

Agilent Mass Profiler Software

Essential Tool Set for Differential Profiling

The Agilent MassHunter Mass Profiler software performs comparative analysis of one or two data sets generated from Agilent time-of-flight (TOF) or quadrupole-TOF (Q-TOF) instruments. The comparative analysis results are displayed in graphical and tabular formats that enable you to quickly identify statistically meaningful differences between features (discrete molecular entities defined by retention time and mass) in the same group or two different groups. The Mass Profiler application can directly query the optional Agilent METLIN Personal Metabolite Database and several web-based public databases, or export results for further analysis.



Our measure is your success.



Mass Profiler comparative analysis

After creating your differential analysis project, you can customize the analysis by editing the parameter settings.

Apply pre-analysis filters to charge state, isotope pattern, abundance level, neutral loss, and mass defect. Specify masses to exclude from the analysis or limit the analysis to specific masses, and set mass and retention time tolerance windows. Align and normalize by specifying internal standards to normalize mass abundance values and correct for retention time shifts in the raw data. The software uses information about user-specified internal standards to normalize abundance values and adjust for retention time shifts across all of the data sets.

Apply filters to show only results of interest in the Feature Summary table and graphical plots. Set thresholds for abundance ratios, differential score, and minimum relative frequency. Filter results based on expression fold change, relative frequencies, or minimum differential score.

For further statistical analyses, export a feature summary to the GeneSpring MS software that provides advanced statistical tools.





Set pre-analysis filters to choose particular data to analyze.



The Log/Log plot of fold changes helps you quickly determine up- or down-regulated features in the samples. Fold change lines in the Log/Log plot represent the constant ratio of abundances between experiment and control groups. In this example, only features with two-fold or greater abundance ratios are displayed.

											Grou	p 1				Group	2							
		E	xpressi	on: 🕫 Bo	th_C	Up_C Dowr	1		217	Feature	s													
	_		Feature	summary					~	Experime	nt(4)			6	Control	1)				T	Comp	arison		
	ID	RT	SD	Mass	SD	Abundance	RSD	Freq.	Mark	RT	Mass	Abundance	RSD	Freq.	RT	Mass	Abundance	RSD	Freq.	BT	Mass	Log2(A1/A2)	Log2(A1/A2)	Diff. Score
1	1	10.933	0.018	193.0735	0.0001	6857493	0.38	8		10.922	193.0735	9290860	0.06		10.945	193.0735	4424126	0.03		4 0.022	-0.0001	1.07	1.07	99.9997
2	2	14.537	0.011	161.0443	0.0002	1962543	1.07	4				0		1	14.537	161.0443	3925086	0.02		4		-16.00	16.00	100.0000
3	3	13.459	0.010	339.0953	0.0001	1478903	1.07	4				0		1	13.459	339.0953	2957806	0.04		4		-16.00	16.00	100.0000
4	4	13.180	0.010	337.0796	0.0001	1256650	1.07	4				0		1	13.180	337.0796	2513300	0.03		4		-16.00	16.00	100.0000
5	5	1.128	0.004	136.0631	0.0001	1200154	0.36	8		1.131	136.0630	1600728	0.03		1 1.125	136.0631	799580	0.03		4 -0.006	0.0000	1.00	1.00	100.0000
6	6	14.587	0.009	232.0729	0.0001	1157221	1.08	4		14.587	232.0729	2314441	0.10		1		0		1	0		16.00	16.00	99.9999
7	7	5.625	0.024	302.0632	0.0002	971597	0.48	8		5.609	302.0631	1410536	0.04		5.642	302.0634	532659	0.03		0.033	0.0003	1.40	1.40	100.0000
8	8	1.681	0.005	227.0900	0.0001	780890	0.75	8		1.681	227.0900	1253252	0.36		1.682	227.0900	308527	0.31		4 0.000	0.0000	2.02	2.02	99.3825
9	9	14.588	0.009	129.0469	0.0001	745544	1.08	4		14.588	129.0469	1491088	0.09		1		0		1	0		16.00	16.00	100.0000
10	10	1.310	0.005	142.1100	0.0000	675075	1.07	4		1.310	142.1100	1350150	0.07		1		0		1	D		16.00	16.00	100.0000
11	11	32.158	0.024	99.0686	0.0000	562693	0.72	6		32.147	99.0686	858214	0.28		\$ 32,180	99.0686	267172	1.15	. :	2 0.033	0.0001	1.68	1.68	97.7119
12	12	15.775	0.008	430.0900	0.0002	540498	0.90	8		15.773	430.0899	991194	0.08		15.776	430.0900	89802	0.03		4 0.003	0.0001	3.46	3.46	100.0000

The Mass Profiler software applies a student's t-test to the differential analysis to check for statistical significance. In the Feature Summary table, the comparison data shows the retention times and mass differences between features from the two groups. If group 1 abundance > group 2 abundance, the feature is upregulated and the feature \log_2 ratio is displayed in red. If group 2 abundance > group 1 abundance, the feature is downregulated and the feature \log_2 ratio is displayed in score is a number between 0 and 100 that represents the relative confidence that the difference in intensity of a feature between the two groups is real. Two methods are available for calculating the differential score, a student's t-test-based method or a support vector machine method.

0	mments							Structu	ure Information		Notes		
						1		Structure	MOL Text		o-Toluric acid 2 Mathubicouric	-	
L						-1			1		o-Methylhippunc	acid	
	Identification Metho DB R RT matchin Expected d Mass RT Abundance	d MFE d MFE g Igno ata variat 0.50 mi 7.5%	rs i + DB lin.mtl wed Da + 5.60 ppm h	Identifica MFG prev DB conf User assi	tion results dicted: 199/217 (8 hits: 101/217 (licting: 24/205 (1 gned: 205/217 (922;] 472;] 22;] 943;]			AT.	0	N-(o-Toluoyi) gly N-(Methybenzoy Glycine, N-(meth 328006_ALDRII Glycine, N-(2-me http://pubch	orgysan cine (jg)scine jbbenzoy() DH thy/benzoy()	
21	nposition		nary: 205 id	entified Feat	ures	Name	Fremula	(Massiren)	ABT MEG Score	CASID	METLINID	KEGGID	HMPID
01	Mass 193.0735	Sumr RT 10.933	nary: 205 ld Feature ID	entified Feat Abundance 6857493	Ures log2(A1/A2) 1.07	Name 2-MethyRippuric acid	Formula C10H11N03	ΔMass(ppm)	ART MFG Score	CAS ID 0.0 42013-20-1	METLIN ID	KEGG ID	HMPID
1	Mass 193.0735 161.0443	Sumr RT 10.933 14.537	nary: 205 Id Feature ID 1 2	entified Feat Abundance 6857493 1962543	ures log2(A1/A2) 1.07 -16.00	Name 2-Methythippuric acid	Formula C10H11N03 C6H905	<u> амазз(ppm)</u> 21 38	ΔRT MFG Score	CAS ID 0.0 42013-20- 0.0	METLIN ID	KEGG ID	HMP ID
	Mass 193.0735 161.0443 339.0953	RT 10.933 14.537 13.459	nary: 205 Id Feature ID 1 2 3	entified Feat Abundance 6857493 1962543 1478903	ures log2(A1/A2) 1.07 -16.00 -16.00	Name 2:MethyRippuric acid	Formula C10H11N03 C6H905 C13H15N407	<u>ДМасс(ppm)</u> 2.1 3.8 -3.3	ΔRT MFG Score 11 11	CAS ID 0.0 42013-20- 0.0 0.0	METLIN ID	KEGG ID	HMPID
1	Mass 193 0735 161 0443 339 0953 337 0796	ET 10.933 14.537 13.459 13.180	nary: 205 Id Feature ID 1 2 3 4	entified Feat Abundance 6857493 1962543 1478903 1256650	ures log2(A1/A2) 1.07 -16.00 -16.00 -16.00	Name 2:Methythippunic acid	Formula C10H11N03 C6H905 C13H15N407 C13H15N407	ΔMassippm) 2.1 3.8 -3.3 -3.1	ΔRT MFG Score 11 11 11	CAS ID 0.0 <u>42013-20-</u> 0.0 0.0 0.0	METLIN ID	KEGG ID	HMPID
No. of the second secon	Mass 193.0735 161.0443 339.0953 337.0796 136.0631	BUMP RT 10.933 14.537 13.459 13.180 1.128	Feature ID / Feature ID / 1 2 3 4 5	Abundance 6857493 1962543 1478903 1256650 1200154	Ures log2(A1/A2) 1.07 -16.00 -16.00 -16.00 1.00	Name 24Methylhippuric acid n-methylhicolinamide	Formula C10H11N03 C8H905 C13H19N407 C13H19N407 C7H9N20	ΔMass(ppm) 2.1 3.8 -3.3 -3.1 5.4	ΔRT MFG Score 11 11 11 11 11 11	CAS ID 0.0 42013-20.7 0.0 0 0.0 0 0.0 114-33-0	METLIN ID 24085	KEGG ID	HMPID
Contraction of the local sector	Mass 193.0735 161.0443 339.0953 337.0796 136.0631 232.0729	NUMP RT 10.933 14.537 13.459 13.180 1.128 14.587	nary: 205 Id Feature ID / 1 2 3 4 5 6	entified Feat Abundance 6857493 1962543 1478903 1256650 1200154 1157221	ures log2(A1/A2) 1.07 -16.00 -16.00 1.00 1.00 1.6.00	Name 2Methythippunic acid n methythicolinamide 31eHaghthooglactic acid	Fomula C10H11N03 C6H905 C13H194407 C13H13H407 C7H9420 C13H1204	۵Mass(ppm) 2.1 3.8 -3.3 -3.1 5.4 3.4	ΔRT MFG Score 1 1 1 1 1 1 1 1 1 1	CAS ID 0.0 42013-201 0.0 0 0.0 0 0.0 114-33-0 8.6 10476-54-1	METLIN ID 24085 2770 2176	KEGG ID	HMPID
	Mass 193 0735 161.0443 339 0953 337.0796 136.0631 232.0729 302.0632	NUMP RT 10.933 14.537 13.459 13.180 1.128 14.587 5.625	nary: 205 Id Feature ID / 1 2 3 4 5 6 7	entified Feat Abundance 6857433 1962543 1478903 125650 1200154 1157221 971597	ures log2(A1/A2) 1.07 -16.00 -16.00 1.00 1.00 1.6.00 1.40	Name 2Mettyhippuric acid nmettyhipcolinamide 3(eNaphthosylactic acid	Fomula C10H11N03 C6H905 C13H15N407 C13H15N407 C7H9X20 C13H1204 C10H12N208	۵Mass(ppm) 21 38 33 33 31 54 34 34 34	ΔRT MFG Score 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	CAS ID 0.0 42013-20-1 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	METLIN ID 24085 3770 2176	KEGG ID	HMPID
1	Mass 193 0735 161.0443 339 0953 337.0796 136 0631 232 0729 302 0632 227.0900	RT 10.933 14.537 13.459 13.180 1.128 14.587 5.625 1.681	nary: 205 Id Feature ID / 1 2 3 4 5 6 7 8	entified Feat Abundance 6857493 1962543 1478903 126650 1200154 1157221 971597 780890	UTES log2(A1/A2) -16.00 -16.00 -16.00 -1.00 -1.00 -1.00 -1.40 -2.02	Name 2MethyReputic acid nmethyRecolmanide 3(aNaphthosySottc acid Deoxycylidine	Formula C10H11N03 C5H505 C13H19N407 C13H19N407 C7H8X20 C13H1204 C10H12N008 C5H13N104	۵۹۹۵۵۵(ppm) 21 38 33 33 -31 54 34 -19 28	ΔRT MFG Score 11 11 11 11 11 11 11 11 11	CAS ID 0.0 4201320. 0.0 0 0.0 0 0.0 114.320 0.0 114.3200 0.0 114.3200 0.0 114.320000000000000000000000000000000000	METLIN ID 24095 2770 2770 2175 2357	KEGG ID	HMPID
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01 1 2 3 4 5 6 7 8 9 10 11 12 13	Mass 193.0735 161.0443 339.0533 337.0796 136.0631 232.0729 302.0632 227.0900 129.0469 142.1100 99.0686 430.0900 145.0525	NUMP RT 10.933 14.537 13.459 13.180 1.128 14.587 5.625 1.681 14.588 1.310 32.158 15.775 13.469	nary: 205 idd Fedure ID / 2 3 4 5 5 6 7 7 8 9 9 10 10 11 11 2 2 13	entified Feat Abundance 6557433 1962543 1478903 1256650 1200154 1157222 971597 780680 745554 675075 562638 564488 495361	UTES log2[A1/A2] 1.07 -16.00 -16.00 1.60 1.00 1.60 2.02 16.00 1.60 1.60 3.46 3.46 2.62	Name 2Methyleparic add nmethylecotraunde 3ENtethnoglande add Desogradde	Fomia C1011103 OFH05 C13113407 C13113407 C1311340 C1311340 C1311340 C1311340 C31120 C3	ΔMass(ppm) 21 38 33 31 54 34 4 4 4 28 4 19 28 41 56 56 417 -29 41	APT MFG Score 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	CASID 2013/201	METUN ID 24025 2720 2720 2025 2025 2025 2025 2025 2	C00891	HMP ID

Agilent METLIN Personal Metabolite Database batch search results include the molecular formulas proposed by the molecular formula generation algorithm, and the MFG probability score.

Identify metabolites and proteins

The Mass Profiler software directly interfaces with several web-based public databases and the optional Agilent METLIN Personal Metabolite Database, enabling you to conveniently launch a search for compound identification from the Mass Profiler application.

For metabolites, save or export METLIN database hits, including molecular formula generation (MFG) results. Export search hits from the METLIN database to a biological pathway analysis application to gain insight about cellular and molecular functions of compounds in the context of functional pathways. For proteins, you can export from the Mass Profiler software a mass list that can be uploaded to the Spectrum Mill software for peptide and protein identification through fast database searches.

Conveniently manage projects, methods, and data

- Create and save projects that specify the group(s) and data files for comparative analysis.
- Save user-specified pre-analysis filters, internal standards, alignment parameters, and results filters to a method that can be applied to user-selected projects. Edit a method to conveniently create a new method.
- Generate inputs to the GeneSpring MS or Spectrum Mill applications from the Feature Summary table or a graphical plot.
- Create a target inclusion list for Agilent Q-TOF MS/MS analysis.
- Export batch summary results .csv files from the METLIN to a biological pathway application to explore relevant biological and chemical information.

About Agilent Technologies

Agilent Technologies is a leading supplier of life science research systems that enable scientists to understand complex biological processes, determine disease mechanisms, and speed drug discovery. Engineered for sensitivity, reproducibility, and workflow productivity, Agilent's life science solutions include instrumentation, microfluidics, software, microarrays, consumables, and services for genomics, proteomics, and metabolomics applications.

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