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Results and Status of an Ongoing Forensic Cheminformatic, Spectral Database

Final Report

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RTI INTERNATIONAL

Abstract

Cheminformatic databases are used for the searching of unknown spectra and the retrieval of chemical data. Many existing commercial and private databases incorporate common mass spectral techniques, such as electron ionization.

The project's original goal was to create a database of spectral information for AccuTOF™-DART® (JEOL USA Inc., Peabody, Massachusetts; IonSense, Inc., Saugus, MA) data. The objectives were to establish standards for data acquisition; maximize data exchange capabilities; determine software needs and develop the foundation of a unified database applicable to multiple disciplines; and begin populating the database with multiple collaboratively collected spectra. Due to a variety of changes and occurrences, the scope of the project was modified with the National Institute of Justice's (NIJ's) approval. This change of scope provided an opportunity to expand the original concept into a cheminformatic database containing spectral data.

Ultimately, the project's purpose was to develop a no-cost, community-driven, peer-reviewed, Web-accessible database of multiple spectral technologies. The intention was to include electron ionization, time-of flight-direct analysis real time (DART-TOF), Fourier transform infrared spectroscopy (FTIR) spectra, and potentially other platforms and configurations relevant to forensic laboratories. Completion of the project involved three phases. The first phase involved determining database organization, management, and capabilities. The second phase was to populate the database with spectra, including existing and newly investigated gas chromatography/ mass spectrometry (GC/MS) spectra. The third phase involved evaluating database efficiency, with a specific interest in the effects of collecting DART-TOF spectra at different instrumental parameters submitted from multiple laboratories.

A stable implementation of the database and Web access utilities has been achieved, and active promotion to the community of users is currently underway. The database includes 2,922 total records representing approximately 5,427 spectra. These records were contributed by the Virginia Department of Forensic Science (VDFS), RTI International[1] (RTI), and the electron ionization (EI)-GC/MS database of the Toxicology Section of the American Academy of Forensic Sciences (AAFS library; Committee Chair–Dr. Graham Jones). The types of instrumental data represented are accurate mass, nominal mass, FTIR, and chromatographic data. Types of compounds submitted to ForensicDB include JWH cannabimimetic compounds; herbal Spice products; drug standards; pharmaceutical preparations; thin layer chromatography (TLC)-separated pharmaceutical preparations; chemical compounds; nylon fibers; and smokeless powders.

This project has resulted in an expanded database tool benefitting a much wider range of forensic chemistry and toxicology. The database now provides a publically available platform with minimal use requirements of the end user for the searching and use of spectral records. The project has provided a means of maintaining and expanding the availability of the widely used AAFS EI-GC-MS database. The project also has provided the flexibility to address data needs for emerging compounds, as well as other forensic chemistry analyses such as photoacoustic FTIR and smokeless powder analyses. To our knowledge, this is a unique database, providing Web-accessible searching of a database of reviewed spectra and inclusion of spectra from multiple spectral methods in one database. The availability of multiple spectral methods in the same database can inform searches for a particular forensic discipline that uses multiple tools for a case investigation, including newer technologies such as DART-TOF. The database is centrally hosted and provided through Web-accessibility, allowing users to access data

[1] RTI International is a trade name of Research Triangle Institute.

collected from new and emerging drugs without having to wait for or routinely purchase a new software update.

The fundamental framework of the database is established and functioning reliably, and community members are contributing spectra and acting as reviewers. The forensic community's use of this database has consistently increased during the project period.

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List of Acronyms

AAFS	American Academy of Forensic Sciences
ATR	attenuated total reflectance
CID	collision-induced dissociation
COTS	commercial off-the-shelf
DART	Direct Analysis in Real Time
DEA	Drug Enforcement Agency
EI	electron ionization
EPA	U.S. Environmental Protection Agency
ESI	electrospray ionization
ESR	electron spin resonance
FTIR	Fourier transform infrared spectroscopy
GC	gas chromatography
GHB	Gamma-Hydroxybutyrate
MDEA	3,4-methylenedioxy-N-ethylamphetamine
MDMA	3,4-methylenedioxy-N-methamphetamine
MS	mass spectrometry
MS/MS	tandem mass spectrometry
NIH	National Institutes of Health
NIJ	National Institute of Justice
NIST 08	NIST/EPA/NIH Mass Spectral Library
NIST	National Institute of Standards and Technology
NMR	nuclear magnetic resonance
PAS	photoacoustic
PCI	positive chemical ionization
QTOF	quadrupole time-of-flight
RTI	RTI International
SI	similarity indexes
SIM	single ion monitoring
SOFT	Society of Forensic Toxicologists
SQL	Structured Query Language
TLC	thin layer chromatography
TOF	time of flight
VDFS	Virginia Department of Forensic Science

Executive Summary

This ForensicDB cheminformatic database project is similar to other types of spectral databases, such as the Integrated Spectral Database System for Organic Compounds (SDBS); the National Institute of Standards and Technology/U.S. Environmental Protection Agency/National Institutes of Health (NIST/EPA/NIH) Mass Spectral Library (NIST 08); the Southern Association of Forensic Scientists database (Forendex); PubChem; and ChemSpider; however, ForensicDB includes direct analysis in real time-time of flight (DART-TOF) spectra. ForensicDB parallels NIST 08 by requesting information on instrumental parameters used for collection to help standardize data submission. It differs from NIST 08 in that it is a free, Web-accessible spectral database with searchable mass and FTIR spectra. All of the data in the data base are freely searchable by chemical structure (or partial structures), metadata, and physicochemical data in the records.

Compared to ChemSpider and SDBS, ForensicDB allows direct electronic comparison of known and unknown spectra contributed by the public. Similar to ChemSpider, ForensicDB is equipped with ACD/Labs software that calculates compound information based on the submitted structure. Additionally, while, NIST 08, ChemSpider, and SDBS are widely available tools for all types of chemists, they are specifically designed for forensic chemists and toxicologists interested in unique chemicals or presentations of chemicals. As a result, NIST 08, ChemSpider, SDBS, and other databases such as PubChem are useful tools to the forensic chemist, but often do not provide data specialized for forensic applications. Forendex provides specialized data, but does not allow users to search by an uploaded spectrum.

A comparison of the available databases and their functionality is shown in **Table ES-1**.

Table ES-1. Comparison of Databases

	ForensicDB	Forendex	NIST 08	SDBS	ChemSpider	PubChem
Web accessible	Y	Y		Y	Y	Y
Community driven	Y	Y			Y	
Physicochemical properties	Y				Y	
Electronic spectrum search	Y		Y			
Electronic structure search	Y		Y		Y	Y
Multiple instrumental methods	Y	Y	Y	Y		
Instrumental parameters	Y	●	Y	●		

● Limited

Research Purpose

The ForensicDB project's purpose was to develop a no-cost (to the end user), community-driven, peer-reviewed, and Web-accessible database. The intention was to include electron ionization (EI), DART, and FTIR spectra and, potentially, other platforms and configurations relevant to forensic laboratories. The advent of DART into the forensic and scientific community increases the need to integrate this instrumental method into a reviewable, reliable, and centrally located database. Integration of several spectral methods aids in the interpretation of DART spectra to determine the identity of the source material. A database that houses several instrumental techniques is advantageous because there is greater

certainty of accurate identification if the same compound has a high spectral similarity for several methods.

DART technology has the potential to contribute to analyses in forensic applications, such as postmortem, court-directed, and workplace drug testing; controlled substances; trace evidence; and identification of unknown substances. The ability to analyze these data and to interpret the resulting spectra is a crucial component in realizing the potential of this technology. By providing a tool for the interpretation of DART-TOF data, this work will enhance the utility of the AccuTOF™-DART® (JEOL USA Inc., Peabody, Massachusetts; IonSense, Inc., Saugus, MA) instrument, thereby facilitating the implementation of rapid and simple drug-screening methods for forensic toxicology and other forensic analyses. The database and the framework for the inclusion of data will likely influence the use of the data in forensic applications, as well as the forensic acceptability of DART-TOF test results. The growing population of DART-TOF users likely will find such a database an essential tool for using the instrument. Continued addition of data and maintenance of the database requires that this be an ongoing program.

Research Design and Methods

While this project originally set out to produce a database of DART-TOF spectra, for various reasons, the project's scope expanded and changed with National Institute of Justice's (NIJ's) final approval. The result has been a much more broadly applicable and unique database and library of multiple spectral data on compounds of forensic interest, as well as a new platform capable of housing searchable data from multiple spectral data platforms.

Although this report is a final report for the current funding, it also serves as current status report for the database program, as it is an ongoing project that continues to grow and evolve both in its scope, its users, and its technologies.

The Project as Originally Proposed

Many investigators realize the need for a database containing DART-TOF spectra and, as a result, there has been independent development of databases of standards against which to compare sample spectra. These databases have varying degrees of functionality, and currently, none allow for the matching of unknown spectra against a library of known spectra—either for the identification of compounds within the unknown spectra (such as the identification of metabolites of cocaine in a blood specimen), or for the identification of a mixture of substances (such as the identification of an unknown white powder as flour or cocaine). The process of standardizing a set of DART-TOF data collection parameters and subsequently compiling a database of drug spectra run under these conditions would allow DART-TOF systems to become extremely useful in a forensic setting.

The original goal of this project was to create a database of spectral information for AccuTOF-DART data. The objectives were to establish standards for data acquisition; maximize data exchange capabilities; determine software needs and develop the foundation of a unified database applicable to multiple disciplines; and begin populating the database with multiple collaboratively collected spectra. This project was intended to be a collaborative effort, with RTI International (RTI) serving as the primary contributor working with the FBI Laboratory, Virginia Department of Forensic Sciences (VDFS), Ames Laboratory, and Aberdeen Proving Ground as collaborators, and xk Inc. (Clackamas, Oregon) as the software developer. This project covered a range of DART-TOF applications and contributions. The software development originally intended to capitalize on the commercial off-the-shelf platform, which was developed by xk, Inc., in cooperation with the FBI for analyzing XRF/XRD data. In initial tests, it appeared that DART-TOF data collected using the Mass Center software by JEOL (Tokyo, Japan) could be easily incorporated with little modification of the existing software. Hence, this was the software originally proposed for this project.

The Project as Implemented

In the first year of the project, multiple changes occurred, which caused RTI to modify its scope of the project and the budget. JEOL and IonSense (Saugus, Massachusetts) reached an agreement and began marketing the DART source to be available on mass spectrometer platforms other than the JEOL AccuTOF. JEOL is the manufacturer of the AccuTOF instrument, and IonSense, Inc. is the manufacturer of the DART. At the time of the proposal, the JEOL TOF was the only MS instrument that could be used with the DART due to contracted negotiations among manufacturers. Under a new agreement finalized after RTI's proposal submission, the DART can now be used on any other type of mass spectral unit by any other manufacturer (e.g., an Agilent TOF or an AB Sciex QTRAP™). While there are not yet a significant number of DART units, for the future usefulness of the database, RTI wanted to design a database that could accommodate data from other MS platforms and from multiple software sources. This change created a cost-prohibitive amount of potential development to modify existing off the shelf software to accomplish multiple platform configurations and would have required end users of ForensicDB to purchase software to use the database.

In addition, JEOL was resistant to alterations of Mass Center software to support database functions. As mentioned, a desired goal of the ForensicDB project was to create a resource that did not require end users to buy software to use the database. Another manufacturer, ACD/Labs (Toronto, Canada) was able to offer a suite of commercial off-the-shelf (COTS) software (ACD/Labs SpecDB), which provided a mechanism for accepting data from many platforms. ACD/Labs also offered a COTS product known as WebLibrarian, which allows a Web-based portal for end users to access the database for searches without any software requirements beyond Internet access and Internet Explorer 6.0 or higher. The backbone of ForensicDB runs out of an Oracle environment. These features provided many advantages to the database concept.

The ACD/Labs software also allowed for expansion of the project from the original concept of containing only accurate mass data from the AccuTOF-DART. This software enhancement would allow for inclusion of more traditional mass spectral technologies in forensic applications, including nominal mass EI-GC-MS spectra; optical spectrometry data such as FTIR; and chromatograms and images. Inclusion of these items in the database significantly improves its utility to drug chemistry, toxicology, and forensic chemistry applications. Thus, the software change broadens the usefulness of the database beyond just DART users while providing complimentary spectral data to better inform DART-TOF searches.

Several changes in partnership also occurred in the early stages of the project. VDFS remains as a partner in the project; however, Aberdeen Proving Ground (Edgewood Chemical and Biological Center) had significant funding changes, and the FBI Laboratory experienced staffing changes and restructuring of the chemistry unit, causing both partners to withdraw from the project. In addition, Ames Laboratory was unable to obtain a controlled substance license, which prohibited them from participating in collection of most spectra of interest.

The unforeseen need to modify the scope of the original project proved a substantial benefit because it provided a means of expanding the original database concept. ForensicDB is now a broadly applicable forensic cheminformatic database containing multiple spectral data types. Several benefits of the expanded project include the following:

1. The AAFS EI-GC-MS drug database has been hosted and maintained by Dr. Graham Jones at the Alberta Office of the Chief Medical Examiner; Dr. Jones is also the Chair of the MS database committee in the Toxicology Section of AAFS. After many years of curating this collection, Dr. Jones desired a mechanism by which the AAFS EI-GC-MS database could remain viable. Including these data in ForensicDB gives the data a more permanent location and provides a means of maintaining and expanding the availability of the widely used AAFS MS database. This

change in hosting will also provide a means of better tracking the use of the AAFS data. In its current hosting, there is no mechanism to track how often data are downloaded.

2. To our knowledge, ForensicDB is a unique database because it provides the ability to search a given spectrum against a Web-accessible database of reviewed spectra and have spectra from multiple spectral methods available in the same database. In addition, ForensicDB provides an accessible resource to forensic laboratories of all sizes, both large, well-funded laboratories that can use this as a supplement to local libraries (such as NIST and Wiley databases), as well as smaller laboratories that cannot afford to continually update their libraries and are very dependent on no-cost libraries, such as the AAFS library.
3. ForensicDB is of significant utility to toxicology, drug chemistry, trace chemical analyses, and any other disciplines using chemical identification. This is a substantially larger group of potential users than just DART-TOF users. In addition, DART-TOF users benefit from the additional information, making DART-TOF a more useful technology.
4. The availability of multiple spectral methods in the same database can inform searches for DART-TOF data, making DART-TOF a more viable tool.
5. This centrally hosted architecture provides for greater flexibility in the future to accommodate growing data needs and to provide access to the most up-to-date information. Also, because ForensicDB is Web-accessible, users can access data collected from new and emerging drugs without having to wait for or purchase a new software download.

Database Structure

Key contributors to the construction, management, and survival of the database include curators, collaborators, reviewers, and the community. **Figure ES-1** shows a schematic of the database structure. Management of ForensicDB is similar to a peer-reviewed journal, in that the curator acts as the editor and the collaborators act as the associate editors. The curator (RTI) is responsible for creating and maintaining the database and Web server and providing the tools necessary to access and update the database. Collaborators are essential in working with the curator to develop the intention, design, and need of the database. They are also influential in assisting the curator with creating requirements for standardization of spectral submission and criteria for evaluating spectra. Collaborators also are responsible for processing the spectral data into an appropriate format for inclusion in the public database. Reviewers evaluate each submitted spectrum according to established evaluation criteria. The community acts as the driving force of ForensicDB, strengthening the database by contributing their spectral data. The survival of ForensicDB is dependent upon the public's continued use, participation, and comments on database improvement, as well as on the public utilizing the database as part of their analytical scheme of analysis.

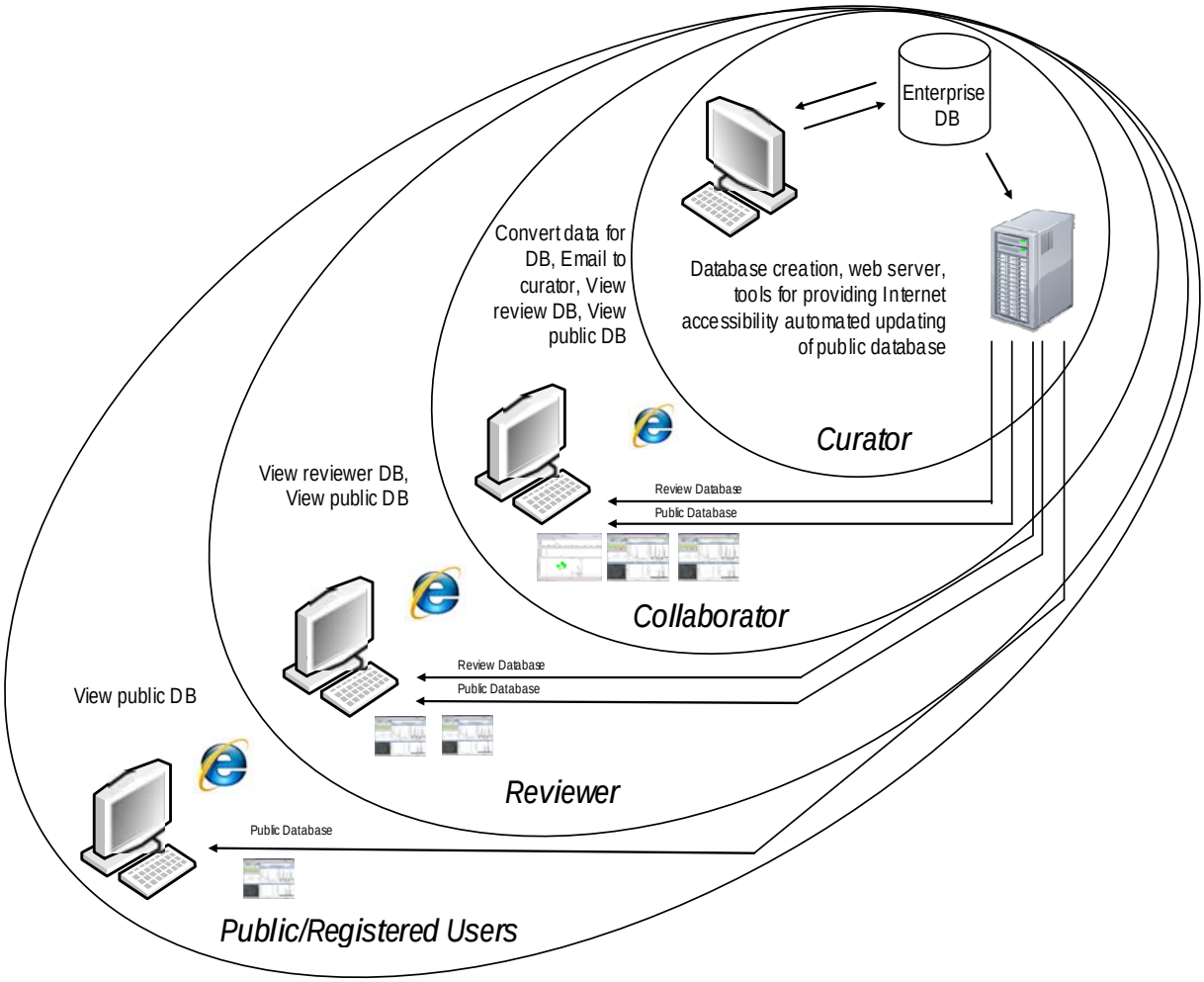

Figure ES-1. Database structure and functionality.

Database Organization

Organization of ForensicDB is based on chemical structure—the only truly unambiguous means of referring to any given compound. **Figure ES-2** illustrates the organization of ForensicDB. A record indicates a specific compound structure and name, analyzed by a particular institution from a specific source material. Thus, multiple records may exist for a specific compound, reflecting a change in the major record features.

Each record may contain multiple documents that indicate spectral method and instrumental parameters. Some of the general requirements for all submissions are spectral method, instrument type, scan range, and data reduction method. Other parameters are requested based on the instrumental technique, such as spectral resolution and number of scans co-added for FTIR data. Specific requirements for DART spectra include gas heater temperature, gas-flow rate, type of sample introduction, and orifice 1 voltage.

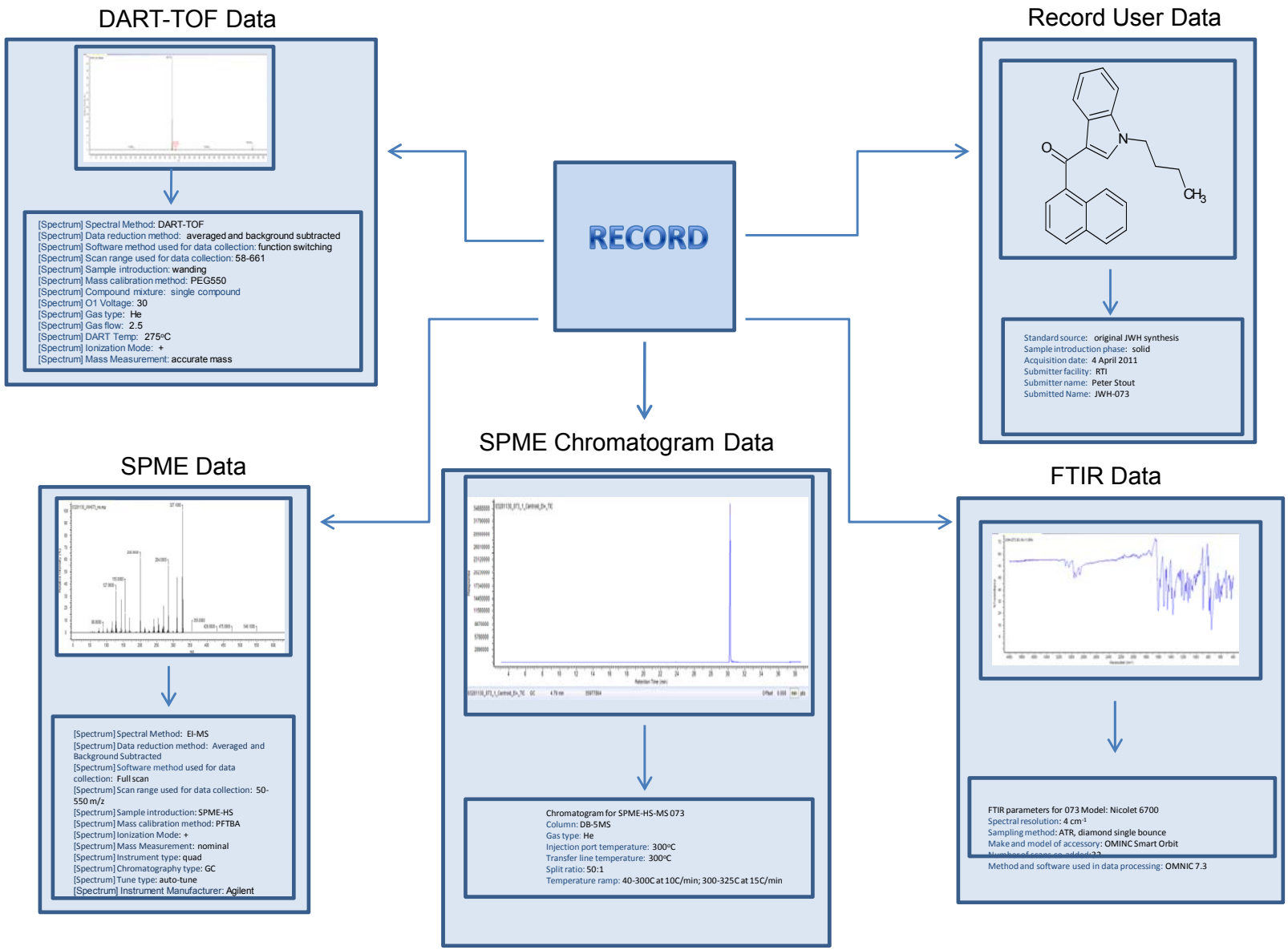

Figure ES-2. Database organization.

Within each record, there is one structure, but in some cases, there may be a structure on each document within a record. This would occur when analyzing a mixture such as the herbal Spice materials. A chromatogram of the Spice material is a document without a structure, but the mass spectrum of an isolated compound within the mixture (e.g., active JWH compound) contains the corresponding structure within the document. The ACD/Labs software calculates physicochemical properties of the structure, which are then housed within a record. Such properties include pKa, monoisotopic mass, and protonated exact mass.

We have tried to standardize the submission of record and document information; however, we were unable to collect the required information of the AAFS spectra because these are historic records. Our intention is to supplement these data with more complete records over time.

Findings (Current Status of Database)

ForensicDB currently includes 2,922 total records representing approximately 5,427 spectra. These records were contributed by VDFS, RTI, and the AAFS Toxicology Section through the EI-GC-MS database (AAFS library). The types of instrumental data represented are accurate mass, nominal mass, FTIR, and chromatographic data. The types of compounds submitted to ForensicDB include JWH cannabimimetic compounds; herbal Spice products; drug standards; pharmaceutical preparations; thin layer chromatography (TLC)–separated pharmaceutical preparations; chemical compounds; nylon fibers; and smokeless powders.

Table ES-2 shows the number of spectra submitted per instrumental method.. The public database includes 2,127 EI-MS spectra submitted by Dr. Graham Jones (AAFS) and VDFS. There are 825 AccuTOF-DART records representing 3,300 spectra submitted by RTI and VDFS. The DART spectra collected at both institutions were analyzed under the same instrumental parameters, and each compound record collected using DART contains a document at 20 V, 30 V, 60 V, and 90 V orifice 1 voltages to illustrate characteristic fragmentation patterns. RTI submitted 28 spectra of JWH compounds collected using electrospray ionization quadrupole time-of-flight (ESI-QTOF).

Table ES-2. Number of Spectra Submitted Per Instrumental Method

Data Type	Documents	Submitter
ForensicDB		
EI-MS	2,077	Graham Jones
	50	VDFS
AccuTOF-DART	2,916	VDFS
	384	RTI
ESI-QTOF	28	RTI
Process and Review Phase		
Chromatography	190	VDFS
	26	RTI
FTIR	81	RTI
	75	Ames
AccuTOF-DART	1,400	RTI
SPME-HS-MS	26	RTI

There are currently 1,798 spectra that are at various points in the processing and review stage. Among these are 95 records of smokeless powder data submitted by VDFS. Each smokeless powder record

includes a document for attenuated total reflectance (ATR)-FTIR, EI-GC/MS, and positive chemical ionization (PCI) GC/MS chromatogram; multi-voltage AccuTOF-DART spectra (20 V, 30 V, 60 V, 90 V); and a picture showing morphological characteristics. There are 26 records of Spice material collected using headspace solid-phase microextraction (HS-SPME-GC-MS). Each Spice material record includes a chromatogram labeled with the identified JWH compound present in the Spice mixture and the corresponding mass spectrum from the chromatogram appended to the record. There are also four AccuTOF-DART spectra included for each Spice material record, as well as the front and back package label and a picture of the Spice material. There are 308 DART records (1,232 spectra) of JWH compounds and 42 DART records (168 spectra) of drug standards from RTI in the processing and review phase. The large collection of data on Spice and JWH compounds is one demonstration of the advantage of having a continually updated library. Rather than having to buy an updated library, new compounds are added to this database and data are available for users as they are added.

Ames Laboratory plans to submit spectra of 75 single nylon fibers collected using photoacoustic (PAS)-FTIR. Before collecting data, the laboratory conducted a preliminary study to determine optimal collection parameters. The resolution was 4 cm^{-1}, and the scanning speed was 2.5 kHz. Ames Laboratory has been collecting and evaluating data while writing in-house software that enables multidimensional library searches and automates search optimization.

Conclusions

The original goal of this project was to create a database of spectral information for AccuTOF-DART data. The objectives were to establish standards for data acquisition; maximize data exchange capabilities; determine software needs and develop the foundation of a unified database applicable to multiple disciplines; and begin populating the database with multiple collaboratively collected spectra. Due to a variety of changes and occurrences, the project scope was modified. This provided an opportunity to expand the original concept into a cheminformatic database containing spectral data.

The result has been an expanded database tool with benefits to a much wider range of forensic chemistry and toxicology. The database now provides a publically available platform with minimal use requirements of the end user for the searching and use of spectral records. The project also has provided a means of maintaining and expanding the availability of the widely used AAFS EI-GC-MS database.

In addition, the project provided the flexibility to address data needs for emerging compounds, other forensic chemistry analyses such as photoacoustic FTIR and smokeless powder analyses. To the best of our knowledge, ForensicDB is a unique database in that it provides the ability to search a given spectrum against a Web-accessible database of reviewed spectra and have spectra from multiple spectral methods available in the same database. The availability of multiple spectral methods in the same database can inform searches for DART-TOF data, making DART-TOF a more viable tool. Also, because the database is centrally hosted and provided through Web-accessibility, it allows users to access data collected from new and emerging drugs without having to wait for or purchase a new software update.

The fundamental framework of the database has been established and is functioning reliably. The forensic user community is steadily increasing around this cheminformatic tool, and community members are interested in sharing spectra and contributing as reviewers.

1. Introduction

1.1 Statement of the Problem

Spectral and cheminformatic databases are provided through both private and commercial organizations. Many private databases are small and incorporate compounds specific to the owning company or organization. An example of a private database is the American Academy of Forensic Science (AAFS) Integrated Spectral Database System for Organic Compounds (SDBS) (AAFS, 2010). Although commercial databases contain more compounds, they can be expensive, and often include software designed to be uploaded on a single computer (Nip and Kuehl, 2000). When these commercial databases are not updated as newer downloads become available and different institute computers use have different software versions, users may not have the most reliable data and may not know they are using outdated information (Nip and Kuehl, 2000).

Electron ionization mass spectrometry (EI-MS) is a common analytical technique used in controlled substances and toxicology. Many private and commercial databases incorporate EI-MS spectra and are used as part of the analysis process. An advantage of these databases is that EI-MS collection parameters have been standardized to 70 eV. Several spectral databases allow for searching compounds and spectra, and these databases include a variety of compounds, are interactive, and incorporate advanced features that aid in compound identification.

Some of these databases include the SDBS, ChemSpider, and the National Institute of Standards and Technology/U.S. Environmental Protection Agency/National Institutes of Health (NIST/EPA/NIH) Mass Spectral Library (NIST 08). The SDBS is a free online database managed by the National Institute of Advanced Industrial Science and Technology (SDBS, 2011). It contains spectra from six instrumental techniques, including EI-MS, Fourier transform infrared spectroscopy (FTIR), 1H and 13C nuclear magnetic resonance (NMR), laser Raman, and electron spin resonance (ESR)(SDBS, 2011). Data on the SDBS are searched by compound name, molecular weight, formula, ion peaks, and NMR shifts (SDBS, 2011). The SDBS does not allow for direct comparison of a known and unknown spectrum and assumes that the sample has already been identified. Not all of these instrumental techniques are routinely used in forensic science.

ChemSpider is a free online chemistry search engine—maintained by the Royal Society of Chemistry—that includes chemical information on a variety compounds (Royal Society of Chemistry, 2011). Registered users with curator and depositor access contribute spectra and compound information and are able to remove or post comments about inaccurate information (Royal Society of Chemistry, 2010). ChemSpider provides several resources for the scientific community when searching for a compound, as well as provides references for a compound's pharmacology, chemical analysis, and calculated properties provided by Advanced Chemistry Development Labs (ACD/Labs Ontario, Canada) (Royal Society of Chemistry, 2007; 2011). Calculated properties include molar volume, surface tension, boiling point, and LogP. ChemSpider is useful for finding information when the compound is known, but it does not allow for electronic spectral comparison.

NIST/EPA/NIH developed the commercial Mass Spectral Library NIST 08 in 2008 (NIST Mass Spectrometry Data Center, 2008). The software is not Web-accessible and its cost can be significant. Purchasing the new NIST 11 Standard Version would cost the end user $2,295, and to upgrade to NIST 11 Standard Version from an older version would cost $1,295 (Scientific Instrument Services Inc., 2011). Due to the price, the database may not be readily accessible to small and/or private laboratories. The NIST 08 version contains EI and tandem mass spectrometry (MS/MS) spectra. Reference spectra retrieved from this search include collection parameters such as instrument type, inlet, and instrument

model (NIST Mass Spectrometry Data Center, 2008). These parameters help the user determine reasons for spectral variability if a reference match is not found. This commercial package allows for direct comparison of a known and unknown spectrum; however, as new compounds are synthesized and become available in the illicit market, users must wait to purchase an updated database version.

All three databases discussed provide useful information to the scientific community. Much of the data are of EI-GC-MS spectra, which does not help with interpretation of newer analytical techniques. Direct analysis in real time (DART) has emerged as a useful screening tool in forensic analysis (Steiner and Larson, 2009). Dr. Robert Cody, a co-inventor of DART, created the SearchFromList software as part of purchasing a DART source. DART users create lists and spectra within SearchFromList for searching (Steiner, 2008); however, the degree of peer-review is unknown, and the incorporated spectra are not centrally located for shared laboratory use.

Currently, there is no centrally located and actively reviewed public database for DART-TOF spectra. Laboratories such as the Virginia Department of Forensic Science (VDFS) have developed their own in-house controlled substances library to search against unknown samples; however, this library is not readily accessible by the public and may not be applicable to other forensic disciplines. Development of a unified database of DART spectra is vital for the expansion of DART into routine forensic analyses. RTI has initiated the development of a standardized and centrally located database of multiple spectral methodologies. The intention is to include nominal mass (EI-MS), accurate mass (DART-TOF), and FTIR spectra.

This cheminformatic database project, known as ForensicDB, is similar to SDBS, NIST 08, and ChemSpider, and the Southern Association of Forensic Scientists database (Forendex), but includes DART-TOF spectra. ForensicDB parallels NIST 08 by requesting information on instrumental parameters used for collection to help standardize data submission. It differs from NIST 08 in that it is a free, Web-accessible spectral database with searchable mass and FTIR spectra, as well as searchable structure and other physicochemical data on compounds in records. Compared to ChemSpider and SDBS, ForensicDB allows direct electronic comparison of known and unknown spectra contributed by the public. Similar to ChemSpider, ForensicDB is equipped with ACD/Labs software that calculates compound information based on the submitted structure. Additionally, while, NIST 08, ChemSpider, and SDBS are widely available tools for chemists, they are efforts designed for chemists of all types, not necessarily forensic chemists and toxicologists interested in unique chemicals or presentations of chemicals. NIST 08, ChemSpider, and SDBS, as well as other databases such as PubChem, are useful tools to the forensic chemist, but often do not provide data specialized for forensic applications. Forendex provides specialized data, but does not allow users to search based on an uploaded spectrum.

The forensic utility of current spectral databases vary due to the existence of relevant compounds and spectral methods, data quality, accessibility, and the ability to search against reference spectra. Forensic applications of these databases routinely contain spectra from traditional instrumentation, such as EI-GC/MS and do not allow for cross searching of other spectral methods. The advent of DART into the forensic and scientific community increases the need to integrate this instrumental method into a reviewable, reliable, and centrally located database. Integration of several spectral methods aids in the interpretation of DART-TOF spectra to determine the identity of the source material. A database that houses several instrumental techniques is advantageous because there is greater certainty of accurate identification if the same compound has a high spectral similarity for several methods (Kornakova et al., 2005).

A comparison of available databases and their functionality is shown in **Table 1**.

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Instrumental parameters	Y	●	Y	●		

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While this project originally set out to produce a database of DART-TOF spectra, for various reasons, this objective had to change. The result for the project has been a much more broadly applicable and unique database and library of multiple spectral data on compounds of forensic interest, as well as a new platform capable of housing searchable data from multiple current and potential future spectral data platforms.

Although this report is a final report for the current funding, it also serves as a current status report of the database, which is an ongoing project that continues to grow and evolve both in its scope and in its technologies.

1.2 Literature Review

In discussions with DART-TOF users, it was apparent that there were a variety of issues to address. Currently, mass spectral databases, such as those available from NIST and the Society of Forensic Toxicologists (SOFT), are limited to spectra from EI instruments, typically from quadrupole mass spectrometers. EI spectral databases are integral parts of the analytical scheme, allowing for fast computer searching of, in most cases, reliable data. Many of these databases are currently available, both commercially (NIST and Wiley) and privately (AAFS Toxicology Section drug spectral library). The advantage of these data is that most instruments that use these databases are run under similar ionization and calibration conditions. Although such databases contain spectra representing a large number of compounds and can be essential tools for toxicologists and chemists, the spectra in the databases have limited utility in interpreting DART-TOF data. DART ionization produces charged forms of the compounds in a sample and provides a high-resolution, accurate mass determination for each form (Cody, 2005). When DART ionization occurs, fragmentation of molecules does not occur in the same way as it

does with EI. DART-TOF data collection is currently a matter of operator choice when it comes to determining the conditions needed for operation. Variability occurs due to the chemical properties of the analyte, and different operators may choose different ionization parameters based on their knowledge, experience, or available equipment.

RTI previously worked on evaluating the application of DART-TOF to screening postmortem toxicology samples as part of a previous NIJ grant project (2006-DN-BX-K014). We have evaluated the detection of 112 compounds and metabolites common to postmortem toxicology analyses (Mindenet al., 2007). We also have been evaluating the detection of these compounds in urine (Stout et al., 2007) and in blood and tissues (Stout et al., 2008). As part of another grant project with NIJ (2006-DN-BX-K019, Analysis of Cocaine Analytes in Human Hair: Evaluation of Concentration Ratios in Different Hair Types, Cocaine Sources, Drug User Populations, and Surface Contaminated Specimens), RTI analyzed 25 illicit cocaine samples by AccuTOF-DART and compared the results with conventional cocaine signature analysis conducted by the Drug Enforcement Agency (DEA) (Ropero-Miller et al., 2008). A variety of applications of DART-TOF have been explored by multiple investigators.

Ames Laboratory, in association with Iowa State University, has been investigating the utility of DART-TOF for forensic analysis of ink samples using a revolutionary mass spectrometry method (NIJ Grant No. 2006-DN-BX-K017, Principal Investigator: Dr. John McClelland). This project is applying DART-TOF mass spectrometry to the analysis of ink on questioned documents. DART-TOF MS analysis neither requires removal of samples from the document nor destroys the document, so it preserves the evidence. The mass spectra can be obtained in only a few minutes and contain substantial detail that is highly characteristic of individual inks. The main goal of the project has been to develop a comprehensive, vetted, computer-searchable library of mass spectra of ink samples that forensic investigators can use to identify the make and model of pen used to produce the writing being examined.

In 2003, Aberdeen Proving Ground (including Edgewood Chemical Biological Center [ECBC]; Principal Investigators: Dr. James Laramee and Dr. H. Dupont Durst) began developing an accurate, sensitive, and easy-to-use detection system that reliably analyzes a wide range of toxic substances. This system exploits the nucleophilic nature of nerve agents to attract protons. The project thrust has been to focus on V-series agents and agents recalcitrant to antidote. Aberdeen Proving Ground has unique experience and access to chemical agents and explosives.

The Commonwealth of Virginia, Department of Forensic Science (Principle Investigator, Mr. Robert Steiner), has been assessing the applicability of DART-TOF to controlled substance evidence. Analytical protocols for the forensic analysis of controlled substances have recently changed dramatically to provide added integrity to the results. These changes have typically involved performing additional examinations of multiple case specimens. This translates into an added time component for completing the analysis for any one case. An example of an application in which DART-TOF would provide fast results is confirmation of active ingredients in pharmaceutical preparations after initial physical identification from tablet markings. Another is screening of multiple specimens with little to no sample preparation, especially liquids that normally require extraction steps. The DART-TOF system has the potential to reduce considerably the amount of time spent per specimen in the analytical scheme, thereby increasing the laboratory throughput and reducing backlogs.

Since early 2005, DART-TOF has been used at the FBI Laboratory in Quantico, VA (Principle Investigator, Marc LeBeau) for several applications (McClelland et al., 2007; Jones et al., 2008). The FBI laboratory has the distinction of having the first production unit of the DART source. The FBI has investigated the use of DART-TOF to rapidly and quantitatively analyze Gamma-Hydroxybutyrate (GHB) in urine. They have also investigated automated sampling technologies to improve sample throughput and the quality of sample introduction. This has been necessary for attempts at quantitative

analysis. A challenge that the FBI is commonly presented with is the identification of an unknown material and determination of any threat the material may pose. Additionally, the FBI is often presented with product tampering cases in which DART-TOF again promises unique strengths. In many toxicological investigations, the suspected source of the poison may be received in addition to biological specimens such as blood or urine. Often, the most direct route to toxicant identification is primary analysis of suspect source material. However, analysis of seized food, beverage, and other commercial products is typically time consuming and laborious. A DART-TOF instrument offers the forensic examiner a tool for rapidly identifying such adulterations in bulk samples.

JEOL (Tokyo, Japan) developed the first generation of software to identify mass spectral peaks in unknown spectra based on their theoretical monoisotopic mass. Although this software has proven to be useful, it has limitations because some compounds do not produce spectra that are consistent with the theoretical monoisotopic mass. They have extended this functionality to include forward and reverse matching against a library of acquired spectra, but this still has limited database capabilities. Furthermore, the software can only match one adduct formation possibility at a time, requiring users to perform multiple steps to complete database processing. These limitations highlight the need for a database that would allow searches based on theoretical exact mass and on actual spectra obtained from multiple instruments by many users. DART-TOF has been used in multiple forensic fields for analyzing and identifying many materials; however, its full utility will not be realized until a unified database of its spectra is available. At this time, a unique opportunity exists to develop the framework for such a database because DART-TOF is a very new technology with limited development of user preferences and a small core of users with established communications.

1.3 Objectives of the Research

1.3.1 The Project as Originally Proposed

Many investigators have realized the need for a database containing DART-TOF spectra and independently began developing databases of standards against which to compare sample spectra. These databases have varying degrees of functionality, and currently, none allow for the matching of unknown spectra against a library of known spectra, either for the identification of compounds within the unknown spectra (such as the identification of metabolites of cocaine in a blood specimen) or for the identification of a mixture of substances (such as the identification of an unknown white powder as flour or cocaine). The process of standardizing a set of DART-TOF data collection parameters and subsequently compiling a database of drug spectra run under these conditions would allow DART-TOF systems to become extremely useful in a forensic setting. The original goal of this project was to create a database of spectral information for AccuTOF-DART data. The objectives were to establish standards for data acquisition; maximize data exchange capabilities; determine software needs and develop the foundation of a unified database applicable to multiple disciplines; and begin populating the database with multiple collaboratively collected spectra.

This project was intended to be a collaborative effort of RTI as the primary contributor with the FBI, VDFS, Ames Laboratory, and Aberdeen Proving Ground as collaborators, and with xk Inc. (Clackamas, Oregon) as the software developer. This covered a range of DART-TOF applications and contributions. The software development originally intended to capitalize on the commercial off-the-shelf product developed by xk Inc., in cooperation with the FBI, for analyzing XRF/XRD data. In initial tests, it had appeared that DART-TOF data collected using the Mass Center software by JEOL could be easily incorporated with little modification of the existing software; hence, this was the software originally proposed for this project.

1.3.2 The Project as Implemented

In the first year of the project, multiple changes occurred, causing RTI to modify its scope of the project and the budget. JEOL and IonSense (Saugus, Massachusetts) reached an agreement and began marketing the DART source to be available on MS platforms other than the JEOL AccuTOF. JEOL is the manufacturer of the AccuTOF instrument, and IonSense is the manufacturer of the DART. At the time of the proposal, the JEOL TOF was the only mass spectrometer instrument that the DART could be used with due to contracted negotiations among manufacturers. Under a new agreement, the DART can now be used on any other type of mass spectral unit by any other manufacturer (e.g., an Agilent TOF or an AB Sciex QTRAP^{TM}). While there are not yet a significant number of DART units, for the future usefulness of the database, RTI wanted to design a database that could accommodate data from other MS platforms and from multiple software sources. This change created a cost prohibitive amount of potential development to modify existing commercial off-the-shelf (COTS) software to accomplish this, and still would require that end users of the database purchase software to use the database.

In addition, JEOL was resistant to alterations of Mass Center software to support database functions. As mentioned, a desired goal of the ForensicDB project was to create a resource that did not require end users to buy software to use the database. Another manufacturer, ACD/Labs (Toronto, Canada) was able to offer a suite of COTS software (ACD/Labs SpecDB), which provided a mechanism for accepting data from many platforms. ACD/Labs also offered a COTS product known as WebLibrarian, which allows a Web-based portal for end users to access the database for searches without any software requirements beyond Internet access and Internet Explorer 6.0 or higher. The backbone of ForensicDB runs out of an Oracle environment. These features provided many advantages to the database concept.

The ACD/Labs software also allowed for expansion of the project from the original concept of containing only accurate mass data from AccuTOF-DART data. This software enhancement would allow for inclusion of more traditional mass spectral technologies in forensic applications, including nominal mass EI-GC-MS spectra along with optical spectrometry data such as FTIR data, and chromatograms and images. Inclusion of these items in the database significantly improves its utility to drug chemistry, toxicology and forensic chemistry applications. Thus, the software change broadens the usefulness of the database beyond just DART users while providing complementary spectral data to better inform DART-TOF searches.

Several changes in partnership also occurred in the early stages of the project. VDFS remains as a partner in the project; however, Aberdeen Proving Ground (Edgewood Chemical and Biological Center) had significant funding changes, and the FBI Laboratory experienced staffing changes and restructuring of the chemistry unit, causing both partners to withdraw from the project. In addition, Ames Laboratory was unable to obtain a controlled substance license, which prohibited them from participating in collection of most spectra of interest.

The unforeseen need to modify the scope of the original project proved a substantial benefit because it provided a means of expanding the original database concept. ForensicDB is now a broadly applicable forensic cheminformatic database containing multiple spectral data types. Several benefits of the expanded project include the following:

1. The AAFS EI-GC-MS drug database has been hosted and maintained by Dr. Graham Jones at the Alberta Office of the Chief Medical Examiner; Dr. Jones is also the Chair of the MS database committee in the Toxicology Section of AAFS. After many years of curating this collection, Dr. Jones desired a mechanism by which the AAFS EI-GC-MS database could remain viable. Including these data in ForensicDB gives the data a more permanent location and provides a means of maintaining and expanding the availability of the widely used AAFS MS database. This

change in hosting will also provide a means of better tracking the use of the AAFS data. In its current hosting, there is no mechanism to track how often data are downloaded.

2. To our knowledge, ForensicDB is a unique database because it provides the ability to search a given spectrum against a Web-accessible database of reviewed spectra and have spectra from multiple spectral methods available in the same database. In addition, ForensicDB provides an accessible resource to forensic laboratories of all sizes, both large, well-funded laboratories that can use this as a supplement to local libraries (such as NIST and Wiley databases), as well as smaller laboratories that cannot afford to continually update their libraries and are very dependent on no-cost libraries, such as the AAFS library.
3. ForensicDB is of significant utility to toxicology, drug chemistry, trace chemical analyses, and any other disciplines using chemical identification. This is a substantially larger group of potential users than just DART-TOF users. In addition, DART-TOF users benefit from the additional information, making DART-TOF a more useful technology.
4. The availability of multiple spectral methods in the same database can inform searches for DART-TOF data, making DART-TOF a more viable tool.
5. This centrally hosted architecture provides for greater flexibility in the future to accommodate growing data needs and to provide access to the most up-to-date information. Also, because ForensicDB is Web-accessible, users can access data collected from new and emerging drugs without having to wait for or purchase a new software download.

1.3.3 New and Emerging Drugs

After rescoping the project, growing concern about "legal high" drugs has highlighted the advantage of the new structure of ForensicDB to address the changing needs in the forensic chemistry community. Spice blends, such as Spice Gold, Spice Diamond, Spice Silver, K2, Skunk, and Smoke are marketed as incense and are being sold over the Internet and in local headshops to users who smoke the mixtures for their marijuana-like effects (Vardakou et al., 2010). While the packaging for these products list only natural herbs as ingredients (many of which are not actually present in the blends), chemical analysis has revealed that they contain synthetic cannabinoids. Most of these synthetic cannabinoids were originally synthesized by Dr. John Huffman at Clemson University for research concerning the cannabinoid receptor system. Many of the synthetic cannabinoids are structurally distinct from Δ^9-tetrahydrocannabinol (THC) and are still legal in some states. Hence, they provide an alternative to cannabis for people seeking to avoid potential judicial consequences of marijuana use or those wanting to become intoxicated and still pass a drug test, factors that also increase their attraction for adolescents and young adults. As knowledge of the intoxicating effects of Spice products has spread over the Internet, their use has been increasing to the point that they are now collectively considered a "drug of concern" by the U.S. Department of Justice National Drug Intelligence Center and Drug Enforcement Administration (2010). The limited availability of these compounds will limit the forensic community's ability to analyze these compounds. RTI is in a unique position to accomplish this task as the entire JWH series of compounds has been transferred to RTI.

A similar method of marketing synthetic stimulants has been in "bath salts" or "plant food" sold over the Internet and in local headshops under names such as White China, Vanilla Sky, Ivory Wave, Euphoria, and White Lightning. Again, the packaging for these materials do not list names of drugs they have been found to contain, such as mephedrone, 3,4-methylenedioxypyrovalerone, and methylone. Many of the same concerns about Spice and synthetic cannabinoids also apply to these drugs.

Even more recently, a synthetic "legal high" cocaine analog known as RTI-126 (2β-[1,2,4-Oxadiazol-5-methyl]-3β-phenyltropane) has been found and described (Casale and Hays, 2011). While it does not

appear that RTI-126 is widespread due to the challenging nature of its synthetic pathway, there are still several hundred related analog compounds in the investigational series.

According to testimony by Joseph T. Rannazzisi, Deputy Assistant Administrator of the Office of Diversion Control, Drug Enforcement Administration given at the Senate Caucus on International Narcotics Control on April 6, 2011, "Both synthetic cannabinoids and synthetic stimulants are 'designer drugs' that are manufactured and distributed in an attempt to circumvent the Controlled Substances Act. They are marketed in a manner so as to mask their intended purpose and are labeled with a statement that the package contents are 'not for human consumption,' or are 'for novelty use only.' The purpose of this statement is to circumvent the Controlled Substance Analogue Enforcement Act of 1986 (as amended), which states that controlled substance analogues shall, '*to the extent intended for human consumption*,' be treated as a controlled substance in Schedule I. 21 U.S.C. § 813 (emphasis added)" (http://www.justice.gov/dea/speeches/110412_testimony.pdf, accessed June 2011). Currently, there is significant concern in the forensic community about how to identify these compounds from both a drug chemistry perspective and from a forensic toxicology perspective. Suppliers are able to quickly change which drugs are added to the material, requiring law enforcement, forensic scientists, and medical personnel to adapt quickly as well.

All of these drugs have presented a significant challenge for identification in both forensic chemistry and in forensic toxicology. Likely, this is a trend to expect for the near future of clandestine chemists seeking compounds reported in the pharmaceutical literature that have a high binding affinity for a useful receptor (ones at which illicit drugs are agonists) with an easy synthetic pathway and are structurally outside of legal control. This is potentially tens of thousands of possible compounds. Data for the forensic community will be essential.

2. Project Methods Database Structure and Functionality

ForensicDB is a Web site composed of a collection of applications that allow public users to view cheminformatic data for a given spectrum and to search these data by providing various known parameters. To achieve its functionality, ForensicDB uses the unique features and functionality of three core software suites: Microsoft's ASP.net server, Oracle Enterprise, and ACD/Labs Web Librarian (Web Librarian).

The base software suite in use on ForensicDB is Microsoft's ASP.net server, which provides the platform for the ACD/Labs Web Librarian software suite and serves the basic HTML pages necessary for www.forensicDB.org to function, In additional, the platform opens a wide variety of objects to enhance functionality beyond standard HTML. The ASP suite was chosen because of its functionality and its compatibility with the ACD/Labs software.

The second software suite necessary to run ForensicDB is ACD/Labs COTS platform Web Librarian. The Web Librarian suite was substantially developed for such a purpose before the existence of ForensicDB and met the needs of this project without significant changes to the software code; however, it was extended to work with a publicly available Web site and database. Because of Web Librarian's legacy with Oracle and ASP.net, these extensions were natural and quickly accomplished.

The third software suite necessary to ForensicDB is Oracle Enterprise—a large and capable data storage platform made for applications that must store vast amounts of data. The enterprise version of Oracle Enterprise used in ForensicDB is known for performance when dealing with large result sets, and as such, it was a natural fit for a cheminformatics database.

These three suites have been designed to operate in two ways: (1) through a workflow process initiated by the end user and (2) through a maintenance process initiated by the database curators or contributors. The first process is initiated by the end user by visiting the Web site (www.forensicDB.org), which the user can locate through many outlets, such as a search engine, email notification, or promotional flyer. Next, the user must login to the Web site or create an account. This functionality is handled by the ASP.net platform. Once the user is logged in, he/she may select the database they want to search; the navigation to and selection of the database is handled by ACD/Labs Web Librarian. Then, the user can browse or search the database; this functionality is made possible by the interplay between Web Librarian and Oracle Enterprise. If the user chooses to browse the database, Web Librarian sends a command to Oracle Enterprise using Structured Query Language (SQL) to select all records. The search function is initiated through Web Librarian when the user chooses this option. Next, the user may select any number of parameters to search, such as by spectrum, molecular weight, or compound name. Web Librarian interprets the user-provided parameters and values and translates these into a SQL query statement to be run against the public database in Oracle Enterprise.

The second workflow process is a maintenance process initiated by ForensicDB curators or contributors (discussed in Section 2.1, *Database Management*). This process is intended to result in the addition of new records to the database or the revision of existing records. Tools for this process include SpecDB, a complimentary program for Web Librarian. Records may be submitted to curators by contributors through various means and in various formats. RTI will accept these records and begin a quality assurance process that involves verifying, cleaning, organizing, and testing the record before including it in the public database. The processing of such records is completed by RTI staff or voluntary contributors, and record quality is ensured by project directors.

2.1 Database Management

Key contributors to the construction, management, and survival of ForensicDB include the curator, collaborators, reviewers, and the community. **Figure 1** shows a schematic of the database structure. Management of ForensicDB is similar to a peer-reviewed journal in that the curator acts as the editor and the collaborators act as the associate editors. The curator (RTI) is responsible for creating and maintaining the database and Web server and providing the tools necessary to access and update the database. Collaborators work with the curator to develop the intention, design, and need of the database and are influential in assisting the curator with creating requirements for standardization of spectral submission and criteria for evaluating spectra. In addition, collaborators are responsible for processing the spectral data into an appropriate format for inclusion in the public database. The reviewers evaluate each submitted spectrum according to established evaluation criteria. The community acts as the driving force of this cheminformatic database, strengthening ForensicDB by contributing their spectral data. The survival of ForensicDB is dependent upon the public's continued use, participation, and comments on database improvement, as well as on public utilizing the database as part of their analytical scheme of analysis.

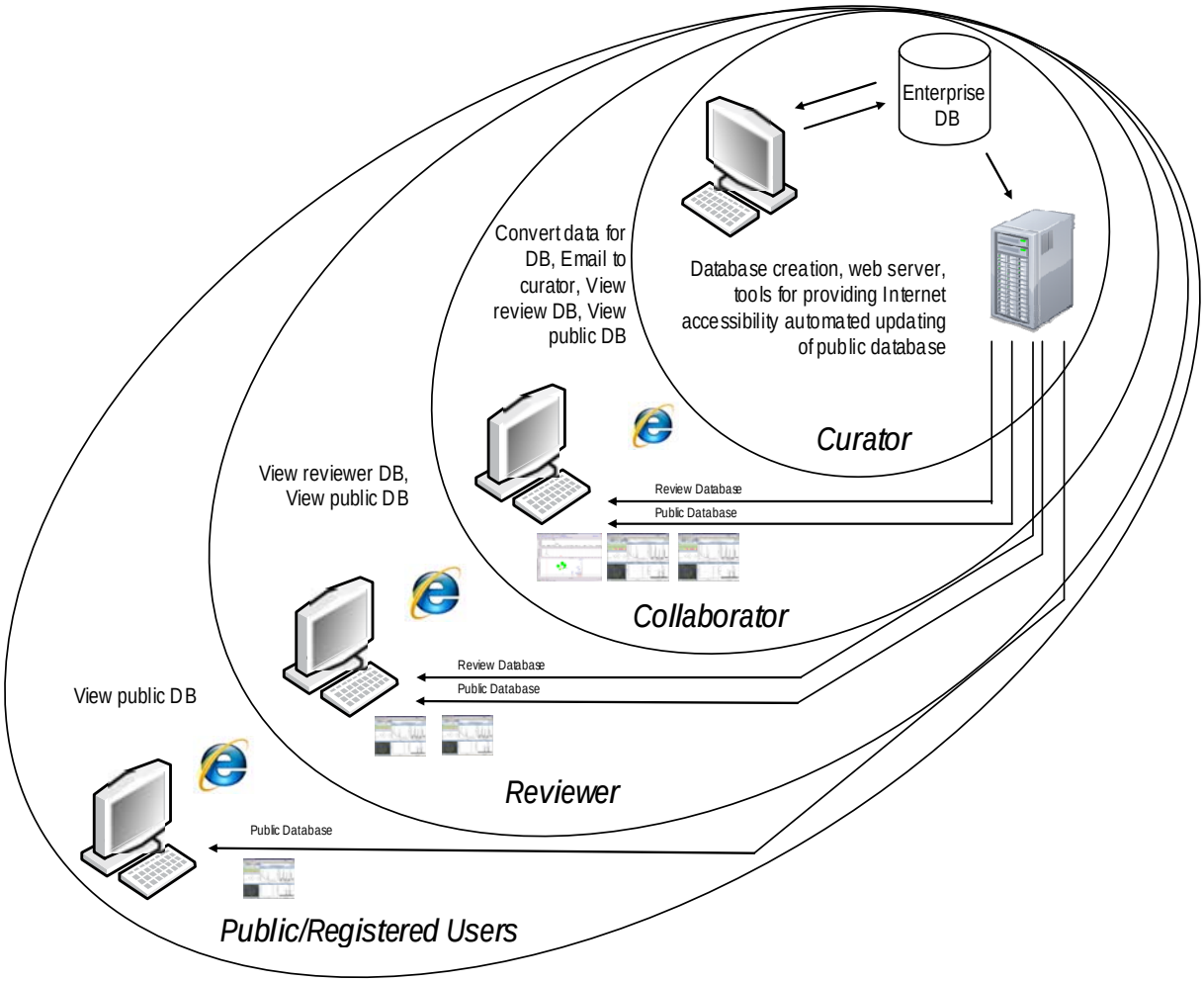

Figure 1. Database structure and functionality.

While the majority of records currently in ForensicDB have come from large libraries of spectra, the intention is to provide a Web portal where registered users can upload their records for submission. Once records have been submitted, collaborators process the data into an acceptable file format and attach correct documents to records with corresponding metadata. The spectral submissions are then uploaded into an editorial review board, and the curator sends an automatic e-mail containing the Web link to two external reviewers to evaluate the spectra based on established criteria. Evaluations are completed online in a Collaboration Database, accessible only by the curator and reviewers. Reviewers are assigned to specific spectra based on their area of expertise. Each instrumental method included in the database has its own criteria to reflect the qualitative spectral differences in techniques.

Reviewers first check to make sure that all information required of the submitter has been provided and that there are no misspellings of the compound name, record information, or document information.

For all spectra, the fragmentation pattern must be reasonable based on the structure and ionization method. In evaluation of DART spectra, the presence of a protonated or deprotonated molecule must be determined. If accurate mass was used for collection and the protonated molecule is present, then the experimental exact mass must be within ±5 mDa of the compound's calculated exact mass. Since increased orifice 1 voltages cause more fragmentation, the reviewer starts at the lowest voltage to locate

the intact molecule. If a protonated or deprotonated molecule cannot be located, then the reviewer tries to determine the reasons for its absence (e.g., instability of the molecule, loss of a water molecule).

Evaluation of each spectrum at all submitted orifice 1 voltages is conducted to determine if the fragmentation is reasonable. Knowledge of DART ionization and the compound of interest are used in examination of fragment ions. Reviewers also look at ^{13}C isotope ratios to make sure they are consistent in each prominent peak. A comparison of the submitted compound spectrum to other spectra of the same compound is performed, and significant differences are noted and discussed with the curator.

The database curator reviews the data and the reviewers' recommendations on whether the spectra should be accepted, rejected, or accepted with revisions. Such revisions may include submission of a structure, inclusion of required instrumental parameters, standard source lot number, and other information required for a complete submission, or submission of a better spectrum based on reviewers' comments. If all criteria are met, the spectra are approved and moved into ForensicDB for public accessibility. Otherwise, rejected spectra may be moved into the Rejected Database, or the contributing user may be contacted to determine if better spectra can be submitted.

A customized code has been created with ACD/Labs to help manage the review process. Currently, the workflow is to have submitted records built to the collaboration data schema— a subsection of the Oracle database that is not publically accessible but can be accessed by reviewers. The reviewer is presented with a voting form to enter recommendations and comments. The curator then evaluates these comments and corrects, rejects, or works with the submitters to finalize the record before "publication" to the public database schema.

2.2 Database Organization

Organization of ForensicDB is based on chemical structure —the only truly unambiguous means of referring to any given compound. **Figure 2** illustrates the organization of ForensicDB. A record indicates a specific compound structure and name, analyzed by a particular institution from a specific source material. Thus, multiple records may exist for a specific compound, reflecting a change in the major record features. Each record may contain multiple documents that indicate spectral method and instrumental parameters. Some of the general requirements for all submissions are spectral method, instrument type, scan range, and data reduction method. Other parameters are requested based on the instrumental technique, such as spectral resolution and number of scans co-added for FTIR data. Specific requirements for DART spectra include gas heater temperature, gas flow rate, type of sample introduction, and orifice 1 voltage.

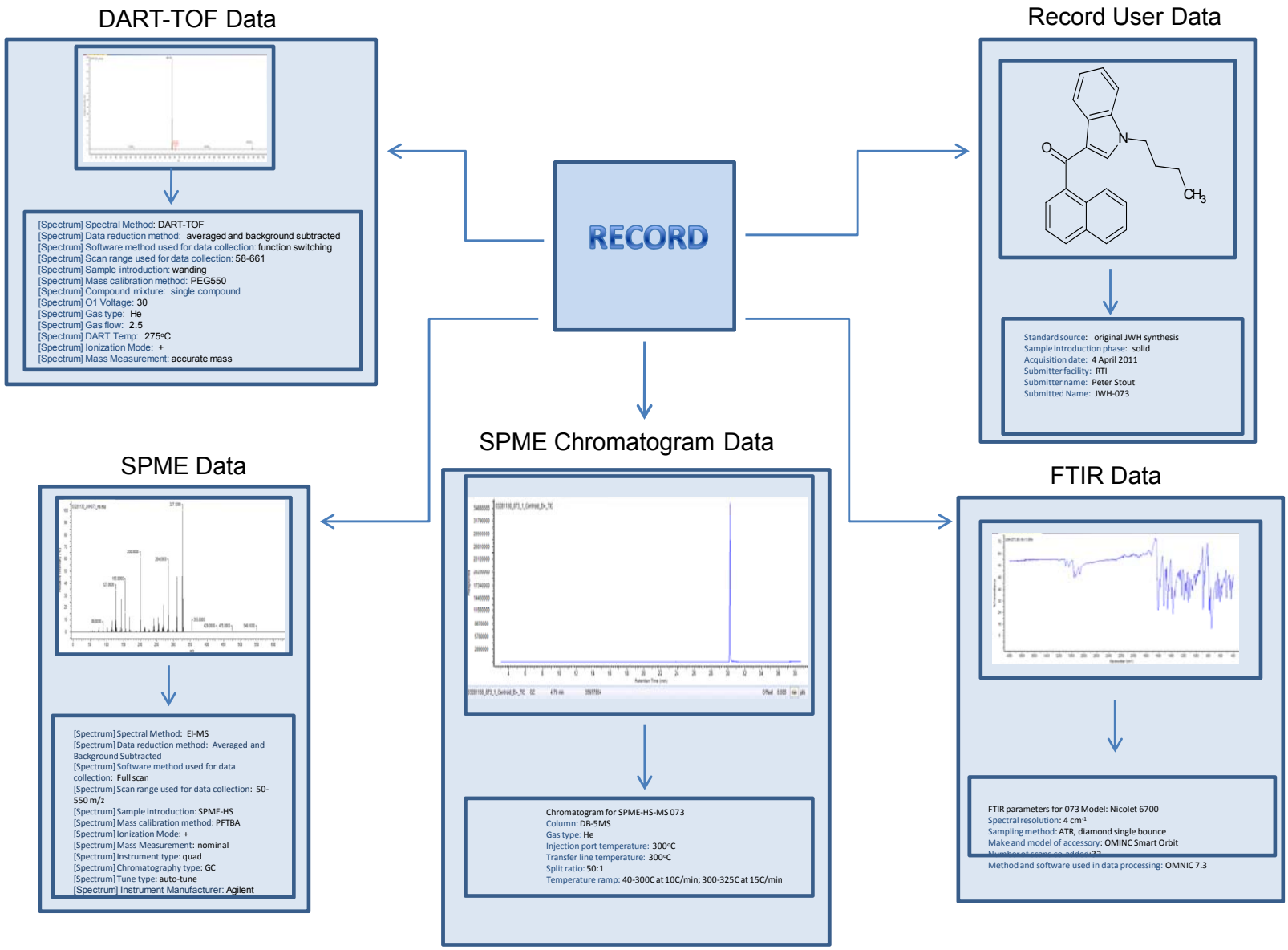

Figure 2. Database organization.

There is one structure within each record, although in some cases, there may be a structure on each document within a record. This would occur when analyzing a mixture such as the herbal Spice materials. A chromatogram of the Spice material is a document without a structure, but the mass spectrum of an isolated compound within the mixture (e.g., active JWH compound) contains the corresponding structure within the document. The ACD/Labs software calculates physicochemical properties of the structure, which are then housed within a record. Such properties include pKa, monoisotopic mass, and protonated exact mass.

We have tried to standardize the submission of record and document information; however, we were unable to collect the required information of the AAFS spectra since these are historic records. Our intention is to supplement these with more complete records over time.

2.3 Database Functionality

Figure 3 shows the main searching features of ForensicDB, which include searching by structure, spectrum, and user data. The structure can be uploaded or created using the provided drawing applet and searched by exact structure, substructure, or structure similarity. **Figure 4** shows the settings dialog box where the user can customize their search depending on whether similarity or substructure search is conducted. Some options include selecting a particular search algorithm and accounting for structures with chiral centers and double bonds.

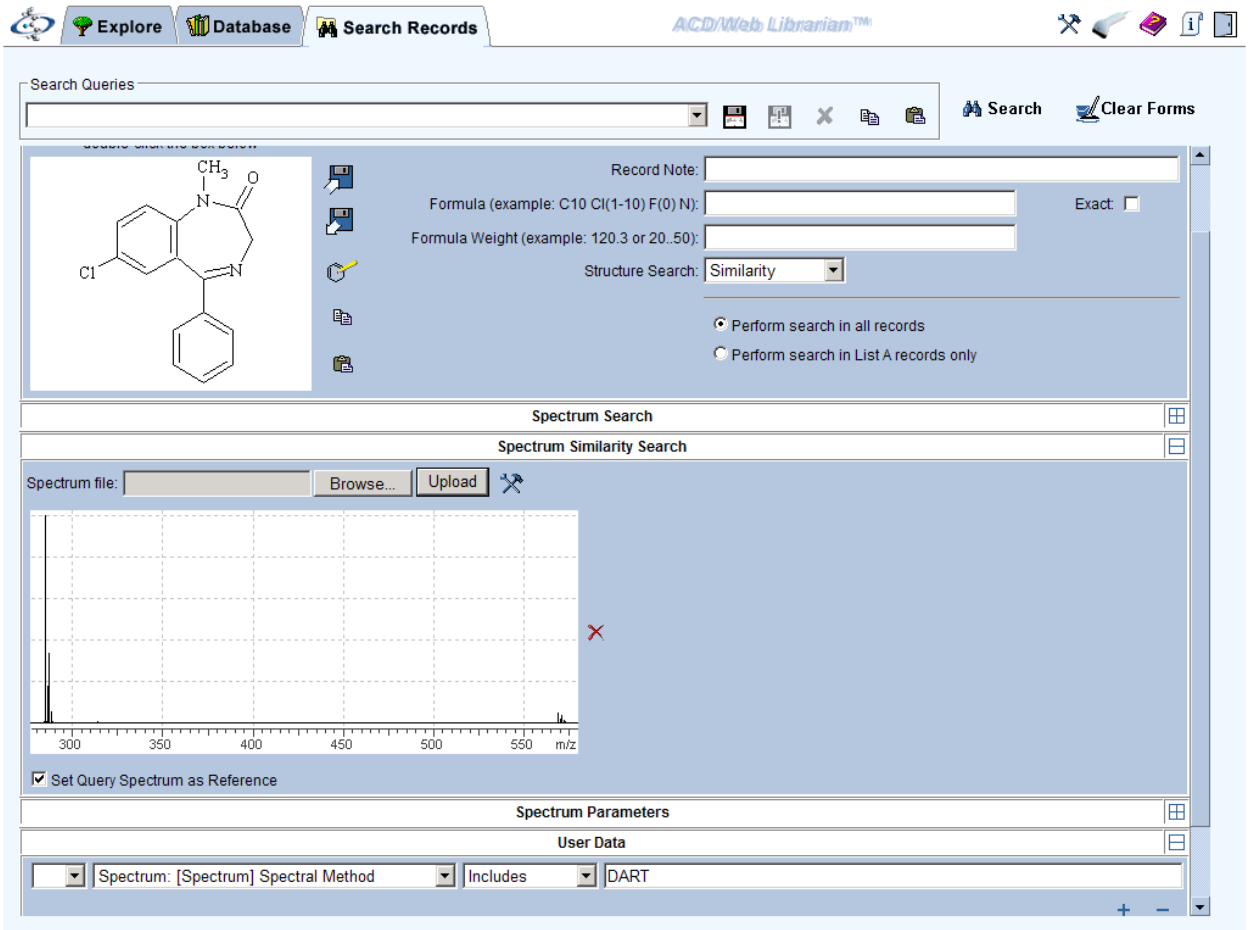

Figure 3. Database search options.

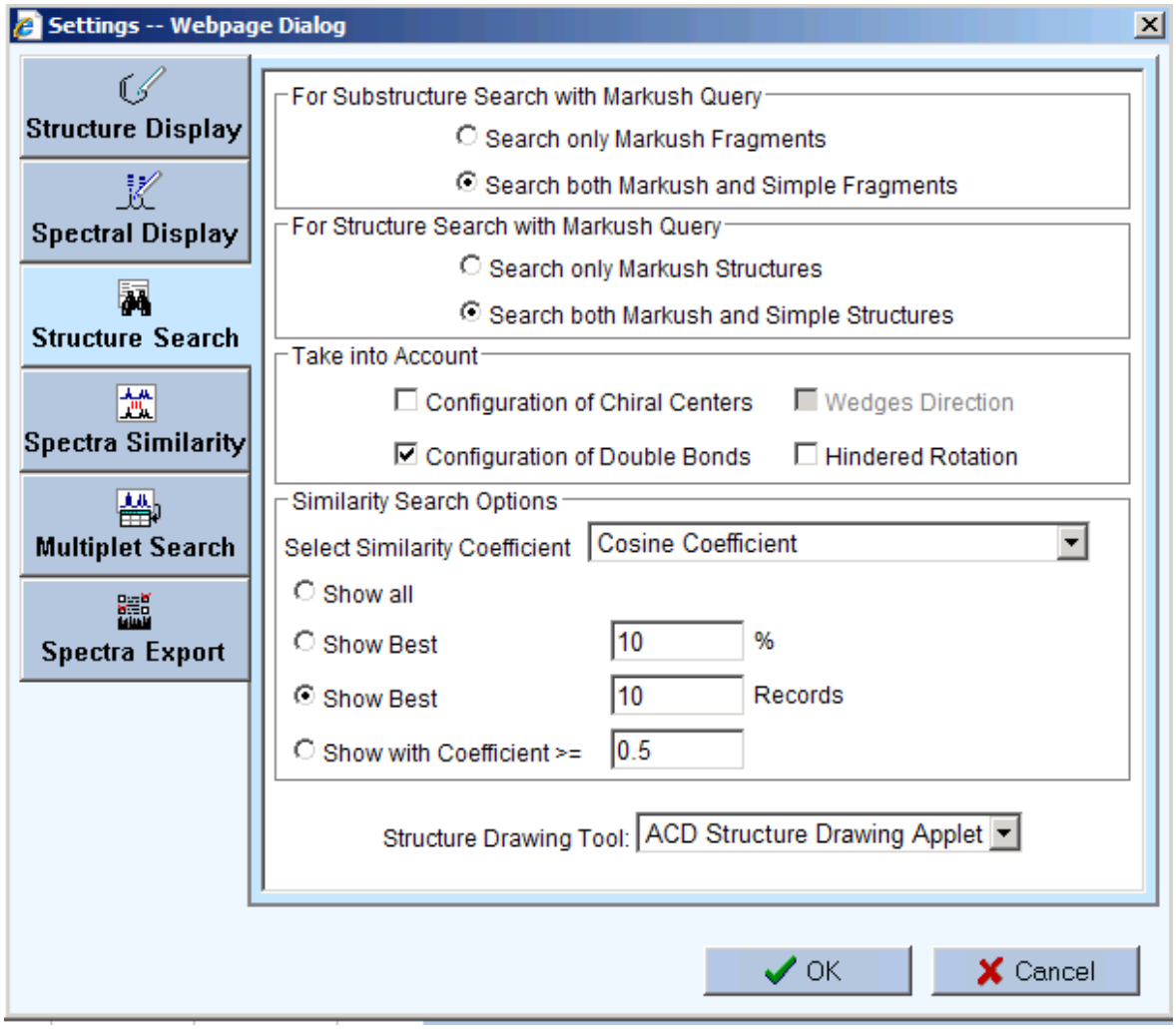

Figure 4. Structure search settings.

Users can upload their unknown spectrum to search against the database by spectral similarity. The spectrum can be set to mirror the reference spectrum. Setting the searched spectrum as a reference was not an original database function, but ACD/Labs worked with RTI to create this feature for the end users. The resulting spectra can be narrowed down by options within the settings dialog box in **Figure 5**.

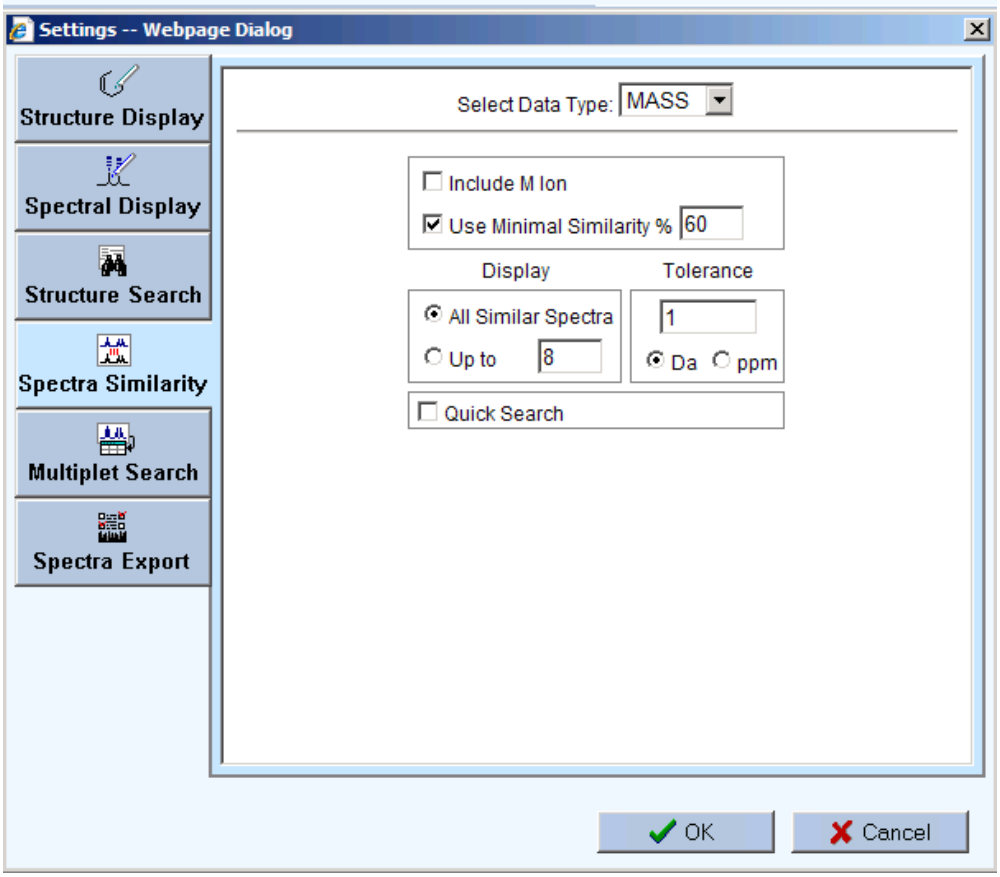

Figure 5. Spectral similarity search settings.

In the case of mass spectra, the data can be narrowed down by minimal percent similarity, number of resulting spectra, and tolerance level. The settings used to narrow search results vary due to the type of spectral method being searched. Another function within spectral similarity search is the ability to search by .CSV, which allows users to search spectra directly from Agilent instrumentation. ForensicDB was originally not able to handle .CSV files, but again, ACD/Labs worked to resolve this issue. **Figure 6** shows the Search CSV button circled in red.

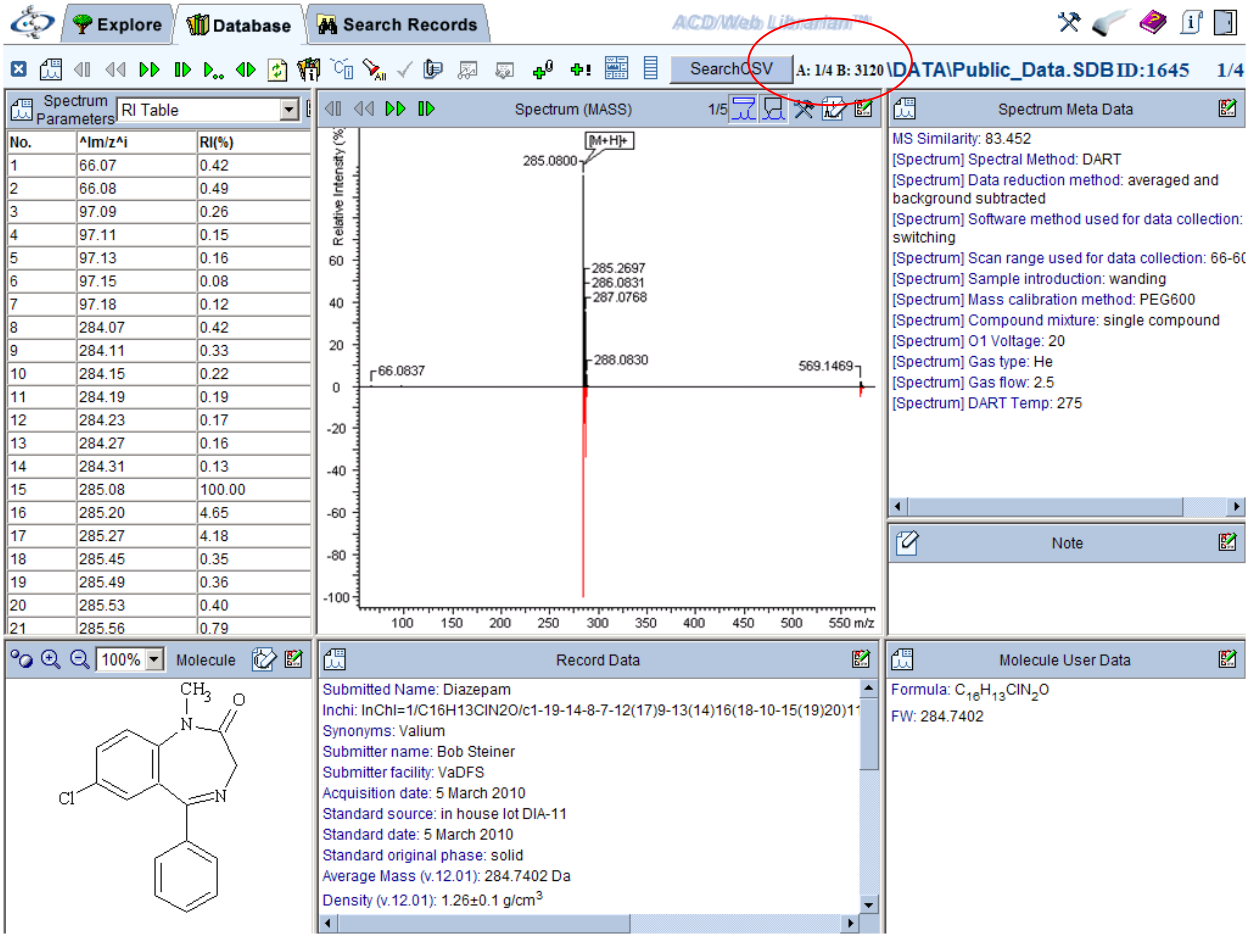

Figure 6. Search by CSV function.

Information in document and record forms can be searched in the user data field. This can be used separately or in conjunction with other searches, as shown in Figure 3, where the search is for the spectrum, but the search occurs only within DART data. Some examples of user data searching include searching by submitted name, instrumental technique, or formula weight.

A diazepam DART spectrum at 20 V was used as an example to illustrate searching in ForensicDB. **Figure 7** shows the dialog box indicating that four reference spectra resulted from the search. Three of the reference spectra were for diazepam, and one was from mazindol. The spectra from diazepam had a percent similarity greater than 80%, while mazindol was at 73%. **Figure 8** shows a comparison of the searched spectrum with a diazepam spectrum from the database. The user can generate a report by selecting information from the database layout (**Figure 9)**; this report can then be used as part of the user's case notes.

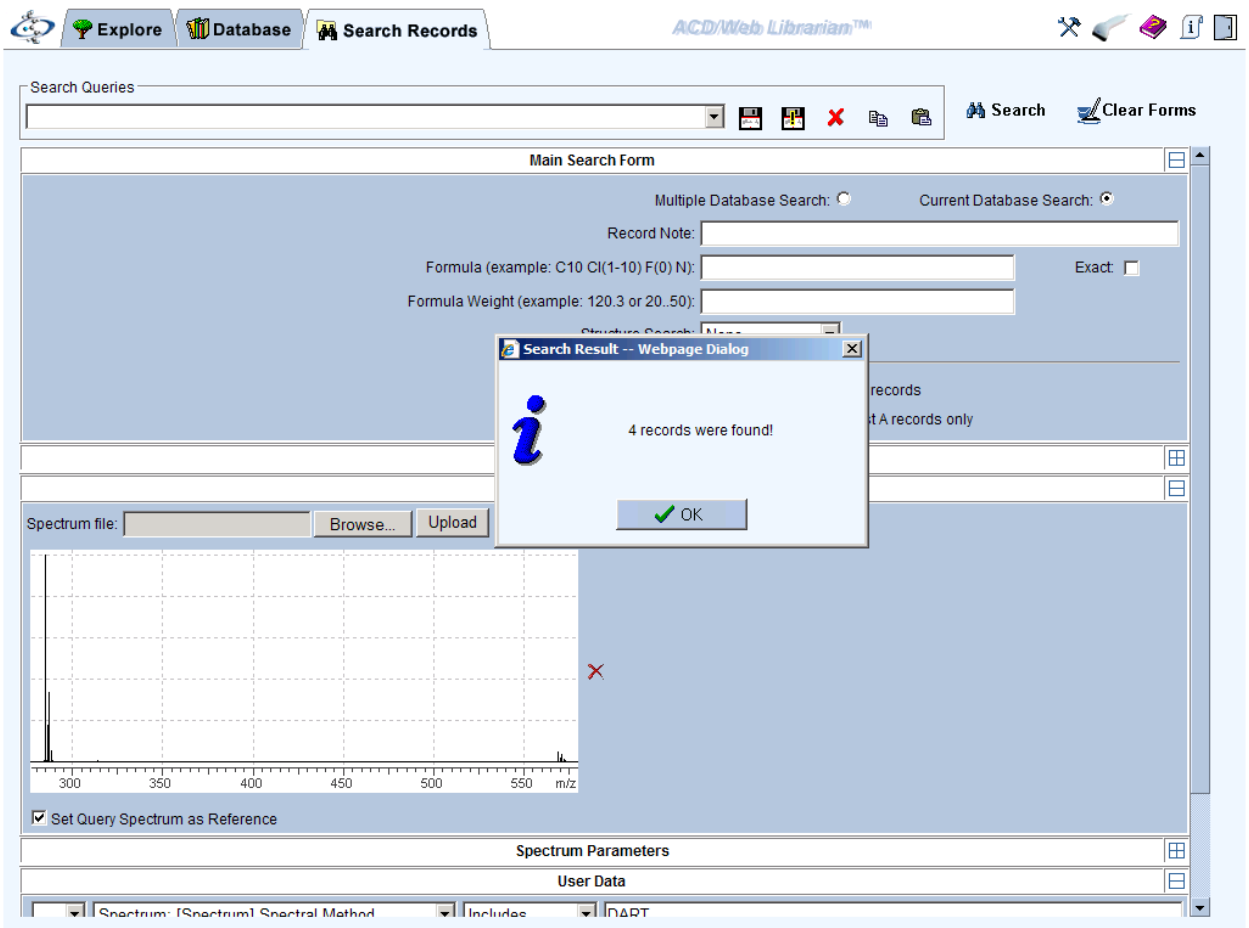

Figure 7. Search results for diazepam DART spectrum at 20 V.

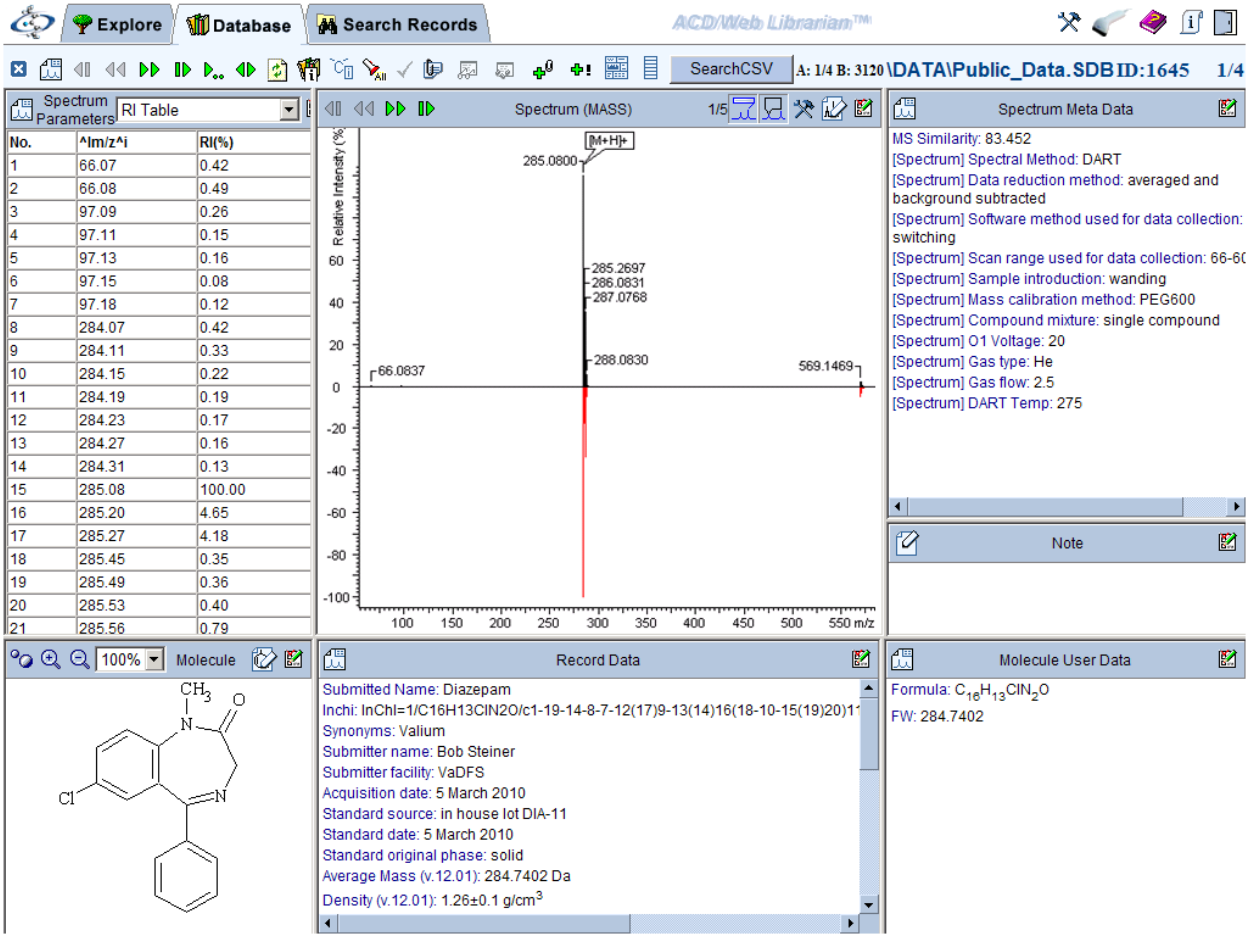

Figure 8. Spectral comparison of search results for diazepam DART spectrum at 20 V.

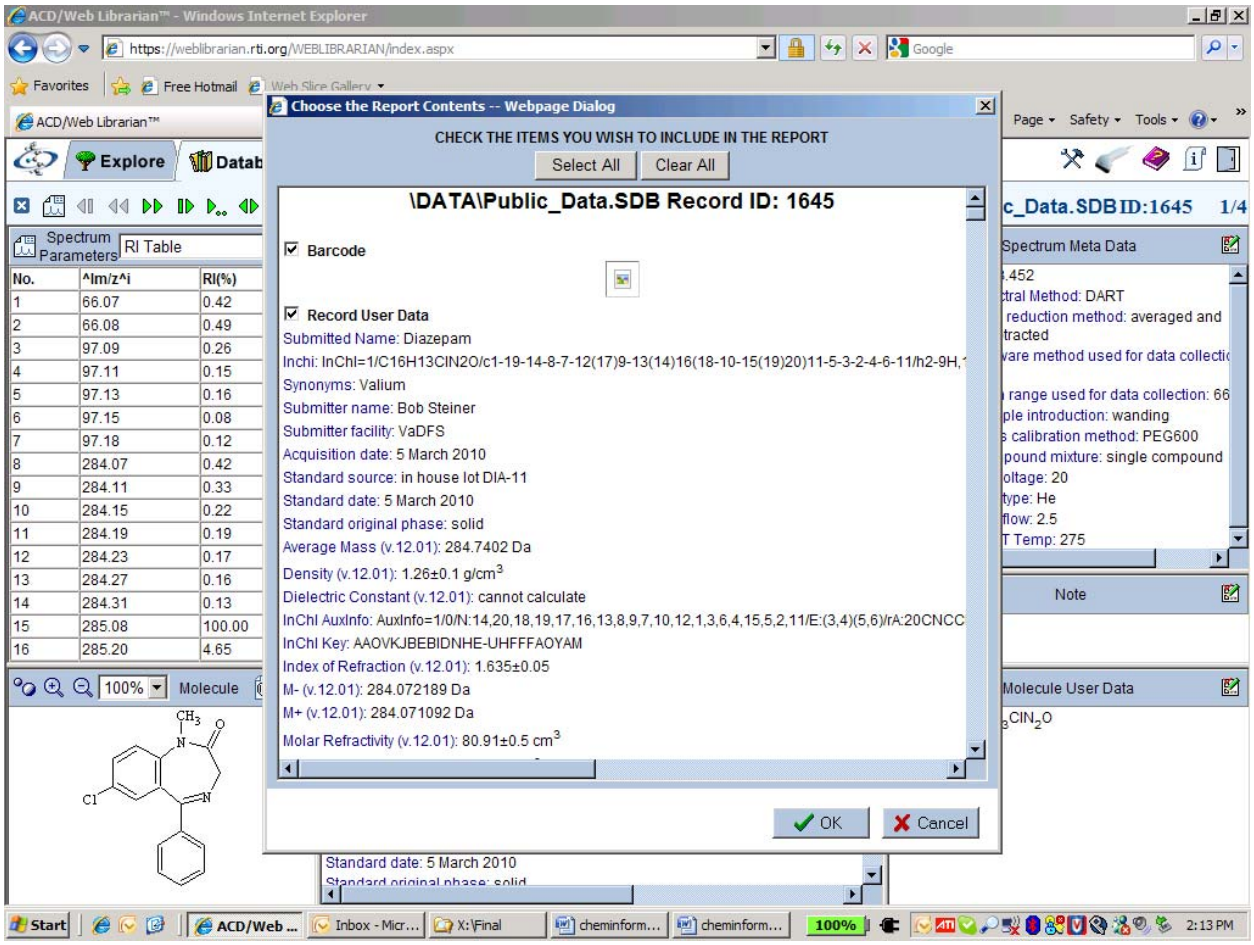

Figure 9. Creating a report from search results.

Figure 8 also shows the standard database layout. The user's view is customizable by the user and remains intact for their account. There are a wide variety of tools available to the user for analyzing the data. The spectrum is shown in the middle and can be set as a different window. In addition, the user can zoom in on specific ions. Documents with reported instrumental parameters can be found in the right corner, along with the percent similarity from a spectral similarity search. Record information can be found at the bottom of the layout. This also includes automatic calculations based off the structure. The structure is shown at the bottom left corner of the database layout. The top left corner contains a table of relative intensities for each fragment ion within the spectrum.

3. Results and Discussion of Database Status

3.1 Current Status of the Database

ForensicDB currently includes 2,922 total records representing approximately 5,427 spectra. These records were contributed by the VDFS, RTI, and AAFS Toxicology Section's EI-GC-MS database (AAFS library). The types of instrumental data represented are accurate mass, nominal mass, FTIR, and chromatographic data. The types of compounds submitted to ForensicDB include JWH cannabimimetic compounds, herbal Spice products, drug standards, pharmaceutical preparations, TLC-separated pharmaceutical preparations, chemical compounds, nylon fibers, and smokeless powders.

Table 2 shows the number of spectra submitted per instrumental method. Some of the data within Table 2 are presented as their own record, or are attached as a document to an existing record of the same source material, lot, and submitting institution. The public database includes 2,127 EI-MS spectra submitted by Dr. Graham Jones (AAFS Committee Chair) and VDFS. There are 825 AccuTOF-DART records representing 3,300 spectra submitted by RTI and VDFS. The DART spectra collected at both institutions were analyzed under the same instrumental parameters. To illustrate the characteristic fragmentation patterns, each compound record collected using DART contains a document at 20 V, 30 V, 60 V, and 90 V orifice 1 voltages. RTI submitted 28 spectra of JWH compounds collected using ESI-QTOF.

Table 2. Number of Spectra Submitted Per Instrumental Method

Data Type	Documents	Submitter
ForensicDB		
EI-MS	2,077	AAFS
	50	VDFS
AccuTOF-DART	2,916	VDFS
	384	RTI
ESI-QTOF	28	RTI
Process and Review Phase		
Chromatography	190	VDFS
	26	RTI
FTIR	81	RTI
	75	Ames
AccuTOF-DART	1,400	RTI
SPME-HS-MS	26	RTI

There are currently 1,798 spectra that are at various points in the processing and review stage. Among these are 95 records of smokeless powder data submitted by VDFS. Each smokeless powder record includes a document for attenuated total reflectance (ATR)-FTIR, EI-GC-MS, and positive chemical ionization (PCI) GC-MS chromatogram; an AccuTOF-DART spectrum at 20 V, 30 V, 60 V, and 90 V; and a picture showing the morphological characteristics. There are 26 records of Spice material collected using headspace solid-phase microextraction (HS-SPME-GC-MS). Each Spice material record includes a chromatogram labeled with the identified JWH compound present in the Spice mixture and the corresponding mass spectrum from the chromatogram appended to the record. There are also 4 AccuTOF-DART spectra included for each Spice material record, as well as the front and back package label and a picture of the Spice material. There are 308 DART records (1,232 spectra) of JWH compounds and -42 DART records (168 spectra) of drug standards from RTI in the processing and review phase.

Ames Laboratory plans to submit spectra of 75 single nylon fibers collected using photoacoustic (PAS)-FTIR. Before collecting data, the laboratory conducted a preliminary study to determine optimal collection parameters. The resolution was 4 cm^{-1} and scanning speed was 2.5 kHz. Ames Laboratory has been collecting and evaluating data while writing in-house software that enables multidimensional library searches and automates search optimization. To evaluate search quality, one can measure N different fiber products by recording M spectra of different filaments of the same product. A good algorithm provides large similarity indexes (SI) for correct matches (970±25) and small SI for incorrect matches (100–800). The best algorithm has low variance and large SI for correct hits, but also must have a large difference between average correct and incorrect match. Ten randomly picked nylon fiber samples were measured using a PAS detector accessory in an FTIR. A set of four nylon fibers with visually similar spectra were selected from this set of 10. A single fiber was fixed between two brass clamps inside the PAS detector's

sample cup. For each of the four fiber types, 3–4 different fibers were mounted and then measured individually in the mid-IR range (400–5000 cm^{-1}), with similar experiments being done on multiple days. When a spectrum from one of the four fiber types is searched against other all curves using the DPN (i.e., dot product of normalized curves) method, the search returns a higher SI for all spectra of the same fiber type as compared to other fiber types. PAS-FTIR spectra have been measured for 70 single nylon fibers and 10 olefin single fibers. Ames Laboratory continues to work on data acquisition and searching ability.

There were some issues that were presented by inclusion of the AAFS data. When these spectra were imported into ForensicDB, a script was created to attach the correct structure based on the submitted name. These structures were pulled from ACD/Labs dictionary within ChemSketch. Approximately 300 spectra were without structures due to non-standardized naming or typographical issues. RTI has resolved these issues and attached the correct structures to the AAFS records. Once the structures were attached, physicochemical properties were calculated and added to the record. RTI also has added synonyms to all AAFS records because they were not previously included.

ForensicDB is used by more than 400 forensic professionals from around the world. More than two-thirds of the user population resides within the United States, and all 50 states have more than one forensic professional using ForensicDB. Some professionals have contacted RTI about specific compounds in the database to solve cases brought up within their jurisdiction. In addition to the substantial and still growing population of users within the United States, ForensicDB enjoys patronage from residents in other countries. Many currents users are from Canada; a growing number of users are appearing from regions in South America and Europe; and some users are from as far away as Egypt, Zambia, or Australia. .

3.2 Database Efficiency

The objective of this part of the project was to determine the efficiency of searching spectra against reference spectra in ForensicDB. Both AccuTOF-DART and GC-MS data were evaluated. Since collection of DART spectra is not standardized across laboratories, it was of interest to determine whether commonly altered DART parameters would affect database searching.

A unique function of AccuTOF is its ability to collect spectral data at four different voltages in one second. This feature, known as function switching, uses collision-induced dissociation (CID) to create fragmentation (Steiner and Larson, 2009). Function switching occurs at the inlet (orifice 1) of the mass spectrometer, which is located directly after the ion source and ambient sampling gap. DART spectra were collected at orifice 1 voltages of 20 V, 30 V, 60 V, and 90 V. An issue with function switching is that it sacrifices sensitivity for more spectral detail. Collection of a spectrum at a single voltage for the entire one second allows for the detection of more ions, thereby increasing sensitivity of fragment ions. The use of function switching was evaluated to determine whether this decrease in sensitivity had an effect on database searching ability.

Fifty drug standards were collected at VDFS using GC/MS, and these were searched against the AAFS EI data. Forty-eight of the fifty searched spectra yielded the correct reference spectrum in the top three of the "hit list." The search results for 3,4-methylenedioxy-N-ethylamphetamine (MDEA) and 3,4-methylenedioxy-N-methamphetamine (MDMA) were not matched to the correct reference spectrum, because the database did not include these two compounds (subsequently, these spectra have been added to the database).

Twenty-five drug standards were collected at RTI using the same AccuTOF-DART parameters set at VDFS (**Table 3).** Previous optimization of DART parameters as a screening method for controlled substances at VDFS was determined by Steiner and Larson (2009). An investigation into the effects of different instrumental parameters was determined by holding all parameters constant, except that the gas

heater temperature was lowered to 200° C and the grid electrode was increased to 350 V. These changes in parameters were collected at RTI and searched against VDFS reference spectra.

Table 3. VDFS AccuTOF-DART Parameters, Operated in Positive Ion Mode on Mass Center Software (Version 1.3.4m)

Parameters	
Orifice 1: Function Switching (20, 30, 60, 90 V)	Orifice 2: 5 V
Orifice 1: 80°C	Gas Heater: 275°C
Electrode 1: 150 V	Electrode 2: 250 V
Ring Lens: 3-6 V	Reflectron: 910 V (tune dependent)
Ion Peak: 600 V	He Flow Rate: 2.5 L/min
Discharge Electrode Needle: 4,000 V	Mass Range: 66 to 600 Da

Table 4 shows three sets of search results of the drug standards collected under function switching at 20, 30, 60, and 90 V. The first search was of data collected using VDFS parameters, the second with gas temperature lowered to 200 °C, and the third with the grid electrode increased to 350 V. In searches from all three sets of parameters, the correct reference spectrum appeared in the top three of the percent similarity "hit list" 90–95 % of the time.

Table 4. Function Switching Search Results

'Hit List'	Temperature: 275 °C Grid electrode: 250 V Percentage (%)	Temperature: 200 °C Grid electrode: 250 V Percentage (%)	Temperature: 275 °C Grid electrode: 350 V Percentage (%)
First	81	73	85
Second	8	14	8
Third	4	3	2
Fourth +	5	7	2
No match	2	3	3

Table 5 shows search results from the standards collected under VDFS parameters using orifice 1 voltages at 20 and 30 V (without function switching). Despite variations in this parameter, the correct reference spectrum was observed in the top three of the hit list in 96% of the searched spectra. **Figure 10** shows cocaine, dextromethorphan, and amphetamine collected with and without function switching using VDFS parameters. These 20 and 30 V spectra of these compounds were plotted against their protonated molecule area counts. The graph demonstrates that function switching does cause decreased sensitivity; however, this study showed that data collected without function switching could be searched in ForensicDB against reference spectra collected with function switching.

Table 5. Search Results without Function Switching

'Hit List'	Temperature: 275 °C Grid electrode: 250 V Percentage (%)
First	74
Second	16
Third	6
Fourth +	2
No match	2

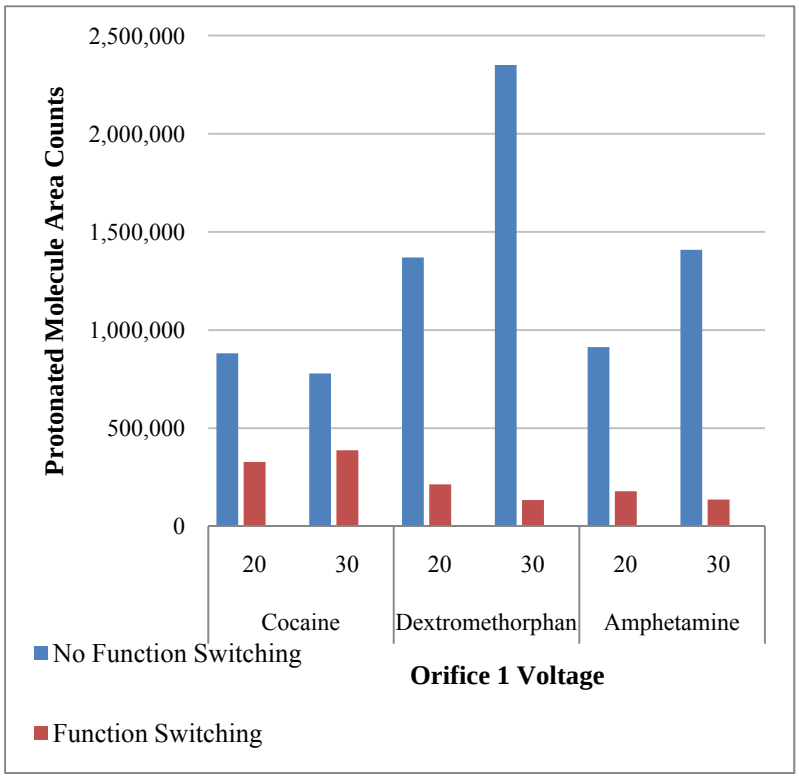

Figure 10. Illustration of effect of function switching on sensitivity.

These results indicate that increasing the grid electrode voltage from 250 to 350 V and decreasing gas temperature from 275 to 200 °C did not cause enough spectral variability to affect the ability of ForensicDB to narrow compound identification. Searching data collected without function switching against a database populated with data collected using function switching does not affect database efficiency. These results also provided a preliminary investigation into inter-laboratory reproducibility, since these spectra were collected at different institutions.

4. Conclusions

4.1 Discussion of Findings

The original goal of this project was to create a database of spectral information for AccuTOF-DART data. The objectives were to establish standards for data acquisition; maximize data exchange capabilities; determine software needs and develop the foundation of a unified database applicable to multiple disciplines; and begin populating the database with multiple collaboratively collected spectra. Due to a variety of changes and occurrences, the project scope was modified, which provided an opportunity to expand the original concept into a cheminformatic database containing spectral data.

The result has been an expanded database tool with benefits to a much wider range of forensic chemistry and toxicology. The database now provides a publically available platform for the searching and use of spectral records, with minimal use requirements of the end user. In addition, the project has provided a means of maintaining and expanding the availability of the widely used AAFS EI-GC-MS database and the flexibility to address data needs for emerging compounds, other forensic chemistry analyses such as photoacoustic FTIR, and smokeless powder analyses. To the best of our knowledge, ForensicDB is a unique database because it provides the ability to search a given spectrum against a Web-accessible database of reviewed spectra and have spectra from multiple spectral methods available in the same

database. The availability of multiple spectral methods in the same database can inform searches for DART-TOF data, making it a more viable tool. In addition, because the database is centrally hosted and Web-accessible it allows users to access data collected from new and emerging drugs without having to wait for or purchase a new software update.

The forensic user community is steadily increasing around this cheminformatic tool. The fundamental framework of the database has been established and is functioning reliably, and community members are interested in sharing spectra and contributing as reviewers.

4.2 Implications for Policy and Practice

This database provides a unique opportunity to help standardize analyses by DART-TOF, thus improving the utility of this technology in the field. The database also can serve as a mechanism to improve the availability of standardized data of known quality to all laboratories for use. This will help improve the quality and reliability of local database searches conducted by laboratories. While it is not and should not be the intention of the database project to replace the use of a concurrently run known standard material for the definitive interpretation of case samples, it can provide a means otherwise unavailable for improving the analyst's ability to identify unusual compounds. The user's ability to search and refine searches using multiple spectral data and then have records returned from potentially multiple institutions and multiple source materials can provide a much higher confidence that the laboratory is providing analyses that are consistent with the wider community.

As the database grows in its acceptance in the user community and the community's willingness to use and contribute increases, the database also will provide a forum to improve the quality of forensic chemistry work. Use of accurate mass determination is very new to the forensic arena, and the community has a long way to go to understand appropriate acceptance criteria. Even for legacy technologies, there are obvious needs for improving understanding and practices. For instance, in one of the demo sessions, an attendee asked "Our laboratory uses all single ion monitoring (SIM), can SIM data be searched in the database?" This provided the opportunity to discuss with community members that identification by a limited SIM method, and library searching based on limited SIM data, are not appropriate analysis procedures. The question and discussion was illustrative of the limited access that some practitioners have to information about what analysis procedures are appropriate.

Currently, community understanding of what constitutes valid and appropriate mass spectral data is of particular interest because the U.S. Department of Health and Human Services has recently allowed tandem mass spectral and high-resolution mass spectral technologies to be used in regulated workplace drug testing. This was done as a prelude to discussions about how to incorporate alternate matrix testing (hair, oral fluid, and sweat) and, potentially, alternative screening and confirmation workflows to include mass spectral screening instead of the traditional immunoassay. A broad understanding of what acceptable high-resolution mass spectra are is essential for this effort.

Not only does ForensicDB provide an accessible repository of data, but it also will serve as an anchor tool for the community of forensic chemists and toxicologists to improve and support reliable, consistent, and valid analyses for case samples.

4.3 Implications for Further Research

Although this report is a final report for the current funding, it also serves as an interim report for the ForensicDB program. The database has additional funding under NIJ award 2010-DN-BX-K177 to expand the capabilities of the database. Under this additional funding, the database will upgrade server capabilities to meet the growing user demand and to increase the stability of the Web services. Also, this funding will seek to aggressively promote and expand the use of the database.

The recent epidemic of "legal high" compounds has highlighted the challenges to the laboratories for staying ahead of illicit trends. The possibility of thousands of potential compounds being marketed has taxed the laboratory and regulatory ability to respond. The database cannot replace concurrently run standards for positive identification in case work, but it can provide a mechanism for access to spectral data on new compounds that are otherwise lacking for the community.

Continuation of the database will allow the user community to continue to grow and mature. This is a lengthy process of establishing the database as a trusted resource in the community and educating the community on how to effectively use the many powerful tools available. Thus, continued and regular outreach and promotion are integral parts of this effort.

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6. Dissemination of Research Findings

The development of ForensicDB has been presented as platform presentations at several national and international forensic science conferences; as at an ACD/Labs software user group meeting; and at multiple professional meetings (**Table 6**). The intention is to present updates of ForensicDB at other upcoming conferences, such as the American Society for Mass Spectrometry conference in September 201. It is also of interest to present at an international ACD/Labs user group meeting.

We continue to look for presentation opportunities and also have a manuscript in process to submit for publications. Currently, a manuscript of the database project is being prepared for submission to the journal *Analytical Chemistry* for publication, and we have done interviews for an editorial in *Scientific Computing World* for their August/September issue examining cheminformatics in forensics.

Table 6. Presentations at Scientific Meetings

Location and Date of Presentation	Title
American Academy of Forensic Sciences 2010	Development of a Web-Accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories
Society of Forensic Toxicologists 2010*	Development of a Web-Accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories
Canadian Society of Forensic Science 2010	Overview of a public Web-accessible cheminformatics database for shared utilization by forensic laboratories
American Academy of Forensic Sciences 2011	Development of a Web-Accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories
ACD/Labs North American Users' Meeting 2011	Development of a Web-Accessible Cheminformatic Spectral Database for Shared Utilization by Forensic Laboratories
Society of Forensic Toxicologists/ The International Association of Forensic Toxicologists 2011	Status Update for ForensicDB: Inclusion of Synthetic Cannabinoids in a Web-Accessible Database for Shared Utilization by Forensic Laboratories

*A demonstration of www.ForensicDB.org was performed at the RTI Exhibitor Booth at SOFT 2010.

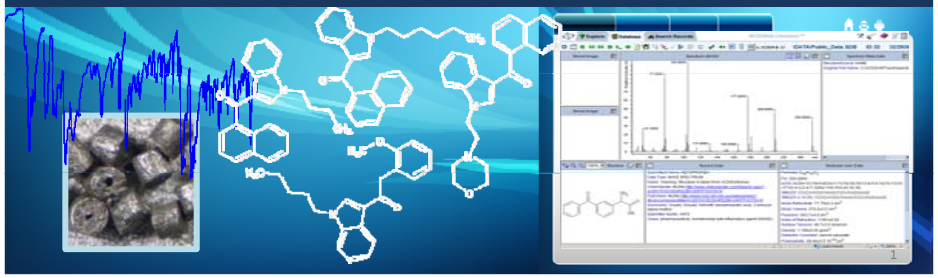
RTI's exhibit booth at the SOFT 2010 meeting included specific demonstrations of ForensicDB, and we plan to repeat those demonstrations at RTI's booth at the SOFT-TIAFT 2011 meeting (September 2011). The SOFT 2010 meeting had an attendance of roughly 1,000 people, and it is estimated that SOFT-TIAFT 2011 will have roughly 1,500 attendees, with a significant international attendance.

In order to familiarize such a diverse user population to ForensicDB's Web-based environment, RTI has offered five training sessions via a Web-deliverable virtual classroom. The virtual classroom environment allows RTI to reach out to users populations in otherwise remote areas of the globe. This feature has helped promote the availability and use of ForensicDB to many forensic professionals, both within and outside of the United States.

These classes have been popular with the global forensic science community, with more than 150 students attending the first two classes. RTI plans to continue offering these classes once a month. In each virtual classroom, we have experienced a myriad of questions about ForensicDB, and we have noted a high level of interest among classroom participants. Many users are excited to see the project expand to include more compounds. Toxicologists and laboratory professionals show growing interest in cannabimimetic compounds, while law enforcement professionals show an interest in explosives and accelerants. Due to the nature of ForensicDB's data structure, it will be possible to include such diverse compounds in the future as we continue to expand the project.

www.ForensicDB.org

A Web-Accessible Spectral Database for Shared Utilization by Forensic Laboratories



Overview

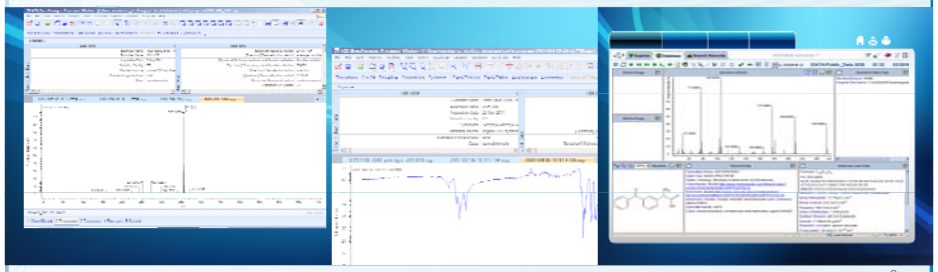
Database Partners

- National Institute of Justice
- Virginia Department of Forensic Science
- ACD Labs
- The Ames Laboratory
- Dr. Graham Jones

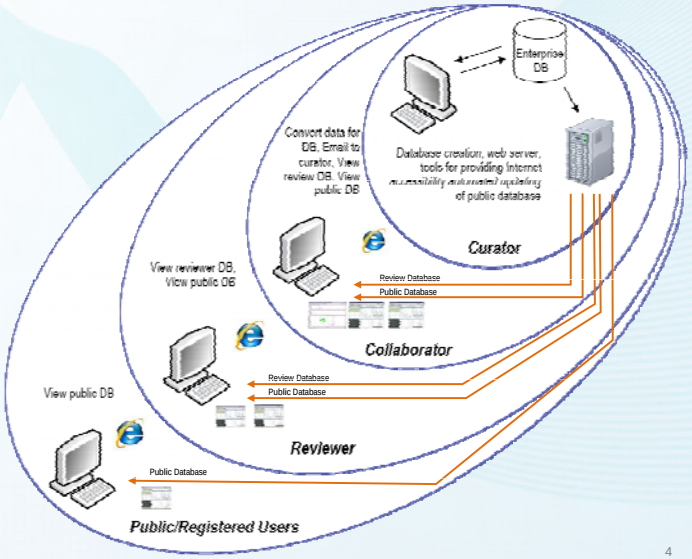
"This project was supported by Award No. 2008-DN-BX-K180 and 2010-DN-BX-K177, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this program are those of the authors and do not necessarily reflect those of the Department of Justice."

Purpose

- Create a no-cost and Web-accessible spectral database
- Create a Web-portal to simplify submissions
- Peer-review of spectral data
- Encourage community involvement



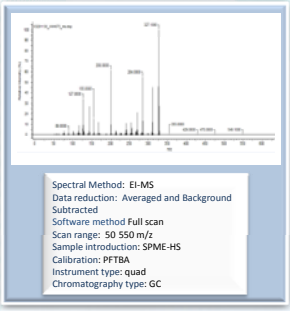
Database Structure



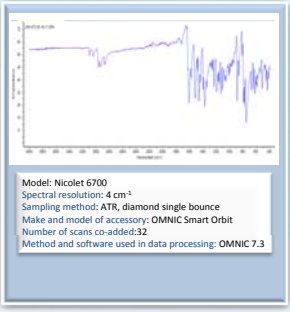
Database Structure

Complete Record:
Contains multiple spectra and images depending on record

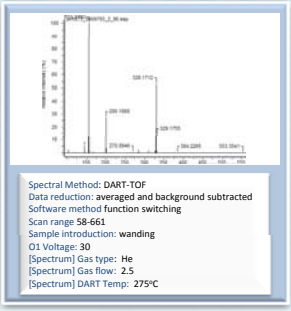
RECORD



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

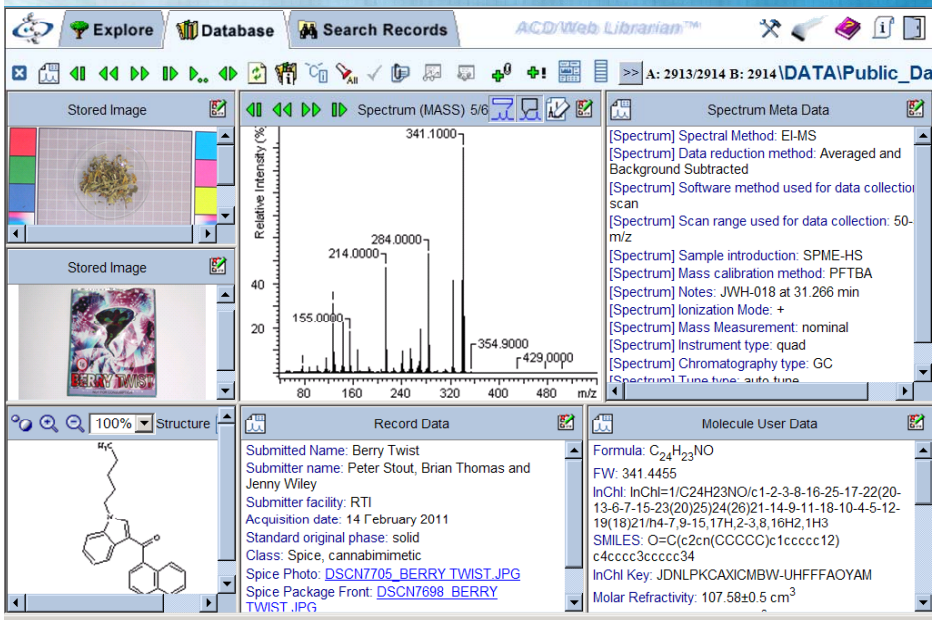


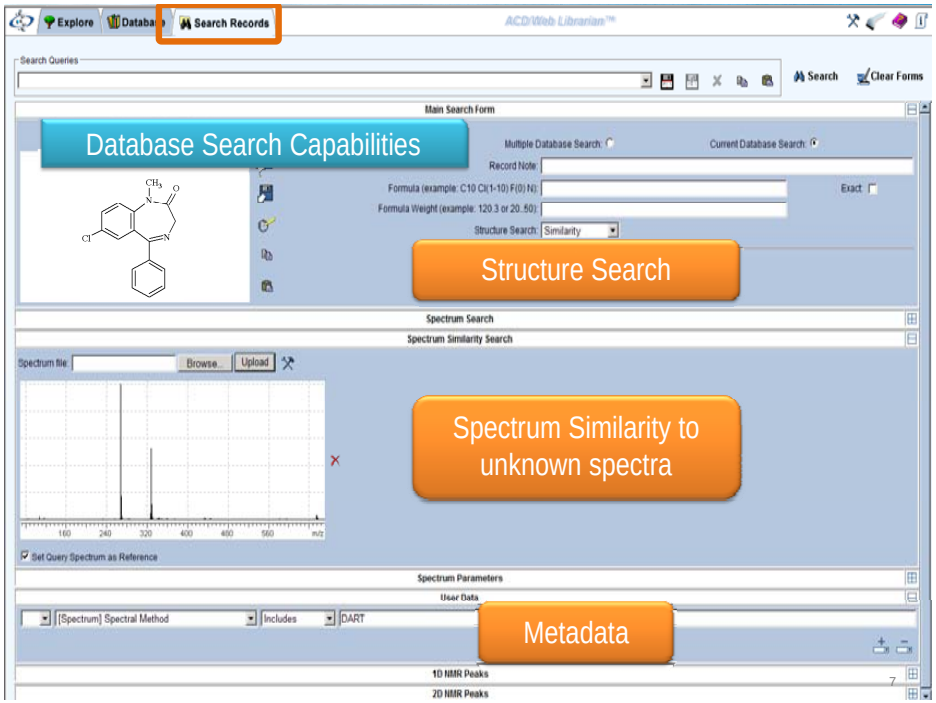
Model: Nicolet 6700
Spectral resolution: 4 cm-1
Sampling method: ATR, diamond single bounce
Make and model of accessory: OMNIC Smart Orbit
Number of scans co-added:32
Method and software used in data processing: OMNIC 7.3



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

ForensicDB Standard Layout





THANK YOU AND CONTACT INFO
(links are active in the PDF document)

forensicDB@rti.org

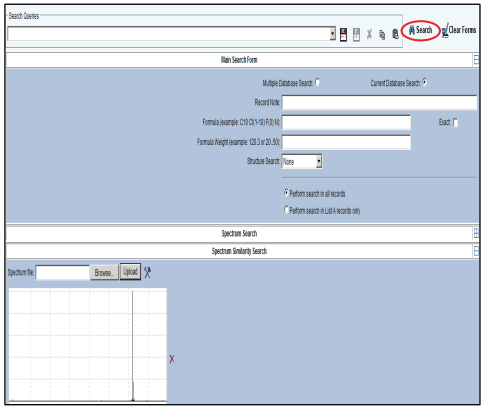
Demo Event Notification List

Printable Quickstart Guide

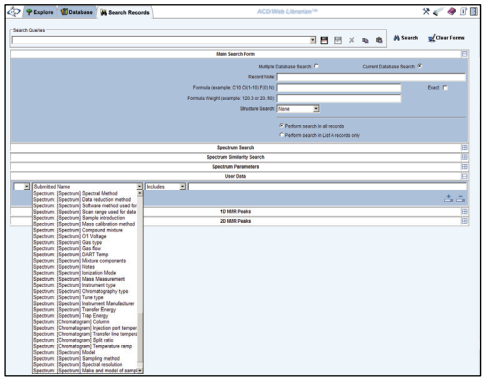
RTI INTERNATIONAL

Cheminformatics Database
www.forensicdb.org

Database Searching

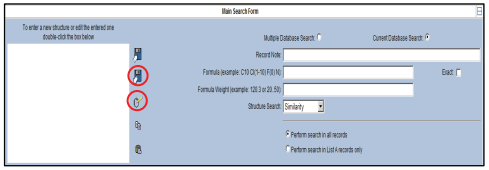


Upload spectrum in Spectrum Similarity Search section.



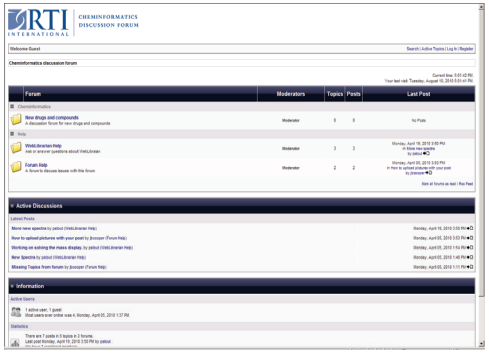
Narrow down search results by choosing information from the User Data drop down box. In the near future an option for searching all fields within ForensicDB with a one click button option will be added.

Database Searching



Upload or draw a structure to search by similarity, substructure, or exact structure.

Keep informed about updates and post comments and questions using the **Forum** tab found on www.forensicdb.org homepage.



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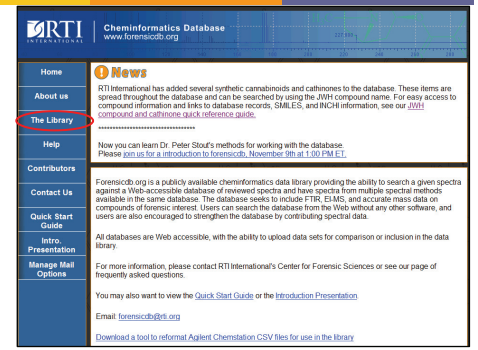
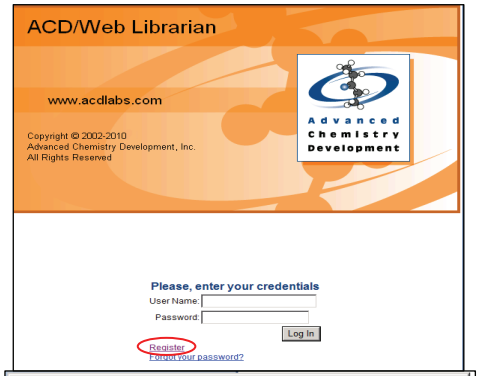
Phone: 866.252.8415
Fax: 919.541.7042
E-mail: forensicdb@rti.org

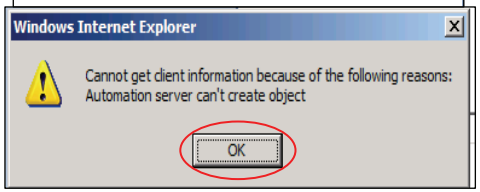
Web Accessible Spectral Database: ForensicDB.org

Register at www.forensicdb.org to access reviewed spectral data, and perform spectra, structure and Meta-data searching.

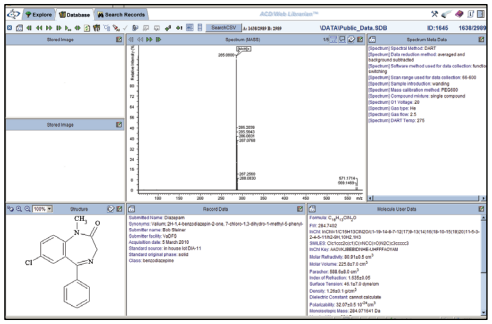
This Website is supported by
NIJ Cooperative Agreement **2008-DN-BX-K180 and 2010-DN-BX-K177**

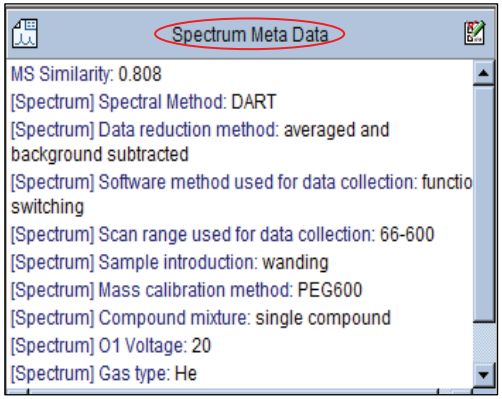


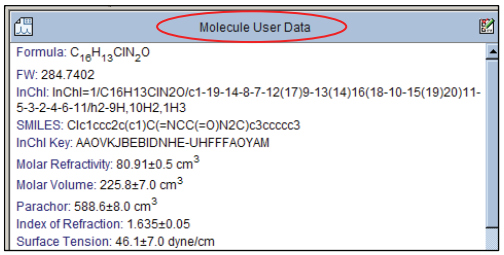


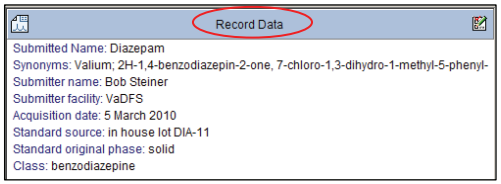


ForensicDB Layout









Navigation

Go to next spectrum

Go to last spectrum

Change spectral settings

Change database properties

View all database spectra

Help manual

Log out

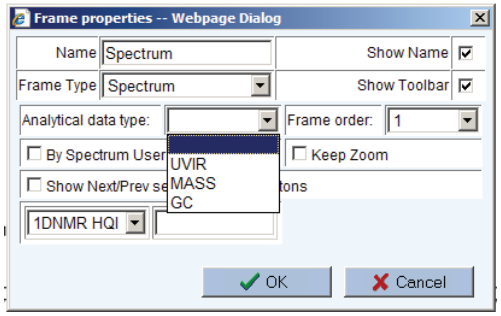
Switch between database view and search options

ForensicDB is composed of Records with appending Documents (spectra). Record information can be found in the Record Data section, which remains the same for all of the appending Documents. Document information is found in the Spectrum Meta Data section, which indicates instrumental parameters used for collection. ForensicDB includes nominal mass, accurate mass, and FTIR data. Calculated properties from the structure are found in the Molecule User Data section.

ForensicDB Layout

The above shows one of four Documents within a Record

Select the properties button in the top right corner of the spectrum window to view different analytical methods



Select appropriate analytical method