DART-MS Libraries

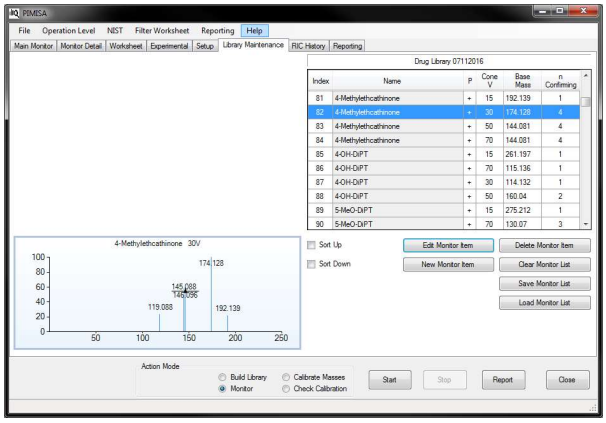
The PIMISA™ Software

Reverse library search software for DART®-MS: Transform mass spectral data into simple, high confidence answers with PIMISA by matching key ions and identifying compounds on the basis of mass, isotopic pattern, and fragmentation patterns generated by using in source fragmentation.

Key Benefits and Features

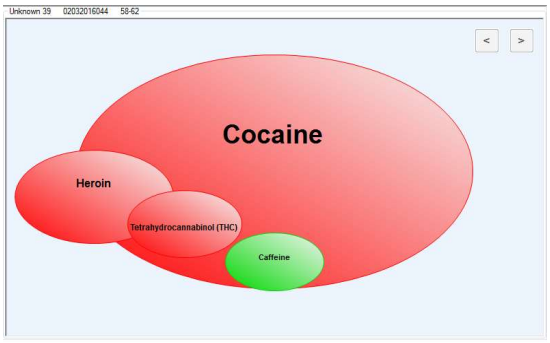
PIMISA identifies compounds on the basis of nominal or accurate mass, isotopic pattern, fragmentation pattern, relative ion intensity and ionization polarity. Features include:

- Capability to create your own searchable library of multi-cone voltage (in-source CID) DART-MS spectra.
- Permits searching against the NIST DART-MS library database for drugs of abuse.
- Identify compounds by matching key target ions present in your spectra with ions from reference spectra (reverse search) leading to high confidence identifications.
- Provides easy-to-understand visual display of compounds identified and semi-quantitative assessment of each one.
- Compatible with Waters MassLynx .Raw data format.



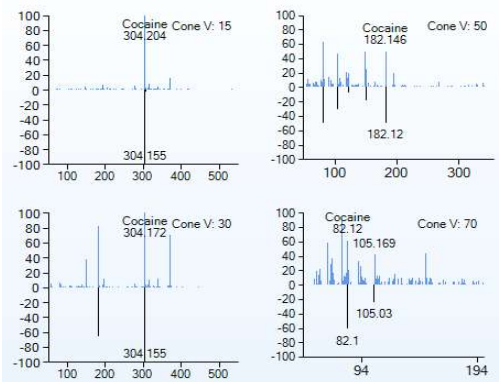
Simple Answers

Detected compounds are indicated by using colored bubbles to indicate importance or relevance. Relative abundance of the molecular ion is used to provide semi-quantitative information.



Reverse Library Search

Reverse library search is the process where key target ions from the library reference spectrum are searched and matched against all of the ions in the sample spectrum. All non-targeted ions in the spectrum are disregarded as shown in the figure to the left.

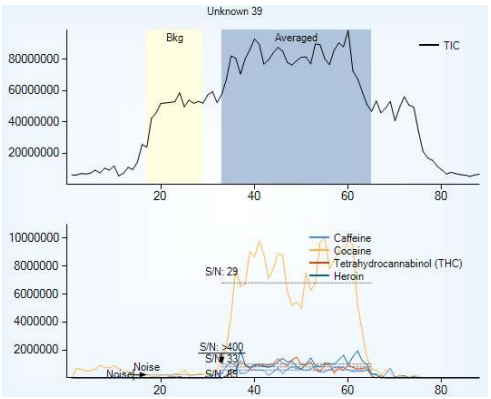


The average match score of each cone voltage spectrum (up to 4) based on mass, relative ion intensity and isotopic pattern is provided.

Detected Analytes

ID	Analyte Name	MW	Match Score	Level
254	Cocaine	303.147	0.975	7200000
331	Heroin	369.158	0.986	1150000
610	Tetrahydrocannabinol (THC)	314.225	0.912	598000
214	Caffeine	194.08	0.922	447000

Extracted Ion Chronograms



TIC and extracted ion chronograms (EIC) of the detected analytes are provided for verifying the presence of each analyte. A signal-to-noise ratio based on intensity is also calculated for verifying analyte presence.