# Detection and Identification of Illicit Drugs and Cutting Agents in Seized Street Drugs:

## Benchtop NMR Spectrometer & Databasing Software


## ACD/Labs User Meeting

Susanne D. Riegel, Alexander F. G. Maier,
Dimitris Argyropoulos,
Marie Lange, Marion Baumgarte

*Baltimore, MD*
*March 8th, 2020*

nanalysis

ACD/Labs

# NMR Instruments and Field Strength


**High Field**
High Resolution
Spectrometer

**Low Field**
High Resolution
Spectrometer


**Low Field**
Low Resolution
Relaxometer

Resolution, Sensitivity, Cost, Field Homogenity, Expertise

Reaction Monitoring

QA/QC by Relaxation &
Diffusion variables

Absolute
Configuation

Structural
Elucidation

Industrial Applications

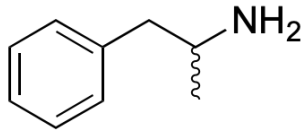
Academic Teaching

Robustness, Accessibility

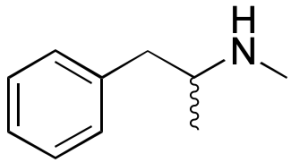
Dalitz, F.; Cudaj, M.; Maiwald, M.; Guthausen, G.; *Prog. Nuc. Mag. Reson. Spec.* **2012**, *60*, 52

# Illegal Drugs

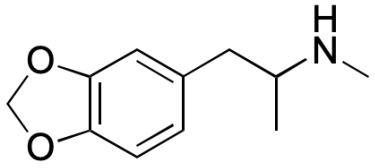
- Typically classified by:
  - Legal Classification – e.g., Schedule I, Class A
  - Effect – e.g., depressant, stimulant, hallucinogen
  - Molecular Structure – e.g., cannabinoids, opioids, phenethylamines




**Amphetamine**
Stimulant

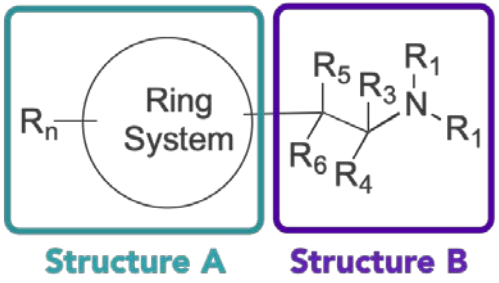



**Methamphetamine**
Stimulant

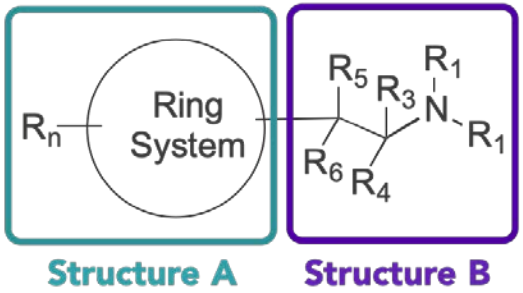



**MDMA**
Psychedelic, entactogen

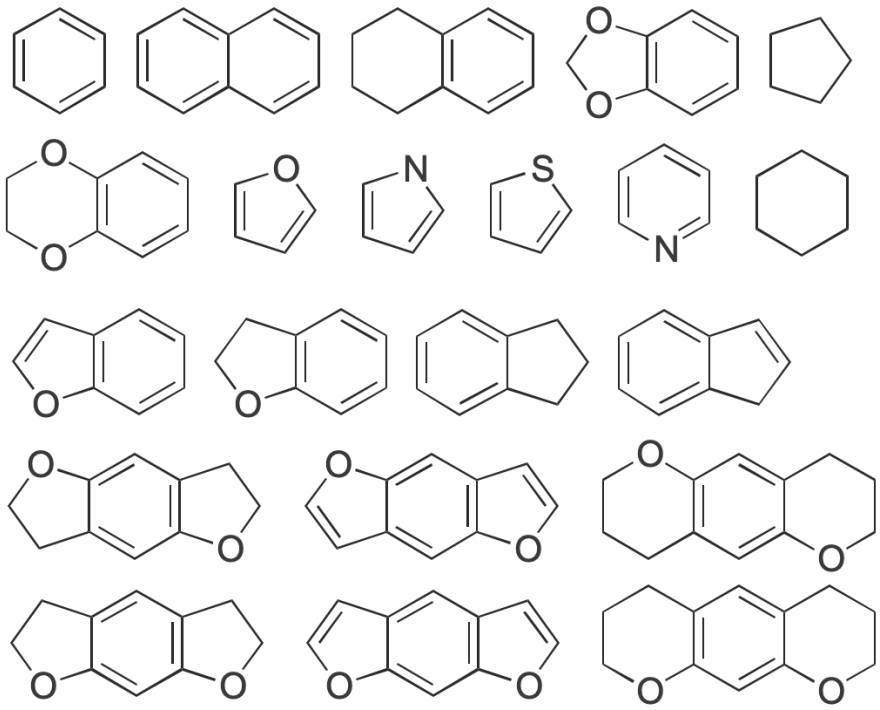
- Designer Drugs – synthetic analog of a legal restricted or prohibited drug devised to avoid drug detection and identification.



# New Psychoactive Substances* (from 2-phenyethylamine)




**Ring System =**



**$R_1$ or $R_2$ =**

H, F, Cl, Br, I
linear alkyl to $C_6$
cycloalkyl to $C_6$
benzyl
alkenyl to $C_6$
alkylcarbonyl to $C_6$
hydroxyl
amino
heterocycles with N

**$R_3$, $R_4$, $R_5$ or $R_6$ =**

H, F, Cl, Br, I
linear alkyl to $C_{10}$
cycloalkyl to $C_{10}$
benzyl, phenyl
alkenyl to $C_{10}$
alkinyl to $C_{10}$
hydroxyl
alkoxy to $C_{10}$
alkylsulfanyl to $C_{10}$
alkyloxycarbonyl to $C_{10}$

** Defined by EU 2015/1535 'Act to combat the distribution of new psychoactive substance'*

# Why Benchtop NMR Spectroscopy?

| | Nik Wipes | IR | HPLC | High-field NMR | Benchtop NMR |
|---|---|---|---|---|---|
| **Sample Prep** | ✓ Easy | ✓ Easy | X Tedious | ✓ Easy | ✓ Easy |
| **Sample Conc** | ~ Medium | ~ Low-medium | ✓ Low | ~ Low-medium | ~ Medium |
| **Analysis Time** | ✓ <1 min | ✓ <1 min | X >15 min | ✓ <1 min | ✓ <1 min |
| **Location** | ✓ On-site | ✓ On-site | X Off-site | X Off-site | ✓ On-site |
| **Standards** | X Required | X Required | X Required | ✓ Not Required | ✓ Not Required |
| **Quantitative** | X | X with calibration | X with calibration | ✓ w/o calibration | ✓ w/o calibration |
| **Capital Cost** | $ | $ | $$ | $$$$ | $$ |
| **Operating Expenditure** | $ | $ | $$ | $$$ | $ |

# Considerations for Mobile Laboratory


- Stability – temperature (AC & simple heating block), vibration (soft or hard)
- Mounting
- Power consumption
- Automation
- Accuracy/reliability

# Sample Preparation and $^1$H NMR Acquisition

## SAMPLE PREP:

### Reference Standards

- 60 µmol of sample dissolved in ~0.6 mL DMSO-$d_6$ or $D_2O$ (if insoluble)
- Vial capped and agitated until dissolved completely.
- Transferred to NMR tube

### Unknown Search Queries

- ~30 mg of an unknown drug sample dissolved/suspended in vials of ~0.6 mL DMSO-$d_6$ and $D_2O$
- Vials were capped and agitated for 1 min
- Liquid phase transferred to NMR tube

## $^1$H NMR DATA ACQUISITION (performed at LKA):

1D $^1$H NMR spectrum at 60 MHz

SW = 80 ppm
SW center = 20 ppm
np = 8192

scan delay = 1 s
ns = 16 or 64
time = 1 min or 4 min

## PRE-PROCESSING (ACD/Labs Macro for automatic processing):

- Zero Fill
- Phase
- Baseline
- solvent detection

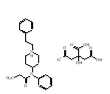
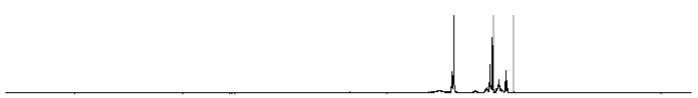
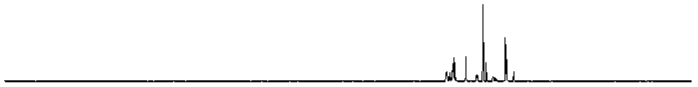
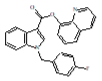
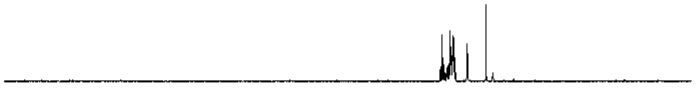
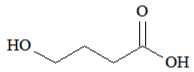
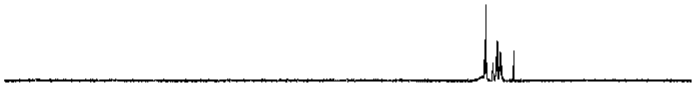
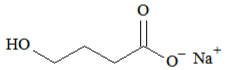
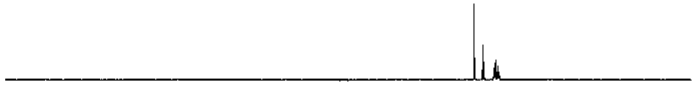
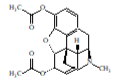
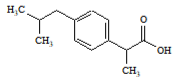
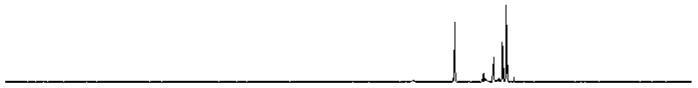
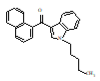
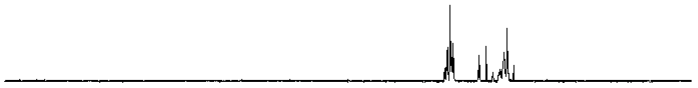
LANDESKRIMINALAMT NIEDERSACHSEN

# Database

ACD/Spectrus DB: Database Window - [C:\NANALYSIS\COLLABORATIONS\ACDLABS\DATABASE COMPARISON\KTI.CFD]

Database View Record Search Lists Plates Options ACD/Labs Help

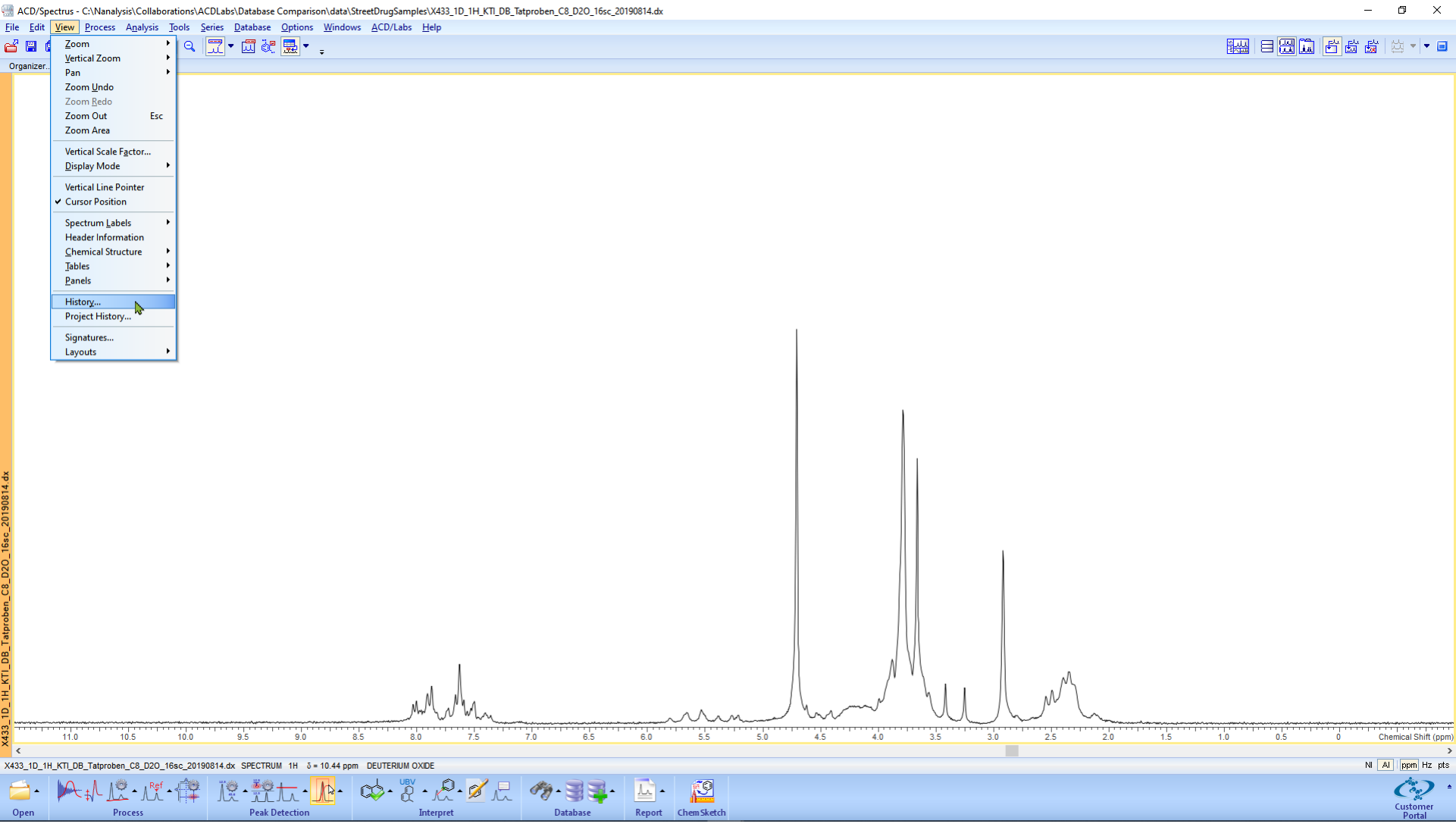
Tile | Table | Default (One Record) | Search Query

| #List | # | Structure | Spectrum | Formula | Trivial Name |
|---|---|---|---|---|---|
| | 94 |  |  | $C_{28}H_{36}N_2O_8$ | Fentanyl citrate |
| | 95 |  |  | $C_{21}H_{22}FN_3O_3$ | FUB-AMB (AMB-FUBINACA) |
| | 96 |  |  | $C_{25}H_{17}FN_2O_2$ | FUB-PB-22 |
| | 97 |  |  | $C_4H_8O_3$ | GHB |
| | 98 |  |  | $C_4H_7NaO_3$ | GHB Na |
| | 99 |  |  | $C_{21}H_{23}NO_5$ | Heroin |
| | 100 |  |  | $C_{13}H_{18}O_2$ | Ibuprofene |
| | 101 |  |  | $C_{24}H_{23}NO$ | JWH-018 |

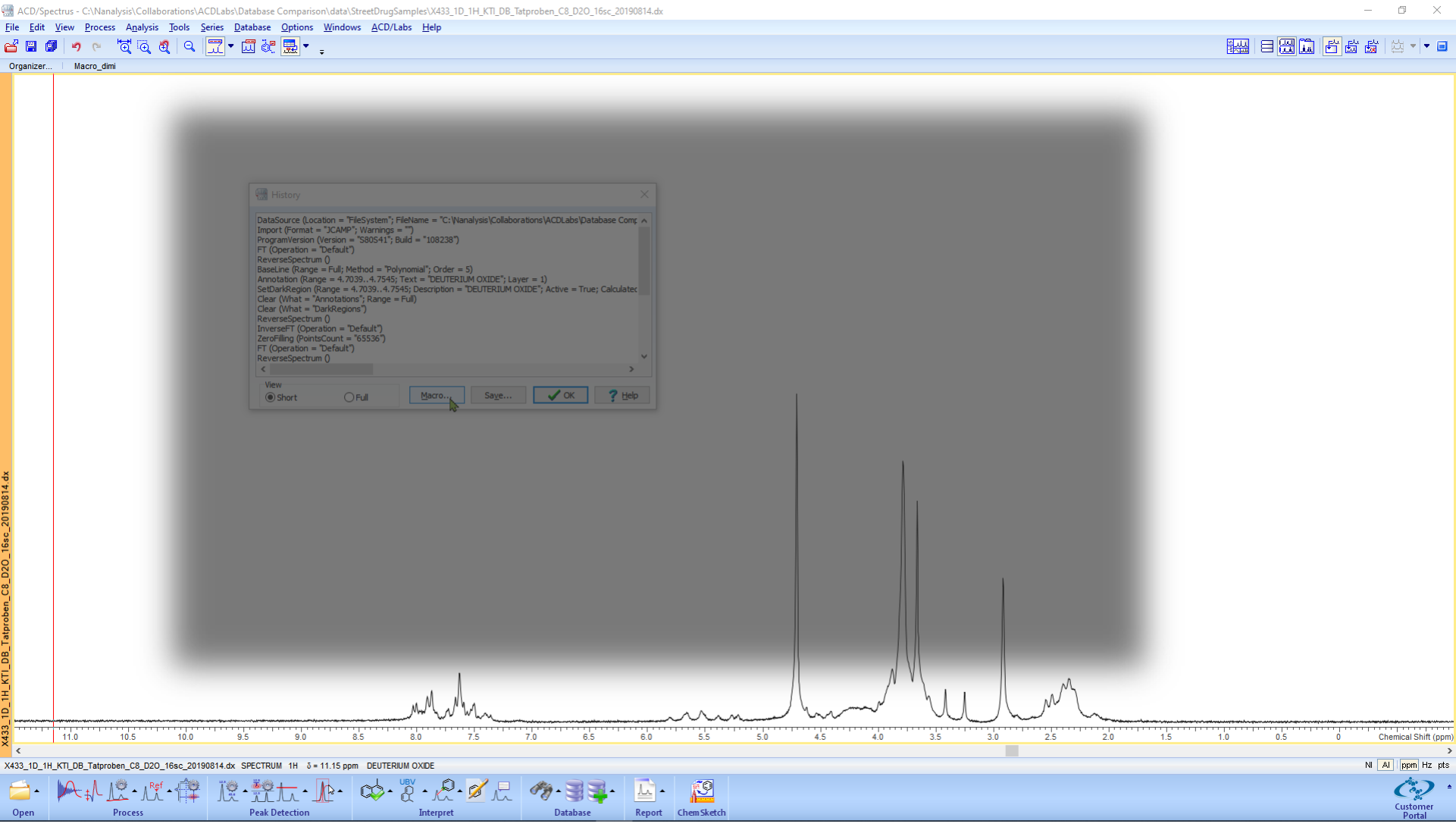
ID: 323 | A: 94/171 | B: 14 | Last Updated: 28/02/2020 19:00 | Single DB

1-ChemSketch | 2-Database | 3-Processor

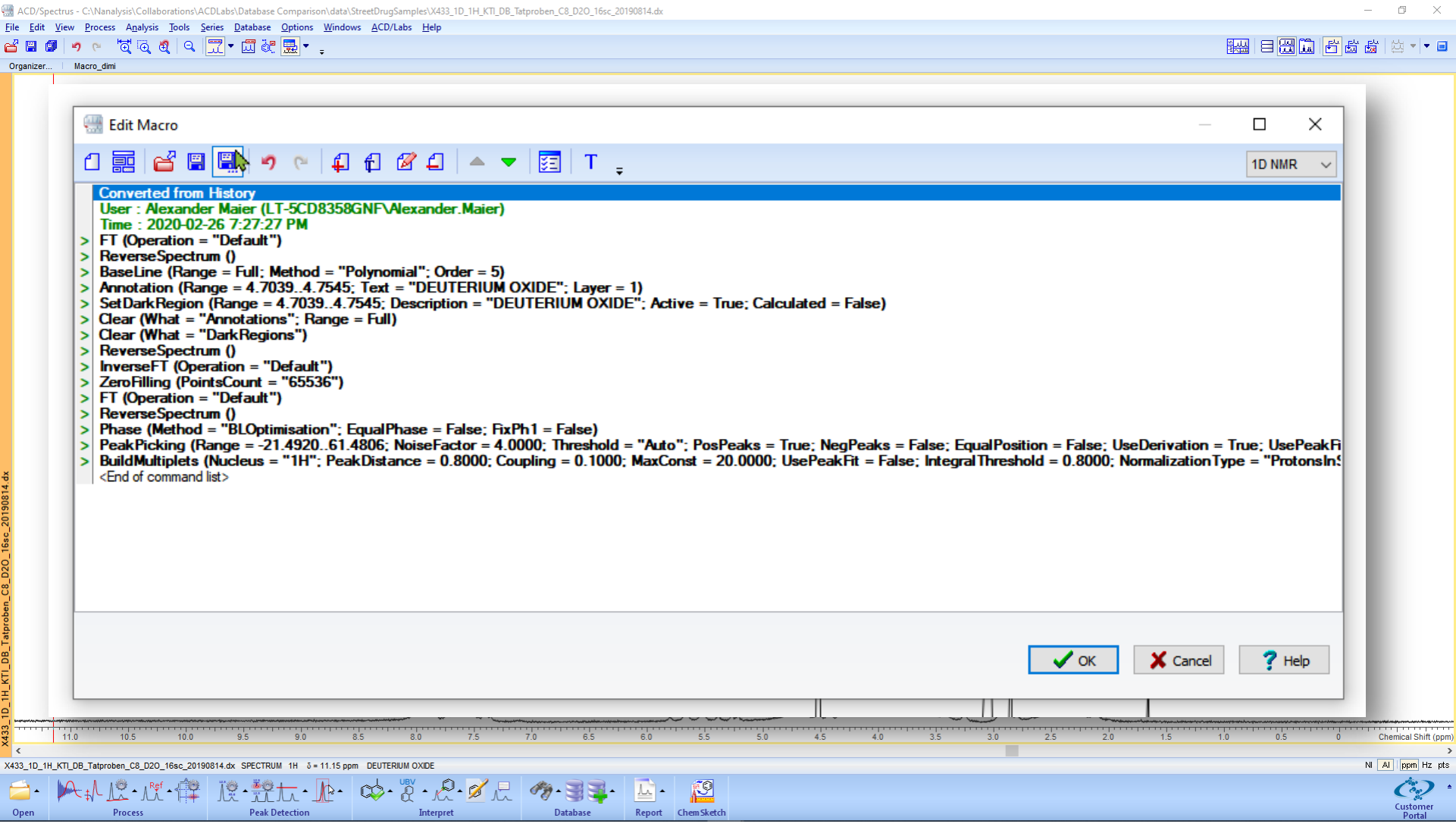
# Creating a Macro



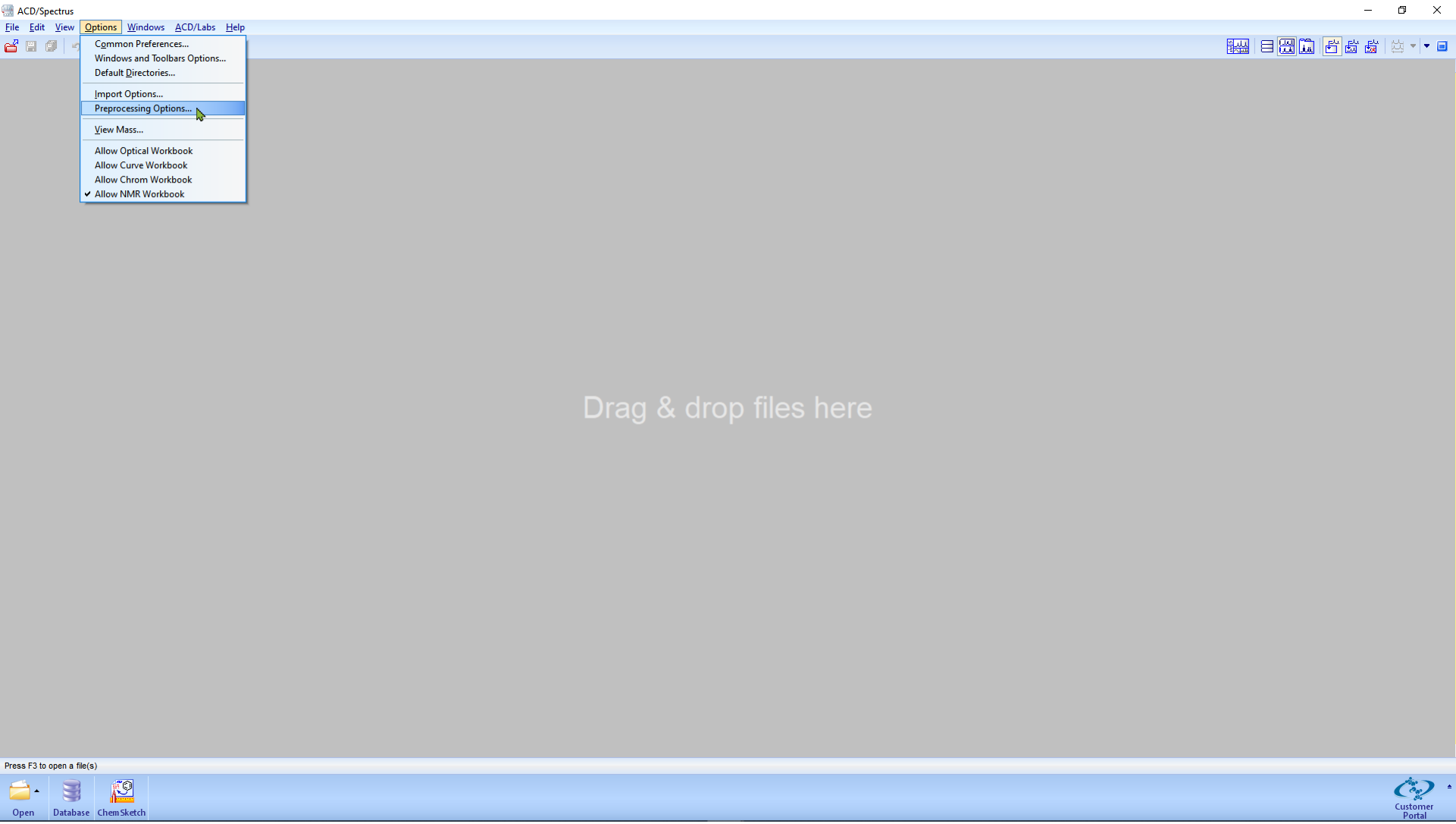
# Creating a Macro



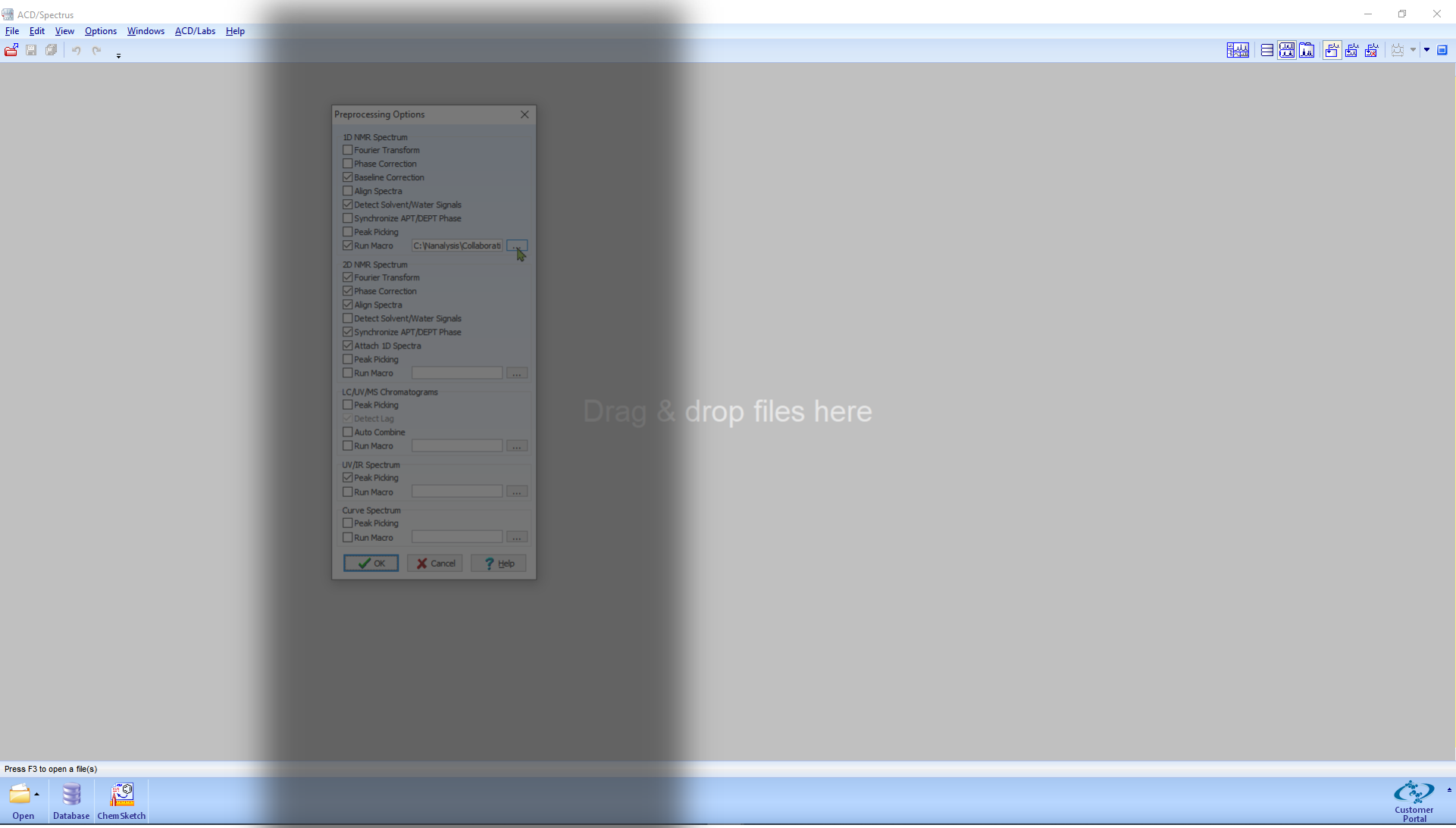
# Creating a Macro



# Automated Preprocessing: Apply Macro



# Automated Preprocessing: Apply Macro



# Case Study: Unknown Street Drug

1. Sample Prep of Unknown:

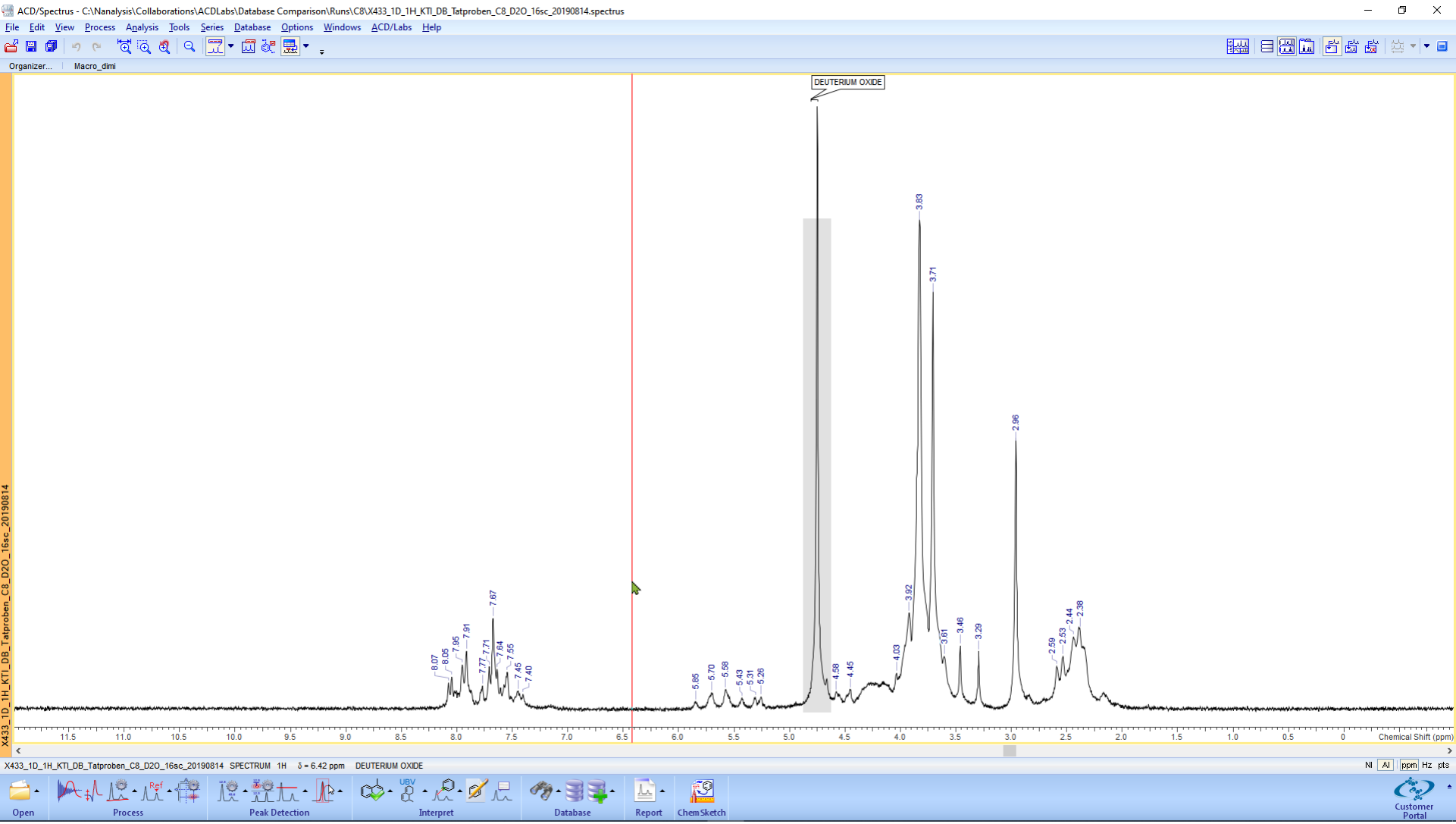
- Spatula of unknown added to vial of ~0.6 mL $D_2O$
- Sealed and agitated for 1 min
- Liquid phase transferred to NMR tube

2. $^1H$ NMR Spectra Acquisition

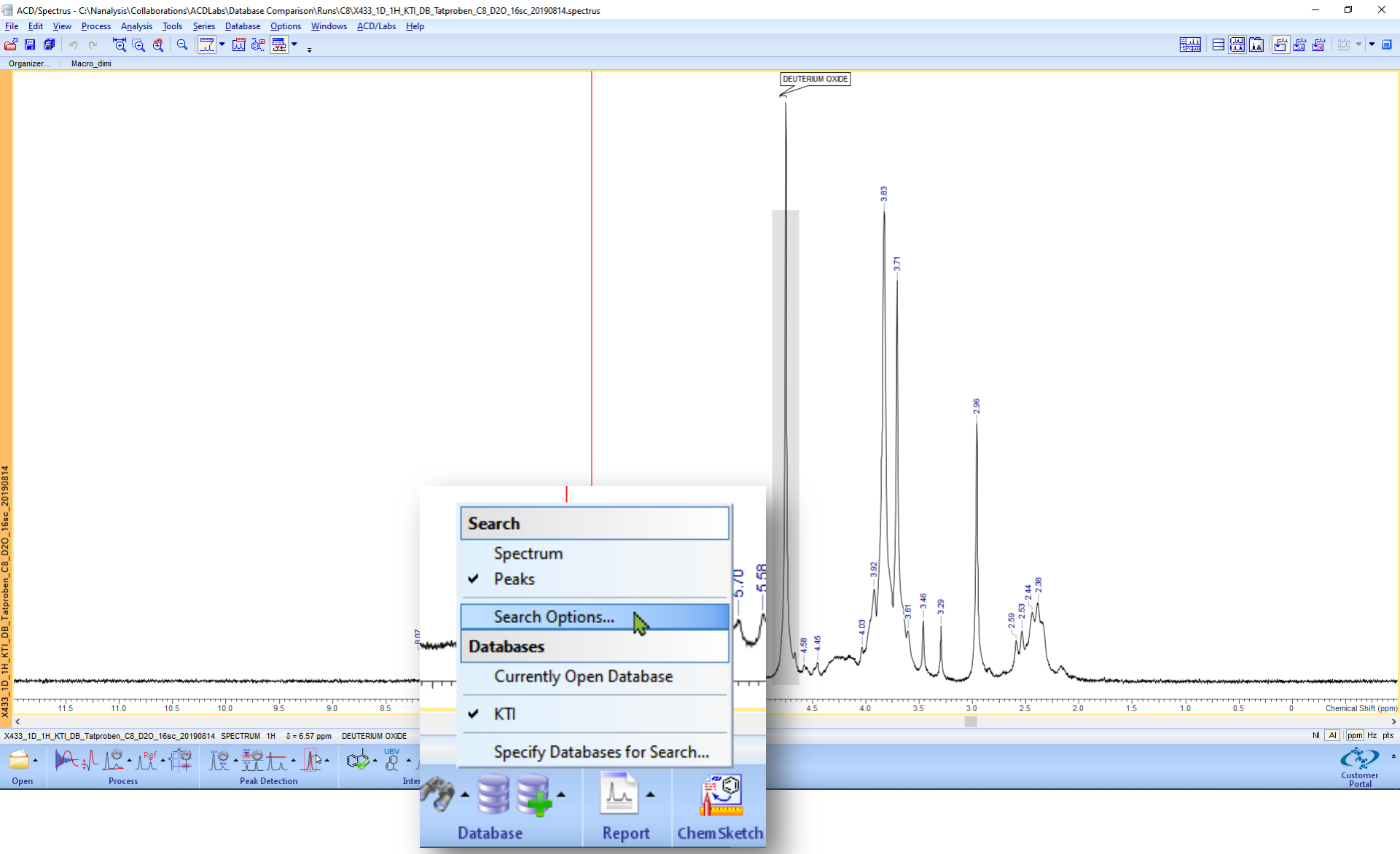
3. Load into ACD/Spectrus

- Auto Preprocessing Macro
- Peak Search with ACD/Spectrus DB

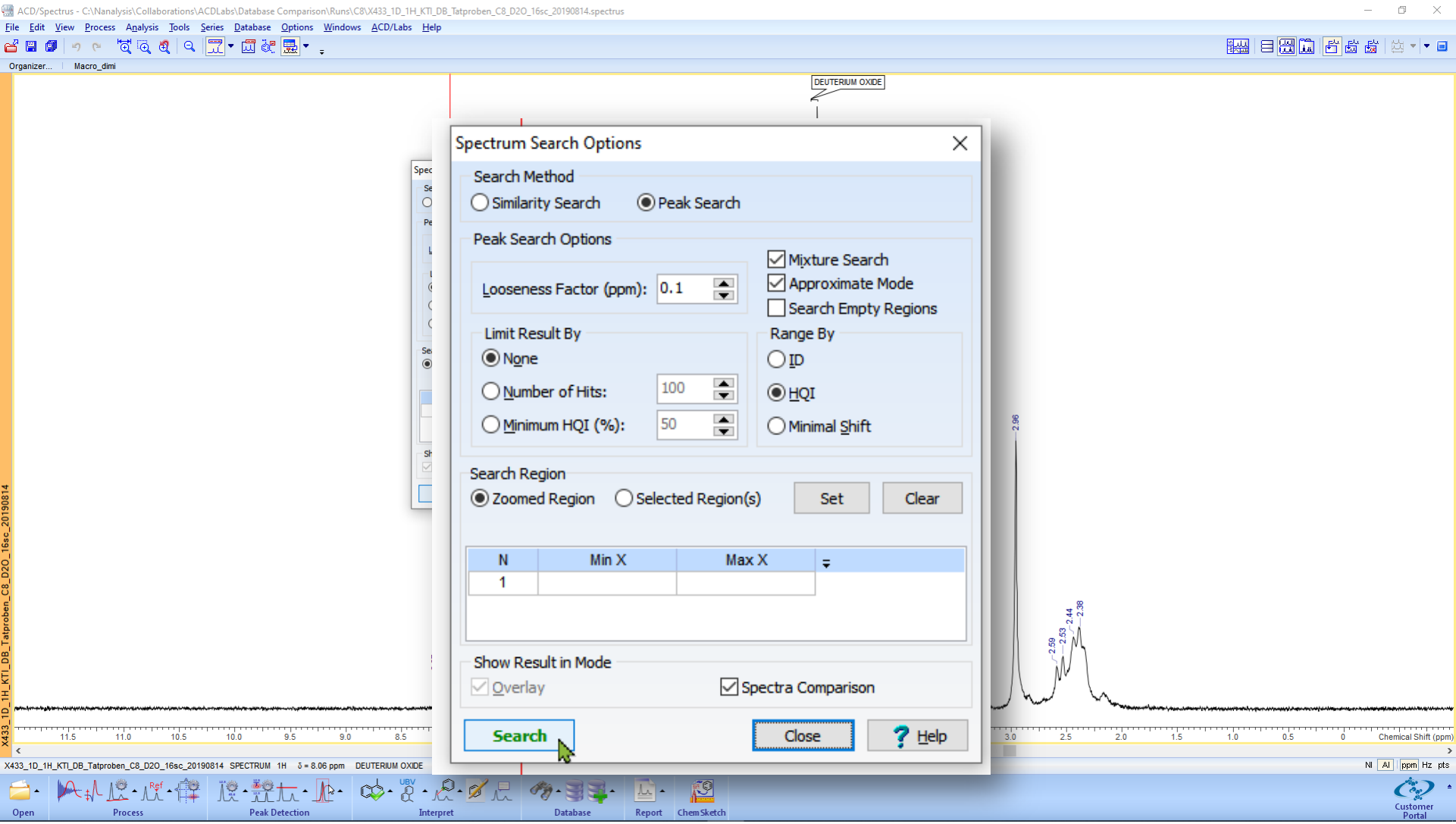
# Open Unknown $^{1}$H NMR Spectra into ACD/Labs



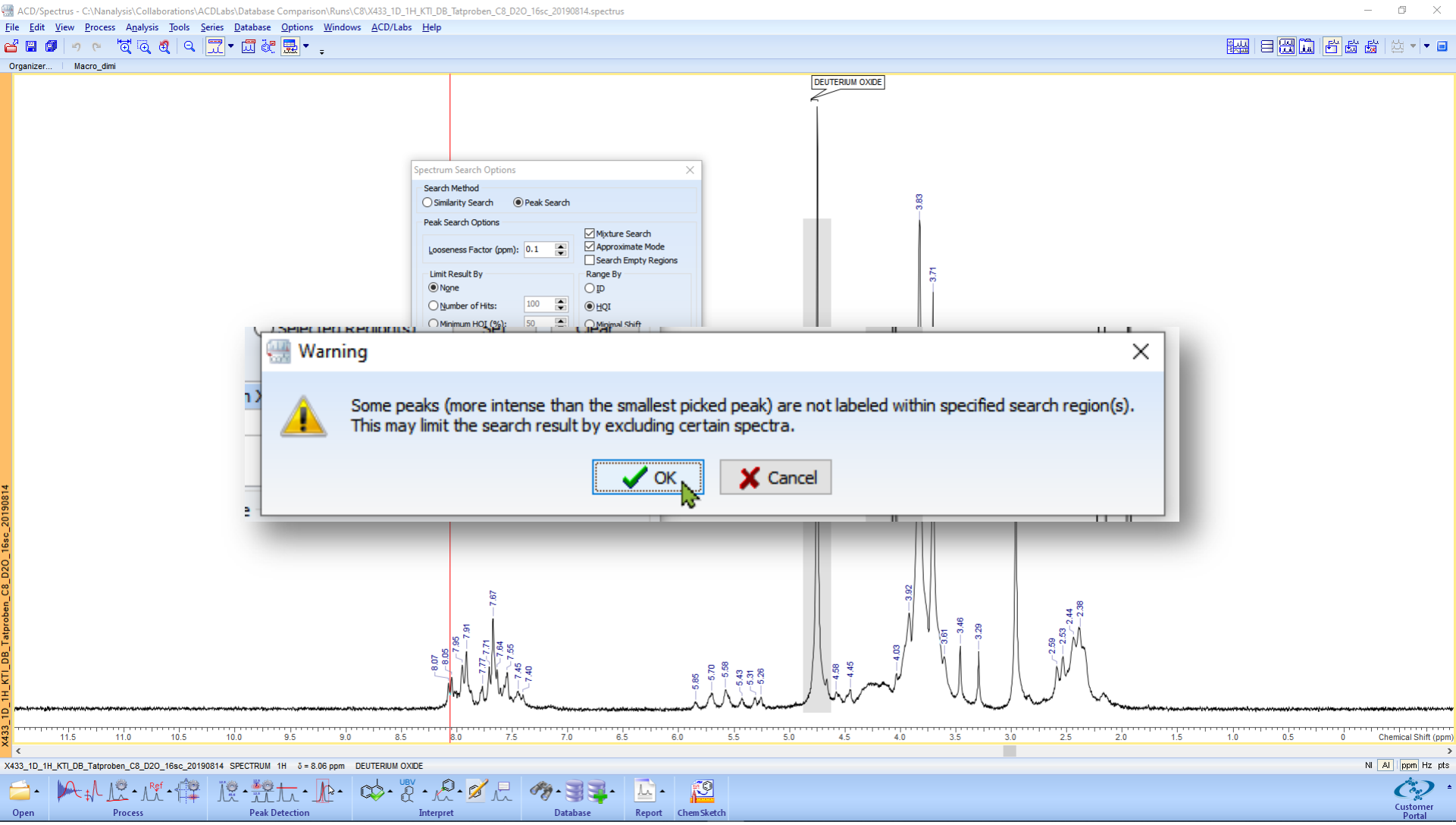
# Search Database



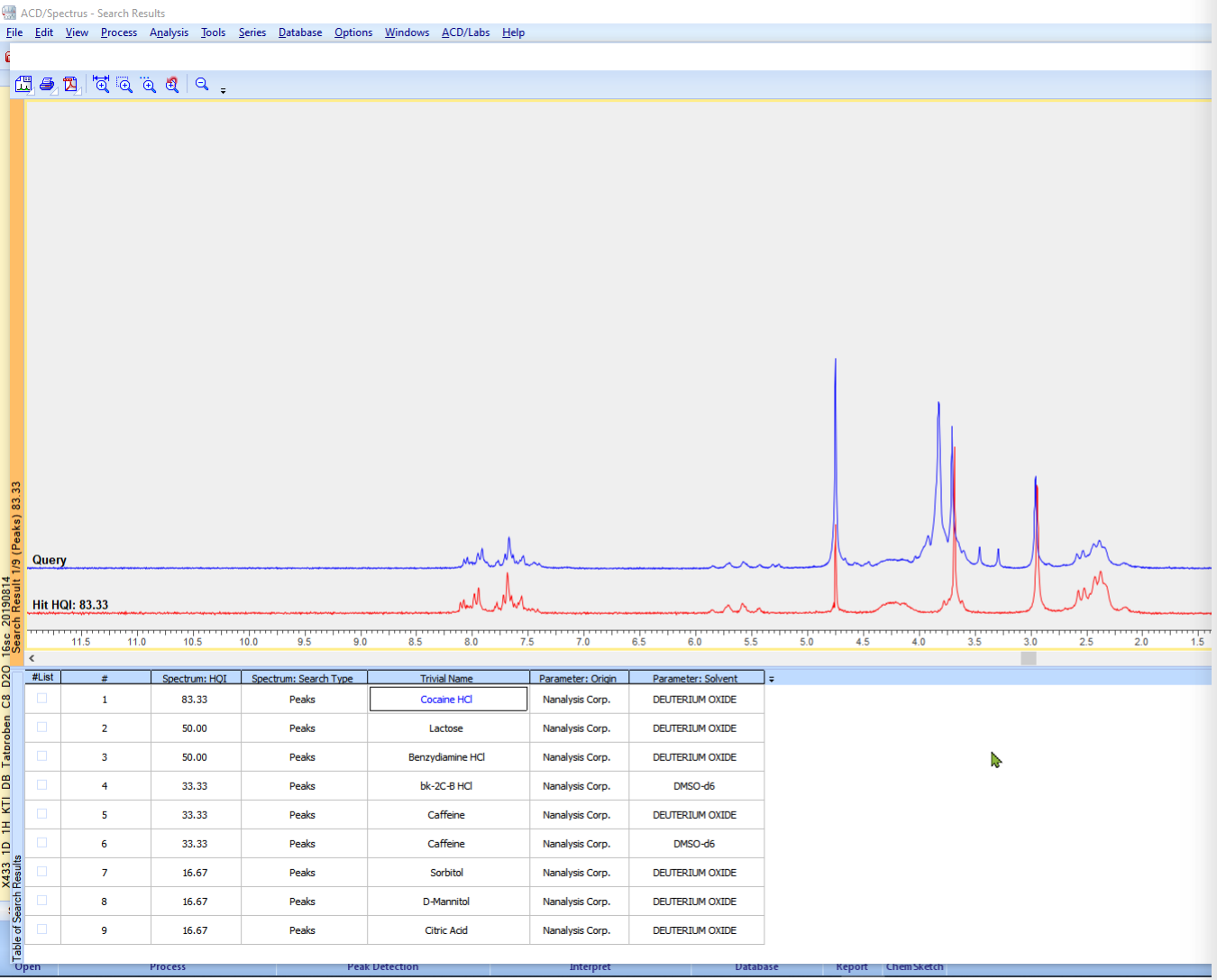
# Database Search Options



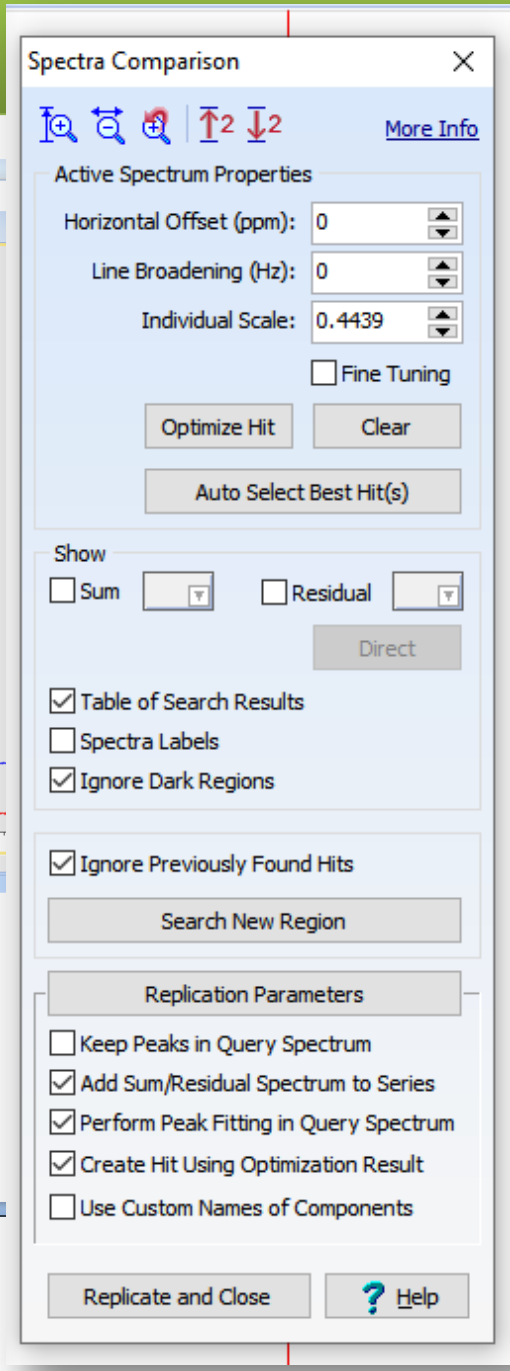
# Database Search



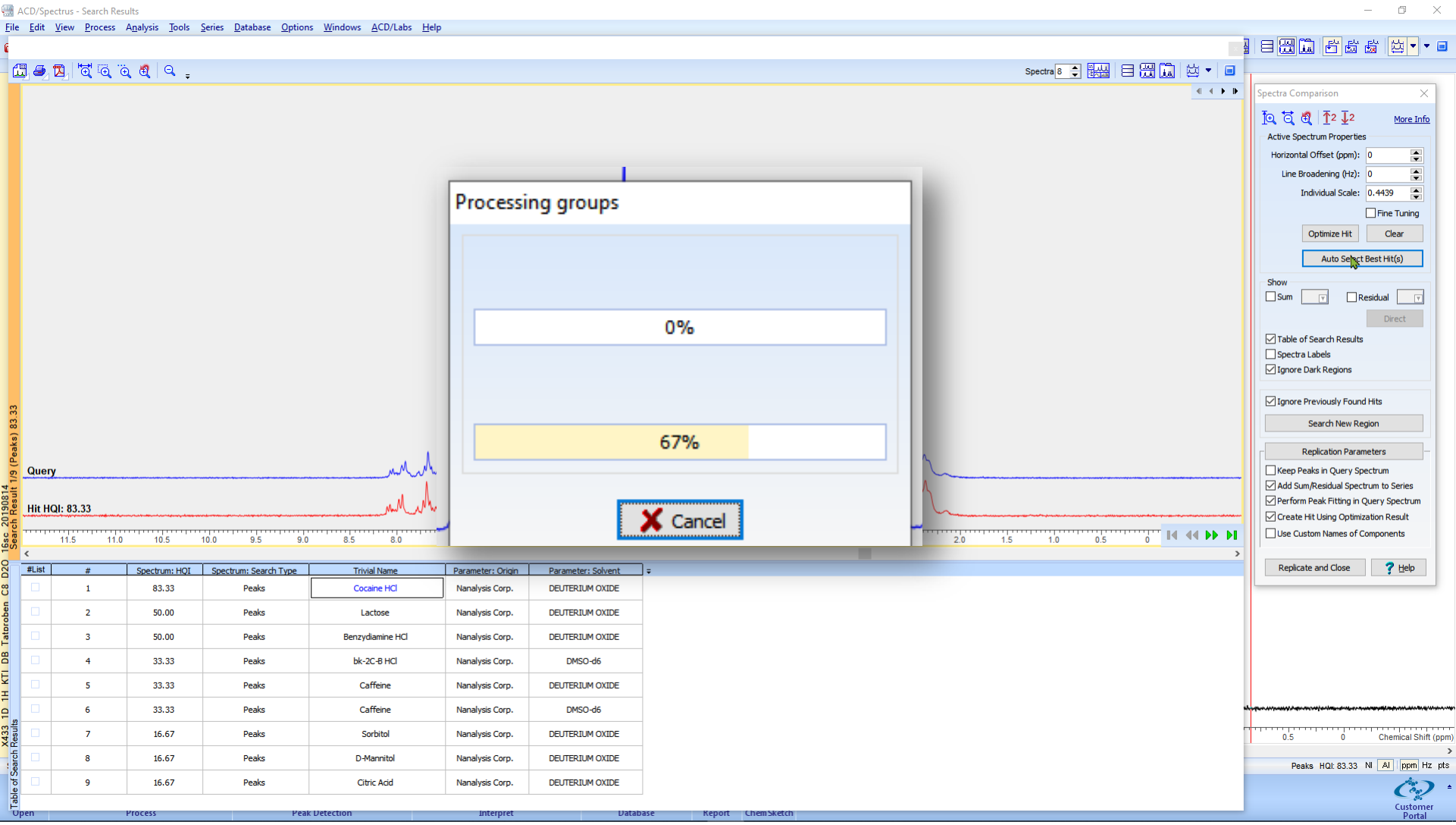
# First Database Hits: Cocaine




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |



# Auto Select Best Hits

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| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Database Best Hits


| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
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| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
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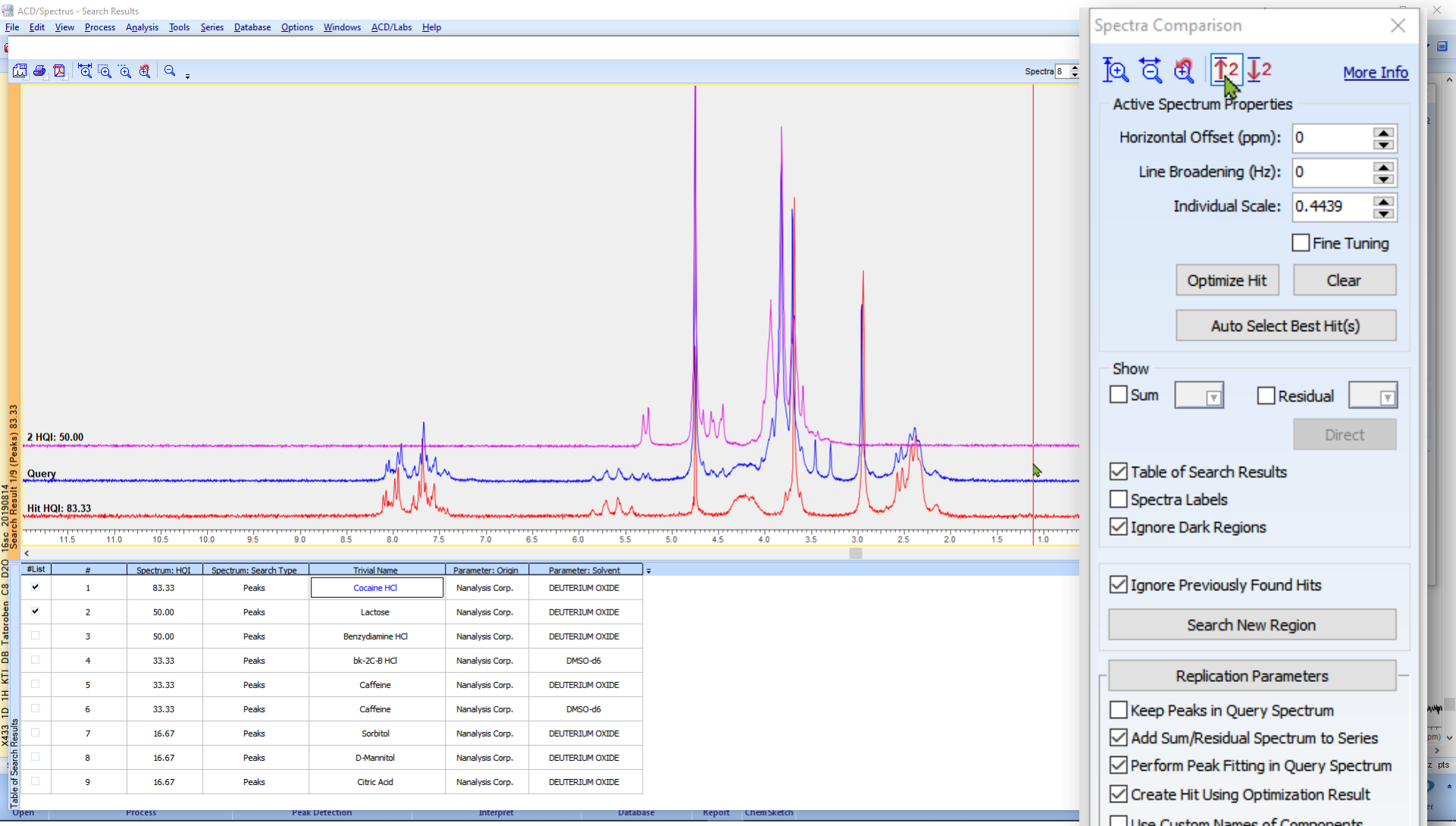
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Adjust Intensity

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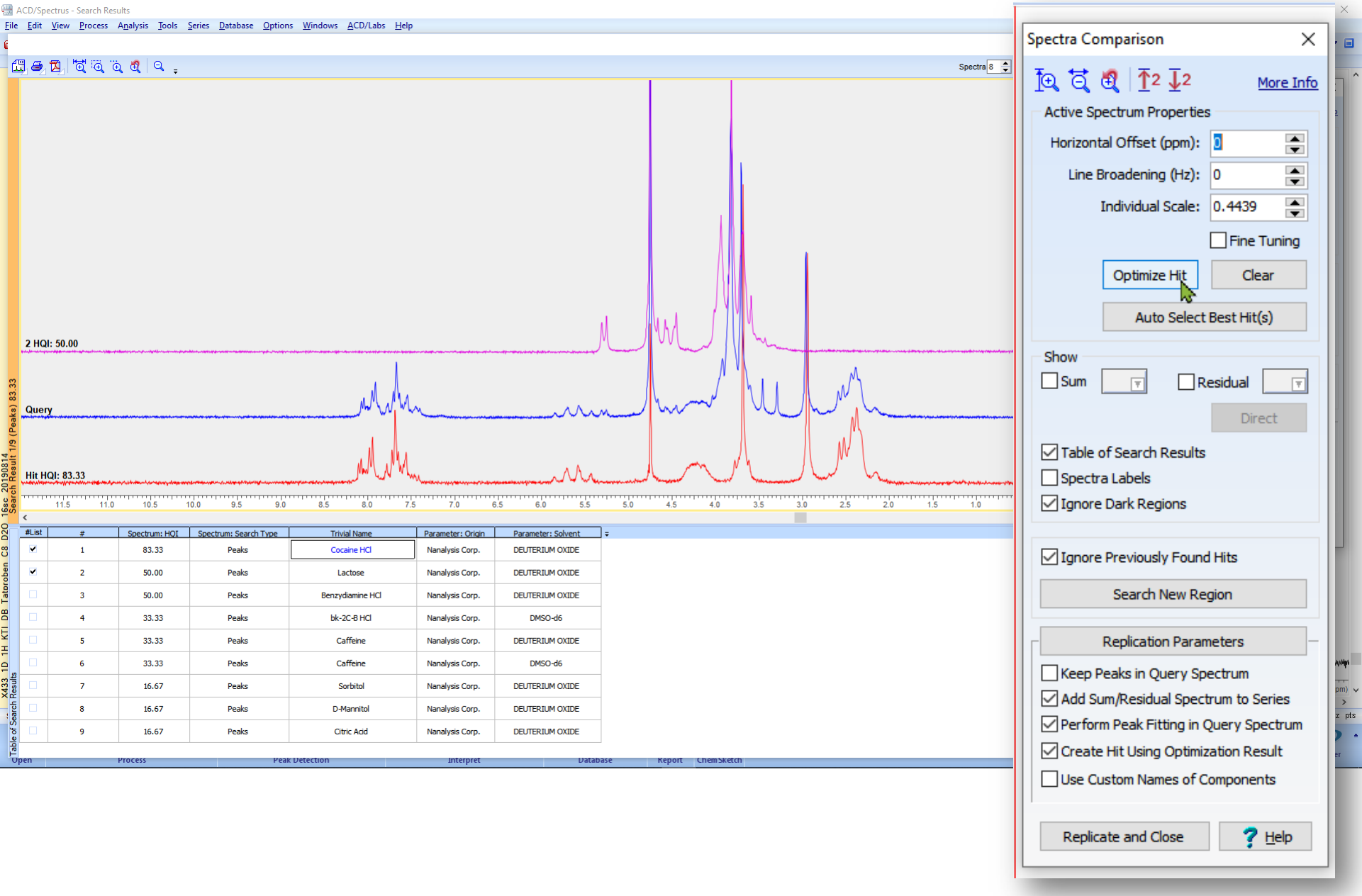
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Optimize Hit




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
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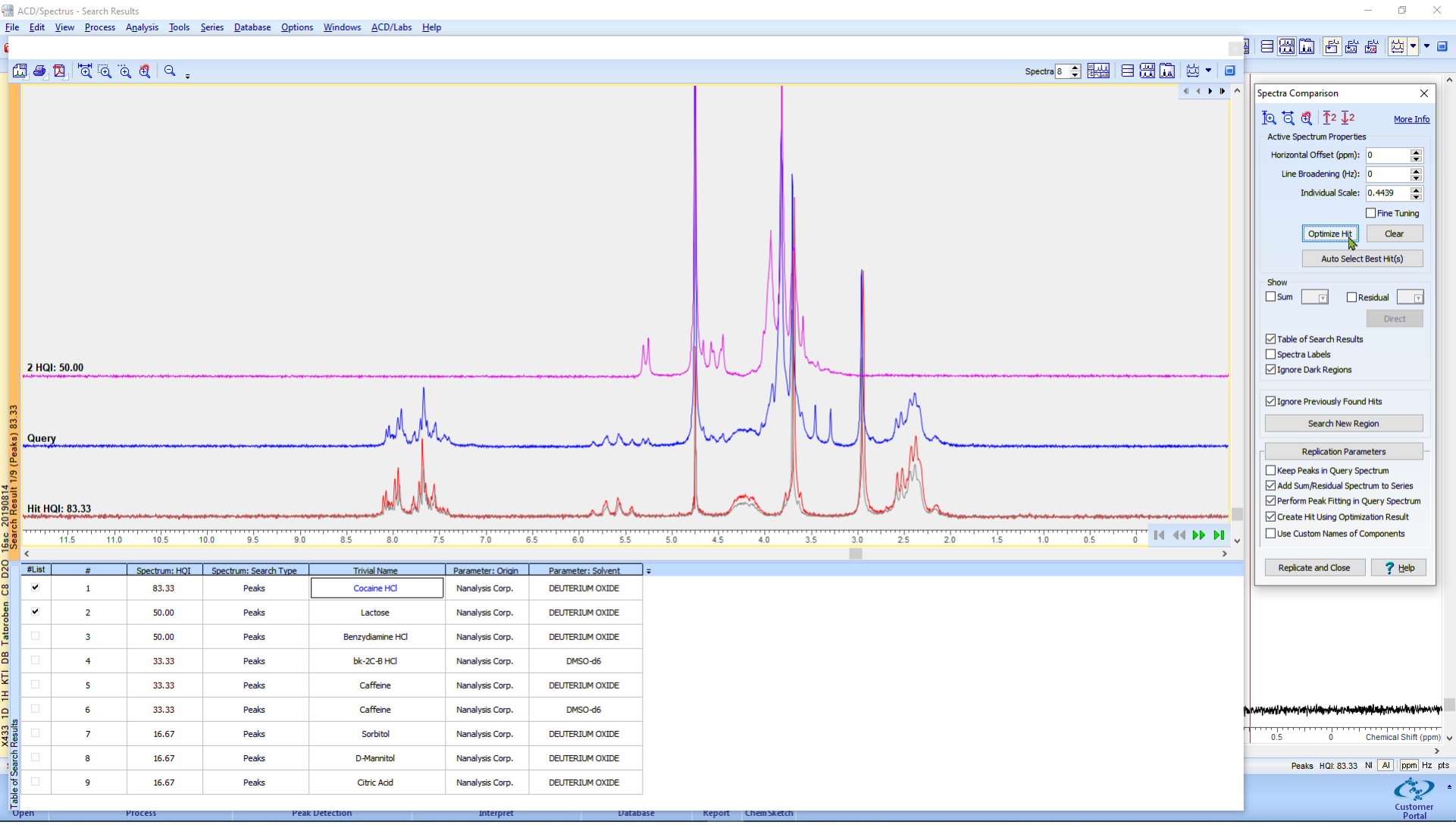
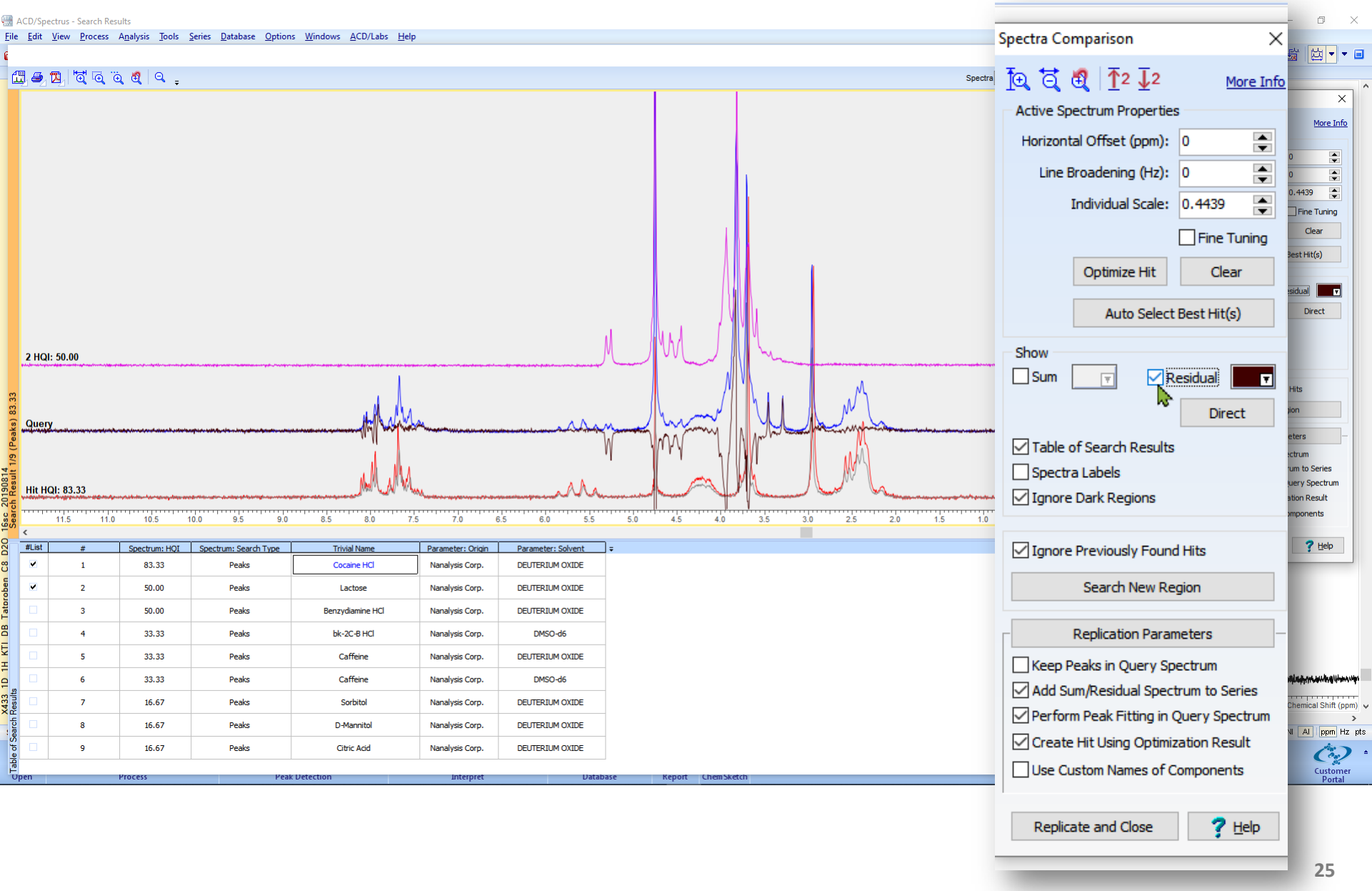
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Optimize hit for Cocaine



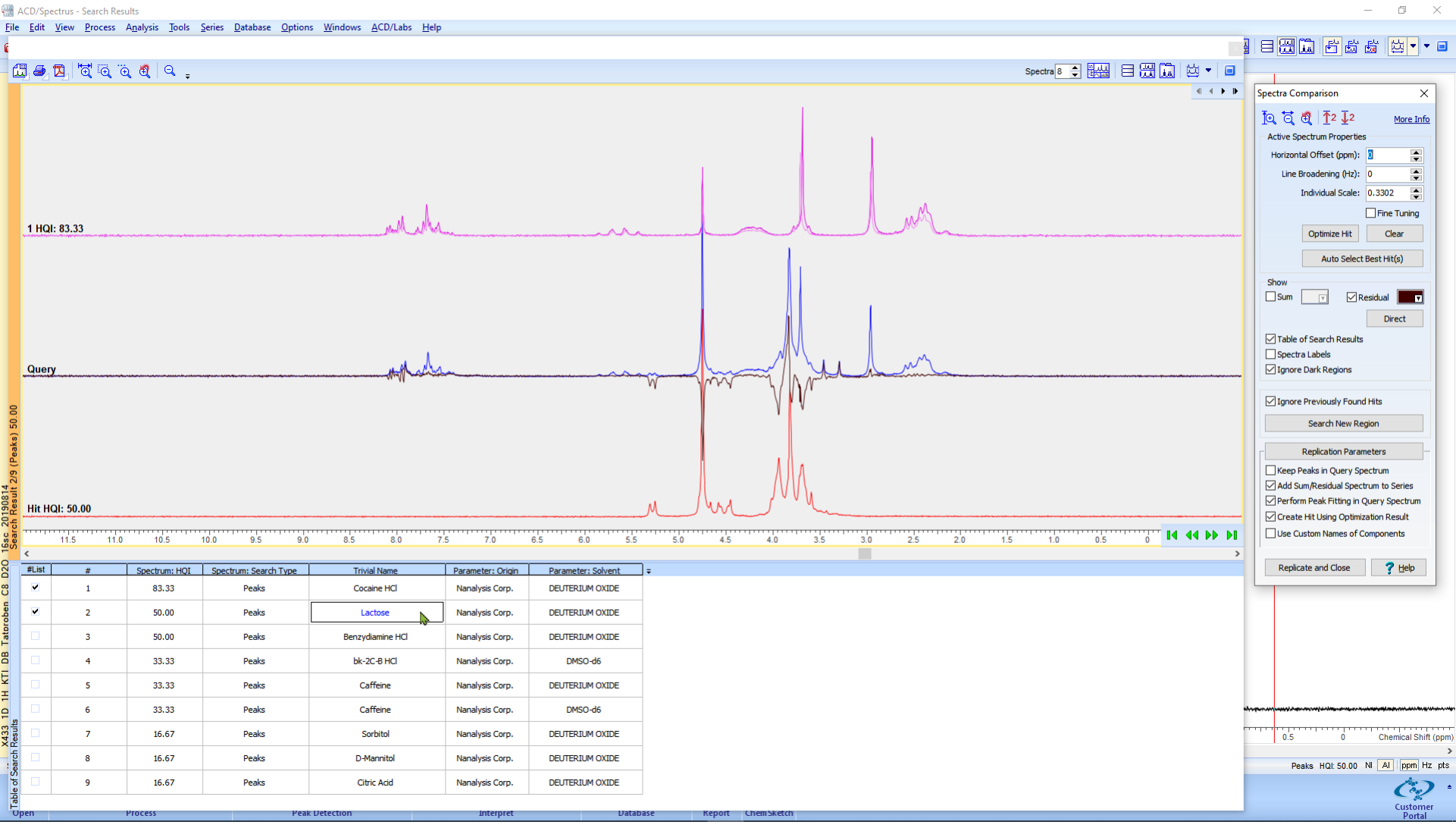

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Residuals of Best Fit for Unknown & Cocaine Std




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

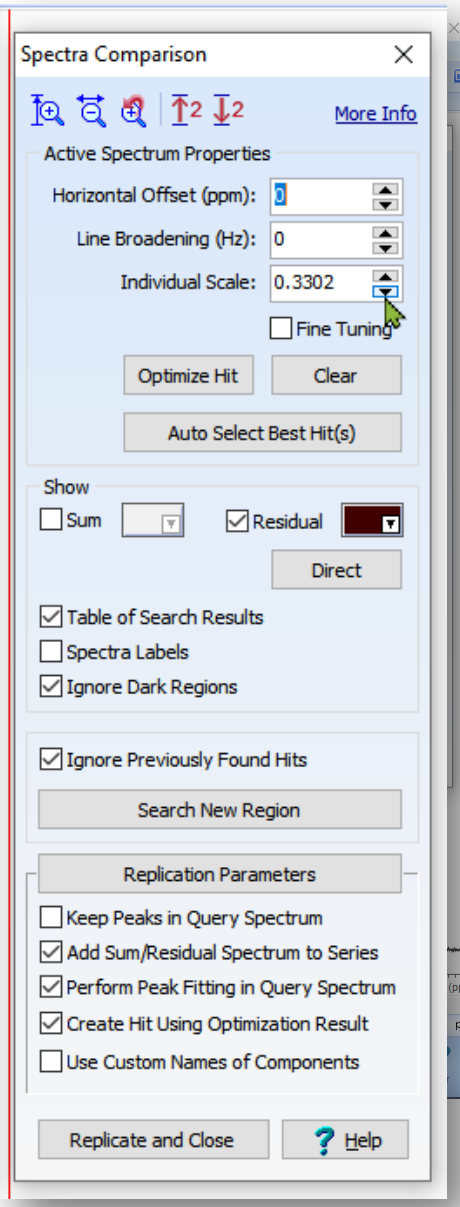
# Optimize Hit for Lactose



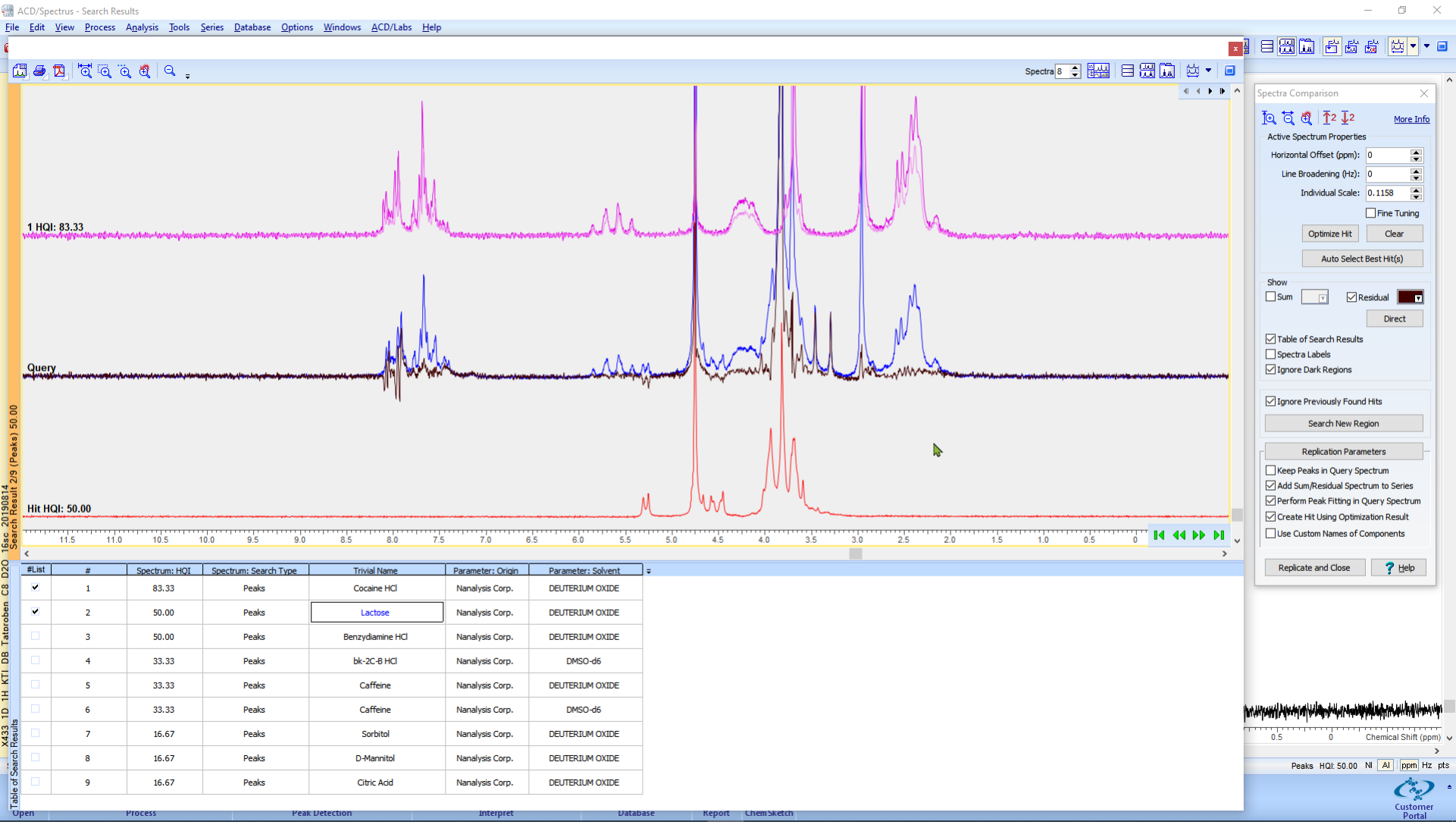

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Manually Change Intensity


| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✓ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✓ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

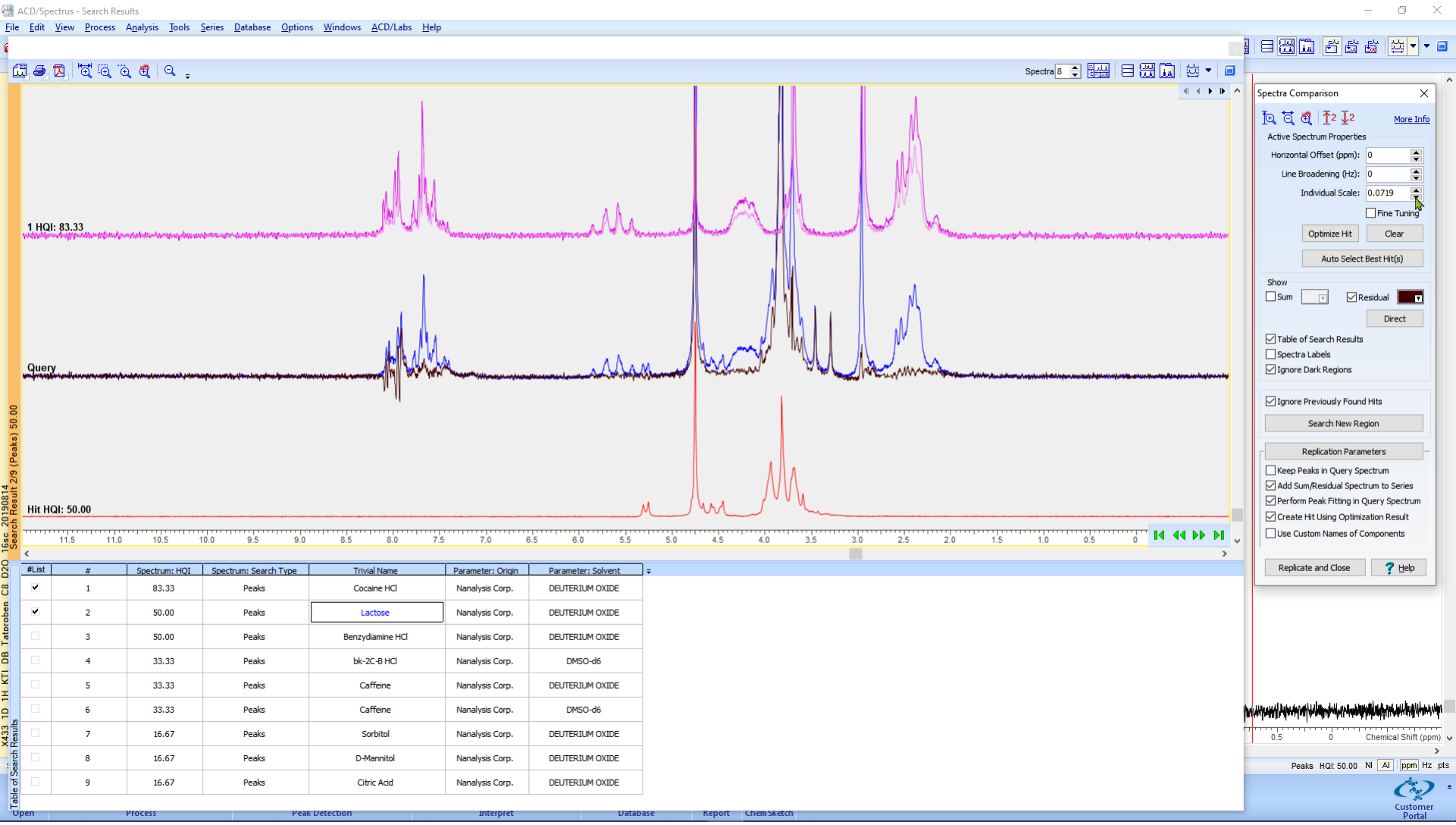


# Manually Change Intensity



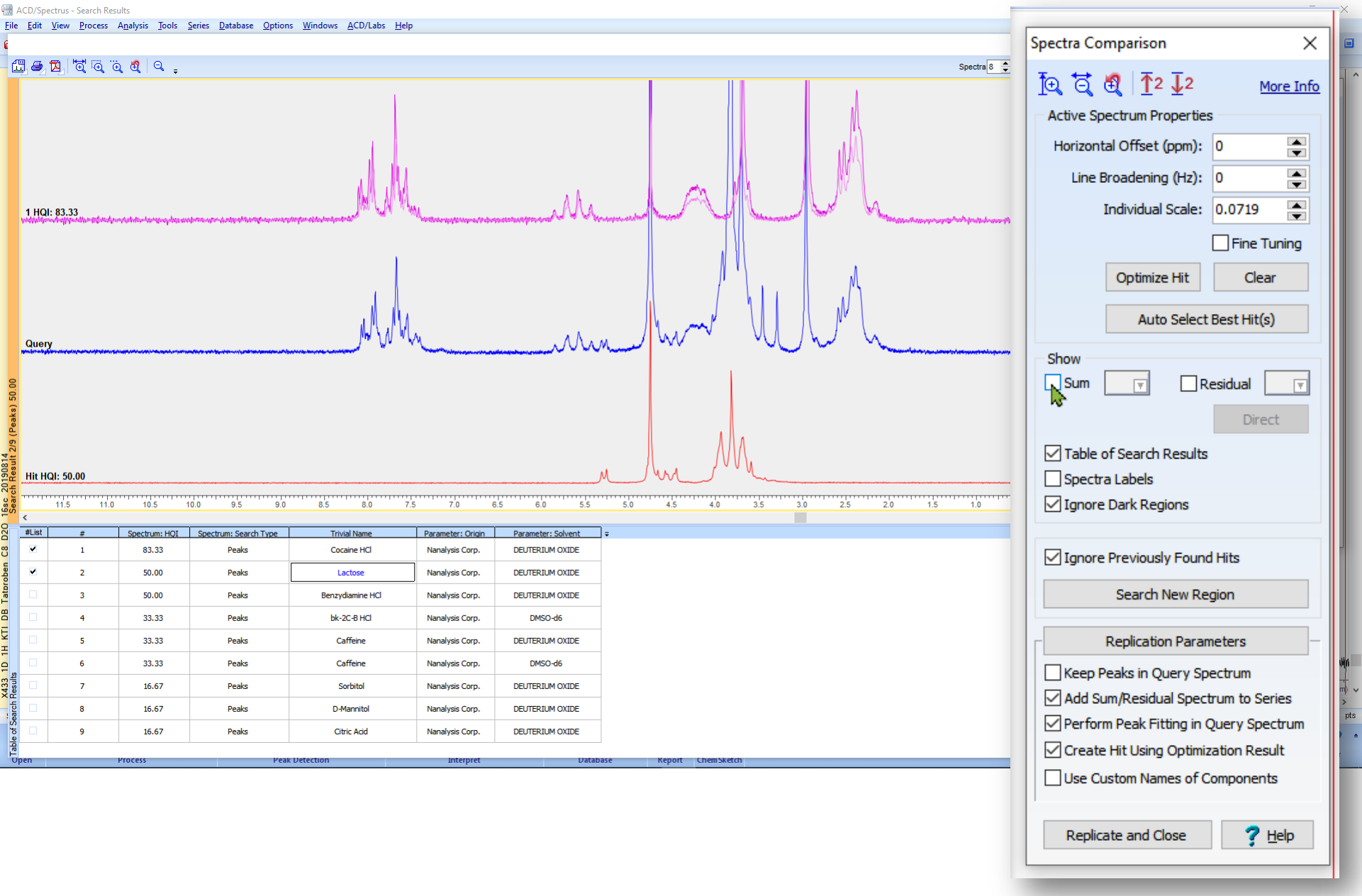

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Manually Change Intensity



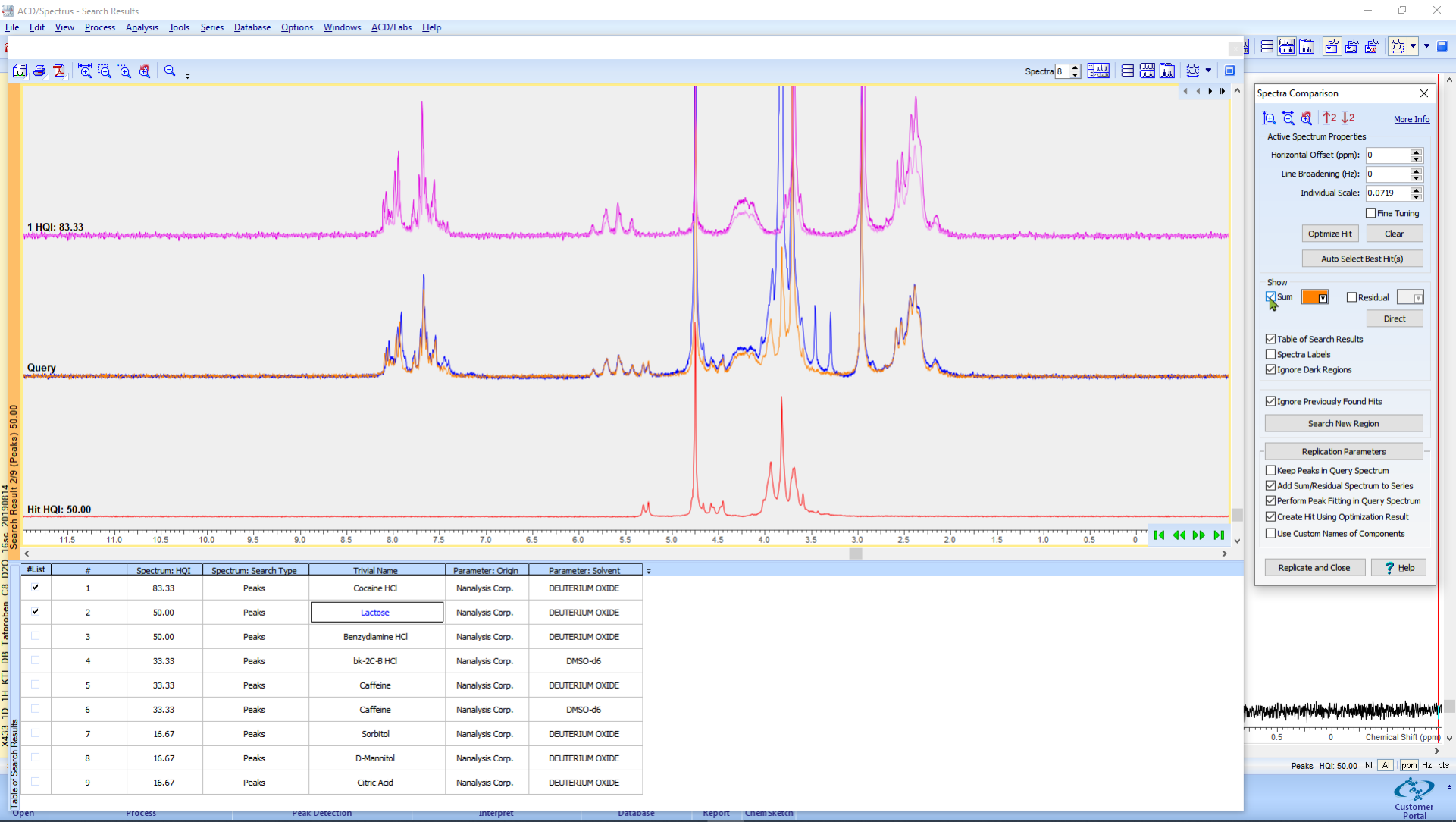

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visualize Sum Instead of Residuals



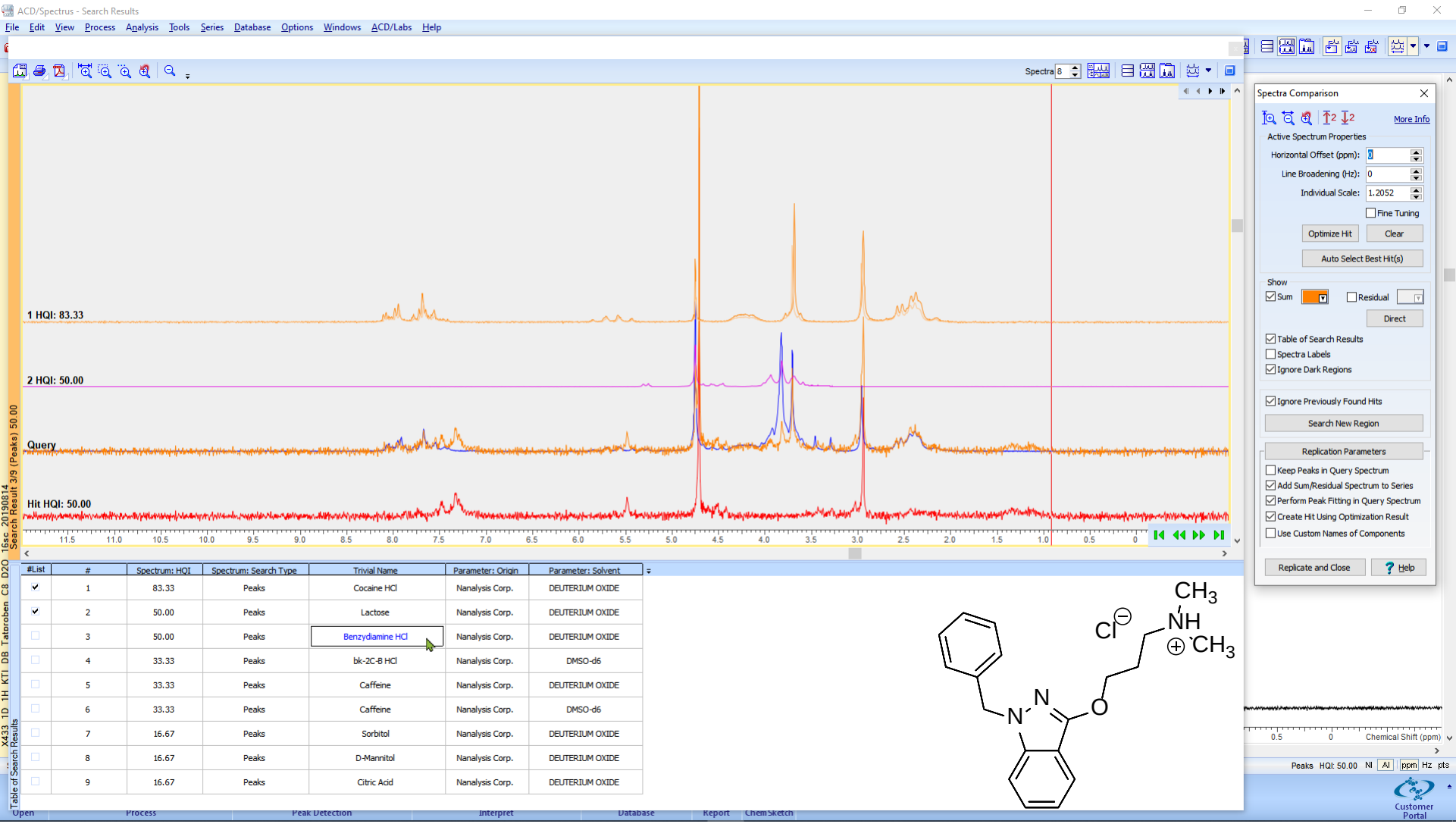

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Sum of Database Components on Unknown



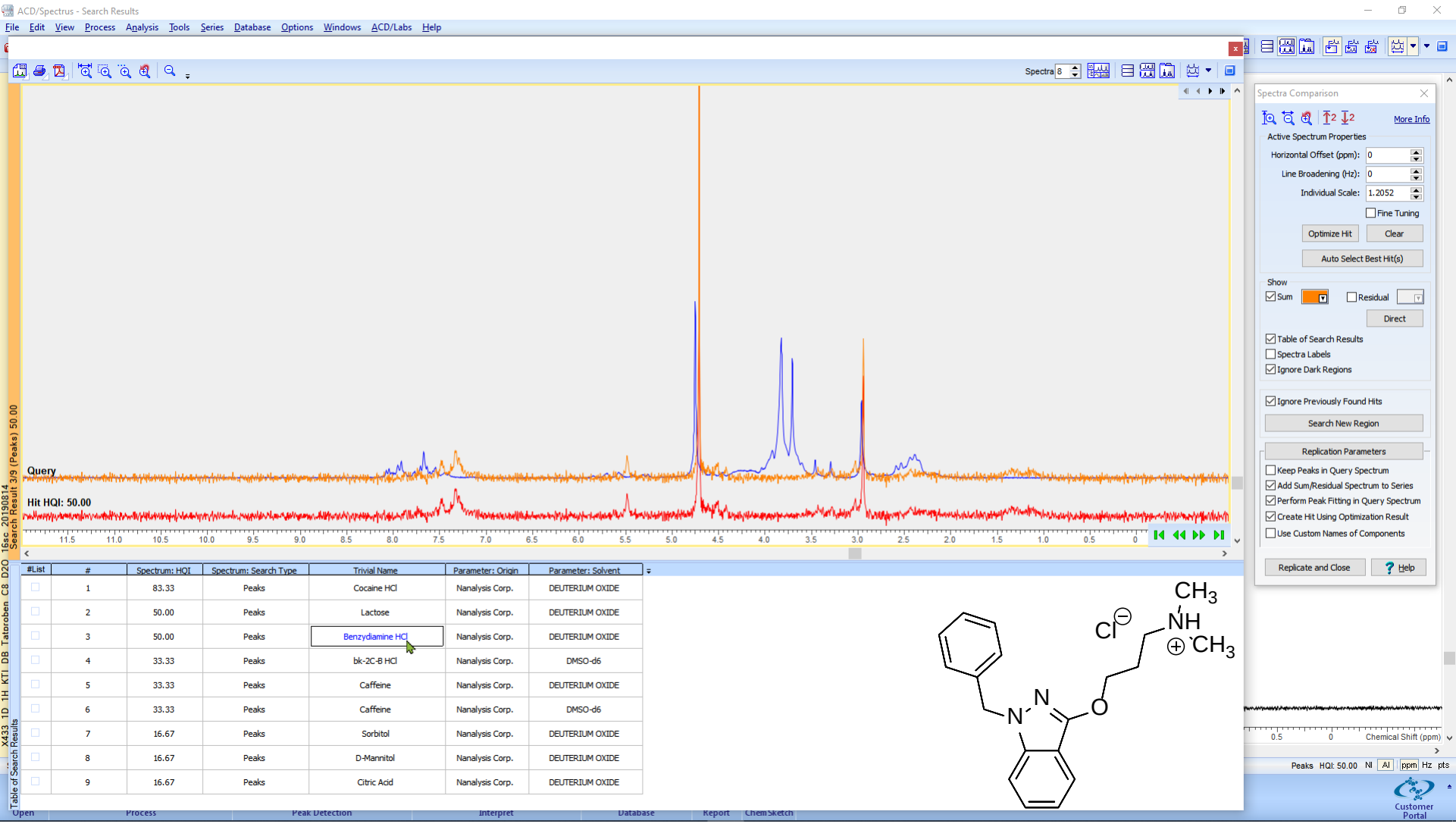

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Manually Investigate Other Potential Hits



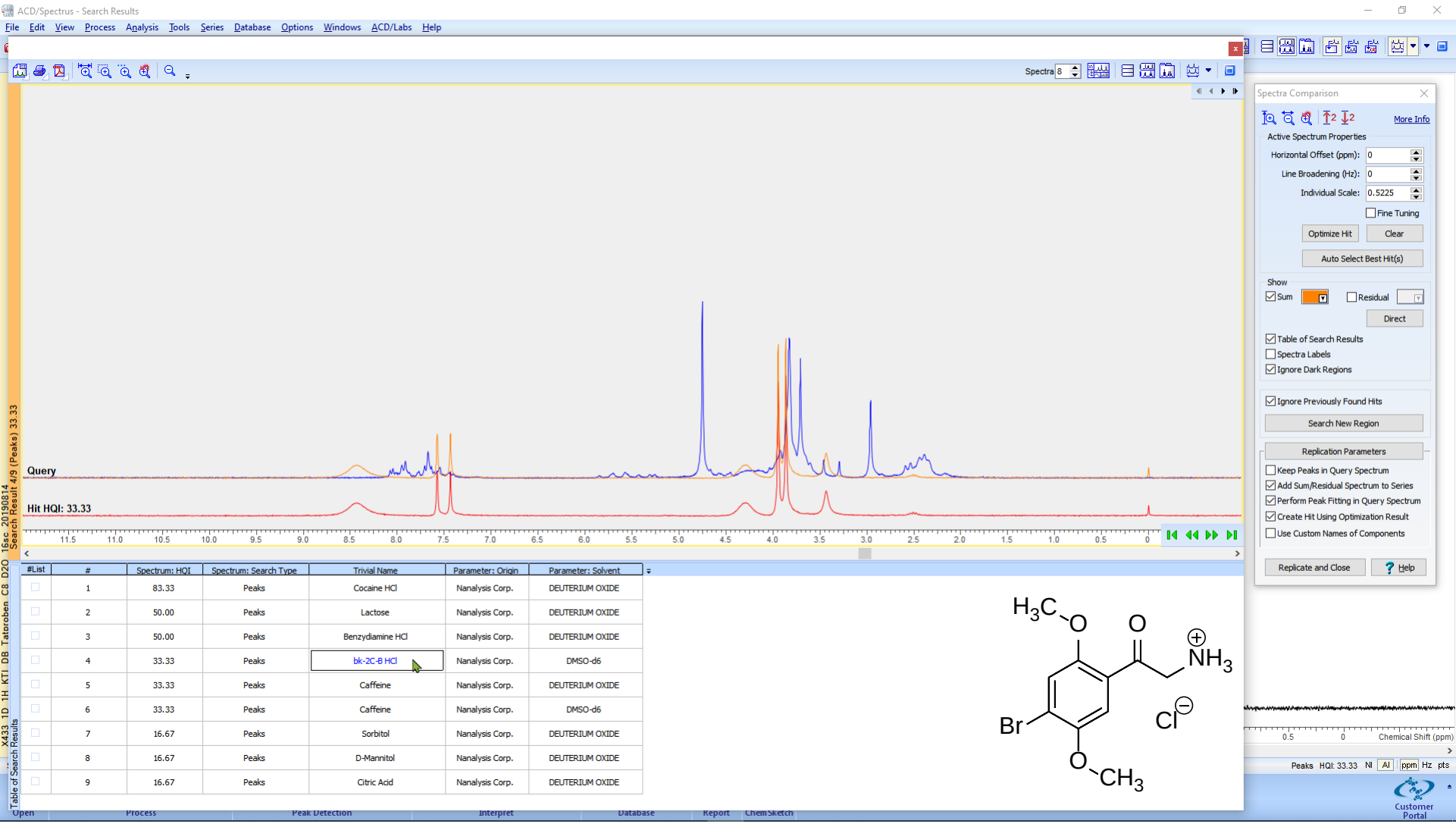

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visualize Inspect Benzydiamine HCl




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visually Inspect bk-2C-B HCl




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
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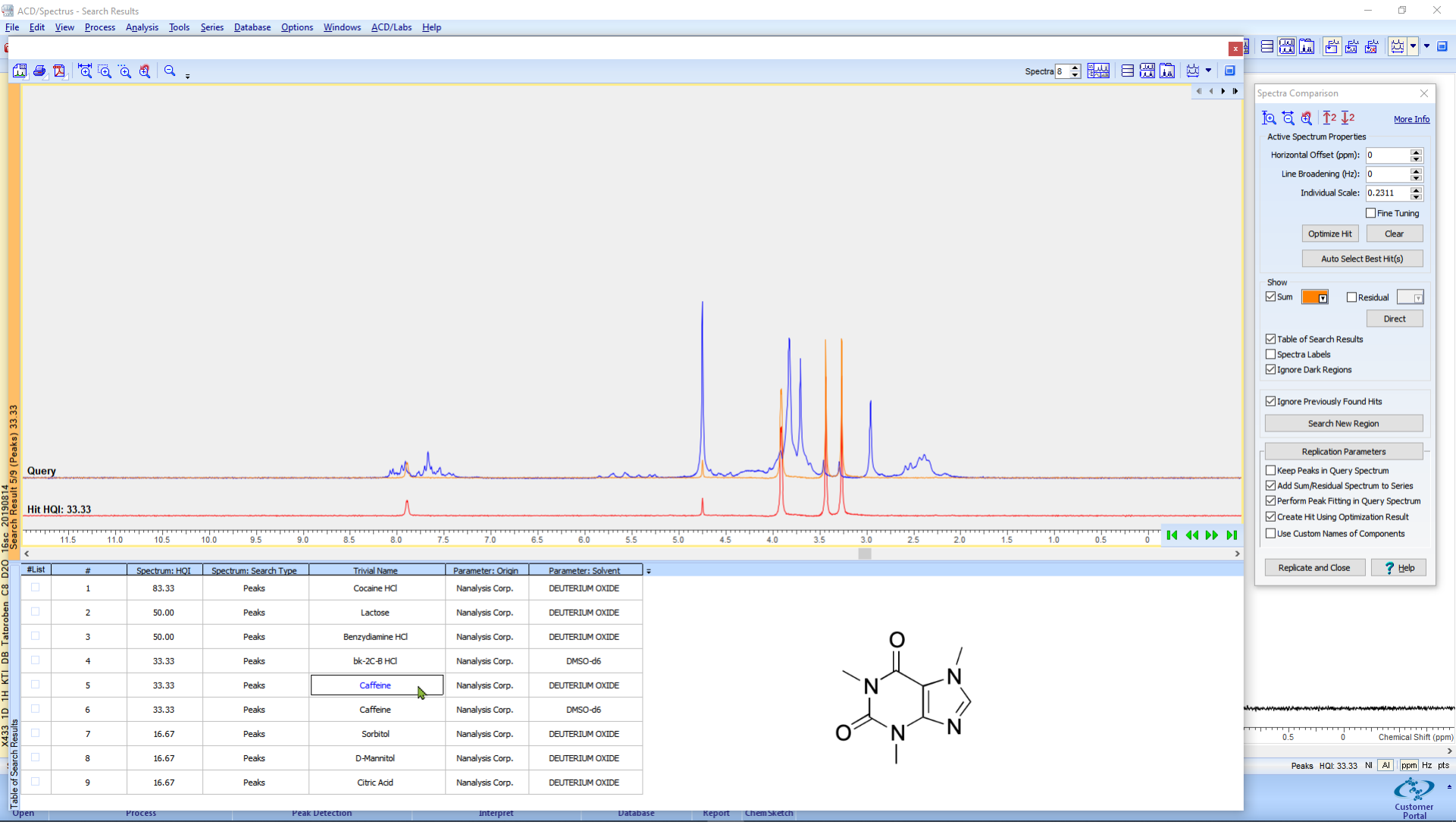
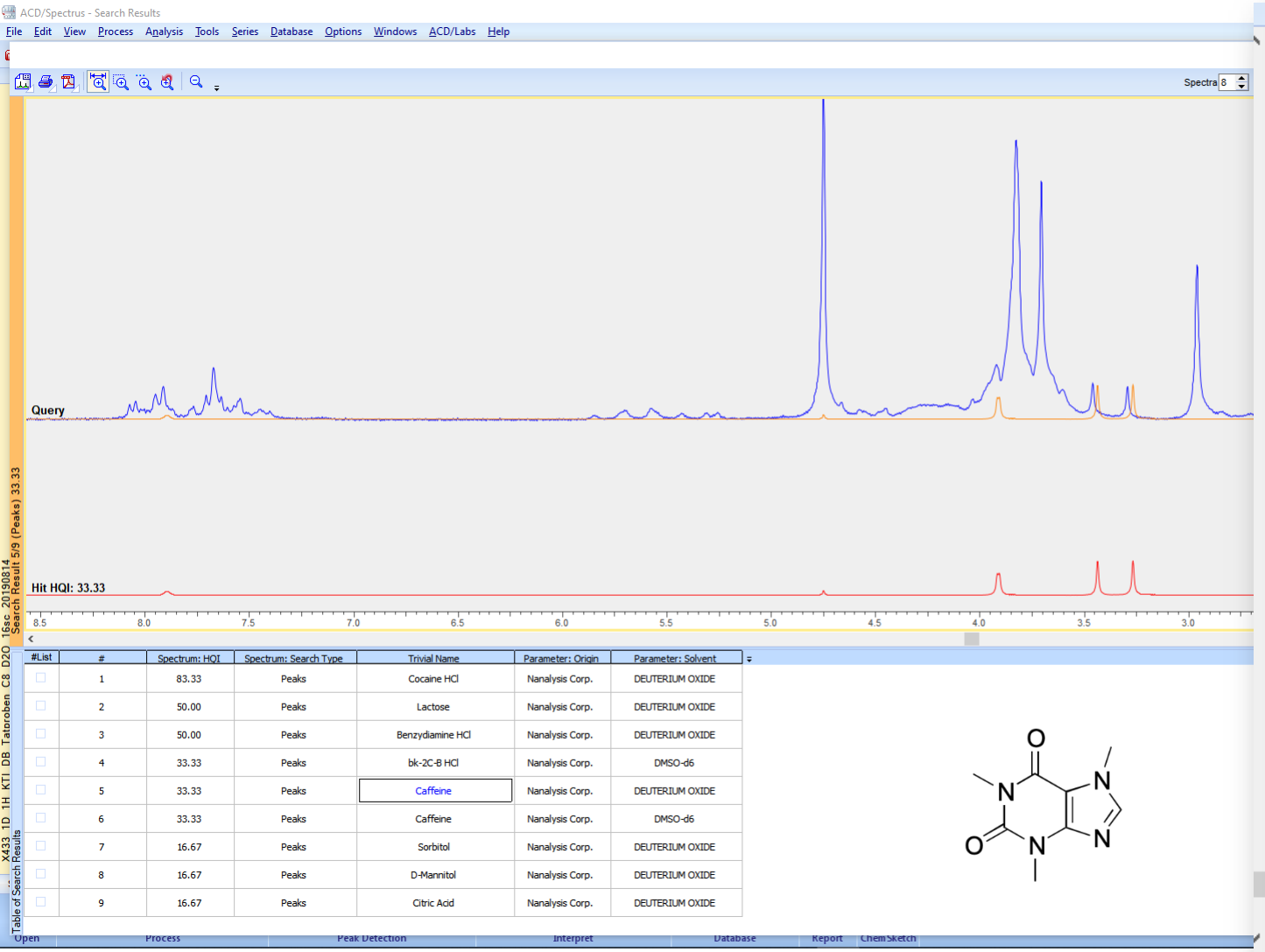
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visually Inspect Caffeine



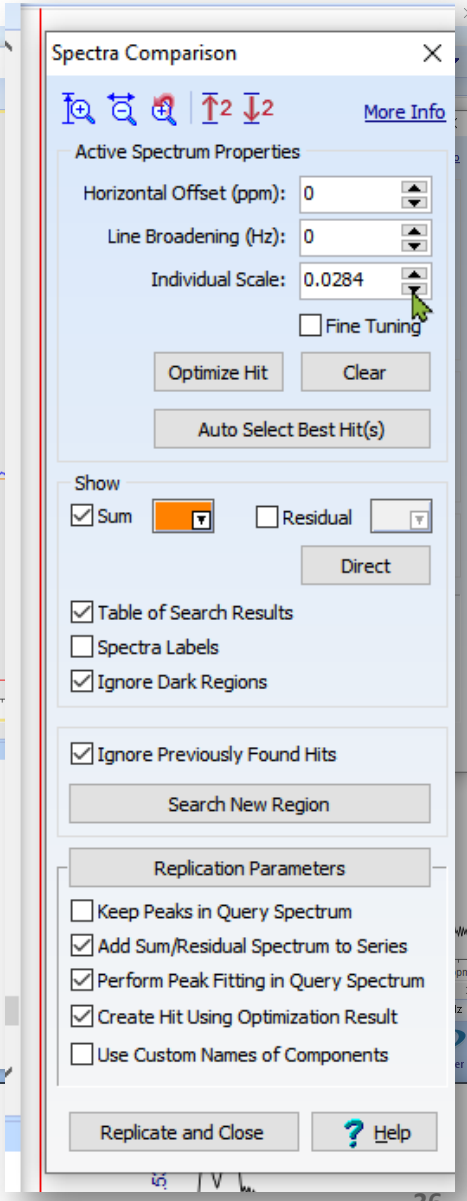

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Optimize Intensity

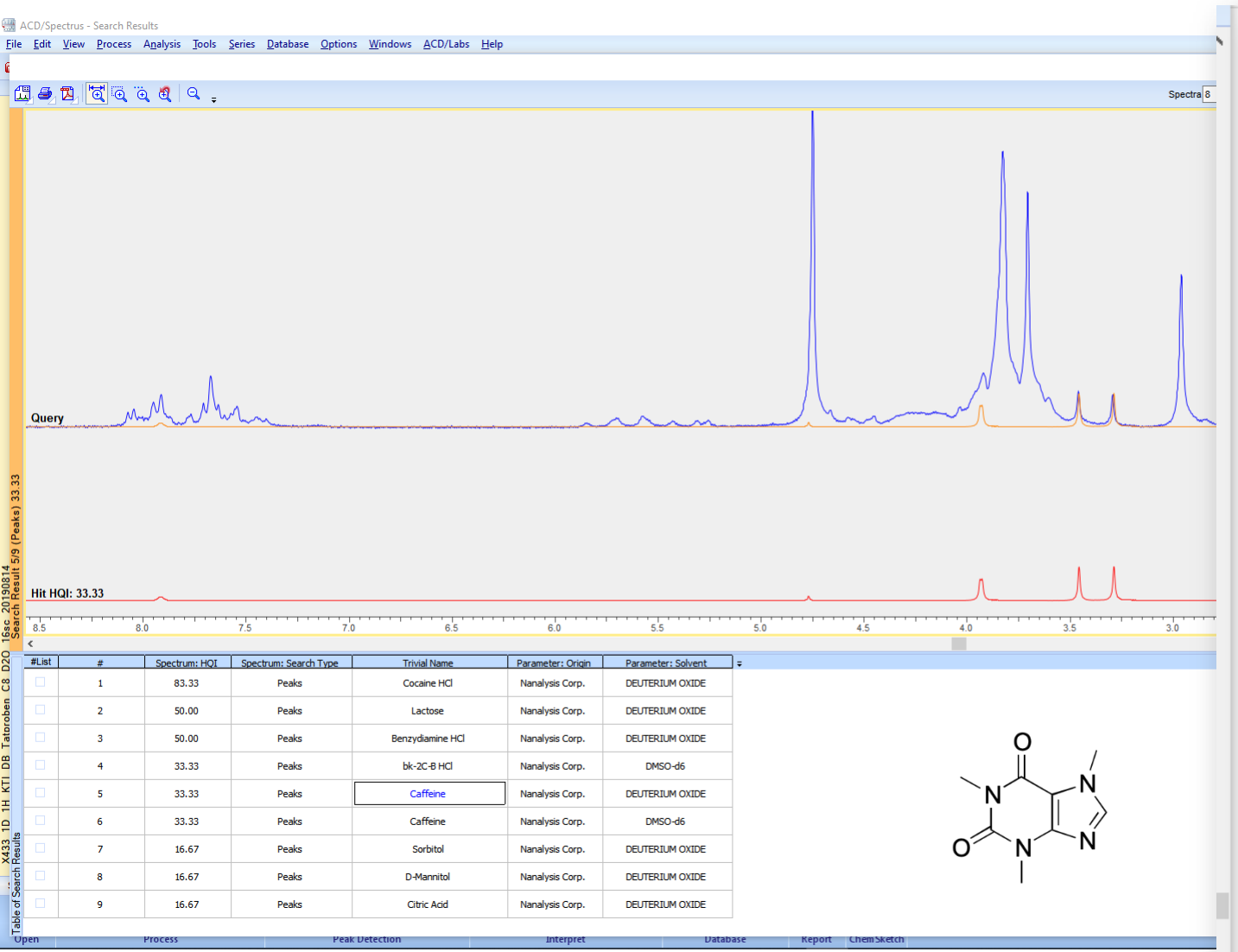



| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |



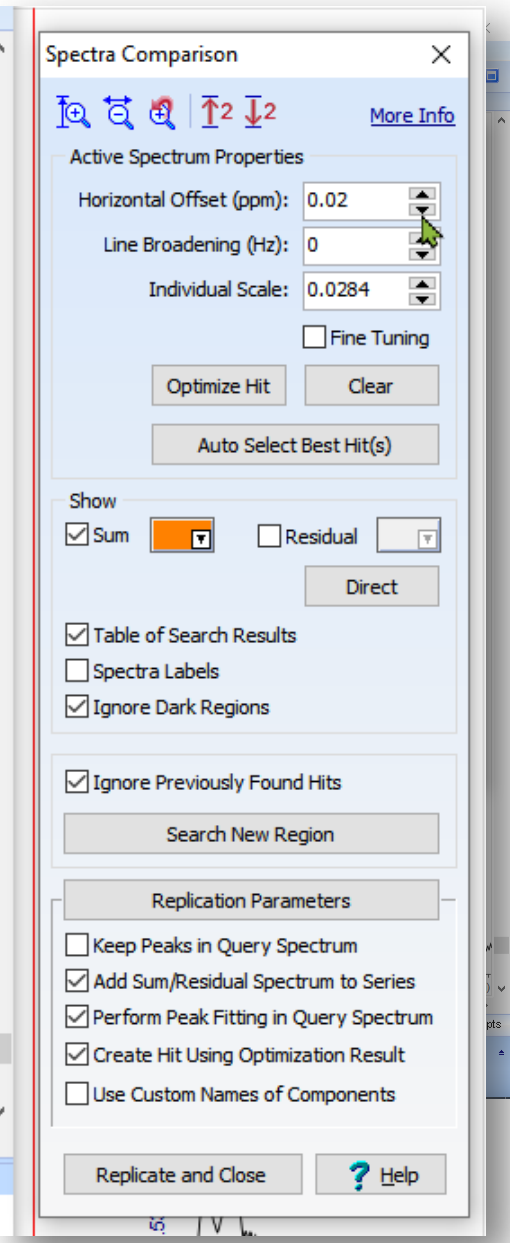


# Horizontal Offset Adjustment

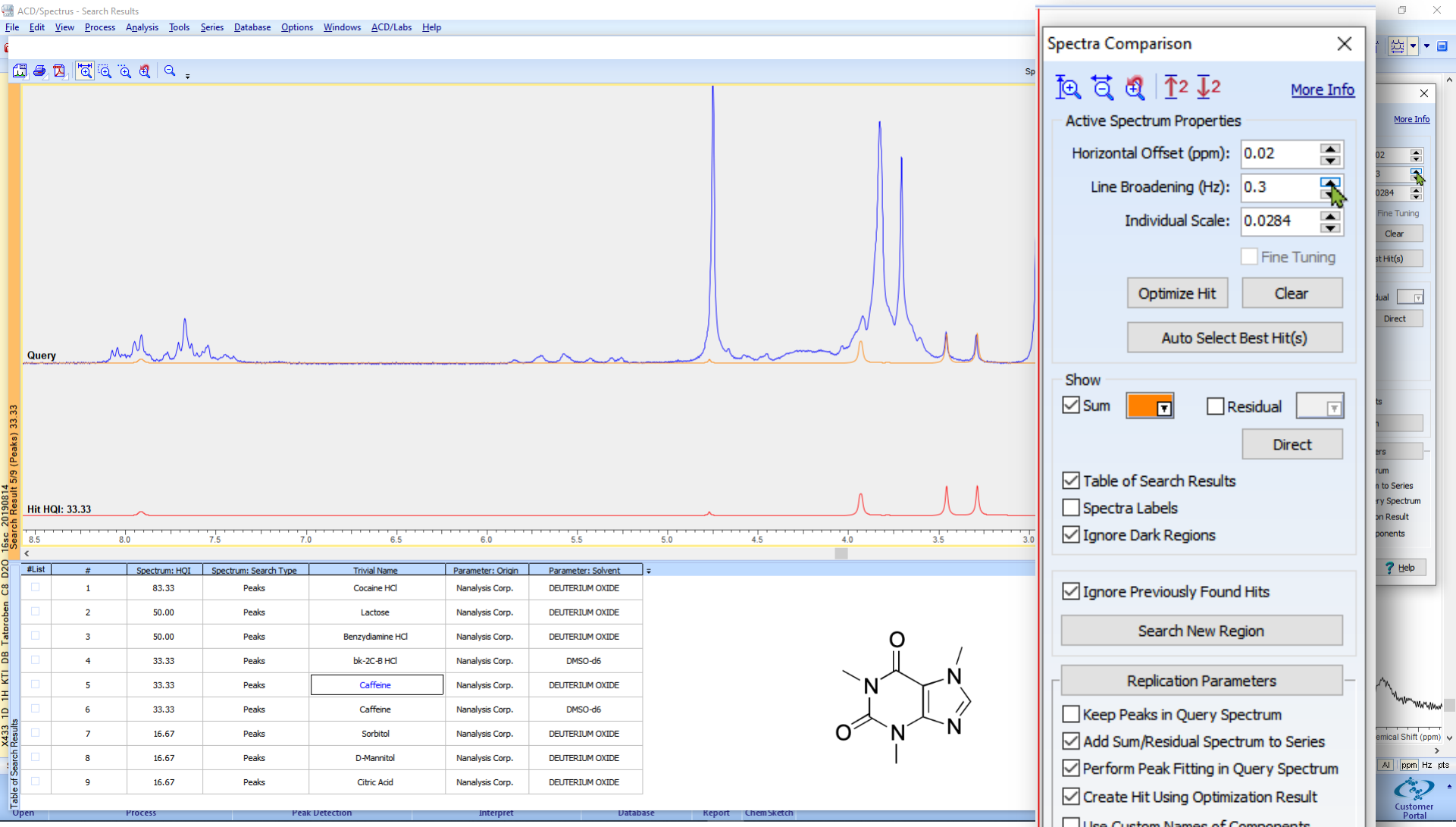



| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |



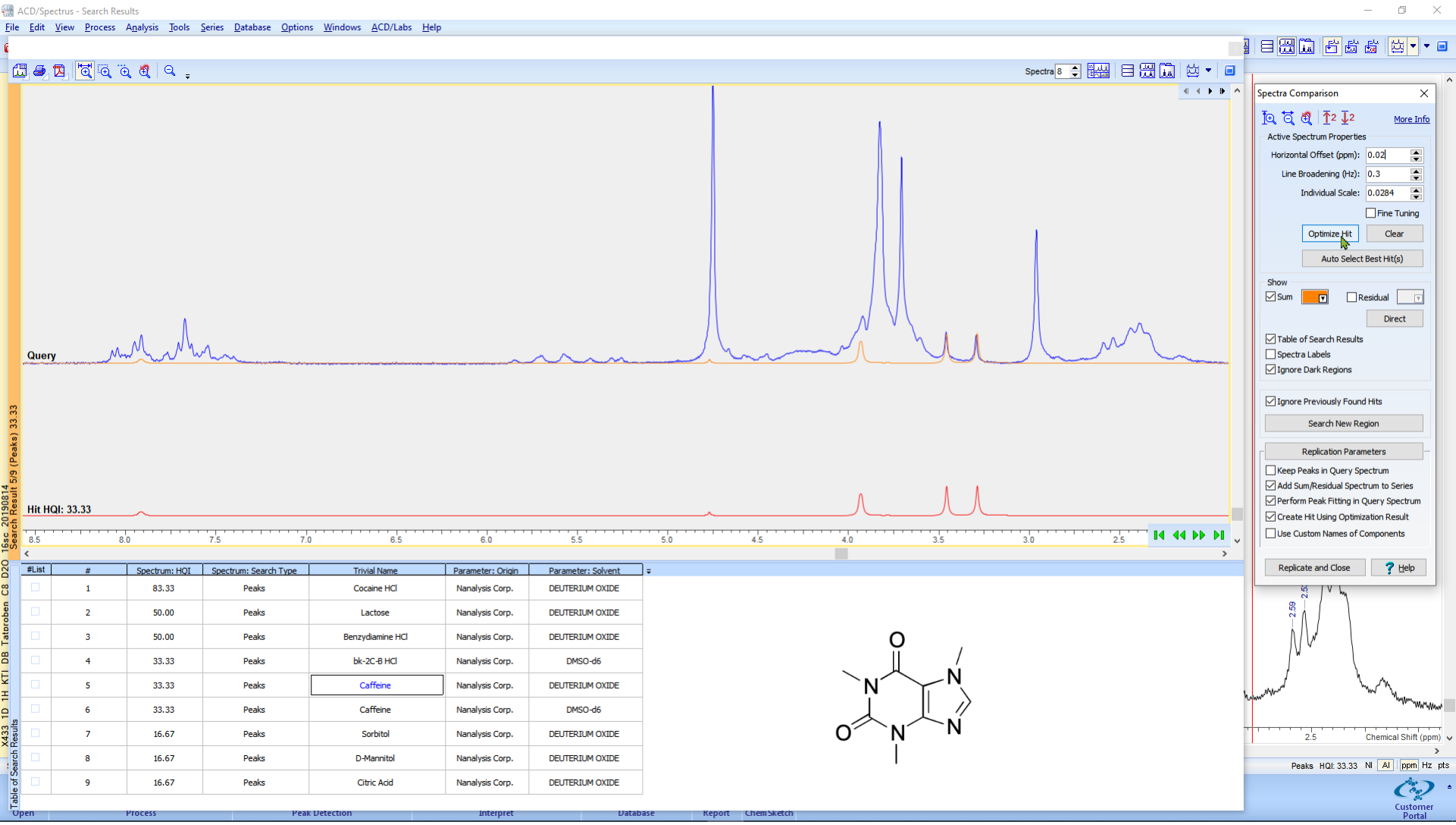


# Line Broadening Adjustment



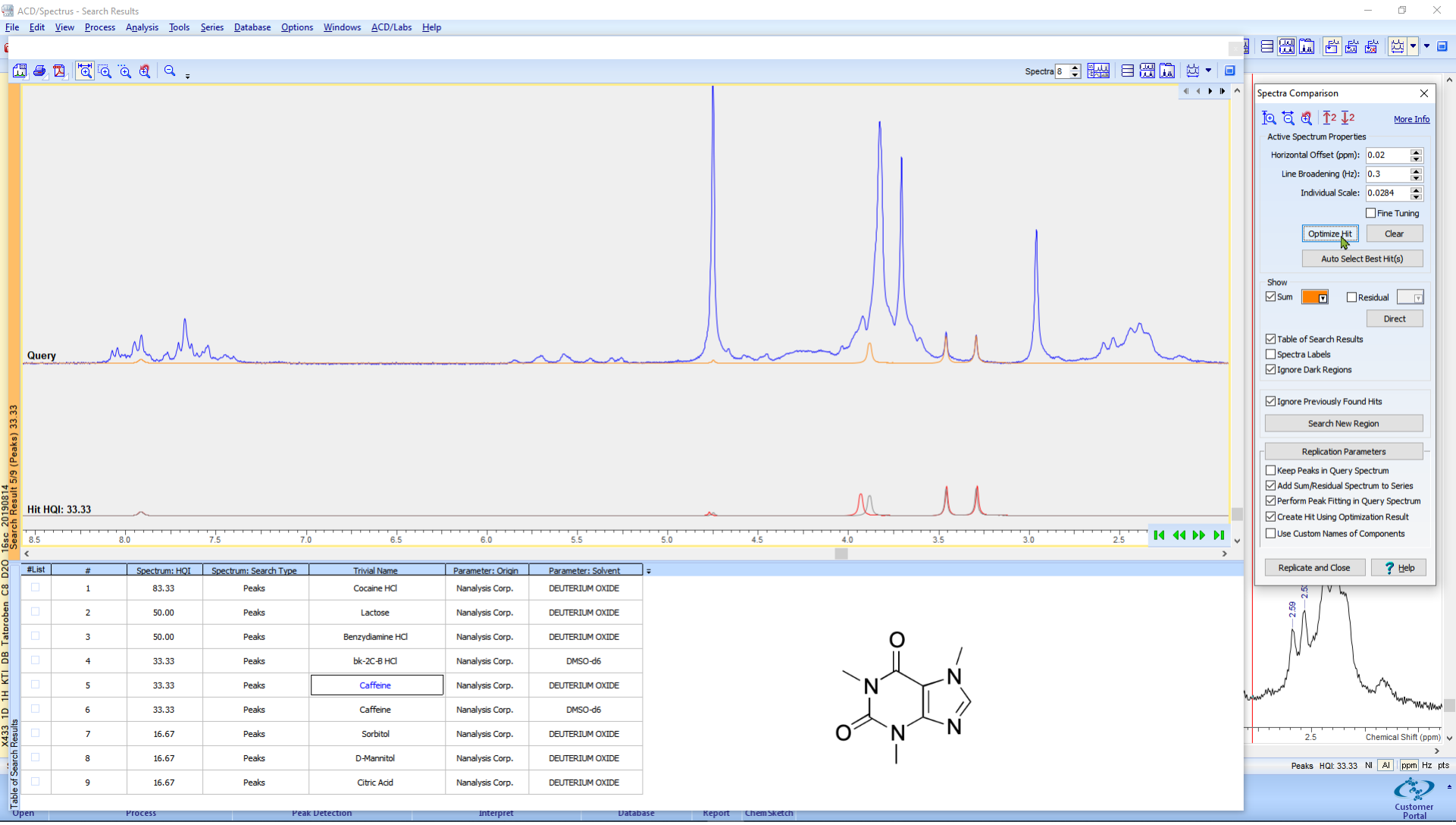

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Optimize Hit



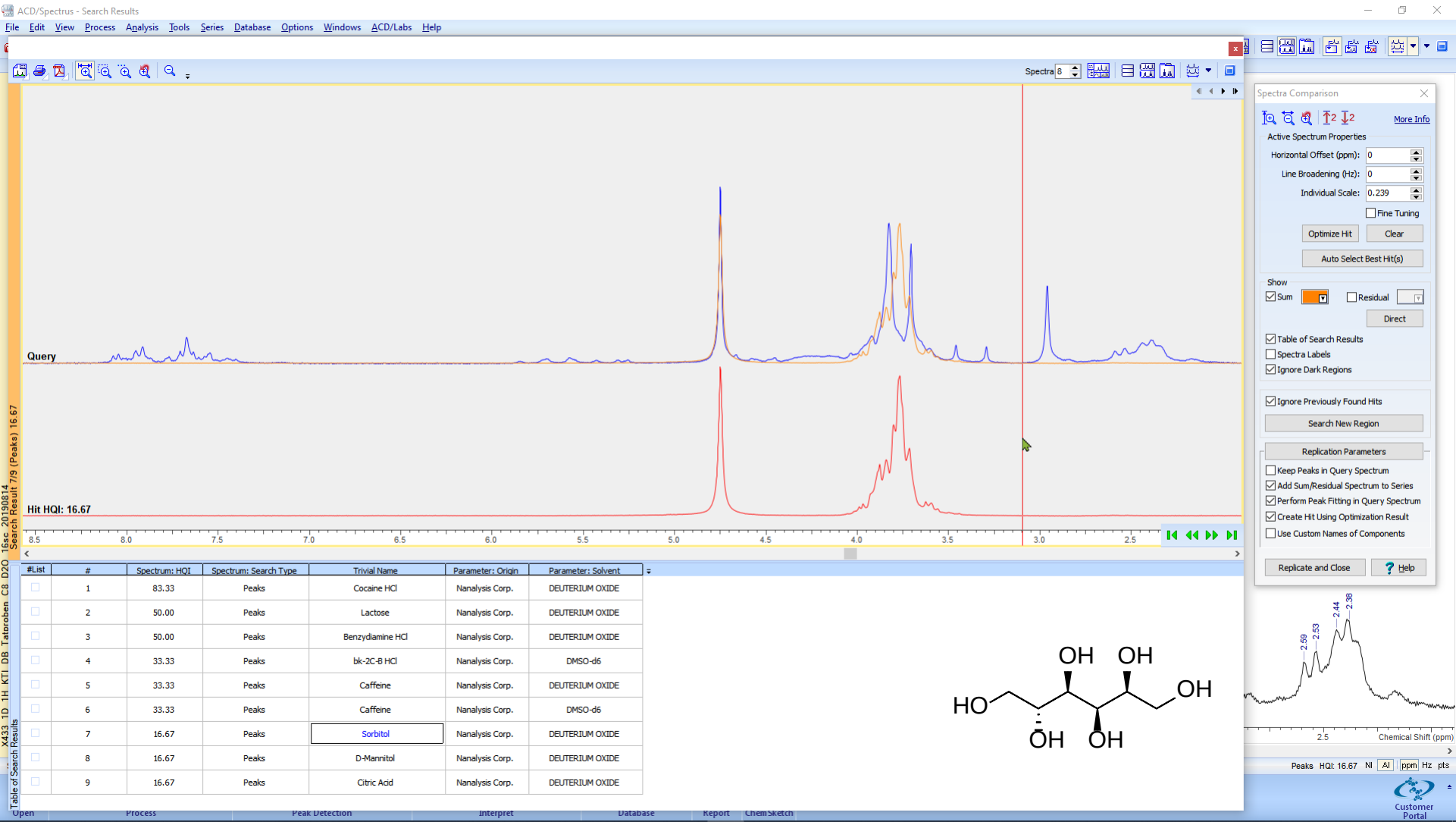

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Caffeine Optimized



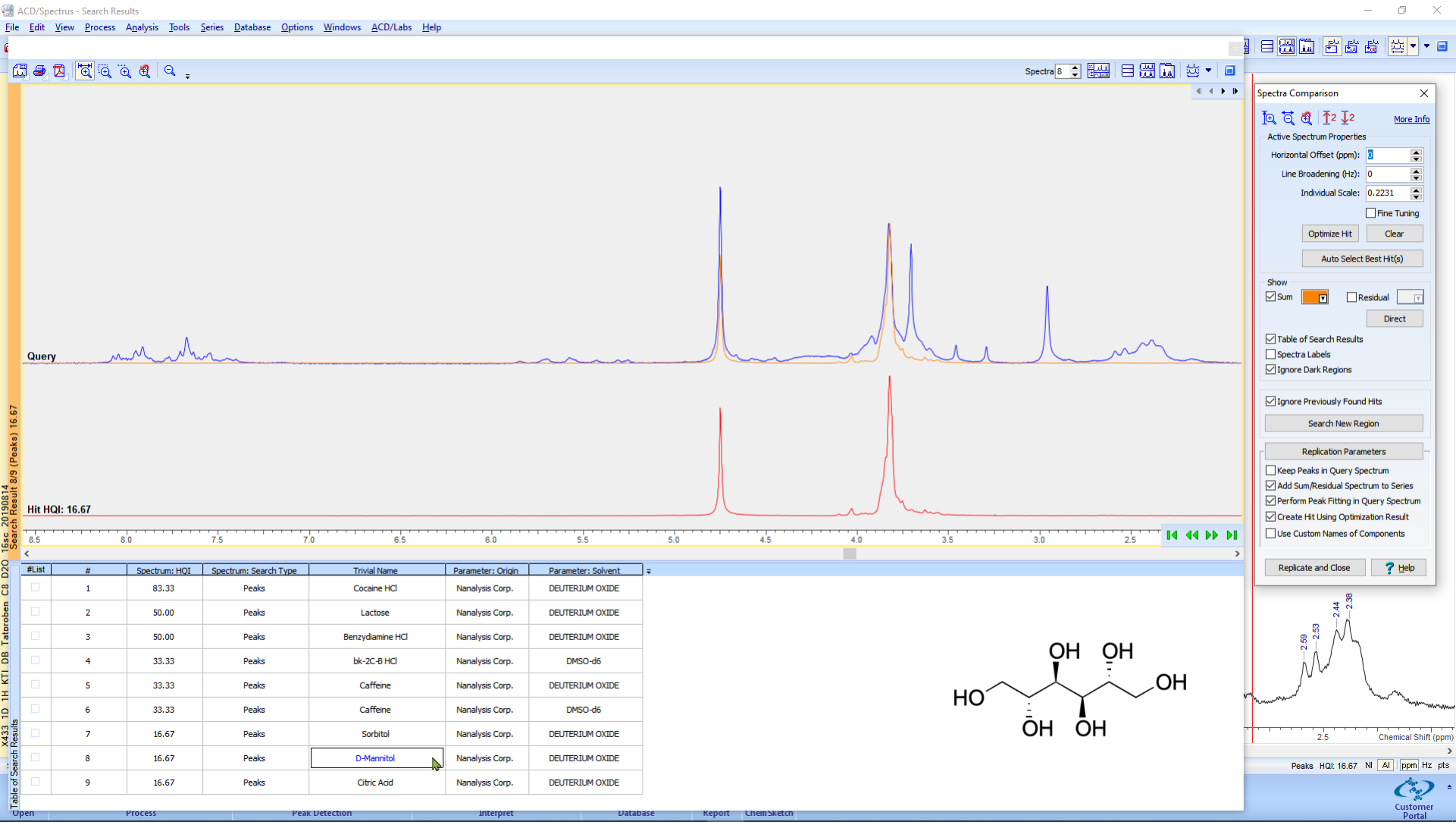

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visually Inspect Sorbitol



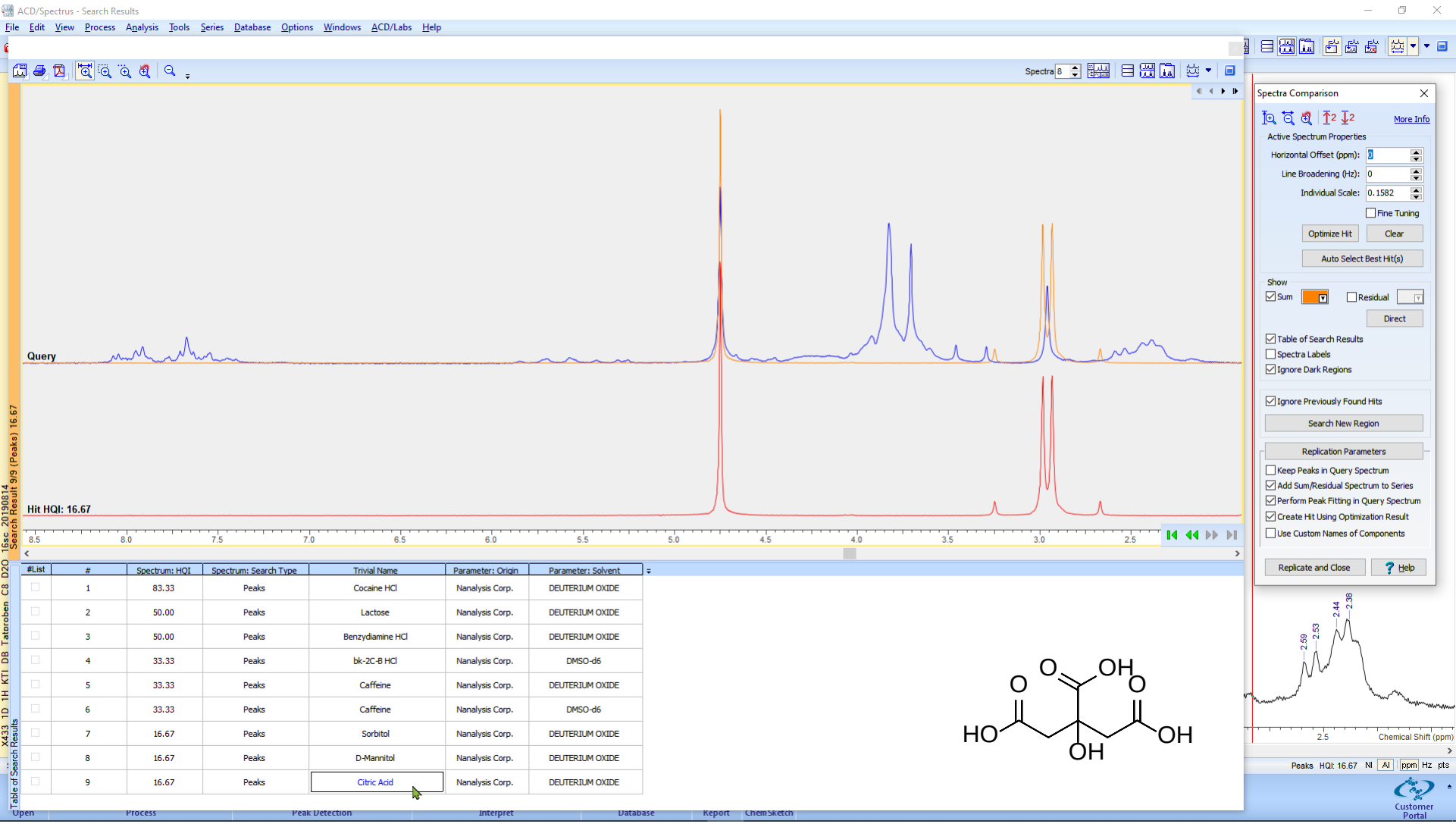

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visually Inspect D-Mannitol



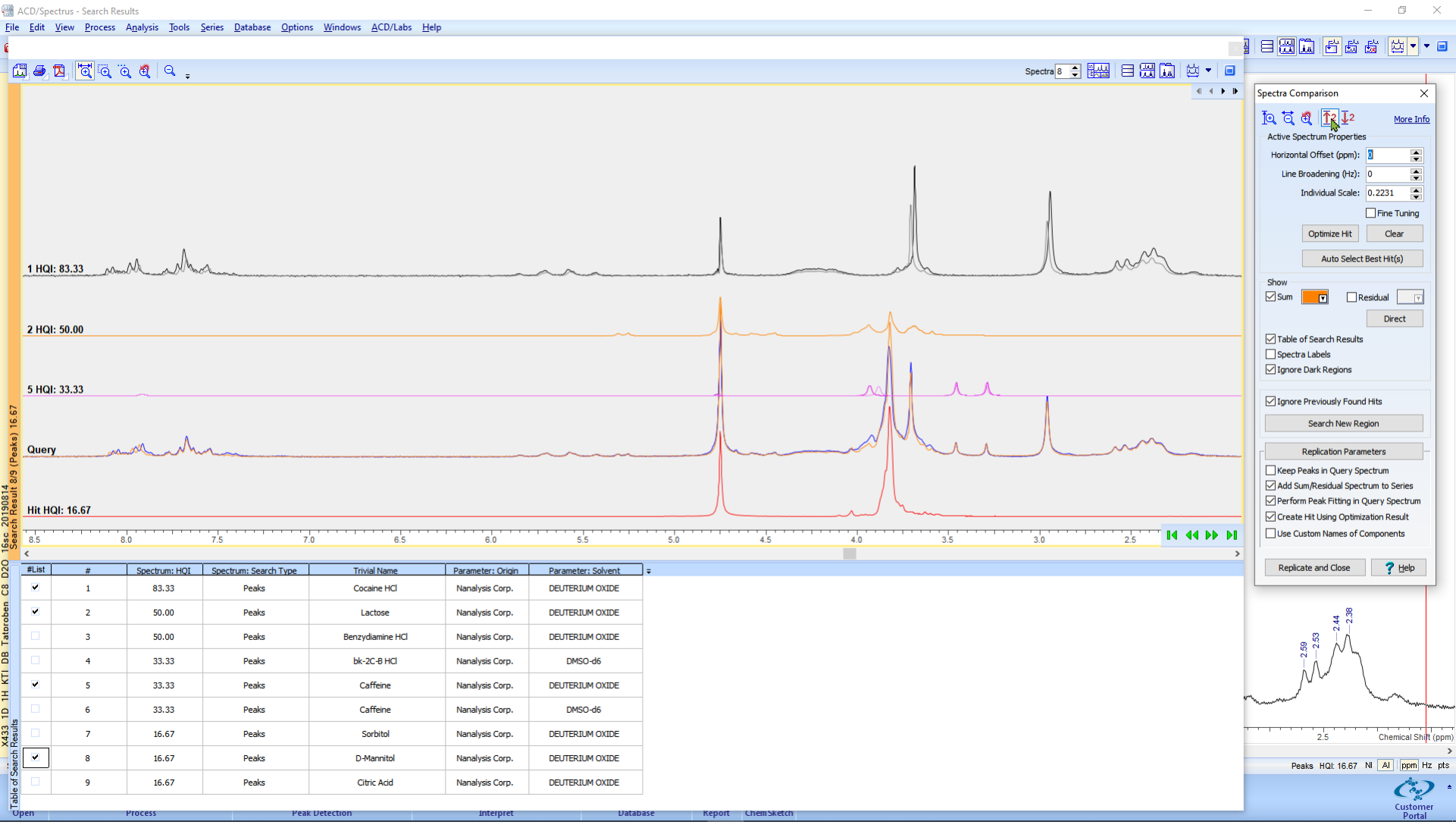

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Visually Inspect Citric Acid



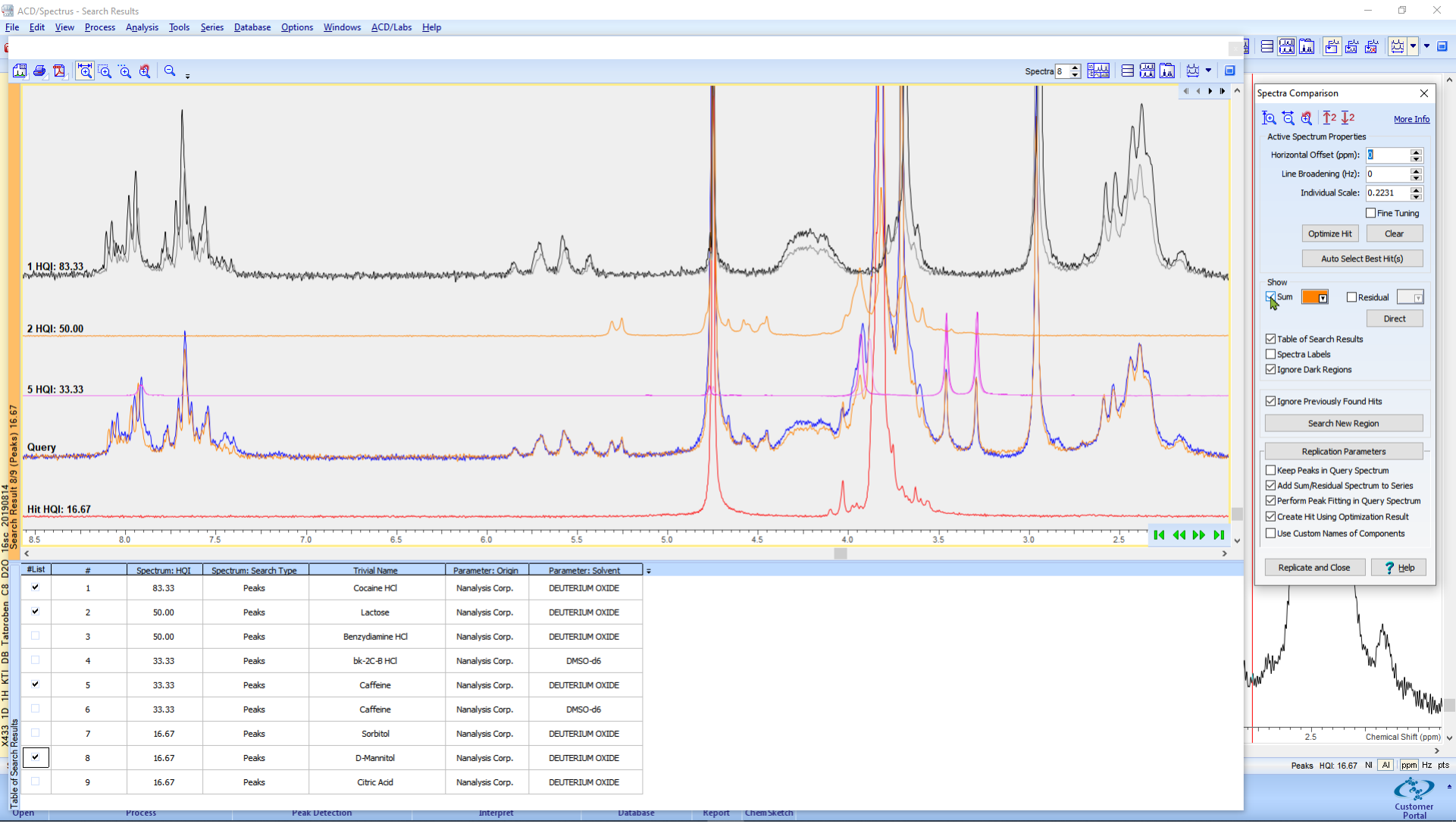

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Select all Matching Components



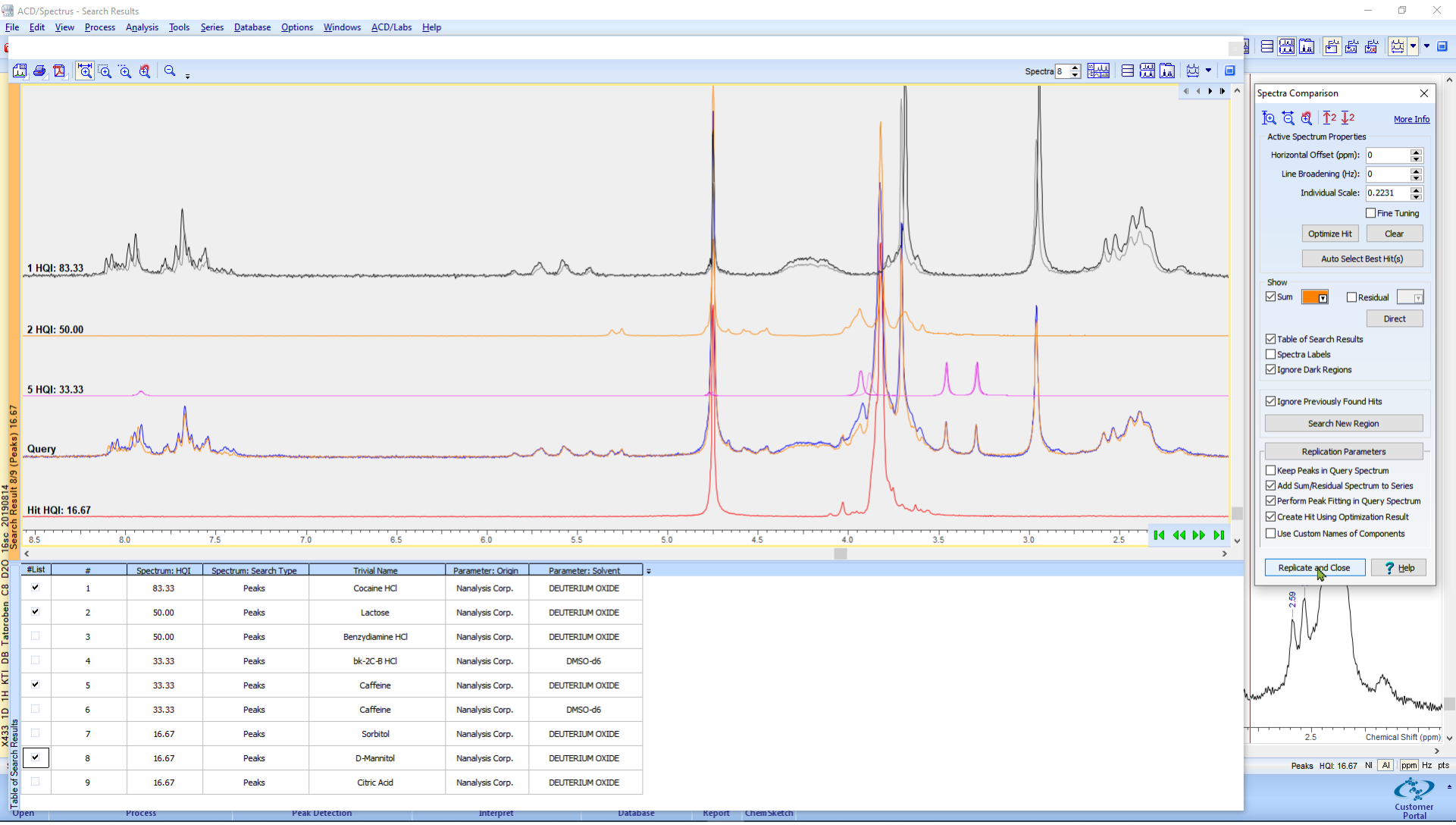

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| ✔ | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Inspect Matching Components: Sum



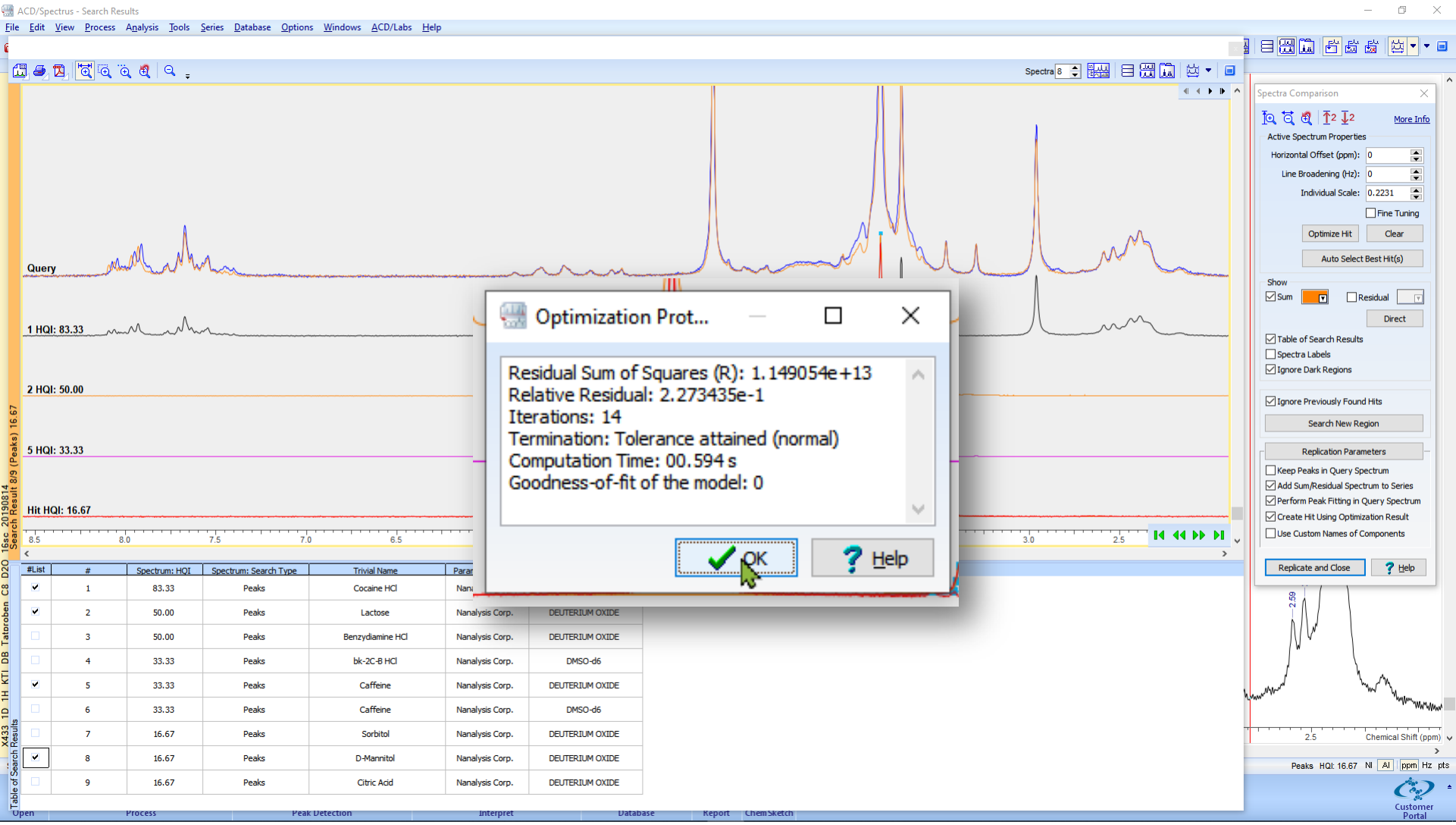

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| ✔ | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Case Study: Cocaine cont.



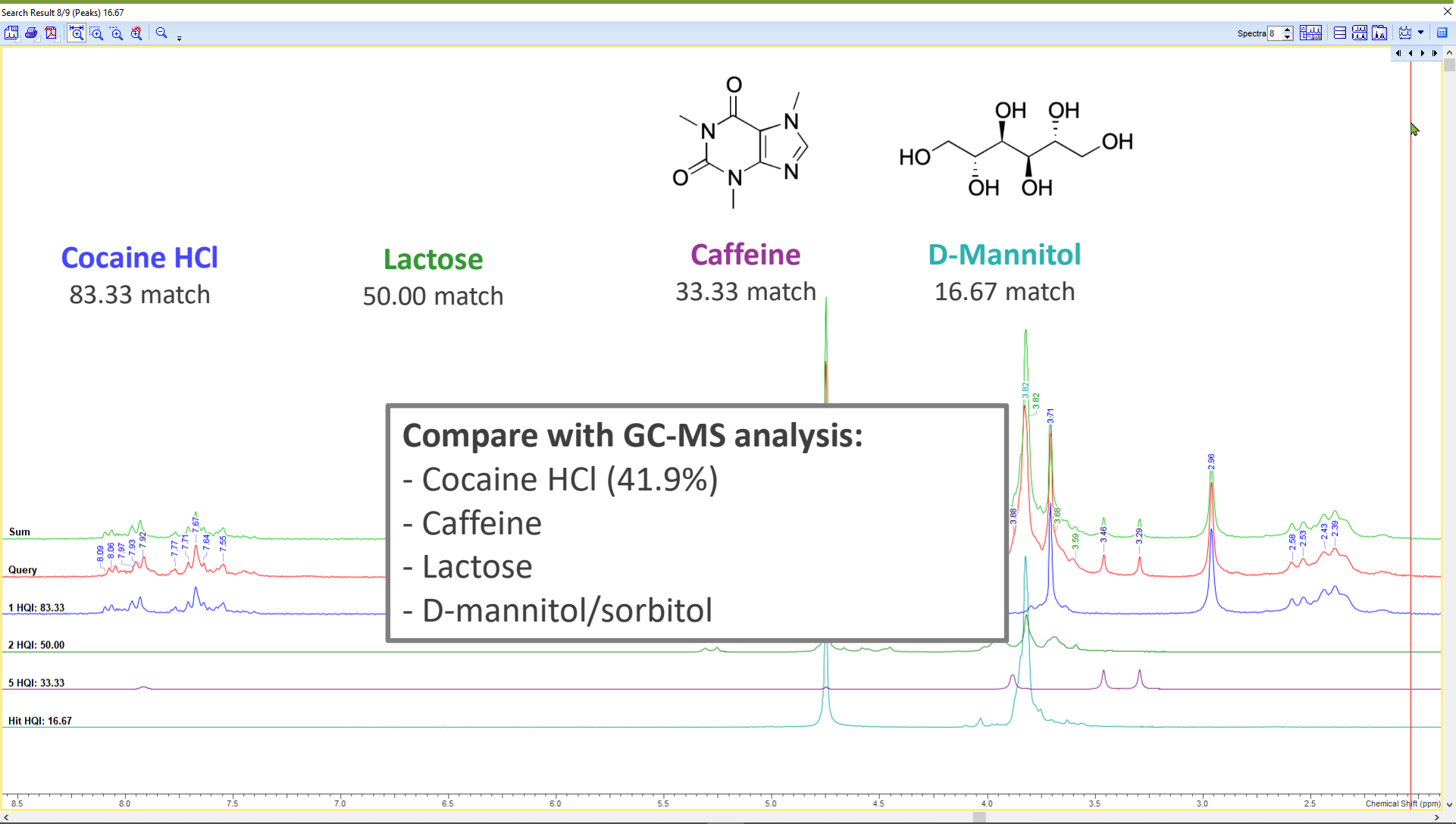

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| ✔ | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Case Study: Cocaine cont.




| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parar | |
|---|---|---|---|---|---|---|
| ✔ | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 3 | 50.00 | Peaks | Benzydiamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| ✔ | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| ✔ | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

# Report: Street Drug Cocaine HCl



# Conclusions and Future Work

- Successfully acquired and built database for 150+ illicit drugs and cutting agents
- Peak pick allowed relatively automatic identification of peaks
- Want to develop fingerprinting/similarity structures flags

# Thanks and Acknowledgments


**Nanalysis**
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