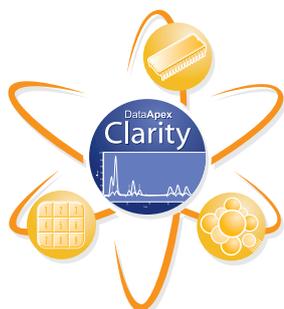


Clarity MS Extension



Software module for processing data from Mass Spectrometry Detectors

The Clarity MS module is a tool for processing data acquired by MS detectors. Spectral data, together with chromatograms, add a third dimension to data analysis.

The Clarity MS module expands Clarity capabilities by providing interactive spectral analysis, peak purity analysis and compound identification based on a spectral library search. MS spectral data can be displayed in the Chromatogram window and printed on reports. Clarity also works with NIST libraries.

The MS Extension is an optional addition to Clarity software, it cannot be used as a standalone program.

CLARITY SOFTWARE

CONTROLS

EXTENSIONS

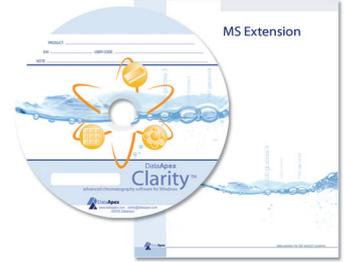
HARDWARE

Clarity MS Extension

Software module for processing 3D data from MS detectors

The MS Extension is an optional, fully integrated addition to Clarity software. It can be ordered as a part of new software or as an extension to existing software.

The MS Extension is fully compatible with both LC Control and GC Control to evaluate the data from both liquid and gas chromatography. On stations with the MS extension activated, new GC-MS and LC-MS types of instruments will become available in the configuration. The MS Extension is also compatible with Clarity Offline software.



Features

MS Data: All data is saved in a single file; a chromatogram on any m/z or a spectrum at any point on the time axis can be simply recalled after an analysis for review. MS spectra acquired using an MS detector may be interactively selected from a chromatogram for visual inspection and comparison. The spectra may also be used for peak purity determinations and component identification through spectral libraries.

MS Method: The Clarity MS method allows any compound to be quantified on any m/z, TIC, BPI or external signals. The identity of the compound can be confirmed using Spectral Library Search and Peak Purity analysis.

Peak Purity: This analysis helps to discover hidden impurities. Purity is calculated from 5 or all spectra within the peak. Peak Purity analysis can be optimized by setting custom preferences relating to the purity threshold, m/z range restriction and intensity threshold.

Spectral Library: The Clarity software works flawlessly with NIST libraries, comparing the peak spectra with the spectra of an unlimited number of spectra from multiple libraries. Spectra stored in a Spectral Library may include retention indices and analysis parameters. The Spectral Library Search can perform automatic identification of integrated/calibrated components (peaks). The library search may be constrained by the RT Window and/or by m/z ions used. Background Correction option is also available.

Import/Export Data: Spectral data can be imported/exported in several formats to or from the Clarity software, including netCDF, mzML and mzXML formats.

Reports: Users can easily include MS report sections, graphs and tables into the report in the intuitive Report Setup dialog.

Instrument Control: Control modules for several MS detectors, both for LC and GC, are being developed at the moment. Please contact sales@dataapex.com to find out about the availability of your MS detector control module.

Specification

- Part No.: A38
- Related Products: Clarity (p/n C50) - required
Clarity offline (p/n C59)
LC Control (p/n A24) or GC Control (p/n A23)

The screenshot displays the Clarity MS Extension software interface. The main window shows a chromatogram with a peak at approximately 9.60 minutes. Below the chromatogram is a mass spectrum plot showing relative intensity versus m/z. A table titled 'Result Table (2010 - DHS_600 - TIC)' lists various compounds with their retention times, peak purities, and EIC values. An 'MS Search' dialog box is open, showing search parameters and a table of search results. The search results table includes columns for Match, RT, Peak, Compound Name, Library, ID, Formula, MS, and CAS No. The 'Method Setup Demo_MS' dialog box is also visible, showing options for peak purity and conformity of the whole spectrum.

Compound Name	Retn. Time [min]	Peak Purity	EIC 1 - Reference m/z 1	EIC 2 - Reference m/z 2	EIC 3 - Reference m/z 3	EIC 4 - Reference m/z 4	Conformity	Calibration
1 Methylene Chloride	4.811	483	49.0	84.0	66.0	25.0	20.0	100
2 Hexane	5.762	686	57.0	41.0	47.0	43.0	54.0	99
3 Ethyl Acetate	6.845	743	43.0	61.0	70.0	51.0	44.0	99
4 Trichloroethane	7.168	891	82.0	85.0	78.0	49.0	8.0	99
5 Benzene	7.723	795	78.0	77.0	17.0	32.0	17.0	100
6 Hexane, 2,2-dimethyl-	7.857	746	86.0	57.0	32.0	12.0	8.0	99
7 Trichloroethylene	8.407	848	132.0	104.0	104.0	95.0	11.0	100
8 2-Butanone, 3-methyl-	8.928	866	43.0	86.0	1.0	44.0	11.0	100
9 2-Pentanone	9.728	955	57.0	86.0	4.0	71.0	41.0	99
10 Butanoic acid, methyl ester	9.808	733	74.0	62.0	38.0	71.0	41.0	97
11 Toluene	9.808	955	92.0	92.0	68.0	11.0	10.0	100
12 Trichloroethylene	10.447	899	156.0	84.0	75.0	11.0	69.0	100
13 Hexanal	10.252	947	44.0	43.0	63.0	46.0	69.0	99
14 Benzene, 1,3-dimethyl-	10.897	702	81.0	206.0	65.0	77.0	8.0	100
15 p-Xylene	11.338	631	51.0	296.0	47.0	77.0	7.0	100
16 Hexane, isobran-	11.489	983	171.0	171.0	303.0	179.0	89.0	99
17 Decane	12.099	966	57.0	71.0	38.0	23.0	43.0	99
Total								