

SmileQ Software

NMR

Analytical

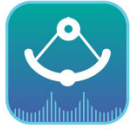


SMILEQ Spectral Management Interface Launching Engine for Q-NMR

The optimum environment for quantitative analysis, combining the ease of use of the main application with an efficient workflow for quantitative analysis.

SMILEQ plugin is a software tool for quantitative NMR analysis

- Quantitative NMR analysis by the internal standard method (for purity and molar concentration)
- The use of the standard material information library is available.
- Analysis using analysis files (analysis templates)
- Batch processing (batch analysis of multiple data)
- Report generation (individual reports and summary reports)
- Automatic quantitative NMR analysis (from measurement to report generation)
- Cooperates with Delta software on the JEOL NMR system



smileq

Delta 

Set Your Sample



Select Analytical Method

Input Sample Weight

qNMR Seamless

GET YOUR REPORT

Method Template

Quantitative Calculation

Report Creation


smileq



SMILEQ widget

Easy to set parameters for qNMR analysis

Report qNMR

Save your time to put together calculation result

Batch analysis qNMR

More comfortable environment multiple qNMR data analysis

SMILEQ

Analysis Mode: Internal Standard

Analyte Details

Name: butylparaben

Molar Mass (g/mol): 194.227

Mass (mg): 91.1133 Volume (mL): 18

Reference Details

Name: DMSO

Reference Filter: 99.5

Purity (%): 94.13

Molar Mass (g/mol): 18.2033

Mass (mg): 18.2033 Volume (mL): 18

Molarity (mmol/L): 10.69875

Target Signal Table

Calc	Pos (ppm)	Start (ppm)	End (ppm)	# Nuclei
<input checked="" type="checkbox"/>	0.939	0.907	0.969	3
<input checked="" type="checkbox"/>	1.444	1.383	1.502	2
<input checked="" type="checkbox"/>	1.693	1.644	1.739	2
<input checked="" type="checkbox"/>	6.889	6.866	6.913	2
<input checked="" type="checkbox"/>	7.868	7.845	7.892	2

Estimate #Nuclei

Calculation Options

Method: Sum Peaks

Decimal Places: 3

Apply

SMILEQ

Analysis Mode: External Std - Analyte

Analyte Details

Name: butylparaben

Molar Mass (g/mol): 194.227

Mass (mg): 91.1133 Volume (mL): 18

Reference Spectra

-- No Checked --

Show in quantity table: Avg. Refs Each Ref

Correction

PULCON: All

SOLCOR

Target Signal Table

Calc	Pos (ppm)	Start (ppm)	End (ppm)	# Nuclei
<input checked="" type="checkbox"/>	0.939	0.907	0.969	3
<input checked="" type="checkbox"/>	1.444	1.383	1.502	2
<input checked="" type="checkbox"/>	1.693	1.644	1.739	2
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SMILEQ

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<input checked="" type="checkbox"/>	7.868	7.845	7.892	2

Estimate #Nuclei

Calculation Options

Method: Sum Peaks

Decimal Places: 3

Quantitative Result

Purity Average: -1.225.781 %

Molarity Average: -3181.011 mmol/L

Update

¹H qNMR

Pos (ppm)	Start (ppm)	End (ppm)	Sum Integral	Peaks Area	# Nuclei	Purity (%)	Molarity (mmol/L)
0.939	0.907	0.969	90408.348	99578.102	3	-12230.179	-3187.370
1.444	1.383	1.502	60337.770	46553.668	2	-12243.478	-3190.836
1.693	1.644	1.739	60087.067	49356.817	2	-12192.607	-3177.578
6.889	6.866	6.913	60090.094	52957.122	2	-12193.221	-3177.738
7.868	7.845	7.892	59972.970	52838.472	2	-12169.455	-3171.544

Parameters

Analyte

Name: butylparaben

Molar Mass: 194.227 g/mol

Weight: 91.1133 mg

Volume: 18 mL

Reference

Name: DMSO

Purity: 99.5 %

Molar Mass: 18.2033 g/mol

Weight: 18.2033 mg

Volume: 18 mL

Molarity: 10.69875 mmol/L

Calculation Options

Method: Sum

Delta Method: Prescribed

Purity

Average: -1.22e+04 %

SD: 30.279 %

RSD: -0.248 %

Molarity

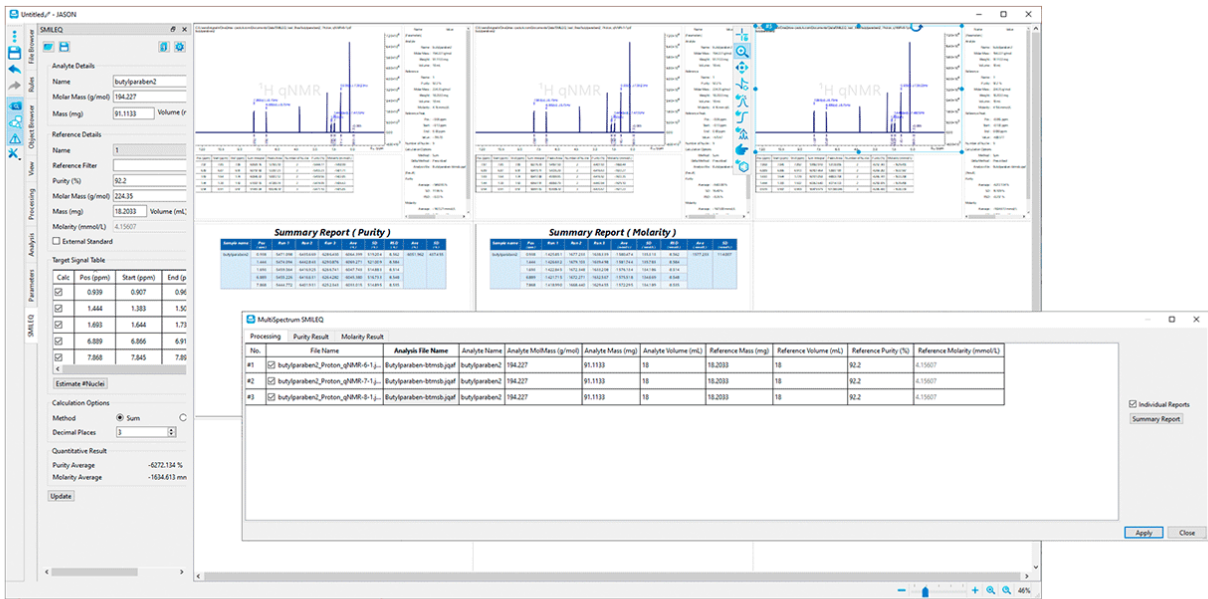
Average: -3.18e+03 mmol/L

SD: 7.891 mmol/L

RSD: -0.248 %



Report qNMR



• Multispectrum qNMR

Uncertainty of the Purity (according to ISO 24583)

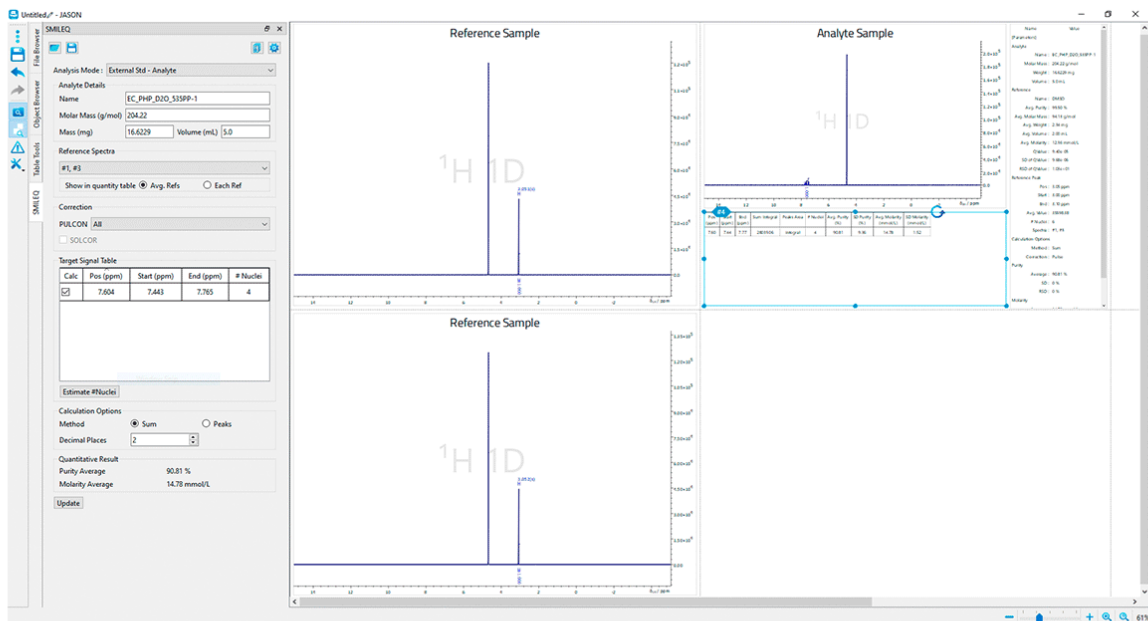
Sample name	Pos (ppm)	Run 1 (%)			Run 2 (%)			Run 3 (%)			Signals		Sample solutions		All Sample solutions	
		Ave	SD	CV	Ave	SD	CV	Ave	SD	CV	Ave	SD	Ave	SD		
butyl parahydroxybenzoate 1	7.86	99.49	0.16	0.16	99.57	0.16	0.16	99.79	0.16	0.16	99.62	0.16	99.72	0.14	99.66	0.08
	6.90	99.63	0.12	0.12	99.56	0.12	0.12	99.79	0.12	0.12	99.66	0.12				
	1.71	99.59	0.14	0.14	99.59	0.14	0.14	99.83	0.14	0.14	99.67	0.14				
	1.41	99.95	0.03	0.03	99.99	0.03	0.03	100.00	0.03	0.03	99.98	0.03				
	0.86	99.82	0.06	0.06	99.70	0.06	0.06	99.79	0.06	0.06	99.77	0.06				
	4.21	99.58	0.11	0.11	99.58	0.11	0.11	99.77	0.11	0.11	99.64	0.11				
butyl parahydroxybenzoate 2	7.86	99.91	0.31	0.31	99.65	0.31	0.31	99.30	0.31	0.31	99.62	0.31	99.73	0.12	99.66	0.08
	6.90	99.78	0.17	0.17	99.58	0.17	0.17	99.44	0.17	0.17	99.60	0.17				
	1.71	100.01	0.33	0.33	99.83	0.33	0.33	99.38	0.33	0.33	99.74	0.33				
	1.41	99.99	0.08	0.08	99.94	0.08	0.08	99.84	0.08	0.08	99.93	0.08				
	0.86	99.82	0.09	0.09	99.79	0.09	0.09	99.65	0.09	0.09	99.76	0.09				
	4.21	100.12	0.36	0.36	99.80	0.36	0.36	99.39	0.36	0.36	99.77	0.36				
butyl parahydroxybenzoate 3	7.86	99.65	0.25	0.25	99.26	0.25	0.25	99.17	0.25	0.25	99.36	0.25	99.59	0.19	99.66	0.08
	6.90	99.61	0.15	0.15	99.50	0.15	0.15	99.31	0.15	0.15	99.47	0.15				
	1.71	99.83	0.23	0.23	99.41	0.23	0.23	99.44	0.23	0.23	99.56	0.23				
	1.41	99.85	0.05	0.05	99.87	0.05	0.05	99.94	0.05	0.05	99.89	0.05				
	0.86	99.73	0.00	0.00	99.73	0.00	0.00	99.73	0.00	0.00	99.73	0.00				
	4.21	99.70	0.15	0.15	99.50	0.15	0.15	99.41	0.15	0.15	99.54	0.15				

Uncertainty Budget (according to ISO 24583)

Source of uncertainty	Unit	Value	Standard uncertainty	Sensitivity coefficient	Relative standard uncertainty
NMR experiments	%	99.77	0.36	1.00	0.36
Measurement repeatability	%	99.77	0.36	1.00	0.36
Variations from different signals selected	%	99.59	0.19	1.00	0.19
Variations from qNMR sample solution preparations	%	99.68	0.08	1.00	0.08
Purity of standard	%	100.00	0.3	1.00	0.25
Combined standard uncertainty (%)					0.49
Coverage factor					2
Expanded uncertainty (%)					0.97



• ISO Compliant analysis



External Standard Analysis

SMILEQ is the software that meets all your expectations

Complete confidence

SMILEQ is developed by JEOL, the global provider of specialised NMR labs.

No surprises

You can enjoy the free trial for 46 days. Our technical assistance team always guides you.

Thought for everyone

From single sample to multiple spectra, internal or external standard, and ISO compliant qNMR analysis, SMILEQ has something to offer every user

Request contact, and in less than 24 hours, our expert technicians will guide you in everything you need.



Name *

Email address *

Telephone

Brief description of the issue *

Thank you for your message. It has been sent.

×

There was an error trying to send your message. Please try again later.

×

CONTACT YOUR EXPERT