

AssureSST

System Suitability Test
 User Manual
 Version 003

Innovation with Integrity

NMR

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1 Overview

AssureSST runs a user-selected set of experiments to monitor instrument performance. AssureSST is configured and controlled through the IconNMR automation software package which uses TopSpin to acquire and evaluate data. Upon completion of the SST, a PDF report is generated summarizing the specifications tested and the results obtained.

2 AssureSST Configuration

AssureSST parameters on the spectrometer are accessed through the IconNMR Configuration window (command "iconc" from the TopSpin command line). In the resulting window, select **AssureSST** in the pane on the left. The AssureSST section has three tabs (1) **System Suitability Test (SST)**, which allows the user to activate SST, schedule tests, and print reports (2) **SST Standard Tests**, which allows the user to select from the standard tests and set the specifications for SST, and (3) **SST User Tests**, which allows the user to set up the acquisition parameter set and analysis method for their own tests. Setup for AssureNMR is discussed in Chapter 7.

The SST (up to six individual standard experiments plus up to four user-defined experiments) as a whole must pass before any other samples queued in IconNMR can be acquired while under AssureNMR operation. The six standard tests are covered in the chapter *SST Standard Tests Tab* [> 5]. The user-defined tests are covered in section *SST User Tests* [> 11]. The user can modify this behavior through the IconNMR Configuration window, by selecting the **Fail Safe/Error Handling** window under Automation from the pane on the left. Unchecking the box beside 'Stop the run when 'Assure' System Suitability Test reports specification failure' allows queued samples to run even after the SST fails.



Any changes to the System Suitability Test (e.g. changing a specification or turning off one of the tests) immediately invalidates the previous suitability run. Thus, after a change, the test will be automatically queued when starting IconNMR even if the last successful SST was within the time specified.

It is possible to queue the SST at any time as NMR SuperUser (Chapter Running IconNMR: Supervisor).

AssureSST

System Suitability Test

User Manual





Figure 2.1: Error Handling options that affect AssureSST.



User Manual



2.1 System Suitability Test (SST) Tab

🌢 IconNMR: Configuration		-	×
<u>F</u> ile <u>H</u> elp			
File Help User Strings	AssureSST System Suitability Test (SST) SST Standard Tests SST User Tests System Suitability Test Enable System Suitability Test (Requires ASSURE-SST License) Perform test: O n demand' Every Status Aday(s) at these times: (hk:mm,hk:mm,) QB:30 SST User INTRA-BRKR-CORP\Ar ~ Log Directory C:\Users\amplity.freund\.topspin1\SystemSuitabilityTest Cload/Save shim set before/after first test Image: Continuous AssureNMR Shim Linewidth Check based on NMR reference peak		
Analysis/Quantification ToolBox Setup Accounting	Continuous AssureNMR Shim Linewidth Check based on NMR reference peak Peak test cutoff linewidth 1.25 Hz		
Search			

Figure 2.2: The System Suitability Test (SST) tab in the AssureSST section of the IconNMR Configuration window.

To activate AssureSST, check the first box on the **System Suitability Test (SST)** tab, 'Enable System Suitability Test (Requires ASSURE-SST License)'. Note that the AssureSST license is included with AssureNMR.

The System Suitability Test is automatically queued for acquisition as required to meet the time set in the entry for 'Perform test every: x day(s) at these times: (hh:mm,hh:mm,...)'. Note the times use a 24-hour format. If other samples are queued (e.g. for AssureNMR analysis) at the time when the SST is required, then the data acquisition of the queued samples will wait until the SST has been performed successfully. Strategies and flexibility in the SST were designed to accommodate experiments which might exceed the available time. Experiments that run past the set time for the next SST will remain in the queue until sufficient time is available to run the sample(s).

The option to 'Load/Save shim set before/after first test' provides a mechanism for AssureSST to adjust to shim changes over time. This is done through a default shim file that is used for all samples including the system suitability test samples. Once a ¹H Lineshape suitability test has been completed successfully, the shim set is updated by writing to 'IconNMRShimSet.probeName' where the probeName extension is the name from the edprobe table for the current probe. For more information on probe identification, type "help edprobe" in TopSpin.

When 'Load/Save shim set before/after first test' is checked, it loads the shims saved as 'IconNMRShimSet.probeName' before shimming. In this case, the solvent dependent shim files in the **Solvent/Probe Dependencies** are not used.

- To use this feature, check the box 'Load/Save shim set before/after first test'.
- Save the desired starting shims by typing "wsh IconNMRShimSet.probeName" from the TopSpin command line.

The SST as a whole is the criterion for a properly functioning spectrometer for the purposes of the AssureNMR software. As a result, failure of any component test is reported after the complete set of required tests is measured. For example, if the system administrator requires four tests (¹H Lineshape, ¹H Sensitivity, ¹³C sensitivity and Temperature) for the SST, then all four tests must be completed before a final 'system pass' or 'system fail' result is obtained. Optionally, the user may select 'Stop system test



after any failure' to immediately halt the acquisition after any test fails. When this box is checked then the tests will stop after the first failed system suitability test and all subsequent system suitability tests will be cancelled until the issue is resolved and AssureSST is restarted.

• Check 'Stop system test after any failure' to halt the SST after any failed test.

Automatic generation of a PDF report (see example in Chapter Reports) for SST results occurs when the 'Print the report' option is active. The administrator can customize the 'Company/Institution' and 'System ID' in the report by filling in the corresponding fields.

Report Options	
Print the report (Su	itable Adobe Reader Installed) Paper Size 🔘 A4 💿 Letter
Company/Institution:	Bruker
System ID:	10028098

Figure 2.3: Report Options for AssureSST

Results from the SST are recorded in a log file written to the SST directory selected in the IconNMR Configuration window. Each of the experiments chosen on the **SST Standard Tests** tab and the **SST User Tests** tab will be run during the SST. An example log file from an SST is shown in Chapter Log File from the System Suitability Test.

The 'Activate Single Peak Linewidth Check' enables continuous monitoring of lineshape for every sample acquired with IconNMR for spectral quality control. When used with the proper processing AU (proc_assureshim) and a sample that has an NMR reference signal at 0 ppm, the system uses the halfwidth of the reference to determine whether the spectrum is of a high enough quality to be passed on for analysis. The threshold cutoff for half height should be at or below the value specified as the 'Peak test cutoff frequency' (in Hertz). A sample with a larger half width will be re-shimmed and re-acquired. Two consecutive sample failures results in automatic queuing of the System Suitability Test.

AssureSST System Suitability Test

User Manual



2.2 SST Standard Tests Tab

6		
leip	A	
er Settings	AssureSST	
User Manager	a second s	
Composite Experiments	System Suitability Test (SST) SST Standard Tests SST User Tests	
Additional Users	Shim Program topshim ordmax=8 tuneaxyz 🔹	Shim Program topshim ordmax=8 tuneaxyz 👻
Originator Items	Line stable -	See lucius
itomation	Linewidens	signal region
Master Switches	Linewidth at 0.55% of signal height < 8	iz Left limit 3 ppm Right limit 2 ppm
Automation Window	Linewidth at 0.11% of signal height < 16	Iz Noise region
Virtual Parameter Sets	Resolution Halfwidth < 8	Iz Left limit 7 ppm Right limit 2.8 ppm
Tuning/Matching	Left Plot Limit 8.64	ppm Noise delta 2 ppm S/N > 135 :1
Lock/Shim Options	Right Plot Limit 7.44	
Dependencies	7.44	
AutoCalibrate	¹¹ C Sensitivity Test	¹³ E Sensitivity Test
- Priority	Perform 12C Sensitivity Test Sample Time @ 100/ 50	Perform ¹⁹ F Sensitivity Test
Temperature Handling	Sample type @ 10% EB	
LC-NMR Options	Sample Position 3	Sample Position 4
SampleTrack Options	Shim Program	Shim Program
- Fail Safe / Error Handling	Signal major	Signal region
· Web Interface	Signer region	
ptions	Left limit 140 ppm Right limit 120	pm Left limit -62.5 ppm Right limit -63.5 ppm
sureNMR	Noise region	Noise region
sureSST	Left limit 124 ppm Right limit 80	ipm Left limit -60.5 ppm Right limit -61.5 ppm
alysis/Quantification	Sample Position 40 ppm S/N > 20	1 Noise delta 1 ppm S/N > 100 :1
olBox Setup		
counting	¹¹ P Sensitivity Test	Temperature Test/Adjustment
	Perform ³¹ P Sensitivity Test	Perform Temperature Test/Adjustment
	Sample Position 5	Sample Position 6
	Sample - 330001	
	Shim Program 🔹	Shim Program 🔹
	Signal region	
	Left limit -10 ppm Right limit -20	Requested Temperature 298 K
	Noire region	Tolerance 01 K
	Left limit -3.5 ppm Right limit -8.5	pm Sample Type @ 99.8% MeOD 🕥 4% Methanol 💿 Glycol
	Noise delta 5 ppm S/N > 10	
	Water Suppression Test	¹ H gNMR Performance Qualification Test
	Perform Water Suppression Test	Perform Quantification Performance Test
	Sample Position 7	Sample Position 27
	Shim Program	Shim Program topshim ordmax=8 tuneaxyz
		Lot No. Ampule B
	Linewidth at 50% of DSS signal (40	te Value Uncertainty
	Calculated a topo of the single Calculated and the single	· verue uncertainty
	Linewidth at 10% of DSS signal < 80	z 1,2,4,5- i etrachioro-3-nitrobenzene 4.999 mg/g 0.050 mg/g
	Anomeric Proton Splitting\nat ca. 5.25ppm < 36	1,3,5-Trimethosybenzene 23.501 mg/g 0.050 mg/g
	Anomeric Proton Sensitivity > 64	L Confidence Level 95.0 V So Default 95%, please refer to manual for details

Figure 2.4: The SST Standard Tests tab in the AssureSST section of the IconNMR Configuration window.

The **SST Standard Tests** tab gives the user access to a set of six preset tests. These tests can be turned on and off, the sample positions can be specified, details for the analyses can be input, and criteria for passing the tests can be set from this tab. The details for each test are in the following sections.

2.2.1 ¹H Lineshape

Also referred to as the humptest, this test automatically measures and determines the ¹H lineshape using the GLP ¹H lineshape standard sample, chloroform in acetone. (See Chapter 13 for the correct sample.) The width of the chloroform line at 0.55% height and 0.11% height is calculated with a double exponential fit along the left and right side of the signal. The resolution test is also performed and evaluates the width of the chloroform signal at half height. These values are compared with the specifications set in this window. The test is passed if the results are less than or equal to the defined values.

- Check the 'Perform Lineshape Test' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS).
- Enter the desired values for an acceptable lineshape test for the (1) 'Linewidth at 0.55% of signal height', (2) 'Linewidth at 0.11% of sample height' and (3) the 'Resolution Halfwidth' (linewidth at 50% of signal height).





AssureSST



The lineshape and sensitivity values are specific to the probe. When the probe is changed, the values must be updated to correspond to the current probe in the SST Standard Tests tab of the IconNMR Configuration window. If the probe has been used previously, stored parameters will be loaded for that probe.

1H Lineshape Humptest				
Perform Lineshape Test				
Sample Position 1+				
Linewidths				
Linewidth at 0.55% of signal height	<	8	Hz	
Linewidth at 0.11% of signal height	<	16	Hz	
Resolution Halfwidth	<	0.8	Hz	
Left Plot Limit 8.64 ppm	1	Right Plot Lim	nit	7.44 ppm

Figure 2.5: ¹H Lineshape Humptest parameters on the SST Standard Tests tab.

2.2.2 ¹H Sensitivity

This test automatically measures and determines the ¹H sensitivity. The ¹H sensitivity standard sample is 0.1% ethylbenzene in chloroform-d for all probes. The height of the biggest signal between the signal limits is calculated. A noise window of width 'Noise delta' in ppm is shifted in 25 steps along the spectrum between the noise limits. Each time, the noise value is determined and the signal-to-noise (S/ N) ratio is calculated with respect to the height of the biggest signal within the signal limits. The best value must meet the specification defined in the S/N box.

- Check the 'Perform ¹H Sensitivity Test' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS).
- Enter the desired 'Signal region' (Left and Right limits) to be used for the signal peak.
- Enter the desired 'Noise region' (Left and Right limits).
- Enter the 'Noise delta' (width of the noise range) in ppm.
- Enter the 'S/N' requirement for a successful test.

1H Sensitivity Test					
Perform 1H Ser	sitivity Test				
Sample Position	2 ≑				
Signal region					
Left limit	3	ppm	Right limit	2	ppm
Noise region					
Left limit	7	ppm	Right limit	2.8	ppm
Noise delta	2	ppm	S/N >	135	:1

Figure 2.6: ¹H Sensitivity Test parameters on the System Suitability Test (SST) tab.

¹³C Sensitivity 2.2.3

This test automatically measures and determines the ¹³C sensitivity. The typical sample used for the ¹³C Sensitivity Test is 10% ethylbenzene in cholorform-d for all probes. The ASTM (American Society for Testing and Materials) sample (40% p-Dioxane in benzene-d6) may also be used. The height of the biggest signal within the signal limits is calculated. A noise window of 'Noise delta' ppm is shifted in 25 steps along the spectrum between the noise limits. Each time, the noise value is determined and the signal-to-noise ratio is calculated with respect to the height of the biggest signal. The best value must meet the specification defined in the S/N box.



- Check the 'Perform ¹³C Sensitivity Test' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS)
- Select the Sample Type, either 10% ethylbenzene or the ASTM sample.
- Enter the desired 'Signal region' (Left and Right limits) to be used for the signal peak.
- Enter the desired 'Noise region' (Left and Right limits).
- Enter the 'Noise delta' (width of the noise range) in ppm.
- Enter the 'S/N' requirement for a successful test.

13C Sensitivity Test	:				
Perform 13C Se	nsitivity Test		Sample Type	10% EB	
Sample Position	3 ≑			ASTM	
Signal region					
Left limit	140	ppm	Right limit	120	ppm
Noise region					
Left limit	124	ppm	Right limit	80	ppm
Noise delta	40	ppm	S/N >	20	:1

Figure 2.7: ¹³C Sensitivity Test parameters on the SST Standard Tests tab.

2.2.4 ¹⁹F Sensitivity

This test automatically measures and determines the ¹⁹F Sensitivity. The typical sample used for the ¹⁹F Sensitivity Test is 0.05% trifluorotoluene in chloroform-d for all probes. The height of the biggest signal between the signal limits is calculated. A noise window of 'Noise delta' ppm is shifted in 25 steps along the spectrum between the noise limits. Each time, the noise value is determined and the signal-to-noise ratio is calculated with respect to the height of the biggest signal. The best value must meet the specification defined in the S/N box.

- Check the 'Perform ¹⁹F Sensitivity Test' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS).
- Enter the desired 'Signal region' (Left and Right limits) to be used for the signal peak.
- Enter the desired 'Noise region' (Left and Right limits).
- Enter the 'Noise delta' (width of the noise range) in ppm.
- Enter the 'S/N' requirement for a successful test.

F19 Sensitivity Test					
Perform F19 Se	nsitivity Test				
Sample Position	4 🜩				
Signal region					
Left limit	-62	ppm	Right limit	-63.5	ppm
Noise region					
Left limit	-60.5	ppm	Right limit	-61.5	ppm
Noise delta	1	ppm	<mark>S/N</mark> >	100	:1

Figure 2.8: ¹⁹F Sensitivity Test parameters on the SST Standard Tests tab.

2.2.5 ³¹P Sensitivity

This test automatically measures and determines the ³¹P Sensitivity. The typical sample used for the ³¹P Sensitivity Test is 0.0485 M triphenylphosphate in acetone-d6 for all probes. The height of the biggest signal between the signal limits is calculated. A noise window of 'Noise delta' ppm is shifted in 25 steps



along the spectrum between the noise limits. Each time, the noise value is determined and the signal-tonoise ratio is calculated with respect to the height of the biggest signal. The best value must meet the specification defined in the S/N box.

- Check the 'Perform ³¹P Sensitivity Test' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS).
- Enter the desired 'Signal region' (Left and Right limits) to be used for the signal peak.
- Enter the desired 'Noise region' (Left and Right limits).
- Enter the 'Noise delta' (width of the noise range) in ppm.
- Enter the 'S/N' requirement for a successful test.

P31 Sensitivity Tes	st				
Perform P31 Ser	nsitivity Test				
Sample Position	5 ≑				
Signal region					
Left limit	-10	ppm	Right limit	-20	ppm
Noise region					
Left limit	-3.5	ppm	Right limit	-8.5	ppm
Noise delta	5	ppm	S/N >	10	:1

Figure 2.9: ³¹P Sensitivity Test parameters on the SST Standard Tests tab.

2.2.6 Temperature Test with Automatic Adjustment

This test automatically measures and, if necessary, adjusts the temperature to the temperature specified in 'Requested Temperature'. The experiment is designed to run after the other components of the SST. In the example below, the temperature is measured with the 99.8% Methanol-d4 Temperature Calibration Standard which has a linear range from 282 K to 330 K. The method will attempt to adjust the temperature to the set point five times before failing. The final observed temperature after adjustment is recorded in the status parameters under the entry for USERA1.

- Check the 'Perform Temperature Test/Adjustment' box to require this experiment to run as part of the SST.
- Set the 'Sample Position' to the holder position of the desired temperature calibration standard in the sample changer (SampleCase, SampleJet, SampleXpress, BACS).
- Enter the 'Requested Temperature' and 'Sample Type'.

Temperature Test	t/Automatic Ad	justme	ent	
Perform Temp	erature Test/A	djustm	ent	
Sample Position	<mark>6</mark> ‡			
Requested Temperature	298	к		
Tolerance	0.1	к		
Sample Type:	99.8% MeC	DD	Ø 4% Methanol	80% Glycol

Figure 2.10: Temperature Test parameters on the SST Standard Tests tab.

2.2.7 Water Suppression Test

This test will determine 2 factors important for the GLP Water Suppression standard sample, 2mM Sucrose + 0.5mM DSS in 90% H_2O + 10% D_2O ; the suppression quality and the sensitivity level of the anomeric sucrose signal at 5.25ppm. A resolution test of the lineshape of DSS is also performed. The test is passed if the lineshape results are less than or equal to the defined values for lineshape and the



percent splitting value of the anomeric proton splitting. The test also requires that the best value for proton sensitivity must be greater than or equal to the defined value for Anomeric Proton Sensitivity. Note that the test assumes the position of water to be 4.7ppm. There is no scout for the optimal water resonance.

- Check the 'Perform Water Suppression Test' box to require this experiment to run as part of the SST.
- Set the "Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS.)
- Select the Shim program to use a shim program different from the default for IconNMR or default for the solvent.
- Enter the desired values for an acceptable lineshape test for the (1) 'Linewidth at 50% of DSS signal', (2) 'Linewidth at 10% of DSS Signal', (3) 'Anomeric Proton Splitting\nat ca. 5.25ppm'.

Water Suppression Test Perform Water Suppression Test			
Sample Position 7			
Shim Program			~
Linewidth at 50% of DSS signal	<	40	Hz
Linewidth at 10% of DSS signal	<	80	Hz
Anomeric Proton Splitting\nat ca. 5.25ppm	<	36	%
Anomeric Proton Sensitivity	>	64	:1

2.2.8 ¹H qNMR Performance Quantification (PQ) Test

This test will measure the potency of a certified quantification reference material (CRM). This CRM is available in ready-to-use sealed ampules from Merck KGaA¹ (formerly Sigma-Aldrich) as Bruker quantitative PQ (qPQ) Certified Reference Material (Product No. 42350). For exact conditions to follow, please refer directly to the prevailing SOP for this method and for your facility. However, the Bruker BioSpin recommendation is to use either freshly prepared samples of the quantification reference material, or a sealed NMR tube of same. Note that the sample must only be used within the validity period of the reference sample as given on the certificate.

Data on the certificate delivered with each lot of the material (see an example in figure (qPQ.1) must be used to complete the information in the qPQ test box, a typical example of which is shown further below in figure qPQ.2.

- Check the 'Perform qPQ Test' box to require this experiment to run as part of the SST.
- Set the "Sample Position' to the holder position of the standard sample in the sample changer (SampleCase, SampleJet, SampleXpress, BACS.)
- Select the Shim program to use a shim program different from the default for IconNMR or default for the solvent.
- The following information will be found on the Certificate of Analysis delivered with the sample and must be manually transcribed into the qPQ test tab:
 - Lot. No.
 - 1,2,4,5-Tetrachloro-3-nitrobenzene certified value for mass and uncertainty
 - 1,3,5-Trimethoxybenzene certified value for mass and uncertainty

¹1 The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the U.S. and Canada.

AssureSST System Suitability Test User Manual







Certificate of Analysis – Certified Reference Material

Biukei qualitita	roduced in double accomment
Product no.:	42350 ISO/IEC 17034
Lot no.:	BCBZ9945
Description of CRM:	1,3,5-Trimethoxybenzene (TMXB) and 1,2,4,5-Tetrachloro-3-nitrobenzene (TCNB) in DMSO-d ₆ (solution)
Expiry date:	DEC 2020
Storage:	20-25°C; storage under Argon
Chemical formula:	$C_9H_{12}O_3$ (TMXB); $C_6HCl_4NO_2$ (TCNB)
Molecular mass:	168.19 g/mol (TMXB); 260.89 g/mol (TCNB)

Constituents	Certified value	Expanded uncertainty, $U=k \cdot u \ (k=2)$				
1,2,4,5-Tetrachloro-3-nitrobenzene	23.51 mg/g	0.18 mg/g				
1,3,5-Trimethoxybenzene	5.00 mg/g	0.04 mg/g				

Figure 2.11: Excerpt of a typical CoA for the PQ reference material.

The field for 'Limit for qPQ-Test Result (100% ±)±)' defines the acceptance criterion for the ¹H qNMR Performance Quantification (PQ) Test. The value is calculated automatically from the given uncertainties of each component and the selected confidence level. The field 'Limit for qPQ-Test Result (100% ±)' cannot be edited. Choosing a different confidence level allows for adjustment of the acceptance criterion.

¹ H qNMR Performance Qualification Te	est			
Perform Quantification Performance Te	est			
Sample Position	8			
Shim Program	topshim			~
Lot No.	BCBZ9945			
	Value		Uncertainty	
1,2,4,5-Tetrachloro-3-nitrobenzene	23.51	mg/g	0.18	mg/g
1,3,5-Trimethoxybenzene	5.000	mg/g	.04	mg/g
Confidence Level	95.0 ~	%	Default 95%,	please refer to manual for details
Limit for qPQ-Test Result (100% \pm)	1.18	%		

Figure 2.12: qPQ Test Parameters on the qPQ test tab.

Upon completion of the test, the results of the qPQ test – Pass if the result lies within the calculated limit or Fail, if without, are automatically appended to the SST test report pdf.

User Manual



2.3 SST User Tests

SST also allows users to specify their own tests. For analysis purposes, the tests are classified as lineshape tests or sensitivity tests. The user must supply information about the solvent, the parameter set to use, and the sample position. In the parameter set, the acquisition au program (AUNM) must be au_zgglp and the processing au program (AUNMP) must be proc_1dglp. The user must also supply the information for the analysis – linewidths and plot region for the lineshape tests, signal and noise regions for the sensitivity tests – interactively on the **SST User Tests** tab.

System Suitability	Test (SST) SST Stan	dard Tests SST U	Jser Tests								
User Defined Lines	hape Test1		User Defined Sensitivity Test1								
📝 Perform User 🛛	Defined Lineshape Tes	Perform User Defined Sensitivity Test1									
Description	Lineshape for wate	r sample			Description	Description Sensitivity for my test sample					
Solvent	H2O+D2O 90%H	120 and 10%D2(•		Solvent	CDCI3		-			
Parameter Set	WATERSUP		Parameter Set	eter Set PROSENS -							
Sample Position	7 ≑				Sample Position	8‡					
Linewidths					Signal region						
Linewidth at 0.5	5% of signal height	< 10	Hz		Left limit	3	ppm	Right limit	2	ppm	
Linewidth at 0.1	1% of signal height	< 20	Hz		Noise region						
Resolution Half	width	< 1.0	Hz		Left limit	7	ppm	Right limit	2.8	ppm	
Left Plot Limit	6 pr	om Right Plot Lim	it 5	ppm	Noise delta	2	ppm	S/N >	500	:1	
User Defined Lines	hape Test2				User Defined Sensi	tivity Test2					
🔲 Perform User D	, efined Lineshape Tes	t2			Perform User D	efined Sensitiv	ity Test	2			
Description	Lineshape nonspin	ning			Description	Description User Defined Sensitivity Test 2					
Solvent	Acetone		•		Solvent	CDCI3		•			
Parameter Set	PROHUMP		•		Parameter Set	PROSENS		-			
Sample Position	9‡				Sample Position	10‡					
Linewidths					Signal region						
Linewidth at 0.5	5% of signal height	< 6	Hz		Left limit	3	ppm	Right limit	2	ppm	
Linewidth at 0.11	1% of signal height	< 12	Hz		Noise region						
Resolution Half	width	< 0.6	Hz		Left limit	7	ppm	Right limit	2.8	ppm	
Resolution nair	wiciui	0.0									

Figure 2.13: SST User Tests tab for SST, with one lineshape test and one sensitivity test activated.

3 Data Organization and Final PDF Report

AssureSST automatically places the SST data in the first directory listed in the Data Directories window for the SST user in the **User Manager** of the IconNMR Configuration window. The generated data directory name uses the following date-stamped format *SST_{YYY_MM_DD_HH_MM_SS}*. Each directory will contain all of the data for a queued System Suitability Test.

Within the data directory for the last experiment that makes up the SST, a PDF report (see the example in Chapter 9.2) is stored which summarizes which tests were run, the criteria, and the results of each test including a pass or fail notation.

4 Assure-SST Reference Standards

300 MHz / 5mm Room Temperature						
Description	Part No.					
Lineshape - 3% Chloroform	Z10230					
1H Sensitivity - 0.1% Ethylbenzene, 40mm filling	Z10901					



User Manual

13C Sensitivity - 10% Ethylbenzene	Z10153							
19F Sensitivity – 0.05% Trifluorotoluene	Z10234							
31P Sensitivity – 0.0485 M Triphenylphosphate	Z10201							
NMR Thermometer 99.8% Methanol-d4	Z10627							
Water Suppression - 2mM sucrose	Z10246							
400 – 900 MHz / 5mm Room Tempera	ture							
Description	Part No.							
Lineshape - 1% Chloroform	Z10248							
1H Sensitivity - 0.1% Ethylbenzene, 40mm filling	Z10901							
13C Sensitivity - 10% Ethylbenzene	Z10153							
19F Sensitivity – 0.05% Trifluorotoluene	Z10234							
31P Sensitivity – 0.0485 M Triphenylphosphate	Z10201							
NMR Thermometer 99.8% Methanol-d4	Z10627							
Water Suppression - 2mM sucrose	Z10246							
400 – 900 MHz / 5mm CryoProbe								
Description	Part No.							
Description Lineshape - 0.3% Chloroform, 40mm filling	Part No. Z10903							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling	Part No. Z10903 Z10901							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene	Part No. Z10903 Z10901 Z10153							
Description Lineshape - 0.3% Chloroform, 40mm filling1H Sensitivity - 0.1% Ethylbenzene, 40mm filling13C Sensitivity - 10% Ethylbenzene19F Sensitivity - 0.05% Trifluorotoluene	Part No. Z10903 Z10901 Z10153 Z10234							
DescriptionLineshape - 0.3% Chloroform, 40mm filling1H Sensitivity - 0.1% Ethylbenzene, 40mm filling13C Sensitivity - 10% Ethylbenzene19F Sensitivity - 0.05% Trifluorotoluene31P Sensitivity - 0.0485 M Triphenylphosphate	Part No. Z10903 Z10901 Z10153 Z10234 Z10201							
Description Lineshape - 0.3% Chloroform, 40mm filling1H Sensitivity - 0.1% Ethylbenzene, 40mm filling13C Sensitivity - 10% Ethylbenzene19F Sensitivity - 0.05% Trifluorotoluene31P Sensitivity - 0.0485 M TriphenylphosphateNMR Thermometer 99.8% Methanol-d4	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627							
Description Lineshape - 0.3% Chloroform, 40mm filling1H Sensitivity - 0.1% Ethylbenzene, 40mm filling13C Sensitivity - 10% Ethylbenzene19F Sensitivity - 0.05% Trifluorotoluene31P Sensitivity - 0.0485 M TriphenylphosphateNMR Thermometer 99.8% Methanol-d4Water Suppression - 2mM sucrose	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose 600 – 900 MHz / 1 mm Room Tempera	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose 600 – 900 MHz / 1 mm Room Tempera Description	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose 600 – 900 MHz / 1 mm Room Tempera Description Lineshape - 3% Chloroform	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose 600 – 900 MHz / 1 mm Room Tempera Description Lineshape - 3% Chloroform 1H Sensitivity - 0.1% Ethylbenzene	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
Description Lineshape - 0.3% Chloroform, 40mm filling 1H Sensitivity - 0.1% Ethylbenzene, 40mm filling 13C Sensitivity - 10% Ethylbenzene 19F Sensitivity - 0.05% Trifluorotoluene 31P Sensitivity - 0.0485 M Triphenylphosphate NMR Thermometer 99.8% Methanol-d4 Water Suppression - 2mM sucrose 600 – 900 MHz / 1 mm Room Tempera Description Lineshape - 3% Chloroform 1H Sensitivity - 0.1% Ethylbenzene 13C Sensitivity - 10% Ethylbenzene	Part No. Z10903 Z10901 Z10153 Z10234 Z10201 Z10627 Z10246							
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600 – 900 MHz / 1.7mm CryoProbe								
Description	Part No.							
Lineshape - 1% Chloroform	Z10717							
1H Sensitivity - 0.1% Ethylbenzene	Z10718							
13C Sensitivity - 10% Ethylbenzene	Z10723							
19F Sensitivity – 0.05% Trifluorotoluene	Z10728							
31P Sensitivity – 0.0485 M Triphenylphosphate	Z10722							
NMR Thermometer 99.8% Methanol-d4	Z10734							
Water Suppression - 2mM sucrose	Z10246							

5 Contact

Manufacturer

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Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

https://www.bruker.com/service/information-communication/helpdesk.html



System Suitability Test

User Manual



/ 18

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