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Introducing GSD - 2D

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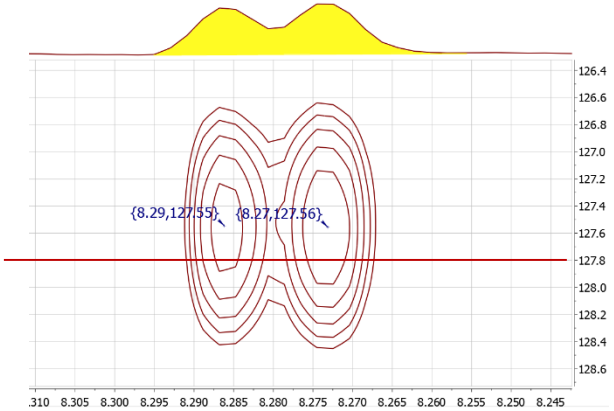
in the Quantitative 2D NMR Workshop

2D Integration Procedures

Semi-quantitative approaches

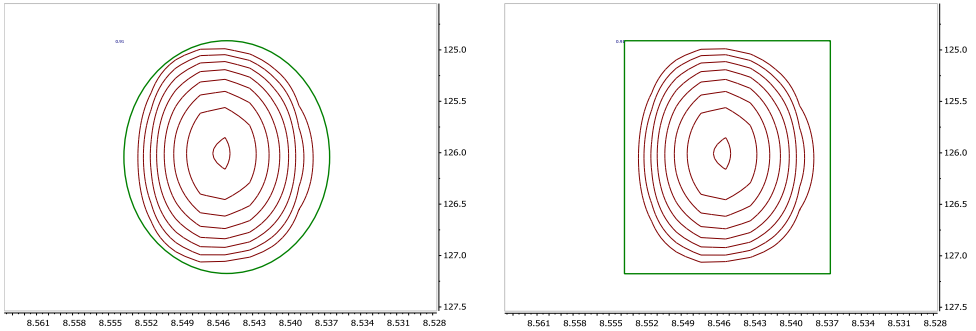
- Peak heights
- 1D areas in cross sections



Quantitative approaches

- Numerical integration

$$V = \sum_{i,j} h_{ij}$$



2D Integration Procedures

Numerical integration: $V = \sum_{i,j} h_{ij}$

Pros

- Simple to use and automate
- Fast
- Lineshape insensitive

Cons

- **Sensitive to integration region size**
- **Affected by baseline (plane) offsets**
- **Problems with overlapped cross peaks**

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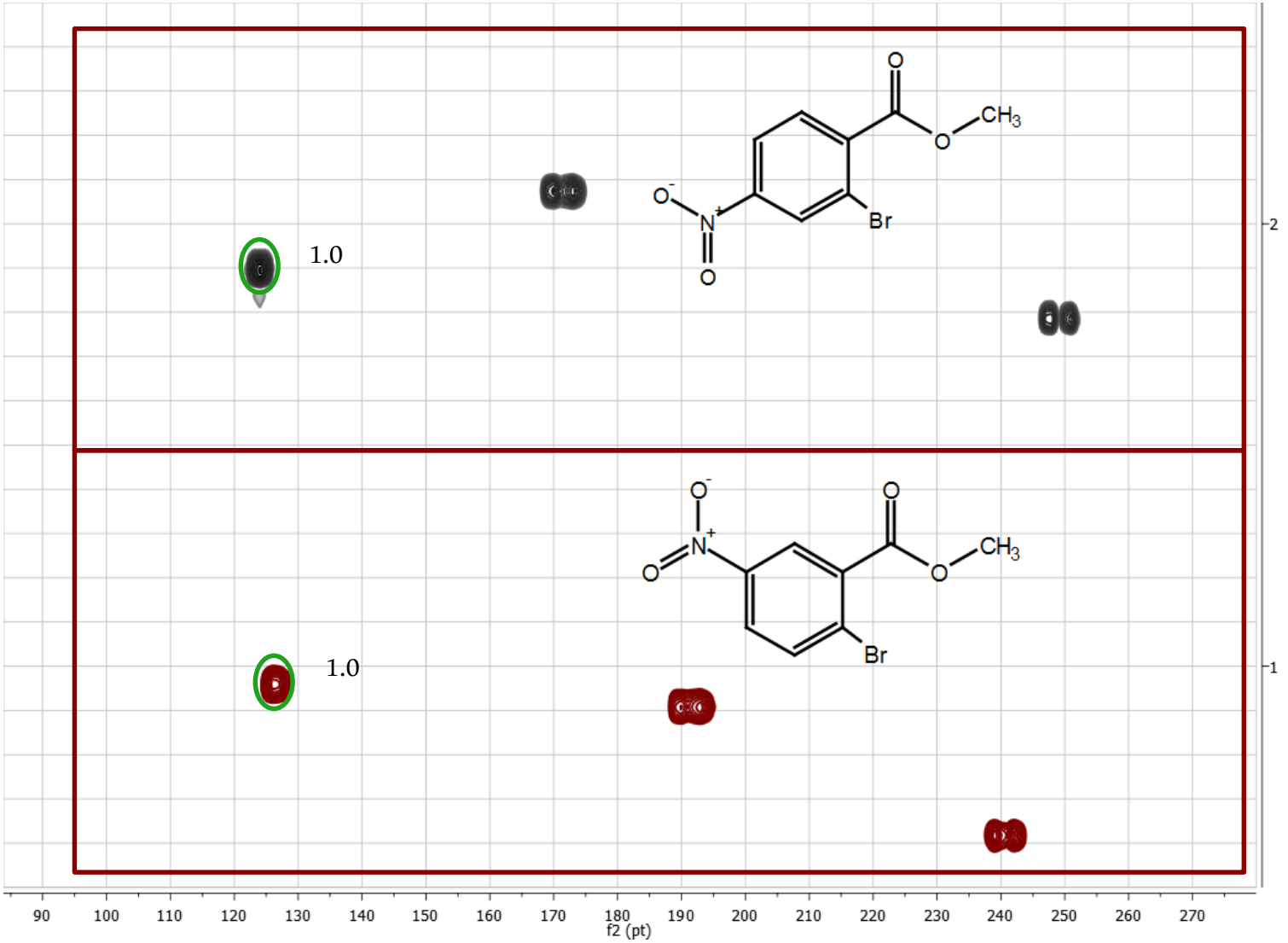
2D Integration in the F-domain



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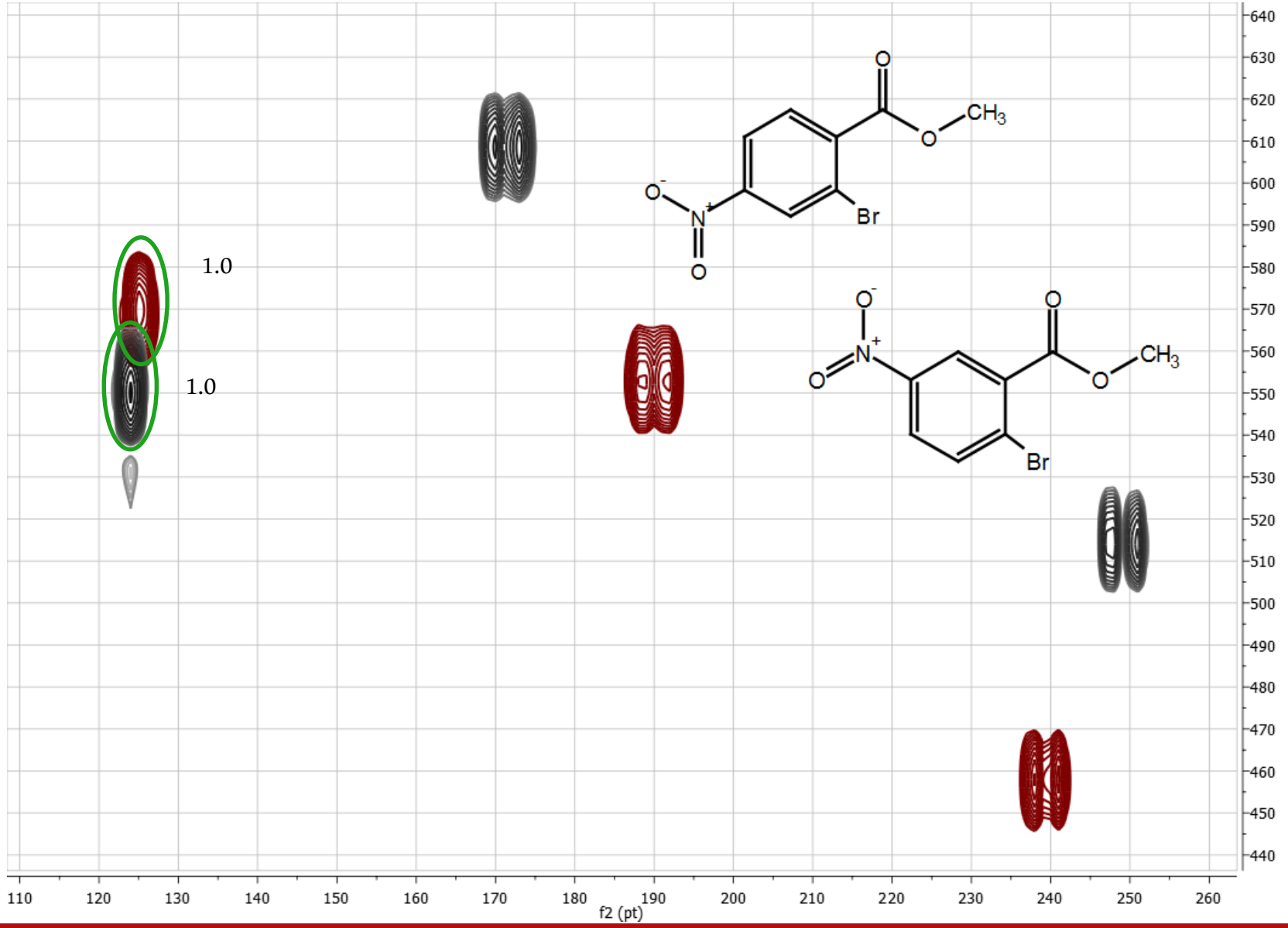

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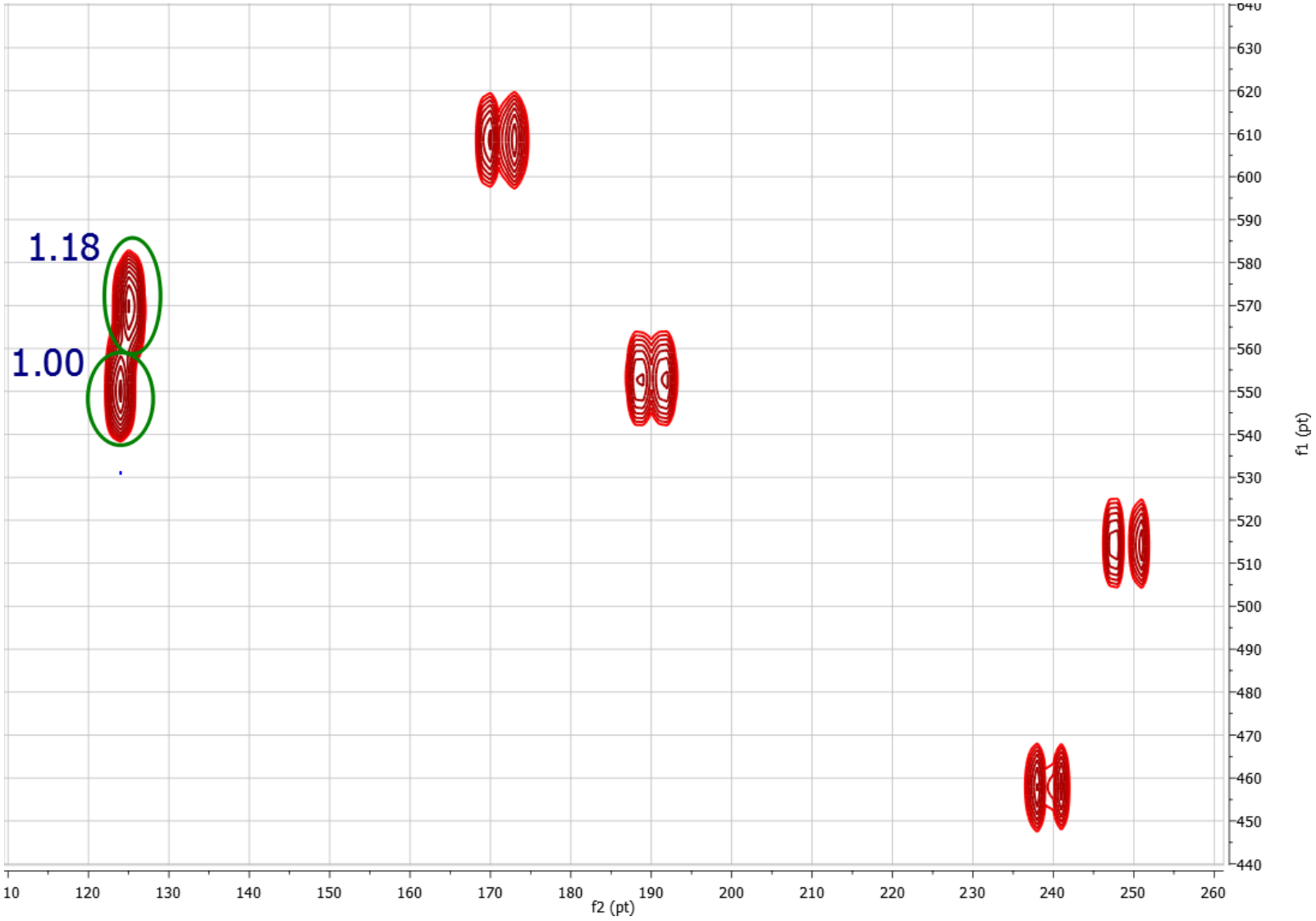
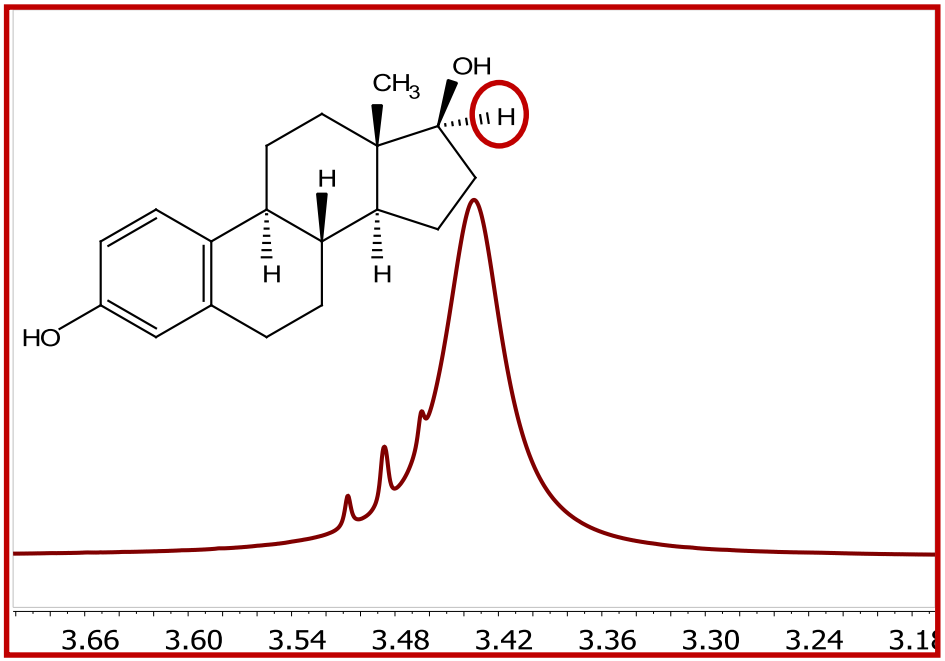
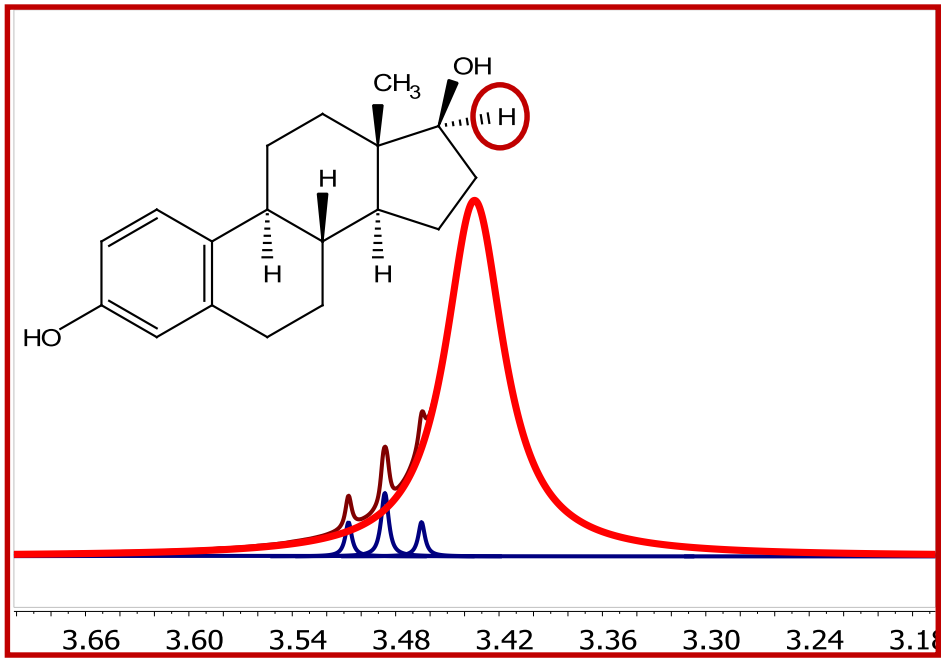


DECONVOLUTION – GSD 1D

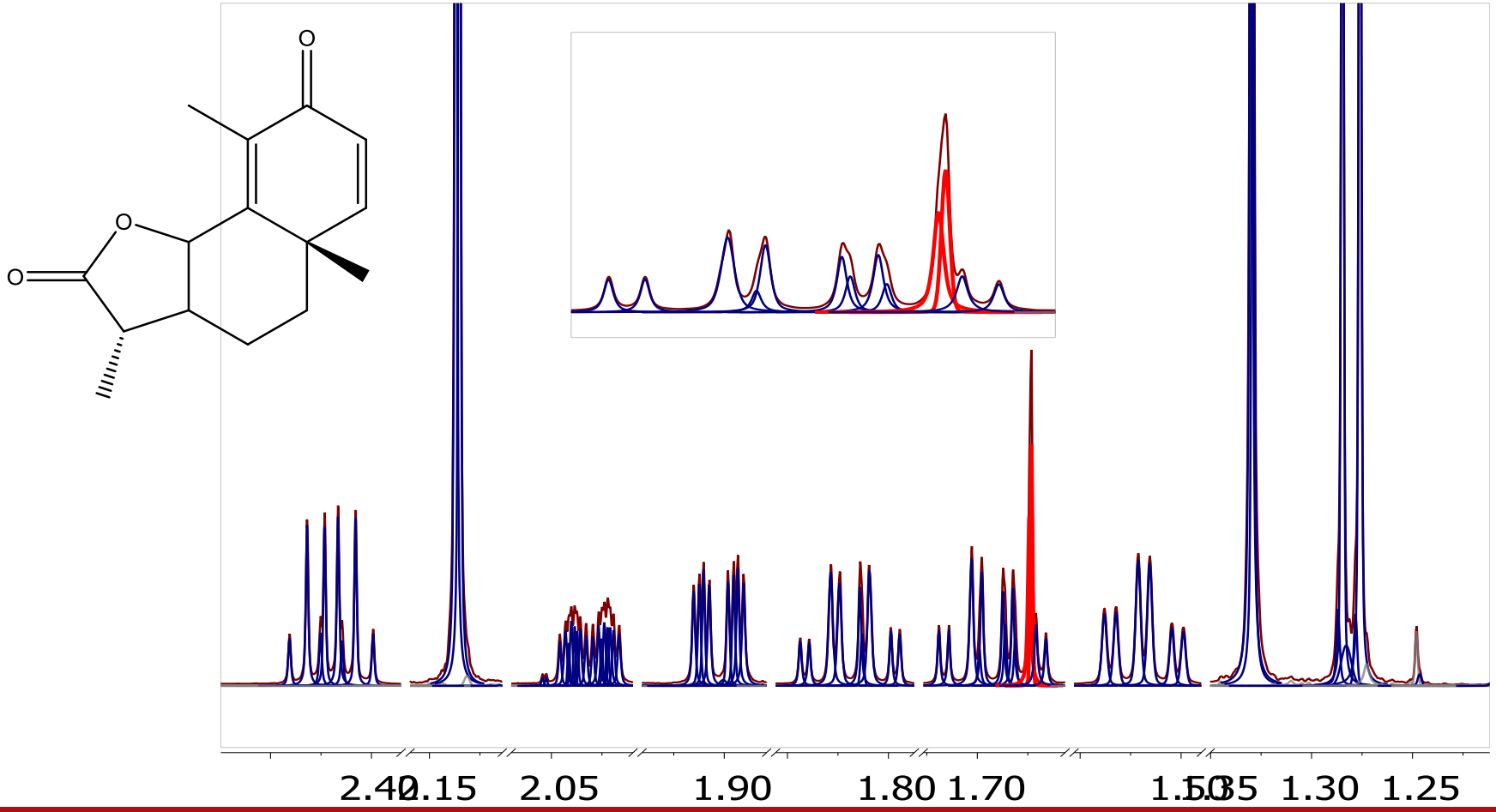
Resolving Overlapping peaks





Towards better 2D Integration Procedures

DECONVOLUTION – GSD 1D

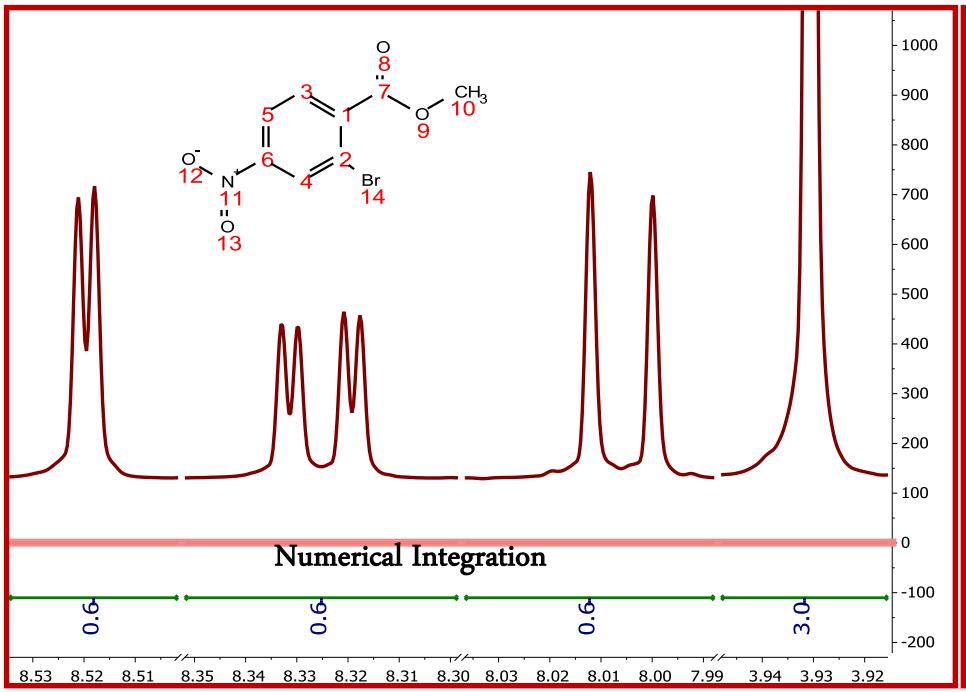


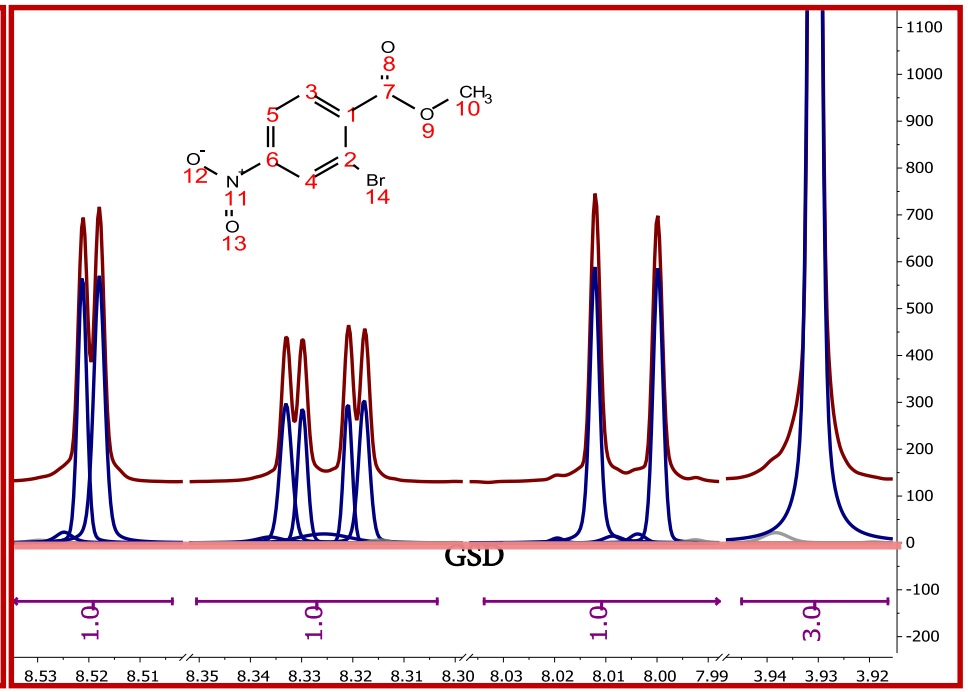
GSD 1D Main Properties

- Fully automatic
- Baseline insensitive
- Resolution Enhancement
- Lineshape adaptable

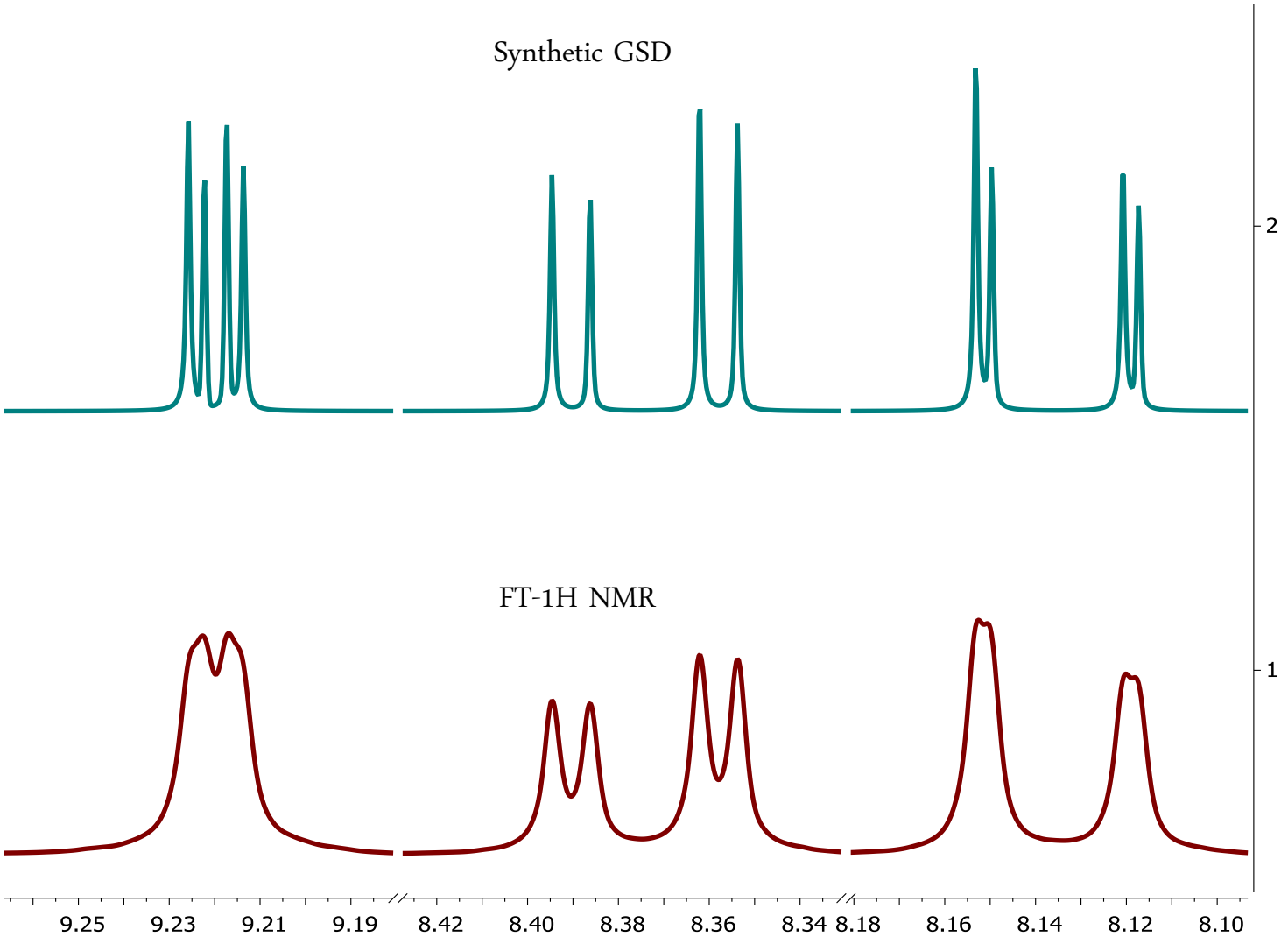
GSD 1D – BASELINE INSENSITIVE

Numerical vs GSD Integration





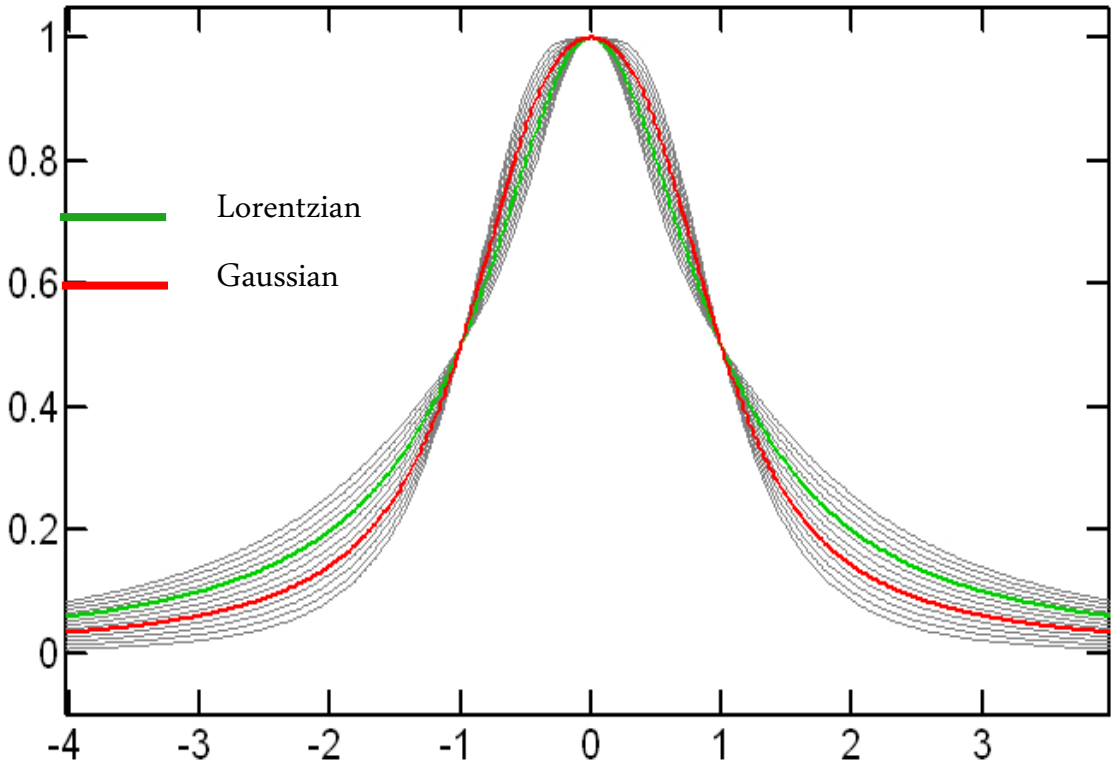
GSD 1D – RESOLUTION ENHACEMENT



GSD 1D – Generalized Lorentzian Shape

$$GL(p,x) = \frac{1-p}{1+x^2} + p\frac{1+x^2/2}{1+x^2+x^4}$$

- GL covers a wider range of lineshapes compared to Lorentzian or Gaussian
- Because it is a rational function, its integral and imaginary parts are easy to evaluate



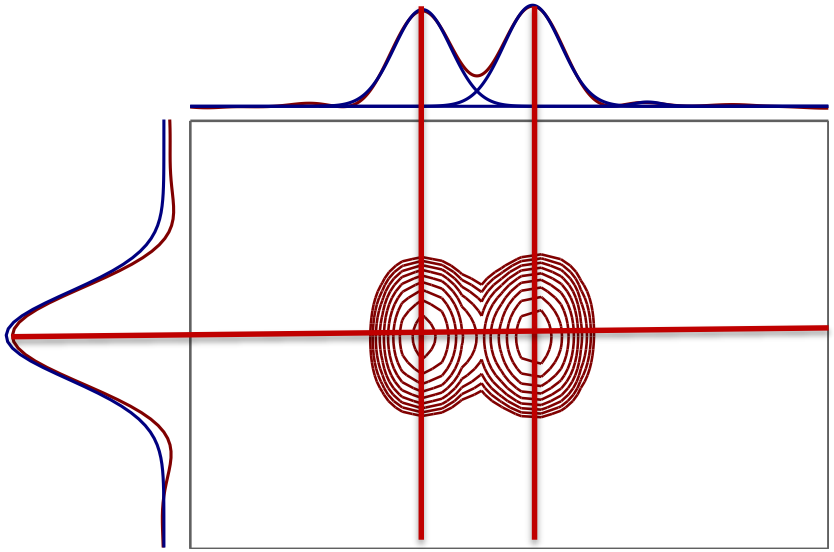
Introducing Ortho-GSD 2D

$$V = \iint S(x,y)dxdy$$

... and assuming that the 2D peak shape can be approximated by

$$V = \iint f(x;Wx,Kx)f(x;Wx,Kx)dxdy$$

... where Wx,Wy,Kx,Ky are some parameters, we have ...

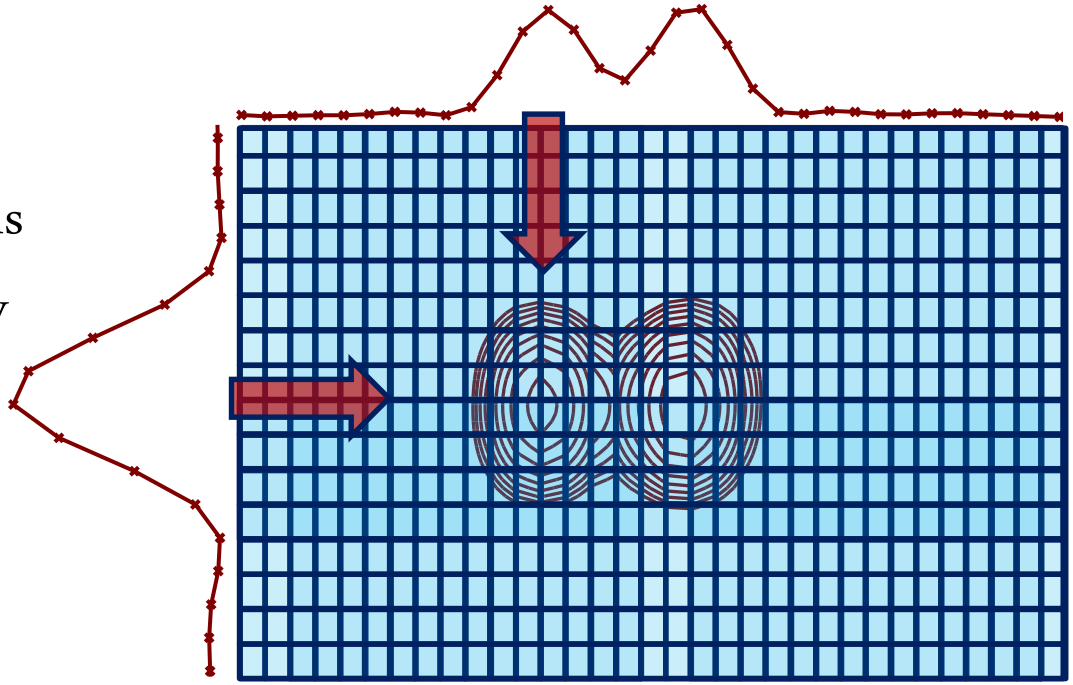


$$V_{GL} = \frac{HW_xW_y\pi^2}{16}\left[\left(\sqrt{3-2}\right)K_x + 2\right]\left[\left(\sqrt{3-2}\right)K_y + 2\right]$$

From GSD **1D** to GSD **2D**

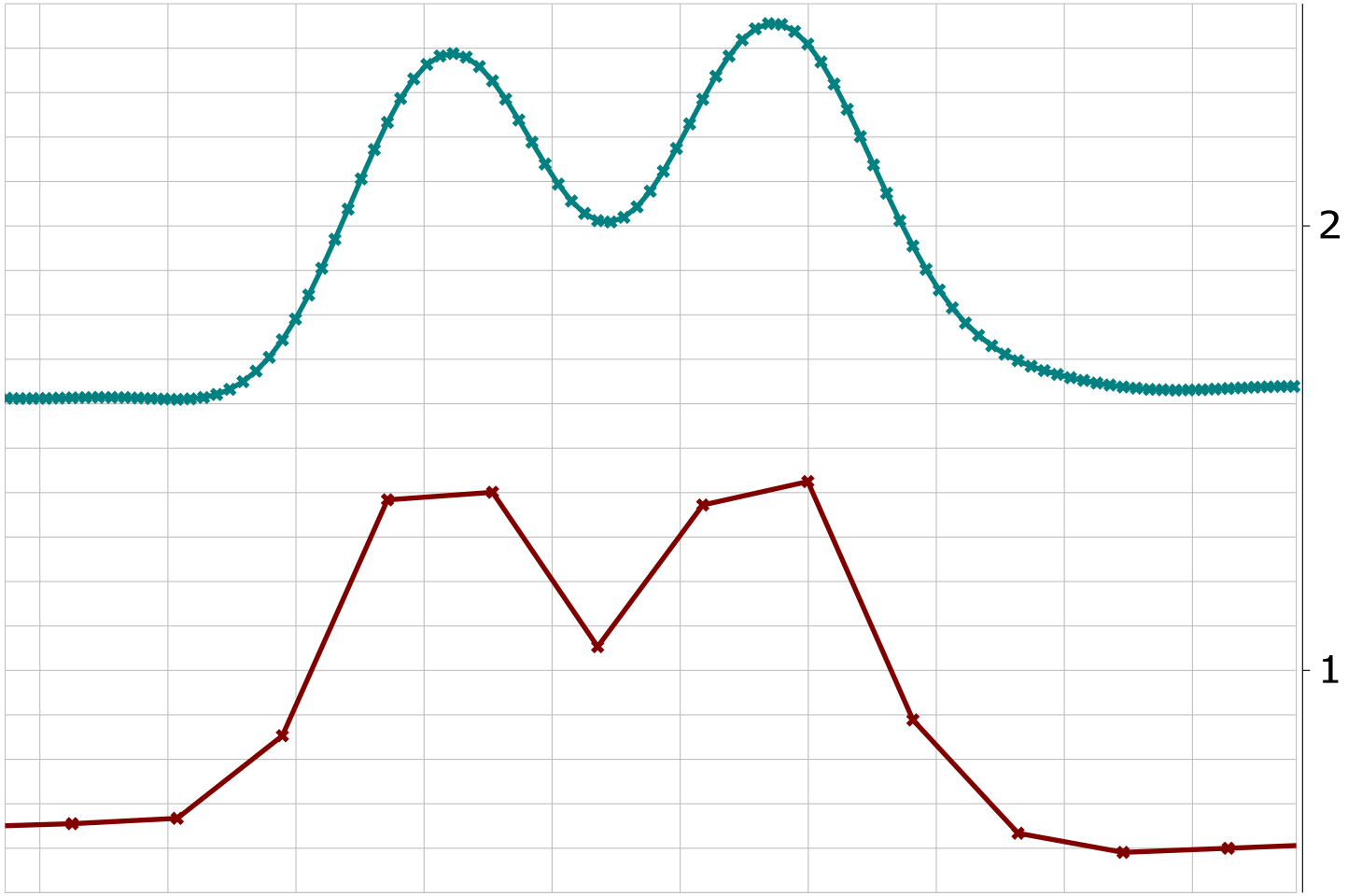
1. 1D GSD along all rows
2. 1D GSD along all columns
3. If there is a cross-intensity

   => **2D GSD peak**



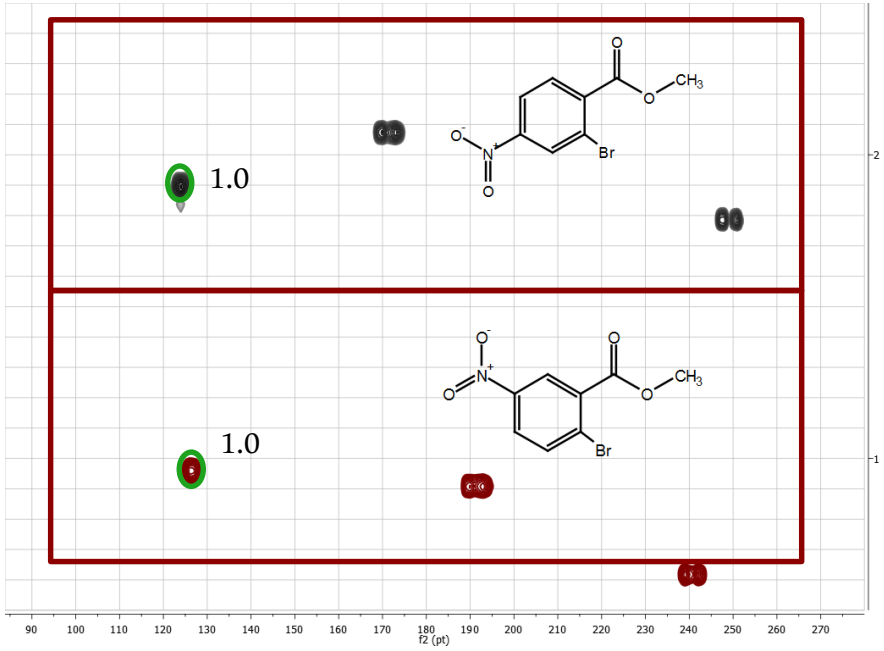
2D Integration in the F-domain

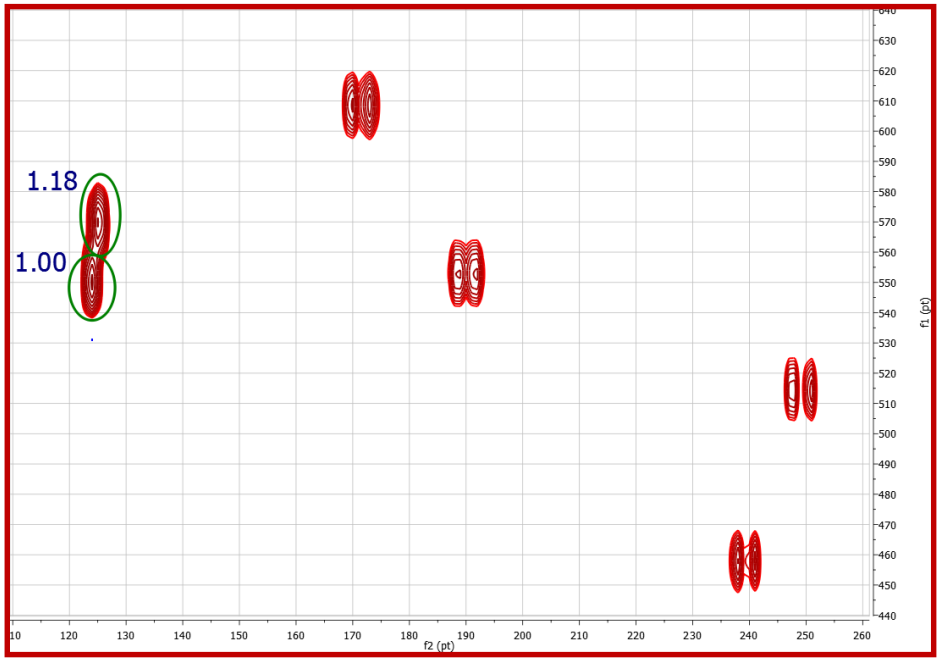
Oversampling of 1D cuts



Some Results

Numerical integration did not produce accurate results, due to overlap.





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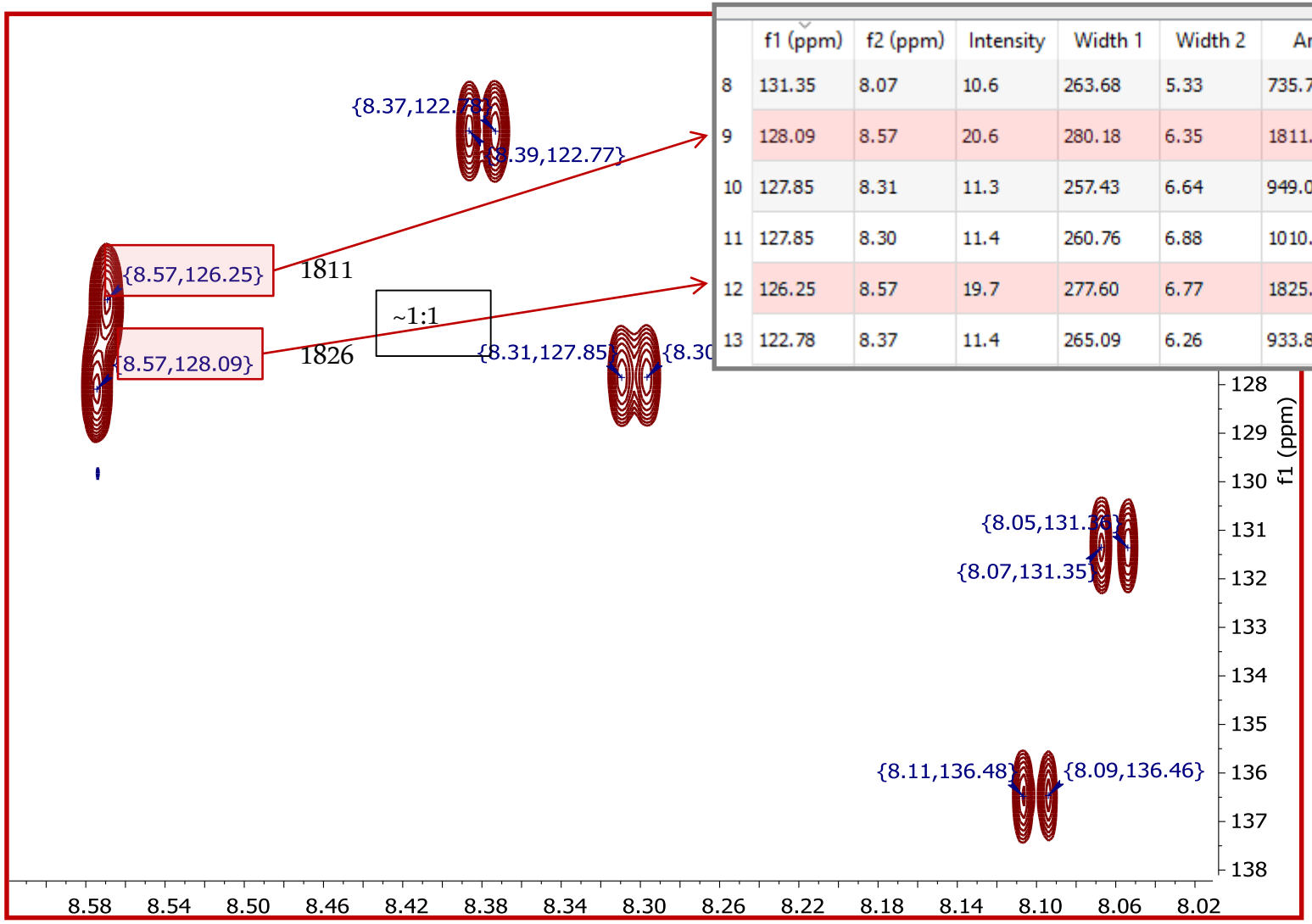
2D Integration in the F-domain

Some Results



	f1 (ppm)	f2 (ppm)	Intensity	Width 1	Width 2	Area	Type	Flags
8	131.35	8.07	10.6	263.68	5.33	735.73	Compound	None
9	128.09	8.57	20.6	280.18	6.35	1811.07	Compound	None
10	127.85	8.31	11.3	257.43	6.64	949.00	Compound	None
11	127.85	8.30	11.4	260.76	6.88	1010.54	Compound	None
12	126.25	8.57	19.7	277.60	6.77	1825.59	Compound	None
13	122.78	8.37	11.4	265.09	6.26	933.81	Compound	None

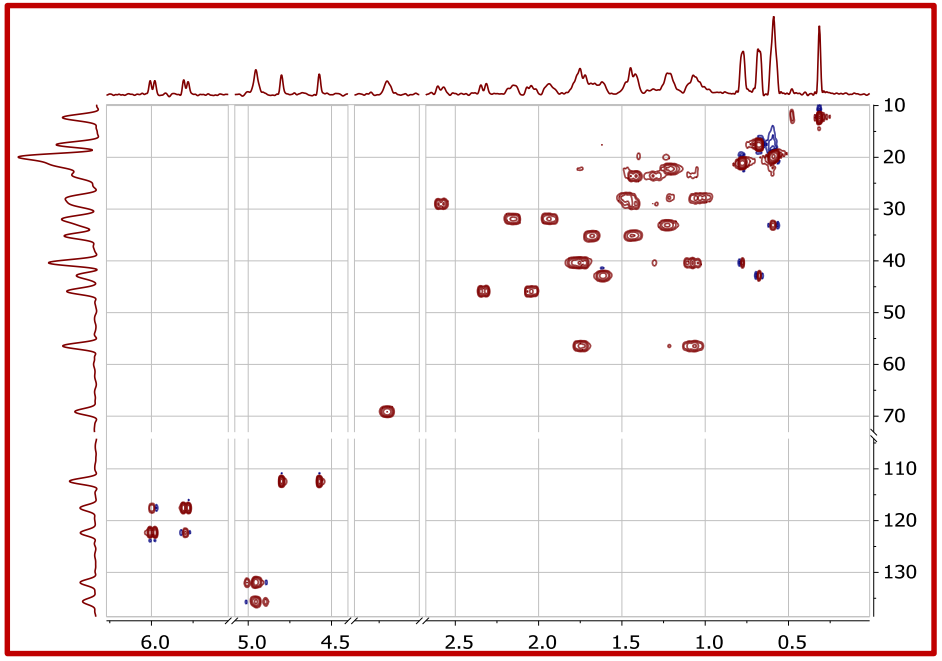
Some Results

NUMERICAL INTEGRATION

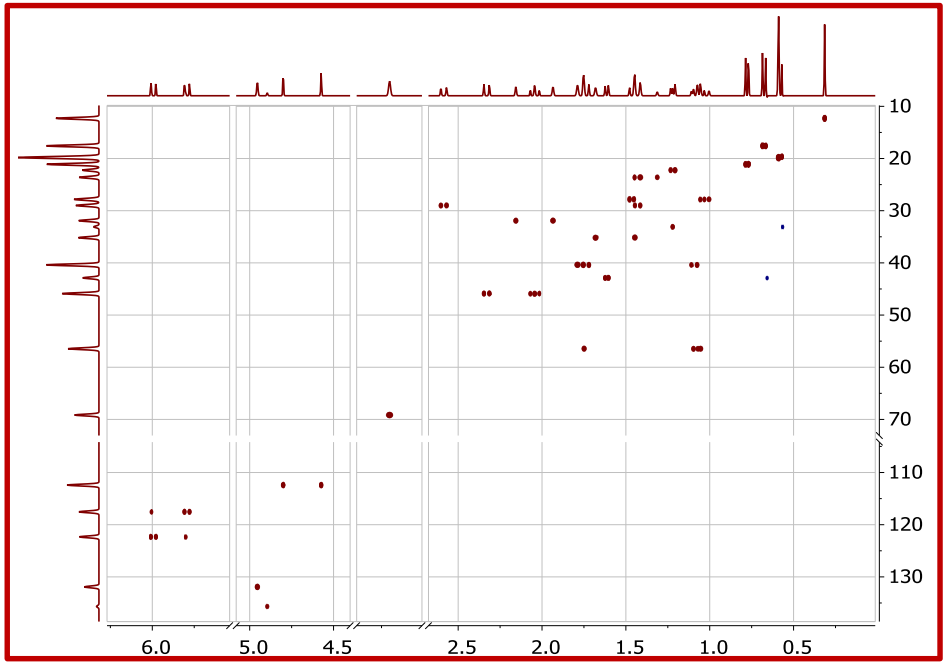
GSD-2D INTEGRATION

Some Results

Original spectrum

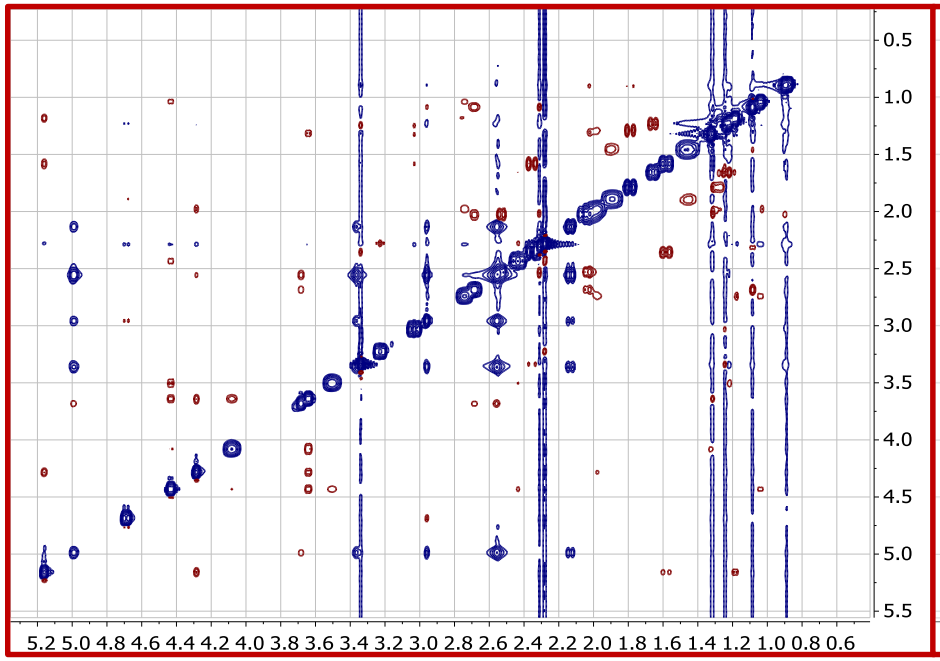


2D-GSD synthesized spectrum



Some Results

Original spectrum



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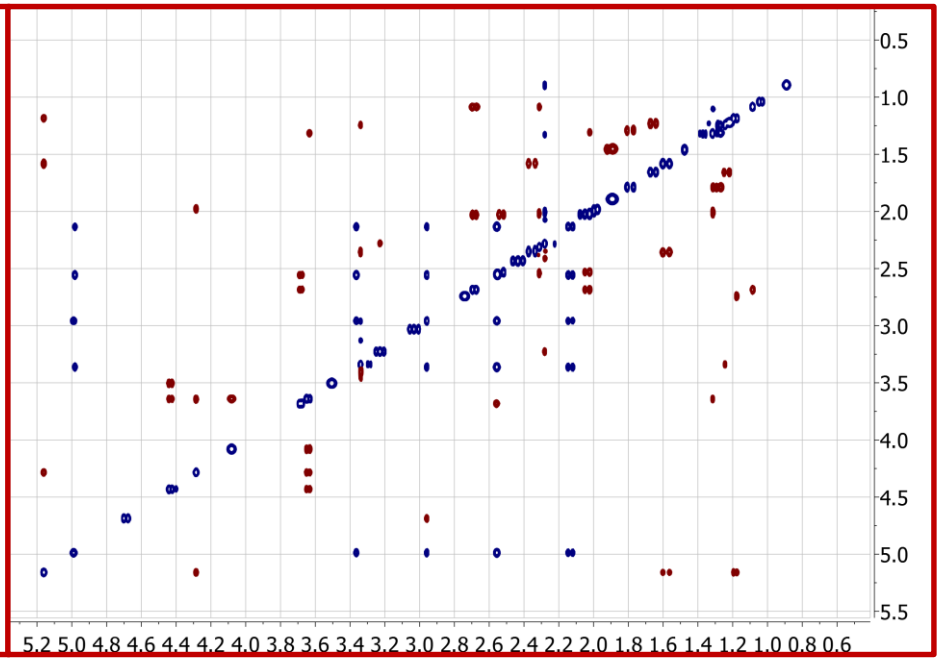
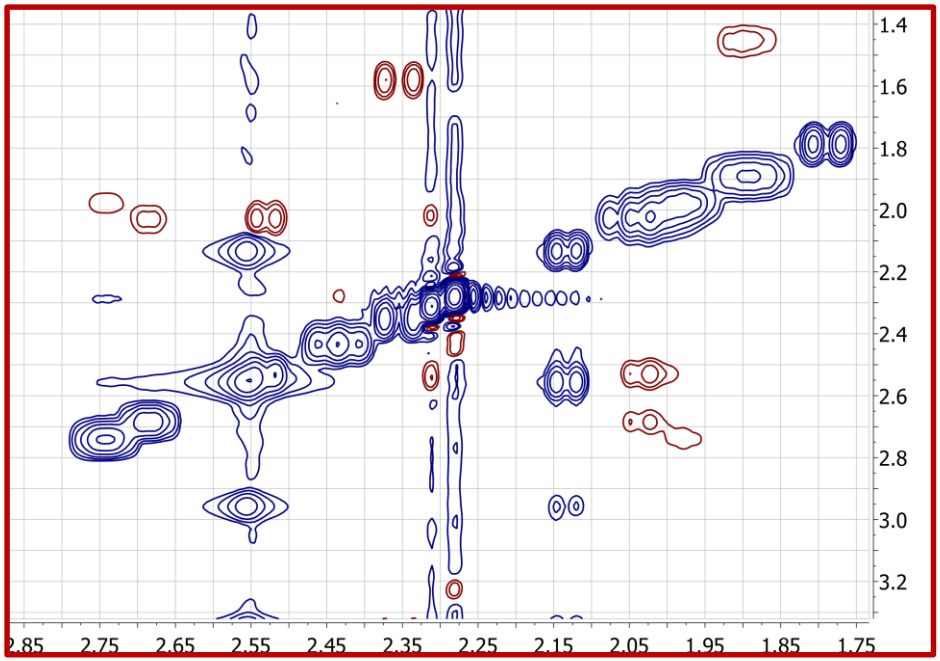
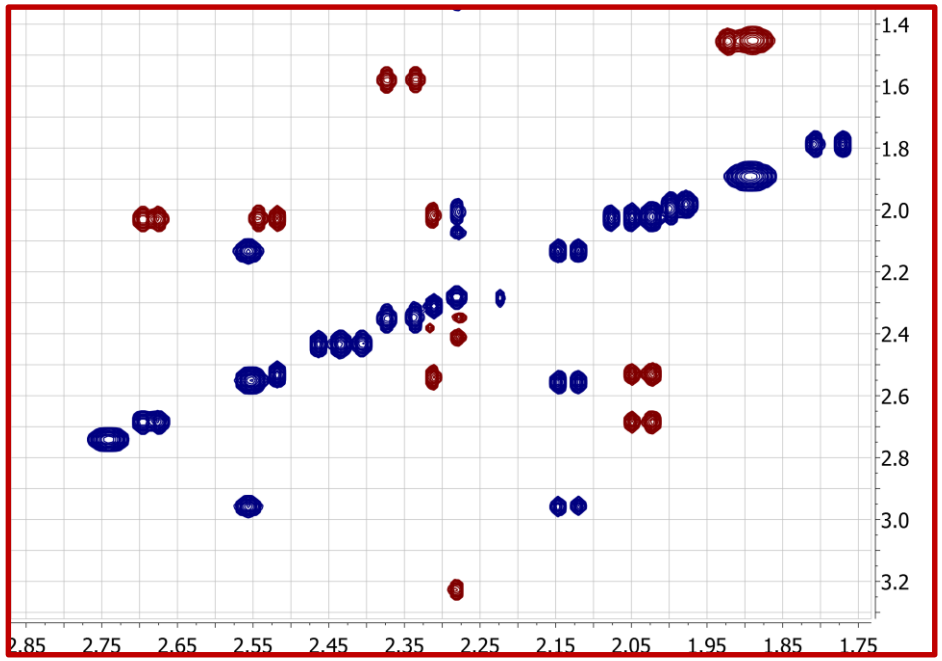


Some Results

Original spectrum



2D-GSD synthesized spectrum



To - Do

1. Comprehensive analysis of algorithm's performance:
    1. Tuning of algorithm parameters
    2. False positives
    3. Missing peaks
2. Quantitive analysis of the determined Volumes
3. New lineshapes?