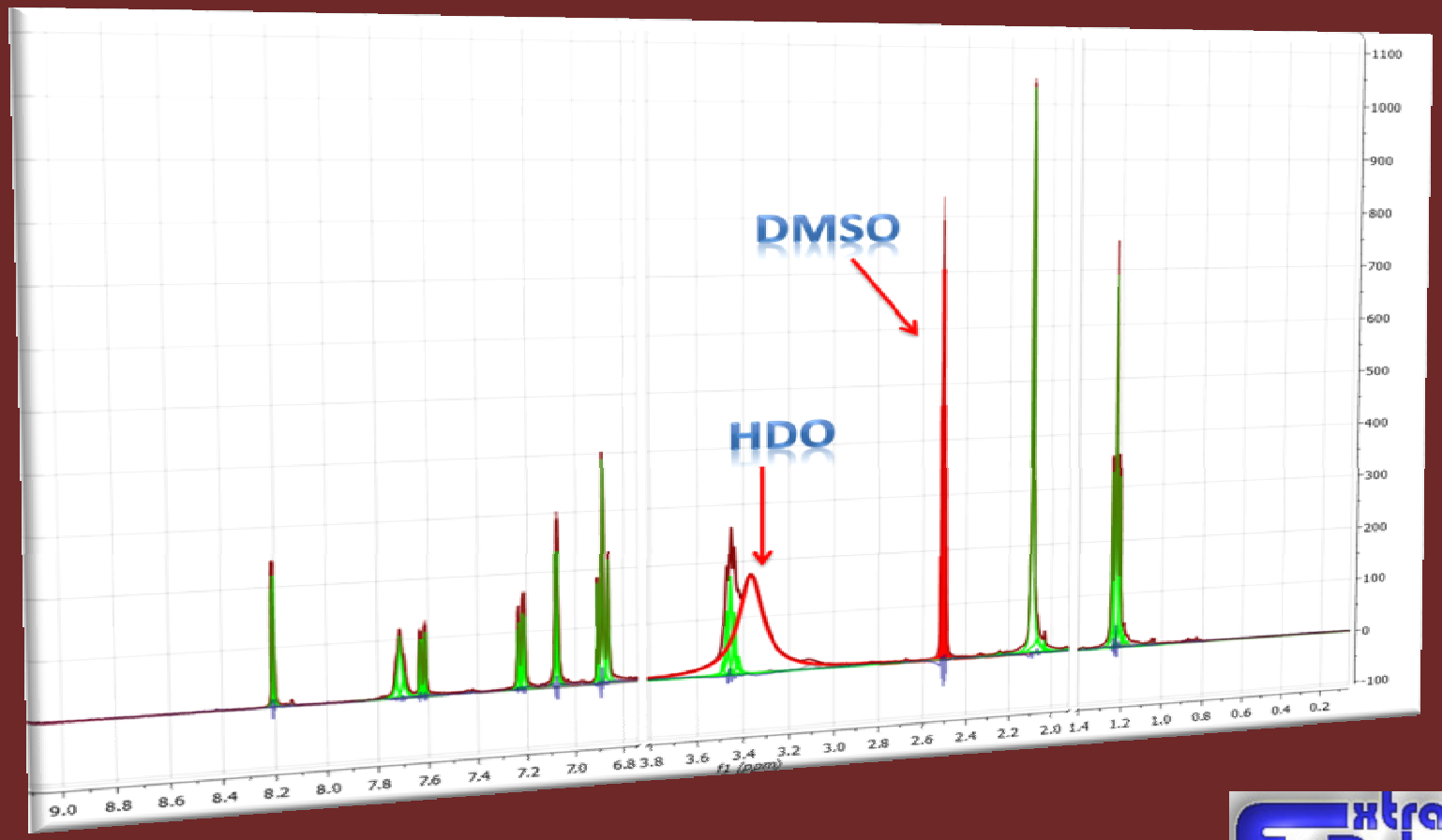
Automatic Solvent Recognition wizard:
example of an AI at work

Stan Sykora, Carlos Cobas,
Felipe Seoane, Pablo Monje, Esther Vaz, et al



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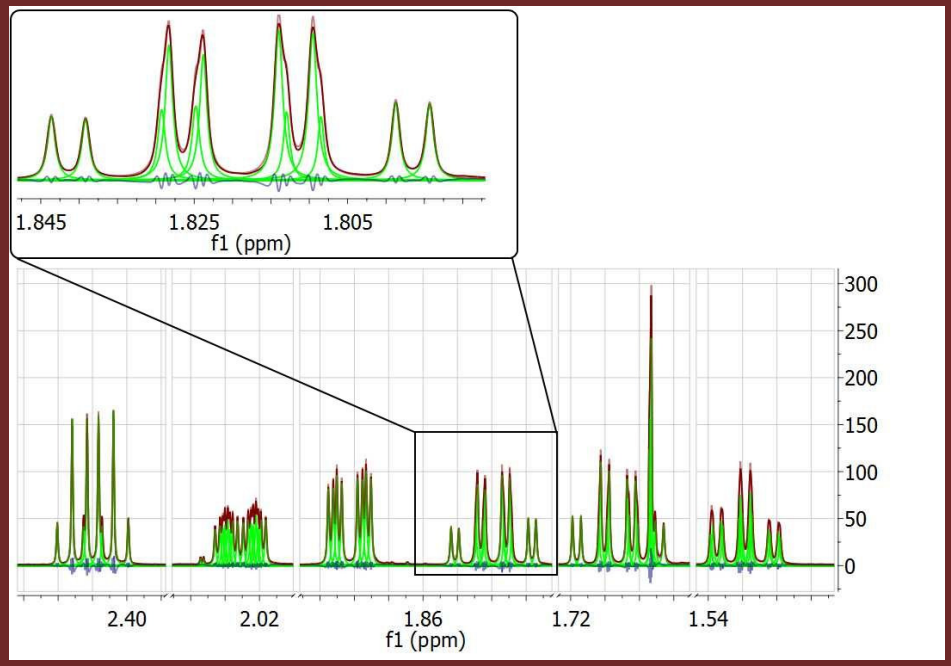
GSD – Global Spectral Deconvolution

f-domain algorithm which automatically decomposes sets of superposed *Lorentzians* and *near-Lorentzians* and ends up in a **GSD Peaks List**

GSD is a standard feature of Mnova,
subject to continuous developmnet



GSD has been born in 2008
and presented in detail at several meetings in 2009 and 2010

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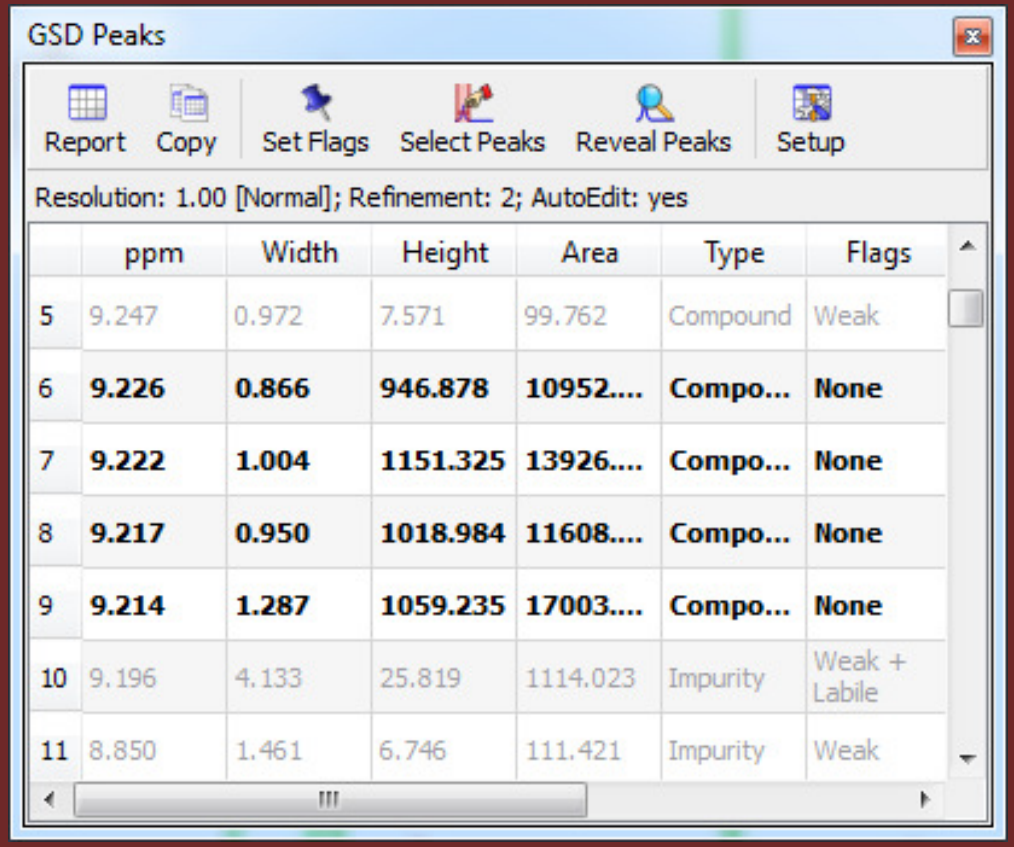
GSD Peaks Editing

Peaks editing brings in

specific NMR know-how

by **classifying** of the peaks in an GSD List



	ppm	Width	Height	Area	Type	Flags
5	9.247	0.972	7.571	99.762	Compound	Weak
6	**9.226**	**0.866**	**946.878**	**10952....**	**Compo...**	**None**
7	**9.222**	**1.004**	**1151.325**	**13926....**	**Compo...**	**None**
8	**9.217**	**0.950**	**1018.984**	**11608....**	**Compo...**	**None**
9	**9.214**	**1.287**	**1059.235**	**17003....**	**Compo...**	**None**
10	9.196	4.133	25.819	1114.023	Impurity	Weak + Labile
11	8.850	1.461	6.746	111.421	Impurity	Weak

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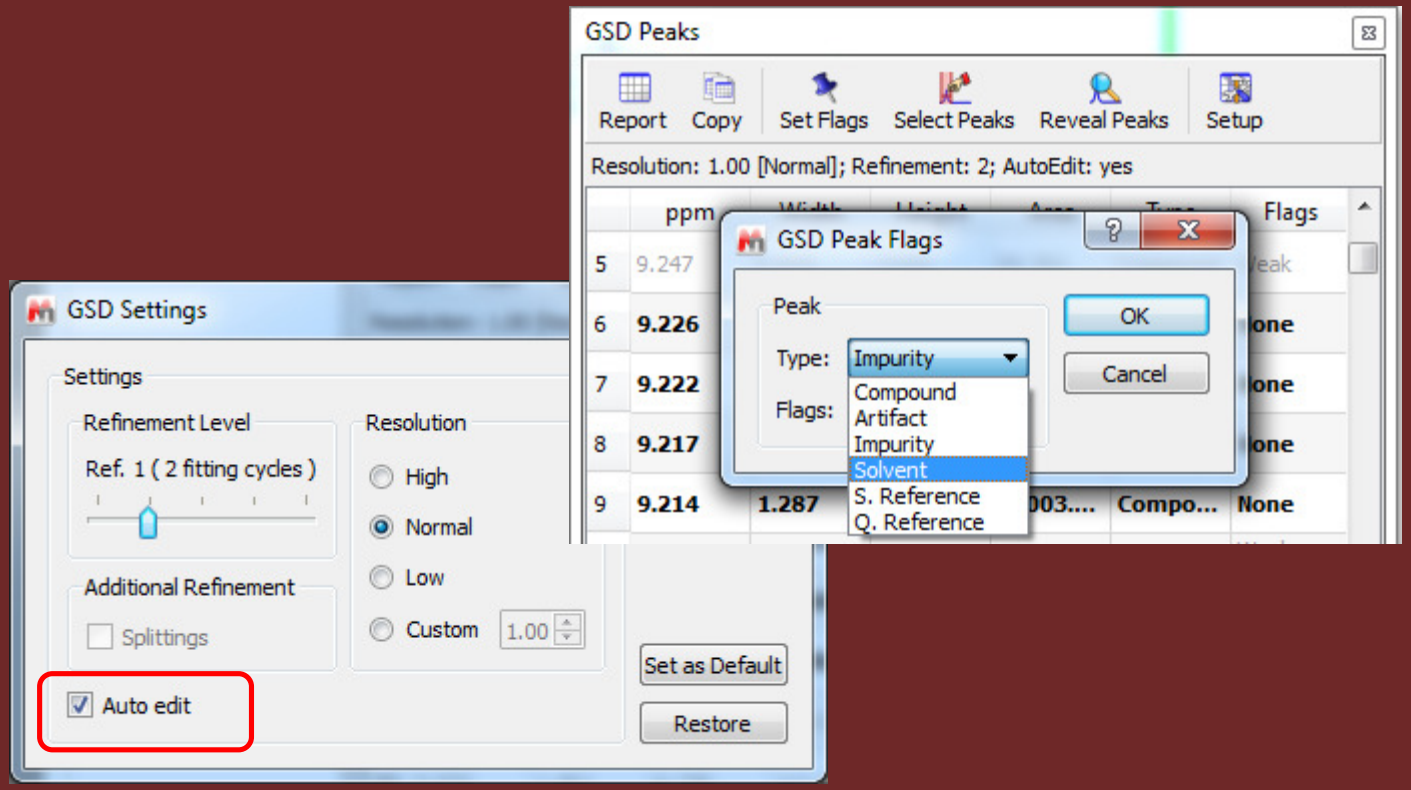
GSD Peaks Editing Modes

- ✓ Manual: Always accessible
- ✓ Automatic: An optional GSD feature always used in ASV



AutoEdit does not exclude subsequent manual peaks editing
(transparently followed by PostEdtit)

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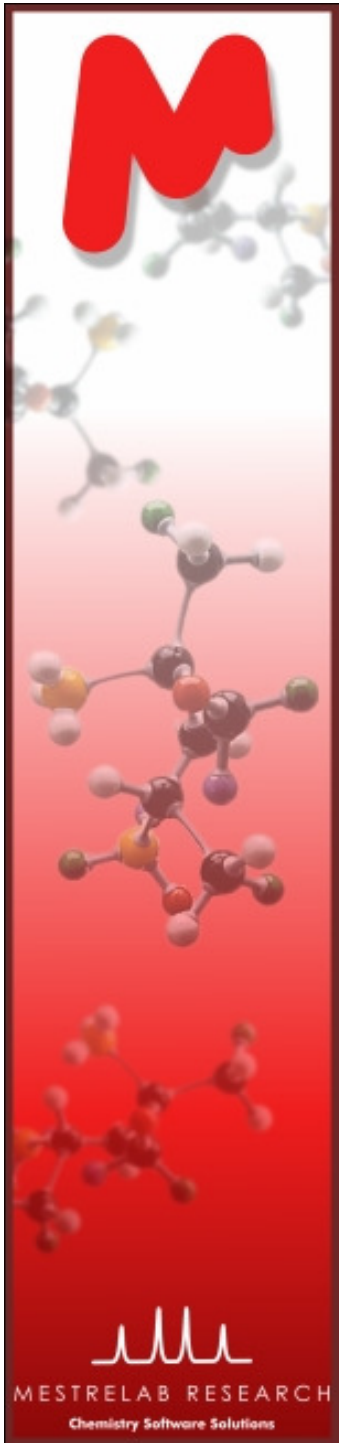
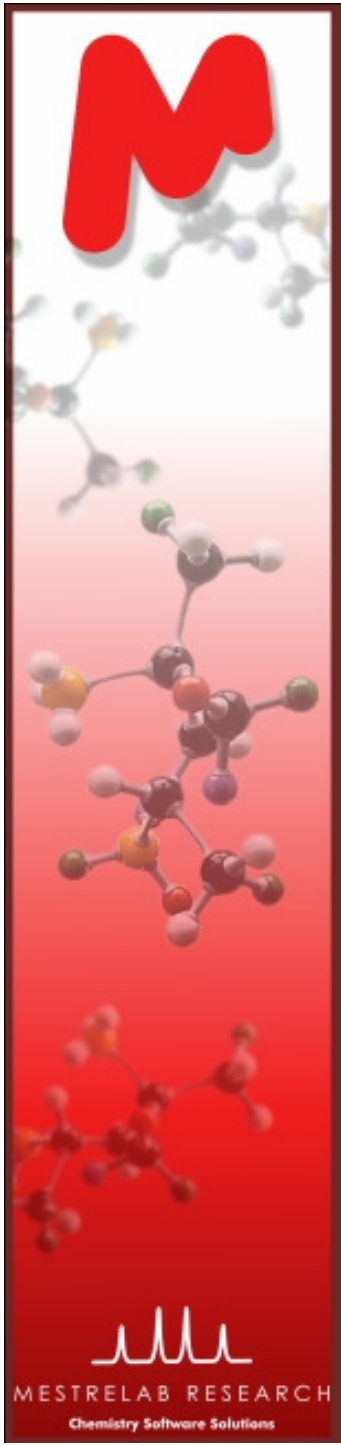


The GSD Auto-Edit algorithm: what is it up to

- ✓ Reference peaks recognition
- ✓ ^{13}C satellites recognition (where possible)
- ✓ Solvent peaks recognition (primary and secondary)
- ✓ Labile peaks recognition
- ✓ J-coupling multiplets recognition
- ✓ Impurity peaks recognition
- ✓ Weak peaks labeling



GSD Auto Editing results

Peak Types:

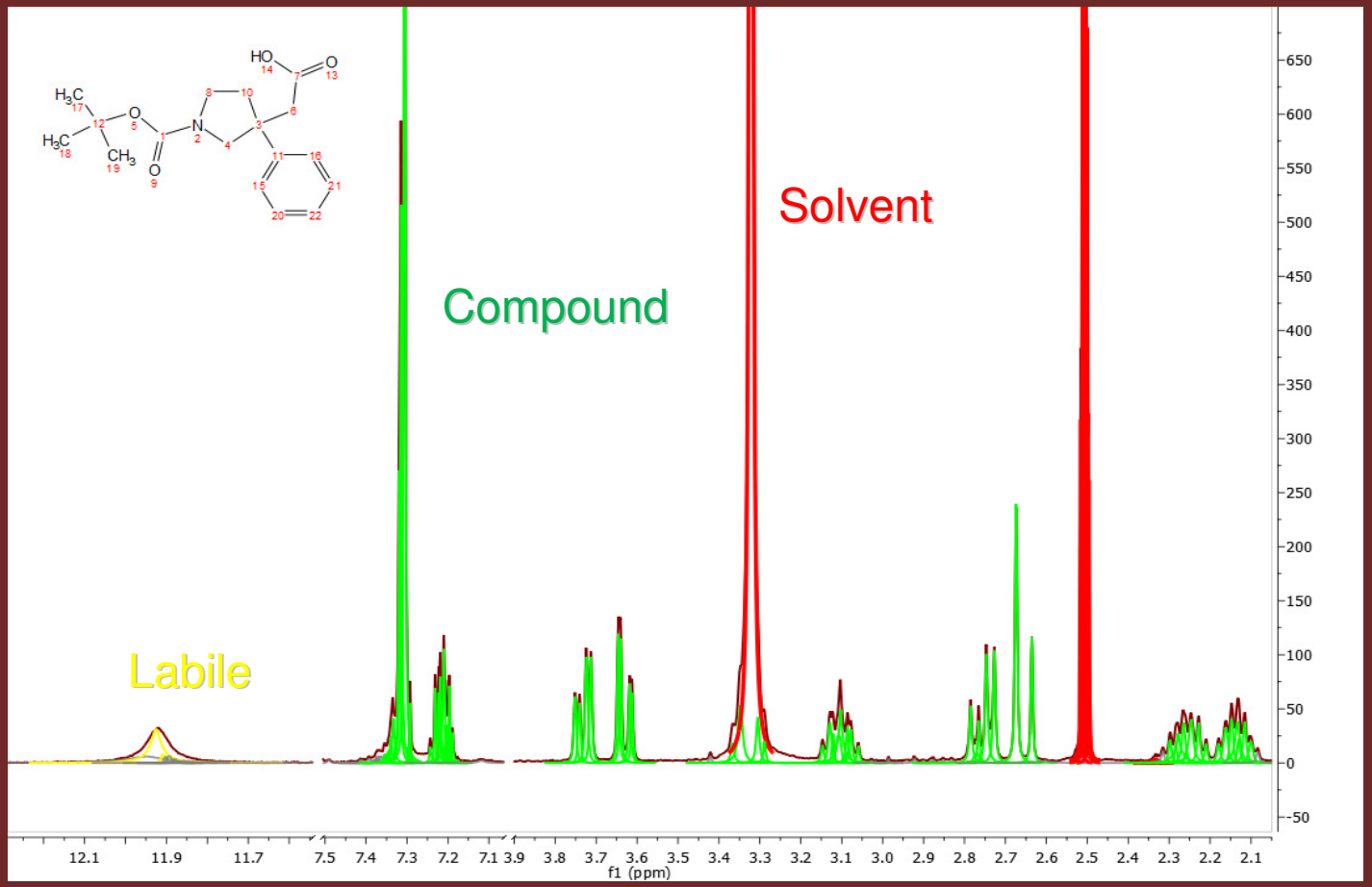
pt_Compound,
pt_Artifact,
pt_Impurity,
pt_Solvent,
pt_SReference,
pt_QReference

Peak Flags:

pf_SetByUser
pf_Hidden
pf_Weak
pf_C13Satellite
pf_Rotational
pf_Labile
pf_HasC13Sats

What can one do with the Edited Peaks List

a) Color-labeled peak plots of the edited peaks



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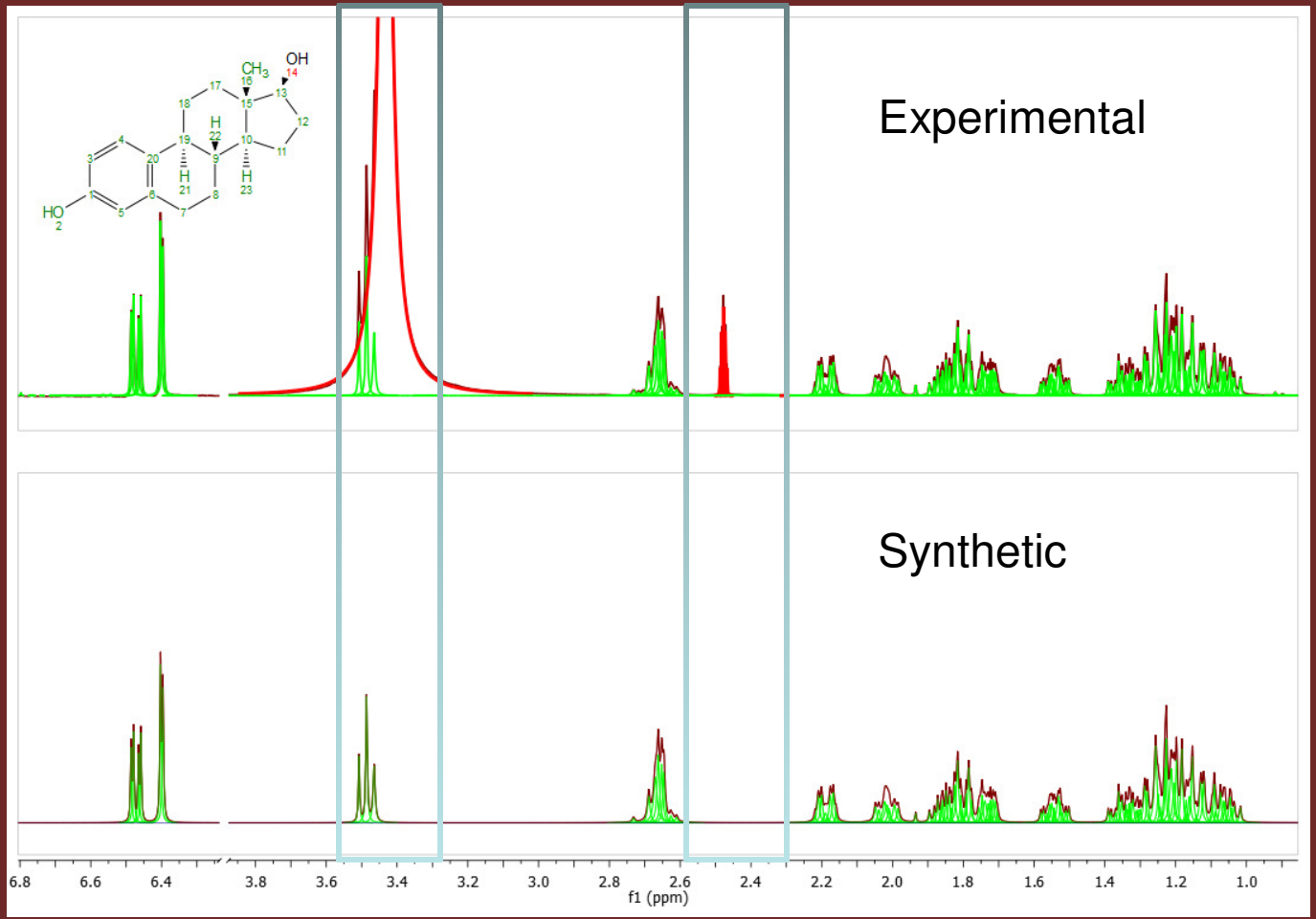
What can one do with the Edited Peaks List

b) Synthetic spectra of any desired category of peaks



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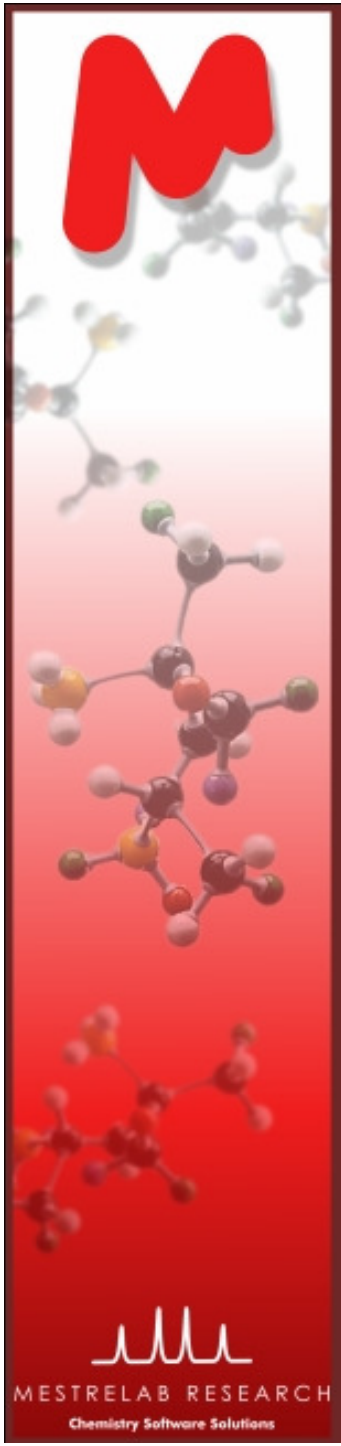
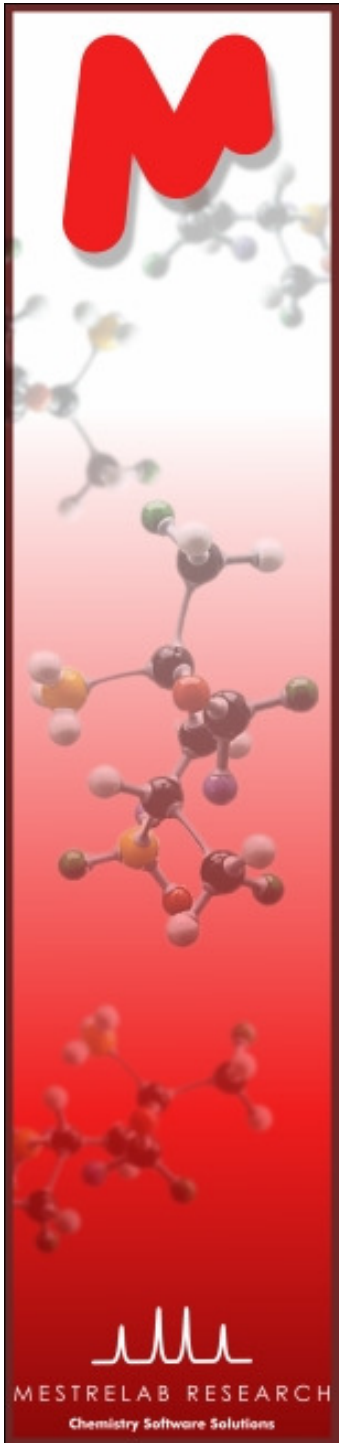


What can one do with the Edited Peaks List ?

c) Good editing is an essential pre-requisite of …

… ASV !

Automatic Structure Verification



Solvent recognition

Possibly the most important and tricky part of **AutoEdit**

Human solvent recognition:

Based on a few imperfect rules and lots of intuition

Automatic solvent recognition:

Based on a long list of imperfect scoring tests

Primary and secondary solvent signals:

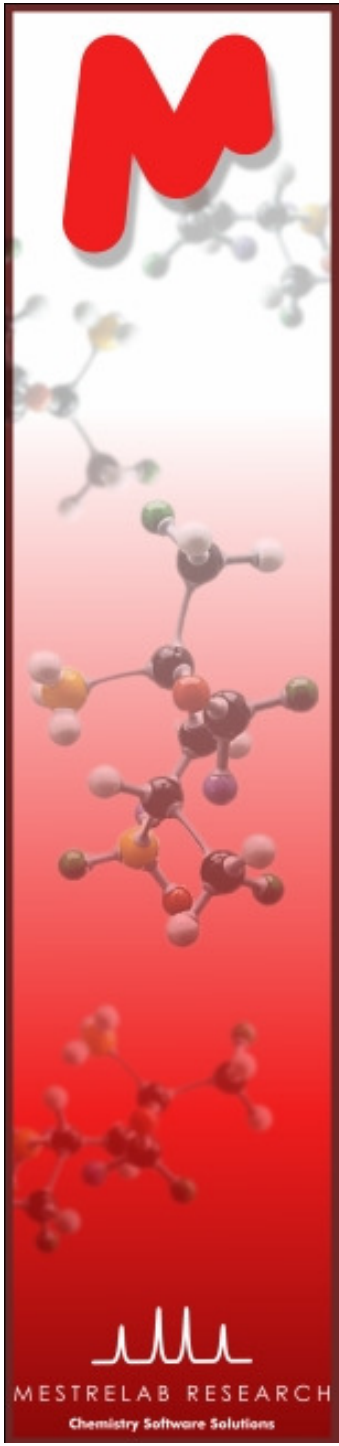
Primary solvent recognition is relatively easy

Secondary solvent signals (water) often present problems

Basic development rule:

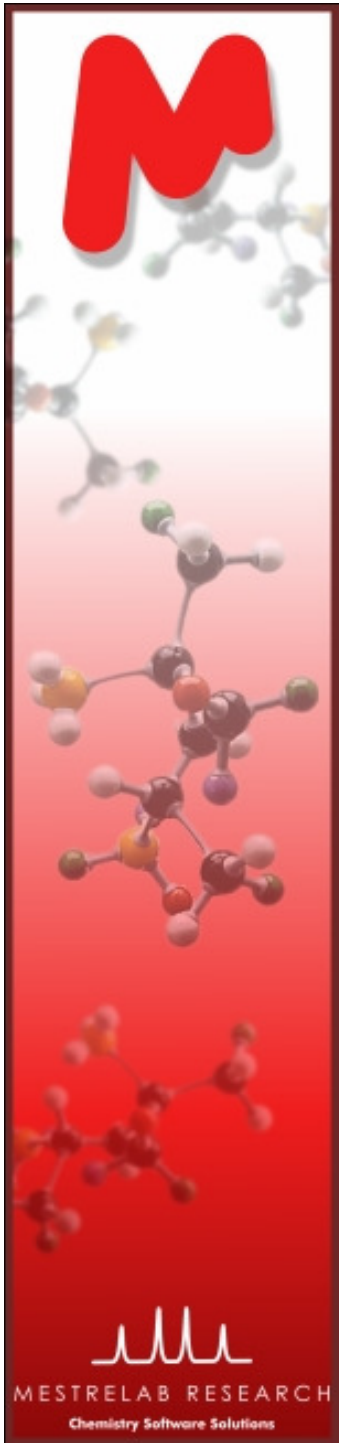
How the hell does Tony know that this peak belongs to solvent !!!

(if you ask him, he does not know)



Solvent description

```
DWORD SdFlags;      // See the FFP_Flags enum in EbPeaks.h
                    // Main Multiplet:
REAL  Shift;              // typical main multiplet shift value
REAL  ShiftLoPpm;         // low limit of main multiplet in ppm
REAL  ShiftHiPpm;         // high limit of main multiplet in ppm
DWORD Npeaks;             // number of main peaks (may not be 0)
REAL  JHz;                // coupling constant
REAL  Pweights[5];        // array of relative weights of the peaks
                    // Satellite Peaks:
REAL  SatWeight;          // satelites relative weight (0.011 or 0)
REAL  JSatHz;             // satelites coupling constant
REAL  SatShiftPpm;        // satelites relative isotope shift
                    // Associated Multiplet:
DWORD Npeaks2;            // number of peaks (may bee 0)
REAL  Weight2;            // relative weight (typical)
REAL  ShiftPpm2;          // relative isotope shift
REAL  JHz2;               // coupling constant
REAL  Pweights2[5];       // array of relative weights of the peaks
```



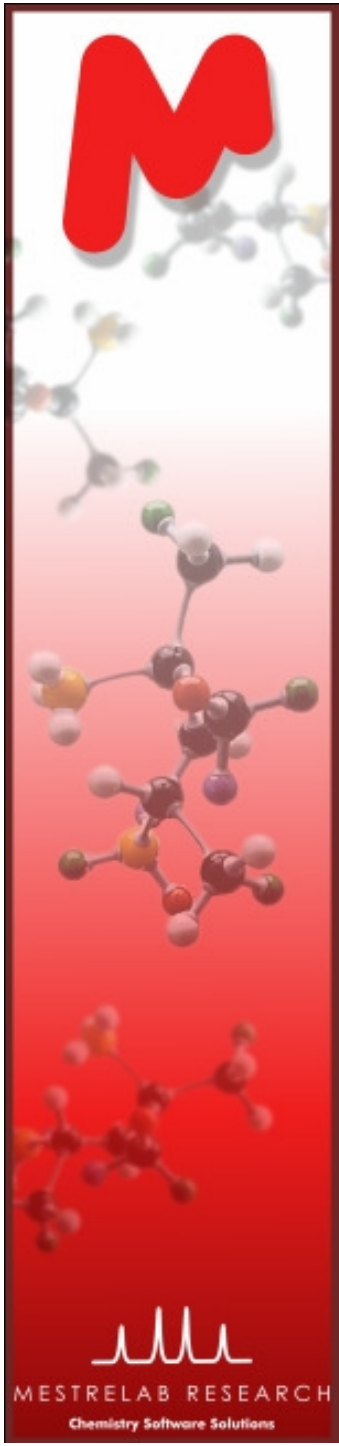
Solvent descriptors

Typically, a solvent entry in Mnova contains two Solvent Descriptors:

- One for the **primary solvent** peaks and
- One for the **secondary solvent** peaks (usually water)

However, it could contain any number of them (even a typical impurity might be nominally considered part of the solvent)

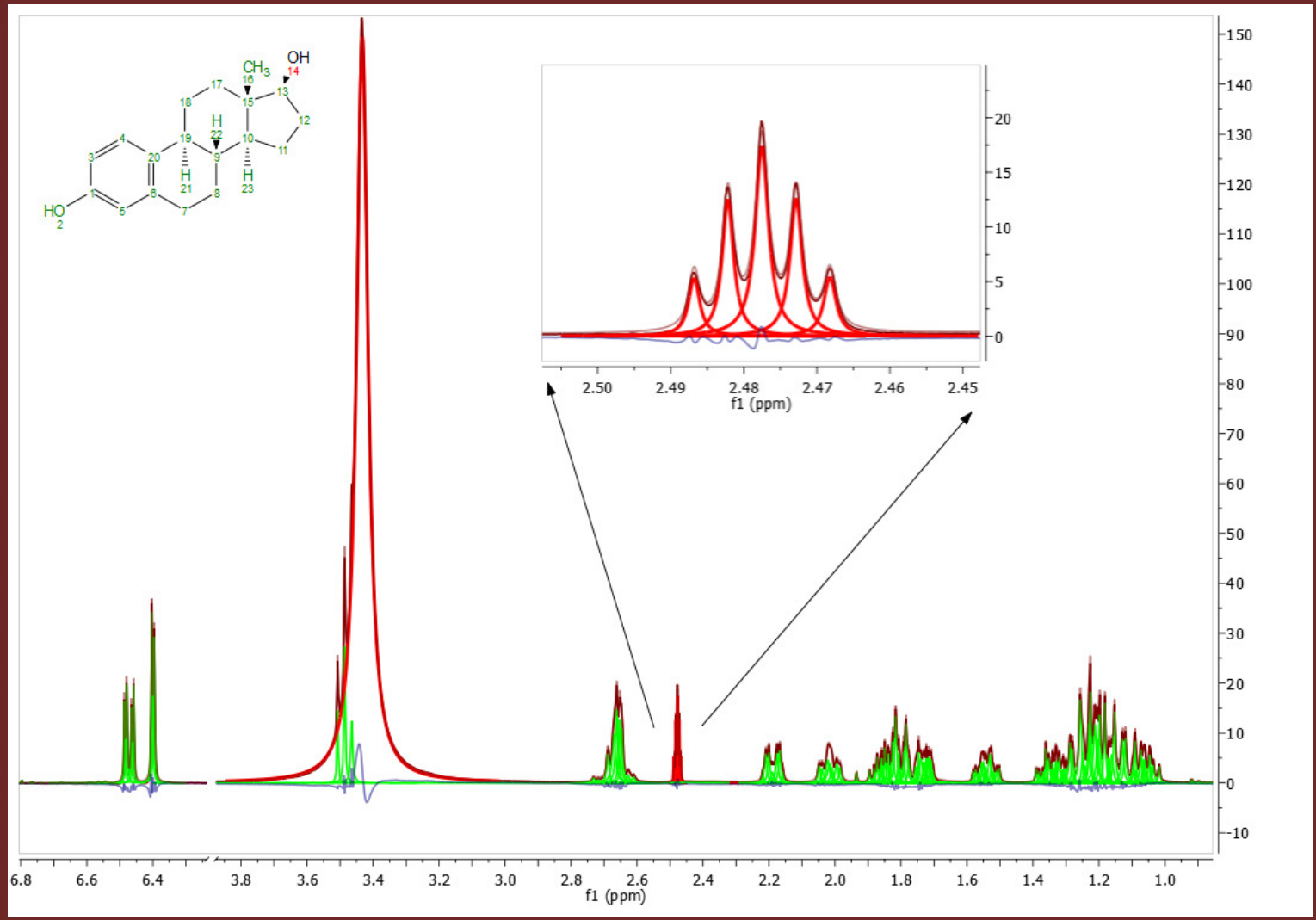
Coming soon:
Possibility to easily edit and add solvent description XML files.



Solvent recognition algorithm

- ✓ Look for the central peak of a solvent multiplet
- ✓ Scan all peaks in the admissible range
- ✓ Associate a full-fledged scoring system with each peak
- ✓ Scan on all of these criteria (if pertinent):
  - Position
  - Width
  - Height
  - Kurtosis
  - Presence of J-coupling multiplet peaks
    - J-HD coupling constant value
    - Relative intensities
  - Presence of 13C satellite peaks
    - Relative intensites
    - J-CH coupling value
    - J-CH isotope shift
  - Presence of secondary J-coupling multiplet
    - Relative intensities
    - J-HD coupling in secondary multiplet

Some examples



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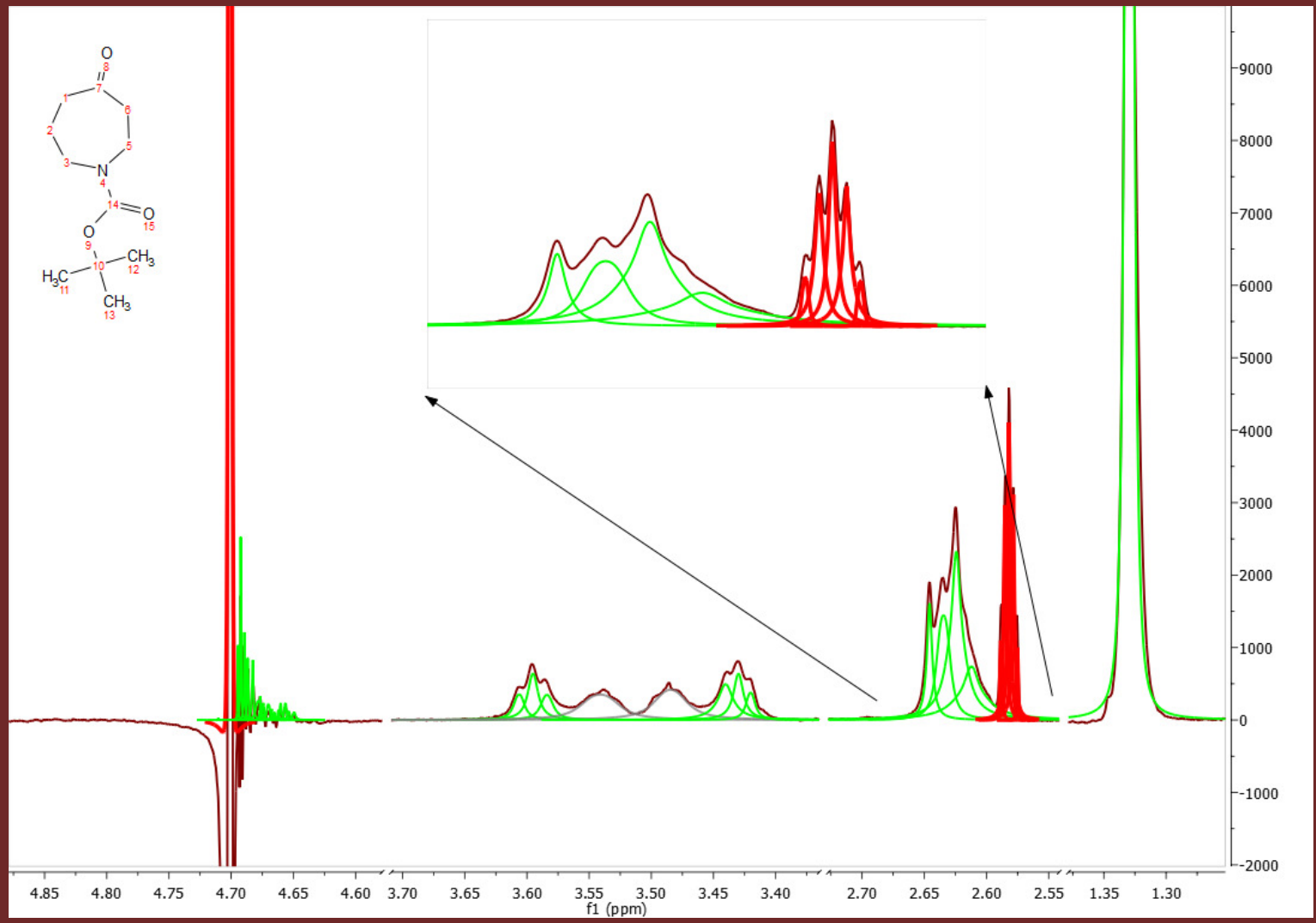
Some examples



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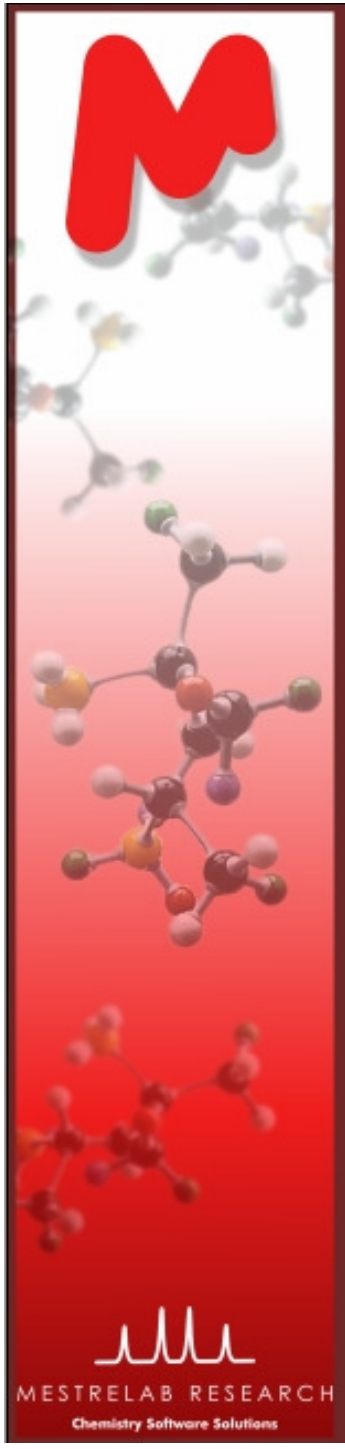

Thank You for your Patience

Any Questions ?

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