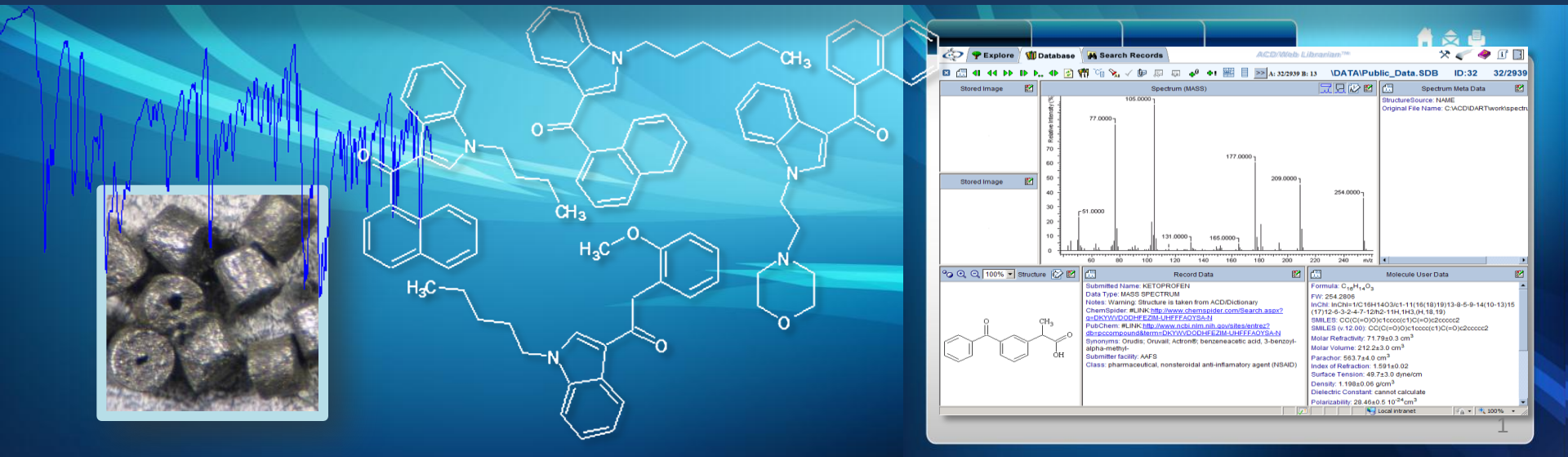
Demo of Online Database Resources for the Identification of Novel and Emerging Drugs

Peter R. Stout, PhD



Forensic Technology Center of Excellence

Commercial Disclaimer

Overview

Outline

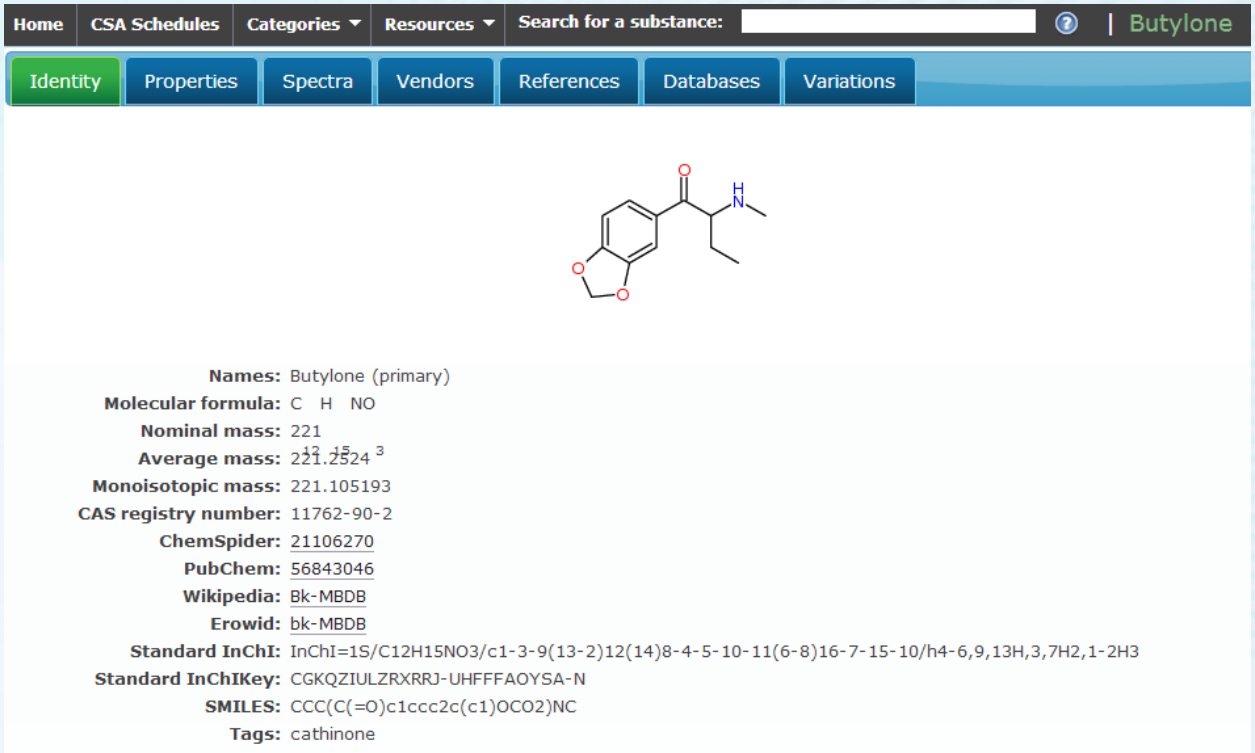
- Overview of existing databases and resources

Cayman Chemical Library

- 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

Forendex

- 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

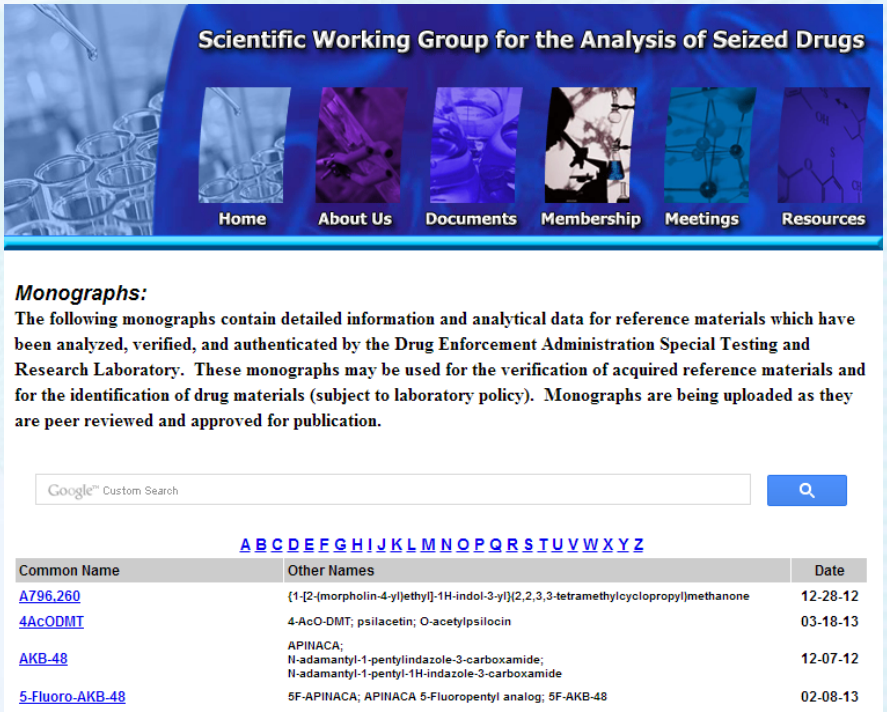


Forensic Drug Review

- 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

SWGDRUG Mass Spectral Library and Drug Monographs

- 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

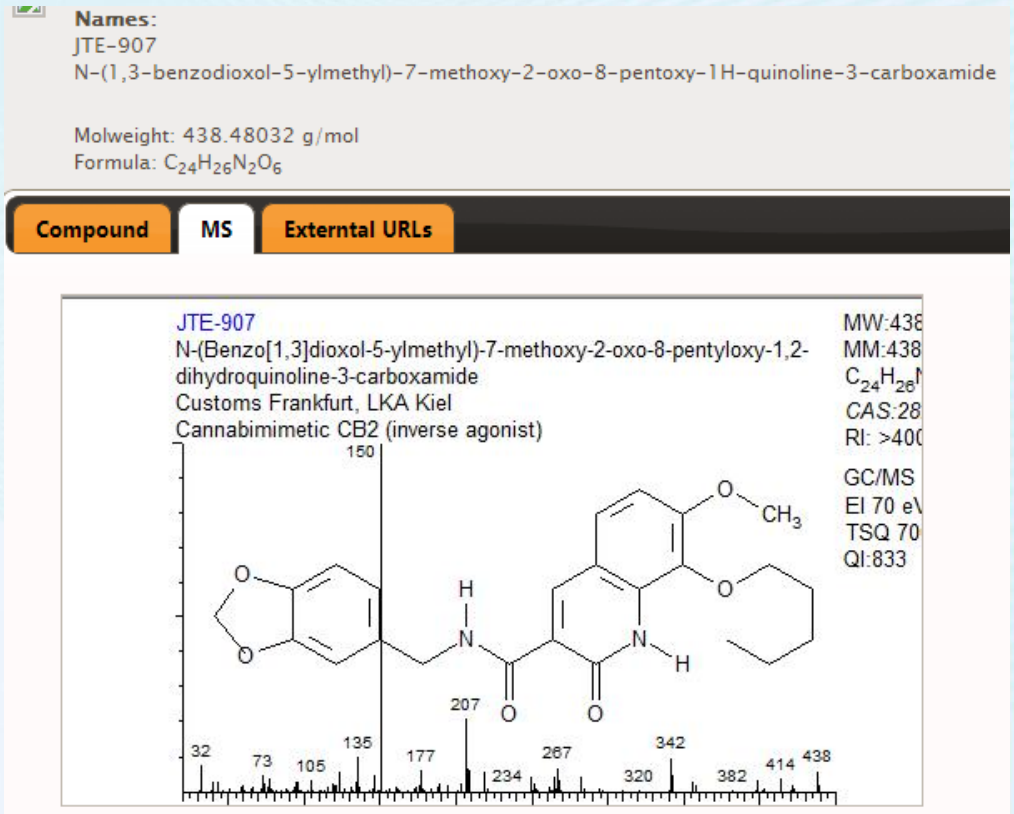


AAFS Mass Spectral Library

- 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

Designer Drugs Online 2012

- 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



Designer Drug Trends

- 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

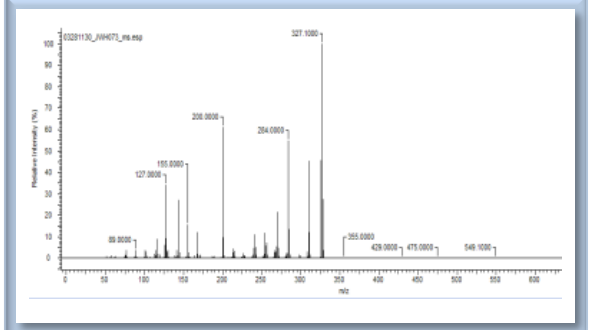
ForensicDB

- 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

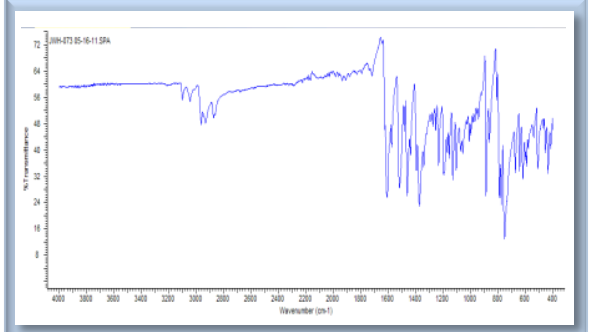
ForensicDB: Database Structure

Complete Record

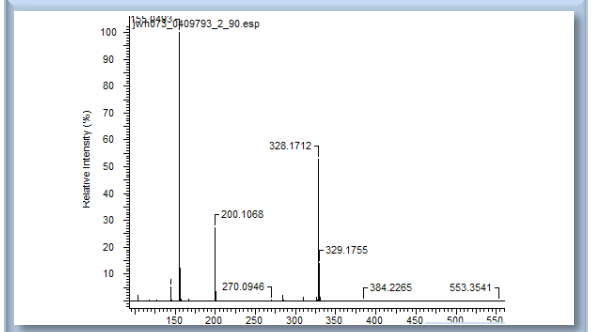
RECORD



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: 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

Database Search Capabilities

Main Search Form

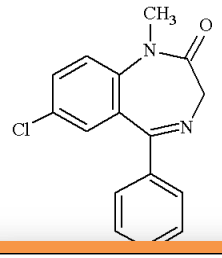
Multiple Database Search: ○ Current Database Search: ●

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

Spectru

560 m/z

Set

Spectrum Similarity

Spectrum Parameters

User Data

Includes DART

Metadata

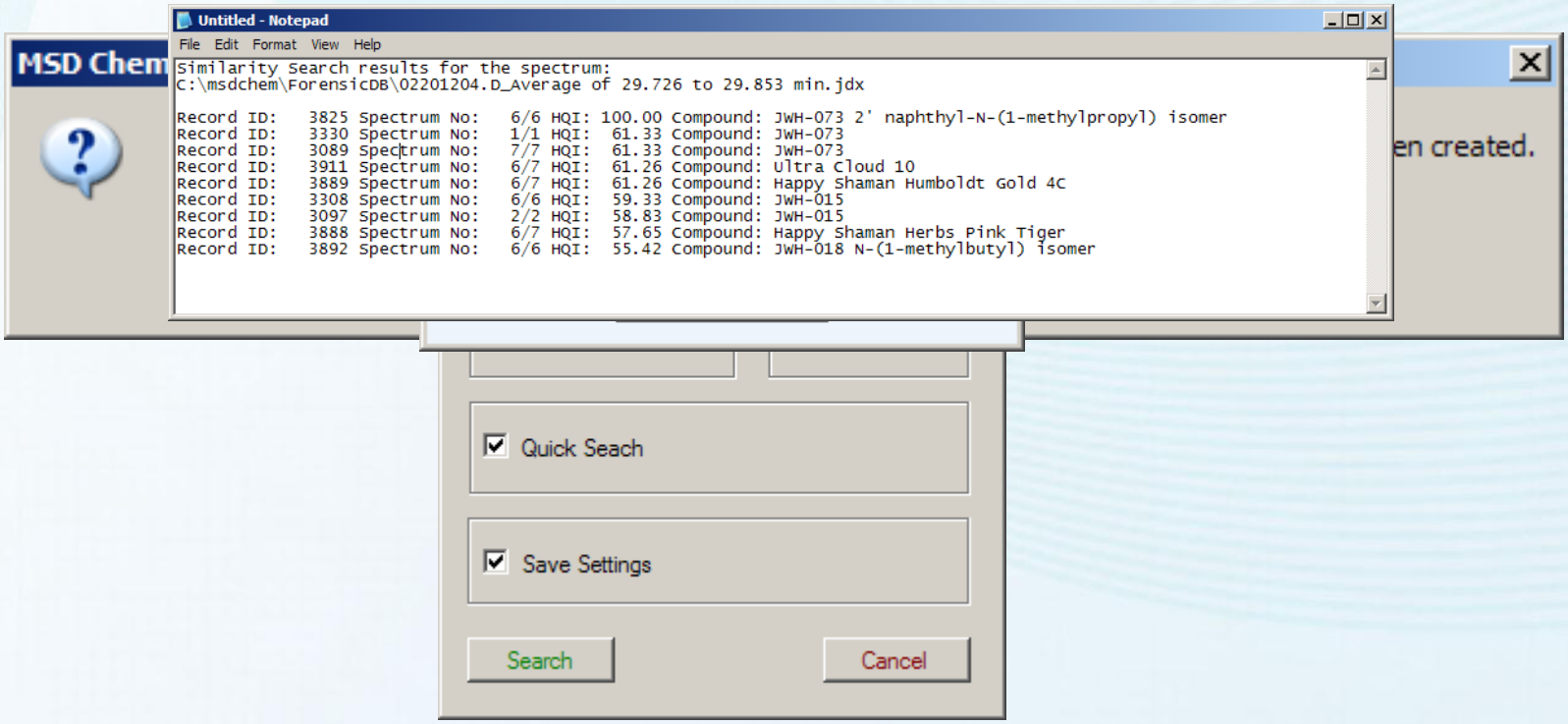
- Spectrum: MS Similarity
- Spectrum: StructureSource
- Spectrum: Original File Name
- Spectrum: [Spectrum] Spectral Method
- Spectrum: [Spectrum] Data reduction method
- Spectrum: [Spectrum] Software method used for
- Spectrum: [Spectrum] Scan range used for data
- Spectrum: [Spectrum] Sample introduction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

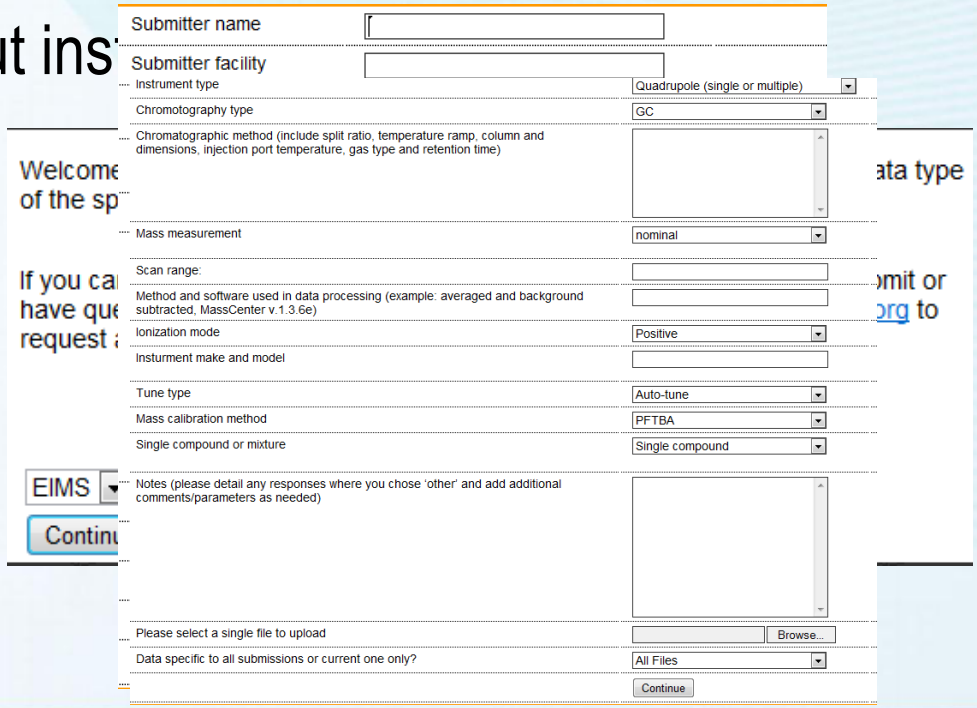
ForensicDB: Agilent ChemStation

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



ForensicDB: Web-portal

- 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



Other Database Resources

- 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

RTI INTERNATIONAL

Cheminformatics Database

www.forensicdb.org