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# Automatic Structure Verification: current status

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# What is ASV? Part I

Molecule versus experimental spectra (1D, 2D, MS, ...):  
Questions to ask: *Might it fit? Is it definitely ruled out?*

Automatic (ASV) versus  
Computer Assisted (CASV) structure verification  
Necessity/possibility to cover both aspects

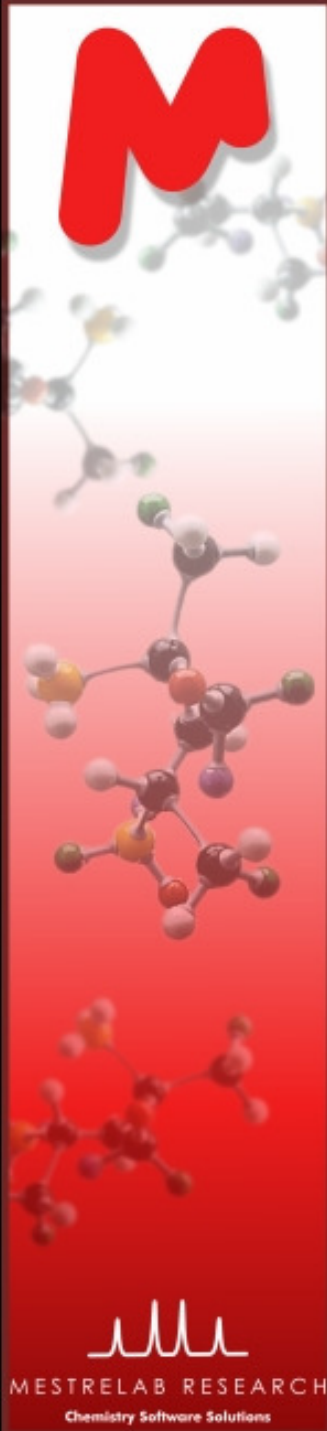
The NMR branch of Mnova ASV is based on  
NMR predictions and  
General rules of the NMR trade (quantitative aspects)

Practical issues to live with:

Real-life spectra: complete with  
solvent peaks, artifact peaks, quantitation errors

Real-life predictions of parameters:  
Error bounds, inversions, almost totally uncertain labiles

Target: Small and medium-sized molecules with  
well-defined peaks & multiplets





## What is ASV? Part II

First of all, it is a **scoring system** (a math concept) based on a library of **ASV tests**.

It is organized into **ASV tasks**, each task comprising a number of ASV tests.

User Interface covers:

Simple tests (one molecule against one spectrum) and various batch modes and scripts

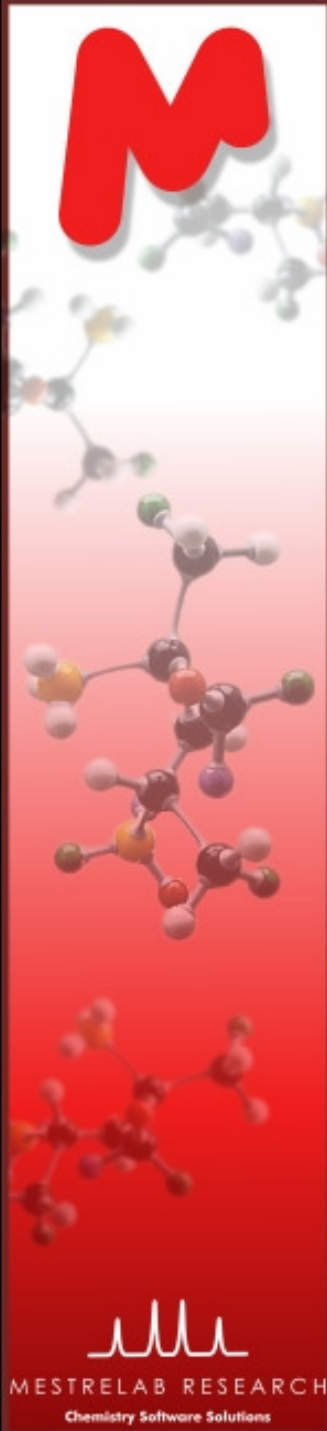
It allows to combine 1D and 2D spectra (HSQC)

It also allows to combine NMR and MS data

Coming soon:

User scripting of custom ASV tasks





# Exploitation of 1D spectra in Mnova ASV

Pre-requisites: GSD with Auto-Edit

Solvent recognition

Labile peaks recognition

Impurities recognition

Efficient J-coupling multiplets recognition

Currently implemented tools for ASV tests:

Novel spectrum similarity metric

Bayesian Number of Nuclides assessments

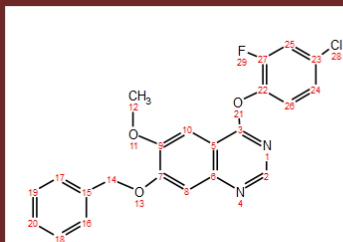
Similarity metric extension for prediction error bounds

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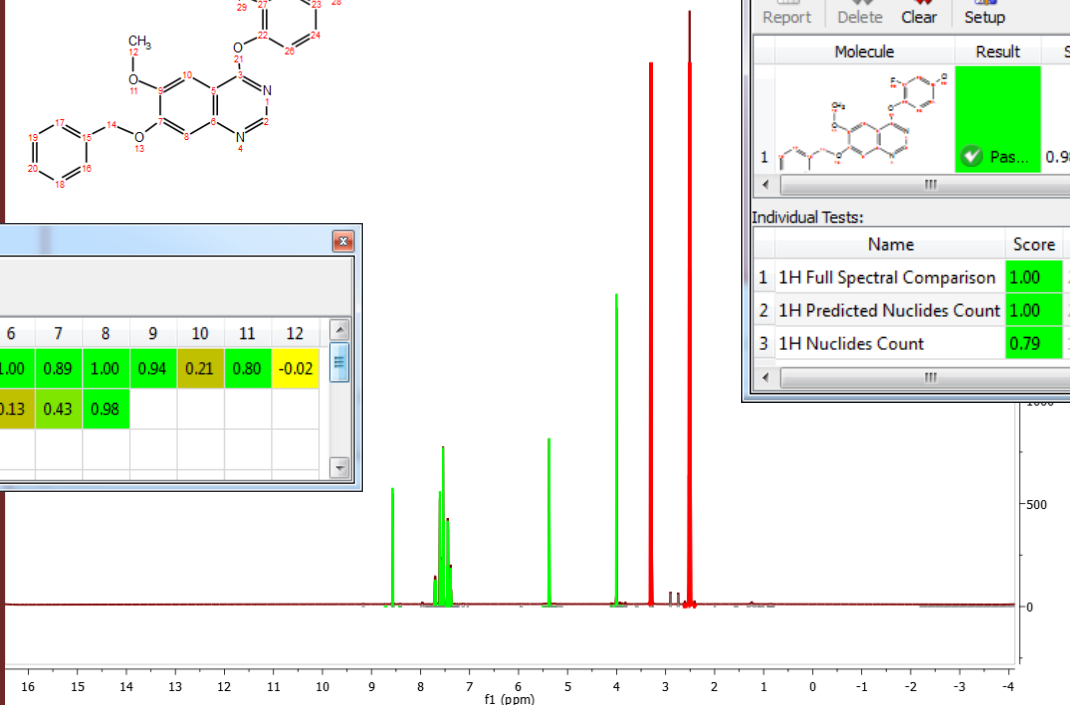
## Present Status

The system is fully operative and already quite good

We now go as far as one can go short of complete assignments of nuclei to spectral multiplets



	1	2	3	4	5	6	7	8	9	10	11	12
A	0.99	0.89	1.00	0.98	0.90	1.00	0.89	1.00	0.94	0.21	0.80	-0.02
B	0.15	0.99	0.98	0.99	0.74	0.13	0.43	0.98				
C												



Molecule	Result	Score	Significance
	✓ Pas...	0.98	4

Name	Score	Significance	Dist
1 1H Full Spectral Comparison	1.00	2	0.041
2 1H Predicted Nuclides Count	1.00	2	0.000
3 1H Nuclides Count	0.79	1	0.894





# Perspectives

ASV has been so far rarely attempted  
and it never reached maturity for widespread use

Its development will probably continue for decades:  
it is a new category of NMR software

## Planned short-term steps:

Ongoing improvements due to  
better recognition of solvent and labile peaks

Enumeration of all possible assignments  
and scoring on all of them.

This will involve the J-structure of the multiplets





# Invitation

You are ALL invited to join the ASV bandwagon

You will get a useful, working product  
becoming better and better

And YOU will be able to actively contribute  
to its development

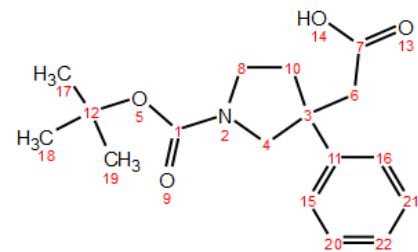
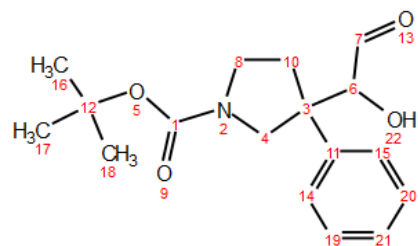


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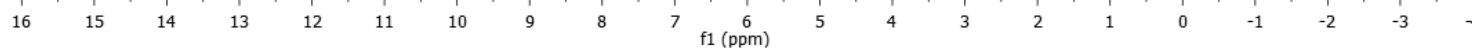
## Example #1

One spectrum, two (or more) molecules



	Name	Score	Significance	Distance
1	1H Full Spectral Comparison	1.00	2	0.0422
2	1H Predicted Nuclides Count	-0.87	8	0.0210
3	1H Nuclides Count	-0.03	2	0.4851

	Name	Score	Significance	Distance
1	1H Full Spectral Comparison	1.00	2	0.0245
2	1H Predicted Nuclides Count	1.00	2	0.0016
3	1H Nuclides Count	0.36	2	0.6807

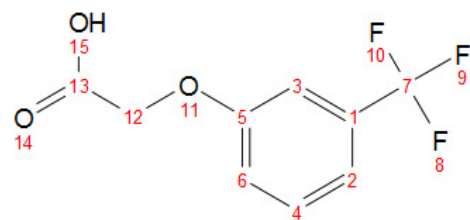




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## Example #2a

Failure due to bad solvent recognition

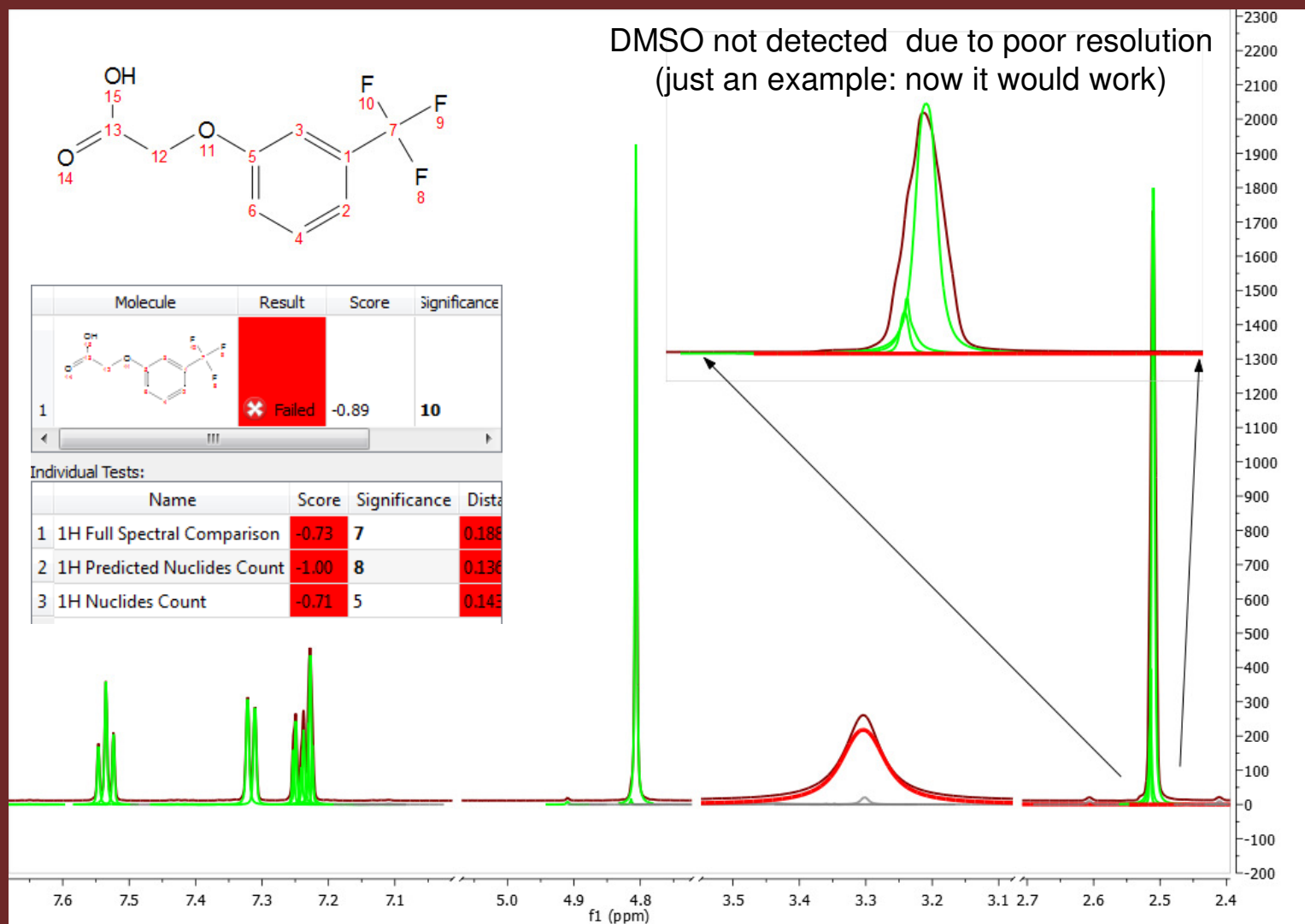


	Molecule	Result	Score	Significance
1		<b>Failed</b>	<b>-0.89</b>	<b>10</b>

Individual Tests:

	Name	Score	Significance	Dist
1	1H Full Spectral Comparison	<b>-0.73</b>	<b>7</b>	<b>0.188</b>
2	1H Predicted Nuclides Count	<b>-1.00</b>	<b>8</b>	<b>0.136</b>
3	1H Nuclides Count	<b>-0.71</b>	<b>5</b>	<b>0.143</b>

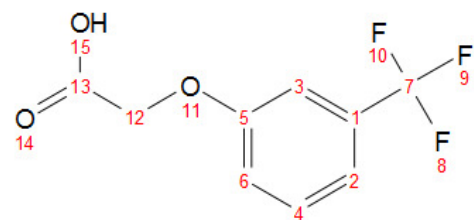
DMSO not detected due to poor resolution  
(just an example: now it would work)



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## Example #2b

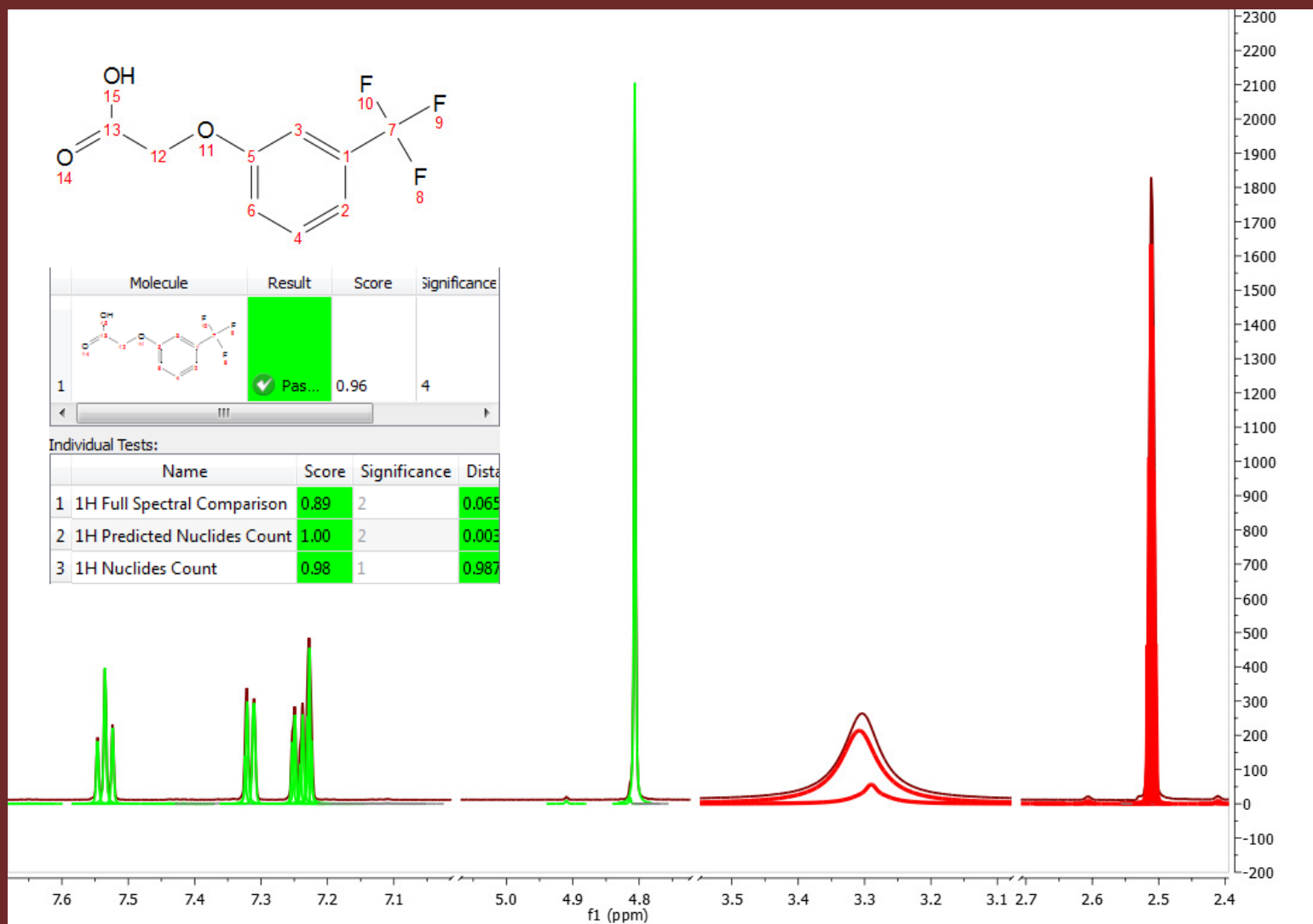
Success after manual marking of the solvent (CASV)



Molecule	Result	Score	Significance
	<input checked="" type="checkbox"/> Pas...	0.96	4

Individual Tests:

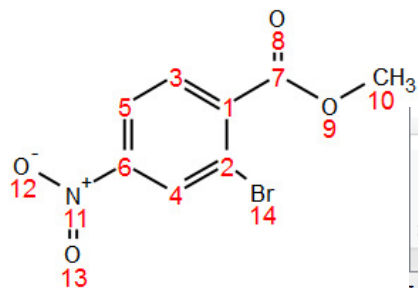
Name	Score	Significance	Dist
1 1H Full Spectral Comparison	0.89	2	0.065
2 1H Predicted Nuclides Count	1.00	2	0.003
3 1H Nuclides Count	0.98	1	0.987



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## Example #3

One molecule, two (or more) spectra



Molecule	Result	Score	Significance
1	✓ Pas...	0.99	4

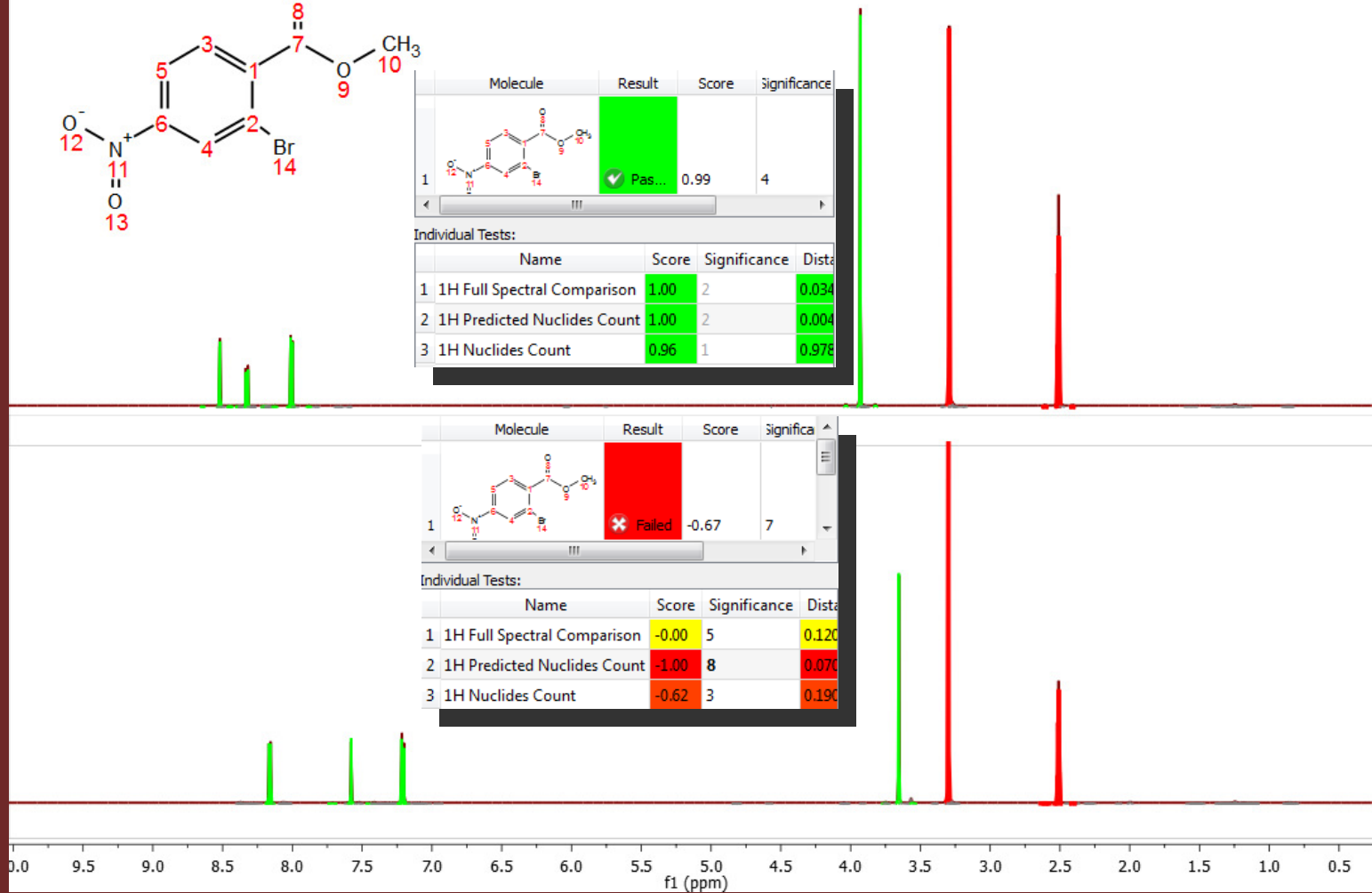
Individual Tests:

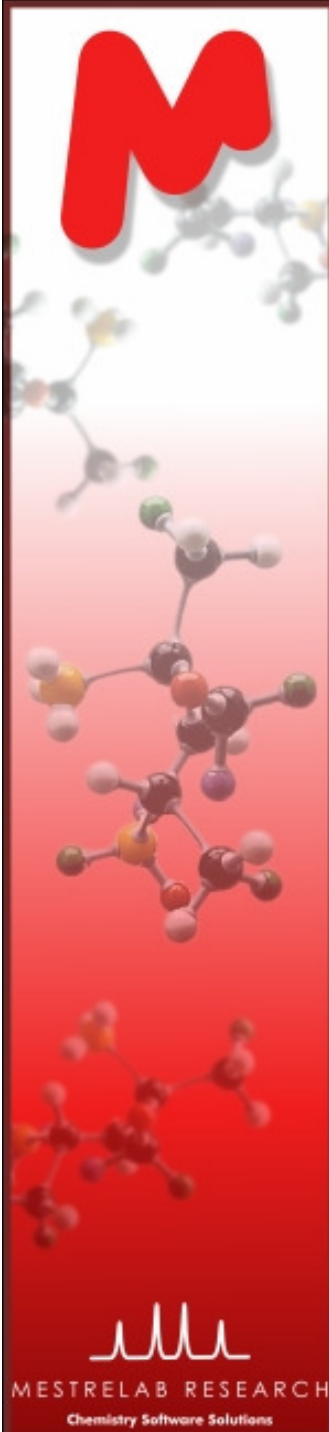
Name	Score	Significance	Dist
1 1H Full Spectral Comparison	1.00	2	0.034
2 1H Predicted Nuclides Count	1.00	2	0.004
3 1H Nuclides Count	0.96	1	0.978

Molecule	Result	Score	Significance
1	* Failed	-0.67	7

Individual Tests:

Name	Score	Significance	Dist
1 1H Full Spectral Comparison	-0.00	5	0.120
2 1H Predicted Nuclides Count	-1.00	8	0.070
3 1H Nuclides Count	-0.62	3	0.190





**Thank You** for your **Patience**

Any Questions ?

SMASH 2010, Portland, OR, USA

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