

Detection and Identification of Illicit Drugs and Cutting Agents in Seized Street Drugs: Benchtop NMR Spectrometer & Databasing Software



ACD/Labs User Meeting

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*Baltimore, MD
March 8th, 2020*

NMR Instruments and Field Strength



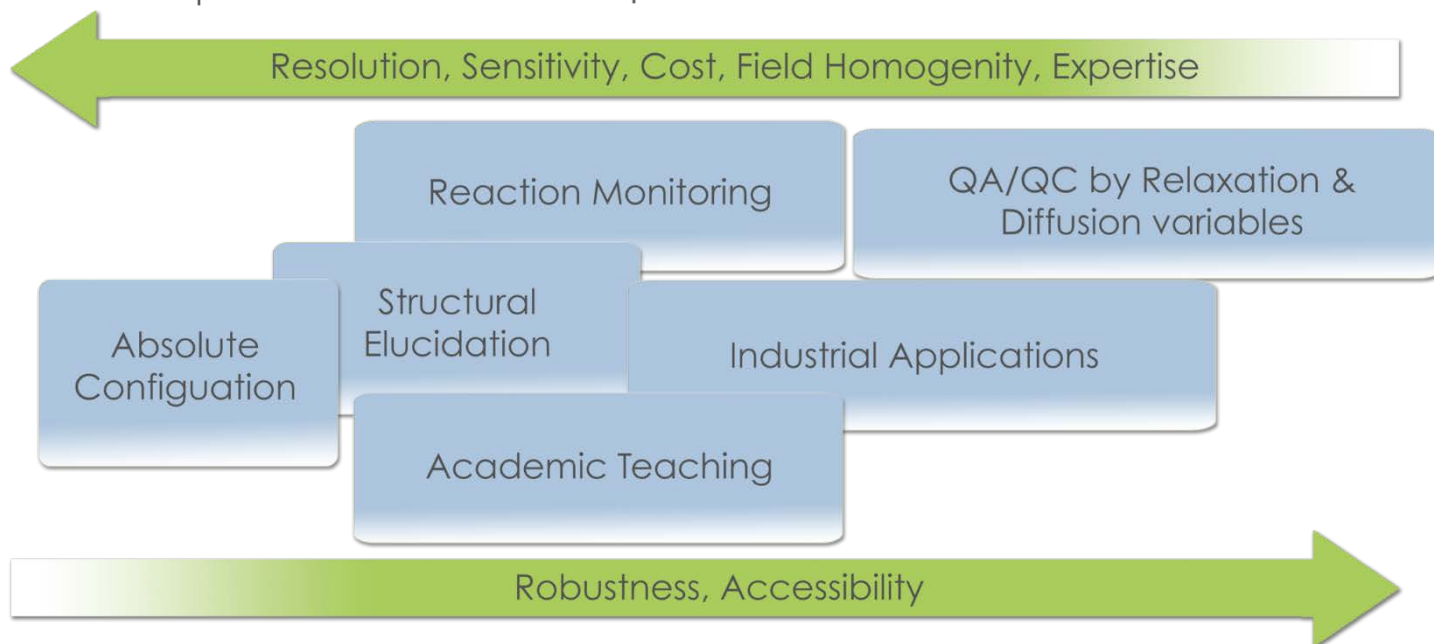
High Field
High Resolution
Spectrometer



Low Field
High Resolution
Spectrometer

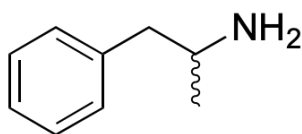


Low Field
Low Resolution
Relaxometer

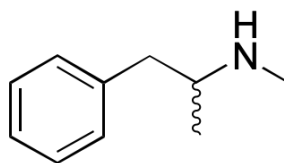


Illegal Drugs

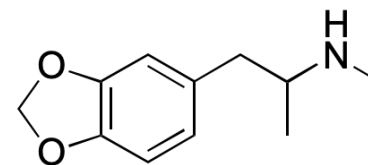
- Typically classified by:
 - Legal Classification – e.g., Schedule I, Class A
 - Effect – e.g., depressant, stimulant, hallucinogen
 - Molecular Structure – e.g., cannabinoids, opioids, phenethylamines



Amphetamine
Stimulant

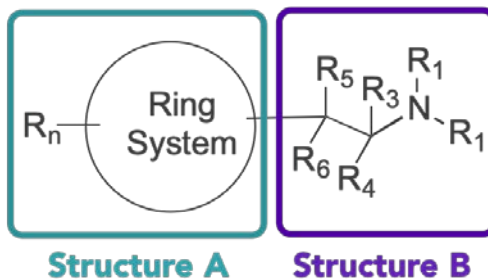


Methamphetamine
Stimulant

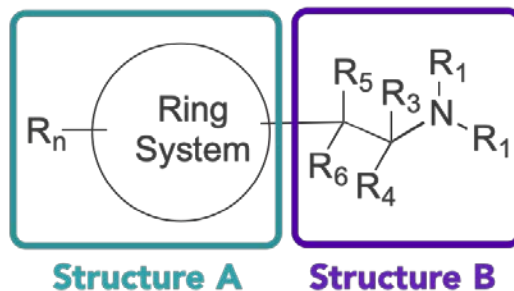


MDMA
Psychedelic, entactogen

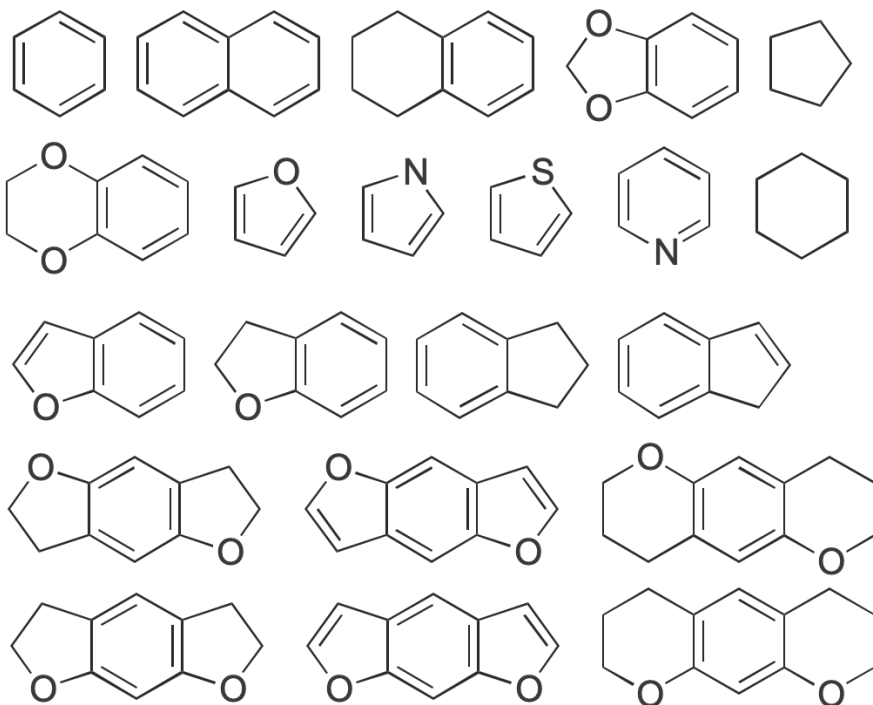
- Designer Drugs – synthetic analog of a legal restricted or prohibited drug devised to avoid drug detection and identification.



New Psychoactive Substances* (from 2-phenylethylamine)



Ring System =



R₁ or R₂ =

H, F, Cl, Br, I
 linear alkyl to C₆
 cycloalkyl to C₆
 benzyl
 alkenyl to C₆
 alkylcarbonyl to C₆
 hydroxyl
 amino
 heterocycles with N

R₃, R₄, R₅ or R₆ =

H, F, Cl, Br, I
 linear alkyl to C₁₀
 cycloalkyl to C₁₀
 benzyl, phenyl
 alkenyl to C₁₀
 alkynyl to C₁₀
 hydroxyl
 alkoxy to C₁₀
 alkylsulfanyl to C₁₀
 alkyloxycarbonyl to C₁₀

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 ^1H NMR Acquisition

SAMPLE PREP:

Reference Standards

- 60 μmol of sample dissolved in
~0.6 mL $\text{DMSO-}d_6$ 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 $\text{DMSO-}d_6$ and D_2O
- Vials were capped and agitated for 1 min
- Liquid phase transferred to NMR tube

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

1D ^1H 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

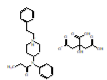

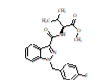

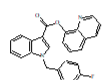

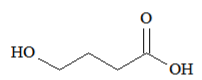

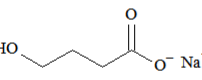

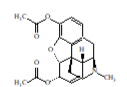

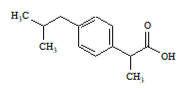

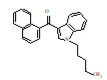



PRE-PROCESSING (ACD/Labs Macro for automatic processing):

- Zero Fill
- Baseline
- Phase
- solvent detection

Database

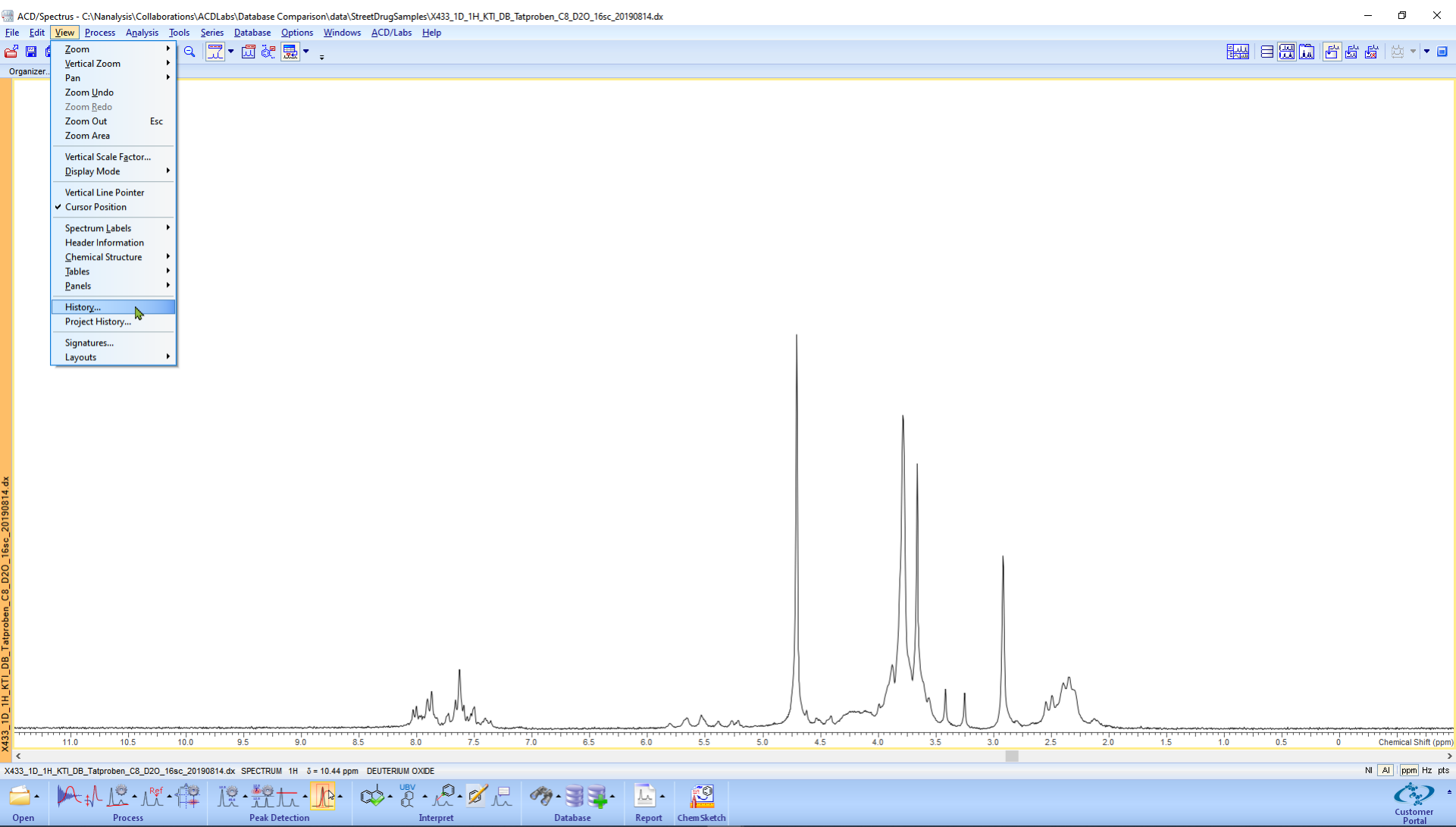
ACD/Spectrum DB: Database Window - [C:\NANALYSIS\COLLABORATIONS\ACDLABS\DATABASE COMPARISON\KTL.CFD]

| #List | # | Structure | Spectrum | Formula | Trivial Name |
|-------------------------------------|-----|---|--|-----------------------|------------------------|
| <input checked="" type="checkbox"/> | 94 |  |  | $C_{28}H_{36}N_2O_8$ | Fentanyl citrate |
| <input type="checkbox"/> | 95 |  |  | $C_{21}H_{22}FN_3O_3$ | FUB-AMB (AMB-FUBINACA) |
| <input type="checkbox"/> | 96 |  |  | $C_{25}H_{17}FN_2O_2$ | FUB-PB-22 |
| <input type="checkbox"/> | 97 |  |  | $C_4H_8O_3$ | GHB |
| <input type="checkbox"/> | 98 |  |  | $C_4H_7NaO_3$ | GHB Na |
| <input type="checkbox"/> | 99 |  |  | $C_{21}H_{23}NO_5$ | Heroin |
| <input type="checkbox"/> | 100 |  |  | $C_{13}H_{18}O_2$ | Ibuprofen |
| <input type="checkbox"/> | 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

ACD/Spectrus - C:\Nanalysis\Collaborations\ACDLabs\Database Comparison\data\StreetDrugSamples\X433_1D_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.dx

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Macro_dimi

History

```
DataSource (Location = "FileSystem"; FileName = "C:\Nanalysis\Collaborations\ACDLabs\Database Comparison\data\StreetDrugSamples\X433_1D_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.dx")
Import (Format = "JCAMP"; Warnings = " ")
ProgramVersion (Version = "580541"; Build = "108238")
FT (Operation = "Default")
ReverseSpectrum ()
Baseline (Range = Full; Method = "Polynomial"; Order = 5)
Annotation (Range = 4.7039..4.7545; Text = "DEUTERIUM OXIDE"; Layer = 1)
SetDarkRegion (Range = 4.7039..4.7545; Description = "DEUTERIUM OXIDE"; Active = True; Calculate)
Clear (What = "Annotations"; Range = Full)
Clear (What = "DarkRegions")
ReverseSpectrum ()
InverseFT (Operation = "Default")
ZeroFilling (PointsCount = "65536")
FT (Operation = "Default")
ReverseSpectrum ()
```

View
☒ Short ☐ Full **Macro...** Save... ☒ OK ☐ Help

X433_1D_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.dx SPECTRUM 1H $\delta = 11.15$ ppm DEUTERIUM OXIDE

NI Al ppm Hz pts

Open Process Peak Detection Interpret Database Report Chem Sketch Customer Portal

The screenshot displays the ACD/Spectrus software interface. The main window shows a 1H NMR spectrum with chemical shift in ppm on the x-axis (ranging from 11.0 to 0.0) and intensity on the y-axis. A prominent peak is visible at approximately 4.7 ppm, labeled 'DEUTERIUM OXIDE'. A 'History' window is open, showing a list of commands executed, including 'DataSource', 'Import', 'ProgramVersion', 'FT', 'ReverseSpectrum', 'Baseline', 'Annotation', 'SetDarkRegion', 'Clear', 'InverseFT', 'ZeroFilling', and 'FT'. The 'Macro...' button is highlighted in the History window. The bottom toolbar contains icons for 'Open', 'Process', 'Peak Detection', 'Interpret', 'Database', 'Report', 'Chem Sketch', and 'Customer Portal'.

Creating a Macro

ACD/Spectrus - C:\Analysis\Collaborations\ACDLabs\Database Comparison\data\StreetDrugSamples\X433_1D_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.dx

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Macro_dimi

Edit Macro

1D NMR

Converted from History

User : Alexander Maier (LT-5CD8358GNF\Alexander.Maier)
Time : 2020-02-26 7:27:27 PM

- > FT (Operation = "Default")
- > ReverseSpectrum ()
- > BaseLine (Range = Full; Method = "Polynomial"; Order = 5)
- > Annotation (Range = 4.7039..4.7545; Text = "DEUTERIUM OXIDE"; Layer = 1)
- > SetDarkRegion (Range = 4.7039..4.7545; Description = "DEUTERIUM OXIDE"; Active = True; Calculated = False)
- > Clear (What = "Annotations"; Range = Full)
- > Clear (What = "DarkRegions")
- > ReverseSpectrum ()
- > InverseFT (Operation = "Default")
- > ZeroFilling (PointsCount = "65536")
- > FT (Operation = "Default")
- > ReverseSpectrum ()
- > Phase (Method = "BLOptimisation"; EqualPhase = False; FixPh1 = False)
- > PeakPicking (Range = -21.4920..61.4806; NoiseFactor = 4.0000; Threshold = "Auto"; PosPeaks = True; NegPeaks = False; EqualPosition = False; UseDerivation = True; UsePeakFit = True)
- > BuildMultiplets (Nucleus = "1H"; PeakDistance = 0.8000; Coupling = 0.1000; MaxConst = 20.0000; UsePeakFit = False; IntegralThreshold = 0.8000; NormalizationType = "ProtonsIn")

<End of command list>

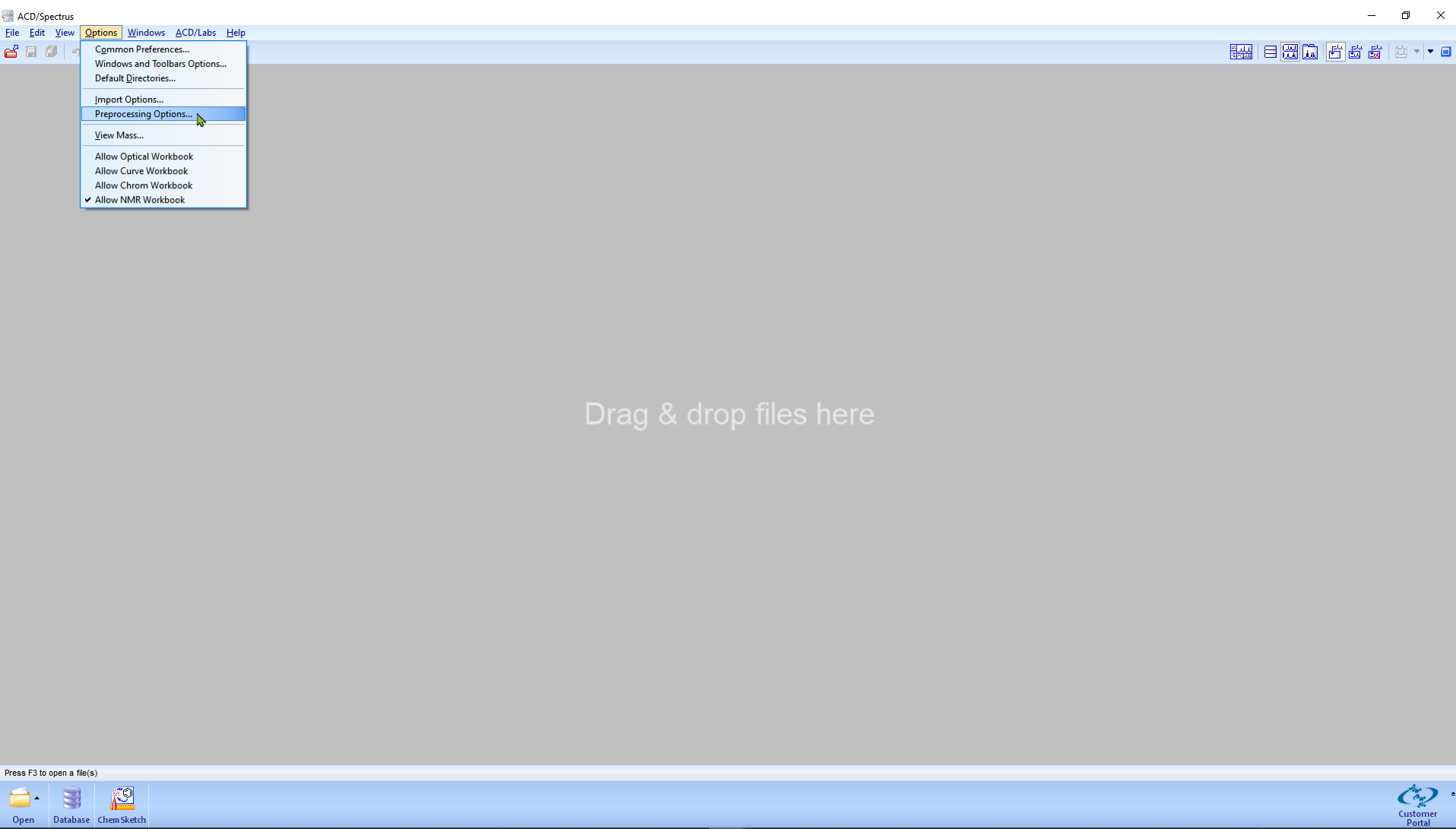
OK Cancel Help

X433_1D_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.dx SPECTRUM 1H δ = 11.15 ppm DEUTERIUM OXIDE

Open Process Peak Detection Interpret Database Report ChemSketch

NI AI ppm Hz pts Customer Portal

Automated Preprocessing: Apply Macro




Automated Preprocessing: Apply Macro

ACD/Spectrus


File Edit View Options Windows ACD/Labs Help

Preprocessing Options


1D NMR Spectrum

- ☐ Fourier Transform
- ☐ Phase Correction
- ☒ Baseline Correction
- ☐ Align Spectra
- ☒ Detect Solvent/Water Signals
- ☐ Synchronize APT/DEPT Phase
- ☐ Peak Picking
- ☒ Run Macro 


2D NMR Spectrum

- ☒ Fourier Transform
- ☒ Phase Correction
- ☒ Align Spectra
- ☐ Detect Solvent/Water Signals
- ☒ Synchronize APT/DEPT Phase
- ☒ Attach 1D Spectra
- ☐ Peak Picking
- ☐ Run Macro 


LC/UV/MS Chromatograms




- ☐ Peak Picking
- ☒ Detect Lag
- ☐ Auto Combine
- ☐ Run Macro 

UV/IR Spectrum

- ☒ Peak Picking
- ☐ Run Macro 

Curve Spectrum

- ☐ Peak Picking
- ☐ Run Macro 

Drag & drop files here

Press F3 to open a file(s)

Open Database ChemSketch

Customer Portal

Case Study: Unknown Street Drug

1. Sample Prep of Unknown:

- Spatula of unknown added to vial of ~0.6 mL D₂O
- Sealed and agitated for 1 min
- Liquid phase transferred to NMR tube

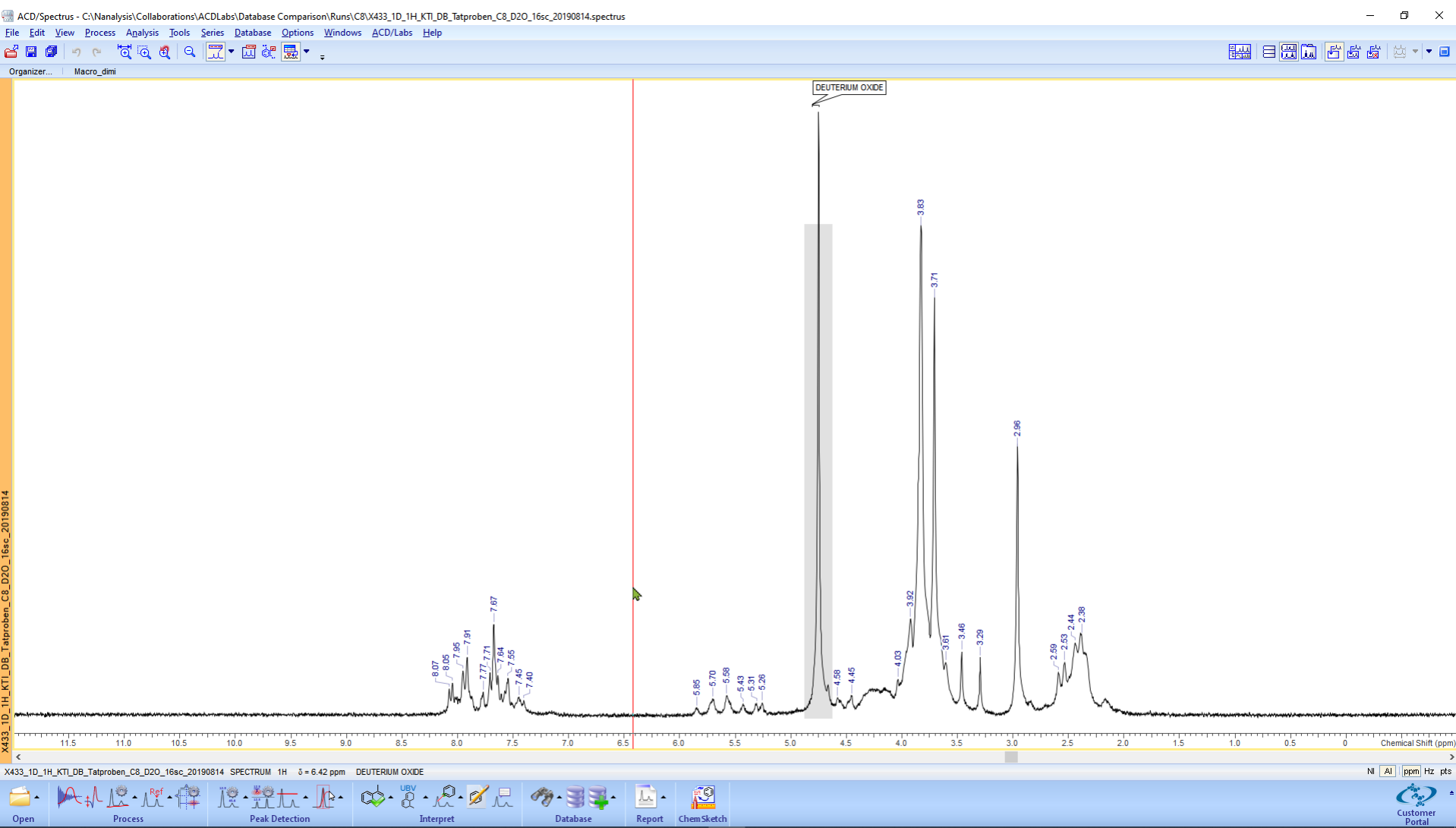
2. ¹H NMR Spectra Acquisition

3. Load into ACD/Spectrus

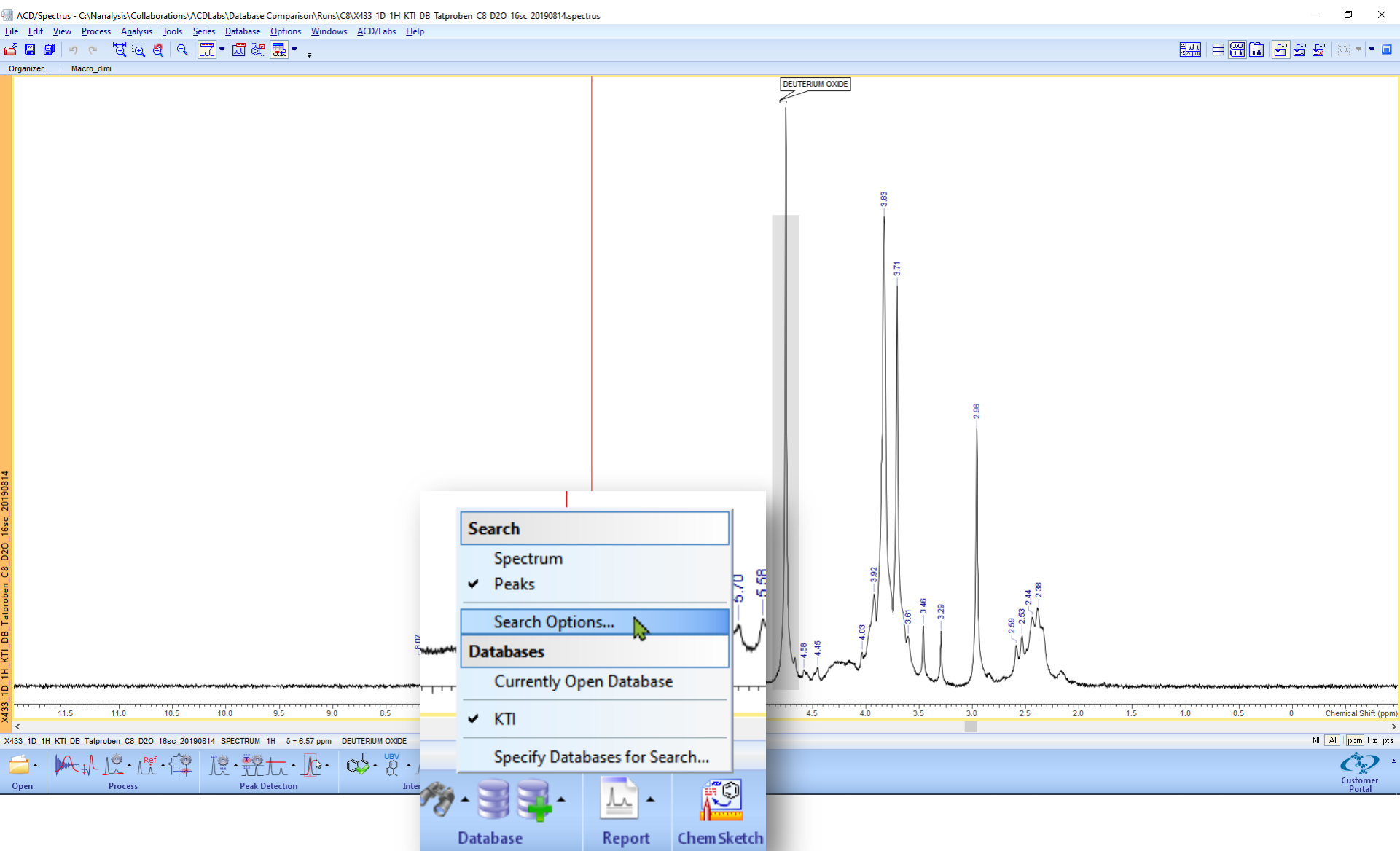
- Auto Preprocessing Macro
- Peak Search with ACD/Spectrus DB



Open Unknown ^1H NMR Spectra into ACD/Labs



Search Database



Database Search Options

ACD/Spectrus - C:\Analysis\Collaborations\ACDLabs\Database Comparison\Runs\C8\X433_ID_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814.spectrum

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Macro_dimi

DEUTERIUM OXIDE

Spectrum Search Options

Search Method
☐ Similarity Search ☒ Peak Search

Peak Search Options

Looseness Factor (ppm): 0.1

☒ Mixture Search
☒ Approximate Mode
☐ Search Empty Regions

Limit Result By
☒ None
☐ Number of Hits: 100
☐ Minimum HQI (%): 50

Range By
☐ ID
☒ HQI
☐ Minimal Shift

Search Region
☒ Zoomed Region ☐ Selected Region(s) Set Clear

| N | Min X | Max X |
|---|-------|-------|
| 1 | | |

Show Result in Mode
☒ Overlay ☒ Spectra Comparison

Search Close ? Help

X433_ID_1H_KTI_DB_Tatproben_C8_D2O_16sc_20190814 SPECTRUM 1H $\delta = 8.06$ ppm DEUTERIUM OXIDE

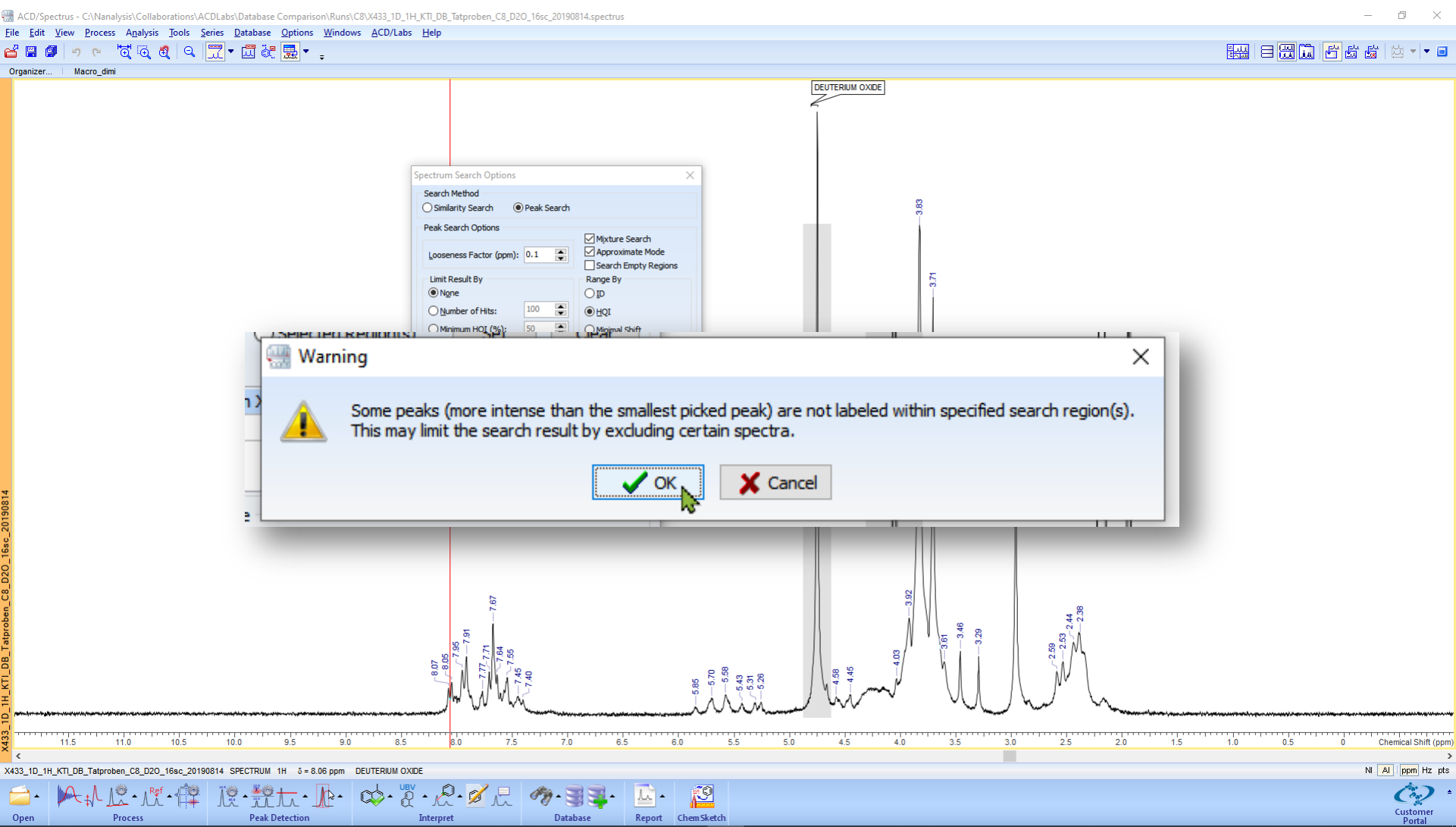
Open Process Ref Peak Detection Interpret Database Report ChemSketch

Customer Portal

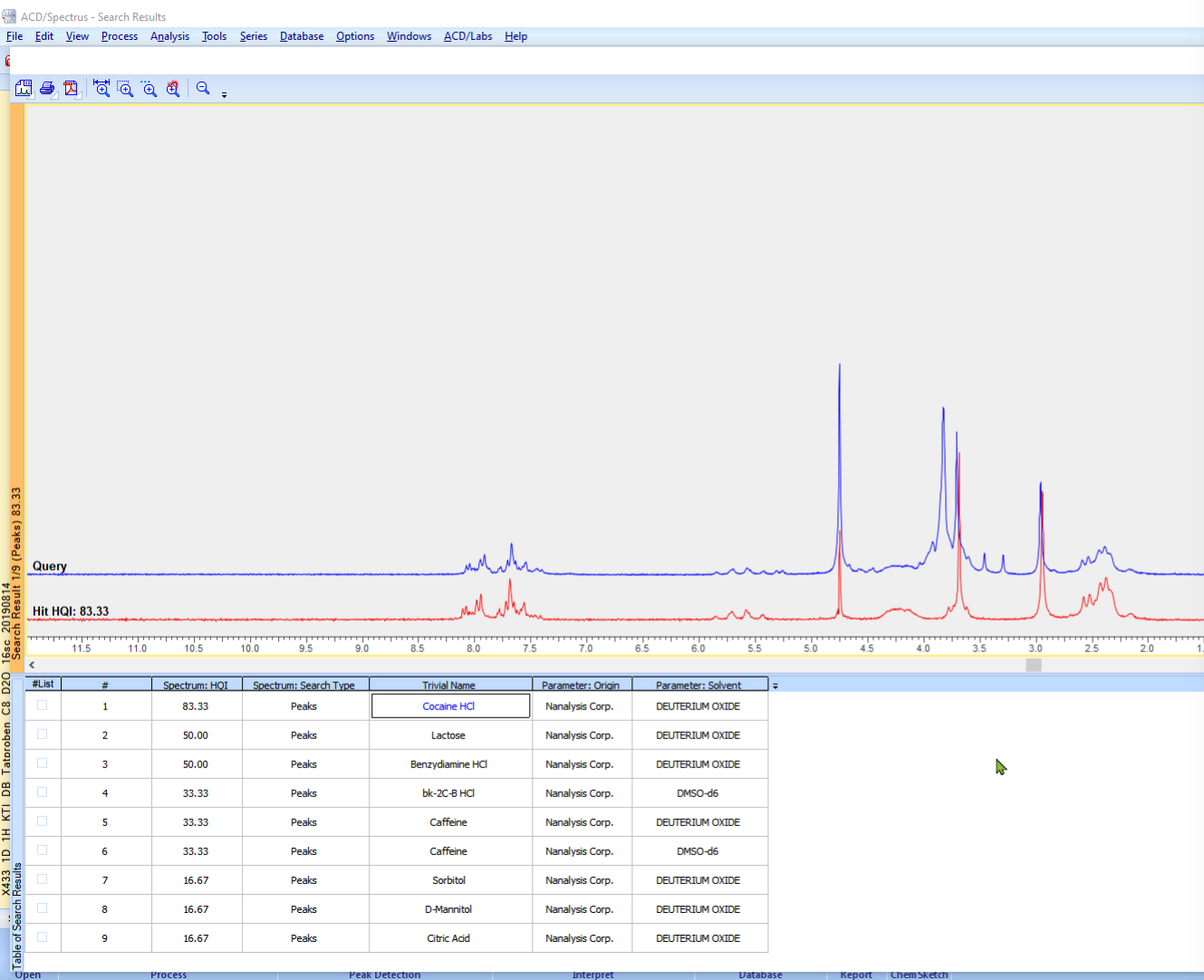
Chemical Shift (ppm)

2.98 2.59 2.53 2.44 2.38

Database Search



First Database Hits: Cocaine



Spectra Comparison

More Info

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.4439

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Auto Select Best Hits

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

Query

Hit HQI: 83.33

Processing groups

0%

67%

Cancel

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.4439

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

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

Open Process Peak Detection Interpret Database Report Chem Sketch

Table of Search Results

X433 1D 1H KTI DB Tairöben C8 D20 16sc 20190314 Search Result 1/9 (Peaks) 83.33

Peaks HQI: 83.33 NI AI ppm Hz pts

Customer Portal

Database Best Hits



Adjust Intensity

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

2 HQI: 50.00

Query

Hit HQI: 83.33

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

Open Process Peak Detection Interpret Database Report Chem Sketch

Spectra Comparison

[More Info](#)

Active Spectrum Properties

Horizontal Offset (ppm):

Line Broadening (Hz):

Individual Scale:

☐ Fine Tuning

Show

☐ Sum ☐ Residual

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Optimize Hit

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

2 HQI: 50.00

Query

Hit HQI: 83.33

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

| #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 | Benzylamine 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 |

Open Process Peak Detection Interpret Database Report Chem Sketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.4439

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close Help

Optimize hit for Cocaine

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

2 HQI: 50.00

Query

Hit HQI: 83.33

Table of Search Results

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

Open Process Peak Detection Interpret Database Report ChemSketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.4439

☐ Fine Tuning

Optimize Hit

Clear

Auto Select Best Hit(s)

Show

☐ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close

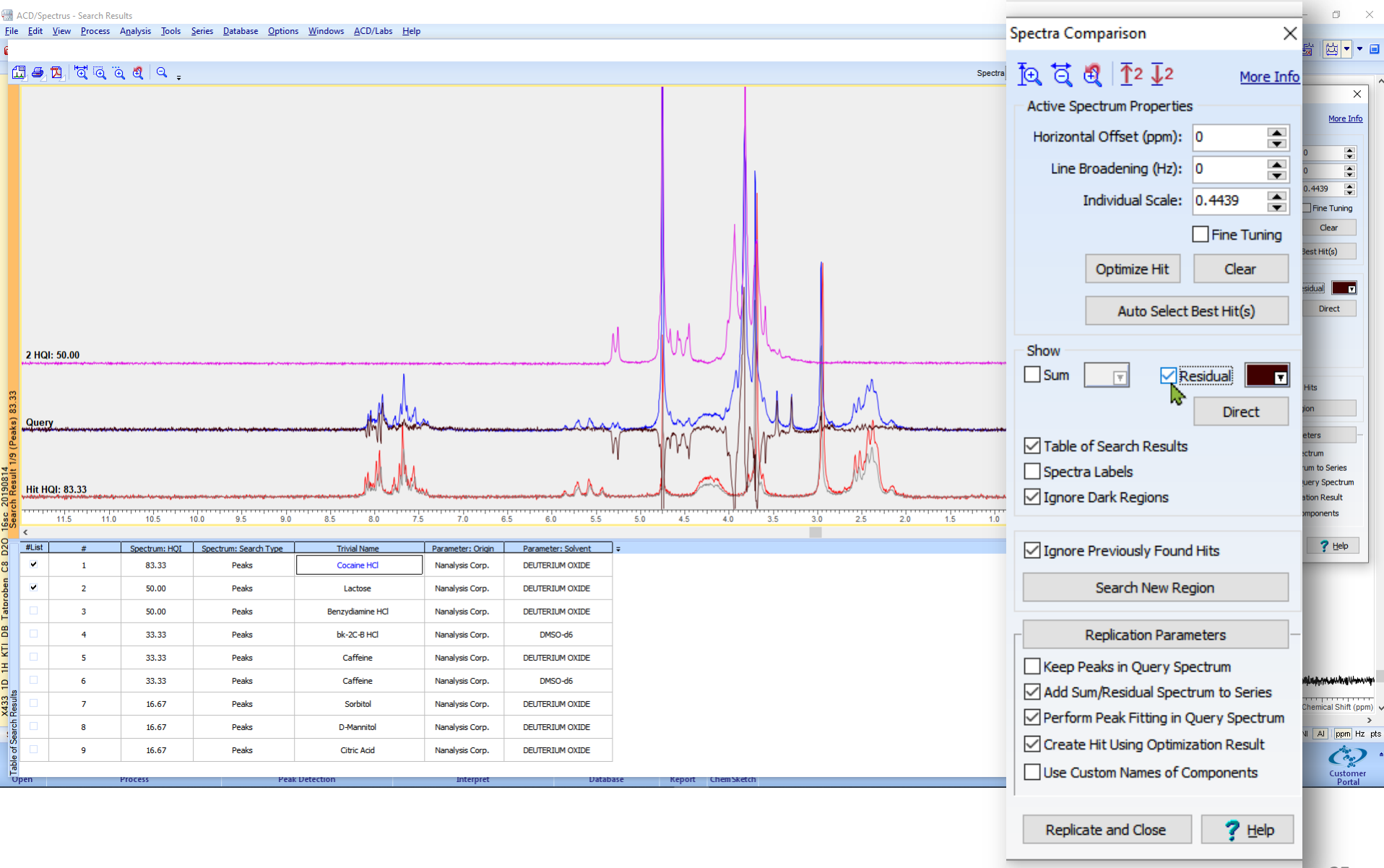
Help

Peaks HQI: 83.33 NI ppm Hz pts

Chemical Shift (ppm)

Customer Portal

Residuals of Best Fit for Unknown & Cocaine Std



Optimize Hit for Lactose

ACD/Spectrum - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

1 HQI: 83.33

Query

Hit HQI: 50.00

Table of Search Results

| #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 | Benzylamine 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 |

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.3302

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☒ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Peaks HQI: 50.00 NI All ppm Hz pts

Customer Portal

Manually Change Intensity

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

1 HQI: 83.33

Query

Hit HQI: 50.00

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

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

Open Process Peak Detection Interpret Database Report Chem Sketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.3302

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☐ Residual ☒ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

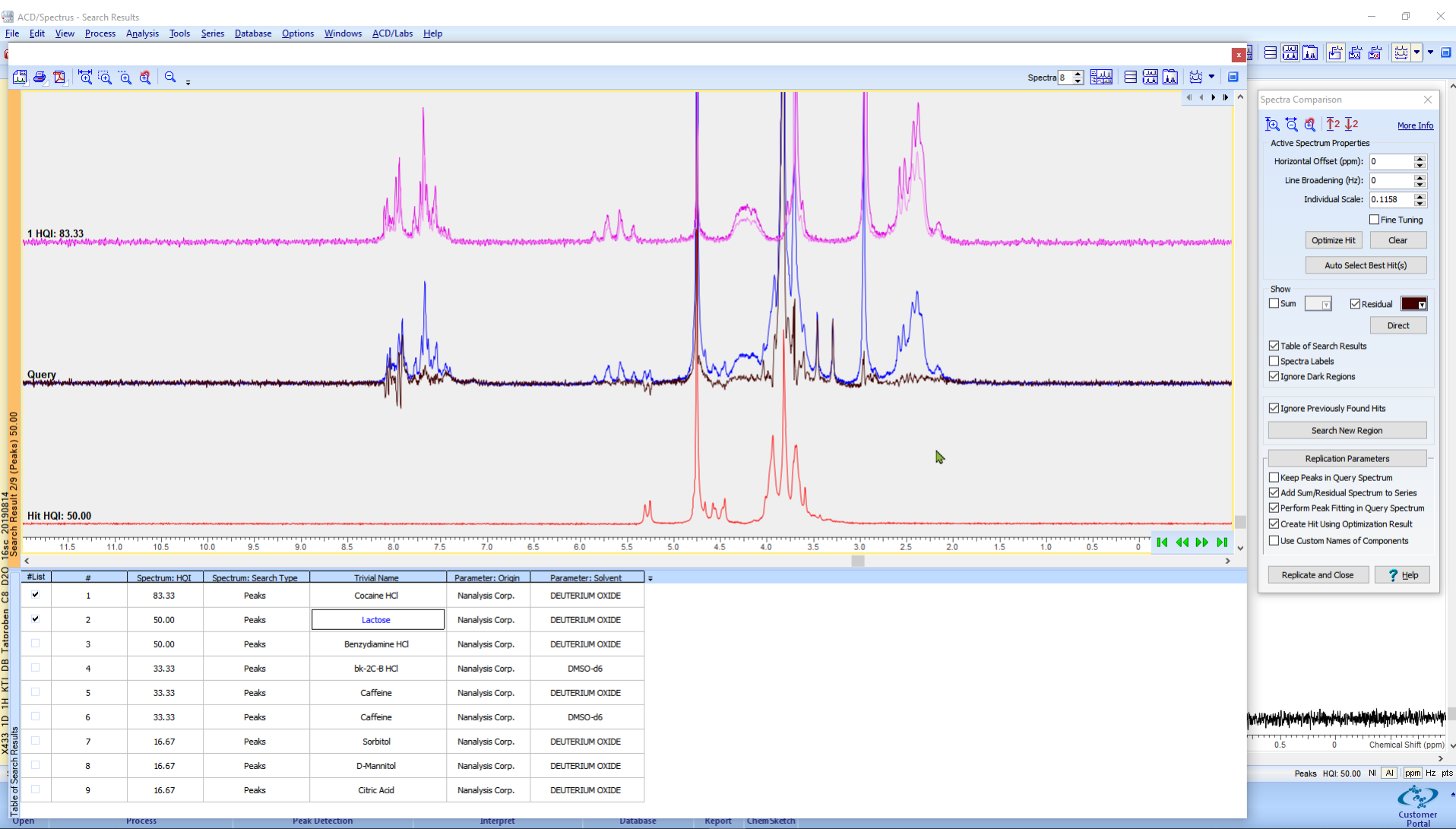
☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Manually Change Intensity



Manually Change Intensity

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

1 HQI: 83.33

Query

Hit HQI: 50.00

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.0719

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☐ Sum ☒ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

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

Open Process Peak Detection Interpret Database Report Chem Sketch

Peaks HQI: 50.00 NI All ppm Hz pts

Customer Portal

Visualize Sum Instead of Residuals

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

1 Hit: 83.33

Query

Hit Hit: 50.00

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

| #List | # | Spectrum: Hit | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|-------------------------------------|---|---------------|-----------------------|-----------------|-------------------|--------------------|
| <input checked="" type="checkbox"/> | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input checked="" type="checkbox"/> | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 3 | 50.00 | Peaks | Benzylamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

Open Process Peak Detection Interpret Database Report Chem Sketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.0719

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

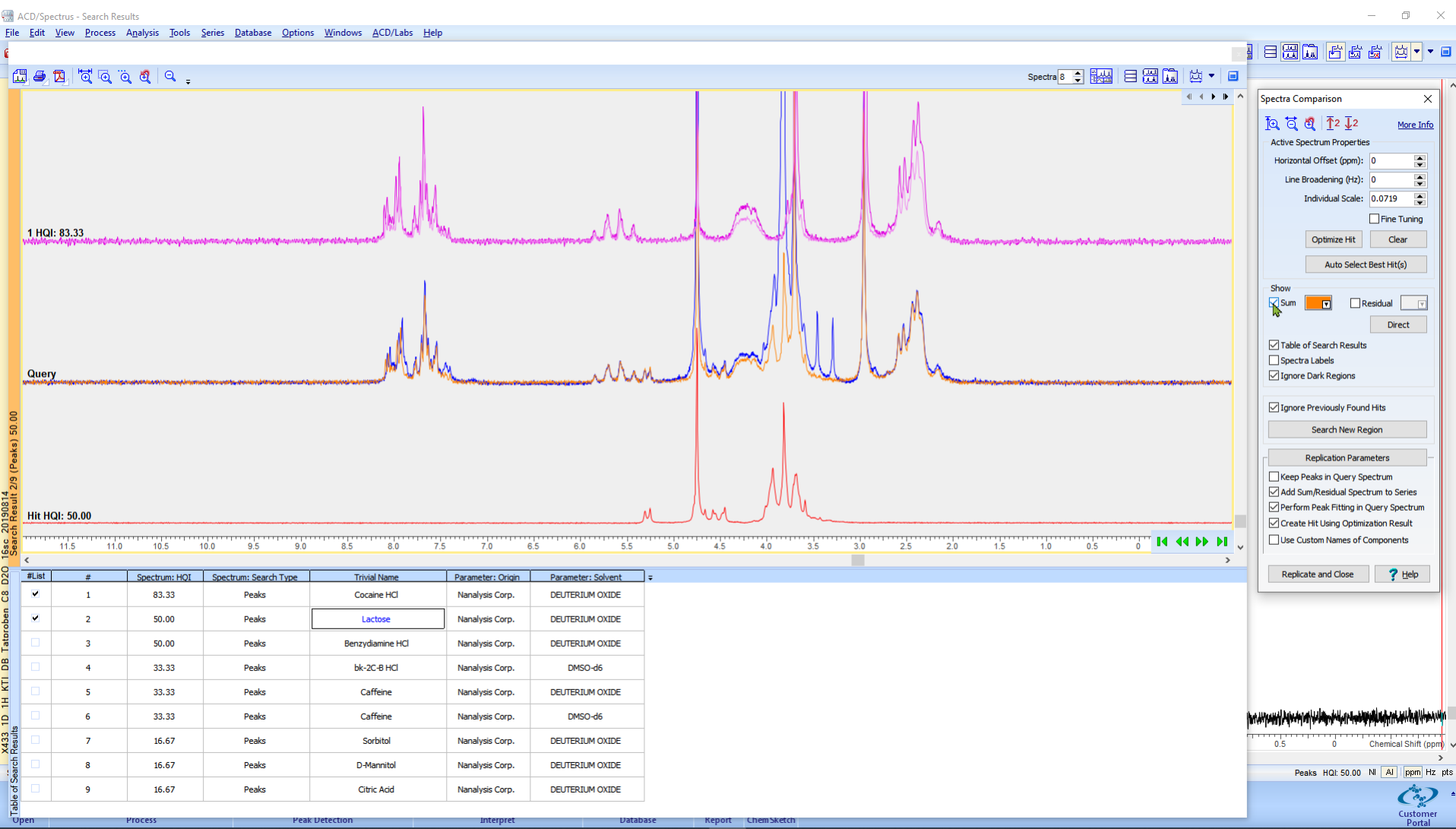
☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close Help

Sum of Database Components on Unknown



Manually Investigate Other Potential Hits

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

1 HQI: 83.33

2 HQI: 50.00

Query

Hit HQI: 50.00

Table of Search Results

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

Chemical Structure:

CN(C)[CH+]([O-])CCOC1=CN(Cc2ccccc2)C3=CC=CC=C13

Peaks HQI: 50.00 N | ppm Hz pts

Customer Portal

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 1.2052

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Visualize Inspect Benzydiamine HCl

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

Query
Hit HQI: 50.00

Search Result 3/9 (Peaks) 50.00

Table of Search Results

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

Chemical Structure: CN(C)[CH+]CCOC1=CN(Cc2ccccc2)C3=CC=CC=C31

Peaks HQI: 50.00 N | ppm Hz pts

Customer Portal

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 1.2052

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

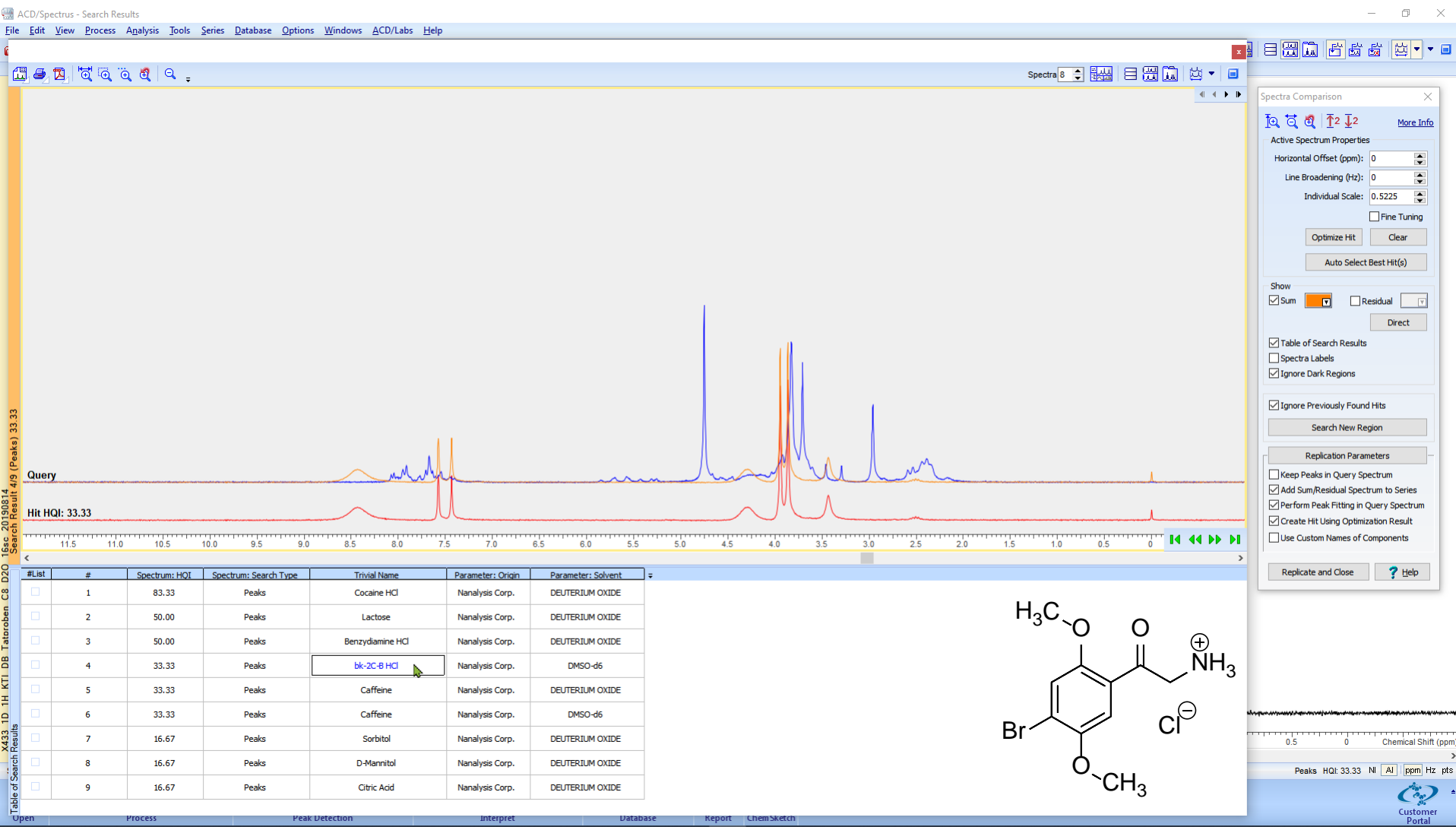
☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Visually Inspect bk-2C-B HCl



Visually Inspect Caffeine

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

Query

Hit HQI: 33.33

| #List | # | Spectrum: HQI | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|--------------------------|---|---------------|-----------------------|-----------------|-------------------|--------------------|
| <input type="checkbox"/> | 1 | 83.33 | Peaks | Cocaine HCl | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 2 | 50.00 | Peaks | Lactose | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 3 | 50.00 | Peaks | Benzylamine HCl | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 4 | 33.33 | Peaks | bk-2C-B HCl | Nananalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 5 | 33.33 | Peaks | Caffeine | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 6 | 33.33 | Peaks | Caffeine | Nananalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 7 | 16.67 | Peaks | Sorbitol | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 8 | 16.67 | Peaks | D-Mannitol | Nananalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 9 | 16.67 | Peaks | Citric Acid | Nananalysis Corp. | DEUTERIUM OXIDE |

Table of Search Results

Open Process Peak Detection Interpret Database Report ChemSketch

Chemical structure of Caffeine: CN1C=NC2=C1C(=O)N(C(=O)N2C)C

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.2311

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Peaks HQI: 33.33 NI All ppm Hz pts

Customer Portal

Optimize Intensity

ACD/Spectrum - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

Query

Hit HQI: 33.33

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

Table of Search Results

Open Process Peak Detection Interpret Database Report Chem Sketch

Chemical Structure: CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.0284

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Horizontal Offset Adjustment

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

Query

Hit HQI: 33.33

Table of Search Results

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

Open Process Peak Detection Interpret Database Report Chem Sketch

Chemical Structure: CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0.02

Line Broadening (Hz): 0

Individual Scale: 0.0284

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close Help

Line Broadening Adjustment

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Query

Hit HQT: 33.33

Table of Search Results

| #List | # | Spectrum: HQT | Spectrum: Search Type | Trivial Name | Parameter: Origin | Parameter: Solvent |
|--------------------------|---|---------------|-----------------------|-----------------|-------------------|--------------------|
| <input type="checkbox"/> | 1 | 83.33 | Peaks | Cocaine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 2 | 50.00 | Peaks | Lactose | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 3 | 50.00 | Peaks | Benzylamine HCl | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 4 | 33.33 | Peaks | bk-2C-B HCl | Nanalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 5 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 6 | 33.33 | Peaks | Caffeine | Nanalysis Corp. | DMSO-d6 |
| <input type="checkbox"/> | 7 | 16.67 | Peaks | Sorbitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 8 | 16.67 | Peaks | D-Mannitol | Nanalysis Corp. | DEUTERIUM OXIDE |
| <input type="checkbox"/> | 9 | 16.67 | Peaks | Citric Acid | Nanalysis Corp. | DEUTERIUM OXIDE |

Open Process Peak Detection Interpret Database Report Chem Sketch

Chemical Structure: CN1C=NC2=C1C(=O)N(C)C2=O

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0.02

Line Broadening (Hz): 0.3

Individual Scale: 0.0284

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual

Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Optimize Hit

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra 8

Query

Hit HQI: 33.33

Table of Search Results

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

Chemical Structure: CN1C=NC2=C1C(=O)N(C)C(=O)N2C

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0.02

Line Broadening (Hz): 0.3

Individual Scale: 0.0284

☐ Fine Tuning

Optimize Hit

Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

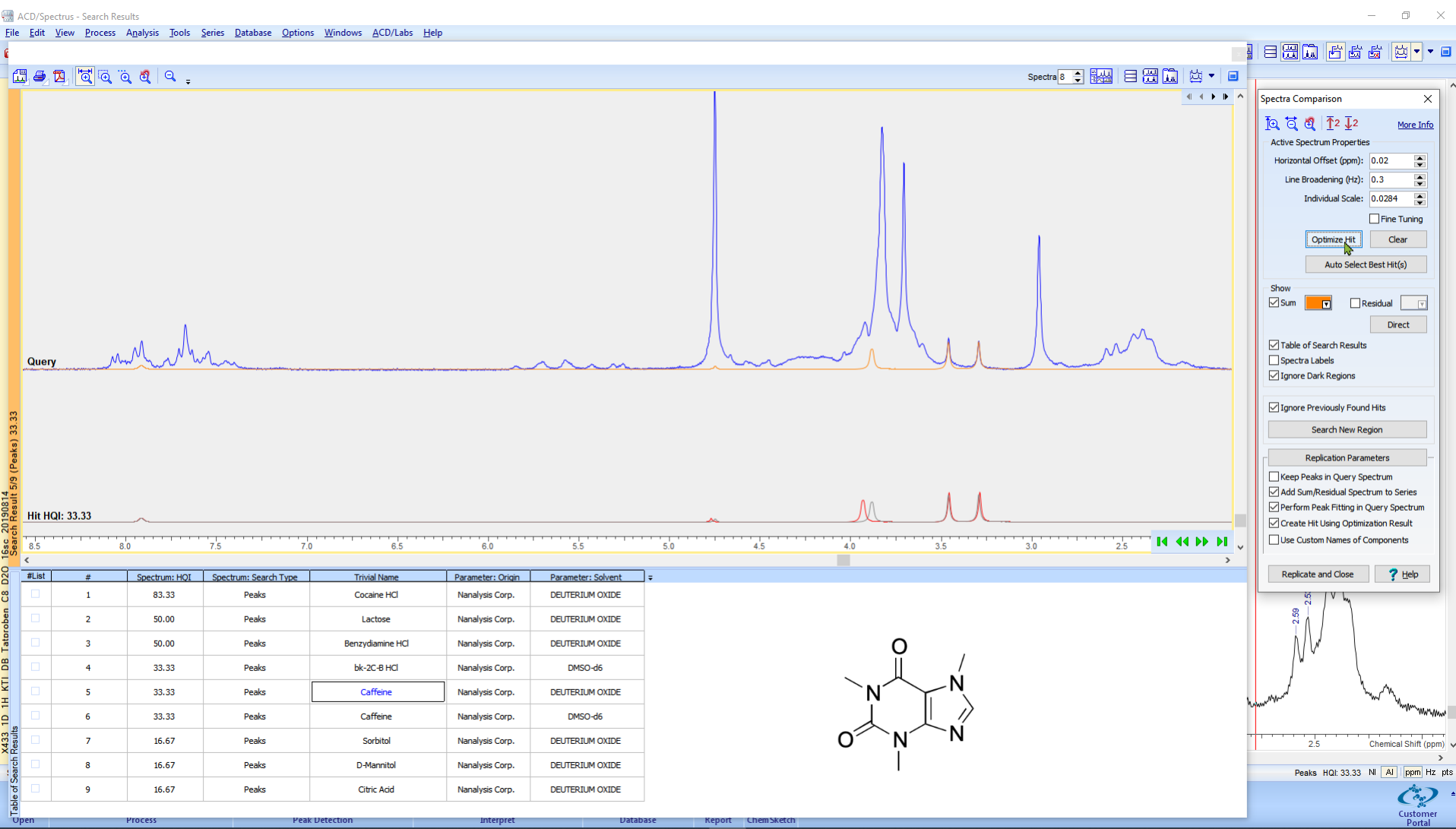
Replicate and Close

Help

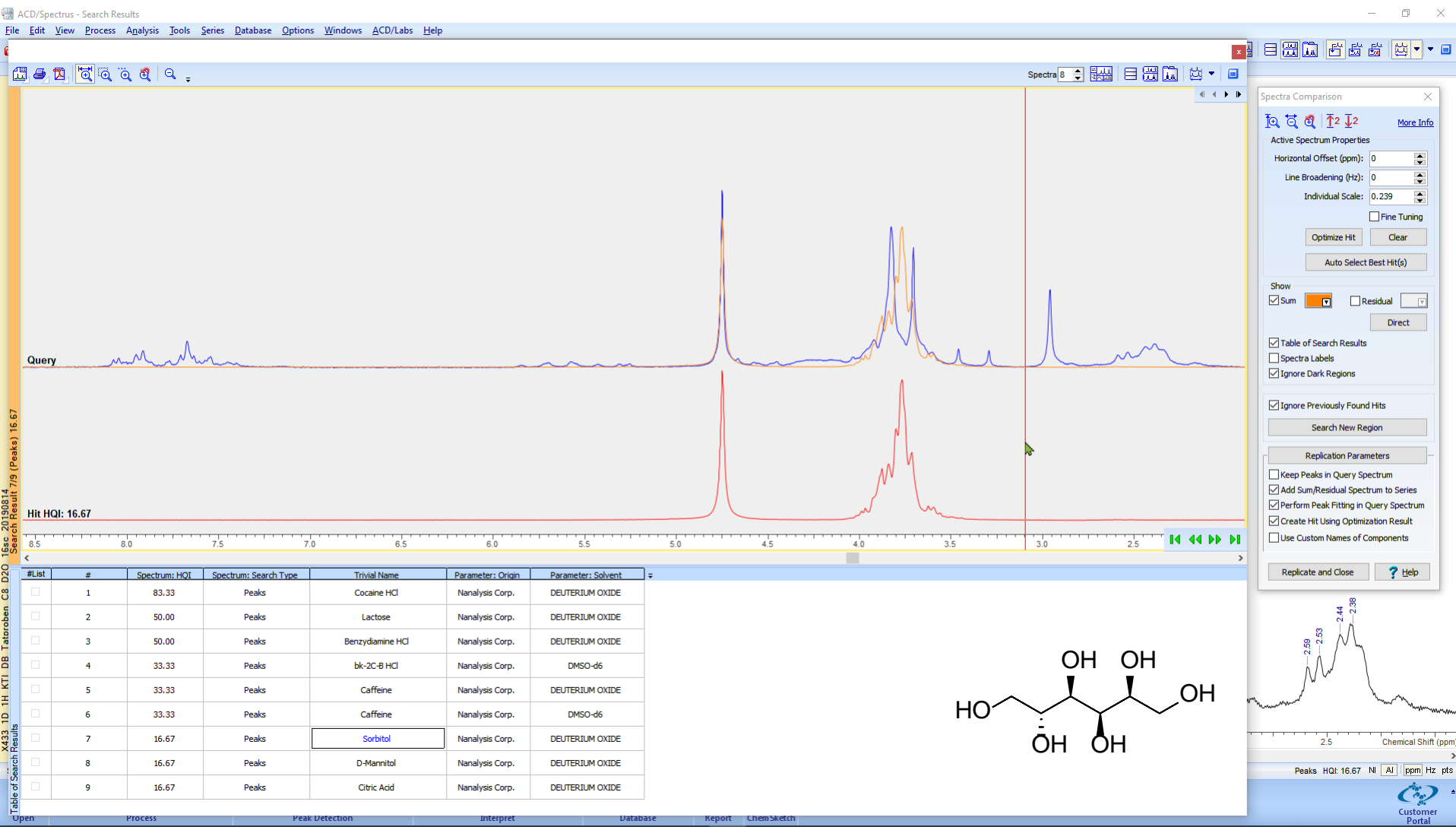
Peaks HQI: 33.33 NI All ppm Hz pts

Customer Portal

Caffeine Optimized



Visually Inspect Sorbitol



Visually Inspect D-Mannitol

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

Query

Hit HQI: 16.67

Table of Search Results

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

Chemical Structure: D-Mannitol

OC[C@H](O)[C@H](O)[C@@H](O)[C@@H](O)CO

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.2231

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☐ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Peaks HQI: 16.67 NI All ppm Hz pts

Customer Portal

Visually Inspect Citric Acid

ACD/Spectrus - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

Query

Hit HQI: 16.67

Table of Search Results

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

Open Process Peak Detection Interpret Database Report ChemSketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.1582

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Chemical Shift (ppm)

Peaks HQI: 16.67 NI All ppm Hz pts

Customer Portal

Chemical structure of Citric Acid: OC(CC(=O)O)(O)C(=O)O

Select all Matching Components

ACD/Spectrum - Search Results

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Spectra: 8

1 HQI: 83.33

2 HQI: 50.00

5 HQI: 33.33

Query

Hit HQI: 16.67

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5

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

Open Process Peak Detection Interpret Database Report ChemSketch

Spectra Comparison

Active Spectrum Properties

Horizontal Offset (ppm): 0

Line Broadening (Hz): 0

Individual Scale: 0.2231

☐ Fine Tuning

Optimize Hit Clear

Auto Select Best Hit(s)

Show

☒ Sum ☐ Residual ☐ Direct

☒ Table of Search Results

☐ Spectra Labels

☒ Ignore Dark Regions

☒ Ignore Previously Found Hits

Search New Region

Replication Parameters

☐ Keep Peaks in Query Spectrum

☒ Add Sum/Residual Spectrum to Series

☒ Perform Peak Fitting in Query Spectrum

☒ Create Hit Using Optimization Result

☐ Use Custom Names of Components

Replicate and Close ? Help

Peaks HQI: 16.67 NI AI ppm Hz pts

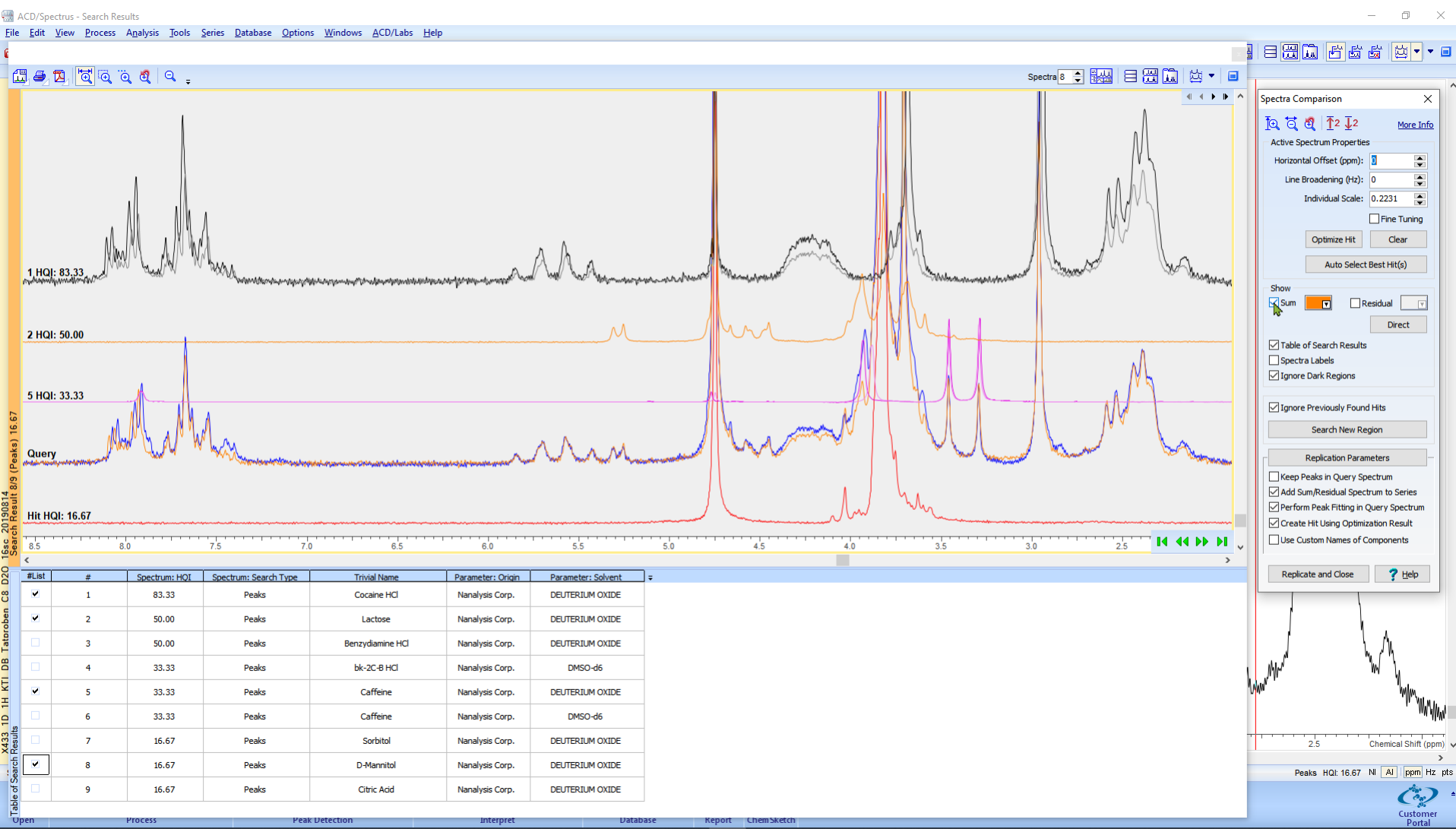
Chemical Shift (ppm)

2.5 2.0 1.5 1.0 0.5 0.0

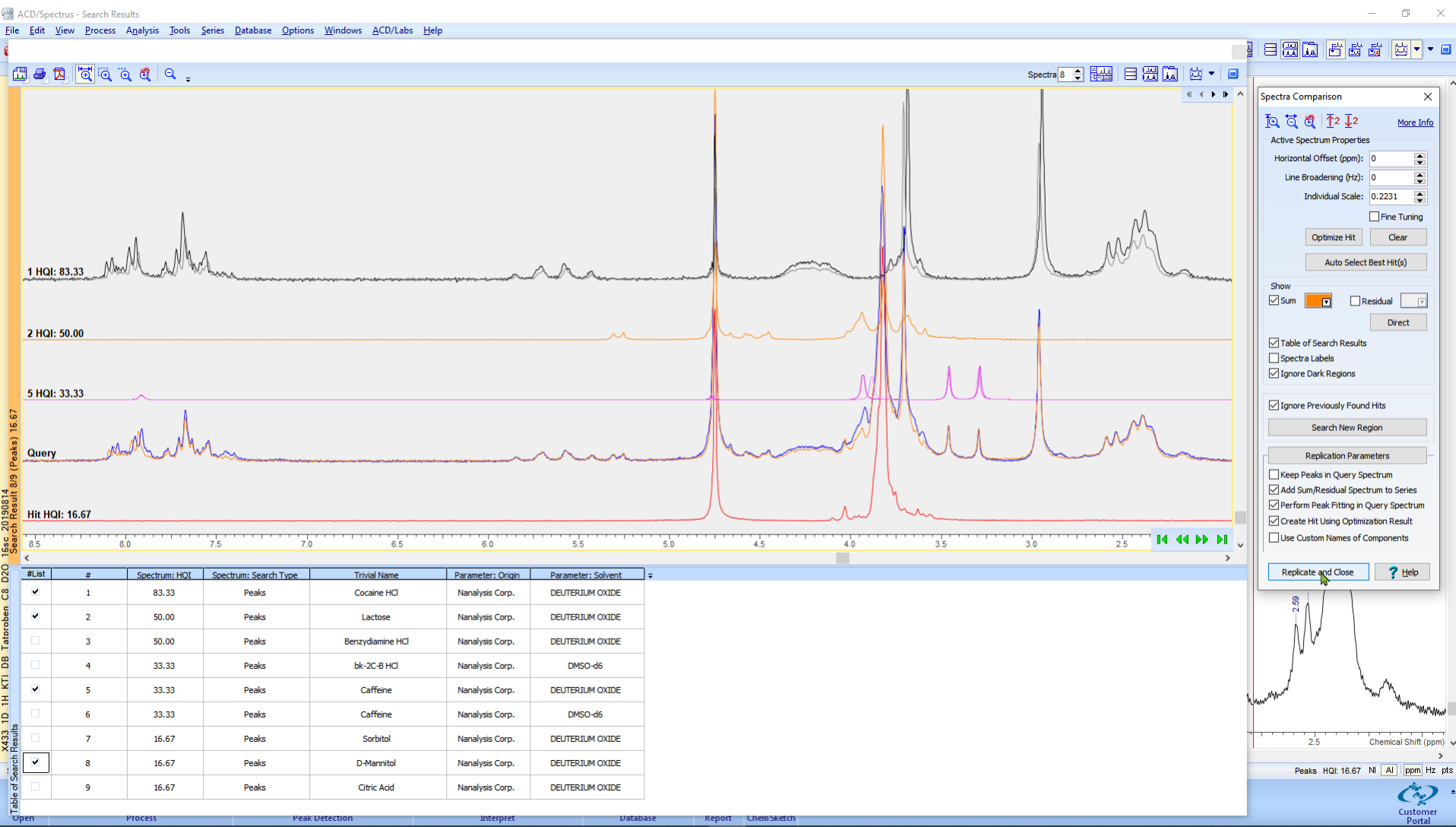
2.59 2.53 2.44 2.38

Customer Portal

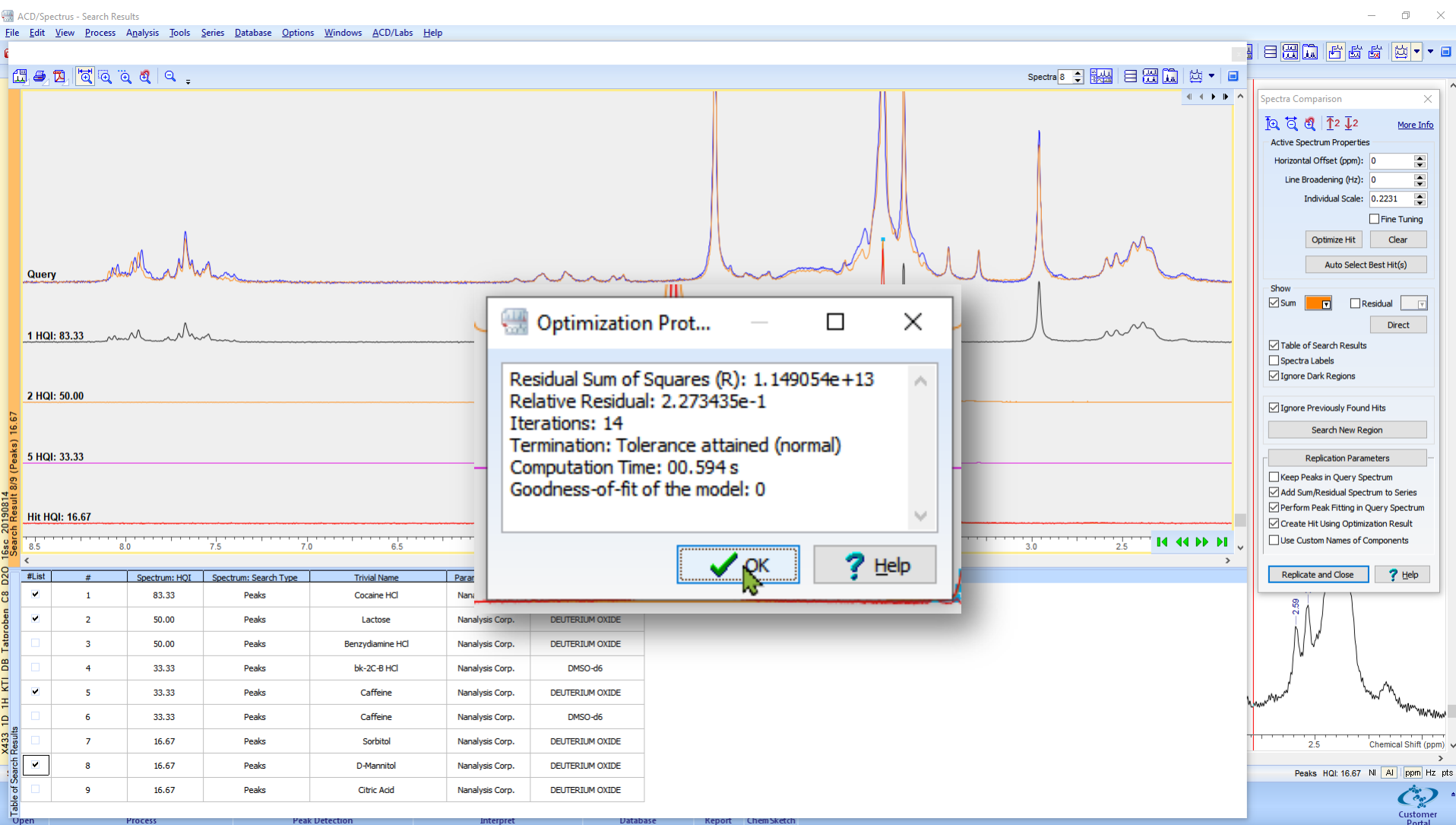
Inspect Matching Components: Sum



Case Study: Cocaine cont.



Case Study: Cocaine cont.

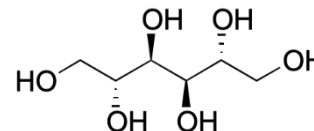
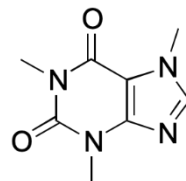


Report: Street Drug Cocaine HCl

Search Result 8/9 (Peaks) 16.67



Spectra 8



Cocaine HCl

83.33 match

Lactose

50.00 match

Caffeine

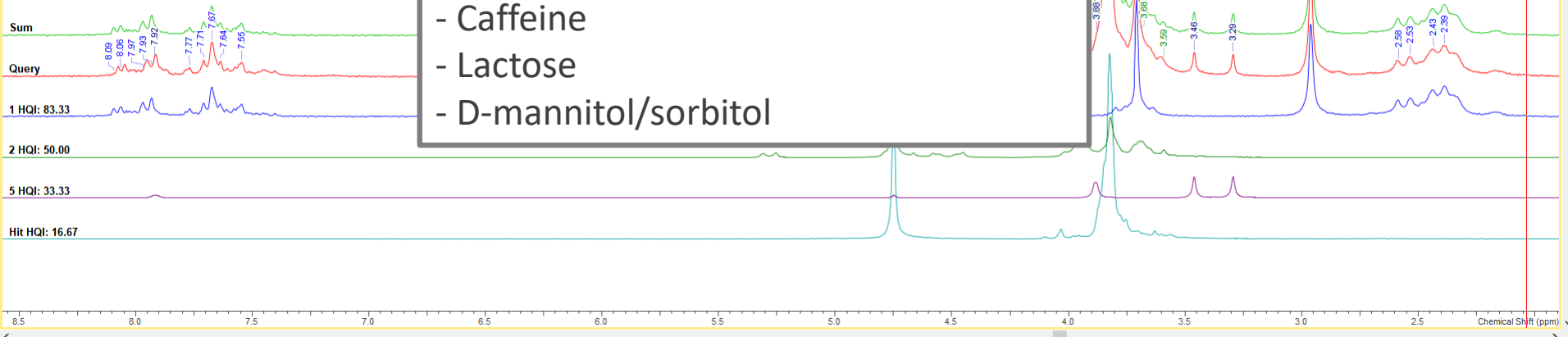
33.33 match

D-Mannitol

16.67 match

Compare with GC-MS analysis:

- Cocaine HCl (41.9%)
- Caffeine
- Lactose
- D-mannitol/sorbitol



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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Adam Paulson
Amro Hussein



ACD/Labs

ACD/Labs

Michel Riese



**LANDESKRIMINALAMT
NIEDERSACHSEN**

Kriminaltechnisches Institut

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