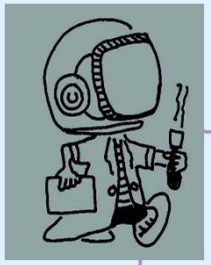
Based on presentation in Turku XXXIX Finnish NMR symposium, June 7-9th 2017

VIRTUAL ^{13}C-^{13}C COUPLED 1D HSQC SPECTRA – A NEW DIMENSION OF QMSA:



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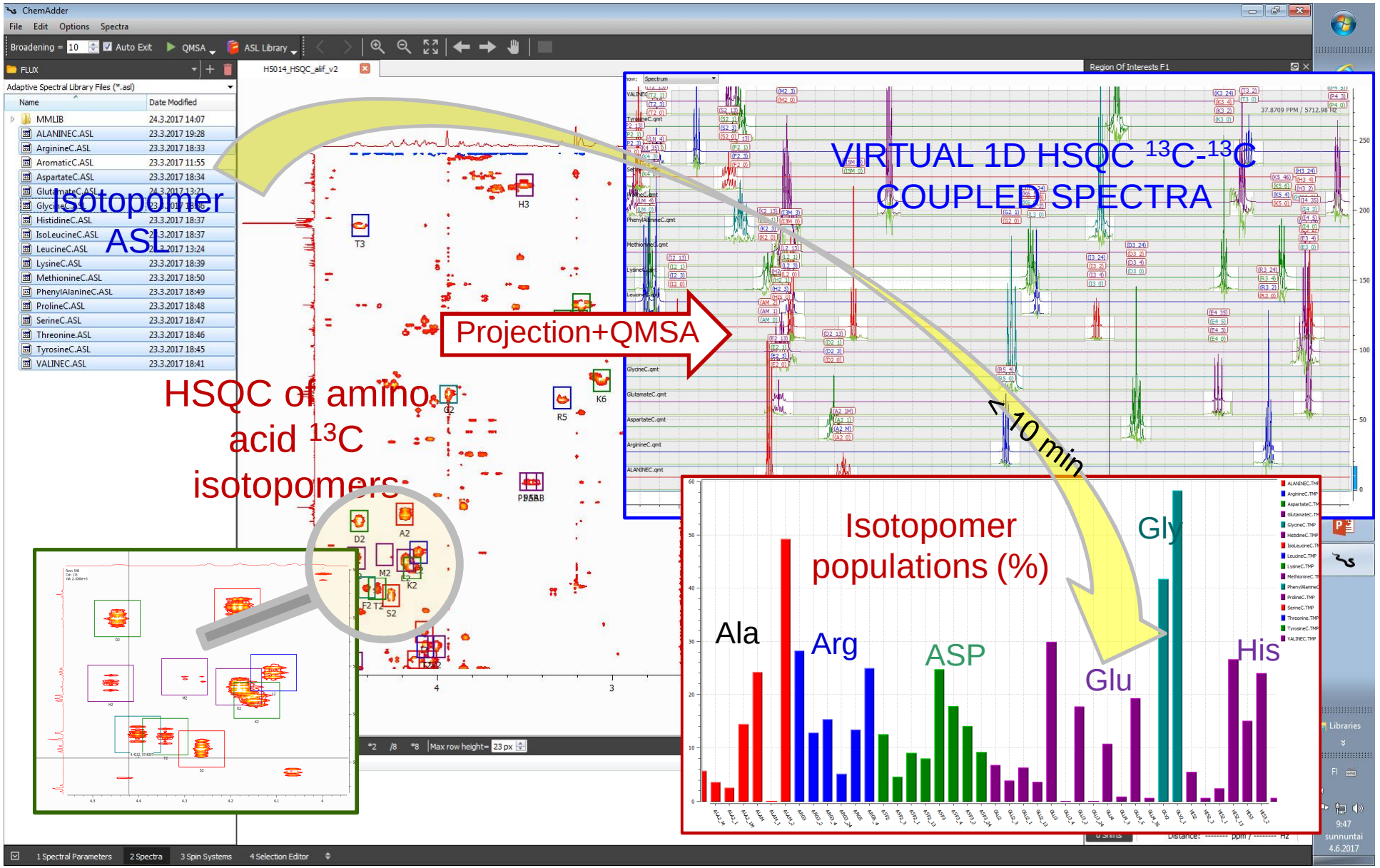
Tools for analyses of 2D spectra:

From 2D to 1D

VIRTUAL 1D HSQC ^{13}C-^{13}C COUPLED SPECTRA:
from of 2D to 1D spectra
...analyzable by QMSA !

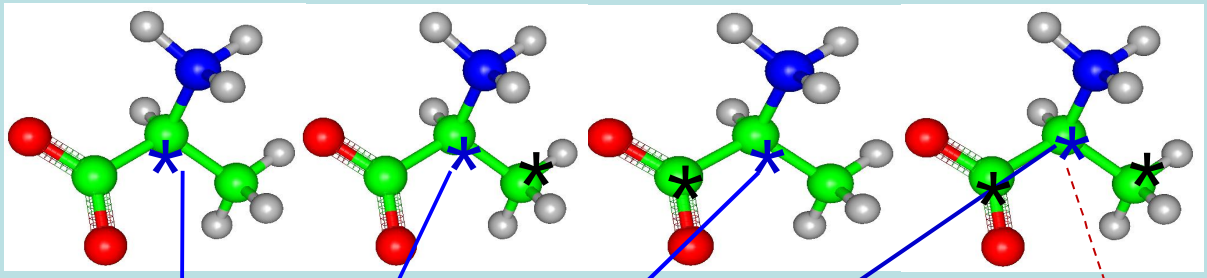
Metabolic flux analysis

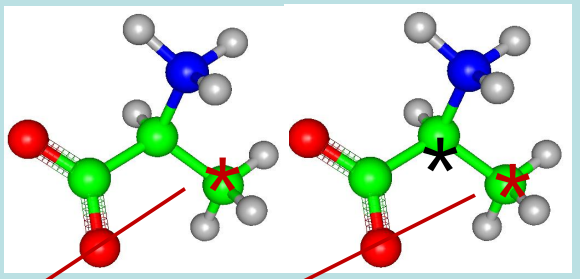
VIRTUAL 1D HSQC ^{13}C-^{13}C COUPLED SPECTRA: from 2D to 1D spectra:

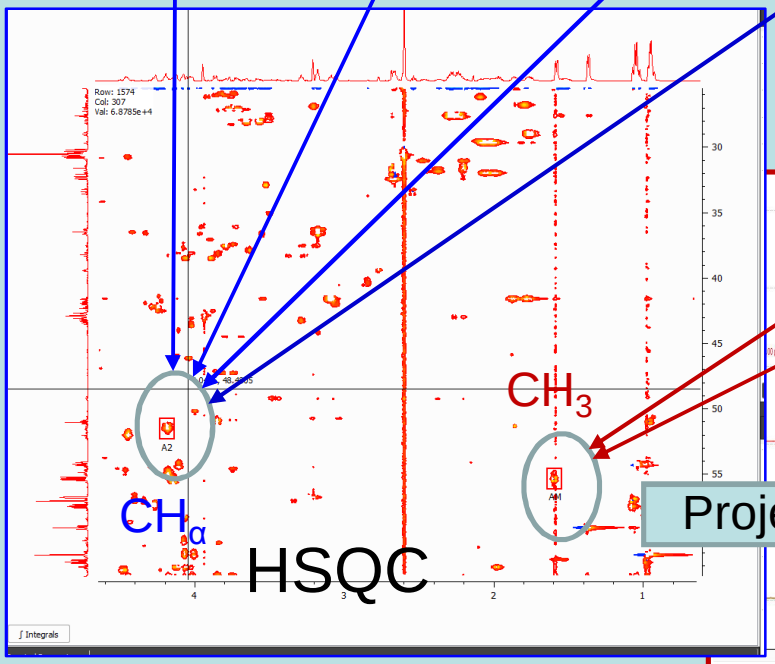


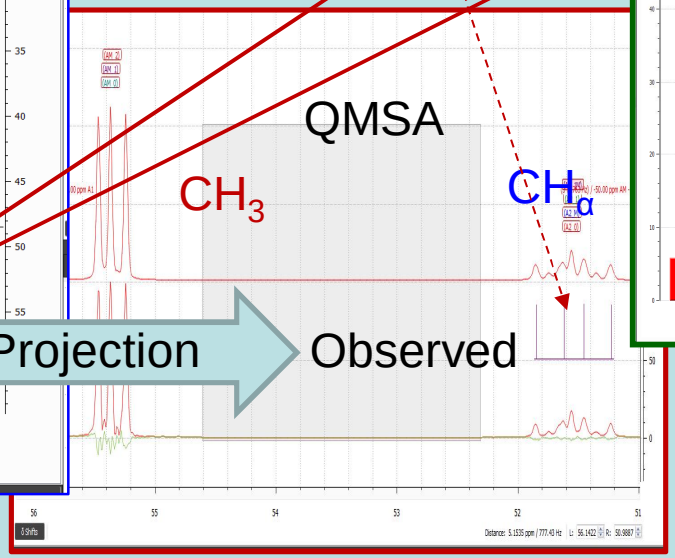
HSQC of amino acid ^{13}C isotopomers 2D spectrum to VIRTUAL 1D spectra: metabolic flux analysis

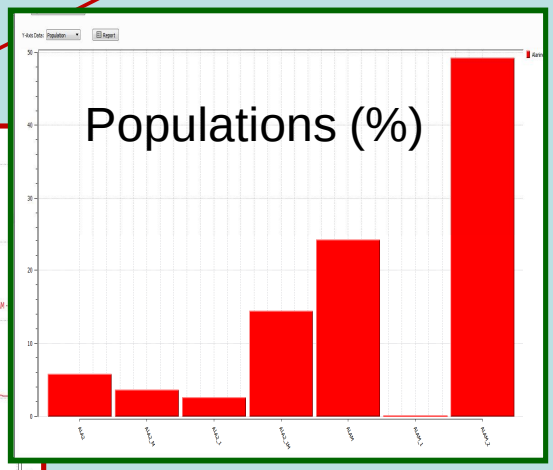
Alanine ^{13}C isotopomers:











ALANINE ^{13}C isotopomer ASL-file

```
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TIME: 23.03.2017  19:28:52

&CONTROL PARAMETERS & FIT INFO:
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        SPECTRUM = C:\CHEMADDER\ASLIBS\FLUX\ALANINEC.QMT ; ND => (RE)READ ORIGINAL!
         PROFILE = C:\CHEMADDER\ASLIBS\FLUX\HSQC_PROFILE.TXT ; OPTIONS/ADDER PROFILE
           FIELD = 150.85400571      ; FOR 1H in MHZ, USED TO TRANSFORM SHIFTS TO HZ
POINT RESOLUTION = 1.37374375        ; DATA-POINT-RESOLUTION (HZ)
      LINE WIDTH = 5.098             ; 0.0 = USE SPECIES DEFAULT (HZ)
        GAUSSIAN = 75.076            ; GAUSSIAN % IN LINE-SHAPE (CAN BE >100%)
            RRMS = 0.4896            ; % FROM MAX. INTENSITY
        QM LINES = 14                ; NO. OF QM LINES

&CHEMICAL SHIFTS(PPM):
ALA2  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.057515[OBS=  0.157384] MWGT=   89.09 SLOPE=  1.0000 ROI= A2
 A2_0     / 1    51.555737  1*1*1  STAT=Y  PRED= 51.5557 RANGE= 0.1000 WIDTH(Y)= 6.875 RESP(N)= 1.0000 SDEV= 0.000005 LOCAL= 11.905 HSQC= A_H2
ALA2_M  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.036609[OBS=  0.320168] MWGT=   89.09 SLOPE=  1.0000 ROI= A2
 A2_M     / 2    51.552856  1*1*1  STAT=Y  PRED= 51.5529 RANGE= 0.1000 WIDTH(Y)= 7.641 RESP(N)= 1.0000 SDEV= 0.000005 LOCAL= 11.832 HSQC= A_H2
 AM       / 2   -50.000000  1*1*1  STAT=N
ALA2_1  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.027389[OBS=  0.010799] MWGT=   89.09 SLOPE=  1.0000 ROI= A2
 A2_1     / 3    51.546642  1*1*1  STAT=Y  PRED= 51.5466 RANGE= 0.1000 WIDTH(Y)= 7.661 RESP(N)= 1.0000 SDEV= 0.000006 LOCAL= 16.540 HSQC= A_H2
 A1       / 3   150.000000  1*1*1  STAT=N
ALA2_1M  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.141620[OBS=  0.004400] MWGT=   89.09 SLOPE=  1.0000 ROI= A2
 A2_1M    / 4    51.542381  1*1*1  STAT=Y  PRED= 51.5424 RANGE= 0.1000 WIDTH(Y)= 7.893 RESP(N)= 1.0000 SDEV= 0.000005 LOCAL= 18.397 HSQC= A_H2
 AM       / 4   -50.000000  1*1*1  STAT=N
 A1       / 4   150.000000  1*1*1  STAT=N
*
ALAM  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.241187[OBS=  0.123688] MWGT=   89.09 SLOPE=  1.0000 ROI= AM
 AM_0     / 5    55.366291  1*1*1  STAT=Y  PRED= 55.3663 RANGE= 0.1000 WIDTH(Y)= 4.758 RESP(N)= 1.0000 SDEV= 0.000001 LOCAL= 9.973 HSQC= A_ME
ALAM_1  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.004035[OBS=  0.047995] MWGT=   89.09 SLOPE=  1.0000 ROI= AM
 AM_1     / 6    55.363174  1*1*1  STAT=Y  PRED= 55.3632 RANGE= 0.1000 WIDTH(N)= 5.103 RESP(N)= 1.0000 SDEV= 0.000001 LOCAL= 9.845 HSQC= A_ME
 A1       / 6   150.000000  1*1*1  STAT=N
ALAM_2  2*SPIN= 1 SPECIES=13C POPULATION(Y)=  0.491644[OBS=  0.069093] MWGT=   89.09 SLOPE=  1.0000 ROI= AM
 AM_2     / 7    55.353104  1*1*1  STAT=Y  PRED= 55.3531 RANGE= 0.1000 WIDTH(Y)= 5.013 RESP(N)= 1.0000 SDEV= 0.000001 LOCAL= 10.290 HSQC= A_ME
 A2       / 7   100.000000  1*1*1  STAT=N

&COUPLING CONSTANTS:
ALA2_M
 J_A2M      34.1763   J A2_M     AM         STAT=Y  PRED= 34.176 RANGE= 0.500 SDEV= 0.3698
ALA2_1
 J_A12      59.2220   J A2_1     A1         STAT=Y  PRED= 59.222 RANGE= 0.750 SDEV= 0.3698
ALA2_1M
 J_A2M      34.1763   J A2_1M    AM         STAT=Y  PRED= 34.176 RANGE= 0.500 SDEV= 0.3698
 J_A12      59.2220   J A2_1M    A1         STAT=Y  PRED= 59.222 RANGE= 0.750 SDEV= 0.3698
ALAM_1
 J_A1M      16.3594   J AM_1     A1         STAT=N  PRED= 16.359 RANGE= 0.350 SDEV= 0.3698
ALAM_2
 J_A2M      34.1763   J AM_2     A2         STAT=Y  PRED= 34.176 RANGE= 0.500 SDEV= 0.3698

&CONSTRAINTS
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&ASL TEMPLATES AT:  150.854006 MHZ
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      1   7777.019531      0.991059    1    1
      2  ALA2_M
      2   7793.504395      0.492330    1    2
      3   7759.160645      0.488901    1    2
      3  ALA2_1
      4   7804.494629      0.473340    1    4
      5   7745.423340      0.476845    1    4
      4  ALA2_1M
      6   7820.979492      0.236949    1    6
      7   7786.635742      0.234082    1    6
      8   7761.908203      0.241858    1    6
      9   7727.564941      0.236420    1    6
      5  ALAM
     10   8351.244141      0.879902    1    9
      6  ALAM_1
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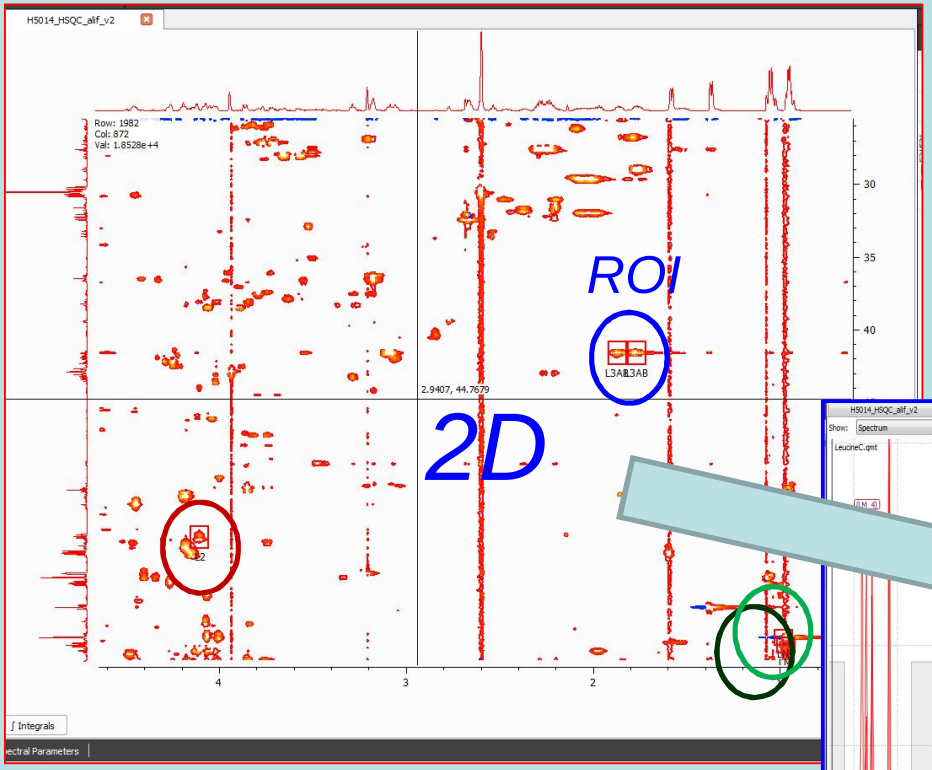
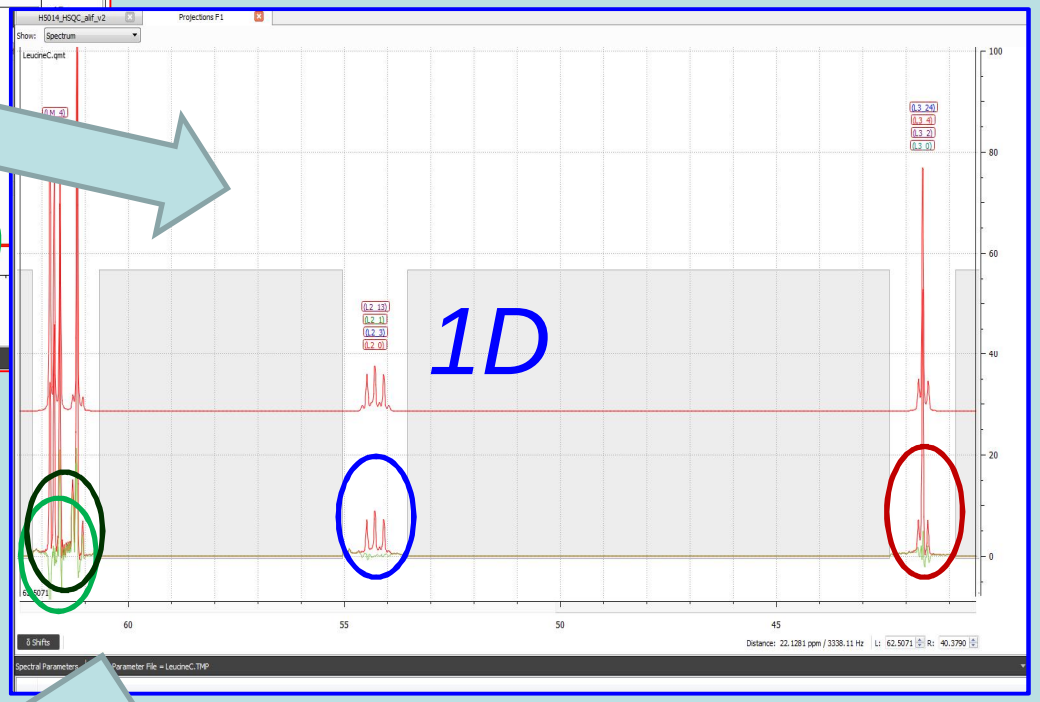
Shifts

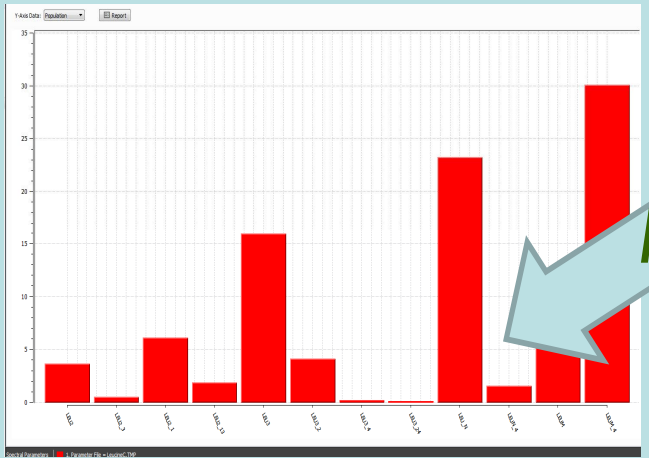
Couplings

ROI = Region of Interest

Leusine ^{13}C isotopomer spectra



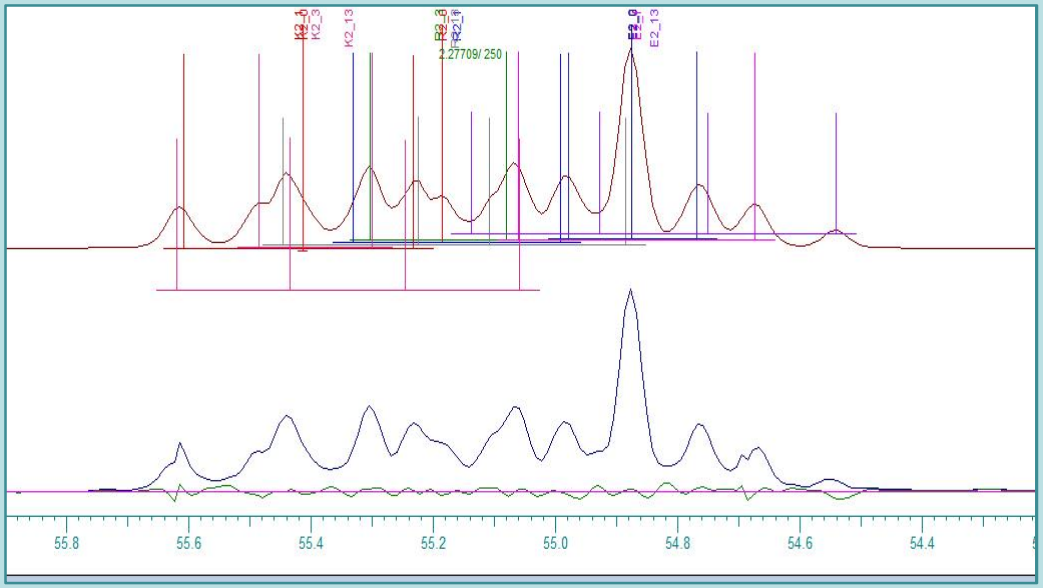




Report

Analysis of overlapping signals

Arg2_Lys2_Glu2_Leu2 multiplets overlap seriously with each others but they can (must) be analysed together:



If an overlapping signal is unknown, it can be described by a dummy multiplet!
In this way more data are got to analysis !

The couplings for the model are obtained from other signals, this fitting gives only populations.


Laksfjord, Norway May 2017
http://chemadder.com