NMR Software

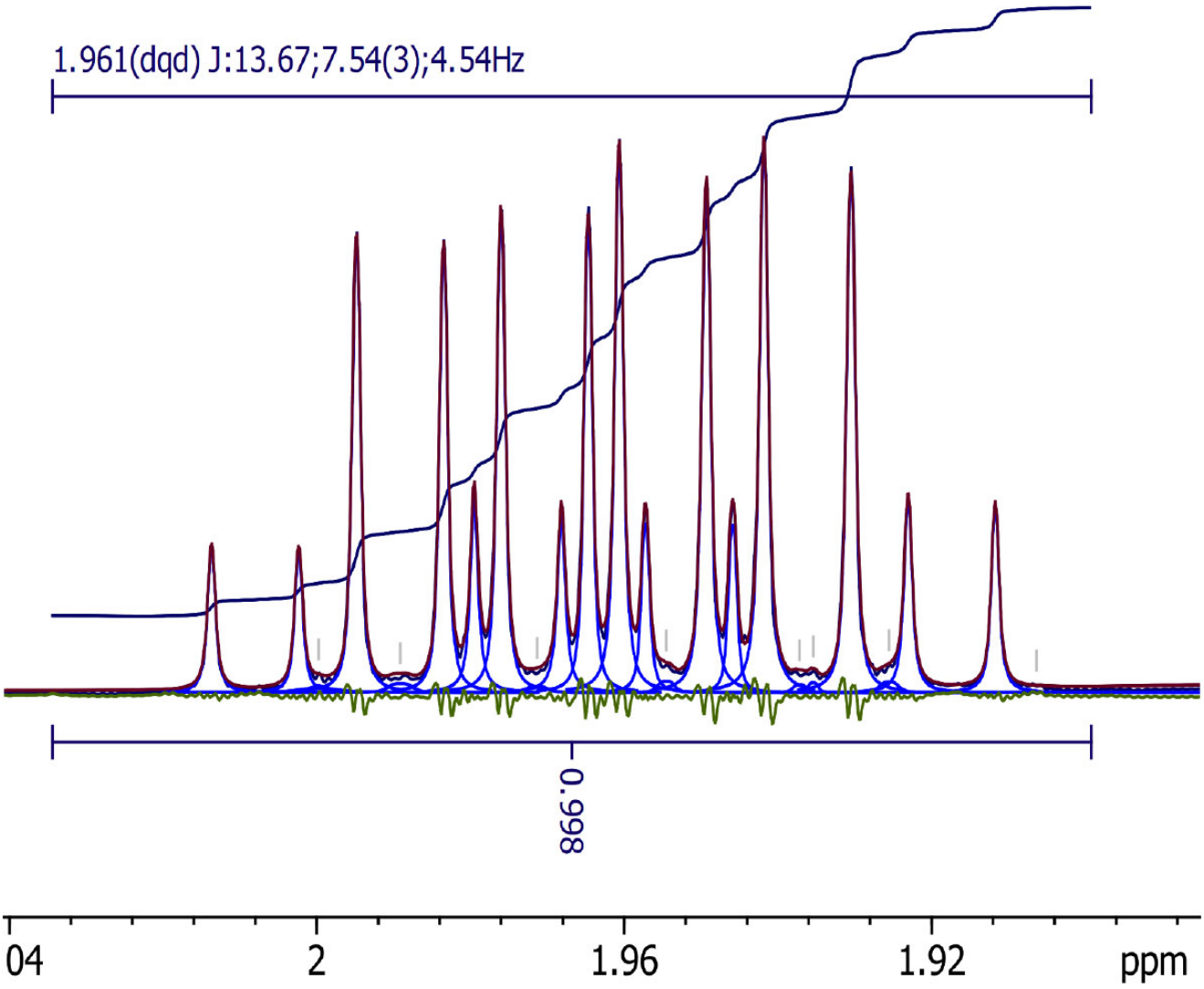
Specialised software for NMR laboratories
Kit of NMR tools prepared to get the most out of your nuclear magnetic resonance data

Simplified user experience

One of the distinguishing features of JASON is the data canvas. As data files are opened, they are displayed on the canvas, which can be extended both horizontally and vertically to accommodate as much data as the computer’s working memory can deal with. Navigating the canvas is done using the mouse to scroll and zoom or by specific data, objects using the object browser. In addition, related data sets and objects can be linked with a shared cursor for spectral analysis

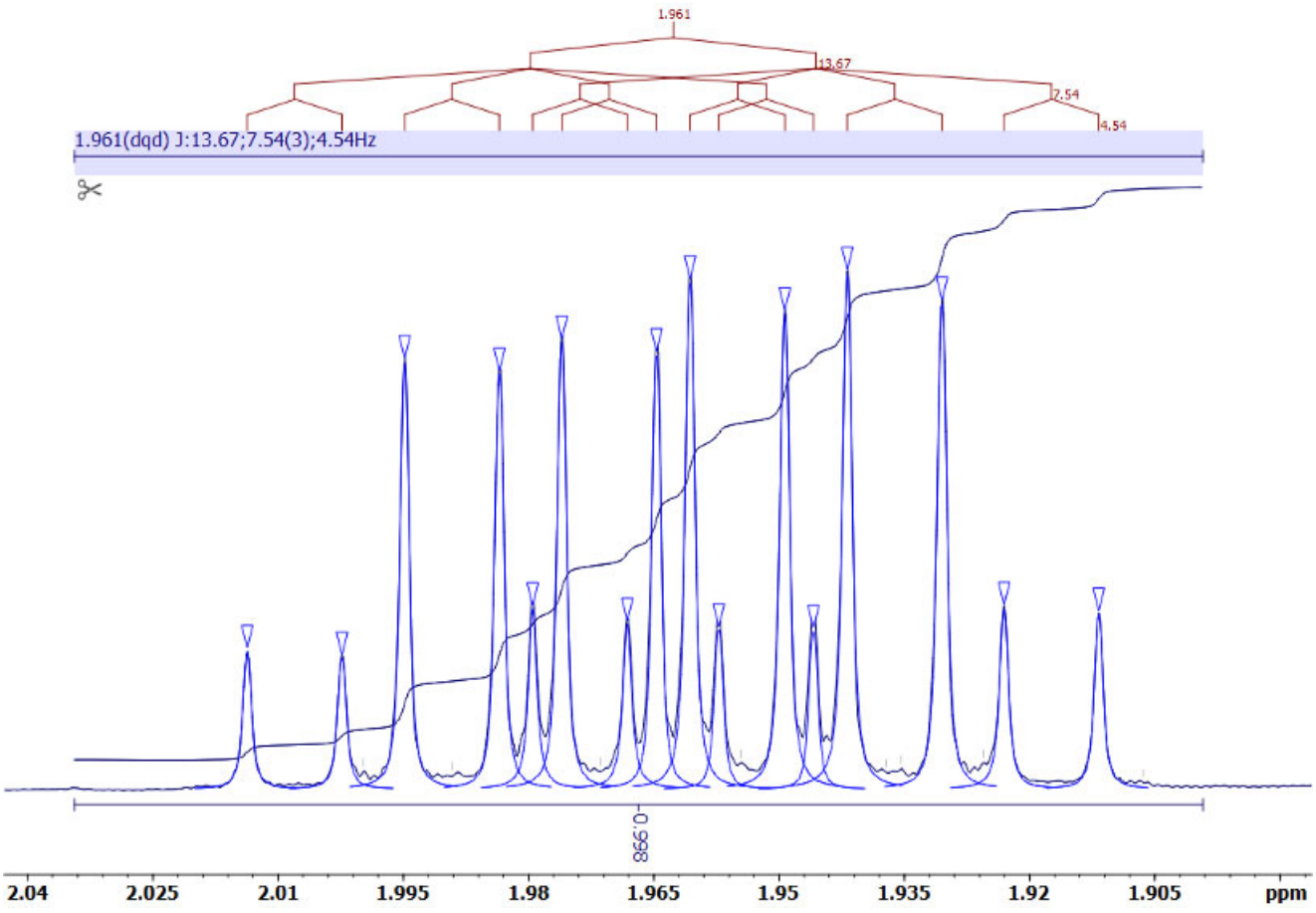
State-of-the-art peak picking

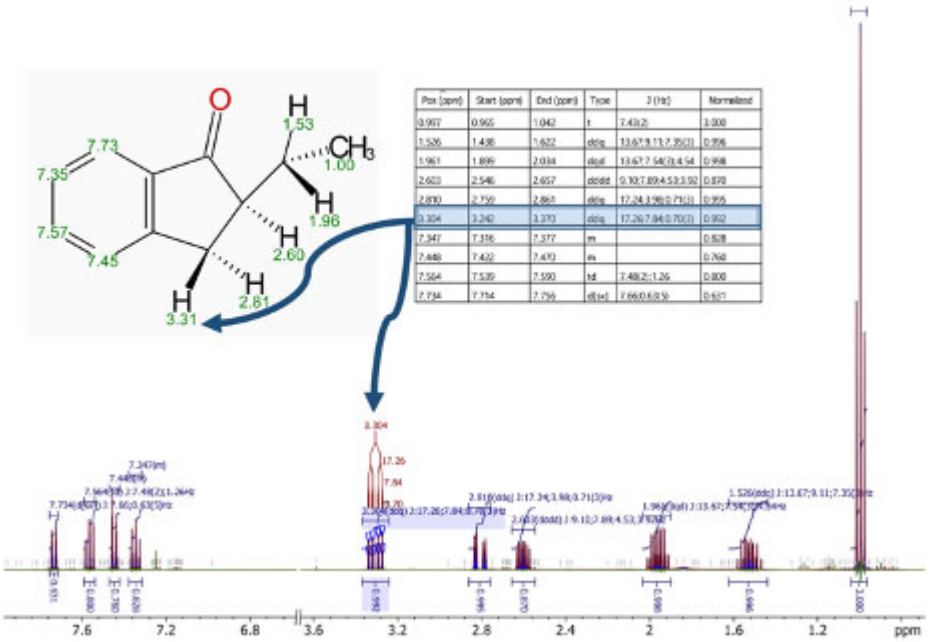
Any NMR processing software worth its salt should include robust peak picking functionality. JASON is no exception and combines peak picking with spectral deconvolution providing the facility to break down a spectrum into a list of peak parameters at a button push.



Optimised workflows multiplet analysis

JASON can group peaks into multiplets and perform first order multiplet analysis to maximise the structural information obtained from a 1H spectrum. This can be done automatically across the entire spectrum or manually on specific spectral regions. Multiplets can be reported as a table within JASON or in journal format.





Draw, modify molecule

Molecular structures can be imported into JASON as .mol or .sdf files. They can also be drawn from scratch with the easy-to-use and intuitive molecular drawing facility. The structures can be linked to spectral data sets to assist in

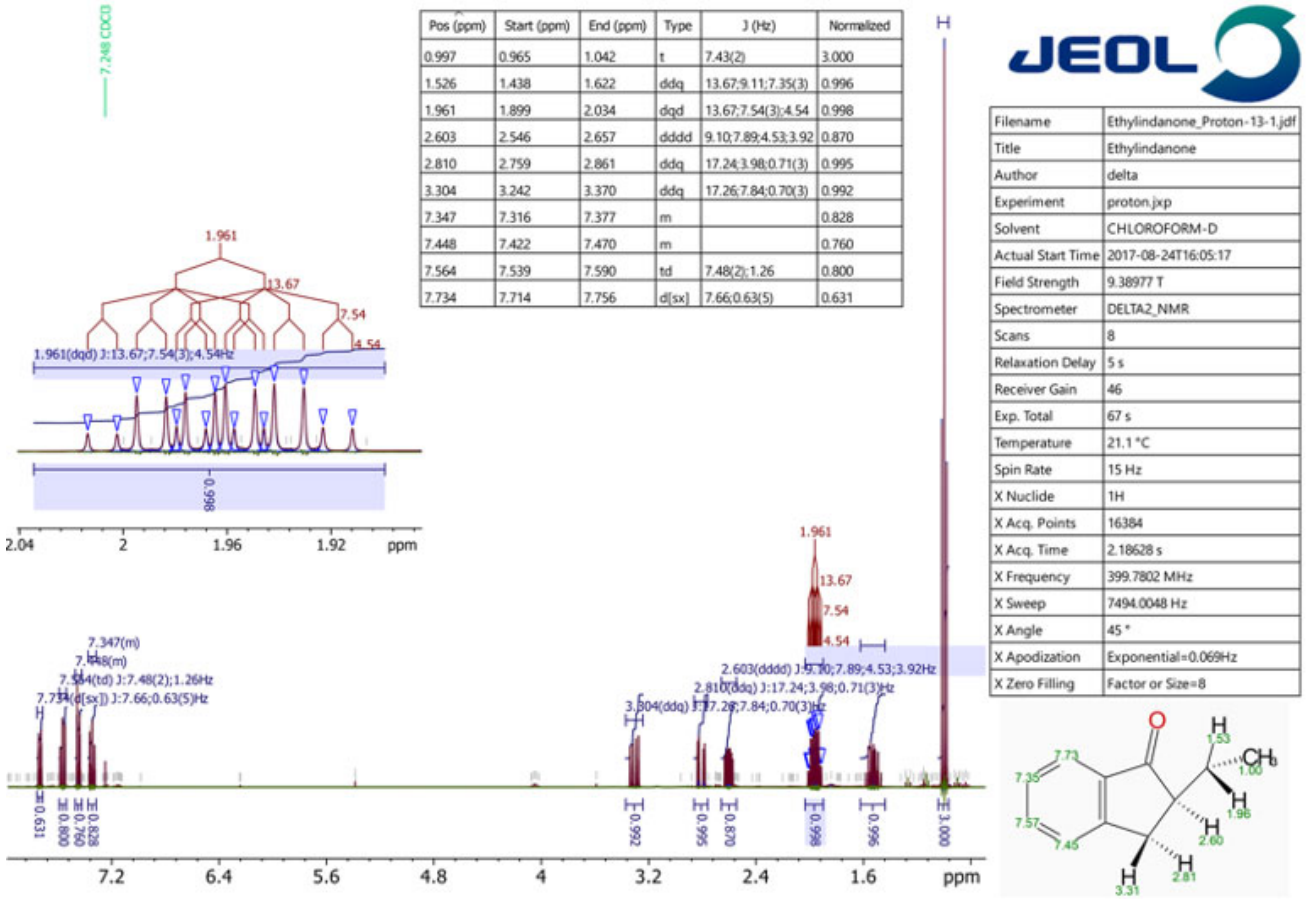
structural analysis and assignment.

Predict NMR

JASON contains a hybrid prediction method, an increment based and a HOSE code approach.When there’s a good representation of the molecule in the database the predictions will be performed with the latter.

Create reports

In addition to displaying spectra and molecular structures on the canvas. It is also possible to create various tables within JASON: Parameter tables, Peak list, and Multiplet tables. In addition, images can be imported, and free text objects can be added to the canvas providing the ability to configure, save and print reports.



Pos (ppm)	Start (ppm)	End (ppm)	Type	J (Hz)	Normalized
0.997	0.965	1.042	t	7.43(2)	3.000
1.526	1.438	1.622	ddq	13.67;9.11;7.35(3)	0.996
1.961	1.899	2.034	dqd	13.67;7.54(3);4.54	0.998
2.603	2.546	2.657	dddd	9.10;7.89;4.53;3.92	0.870
2.810	2.759	2.861	ddq	17.24;3.98;0.71(3)	0.995
3.304	3.242	3.370	ddq	17.26;7.84;0.70(3)	0.992
7.347	7.316	7.377	m		0.828
7.448	7.422	7.470	m		0.760
7.564	7.539	7.590	td	7.48(2);1.26	0.800
7.734	7.714	7.756	d[sx]	7.66;0.63(5)	0.631

Filename	Ethylindanone_Proton-13-1.jdf
Title	Ethylindanone
Author	delta
Experiment	proton.jxp
Solvent	CHLOROFORM-D
Actual Start Time	2017-08-24T16:05:17
Field Strength	9.38977 T
Spectrometer	DELTA2_NMR
Scans	8
Relaxation Delay	5 s
Receiver Gain	46
Exp. Total	67 s
Temperature	21.1 °C
Spin Rate	15 Hz
X Nuclide	1H
X Acq. Points	16384
X Acq. Time	2.18628 s
X Frequency	399.7802 MHz
X Sweep	7494.0048 Hz
X Angle	45 °
X Apodization	Exponential=0.069Hz
X Zero Filling	Factor or Size=8

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