



# METLIN Metabolite Personal Compound Database and Library for Accurate-Mass LC/MS

More confident identification of endogenous metabolites for metabolomics

## METLIN PCD

- Includes masses, chemical formulas and structures for approximately 25,000 endogenous and exogenous metabolites, lipids, and di- and tri-peptides
- Many entries include CAS, HMP, LMP, or KEGG identifiers as well as web links to associated database entries
- Includes 679 compounds with retention times that have been determined using a standardized reversed-phase method providing more confident compound identification by using accurate mass and retention time (AMRT)

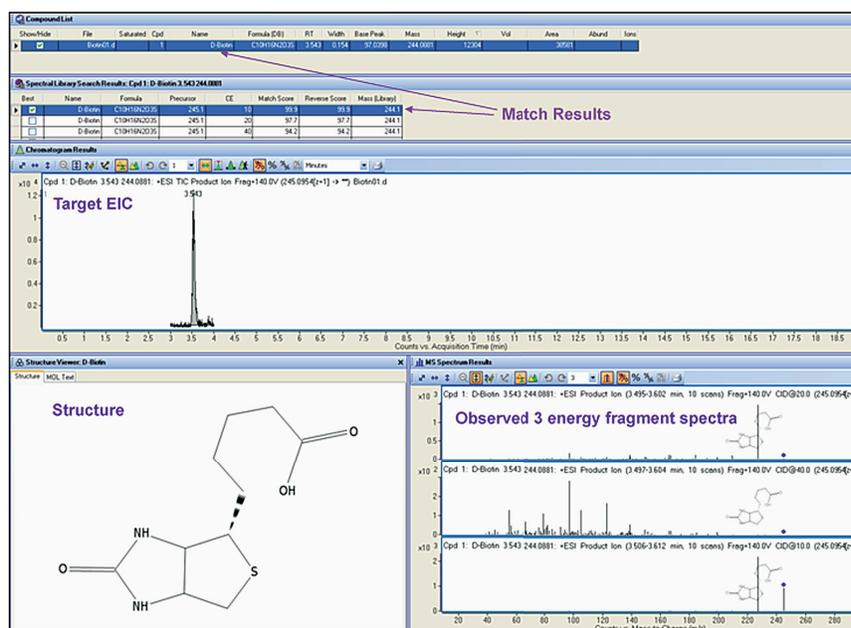
## METLIN PCDL

- Includes all compounds contained in METLIN PCD, and additionally accurate mass Q-TOF MS/MS library reference spectra for 2278 compounds
- Generates higher confidence compound ID by matching unknown Q-TOF MS/MS spectra to the spectral library

## Identify endogenous metabolites with confidence using METLIN Metabolite Personal Compound Database and Library

Compound identification is a key element in untargeted metabolomics experiments. The level of confidence in the identification is directly dependent on the quality of the database used to assign compound identity. The METLIN metabolite database, created by Gary Siuzdak, PhD, is one of the most comprehensive and widely used metabolite databases in the world today.

Agilent Technologies is the exclusive provider of the METLIN Personal Compound Database (PCD) and now the new accurate mass MS/MS Library (PCDL). The software resides on your local PC and facilitates faster, easier, compound identification for metabolomics research.



MS/MS Library match example – Biotin in positive ion mode



## Seamless Integration with Mass Profiler Professional (MPP)

Using a combination of advanced processing capabilities and powerful statistical and mathematical models to analyze complex MS data sets, MPP easily lets you classify, compare and analyze sample groups via differential analysis in metabolomics studies. MPP now runs in a Windows 7 as a native 64-bit application with capacity for faster processing and support for much larger sample sets.

MPP includes an integrated ID Browser that mirrors MassHunter's qualitative analysis functionality to allow identification using METLIN PCD for LC/MS TOF data and EI library for GC/MS data.

m/z	Abund	Charge	Sat
175.119	88894	1	
176.1253	17990	1	
177.1277	2687	1	
197.101	19806	1	
387.1842	901	1	

Label	CAS	Name	Cpd	HMP	KEGG	LMP	Notes	Hits (DB)
Cpd 67: 1-Oleoyl-Lysophosphatidic acid		1-Oleoyl-Lysoph.	67	HMDB00443				
Cpd 49: 2,3-Diphospho-D-Glyceric Acid	138-81-8	2,3-Diphospho-	49				Geigy vol 3 p.112	
Cpd 1: Arginine		Arginine	1				Positive MS/MS	
Abund Match	CAS	Cpd ID	Name	Mass (DB)	Database Search Match Score	Formula	HMP	Identification Techni
23.14	74-79-3	11	Arginine	174.1117	65.49	C5 H14 N4 O2		DBS
23.14		5784	D-Arginine	174.1117	65.49	C5 H14 N4 O2	HMDB03416	DBS
Label	CAS	Name	Cpd	HMP	KEGG	LMP	Notes	Hits (DB)
Cpd 59: Asp Met Asp		Asp Met Asp	59					
Cpd 41: cyclic adenosine diphosphate ribose	119340-53-3	cyclic adenosine..	41					
Cpd 2: Gly Phe Phe		Gly Phe Phe	2					
Cpd 8: Granisetron metabolite 1		Granisetron met.	8				antibiotic activit.	
Cpd 7: Hemigossypol		Hemigossypol	7		C09680	LMPRO1030033		
Cpd 29: His Pro Asn		His Pro Asn	29					
Cpd 37: Hydroquinone disulfate	2458-55-1	Hydroquinone di..	37				Poison, Disinfect.	

MassHunter ID Browser identifies compounds from an entity list generated by MPP. In this example, results for mass 174.1117 matched against the METLIN database reveals it to be arginine; molecular formula, database match score, name, KEGG and CASS ID are also shown.

## Ordering information

G3849AA MassHunter Workstation for TOF/Q-TOF B.04.00 Upgrade  
G3338AA MassHunter Workstation Offline Software B.04.00 Upgrade  
G6825AA MassHunter METLIN Metabolite PCD  
G3874AA MassHunter METLIN Metabolite PCDL  
G3835AA MassHunter Mass Profiler Professional B.02.01  
G1668AA High-End LC/MS PC Workstation (Windows 7, 64-bit)

[www.agilent.com/chem/metlin](http://www.agilent.com/chem/metlin)

© Agilent Technologies, Inc., 2011  
Published in USA, April 18, 2011  
Publication Number 5990-7928EN