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A NEW DIMENSION OF QMSA: SPECTRA OF MILLIONS TRANSITIONS

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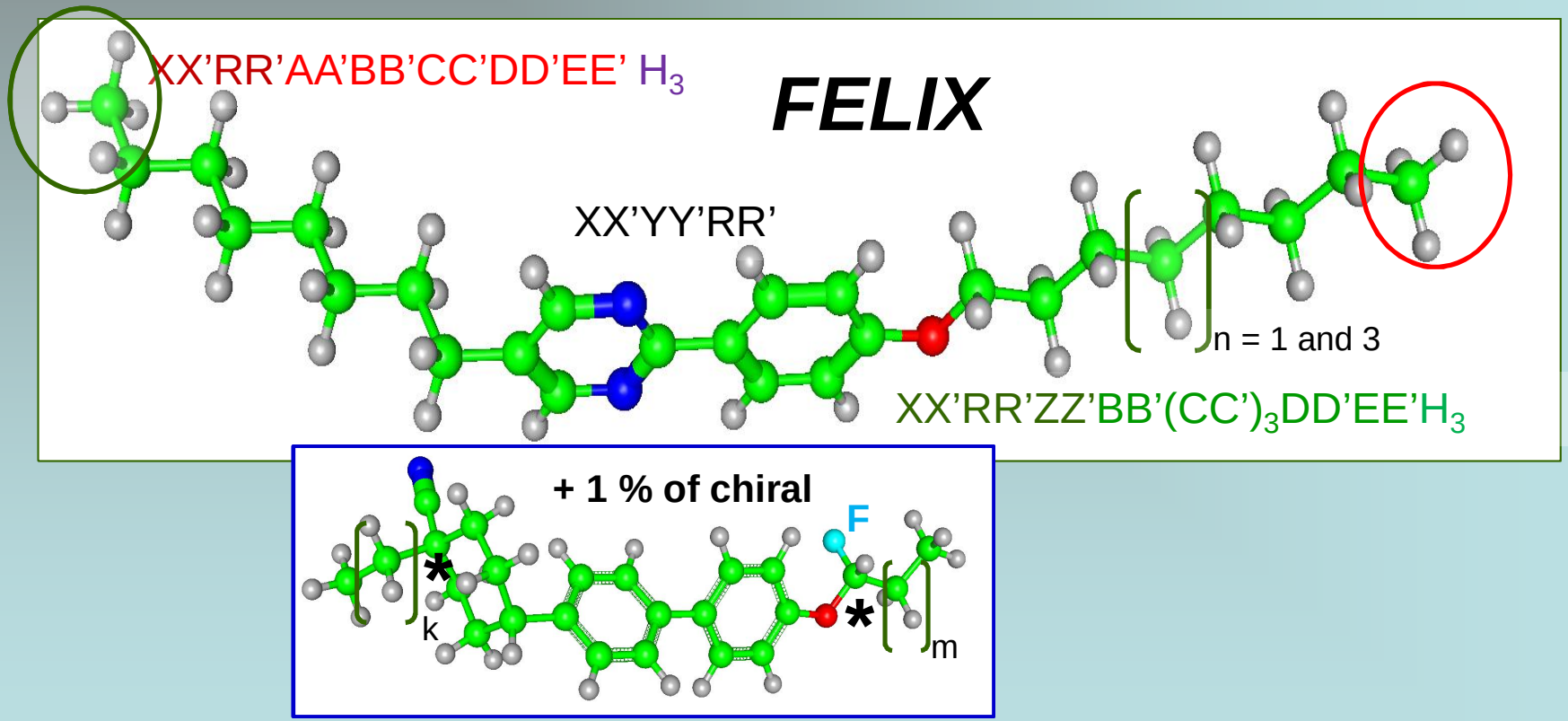
QMSA of total ^{1}H NMR and 1D TOCSY spectra of *FELIX chiral nematic solvent*

An example of a large, very tightly coupled spin-system, solved by QMSA of 1D TOCSY spectra

29 spin-particles (60 protons) in 4 sub-systems

Totally > 30 000 000 non-zero intensity transitions !



QMSA of Ph-$(CH_2)_7CH_3$

Experimental: ^{1}H TOCSY spectrum in which *response factors* of the CH_n protons decay from 1.00 (XX') to 0.26 (K_3)

SpinAdder treats as an XX'RR'AA'BB'CC'DD'EE'K_3 –system:
Simulation time: < 60 sec
Theoretical transitions: 58 048 992
non-zero intensities: 5 442 2281 (99.8% of theor. intensity)
non-zero intensities: 2 223 827 (97.5% of theor. intensity)
Lines after packing: 129 871 (packing criterium 0.010 Hz)
For AA'BB'CC'DD'EE' all the ^{2}J, ^{3}J and ^{4}J are not well-defined by the spectrum, they were taken from analysis of heptane (MRC) and kept constant during iteration.

ALL THE CH_2 SHIFTS WELL-DEFINED, see THE ORDER: A-B-E-C-D !
ANALYSIS EXPLAINS THE ODD SHAPE OF THE **CH_3-SIGNAL** (593 non-denerate lines within ca. 18 Hz) !

FELIX of MILLIONS TRANSITIONS

QMSA of the octanol and decanol ethers

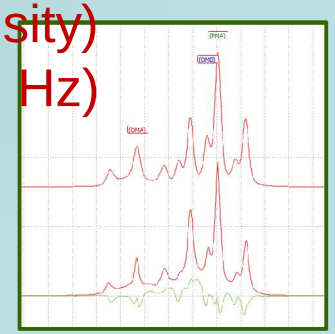
Experimental: normal 1H spectrum

Spin-systems:

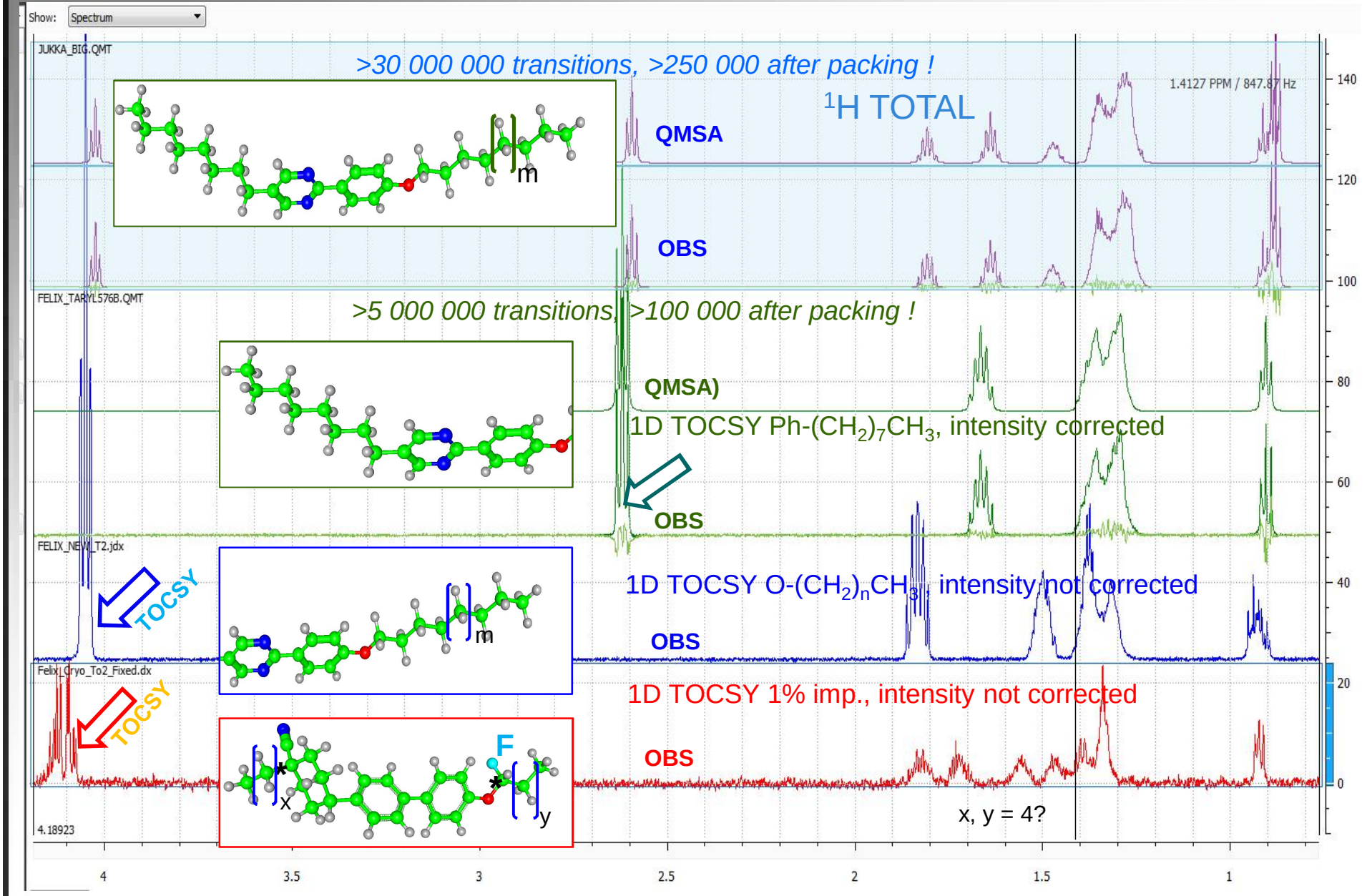
XX'RR'AA'BB'CC'DD'EE' H_3(50 mol%, octane system) +
XX'RR'ZZ' BB'CC'DD'EE'H_3 (24 mol%, octanol system)+
XX'RR'ZZ'BB'$(CC')_3$DD'EE'H_3 (21 mol%, decanol system) +
XX'YY'ZZ' (100 mol%)
(1 mol% *chiral impurity* with F, not included in QMSA)

Simulation time: 6 min

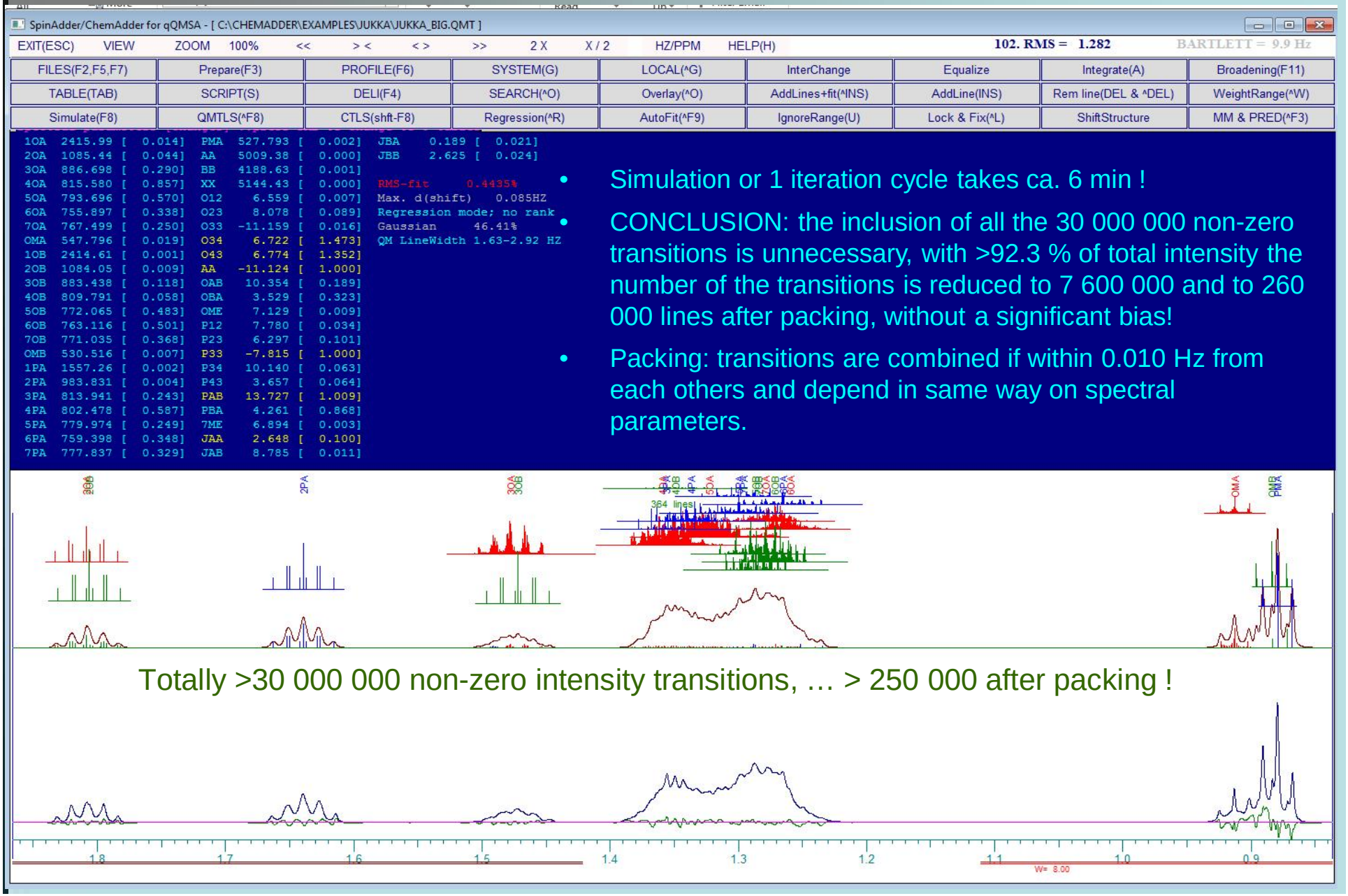
Theoretical transitions: 265 648 994
non-zero intensities: 32 680 248 (99.9% of theor. intensity)
non-zero intensities: 7 689 098 (92.8% of theor. intensity)
Lines after packing: 265 690 (packing criterium 0.010 Hz)
The order of CH_2-signals unclear
Explains the CH_2 signal:



*QMSA of total ^{1}H NMR and **1D TOCSY** spectra of FELIX chiral nematic solvent - lessons for old snakes*



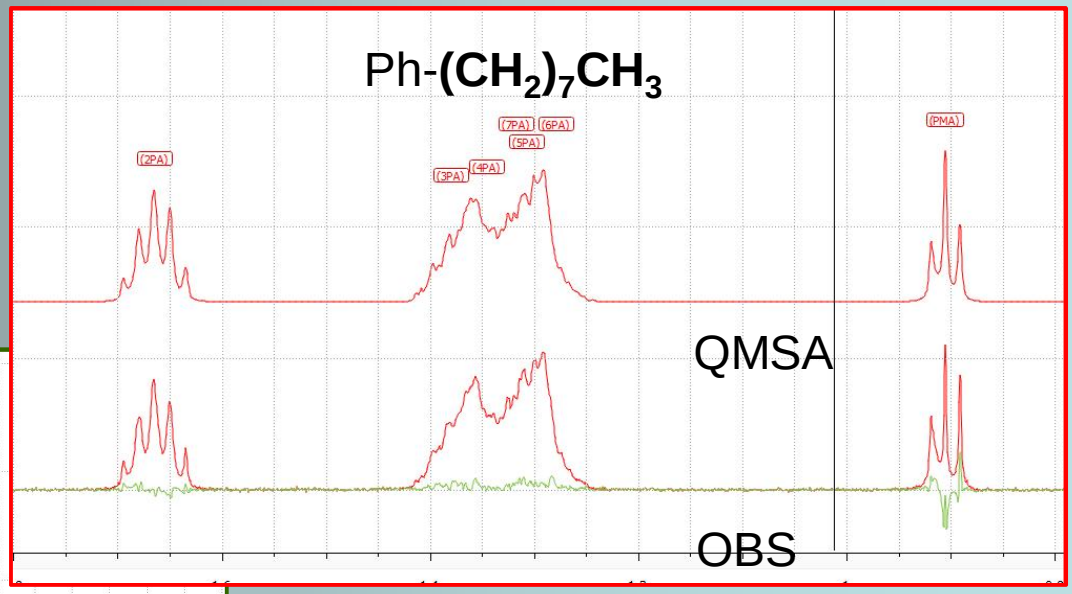
SpinAdder *display of QMSA of FELIX total ^{1}H NMR spectrum*

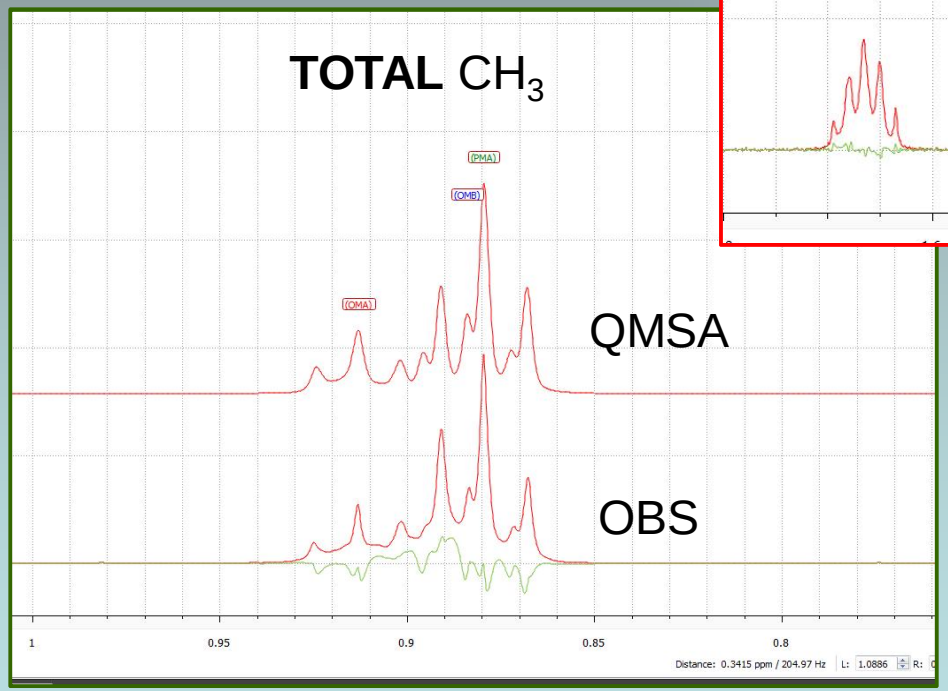


- Simulation or 1 iteration cycle takes ca. 6 min !
- CONCLUSION: the inclusion of all the 30 000 000 non-zero transitions is unnecessary, with >92.3 % of total intensity the number of the transitions is reduced to 7 600 000 and to 260 000 lines after packing, without a significant bias!
- Packing: transitions are combined if within 0.010 Hz from each others and depend in same way on spectral parameters.

Totally >30 000 000 non-zero intensity transitions, … > 250 000 after packing !

CH_3 QMSA


Ph-$(CH_2)_7CH_3$
(2PA)
(3PA)
(4PA)
(5PA)
(6PA)
(7PA)
(PMA)
QMSA
OBS


TOTAL CH_3
(OMA)
(OMB)
(PMA)
QMSA
OBS
1
0.95
0.9
0.85
0.8
Distance: 0.3415 ppm / 204.97 Hz
L: 1.0886
R: