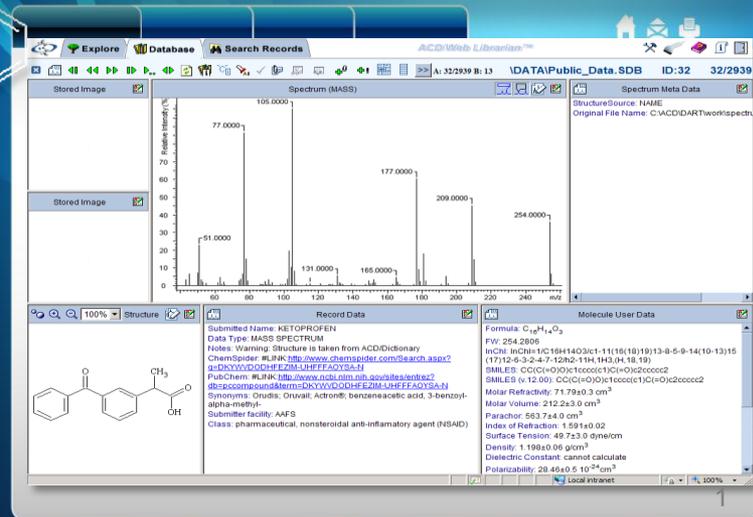
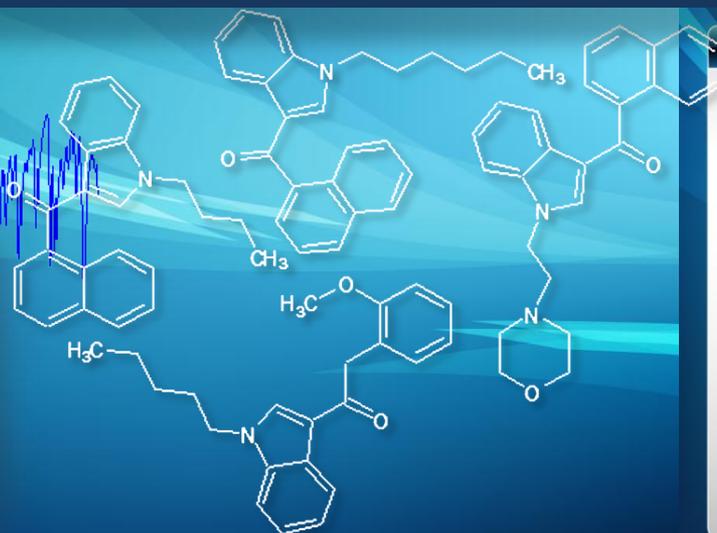
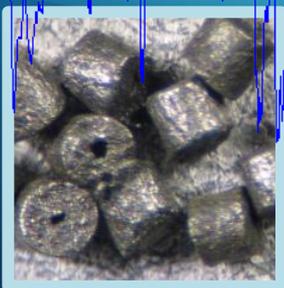


Demo of Online Database Resources for the Identification of Novel and Emerging Drugs

Peter R. Stout, PhD







CAUTION:
THIS PRESENTATION
MENTIONS
COMMERCIAL
NAMES

Outline

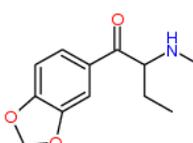
- Overview of existing databases and resources

- 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: C₁₂ H₁₅ NO₃

Nominal mass: 221

Average mass: 221.2524³

Monoisotopic mass: 221.105193

CAS registry number: 11762-90-2

ChemSpider: [21106270](#)

PubChem: [56843046](#)

Wikipedia: [Bk-MBDB](#)

Erowid: [bk-MBDB](#)

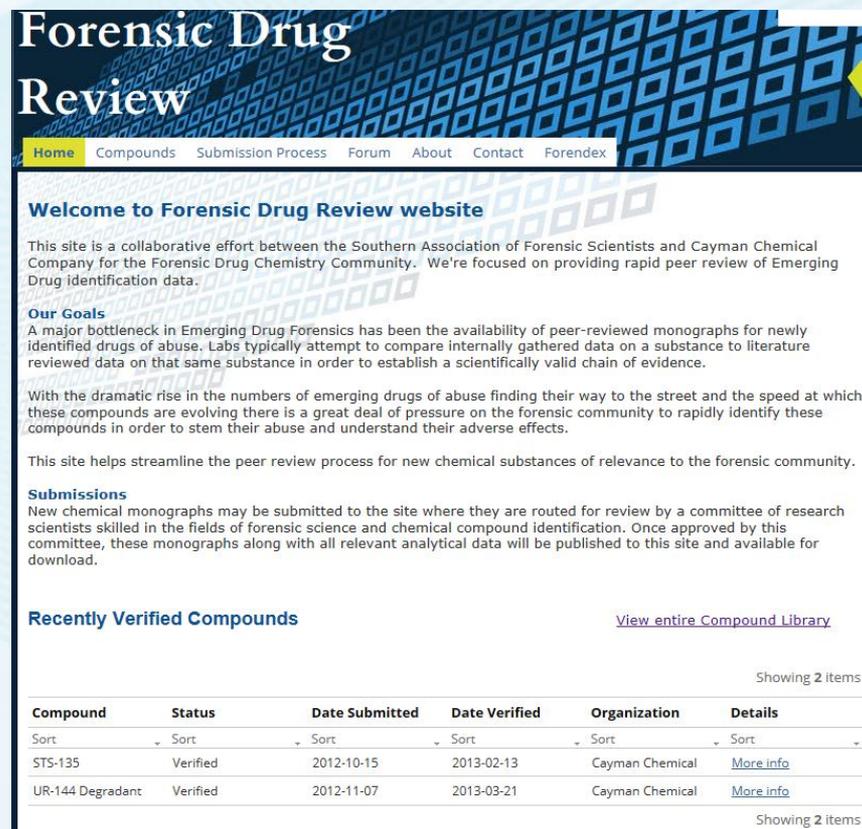
Standard InChI: InChI=1S/C12H15NO3/c1-3-9(13-2)12(14)8-4-5-10-11(6-8)16-7-15-10/h4-6,9,13H,3,7H2,1-2H3

Standard InChIKey: CGKQZIULZRXRJ-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.

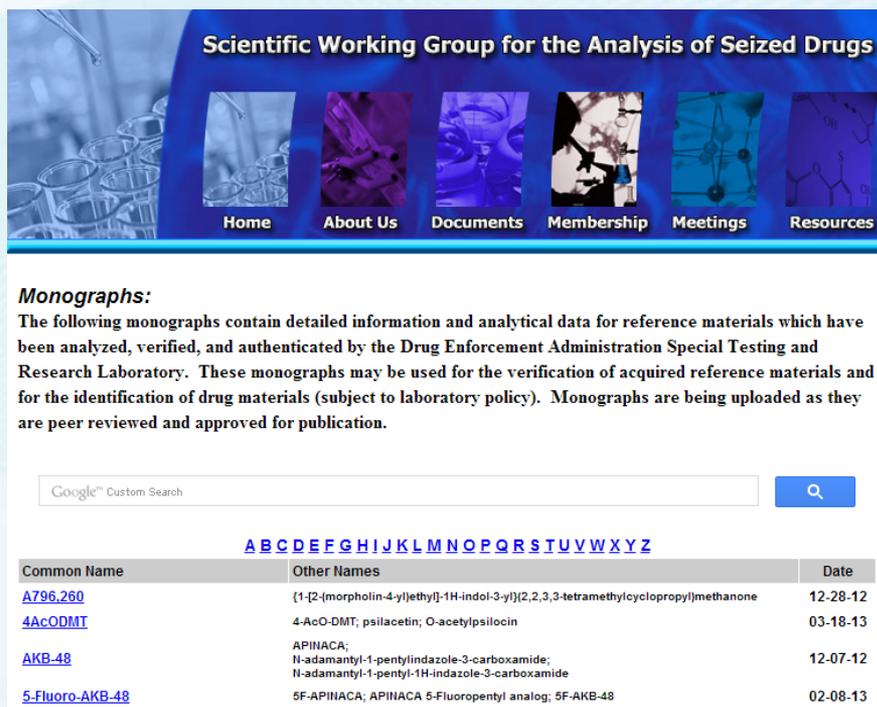
Recently Verified Compounds [View entire Compound Library](#)

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	More info
UR-144 Degradant	Verified	2012-11-07	2013-03-21	Cayman Chemical	More info

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

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

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

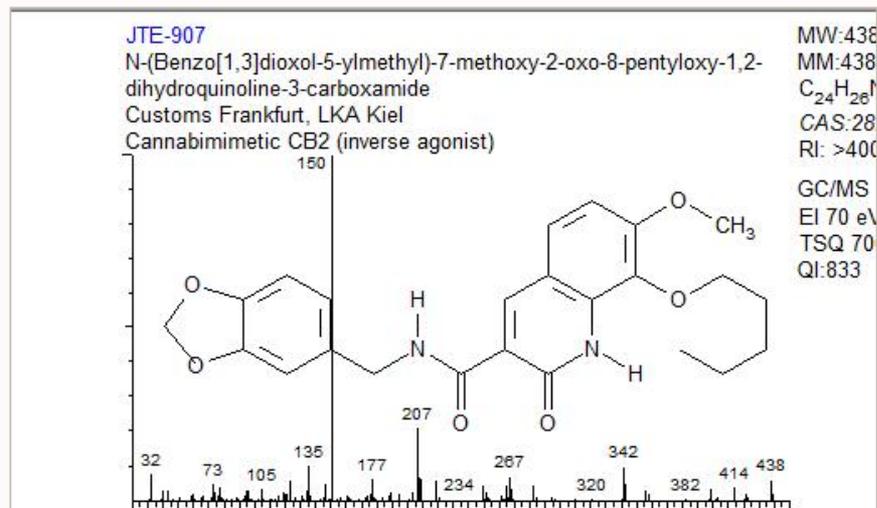
- EI-MS data freely downloadable in Agilent ChemStation or other platform as requested
- Over 2,800 spectra of pure compounds, metabolites and breakdown products
- Includes replicate spectra
- Spectra verified against independent library

- 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: C₂₄H₂₆N₂O₆

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



[About](#) [Research](#) [Policy](#) [Resources](#) [Partners](#) [Contact](#)

DESIGNER DRUGS
THE TRENDS REPORT

Emerging Drug Spotlight,
Synthetic Cannabinoid XLR-11 

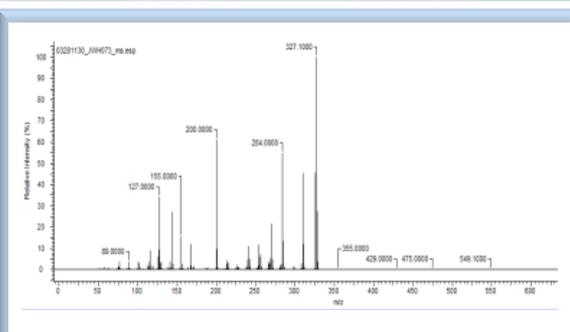
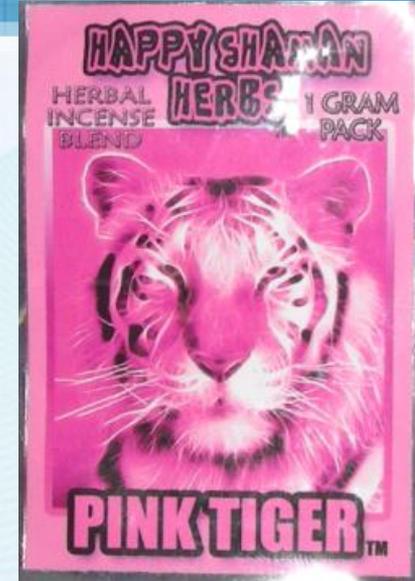
About Designer Drug Trends online...

The mission of Designer Drug Trends is to provide a comprehensive resource in the incredibly dynamic and quickly growing designer/synthetic drug market. We are funded and managed by NMS Labs and much of the information has been compiled by legislative and regulatory specialists at Gordon Thomas Honeywell - GA, but the purpose of the site is to provide public and private industry members, specialized scientists and researchers, and the general public a single and authoritative source on the rapidly evolving designer drug epidemic. Never before have so many reliable and comprehensive resources been pulled together for the purpose of providing a holistic look at designer drug problem. We invite everyone to tour the site, which includes resources for everyone from parents to scientists!

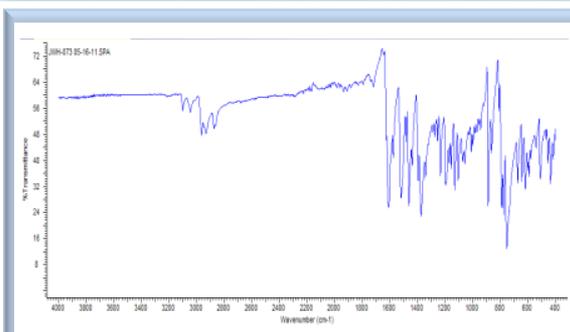
- Free, Web-accessible and searchable database
- Over 3,200 records that include one or more instrumental techniques
 - FTIR, EI-MS, DART-TOF, and ESI-QTOF spectra from various contributors
- Replicate spectra
- Peer review process
- Frequent updates
- Download single records as JACAMP files

Complete Record

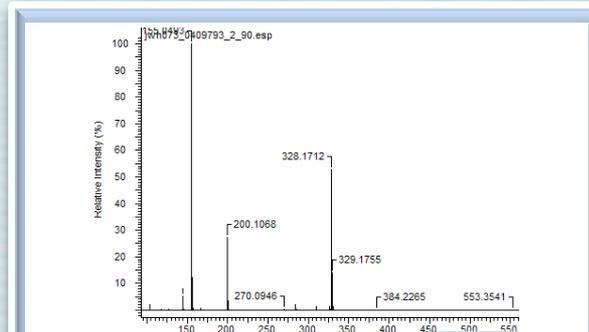
RECORD



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⁻¹
 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

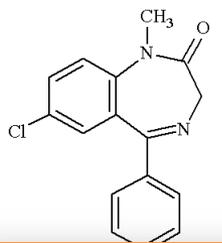


Spectral Method: DART-TOF
 Data reduction: averaged and background subtracted
 Software method function switching
 Scan range 58-661
 Sample introduction: wandung
 O1 Voltage: 30
 [Spectrum] Gas type: He
 [Spectrum] Gas flow: 2.5
 [Spectrum] DART Temp: 275°C



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: Similarity

Structure Search

Spectrum Search

Spectrum Similarity Search

Spectrum Similarity

Spectrum Parameters

User Data

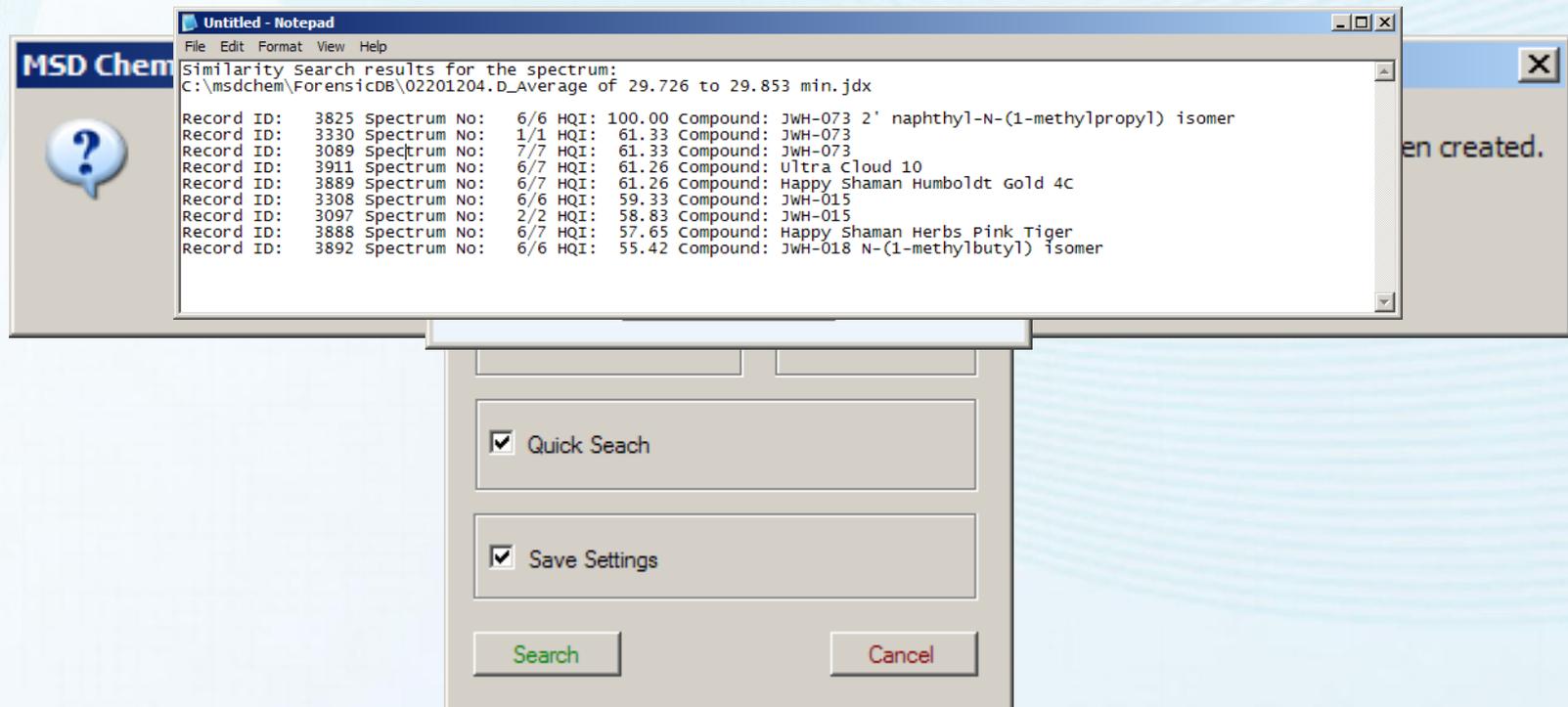
Includes

Metadata

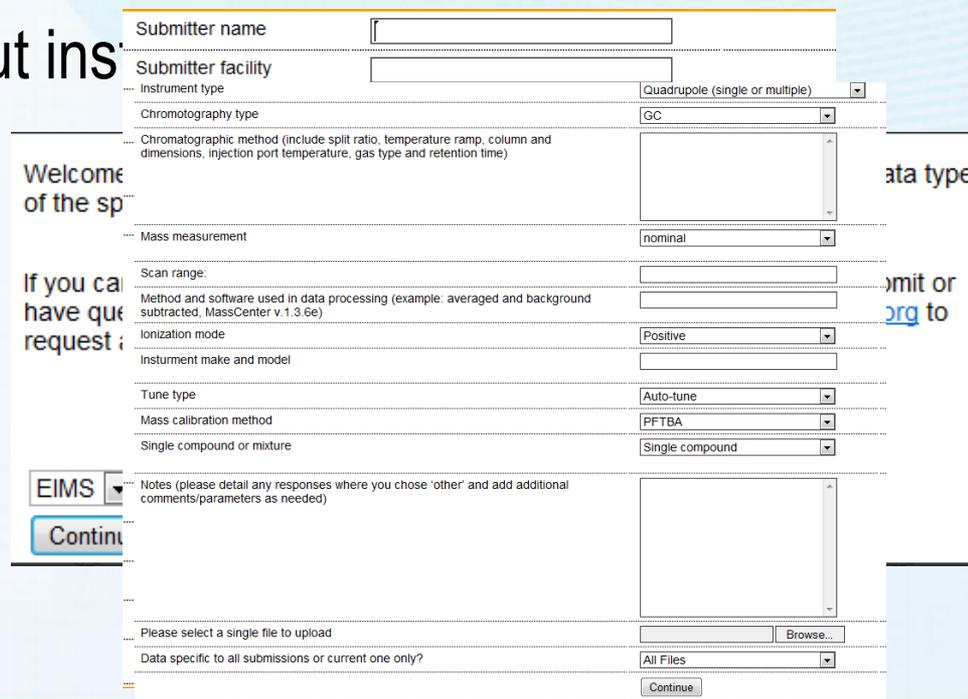
- Spectrum: MS Similarity
- Spectrum: StructureSource
- Spectrum: Original File Name
- Spectrum: [Spectrum] Spectral Method
- Spectrum: [Spectrum] Data reduction method
- Spectrum: [Spectrum] Software method used for
- Spectrum: [Spectrum] Scan range used for data
- Spectrum: [Spectrum] Sample introduction
- 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



- 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 options:

- Submitter name:
- Submitter facility:
- Instrument type:
- Chromatography type:
- Chromatographic method (include split ratio, temperature ramp, column and dimensions, injection port temperature, gas type and retention time):
- Mass measurement:
- Scan range:
- Method and software used in data processing (example: averaged and background subtracted, MassCenter v.1.3.6e):
- Ionization mode:
- Instrument make and model:
- Tune type:
- Mass calibration method:
- Single compound or mixture:
- Notes (please detail any responses where you chose 'other' and add additional comments/parameters as needed):
- File upload:
- Data specific to all submissions or current one only?:
-

On the left side of the form, there is a dropdown menu for "EIMS" and a "Continue" button. On the right side, there is a "Data type" label and a "Submit or org to" label.

- 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

forensicDB@rti.org

pstout@rti.org