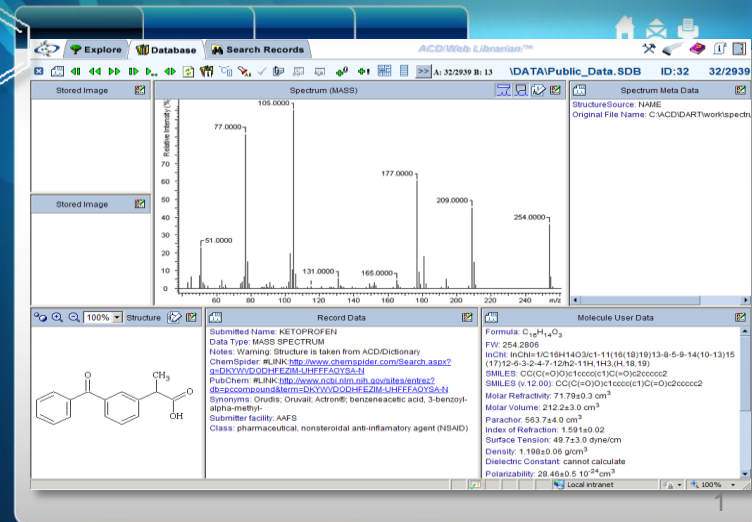
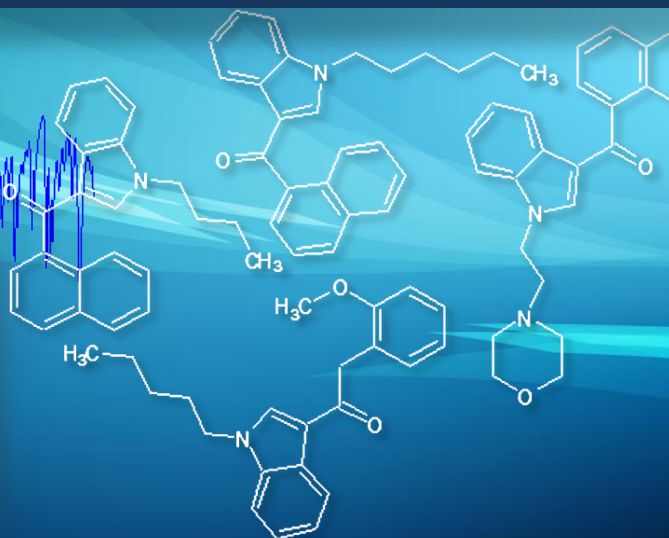
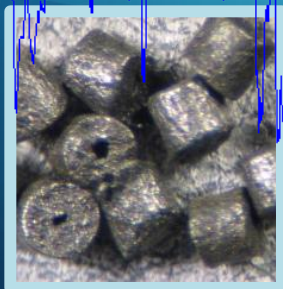


# Demo of Online Database Resources for the Identification of Novel and Emerging Drugs

Peter R. Stout, PhD





[www.forensicCOE.org](http://www.forensicCOE.org)





## Outline

- Overview of existing databases and resources

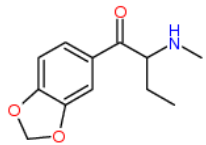
- EI-MS spectra of their forensic related compounds
  - Over 280 synthetic cannabinoids including parent compounds, isomers and metabolites
  - Over 200 emerging drug compounds of different classes
- Free download in NIST and Agilent ChemStation formats
- Frequently updated
- Each version includes a change log



- Reference site of emerging compounds
- Over 300 compounds with FITR and EI-MS spectra as PDF files from various contributors
- Links to other databases, references, and vendors
- Name search
- Structure properties
- Active forum

Home CSA Schedules Categories ▾ Resources ▾ Search for a substance:  ? | Butylone

Identity Properties Spectra Vendors References Databases Variations



**Names:** Butylone (primary)

**Molecular formula:** C<sub>12</sub> H<sub>15</sub> NO<sub>3</sub>

**Nominal mass:** 221

**Average mass:** 221.2524<sup>3</sup>

**Monoisotopic mass:** 221.105193

**CAS registry number:** 11762-90-2

**ChemSpider:** [21106270](#)

**PubChem:** [56843046](#)

**Wikipedia:** [Bk-MBDB](#)

**Erowid:** [bk-MBDB](#)

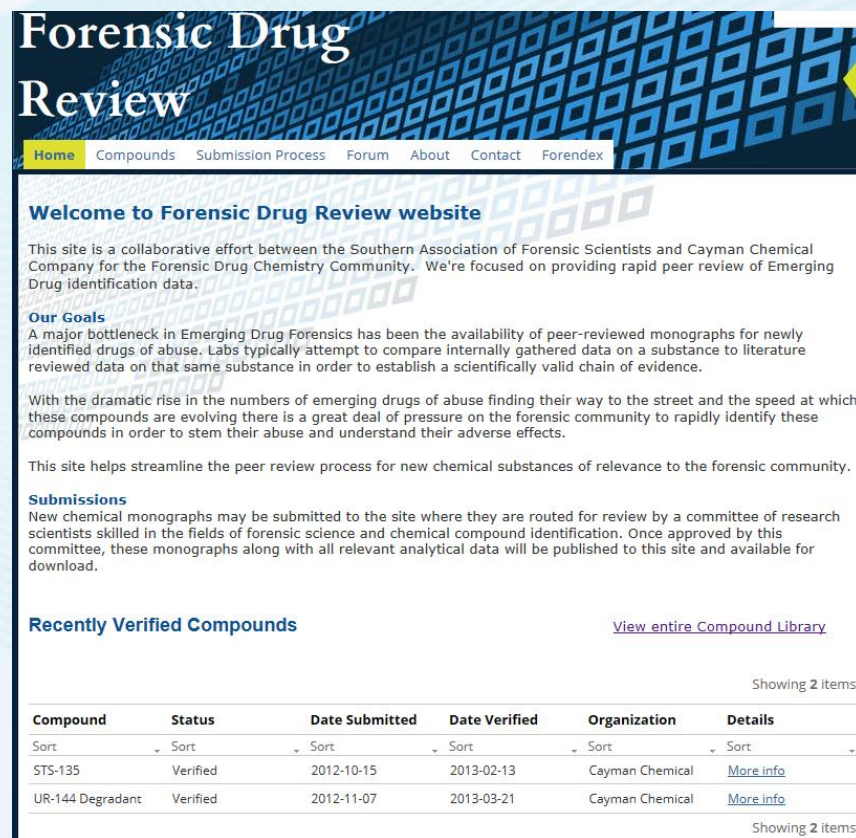
**Standard InChI:** InChI=1S/C12H15NO3/c1-3-9(13-2)12(14)8-4-5-10-11(6-8)16-7-15-10/h4-6,9,13H,3,7H2,1-2H3

**Standard InChIKey:** CGKQZIULZRXRRJ-UHFFFAOYSA-N

**SMILES:** CCC(C(=O)c1ccc2c(c1)OCO2)NC

**Tags:** cathinone

- Collaboration between Cayman Chemical and SAFS
- PDF of verified compounds from various contributors
- Includes NMR, EI-MS, and FTIR
- Review and Editorial Committee
- Submission Process



**Forensic Drug Review**

Home Compounds Submission Process Forum About Contact Forendex

**Welcome to Forensic Drug Review website**

This site is a collaborative effort between the Southern Association of Forensic Scientists and Cayman Chemical Company for the Forensic Drug Chemistry Community. We're focused on providing rapid peer review of Emerging Drug Identification data.

**Our Goals**

A major bottleneck in Emerging Drug Forensics has been the availability of peer-reviewed monographs for newly identified drugs of abuse. Labs typically attempt to compare internally gathered data on a substance to literature reviewed data on that same substance in order to establish a scientifically valid chain of evidence.

With the dramatic rise in the numbers of emerging drugs of abuse finding their way to the street and the speed at which these compounds are evolving there is a great deal of pressure on the forensic community to rapidly identify these compounds in order to stem their abuse and understand their adverse effects.

This site helps streamline the peer review process for new chemical substances of relevance to the forensic community.

**Submissions**

New chemical monographs may be submitted to the site where they are routed for review by a committee of research scientists skilled in the fields of forensic science and chemical compound identification. Once approved by this committee, these monographs along with all relevant analytical data will be published to this site and available for download.

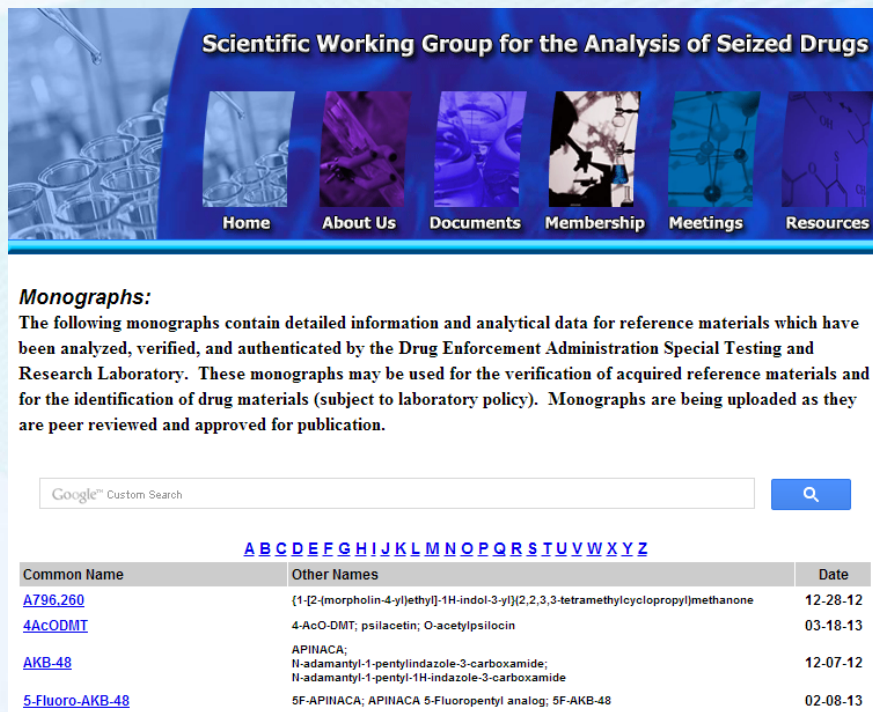
**Recently Verified Compounds** [View entire Compound Library](#)

Showing 2 items

Compound	Status	Date Submitted	Date Verified	Organization	Details
Sort	Sort	Sort	Sort	Sort	Sort
STS-135	Verified	2012-10-15	2013-02-13	Cayman Chemical	<a href="#">More info</a>
UR-144 Degradant	Verified	2012-11-07	2013-03-21	Cayman Chemical	<a href="#">More info</a>

Showing 2 items

- Freely downloadable in several formats
- Approximately 1,835 spectra of parent compounds, metabolites, and derivatized compounds from various contributors
- No replicate spectra
- Drug monographs
  - peer reviewed data
  - NMR
  - FTIR
  - EI-MS



**Scientific Working Group for the Analysis of Seized Drugs**

Home About Us Documents Membership Meetings Resources

**Monographs:**  
The following monographs contain detailed information and analytical data for reference materials which have been analyzed, verified, and authenticated by the Drug Enforcement Administration Special Testing and Research Laboratory. These monographs may be used for the verification of acquired reference materials and for the identification of drug materials (subject to laboratory policy). Monographs are being uploaded as they are peer reviewed and approved for publication.

Google Custom Search

ABCDEFGHIJKLMNOPQRSTUVWXYZ

Common Name	Other Names	Date
<a href="#">A796.260</a>	{1-[2-(morpholin-4-yl)ethyl]-1H-indol-3-yl}(2,2,3,3-tetramethylcyclopropyl)methanone	12-28-12
<a href="#">4AcODMT</a>	4-AcO-DMT; psilacetin; O-acetylpsilocin	03-18-13
<a href="#">AKB-48</a>	APINACA; N-adamantyl-1-pentylindazole-3-carboxamide; N-adamantyl-1-pentyl-1H-indazole-3-carboxamide	12-07-12
<a href="#">5-Fluoro-AKB-48</a>	5F-APINACA; APINACA 5-Fluoropentyl analog; 5F-AKB-48	02-08-13



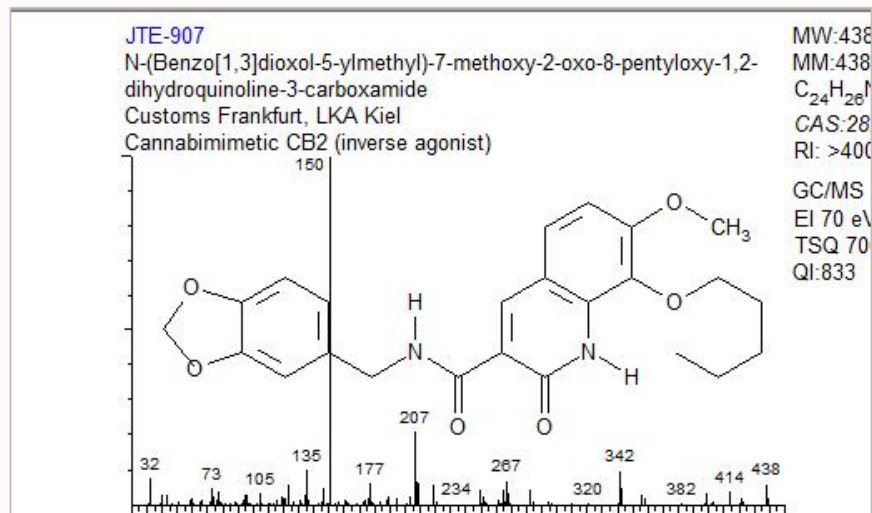
- EI-MS data freely downloadable in Agilent ChemStation or other platform as requested
- Over 2,800 spectra of pure compounds, metabolites and breakdown products
- Includes replicate spectra
- Spectra verified against independent library

- Freely available EI-MS data
- Not downloadable
- Merged with commercial Mass Spectra of Designer Drugs database yearly
- Searchable by name, fragment and relative intensity
- E-mail sent to registered users with newly emerged drugs
- Reviewed and given a computerized Quality Index
- Molecular Index of Cannabimimetics

**Names:**  
JTE-907  
N-(1,3-benzodioxol-5-ylmethyl)-7-methoxy-2-oxo-8-pentoxo-1H-quinoline-3-carboxamide

Molweight: 438.48032 g/mol  
Formula: C<sub>24</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>

**Compound**   **MS**   **External URLs**



- Provided by NMS Labs
- Online resource for a variety of sectors including scientists, police officers, and policy makers
- Links to research, state-by-state policy and webinars

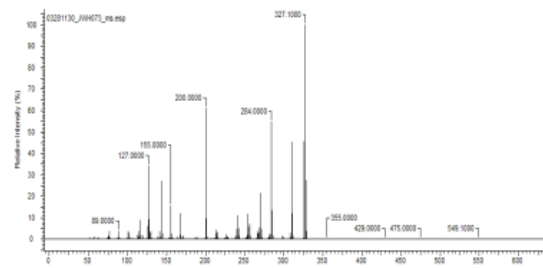




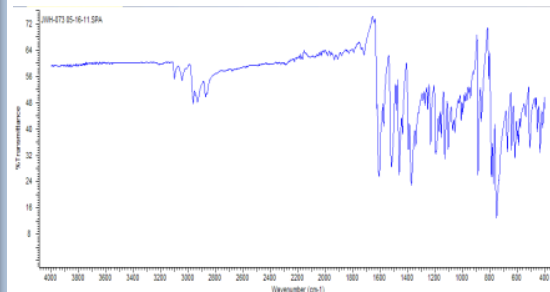
- Free, Web-accessible and searchable database
- Over 3,200 records that include one or more instrumental techniques
  - FTIR, EI-MS, DART-TOF, and ESI-QTOF spectra from various contributors
- Replicate spectra
- Peer review process
- Frequent updates
- Download single records as JACAMP files

## Complete Record

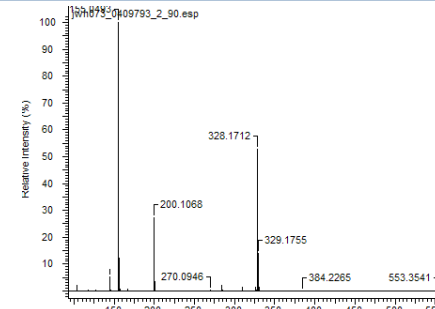
RECORD



Spectral Method: EI-MS  
Data reduction: Averaged and Background Subtracted  
Software method Full scan  
Scan range: 50-550 m/z  
Sample introduction: SPME-HS  
Calibration: PFTBA  
Instrument type: quad  
Chromatography type: GC



Model: Nicolet 6700  
Spectral resolution: 4 cm<sup>-1</sup>  
Sampling method: ATR, diamond single bounce  
Make and model of accessory: OMNIC Smart Orbit  
Number of scans co-added: 32  
Method and software used in data processing: OMNIC 7.3



Spectral Method: DART-TOF  
Data reduction: averaged and background subtracted  
Software method function switching  
Scan range 58-661  
Sample introduction: wanding  
O1 Voltage: 30  
[Spectrum] Gas type: He  
[Spectrum] Gas flow: 2.5  
[Spectrum] DART Temp: 275°C



Explore



Database



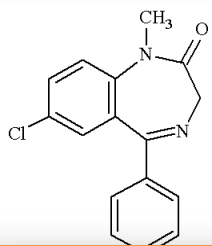
Search Records



Search Clear Forms

Main Search Form

# Database Search Capabilities



Multiple Database Search: ☐

Current Database Search: ☒

Record Note:

Formula (example: C10 Cl(1-10) F(0) N):

Exact: ☐

Formula Weight (example: 120.3 or 20..50):

Structure Search:

Structure Search

Spectrum Search

Spectrum Similarity Search

Spectrum Similarity

Spectrum Parameters

User Data

Metadata

- Spectrum: MS Similarity
- Spectrum: StructureSource
- Spectrum: Original File Name
- Spectrum: [Spectrum] Spectral Method
- Spectrum: [Spectrum] Data reduction method
- Spectrum: [Spectrum] Software method used for
- Spectrum: [Spectrum] Scan range used for data
- Spectrum: [Spectrum] Sample introduction
- Spectrum: [Spectrum] Mass calibration method
- Spectrum: [Spectrum] Compound mixture
- Spectrum: [Spectrum] O1 Voltage
- Spectrum: [Spectrum] Gas type
- Spectrum: [Spectrum] Gas flow
- Spectrum: [Spectrum] DART Temp
- Spectrum: Mass Calibration
- Spectrum: Data Reduction Method
- Spectrum: Software For Data Collection
- Spectrum: Spectral Method
- Spectrum: Scan Range
- Spectrum: Instrument type
- Spectrum: Chromatography type
- Spectrum: Tune type
- Spectrum: Instrument manufacturer
- Spectrum: Mass Measurement
- Spectrum: Ionization Mode
- Spectrum: [Spectrum] Mixture components
- Spectrum: [Spectrum] Notes
- Spectrum: [Spectrum] Ionization Mode
- Spectrum: [Spectrum] Mass Measurement
- Spectrum: [Spectrum] Compound /Mixture

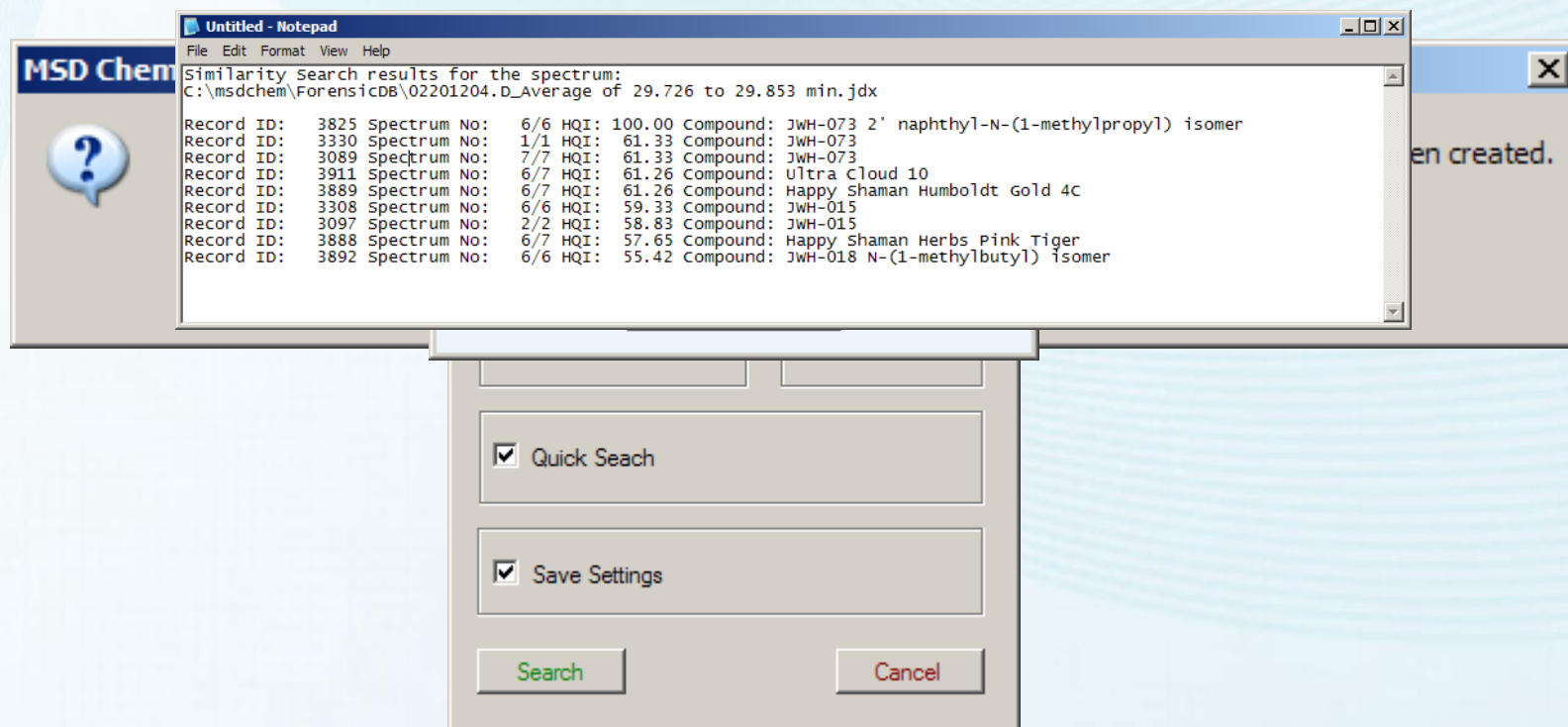


1D NMR Peaks

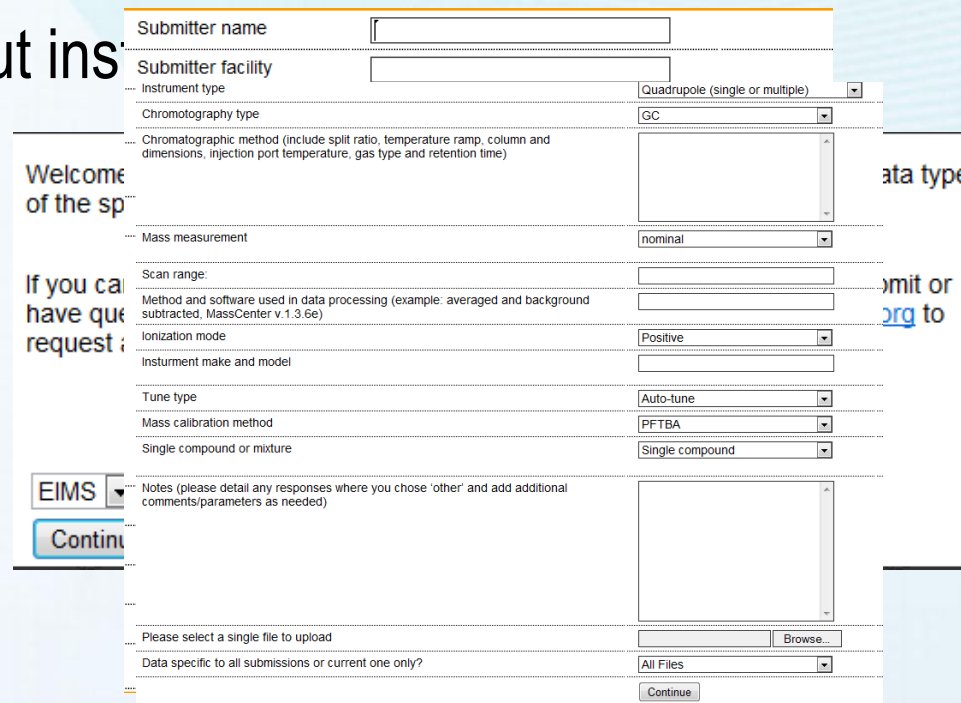
2D NMR Peaks



- Developed macros and applications for Agilent Chemstation
- Downloadable from database homepage
- Allows creation of a JACAMP
- Search ForensicDB directly from Agilent Chemstation



- Developed a Web-portal
- Allows the community to submit spectral data
- Includes submission for EI-MS, DART-TOF, FTIR and other spectral methods
- Users fill out record information
- Users fill out ins



The screenshot shows a web form for submitting spectral data. The form includes the following fields and sections:

- Submitter name:** Text input field.
- Submitter facility:** Text input field.
- Instrument type:** Dropdown menu with "Quadrupole (single or multiple)" selected.
- Chromatography type:** Dropdown menu with "GC" selected.
- Chromatographic method (include split ratio, temperature ramp, column and dimensions, injection port temperature, gas type and retention time):** Text area.
- Mass measurement:** Dropdown menu with "nominal" selected.
- Scan range:** Text input field.
- Method and software used in data processing (example: averaged and background subtracted, MassCenter v.1.3.6e):** Text input field.
- Ionization mode:** Dropdown menu with "Positive" selected.
- Instrument make and model:** Text input field.
- Tune type:** Dropdown menu with "Auto-tune" selected.
- Mass calibration method:** Dropdown menu with "PFTBA" selected.
- Single compound or mixture:** Dropdown menu with "Single compound" selected.
- EIMS:** A button labeled "EIMS" with a dropdown arrow.
- Notes (please detail any responses where you chose 'other' and add additional comments/parameters as needed):** Text area.
- Continue:** A blue button labeled "Continue".
- Please select a single file to upload:** A text input field with a "Browse..." button.
- Data specific to all submissions or current one only?:** Dropdown menu with "All Files" selected.
- Continue:** A button labeled "Continue".

On the left side of the form, there is a sidebar with the following text:

- Welcome of the sp
- If you can have que request

On the right side of the form, there is a sidebar with the following text:

- ata type
- Submit or org to

- NIST Chemistry WebBook
- Wiley Registry of Mass Spectral Data
- Mass Spectra of Designer Drugs
- MS and GC data of Drugs Poisons, Pesticides, Pollutants, and Their Metabolites
- Wiley Registry of Tandem MS Data
- NIST/EPA/NIH Mass Spectral Library
- Instrumental Data for Drug Analysis



## THANK YOU AND CONTACT INFO



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[pstout@rti.org](mailto:pstout@rti.org)