Simple export from ADAP-KDB

Names given for each match are based on experimental or empirical data contained within the database. These do not necessarily differentiate between isomeric forms.

Click here to see results

Description of the compound annotation results:		
This export shows a single top match for each measured feature. Every match displays the following information:		
Index	File index	Index of the input files submitted by users.
	Numerical Signal ID assigned by ADAP-KDB	ADAP-KDB automatically assigns a numerical signal ID to each signal in the input file that a user submits to ADAP-KDB for compound annotation.
	Match #	One signal might have multiple matching candidates, the "Match Index" is a unique identifier for each matching candidate for a signal.
Information Measured or Calculated from Mass Spectrometry Data	Query Signal Name	Unique identifier of the query signal submitted by a user.
	Retention Time (min)	Retention time (RT) of the signal. If the signal contains multiple adducts grouped together, the RT here is the average of the individual RT of each adduct.
	Precursor m/z	The measured m/z of each signal. If the signal contains multiple adducts grouped together, the precusor ion is listed with the order of intensity from high to low.
	Adduct	Calculated by data preprocessing software tools
	Neutral Mass (Da)	Calculated by data preprocessing software tools
	With Fragmentation Spectrum or not	A boolean value indicating if there are fragmentation spectra associated with the underlying compound.
Library Matching Results	Retention Time Error (min)	The difference between measured RT and retention time in the library.
	Precursor Mass Error (ppm)	(a) For signals that contains multiple adducts grouped together, this "Precursor Mass Error" is "Predicted Neutral Mass" minus "Library Exact Mass".
		(b) For signals that contains only one peak and therefore an adduct cannot be assigned to the signal, this Precursor Mass Error is "Precursor m/z" minus "Predicted Adduct" minus "Library Exact Mass".
	Matching Adduct	When data preprocessing software tool cannot provide the neutral mass for this signal, the library matching algorithm computes the neutral mass for each possible adduct. The assumed adduct that match with the measured “Precursor m/z” is listed here as the “Matching Adduct”.
	Isotopic Similarity	The similariy between the measured isotopic pattern and the therotical isotopic pattern of the matching library compound with predicted adduct.
	Fragmentation Score by matching with Experimental spec	a) The similarity score between the measured MS/MS pattern and the library MS/MS data based on the same adduct. If the signal has multiple adducts, the MS/MS similarity will be conducted based on each adduct specifically. The highest mimilarity value will be reported as the general fragmentation score.
		b) The similarity score for indivudal adduct will be reported in the advanced export.
	Fragmentation score by matching with theoretical spectra	The similarity score between the measured MS/MS and the predicted MS/MS.
	Ontology Level	
	Is this the best match?	A check mark indicating that this is the best match suggested by ADAP-KDB.
Compound Information	Compound ID	Unique identifier of library compounds. It could be Pubchem ID, HMDB ID or CAS.
	Compound Name	This is normally the most commonly used name of the compound.
	Chemical Formula	Chemical formula based on the structure of the compound. This information is automatically included in sdf files.
	Library Monoisotopic Exact Mass (Da)	The therotical exact mass that caculated from chemical structrue which is automatically included in sdf files
	Library Retention Time (min)	Retention time of the compound in the library
	CAS NO	CAS Registry Number
	HMDB ID	Human Metabolome Database Identifier
	PubChem ID	PubChem Identifier
	InChI Key	International Chemical Identifier (InChI) Key
	Library Category	Category of the matching library. For example, microbiome, foodome, enviromental, etc
Misc	Notes	Any notes that the user wants to add.

The following ontology levels are used to express the confidence of each match:

Matches against in-house libraries	OL_1	Match is based on the spectral similarity, neutral mass error, and retention time error.
	OL_2a	Match is based on the neutral mass error and retention time error.
	OL_2b	Match is based on the spectral similarity and retention time error.
Matches against public lirbaries	PD_A	Match is based on the spectral similarity and neutral mass error.
	PD_B	Match is based on the predicted spectral similarity and neutral mass error.
	PD_C	Match is based on the isotopic distribution similarity and neutral mass error.
	PD_D	Match is based on the neutral mass error only.