TopSpin

Regulatory Compliance

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An audit trail for all manipulations and evaluations performed with a data file is automatically stored with the data. The audit trail function is always active and cannot be switched off.

The audit trail shows, for each data manipulation, a WHEN/WHO/WHERE/WHAT entry including all functional parameters.

The audit trail is a readable ASCII file protected by a hash code, and it is linked with the NMR data. For this reason, illegal manipulations of the data or the audit trail can be detected using a respective TopSpin function.

Example file: em, ft, pk performed

```
##TITLE= Audit trail, TOPSPIN    Version 2.1.a
##JCAMPDX= 5.01
##ORIGIN= Bruker BioSpin GmbH
##OWNER= bg
$$ C:/Bruker/TOPSPIN/data/blood/nmr/phspot-12/10/pdata/1/auditp.txt
##AUDIT TRAIL=  $$ (NUMBER, WHEN, WHO, WHERE, PROCESS, VERSION, WHAT)
(    1,<2006-12-11 15:29:52.750 +0
       <em LB = 1 SI = 128K
         data hash MD5: 128K
         96 E3 89 1B 0A 2F 17 73 30 FC 6B 84 58 9B 38 4F>)
(    2,<2006-12-11 15:29:54.953 +0100>,<bg>,<EOS4>,<procld>,<TOPSPIN 2.1.a>,
       <ft FT_mod = 6 PKNL = 1 SI = 128K
         dat  hash MD5: 128K
         DE 65  5 A7 DA DB 9F 1B 6E 5F 13 A3 8A F7 5F 56>)
(    3,<2006-12-11 15:29:56.765 +0100>,<bg>,<EOS4>,<procld>,<TOPSPIN 2.1.a>,
       <pk PHC0 = 19 .6327 PHC1 = 20.1901
         data hash MD5: 128K
         8B A5 68 14 99 9C  0 BE 63 66 7F DE 73 BA 14 00>)
##END=

$$ hash MD5
$$ 0E AB 0F 07 A7 42 FE 8B 5
```

em with parameters *LB, SI*

ft with parameters *FT_mod, SI, PKNL*

Electronic Signatures

TopSpin supports electronic signatures of NMR datasets.

Electronic signatures display: *User, signature meaning, comment, date/time*

**Electronic signatures are part of the audit trail file**

Signatures cannot be deleted, changed, overwritten or copied to another data file

Electronic Signatures

Electronic signature entry…

```
(    4,<2006-12-11 15:44:35.125 +0100>,<bg/fxm>,<EOS4>,<dataserver>,<TOPSPIN 2.1.a>,
      <Electronic Signature:
```

…in the audit trail file

```
       USER ID      fxm
       USER NAME    Franz X. Maier
       MEANING      Spectrum approved by operator
       COMMENT      Blood plasma spectrum
      data hash MD5: 128K
      8B A5 68 14 99 9C C0 BE 63 66 7F DE 73 BA 14 00>)
```

Electronic Signatures
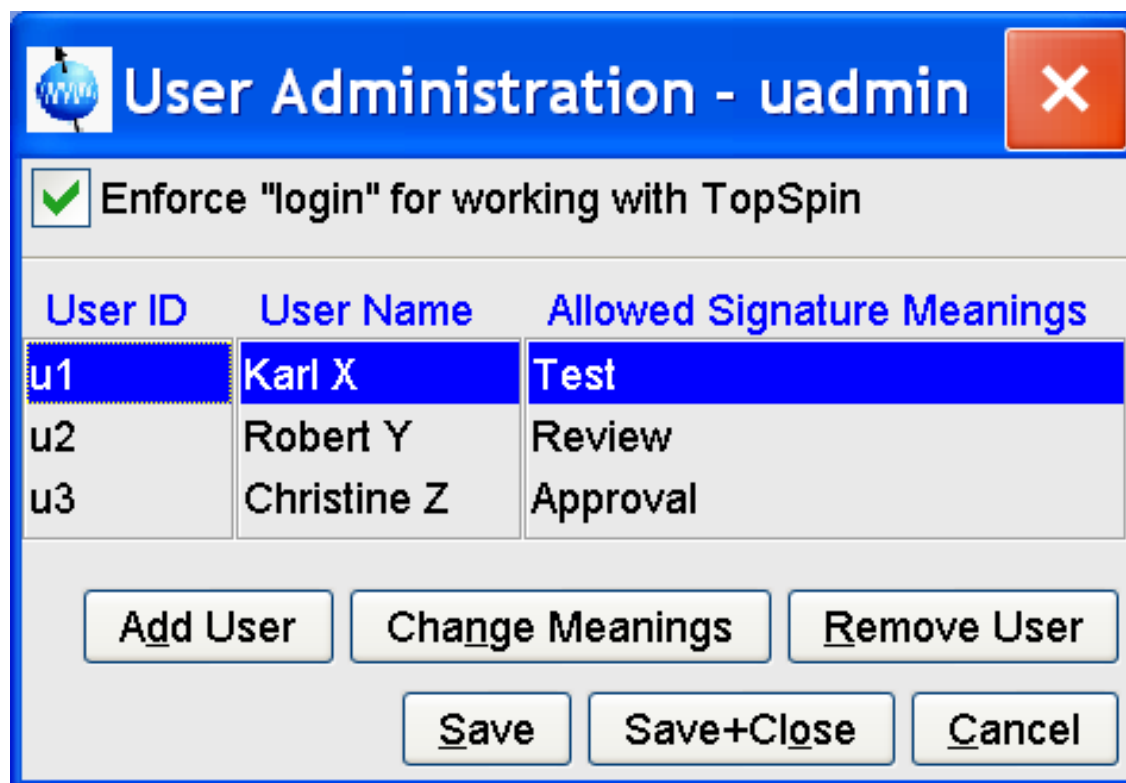
Electronic signature...

...on the data plot

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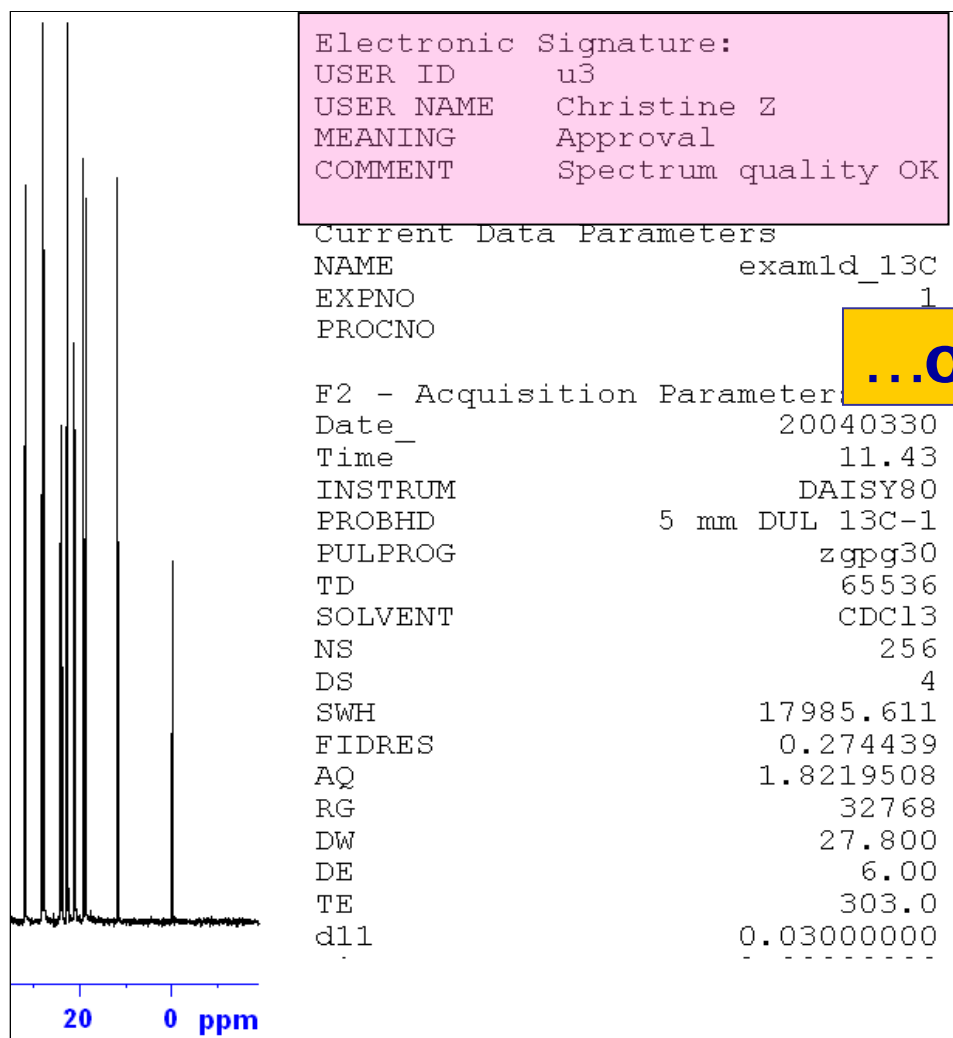
TopSpin (from 2.0 on) offers an operating system independent internal user management

If enabled, a separate login with user ID and password is necessary to be able to work with TopSpin

After a specified time of inactivity TopSpin locks itself automatically. Only the last logged in user or a the NMR administrator may unlock TopSpin using their respective password

Internal users setup dialog

21 CFR Part 11 Compliance Document

Delivered with TopSpin as PDF, 12 pages

TopSpin

21 CFR Part 11 Compliance Document

(Version: July 26th, 2005)

Compliance Table for Subpart B: Electronic Records

Section	Text of 21 CFR Part11	Status	Implementation in TopSpin
11.10	Persons who use closed systems to create, modify, maintain, or transmit electronic records shall employ procedures and controls designed to ensure the authenticity, integrity, and, when appropriate, the confidentiality of electronic records, and to ensure that the signer cannot readily repudiate the signed record as not genuine. Such procedures and controls shall include the following:	System owner	It is assumed that TopSpin is run as a closed system. If TopSpin shall be run in an open system the system owner has to establish suitable measures to prevent unauthorized access to the whole system or part of it.
11.10(a)	Validation of systems to ensure accuracy, reliability, consistent intended performance, and the ability to discern invalid or altered records.	Complies	• TopSpin is validated based on a validation SOP. • The output of Bruker's TopSpin validation suites are available. • All departments of Bruker BioSpin GmbH are ISO 9001:2000 certified. • Additional information about complete spectrometer system validation is available in the document *GLP Requirements* (Bruker Order Number Z31619).
11.10(b)	The ability to generate accurate and complete copies of record in both human readable and electronic form suitable for inspection, review, and copying by the agency. Persons should contact the agency if there are any questions regarding the ability of the agency to perform such review and copying of the electronic records.	Complies	• TopSpin data may be viewed using the "-developer" option at TopSpin startup. No license is required for this case. • TopSpin data sets can be exported in JCAMP-DX format (which is an internationally standardized ASCII coded data exchange format). TopSpin JCAMP-DX files are as secure as TopSpin binary files and include the audit trails and possibly applied electronic signatures.