

Apéndice A

Tabla S1. Metabolitos identificados putativamente hasta el nivel 2, según el sistema propuesto por la sociedad de metabolómica. Los espectros de referencia fueron tomados del programa libre CFM-ID (v 4.0). ([CFM-ID \(wishartlab.com\)](http://wishartlab.com)).

Metabolito	<i>m/z</i>	Aducto	Iones fragmento. Exp	Iones fragmento. Ref
1-metoxifenantreno	226.1224	[M+NH ₄] ⁺	226.1224	226.1227
			209.0955	209.0961
			153.0700	153.0697
			151.0550	151.0542
1-fenil-2-hexanona	177.1273	[M+H] ⁺	177.1273	177.1274
			57.0341	57.0335
			57.0705	57.0700
			119.0857	119.0855
Ácido L- argininosuccínico	291.1294	[M+H] ⁺	291.1294	291.1299
			89.0231	89.0233
			85.0760	85.0762
			130.0610	130.0611
Fenilacetaldehído	121.0650	[M+H] ⁺	121.0650	121.0648
			91.0545	91.0542
			93.0700	93.0699
			77.0380	77.0386
L-valina	118.0864	[M+H] ⁺	118.0864	118.0862
			72.0813	72.0808
			55.0545	55.0542
			56.0490	56.0494
Estearamida	284.2945	[M+H] ⁺	284.2945	284.2947
			71.0860	71.0855
			97.1015	97.1012
			57.0692	57.0698
Urato-3-ribonucleósido	301.0793	[M+H] ⁺	301.0793	301.0778
			169.0365	169.0356
			151.0255	151.0251

Ácido 11-amino-undecanoico	202.1800	[M+H] ⁺	202.1800	202.1802
			184.1700	184.1696
			89.0590	89.0597
			72.0815	72.0808
Ácido 5-amino-pentanoico	140.0682	[M+Na] ⁺	140.0682	140.0682
			56.0497	56.0495
			55.0545	55.0542
Glicerol	115.0369	[M+Na] ⁺	115.0368	115.0365
			57.0341	57.0349
			75.0446	75.0440
2-(3-fenilpropil) piridina	198.1276	[M+H] ⁺	198.1276	198.1277
			91.0500	91.0495
			65.0395	65.0386
Dodecanamida	200.2008	[M+H] ⁺	200.2008	200.2009
			183.1745	183.1743
			55.0545	55.0542
			57.0700	57.0699
Pipericina	336.3257	[M+H] ⁺	336.3257	336.3266
			72.0813	72.0813
			57.0705	57.0704
			68.0500	68.0500
Creatina	132.0768	[M+H] ⁺	132.0768	132.0766
			115.0545	115.0502
			90.0552	90.0550
			72.05774	72.0556
MG(i-18:0/0:0/0:0)	381.2970	[M+Na] ⁺	381.2970	381.2975
			267.2685	267.2682
			99.1170	99.1168
			249.2585	249.2577
Ácido fenilacético	154.0862	[M+NH ₄] ⁺	154.0862	154.0862
			91.9545	91.9542
			65.0385	65.0386
			119.0495	119.0491
D-glucosamina	180.0865	[M+H] ⁺	180.0865	180.0866
			162.0765	162.0761
			144.0660	144.0655
			60.0440	60.0444
Armillarina	415.2110	[M+H] ⁺	415.2110	415.2115
			95.0859	95.0855

			97.1015	97.1017
			135.0441	135.0446
Ácido L-glutámico	170.0422	[M+Na] ⁺	170.0422	170.0423
			84.0445	84.0444
			85.0286	85.0284
			56.0491	56.0495
Espermidina	146.1651	[M+H] ⁺	146.1651	146.1652
			129.1384	129.1386
			70.0655	70.0651
			72.0815	72.0808
Ácido fenilglioxílico	151.0389	[M+H] ⁺	151.0389	151.0389
			105.0337	105.0335
			133.0280	133.0285
Fosfocreatina	194.0320	[(M+H)-H ₂ O] ⁺	194.0320	194.0325
			130.0612	130.0611
			132.0768	132.0768
Linoleamida	280.2632	[M+H] ⁺	280.2632	280.2635
			95.0860	95.0855
			121.1015	121.1012
			262.2532	262.2529
Isopropilmaleato	159.0651	[M+H] ⁺	159.0651	159.0652
			97.0650	97.0648
			95.0495	95.0491
Ácido 9,10-epoxiesteárico	321.2398	[M+Na] ⁺	321.2398	321.2400
			57.0600	57.0698
			95.0860	95.0855
Fosfoserina	207.9981	[M+Na] ⁺	207.9981	207.9981
			80.9735	80.9736
			140.0109	140.0107
Dihidrouracilo	132.0768	[M+NH ₄] ⁺	132.0768	132.0767
			72.0449	72.0445
			87.0584	87.0555
			115.0545	115.0502
N-butiril-L-homoserina lactona	172.0967	[M+H] ⁺	172.0967	172.0968
			100.0395	100.0393
			102.0552	102.0550
			154.0861	154.0862
7-hexadecenal	239.2367	[M+H] ⁺	239.2367	239.2369
			221.2263	221.2264

			125.1327	125.1325
			109.1009	109.1012
MG(16:0/0:0/0:0)	331.2839	[M+H] ⁺	331.2839	331.2848
			257.2485	257.2481
			299.2945	299.2950
Ácido 10-oxo-nonadecanoico	313.2733	[M+H] ⁺	313.2734	313.2737
			57.0340	57.0334
			55.0548	55.0542
			71.0496	71.0491
Ácido α -linolénico	279.2315	[M+H] ⁺	279.2319	279.2319
			63.0229	63.0229
			81.0699	81.0699
			95.0855	95.0855
Pantotenato	202.1073	[(M+H)-H ₂ O] ⁺	–	–
Ácido 5-oxo-heneicosanoico	341.3046	[M+H] ⁺	341.3046	341.3050
			305.2840	305.2839
			323.2945	323.2945
			95.0851	95.0855
Ácido linoleil hidroxámico	296.2580	[M+H] ⁺	296.2580	296.2684
			121.1013	121.1012
			200.1647	200.1645
			83.0858	83.0855
Ácido 3-hidroxifenilacético	170.0811	[M+NH ₄] ⁺	170.0811	170.0812
			63.0230	63.0229
			65.0389	65.0386
1-metilpirrolinio	107.0706	[M+Na] ⁺	107.0705	107.0705
			57.0705	57.0698
			55.0549	55.0542
			53.0392	53.0386
Ser Arg Tyr	425.2140	[M+H] ⁺	–	–
Pro Lys Asn	358.2078	[M+H] ⁺	–	–
Ácido 2,4,12-octadecatrienoico isobutilamida	334.3102	[M+H] ⁺	334.3102	334.3104
			57.0700	57.0698
			261.2215	261.2213
CDP-ribitol	560.0643	[M+Na] ⁺	560.0643	560.0653
			410.0725	410.0724
			292.9830	292.9822
			502.0625	502.0622

			202.2163	202.2165
10-dodecen-1-ol	202.2164	$[M+NH_4]^+$	97.1015	97.1012
			69.0704	69.0700
			57.0704	57.0700
Dehidrofitoesfingosina	316.2843	$[M+H]^+$	316.2842	316.2846
			71.0849	71.0855
			298.2741	298.2741
			225.2213	225.2213
Ácido fosfohidroxipirúvico	92.9961	$[M+2H]^{++}$	–	–
L-homofenilalanina	180.1018	$[M+H]^+$	180.1018	180.1019
			134.0966	134.0964
			117.0700	117.0698
3-oxo-3-fenilpropanoato	165.0546	$[M+H]^+$	165.0546	165.0546
			119.0492	119.0491
			105.0337	105.0335
L-lisina	129.1023	$[(M+H)-H_2O]^+$	–	–
Fosfato de N-metiletanolamina	156.0421	$[M+H]^+$	156.0421	156.0420
			80.9740	80.9736
			58.0655	58.0651
			98.9844	98.9842
Citosina	112.0508	$[M+H]^+$	112.0508	112.0505
			69.0445	69.0447
			95.0239	95.0239
3-hidroxibenzaldehído	123.0442	$[M+H]^+$	123.0442	123.0441
			95-0495	95-0491
			105.0332	105.0335
			51.0231	51.0230
sn-glicero-3-fosfocolina	130.0629	$[M+2H]^{++}$	130.0629	130.0627
			79.0547	79.0542
			92.0498	92.0495
L-histidina	156.0766	$[M+H]^+$	156.0766	156.0768
			110.0715	110.0712
			93.0450	93.0447
			83.0607	83.0604
Ácido N-carbamoilglutámico	171.0400	$[(M-H)-H_2O]^-$	–	–
Ácido octadecanedioico	313.2377	$[M-H]^-$	313.2377	313.2388
			295.2275	295.2279
			59.0139	59.0139

Arg Arg Met	496.2240	[M+Cl] ⁻	-	-
Ácido 3-oxohexadecanoico	329.2326	[(M+HCOOH)-H] ⁻	329.2333	329.2333
			59.0138	59.0138
			57.0346	57.0346
Oxaloglutarato	203.0197	[M-H] ⁻	203.0197	203.0197
			185.0095	185.0092
			141.0193	141.0193
			113.0245	113.0244
Ácido 12-hidroxiesteárico	299.2585	[M-H] ⁻	299.2585	299.2592
			281.2481	281.2486
			213.1493	213.1496
			129.1280	129.1285
4-fosfopantoato	227.0317	[M-H] ⁻	227.0317	227.0326
			78.9584	78.9591
			183.0431	183.0428
			96.9697	96.9696
Ácido 6-fosfogluconico	275.0167	[M-H] ⁻	275.0167	275.0173
			231.0266	231.0275
			96.9684	96.9696
			78.9578	78.9590
Ácido 10-oxo-11-octadecenoico	295.2270	[M-H] ⁻	295.2270	295.2278
			277.2175	277.2173
			183.1021	183.1026
			111.1165	111.1179
Trp Arg Val	494.2276	[M+Cl] ⁻	-	-