





Structural complexity of metabolites.



Keys to identifying chemical structures (putative/definitive) by mass spectrometry

- o Retention time in LC
- Accurate mass
- Isotope distribution
- Nitrogen rule
- Fragmentation pattern of a precursor ion
- Comparison with authentic standards (definitive)

Moco et al. Trends in Analytical Chemistry, 2007



Platform to process untargeted metabolomic data

- XCMS (developed by the Siuzdak Lab at the Scripps Research Institute) Online, is a web-based version that allows users to easily upload and process LC-MS data. It is a bioinformatics platform to identify endogenous metabolites..
- METLIN ((<u>http://metlin.scripps.edu</u>) is a metabolite database for metabolomics containing over 64,000 structures and it also has comprehensive tandem mass spectrometry data on over 10,000 molecules at different collision energies.
- Provides an annotated list of known metabolites, their masses, chemical forms and structures.



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19	56 967267e DOWN	248.1261	19.52	6.452	44 183	7.890	78				See parameter	144
22	1.9 9.93395e DOWN	253.0369	13.74	139.227	1,061,319	563,804 (798M)-	15				antipica tah Tor e adarmalah	
21	4.2 1.07130e UP	342,0106	18.78	1.834	3,852	15,140	119					
22	1.8 1.21423# UP	212 (23)	10.72	17,852	37,542	68.907	40					
24	2.5 1.50678e DOWN	587.3766	19.95	- 554	7.036	2,762	37					
25	17.1 (1.52230e DOWN	228.1000	20.66	1.572	97,120	5.871	129					
27	17 215436e UP	263.0063	10.74	5,892	21,778	37,391	40					
28	1.6 2 18376¢ DOWN	334 1315	.14,67	1,011	163,607	101,710	28					
29	5.5.2.17097e DOWN	443.1640	11.60	9,675	102,105	18.013 (212)(4)	87					
31	1.8-2.74162#.DOWN	263.1134	9.95	9.372	17,274	41,811	68					
25	2.1.2.76251e DOWN	605.2895	15.91	1,219	19,355	9,331	21					
34	1.5.3319444 DOWN	304.1076	11.54	2,290	67,825	42,308	97					
26	1.6 .1.84743e DOWN	254 1500	14.19	4,907	48,765	31,912	13		1	M	1.000	1.000000
28	1.4.4.022998-DOWN	634-0789	11.92	6.591	2(37)	41.574	43		100	w Natio	A006	a composi





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	447	18.4	B DOBET UP	240 2588	17.09	872	120	3,277	17					
	1957	. 9.2	0.15752 DOWN	241.0796	8.53	4,139	25.179	22,897	56			standard had been to		
	332		100546.UP	241.1070	18.52	4.140	18,272	21,889	55					
	405	27.4	0.00042 DOWN	241.3579	15.22	79.054	19,412	411741 (6708)	37	-				
	227	12	0.00256 DOWN	241.1112	12.74	7,118	109.918	90.558	24					
	748	2.1	8.82230 UP	241.3983	17.50	758	.23	820	17					
	3045	1.0	8.52756 UP	241.8992	26.05	5.383	47.582	45,418	19				1.00	
	2887	- 11	8.46254 UP	242.877%	4.14	1.042	20,793	22,134	121					_
	2157	10.4	8 28734 DONN	242.1993	10.24	3,875	4,258	18 134 H 194	17					1
	1424	1.5	0.07744.UP	242 9418	3.58	611	5.311	7.766	140					(Second
	823	1.8	9.92712 UP	243.0374	10.59	1.537	9,975	18.921	78					Promotional
	789	12	0.02026 UP	243.0579	10.55	1,537	15,475	18,175	78				-	
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atty Acyls [F	A] (W)> Eicosanoids [FA	03]		
LM_ID	Common Name	Systematic Name	Formula	Mas
LMFA03000001	8(9)-EpETE	(+/-)-8(9)-epoxy-5Z,11Z,14Z,17Z-	C20H30O3	318.2
LMFA0300002	11(12)-EpETE	(+/-)-11(12)-epoxy-5Z,8Z,14Z,17Z-	C20H30O3	318.2
	44(48) 5-575			
LMFA03000003	T4(T2)-EDELE	(+/-)-14(15)-epoxy-52,02,112,172-	C20H30O3	318.2
MFA03000003	17(18)-EpETE	(+/-)-14(15)-epoxy-52,82,112,172- eicosatetraenoic acid (+/-)-17(18)-epoxy-52,82,112,142-	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃	318.2
LMFA03000003	17(13)-EPETE 17(18)-HEDE	<pre>(+/-)-14(15)-epoxy-52,82,112,172- eicosatetraenoic acid (+/-)-17(18)-epoxy-52,82,112,142- eicosatetraenoic acid 11R-hydroxy-12E,142-eicosadienoic acid</pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃	310.; 318.; 324.;
LMFA03000003 LMFA03000004 LMFA03000005 LMFA03000006	17(13)-EpETE 11(R)-HEDE 17R,185-EpETE	<pre>(+/-)-14(3)-epoxy-32.82.112.172- eicosatetraenoic act/32.82.112.172- eicosatetraenoic act/32.82.112.142- eicosatetraenoic acid 11R-hydroxy-12E.142-eicosatenoic acid 17R,103-epoxy-52.82.112.142-</pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃	310.2 318.2 324.2 310.2
LMFA03000003 LMFA03000004 LMFA03000005 LMFA03000006	17(13)*EPETE 17(18)-EPETE 11(R)-HEDE 17R,105-EPETE 15(R)-HEDE	(+7)-24(13)-epoxy-32.02,112,172- eicosatetraencie activatione activation a	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₆ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃	310.2 318.2 324.2 310.2
LMFA03000003 LMFA03000004 LMFA03000005 LMFA03000006 LMFA03000000	17(13)-EpETE 11(R)-HEDE 17R.105-EpETE 15(R)-HEDE 15-HEDE 115-HEDE	(47) 1413 https://www.sci.uk.org/ city.org/ ecoasterisense/ science/ 11R-hydroxy-12E,142-eicosadienoic acid 11R-hydroxy-12E,142-eicosadienoic acid 13R-hydroxy-12E,142-eicosadienoic acid 13S-hydroxy-12E,142-eicosadienoic acid 13S-hydroxy-12E,142-eicosadienoic acid	$C_{20}H_{30}O_3$ $C_{20}H_{30}O_3$ $C_{20}H_{30}O_3$ $C_{20}H_{30}O_3$ $C_{20}H_{30}O_3$ $C_{20}H_{30}O_3$	310.2 318.2 324.2 310.2 324.2 324.2
LMFA03000003 LMFA03000005 LMFA03000005 LMFA03000006 LMFA03000009 LMFA03000009	14(12)-EPETE 17(10)-EPETE 17R,10S-EPETE 17R,10S-EPETE 15(R)-HEDE 11S-HEDE Prostancic acid skeleton	(+/>)-1413)-pipoy/32.02.112.172- (+/>)-11(3)-pipoy/32.02.112.172- eicosatetraenoic acid 118-hydroxy-120.142-eicosadienoic acid 178.185-epoxy-52.02.112.142- eisosatetraenoic acid 158-hydroxy-120.142-eicosadienoic acid 115-hydroxy-120.142-eicosadienoic acid 115-hydroxy-120.142-eicosadienoic acid	$\begin{array}{c} C_{20}H_{30}O_3\\ \\ C_{20}H_{30}O_3\\ \\ C_{20}H_{30}O_3\\ \\ C_{20}H_{30}O_3\\ \\ C_{20}H_{30}O_3\\ \\ C_{20}H_{30}O_3\\ \\ \end{array}$	310.2 318.2 324.2 310.2 324.2 324.2
LMFA03000003 LMFA03000005 LMFA03000006 LMFA03000000 LMFA03000009 LMFA03010000 LMFA03010000	14(12)-EDBIE 11(R)-HEDE 17(R)-HEDE 17/R,105-EDETE 15(R)-HEDE 115-HEDE Prostanoic acid skeleton 6-keto-POFia	<pre>(H/C):14135-general/24.2011.2.172- (H/C):11(3)-general/24.2011.2.142- eicosatetraenoic acid 11R-hydroxy-128,142-eicosadienoic acid 17R-188-genery-52.02.112.142- eicosatetraenoic acid 11Sh-hydroxy-128,142-eicosadienoic acid 11Sh-hydroxy-128,142-eicosadienoic acid 11Sh-hydroxy-128,142-eicosadienoic acid - </pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₆ O ₃ - C ₂₀ H ₃₆ O ₆	310.2 318.2 324.2 310.2 324.2 324.2 - 370.2
LMFA03000003 LMFA03000005 LMFA03000005 LMFA03000006 LMFA03000000 LMFA03010000 LMFA03010000 LMFA03010000	14(13)-EpETE 17(10)-EpETE 11(R)-HEDE 17R,105-EpETE 15(R)-HEDE 135-HEDE Prostancic acid skeleton 6-keto-DGF1a PGF2a	(47)-14135-discoverga2.02.012.172. (47)-11(3)-peopy-52.02.112.142- eicosatetraenoic acid 118-hydroxy-126,142-eicosadienoic acid 138-hydroxy-126,142-eicosadienoic acid 115-hydroxy-126,142-eicosadienoic acid 115-hydroxy-126,142-eicosadienoic acid 115-hydroxy-126,142-eicosadienoic acid 6-oxo-95,118,155-trihydroxy-136- prostenoic acid 95,118,155-trihydroxy-25,136-	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₆ O ₃ - C ₂₀ H ₃₆ O ₆ C ₂₀ H ₃₄ O ₆	310.3 318.3 324.2 310.2 324.2 324.2 324.2 - 370.2 354.2
LMFA03000003 LMFA03000005 LMFA03000005 LMFA03000006 LMFA03000000 LMFA03010000 LMFA03010000 LMFA03010000 LMFA03010000	17(13)-Eperte 17(13)-Eperte 17(R)-HEDE 17(R,105-EpErte 15(R)-HEDE Prostancic acid skeleton 6-kato-PGP1a PGP2a PGP2a PGP2	<pre>(+/-):1413):emony2=2.0:112.172- (+/-):1413):emony2=2.0:112.172- eicosatetrienoic acid 178.h03:emony52.02.112.142- eicosatetrienoic acid 178.h03:emony52.02.112.142- eicosatetrienoic acid 189.hydroxy-112.13E-eicosadienoic acid 119-hydroxy-122.142-eicosadienoic acid - - - </pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₆ O ₃ - C ₂₀ H ₃₆ O ₃ - C ₂₀ H ₃₄ O ₆ C ₂₀ H ₃₄ O ₅	310.2 310.2 324.2 310.2 324.2 324.2 324.2 370.2 354.2 354.2
LMFA03000003 LMFA03000004 LMFA03000006 LMFA03000000 LMFA03000000 LMFA03010000 LMFA03010002 LMFA03010003 LMFA03010004	14(13)-IghTE 11(R)-IHEDE 17R,168-EpHTE 17R,168-EpHTE 115(R)-IHEDE Prostanoic acid skeleton 6-keto-PGF1a PGF2a PGF2 (W) PGF2 (W)	<pre>(+/-):1415)-genovy52.02.112.172- eicosateriaenov52.02.112.142- eicosateriaenoic acid 11R-hydroxy-128.142-eicosadienoic acid 11R-hydroxy-128.142-eicosadienoic acid 11S-hydroxy-128.142-eicosadienoic acid 11S-hydroxy-128.142-eicosadienoic acid 11S-hydroxy-128.142-eicosadienoic acid 95.11R.155-trihydroxy-52.136- prostanicaeid 95.11R.155-trihydroxy-52.136- genose-13R.155.454,740-552.136- 95.136-dhydroxy-11-oxo-52.136-</pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ - C ₂₀ H ₃₆ O ₃ - C ₂₀ H ₃₆ O ₆ C ₂₀ H ₃₄ O ₆ C ₂₀ H ₃₄ O ₅ C ₂₀ H ₃₂ O ₅	310.2 310.2 324.2 324.2 324.2 - 370.2 354.2 352.2 352.2
LMFA0300003 LMFA03000004 LMFA03000005 LMFA03000005 LMFA03000000 LMFA03000000 LMFA03010000 LMFA03010000 LMFA03010003 LMFA03010003 LMFA03010003	14(13)-IghtTE 11(R)-HEDE 17R,105-EpITE 13R-HEDE 13R-HEDE 1313-HEDE Prostancic acid skeleton 6-kete-0611a PGF2a PGE2 (W) PGD4 1	<pre>(H/C):1413):epicovy22.02.112.172- (H/C):11(8)-epicovy52.02.112.142- eicosatetraenoic acid 11R-http://straenoic.acid 11R-http://straenoic.acid 13R-htydrosy-12.12.132-eicosadienoic acid 13B-htydrosy-12.12-13E-eicosadienoic acid 13B-htydrosy-12.13E-eicosadienoic acid 13B-htydrosy-12.13E-eicosadienoic acid 13B-htydrosy-12.13E-eicosadienoic acid </pre>	C20H30O3 C20H30O3 C20H30O3 C20H30O3 C20H30O3 C20H30O3 C20H30O3 - C20H36O3 C20H36O8 C20H36O8 C20H36O8 C20H36O8 C20H32O8	310.2 310.2 324.2 3354.2 3354.2 3354.2 3354.2 3354.2 3354.2 3354.2 3354.2 3354.2
LMFA03000003 LMFA03000003 LMFA03000003 LMFA03000003 LMFA03000003 LMFA03000001 LMFA03010000 LMFA030100003 LMFA03010004 LMFA03010004 LMFA03010004	14(13)-EpiTE 17(10)-EpiTE 17(10)-EpiTE 17R,105-EpiTE 13R-HEDE 13R-HEDE Prostancic add skeleton 6-keto-DFI1a PGF2a PGF2a PGF2 PGF2-44	<pre>(+/-):1413):epicovy22.02.112.172- (+/-):1(18)-epicvy-52.02.112.142- eicosatetraenoic acid 118-hydrosy-12.0.142-eicosadienoic acid 118-hydrosy-12.0.142-idosadienoic acid 119-hydrosy-12.0.142-eicosadienoic acid 119-hydrosy-12.0.142-eicosadienoic acid 119-hydrosy-12.0.142-eicosadienoic acid 95.118.158-trihydrosy-52.138- prostenoic acid 95.118-158-trihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-dihydrosy-52.138- prostenoic acid 95.158-138-trihydrosy-52.138-</pre>	C2043003 C2043003 C2043003 C2043003 C2043003 C2043003 C2043003 - C2043003 C2043003 C2043005 C2043005 C2043205 C2043205 C2043204	310.1 318.2 324.1 310.2 324.2 324.2 324.2 324.2 324.2 324.2 324.2 352.2 352.2 352.2 352.2 356.2
LMFA03000003 LMFA03000004 LMFA03000005 LMFA03000005 LMFA03000005 LMFA03010000 LMFA03010003 LMFA03010003 LMFA03010004 LMFA03010005 LMFA03010005	14(13)-IgnTE 17(10)-IgnTE 17(10)-IgnTE 17k.165-EpITE 17k.165-EpITE 176:1465-E Prostancic acid skeleton 6-keto-POF1a POF2a POF2	<pre>(+/-):1415)-genovy22.02.112.172- eicosateriaenoix acid 11R-hydroxy-128.02.112.142- eicosateriaenoix acid 11R-hydroxy-128.0142-eicosadienoix acid 11S-hydroxy-128.0142-eicosadienoix acid 11S-hydroxy-128.0142-eicosadienoix acid 11S-hydroxy-128.0142-eicosadienoix acid 11S-hydroxy-128.0142-eicosadienoix acid 55.018.118.015-trihydroxy-52.136- prostadienoix acid 95.118.155-trihydroxy-52.136- prostadienoix acid 95.138.55.138.01-00002.136- prostadienoix acid 95.138.155.118.010002.136- prostadienoix acid 95.138.155.118.010002.136- prostadienoix acid 95.118.155-trihydroxy-52.136- prostadienoix acid 95.136- prostadienoix acid 95.136- prostad</pre>	C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₃ - C ₂₀ H ₃₀ O ₃ C ₂₀ H ₃₀ O ₅ C ₂₀ H ₃₀ O ₅	310.2 318.2 324.2 324.2 324.2 324.2 324.2 324.2 354.2 352.2 352.2 352.2 356.2
LMFA03002003 LMFA03002004 LMFA03002005 LMFA03002005 LMFA03002005 LMFA03002005 LMFA03002003 LMFA03010003 LMFA03010003 LMFA03010005 LMFA03010005 LMFA03010005	14(13)-IghTE 17(10)-EpITE 17(10)-EpITE 176.163-EpITE 176.163-EpITE 175.163-EDE Prostancic acid skeleton 6-keto-PGF1a PGF2a PGE2 (W) PGD2 (W) PGD4 PGF2a-d4 PGF2a-d4	<pre>(+/-):1413):epicovg22 (+/-):11(3):epicovg22.02:112:142- eicosatetraenoic acid 17R.103-epicovg-52.02:112:142- eicosatetraenoic acid 17R.103-epicovg-52.02:112:142- eicosatetraenoic acid 19R-hydroxy-12:0:142-eicosadienoic acid 113-hydroxy-12:0:142-eicosadienoic acid 113-hydroxy-12:132-eicosadienoic acid 113-hydroxy-12:132-eicosadienoic acid 0: </pre>	C20H30C3 C20H30C3 C20H30C3 C20H30C3 C20H30C3 C20H30C3 C20H30C3 - C20H30C4 C20H30C4 C20H30C4 C20H30C4 C20H30C4 C20H32C4 C20H32C4 C20H32C4 C20H32C4 C20H32C4	310.: 318.: 324.: 325.: 325.: 325.: 325.: 325.: 325.: 325.: 325.: 325.: 325.:
MEAD300003 MEAD300003 MEAD300003 MEAD300003 MEAD300003 MEAD300003 MEAD30003 MEAD301003 MEAD301003 MEAD301003 MEAD301003 MEAD301003 MEAD301003 MEAD301003	14(13)+IBHTE 17(18)-IBHTE 17(18)-IBHTE 17R,188-EPITE 13R-HEDE 13R-HEDE Prostanoic acid skeleton 6-kete-DGP1a PGF2a PGF2a PGF2a PGF2 PGF2 PGF2 PGF2 PGF2-d4 PGF2-d4	<pre>(+/-):1413):epicony22.02.112.172- (+/-):1(3):epicony22.02.112.142- eicosatetraenoic acid 118.hydrosy125.142-eicosadienoic acid 118.hydrosy125.142-eicosadienoic acid 119.hydrosy125.142-eicosadienoic acid 119.hydrosy125.142-eicosadienoic acid 119.hydrosy125.142-eicosadienoic acid 95.118.155-trihydrosy-52.136- prostancia acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 95.118.155-trihydrosy-52.136- prostadienoic acid 111.155-thydrosy-52.136- prostadienoic acid 95.118.155-thydrosy-52.136- prostadienoic acid 95.118.155-thydrosy-52.136- prostadienoic acid 111.155-thydrosy-52.136- prostadienoic acid 111.155-thydrosy-51.155- prostadienoic acid 1115-1111.155-1115-11155- prostadieno</pre>	C20430C3 C20430C3 C20430C3 C20430C3 C20430C3 C20430C3 C20430C3 C20430C3 C20430C3 C20432C3 C20432C3 C20432C3 C20432C3 C20432C3 C20432C4 C2042C4	310. 318. 324. 310. 324. 325. 352. 355. 356.

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Conclusions

- Identifying unknown metabolites is a significant analytical challenge in metabolomics and it requires integrated analytical and bioinformative approaches.
- Data processing and data analysis are important for putative identifications.
- The use of high-resolution MS and MSⁿ provides important information to propose structures of fragment and precursor ions.
- Only an integrated approach can describes multitude of metabolites present in a biological sample.