PULSE PROGRAM CATALOGUE: II. BIOMOLECULAR NMR EXPERIMENTS

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TOPSPIN v3.0
NMRGuide

UAB

31-03-2010
Part Number --------

2D HSQC
3D HCCH-TOCSY experiments
HCP Quantitative
P-FIDS

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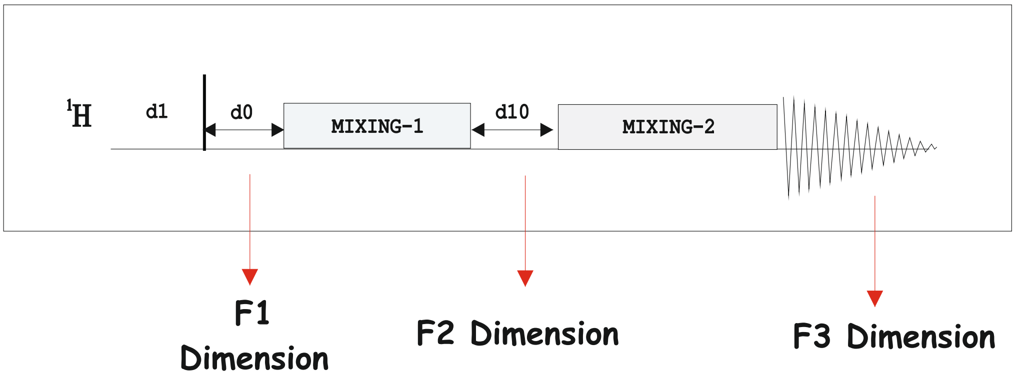
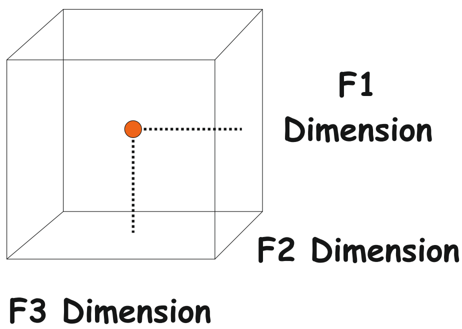
BASIC
3D HOMONUCLEAR
EXPERIMENTS

General Scheme for 3D Homonuclear Experiments



The delays d0 and d10 represent two independent variable periods that provide two independent frequency dimensions (F2 and F3). The third dimension is directly generated from the FID period (F1 Dimension), as in 1D or 2D experiments.

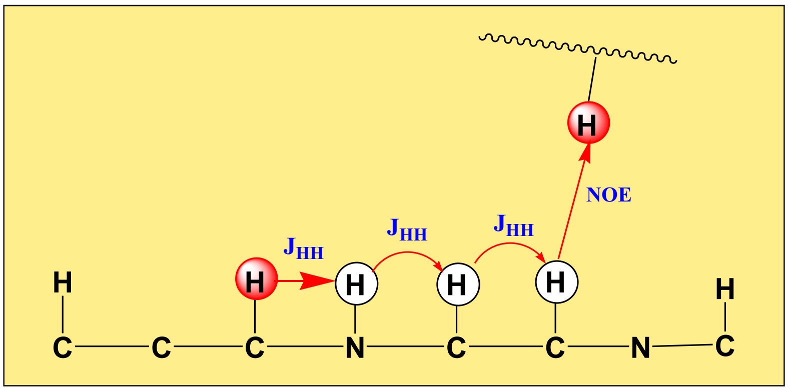


3D Homonuclear Experiments

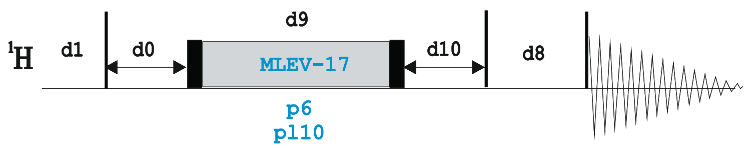
- 3D TOCSY-NOESY experiment (**mlevnoesy3d**)
- 3D TOCSY-ROESY experiment (**mlevroesy3d**)
- 3D NOESY-TOCSY experiment (**noesymlev3d**)
- 3D NOESY-TOCSY experiment using presaturation (**noesymlevpr3d**)
- 3D NOESY-NOESY experiment using presaturation (**noesynoesypr3d**)

Also see related 2D NOESY, 2D ROESY and 2D TOCSY experiments

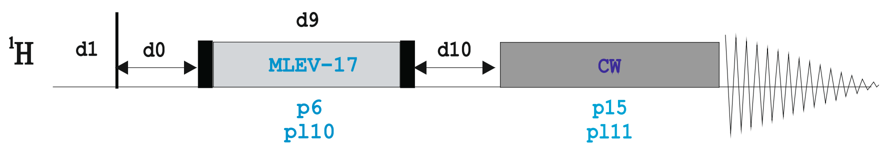
References:
A. Bax & D.G. Davis, J. Magn. Reson. 65, 355-360 (1985)
A. Bax & D.G. Davis, J. Magn. Reson. 63, 207-213 (1985)

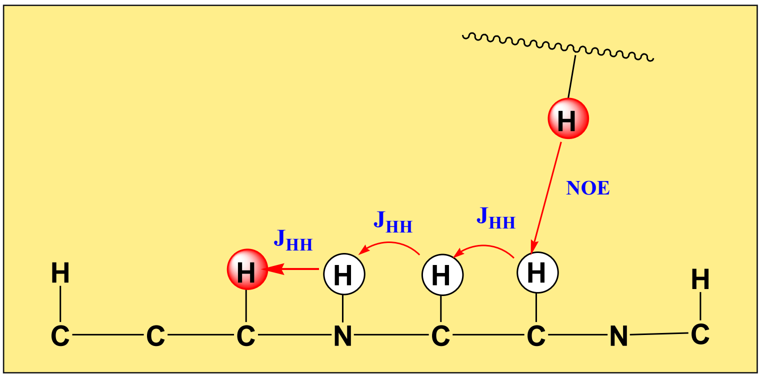


mlevnoesy3d

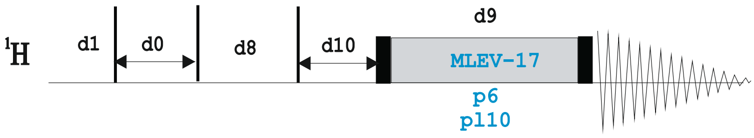


mlevroesy3d

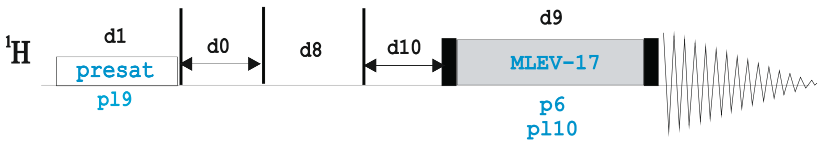


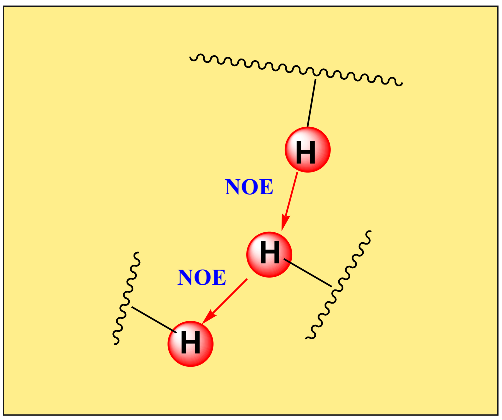


noesymlev3d



noesymlevpr3d





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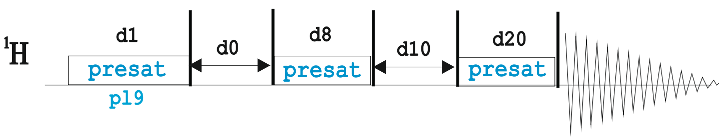

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BASIC 3D X-EDITED
TOCSY EXPERIMENTS

3D Basic X-edited TOCSY

- 3D ^{1}H-^{13}C TOCSY-HMQC experiment using presaturation (**mlevhmqcpr3d**)
- 3D ^{1}H-^{13}C HMQC-TOCSY experiment using BIRD (**hmqcmlevbi3d**)

- 3D ^{1}H-^{13}C HSQC-TOCSY experiment using echo/antiecho, adiabatic pulses and MLEV-17 (**hsqcetgpml3d.2**)
- 3D ^{1}H-^{13}C HSQC-TOCSY experiment using PEP, adiabatic pulses and DIPSI-2 (**hsqcdietgpsisp3d.2**)

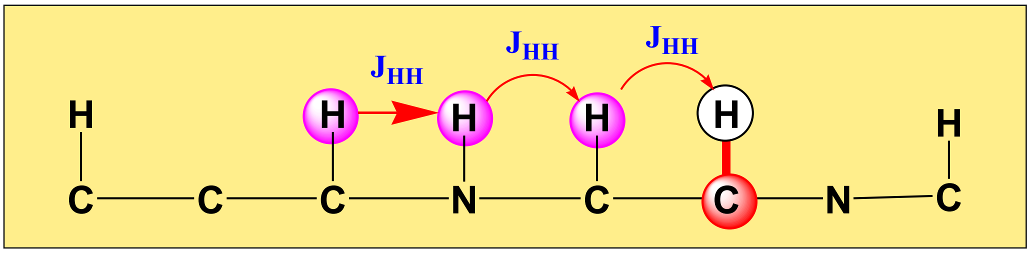
Also see:
2D TOCSY experiment
2D HSQC-TOCSY experiments and Measurement of long-range proton-carbon coupling constants
3D TOCSY-HSQC experiments
2D X-filtered/edited TOCSY experiments

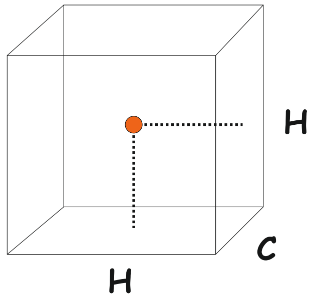
Other Protein NMR experiments involving TOCSY:
HCCH-TOCSY Experiment
HCC(CO)NH Experiment
13C-13C TOCSY

References:

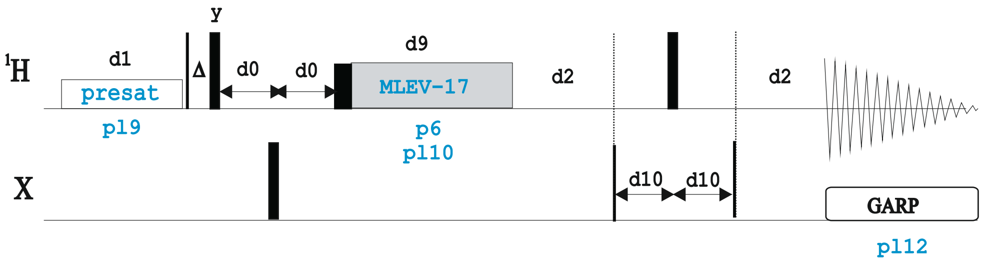
A. Bax and S. Subramanian, J. Magn. Reson. 67, 565-569 (1986)
A. Bax & D.G. Davis, J. Magn. Reson. 65, 355-360 (1985)

TOCSY-HMQC

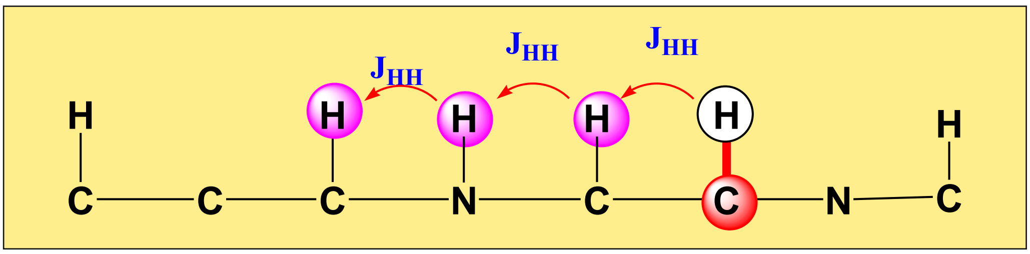


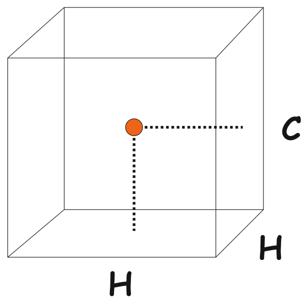


mlevhmqcpr3d

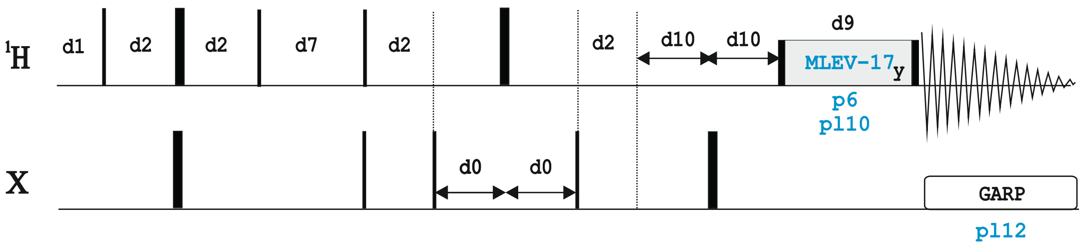


HMQC-TOCSY

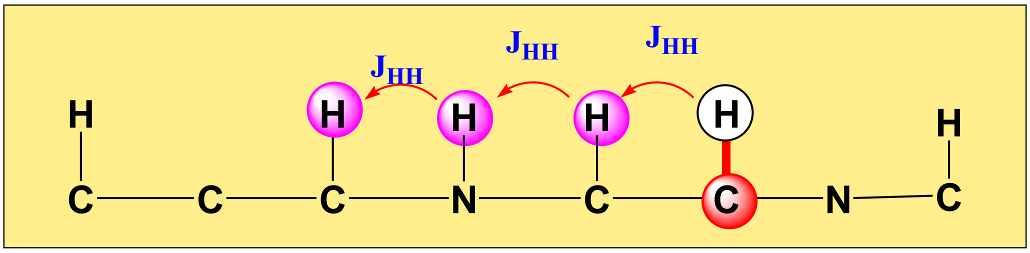


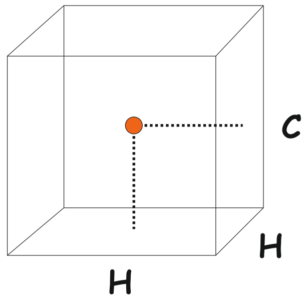


hmqcmlevbi3d

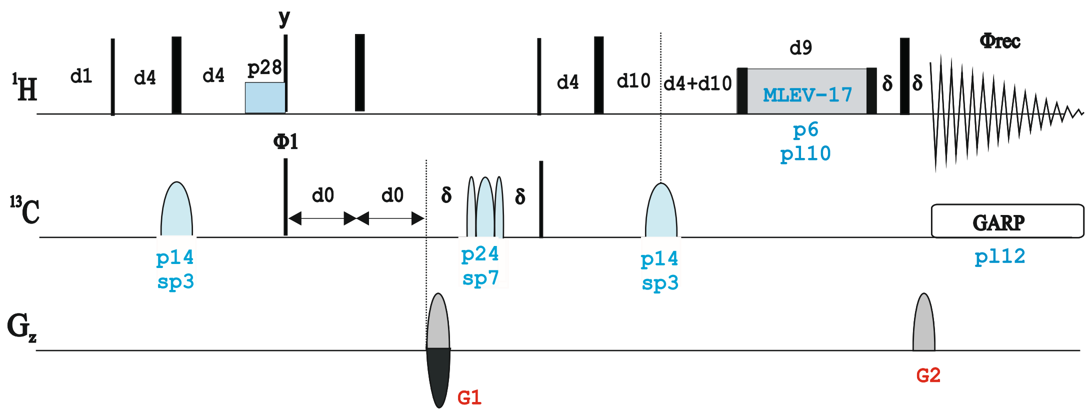


HSQC-TOCSY

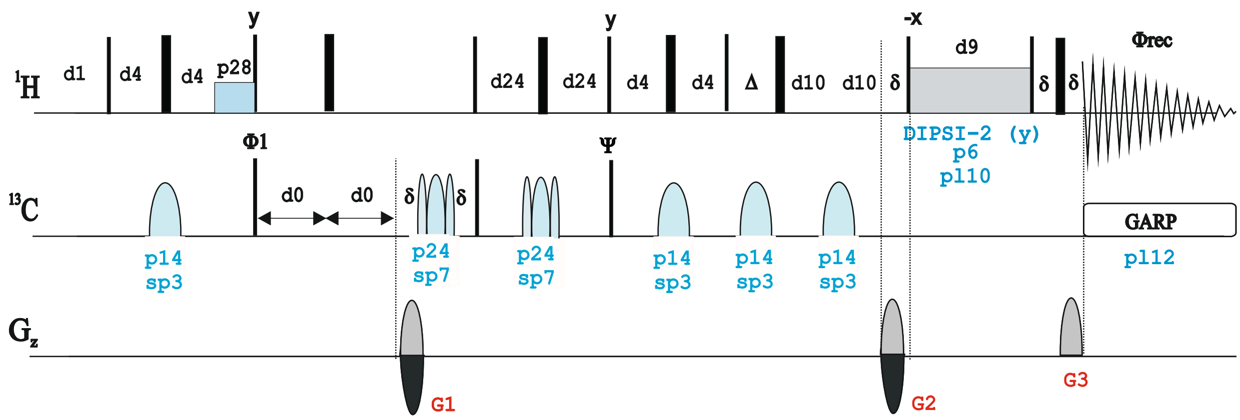




hsqcetgpml3d.2



hsqcdietgpsisp3d.2



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3D TOCSY-HSQC
EXPERIMENTS

3D TOCSY-HSQC

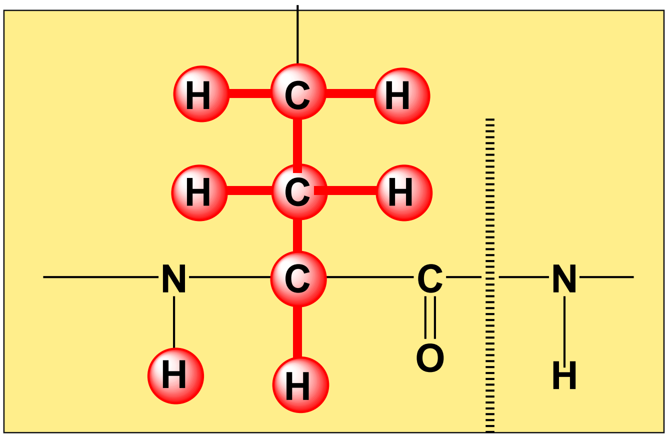
Gradient-enhanced from f2 channel:

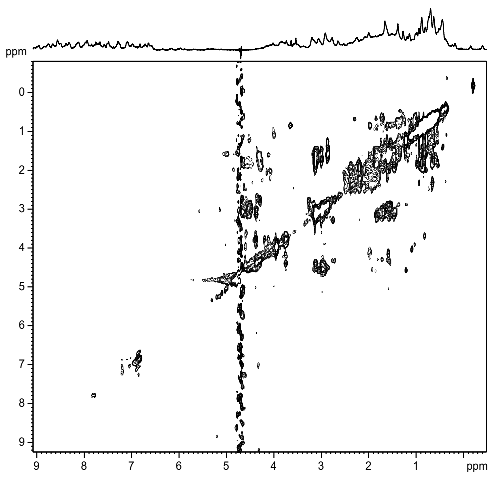
- ge-3D ^{1}H-^{13}C TOCSY-HSQC experiment using echo-antiecho (**mlevhsqcetgp3d** | MLEVHSQCETGP3D)

Gradient-enhanced from f3 channel:

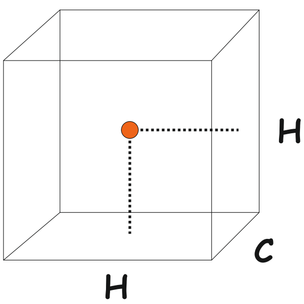
- ge-3D ^{1}H-^{15}N TOCSY-HSQC with MLEV using echo-antiecho (**mlevhsqcetf3gp3d** | MLEVHSQCETF3GP3D)
- ge-3D ^{1}H-^{15}N TOCSY-HSQC with DIPSI-2 and PEP (**dipsihsqcf3gpsi3d** | DIPSIHSQCF3GPSI3D)
- ge-3D ^{1}H-^{15}N TOCSY-HSQC with DIPSI-2 using TROSY (**dipsitretf3gp3d** | DIPSITRETF3GP3D)

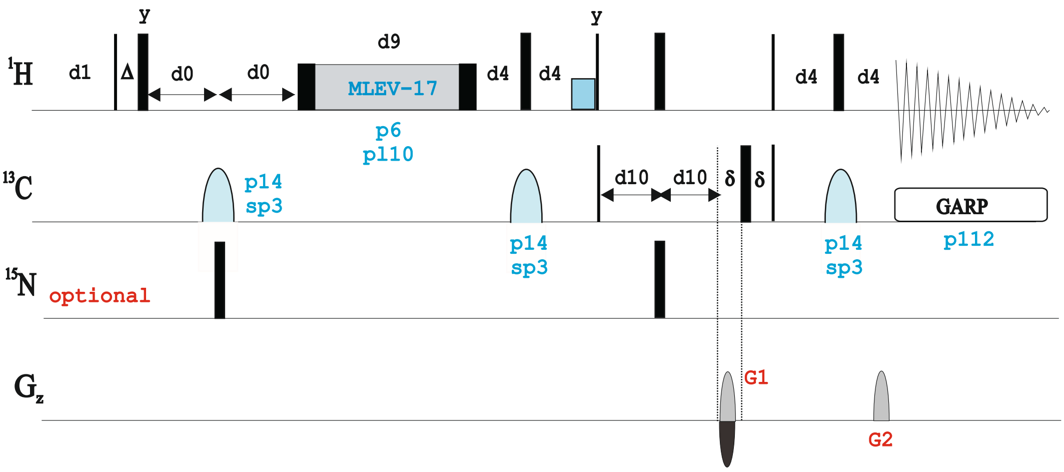
Also see:
2D TOCSY experiment
2D & 3D HSQC-TOCSY experiments
2D X-filtered/edited TOCSY experiments



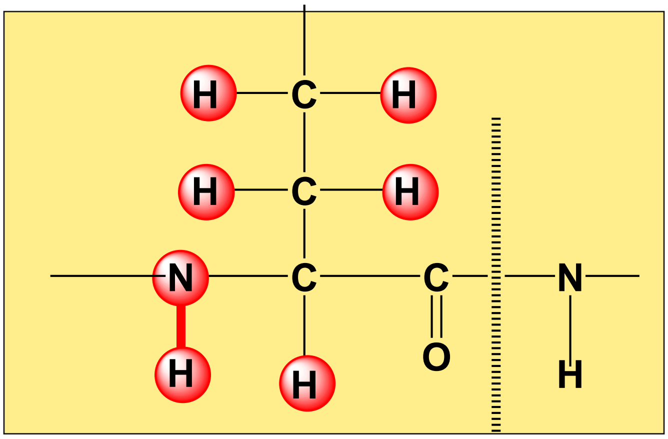


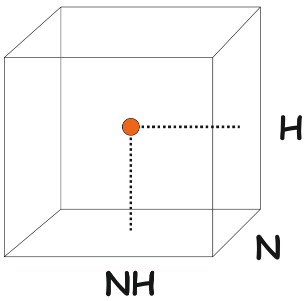
mlevhsqcetgp3d



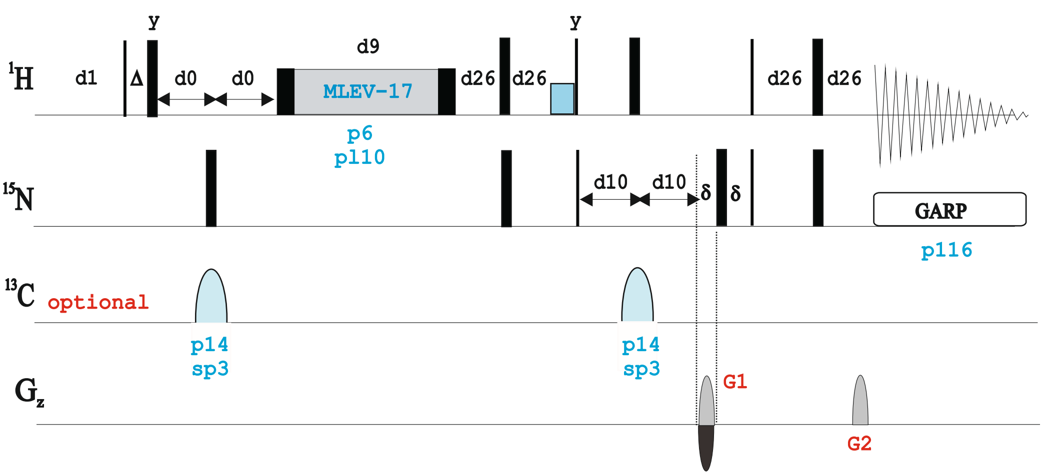


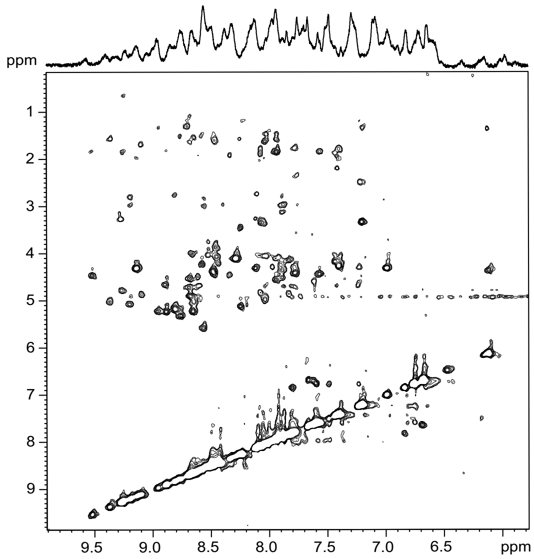
References:
1. A. Bax & D.G. Davis, J. Magn. Reson. 65, 355-360 (1985)
2. A.L. Davis, J. Keeler, E.D. Laue & D. Moskau, J. Magn. Reson. 98, 207-216 (1992)
3. A.G. Palmer III, J. Cavanagh, P.E. Wright & M. Rance, J. Magn. Reson. 93, 151-170 (1991)
4. L.E. Kay, P. Keifer & T. Saarinen, J. Am. Chem. Soc. 114, 10663-5 (1992)
5. J. Schleucher et al., Angew. Chem. 114(10), 1518 (1993)



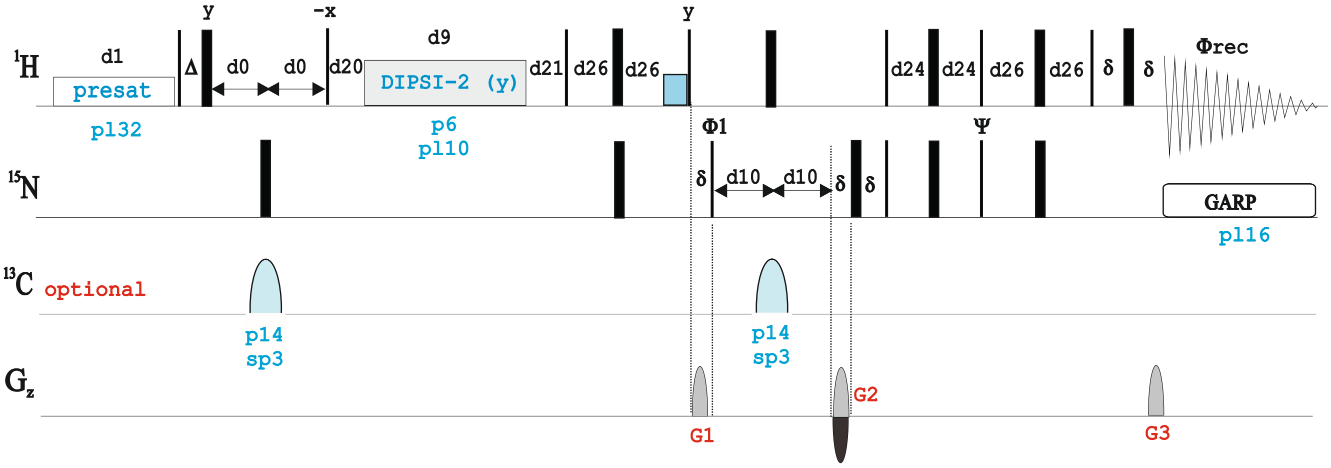


mlevhsqcetf3gp3d

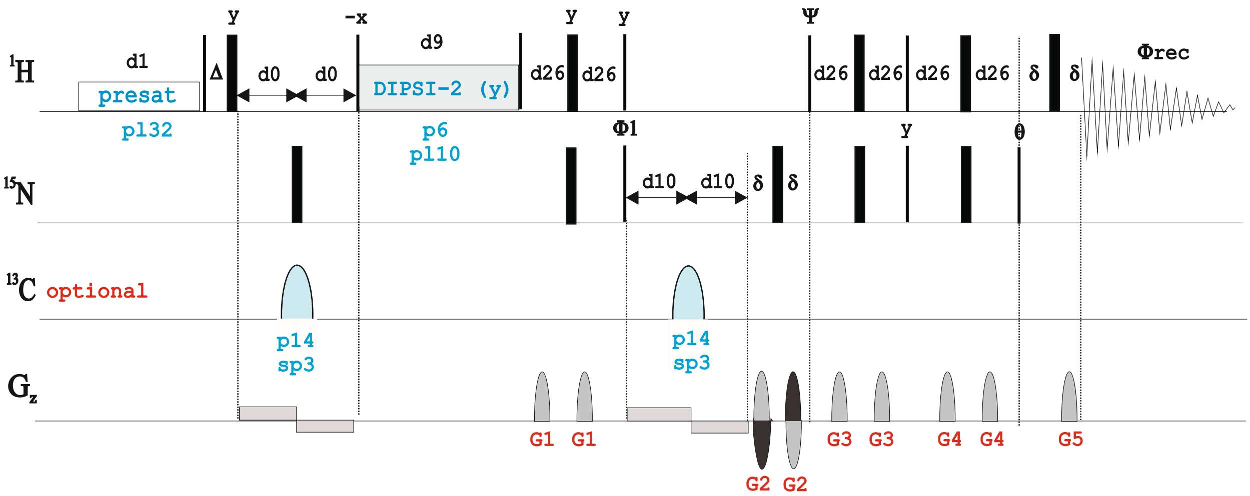




dipsihsqcf3gpsi3d



dipsitretf3gp3d



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2D 13C/15N-FILTERED
TOCSY EXPERIMENTS

2D $^{13}C/^{15}N$-filtered TOCSY

ge-2D w_1-$^{13}C,^{15}N$-filtered TOCSY experiment

- ge-2D w_1-$^{13}C,^{15}N$-filtered TOCSY using DIPSI2 and WATERGATE (**dipsi2gpphwgx1**)

ge-2D w_2-$^{13}C,^{15}N$-filtered TOCSY experiment

- ge-2D w_2-$^{13}C,^{15}N$-filtered TOCSY using DIPSI2 and WATERGATE (**dipsi2gpphwgx2**)

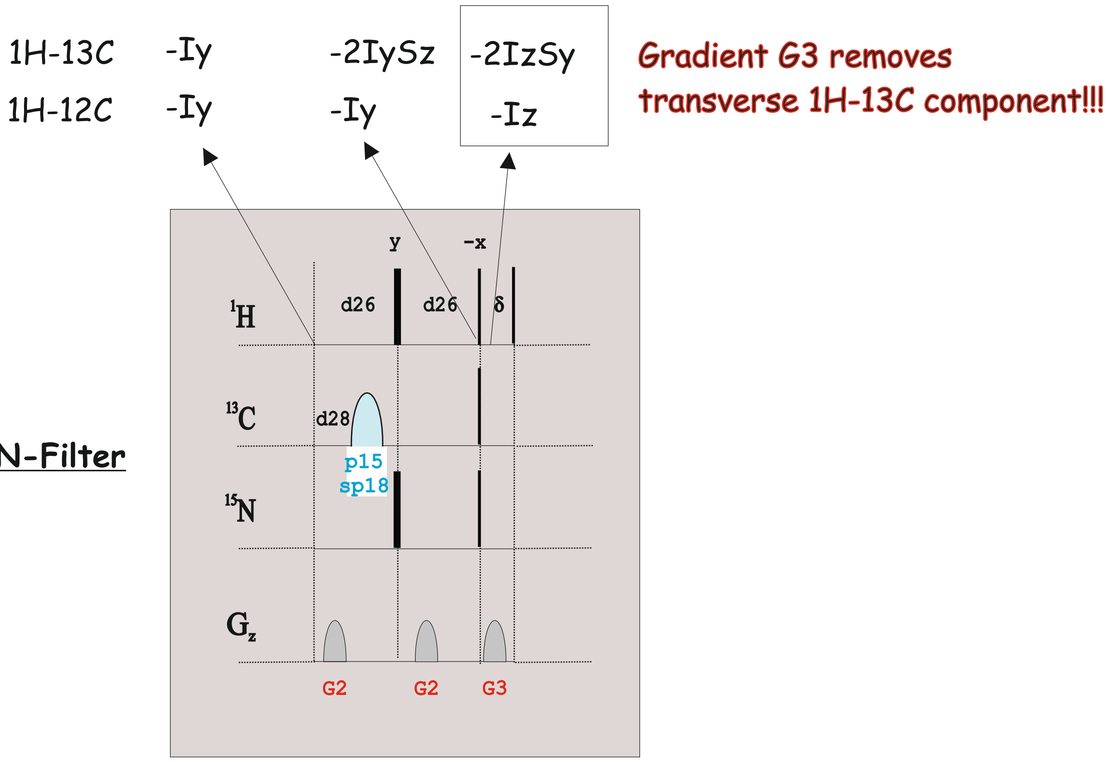
ge-2D w_1,w_2-$^{13}C,^{15}N$-filtered TOCSY experiment

- Phase-sensitive ge-2D w_1,w_2 $^{13}C,^{15}N$ -filtered TOCSY using DIPSI2 and WATERGATE (selective pulses) (**dipsi2gpphwgxf**)

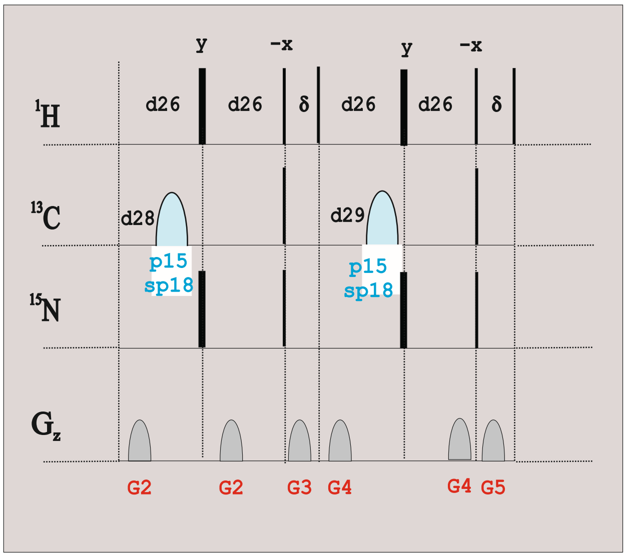
Also see:
2D TOCSY experiment
3D TOCSY-HSQC and 3D HSQC-TOCSY experiments

1. A.L. Breeze, Prog. NMR Spectrosc. 36, 323-372 (2000).
2. C. Zwahlen, P. Legault, S.J.F. Vincent, J. Greenblatt, R. Konrat & L.E. Kay, J. Am. Chem. Soc. 119 6711-6721 (1997).
3. K. Ogura, H. Terasawa & F. Inagaki, J. Biomol. NMR 8, 492-498 (1996).
4. J. Iwahara, J.M. Wojciak & R.T. Clubb, J. Biomol. NMR 19, 231-241 (2001).

Single 13C,15N-Filter

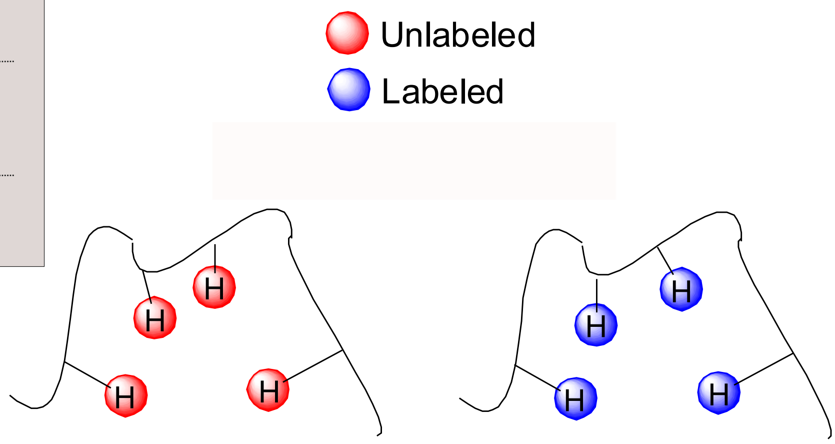


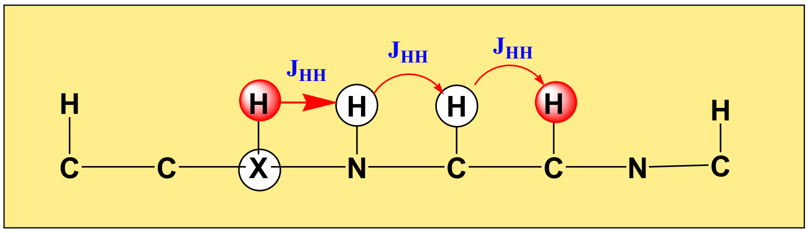
Double 13C,15N-Filter



d26: 1/(4*J(NH))
d28: 1/(4*J(CH)min)
d29: 1/(4*J(CH)max)

Differentiation between TOCSY in labeled/unlabeled Compounds





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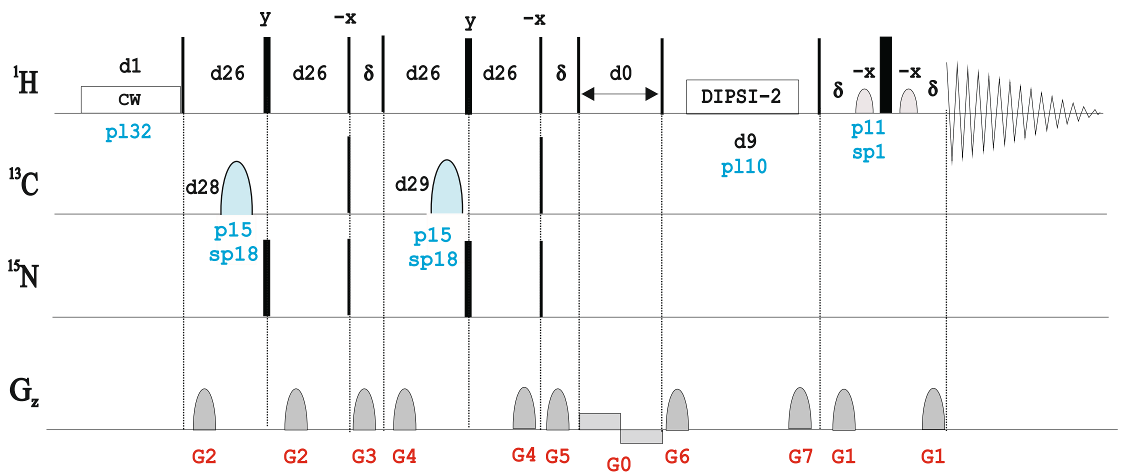

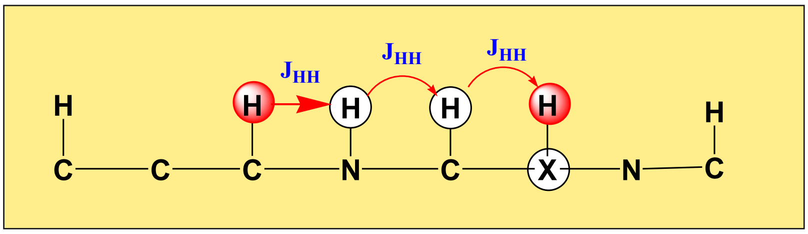

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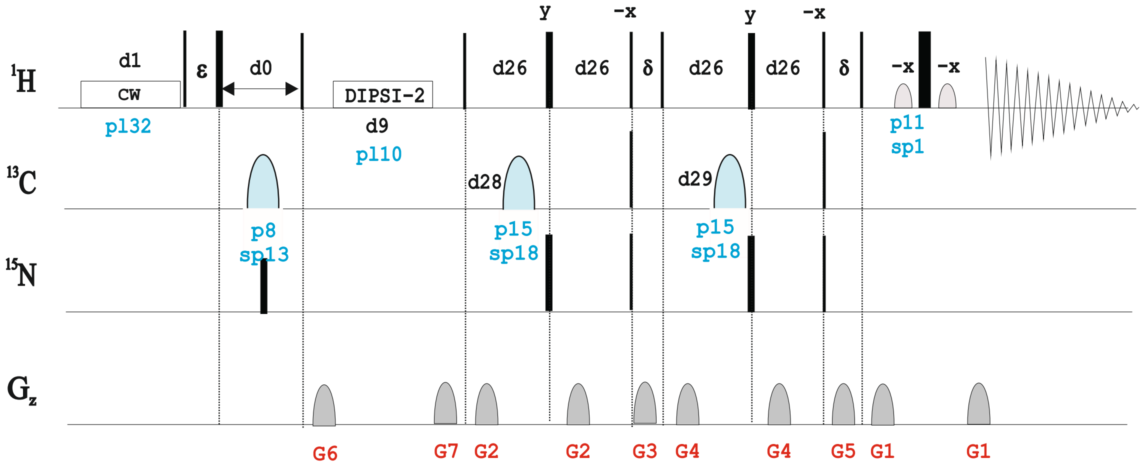

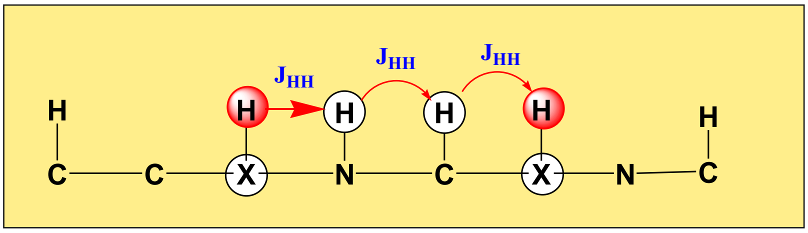

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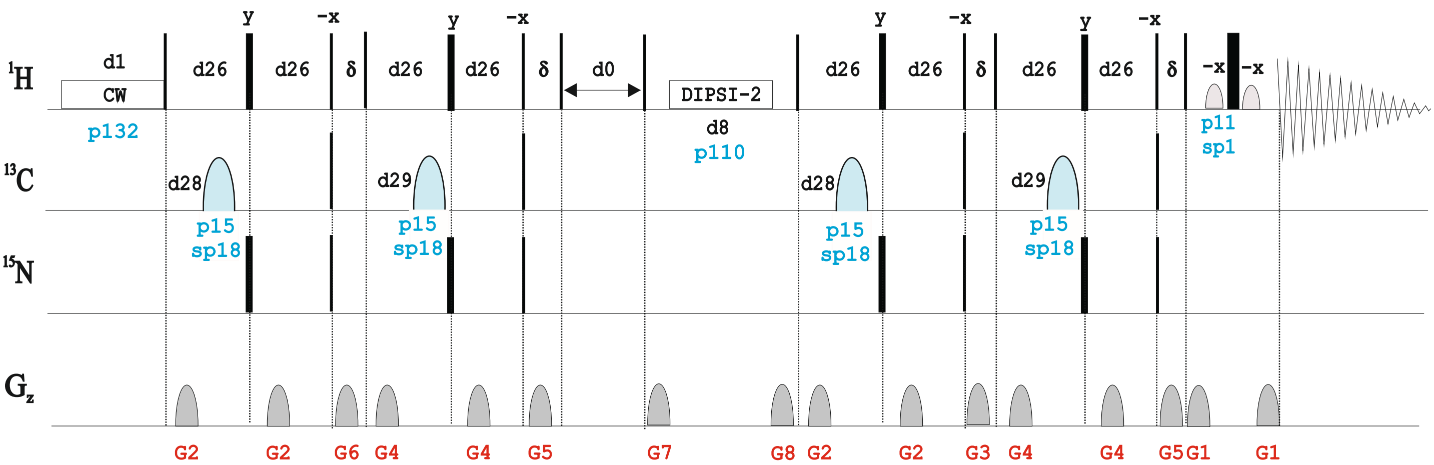

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3D HCCH-COSY
3D HCCH-TOCSY

HCCH-COSY / HCCH-TOCSY

- **HCCH-COSY**

  3D HC(C)H-COSY experiment (**hcchcogp3d** | HCCHCOGP3D)
  3D (H)CCH-COSY experiment (**hcchcogp3d2**)
  3D (H)CCH-COSY experiment using TROSY for aromatic residues (**trhcchcogp3d**)

  4D HCCH-COSY experiment (**hcchcogp4d**)

- **HCCH-TOCSY**

  3D HC(C)H-TOCSY experiment (**hcchdigp3d** | HCCHDIGP3D)
  3D (H)CCH-TOCSY experiment (**hcchdigp3d2** | HCCHDIGP3D2)
  3D HC(C)H-TOCSY using adiabatic TOCSY experiment (**hcchatgp3d** | HCCHATGP3D)
  3D (H)CCH-TOCSY using adiabatic TOCSY experiment (**hcchatgp3d2**)

  4D HCCH-TOCSY experiment (**hcchdigp4d**)

- **ge-2D Long-range HCCH correlation**

  Phase-sensitive ge-2D Long-range (H)C(C)H using echo-antiecho (**hcchetgplr**)

Also see 3D HCCH-E.COSY experiments for J measurement

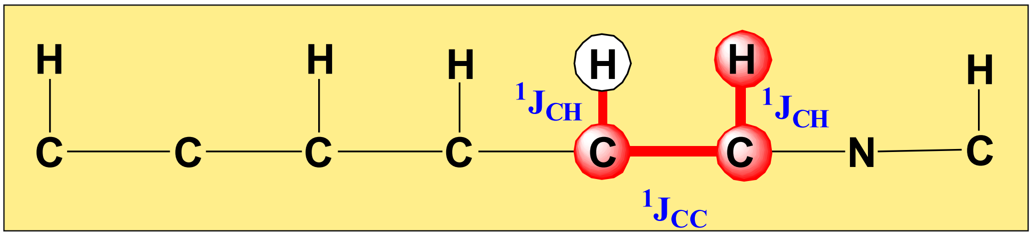
- 3D HC(C)H[HA]-E.COSY (hcchecosgp3d | HCCHECOSGP3D) - 3J[HA-HB] via E.COSY
- 3D HC(C)H[CO]-E.COSY (hcchcosygp3d | HCCHCOSYGP3D) - 3J[CO-HB] via E.COSY
- 3D (H)C(C)CH[CO]-E.COSY (hccccosygp3d | HCCCCOSYGP3D) - 3J[CG-CO] via E.COSY

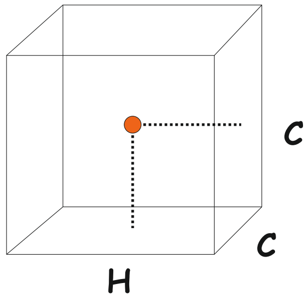
Also see HCCH-type experiments in "Nucleic Acids Experiments"

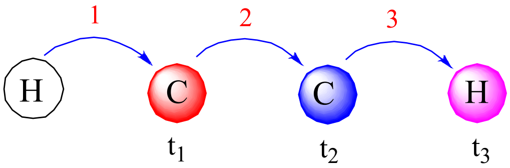
- 3D TROSY-(H)CCH-COSY for intra-base correlation (na_trhcchco3d)
- 3D H(C)CH-E.COSY experiment (na_hcchecgp3d | NA_HCCHECGP3D)
- 3D HCC-TOCSY-CCH-COSY experiment (na_hcchfwdigp3d | NA_HCCHFWDIGP3D)
- 3D HCC-TOCSY-CCH-E.COSY experiment (na_hcchfwdiecgp3d | NA_HCCHFWDIECGP3D)
- 3D HCC-TOCSY-CCH-E.COSY experiment using jump-and-return (11) (na_hcchfwdiecgpjr3d)
- 3D forward directed quantitative gamma HCCH-TOCSY (na_ghcchfwdigp3d | NA_GHCCHFWDIGP3D)

Related Experiments:
HCC(CO)NH Experiment
13C-13C TOCSY

References:
1. L.E. Kay, G.Y. Xu, A.U. Singer, D.R. Muhandiram & J. D. Forman-Kay J. Magn. Reson. B 101, 333 - 337 (1993))
2. W.Peti, C. Griesinger & W. Bermel, J. Biomol. NMR 18, 199 - 205 (2000)

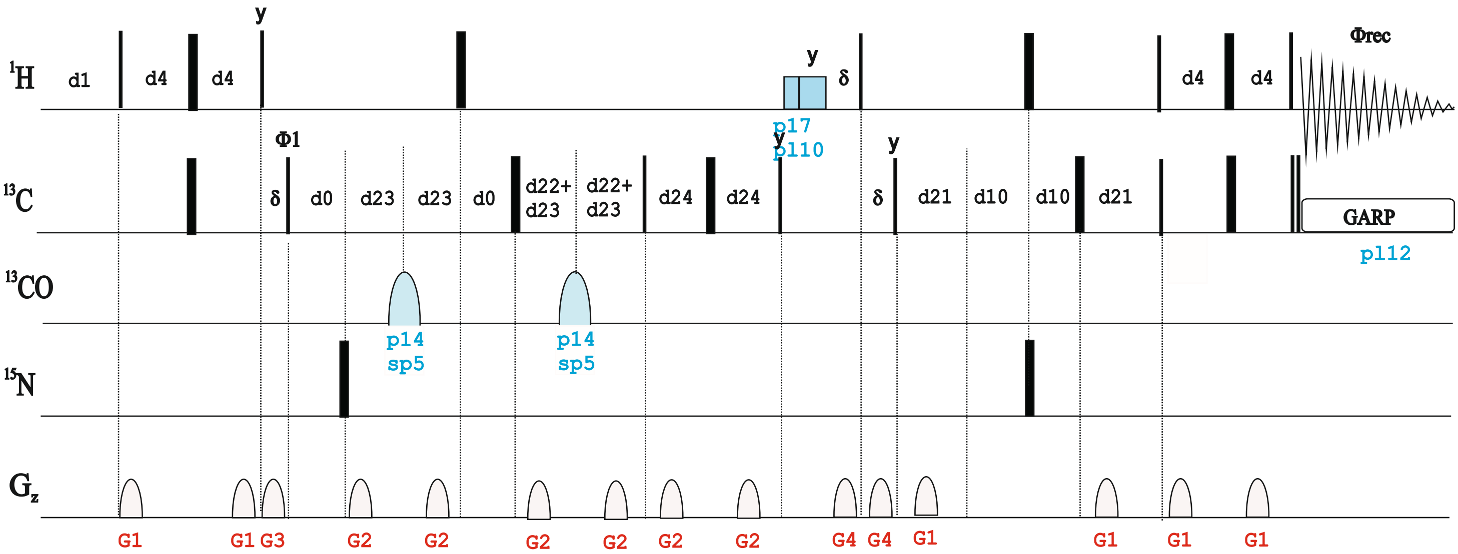




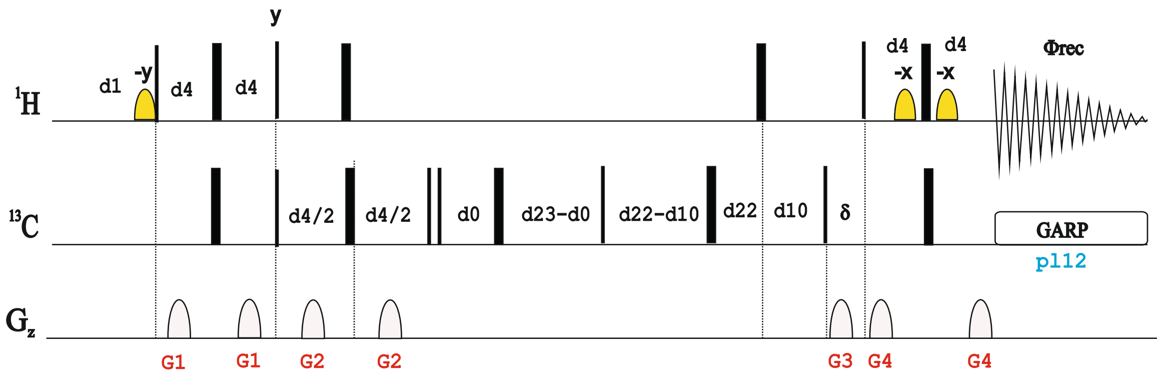


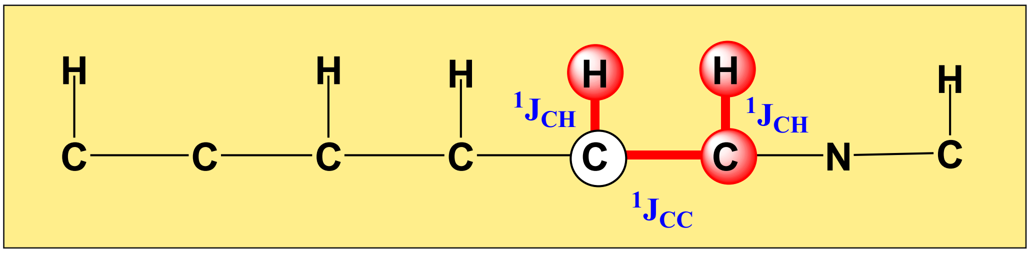
d4 : 1/(4J(CH)) - tau a [1.6 msec]
d21: 1/(6J'(CH)) - tau c [1.1 msec]
d22: d22+d23*2+t2max*0.5 = 1/(4J(CC)) : 3.6m-d23*2-(in0*td1/4)
d23: tau b [475 usec]
d24: 1/(4J(CC)) [3.6 msec]

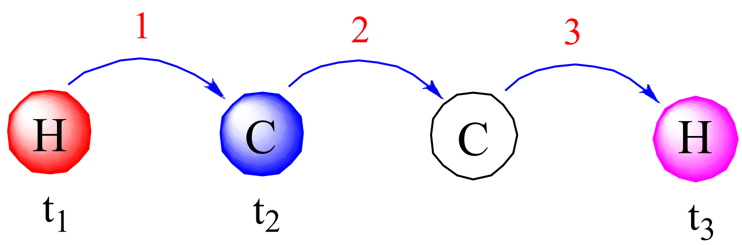
hcchcogp3d2

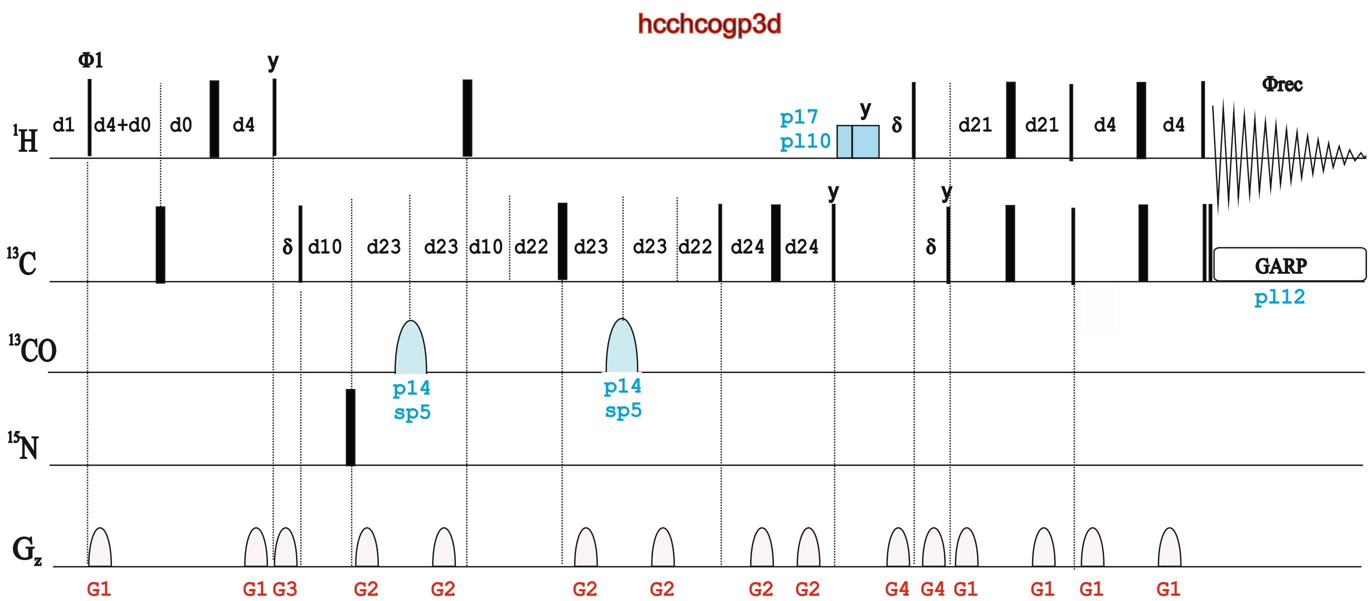


trhcchcogp3d






1
2
3
H
C
C
H
t_1
t_2
t_3


hcchcogp3d
Φ1
y
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d4
p17
p110
δ
d21
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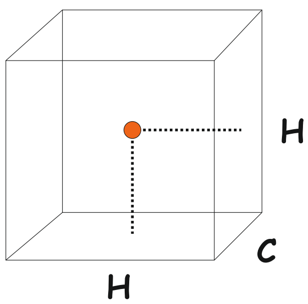
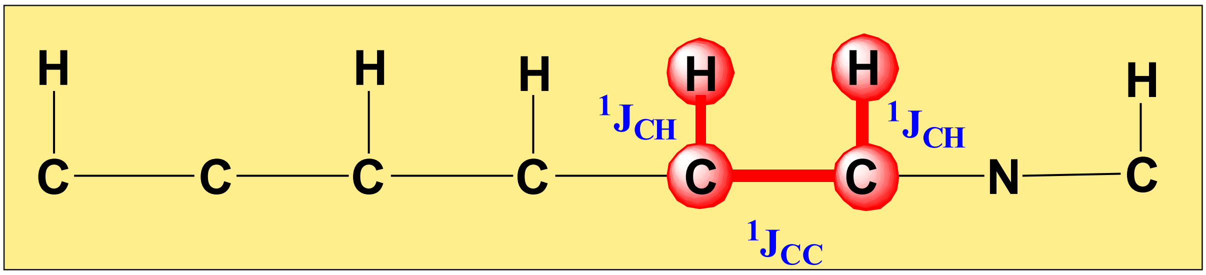
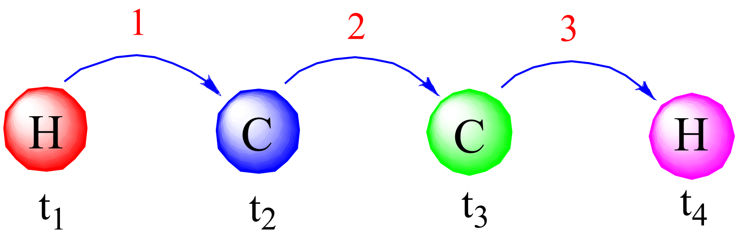
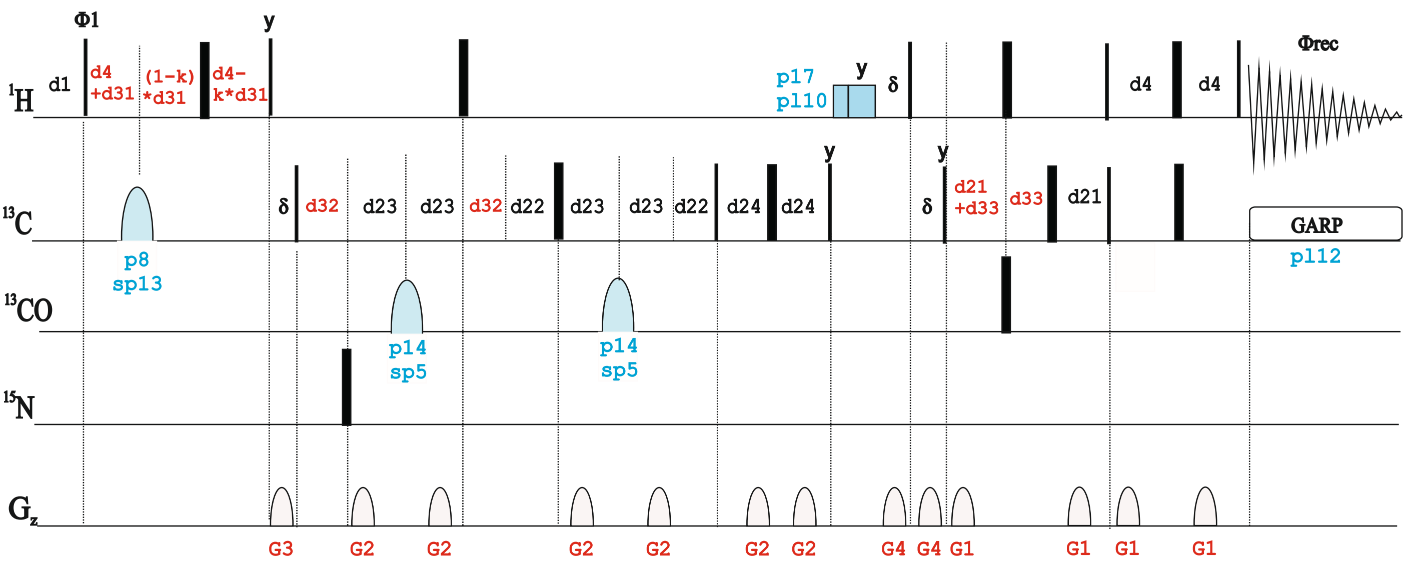
d4
Φrec
GARP
p112
δ
d10
d23
d23
d10
d22
d23
d23
d22
d24
d24
p14
sp5
p14
sp5
G1
G1 G3
G2
G2
G2
G2
G2
G2
G4
G4
G1
G1
G1
G1

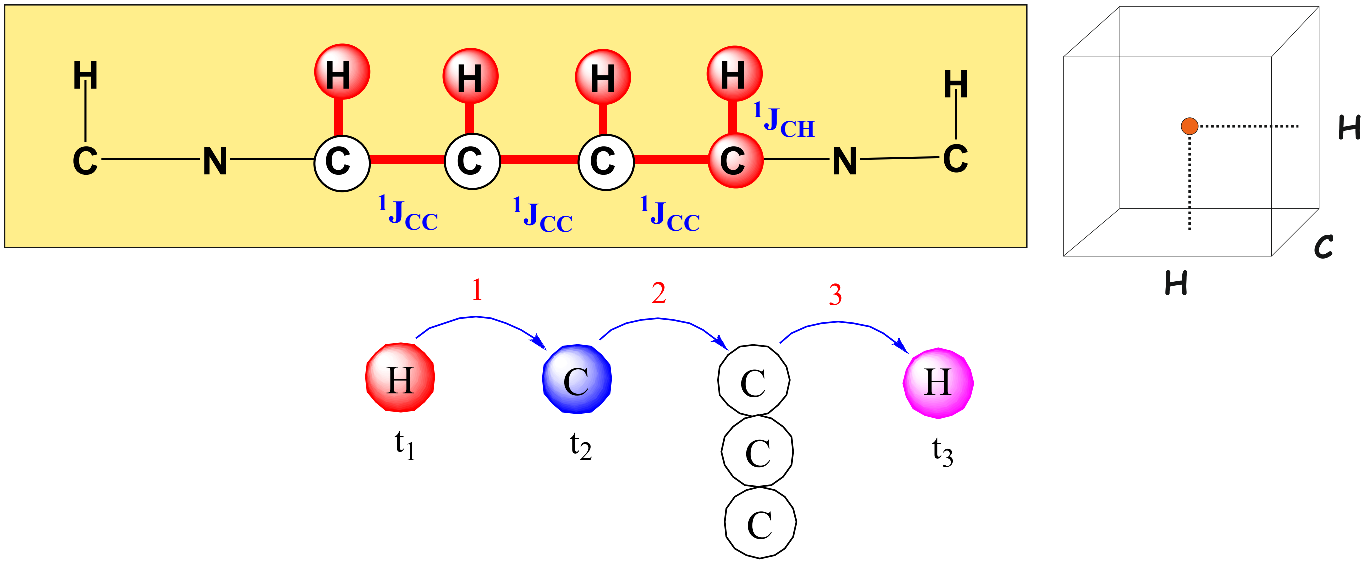



H
C
N
$^1J_{CH}$
$^1J_{CC}$


1
2
3
H
C
C
H
t_1
t_2
t_3
t_4

hcchcogp4d


Φ1
y
Φrec
^{1}H
d1
d4 +d31
(1-k) *d31
d4- k*d31
p17
p110
δ
d4
^{13}C
p8
sp13
d32
d23
d22
d24
d21 +d33
d33
d21
GARP
p112
^{13}CO
p14
sp5
^{15}N
G_z
G3
G2
G4
G1



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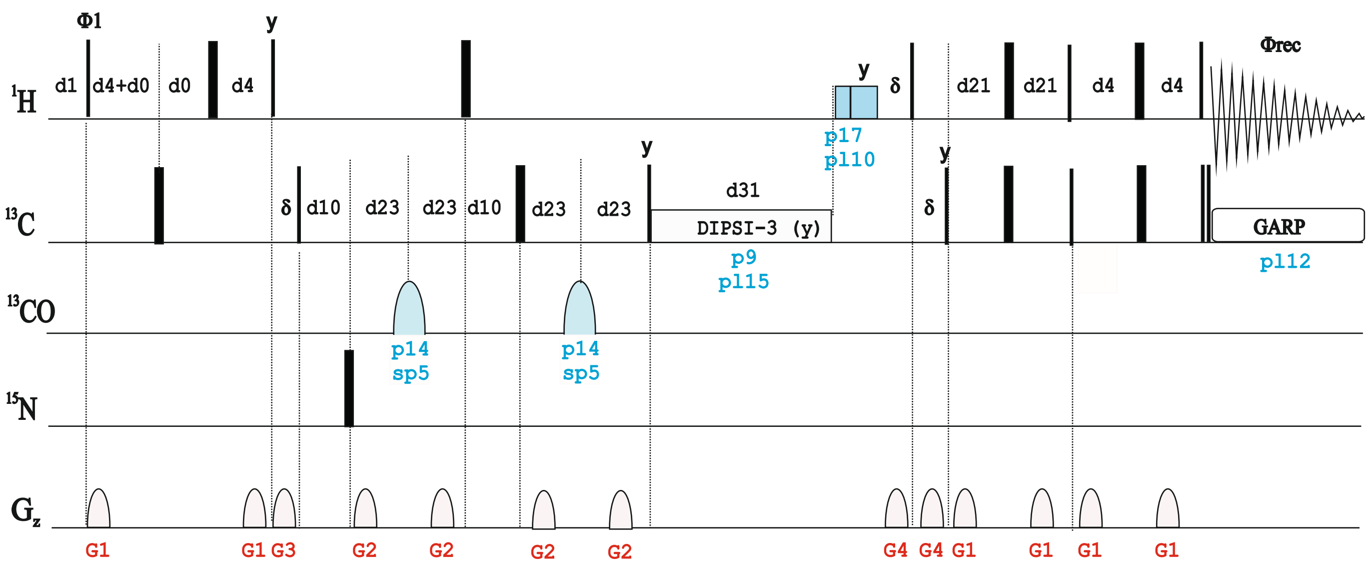
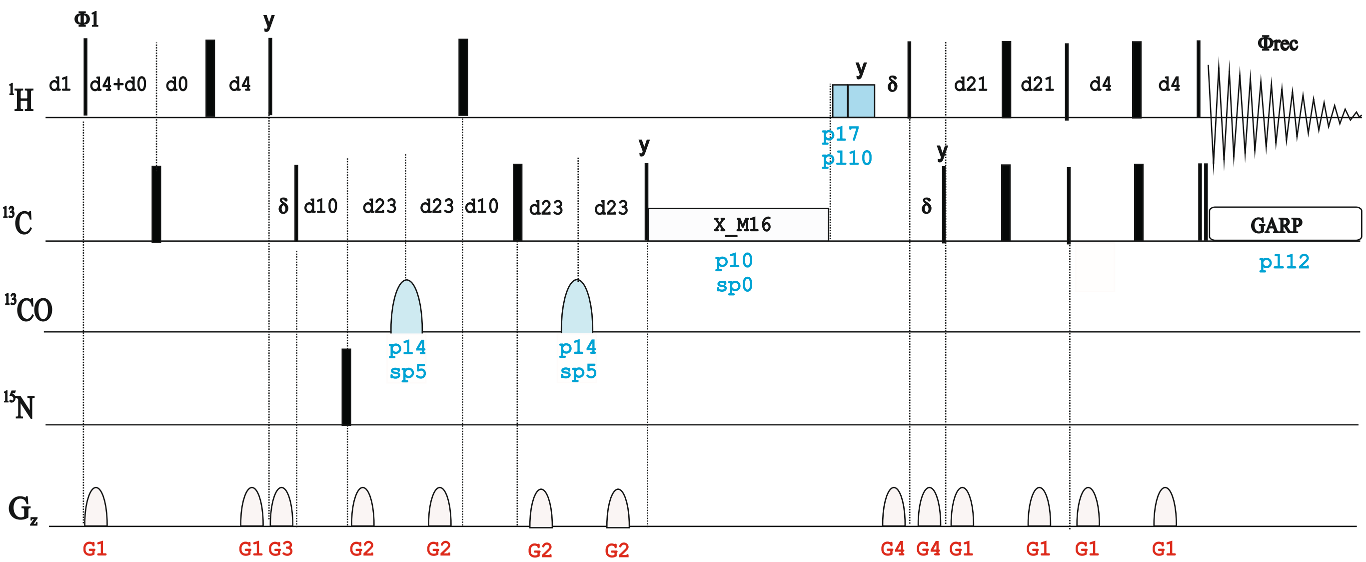
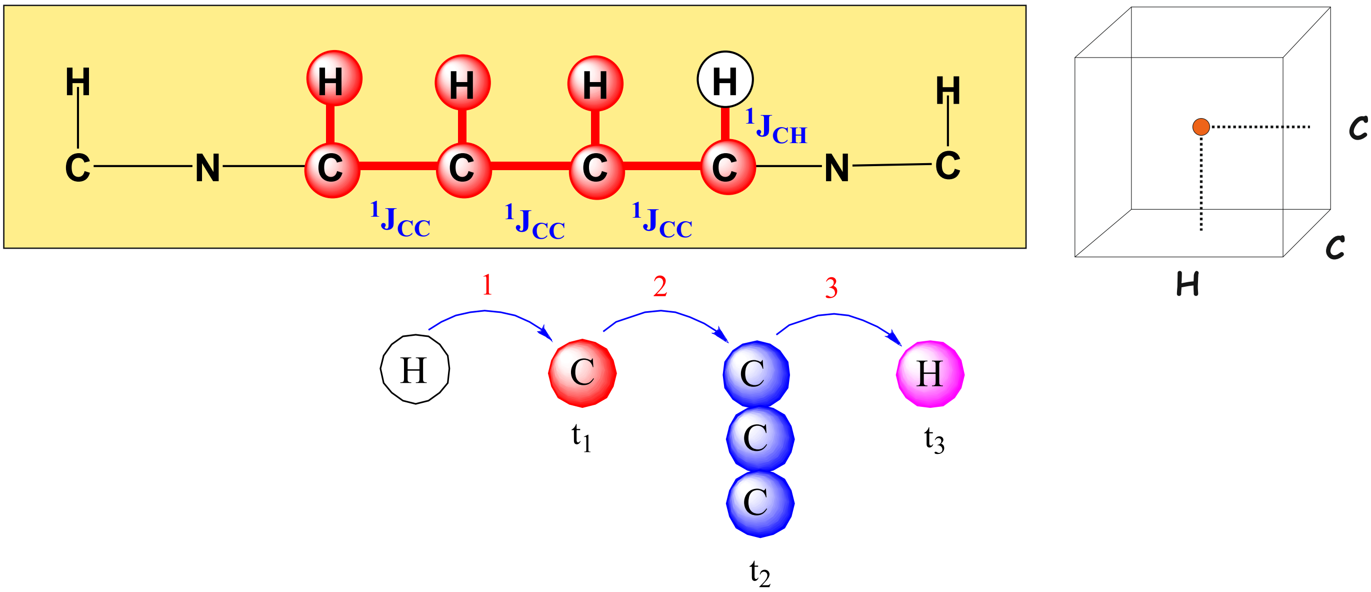
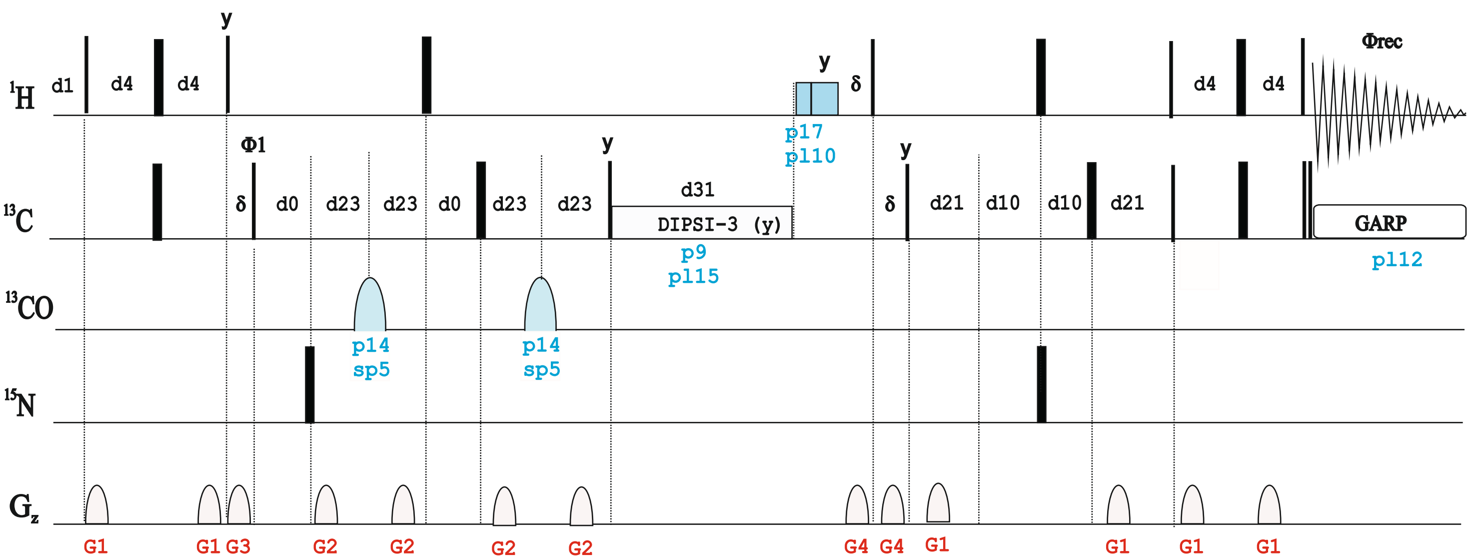


hcchatgp3d

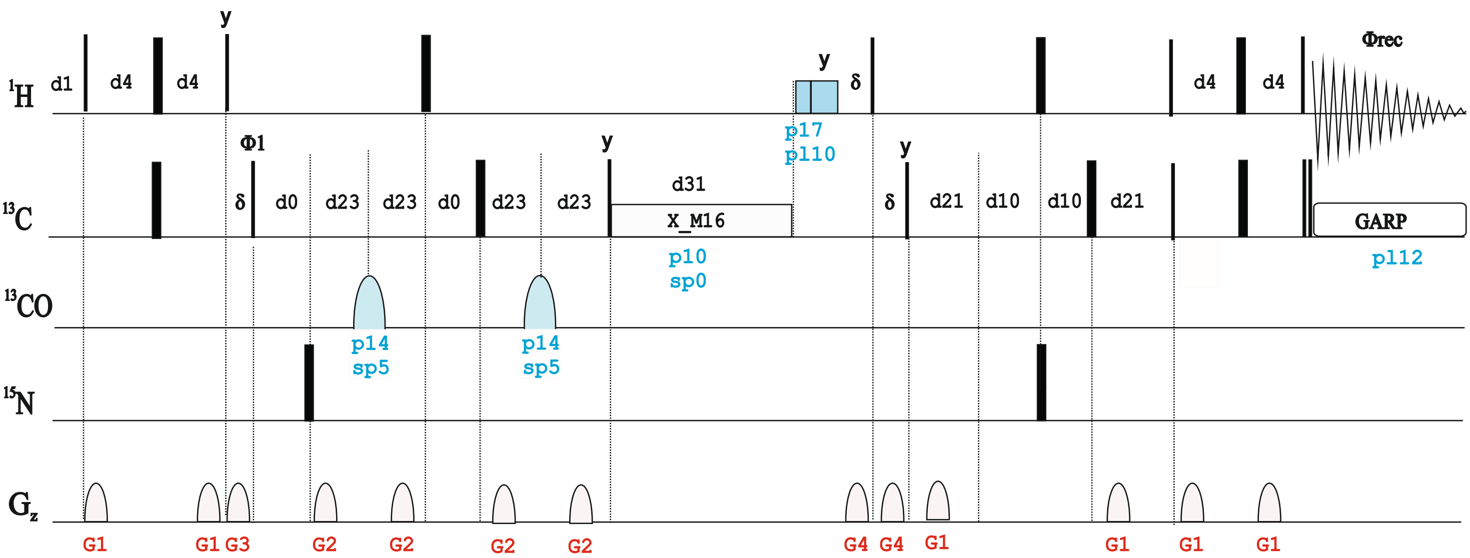


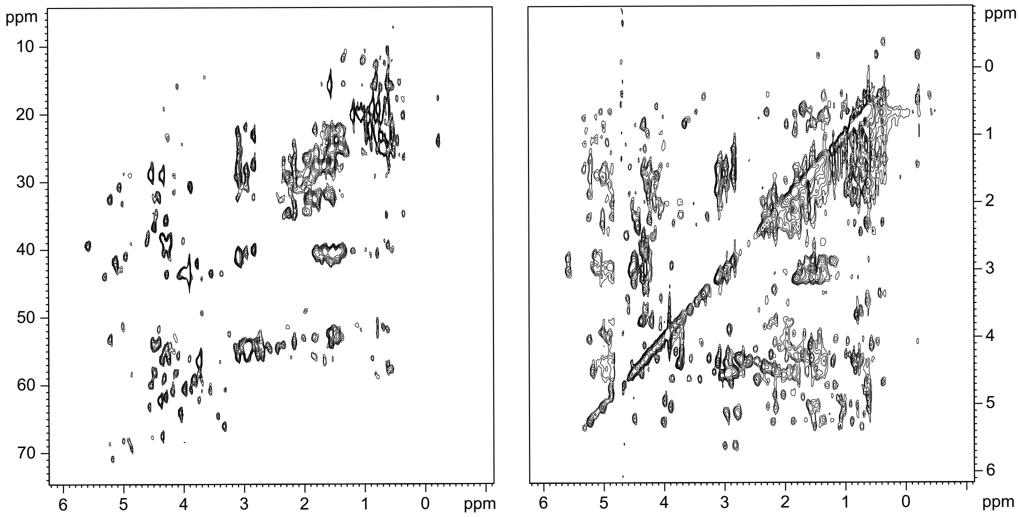


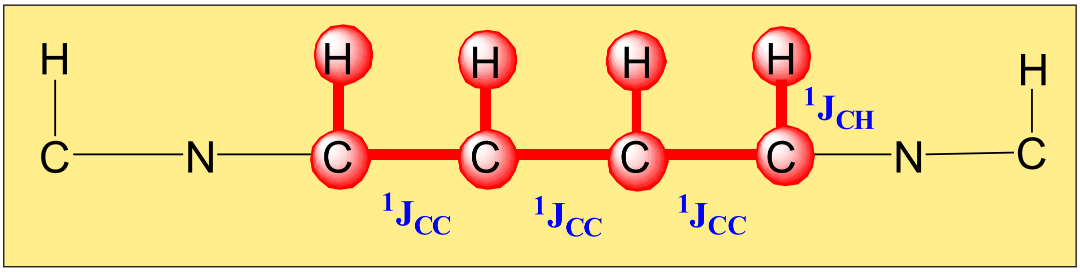
hcchdigp3d2

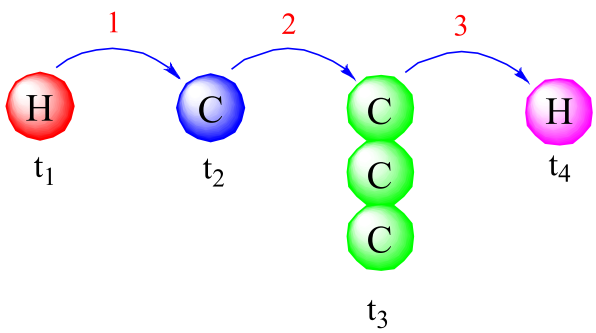


hcchatgp3d2

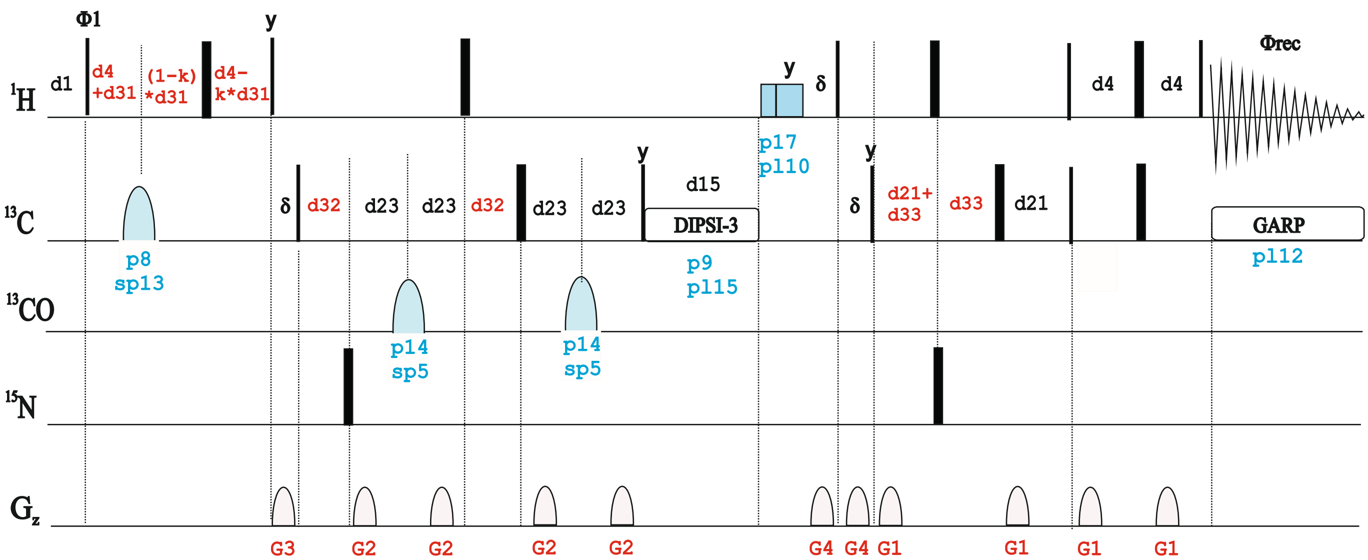



ppm
10
20
30
40
50
60
70
6 5 4 3 2 1 0 ppm
ppm
0
1
2
3
4
5
6
6 5 4 3 2 1 0 ppm


H
C
N
C
H
1JCH
1JCC
1JCC
1JCC

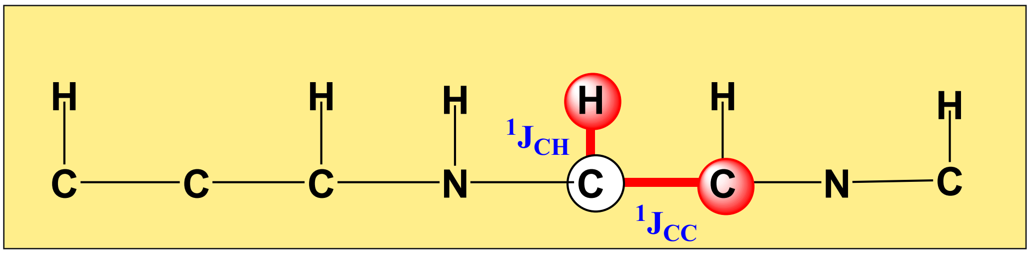

1
2
3
H
C
C
C
C
H
t1
t2
t3
t4

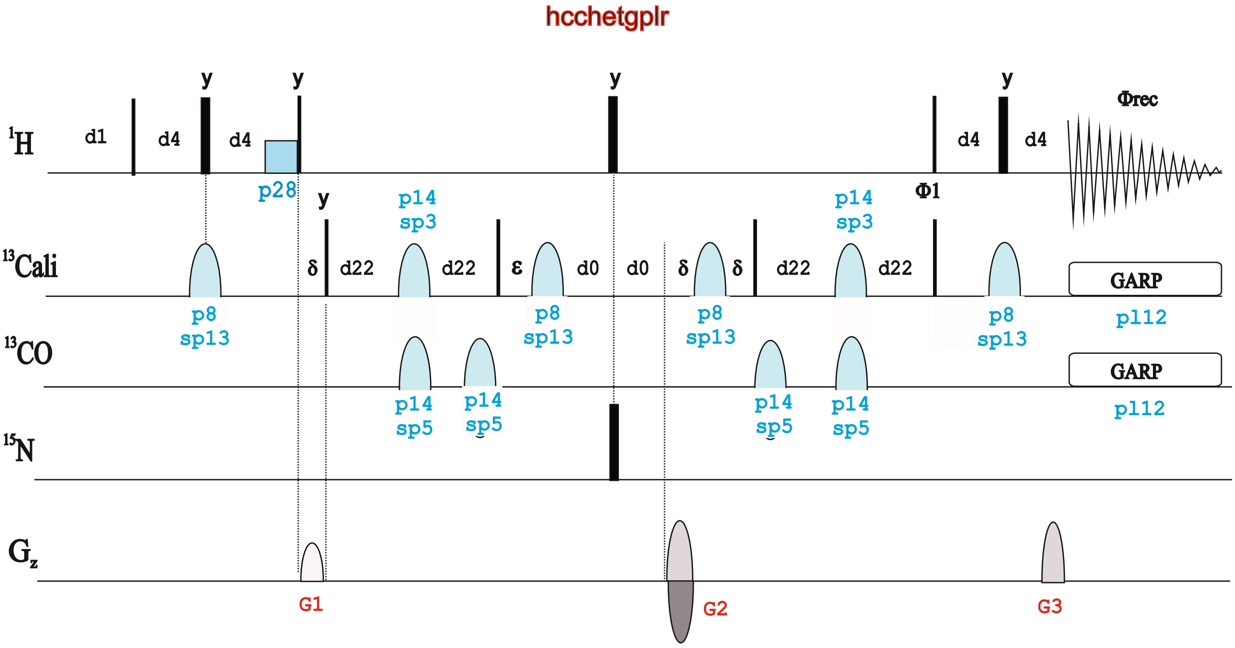
hcchdigp4d


Φ1
y
Φrec
1H
d1
d4 +d31
(1-k) *d31
d4- k*d31
y
δ
d4
d4
p17 p110
13C
p8 sp13
δ
d32
d23
d23
d32
d23
d23
y
d15
DIPSI-3
p9 p115
δ
y
d21+ d33
d33
d21
GARP
p112
13CO
p14 sp5
p14 sp5
15N
Gz
G3 G2 G2 G2 G2 G4 G4 G1 G1 G1 G1

2D (H)C(C)H:

A. Bax, D. Max & D. Zax, J. Am. Chem. Soc. 114, 6923-6925 (1992)





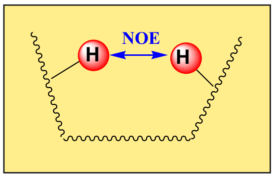
BRUKER PULSE PROGRAM CATALOGUE

NMRGuide

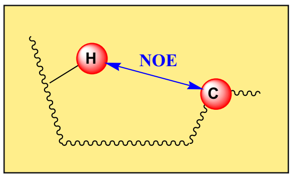
3D NOESY-HSQC EXPERIMENTS

Edited NOESY experiments for labeled proteins:

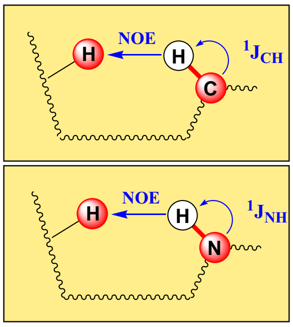
2D NOESY
2D ROESY



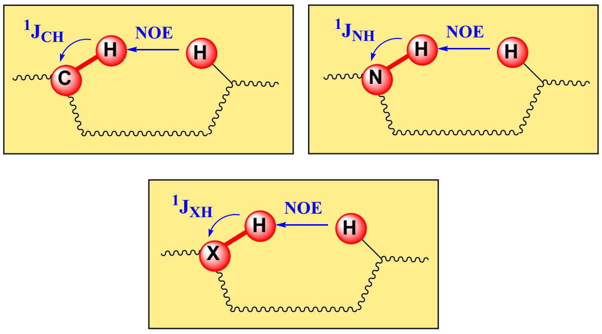
2D HOESY



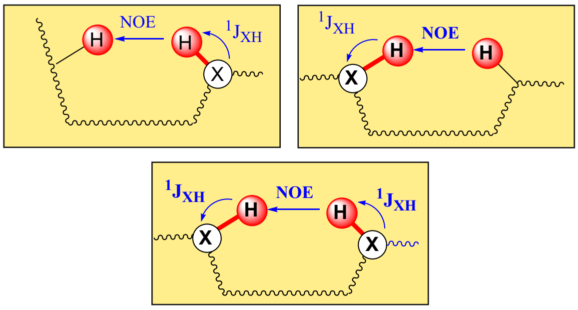
2D/3D HSQC-NOESY



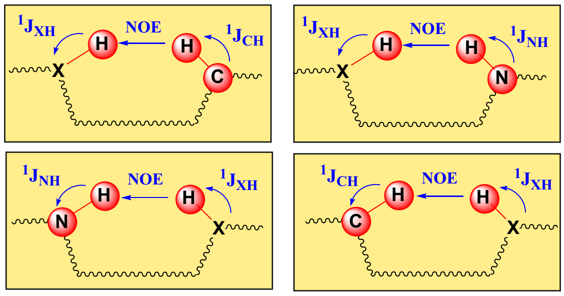
2D/3D NOESY-HSQC

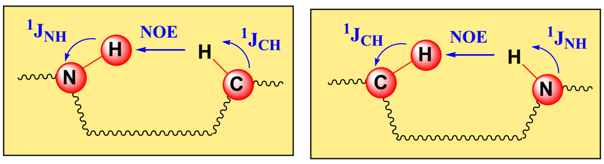


2D/3D w1/w2 12C,14N-Edited NOESY

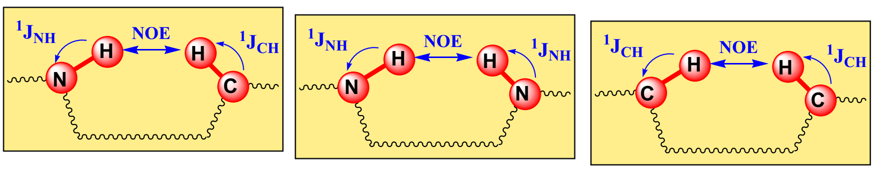


3D w3 12C,14N-Edited HSQC-NOESY
3D w1 12C,14N-Edited NOESY-HSQC





3D HSQC-NOESY-HSQC



4D HSQC-NOESY-HSQC

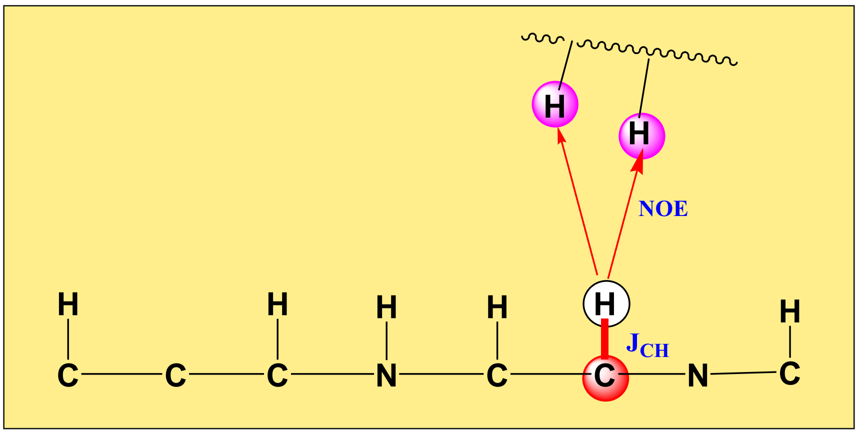
3D Basic X-edited NOESY

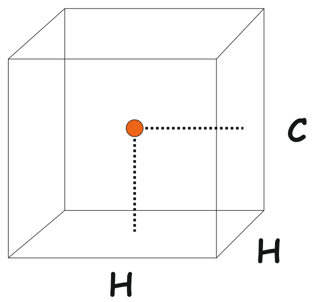
- 3D ^{1}H-^{13}C NOESY-HMQC experiment using presaturation (**noesyhmqcpr3d**)
- 3D ^{1}H-^{13}C HMQC-NOESY experiment using BIRD (**hmqcnoesybi3d**)

Also see:
2D HMQC and 2D NOESY experiments
2D & 3D HSQC-NOESY Experiments
3D NOESY-HSQC Experiments

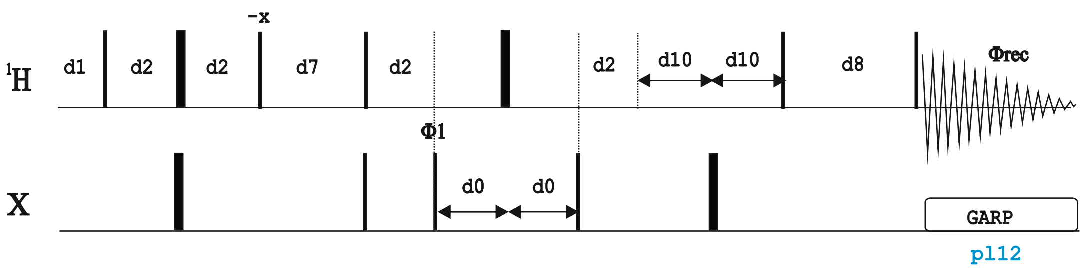
References:

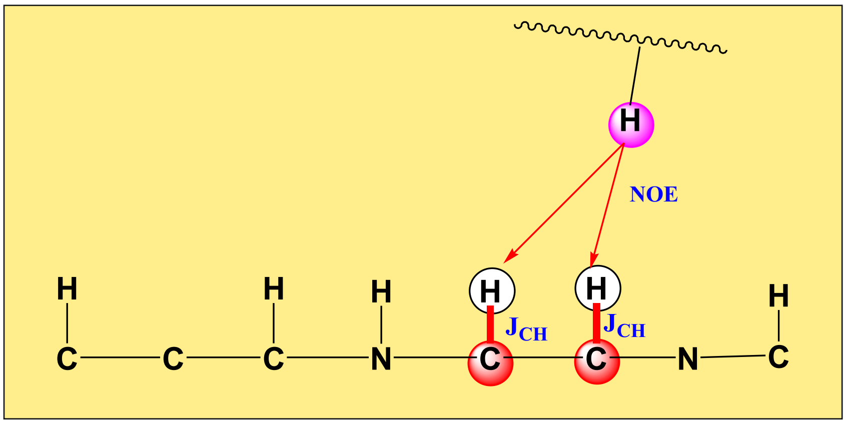
A. Bax and S. Subramanian, J. Magn. Reson. 67, 565-569 (1986)
A. Bax & D.G. Davis, J. Magn. Reson. 65, 355-360 (1985)

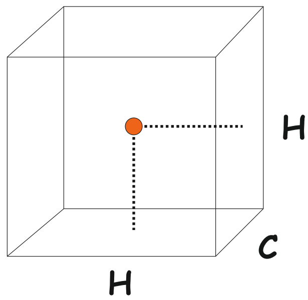




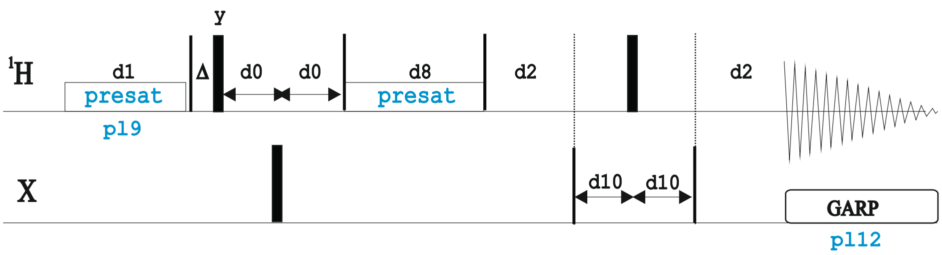
hmqcnoesybi3d

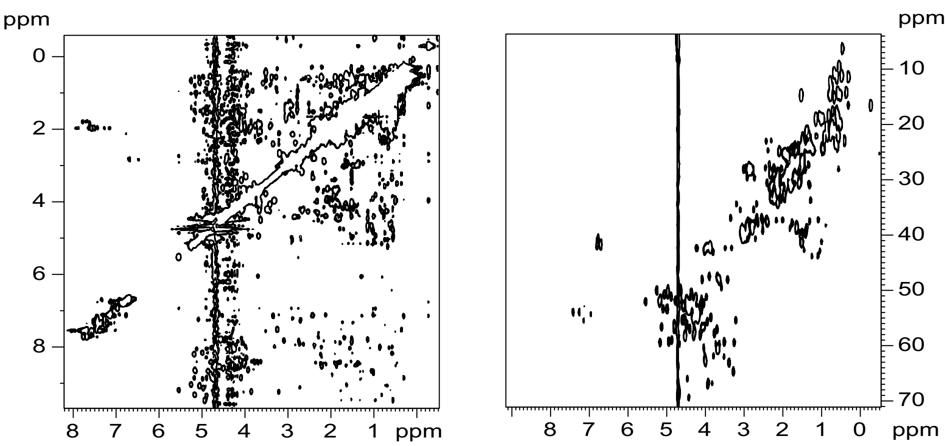






noesyhmqcpr3d





3D NOESY-HSQC / 3D NOESY-HMQC

- **Gradient-enhanced from f2 channel:**

  3D ^{1}H-^{13}C NOESY-HSQC experiment
  - using echo-antiecho (**noesyhsqcetgp3d** | NOESYHSQCETGP3D)
  - using PEP (**noesyhsqcetgpsi3d** | NOESYHSQCETGPSI3D)

- **Gradient-enhanced from f3 channel:**

  3D ^{1}H-^{15}N NOESY-HSQC experiment
  - using echo-antiecho (**noesyhsqcetf3gp3d** | NOESYHSQCETF3GP3D)
  - using PEP (**noesyhsqcf3gpsi3d** | NOESYHSQCF3GPSI3D)
  - using PEP and water flip-back (**noesyhsqcfpf3gpsi3d** | NOESYHSQCFPF3GPSI3D)
  - using WATERGATE with 3919 (**noesyhsqcf3gp193d** | NOESYHSQCF3GP193D)
  - using WATERGATE with shaped pulses (**noesyhsqcf3gpwg3d**)
  - using TROSY (**noesytretf3gp3d** | NOESYTRETF3GP3D)
  - using ZQ-TROSY and WATERGATE (**noesytzgp3d** | NOESYTZGP3D)
  - using TROSY for aromatic residues and WATERGATE (**noesytrosyargpphwg**)

  3D ^{1}H-^{15}N NOESY-HMQC experiment
  - using WATERGATE (**noesyhmqcf3gpph3d**)

- **Gradient-enhanced from f2 and f3 channel:**

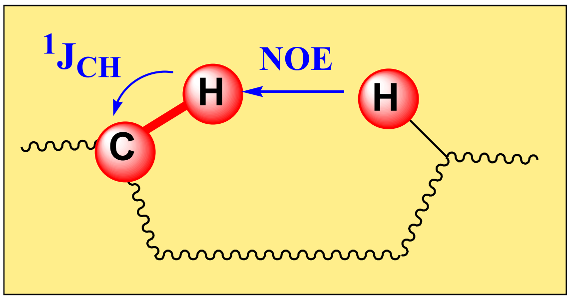
  3D NOESY-^{13}C,^{15}N-HSQC experiment
  - with simultaneous evolution (**noesyhsqcgpsm3d.2** | NOESYHSQCGPSM3D.2)
  - with simultaneous evolution, sensitivity improvement and adiabatic 13C pulses (**noesyhsqcgpsismsp3d** | NOESYHSQCGPSISMSP3D)

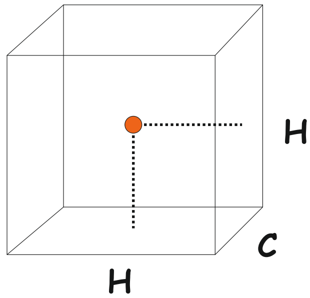
Also see NOESY-HSQC experiments in Nucleic Acid Experiments:
3D ^{1}H-^{13}C NOESY-CT-HSQC using echo-antiecho (na_noesyhsqcctetgp3d)
3D ^{1}H-^{13}C NOESY-HSQC using WATERGATE and refocusing of J(C5C6) during t_1 (na_c6noesyhsqcgp3d)
3D ^{1}H-^{15}N NOESY-HSQC using WATERGATE (na_noesyhsqcf3gpwg3d)

Related Experiments:
2D NOESY
3D NOESY-HSQC
3D HSQC-NOESY-HSQC
2D & 3D X-filtered/edited NOESY

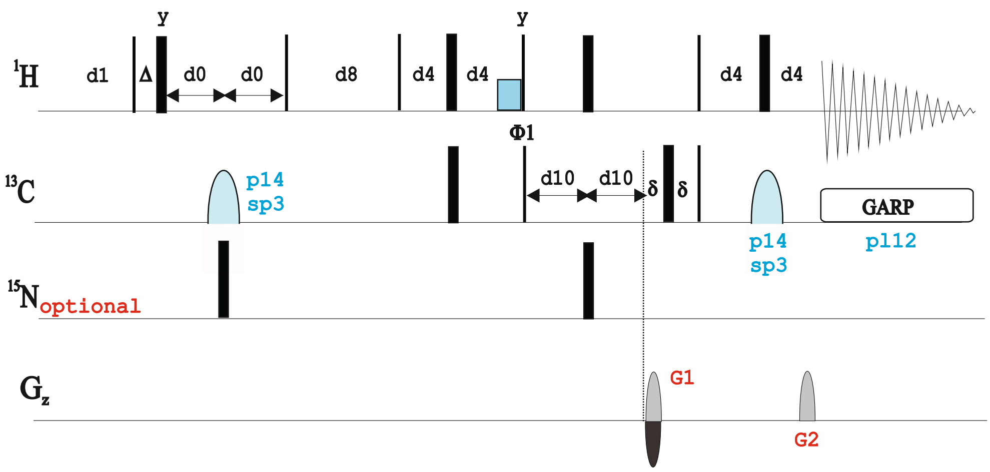
NOESY-HSQC:

1. A.L. Davis, J. Keeler, E.D. Laue & D. Moskau, J. Magn. Reson. 98, 207-216 (1992)
2. O. Zhang, L.E. Kay, J.P. Olivier & J.D. Forman-Kay, J. Biomol. NMR 4, 845 - 858 (1994)
3. G. Zhu, X.M. Kong & K.H. Sze, J. Biomol. NMR 13, 77-81 (1999)
4. K.V. Pervushin, G. Wider, R. Riek & K. Wuethrich, PNAS, 96, 9607-9612 (1999)





noesyhsqcetgp3d



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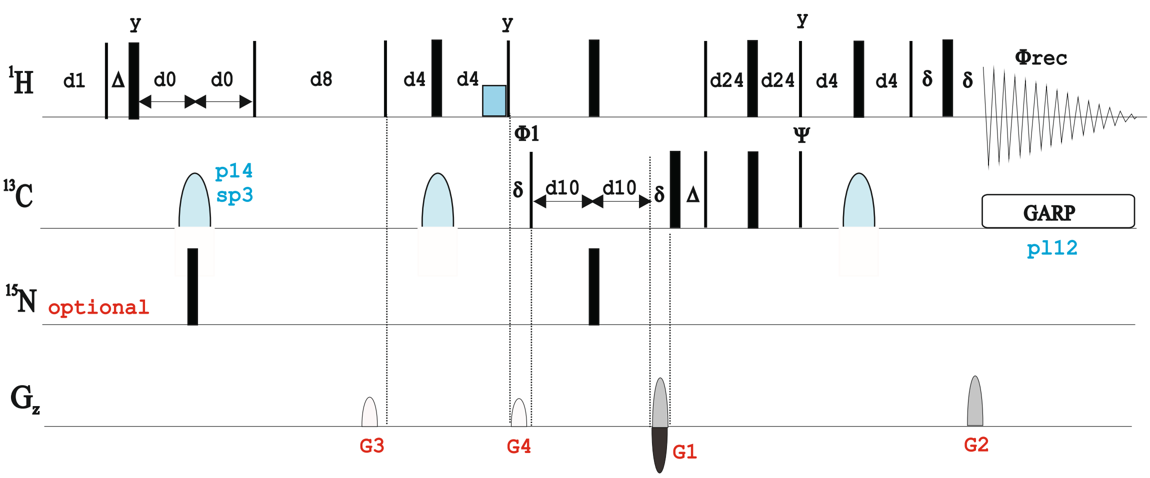
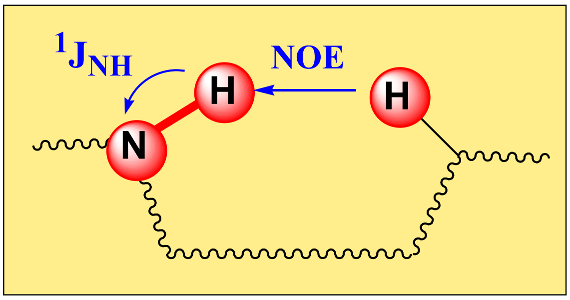
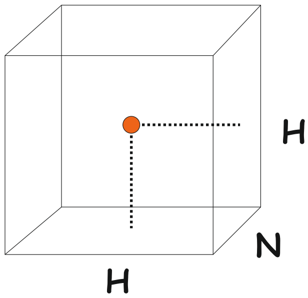
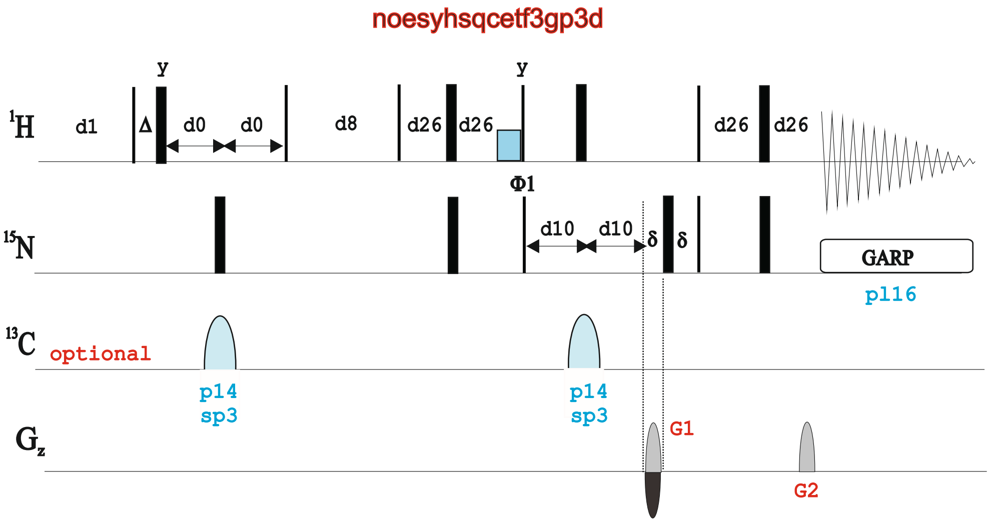



1JNH
NOE
H
H
N


H
N
H


noesyhsqcetf3gp3d
1H
d1
Δ
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d0
d0
d8
d26
d26
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d26
d26
Φ1
15N
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d10
δ
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GARP
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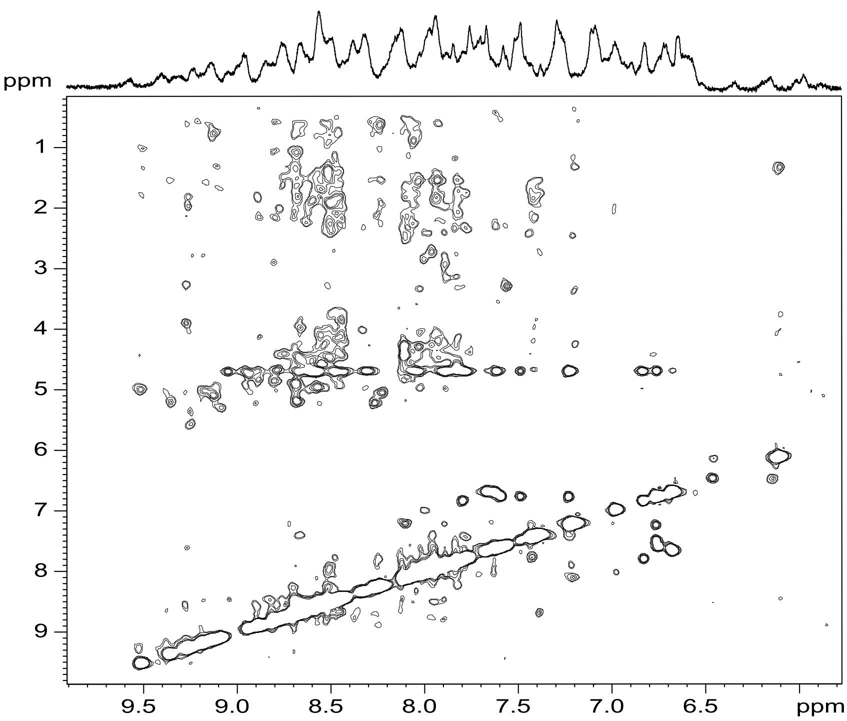
13C
optional
p14
sp3
p14
sp3
Gz
G1
G2


ppm
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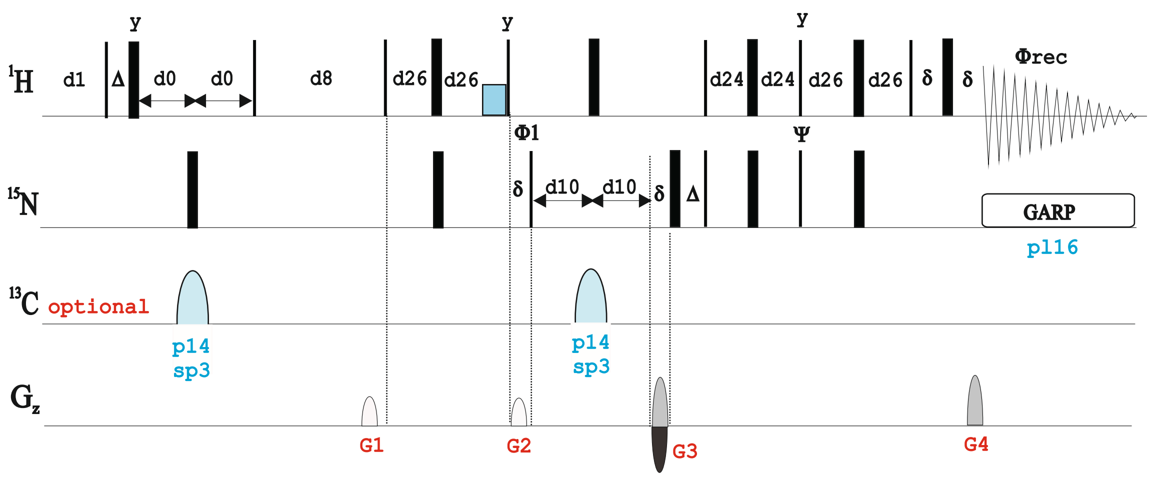
8.0
7.5
7.0
6.5
ppm

noesyhsqcf3gpsi3d



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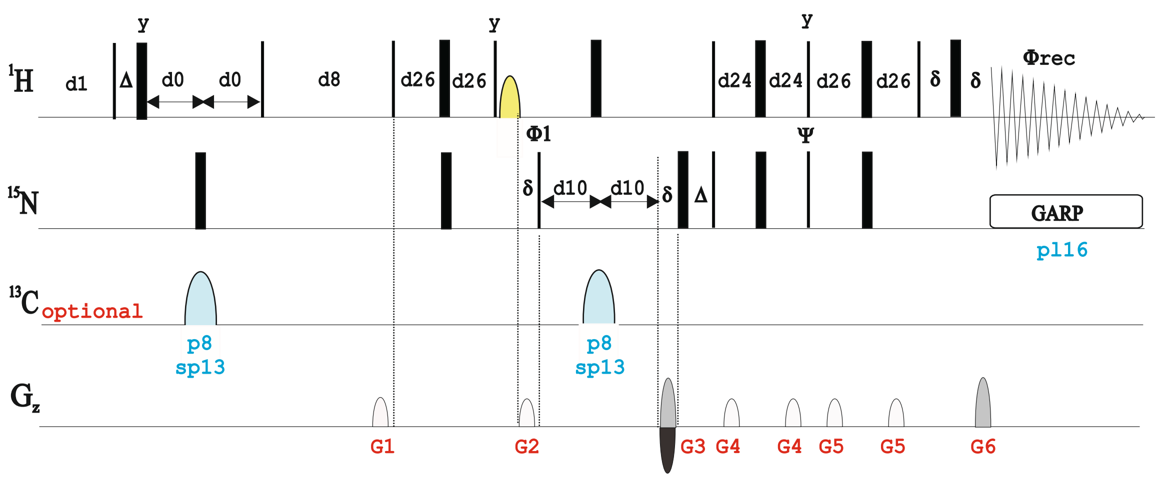

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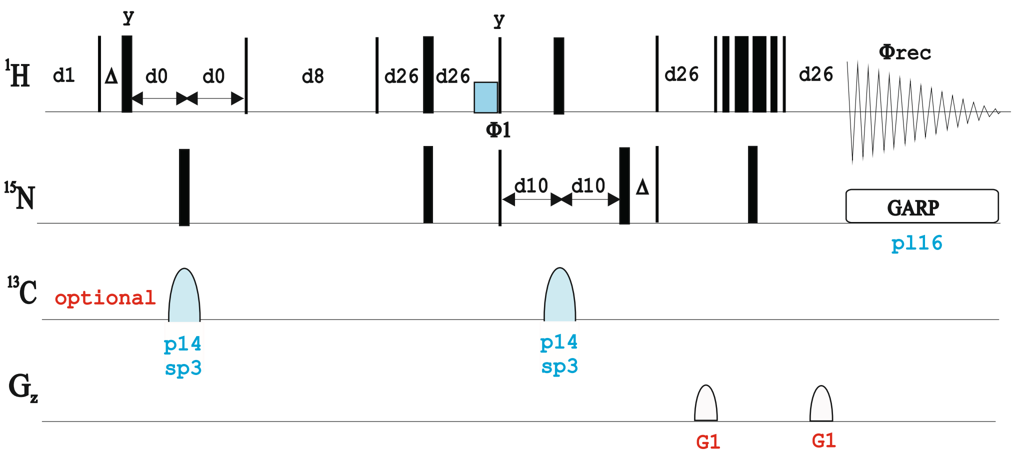

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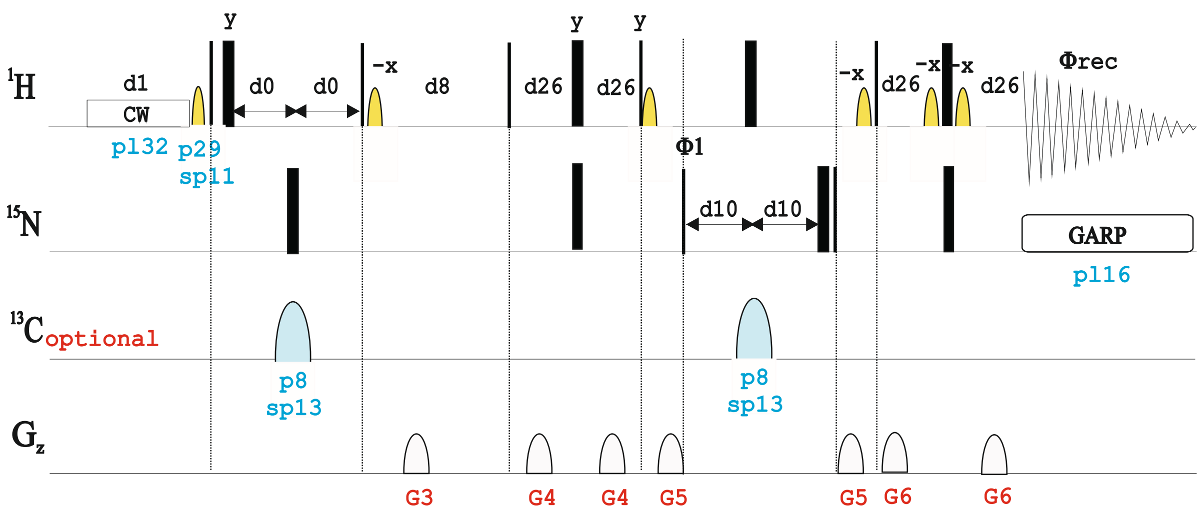
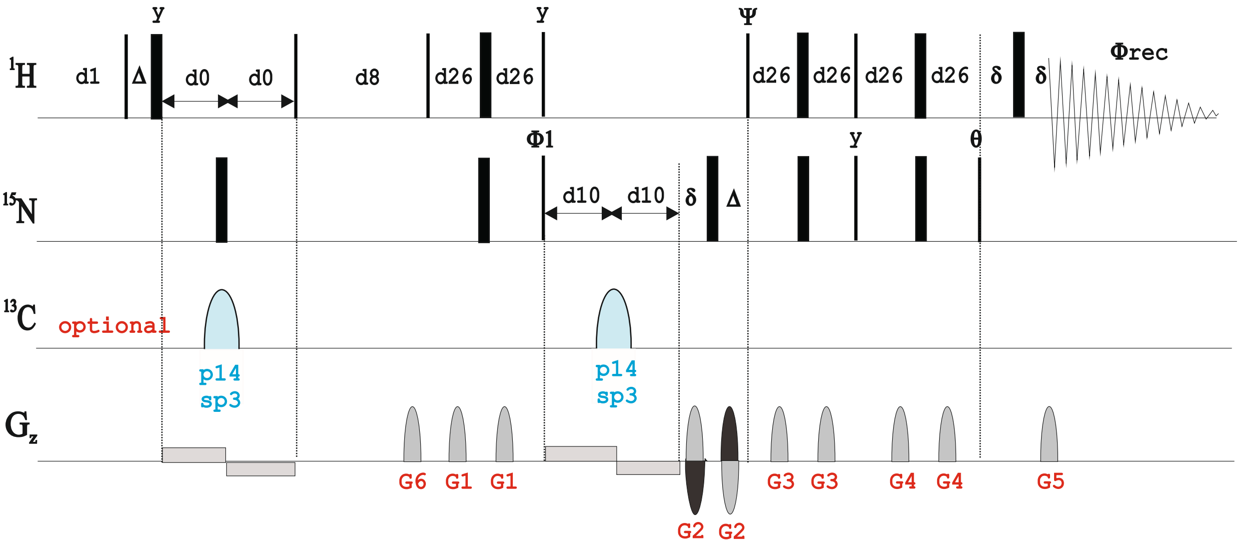


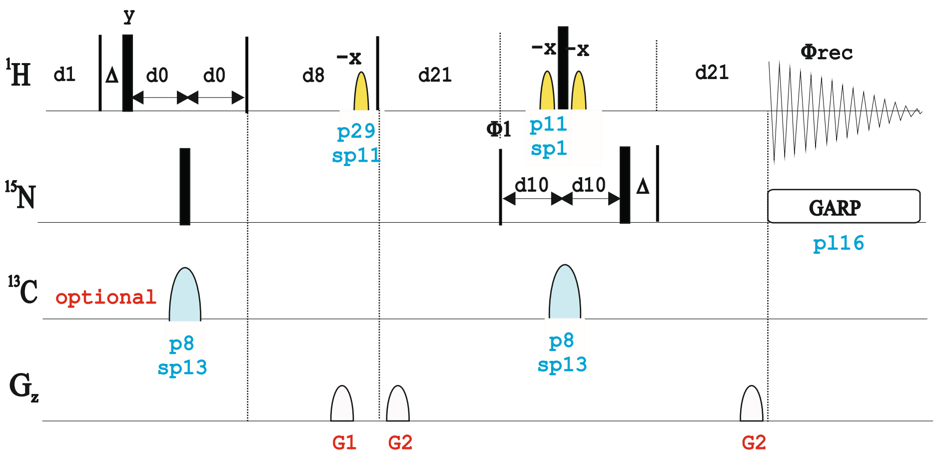
NOESY-TROSY

noesytretf3gp3d



NOESY-HMQC

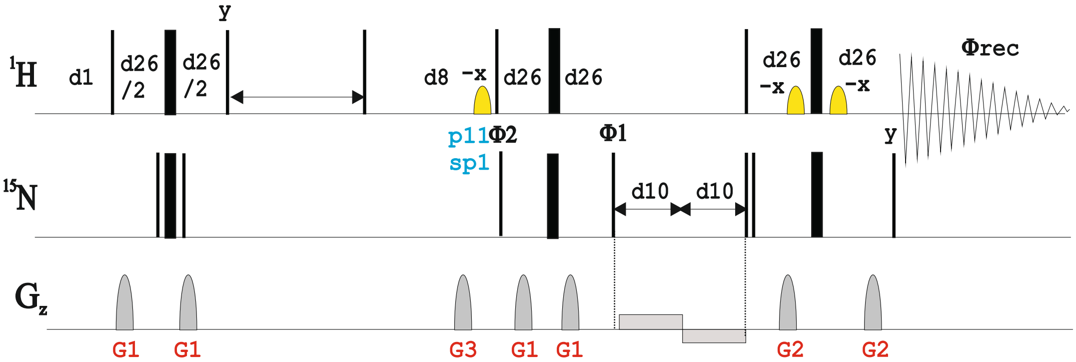
noesyhmqcf3gpph3d



NOESY-ZQ-TROSY

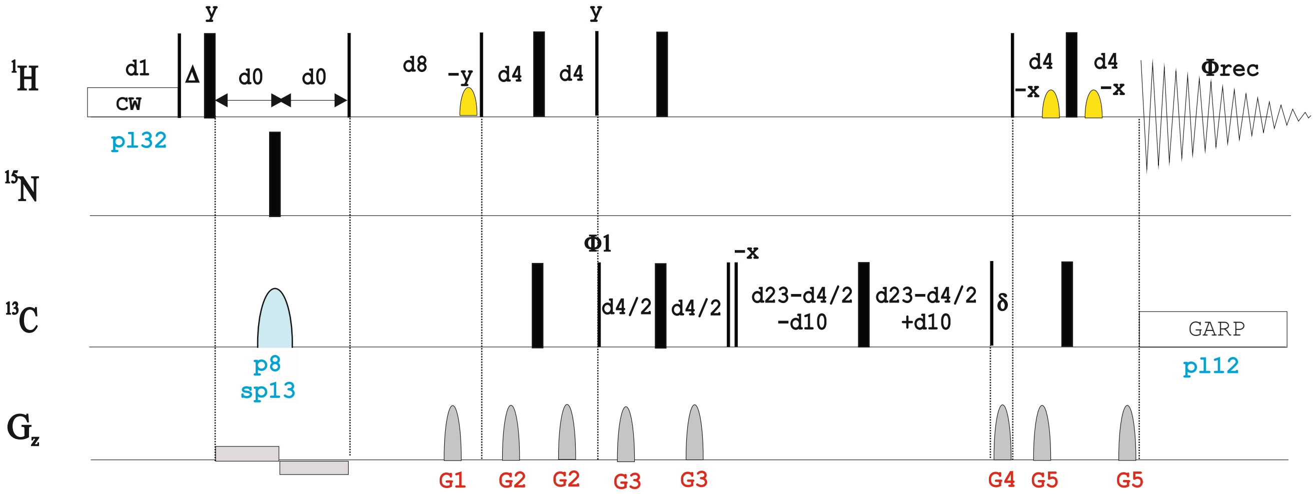
K.V. Pervushin, G. Wider, R. Riek & K. Wuethrich, Proc. Natl. Acad. Sci USA 96, 9607-9612 (1999)

noesytzgp3d



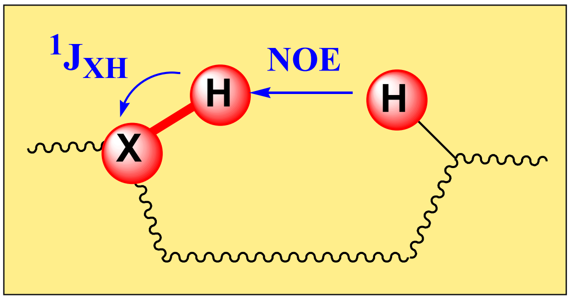
NOESY-TROSY for Aromatic Residues

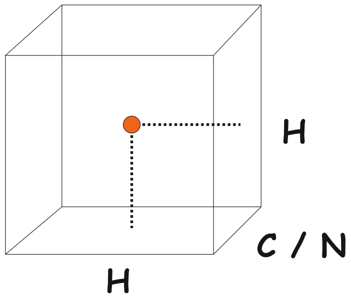
noesytrosyargpphwg



NOESY-13C,15N-HSQC

S.M. Pascal, D.R. Muhandiram, T. Yamazaki, J.D. Forman-Kay & L.E. Kay, J. Magn. Reson. B103, 197 - 201 (1994)





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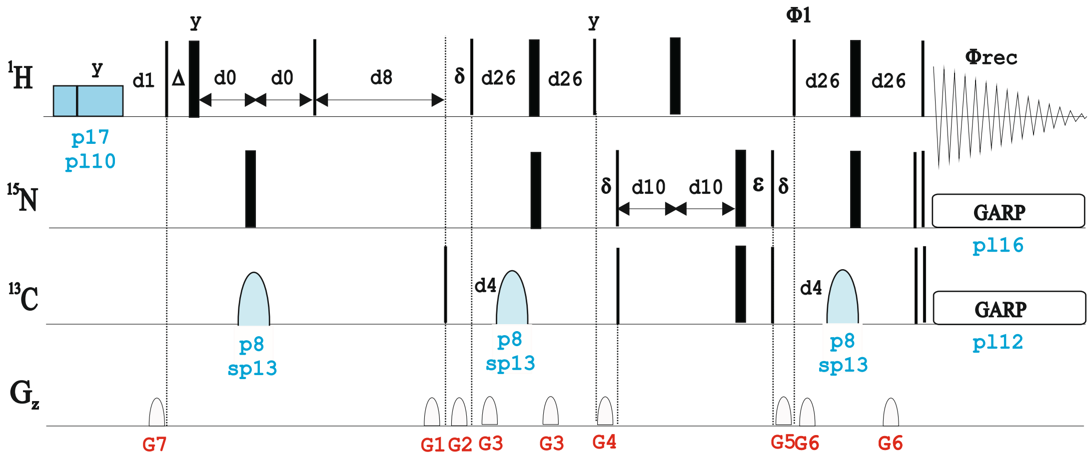

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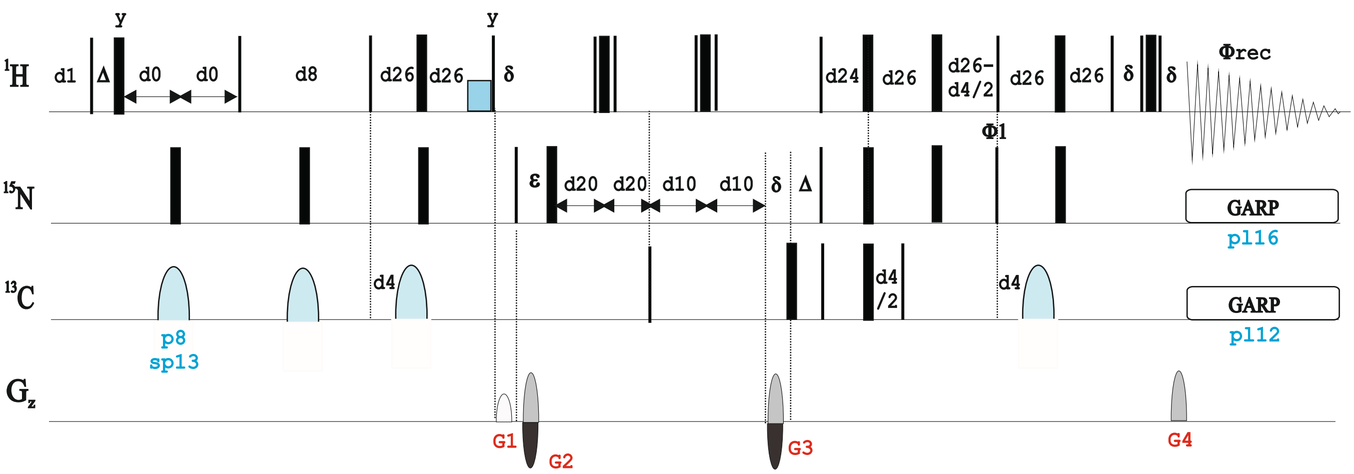

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NMRGuide

3D and 4D
HSQC-NOESY-HSQC
EXPERIMENTS

3D HSQC-NOESY-HSQC

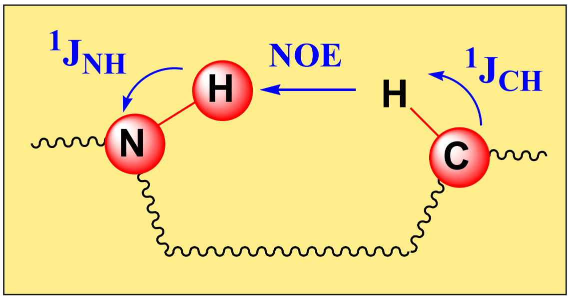
- 3D ^{1}H-^{13}C HSQC-NOESY- ^{1}H-^{15}N HSQC (**noesycngp3d** | NOESYCNGP3D)
- 3D ^{1}H-^{15}N HSQC-NOESY- ^{1}H-^{13}C HSQC (**noesyncgp3d** | NOESYNCGP3D)

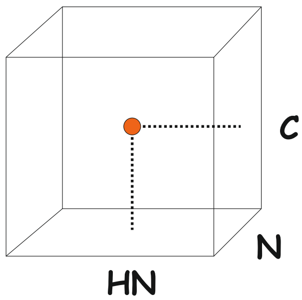
4D HSQC-NOESY-HSQC
4D HSQC-NOESY-HMQC
4D HMQC-NOESY-HMQC

- ^{13}C-^{13}C
  - 4D ^{1}H-^{13}C HSQC-NOESY- ^{1}H-^{13}C HSQC (**hsqcnoesyhsqcccgp4d** | HSQCNOESYHSQCCCGP4D)
- ^{13}C-^{15}N
  - 4D ^{1}H-^{13}C HSQC-NOESY- ^{1}H-^{15}N HSQC (**hsqcnoesyhsqccngp4d** | HSQCNOESYHSQCCNGP4D)
  - 4D ^{1}H-^{13}C HSQC-NOESY- ^{1}H-^{15}N HMQC (**hsqcnoesyhmqccngp4d**)
  - 4D ^{1}H-^{13}C HMQC-NOESY- ^{1}H-^{15}N HSQC (**hmqcnoesyhmqcncgp4d**)
- ^{15}N-^{13}C
  - 4D ^{1}H-^{15}N HSQC-NOESY- ^{1}H-^{13}C HSQC (**hsqcnoesyhsqcncgp4d** | HSQCNOESYHSQCNCGP4D)
- ^{15}N-^{15}N
  - 4D ^{1}H-^{13}C HSQC-NOESY- ^{1}H-^{15}N HSQC (**hsqcnoesyhsqcnngp4d** | HSQCNOESYHSQCNNGP4D)
  - 4D ^{1}H-^{13}C HMQC-NOESY- ^{1}H-^{15}N HMQC (**hmqcnoesyhmqcnngp4d**)

Related Experiments:
2D NOESY
3D NOESY-HSQC
2D & 3D X-filtered/edited NOESY

References:
T. Diercks, M. Coles & H. Kessler, J. Biomol. NMR, 15, 177-180 (1999)





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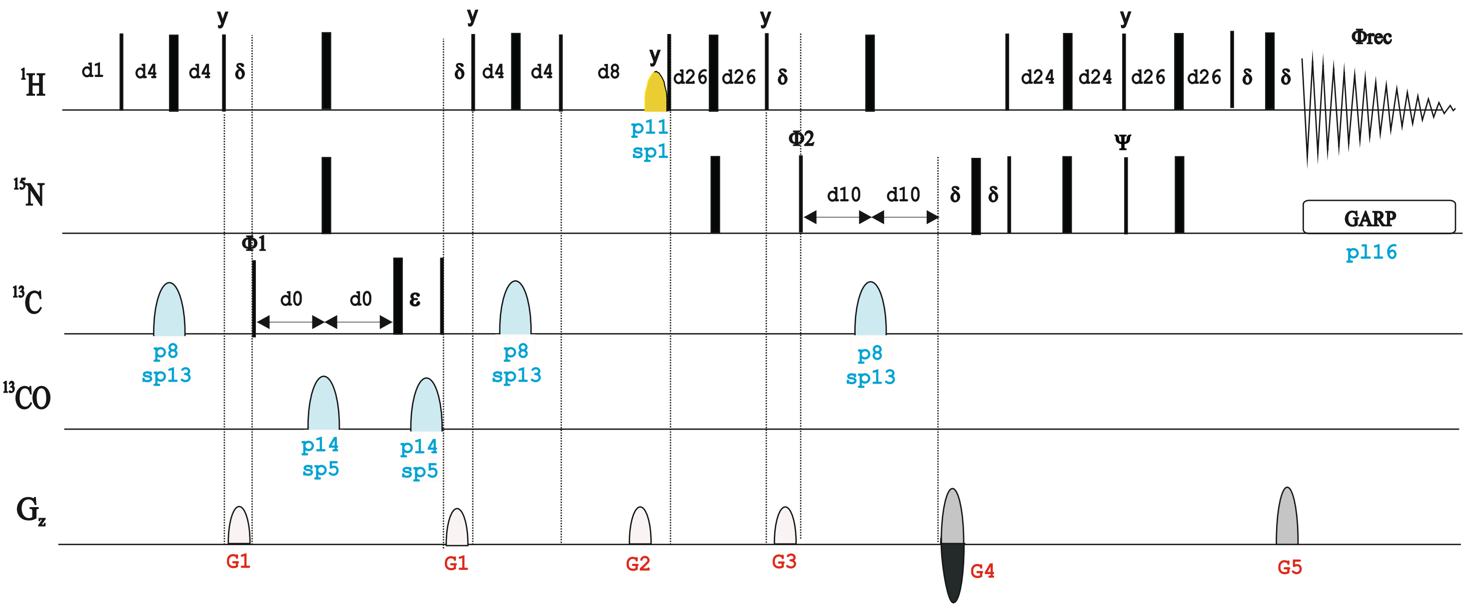

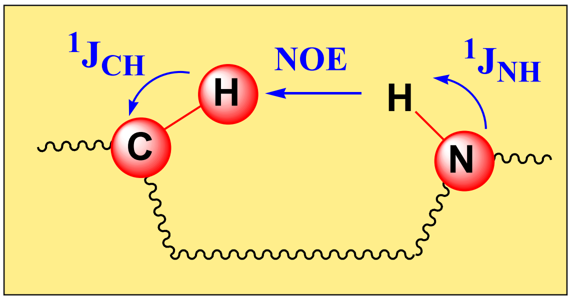

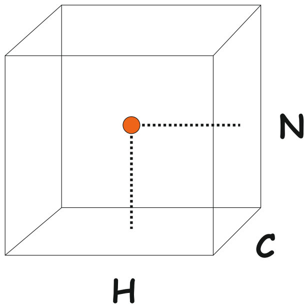

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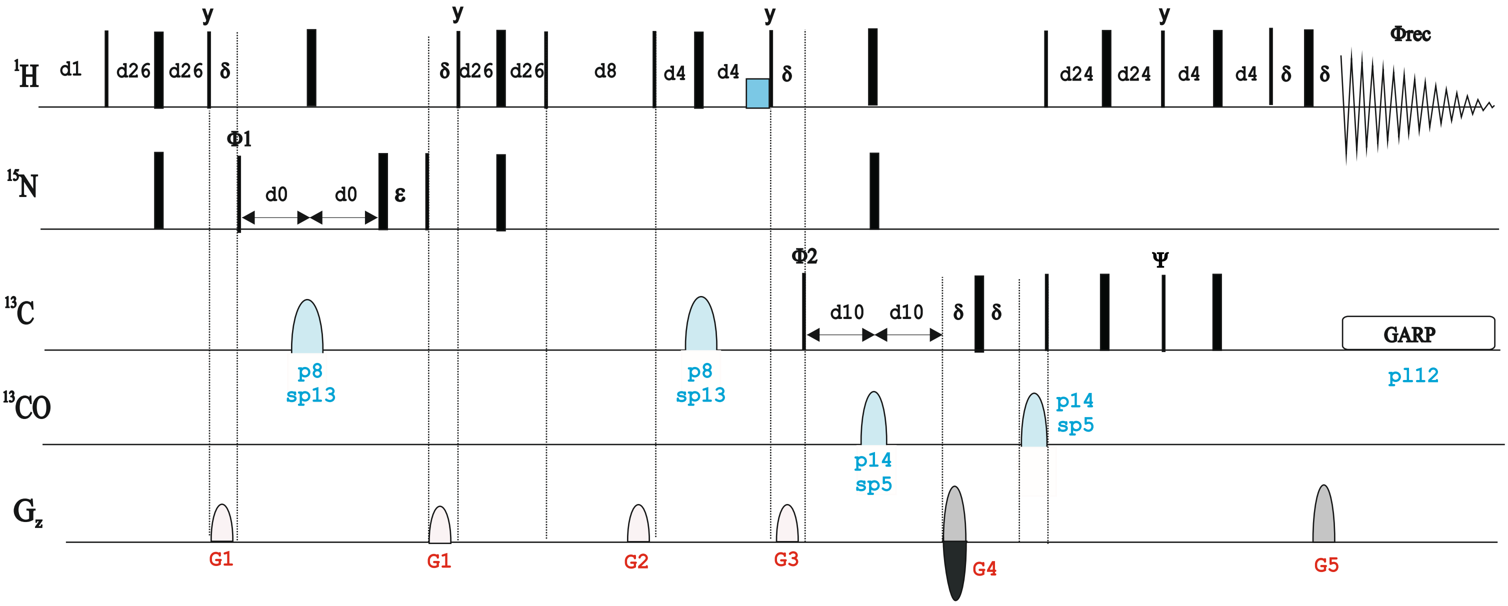

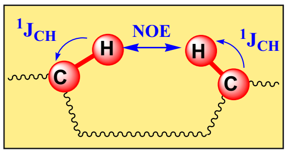

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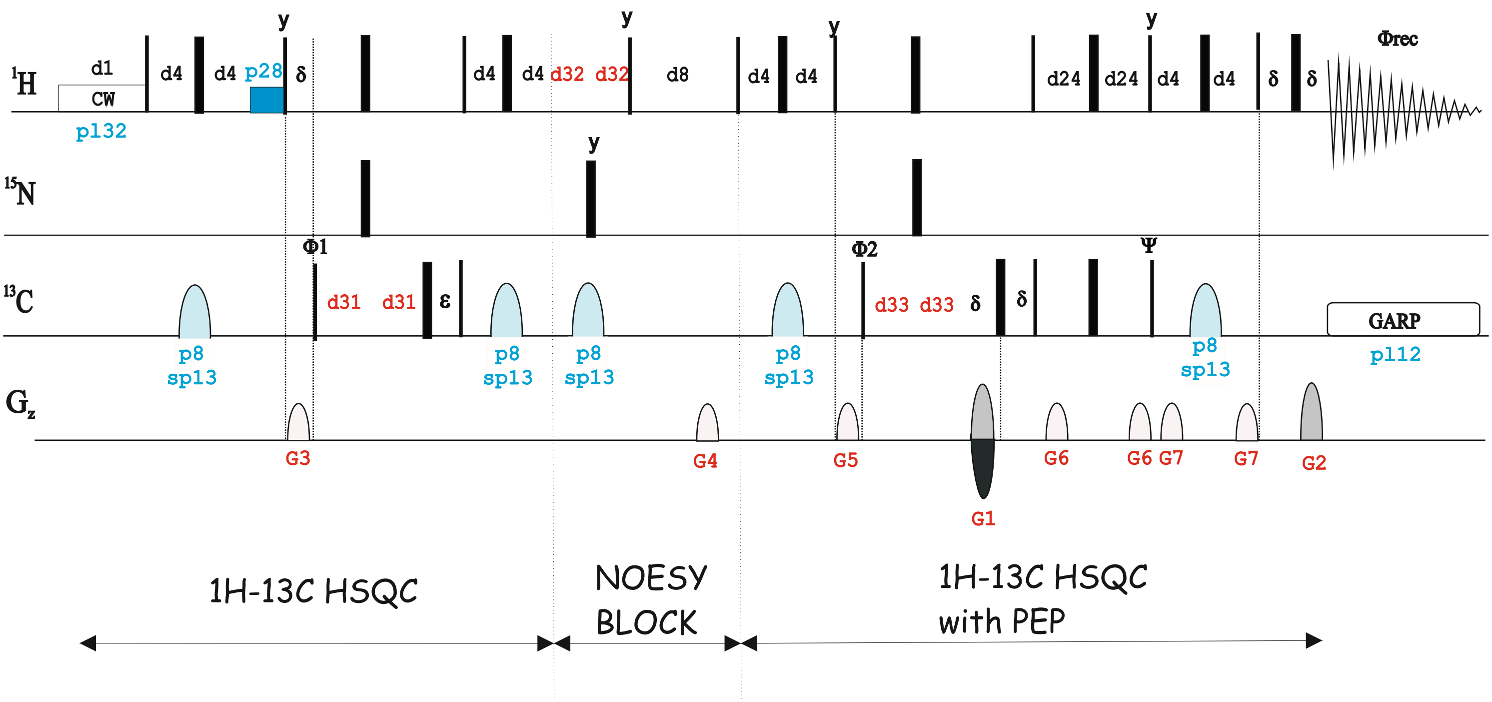

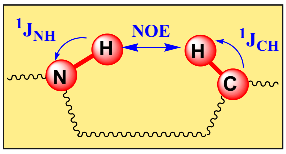

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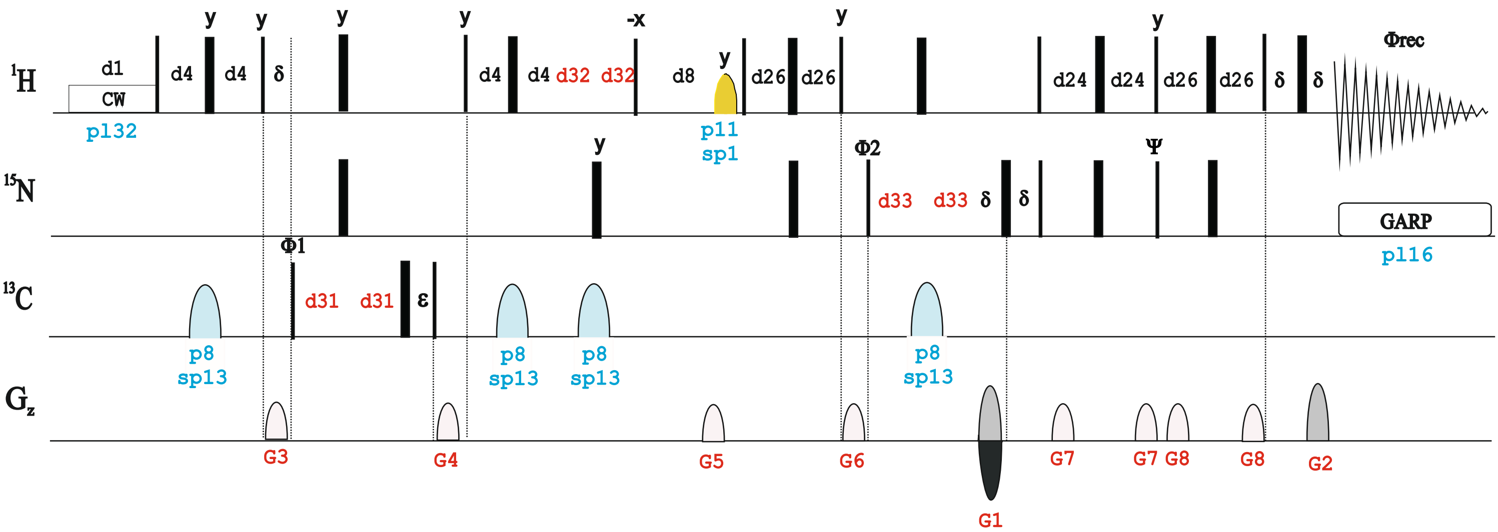

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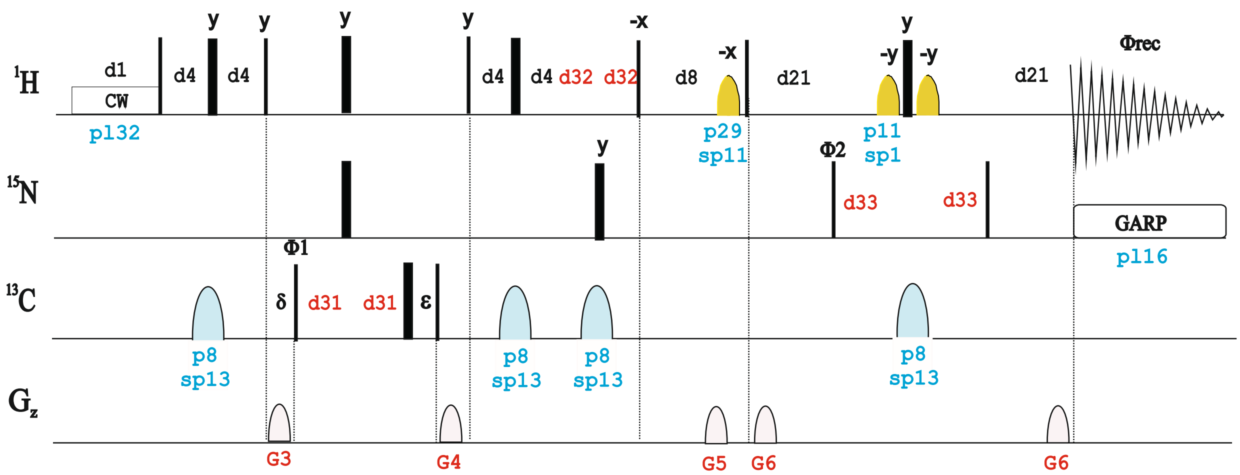

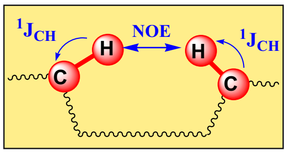

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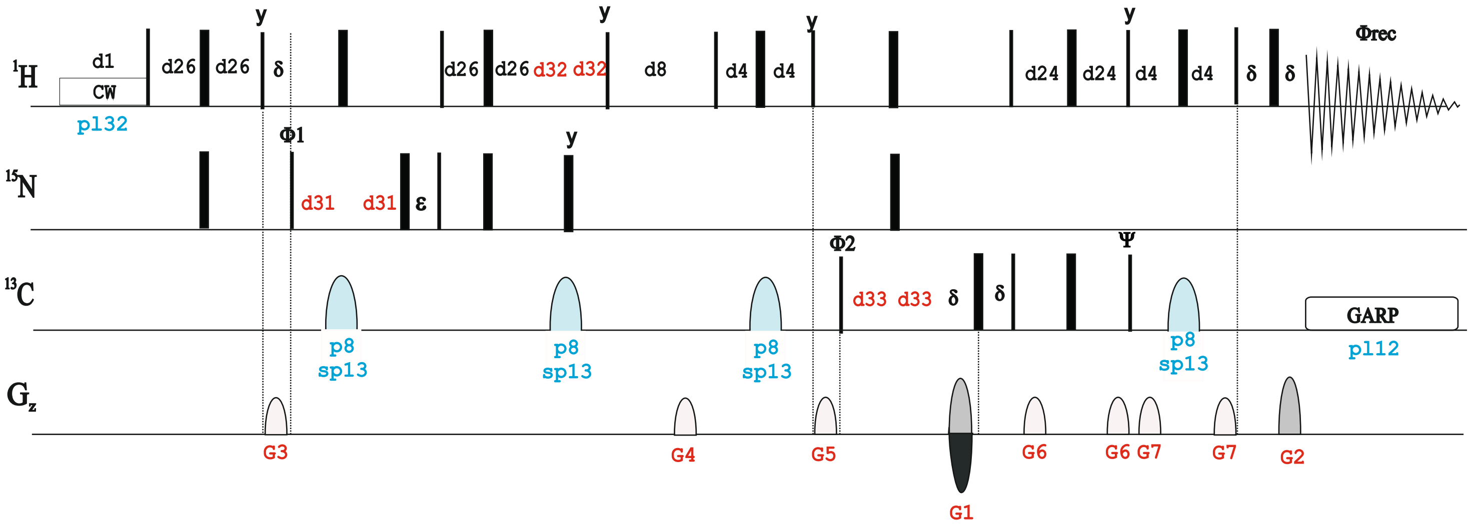

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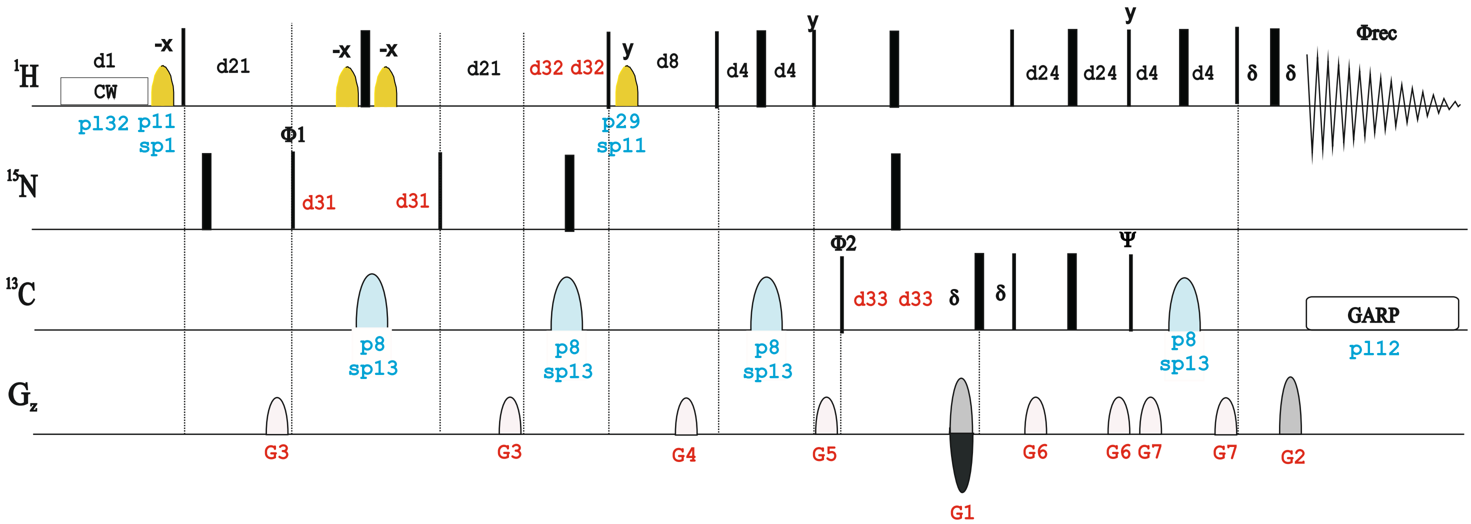

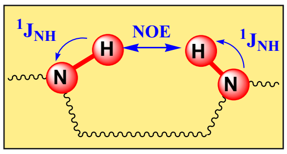

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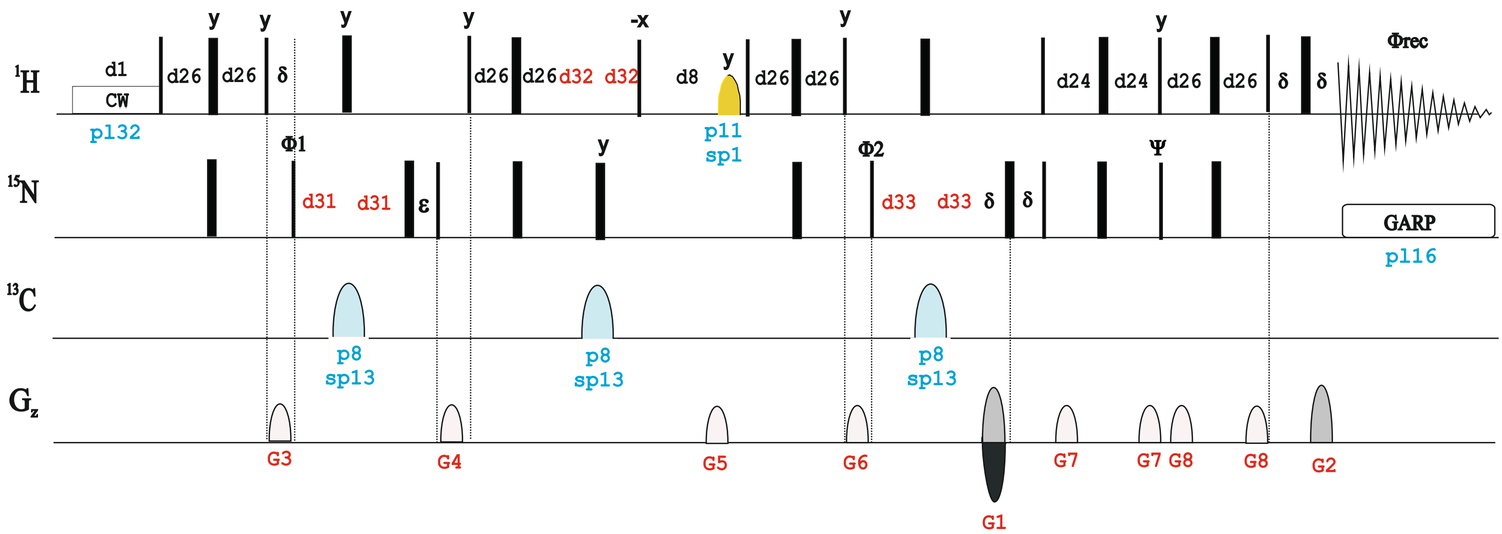

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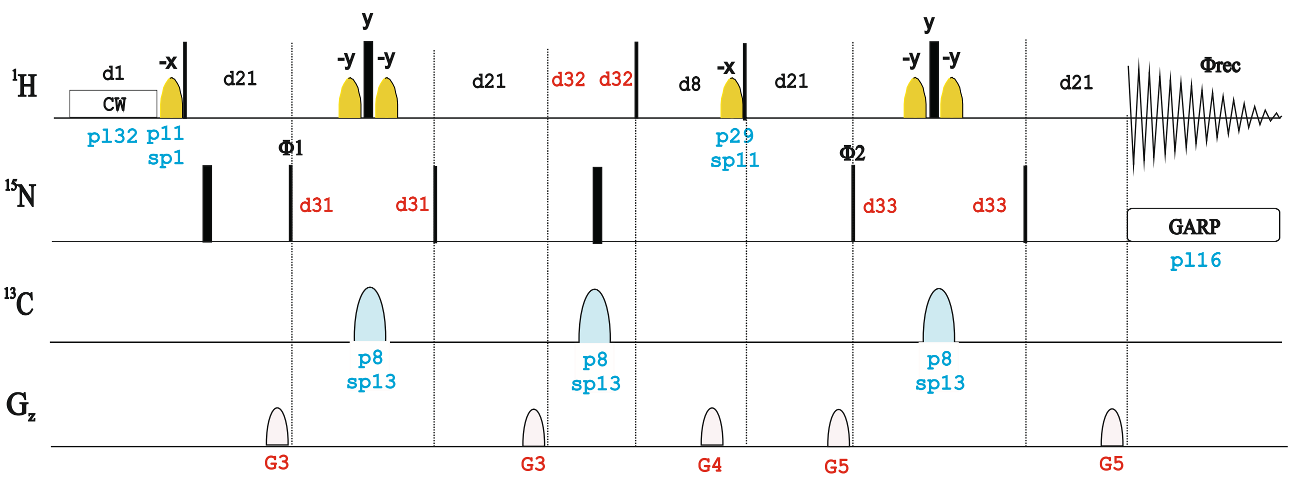

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NMRGuide

2D X-FILTERED/EDITED
NOESY EXPERIMENTS

2D X-Filtered/edited NOESY

ge-2D w_1,w_2 ^{13}C-filtered/edited NOESY experiment

- Phase-sensitive ge-2D w_1,w_2 ^{13}C-filtered/edited NOESY with presaturation (**noesygpphprxf** | NA_NOESYGPPHPRXF)
- Phase-sensitive ge-2D w_1,w_2 ^{13}C-filtered/edited NOESY with WATERGATE (3-9-19) (**noesygpphxf19**| NA_NOESYGPPHXF19)

ge-2D w_1,w_2-^{15}N-filtered/edited NOESY experiment

- Phase-sensitive ge-2D w_1,w_2-^{15}N-filtered/edited NOESY using WATERGATE (3-9-19) (**noesyf3gpphxf19**| NOESYF3GPPHXF19)

ge-2D w_1-^{13}C,^{15}N-Doubly Filtered NOESY experiment

- ge-2D w_1-^{13}C,^{15}N-Doubly Filtered NOESY using WATERGATE (**noesygpphwgx1**| NOESYGPPHWGX1)

ge-2D w_2-^{13}C,^{15}N-Doubly Filtered NOESY experiment

- ge-2D w_2-^{13}C,^{15}N-Doubly Filtered NOESY using WATERGATE (**noesygpphwgx2**| NOESYGPPHWGX2)

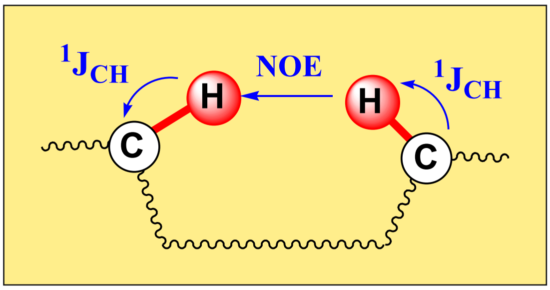
ge-2D w_1,w_2-^{13}C,^{15}N-Doubly Filtered NOESY experiment

- Phase-sensitive ge-2D w_1,w_2 ^{13}C,^{15}N -Doubly Filtered NOESY with WATERGATE (selective pulses) (**noesygpphwgxf**| NOESYGPPHWGXf)
- Phase-sensitive ge-2D w_1,w_2 ^{13}C,^{15}N-Doubly Filtered NOESY with WATERGATE (selective pulses) (**noesygpphwgxf.2**| NOESYGPPHWGXf.2)

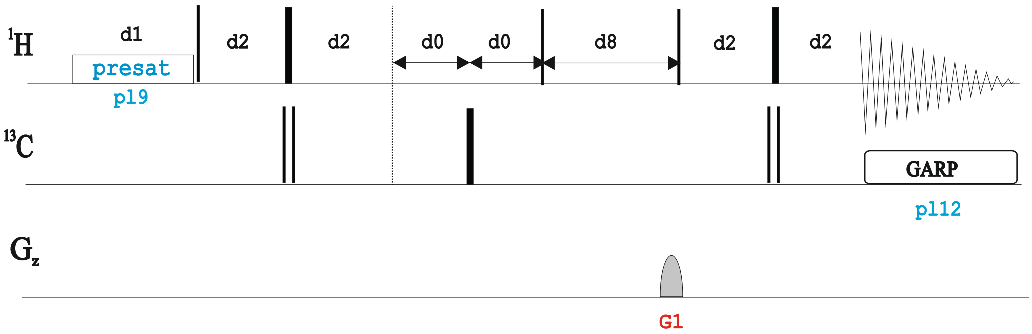
Related Experiments:
2D NOESY
3D NOESY-HSQC
3D X-filtered/edited NOESY
3D and 4D HSQC-NOESY-HSQC

References:

1. A.L. Breeze, Prog. NMR Spectrosc. 36, 323-372 (2000)
2. C. Zwahlen, P. Legault, S.J.F. Vincent, J. Greenblatt, R. Konrat & L.E. Kay, J. Am. Chem. Soc. 119 6711-6721 (1997)
3. K. Ogura, H. Terasawa & F. Inagaki, J. Biomol. NMR 8, 492-498 (1996)
4. J. Iwahara, J.M. Wojciak & R.T. Clubb, J. Biomol. NMR 19, 231-241 (2001)



noesygpphprxf



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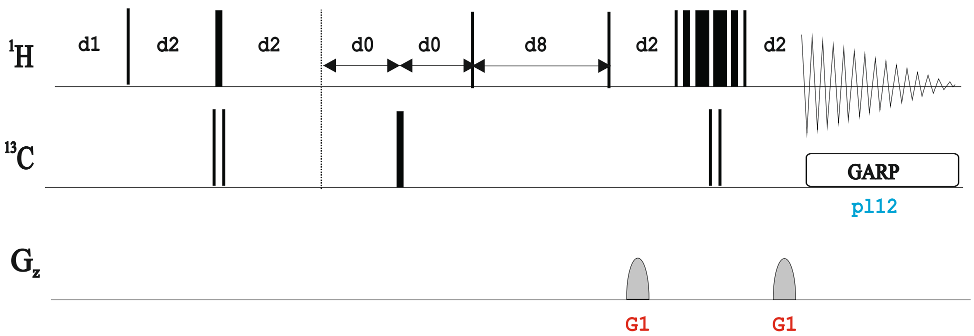
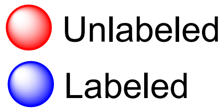
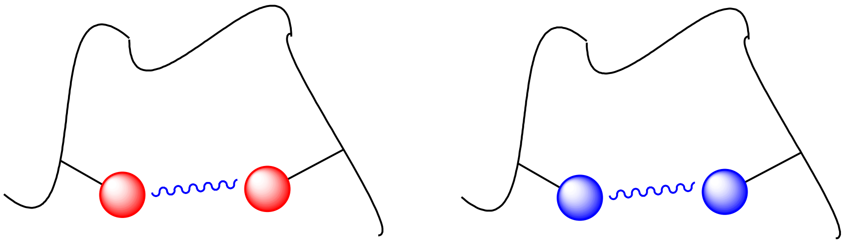
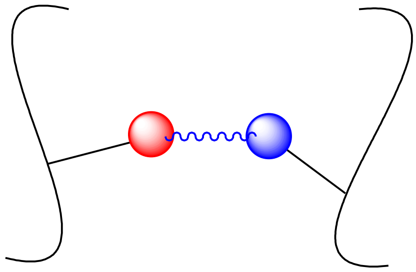


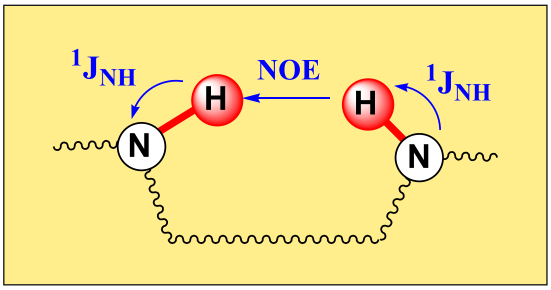


Intramolecular NOEs



Intermolecular NOEs





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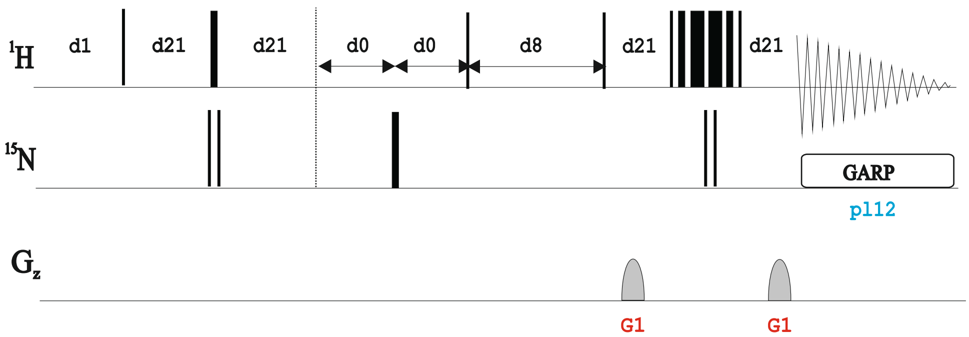
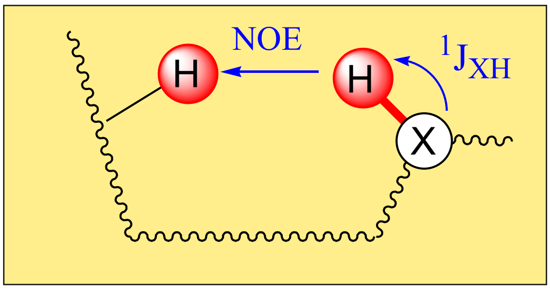
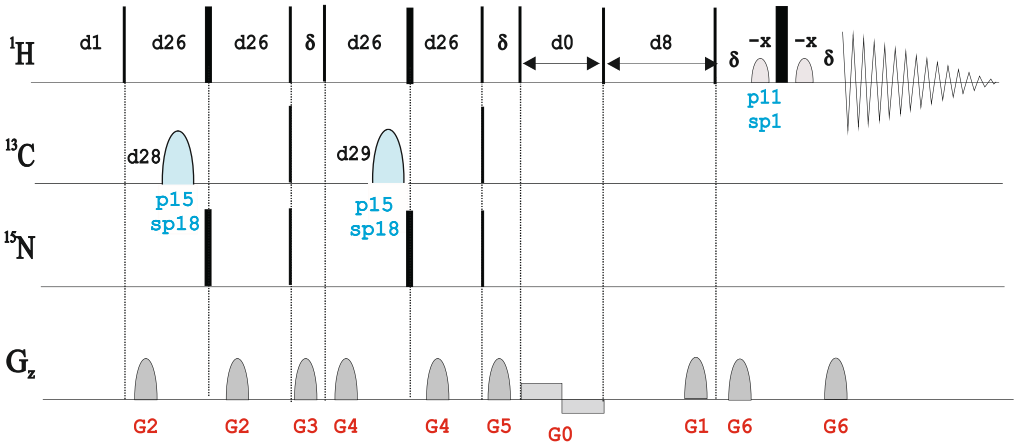


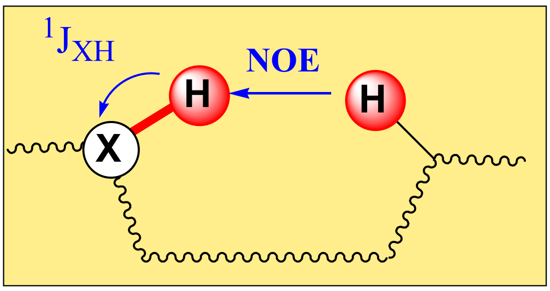
w1-13C,15N-Doubly Filtered NOESY
H[C12,N14] (t1) -> H (t2)



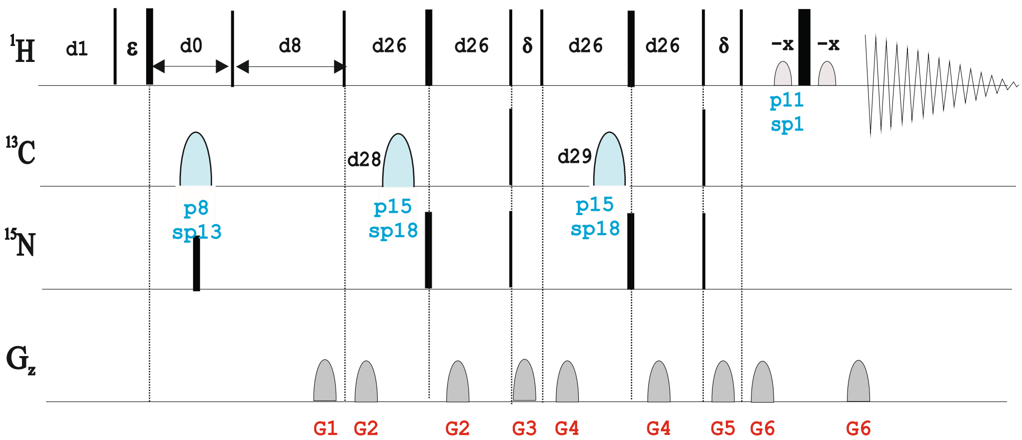
noesygpphwgx1



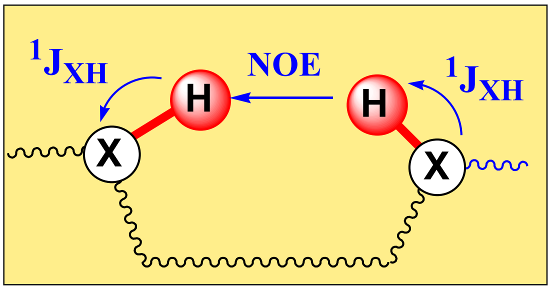
w2-13C,15N-Doubly Filtered NOESY
H (t1) -> H[C12,N14] (t2)



noesygpphwgx2



w1,w2-13C,15N-Doubly Filtered NOESY
H[C12,N14] (t1) -> H[C12,N14] (t2)



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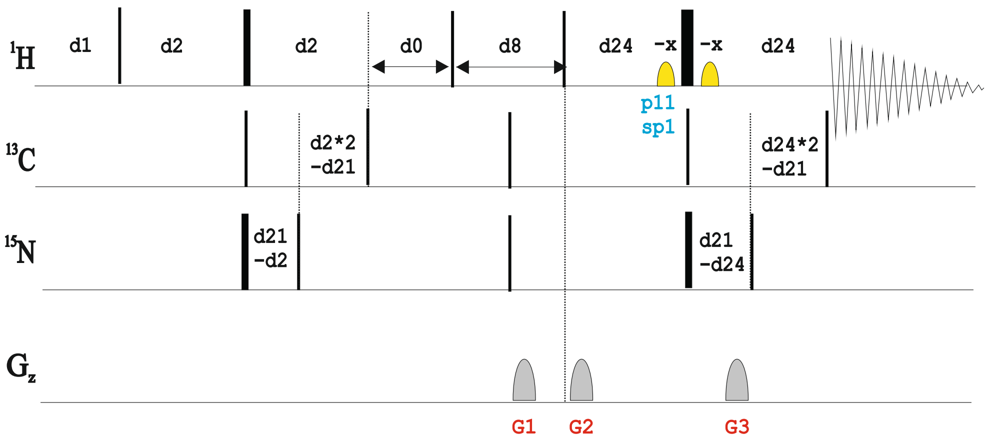
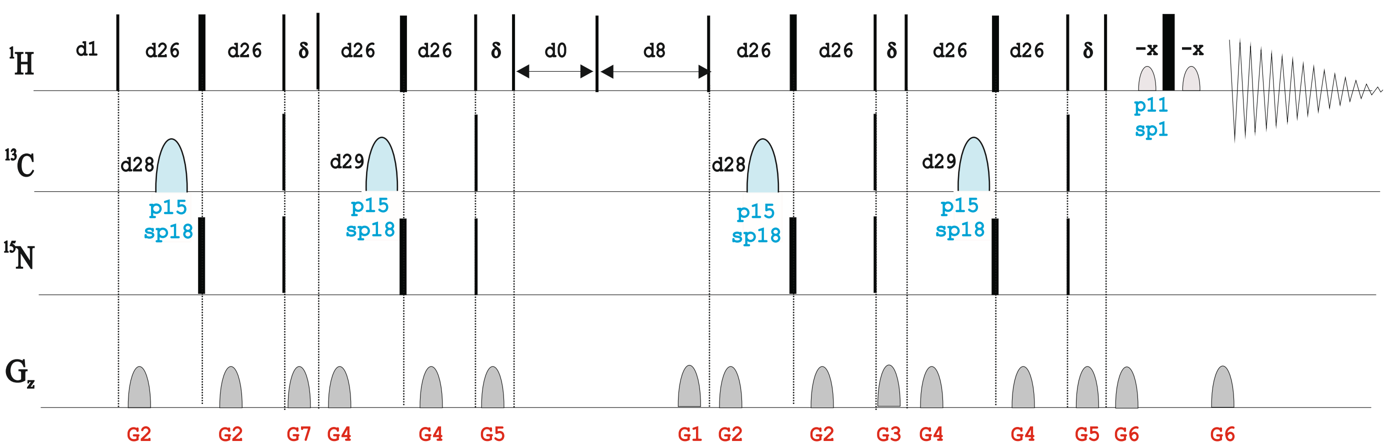


noesygpphwgxf.2



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NMRGuide

3D DOUBLY-13C,15N-FILTERED
HSQC-NOESY & NOESY-HSQC
EXPERIMENTS

3D X-Filtered HSQC-NOESY
3D X-Filtered NOESY-HSQC

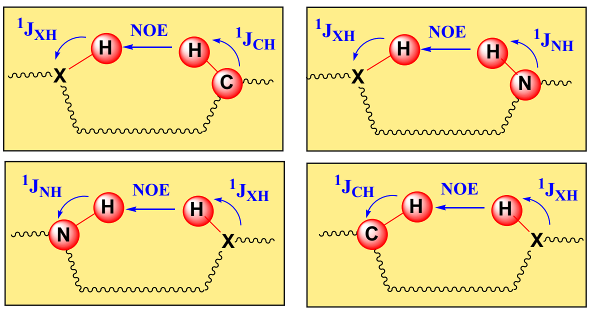
ge-3D ^{13}C,^{15}N-Doubly Filtered HSQC-NOESY experiment

- W_3-^{13}C,^{15}N-Doubly Filtered 3D ^{1}H-^{13}C-HSQC-NOESY using WATERGATE (**hsqcgpnowgx33d**| HSQCGPNOWGX33D)
- W_3-^{13}C,^{15}N-Doubly Filtered 3D ^{1}H-^{15}N-HSQC-NOESY using WATERGATE (**hsqcf3gpnowgx33d** | HSQCF3GPNOWGX33D)

ge-3D ^{13}C,^{15}N-filtered/edited NOESY-HSQC experiment

- w_1-^{13}C,^{15}N- Filtered 3D NOESY-^{1}H-^{13}C-HSQC using WATERGATE (**noesyhsqcgpwgx13d**| NOESYHSQCGPWGX13D)
- w_1-^{13}C,^{15}N- Filtered 3D NOESY-^{1}H-^{15}N-HSQC using WATERGATE (**noesyhsqcf3gpwgx13d**| NOESYHSQCF3GPWGX13D)
- w_1-^{13}C,^{15}N- Filtered 3D NOESY-^{1}H-^{15}N-HSQC using PEP and echo-antiecho (**noesyhsqcfpf3gpsix13d**)
- 3D w_1-^{12}C/^{14}N- Filtered NOESY-^{13}C, ^{15}N-HSQC experiment with simultaneous evolution and editing between labeled-unlabeled part (**noesyhsqcedgpsm3d** | NOESYHSQCEDGPSM3D)
- 3D w_1-^{12}C/^{14}N- Filtered NOESY-^{13}C, ^{15}N-HSQC experiment with simultaneous evolution, sensitivity improvement and editing between labeled-unlabeled part (**noesyhsqcedgpsism3d** | NOESYHSQCEDGPSISM3D)

Also see:
NOESY, NOESY-HSQC, HSQC-NOESY, and HSQC-NOESY-HSQC experiments



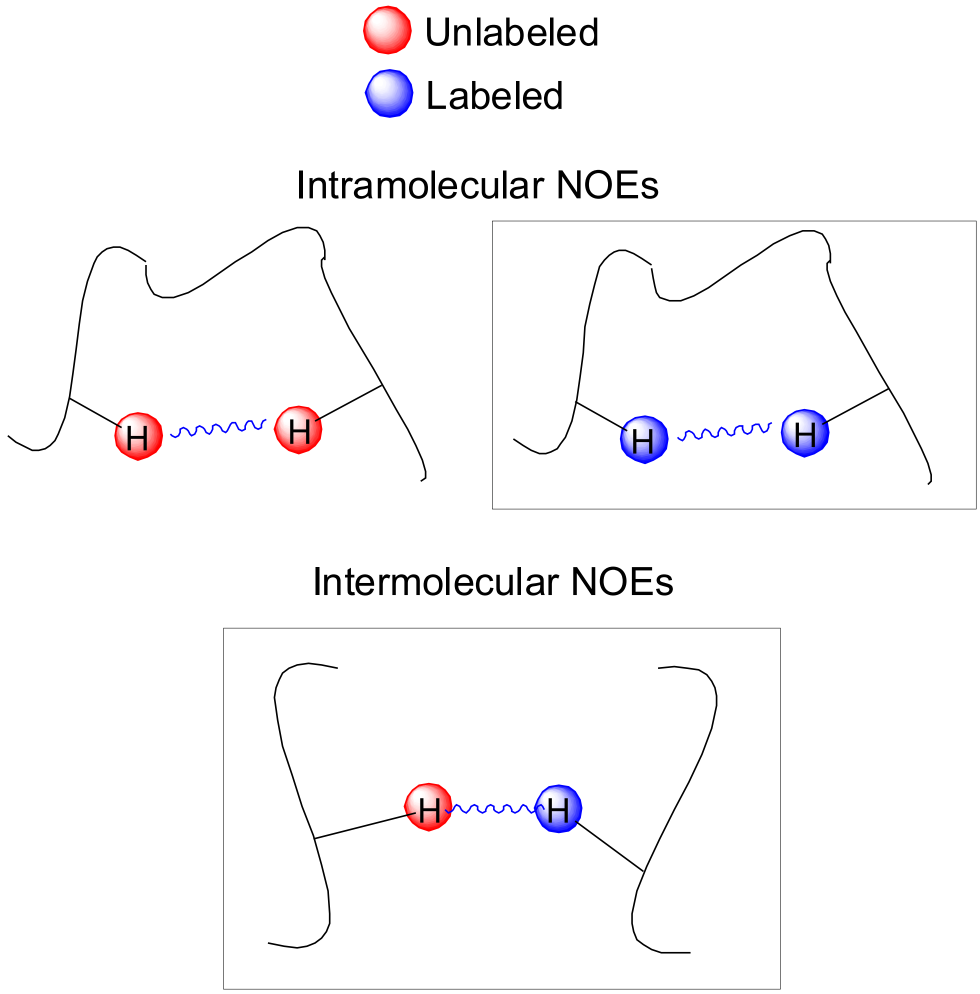
w3-Filtered 3D HSQC-NOESY

w1-Filtered 3D NOESY-HSQC

References:
1. A.L. Breeze, Prog. NMR Spectrosc. 36, 323-372 (2000)
2. C. Zwahlen, P. Legault, S.J.F. Vincent, J. Greenblatt, R. Konrat & L.E. Kay, J. Am. Chem. Soc. 119 6711-6721 (1997)
3. K. Ogura, H. Terasawa & F. Inagaki, J. Biomol. NMR 8, 492-498 (1996)
4. J. Iwahara, J.M. Wojciak & R.T. Clubb, J. Biomol. NMR 19, 231-241 (2001)

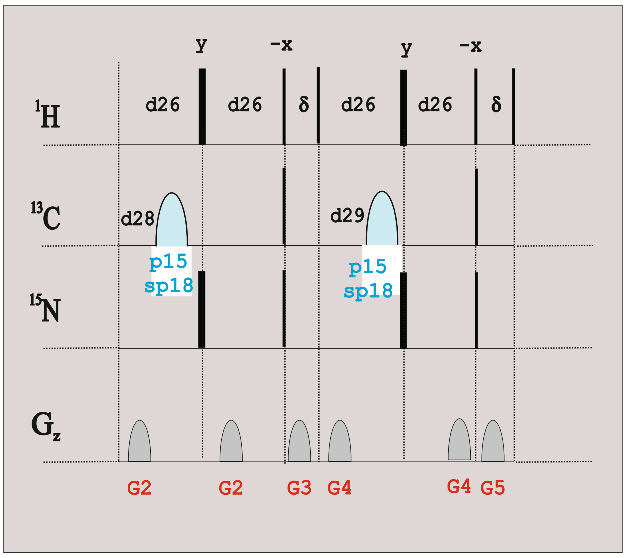
In a mixture of a 13C,15N-compound and a natural-abundance 12C,14N compound there is some different NOE pathways:
i) Intramolecular Unlabeled-Unlabeled NOEs
ii) Intramolecular Labeled-Labeled NOEs
iii)Intermolecular Labeled-Unlabeled NOEs

X-Filtered/Edited NOESY experiments can distinguish between them:



All these experiments use a Double 13C,15N-Filter

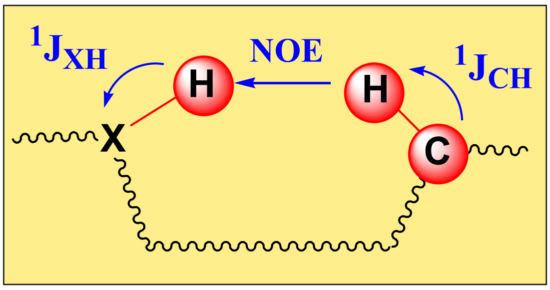
(see X-filtered TOCSY experiments)

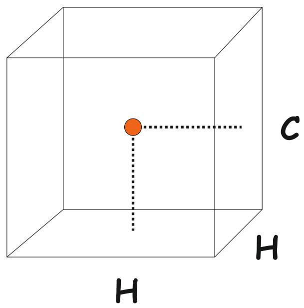


d26: 1/(4*J(NH))
d28: 1/(4*J(CH)min)
d29: 1/(4*J(CH)max)

w3-13C,15N-Doubly Filtered 13C-HSQC-NOESY experiment

C13 (t1) -> H[C13] (t2) -> H[C12,(N14)] (t3)





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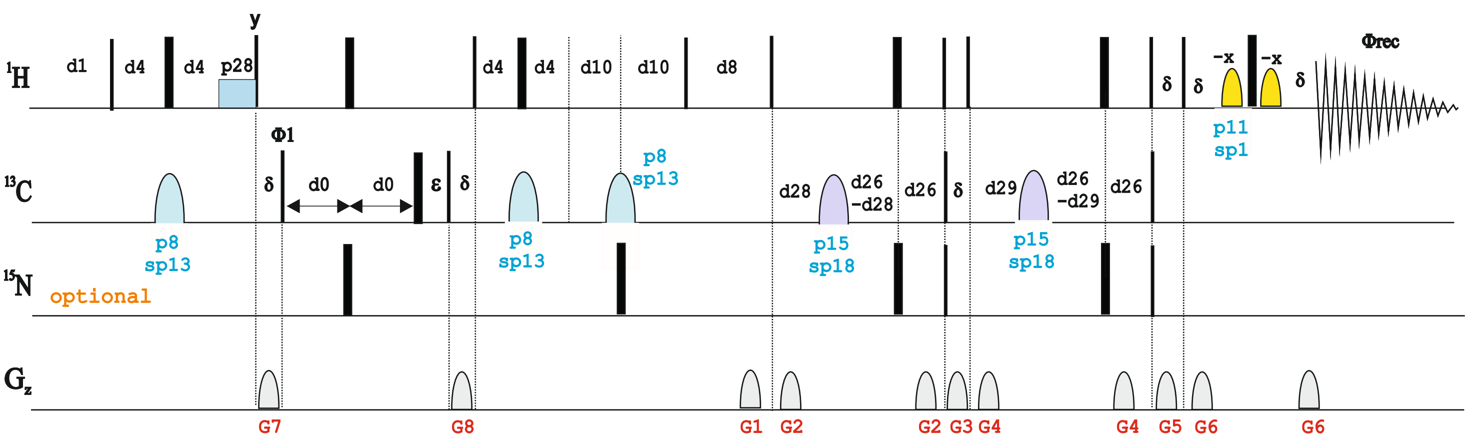
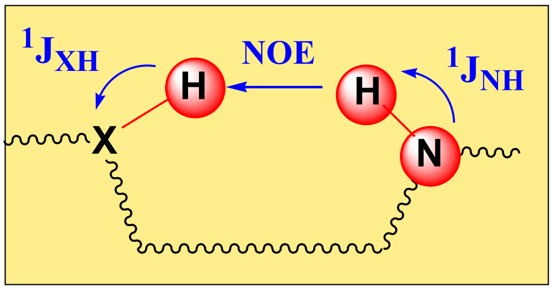
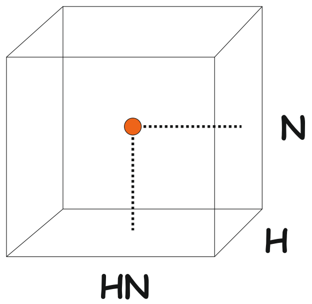


w3-13C,15N-Doubly Filtered 15N-HSQC-NOESY experiment

N15 (t1) -> H[N15] (t2) -> H[(C12),N14] (t3)





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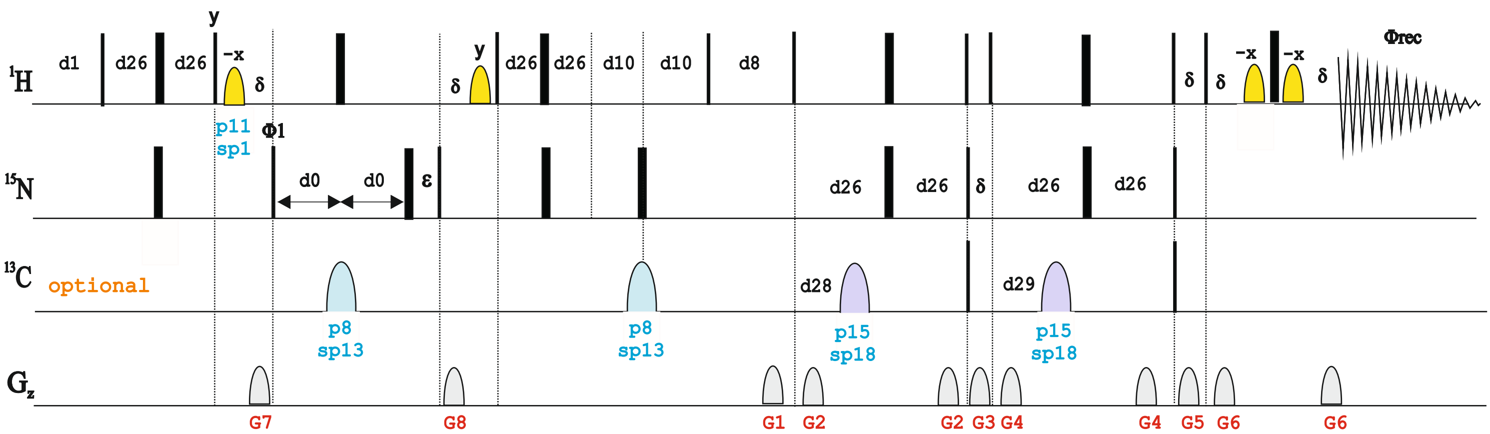
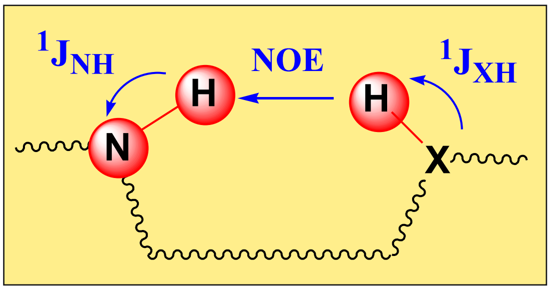
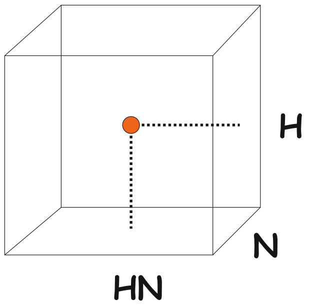


w1-13C,15N-Doubly Filtered NOESY-HSQC experiment

H[(C12),N14] (t1) -> N15 (t2) -> H[N15] (t3)





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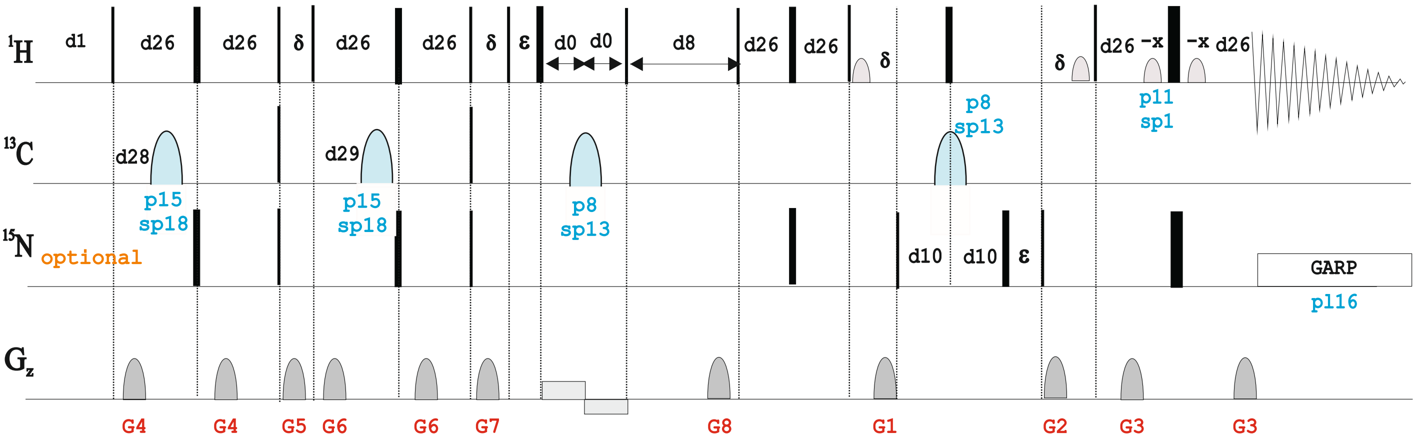

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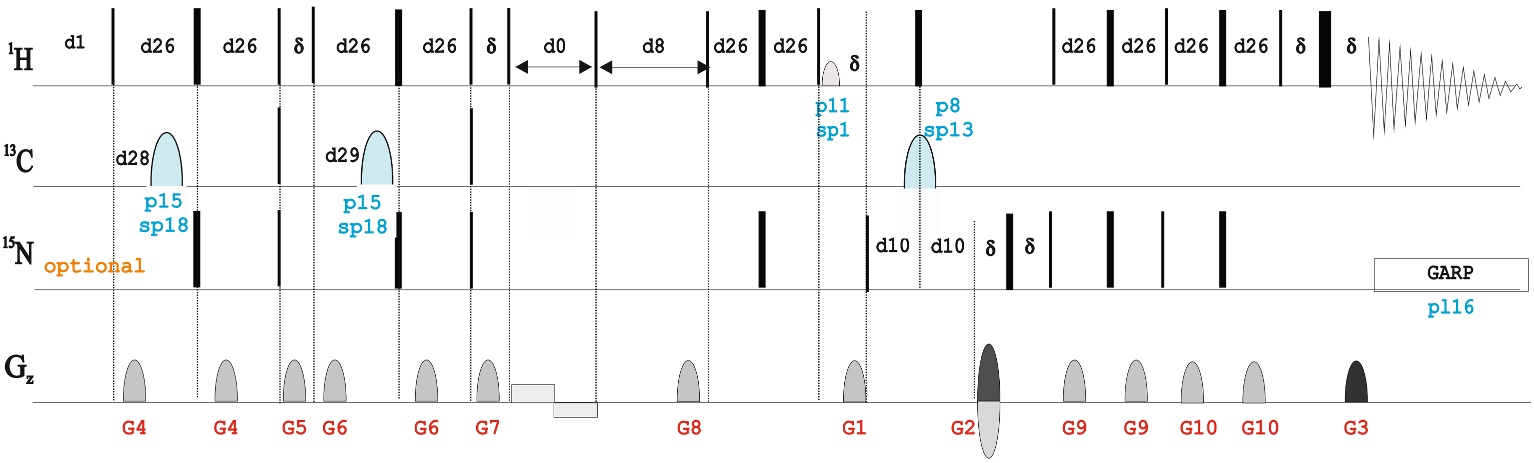
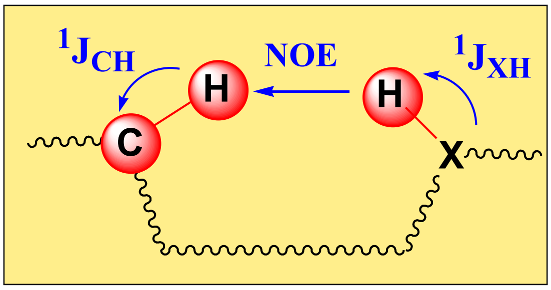
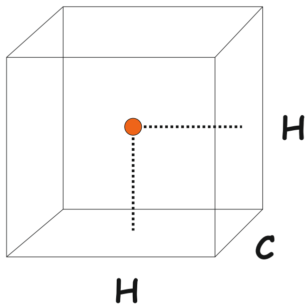


w1-13C,15N-Doubly Filtered NOESY-HSQC experiment

H[(C12),N14] (t1) -> C13 (t2) -> H[C13] (t3)





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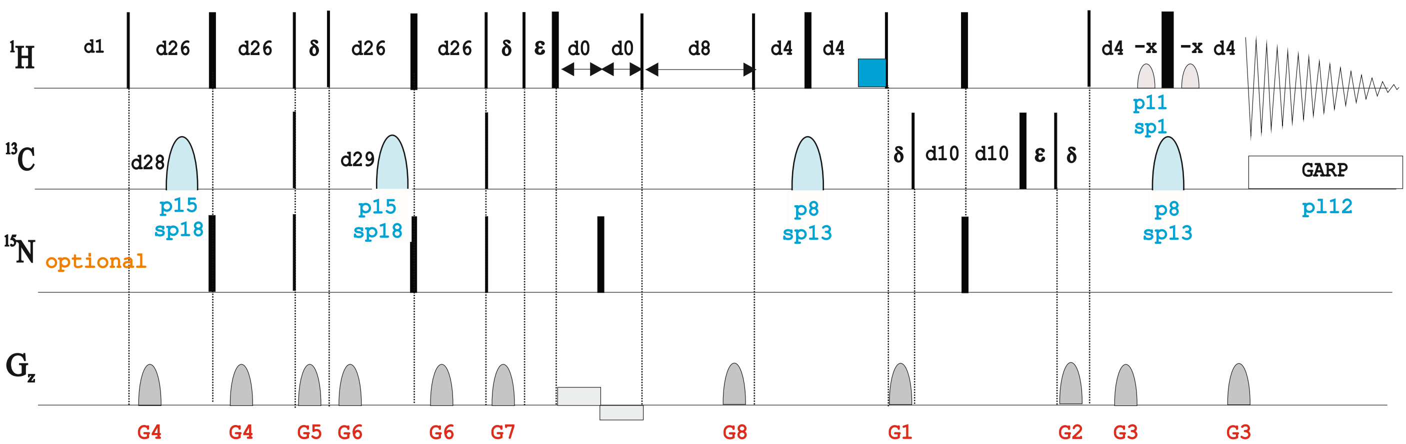
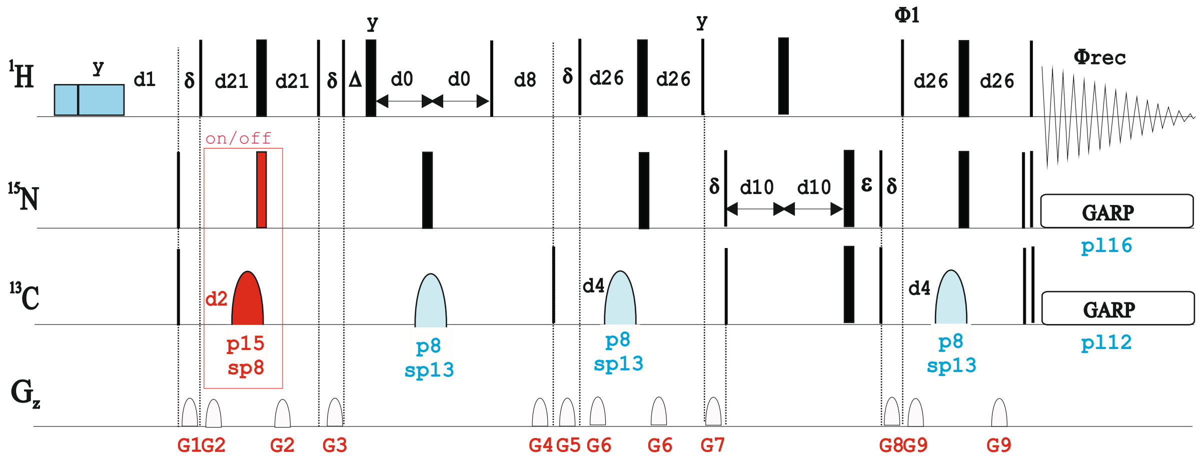


12C,14N vs 13C,15N-edited NOESY-HSQC:

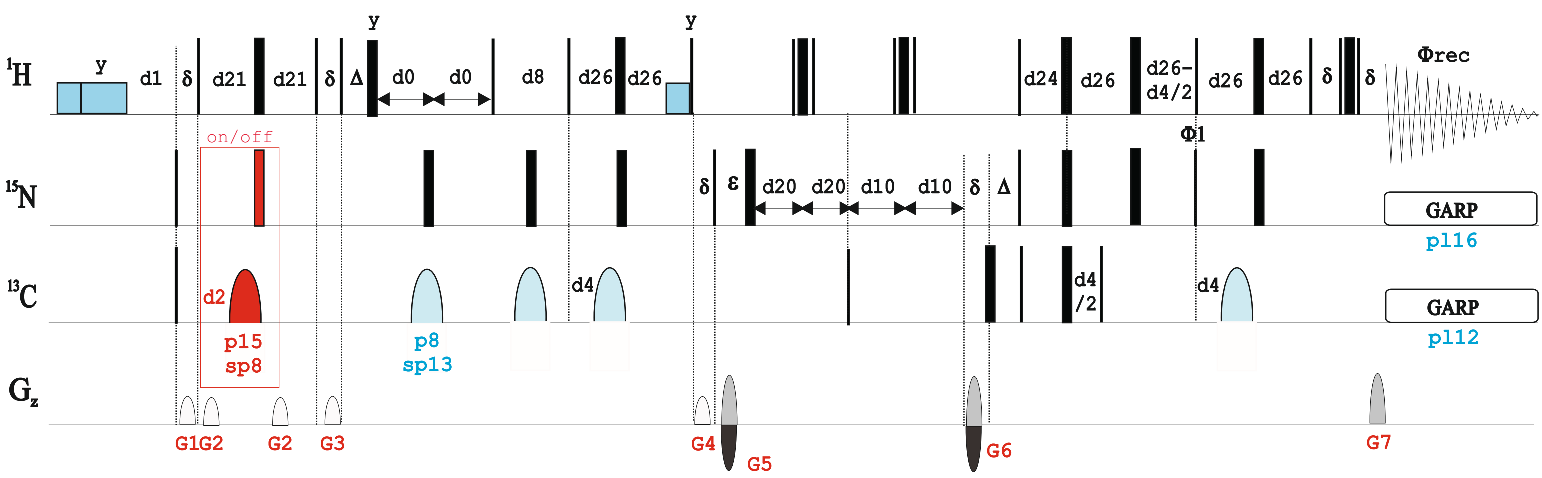
C. Eichmueller, W. Schueler, R. Konrat & B. Kraeutler, J. Biomol. NMR 21, 107-116 (2001)

noesyhsqcedgpsm3d



;use AU-program split [2 F2] to create separate datasets

noesyhsqcedgpsism3d



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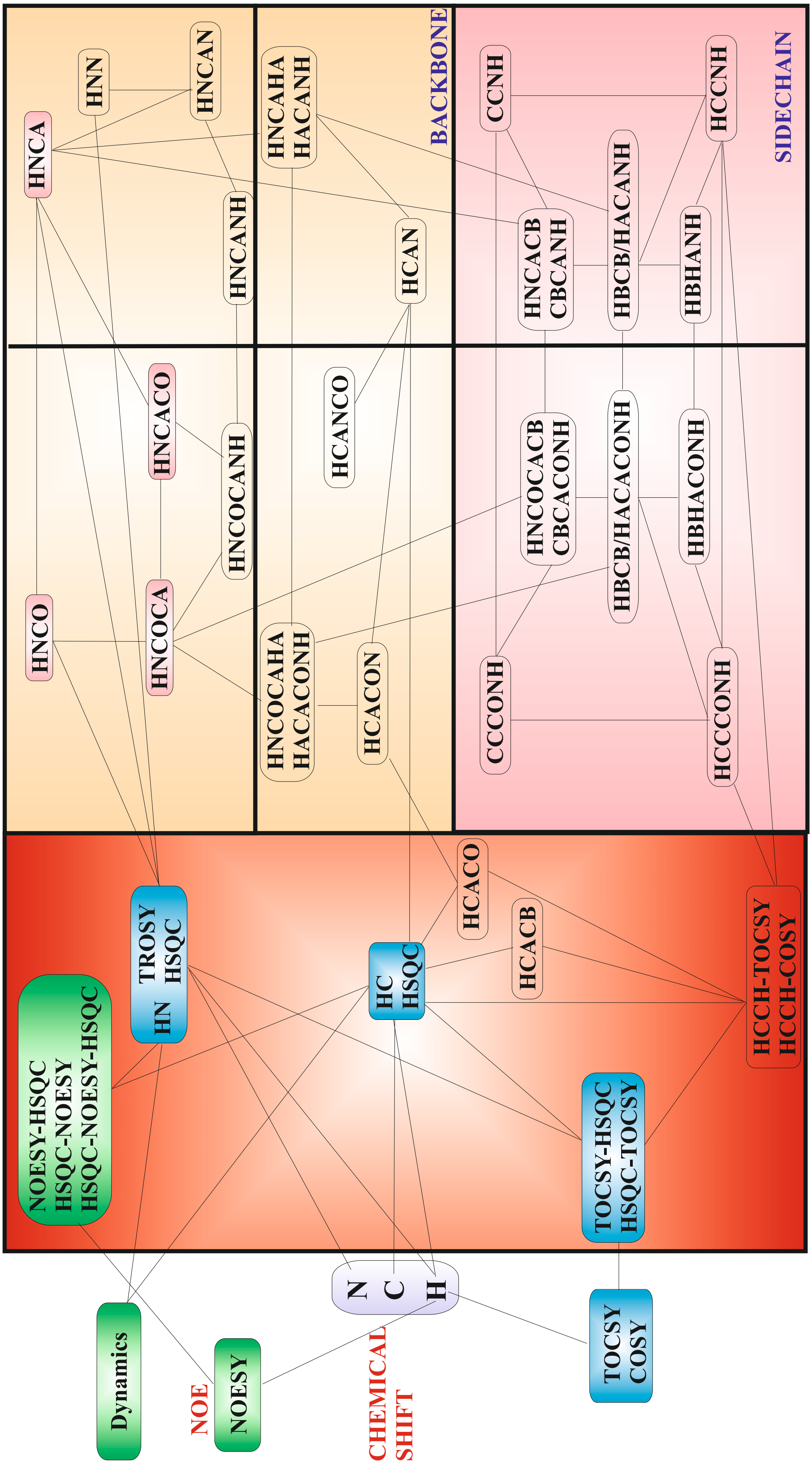
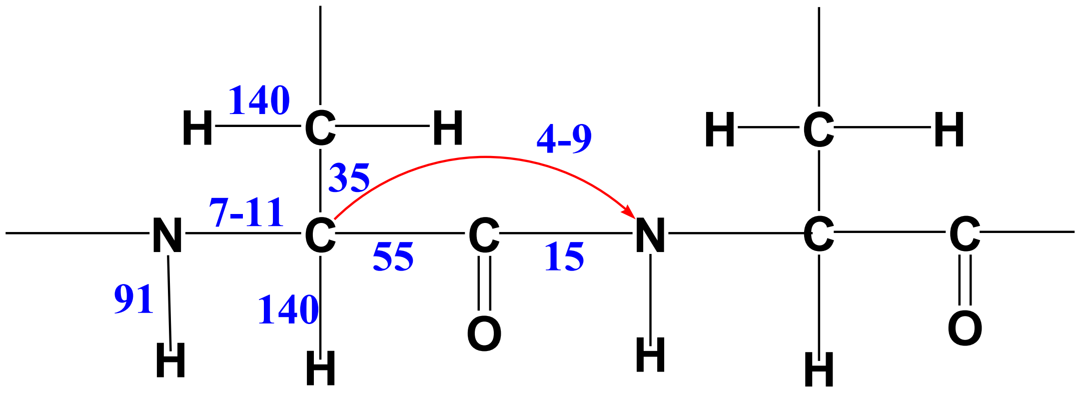
PROTEIN NMR
BACKBONE EXPERIMENTS


BACKBONE
SIDECHAIN
HNCA
HNN
HNCAN
HNCANH
HNCAHA
HACANH
HCAN
CCNH
HCCNH
HNCACB
CBCANH
HBCB/HACANH
HBHANH
HNCO
HNCOCA
HNCACO
HNCOCANH
HCANCO
HNCOCAHA
HACACONH
HCACON
HNCOCACB
CBCACONH
HBCB/HACACONH
HBHACONH
CCCONH
HCCCONH
NOESY-HSQC
HSQC-NOESY
HSQC-NOESY-HSQC
TROSY
HN HSQC
HC HSQC
HCACO
HCACB
HCCH-TOCSY
HCCH-COSY
TOCSY-HSQC
HSQC-TOCSY
N
C
H
Dynamics
NOE
NOESY
CHEMICAL
SHIFT
TOCSY
COSY

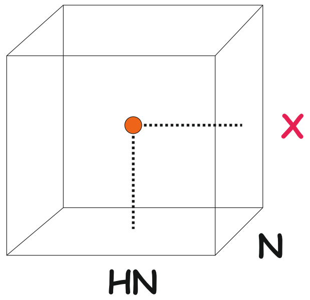
Interpulse delays are optimized as a function of the following heteronuclear coupling constants:



Identifier	Power	Duration	spnam	cpdprg	Description	Remarks
			PROTON PULSES & POWER LEVELS			
p1,p2	pl1				High Power Pulse	
p6	pl10	25u			TOCSY	
p15	pl11				ROESY	Power as 125u pulse
p26,pcpd1	pl19	55-65u		dipsi2	Decoupling pulse	
p11	sp1	1.5-2m	SINC1.1000		Water flipback pulse	
			CARBON PULSES & POWER LEVELS			
p3,p4	pl2				High Power Pulse	
p9	pl15	25u		dipsi3	CC-TOCSY or HC-Cross polarization	
p13	sp2	320u	Q5.1000		on-resonance 90° (Cali or CO)	
p13	sp8	320u	Q5tr.1000		on-resonance time-reversed 90° (Cali or CO)	
p14	sp3	256u	Q3.1000		on-resonance 180° (Cali or CO)	
p14	sp5/sp7	256u	Q3.1000		off-resonance 180° (Cali or CO)	
		1500u	Q5.1000		on-resonance 90° (CA)	
		1500u	Q5tr.1000		on-resonance time-reversed 90° (CA)	
p24	sp9	1000u	Q3.1000		on-resonance 180° (CA)	
p24	sp7	2000u	Crp60comp.4		Adiabatic 180° refocusing	Power as 25u pulse
p8	sp13	500u	Crp60,0.5,20.1		Adiabatic 180° inversion	Power as 25u pulse
pcpd2	pl12	60u-80u		garp	Low Power Pulse for broadband decoupling	
pcpd2, p31	sp15,pl13	1500u	Crp42,1.5,20.2	p5m4sp180.p31	Adiabatic Decoupling	Power as GARP + 2dB
		750u	Crp42,1.5,20.3		Adiabatic Bilev	
pcpd2, p31	sp15,pl28	768u	Q3.1000	mlevsp180.p31	CA or CO selective decoupling	
pcpd2, p31	sp15,pl28	100u	Gauss5.256	mlevsp180.p31	Selective CO Decoupling	Power as 25u pulse
			NITROGEN PULSES & POWER LEVELS			
p21,p22	pl3				High Power Pulse	
pcpd3	pl16	200-300u		garp	Low Power Pulse for broadband decoupling	
			DEUTERIUM PULSES & POWER LEVELS			
pcpd4	pl17	250u		garp	Low Power Pulse for broadband decoupling	

Delay	Coupling Constant	length (ms)	Remarks	Experiment
d3	1/(3JCH)	2.2		
d4	1/(4JCH)	1.6-1.8		
d21	1/(6JCH)	1.1		
d21	1/(2JNH)	5.5		
d22	1/(4JCOCA)	4.0		
d22	1/(2JCOCA)	3.6	Two-bond	
d22	1/(2JCOCA)	4.4	One-bond	
d23	1/(2JNCO)	12.0		
d24	1/(4JCC)	3.6		
d26	1/(4JNH)	2.3		
d21	T(N)	12.4		
d23	T(C)	12.0	2T=24ms<1/4JCH	

H(N)-Detection



HN,N,CO
HNCO
HN(CA)CO
(HACA)CONH

HN,N,CA
HNCA
HN(CO)CA
SeqHNCA
IntraHNCA

HN,N,N
(H)N(CA)NNH
(H)N(COCA)NNH

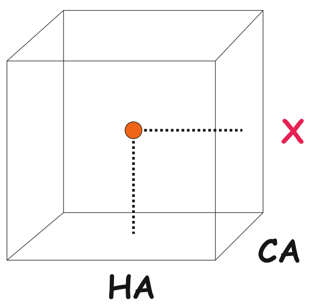
NH,N,HN
H(NCA)NNH
H(NCOCA)NNH

HN,N,HA
HN(CA)HA
HA(CA)NH
HA(CACO)NH

HN,N,Cali
CBCA(CO)NH
HN(CO)CBCA
CBCANH
SeqCBCANH
IntraCBCANH
HNCBCA
CCANH
CCA(CO)NH
CC(CO)NH
(H)CC(CO)NH

HN,N,Hali
HBHA(CO)NH
HBHANH
H(CC)(CO)NH

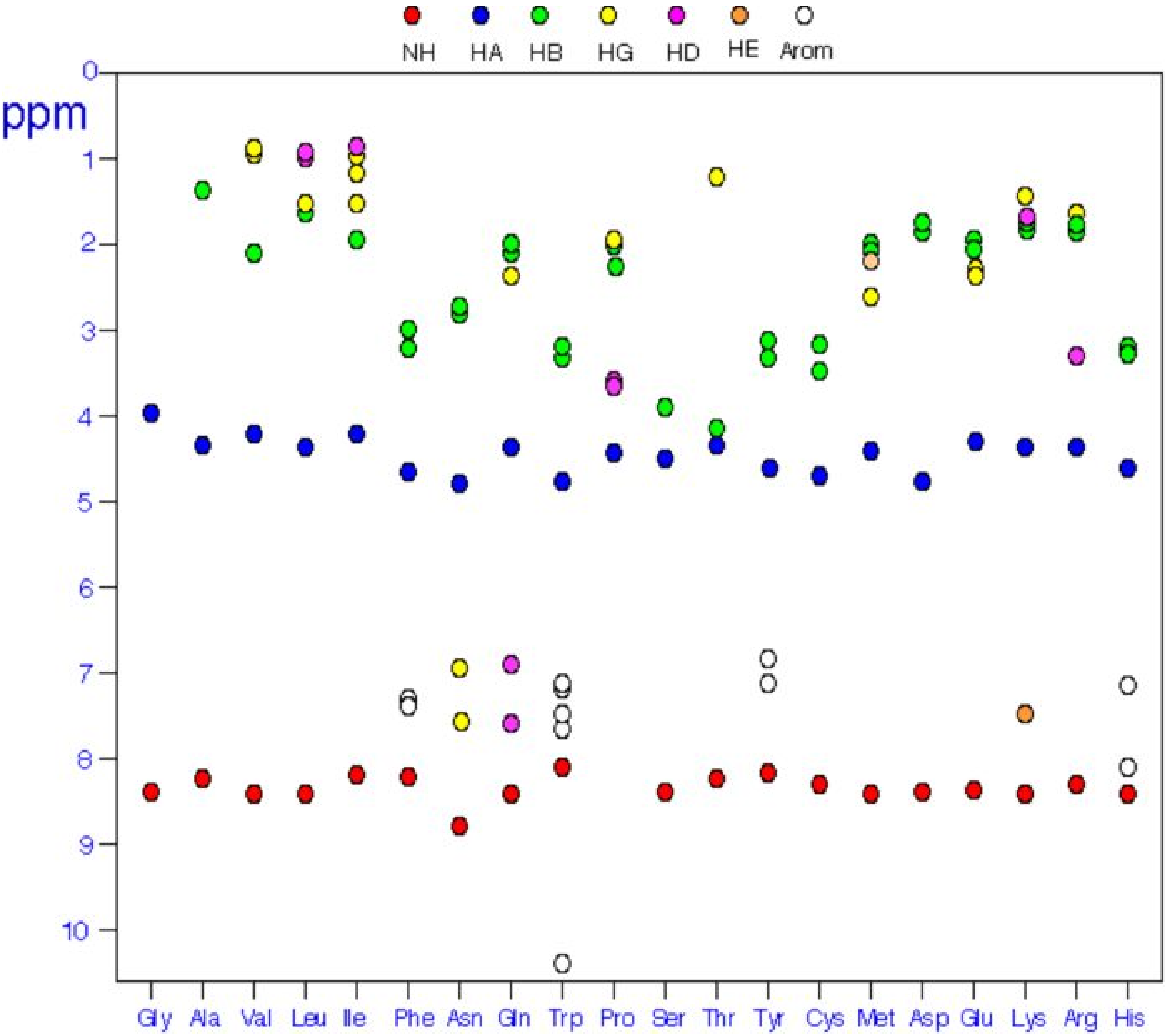
HA-Detection



HA,CA,CO
HACACO

HA,CA,N
HACAN
HACA(CO)N
HCBCA(CO)N

1H Chemical Shifts of random-coil 20 aa



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3D HNCO

Experiment Description

The HNCO experiment correlates the NH group (d(NH) and d(N)) with the carbonyl carbon (d(CO)) of the preceding residue. It is the basis for more complicated triple-resonance 3D, 4D ... NMR pulse sequences

Sample Requirements

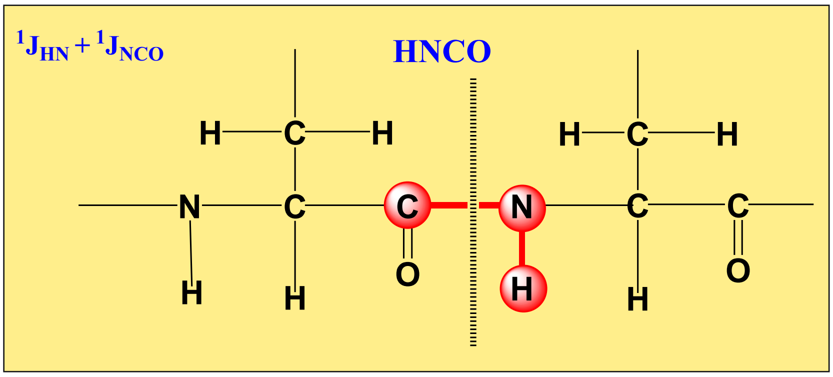
13C,15N-doubly labeled protein

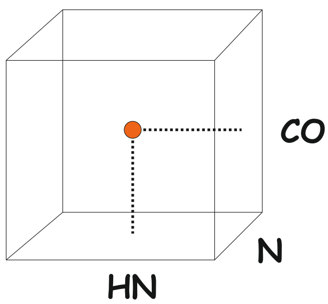
Hardware Requirements

Triple Channel Configuration

References

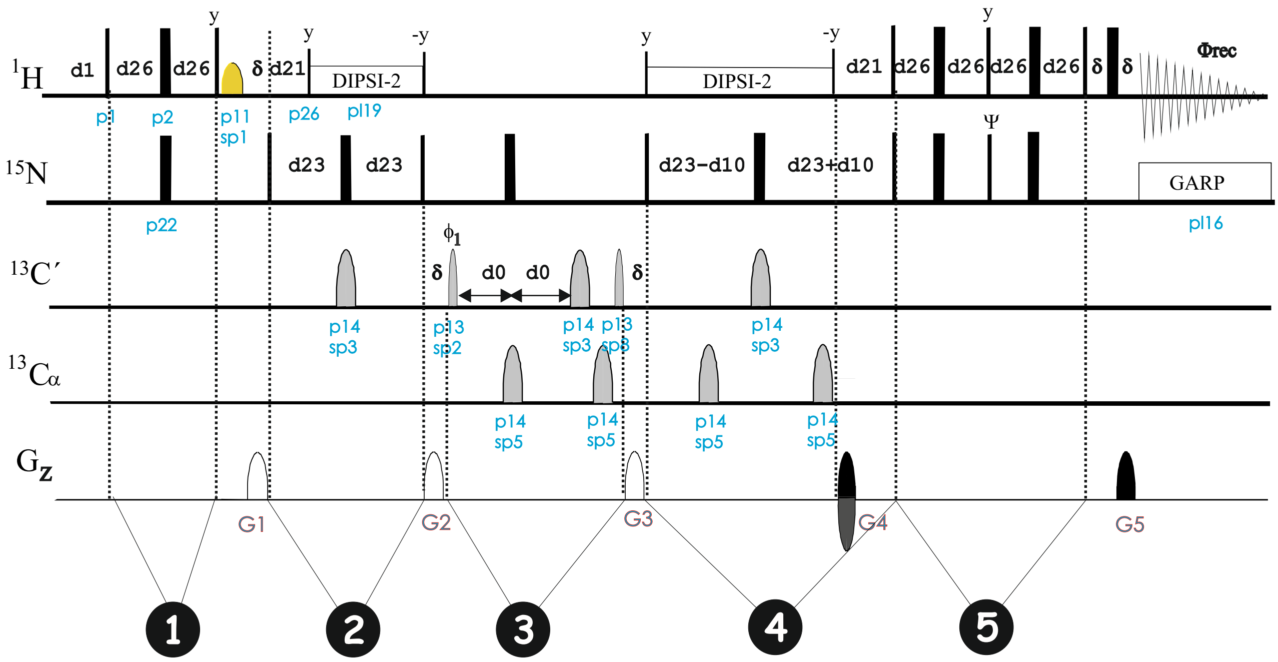
1. S. Grzesiek & A. Bax, J. Magn. Reson. 96, 432 - 440 (1992)
2. J. Schleucher, M. Sattler & C. Griesinger, Angew. Chem. Int. Ed. 32, 1489-1491 (1993)
3. L.E. Kay, G.Y. Xu & T. Yamazaki, J. Magn. Reson. A109, 129-133 (1994)
4. T. Schulte-Herbrueggen & O.W. Sorensen, J. Magn. Reson. 144, 123 - 128 (2000)





Understanding 3D Triple-Resonance NMR Experiments

hncogp3d



1	1H-15N INEPT transfer: Iz to 2IxNz
2	Concatenated Fixed period consisting of J(NH) refocusing and INEPT 15N-CO: 2IxNz-to-2IzNy-to-2NyCOz
3	CO evolution period consisting of δ(CO) evolution and J(CO-N) decoupling and δ(CO) evolution and J(CO-CA) decoupling: -2NzCOy(cos w(CO)t1)
4	Concatenated Constant-time 15N evolution period consisting of: i) δ(N) evolution and J(N-H) evolution, ii) δ(N) evolution and J(N-CA) refocusing and iii) δ(N) evolution and J(N-CO) decoupling: -2NyIz cos (w(CO)t1)exp(iw(N)t2)
5	1H-15N INEPT-PEP transfer consisting of two retro-INEPT like blocks: [Ix(cosw(N)t2)+Iy(sin(w(N)t2)]cos(w(CO)t1)

Concatenated Periods in 3D Triple-Resonance NMR Experiments

Fixed period
Overall Duration: 2d23

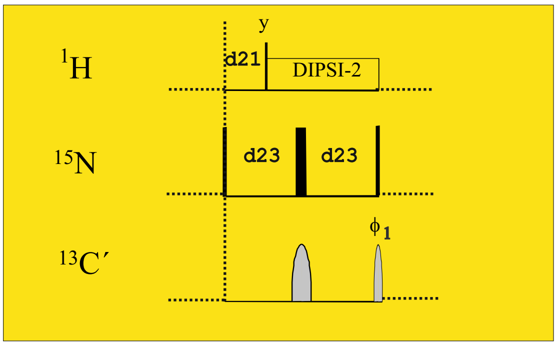
^{1}H Chemical shift: d25 - (d23-d25) - d23 = 2d25-2d23

X Chemical shift: d25 + (d23-d25) - d23 = 0

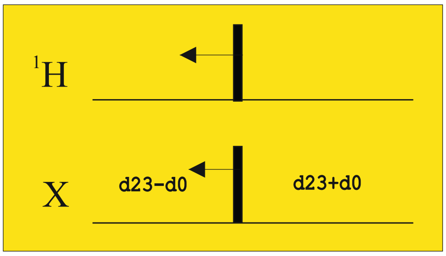
J(XH) Coupling Constant: d25 - (d23-d25) + d23 = 2d25

J(HH) and J(XX) Coupling Constant: d25 + (d23-d25) + d23 = 2d23

A related building block is largely used in 3D experiments in which J(XY) evolves during d23 whereas J(HH) is refocused during d25 and decoupled



Constant-time 15N-evolution periods



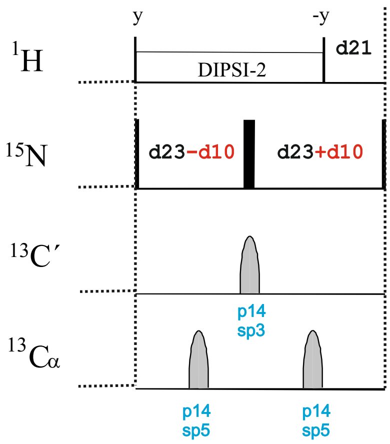
Variable Constant-time period
Overall Duration: 2d23

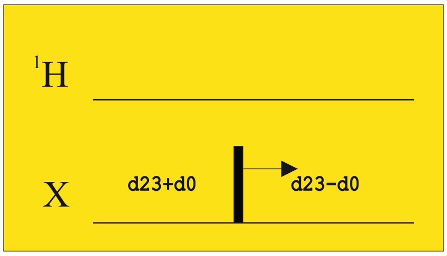
^{1}H Chemical shift: (d23 - d0) - (d23 + d0) = -2d0

X Chemical shift: (d23 - d0) - (d23 + d0) = -2d0

J(XH) Coupling Constant: (d23 - d0) + (d23 + d0) = 2d23

J(HH) and J(XX) Coupling Constant: (d23 - d0) + (d23 + d0) = 2d23





Variable Constant-time period

Overall Duration: 2d23

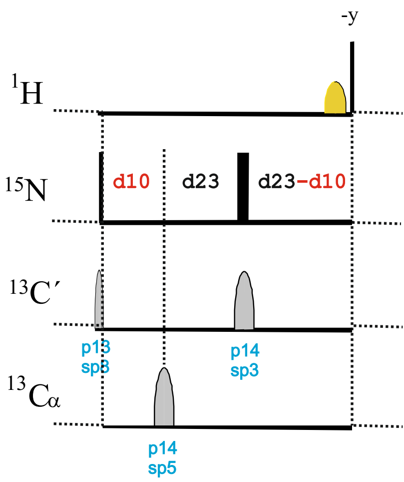
^{1}H Chemical shift: (d23 + d0) + (d23 - d0) = 2d23

X Chemical shift: (d23+d0) - (d23-d0) = 2d0

J(XH) Coupling Constant: (d23+d0) - (d23-d0) = 2d0

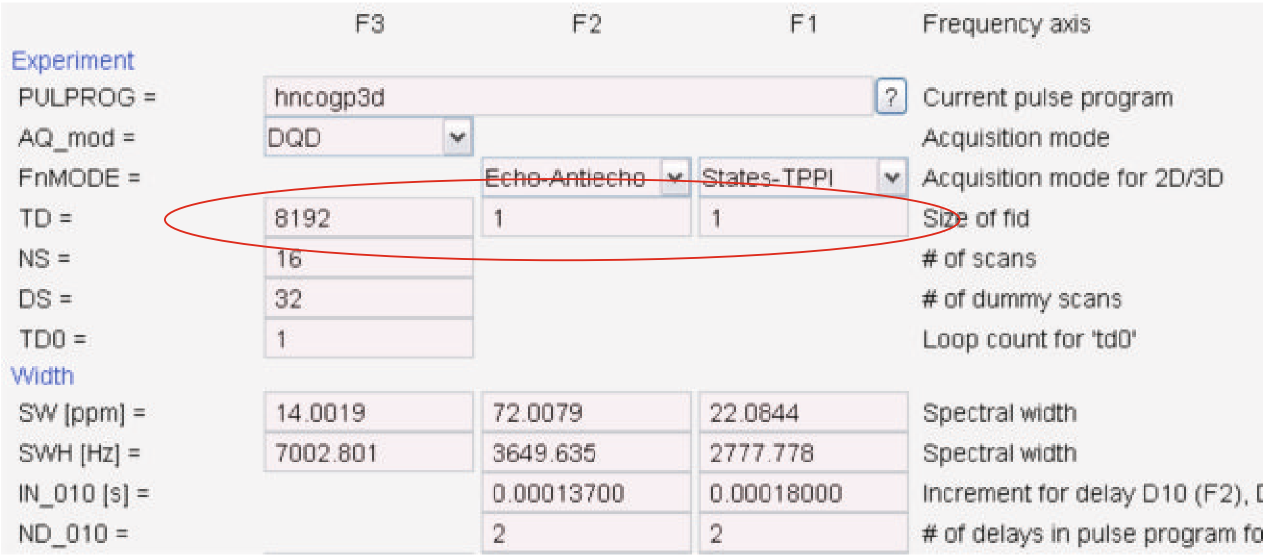
J(HH) and J(XX) Coupling Constant: (d23+d0) + (d23-d0) = 2d23

trhncogp3d



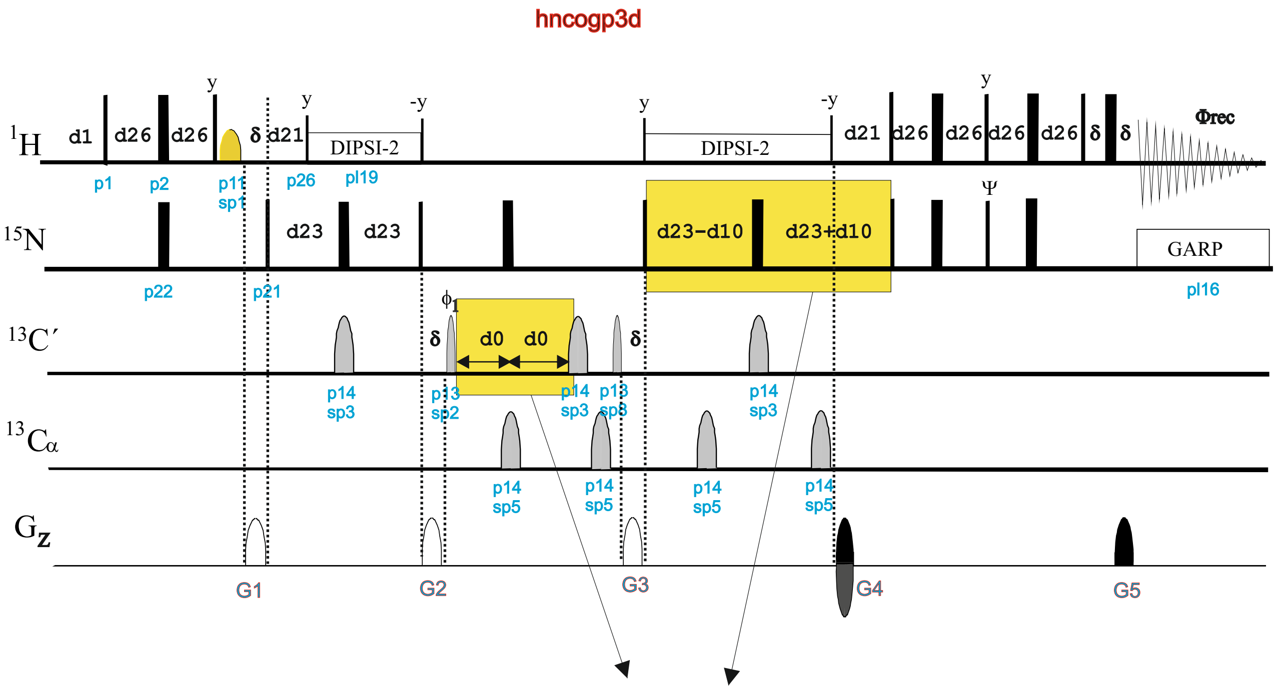
Practical fine adjustment of pulse lengths and power levels.

1. Load the basic parameter set for the HNCO experiment: **rpar HNCOGP3D all**
2. Load the basic pulses and power levels according to your available probehead: **getprosol**
3. Change the parmode in eda from 3D to 1D (see mc command) and then set td in the indirect F1 and F2 dimensions to 1. Also increases td in the detected dimension up to 8K, for instance.



	F3	F2	F1	Frequency axis
Experiment				
PULPROG =	hncogp3d			Current pulse program
AQ_mod =	DQD			Acquisition mode
FnMODE =		Echo-Antiecho	States-TPPI	Acquisition mode for 2D/3D
TD =	8192	1	1	Size of fid
NS =	16			# of scans
DS =	32			# of dummy scans
TD0 =	1			Loop count for 'td0'
Width				
SW [ppm] =	14.0019	72.0079	22.0844	Spectral width
SWH [Hz] =	7002.801	3649.635	2777.778	Spectral width
IN_010 [s] =		0.00013700	0.00018000	Increment for delay D10 (F2), D
ND_010 =		2	2	# of delays in pulse program fo

4. Set **ns** and start acquisition with **rga** and **zg**.
5. When the data is transformed with ef, the program asks for the procno number.
If you type 2, for instance, the corresponding 1D H(NCO) spectrum is displayed in the "filename 1 2" file

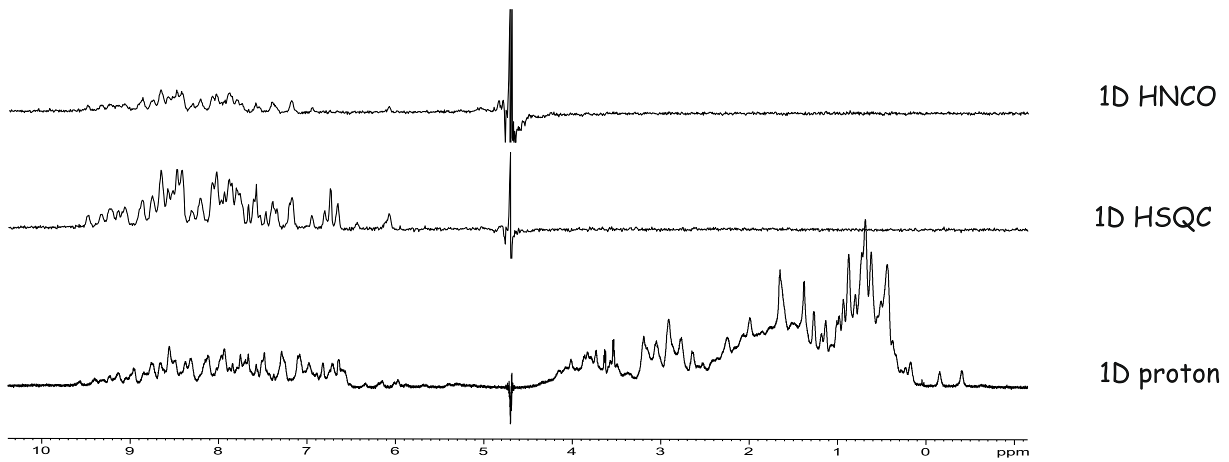


In the 1D H(NCO) experiment, d0 and d10 are fixed to a minimum fixed value of 3us.

6. Once the 1D data shows signals in the NH region, the overall signal must be maximized by individual optimization of the different parameters of the sequence. This process is performed from the "1 2" file and executing the **popt** program. In the case of hncogp3d the most important pulses are:

Hard 1H pulse (p1) at pl1
Water 90 selective 1H pulse (p11) at sp1
Hard 15N 90 pulse (p21) at pl3
Selective 13CO 180° pulse (p14) at sp3
Selective 13CO 90° pulse (p13) at sp2 and sp8
Selective 13CA 180° pulse (p14) at sp5

Usually, pulse length are fixed and the power level is varied over an specific range up to a maximum value is obtained.

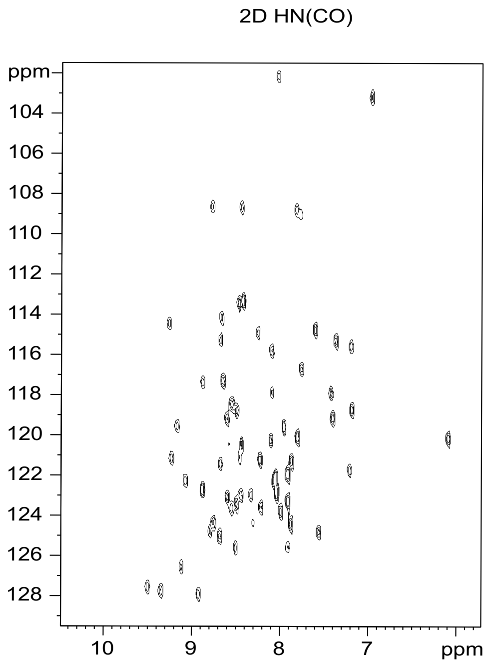


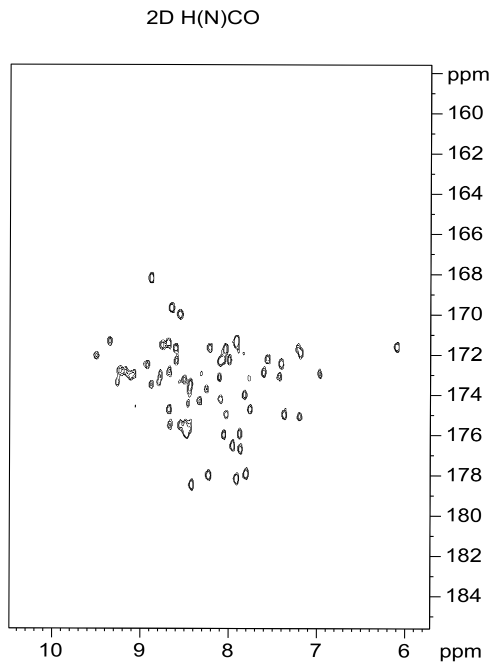
Although sequences included into the pp directory are highly robust, this same 1D calibration protocol based on the use of **zg/popt** can be used to optimize other parameters and to design better alternatives or modify the exisiting ones according to the used sample conditions:

Required number of scans
Setting of delay durations
Check for proper gradient strengths
Use of alternative purgue gradients
Use of additional water flip-back pulses
Check for proper and minimum phase cycling
.....

Recording 2D Planes:

Once the acquisition parameters have been finely adjusted, it is recommended to record the first 2D planes of the 3D spectrum. This is automatically set from the original dataset and setting the corresponding td values according to the required resolution in each dimension. Thus, an 2D HN(CO) spectrum is acquired by setting td to 2k(1H), 64(N) and 1(CO) in eda. Otherwhise, a 2D H(N)CO spectrum is acquired by setting td to 2k(1H), 1(N) and 64(CO), for instance. These preliminary spectra could be also used to check for useful offsets and spectral windows in each dimension.





Experiment Version vs Labeling Strategy and Protein Size:

Basically, all 3D experiments can be designed with different pulse timings as a function of sample requirements and performance. The most typical approaches are:

i) **PEP Block** in step 5: Maximum Theoretical sensitivity for IS spin systems
ii) **WATERGATE Block** in step 5: Better solvent suppression
iii) **TROSY Block** in step 5: TROSY editing for large proteins. heteronuclear decoupling is removed during N evolution and during acquisition.

1. Conventional
2. Echo/Antiecho

iv) **2H-decoupling** during CA evolution: For 2H-labeled Proteins

3D HNCO experiment

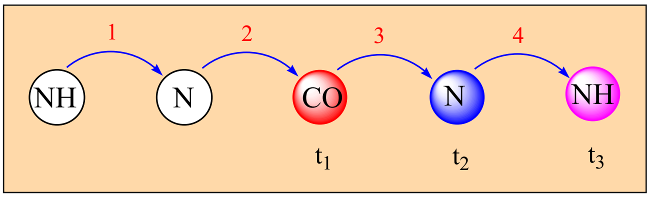
- 3D HNCO using PEP (**hncogp3d** | HNCOGP3D)
- 3D HNCO using WATERGATE (**hncogpwg3d** | HNCOGPWG3D)
- 3D HNCO using TROSY (**trhncogp3d** | TRHNCOGP3D):
    - using echo-antiecho gradient (**trhncoetgp3d** | TRHNCOETGP3D)
    - with ^{2}H-decoupling (**trhncogp2h3d** | TRHNCOGP2H3D)

Also see:
3D APSY-HNCO experiment:
Reduced-Dimensionality (3,2)-HNCO (rd_hnco_32 | APSY_HNCO_32)

3D SOFAST/BEST-HNCO experiment:
3D BEST-HNCO (b_hncogp3d | B_HNCOGP3D)
3D BEST-HNCO using TROSY (b_trhncogp3d)
3D BEST-intraHNCO (b_hncoigp3d | B_HNCOIGP3D)
3D BEST-intraHNCO using TROSY (b_trhncoigp3d)

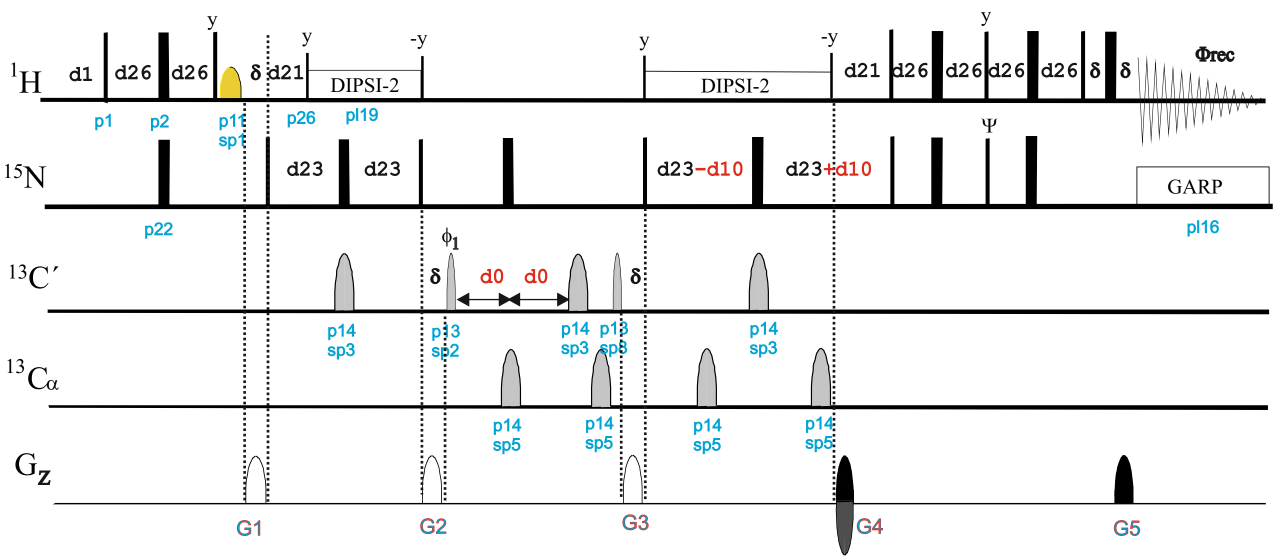
3D HNCO-type experiments for T1, T2 and T1(rho) relaxation measurements
3D HNCO-type experiments for J measurements
3D HNCO-type experiments for RDC measurements
3D HNCO-type experiments for Hydrogen-Bonds J measurements
3D Carbon-Detected HNCO experiments

Related Experiments:
intra-HNCO, HN(CA)CO experiments

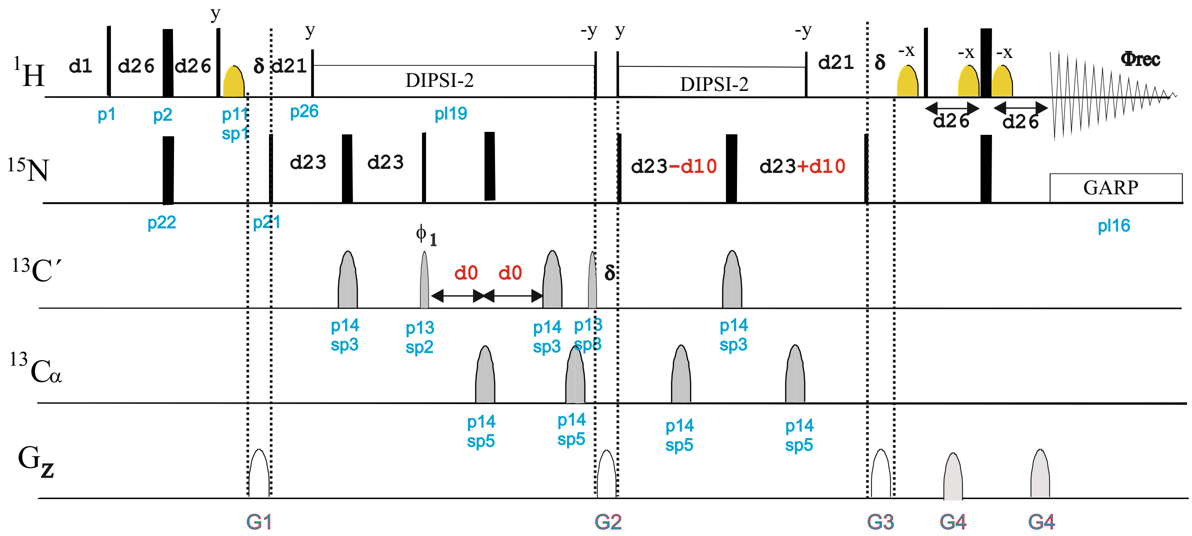


d26=1/4J(NH)=2.5m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m

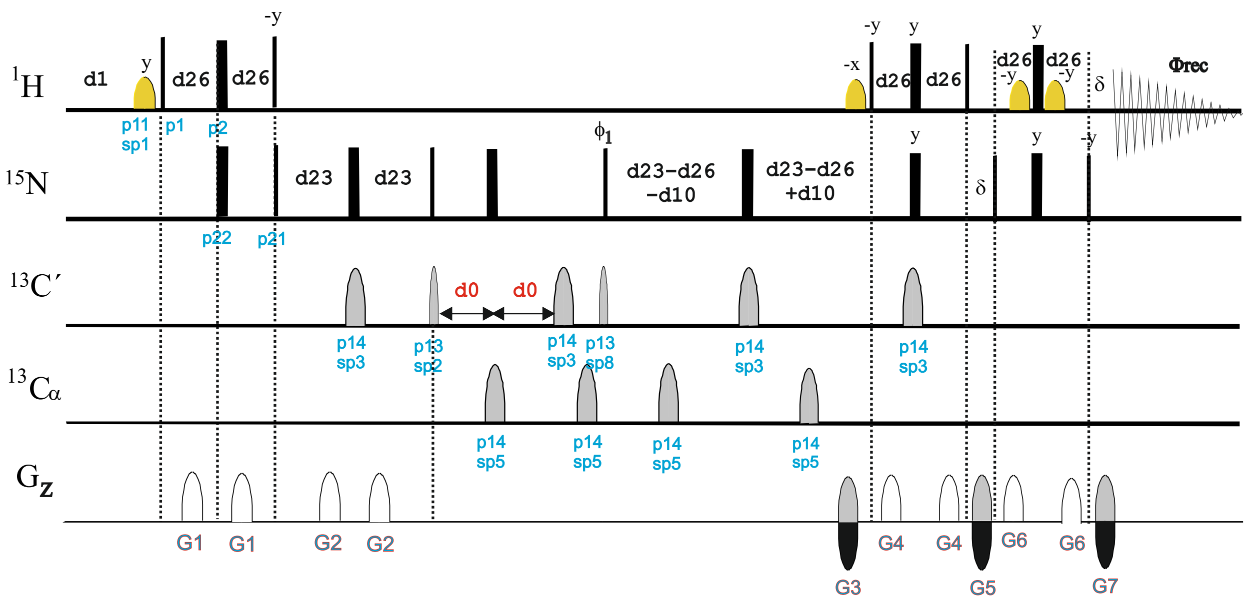
hncogp3d



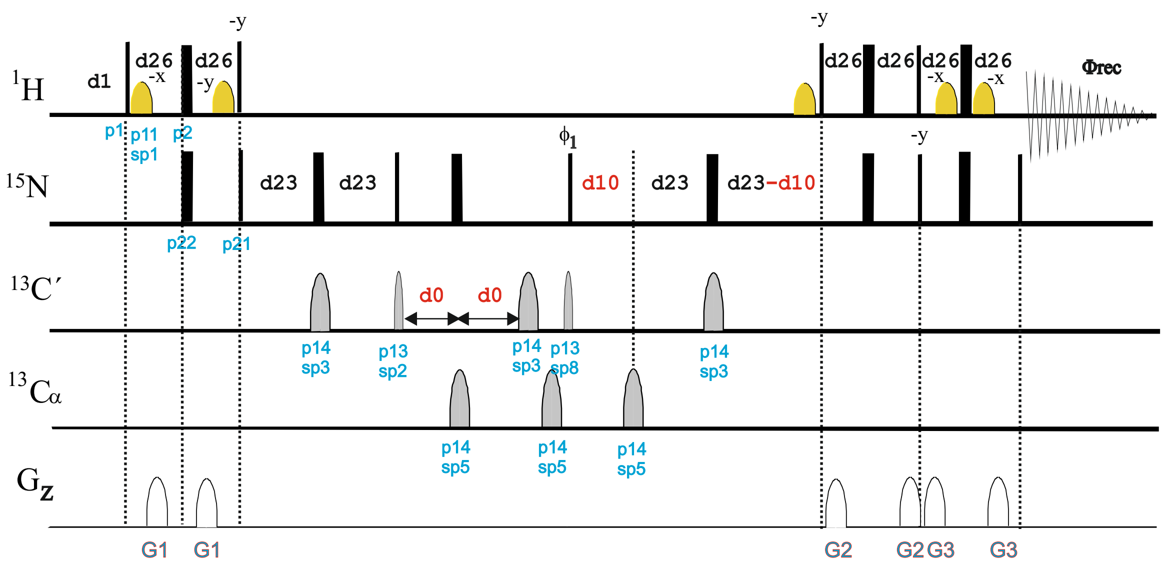
hncogpwg3d



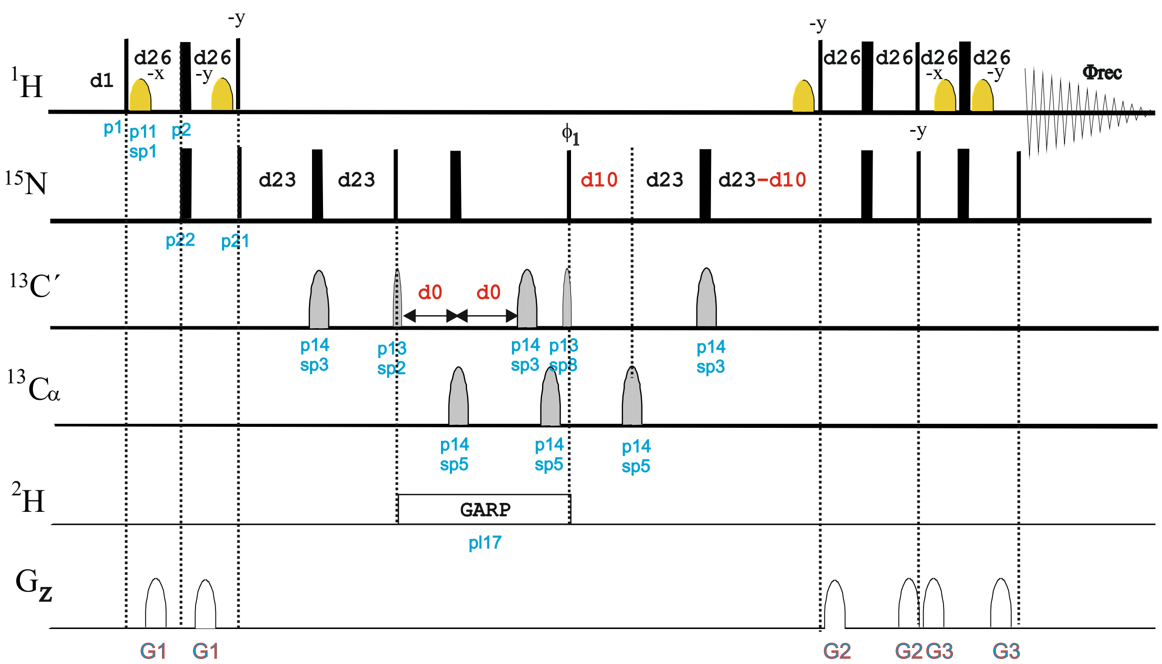
trhncoetgp3d



trhncogp3d



trhncogp2h3d



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3D HNCA

Experiment Description

The HNCA experiment correlates the NH group (d(NH) and d(N)) with the alpha carbon carbon (d(CA)) of the same and of the preceding residue.

Sample Requirements

13C,15N-doubly labeled protein

Hardware Requirements

Triple Channel Configuration

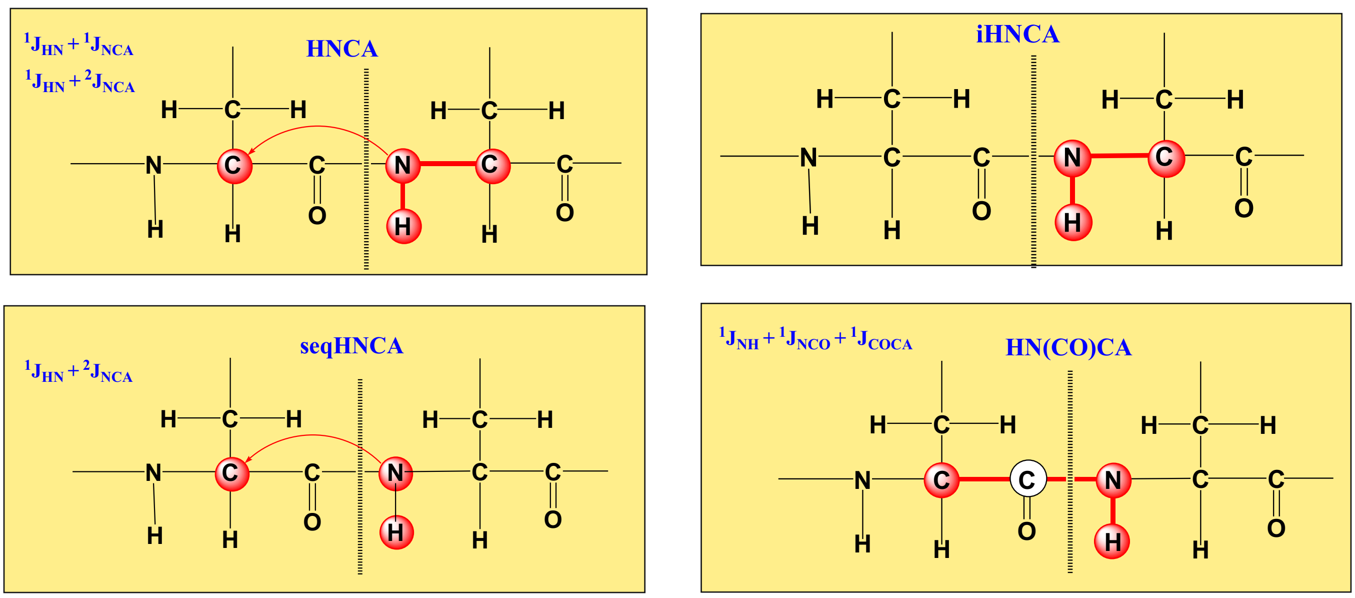
References

1. S. Grzesiek & A. Bax, J. Magn. Reson. 96, 432 - 440 (1992)
2. J. Schleucher, M. Sattler & C. Griesinger, Angew. Chem. Int. Ed. 32, 1489-1491 (1993).
;3. L.E. Kay, G.Y. Xu & T. Yamazaki, J. Magn. Reson. A109, 129-133 (1994))

Main Features:

1. HNCA provides one inter-residue and one intra-residue cross peak.
2. The intensity of the HNCA peaks are less intense than in the HNCO experiment.
3. The inter-residue cross peak is generally less intense than the intra-residue cross peak

Comparison of different 3D experiments detecting HN, N and CA



3D HNCA experiment

- 3D HNCA using PEP (**hncagp3d** | HNCAGP3D)
  - with ^{2}H-decoupling (**hncagp2h3d** | HNCAGP2H3D)
- 3D HNCA using WATERGATE (**hncagpwg3d** | HNCAGPWG3D)
  - with ^{2}H-decoupling (**hncagpwg2h3d** | HNCAGPWG2H3D)
- 3D HNCA with selective Cb/C=O decoupling (**hncadhgp3d**)
- 3D HNCA using TROSY(**trhncagp3d2.2** | TRHNCAGP3D2.2) :
  - using echo-antiecho gradient (**trhncaetgp3d** | TRHNCAETGP3D)
  - using echo-antiecho gradient and with ^{2}H-decoupling (**trhncaetgp2h3d** | TRHNCAETGP2H3D)
  - with HMQC steps (**trhncagp3d.2** | TRHNCAGP3D.2)
  - with ^{1}H?-decoupling (**trhncagp3d2** | TRHNCAGP3D2)
  - with ^{1}H?-decoupling and HMQC steps (**trhncagp3d** | TRHNCAGP3D)
  - with ^{2}H-decoupling and HMQC steps (**trhncagp2h3d** | TRHNCAGP2H3D)
  - with ^{2}H-decoupling (**trhncagp2h3d2** | TRHNCAGP2H3D2)

Also see:

3D APSY-HNCA experiment:

Reduced-Dimensionality (3,2)-HNCA (rd_hnca_32 | APSY_HNCA_32)

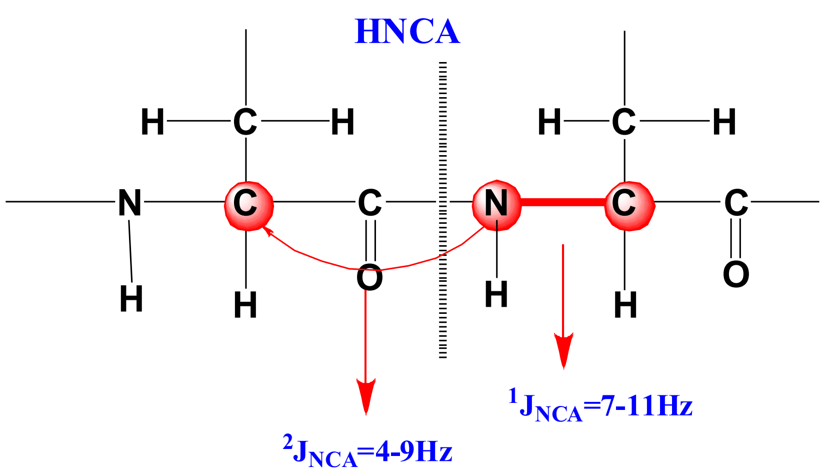
3D SOFAST/BEST-HNCO experiments:

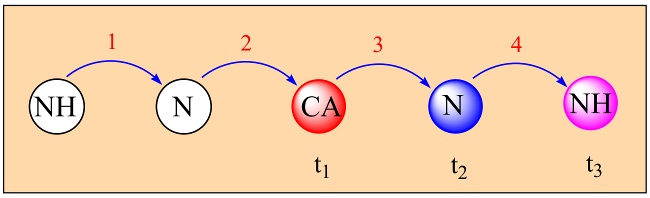
3D BEST-HNCA (b_hncagp3d | B_HNCAGP3D)
3D BEST-HNCA using TROSY (b_trhncagp3d)

3D HNCA-type experiments for J measurements
3D HNCA-type experiments for RDC measurements
3D Carbon-Detected HNCA experiments

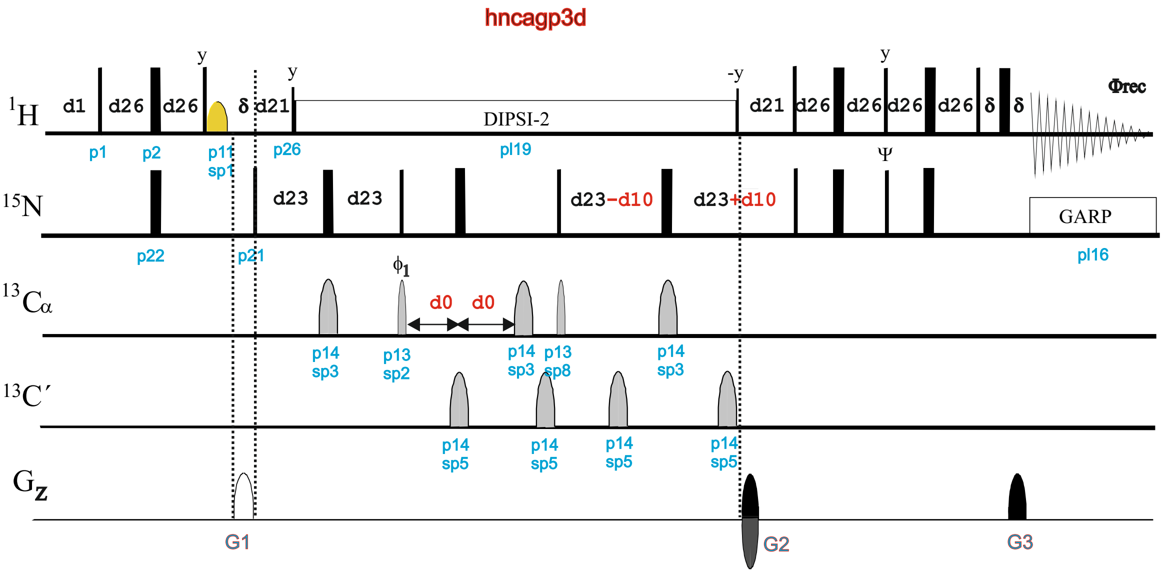
Related Experiments:
intra-HNCA, sequential-HNCA, HN(CO)CA

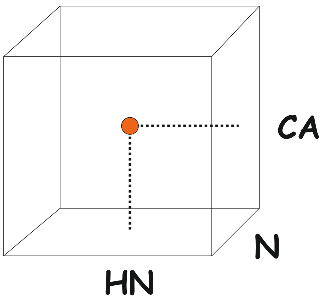
In all experimentos involving a N-CA transfer, two complementary pathways are involved:



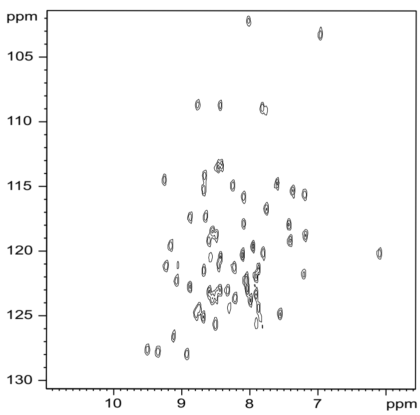


d26=1/4J(NH)=2.5m
d21=1/2J(NH)=5.5m
d23=1/4J(NCA)=12m

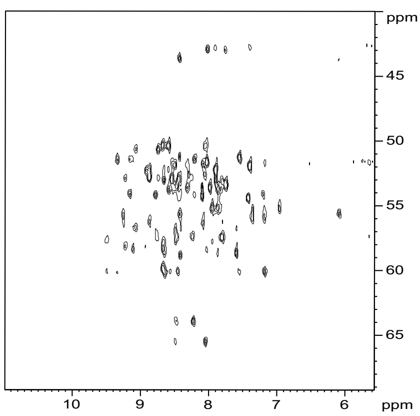


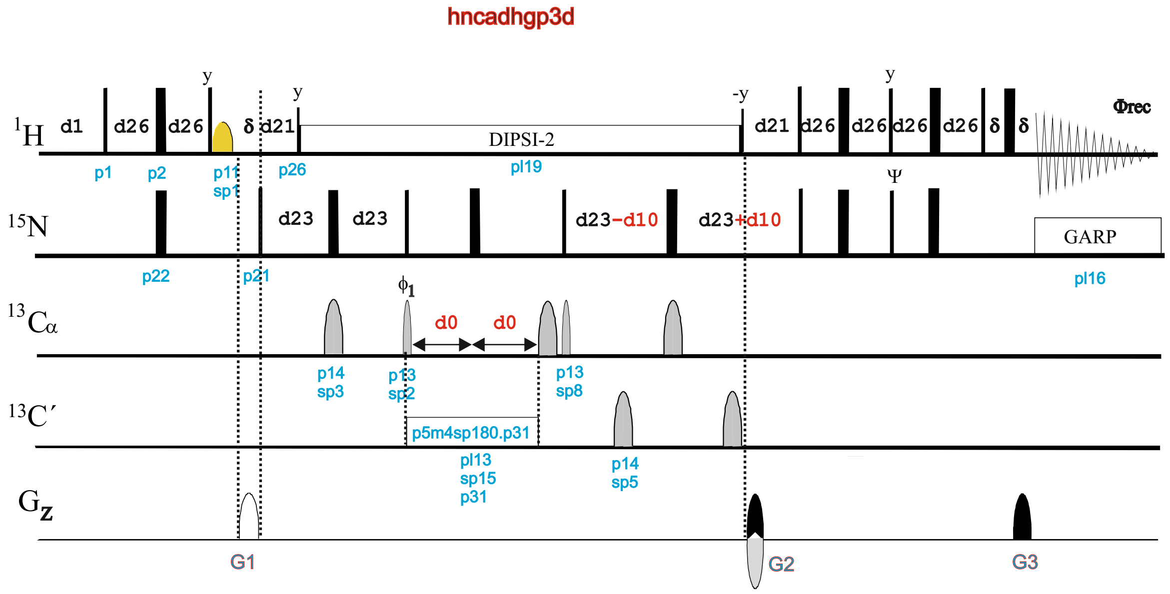


2D HN(CA)

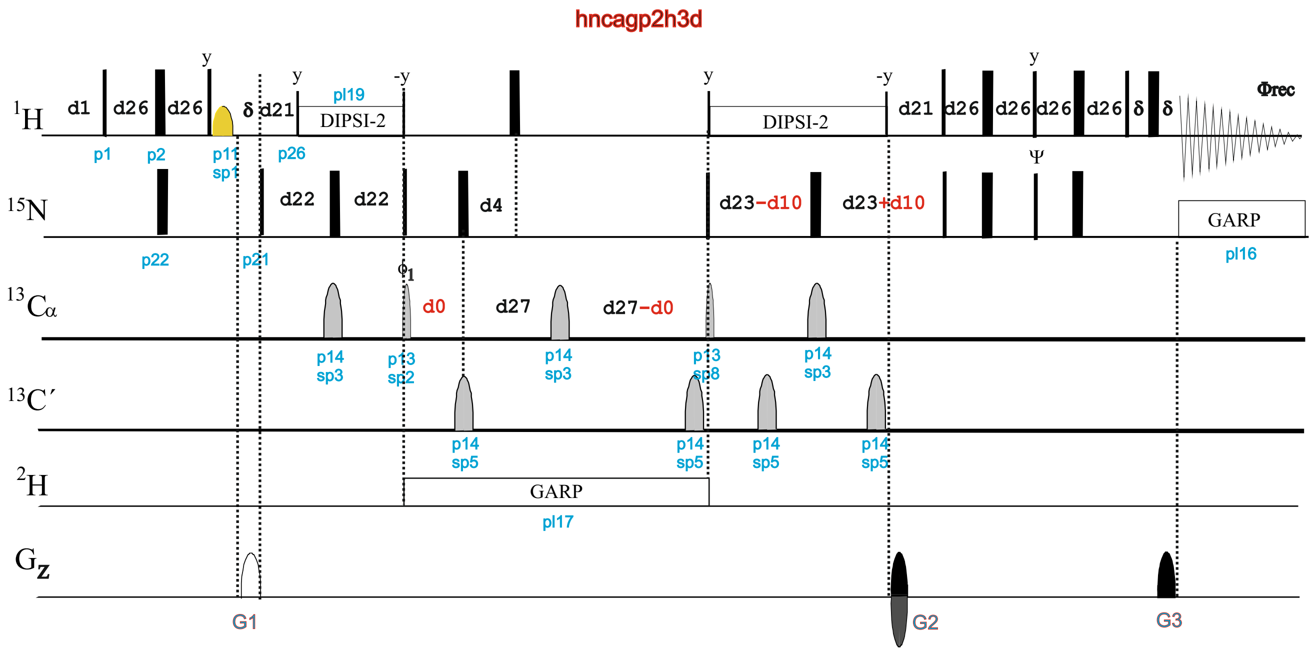


2D H(N)CA

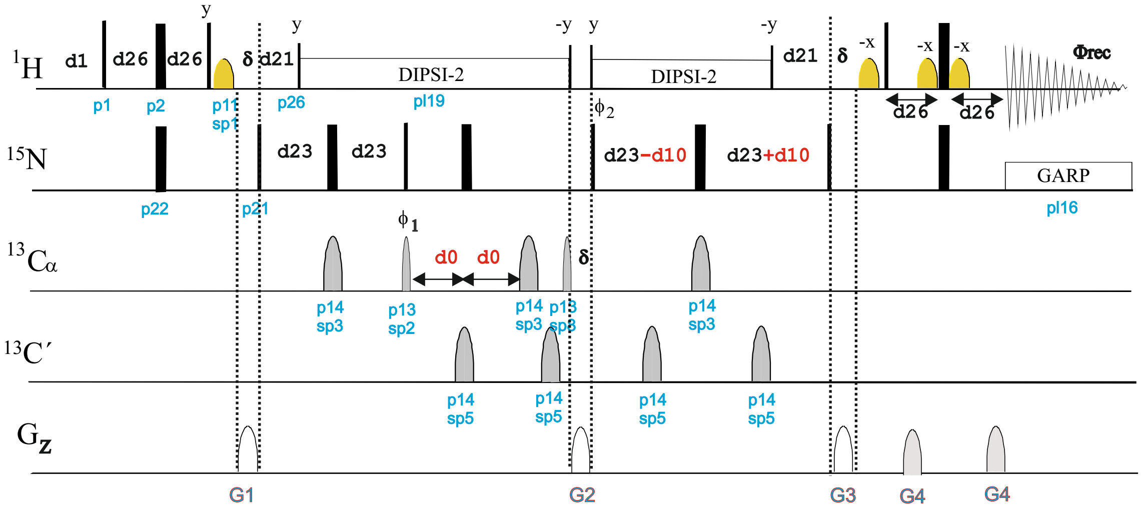




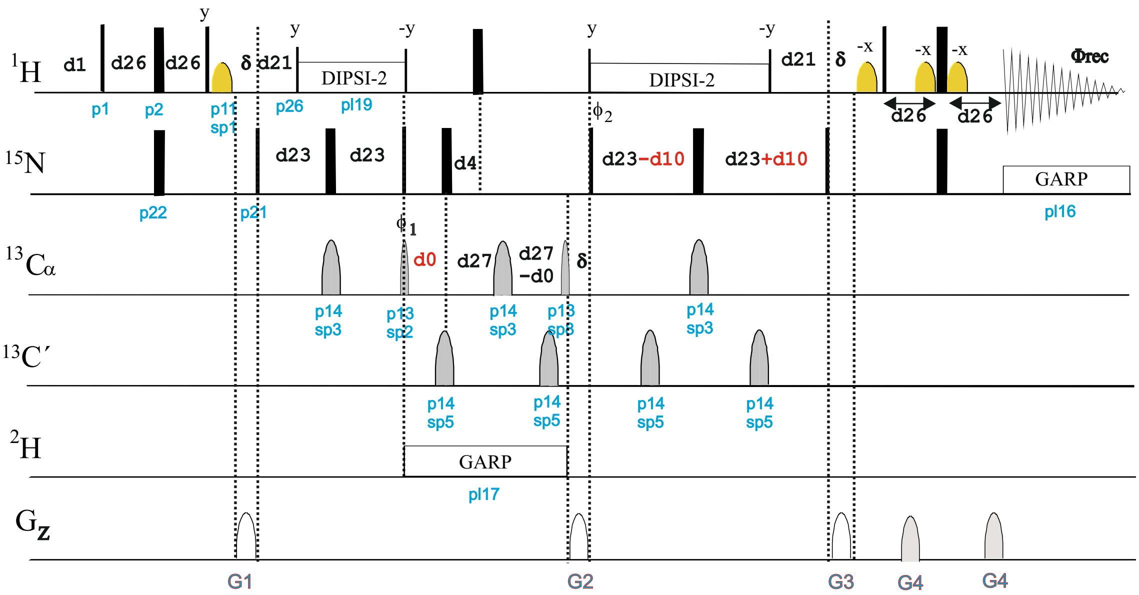
Selective CB/CO Decoupling:
H. Matsuo, E. Kupce, H. Li & G. Wagner, J. Magn. Reson. B 113, 91-96 (1996)



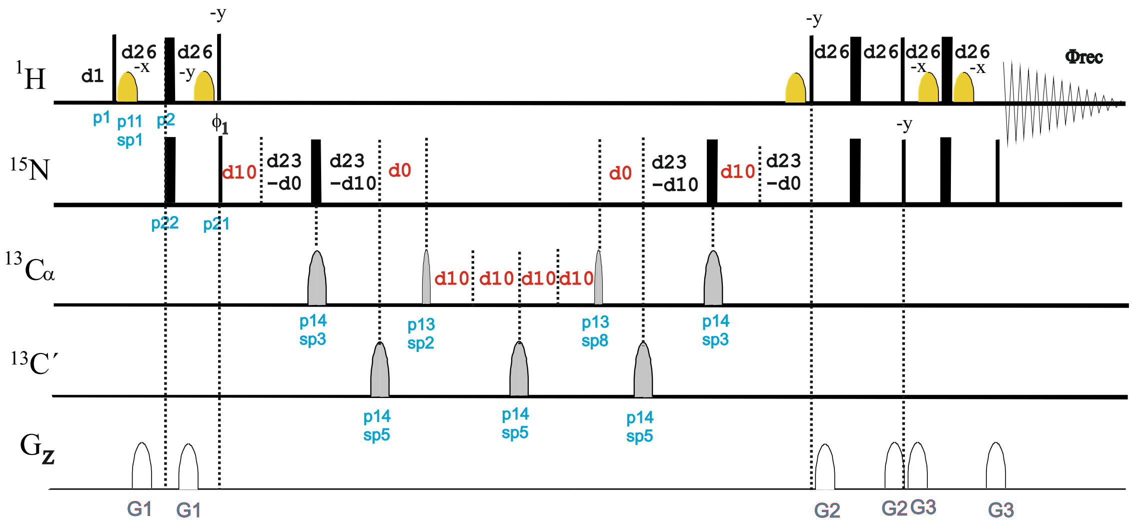
hncagpwg3d



hncagpwg2h3d



trhncagp3d



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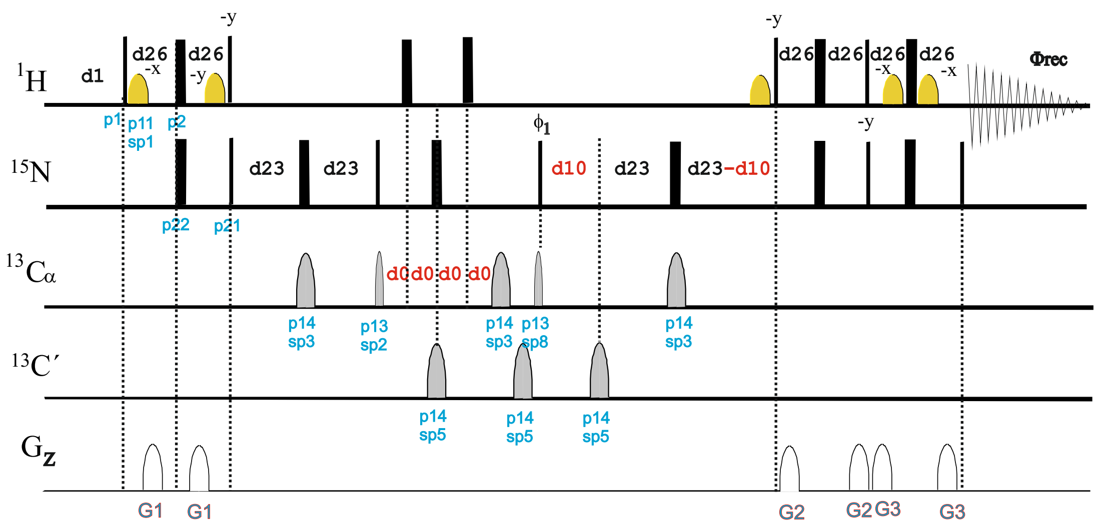
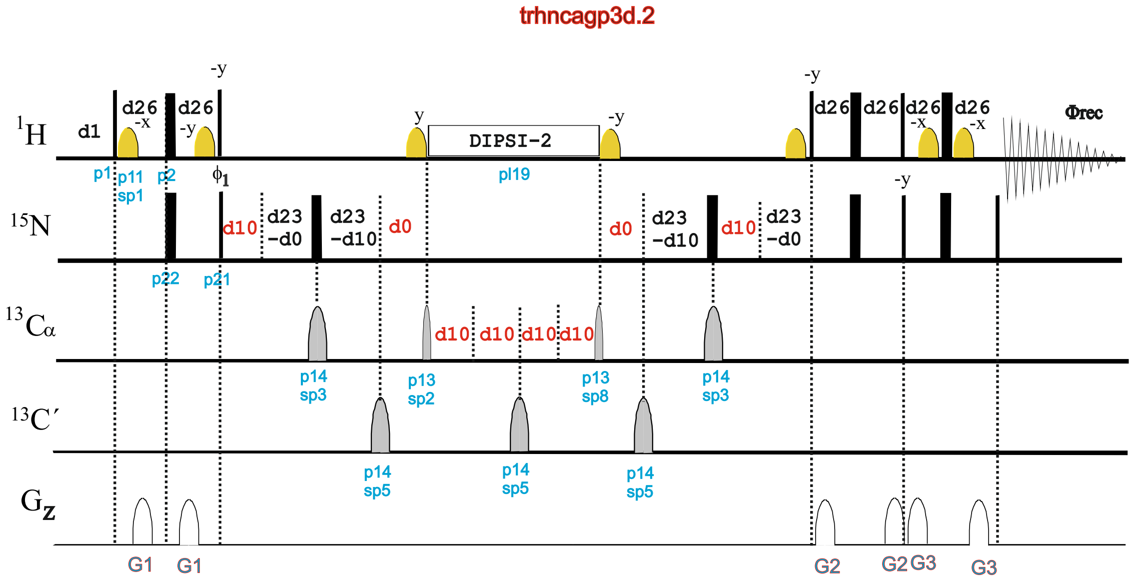
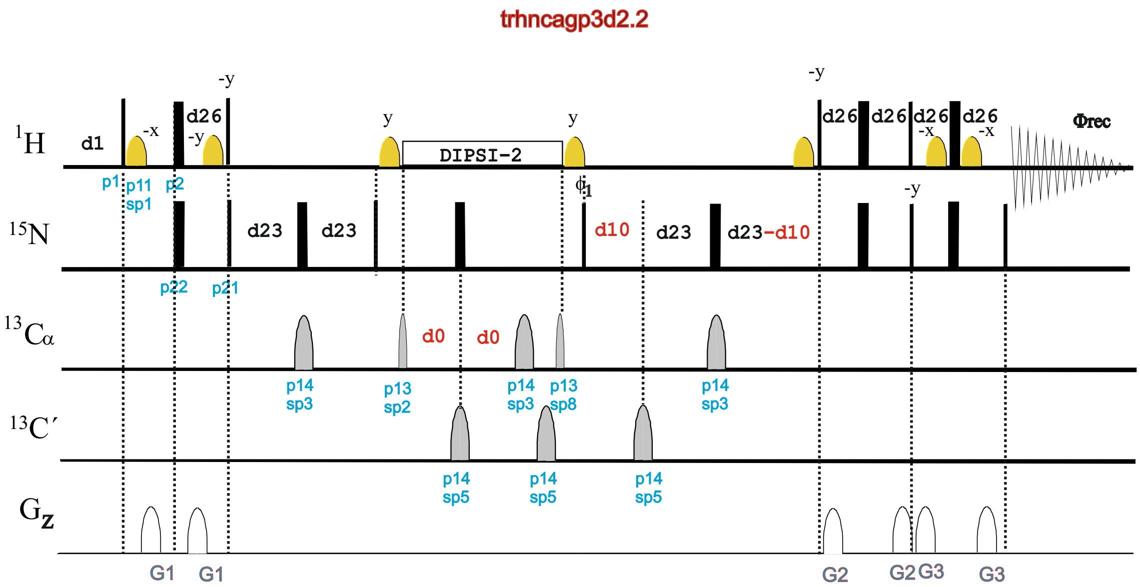



trhncagp3d.2
1H
15N
13Cα
13C′
Gz
d1
d26
d23
-d0
-d10
d10
d0
DIPSI-2
Φrec
p1
p11
sp1
p2
p22
p21
pl19
p13
sp2
sp8
p14
sp3
sp5
G1
G2
G3


trhncagp3d2.2
1H
15N
13Cα
13C′
Gz
d1
d26
d23
d23-d10
d10
d0
DIPSI-2
Φrec
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p22
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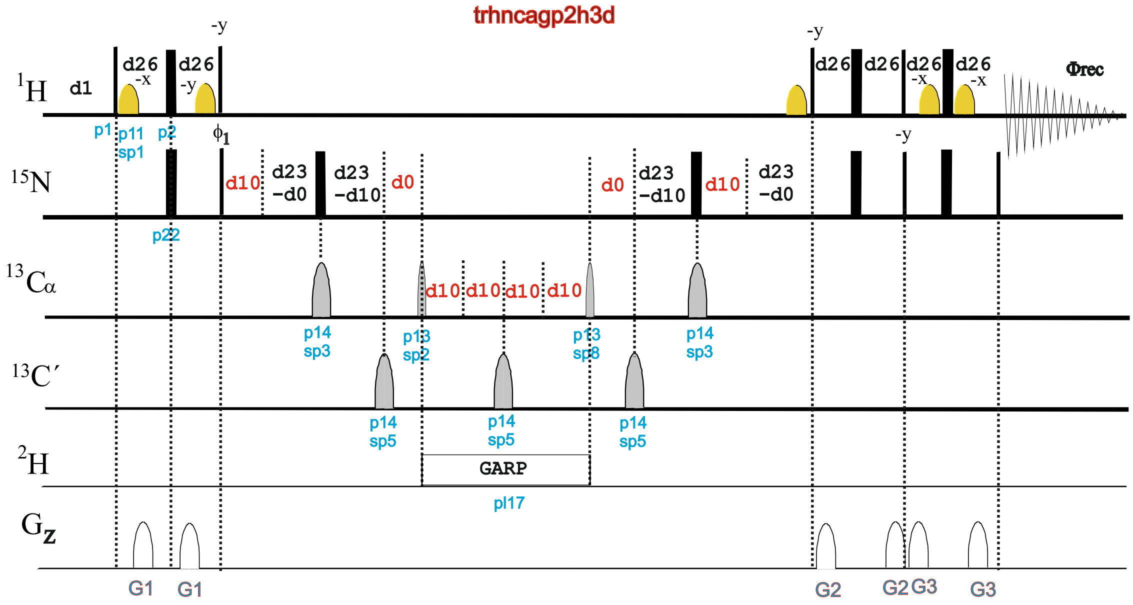
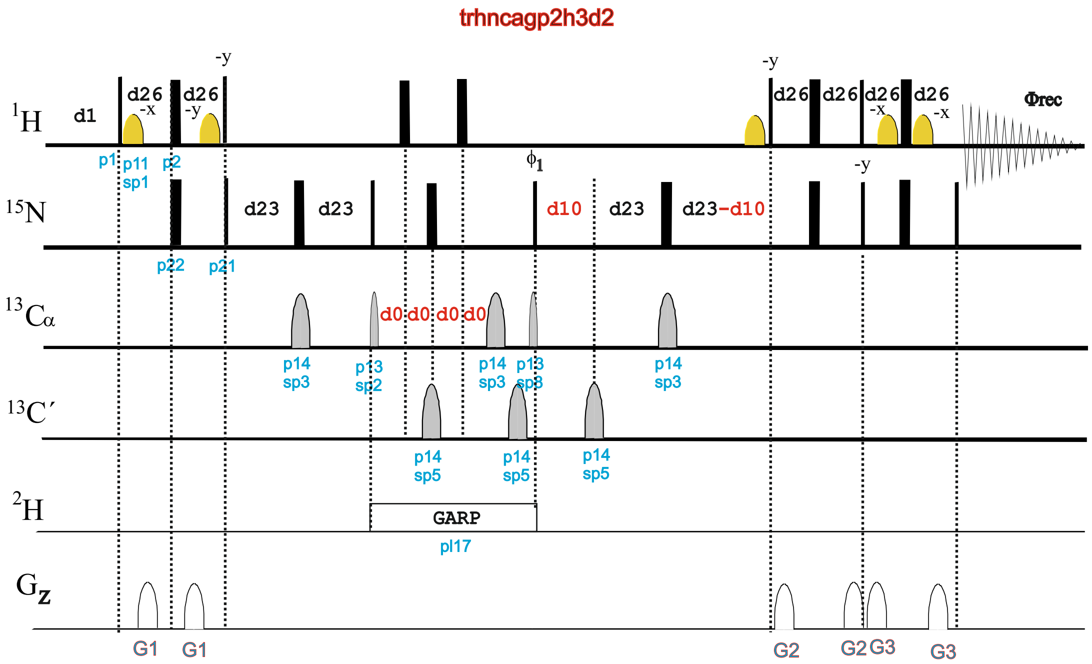
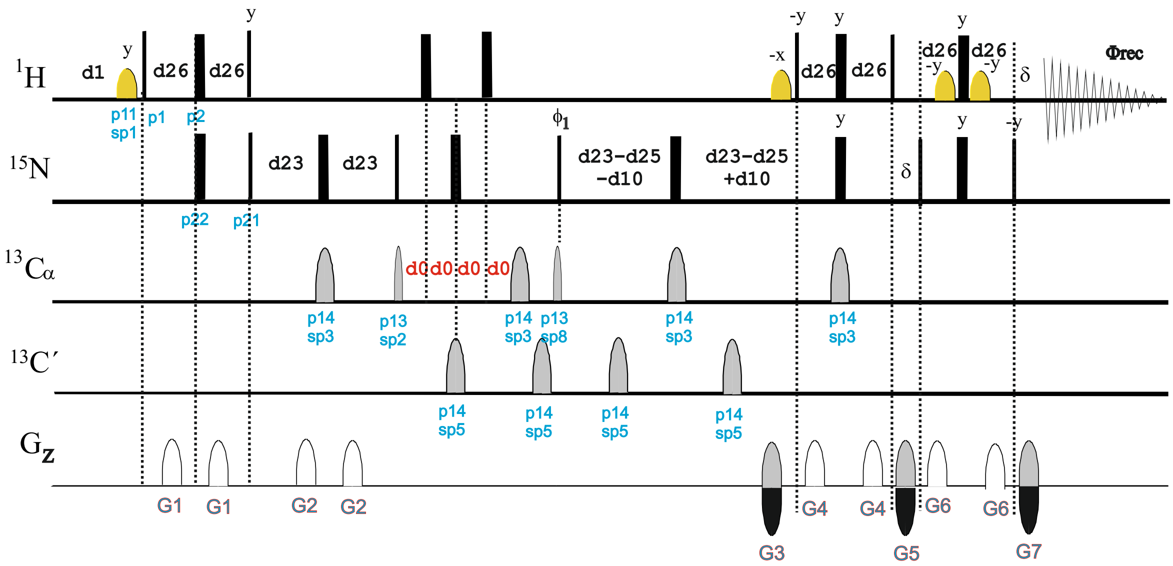
p14
sp3
sp5
G1
G2
G3

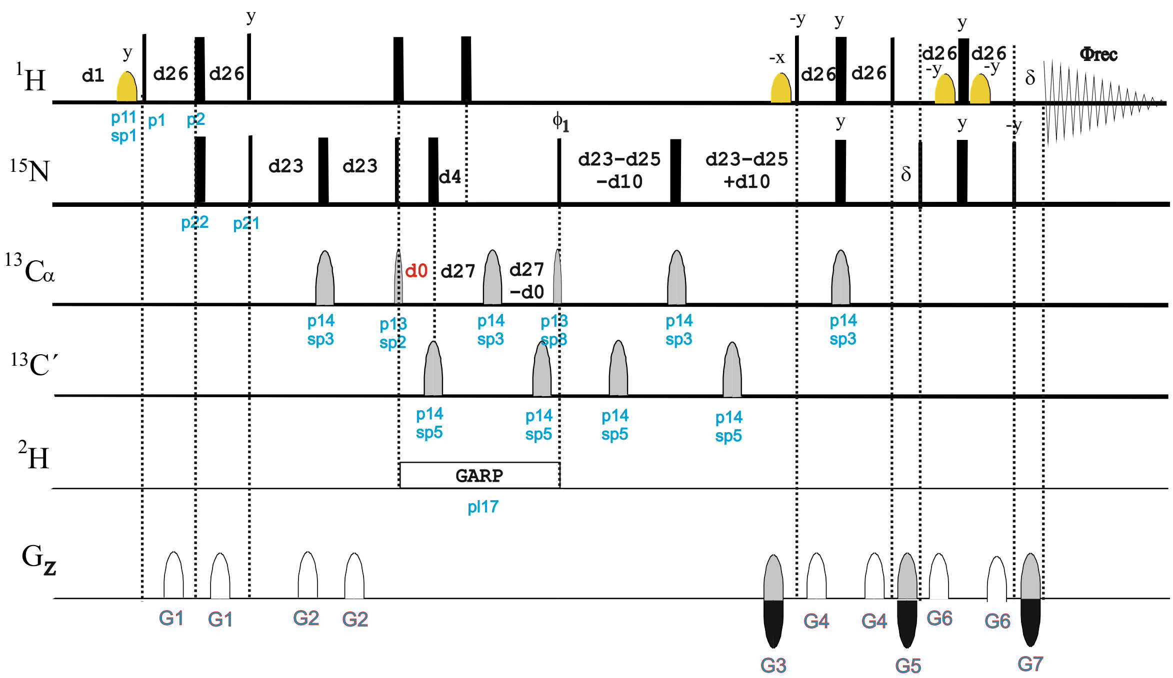

trhncagp2h3d
^{1}H
d1
d26
d26
Φrec
^{15}N
^{13}Cα
^{13}C′
^{2}H
GARP
pl17
G$_z$
G1
G1
G2
G2
G3
G3


trhncagp2h3d2
^{1}H
d1
d26
d26
Φrec
^{15}N
d23
d10
d23-d10
^{13}Cα
^{13}C′
^{2}H
GARP
pl17
G$_z$
G1
G1
G2
G2
G3
G3

trhncaetgp3d



trhncaetgp2h3d



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NMRGuide

3D HN(CA)CO

HNCACO Experiment

3D HN(CA)CO experiment

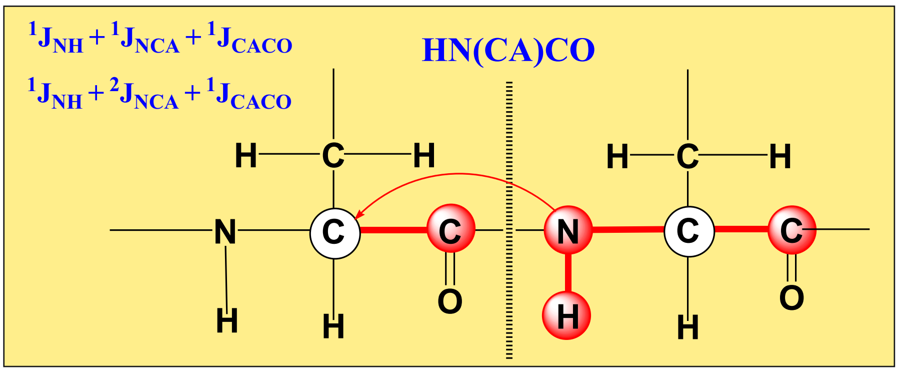
- 3D HN(CA)CO using PEP (**hncacogp3d** | HNCACOGP3D)
  - with ^{2}H-decoupling and suppression of protonated carbons (**hncacogp2h3d** | HNCACOGP2H3D)
  - with ^{2}H-decoupling (**hncacogp2h3d.2** | HNCACOGP2H3D.2)
- 3D HN(CA)CO using WATERGATE (**hncacogpwg3d** | HNCACOGPWG3D)
  - with ^{2}H-decoupling and suppression of protonated carbons (**hncacogpwg2h3d** | HNCACOGPWG2H3D)
- 3D HN(CA)CO using TROSY (**trhncacogp3d** | TRHNCACOGP3D)
  - with ^{2}H-decoupling (**trhncacogp2h3d** | TRHNCACOGP2H3D)
  - using echo-antiecho gradient (**trhncacoetgp3d** | TRHNCACOETGP3D)
  - using echo-antiecho gradient and with ^{2}H-decoupling (**trhncacoetgp2h3d** | TRHNCACOETGP2H3D)

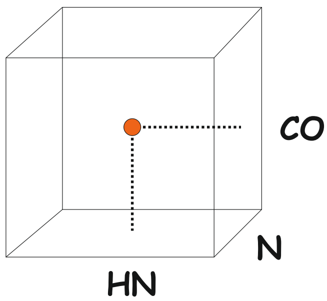
4D HNCACO experiment

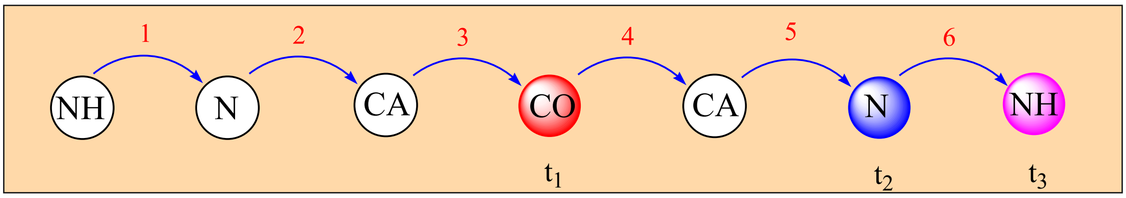
- 4D HNCACO using PEP (**hncacogp4d**)
  - with ^{2}H-decoupling (**hncacogp2h4d**)
- 4D HNCACO using WATERGATE (**hncacogpwg4d**)
  - with ^{2}H-decoupling (**hncacogpwg2h4d**)
- 4D HNCACO using TROSY (**trhncacogp4d**)
  - with ^{2}H-decoupling (**trhncacogp2h4d**)
  - using echo-antiecho gradient (**trhncacoetgp4d**)
  - using echo-antiecho gradient and with ^{2}H-decoupling (**trhncacoetgp2h4d**)

Also see:
3D SOFAST/BEST-HN(CA)CO experiment
3D BEST-HN(CA)CO (**b_hncacogp3d** | **B_HNCACOGP3D**)
3D BEST-HN(CA)CO using TROSY (**b_trhncacogp3d**)
4D BEST-HNCACO (**b_hncacogp4d**)
3D CO-Detected (H)NCACO experiments

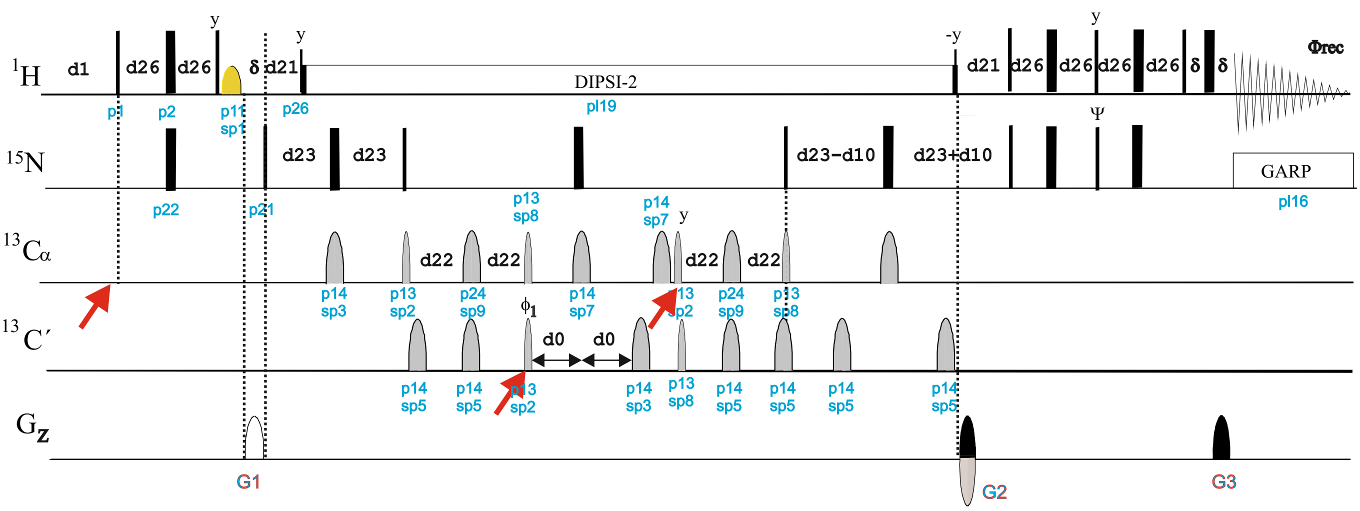
Related Experiments:
HNCO Experiment



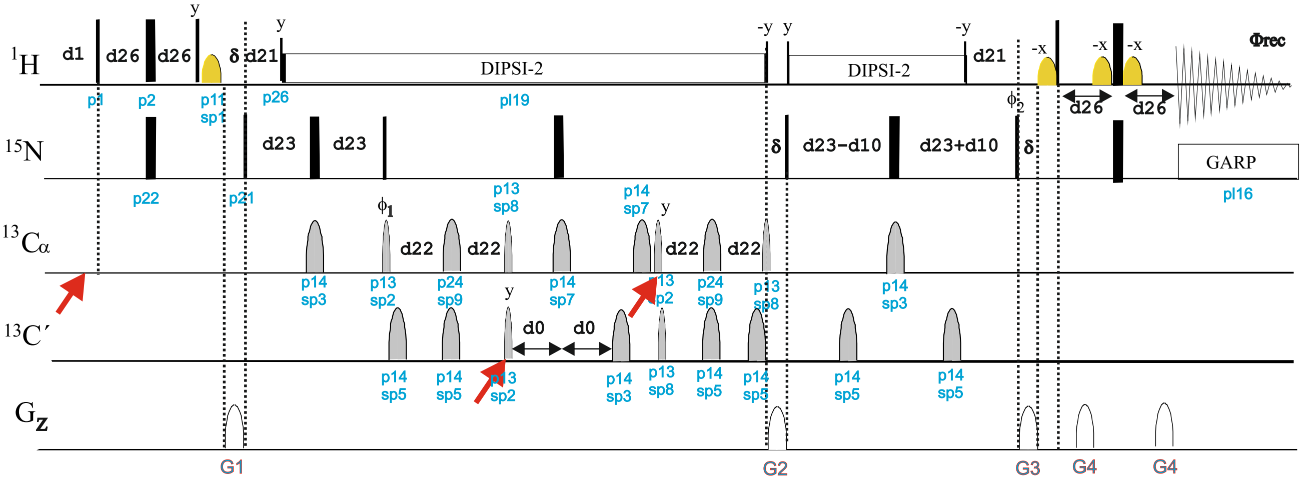




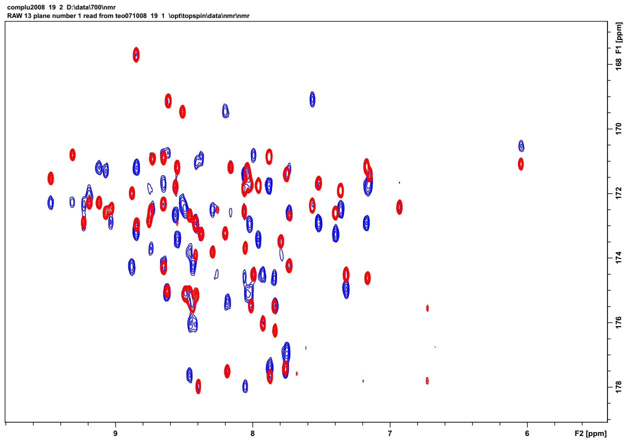
hncacogp3d



hncacogpwg3d

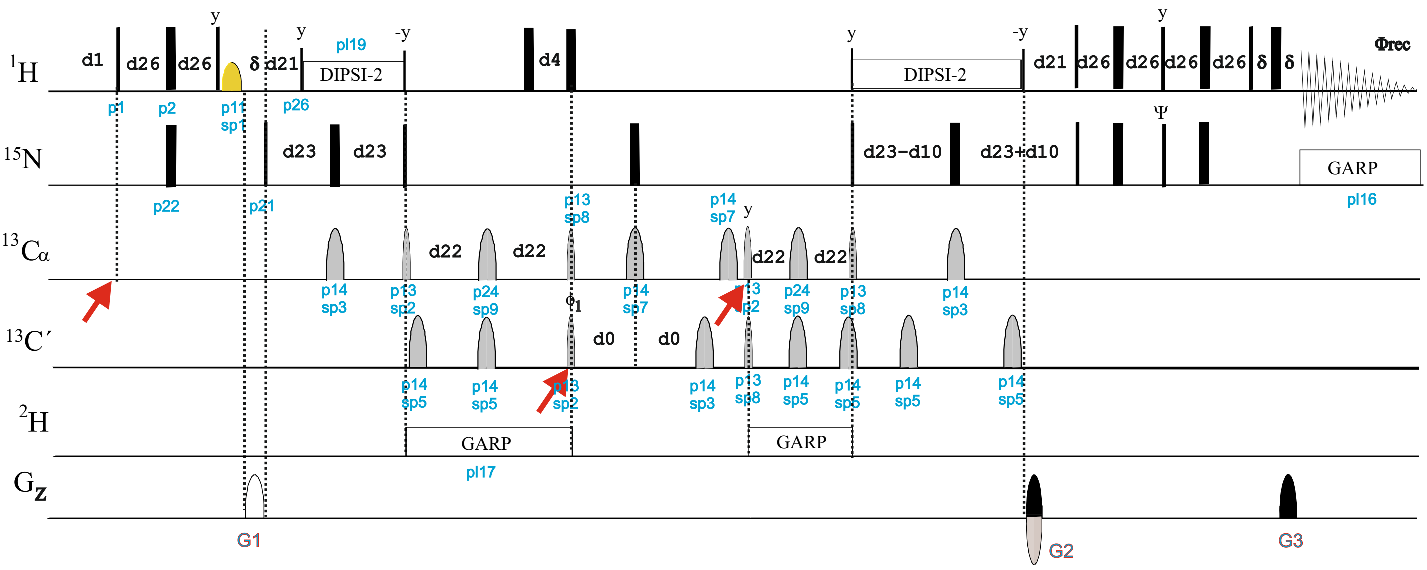


d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m
d22=1/4J(COCA)=4m
d4=1/4J(CH)=1.7m

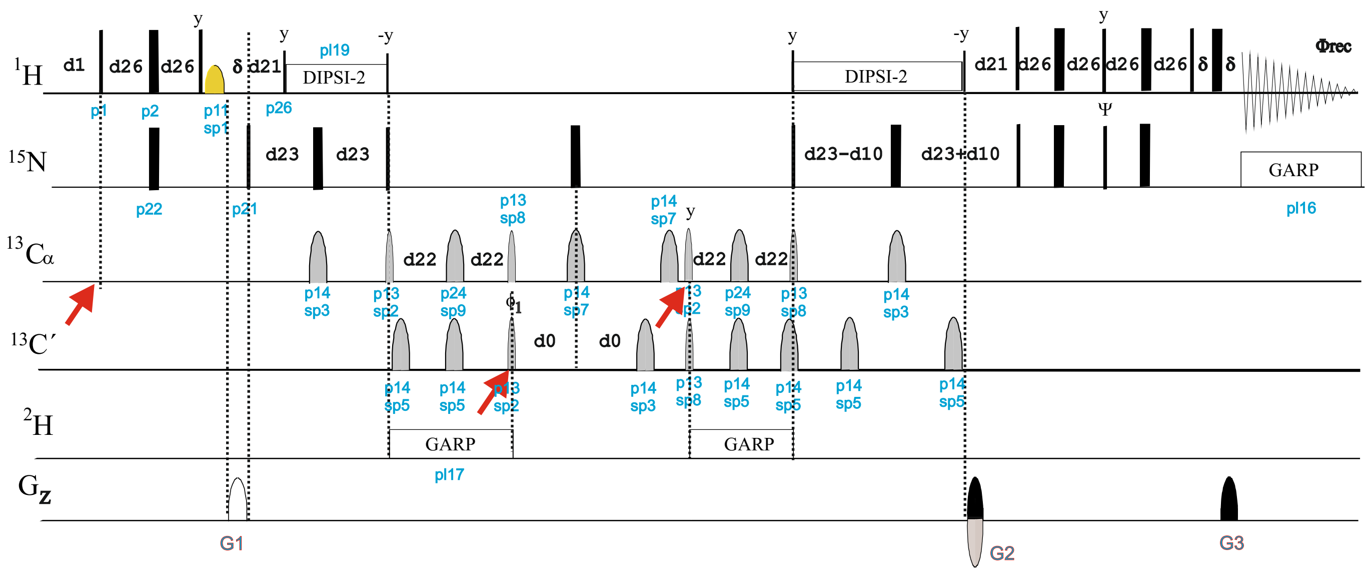


HNCO (blue)
vs
HN(CA)CO (red)

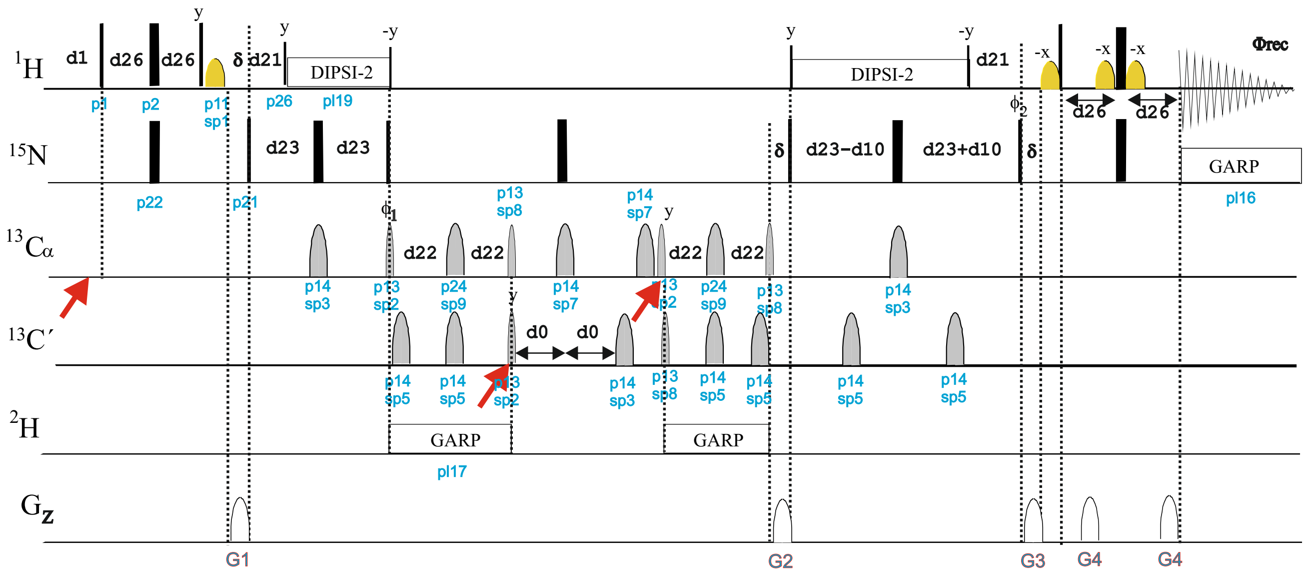
hncacogp2h3d



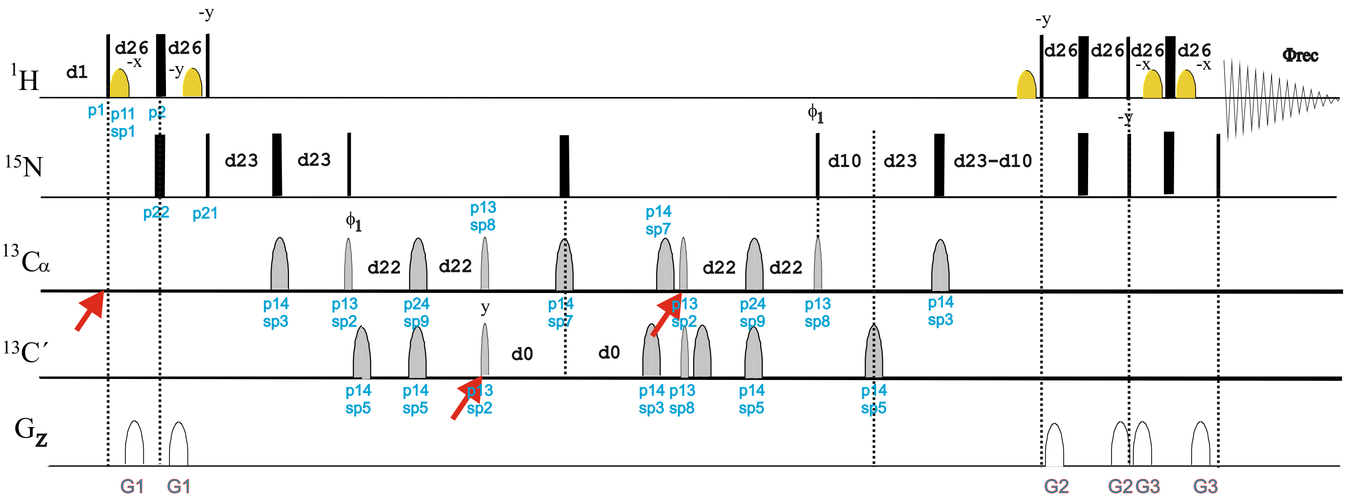
hncacogp2h3d.2



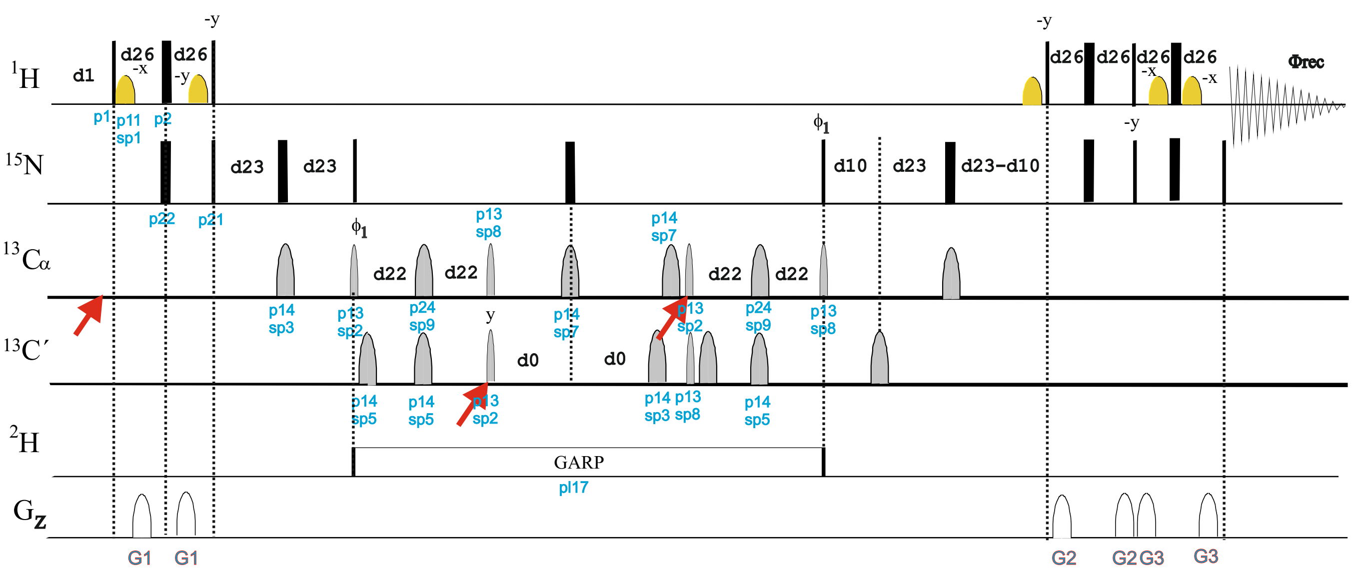
hncacogpwg2h3d



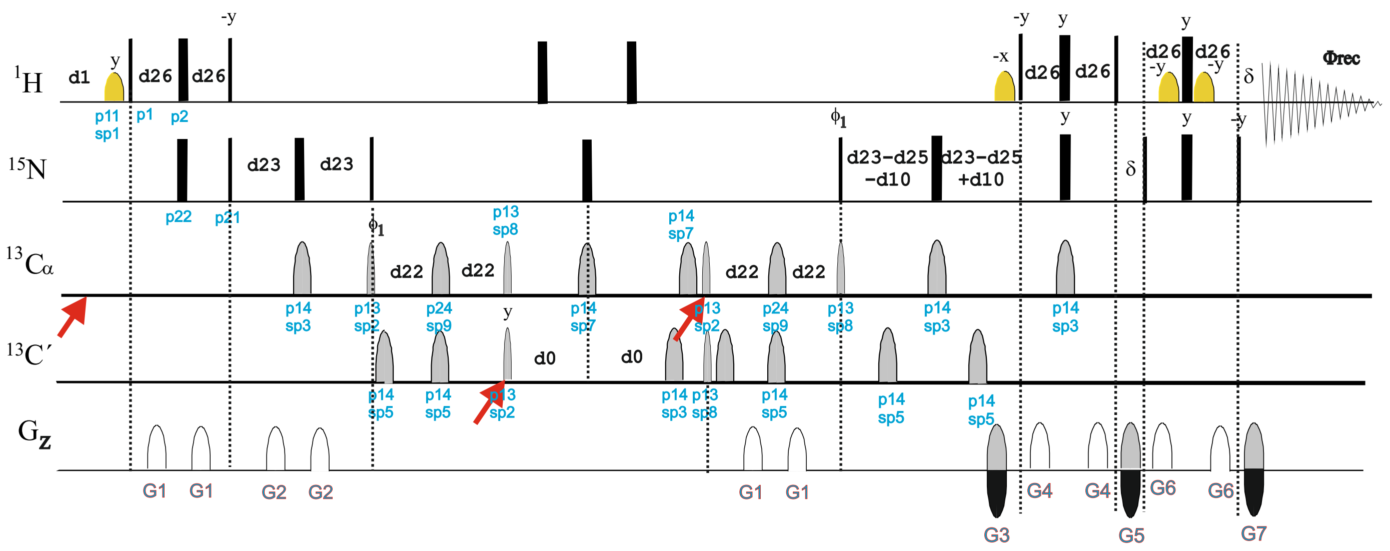
trhncacogp3d



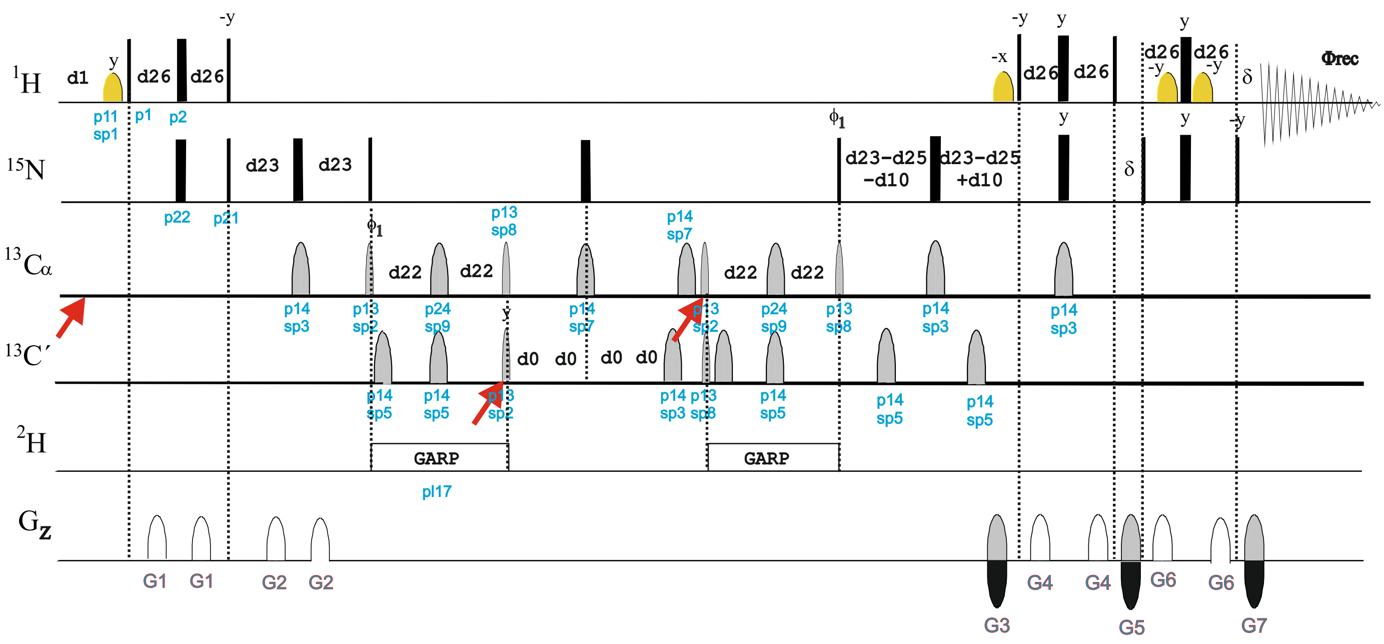
trhncacogp2h3d



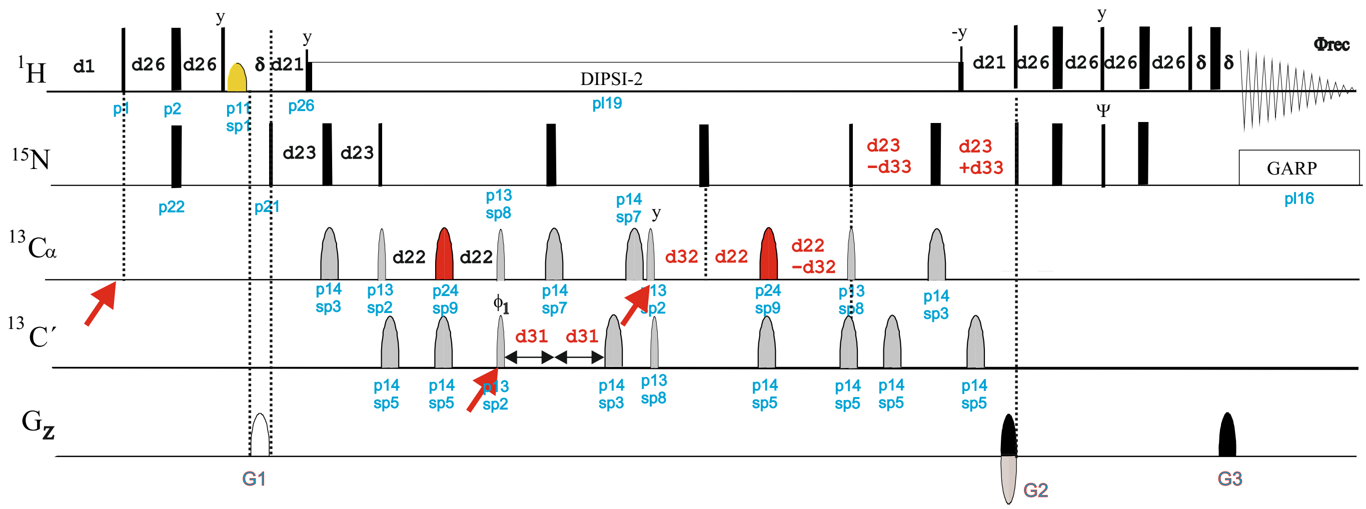
trhncacoetgp3d



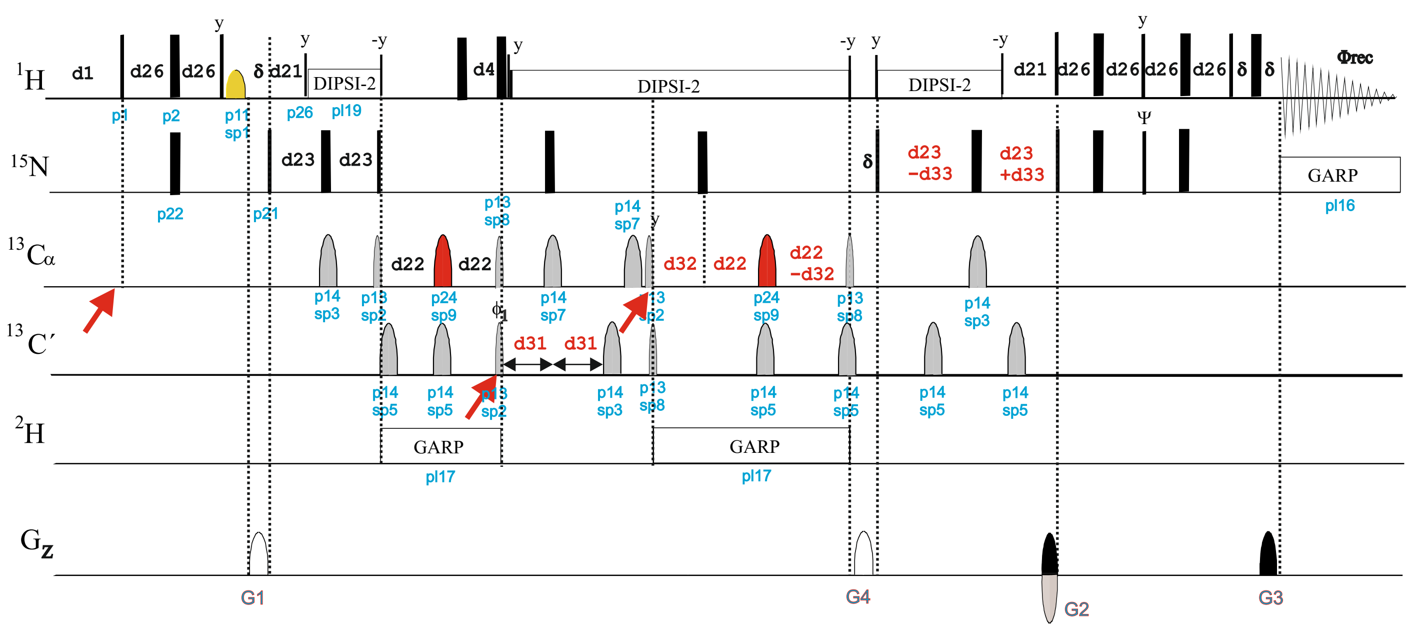
trhncacoetgp2h3d



hncacogp4d



hncacogp2h4d



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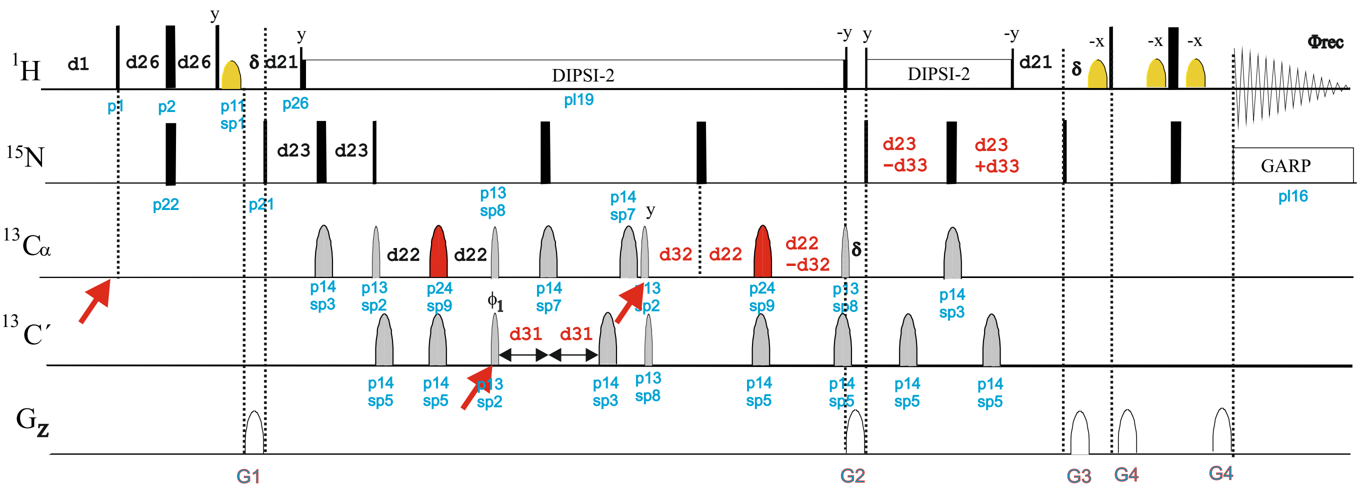

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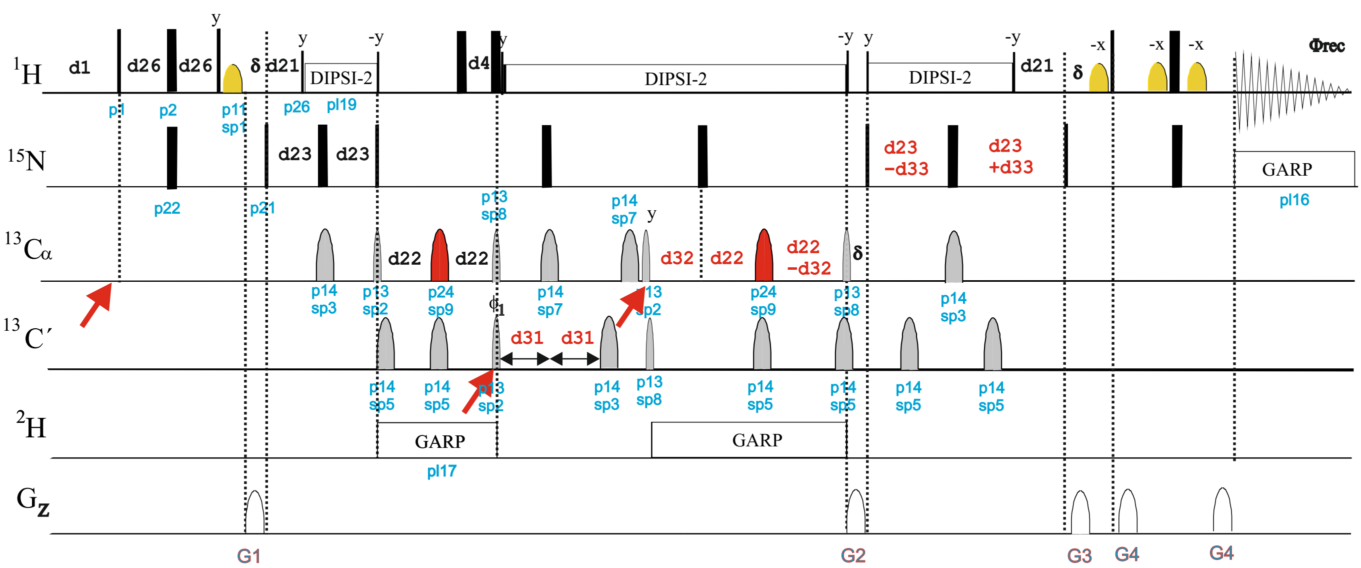
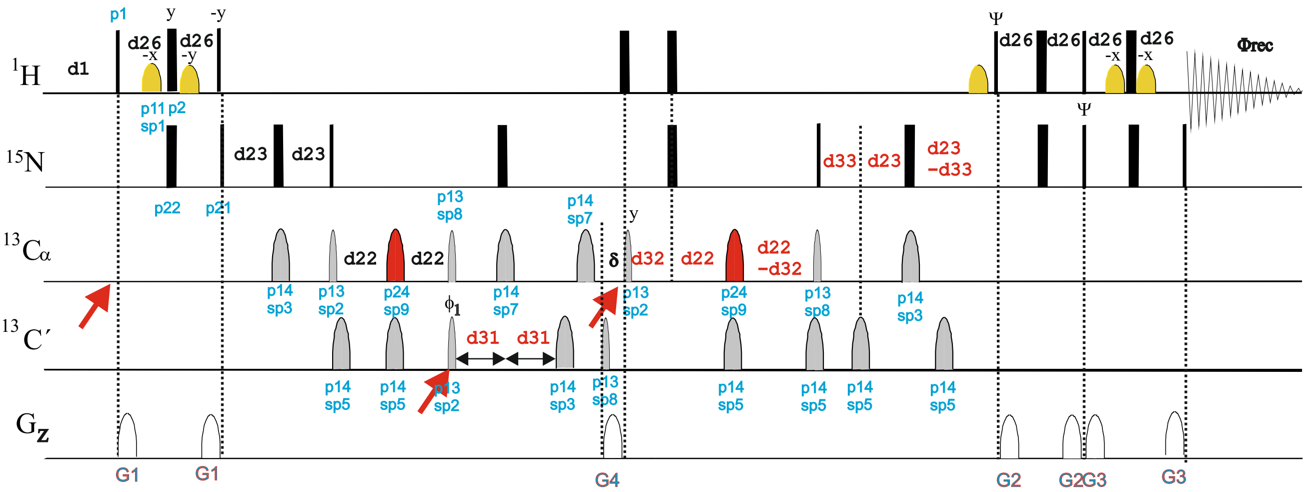
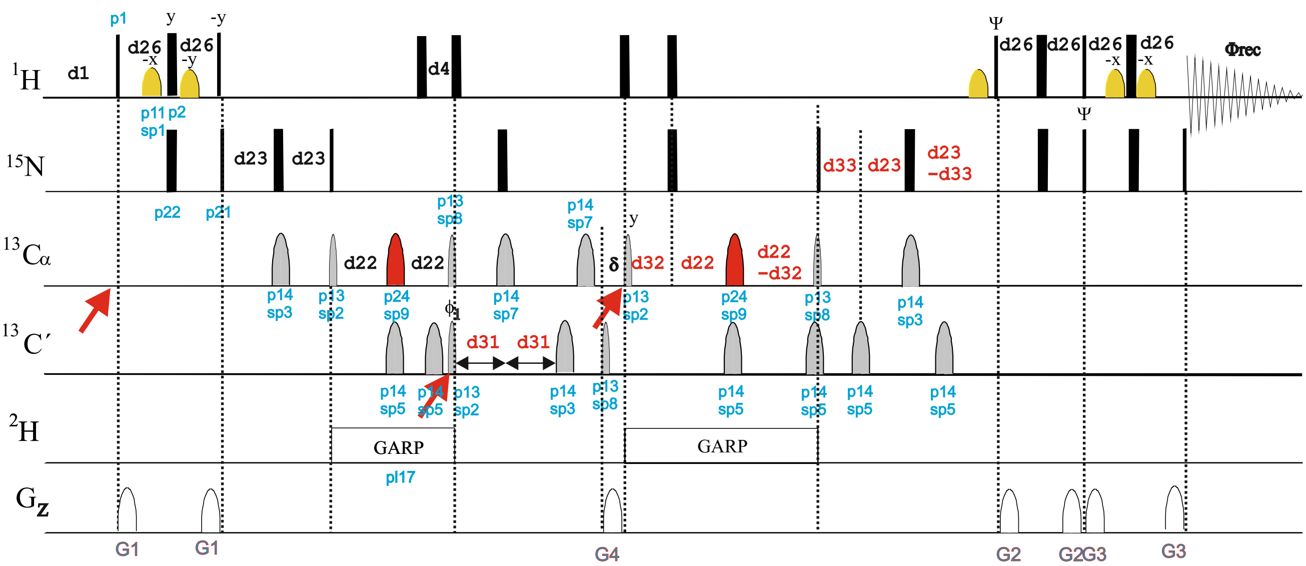


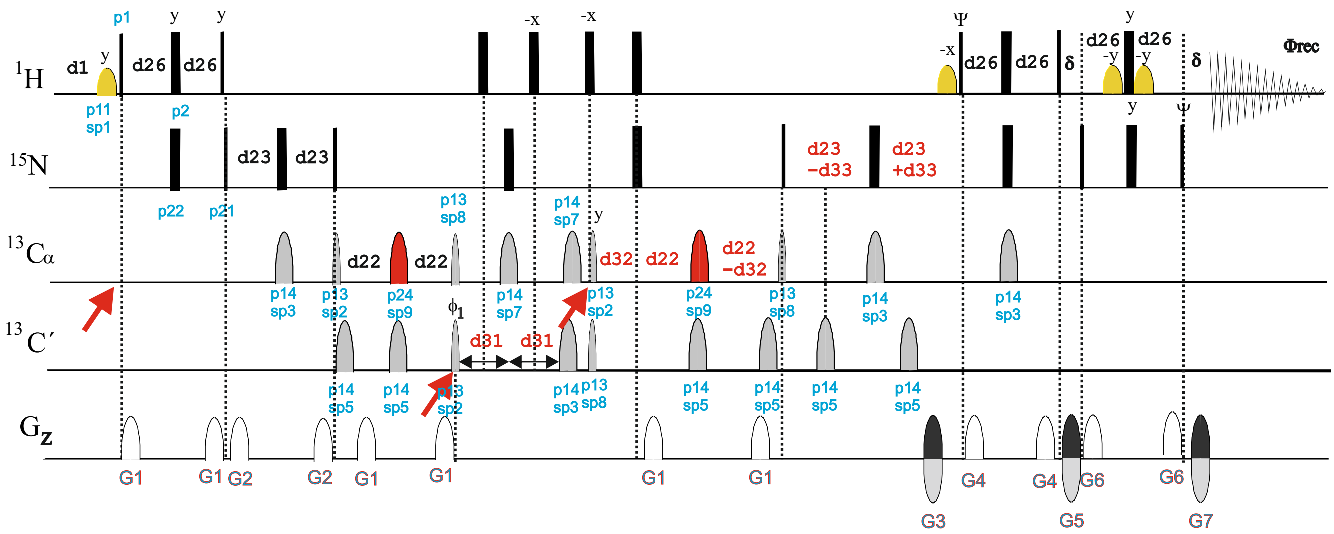
trhncacogp4d



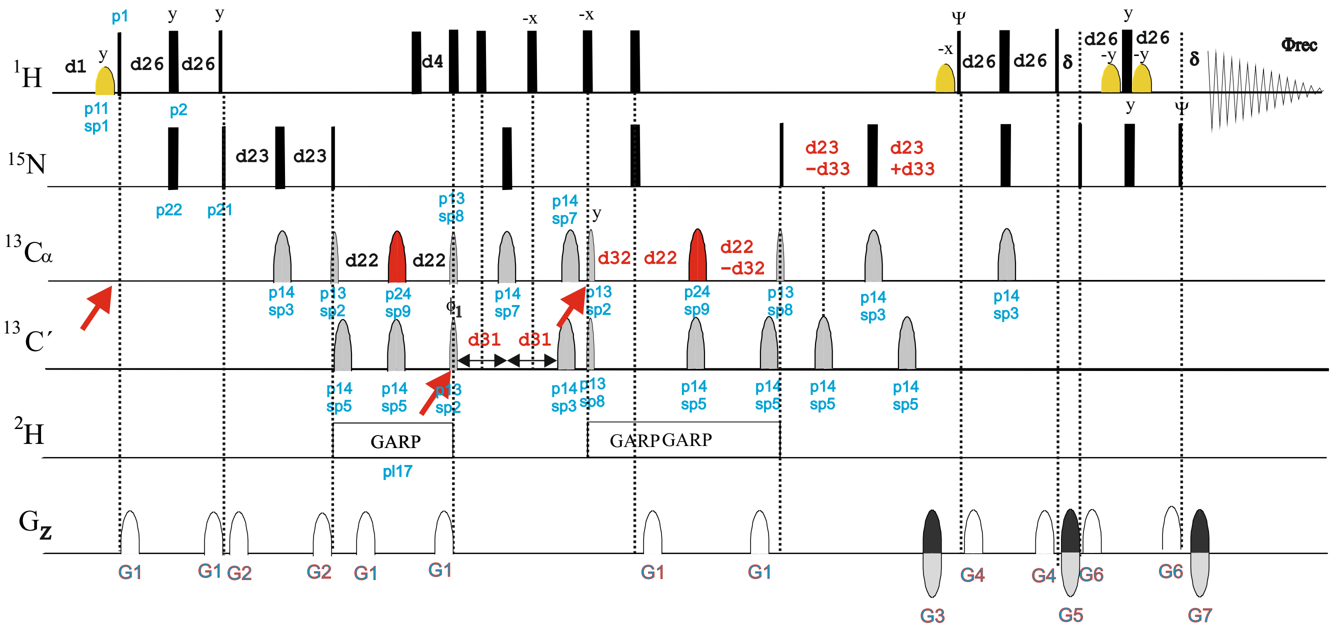
trhncacogp2h4d



trhncacoetgp4d



trhncacoetgp2h4d



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NMRGuide

3D HN(CO)CA

HNCOCA Experiment

3D HN(CO)CA experiment

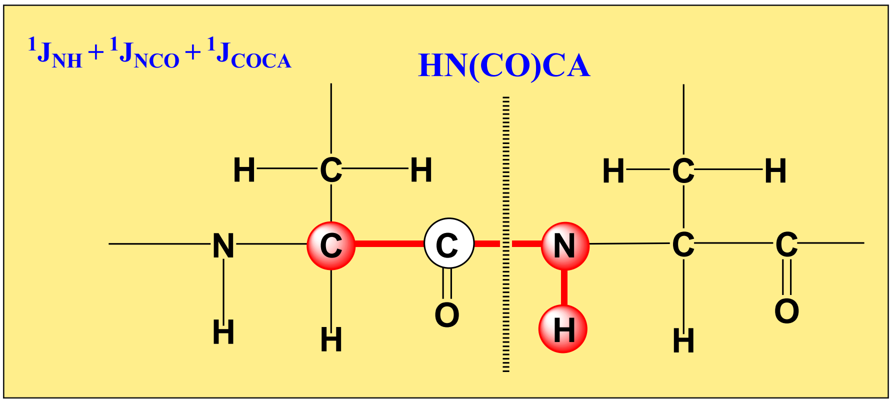
- 3D HN(CO)CA using PEP (**hncocagp3d** | HNCOCAGP3D)
    - with ^{2}H-decoupling (**hncocagp2h3d** | HNCOCAGP2H3D)
- 3D HN(CO)CA using WATERGATE (**hncocagpwg3d** | HNCOCAGPWG3D)
    - with ^{2}H-decoupling (**hncocagpwg2h3d** | HNCOCAGPWG2H3D)
- 3D HN(CO)CA using TROSY (**trhncocagp3d** | TRHNCOCAGP3D):
    - with ^{2}H-decoupling (**trhncocagp2h3d** | TRHNCOCAGP2H3D)
    - using echo-antiecho gradient (**trhncocaetgp3d** | TRHNCOCAETGP3D)
    - using echo-antiecho gradient and with ^{2}H-decoupling (**trhncocaetgp2h3d** | TRHNCOCAETGP2H3D)

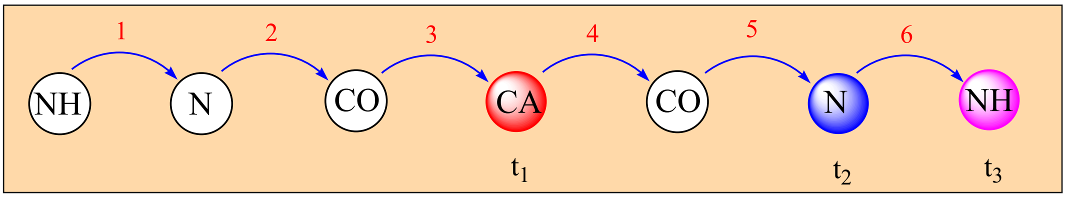
4D HNCOCA experiment

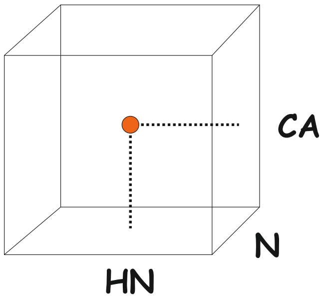
- 4D HNCOCA using PEP (**hncocagp4d**)
    - with ^{2}H-decoupling (**hncocagp2h4d**)
- 4D HNCOCA using WATERGATE (**hncocagpwg4d**)
    - with ^{2}H-decoupling (**hncocagpwg2h4d**)
- 4D HNCOCA using TROSY (**trhncocagp4d**)
    - with ^{2}H-decoupling (**trhncocagp2h4d**)
    - using echo-antiecho gradient (**trhncocaetgp4d**)
    - using echo-antiecho gradient and with ^{2}H-decoupling (**trhncocaetgp2h4d**)

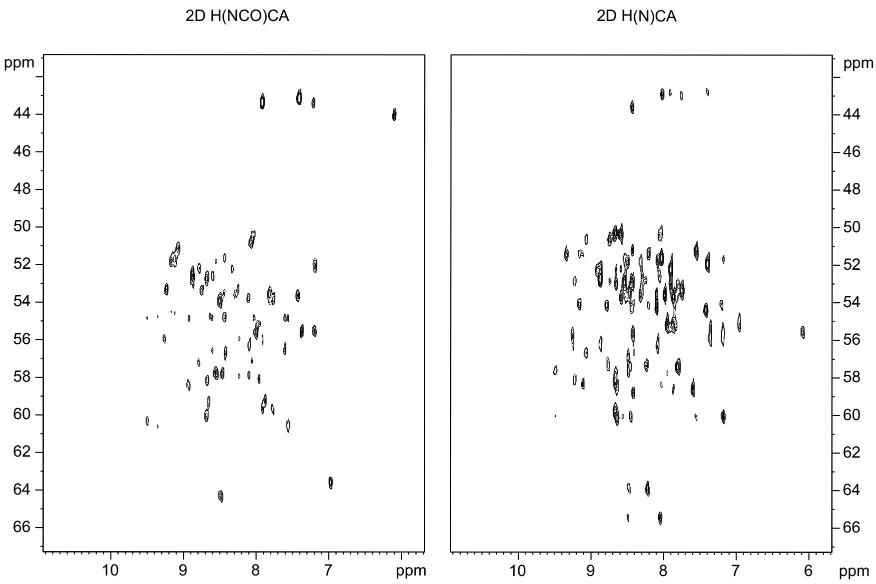
Also see:
SOFAST/BEST-HN(CO)CA experiment
    3D BEST-HN(CO)CA (b_hncocagp3d | B_HNCOCAGP3D)
    3D BEST-HN(CO)CA using TROSY (b_trhncocagp3d)
    4D BEST-HNCOCA (b_hncocagp4d)
3D APSY-HNCOCA experiment
    Reduced-Dimensionality (4,2)-HNCOCA (rd_hncoca_42 | APSY_HNCOCA_42)
3D (H)NCOCA in "Carbon-Detected Experiments"
3D HNCO-type experiments for J measuring

Related Experiments:
intra-HNCA, HNCA

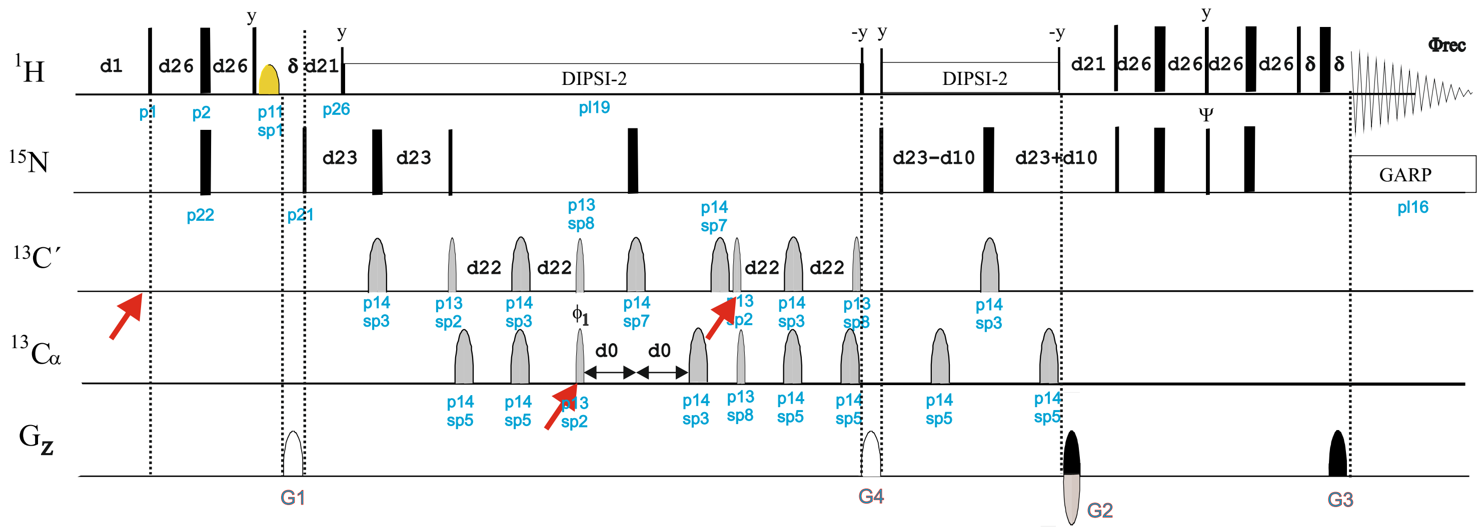

$^1J_{NH} + ^1J_{NCO} + ^1J_{COCA}$
HN(CO)CA
H
C
N
O


1
2
3
4
5
6
NH
N
CO
CA
CO
N
NH
t_1
t_2
t_3

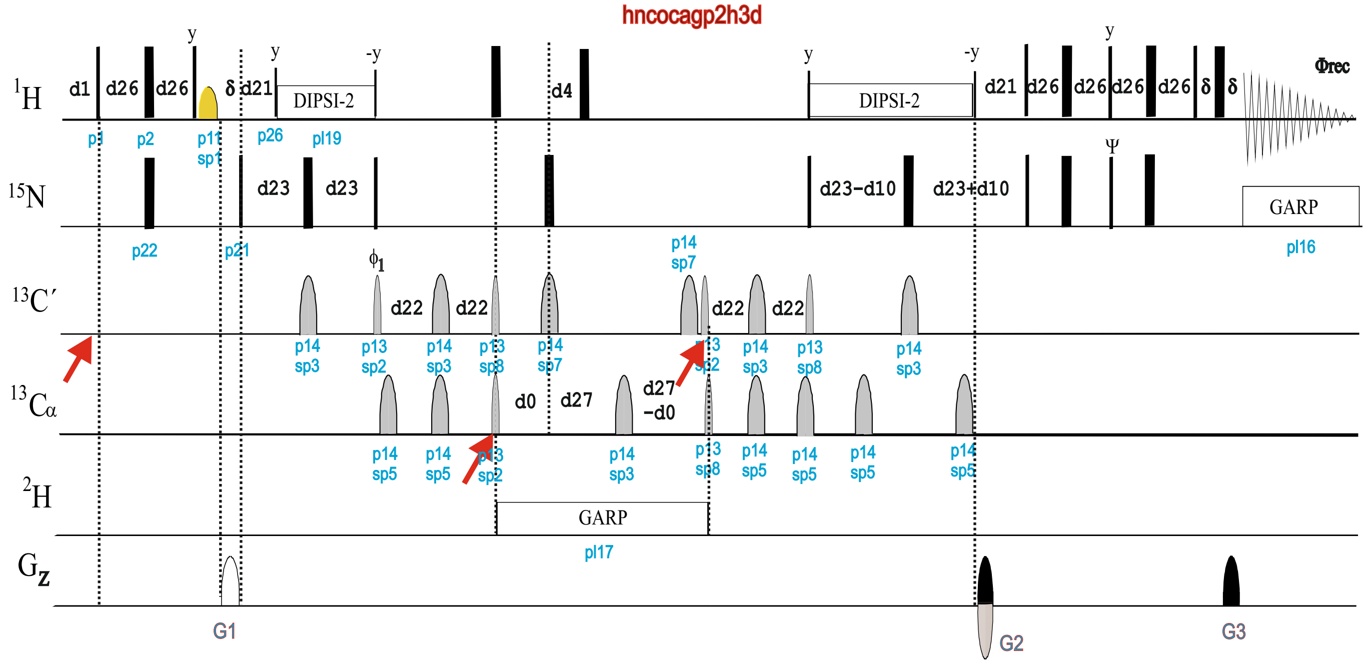

CA
N
HN


2D H(NCO)CA
2D H(N)CA
ppm
44
46
48
50
52
54
56
58
60
62
64
66
10
9
8
7
6
ppm

hncocagp3d



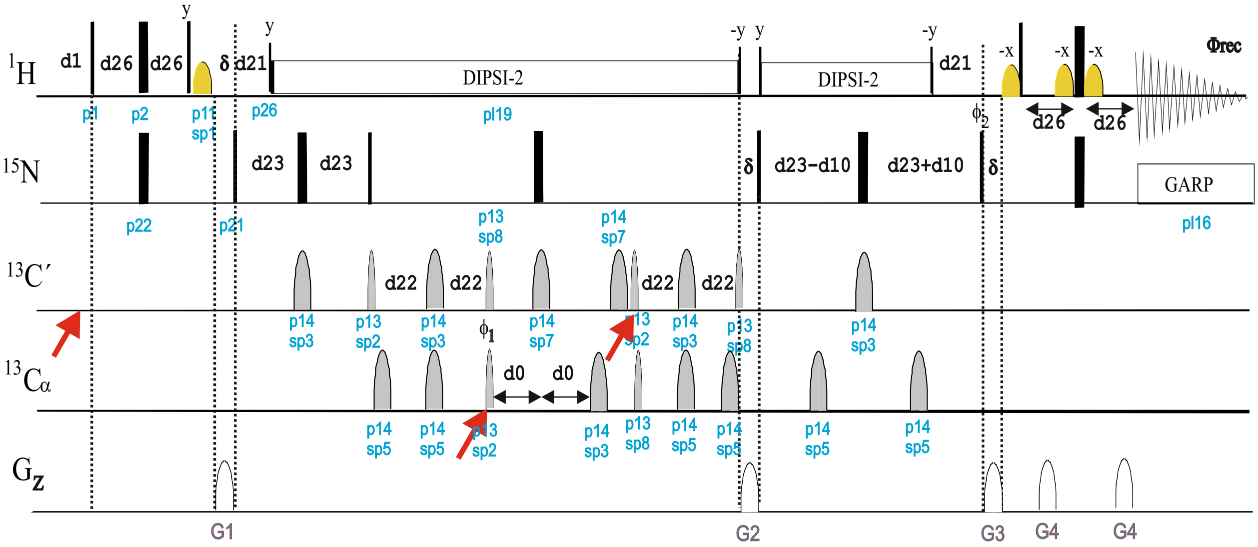
hncocagp2h3d



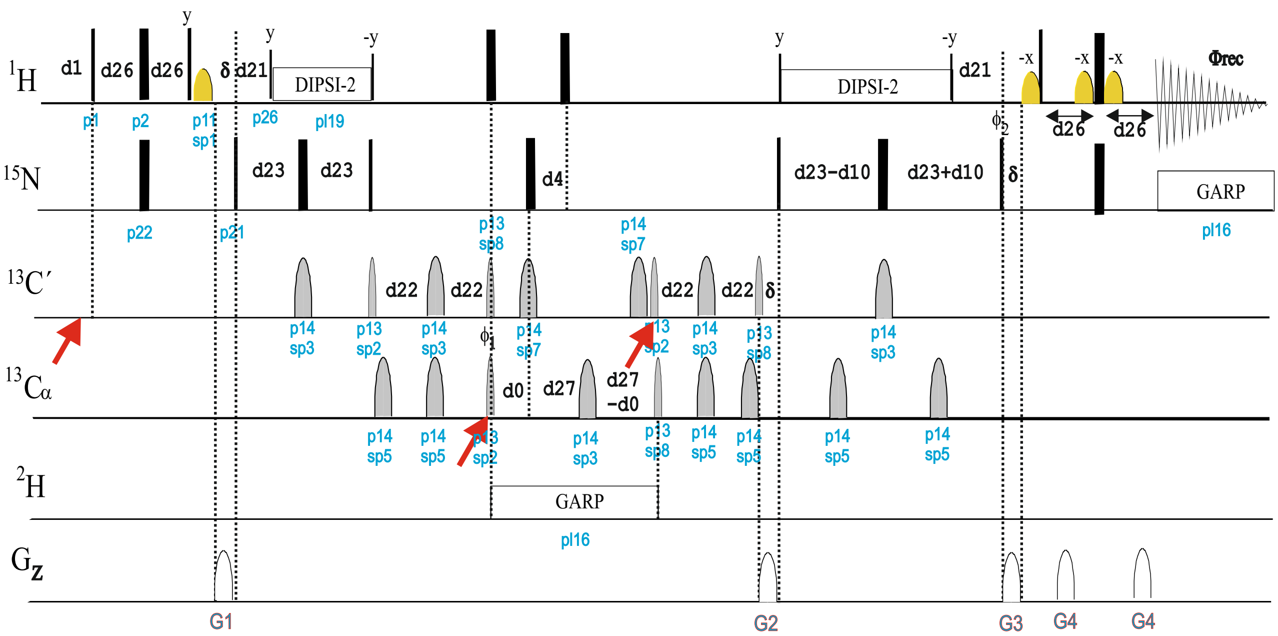
d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m
d22=1/4J(COCA)=4m

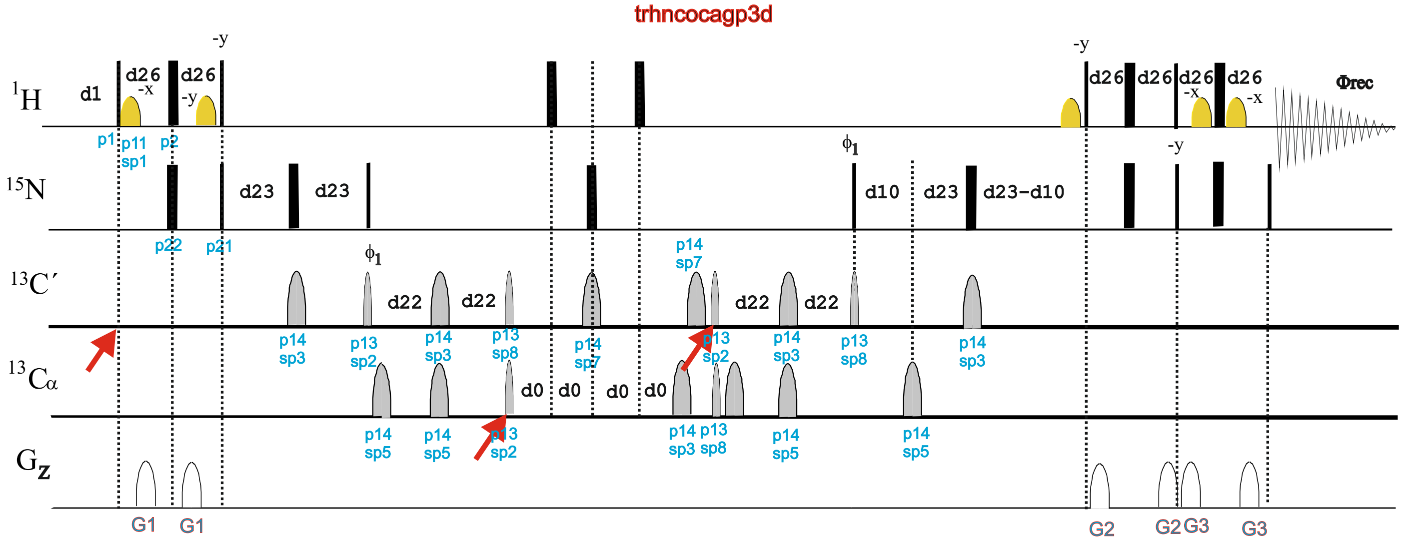
d27=CT(CA)=13.8m
d4=1/4J(CH)=1.7m

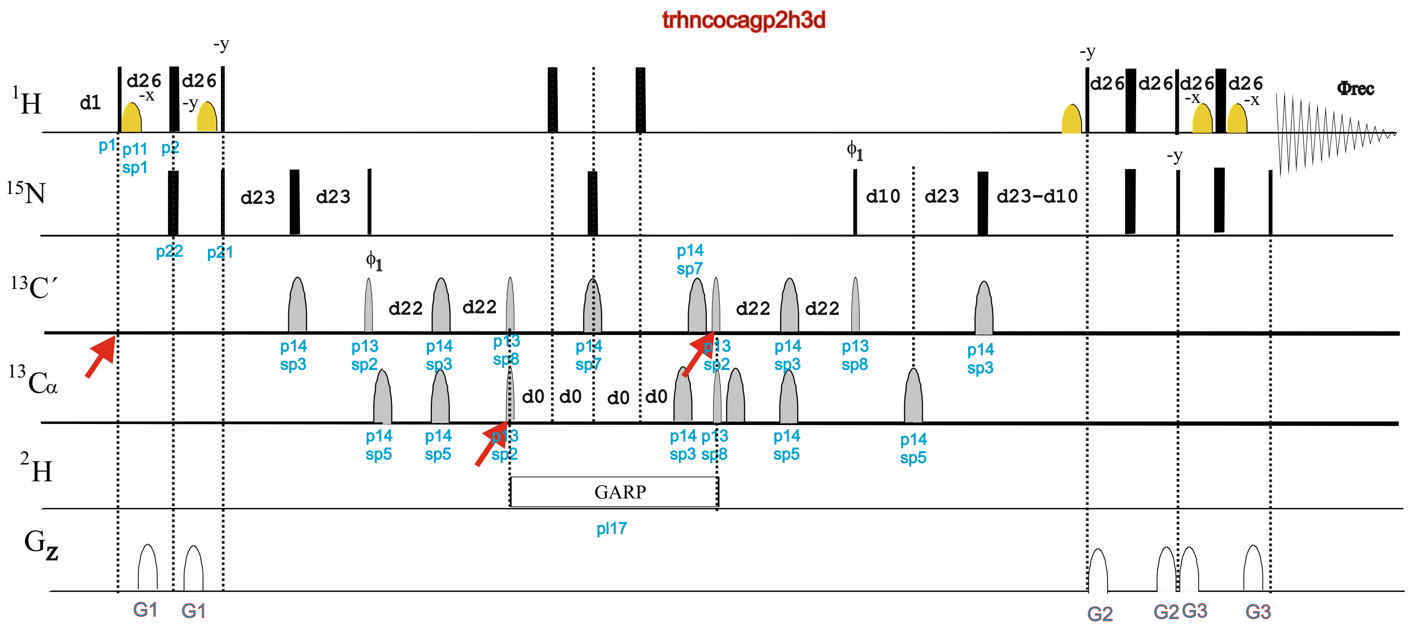
hncocagpwg3d



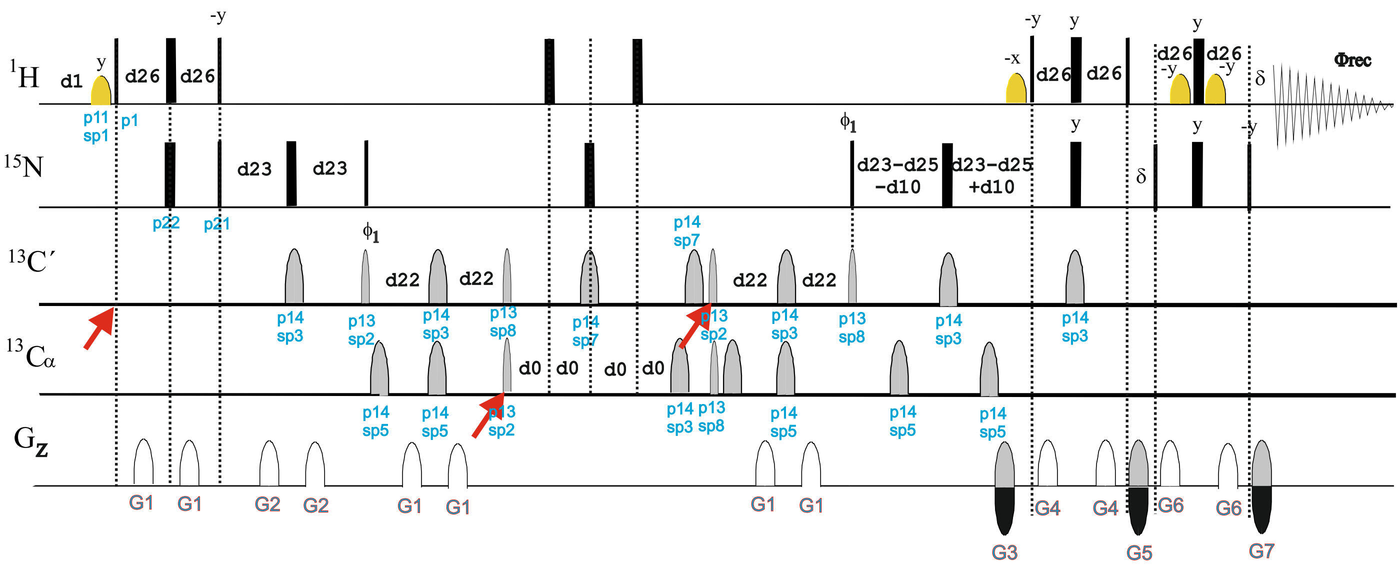
hncocagpwg2h3d



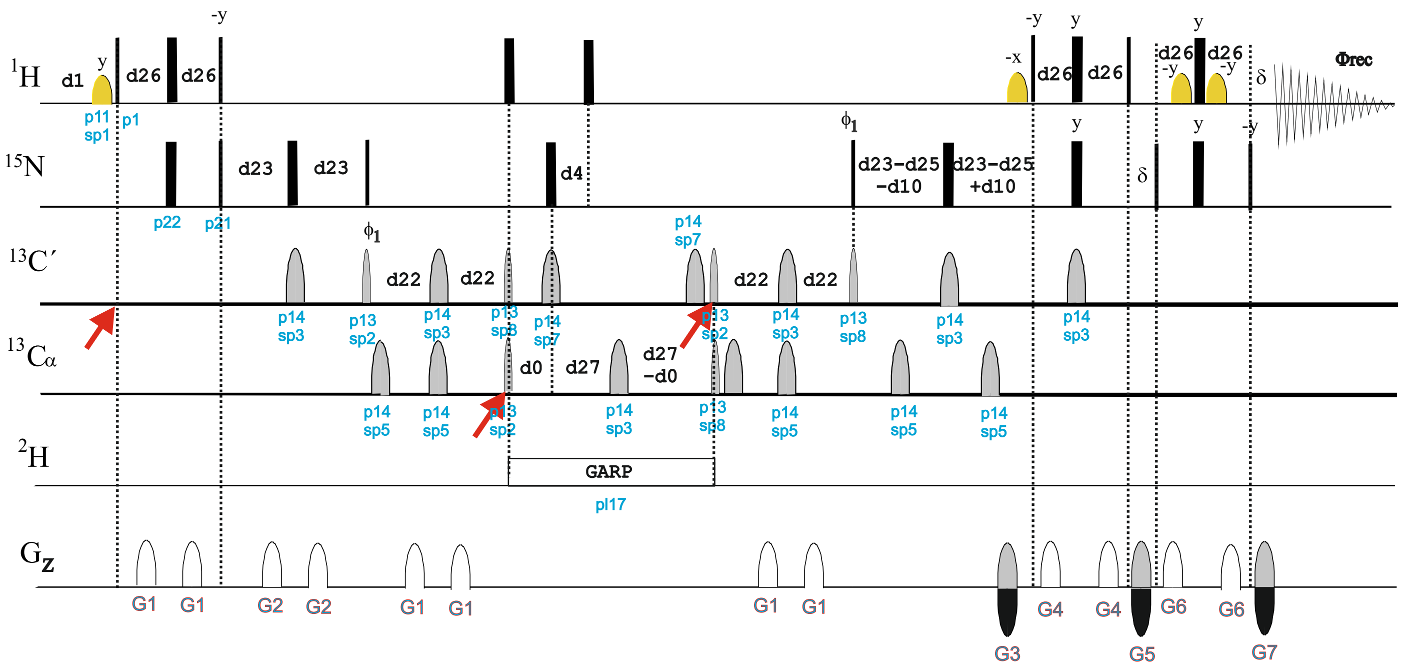

trhncocagp3d
1H
15N
13C′
13Cα
Gz
d1
d26
d23
d22
d0
d10
d23-d10
Φrec
G1
G2
G3

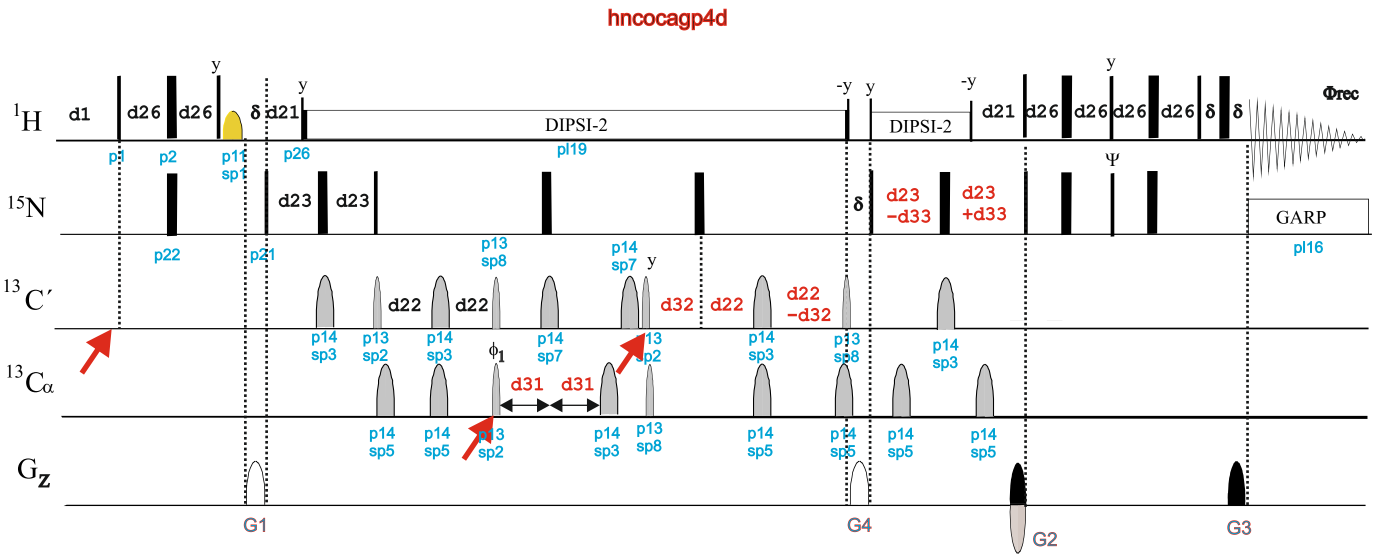

trhncocagp2h3d
1H
15N
13C′
13Cα
2H
Gz
GARP
pl17
Φrec
G1
G2
G3

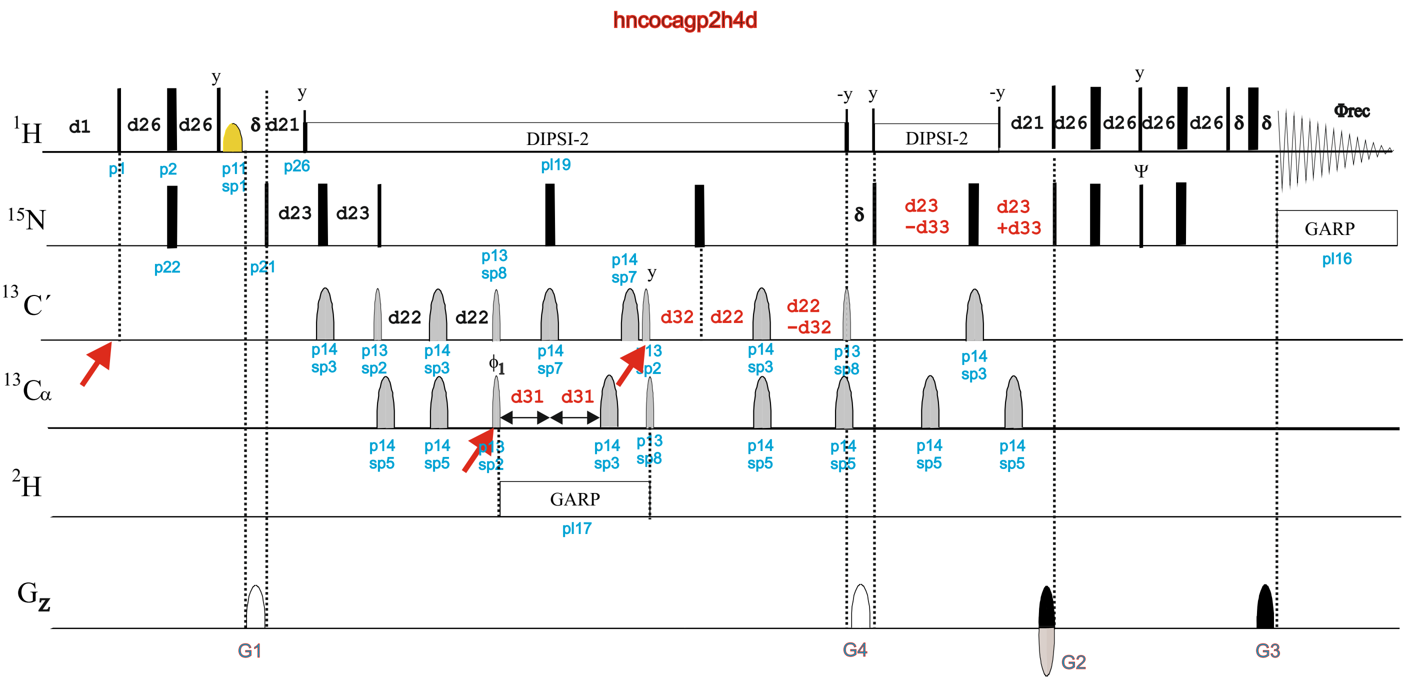
trhncocaetgp3d



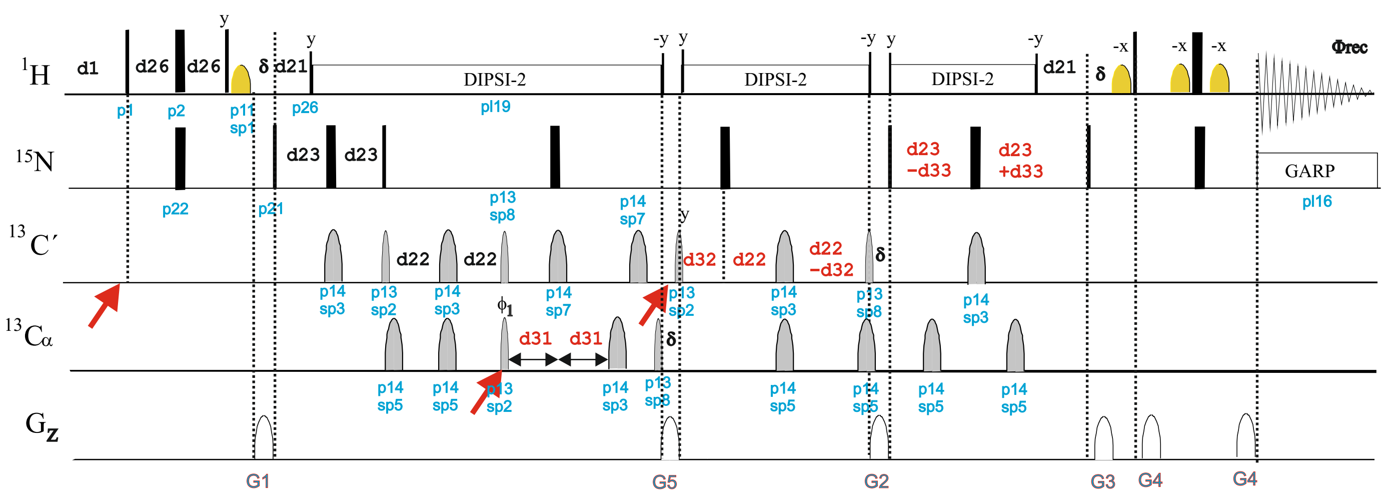
trhncocaetgp2h3d



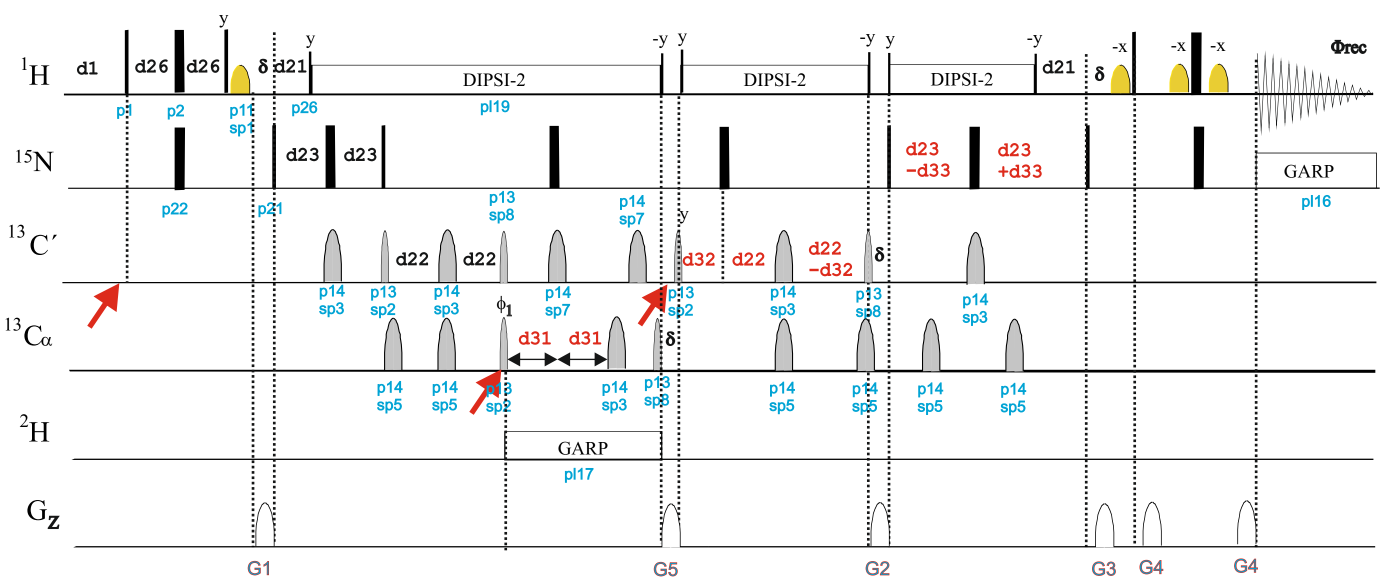

hncocagp4d
1H
15N
13C′
13Cα
Gz
d1
d26
d21
DIPSI-2
pl19
GARP
pl16
Φrec
d23
d23 −d33
d23 +d33
d22
d22 −d32
d32
d31
G1
G4
G2
G3


hncocagp2h4d
1H
15N
13C′
13Cα
2H
Gz
d1
d26
d21
DIPSI-2
pl19
GARP
pl16
pl17
Φrec
d23
d23 −d33
d23 +d33
d22
d22 −d32
d32
d31
G1
G4
G2
G3

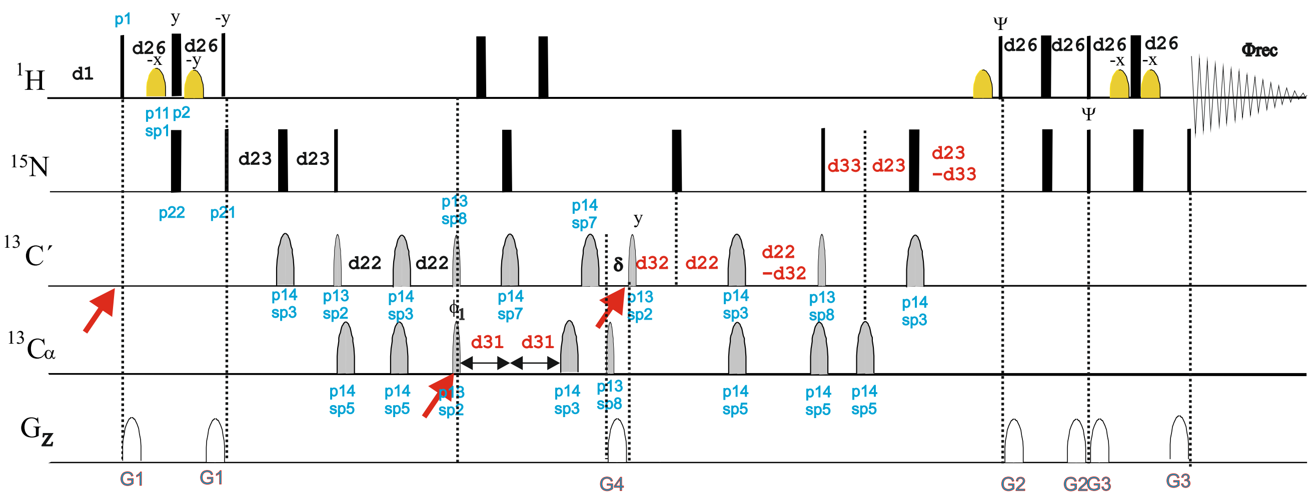
hncocagpwg4d



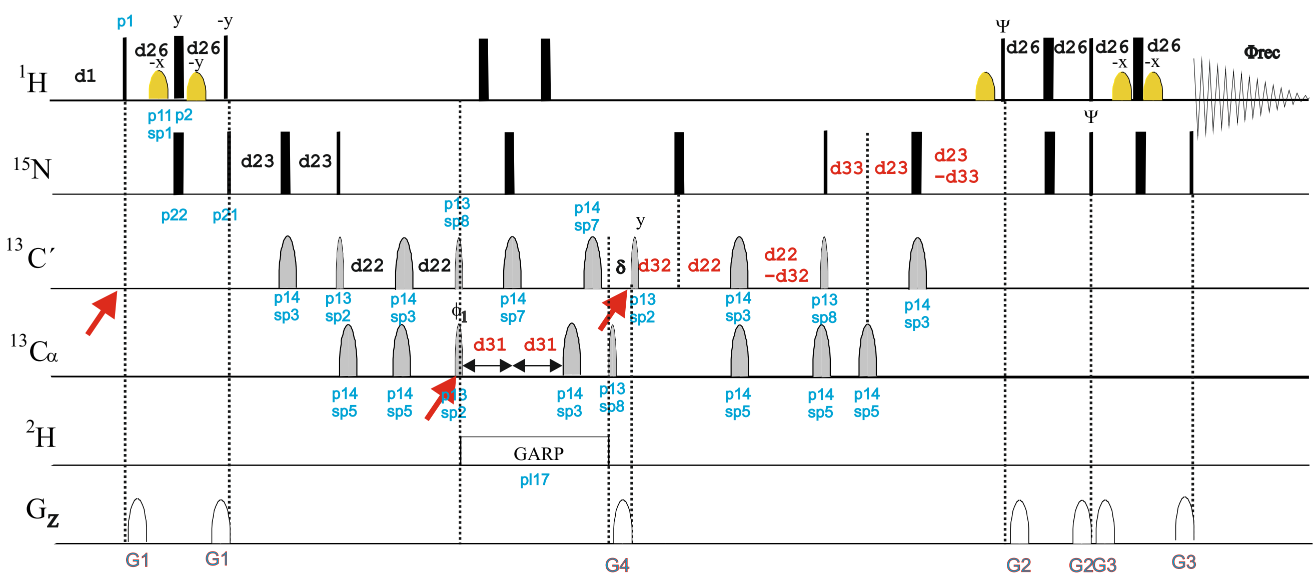
hncocagpwg2h4d



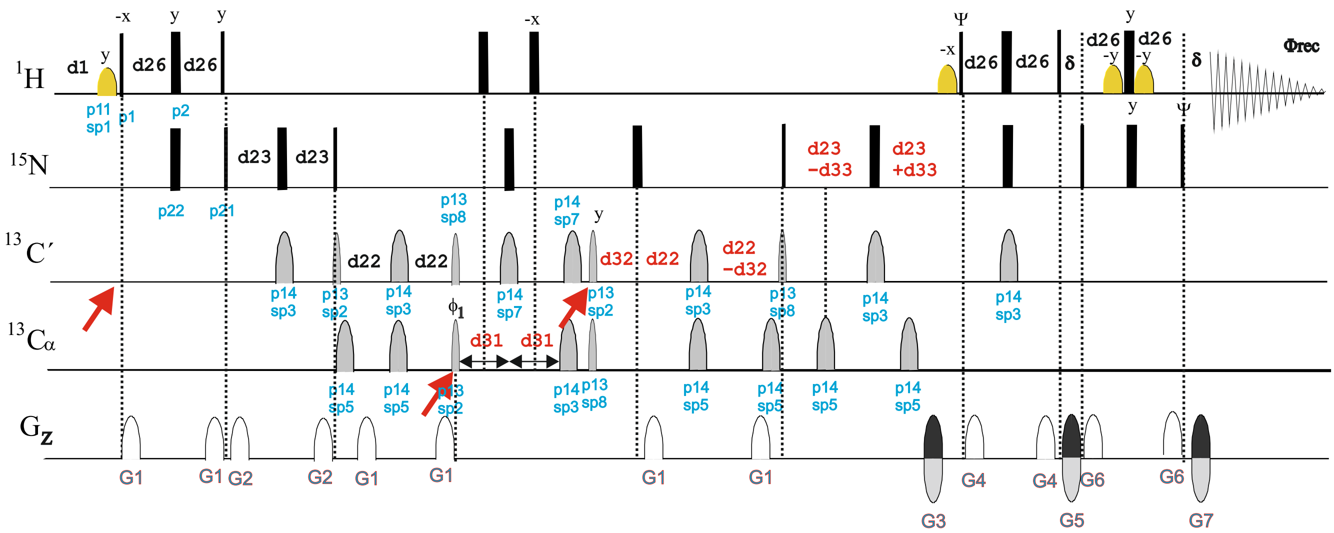
trhncocagp4d



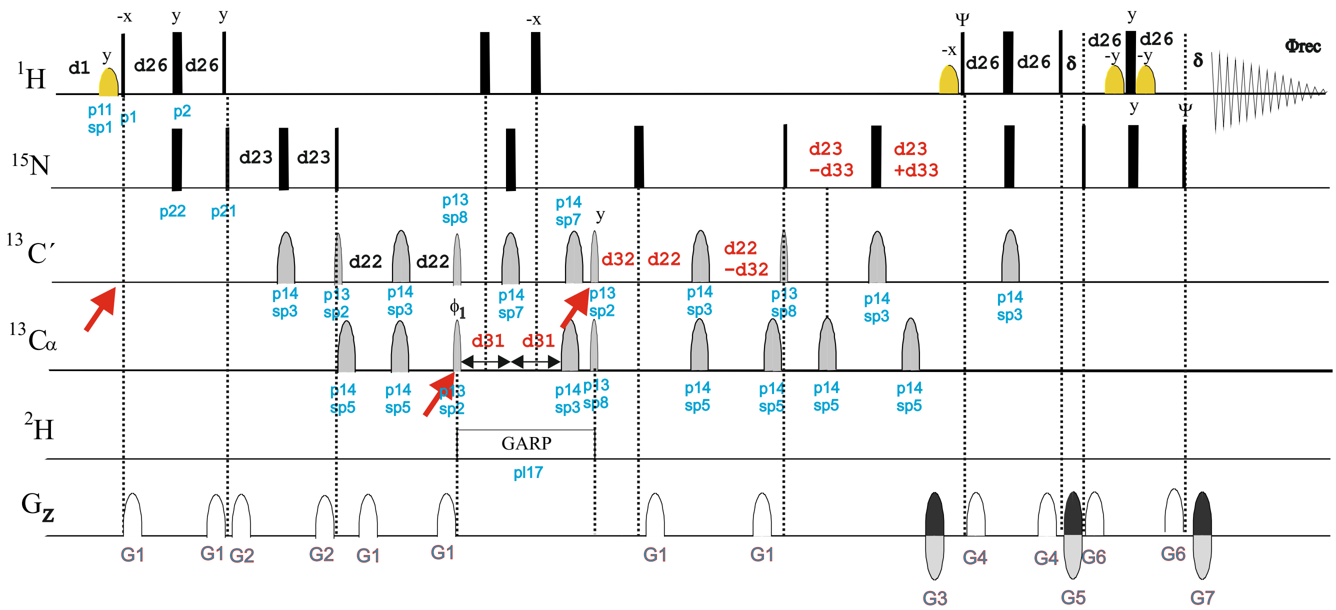
trhncocagp2h4d



trhncocaetgp4d



trhncocaetgp2h4d



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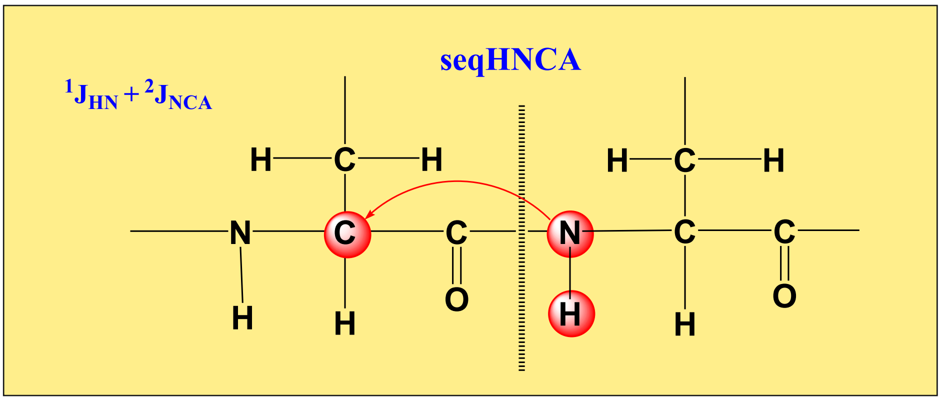
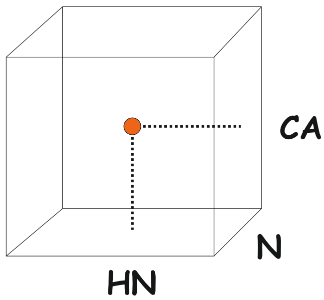
3D SEQUENTIAL HNCA

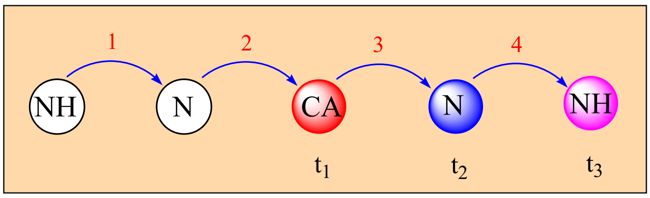
3D sequential-HNCA experiment

- 3D Sequential HNCA using TROSY (**seqtrhncagp3d** | SEQTRHNCAGP3D)
  - with ^{2}H-decoupling (**seqtrhncagp2h3d** | SEQTRHNCAGP2H3D)
  - with gradient echo-antiecho (**seqtrhncaetgp3d** | SEQTRHNCAETGP3D)
  - with gradient echo-antiecho and with ^{2}H-decoupling (**seqtrhncaetgp2h3d** | SEQTRHNCAETGP2H3D)

Also see: HNCA, intra-HNCA, HN(CO)CA



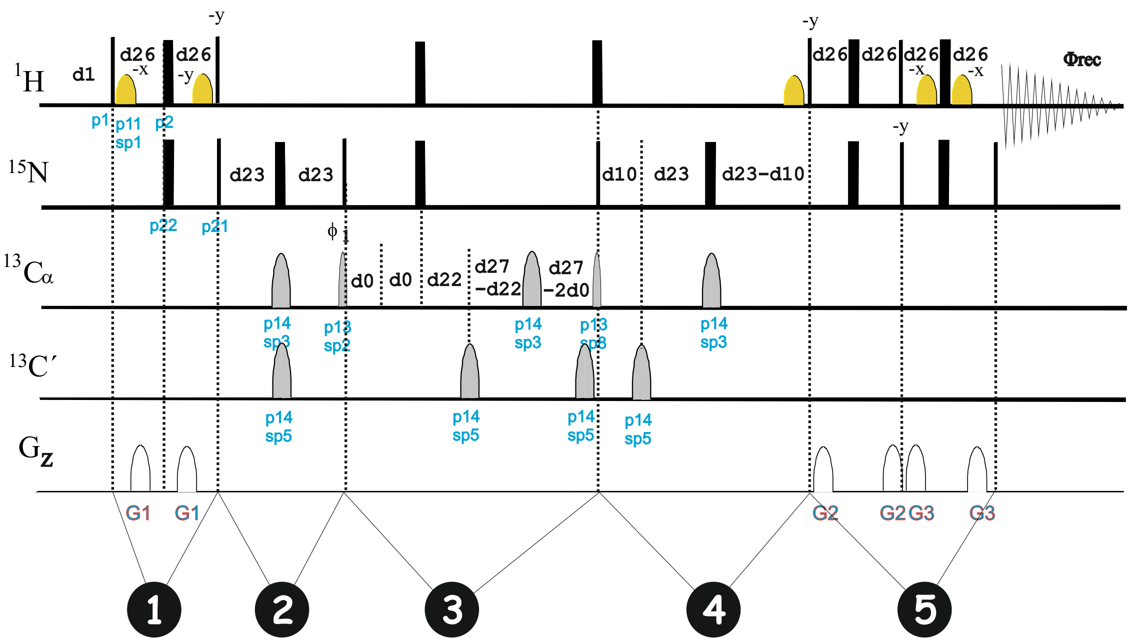




d26=1/4J(NH)=2.3m
d23=1/4J(NCA)=12m
d22=1/4J(CACO)=4.5m
d27=1/4J(CACB)=13.3m
d25=1/4J(NH)=2.3m

Identification of evolution elements

seqtrhncagp3d



1. 1H-15N INEPT transfer

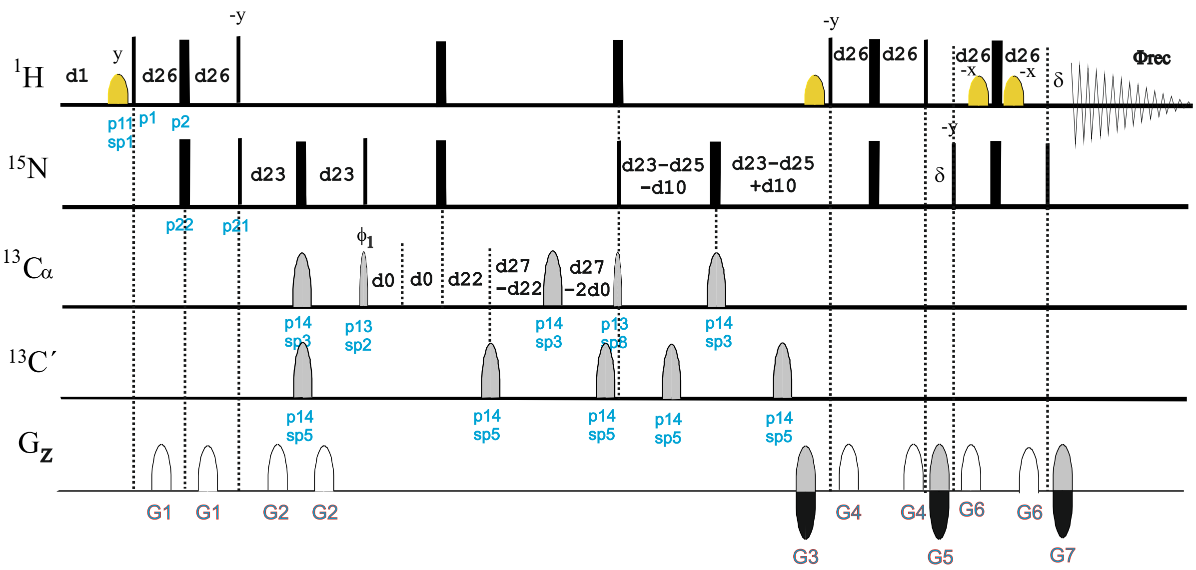
2. Concatenated Fixed period consisting of:
   J(NH) evolution
   INEPT 15N-CA
   INEPT 15N-CO

3. Concatenated Constant-time CA evolution period consisting of:
   δ(CA) evolution and J(CA-N) decoupling
   δ(CA) evolution and J(CA-H) decoupling
   δ(CA) evolution and J(CA-CO) refocusing

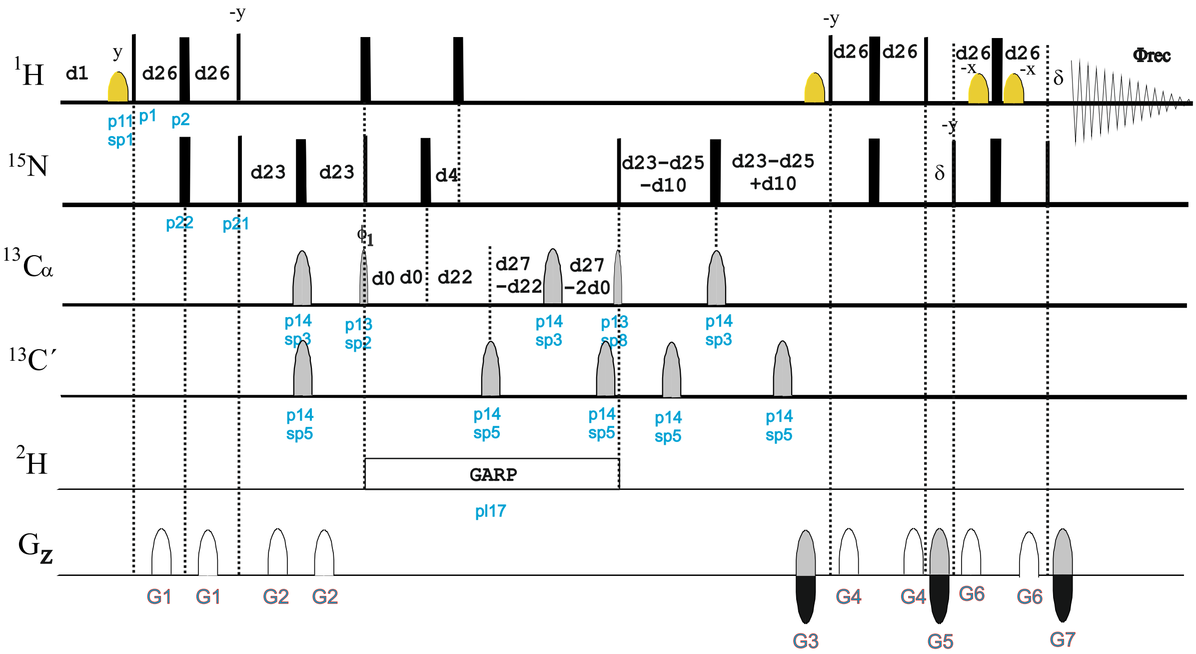
4. Concatenated Constant-time 15N evolution period consisting of:
   δ(N) evolution and J(N-H) evolution
   δ(N) evolution and J(N-CA) refocusing
   δ(N) evolution and J(N-CO) decoupling

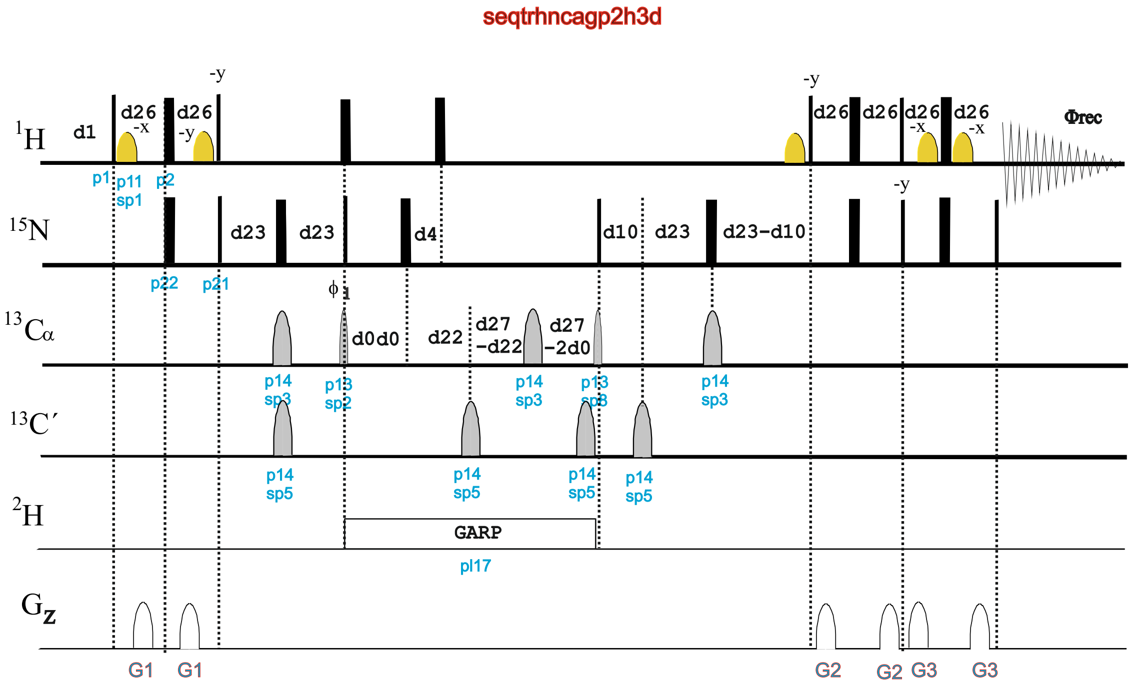
5. 1H-15N TROSY transfer consisting of two retro-INEPT like blocks

seqtrhncaetgp3d



seqtrhncaetgp2h3d




seqtrhncagp2h3d
1H
15N
13Cα
13C′
2H
Gz
d1
d26
d23
d4
d0
d22
d27
-d22
-2d0
d10
d23-d10
GARP
pl17
Φrec
p1
p11
sp1
p2
p22
p21
p14
sp3
sp5
p13
sp2
sp8
G1
G2
G3

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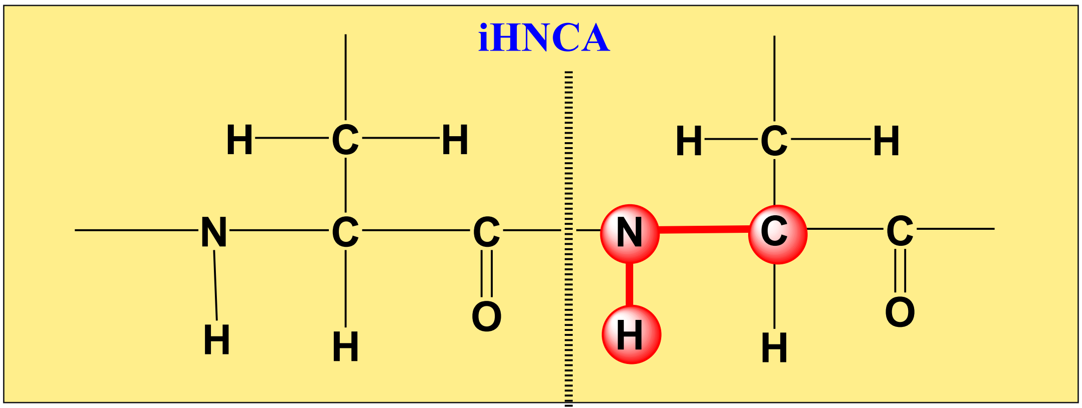
3D INTRA-HNCA

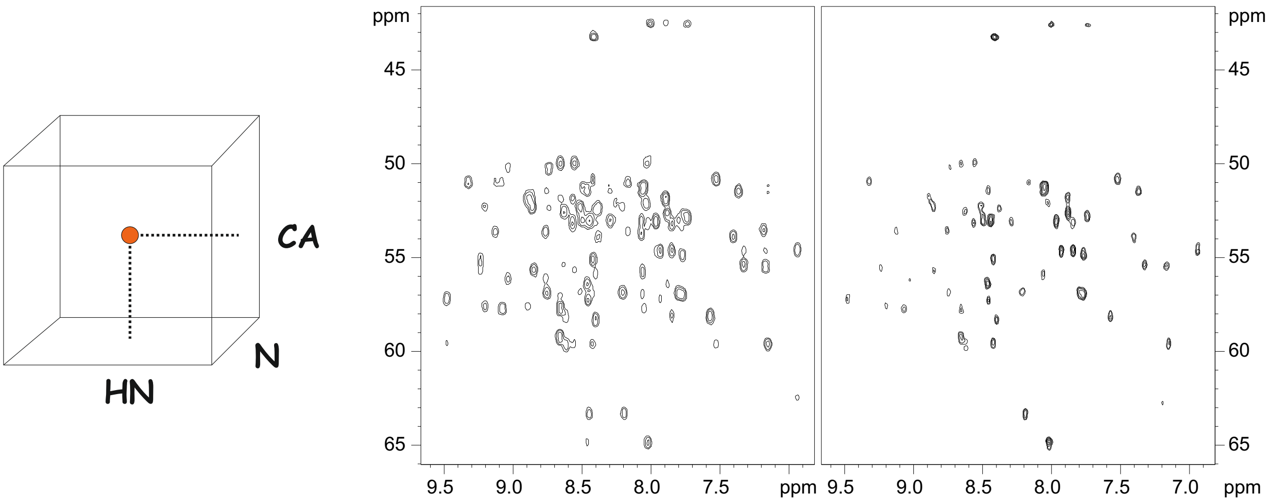
3D intra-HNCA experiment

- 3D Intra-HNCA using PEP (**hncaigp3d** | HNCAIGP3D)
  - with ^{2}H-decoupling (**hncaigp2h3d** | HNCAIGP2H3D)
- 3D Intra-HNCA using WATERGATE (**hncaigpwg3d** | HNCAIGPWG3D)
  - with ^{2}H-decoupling (**hncaigpwg2h3d** | HNCAIGPWG2H3D)
- 3D Intra-HNCA using TROSY (**trhncaigp3d** | TRHNCAIGP3D)
  - with ^{2}H-decoupling (**trhncaigp2h3d** | TRHNCAIGP2H3D)
  - with gradient echo-antiecho (**trhncaietgp3d** | TRHNCAIETGP3D)
  - with gradient echo-antiecho and with ^{2}H-decoupling (**trhncaietgp2h3d** | TRHNCAIETGP2H3D)

Also see:
3D SOFAST/BEST-intraHNCA experiment
3D BEST-intraHNCA (b_hncaigp3d | B_HNCAIGP3D)
3D BEST-intraHNCA using TROSY (b_trhncaigp3d)

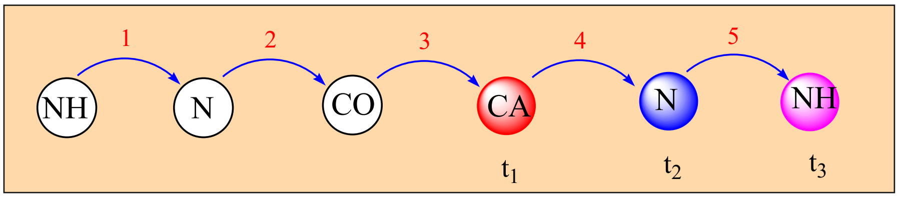
Related Experiments:
seq-HNCA, HNCA, HN(CO)CA





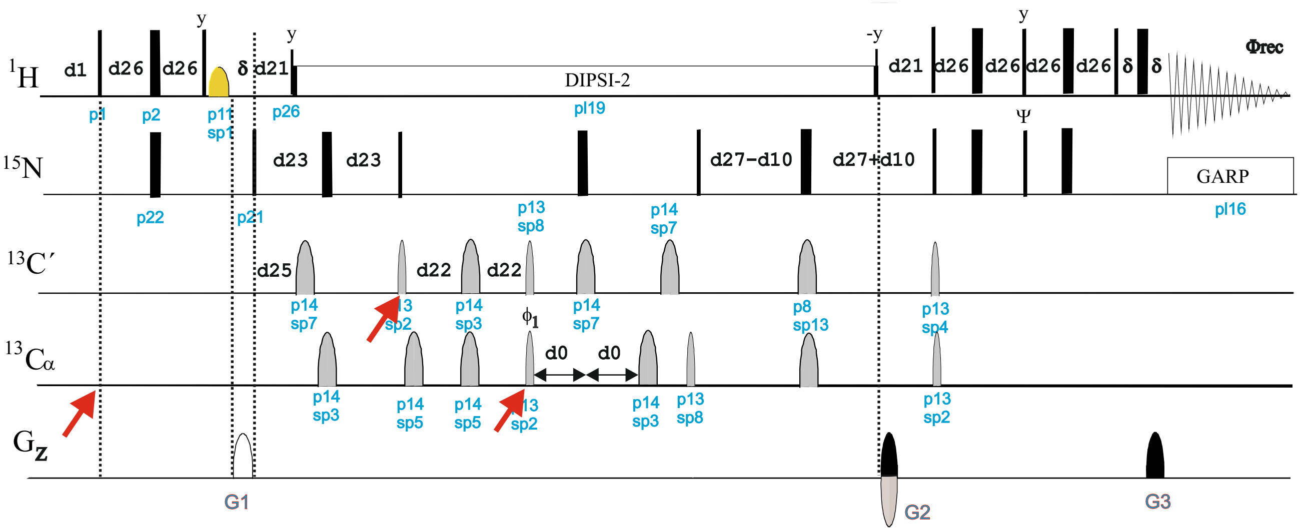
2D H(N)CA

2D intra-H(N)CA

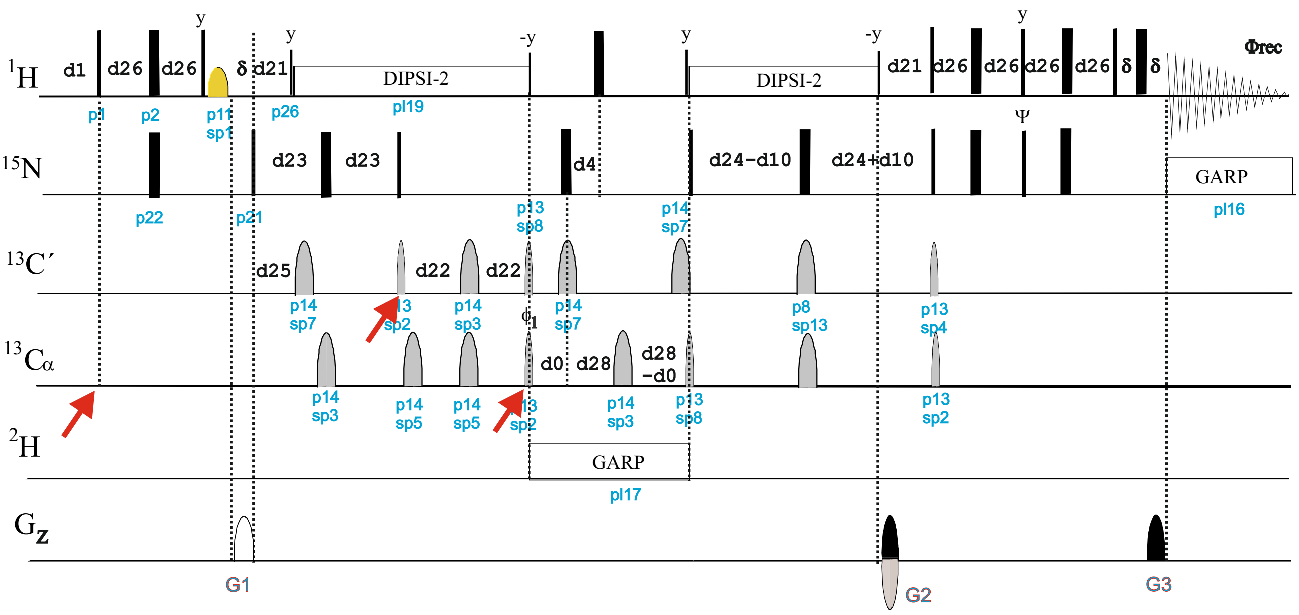


d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCA)=26m
d22=1/4J(CACO)=4.2m
d27=1/4J(NCA)&1/4J(NCO)=15.8m
d25=1/4J(NCO)=16.5m

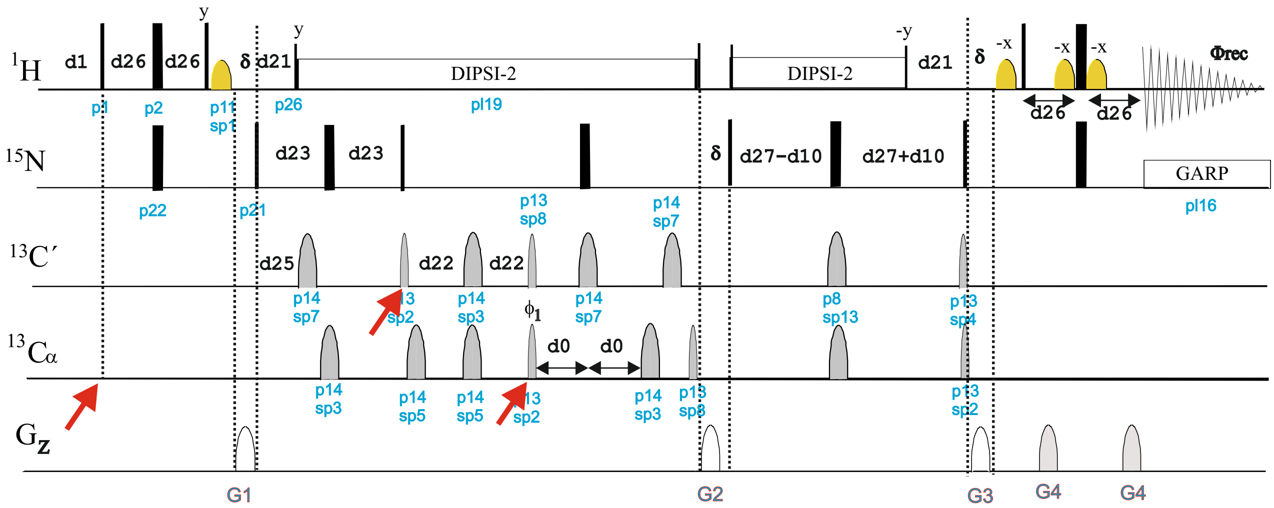
hncaigp3d



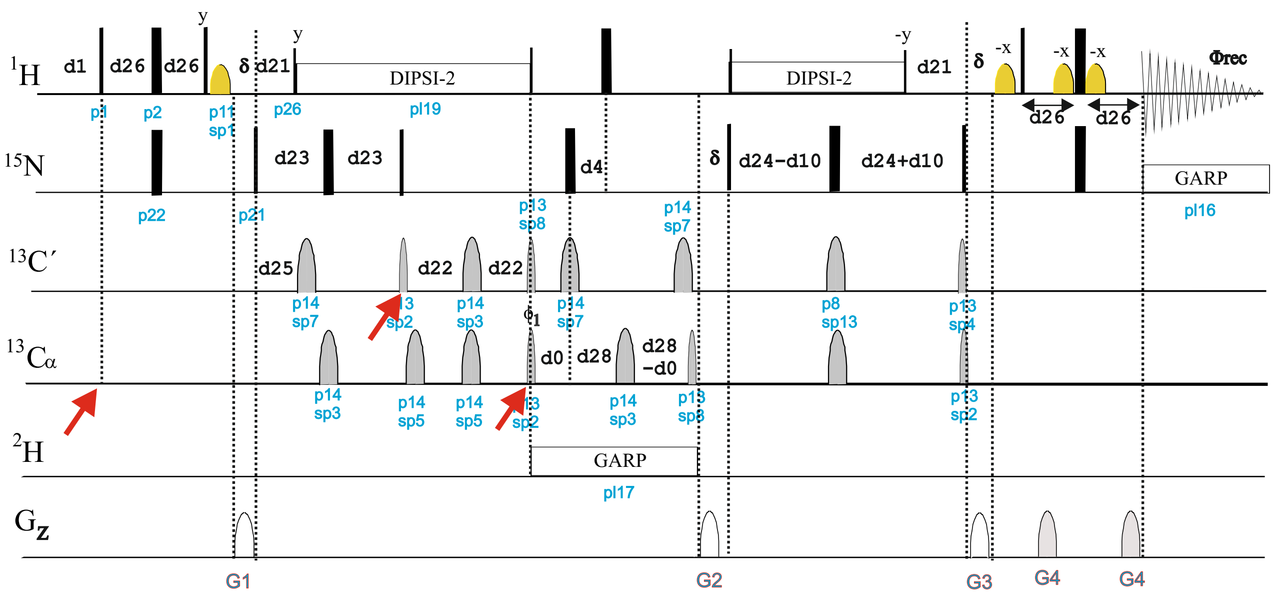
hncaigp2h3d



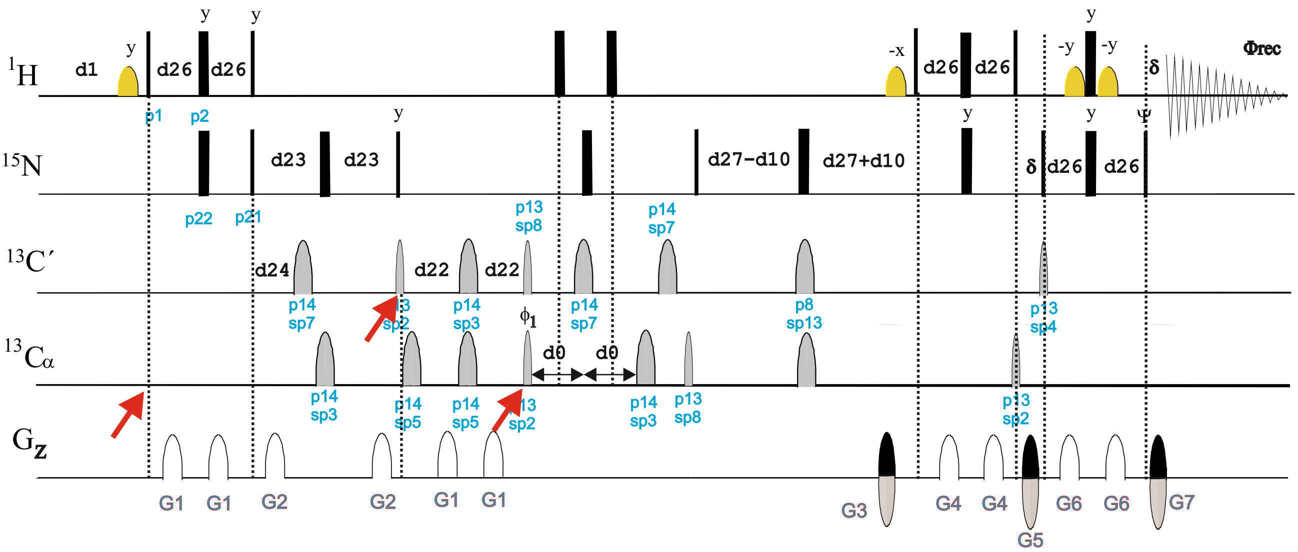
hncaigpwg3d



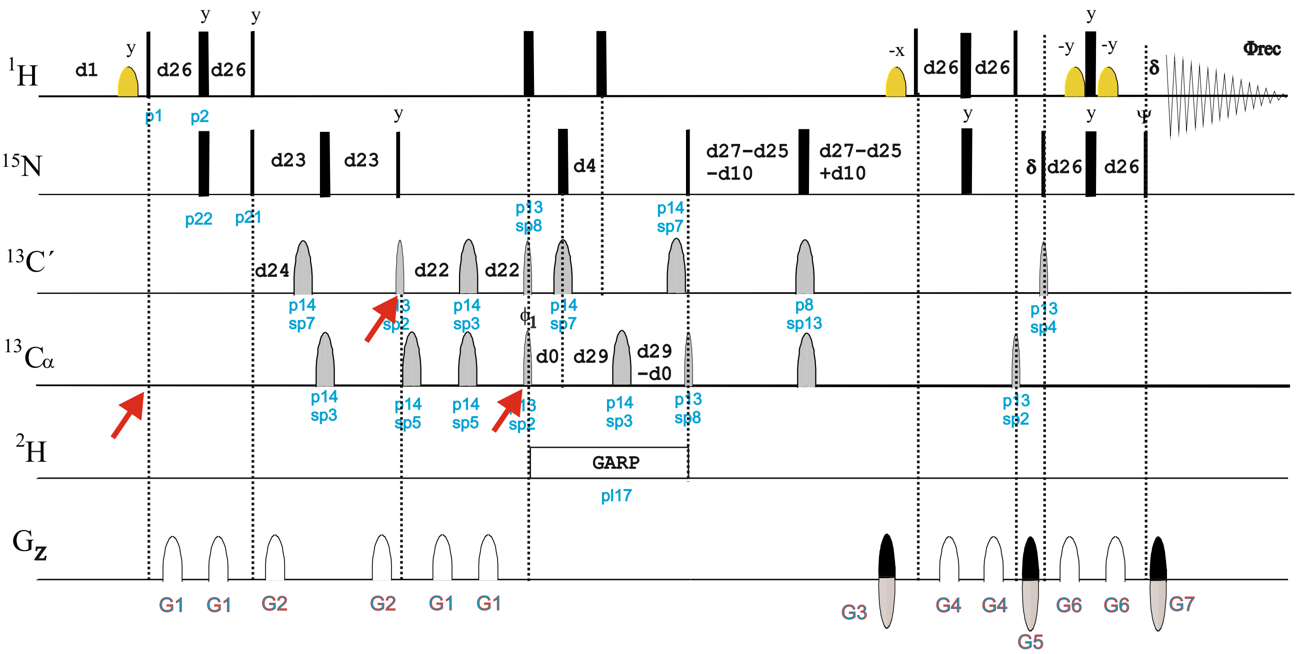
hncaigpwg2h3d



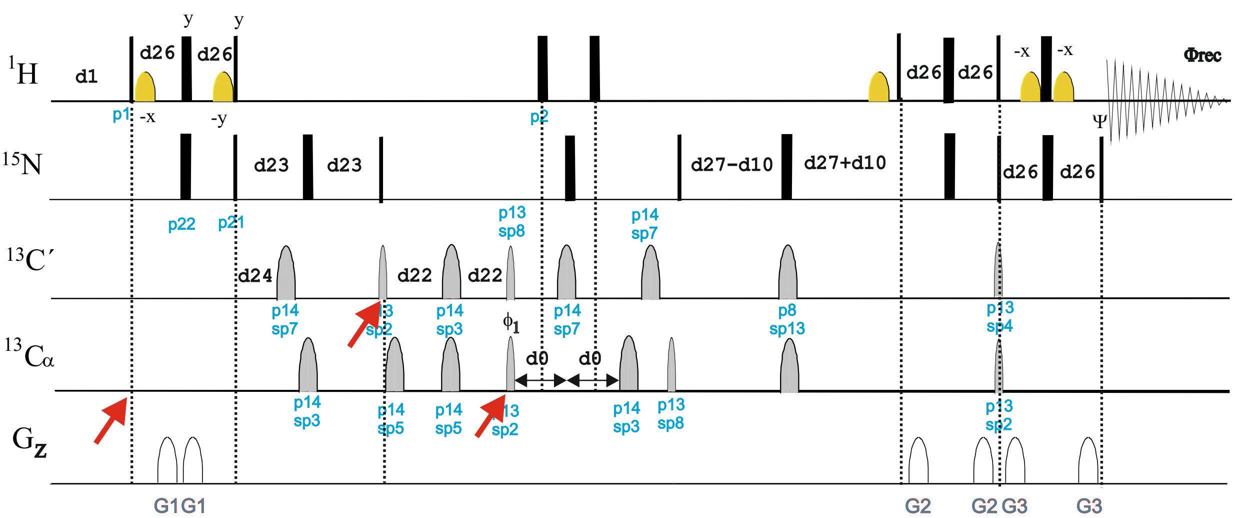
trhncaietgp3d



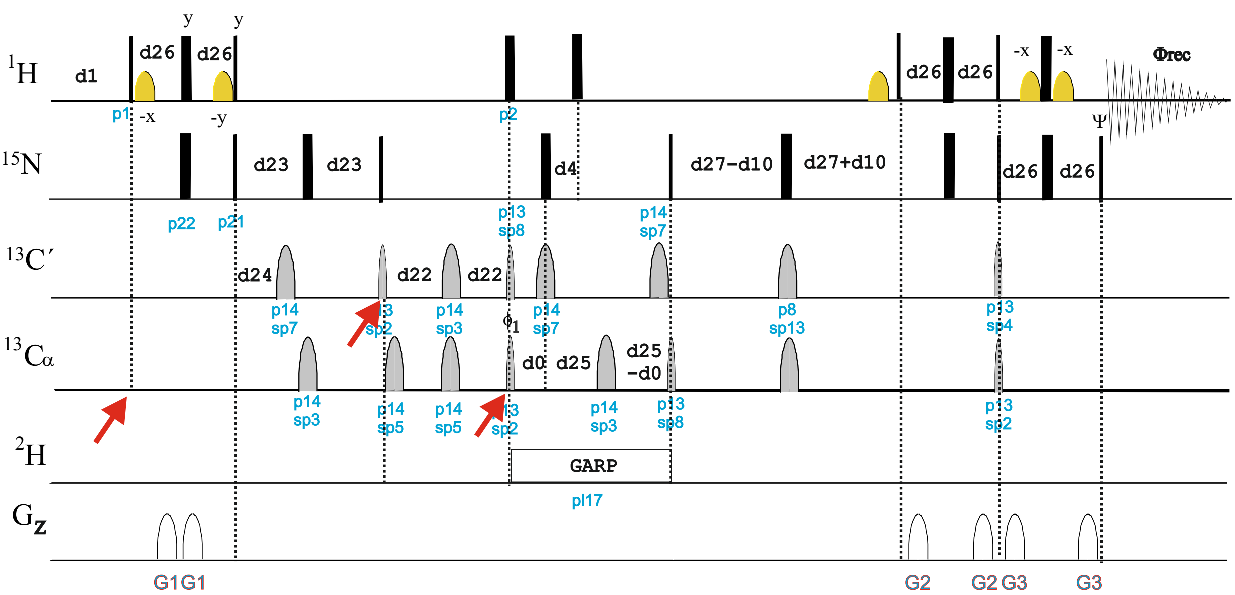
trhncaietgp2h3d



trhncaigp3d



trhncaigp2h3d



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3D HNCANNH

HNCANNH Experiment

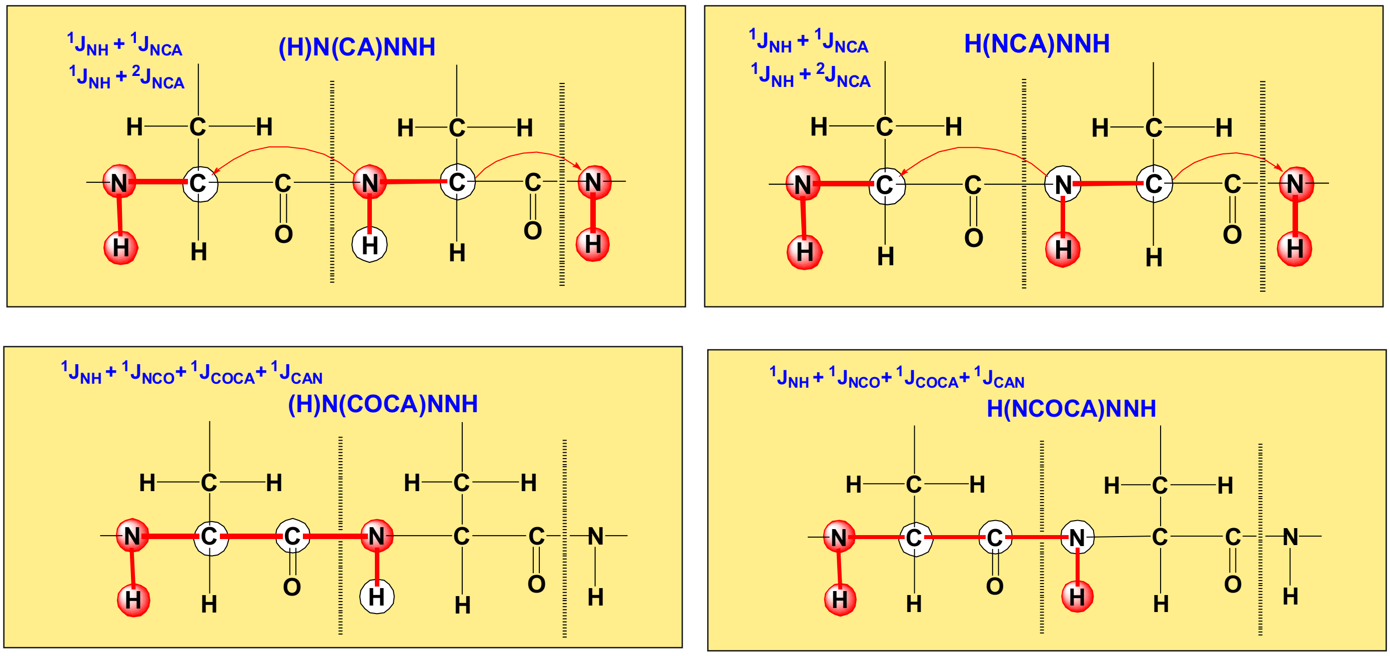
3D (H)N(CA)NNH experiment

- 3D (H)N(CA)NNH (**hncannhgp3d** | HNCANNHGP3D)
- 3D (H)N(CA)NNH with ^{2}H-decoupling (**hncannhgp2h3d** | HNCANNHGP2H3D)
- 3D (H)N(CA)NNH using WATERGATE (**hncannhgpwg3d**)
- 3D (H)N(CA)NNH using WATERGATE and ^{2}H-decoupling (**hncannhgpwg2h3d**)
- 3D (H)N(CA)NNH using TROSY (**trhncannhgp3d**)
- 3D (H)N(CA)NNH using TROSY and ^{2}H-decoupling (**trhncannhgp2h3d**)
- 3D (H)N(CA)NNH using TROSY and echo-antiecho (**trhncannhetgp3d**)
- 3D (H)N(CA)NNH using TROSY, echo-antiecho and ^{2}H-decoupling (**trhncannhetgp2h3d**)

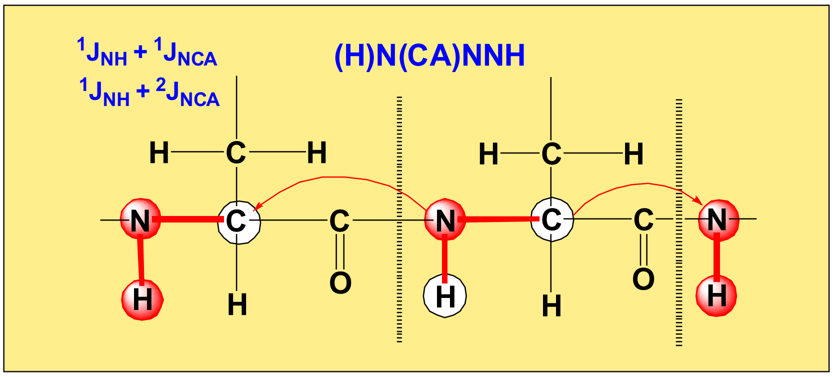
3D H(NCA)NNH experiment

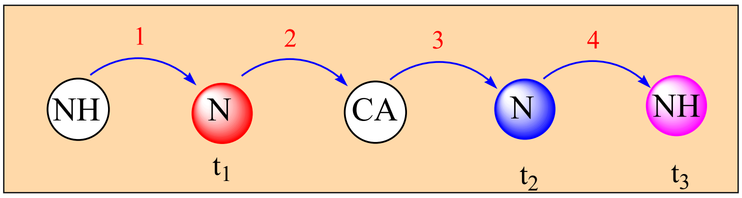
- 3D H(NCA)NNH (**hncannhgp3d.2**)
- 3D H(NCA)NNH with ^{2}H-decoupling (**hncannhgp2h3d.2**)
- 3D H(NCA)NNH using WATERGATE (**hncannhgpwg3d.2**)
- 3D H(NCA)NNH using WATERGATE and ^{2}H-decoupling (**hncannhgpwg2h3d.2**)
- 3D H(NCA)NNH using TROSY (**trhncannhgp3d.2**)
- 3D H(NCA)NNH using TROSY and ^{2}H-decoupling (**trhncannhgp2h3d.2**)
- 3D H(NCA)NNH using TROSY and echo-antiecho (**trhncannhetgp3d.2**)
- 3D H(NCA)NNH using TROSY, echo-antiecho and ^{2}H-decoupling (**trhncannhetgp2h3d.2**)

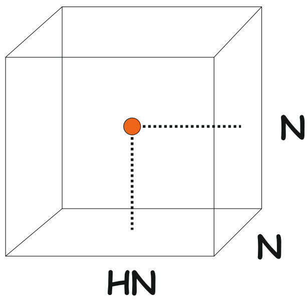
Also see:
HNCOCANNH Experiment

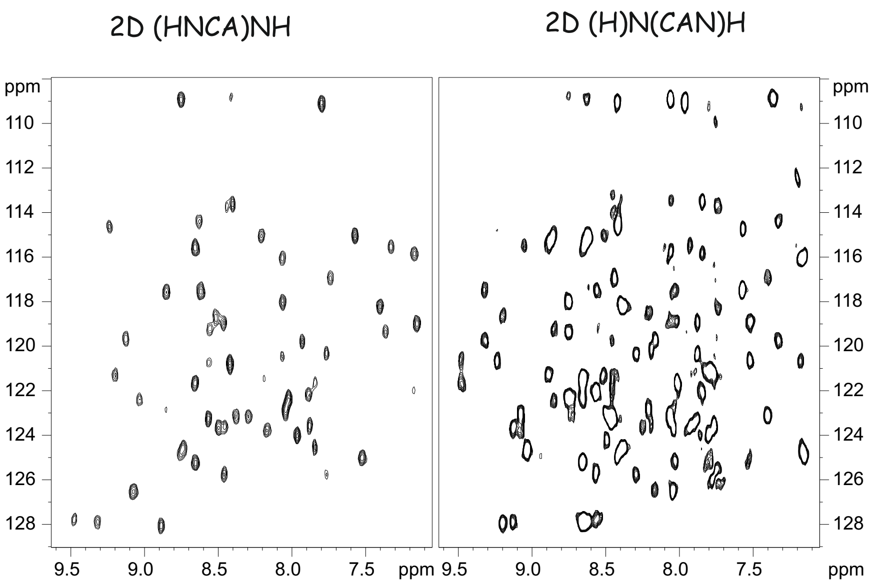


R. Weisemann, H. Rueterjans & W. Bermel, J. Biomol. NMR 3, 113-120 (1993)

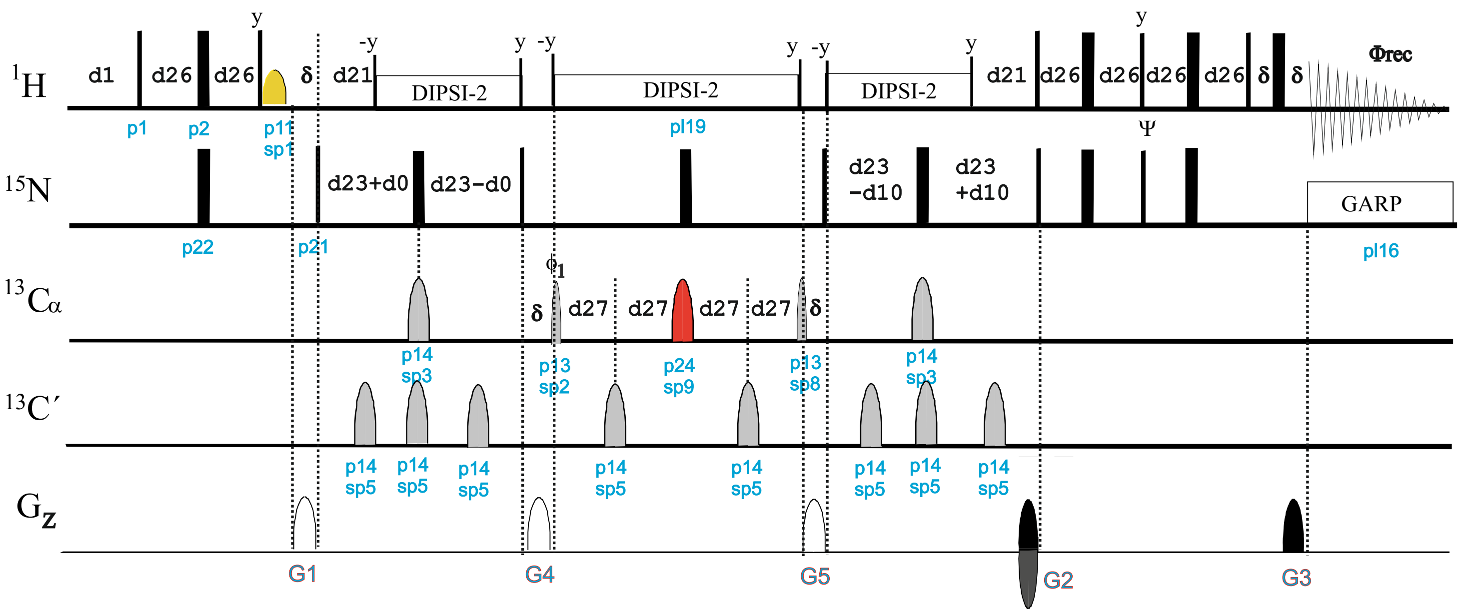






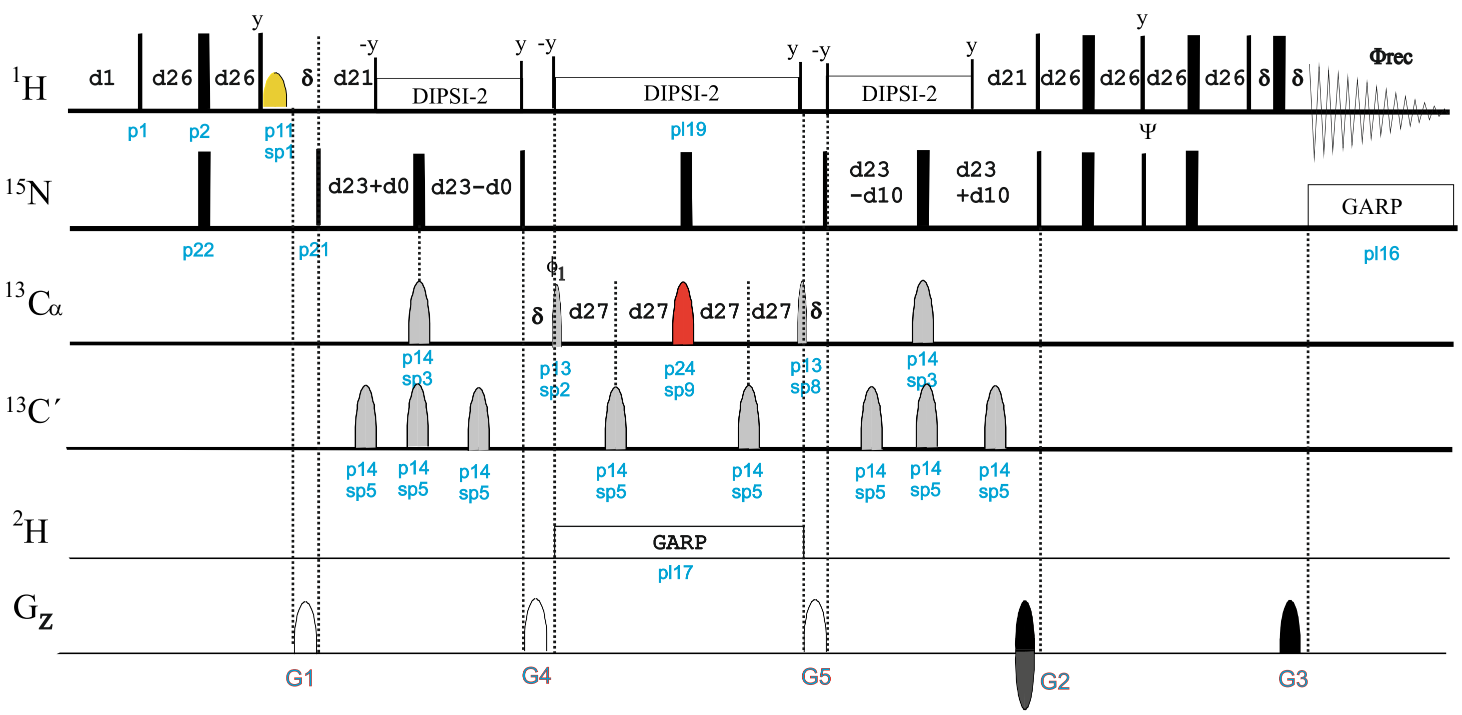


hncannhgp3d

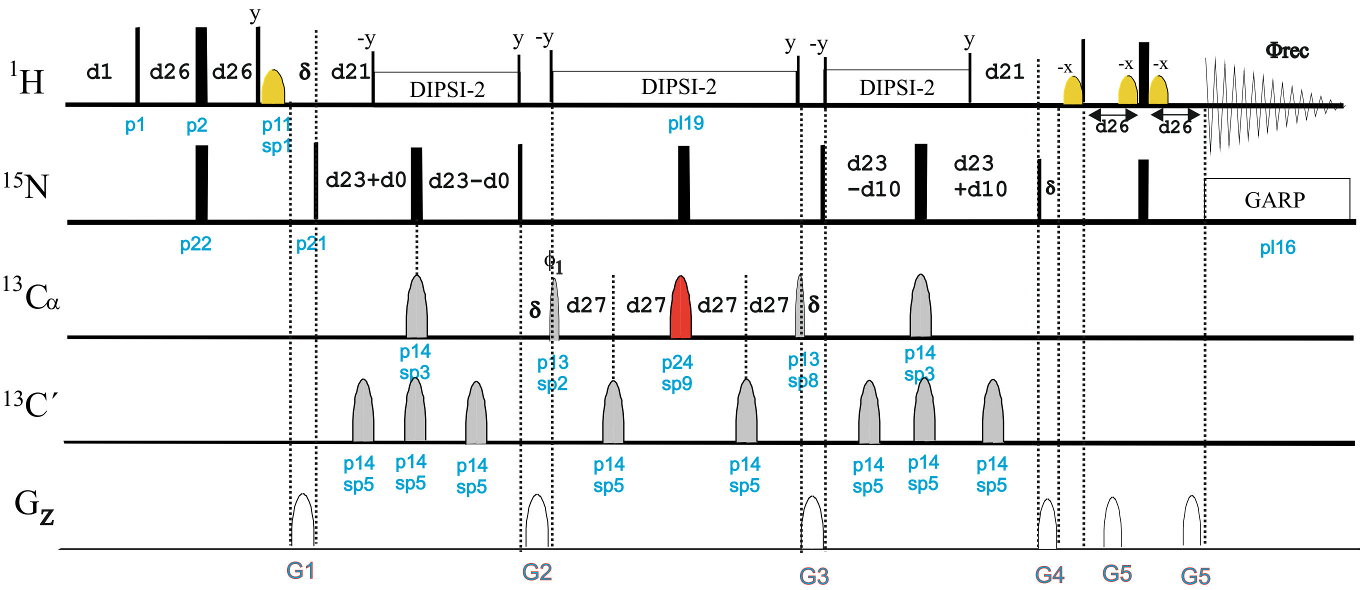


d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d26: 1/(4J'(NH)	[2.3 msec]
d27: 1/(4J`(NCa)	[12.5 msec]

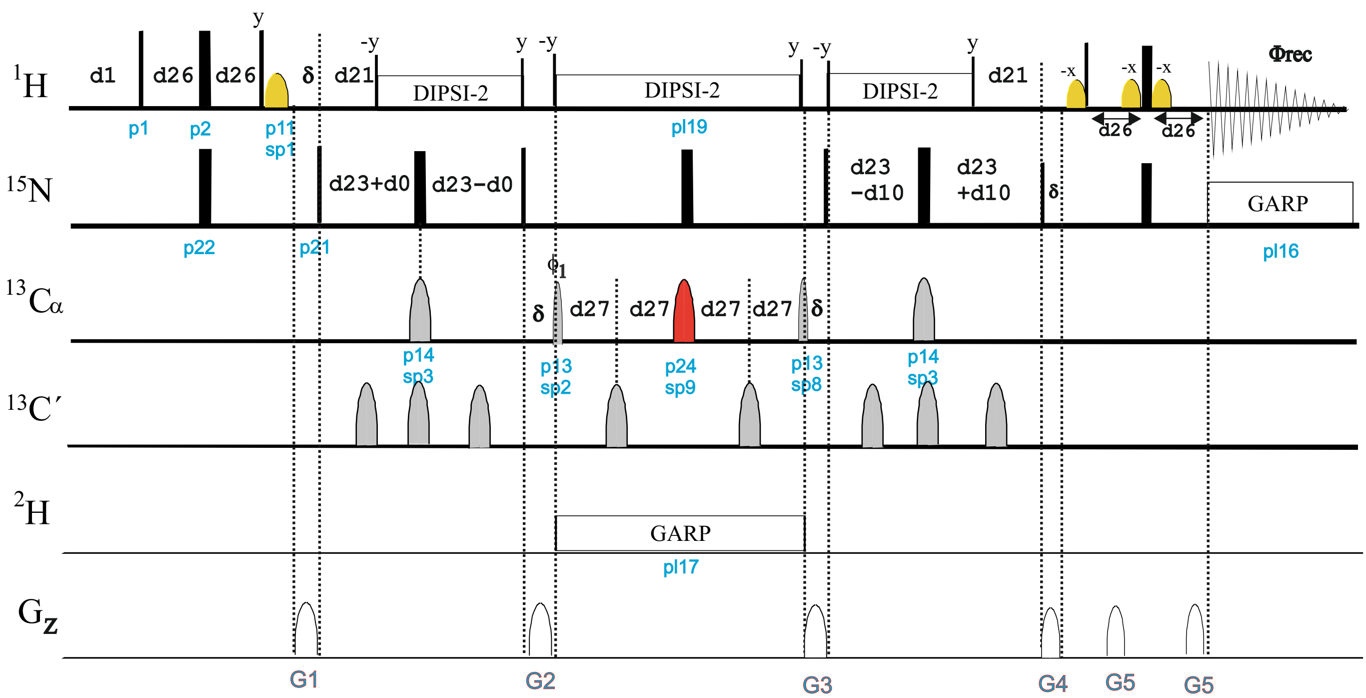
hncannhgp2h3d



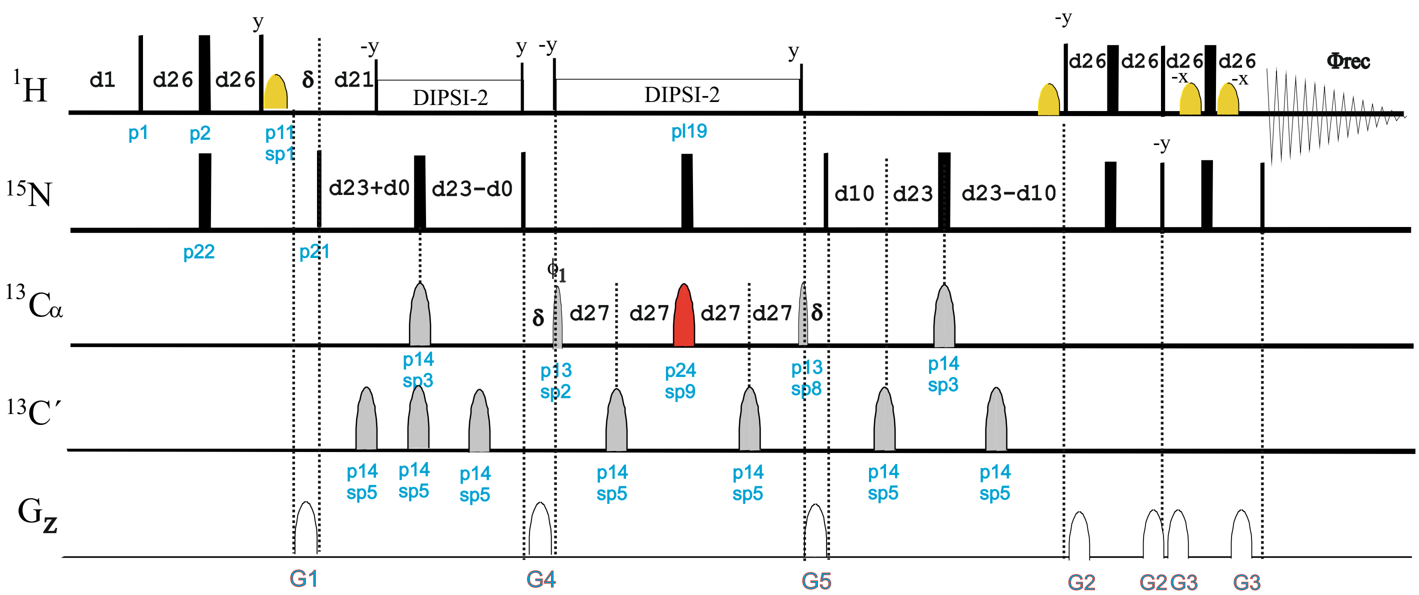
hncannhgpwg3d



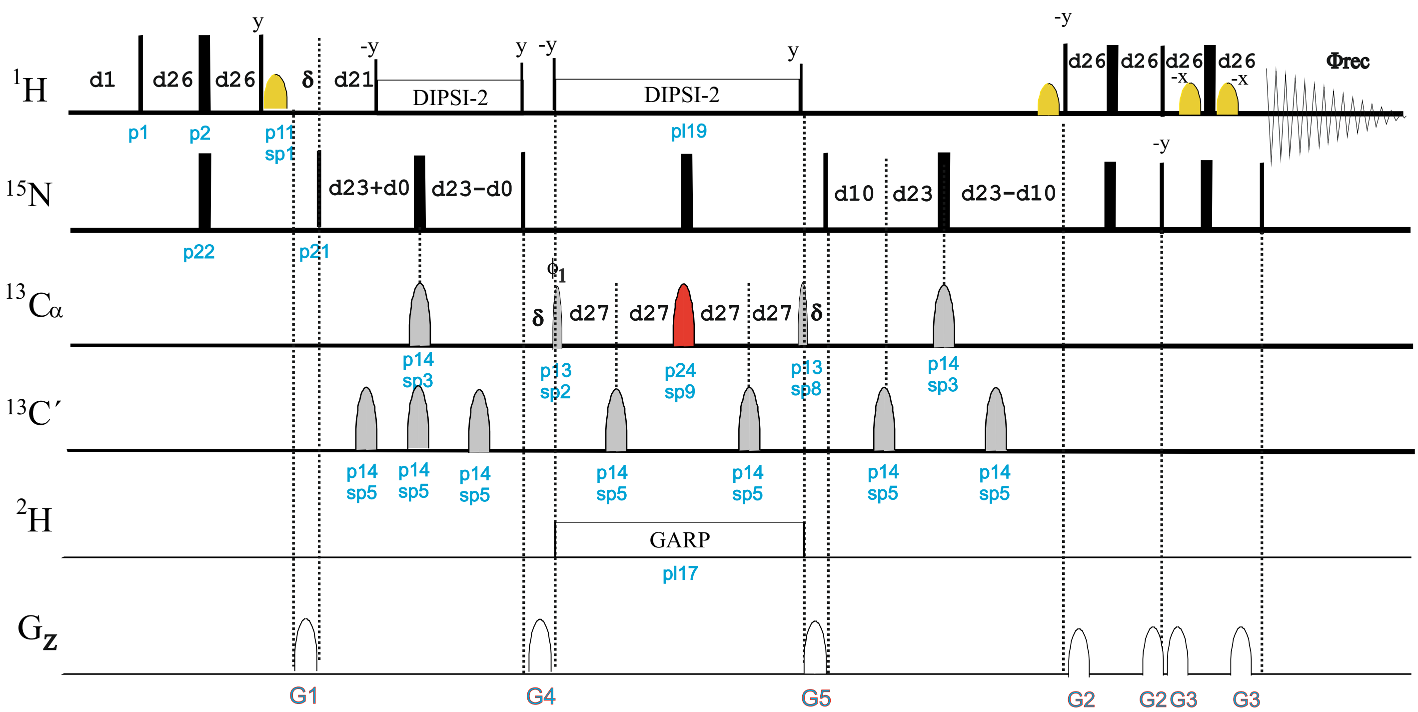
hncannhgpwg2h3d



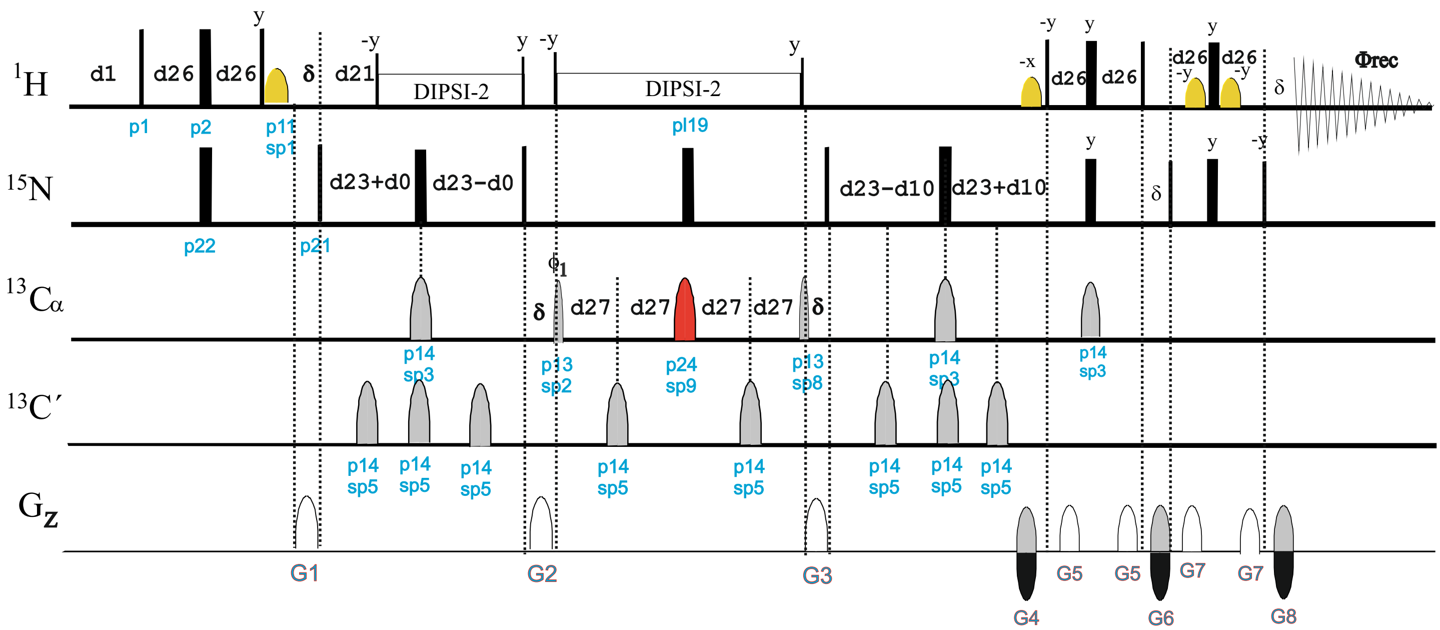
trhncannhgp3d



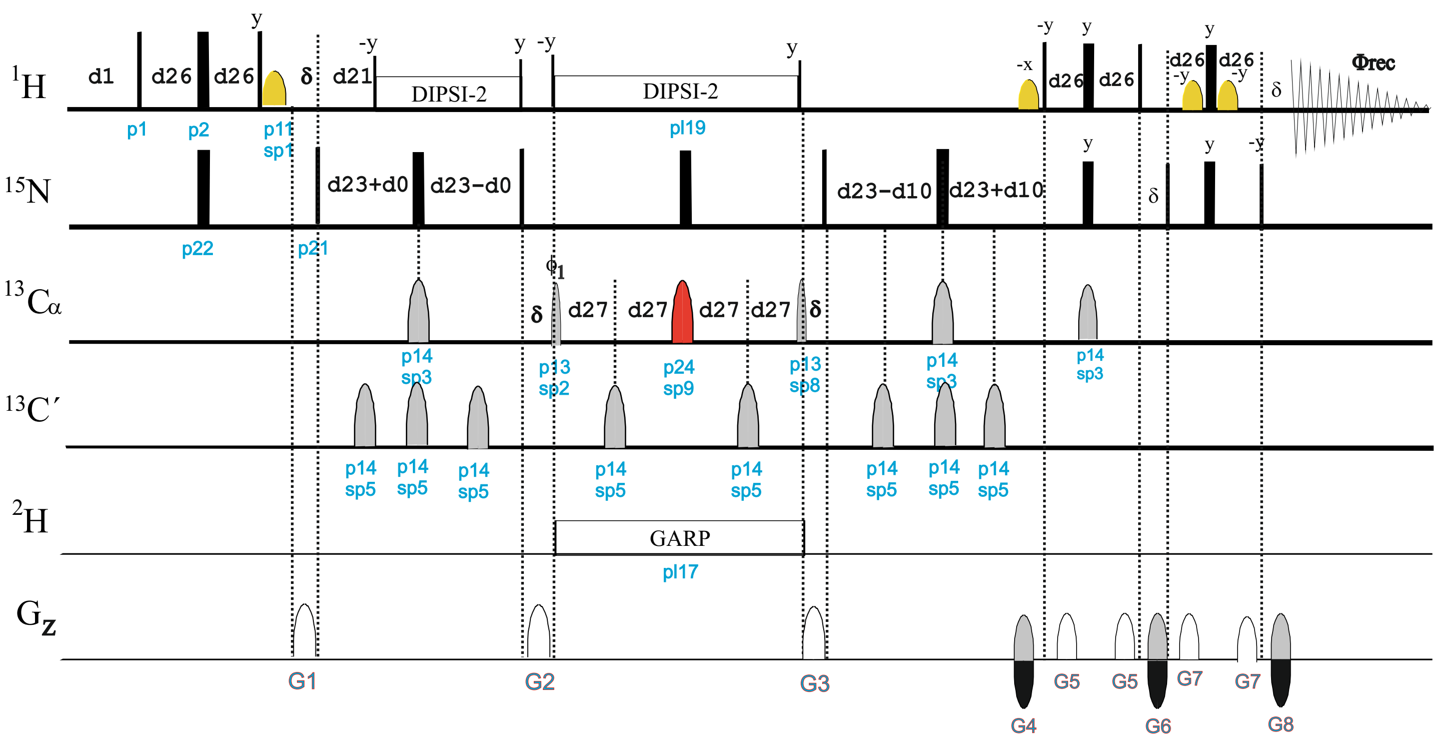
trhncannhgp2h3d

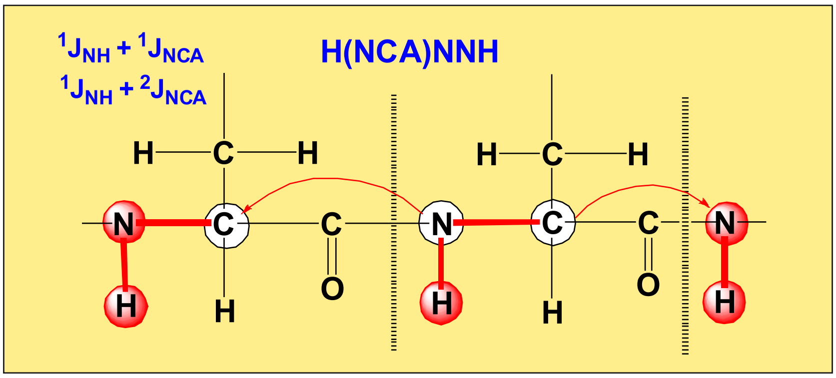


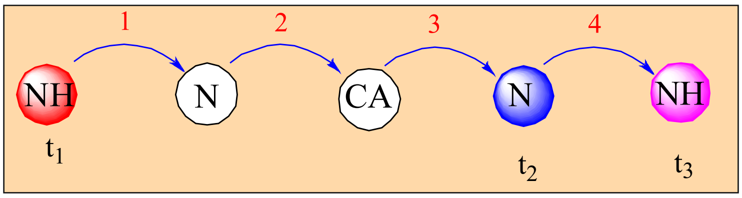
trhncannhetgp3d

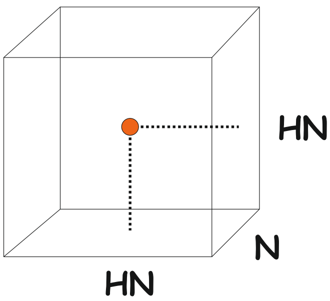


trhncannhetgp2h3d

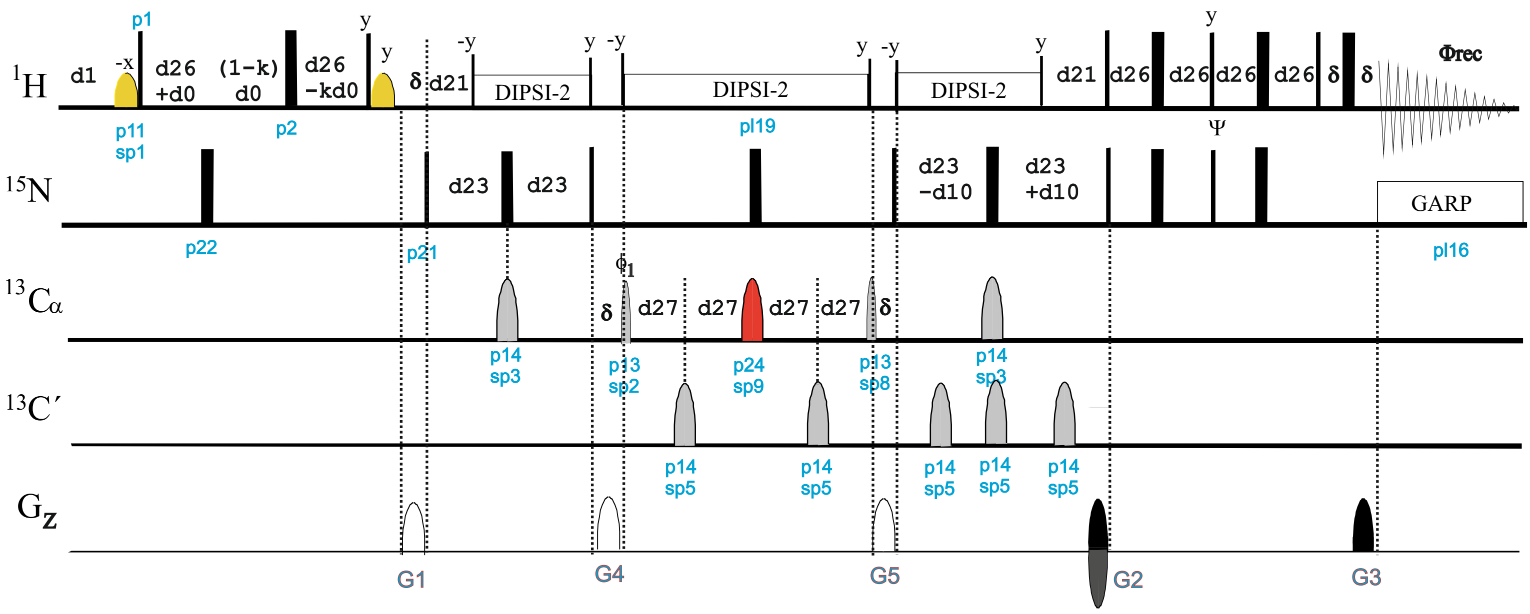



$^1J_{NH} + {}^1J_{NCA}$
$^1J_{NH} + {}^2J_{NCA}$
H(NCA)NNH

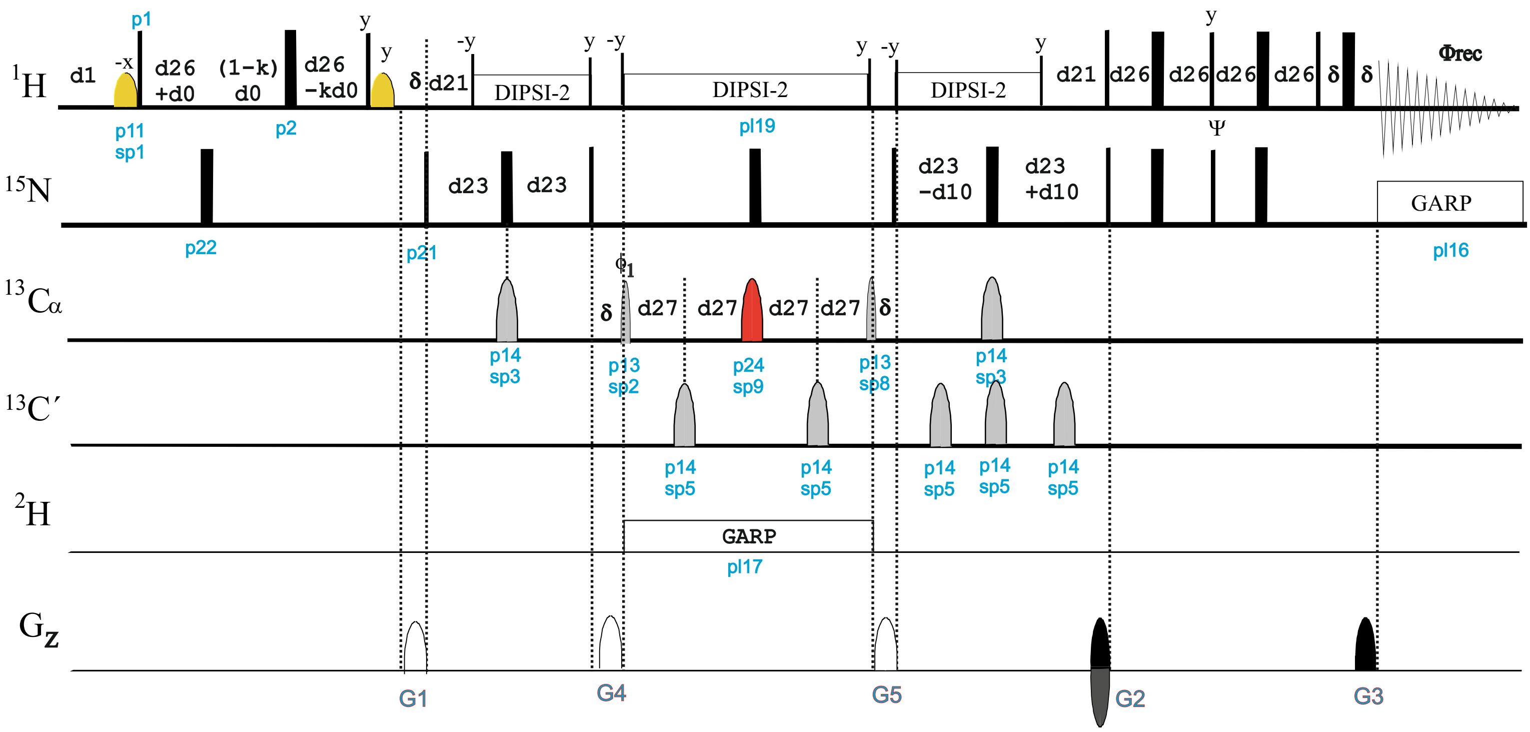

1
2
3
4
NH
N
CA
N
NH
t_1
t_2
t_3


HN
N
HN

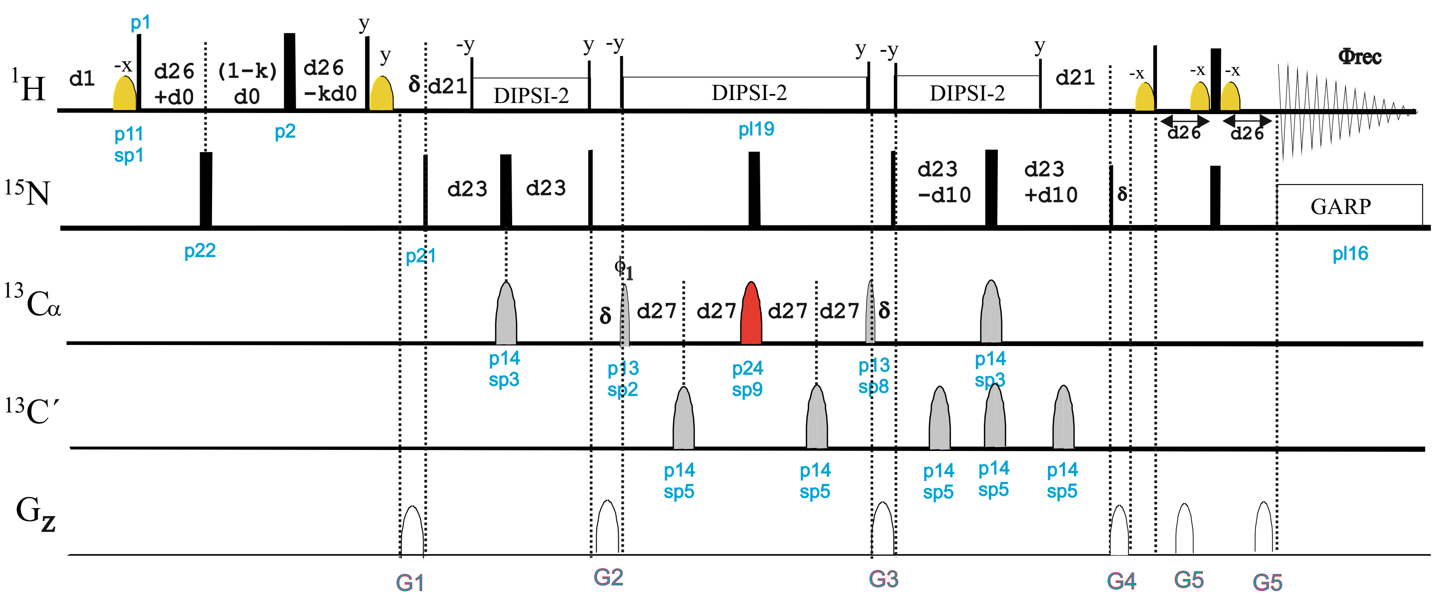
hncannhgp3d.2



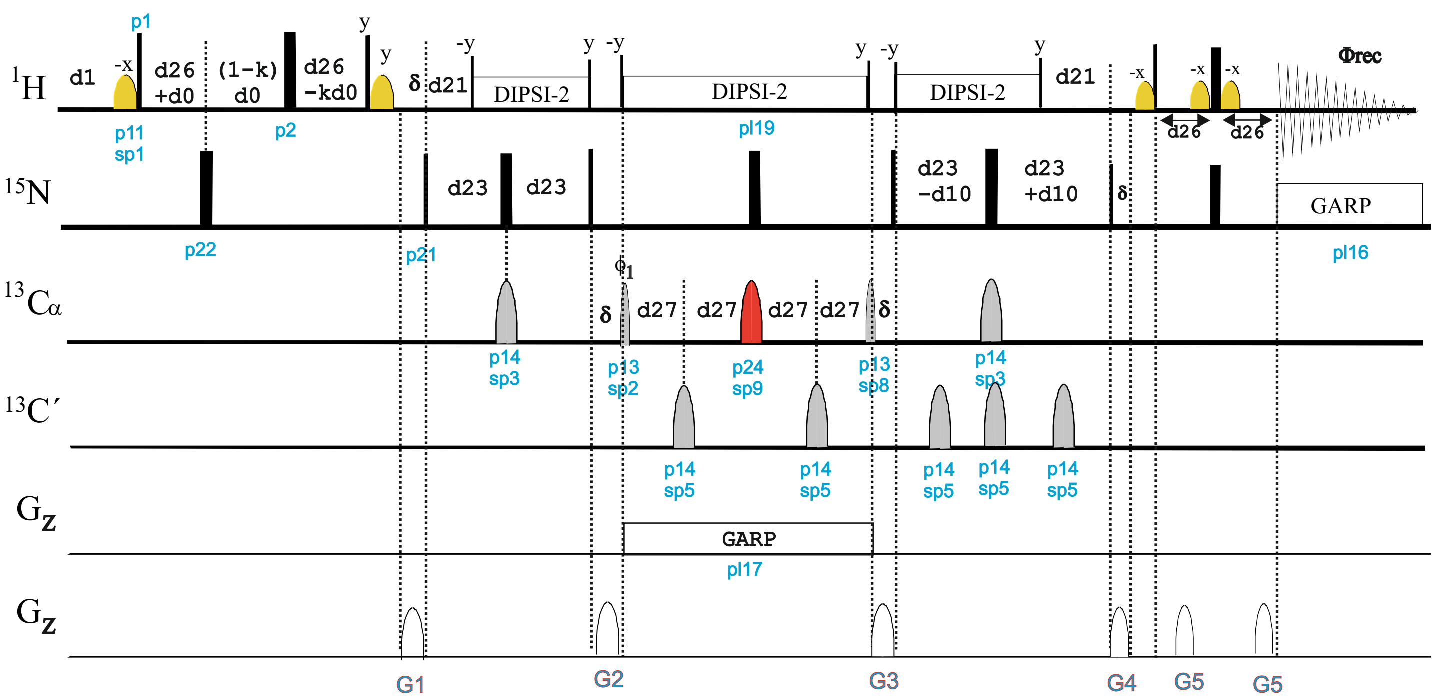
hncannhgp2h3d.2



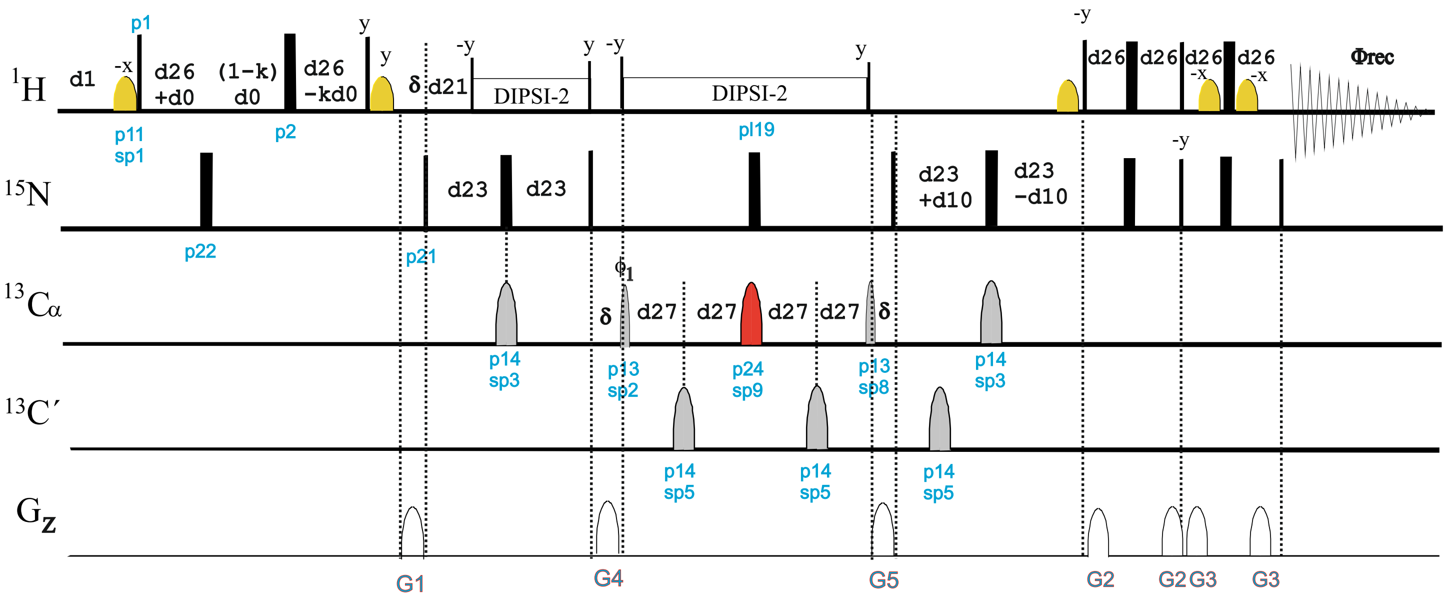
hncannhgpwg3d.2



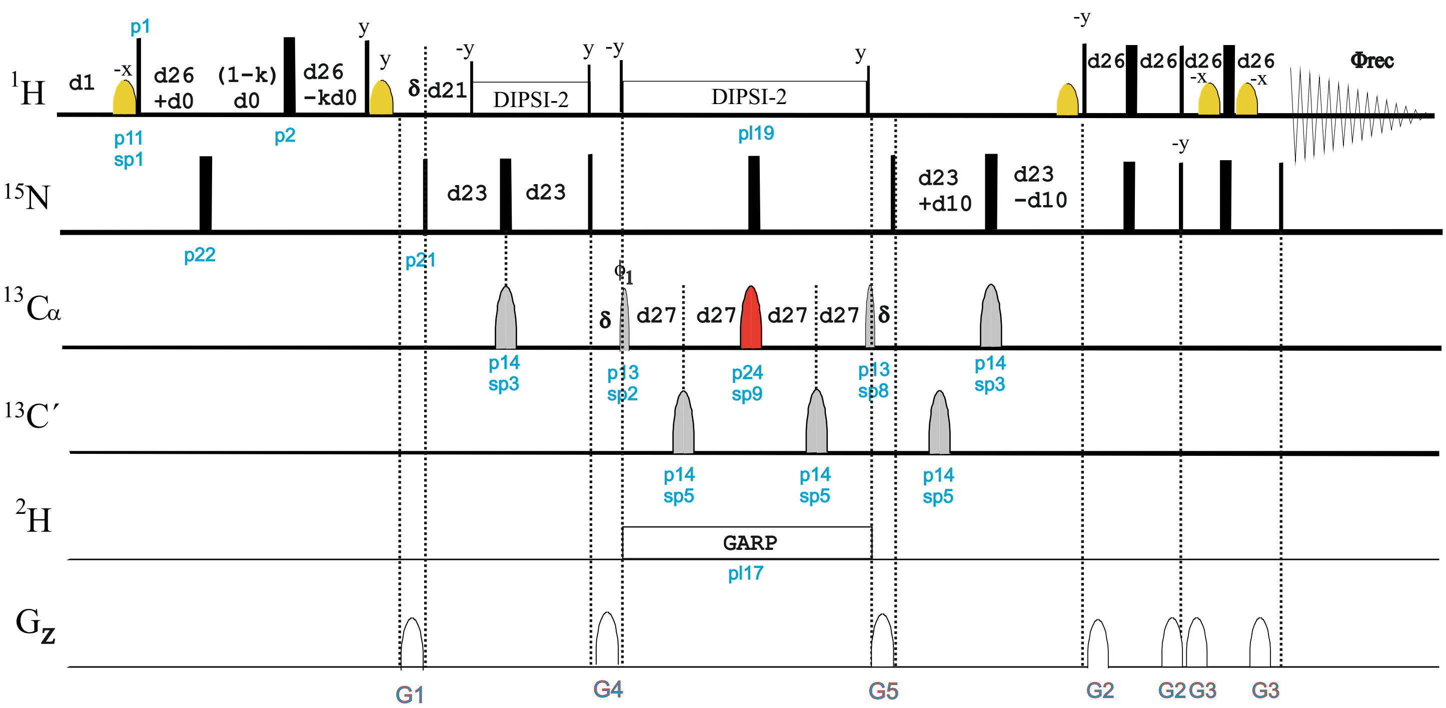
hncannhgpwg2h3d.2



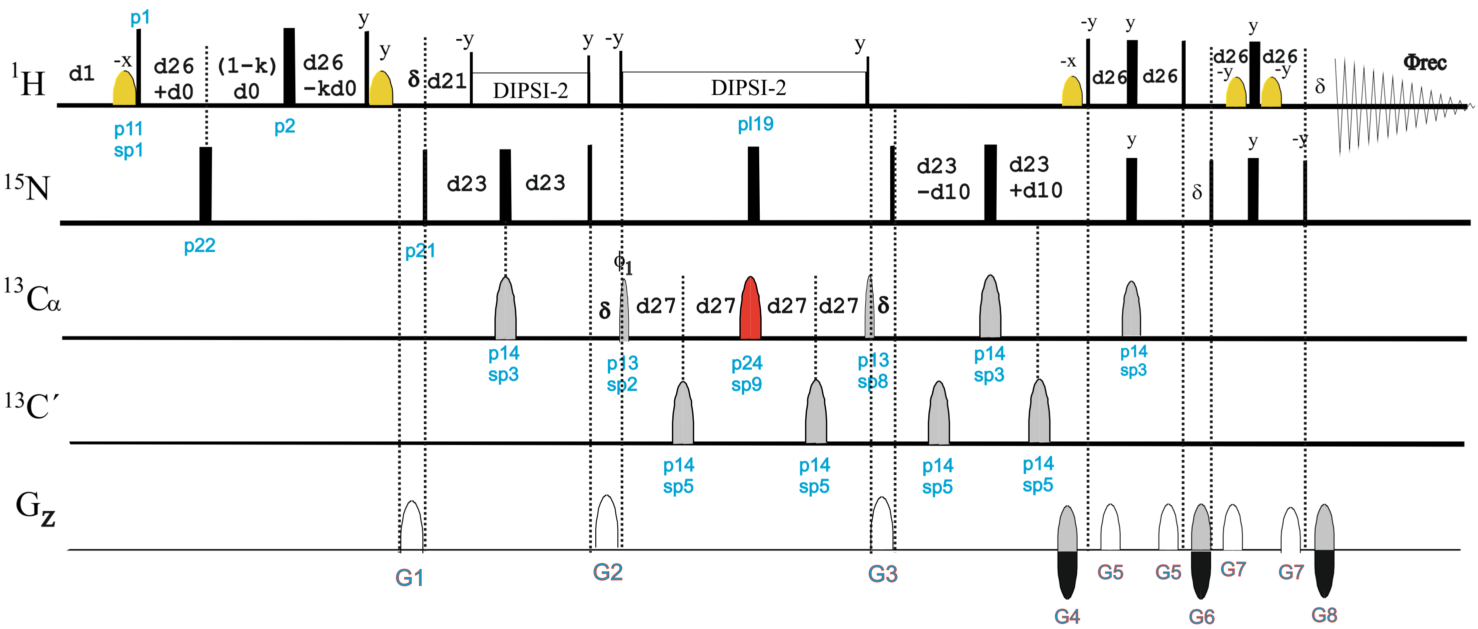
trhncannhgp3d.2



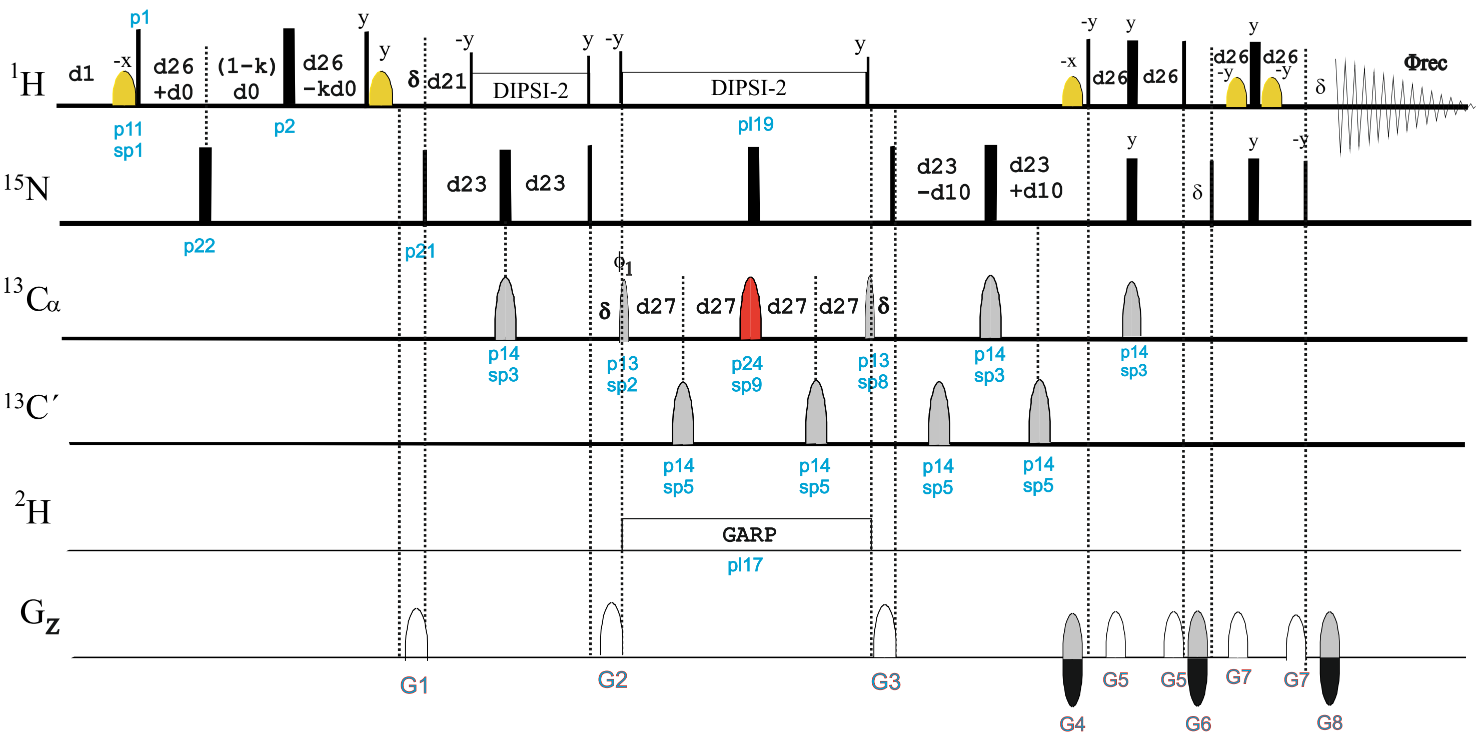
trhncannhgp2h3d.2



trhncannhetgp3d.2



trhncannhetgp2h3d.2



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3D HNCOCANNH

HNCOCANNH Experiment

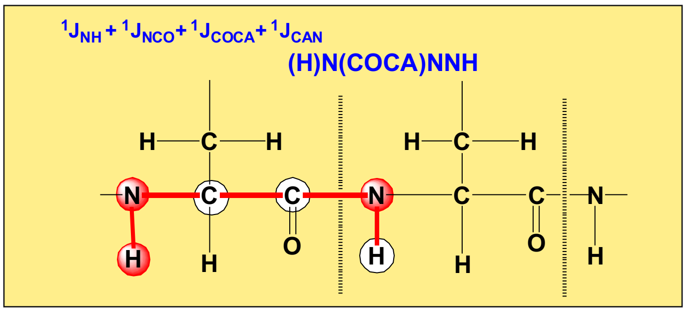
3D (H)N(COCA)NNH experiment

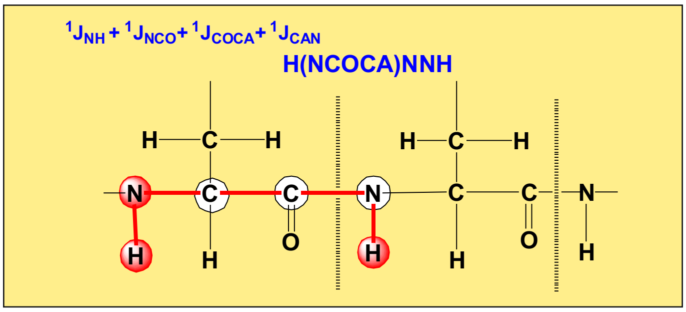
- 3D (H)N(COCA)NNH (**hncocannhgp3d**)
- 3D (H)N(COCA)NNH with ^{2}H-decoupling (**hncocannhgp2h3d**)
- 3D (H)N(COCA)NNH using WATERGATE (**hncocannhgpwg3d**)
- 3D (H)N(COCA)NNH using WATERGATE and ^{2}H-decoupling (**hncocannhgpwg2h3d**)
- 3D (H)N(COCA)NNH using TROSY (**trhncocannhgp3d**)
- 3D (H)N(COCA)NNH using TROSY and ^{2}H-decoupling (**trhncocannhgp2h3d**)
- 3D (H)N(COCA)NNH using TROSY and echo-antiecho (**trhncocannhetgp3d**)
- 3D (H)N(COCA)NNH using TROSY, echo-antiecho and ^{2}H-decoupling (**trhncocannhetgp2h3d**)

3D H(NCOCA)NNH experiment

- 3D H(NCOCA)NNH (**hncocannhgp3d.2**)
- 3D H(NCOCA)NNH with ^{2}H-decoupling (**hncocannhgp2h3d.2**)
- 3D H(NCOCA)NNH using WATERGATE (**hncocannhgpwg3d.2**)
- 3D H(NCOCA)NNH using WATERGATE and ^{2}H-decoupling (**hncocannhgpwg2h3d.2**)
- 3D H(NCOCA)NNH using TROSY (**trhncocannhgp3d.2**)
- 3D H(NCOCA)NNH using TROSY and ^{2}H-decoupling (**trhncocannhgp2h3d.2**)
- 3D H(NCOCA)NNH using TROSY and echo-antiecho (**trhncocannhetgp3d.2**)
- 3D H(NCOCA)NNH using TROSY, echo-antiecho and ^{2}H-decoupling (**trhncocannhetgp2h3d.2**)

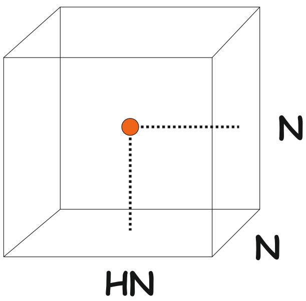
Also see:
HNCANNH Experiment

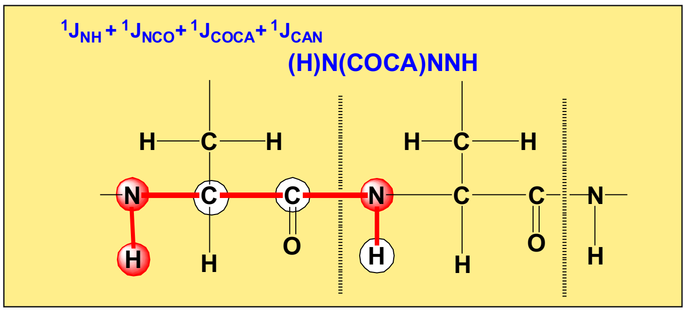




References:

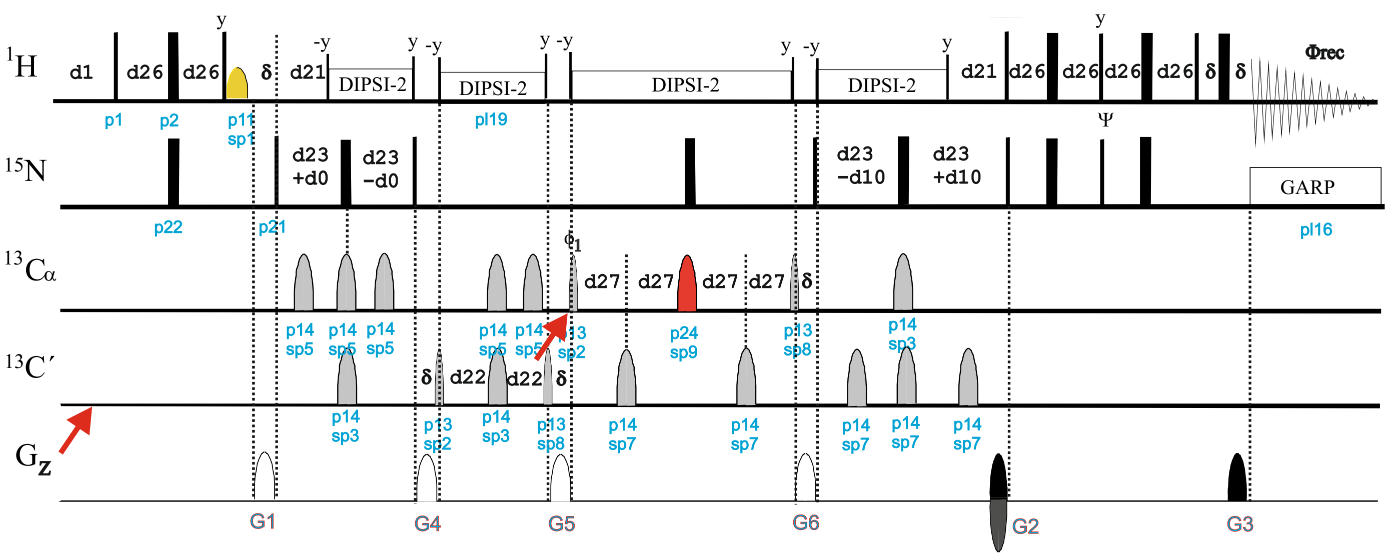
1. C. Bracken, A.G. Palmer & J. Cavanagh, J. Biomol. NMR 9, 94-100 (1997)
2. S.C. Panchal, N.S. Bhavesh & R.V. Hosur, J. Biomol. NMR 20, 135-147 (2001)
3. Z.-Y. J. Sun, D.P. Frueh, P. Selenko, J.C. Hoch & G. Wagner, J. Biomol. NMR 33, 43-50 (2005)



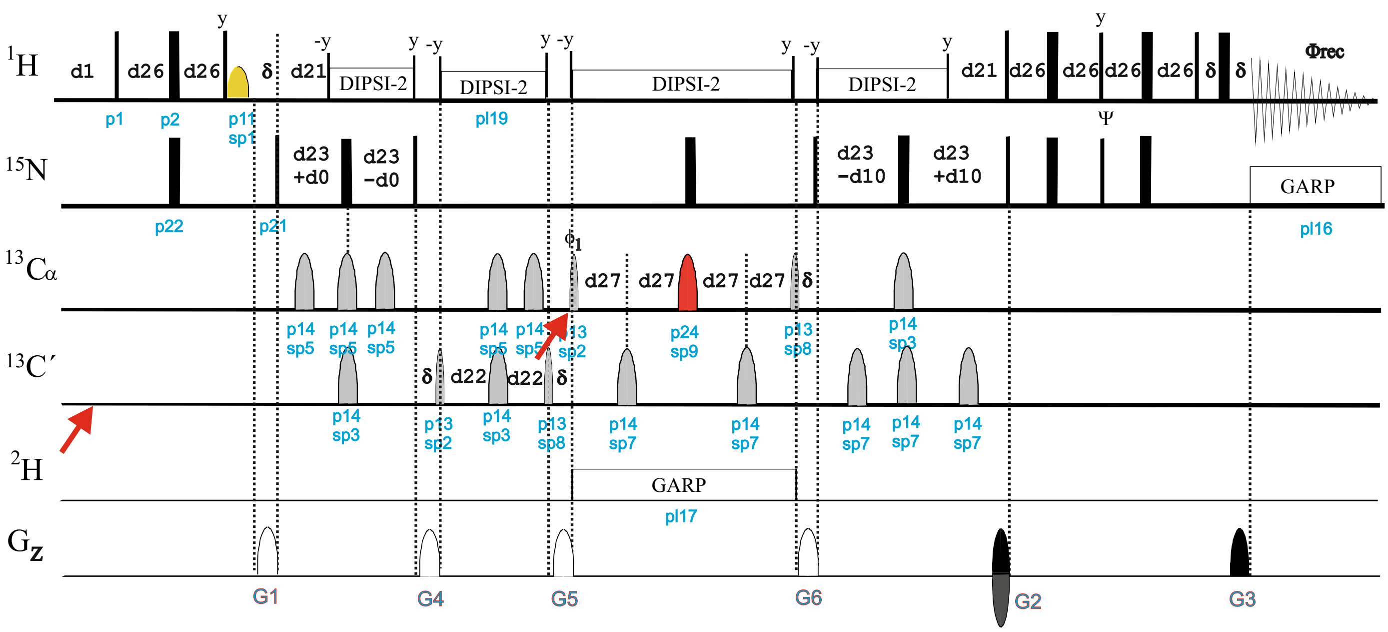


d21: 1/(2J(NH) [5.5 msec]
d22: 1/(4J(COCa)) [4.5 msec]
d23: 1/(4J(NCa) [12.4 msec]
d26: 1/(4J'(NH) [2.3 msec]
d27: 1/(4J`(NCa) [12.5 msec]

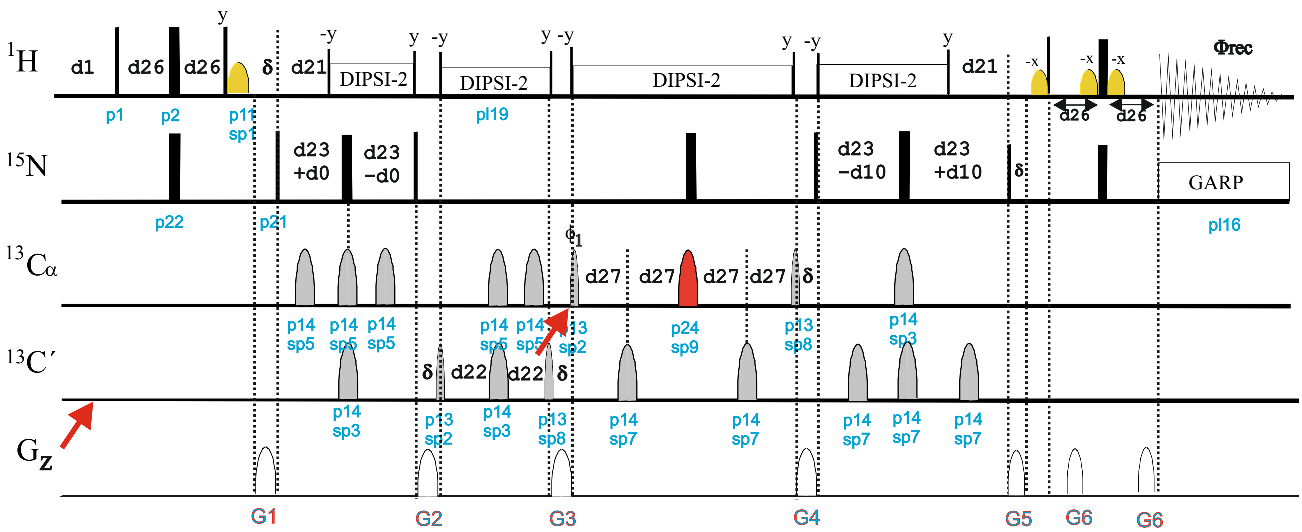
hncocannhgp3d



hncocannhgp2h3d



hncocannhgpwg3d



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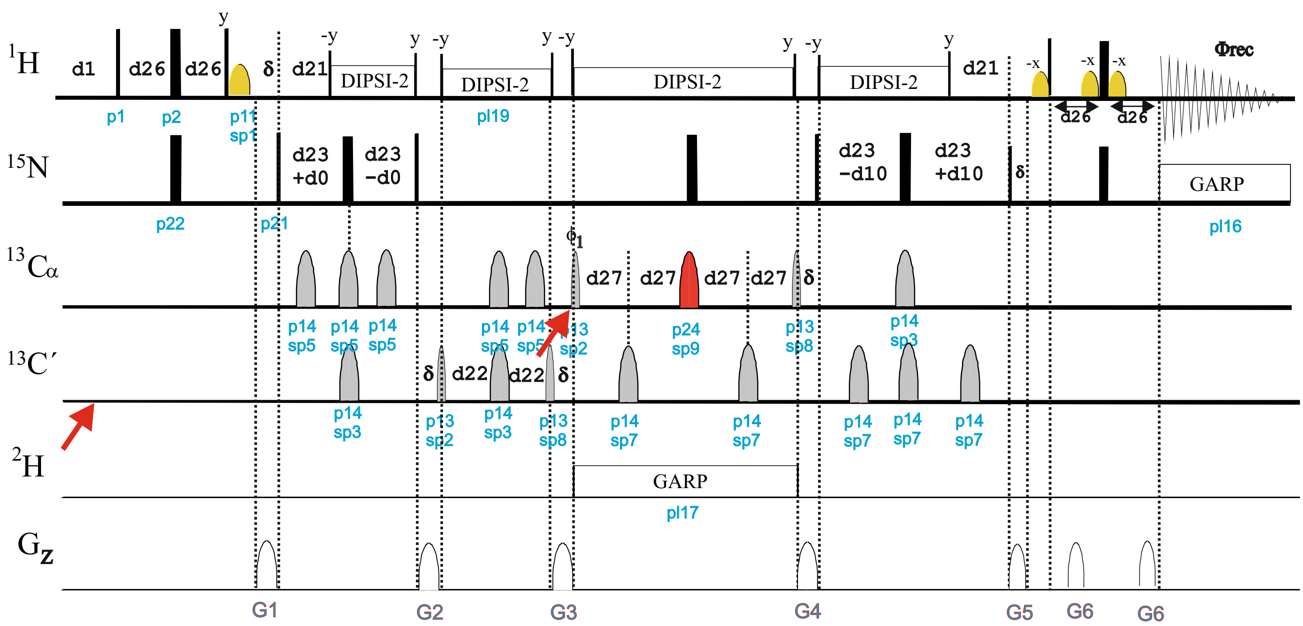
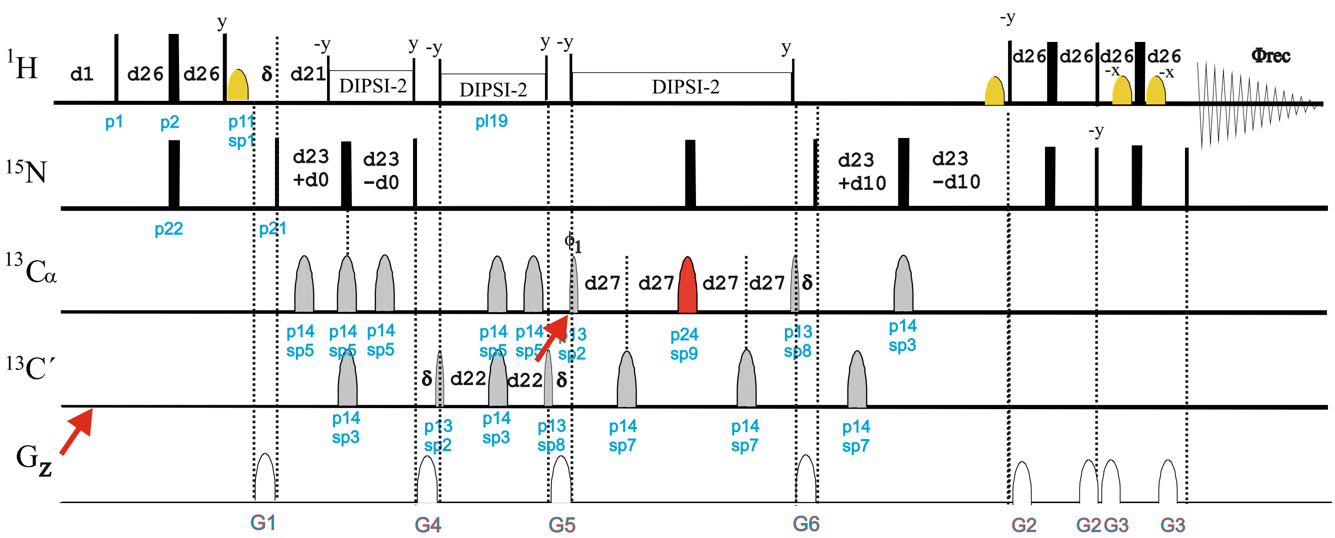
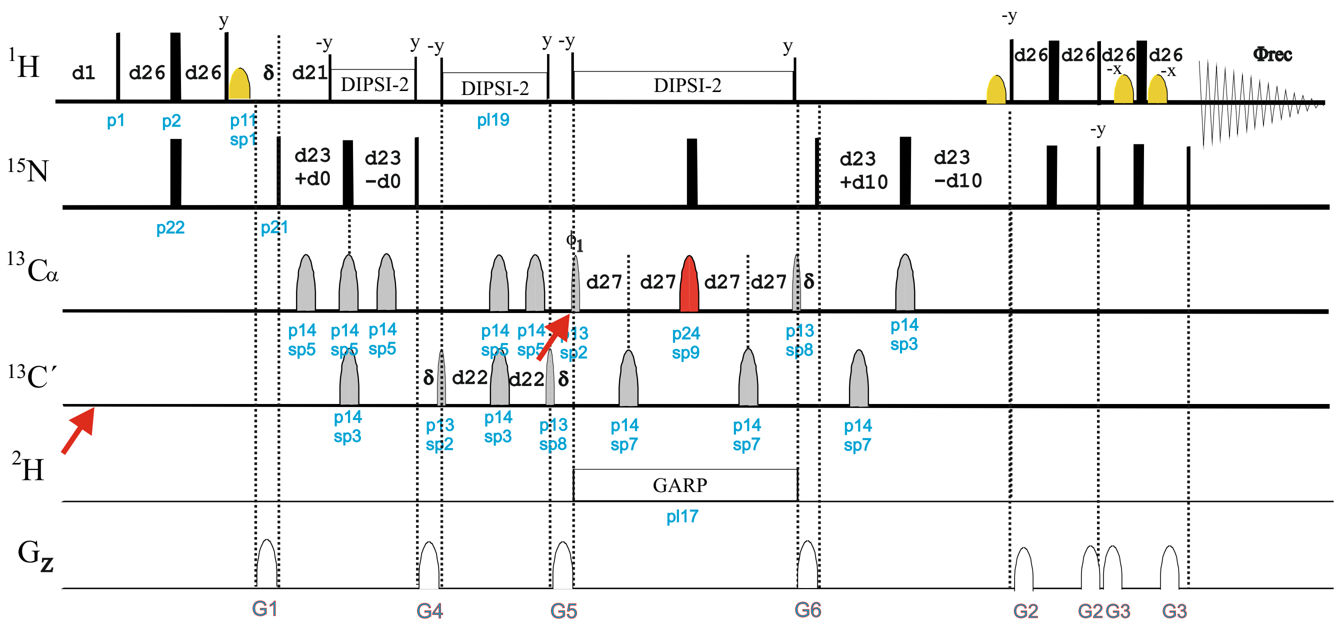


trhncocannhgp3d



trhncocannhgp2h3d



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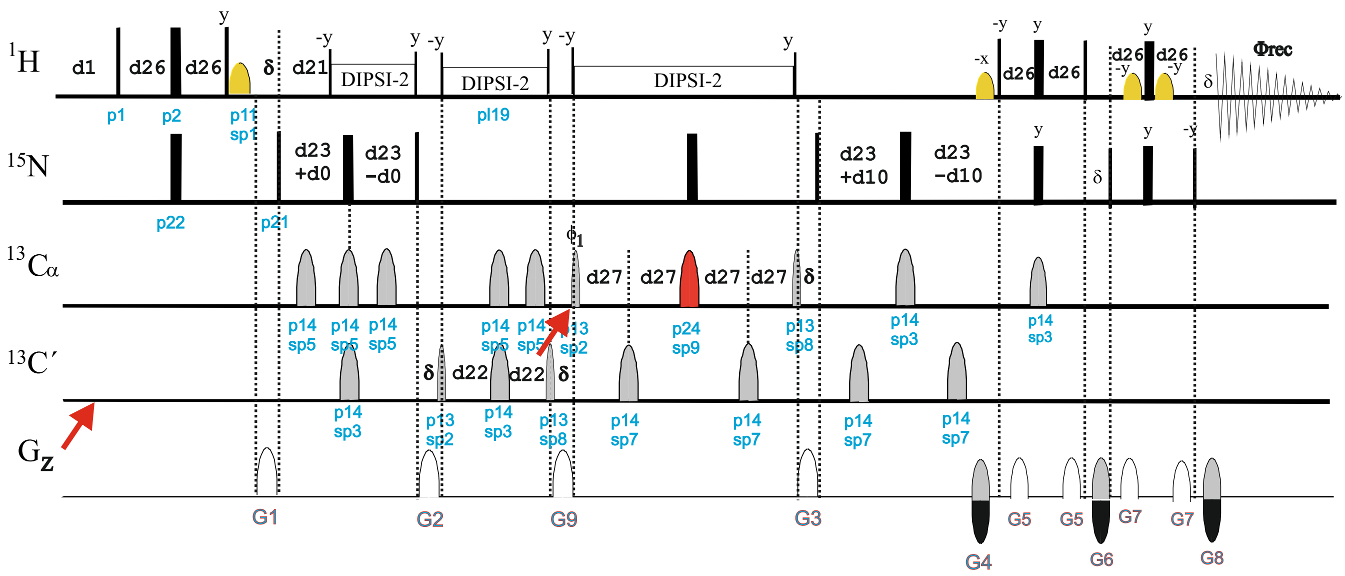
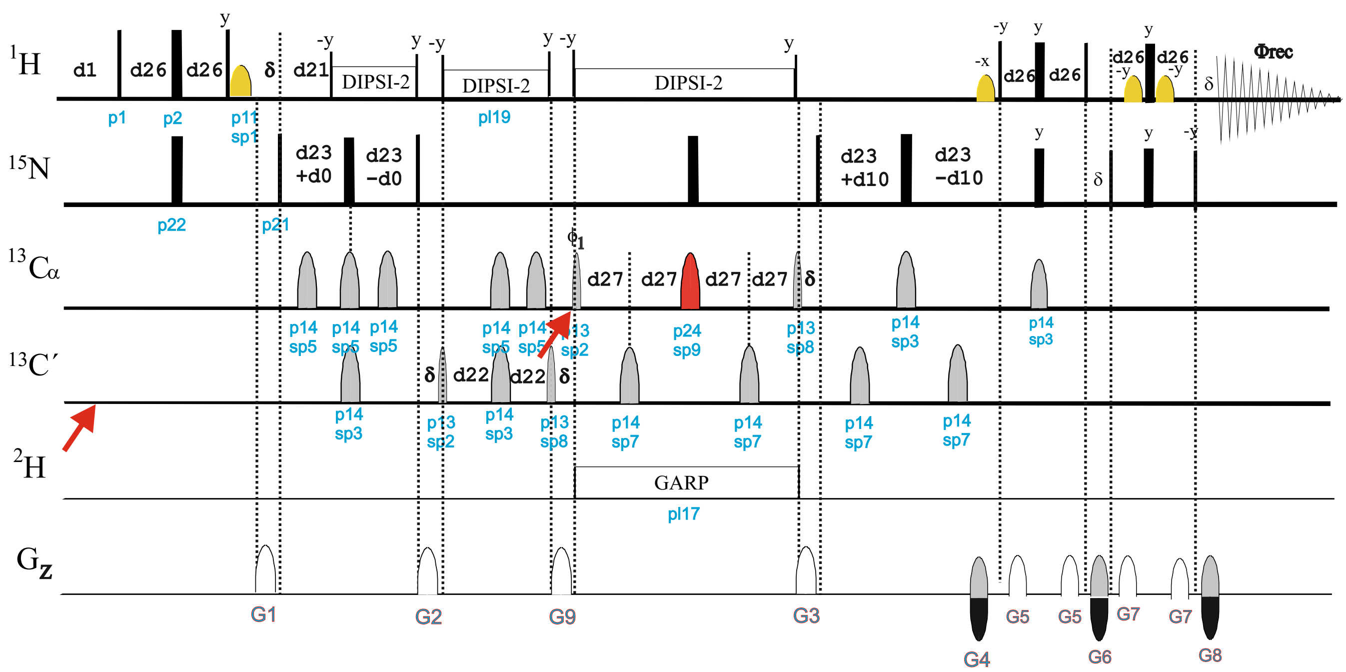
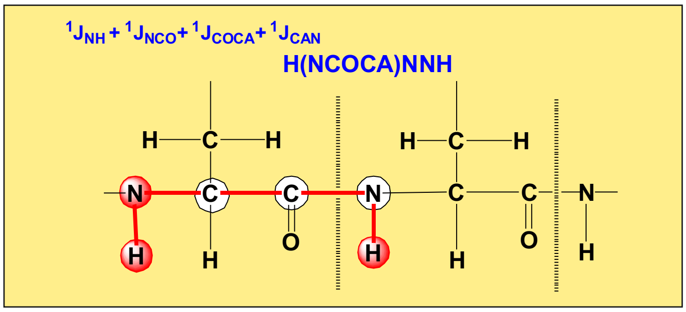
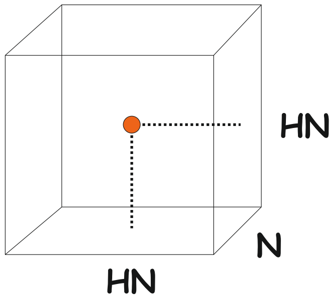


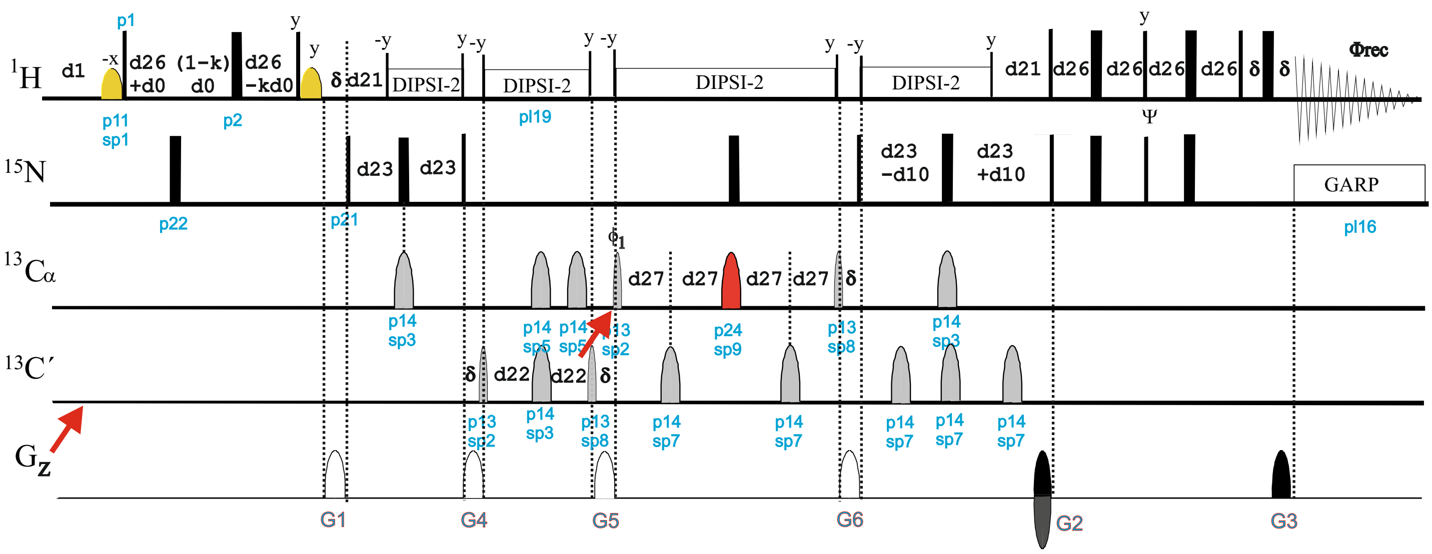
trhncocannhetgp2h3d







hncocannhgp3d.2



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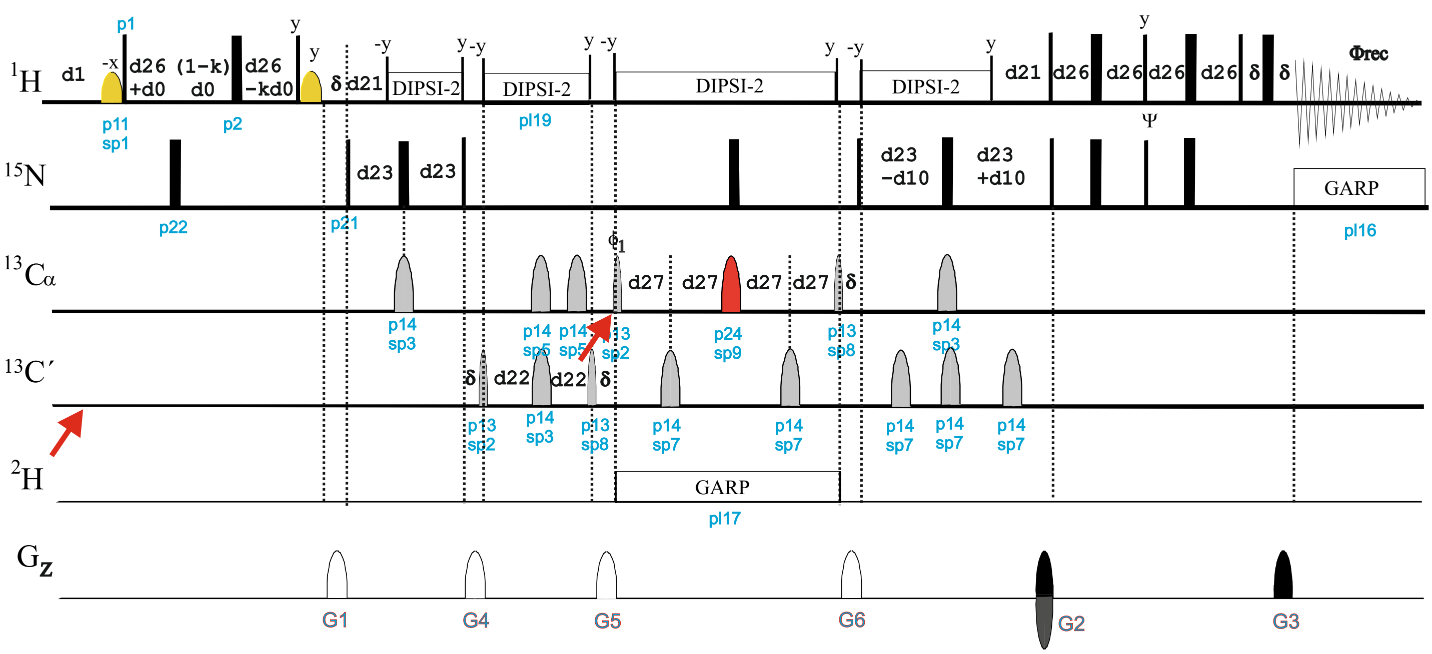
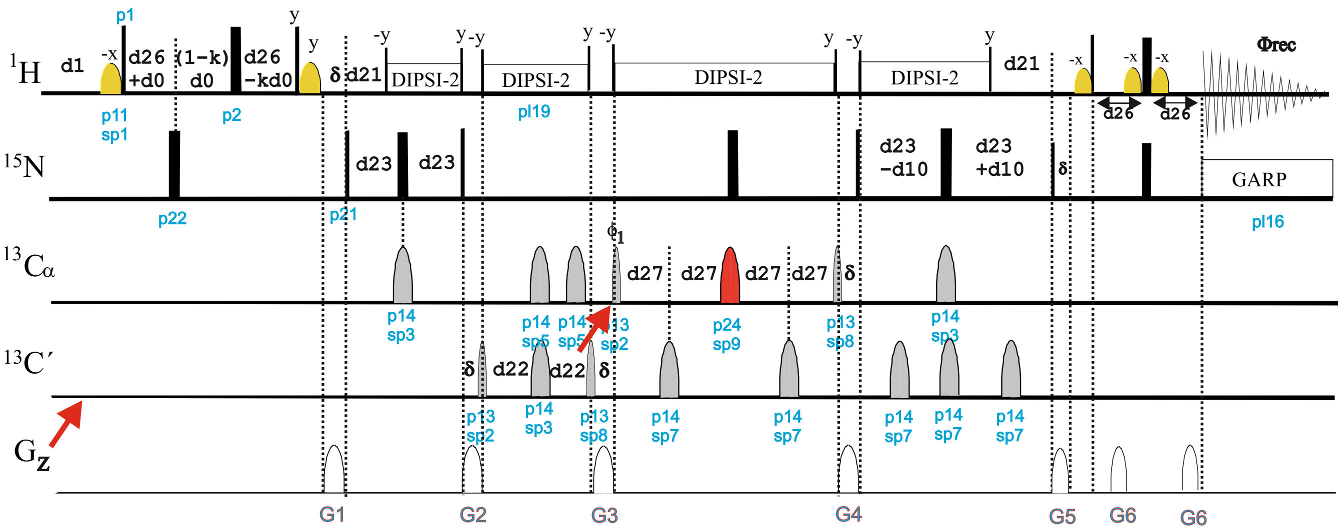
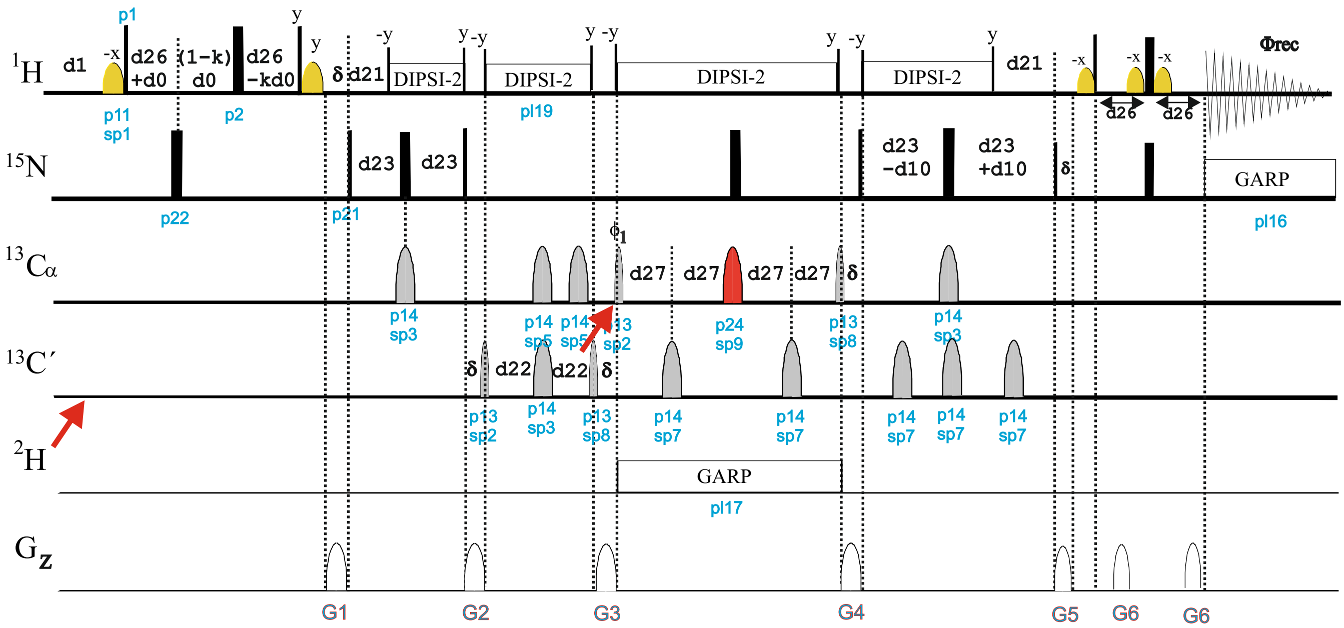


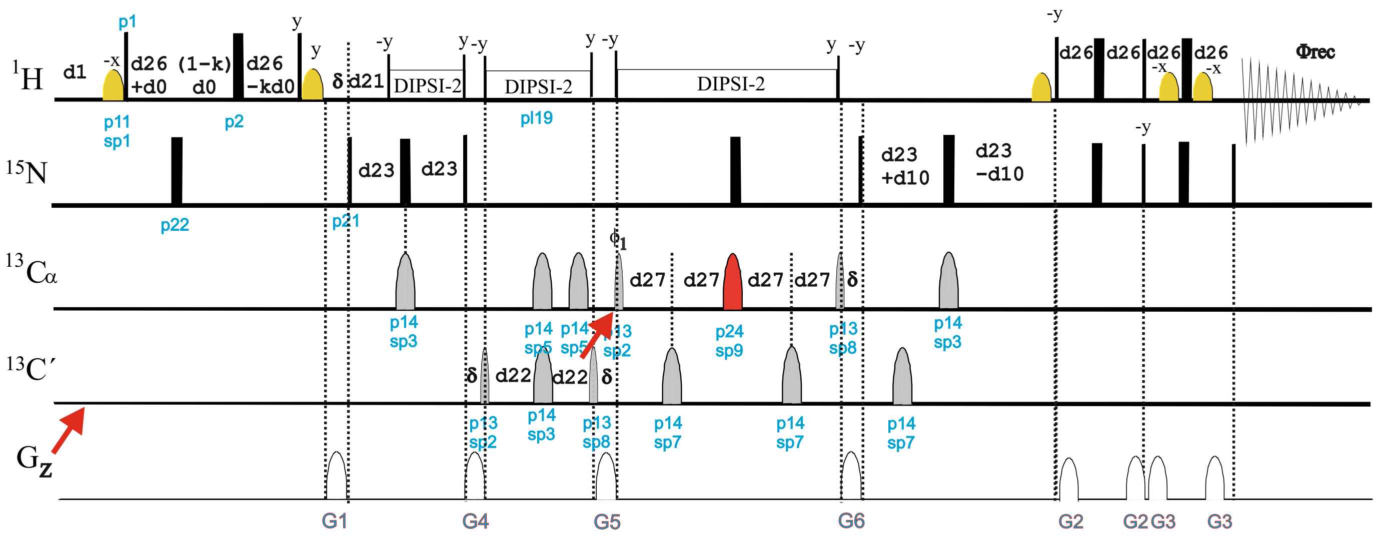
hncocannhgpwg3d.2



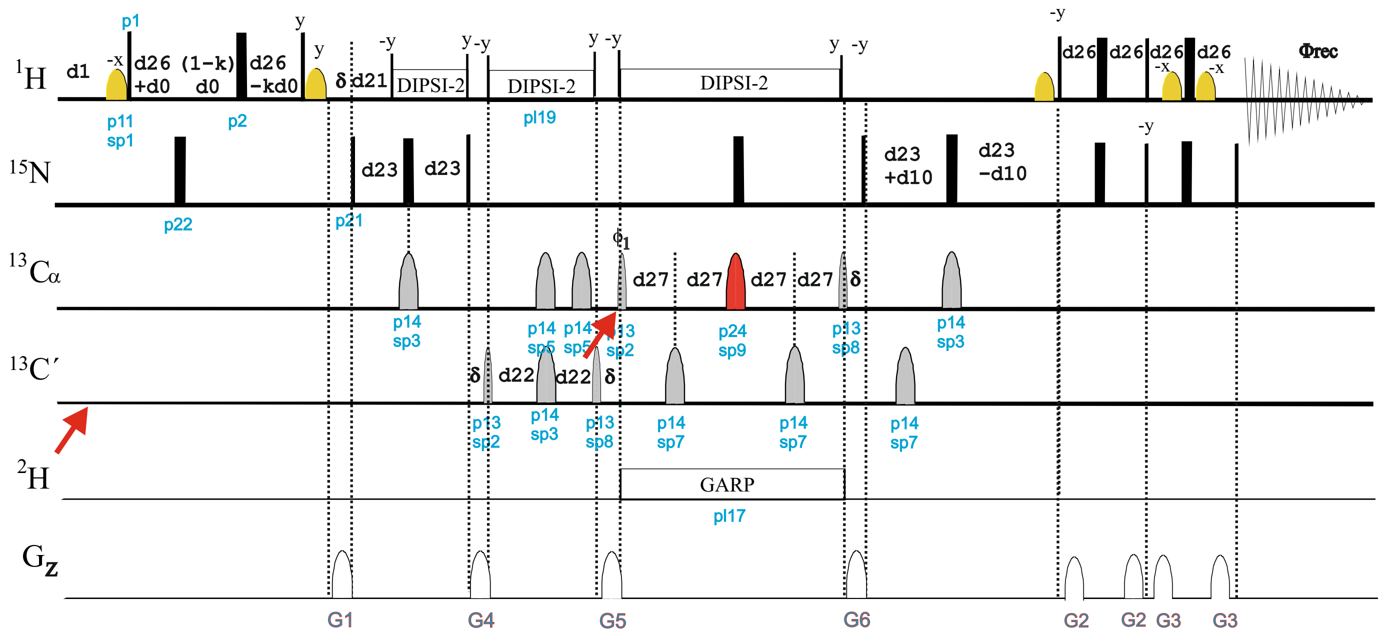
hncocannhgpwg2h3d.2



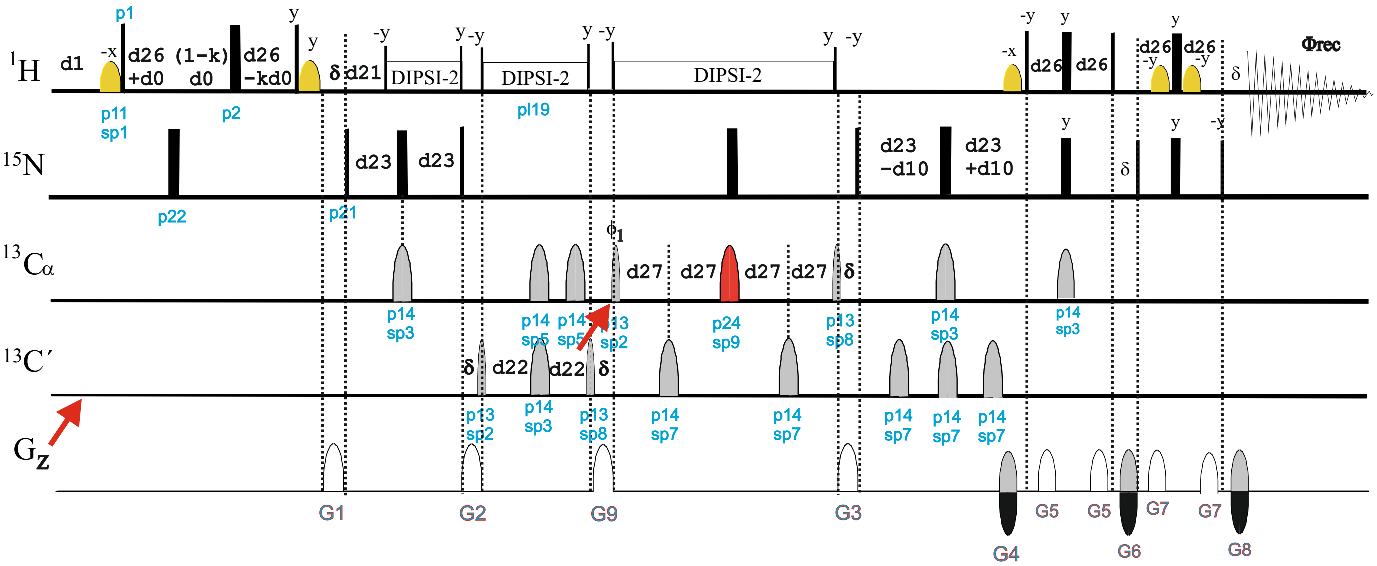
trhncocannhgp3d.2



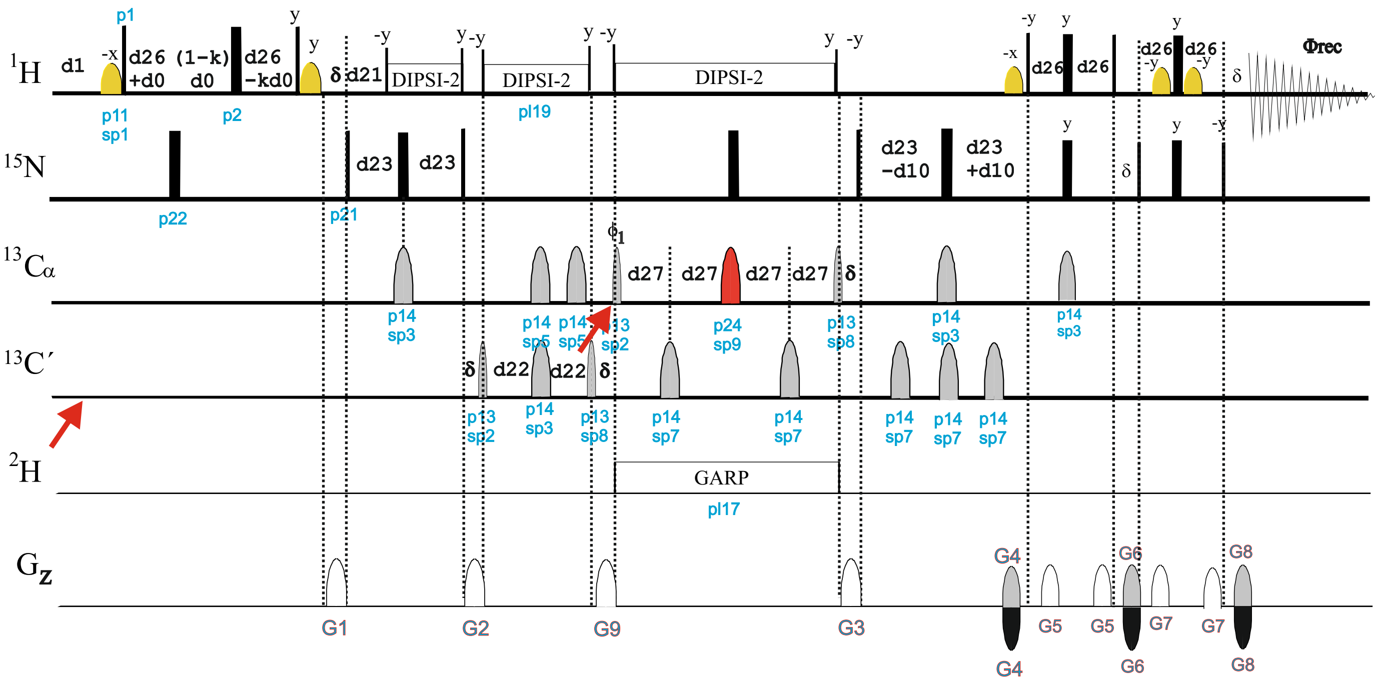
trhncocannhgp2h3d.2



trhncocannhetgp3d.2



trhncocannhetgp2h3d.2



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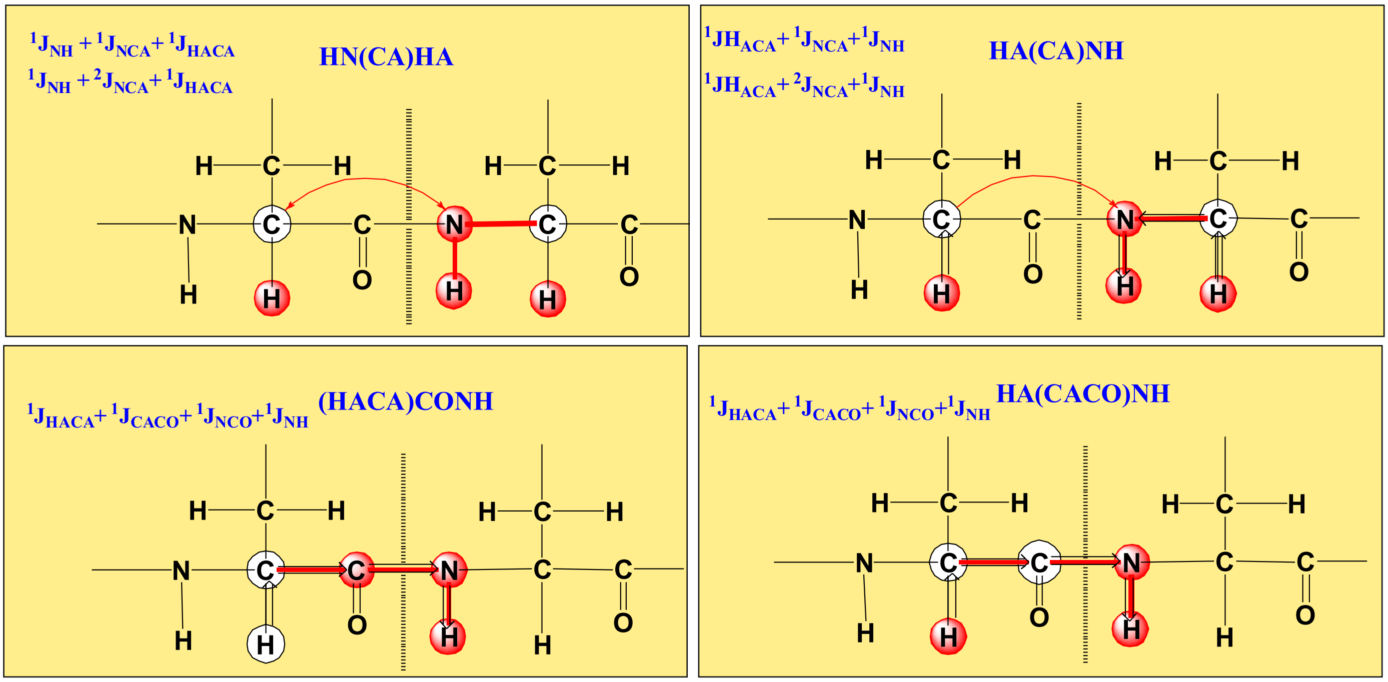
3D HN(CA)HA
3D HA(CA)NH
3D HA(CACO)NH

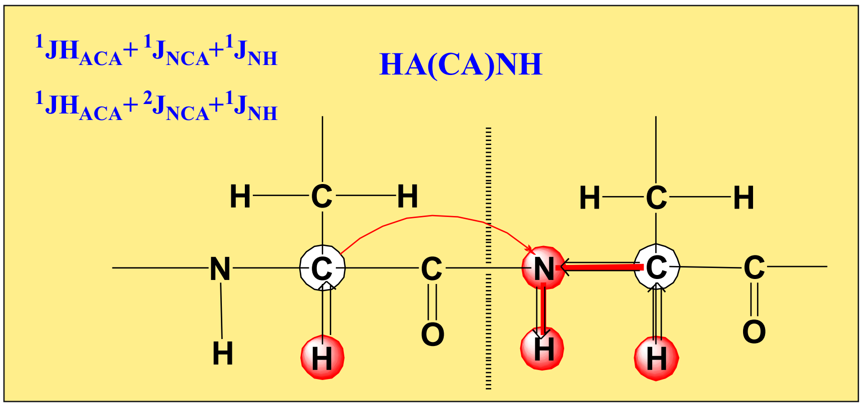
Miscellaneous NH-Detected Backbone Experiments

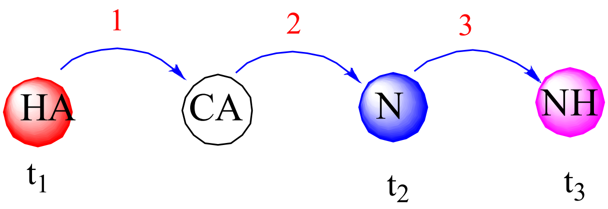
- 3D HA(CA)NH using WATERGATE (**hanhgpwg3d**)

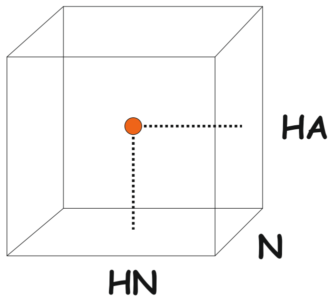
- 3D HA(CACO)NH using WATERGATE (**haconhgpwg3d**)
- 3D (HACA)CONH using PEP (**hcaconhgp3d**)
- 3D (HACA)CONH using WATERGATE (**hcaconhgpwg3d**)

- 3D HN(CA)HA (**hncah3d**)

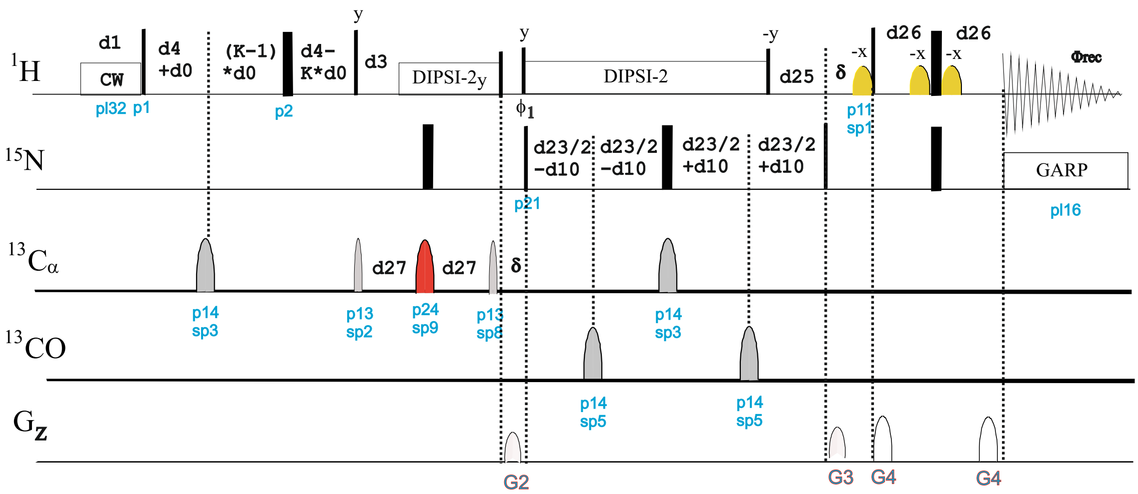




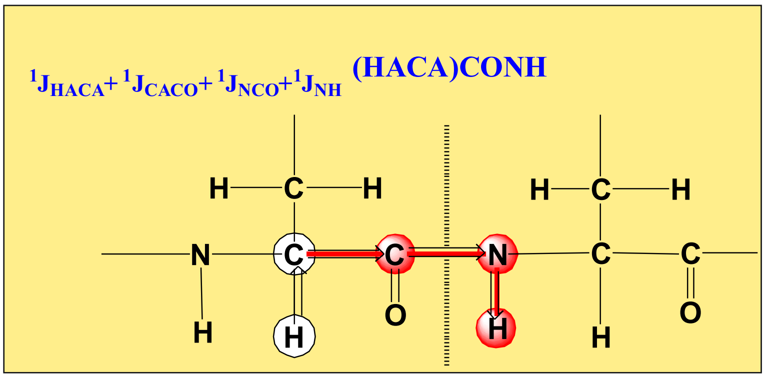




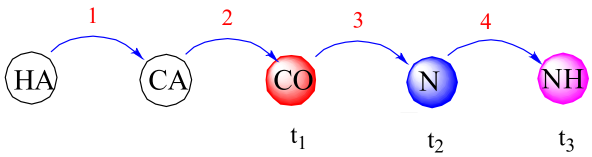
hanhgpwg3d



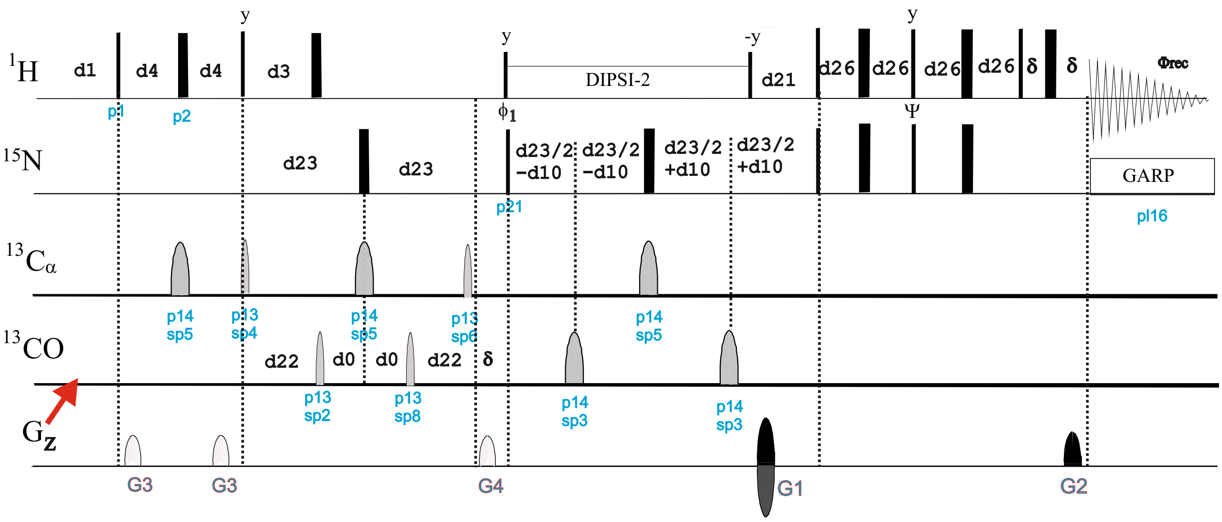
d3 : 1/(3J(CH))	[2.2 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d21: 1/(4J(NCa)), T(N)	[12.4 msec]
d25: 1/(2J(NH))	[5.5 msec]
d26: 1/(4J(NH))	[2.3 msec]
d27: 1/(4J'(NCa))	[11 msec]



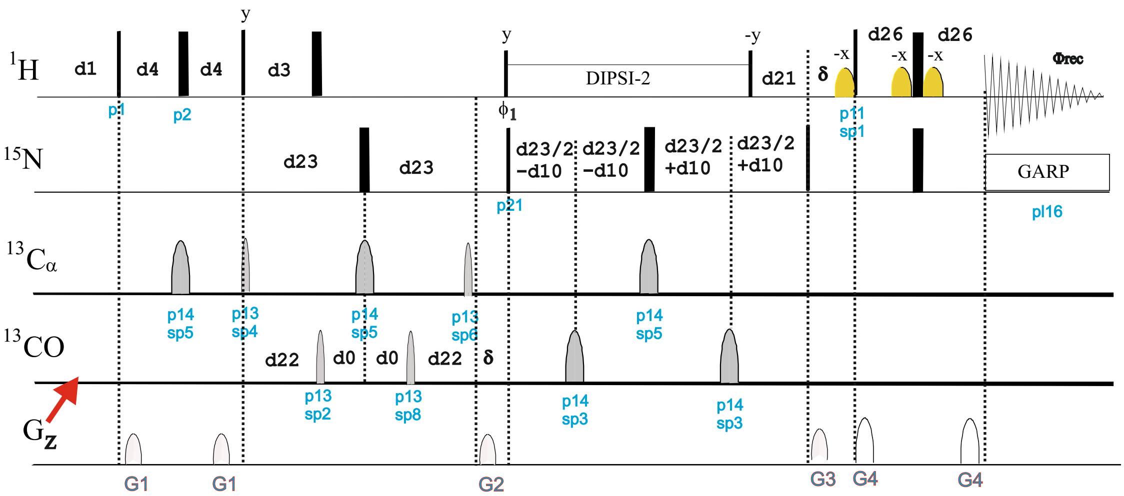
R. Folmer & G. Otting, J. Biomol. NMR 16, 229-233 (2000)



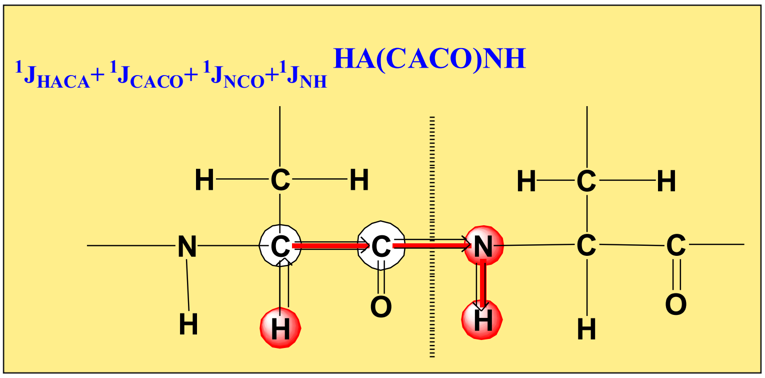
hcaconhgp3d

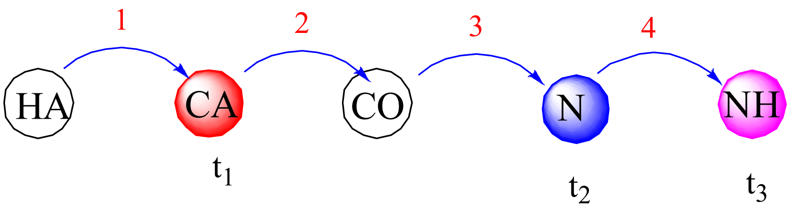


hcaconhgpwg3d

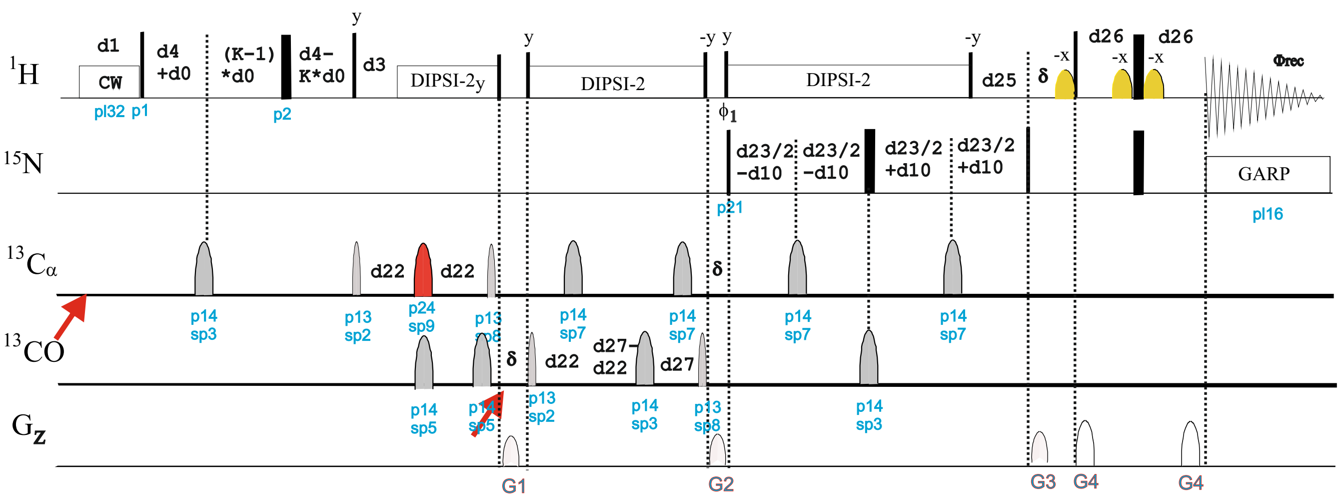


d3 : 1/(6J(HCa))	[1.16 msec]
d4 : 1/(4J(HCa))	[1.5 msec]
d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCa))	[12.4 msec]
d26: 1/(4J'(NH))	[2.3 msec]

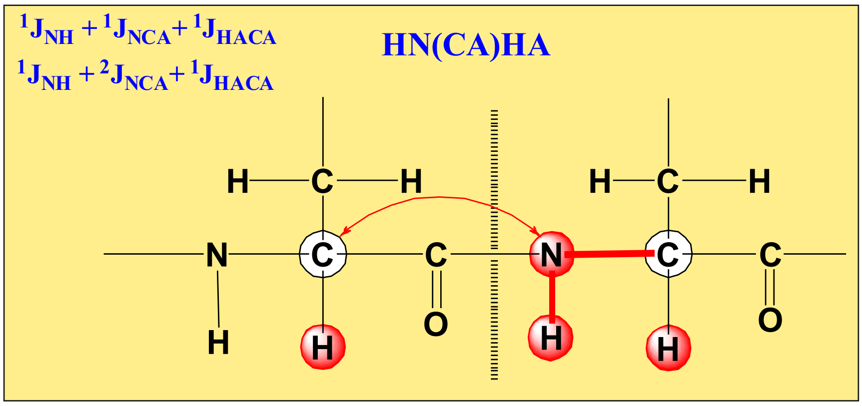


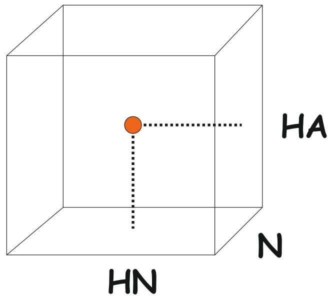


haconhgpwg3d

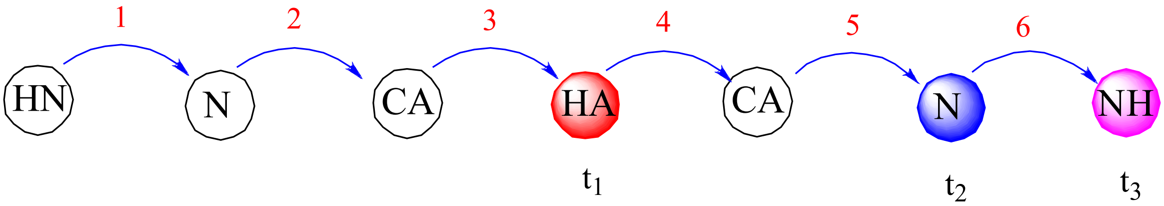


d3 : 1/(3J(CH))	[2.2 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d22: 1/(4J'(CaCO))	[4.4 msec]
d23: 1/(4J(NCO)), T(N)	[12.4 msec]
d25: 1/(2J(NH))	[5.5 msec]
d26: 1/(4J(NH))	[2.3 msec]
d27: 1/(4J'(NCO))	[12.4 msec]

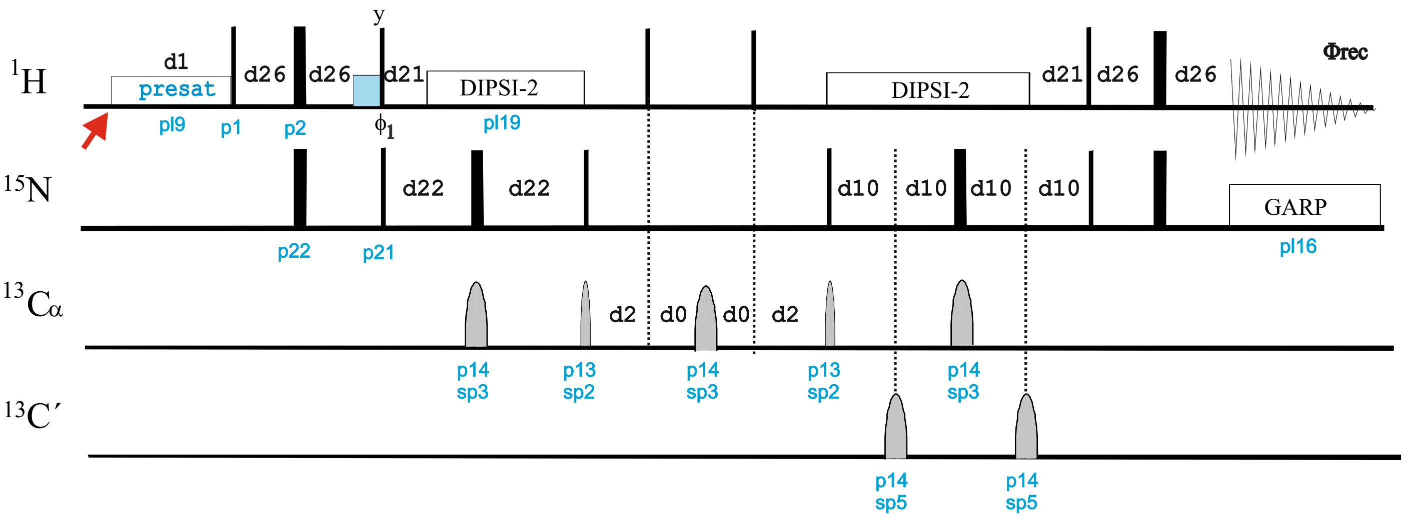




; S. Seip, J. Balbach & H. Kessler, J. Magn. Reson. 100,
; 406-410 (1992)



hncah3d



d2 : 1/(2J(CH))	[3 msec]
d21: 1/(2J`(NH))	[4.5 msec]
d22: 1/(4J(N-Ca))	[11 msec]
d26: 1/(4J(NH))	[2.75m]

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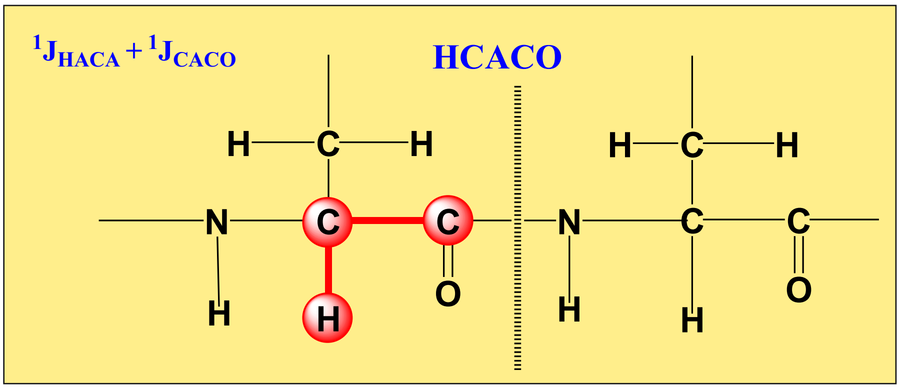
HA-DETECTED
BACKBONE EXPERIMENTS

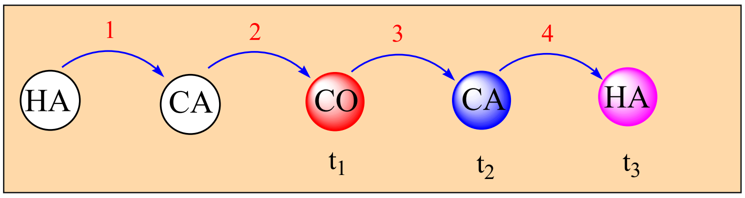
HA-Detected Backbone Experiments

- 3D HCACO experiment (**hcacogp3d** | HCACOGP3D)

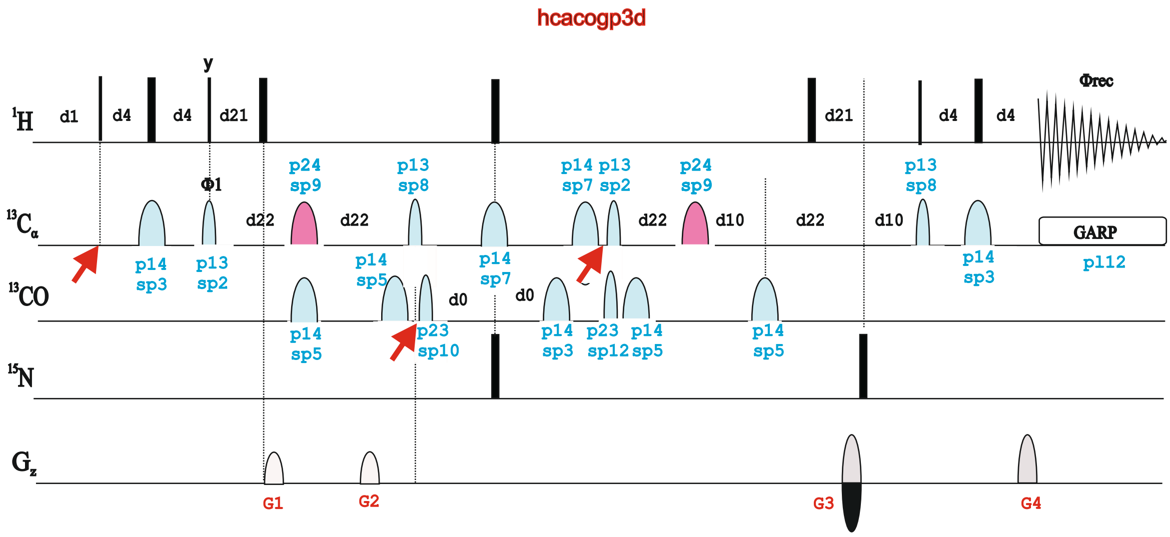
  Also see:
  3D HCACO-type experiments for J measuring
  ^{13}C-detected CACO-type experiments

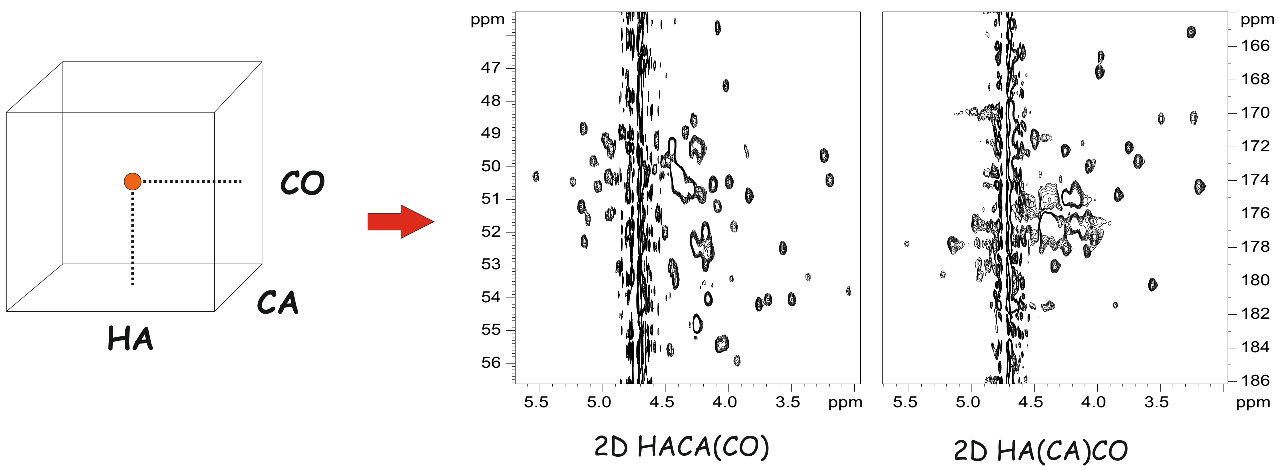
- 2D H(CA)N with ^{2}H-decoupling (**hcangp2h**)
- 3D HCAN using PEP (**hcangp3d**)
- 2D H(CACO)N with ^{2}H-decoupling (**hcacongp2h**)
- 3D HCA(CO)N using PEP (**hcacongp3d**)
- 3D HCBCA(CO)N (**hcbcacongp3d**)





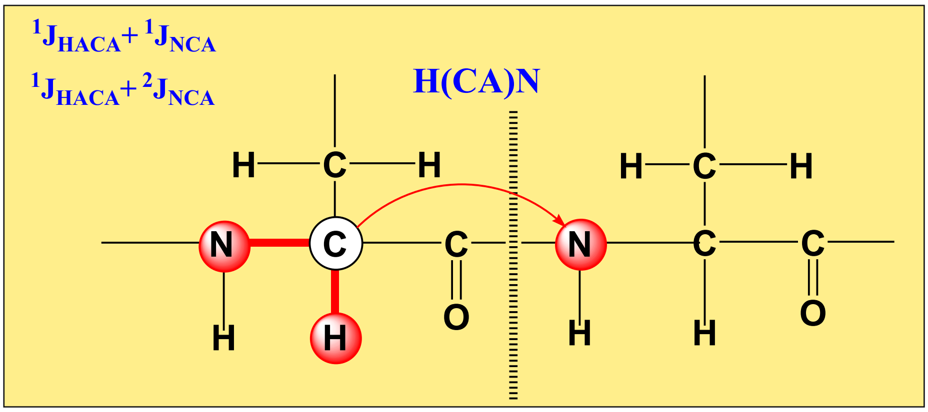
d4=1/4J(CAHA)=1.7m
d21=1/4J(CH) or 1/6J(CH)=1.7m or 1.2m
d22=1/4J(CACO)=4.5m

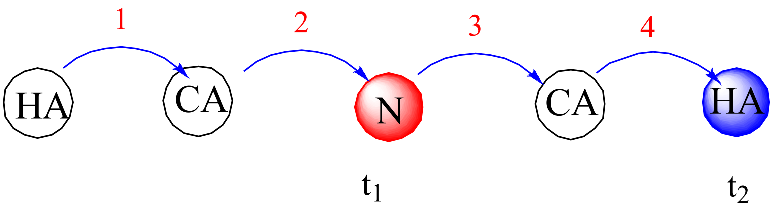


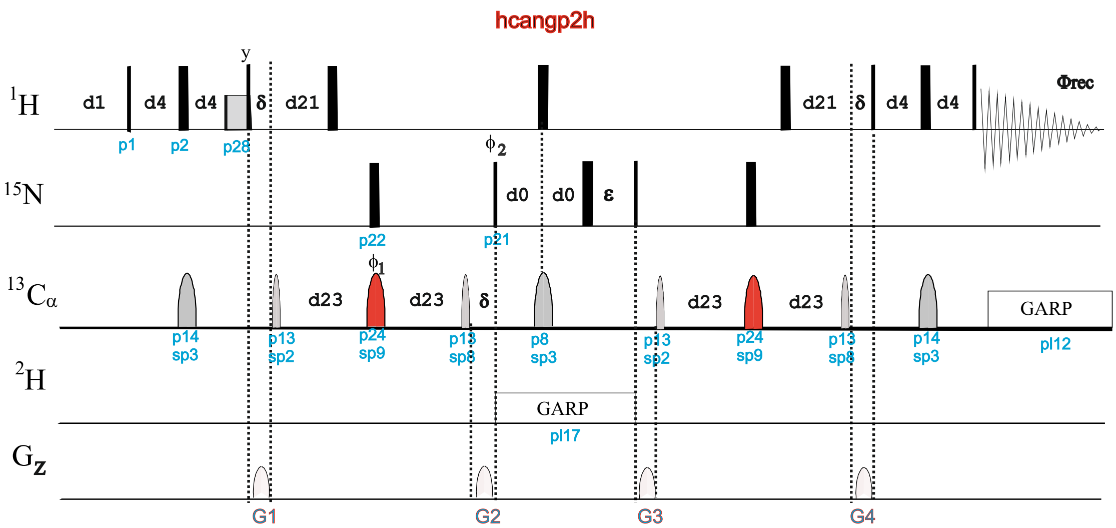


2D H(CA)N Experiment

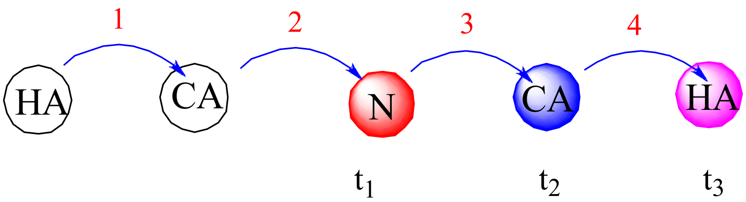
A.C. Wang, S. Grzesiek, R. Tschudin, P.J. Lodi & A. Bax, J. Biomol. NMR 5, 376-382 (1995)

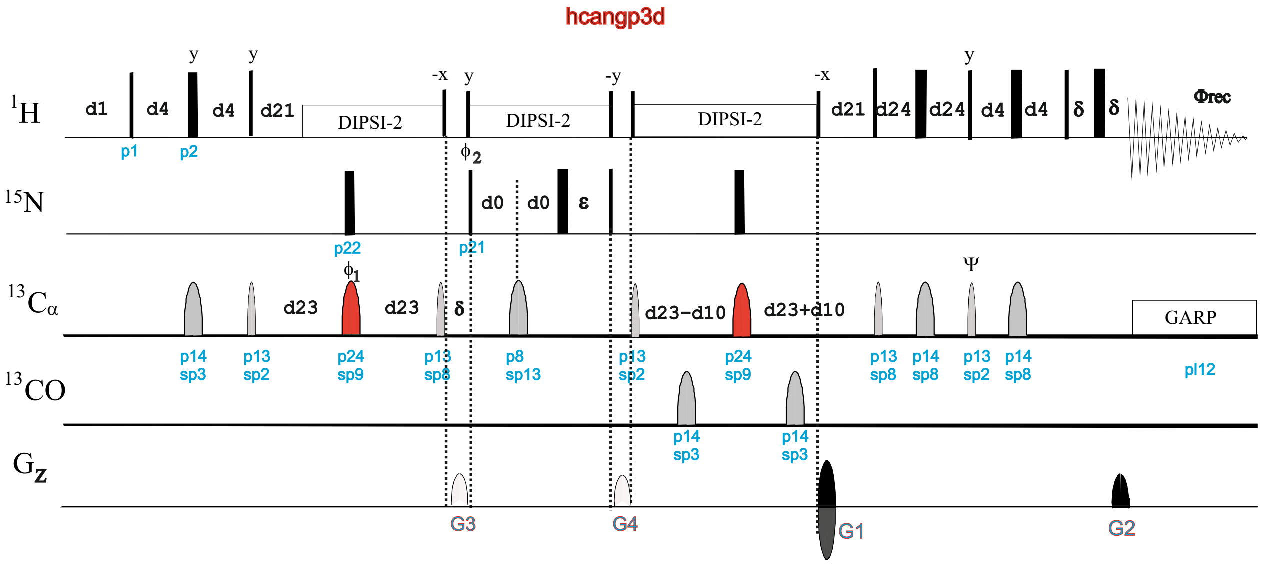


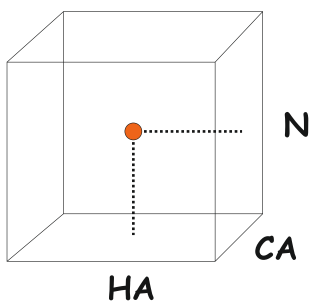




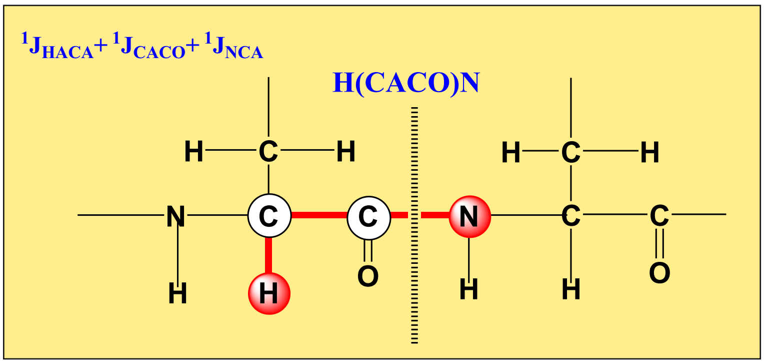
3D HCAN Experiment

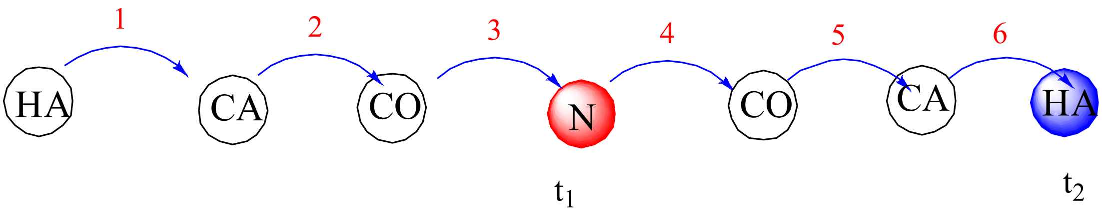




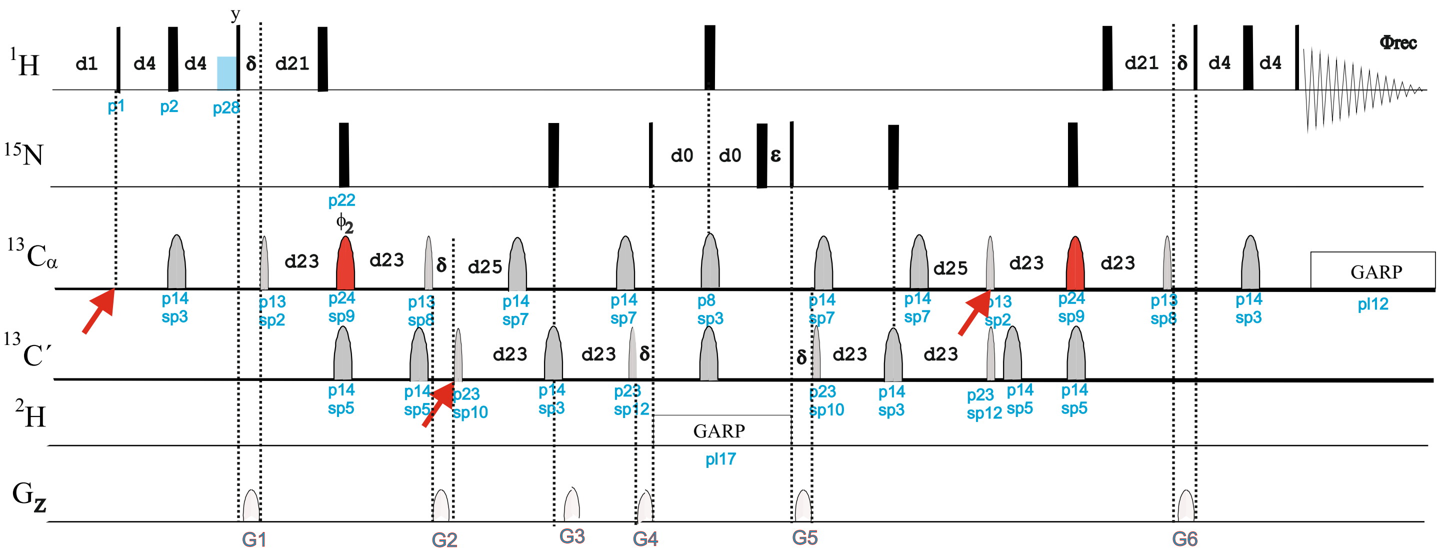


2D H(CACO)N Experiment



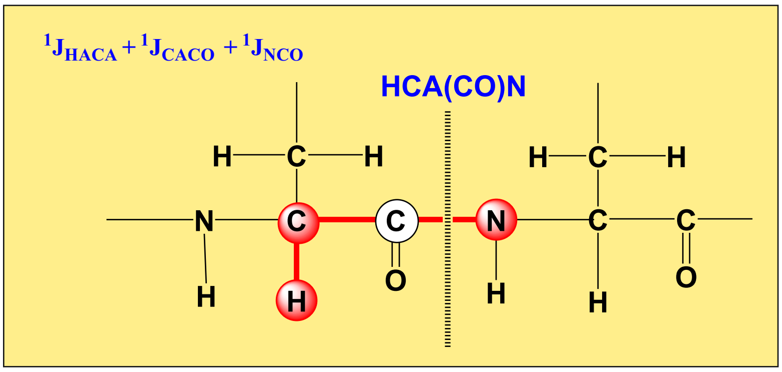


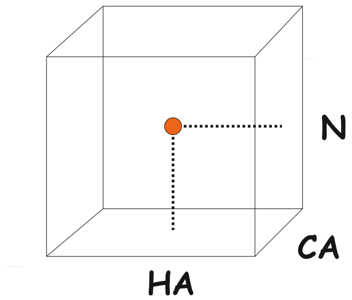
hcacongp2h

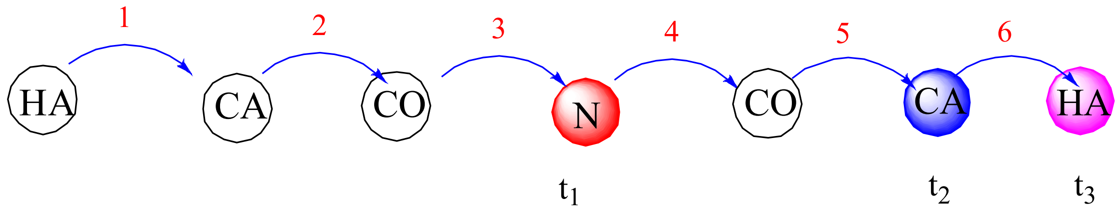


d4 : 1/(4J(HCa))	[1.5 msec]
d21: 1/(4J`(HCa))	[1.55 msec]
d22: 1/(4J(CaCO))	[4.5 msec]
d23: 1/(4J(NCO))	[13.1 msec]
d25: 1/(4J`(CaCO))	[4.5 msec]

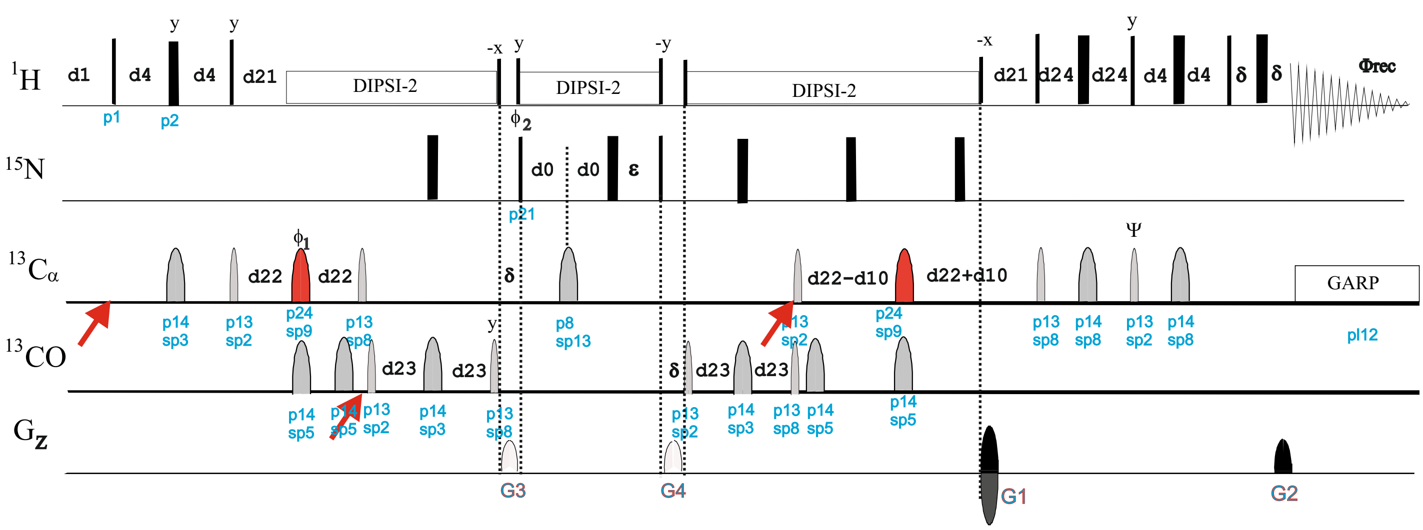
2D HCA(CO)N Experiment







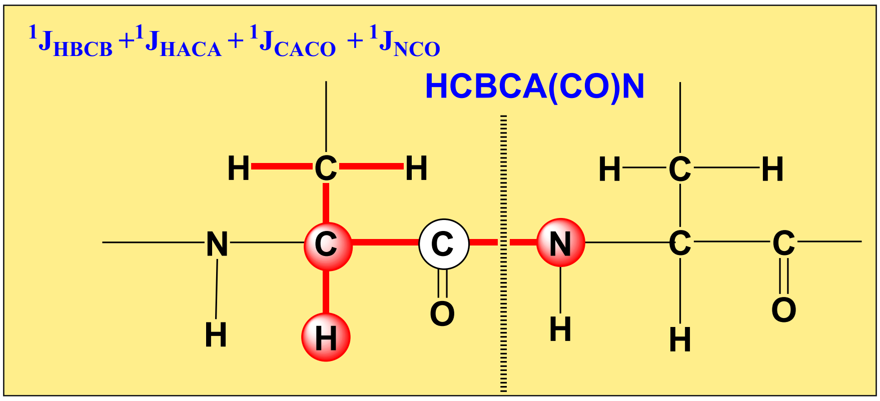
hcacongp3d

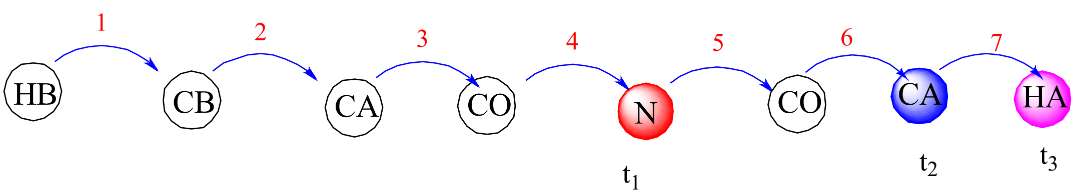


d4 : 1/(4J(HCa)) [1.6 msec]
d21: 1/(3J(HCa)) [2.2 msec]
d22: 1/(4J(CaCO)) [4.5 msec]
d23: 1/(4J(NCa)) [12 msec]
d24: 1/(8J(HCa)) for all multiplicities
1/(4J(HCa)) for CH

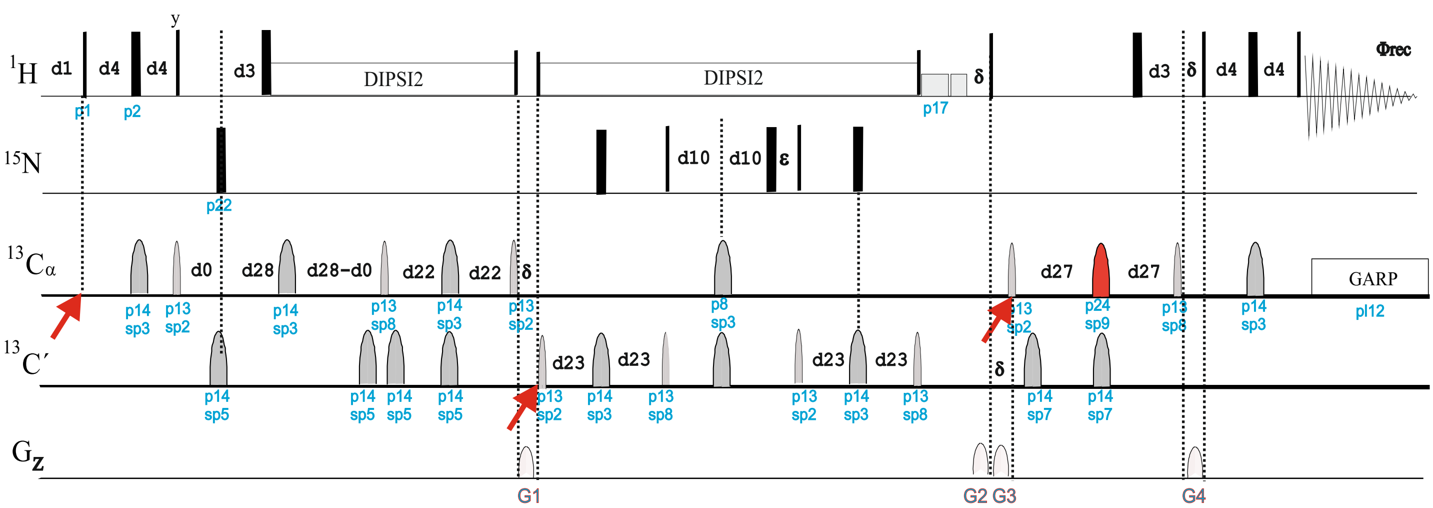
2D HCBCA(CO)N Experiment

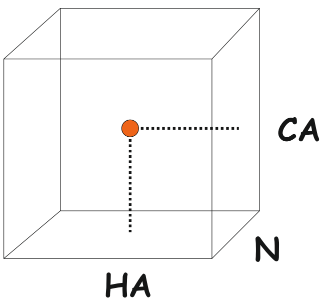
1. V. Kanelis, L. Donaldson, D.R. Muhandiram, D. Rotin, J.D. Foreman-Kay & L.E. Kay, J. Biomol. NMR 16, 253-259 (2000))
2. A.C. Wang, S. Grzesiek, R. Tschudin, P.J. Lodi & A. Bax, J. Biomol. NMR 5, 376-382 (1995))





hcbcacongp3d





d3 : 1/(6J(HCa))	[1.1 msec]
d4 : 1/(4J(HCa))	[1.6 msec]
d22: 1/(4J'(COCa)	[3.6 msec]
d23: 1/(4J(NCO)	[12 msec]
d27: 1/(4J(COCa)	[4.2 msec]
d28: 1/(8J(CaCb))	[3.6 msec]

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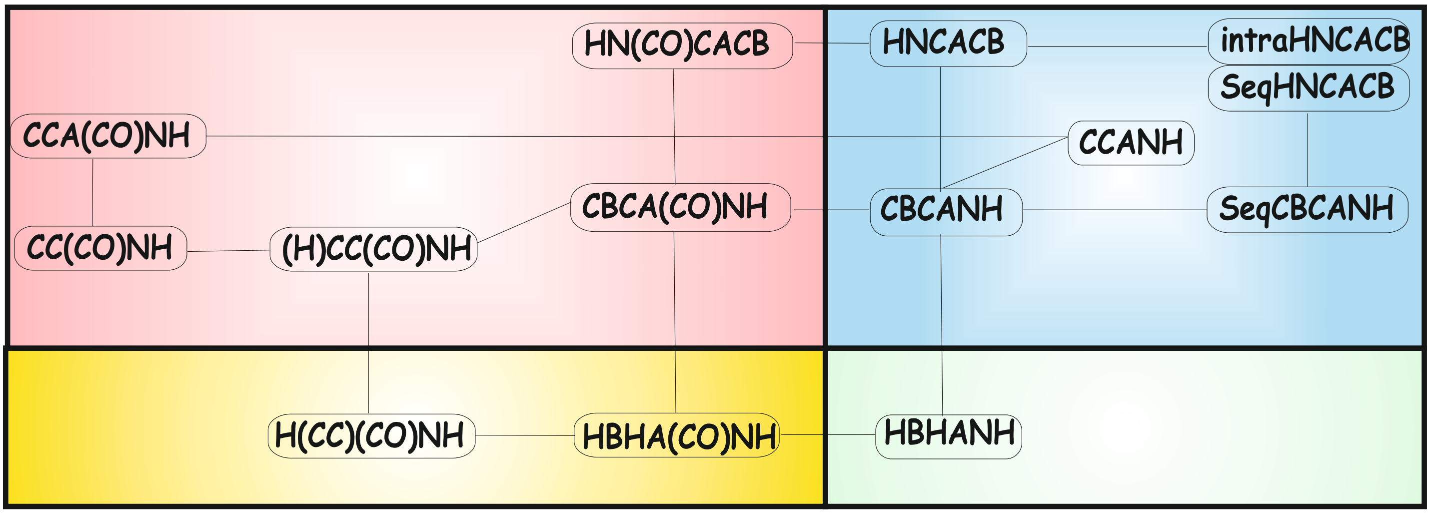
NMRGuide

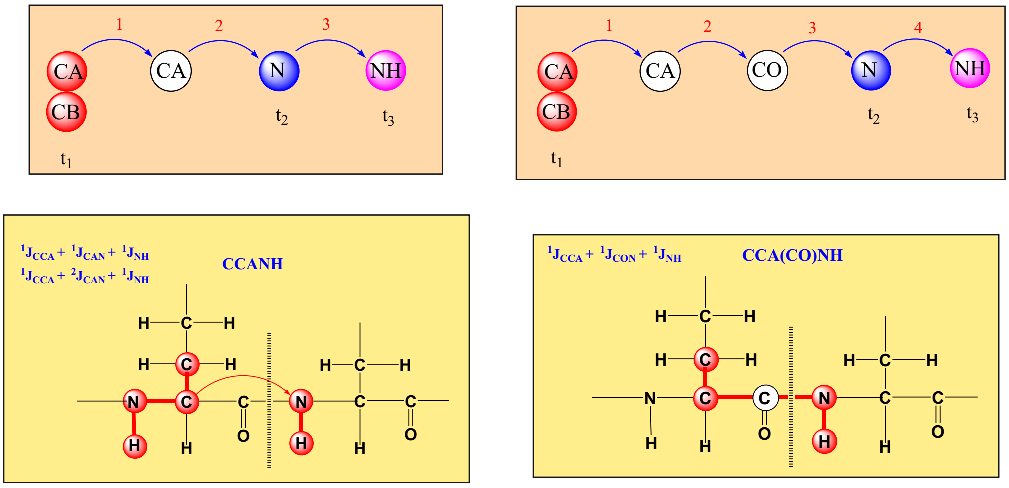
PROTEIN NMR.
BACKBONE-SIDECHAIN
3D EXPERIMENTS

3D BACKBONE-SIDECHAIN



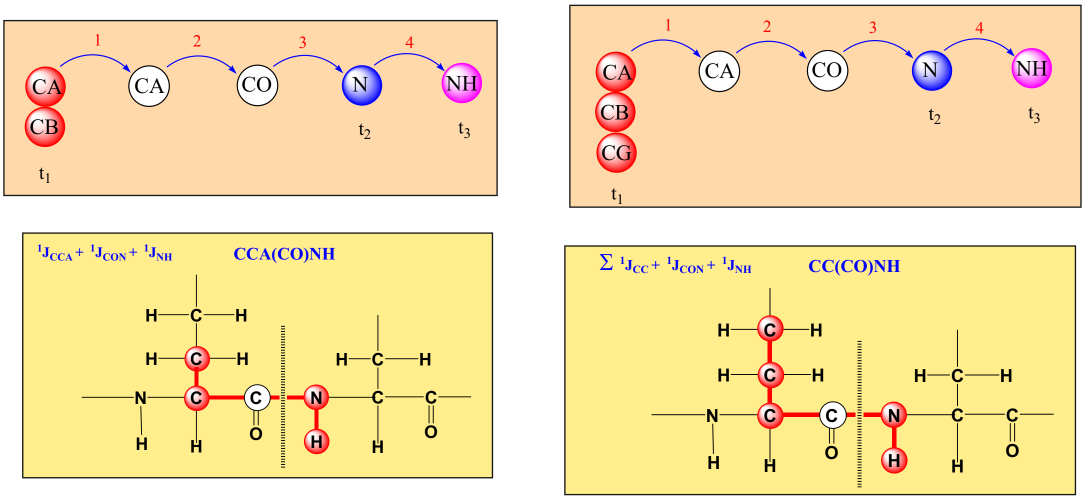
A. Experiments Involving CO into the Magnetization Transfer Mechanism

Example: **CCANH vs CCA(CO)NH:**

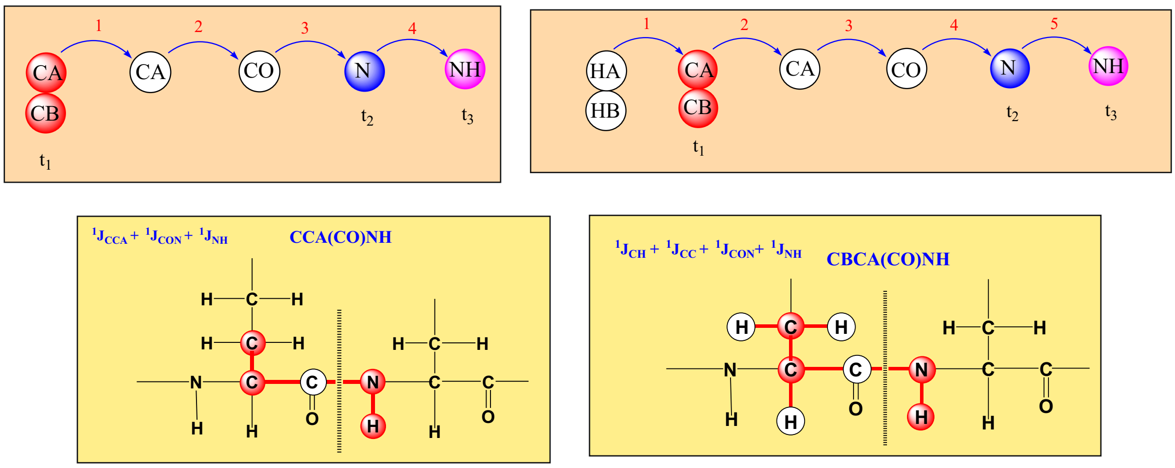


Other examples:
CBCA(CO)NH vs CBCANH
HN(CO)CACB vs HNCACB

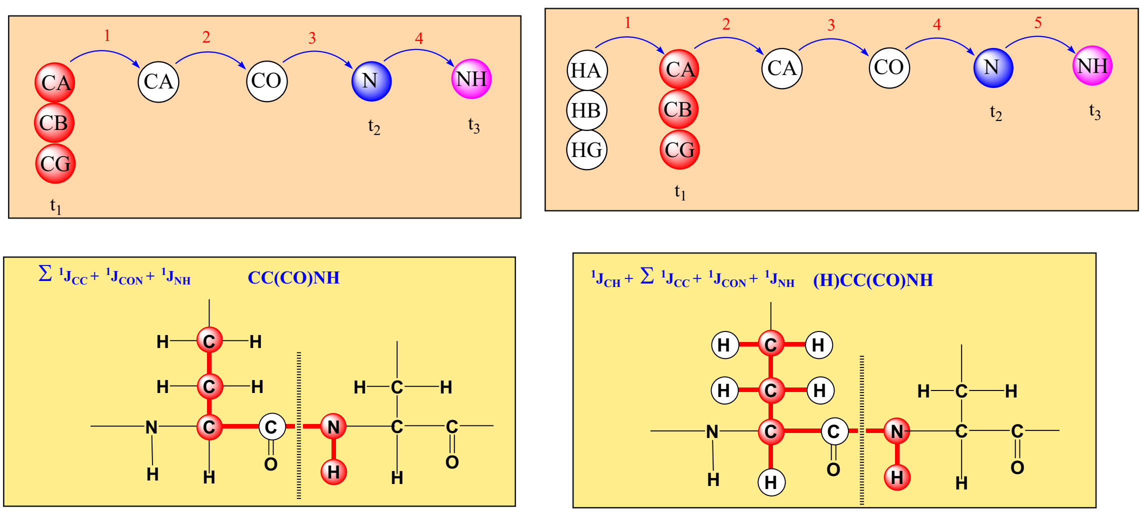
B. COSY vs TOCSY CC Transfer. Example: CCA(CO)NH vs CC(CO)NH



C. Starting from 13C or from 1H. Example1: CCA(CO)NH vs CBCA(CO)NH

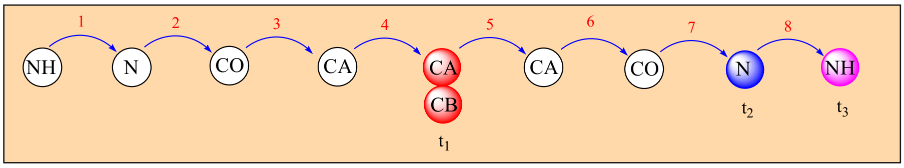


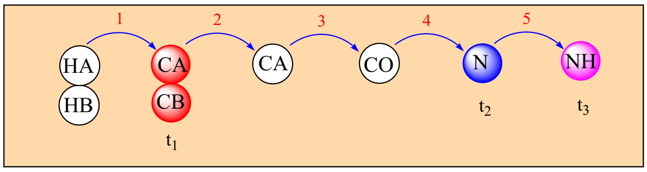
Example 2: CC(CO)NH vs (H)CC(CO)NH:

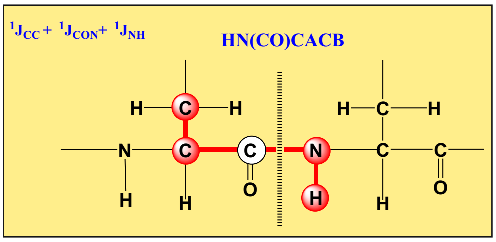


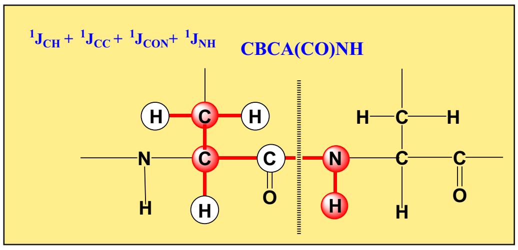
D. Out-and-back vs Out-and-Stay. Examples: HN(CO)CACB vs CBCA(CO)NH

Other examples: HNCACB vs CBCANH









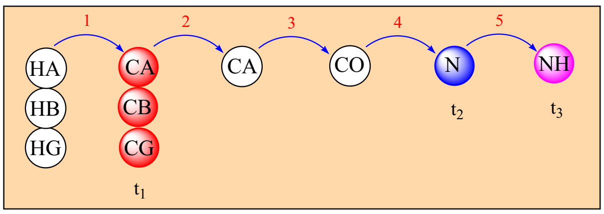
E. Evolving Aliphatic Carbons or Aliphatic protons.

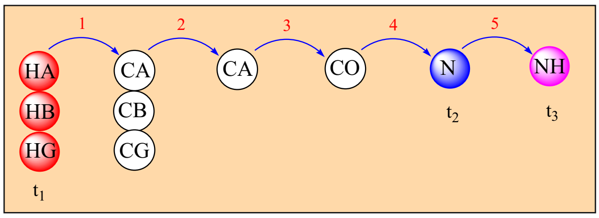
Example (H)CC(CO)NH vs H(CC)(CO)NH:

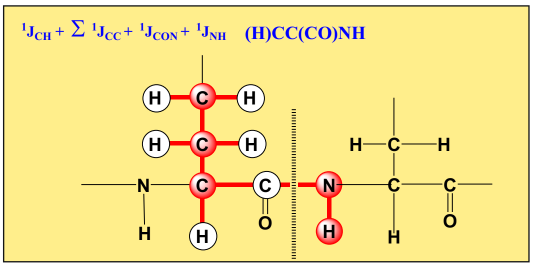
Other examples:

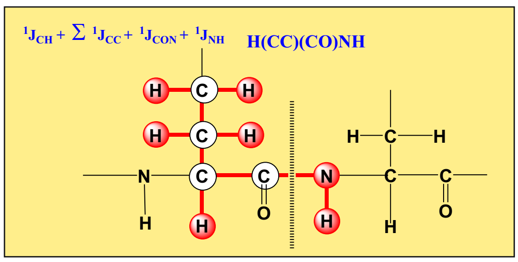
CBCA(CO)NH vs HBHA(CO)NH

CBCANH vs HBHANH









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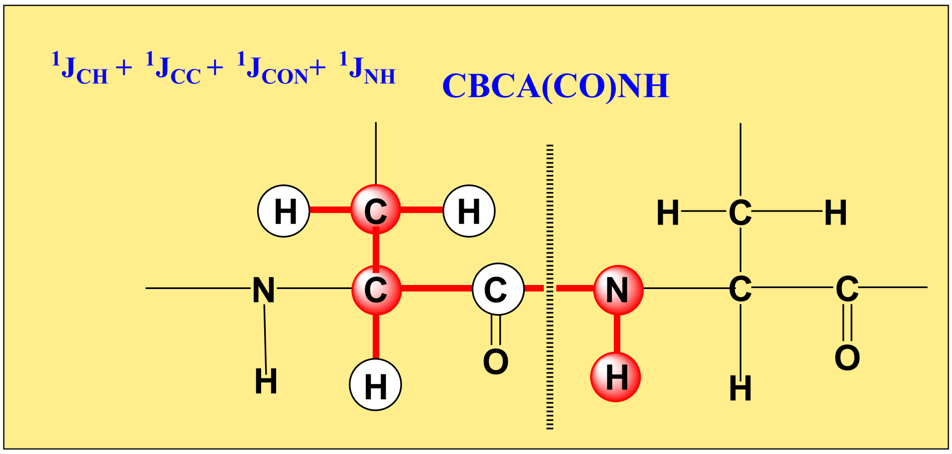
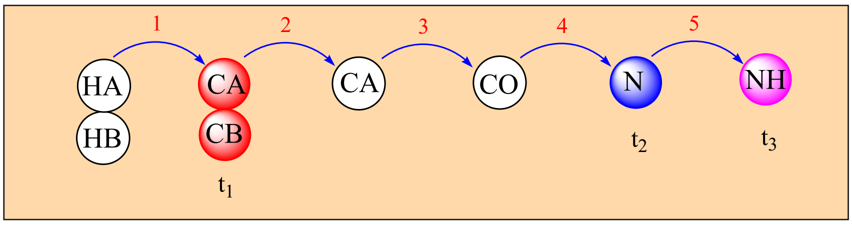
3D CBCACONH

CBCACONH experiment

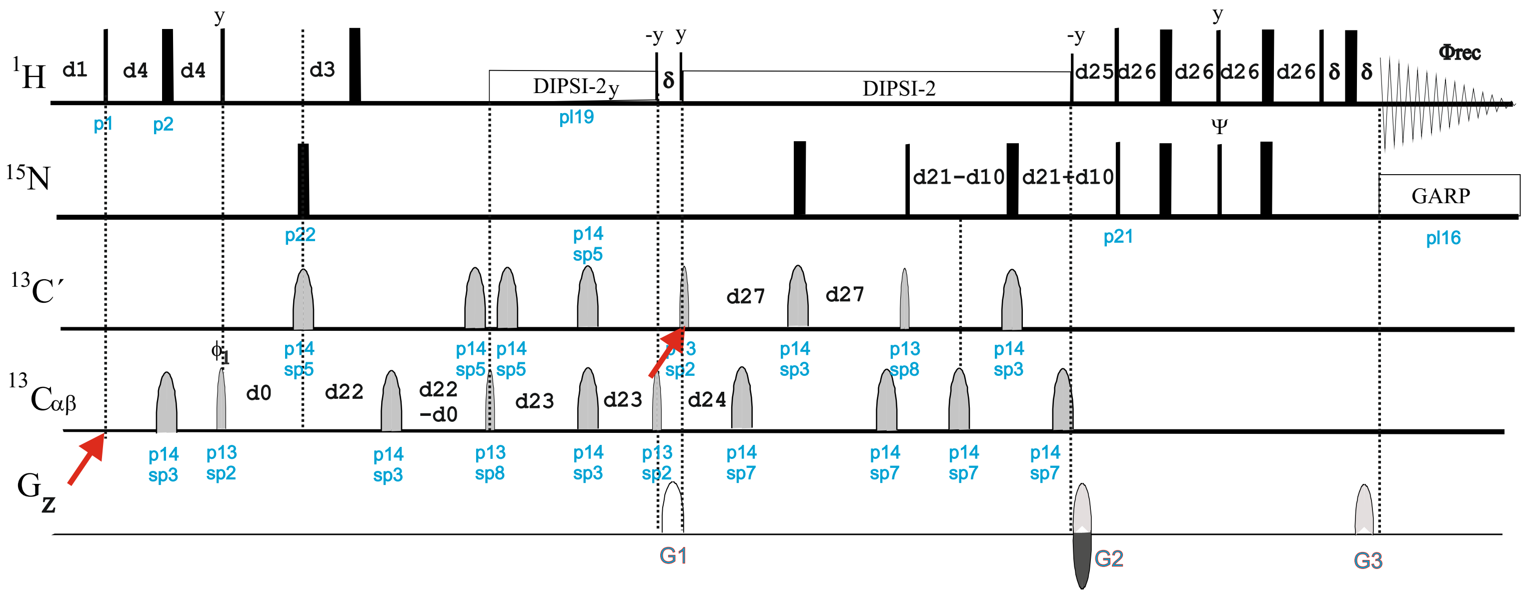
- 3D CBCA(CO)NH using PEP (**cbcaconhgp3d** | CBCACONHGP3D)
- 3D CBCA(CO)NH using WATERGATE (**cbcaconhgpwg3d** | CBCACONHGPWG3D)
- 3D CBCA(CO)NH using WATERGATE and filter por CG (**cbcaconhgpwg3d.2**)
- 3D CBCA(CO)NH using TROSY (**trcbcaconhgp3d** | TRCBCACONHGP3D)
- 3D CBCA(CO)NH using TROSY and gradient echo-antiecho (**trcbcaconhetgp3d** | TRCBCACONHETGP3D)
- 4D CBCACONH using WATERGATE (**cbcaconhgpwg4d**)
- 5D HBHACBCACONH using WATERGATE (**hbhacbcaconhgpwg5d**)

Also see:
CBCANH experiments
HN(CO)CACB experiments
HCCCONH experiments

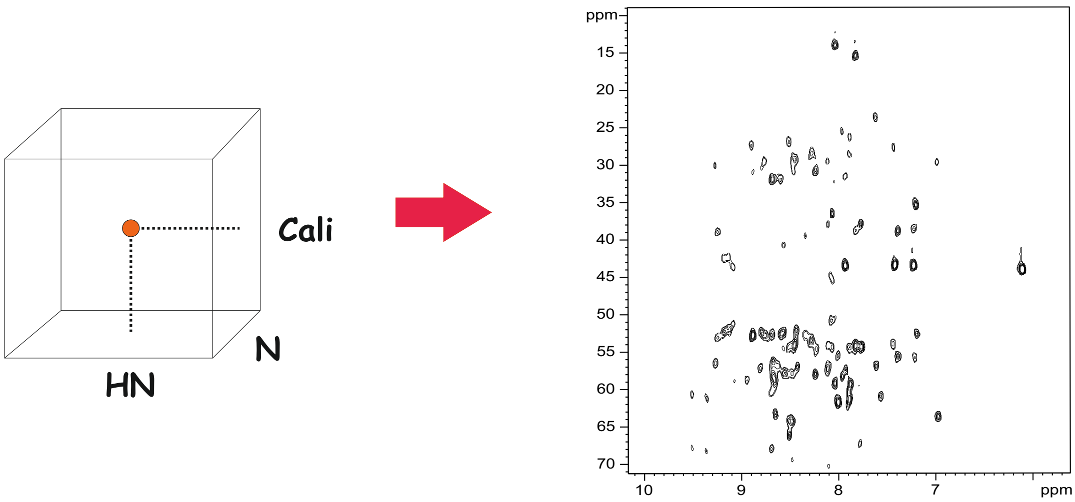




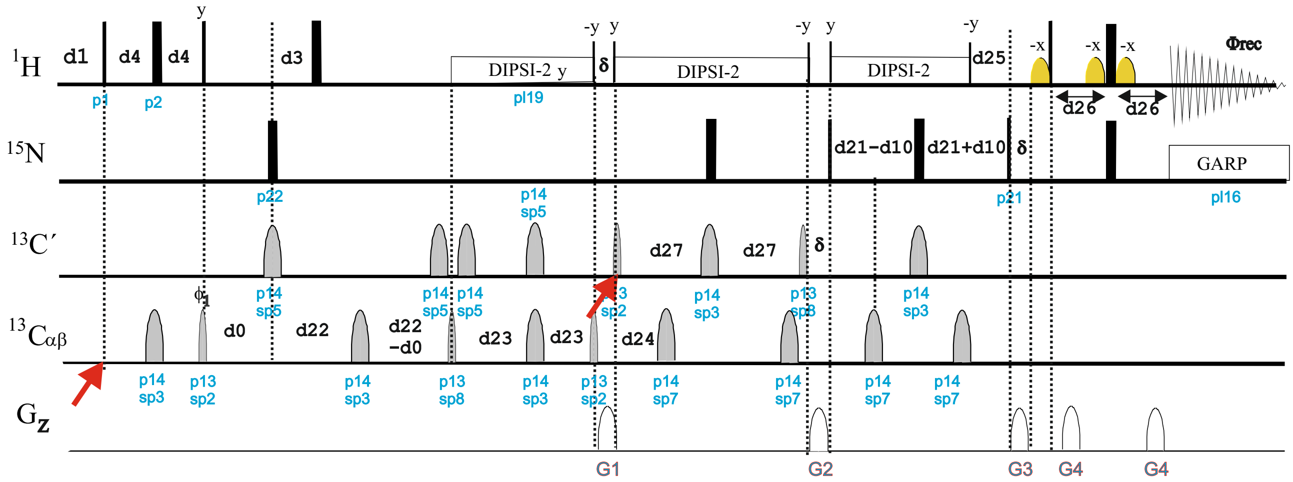
cbcaconhgp3d



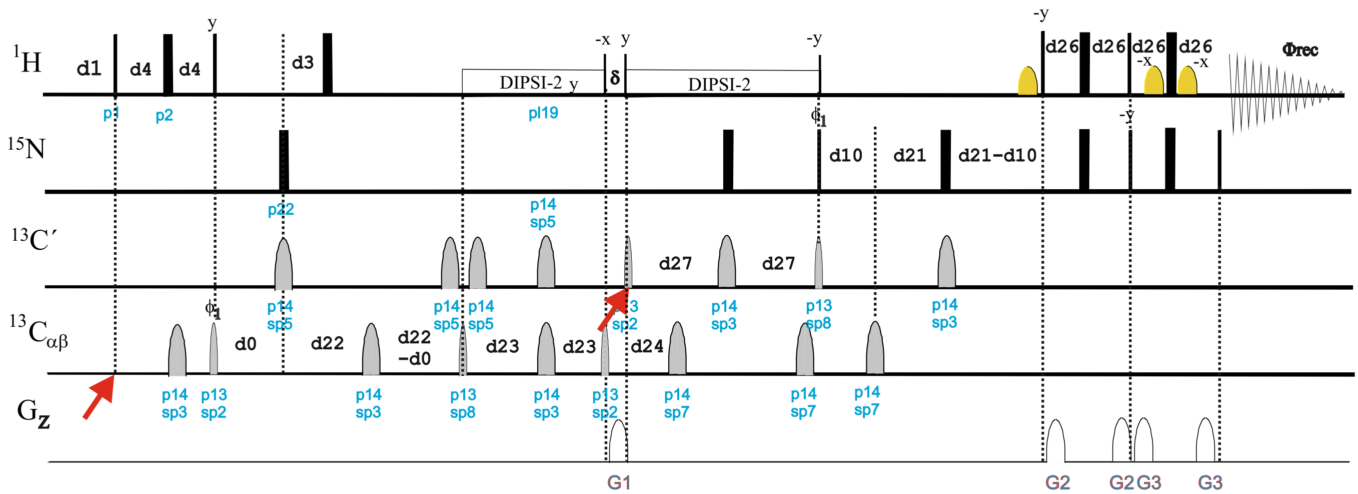
d4=1/4J(CH)=1.7m	d27=1/4J(NCO)=12.4m
d3=1/6J(CH)=1.1m	d21=1/4J(NCO)=12.4m
d22=1/4J(CBCA)=3.6m	d25=1/2J(NH)=5.5m
d23=1/4J(CBCA)=3.6m	d26=1/4J(NH)=2.3m
d24=1/4J(CACO)=4.4m	



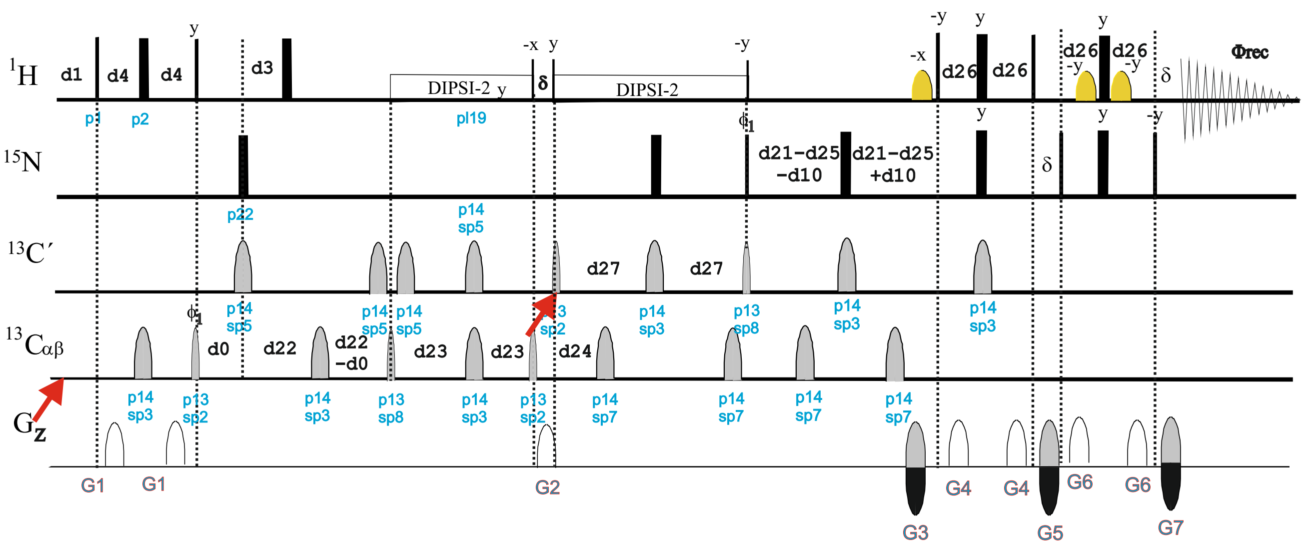
cbcaconhgpwg3d



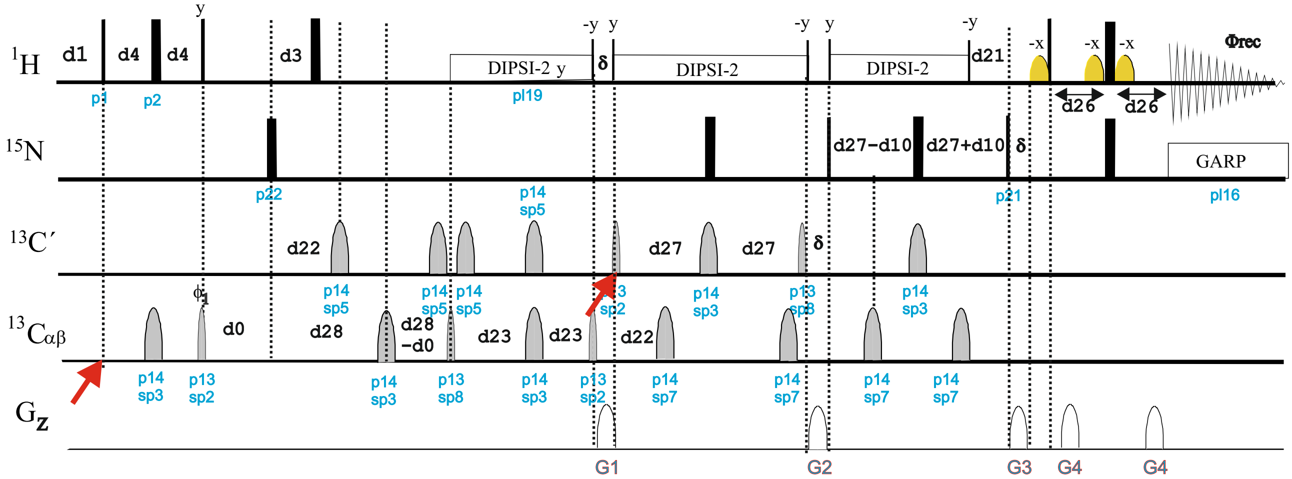
trcbcaconhgp3d



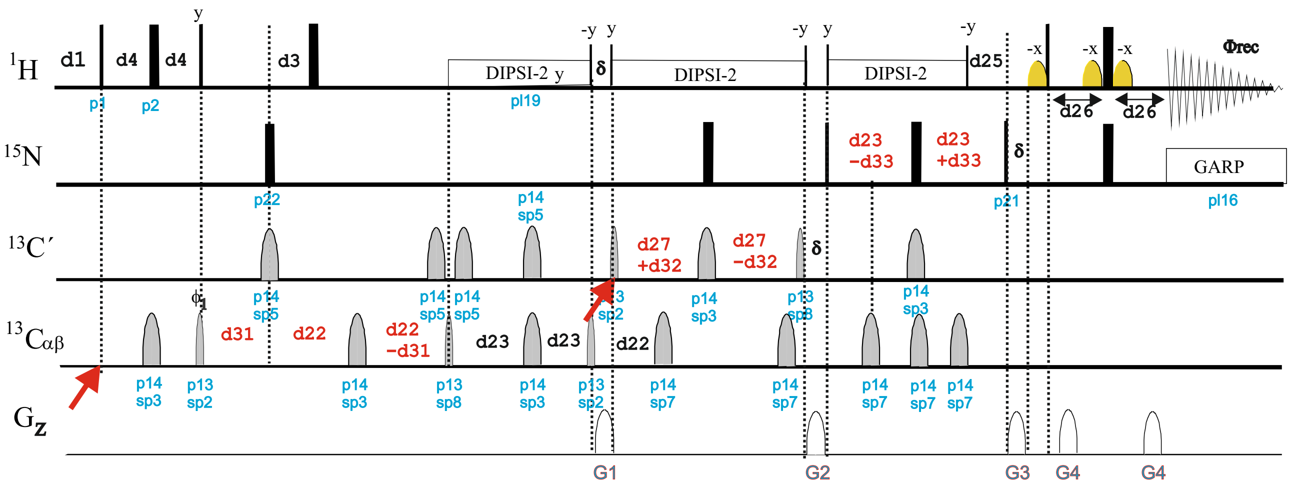
trcbcaconhetgp3d



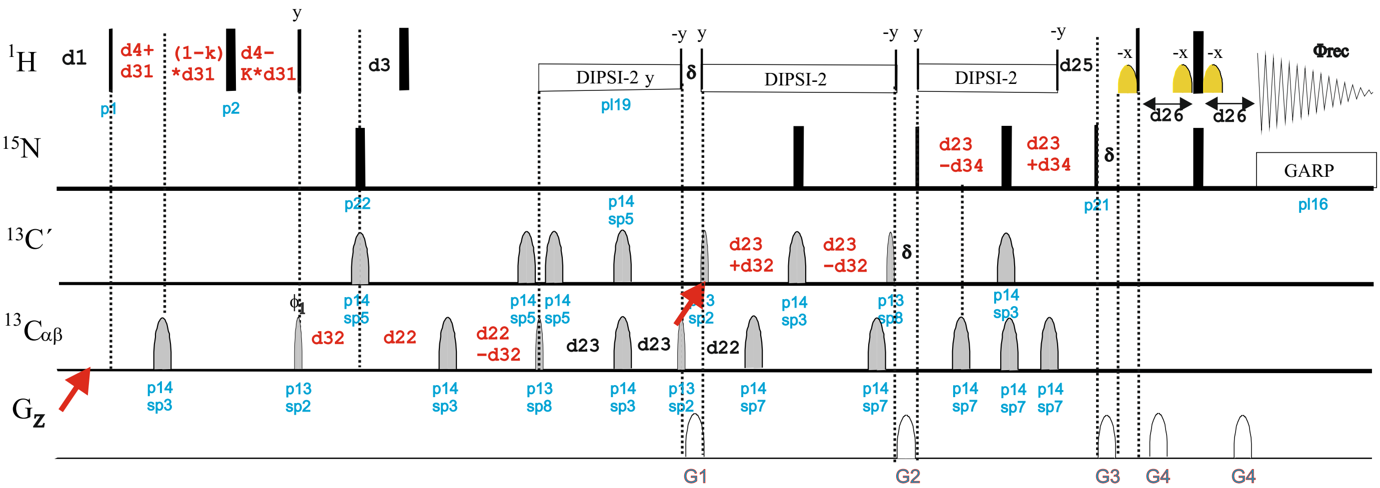
cbcaconhgpwg3d.2



cbcaconhgpwg4d



hbhacbcaconhgpwg5d



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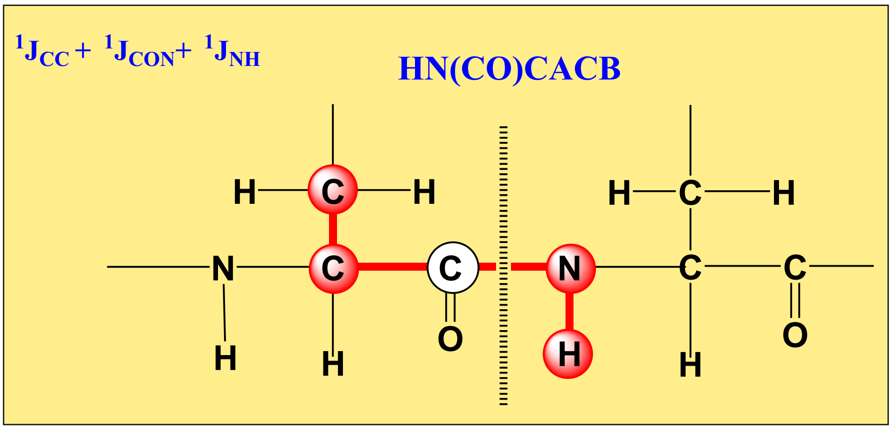
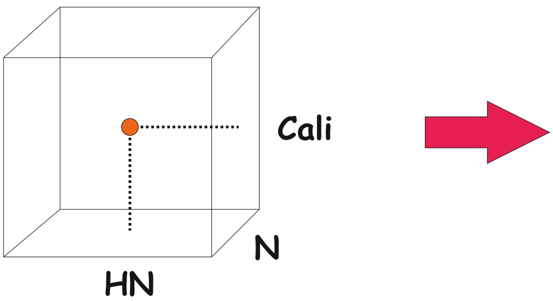
3D HN(CO)CACB

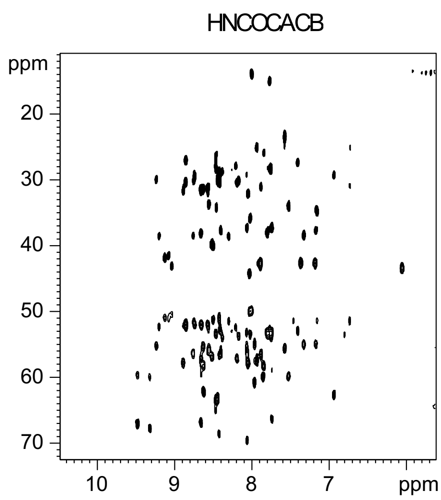
3D HN(CO)CACB experiment

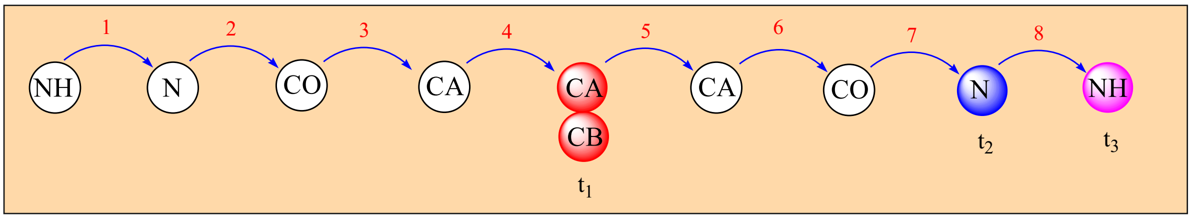
- 3D HN(CO)CACB using PEP (**hncocacbgp3d** | HNCOCACBGP3D):
  - with ^{2}H-decoupling (**hncocacbgp2h3d** | HNCOCACBGP2H3D)
- 3D HN(CO)CACB using WATERGATE (**hncocacbgpwg3d** | HNCOCACBGPWG3D)
  - with ^{2}H-decoupling (**hncocacbgpwg2h3d** | HNCOCACBGPWG2H3D)
- 3D HN(CO)CACB using TROSY (**trhncocacbgp3d** | TRHNCOCACBGP3D):
  - with ^{2}H-decoupling (**trhncocacbgp2h3d** | TRHNCOCACBGP2H3D)
  - using gradient echo-antiecho (**trhncocacbetgp3d** | TRHNCOCACBETGP3D)
  - using gradient echo-antiecho and with ^{2}H-decoupling (**trhncocacbetgp2h3d** | TRHNCOCACBETGP2H3D)

Also see:
APSY-HNCOCACB experiment
Reduced-Dimensionality (3,2)-HNCOCACB (rd_hncocacb_32 | APSY_HNCOCACB_32)
SOFAST/BEST-HNCOCACB experiment
3D BEST-HN(CO)CACB (b_hncocacbgp3d | B_HNCOCACBGP3D)
3D BEST-HN(CO)CACB using TROSY (b_trhncocacbgp3d)
4D BEST-HNCOCACB (b_hncocacbgp4d)
3D HNCACB and CBCA(CO)NH experiments

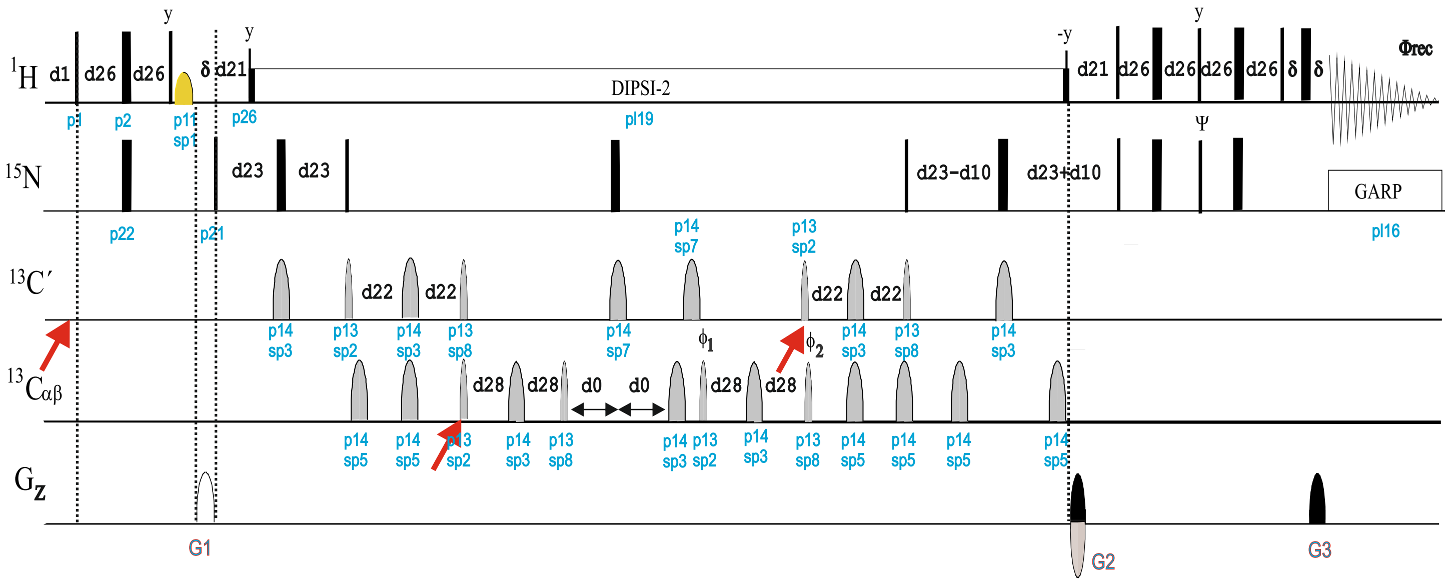




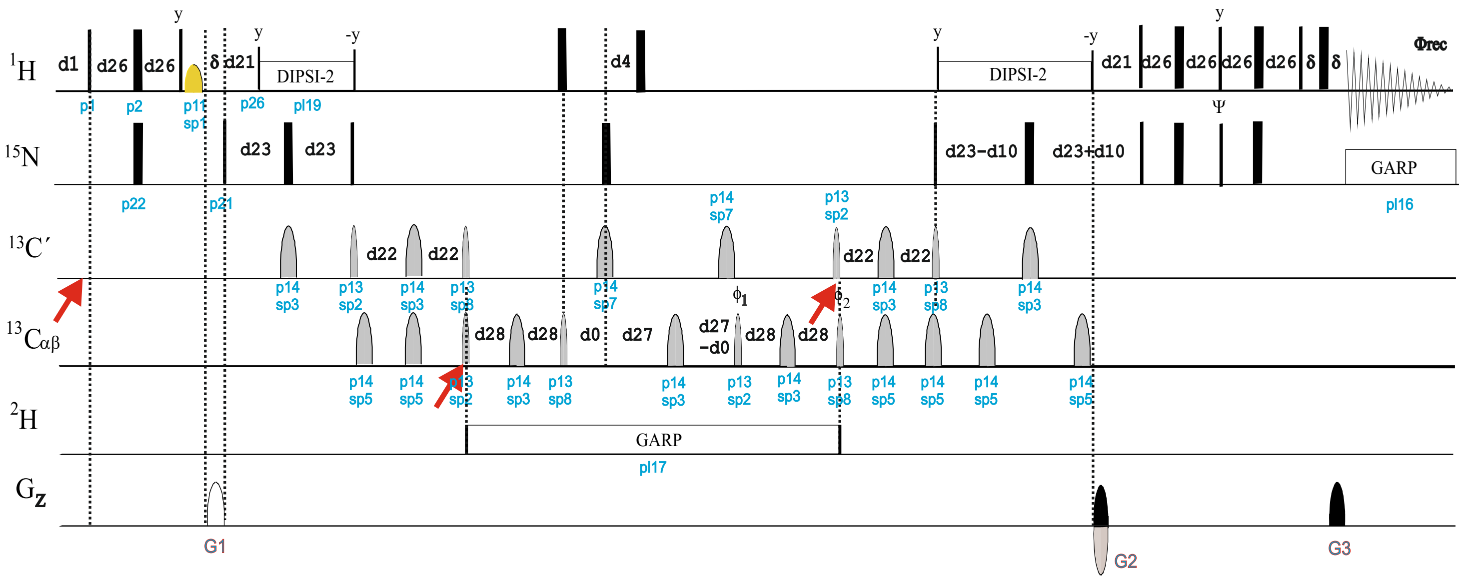




hncocacbgp3d

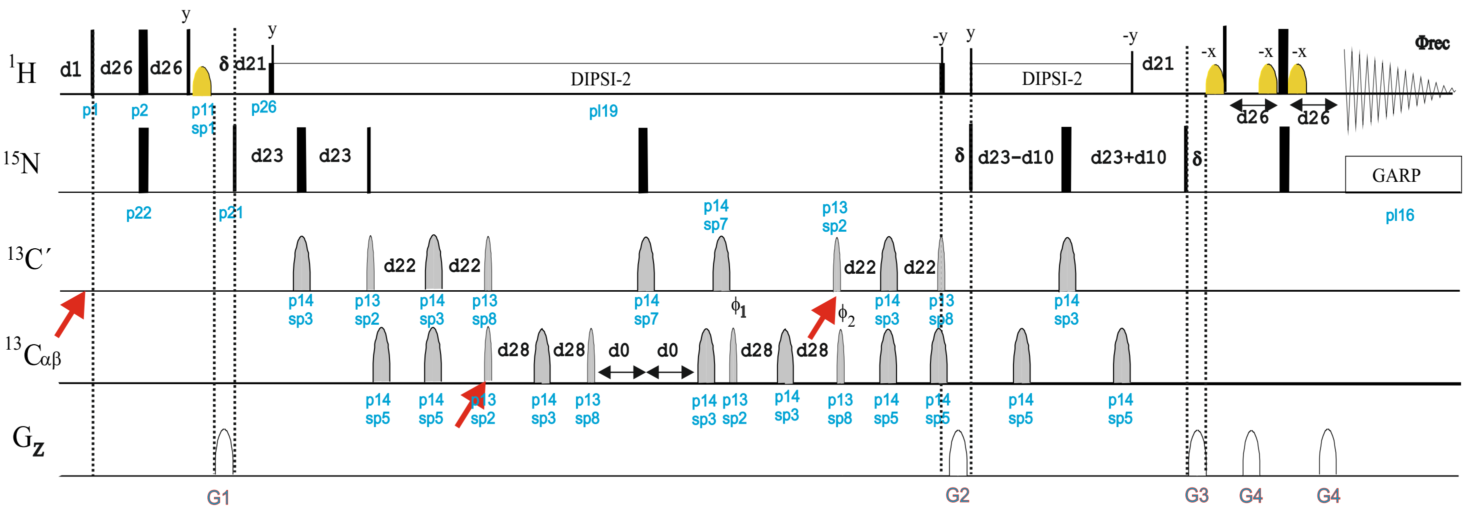


hncocacbgp2h3d



d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m
d22=1/4J(CACO)=4m
d28=1/4J(CACB)=3.6m

hncocacbgpwg3d



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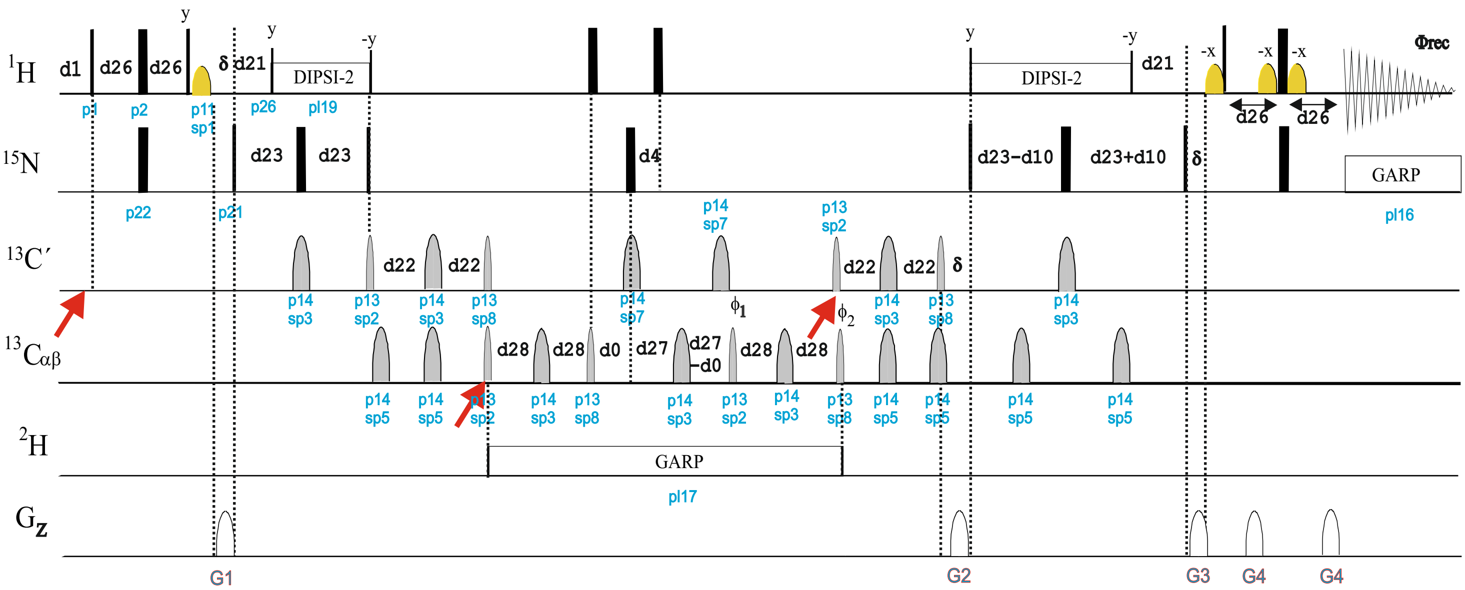
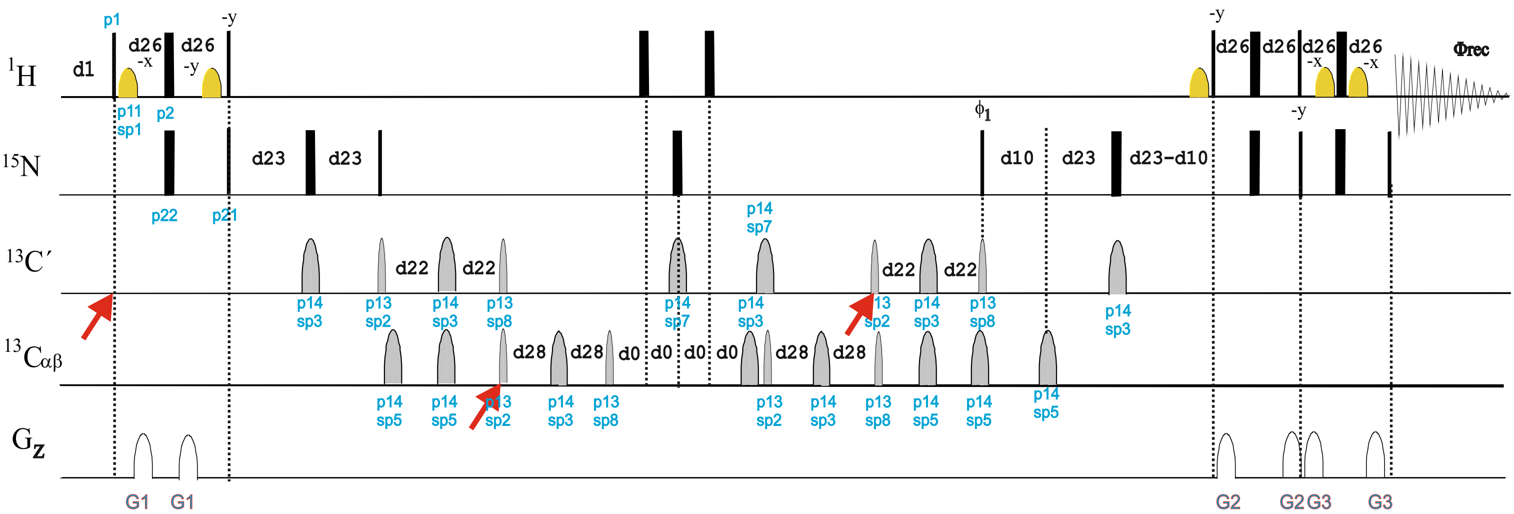


trhncocacbgp3d



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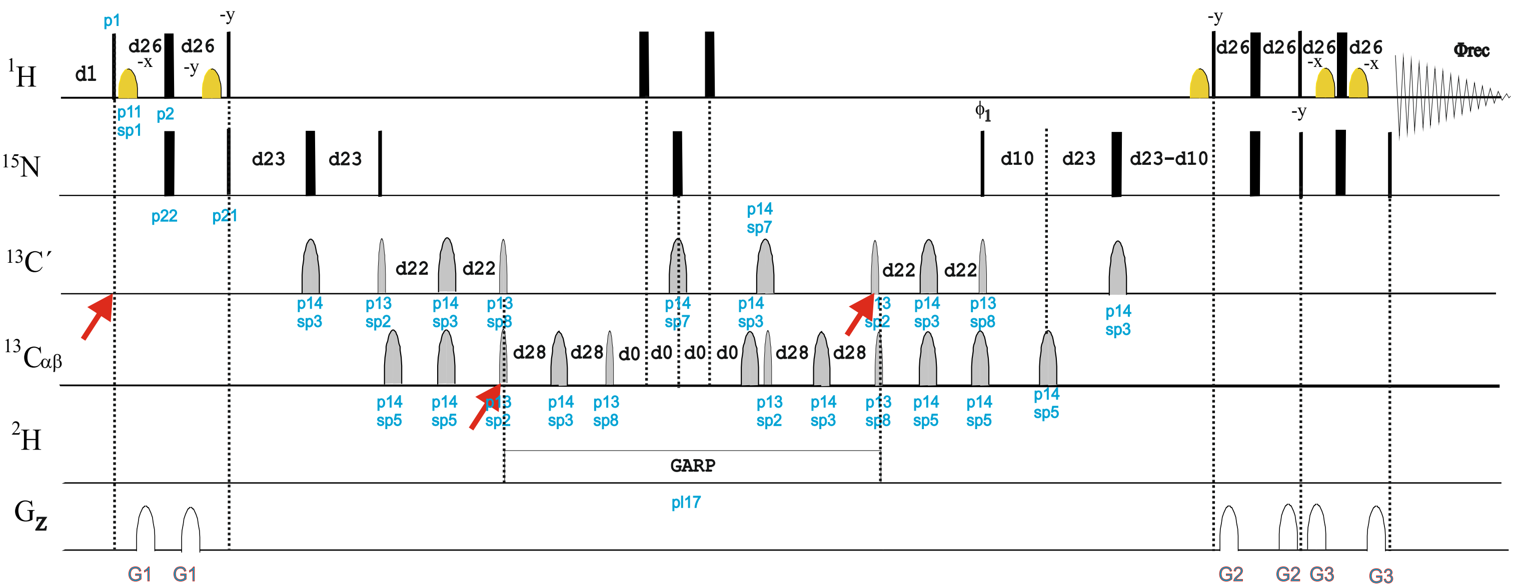
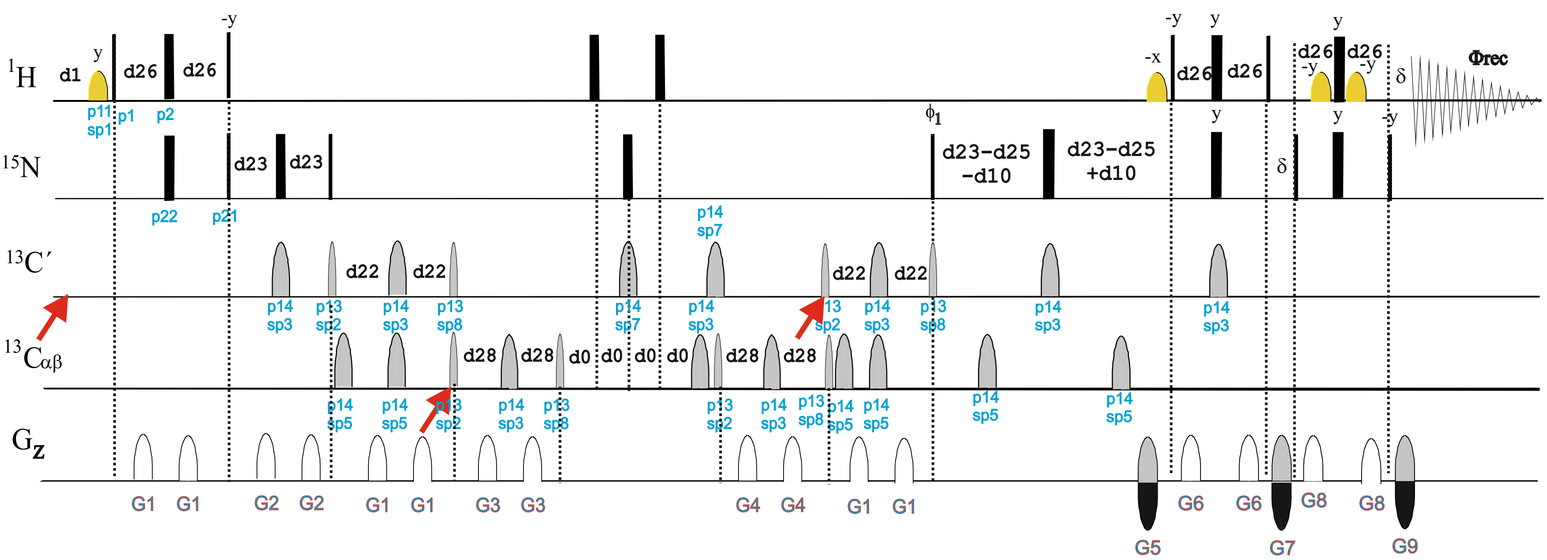
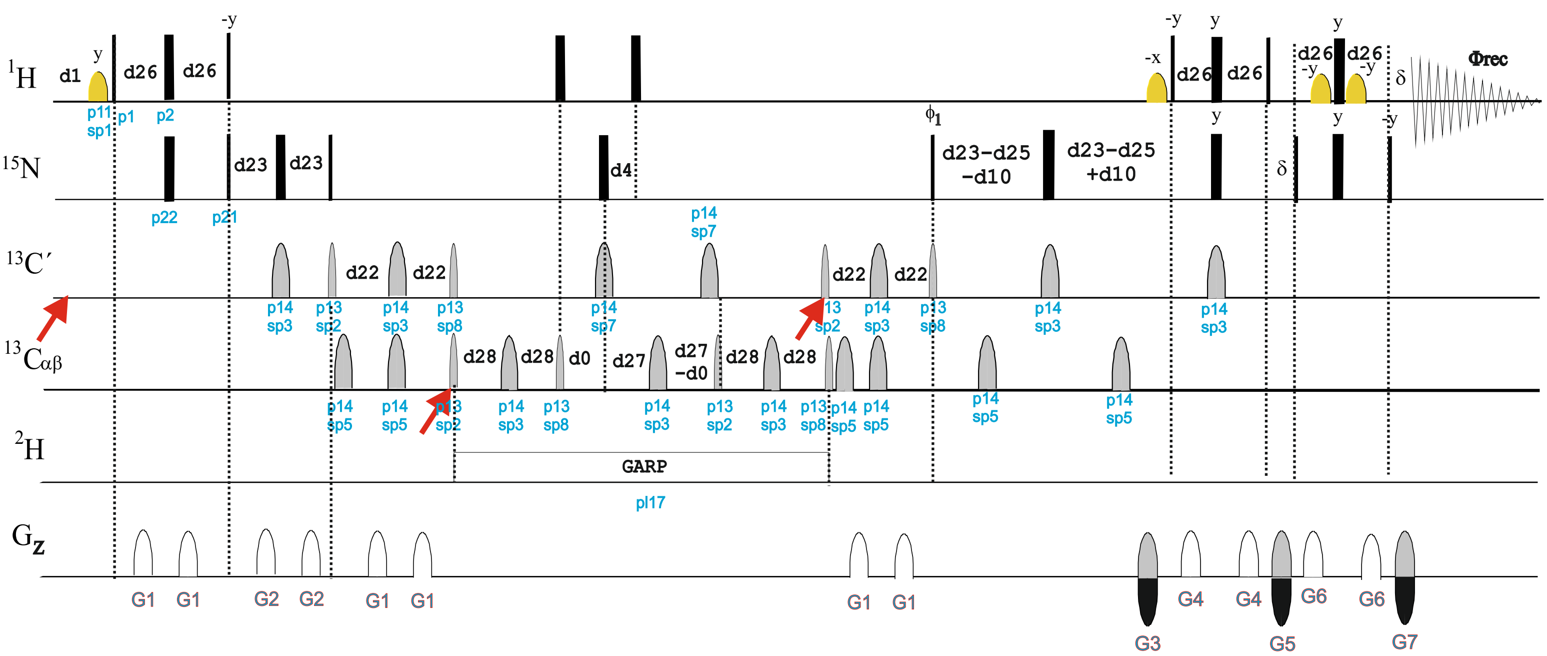


trhncocacbetgp3d



trhncocacbetgp2h3d



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3D CBCANH

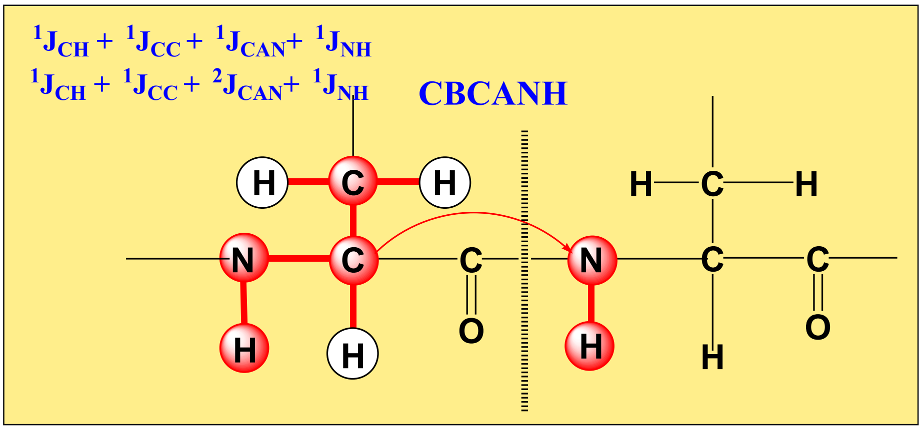
CBCANH experiment

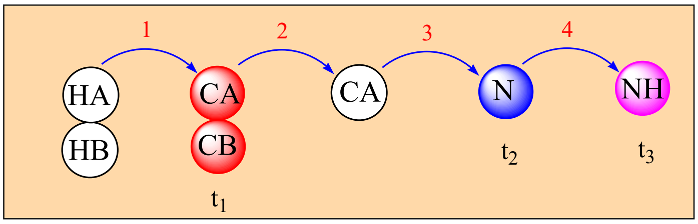
- 3D CBCANH using PEP (**cbcanhgp3d** | CBCANHGP3D)
- 3D CBCANH using WATERGATE (**cbcanhgpwg3d** | CBCANHGPWG3D)
- 3D CBCANH using TROSY (**trcbcanhgp3d** | TRCBCANHGP3D)
- 3D CBCANH using TROSY and gradient echo-antiecho (**trcbcanhetgp3d** | TRCBCANHETGP3D)

- 4D HBHACBCANH using WATERGATE (**hbhacbcanhgpwg4d**)

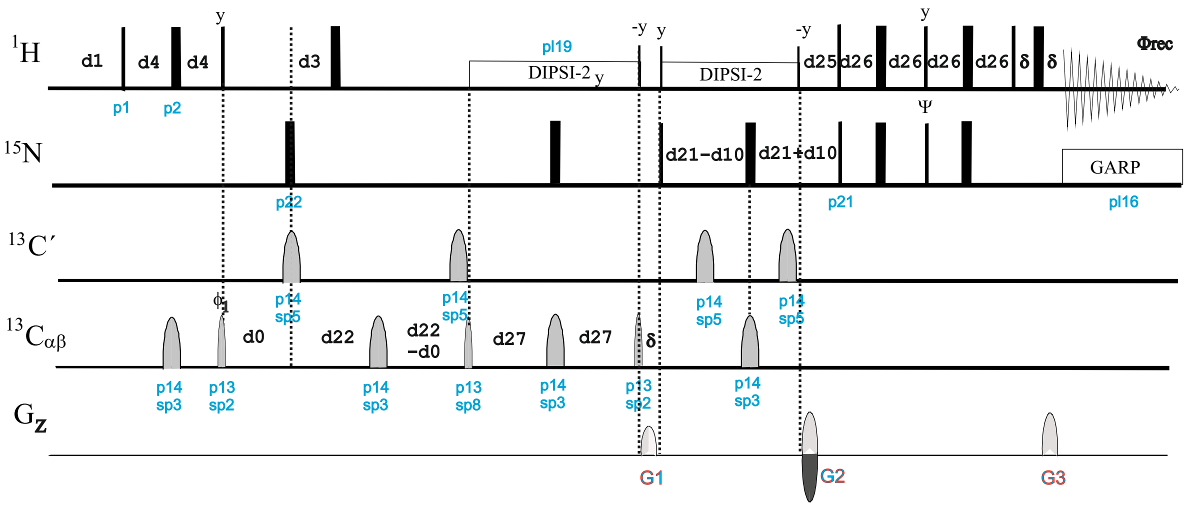
Also see:
HNCACB experiments
Sequential CBCANH experiments
CBCA(CO)NH experiments
CCANH experiments

References:
S. Grzesiek & A. Bax, J. Magn. Reson. 99, 201-207 (1992)

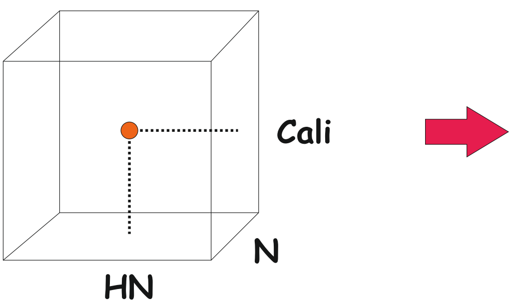


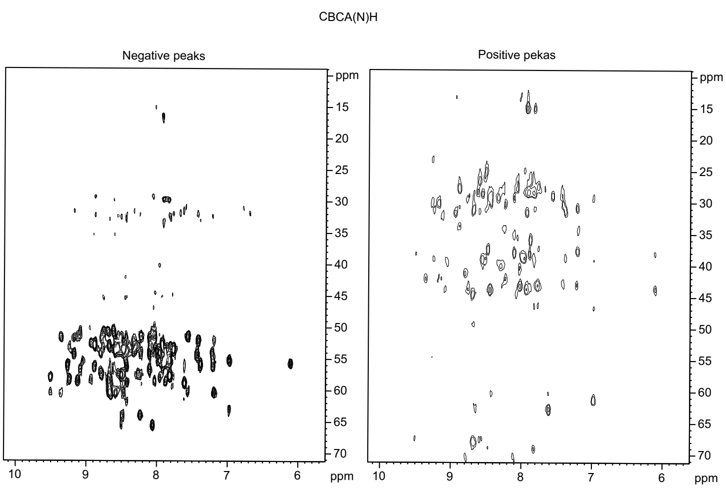


cbcanhgp3d

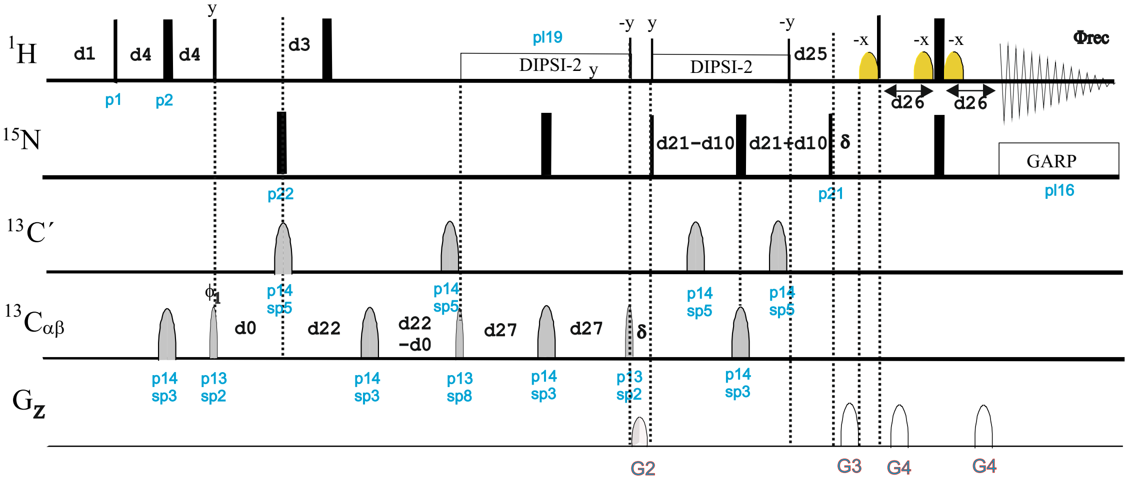


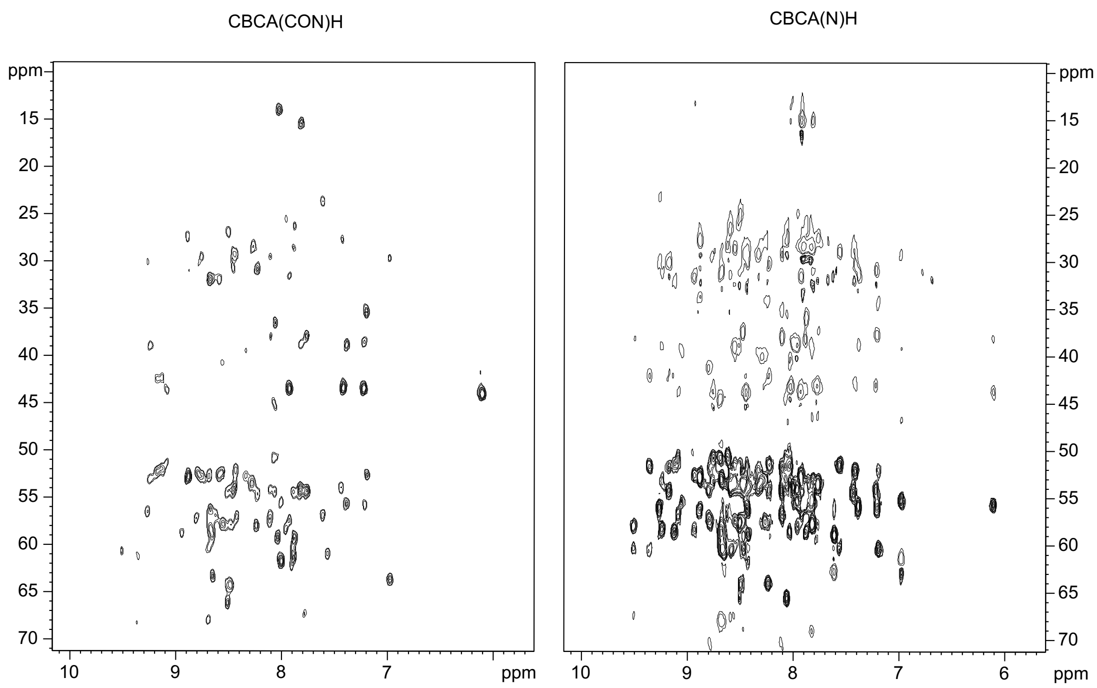
d4=1/4J(CH)=1.7m
d3=1/6J(CH)=1.1m
d22=1/4J(CBCA)=3.6m
d27=1/4J(NCO)=11m
d21=1/4J(NCO)=12.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m



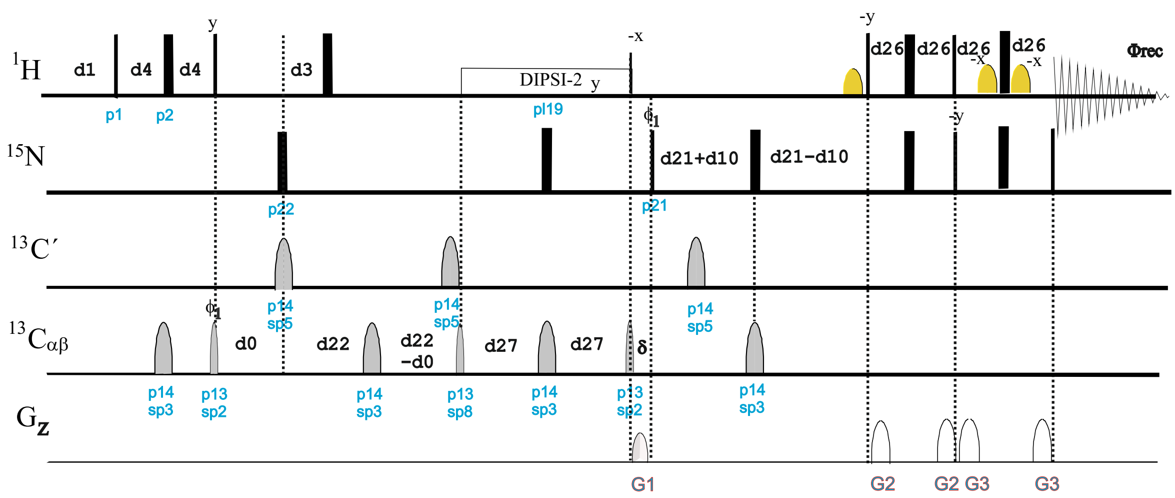


cbcanhgpwg3d

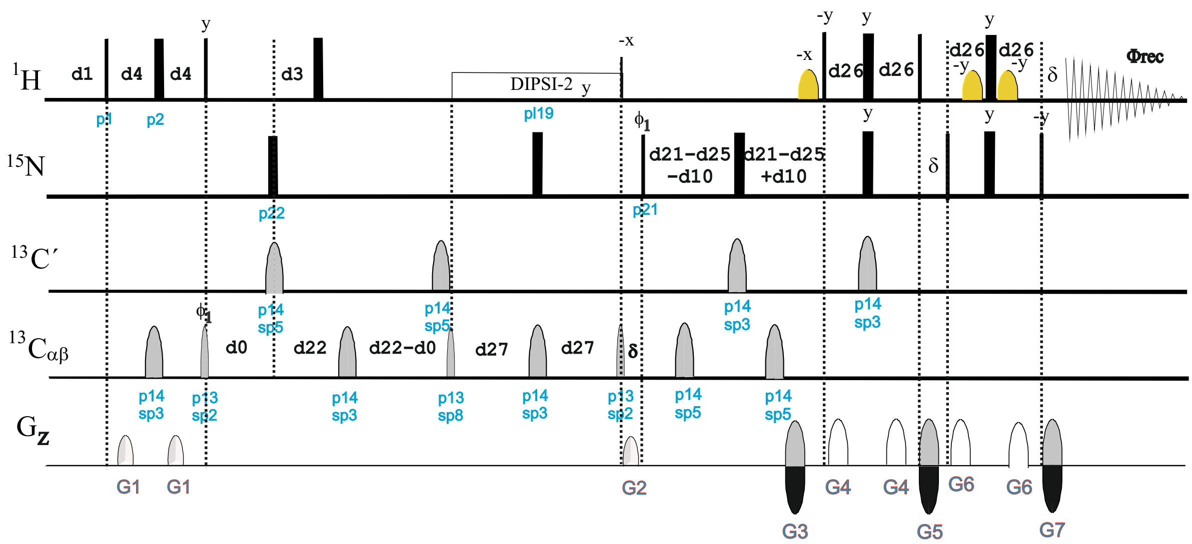




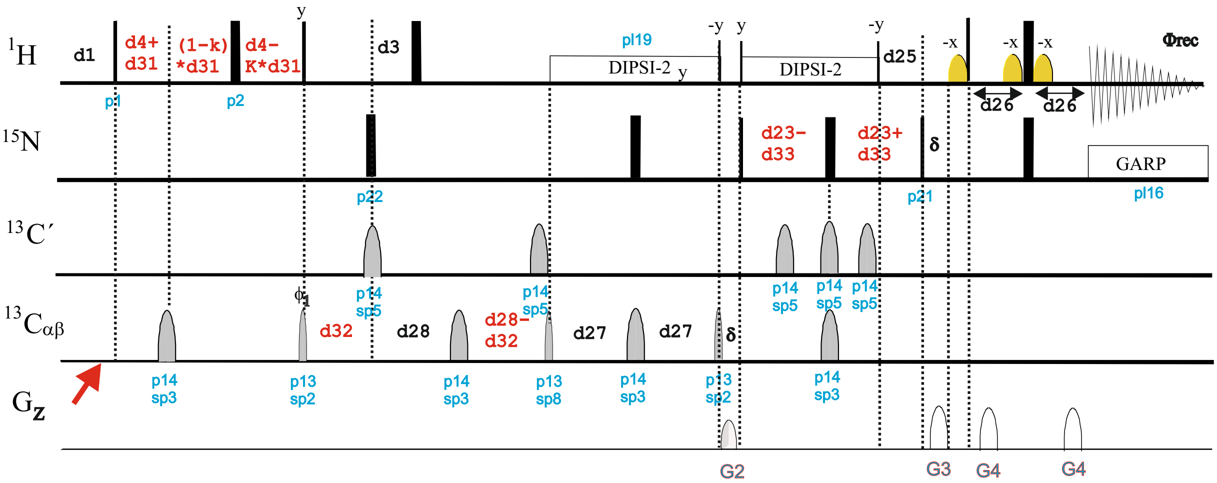
trcbcanhgp3d



trcbcanhetgp3d



hbhacbcanhgpwg4d



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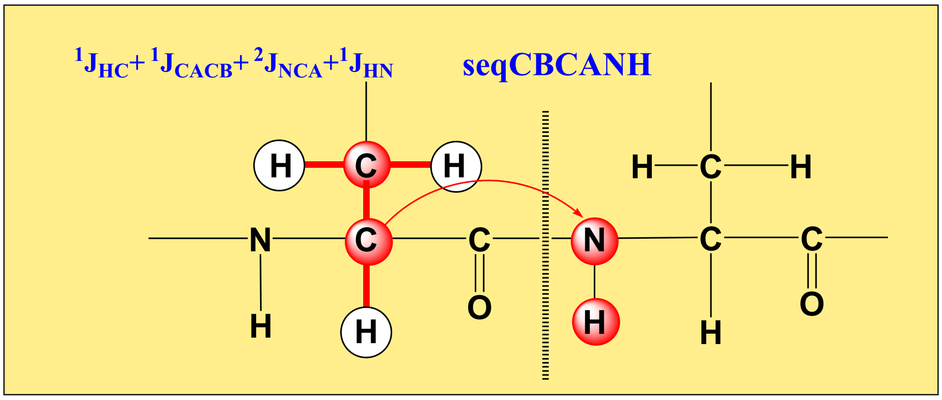
3D SEQUENTIAL CBCANH

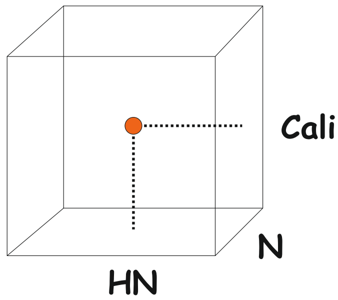
3D Sequential CBCANH experiment

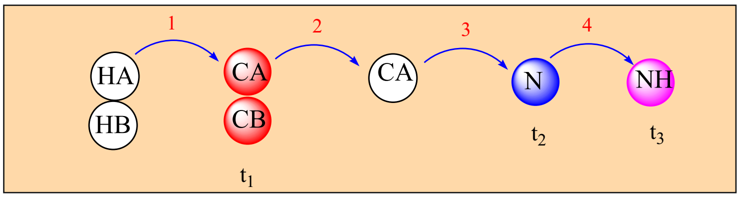
- 3D Sequential CBCANH using TROSY (**seqtrcbcanhgp3d** | SEQTRCBCANHGP3D)

Also see:
CBCANH experiments
Sequential HNCACB experiment

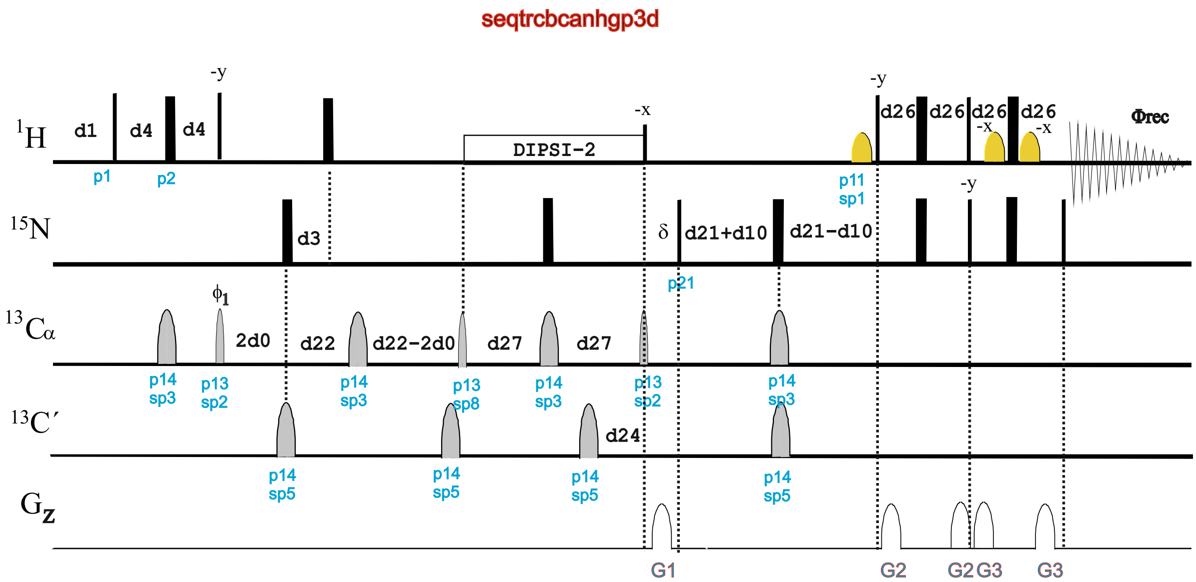
Ref: A. Meissner & O.W. Sorensen, J. Magn. Reson. 151, J. Biomol. NMR 20, 188-180 (2001))







d26=1/4J(NH)=2.3m
d21=1/4J(NCA)=12.4m
d22=1/8J(CACB)=3.6m
d27=1/4J(NCA)=11m
d24=1/4J(CACO)=4.5m
d4=1/4J(CH)=1.7m
d3=1/6J(CH)=1.1m



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3D HNCACB

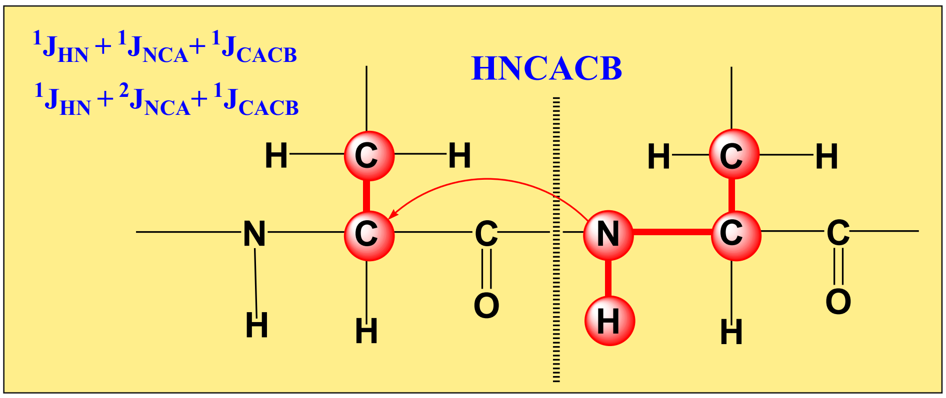
3D HNCACB experiment

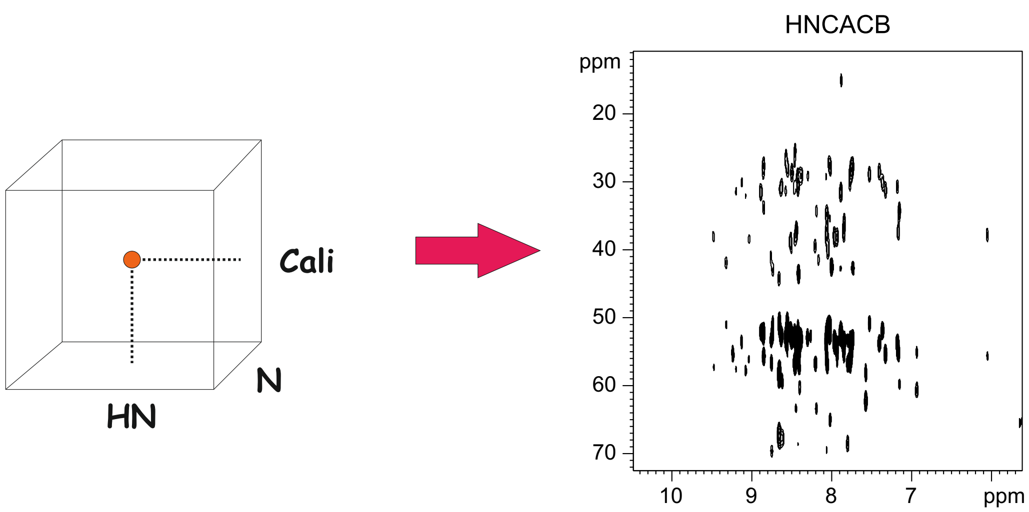
- 3D HNCACB using PEP (**hncacbgp3d** | HNCACBGP3D):
  - with ^{2}H-decoupling (**hncacbgp2h3d** | HNCACBGP2H3D)
- 3D HNCACB using WATERGATE (**hncacbgpwg3d** | HNCACBGP2H3D)
  - with ^{2}H-decoupling (**hncacbgpwg2h3d** | HNCACBGPWG2H3D)
- 3D HNCACB using TROSY (**trhncacbgp3d** | TRHNCACBGP3D) :
  - with ^{2}H-decoupling (**trhncacbgp2h3d** | TRHNCACBGP2H3D)
  - with gradient echo-antiecho (**trhncacbetgp3d** | TRHNCACBETGP3D)
  - with gradient echo-antiecho and with ^{2}H-decoupling (**trhncacbetgp2h3d** | TRHNCACBETGP2H3D)

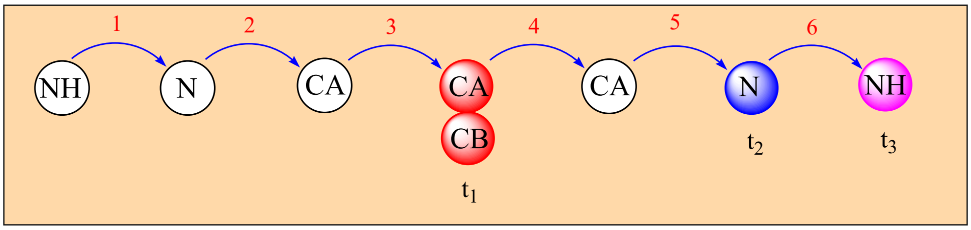
Also see:
3D APSY-HNCACB experiment
Reduced-Dimensionality (3,2)-HNCACB (**rd_hncacb_32** | **APSY_HNCACB_32)**
3D SOFAST/BEST-HNCACB experiment
3D BEST-HNCACB (**b_hncacbgp3d** | **B_HNCACBGP3D**)
3D BEST-HNCACB using TROSY (**b_trhncacbgp3d**)
3D HNCACB for J Measurements
3D HNCACB[CO]-E.COSY (**hncacbgpjc3d** | HNCACBGPJC3D) - 3J[CO-CB] via E.COSY

3D HNCA(CO)CB and CBCANH experiments
3D intra-HNCACB & 3D sequential-HNCACB experiments

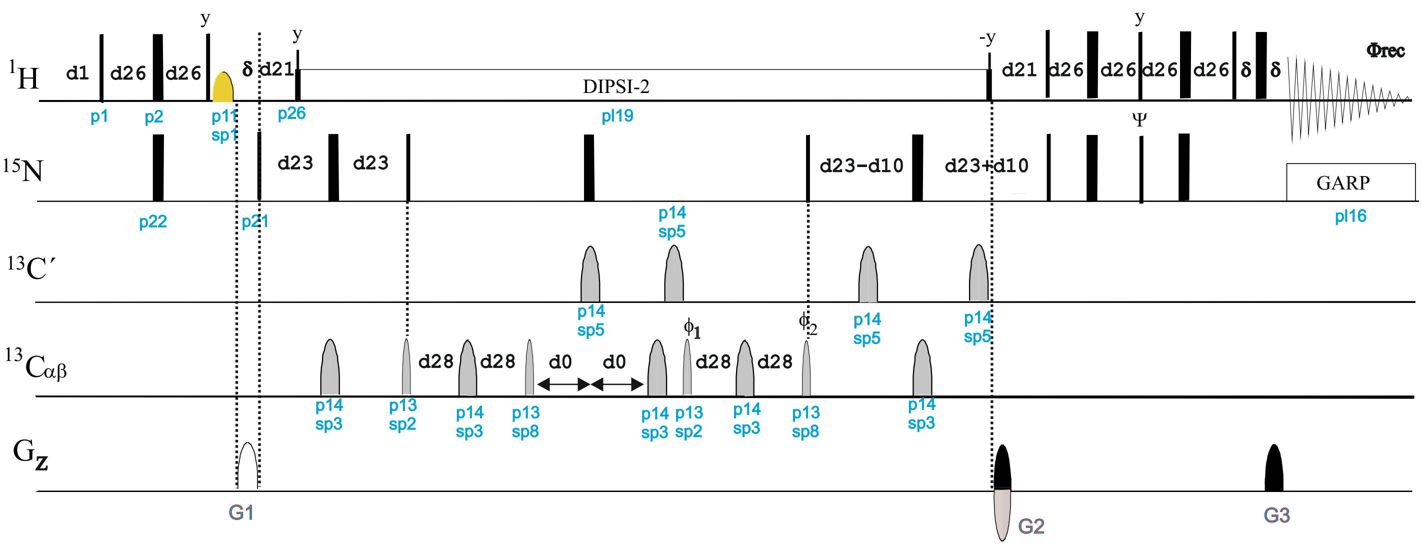
1. M. Wittekind & L. Mueller, J. Magn. Reson. B 101, 201-205 (1993)
2. D.R. Muhandiram & L.E. Kay, J. Magn. Reson. B 103, 203-216 (1994)





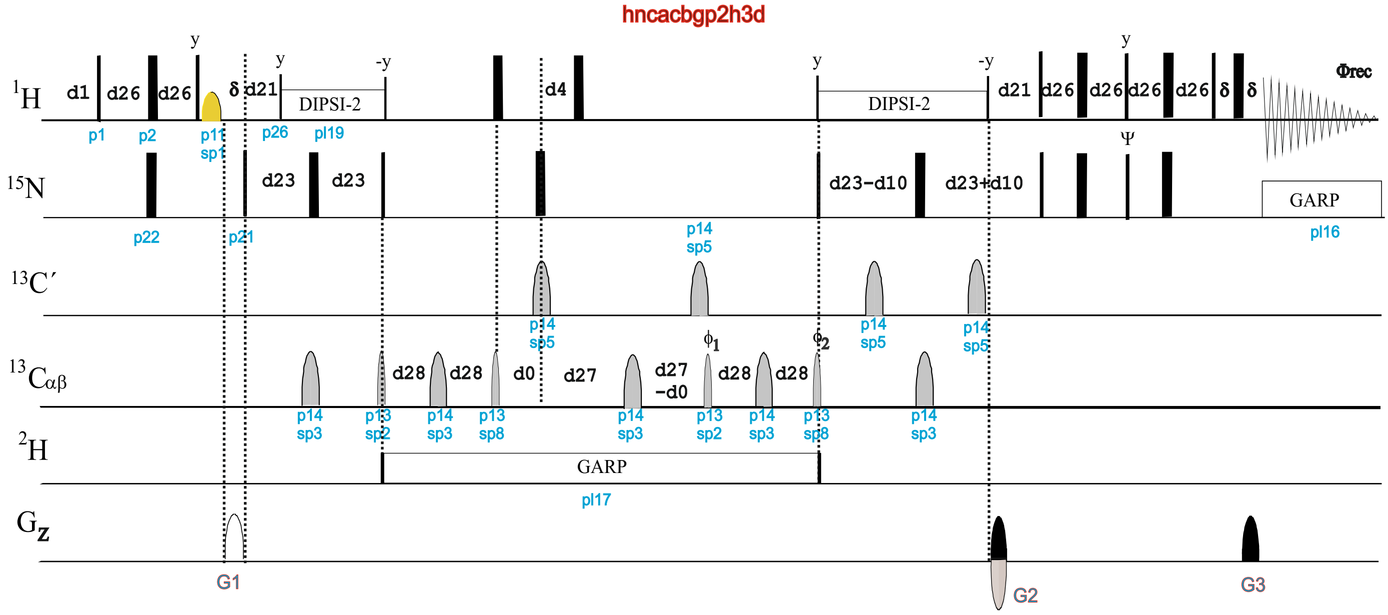


hncacbgp3d



d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12.4m
d28=1/4J(CACB)=3.6m
if ZGOPTNS=LABEL_CB d28=7.2m

hncacbgp2h3d



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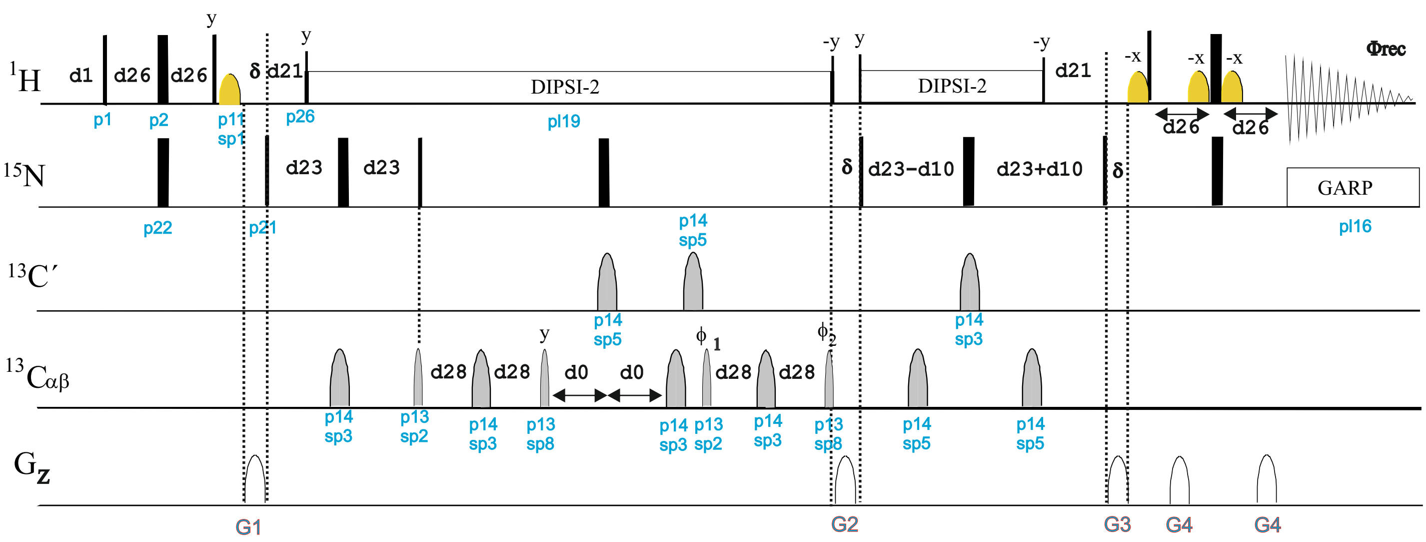

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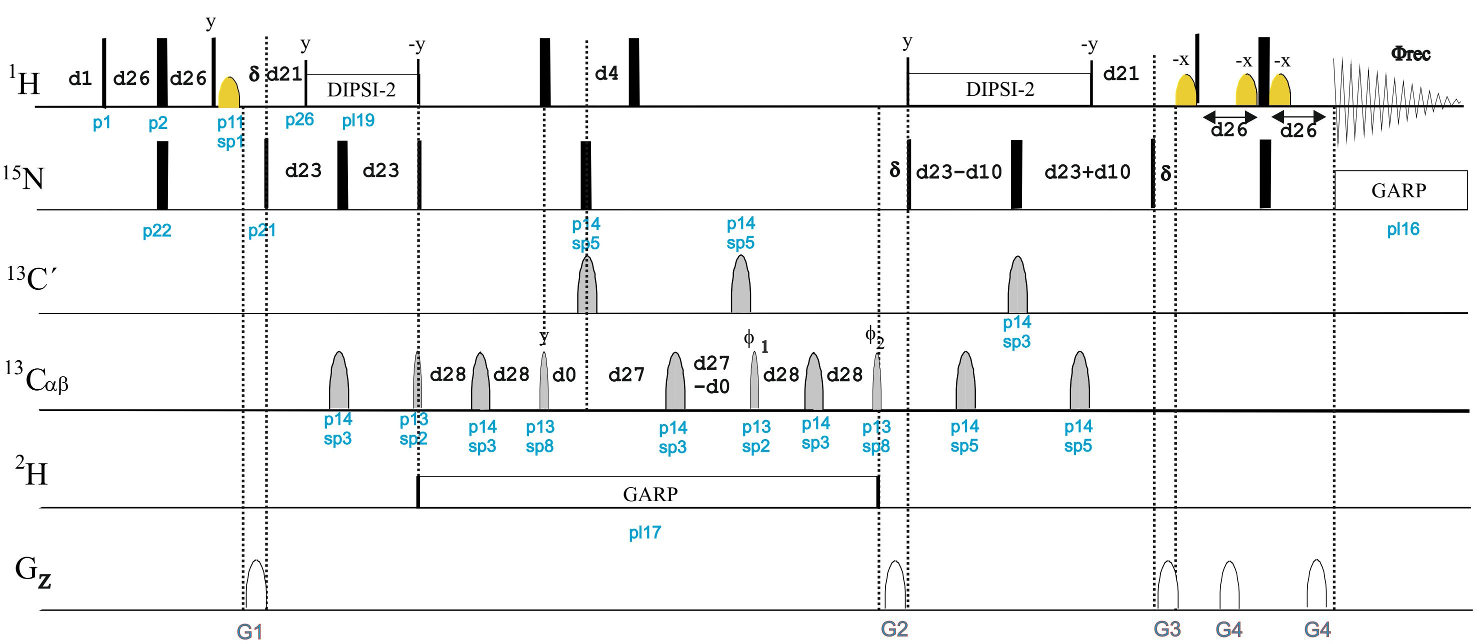
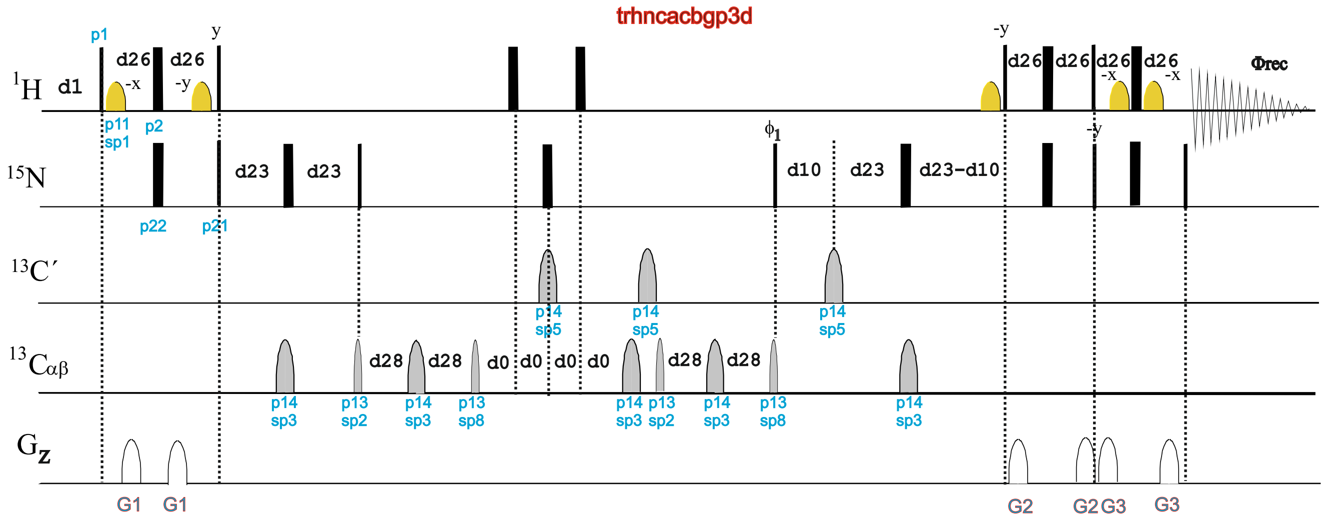
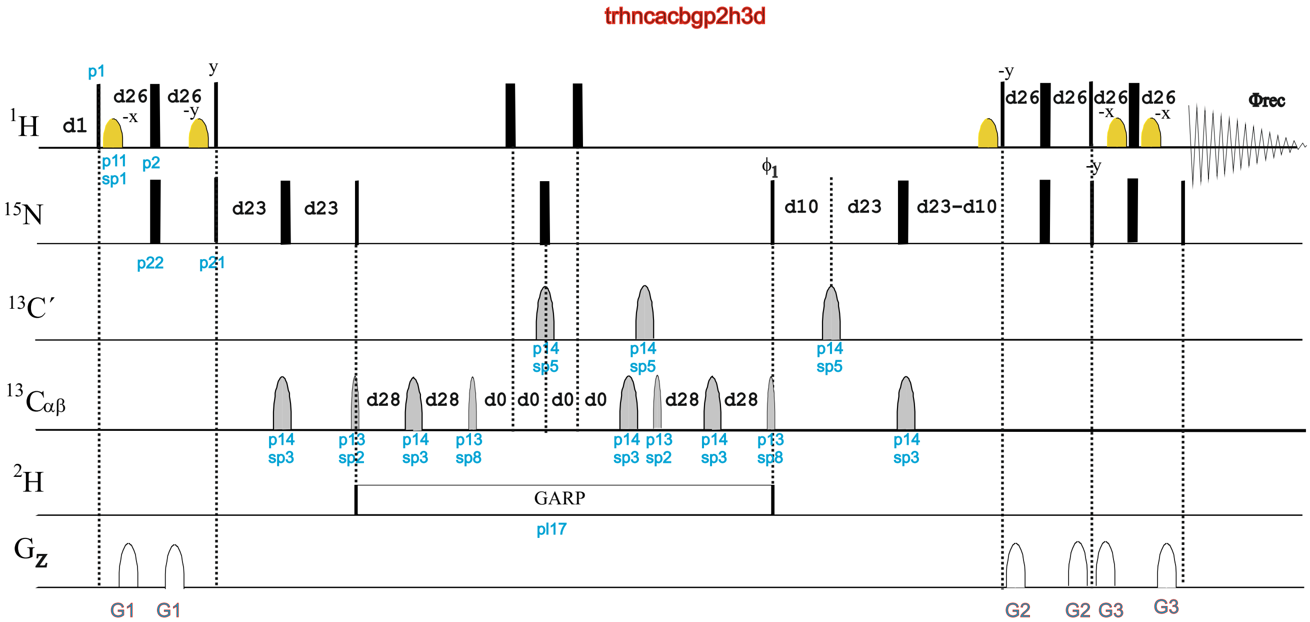
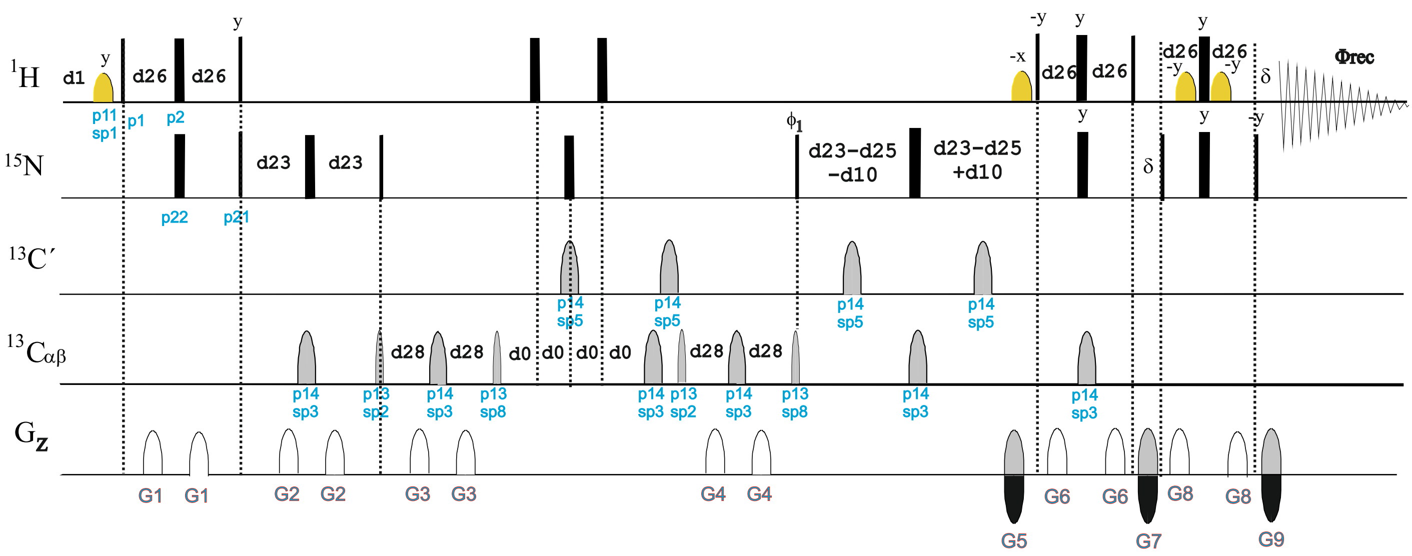



trhncacbgp3d
1H
15N
13C′
13Cαβ
Gz
d1
d26
d23
d28
d0
d10
d23-d10
Φrec
G1
G2
G3


trhncacbgp2h3d
1H
15N
13C′
13Cαβ
2H
Gz
GARP
pl17
G1
G2
G3

trhncacbetgp3d



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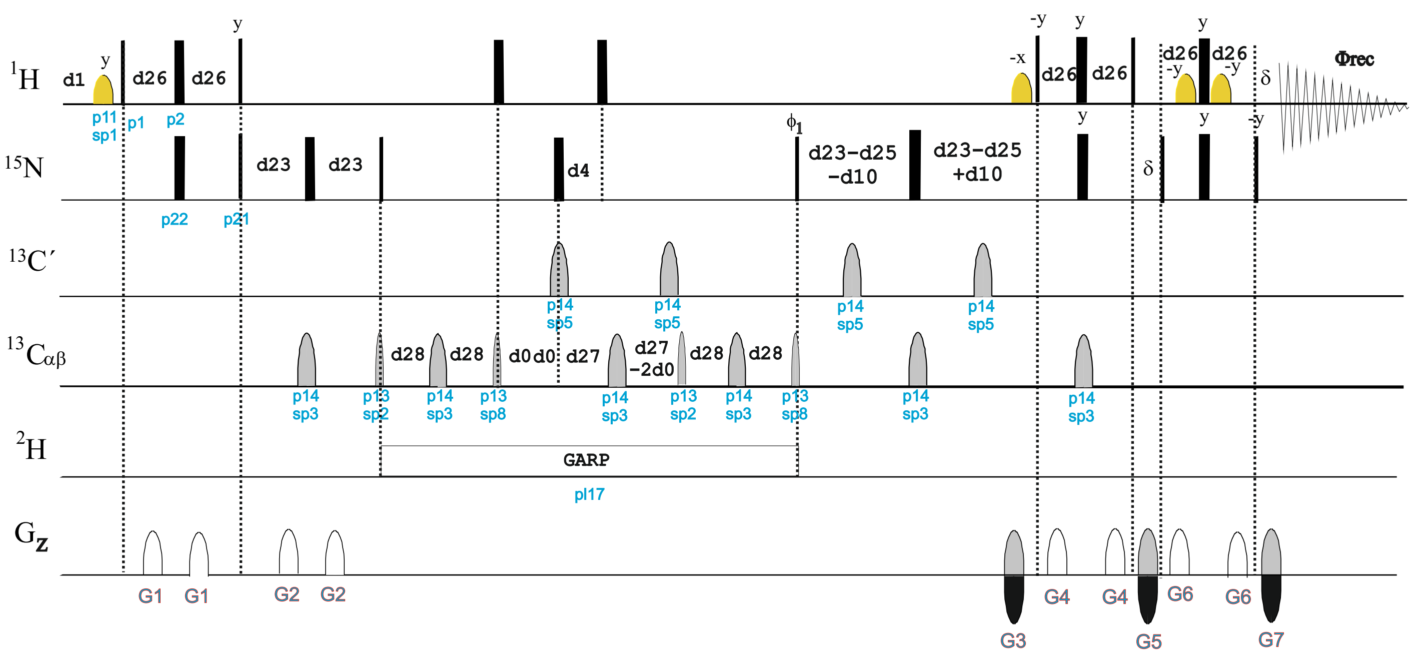

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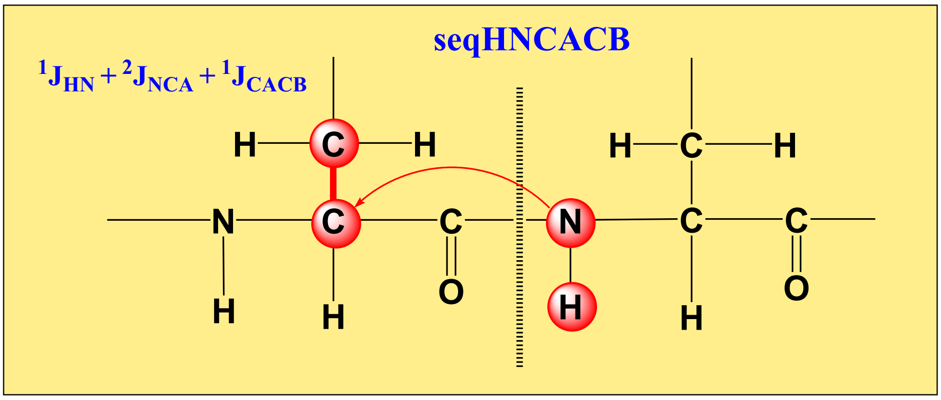
3D SEQUENTIAL HNCACB

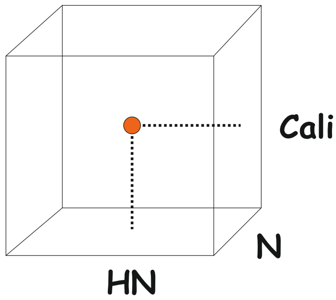
3D Sequential-HNCACB experiment

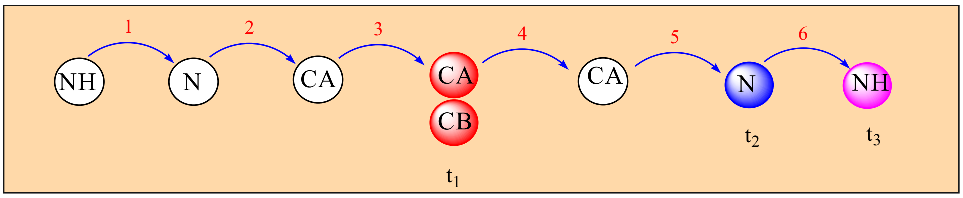
- 3D Sequential HNCACB using TROSY (**seqtrhncacbgp3d** | SEQTRHNCACBGP3D)
  - with ^{2}H-decoupling (**seqtrhncacbgp2h3d** | SEQTRHNCACBGP2H3D)
  - Using gradient echo-antiecho (**seqtrhncacbetgp3d** | SEQTRHNCACBETGP3D)
  - Using gradient echo-antiecho and with ^{2}H-decoupling (**seqtrhncacbetgp2h3d** | SEQTRHNCACBETGP2H3D)

Also see:
3D HNCACB and intra-HNCACB experiments
3D sequential CBCANH experiments

References:
A. Eletsky, A. Kienhoefer & K. Pervushin, J. Biomol. NMR 20, 188-180 (2001)

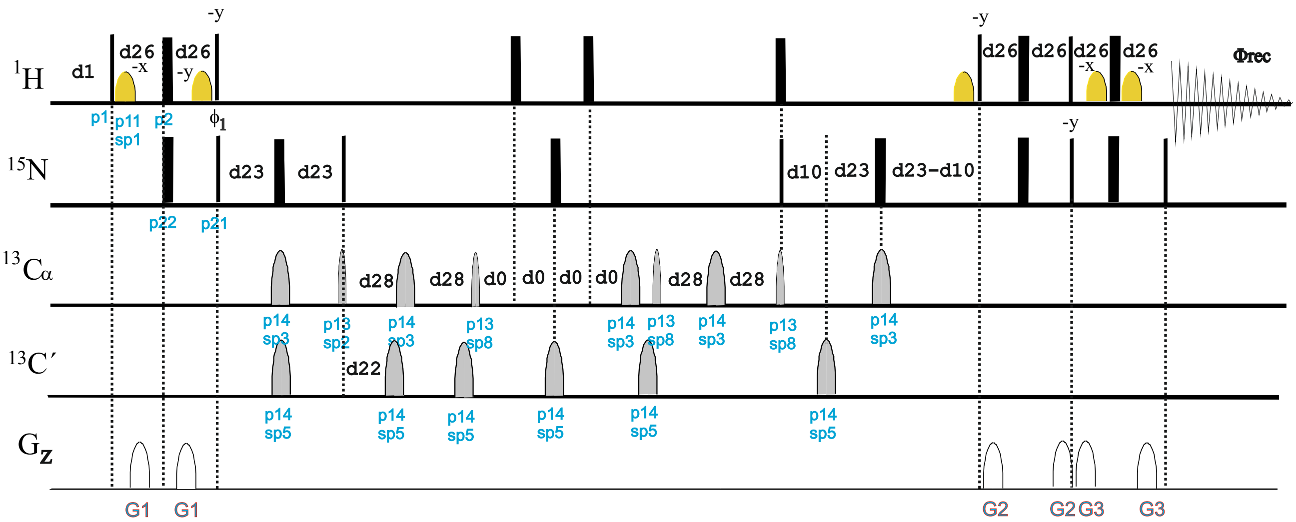




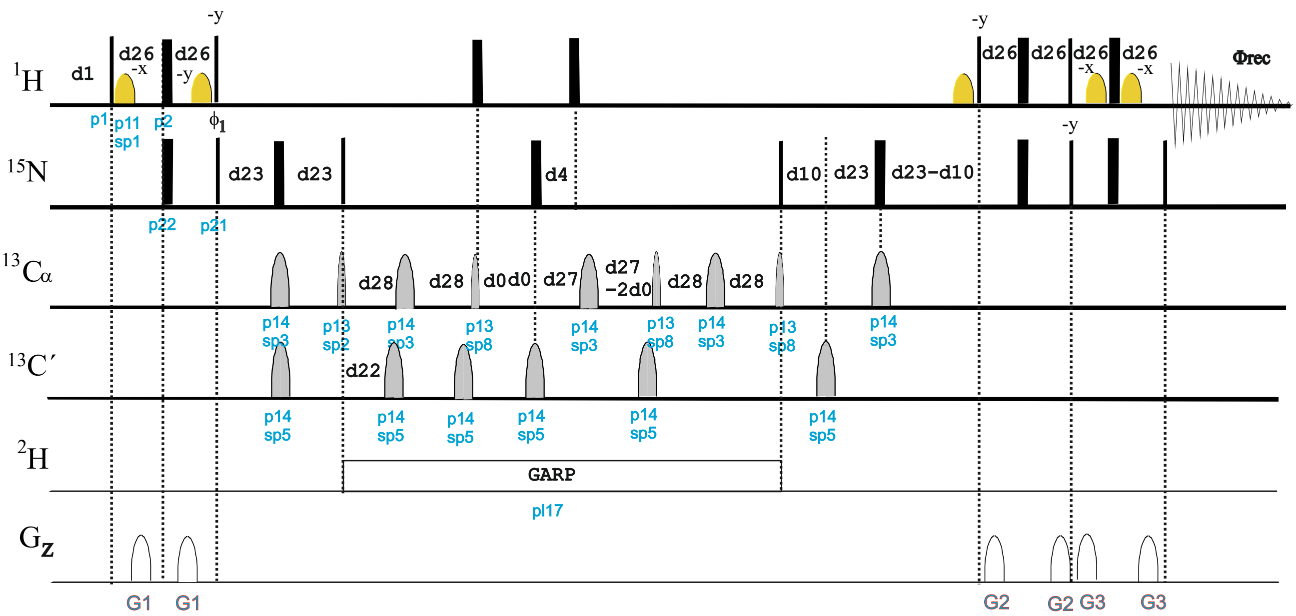


d26=1/4J(NH)=2.3m
d23=1/4J(NCA)=12m
d22=1/4J(CACO)=4.5m
d28=1/8J(CACB)=5m
d25=1/4J(NH)=2.3m

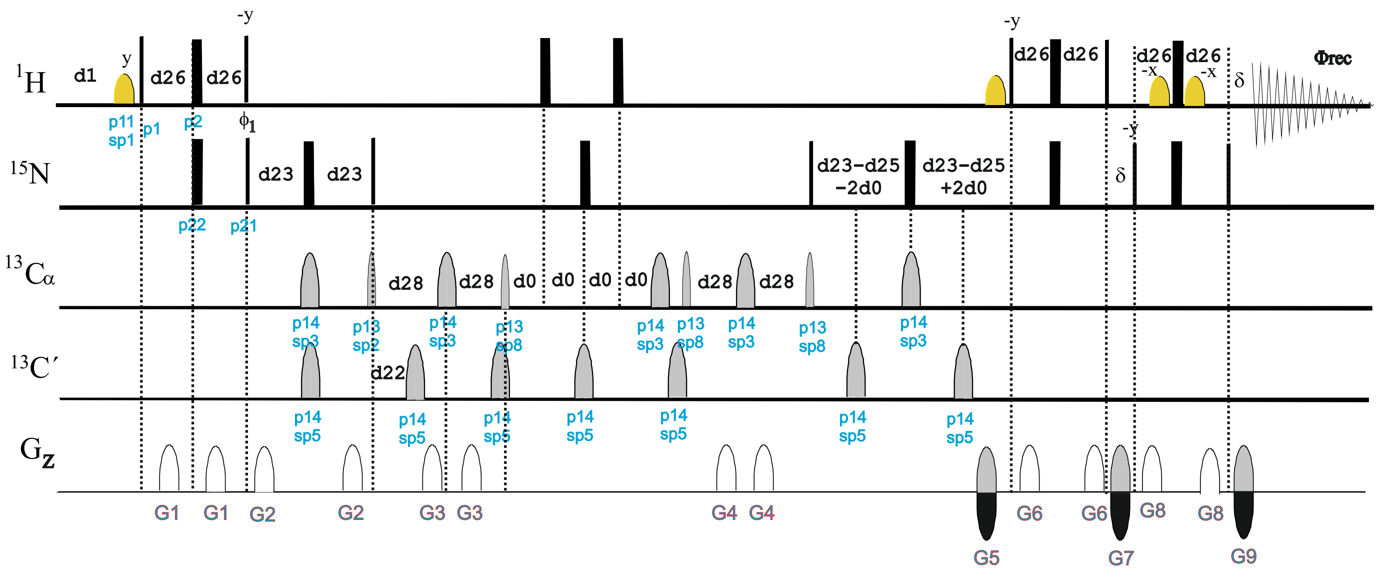
seqtrhncacbgp3d



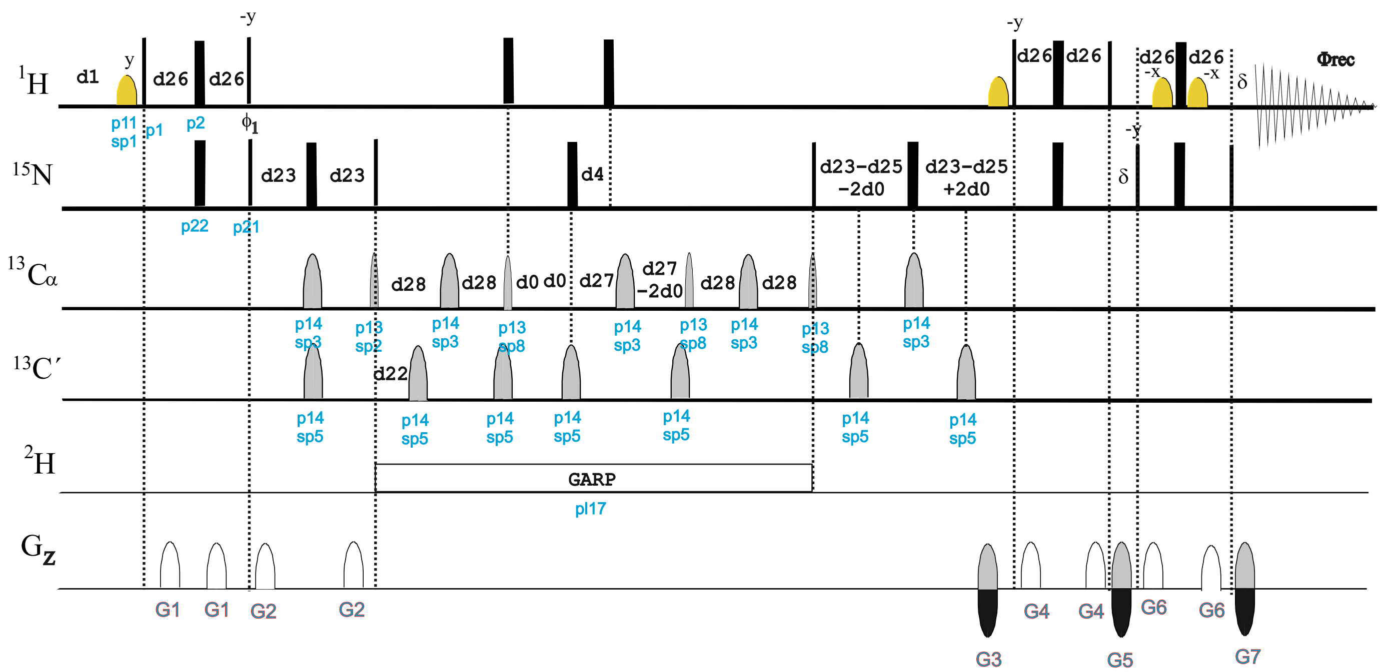
seqtrhncacbgp2h3d



seqtrhncacbetgp3d



seqtrhncacbetgp2h3d



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3D Intra-HNCACB

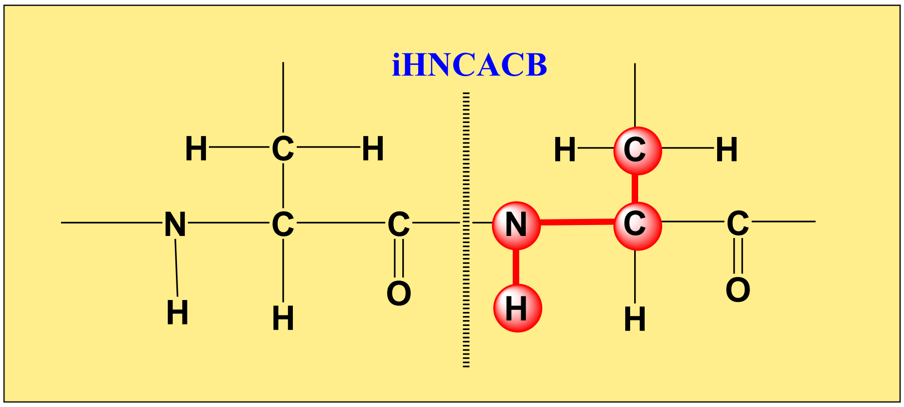
3D intra-HNCACB experiment

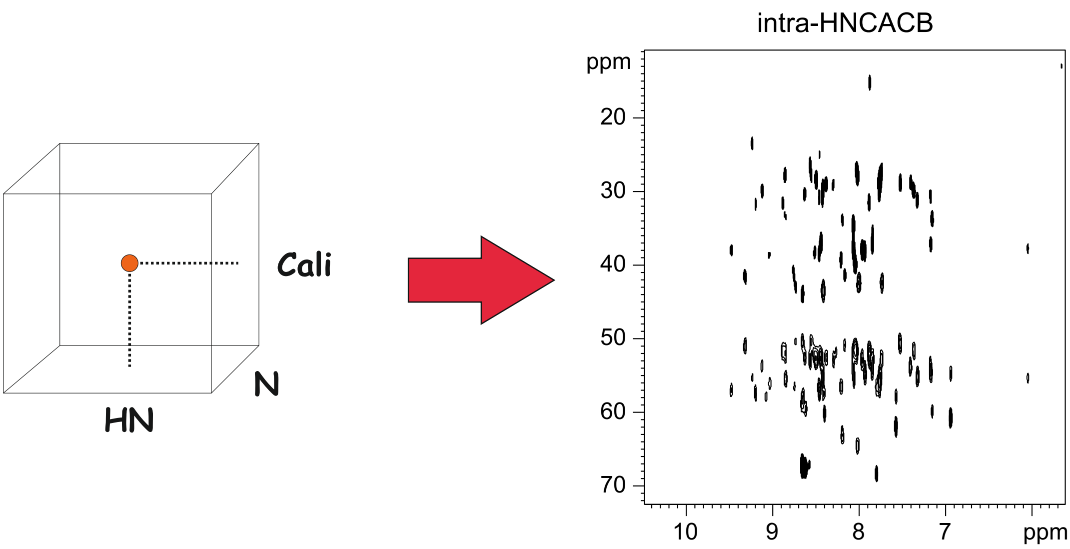
- 3D Intra-HNCACB using PEP (**hncacbigp3d** | HNCACBIGP3D)
  - with ^{2}H-decoupling (**hncacbigp2h3d** | HNCACBIGP2H3D)
- 3D Intra-HNCACB using WATERGATE (**hncacbigpwg3d** | HNCACBIGPWG3D)
  - with ^{2}H-decoupling (**hncacbigpwg2h3d** | HNCACBIGPWG2H3D)
- 3D Intra-HNCACB using TROSY (**trhncacbigp3d** | TRHNCACBIGP3D)
  - with ^{2}H-decoupling (**trhncacbigp2h3d** | TRHNCACBIGP2H3D)
  - With gradient echo-antiecho (**trhncacbietgp3d** | TRHNCACBIETGP3D)
  - With gradient echo-antiecho and with ^{2}H-decoupling (**trhncacbietgp2h3d** | TRHNCACBIETGP2H3D)

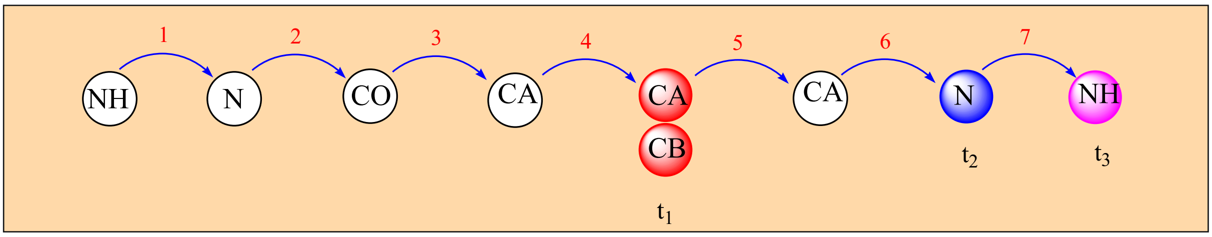
Also see:
3D SOFAST/BEST intra-HNCACB experiment
3D BEST-intraHNCACB (**b_hncacbigp3d** | **B_HNCACBIGP3D**)
3D BEST-intraHNCACB using TROSY (**b_trhncacbigp3d**)

3D HNCACB and sequential-HNCACB experiments

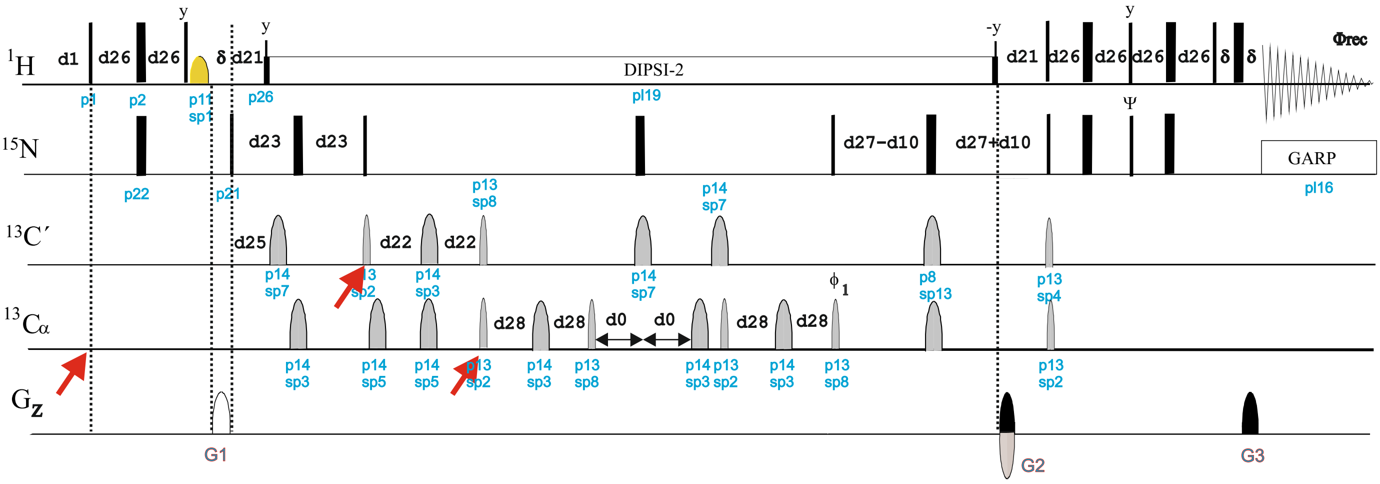
D.Nietlispach, Y. Ito & E.D. Laue, J. Am. Chem. Soc. 124, 11199-11207 (2002)





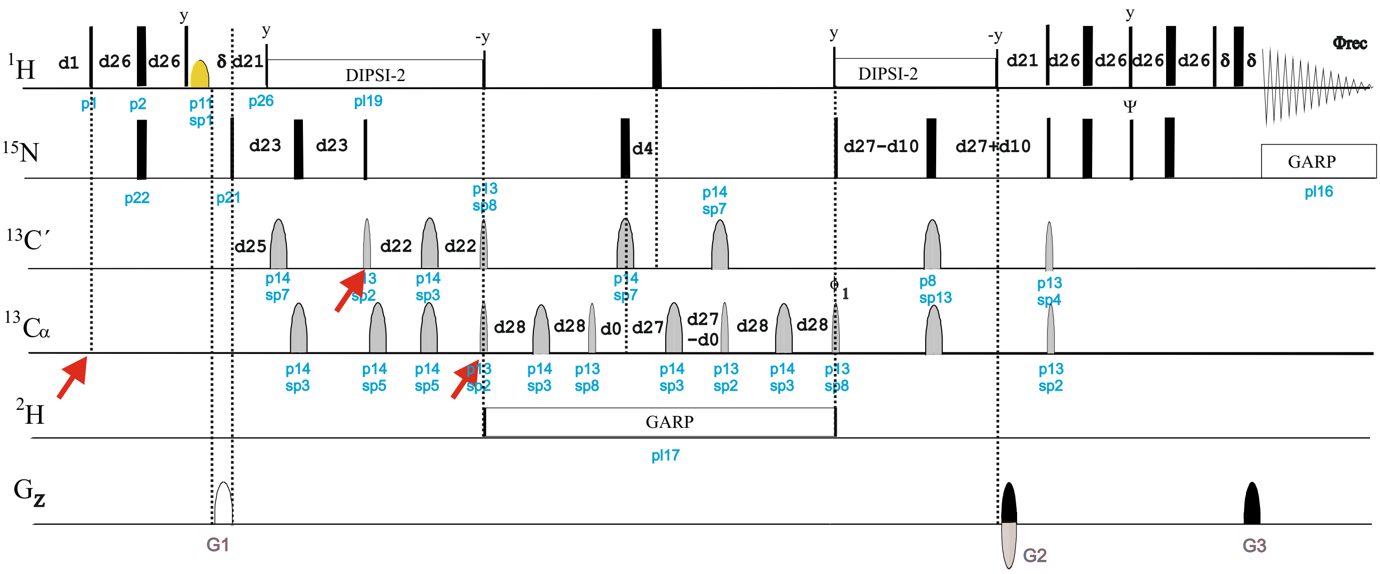


hncacbigp3d

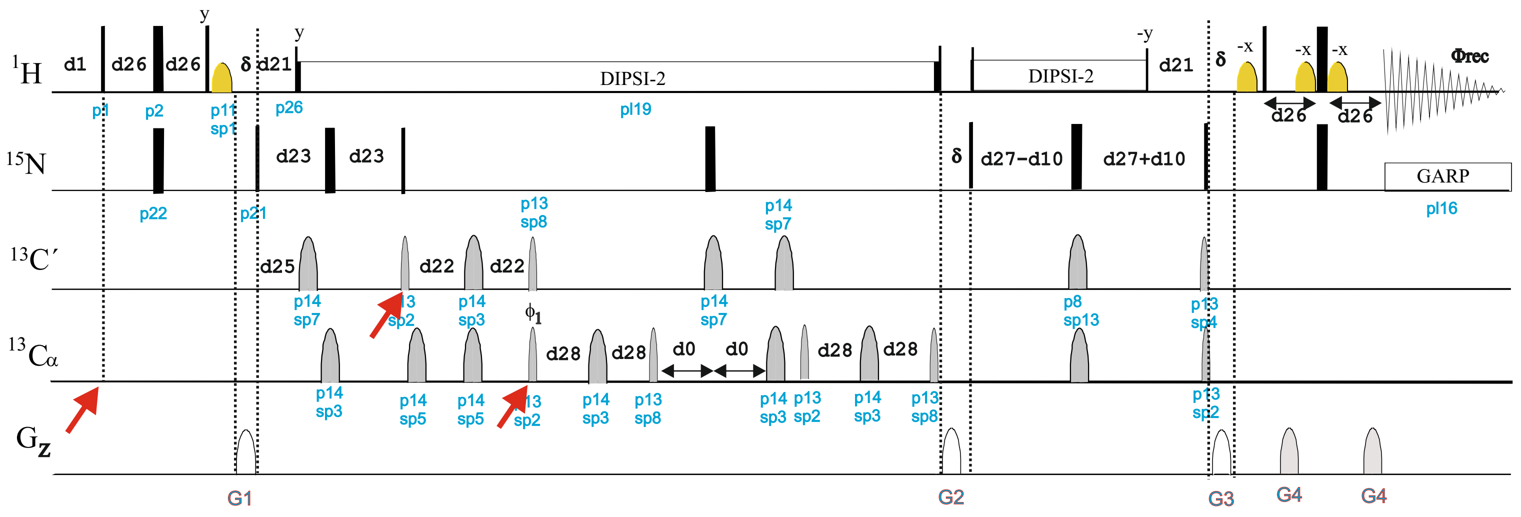


d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCA)=26m
d22=1/4J(CACO)=4.2m
d27=1/4J(NCA)&1/4J(NCO)=15.8m
d25=1/4J(NCO)=16.5m
d28: 1/(8J(CaCb)) =3.6m (7.2m if **ZGOPTNS=-DLABEL_CB**)

hncacbigp2h3d



hncacbigpwg3d



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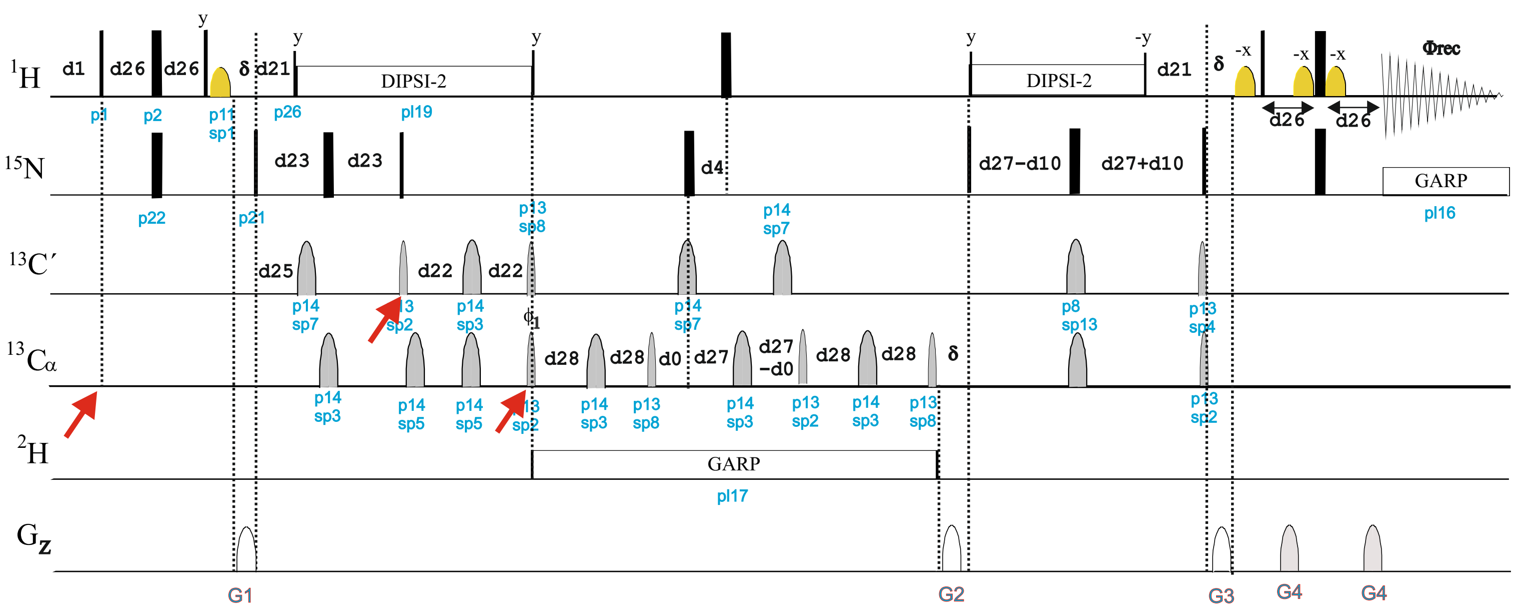
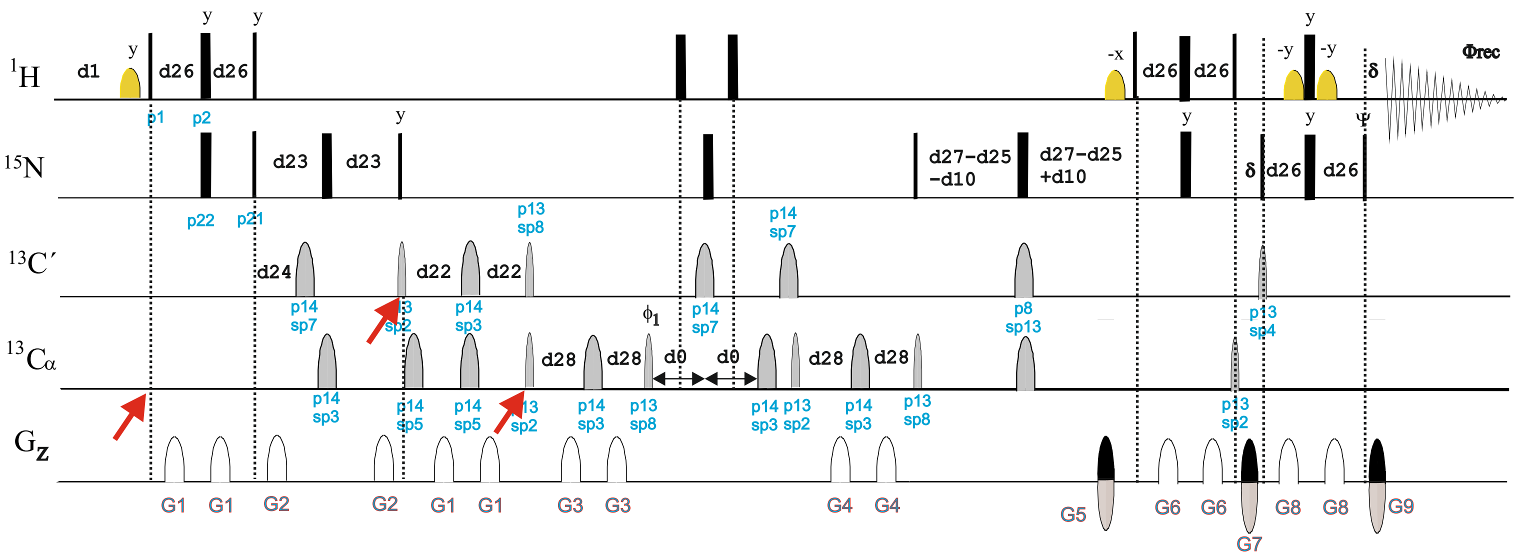
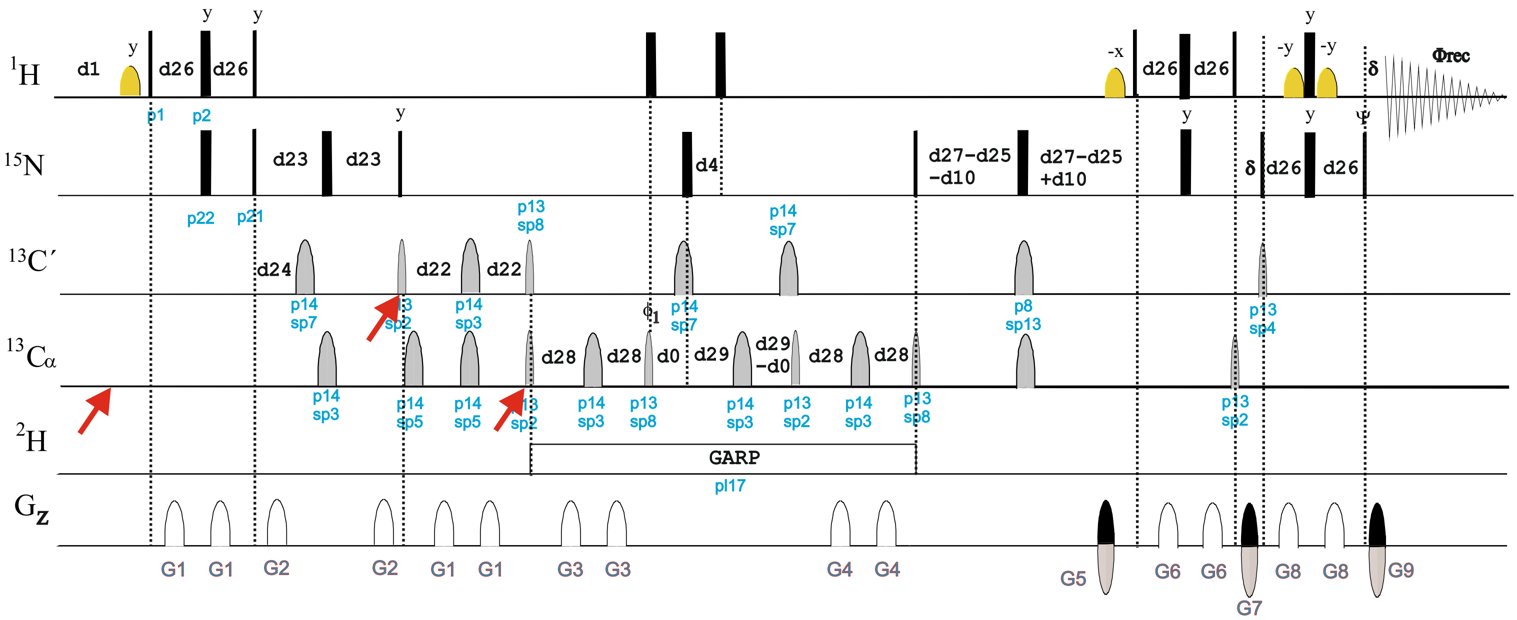


trhncacbietgp3d



trhncacbietgp2h3d



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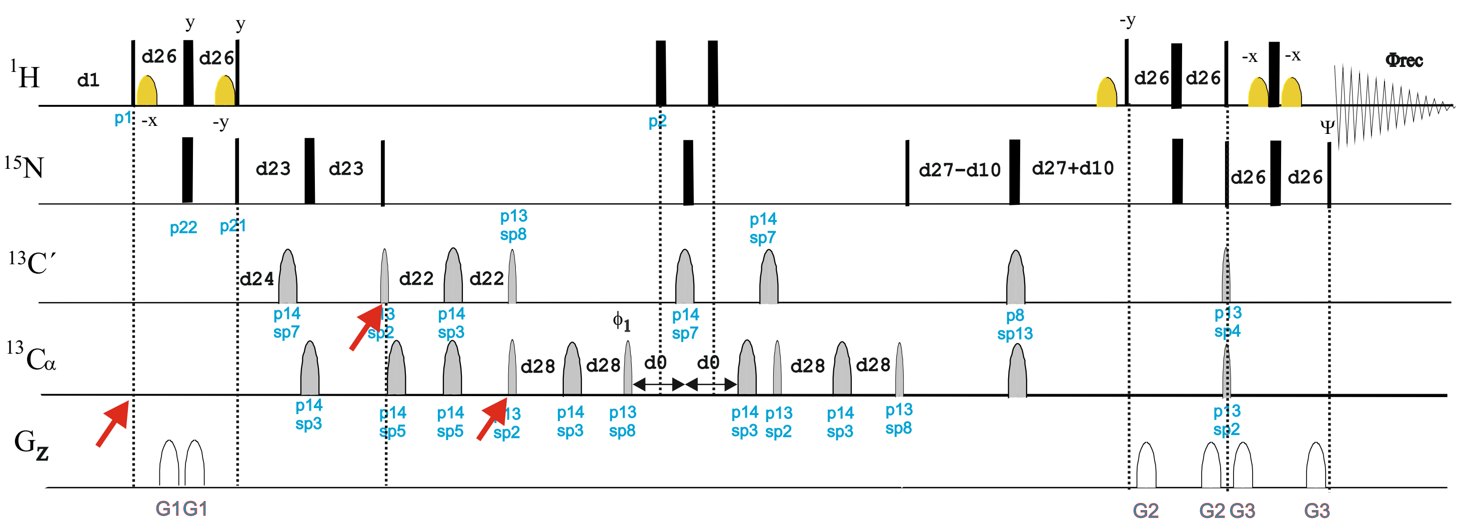

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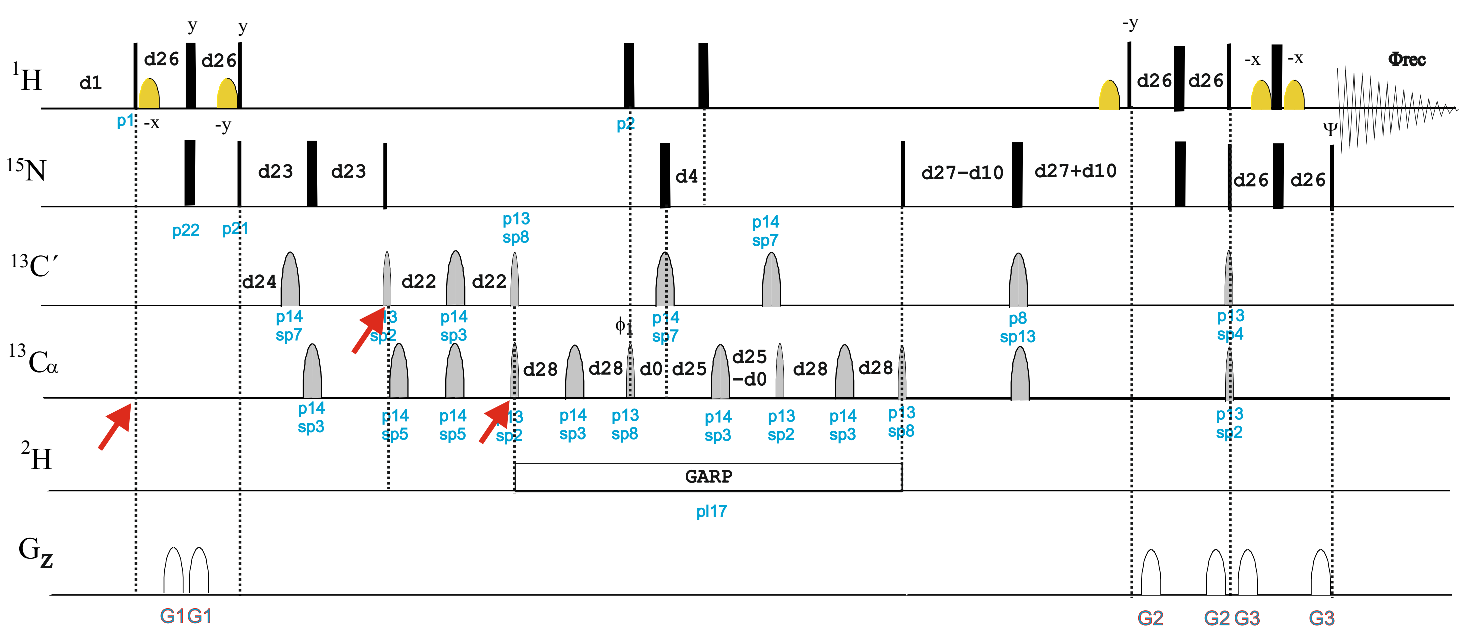

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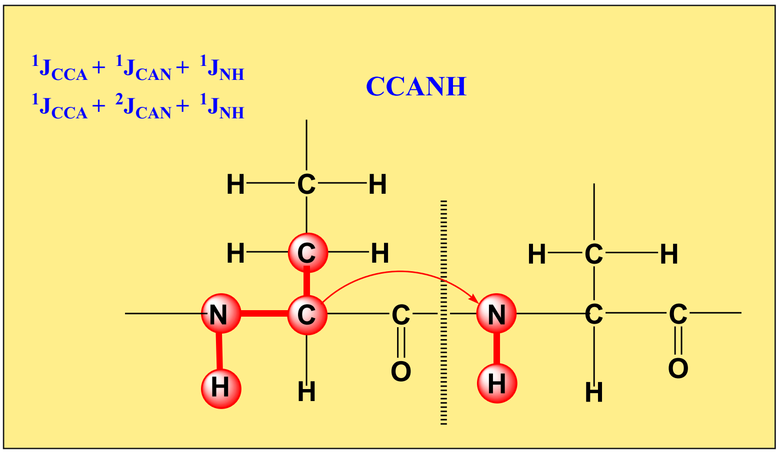
3D CCANH

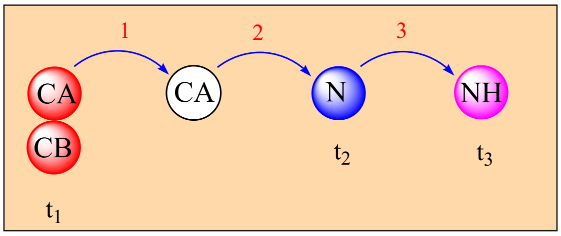
3D CCANH experiment

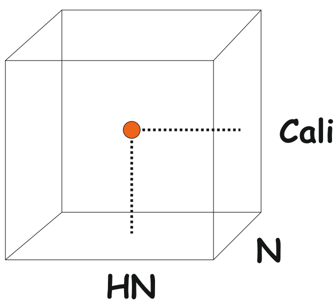
- 3D CCANH using PEP (**ccanhgp3d** | CCANHGP3D)
- 3D CCANH using PEP with ^{2}H-decoupling (**ccanhgp2h3d** | CCANHGP2H3D)
- 3D CCANH using PEP and ^{1}H-NOE (**ccanhgp3d.2** | CCANHGP3D.2)

Also see:
CCA(CO)NH and 3D CC(CO)NH experiments
3D & 4D HCCCONH Experiments

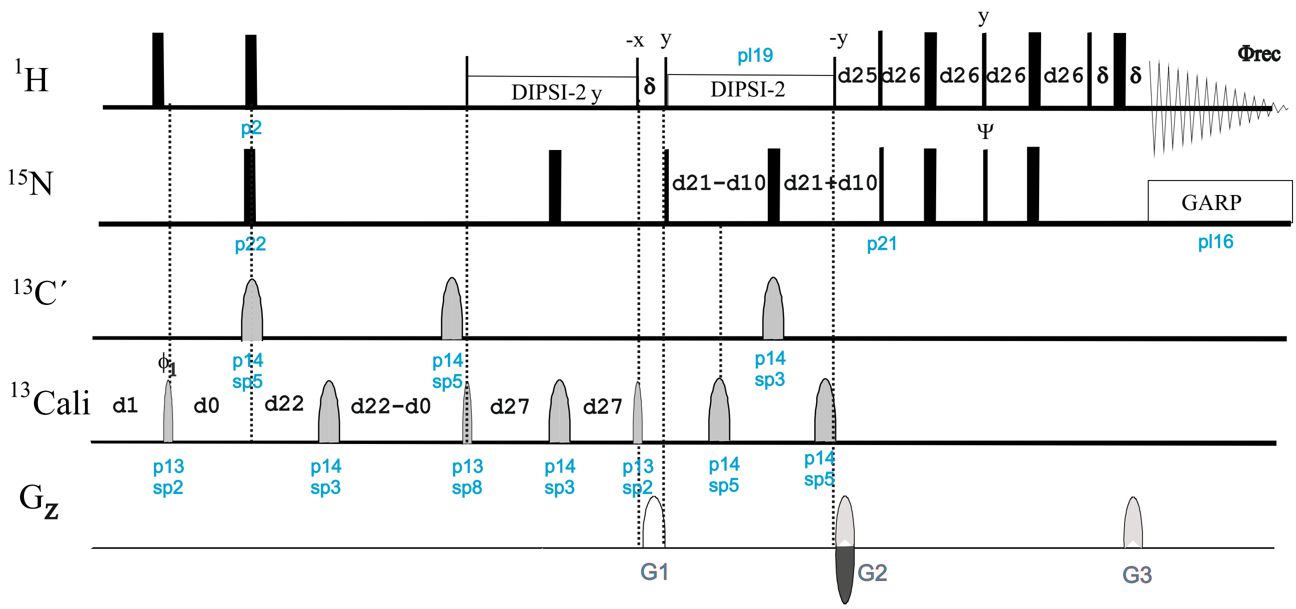
S. Grzesiek & A. Bax, J. Biomol. NMR 3, 185-204 (1993)





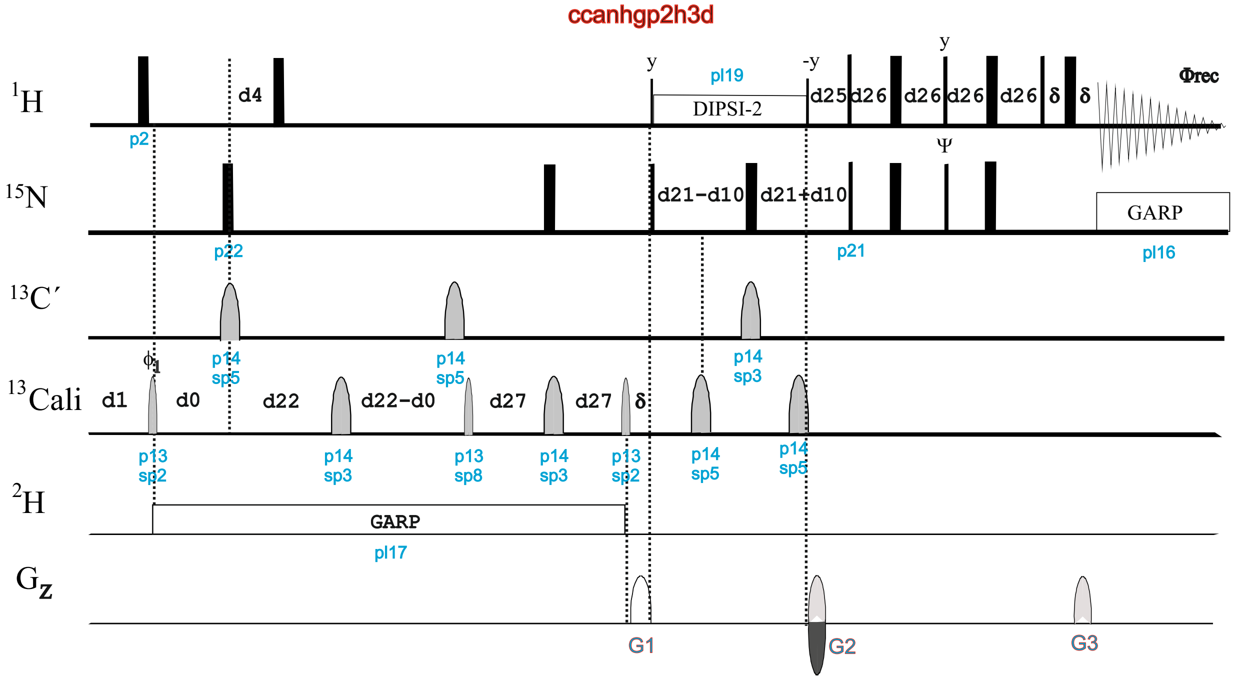


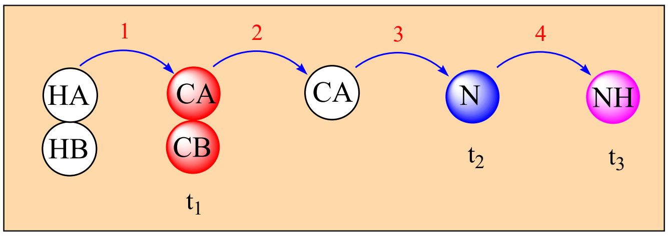
ccanhgp3d



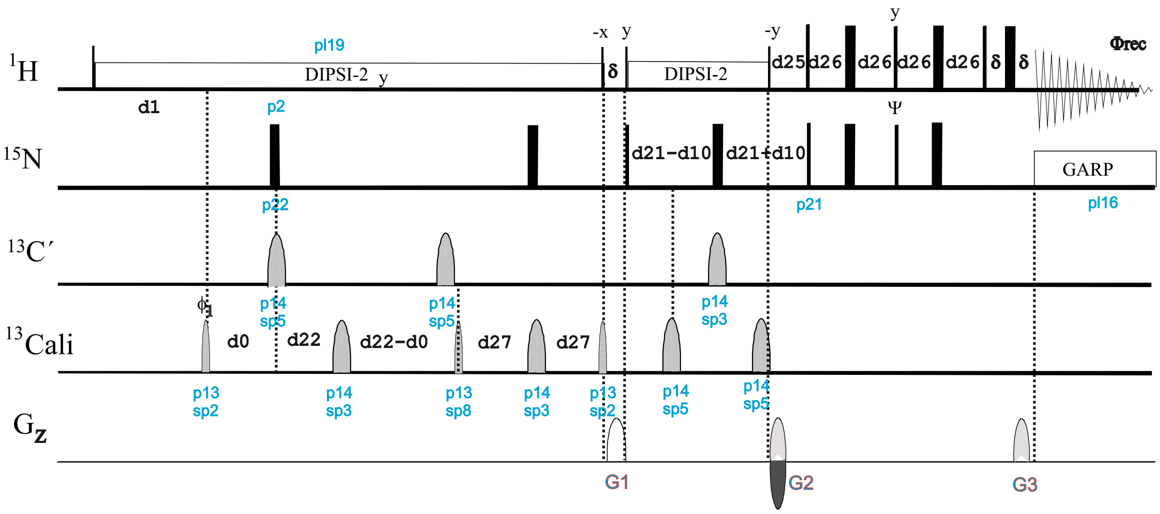
d21=1/4J(NCO)=12.4m
d22=1/4J(CC)=3.6m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m
d27=1/4J(CACO)=11m

ccanhgp2h3d




1
2
3
4
HA
HB
CA
CB
CA
N
NH
t_1
t_2
t_3

ccanhgp3d.2


^{1}H
^{15}N
^{13}C′
^{13}Cali
G_z
pl19
DIPSI-2 y
DIPSI-2
-x
y
-y
δ
d25
d26
Φrec
Ψ
d1
p2
d21-d10
d21+d10
GARP
p22
p21
pl16
p14
sp5
sp3
ϕ_1
d0
d22
d22-d0
d27
p13
sp2
sp8
G1
G2
G3

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3D CCA(CO)NH
3D CC(CO)NH

CCA(CO)NH and CC(CO)NH Experiments

3D CCA(CO)NH experiment

- 3D CCA(CO)NH using PEP (**ccaconhgp3d** | CCACONHGP3D)
- 3D CCA(CO)NH using PEP with ^{2}H-decoupling (**ccaconhgp2h3d** | CCACONHGP2H3D)
- 3D CCA(CO)NH using PEP and ^{1}H-NOE (**ccaconhgp3d.2** | CCACONHGP3D.2)

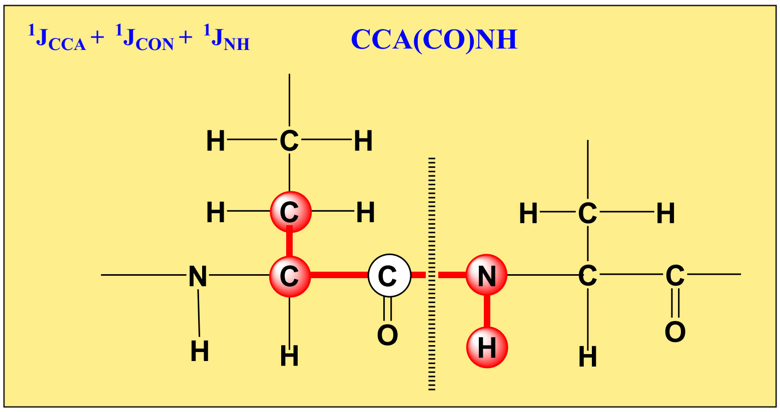
3D CC(CO)NH experiment

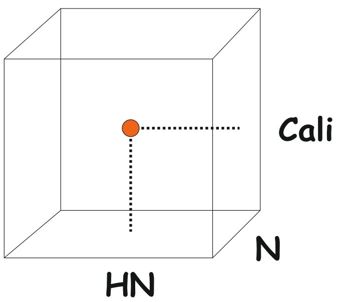
- 3D CC(CO)NH using PEP (**ccconhgp3d** | CCCONHGP3D)
- 3D CC(CO)NH using PEP with ^{2}H-decoupling (**ccconhgp2h3d** | CCCONHGP2H3D)

Also see:
3D CBCACONH, 3D CCANH, 3D (H)CC(CO)NH and H(CCCO)NH experiments

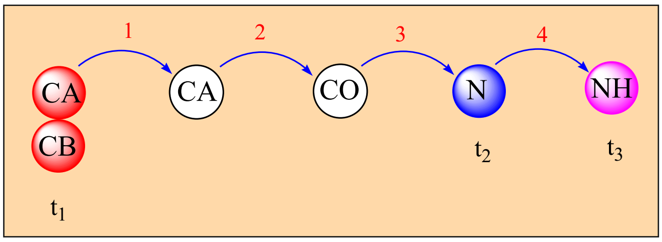
References:

S. Grzesiek & A. Bax, J. Biomol. NMR 3, 185-204 (1993)





d21=1/4J(NCO)=12.4m
d22=1/4J(CC)=3.6m
d23=1/4J(CBCA)=3.6m
d24=1/2J(CBCA)=4.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m
d27=1/4J(CACO)=12.4m



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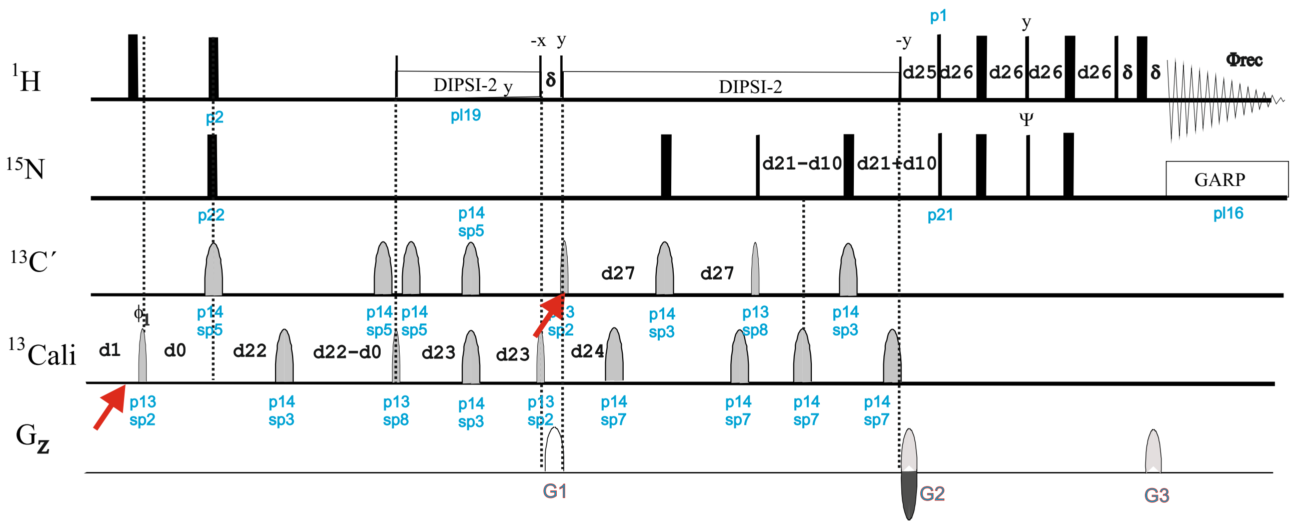

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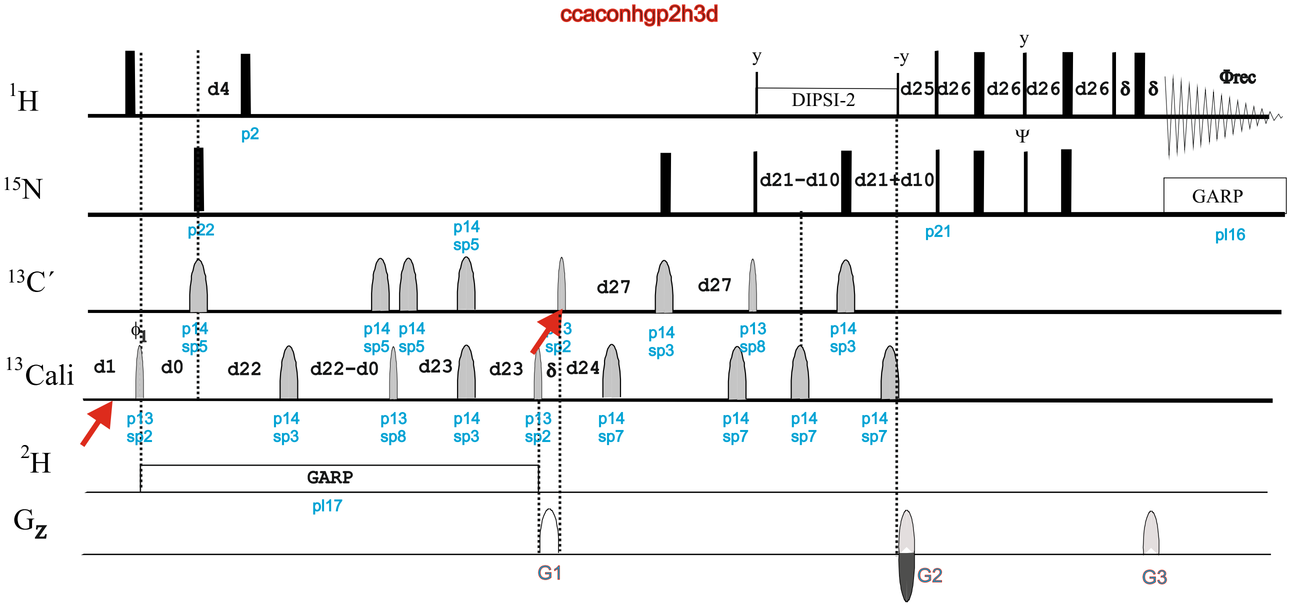
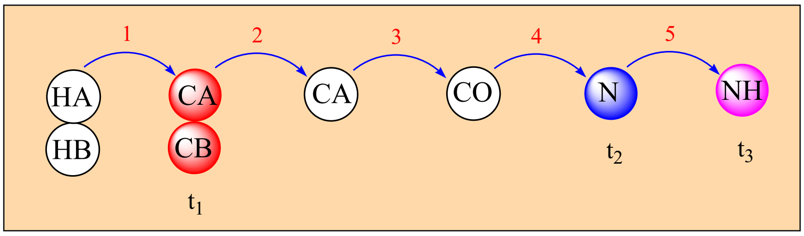
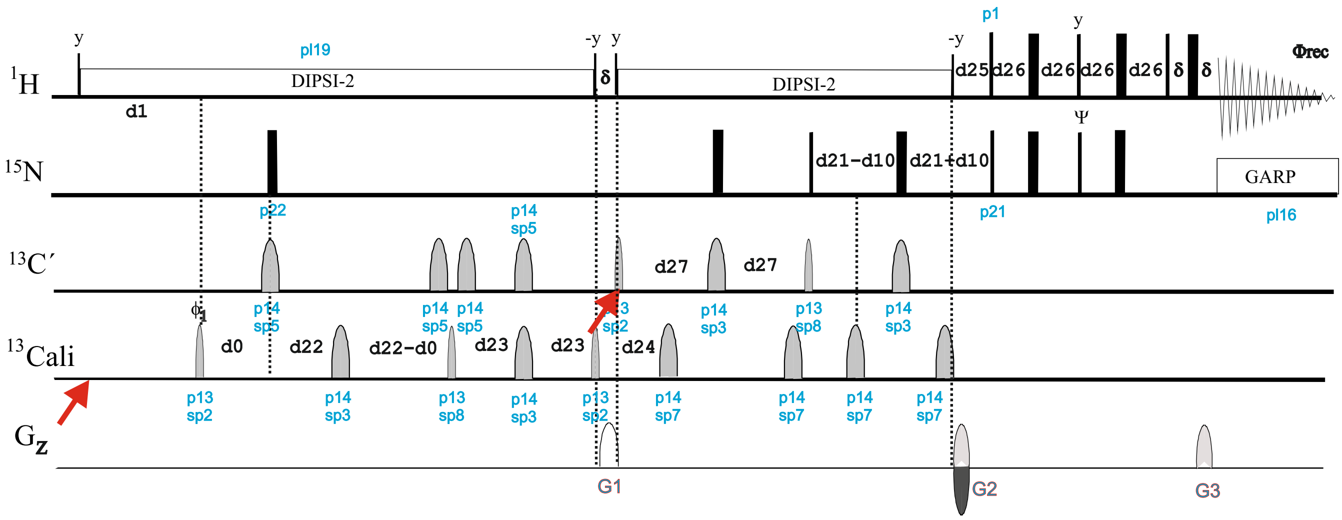
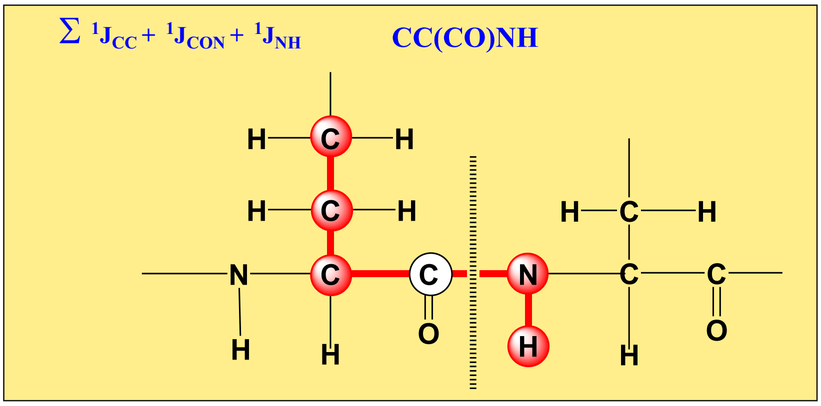




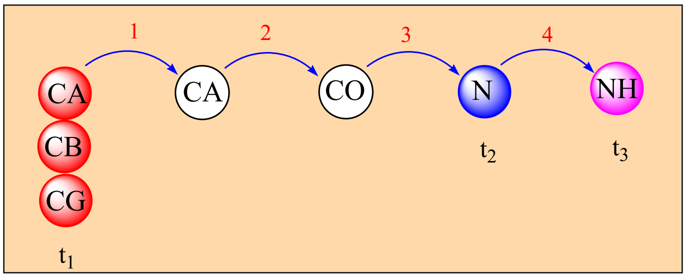
ccaconhgp3d.2

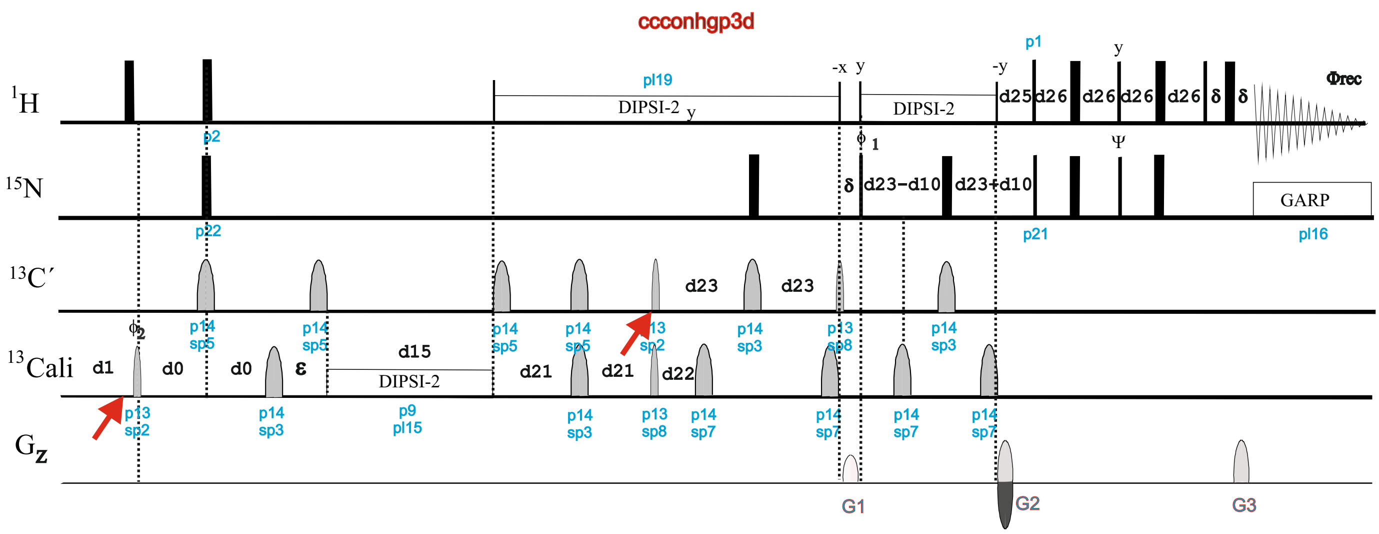




References:

1. G.T. Montelione, B.A. Lyons, S.D. Emerson & M. Tashiro, J. Am. Chem. Soc. 114, 10974-75 (1992)
2. S. Grzesiek, J. Anglister & A. Bax, J. Magn. Reson. 101 B, 114-9 (1993)
3. B.A. Lyons & G.T. Montelione, J. Magn. Reson. 101 B, 206-9 (1993)
4. T.M. Logan, E.T. Olejniczak, R.X. Xu & S.W. Fesik, J. Biomol. NMR 3, 225-31 (1993)
5. R.T. Clowes, W. Boucher, C.H. Hardman, P.J. Domaille & E.D. Laue, J. Biomol. NMR 3, 349-354 (1993)
6. T. Carlomagno, M. Maurer, M. Sattler, M.G. Schwendinger, S.J. Glaser & C. Griesinger, J. Biomol. NMR 8, 161-170 (1996)





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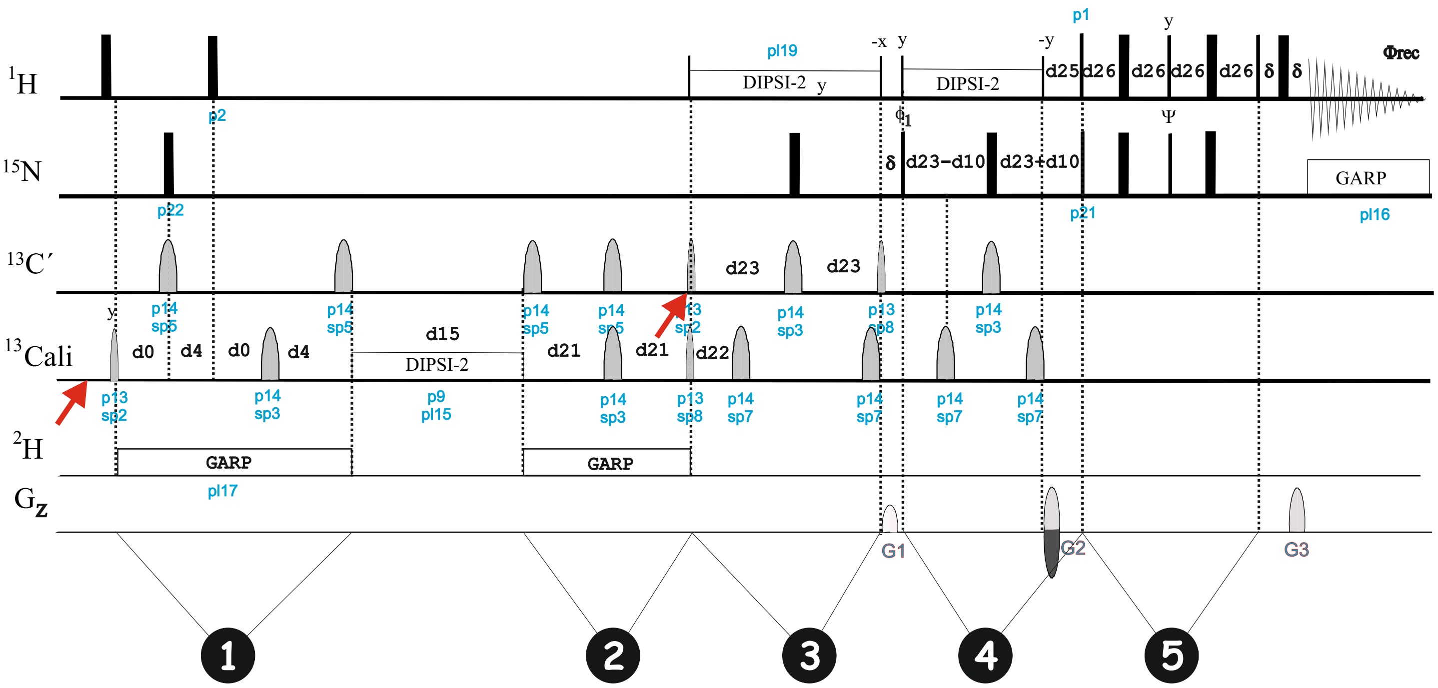

d15:TOCSY mixing time [12 msec]
d21=1/4J(CACO)=3.6m
d22=1/2J(CACO)=4.4m
d23=1/4J(NCO)=12.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m
d4=1/4J(CH)=1.7m

1 Variable Cali evolution period consisting of:
δ(CAli) evolution and J(CAli-CO) decoupling
δ(CAli) evolution and J(CAli-N) decoupling
δ(CAli) evolution and J(CAli-2H) decoupling
δ(CAli) evolution and J(CAli-H) defocusing
δ(CAli) evolution and J(CAli-Cali) evolution

2 Cali-CO INEPT transfer

3 CO-N INEPT transfer
J(CO-H) decoupling
J(CO-H) refocusing

4 Concatenated Constant-time 15N evolution period consisting of:
δ(N) evolution and J(N-H) evolution
δ(N) evolution and J(N-CO) refocusing
δ(N) evolution and J(N-Cali) decoupling

5 1H-15N TROSY transfer consisting of two retro-INEPT like blocks

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HCC(CO)NH EXPERIMENTS

HCC(CO)NH experiments

3D (H)CC(CO)NH Experiment

- 3D (H)CC(CO)NH using PEP (**hccconhgp3d3** | HCCCONHGP3D3)
- 3D (H)CC(CO)NH using WATERGATE (**hccconhgpwg3d3** | HCCCONHGPWG3D3)
- 3D (H)CC(CO)NH using TROSY (**trhccconhgp3d3** | TRHCCCONHGP3D3)
  - With gradient echo-antiecho (**trhccconhetgp3d3** | TRHCCCONHETGP3D3)
  - With additional gradient (**trhccconhgp3d3.2** | TRHCCCONHGP3D3.2)
  - With additional gradient and with gradient echo-antiecho (**trhccconhetgp3d3.2** | TRHCCCONHETGP3D3.2)

3D H(CC)(CO)NH Experiment

- 3D H(CC)(CO)NH using PEP (**hccconhgp3d2** | HCCCONHGP3D2)
  - with ^{1}H-^{13}C CP transfer (**hccconhgp3d1** | HCCCONHGP3D1)
- 3D H(CC)(CO)NH using WATERGATE (**hccconhgpwg3d2** | HCCCONHGPWG3D2)
- 3D H(CC)(CO)NH using TROSY (**trhccconhgp3d2** | TRHCCCONHGP3D2)
  - With gradient echo-antiecho (**trhccconhetgp3d2** | TRHCCCONHETGP3D2)

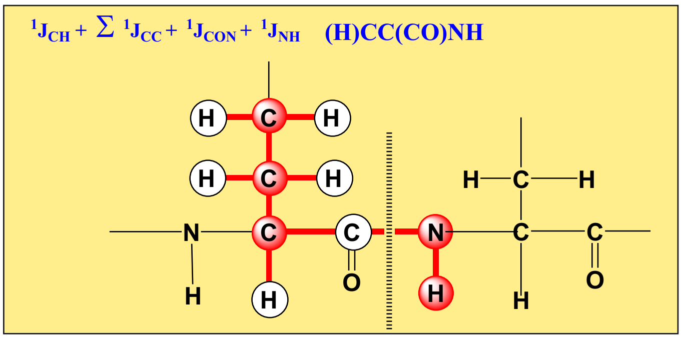
4D HCC(CO)NH Experiment

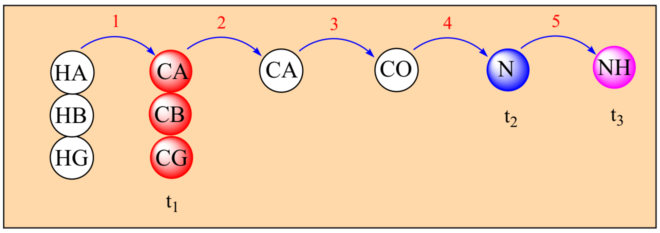
- 4D HCC(CO)NH using WATERGATE (**hccconhgpwg4d**)

Also see:
3D HBHA(CO)NH experiment
3D CC(CO)NH & CCA(CO)NH experiments
3D CBCA(CO)NH experiment

References:

1. G.T. Montelione, B.A. Lyons, S.D. Emerson & M. Tashiro, J. Am. Chem. Soc. 114, 10974-75 (1992)
2. S. Grzesiek, J. Anglister & A. Bax, J. Magn. Reson. 101 B, 114-9 (1993)
3. B.A. Lyons & G.T. Montelione, J. Magn. Reson. 101 B, 206-9 (1993)
4. T.M. Logan, E.T. Olejniczak, R.X. Xu & S.W. Fesik, J. Biomol. NMR 3, 225-31 (1993)
5. R.T. Clowes, W. Boucher, C.H. Hardman, P.J. Domaille & E.D. Laue, J. Biomol. NMR 3, 349-354 (1993)
6. T. Carlomagno, M. Maurer, M. Sattler, M.G. Schwendinger, S.J. Glaser & C. Griesinger, J. Biomol. NMR 8, 161-170 (1996)





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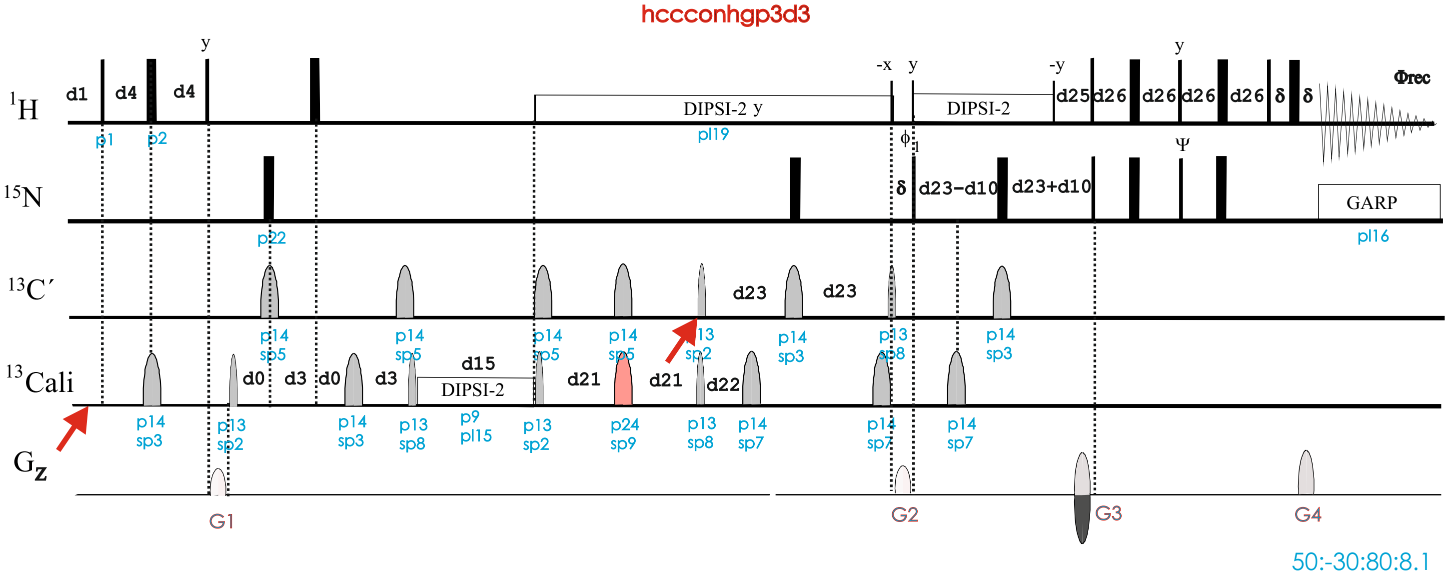

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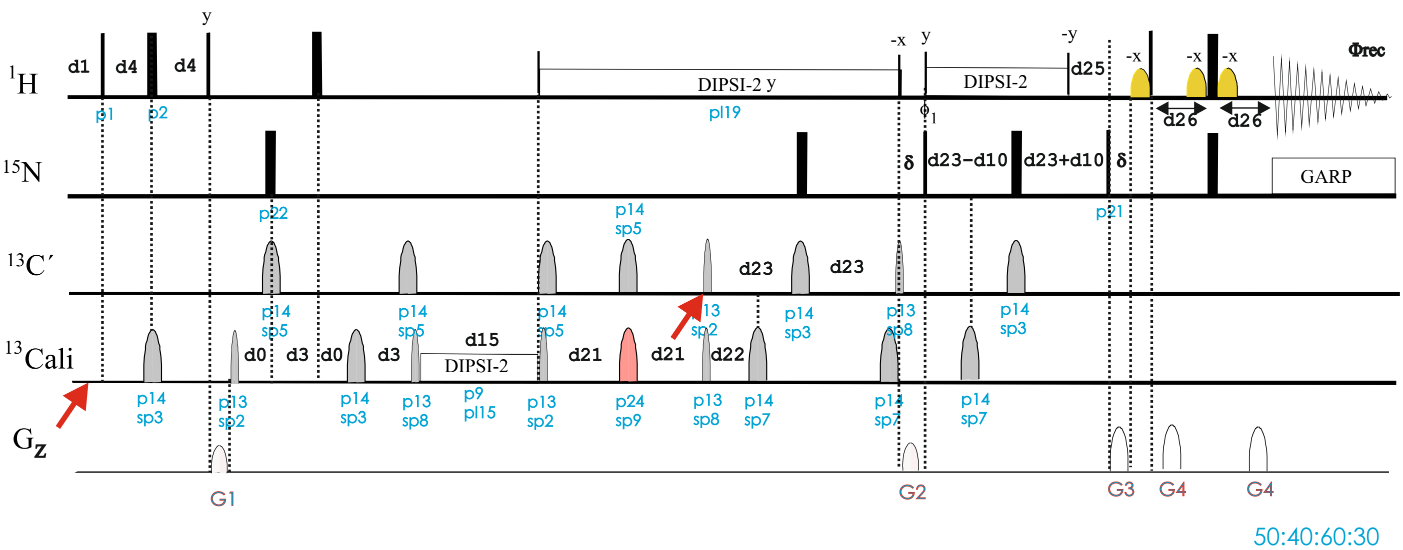

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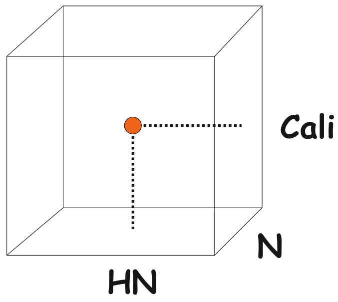
d21=1/2J(CACO)=3.6m
d22=1/2J(CACO)=4.4m
d23=1/4J(NCO)=12.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m



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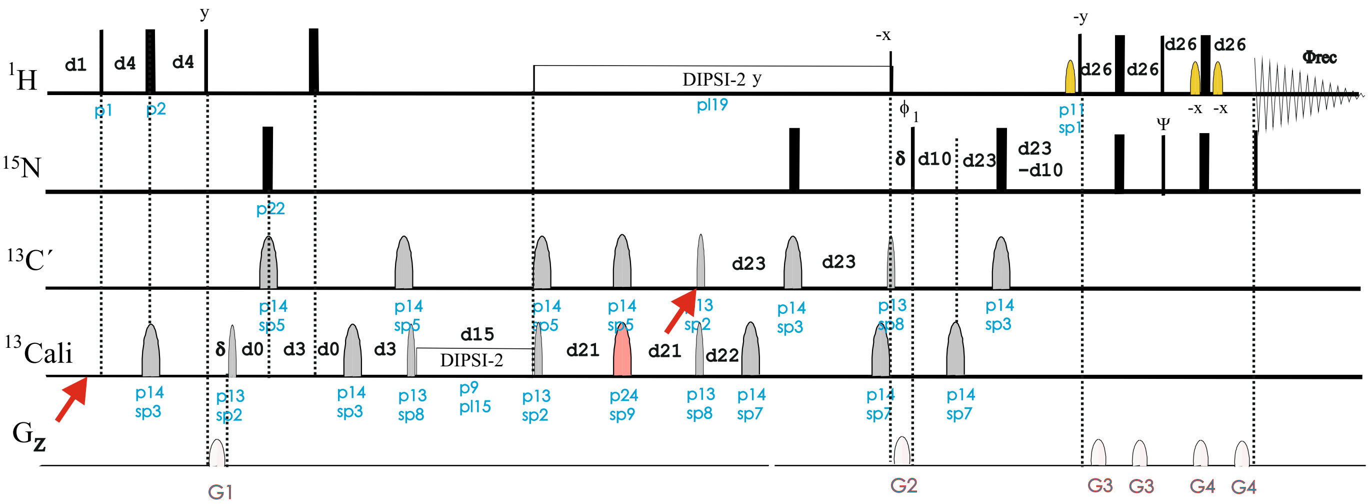

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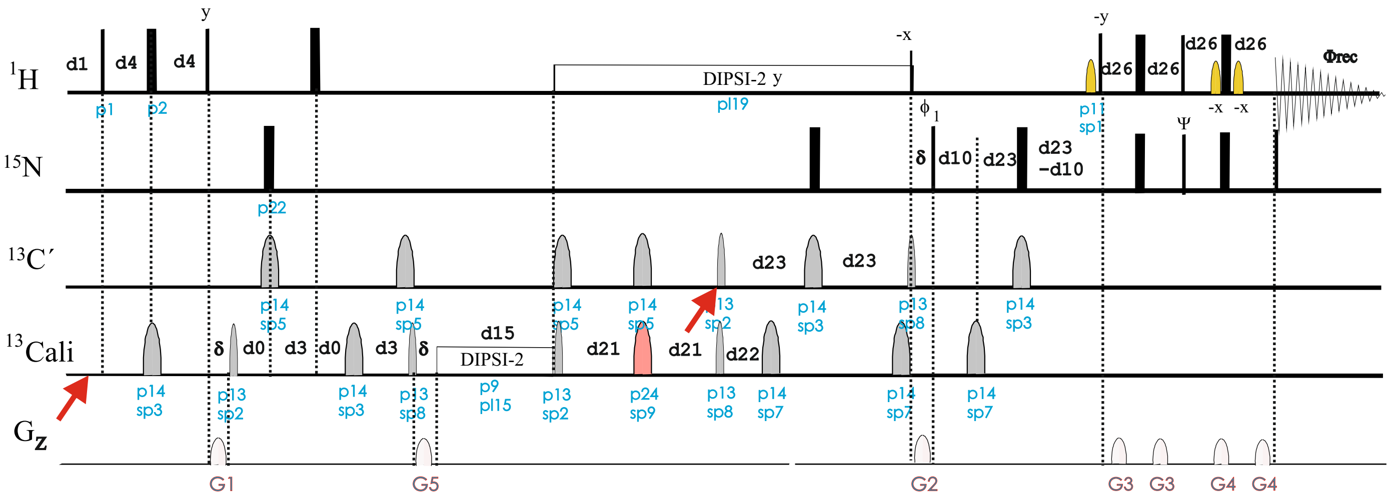

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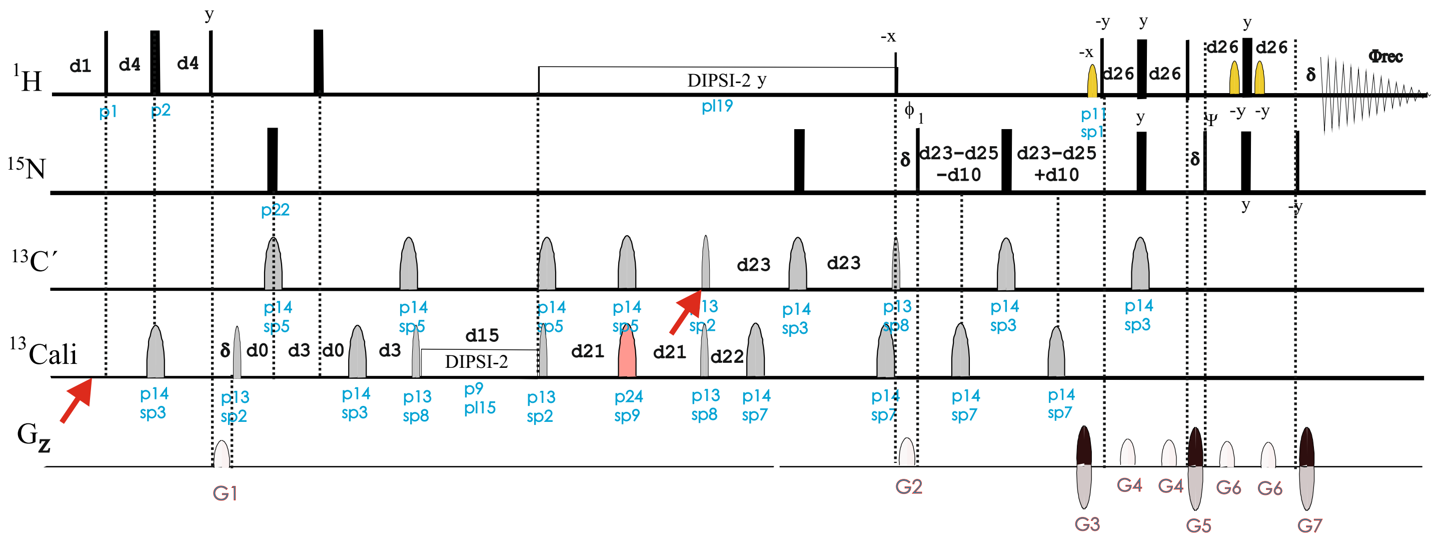

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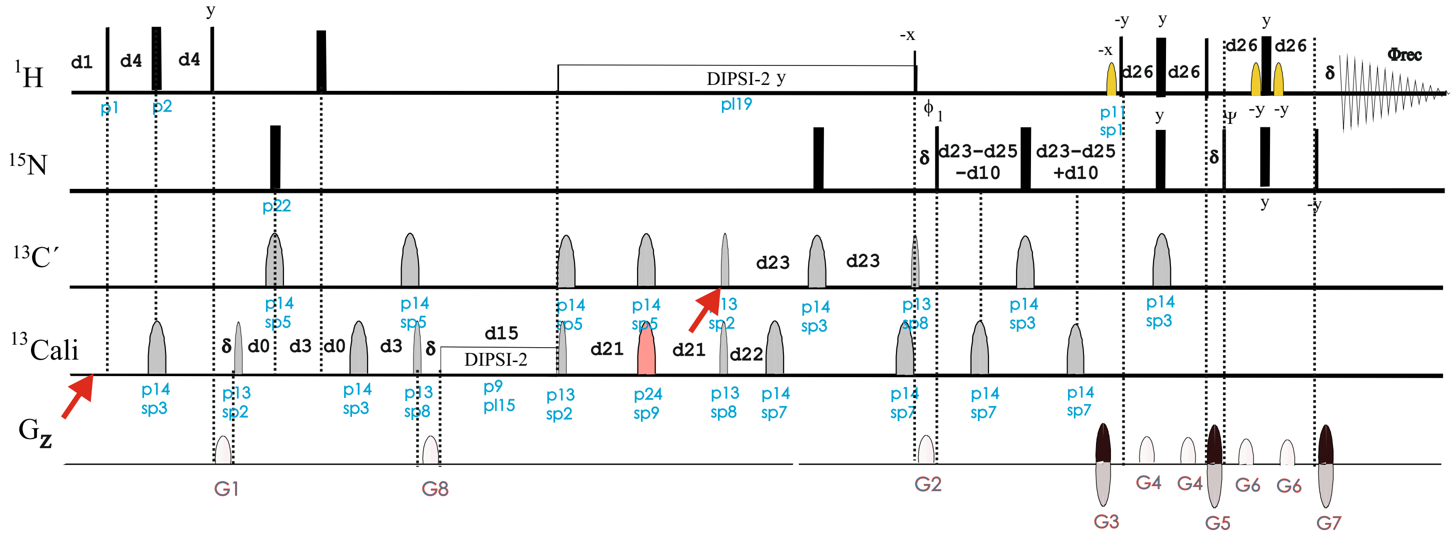

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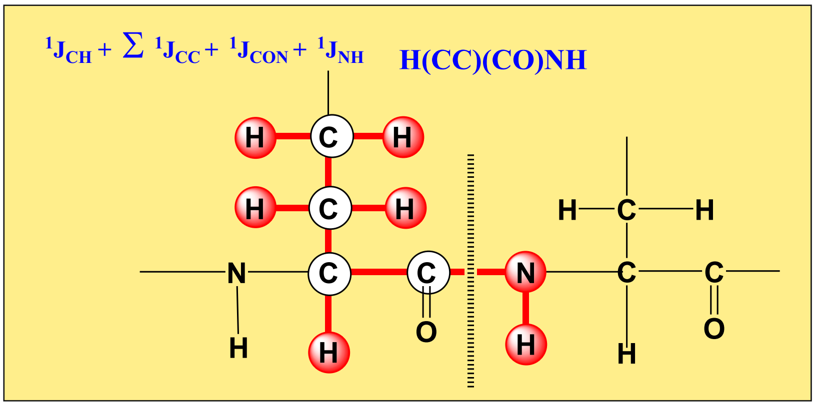

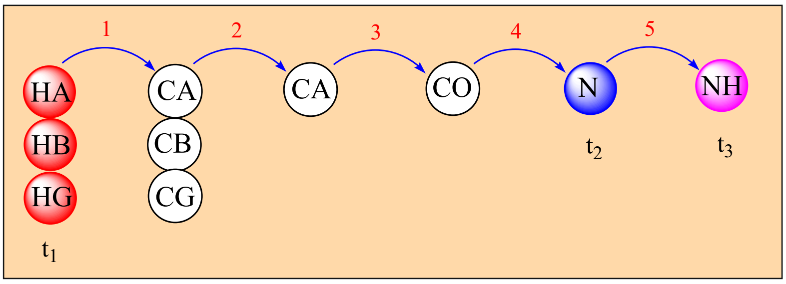

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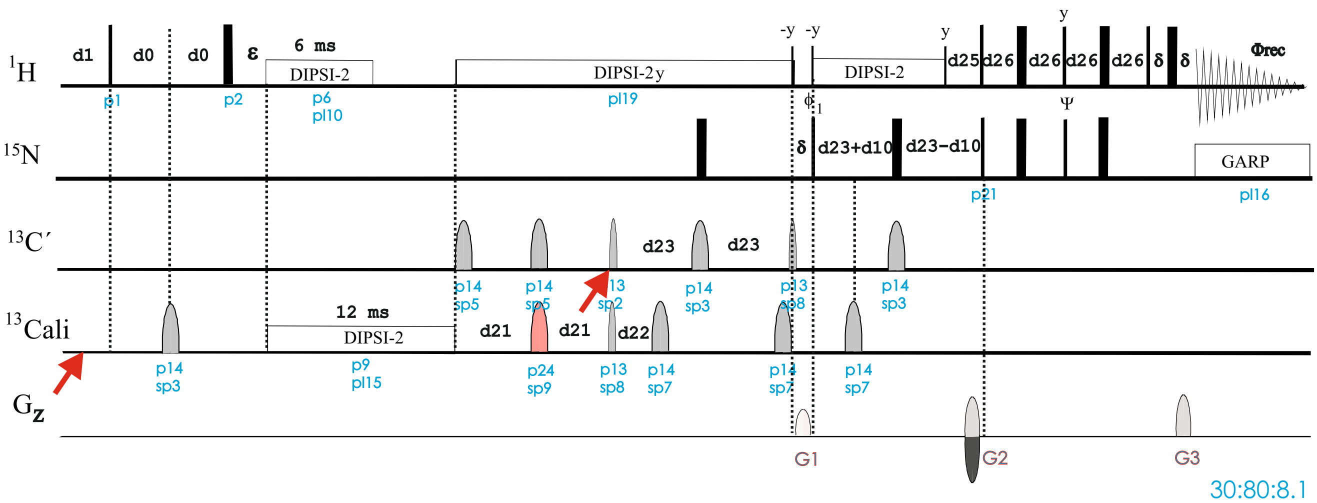

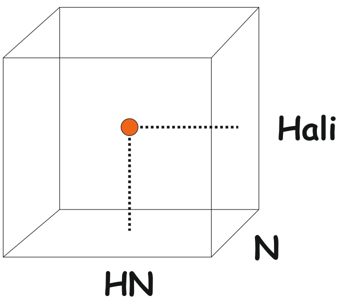

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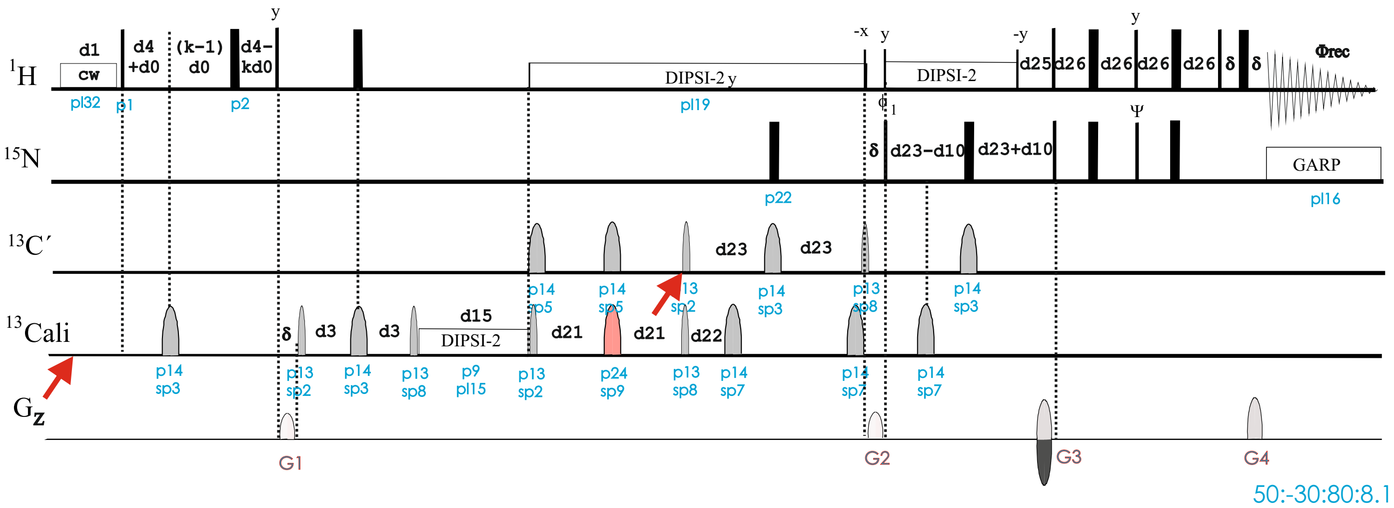
d21=1/2J(CACO)=3.6m
d22=1/2J(CACO)=4.4m
d23=1/4J(NCO)=12.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m

hccconhgp3d2



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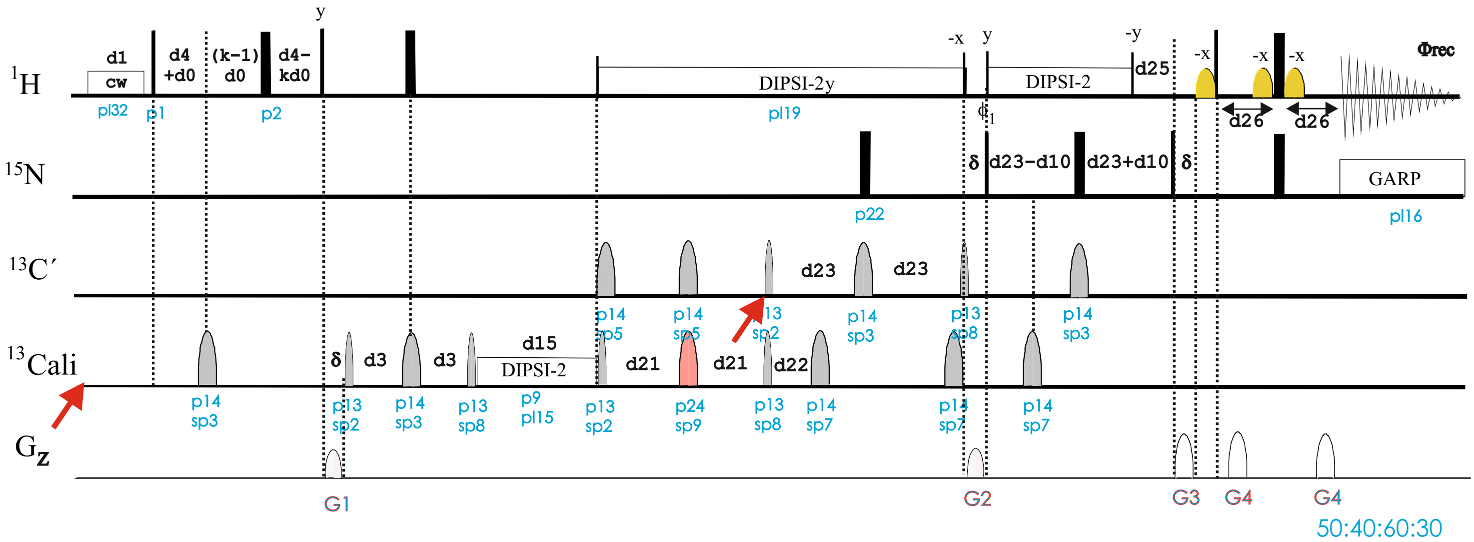

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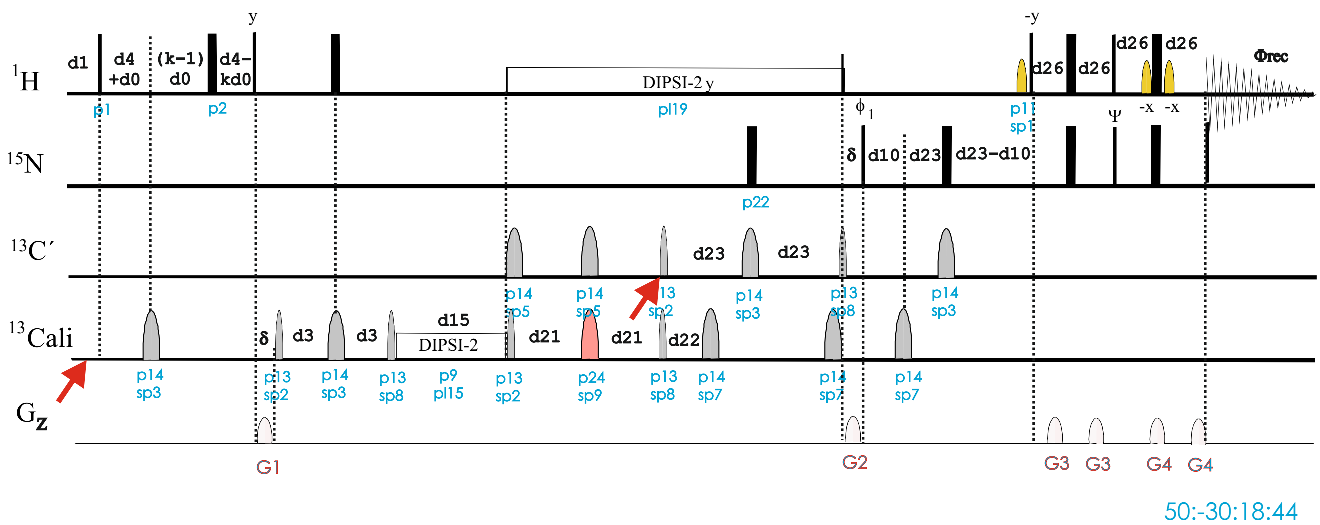

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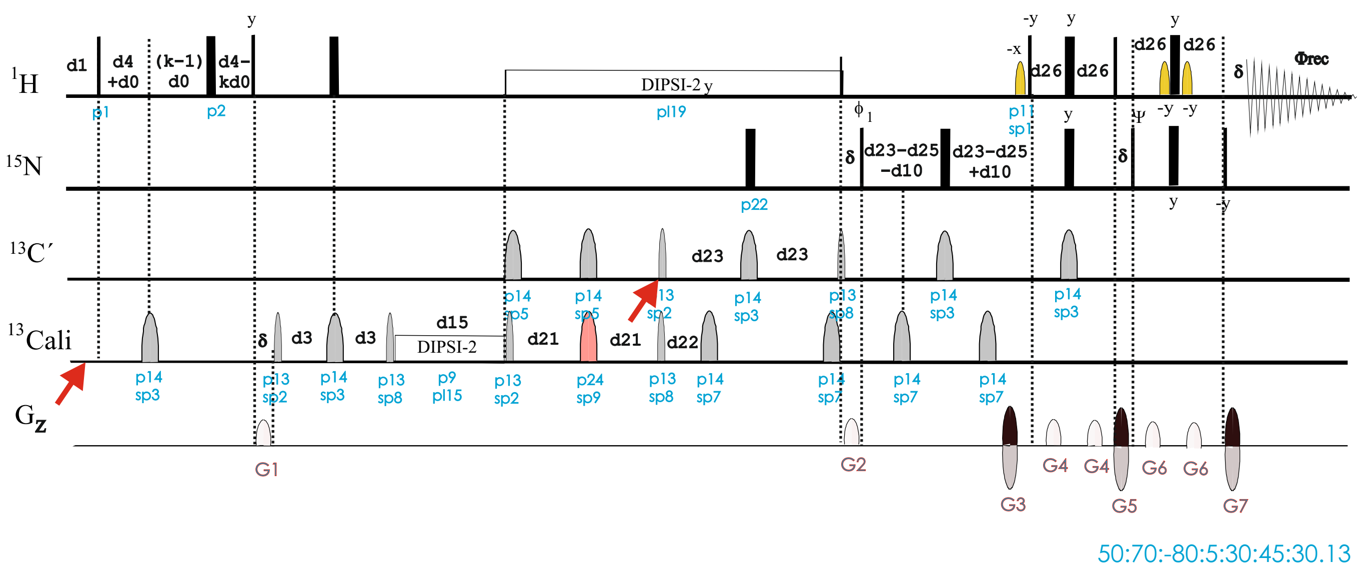

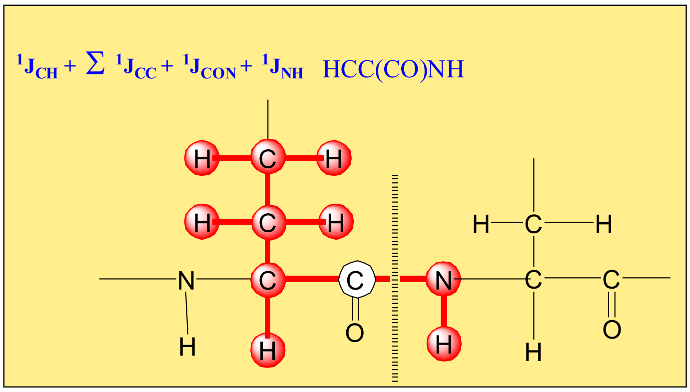

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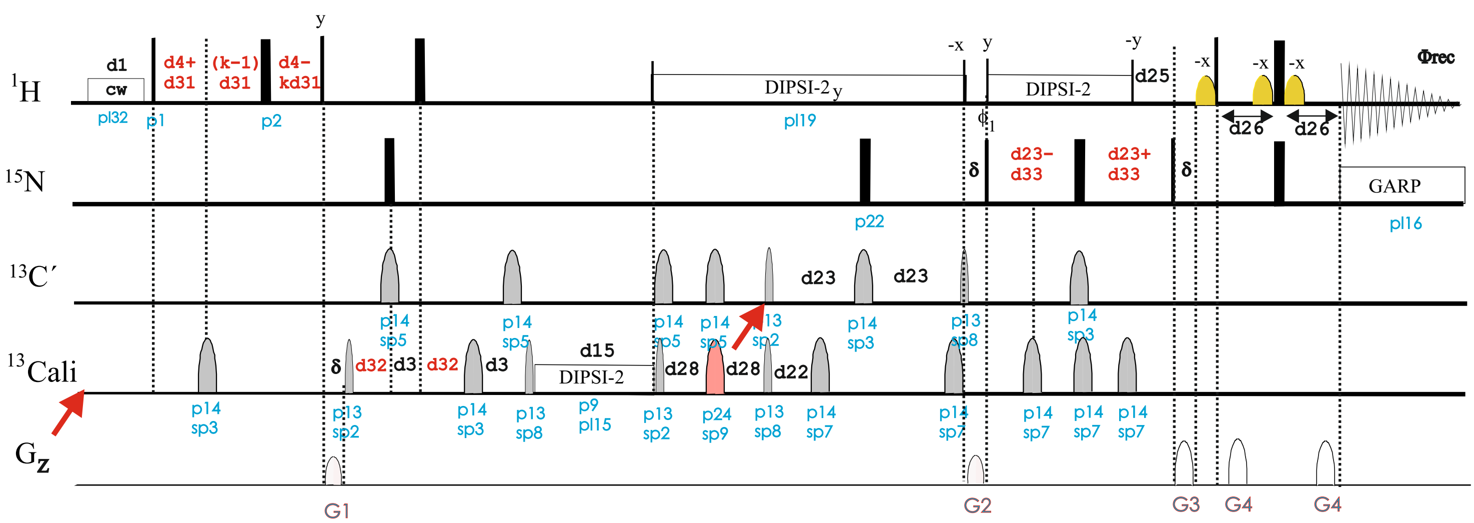

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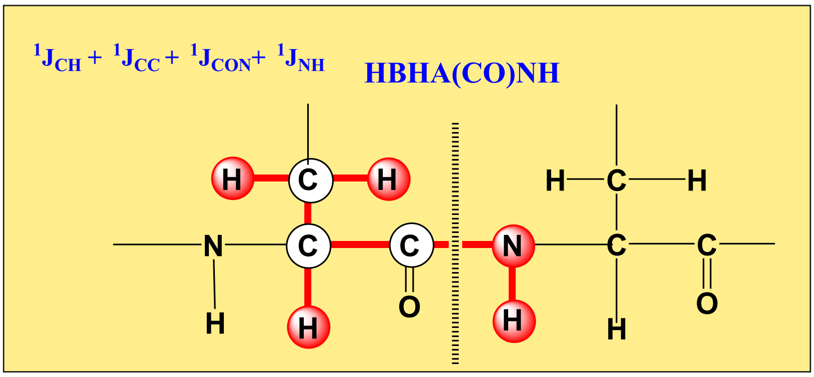
3D HBHA(CO)NH

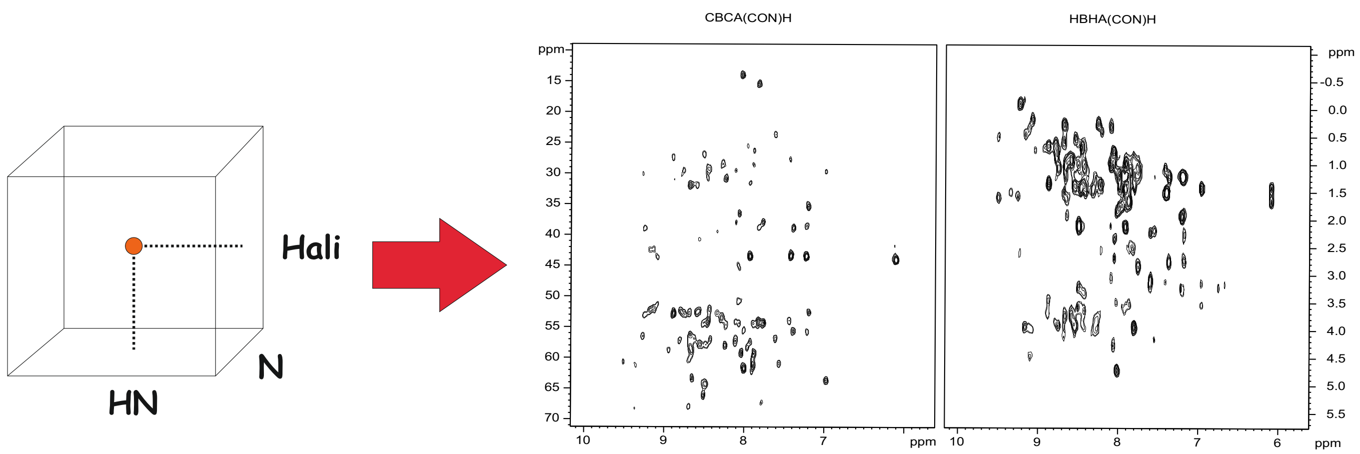
HBHACONH experiment

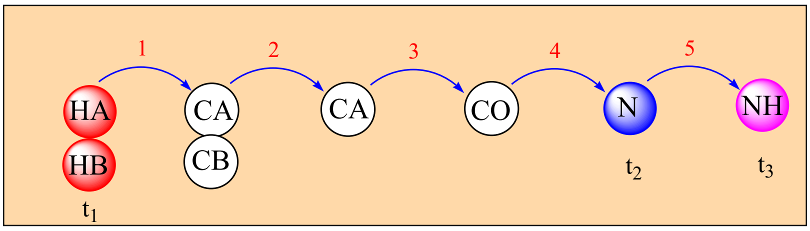
- 3D HBHA(CO)NH with PEP (**hbhaconhgp3d** | HBHACONHGP3D)
- 3D HBHA(CO)NH using WATERGATE (**hbhaconhgpwg3d** | HBHACONHGPWG3D)
- 3D HBHA(CO)NH using TROSY (**trhbhaconhgp3d** | TRHBHACONHGP3D)
- 3D HBHA(CO)NH using TROSY and gradient echo-antiecho (**trhbhaconhetgp3d** | TRHBHACONHETGP3D)

- 4D HBHACONH using WATERGATE (**hbhaconhgpwg4d**)

Also see:
3D HBHANH experiment
3D CBCA(CO)NH experiment
3D H(CC)(CO)NH experiment







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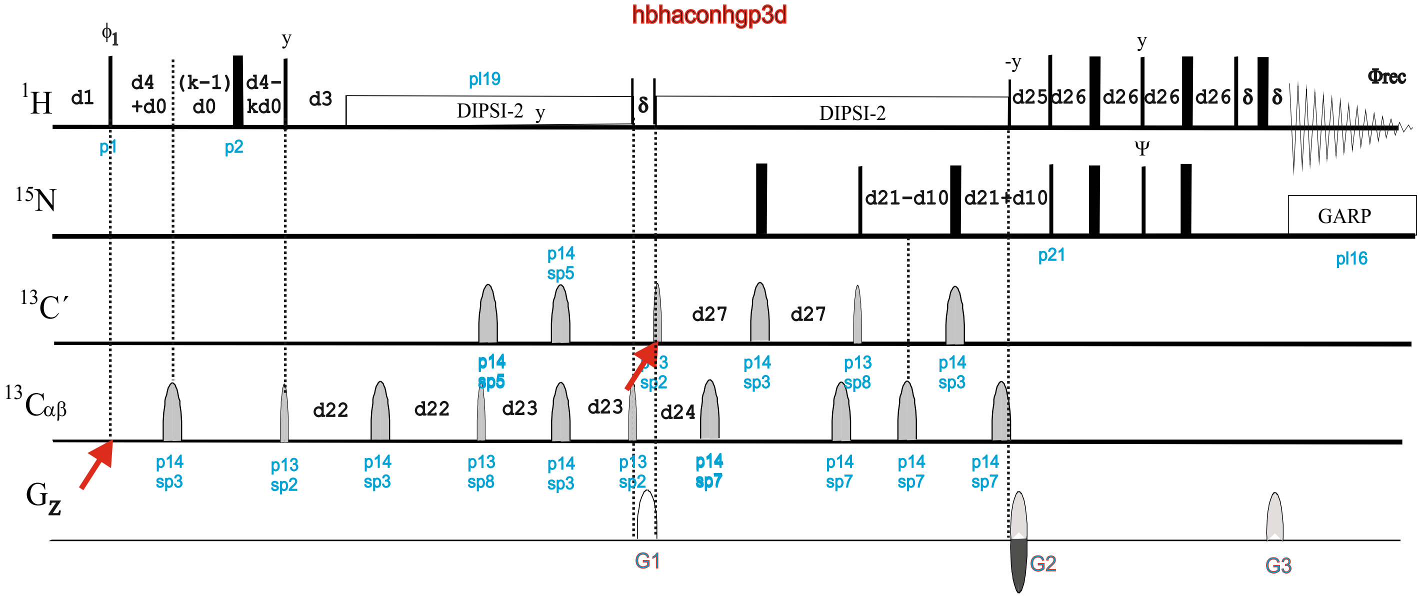
d3=1/6J(CH)=2.2m
d21=1/4J(NCO)=12.4m
d22=1/4J(CACB)=3.6m
d23=1/4J(CACO)=3.6m
d24=1/2J(CACO)=4.4m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m
d27=1/4J(NCO)=12.4m

hbhaconhgp3d



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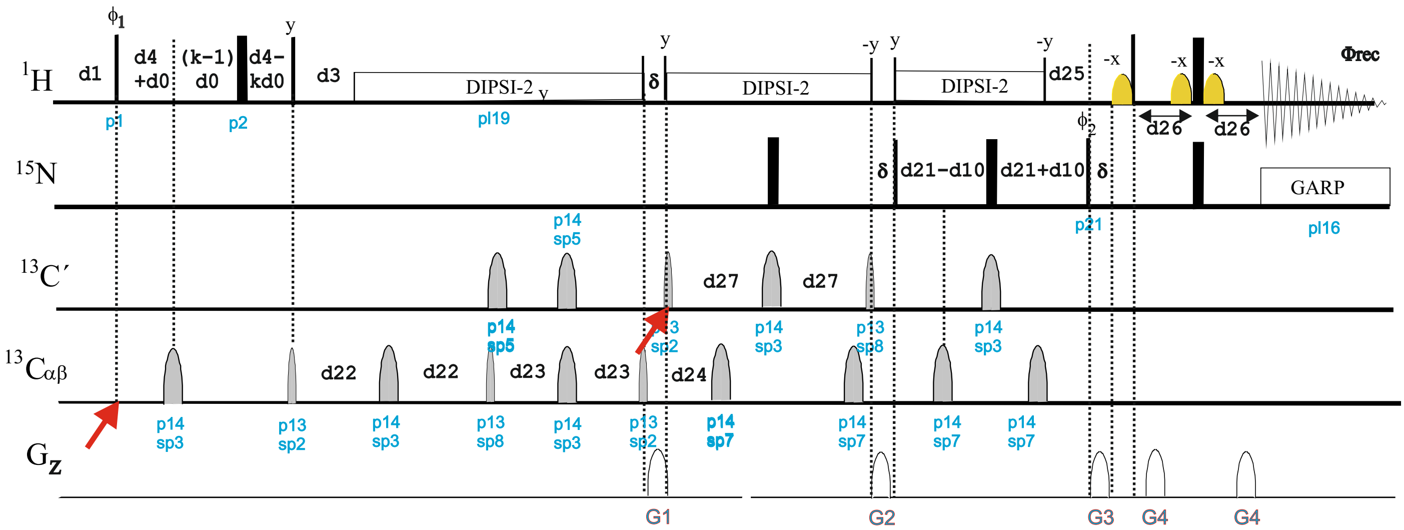

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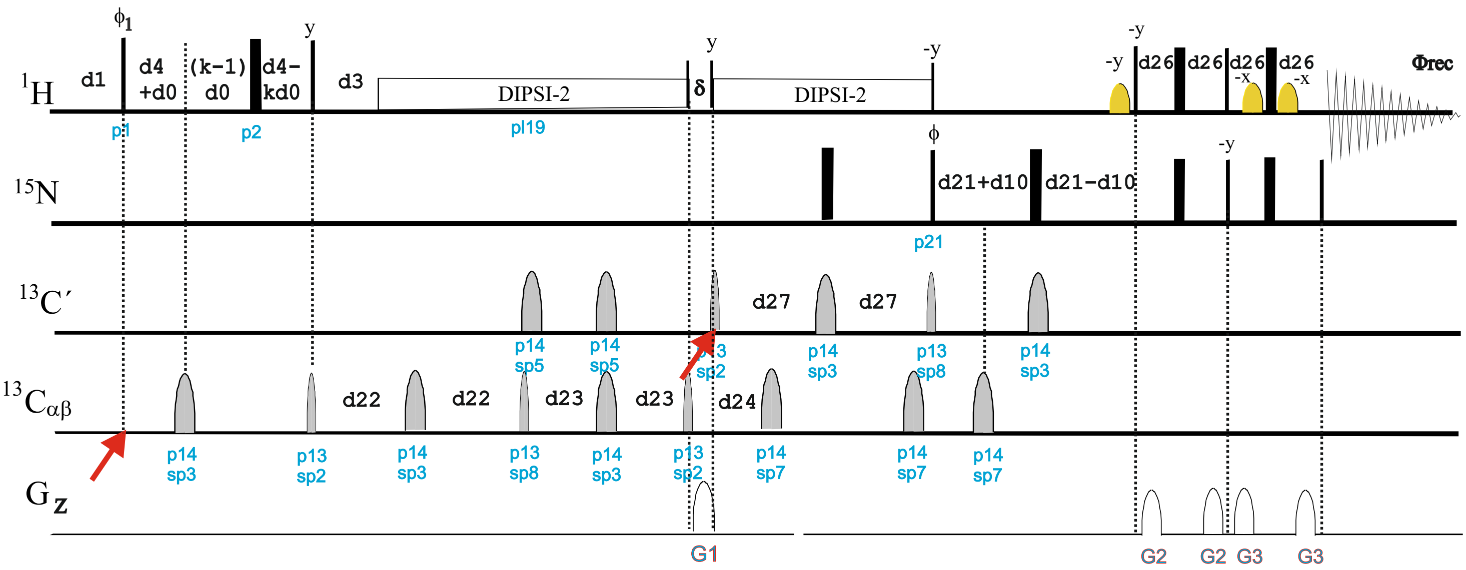

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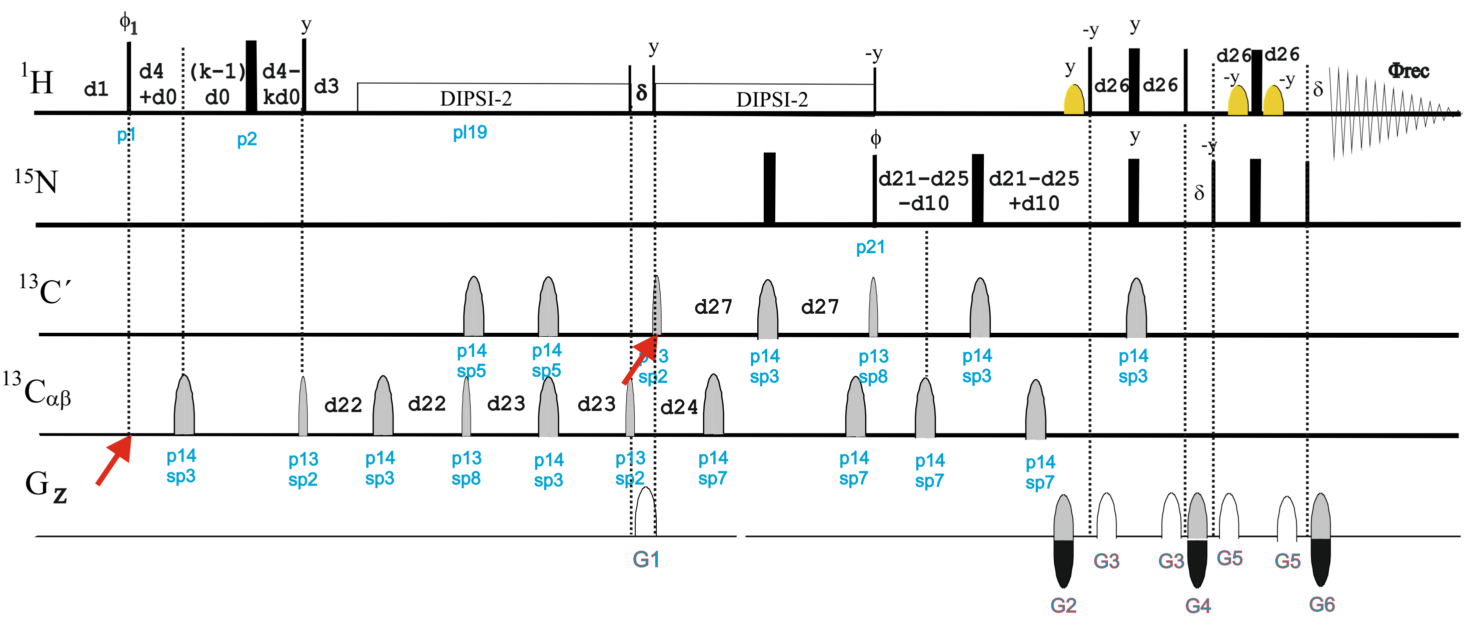

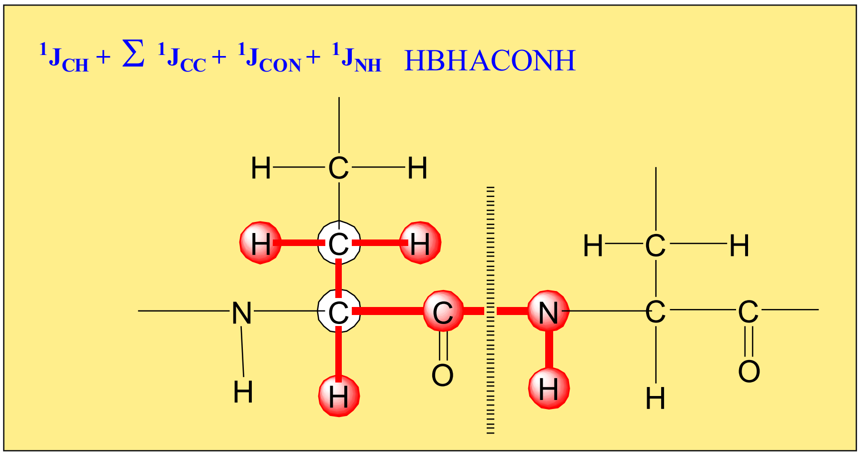

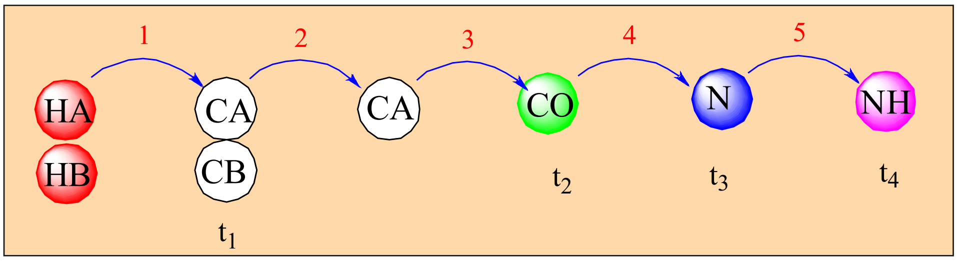

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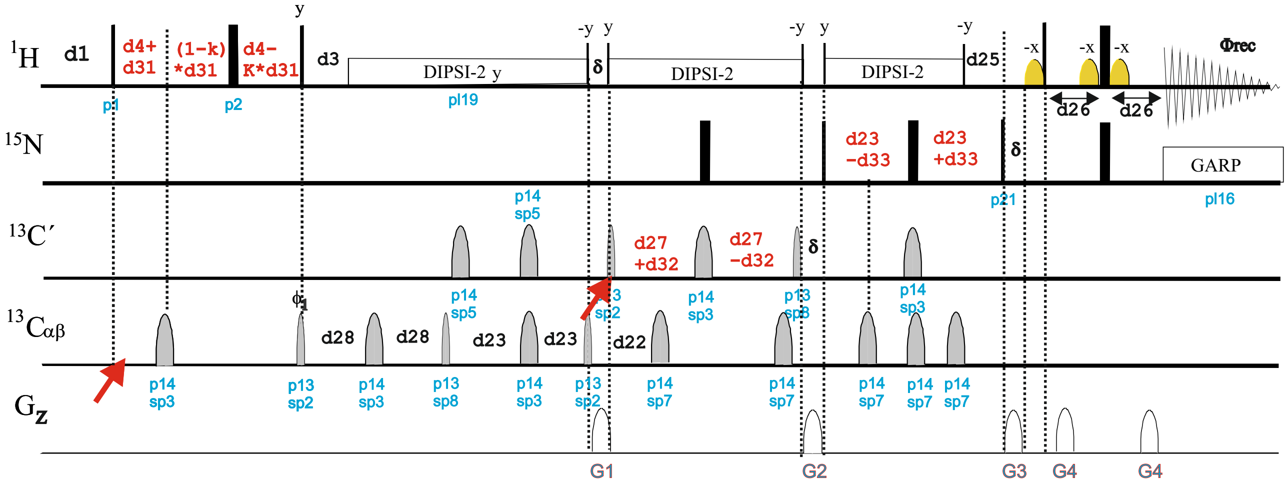

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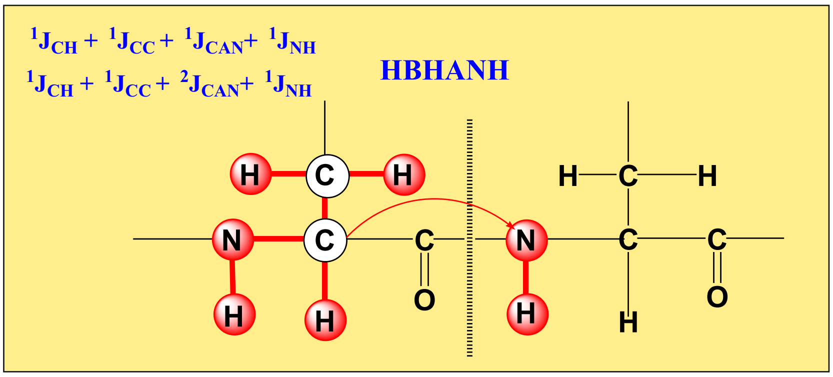
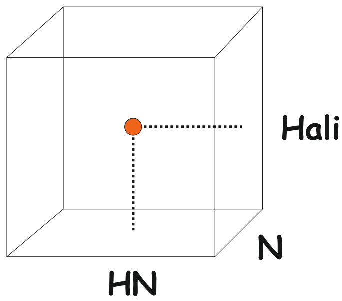
3D HBHANH

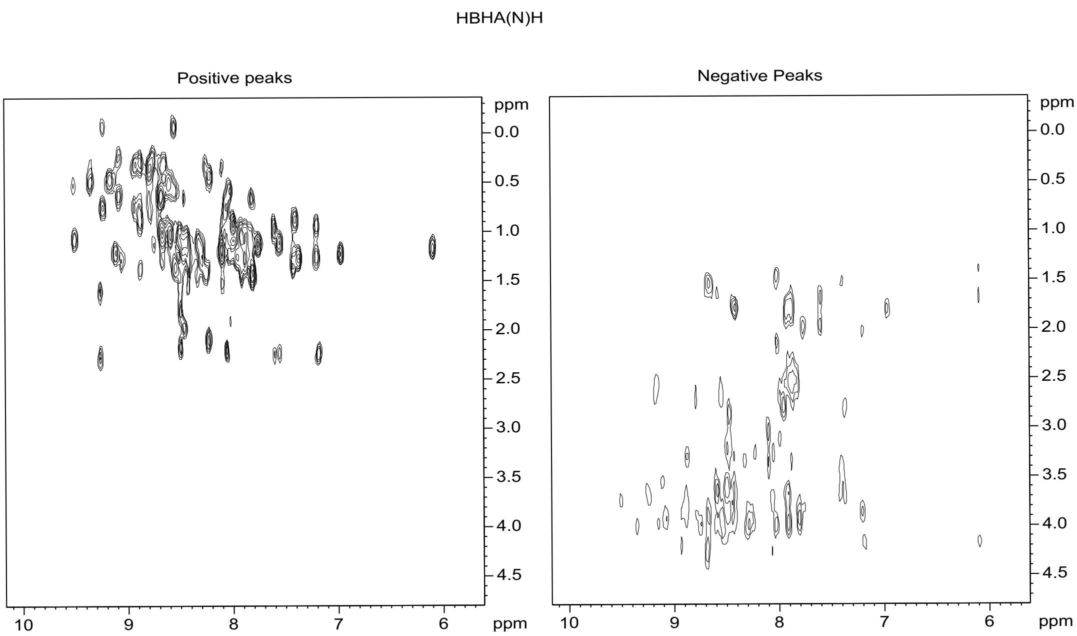
3D HBHANH experiment

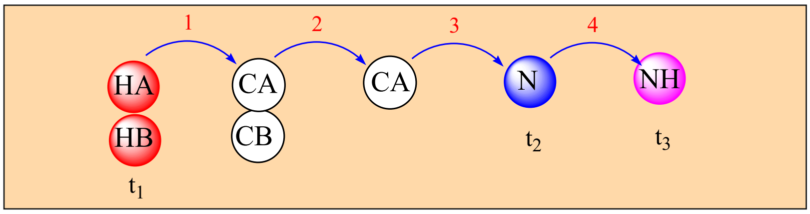
- 3D HBHANH using PEP (**hbhanhgp3d**) | HBHANHGP3D)
- 3D HBHANH using WATERGATE (**hbhanhgpwg3d**) | HBHANHGPWG3D)
- 3D HBHANH using TROSY (**trhbhanhgp3d** | TRHBHANHGP3D)
- 3D HBHANH using TROSY and gradient echo-antiecho (**trhbhanhetgp3d** | TRHBHANHETGP3D)

Also see:
3D HBHA(CO)NHexperiment









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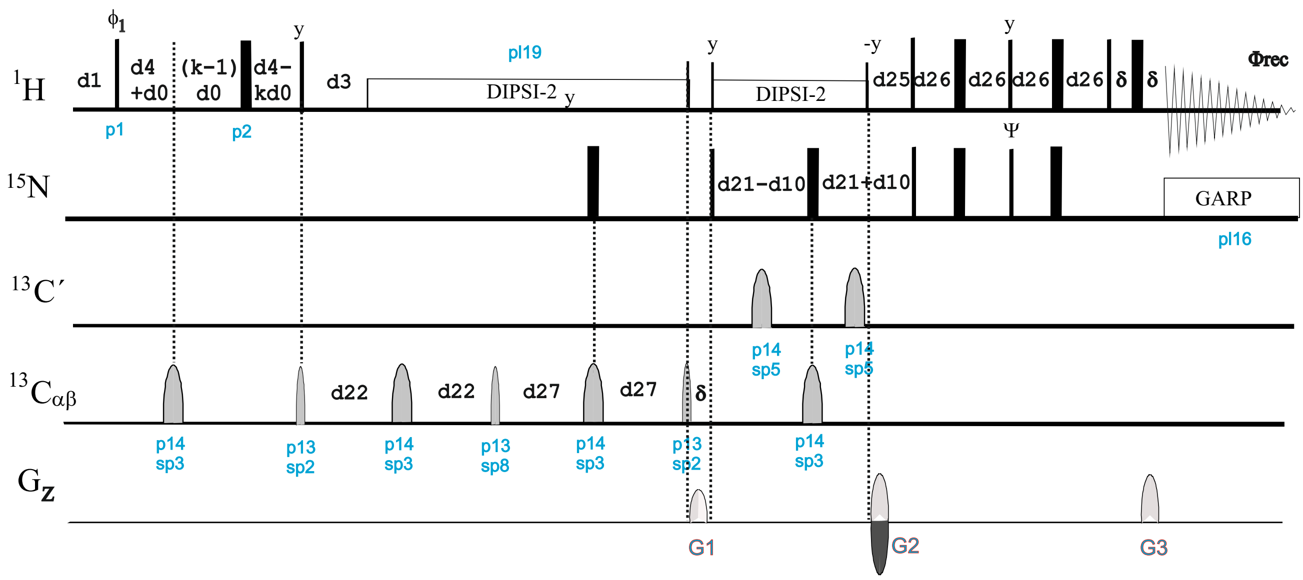
d3=1/6J(CH)=2.2m
d21=1/4J(NCO)=12.4m
d22=1/4J(CACB)=3.6m
d25=1/2J(NH)=5.5m
d26=1/4J(NH)=2.3m
d27=1/4J(NCO)=12.4m

hbhanhgp3d



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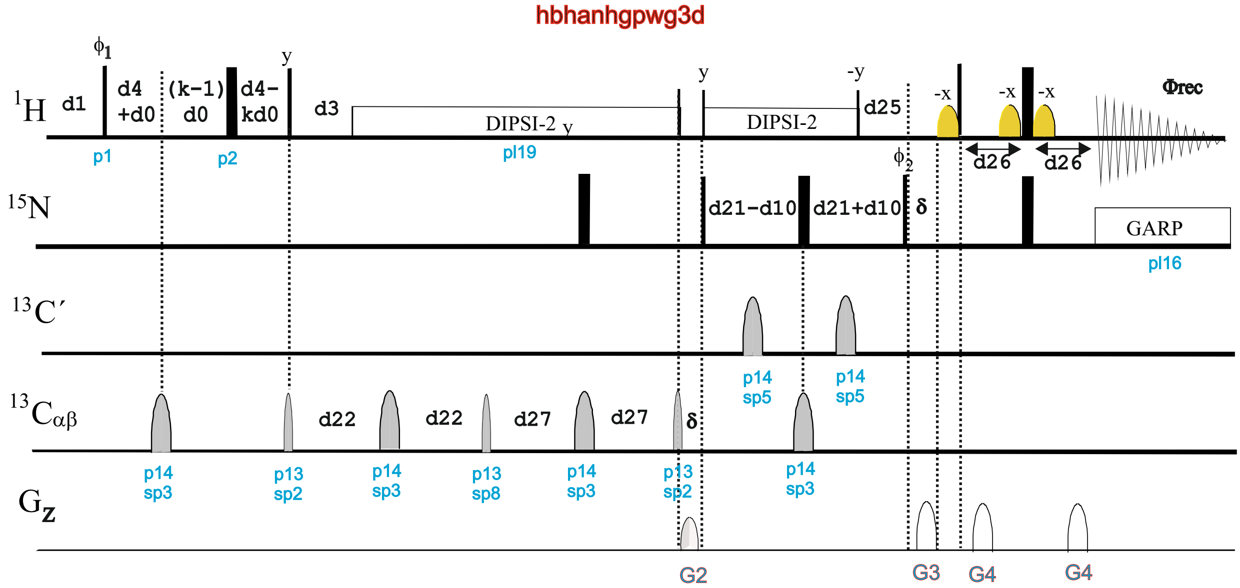
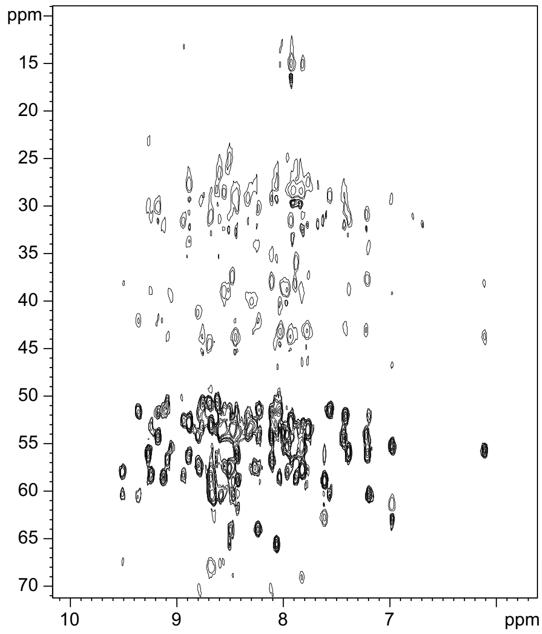
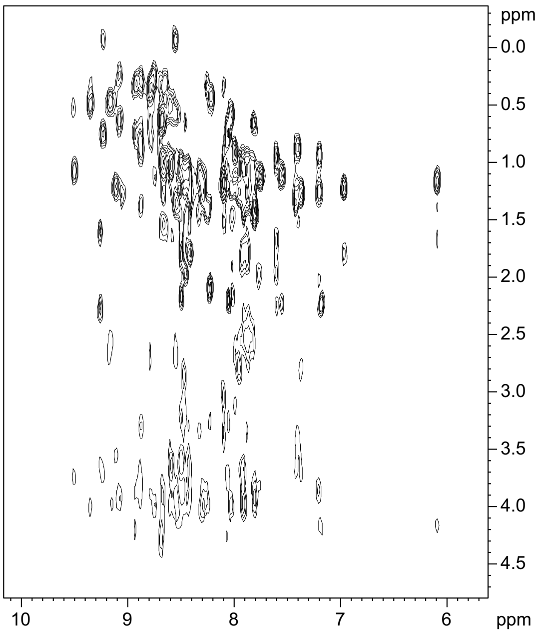


CBCA(N)H



HBHA(N)H



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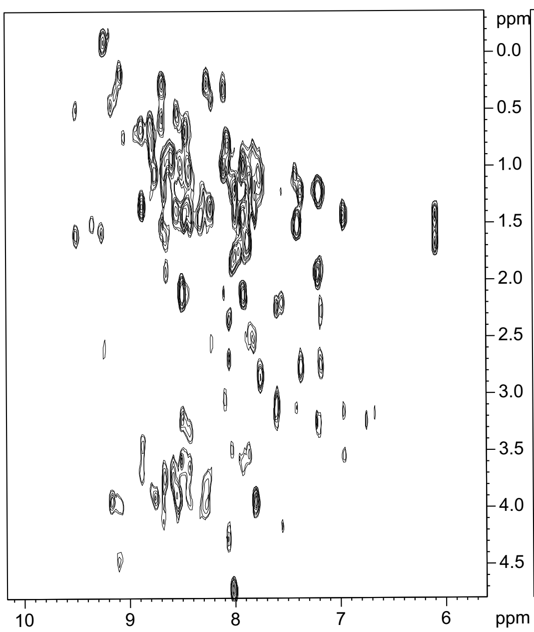

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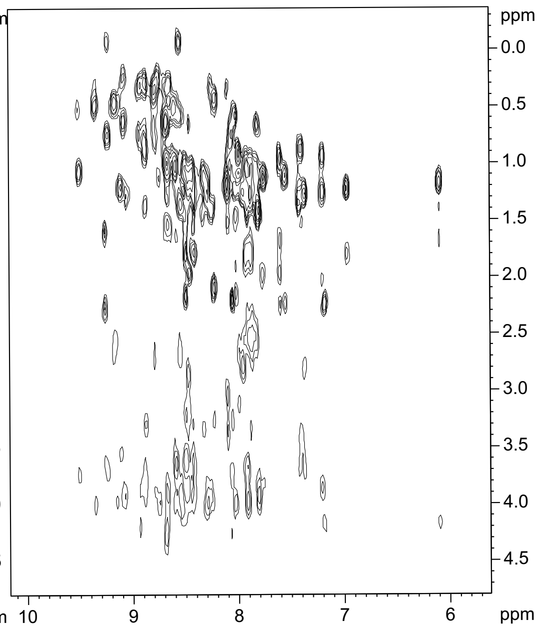

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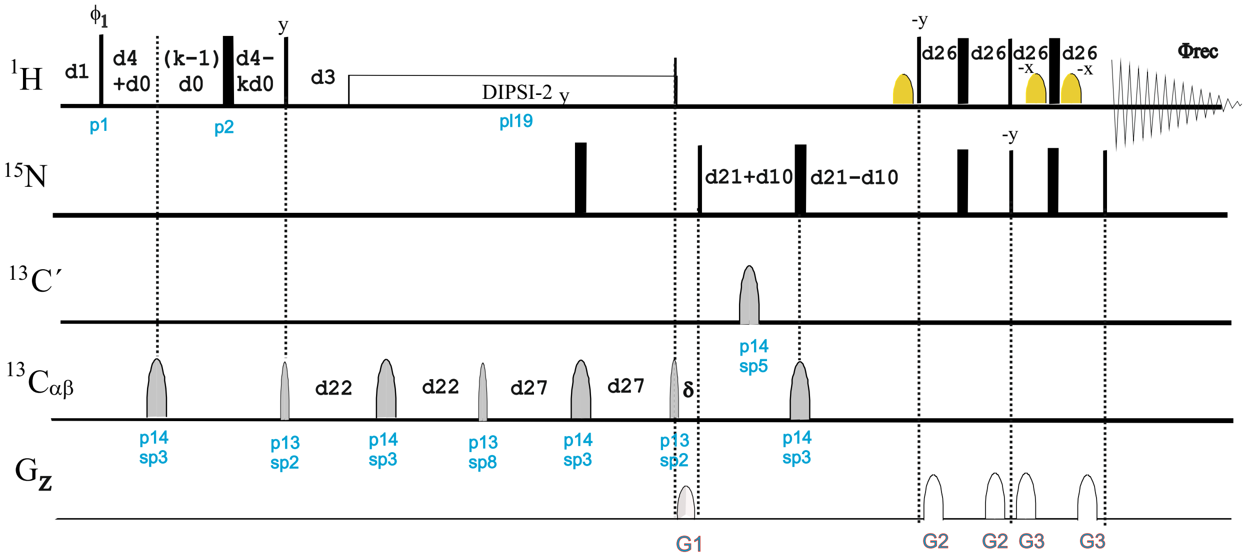

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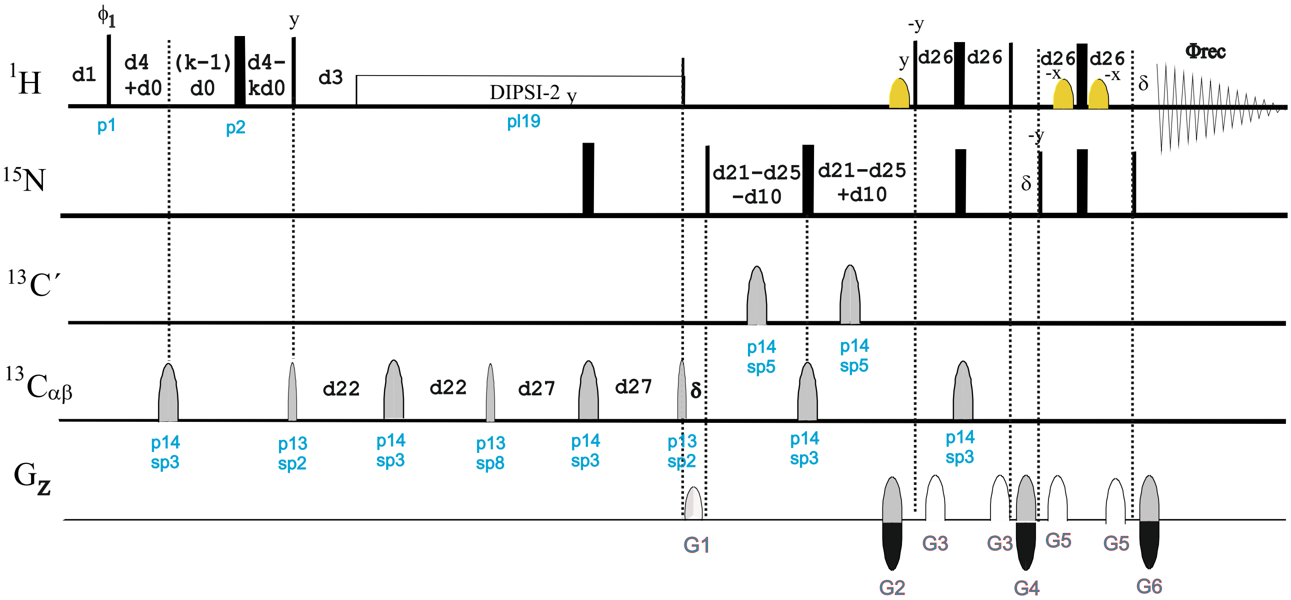

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REDUCED-DIMENSIONALITY
(APSY) NMR
EXPERIMENTS

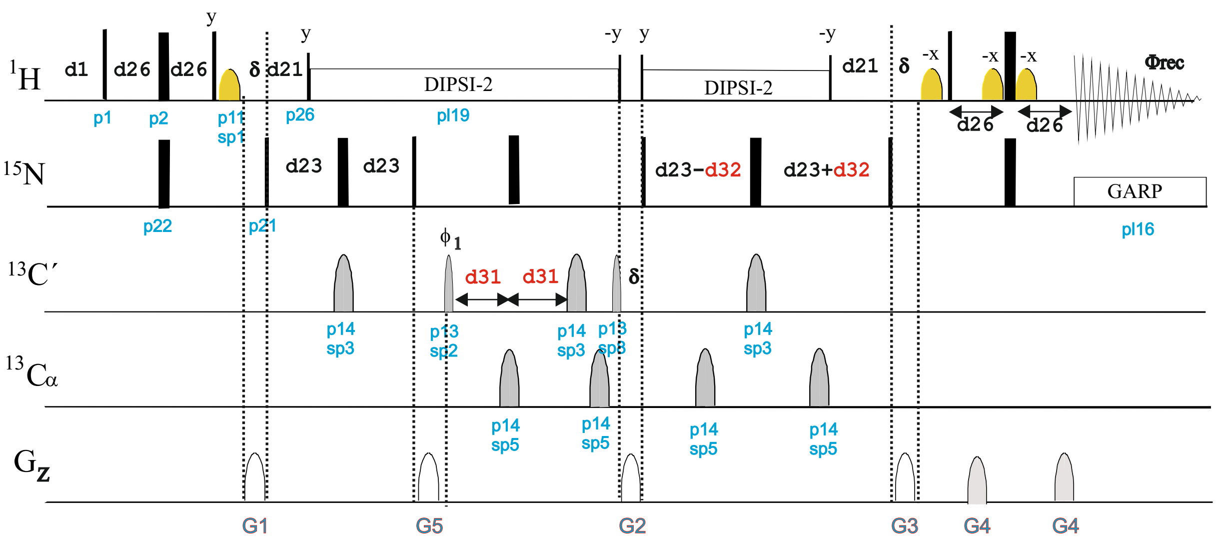
S. Hiller, F. Fiorito. K. Wuethrich & G. Wider, Proc. Natl. Acad. Sci. USA 102, 10876-10881 (2005).
F. Fiorito, S. Hiller, G. Wider & K. Wuethrich, J. Biomol. NMR 35, 27-37 (2006)

Reduced-Dimensionality (RD) /APSY NMR Experiments

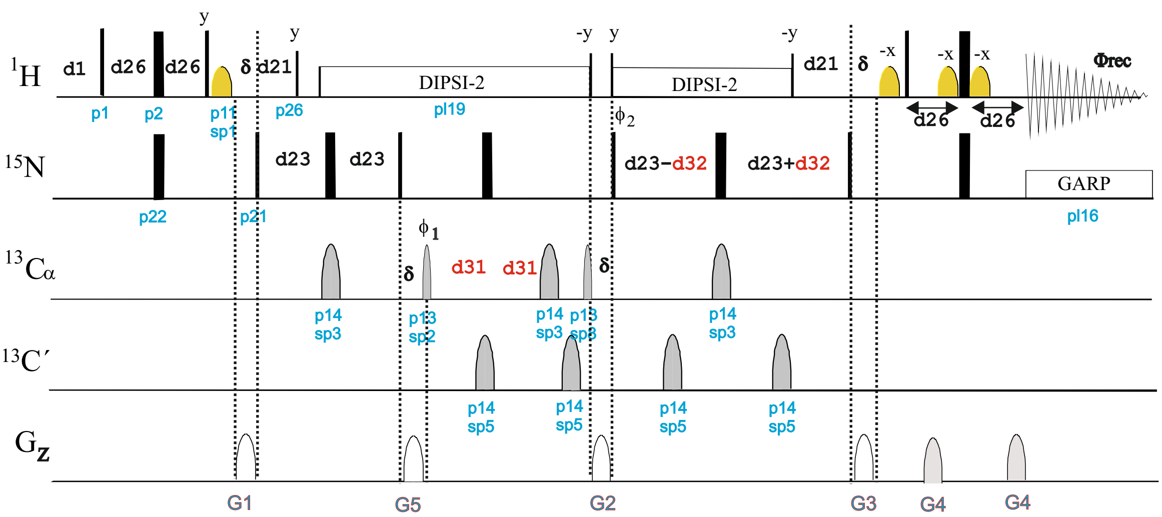
- Reduced-Dimensionality (3,2)-HNCA (**rd_hnca_32 | APSY_HNCA_32)**
- Reduced-Dimensionality (3,2)-HNCACB (**rd_hncacb_32 | APSY_HNCACB_32)**
- Reduced-Dimensionality (3,2)-HNCOCACB (**rd_hncocacb_32 | APSY_HNCOCACB_32)**
- Reduced-Dimensionality (6,2)-HNCOCANH (**rd_hncocanh_62 | APSY_HNCOCANH_62)**
- Reduced-Dimensionality (3,2)-HNCO (**rd_hnco_32 | APSY_HNCO_32)**
- Reduced-Dimensionality (4,2)-HNCOCA (**rd_hncoca_42 | APSY_HNCOCA_42)**

See the original experiments

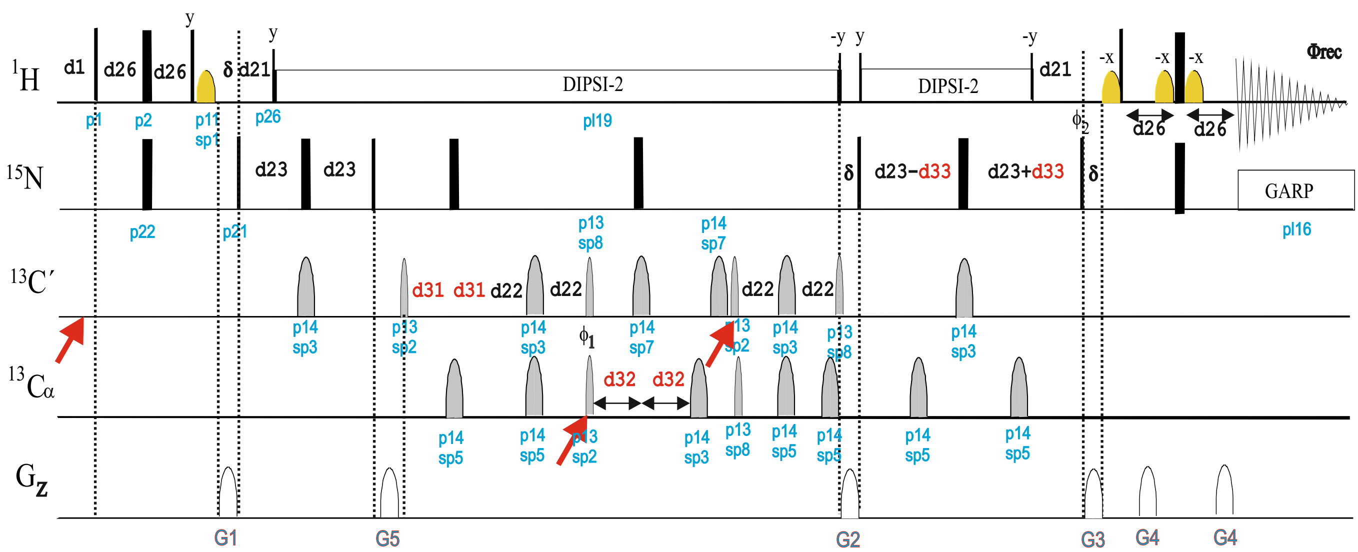
rd_hnco_32



rd_hnca_32



rd_hncoca_42



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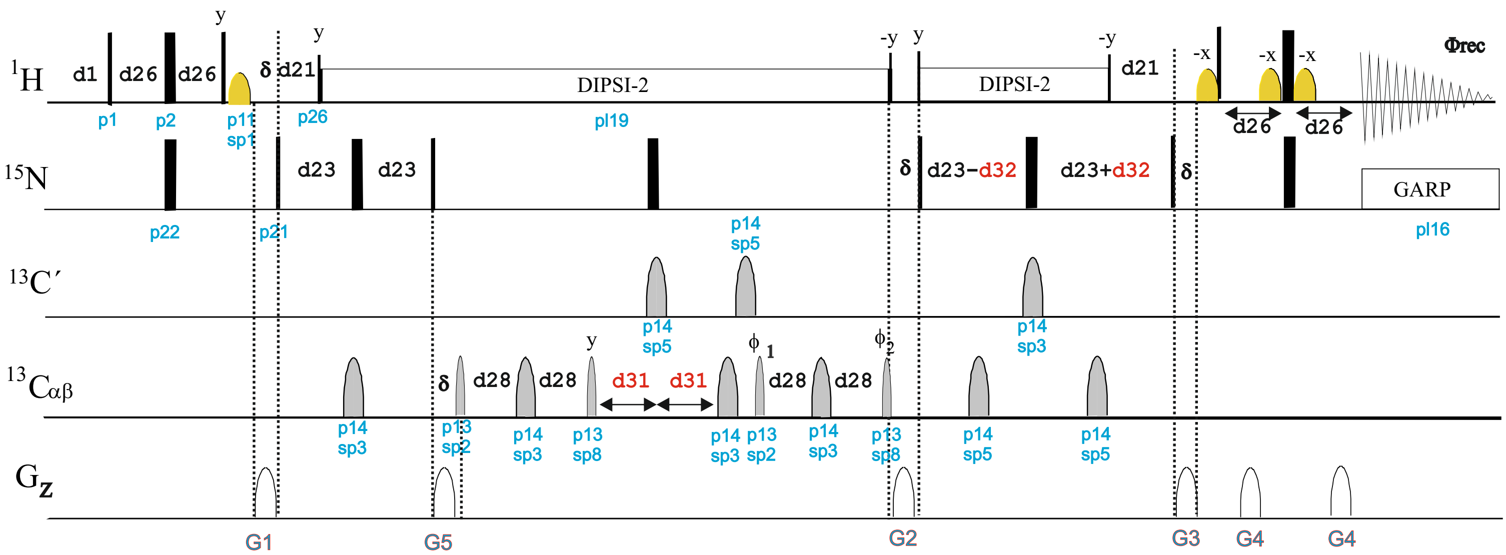

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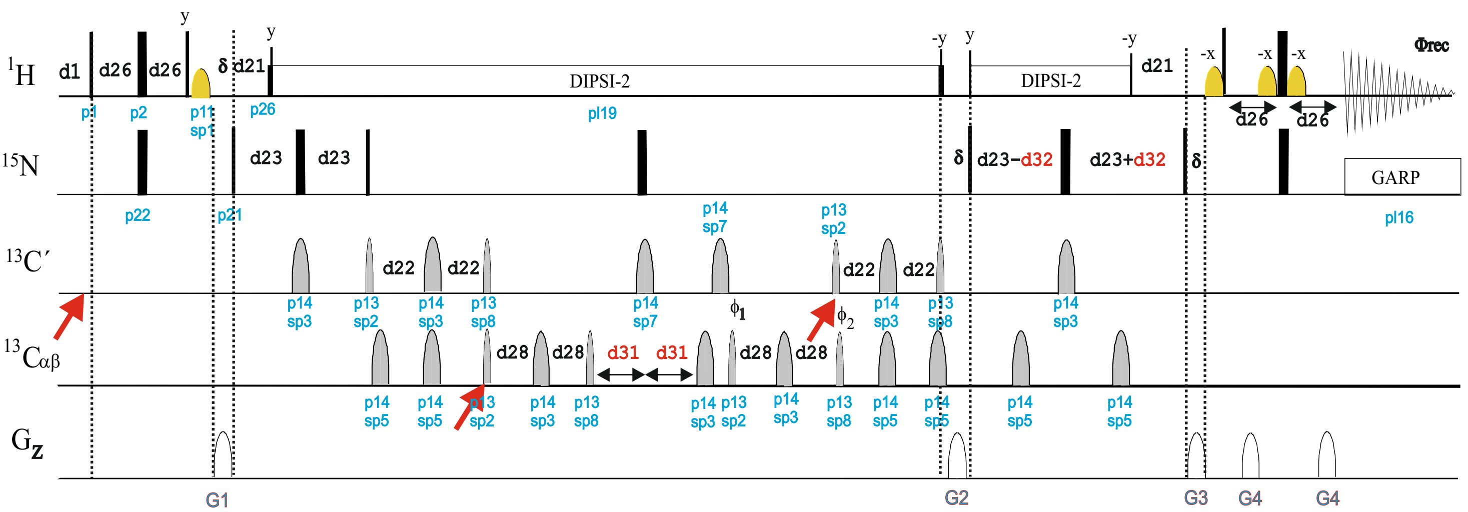

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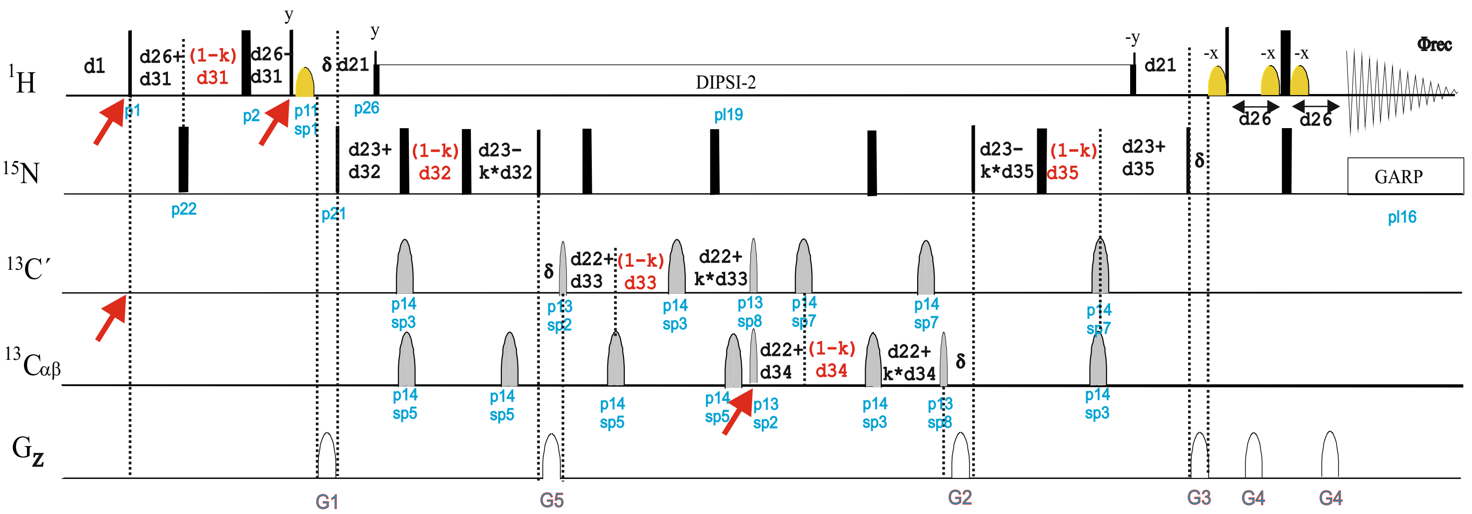

A Decription of the usage of the APSY techmique in TOPSPIN can be found in the ***APSY Manual*** (see **Help** menu in Topspin)

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2D & 3D
BEST/SOFAST
NMR EXPERIMENTS

SOFAST/BEST NMR Experiments

2D SOFAST/BEST Experiments

- 2D Sofast-HMQC (**sfhmqcf3gpph | SFHMQCF3GPPH)**
- 2D Sofast-HMQC with inversion of water/aliphatic protons (**hetsfhmqcf3gpph)**
- 2D Sofast-HMQC with sensitivity improved (**sfhmqcf3gpphiasi)**
- 2D BEST-HSQC (**b_hsqcetf3gpsi | B_HSQCETF3GPSI**)
- 2D BEST-TROSY (**b_trosyf3gpph**)
- 2D BEST-TROSY with sensitivity improved (**b_trosyetf3gpsi**)

3D SOFAST/BEST Experiments

- 3D BEST-HNCO (**b_hncogp3d | B_HNCOGP3D**)
- 3D BEST-HNCO using TROSY (**b_trhncogp3d**)
- 3D BEST-intraHNCO (**b_hncoigp3d | B_HNCOIGP3D**
- 3D BEST-intraHNCO using TROSY (**b_trhncoigp3d**)
- 3D BEST-HNCA (**b_hncagp3d | B_HNCAGP3D**)
- 3D BEST-HNCA using TROSY (**b_trhncagp3d)**
- 3D BEST-intraHNCA (**b_hncaigp3d | B_HNCAIGP3D**)
- 3D BEST-intraHNCA using TROSY (**b_trhncaigp3d**)
- 3D BEST-HN(CO)CA (**b_hncocagp3d | B_HNCOCAGP3D**)
- 3D BEST-HN(CO)CA using TROSY (**b_trhncocagp3d**)
- 3D BEST-HN(CA)CO (**b_hncacogp3d | B_HNCACOGP3D**)
- 3D BEST-HN(CA)CO using TROSY (**b_trhncacogp3d**)
- 3D BEST-HNCACB (**b_hncacbgp3d | B_HNCACBGP3D**)
- 3D BEST-HNCACB using TROSY (**b_trhncacbgp3d**)
- 3D BEST-intraHNCACB (**b_hncacbigp3d | B_HNCACBIGP3D**)
- 3D BEST-intraHNCACB using TROSY (**b_trhncacbigp3d**)
- 3D BEST-HN(CO)CACB (**b_hncocacbgp3d | B_HNCOCACBGP3D)**
- 3D BEST-HN(CO)CACB using TROSY (**b_trhncocacbgp3d)**

4D SOFAST/BEST Experiments

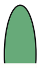
- 4D BEST-HNCACO (**b_hncacogp4d**)
- 4D BEST-HNCOCA (**b_hncocagp4d**)
- 4D BEST-HNCOCACB (**b_hncocacbgp4d)**

See the original experiments

NH-selective shaped pulses for BEST/Sofast NMR Experiments:

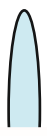
p39
sp23

p39: f1 channel - 120 degree shaped pulse for excitation
sp23= Pc9_4_120.1000 (120o) (3.0ms at 600.13 Mhz)
(or Q5.1000 (90o) (2.0ms at 600.13 MHz))



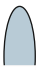
p40
sp24

p40: f1 channel - 180 degree shaped pulse for refocussing
sp24= Rsnob.1000 (1.0ms at 600.13 Mhz)



p41
sp25

p41: f1 channel - 90 degree shaped pulse for excitation
sp25=sp27= Pc9_4_90.1000 (3.0ms at 600.13 Mhz)

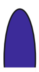


p42
sp26

p42: f1 channel - 180 degree shaped pulse for refocussing
sp26= Reburp.1000 (2.0ms at 600.13 Mhz)

p43
sp28

p43: f1 channel - 90 degree shaped pulse for excitation
sp28= Eburp2.1000 (1.92ms at 600.13 Mhz)
sp29= Eburp2tr.1000 (1.92ms at 600.13 Mhz)



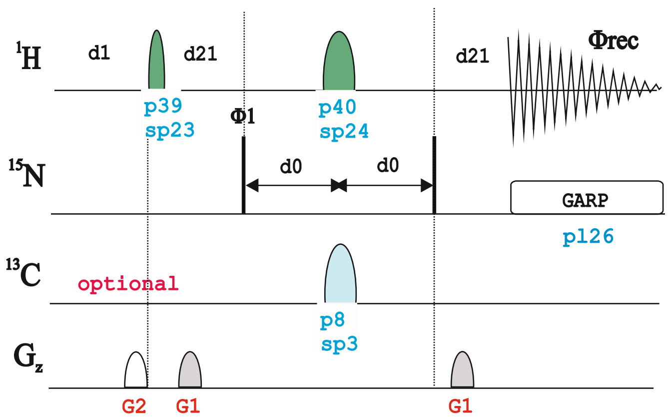
p44
sp30

p44: f1 channel - 180 degree shaped pulse for refocussing
sp30= Bip720,50,20.1 (200us at 600.13 MHz)

BEST-NMR:

1. P. Schanda, H. v. Melckebeke & B. Brutscher, J. Am. Chem. Soc. 128, 9042-9043 (2006)
2. E. Lescop, P. Schanda & B. Brutscher, J. Magn. Reson. 187 163-169 (2007)

sfhmqcf3gpph



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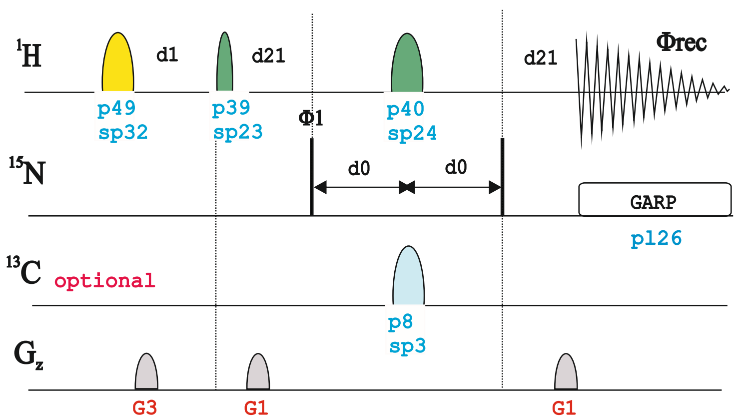
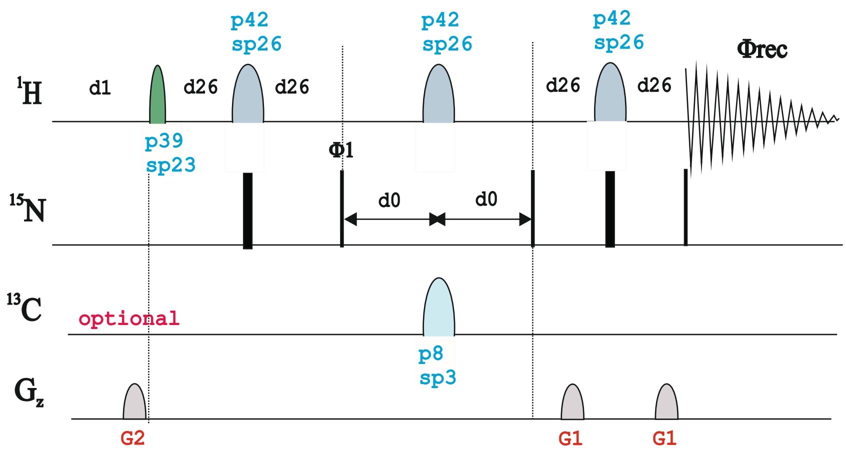
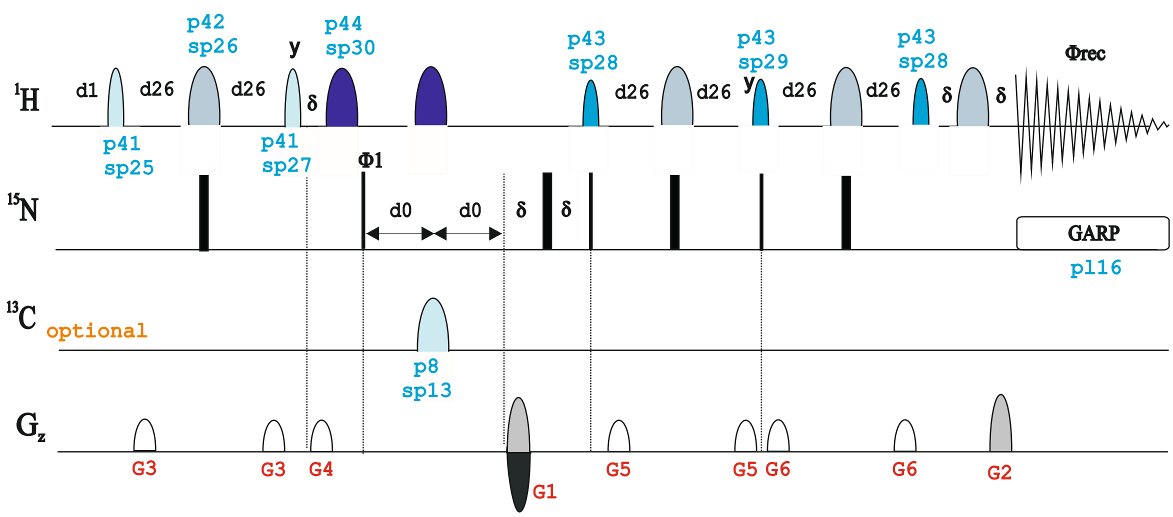


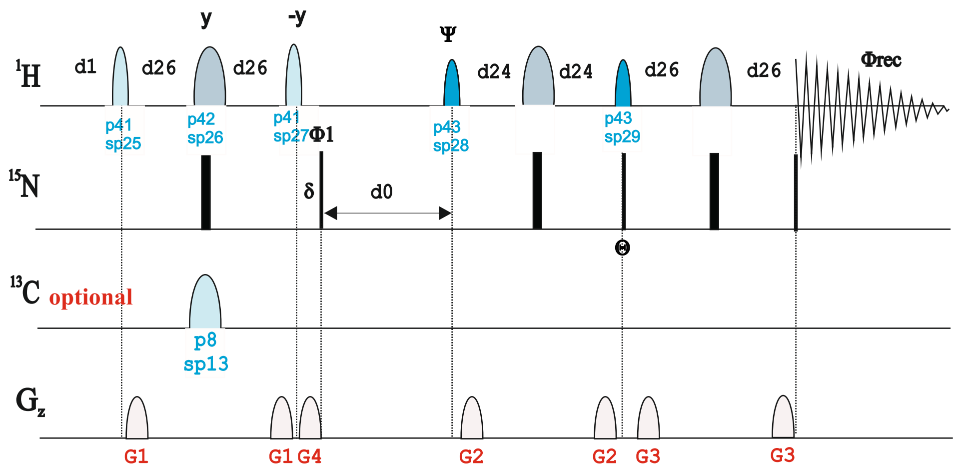
sfhmqcf3gpphiasi



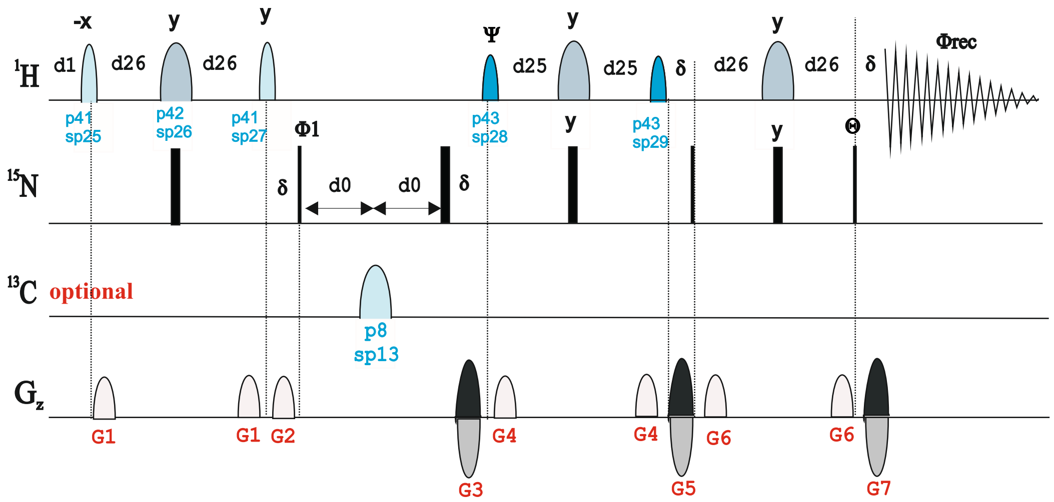
b_hsqcetf3gpsi

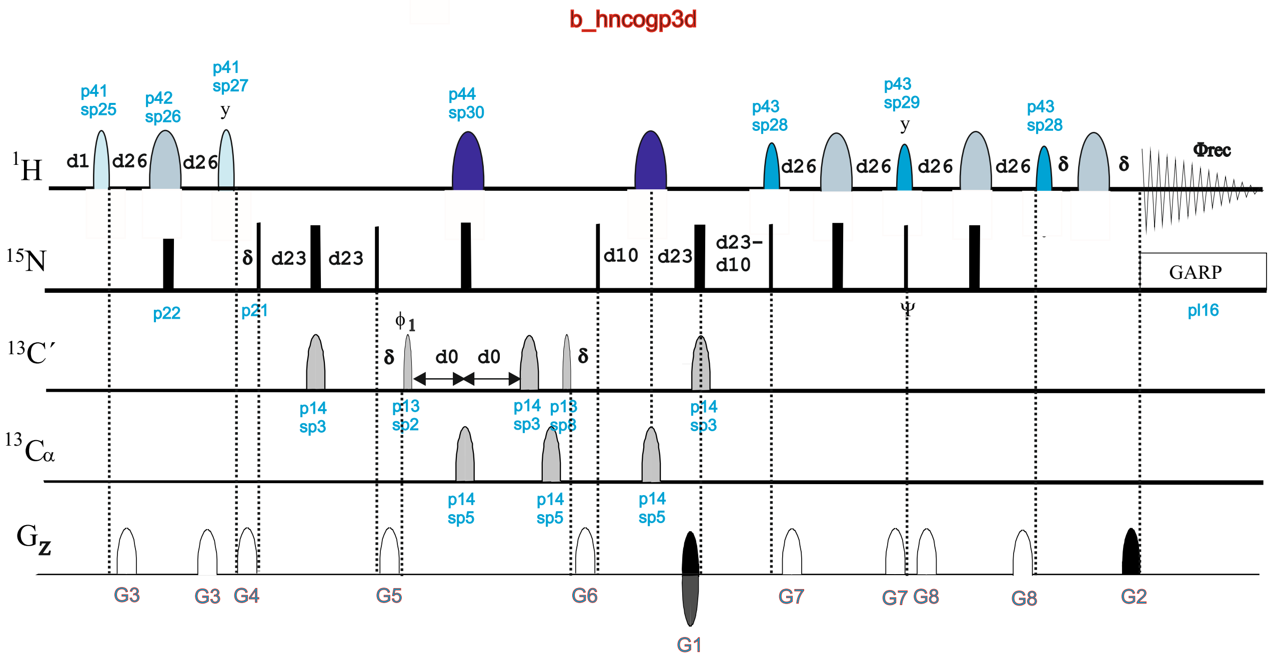


b_trosyf3gpph



b_trosyetf3gpsi




b_hncogp3d
p41
sp25
p42
sp26
p41
sp27
y
p44
sp30
p43
sp28
p43
sp29
y
p43
sp28
Φrec
d1
d26
d26
d26
d26
d26
d26
δ
δ
δ
d23
d23
d10
d23
d23-
d10
GARP
p22
p21
pl16
Ψ
ϕ1
δ
d0
d0
δ
p14
sp3
p13
sp2
p14
sp3
p13
sp8
p14
sp3
p14
sp5
p14
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sp5
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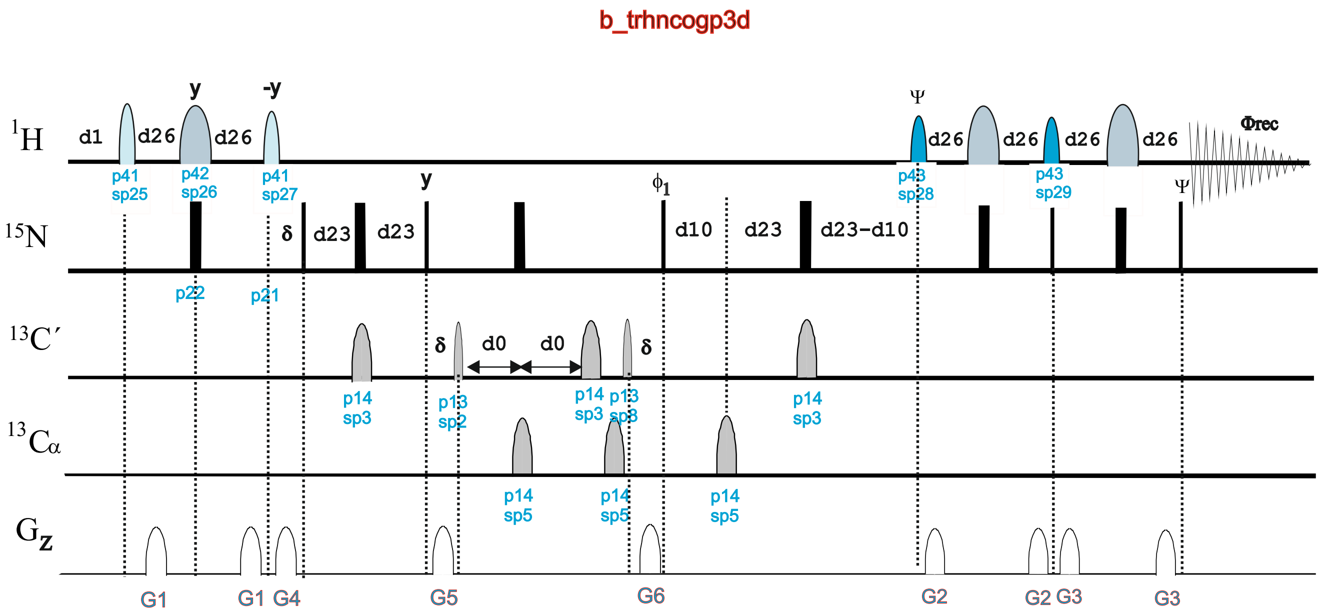
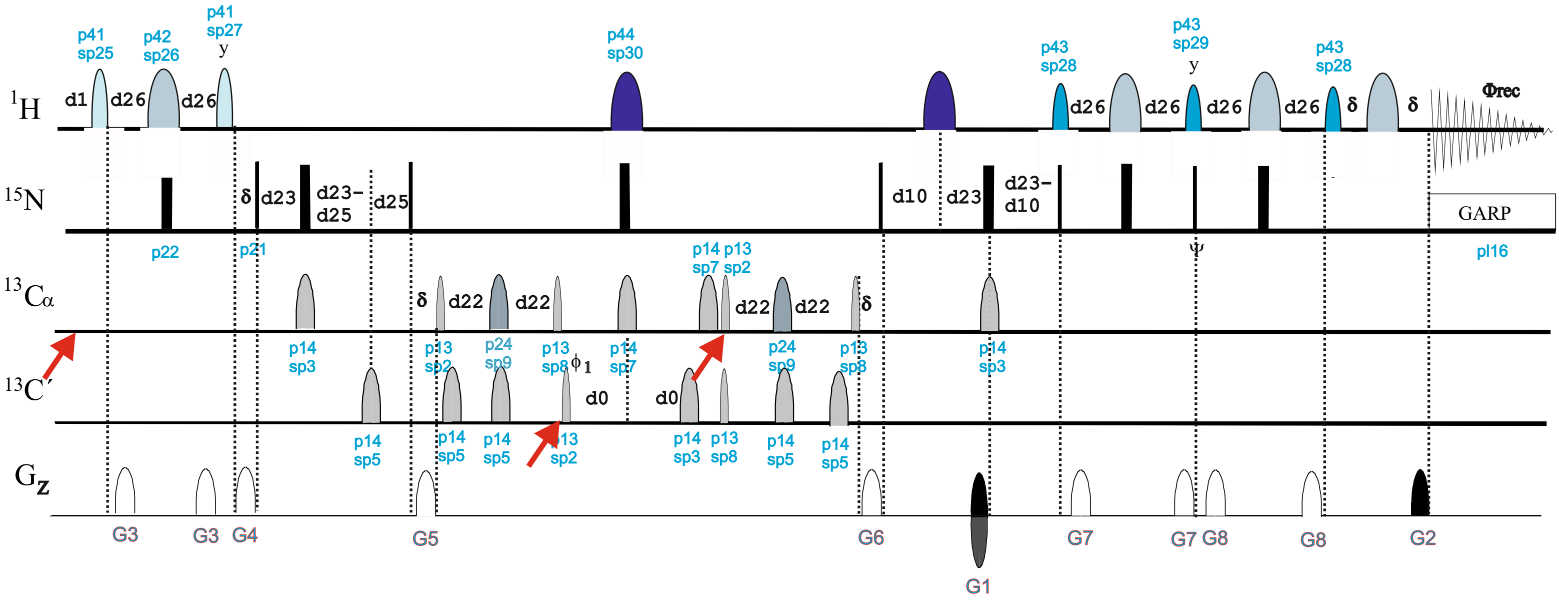
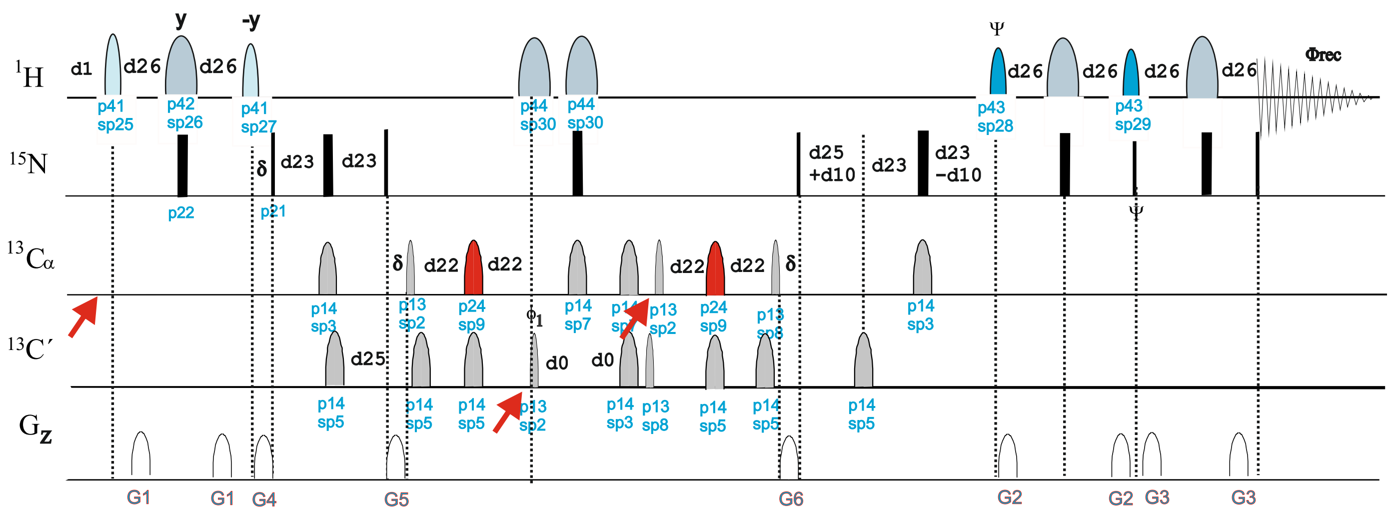
G3
G4
G5
G6
G1
G7
G7
G8
G8
G2


b_trhncogp3d
y
-y
Ψ
Φrec
d1
d26
d26
d26
d26
d26
d26
p41
sp25
p42
sp26
p41
sp27
y
ϕ1
p43
sp28
p43
sp29
Ψ
δ
d23
d23
d10
d23
d23-d10
p22
p21
δ
d0
d0
δ
p14
sp3
p13
sp2
p14
sp3
p13
sp8
p14
sp3
p14
sp5
p14
sp5
p14
sp5
G1
G1
G4
G5
G6
G2
G2
G3
G3

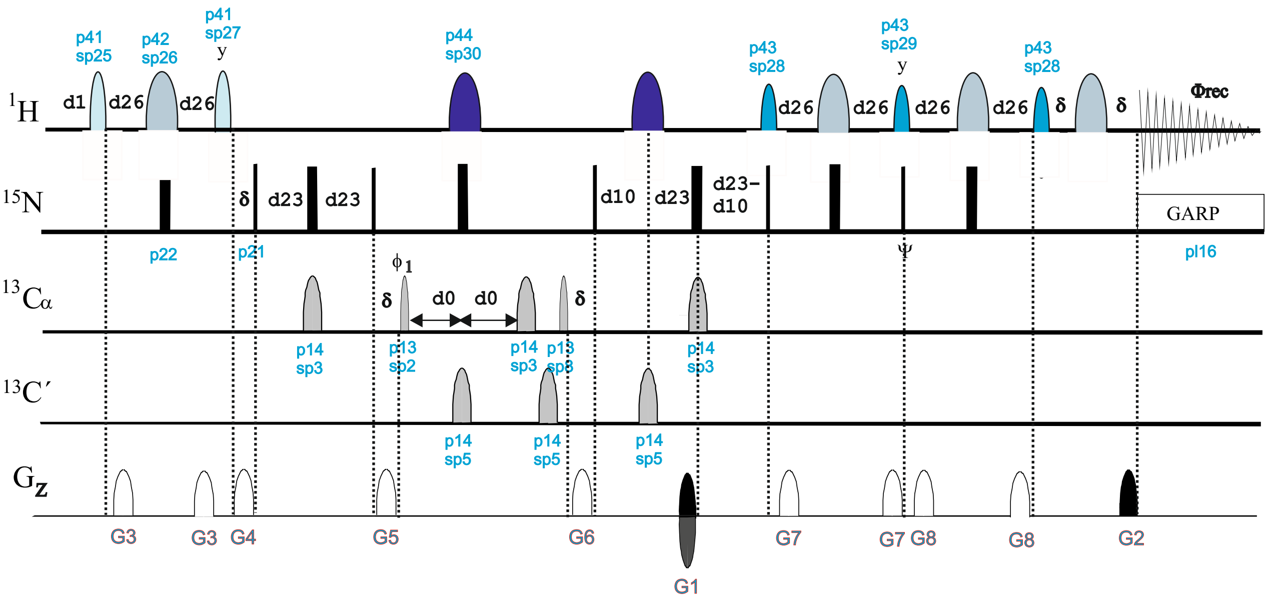
b_hncoigp3d



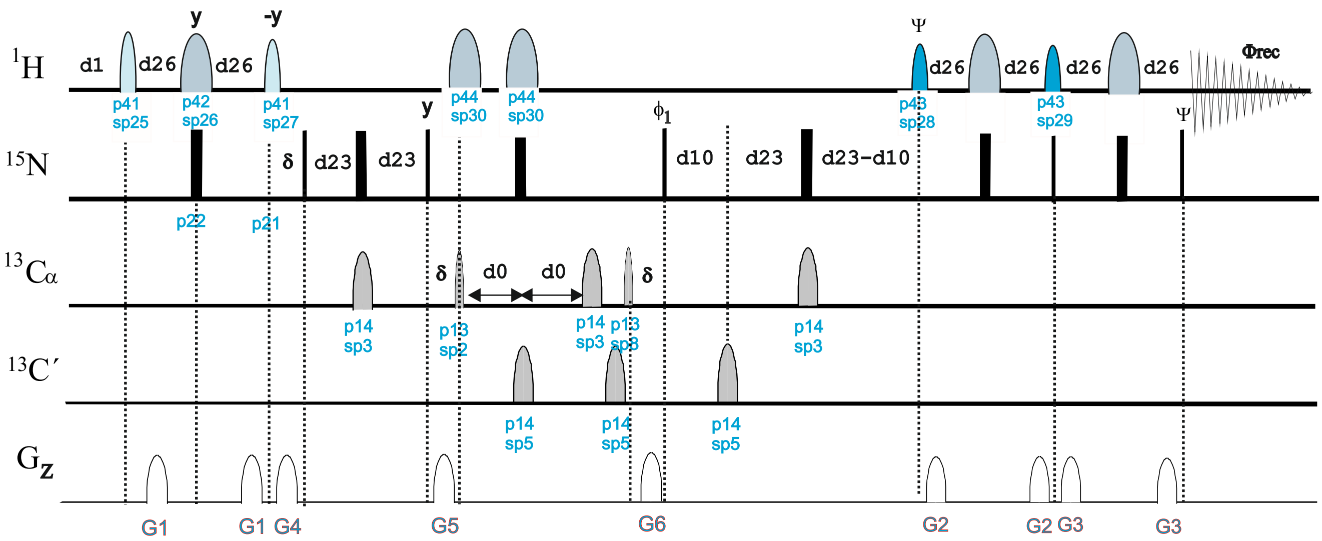
b_trhncoigp3d



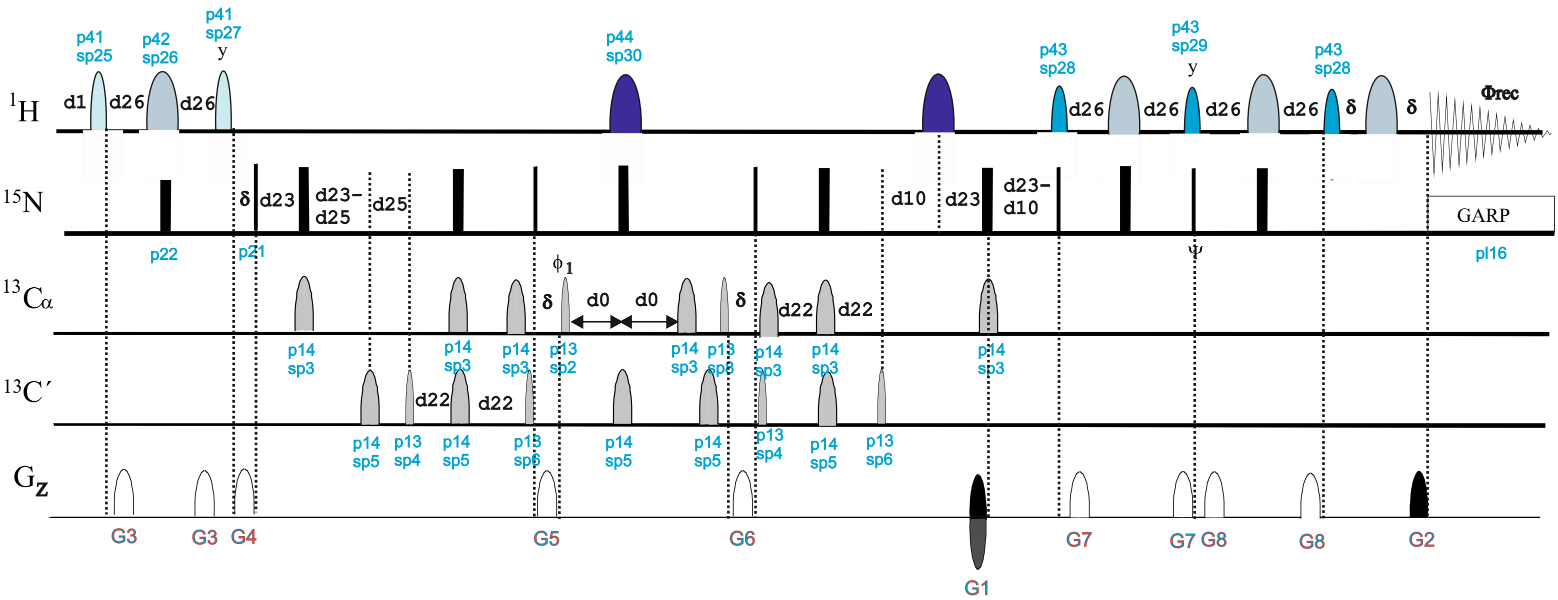
b_hncagp3d



b_trhncagp3d



b_hncaigp3d



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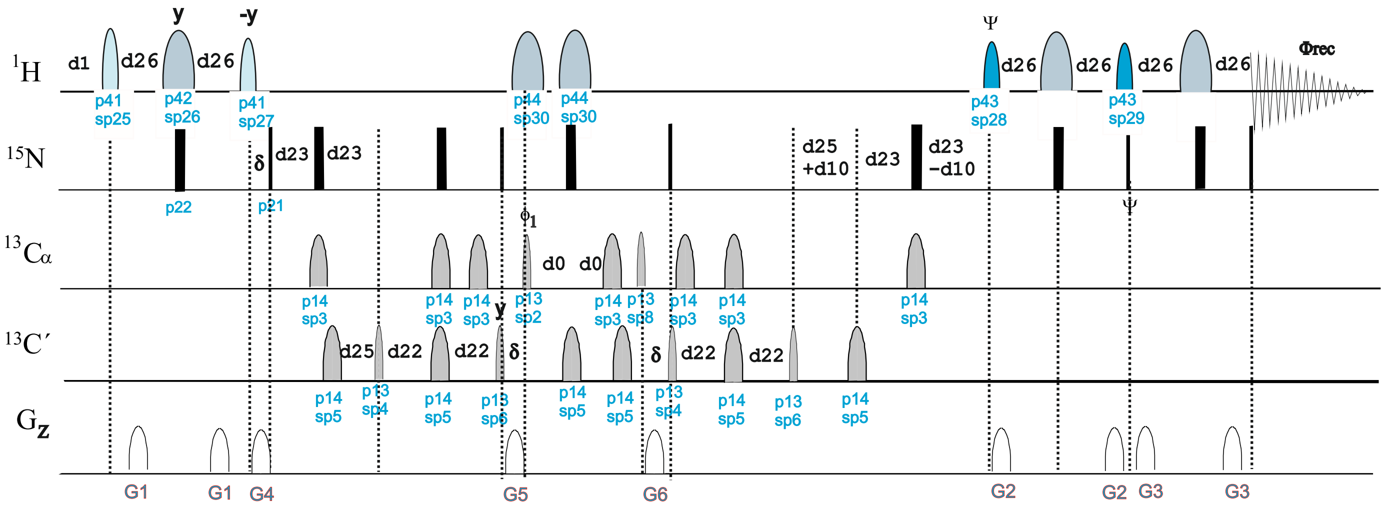

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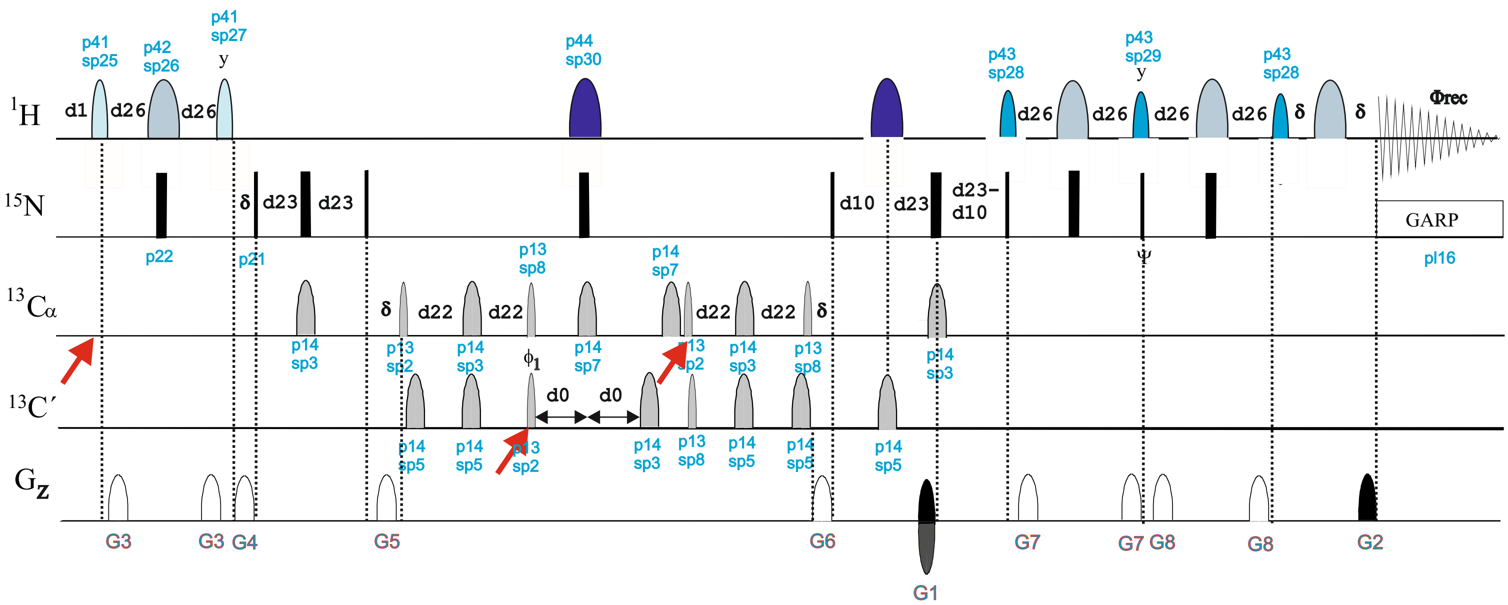

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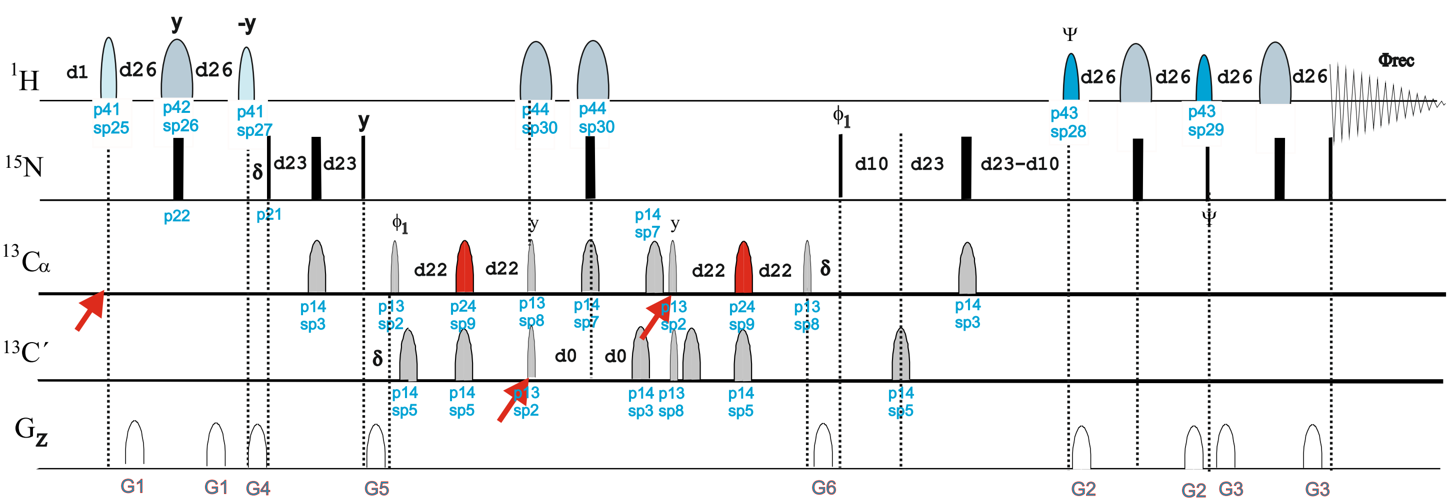
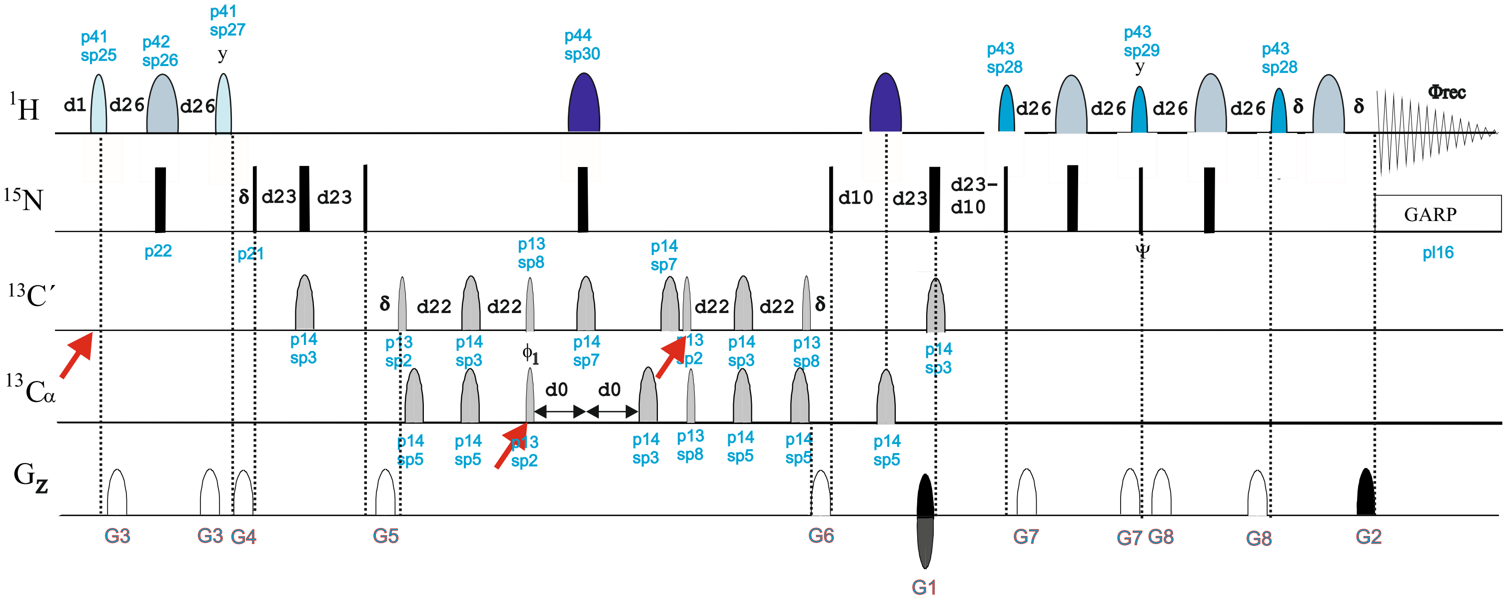
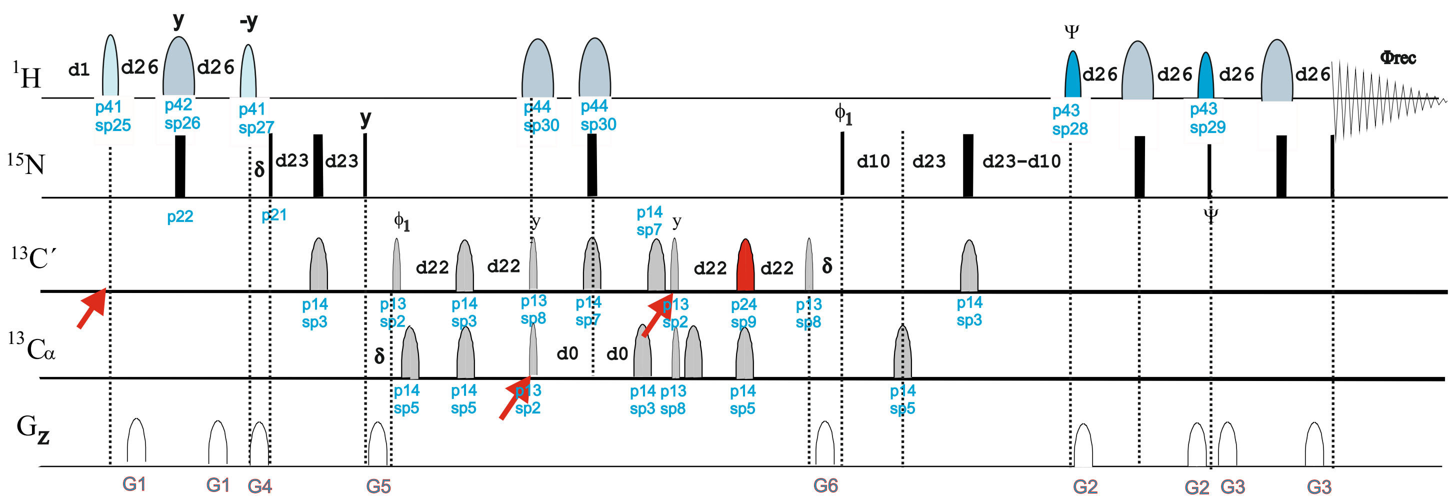


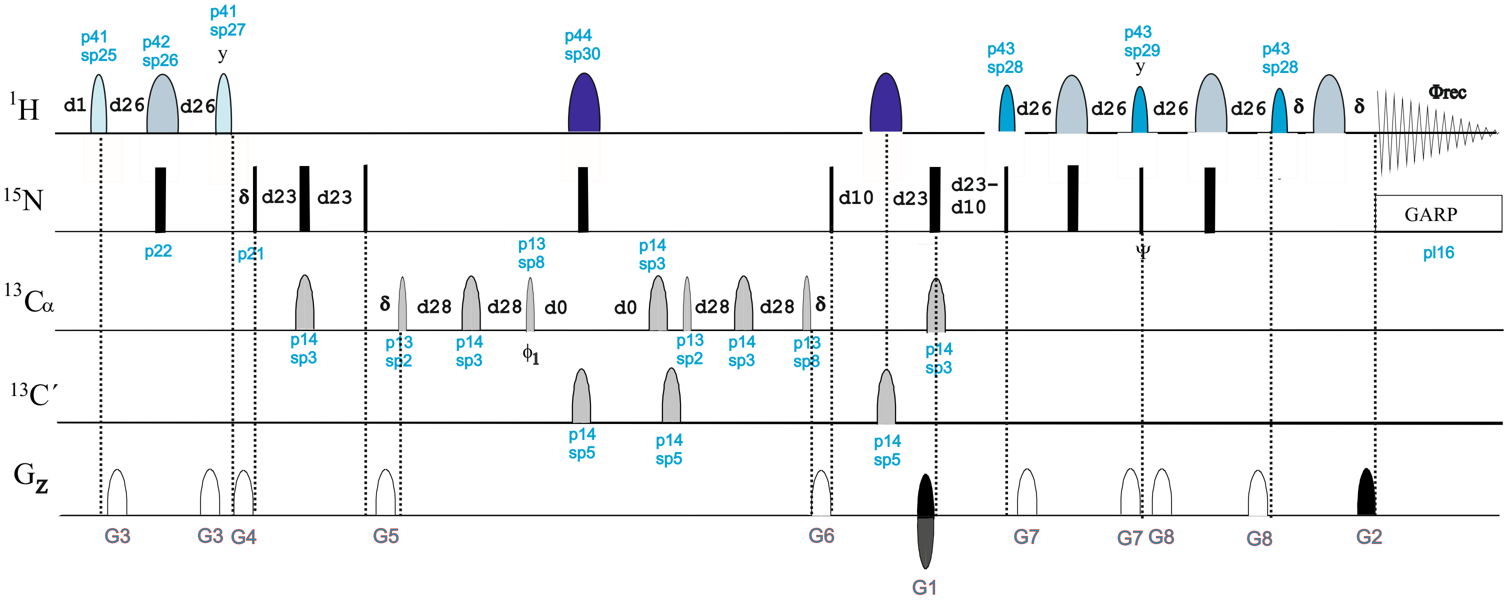
b_hncocagp3d



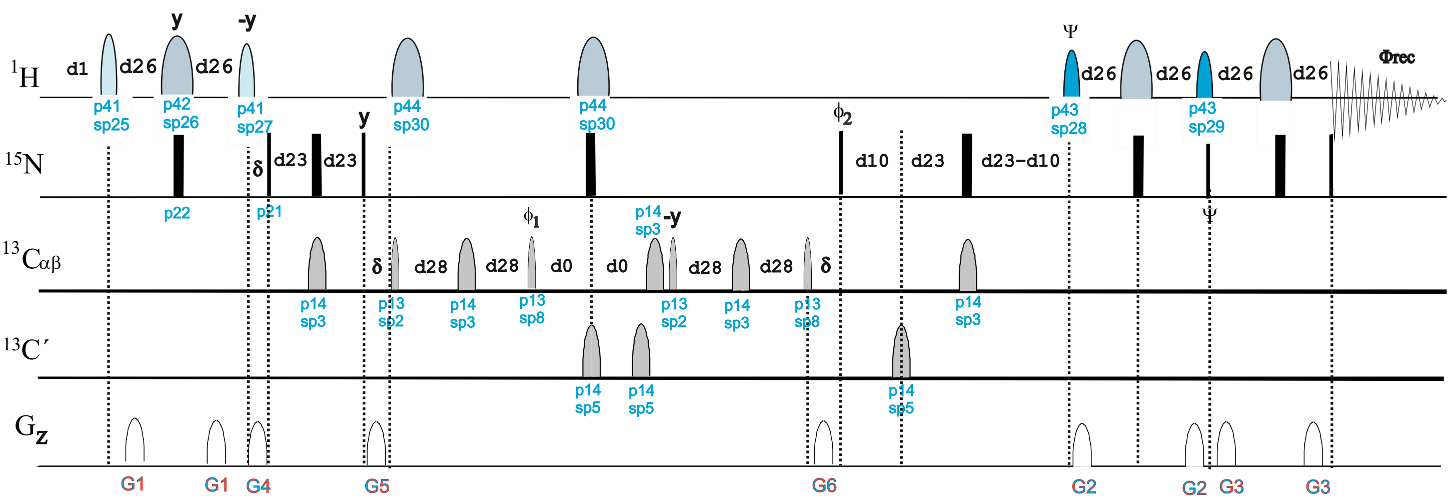
b_trhncocagp3d



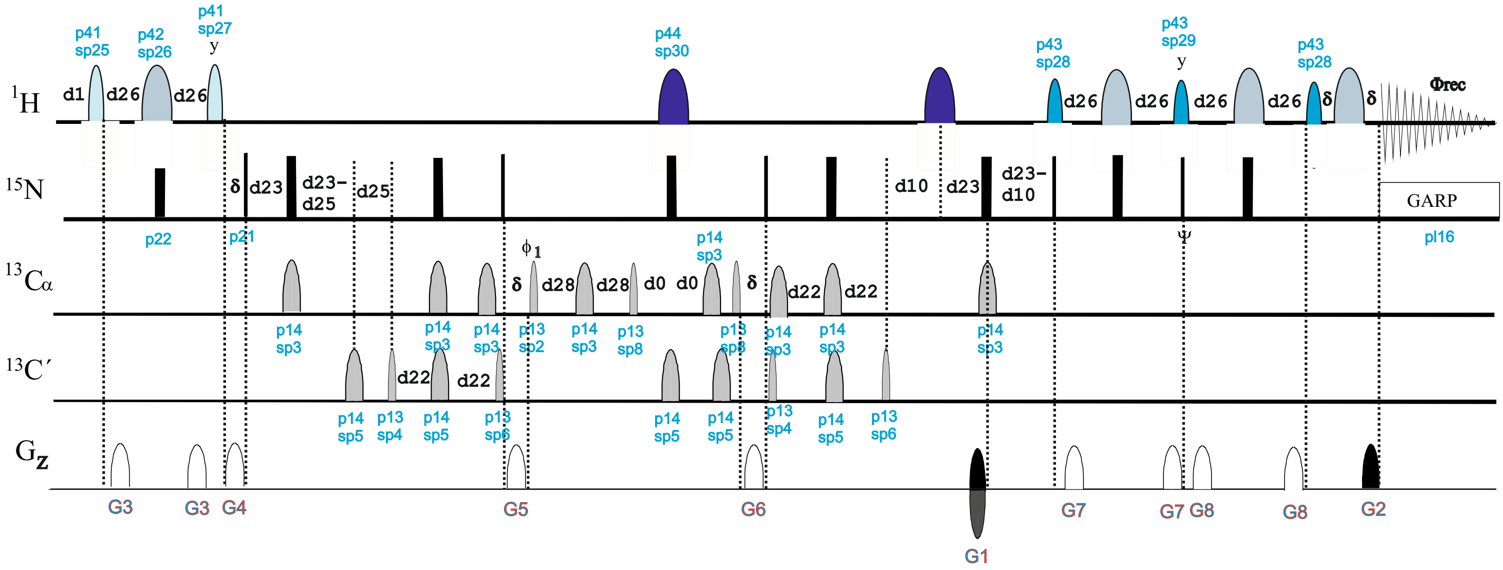
b_hncacbgp3d



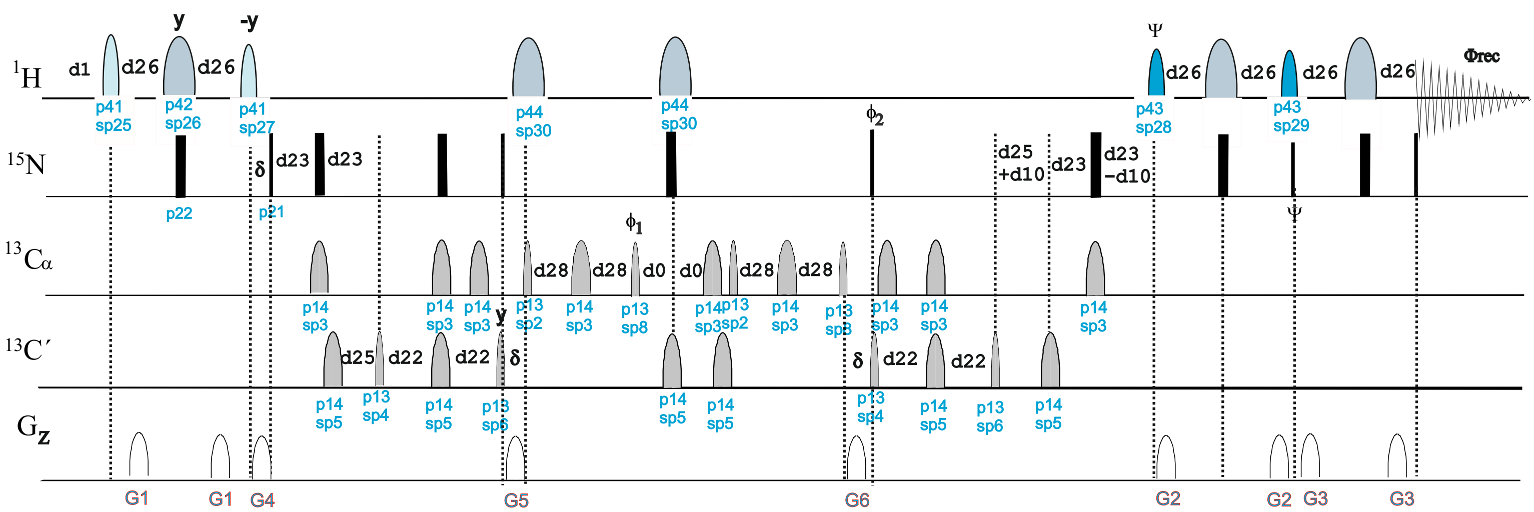
b_trhncacbgp3d



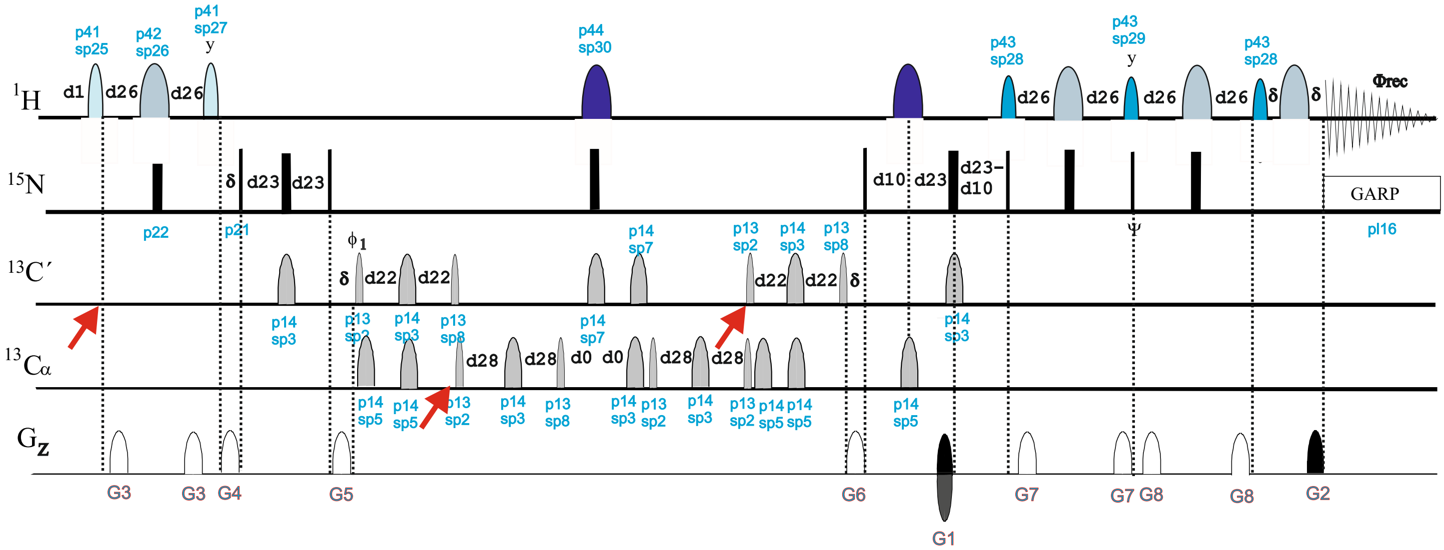
b_hncacbigp3d



b_trhncacbigp3d



b_hncocacbgp3d



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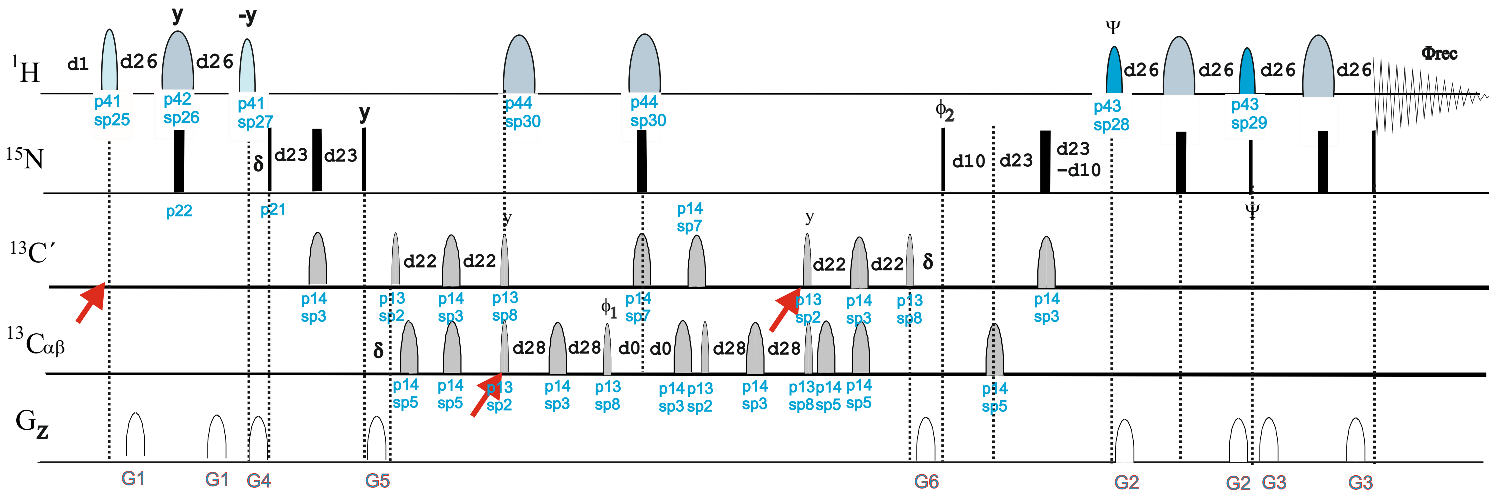


BRUKER
PULSE PROGRAM
CATALOGUE

NMRGuide

AMINO-ACID TYPE_SELECTIVE
MUSIC EXPERIMENTS

General Description:

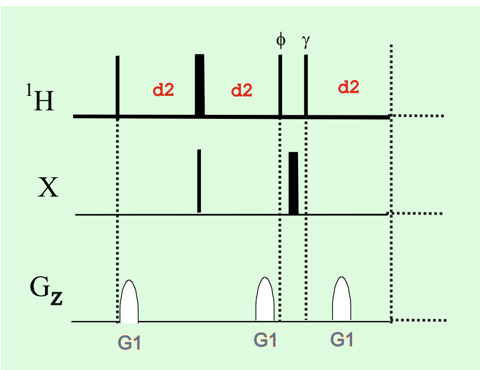
Amino-Acid Type-Selective Experiments are a set of triple-resonance NMR experiments alternatives to the conventional experiments, designed to provide specific information of particular amino-acids. Some of the main features:

1. Sequential and aa-type information is obtained.
2. Reduction of number of peaks and signal overlapping.
3. Unambiguous assignment for some aa.
3. NMR Pulse sequences are mainly based on the original CBCACONH and CBCANH experiments
   A. CBCACONH-type experiments provide a single cross-peak from the sequential inter-residue i+1 correlation due to CO is involved.
   B. CBCANH-type experiments provide to different cross peaks, from intra- and inter-residue connectivites by means of the similar 1J(NCA) and 2J(NCA) coupling pathways.
4. They can be recorded as a 2D 1H-15N or 3D HNCO- or HNCA-type maps (**see ZGOPTNS**).
5. Main keys are the initial CH2-, CH3- or NH2-selected transfer steps (see MUSIC element) and the use of specific offset, selective pulses on specific regions and delays optimization.

References of Amino-Acid Type-Selective MUSIC Experiments:

1. P. Schmieder, M. Leidert, M. Kelly & H. Oschkinat, J. magn. Reson. 131, 199-202 (1998).
2. M. Schubert, M. Smalla, P. Schmieder & H. Oschkinat, J. Magn. Reson. 141, 34-43 (1999)
3. M. Schubert, L. Ball, H. Oschkinat & P. Schmieder, J. Biomol. NMR 17, 331-335 (2000)
4. 3. M. Schubert, H. Oschkinat & P. Schmieder, J. Biomol. NMR 20, 379-384 (2001)
5. M. Schubert, H. Oschkinat & P. Schmieder, J. Magn. Reson. 148, 61-72 (2001).
6. M. Schubert, H. Oschkinat & P. Schmieder, J. Magn. Reson. 153, 186-192 (2001)
7. M. Schubert, D. Labudde, D. Leitner, H. Oschkinat & P. Schmieder, J. Biomol. NMR 31, 115-127 (2005).

The MUSIC (Multiplicity Selective In-Phase Coherence Transfer) Element:



Phase Cycles for:
CH2 or NH2 selection

ϕ 0°
γ 45°,135°225°,315°
rec 0°,180°

Ch3 selection

ϕ 0°
γ 30°,90°,150°,210°,270°,330°
rec 0°,180°

d2=1/2J=3.6ms(CH2 or Ch3) or 5.5ms(NH2)

AminoAcid-selective (MUSIC) Experiments

- 3D MUSIC Metionine (Met - M) with CH2 selection (**music_cm_3d**)
- 3D MUSIC - Metionine (Met - M) with CH2 selection (**music_cm_3d_2**)

- 3D MUSIC - Glutamic (Glu - E) or Aspartic (Asp - D) with CH2 selection (**music_de_3d**)
- 3D MUSIC - Glutamic (Glu - E) or Aspartic (Asp - D) with CH2 selection (**music_de_3d_2**)

- 3D MUSIC - PhenylAlanine (Phe - F)/Hystidine (His-H)/ Tyrosine (Tyr-Y) or Triptophan (Trp - W) with CH2 selection (**music_fhyw_3d**)
- 3D MUSIC - PhenylAlanine (Phe - F)/Hystidine (His-H)/ Tyrosine (Tyr-Y) or Triptophan (Trp - W) with CH2 selection (**music_fhyw_3d_2**)

- 3D MUSIC - Glycine (Gly - G) or Asparagine (Asn - N)/Glutamine (Gln - Q) with CH2 selection (**music_gly_3d**)
- 3D MUSIC - Glycine (Gly - G) or Asparagine (Asn - N)/Glutamine (Gln - Q) with CH2 selection (**music_gly_3d_2**)

- 3D MUSIC - Serine (Ser - S) with CH2 selection (**music_ser_3d**)
- 3D MUSIC - Serine (Ser - S) with CH2 selection (**music_ser_3d_2**)

- 3D MUSIC - Lysine (Lys - K) and/or Arginine (Arg- R) (**music_kr_3d**)
- 3D MUSIC - Lysine (Lys - K) and/or Arginine (Arg- R) (**music_kr_3d_2**)

- 3D MUSIC - Isoleucine (Ile - I) with CH3 selection (**music_ile_3d**)
- 3D MUSIC - Isoleucine (Ile - I) with CH3 selection (**music_ile_3d_2**)

- 3D MUSIC - Leucine (Leu - L)/ Alanine (Ala-A) or Valine (Val - V)/Isoleucine (Ile-I)/ Alanine (Ala-A)with CH3 selection (**music_lavia_3d**)
- 3D MUSIC - Leucine (Leu - L)/ Alanine (Ala-A) or Valine (Val - V)/Isoleucine (Ile-I)/ Alanine (Ala-A)with CH3 selection (**music_lavia_3d_2**)

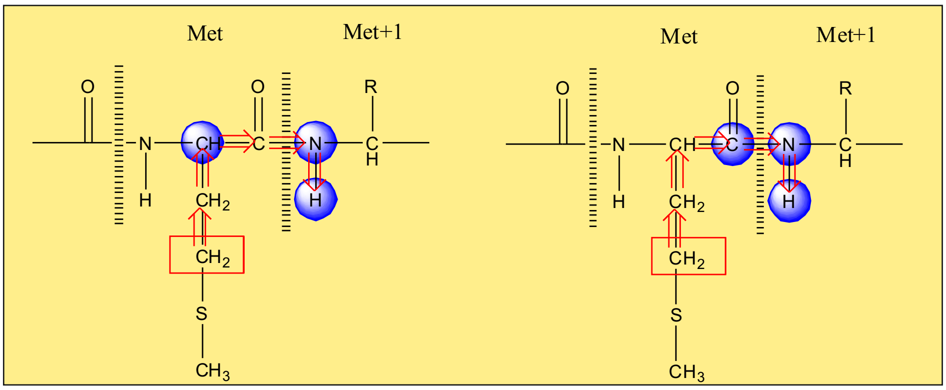
- 3D MUSIC - Valine (Val - V)/Isoleucine (Ile - I) or Theonine (Thr - T)/Alanine (Ala - A)with CH3 selection (**music_tavi_3d**)
- 3D MUSIC - Valine (Val - V)/Isoleucine (Ile - I) or Theonine (Thr - T)/Alanine (Ala - A)with CH3 selection (**music_tavi_3d_2**)

- 3D MUSIC - Proline (Pro - P) (**music_pro_1_3d**)
- 3D MUSIC - Proline (Pro - P) (**music_pro_1_3d.2**)
- 3D MUSIC - Proline (Pro - P) (**music_pro_2_3d**)
- 3D MUSIC - Proline (Pro - P) (**music_pro_2_3d.2**)

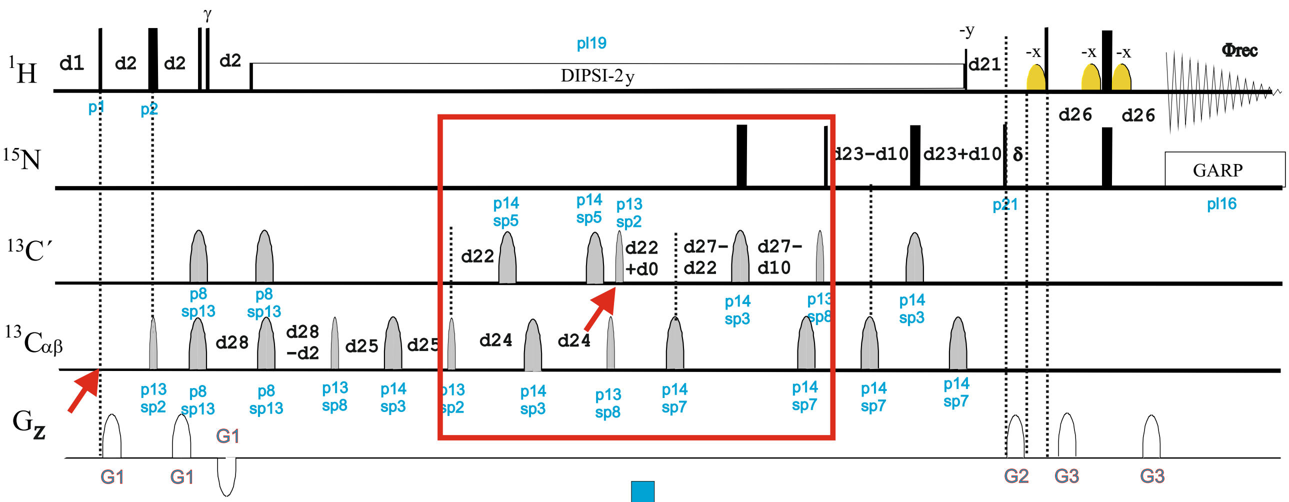
- 3D MUSIC - Glutamine (Gln - Q) or Asparagine (Asn - N) with NH2 selection (**music_qn_3d**)
- 3D MUSIC - Glutamine (Gln - Q) or Asparagine (Asn - N) with NH2 selection (**music_qn_3d_2**)

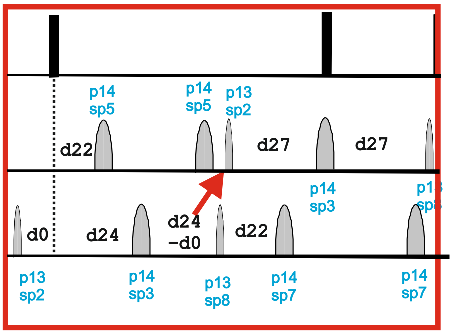
- 2D MUSIC - Triptophan (Trp - W)(**music_trpe_2d**)

MUSIC-Metionine: $(CH_2C)CA(CO)NH$ and $(CH_2CCA)CONH$



music_cm_3d

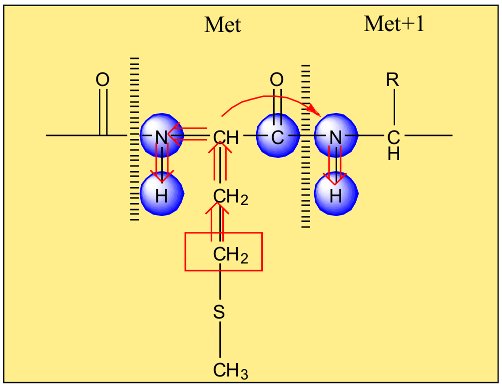




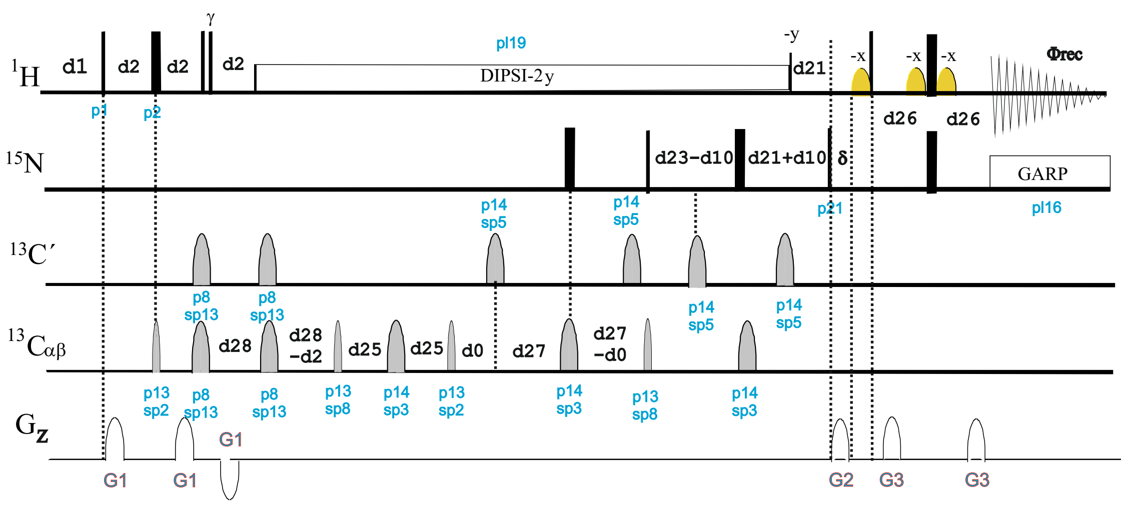
ZGOPTNS:
no option: 3D $(CH_2C)CA(CO)NH$ NH(Met+1)
LABEL CO:_3D $(CH_2CCA)CONH$ NH(Met+1)

d2 : 1/(2J(CH) [3.5 msec]
d21: 1/(2J(NH) [5.5 msec]
d22: 1/(4J(CaCO) [4.5 msec]
d23: 1/(4J(NCO) [12.4 msec]
d24: n/(4J(CC) [20 msec]
or 1/(4J(CC) (LABEL_CO) [5.2 msec]
d25: 1/(4J(CC) [6.0 msec]
d26: 1/(4J(NH) [2.3 msec]
d27: 1/(4J(NCO) [12.4 msec]
d28: 1/(4J(CC) [6.0 msec]
Possible breakthrough: Glu, Gly, Lys, Ser, Val

MUSIC-Metionine: $(CH_2C)CANH$



music_cm_3d_2

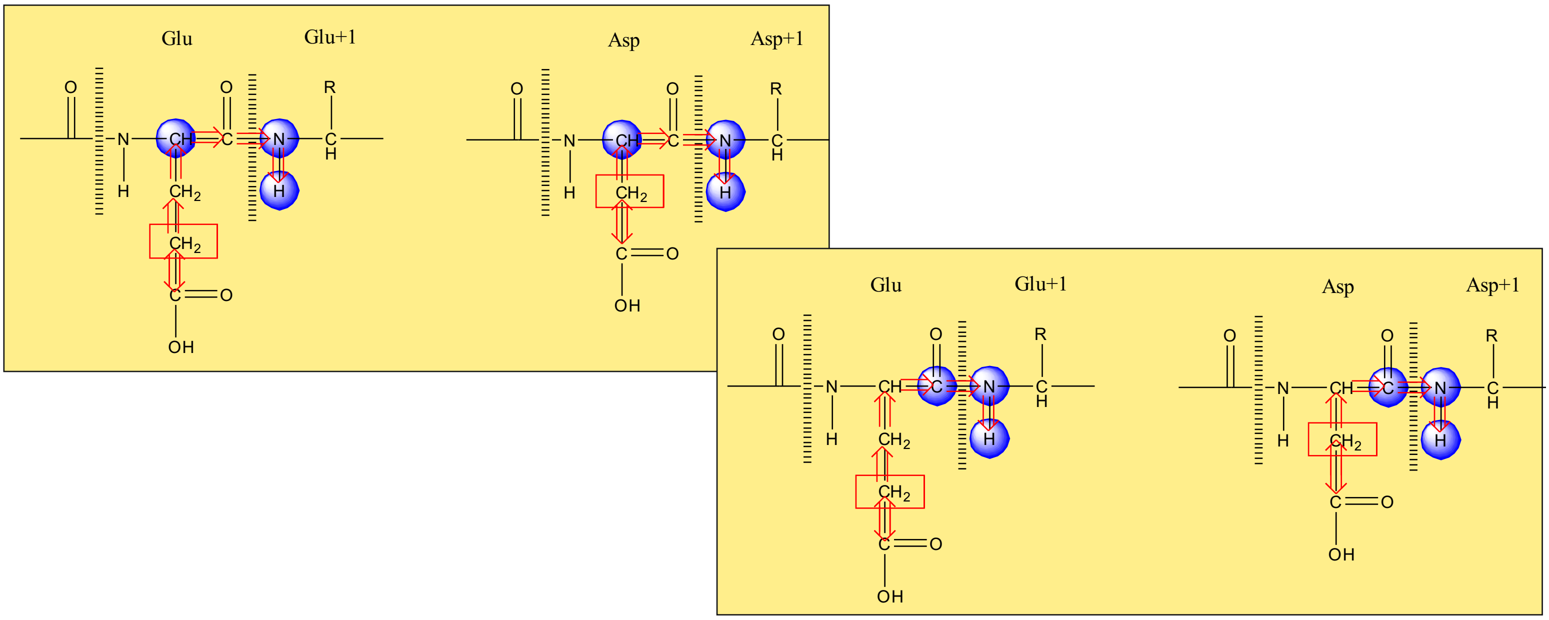


ZGOPTNS

no option: 3D $(CH_2C)CANH$ NH(Met) and NH(Met+1)

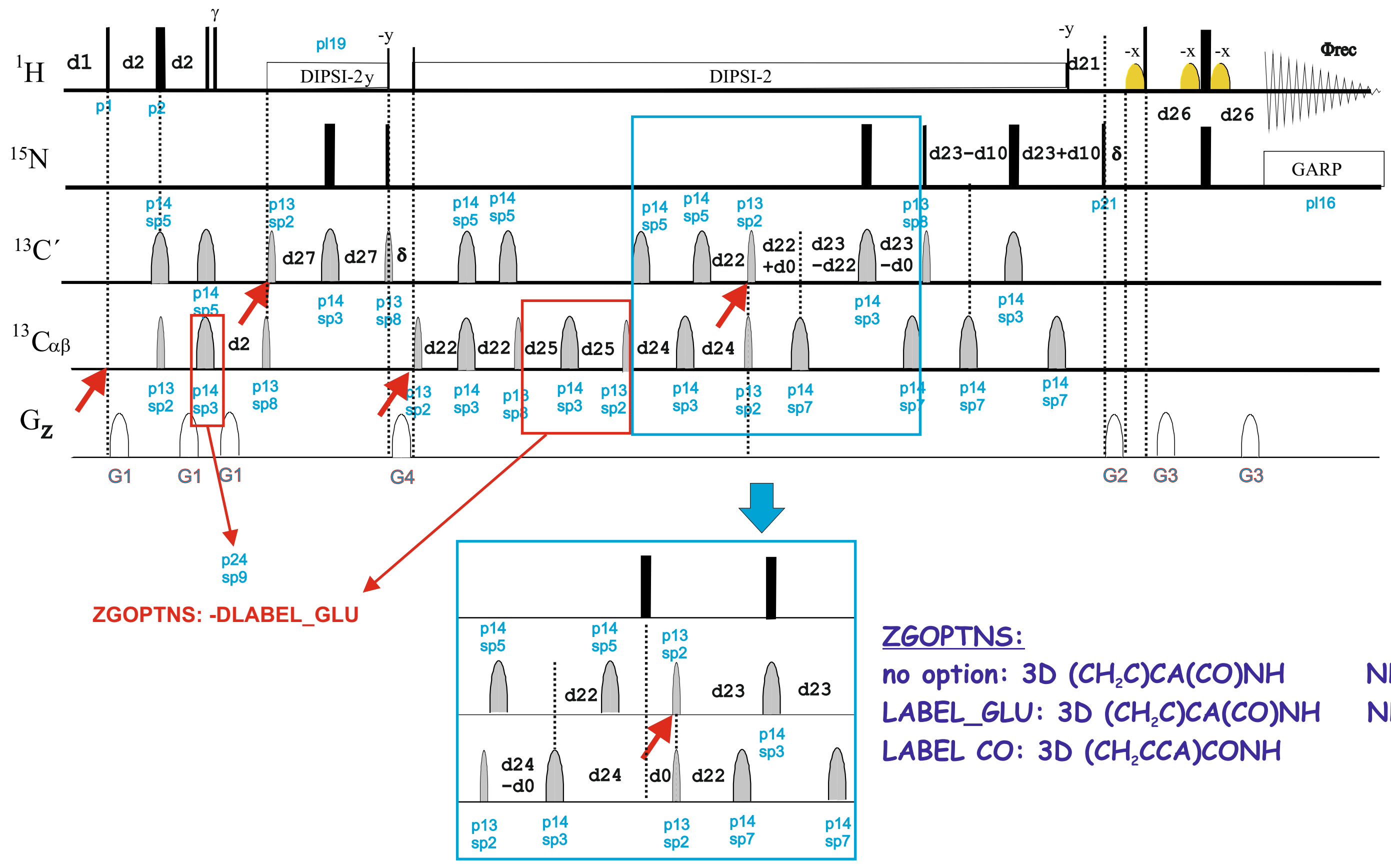
d2 : 1/(2J(CH))	[3.5 msec]
d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d25: 1/(4J(CC)	[6.0 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa)	[8.2 msec]
d28: 1/(4J(CC)	[6.0 msec]

MUSIC-Glu/Asp: $(CH_2COC)CA(CO)NH$ and $(CH_2COCCA)CONH$



music_de_3d

ZGOPTNS: -DLABEL_CO



ZGOPTNS: -DLABEL_GLU

ZGOPTNS:

no option: 3D $(CH_2C)CA(CO)NH$ NH(Asp+1)

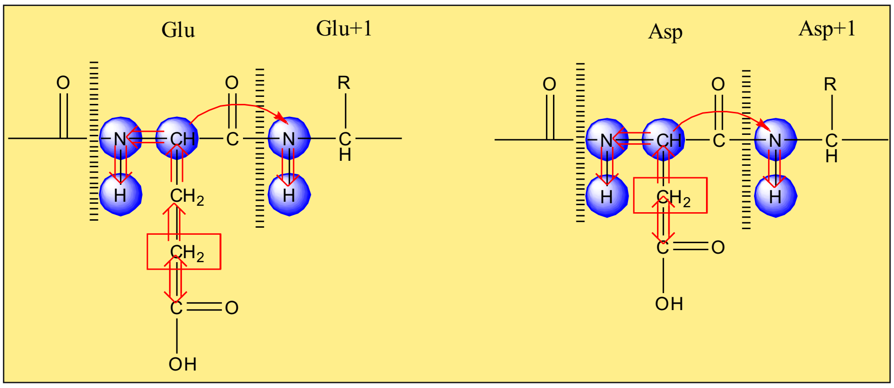
LABEL_GLU: 3D $(CH_2C)CA(CO)NH$ NH(Glu+1)

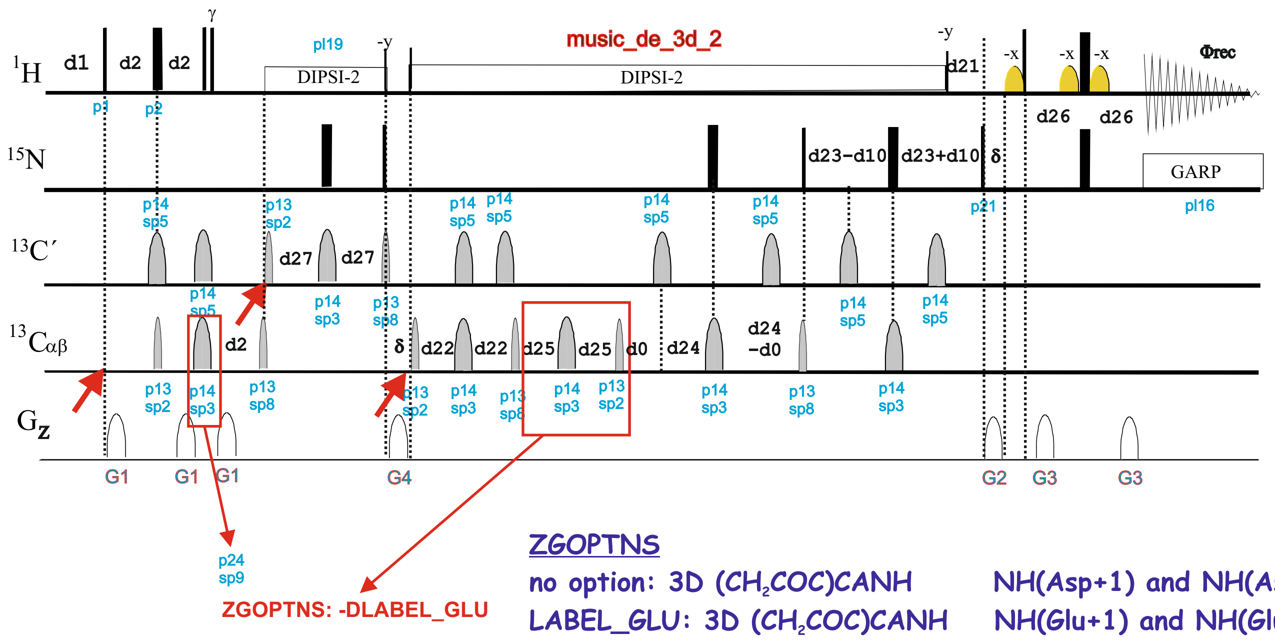
LABEL CO: 3D $(CH_2CCA)CONH$

d2 : 1/(2J(CH) = [4.0 msec]
d21: 1/(2J(NH) = [5.5 msec]
d22: 1/(4J(CaCO) = [4.5 msec]
d23: 1/(4J(NCO) = [12.4 msec]

d24: n/(4J(CC) = [20 msec]
or 1/(4J(CC) (LABEL_GLU) = [9.0 msec]
or 1/(4J(CC) (LABEL_CO) = [4.5 msec]
d25: 1/(4J(CC) = [4.5 msec]
d26: 1/(4J(NH) = [2.3 msec]
d27: 1/(4J(NCO(s)) = [16.0 msec]

MUSIC-Glu/Asp: $(CH_2COC)CANH$





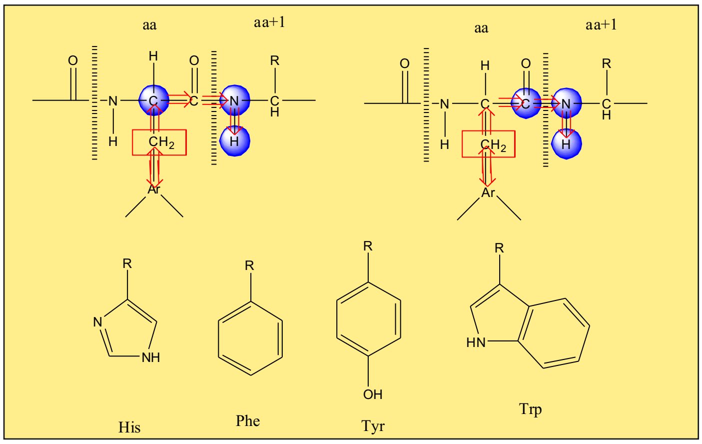
ZGOPTNS

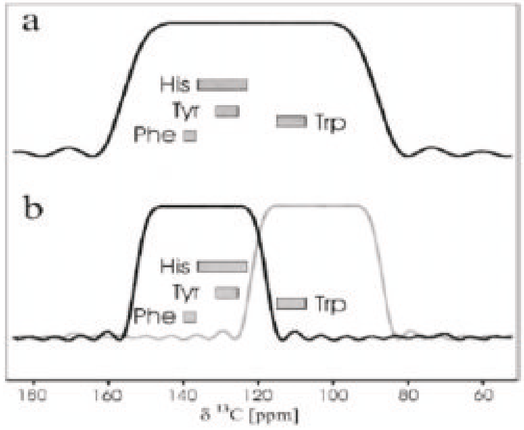
no option: 3D $(CH_2COC)CANH$ NH(Asp+1) and NH(Asp)

LABEL_GLU: 3D $(CH_2COC)CANH$ NH(Glu+1) and NH(Glu)

;d2 : 1/(2J(CH))	[4.0 msec]
;d21: 1/(2J(NH)	[5.5 msec]
;d22: 1/(4J(COCa)	[4.5 msec]
;d23: 1/(4J(NCa)	[12.4 msec]
;d24: 1/(4J(CC)	[9.0 msec]
;d25: 1/(4J(CC)	[4.5 msec]
;d26: 1/(4J(NH)	[2.3 msec]
;d27: 1/(4J(NCO(s))	[16.0 msec]

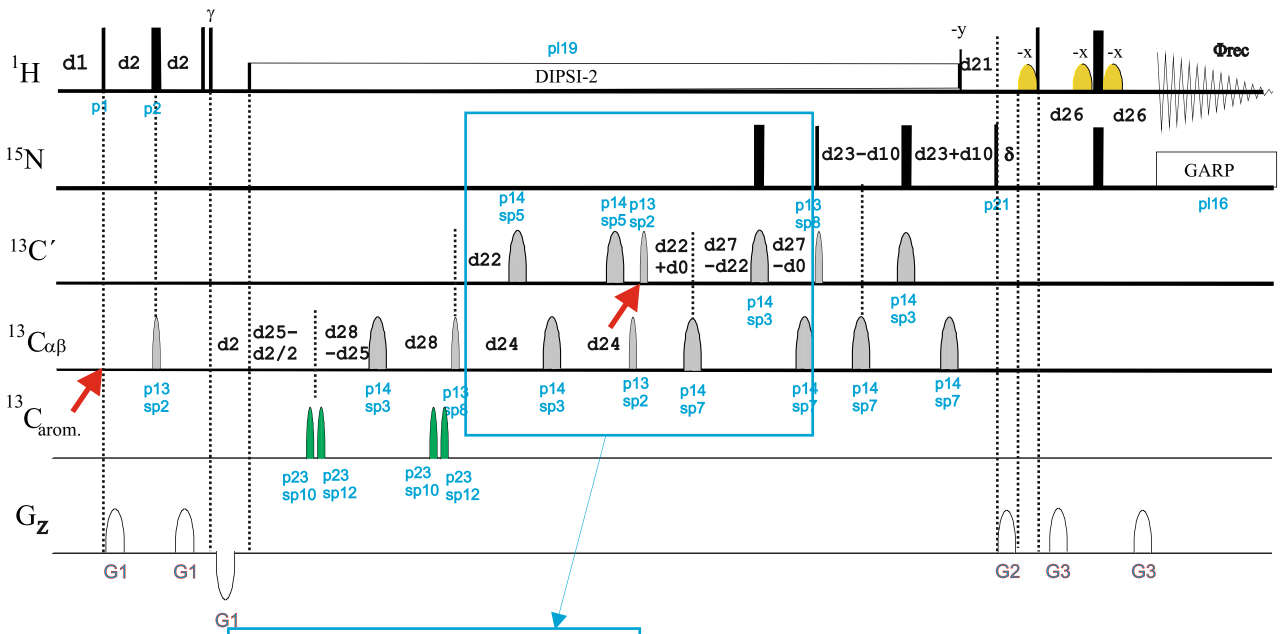
MUSIC-Aromatic: $(CH_2)CA(CO)NH$ and $(CH_2CA)CONH$

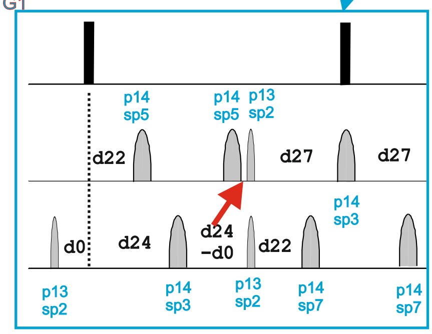




music_fhyw_3d

ZGOPTNS: -DLABEL_CO



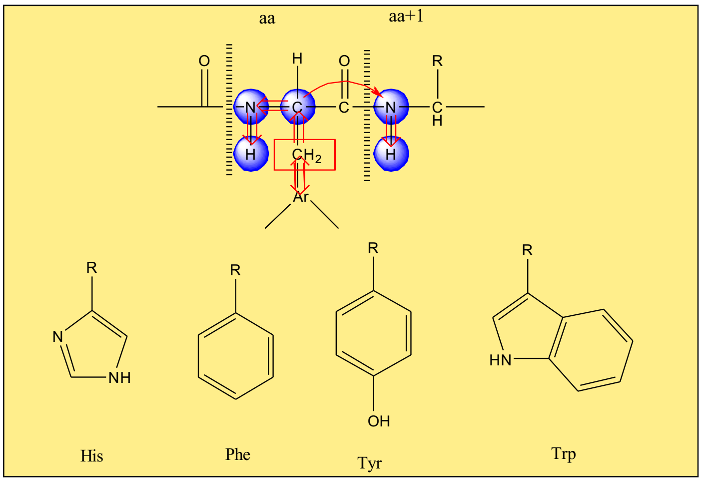


ZGOPTNS:

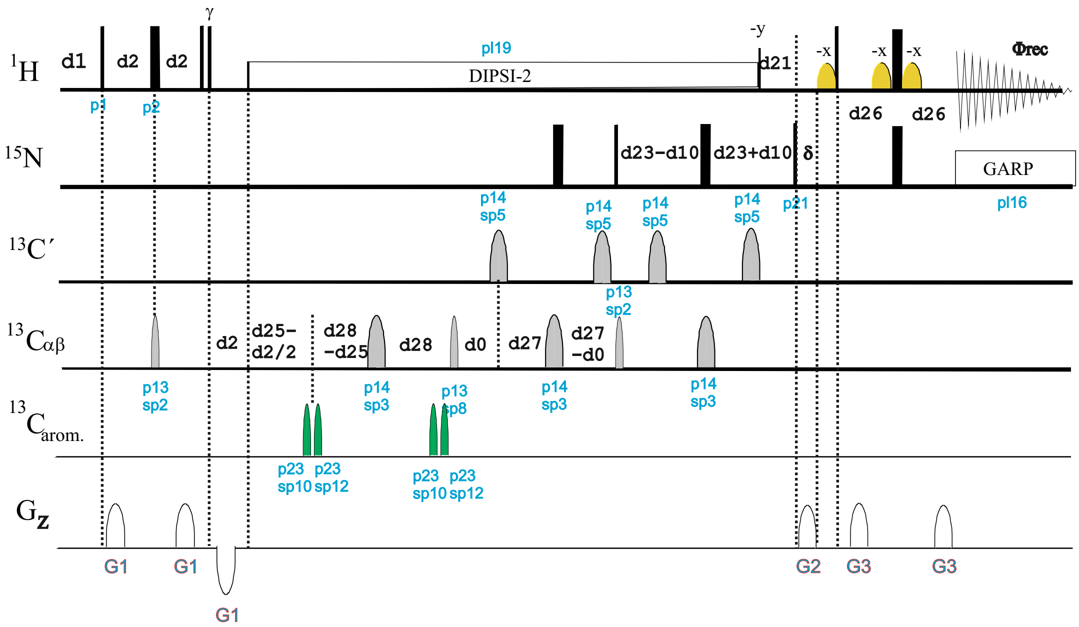
no option: 3D $(CH_2C)CA(CO)NH$ NH((Phe,Tyr,Hys)+1)
LABEL_TRP: 3D $(CH_2C)CA(CO)NH$ NH(Trp+1)
LABEL_CO: 3D $(CH_2CCA)CONH$

d2 : 1/(2J(CH))	[3.5 msec]	d25: 1/(4J(CC)	[7.05 msec]
d21: 1/(2J(NH)	[5.5 msec]	d26: 1/(4J(NH)	[2.3 msec]
d22: 1/(4J(CaCO)	[4.5 msec]	d27: 1/(4J(NCO)	[11.4 msec]
d23: 1/(4J(NCO)	[12.4 msec]	d28: 1/(4J(CC)	[7.1 msec]
d24: n/(4J(CC)	[20 msec]		
or 1/(4J(CC) (LABEL_CO)	[4.5 msec]		

MUSIC-Aromatic: (CH$_2$)CANH



music_fhyw_3d_2



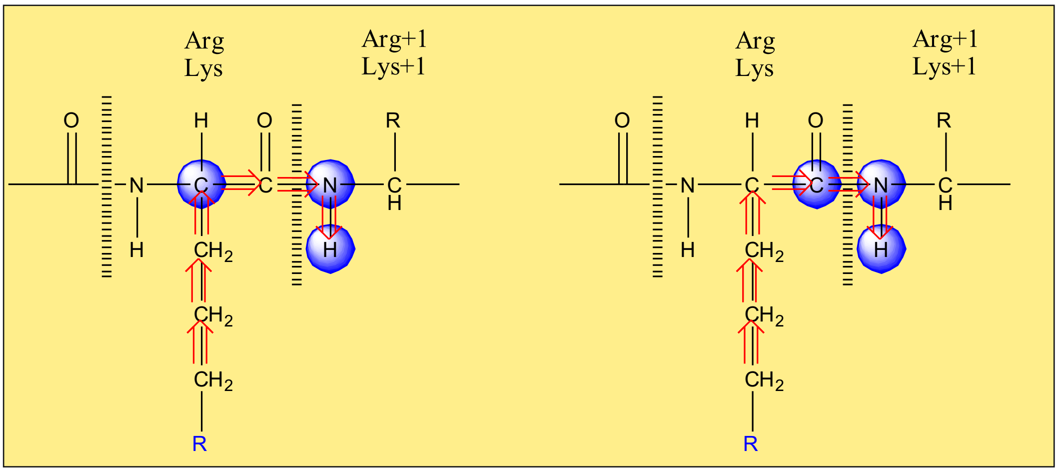
ZGOPTNS:

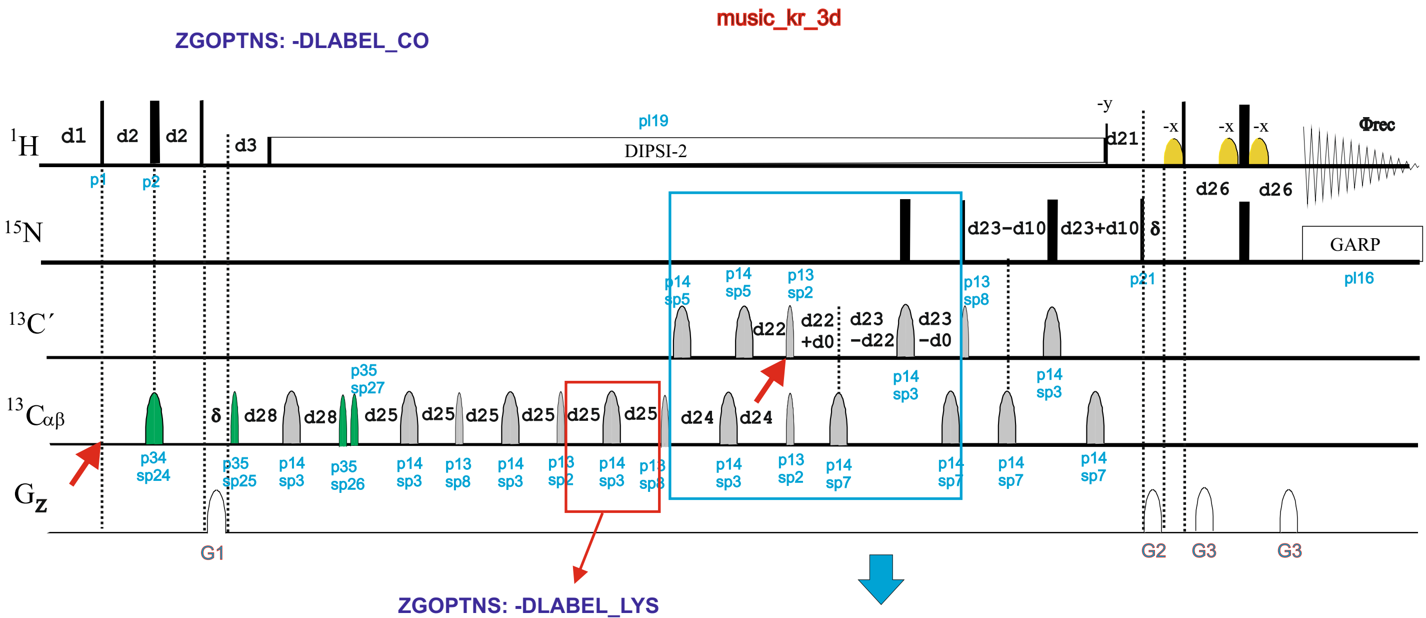
no option: 3D (CH$_2$C)CANH NH((Phe,Tyr,Hys)) and NH((Phe,Tyr,Hys)+1)

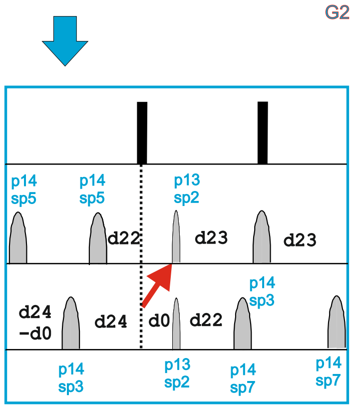
LABEL_TRP: 3D (CH$_2$C)CANH NH(Trp) and NH(Trp+1)

d2 : 1/(2J(CH)) [3.5 msec]
d21: 1/(2J(NH) [5.5 msec]
d23: 1/(4J(NCa) [12.4 msec]
d25: 1/(4J(CC) [7.05 msec]
d26: 1/(4J(NH) [2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa) [9.0 msec]
d28: 1/(4J(CC) [7.1 msec]

MUSIC-Arg/Lys: (CH_2C)CA(CO)NH and (CH_2CCA)CONH



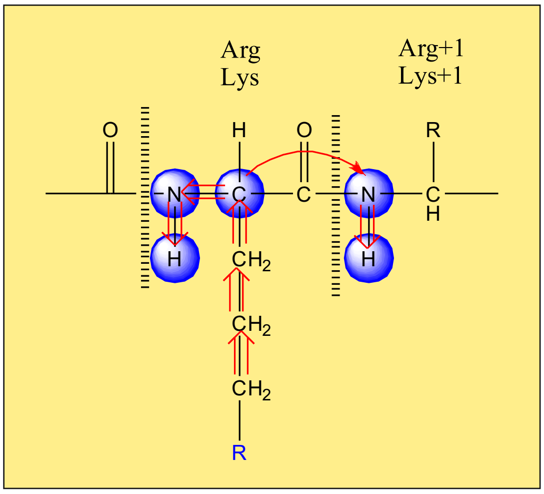




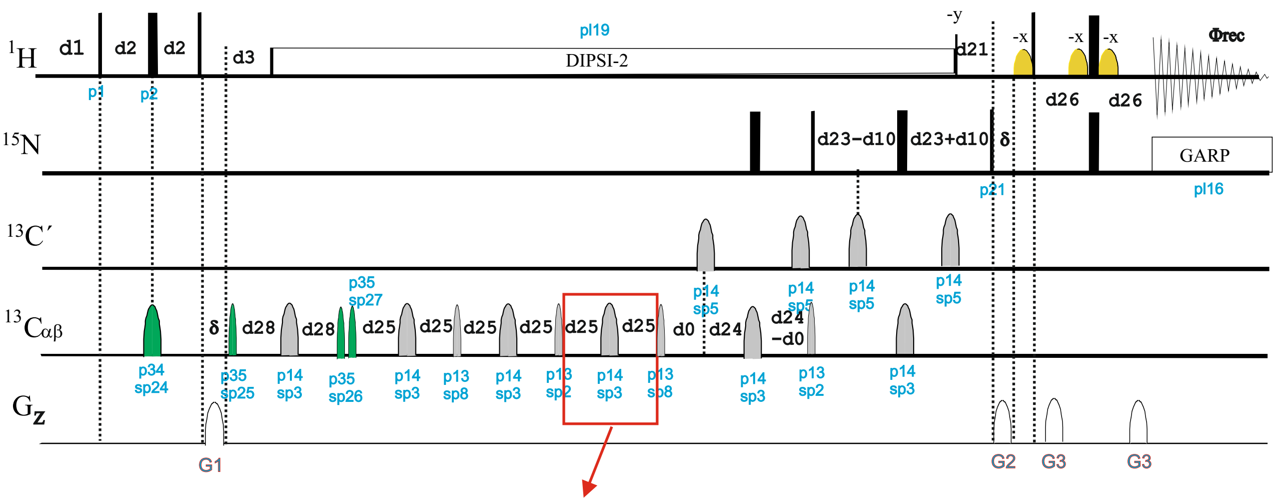
ZGOPTNS
no options: 3D (HC)CA(CO)NH NH(Arg+1)
LABEL_LYS: 3D (HC)CA(CO)NH NH(Arg+1) and NH(Lys+1)
LABEL_CO: 3D (HCCA)CONH NH(Arg+1) and NH(Lys+1)

d3 : 1/(4J(CH))	[2.1 msec]	d24: n/(4J(CC))	[19.5m msec]
d4 : 1/(4J(CH))	[2.0 msec]	or 1/(4J(CC) (LABEL_LYS)	[8.8 msec]
d21: 1/(2J(NH)	[5.5 msec]	or 1/(4J(CC) (LABEL_CO)	[4.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]	d25: 1/(4J(CC)	[5.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]	d26: 1/(4J(NH)	[2.3 msec]
		d28: 1/(8J(CC)	[3.5 msec]

MUSIC-Arg/Lys (CH$_2$C)CANH



music_kr_3d_2



ZGOPTNS: -DLABEL_LYS

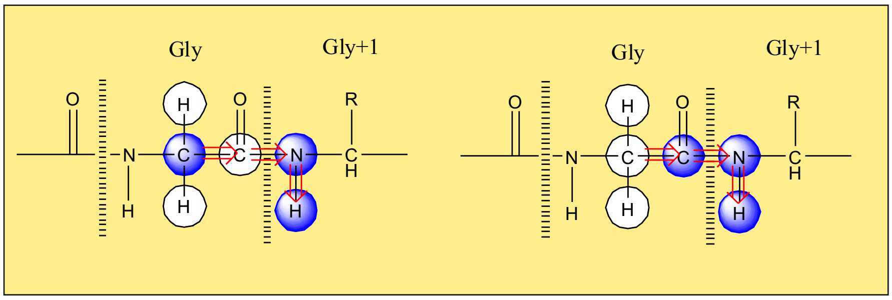
ZGOPTNS

no options: 3D (HC)CANH NH(Arg, Arg+1)

LABEL_LYS: 3D (HC)CANH NH(Arg, Arg+1) and NH(Lys, Lys+1)

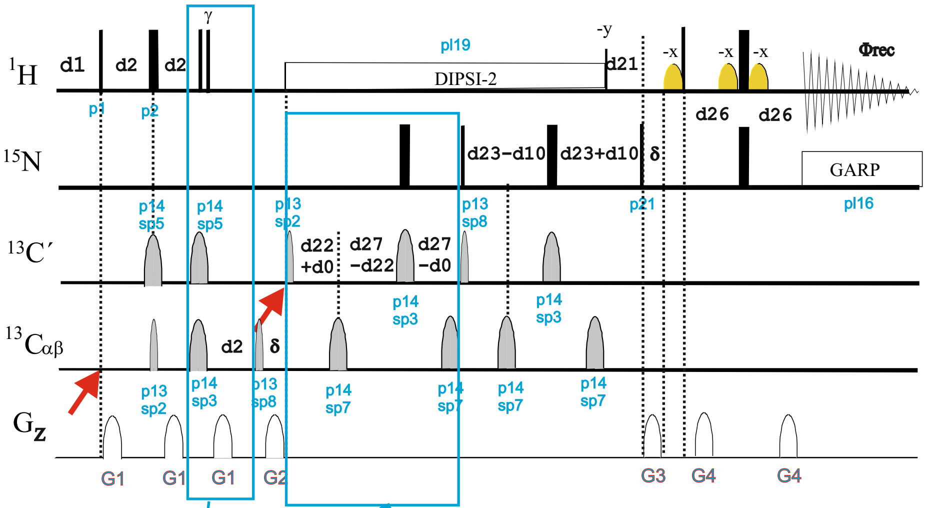
d3 : 1/(4J(CH))	[2.1 msec]
d4 : 1/(4J(CH))	[2.0 msec]
d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d24: 1/(4J(CbCa) and 1/(4J(NCa)	[9.0 msec]
d25: 1/(4J(CC)	[5.5 msec]
d26: 1/(4J(NH)	[2.3 msec]
d28: 1/(8J(CC)	[3.5 msec]

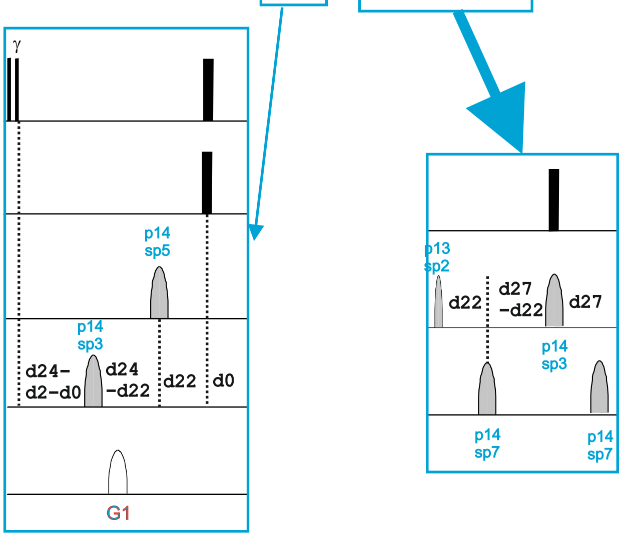
MUSIC-Glycine: $CH_2(CO)NH$ and $(CH_2)CONH$



ZGOPTNS: -DLABEL_CO

music_gly_3d





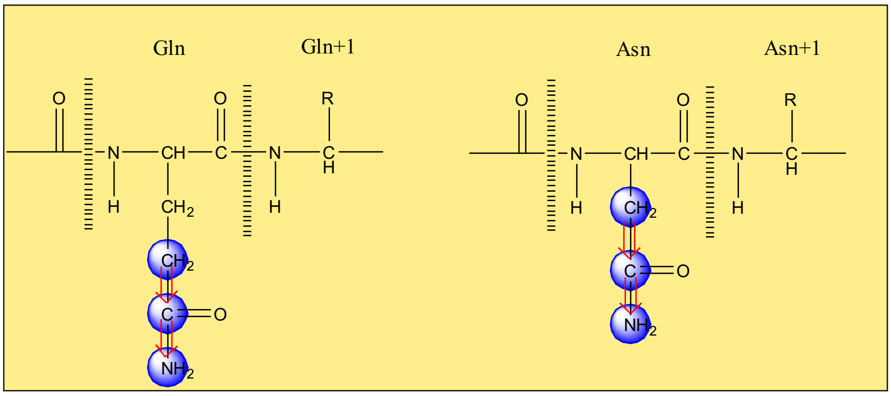
ZGOPTNS

no option: 3D $(CH_2)CA(CO)NH$ NH(Gly+1)

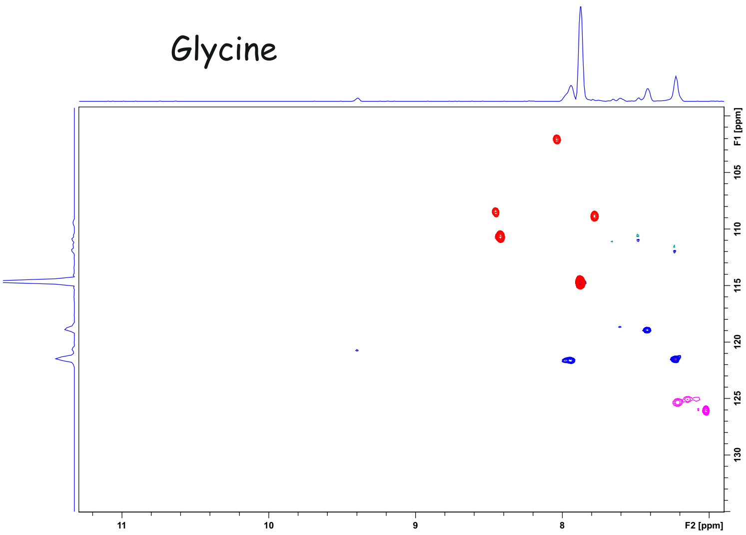
LABEL_GLY: 3D $(CH_2)CA(CO)NH$ NH(Gly+1)

LABEL_CO: 3D $(CH_2CA)CONH$

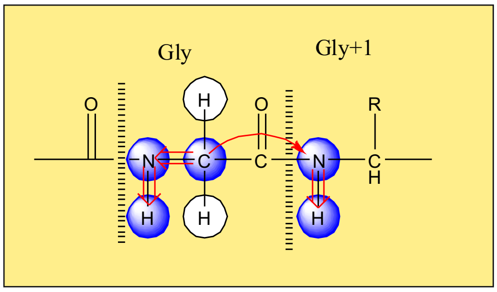
Also can be observed:



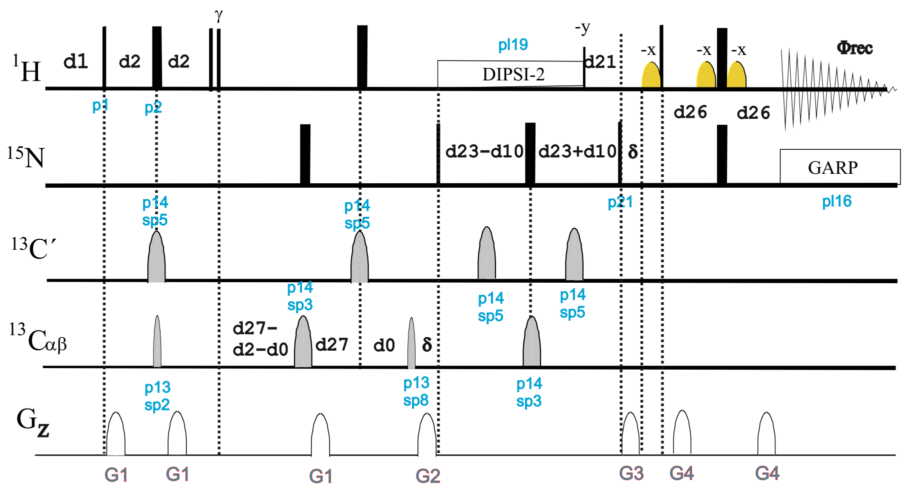
d2 : 1/(2J(CH))	[3.5 msec]
d21: 1/(4J(NH)	[2.9 msec]
or 1/(2J(NH) (LABEL_GLY)	[5.9 msec]
d22: 1/(4J(CaCO)	[4.4 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: 1/(4J(NCa)	[13.8 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO)	[12.4 msec]



MUSIC-Glycine: CH_2NH



music_gly_3d_2

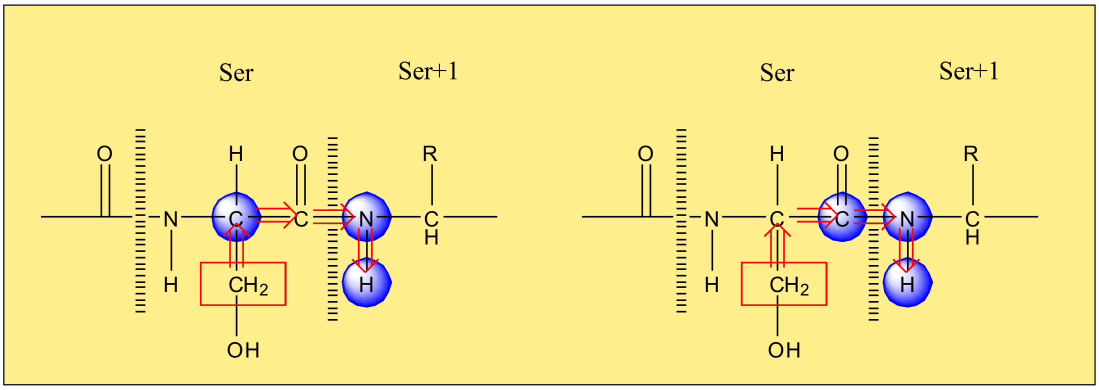


ZGOPTNS

no option: 3D (CH_2)CANH NH(Gly+1) and NH(Gly)

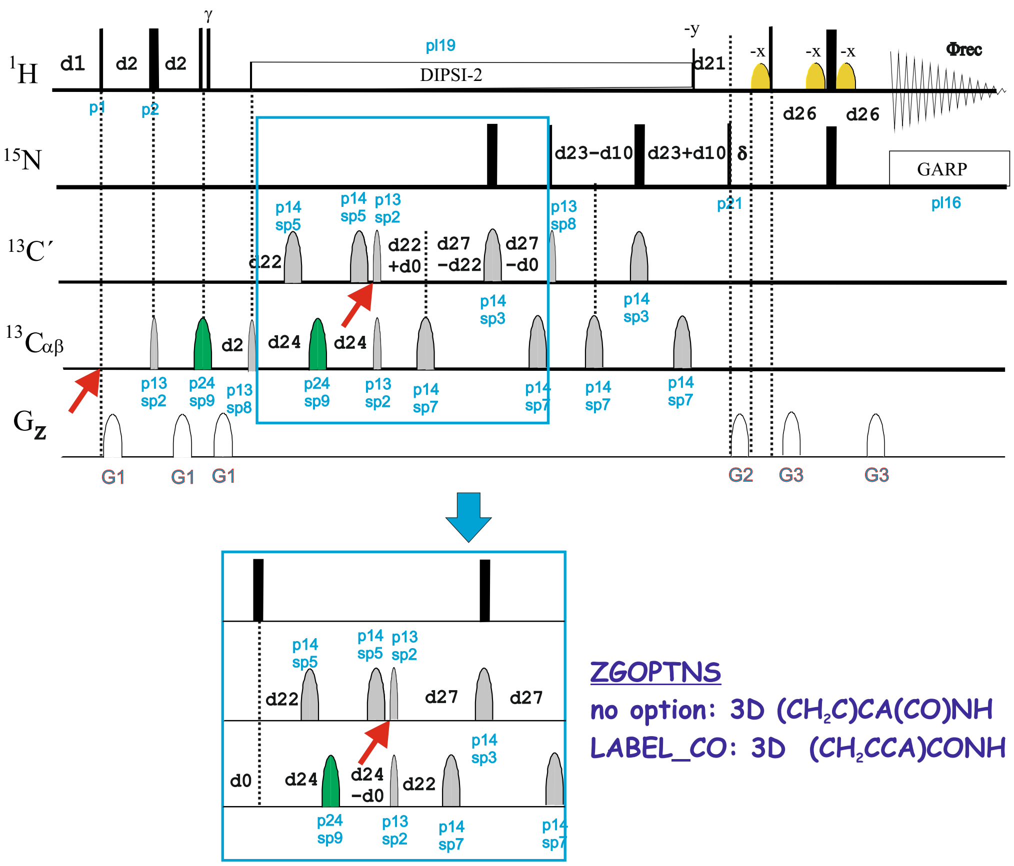
LABEL_GLY: 3D (CH_2)CANH NH(Gly+1) and NH(Gly)

MUSIC-SER: $(CH_2)CA(CO)NH$ and $(CH_2CA)CONH$



music_ser_3d

ZGOPTNS: -DLABEL_CO



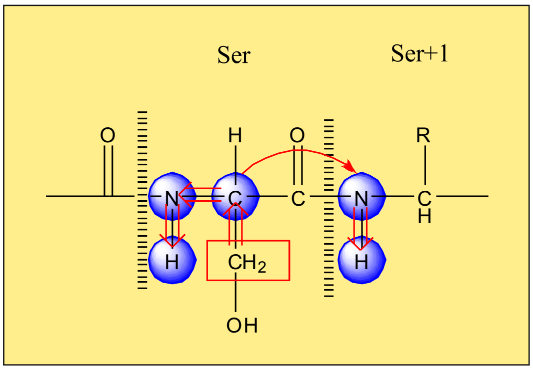
ZGOPTNS

no option: 3D $(CH_2C)CA(CO)NH$ NH(Ser+1)

LABEL_CO: 3D $(CH_2CCA)CONH$

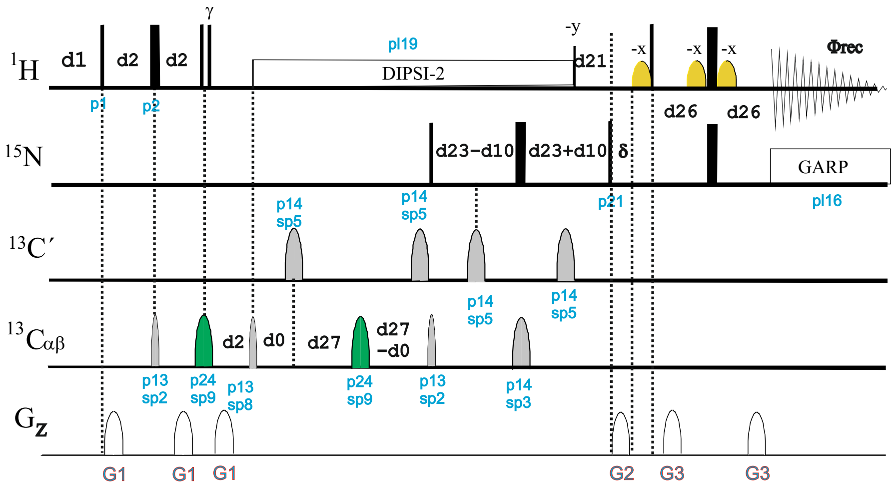
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: n/(4J(CC)	[17 msec]
or 1/(4J(CC) (LABEL_CO)	[5.3 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO)	[12.4 msec]

MUSIC-SER: $(CH_2)CANH$



d2 : 1/(2J(CH))	[3.5 msec]
d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa)	[8.2 msec]

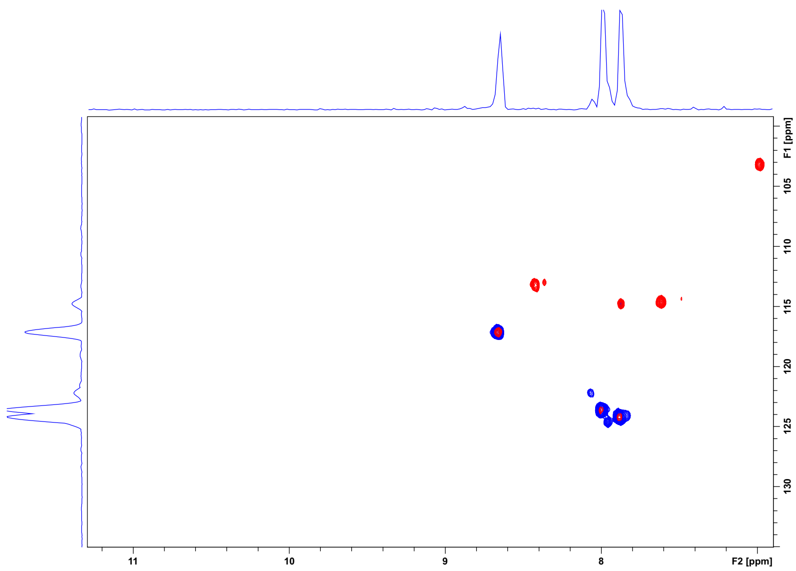
music_ser_3d_2



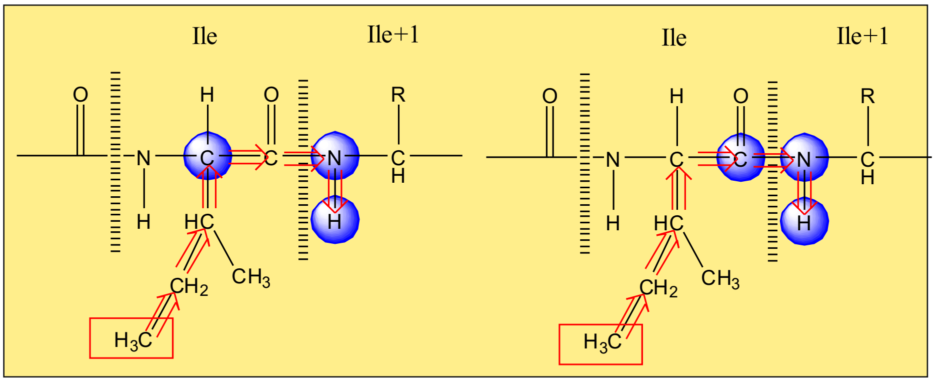
ZGOPTNS

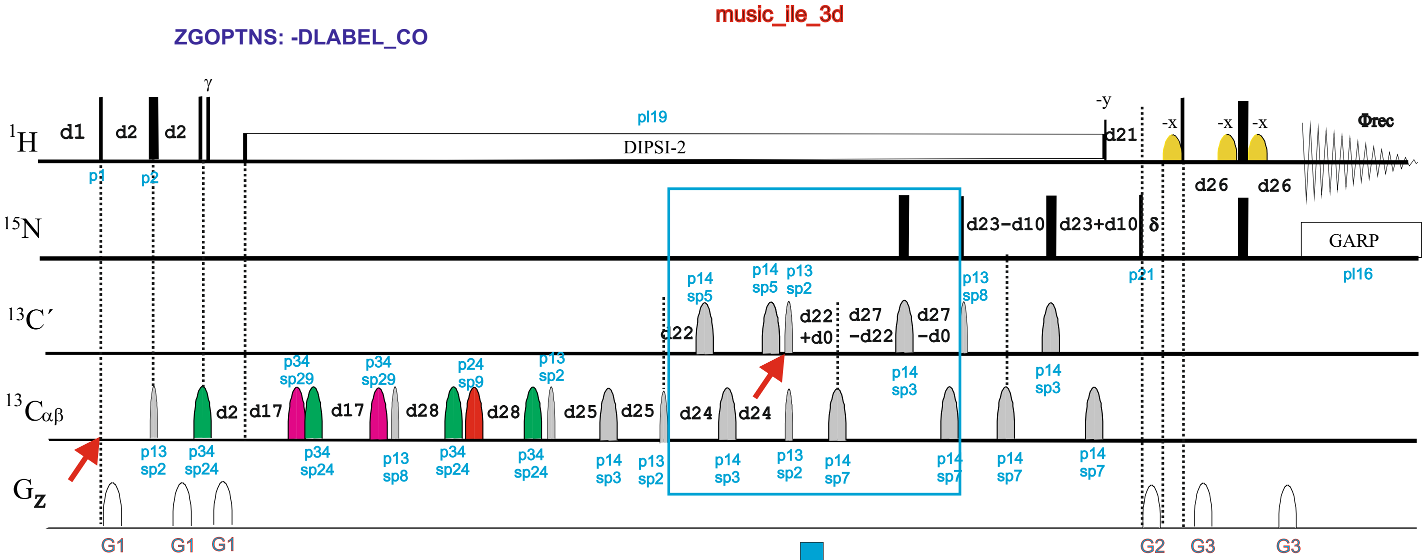
no options: 3D $(CH_2C)CANH$ NH(Ser+1) and NH(Ser)

Serine

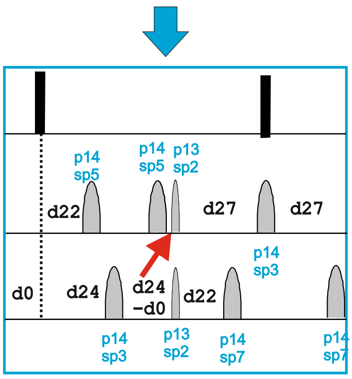


MUSIC-Isoleucine: $(CH_3C)CA(CO)NH$ and $(CH_3CCA)CONH$



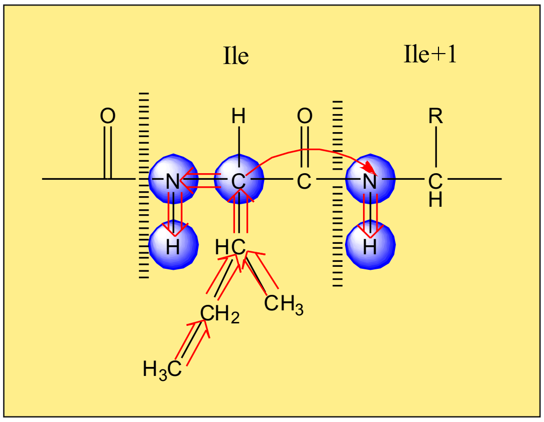


ZGOPTNS
no option: 3D $(CH_3C)CA(CO)NH$ NH(Ile+1)
LABEL_CO: 3D $(CH_3CCA)CONH$

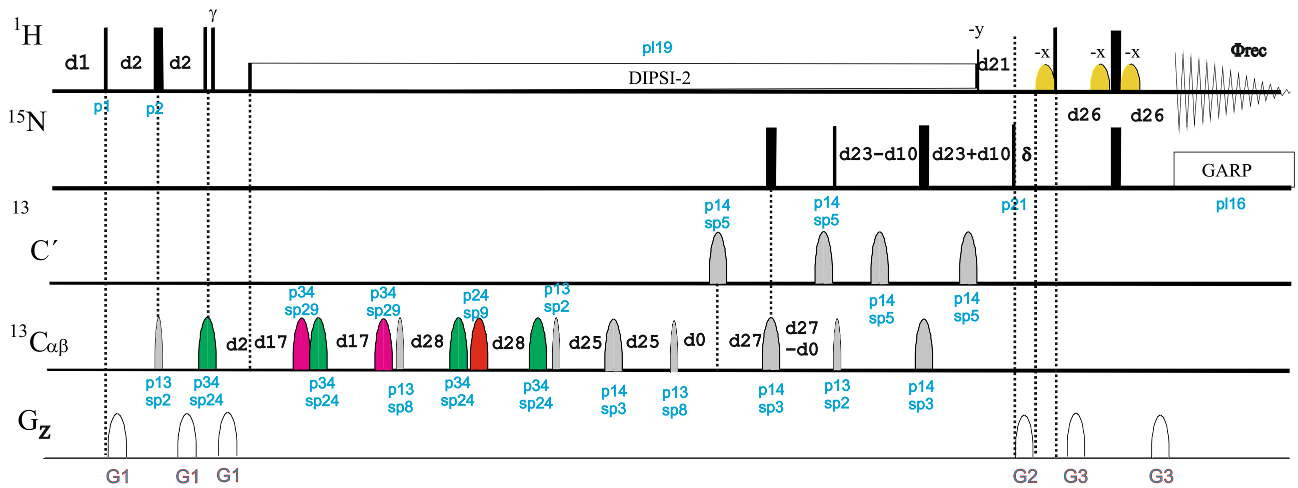


d2 : 1/(2J(CH))	[4.0 msec]
d17: 1/(4J(CC)	[7.0 msec]
d21: 1/(2J(NH)	[5.9 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: n/(4J(CC)	[19 msec]
or 1/(4J(CC) (LABEL_CO)	[4.5 msec]
d25: 1/(4J(CC)	[4.0 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO)	[12.4 msec]
d28: 1/(4J(CC)	[7.0 msec]

MUSIC-Isoleucine: $(CH_3C)CANH$



music_ile_3d_2

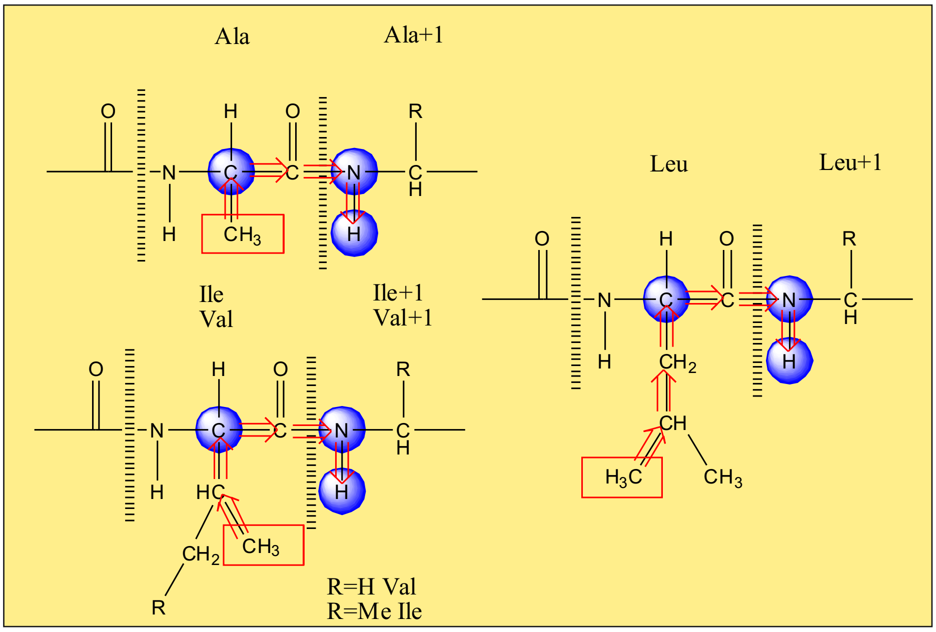


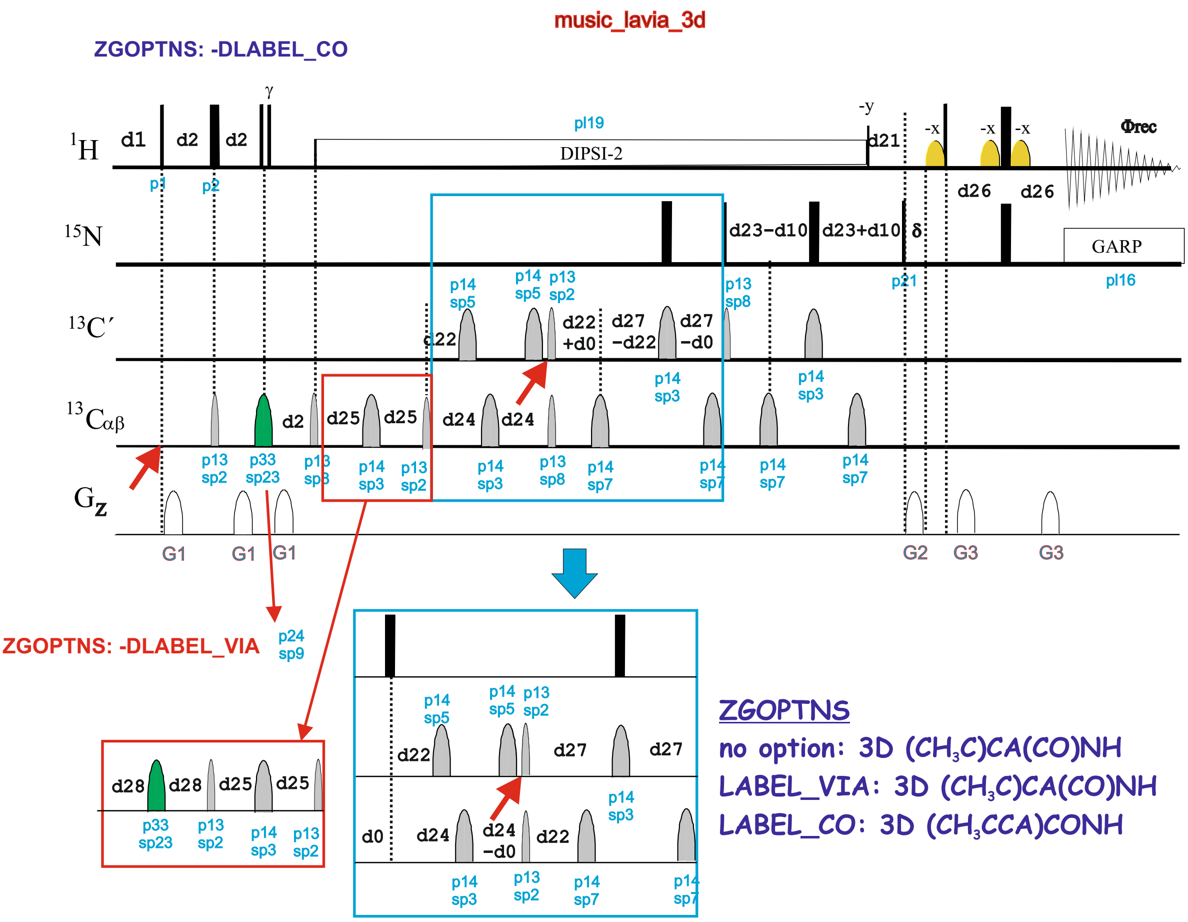
ZGOPTNS

no options: 3D $(CH_3C)CANH$ NH(Ile+1) and NH(Ile)

d2 : 1/(2J(CH))	[4.0 msec]
d17: 1/(4J(CC)	[7.0 msec]
d21: 1/(2J(NH)	[5.9 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d25: 1/(4J(CC)	[4.0 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa)	[9.0 msec]
d28: 1/(4J(CC)	[7.0 msec]

MUSIC-LAVIA: $(CH_3C)CA(CO)NH$ and $(CH_3CCA)CONH$



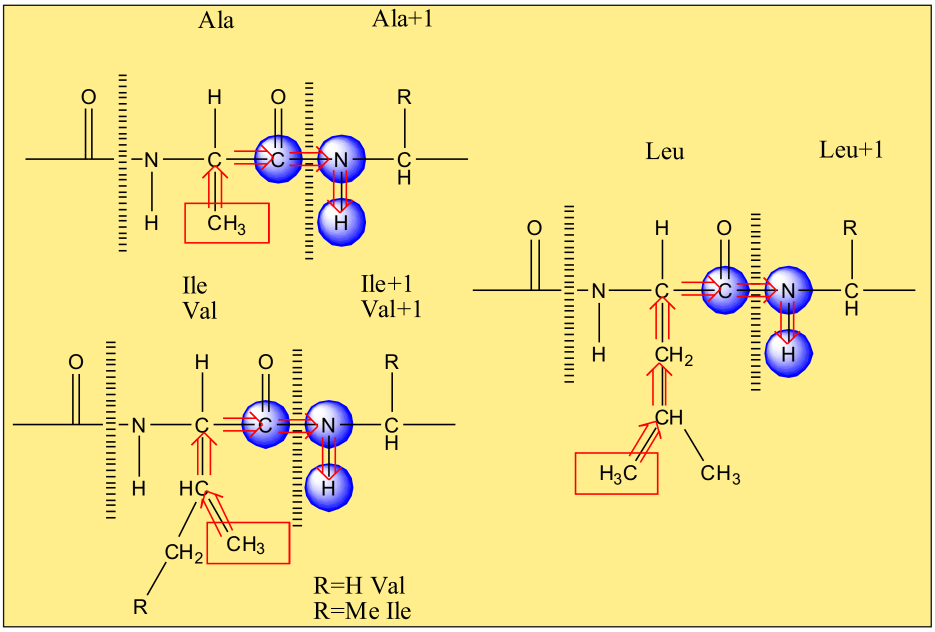


ZGOPTNS

no option: 3D $(CH_3C)CA(CO)NH$ NH((Leu,Ala)+1)

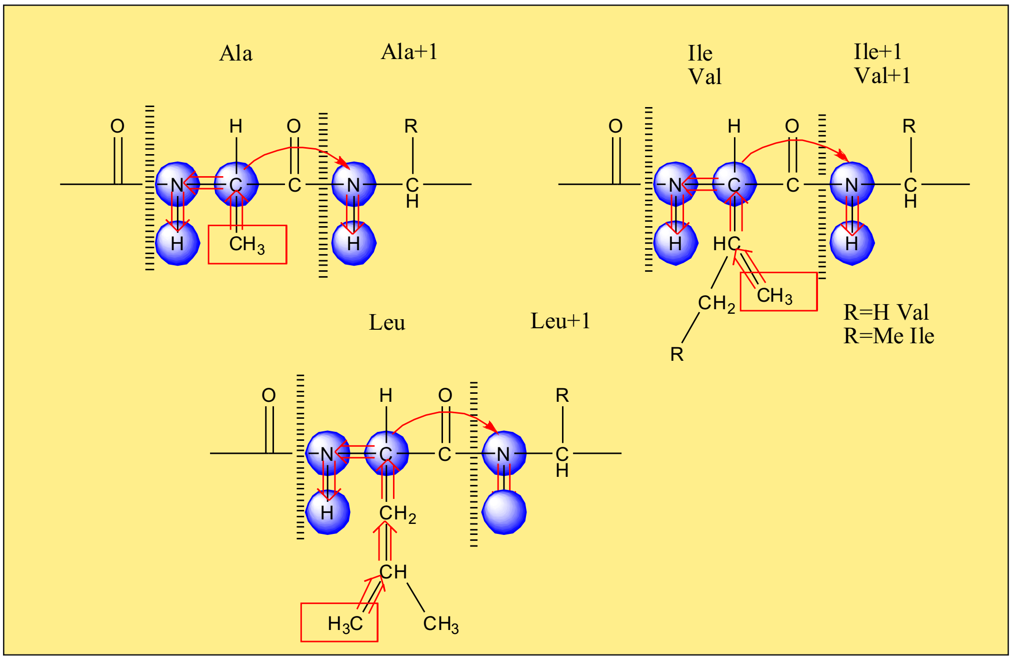
LABEL_VIA: 3D $(CH_3C)CA(CO)NH$ NH((Val,Ile,Ala)+1)

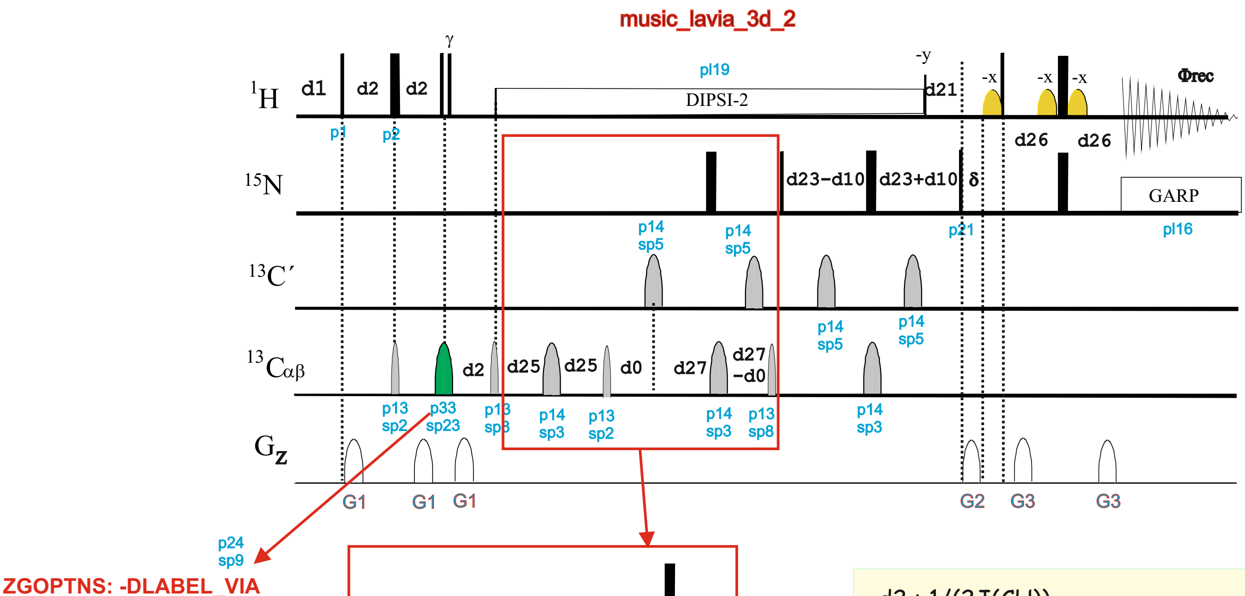
LABEL_CO: 3D $(CH_3CCA)CONH$

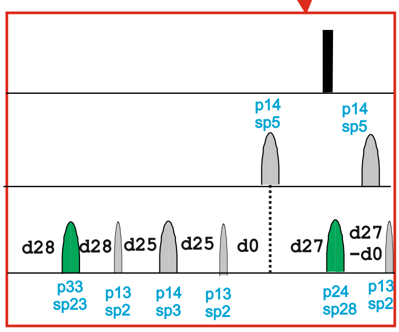


d2 : 1/(2J(CH))	[4.0 msec]
d21: 1/(2J(NH)	[5.9 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: n/(4J(CC)	[19 msec]
or n/(4J(CC) (LABEL_VIA)	[17 msec]
or 1/(4J(CC) (LABEL_CO)	[4.5 msec]
d25: 1/(4J(CC)	[7.0 msec]
or 1/(8J(CC) (LABEL_VIA)	[4.0 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO)	[12.4 msec]
d28: 1/(8J(CC)	[3.6 msec]

MUSIC-LAVIA: (CH_3C)CANH







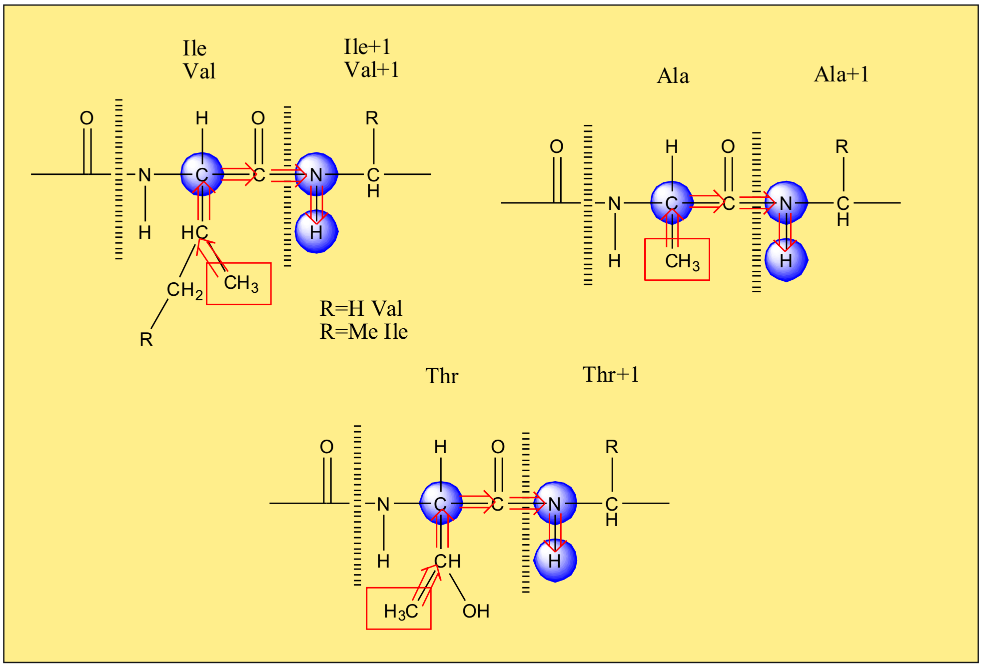
d2 : 1/(2J(CH))		[4.0 msec]
d21: 1/(2J(NH)		[5.9 msec]
d23: 1/(4J(NCa)		[12.4 msec]
d25: 1/(4J(CC)		[7.0 msec]
	or 1/(8J(CC) (LABEL_VIA)	[4.0 msec]
d26: 1/(4J(NH)		[2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa)		[9.0 msec]
d28: 1/(8J(CC)		[3.6 msec]

ZGOPTNS

no options: 3D (CH_3C)CANH NH((Leu,Ala)+1) and NH((Leu,Ala))

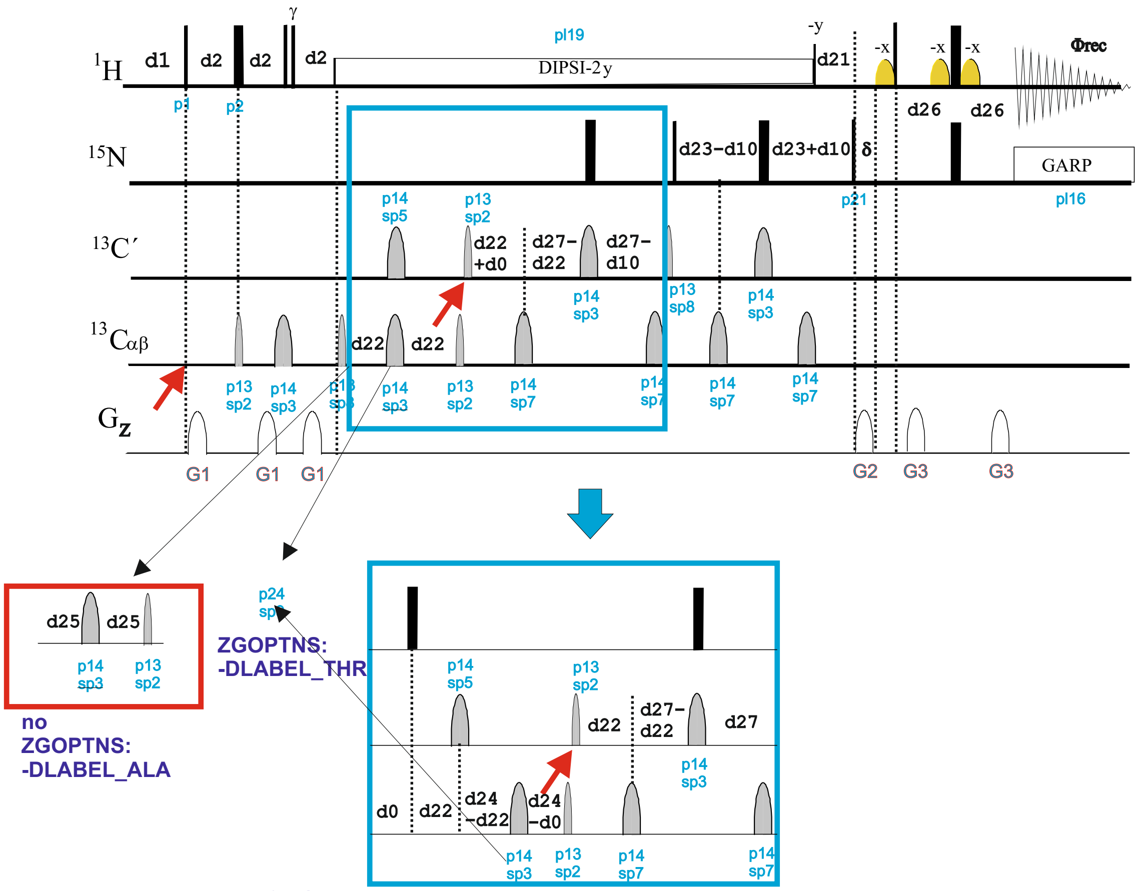
LABEL_VIA: 3D (CH_3C)CANH NH((Val,Ile,Ala)+1) and NH((Val,Ile,Ala))

MUSIC-TAVI: $(CH_3C)CA(CO)NH$ and (CH3CCA)CONH



music_tavi_3d

ZGOPTNS: -DLABEL_CO, -DLABEL_ALA



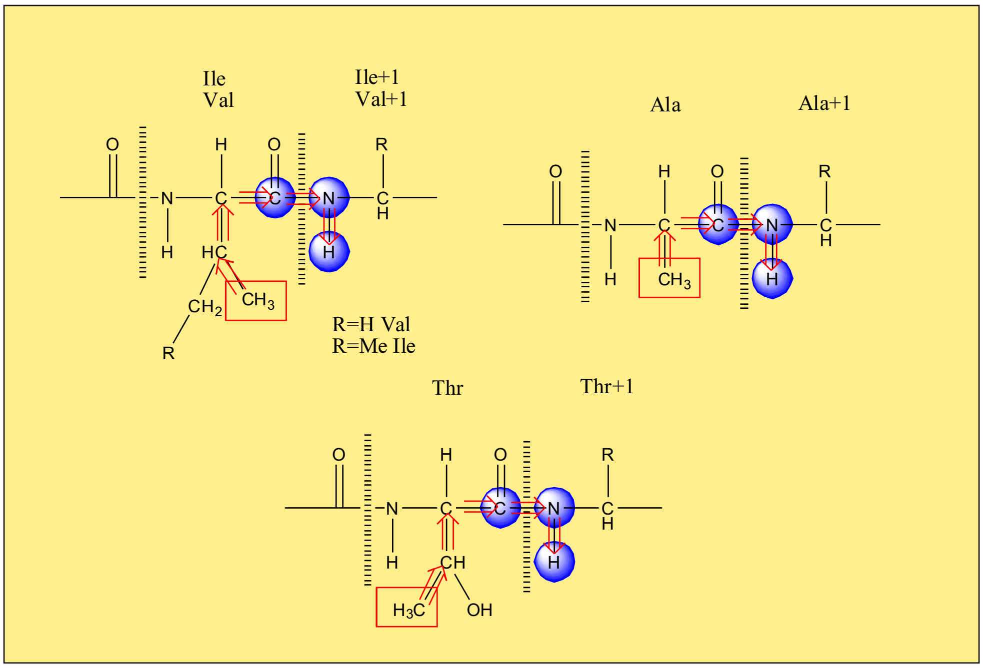
ZGOPTNS

no options: 3D $(CH_3C)CA(CO)NH$ NH((Thr,Ala,Val,Ile)+1)

LABEL_ALA: 3D $(CH_3C)CA(CO)NH$ NH((Ala+1))

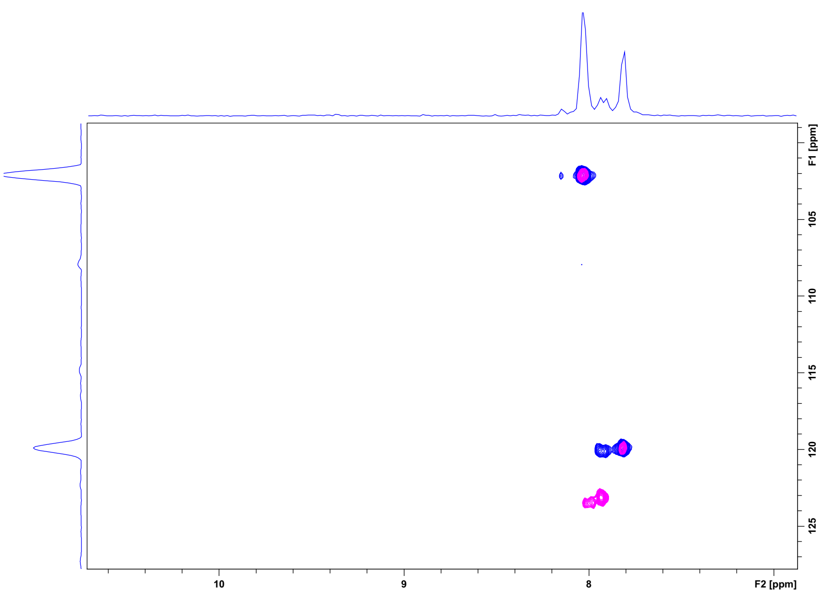
LABEL_THR: 3D $(CH_3C)CA(CO)NH$ NH((Thr,Ala)+1)

LABEL_CO: 3D $(CH_3CCA)CONH$

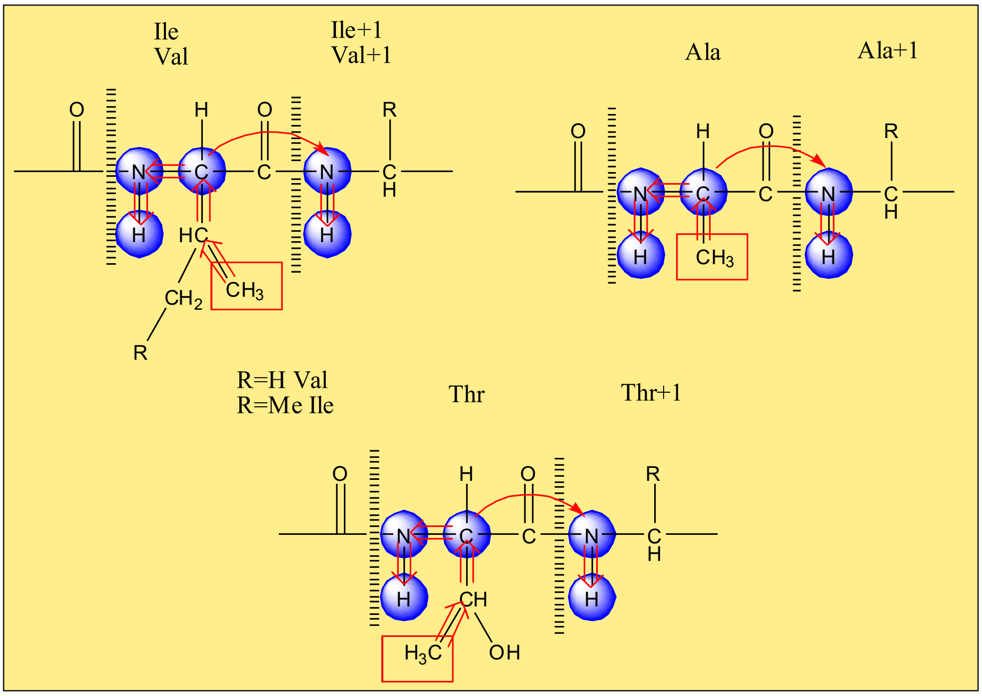


d2 : 1/(2J(CH))	[4.0 msec]
d21: 1/(2J(NH)	[5.9 msec]
d22: 1/(4J(CaCO)	[4.4 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: n/(4J(CC)	[17 msec]
d25: 1/(4J(CC)	[5.5 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO)	[12.4 msec]

TAVI

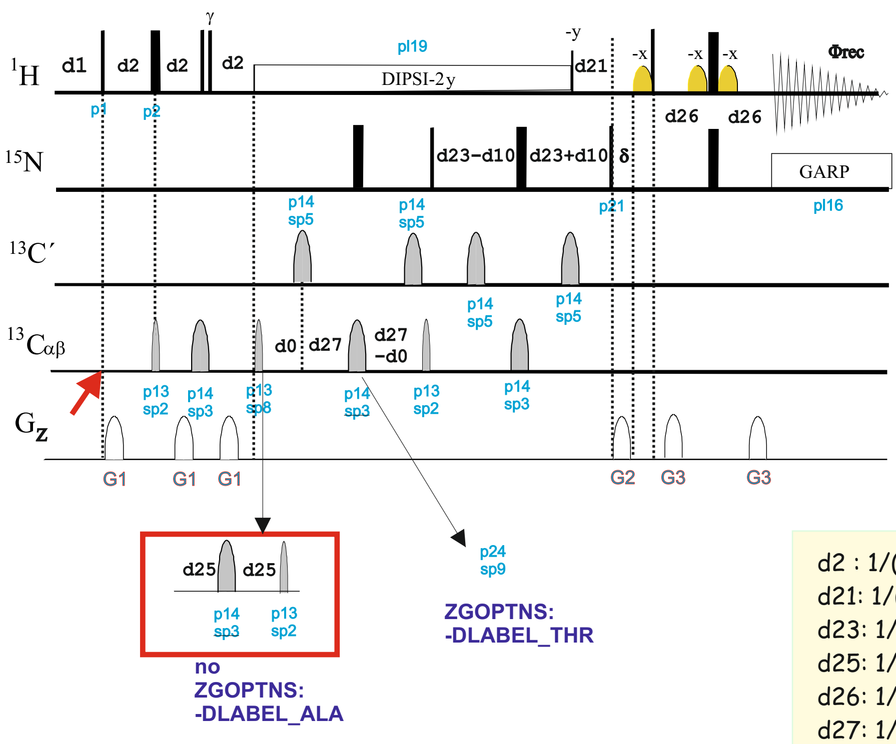


MUSIC-TAVI: (CH3C)CANH



music_tavi_3d_2

ZGOPTNS: -DLABEL_ALA



d2 : 1/(2J(CH))	[4.0 msec]
d21: 1/(2J(NH)	[5.9 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d25: 1/(4J(CC)	[5.5 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(CbCa) and 1/(4J(NCa)	[8.2 msec]

ZGOPTNS

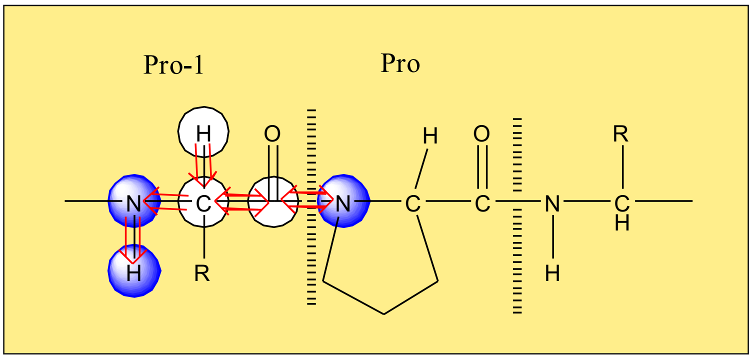
no options: 3D (CH_3C)CANH NH((Thr,Ala,Val,Ile)+1) and NH(Thr,Ala,Val,Ile)

LABEL_ALA: 3D (CH_3C)CANH NH((Ala+1) and NH(Ala)

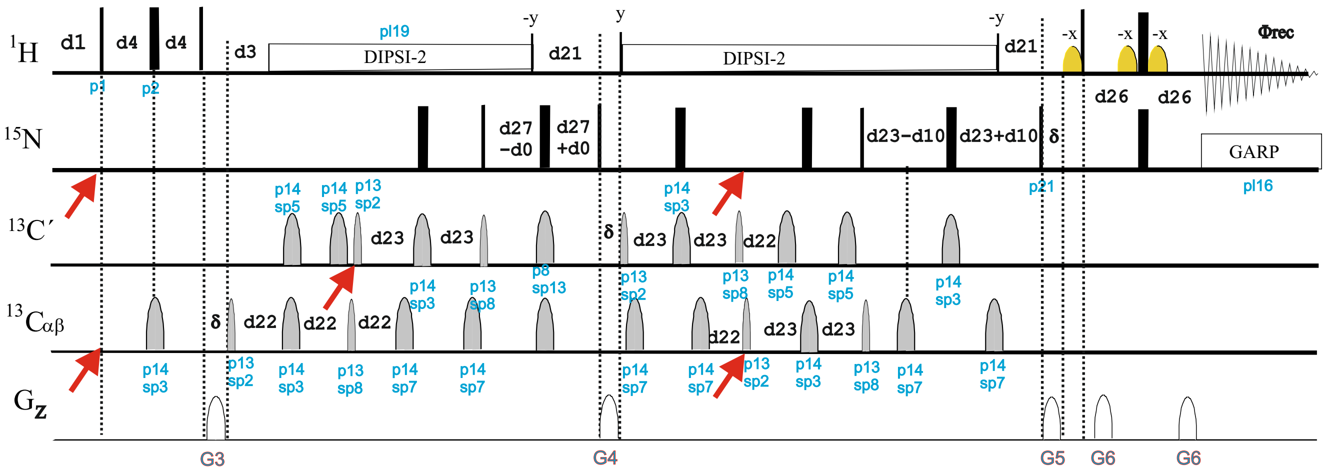
LABEL_THR3D (CH_3C)CANH NH((Thr,Ala)+1) and NH(Thr,Ala)

MUSIC-Proline: (HACACO)N(COCA)NH

Ref: M. Schubert, L. Ball, H. Oschkinat & P. Schmieder, J. Biomol. NMR 17, 331-335 (2000)



music_pro_1_3d

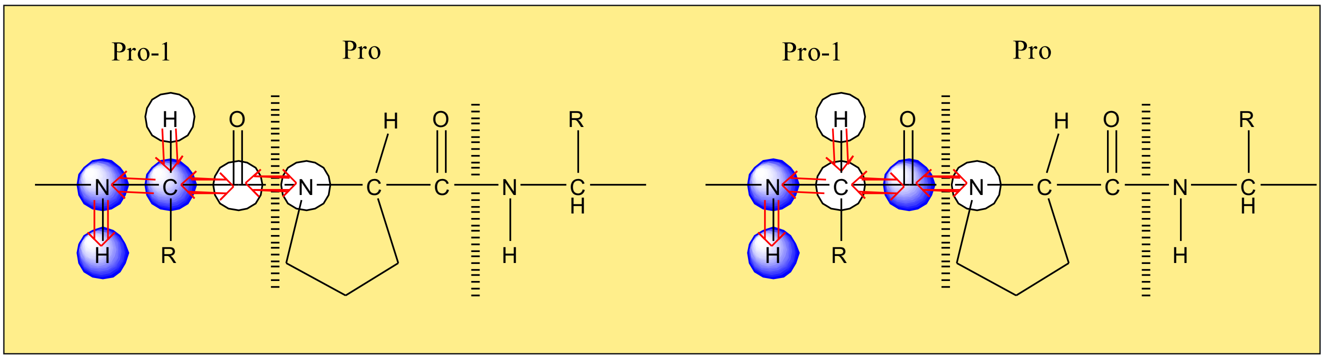


ZGOPTNS

no options: 3D (HACACO)N(COCA)NH NH(Pro-1)

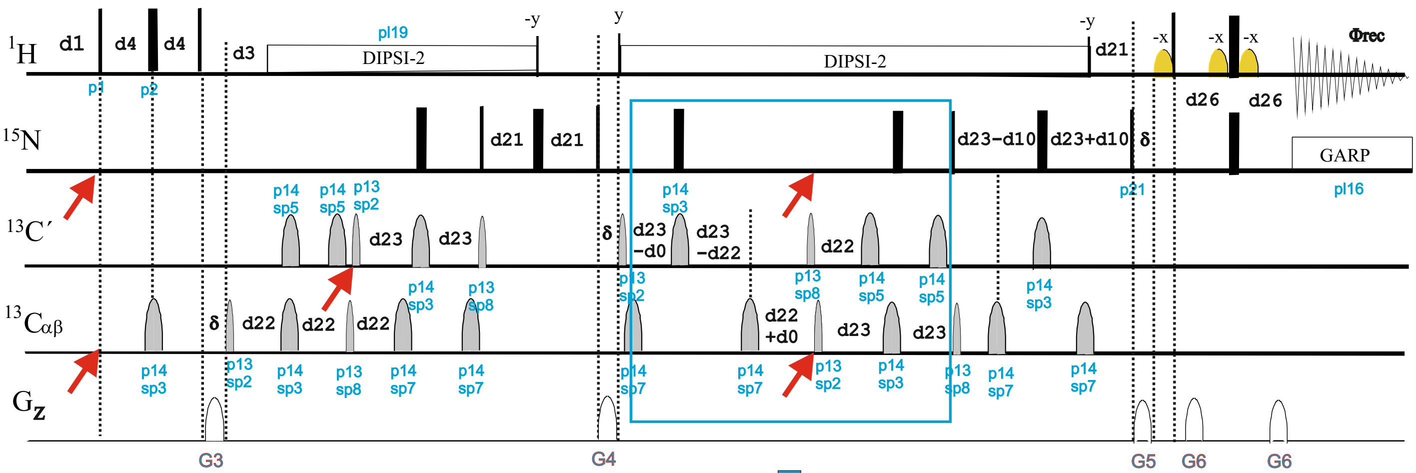
d3 : 1/(4J(CH))	[2.1 msec]
d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NC)	[12.4 msec]
d26: 1/(4J(NH)	[2.3 msec]

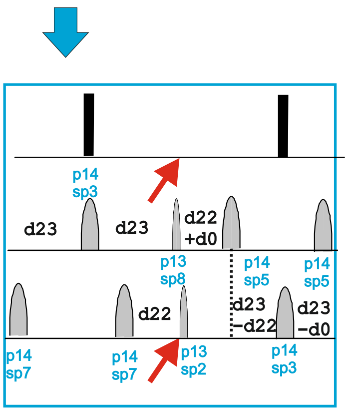
MUSIC-Proline: (HACACONCO)CANH and (HACACON)CO(CA)NH



music_pro_1_3d.2

ZGOPTNS: -DLABEL_CO





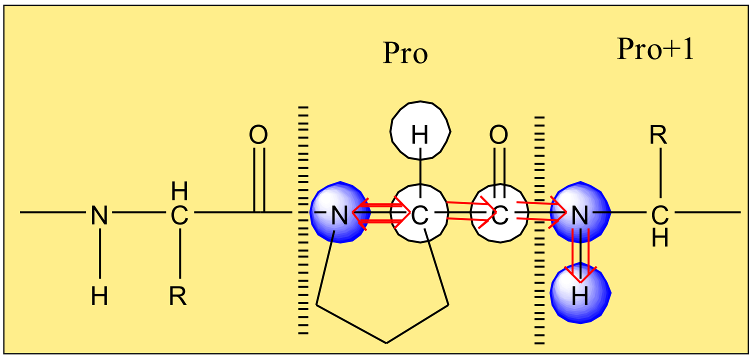
ZGOPTNS

no options: 3D (HACACONCO)CANH NH(Pro-1)

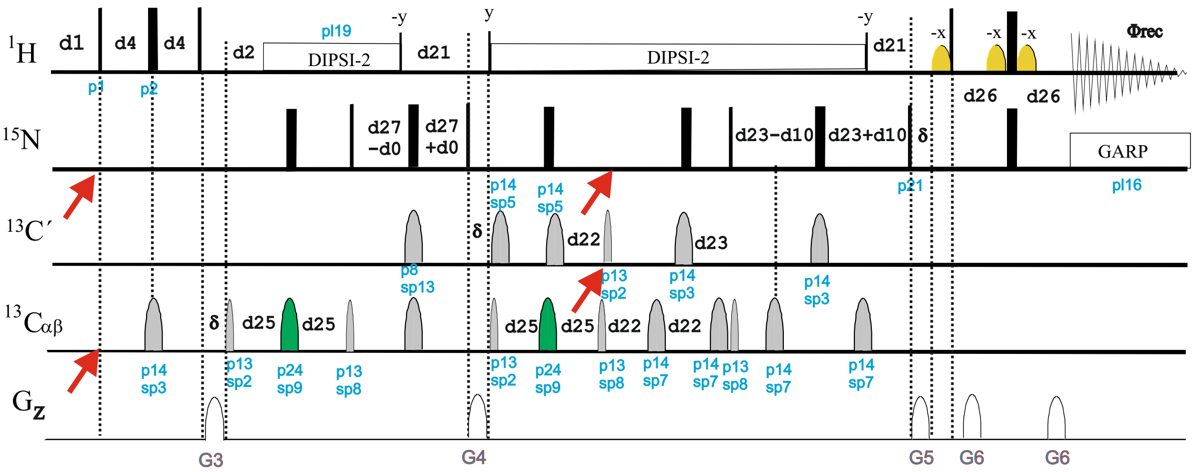
LABEL_CO: 3D (HACACON)CO(CA)NH

d3 : 1/(4J(CH))	[2.1 msec]
d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(CaCO))	[4.5 msec]
d23: 1/(4J(NC))	[12.4 msec]
d26: 1/(4J(NH))	[2.3 msec]

MUSIC-Proline: (HACA)N(CACO)NH



music_pro_2_3d

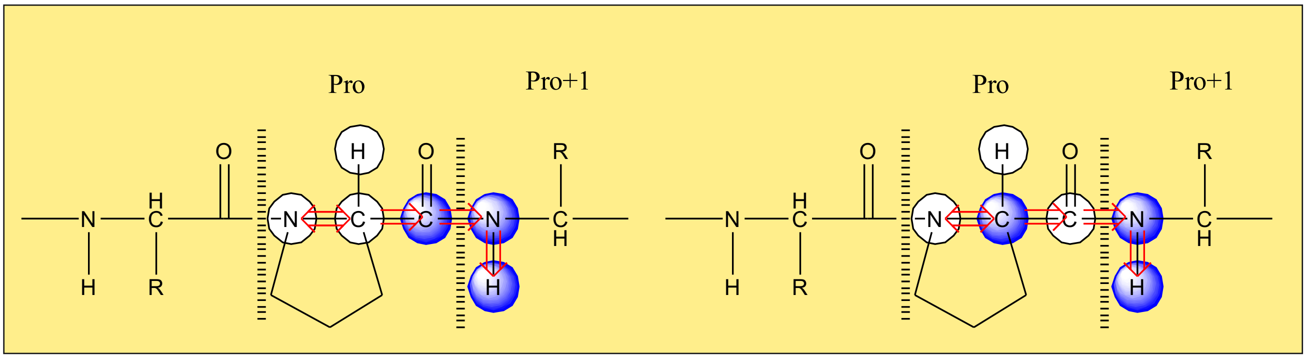


ZGOPTNS

no options: 3D (HACA)N(CACO)NH NH(Pro+1)

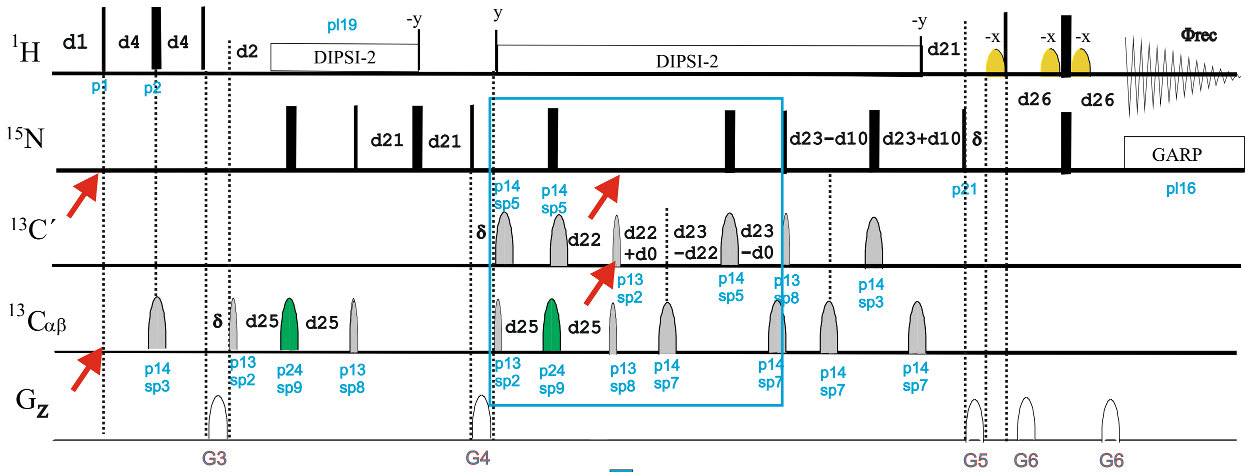
d2 : 1/(2J(CH))	[3.4 msec]
d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d25: 1/(4J(NCa)	[7.0 msec]
d26: 1/(4J(NH)	[2.3 msec]

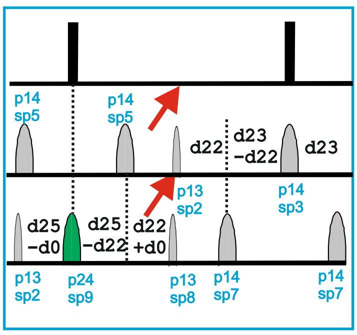
MUSIC-Proline: (HACANCA)CONH and (HACAN)CA(CO)NH



music_pro_2_3d.2

ZGOPTNS: -DLABEL_CO





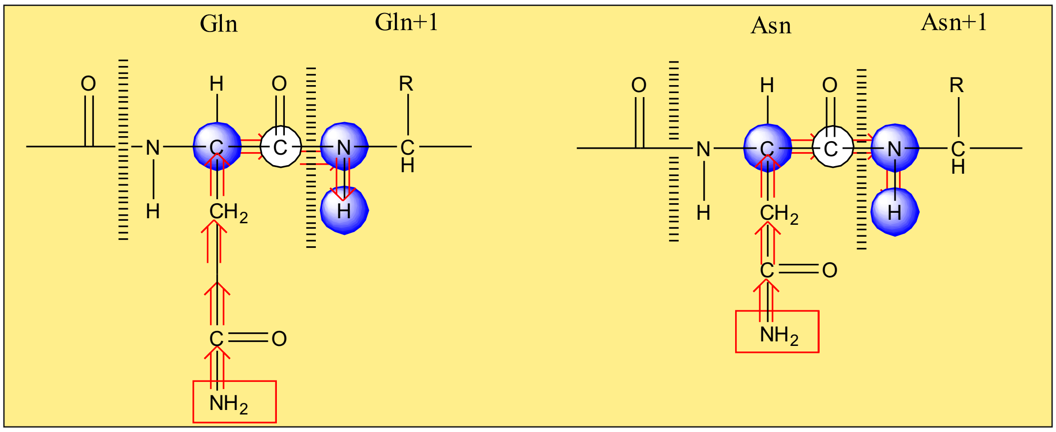
ZGOPTNS

no options: 3D (HACANCA)CONH NH(Pro+1)

LABEL_CO: 3D (HACAN)CA(CO)NH

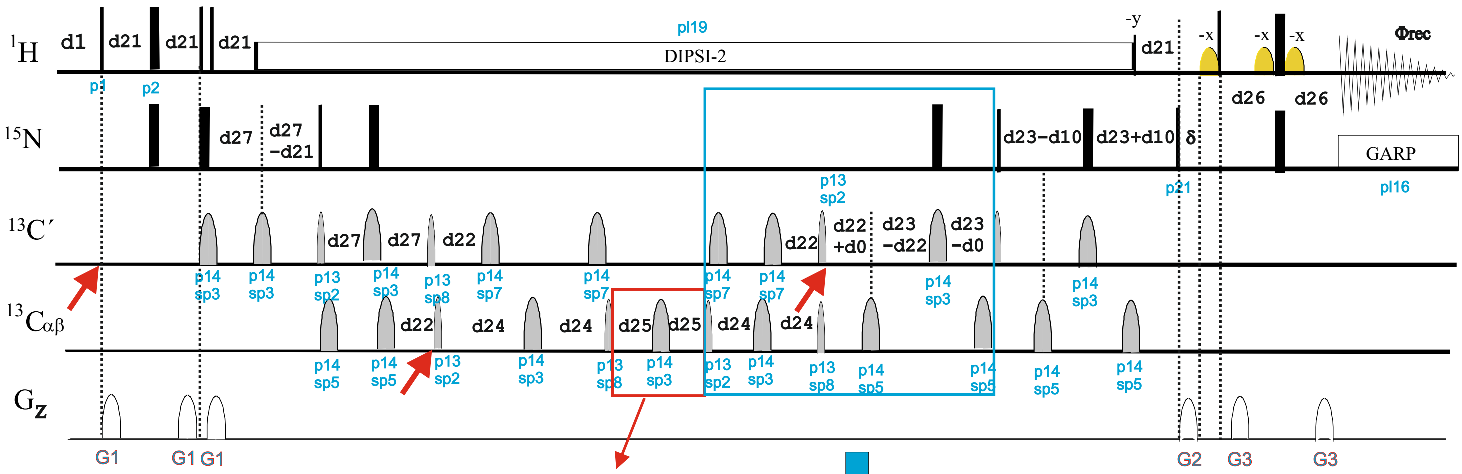
d2 : 1/(2J(CH))	[3.4 msec]
d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(CaCO))	[4.5 msec]
d23: 1/(4J(NCO))	[12.4 msec]
d25: 1/(4J(NCa))	[7.0 msec]
d26: 1/(4J(NH))	[2.3 msec]

MUSIC-GLN/ASN: $(NH_2COC)CA(CO)NH$ and $(NH_2COCCA)CONH$

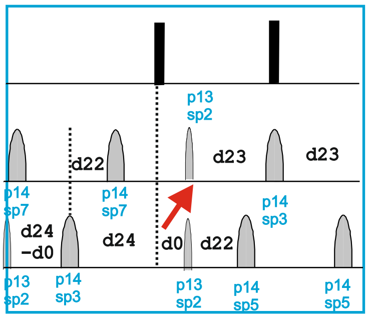


music_qn_3d

ZGOPTNS: -DLABEL_CO



ZGOPTNS: -DLABEL_GLN



ZGOPTNS

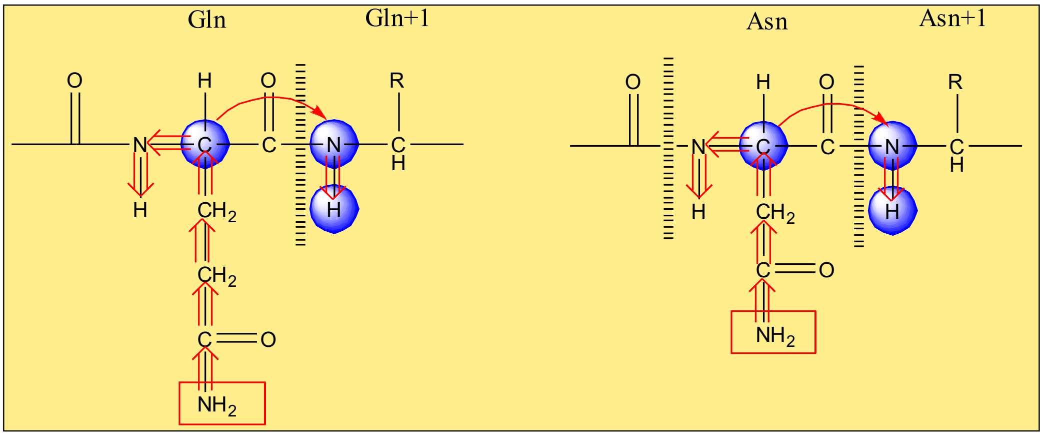
no options: 3D $(NH_2COC)CA(CO)NH$ NH(Asn+1)

LABEL_GLN: 3D $(NH_2COC)CA(CO)NH$ NH((Gln,Asn)+1)

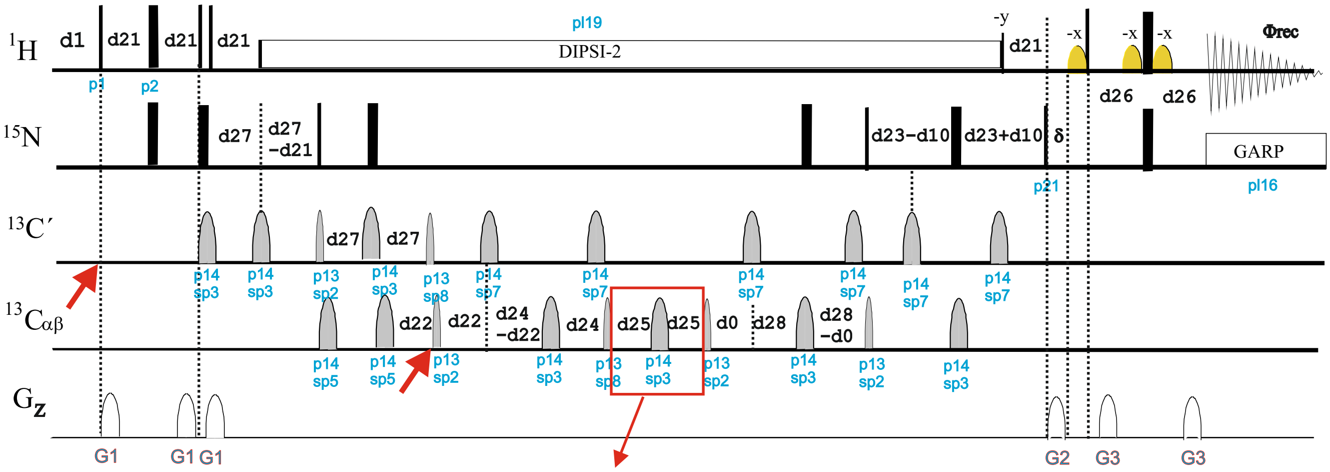
LABEL_CO: 3D $(NH_2COCCA)CONH$

d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCO)	[12.4 msec]
d24: 1/(4J(CC)	[5.2 msec]
d25: 1/(4J(CC)	[6.8 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO(s))	[14.2 msec]

MUSIC-GLN/ASN: $(NH_2COC)CANH$



music_qn_3d_2



ZGOPTNS

no options: 3D $(NH_2COC)CANH$ NH(Asn+1)

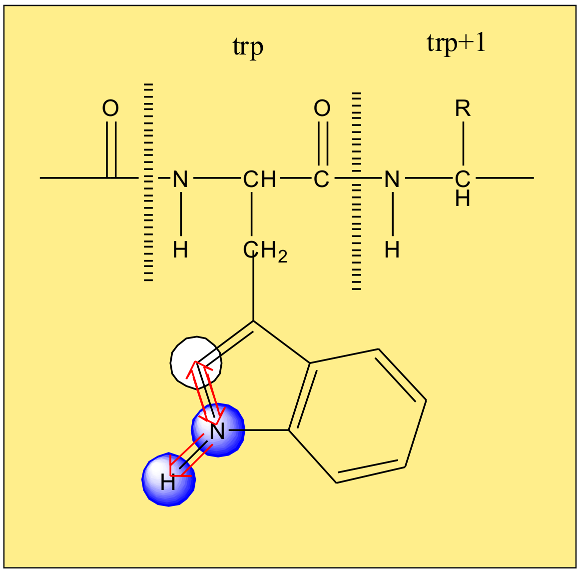
LABEL_GLN: 3D $(NH_2COC)CANH$ NH((Gln, Asn)+1)

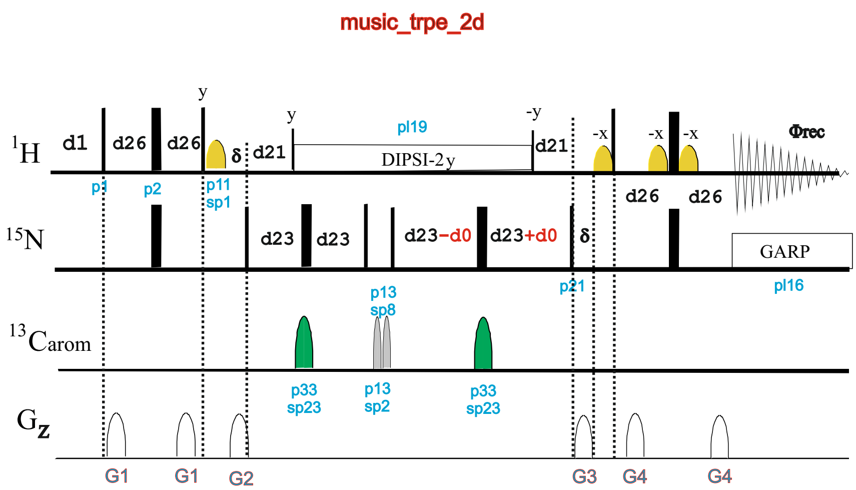
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(CaCO)	[4.5 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d24: 1/(4J(CC)	[5.2 msec]
d25: 1/(4J(CC)	[6.8 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J(NCO(s))	[14.2 msec]
d28: 1/(4J(CC)	[7.0 msec]
or 1/(4J(CC) (LABEL_GLN)	[9.0 msec]

MUSIC-TRP: 2D (HENECE)NH

Reference:

M. Schubert, H. Oschkinat & P. Schmieder, J. Magn. Reson. 153, 186-192 (2001)





d21: 1/(2J(NH)) [5.5 msec]
d23: 1/(4J(NC)) [12.4 msec]
d26: 1/(4J(NH)) [2.3 msec]

BRUKER
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NMRGuide

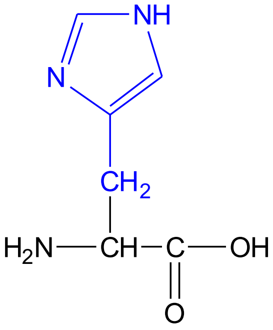
AROMATIC-SPECIFIC
NMR EXPERIMENTS

Aromatic-Specific Experiments

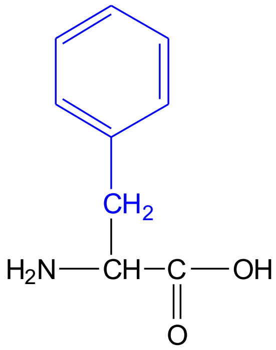
- 2D (HB)CB(CGCD)HD (**hbcbcgcdhdgp**)
- 2D (HB)CB(CGCDCE)HE (**hbcbcgcdcehegp**)

- 2D (HB)CB(CGCC-TOCSY)Har (**hbcbcgcchargp**)

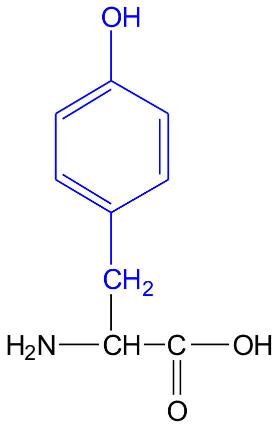
- 3D Har(CC-TOCSY-CGCBCACO)NH (**hcccgcbcaconhgp3d**)
- 3D Har(CC-TOCSY-CGCBCACO)NH using WATERGATE (**hcccgcbcaconhgpwg3d**)
- 3D Har(CC-TOCSY-CGCBCACO)NH using TROSY (**trhcccgcbcaconhgp3d**)
- 3D Har(CC-TOCSY-CGCBCACO)NH using TROSY and echo-antiecho (**trhcccgcbcaconhetgp3d**)



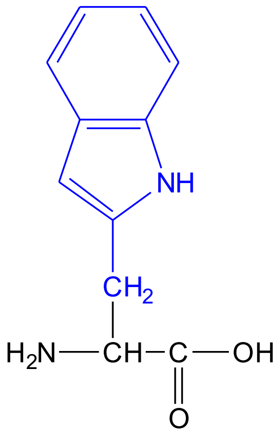
Histidine (His)



Phenylalanine (Phe)



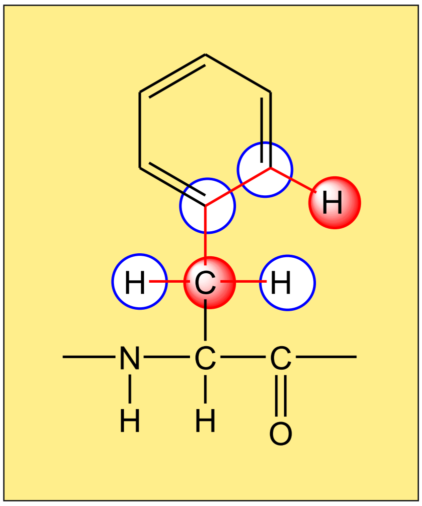
Tyrosine (Tyr)



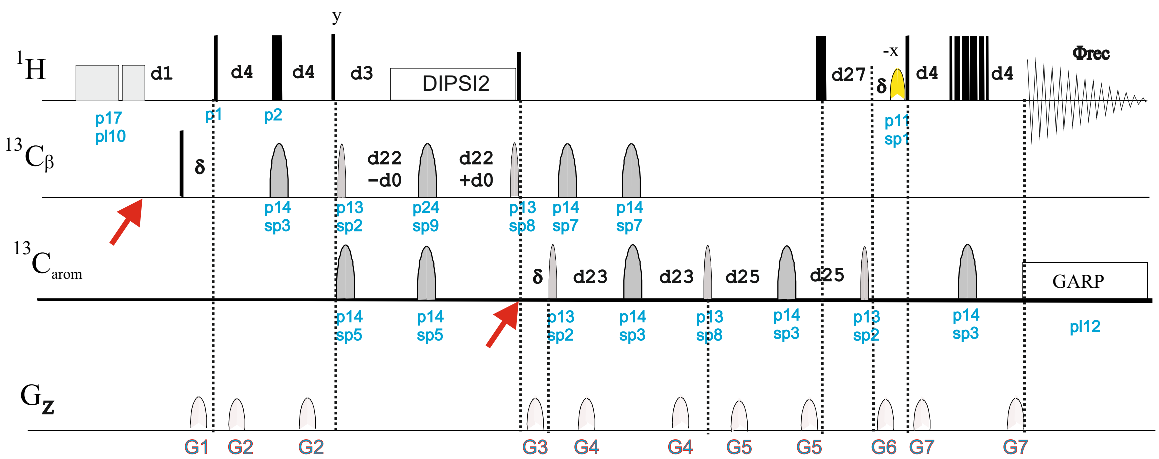
Tryptophan (Trp)

References:
1. T. Yamazaki, J.D. Forman-Kay & L.E. Kay, J. Am. Chem. Soc. 115, 11054-11055 (1993)
2. F. Loehr, R. Haensel, V.V. Rogov & V. Doetsch,J. Biomol. NMR 37, 205-224 (2007)

2D (HB)CB(CGCD)HD

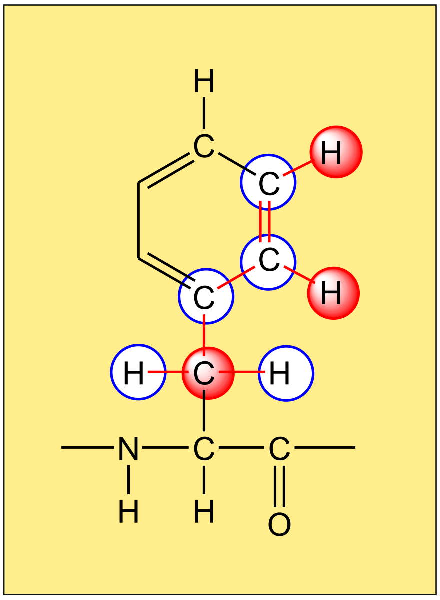


hbcbcgcdhdgp

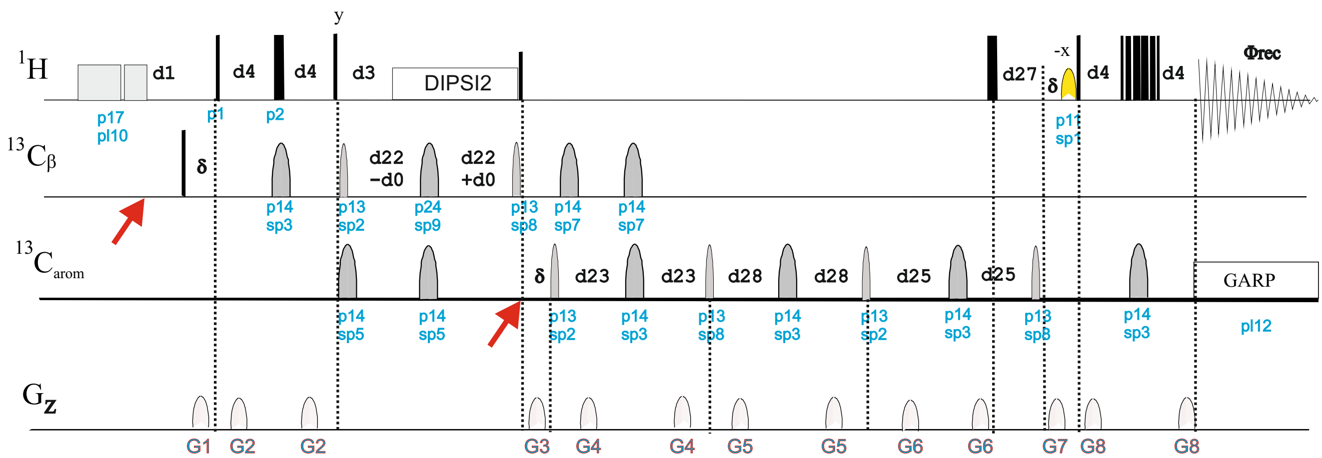


d3 : 1/(3J'(HbCb))	[1.8 msec]
d4 : 1/(4J(HbCb))	[1.7 msec]
d21: 1/(4J'(HeCe))	[1.25 msec]
d22: 1/(4J(CbCg))	[4.4 msec]
d23: 1/(4J'(CbCg)) and 1/(4J(CgCd))	[2.7 msec]
d25: 1/(4J'(CgCd))	[2.1 msec]
d27: 1/(4J(HdCd))	[1.4 msec]

2D (HB)CB(CGCDCE)HE

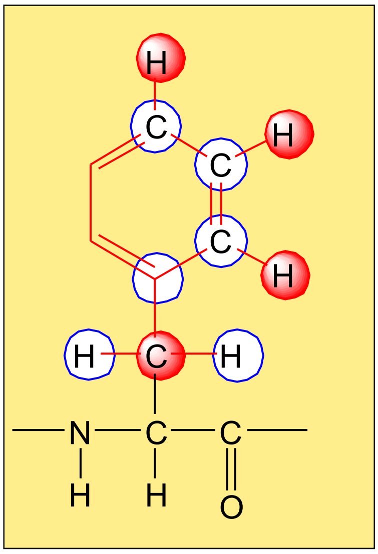


hbcbcgcdcehegp

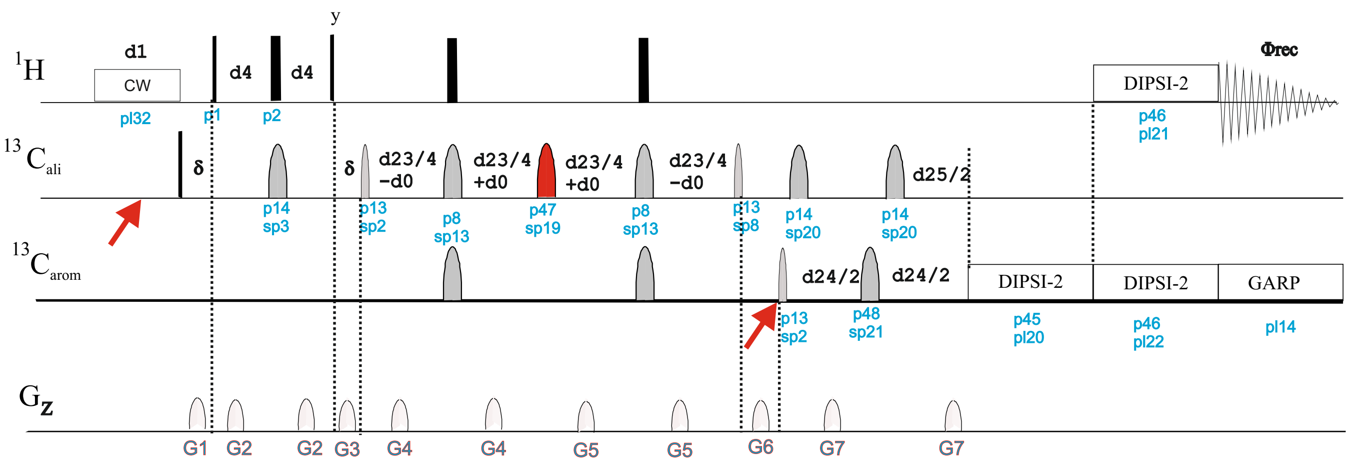


d3 : 1/(3J'(HbCb))	[1.8 msec]
d4 : 1/(4J(HbCb))	[1.7 msec]
d21: 1/(4J'(HeCe))	[1.25 msec]
d22: 1/(4J(CbCg))	[4.4 msec]
d23: 1/(4J'(CbCg)) and 1/(4J(CgCd))	[2.7 msec]
d25: 1/(4J'(CdCe))	[2.1 msec]
d27: 1/(4J(HeCe))	[1.4 msec]
d28: 1/(4J'(CgCd)) and 1/(4J(CdCe))	[3.8 msec]

2D (HB)CB(CGCC_TOCSY)Har



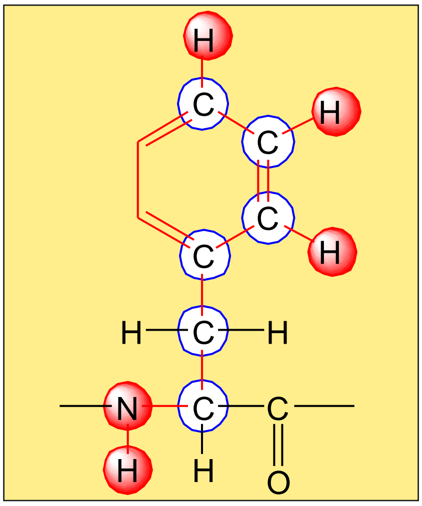
hbcbcgcchargp



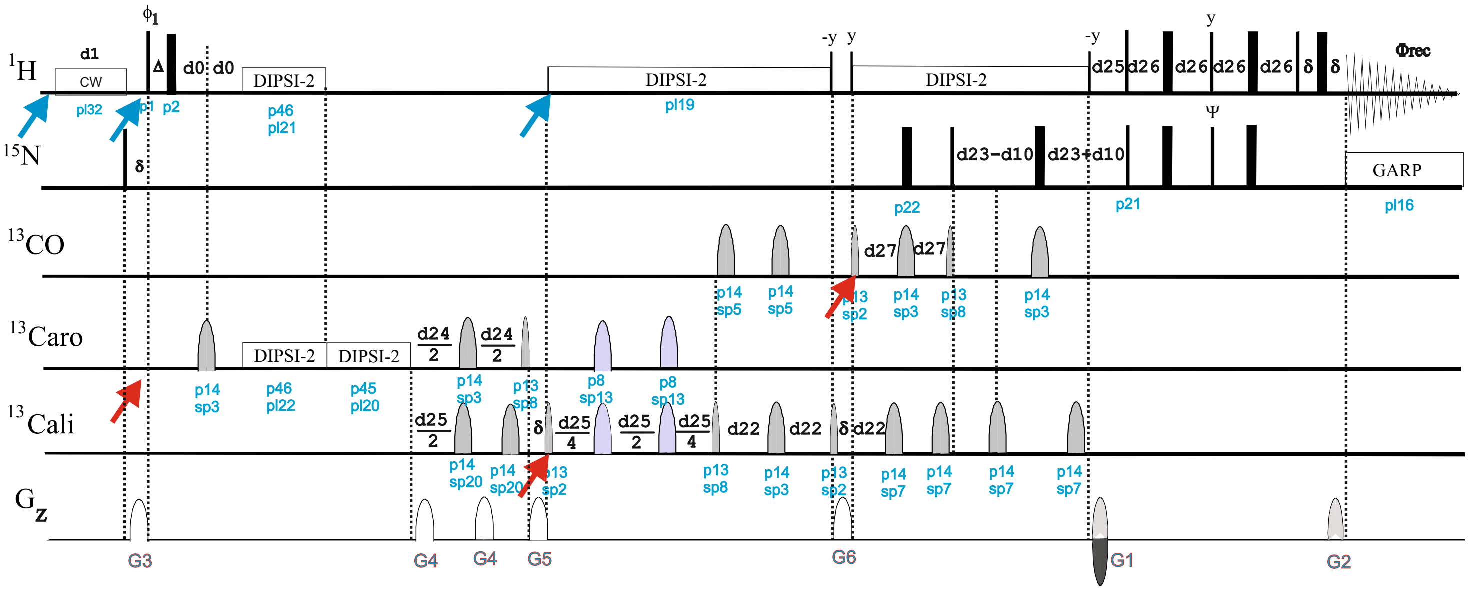
d4 : 1/(4J(HbCb)) [1.7 msec]
d23: 1/(2J'(CbCg)) and 5/(4J'(HbCb)) [9.0 msec]
d24: 1/(J(CgCd))
Phe, Trp [11.5 msec]
Tyr [15.0 msec]
all [17.4 msec]
d25: 1/(2J(CbCg)) [10.4 msec]

cnst24: Caromatic chemical shift (offset, in ppm) [130 ppm]
cnst30: Cbeta(aro) chemical shift (offset, in ppm) [35 ppm]
cnst51: Calpha(aro) chemical shift (offset, in ppm) [59 ppn]
cnst52: Caromatic chemical shift (offset, in ppm)
Phe [141 ppm]
Trp [111 ppm]
Tyr [129 ppm

3D Har(CC-TOCSY-CGCBCACO)NH

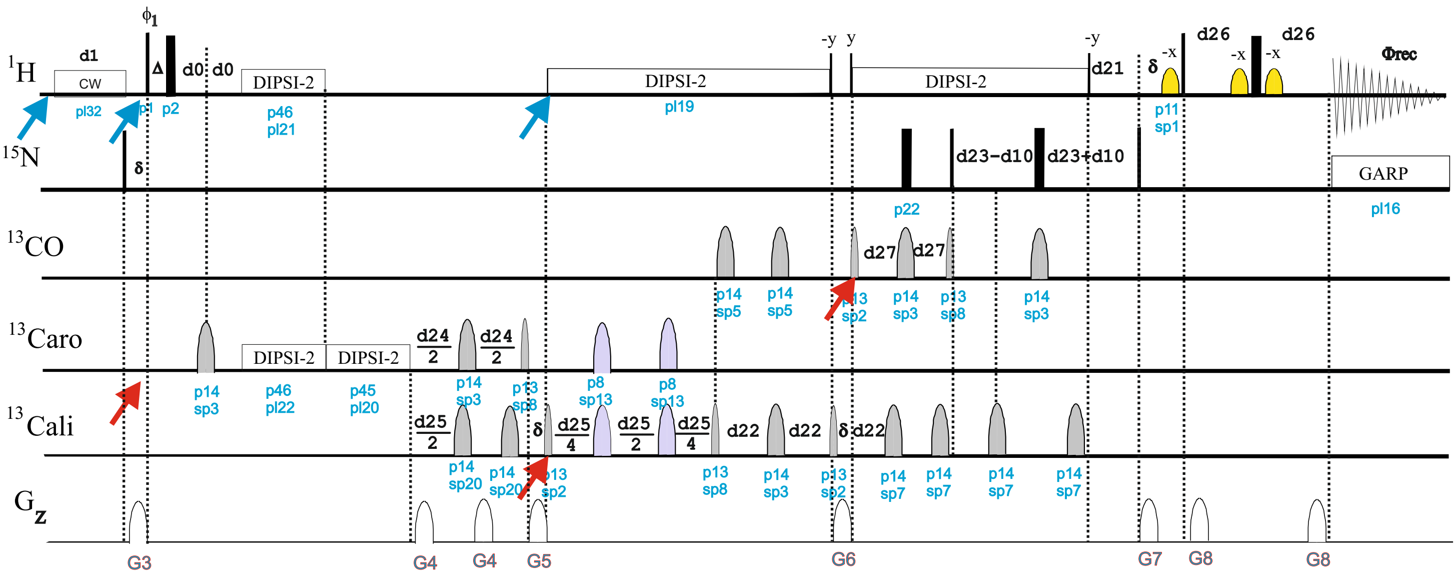


hcccgcbcaconhgp3d

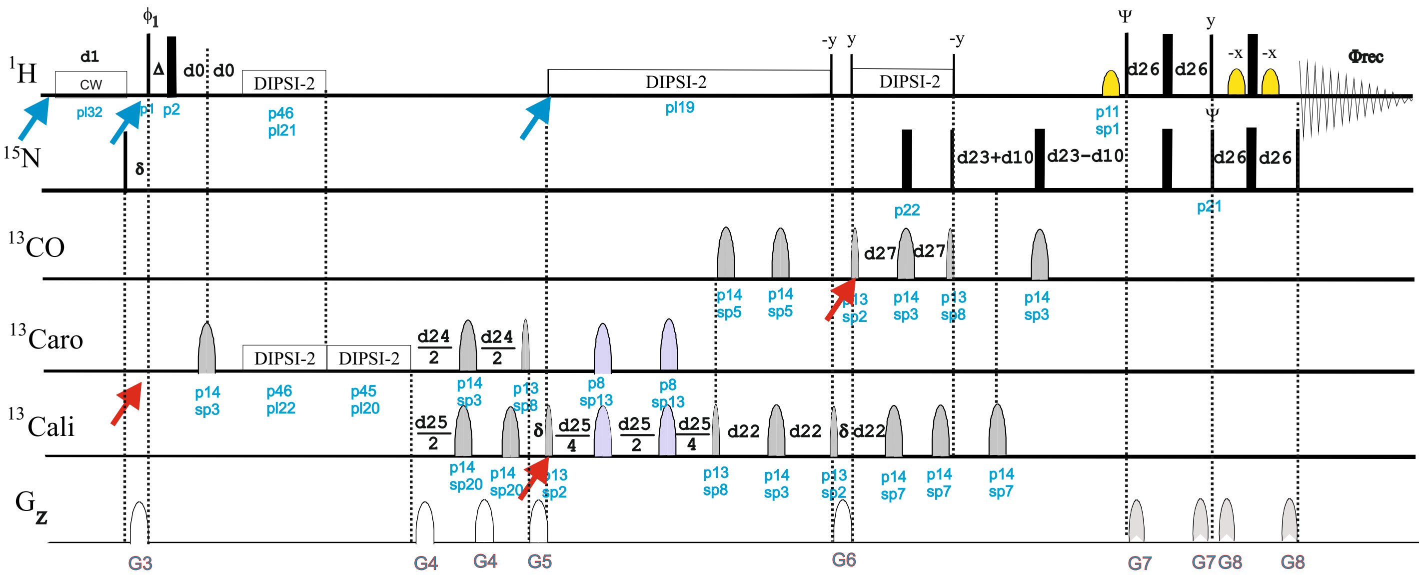


d21: 1/(2J(NH)) [5.5 msec]
d22: 1/(4J(CaCO)) [4.6 msec]
d23: 1/(4J(NCO) [12.4 msec]
d24: 1/(J(CgCd)) [17.4 msec]
d25: 1/(2J(CbCg)) [10.4 msec]
d26: 1/(4J'(NH) [2.3 msec]
d27: 1/(4J'(NCO) [11.0 msec]

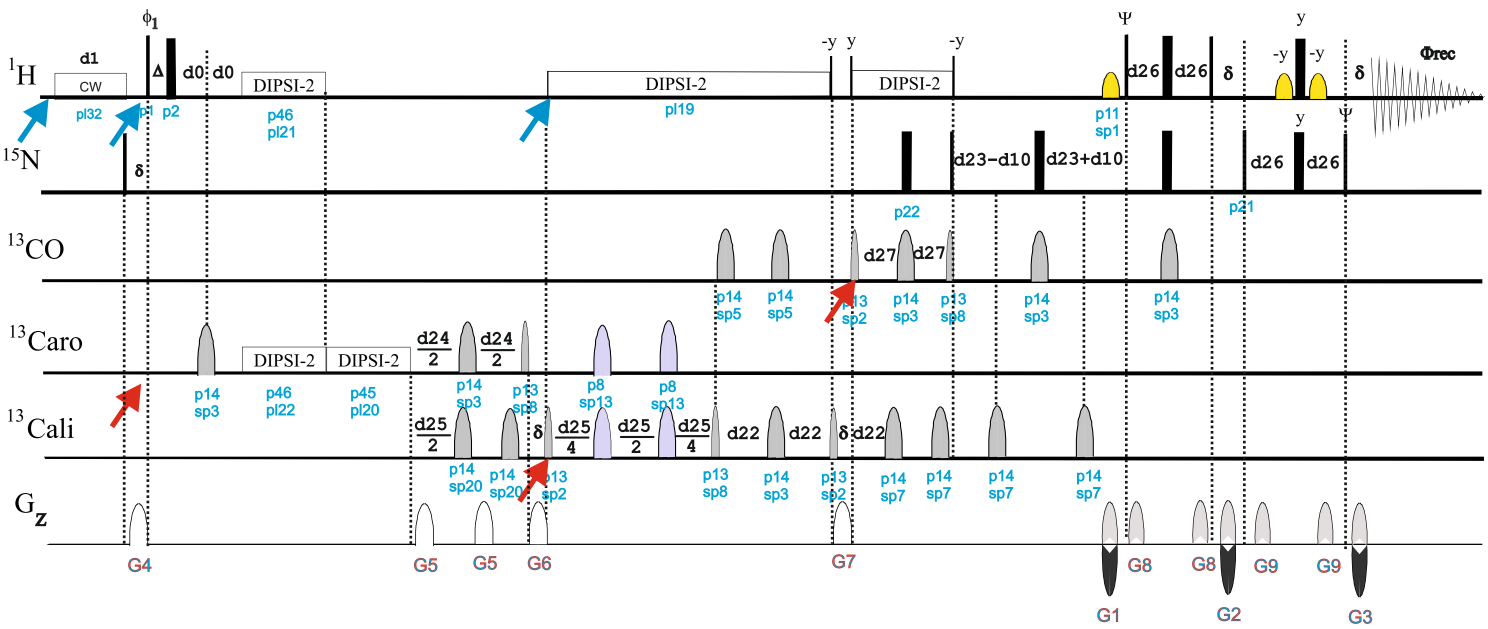
hcccgcbcaconhgpwg3d



trhcccgcbcaconhgp3d



trhcccgcbcaconhetgp3d



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NMRGuide

METHYL-SELECTIVE NMR EXPERIMENTS

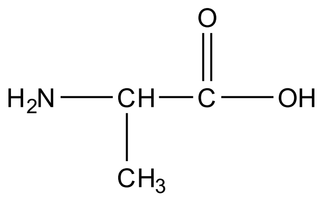
Methyl-selective Experiments

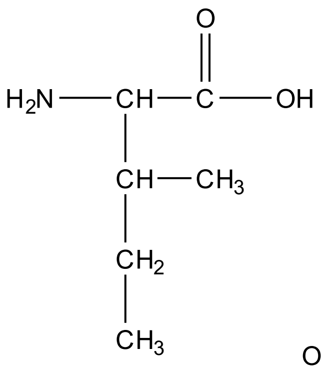
- 3D (Hme)Cme([C])CA experiment using WATERGATE (**hmcmcbcagpwg3d**)
- 3D (Hme)Cme([C]CA)CO experiment using WATERGATE (**hmcmcbcacogpwg3d**)
- 3D (Hme)Cme([C]CA)NH experiment using WATERGATE (**hmcmcbcanhgpwg3d**)
- 3D Hme (Cme[C]CA)NH experiment using WATERGATE (**hmcmcbcanhgpwg3d.2**)
- 3D (Hme)Cme([C]CACO)NH experiment using WATERGATE (**hmcmcbcaconhgpwg3d**)

Also see:
Amino-Acid-Type Experiments with CH3-selection
All Backbone-Sidechain experiments: (H)CC(CO)NH, CC(CO)NH, CCA(CO)NH, CCANH, CBCACONH, CBCANH ....

V. Tugarinov & L.E. Kay, J. Am. Chem. Soc. 125, 13868-13878 (2003)

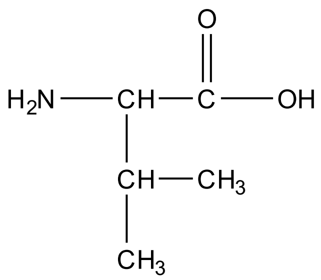
Ala

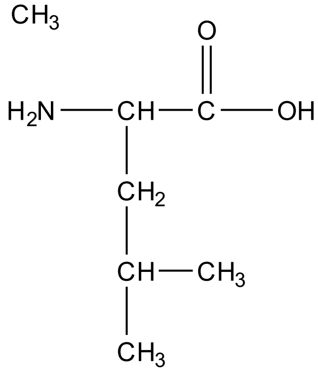




Ile

Val



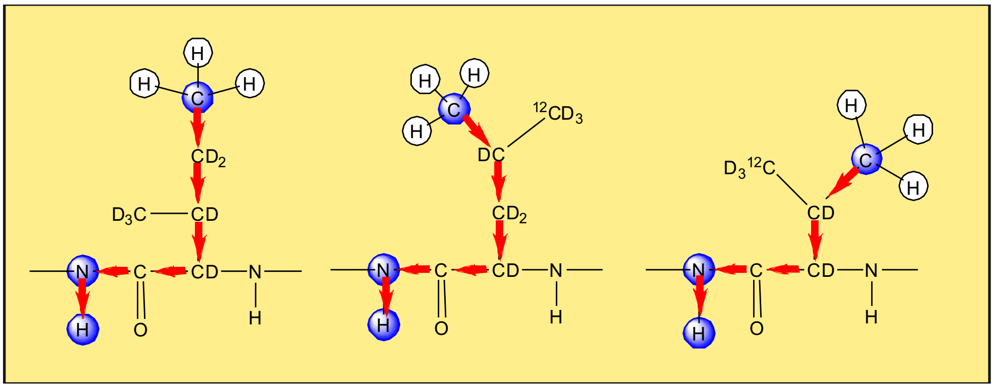


Leu

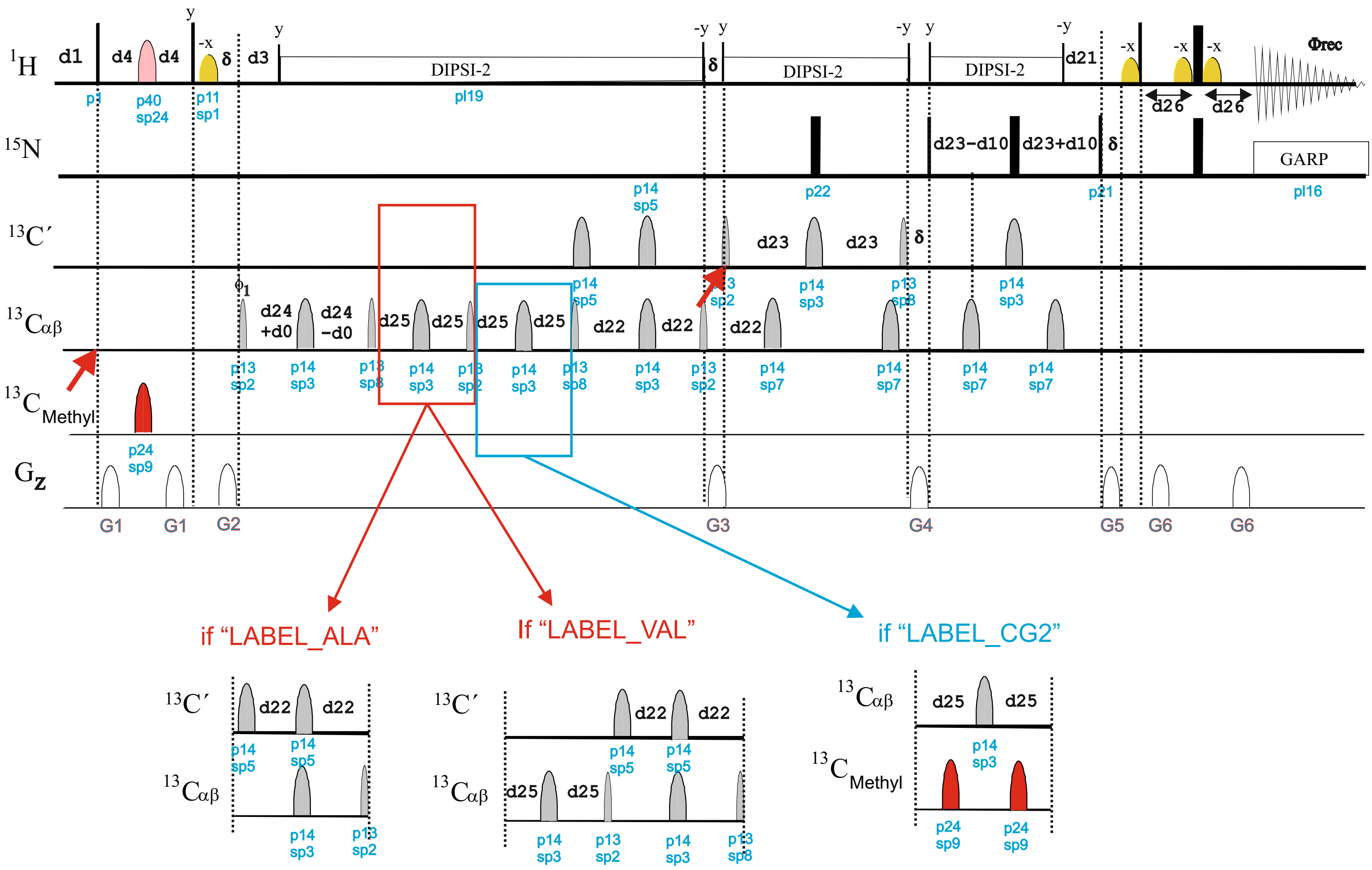
ZGOPTNS options (in eda) In **ALL EXPERIMENTS**:

no option all methyl groups
LABEL_ALA: one transfer step along sidechain: methyl groups
in Cb position only (option **-DLABEL_ALA**)
;LABEL_VAL: two transfer steps along sidechain: methyl groups
in Cg position only (option **-DLABEL_VAL**)
;LABEL_CG2: refocussing pulse for Ile Cg2 (depending on labelling
scheme) (option **-DLABEL_CG2**)

3D (Hme)Cme([C]CACO)NH

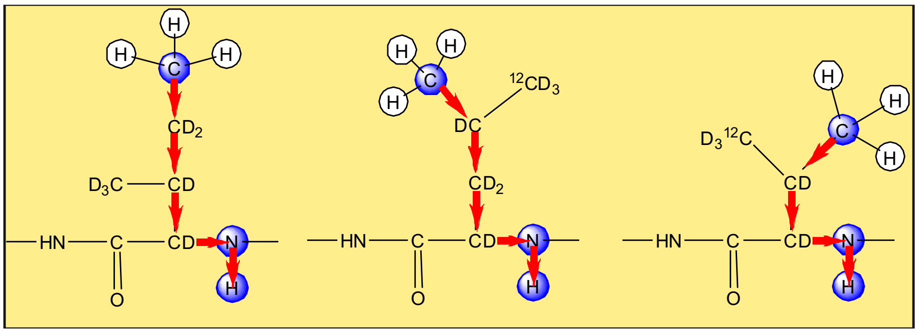


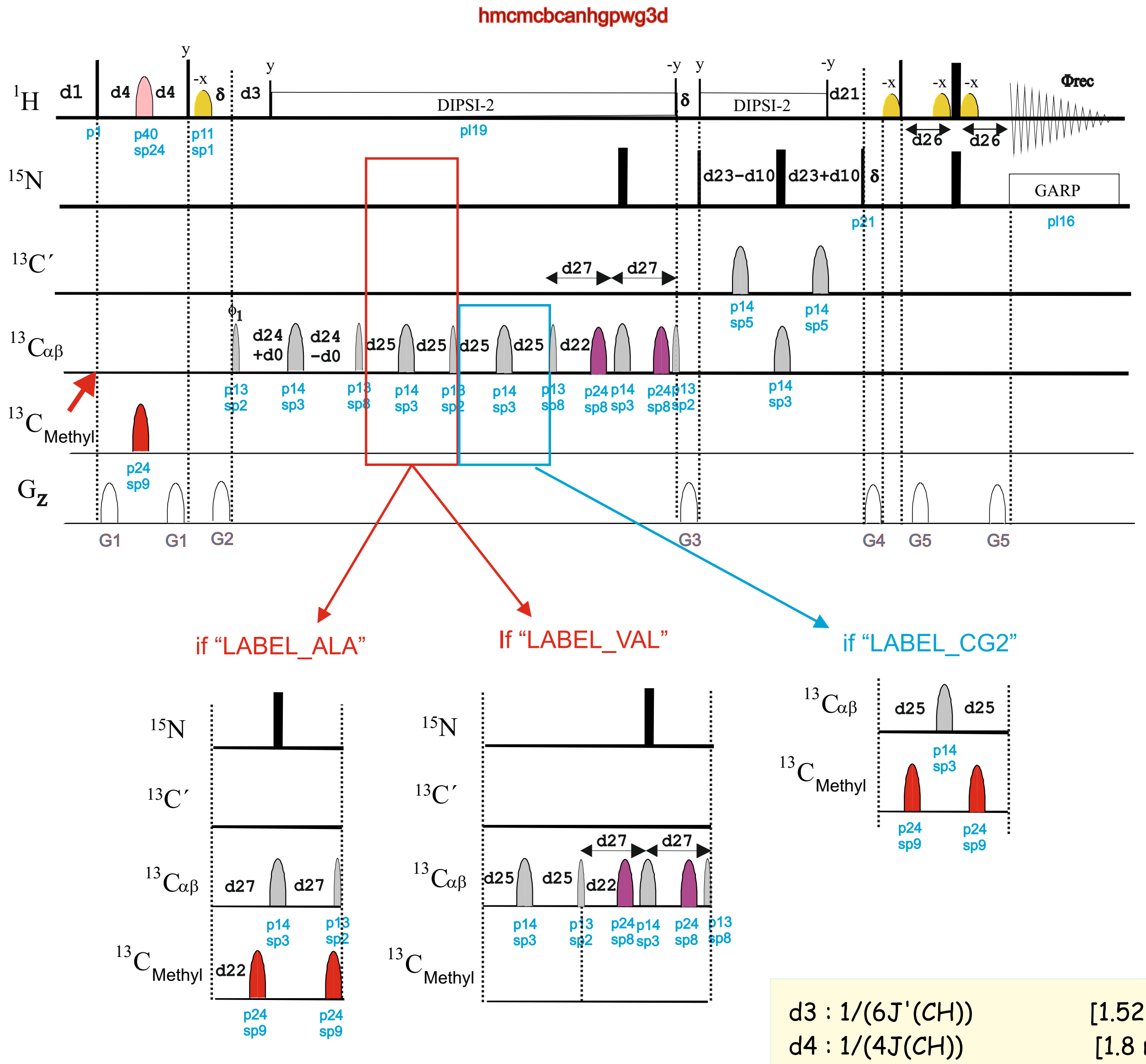
hmcmcbcaconhgpwg3d



d3 : 1/(6J'(CH))	[1.52 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(CaCO))	[4.5 msec]
d23: 1/(4J(NCa))	[12.4 msec]
d24: 1/(4J(CmeC))	[7 msec]
d25: 1/(4J'(CC))	[5 msec]
d26: 1/(4J(NH))	[2.3 msec]

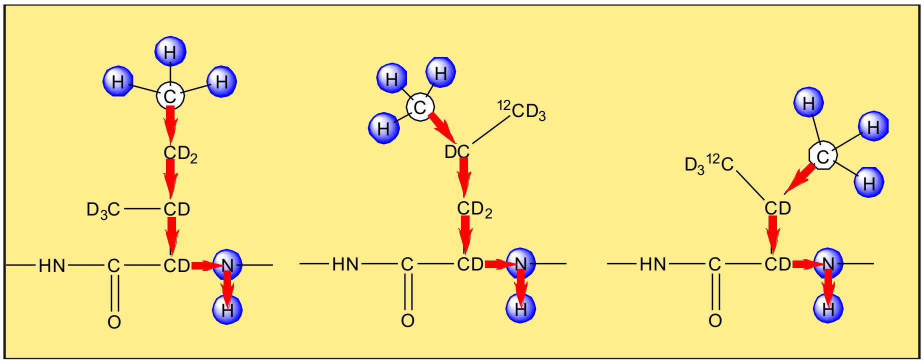
3D (Hme)Cme([C]CA)NH



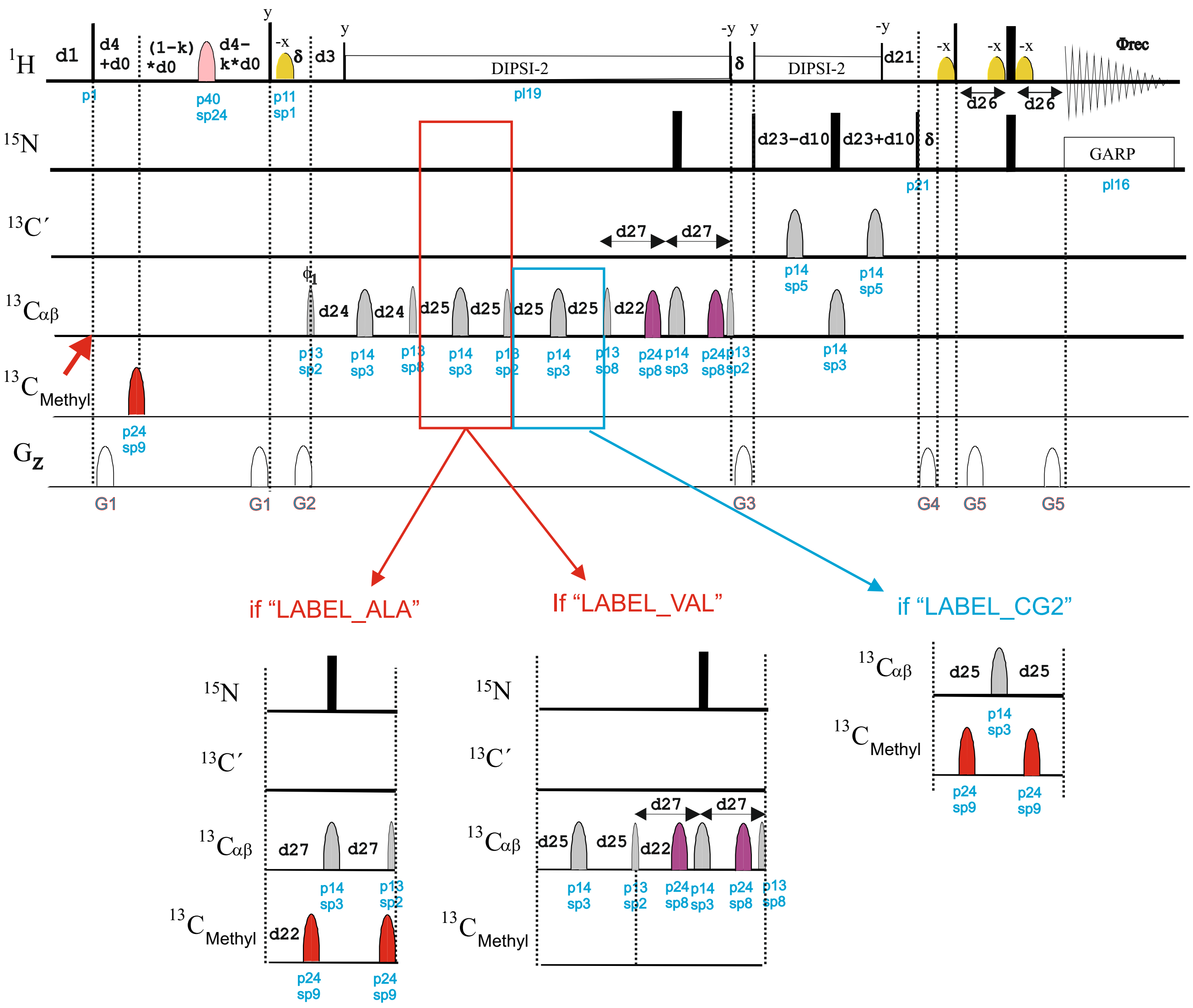


d3 : 1/(6J'(CH))	[1.52 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(8J'(CC))	[2.7 msec]
d23: 1/(4J(NCa)	[12.4 msec]
d24: 1/(4J(CmeC))	[7 msec]
d25: 1/(4J'(CC))	[5 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J'(NCa)	[10.0 msec]

3D Hme(Cme[C]CA)NH



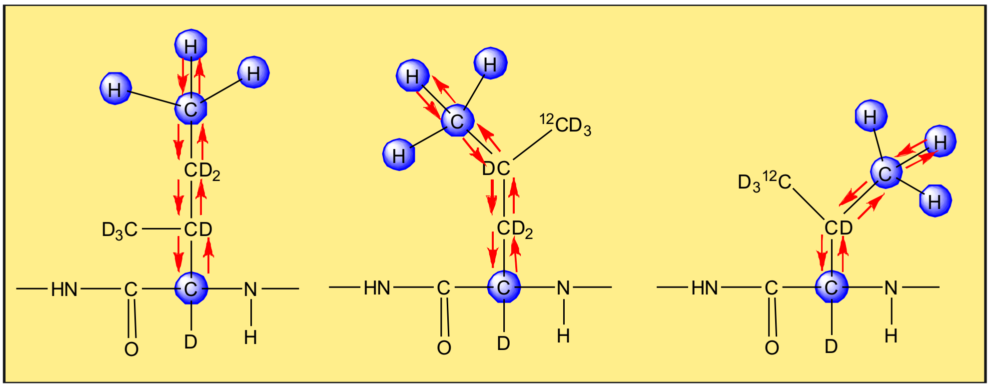
hmcmcbcanhgpwg3d2

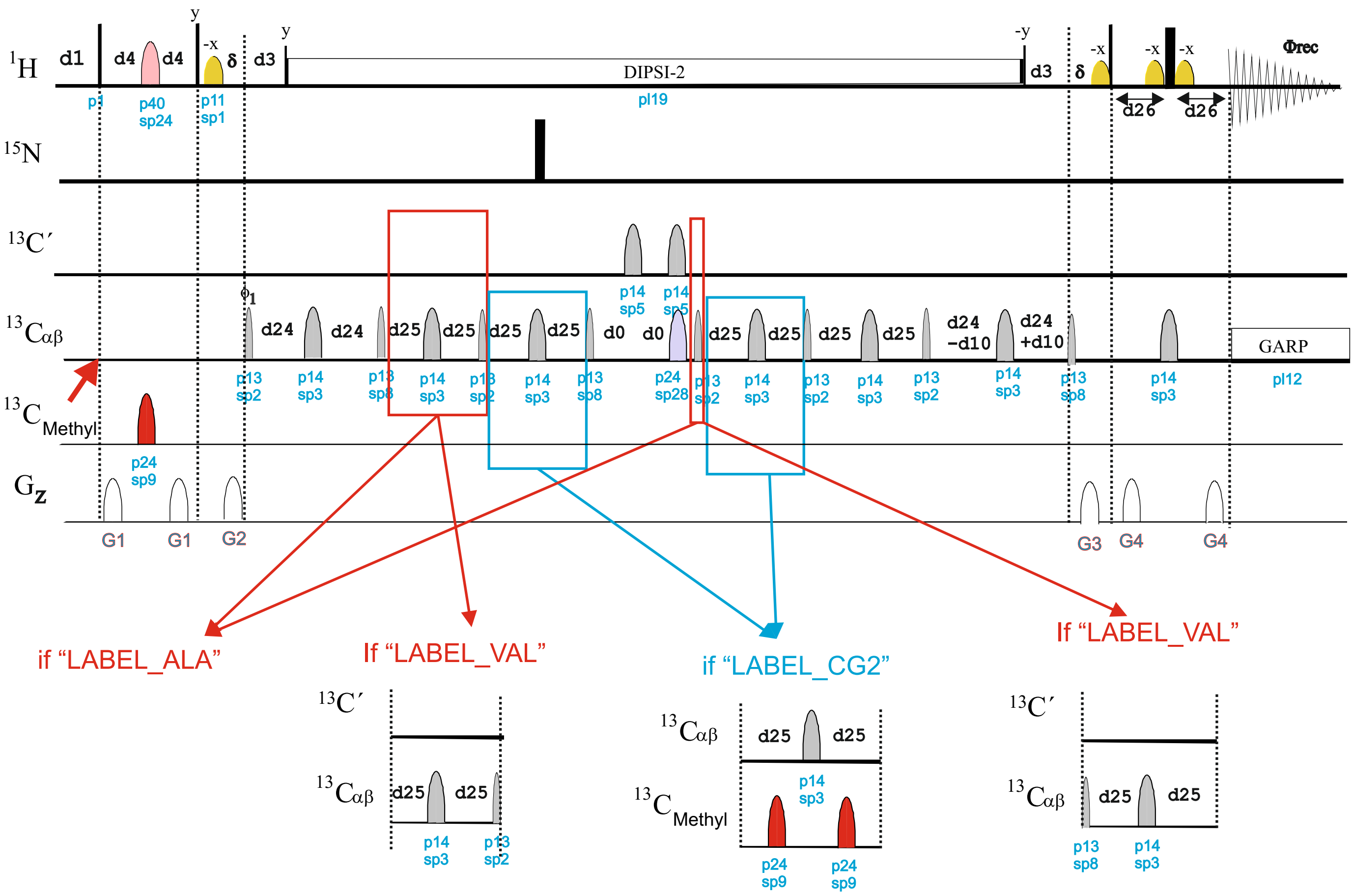


d3 : 1/(6J'(CH))	[1.52 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(8J'(CC))	[2.7 msec]

d23: 1/(4J(NCa)	[12.4 msec]
d24: 1/(4J(CmeC))	[7 msec]
d25: 1/(4J'(CC))	[5 msec]
d26: 1/(4J(NH)	[2.3 msec]
d27: 1/(4J'(NCa)	[10.0 msec]

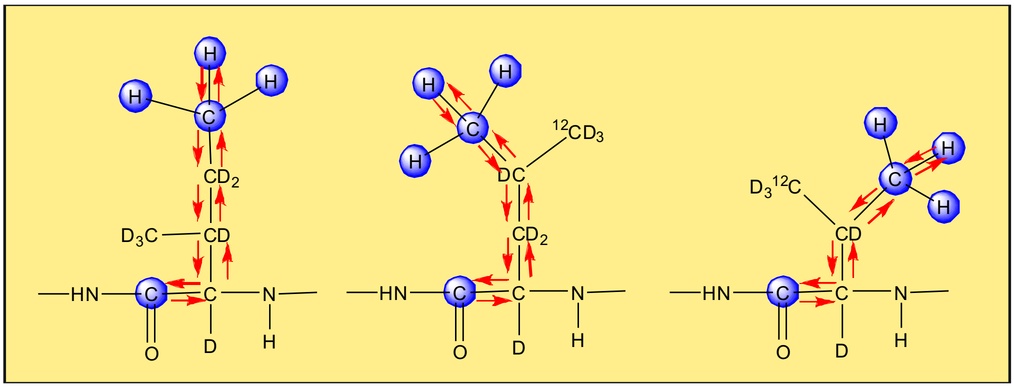
3D (Hme)Cme([C])CA

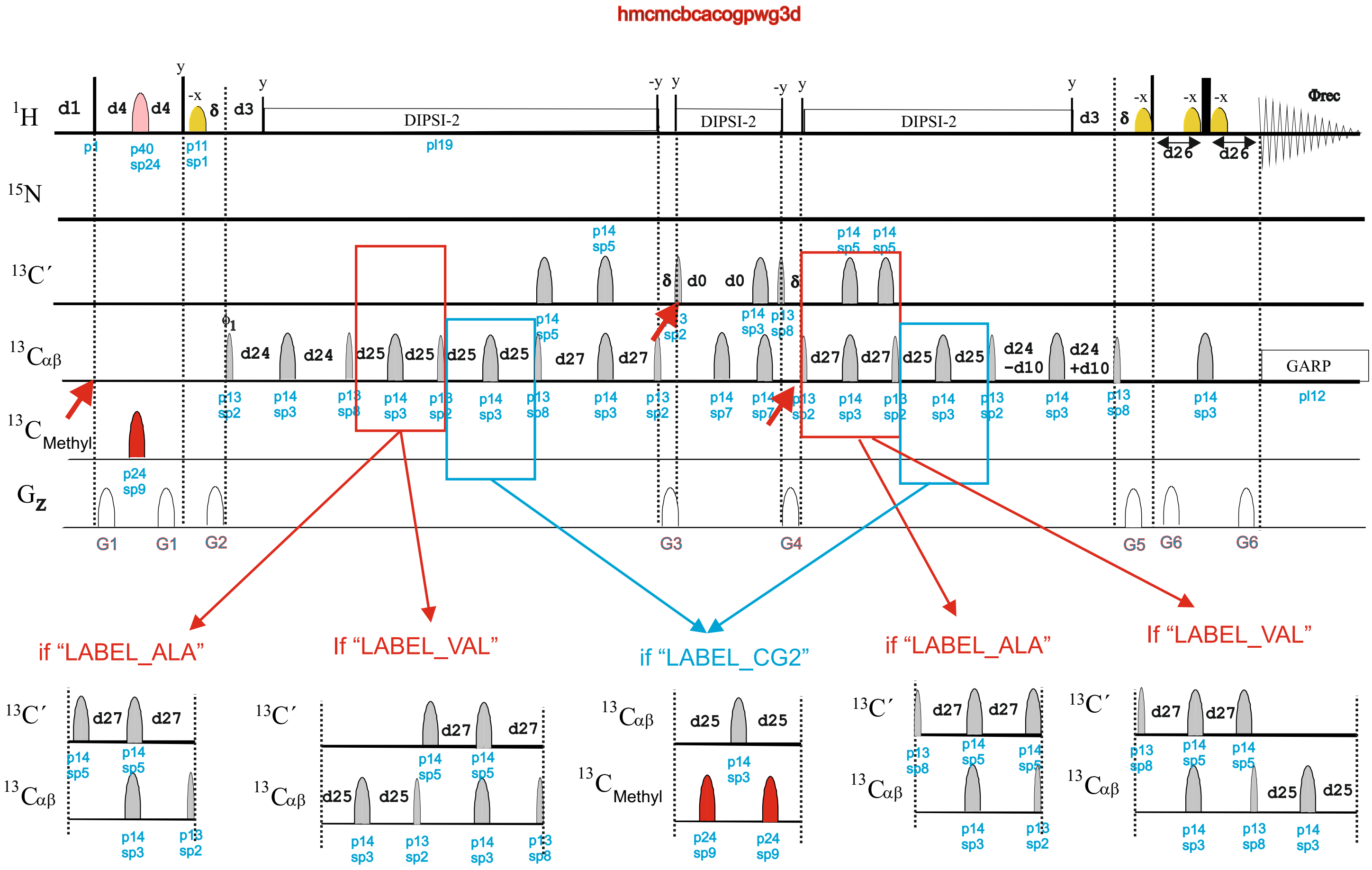




d3 : 1/(6J'(CH))	[1.52 msec]
d4 : 1/(4J(CH))	[1.8 msec]
d24: 1/(4J(CmeC))	[7 msec]
d25: 1/(4J'(CC))	[5 msec]

3D (Hme)Cme([C]CA)CO





d3 : 1/(6J'(CH)) [1.52 msec]
d4 : 1/(4J(CH)) [1.8 msec]
d24: 1/(4J(CmeC)) [7 msec]
d25: 1/(4J'(CC)) [5 msec]
d27: 1/(4J''(CC)), 1/(4J(CaCO)) [4.75 msec]

BRUKER
PULSE PROGRAM
CATALOGUE

NMRGuide

2D & 3D CARBON-DETECTED
EXPERIMENTS

Main Features of carbon-detected experiments

Experiment Description

Shorter pulse sequences.
No need for solvent suppression techniques.
Avoid radiation damping.
Applied in spectra with low dispersion and on samples with low proton density.
Excellent chemical shift dispersion for carbonyl CO nuclei.

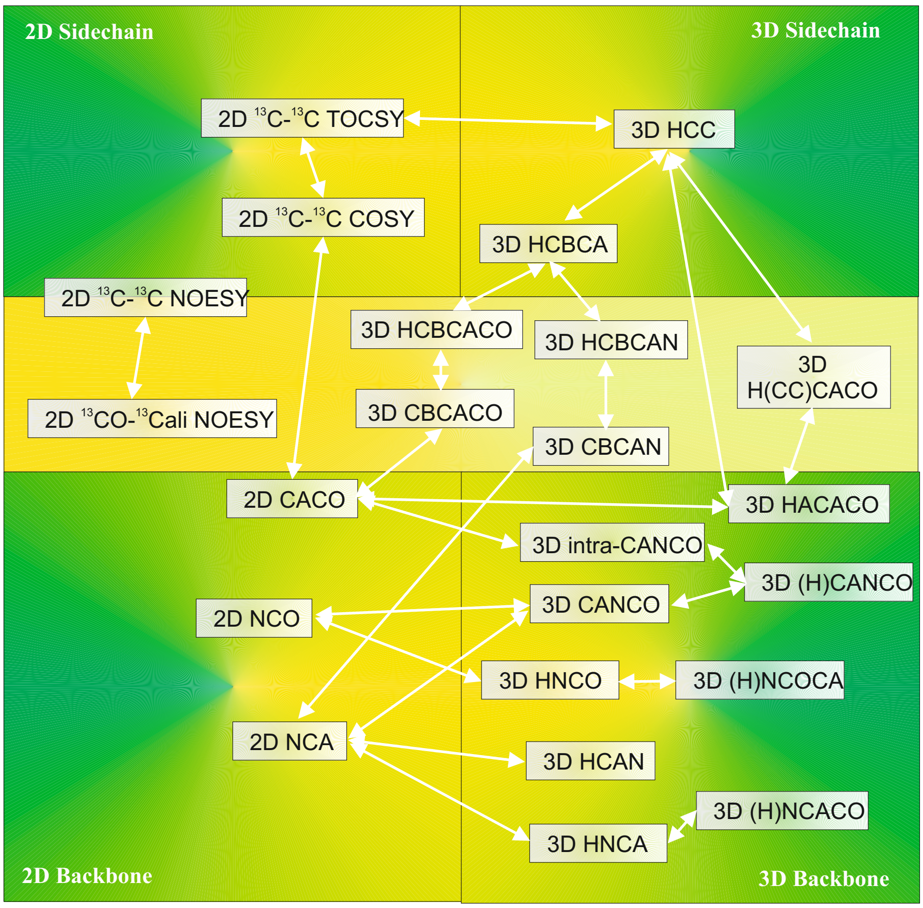
Sample Requirements

Usually applied on doubly-labelled 13C15N-labeled protein. Particular interesting in proteins showing fast relaxation properties such a paramagnetic or very large proteins. Also useful for labeled nucleic acids having low proton densities and low spectral dispersion.

Hardware Requirements

Carbon-detected experiments are best performed on a sensitivity-optimized cryoprobe dedicated for 13C detection but it is not mandatory. In most cases, it is also necessary triple-resonance (1H, 13C, 15N) and z-gradient capabilities.

Carbon-Detected NMR Experiments



Experimental details for carbon-detected experiments

Offsets

1H at 4.7ppm (o2p)
15N at 118ppm (o3p)
13CO at 173ppm (cnst21)
13CA at 55 ppm (cnst22)
13Cali at 39ppm (cnst23)

Decoupling/Mixing

From f2 channel: 1H CPD with 3.0KHz Waltz-16 (pcpd2 at pl12)
From f3 channel: 15N CPD with 1KHz GARP-4 (pcpd3 at pl16)

13C TOCSY with 10KHz FLOPSY-16 (pl10)

Spectral Widths

18-24ppm for CO
42 ppm for 15N
48 ppm for CA
75-80 ppm for Cali

Typical 13C pulses from F1 channel (For 600MHz spectrometer)

p11 sp23: 90° Cali/CO on- resonance (320us (Q5 and Q5tr))
P12 sp24: 180° Cali/CO on-resonance (256us (Q3))
p11 sp25: retro 90° Cali/CO on-resonance (320us (Q5 and Q5tr))
p12 sp26: 180° CO/Cali off-resonance with respect to Cali/CO (256us (Q3))
p12 sp27: 180° CO/CA off-resonance with respect to CA/CO (256us (Q3))
p25 sp28: 180° Selective CA on-resonance (1 ms (Q3))
p12 sp29: 180° Cali off-resonance with respect to CA (256us (Q3))
p30 sp30: Simultaneous 180° CA and CO (symmetrically modulated)

p8 sp13: 180° adiabatic for inversion (500us(Chirp))
p24 sp7: 180° adiabatic for refocusing (2000us(Composite chirp))

Very Important!!: In all pulse programs the syntax

prosol relations=<triple_c>

is included for automated acquisition/set-up using edprosol/getprosol. This file is defined in the following directory:

$TOPSPINHOME/conf/instr/spect/prosol/relations/triple_c

2D Carbon-Detected Experiments

- 2D CC COSY
  - Conventional (**c_cosy**)
  - Constant-time (**c_cosy_ct** / **c_cosy2_ct**)
- 2D CC NOESY
  - Conventional (**c_ccnoesy**)
  - 2D CC NOESY (**c_ccnoesy2**)
  - Constant-time (**c_ccnoesy_ct**)
- 2D CC TOCSY
  - Conventional (**c_ccflopsy16**)
  - With DIPAP for virtual decoupling **(c_ccflopsy16_ia)**
  - Constant-time (**c_ccflopsy16_ct**)
  - Constant-time with DIPAP for virtual decoupling **(c_ccflopsy16_ctia)**
- 2D CACO
  - Using HSQC (**c_caco**)
  - with IPAP for virtual decoupling **(c_caco_ia)**
  - with S3E for virtual decoupling **(c_caco_s3)**
  - Using HMQC (**c_coca_mq** | **c_coca_mq.2**)
- 2D COCA
  - Using HSQC **(c_coca)**
  - with DIPAP for virtual decoupling **(c_coca_ia)**
- 2D CON
  - Using HMQC (**c_con_mq**)
  - Using HSQC (**c_con_sq**)
  - Using HSQC with IPAP for virtual decoupling **(c_con_iasq)**
  - Using HMQC with IPAP for virtual decoupling **(c_con_mqia)**
- 2D CAN
  - Using HMQC (**c_can_mq**)
  - Using HMQC (**c_can_mq.2**)
  - Using HSQC with DIPAP for virtual decoupling **(c_can_iasq)**

3D Carbon-Detected Experiments
For Backbone Assignments

- 3D HCACO
  - (*) With CO detection (**c_hcaco_3d**)
  - With CO detection and with IPAP for virtual decoupling **(c_hcaco_ia3d)**
  - With CO detection and with S3E for virtual decoupling **(c_hcaco_s33d)**
  - With CO detection and using HMQC **(c_hacaco_3d)**
- 3D HCAN
  - (*) With CA detection **(c_hcan_3d)**
  - With CA detection and with DIPAP for virtual decoupling **(c_hcan_ia3d)**
- 3D CANCO
  - (*) With CO detection (**c_canco_3d**)
  - With CO detection and with IPAP for virtual decoupling **(c_canco_ia3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_canco_ia3d.2)**
  - (*) (H)CANCO starting from HA and with CO detection **(c_hcanco_3d)**
  - (H)CANCO starting from HA and with CO detection and with IPAP for virtual decoupling **(c_hcanco_ia3d)**
- 3D intra-CANCO
  - (*) With CO detection **(c_cancoi_3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_cancoi_ia3d)**
  - (*) Intra-(H)CANCO starting from HA and with CO detection **(c_hcancoi_3d)**
  - Intra-(H)CANCO starting from HA and with CO detection and with IPAP for virtual decoupling **(c_hcancoi_ia3d)**
- 3D HNCA
  - (*) With CA detection **(c_hnca_3d)**
  - With CA detection and with DIPAP for virtual decoupling **(c_hnca_ia3d)**
- 3D HNCO
  - (*) With CO detection **(c_hnco_3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_hnco_ia3d)**
- 3D (H)NCACO
  - (*) With CO detection **(c_hncaco_3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_hncaco_ia3d)**
  - With CO detection and with S^3E for virtual decoupling **(c_hncaco_s33d)**
- 3D (H)NCOCA
  - (*) With CA detection **(c_hncoca2_3d)**
  - With CA detection and with DIPAP for virtual decoupling **(c_hncoca2_ia3d)**
  - (*) (H)N(CO)CACO with CO detection **(c_hncoca_3d)**
  - (H)N(CO)CACO with CO detection and with IPAP for virtual decoupling **(c_hncoca_ia3d)**

(*) NOTE: These pulse programs have been moved to pp.dextra directory

3D Carbon-Detected Experiments
For Sidechain Assignments

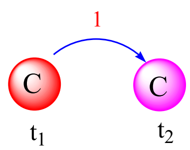
- 3D HCC CT-TOCSY (**c_hccflopsy16_3d**)
- 3D HCBCA
  - (*) With CA detection **(c_hcbca_3d)**
  - With CA detection and with DIPAP for virtual decoupling **(c_hcbca_ia3d)**
- 3D HCB(CA)CO
  - (*) With CO detection **(c_hcbcaco_3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_hcbcaco_ia3d)**
  - With CO detection and with S^3E for virtual decoupling **(c_hcbcaco_s33d)**
- 3D CBCACO
  - (*) With CO detection **(c_cbcaco_3d)**
  - With CO detection and with IPAP for virtual decoupling **(c_cbcaco_ia3d)**
  - With CO detection and with S^3E for virtual decoupling **(c_cbcaco_s33d)**
- 3D CCCO
  - With CO detection and with IPAP for virtual decoupling **(c_ccco_ia3d)**
  - With CO detection and with S^3E for virtual decoupling **(c_ccco_s33d)**
- 3D CBCACON
  - With CO detection and with IPAP for virtual decoupling **(c_cbcacon_ia3d)**
- 3D CCCON
  - With CO detection and with IPAP for virtual decoupling **(c_cccon_ia3d)**
- 3D CBCANCO
  - With CO detection and with IPAP for virtual decoupling **(c_cbcanco_ia3d)**
- 3D (H)CBCAN
  - (*) With CA detection **(c_hcbcan_3d)**
  - With CA detection with DIPAP for virtual decoupling **(c_hcbcan_ia3d)**

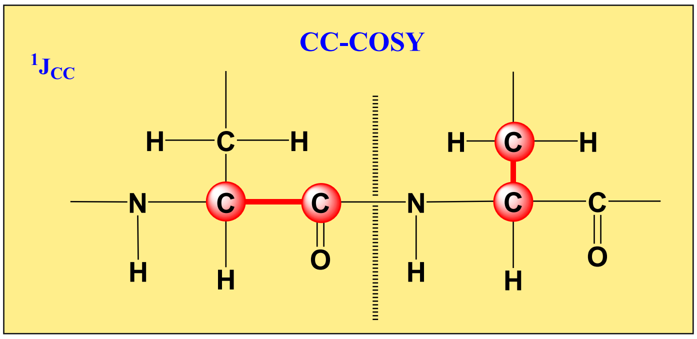
(*) NOTE: These pulse programs have been moved to pp.dextra directory

2D ^{13}C-^{13}C COSY Experiment

Experiment Description

The 2D CC COSY experiment allows to obtain a homonuclear CC correlation mapto trace out through-bond carbon-carbon connectivities in 13C-labeled proteins





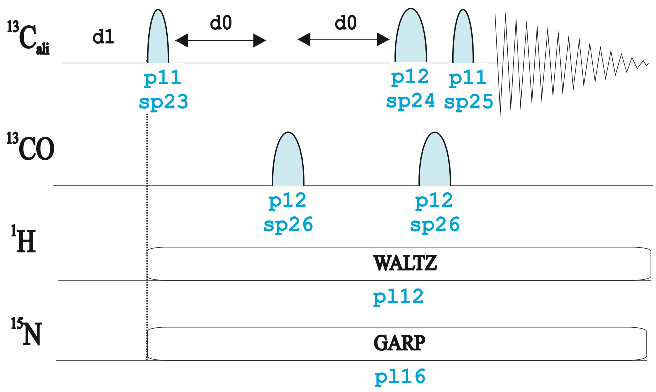
Related Experiments

2D COCA
2D CC and 3D HCC TOCSY

References:

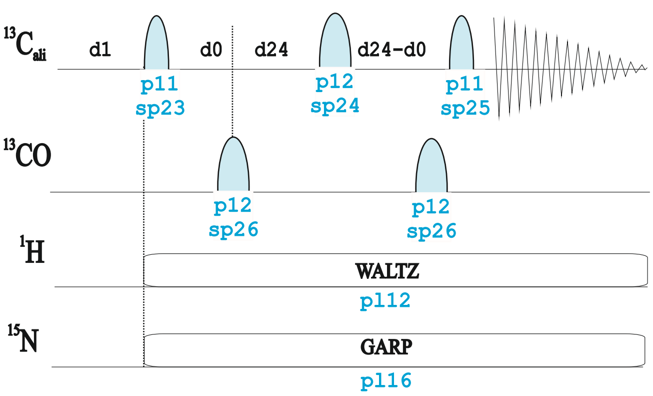
1. T.E. Machonkin, W.M. Westler & J.L Markley, J. Am. Chem. Soc. 124, 3204-3205 (2002)
2. W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Am. Chem. Soc. 125, 16423-16429 (2003)

c_cosy

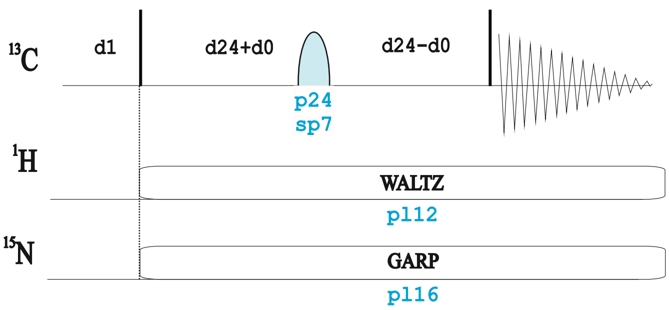


d24=1/4J(CC)=5ms

c_cosy_ct



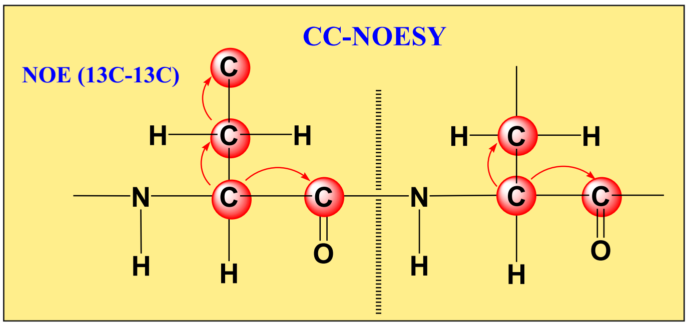
c_cosy2_ct



2D ^{13}C-^{13}C NOESY Experiment

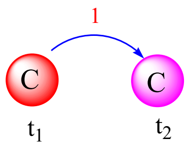
Experiment Description

The 2D CC NOESY experiment allows to obtain a homonuclear CC correlation mapto trace out through-space carbon-carbon interactions in 13C-labeled proteins

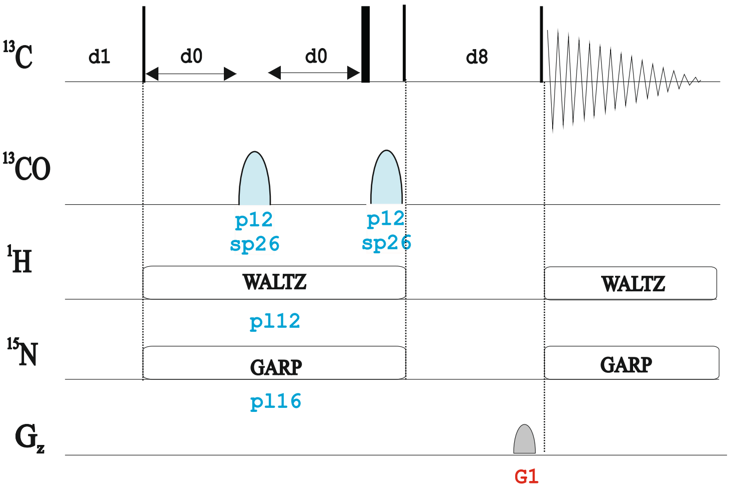


Related Experiments

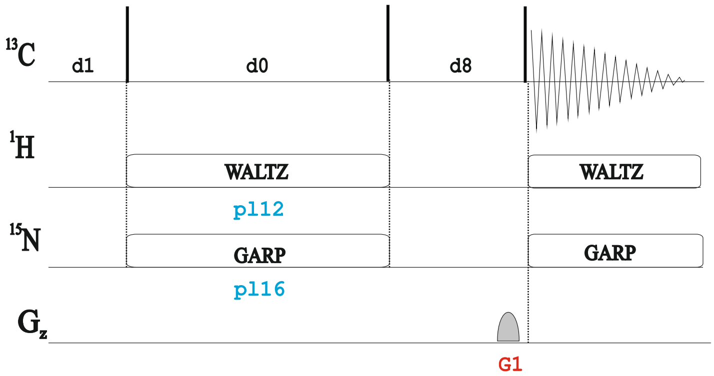
2D CC COSY and 2D CC TOCSY



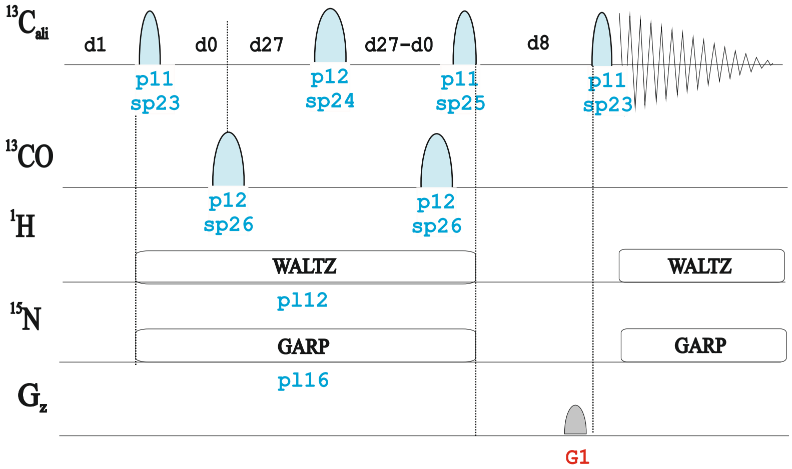
c_ccnoesy



c_ccnoesy2



c_ccnoesy_ct



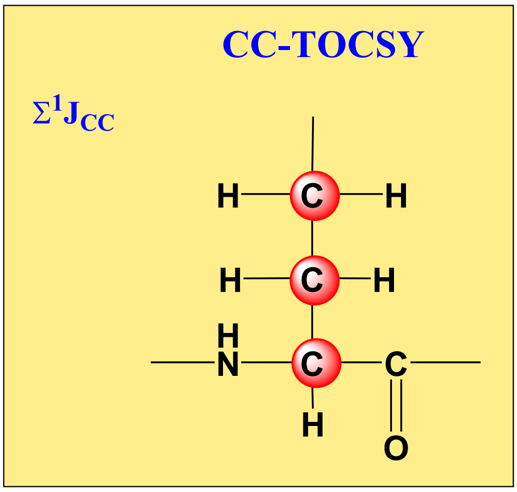
d8=NOE mixing time
d27=1/2J(CACB)=13.3ms

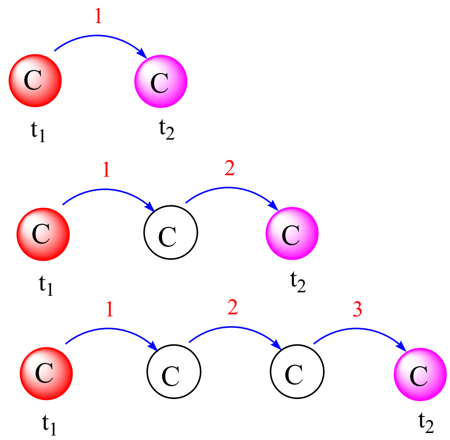
References:
1. W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Am. Chem. Soc. 125, 16423-16429 (2003)
2. I. Bertini, I.C. Felli, R. Kuemmerle, D. Moskau & R. Pierattelli, J. Am. Chem. Soc. 126, 464-465 (2004)

2D ^{13}C-^{13}C TOCSY Experiment

Experiment Description

The 2D CC TOCSY experiment is a 13C-start, 13C-detected TOCSY scheme that allows to trace out through-bond CC connectivities via 1J(CC) in 13C-labeled proteins. Homonuclear CC splitting in the acquisition dimension can be removed by selective homonuclear decoupling during acquisition or virtually using the DIPAP approach (05JMR404).





NMR Spectrum

The experiment provides a 2D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to 1J(CC) coupling.

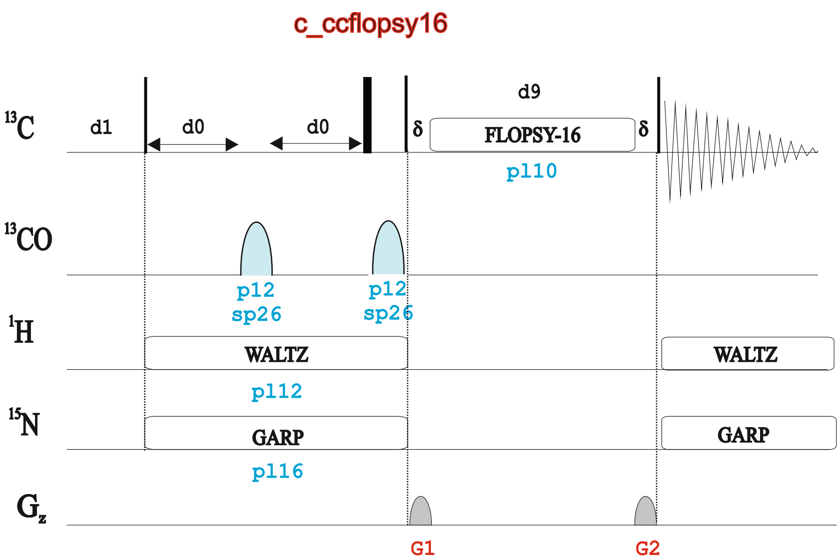
References:

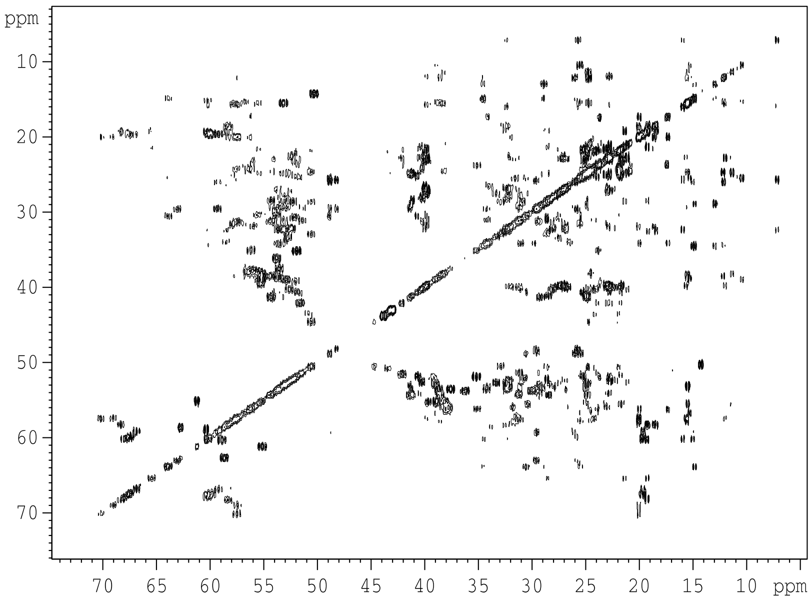
1. A. Eletsky, O.Moreira, H. Kovacs & K. Pervushin, J. Biomol. NMR 26, 167-179 (2003)
2. ;W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)
3. L. Duma, S. Hediger, A. Lesage & L. Emsley, J. Magn. Reson. 164, 187-195 (2003))

Related Experiments

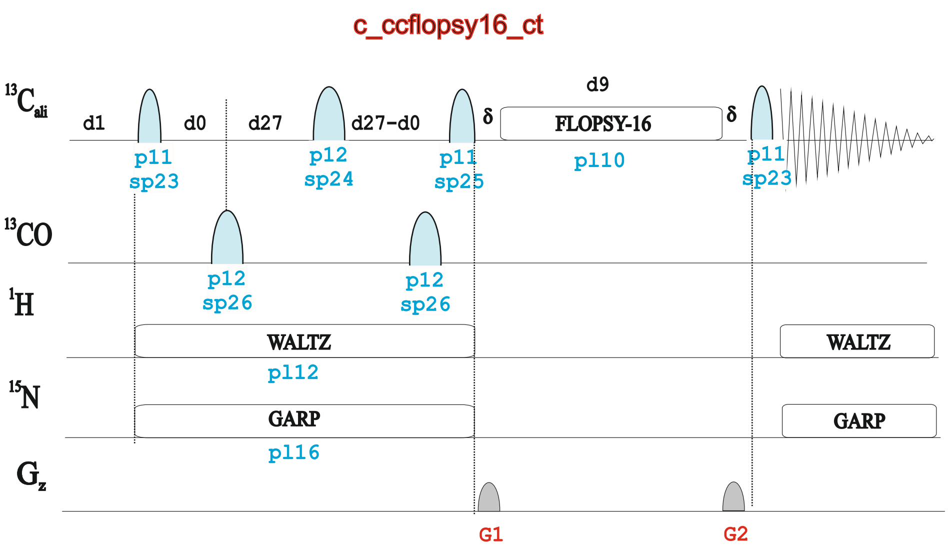
2D CC COSY and 2D CC NOESY
3D carbon-detected HCC TOCSY

3D HCCH-type experiments

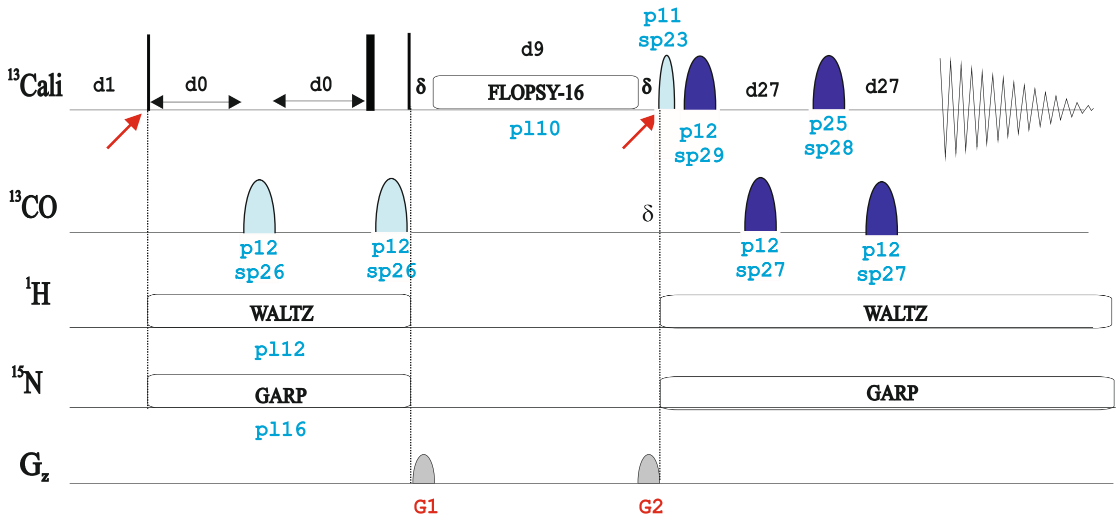




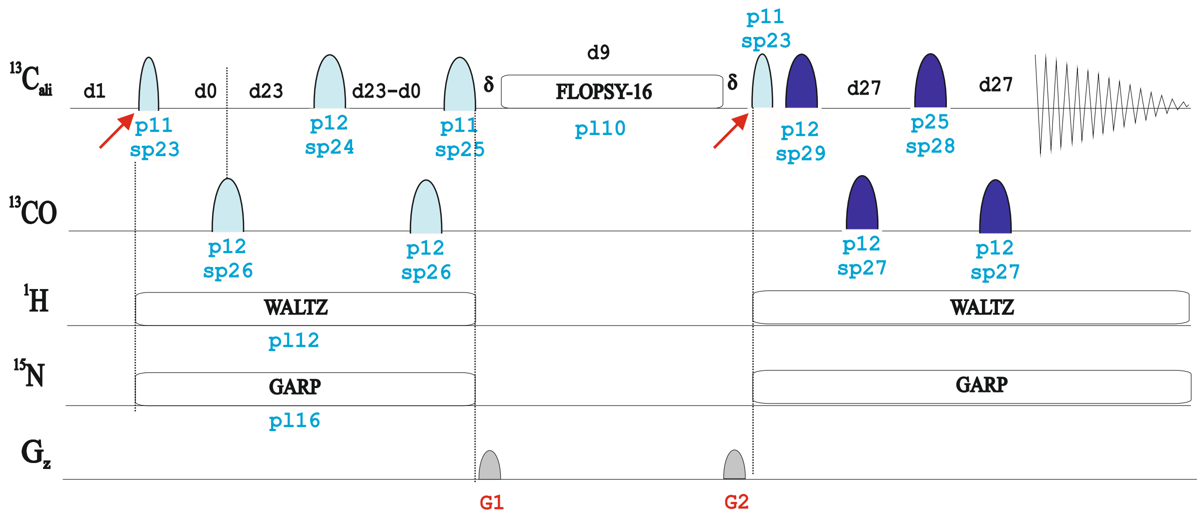
d9=TOCSY mixing time
d27=1/2J(CACB)=13.3ms
or =1/8J(CACB)=3.6ms (DIPAP)
d22=1/4J(COCA)=4.5ms
d23=1/2J(CACB)=13.3ms (DIPAP)



c_ccflopsy16_ia



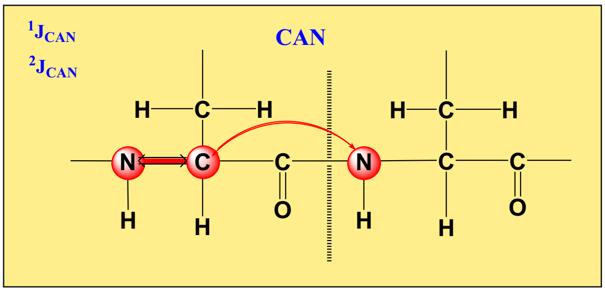
c_ccflopsy16_ctia



2D CAN Experiment

Experiment Description

The 2D CAN experiment is a CA-detected experiment that allows the correlation between the chemical shifts of the CA(i) carbon with the Nitrogen of the same (i) and the next (i+1) residue in doubly-labeled 13C/15N proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



NMR Spectrum

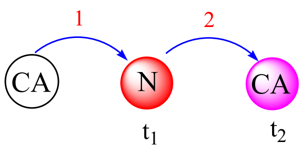
The experiment provides a 2D correlation map in which each CA in the acquisition dimension is correlated to two different N chemical shifts.

Related Experiments

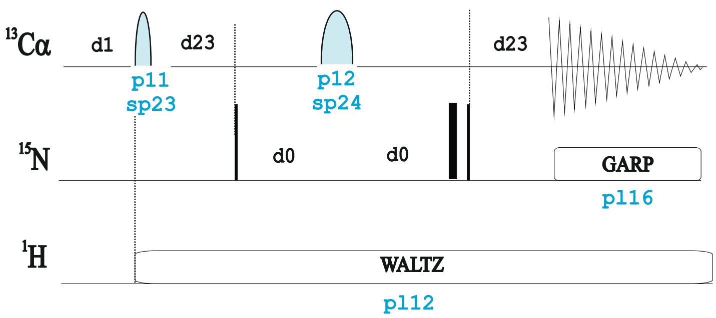
3D HCAN

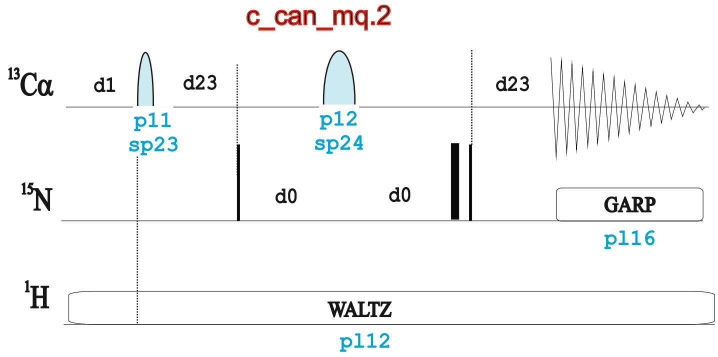
References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli,_ P.R. Vasos, Angew. Chem. Int. Ed 44, 3089-3092 (2005)

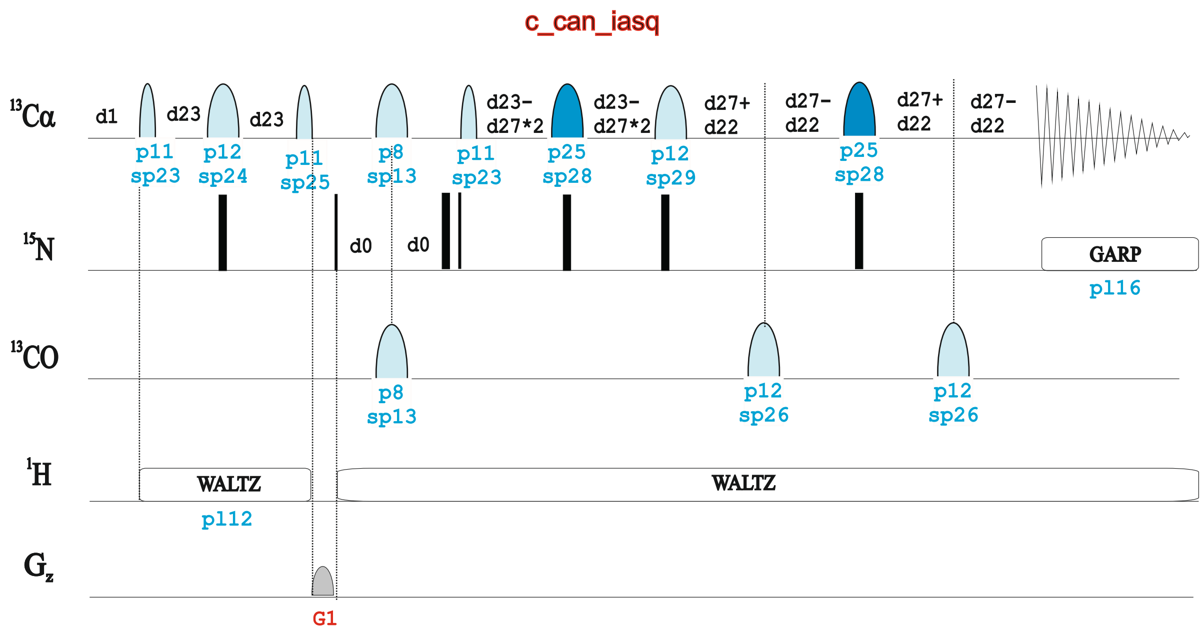


c_can_mq





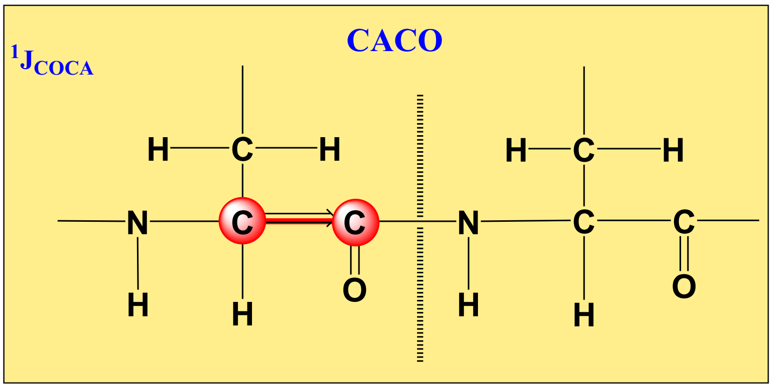
d27=1/8J(CACB)=3.6ms
d22=1/4J(COCA)=4.5ms
d23=1/2J(CAN)=25ms (in mq experiments)
or =1/4J(CAN)=12.4ms (in sq experiments)



2D CACO Experiment

Experiment Description

The 2D CACO experiment is a CO-detected that allows the correlation between the chemical shifts of the CA and CO carbons of the same residue in 13C-labeled proteins.
Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclea decoupling during acquisition or virtually using the IPAP approach (05JMR404).



The CACO experiment can be driven in a out-and-stay way (c_caco) or using a out-and-back transfer (c_coca_mq).

NMR Spectrum

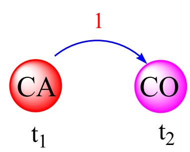
The experiment provides a 2D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to 1J(CACO) coupling

References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

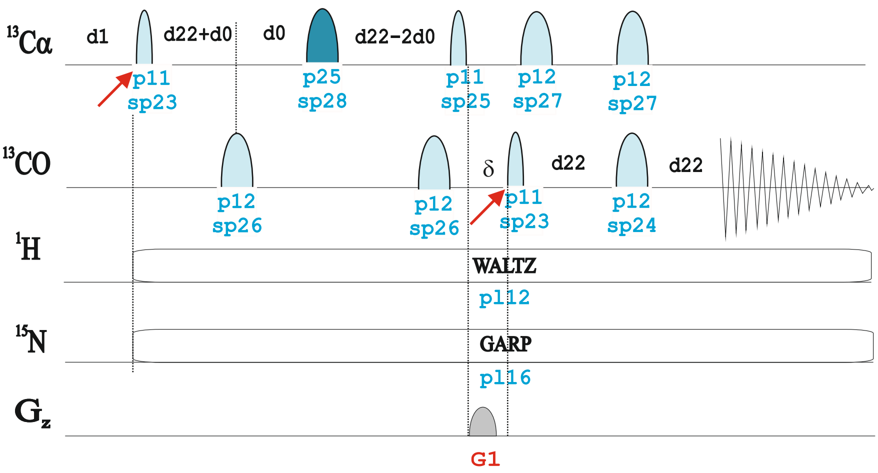
Related Experiments

2D COCA
3D HCACO

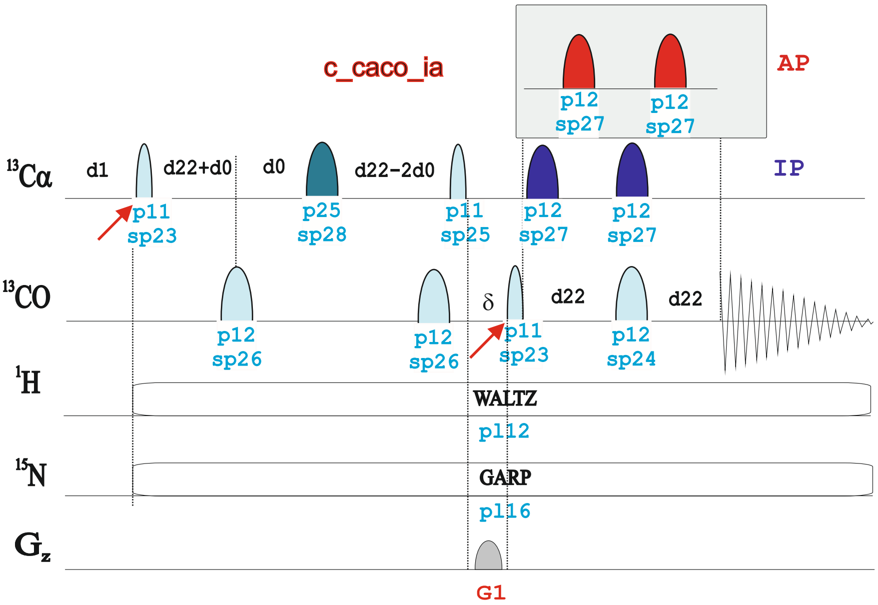


d22=1/4J(COCA)=4.5ms

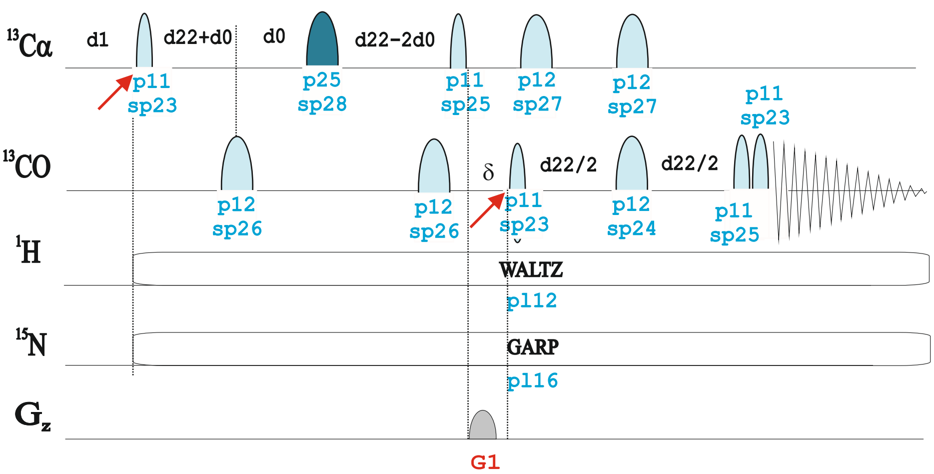
c_caco

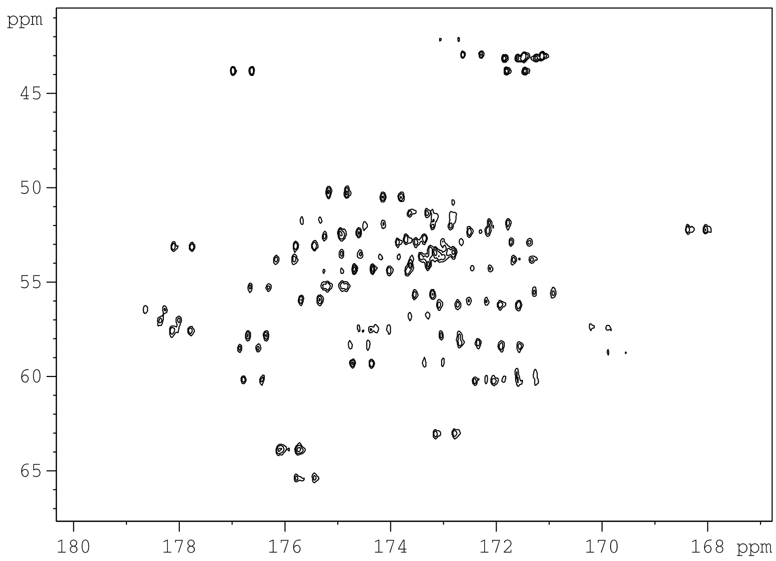


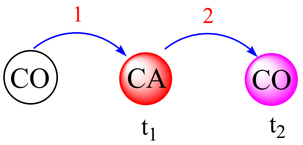
c_caco_ia



c_caco_s3



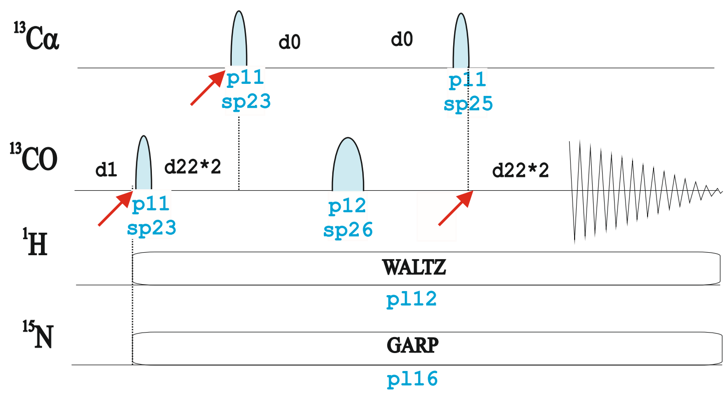




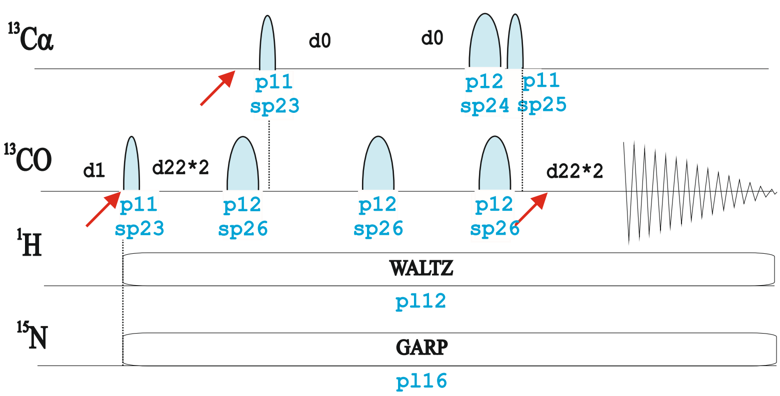
References:

1. M. Kostic, S.S. Pochapsky & T.C. Pochapsky, J. Am. Chem. Soc. 124, 9054-9055 (2002)
2. W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Am. Chem. Soc. 125, 16423-16429 (2003)

c_coca_mq



c_coca_mq.2



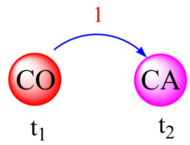
2D COCA Experiment

Experiment Description

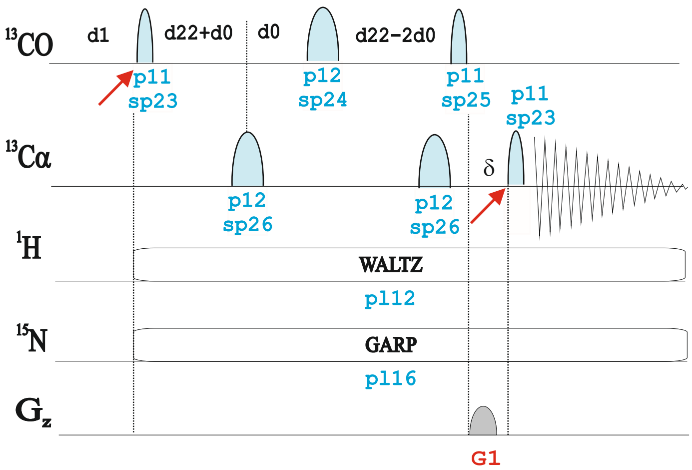
The 2D COCA experiment is the equivalent CA-deteted experiment of the CO-detected CACO experiment

References:

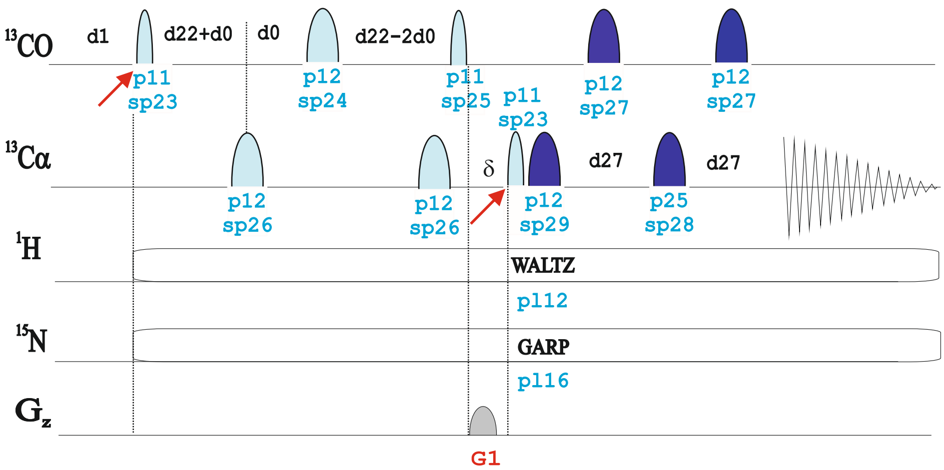
W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)



c_coca



c_coca_ia

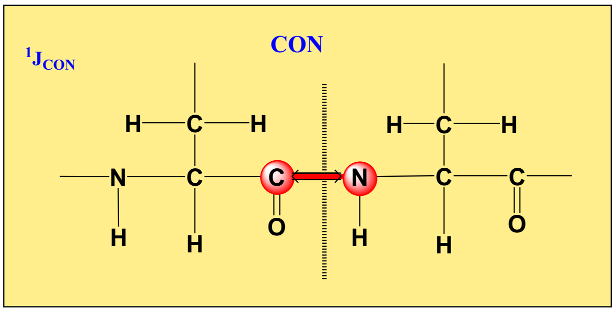


d27=1/8J(CACB)=3.6ms
d22=1/4J(COCA)=4.5ms

2D CON Experiment

Experiment Description

The 2D CON experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the carbonyl CO carbo and the amide N of the next residue in doubly 13C/15N-labeled proteins. Homonuclear CO-CA splitting (55Hz) in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach.



Related Experiments

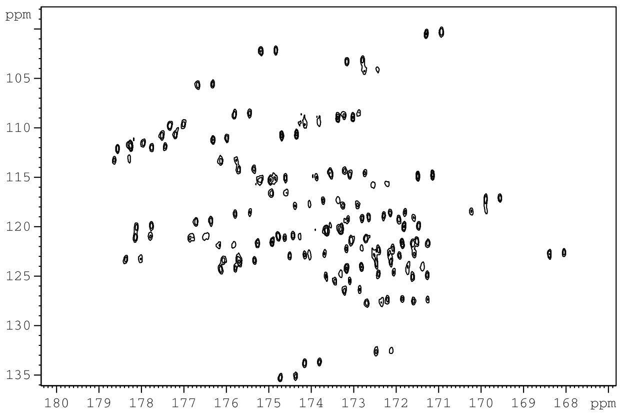
3D HNCO

NMR Spectrum

The experiment provides a 2D correlation map in which each cross-peak corresponds to the CO-N bond connectivity

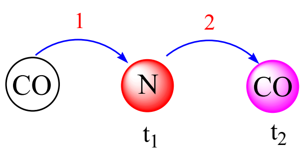
References:

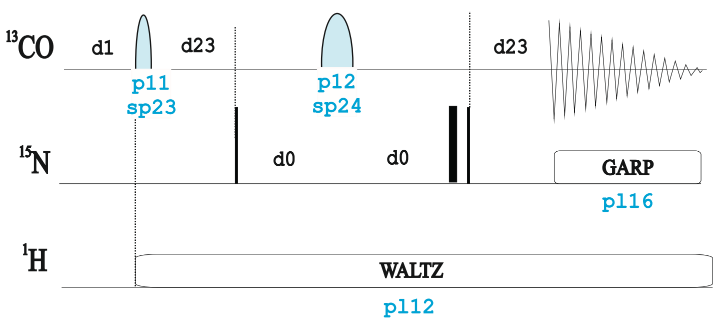
1. M. Kostic, S.S. Pochapsky & T.C. Pochapsky, J. Am. Chem. Soc. 124, 9054-9055 (2002)
2. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005))



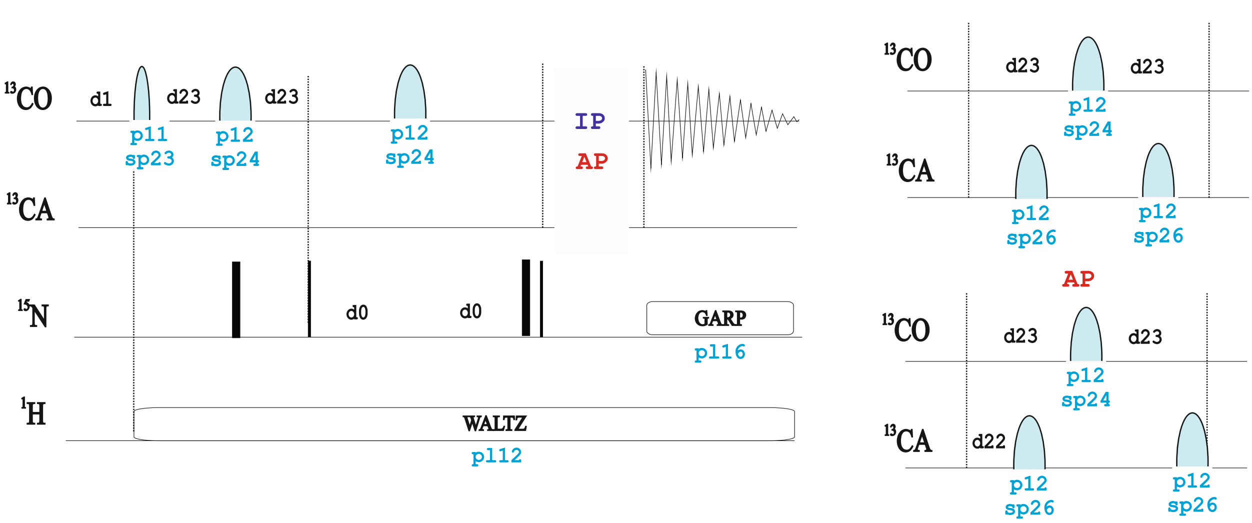
d23=1/2J(NCO)=25ms (in mq experiments)
or =1/4J(NCO)=12.5ms (in sq experiments)
d22=1/4J(COCA)=4.5ms

c_con_mq

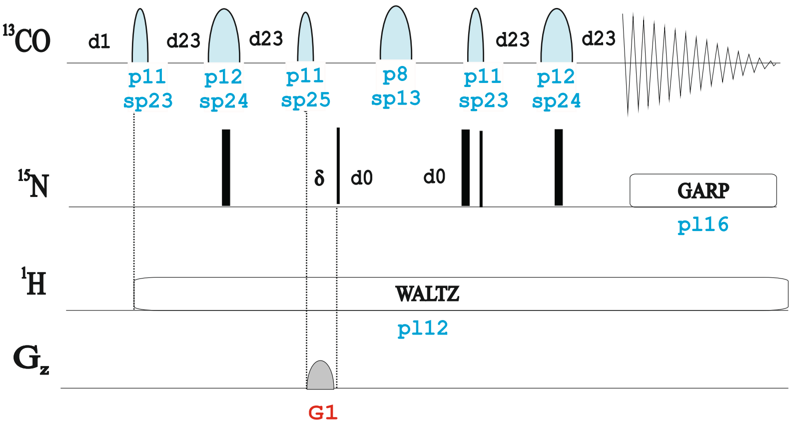




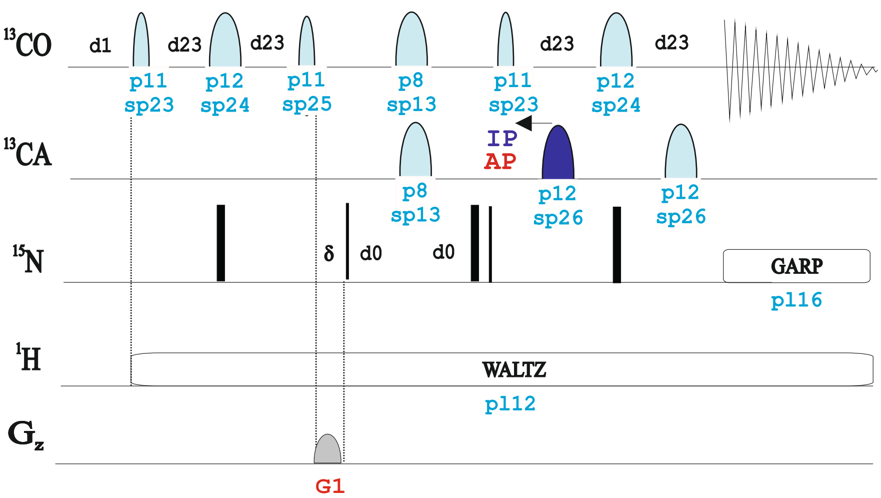
c_con_mqia



c_con_sq



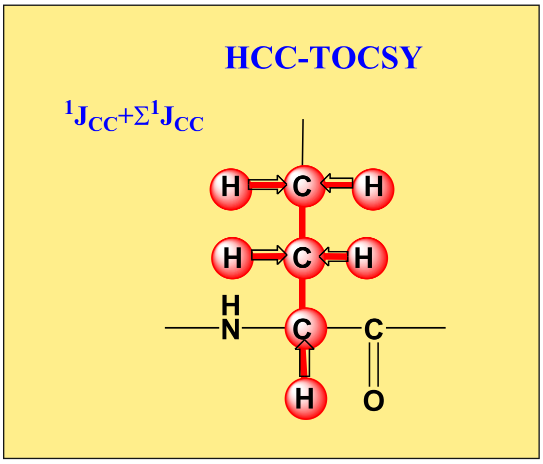
c_con_iasq



3D HCC-TOCSY Experiment

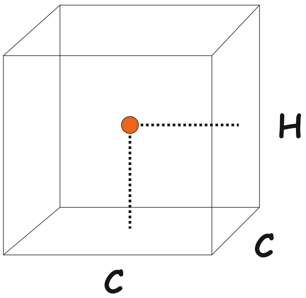
Experiment Description

The 3D HCC-TOCSY experiment is a C-detected experiment that allows the correlation between all sidechain 1H and aliphatic 13C of the same residues in 13C-labeled proteins.



NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak correspond to a HC-C connectivity.

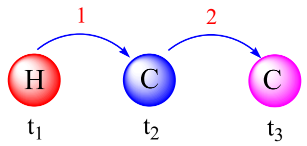


References:

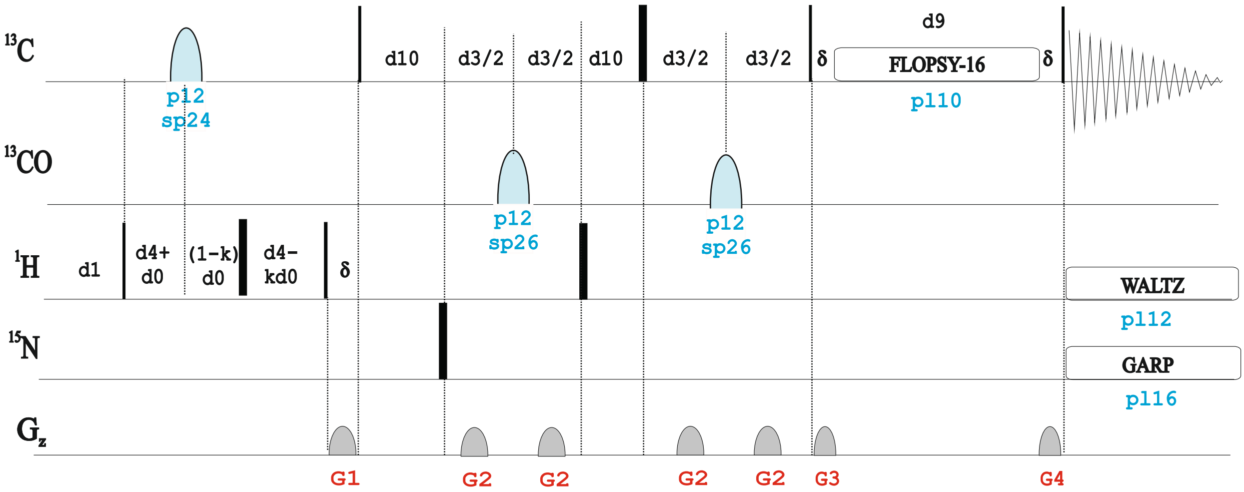
Z. Serber, C. Richter & V. Doetsch, ChemBioChem. 2, 247-251 (2001)

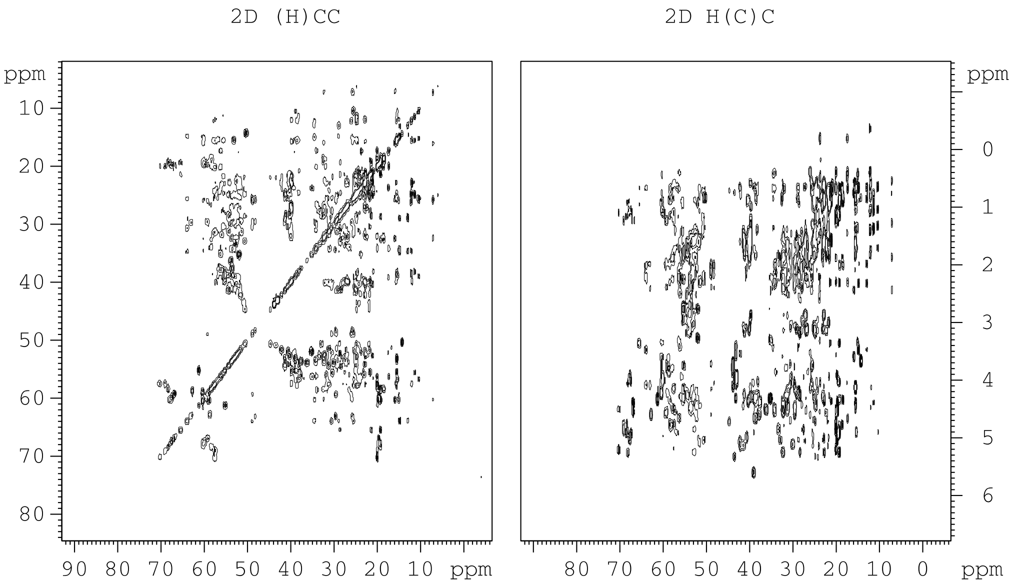
Related Experiments

2D CC COSY and CC-TOCSY experiment



c_hccflopsy16_3d



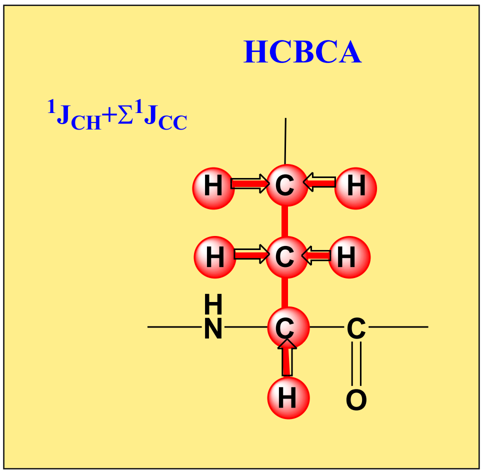


d9 is the TOCSY mixing time
d3=1/6J(CH)=0.95ms
d4=1/4J(CH)=1.8ms

3D HCBCA Experiment

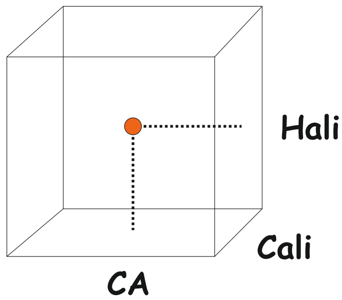
Experiment Description

The 3D HCBCA experiment is a carbon-detected experiment that allows to obtain the sidechain H, CB and CA connectivities in 13C-labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).



NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to 1J(CACO) coupling

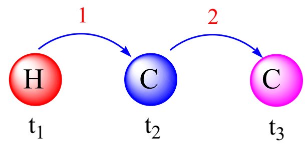


References:

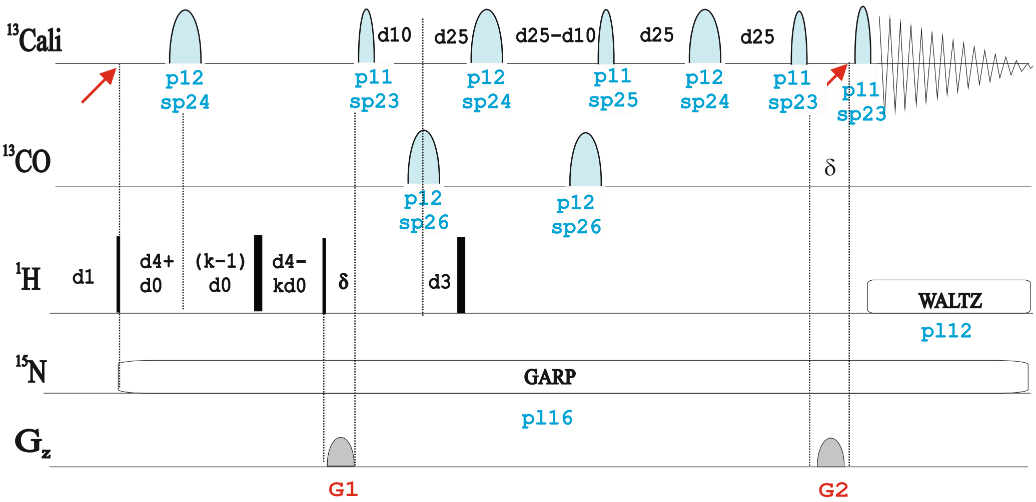
1. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)
2. L. Duma, S. Hediger, A. Lesage & L. Emsley, J. Magn. Reson. 164, 187-195 (2003)

Related Experiments

2D CC TOCSY
3D HCC TOCSY

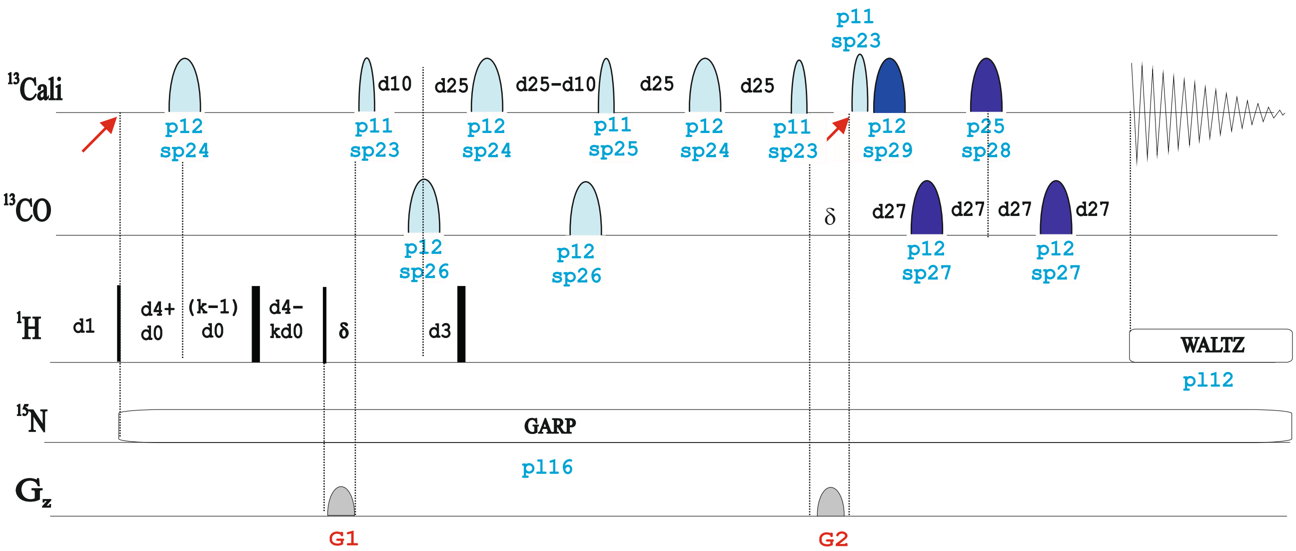


c_hcbca_3d



d25=1/8J(CACB)=4.0ms
d22=1/4J(COCA)=4.5ms
d27=1/4J(CACB)=7.2ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

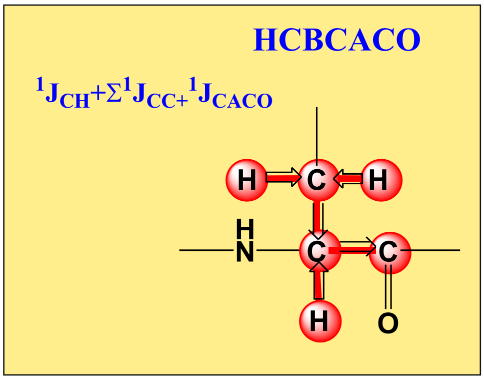
c_hcbca_ia3d



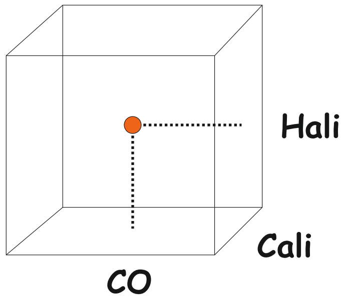
3D HCBCACO Experiment

Experiment Description

The 3D HCBCACO experiment is a CO-detected that allows the correlation between the chemical shifts of the sidechain protons and the CB, CA and CO carbons of the same residue in 13C-labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach.



NMR Spectrum

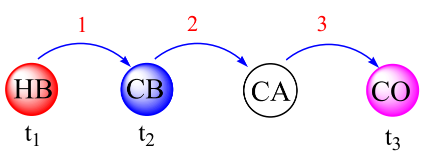


References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

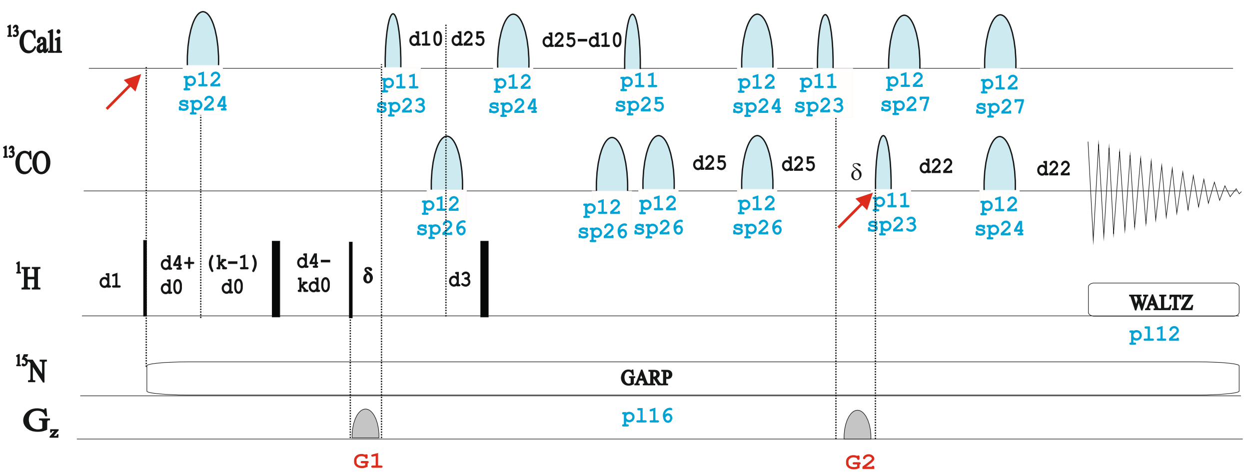
Related Experiments

2D CC TOCSY
3D HCC TOCSY and HCBCA experiments

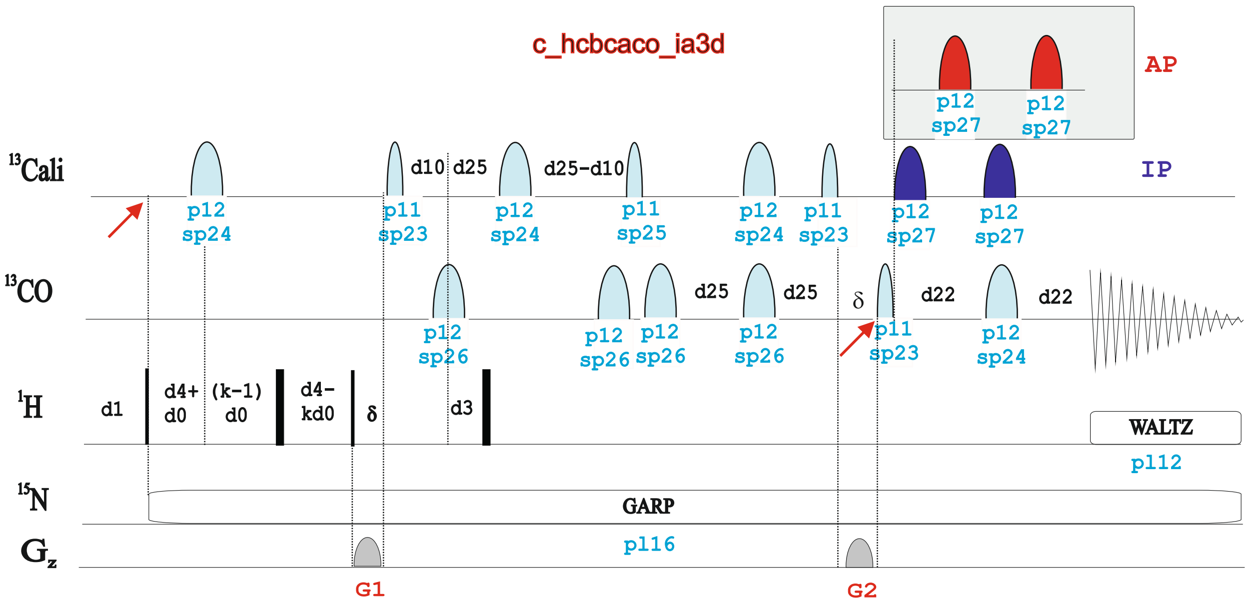


d25=1/8J(CACB)=4.0ms
d22=1/4J(COCA)=4.5ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

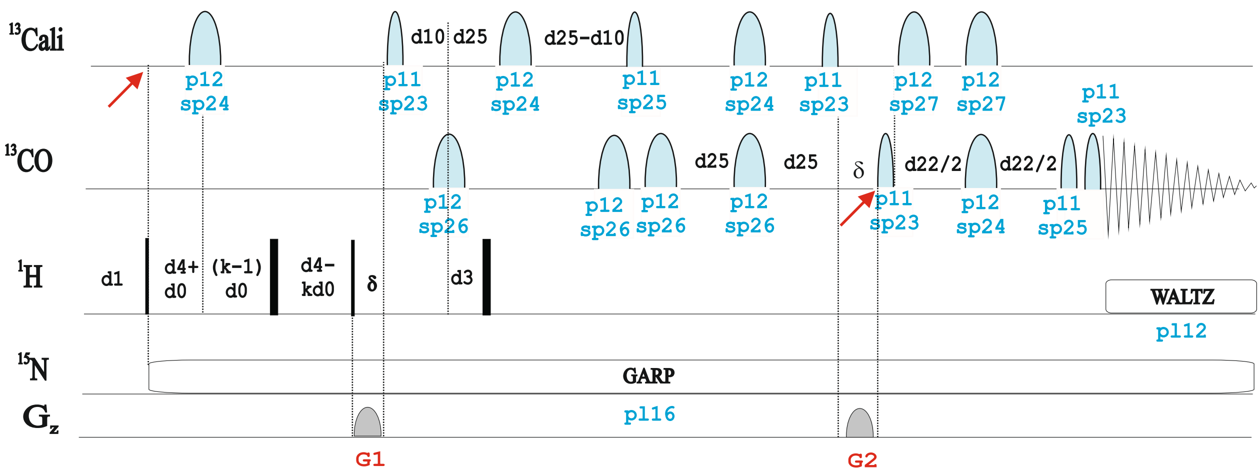
c_hcbcaco_3d



c_hcbcaco_ia3d



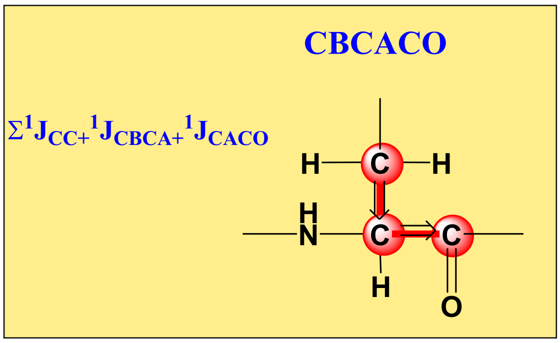
c_hcbcaco_s33d



3D CBCACO Experiment

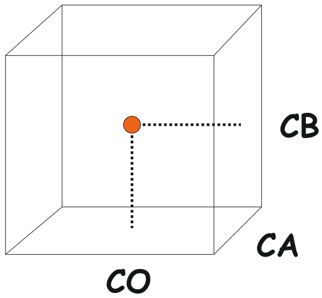
Experiment Description

The 3D CBCACO experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the sidechain CB, CA and CO carbons of the same residue in 13C-labele proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404)



NMR Spectrum

The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to 1J(CACO) coupling

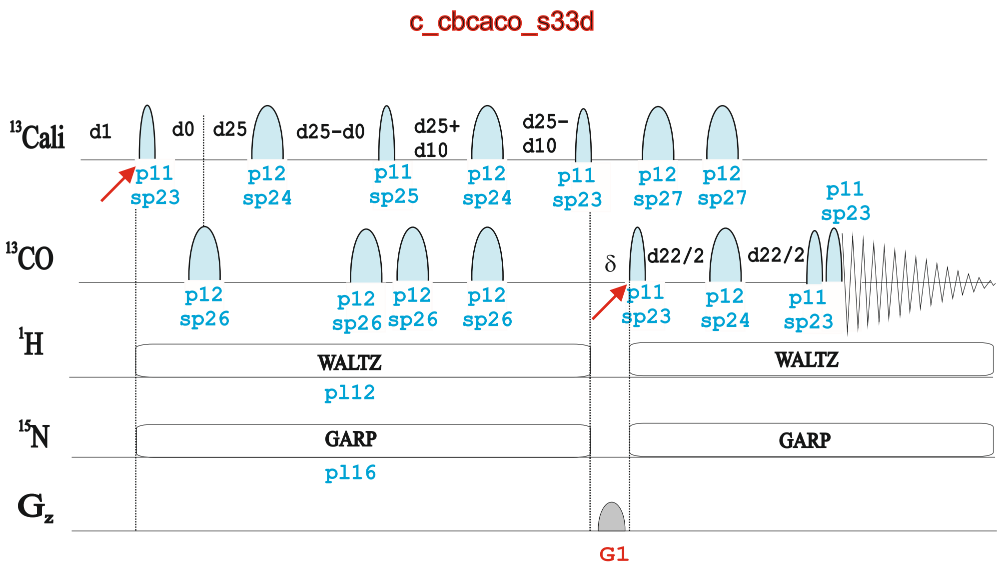


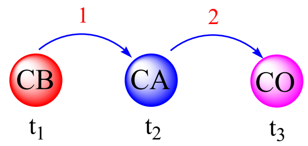
References:

W. Bermel, I. Bertini, L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, & P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

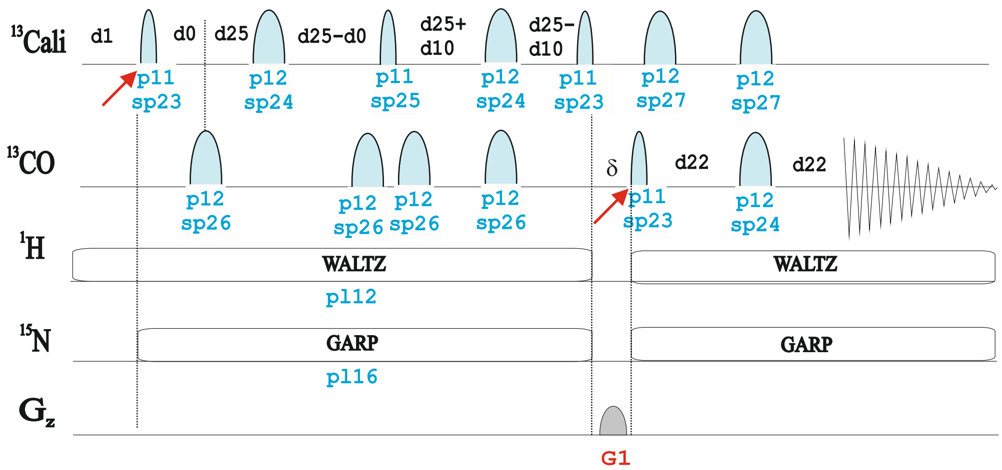
Related Experiments

2D CC COSY and TOCSY
2D CACO
3D HCACO



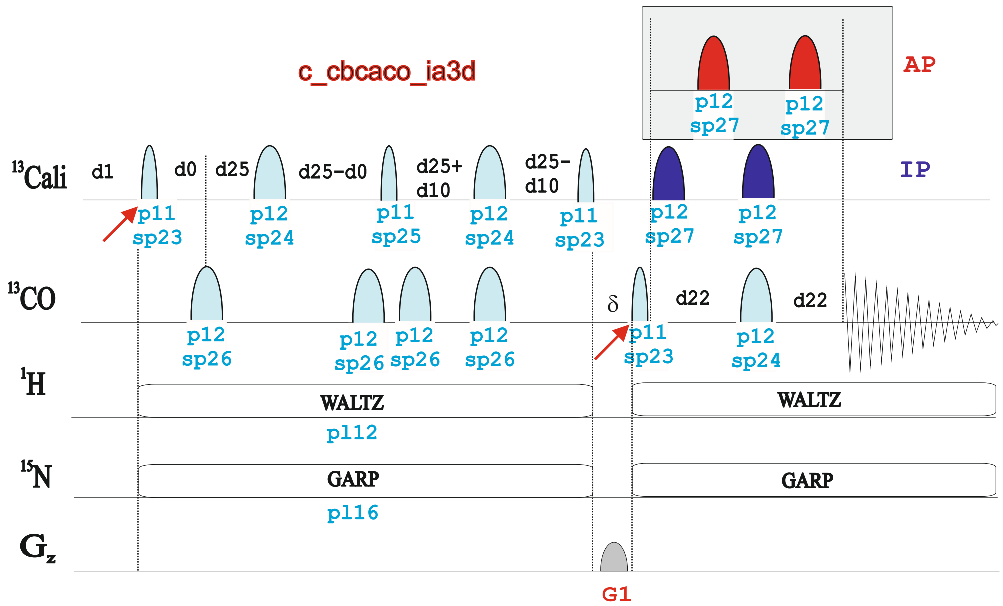


c_cbcaco_3d

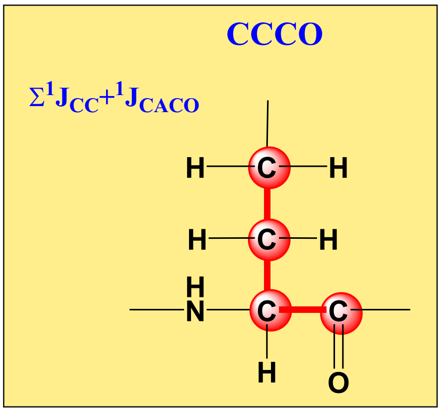


d22=1/4J(COCA)=4.5ms
d25=1/8J(CACB)=5.0ms

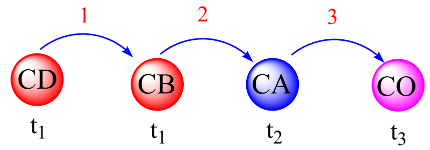
c_cbcaco_ia3d



3D CCCO Experiment

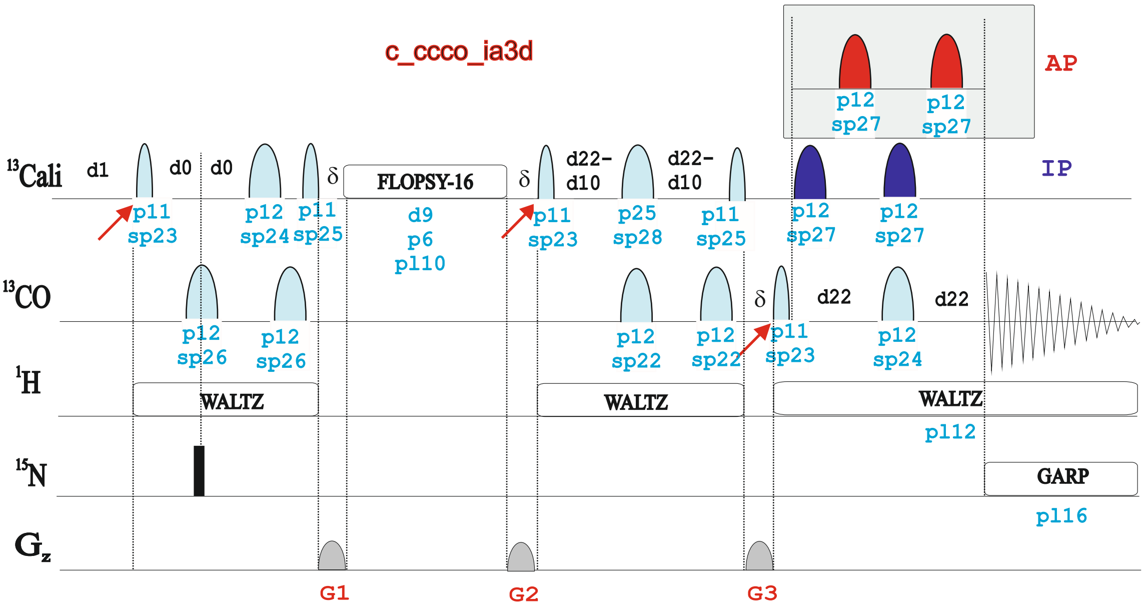


W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006)

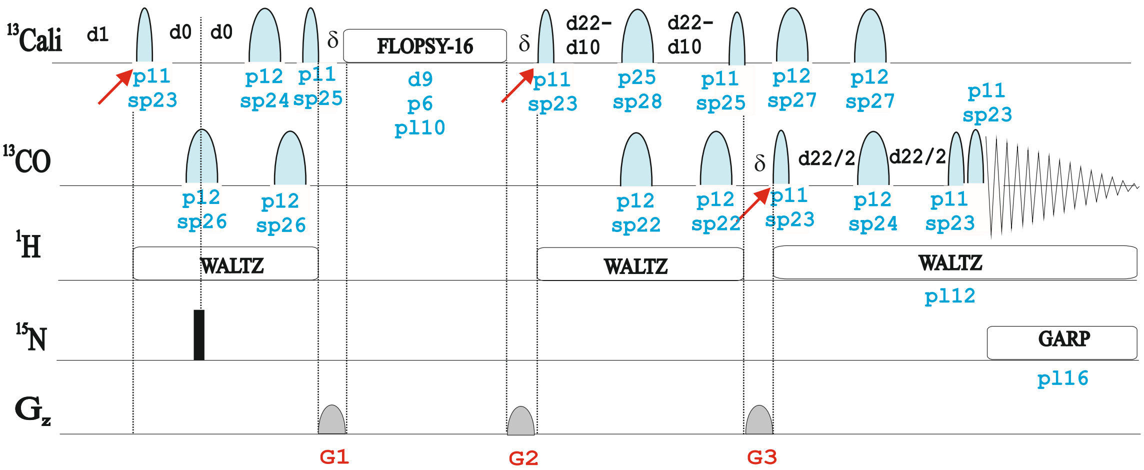


d22: 1/(4J(COCa)) [4.5 msec]

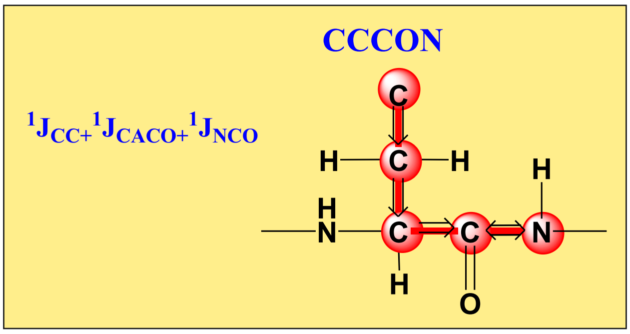
c_ccco_ia3d



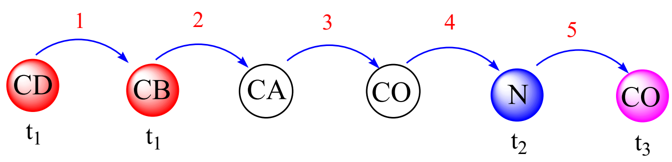
c_ccco_s33d

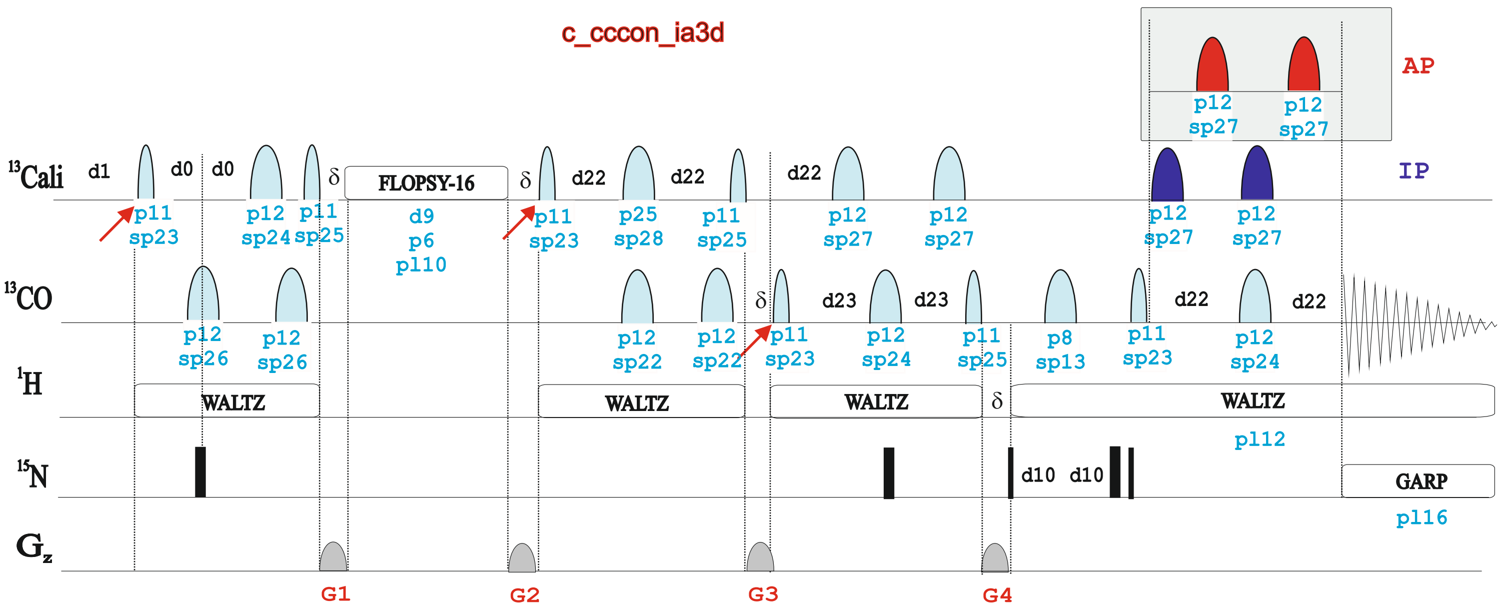


3D CCCON Experiment



W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006)





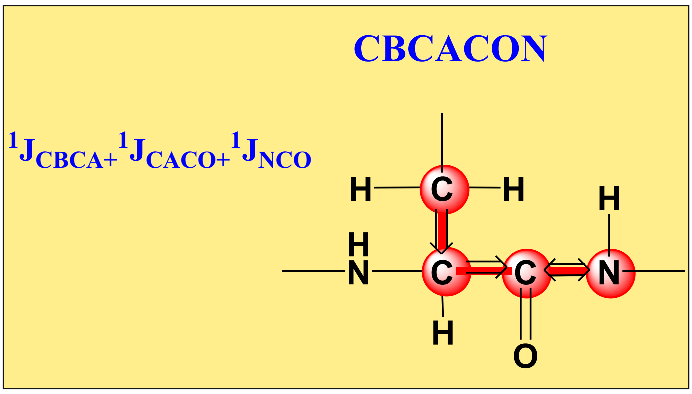
d22: 1/(4J(COCa)) [4.5 msec]
d23: 1/(4J(NCO)) [12.5 msec]
d9 : TOCSY mixing time [12 msec]

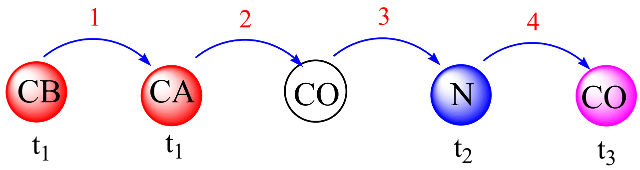
3D CBCACON Experiment

Experiment Description

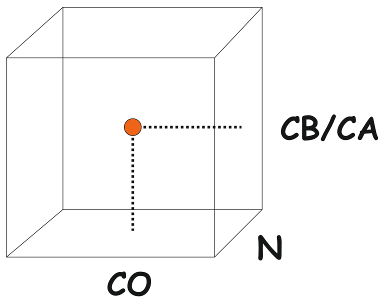
The 3D CBCACON experiment is a CO-detected experiment that allows to assign intra-residue CA, CB, CO and N chemical shifts in doubly-labeled 13C/15N proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach.

W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006)

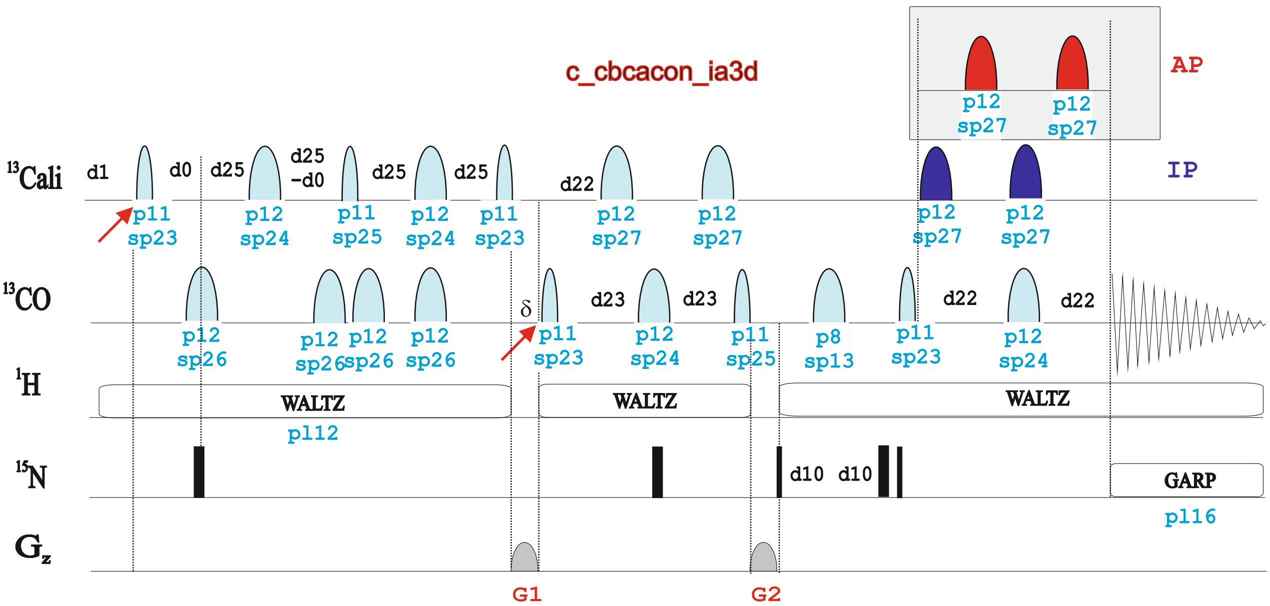




NMR Spectrum



d22=1/4J(COCA)=4.5ms
d23=1/4J(CON)=12.5ms
d25=1/8J(CACB)=5.0ms



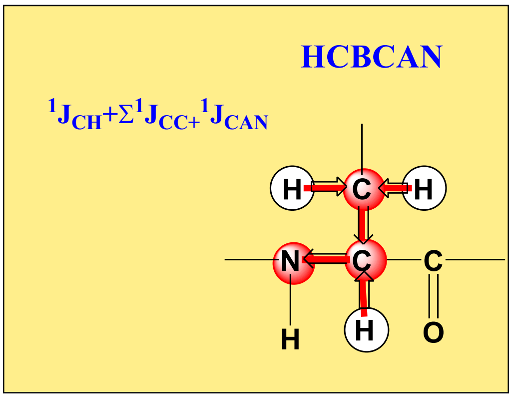
3D (H)CBCAN Experiment

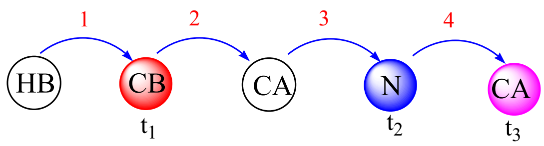
Experiment Description

The 3D (H)CBCAN experiment is a CA-detected experiment that allows to assign intra-residue CA, CB and N chemical shifts in doubly-labeled 13C/15N proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach.

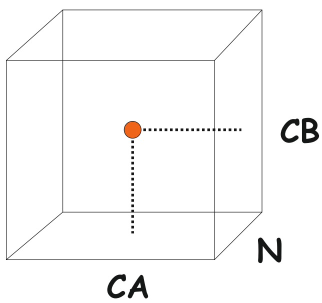
References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)





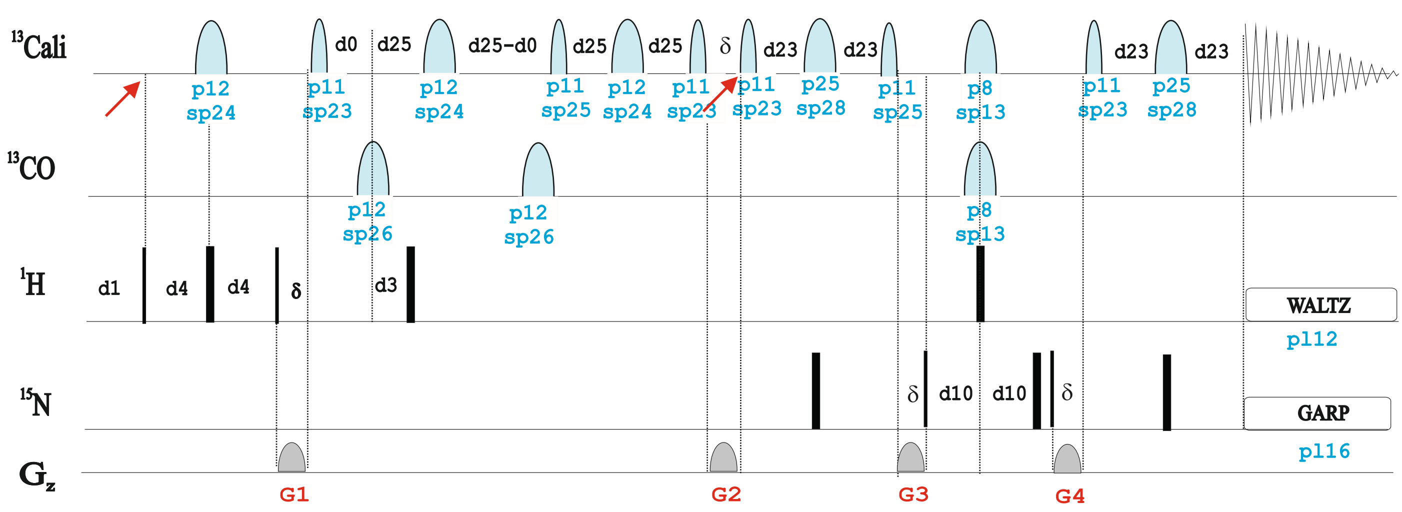
NMR Spectrum



Related Experiments

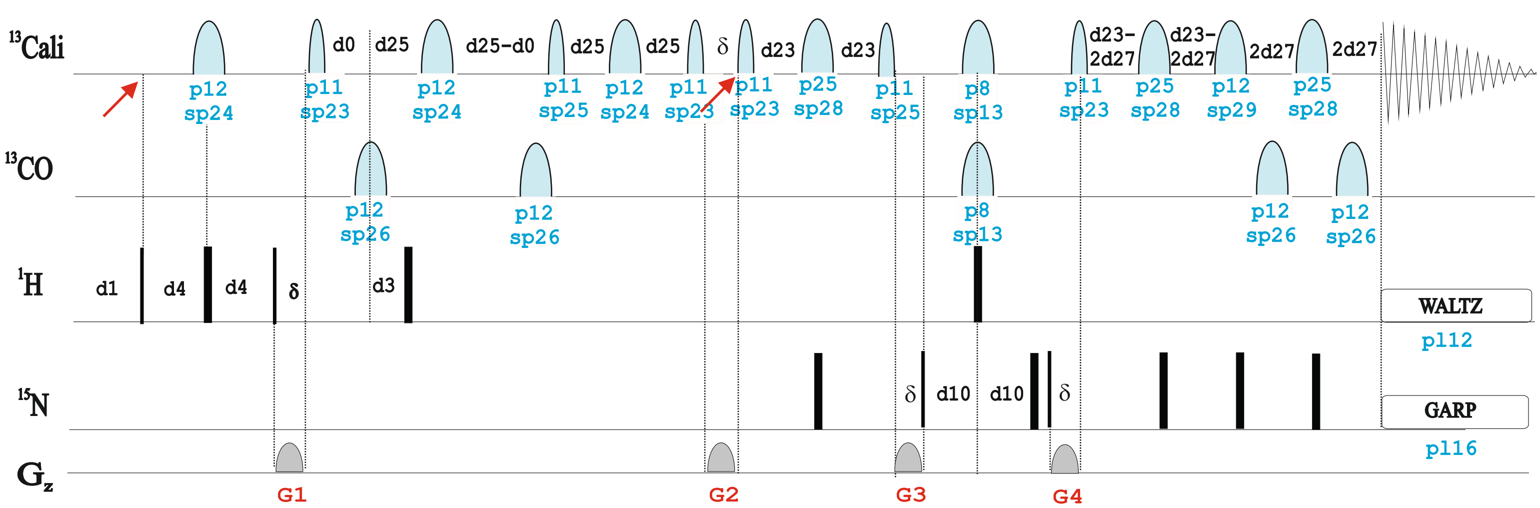
3D HCC TOCSY

c_hcbcan_3d



d22=1/4J(COCA)=4.5ms
d25=1/8J(CACB)=4.0ms
d23=1/4J(NCA)=12.4ms
d27=1/8(CACB)=3.6ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

c_hcbcan_ia3d



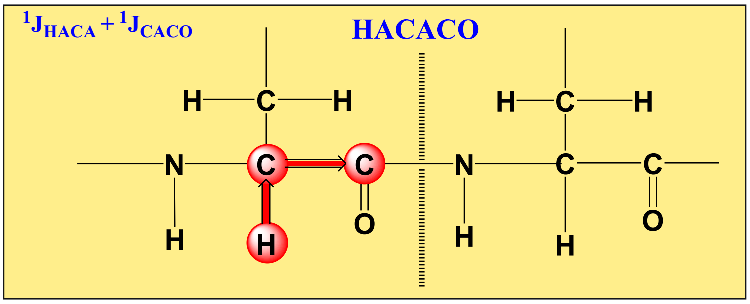
3D CO-Detected HCACO Experiment

Experiment Description

The 3D HCACO experiment is a CO-detected experiment that allows the correlation between the chemical shifts of the CA and CO carbons of the same residue in 13C-labeled proteins. Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach (05JMR404).

Related Experiments

2D COCA
3D HA-detected HCACO



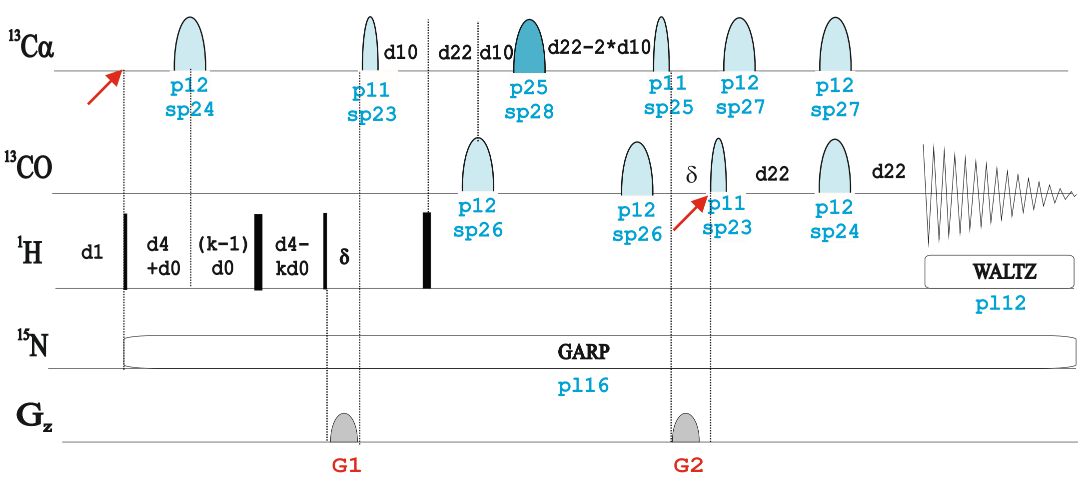
NMR Spectrum

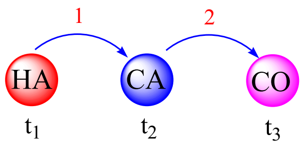
The experiment provides a 3D correlation map in which each cross-peak displays a doublet in the acquisition dimension due to 1J(CACO) coupling.

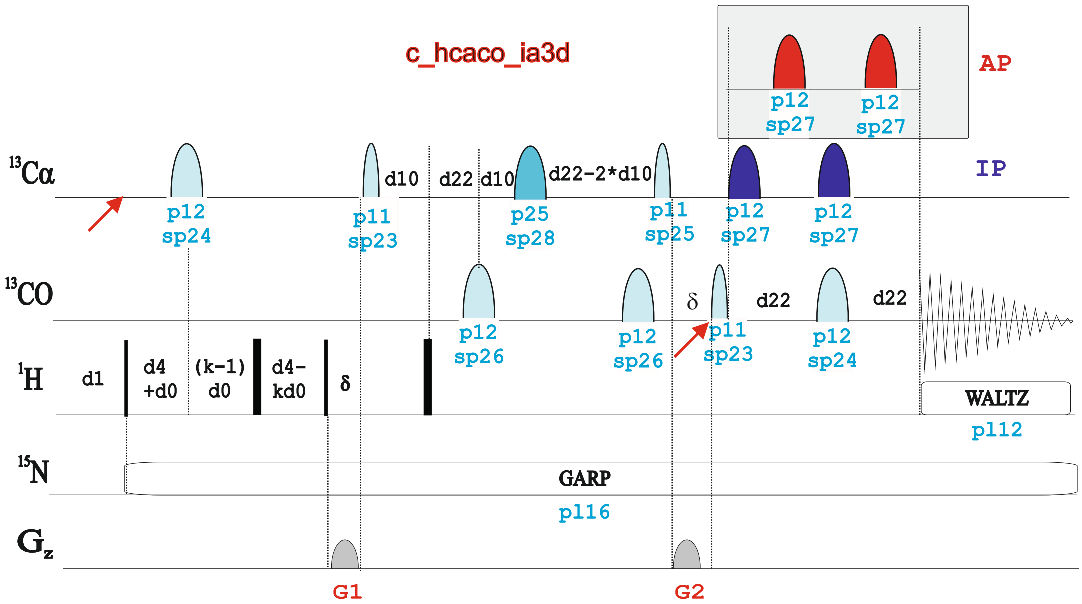
References:

1. Z. Serber, C. Richter, D. Moskau, J.-M. Boehlen, T. Gerfin, D. Marek, M. Haeberli, L. Baslgia, F. Laukien, A.S. Stern, J.C. Hoch & V. Doetsch, J. Am. Chem. Soc. 122, 3554-3555 (2000)
2. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005).
3. K. Pervushin & A. Eletsky, J. Biomol. NMR 25, 147-152 (2003)

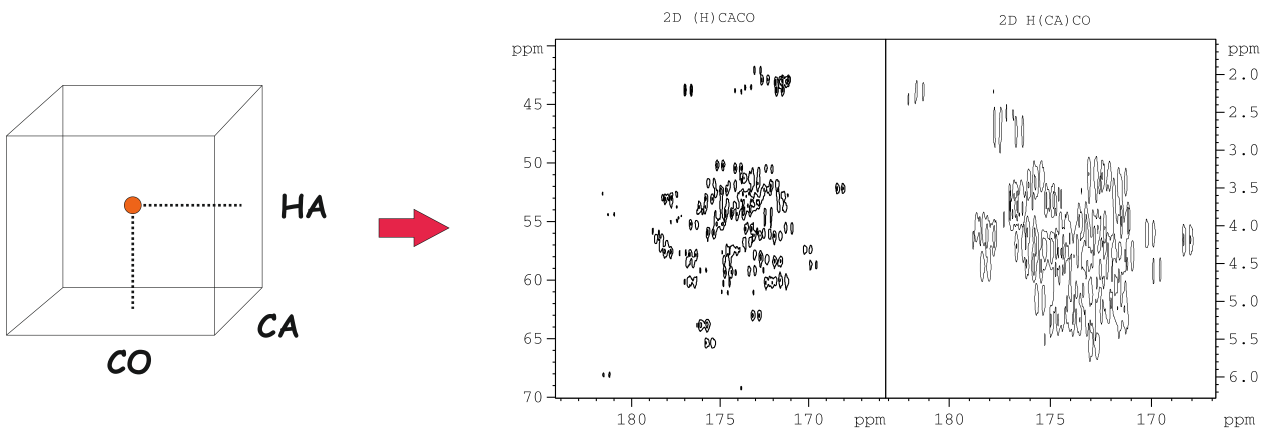
c_hcaco_3d



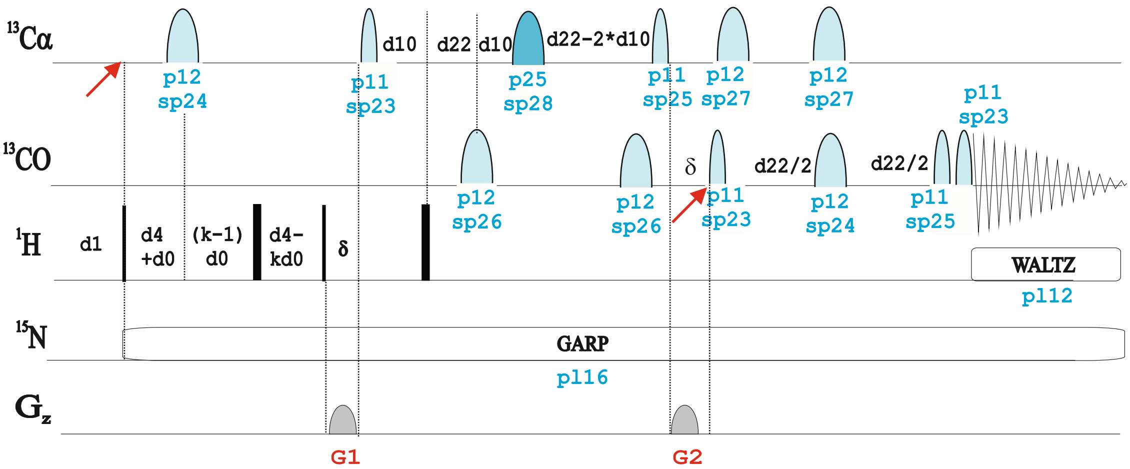




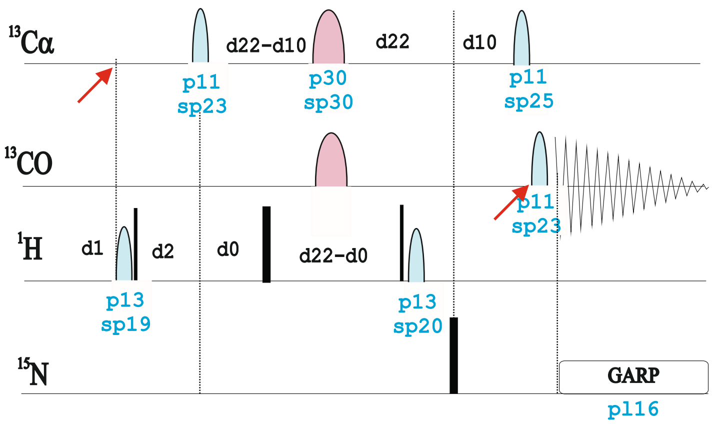
d22=1/4J(COCA)=4.5ms
d2=1/2J(CHA)=3.2ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms



c_hcaco_s33d



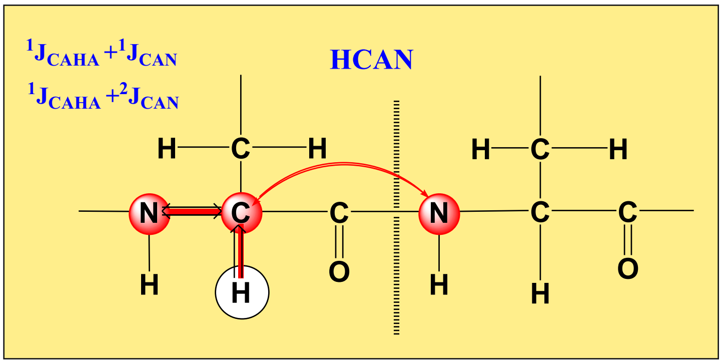
c_hacaco_3d



3D HCAN Experiment

Experiment Description

The 3D HCAN experiment is a CA-detected experiment that correlates the CA-HA of a given residue with the N chemical shift of the same and the next residue in doubly-labeled 13C/15N proteins.

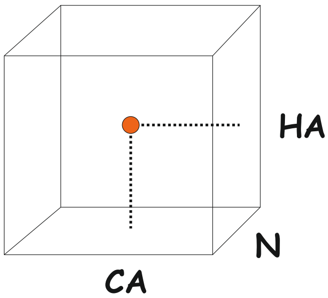


Related Experiments

2D CAN
3D HNCA

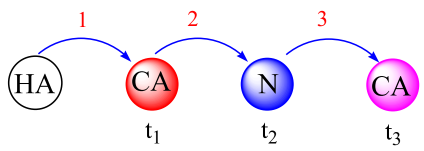
NMR Spectrum

A 3D H,N,C map is obtained

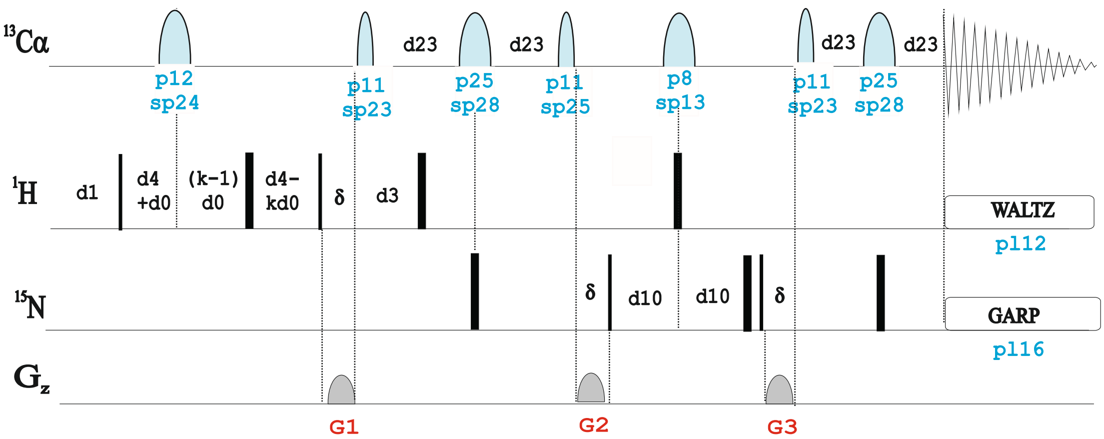


References:

1. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

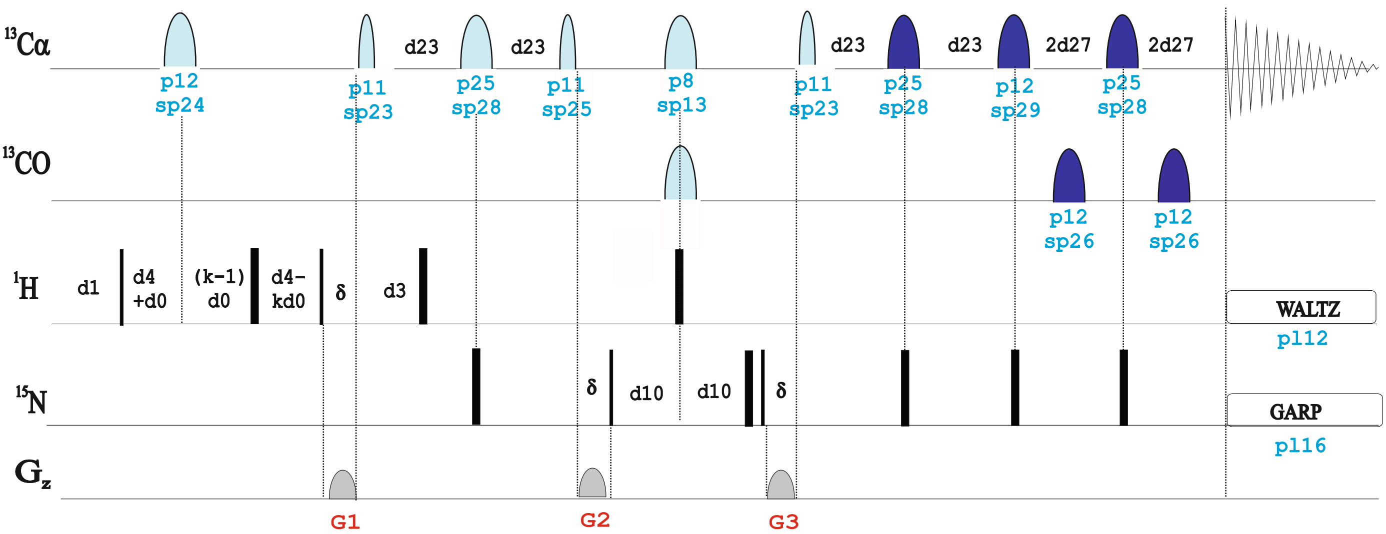


c_hcan_3d



d23=1/4J(NCA)=12.4ms
d22=1/4J(COCA)=4.5ms
d27=1/8J(CACB)=3.6ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

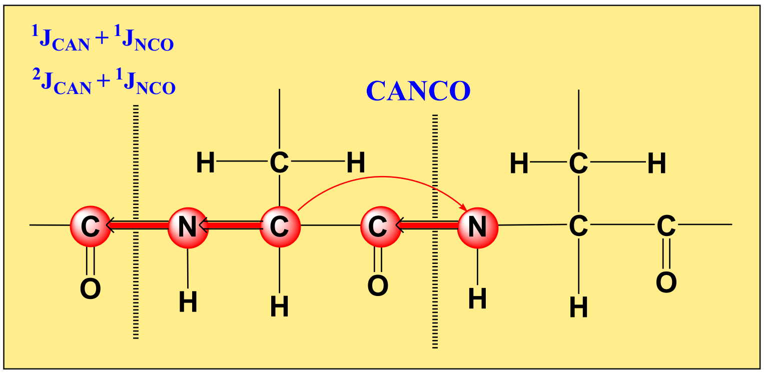
c_hcan_ia3d



3D CANCO Experiment

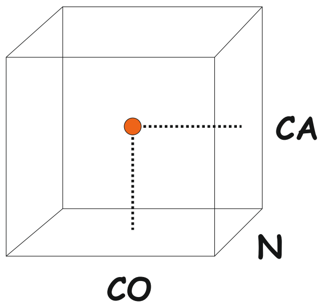
Experiment Description

The 3D CANCO experiment is a CO-detected experiment that allows the correlation betwee the chemical shifts of the CA and the CO of the same and the previous residues and the N of the same and the next residue in doubly-labeled 13C/15N proteins.
Homonuclear CO-CA splitting in the acquisition dimension can be removed by homonuclear decoupling during acquisition or virtually using the IPAP approach.



Related Experiments

3D HNCACO experiment
3D intra-CANCO and (H)CANCO experiments

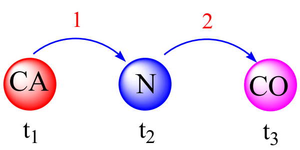


NMR Spectrum

The experiment provides a 3D correlation map in which each CA nucleus displays two different connectivities

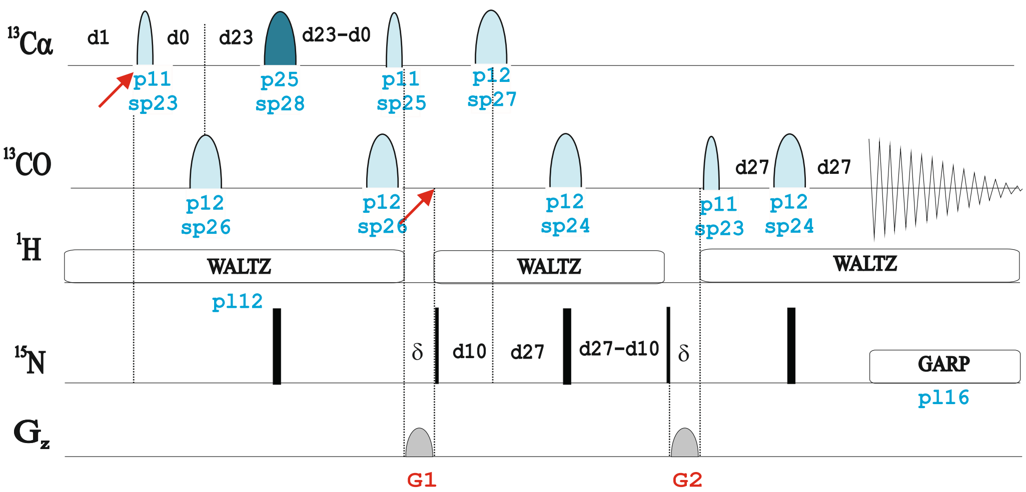
References:

1. I. Bertini, L. Duma, I.C. Felli, M. Fey, C. Luchinat, R. Pierattelli & P. Vasos, Angew. Chem. Int. Ed. 43, 2257-2259 (2004)
2. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

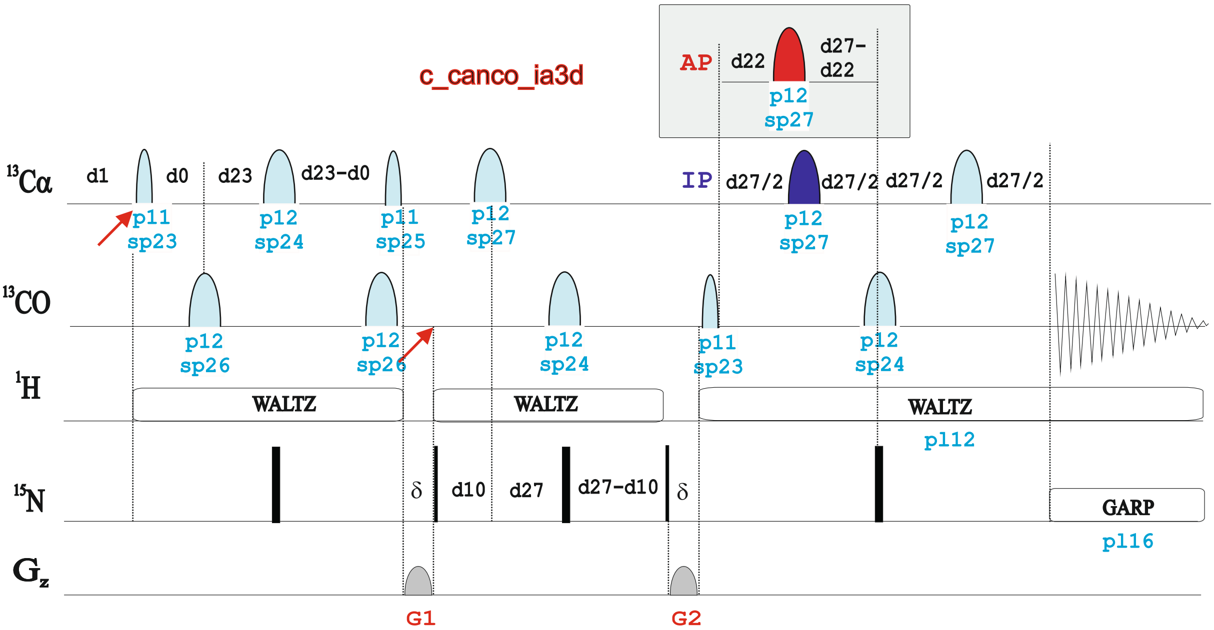


d23=1/4J(NCA)=12.4ms
d22=1/4J(COCA)=4.5ms
d27=1/4J(NCO)=16.0ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

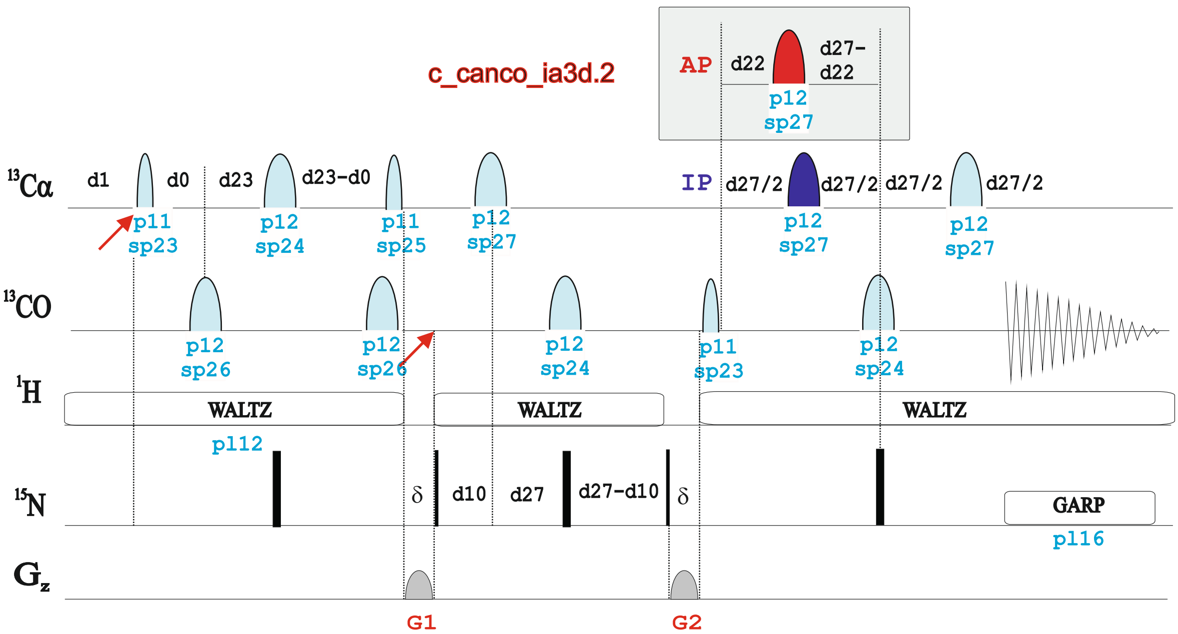
c_canco_3d



c_canco_ia3d



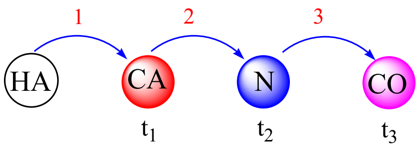
c_canco_ia3d.2

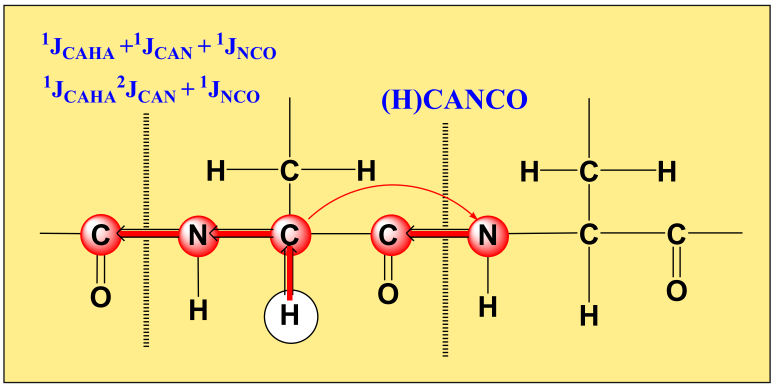


3D (H)CANCO Experiment

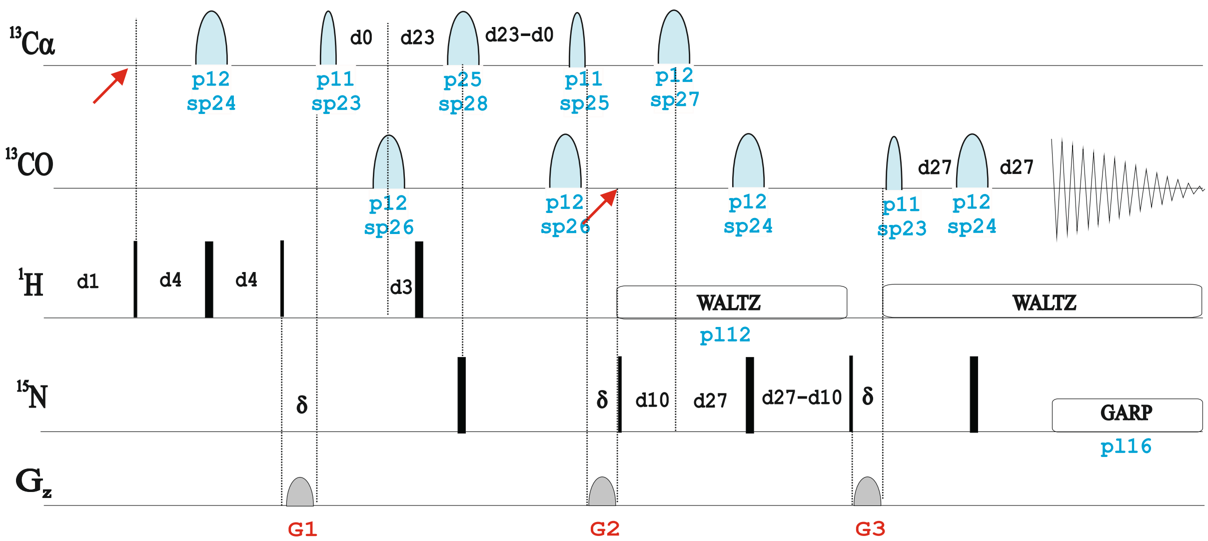
Experiment Description

Variant of the CANCO experiment that starts from the HA protons.

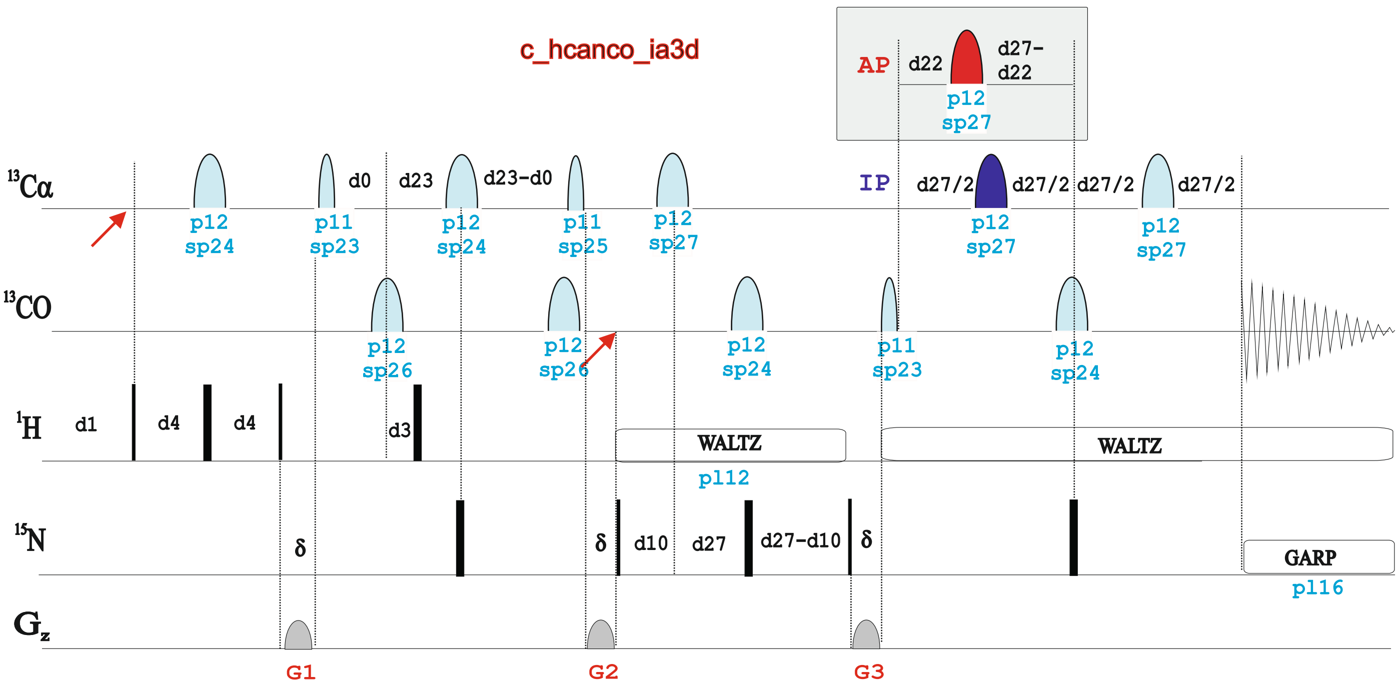




c_hcanco_3d



c_hcanco_ia3d

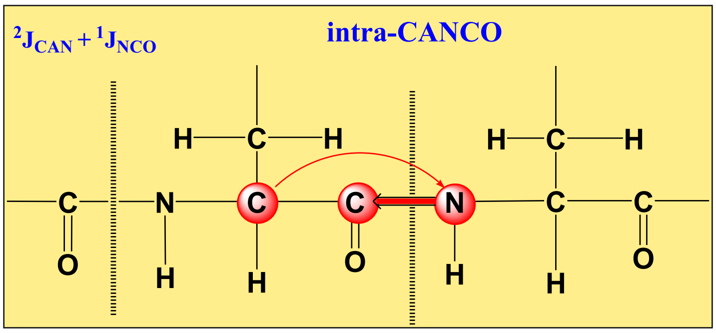


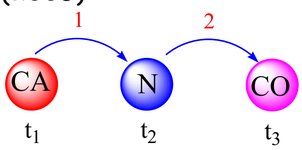
3D intra-CANCO Experiment

Experiment Description

Variant of the CANCO experiment that provides exclusively intra-residue CANCO connectivities.

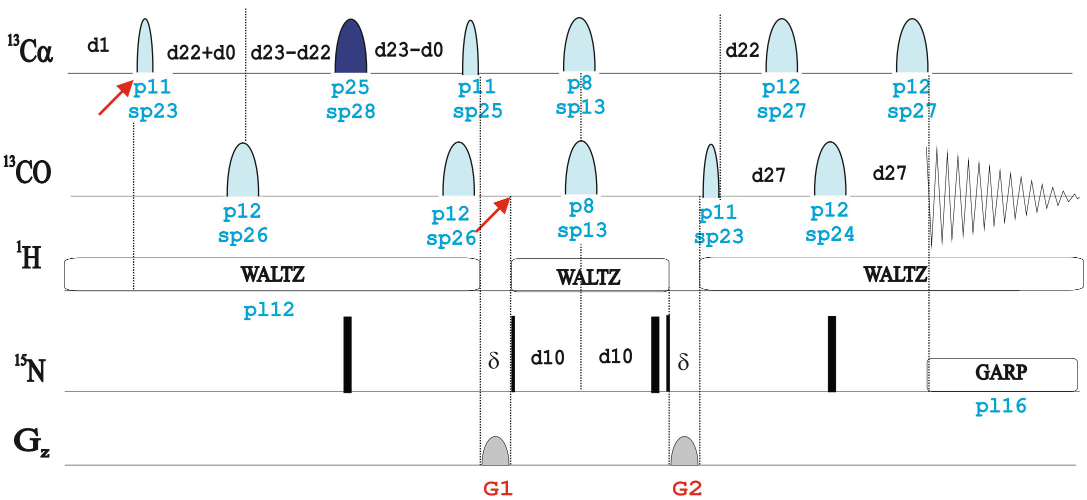
1. W. Bermel, I. Bertini, I.C. Felli, R. Pierattelli & P. Vasos, J. Magn. Reson. 172, 324-328 (2005)
2. W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)



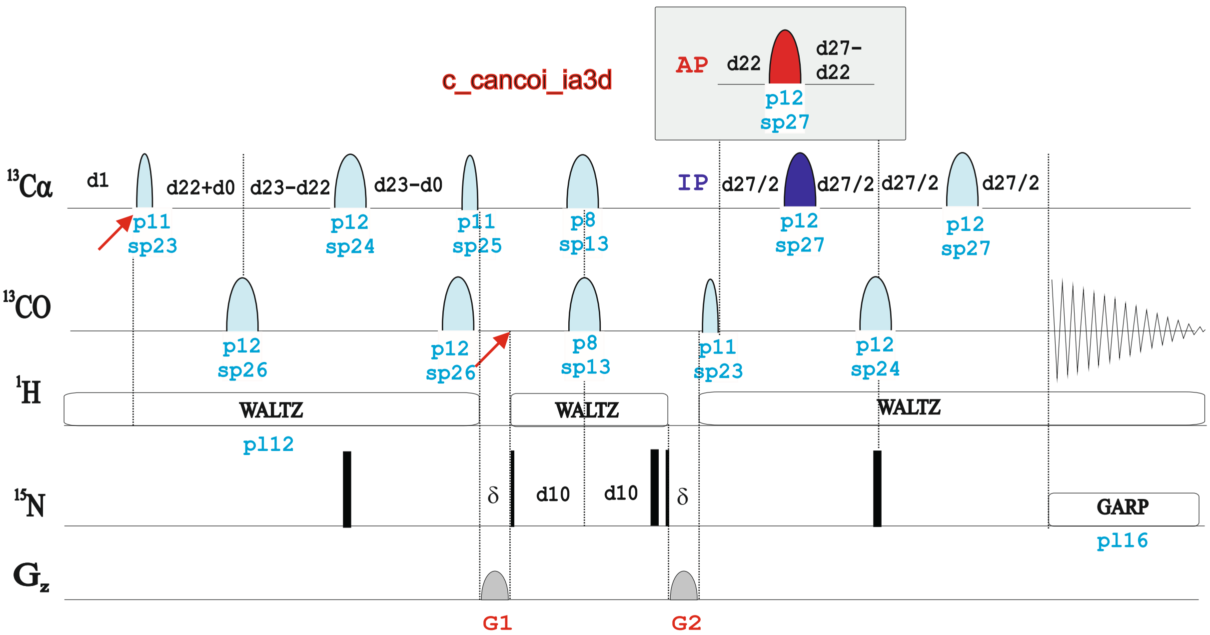


d22: 1/(4J(COCa)) = [4.5 msec]
d23: 1/(4J(NCa)) and 1/(2J(CaCb)) = [13.3 msec]
d27: 1/(4J(NCO)) = [16.0 msec]

c_cancoi_3d



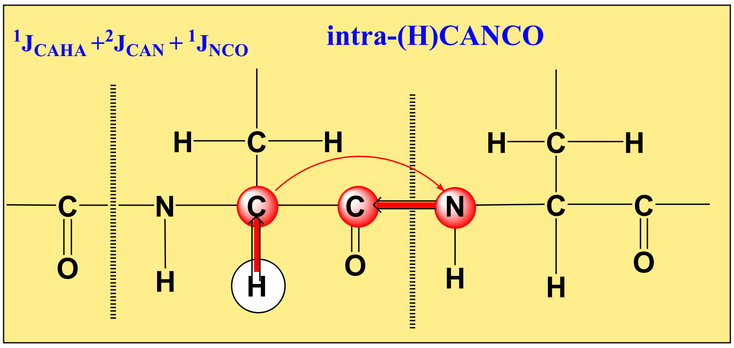
c_cancoi_ia3d

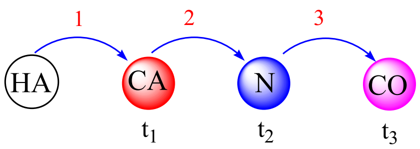


3D intra-(H)CANCO Experiment

Experiment Description

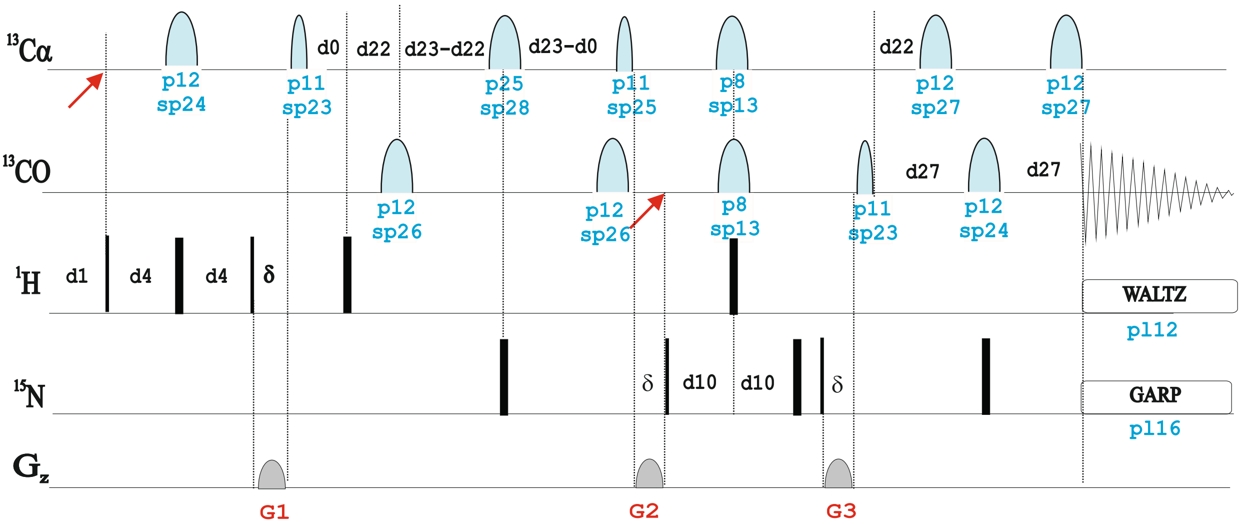
Variant of the intra-CANCO experiment that starts from the HA protons.



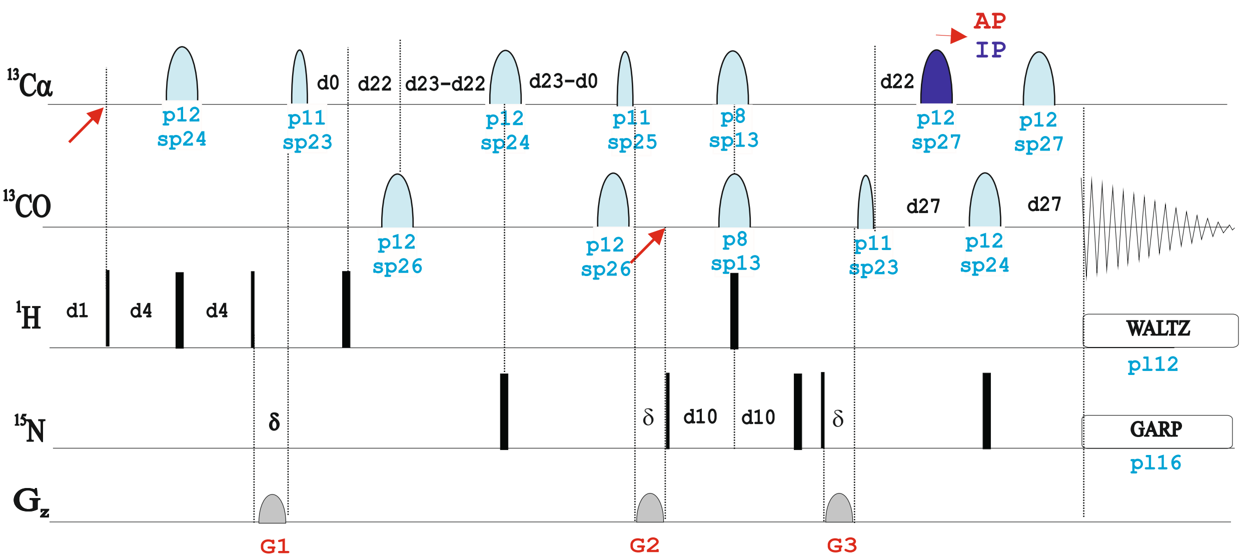


;d3 : 1/(6J(HCa)) [1.1 msec]
;d4 : 1/(4J(HCa)) [1.8 msec]
;d22: 1/(4J(COCa)) [4.5 msec]
;d23: 1/(4J(NCa)) and 1/(2J(CaCb)) [13.3 msec]
;d27: 1/(4J(NCO)) [16.0 msec]

c_hcancoi_3d



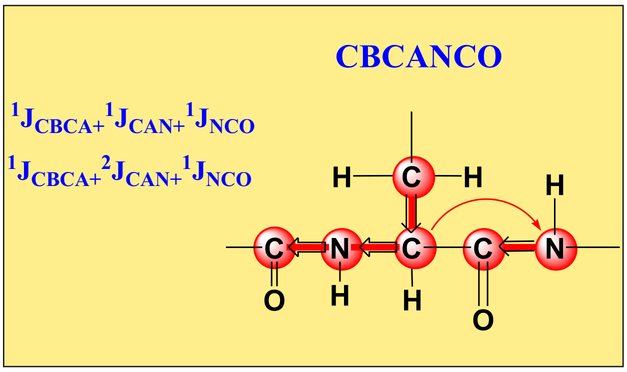
c_hcancoi_ia3d



3D CBCANCO Experiment

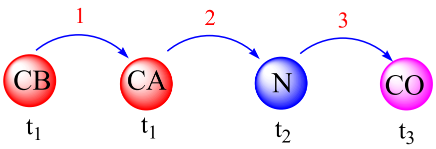
Experiment Description

Variant of the CANCO experiment incorporating an initial CB-CA transfer
The experiment provides intra- and inter-residue between CB,CA and CO,N connectivities

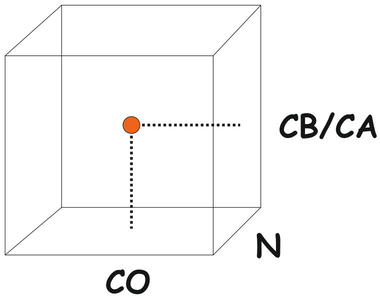


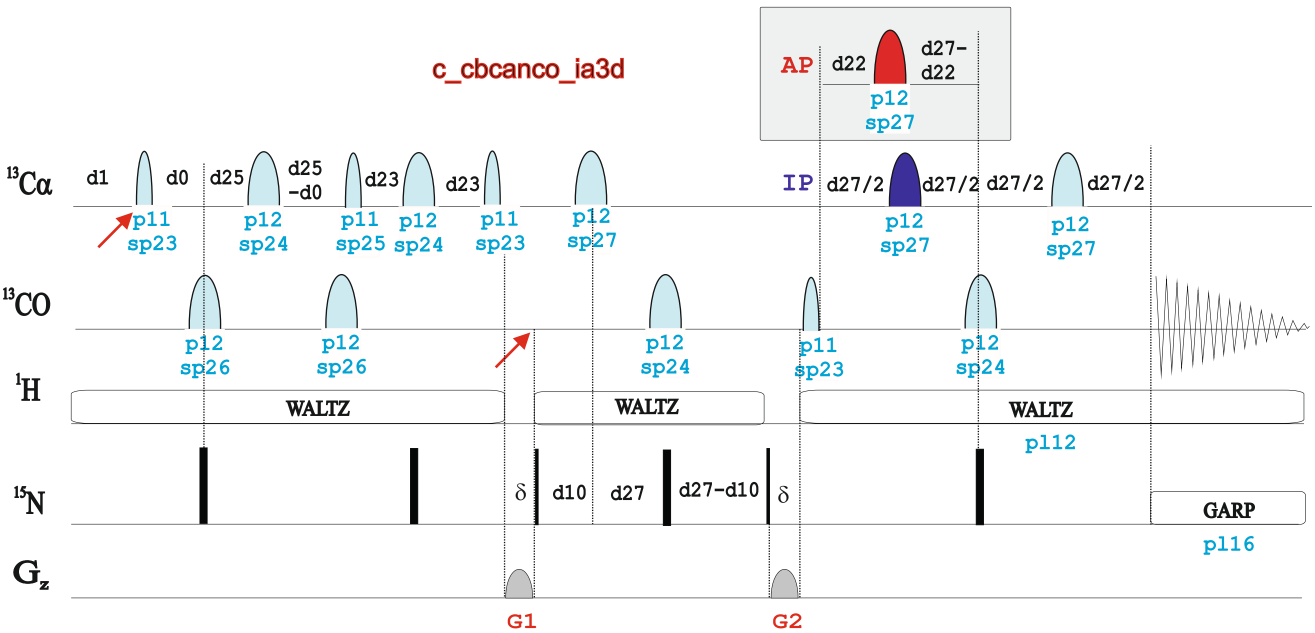
References:

W. Bermel, I. Bertini, I.C. Felli, R. Kuemmerle & R. Pierattelli, J. Magn. Reson. 178, 56-64 (2006)



d23=1/4J(NCA)=12.4ms
d22=1/4J(COCA)=4.5ms
d27=1/4J(NCO)=16.0ms
d3=1/6J(CHA)=1.1ms
d4=1/4J(CHA)=1.8ms

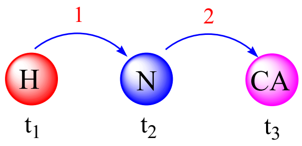


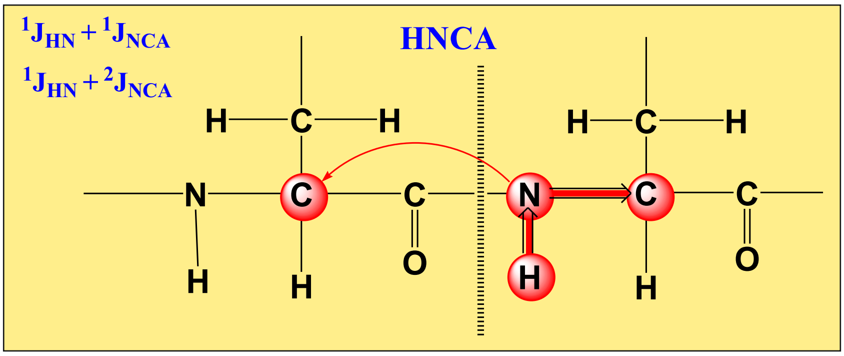


3D CA-detected HNCA Experiment

Experiment Description

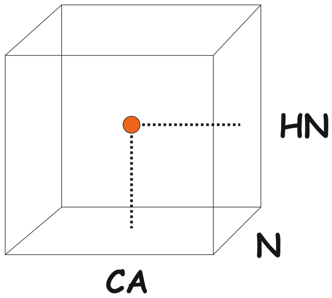
The 3D CA-detected HNCA experiment is an out-and-stay version of the conventional HNCA experiment





NMR Spectrum

The experiment provides the same 3D HNCA correlation map



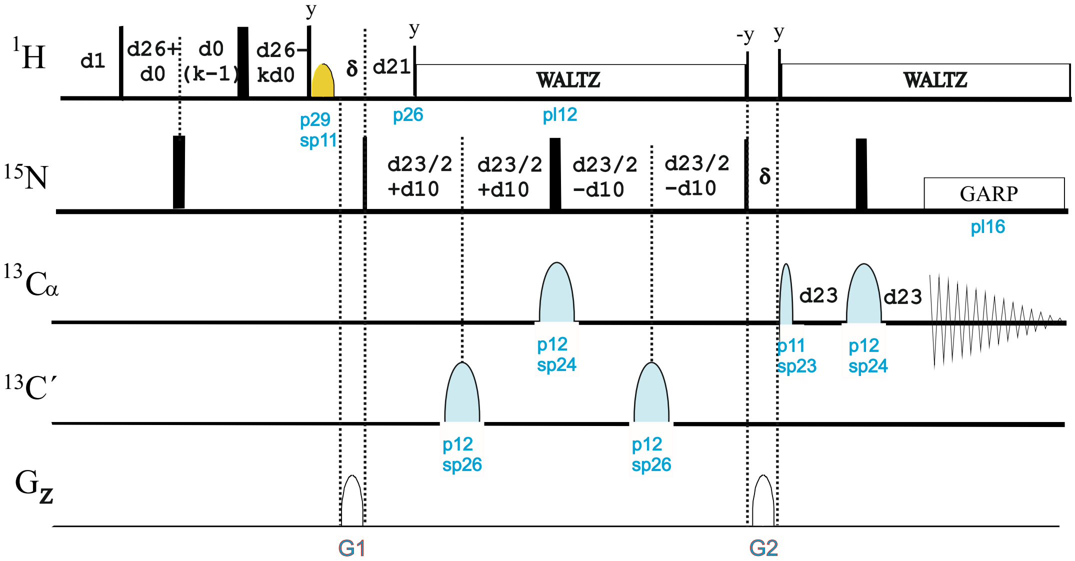
References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

Related Experiments.

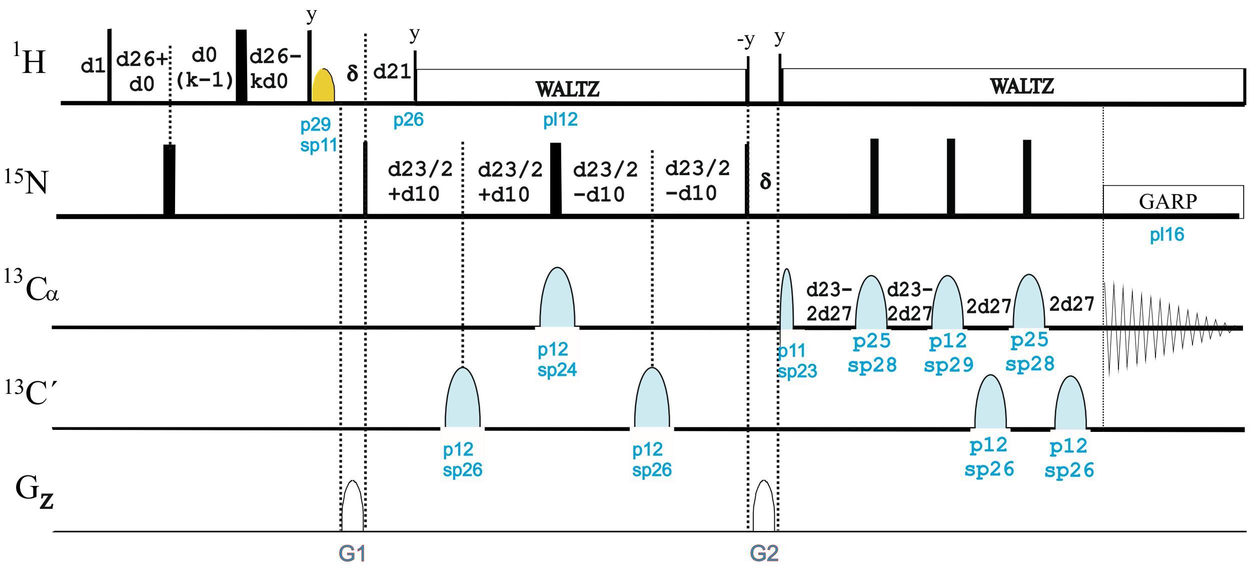
3D HA-Detected HNCA

c_hnca_3d



d21=1/2J(NH)=5.5ms
d22=1/4J(COCA)=4.5ms
d23=1/4J(NCA)=12.4ms
d26=1/4J(NH)=2.3ms
d27=1/8(CACB)=3.6ms

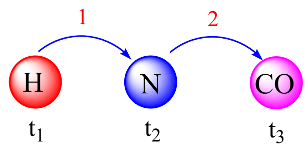
c_hnca_ia3d

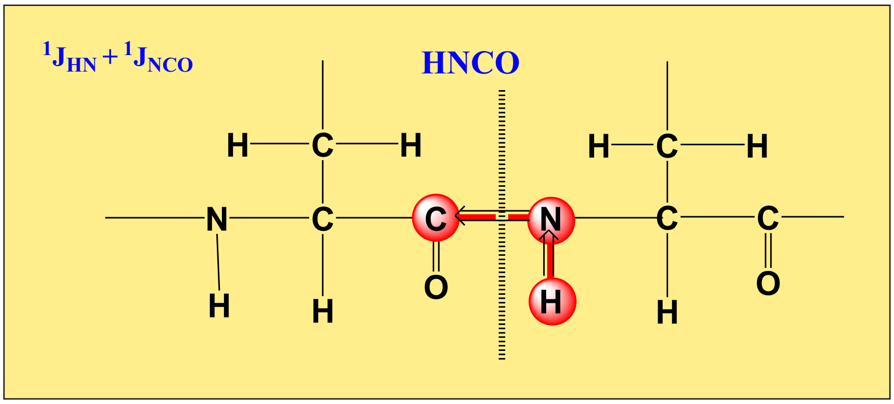


3D CO-detected HNCO Experiment

Experiment Description

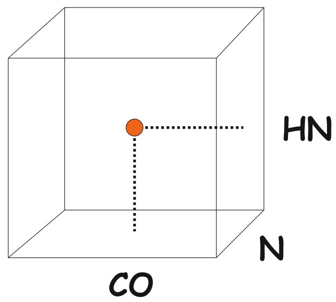
The 3D CO-detected HNCO experiment is an out-and-stay version of the conventional HNCO experiment





NMR Spectrum

The experiment provides the same 3D HNCO correlation map



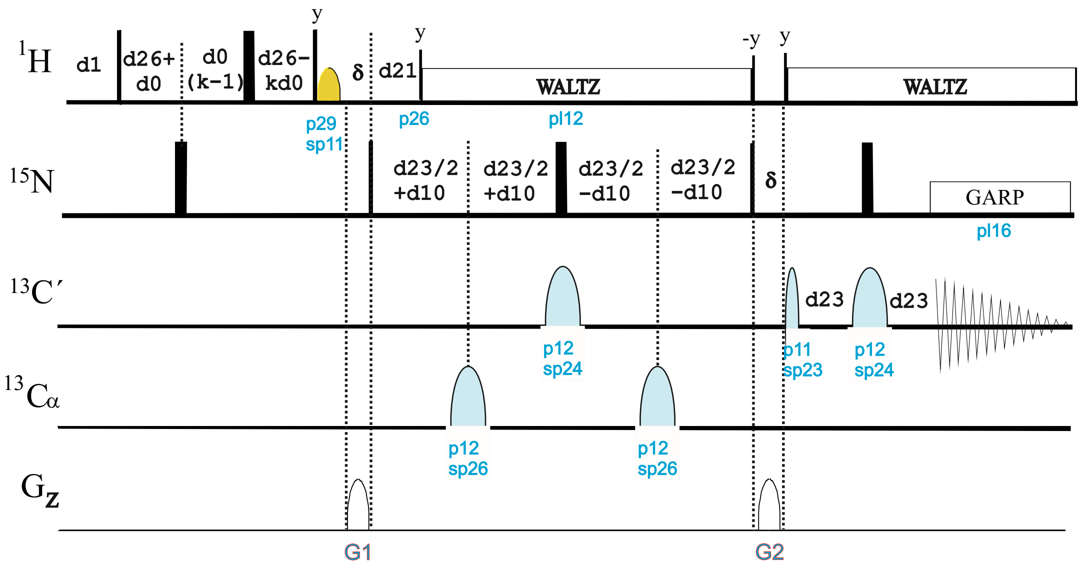
References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

Related Experiments.

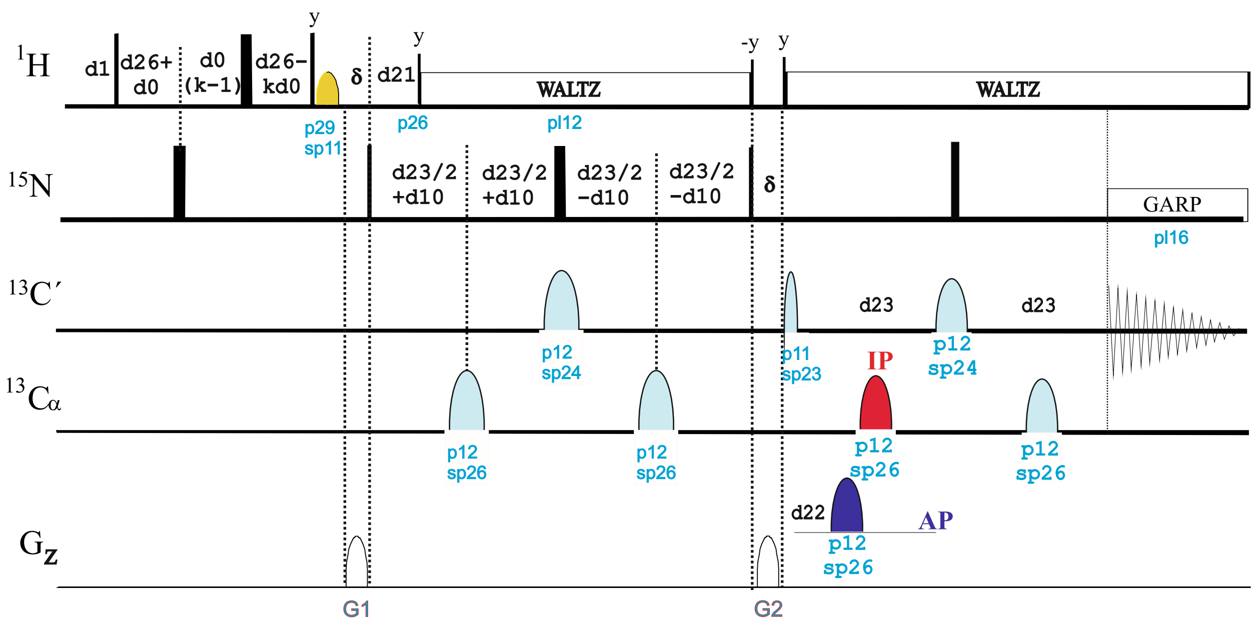
3D HN-Detected HNCO

c_hnco_3d



d21=1/2J(NH)=5.5ms
d22=1/4J(COCA)=4.5ms
d23=1/4J(NCA)=12.4ms
d27=1/8(CACB)=3.6ms

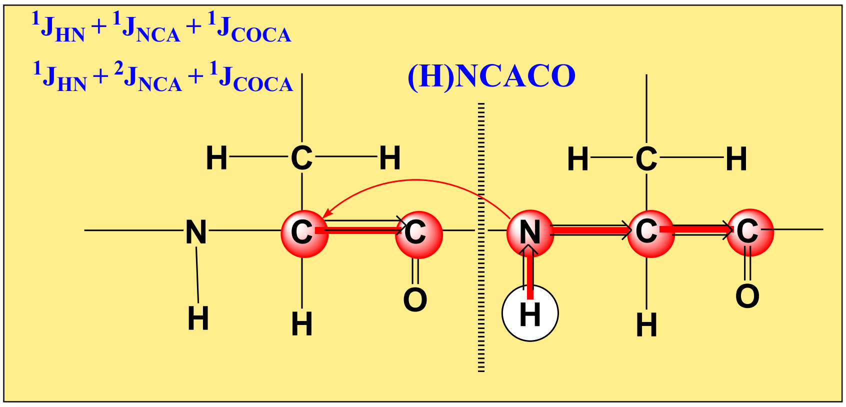
c_hnco_ia3d



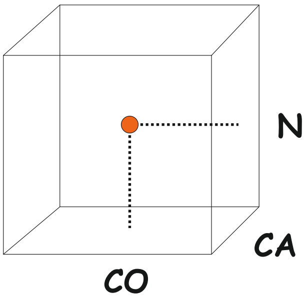
3D CO-detected (H)NCACO Experiment

Experiment Description

The 3D CO-detected HNCACO experiment is an out-and-stay version of the conventional1H-detected HNCACO experiment. Each nitrogen is correlated to CA and CO carbons of the same and the previous residue.



NMR Spectrum



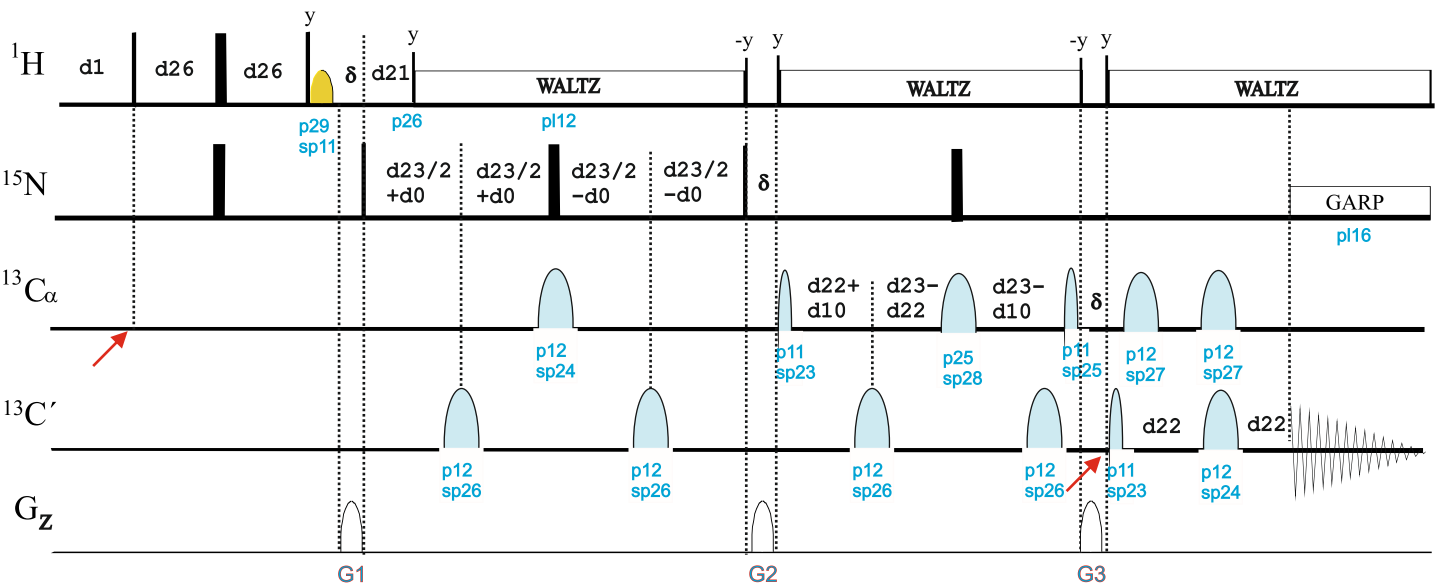
References:

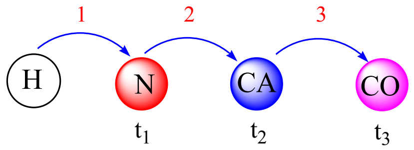
W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

Related Experiments.

3D HN-Detected HNCACO

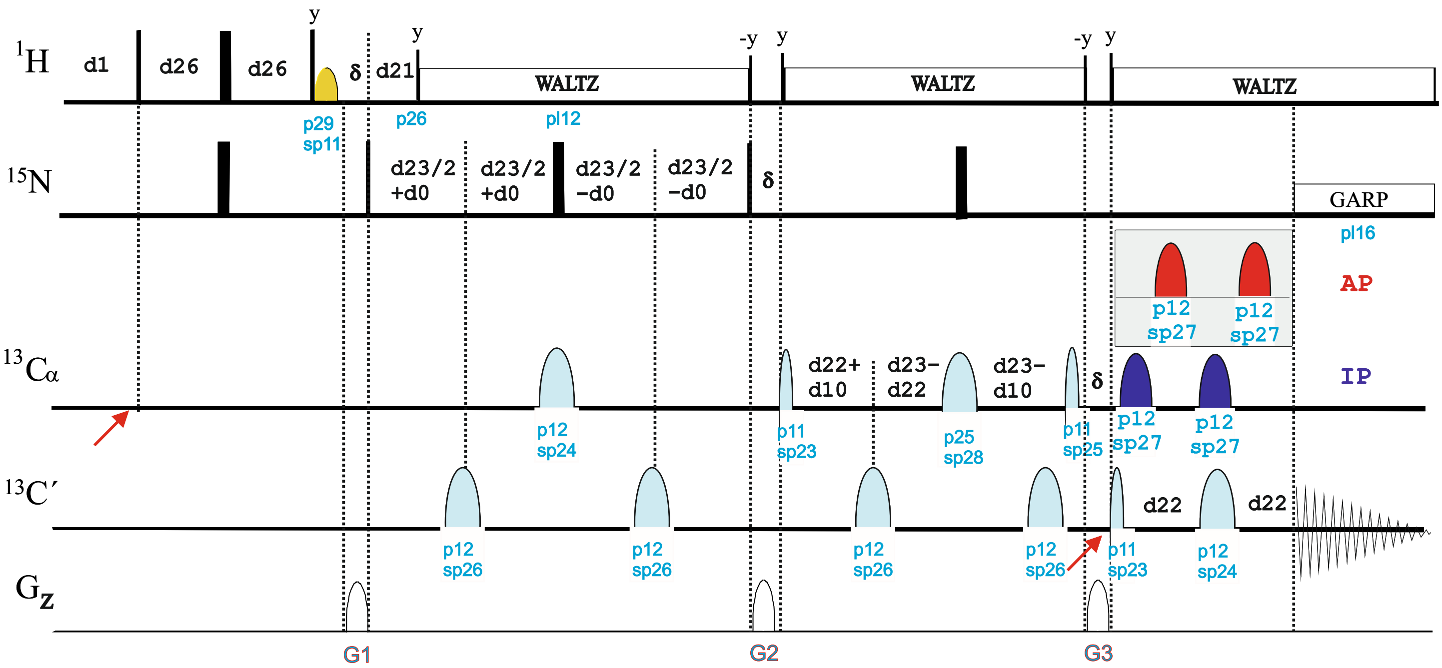
c_hncaco_3d



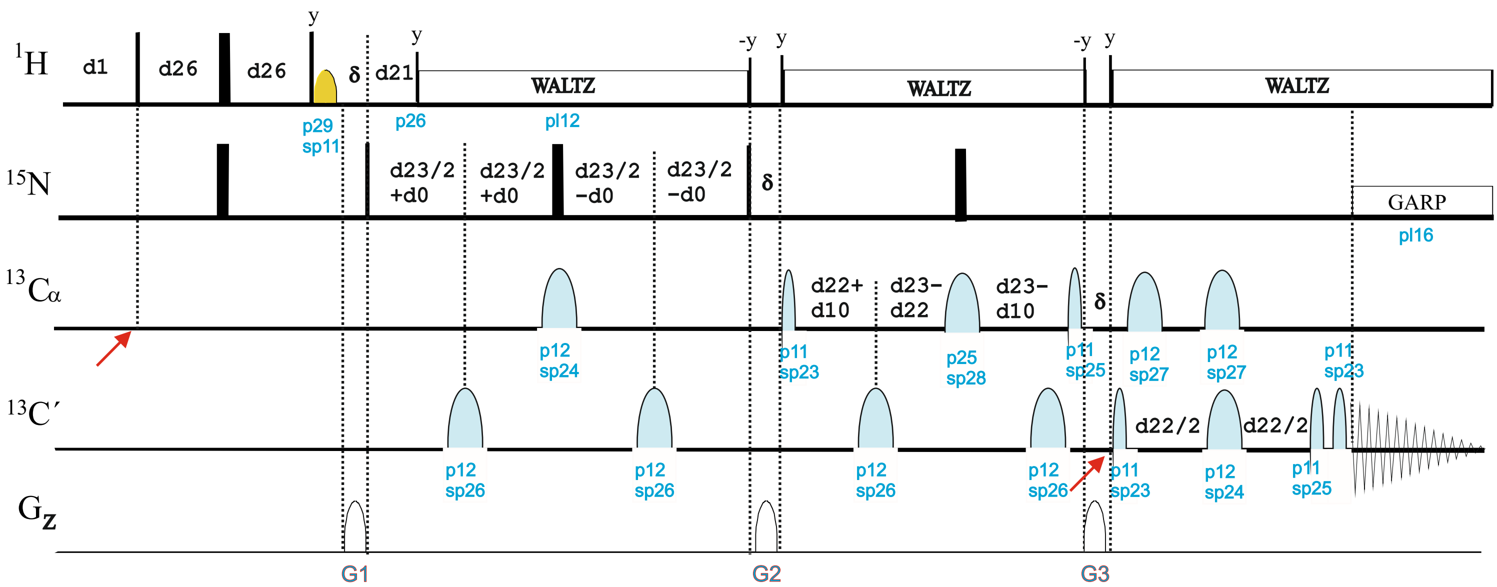


d21=1/2J(NH)=5.5ms
d22=1/4J(COCA)=4.5ms
d23=1/4J(NCA)=12.4ms
d26=1/4J(NH)=2.3ms

c_hncaco_ia3d



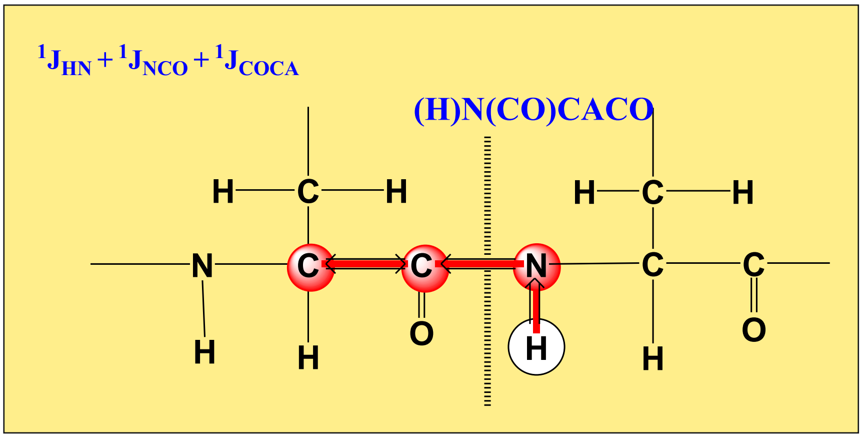
c_hncaco_s33d



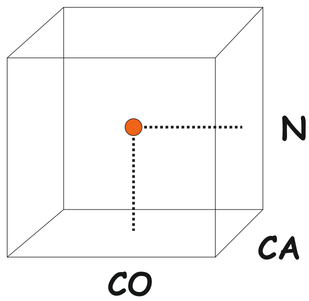
3D CO-detected (H)NCOCA Experiment

Experiment Description

The 3D (H)N(CO)CACO is the CO-detected equivalent of the HNCOCA experiment, in which a nitrogen nucleus is correlated to the CO and CA carbons of the previous residue.



NMR Spectrum

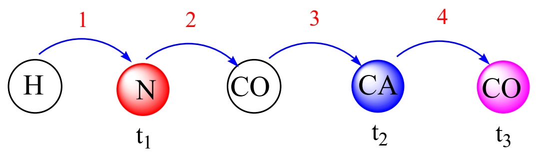


References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

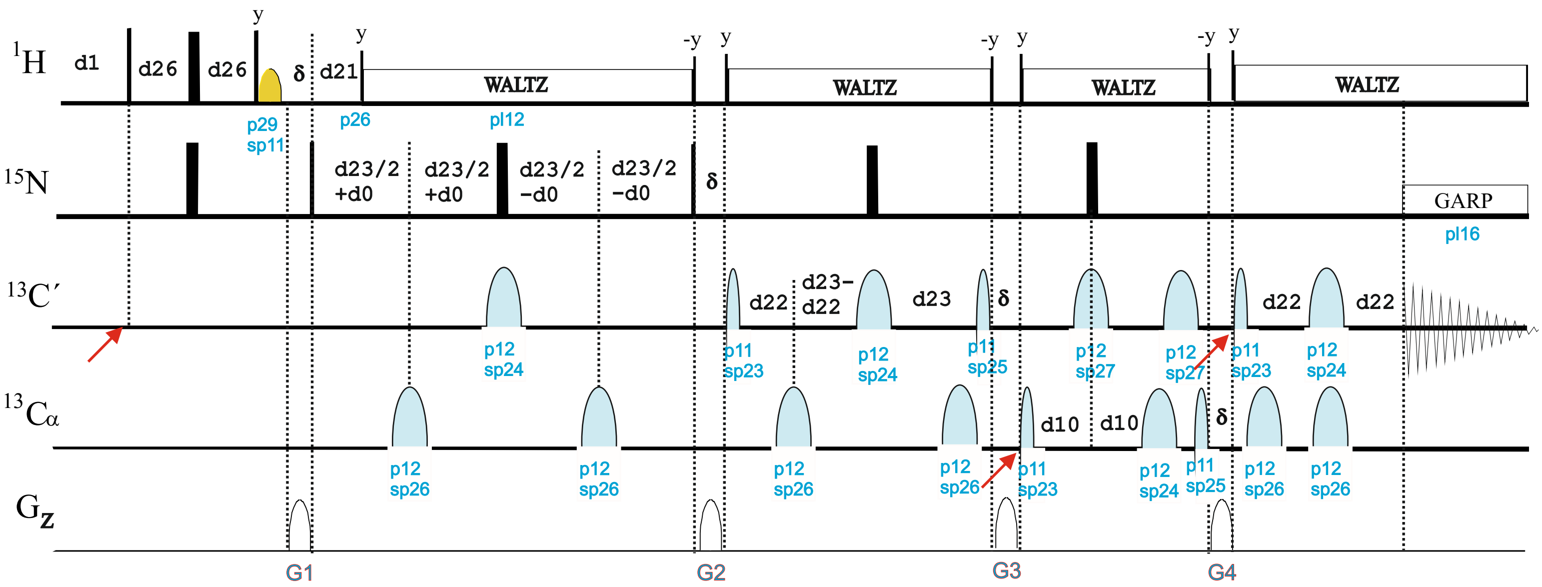
Related Experiments.

3D HN-Detected HNCOCA
CA-detected (H)NCOCA

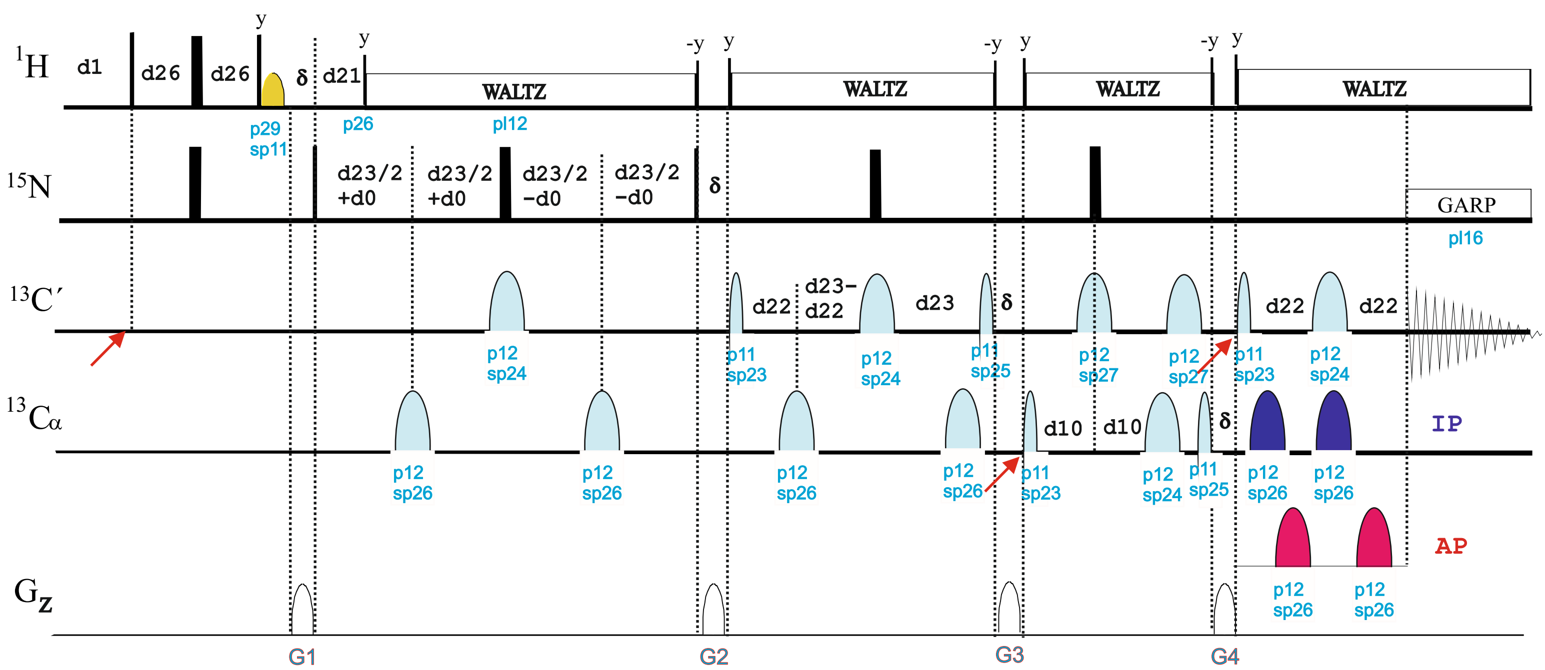


d21=1/2J(NH)=5.5ms
d22=1/4J(COCA)=4.5ms
d23=1/4J(NCO)=12.4ms
d26=1/4J(NH)=2.3ms

c_hncoca_3d



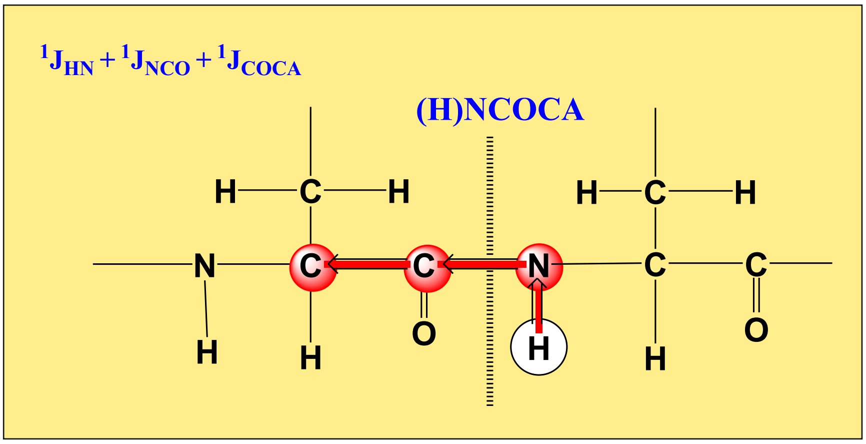
c_hncoca_ia3d



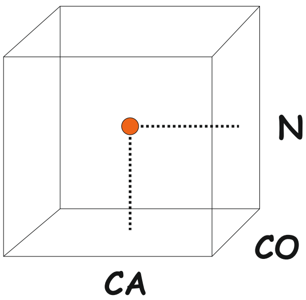
3D CA-detected (H)NCOCA Experiment

Experiment Description

The 3D CA-detected HNCOCA experiment is an out-and-stay version of the conventional 1H-detected HNCOCA experiment. Each nitrogen is correlated to CA and CO carbons of the same and the previous residue.



NMR Spectrum

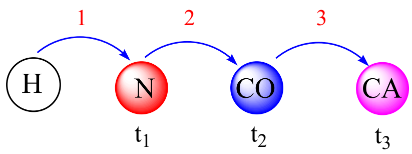


References:

W. Bermel, I. Bertini,L. Duma, I.C. Felli, L. Emsley, R. Pierattelli, P.R. Vasos, Angew. Chem. Int. Ed. 44, 3089-3092 (2005)

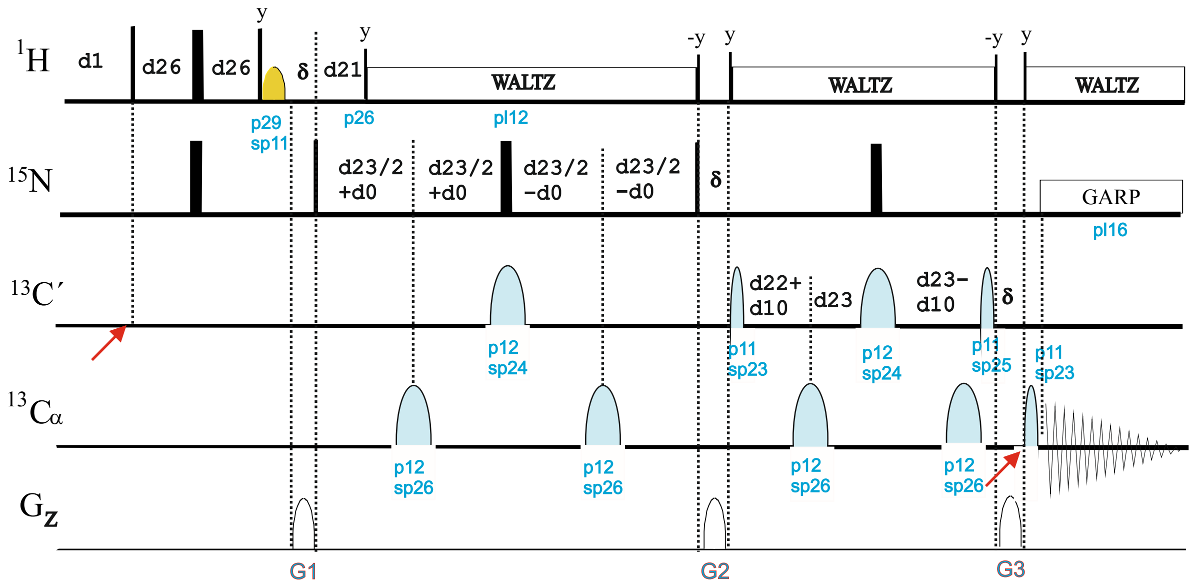
Related Experiments

1H-detected HNCOCA
CO-detected (H)NCOCA
CANCO and i-CANCO

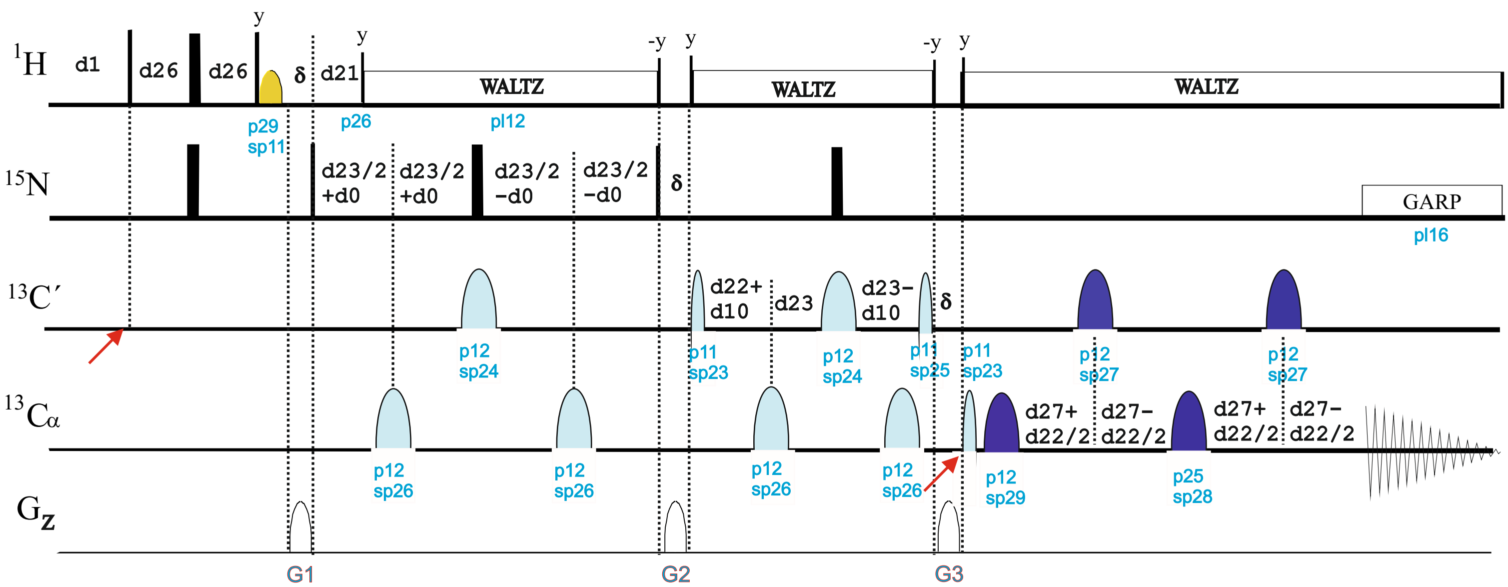


d21=1/2J(NH)=5.5ms
d22=1/4J(COCA)=4.5ms
d23=1/4J(NCA)=12.4ms
d26=1/4J(NH)=2.3ms
d27=1/8(CACB)=3.6ms

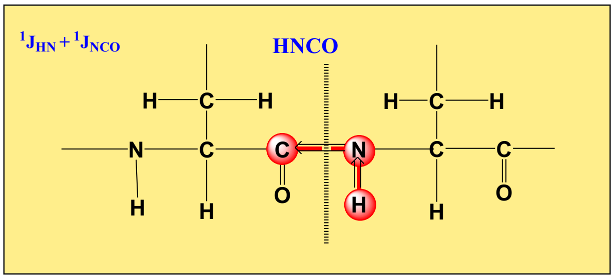
c_hncoca2_3d

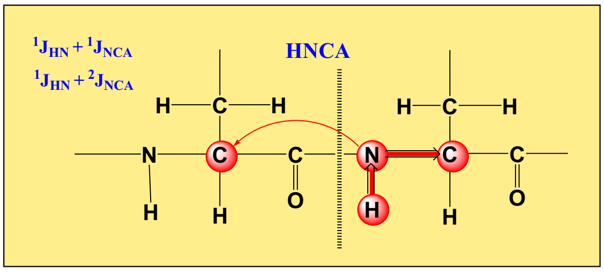


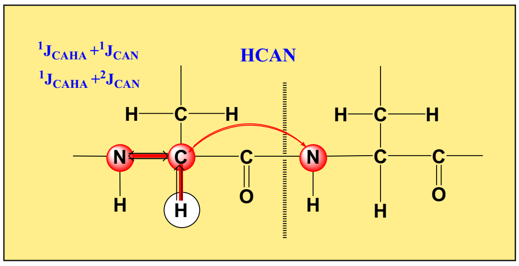
c_hncoca2_ia3d

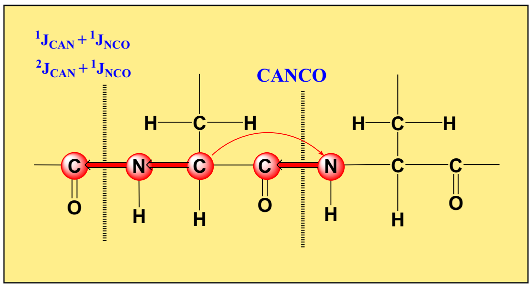


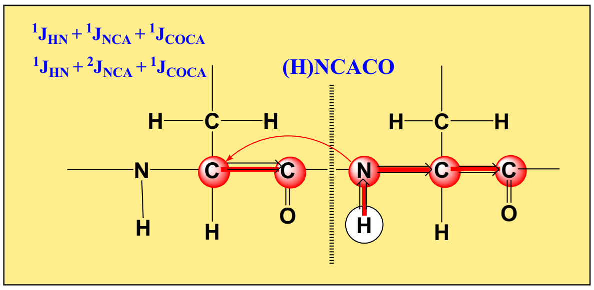
Summary of C-detected backbone CN experiments

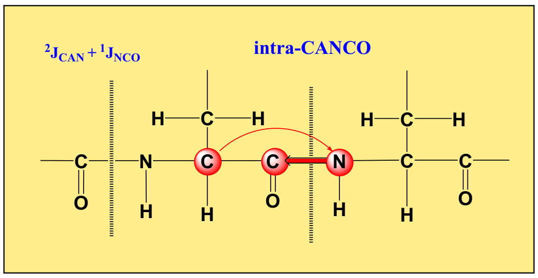


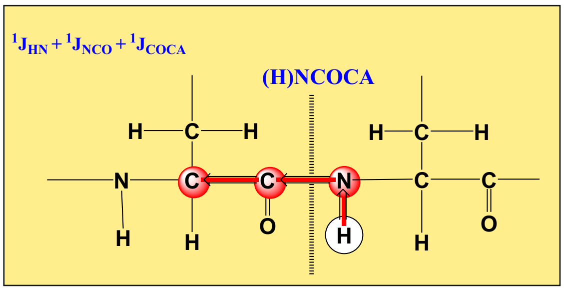












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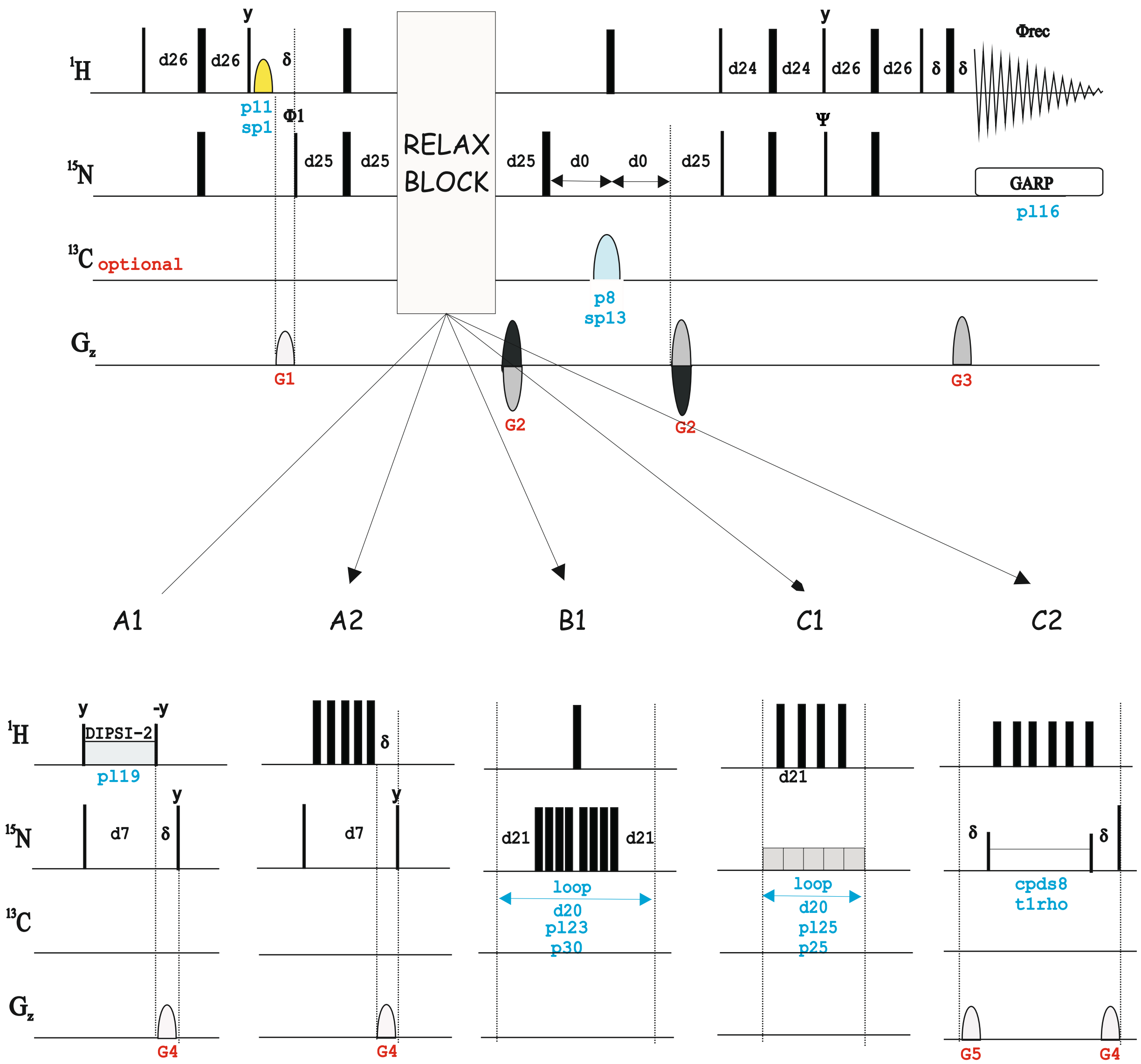
2D HSQC EXPERIMENTS FOR THE MEASUREMENT OF T1, T2, T1RHO RELAXATION TIMES AND HETERONUCLEAR NOEs.

NMR Experiment: Relaxation Rates Measurement

Pulprog (3D mode)	Parameter Set	pp (2D mode)	TROSY version
A1. hsqct1etf3gpsi3d	HSQCT1ETF3GPSI3D	hsqct1etf3gpsi3d	trt1etf3gpsi3d
A2. hsqct1etf3gpsi3d.2	HSQCT1ETF3GPSI3D.2	hsqct1etf3gpsi3d.2	
B1. hsqct2etf3gpsi3d	HSQCT2ETF3GPSI3D	hsqct2etf3gpsi3d	trt2etf3gpsi3d
C1. hsqctretf3gpsi3d	HSQCTRETF3GPSI3D	hsqctretf3gpsi3d	
C2. hsqctretf3gpsi3d.2	HSQCTRETF3GPSI3D.2		

General Scheme



2D HSQC experiments for ^{13}C Relaxation Measurements (from f2 channel)

- **Heteronuclear ^{13}C-^{1}H NOEs:**

  Phase sensitive ge-2D ^{1}H-^{13}C HSQC to measure heteronuclear ^{13}C -^{1}H NOEs using PEP (**hsqcnoegpsi** | HSQCNOEGPSI)
  Phase sensitive ge-2D ^{1}H-^{13}C HSQC to measure heteronuclear ^{13}C -^{1}H NOEs using PEP and refocusing adiabatic ^{13}C pulses (**hsqcnoegpsi.2** | HSQCNOEGPSI)

- **T_1 (C):**

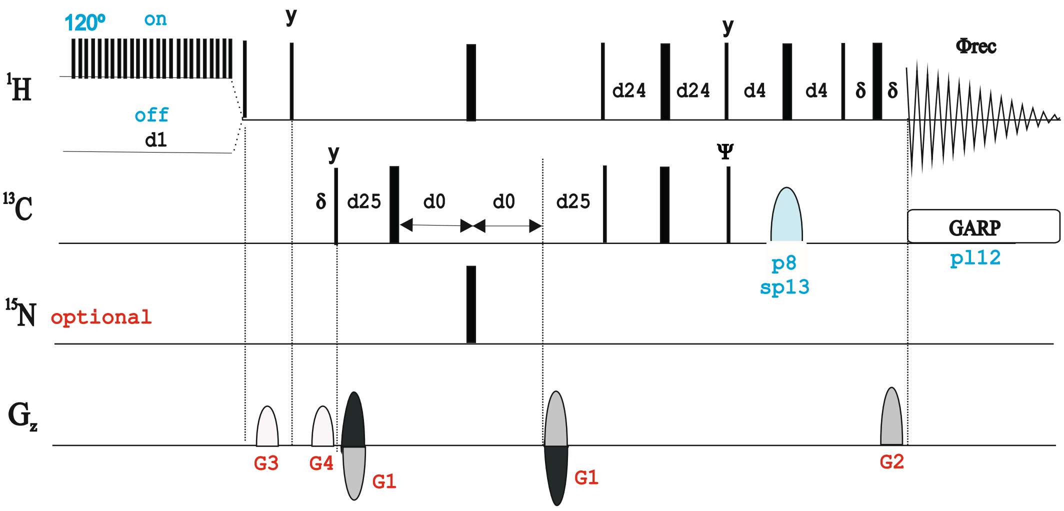
  Phase-sensitive ge-2D ^{1}H-^{13}C HSQC to measure ^{13}C T_1 relaxation times using PEP, 180° ^{1}H pulses and acquired as pseudo-3D (**hsqct1etgpsi3d**).
  Phase-sensitive ge-2D ^{1}H-^{13}C HSQC to measure ^{13}C T_1 relaxation times using PEP,180° ^{1}H pulses, refocusing adiabatic ^{13}C pulses and acquired as pseudo-3D (**hsqct1etgpsi3d.2**).

- **T_2 (C):**

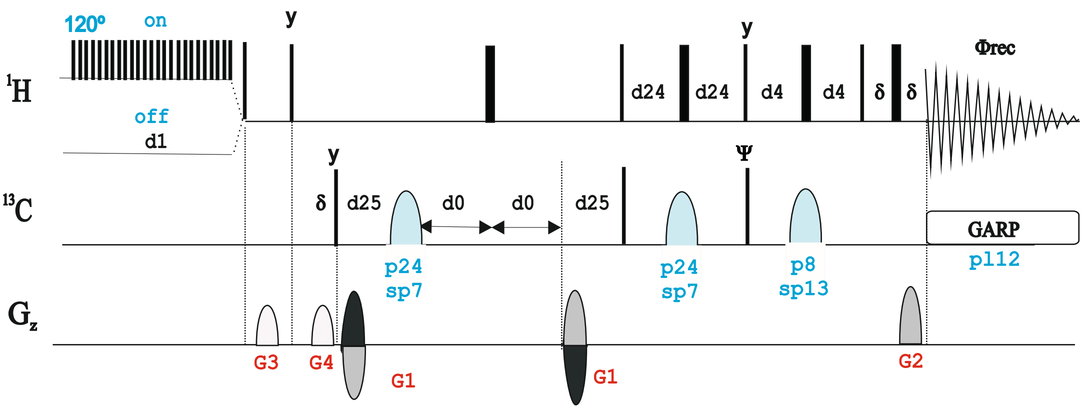
  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{13}C T_2 relaxation times using PEP and refocusing adiabatic ^{13}C pulses (**hsqct2etgpsi3d.2**)

Also see:
T1 & T2 Relaxation
3D HNCO for Relaxation Measurements

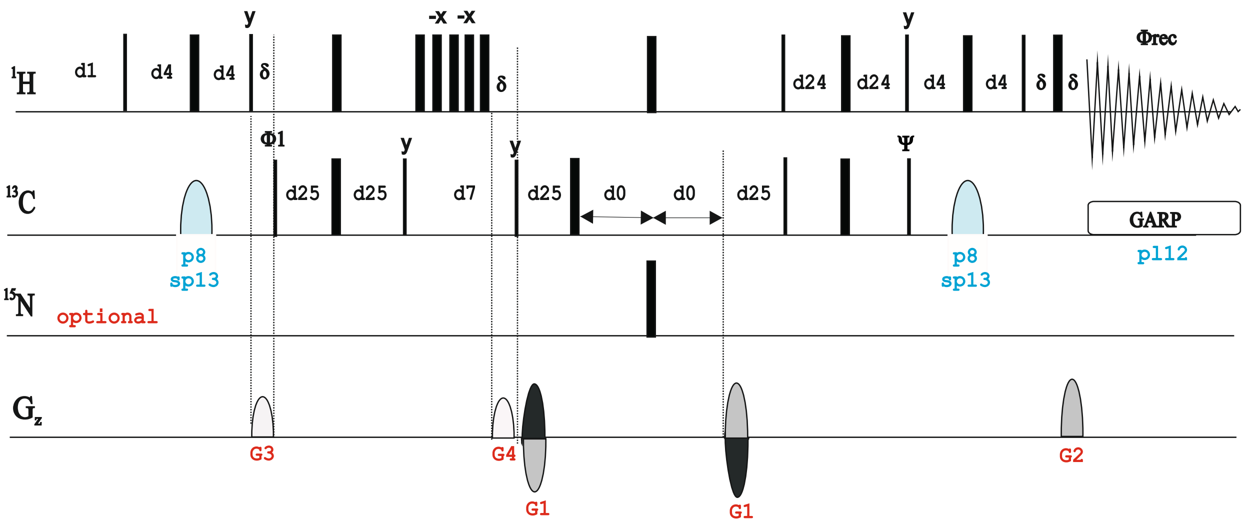
hsqcnoegpsi



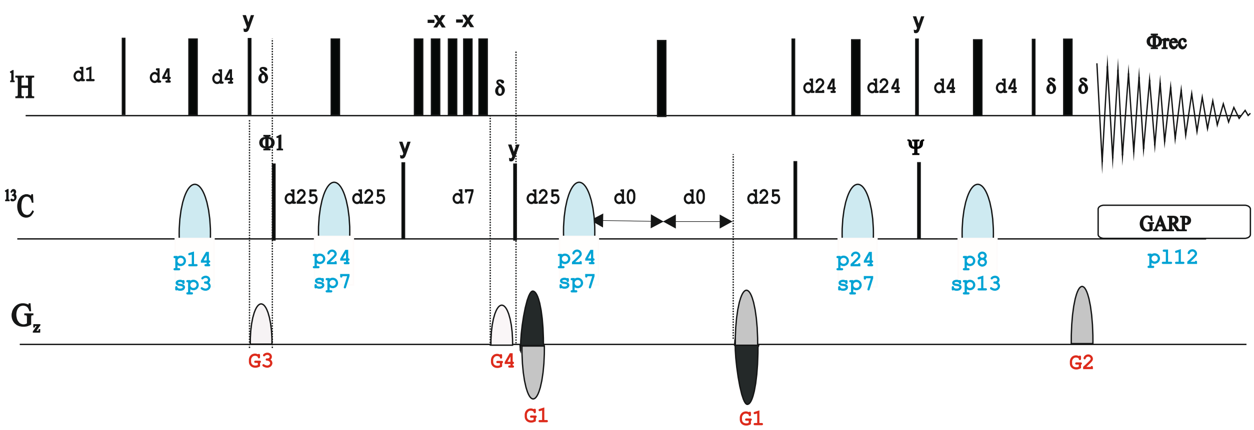
hsqcnoegpsi.2



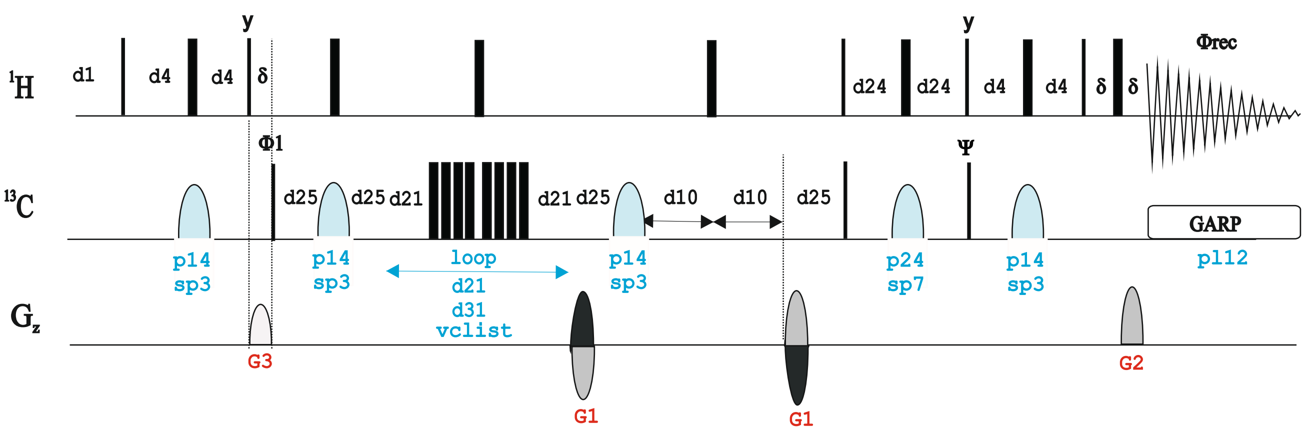
hsqct1etgpsi3d



hsqct1etgpsi3d.2



hsqct2etgpsi3d.2



2D HSQC experiments for ^{15}N Relaxation Measurements (from f3 channel)

- **Heteronuclear ^{15}N-^{1}H NOEs:**

  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure heteronuclear ^{15}N-^{1}H NOEs using PEP (**hsqcnoef3gpsi** | HSQCNOEF3GPSI)
  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure heteronuclear ^{15}N-^{1}H NOEs using TROSY (**trnoef3gpsi** | TRNOEF3GPSI)

- **T_1 (N):**

  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_1 relaxation times using PEP:
  Using 1H-decoupling (**hsqct1etf3gpsi** | HSQCT1ETF3GPSI)
  Using 1H-decoupling acquired as pseudo-3D (**hsqct1etf3gpsi3d** | HSQCT1ETF3GPSI3D)
  Using 180 1H pulses (**hsqct1etf3gpsi.2** | HSQCT1ETF3GPSI.2)
  Using 180 1H pulses acquired as pseudo-3D (**hsqct1etf3gpsi3d.2** | HSQCT1ETF3GPSI3D.2)
  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_1 relaxation times using TROSY:
  Using 1H-decoupling (**trt1etf3gpsi** | TRT1ETF3GPSI)
  Using 1H-decoupling acquired as pseudo-3D (**trt1etf3gpsi3d**)
  Using 180 1H pulses acquired as pseudo-3D (**trt1etf3gpsi3d.2**)

- **T_2 (N):**

  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_2 relaxation times using PEP:
  Acquired as individual 2D data (**hsqct2etf3gpsi** | HSQCT2ETF3GPSI):
  Acquired as pseudo-3D (**hsqct2etf3gpsi3d** | HSQCT2ETF3GPSI3D)
  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_2 relaxation times using TROSY:
  Acquired as individual 2D (**trt2etf3gpsi** | TRT2ETF3GPSI)
  Acquired as pseudo-3D (**trt2etf3gpsi3d**)

- **T_{1rho} (N):**

  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_{1rho} relaxation times using PEP:
  Acquired as individual 2D data (**hsqctretf3gpsi** | HSQCTRETF3GPSI)
  Acquired as pseudo-3D (**hsqctretf3gpsi3d** | HSQCTRETF3GPSI3D)
  With adiabatic ramping and acquired as pseudo-3D (**hsqctretf3gpsi3d.2** | HSQCTRETF3GPSI3D.2)
  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N T_{1rho} relaxation times using TROSY:
  Acquired as pseudo-3D (**trtretf3gpsi3d**)

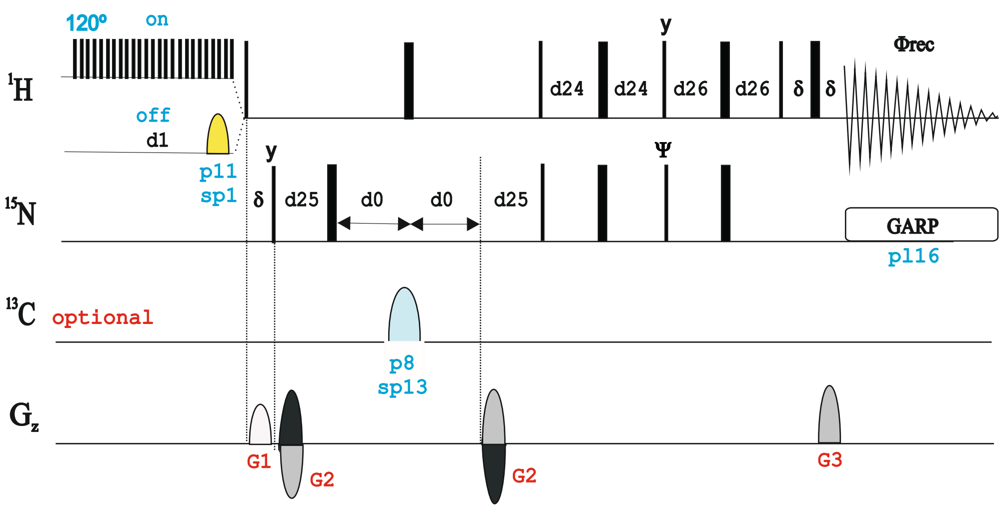
- **$R_{exchange}$ (N):**

  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N-R(exchange) using PEP and Relaxation-dispersion (**hsqcrexetf3gpsi3d** | HSQCTREXETF3GPSI3d)
  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N-R(exchange) using TROSY and Relaxation-dispersion (**trrexetf3gpsi3d**)
  Phase sensitive ge-2D ^{1}H-^{15}N HSQC to measure ^{15}N-exchange
  Using PEP (**hsqcetexf3gp**)
  Using WATERGATE (**hsqcexf3gpwgph**)
  Using TROSY (**tretexf3gp**)

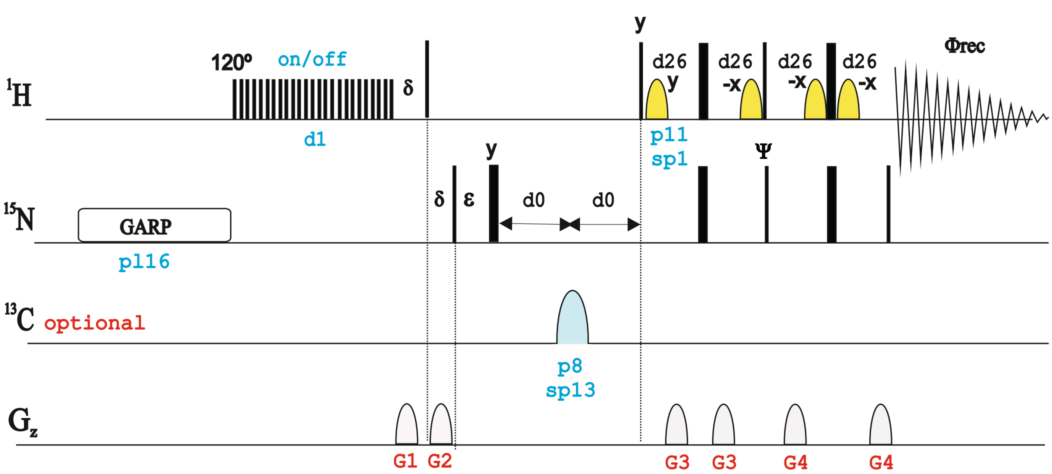
- **Cross-correlation:**

  Phase-sensitive ge-2D ^{1}H-^{15}N HSQC to measure N-15 / H-1 cross correlation (**hsqcccf3gpphwg**)

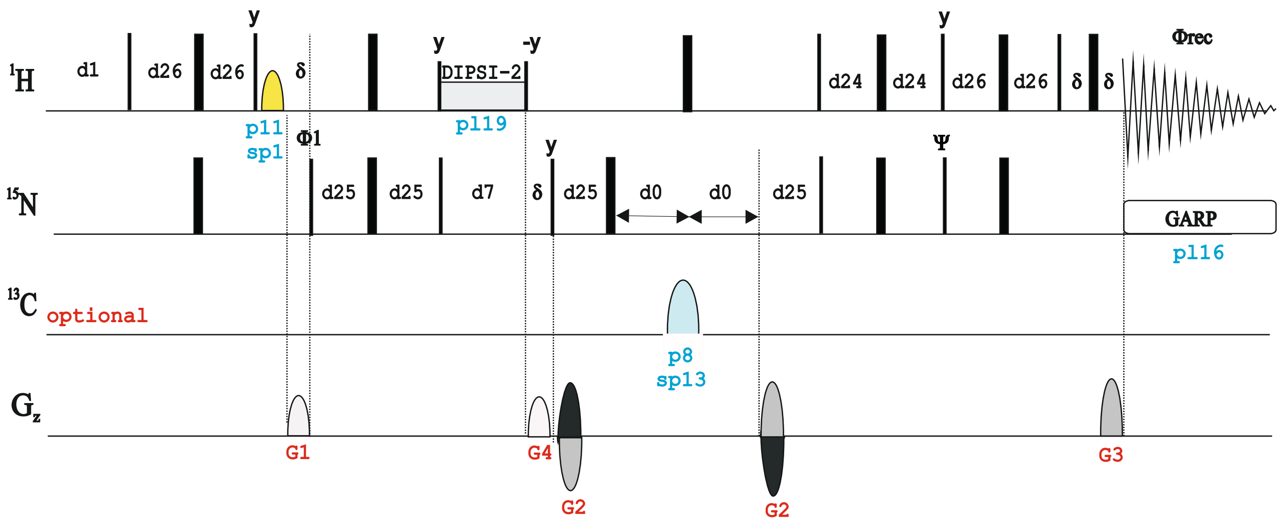
hsqcnoef3gpsi



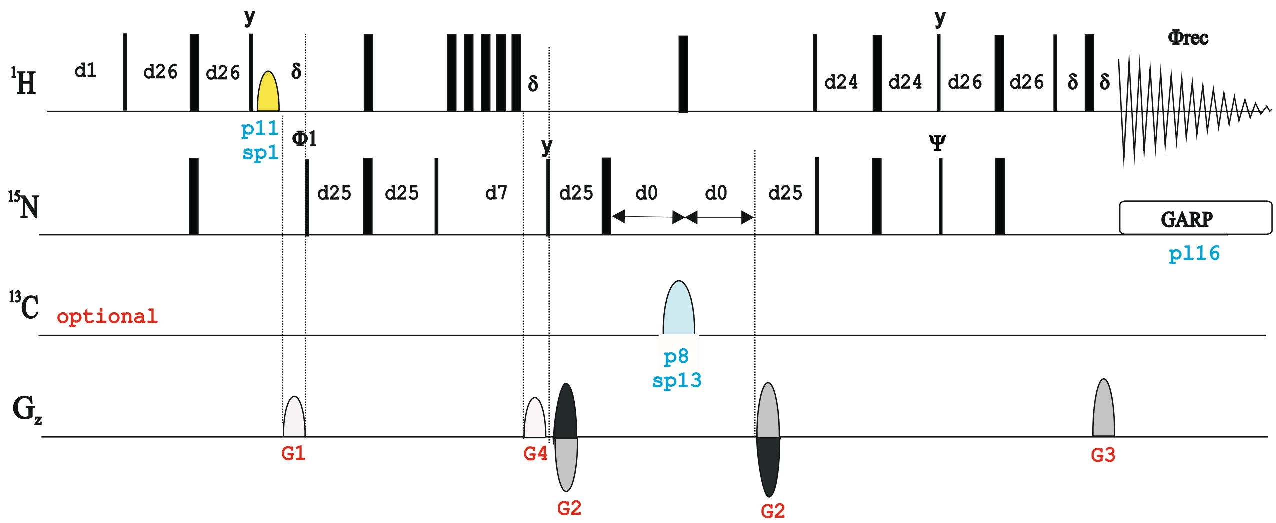
trnoef3gpsi



hsqct1etf3gpsi3d
hsqct1etf3gpsi

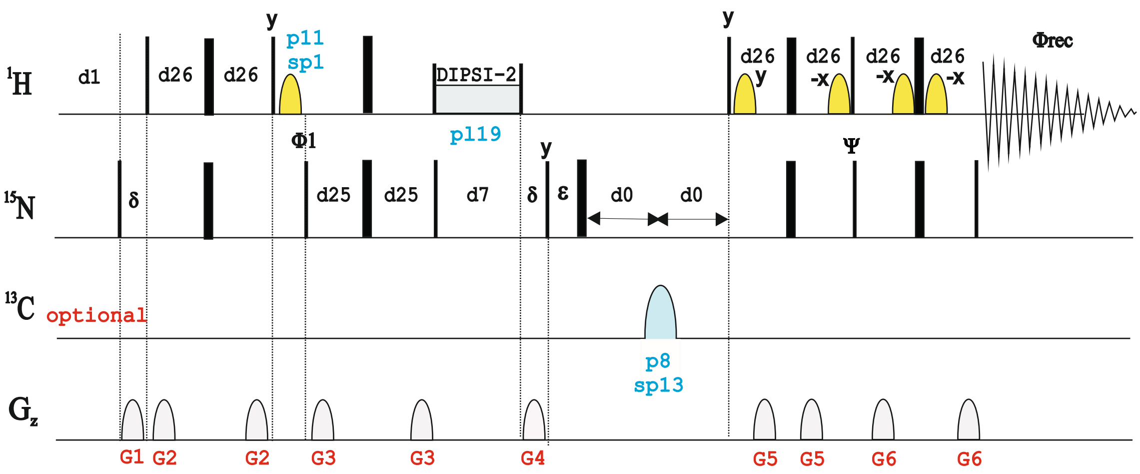


hsqct1etf3gpsi3d.2
hsqct1etf3gpsi.2



trt1etf3gpsi

trt1etf3gpsi3d



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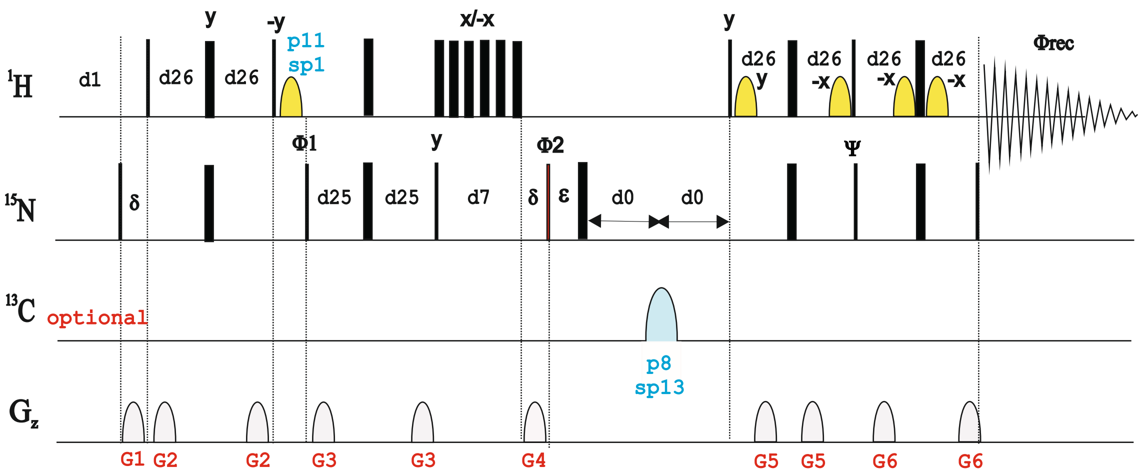

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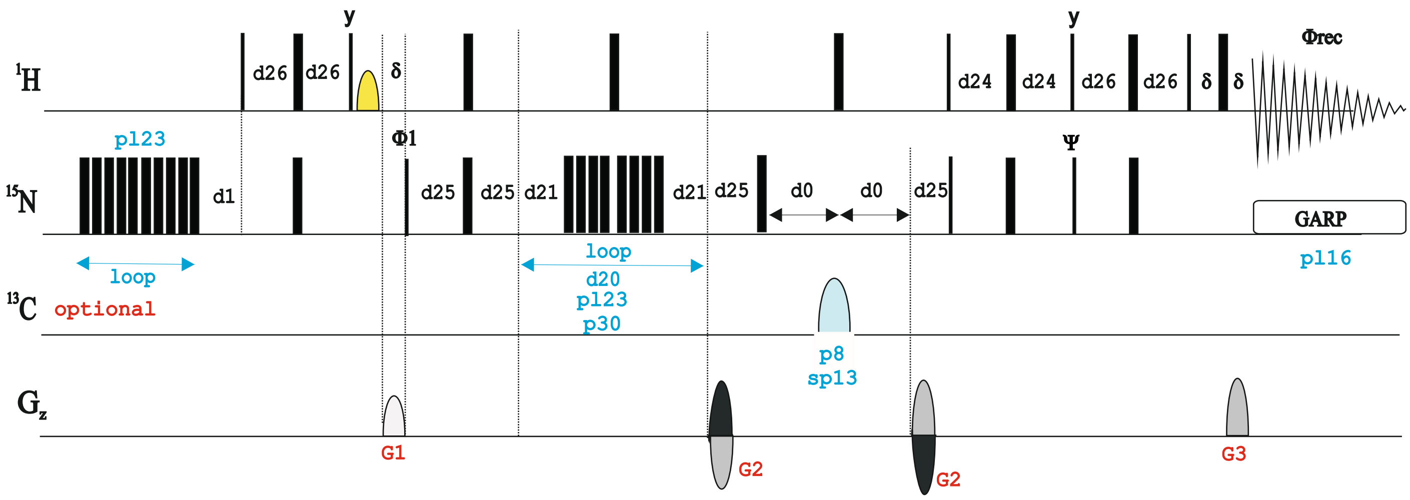

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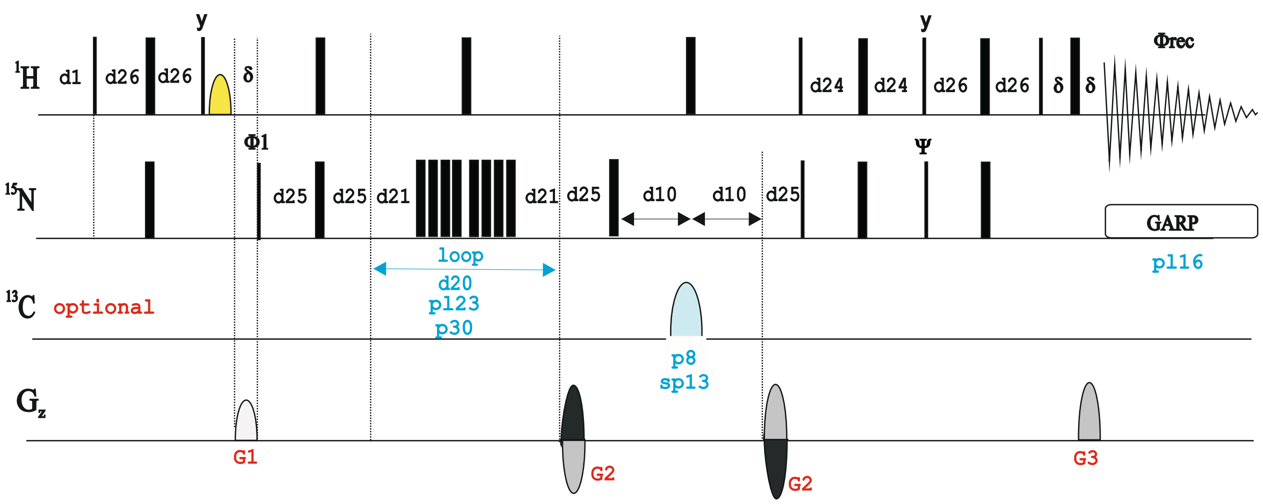
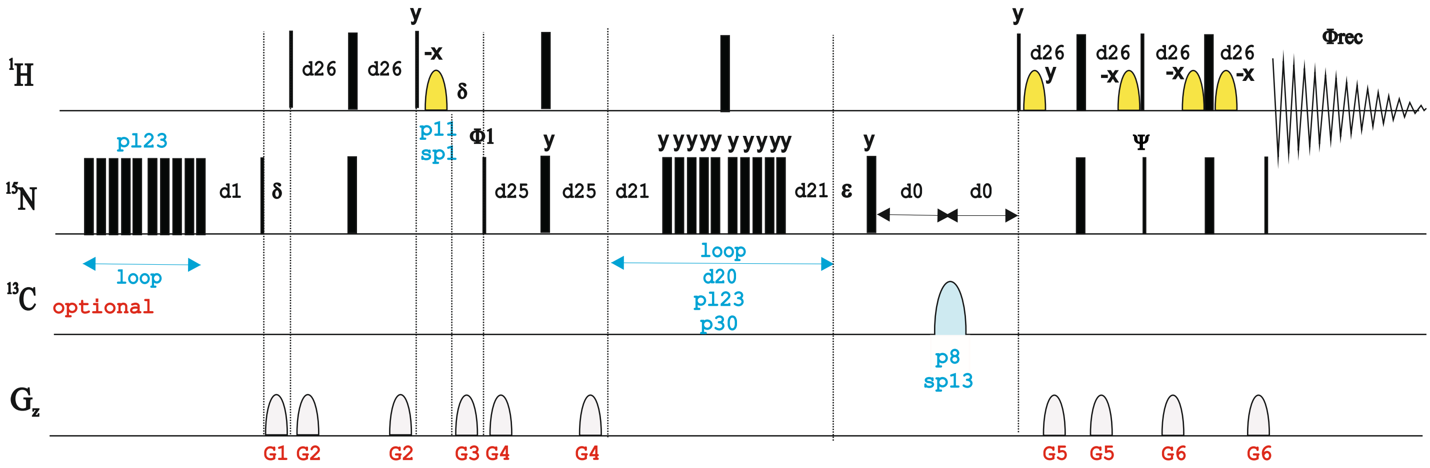
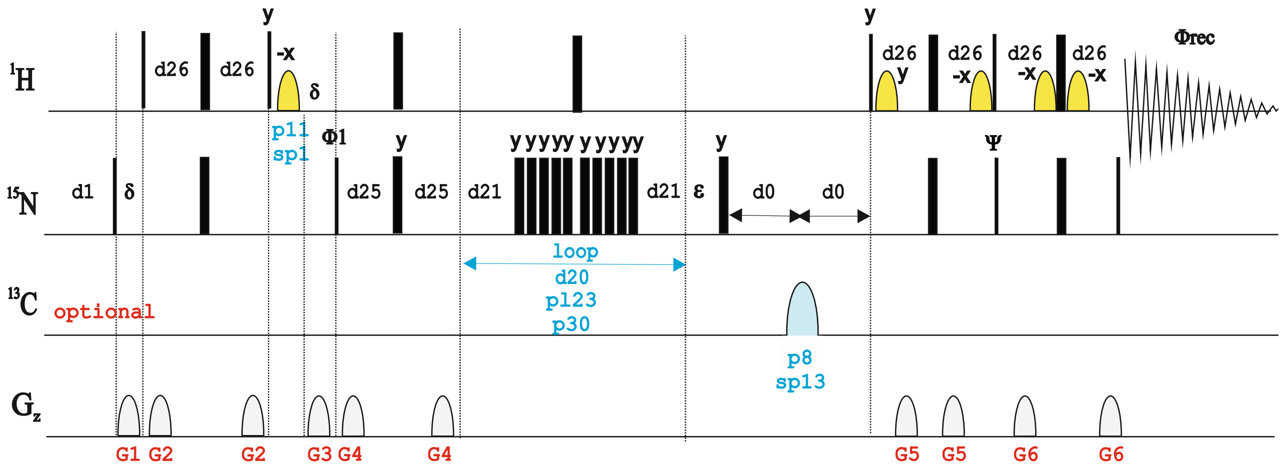


trt2etf3gpsi



trt2etf3gpsi3d



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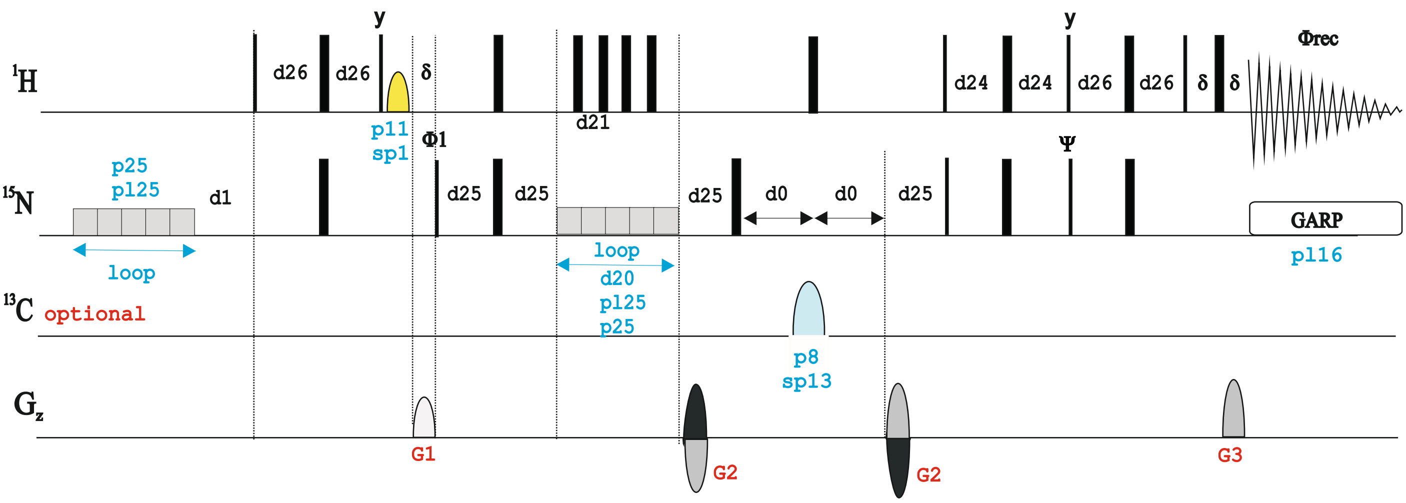

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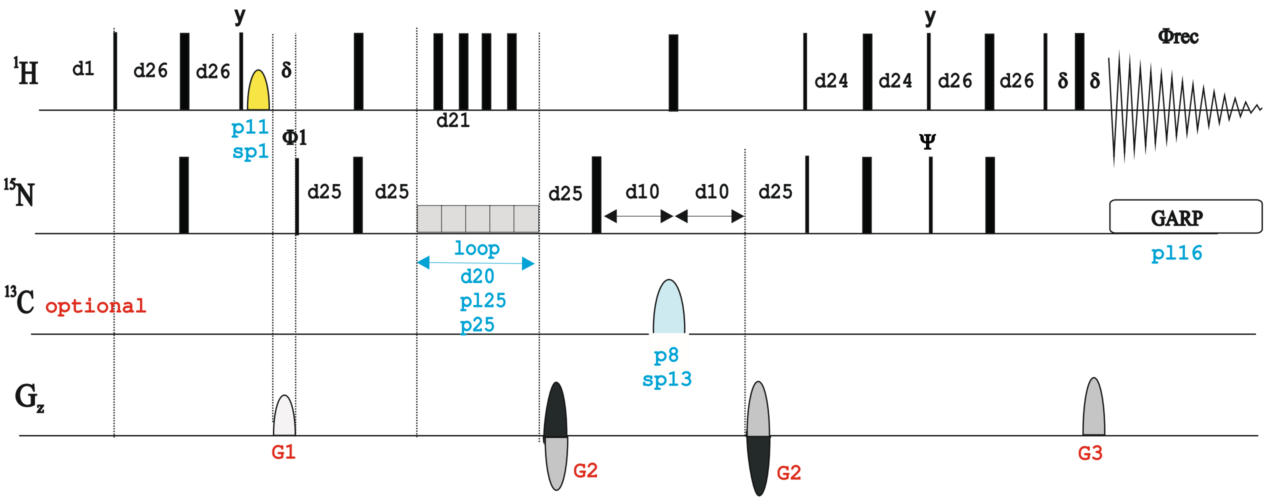
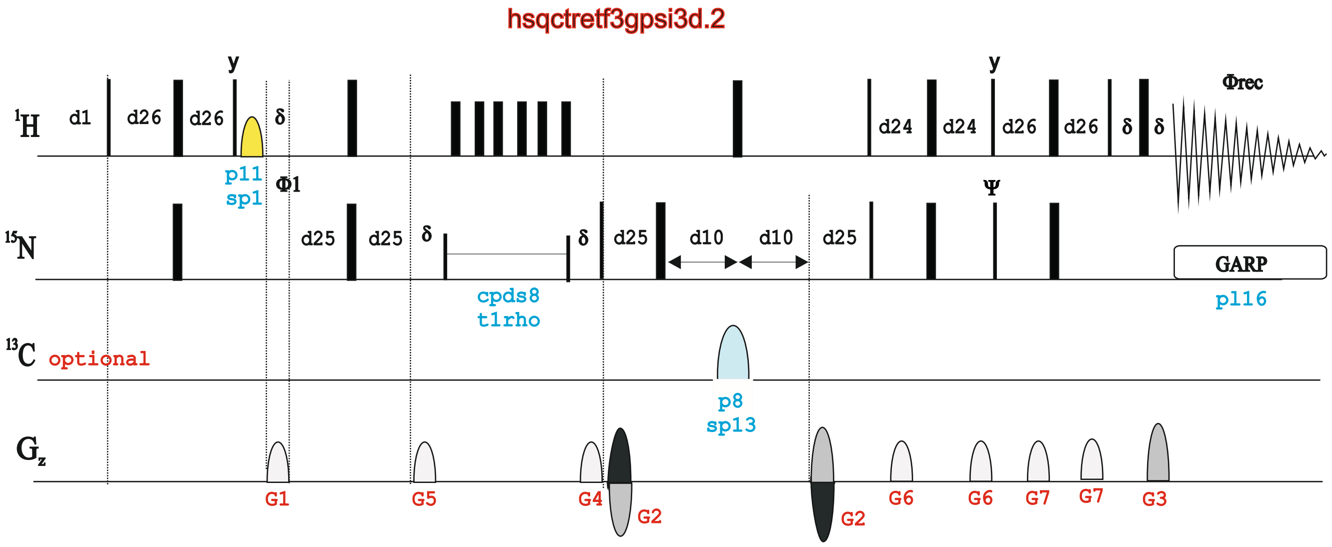
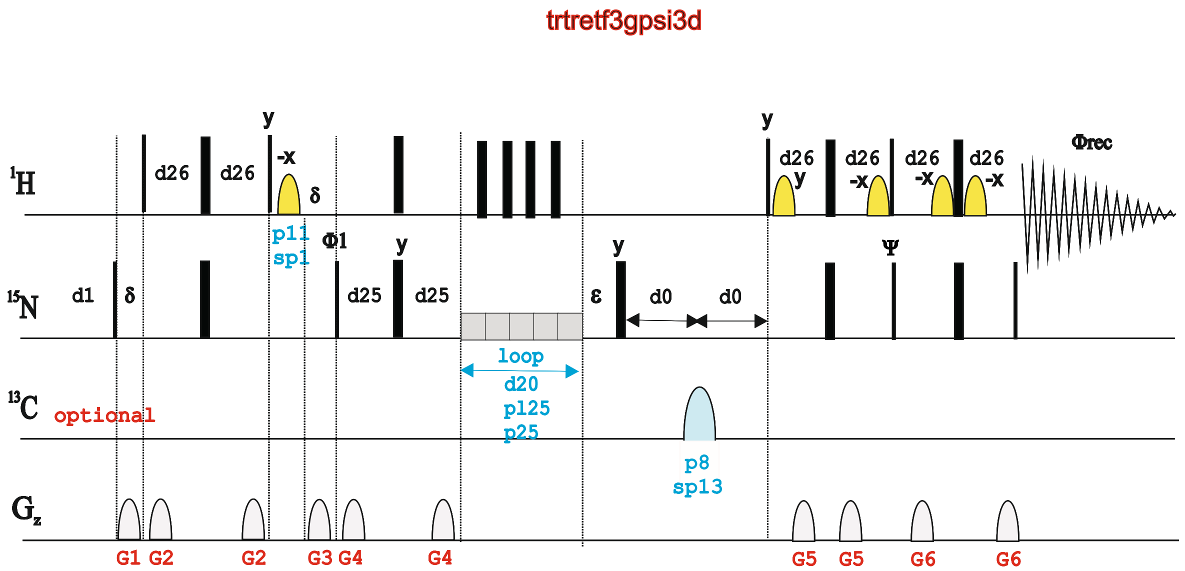
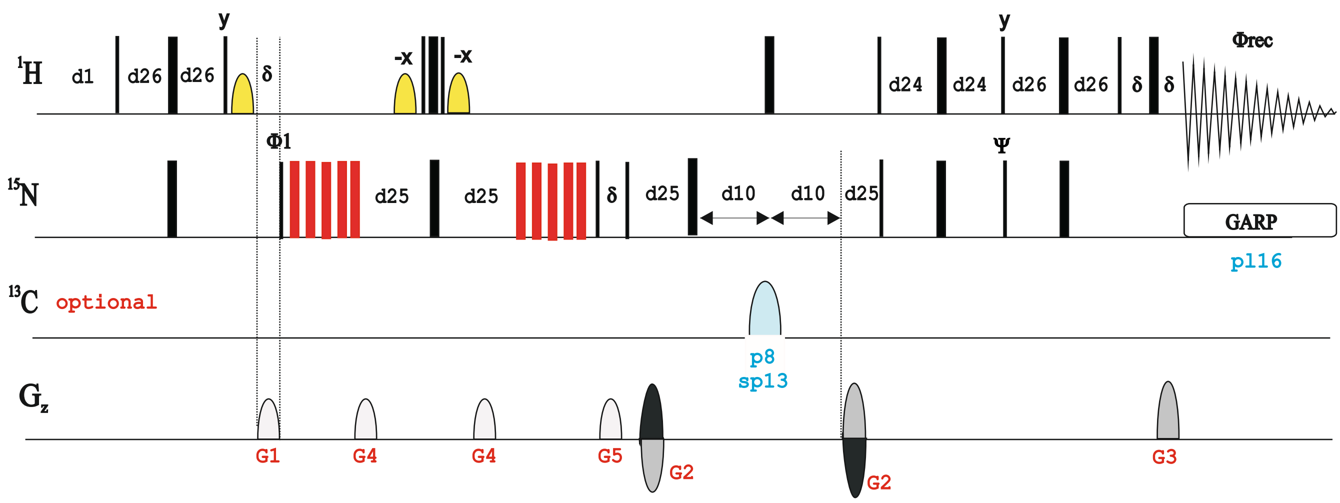



hsqctretf3gpsi3d.2
¹H
d1
d26
d26
y
δ
p11
sp1
Φ1
d24
d24
y
d26
d26
δ
δ
Φrec
¹⁵N
d25
d25
δ
δ
d25
d10
d10
d25
Ψ
cpds8
t1rho
GARP
p116
¹³C
optional
p8
sp13
Gz
G1
G5
G4
G2
G2
G6
G6
G7
G7
G3


trtretf3gpsi3d
¹H
d26
d26
y
-x
δ
p11
sp1
Φ1
y
d26
y
d26
-x
d26
-x
d26
-x
Φrec
¹⁵N
d1
δ
y
d25
d25
y
ε
d0
d0
Ψ
loop
d20
p125
p25
¹³C
optional
p8
sp13
Gz
G1
G2
G2
G3
G4
G4
G5
G5
G6
G6

hsqcrexetf3gpsi3d



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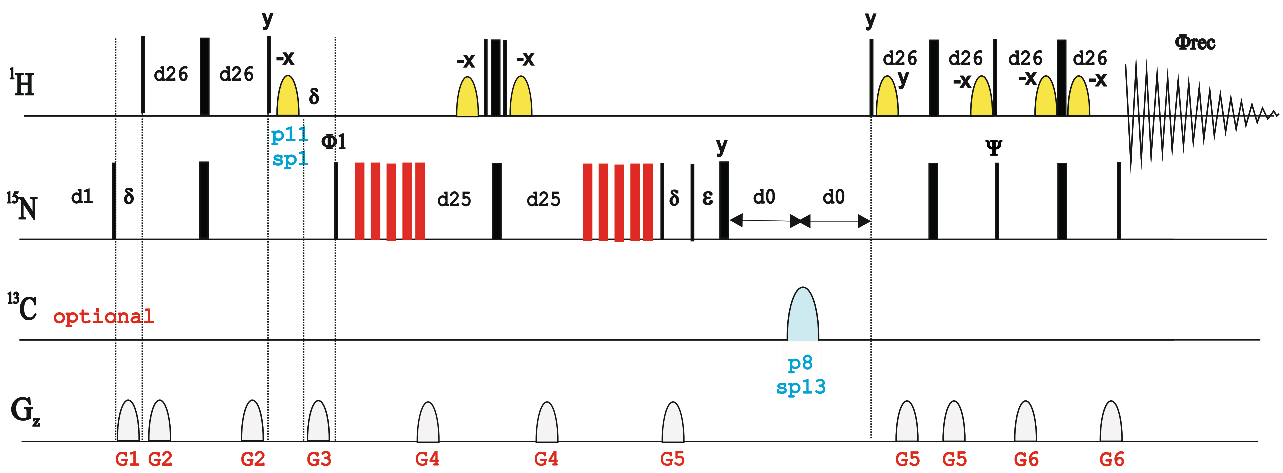

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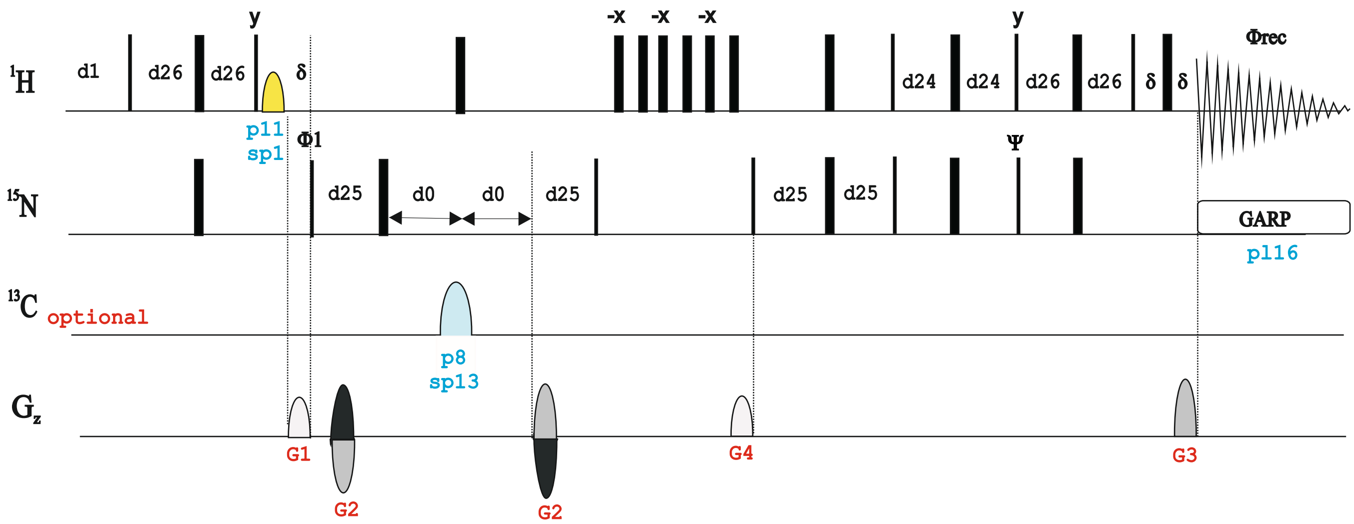

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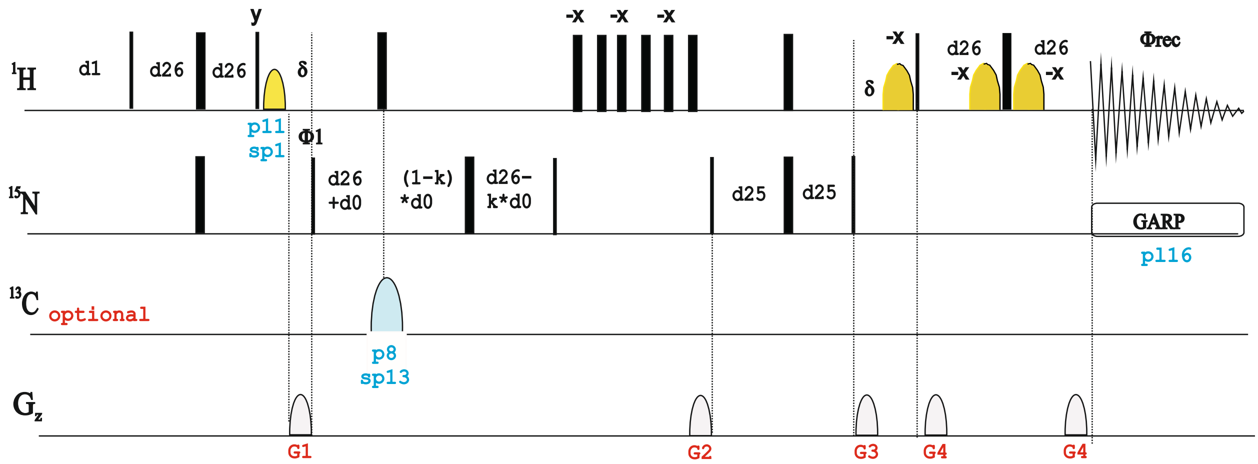
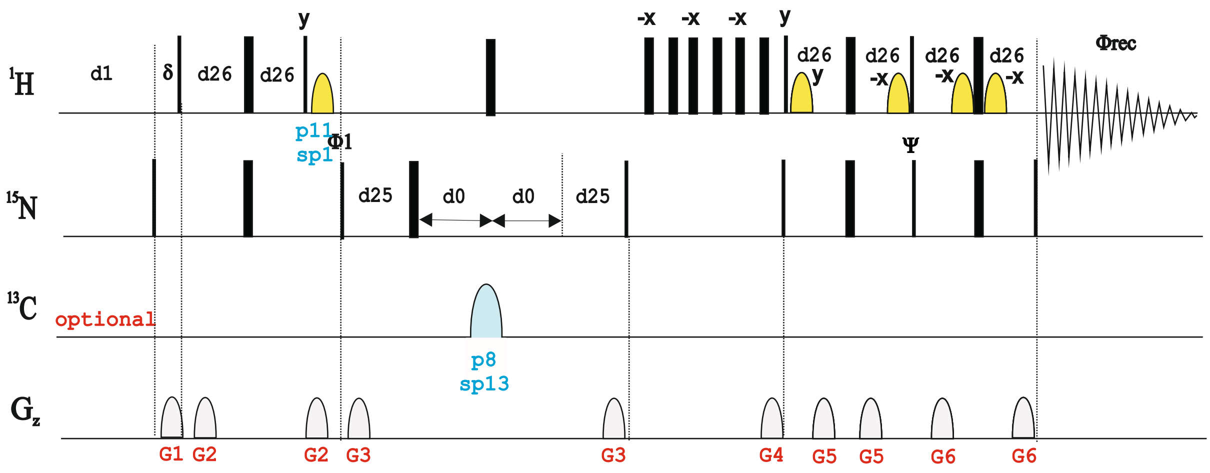


tretexf3gp



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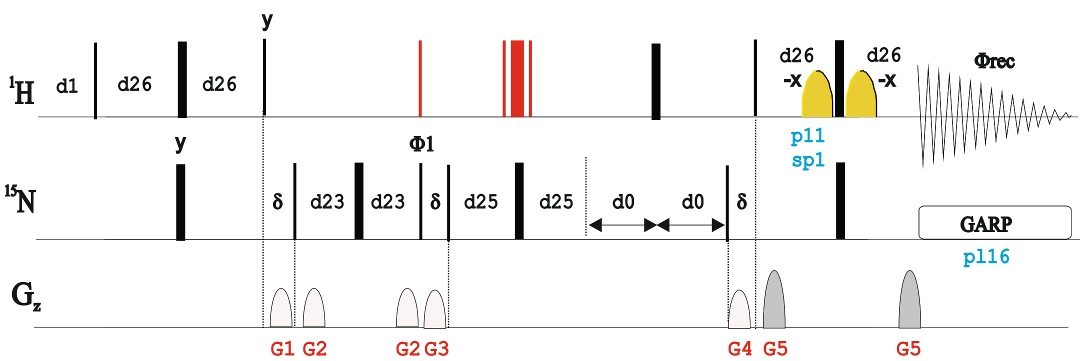

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3D HNCO EXPERIMENTS FOR
THE MEASUREMENT OF T1, T2 AND T1RHO
RELAXATION TIMES.

3D HNCO experiments for ^{15}N Relaxation Measurements

- **Heteronuclear ^{15}N-^{1}H NOEs:**

  3D HNCO to measure heteronuclear ^{15}N-^{1}H NOEs using PEP (**hnconoef3gpsi**)

- **T_1 (N):**

  3D HNCO to measure ^{15}N T_1 relaxation times
  Using PEP (**hncot1f3gpsi**)
  Using TROSY (**trhncot1f3gp**)

- **T_2 (N):**

  3D HNCO to measure ^{15}N T_2 relaxation times
  Using PEP (**hncot2f3gpsi**)
  Using TROSY (**trhncot2f3gp**)

- **T_{1rho} (N):**

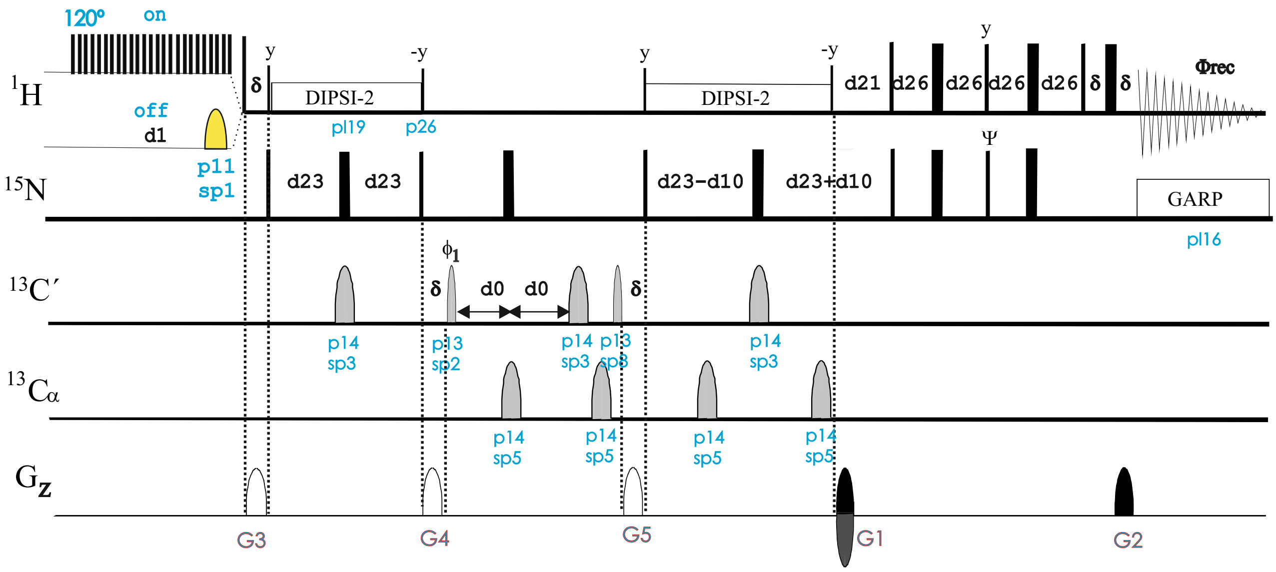
  3D HNCO to measure ^{15}N T_{1rho} relaxation times
  Using PEP (**hncotrf3gpsi**)
  Using TROSY (**trhncotrf3gp**)

- **$R_{exchange}$ (N):**

  3D HNCO to measure ^{15}N $R_{exhange}$
  Using PEP (**hncorexf3gpsi**)
  Using TROSY (**trhncorexf3gp**)

Also see:
T1 & T2 Relaxation
2D HSQC Experiments for Relaxation Measurements

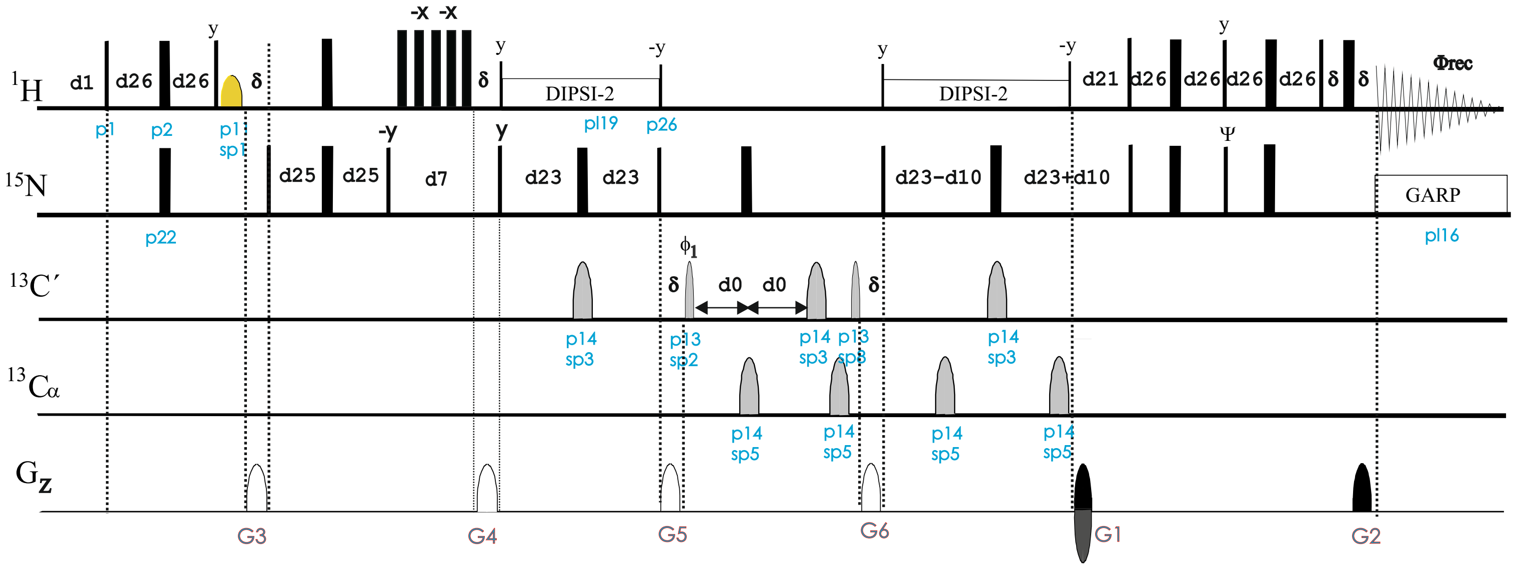
hnconoef3gpsi



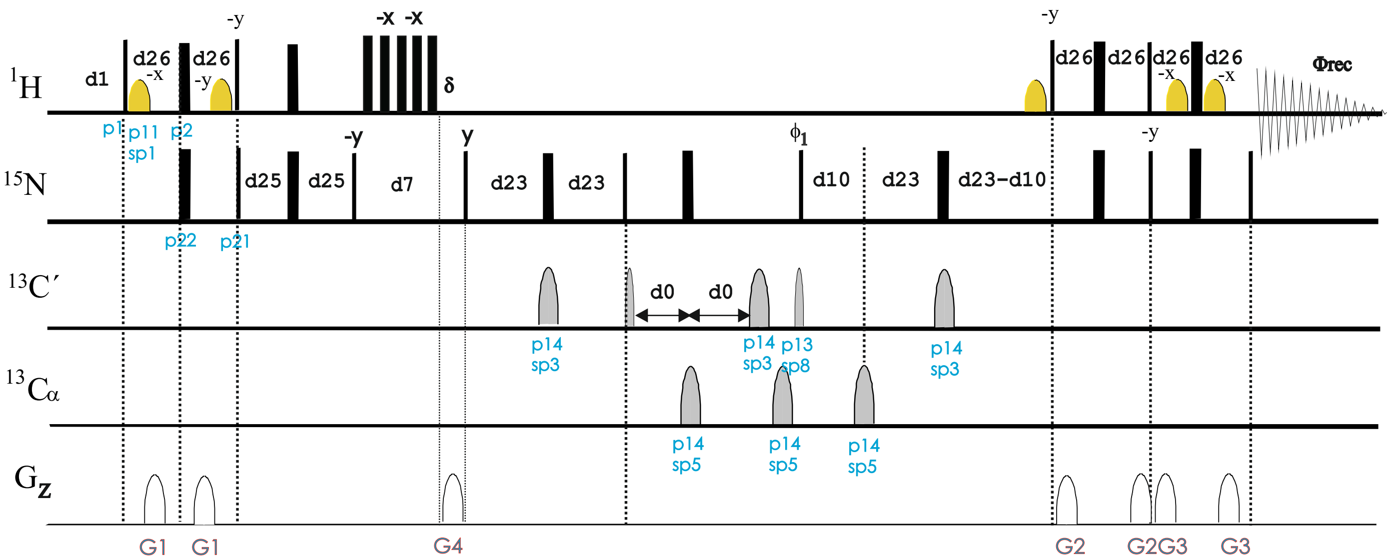
References:

V. Tugarinov, W.-Y. Choy, E. Kupce & L.E. Kay, J. Biomol. NMR 30, 347-352 (2004)

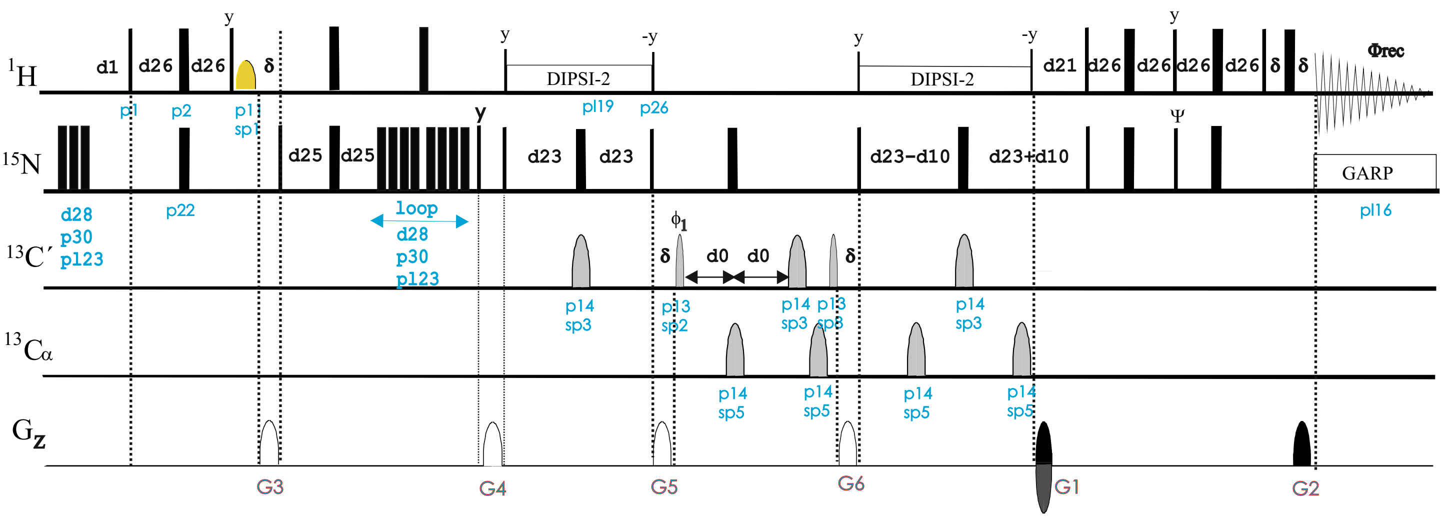
hncot1f3gpsi



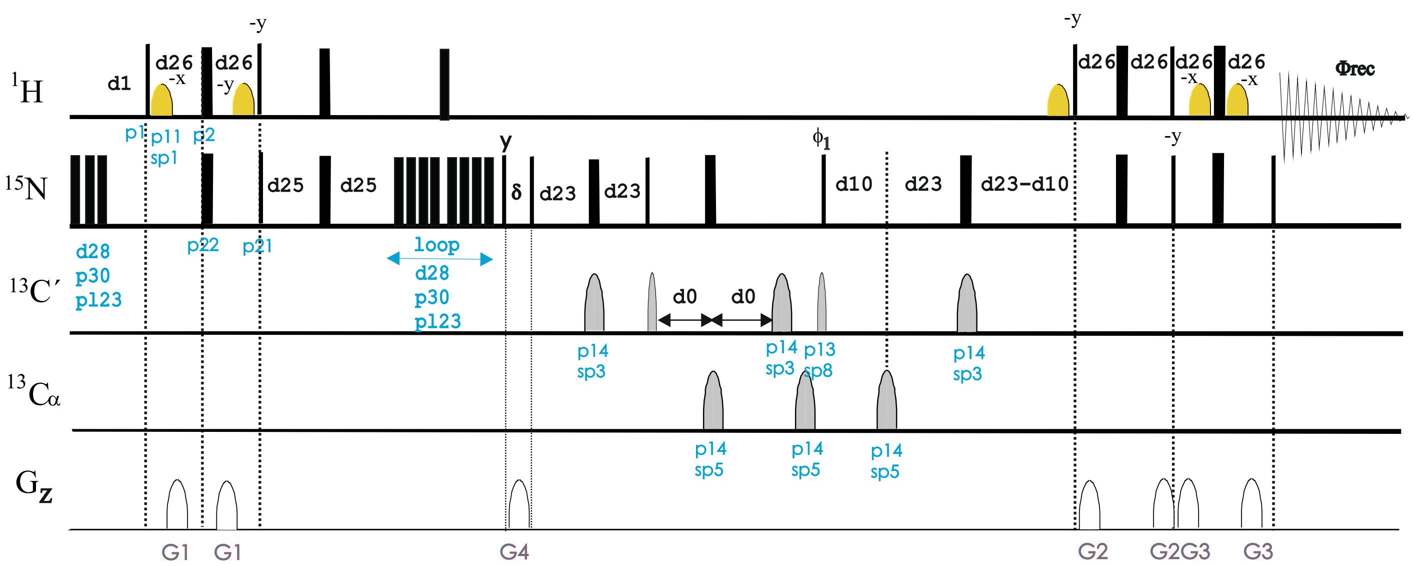
trhncot1f3gp



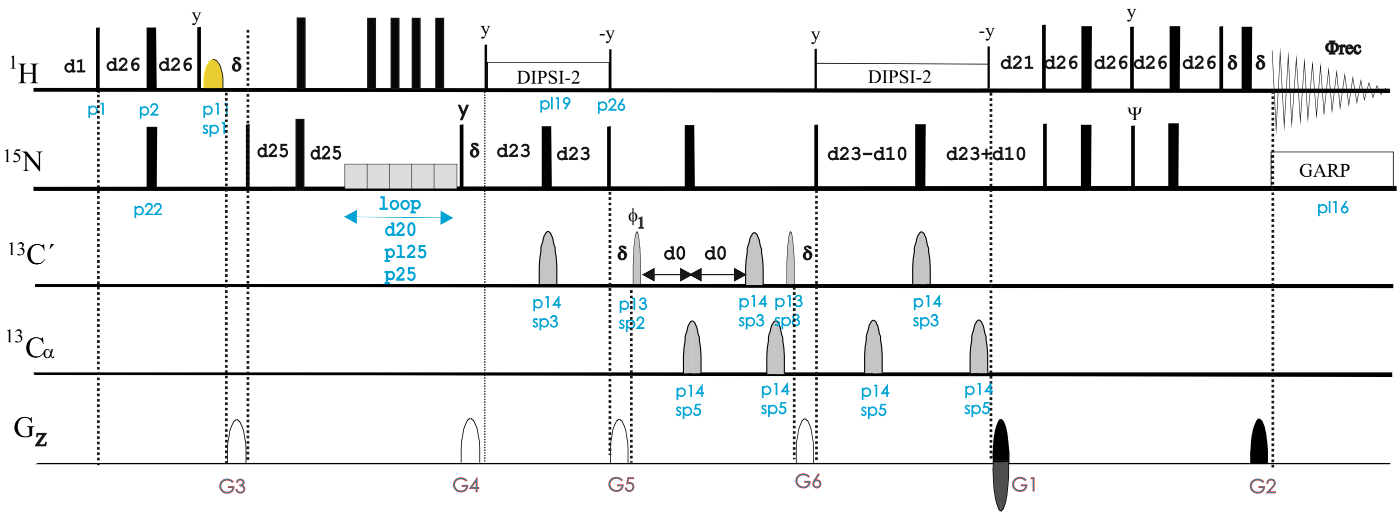
hncot2f3gpsi



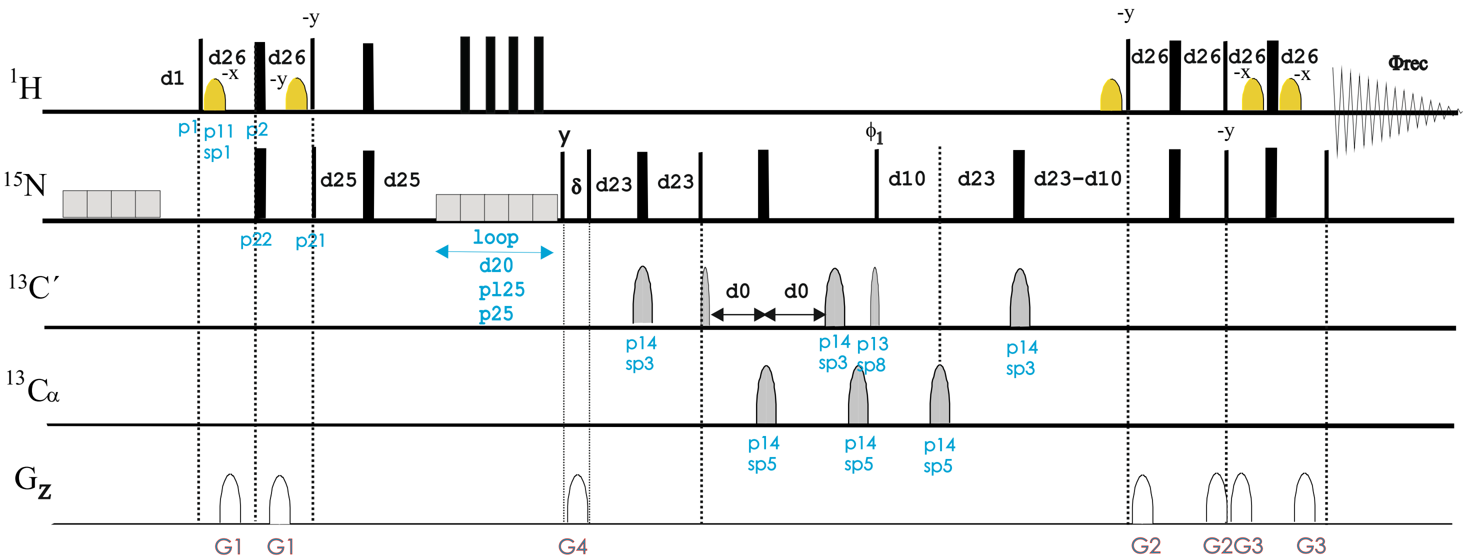
trhncot2f3gp



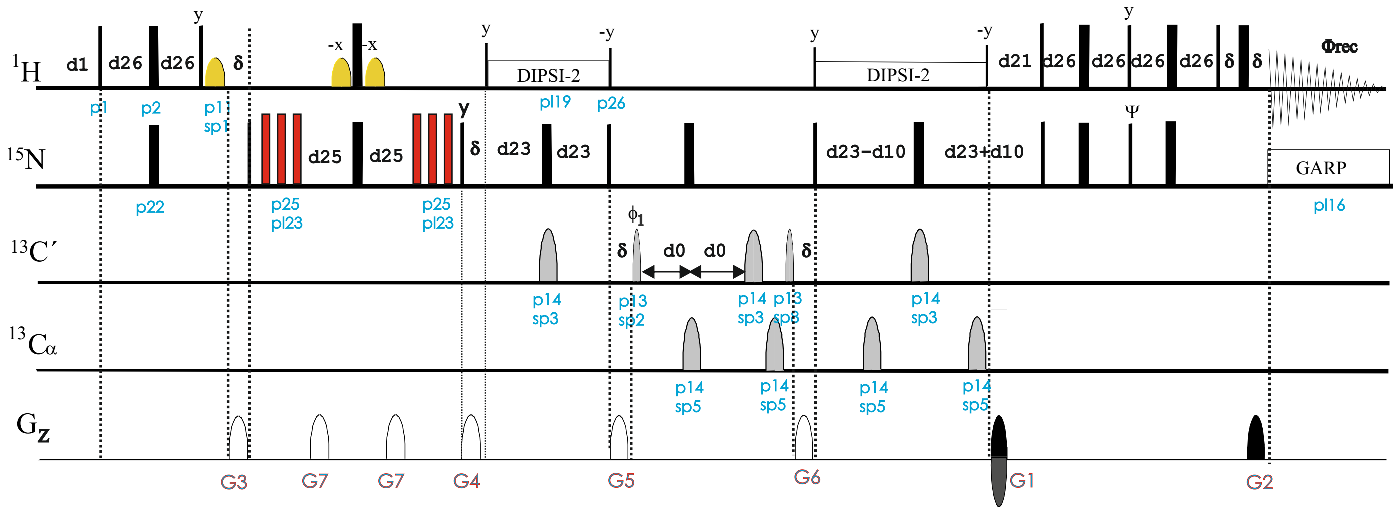
hncotrf3gpsi



trhncotrf3gp



hncorexf3gpsi



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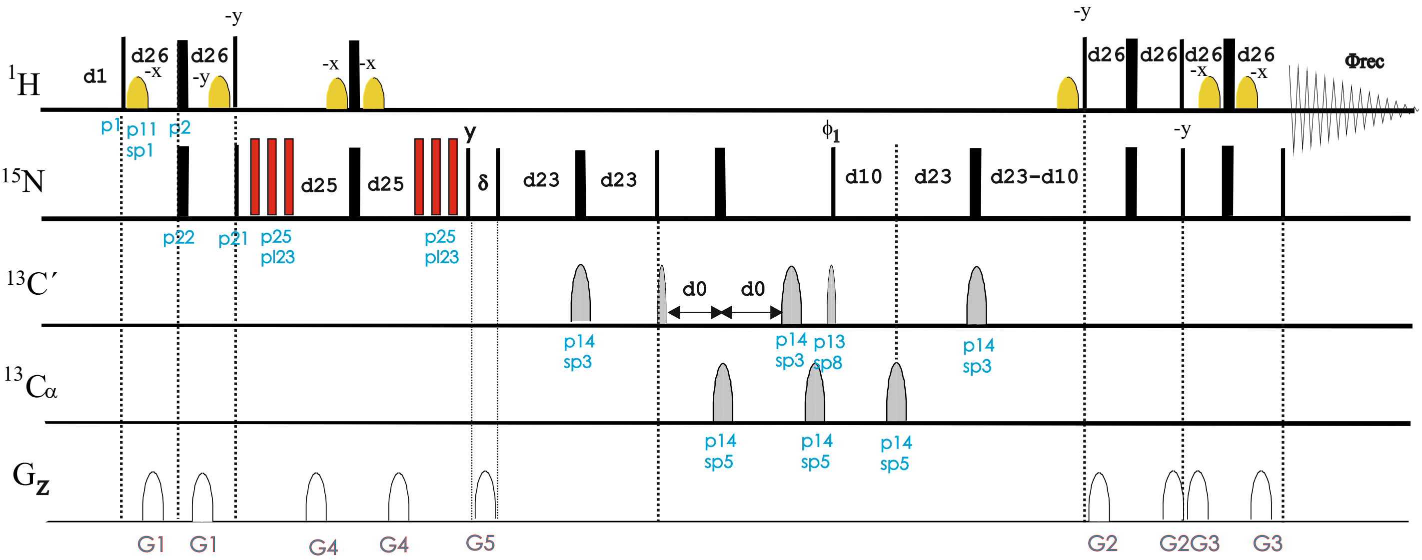

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PROTEIN NMR
COUPLING CONSTANTS

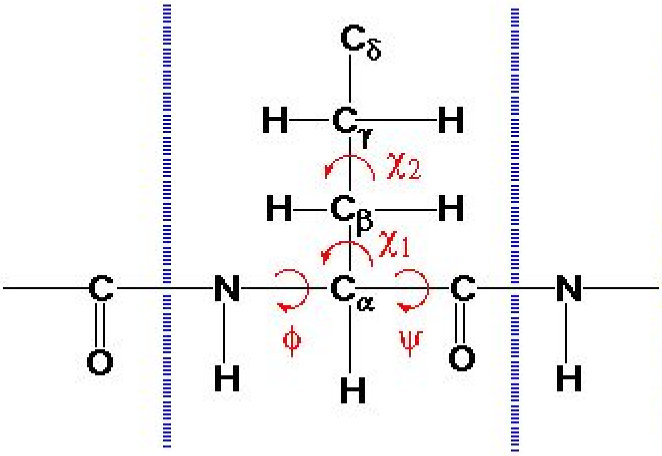
Protein NMR

Coupling Constants

Tutorials: J Backbone
Tutorials: J Sidechain
Tutorials: J Miscellaneous

NMR Experiments

- Introduction
- Determination
- J-Resolved
- Spin-State Selective
- E.COSY
- TROSY/antiTROSY
- J-scaling
- J-Quantitative
- DQ-ZQ



Scalar Couplings (J)

- One-bond
- Two-bond
- Three-bond

- Backbone Three-bond ϕ
- Backbone Three-bond ω
- Backbone Three-bond ψ
- Sidechain Three-bond χ_1
- Sidechain Three-bond χ_2

Dipolar Couplings (D)

- Introduction
- Anisotropic Media
- NMR Experiments
- Structure Calculation

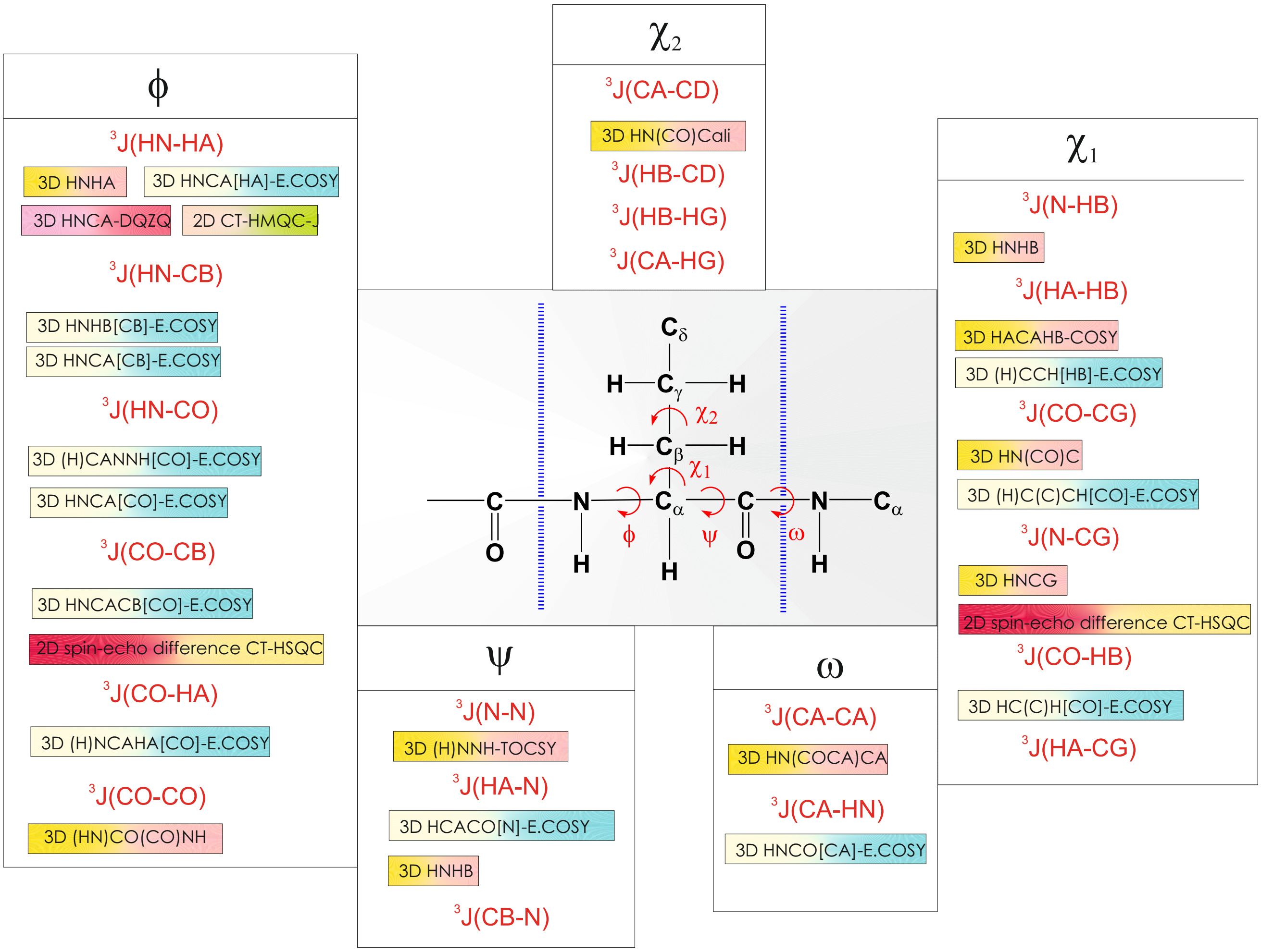
- Applications

Cross-Hydrogen Bond (^hJ)

- Introduction
- NMR Experiments
- Applications

2D Experiments | 3D Double-Resonance Experiments
3D Triple-Resonance Experiments

General Reading: 76PROG41, B03ZER147


φ
3J(HN-HA)
3D HNHA
3D HNCA[HA]-E.COSY
3D HNCA-DQZQ
2D CT-HMQC-J
3J(HN-CB)
3D HNHB[CB]-E.COSY
3D HNCA[CB]-E.COSY
3J(HN-CO)
3D (H)CANNH[CO]-E.COSY
3D HNCA[CO]-E.COSY
3J(CO-CB)
3D HNCACB[CO]-E.COSY
2D spin-echo difference CT-HSQC
3J(CO-HA)
3D (H)NCAHA[CO]-E.COSY
3J(CO-CO)
3D (HN)CO(CO)NH
χ2
3J(CA-CD)
3D HN(CO)Cali
3J(HB-CD)
3J(HB-HG)
3J(CA-HG)
χ1
3J(N-HB)
3D HNHB
3J(HA-HB)
3D HACAHB-COSY
3D (H)CCH[HB]-E.COSY
3J(CO-CG)
3D HN(CO)C
3D (H)C(C)CH[CO]-E.COSY
3J(N-CG)
3D HNCG
2D spin-echo difference CT-HSQC
3J(CO-HB)
3D HC(C)H[CO]-E.COSY
3J(HA-CG)
ψ
3J(N-N)
3D (H)NNH-TOCSY
3J(HA-N)
3D HCACO[N]-E.COSY
3D HNHB
3J(CB-N)
ω
3J(CA-CA)
3D HN(COCA)CA
3J(CA-HN)
3D HNCO[CA]-E.COSY

PROTEIN NMR
COUPLING CONSTANTS

Phi Backbone Coupling Constant

- 3D HNHA experiment (**hnhagp3d** | HNHAGP3D) - 3J(HN-HA) via quantitative-J
- 3D HNCA[HA,CB]-E.COSY (**hncaecosgp3d** | HNCAECOSGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via E.COSY
- 3D HNCA[HA]-E.COSY (**hncaecosgp3d2** | HNCAECOSGP3D2) - 3J[H(N)-HA] via E.COSY
- 3D DQ/ZQ HNCA (**hncadqzqgp3d** | HNCADQZQGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via DQ/ZQ
- 2D CT-HMQC-J (**hmqcjgp** | HMQCJGP) - 3J[H(N)-HA] via J-modulation
- 3D HNHB[CB]-E.COSY (**hnhbecosgp3d** | HNHBECOSGP3D) - 3J[H(N)-CB] via E.COSY
- 3D HNCA[CB]-E.COSY (**hncajcgp3d** | HNCAJCGP3D) - 3J[H(N)-CB] via E.COSY
- 3D (H)CANNH[CO]-E.COSY (**hcannhgp3d** | HCANNHGP3D) - 3J[H(N)-CO] via E.COSY
- 3D HNCA[CO]-E.COSY (**hncacosygp3d** | HNCACOSYGP3D) - 3J[H(N)-CO] via E.COSY
- 3D HNCACB[CO]-E.COSY (**hncacbgpjc3d** | HNCACBGPJC3D) - 3J[CO-CB] via E.COSY
- 2D spin-echo difference CT-HSQC (**hsqccte tgpjclr** | HSQCCTETGPJCLR) - 3J[CO-CB] via spin-echo difference
- 3D (H)NCAHA[CO]-E.COSY (**hncahagp3d** | HNCAHAGP3D) - 3J[HA-CO] via E.COSY
- 3D (HN)CO(CO)NH (**hncocogp3d** | HNCOCOGP3D) - 3J[CO-CO] via quantitative-J

Psi Backbone Coupling Constant

- 3D (H)NNH-TOCSY (**hnnhdigp3d** | HNNHDIGP3D) - 3J[N-N] via quantitative-J
- 3D HCACO[N]-E.COSY (**hcacogpjc3d** | HCACOGPJC3D) - 3J[HA-N] via E.COSY
- 3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J

Omega Backbone Coupling Constant

- 3D HN(COCA)CA (**hncocacagp3d** | HNCOCACAGP3D) - 3J[CA-CA] via quantitative-J
- 3D HNCO[CA]-E.COSY (**hncoecosgp3d** | HNCOECOSGP3D) - 3J[H(N)-CA] via E.COSY

Chi1 Sidechain Coupling Constant

- 3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J
- 3D HACAHB-COSY (**hacahbcosygp3d** | HACAHBCOSYGP3D) - 3J[HA-HB] via quantitative-J
- 3D HN(CO)C (**hncocgp3d** | HNCOCGP3D) - 3J[CG-CO] via quantitative-J
- 3D HC(C)H[HA]-E.COSY (**hcchecosgp3d** | HCCHECOSGP3D) - 3J[HA-HB] via E.COSY
- 3D HC(C)H[CO]-E.COSY (**hcchcosygp3d** | HCCHCOSYGP3D) - 3J[CO-HB] via E.COSY
- 3D (H)C(C)CH[CO]-E.COSY (**hccccosygp3d** | HCCCCOSYGP3D) - 3J[CG-CO] via E.COSY
- 3D HNCG (**hncggp3d.1** | HNCGGP3D.1) - 3J[N-CG] via quantitative-J
- 3D HNCG (**hncggp3d.2** | HNCGGP3D.2) - 3J[N-CG] via quantitative-J
- 2D spin-echo difference CT-HSQC (**hsqcetfpf3gpjcsi** | HSQCETFPFGPJCSI) - 3J[N-CG] via spin-echo difference

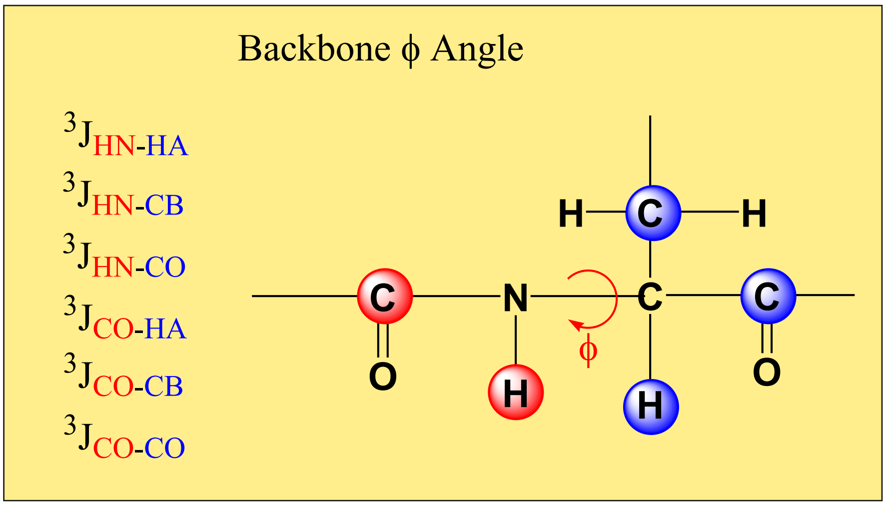
Chi2 Sidechain Coupling Constant

- 3D HN(CO)CACali (**hncocacgp3d** | HNCOCACGP3D) - 3J[CA-CD] via quantitative-J

BRUKER
PULSE PROGRAM
CATALOGUE

NMRGuide

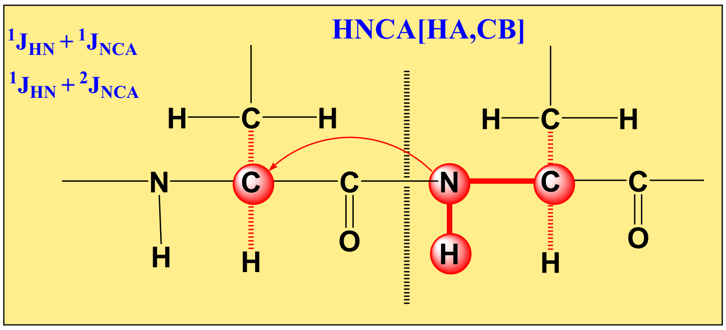
PROTEIN NMR
COUPLING CONSTANTS
PHI BACKBONE ANGLE



Phi Backbone Coupling Constant

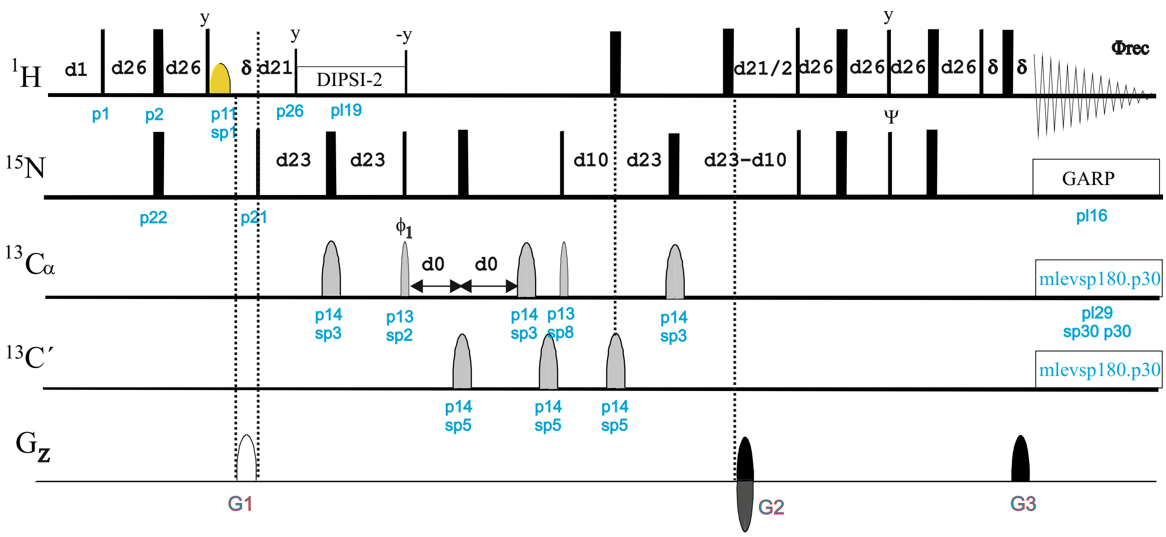
- 3D HNHA experiment (**hnhagp3d** | HNHAGP3D) - 3J(HN-HA) via quantitative-J
- 3D HNCA[HA,CB]-E.COSY (**hncaecosgp3d** | HNCAECOSGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via E.COSY
- 3D HNCA[HA]-E.COSY (**hncaecosgp3d2** | HNCAECOSGP3D2) - 3J[H(N)-HA] via E.COSY
- 3D DQ/ZQ HNCA (**hncadqzqgp3d** | HNCADQZQGP3D) - 3J[H(N)-HA] and 3J[H(N)-CB] via DQ/ZQ
- 2D CT-HMQC-J (**hmqcjgp** | HMQCJGP) - 3J[H(N)-HA] via J-modulation
- 3D HNHB[CB]-E.COSY (**hnhbecosgp3d** | HNHBECOSGP3D) - 3J[H(N)-CB] via E.COSY
- 3D HNCA[CB]-E.COSY (**hncajcgp3d** | HNCAJCGP3D) - 3J[H(N)-CB] via E.COSY
- 3D (H)CANNH[CO]-E.COSY (**hcannhgp3d** | HCANNHGP3D) - 3J[H(N)-CO] via E.COSY
- 3D HNCA[CO]-E.COSY (**hncacosygp3d** | HNCACOSYGP3D) - 3J[H(N)-CO] via E.COSY
- 3D HNCACB[CO]-E.COSY (**hncacbgpjc3d** | HNCACBGPJC3D) - 3J[CO-CB] via E.COSY
- 2D spin-echo difference CT-HSQC (**hsqcctetgpjclr** | HSQCCTETGPJCLR) - 3J[CO-CB] via spin-echo difference
- 3D (H)NCAHA[CO]-E.COSY (**hncahagp3d** | HNCAHAGP3D) - 3J[HA-CO] via E.COSY
- 3D (HN)CO(CO)NH (**hncocogp3d** | HNCOCOGP3D) - 3J[CO-CO] via quantitative-J

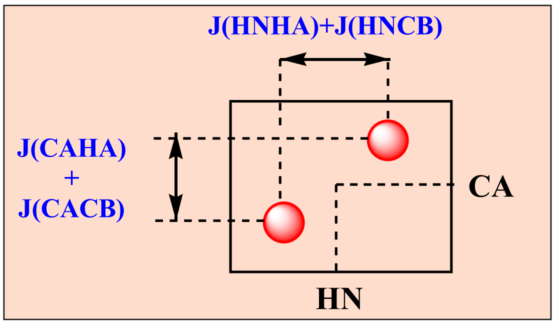
3D HNCA[HA,CB]-E.COSY Experiment

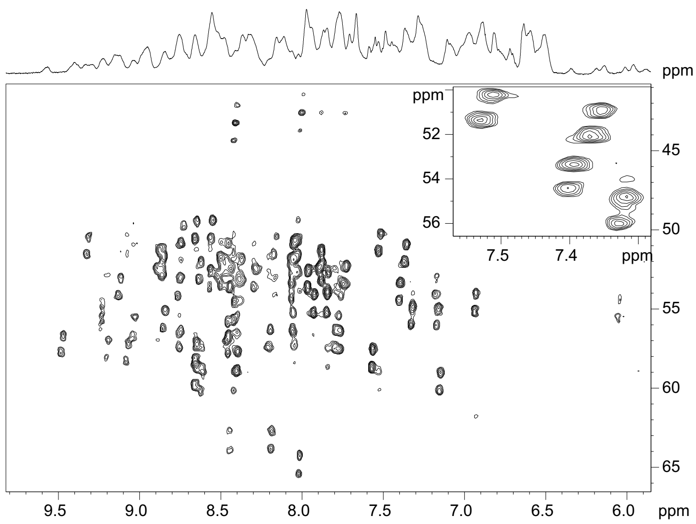


J(HN-HA)
J(HN-CB)
E.COSY

hncaecosgp3d

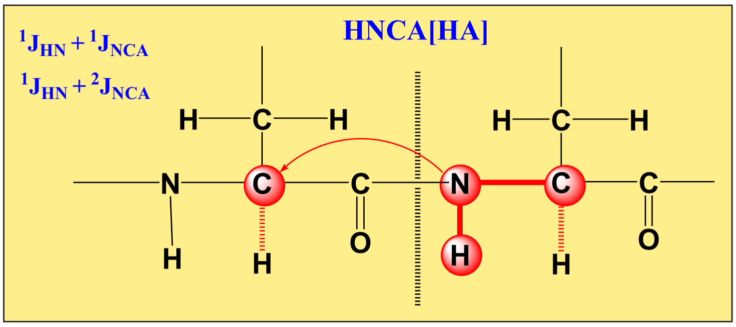






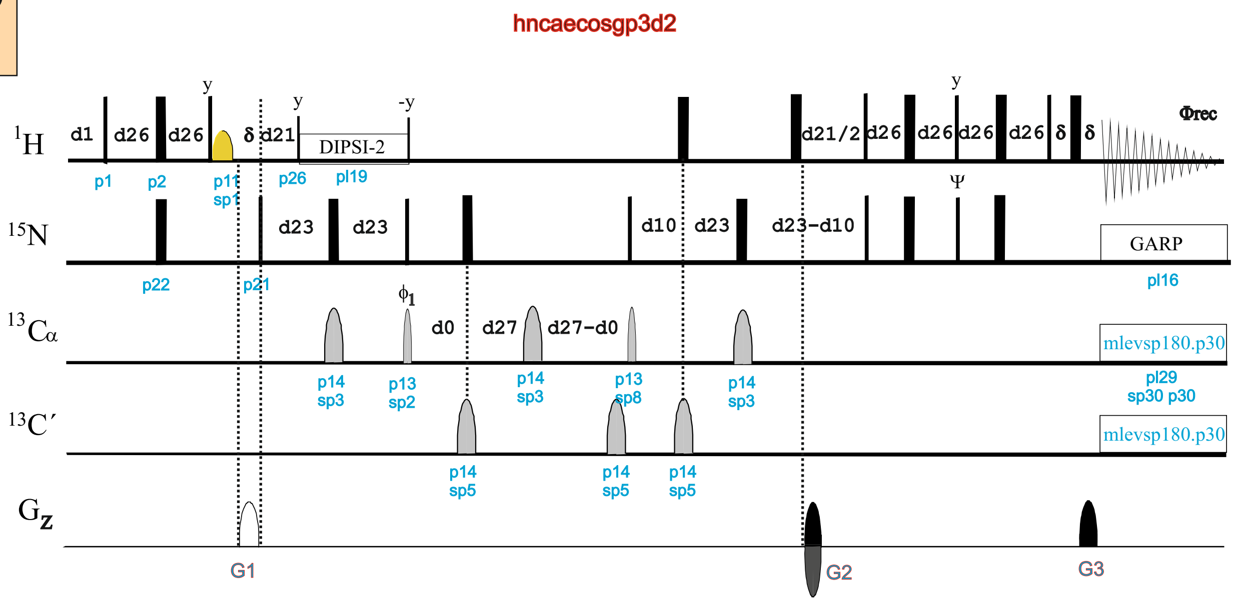
R.Weisemann, H. Rueterjans, H. Schwalbe, J. Schleucher, W. Bermel & C. Griesinger, J. Biomol. NMR 4, 231-240 (1994)

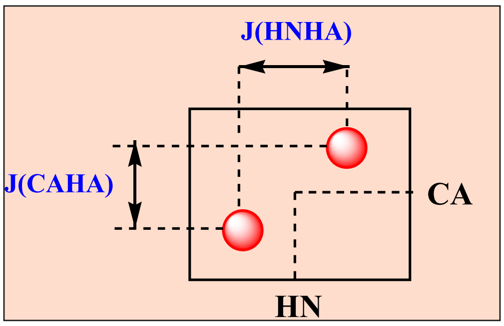
3D HNCA[HA]-E.COSY Experiment

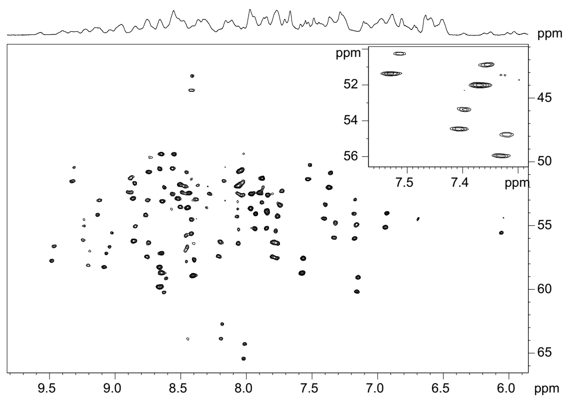


d21: 1/(2J(NH) [5.5 msec]
d23: 1/(4J(NCa) [12 msec]
d26: 1/(4J'(NH) [2.3 msec]
d27: constant time delay T(C) [13.3 msec]

J(HN-HA)
E.COSY





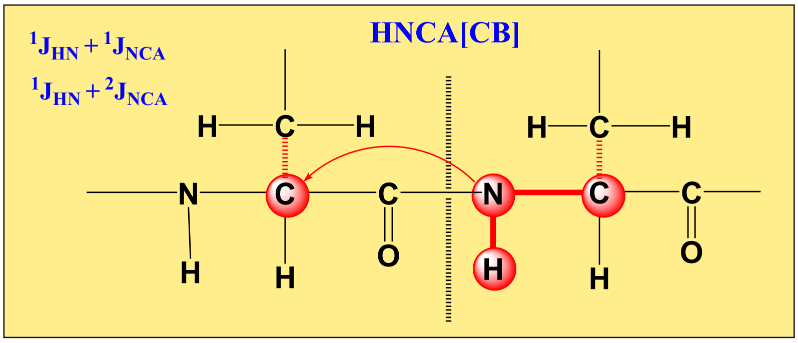


R.Weisemann, H. Rueterjans, H. Schwalbe, J. Schleucher, W. Bermel & C. Griesinger, J. Biomol. NMR 4, 231-240 (1994).

Related Experiments:

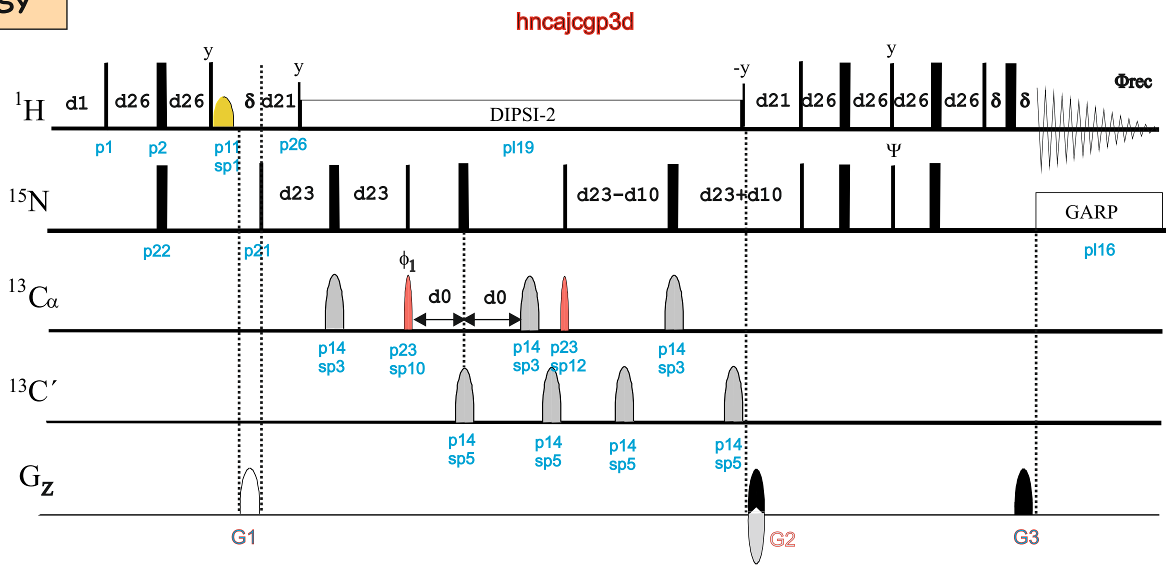
See original 3D HNCA Experiment

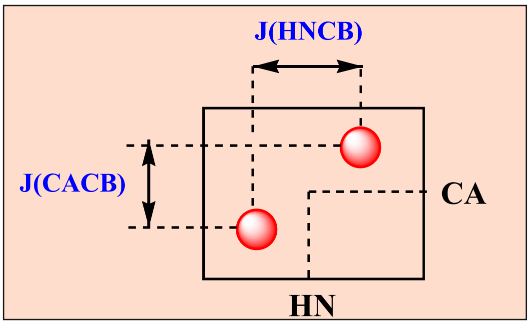
3D HNCA[CB]-E.COSY Experiment



d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12 msec]
d26: 1/(4J'(NH)	[2.3 msec]

J(HN-CB)
E.COSY



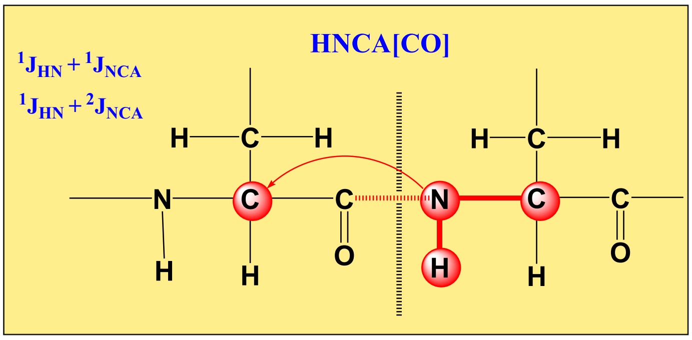


A.C. Wang & A. Bax, J. Am. Chem. Soc. 118, 2483-2494 (1996)

Related Experiments:

See original 3D HNCA Experiment

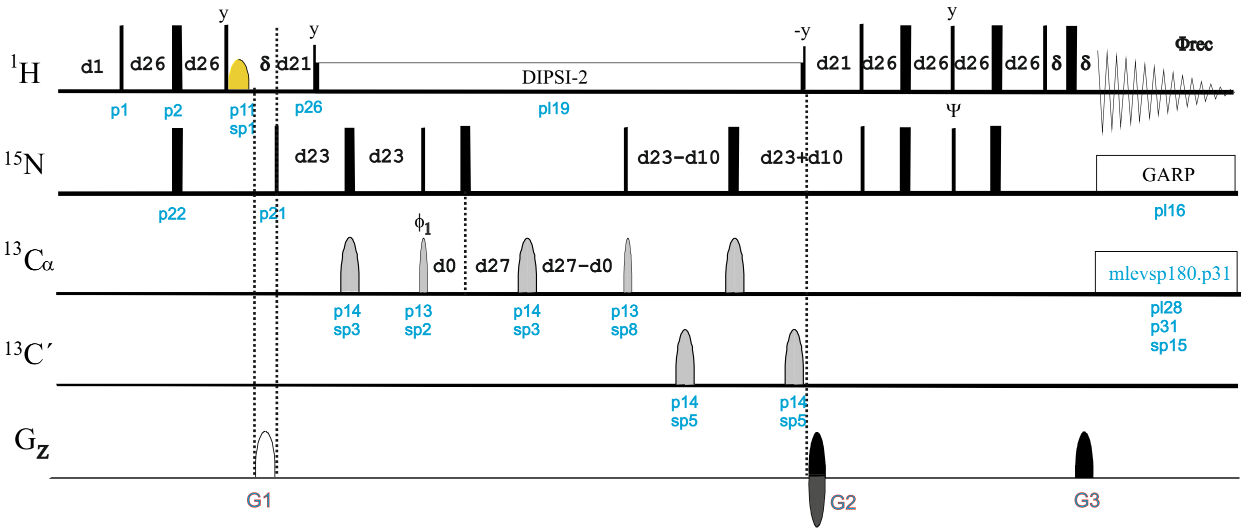
3D HNCA[CO]-E.COSY Experiment

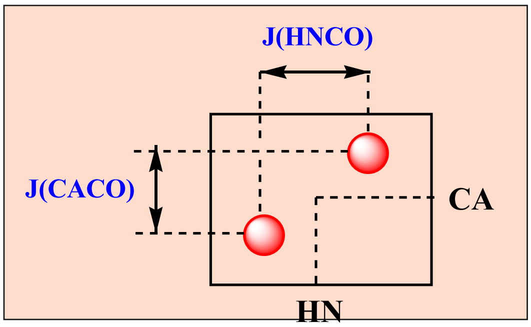


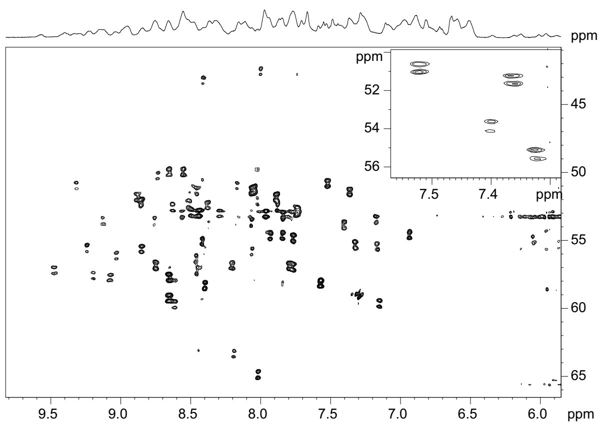
d21: 1/(2J(NH) [5.5 msec]
d23: 1/(4J(NCa) [12 msec]
d26: 1/(4J'(NH) [2.3 msec]
d27: constant time delay T(C) [13.3 msec]

J(HN-CO)
E.COSY

hncacosygp3d







References:

R.Weisemann, H. Rueterjans, H. Schwalbe, J. Schleucher, W. Bermel & C. Griesinger, J. Biomol. NMR 4, 231-240 (1994)

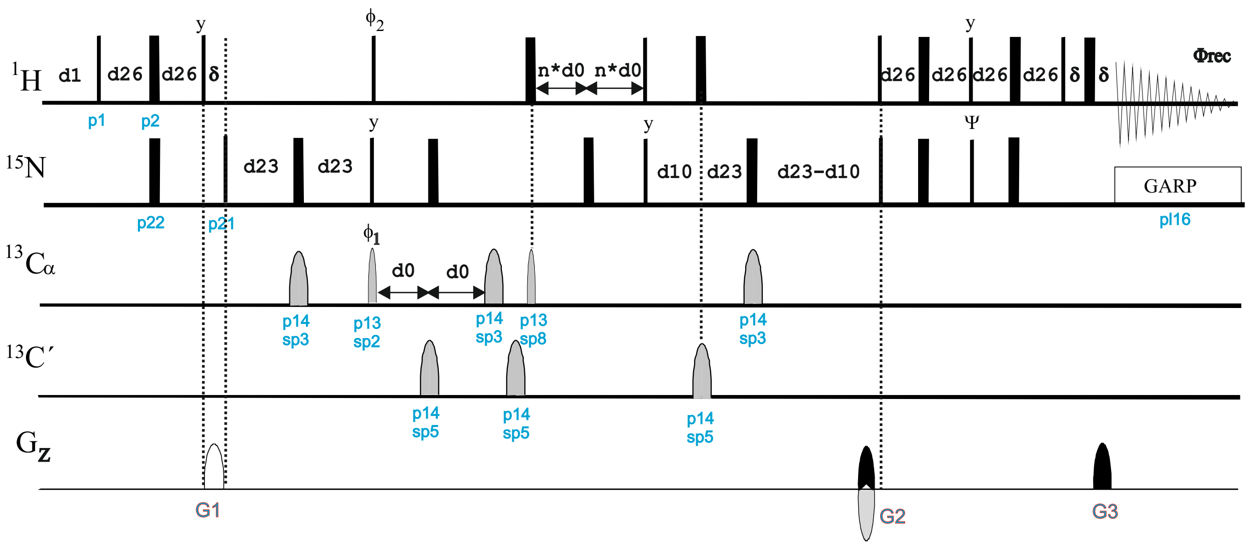
Related Experiments:

See original 3D HNCA experiment

3D DQ/ZQ-HNCA Experiment

J(HN-HA) and J(HN-CB)
DQ/ZQ

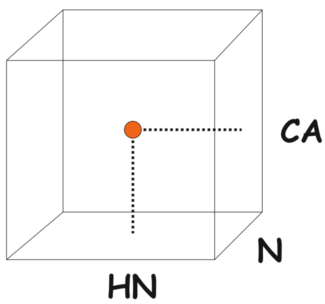
hncadqzqgp3d



d23: 1/(4J(NCa)   [13.5 msec]
d26: 1/(4J'(NH)   [2.6 msec]

Acquisition and Processing

DQ+ZQ and DQ-ZQ Data are recorded in interleaved mode
Processing:
use AU-program split [ipap 2]



References:

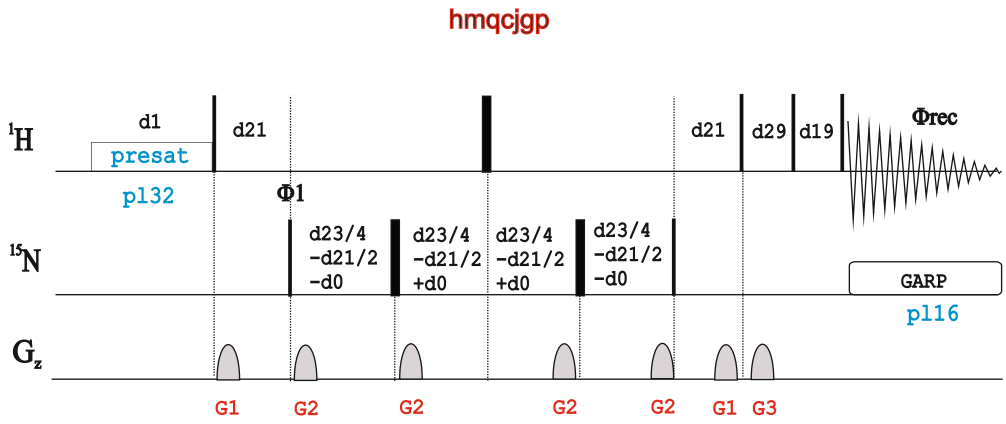
A. Rexroth, P. Schmidt, S. Salma, T. Geppert, H. Schwalbe & C. Griesinger, J. Am. Chem. Soc. 117, 10389-10390 (1995)

Related Experiments:

See original 3D HNCA Experiment

2D J-Modulated CT-HMQC Experiment

J(HN-HA)
J-modulation



d21: 1/(2J(NH) [5.3 msec]
d23: overall constant time for J-modulation : 4*T + 2*d21
d29: z-filter delay (delta) [2 msec]

References:

H. Kuboniwa, S. Grzesiek, F. Delaglio & A. Bax, J. Biomol NMR 4, 871-878 (1994)

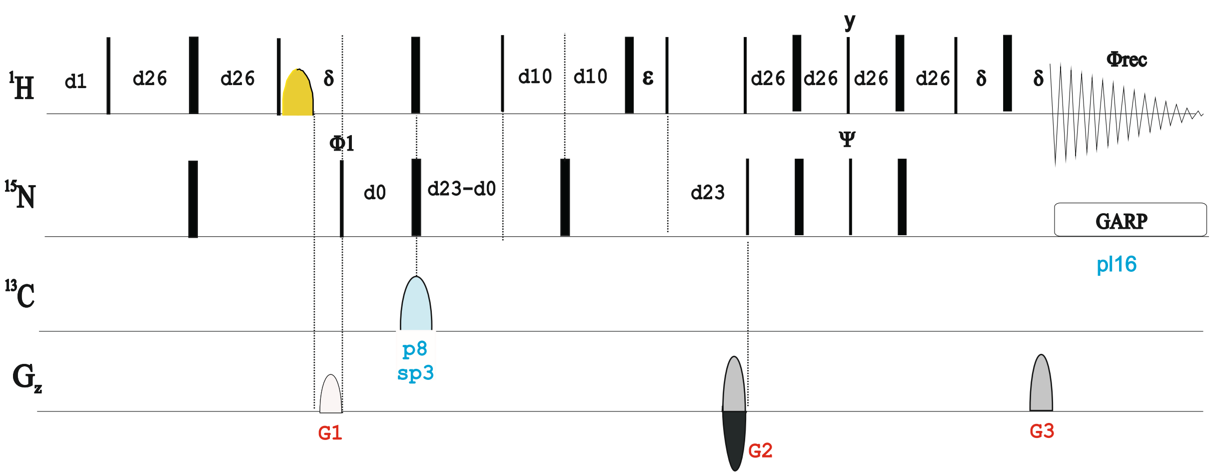
Related Experiments:

See original 2D HMQC and CT-HMQC experiments

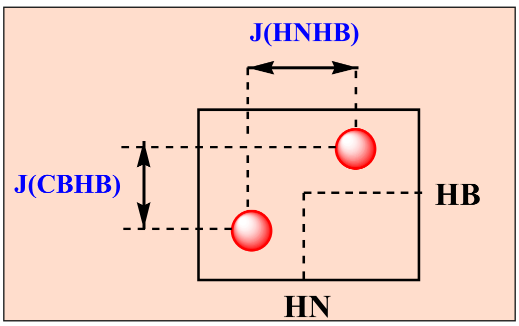
3D HNHB[CB]-E.COSY Experiment

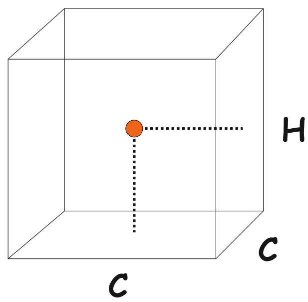
J(HN-CB)
E.COSY

hnhbecosgp3d



d23: constant time delay T(N)	[37.8 msec]
d26: 1/(4J'(NH)	[2.3 msec]





References:

F. Loehr & H. Rueterjans, J. Biomol. NMR 13, 263 - 274 (1999)

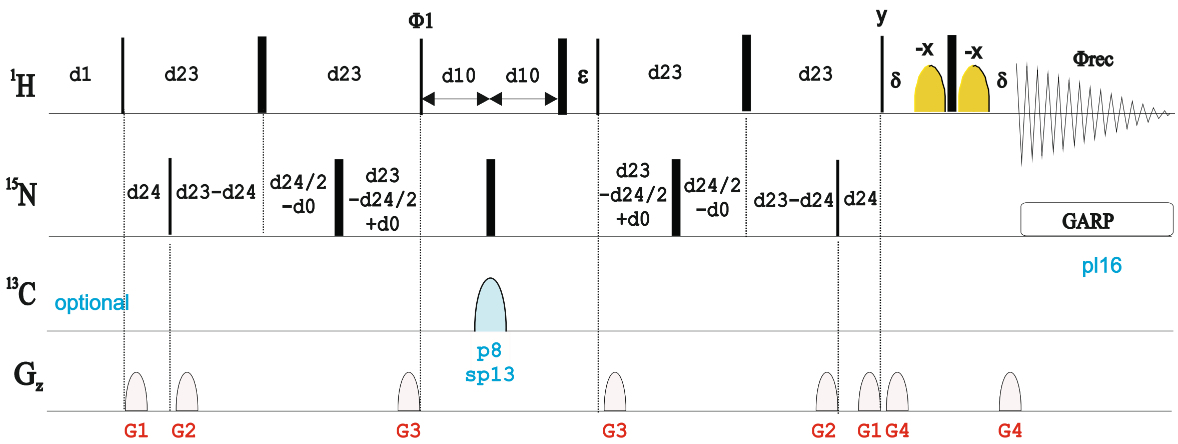
Related Experiments:

See original 3D HNHB experiment

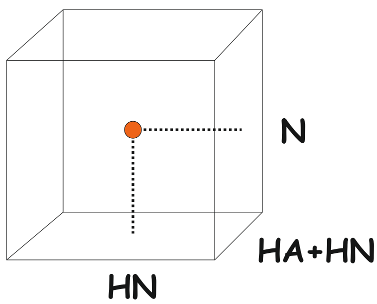
3D HNHA Experiment

J(HN-HA)
J-quantitative

hnhagp3d



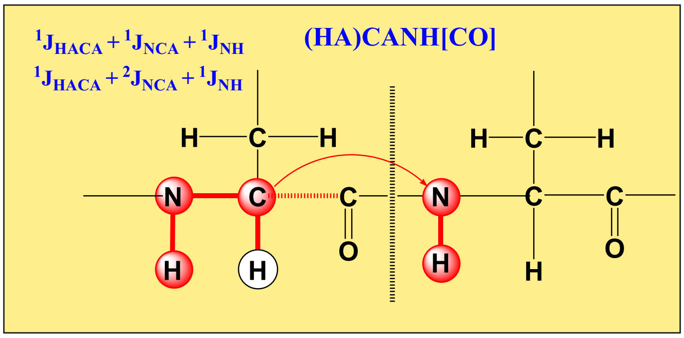
d23: 1/(4J(HNHa))	[13.05 msec]
d24: 1/(2J(NH))	[4.5 msec]



References:

1. G.W. Vuister & A. Bax, J. Am. Chem. Soc. 115, 7772-7777 (1993)
2. G.W. Vuister & A. Bax, J. Biomol NMR 4, 193-200 (1994)

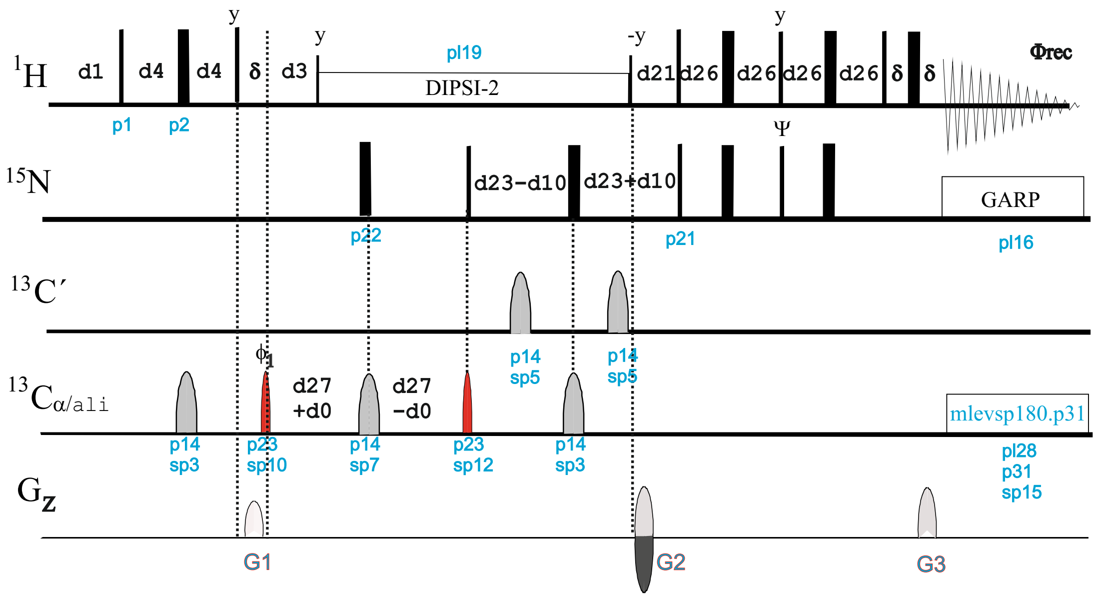
3D (H)CANNH[CO]-E.COSY Experiment

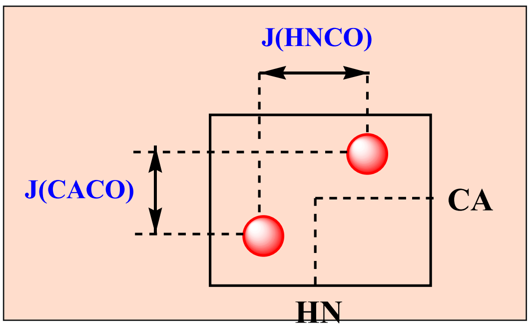


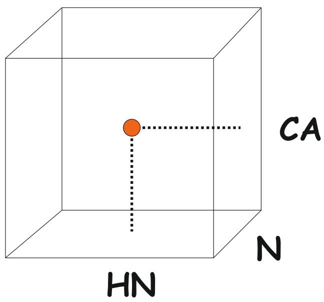
d3 : 1/(3.4J(CH) [2.0 msec]
d4 : 1/(4J(CH) [1.7 msec]
d21: 1/(2J(NH) [5.5 msec]
d23: 1/(4J(NCa) [12 msec]
d26: 1/(4J'(NH) [2.3 msec]
d27: constant time delay T(C) [13.3 msec]

J(HN-CO)
E.COSY

hcannhgp3d







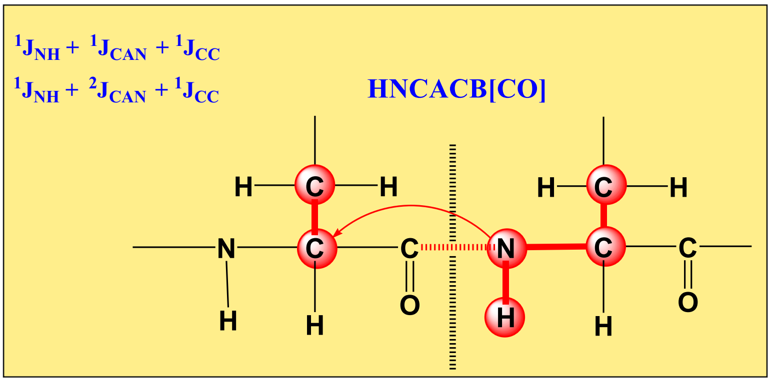
References:

F. Loehr & H. Rueterjans, J. Biomol. NMR 5, 25-36 (1995)

Related Experiments:

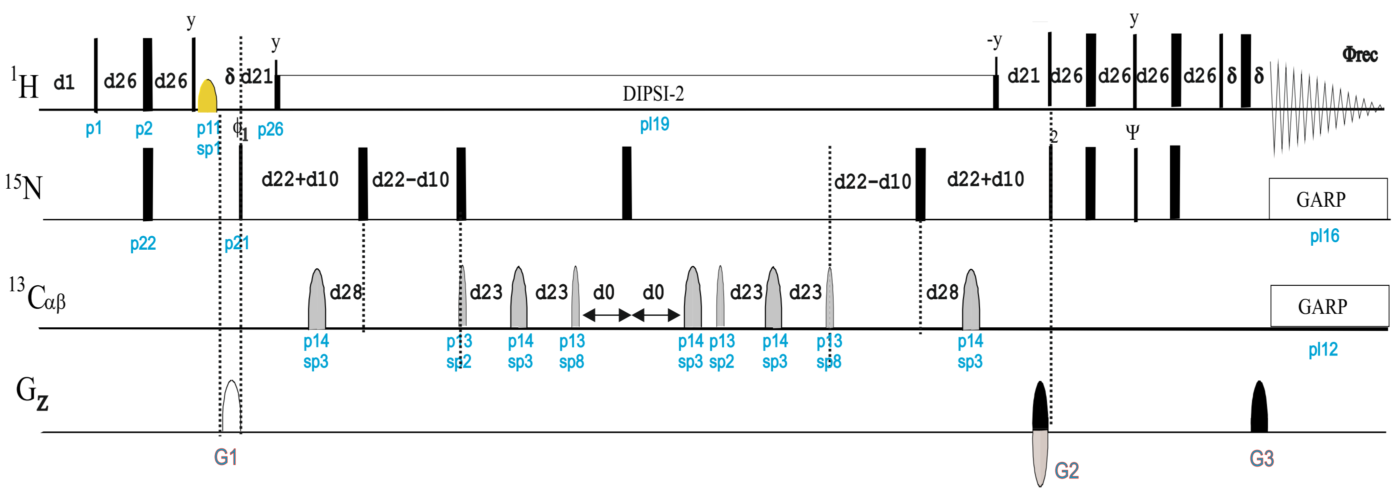
See original 3D HACANH experiment

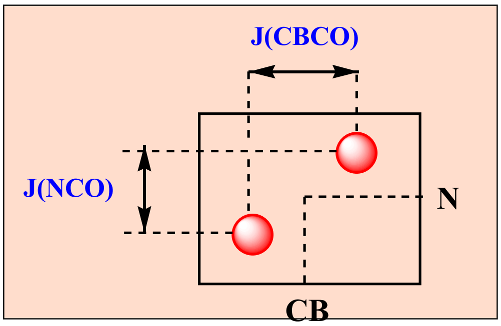
3D HNCACB[CO] Experiment



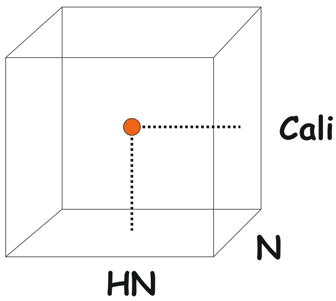
J(CO-CB)
E.COSY

hncacbgpjc3d





d21: 1/(2J(NH)) [5.5 msec]
d22: T(N) [17.6 msec]
d23: 1/(4J(CaCb) [6.7 msec]
d26: 1/(4J'(NH) [2.3 msec]
d28: T(N) - [1/(4J(NCa)opt] [2.1 msec]



References:

F. Loehr & H. Rueterjans, J. Biomol. NMR 13, 263-274 (1999)
J.-S. Hu & A. Bax, J. Biomol. NMR 11, 199-203 (1998)

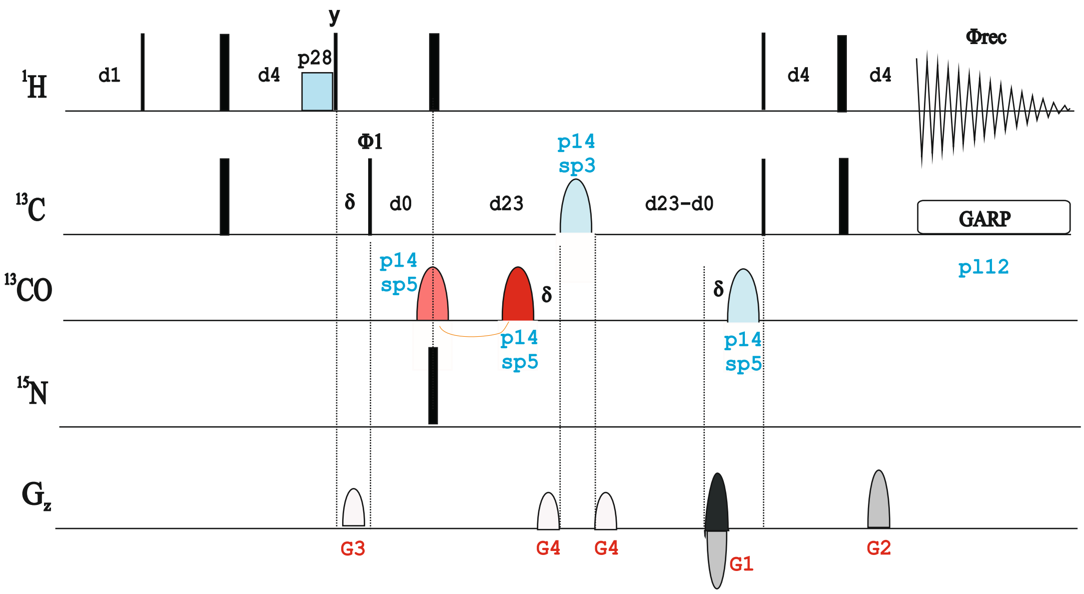
Related Experiments:

See original 3D HNCACB experiment

2D Spin-echo Difference CT-HSQC Experiment

J(CO-CB)
spin-echo difference

hsqcctetgpjclr



d4 : 1/(4J)CH [1.7 msec]
d23: constant time delay T(C) [28.7 msec]
2T = n/1J(CC)
d31: effective delay for J-evolution

References:

S. Grzesiek, G.W. Vuister & A. Bax, J. Biomol. NMR 3, 487-493 (1993)

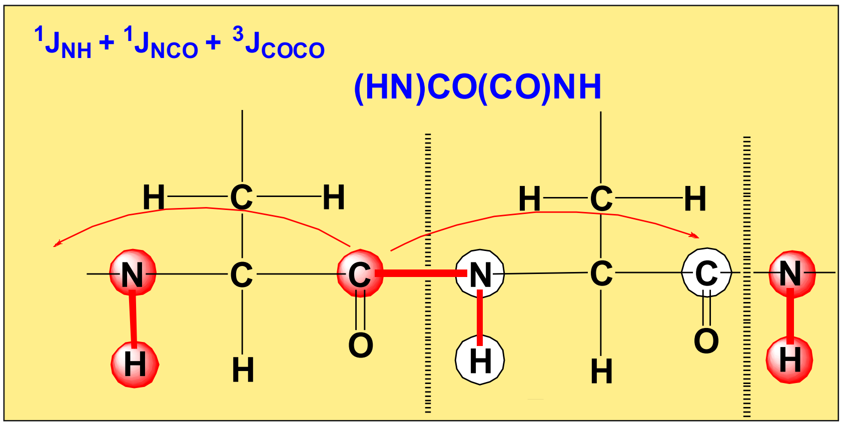
Related Experiments:

See original 2D CT-HSQC experiment

Processing:

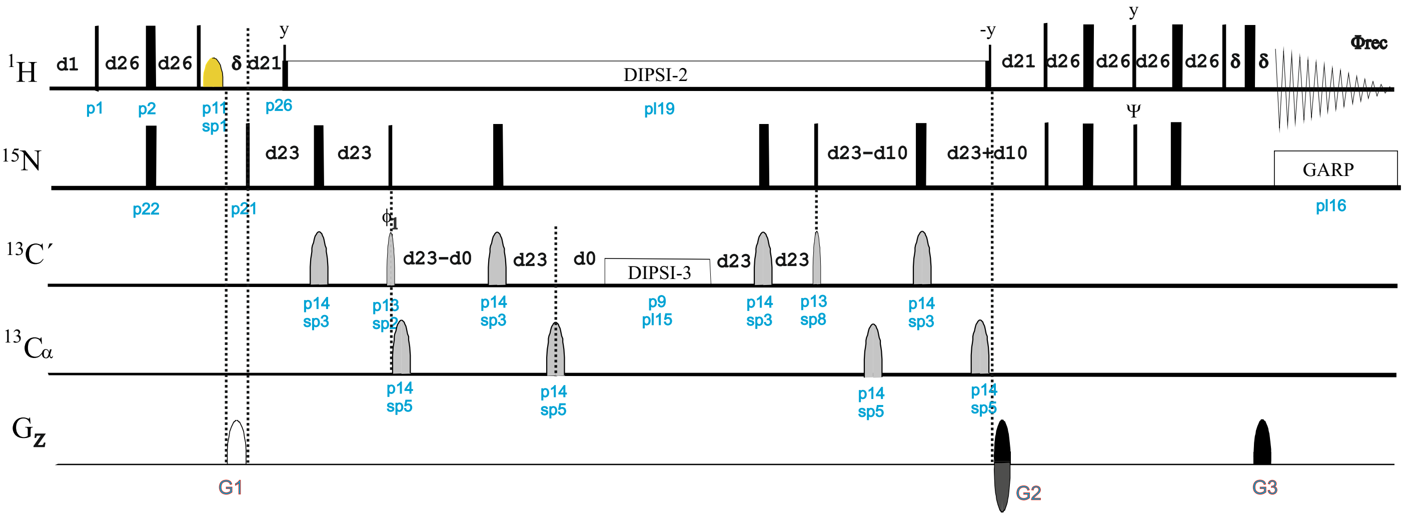
Two data are recorded in an interleaved mode.
Use AU-program split [2] to split data

3D (HN)CO(CO)NH Experiment

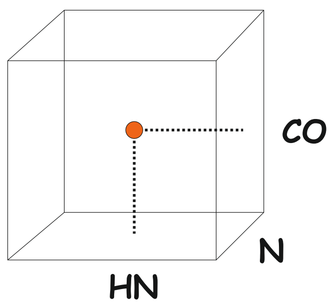


J(CO-CO)
J-quantitative

hncocogp3d



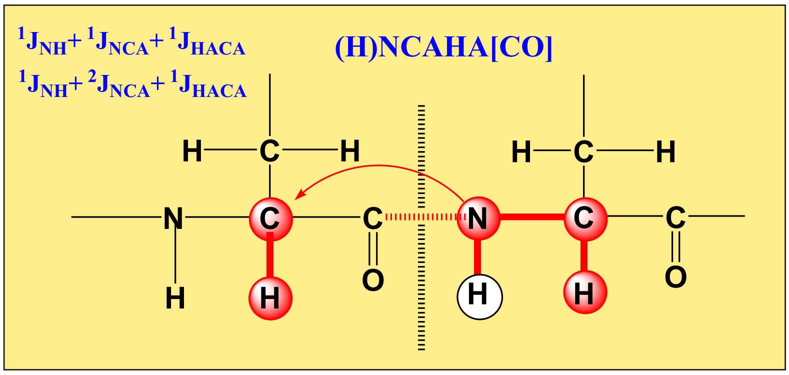
d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCO)	[13.5 msec]
d26: 1/(4J'(NH)	[2.3 msec]
d31: length of DIPSI-3 cycle	



References:

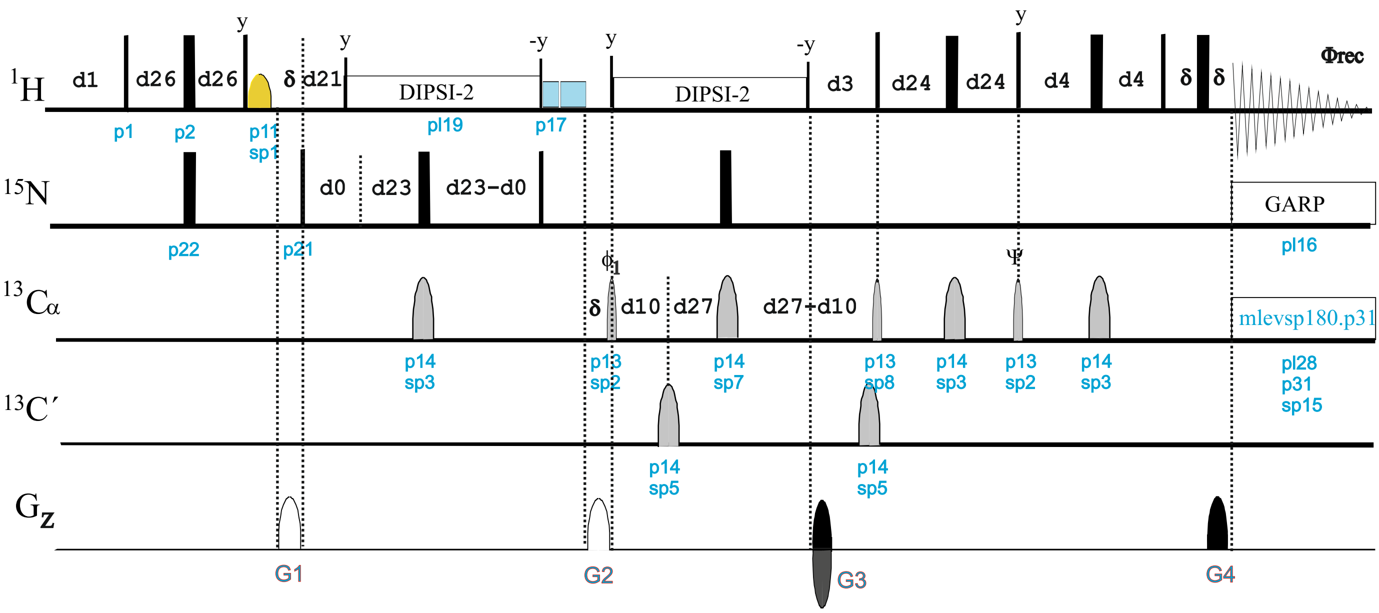
S. Grzesiek & A. Bax, J. Biomol. NMR 9, 207-211 (1997)
J.-S. Hu & A. Bax, J. Am. Chem. SOc. 118, 8170-8171 (1996)

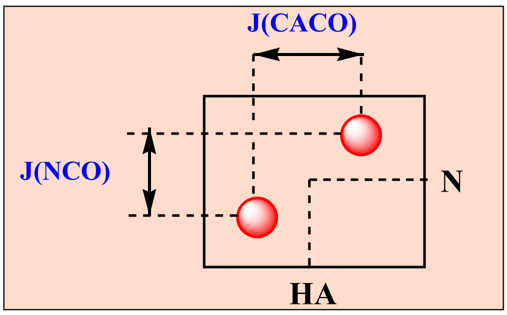
3D (H)NCAHA[CO]-E.COSY Experiment



J(HA-CO)
E.COSY

hncahagp3d





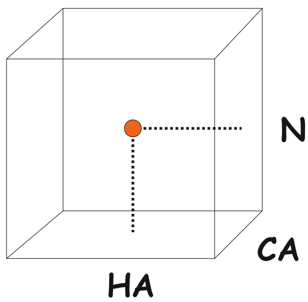
d3 : 1/(3.2J(CH)) [2.1 msec]
d4 : 1/(4J(CH)) [1.7 msec]
d21: 1/(2J(NH)) [5.5 msec]
d23: 1/(4J(NCa)) [15.5 msec]
d24: 1/(8J)CH for all multiplicities
1/(4J)CH for CH
d26: 1/(4J'(NH)) [2.3 msec]
d27: constant time delay T(C) [13.3 msec]

References:

F. Loehr & H. Rueterjans, J. Biomol. NMR 5, 25 - 36 (1995)

Related Experiment:

See the original HNCAHA Experiment



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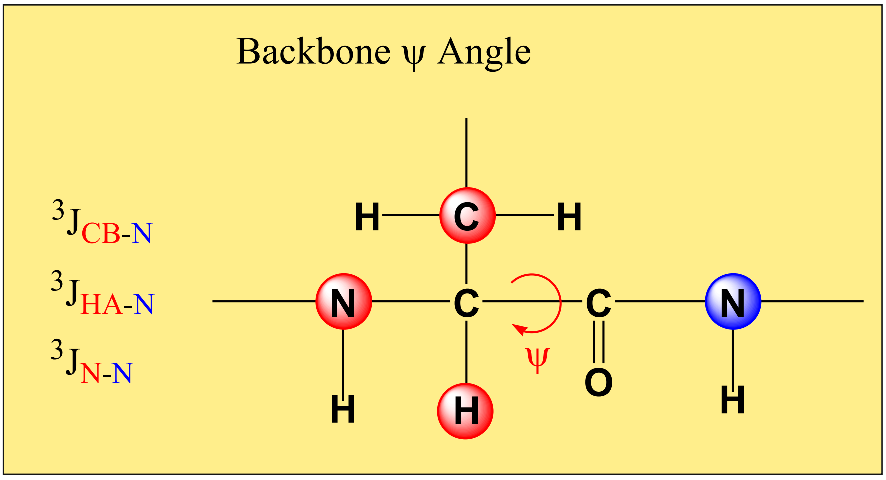
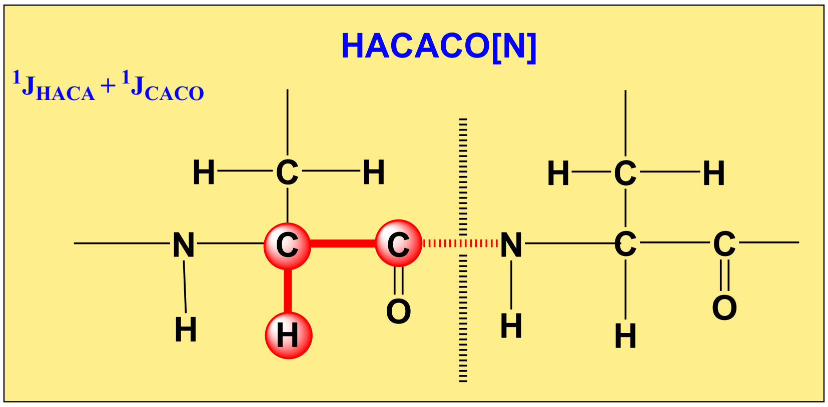
COUPLING CONSTANTS
PSI BACKBONE ANGLE



Psi Backbone Coupling Constant

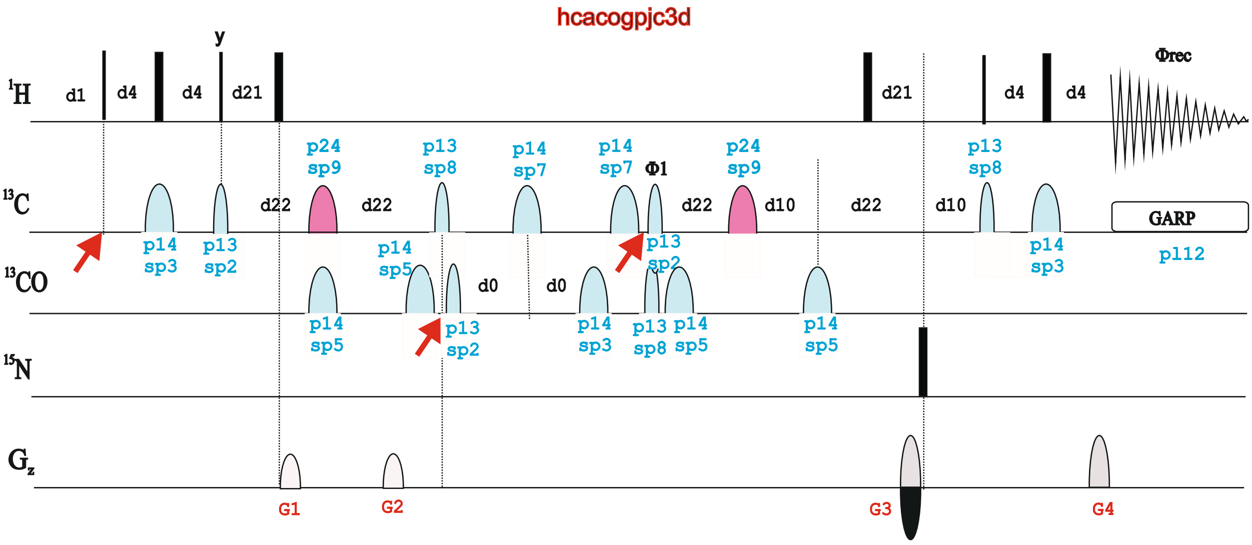
- 3D (H)NNH-TOCSY (**hnnhdigp3d** | HNNHDIGP3D) - 3J[N-N] via quantitative-J
- 3D HCACO[N]-E.COSY (**hcacogpjc3d** | HCACOGPJC3D) - 3J[HA-N] via E.COSY
- Also see in Ch1 Sidechain Coupling Constants:
  3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J

3D HACACO[N]-E.COSY Experiment

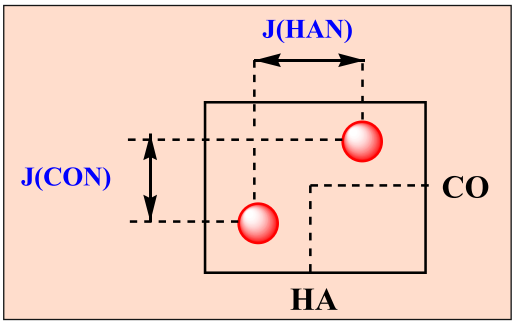


J(HA-N)
E.COSY

hcacogpjc3d



d4 : 1/(4J(HCa)) [1.7 msec]
d21: 1/(4J`(HCa)) for CH [1.7 msec]
1/(6J`(HCa)) for CH and CH2 [1.2 msec]
d22: 1/(4J(CaCO)) [4.5 msec]

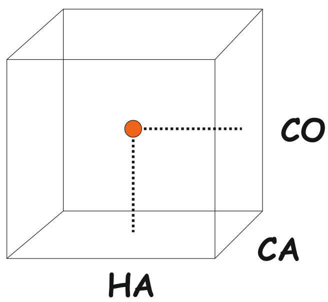


References:

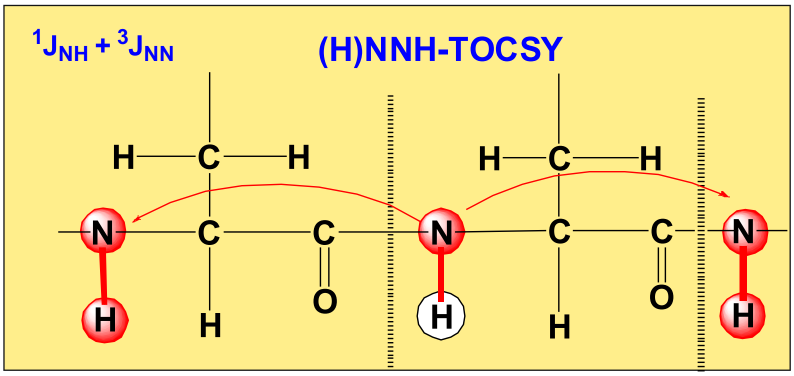
A.C. Wang & A. Bax, J. Am. Chem. Soc. 117, 1810-1813 (1995))
;(L.E. Kay et al., J. Magn. Reson 89, 496 - 514 (1990)

Related Experiments:

See the original 3D HCACO Experiment

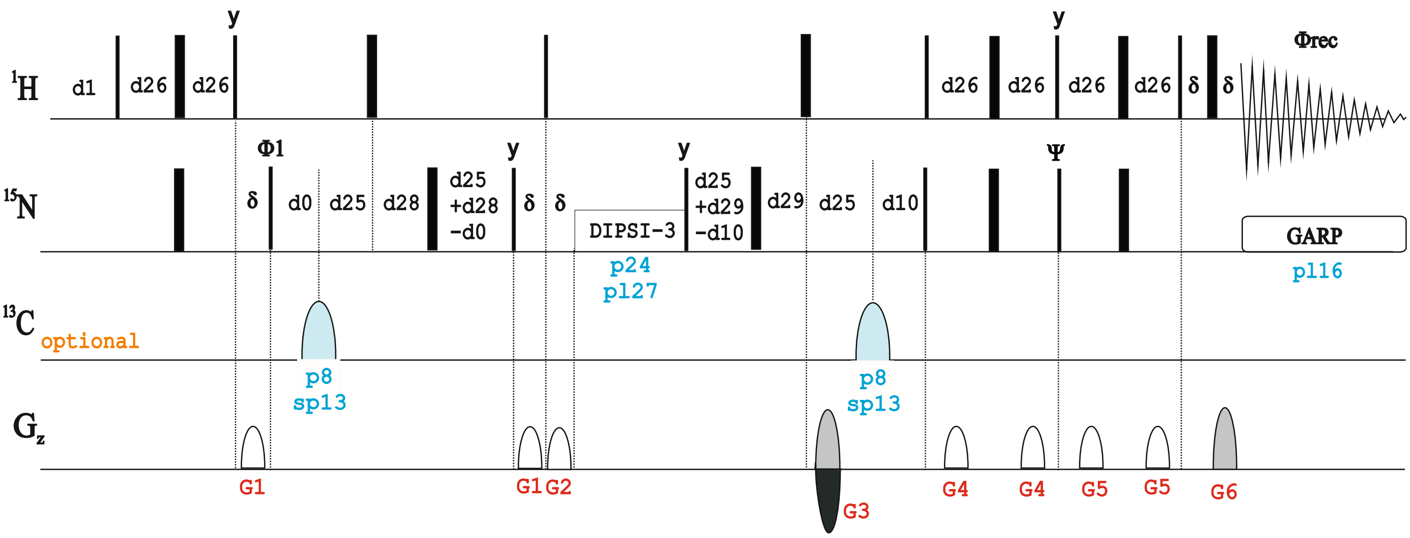


3D (H)NNH-TOCSY Experiment

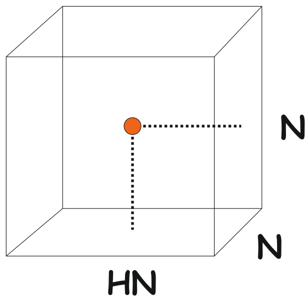


J(N-N)
J-quantitative

hnnhdigp3d



d25: 1/(4J(NH) [2.75 msec]
d26: 1/(4J'(NH) [2.3 msec]
d31: length of DIPSI-3 cycle



References:

F. Loehr & H. Rueterjans, J. Magn. Reson. 132, 130-137 (1998)
K. Theis, A.J. Dingley, A. Hoffmann, J.G. Omichinski & S. Grzesiek, J. Biomol. NMR 10, 403-408 (1997)

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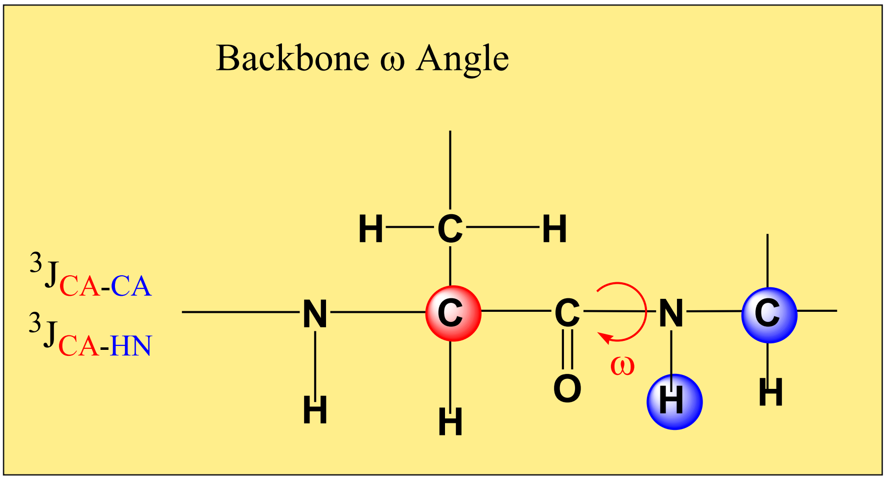
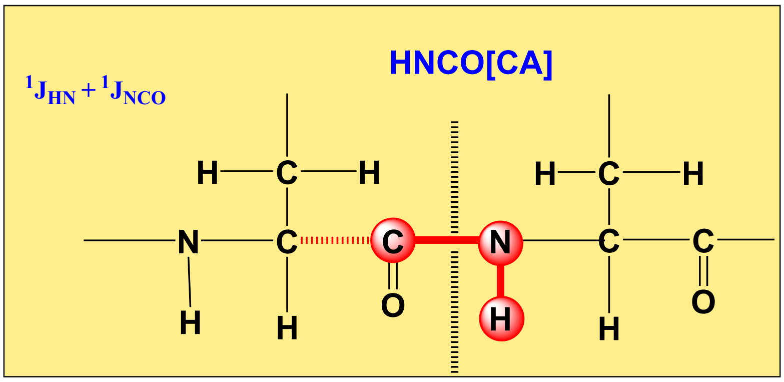
COUPLING CONSTANTS
OMEGA BACKBONE ANGLE



Omega Backbone Coupling Constant

- 3D HN(COCA)CA (**hncocacagp3d** | HNCOCACAGP3D) - 3J[CA-CA] via quantitative-J
- 3D HNCO[CA]-E.COSY (**hncoecosgp3d** | HNCOECOSGP3D) - 3J[H(N)-CA] via E.COSY

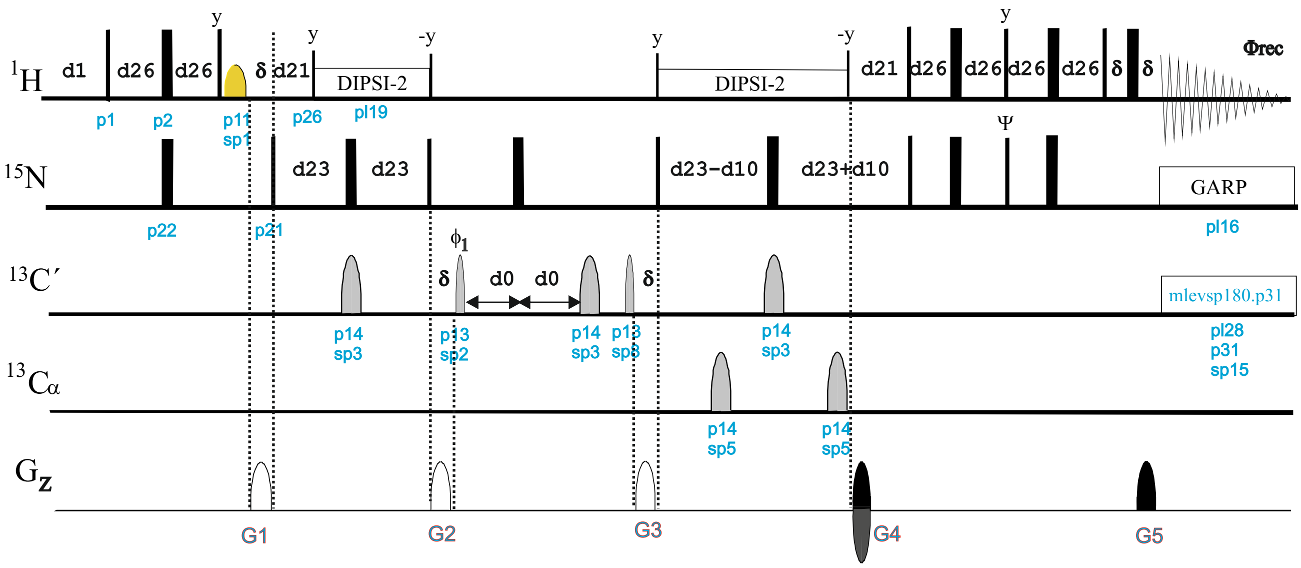
3D HNCO[CA]-E.COSY Experiment

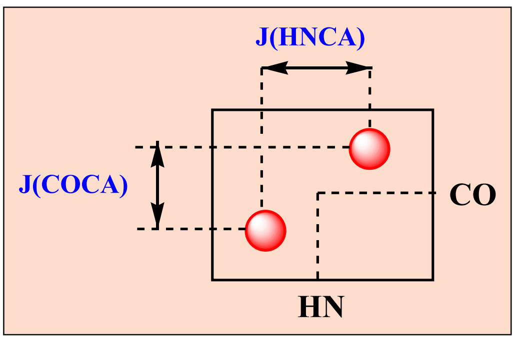


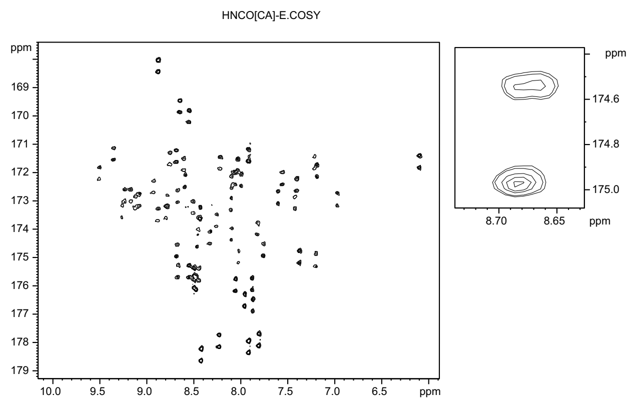
J(HN-CA)
E.COSY

d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCO)	[12 msec]
d26: 1/(4J'(NH)	[2.3 msec]

hncoecosgp3d

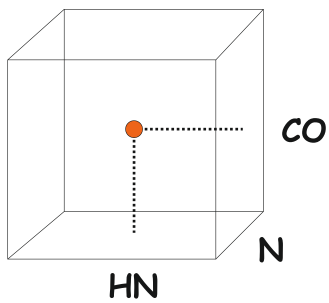






References:

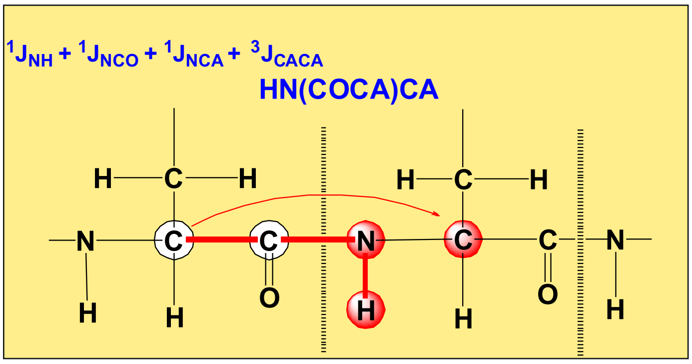
M. Hennig, W. Bermel, H. Schwalbe & C. Griesinger, J. Am. Chem. Soc. 122, 6268-6277 (2000)



Related Experiments:

See original 3D HNCO experiment

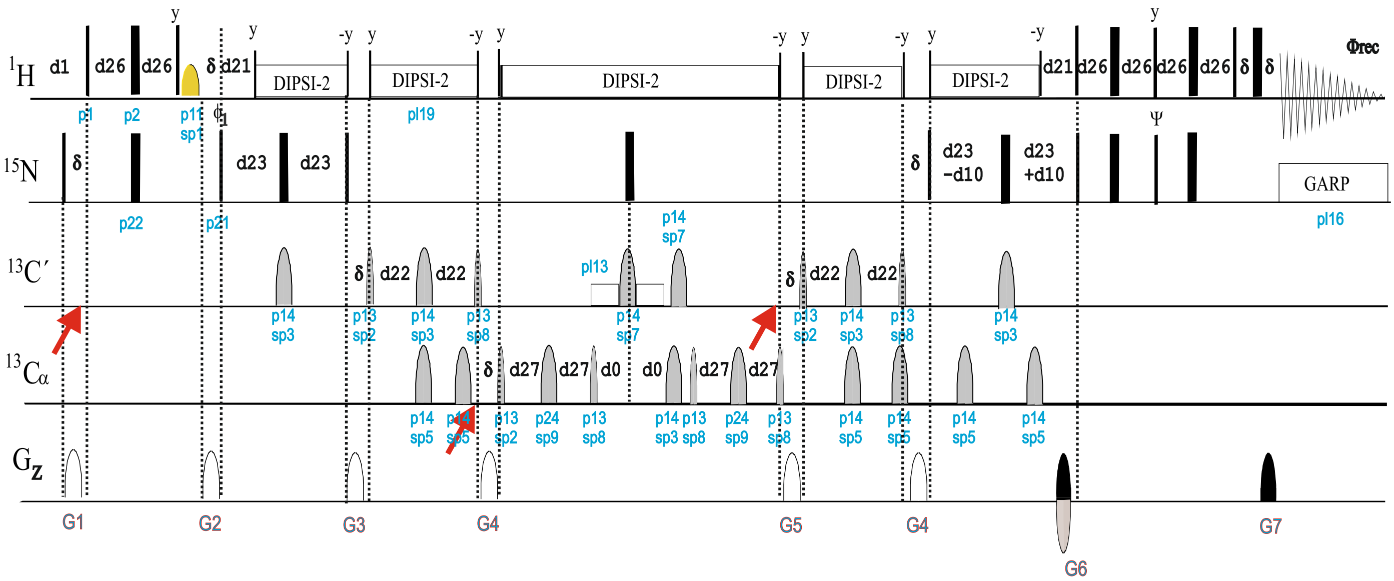
3D HN(COCA)CA Experiment



J(CA-CA)

J-quantitative

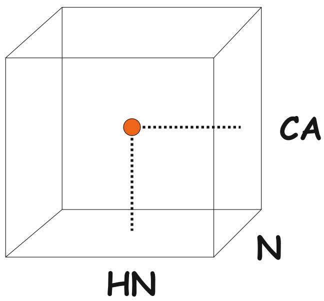
hncocacagp3d



d21: 1/(2J(NH)	[5.5 msec]
d22: 1/(4J(COCa)	[4.55 msec]
d23: 1/(4J(NCO)	[12.8 msec]
d26: 1/(4J'(NH)	[2.4 msec]
d27: 1/(4J'(CaCa)	[28.6 msec]

References:

M. Hennig, W. Bermel, H. Schwalbe & C. Griesinger, J. Am. Chem. Soc. 122, 6268-6277 (2000)



Related Experiments:

See original 3D HNCOCA experiment

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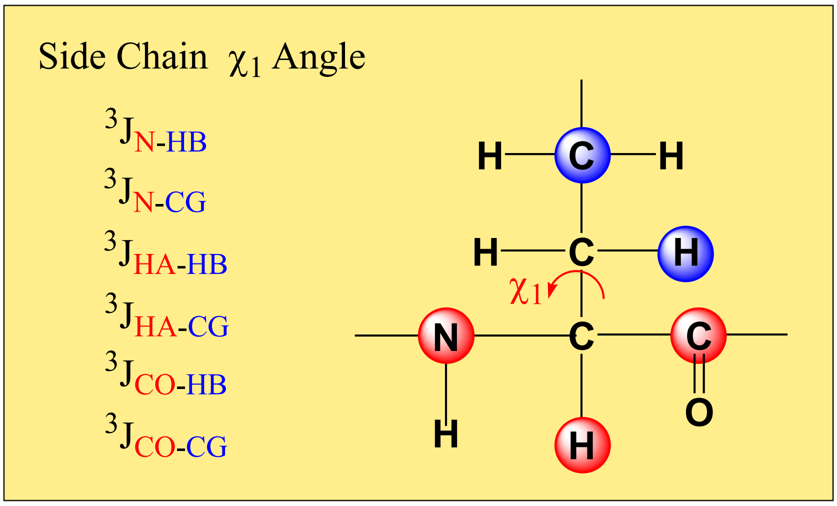
CHI1 SIDECHAIN ANGLE



Chi1 Sidechain Coupling Constant

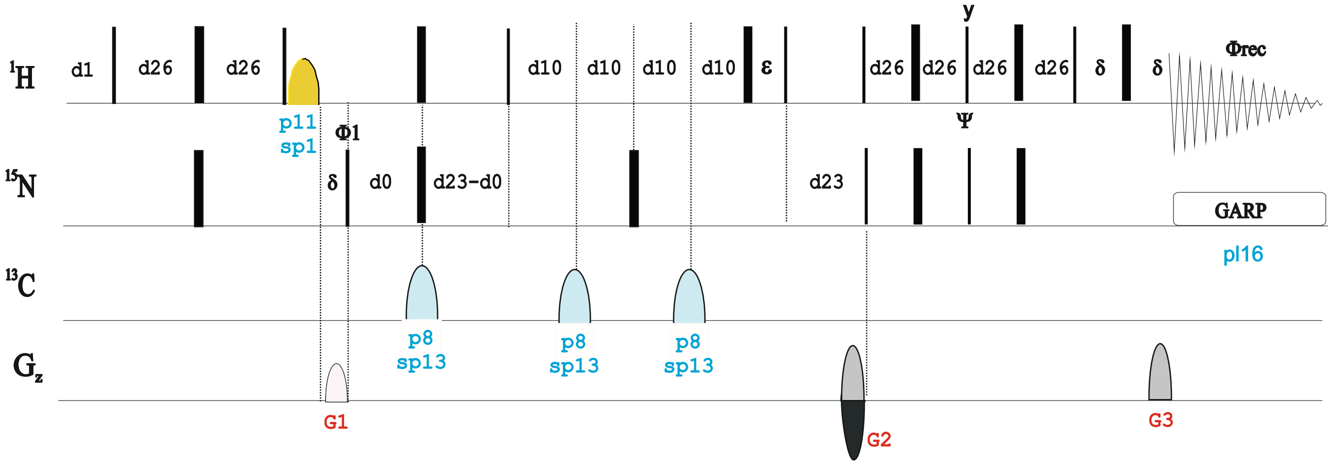
- 3D HNHB (**hnhbgp3d** | HNHBGP3D) - 3J[HN-HA] and 3J[HN-HB] via quantitative-J
- 3D HACAHB-COSY (**hacahbcosygp3d** | HACAHBCOSYGP3D) - 3J[HA-HB] via quantitative-J
- 3D HN(CO)C (**hncocgp3d** | HNCOCGP3D) - 3J[CG-CO] via quantitative-J
- 3D HC(C)H[HA]-E.COSY (**hcchecosgp3d** | HCCHECOSGP3D) - 3J[HA-HB] via E.COSY
- 3D HC(C)H[CO]-E.COSY (**hcchcosygp3d** | HCCHCOSYGP3D) - 3J[CO-HB] via E.COSY
- 3D (H)C(C)CH[CO]-E.COSY (**hccccosygp3d** | HCCCCOSYGP3D) - 3J[CG-CO] via E.COSY
- 3D HNCG (**hncggp3d.1** | HNCGGP3D.1) - 3J[N-CG] via quantitative-J
- 3D HNCG (**hncggp3d.2** | HNCGGP3D.2) - 3J[N-CG] via quantitative-J
- 2D spin-echo difference CT-HSQC (**hsqcetfpf3gpjcsi** | HSQCETFPFGPJCSI) - 3J[N-CG] via spin-echo difference

3D HNHB Experiment

J(N-HB), J(N-HA)

J-quantitative

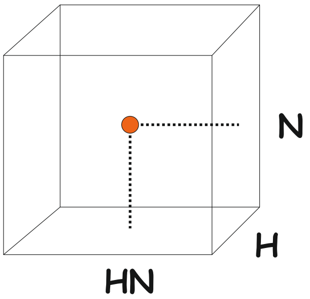
hnhbgp3d



d23: constant time delay T(N)	[37.8 msec]
d26: 1/(4J'(NH)	[2.3 msec]

References:

1. S.J. Archer, M. Ikura, D.A. Torchia & A. Bax,
J. Magn. Reson. 95, 636-641 (1991)
2. P.Duex, B. Whitehead, R. Boelens, R. Kaptein & G.W. Vuister,
J. Biomol. NMR 10, 301-306 (1997)
3. F. Loehr & H. Rueterjans, J. Biomol. NMR 13, 263 - 274 (1999)



Related Experiments:

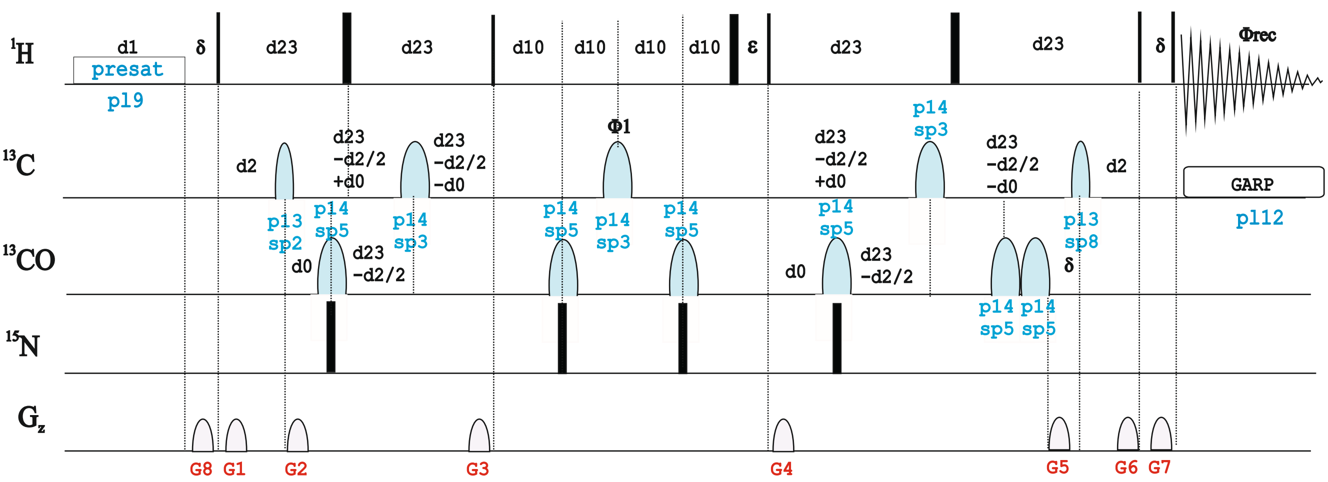
See also: 3D HNHB-E.COSY experiment

3D HACAHB-COSY Experiment

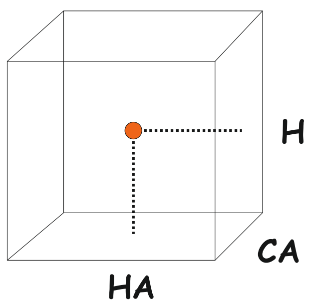
J(HA-HB)

J-quantitative

hacahbcosygp3d



d2 : 1/(2J(CH)) [3.4 msec]
d23: 1/(4J'(HaHb)) [8.7 msec]

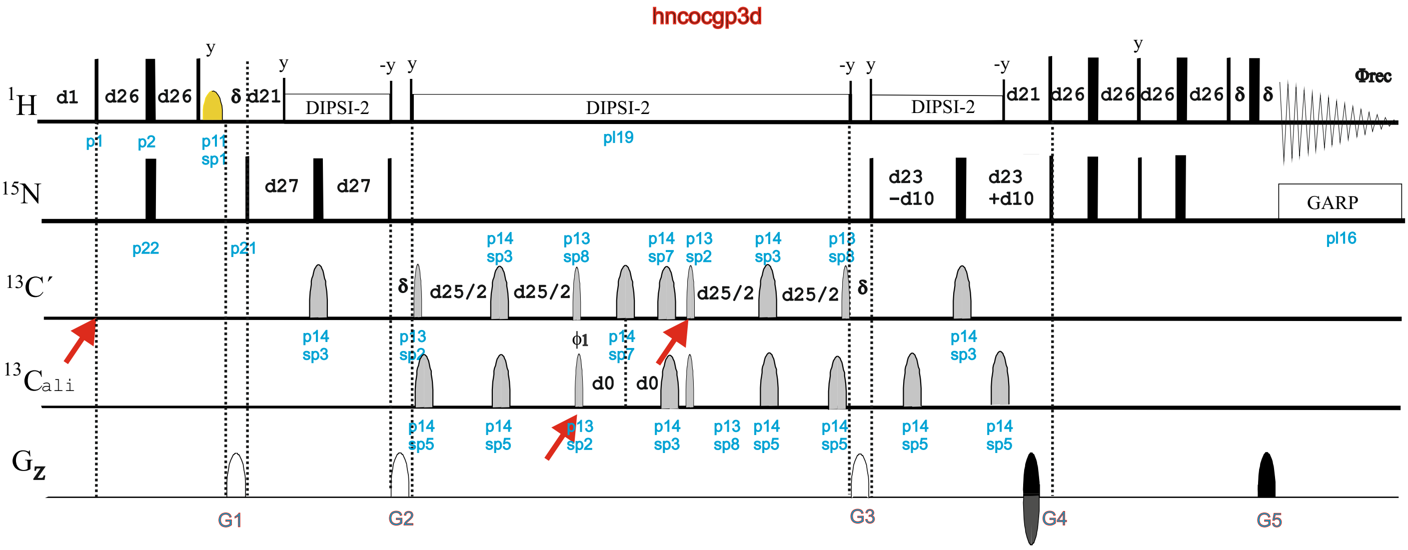


References:

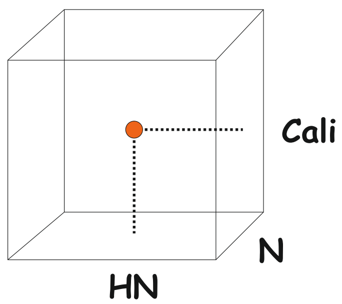
S. Grzesiek, H. Kuboniwa, A.P. Hinck & A. Bax, J. Am. Chem. Soc. 117, 5312-5315 (1995)

3D HN(CO)C Experiment

J(CG-CO)
J-quantitative



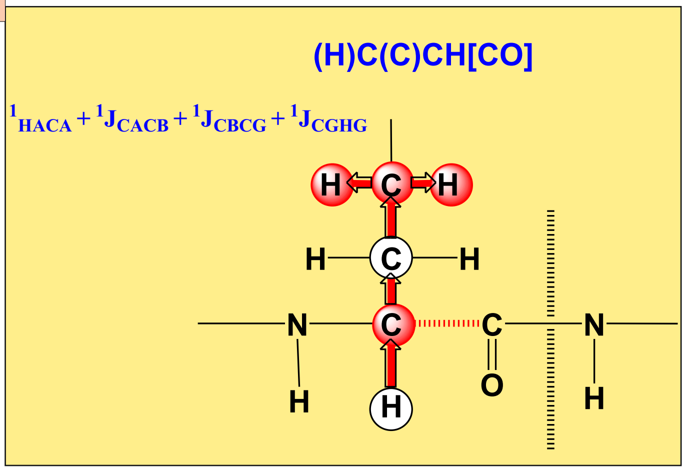
d21: 1/(2J(NH)) [5.4 msec]
d23: 1/(4J(NCO)) [13.8 msec]
d25: cross peak experiment: 1/(2J(CgCO)) [56.1 msec]
reference exepriment: [46.7 msec]
d26: 1/(4J'(NH)) [2.3 msec]
d27: 1/(4J'(NCO)) [12.5 msec]



References:

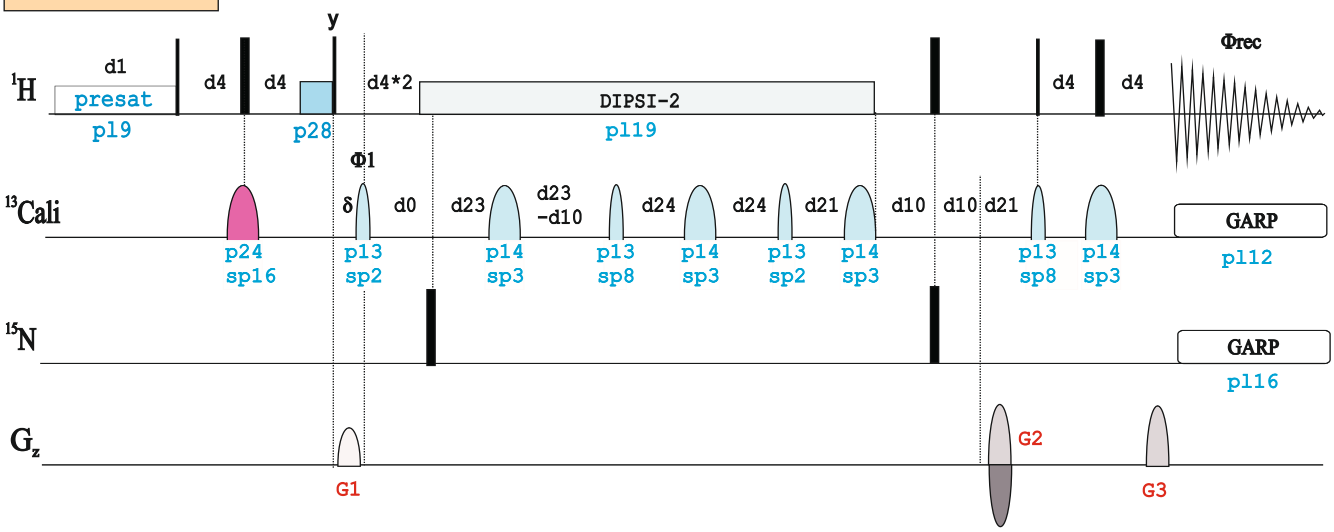
J.-S. Hu & A. Bax, J. Am. Chem. Soc. 119, 6360 - 6368 (1997)

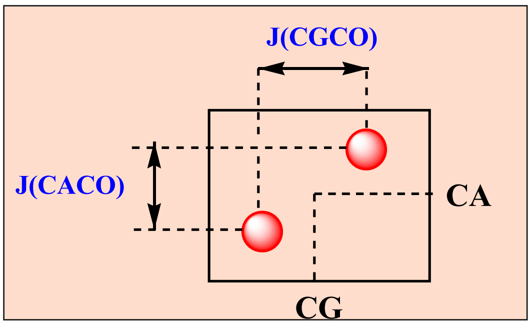
3D (H)C(C)CH[CO]-E.COSY Experiment



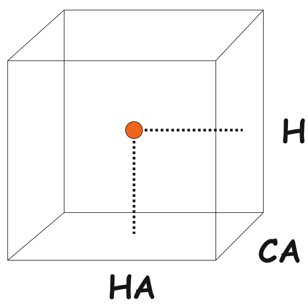
J(CG-CO)
E.COSY

hccccosygp3d





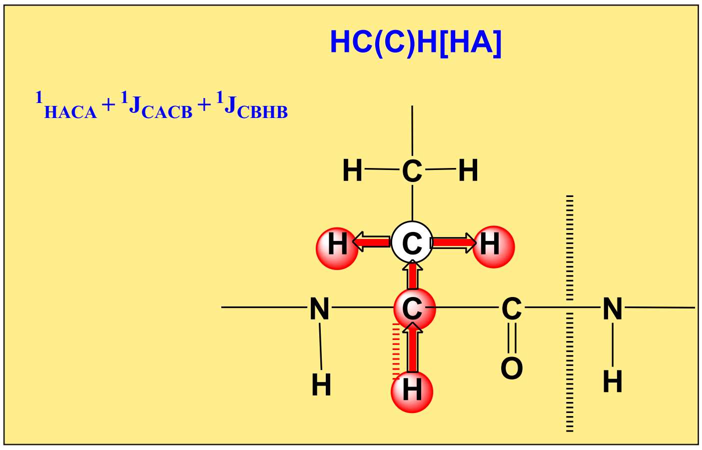
d21: 1/(5J'(CH))	[1.38 msec]
d23: 1/(4J(CC))	[7.2 msec]
d24: 1/(6.65J'(CC))	[4.3 msec]



References:

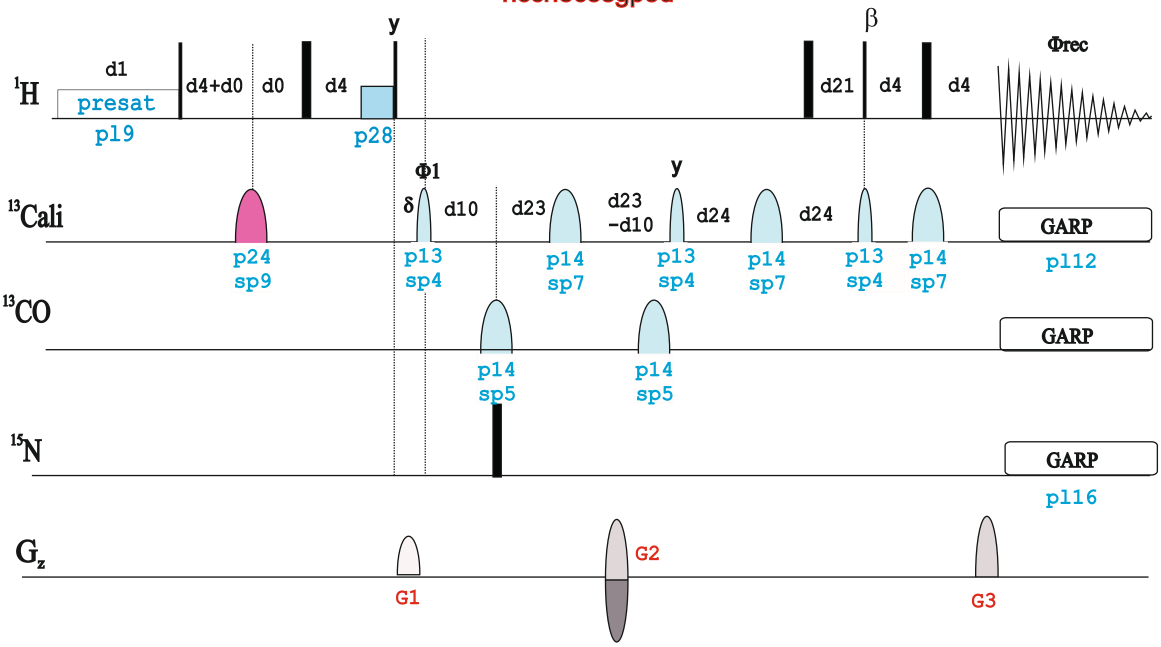
1. H. Schwalbe, A. Rexroth, U. Eggenberger, T. Geppert & C. Griesinger, J. Am. Chem. Soc. 115, 7878-7879 (1993)
2. Y. Karimi-Nejad, J.M. Schmidt, H. Rueterjans, H. Schwalbe & C. Griesinger, Biochemistry 33, 5481-5492 (1994)

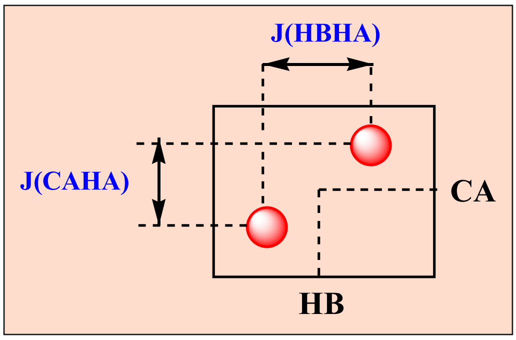
3D HC(C)H[HA]-E.COSY Experiment



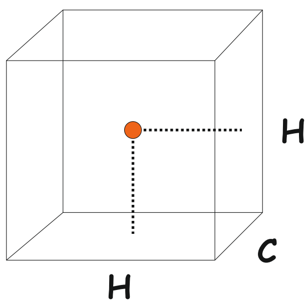
J(HB-HA)
E.COSY

hcchecosgp3d





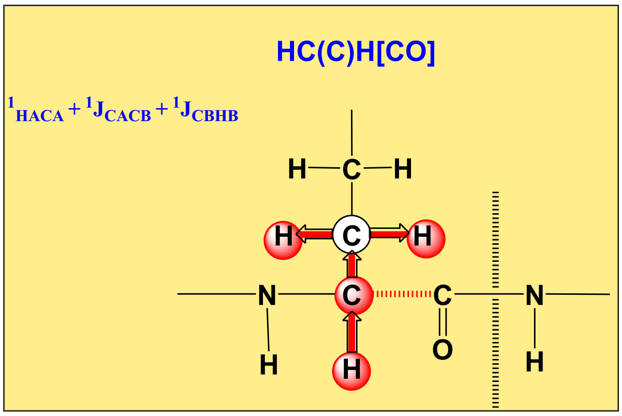
d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(8J'(CH))	[0.85 msec]
d23: 1/(4J(CC))	[7.2 msec]
d24: 1/(4J'(CC))	[3.6 msec]



References:

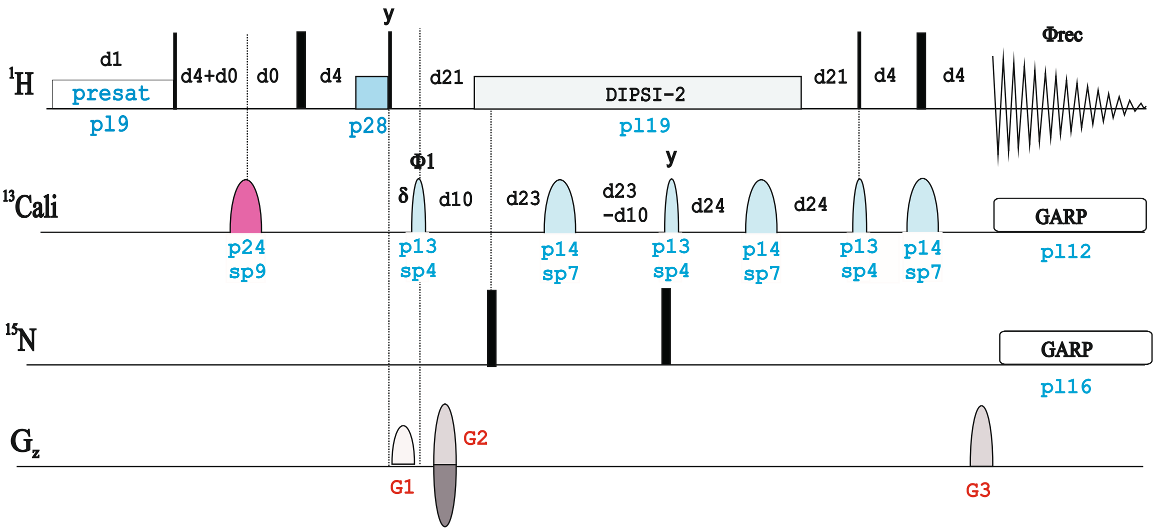
1. Y. Karimi-Nejad, J.M. Schmidt, H. Rueterjans, H. Schwalbe & C. Griesinger, Biochemistry 33, 5481-5492 (1994)
2. ;U. Eggenberger, Y. Karimi-Nejad, H. Thuering, H. Rueterjans & C. Griesinger, J. Biomol. NMR 2, 583-590 (1992)

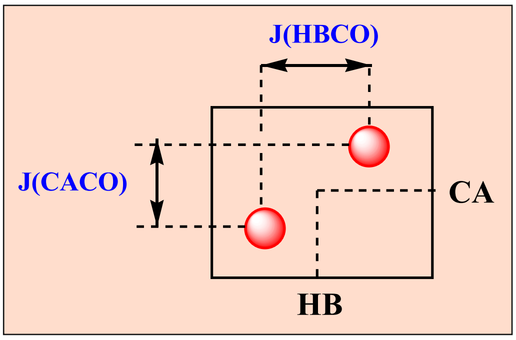
3D HC(C)H[CO]-E.COSY Experiment



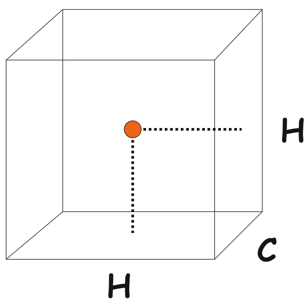
J(HB-CO)
E.COSY

hcchcosygp3d





d4 : 1/(4J(CH))	[1.7 msec]
d21: 1/(4J'(CH))	[1.7 msec]
d23: 1/(4J(CC))	[7.2 msec]
d24: 1/(4J'(CC))	[3.6 msec]



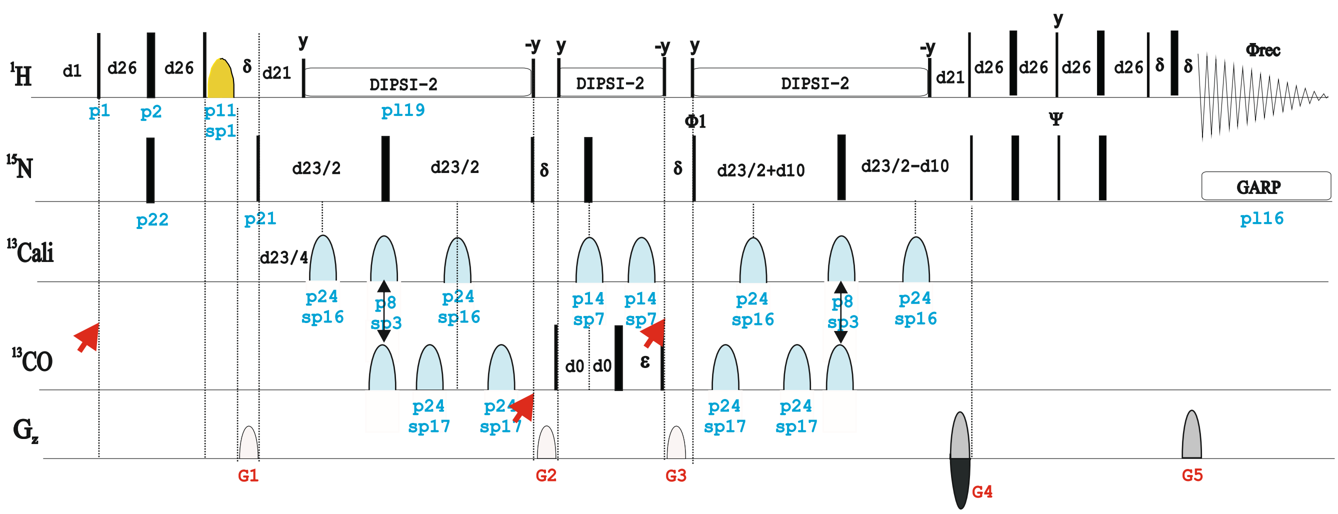
References:

1. Y. Karimi-Nejad, J.M. Schmidt, H. Rueterjans, H. Schwalbe & C. Griesinger, Biochemistry 33, 5481-5492 (1994)
2. U. Eggenberger, Y. Karimi-Nejad, H. Thuering, H. Rueterjans & C. Griesinger, J. Biomol. NMR 2, 583-590 (1992)

3D HNCG Experiment

J(N-CG)
J-quantitative
Reference experiment

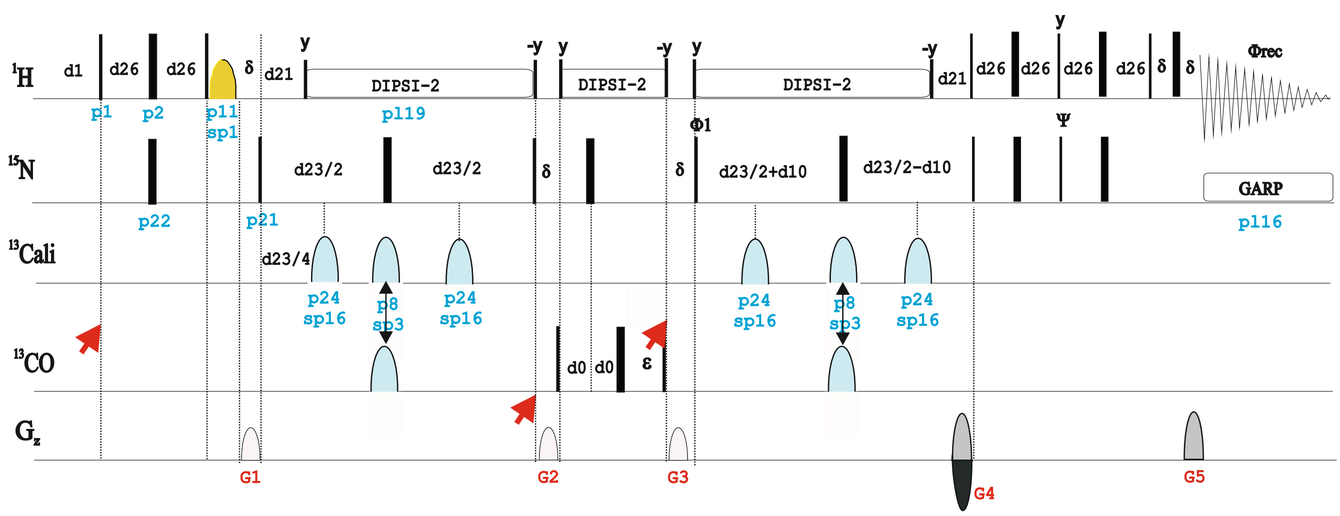
hncggp3d.1



d21: 1/(2J(NH) [5.5 msec]
d23: 1/(2J(NCg) = 2*T(N) [66.6 msec]
d26: 1/(4J'(NH) [2.3 msec]

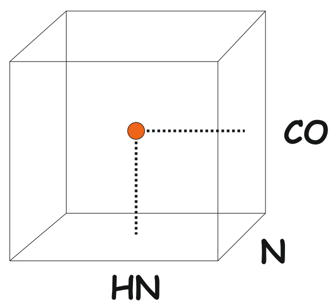
J(N-CG)
J-quantitative
Cross-peak experiment

hncggp3d.2



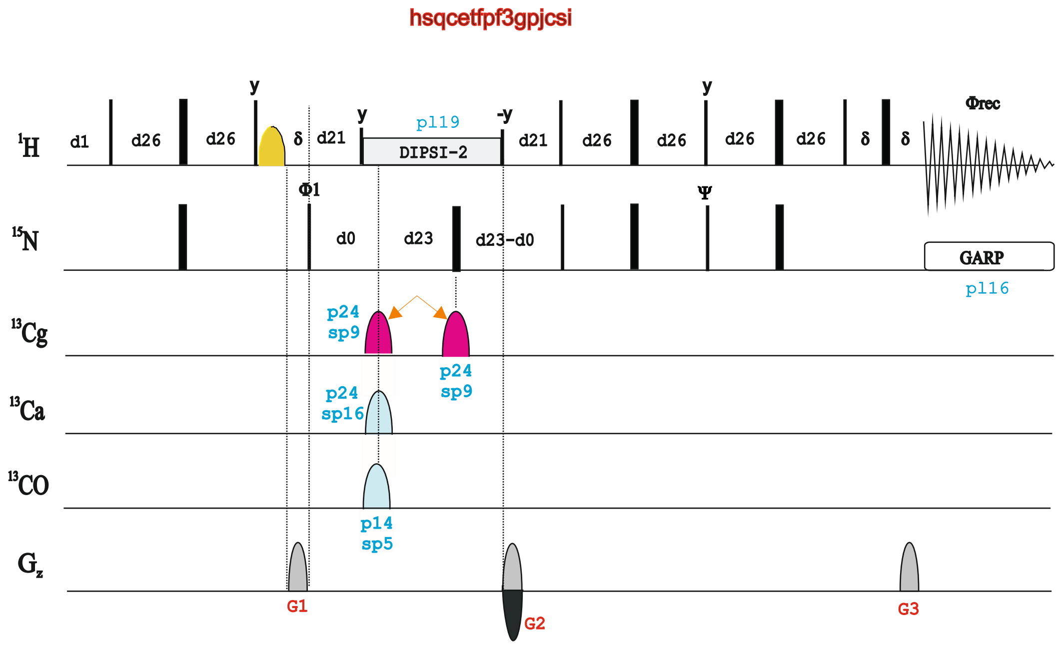
References:

1. J.-S. Hu & A. Bax, J. Biomol. NMR 9, 323-328 (1997)
2. R. Konrat, D.R. Muhandiram, N.A. Farrow & L.E. Kay, J. Biomol. NMR 9, 409-422 (1997)



2D Spin-Echo Difference CT-HSQC Experiment

J(N-CG)
spin-echo difference



d21: 1/(2J(NH)	[5.5 msec]
d23: constant time delay T(N)	[100 msec]
d26: 1/(4J'(NH)	[2.3 msec]

References:

J.-S. Hu & A. Bax, J. Biomol. NMR 9, 323-328 (1997)

Related Experiments:

Also See the original 2D CT-HSQC Experiment

Processing:

Two data are recorded ina interleaved mode
Use AU-program split [2] to split data

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COUPLING CONSTANTS
CHI2 SIDECHAIN ANGLE

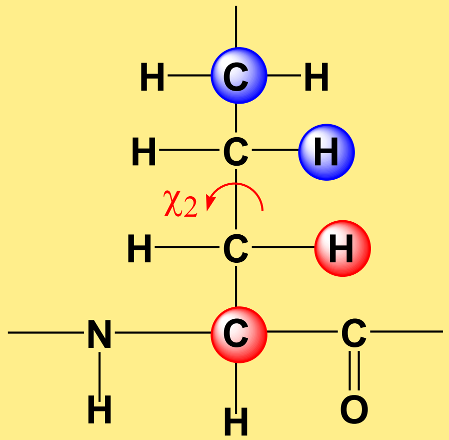
Side Chain χ_2 Angle

$^3J_{HB\text{-}CD}$

$^3J_{HB\text{-}HG}$

$^3J_{CA\text{-}HG}$

$^3J_{CA\text{-}CD}$



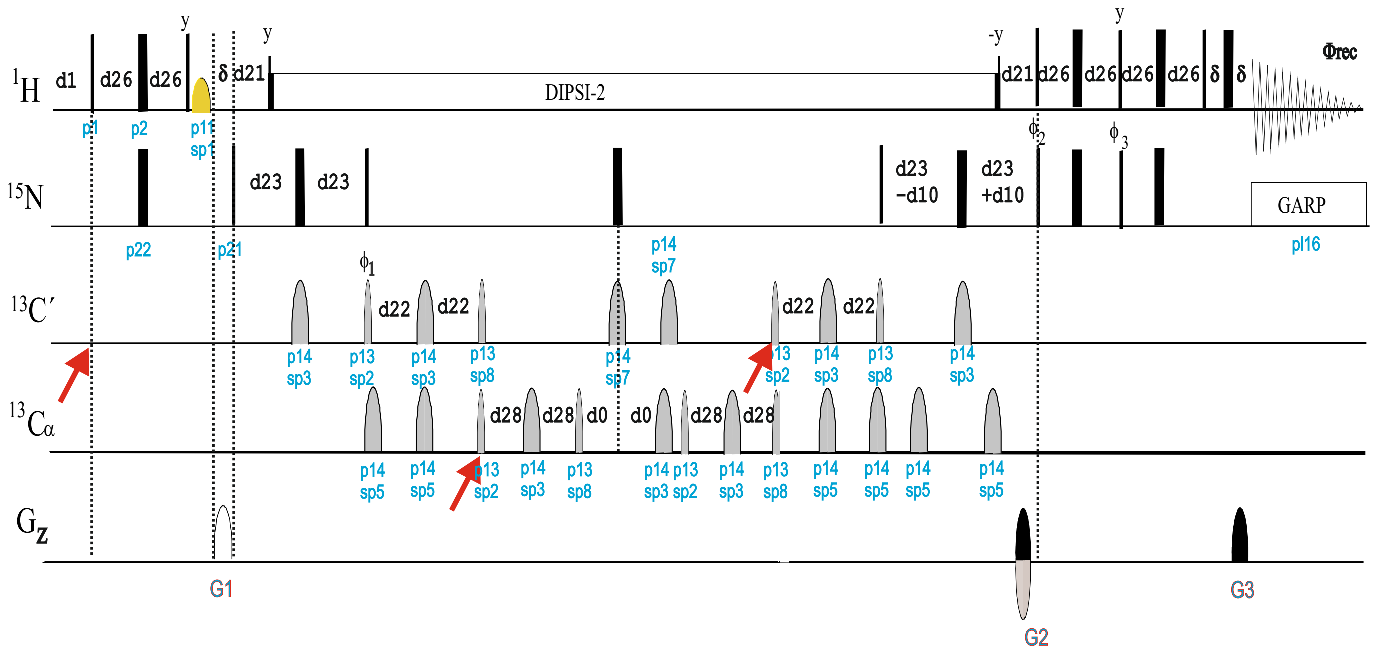
Chi2 Sidechain Coupling Constant

- 3D HN(CO)CACali (**hncocacgp3d** | HNCOCACGP3D) - 3J[CA-CD] via quantitative-J

J(CA-CD)
J-quantitative

d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(COCa))	[4.5 msec]
d23: 1/(4J(NCO))	[15 msec]
d26: 1/(4J'(NH))	[2.5 msec]
d28: 1/(4J(CaCd))	[28.2 msec]

hncocacgp3d



References:

M. Hennig, D. Ott, P. Schulte, R. Loewe, J. Krebs, T. Vorherr,
W. Bermel, H. Schwalbe & C. Griesinger, J. Am. Chem. Soc. 119, 5055-5056 (1997)

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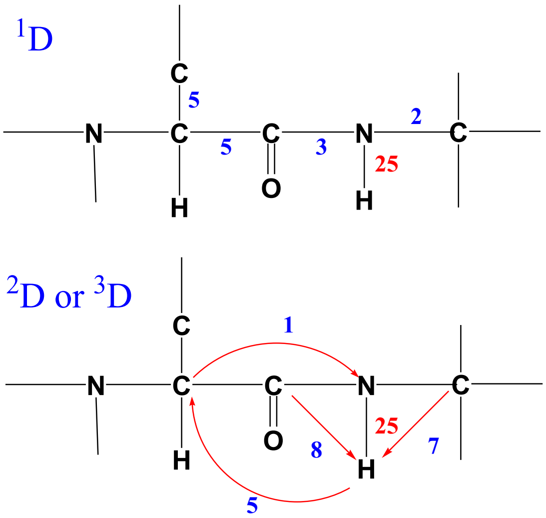
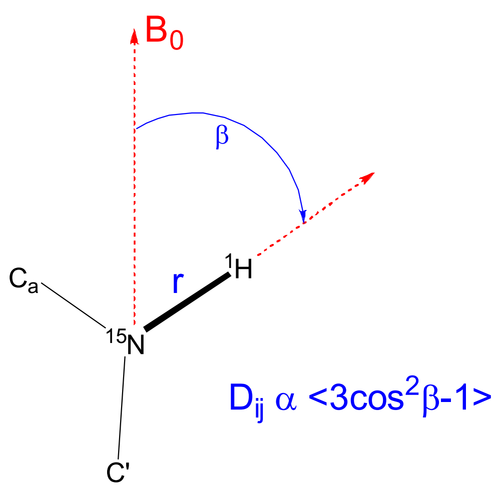
3D IPAP-HNCO & -IPAP-HNCA
FOR RDC MEASUREMENTS

3D HNCO and HNCA experiments for RDC measurements:

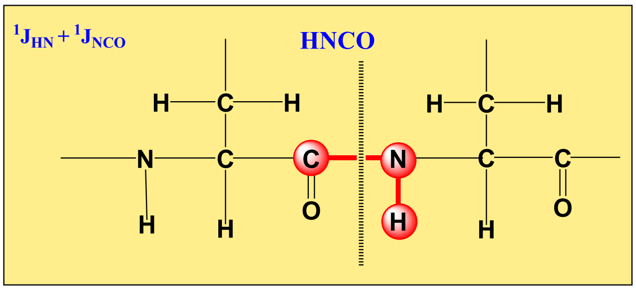
- 3D IPAP-HNCO to measure $^1J(NH)$ (**hncogpia**)
- 3D IPAP-J-HNCO to measure $^1J(CA\text{-}CO)$ and $^3J(HN\text{-}CA)$:
  - Using PEP (**hncogprc3d1** | HNCOGRPC3D1)
  - Using WATERGATE (**hncogprcwg3d1** | HNCOGRPCWG3D1)
  - Using TROSY (**trhncogprc3d1** | TRHNCOGRPC3D1)
- 3D IPAP-J-HNCO to measure $^{1,2}J(N\text{-}CA)$ and $^3J(HN\text{-}CA)$:
  - Using PEP (**hncogprc3d2** | HNCOGRPC3D2)
  - Using WATERGATE (**hncogprcwg3d2** | HNCOGRPCWG3D2)
  - Using TROSY (**trhncogprc3d2** | TRHNCOGRPC3D2)
- 3D IPAP-J-HNCO to measure $^1J(N\text{-}CO)$:
  - Using PEP (**hncogprc3d3** | HNCOGRPC3D3)
  - Using WATERGATE (**hncogprcwg3d3** | HNCOGRPCWG3D3)
  - Using TROSY (**trhncogprc3d3** | TRHNCOGRPC3D3)
- 3D J-HNCO (CA) to measure $^1J(CA\text{-}CB)$:
  - Using PEP (**hncogprc3d4** | HNCOGRPC3D4)
  - Using WATERGATE (**hncogprcwg3d4** | HNCOGRPCWG3D4)
  - Using TROSY (**trhncogprc3d4** | TRHNCOGRPC3D4)
- 3D IPAP-J-HNCO (CA) to measure $^1J(CA\text{-}HA)$ and $^1J(CA\text{-}CB)$:
  - Using PEP (**hncogprc3d5** | HNCOGRPC3D5)
  - Using WATERGATE (**hncogprcwg3d5** | HNCOGRPCWG3D5)
  - Using TROSY (**trhncogprc3d5** | TRHNCOGRPC3D5)
- 3D IPAP-J-HNCO to measure $^1J(H\text{-}N)$ and $^3J(HN\text{-}CA)$:
  - Using PEP (**hncogprc3d6** | HNCOGRPC3D6)
  - Using WATERGATE (**hncogprcwg3d6** | HNCOGRPCWG3D6)
  - Using TROSY (**trhncogprc3d6** | TRHNCOGRPC3D6)
- 3D IPAP-J-HNCO to measure $^1J(N\text{-}CO)$:
  - Using PEP (**hncogprc3d7**)
  - Using WATERGATE (**hncogprcwg3d7**)
  - Using TROSY (**trhncogprc3d7**)

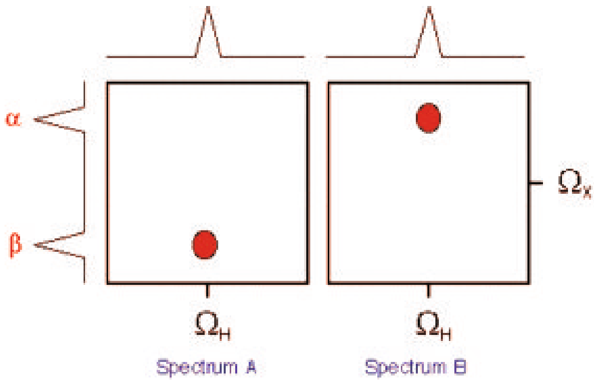
- 3D IPAP-J-HNCA to measure $^1J(CA\text{-}HA)$:
  - Using PEP (**hncagprc3d1**)
  - Using WATERGATE (**hncagprcwg3d1**)
  - Using TROSY (**trhncagprc3d1**)

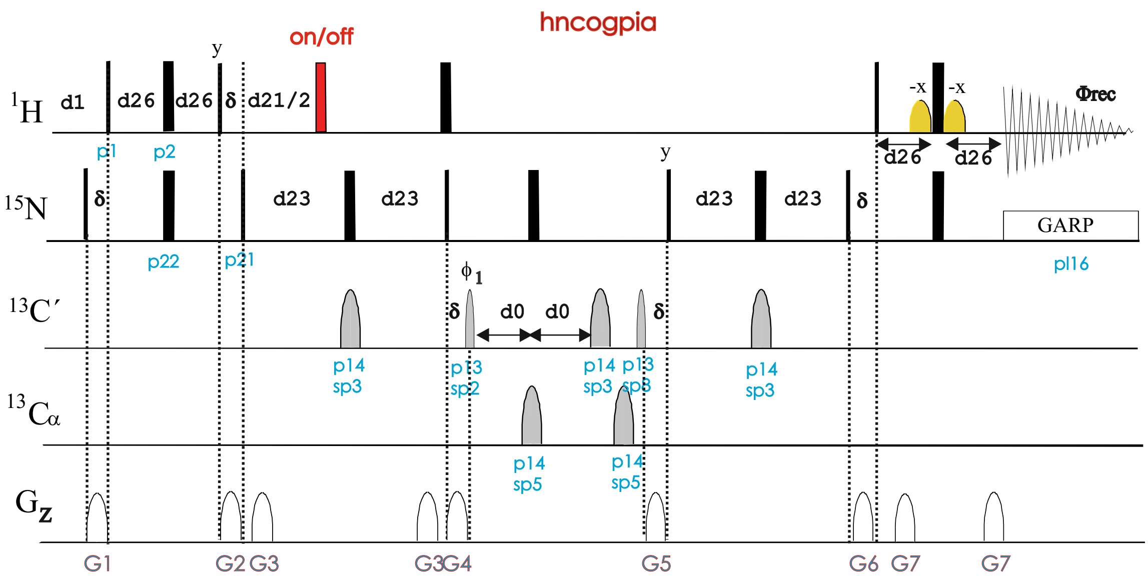




3D IPAP-HNCO: J(NH)







Processing:

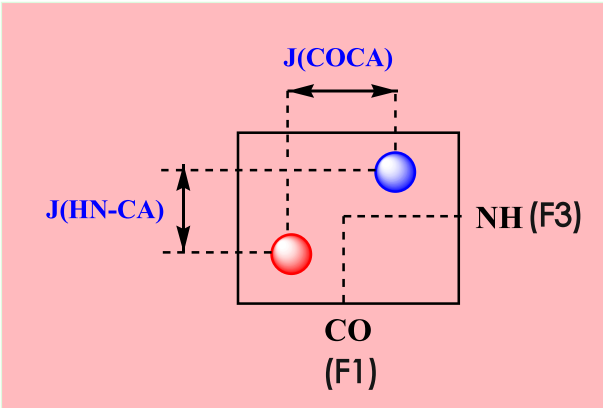
Two data are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data

d21: 1/(2J(NH))	[5.3 msec]
d23: 1/(4J(NCO))	[13.5 msec]
d26: 1 /(4J'(NH))	[2.5 msec]

Reference:

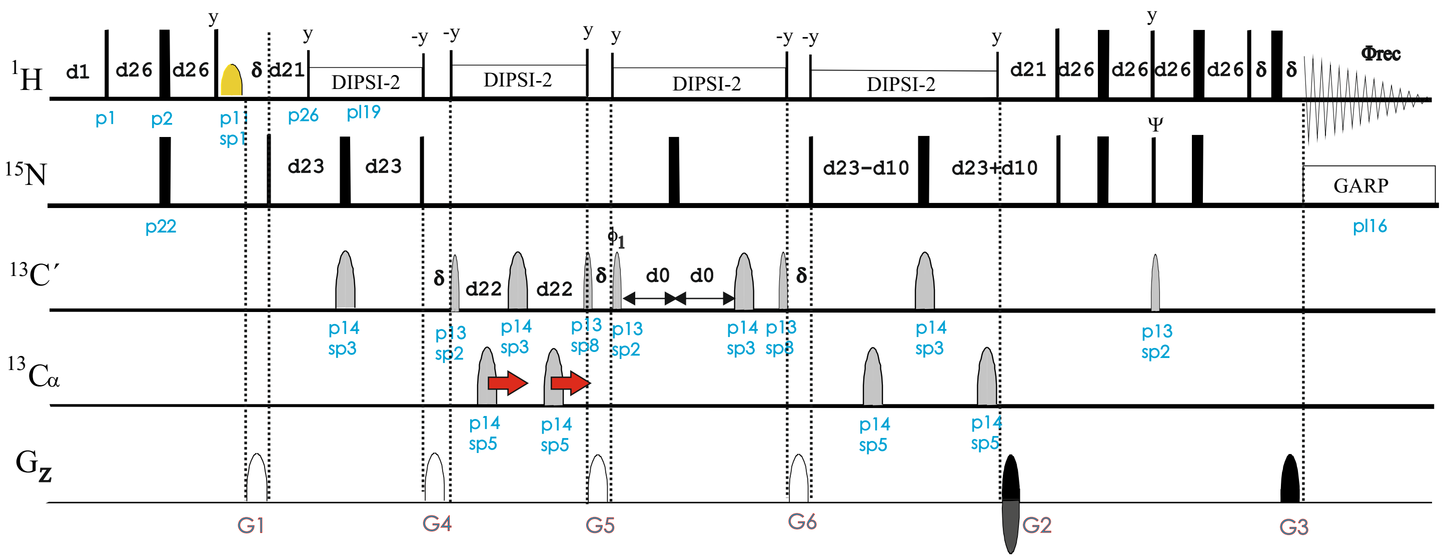
M.Ottiger, F. Delaglio & A. Bax, J. Magn. Reson.
131, 373-378 (1998)

3D IPAP-J-HNCO: 1J(CA-CO) and 3J(HN-CA)



d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m
d22=1/4J(COCA)=4.3m

hncogprc3d1



S3 Editing of CA prior to CO evolution
F1(H) -> F3(N) -> F2(C=O,J(Ca),t1) -> F3(N,t2) -> F1(H,t3).

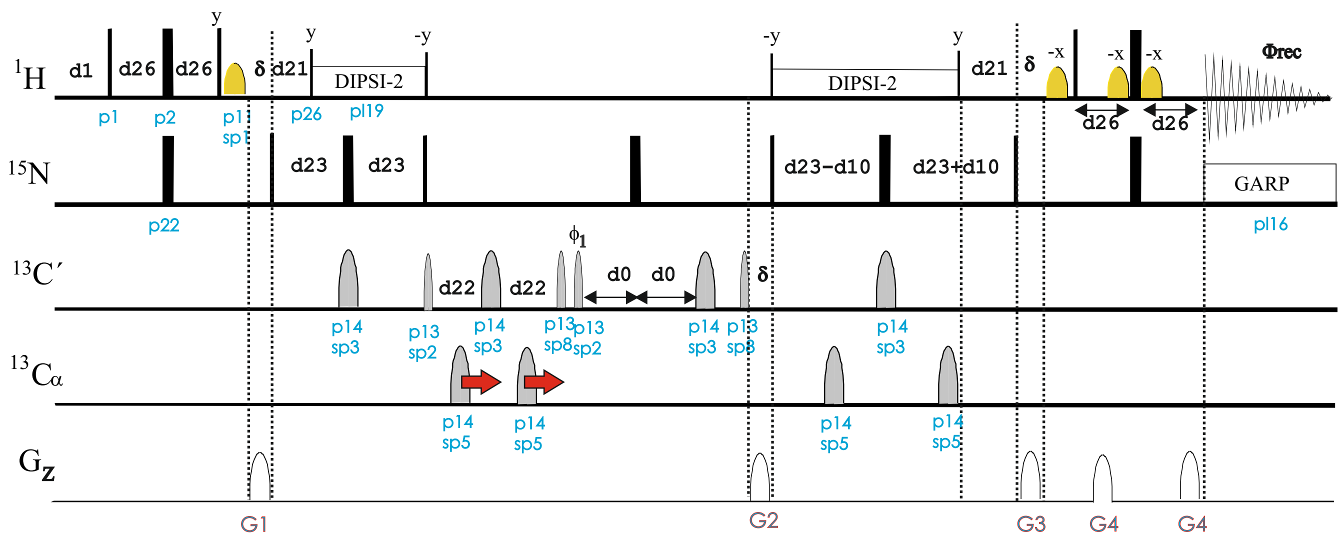
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+AP amd IP-AP)

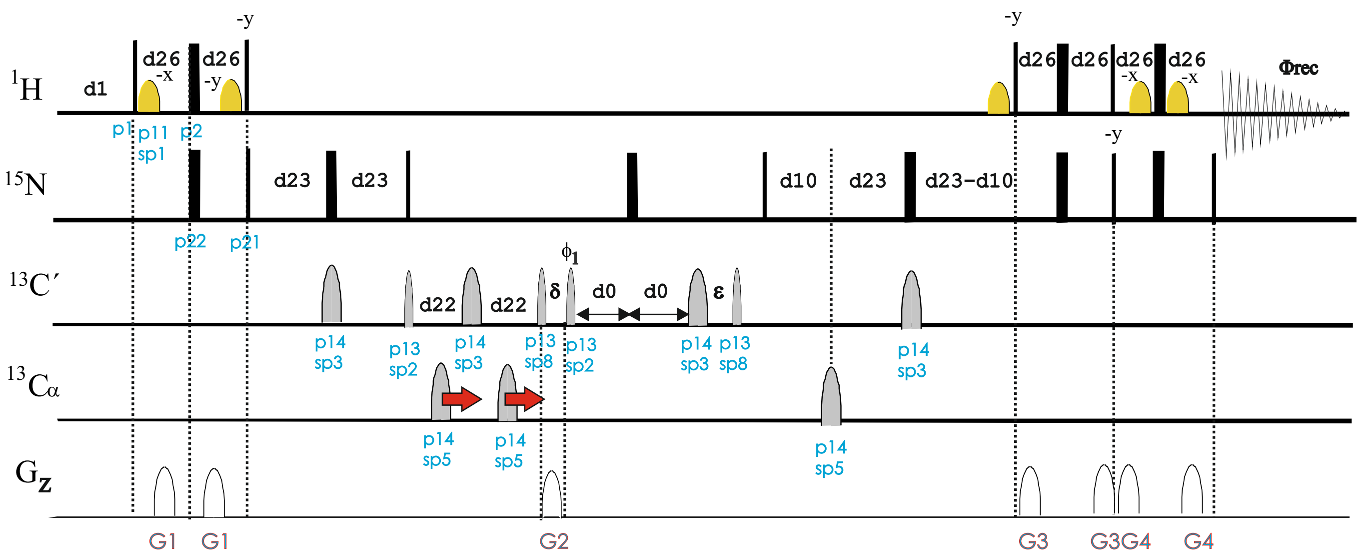
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

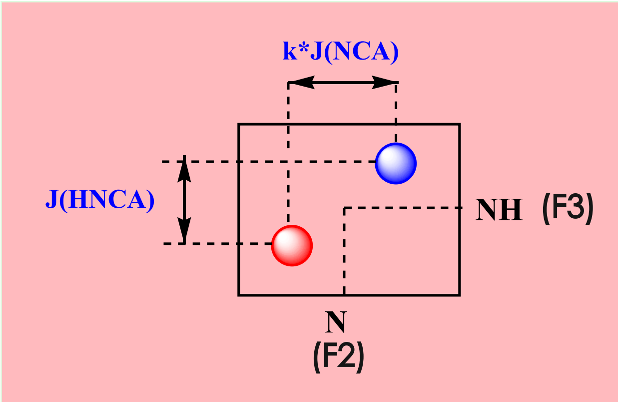
hncogprcwg3d1



trhncogprc3d1

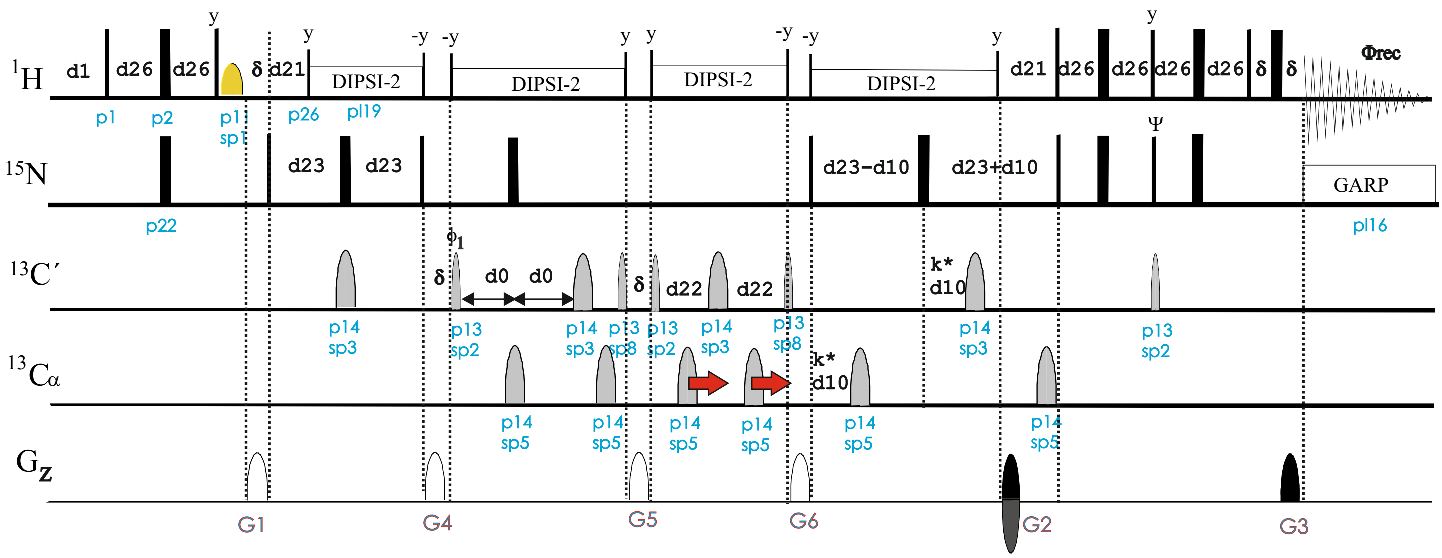


3D IPAP-J-HNCO: 1J(N-CA), 2J(N-CA) and 2J(HN-CA), 3J(HN-CA)



d26=1/4J(NH)=2.3m
d21=1/2J(NH)=5.5m
d23=1/4J(NCO)=12m
d22=1/4J(COCA)=4.3m

hncogprc3d2



S3 Editing of CA prior to NH evolution.
F1(H) -> F3(N) -> F2(C=O,t1) -> F3(N,t2,J(Ca)) -> F1(H,t3)

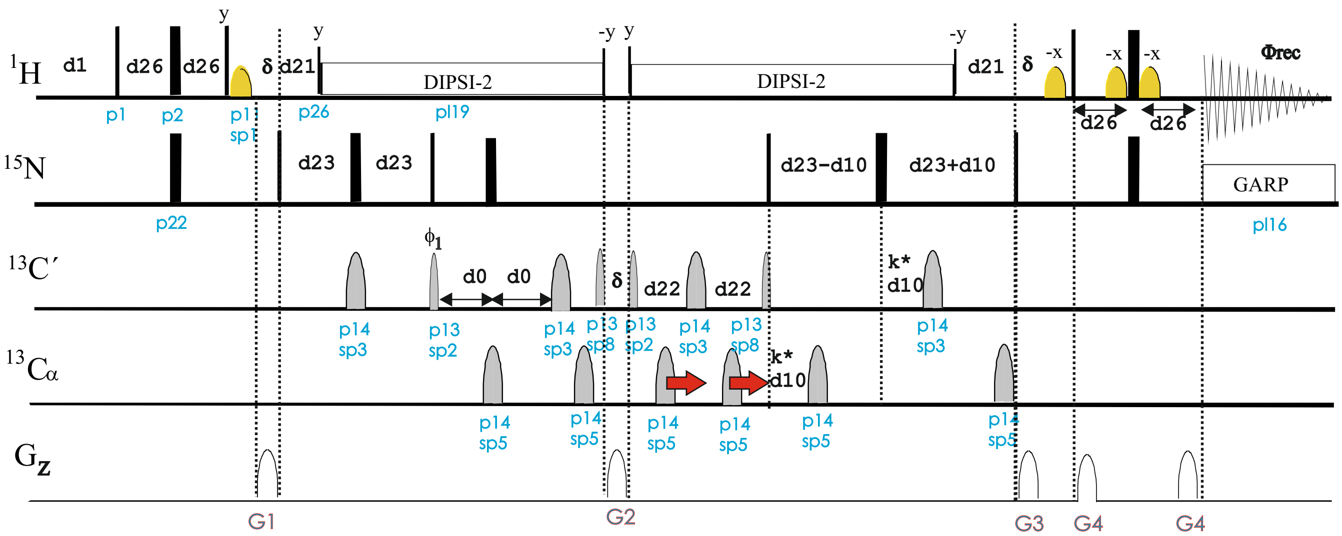
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

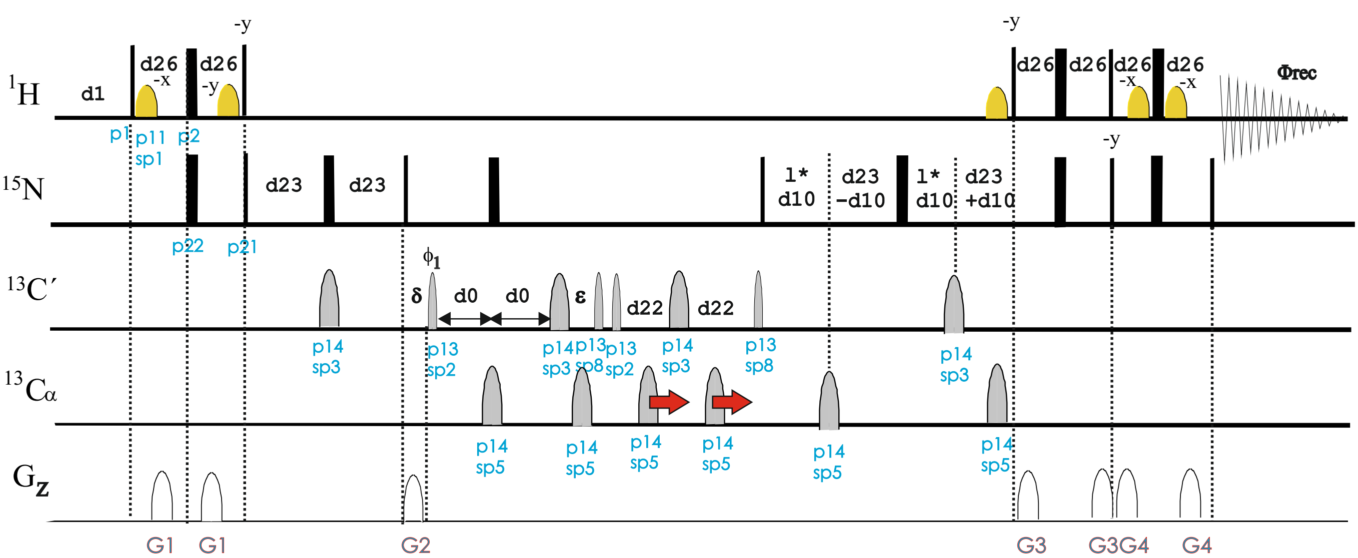
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

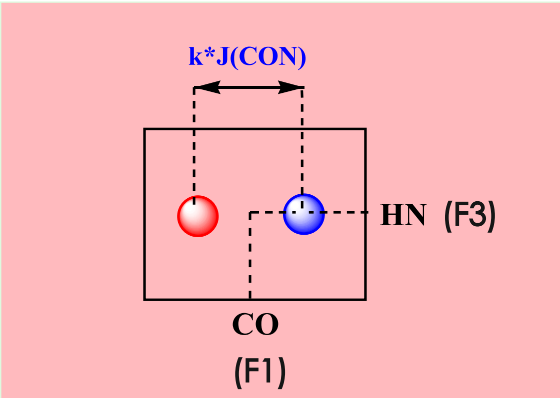
hncogprcwg3d2



trhncogprc3d2

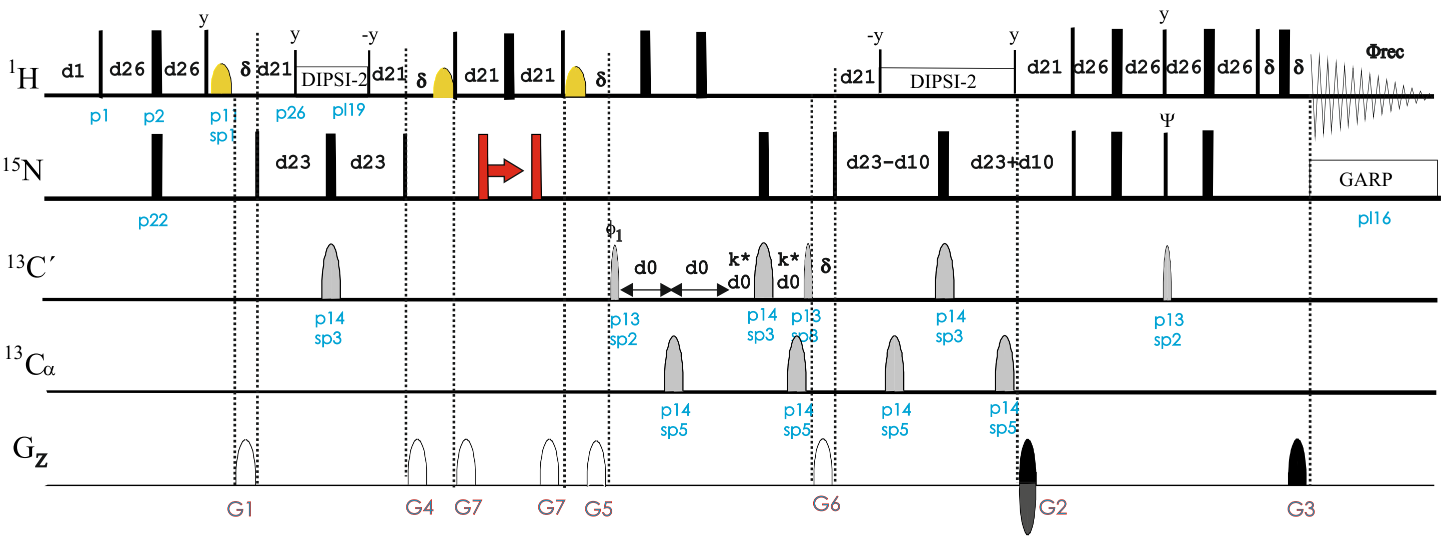


3D IPAP-J-HNCO: 1J(N-CO)



d21: 1/(2J(NH))	[5.5 msec]
d23: 1/(4J(NCO))	[12 msec]
d26: 1/(4J'(NH))	[2.3 msec]

hncogprc3d3



Editing of N prior to CO evolution.
F1(H) -> F3(N) -> F1(H,J(N)) -> F2(C=O,t1) -> F3(N,t2) -> F1(H,t3)

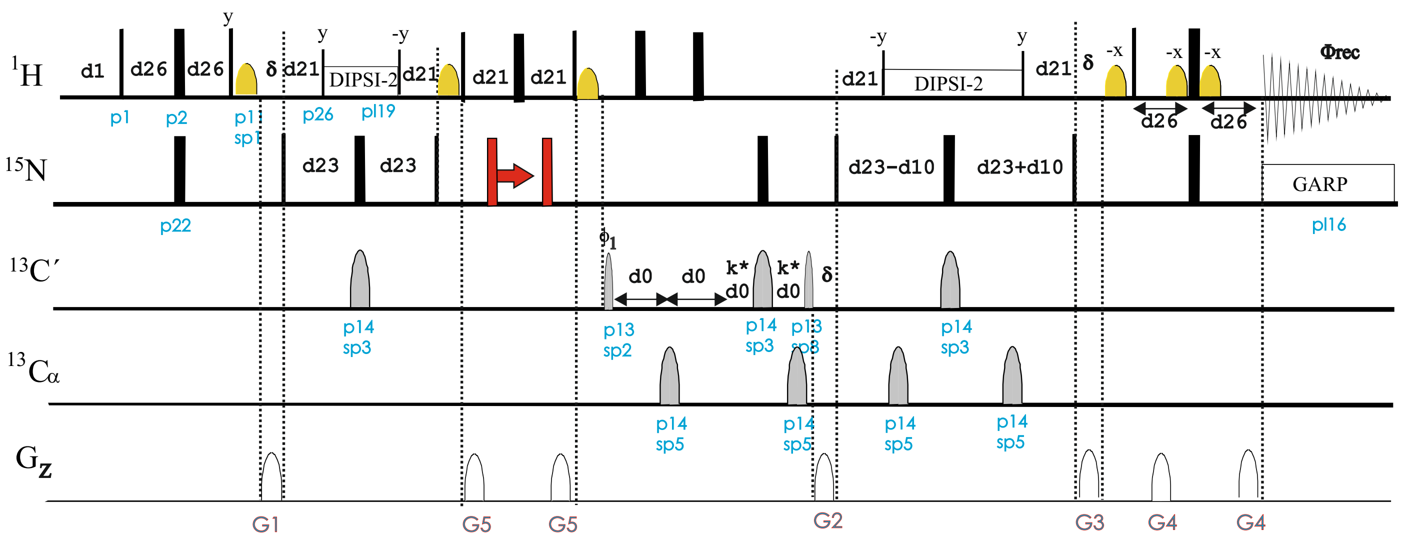
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

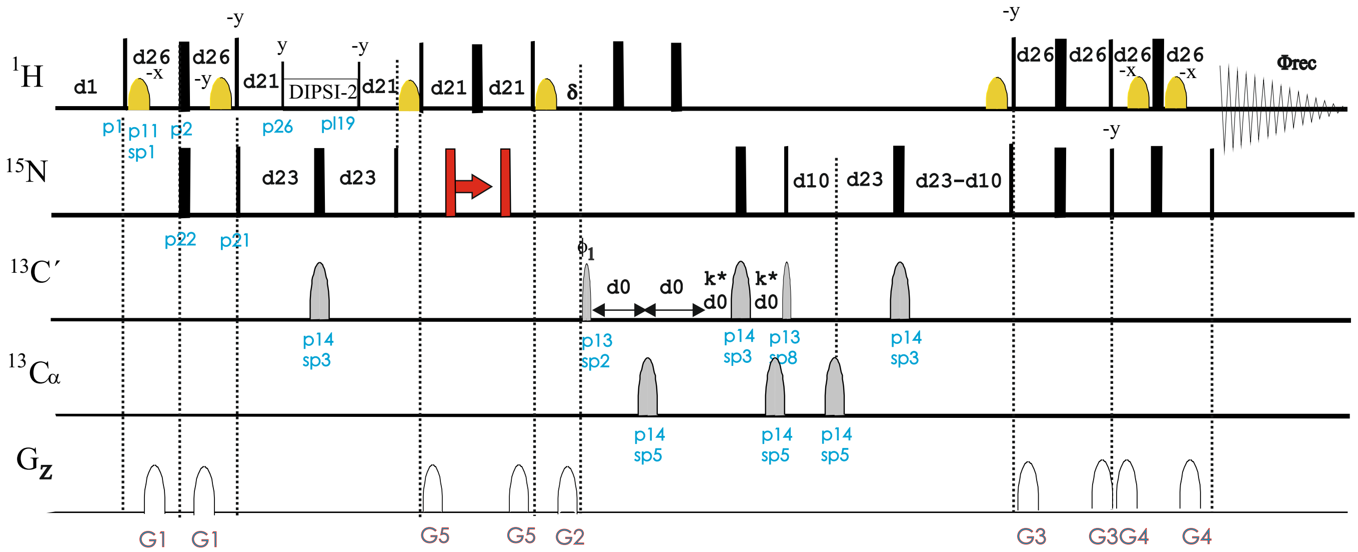
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

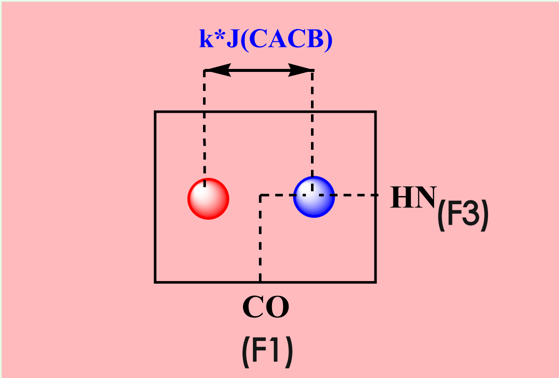
hncogprcwg3d3



trhncogprc3d3

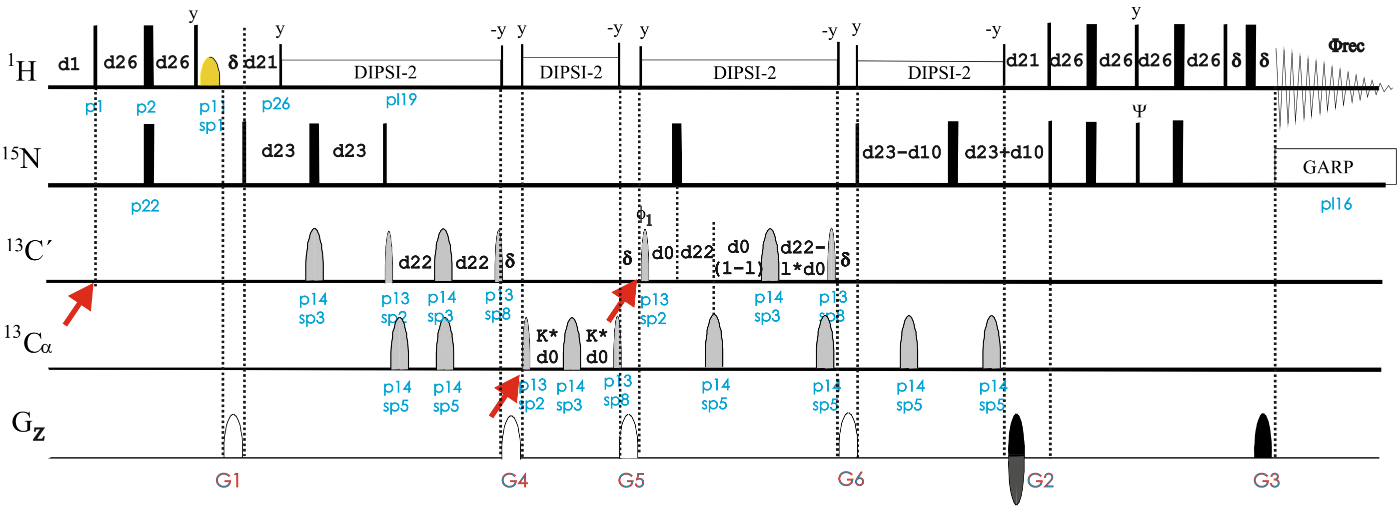


3D J-HNCO: 1J(CA-CB)



d21: 1/(2J(NH)) [5.5 msec]
d22: 1/(4J(COCa)) [4.5 msec]
d23: 1/(4J(NCO)) [12 msec]
d26: 1/(4J'(NH)) [2.3 msec]

hncogprc3d4



Editing of N prior to CO evolution.
F1(H) -> F3(N) -> F2(C=O) -> F2(Ca,J(Cb)) -> F2(C=O,t1) -> F3(N,t2) -> F1(H,t3)

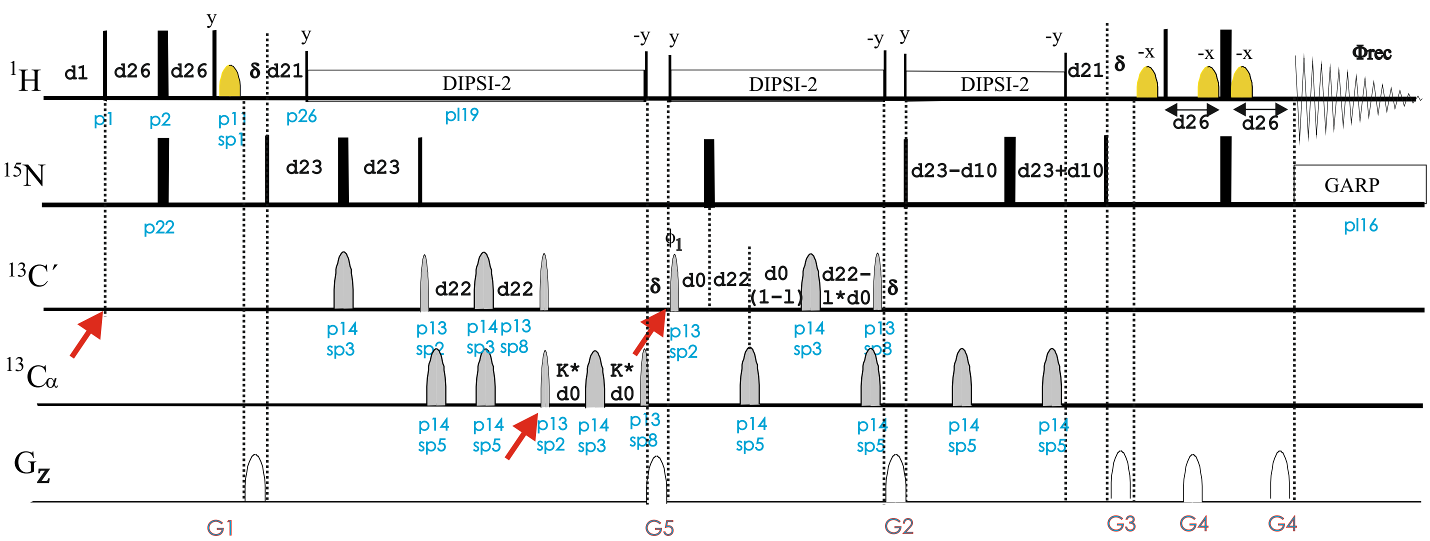
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

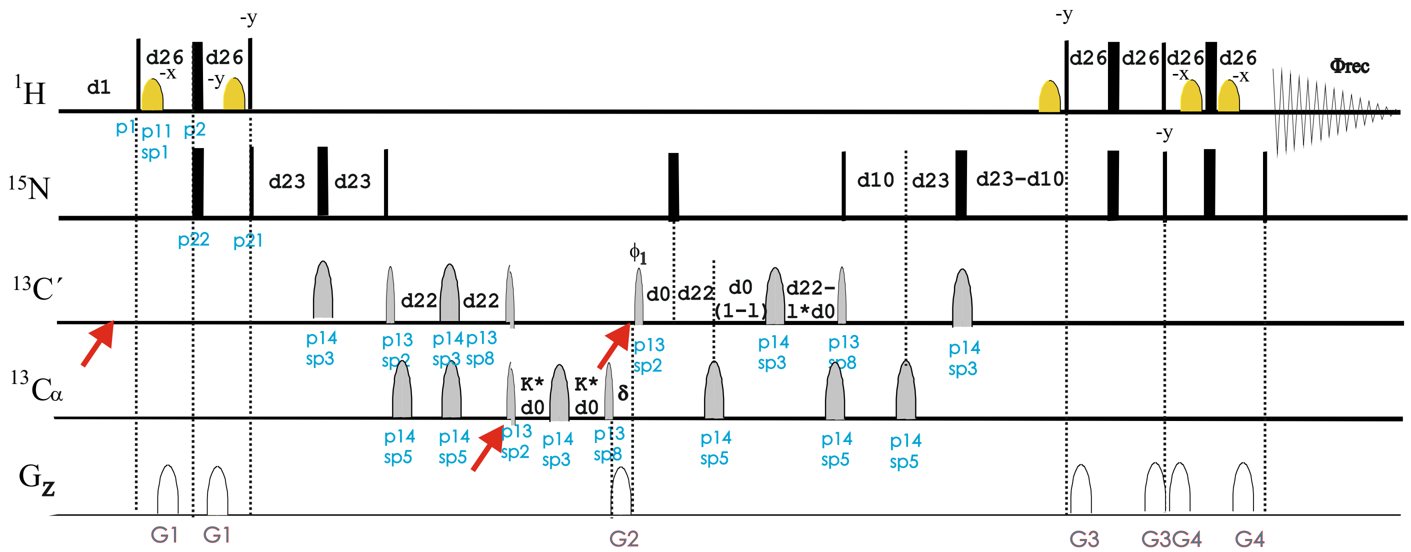
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

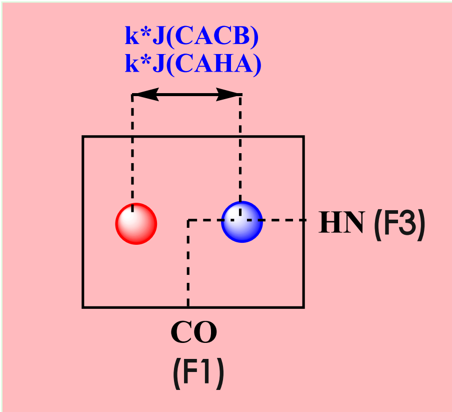
hncogprcwg3d4



trhncogprc3d4

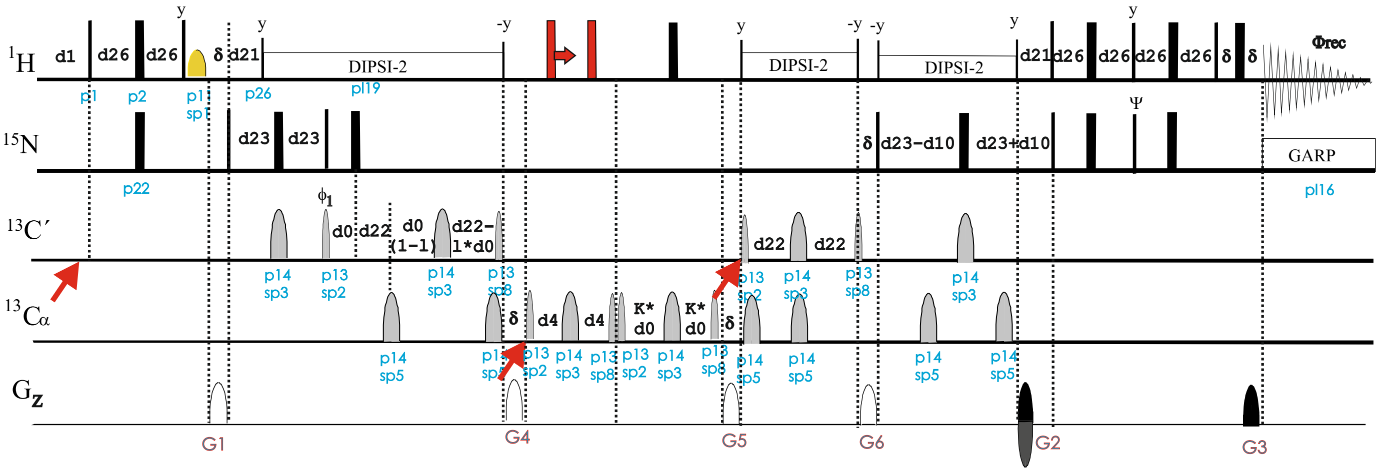


3D IPAP-J-HNCO: 1J(CA-HA) and 1J(CA-CB)



d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(COCa))	[4.5 msec]
d23: 1/(4J(NCO))	[12 msec]
d26: 1/(4J'(NH))	[2.3 msec]

hncogprc3d5



Editing of CA after the CO evolution.
F1(H) -> F3(N) -> F2(C=O,t1) -> F2(Ca,J(Ha)) -> F2(C=O) -> F3(N,t2) -> F1(H,t3)

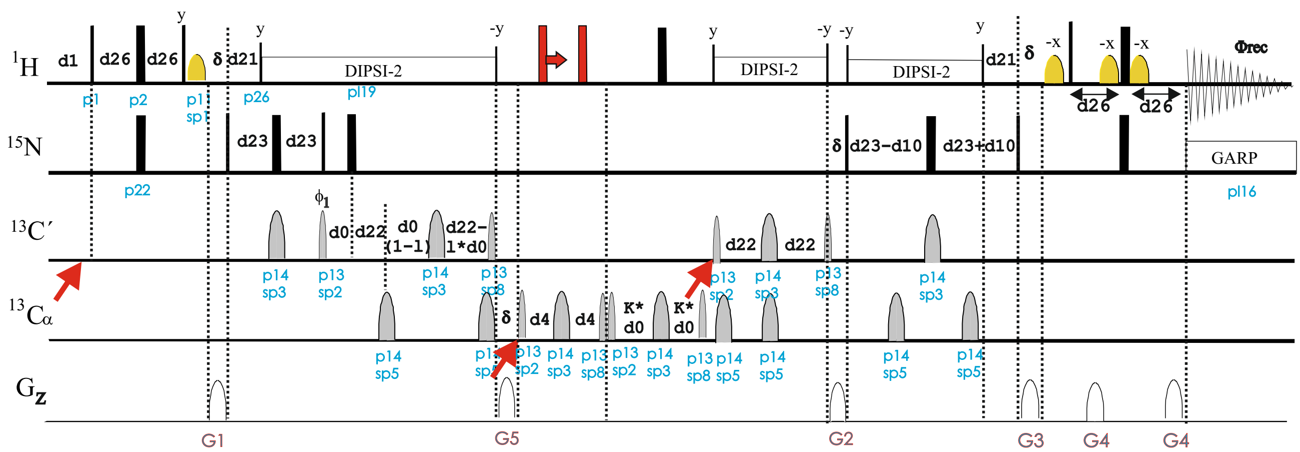
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

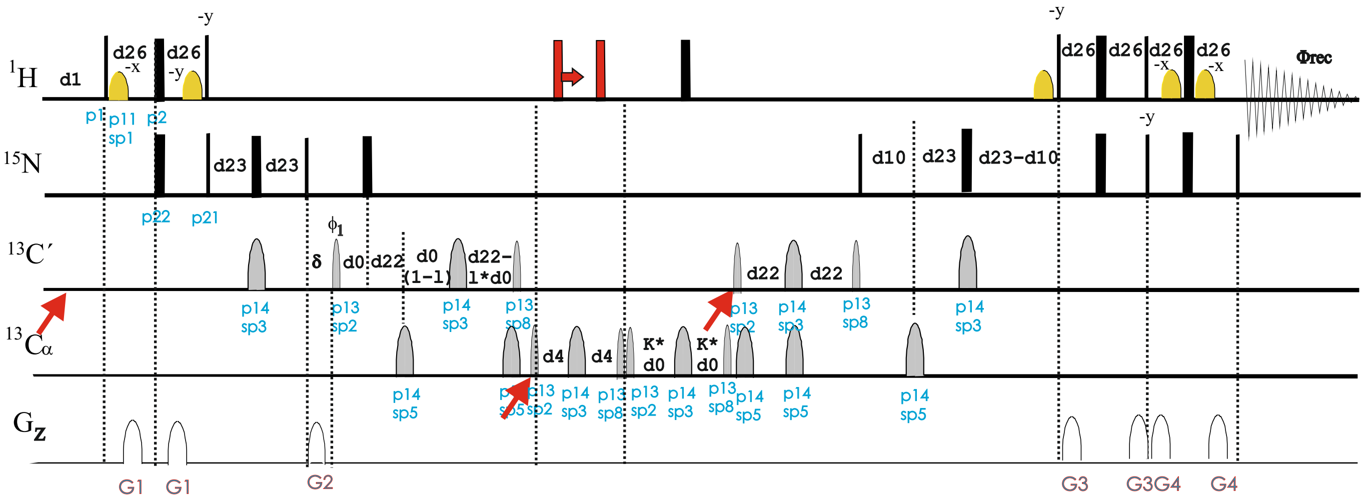
Reference:

D. Yang, J.R. Tolman, N.K. Goto & L.E. Kay, J. Biomol. NMR 12, 325-332 (1998)

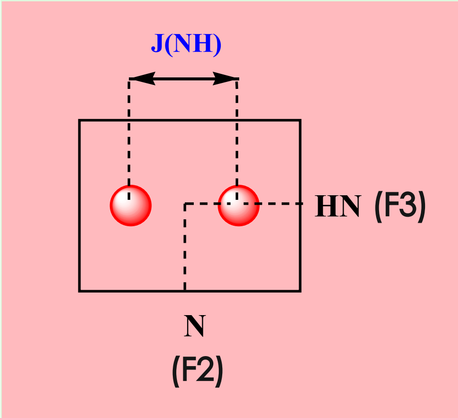
hncogprcwg3d5



trhncogprc3d5

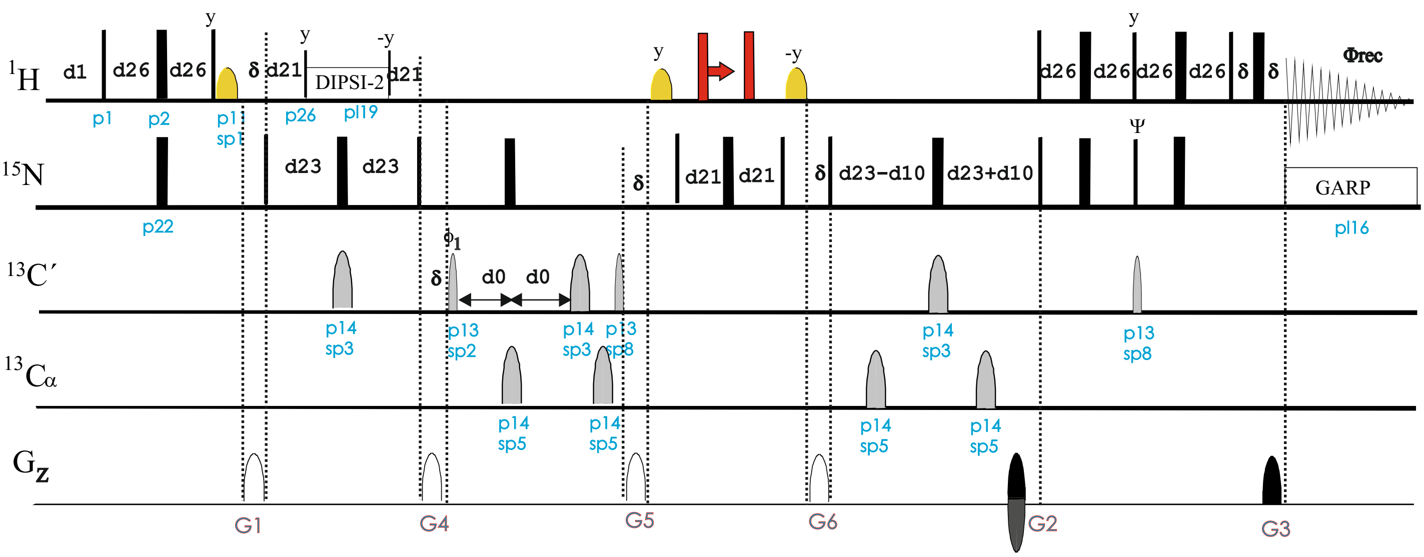


3D IPAP-J-HNCO: 1J(HN)



d21: 1/(2J(NH))	[5.5 msec]
d22: 1/(4J(COCa))	[4.5 msec]
d23: 1/(4J(NCO))	[12 msec]
d26: 1/(4J'(NH))	[2.3 msec]

hncogprc3d6



Editing of HN pior to N evolution.
F1(H) -> F3(N) -> F2(C=O,t1) -> F3(N,J(H(N),t2) -> F1(H,t3)

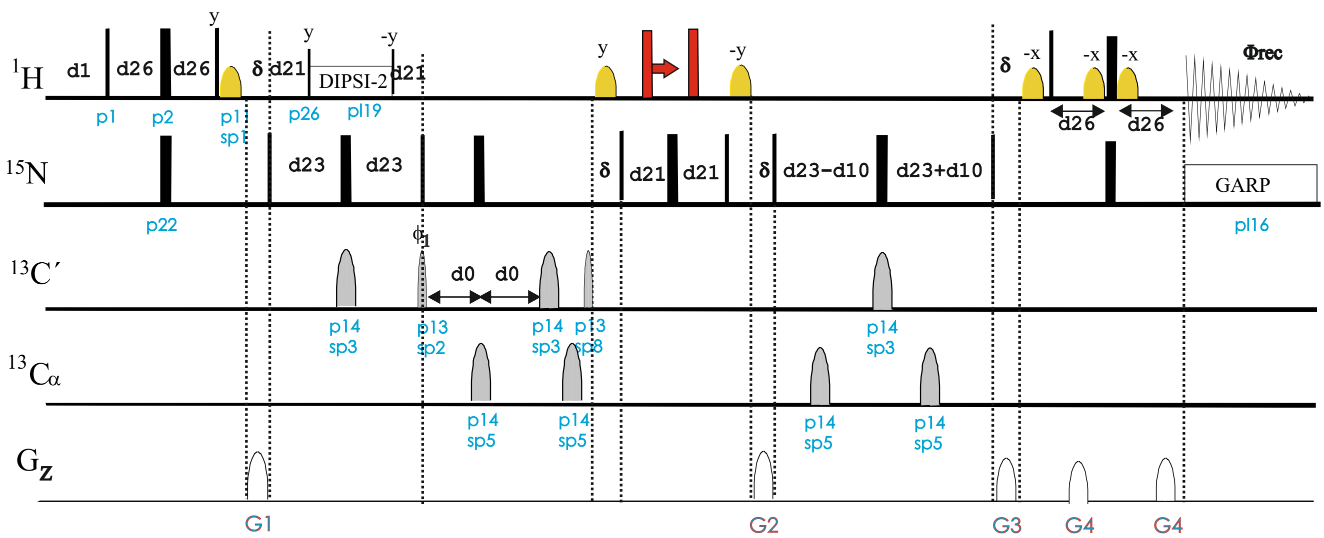
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

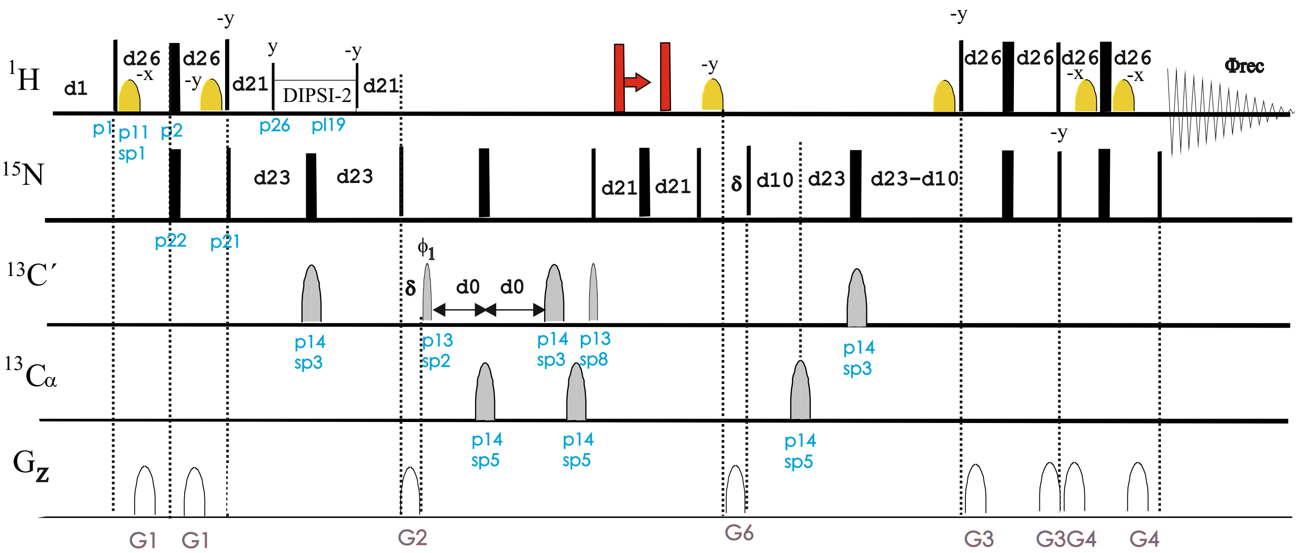
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

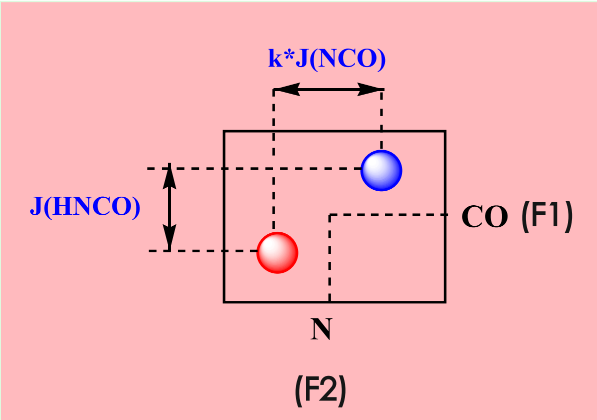
hncogprcwg3d6



trhncogprc3d6

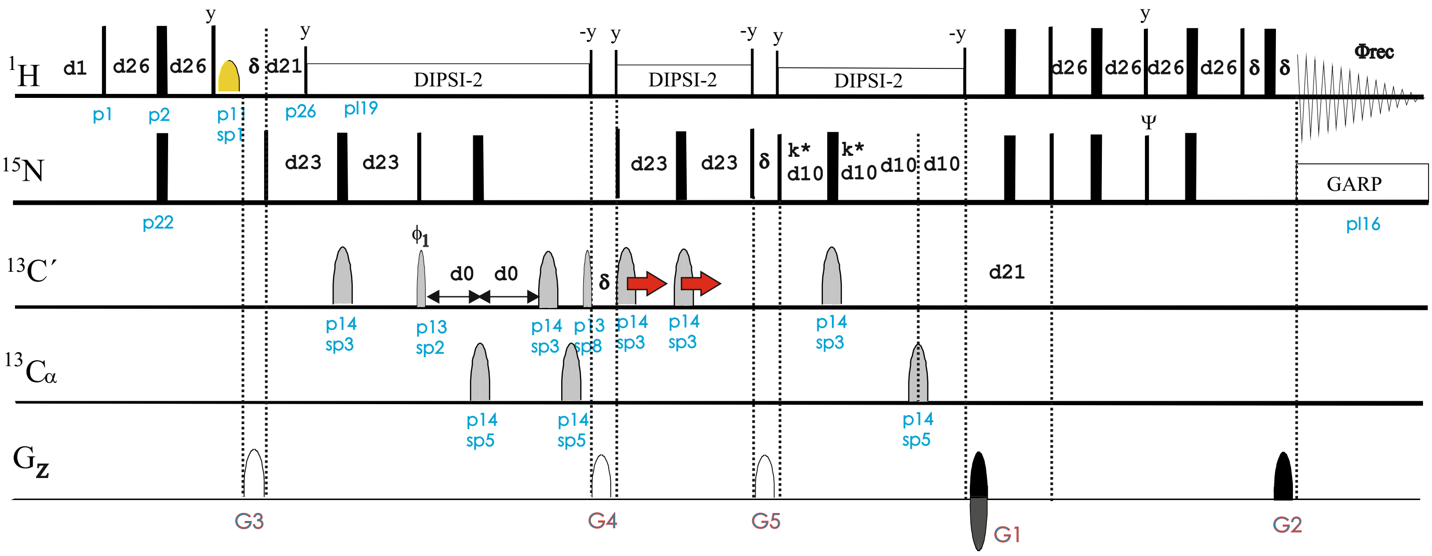


3D IPAP-J-HNCO: 1J(NCO) and 2J(HNCO)



d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCO)	[12 msec]
d26: 1/(4J'(NH)	[2.3 msec]

hncogprc3d7



Editing of CO pior to N evolution.
F1(H) -> F3(N) -> F2(C=O,t1) -> F3(N,J(C'),t2) -> F1(H,t3)

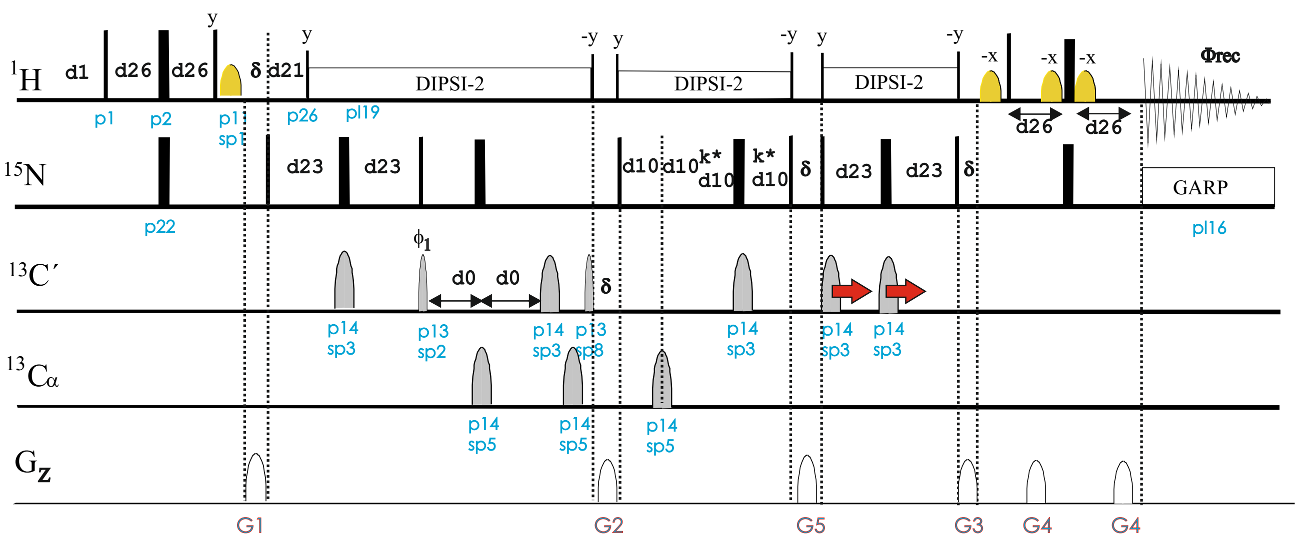
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

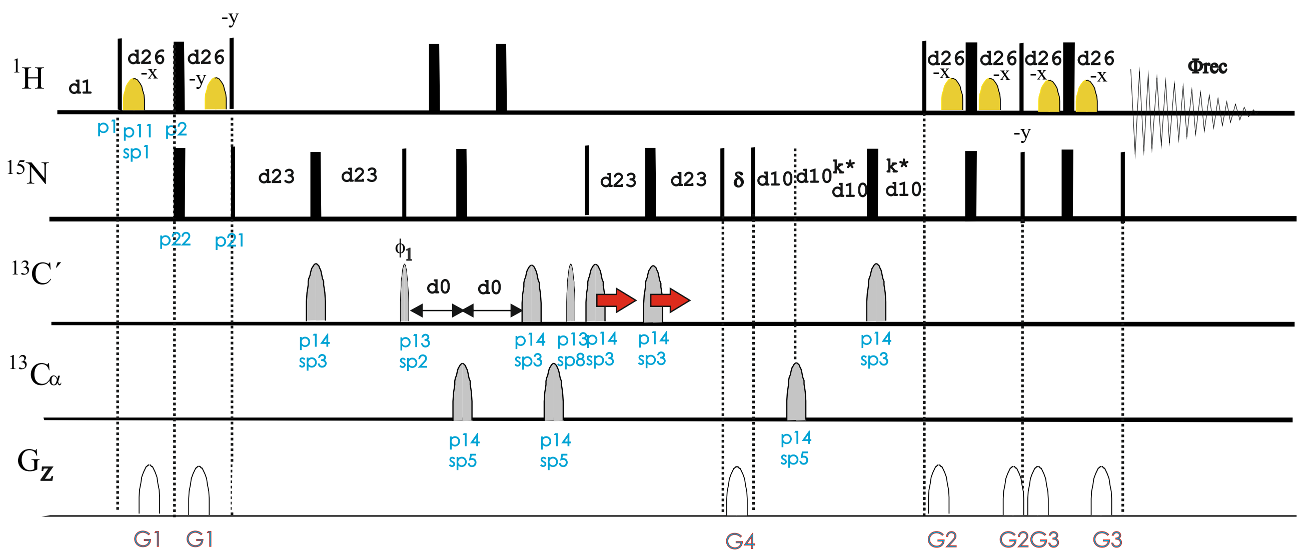
Reference:

P. Permi, P.R. Rosevear & A. Annila, J. Biomol. NMR 17, 43-54 (2000)

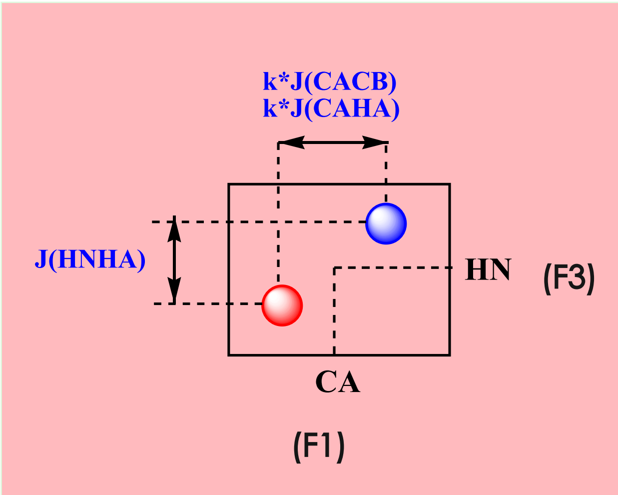
hncogprcwg3d7



trhncogprc3d7

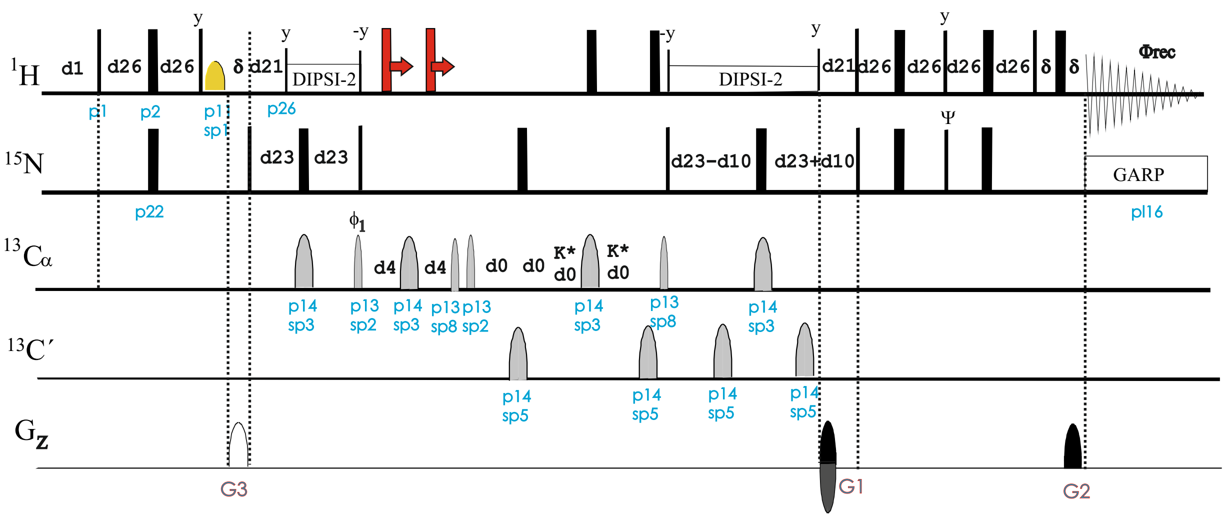


3D IPAP-J-HNCA: 1J(CA-HA) and 1J(CACB)



d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(4J(NCa)	[12 msec]
d26: 1/(4J'(NH)	[2.3 msec]

hncagprc3d1



S3 Editing of HA pior to CA evolution.
F1(H) -> F3(N) -> F2(Ca,J,t1) -> F3(N,t2) -> F1(H,t3)

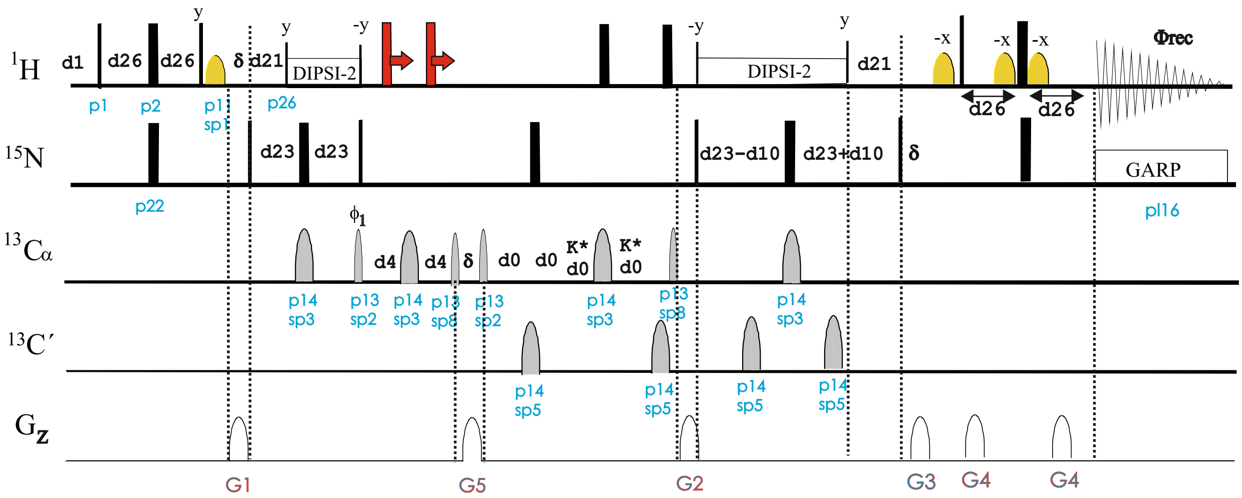
Processing:

Two data (IP and AP) are recorded in a interleaved mode.
Use AU-program split [ipap 2] to split data (IP+ap and IP-AP)

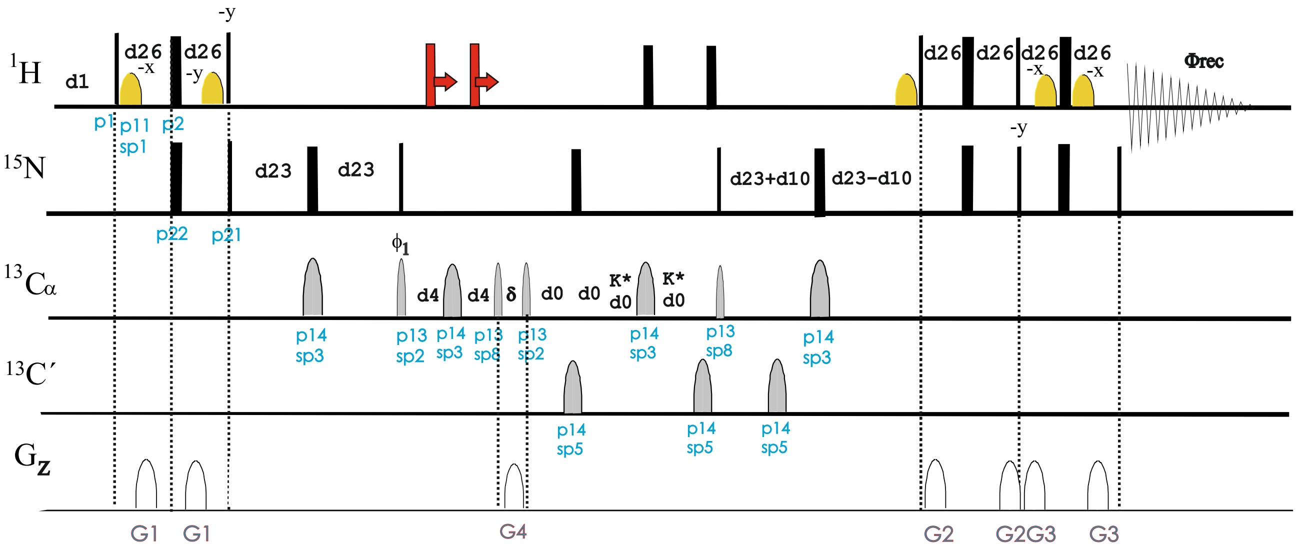
Reference:

P. Permi, J. Biomol. NMR 27, 341-349 (2003)

hncagprcwg3d1



trhncagprc3d1



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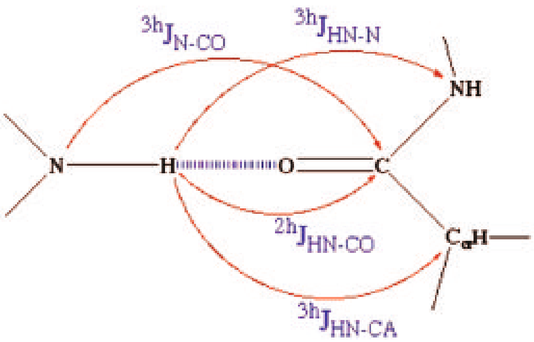
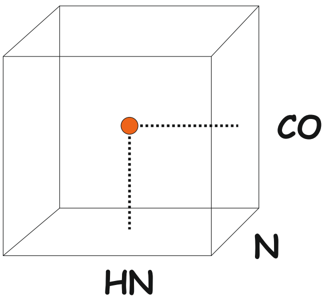
PROTEIN NMR
COUPLING CONSTANTS
THROUGH-HYDROGEN BONDS

Through-Hydrogen-bond 3D HNCO experiments

- 3D Hydrogen bond-HNCO (**hncogphb3d | HNCOGPHB3D**)
- 3D Hydrogen bond-HNCO with ^{13}C decoupling (**hncogphb3d.2**)
- 3D Hydrogen bond-HNCO without decoupling to enhance TROSY effect without spin-state selection (**hncogphb3d2 | HNCOGPHB3D2**)
- 3D Hydrogen bond-HNCO using TROSY (**trhncogphb3d**)

Also see:
The original 3D HNCO Experiment.



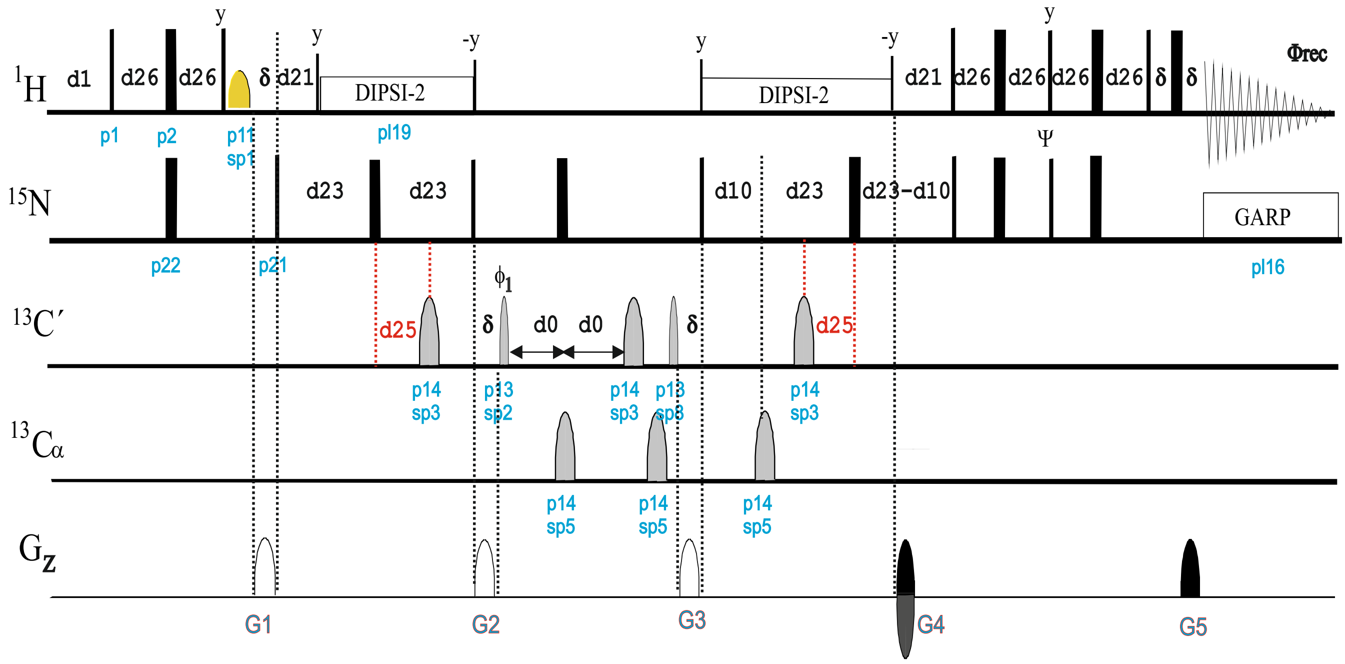


d21: 1/(2J(NH)	[5.5 msec]
d23: 1/(1J(NCO)	[66.6 msec]
d25: 1/(4J(NCO)	[16.6 msec]
d26: 1/(4J'(NH)	[2.3 msec]

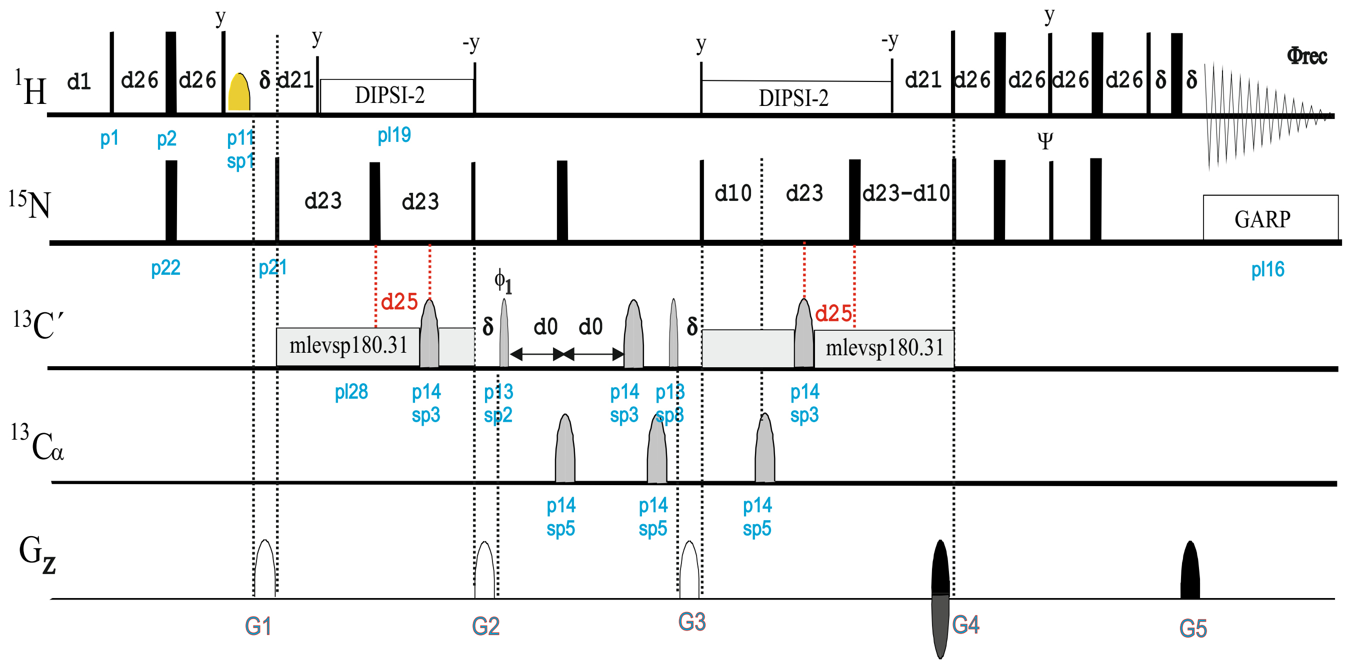
References:

1.F. Cordier & S. Grzesiek, J. Am. Chem. Soc. 121, 1601-1602 (1999)

hncogphb3d



hncogphb3d.2



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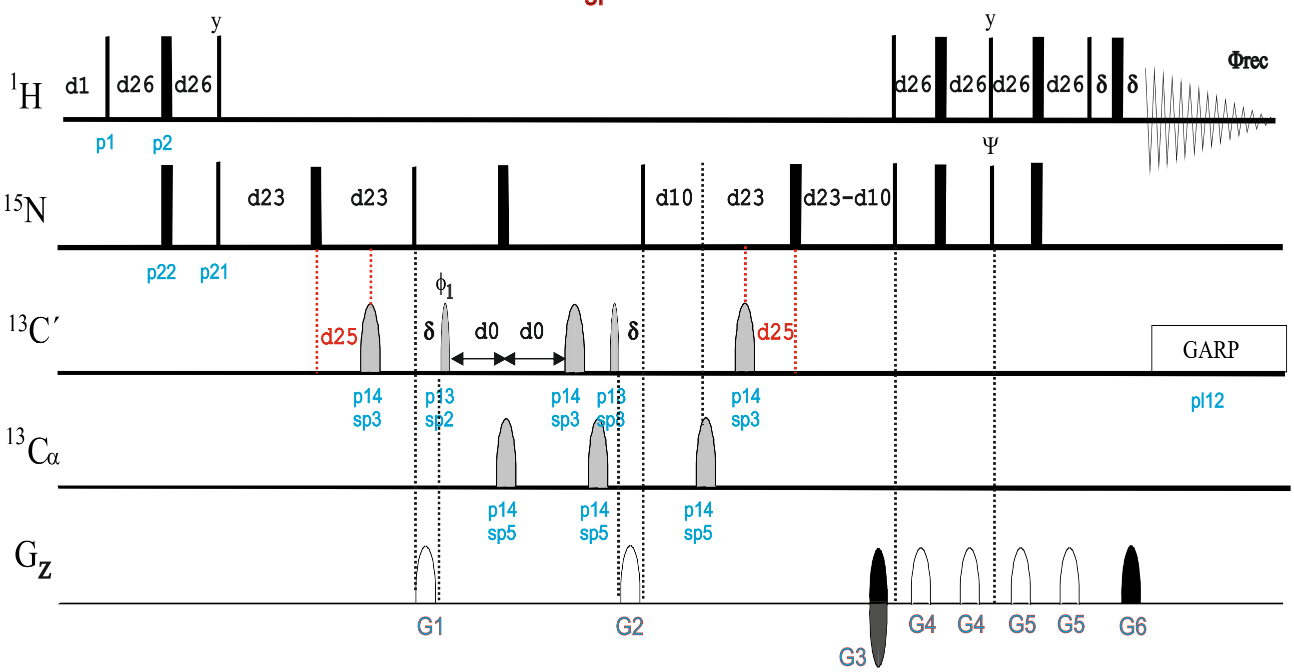
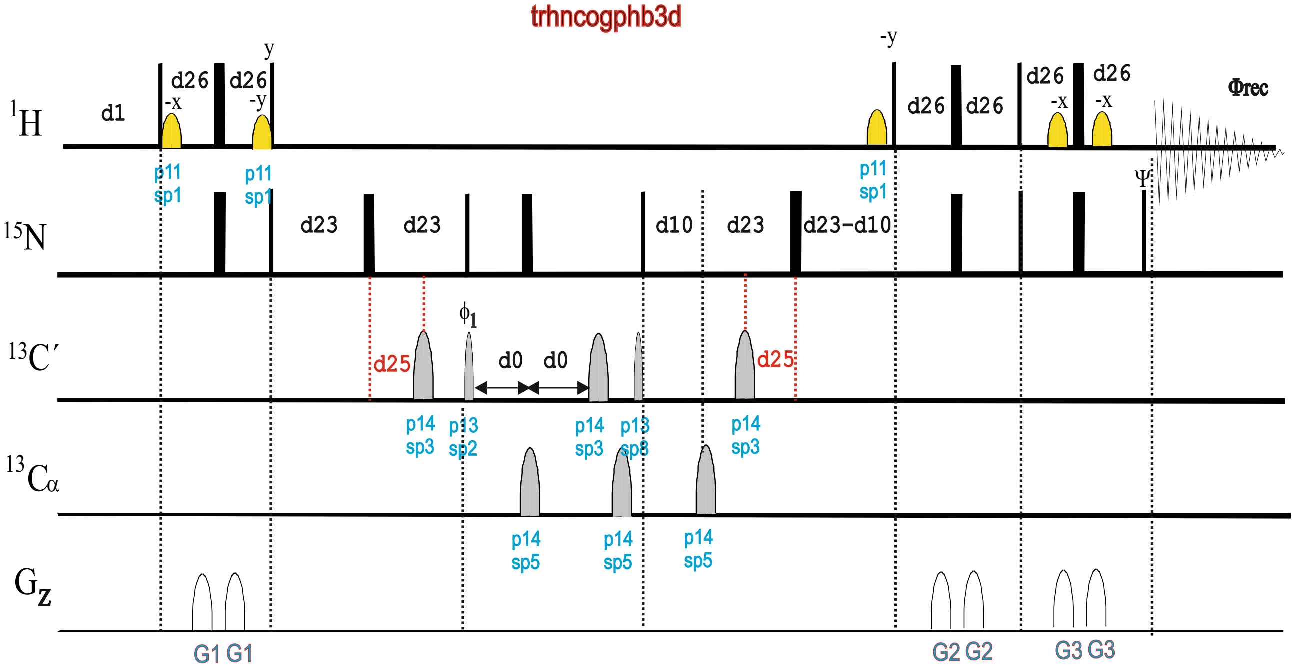


trhncogphb3d



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NMRGuide

2D & 3D NUCLEIC-ACID
NMR EXPERIMENTS.
INTRODUCTION

References:

1. S.S. Wijmenga and B.N.M. van Buuren, "The use of NMR methods for conformational studies of nucleic acids, Prog. Nucl. Magn. Reson., 32, 287-387 (1998).
2. B. Fürtig, C. Richter, J. Wöhnert, and H. Schwalbe, "NMR of RNA", ChemBioChem, 4, 936-962(2003).

1. Sugar Assignment

   H and H/C experiments
   Sugar puckering
   Measurement of J(CH) and J(HH)

2. Sequential assignment via phosphodiester linkage

   H/P and H/C/P experiments
   Measurement of J(PH) and J(PC)
   NOE contacts

3. Sugar-to-base connectivities

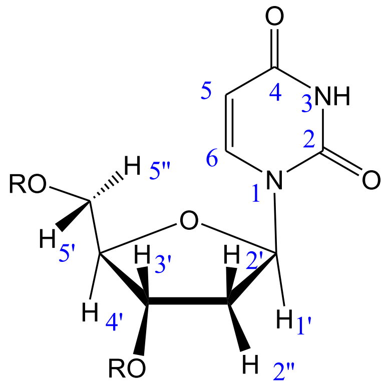
   H/C/N experiments
   NOE contacts

4. Intra-base assignment

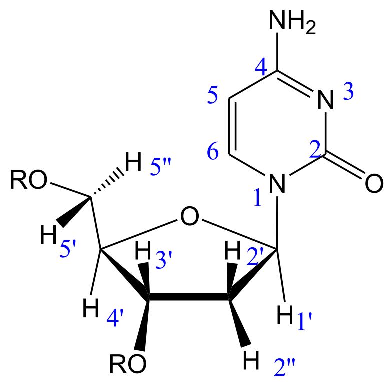
   H/N, H/C and H/C/N experiments

5. Base-pairing identification

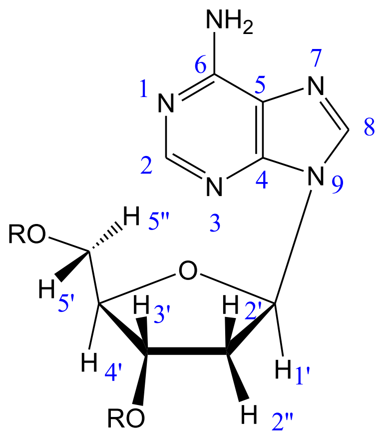
   Through-hydrogen-bond H/N experiments
   NOE contacts



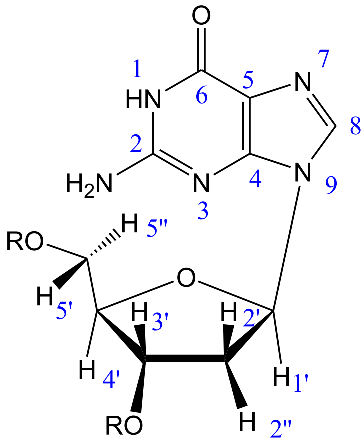
Uridine



Cytosine, C



Adenine, A



Guanine, G

	N1	C2	N3(H)	C4	C5(H5)	C6(H6)	N(H_2)
U	142-146	154	156-162 (13-14)	169	102-107 (5.0-6.0)	137-144 (6.9-7.9)	-
C	150-156	159	210	166-168	94-99 (5.0-6.0)	136-144 (6.9-7.9)	94-98 (6.7-7.0 & 8.1-8.8)

	N1(H)	C2(H2)	N3	C4	C5	C6	N7	C8(H8)	N9	N(H_2)
A	214-216	152-156 (7-8)	220-226	149-151	119-121	157-158	224-232	137-142 (7.7-8.5)	166-172	82-84 (5-6 & 7.8)
G	146-149 (12-13.6)	156	167	152-154	117-119	161	228-238	131-138 (7.5-8.3)	166-172	72-76 (5-6 & 8-9)

	C1'	C2'	C3'	C4'	C5'
Sugar	87-94	70-78	70-78	82-86	63-68
	(5-6	4.4-5.0	4.4-5.0	3.8-4.3	3.8-4.3)

Main Features of nucleic acid (NA) experiments

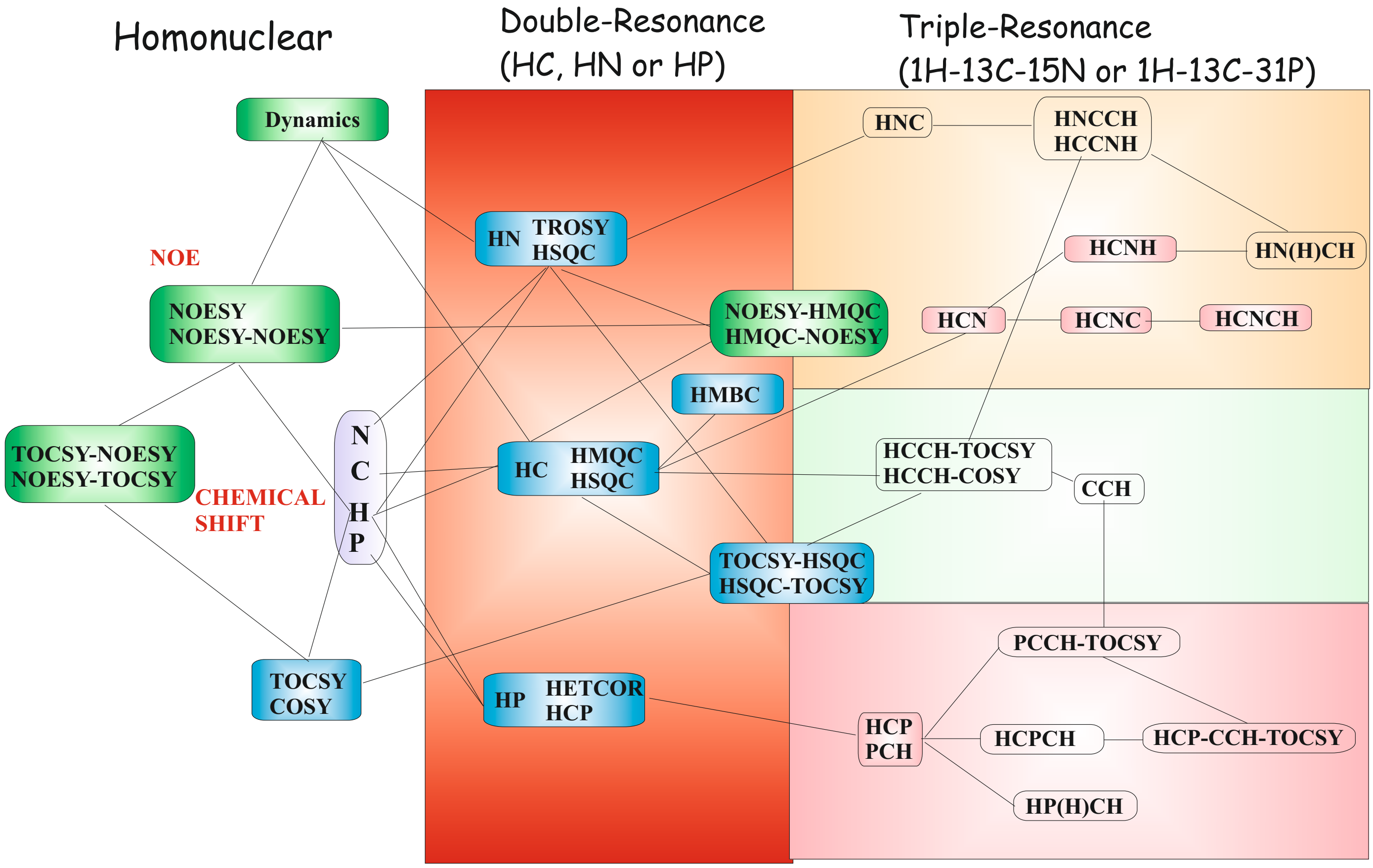
NAs usually present poor degeneracy and important conformational flexibility. Thus, 1H NMR spectra of NAs can be difficult to analyze because of their low proton density and important resonance overlapping due to poor 1H chemical shift dispersion. However, small NAs can be studied using the same1D and 2D NMR experiments dedicated to study natural-abundance organic molecules. Higher NAs would require double- and triple-resonance NMR experiments involving low-sensitive 13C or 15N nuclei.

Sample Requirements

Unlabeled NAs can be analyzed with typical 1D and 2D NMR homo- and heteronuclear NMR experiments. In compllex NAs, more sophisticated and specifically designed 15N and Triple-resonance HCX experiments can require selective 13C/15N labeling or 13C15N-doubly labeled samples.

Hardware Requirements

NAs experiments are best recorded on triple-resonance 1H,13C,15N or 1H,13C,31P inverse probeheads with z-gradients capabilities.



Experimental details for nucleic-acid experiments

Offsets

F1 channel: 1H (o1p)
F2 channel: 13C (o2p)
F3 channel: 15N (o3p) in HN-type or HCN-type experiments
F3 channel: 31P (o3p) in HP-type or HCP-type experiments

Mixing/Decoupling

From f2 channel:
13C CPD with GARP (pcpd2=80us at pl12)
13C-13C TOCSY with FLOPSY-16 (p9 at pl15)

From f3 channel:
15N CPD with GARP (pcpd3=200us at pl16)
31P CPD with GARP (pcpd3 at pl16)

Typical 13C pulses from F2 channel

p13 sp2: 90° C on- resonance (320us , spnam2=Q5.1000)
P14 sp3: 180° C on-resonance (256us, spnam3= Q3.1000)
p13 sp8: retro-90° C on-resonance (320us, spnam8= Q5tr.1000)
p14 sp5: 180° C off-resonance (256us, spnam5=Q3.1000)

p8 sp13: 180° adiabatic for inversion (500us using CHIRP , spnam13=Crp60,0.5,20.1)

Typical 15N pulses from F3 channel

p30 sp9: 180° N1/N9 on- resonance (700us , spnam9=Q3.1000)

Very Important!!: In all pulse programs the syntax

prosol relations=<triple_na>

is included for automated acquisition/set-up using edprosol/getprosol. This file is defined in the following directory:

$TOPSPINHOME/conf/instr/spect/prosol/relations/triple_na

Specific Nucleic Acid NMR

- **3D HC and HN NOESY Experiments:**

3D ^{1}H-^{13}C NOESY-CT-HSQC using echo-antiecho (**na_noesyhsqcctetgp3d**)
3D ^{1}H-^{13}C NOESY-HSQC using WATERGATE and refocusing of J(C5C6) during t_1 (**na_c6noesyhsqcgp3d**)
3D ^{1}H-^{15}N NOESY-HSQC using WATERGATE (**na_noesyhsqcf3gpwg3d**)

- **2D and 3D HCN-Type Experiments:**

HCN experiment
3D using echo-antiecho (**na_hcnetgpsi3d** | NA_HCNETGPSI3D)
3D using echo-antiecho and selective pulses (**na_hcnetgpsisp3d** | NA_HCNETGPSISP3D)
3D using MQ (**na_hcnmq3d**)
3D using MQ and selective 1H pulses (**na_hcnmqsp3d**)
3D using TROSY (**na_trhcnph3d**)
3D using TROSY and gradient selection (**na_trhcnetsi3d**)
2D H(C)N using TROSY (**na_trhcnph**)
2D H(C)N using TROSY and gradient selection (**na_trhcnet**)
2D H(C)N using MQ (**na_hcnmqgpphpr** | NA_HCNMQGPPHPR)
HCNCH experiment
2D H(CNC)H (**na_hcnchgpjrphsp** | NA_HCNCHGPJRPHSP)
3D H(C)N(C)H using MQ (**na_hcnchgpmqsp3d**)
3D H(C)N(C)H using MQ and TROSY (**na_trhcnchmqsp3d**)
3D H(C)N(C)H using MQ, TROSY and WATERGATE (**na_trhcnchmqspwg3d**)
3D (H)CN(C)H using MQ, TROSY and WATERGATE (**na_trhcnchmqspwg3d2**)
3D (HC)N(C)CH-COSY using MQ (**na_hcncchcomq3d**)
3D (HC)N(C)CH-TOCSY using MQ (**na_hcncchdimq3d**)
2D H(CN)H using WATERGATE (**na_hcnhgpph19** | NA_HCNHGPPH19)
2D H(CN)C (**na_h68c68n19c42**)
HCCNH experiment
3D H(6/8)(CCC)NH (**na_hccnhdigpwg3d** | NA_HCCNHDIGPWG3D)
3D H(CC)NH-COSY (**na_h5c5c4n3h_3d**)
3D H(CC)NH-TOCSY (**na_h56c56c4n3h_3d**)
3D (H)C(C)NH-TOCSY (**na_h56c56c4n3h_3d2**)
2D H(NC6)C5 (**na_hnc6c5etgpsi**)
3D (H)N(C)CH (**na_hncch3d**)

3D TROSY-(H)CCH-COSY for intra-base correlation (**na_trhcchco3d**)

- **Observation HN-N hydrogen bonds:**

2D HNN-COSY (**na_hnncosygpphwg** | NA_HNNCOSYGPPHWG)
2D HNN-COSY using shaped ^{15}N 180° pulses (**na_hnncosygpphspwg**)
2D HNN-COSY using TROSY and shaped ^{15}N 180° pulses (**na_trhnncosygpphspwg**)

- **2D and 3D HC Experiments to determine J(HH) and J(CH) :**

3D H(C)CH-E.COSY experiment (**na_hcchecgp3d** | NA_HCCHECGP3D)
3D HCC-TOCSY-CCH-COSY experiment (**na_hcchfwdigp3d** | NA_HCCHFWDIGP3D)
3D HCC-TOCSY-CCH-E.COSY experiment (**na_hcchfwdiecgp3d** | NA_HCCHFWDIECGP3D)
3D HCC-TOCSY-CCH-E.COSY experiment using jump-and-return (11) (**na_hcchfwdiecgpjr3d**)
3D forward directed quantitative gamma HCCH-TOCSY (**na_ghcchfwdigp3d** | NA_GHCCHFWDIGP3D)
2D ^{1}H-^{13}C HSQC for measuring J_{CH} in sugars (**na_hsqcetgpjcsp** | NA_HSQCETGPJCSP)

- **2D and 3D HP Experiments:**

2D CT HH-{^{31}P}-COSY with presaturation to measure J(H3'-P) (**na_hpcosyphpr** | NA_HPCOSYPHPR)

2D ^{1}H-^{31}P HETCOR experiment
Using echo-antiecho (**na_xhcoetf3gp**)
Constant-time using echo-antiecho (**na_xhcoctetf3gp**)
Constant-time without gradient selection (**na_hpctco**)
Constant-time without gradient selection using jr (**na_hpctcojr**)

2D ^{1}H-^{31}P HSQC experiment
Using CPMG (**na_hsqcetf3gpxy**)
Using CPMG and jump-and-return (**na_hsqcf3gpjrphxy**)

2D ^{1}H-^{31}P Hetero-TOCSY using cross-polarization (**na_hpdi**)

2D ^{1}H-^{31}P HSQC-NOESY using CPMG (**na_hsqcf3gpnophxy**)

2D ^{1}H-^{31}P Hetero-TOCSY-NOESY
Using cross-polarization (**na_hpdino)**
Using WATERGATE and cross-polarization (**na_hpdino19)**
3D using cross-polarization (**na_hpdino3d)**
3D using WATERGATE and cross-polarization (**na_hpdino193d)**

- **2D and 3D HCP Experiments:**

HCP Experiment
3D HCP using sensitivity-enhancement (**na_hcpetgpsi3d** | NA_HCPETGPSI3D)

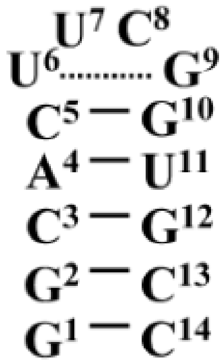
3D HCP-TOCSY
Using CC TOCSY and presaturation (**na_hcpdigp3d**)
Using CC TOCSY and jump-and-return (11) (**na_hcpdigpjr3d**)
Using CC TOCSY and echo-entiecho (**na_hcpdietgp3d**)
Using CC TOCSY and sensitivity-enhancement (**na_hcpdietgpsi3d** | NA_HCPDIETGPSI3D)

PHCH Experiment
3D P(H)CH using HMQC and echo-antiecho (**na_hpccoetf3gp3d)**
3D Constant-time P(H)CH using HMQC (**na_hpcctco3d)**
3D Constant-time P(H)CH using HMQC and echo-antiecho (**na_hpccoctetf3gp3d)**
3D Hetero-TOCSY-COSY using HMQC and cross-polarization (**na_hpdico3d)**

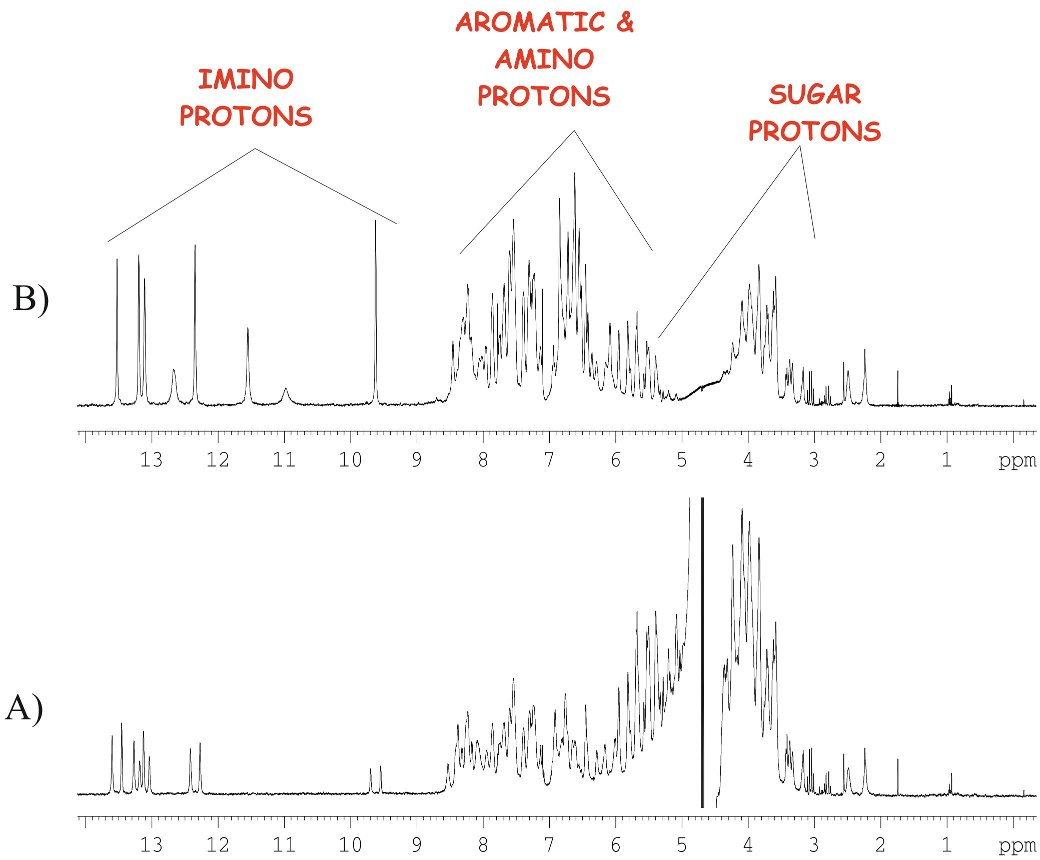
PCH Experiment
2D P(C)H using HC INEPT transfer **(na_pcchco)**
2D P(C)H using HC cross-polarization **(na_pcchdi)**
2D P(CCC)H using CC TOCSY and HC cross-polarization **(na_pcchdi2)**

2D quantitative HC(P) for determination of J(CP) (**na_hcpqetgpsi.1** | NA_HCPQETGPSI.1 and **na_hcpqetgpsi.2** | NA_HCPQETGPSI.2)
2D P-FIDS experiment to measure J(HP) and J(CP) (**na_pfidsetgpsi** | NA_PFIDSETGPSI)

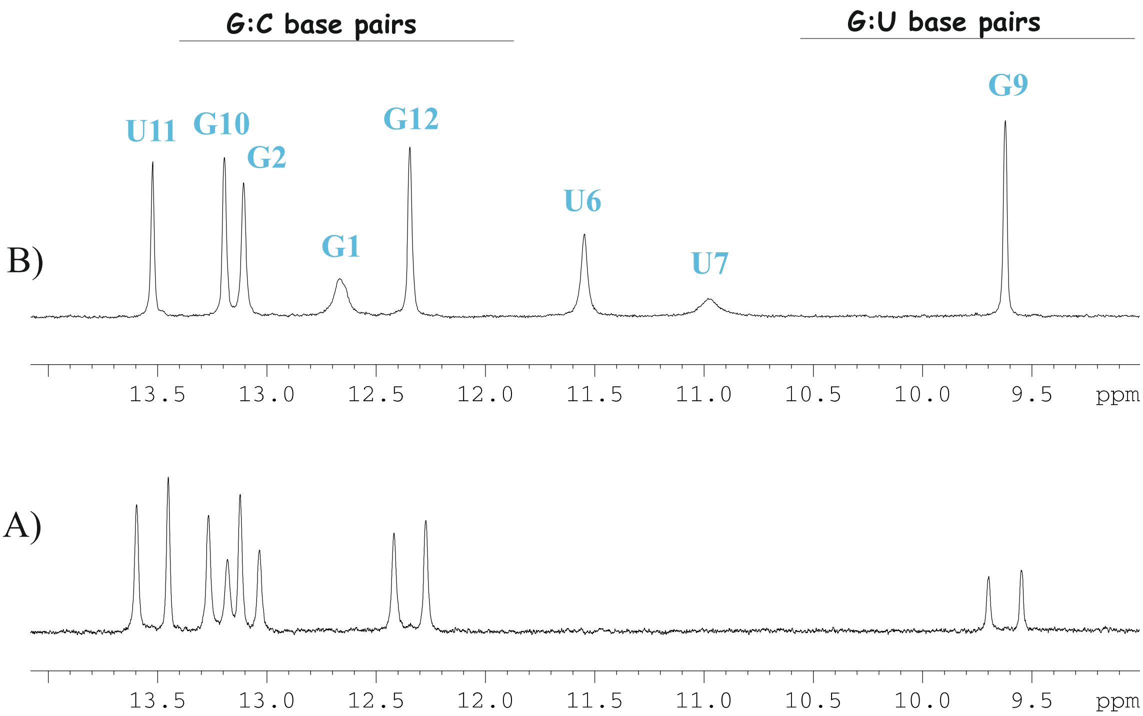
All NMR spectra shown in this chapter correspond to a 1mM sample of doubly-labeled 13C/15N RNA 14-mer 5'-GGCACUUCGGUGCC-3' (commercially available from Silantes) dissolved in 90% H2O/10% D2O (courtesy from Dr. W. Bermel - Bruker Biospin, Kalshruhe). Experiments were recorded in a 600MHz AVANCE spectrometer equipped with a 5mm TXI probehead.



A) 1H spectrum using presaturation (zgpr)
B) 1H spectrum using water suppression using WATERGATE and heteronuclear 15N decoupling during 1H acquisition.



Expansions of the lowfield imino NH region.



Important classical 2D experiments to study NAs:

- 2D 1H-1H COSY and TOCSY experiments for assignment of ribose spin systems

- 2D 1H-1H NOESY experiment for intra- and inter-residue connectivities, and also for base pairing

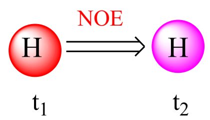
- 2D 1H-13C and 1H-15N HMQC i HSQC experiments to identify directly-attached CH and NH spin systems.

- 2D 1H-13C HMBC and 2D long-range optimized HSQC to trace out two- and three-bond away proton-carbon and proton-nitrogen connectivities. Very useful for the assignment of non-protonated carbon and nitrogen in the base noiety.

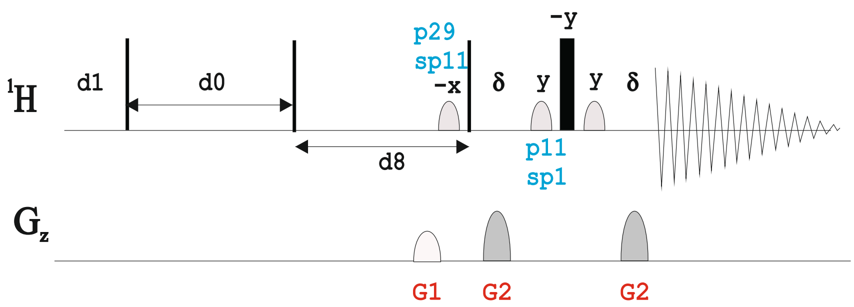
2D NOESY Experiment

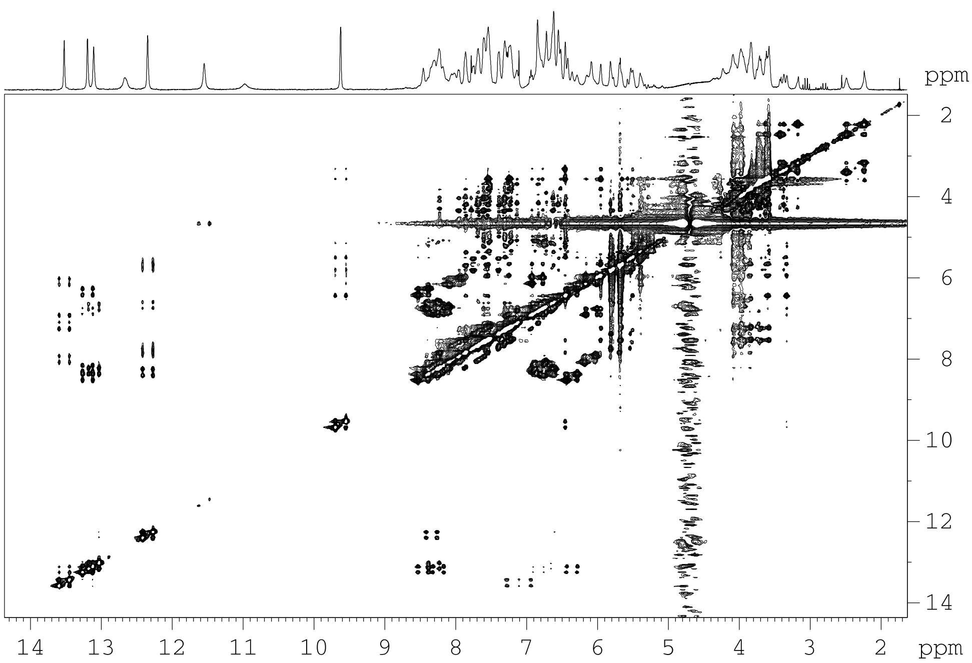
NOESY experiment is an important tool for conformational studies of nucleic acids. It can be run on unlabeled and labeled nucleic acids. Important NOE contacts for sequential assignments are imino-to-imino, imino-to-amino, and imino-to-nonechangeable proton regions. Information on base pairing and hydrogen bonding can be also extarcted from NOE imino cross-peaks.

See all available NOESY schemes in the 2D NOESY chapter or also 3D X-edited NOESY experiments.



noesyfpgpphwg





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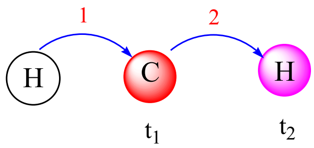
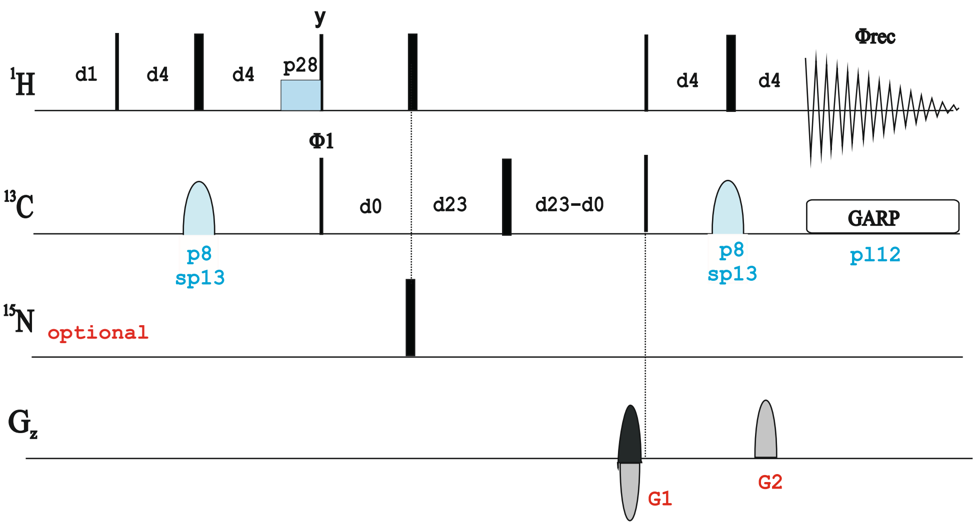
NUCLEIC-ACID NMR
2D & 3D HCN EXPERIMENTS

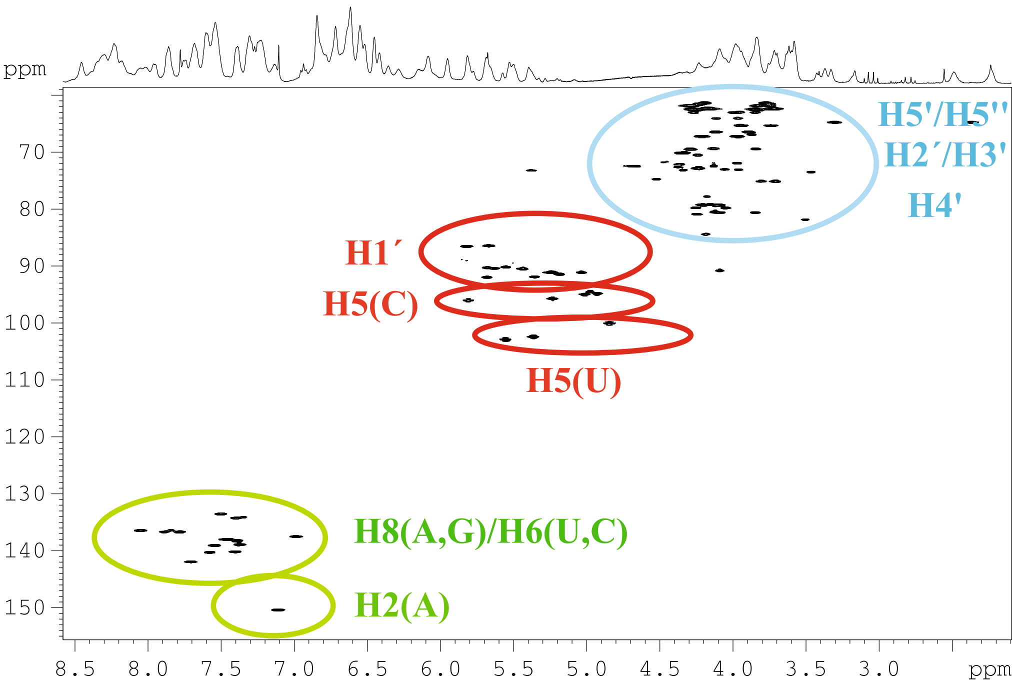
2D Constant-time HSQC/HMQC Experiment

1H-13C correlation experiments can be recorded as usual for both unlabeled and 13C-labeled NAs. IN the later, constant-time experiments are recommended to refocus J(CC) during the indirect F1 dimension. See the corresponding 2D HSQC and HMQC chapters for all availables pulse programs.



hsqcctetgpsp.2

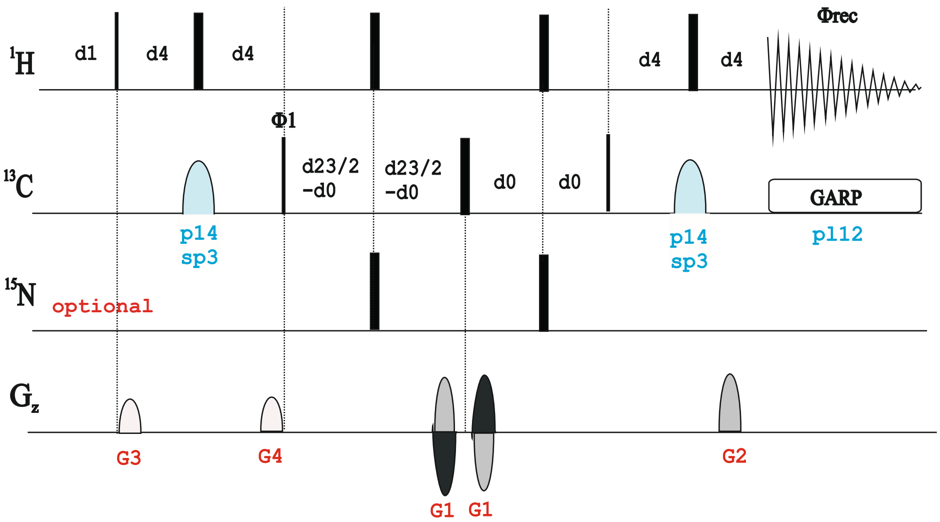


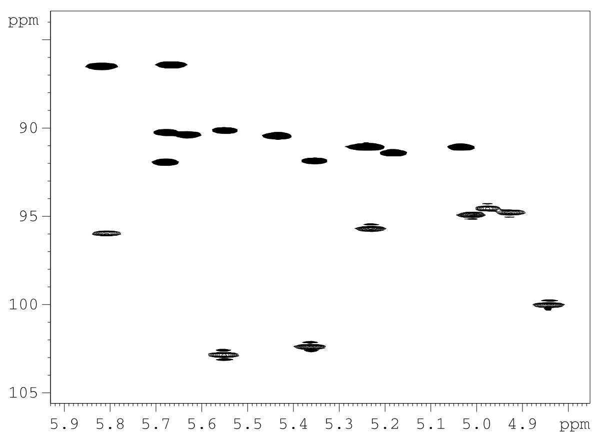


d1=1.5s
d4=1/4J(CH)=1.72ms
(optimized to cnst2=145Hz)
d23=CT(C) period=8.8ms

For a complete assignment, See Fig. 6 in 04jb69-28

hmqcctetgp

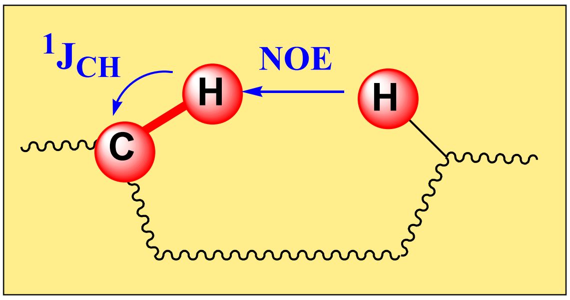


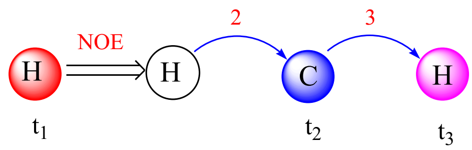


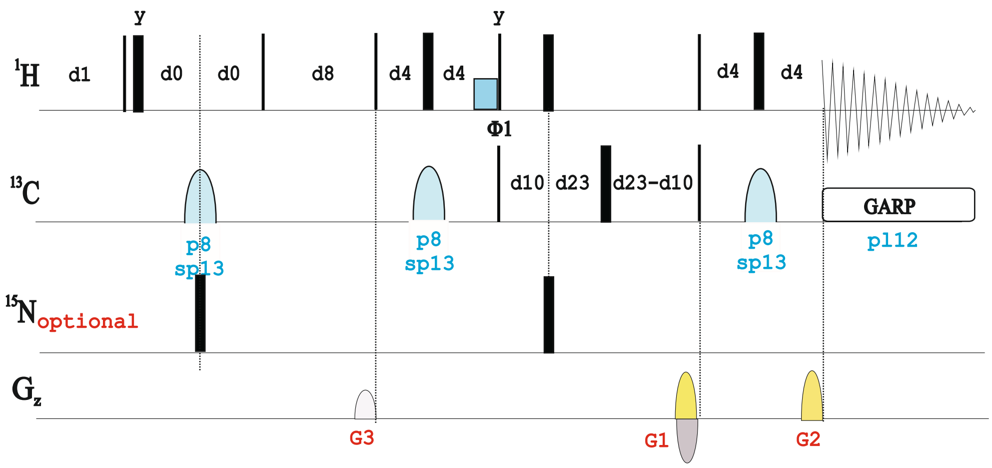
d1=1.5s
d4=1/4J(CH)=1.72ms
(optimized to cnst2=145Hz)
d23=CT(C) period=8.8ms

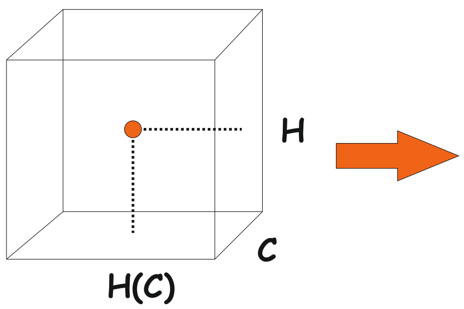
3D Constant-time ^{1}H-^{13}C NOESY-HSQC Experiment

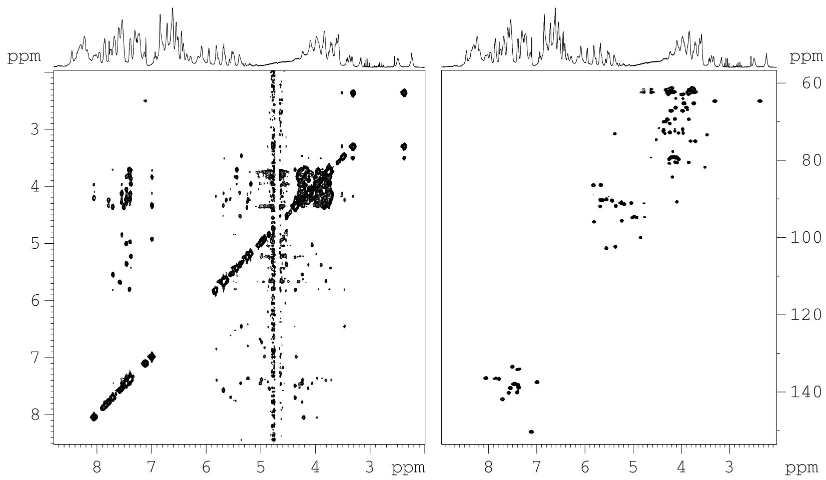
Constant-time version of the 3D NOESY-HSQC experiment to be applied on 13C-labeled NAs. Useful to remove J(CC) splitting from the indirect C dimension. The experiment allows to detect intra-residue 1H-1H NOE contacts between individual sugar rings and their connected bases.







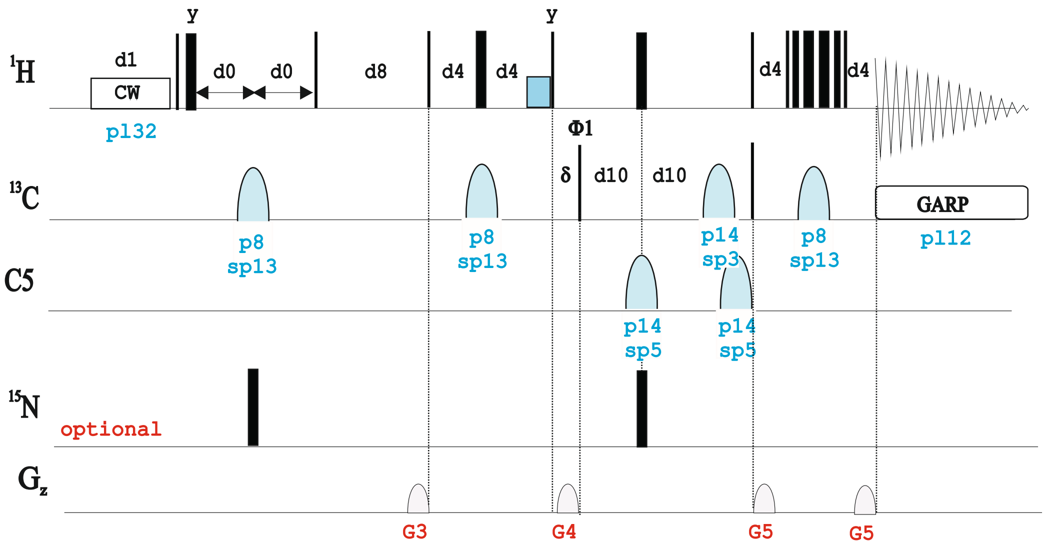


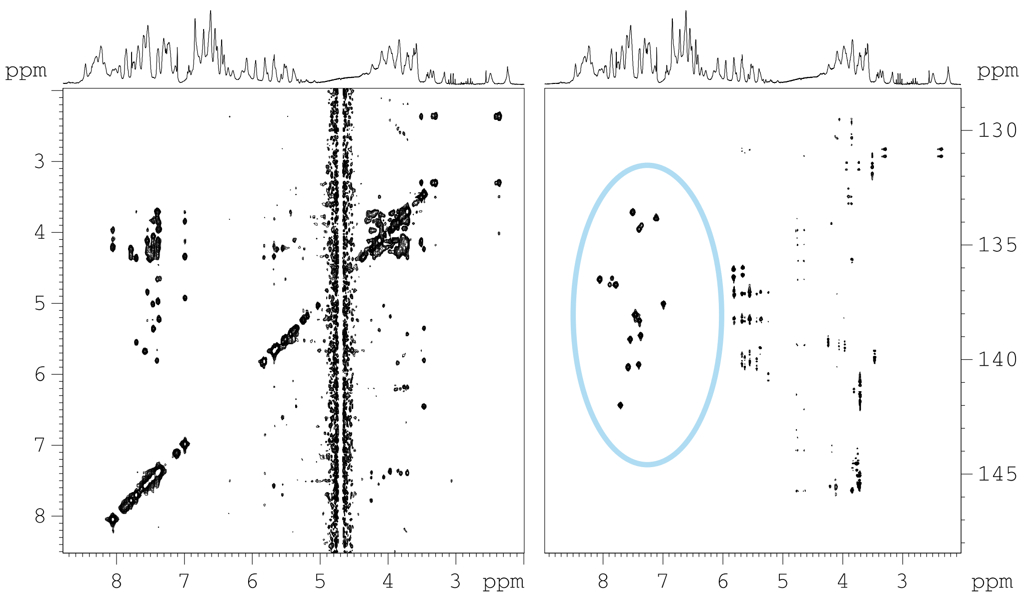


d1=1.5s
d8=NOESY mixing time=100ms
d4=1/4J(CH)=1.72ms
(optimized cnst2=145Hz)
d23=CT(C) period=8.8ms

Non-constant-time version of the 3D NOESY-HSQC experiment with selective refocusing of the H(C6C5) coupling constant by means of 180° 13C selective pulses (p14=1ms, spnam3=Q3)) on C5 during the indirect d10 period.

na_c6noesyhsqcgp3d



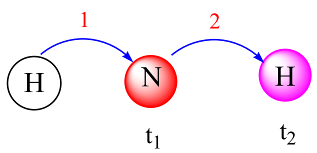


d1=1.5s
d8=NOESY mixing time=100ms
d4=1/4J(CH)=1.25ms (optimized to cnst2=200Hz)
SW in the C dimension reduced to 16.5ppm

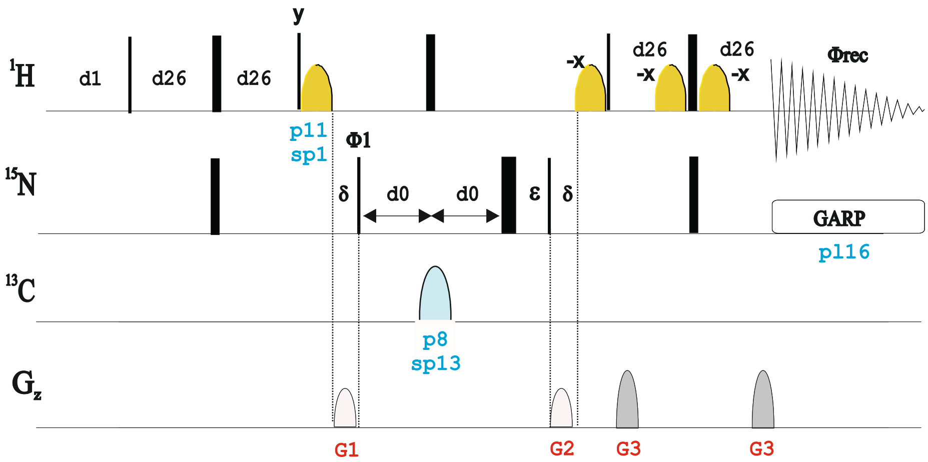
2D ^{1}H-^{15}N HSQC Experiment

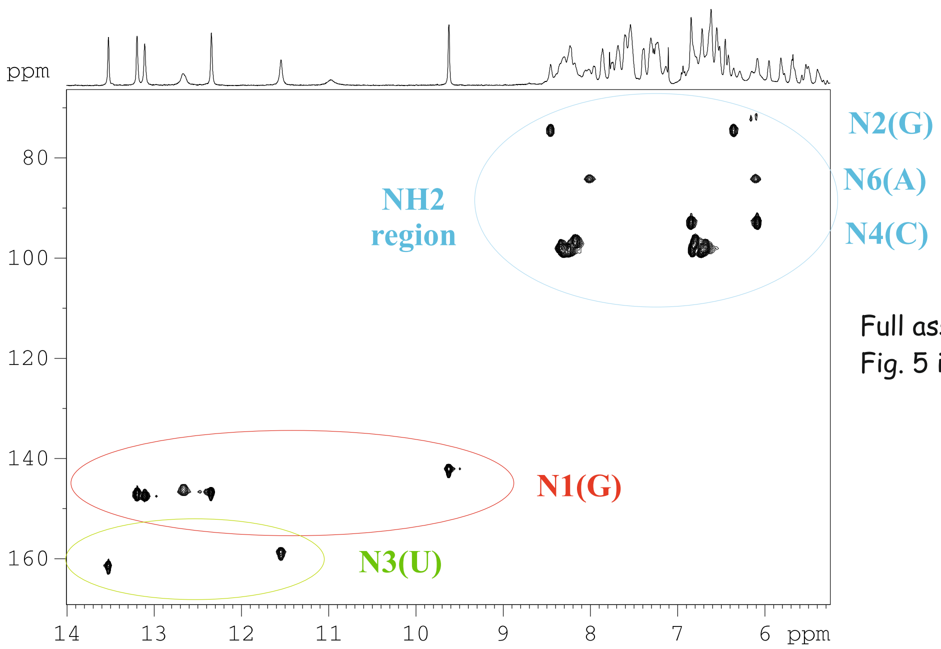
Experiment Description

Assignment of exchangeable imino and amino protons with their directly-attached nitrogen nuclei in H2O.



hsqcfpf3gpphwg



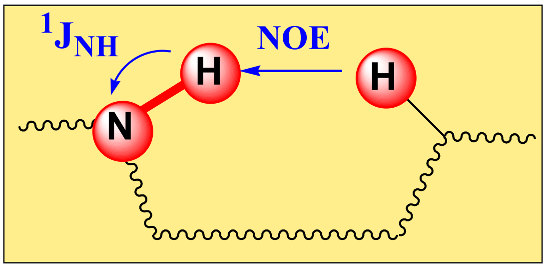


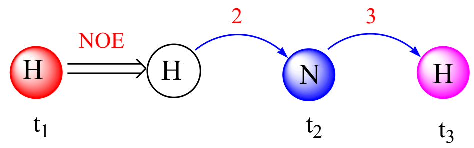
Full assignment:
Fig. 5 in 04jb69-28

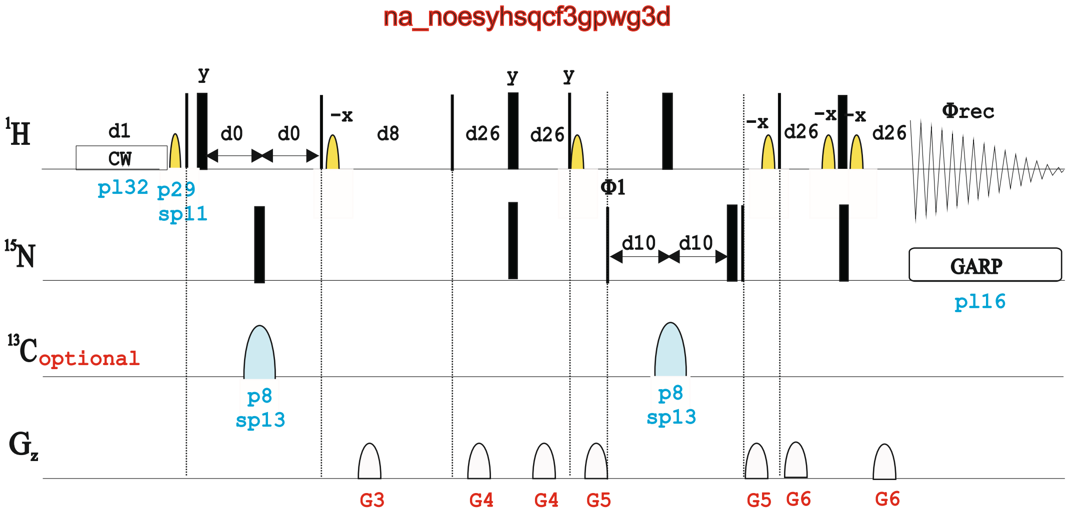
d1=1.5s
p11=90° water selective=1ms (Squa100.1000)
d26=1/4J(NH)=2.77ms
(optimized cnst4=90Hz)

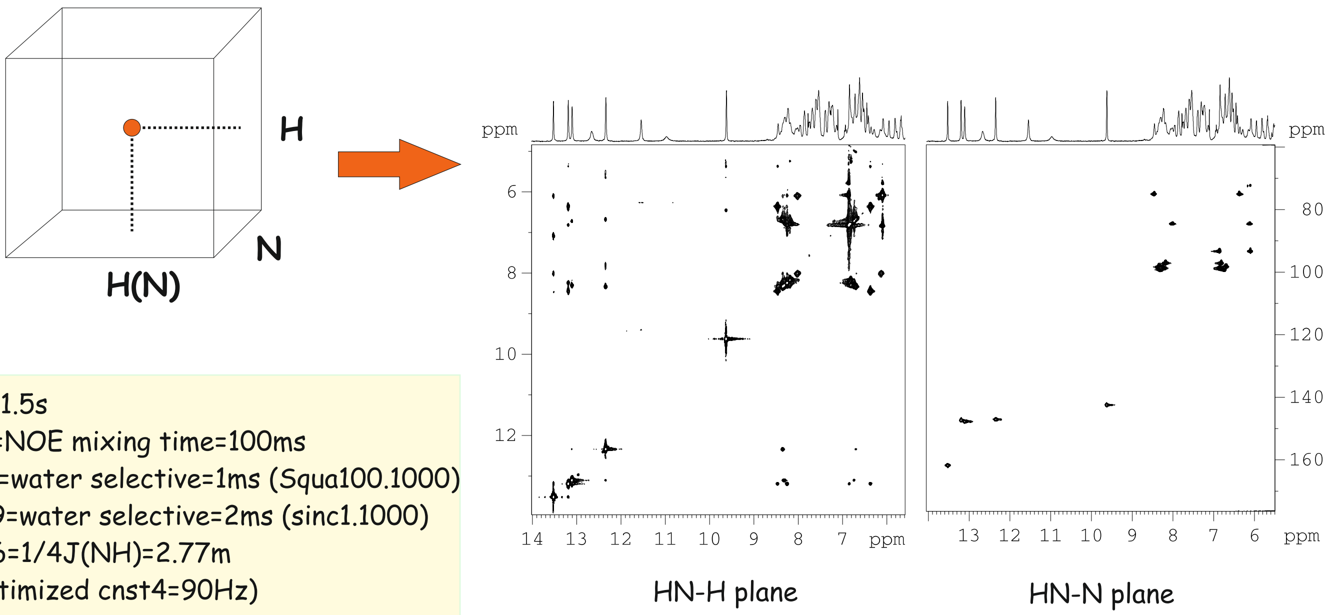
3D ^{1}H-^{15}N NOESY-HSQC Experiment

Sequential assignment of exchangeable imino and amino groups via NOE contacts.Three important connectivities: imino-to-imino, imino-to-amino, and amino-to-non exchangeable aromatic and sugar protons







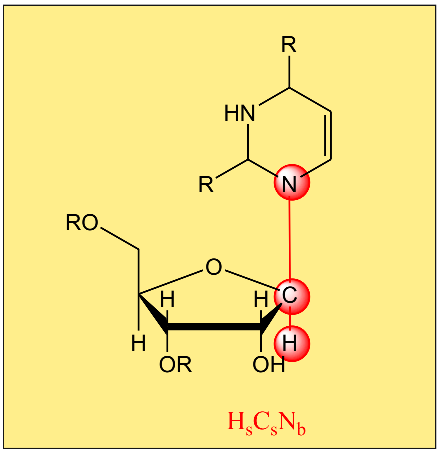


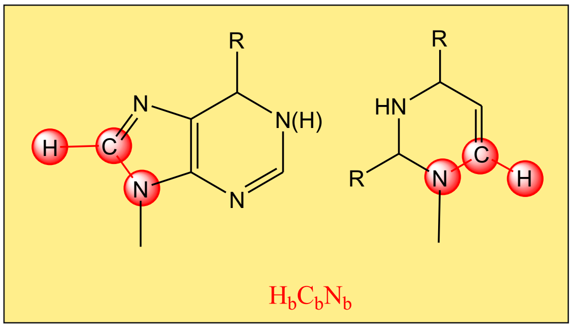
d1=1.5s
d8=NOE mixing time=100ms
p11=water selective=1ms (Squa100.1000)
p29=water selective=2ms (sinc1.1000)
d26=1/4J(NH)=2.77m
(optimized cnst4=90Hz)
ZGOPTNS=-DLABEL_CN

3D HCN Experiment

Experiment Description:

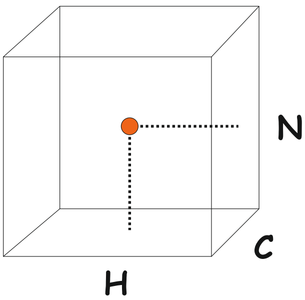
This experiment provides sugar-to-base and intrabase HCN connectivities in isotopically labeled nucleotides. Several 2D and 3D versions of this out-and-back HCN experiment incorporating SQC, MQC and TROSY effects are available.





NMR Spectrum

The experiment provides a 3D correlation map. As a function of experimental conditions, both type of correlations can be observed in the same spectrum. Otherwise, selective HsCsNb or HbCbNb spectra can also be obtained.

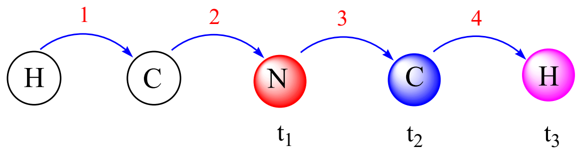


References:

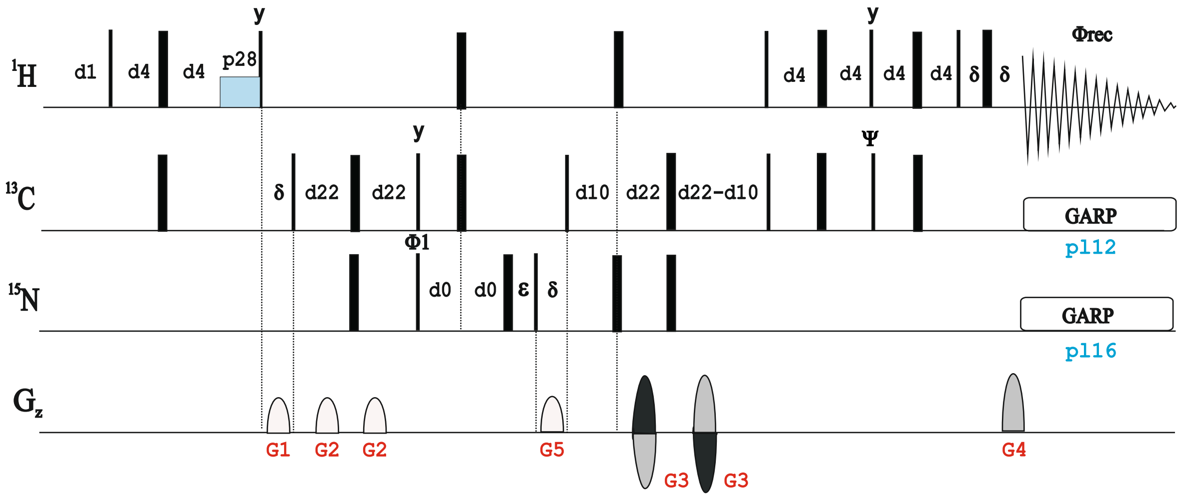
V. Sklenar, R.D. Peterson, M.R. Rejante & J. Feigon, J. Biomol. NMR 3, 721 - 727 (1993)

Related Experiments

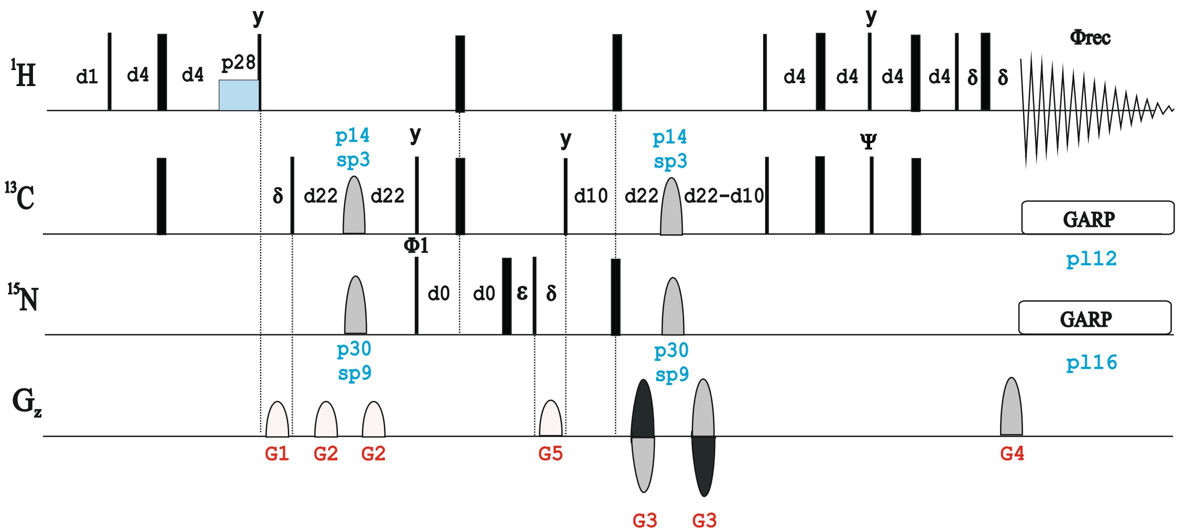
HCNCH
HCNH



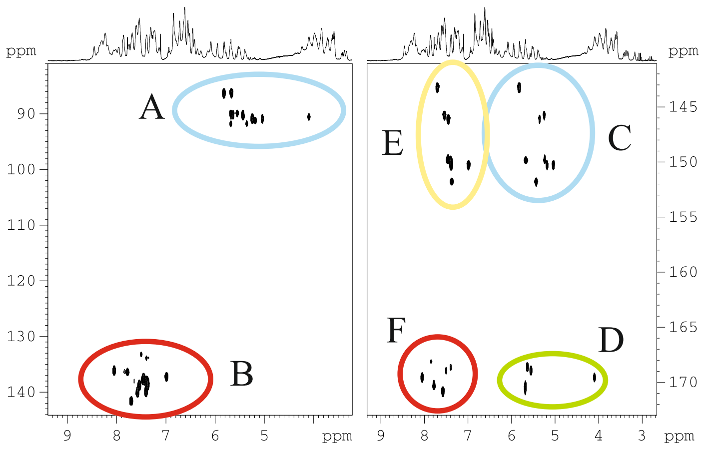
na_hcnetgpsi3d



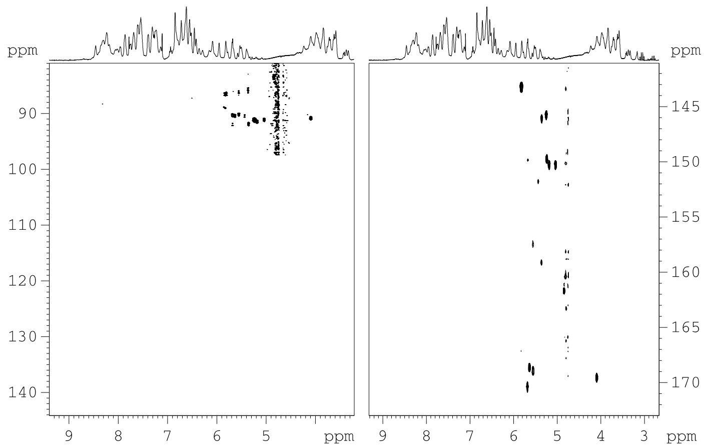
na_hcnetgpsisp3d



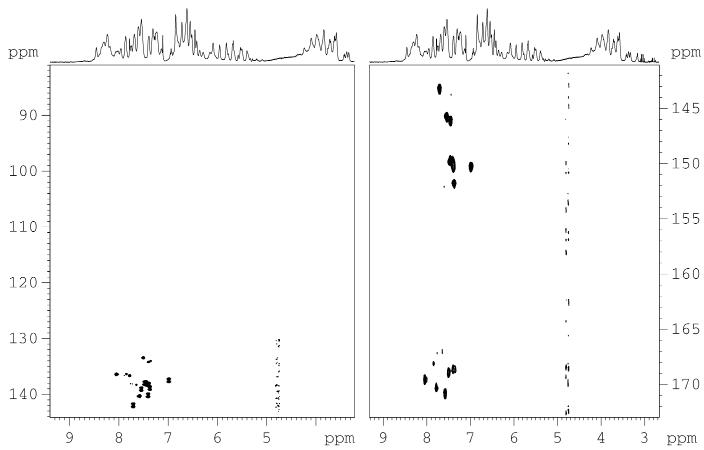
The 2D HC(N) plane can be separated in two areas: A) sugar area (blue) displaying the anomeric H1'-C1' correlations; and B) base area (red) displaying the olefinic H6C6(U,C) and H8C8(A,G) correlations.
The 2D H(C)N plane displays four different sugar-to-base correlations C) H1'-to-N1(U,C) (blue area); D) H1'-to-N9(A,G) (green area); E) H6(U,C)-to-N1(U,C) (yellow area); and F) H8(A,G)-to-N9(A,G) (red area).



d1=1.5s
d4=1/4J(CH)=1.40ms for all J(HC) ,
J(H8C8) and J(H6C6)
d22=1/4J(CN)=17.5ms for all J(N1C1'), J(N9C1'),
J(N1C6), and J(N9C8)
p14=2.6ms (spnam3=q3_rna_c68c1.256)
o2p=113.45ppm
p30=700us(spnam9=Q3.1000)



d1=1.5s
d4=1/4J(CH)=1.56ms for J(H1'C1')
d22=1/4J(CN)=15ms for J(N1C1'), J(N9C1')
p14=1.0ms (spnam3=Q3.1000)
o2p=89.19ppm
p30=700us(spnam9=Q3.1000)
Reduced SW in the C dimension=16.5ppm



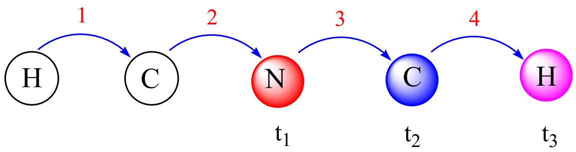
d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d22=1/4J(CN)=15ms for J(N1C6), and J(N9C8)
p14=1.0ms (spnam3=Q3.1000)
o2p=137.7ppm
p30=700us(spnam9=Q3.1000)
Reduced SW in the C dimension=16.5ppm

3D MQ-HCN Experiment

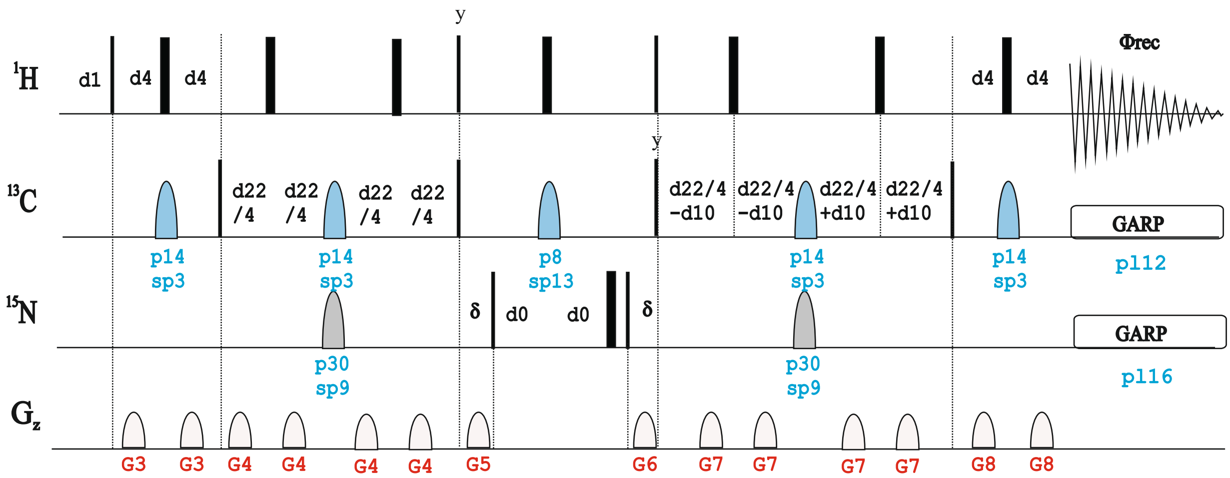
Experiment Description:

Version of the HCN experiment that involves multiple-quantum coherences (MQC) instead of SQC to enhance relaxation features.

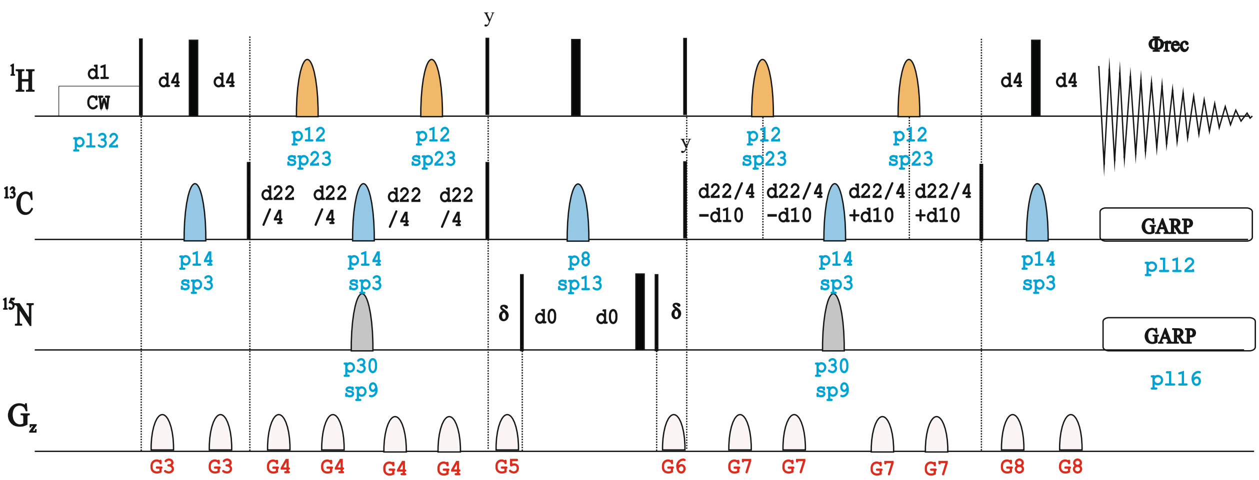
J.P. Marino, J.L. Diener, P.B. Moore & C. Griesinger, J. Am. Chem. Soc. 119, 7361-7366 (1997)

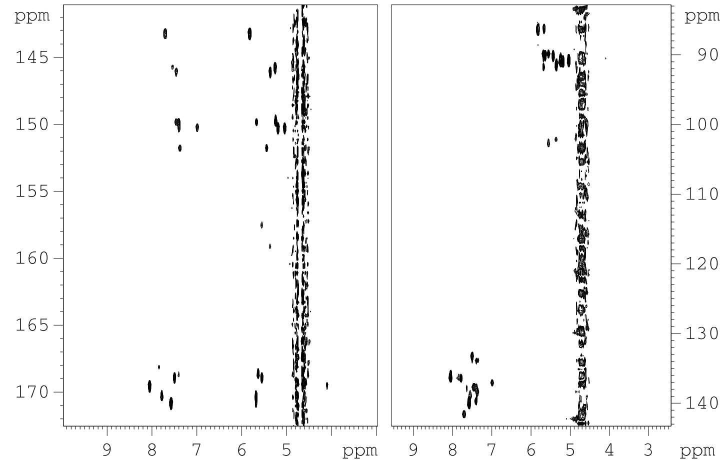


na_hcnmq3d

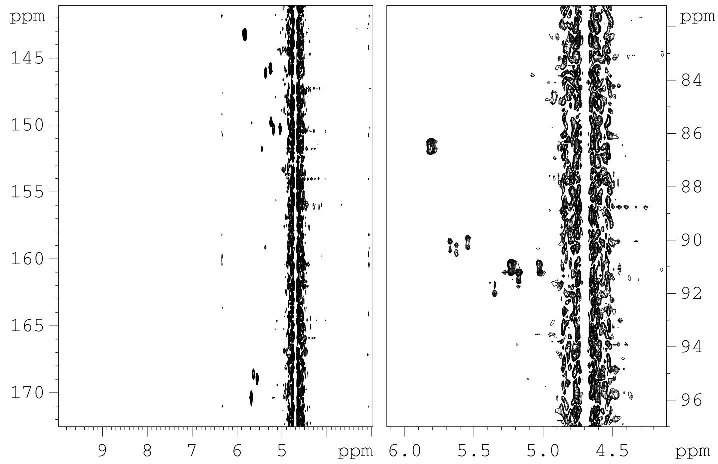


na_hcnmqsp3d

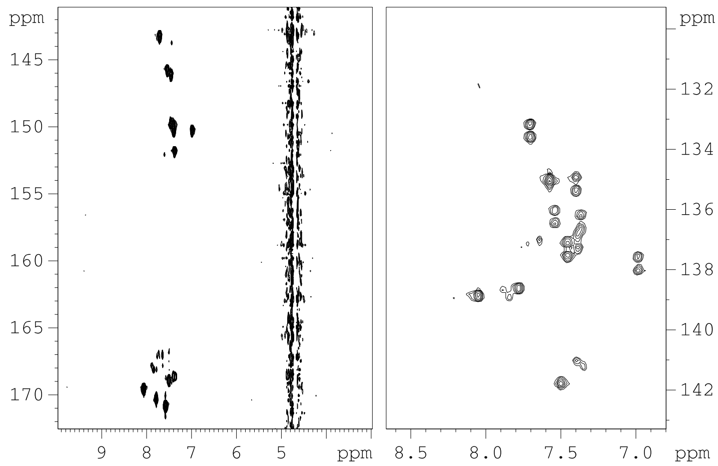




d1=1.5s
d4=1/4J(CH)=1.40ms for all J(H1'C1') ,
J(H8C8) and J(H6C6)
d22=1/4J(CN)=16.0ms for all J(N1C1'), J(N9C1'),
J(N1C6), and J(N9C8)
p14=2.6ms (spnam3=q3_rna_c68c1.256)
o2p=113.45ppm
p30=700us(spnam9=Q3.1000)
p12=1.65ms (spnam23=reburp.1000)



d1=1.5s
d4=1/4J(CH)=1.56ms for J(H1'C1')
d22=1/4J(CN)=16ms for J(N1C1'), J(N9C1')
p14=1.0ms (spnam3=Q3.1000)
o2p=89.19ppm
p30=700us(spnam9=Q3.1000)
p12=3.30ms (spnam23=reburp.1000)
Reduced SW in the C dimension=16.5ppm



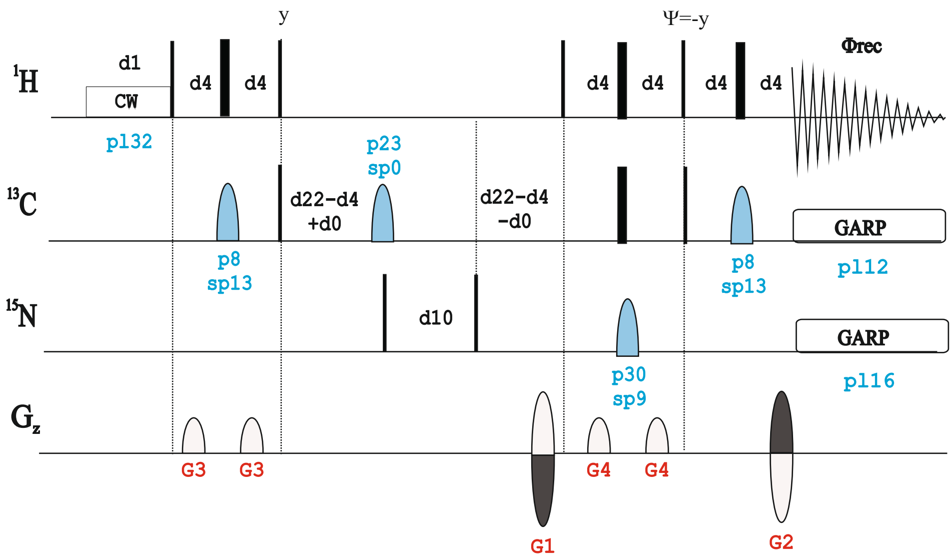
d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d22=1/4J(CN)=16ms for J(N1C6), and J(N9C8)
p14=1.0ms (spnam3=Q3.1000)
o2p=137.7ppm
p30=700us(spnam9=Q3.1000)
p12=3.30ms (spnam23=reburp.1000)
Reduced SW in the C dimension=16.5ppm

3D TROSY-HCN Experiment

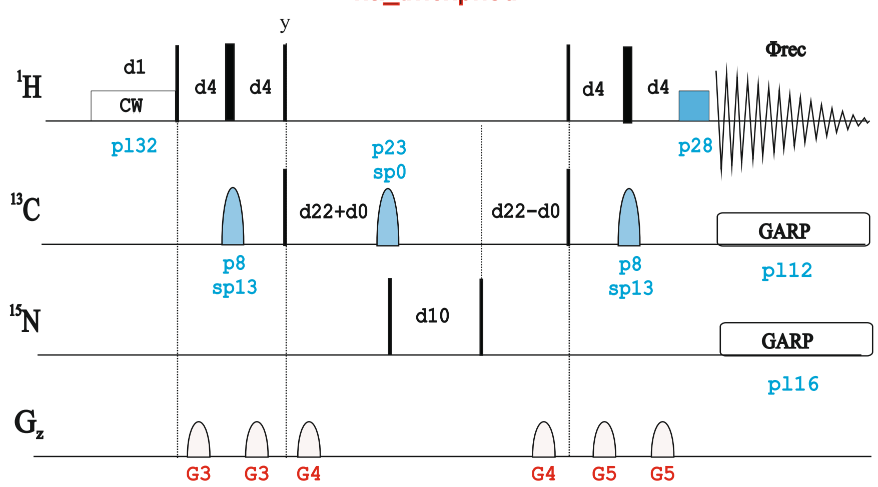
Version of the HCN experiment that involves multiple-quantum coherences (MQC) and TROSY effects instead of SQC to enhance relaxation features.

1. R. Fiala, J. Czernek & V. Sklenar, J. Biomol. NMR 16, 291-302 (2000)
2. R. Riek, K. Pervushin, C. Fernandez, M. Kainosho & K. Wuethrich, J. Am. Jacs. Soc. 123, 658-664 (2001)
3. B. Brutscher & J.-P. Simorre, J. Biomol. NMR 21, 367-372 (2001)

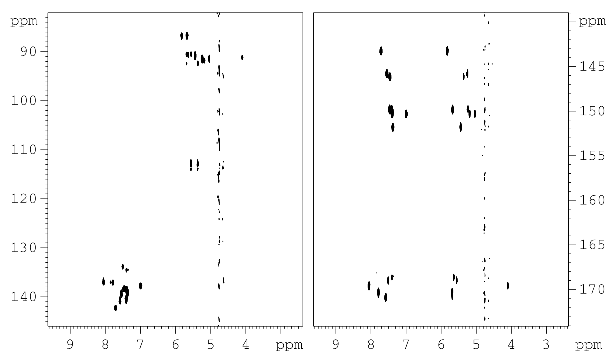
na_trhcnetsi3d



na_trhcnph3d



d1=1.5s
d4=1/4J(CH)=1.40ms for all J(H1'C1') , J(H8C8) and J(H6C6)
d22=1/2J(CN)=30ms for all J(N1C1'), J(N9C1'), J(N1C6), and J(N9C8)
p23=0ms (spnam3=q3_rna_c68c1.256)
o2p=113.45ppm
p30=700us(spnam9=Q3.1000)



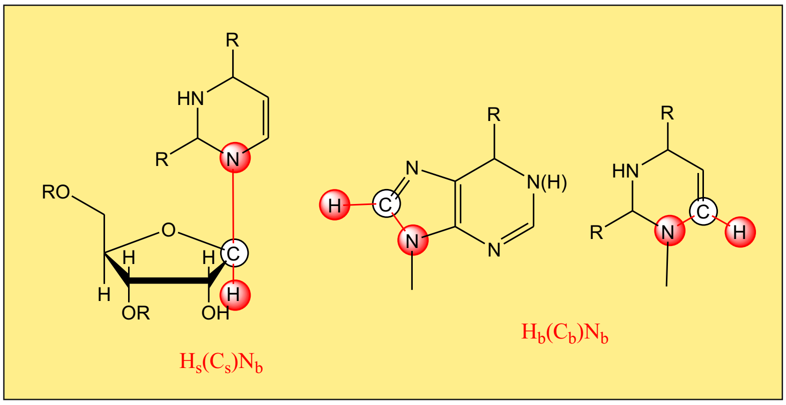
2D TROSY-H(C)N Experiment

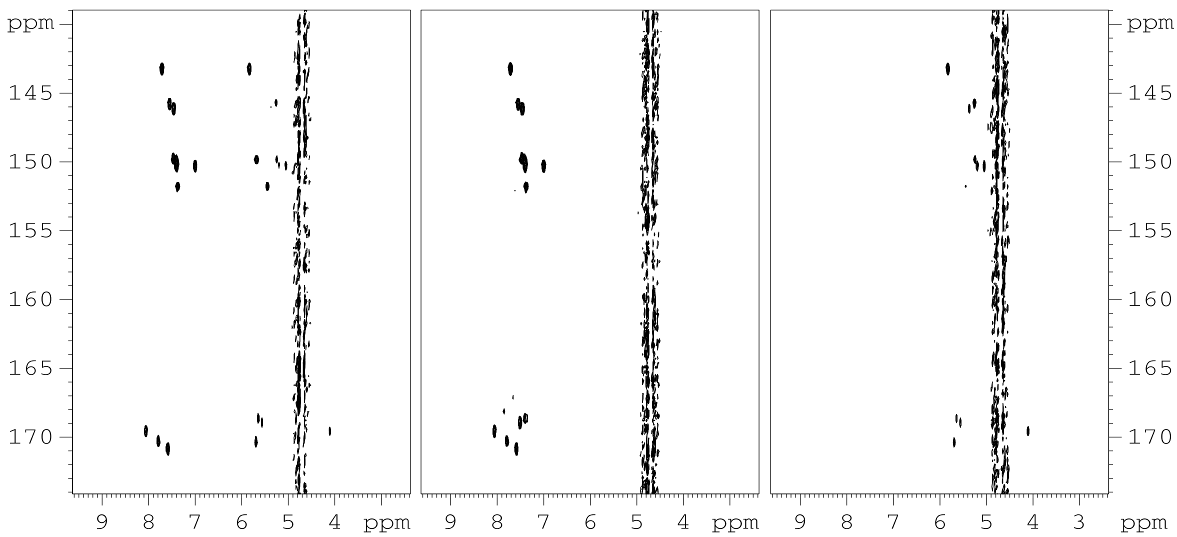
Experiment Description:

2D TROSY version of the HCN experiment in which the 2D H(C)N plane is obtained

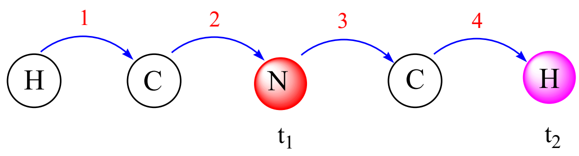
References:

R. Fiala, J. Czernek & V. Sklenar, J. Biomol. NMR 16, 291-302 (2000)

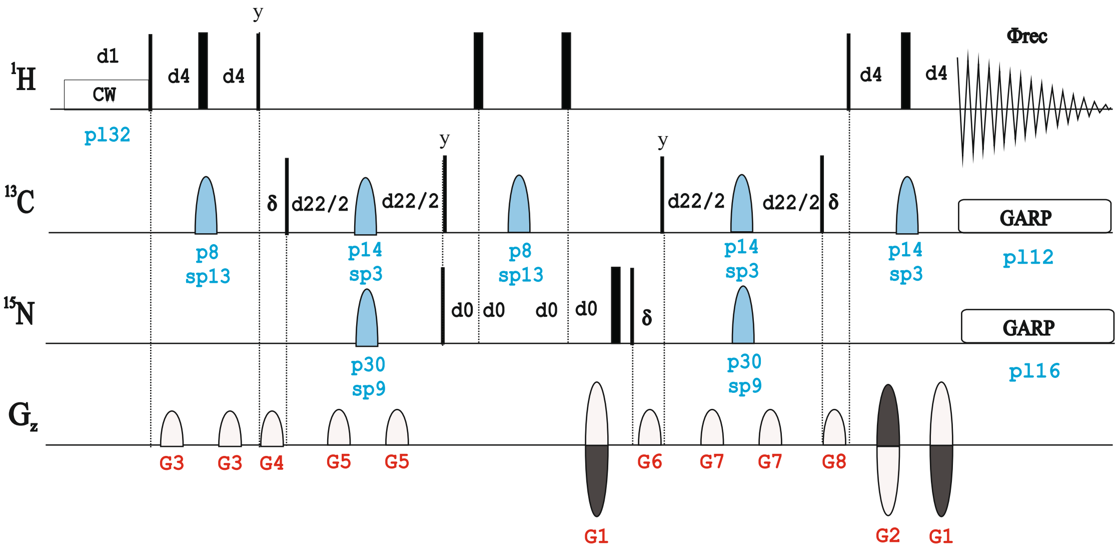




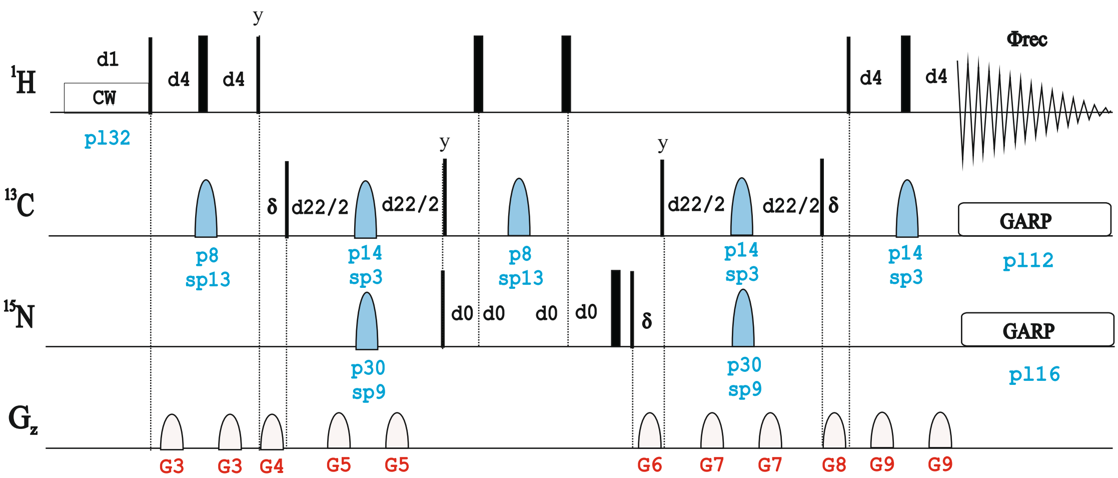
The same acquisition parameters as discussed in the 3D HCN experiments



na_trhcnet



na_trhcnph



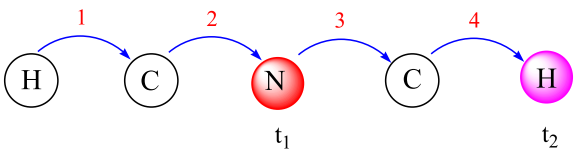
2D MQ-H(C)N Experiment

Experiment Description:

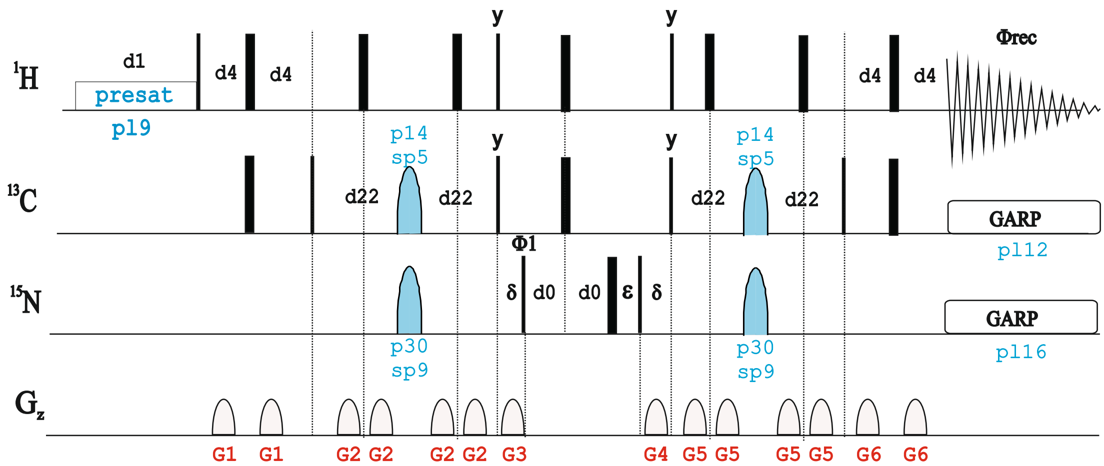
2D MQ version of the HCN experiment in which the 2D H(C)N plane is obtained.

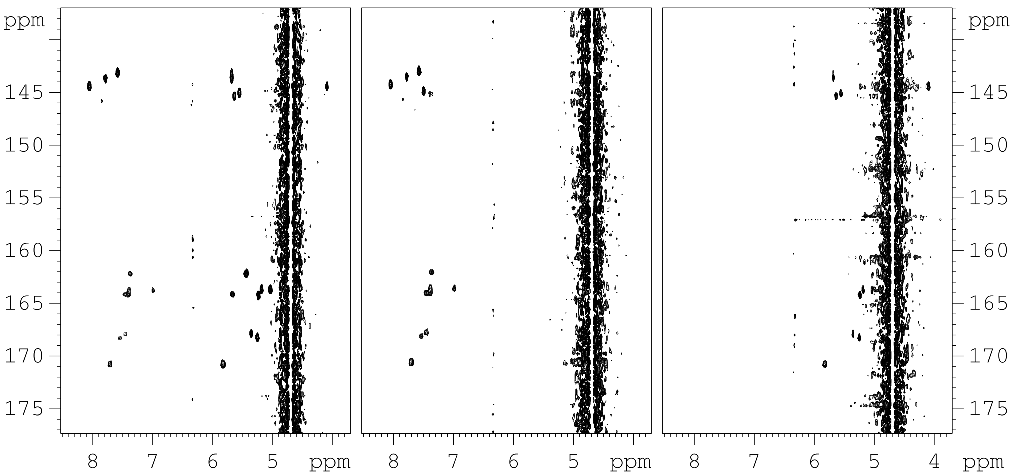
References:

1. J.P. Marino, J.L. Diener, P.B. Moore & C.Griesinger, J. Am. Chem. Soc. 119, 7361 - 7366 (1997)
2. V. Sklenar, T. Diekmann, S.E. Butcher & J.Feigon, J. Magn. Res. 130, 119 - 124 (1998)



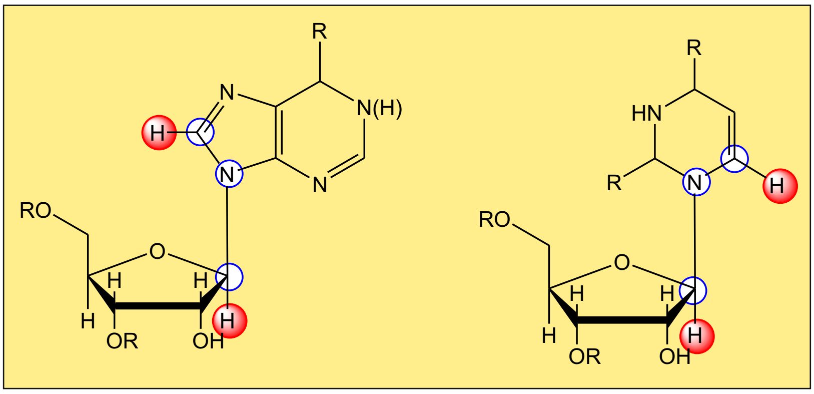
na_hcnmqgpphpr





The same acquisition parameters as discussed in the 3D HCN experiments

2D H(CNC)H Experiment

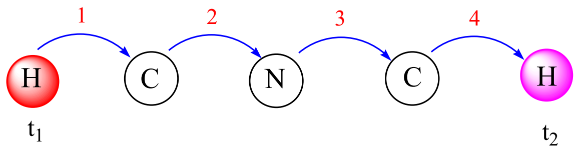


Experiment Description

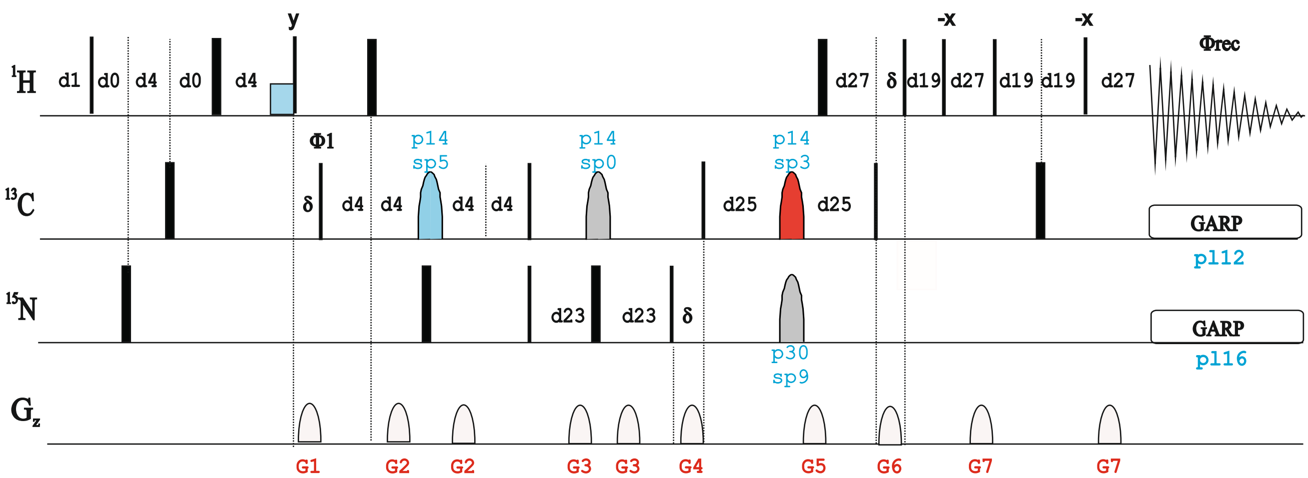
2D version of the HCNCH experiment that allows to correlate the anomeric proton of the sugar ring with the H6/H8 of the connected base in isotopically labeled oligonucleotides.

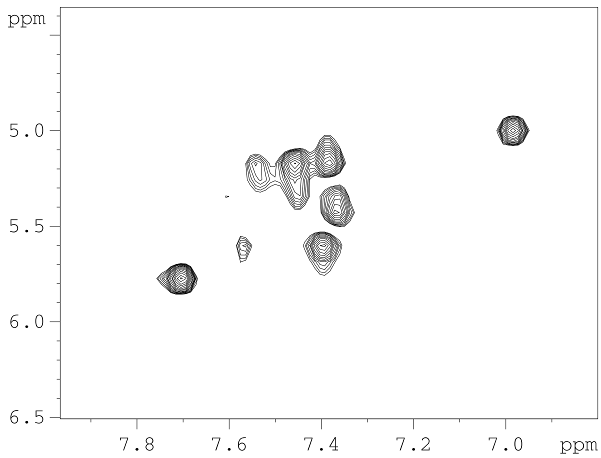
References:

V. Sklenar, R.D. Peterson, M.R. Rejante, E. Wang & J. Feigon, J. Am. Chem. Soc. 115, 12181 - 12182 (1993)



na_hcnchgpjrphsp



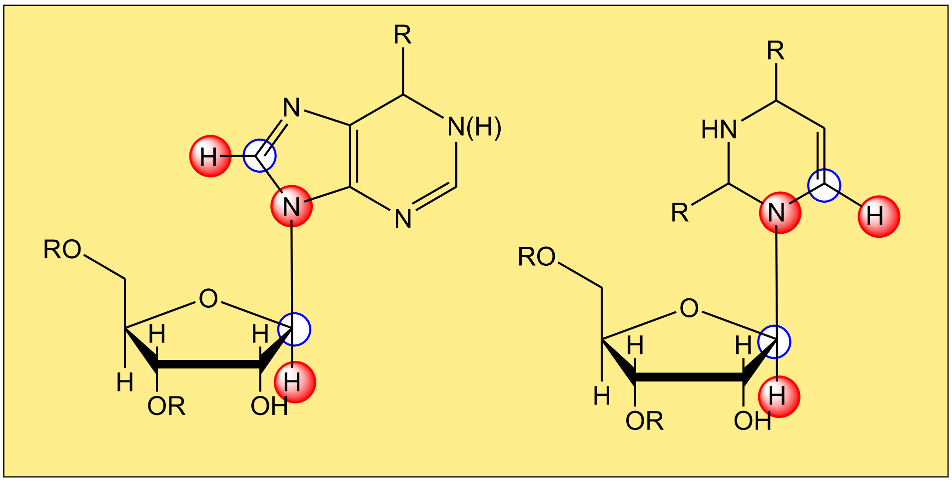


d1=1.5s
d4=1/4J(CH)=1.56ms
d23=1/4J(CN)=17ms
d25=1/4J(CN)=16ms
d27=1/4J/CH)=1.25ms
d19=134us
p14=1ms (spnam3=spnam5=Q3.1000 and spnam0=q3_rna_c68c1.1000)
o2p=113.5 ppm

3D H(C)N(C)H Experiment

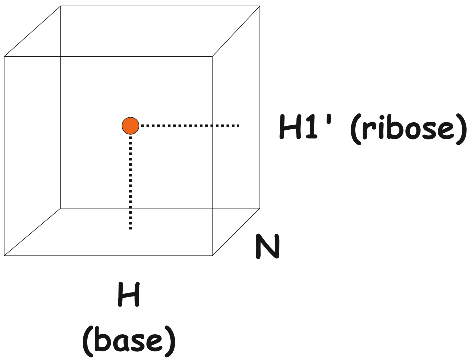
Experiment Description:

3D version of the HCNCH experiment that allows to correlate the two different HCN correlations observed in the HCN experiment. The experiment starts from the H1'-C1' ribose pair, N1/9 is allowed to evolve in an indirect dimension and finally the H6C6/H8C8 base proton is detected.



NMR Spectrum

The experiment provides a 3D correlation map

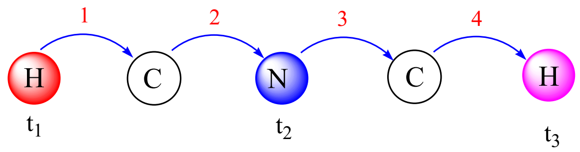


References:

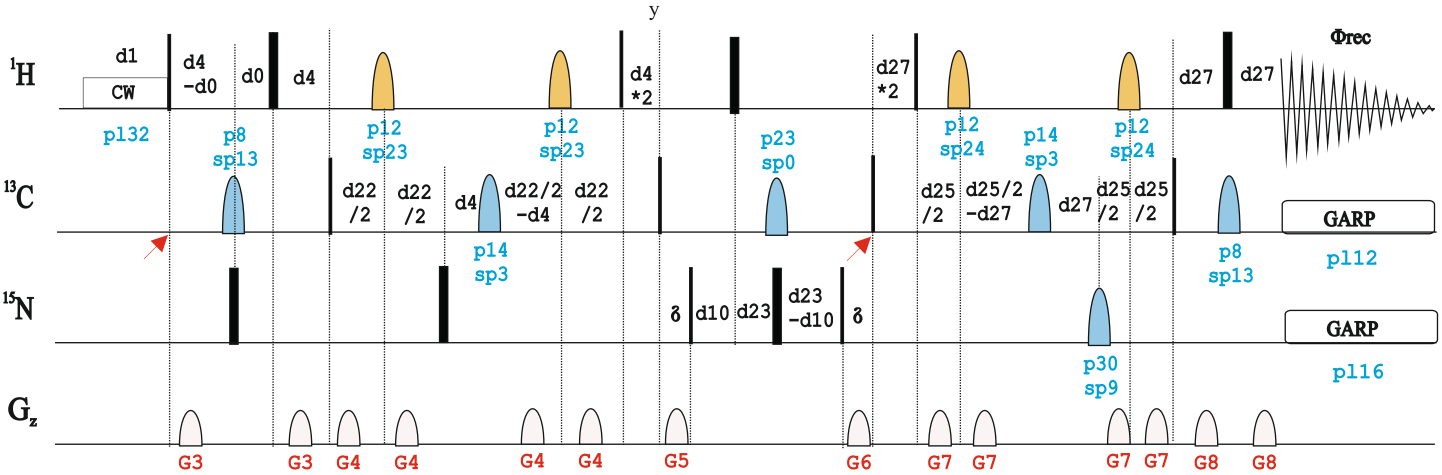
R. Fiala, F. Jiang & V. Sklenar, J. Biomol. NMR 12, 373-383 (1998)

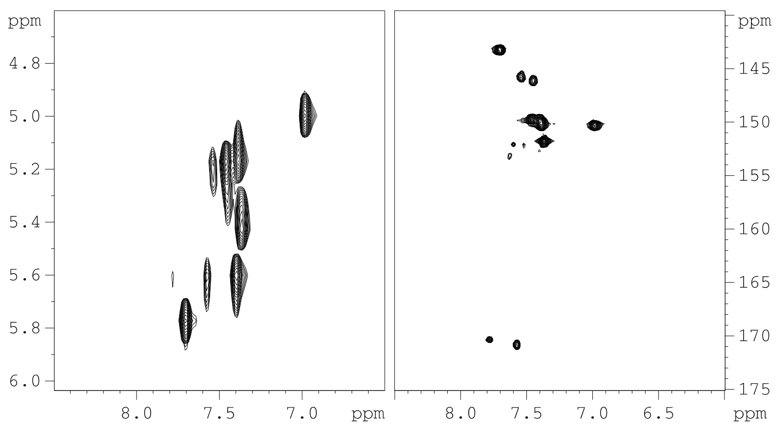
Related Experiments

HCN experiment



na_hcnchmqsp3d

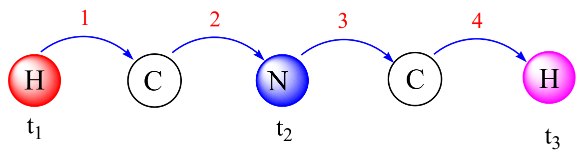




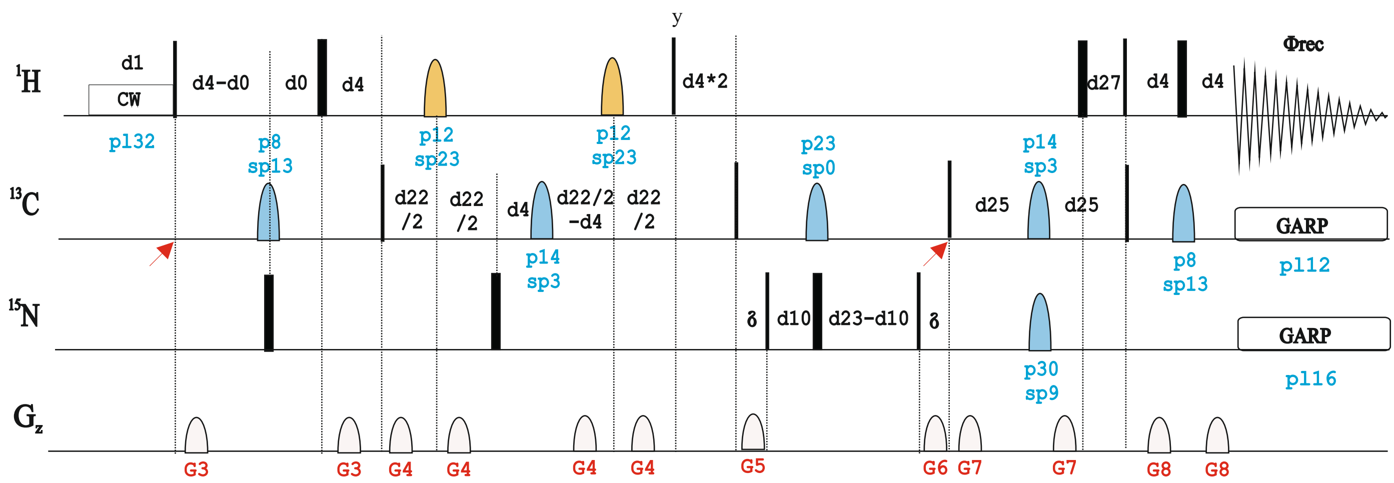
d1=1.5s
d4=1/4J(C1'H1')=1.6ms
d22=1/4J(C1'N)=18ms
d23=1/4J(C1'N, C6/8N)=17ms
d25=1/4J(C6/8N)=16ms
d27=1/4J/C6/8H6/8)=1.25ms
p12=3.3ms (spnam23=spnam24=reburp.1000)
p14=1ms (spnam3=spnam5=Q3.1000
p23=0 (spnam0=q3_rna_c68c1.1000)
cnst21=89.19 (C1' chemical shift)
cnst22=137.7 (C6C(chemical shift)

3D TROSY MQ-H(C)N(C)H Experiment

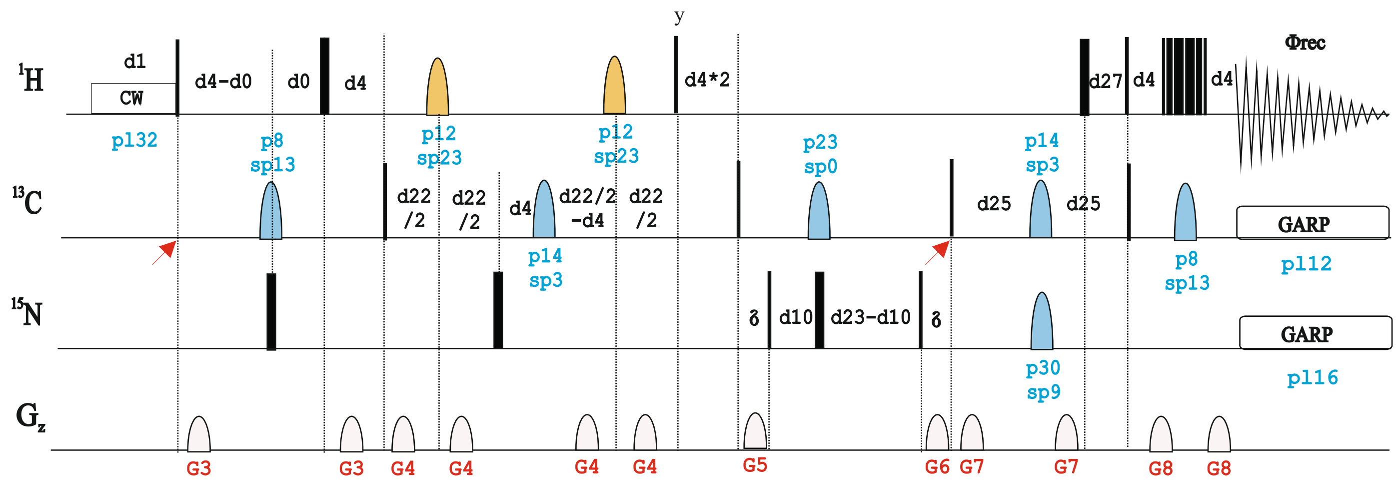
R. Fiala, J. Czernek & V. Sklenar, J. Biomol. NMR 16, 291-302 (2000)



na_trhcnchmqsp3d



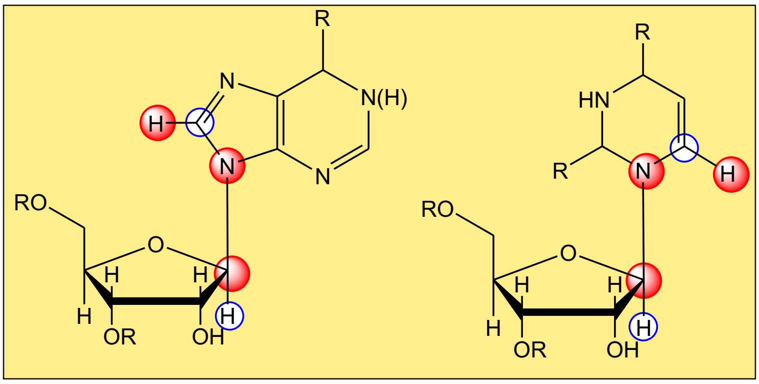
na_trhcnchmqspwg3d

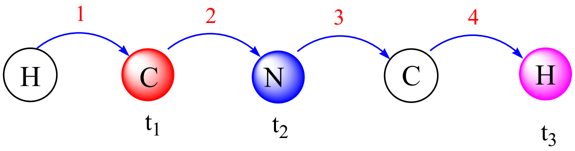


3D TROSY (H)CN(C)H Experiment

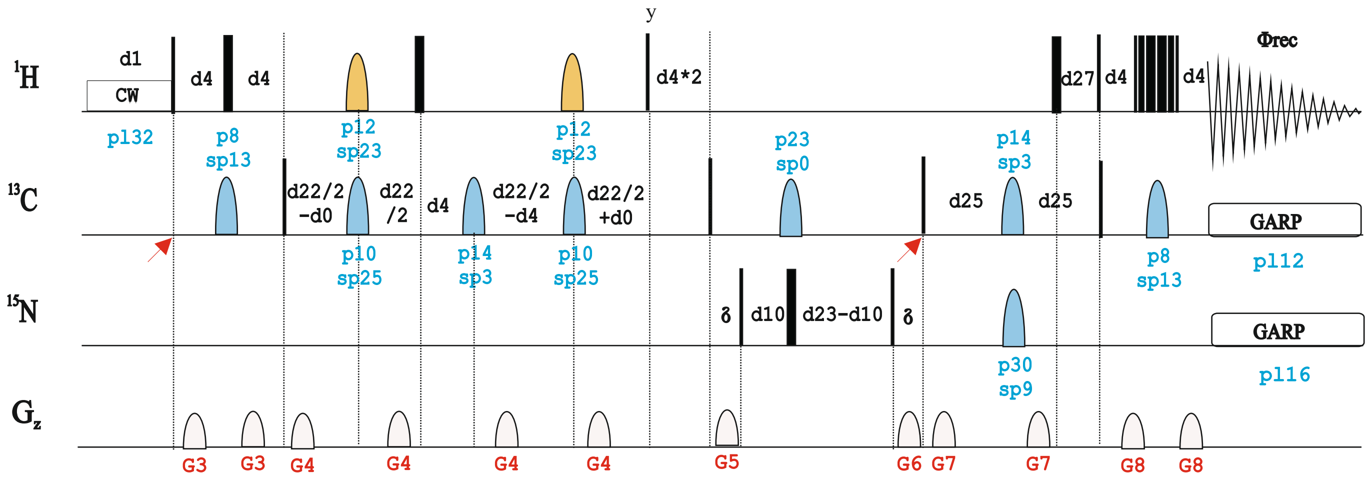
TROSY version of the 3D HCNCH experiment in which C1' chemical shift evolves instead of the H1' chemical shift.

R. Fiala, J. Czernek & V. Sklenar, J. Biomol. NMR 16, 291-302 (2000)

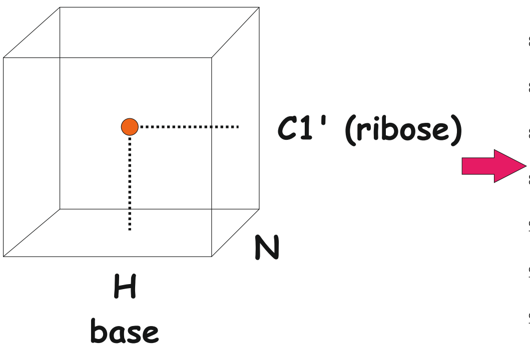


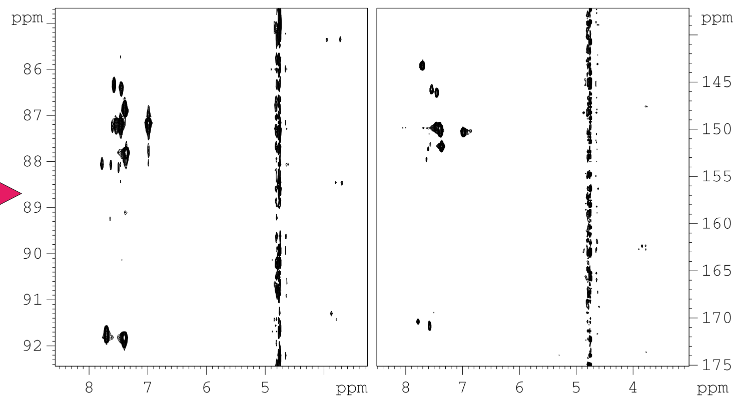


na_trhcnchmqspwg3d2



The experiment yields a 3D map correlation the sugar C1' carbno with the N1/N9 nitrogen and the H2/H8 protons of the connected base.





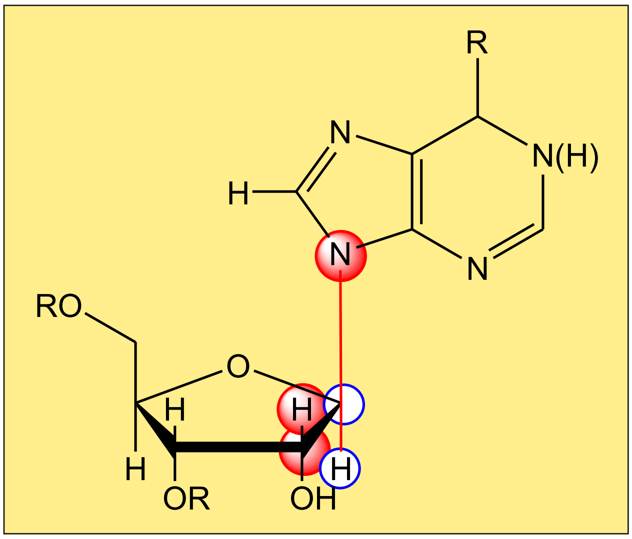
d1=1.5s
d4=1/4J(C1'H1')=1.6ms
d22=1/4J(C1'N)=18ms
d23=1/4J(C1'N, C6/8N)=17ms
d25=1/4J(C6/8N)=16ms
d27=1/4J/C6/8H6/8)=1.25ms

p12=3.3ms (spnam23=spnam24=reburp.1000)
p14=1ms (spnam3=spnam5=Q3.1000
p23=0 (spnam0=q3_rna_c68c1.1000)
cnst21=89.19 (C1' chemical shift)
cnst22=137.7 (C6C8 chemical shift)
cnst23=72 (C2' chemical shift)

3D MQ-(HC)N(C)CH-COSY Experiment

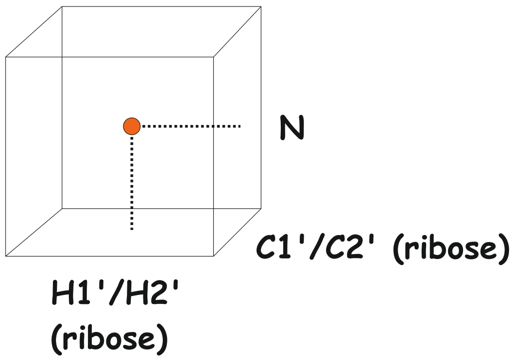
Experiment Description:

This experiment (HCN-CCH COSY) uses the good chemical shift dispersion of N1/N9 to assign the ribose spin system via a C1' to C2' COSY transfer after an initial HCNC transfer.



NMR Spectrum

The experiment provides a 3D correlation map

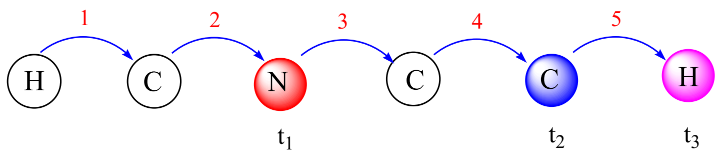


References:

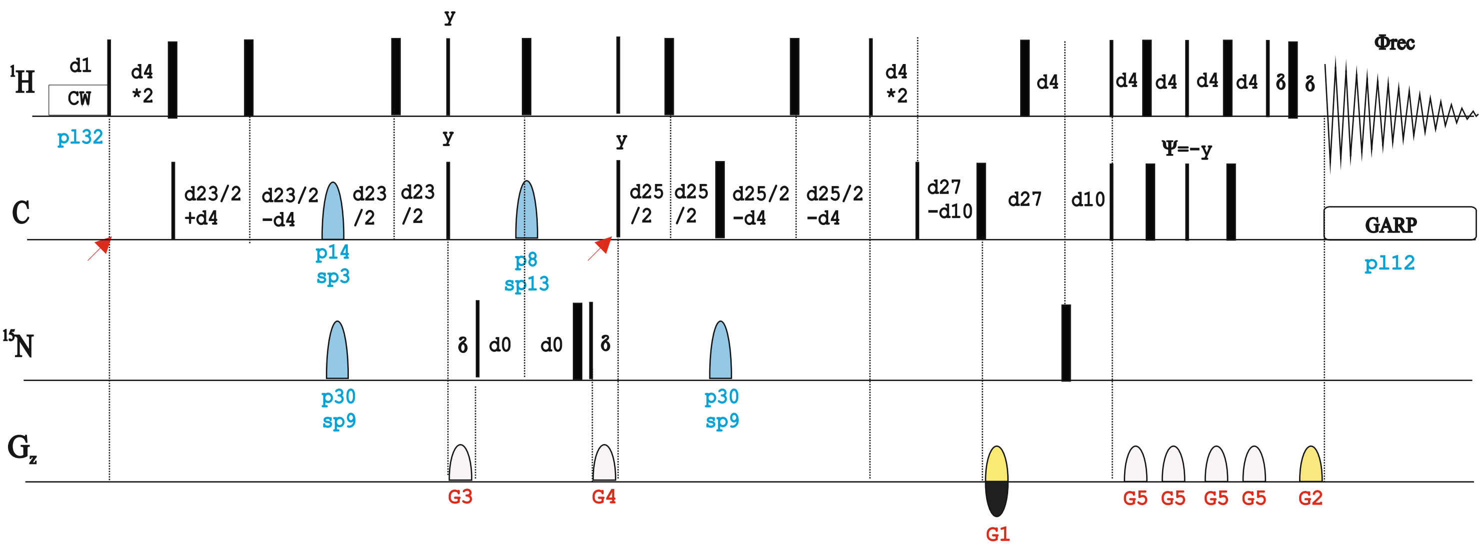
W. Hu, L. Jiang & Y.Q. Gosser, J. Magn. Reson. 145, 147-151 (2000)

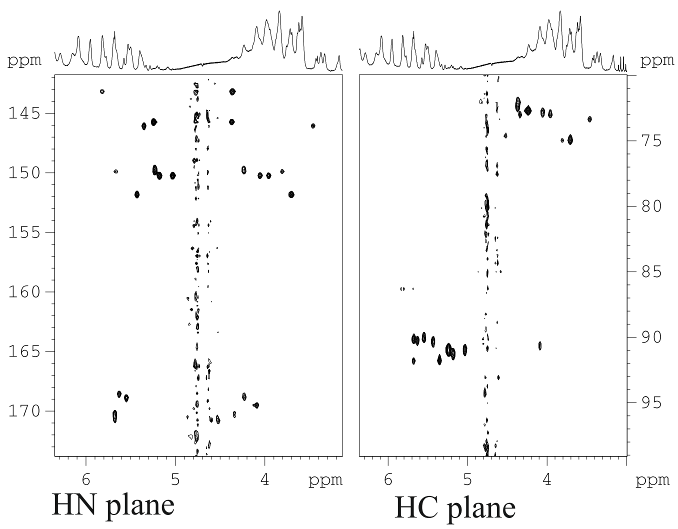
Related Experiments

HCN-CCH TOCSY



na_hcncchcomq3d



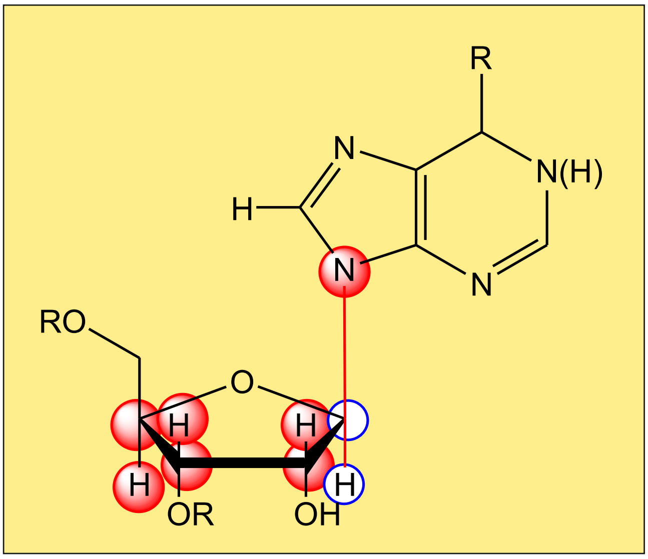


d1=1.5s
d4=1/4J(C1'H1')=1.56ms
d23=1/4J(C1'N)=18ms
d25=1/4J(C1'N)=15ms
d27=1/8J/C1'C2')=3.25ms
cnst21=C1' chemical shift=90ppm
cnst23=C2' chemical shift=72 ppm
o2p=79ppm
p14=1ms (spnam3=Q3.1000)
o3p=160 ppm
p30=700us (spnam9=Q3.1000)

3D MQ-(HC)N(C)CH-TOCSY Experiment

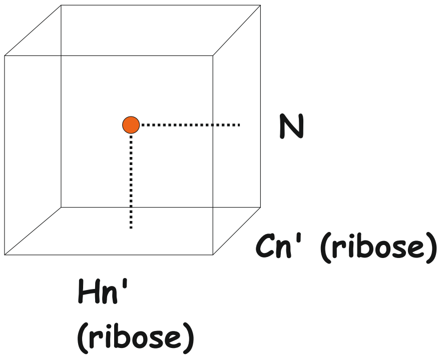
Experiment Description:

This experiment (HCN-CCH TOCSY) uses the good chemical shift dispersion of N1/N9 to assign the ribose spin system via a C1' to Cn' TOCSY transfer after an initial HCNC transfer.



NMR Spectrum

The experiment provides a 3D correlation map

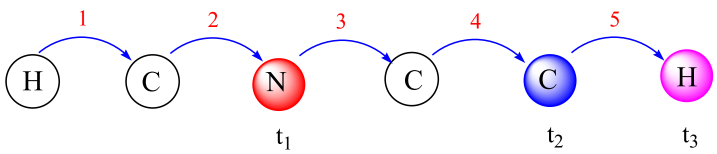


References:

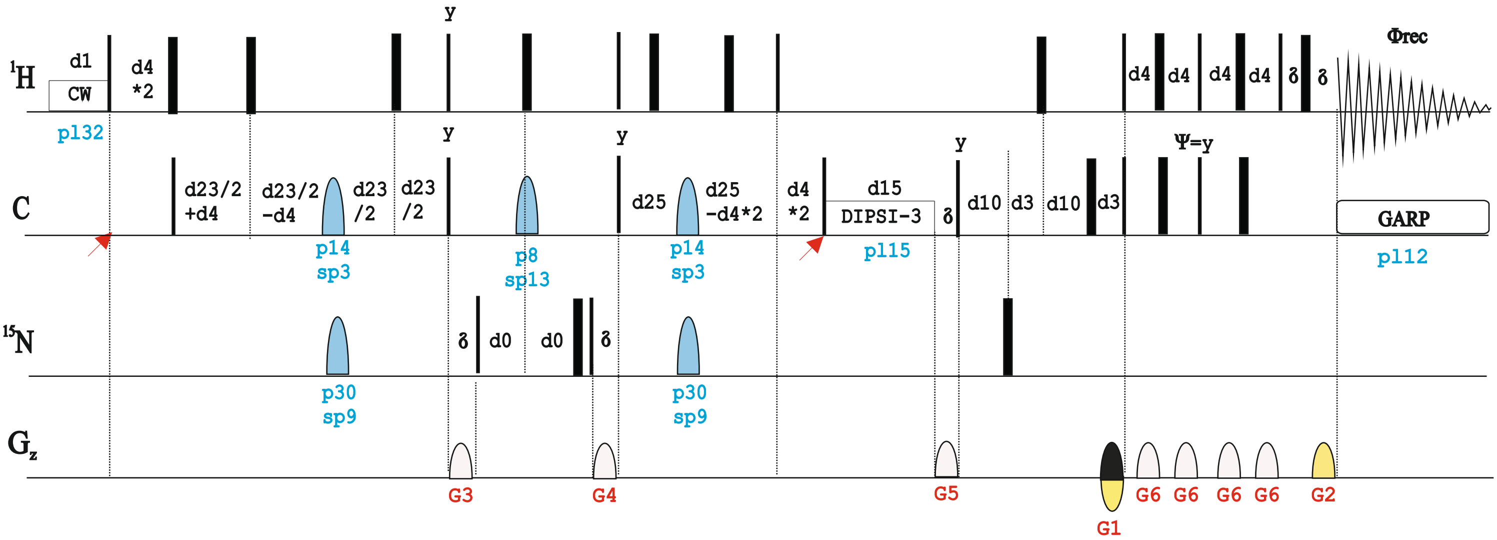
W. Hu, L. Jiang & Y.Q. Gosser, J. Magn. Reson. 145, 147-151 (2000)

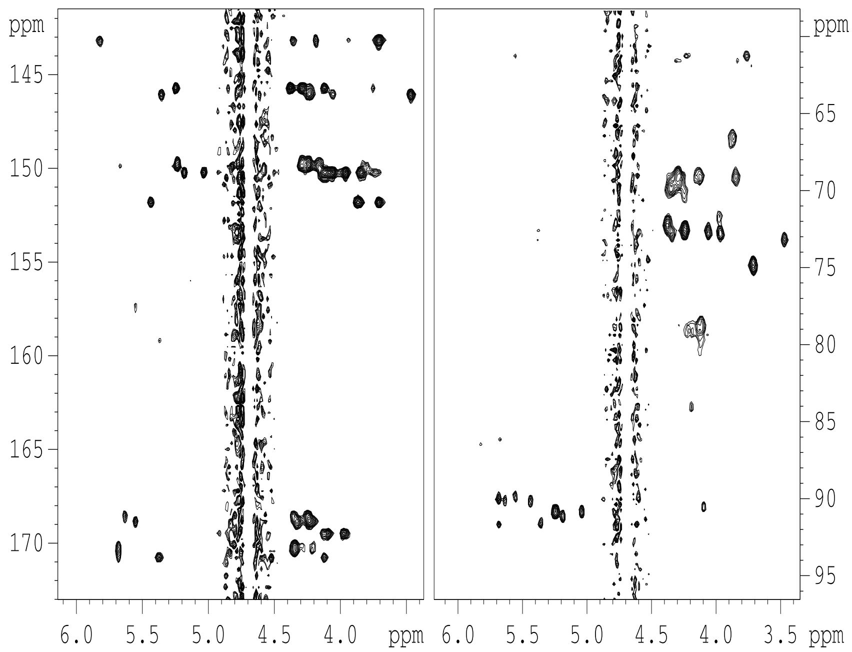
Related Experiments

HCN-CCH COSY



na_hcncchdimq3d





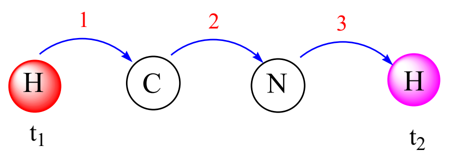
d1=1.5s
d4=1/4J(C1'H1')=1.56ms
d3=1/4J(C'H')=0.95ms
d15= CC TOCSY= 12 ms
d23=1/4J(C1'N)=18ms
d24=1/8J(C'H')=0.78ms
d25=1/4J(C1'N)=15ms
d27=1/8J/C1'C2')=3.25ms
cnst21=C1' chemical shift=90ppm
cnst23=C2' chemical shift=72 ppm
o2p=79ppm
p14=1ms (spnam3=Q3.1000)
o3p=160 ppm
p30=700us (spnam9=Q3.1000)

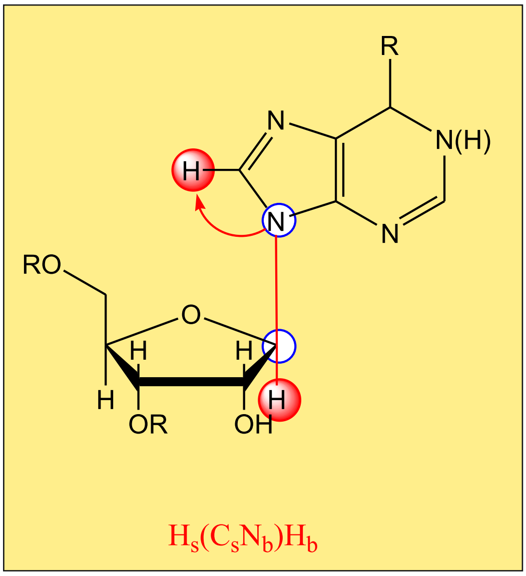
2D H(CN)H Experiment

Experiment Description:

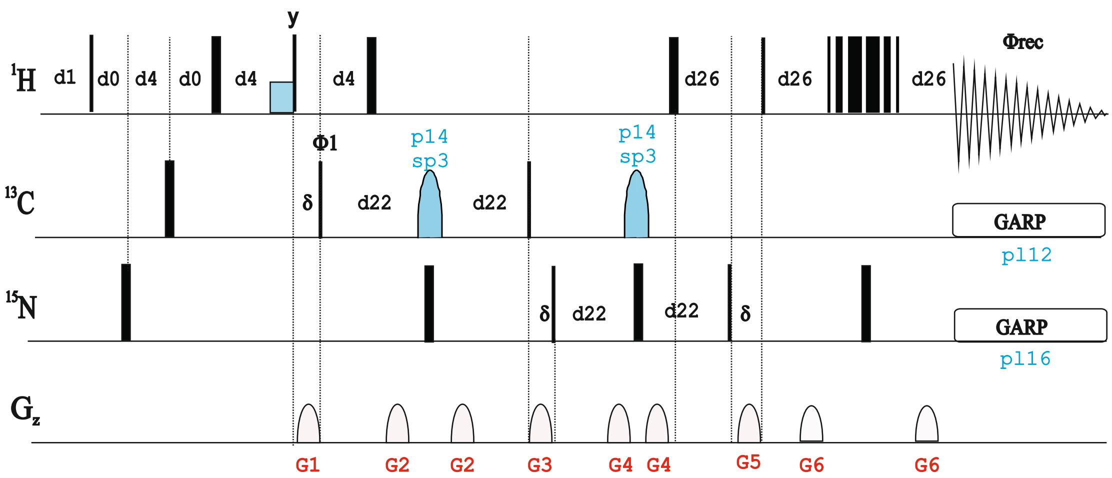
Experiment alternative to the HCNCH experiment that allows to correlate the H1' ribose proton with the base H6/8 protons via 2J(N1/9-H6/8) coupling constant

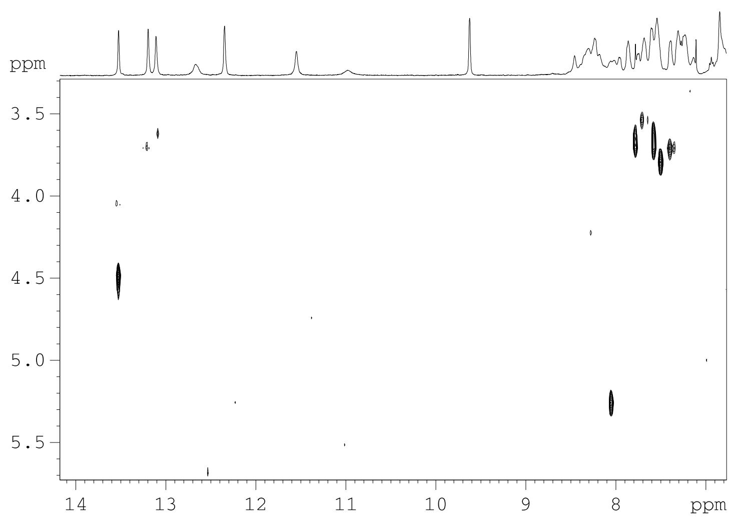
S .Tate, A. Ono & M. Kainosho, J. Am. Chem. Soc. 116, 5977 - 5978 (1994).





na_hcnhgpph19



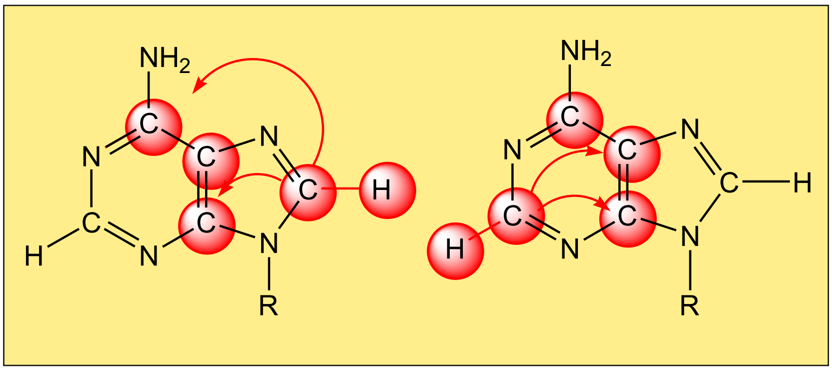


d1=1.5s
d4=1/4J(CH)=1.56ms
d22=1/4J(CN)=18.0ms
d26=1/4J(NH)=15ms (long-range)
p14=1ms (spnam3=Q3.1000)
o2p=89.19ppm

3D TROSY-(H)CCH-COSY Experiment

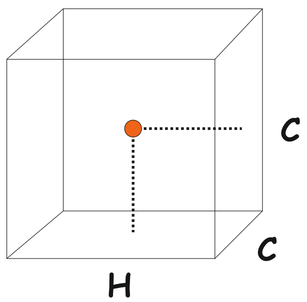
Experiment Description:

Experiment that correlates the adenine H2 and H8 protons in 13C-labeled NAs molecules. The experiment provides 13C chemical shifts of all carbon nuclei in the adenine base and also thelong-range H8-C4/C5/C8 correlation in guanines (01jb173-20).



NMR Spectrum

The experiment provides a 3D correlation map

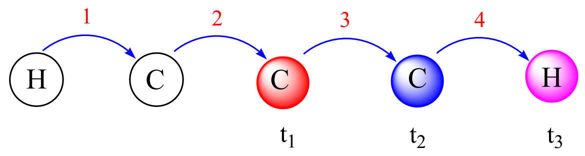


References:

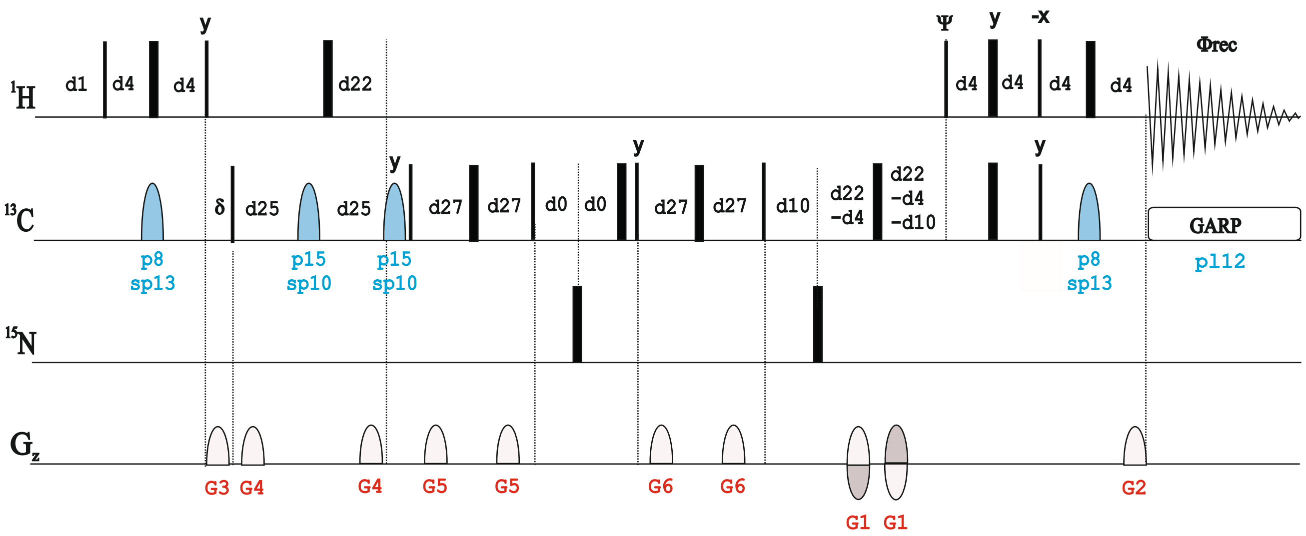
B. Simon, K. Zanier & M. Sattler, J. Biomol. NMR 20, 173-176 (2001)

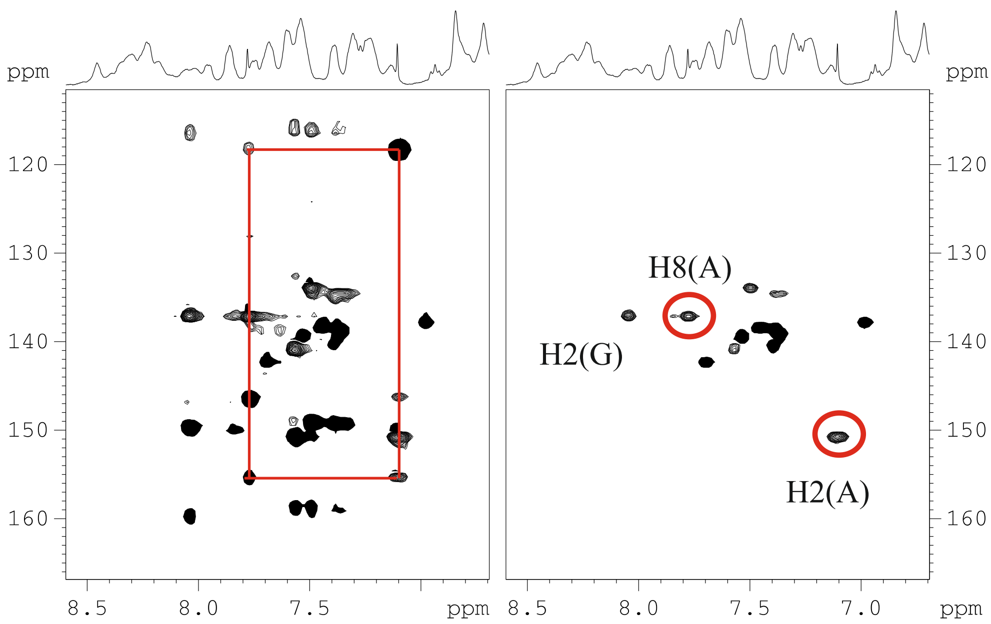
Related Experiments

2D 1H-13C HMBC



na_trhcchco3d



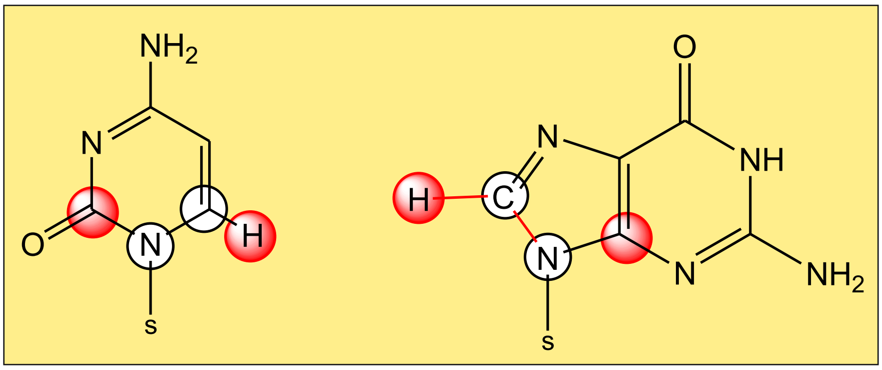


d1=1.5s
d4=1.25ms
cnst28=4.69 C5 offset
d22=1/4J(C2C5) and
1/4(C8C4/C6)=14.2ms
d25=1/2J(C5C6)=7.12ms
d27=1/4J(C5C4/C6)=1ms
o2p=140ppm
p15=90 pulse C5 off-resonance

2D H(CN)C Experiment

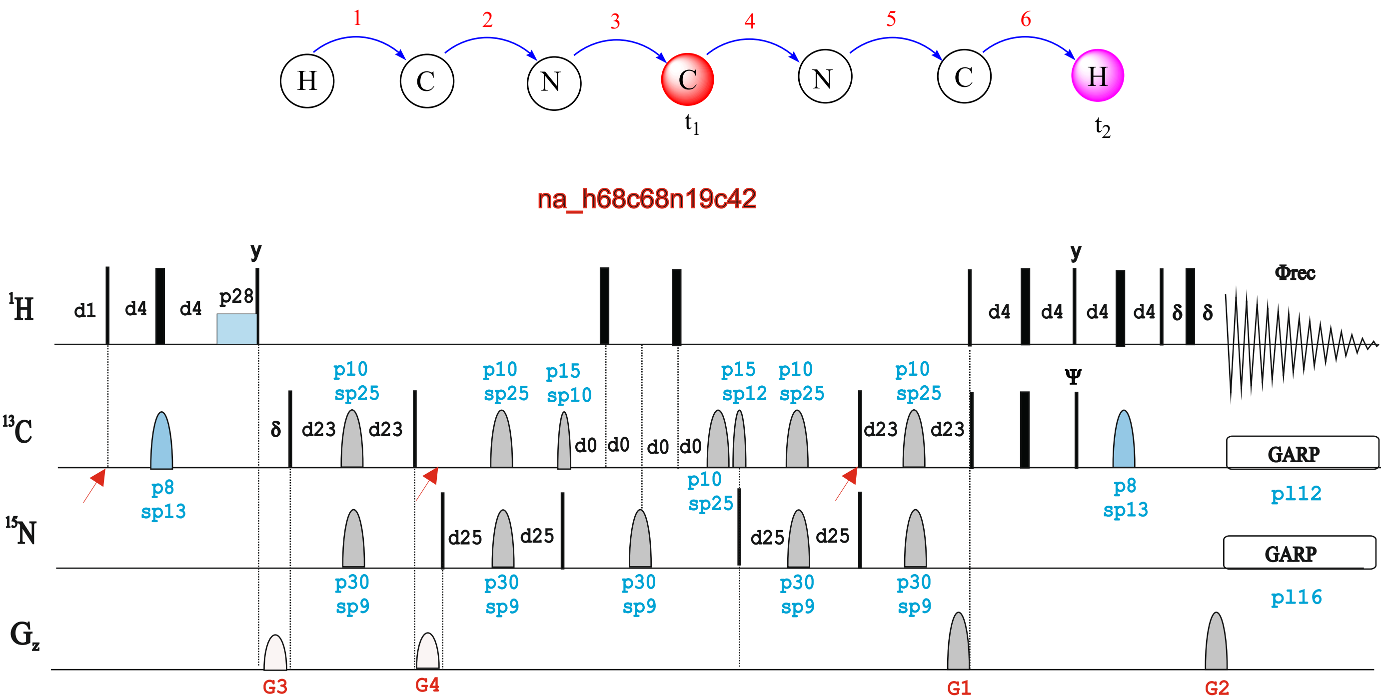
Experiment Description:

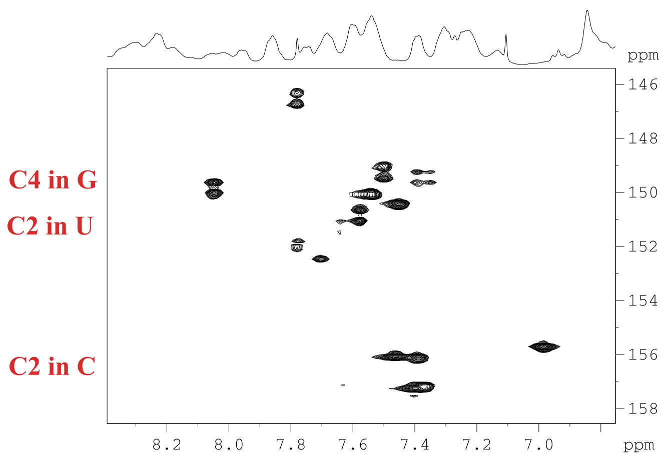
The H(CN)C experiment (also referred as H(6/8)C(6/8)N(1/9)C(2/4)) correlates the aromatic H6/8 protons of the base with the non-protonated C2/4 carbons via the C6/8 and N1/9 centers.



References:

B. Fuertig, C. Richter, W. Bermel & H. Schwalbe, J. Biomol. NMR 28, 69-79 (2004)



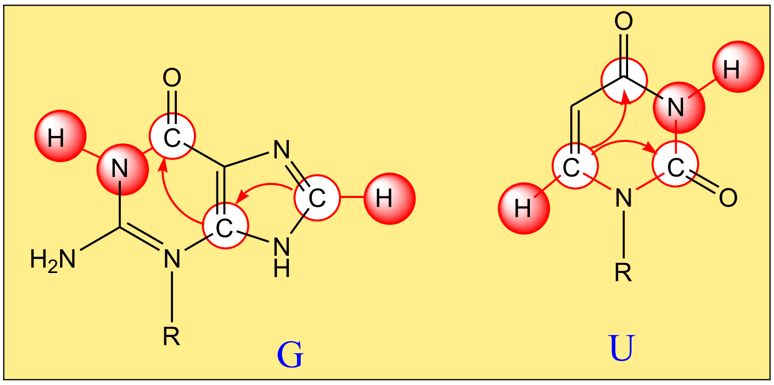


d1=1.5s
d4=1/4J(CH)=1.25ms for J(H8C8) and J(H6C6)
d23=1/4J(CN)=15ms for J(N1C6), and J(N9C8)
d25=1/4J(CN)=15ms for J(N1C2), and J(N9C4)
o2p=cnst27=152ppm
cnst22=137.7=chemical shift C6(CU)/C8(AG)
p30=700us(spnam9=Q3.1000)
p10=
p15=
Reduced SW in the C dimension=16.5ppm

3D H(6/8)(CCC)NH Experiment

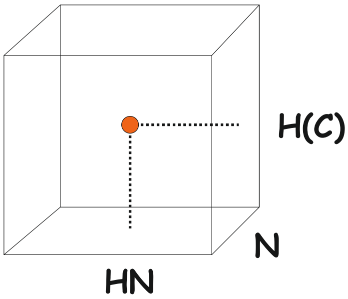
Experiment Description:

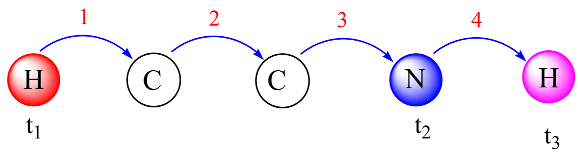
The HCCNH-TOCSY experiment allows the correlation between the exchangeable imino NH groups with H8 in guanines and H6 in uridines.



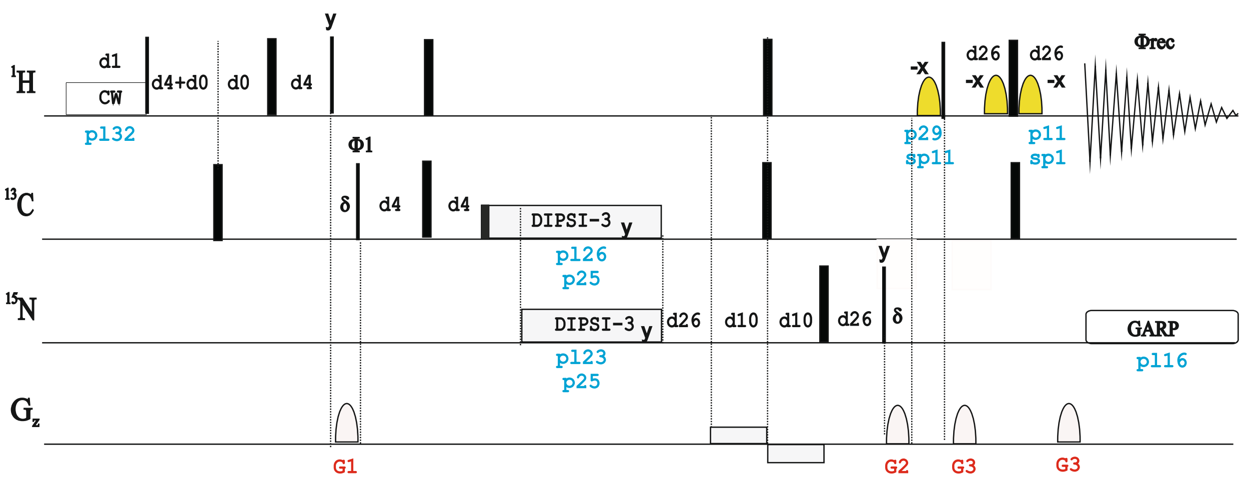
References:

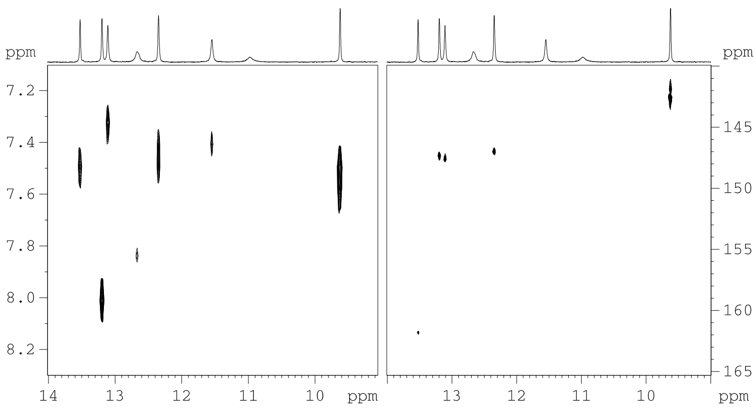
V. Sklenar, T. Dieckmann, S. E.Butcher & J. Feigon, J. Biomol. NMR 7, 83 - 87 (1996)





na_hccnhdigpwg3d





d1=1.5s
d4=1/4J(CH)=12.5ms
optimized for cnst2=200Hz
d26=1/4J(NH)=2.77ms
optimized for cnst4=90Hz
p29=p11=1ms (Squa100.1000)
p25=245us
l1=1
l1=3
o2p=149 ppm

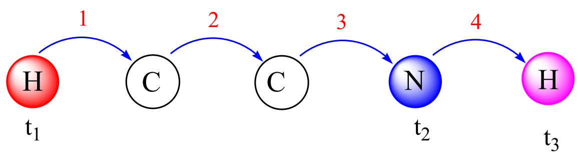
3D H(CC)NH-COSY Experiment

Experiment Description:

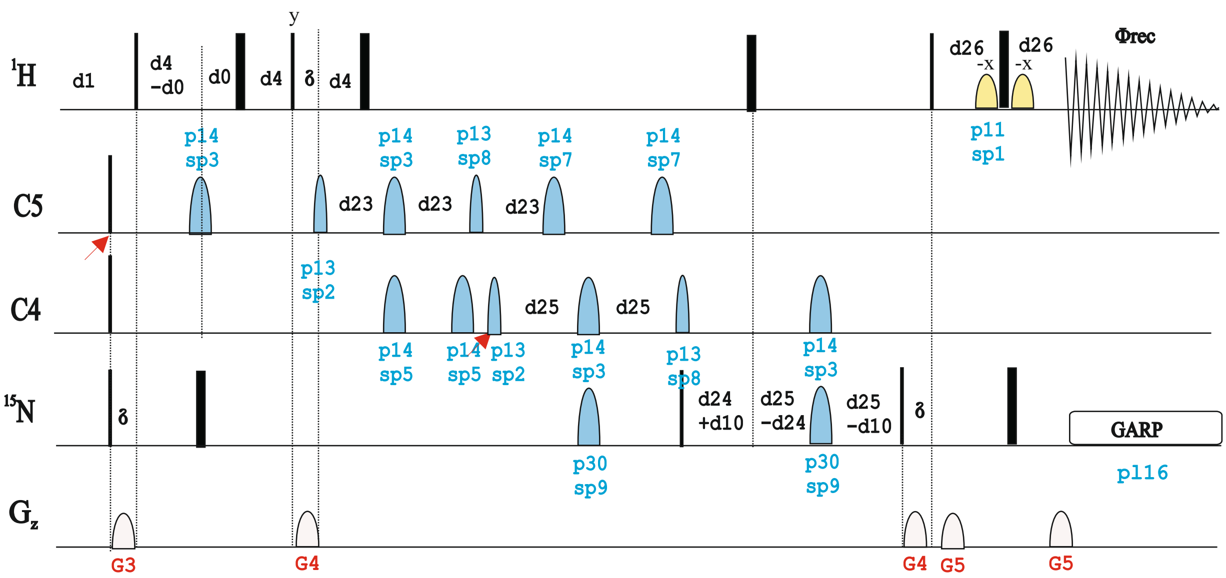
The HCCNH experiment allows the correlation of the exchangeable NH and NH2 spin systems with the H5 and H6 protons in U and C via a CC COSY transfer.
The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH2 groups.

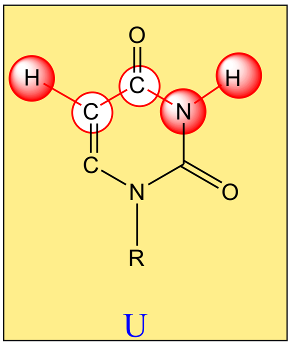
References:

J. Woehnert, R. Ramachandran, M. Goerlach & L.R. Brown, J. Magn. Reson. 139, 430-433 (1999)

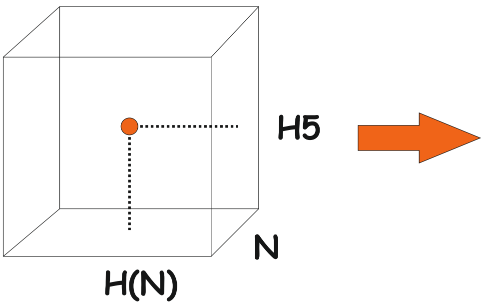


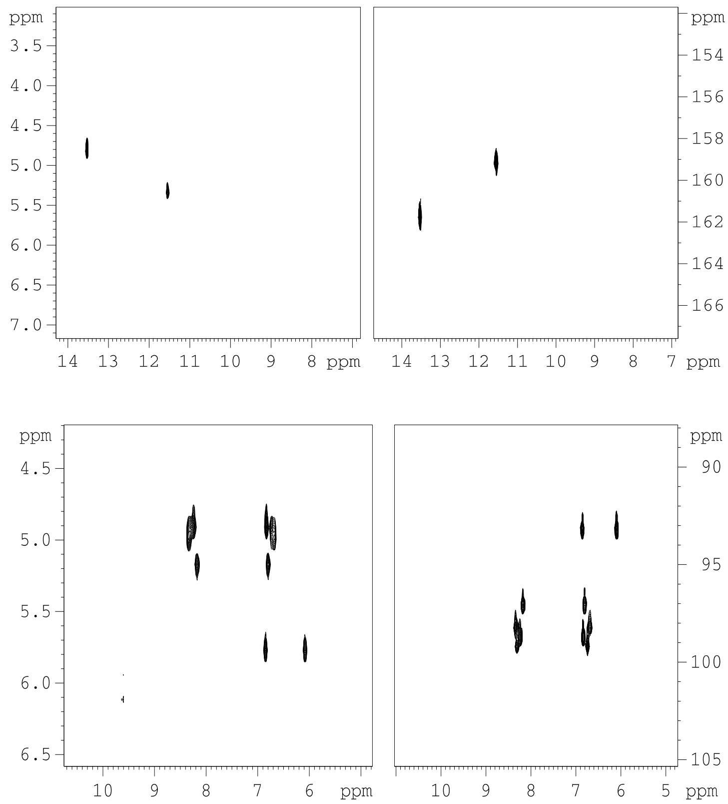
na_h5c5c4n3h_3d

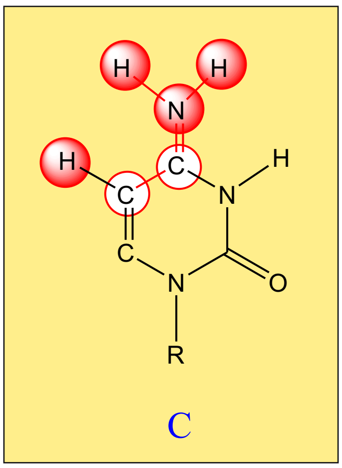




d1=1.5s
d4=1/4J(C5H5)=1.25ms
d23=1/4J(C5C4)=4.1ms
d24=1/4J(NH) for U=2.78ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
p11=1 ms (spnam1=Squa100.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3/5/7=Q3.1000)
cnst24=C4(C/U) chemical shift=169ppm
cnst28=C5(C/U) chemical shift=105ppm
o3p=160ppm (for U)
p30=700us (spnam9=Q3.1000)







d1=1.5s
d4=1/4J(C5H5)=1.25ms
d23=1/4J(C5C4)=4.1ms
d24=1/8J(NH) for C=1.39ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
p11=1 ms (spnam1=Squa100.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3/5/7=Q3.1000)
cnst24=C4(C/U) chemical shift=169ppm
cnst28=C5(C/U) chemical shift=105ppm
o3p=100ppm (for C)
p30=700us (spnam9=Q3.1000)

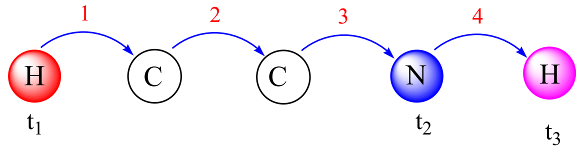
3D H(CC)NH-TOCSY Experiment

Experiment Description:

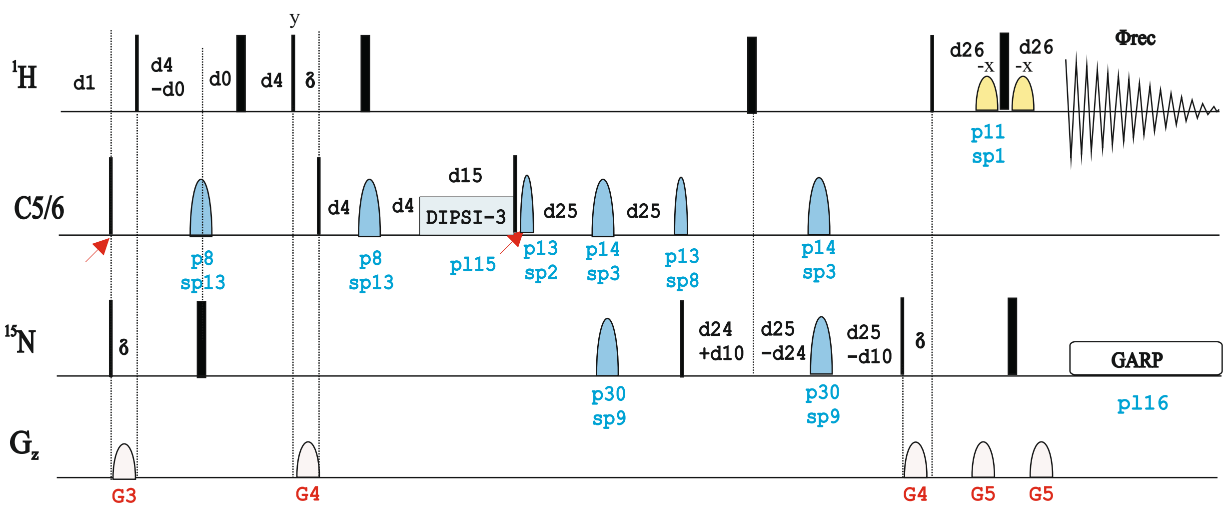
The HCCNH-TOCSY experiment allows the correlation of the exchangeable NH and NH spin systems with the H5 and H6 protons in U and C via a CC TOCSY transfer.
The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH2 groups.

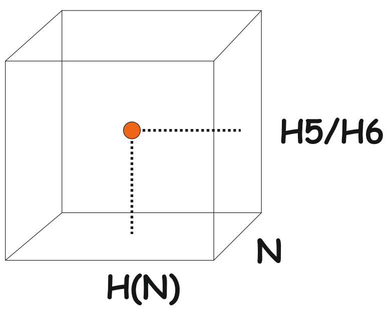
References:

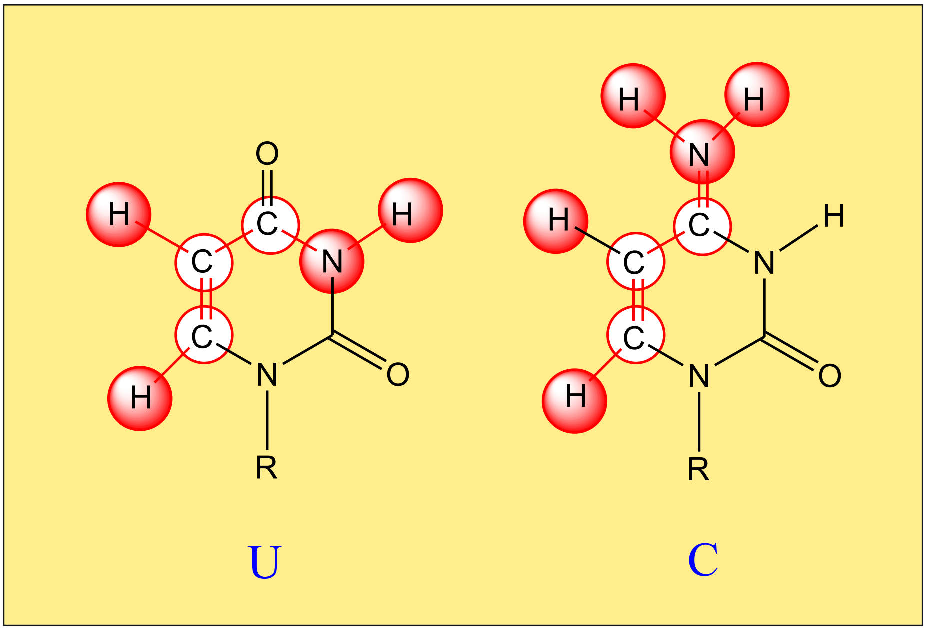
J. Woehnert, M. Goerlach & H. Schwalbe, J. Biomol. NMR 26, 79-83 (2003).

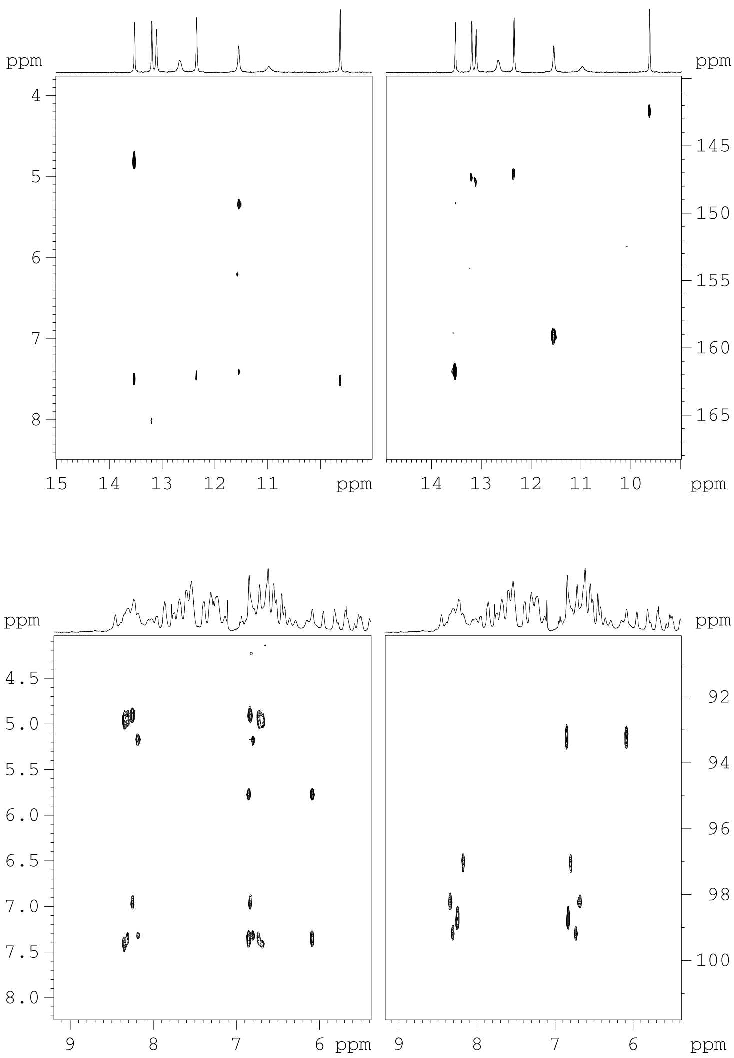


na_h56c56c4n3h_3d









d24=1/4J(NH) for U=2.78ms
o3p=160ppm (for U)

d1=1.5s
d4=1/4J(C5H5)=1.25ms
d24=1/4J(NH) for U or 1/8J(NH) for C
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
d15=CC TOCSY=19.5ms
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3=Q3.1000)
p30=700us (spnam9=Q3.1000)
cnst24=169ppm (C4 in C/U)
cnst28=105ppm (C5 in C/U)
o2p=89.19ppm
o3p=160ppm (for U) or 100ppm(for C)

d24=1/8J(NH) for U=1.39ms
o3p=100ppm (for C)

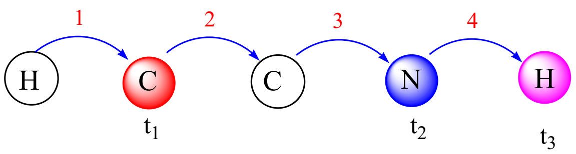
3D (H)C(C)NH-TOCSY Experiment

Experiment Description:

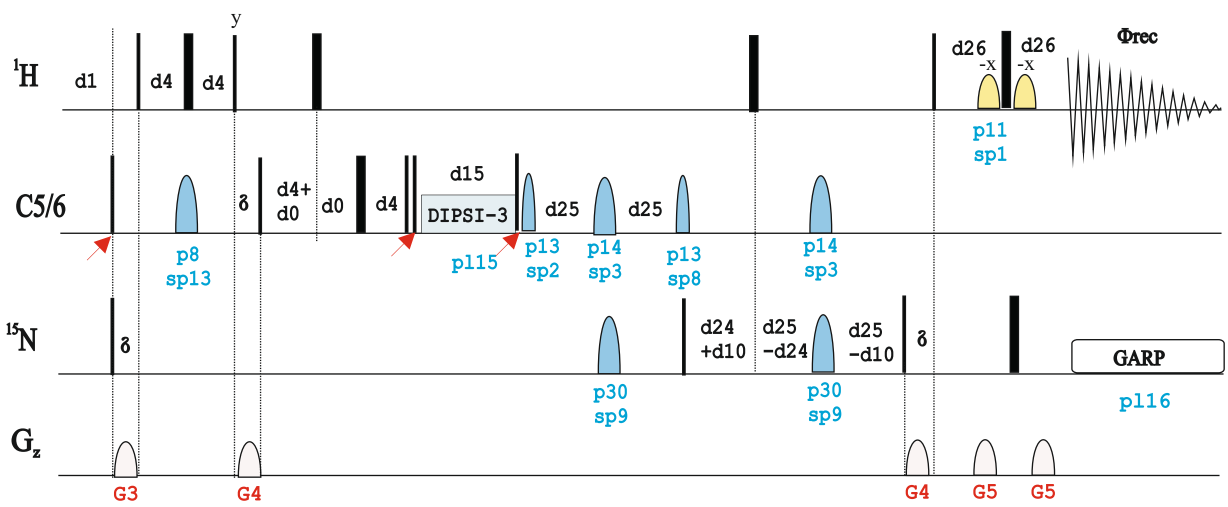
The HCCNH-TOCSY experiment allows the correlation of the exchangeable NH and NH spin systems with the C6 carbons in U and C via a CC TOCSY transfer.
The experiment starts from the aromatic CH spin system and detects H(N). It can be separately optimized for imino NH or for amino NH2 groups.

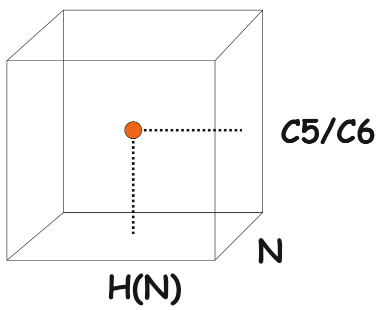
References:

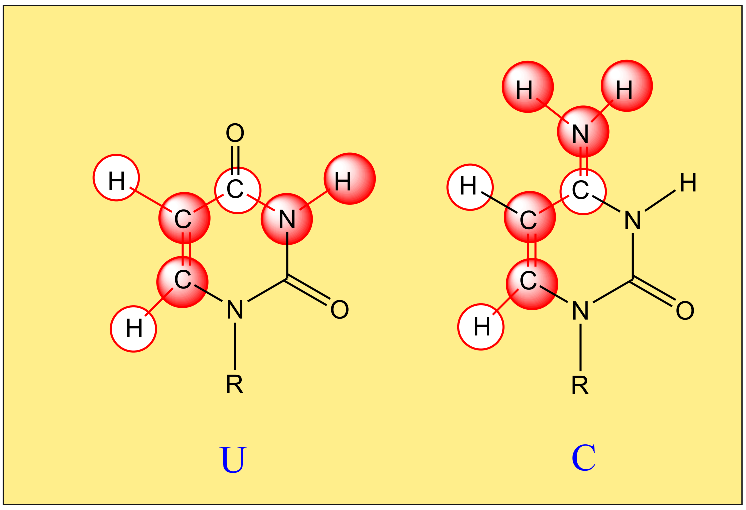
J. Woehnert, M. Goerlach & H. Schwalbe,J. Biomol. NMR 26, 79-83 (2003)

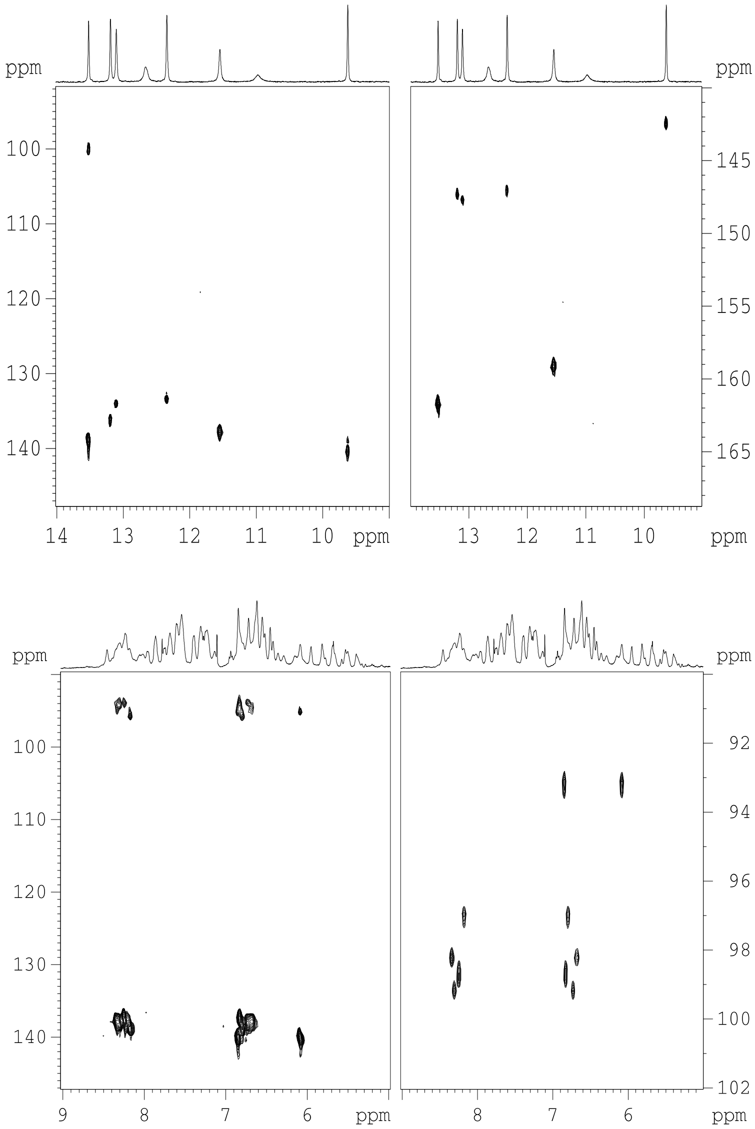


na_h56c56c4n3h_3d2









d24=1/4J(NH) for U=2.78ms
o3p=160ppm (for U)

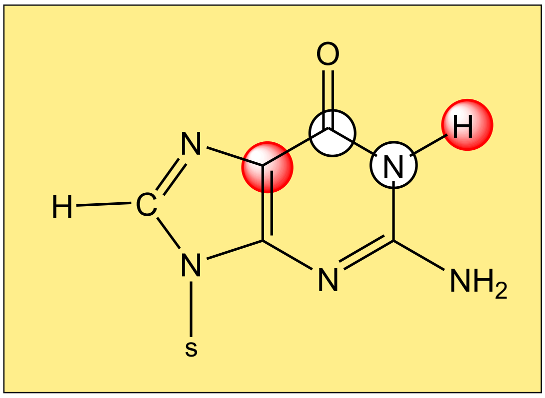
d1=1.5s
d4=1/4J(C5H5)=1.25ms
d25=1/4J(C4N)=10ms
d26=1/4J(NH)=2.5ms
d15=CC TOCSY=19.5ms
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
p14=1ms (spnam3=Q3.1000)
p30=700us (spnam9=Q3.1000)
cnst22=137ppm (C6 in C7U)
cnst24=169ppm (C4 in C/U)
cnst28=105ppm (C5 in C/U)
o2p=121.35ppm

d24=1/8J(NH) for C=1.39ms
o3p=100ppm (for C)

2D H(NC)C Experiment

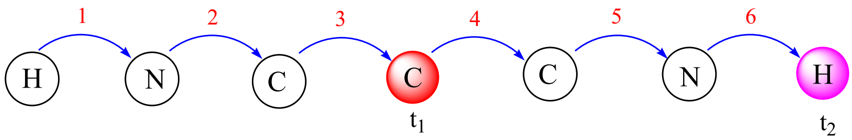
Experiment Description:

The H(NC)C experiment allows the assignment of C5 carbon in G residues from imino NH proton via the C6 carbon (04jb69). The pulse scheme is a variant of the out-and-back HNCOCA experiment.

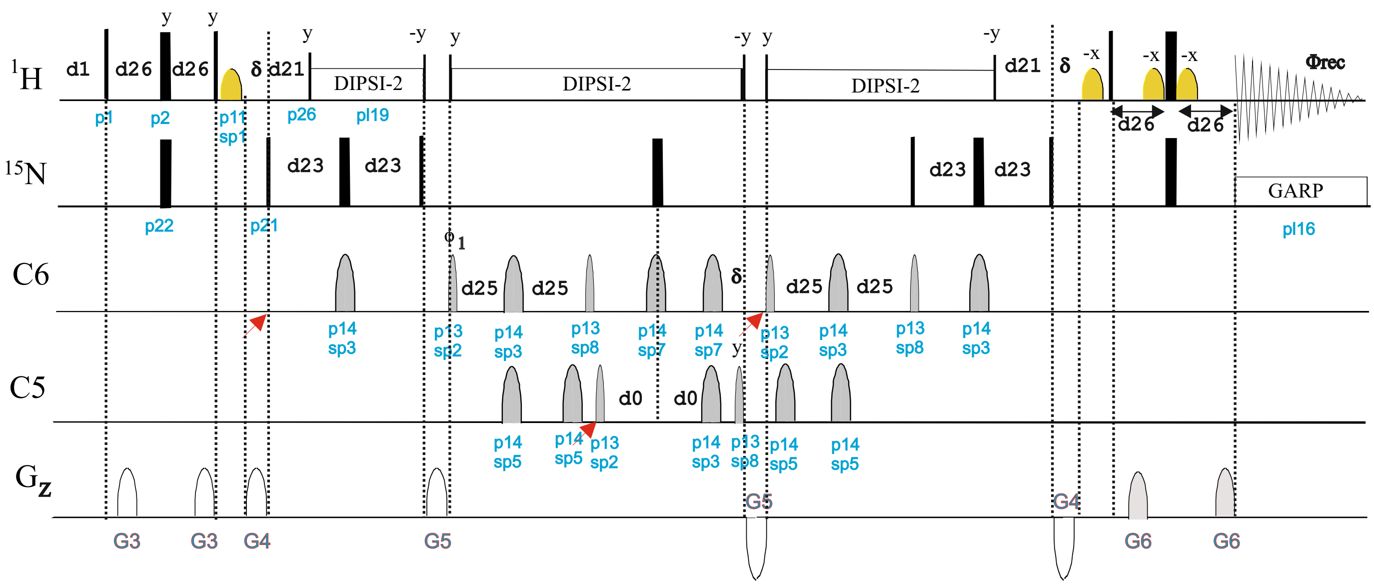


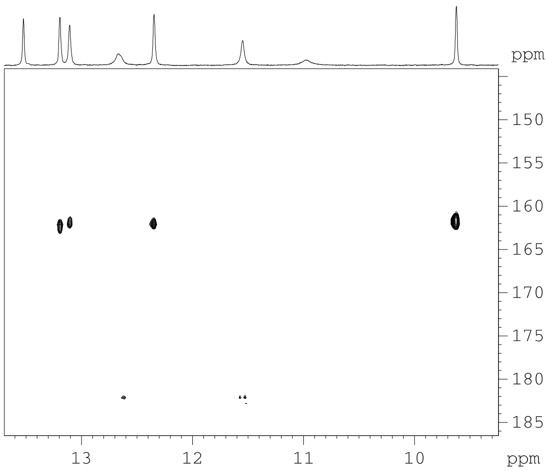
References:

B. Fuertig, C. Richter, W. Bermel & H. Schwalbe, J. Biomol. NMR 28, 69-79 (2004)



na_hnc6c5etgpsi





d1=1.5s
d26=1/4J(NH)=2.78ms
d23=1/4J(C6N)=25ms
d25=1/4J(C6C5)=2.8ms
d21=1/2J/NH)=5.56ms
p11=1s (spnam1=Squa100.1000)
p14=1ms (spnam3/5/7=Q3.1000)
p13=1ms (spnam2=Q5.1000 and spnam8=Q5tr.1000)
cnst25=C6(G) chemical shift=160ppm
cnst26=C5(G) chemical shift=119ppm
o2p=C5 chemical shift=165ppm
o3p=160ppm

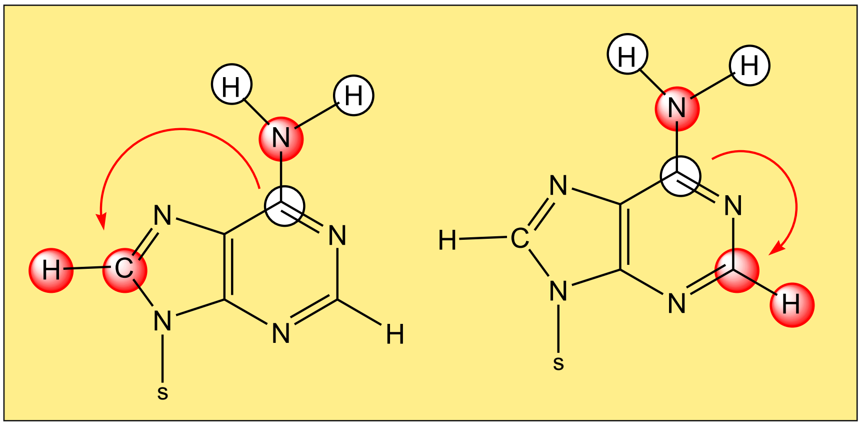
3D (H)N(C)CH Experiment

Experiment Description:

The 3D HNCCH experiment allows the correlation of the imino N nitrogen with the H2/C2 and H8/C8 spin systems in adenines.

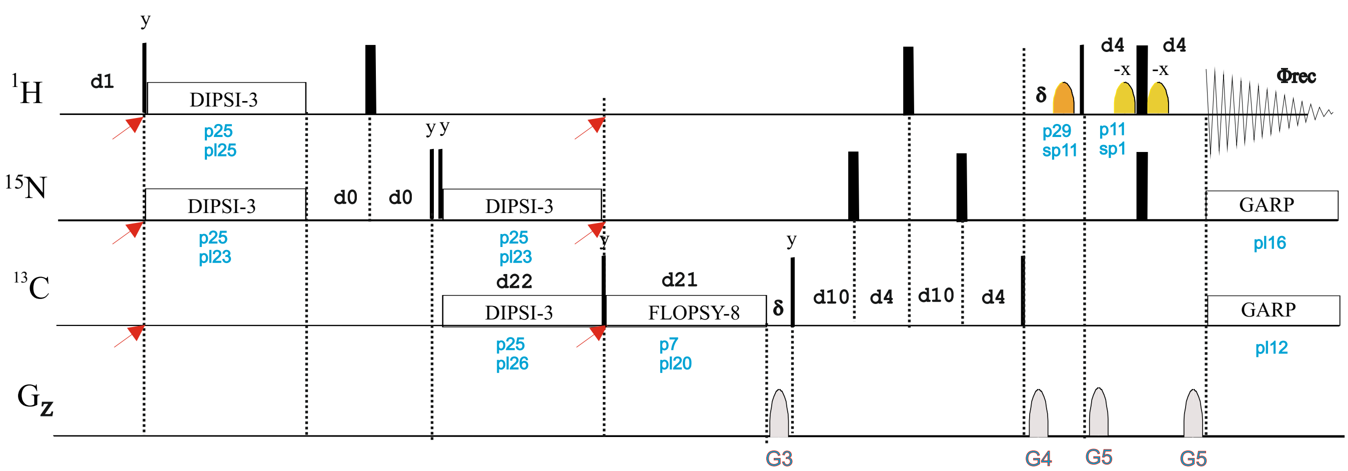
References:

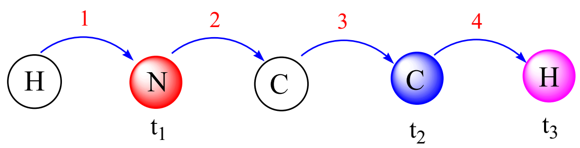
J.-P. Simorre, G.R. Zimmermann, L. Mueller & A. Pardi, J. Am. Chem. Soc. 118, 5316-5317 (1996)

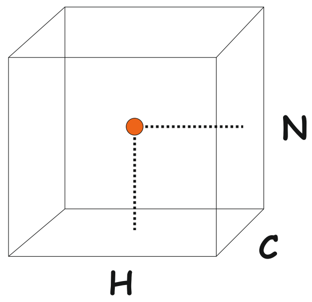


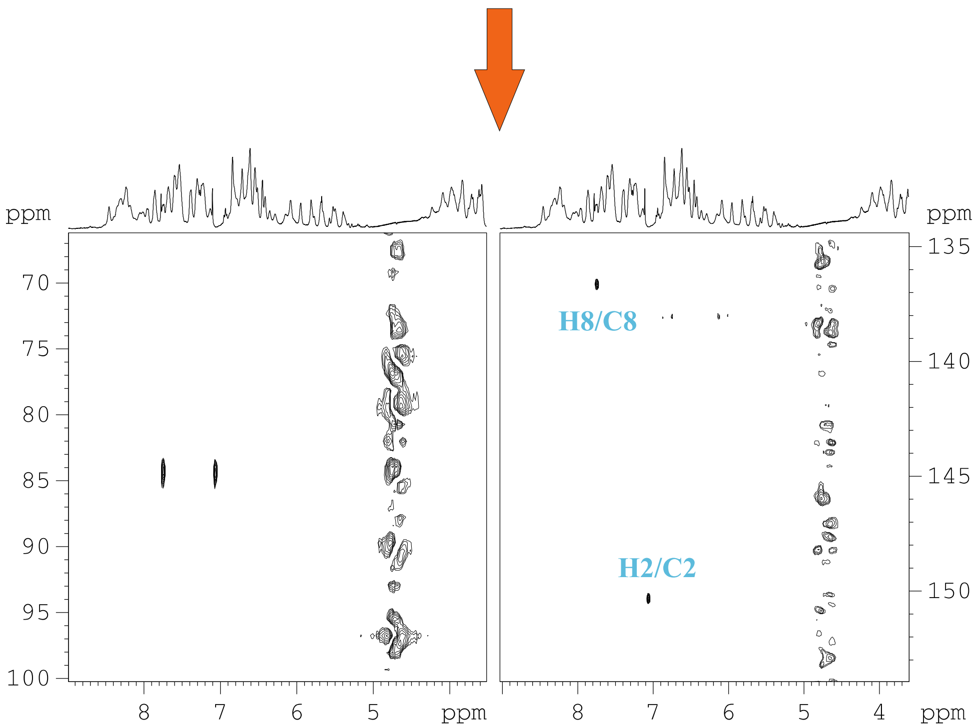
The experiment uses three different cross-polarization transfer schemes. First, a heteronuclear cross-polarization (HCP) transfer from 1H to 15N. Then, another HC transfer from N to C followed by a homonuclear TOCSY CC transfer

na_hncch3d









d1=1.5s
d4=1/4J(CH)=1.25ms
p11=p29=1s (spnam1=Squa100.1000)
p25=226us
d21=CC TOCSY=38ms
d22=CN TOCSY=45ms
o1p=cnst18=4.7ppm
cnst19=NH chemical shift
cnst25=C6 chemical shift=160ppm
o2p=cnst29=145 ppm (Caro)
o3p=cnst31=81ppm (NH2)

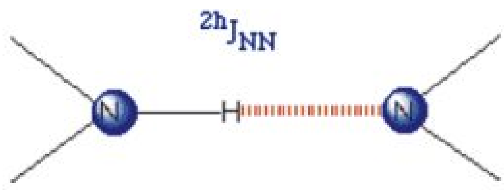
3D hydrogen-bond HNN Experiment

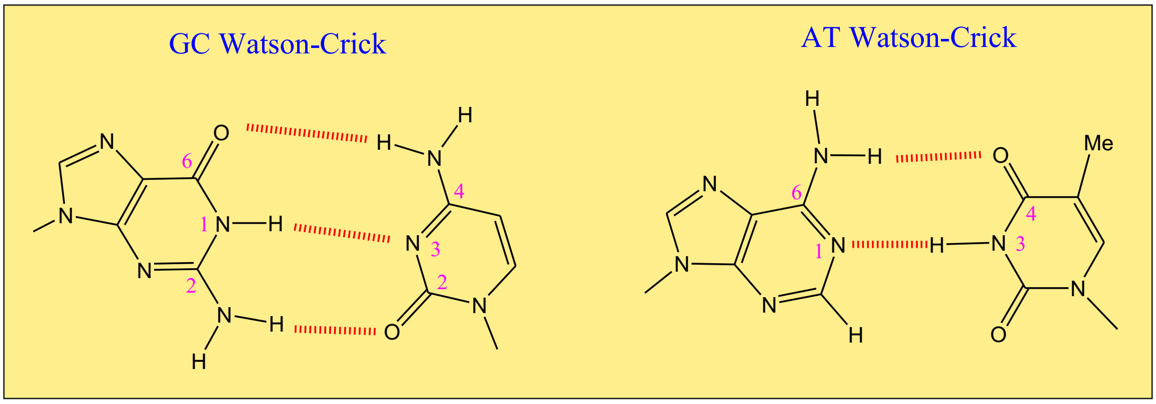
Experiment Description:

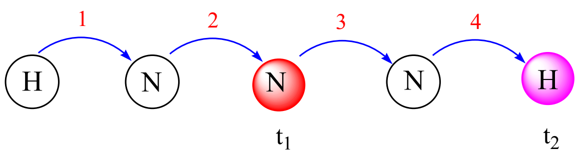
Experiment to detect hydrogen-bond NH-N connectivities (98jacs8293, 20NAR1585-28).

References:

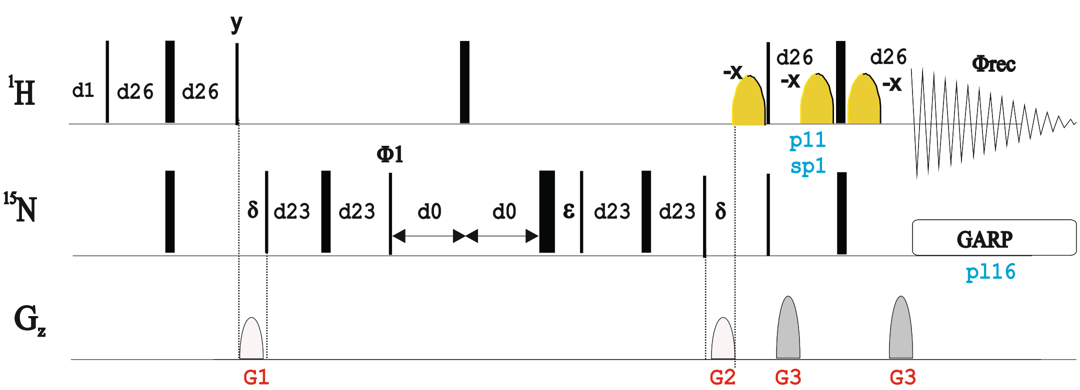
A.J. Dingley & S. Grzesiek, J. Am. Chem. Soc. 120, 8293 - 8297 (1998)

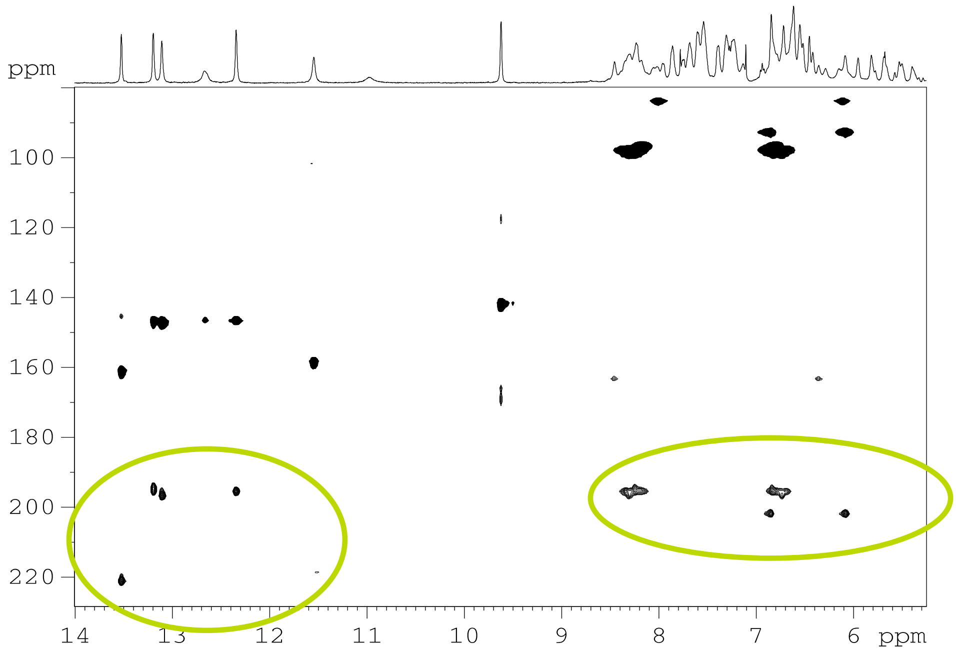






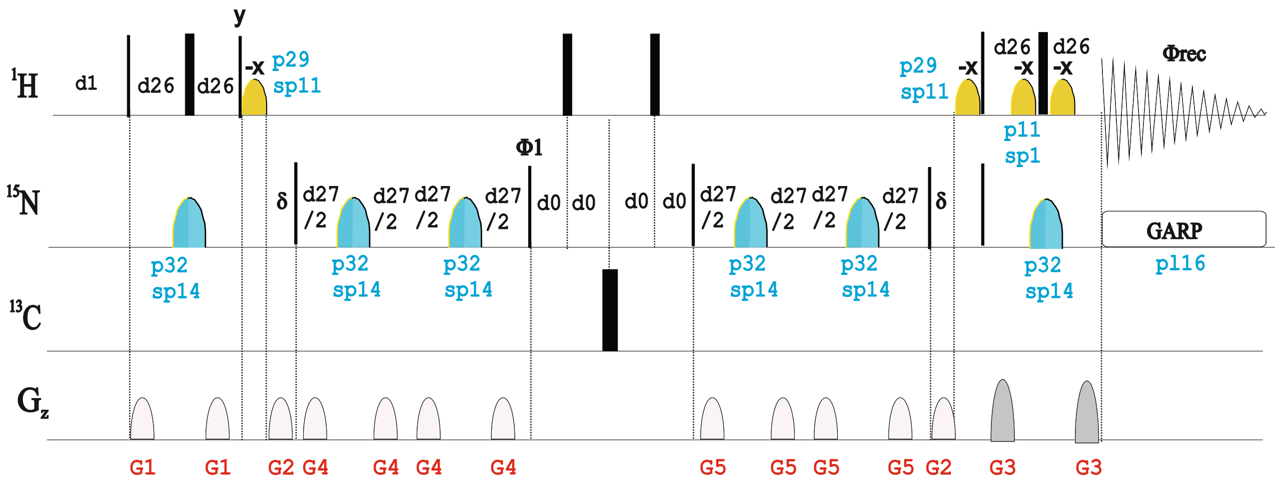
na_hnncosygpphwg



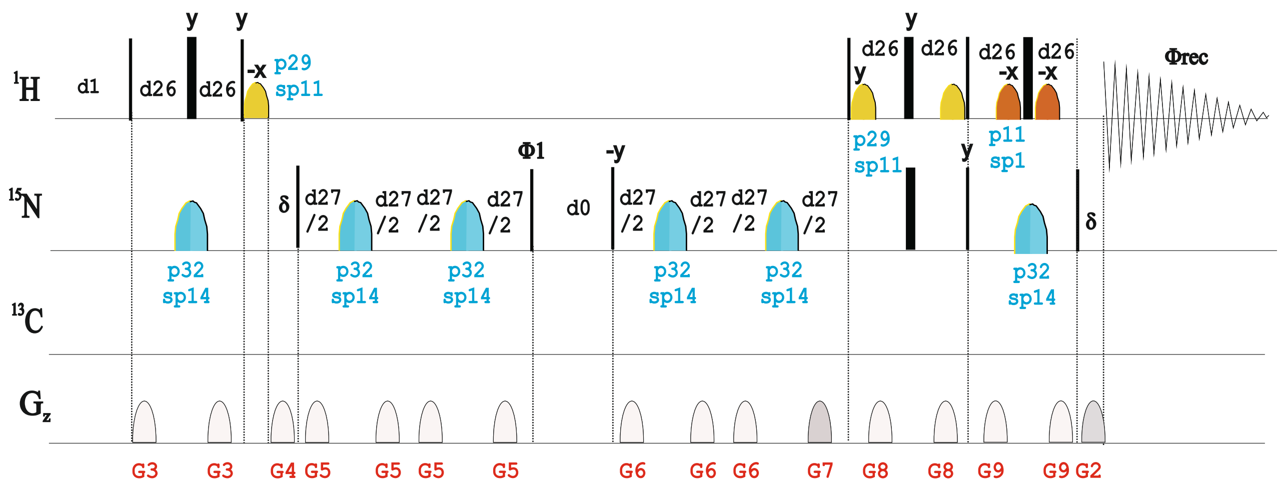


d1=1.5s
p11=90° water selective
=1ms (Squa100.1000)
d26=1/4J(NH)=2.25ms
d23=1/4J(NN)=15ms

na_hnncosygpphspwg



na_trhnncosygpphspwg



BRUKER
PULSE PROGRAM
CATALOGUE

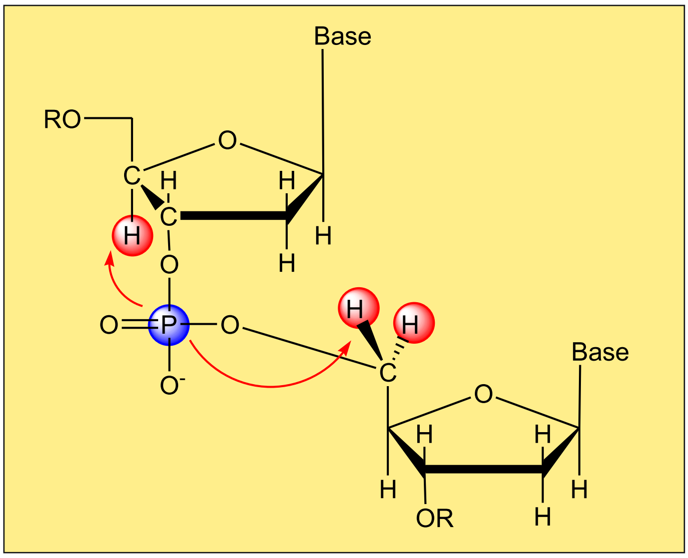
NMRGuide

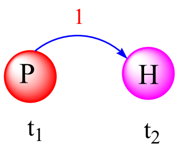
NUCLEIC-ACID NMR
2D & 3D HCP EXPERIMENTS

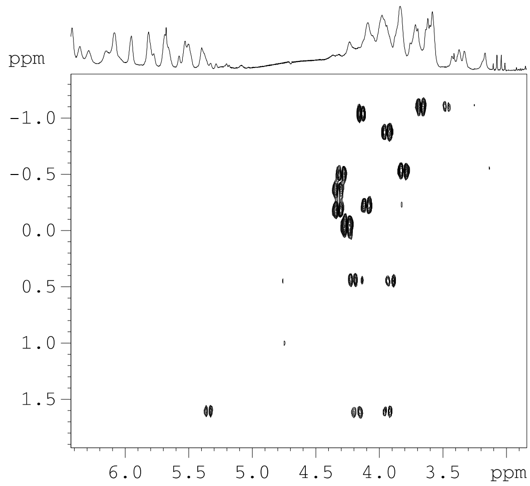
2D 31P-1H HETCOR or HP COSY Experiment

Experiment Description

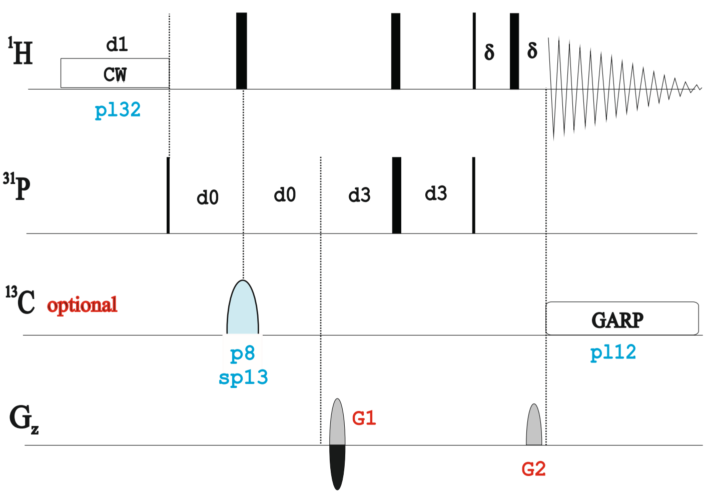
Experiment to achieve sequential backbone assignment via through-bond J(H3´(i)P(i)) and J(H5'/H5''(i+1)P(i)) connectivities in unlabeled and 13C-labeled NAs.
The pulse sequence uses a direct 31P-to-1H INEPT-like transfer and can be also driven in a constant-time mode..







na_xhcoetf3gp

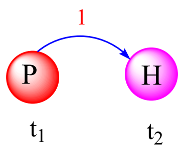


d1=1.5 s
d3=1/6J(PH)=16.6 ms
(optimized cnst2=10Hz with cnst11=6)
o3p=0 ppm
o2p=77 ppm

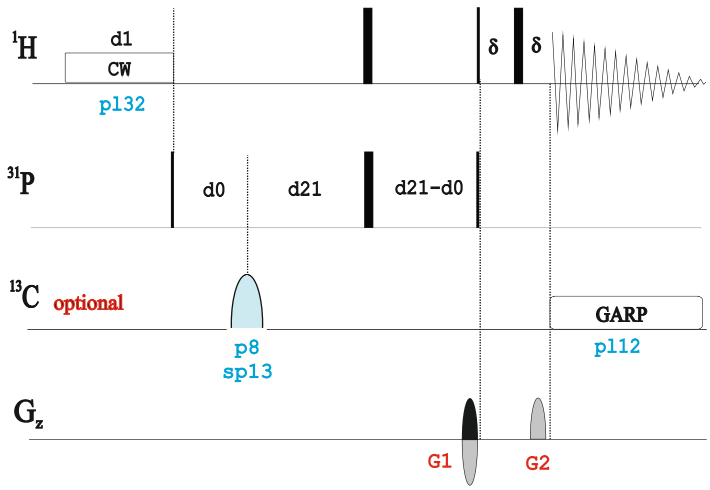
2D Constant-time HP COSY Experiment

Experiment Description:

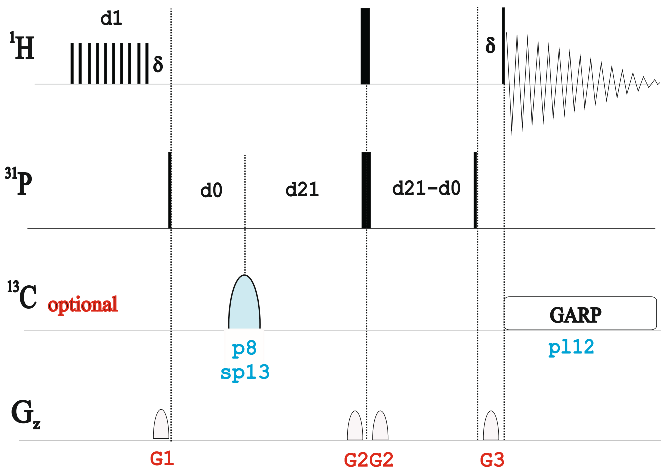
Constant-time version of the 1H-31P HETCOR or HP-COSY experiment

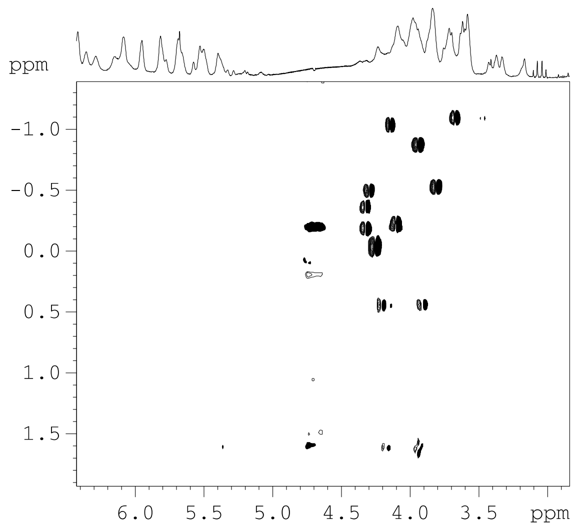


na_xhcoctetf3gp

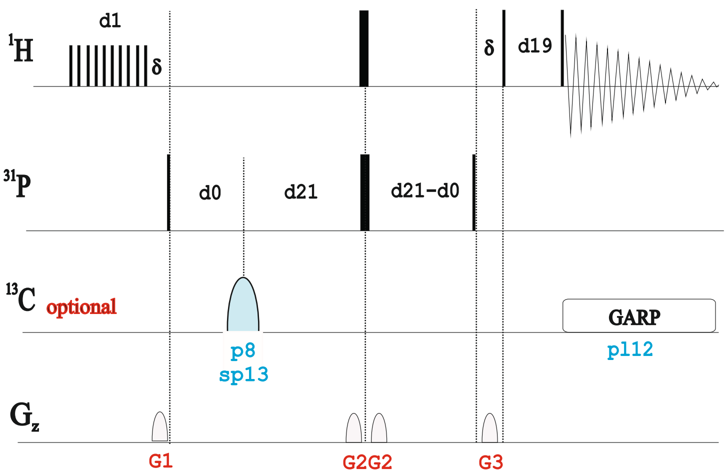


na_hpctco





na_hpctcojr

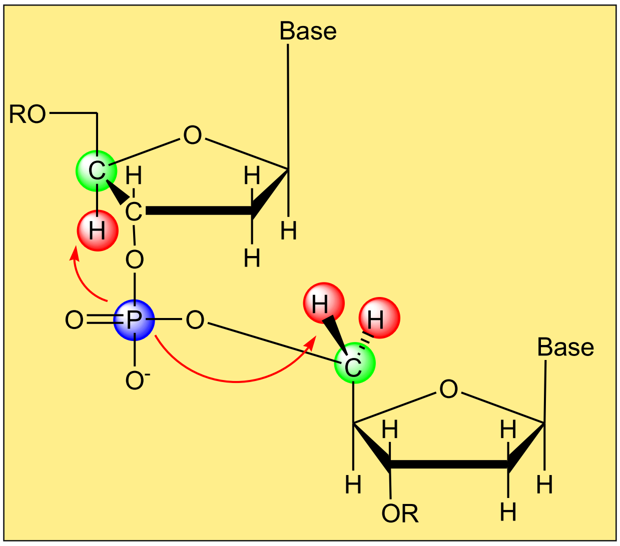


d1=1.5 s
d21=1/4J(PH)=22 ms
(optimized cnst4=11Hz)
o3p=0 ppm
o2p=77 ppm

3D CT PHCH Experiment

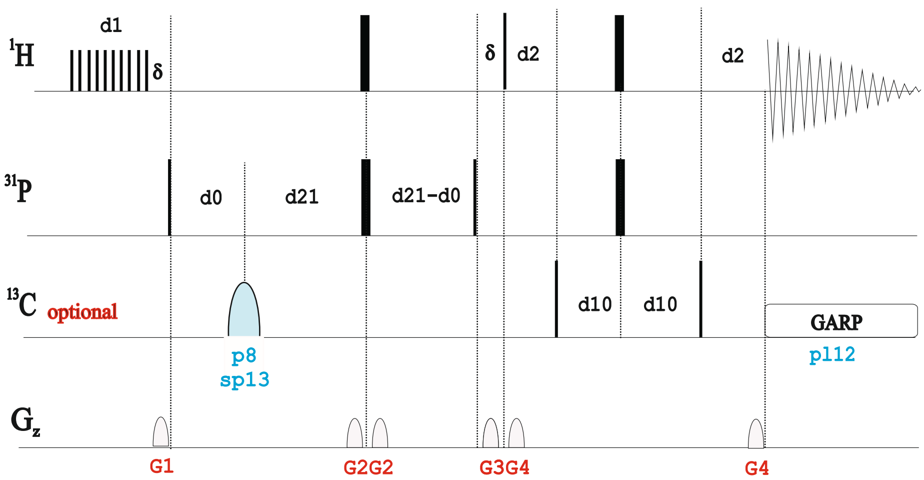
Experiment Description

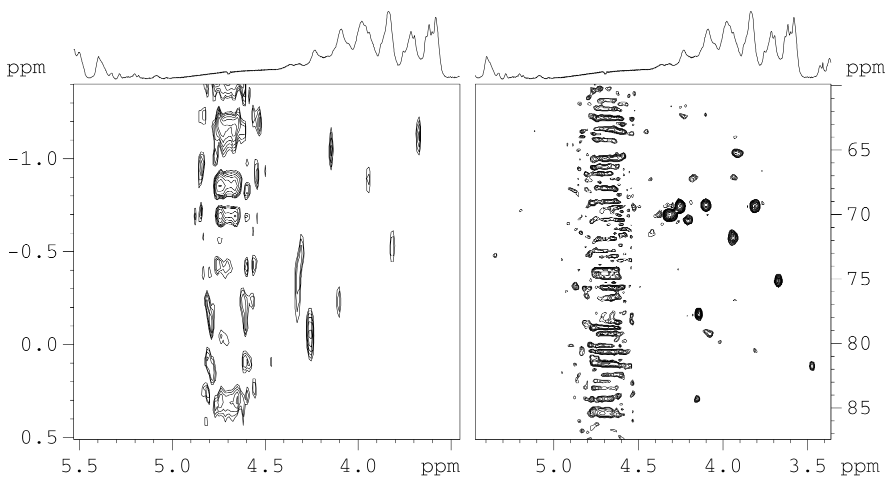
The 3D constant-time version of the P(H)CH experiment extends the backbone assignment of the HP experiment to C3'(i) and C5'(i+1) carbons by means a 1H-13C HMQC building block.



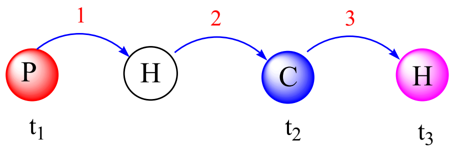
References:

1. T. Carlomagno, M. Hennig & J.R. Williamson, J. Biomol. NMR 22, 65-81 (2002)
2. G. Varani, F. Aboul-ela, F. Allain & C.C. Gubser, J. Biomol. NMR 5 315-320 (1995))

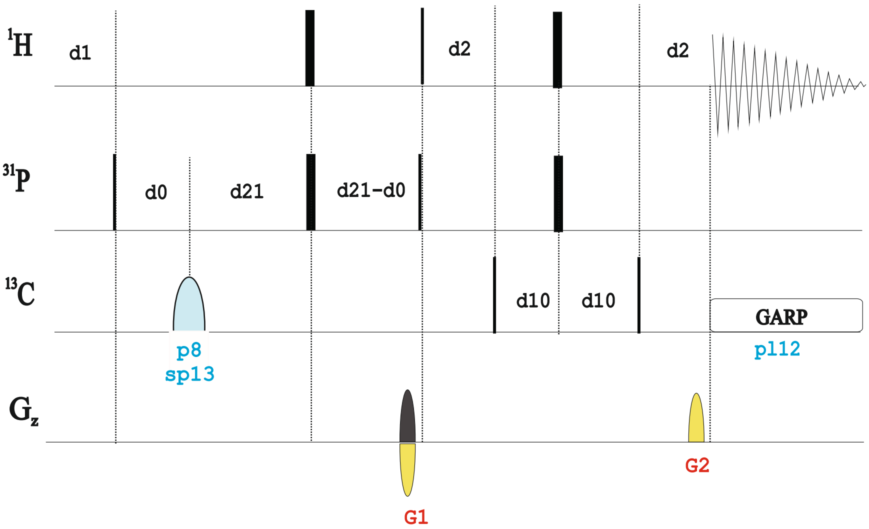




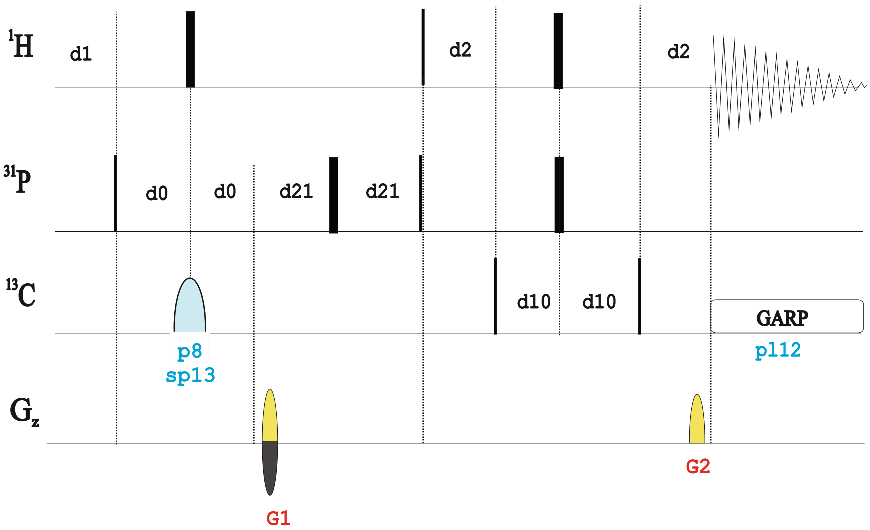
d1=1.5 s
d21=1/4J(PH)=22.7ms
(optimized cnst4=J(PH)=11Hz)
d2=1/2J(CH)=3.44ms
(optimized cnst2=J(CH)=145Hz)



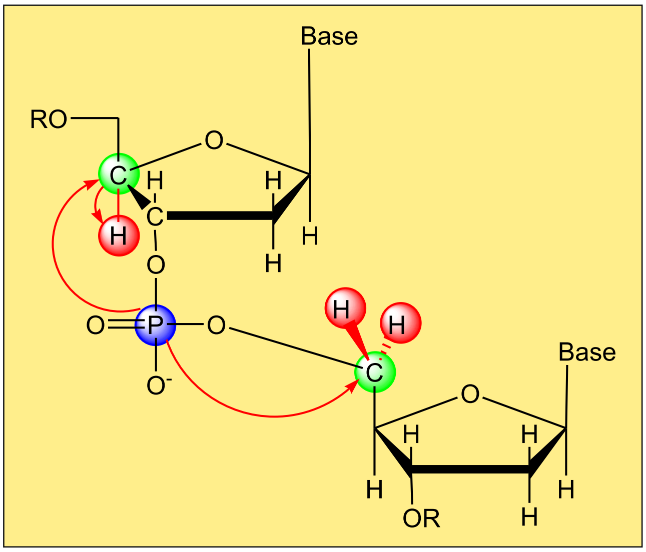
na_hpccoctetf3gp3d



na_hpccoetf3gp3d



2D P(C)H Experiment

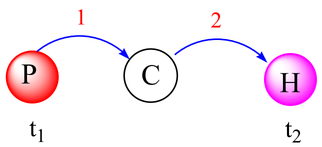


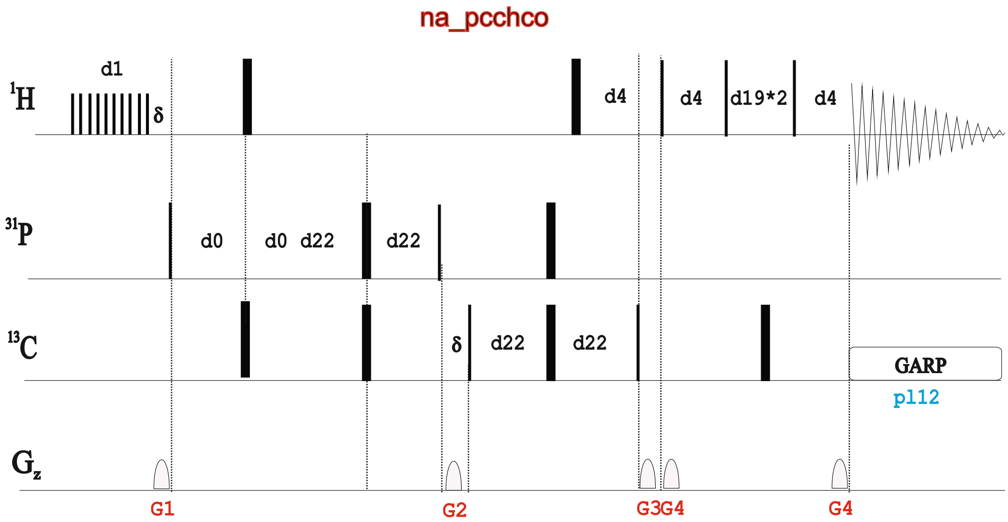
Experiment Description

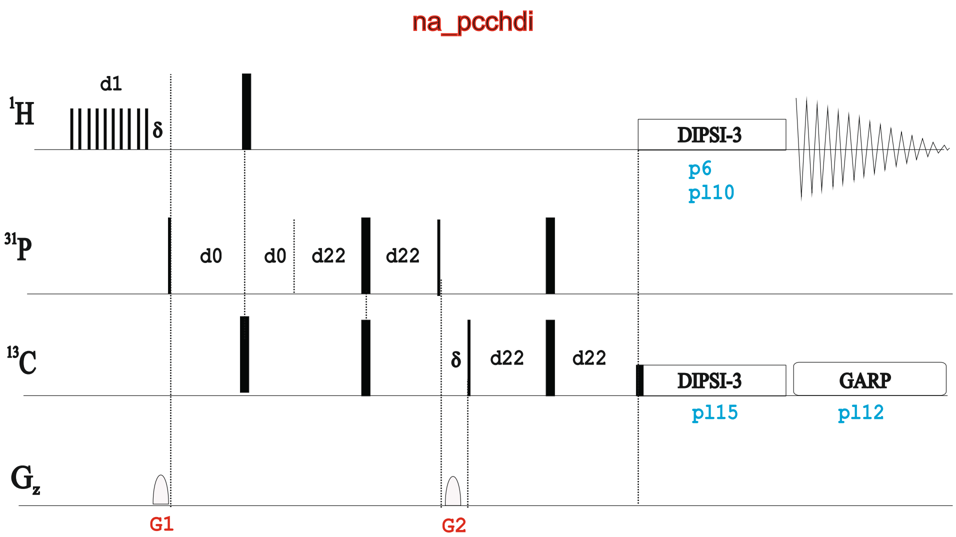
Experiment to achieve backbone PH assignment by through-bond coherence transfer P-to-C via J(C4'(i)-P(i)) and J(C4'(i+1)-p(i)) followed by an INEPT or cross-polarization C-to-H transfer.

References:

S.S. Wijmenga, H.A. Heus, H.A.E. Leeuw, H. Hoppe, M. van der Graaf & C.W. Hilbers, J. Biomol. NMR 5, 82-86 (1995)







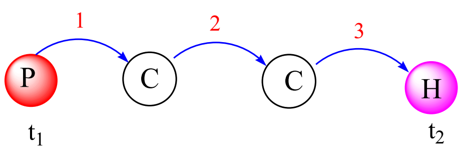
2D P(CC)H Experiment

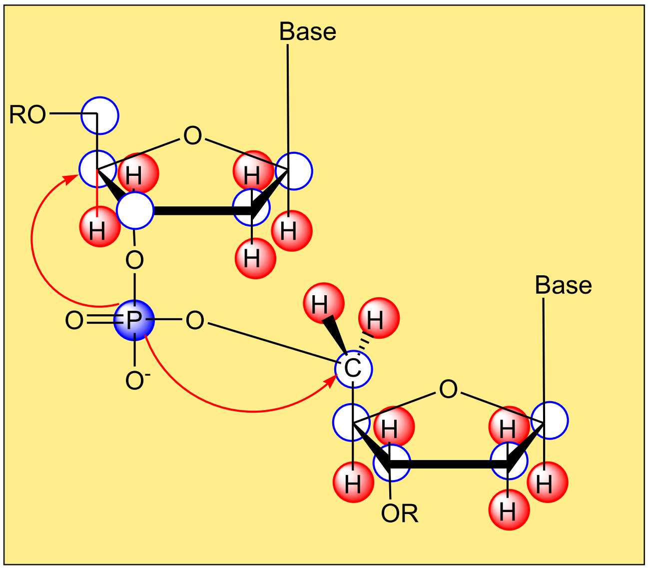
Experiment Description

Extension of the P(C)H experiment in which after the P-to-C transfer, a C-C TOCSY transfer relays the information through all carbons of the ribose ring and, finally, a C-to-P cross-polarization scheme allows to detect all ribose protons

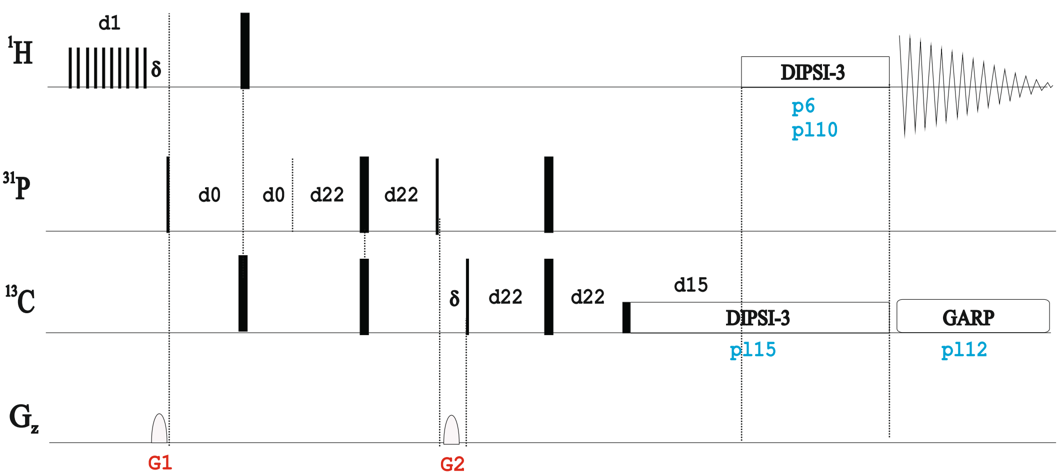
References:

S.S. Wijmenga, H.A. Heus, H.A.E. Leeuw, H. Hoppe, M. van der Graaf & C.W. Hilbers, J. Biomol. NMR 5, 82-86 (1995).



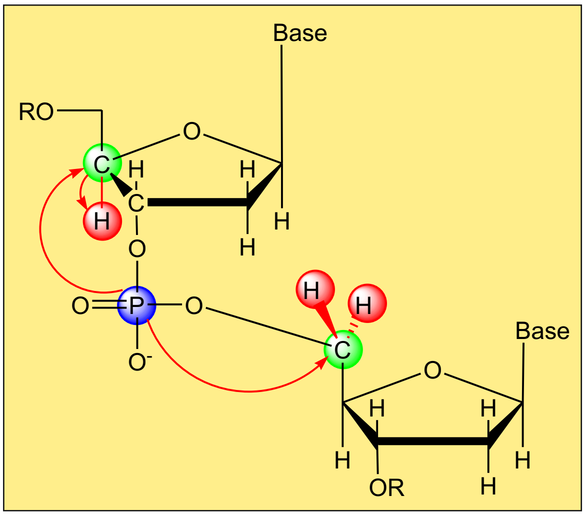


na_pcchdi2



d15: TOCSY mixing time (CC) [13 msec]
d22: 1/(4J(CP)) [12.5 msec]

3D HCP Experiment

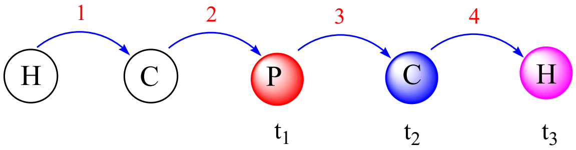


Experiment Description:

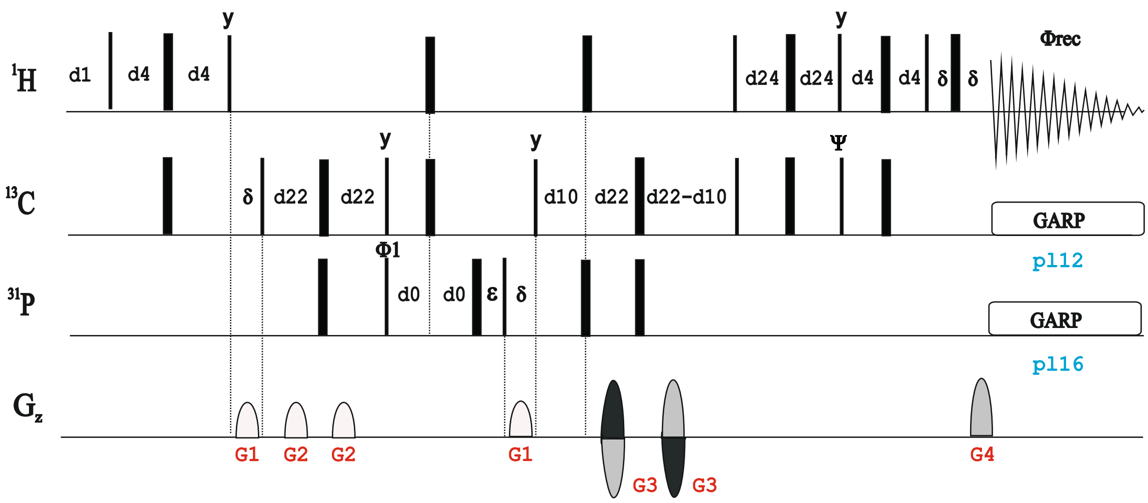
Out-and-back pulse scheme to correlate backbone P, C and H in a 3D experiment (94jacs6472).

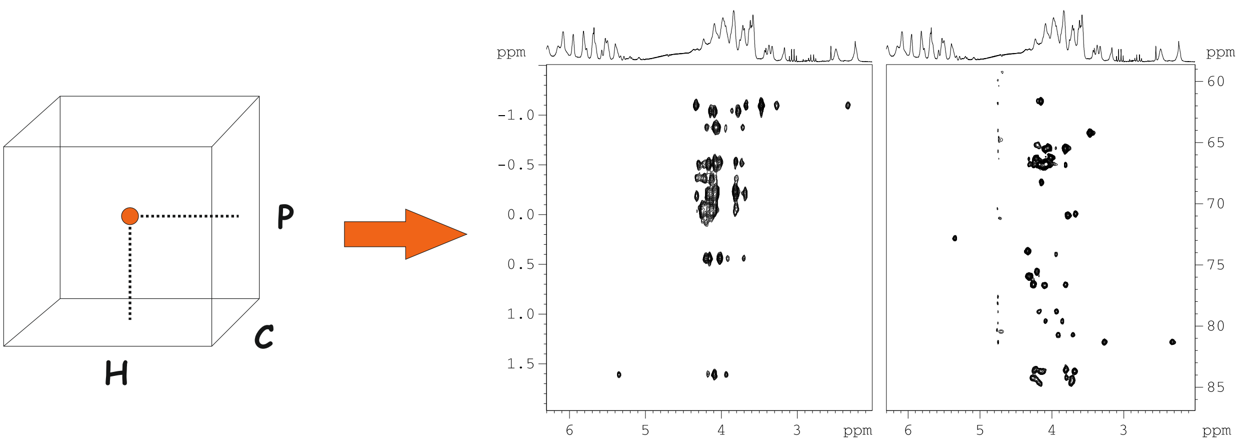
References:

J.P. Marino, H. Schwalbe, C. Anklin, W. Bermel, D.M. Crothers & C. Griesinger, J. Am. Chem. Soc. 116, 6472 - 6473 (1994)



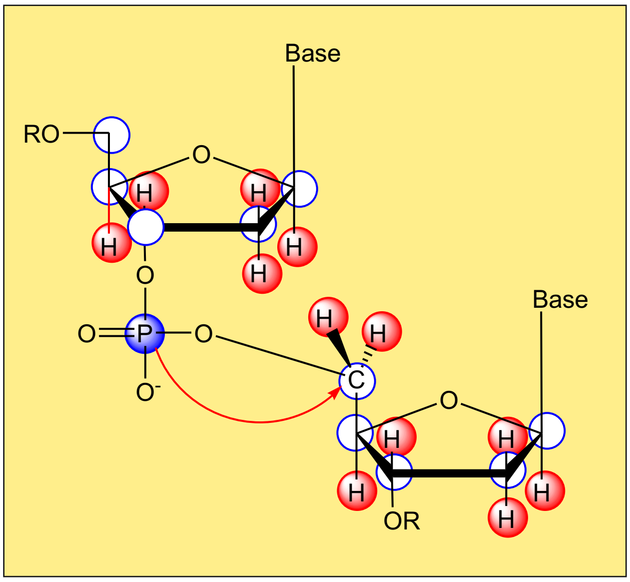
na_hcpetgpsi3d





d1=1.5 s
d4=1/4J(CH)=1.6 ms (optimized cnst2=J(CH)=155Hz)
d22=1/8J(CP)=12.5ms (optimized cnst5=J(CP)=10Hz)
d24=0.8 ms (optimized cnst11=8)

3D HCP-TOCSY Experiment



Experiment Description:

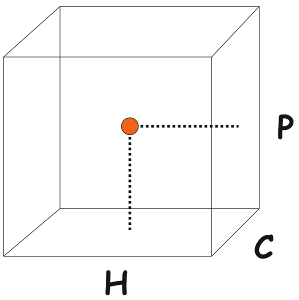
Variant of the 3D HCP experiment in which a CC TOCSY transfer has been included to involve all carbons and protons of the ribose ring (95JB87-5), in particular, the well dispersed anomeric H1' protons.

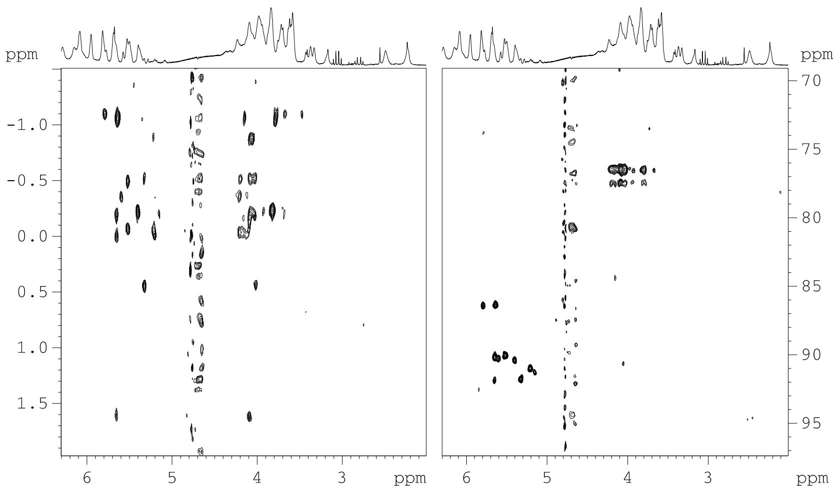
References:

J.P. Marino, H. Schwalbe, C. Anklin, W. Bermel, D.M. Crothers & C. Griesinger, J. Biomol. NMR 5, 87 - 92 (1995)

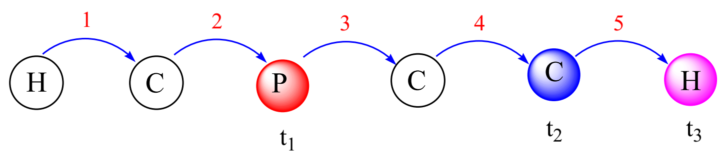
NMR Spectrum

The out-and-back experiment provides a 3D 1H, 13C, 31P correlation map

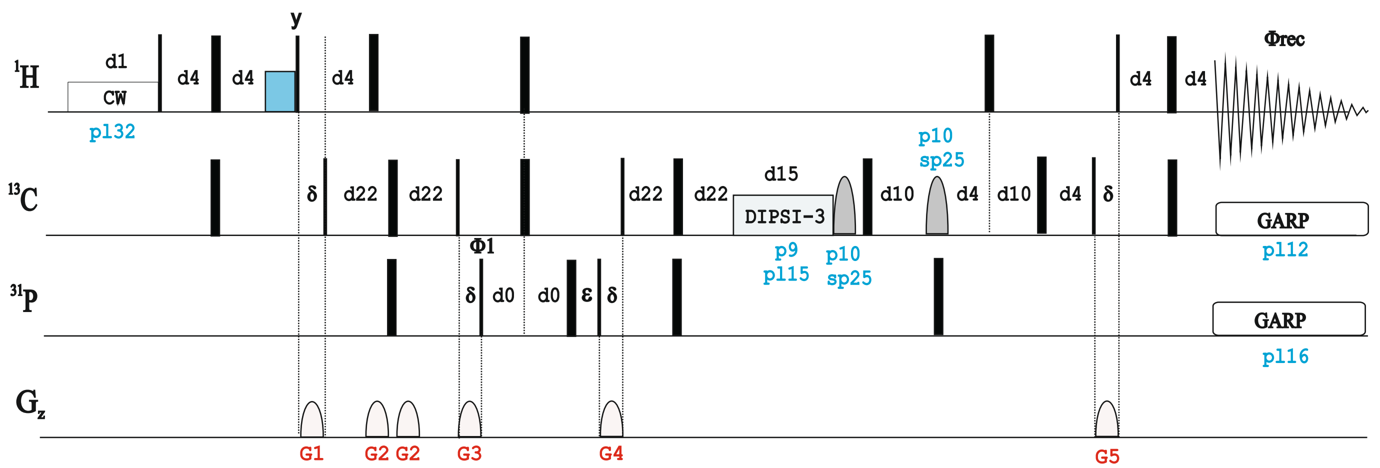




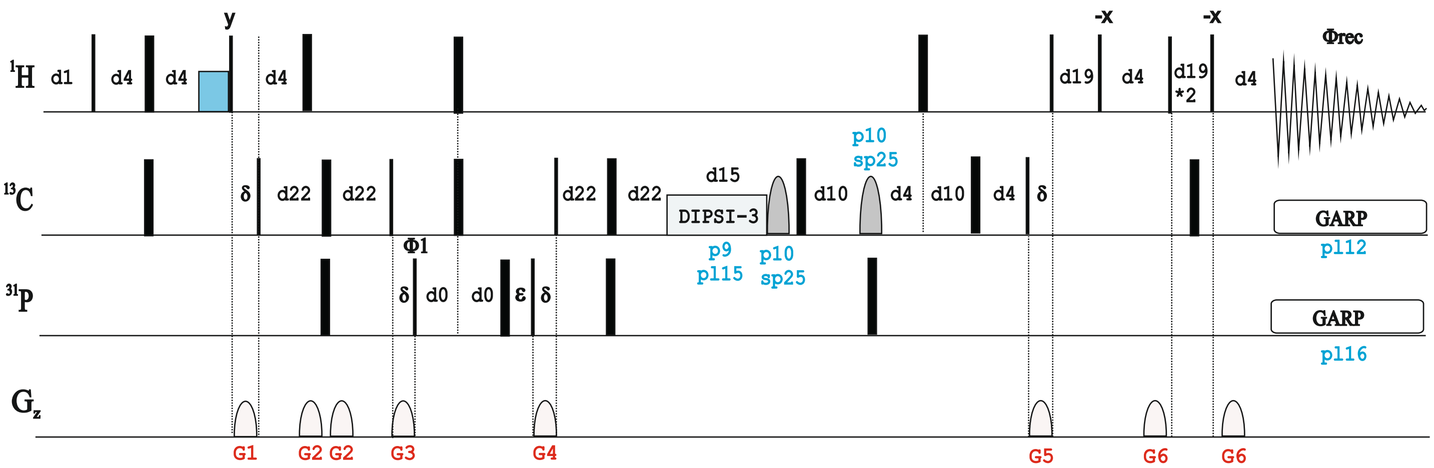
d1=1.5 s
d4=1/4J(CH)=1.6 ms
(optimized cnst2=J(CH)=155Hz)
d22=1/8J(CP)=12.5ms
(optimized cnst5=J(CP)=10Hz)
d15=CC TOCSY mixing=11 ms



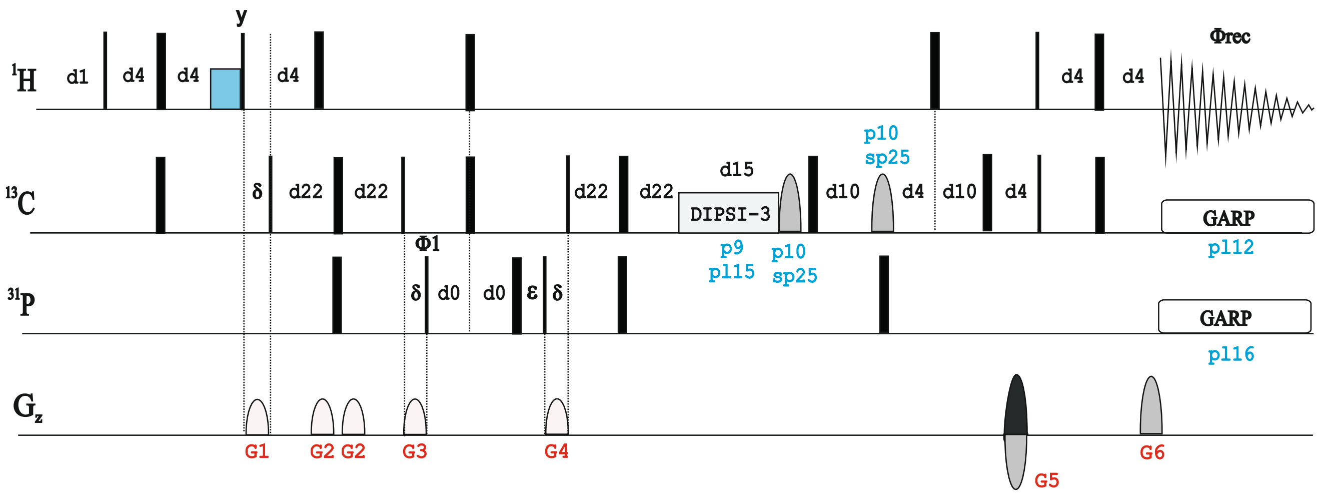
na_hcpdigp3d



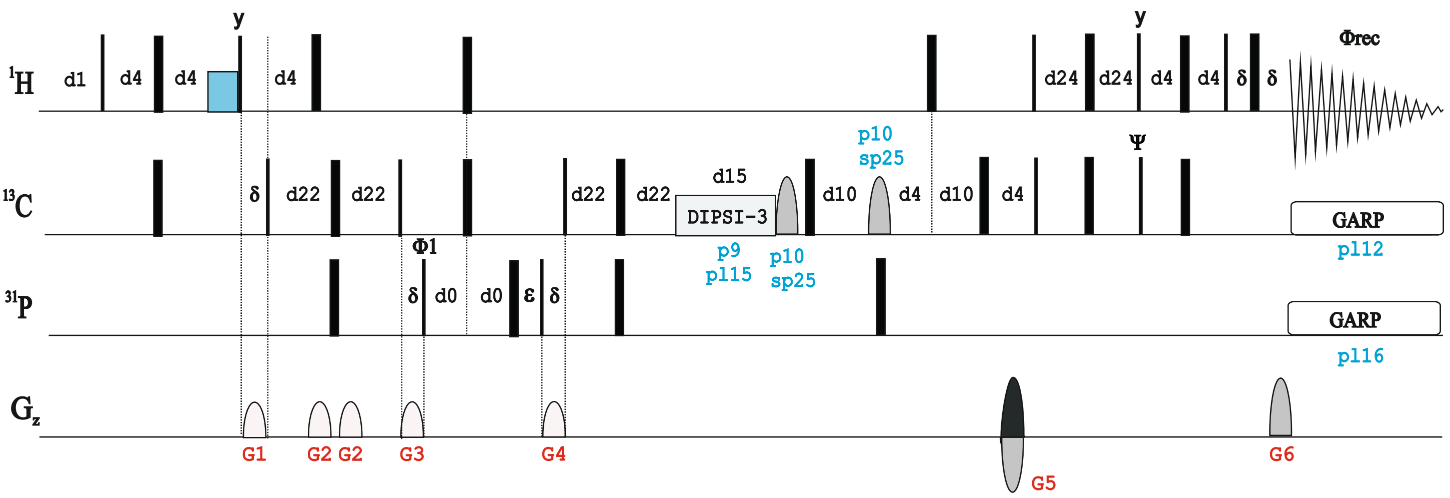
na_hcpdigpjr3d

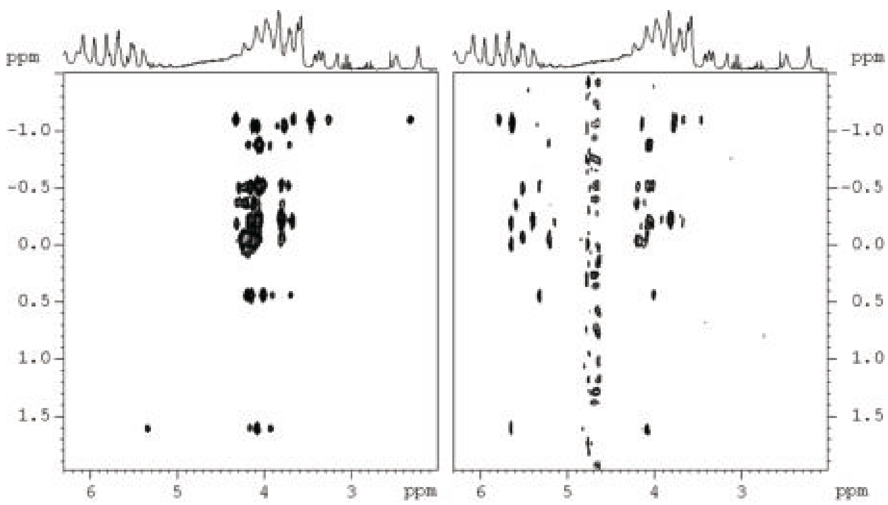


na_hcpdietgp3d



na_hcpdietgpsi3d





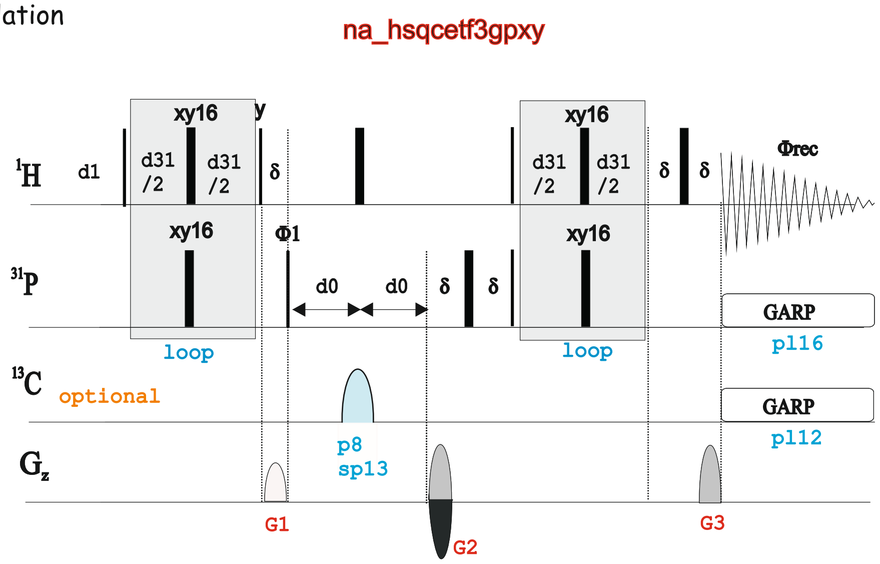
2D 1H-31P HSQC using CPMG-XY16 Experiment

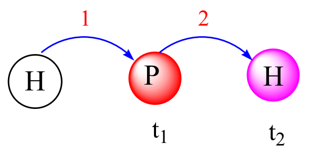
Experiment Description:

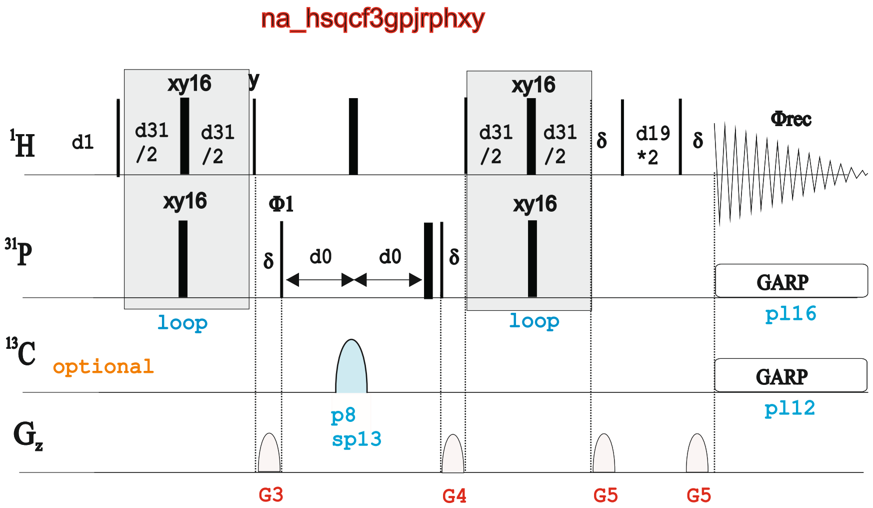
Modified version of the long-range optimized 1H-31P HSQC experiment in which a CPMG-XY16 pulse train is included to avoid 1H-1H mpdulation and exchange processes.

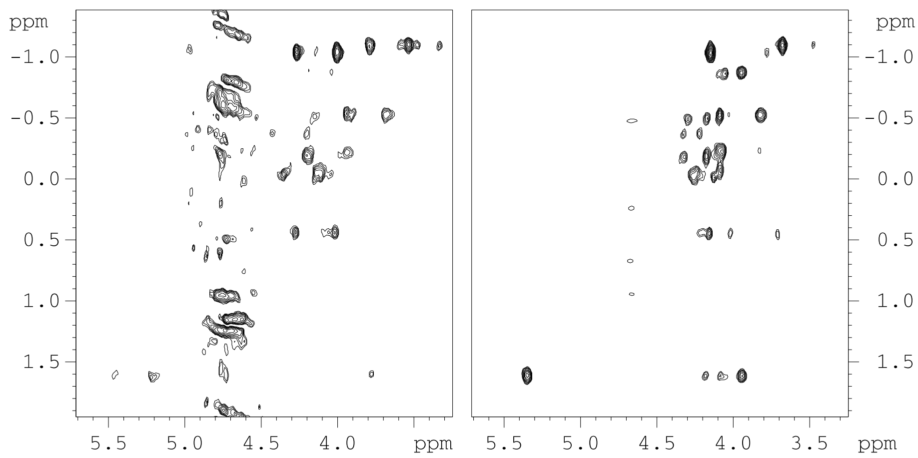
References:

B. Luy & J.P. Marino, J. Am. Chem. Soc. 123, 11306-11307 (2001)









hsqcetf3gp vs hsqcetf3gpxy

d1=1.5 s
d26=1/4J(PH)=12.5 ms
(optimized cnst4=J(PH)=J(20Hz)
d21=delay in CY16-CPMG=100us

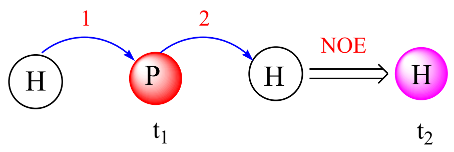
2D 1H-31P HSQC-NOESY using CPMG-XY16 Experiment

Experiment Description:

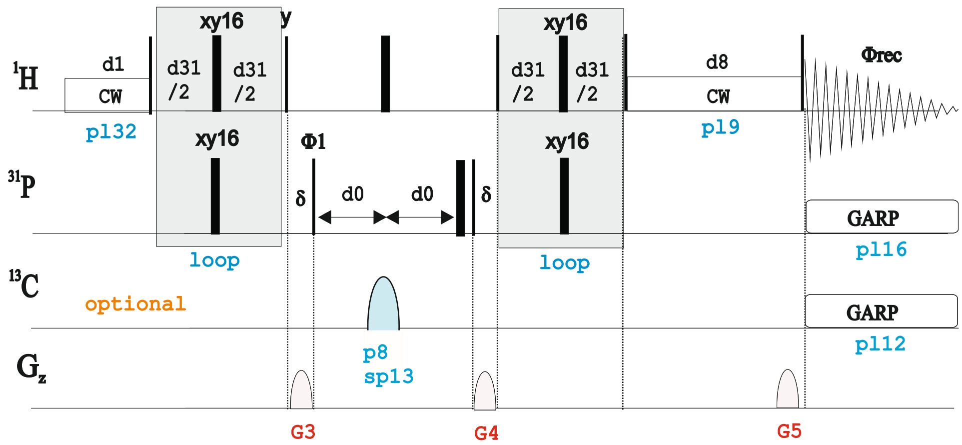
Modified HSQC-NOESY pulse scheme involving CPMG-XY16 transfer during the INEPT periods.

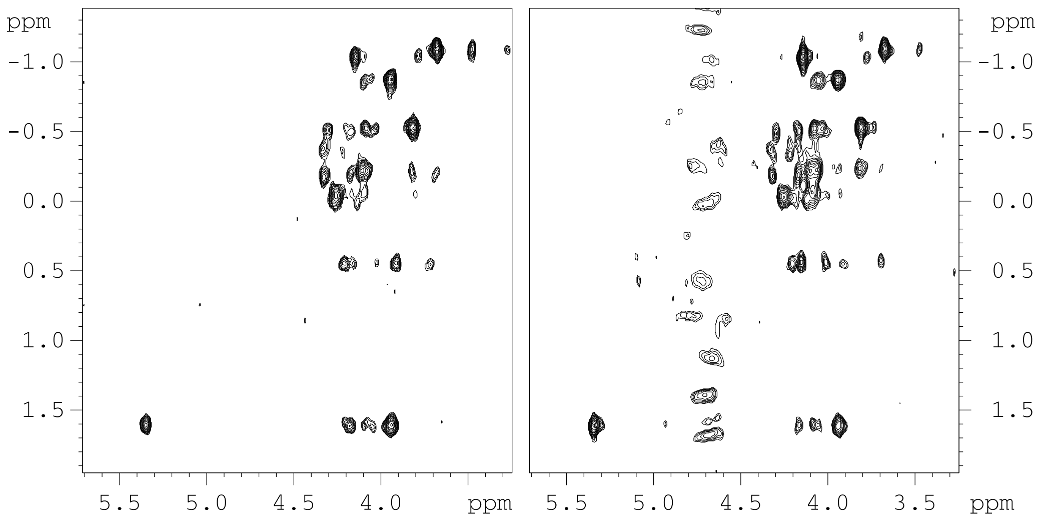
References:

B. Luy & J.P. Marino,
J. Am. Chem. Soc. 123,
11306-11307 (2001)



na_hsqcf3gpnophxy





hpdino vs hsqcetf3gpnoxy

d1=1.5 s
d26=1/4J(PH)=12.5ms
(optimized cnst4=J(PH)=20Hz)
d21=delay in CY16-CPMG=100us
d8=NOE mixing time

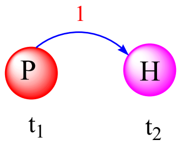
2D 1H-31P HeteroTOCSY Experiment

Experiment Description:

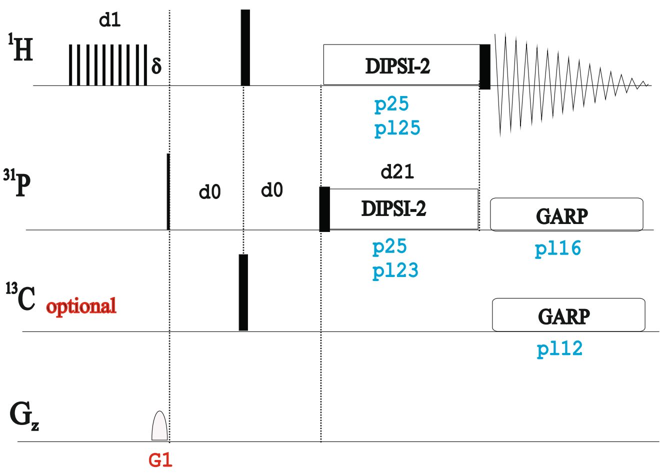
Experiment to correlate 31P and 1H chemical shifts that uses Heteronuclear cross-polarization for magnetization transfer from 31P to 1H via J(PH).

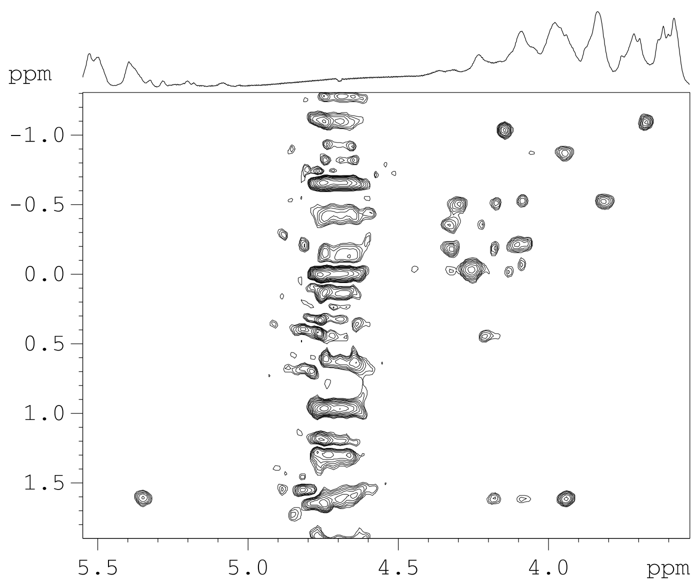
References:

G.W. Kellogg, J. Magn. Reson. 98, 176-182 (1992)



na_hpdi





d1=1.5 s
d21=1/6J(PH)=20 ms
(heteroTOCSY mixing)

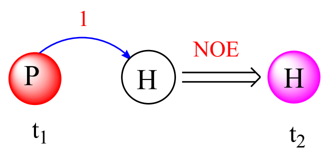
2D HeteroTOCSY-NOESY Experiment

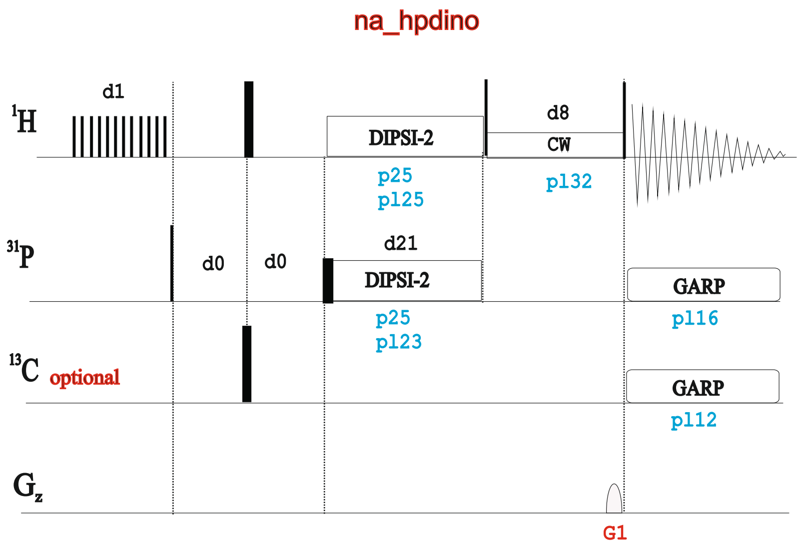
Experiment Description

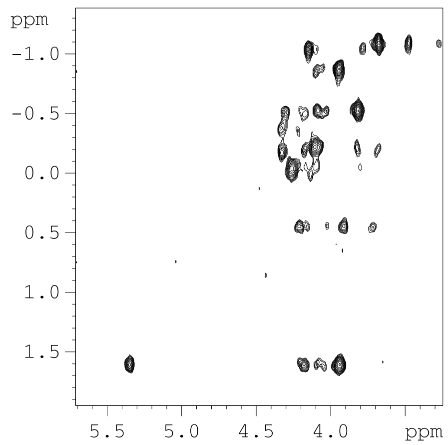
2D Cross-polarization version of a 31P-edited NOESY experiment.

References:

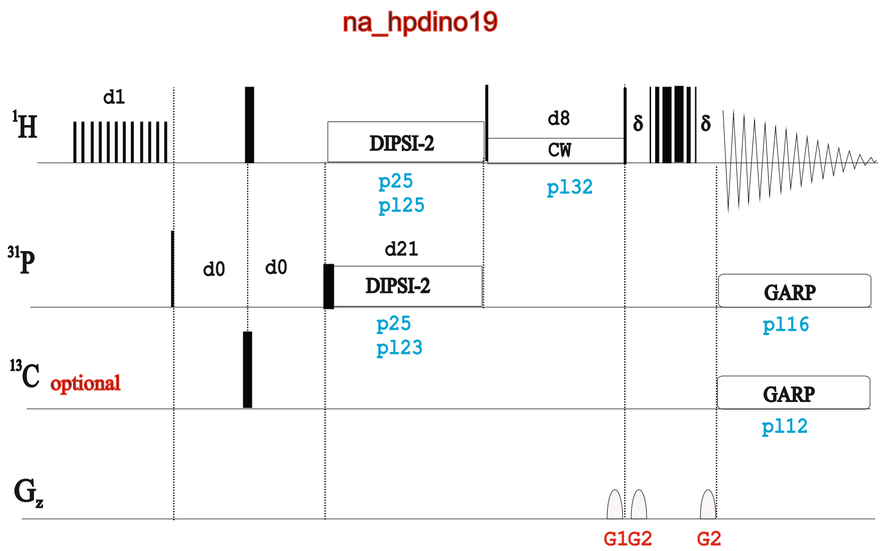
G.W. Kellogg, A.A. Szewczak & P.B. Moore, J. Am. Chem. Soc. 114, 2727-2728 (1992)







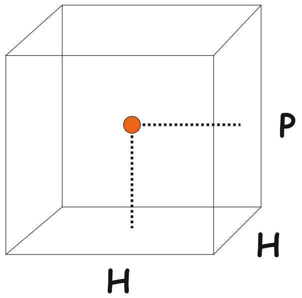
d1=1.5 s
d21=1/6J(PH)=20 ms
(heteroTOCSY mixing)



3D HeteroTOCSY-NOESY Experiment

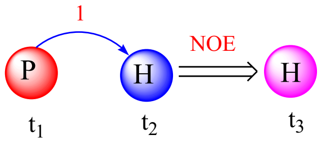
Experiment Description

3D Cross-polarization version of a P-edited 1H-1H NOESY experiment that provides a 3D P,H,H map.

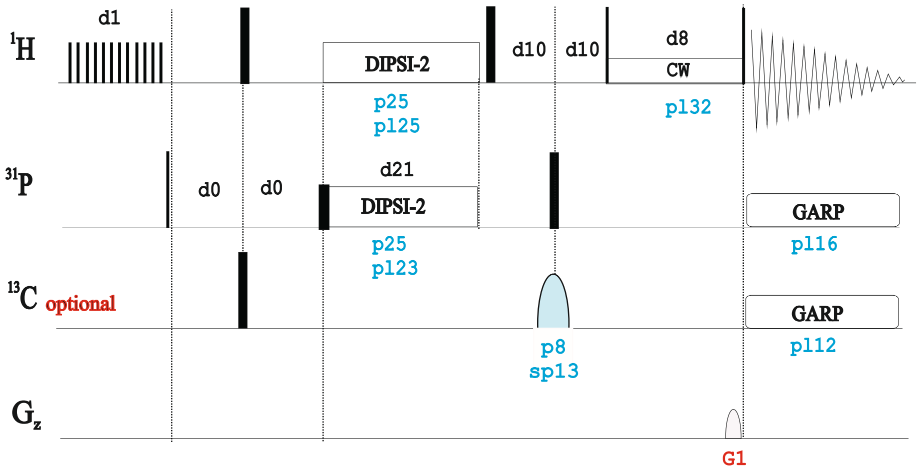


References:

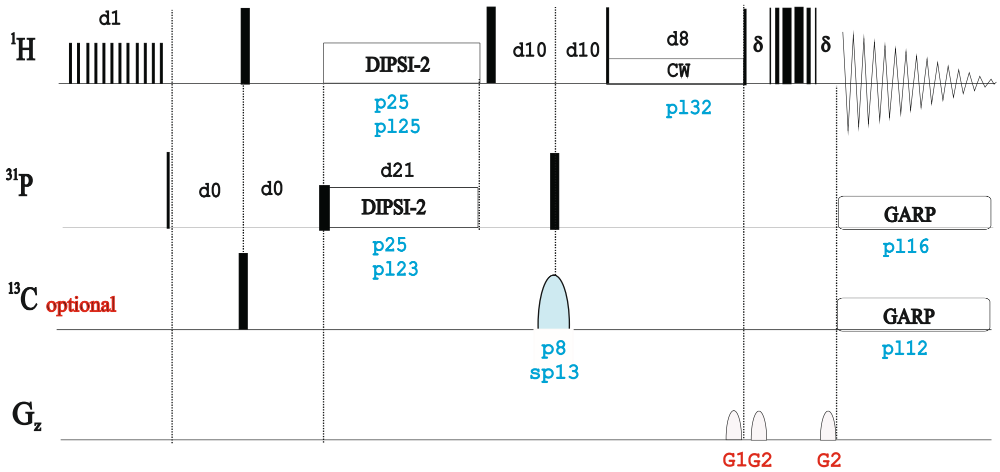
G.W. Kellogg & B.I. Schweitzer, J. Biomol. NMR 3, 577-595 (1993)



na_hpdino3d



na_hpdino193d



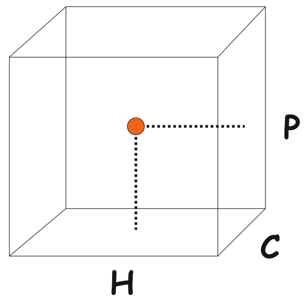
3D HeteroTOCSY-COSY Experiment

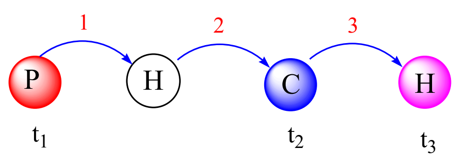
Experiment Description

3D version of the PHCH experiment that uses cross-polarization for P-to-H transfer. The experiment provides a 3D correlation P;C;H map.

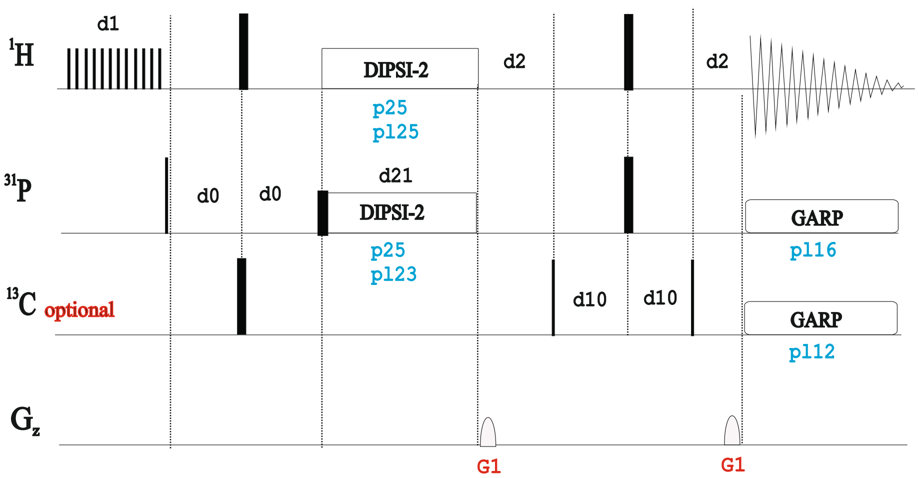
References:

G. Varani, F. Aboul-ela, F. Allain & C.C. Gubser,
J. Biomol. NMR 5 315-320 (1995)





na_hpdico3d



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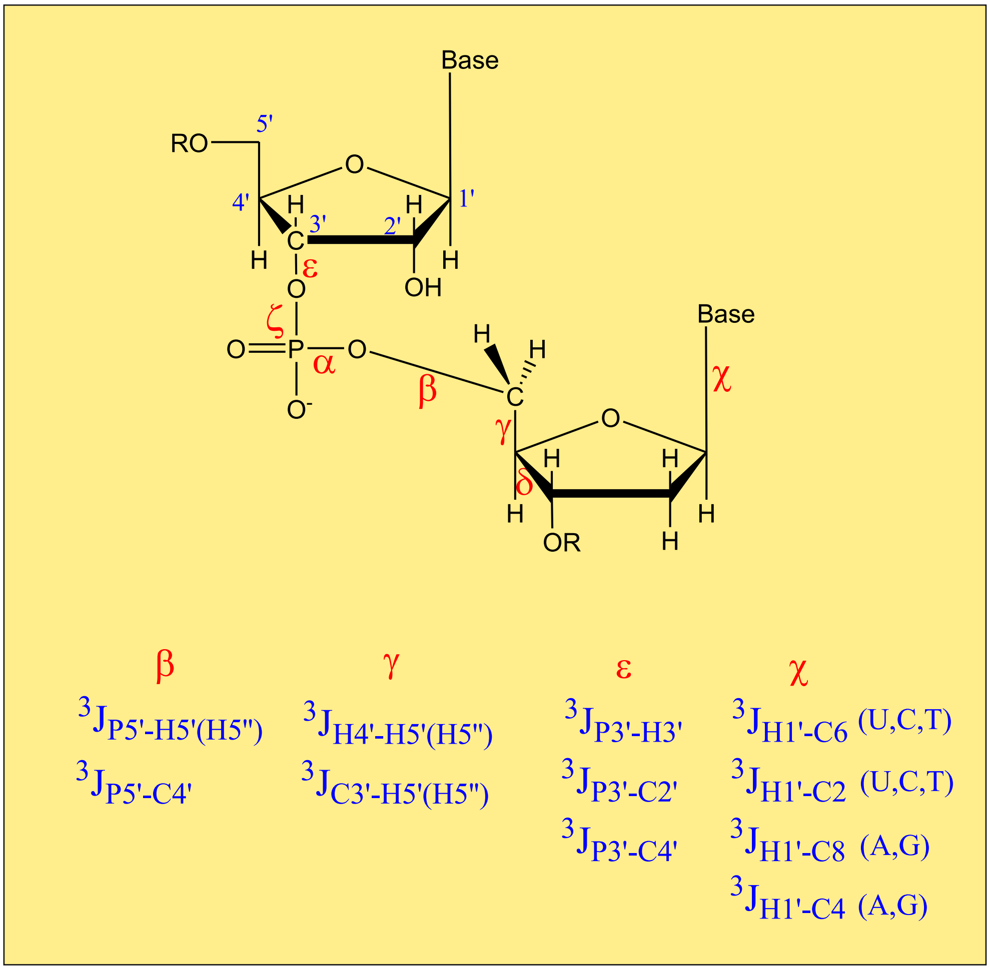
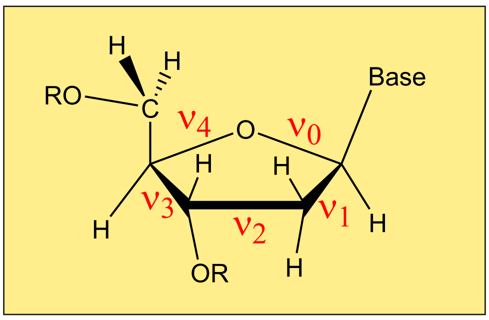




2D HSQC Experiment for measuring J(CH)

Experiment Description

Modified sensitivity-improved HSQC pulse scheme for the stereospecific assignment of H5'/H5'' diastereotopic protons in NAs by measurement o fhomonuclear J(H4'H5') and heteronuclear J(C4'H5') coupling constants.

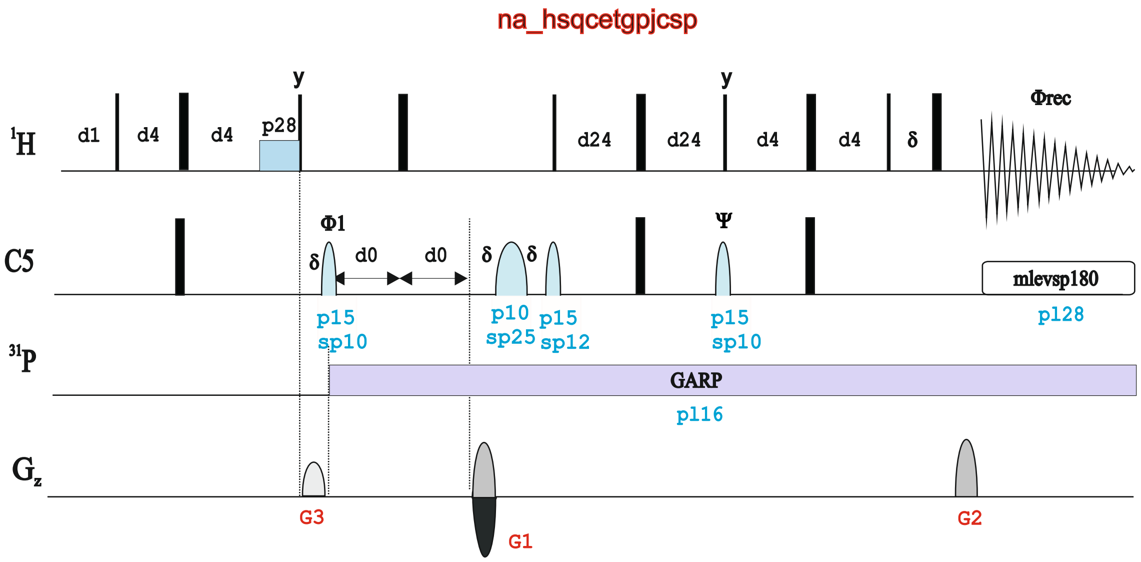
Also useful for measurement of J(C2'H1') via N in 13C/15N labeled Nas

References:

J.P. Marino, H. Schwalbe, S.J. Glaser, C. Griesinger,J. Am. Chem. Soc. 118, 4388 - 4395 (1996) .

Related Experiments:

Also see the original 2D HSQC experiment.



p15=2 ms (Q5/Q5tr)
p10=2 ms (Q3)
pl28= Selective C5 decoupling

3D H(C)CH-E.COSY Experiment

Experiment Description:

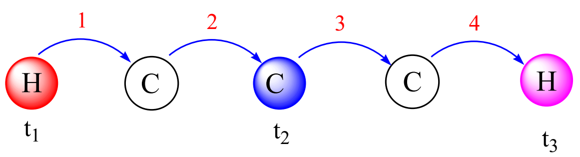
Modified HCCH-COSY pulse scheme to measure J(CH) in ribose rings.

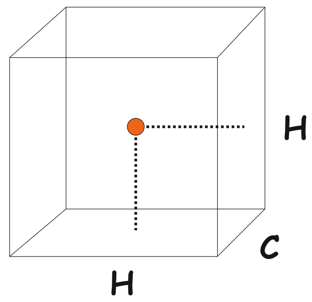
References:

1. L.E. Kay, G.Y. Xu, A.U. Singer, D.R. Muhandiram & J. D. Forman-Kay J. Magn. Reson. B 101, 333 - 337 (1993)
2. H. Schwalbe, J.P. Marino, G.C. King, R. Wechselberger, W. Bermel & C. Griesinger, J. Biomol. NMR 4, 631 - 644 (1994)

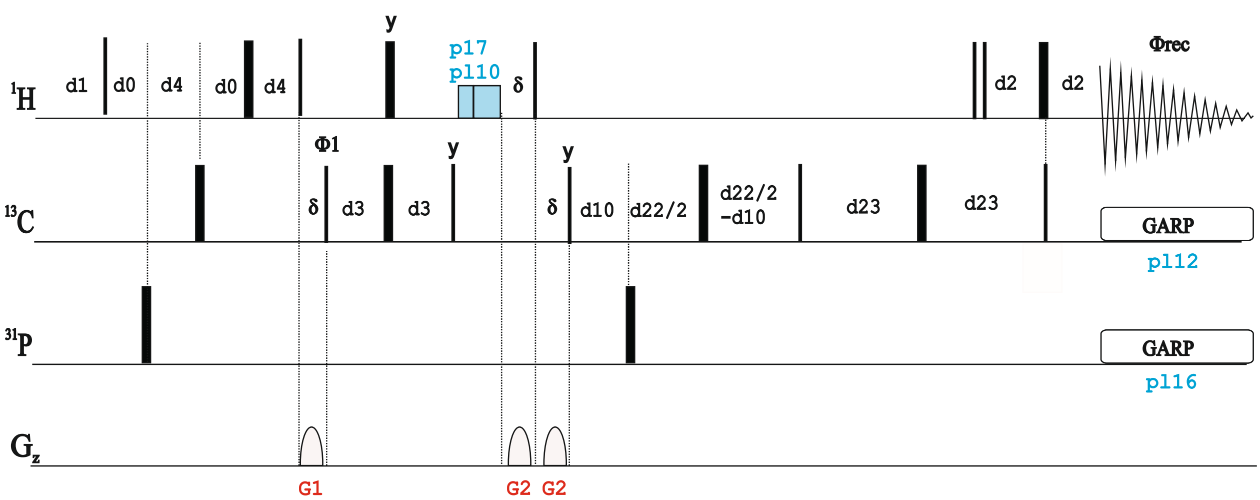
Related Experiments:

Also see other HCCH-type experiments





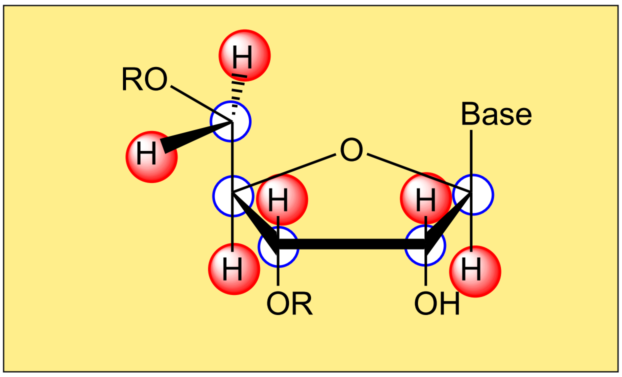
na_hcchecgp3d



d2=1/2J(CH)
d4=1/4J(CH)=1.6ms
d3=1/4J(CH)
d23=1/8J(CC)=3.1ms
d22=Constant-time C period.
For all correlations 3/4J(CC)=18.8ms
For C1' and C5' 1/2J(CC)=12.5ms

3D H(C)CH-TOCSY Experiment

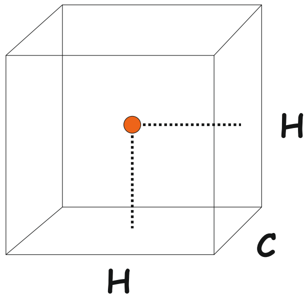
Experiment Description

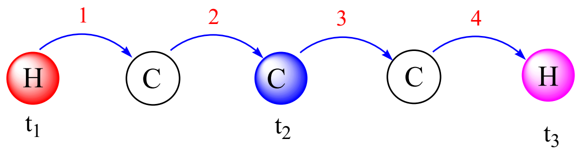


Specific HCCH-TOCSY experiment to identify all 1H and 13C nuclei belonging to the same sugar ring in 13C-labeled NAs. Alternative to classical COSY and TOCSY experiment. ALso see other HCCH-COSY and HCCH-TOCSY experiments.

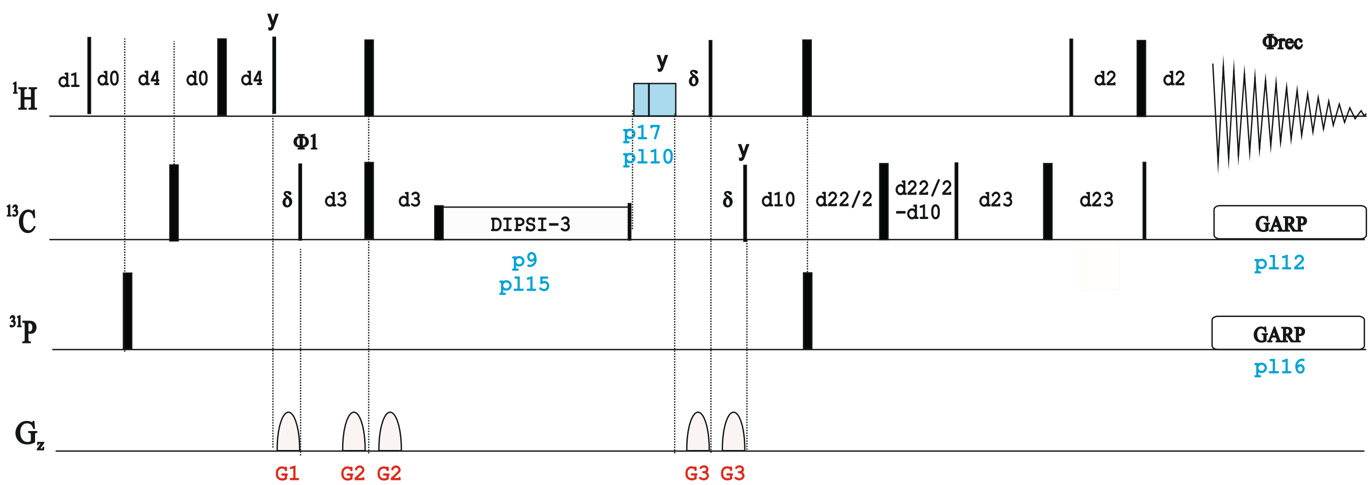
References:

L.E. Kay, G.Y. Xu, A.U. Singer, D.R. Muhandiram & J. D. Forman-Kay J. Magn. Reson. B 101, 333 - 337 (1993)
2. H. Schwalbe, J.P. Marino, S.J. Glaser & C.Griesinger, J. Am. Chem. Soc. 117, 7251 - 7252 (1995)
3. J.P. Marino, H. Schwalbe, S.J. Glaser & C.Griesinger, J. Am. Chem. Soc. 118, 4388 - 4395 (1996)
4. S.J. Glaser, H. Schwalbe, J.P. Marino & C. Griesinger, J. Magn. Res. B 112, 160 - 180 (1996).





na_hcchfwdigp3d



d2=1/2J(CH)
d4=1/4J(CH)=1.6ms
d3=1/4J(CH)
d23=1/8J(CC)=3.1ms
d22=Constant-time C period.
For all correlations 3/4J(CC)=18.8ms
For C1' and C5' 1/2J(CC)=12.5ms

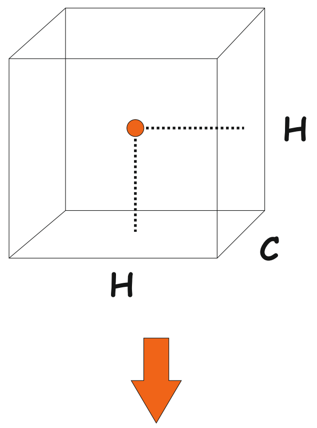
3D H(C)CH-TOCSY E.COSY Experiment

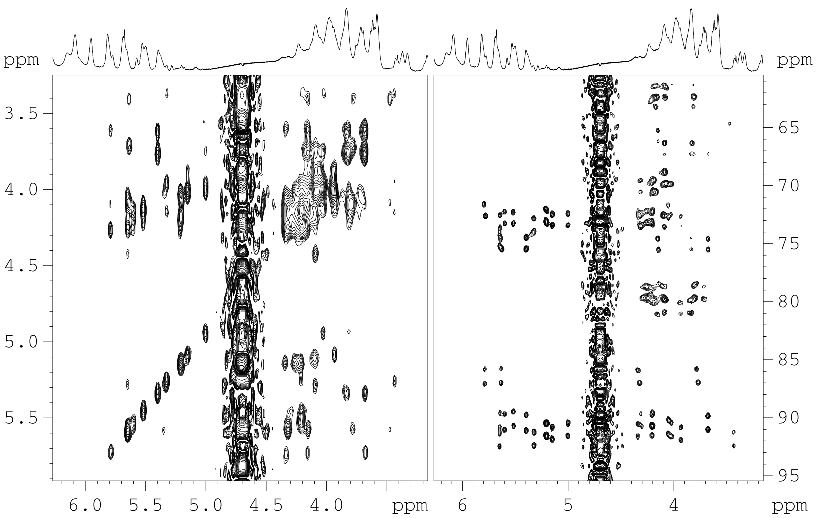
Experiment Description:

E.COSY version of the HCCH-TOCSY experiment to measure J(H4'H5') coupling constants (96jacs4388)

References:

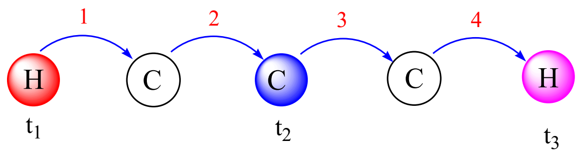
L.E. Kay, G.Y. Xu, A.U. Singer, D.R. Muhandiram & J. D. Forman-Kay J. Magn. Reson. B 101, 333 - 337 (1993)
H. Schwalbe, J.P. Marino, S.J. Glaser & C.Griesinger, J. Am. Chem. Soc. 117, 7251 - 7252 (1995)
J.P. Marino, H. Schwalbe, S.J. Glaser & C.Griesinger, J. Am. Chem. Soc. 118, 4388 - 4395 (1996)
S.J. Glaser, H. Schwalbe, J.P. Marino & C. Griesinger, J. Magn. Res. B 112, 160 - 180 (1996)



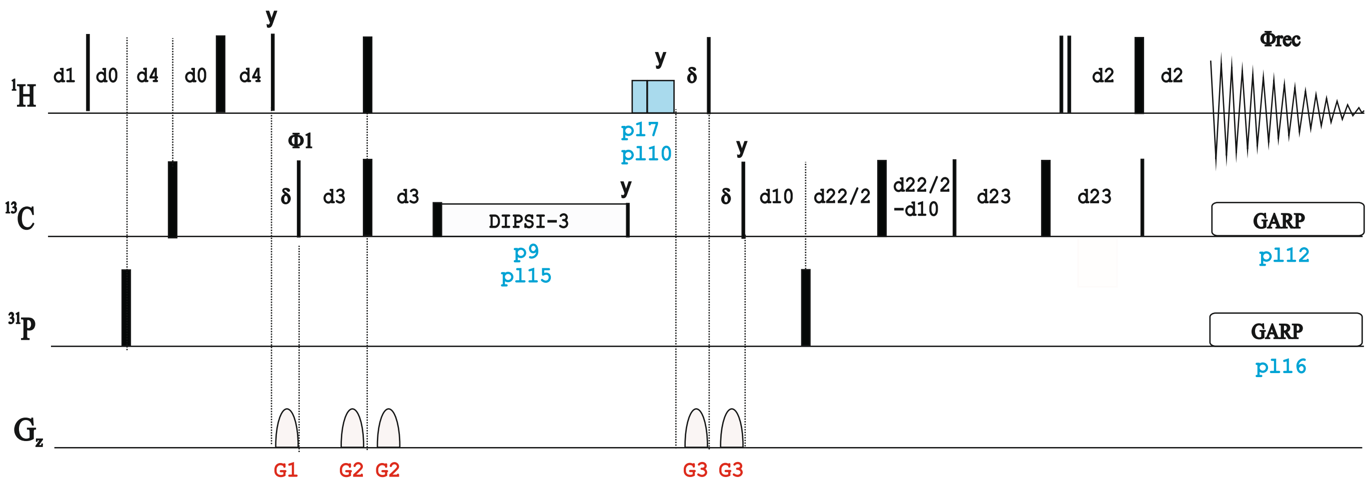


E.COSY pattern in the C dimension of the 2D HC plane

d1=1.5s
d3=1/4J(CH)=1.55ms
d4=1/4J(CH)=1.56ms
(optimized cnst2=160Hz)
d22=CT(C)=7.6ms
d23=1/8J(CC)=3.1ms
(optimized for cnst8=38Hz)
l1=2 for CC TOCSY=9.2ms using p9=26us



na_hcchfwdiecgp3d



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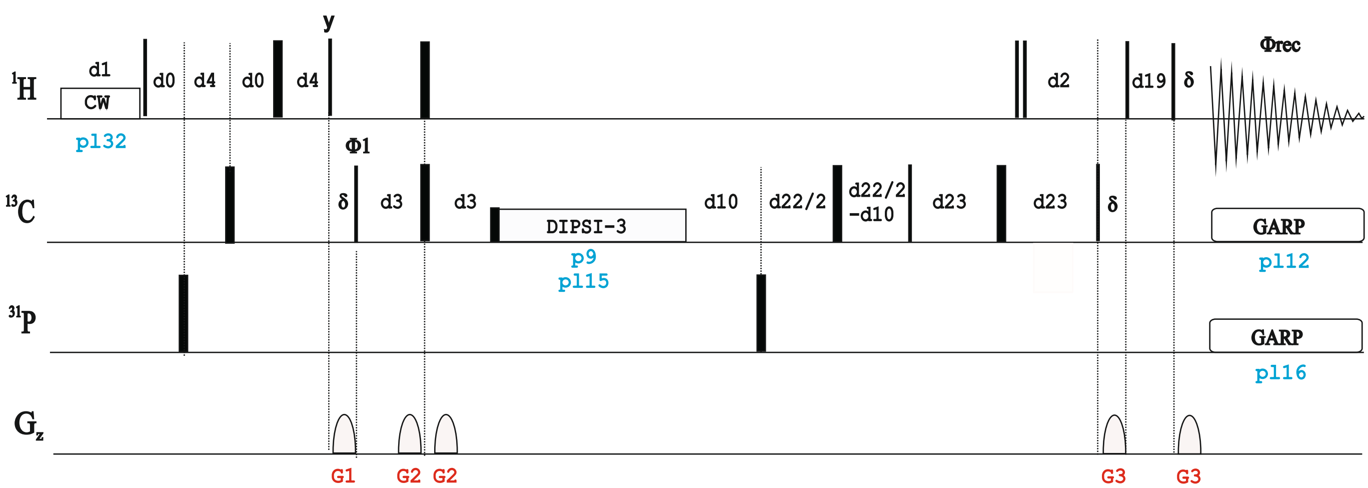


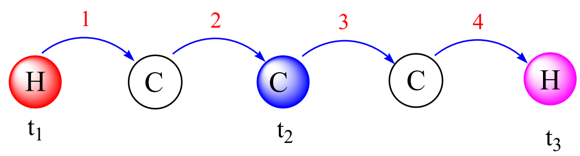
Forward-directed quantitative 3D H(C)CH-TOCSY Experiment

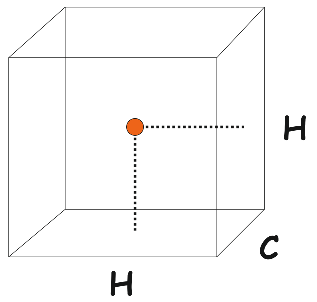
Experiment Description:

Modified HCCH-TOCSY version to measure J(HH) and J(CH) coupling constants

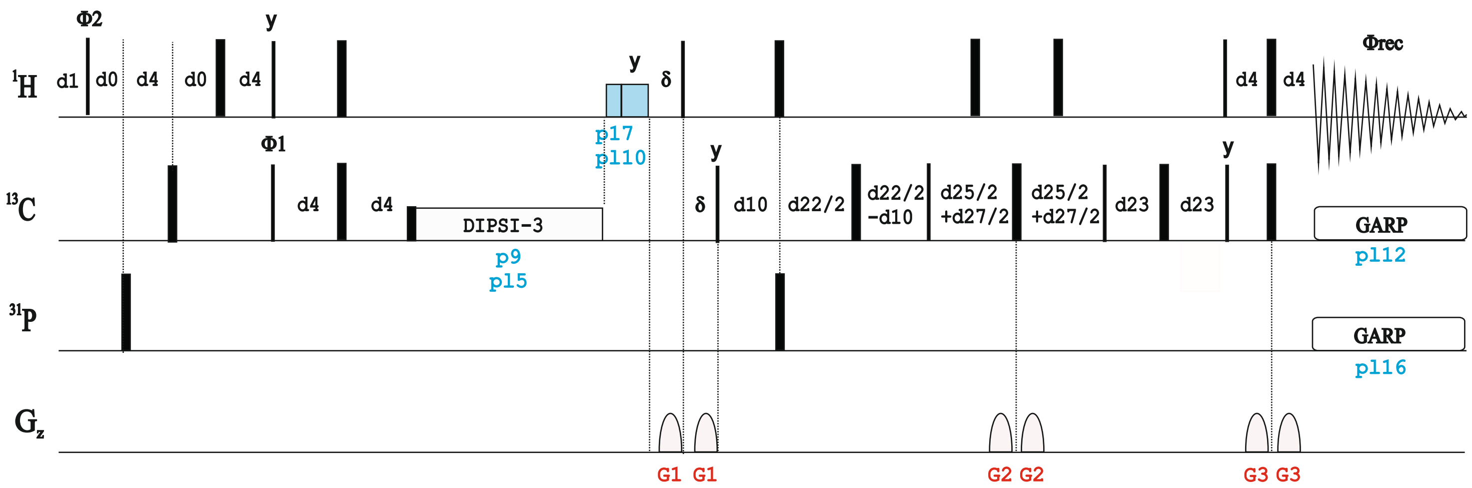
References:

1. I.C. Felli, C. Richter, C. Griesinger & H. Schwalbe, J. Am. Chem. Soc. 121, 1956 - 1957 (1999)
2. C. Richter, C. Griesinger, I.C. Felli, P.T. Cole, G. Varani & H.Schwalbe, J. Bimol. NMR 15, 241 - 250 (1999)





na_ghcchfwdigp3d



d4=1/4J(CH)=1.6ms
d23=1/8J(CC)=3.1ms
d22=Constant-time C period.
For all correlations 3/4J(CC)=18.8ms
For C1' and C5' 1/2J(CC)=12.5ms
d25=development of cross-correlated relaxation=25ms

For reference experiment d27=1/2J(CH)=3.1ms
For cross-peak experiment d27=0

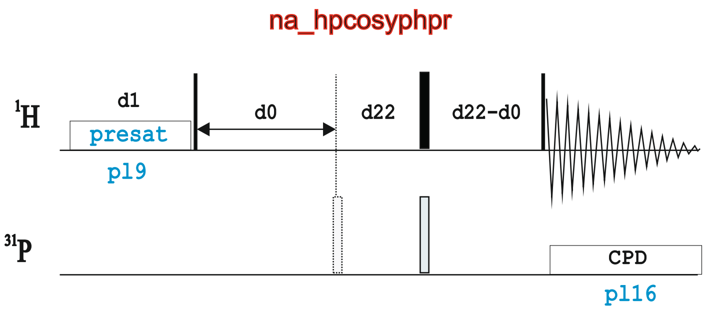
2D Constant-time HH-{31P} COSY Experiment

Experiment Description

Constant-time 1H-1H COSY experiment for the measurement of J(H3-P) coupling constants in NAs (98jmr164-134). Two experiments are recorded varying the position of the 180° 31P pulse.

References:

G.M. Clore, E.C. Murphy, A.M. Gronenborn & A.Bax, J. Magn. Res. 134, 164 - 167 (1998)



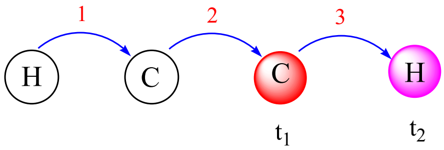
d22: constant time delay T	[25 msec]

2D quantitative HC(P) Experiment

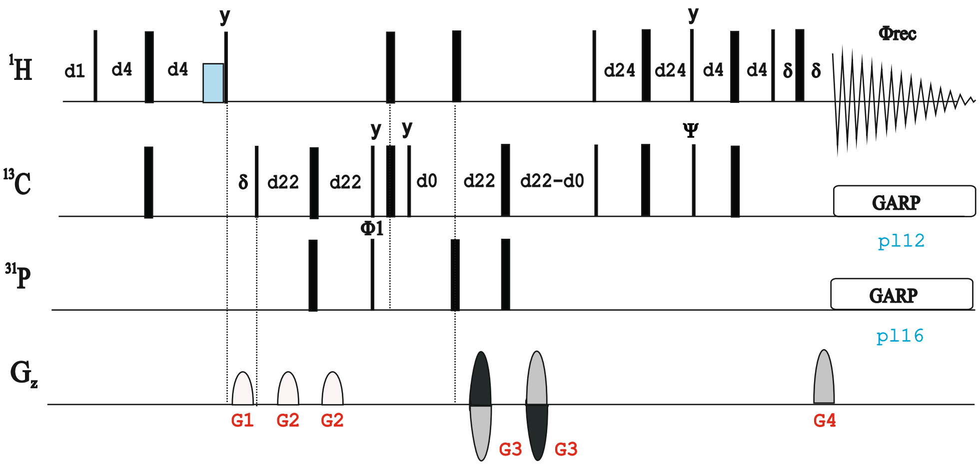
Experiment Description:

Modified 2D version of the put-and-back HCP experiment to measure J(CP) coupling constants. Independent reference-peak and a cross-peak experiment are separately recorded.

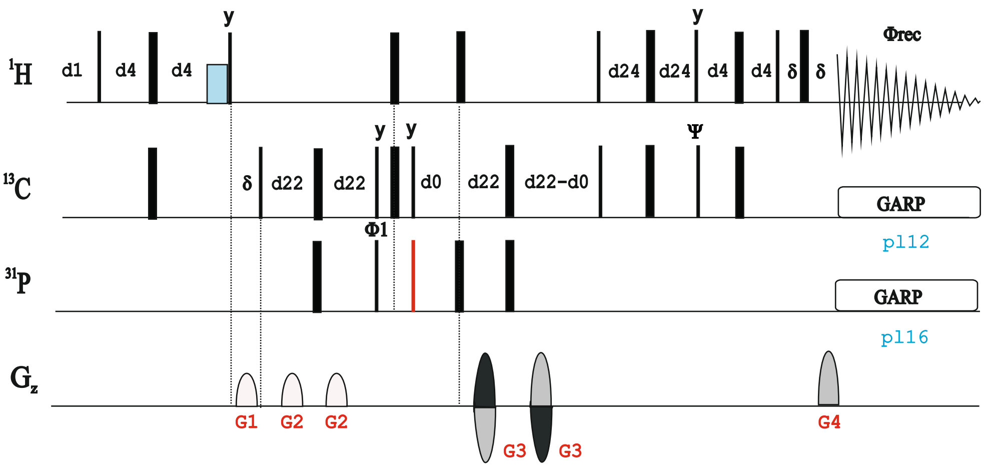
C. Richter, B. Reif, K. Woerner, S. Quant, J.P. Marino, J.W. Engels, C.Griesinger & H.Schwalbe, J. Biomol. NMR 12, 223-230 (1998)

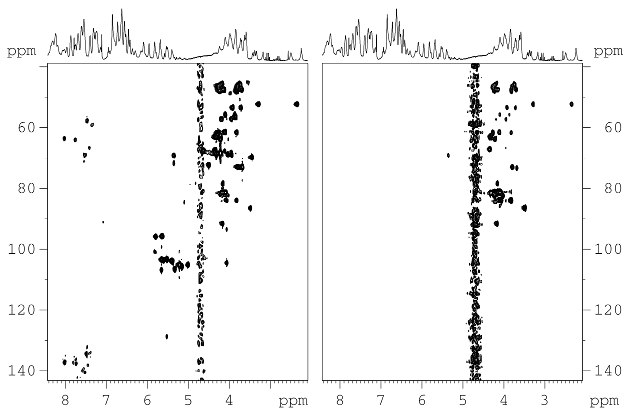


na_hcpqetgpsi.1



na_hcpqetgpsi.2





d1=1.5s
d4=1/4J(CH)=1.6ms
cnst2=J(CH)
cnst5=J(CP)

d22=CT(1/J(CC) for J(CC)=40Hz and
1/4J(C4'-P)=12.5ms
1/4J(C5'-P)=25ms

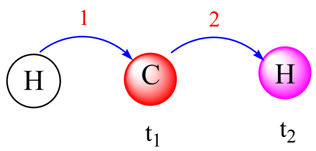
2D P-FIDS Experiment

Experiment Description:

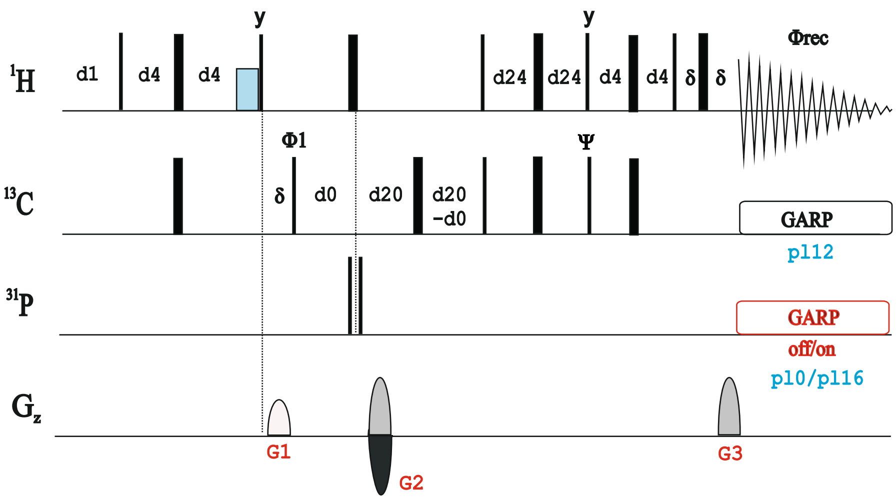
Modified HSQC experiment to measure J(HP) and J(CP) in Nas.
Two experiments are recorded with optional 31P decoupling during 1H acquisition.

References:

1. H. Schwalbe, W. Samstag, J.W. Engels, W. Bermel & C.Griesinger, J. Biomol. NMR 3, 479 - 486 (1993)
2. H. Schwalbe, J.P. Marino, G.C. King, R. Wechselberger, W. Bermel &
C. Griesinger, J. Biomol. NMR 4, 631 - 644 (1994)



na_pfidsetgpsi



d4=1/4J(CH)
d24 optimized as a function of CHn multiplicity
d20=1/2J(CC)=12.5ms or 3/2J(CC)=37.5ms

