

Example CRAFT

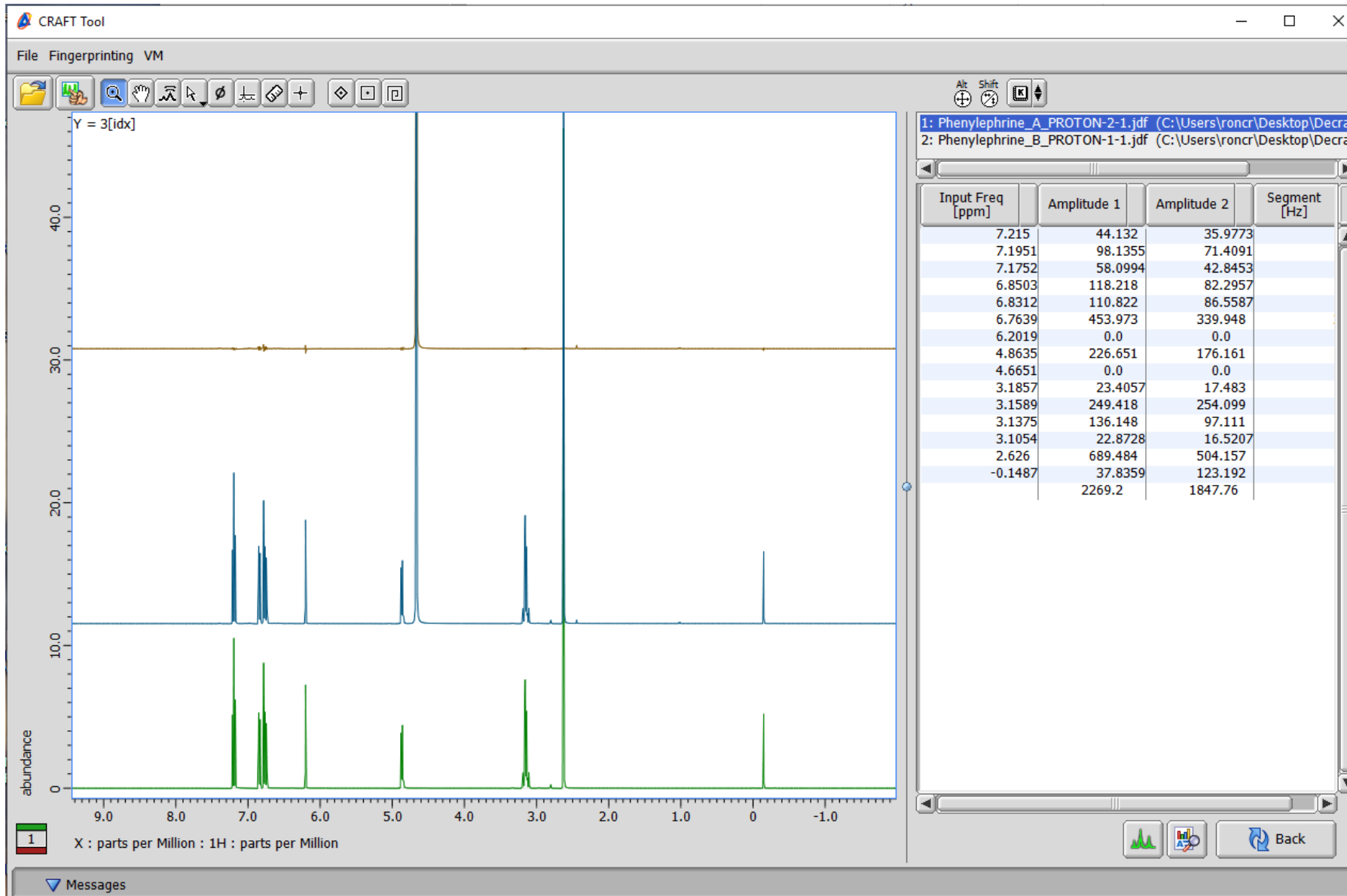
Quick guide to provided example data for Delta-CRAFT in Delta 5.3.1

Example Data

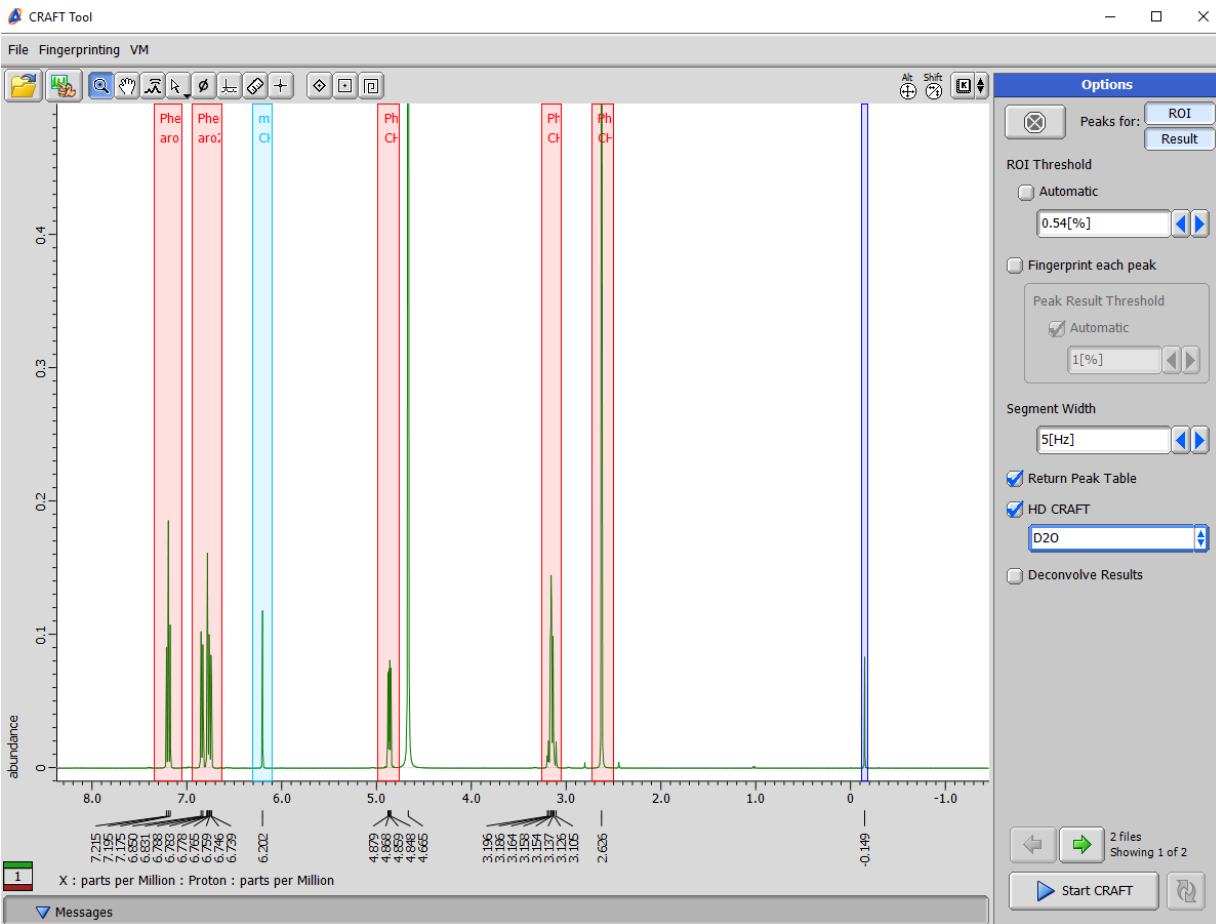
- Raw data fid (.jdf) files are provided for Amikasin (1D & 2D gHSQCAD), Caffiene, Pseudoephedrine HCl, & Phenylephrine HCl.
- All data but the Amikasin were acquired as qNMR purity evaluations using maleic acid as internal standard.
- The Amikasin serves as an example for using 2D CRAFT to greatly enhance the F1 resolution in heteronuclear 2D experiments.

qNMR Sample Information

- Two sets of samples “A & B” for all 3 compounds.
- Caffeine_A = 4.80mg; maleic acid =1.004mg; TSP = 0.254mg. Molecular weight = 194.2 for caffeine & 116.07 for maleic acid.
- Caffeine_B = 4.487mg; maleic acid = 4.192mg; TSP = 1.158mg.
- Phenylephrine_A = 15.40mg; maleic acid=1.004mg;TSP=0.254mg. Molecular weight of Phenylephrine HCl = 203.67
- Phenylephrine_B= 11.23mg; maleic acid=4.192mg; TSP=1.158mg.
- Pseudoeph_A = 15.83mg; maleic acid = 1.004mg; TSP=0.254mg. Molecular weight of pseudoephedrine HCl = 201.69
- Pseudoeph_B=14.74mg; maleic acid = 4.192mg; TSP=1.158mg.



Craft results with no fingerprints - Phenylephrine

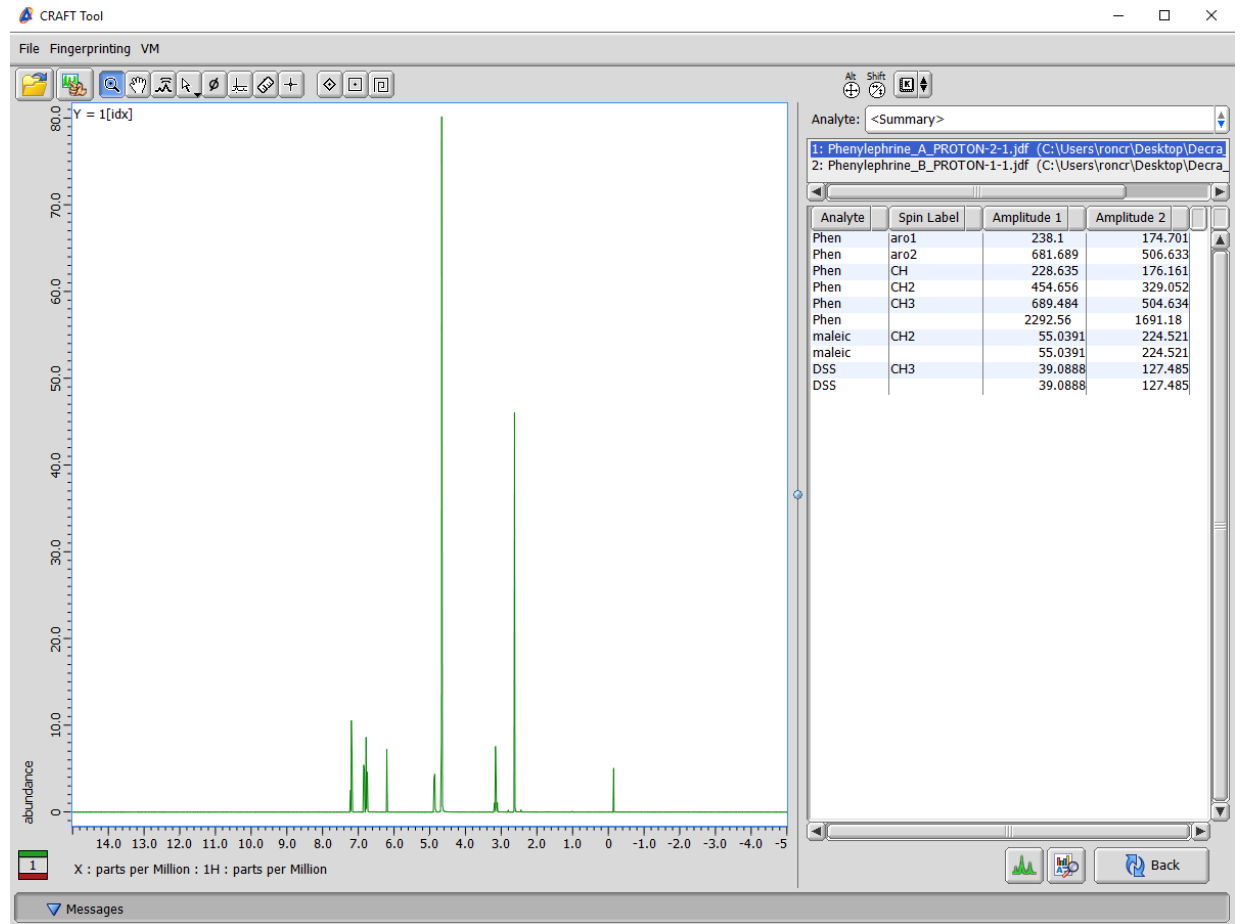


Fingerprints loaded for CRAFT

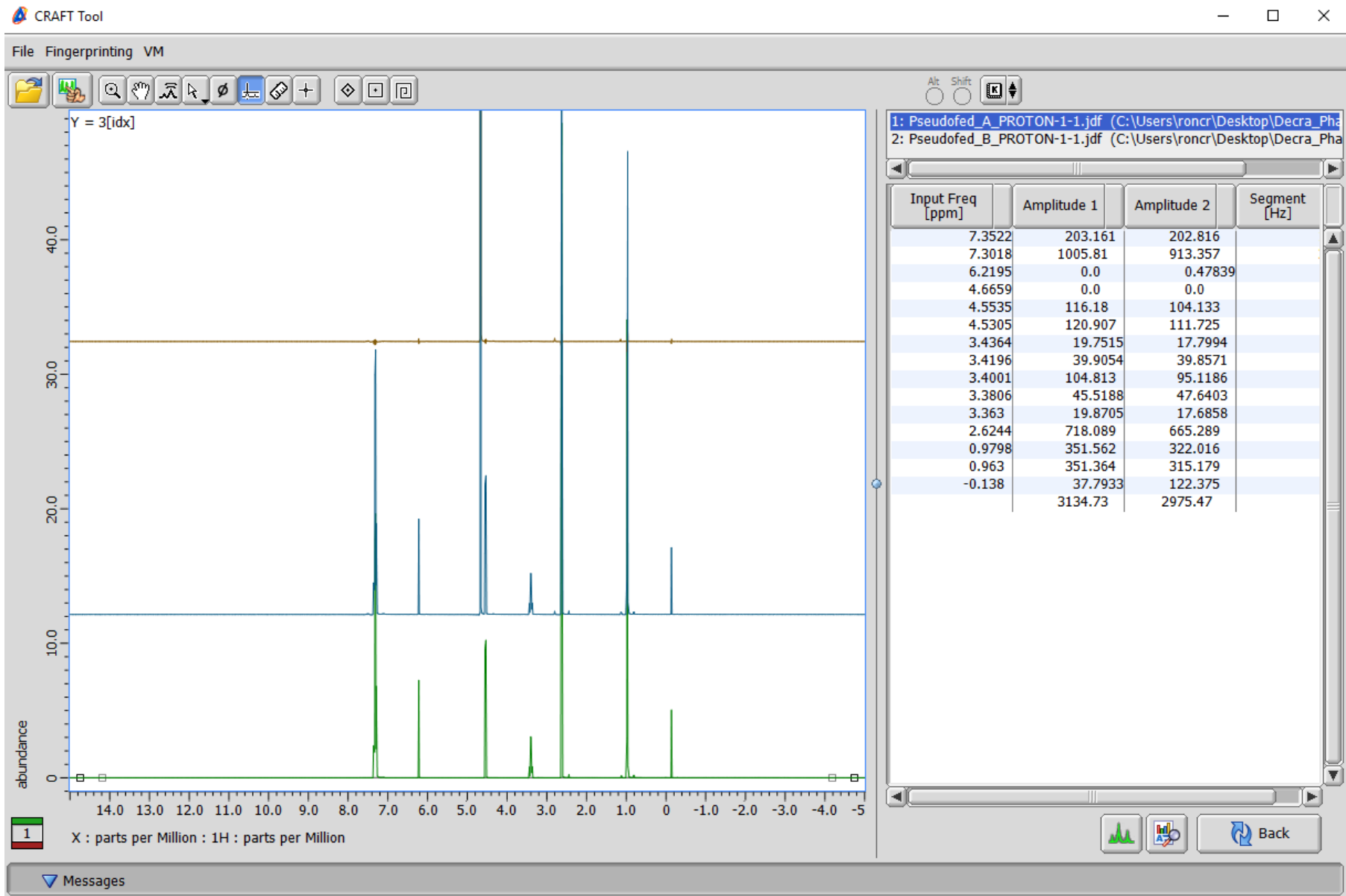
Phenylephrine HCl

Maleic acid

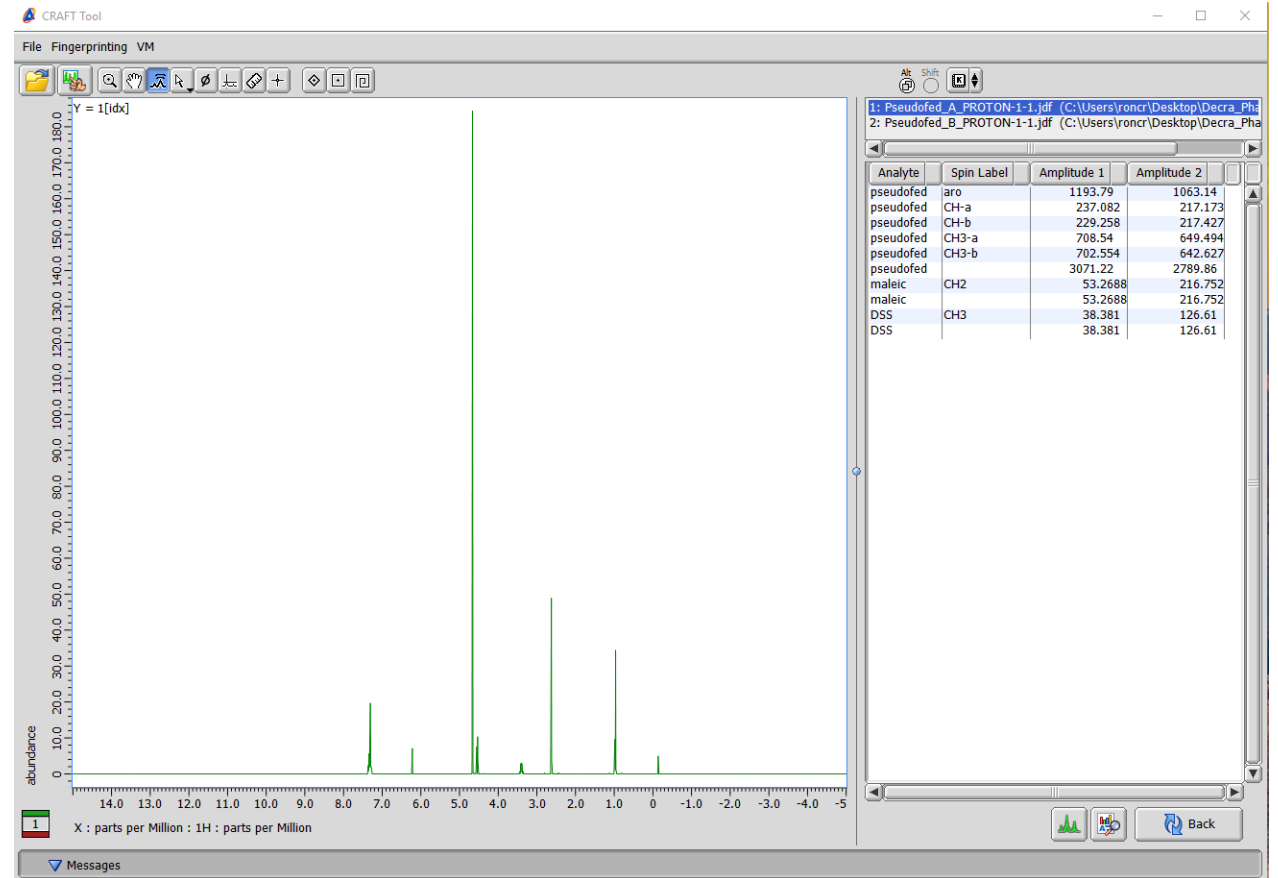
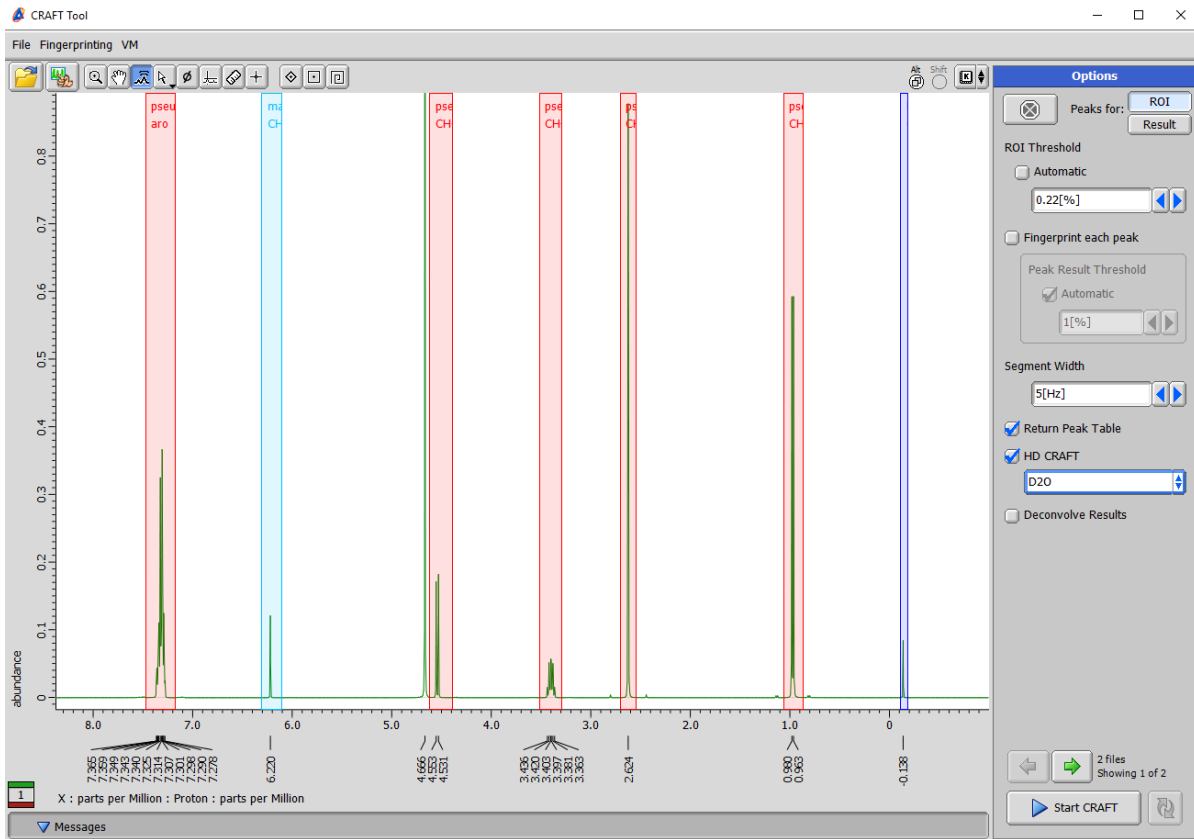
TSP



CRAFT Result with reporting by fingerprints



Craft results with no fingerprints - Pseudofed



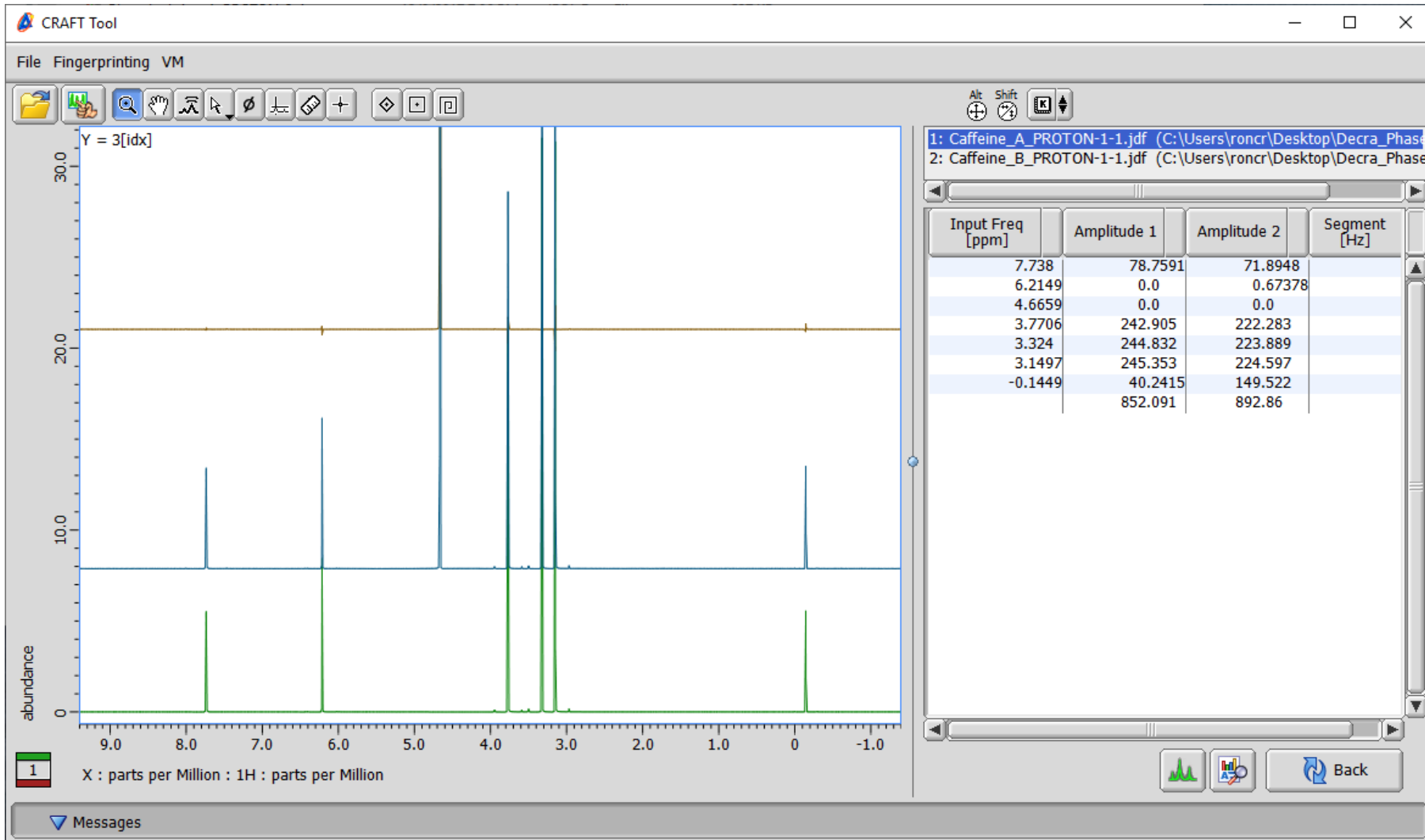
Fingerprints loaded for CRAFT

Pseudofed HCl

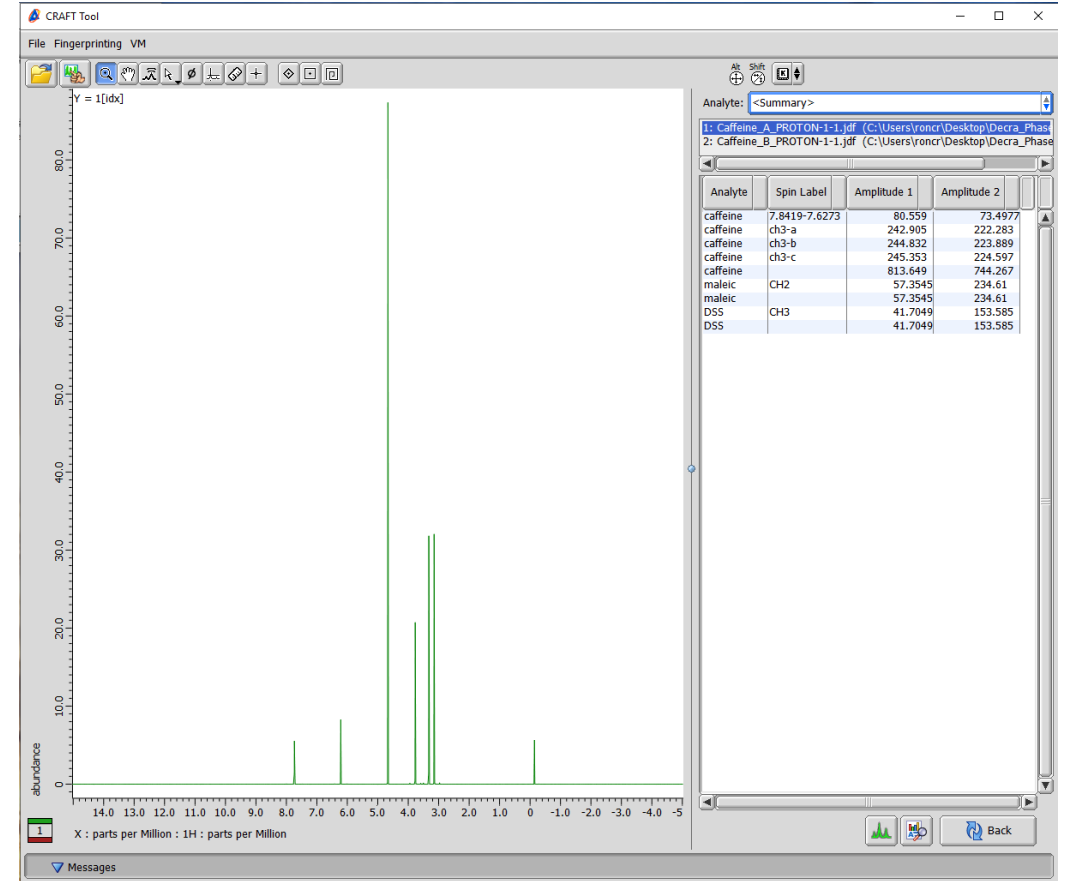
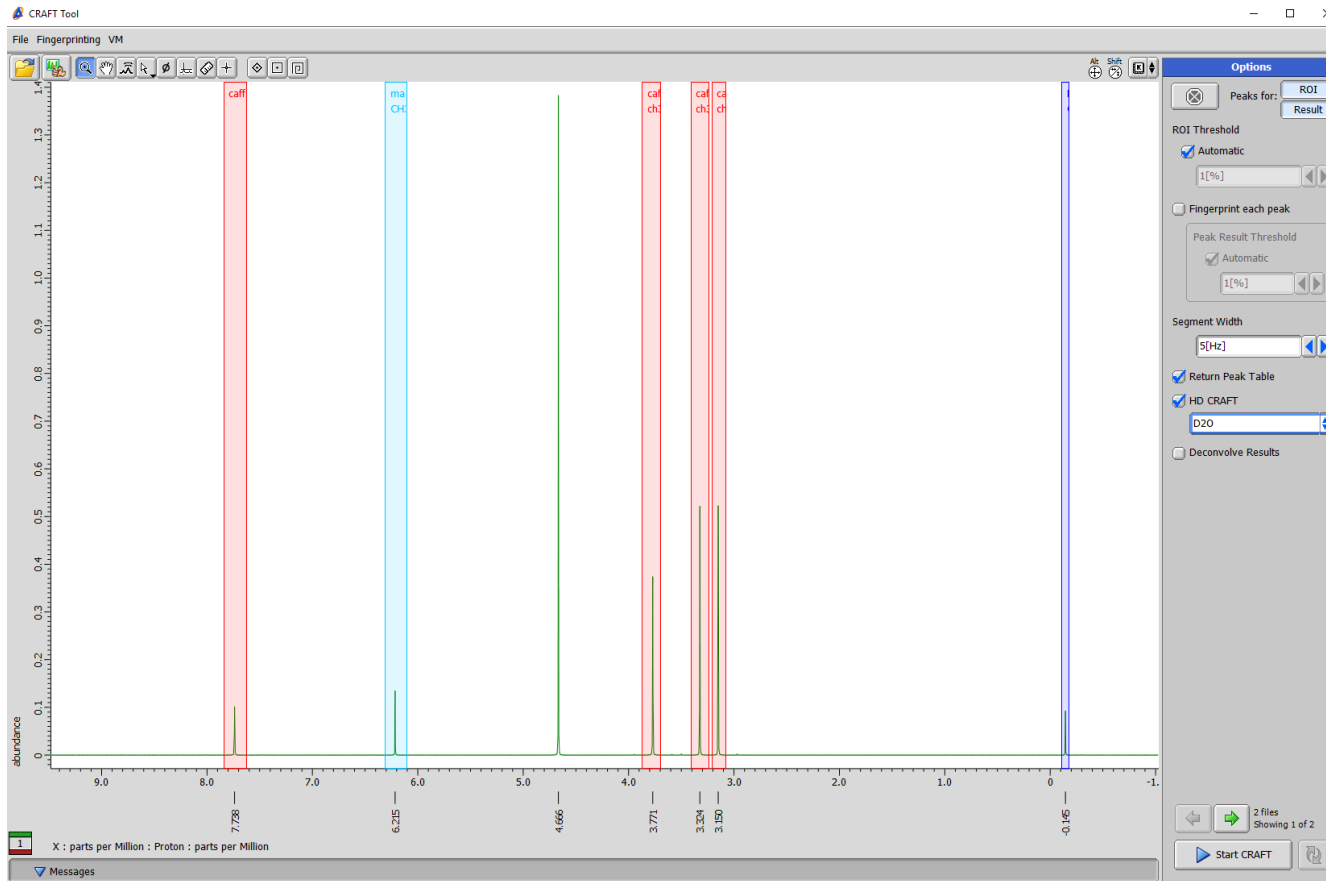
Maleic acid

TSP

CRAFT Result with reporting by fingerprints



Craft results with no fingerprints – Caffeine



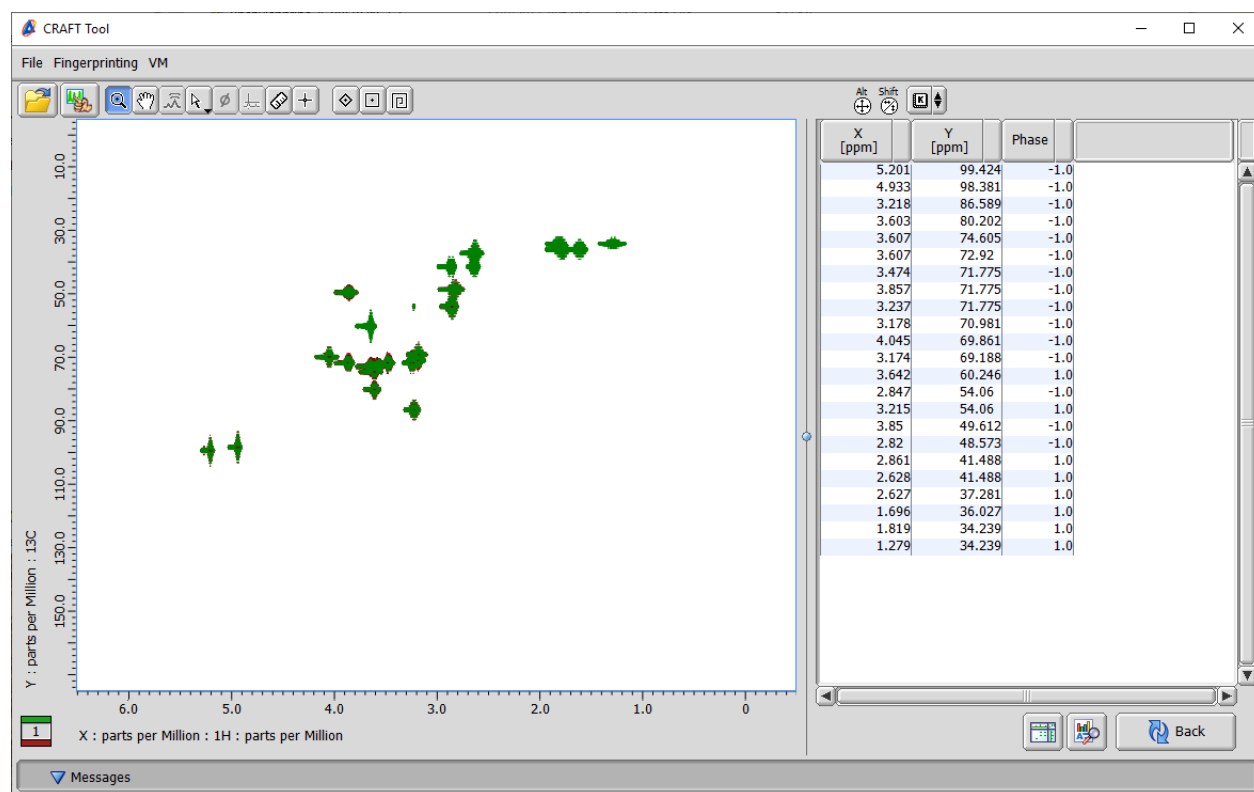
Fingerprints loaded for CRAFT

Caffeine

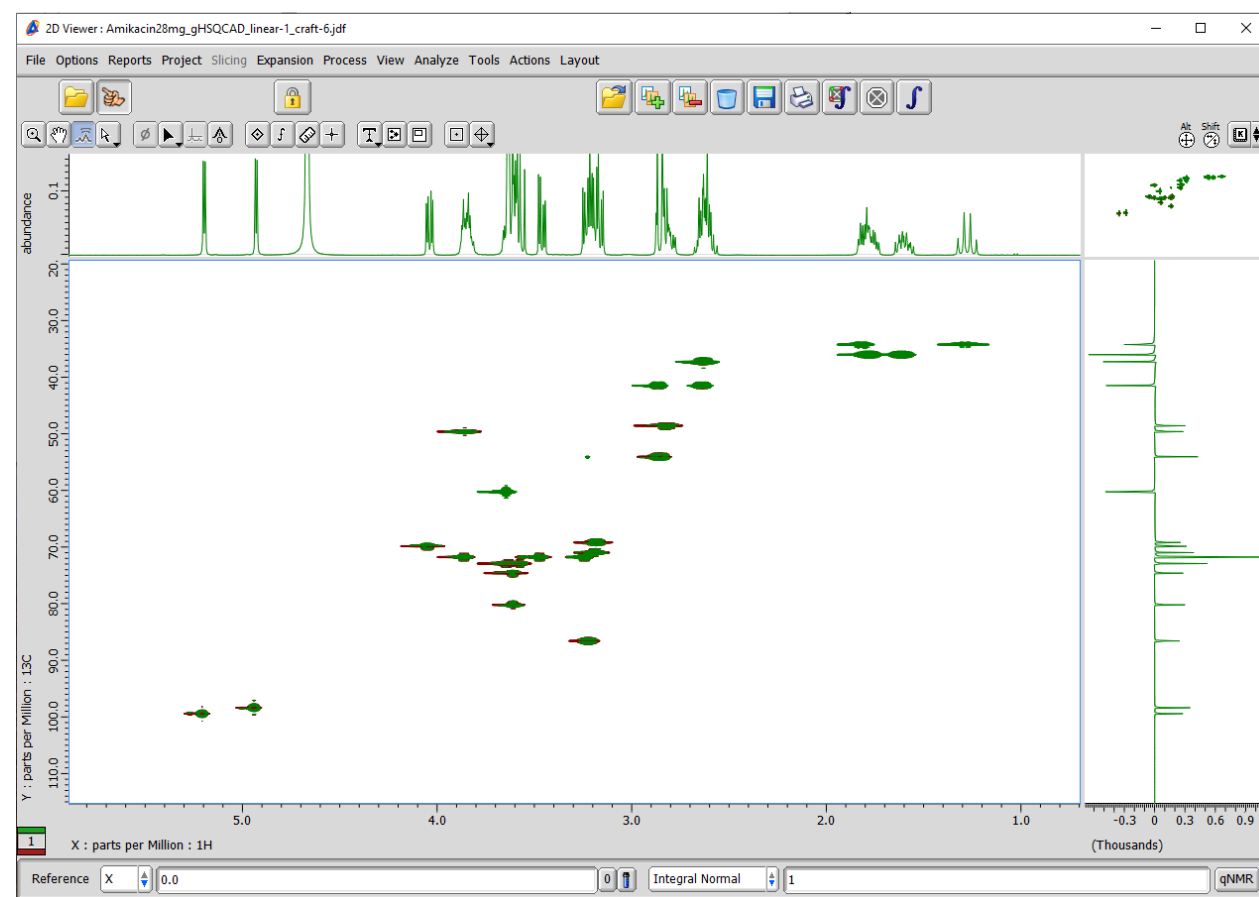
Maleic acid

TSP

CRAFT Result with reporting by fingerprints



2D CRAFT Amikasin with Table



2D CRAFT Amikasin showing extended High-resolution F1 (Y) projection