

Checked	Name	Formula	Annot. Sou	Annot. Sou	Annot. Sou	Annot. Sou	Annot. Sou	Annot. Del	Calc. MW	m/z	RT [min]	Area (Max. # ChemSpis)	# mCloud	# mVault	m1 mCloud	m2 mCloud	m3 mCloud	m4 mCloud	Mass List 1	Mass List 2	Reference	Area: JBI01	Area: JBI01	Peak Rating	Peak Rating	
FALSE	Acetohydroxamic acid	C2 H5 N O2	Full match	Full match	No results	Partial mat	Full match	0.78	75,0329	76,0396	1.96	4162068	10	1	0	99,7	10		4094390	4162068		7,5	7,5			
FALSE	Creatinine	C4 H7 N3 C	Full match	Full match	No results	Partial mat	Full match	-0,35	113,0589	114,0662	1,342	1,03E+08	3	1	0	99,6	10		Single mat	No matche DDA for pr	[M+H]+1	1,03E+08	1,01E+08	8,4	8,4	
FALSE	D-(+)-Pyroglutamic Acid	C5 H7 N O3	Full match	Full match	No results	Full match	Full match	0,2	129,0426	130,0499	2,67	9400175	17	5	0	99,6	10	57,4	Multiple m	No matche DDA for pr	[M+H]+1	9400175	8542528	7,3	6,2	
FALSE	L-(-)-Methionine	C5 H11 N C	Full match	Full match	No results	Full match	Full match	-0,26	149,051	150,0583	1,962	59182065	13	2	0	99,5	95,1		Multiple m	No matche DDA for pr	[M+H]+1	59182065	58736203	8,4	8,4	
FALSE	L-(-)-Citrulline	C6 H13 N3	Full match	Full match	No results	Full match	Full match	0,04	175,0957	176,103	1,281	22908237	7	1	0	99,3	95,1		Single mat	No matche DDA for pr	[M+H]+1	22908237	21663172	9,5	9,5	
FALSE	Acetyl-L-carnitine	C9 H17 N C	Full match	Full match	No results	Full match	Full match	-1,08	203,1155	204,1228	1,962	1,55E+08	10	1	0	99,3	68,5		Single mat	No matche DDA for pr	[M+H]+1	1,55E+08	1,53E+08	8,9	8,9	
FALSE	Caffeine	C8 H10 N4	Full match	Full match	No results	Full match	Full match	-1,25	194,0801	195,0874	4,651	1,02E+08	7	3	0	99,2	68,2		Single mat	Single mat	DDA for pr	[M+H]+1	1E+08	1,02E+08	9,5	9,5
FALSE	Acetyl-L-carnitine	C9 H17 N C	Full match	Full match	No results	Full match	Full match	-0,1	203,1157	204,123	2,143	29828226	10	1	0	99,2	67,9		Single mat	No matche DDA for pr	[M+H]+1	24512950	29828226	6,7	7,3	
FALSE	Acetyl-L-carnitine	C9 H17 N C	Full match	Full match	No results	Full match	Full match	-0,06	203,1158	204,123	2,218	15358697	10	1	0	99,1	67,7		Single mat	No matche DDA for pr	[M+H]+1	12818633	15358697	7,8	7,8	
FALSE	Valine	C5 H11 N C	Full match	Full match	No results	Full match	Full match	-1,24	117,0788	118,0861	1,819	4,96E+08	40	3	0	99	9,9		Multiple m	No matche DDA for pr	[M+H]+1	4,96E+08	4,89E+08	8,4	8,4	
FALSE	DL-Carnitine	C7 H15 N C	Full match	Full match	No results	Full match	Partial mat	-0,26	161,1052	162,1124	1,291	74207483	7	3	0	98,9	66,5		Multiple m	Single mat	DDA for pr	[M+H]+1	74164024	74207483	8,4	8,4
FALSE	Lactamide	C3 H7 N O2	Full match	Full match	No results	Not the tof	Full match	0,21	89,0477	90,05497	1,193	42582384	19	3	0	98,8	9,9		Multiple m	No matche DDA for pr	[M+H]+1	42198896	42582384	7,3	8,4	
FALSE	L-Isoleucine	G6 H13 N C	Full match	Full match	No results	Not the tof	Full match	-0,29	131,0946	132,1019	2,918	1,01E+08	52	4	0	98,8	9,9		Multiple m	No matche DDA for pr	[M+H]+1	1,01E+08	88888057	5,7	6,2	
FALSE	L-Norleucine	G6 H13 N C	Full match	Full match	No results	Not the tof	Full match	-0,93	131,0945	132,1018	3,236	4,78E+08	52	4	0	98,7	9,9		Multiple m	No matche DDA for pr	[M+H]+1	4,78E+08	4,59E+08	8,4	8,4	
FALSE	L-Isoleucine	G6 H13 N C	Full match	Full match	No results	Not the tof	Full match	-0,4	131,0946	132,1019	3,102	1,21E+08	52	4	0	98,6	9,9		Multiple m	No matche DDA for pr	[M+H]+1		1,21E+08		7,3	
FALSE	L-Pyrogutamic acid	C5 H7 N O2	Full match	Full match	No results	Full match	Full match	0,1	129,0426	130,0499	1,214	18827421	17	2	0	98,6	9,9		Multiple m	No matche DDA for pr	[M+H]+1		18827421		8,9	
FALSE	D-(-)-Glutamine	C5 H10 N2	Full match	Full match	No results	Full match	Full match	0,15	146,0692	147,0764	1,214	1,01E+08	29	4	0	98,4	93,7	49,7	Multiple m	No matche DDA for pr	[M+H]+1	1,01E+08		8,9		
FALSE	Paraxanthine	C7 H8 N4 C	Full match	Full match	No results	Full match	Full match	-0,72	180,0646	181,0719	4,19	41991111	6	9	0	98,2	63,5	76	Multiple m	No matche DDA for pr	[M+H]+1	41304284	41991111	8,4	8,4	
FALSE	D-(-)-Glutamine	C5 H10 N2	No match	Invalid ma	No results	No match	No match	-280871	105,0426	106,0499	1,211	34237099	13	4	0	98,2	93,2	48,1	Multiple m	No matche DDA for ot	[M+H]+1	34237099	2353389	8,6	8,6	
FALSE	Kojic acid	G6 H6 O4	No match	Invalid ma	No results	No match	No results	-16,73	142,0242	143,0315	1,953	160265,4	2	2	0	98,1	9,9		No matche	No matche DDA for pr	[M+H]+1		160265,4		4,3	
FALSE	Theobromine	C7 H8 N4 C	Full match	Full match	No results	Full match	Full match	-0,4	180,0647	181,0719	3,958	20883247	6	9	0	97,9	98,29	62,5	Multiple m	No matche DDA for pr	[M+H]+1	19002510	20883247	7,8	8,9	
FALSE	Pipecolic acid	G6 H11 N C	Full match	Full match	No results	Full match	Partial mat	0,26	129,079	130,0863	1,518	4681244	54	4	0	97,8	9,9		Multiple m	Multiple m	DDA for pr	[M+H]+1	4681244	4179992	7	5,3
FALSE	DL-Stachydrine	C7 H13 C N	No match	Invalid ma	No results	No match	No results	-223811	111,0684	144,1019	1,629	33850351	28	3	0	97,8	9,9		No matche	No matche DDA for ot	[M+H+MeC]	33731160	33850351	8,4	8,4	
FALSE	Uric acid	C5 H4 N4 C	Full match	Full match	No results	Full match	Full match	-0,8	168,0282	169,0355	2,402	1,45E+08	4	1	0	97,8	92,2		Single mat	No matche DDA for pr	[M+H]+1	1,45E+08	1,36E+08	8,4	8,4	
FALSE	L-Histidine	G6 H9 N3 C	Full match	Full match	No results	Full match	Full match	-0,09	155,0695	156,0768	1,163	8804469	12	11	0	97,7	92,1	61,9	Multiple m	No matche DDA for pr	[M+H]+1	8804469	7983428	9,5	9,5	
FALSE	Uric acid	C5 H4 N4 C	Full match	Full match	No results	Full match	Full match	-0,89	168,0282	169,0355	2,799	1,9E+08	4	1	0	97,7	92		Single mat	No matche DDA for pr	[M+H]+1	1,88E+08	1,9E+08	8,4	8,4	
FALSE	D-(+)-Proline	C5 H9 N O2	Full match	Full match	No results	Full match	Full match	-0,06	115,0633	116,0706	1,411	2,56E+08	30	2	0	97,5	9,9		Multiple m	Single mat	DDA for pr	[M+H]+1	2,56E+08	2,53E+08	9,5	8,4
FALSE	Indole-3-acetic acid	C10 H9 N C	Full match	Full match	No results	Full match	Full match	-0,15	175,0633	176,0706	6,017	4584430	31	2	0	97,5	9,9		Multiple m	Multiple m	DDA for pr	[M+H]+1	4442144	4584430	8	8
FALSE	Triethyl phosphate	G6 H15 O4	Full match	Full match	No results	Full match	Full match	0,29	182,0709	183,0781	6,12	448536,4	4	1	0	97,2	9,9		Single mat	No matche DDA for pr	[M+H]+1	425105,6	448536,4	6,3	6,3	
FALSE	Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N	Full match	Full match	No results	Full match	No results	-0,74	292,0905	293,0977	7,215	4,06E+08	3	1	0	97,1	90,6		No matche	No matche DDA for pr	[M+H]+1		4,06E+08		7,8	
FALSE	Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N	Full match	Full match	No results	Full match	No results	-0,44	292,0905	315,0798	1,338	1,01E+08	3	1	0	97,1	98,7		No matche	No matche DDA for pr	[M+Na]+1		1,01E+08		7,8	
FALSE	Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N	Full match	Full match	No results	Full match	No results	-1,6	292,0902	293,0975	1,462	1,46E+10	3	1	0	97	98,6		No matche	No matche DDA for pr	[M+H]+1	1,46E+10	1,41E+10	8,4	8,4	
FALSE	Creatine	C4 H9 N3 C	Full match	Full match	No results	Full match	Full match	0,22	131,0695	132,0768	1,414	53041815	10	5	0	97	58,3		Multiple m	Single mat	DDA for pr	[M+H]+1	53041815	50972769	9,5	8,4
FALSE	L-Pyrogutamic acid	C5 H7 N O2	Full match	Full match	No results	Full match	Full match	0,21	129,0426	130,0499	2,41	6356392	17	5	0	96,7	9,8	55,2	Multiple m	No matche DDA for pr	[M+H]+1	6356392	6292629	7,8	7,8	
FALSE	Palmitoyl sphingomyelin	C39 H79 N	Not the tof	Full match	No results	Full match	No results	0,49	702,5679	703,5752	7,135	57806228	5	1	0	96,6	9,8		No matche	No matche DDA for pr	[M+H]+1	53546810	57806228	6,2	6,2	
FALSE	N3,N4-Dimethyl-L-arginine	C8 H18 N4	Full match	Full match	No results	Full match	Full match	0,04	202,143	203,1503	1,548	3730631	8	1	0	96,5	98,5		Single mat	No matche DDA for pr	[M+H]+1	6749183	70370631	8,9	9,5	
FALSE	1-Aminocyclohexanecarboxylic acid	C7 H13 N C	Full match	Full match	No results	Partial mat	Full match	0,22	143,0947	144,1019	1,96	4590679	27	2	0	96,3	55,7		Single mat	Multiple m	DDA for pr	[M+H]+1	4590679	4278186	8	8
FALSE	DL-α-Aminocaprylic acid	C8 H17 N C	Full match	Full match	No results	Full match	Partial mat	0,32	159,126	160,1333	4,662	1119045	16	1	0	96,3	55,6		No matche	Single mat	DDA for pr	[M+H]+1	1015393	1119045	7,2	8,3
FALSE	L-Tyrosine	C9 H11 N C	Full match	Full match	No results	Full match	Partial mat	-0,87	181,0737	182,0881	3,231	2,18E+08	37	3	0	96,2	98,4	53,2	Multiple m	Single mat	DDA for pr	[M+H]+1	2,18E+08	2,1E+08	9,5	9,5
FALSE	Choline	C5 H13 N C	Full match	Full match	No results	Partial mat	Full match	0,15	103,0997	104,107	1,243	34261133	17	1	0	96,1	9,8		Single mat	No matche DDA for pr	[M+H]+1	34261133	31993421	8,4	8,9	
FALSE	1-Methylhistidine	C7 H11 N3	Full match	Full match	No results	Full match	Full match	0,05	169,0851	170,0924	1,177	8508026	13	5	0	96,1	88		Multiple m	No matche DDA for pr	[M+H]+1	8508026	8275173	7,8	8,4	
FALSE	Phloroglucinol	G6 H6 O3	Full match	Full match	No results	Partial mat	Full match	-0,12	126,0317	127,039	0,386	47317585	24	6	0	96	87		Multiple m	Multiple m	DDA for pr	[M+H]+1		47317585		7
FALSE	7-Methylxanthine	G6 H6 N4 C	Full match	Full match	No results	Full match	Full match	-0,05	166,0491	167,0563	3,637	1022761	9	3	0	95,9	9,8		Multiple m	No matche DDA for pr	[M+H]+1	1004414	1022761	7,7	7,7	
FALSE	DL-Tryptophan	C11 H12 N	Full match	Full match	No results	Full match	Partial mat	-1,08	204,0897	205,0969	4,131	2,99E+08	32	4	0	95,9	87,6	44,6	Multiple m	Multiple m	DDA for pr	[M+H]+1	2,63E+08	2,99E+08	9,5	9,5
FALSE	3-Acetyl-2,5-dimethylfuran	C8 H10 O2	No match	Invalid ma	No results	No match	No match	130447,2	156,0787	157,0859	7,044	10669419	14	9	0	94,7	9,7	46,2	No matche	Multiple m	DDA for ot	[M+H]+1	10669419	10425168	4	5,1
FALSE	DL-Homoserine	C4 H9 N O3	Full match	Full match	No results	Full match	Full match	0,31	119,0583	120,0656	1,221	20527488	37	4	0	94,7	49,4		Multiple m	No matche DDA for pr	[M+H]+1	20527488	19810506	8,9	8,9	
FALSE	Maleic hydrazide	C4 H4 N2 C	Full match	Full match	No results	Partial mat	Partial mat	0,27	112,0273	113,0346	3,22	1785911	12	3	0	94	9,7		Single mat	Single mat	DDA for pr	[M+H]+1	1785911	1607252	7,7	7,2
FALSE	3-Acetyl-2,5-dimethylfuran	C8 H10 O2	Full match	Full match	No results	Partial mat	Partial mat	0,03	138,0681	139,0754	7,055	20365137	62	4	0	93,9	9,7	45,7	Single mat	Multiple m	DDA for pr	[M+H]+1	20365137		4	
FALSE	2-Mercaptoethanol	C2 H6 O S	Full match	Full match	No results	Not the tof	Full match	-0,03	78,01393	79,02121	1,357	3,65E+08	3	1	0	93,8	9,7		Single mat	No matche DDA for pr	[M+H]+1	3,65E+08		4,6		
FALSE	NP-021074	C13 H20 O	No match	Invalid ma	No results	No match	No results	85823,11	278,113	279,1203	5,895	2287151	2	1	0	93,3	45,5		No matche	No matche DDA for pr	[M+H]+1	2258744	2287151	4,2	4,2	
FALSE	N-Ethylglycine	C4 H9 N O2	Full match	Full match	No results	Not the tof	Full match	0,04	103,0633	104,0706	1,338	17995528	35	8	0	93,2	9,7		Multiple m	No matche DDA for pr	[M+H]+1	17995528	16561845	7,8	6,2	
FALSE	DL-Arginine	G6 H14 N4	Full match	Full match	No results	Full match	Full match	-0,23	174,1116	175,1189	1,164	45831944	10	2	0	93,2	78,7		Multiple m	No matche DDA for pr	[M+H]+1	45831944	43566952	8,4	7,3	
FALSE	N,N-Dimethylaniline	C8 H11 N	Full match	Full match	No results	Partial mat	Full match	0,18	121,																	

FALSE	Benzothiazole	C7 H5 N S	Full match	Full match	No results	Full match	No results	0,2	135,0143	136,2161	1,449	24862822	5	11	0	77,7	8,9	58,9	No matche	No matche	DDA for pr	[M+H]+1	24862822	1682705	4	0,7
FALSE	N,N-Diisopropylethylamine (DIPEA)	C8 H19 N	Full match	Full match	Full match	Full match	No results	-0,11	129,1517	130,159	7,589	4776793	16	1	0	76,7	8,8		No matche	No matche	DDA for pr	[M+H]+1	4776793		5,3	
FALSE	N,N,N4-Dimethyl-L-arginine	C8 H18 N4	No results	Full match	No results	Partial mat	Full match	-0,07	202,143	203,1502	1,487	1746773	9	1	0	76,5	67,9		Single mat	No matche	DDA for pr	[M+H]+1	1687236	1746773	7,2	7,2
FALSE	Adenosine	C10 H13 N	Not the to	Full match	Full match	Full match	Partial mat	0,07	267,0968	268,1041	3,299	946828	12	1	0	74,8	8,7		Multiple m	Single mat	DDA for pr	[M+H]+1	946828	846085,3	6,1	6,6
FALSE	Methyl indole-3-acetate	C11 H11 N	Full match	Full match	No results	Not the to	Full match	-0,27	189,0789	190,0862	6,493	2051266	29	1	0	74,7	8,7		Multiple m	Multiple m	DDA for pr	[M+H]+1	2039385	2051266	6,1	8,8
FALSE	Methyl 2-(4-acetylamino)-4-amino-4-oxobutanoic acid	C7 H12 N2	Full match	Full match	No results	Partial mat	Full match	-0,16	188,0797	189,087	1,578	94090825	7	3	0	74,6	45,7	42,7	Single mat	No matche	DDA for pr	[M+H]+1	94090825	92148407	6,2	6,2
FALSE	Caprolactam	C6 H11 N	C Full match	Full match	Full match	Partial mat	No results	0,35	113,0842	114,0914	4,443	806117,6	23	1	0	74,4	27		No matche	No matche	DDA for pr	[M+H]+1	729682,3	806117,6	6,8	6,3
FALSE	N,N-Diisopropylethylamine (DIPEA)	C8 H19 N	Full match	Full match	No results	Full match	No results	0,25	129,1518	130,1591	4,458	3168084	16	1	0	73,8	8,7		No matche	No matche	DDA for pr	[M+H]+1	2747234	3168084	5,3	4,8
FALSE	Gabapentin	C9 H17 N	C Full match	Full match	No results	Full match	Partial mat	0,16	171,126	172,1332	1,962	1994978	20	2	0	73,6	8,7		No matche	Single mat	DDA for pr	[M+H]+1	1895789	1994978	8,6	7,5
FALSE	Palmitic acid	C16 H32 O	No match	Invalid ma	No results	No match	No results	66447,34	273,2667	274,274	6,788	18716855	3	1	0	73,5	26,5		No matche	No matche	DDA for pr	[M+H]+1	18036861	18716855	9,5	8,4
FALSE	Bilirubin	C33 H36 N	Not the to	Full match	No results	Full match	Full match	0,19	584,2636	585,2709	6,563	3664575	6	1	0	73,1	8,7		Multiple m	No matche	DDA for pr	[M+H]+1	3424028	3664575	9,1	8,6
FALSE	bicyclo[2.2.2]oct-2-en-1-yl 4-methylbenzene	C15 H18 O	No match	Invalid ma	No results	No match	No match	-14	278,0398	279,1011	3,618	1342137	5	1	0	71,9	25,5		No matche	Single mat	DDA for pr	[M+H]+1	1032429	1342137	5,5	6,6
FALSE	Indole-3-lactic acid	C11 H11 N	Full match	Full match	No results	Not the to	Full match	-0,07	205,0739	206,0812	5,539	1773973	24	2	0	71,8	42,1		Multiple m	Multiple m	DDA for pr	[M+H]+1	1694622	1773973	7,2	7,2
FALSE	N-Methylcaprolactam	C7 H13 N	C Full match	Full match	No results	Not the to	No results	0,03	127,0997	128,107	5,681	2300964	26	1	0	70,6	8,5		No matche	No matche	DDA for pr	[M+H]+1	2193677	2300964	6,4	6,4
FALSE	Thiglic acid	C5 H8 O2	Full match	Full match	No results	Not the to	Full match	0,13	100,0524	101,0597	7,021	26710590	37	1	0	70,2	8,5		Multiple m	No matche	DDA for pr	[M+H]+1	26710590	25095439	4,6	4
FALSE	3-(3,4,5-trimethoxyphenyl)propanoic acid	C12 H16 O	No match	Invalid ma	No results	No match	No match	-75013	222,0892	223,0965	6,88	1782541	64	1	0	70,1	39,8		No matche	Multiple m	DDA for pr	[M+H]+1	1782541	1780556	6,6	6,6
FALSE	1-Tetradecylamine	C14 H31 N	Full match	Full match	No results	Full match	Partial mat	-0,31	213,2456	214,2529	6,917	1529381	5	1	0	68,2	8,4		No matche	Single mat	DDA for pr	[M+H]+1	1351943	1529381	7,7	6,6
FALSE	7-methyl-3-nitroimidazo[1,2-a]pyridine	C8 H7 N3	C No match	Invalid ma	No results	No results	No results	124140,2	199,0333	200,0406	1,155	2735337	0	1	0	67,4	24,1		No matche	No matche	DDA for pr	[M+H]+1	2735337	2516788	7	7,5
FALSE	7-methyl-3-nitroimidazo[1,2-a]pyridine	C8 H7 N3	C No match	Invalid ma	No results	No match	No results	1248322	398,0741	200,0443	1,248	1495208	1	1	0	67,4	24,1		No matche	No matche	DDA for ot	[M+2H]+2	1495208	877081,5	3,9	7,2
FALSE	2-(Phenylthio)-1-[4-(1H-pyrrrol-1-yl)]piperidin	C17 H20 N	No match	Invalid ma	No results	No match	No results	13,64	300,3327	301,141	1,101	18970069	3	8	0	67,4	39,7		No matche	No matche	DDA for pr	[M+H]+1	18970069	16579789	6,2	6,2
FALSE	(S)-(+)-2-Amino-1-propanol	C3 H9 N O	Full match	Full match	No results	Full match	Full match	0,87	75,06848	76,07576	1,303	5630789	10	1	0	67,3	8,4		Multiple m	No matche	DDA for pr	[M+H]+1	5630789	5633026	7	7,5
FALSE	2-[[3S]-1-(3,4-Difluorobenzyl)-3-pyrrolidinyl]	C18 H16 F2	No match	Invalid ma	No results	No match	No results	11,58	314,1267	315,134	6,973	3069537	10	2	0	67,1	8,4		No matche	No matche	DDA for pr	[M+H]+1	2523281	3069537	8	7,5
FALSE	NP-011892	C17 H14 O	No match	Invalid ma	No results	No match	No results	-20,44	314,0726	315,0799	1,57	17521002	1	4	0	65,7	8,3		No matche	No matche	DDA for pr	[M+H]+1	17521002		7,8	
FALSE	NP-011892	C17 H14 O	No match	Invalid ma	No results	No match	No results	-20,62	314,0726	315,0798	1,369	1,17E+08	1	4	0	65	23,9		No matche	No matche	DDA for pr	[M+H]+1		1,17E+08		6,2
FALSE	NP-011892	C17 H14 O	No match	Invalid ma	No results	No match	No results	-20,83	314,0725	315,0798	2,125	1,5E+08	1	3	0	65	23,9		No matche	No matche	DDA for pr	[M+H]+1		1,5E+08		5,7
FALSE	Cortisol	C21 H30 O	Full match	Full match	No results	Full match	Partial mat	-0,22	362,2093	363,2165	6,437	5074129	32	2	0	63,1	56,6		Multiple m	Multiple m	DDA for pr	[M+H]+1	5062200	5074129	7,5	8,6
FALSE	N6-Me-Adenosine	C11 H15 N	Not the to	Full match	No results	Partial mat	Partial mat	0,3	281,1125	282,1198	2,346	1170402	9	1	0	62,6	8,1		Multiple m	Single mat	DDA for pr	[M+H]+1	1142050	1170402	7,2	7,2
FALSE	Aflatoxin B2	C17 H14 O	No match	Invalid ma	No results	No match	No results	69968,43	336,0547	337,0619	1,354	1951352	3	6	0	61,9	8,1		No matche	No matche	DDA for pr	[M+H]+1	1951352		8,6	
FALSE	NP-001223	C10 H18 O	Unused	Invalid ma	No results	No match	No match	181115,7	208,11	209,1172	7,265	2436344	60	4	0	60,9	8		Single mat	Multiple m	DDA for pr	[M+H]+1	2436344	2038967	5,3	7,5
FALSE	1-Methylxanthine	C6 H6 N4	C Full match	Full match	No results	Full match	Full match	0,04	166,0491	167,0564	3,724	845965,6	9	3	0	59,4	8		Multiple m	No matche	DDA for pr	[M+H]+1	802417,4	845965,6	8,5	7,7
FALSE	N-Acetylorithine	C7 H14 N2	Full match	Full match	No results	Full match	Full match	0,27	174,1005	175,1078	1,621	82211076	16	3	0	57,8	7,9	41,6	Multiple m	No matche	DDA for pr	[M+H]+1	8221076	8046765	7,8	7,8
FALSE	Methionine	C5 H11 N	C Full match	Full match	No results	Full match	Full match	0,26	149,0511	150,0584	2,214	1520644	13	2	0	57,6	23,2		Multiple m	No matche	DDA for pr	[M+H]+1		1520644		6,1
FALSE	1,7-Dimethyluric acid	C7 H8 N4	C Full match	Full match	No results	Full match	Full match	0,24	196,0597	197,067	4,009	502156,2	6	3	0	56,2	23		Multiple m	No matche	DDA for pr	[M+H]+1	492656,2	502156,2	7,4	7,9
FALSE	L-2,4-Diaminobutyric acid	C4 H10 N2	Full match	Full match	No results	Full match	Partial mat	0,37	118,0743	119,0816	1,535	8669124	20	17	0	55,9	23	61,8	Single mat	Multiple m	DDA for pr	[M+H]+1	8669124	6544594	6,2	4,6
FALSE	Ecgoneine methyl ester	C10 H17 N	Full match	Full match	No results	Full match	Full match	0,12	199,1209	241,1547	3,216	2129271	22	1	0	55,1	22,9		Single mat	Single mat	DDA for pr	[M+ACN+H]	2129271	1096585	6,4	7,2
FALSE	Bilirubin	C33 H36 N	Not the to	Full match	No results	Full match	Full match	0,3	584,2637	585,2709	5,474	657583,3	6	1	0	54,8	7,7		Multiple m	No matche	DDA for pr	[M+H]+1	657583,3	649035,9	7,9	7,9
FALSE	Thiglic acid	C5 H8 O2	No match	Invalid ma	No results	No match	No match	170176,7	117,079	101,0598	1,019	1431721	40	1	0	53,6	7,7		Multiple m	No matche	DDA for ot	[M+H-NH3]	1431721		4,5	
FALSE	4-[[3-(Diethylamino)propyl]amino]-4-oxobutanoic acid	C11 H20 N	Full match	Full match	No results	Partial mat	Partial mat	0,17	228,1474	229,1547	2,246	1765610	6	2	0	53,3	36,5		Multiple m	Multiple m	DDA for pr	[M+H]+1	1741705	1765610	7,2	5
FALSE	Diphenylamine	C12 H11 N	Full match	Full match	No results	Partial mat	Full match	-1,03	169,089	170,0963	1,242	1364549	15	2	0	52,8	7,6		Multiple m	No matche	DDA for pr	[M+H]+1	1364549		5	
FALSE	NP-003459	C9 H14 O4	No match	Invalid ma	No results	No match	No match	-96784,7	168,0786	169,0859	6,967	81373112	42	1	0	52,1	22,6		Single mat	Multiple m	DDA for pr	[M+H]+1		81373112		5,1
FALSE	4,5-diphenyl-1,3-oxazole-2-thiol	C15 H11 N	No match	Invalid ma	No results	No match	No results	10,33	253,0588	254,066	1,694	1061925	4	1	0	51,7	7,6		No matche	No matche	DDA for pr	[M+H]+1	1061925	1017643	7,7	7,7
FALSE	4-Acetamidobutanoic acid	C6 H11 N	C Full match	Full match	No results	Partial mat	Full match	0,45	145,0714	146,0812	1,35	1865806	29	2	0	51,1	22,5		Multiple m	No matche	DDA for pr	[M+H]+1	393309,5	1865806	2,2	5
FALSE	Cyclohexylamine	C6 H13 N	Full match	Full match	No results	Full match	No results	0,15	99,10481	100,1121	3,505	1980042	17	1	0	50,3	22,5		No matche	No matche	DDA for pr	[M+H]+1	1980042	1817067	7	7,2
FALSE	Hydrolyzed fumonisin B1	C22 H47 N	Full match	Full match	No results	Full match	No results	0,13	405,3455	406,3528	6,825	968928,5	1	1	0	49,9	22,4		No matche	No matche	DDA for pr	[M+H]+1	955475,1	968928,5	8,8	8,3
FALSE	Dihydrothymine	C5 H8 N2	C Full match	Full match	No results	Full match	Full match	0,08	128,0586	129,0659	1,381	17045610	19	1	0	49,8	7,5		Single mat	No matche	DDA for pr	[M+H]+1	16407028	17045610	7,8	8,4
FALSE	5-Ethylcyclohexane-1,3-dione	C8 H12 O2	Full match	Full match	No results	Partial mat	Partial mat	-0,81	140,0836	141,091	7,172	37409656	46	1	0	49,7	22,4		Multiple m	Multiple m	DDA for pr	[M+H]+1		37409656		4
FALSE	INK	C16 H31 N	No match	Invalid ma	No results	No match	No match	-495981	188,1163	189,1235	1,627	390967,9	20	3	0	49,3	7,5		Multiple m	No matche	DDA for pr	[M+H]+1	390967,9		4,9	
FALSE	5-Nitro-o-toluidine	C7 H8 N2	C Full match	Full match	No results	Full match	Full match	-0,17	152,0586	153,0658	3,493	2594898	34	3	0	49	52,9	77,8	Multiple m	No matche	DDA for pr	[M+H]+1	2561561	2594898	8	8
FALSE	N-Acetyl-L-carnosine	C11 H16 N	Not the to	Full match	No results	Full match	Full match	-0,12	268,1272	269,1245	1,962	1370146	12	1	0	48,5	7,4		Single mat	No matche	DDA for pr	[M+H]+1	1248705	1370146	7,2	8,3
FALSE	Guvacoline	C7 H11 N	C No results	Full match	No results	Not the to	Full match	-1,76	141,0787	142,0863	1,955	2143191	18	1	0	48	7,4		Single mat	No matche	DDA for pr	[M+H]+1	1955011	2143191	7,5	7
FALSE	4-Isobutylbenzoic acid	C11 H14 O	Full match	Full match	No results	Partial mat	Partial mat	-0,07	178,0994	179,1066	7,435	3276281	95	2	0	47,9	7,4		Multiple m	Multiple m	DDA for pr	[M+H]+1	3175347	3276281	7	7,5
FALSE	N2-[5-Phenyl-4-(trifluoromethyl)-1,3-thiazol-2-yl]thioacetamide	C15 H9 F3	No match	Invalid ma	No results	No match	No results	-107235	316,0485	317,0559	1,534	6821933	1	1	0	47,2	7,4		No matche	No matche	DDA for ot	[M+H]+1		6821933		5,7

FALSE	[Similar to: NP-017683; ΔMass: -562.4259 Da]	C10 H18 N	Full match	Invalid ma	No results	No results	No match	No results	0.05	382,1086	383,1159	1,244	39980487	1	10	0		46	No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	36377837	39980847	9,5	9,5
FALSE	N-Carbamoyl-2,2,2-trichloroacetamide	C3 H3 Cl3	No results	No results	No results	No results	Full match	No results	0.09	203,926	102,9703	0,998	89764106	1	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	89764106		7,3	
FALSE			No results	No results	No results	No results	Full match	No results		95,91451	96,92179	1,144	42443032	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	42443032	40045536	9,5	8,4
FALSE	Phenylacetylene	C8 H6	Full match	Invalid ma	No results	No results	Full match	No results	-0,17	102,0469	120,0808	3,681	34599633	4	12	0			No match	No match	DDA for ot	[M+NH4] <sup>+</sup> +1	33833701	34599633	9,5	9,5
FALSE		C4 H3 N4	C Full match	No results	No results	No results	No results	No results	-4,59	361,9189	362,9262	1,101	34620138	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	34620138	32980610	8,9	8,9
FALSE			No results	No results	No results	No results	No results	No results		129,9579	130,9652	0,992	79373297	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	70658932	79373297	7,8	5,7
FALSE		C8 H12 O3	Full match	No results	No results	No results	No match	No results	-3,41	218,0254	110,02	0,34	18867348	3	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2		18867348		9,5
FALSE		C2 H7 N2	C Full match	No results	No results	No match	No results	No results	-3,74	215,9433	216,9506	0,982	62847983	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	57448046	62847983	8,4	8,4
FALSE		C2 H2 N4	C Full match	No results	No results	No results	No results	No results	0,8	351,8919	430,9135	1,101	28763618	0	0	0			No match	No match	DDA for pr	[M+DMSO]	28763618	27790758	8,9	8,9
FALSE			No results	No results	No results	No results	No results	No results		178,999	90,50676	0,3	6703940	0	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	5862002	6703940	9,5	8,9
FALSE	4-(2-Hydroxyethyl)phenyl hydrogen sulfate	C6 H12 N4	Full match	No results	No results	No match	No results	No results	-2,71	202,0532	102,0339	0,996	82226748	1	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	82226748	72942572	6,7	6,7
FALSE		C8 H10 O5	No results	No results	No results	Full match	No results	No results	1,93	218,0253	110,0199	7,584	3,97E+08	3	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	3,97E+08	89028761	6,2	5,7
FALSE	3-(4-Chlorophenyl)-3-Methoxypropyl Chloride	C10 H12 Cl	No results	No results	No results	Full match	No results	No results	-4,85	218,0255	110,02	0,304	19553015	6	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	19553015	6135274	6,2	9,5
FALSE	[Similar to: EQH; ΔMass: -244.1196 Da]		No results	Invalid ma	No results	No results	No results	No results		168,0511	169,0584	1,214	34024938	0	10	0		45,8	No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	34024938	33482627	9,5	9,5
FALSE	O-ureido-D-serine	C4 H9 N3	C Full match	No results	No results	No results	Partial mat	No results	2,02	163,0596	82,53709	0,733	55265591	2	0	0			No match	Multiple m	No MS2	[M+2H] <sup>+</sup> +2		55265591		7,3
FALSE		C2 H5 N2	C Full match	No results	No results	No results	No results	No results	-3,85	197,9328	239,9666	0,989	49297987	0	0	0			No match	No match	DDA for pr	[M+ACN+H]	49297987	47380703	7,8	8,4
FALSE			No results	No results	No results	No results	No results	No results		157,9568	158,9641	1,105	36314373	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	36314373	34968664	8,9	8,9
FALSE		C8 H12 O3	Full match	No results	No results	No match	No results	No results	-3,48	218,0254	110,02	7,377	3,18E+08	3	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2		3,18E+08		5,1
FALSE	Diethylpyrocarbonate	C6 H10 O5	Full match	No results	No results	Full match	Full match		-0,01	162,0528	145,0496	1,247	73834250	49	0	0			Multiple m	No match	DDA for pr	[M+H+H2O]	25212433	73834250	9,5	5,1
FALSE		C4 H O13	F Full match	No results	No results	No results	No results	No results	-2,79	287,9147	288,922	1,072	25365367	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	25365367	23468134	8,9	8,4
FALSE		C H3 N2 O6	Full match	No results	No results	No results	No results	No results	2,12	231,9209	232,9282	0,995	51723142	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	49895805	51723142	5,1	5,7
FALSE			No results	No results	No results	No results	No results	No results		103,996	105,0033	0,972	51569590	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	46126481	51569590	7,3	7,3
FALSE		C2 H7 O4	F Full match	No results	No results	No match	No results	No results	-2,63	219,9272	220,9345	1,07	24037010	3	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	24037010	22062132	8,4	8,9
FALSE		C2 H6 N2	C Full match	No results	No results	No results	No results	No results	3,18	122,0331	82,53712	0,974	43481716	0	0	0			No match	No match	DDA for pr	[M+ACN+2]		43481716		5,1
FALSE	[Similar to: 2-(4-chlorophenyl)-2-oxoethyl-2,	C7 H4 O9	F Full match	Invalid ma	No results	No results	No results	No results	-4,96	293,9316	294,9389	1,103	22934414	0	1	0		45,3	No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	22934414	22116505	8,9	9,5
FALSE	3-Amino-2,3,6-trideoxy-α-l-rbo-hexopyran	C6 H13 N	C Full match	No results	No results	Full match	No results	No results	0,08	147,0896	130,0863	1,957	19071582	22	0	0			No match	No match	DDA for pr	[M+H+H2O]	19071582	18597789	8,4	8,4
FALSE	C8-Carnitine	C15 H29 N	Full match	No results	No results	Full match	Full match		-0,59	287,2095	288,2168	5,957	21184994	5	0	0			Multiple m	No match	DDA for pr	[M+H] <sup>+</sup> +1	19104284	21184994	8,4	8,4
FALSE			No results	No results	No results	No results	No results	No results		176,9988	89,50669	7,584	3E+08	0	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2	3E+08	56279126	5,1	6,2
FALSE	Allyltrimethylsilane	C6 H14 Si	No results	No results	No results	Full match	No results	No results	-0,02	114,0865	115,0938	7,209	6878409	5	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	6878409	6596087	6,2	4,6
FALSE	EDDA	C6 H12 N2	Full match	No results	No results	Full match	No results	No results	0,35	176,0798	177,087	1,515	1,17E+08	13	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	1,17E+08	90101093	6,7	4
FALSE			No results	No results	No results	No results	No results	No results		155,113	156,1203	7,305	2,93E+08	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1		2,93E+08		6,2
FALSE			No results	No results	No results	No results	No results	No results		221,8605	222,8678	1,143	15509102	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	15509102	14679023	8,4	8,4
FALSE		C H Cl2 N2	Full match	No results	No results	No match	No results	No results	-3,67	205,8866	206,8939	1,141	17774965	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	17774965	16736469	8,4	8,4
FALSE		C7 H5 N6	C Full match	No results	No results	No match	No match		-2,02	220,0258	111,0202	7,592	1,71E+08	2	0	0			Single mat	No match	DDA for ot	[M+2H] <sup>+</sup> +2	1,56E+08	1,71E+08	6,2	6,2
FALSE		C9 H4 N2	C Full match	No results	No results	No results	No results	No results	-1,67	377,8929	378,9002	1,102	18098696	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	18098696	17138458	8,9	8,9
FALSE		C7 H3 N3	C Full match	No results	No results	No results	No results	No results	-4,13	176,999	89,50675	7,377	2,45E+08	0	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2		2,45E+08		4,6
FALSE	Methyltrifluorosilane	C H3 F3 Si	No results	No results	No results	Full match	No results	No results	2,79	99,99589	101,0032	1,099	48922419	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	48922419	47077516	6,2	4,6
FALSE	2-Amino-6-nitrobenzothiazole	C7 H5 N3	C Full match	No results	No results	Full match	No results	No results	-3,94	195,0095	98,51202	0,34	9722488	4	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2		9722488		9,5
FALSE		C7 H5 N6	C Full match	No results	No results	No match	No match		-1,72	220,0259	111,0202	0,304	12164209	2	0	0			Single mat	No match	DDA for ot	[M+2H] <sup>+</sup> +2	9559016	12164209	9,5	9,5
FALSE	BLAH	S Se	No results	No results	No results	Full match	No results	No results	-1,35	111,8884	112,8957	1,145	17052908	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	17052908	16124631	9,5	9,5
FALSE		C4 H6 O17	Full match	No results	No results	No results	No results	No results	-1,98	419,8793	498,9011	1,101	15327811	0	0	0			No match	No match	DDA for pr	[M+DMSO]	15327811	14654328	8,9	8,9
FALSE		C2 H N5 O	Full match	No results	No results	No results	No results	No results	-4,62	142,9895	143,9968	0,99	39346691	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	39346691		5,1	
FALSE		C3 H3 N2	C Full match	No results	No results	No results	No results	No results	-3,33	367,8658	446,8876	1,102	14718093	0	0	0			No match	No match	DDA for ot	[M+DMSO]	14718093	14332281	8,9	8,9
FALSE		C4 H12 N2	Full match	No results	No results	No results	No results	No results	-4,22	184,025	185,0323	1,207	16848959	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1		16848959		9,5
FALSE		C7 H5 N8	C Full match	No results	No results	No results	No results	No results	0,8	565,8812	566,8885	1,1	12249262	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	12249262	11747883	8,9	8,4
FALSE			No results	No results	No results	No results	No results	No results		140,9513	141,9586	0,318	54404433	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	54404433	4558261	5,1	7,5
FALSE	Citric acid	C6 H8 O7	Full match	No results	No results	Full match	Partial mat		-0,28	192,027	215,0161	2,145	37169594	17	0	0			Multiple m	Single mat	DDA for pr	[M+Na] <sup>+</sup> +1	37169594	36264946	7,8	7,8
FALSE	1-Octanesulfonyl fluoride	C8 H17 F O	No results	No results	No results	Full match	No results	No results	1,37	196,0936	219,0828	1,147	6462999	1	0	0			No match	No match	DDA for pr	[M+Na] <sup>+</sup> +1	6462999	5096178	9,5	9,1
FALSE		C4 H8 N O4	Full match	No results	No results	No match	No results	No results	2,75	165,0196	83,51705	0,994	33566682	4	0	0			No match	No match	No MS2	[M+2H] <sup>+</sup> +2	33566682	30519041	5,1	6,2
FALSE		C2 H N3 O2	Full match	No results	No results	No results	No results	No results	1,08	99,00698	100,0143	0,986	29229400	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	29229400		6,7	
FALSE	9-Decenoylcarnitine	C17 H31 N	Full match	No results	No results	Full match	No results	No results	-0,28	313,2252	314,2325	6,38	15426626	1	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	14357391	15426626	8,9	9,5
FALSE		C4 H N4 O2	Full match	No results	No results	No results	No results	No results	-0,88	309,9055	310,9128	1,103	14770823	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	14770823	14557024	9,5	9,5
FALSE		C5 H2 N5	C Full match	No results	No results	No results	No results	No results	-1,95	178,9994	90,50695	0,339	6466827	0	0	0			No match	No match	DDA for ot	[M+2H] <sup>+</sup> +2		6466827		9,5
FALSE		C3 H5 N2	F Full match	No results	No results	No results	No results	No results	-1,18	131,991	132,9982	0,972	28354978	0	0	0			No match	No match	DDA for pr	[M+H] <sup>+</sup> +1	24144281	28354978	7,3	5,1
FALSE			No results	No results	No results	No results	No results	No results		555,8544	634,876	1,1	9364542	0	0	0			No match	No match	DDA for ot	[M+DMSO]		9364542		8,9
FALSE			No results	No results	No results	No results	No results	No results		1267,738	634,8761	1,098														



FALSE	TEMPO	C9 H19 N	Full match	No results	No results	No results	Full match	No results	-0.05	157,1467	158,1539	7,293	16145697	11	0	0	0	No match	No match	No MS2	[M+H]+1	16145697	13249974	7,3	7,8
FALSE				No results	No results	No results	No results	No results		255,8135	256,8207	1,172	9439791	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	9439791	9223827	8,4	6,7
FALSE		C5 H9 Cl N	Full match	No results	No results	No results	No match	No results	-3.09	260,0039	261,0112	1,232	13831721	1	0	0	0	No match	No match	DDA for pr	[M+H]+1	13391670	13831721	7,3	8,4
FALSE		C3 H2 N3 P	Full match	No results	No results	No results	No match	No results	3.18	110,9999	112,0063	0,983	16736731	1	0	0	0	No match	No match	DDA for pr	[M+H]+1	16736731	16261382	5,7	7,8
FALSE	Phenylac-gln-OH	C13 H16 N	Full match	No results	No results	Full match	Full match		-0.18	264,111	265,1182	4,722	7400760	9	0	0	0	Multiple m	Multiple m	DDA for pr	[M+H]+1	7203945	7400760	8,4	8,9
FALSE	Benzofuran-2-carbonyl chloride	C9 H5 Cl O	No results	No results	No results	Full match	No results		-3.06	179,9973	91,00591	0,3	1798508	6	0	0	0	No match	No match	No MS2	[M+2H]+2	1798508		8,8	
FALSE				No results	No results	No results	No results	No results		156,9875	79,50104	0,981	16465062	0	0	0	0	No match	No match	DDA for ot	[M+2H]+2	16115810	16465062	7,8	5,7
FALSE	Citric acid	C6 H8 O7	Full match	No results	No results	Full match	Partial mat		-0.18	192,027	215,0162	2,388	30123772	19	0	0	0	Multiple m	Single mat	DDA for pr	[M+Na]+1	29995744	30123772	7,8	7,8
FALSE		C9 H7 O P	Full match	No results	No results	No results	No match		1.53	162,0237	82,01913	0,987	15720533	3	0	0	0	No match	No match	DDA for ot	[M+2H]+2	15720533	14525297	5,1	5,7
FALSE		C8 H4 N6 C	Full match	No results	No results	No results	No results	No results	0.54	581,8553	582,8626	1,1	6119765	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	6017929	6119765	8,9	8,9
FALSE				No results	No results	No results	No results	No results		1299,686	650,8501	1,099	5635270	0	0	0	0	No match	No match	DDA for ot	[M+2H]+2	5635270	5433258	8,6	8,6
FALSE		C3 H5 Cl O	Full match	No results	No results	No results	No results	No results	-3.51	409,8499	40,8562	1,124	4830422	0	0	0	0	No match	No match	DDA for ot	[M+H]+1	4830422	4617532	8,6	8,6
FALSE	2-Hydroxyethyl phosphate	C2 H7 O5 P	Full match	No results	No results	Full match	Full match		3.42	142,0036	72,00907	0,983	16481762	1	0	0	0	No match	No match	DDA for ot	[M+2H]+2	16481762	15303482	6,2	5,7
FALSE	Glu-Glu	C10 H16 N	Full match	No results	No results	Full match	Full match		0.02	276,0958	318,1296	1,952	5290670	7	0	0	0	Single mat	No match	DDA for ot	[M+ACN+H]	5204578	5290670	7,5	8
FALSE	γ-Glu-gln	C10 H17 N	Full match	No results	No results	Full match	Full match		-0.31	275,1117	276,1189	1,499	9926095	9	0	0	0	No match	No match	DDA for pr	[M+H]+1	9926095			8,9
FALSE		C5 H N4 O2	Full match	No results	No results	No results	No results	No results	-2.36	179,9833	99,51225	0,305	1519532	0	0	0	0	No match	No match	No MS2	[M+H+NH4]		1519532		8,3
FALSE	C12-Carnitine	C19 H37 N	Full match	No results	No results	Full match	No results		-0.21	343,2722	344,2795	6,918	8727777	5	0	0	0	No match	No match	DDA for pr	[M+H]+1	7427797	8727777	8,4	9,5
FALSE	1-arachidonoyl-sn-glycero-3-phosphocholine	C28 H50 N	Full match	No results	No results	Full match	No results		-0.19	543,3324	544,3397	7,413	13908873	3	0	0	0	No match	No match	DDA for pr	[M+H]+1	13908873		7,8	
FALSE		C4 H6 Cl2 F	Full match	No results	No results	No results	No results	No results	-1.79	341,8615	342,8688	1,134	5824351	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	5824351	5328207	8,4	8
FALSE	Tetrolic Acid	C4 H4 O2	Full match	No results	No results	Full match	Partial mat		0.44	84,02117	117,0547	1,248	19120560	11	0	0	0	Single mat	Single mat	DDA for pr	[M+H+MeC]		19120560		4,6
FALSE				No results	No results	No results	No results	No results		111,0107	112,0179	7,592	66067266	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	61654209	66067266	6,2	6,2
FALSE	Methyl 1,2,2,6,6-pentamethyl-4-piperidyl sel	C21 H39 N	Full match	No results	No results	Full match	Partial mat		-0.13	369,2879	370,2951	7,007	9777091	10	0	0	0	No match	Single mat	DDA for pr	[M+H]+1	8306184	9777091	8,4	8,4
FALSE		C2 H4 Br Cl	Full match	No results	No results	No results	No results	No results	3.73	263,8452	264,8525	1,144	5819265	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	5819265	5242649	8,9	8,6
FALSE	Cyclopentylamine	C5 H11 N	Full match	No results	No results	Full match	Full match		0.19	85,08917	86,09644	2,889	25516281	6	0	0	0	Single mat	No match	DDA for pr	[M+H]+1	25516281	22279835	5,1	6,7
FALSE	Platelet-activating factor	C26 H54 N	Full match	No results	No results	Full match	No match		0.99	523,3643	524,371	7,124	36050639	6	0	0	0	No match	Multiple m	DDA for pr	[M+H]+1		36050639		6,7
FALSE	[Similar to: N-[1-(4-methoxyphenyl)-5-methy			No results	Invalid ma	No results	No results	No results		82,04128	187,0714	1,504	18082503	0	4	0	0	No match	No match	DDA for ot	[2M+Na]+1	18082503		5,7	
FALSE				No results	No results	No results	No results	No results		110,0023	111,0095	0,976	15136647	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	15136647	14218196	7,8	5,1
FALSE				No results	No results	No results	No results	No results		90,01028	218,9837	0,976	12331925	0	0	0	0	No match	No match	DDA for pr	[2M+K]+1	10921892	12331925	7,8	8,4
FALSE				No results	No results	No results	No results	No results		1435,66	718,8374	1,099	4938340	0	0	0	0	No match	No match	DDA for ot	[M+2H]+2	4938340	4800017	8,6	8,6
FALSE		C4 H4 Br O F	Full match	No results	No results	No results	No results	No results	-0.25	237,8345	238,8417	1,143	5055138	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	5055138	4814135	9,1	9,1
FALSE		C2 H4 Br N	Full match	No results	No results	No results	No results	No results	-2.6	273,874	274,8813	1,138	5673359	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	5673359	5342252	8,4	8,6
FALSE	trans-2-Dodecenoylcarnitine	C19 H35 N	Full match	No results	No results	Full match	No results		-0.18	341,2566	342,2638	6,804	10924562	3	0	0	0	No match	No match	DDA for pr	[M+H]+1	10349668	10924562	7,8	8,4
FALSE	Coumarone	C8 H6 O	Full match	Invalid ma	No results	Full match	No results		0.34	118,0419	136,0757	3,232	6427123	6	10	0	0	No match	No match	DDA for pr	[M+NH4]+	6427123	5697173	8,4	8,4
FALSE		C22 H46 N	Full match	No results	No results	No match	No match		4.85	519,3323	520,3396	6,435	1,51E+08	6	0	0	0	Single mat	Single mat	DDA for pr	[M+H]+1	1,44E+08	1,51E+08	5,1	6,2
FALSE		C2 H Cl4 Ni	Full match	No results	No results	No results	No results	No results	-2.65	405,766	406,7725	1,143	4093435	0	0	0	0	No match	No matches	No MS2	[M+H]+1	4093435	3872335	8,6	8,6
FALSE		C6 H3 Cl O	Full match	No results	No results	No results	No results	No results	-4.89	283,9029	284,9101	1,126	4658151	0	0	0	0	No match	No match	No MS2	[M+H]+1	4506313	4658151	8,6	7
FALSE		C3 H5 Cl N	Full match	No results	No results	No results	No results	No results	-0.23	199,9658	241,9997	0,972	11197713	0	0	0	0	No match	No match	No MS2	[M+ACN+H]	11034456	11197713	7,8	8,4
FALSE		C4 H4 O2 P2	Full match	No results	No results	No results	No results	No results	0.52	141,9408	164,93	1,114	6737043	0	0	0	0	No match	No match	DDA for ot	[M+Na]+1	6737043	3791369	7,8	8
FALSE				No results	No results	No results	No results	No results		769,8436	770,8509	1,099	4636765	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	4636765		8,6	
FALSE		C H2 N2 O4	Full match	No results	No results	No match	No results	No results	-3.08	231,9102	232,9174	1,112	3327695	1	0	0	0	No match	No match	DDA for pr	[M+H]+1	3327695	3169619	9,1	9,1
FALSE		C7 H11 N4	Full match	No results	No results	No match	No results	No results	-4.67	278,0403	261,037	1,248	10671974	3	0	0	0	No match	No match	DDA for pr	[M+H+H2O]	10671974	10311111	8,9	8,9
FALSE		C5 H6 N O4	Full match	No results	No results	No match	No results	No results	1.44	175,0037	88,50912	0,339	3157732	1	0	0	0	No match	No match	DDA for ot	[M+2H]+2		3157732		9,1
FALSE				No results	No results	No results	No results	No results		1539,687	770,851	1,097	4885464	0	0	0	0	No match	No match	DDA for ot	[M+2H]+2		4885464		8,6
FALSE		C H2 Cl4 O	Full match	No results	No results	No results	No results	No results	3.32	279,8192	280,8265	1,144	4538312	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	4538312	4158397	9,1	8,6
FALSE				No results	No results	No results	No results	No results		178,0023	90,00841	0,327	4756741	0	0	0	0	No match	No match	DDA for ot	[M+2H]+2	2429684	4756741	5,9	8
FALSE				No results	No results	No results	No results	No results		253,8164	254,8237	1,172	7764920	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	7764920	7083809	8,9	9,5
FALSE		C2 H N4 O2	Full match	No results	No results	No results	No results	No results	-0.73	349,8852	350,8925	1,061	4731438	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	4731438	4412086	8,6	8,6
FALSE	5-Hydroxy-2-furoic acid	C5 H4 O4	Full match	No results	No results	Full match	No results		0.06	128,011	129,0182	2,144	12814129	1	0	0	0	No match	No match	DDA for pr	[M+H]+1	12710345	12814129	8,4	7,8
FALSE		C2 H7 Cl2	Full match	No results	No results	No results	No results	No results	0.84	289,848	290,8553	1,14	4676833	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	4676833	4570947	8	8
FALSE				No results	No results	No results	No results	No results		130,967	113,9637	0,34	3435918	0	0	0	0	No match	No match	DDA for ot	[M+H+H2O]		3435918		9,1
FALSE		C4 H Cl2 O	Full match	No results	No results	No results	No results	No results	-0.01	357,8354	358,8427	1,136	5277924	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	5277924	4740616	8	8
FALSE	2-Keto-glutaramic acid	C5 H7 N O4	Full match	No results	No results	Full match	Full match		0.37	145,0376	187,0713	1,507	33971986	2	0	0	0	Multiple m	Single mat	DDA for pr	[M+ACN+H]		33971986		5,7
FALSE		C H N2 O P	Full match	No results	No results	No results	No results	No results	4.44	87,98304	130,0169	0,974	13288555	0	0	0	0	No match	No match	DDA for ot	[M+ACN+H]	12892904	13288555	5,1	6,2
FALSE				No results	No results	No results	No results	No results		99,01712	82,01383	0,975	12622085	0	0	0	0	No match	No match	DDA for pr	[M+H+H2O]	12622085	11135521	5,7	4
FALSE	[Similar to: L-(+)-Citrulline; ΔMass: 21.9942	C6 H15 N C	Full match	Invalid ma	No results	No results	No results	No results	0	197,0899	198,0972	1,254	12754015	0	1	0	0	No match	No match	DDA for pr	[M+H]+1	12593986	12754015	5,7	8,4
FALSE				No results	No results	No results	No results	No results		291,1069	292,1142	1,442	8476717	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	8281704	8476717	8,9	6,7
FALSE		C8 H15 N2	Full match	No results	No results	No match	No results	No results	0.56	330,0466	331,0539	1,368	8732467	2	0	0	0	No match	No match	DDA for pr	[M+H]+1	8732467		6,2	
FALSE		C3 H2 Cl3 F	Full match	No results	No results	No results	No results	No results	-2.57	415,7948	416,8013	1,139	4180758	0	0	0	0	No match	No match	No MS2	[M+H]+1	4180758	3858768	8	8
FALSE		C3 H N2 O	Full match	No results	No results	No results	No results	No results	3.1	173,9307	174,938	1,106	8174348	0</											

FALSE	Thiomorpholine	C4 H9 N S	Full match	No results	No results	No results	Full match	No results	0,32	103,0456	104,0529	1,962	3384310	2	0	0	0	No match	No match	DDA for pri	[M+H]+1	3384310	3132572	8	8,6
FALSE				No results	No results	No results	No results	No results		87,51355	88,52083	1	1015288	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1015288	857058,1	5	3,4
FALSE		C2 H4 O6 F	Full match	No results	No results	No results	No match	No results	3,71	185,949	186,9563	0,308	15634217	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	14466559	15634217	6,7	7,8
FALSE		C2 H4 N2 C	Full match	No results	No results	No results	No match	No results	-2,59	277,9156	316,8788	1,111	1281640	1	0	0	0	No match	No match	DDA for otl	[M+K]+1	1281640	1151278	8,8	7,2
FALSE	N-Acetyl-N-hydroxyacetamide	C4 H7 N O2	Full match	No results	No results	Full match	Partial mat		0,2	117,0426	118,0499	1,96	3427847	14	0	0	0	Multiple m	Single mat	DDA for pri	[M+H]+1	3427847	3318526	8	7,8
FALSE		C9 H19 N C	Full match	No results	No results	No match	No results		-2,35	235,0886	236,0958	1,508	26870208	2	0	0	0	No match	No match	No MS2	[M+H]+1		26870208		5,1
FALSE	2-Oxirylacetonitrile	C4 H5 N O	Full match	Invalid ma	No results	Full match	No results		0,37	83,03714	84,04442	0,358	50571963	6	20	0	0	No match	No match	DDA for pri	[M+H]+1	50571963	44129303	2,9	4
FALSE	5-Methoxy-1-(D-ribofuranosyl)-2,4(1H,3H)-p	C10 H14 N	Full match	No results	No results	Full match	No results		0,16	274,0801	307,1136	1,96	3295300	2	0	0	0	No match	No match	DDA for otl	[M+H+MeC]	3295300	3231657	8	8
FALSE		C2 H C14 Ni	Full match	No results	No results	No results	No results		3,25	389,7912	390,7985	1,142	3224279	0	0	0	0	No match	No match	No MS2	[M+H]+1	2682693	3224729	8,6	8
FALSE	2-Aminoisobutyric Acid	C4 H9 N O2	Full match	No results	No results	Full match	Full match		0,4	103,0634	104,0706	1,246	3313026	35	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1	3317192	3313026	9,1	8,6
FALSE		C3 H8 Cl O	Full match	No results	No results	No results	No results		0,99	299,8768	300,8841	1,129	3661653	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	3661653	3471252	8	8
FALSE		C2 H C13 N	Full match	No results	No results	No results	No results		0,84	331,8327	332,84	1,141	3435361	0	0	0	0	No match	No match	No MS2	[M+H]+1	3327478	3435361	8	8,6
FALSE				No results	No results	No results	No results			105,9433	106,9506	1,11	7253175	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	7253175	6832726	7,8	7,8
FALSE				No results	No results	No results	No results			88,00107	89,00835	0,339	2493898	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		2493898		9,1
FALSE		C11 H13 Cl	Full match	No results	No results	No results	No results		-3,01	354,0043	355,0115	1,534	6599846	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	6599846		8,4	
FALSE				No results	No results	No results	No results			128,9719	129,9792	0,981	10098808	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	10098808	9460393	7,3	5,7
FALSE		C25 H42 N	Full match	No results	No results	No results	No results		-2,81	590,2783	296,1464	7,316	12902669	0	0	0	0	No match	No match	DDA for otl	[M+2H]+2	12304936	12902669	6,2	7,8
FALSE		C4 H4 N6 C	Full match	No results	No results	No match	No results		1,49	184,0348	185,042	1,111	12259927	4	0	0	0	No match	No match	DDA for pri	[M+H]+1	12248904	12259927	5,7	5,7
FALSE		C4 H4 N4 C	Full match	No results	No results	No results	No results		0,72	393,8669	394,8742	1,102	4083514	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	4083514	4056794	8,6	8,6
FALSE		C2 H5 N2 C	Full match	No results	No results	No results	No results		3,74	327,8907	328,898	0,978	7462217	0	0	0	0	No match	No match	No MS2	[M+H]+1	7141578	7462217	5,7	5,7
FALSE		C53 H86 Ni	Full match	No results	No results	No results	No results		-0,05	980,6033	491,3089	7,395	7983200	0	0	0	0	No match	No match	DDA for otl	[M+2H]+2	7983200	7733356	8,4	8,4
FALSE	Butyl 3,4,5-trimethoxybenzoate	C14 H20 O	Full match	No results	No results	Full match	Partial mat		0,22	268,1311	251,1278	7,264	5039204	5	0	0	0	No match	Multiple m	DDA for pri	[M+H-H2O]	5039204	4419507	8	8
FALSE	(iii) hydride	H2 Sn	No results	No results	No results	Full match	No results		-4,87	121,9173	122,9245	1,109	7001754	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	7001754	6585582	5,1	7,8
FALSE		C13 H2 N6	Full match	No results	No results	No results	No results		-0,66	559,8644	560,8716	1,08	4352789	0	0	0	0	No match	No match	No MS2	[M+H]+1	4352789	4002639	8	8
FALSE		C45 H76 N	Full match	No results	No results	No match	No results		-1,52	781,5623	782,5696	7,16	52030231	49	0	0	0	No match	No match	DDA for pri	[M+H]+1		52030231		6,2
FALSE		C23 H42 N	Full match	No results	No results	No results	No results		-2,89	467,3012	468,3085	6,926	8957842	5	0	0	0	No match	No match	DDA for pri	[M+H]+1	5143749	8957842	8	8,9
FALSE	pdta	C11 H18 N	Full match	No results	No results	Full match	No results		0,33	306,1064	307,1137	1,65	7439311	2	0	0	0	No match	No match	DDA for pri	[M+H]+1	7439311	7044522	7,8	8,4
FALSE		C45 H76 N	Full match	No results	No results	No match	No results		-1,29	781,5625	782,5698	7,272	43784322	49	0	0	0	No match	No match	DDA for pri	[M+H]+1	43784322		5,7	
FALSE		C2 H C14 O	Full match	No results	No results	No results	No results		-3,76	337,7778	338,7851	1,147	3226219	0	0	0	0	No match	No match	No MS2	[M+H]+1	3226219	2193055	9,1	8,6
FALSE	PC(18:1/0:0)	C26 H52 N	Full match	No results	No results	Full match	Full match		3,17	521,3498	522,3557	7,401	2932518	5	0	0	0	Single mat	No match	DDA for otl	[M+H]+1	2782795	2932518	4,2	7,5
FALSE				No results	No results	No results	No results			90,01624	91,02352	0,975	9995331	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		9995331		5,1
FALSE		C2 H5 O7 F	Full match	No results	No results	No results	No results		1,64	203,9497	204,957	1,07	4674244	0	0	0	0	No match	No match	No MS2	[M+H]+1	4674244	4331296	8	8,6
FALSE		C8 H2 Cl N	Full match	No results	No results	No match	No results		-3,24	206,9651	207,9724	1,194	475681,5	1	0	0	0	No match	No match	DDA for otl	[M+H]+1	475681,5	434667	7,9	7,9
FALSE				No results	No results	No results	No results			809,3711	270,7976	1,173	5454052	0	0	0	0	No match	No match	DDA for otl	[M+3H]+3	5454052		8,6	
FALSE		C5 H2 N5 C	Full match	No results	No results	No results	No results		-2,05	178,9993	90,50694	7,582	30216323	0	0	0	0	No match	No match	DDA for otl	[M+2H]+2	30216323	11145592	6,2	5,1
FALSE				No results	No results	No results	No results			119,9736	120,9809	0,99	9804352	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	9248404	9804352	4,6	5,1
FALSE				No results	No results	No results	No results			130,967	113,9637	0,304	1065488	0	0	0	0	No match	No match	No MS2	[M+H-H2O]		1065488		8,3
FALSE	Tilarginine	C7 H16 N4	Full match	No results	No results	Full match	Full match		0,1	188,1273	189,1346	1,229	4466616	8	0	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1	4364692	4466616	7,5	7,5
FALSE				No results	No results	No results	No results			1247,68	624,8474	1,114	1913861	0	0	0	0	No match	No match	No MS2	[M+2H]+2	1913861		9,7	
FALSE	1,1'-[2,6-Dimethyl-4-(3-nitrophenyl)-1,4-dihy	C17 H18 N	Full match	No results	No results	Full match	No results		0,09	314,1267	315,134	7,055	5164646	10	0	0	0	No match	No match	DDA for pri	[M+H]+1	3997375	5164646	8,6	8
FALSE	alpha-Ketoglutaric acid	C5 H6 O5	Full match	No results	No results	Full match	Full match		0,06	146,0215	147,0288	2,144	8545078	6	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1	8545078	8393743	7,3	8,9
FALSE		C2 H2 Br Cl	Full match	No results	No results	No results	No results		2,84	269,7904	270,7976	1,171	5021088	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		5021088		7,5
FALSE	2-Amino-6-nitrobenzothiazole	C7 H5 N3 C	Full match	No results	No results	Full match	No results		-3,58	195,0096	98,51205	7,381	60608138	4	0	0	0	No match	No match	DDA for otl	[M+2H]+2	46622380	60608138	2,9	5,1
FALSE		C34 H45 N	Full match	No results	No results	No match	No results		-4,08	611,3671	612,3744	7,461	8217571	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	5752749	8217571	6,2	8,4
FALSE		C4 H2 Cl4	Full match	No results	No results	No results	No results		-4,3	395,7378	474,76	1,142	2589920	0	0	0	0	No match	No match	No MS2	[M+DMSO-	2589920	2305564	8	8
FALSE		C4 H2 O13	Full match	No results	No results	No results	No results		-3,85	383,8397	462,8616	1,102	3526258	0	0	0	0	No match	No match	DDA for otl	[M+DMSO-	3526258	3490383	8,6	8,6
FALSE				No results	No results	No results	No results			86,98628	87,99355	0,979	8297366	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		8297366		5,1
FALSE		C2 H C14 P	Full match	No results	No results	No results	No results		4,16	195,8578	196,8651	1,168	5823920	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	5823920	5629069	8,9	6,4
FALSE		C2 H3 N7 S	Full match	No results	No results	No results	No results		-3,32	157,0165	79,51555	0,994	8220452	1	0	0	0	No match	No match	DDA for otl	[M+2H]+2	8220452	7022212	5,7	6,2
FALSE	2-Methyl-2,4-thiazolidinedicarboxylic acid	C6 H9 N O4	Full match	No results	No results	Full match	No results		-0,02	191,0252	192,0325	1,794	5916322	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	5916322	5757167	6,2	8,4
FALSE		C44 H80 N	Full match	No results	No results	No results	No results		0	892,5508	447,2827	7,411	7547466	0	0	0	0	No match	No match	DDA for otl	[M+2H]+2	7547466	7008658	6,7	8,4
FALSE		C3 H12 Cl F	Full match	No results	No results	No results	No results		1,76	247,9917	248,999	1,196	3411583	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		3411583		7,8
FALSE		C18 H29 N	Full match	No results	No results	No results	No results		-0,04	475,1914	238,603	1,937	2886140	0	0	0	0	No match	No match	DDA for otl	[M+2H]+2	2886140	2714277	8	7,5
FALSE				No results	No results	No results	No results			1255,704	628,8591	1,081	3718970	0	0	0	0	No match	No match	No MS2	[M+2H]+2	3718970		8	
FALSE		C30 H53 N	Full match	No results	No results	No results	No match		4,49	655,3934	656,4007	7,457	8018230	0	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	5521965	8018230	6,4	8,4
FALSE		C2 H5 N2 C	Full match	No results	No results	No match	No results		1,02	199,9304	241,9642	0,978	6623217	1	0	0	0	No match	No match	No MS2	[M+ACN+H	6597732	6623217	6,7	7,3
FALSE		C12 H7 N	Full match	No results	No results	No results	No results		-3,71	165,0572	83,5359	0,977	7977743	0	0	0	0	No match	No match	No MS2	[M+2H]+2	7977743	6594971	5,1	7,3
FALSE				No results	No results	No results	No results			473,8263	474,8335	0,989	7652747	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	7320004	7652747	5,7	3,5
FALSE				No results	No results	No results	No results			361,8789	362,8861	0,994	8089065	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	7834986	8089065	4,6	5,7
FALSE	ETHYL 1-NITROSOPROLINE	C7 H12 N2	Full match	No results																					

FALSE		C5 H6 Cl3 ?	Full match	No results	No results	No results	No results	No results	2,92	467,8086	468,8149	1,134	2286996	0	0	0	No matche	No matche	No MS2	[M+H]+1	2286996	2134414	8,6	8,6
FALSE				No results	No results	No results	No results	No results		313,7721	314,7794	1,173	3064316	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	3064316	2882215	9,1	8,6
FALSE	2-Amino-6-nitrobenzothiazole	C7 H5 N3 C	Full match	No results	No results	Full match	No results	No results	-3,47	195,0096	98,51206	7,549	9870344	4	0	0	No matche	No matche	DDA for otl	[M+2H]+2	9870344		6,2	
FALSE		C4 H Cl4 N	Full match	No results	No results	No results	No results	No results	1,14	421,74	422,7465	1,144	1971296	0	0	0	No matche	No matche	No MS2	[M+H]+1	1971296	1367695	8,6	8,3
FALSE		C6 H Cl2 O	Full match	No results	No results	No results	No results	No results	-4,27	459,7759	460,7832	1,139	2051402	0	0	0	No matche	No matche	No MS2	[M+H]+1		2051402		8,6
FALSE		C7 H3 Cl Ni	Full match	No results	No results	No results	No results	No results	0,87	571,8267	572,8339	1,116	1520045	0	0	0	No matche	No matche	No MS2	[M+H]+1	1520045	1337910	7,7	8,8
FALSE		C11 H3 N4	Full match	No results	No results	No results	No results	No results	0,01	485,86	486,8673	1,064	2893494	0	0	0	No matche	No matche	No MS2	[M+H]+1	2893494	2714973	5,9	3,7
FALSE		C5 H7 N4 C	Full match	No results	No results	No results	No results	No results	-0,85	439,8635	440,8708	1,077	3362707	0	0	0	No matche	No matche	No MS2	[M+H]+1	3362707	3137360	8	8
FALSE	Glutaric anhydride	C5 H6 O3	Full match	No results	No results	Full match	Full match	Full match	0,15	114,0317	115,039	1,251	25477843	15	0	0	Single mat	No matche	DDA for pri	[M+H]+1		25477843		5,1
FALSE				No results	No results	No results	No results	No results		387,7047	388,712	1,173	3172589	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	3172589	2983934	7,5	8
FALSE		C35 H62 N	Full match	No results	No results	No results	No results	No match	-3,83	699,4197	700,427	7,447	6922140	0	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	4859734	6922140	5,9	8,4
FALSE		C H3 Cl2 O	Full match	No results	No results	No match	No results	No results	4,56	465,722	466,7283	1,146	2070295	42	0	0	No matche	No matche	No MS2	[M+H]+1	2070295		8,6	
FALSE		C7 H Cl O9	Full match	No results	No results	No results	No results	No results	3,28	325,8795	326,8868	1,103	3329882	0	0	0	No matche	No matche	No MS2	[M+H]+1	3329882	3293292	8,6	9,1
FALSE	α,4-Dibromotoluene	C7 H6 Br2	No results	No results	No results	Full match	No results	No results	1,84	247,8841	248,8914	1,113	1775754	3	0	0	No matche	No matche	DDA for pri	[M+H]+1	1775754	1489558	8,8	8,8
FALSE		C35 H73 N	Full match	No results	No results	No results	No results	No results	3,88	684,557	343,2858	7,159	32369620	0	0	0	No matche	No matche	DDA for otl	[M+2H]+2	32369620	30686054	5,7	5,7
FALSE		C9 H7 O3 F	Full match	No results	No results	No match	No match	No match	4,08	194,0141	98,01431	0,299	408416,1	1	0	0	No matche	Single mat	No MS2	[M+2H]+2		408416,1		8,5
FALSE	1-(Tetrahydro-2-furoyl)piperazine	C9 H16 N2	Full match	No results	No results	Full match	Partial mat	Partial mat	-0,16	184,1212	185,1284	4,047	3255076	10	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	2916006	3255076	8	8
FALSE				No results	No results	No results	No results	No results		1391,678	696,8464	1,08	3095868	0	0	0	No matche	No matche	No MS2	[M+2H]+2	3095868	2862176	8	8
FALSE		C47 H82 N	Full match	No results	No results	No results	No match	No results	-0,48	1075,556	359,526	4,234	2916221	1	0	0	No matche	No matche	DDA for otl	[M+3H]+3	2685791	2916221	8,6	8
FALSE				No results	No results	No results	No results	No results		1351,699	676,8568	1,097	2007785	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1951505	2007785	8,6	8,6
FALSE	1-[(9Z)-hexadecenoyl]-sn-glycero-3-phospho	C24 H48 N	Full match	No results	No results	Full match	No match	No match	-0,03	493,3168	494,3241	7,175	8404180	3	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	8404180	7821095	6,7	7,8
FALSE				No results	No results	No results	No results	No results		108,5144	109,5216	0,303	1082665	0	0	0	No matche	No matche	No MS2	[M+H]+1	954754,4	1082665	6,6	8,8
FALSE				No results	No results	No results	No results	No results		140,9513	182,9851	7,185	55893789	0	0	0	No matche	No matche	DDA for pri	[M+ACN+H]		55893789		5,7
FALSE		C4 H5 Cl4 ?	Full match	No results	No results	No results	No results	No results	3,08	457,7799	458,7862	1,14	2159627	0	0	0	No matche	No matche	No MS2	[M+H]+1	2159627	1616034	8	7,7
FALSE	Glycine	C2 H5 N O2	Full match	No results	No results	Full match	Full match	Full match	0,93	75,0321	76,03937	1,166	4970053	10	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	4181326	4970053	7	4,8
FALSE	2-arachidonyl-sn-glycero-3-phosphoethanol	C25 H44 N	Full match	No results	No results	Full match	Full match	No match	0	501,2855	502,2928	6,802	13739508	5	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	13739508	13129170	7,3	7,3
FALSE				No results	No results	No results	No results	No results		219,0288	110,5217	0,339	1741042	0	0	0	No matche	No matche	No MS2	[M+2H]+2		1741042		8,8
FALSE	L-Cysteinylglycine disulfide	C8 H15 N3	Full match	No results	No results	Full match	No results	No results	0,17	297,0454	298,0526	1,179	4022448	4	0	0	No matche	No matche	DDA for pri	[M+H]+1	4022448	3752419	7,5	6,4
FALSE		C6 H2 N2 C	Full match	No results	No results	No match	No results	No results	-4,13	181,9779	182,9851	7,223	54288075	2	0	0	No matche	No matche	DDA for pri	[M+H]+1	54288075		6,2	
FALSE		C29 H41 N	Full match	No results	No results	No results	No results	No results	-2,62	523,3145	524,3218	7,486	6245885	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	4617531	6245885	5,9	8,4
FALSE	3-Hydroxy-2,2-bis(hydroxymethyl)propyl noi	C14 H28 O	Full match	No results	No results	Full match	Partial mat	Partial mat	-0,27	276,1936	277,2009	7,341	3134404	1	0	0	No matche	Single mat	DDA for pri	[M+H]+1	3134404	2718808	8	8
FALSE		C10 H4 N4	Full match	No results	No results	No results	No results	No results	-3,73	561,7985	562,805	1,118	1157975	0	0	0	No matche	No matche	No MS2	[M+H]+1	1157975	1060230	8,8	8,8
FALSE		C5 H3 Br Cl	Full match	No results	No results	No results	No results	No results	4,69	363,7806	364,7878	1,143	1722235	0	0	0	No matche	No matche	No MS2	[M+H]+1	1722235	1627467	8,3	8,3
FALSE	1-arachidonoyl-sn-glycero-3-phosphocholine	C28 H50 N	Full match	No results	No results	Full match	No results	No results	0,19	543,3326	544,3399	7,269	5446376	3	0	0	No matche	No matche	DDA for pri	[M+H]+1	5446376	3457440	7	6,4
FALSE		C16 H14 N	Full match	No results	No results	No match	No match	No match	-3,58	354,1064	355,1137	1,962	2138709	2	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	2138709	2112412	8,6	8,6
FALSE	Furfural	C5 H4 O2	Full match	Invalid ma	No results	Full match	Full match	Full match	0,46	96,02117	97,02846	1,249	5213733	6	12	0	Single mat	No matche	DDA for pri	[M+H]+1	5213733		5,9	
FALSE		C6 H N2 O	Full match	No results	No results	No results	No results	No results	-2,69	435,8722	436,8795	1,111	1269914	0	0	0	No matche	No matche	No MS2	[M+H]+1	1269914		8,3	
FALSE				No results	No results	No results	No results	No results		1367,673	684,8438	1,097	1893212	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1679842	1893212	8,3	9,1
FALSE				No results	No results	No results	No results	No results		329,7461	330,7534	1,173	2908293	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2908293	2841453	8	8
FALSE		C7 H15 N3	Full match	No results	No results	No match	No results	No results	-2,65	219,0685	110,5415	0,969	6912798	3	0	0	No matche	No matche	No MS2	[M+2H]+2	6912798	6512404	5,1	3,5
FALSE				No results	No results	No results	No results	No results		1419,686	710,8504	1,097	1718925	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1641312	1718925	8,3	8,3
FALSE	glu-as	C9 H14 N2	Full match	No results	No results	Full match	No results	No results	0,25	262,0802	263,0875	1,356	6798736	5	0	0	No matche	No matche	DDA for pri	[M+H]+1	6798736	6429320	5,7	6,2
FALSE				No results	No results	No results	No results	No results		91,51506	92,52234	1,029	2176237	0	0	0	No matche	No matche	No MS2	[M+H]+1	2176237		8,6	
FALSE		C7 H6 Br Cl	Full match	No results	No results	No results	No results	No results	-0,76	463,7251	464,7313	1,145	1948735	0	0	0	No matche	No matche	No MS2	[M+H]+1	1276703	1948735	7,7	8
FALSE	carglumic acid	C6 H10 N2	Full match	No results	No results	Full match	No results	No results	0,25	190,059	223,0925	1,283	3182306	11	0	0	No matche	No matche	DDA for pri	[M+H+MeC]	3182306		8,6	
FALSE	Cystine	C6 H12 N2	Full match	No results	No results	Full match	Full match	Full match	0,05	240,0239	241,0311	1,17	4070155	4	0	0	Single mat	No matche	DDA for pri	[M+H]+1	4070155	3687840	9,1	8,6
FALSE	EDDA	C6 H12 N2	Full match	No results	No results	Full match	No results	No results	-0,2	176,0797	177,0869	2,011	7432640	13	0	0	No matche	No matche	DDA for pri	[M+H]+1		7432640		5,7
FALSE		C5 H Cl N2	Full match	No results	No results	No results	No results	No results	-4,35	283,9307	266,9274	1,059	2326058	0	0	0	No matche	No matche	No MS2	[M+H-H2O]	2326058	2219348	8,6	8,6
FALSE	(Z)-dehydrobutyrine	C4 H7 N O2	Full match	No results	No results	Full match	Full match	Full match	-3,63	101,0473	102,0546	1,455	7081408	24	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	7081408	6988444	4	2,4
FALSE				No results	No results	No results	No results	No results		286,8816	287,8888	0,34	1246007	0	0	0	No matche	No matche	DDA for pri	[M+H]+1		1246007		8,8
FALSE	glu-ser	C8 H14 N2	Full match	No results	No results	Full match	No results	No results	-0,04	234,0852	235,0925	2,157	9235353	5	0	0	No matche	No matche	DDA for pri	[M+H]+1		9235353		6,7
FALSE		C9 H11 N2	Full match	No results	No results	No results	No results	No results	-0,44	591,8126	624,8461	1,11	2232711	0	0	0	No matche	No matche	No MS2	[M+H+MeC]		2232711		5,9
FALSE		C2 H8 Cl N	Full match	No results	No results	No results	No results	No results	0,98	222,9391	264,9729	1,198	2213296	0	0	0	No matche	No matche	DDA for otl	[M+ACN+H]	2213296	2031900	8,6	8,6
FALSE		C2 H5 Cl N	Full match	No results	No results	No results	No results	No results	2,19	345,9014	346,9087	0,989	5497329	0	0	0	No matche	No matche	No MS2	[M+H]+1	4851798	5497329	4,8	7
FALSE				No results	No results	No results	No results	No results		76,99153	77,99883	0,333	1869355	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	708660,6	1869355	6,3	7,2
FALSE	Nefiracetam	C14 H18 N	Full match	No results	No results	Full match	Partial mat	Partial mat	0,09	246,1369	247,1441	4,435	2505773	13	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	2385898	2505773	9,1	8,6
FALSE				No results	No results	No results	No results	No results		333,9077	334,915	1,062	2120490	0	0	0	No matche	No matche	No MS2	[M+H]+1	2120490	1959400	8,6	8,6
FALSE		C2 H N2 O3	Full match	No results	No results	No results	No results	No results	-1,16	321,879	322,8868	1,108	1125406	0	0	0	No matche	No matche	No MS2	[M+H]+1		1125406		8,8
FALSE	2,2'-(Decylimino)diethanol	C14 H31 N	Full match	Invalid ma	No results	Full match	No results	No results	0,01	245,2355	246,2428	6,272	2843111	1	2	0	No matche	No matche	DDA for pri	[M+H]+1	2564829	2843111	8	8
FALSE		C2 H Cl2 N	Full match	No results	No results	No results	No results	No results	1,24	423,7364	424,7436	1,143	1755721	0	0	0	No matche	No matche	No MS2	[M+H]+1		1755721		8,3
FALSE	BUTYROLACTONETHIOL	C4 H6 O2 S	Full match	Invalid ma	No results</																			



FALSE		C14 H4 Cl F	Full match	No results	No results	No results	No results	-0.19	759,8148	760,8221	1,11	1304428	1	0	0	0	No matche	No matche	No MS2	[M+H]+1	1304428	8,8		
FALSE		C7 H16 N2	Full match	No results	No results	No results	No results	0,28	240,0958	241,1031	1,282	2801857	1	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2261749	2801857	8,6	8
FALSE		C5 H2 Cl2	Full match	No results	No results	No results	No results	-1,45	449,7478	450,7544	1,144	1677338	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1677338	1534113	7,7	7,7
FALSE			No results	No results	No results	No results	No results		108,0123	109,0196	0,994	5182396	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	5182396	4800889	5,9	5,3
FALSE		C2 H2 Cl2	Full match	No results	No results	No results	No results	2,57	381,7596	382,7669	1,149	2146509	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	2146509	2050467	8,6	7,5
FALSE		C5 H2 N5	Full match	No results	No results	No results	No results	-1,69	178,9994	90,50697	7,432	20082808	0	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2		20082808		5,1
FALSE			No results	No results	No results	No results	No results		451,827	530,8489	1,101	1850460	0	0	0	0	No matche	No matche	No MS2	[M+DMSO-	1850460	1850335	8,3	8,3
FALSE	Guanylmelamine		No results	No results	No results	No results	No results		1383,652	692,8333	1,107	1883461	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2		1883461		8,3
FALSE		C4 H8 N8	Full match	Invalid ma	No results	Full match	No results	1,71	168,0875	169,0948	1,119	4112476	1	10	0	0	No matche	No matche	DDA for pri	[M+H]+1	3950716	4112476	5,3	7
FALSE		C3 H5 N2	Full match	No results	No results	No results	No results	-1,23	339,9246	340,9319	1,077	2631258	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	2631258	2528495	8	8
FALSE			No results	No results	No results	No results	No results		137,8992	138,9065	1,166	3490696	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	3490696	3360527	5,3	4,2
FALSE	thiomorpholine-3-carboxylic acid	C5 H9 N2	Full match	No results	No results	Full match	Full match	0,39	147,0355	148,0427	1,964	1665189	9	0	0	0	Single mat	No matche	DDA for pri	[M+H]+1	1665189	1572729	7,2	8,3
FALSE		C12 H6 N5	Full match	No results	No results	No results	No results	0,3	712,7857	357,4001	0,995	3195827	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	3076141	3195827	4,2	5,3
FALSE	[Similar to: 3-Hydroxy-1-[3-(trifluoromethyl)]		No results	Invalid ma	No results	No results	No results		189,9047	190,912	1,109	3436642	0	3	0	0	No matche	No matche	DDA for pri	[M+H]+1	3436642	3072176	4,8	4,8
FALSE		C9 H25 N4	Full match	No results	No results	No results	No results	3,08	316,1522	334,186	6,891	17910419	1	0	0	0	No matche	No matche	DDA for ott	[M+NH4]+:		17910419		6,2
FALSE		C3 H9 N4	Full match	No results	No results	No results	No results	0,83	164,0287	83,02162	1,103	5654978	0	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2		5654978		4,2
FALSE			No results	No results	No results	No results	No results		295,7931	296,8004	1,145	1538302	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1538302	1507150	8,3	8,3
FALSE	tyrosine O-sulfate	C9 H11 N	Full match	No results	No results	Full match	No results	-0,17	261,0307	262,0379	3,287	2207160	4	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2207160	2056721	8	7,5
FALSE		C2 H4 N O	Full match	No results	No results	No results	No results	4,87	200,9684	201,9757	0,304	789167,9	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	789167,9		9	
FALSE			No results	No results	No results	No results	No results		413,7083	414,7148	1,145	1370690	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1370690	1283533	8,8	8,3
FALSE		C14 H21 O	Full match	No results	No results	No match	No match	0,48	316,1077	317,115	1,144	5063117	2	0	0	0	No matche	Multiple m	No MS2	[M+H]+1	5063117	4874289	4,8	4,8
FALSE			No results	No results	No results	No results	No results		1527,653	764,8339	1,082	2090811	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	2090811	1977402	8	7,5
FALSE		C2 H N6 O	Full match	No results	No results	No results	No results	-3,11	249,9315	250,9388	0,989	5021930	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	5021930	4805488	5,3	3,2
FALSE			No results	No results	No results	No results	No results		219,0289	110,5217	7,55	35306141	0	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2	35306141	7742551	5,1	6,2
FALSE	1,3-Dimethylbutylamine	C6 H15 N	Full match	No results	No results	Full match	Full match	0,31	101,1205	102,1278	7,53	42905725	15	0	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	31680050	42905725	4	5,7
FALSE			No results	No results	No results	No results	No results		287,7615	288,7687	1,168	3101800	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	3101800	2943008	4,8	8
FALSE		C H3 O4 P3	Full match	No results	No results	No results	No results	-4,81	267,8393	268,8466	1,143	1770628	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1770628	1650734	7,7	8,3
FALSE		C10 H10 N	Full match	No results	No results	No results	No results	-1,35	507,8509	508,8582	1,081	2211300	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	2211300	2028603	8	8
FALSE			No results	No results	No results	No results	No results		192,1238	193,1311	1,113	5554087	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	5554087	5059809	5,9	5,3
FALSE		C3 H N4 O	Full match	No results	No results	No results	No results	-0,99	393,7861	394,7927	1,141	1533865	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1		1533865		7,7
FALSE	Methylsulfonylethane	C2 H6 O2 S	Full match	No results	No results	Full match	Full match	0,26	94,00887	95,01615	1,95	2837664	1	0	0	0	Single mat	No matche	DDA for pri	[M+H]+1	2811681	2837664	8	7,5
FALSE			No results	No results	No results	No results	No results		1231,698	616,8564	1,097	1409587	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1409587	1344181	8,3	7,7
FALSE			No results	No results	No results	No results	No results		1335,725	668,8698	1,097	1228120	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1228120	1208551	8,3	8,3
FALSE		C9 H5 Cl O	Full match	No results	No results	No results	No results	1,58	401,8951	402,9024	1,063	1657362	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1657362	1388048	8,3	8,3
FALSE		C11 H19 N	Full match	No results	No results	No match	No results	0,22	369,0665	370,0738	1,391	1972295	1	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1972295	1704449	8	8,3
FALSE		C4 H N2 O	Full match	No results	No results	No results	No results	4,81	217,9033	218,9106	1,004	4624909	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	4507954	4624909	4,8	2,6
FALSE			No results	No results	No results	No results	No results		113,8866	114,8939	1,145	2112972	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	2112972	1979040	9,1	7
FALSE		C3 H N2 O	Full match	No results	No results	No results	No results	4,89	477,7471	478,7541	1,142	1320726	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1320726	1231379	8,3	7,7
FALSE		C11 H12 N	Full match	No results	No results	No results	No results	-3,27	189,0701	207,104	4,13	1858261	0	0	0	0	No matche	No matche	No MS2	[M+NH4]+:	1567217	1858261	7,2	8,3
FALSE	9-Decenoylcarnitine	C17 H31 N	Full match	No results	No results	Full match	No results	-0,18	313,2253	314,2325	6,49	2310097	1	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2264097	2310097	7,5	8
FALSE	Pyrogallol	C6 H6 O3	Full match	No results	No results	Full match	Full match	0,49	126,0318	127,039	1,446	1811858	24	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	1811858		7,2	
FALSE			No results	No results	No results	No results	No results		1487,674	744,8444	1,097	1249997	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1249997		8,3	
FALSE		C H Cl O P2	Full match	No results	No results	No match	No results	4,23	253,8085	254,8158	1,145	1332740	1	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1332740	1242619	7,2	7,7
FALSE	Phenylethyl alcohol	C8 H10 O	No results	Invalid ma	No results	Full match	Full match	0,09	122,0732	123,0805	7,058	45006641	25	10	0	0	Multiple m	Single mat	DDA for pri	[M+H]+1	45006641	23232928	5,7	4
FALSE			No results	No results	No results	No results	No results		1503,648	752,8312	1,097	1142906	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1128036	1142906	8,3	8,8
FALSE			No results	No results	No results	No results	No results		741,8316	742,8389	1,097	1368248	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		1368248		8,3
FALSE	Oleoylecarnitine	C25 H47 N	Full match	No results	No results	Full match	No results	0,04	425,3505	426,3578	7,328	2305457	7	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2305457	2061652	8,6	7,5
FALSE	N-Nonanoylmorpholine	C13 H25 N	Full match	No results	No results	Full match	No results	-0,09	227,1885	228,1958	7,199	4117598	4	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	4117598	4107410	7,5	7,5
FALSE			No results	No results	No results	No results	No results		1519,626	760,8204	1,104	982646,8	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2		982646,8		9,3
FALSE		C2 H2 Cl N	Full match	No results	No results	No results	No results	-0,79	341,772	342,7793	1,147	1577357	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1577357		8,8	
FALSE			No results	No results	No results	No results	No results		311,7751	312,7824	1,173	1953887	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1953887	1822282	8,6	8,3
FALSE	Dimethylcadmium	C2 H6 Cd	No results	Invalid ma	No results	Full match	No results	-4,88	143,9496	144,9569	0,306	395242,6	1	1	0	0	No matche	No matche	DDA for pri	[M+H]+1	395242,6	260244,6	8,2	7,1
FALSE	DL-Lysine	C6 H14 N2	Full match	Invalid ma	No results	Full match	Full match	0,06	146,1055	147,1128	1,164	2155294	18	8	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	2155294		7	
FALSE		C2 H3 N2 C	Full match	No results	No results	No results	No results	2,86	133,9885	134,9958	0,967	3922205	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	3304768	3922205	4,2	5,3
FALSE	Acetonedicarboxylic Acid	C5 H6 O5	Full match	No results	No results	Full match	Full match	0,19	146,0216	129,0183	2,383	7256678	6	0	0	0	Multiple m	No matche	DDA for ott	[M+H-H2O	6896063	7256678	5,7	7,3
FALSE		C9 H14 P2	Full match	No results	No results	No match	No results	4,86	216,0302	109,0224	0,32	1259932	3	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1259932	1083387	4,5	8,8
FALSE		C4 H3 N2 C	Full match	No results	No results	No results	No results	-2,83	411,8557	412,863	1,055	1425737	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	1425737	1201043	8,3	8,8
FALSE			No results	No results	No results	No results	No results		70,02188	71,02915	0,972	4576228	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	4576228		4,8	
FALSE		C5 H14 N2	Full match	No results	No results	No results	No results	-1,09	164,063	83,0388	0,976	3791663	5	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2	3791663	2882505	3,7	5,3
FALSE		C7 H2 O7 F	Full match	No results	No results	No results	No results	0,85	419,7883	420,7956	1,139	1427822	0	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1427822	1302971	7,7	7,7
FALSE		C2 H2 Br Cl	Full match	No results	No results	No results	No results	0,16	411,7118	490,734	1,142	1241276	0	0	0	0	No matche	No matche	No MS2					

FALSE				No results	No results	No results	No results	No results	703,5713	704,5786	7,219	7488641	0	0	0	No matche	No matche	No MS2	[M+H]+1	7488641		5,7	
FALSE			C3 H12 N1	Full match	No results	No results	No results	No results	-1,38	330,0463	331,0536	1,517	3747045	1	0	0	No matche	No matche	DDA for pr	[M+H]+1	3747045	4,2	
FALSE			C5 H10 N C	Full match	No results	No results	No results	No results	0,58	163,0222	164,0294	1,209	1533950	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	1533950	7,7	
FALSE			C4 H C12 O	Full match	No results	No results	No results	No results	-2,99	355,749	356,7562	1,147	1293635	0	0	0	No matche	No matche	No MS2	[M+H]+1	1284933	8,8	
FALSE			N~5~-Isopropyl-L-ornithine	C8 H18 N2	Full match	No results	No results	Full match	No results	-0,32	174,1368	175,1441	1,156	1622828	9	0	0	No matche	No matche	DDA for pr	[M+H]+1	1579080	6,1
FALSE					No results	No results	No results	No results		1199,75	600,8823	1,097	1124070	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1076165	8,8	
FALSE					No results	No results	No results	No results		728,7631	365,3888	1,012	3453881	0	0	0	No matche	No matche	No MS2	[M+2H]+2	3297998	4,8	
FALSE			2,2'-(2-[(2-Hydroxyethyl)amino]ethyl)imino	C6 H20 N2	Full match	No results	No results	Full match	No results	0,09	192,1474	193,1547	1,31	1532565	2	0	0	No matche	No matche	DDA for pr	[M+H]+1	1390834	8,3
FALSE				C6 H3 C12 ?	Full match	No results	No results	No results	No results	-0,01	681,7988	682,8061	1,119	579108,6	0	0	0	No matche	No matche	No MS2	[M+H]+1	579108,6	9
FALSE			Cytosine	C4 H5 N3 C	Full match	No results	No results	Full match	Full match	3,07	111,0436	245,0768	3,218	1692254	8	0	0	Single mat	No matche	DDA for ot	[2M+Na]+1	1692254	8,3
FALSE				C3 H4 C13 ?	Full match	No results	No results	No results	No results	1,71	551,7699	552,7764	1,134	1200876	0	0	0	No matche	No matche	No MS2	[M+H]+1	1187513	7,7
FALSE				C2 H3 C14 ?	Full match	No results	No results	No results	No results	0,83	609,7287	610,7352	1,135	1165931	0	0	0	No matche	No matche	No MS2	[M+H]+1	1165931	7,2
FALSE			Xentrivalpeptide K	C40 H69 N	No results	No results	No results	No results	Full match	-3,97	791,5125	264,8448	1,141	1445237	0	0	0	No matche	Single mat	DDA for ot	[M+3H]+3	1445237	7,7
FALSE					No results	No results	No results	No results	No results		959,6864	480,8505	1,057	1088084	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1088084	8,3
FALSE				C36 H82 N	Full match	No results	No results	No results	No results	-0,75	786,597	787,6043	7,301	8188244	0	0	0	No matche	No matche	No MS2	[M+H]+1		6,2
FALSE				C5 H2 O9 F	Full match	No results	No results	No results	No results	-4,61	299,8881	300,8954	1,091	1304243	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	1304243	7,7
FALSE					No results	No results	No results	No results	No results		84,50828	85,51555	0,976	2796873	0	0	0	No matche	No matche	No MS2	[M+H]+1	2796873	4,2
FALSE				C15 H9 N6	Full match	No results	No results	No results	No results	-0,37	733,8041	734,8114	1,101	1398059	0	0	0	No matche	No matche	No MS2	[M+H]+1	1398059	8,3
FALSE					No results	No results	No results	No results	No results		429,6894	430,6967	1,174	1383140	0	0	0	No matche	No matche	No MS2	[M+H]+1	1377182	8,8
FALSE				C49 H104 ?	Full match	No results	No results	No results	No results	-0,21	972,7014	487,358	0,992	2361976	0	0	0	No matche	No matche	No MS2	[M+2H]+2	2361976	3,2
FALSE			EDDA	C6 H12 N2	Full match	No results	No results	Full match	No results	0,04	176,0797	177,087	2,254	9768589	13	0	0	No matche	No matche	DDA for pr	[M+H]+1		5,7
FALSE			vinylglycine	C4 H7 N O2	Full match	No results	No results	Full match	Full match	0,34	101,0477	102,055	1,963	91898170	24	0	0	Multiple m	No matche	DDA for pr	[M+H]+1	91898170	5,1
FALSE				C H3 C12 O?	Full match	No results	No results	No results	No results	-1,93	481,6961	482,7024	1,147	1170435	0	0	0	No matche	No matche	No MS2	[M+H]+1	1170435	7,7
FALSE					No results	No results	No results	No results	No results		403,6793	404,686	1,173	1861624	0	0	0	No matche	No matche	No MS2	[M+H]+1	1861624	8,3
FALSE					No results	No results	No results	No results	No results		108,0151	109,0224	7,587	24953547	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	24953547	5,1
FALSE			γ-Glu-Ala	C8 H14 N2	Full match	No results	No results	Full match	Partial mat	0,16	218,0903	219,0976	1,366	2886937	9	0	0	No matche	Multiple m	DDA for pr	[M+H]+1	2886937	4,8
FALSE					No results	No results	No results	No results	No results		1331,633	666,824	1,101	1519008	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1519008	8,3
FALSE					No results	No results	No results	No results	No results		92,00806	93,01534	0,993	3870870	0	0	0	No matche	No matche	No MS2	[M+H]+1		5,9
FALSE				C23 H3 N5	Full match	No results	No results	No results	No results	0,46	826,7657	414,3901	0,987	2467947	0	0	0	No matche	No matche	No MS2	[M+2H]+2	2467947	5,3
FALSE				C4 H7 Br C	Full match	No results	No results	No results	No results	1,91	619,7575	620,7639	1,123	848343,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	848343,8	8,8
FALSE				C21 H37 N	Full match	No results	No results	No results	No results	0,06	303,2926	304,2999	7,153	2753629	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	2753629	5,9
FALSE			DL-Ala-DL-Leu	C9 H18 N2	No results	No results	No results	Full match	No results	-0,06	202,1317	203,139	1,962	1217112	6	0	0	No matche	No matche	No MS2	[M+H]+1	1217112	8,3
FALSE					No results	No results	No results	No results	No results		505,619	506,6263	1,173	1283327	0	0	0	No matche	No matche	No MS2	[M+H]+1	1283327	8,8
FALSE			Bacitrocin C	C18 H27 N	Full match	No results	No results	No results	Full match	-3,56	361,2101	362,2174	7,442	9535105	0	0	0	No matche	Single mat	DDA for pr	[M+H]+1	9535105	5,7
FALSE				C9 H19 O6	Full match	No results	No results	No results	No results	-3,52	286,063	287,0703	1,147	729984,8	2	0	0	No matche	No matche	No MS2	[M+H]+1	729984,8	5,7
FALSE			dimethylformamide	C3 H7 N O	Full match	No results	No results	Full match	Full match	1,05	73,05284	74,06012	1,221	4847834	12	0	0	Multiple m	No matche	DDA for pr	[M+H]+1	4847834	4,2
FALSE					No results	No results	No results	No results	No results		71,49484	72,50212	0,993	3768934	0	0	0	No matche	No matche	No MS2	[M+H]+1	3121674	3,2
FALSE			(2E)-decanoic acid	C10 H18 O	Full match	No results	No results	Full match	Full match	0,02	170,1307	171,138	7,341	2498591	160	0	0	Multiple m	Multiple m	DDA for pr	[M+H]+1	2498591	7
FALSE				C5 H2 O6 S	Full match	No results	No results	No results	No results	-3,84	189,9565	190,9638	1,954	1001860	0	0	0	No matche	No matche	No MS2	[M+H]+1	1001860	8,8
FALSE			Diethyl 1,1-cyclopentenedicarboxylate	C11 H18 O4	Full match	No results	No results	Full match	Partial mat	0,1	214,1205	215,1278	7,026	23699888	9	0	0	No matche	Multiple m	DDA for pr	[M+H]+1	23699888	5,1
FALSE				C4 H O14 F	Full match	No results	No results	No results	No results	-1,39	461,7735	462,7803	1,142	1167512	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	1167512	7,7
FALSE				C8 H2 O18	Full match	No results	No results	No results	No results	-1,34	479,8431	480,8503	1,055	1097598	0	0	0	No matche	No matche	No MS2	[M+H]+1		5
FALSE				C21 H33 N	Full match	No results	No results	No results	No results	-3,41	494,1861	248,1003	1,667	4191069	0	0	0	No matche	No matche	DDA for ot	[M+2H]+2	4191069	5,9
FALSE					No results	No results	No results	No results	No results		156,1164	157,1237	7,171	23800652	0	0	0	No matche	No matche	No MS2	[M+H]+1		5,1
FALSE			Safingol	C18 H39 N	Full match	No results	No results	Full match	Full match	0,17	301,2981	302,3054	7,003	2196292	4	0	0	Single mat	No matche	DDA for pr	[M+H]+1	1725003	8,3
FALSE			Furaneol	C6 H8 O3	Full match	No results	No results	Full match	Full match	0,28	128,0474	129,0547	1,47	11073397	31	0	0	Multiple m	Multiple m	DDA for pr	[M+H]+1	9766773	5,1
FALSE					No results	No results	No results	No results	No results		1555,661	778,8378	1,097	965587,4	0	0	0	No matche	No matche	No MS2	[M+2H]+2	929148,2	8,3
FALSE			Phenylethyl alcohol	C8 H10 O	No results	No results	No results	Full match	Full match	0,21	122,0732	123,0805	7,272	10712391	25	0	0	Multiple m	Single mat	DDA for pr	[M+H]+1		4,6
FALSE				C4 H2 O15	Full match	No results	No results	No results	No results	0	383,859	384,8662	1,111	707816,2	0	0	0	No matche	No matche	No MS2	[M+H]+1	669183,4	8,5
FALSE				C18 H27 N	Full match	No results	No results	No results	No results	-3,6	377,205	378,2122	7,491	3958784	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	3318679	4,8
FALSE			1-[[8,11Z,14Z]-icosatrienyl]-sn-glycero-3-ph	C28 H52 N	Full match	No results	No results	Full match	No results	3,44	545,35	568,3394	7,327	2621829	3	0	0	No matche	No matche	DDA for ot	[M+Na]+1	2621829	5,9
FALSE				C11 H3 C12	Full match	No results	No results	No results	No results	-1,79	601,696	602,7033	1,139	1119219	0	0	0	No matche	No matche	No MS2	[M+H]+1		7,5
FALSE			N~2~-Acetyl-L-ornithine	C7 H14 N2	Full match	No results	No results	Full match	Full match	0,22	174,1005	175,1078	1,419	2049523	16	0	0	Multiple m	No matche	DDA for pr	[M+H]+1		8,3
FALSE				C4 H7 C1 N	Full match	No results	No results	No results	No results	-2,11	150,0015	151,0088	0,988	3733453	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	3165617	4,2
FALSE				C4 H N4 O3	Full match	No results	No results	No results	No results	-1,71	183,9783	184,9856	7,582	21878026	0	0	0	No matche	No matche	No MS2	[M+H]+1	18995177	6,2
FALSE			N-(tert-Butoxycarbonyl)-L-leucine	C11 H21 N	Full match	No results	No results	Full match	Full match	0,1	231,1471	232,1544	3,943	1563923	7	0	0	Multiple m	No matche	DDA for pr	[M+H]+1	1407917	6,6
FALSE			4-[Methyl(3R,4R)-4-methyl-1-propionyl]-p	C16 H23 N	Full match	No results	No results	Not the top	No results	-4,03	317,1839	318,1912	7,292	10578816	3	0	0	No matche	No matche	DDA for pr	[M+H]+1	10578816	4,6
FALSE					No results	No results	No results	No results	No results		108,0151	109,0224	0,305	365377,5	0	0	0	No matche	No matche	No MS2	[M+H]+1		8,2
FALSE					No results	No results	No results	No results	No results		285,7644	286,7716	1,171	2374307	0	0	0	No matche	No matche	No MS2	[M+H]+1	2374307	5,3
FALSE				C5 H9 C12 ?	Full match	No results	No results	No match	No results	0,03	305,951	306,9576	1,194	1522019	1	0	0	No matche	No matche	No MS2	[M+H]+1		7,2
FALSE				C H2 Br C14	Full match	No results	No results	No results	No results	-3,18	385,7077	386,715	1,173	1582536	0	0	0	No matche	No matche	No MS2	[M+H]+1	1582536	7,2
FALSE			5-methylisoxazol	C4 H5 N O	Full match	No results	No results	Full match	No results	0,76	83,03718	84,04446	1,006	2856504	6	0	0	No matche	No matche	DDA for pr	[M+H]+1		7,5
FALSE			Piptamine	C23 H41 N	Full match	No results	No results	No results	Full match	0,23	331,324	332,3313	7,305	3063077	0	0	0	No matche	Single mat	DDA for pr	[M+H]+1	3014562	5,3
FALSE				C46 H106 F	Full match	No results	No results	No results	No results	0,05	956,724	479,3693	0,989	2326595	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1926117	2,1
FALSE			3-hydroxyoctanoylcarnitine	C15 H29 N	Full match	No results	No results	Full match	No results	0,12	303,2046	304,2119	5,083	2324946	1	0	0	No matche	No matche	DDA for pr	[M+H]+1	2181472	8
FALSE																							



FALSE	5-hydroxyisouric acid	C5 H4 N4 C	Full match	No results	No results	Full match	Full match	0,01	184,0233	185,0305	2,403	3882762	2	0	0	0	Single mat	No match	DDA for pri	[M+H]+1	3882762	3513151	7,5	8,3
FALSE		C6 H17 N1	Full match	No results	No results	No match	No results	-0,95	308,122	309,1293	1,365	1528380	2	0	0	0	No match	No match	DDA for pri	[M+H]+2	1528380	1360628	7,7	8,8
FALSE		C6 H12 N4	Full match	No results	No results	No results	No results	0,02	188,0732	95,04387	0,972	3523455	0	0	0	0	No match	No match	No MS2	[M+2H]+2	3523455	2634084	3,2	4,8
FALSE		C2 H2 O7 F	Full match	No results	No results	No results	No results	4,01	231,9006	232,9079	1,091	1142378	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1142378	1063583	7,2	7,7
FALSE	5-Hydroxy-DL-tryptophan	C11 H12 N	Full match	No results	No results	Full match	Partial mat	-0,19	220,0848	221,092	3,769	3114180	17	0	0	0	Multiple m	Single mat	DDA for pri	[M+H]+1	3018196	3114180	4,2	7,5
FALSE		C6 H Br O S	Full match	No results	No results	No results	No results	0,68	263,8375	264,8449	1,137	1380917	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		1380917		7,7
FALSE			No results	No results	No results	No results	No results		858,7209	430,3678	0,977	2430380	0	0	0	0	No match	No match	No MS2	[M+2H]+2	2430380	2308064	3,2	7,5
FALSE		C33 H77 N	Full match	No results	No results	No match	No results	0,23	759,5795	760,5868	7,139	16302260	29	0	0	0	No match	No match	DDA for pri	[M+H]+1	16302260		5,7	
FALSE		C2 H Cl4 O	Full match	No results	No results	No results	No results	0,83	513,6526	592,6748	1,145	960418	0	0	0	0	No match	No match	No MS2	[M+DMSO]	925528,2	960418	8,3	7,7
FALSE	glu-ser	C8 H14 N2	Full match	No results	No results	Full match	No results	0,09	234,0852	235,0925	2,37	19058944	5	0	0	0	No match	No match	DDA for pri	[M+H]+1		19058944		5,1
FALSE		C9 H3 N4 C	Full match	No results	No results	No results	No results	0,56	547,8303	548,8376	1,056	885194,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		885194,9		8,8
FALSE	3-BHA	C11 H16 O	Full match	No results	No results	Full match	Partial mat	-0,04	180,115	181,1223	7,204	26867992	36	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	26867992		5,1	
FALSE	Aconitic anhydride	C6 H4 O5	Full match	No results	No results	Full match	No results	0,13	156,0059	157,0132	2,144	3262815	3	0	0	0	No match	No match	DDA for pri	[M+H]+1	3262815	3145023	6,4	7
FALSE		C14 H2 N2	Full match	No results	No results	No results	No results	0,8	469,8824	470,8897	1,065	1129471	0	0	0	0	No match	No match	No MS2	[M+H]+1	1129471	1031867	8,3	8,3
FALSE		C6 H6 Cl4 F	Full match	No results	No results	No results	No results	0,09	515,7389	516,7455	1,136	1115321	0	0	0	0	No match	No match	No MS2	[M+H]+1	846595,1	1115321	8,3	7,7
FALSE	[Similar to: Ethylenediaminetetraacetic acid]	C5 H11 N8	Full match	Invalid mat	No results	No match	No results	0,96	292,0272	293,0344	1,428	366013,1	7	2	0	0	No match	No match	DDA for pri	[M+H]+1		366013,1		8,2
FALSE	CAPROYL SARCOSINE	C13 H25 N	Full match	No results	No results	Full match	No results	-0,04	243,1834	244,1907	6,813	2825432	2	0	0	0	No match	No match	DDA for pri	[M+H]+1	2295570	2825432	7	7
FALSE			No results	No results	No results	No results	No results		643,8258	644,8331	1,082	1484399	0	0	0	0	No match	No match	No MS2	[M+H]+1		1484399		7,7
FALSE	1,6-Hexanediol diacrylate	C12 H18 O	Full match	No results	No results	Full match	Partial mat	-0,17	226,1205	227,1278	7,103	27013033	14	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	27013033		4,6	
FALSE		C20 H43 N	Full match	No results	No results	No results	No results	0,11	361,3193	362,3265	6,82	1789883	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1643335	1789883	8,3	8,3
FALSE	bis(pentamethylene)urea	C11 H20 N	Full match	No results	No results	Full match	No results	0,14	196,1576	197,1649	7,611	3222058	2	0	0	0	No match	No match	DDA for pri	[M+H]+1	2391958	3222058	8,6	8
FALSE		C4 H6 N4 C	Full match	No results	No results	No results	No results	-3,79	190,0331	191,0404	1,279	1704216	0	0	0	0	No match	No match	No MS2	[M+H]+1		1704216		7,7
FALSE	Homocitrulline	C7 H15 N3	Full match	No results	No results	Full match	Full match	0,31	189,1114	190,1187	1,531	1849666	5	0	0	0	Single mat	No match	DDA for pri	[M+H]+1	1849666	1692087	5	3,4
FALSE	Linoleyl carnitine	C25 H45 N	Full match	No results	No results	Full match	No results	0,21	423,335	424,3422	7,213	1603667	2	0	0	0	No match	No match	DDA for pri	[M+H]+1	1603667	1567234	6,6	8,3
FALSE		C4 H6 Cl3	Full match	No results	No results	No results	No results	0,64	525,7675	526,774	1,136	1033536	0	0	0	0	No match	No match	No MS2	[M+H]+1		1033536		8,3
FALSE			No results	No results	No results	No results	No results		259,8902	260,8975	1,105	1595092	0	0	0	0	No match	No match	No MS2	[M+H]+1	1595092	1542050	8,3	8,3
FALSE			No results	No results	No results	No results	No results		1423,626	712,8204	1,078	1281470	0	0	0	0	No match	No match	No MS2	[M+2H]+2	1281470		7,7	
FALSE		C11 H3 N4	Full match	No results	No results	No results	No results	0,01	571,8478	572,8552	1,102	975131,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	975131,7	378840,2	8,3	3,8
FALSE		C39 H74 N	Full match	No results	No results	No match	No results	-4,05	702,5678	352,2912	7,266	15026821	5	0	0	0	No match	No match	No MS2	[M+2H]+2	15026821		4,6	
FALSE	DL-Ornithine	C5 H12 N2	Full match	No results	No results	Full match	Full match	0,45	132,0899	133,0972	1,034	2421631	11	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1		2421631		7
FALSE	2-benzenesulfonamidopyrimidine	C10 H9 N3	Full match	No results	No results	Full match	No match	-2,99	235,0409	118,5277	0,303	910838,3	2	0	0	0	No match	Multiple m	No MS2	[M+2H]+2	619218,6	910838,3	2,5	7,2
FALSE	8-(Hydroxyethylamino)adenine	C7 H10 N6	Full match	No results	No results	Full match	No results	1,29	194,0919	195,0991	1,104	3297633	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	3297633	2986291	5,3	4,8
FALSE	prohydrojasmon	C15 H26 O	Full match	No results	No results	Full match	Partial mat	0,07	254,1882	255,1955	7,436	4467610	26	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	4467610	4037259	5,9	7,5
FALSE		C25 H46 N	Full match	No results	No results	No match	No results	-2,66	511,3274	512,3347	6,878	2620198	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	1886518	2620198	8	8
FALSE		C2 H Cl4 O	Full match	No results	No results	No results	No results	0,89	369,7337	370,741	1,172	1217088	0	0	0	0	No match	No match	No MS2	[M+H]+1	1217088	1178547	8,3	7,7
FALSE	Glycerol	C3 H8 O3	Full match	No results	No results	Full match	Full match	0,56	92,0474	75,04411	1,366	4213494	3	0	0	0	Single mat	No match	DDA for pri	[M+H+H2O]	4213494	1652240	4,2	3,9
FALSE		C6 H8 N6 C	Full match	No results	No results	No results	No results	1,62	180,0763	181,0835	1,111	3727532	0	0	0	0	No match	No match	No MS2	[M+H]+1	3727532	3361190	4,2	6,4
FALSE			No results	No results	No results	No results	No results		1287,652	644,8331	1,077	1474848	0	0	0	0	No match	No match	No MS2	[M+2H]+2		1474848		7,7
FALSE		C3 H2 N2 C	Full match	No results	No results	No results	No results	0,73	367,8756	368,8828	1,093	1048222	0	0	0	0	No match	No match	No MS2	[M+H]+1	1048222	954949,8	7,7	8,3
FALSE		C18 H27 N	Full match	No results	No results	No results	No results	-3,39	377,205	378,2123	7,588	2144860	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1735977	2144860	8,3	8,6
FALSE		C5 H3 N4 C	Full match	No results	No results	No results	No results	2,65	451,8465	452,8537	1,11	601984,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	601984,6	551921,6	8,5	8,5
FALSE		C19 H45 N	Full match	No results	No results	No match	No match	2,23	495,3326	496,3399	6,838	17202062	4	0	0	0	Single mat	No match	DDA for pri	[M+H]+1		17202062		5,1
FALSE	5-methylthioribose	C6 H12 O4	Full match	No results	No results	Full match	Full match	0,15	180,0457	181,0529	1,958	993015,1	3	0	0	0	Single mat	No match	No MS2	[M+H]+1	993015,1	915183,5	7,7	7,2
FALSE			No results	No results	No results	No results	No results		1095,661	548,8378	1,057	920823,3	0	0	0	0	No match	No match	No MS2	[M+2H]+2		920823,3		8,8
FALSE	L-Proline	C5 H9 N O2	Full match	No results	No results	Full match	Partial mat	0,49	115,0634	133,0972	1,039	2287806	30	0	0	0	Multiple m	Single mat	DDA for ori	[M+NH4]+	2287806		6,4	
FALSE	9-Nitrooleate	C18 H33 N	Full match	No results	No results	Full match	Partial mat	0,21	327,241	328,2483	6,628	1830540	3	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	1830540	1775470	7,2	6,6
FALSE			No results	No results	No results	No results	No results		503,6231	504,6294	1,174	1083003	0	0	0	0	No match	No match	No MS2	[M+H]+1	1083003	974236,3	8,3	8,8
FALSE		C6 H12 Cl3	Full match	No results	No results	No results	No results	-1,72	375,9213	376,9286	1,221	1857499	0	0	0	0	No match	No match	No MS2	[M+H]+1	1657003	1857499	8,3	8,3
FALSE			No results	No results	No results	No results	No results		711,8132	712,8205	1,079	1337157	0	0	0	0	No match	No match	No MS2	[M+H]+1		1337157		7,7
FALSE			No results	No results	No results	No results	No results		156,0077	157,0149	0,977	2805670	0	0	0	0	No match	No match	No MS2	[M+H]+1	2805670		4,8	
FALSE		C H2 Cl O5	Full match	No results	No results	No results	No results	4,52	221,8814	222,8886	1,128	1075149	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1075149	969263,2	7,2	7,2
FALSE	4-Amino-4'-fluorobiphenyl	C12 H10 F	No results	No results	No results	Full match	No results	-4,07	187,079	94,54676	0,974	2013774	2	0	0	0	No match	No match	No MS2	[M+2H]+2	2013774	1573745	4,8	3,9
FALSE	N-Acetyl-4-chloro-D-phenylalanyl-4-chloro-D	C69 H91 Cl	No results	No results	No results	Full match	No results	2,48	1451,634	726,8245	1,097	895419,7	1	0	0	0	No match	No match	No MS2	[M+2H]+2	895419,7	732127	8,3	7,9
FALSE		C7 H16 N4	Full match	No results	No results	No match	No match	-2,01	266,0515	267,0588	3,222	1201035	1	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	1132127	1201035	8,3	7,7
FALSE			No results	No results	No results	No results	No results		598,8052	300,4099	1,028	2207100	0	0	0	0	No match	No match	No MS2	[M+2H]+2	2207100	1032960	2,6	7,2
FALSE	N-[(2S)-4-Cyclohexyl-1-ethoxy-1-oxo-2-butan	C15 H27 N	Full match	No results	No results	Not the top	No results	0,1	285,194	286,2013	5,546	1431438	12	0	0	0	No match	No match	DDA for pri	[M+H]+1	1222945	1431438	7,2	6,6
FALSE		C11 H14 O	Full match	No results	No results	Full match	Partial mat	-0,22	194,0943	227,1278	7,112	26353451	97	0	0	0	No match	Multiple m	DDA for pri	[M+H+MeC]		26353451		4
FALSE		C40 H69 N	Full match	No results	No results	No results	No match	0,4	787,4721	788,4794	7,427	3127848	0	0	0	0	No match	Single mat	DDA for pri	[M+H]+1	2283841	3127848	7,5	7,5
FALSE	Hydroxyethyl imidazolidinone	C10 H12 N2	Full match	No results	No results	Full match	Partial mat	0,45	130,0743	131,0816	1,52	7138633	18	0	0	0	No match	Single mat	DDA for pri	[M+H]+1	7138633	3094279	4,6	7,5
FALSE		C3 H10 N2	Full match	No results	No results	No results	No results	0,43	138,0464	139,0536	1,289													

FALSE			No results	No results	No results	No results	No results	461,6382	462,6446	1,159	1162506	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1162506	1058105	8,3	8,8	
FALSE	Pivagabine	C8 H17 N F	Full match	No results	No results	No results	No match	-2,37	189,0832	190,0905	1,479	7037419	2	0	0			Single mat	No matche	DDA for pr	[M+H] <sup>+</sup> +1	3292243	7037419	6,4	6,4
FALSE		C9 H17 N C	Full match	No results	No results	No results	Full match	-0,17	187,1208	188,1281	1,904	1976800	13	0	0			Single mat	No matche	DDA for pr	[M+H] <sup>+</sup> +1	1819075	1976800	7,2	7,5
FALSE			No results	No results	No results	No results	No results		73,00032	74,0076	0,988	1789233	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	1789233	1523025	5,5	2,8
FALSE		C4 H4 O8 S	Full match	No results	No results	No match	No results	3,87	175,9634	176,9707	0,994	2594067	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	2171766	2594067	6,4	5,9
FALSE			No results	No results	No results	No results	No results		507,7079	586,7299	1,139	898899,7	0	0	0			No matche	No matche	No MS2	[M+DMSO]	898899,7	843379,3	8,3	8,3
FALSE		C16 H34 N	Full match	No results	No results	No results	No match	-4,98	538,1765	270,0956	1,549	2653022	1	0	0			No matche	No matche	DDA for ot	[M+2H] <sup>+</sup> +2	2653022	2321816	4,8	5,9
FALSE		C4 H3 N6 C	Full match	No results	No results	No results	No results	3,04	435,8629	436,8702	1,093	930049,9	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	930049,9	792294,2	7,7	7,4
FALSE			No results	No results	No results	No results	No results		103,023	104,0303	0,982	2151942	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	2151942	1894605	5,3	2,6
FALSE	Pentachloroethane	C2 H C15	No results	No results	No results	Full match	No results	-0,98	199,8519	200,8592	1,168	1921216	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1921216	1683488	7	5
FALSE		C10 H3 N C	Full match	No results	No results	No results	No results	0,98	169,0165	85,51555	1,018	1188762	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2		1188762		7,7
FALSE			No results	No results	No results	No results	No results		1345,682	673,8481	1,086	1221949	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2	1221949		7,7	
FALSE			No results	No results	No results	No results	No results		88,99806	90,00534	0,328	867134,9	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	438227,1	867134,9	4,1	7,7
FALSE	Muscimol	C4 H6 N2 C	Full match	No results	No results	No results	Full match	0,31	114,043	115,0502	1,963	1389037	14	0	0			Multiple m	Multiple m	No MS2	[M+H] <sup>+</sup> +1	1389037	1270376	6,6	7,2
FALSE			No results	No results	No results	No results	No results		98,02628	99,03356	1,009	2331445	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	2251672	2331445	4,8	3,2
FALSE		C5 H6 Br N	Full match	No results	No results	No results	No results	0,33	668,6849	669,6922	1,136	784755,2	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1		784755,2		7,9
FALSE	5-hydroxyisouric acid	C5 H4 N4 C	Full match	No results	No results	Full match	Full match	-0,15	184,0232	185,0305	2,794	5992951	2	0	0			Single mat	No matche	DDA for pr	[M+H] <sup>+</sup> +1	5762008	5992951	6,7	6,2
FALSE		C H2 N2 O	Full match	No results	No results	No results	No results	3,82	90,00689	123,0404	0,972	2413336	0	0	0			No matche	No matche	DDA for ot	[M+H+MeC]	2413336		5,3	
FALSE			No results	No results	No results	No results	No results		299,4025	300,4098	0,981	1278822	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1		1278822		6,1
FALSE	Epixine	C24 H37 N	Full match	No results	No results	Full match	Partial mat	-0,09	435,2621	436,2693	7,495	2306399	1	0	0			No matche	Single mat	DDA for pr	[M+H] <sup>+</sup> +1	1863833	2306399	7,2	7,5
FALSE	Methyltrifluorosilane	C H3 F3 Si	No results	No results	No results	Full match	No results	2,9	99,9959	101,0032	3,202	17680985	1	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	17477503	17680985	5,1	5,1
FALSE			No results	No results	No results	No results	No results		87,50183	88,50911	7,584	18999848	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	18999848	3636086	5,1	5,9
FALSE		C2 H2 Cl O	Full match	No results	No results	No results	No results	-2,57	315,8507	316,858	1,135	1053619	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1053619	1022207	6,6	7,2
FALSE		C8 H9 N6 F	Full match	No results	No results	No match	No results	1,03	441,871	442,8782	0,984	1977315	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1878995	1977315	2,8	4,8
FALSE		C2 H5 Br Cl	Full match	No results	No results	No results	No results	-1,34	353,7518	354,7591	1,147	988473,7	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	988473,7	828612,7	8,3	7,9
FALSE	Butyl Parahydroxybenzoate	C11 H14 O	Full match	No results	No results	Full match	Partial mat	0	194,0943	195,1016	7,592	1287069	97	0	0			No matche	Multiple m	DDA for pr	[M+H] <sup>+</sup> +1	1241527	1287069	8,8	7,7
FALSE		C6 H N3 O4	Full match	No results	No results	No results	No results	-3,4	178,9961	180,0034	1,209	996930,4	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	996930,4	944376,3	8,8	7,7
FALSE			No results	No results	No results	No results	No results		1209,707	605,8608	1,087	1083653	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2	1083653	1038430	7,7	7,7
FALSE			No results	No results	No results	No results	No results		659,6545	660,6618	1,141	761345,4	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	761345,4	744024,8	7,9	7,9
FALSE		C17 H3 N6	Full match	No results	No results	No results	No results	-0,35	703,8257	704,833	1,087	1078238	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1		1078238		6,7
FALSE		C7 H11 Cl2	Full match	No results	No results	No results	No results	2,06	333,9367	334,9439	1,223	1583066	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1476363	1583066	6,1	6,1
FALSE		C19 H40 Cl	Full match	No results	No results	No results	No results	0,83	608,1395	647,1026	1,538	1568765	0	0	0			No matche	No matche	DDA for ot	[M+K] <sup>+</sup> +1	1568765		6,1	
FALSE		C12 H28 N	Full match	No results	No results	No match	No results	-3,91	393,1385	394,1457	1,962	971472,3	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	971472,3	957341,3	7,7	7,2
FALSE			No results	No results	No results	No results	No results		1363,598	682,8061	1,119	599899,5	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2	599899,5		7,4	
FALSE			No results	No results	No results	No results	No results		114,9812	115,9885	0,979	1646056	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	1525133	1646056	5	4,5
FALSE		C5 H2 O4	Full match	No results	No results	No results	No results	1,39	125,9955	127,0028	0,973	1246389	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	1246389	1035574	3,9	4,5
FALSE	(Z)-N-16-hydroxyhexadec-9-enoyl-L-alanine	C20 H37 N	Full match	No results	No results	No results	Full match	-0,12	355,2722	356,2795	6,907	1700102	0	0	0			No matche	Single mat	DDA for pr	[M+H] <sup>+</sup> +1	1429076	1700102	7,2	7,2
FALSE		C9 H24 N9	Full match	No results	No results	No match	No results	-0,65	321,1789	322,1861	6,99	8308555	2	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	7477839	8308555	5,7	6,2
FALSE		C8 H2 Br Cl	Full match	No results	No results	No results	No results	1,11	615,6737	616,6804	1,137	774719,1	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	774719,1	377810,8	7,9	7,1
FALSE		C8 H3 N4 C	Full match	No results	No results	No results	No results	-1,02	519,8346	520,8418	1,11	433320,1	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	387638,8	433320,1	8,2	8,5
FALSE		C2 H2 Cl3 F	Full match	No results	No results	No results	No results	4,68	439,7182	440,7255	1,153	1072056	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1072056	968102,8	7,7	3,9
FALSE		C12 H4 Cl F	Full match	No results	No results	No results	No results	0,69	395,8782	396,8854	1,055	787865,7	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	787865,7	723748,4	7,9	7,9
FALSE	N-(tert-Butoxycarbonyl)-L-leucine	C11 H21 N	Full match	No results	No results	Full match	Full match	0,07	231,1471	232,1544	3,881	1070651	7	0	0			Multiple m	No matche	DDA for pr	[M+H] <sup>+</sup> +1	1017375	1070651	7,2	7,7
FALSE		C7 H5 N7	Full match	No results	No results	No match	No results	1,66	187,061	188,0682	3,68	991651,4	1	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	754030,3	991651,4	7,4	8,3
FALSE		C5 H7 O5 F	Full match	No results	No results	No results	No results	-4,51	178,0023	90,00843	7,376	19946952	0	0	0			No matche	No matche	DDA for ot	[M+2H] <sup>+</sup> +2		19946952		5,1
FALSE			No results	No results	No results	No results	No results		561,8356	562,8428	1,107	501483,4	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	381706,7	501483,4	5,4	4,1
FALSE		C6 H3 N5 C	Full match	No results	No results	No results	No results	-0,63	222,9811	223,9884	0,308	8505420	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	8505420		5,1	
FALSE		C16 H36 O	Full match	No results	No results	No results	No results	-0,97	578,1371	290,0758	1,249	1453209	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2	1453209	1351604	8,3	8,3
FALSE			No results	No results	No results	No results	No results		235,9138	236,9211	0,997	2454431	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	2011493	2454431	4,2	4,8
FALSE		C7 H14 N3	Full match	No results	No results	No results	No results	0,49	219,0596	220,0669	1,283	1111652	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	1075318	1111652	8,3	8,3
FALSE			No results	No results	No results	No results	No results		615,8179	616,8252	1,059	750411,3	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1	733136,6	750411,3	4,1	7,9
FALSE		C4 H2 Cl2 C	Full match	No results	No results	No results	No results	0,35	617,6699	618,6772	1,14	788903,4	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> +1		788903,4		7,4
FALSE		C4 H6 N6 C	Full match	No results	No results	No match	No results	1,43	186,0504	187,0577	1,114	2837745	1	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	2754960	2837745	5,9	4,2
FALSE	(±)-Dihydrojasmonic Acid	C12 H20 O	Full match	No results	No results	Full match	Full match	-0,26	212,1412	195,1379	6,907	18181060	19	0	0			Multiple m	Multiple m	DDA for pr	[M+H+H2O]	18181060	15326967	4,6	4,6
FALSE			No results	No results	No results	No results	No results		1513,605	757,8098	1,068	962720,2	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> +2	936865,7	962720,2	4,5	5
FALSE		C4 H2 Cl O	Full match	No results	No results	No match	No results	-4,83	289,8688	290,8761	1,123	747031,9	1	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	672612,7	747031,9	8,5	7,9
FALSE		C H N7 O	Full match	No results	No results	No results	No results	2,47	127,0246	150,0138	1,164	814796,8	0	0	0			No matche	No matche	No MS2	[M+Na] <sup>+</sup> +1	814796,8		8,5	
FALSE			No results	No results	No results	No results	No results		87,52117	88,52844	1	2104216	0	0	0			No matche	No matche	DDA for pr	[M+H] <sup>+</sup> +1	770181,7	2104216	7,9	2,1
FALSE	4-nitrophenyl isocyanate	C7 H4 N2 C	Full match	No results	No results	No results	Full match	4,04	164,0229																

FALSE		C5 H8 N2 C	Full match	No results	No results	No results	No results	No results	-3,28	224,0273	225,0346	1,226	1880136	0	0	0	No matche	No matche	No MS2	[M+H]+1	1880136		6,1		
FALSE			No results	No results	No results	No results	No results	No results		235,8846	236,8918	1,137	916175,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	916175,9	751466,7	8,3	7,4	
FALSE		C16 H29 N	Full match	No results	No results	No results	No results	No results	0,24	299,192	300,1993	6,711	1132194	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1115309	1132194	8,3	7,7	
FALSE		C9 H7 N5 C	Full match	No results	No results	No results	No results	No results	2,1	345,0023	346,0095	0,306	1420098	0	0	0	No matche	No matche	No MS2	[M+H]+1	1142859	1420098	5,5	7,7	
FALSE	(2E)-hexadecenoylcarnitine	C23 H43 N	Full match	No results	No results	Full match	Partial mat		0,12	397,3193	398,3265	7,177	1609373	2	0	0	No matche	Single mat	DDA for pri	[M+H]+1	465803,7	1609373	4,1	7,2	
FALSE			No results	No results	No results	No results	No results			1261,721	631,8676	1,088	1120480	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1120480		7,2		
FALSE			No results	No results	No results	No results	No results			160,9623	161,9696	0,307	1308310	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	561089,6	1308310	3,6	4,5	
FALSE	L-(+)-Alanine	C3 H7 N O2	Full match	No results	No results	Full match	Full match		0,25	89,0477	90,05498	3,267	47017490	19	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	47017490		4		
FALSE			No results	No results	No results	No results	No results			489,6453	490,6526	1,174	773635,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	773635,9	712936,8	5,8	7,9	
FALSE	Furfuralol	C5 H6 O2	Full match	No results	No results	Full match	No results		0,26	98,0368	99,04408	7,092	29907590	16	0	0	No matche	No matche	DDA for pri	[M+H]+1	24623642	29907590	4,6	4,6	
FALSE			No results	No results	No results	No results	No results			145,0226	146,0299	0,964	2315374	0	0	0	No matche	No matche	No MS2	[M+H]+1	2315374		7,2	4,2	
FALSE		C11 H19 N	Full match	No results	No results	No match	No results		3,41	314,1267	315,134	6,804	1227645	10	0	0	No matche	No matche	DDA for pri	[M+H]+1	1170951	1227645	8,8	7,7	
FALSE		C6 H2 Br Cl	Full match	No results	No results	No results	No results		0,94	661,742	662,7489	1,13	558743,6	0	0	0	No matche	No matche	No MS2	[M+H]+1	558743,6	504782,3	7,9	7,9	
FALSE			No results	No results	No results	No results	No results			1193,733	597,8736	1,087	990859,4	0	0	0	No matche	No matche	No MS2	[M+2H]+2	990859,4	771807,2	7,7	7,4	
FALSE		C15 H3 N2	Full match	No results	No results	No results	No results		2,1	463,8655	464,8728	1,057	715574,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	715574,5	680321,9	7,9	7,4	
FALSE	Jasmonic acid	C12 H18 O	Full match	No results	No results	Full match	Full match		-0,28	210,1255	211,1328	7,029	30315118	40	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1	30315118		5,1		
FALSE		C3 H2 Cl N	Full match	No results	No results	No match	No results		-3,14	275,978	276,9852	1,229	1815018	2	0	0	No matche	No matche	No MS2	[M+H]+1	1732572	1815018	5	8,3	
FALSE			No results	No results	No results	No results	No results			1293,669	647,8416	1,087	940328,9	0	0	0	No matche	No matche	No MS2	[M+2H]+2	940328,9		7,7		
FALSE		C2 H N2 O2	Full match	No results	No results	No results	No results		2,99	115,9779	116,9852	0,983	1925005	0	0	0	No matche	No matche	No MS2	[M+H]+1	1686546	1925005	2,3	4,2	
FALSE	N-Boc-L-leucine Methyl Ester	C12 H23 N	Full match	No results	No results	Full match	Partial mat		0,09	245,1627	246,17	4,461	1223467	6	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	1121616	1223467	8,3	7,2	
FALSE		C6 H12 N6	Full match	No results	No results	No results	No results		1,43	184,1075	185,1148	1,093	3357893	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	3204059	3357893	3,7	5,3	
FALSE			No results	No results	No results	No results	No results			1397,695	699,8548	1,088	844728,8	0	0	0	No matche	No matche	No MS2	[M+2H]+2	804754,6	844728,8	7,9	7,7	
FALSE		C25 H53 N	Full match	No results	No results	No match	No match		-2,41	523,3642	524,3715	6,863	18244497	6	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	18244497		5,7		
FALSE	Glutarylcarnitine	C12 H21 N	Full match	No results	No results	Full match	No results		-0,05	275,1369	276,1442	3,346	1030539	3	0	0	No matche	No matche	DDA for pri	[M+H]+1	1002699	1030539	8,3	8,3	
FALSE	Benzyl butyrate	C11 H14 O	Full match	No results	No results	Full match	Full match		-0,11	178,0994	179,1066	7,145	17210590	95	0	0	Multiple m	Multiple m	DDA for ott	[M+H]+1	17210590	13685985	3,5	4	
FALSE		C2 H7 N4 C	Full match	No results	No results	No results	No results		0,91	166,008	84,01126	0,978	1781345	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2	1781345	1586464	7,2	3,9	
FALSE			No results	No results	No results	No results	No results			146,9966	169,9858	1,167	966167,5	0	0	0	No matche	No matche	DDA for pri	[M+Na]+1	966167,5	941266,3	8,3	6,6	
FALSE	(3R,4R,5R,7R)-7-[(1R,2S,5S)-2,5-Dihydroxy-1,	C15 H24 O	Full match	No results	No results	Full match	Partial mat		0,17	284,1624	285,1697	7,094	11093125	7	0	0	No matche	Multiple m	DDA for ott	[M+H]+1	10461666	11093125	3,5	5,7	
FALSE		C8 H3 N6 C	Full match	No results	No results	No match	No match		-0,94	246,0053	247,0126	0,975	1975750	6	0	0	Multiple m	Single mat	No MS2	[M+H]+1	1589648	1975750	4,5	2,1	
FALSE		C4 H4 Br Cl	Full match	No results	No results	No results	No results		-3,76	599,7	600,7063	1,136	709703,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	709703,1	663782,5	7,9	7,4	
FALSE		C12 H8 N8	Full match	No results	No results	No match	No results		-3,5	360,0554	361,0627	2,396	2660308	2	0	0	No matche	No matche	DDA for pri	[M+H]+1	2660308	2376568	7,5	8	
FALSE	(20R)-Cholesta-3,5-diene	C27 H44	Full match	No results	No results	Full match	No results		-0,04	368,3443	369,3516	0,976	2261591	1	0	0	No matche	No matche	No MS2	[M+H]+1		2261591		4,8	
FALSE		C3 H5 N4 C	Full match	No results	No results	No results	No results		-4,92	160,0142	81,01439	1	1564819	0	0	0	No matche	No matche	DDA for ott	[M+2H]+2	1564819		5,5		
FALSE		C5 H12 N6	Full match	No results	No results	No results	No results		2,05	156,1127	157,1199	7,264	15172994	0	0	0	No matche	No matche	No MS2	[M+H]+1	15172994	14514600	5,1	5,1	
FALSE	pyrimidinethione	C4 H4 N2 S	Full match	No results	No results	Full match	No results		-0,44	112,0095	113,0168	0,305	220647,7	1	0	0	No matche	No matche	No MS2	[M+H]+1		220647,7		7,6	
FALSE		C3 H26 O	Full match	No results	No results	No match	No match		-2,35	342,1163	343,1236	1,251	1137725	95	0	0	Multiple m	No matche	No MS2	[M+H]+1	1094720	1137725	4,5	6,1	
FALSE	Triethylamine	C6 H15 N	Full match	No results	No results	Full match	Full match		0,31	101,1205	102,1278	3,21	1136966	16	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	1076459	1136966	7,2	5,5	
FALSE		C52 H71 N	Full match	No results	No results	No results	No results		-0,13	1035,452	346,158	3,277	909055,8	0	0	0	No matche	No matche	DDA for ott	[M+3H]+3	909055,8	831485,3	7,7	7,4	
FALSE	Tris-formaminomethane	C4 H7 N3 C	Full match	No results	No results	Full match	No results		3,26	145,0492	73,53188	0,306	5899740	5	0	0	No matche	No matche	DDA for ott	[M+2H]+2	5899740	3041900	4	3,7	
FALSE		C3 H7 N2 C	Full match	No results	No results	No match	No results		-0,9	179,977	180,9842	0,995	2431178	1	0	0	No matche	No matche	No MS2	[M+H]+1	2431178		4,2		
FALSE			No results	No results	No results	No results	No results			97,00718	98,01445	0,314	360146,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	360146,5	140912,1	8,2	8,2	
FALSE	N-[2-[[2-(Ethylthio)ethyl]thio]ethyl]urea	C7 H16 N2	Full match	No results	No results	Full match	No results		3,38	208,0711	209,0784	1,108	2837370	2	0	0	No matche	No matche	DDA for pri	[M+H]+1	2837370	2510803	4,8	3,2	
FALSE		C2 H Br Cl3	Full match	No results	No results	No results	No results		-1,34	443,6673	444,6736	1,159	825212	0	0	0	No matche	No matche	No MS2	[M+H]+1	825212	823223,6	7,9	8,5	
FALSE		C4 H5 Cl4	Full match	No results	No results	No results	No results		2,73	557,7154	558,7216	1,141	634261,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	634261,3	565393,1	7,9	6,8	
FALSE			No results	No results	No results	No results	No results			1471,699	736,857	1,097	778822,5	0	0	0	No matche	No matche	No MS2	[M+2H]+2	650428,5	778822,5	7,9	7,4	
FALSE		C6 H N8 O4	Full match	No results	No results	No match	No results		0,34	279,9859	280,9932	0,975	1998728	1	0	0	No matche	No matche	No MS2	[M+H]+1	1998728	1935477	7	5,3	
FALSE		C11 H11 Br	Full match	No results	No results	No results	No results		0,14	282,0004	283,0077	4,997	958833,6	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	942791	958833,6	8,3	8,3	
FALSE		C4 H5 N7 C	Full match	No results	No results	No results	No results		1,45	183,0507	184,058	4,856	563273,6	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	5234971	563273,6	4,2	2,6	
FALSE		C4 H5 N7 C	Full match	No results	No results	No results	No results		1,62	183,0508	184,0581	5,131	4391515	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	4167239	4391515	4,2	2,6	
FALSE	6-Cyanopurine	C6 H3 N5	Full match	No results	No results	Full match	No results		-2,91	145,0384	146,0457	1,438	2757627	1	0	0	No matche	No matche	DDA for pri	[M+H]+1	2757627		4,8		
FALSE			No results	No results	No results	No results	No results			629,823	630,8302	1,104	398464,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	222077,4	398464,1	3,8	7,4	
FALSE			No results	No results	No results	No results	No results			1355,639	678,8265	1,114	309185,7	0	0	0	No matche	No matche	No MS2	[M+2H]+2	309185,7		4,3		
FALSE			No results	No results	No results	No results	No results			82,01437	83,02164	1,291	1661651	0	0	0	No matche	No matche	No MS2	[M+H]+1		1661651		5	
FALSE	5-Methyl-2-pyrrolidone	C5 H9 N O	Full match	No results	No results	Full match	No results		0,12	99,06843	100,0757	3,855	2347117	26	0	0	No matche	No matche	DDA for pri	[M+H]+1	2320430	2347117	7,5	7	
FALSE			No results	No results	No results	No results	No results			96,50711	97,51439	0,34	775846,1	0	0	0	No matche	No matche	No MS2	[M+H]+1		775846,1		6,8	
FALSE		C12 H30 N	Full match	No results	No results	No results	No results		-0,78	379,2206	380,2279	7,05	5789766	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	5258224	5789766	4,8	5,7	
FALSE			No results	No results	No results	No results	No results			1481,657	741,8356	1,09	843916,5	0	0	0	No matche	No matche	No MS2	[M+2H]+2	843916,5		7,7		
FALSE		C2 H3 Br Cl	Full match	No results	No results	No results	No results		0,31	401,6826	402,6889	1,145	858516,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	858516,1	803886,2	5	5,2	
FALSE	Butabarbital	C10 H16 N	Full match	No results	No results	No results	Partial mat		0,14	212,1161	213,1234	3,215	1162343	7	0	0	No matche	Multiple m	No MS2	[M+H]+1	1088146	1162343	7,7	7,2	
FALSE	quinolone	C9 H7 N O	Full match	No results	No results	Full match	Full match		0,44	145,0528	146,0601	4,132	992175,2	22	0	0	Multiple m	No matche	No MS2	[M+H]+1	934890,2	992175,2	6,6	7,2	
FALSE		C2 H8 O3 F	Full match	No results	No results	No results	No results		-3,89	141,9943	143,0016	0,983	22												



FALSE	THI	C9 H14 N2	Full match	No results	No results	No results	Full match	No results	0,28	230,0903	263,1239	1,723	1561019	9	0	0	No matche	No matche	DDA for pri	[M+H]+MeC	1430137	1561019	6,1	5,5
FALSE			No results	No results	No results	No results	No results	No results		1425,634	713,8242	1,104	626172,3	0	0	0	No matche	No matche	No MS2	[M+2H]+2	626172,3			8,5
FALSE			No results	No results	No results	No results	No results	No results		375,7249	376,7322	1,174	799487,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	799487,3	714655,9	8,5	5,8
FALSE			No results	No results	No results	No results	No results	No results		112,9564	113,9637	0,318	3305728	0	0	0	No matche	No matche	No MS2	[M+H]+1	3305728		6,1	
FALSE		C H2 Cl O5	Full match	No results	No results	No results	No results	No results	4,41	221,8813	222,8886	1,189	1646199	0	0	0	No matche	No matche	No MS2	[M+H]+1	1646199	1626600	6,4	3,9
FALSE		C16 H3 Br	Full match	No results	No results	No results	No results	No results	1,85	625,7023	626,7091	1,136	717985,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	717985,1	599041,4	7,4	7,9
FALSE		C2 H8 N3 C	Full match	No results	No results	No results	No results	No results	1,07	169,0254	170,0327	2,4	2077803	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	2077803	1947193	7,5	7,5
FALSE		C13 H N4 O	Full match	No results	No results	No results	No results	No results	-2,36	139,9885	140,9957	0,341	1067251	0	0	0	No matche	No matche	DDA for pri	[M+H]+1		1067251		7,2
FALSE	3-epi-3-hydroxymugineic acid	C12 H20 N	Full match	No results	No results	No results	Full match	Full match	0,24	336,117	337,1242	2,268	1754158	1	0	0	Single mati	No matche	DDA for pri	[M+H]+1	1754158	1651578	7,2	6,6
FALSE	Acetyl cyclohexanesulfonoperoxoate	C8 H14 O5	Full match	No results	No results	No results	Not the top	Full match	0,71	222,0564	223,0636	7,154	1524631	7	0	0	Multiple m	Single mati	No MS2	[M+H]+1	498480,7	1524631	4,1	5
FALSE			No results	No results	No results	No results	No results	No results		1409,657	705,8358	1,106	609588,1	0	0	0	No matche	No matche	No MS2	[M+2H]+2	272129,6	609588,1	6	6,8
FALSE	3,5-DIISOPROPYLSALICYLIC ACID	C13 H18 O	Full match	No results	No results	No results	Full match	Partial mat	-0,21	222,1256	255,159	7,187	18418055	36	0	0	Single mati	Multiple m	DDA for pri	[M+H]+MeC		18418055		5,1
FALSE		C7 H4 N4 C	Full match	No results	No results	No results	No match	No results	3,41	224,0189	113,0167	7,565	8527232	1	0	0	No matche	No matche	DDA for ori	[M+2H]+2	8527232	3424961	5,1	6,4
FALSE			No results	No results	No results	No results	No results	No results		140,9513	141,9586	7,41	15451217	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	15451217		5,7	
FALSE		C7 H2 Cl O	Full match	No results	No results	No results	No results	No results	1,68	277,8859	278,8932	1,124	683229,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	683229,7		8,5	
FALSE			No results	No results	No results	No results	No results	No results		401,7278	402,7351	1,148	598985,2	0	0	0	No matche	No matche	No MS2	[M+H]+1	598985,2	549236,6	8,5	7,9
FALSE		C48 H79 N	Full match	No results	No results	No results	No results	No results	1,48	875,5243	438,7694	7,404	1684387	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1684387	1546697	6,6	6,6
FALSE		C17 H5 Cl3	Full match	No results	No results	No results	No results	No results	0,63	567,7438	568,7501	1,128	574317,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	574317,3	569136,4	7,4	7,4
FALSE		C47 H69 N	Full match	No results	No results	No results	No results	No results	-1,43	919,4552	460,7349	4,721	1091844	0	0	0	No matche	No matche	DDA for ori	[M+2H]+2	1046812	1091844	7,2	6,6
FALSE			No results	No results	No results	No results	No results	No results		335,2138	168,6142	0,974	1720596	0	0	0	No matche	No matche	No MS2	[M+2H]+2		1720596		4,5
FALSE		C9 H14 N C	Full match	No results	No results	No match	No results	No results	-3,57	183,0807	184,0879	3,232	913900	7	0	0	No matche	No matche	DDA for pri	[M+H]+1	913900	825843,1	8,8	7,4
FALSE		C4 H Cl O6	Full match	No results	No results	No results	No results	No results	0,93	273,866	274,8733	1,105	1052971	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1052971	1042003	8,3	7,2
FALSE	meprobamate	C9 H18 N2	Full match	No results	No results	No results	Full match	Full match	0,24	218,1267	219,134	1,958	727284,7	21	0	0	Single mati	No matche	DDA for pri	[M+H]+1	695428,3	727284,7	8,5	6,8
FALSE		C6 H6 Cl N	Full match	No results	No results	No results	No match	No results	-4,66	577,7725	578,779	1,121	459237,2	1	0	0	No matche	No matche	No MS2	[M+H]+1	388105,9	459237,2	8,2	7,9
FALSE	1-Piperidine	C5 H9 N	Full match	No results	No results	No results	Full match	Full match	0,56	83,07355	84,08082	1,96	1536023	13	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	1536023	889203,3	6,1	6,1
FALSE			No results	No results	No results	No results	No results	No results		621,5366	622,5439	1,176	556485,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	556485,3	501342,7	7,9	8,5
FALSE			No results	No results	No results	No results	No results	No results		683,8051	684,8124	1,059	665007,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	531142,8	665007,1	3,6	4,7
FALSE			No results	No results	No results	No results	No results	No results		195,1471	196,1543	3,455	875348,8	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	798078,7	875348,8	7,4	7,2
FALSE			No results	No results	No results	No results	No results	No results		519,5969	520,6033	1,175	789022,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	789022,3	754488,4	7,4	7,4
FALSE	Methyltrifluorosilane	C H3 F3 Si	No results	No results	No results	Full match	No results	No results	3,13	99,99592	101,0032	1,384	1906414	1	0	0	No matche	No matche	No MS2	[M+H]+1	1868874	1906414	6,6	1,5
FALSE		C6 H Cl O7	Full match	No results	No results	No results	No results	No results	-2,08	347,8286	426,8505	1,12	499284,8	0	0	0	No matche	No matche	No MS2	[M+DMSO]	499284,8		7,4	
FALSE			No results	No results	No results	No results	No results	No results		734,587	735,5943	1,143	426588,6	0	0	0	No matche	No matche	No MS2	[M+H]+1	426588,6		7,9	
FALSE	Palmitelaidic acid	C16 H30 O	No results	No results	No results	Full match	Full match	Full match	0,78	254,2248	255,2321	1,489	50344573	36	0	0	Single mati	Multiple m	DDA for pri	[M+H]+1		50344573		5,1
FALSE	Lauryldimethylamine oxide	C14 H31 N	Full match	No results	No results	Full match	No results	No results	-0,13	229,2405	230,2478	6,947	1862738	1	0	0	No matche	No matche	No MS2	[M+H]+1	1797739	1862738	6,1	6,6
FALSE		C6 H9 O7 F	Full match	No results	No results	No results	No match	No results	0,12	224,0086	225,0159	1,249	1296605	2	0	0	No matche	No matche	No MS2	[M+H]+1	1296605	1237665	7,2	5
FALSE			No results	No results	No results	No results	No results	No results		433,6836	434,6908	1,173	674656,5	0	0	0	No matche	No matche	No MS2	[M+H]+1		674656,5		8,5
FALSE		C26 H3 N6	Full match	No results	No results	No results	No results	No results	-0,06	779,8006	780,8079	1,082	810450,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	810450,3		7,4	
FALSE		C4 H2 Cl N	Full match	No results	No results	No results	No results	No results	-0,28	569,7401	570,7474	1,136	686516,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	686516,3		7,4	
FALSE	3-Methylglutarylcarnitine	C13 H23 N	Full match	No results	No results	Not the top	No results	No results	0,02	289,1525	290,1598	3,732	911732,3	4	0	0	No matche	No matche	DDA for pri	[M+H]+1	907321,8	911732,3	7,2	6,6
FALSE		C4 H Br Cl3	Full match	No results	No results	No results	No results	No results	-4,73	469,6705	548,6928	1,144	544214,7	0	0	0	No matche	No matche	No MS2	[M+DMSO]	544214,7	515276	7,9	7,4
FALSE			No results	No results	No results	No results	No results	No results		497,6781	498,6848	1,149	459986,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	459986,5	414803,6	7,4	6,8
FALSE			No results	No results	No results	No results	No results	No results		1164,496	583,2554	7,058	1037718	0	0	0	No matche	No matche	No MS2	[M+2H]+2		1037718		7,2
FALSE	Ethyl (2E,4Z)-2,4-hexadecadienoate	C18 H32 O	Full match	No results	No results	Full match	Partial mat		1,06	280,2405	281,2478	1,608	3992987	27	0	0	Multiple m	Single mati	DDA for pri	[M+H]+1		3992987		5,1
FALSE		C2 H N6 O4	Full match	No results	No results	No results	No results	No results	-1,13	235,9515	236,9588	0,986	1447667	0	0	0	No matche	No matche	No MS2	[M+H]+1		1447667		5,1
FALSE		C3 H2 N6 C	Full match	No results	No results	No results	No results	No results	0,9	471,8017	472,809	1,136	685849,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	685849,8		7,4	
FALSE		C6 H6 Cl3 F	Full match	No results	No results	No results	No results	No results	-4,17	322,8824	364,9163	1,196	784455,1	0	0	0	No matche	No matche	No MS2	[M+ACN+H]	784455,1	733115,5	5,8	4,7
FALSE	azidamfenicol	C11 H13 N	No results	No results	No results	Full match	No results	No results	2,35	295,0924	296,0996	1,447	365737,2	7	0	0	No matche	No matche	DDA for pri	[M+H]+1	365737,2		4,3	
FALSE			No results	No results	No results	No results	No results	No results		676,6283	677,6356	1,143	522953,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	522953,8		7,4	
FALSE		C5 H4 N5 C	Full match	No results	No results	No results	No results	No results	-1,63	197,0099	99,51225	7,554	8441568	0	0	0	No matche	No matche	No MS2	[M+2H]+2	8441568	2972457	5,7	2,1
FALSE	N-(3-Methoxyphenyl)-4-(pyrazolo[1,5-b]pyri	C17 H14 N	Full match	No results	No results	Not the top	No results	No results	-4,26	318,1216	319,1288	5,29	1020947	4	0	0	No matche	No matche	DDA for pri	[M+H]+1	955710,4	1020947	7,2	8,3
FALSE	Diethylene glycol n-butyl ether	C8 H18 O3	Full match	No results	No results	No results	No results	No results	-0,08	162,1256	163,1329	0,392	6840645	17	0	0	No matche	No matche	DDA for pri	[M+H]+1	6838397	6840645	3,5	4
FALSE			No results	No results	No results	No results	No results	No results		1187,716	594,8653	1,071	527494,2	0	0	0	No matche	No matche	No MS2	[M+2H]+2	527494,2	510184,8	8,5	7,9
FALSE	2-Nitro-5-sulfidobenzoate	C7 H3 N O4	Full match	No results	No results	Full match	No results	No results	-3,85	196,9775	197,9848	0,33	798744	1	0	0	No matche	No matche	No MS2	[M+H]+1	608043,1	798744	5,8	6,8
FALSE		C2 H4 Cl2 C	Full match	No results	No results	No results	No results	No results	-0,97	575,695	576,7018	1,143	638014,3	0	0	0	No matche	No matche	No MS2	[M+H]+1		638014,3		5,5
FALSE		C39 H81 N	Full match	No results	No results	No results	No results	No results	-0,58	919,5506	460,7826	7,403	1623021	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1623021	1598329	5,5	5,5
FALSE		C8 H8 N5 C	Full match	No results	No results	No match	No results	No results	-1,16	237,0413	119,5279	0,3	212143,8	1	0	0	No matche	No matche	No MS2	[M+2H]+2	212143,8	128477,5	3,8	7,1
FALSE	3,4-DIMETHOXYBENZENEPROPANOL	C11 H16 N O	Full match	No results	No results	Full match	Partial mat		0,1	196,11	197,1172	7,064	25679277	31	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	25679277	20372804	5,1	4
FALSE		C3 H6 N P	Full match	No results	No results	No results	No results	No results	0,44	118,9959	120,0032	1,153	595570,9	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	595570,9	543564,1	5,8	6,3
FALSE	METIPRANOLOL	C17 H27 N	Full match	No results	No results	Full match	Partial mat		0,33	309,1941	310,2014	5,934	1111776	13	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	1036958	1111776	7,7	7,7
FALSE		C H2 Cl O14	Full match	No results	No results	No results	No results	No results	-2,85	493,7215	494,7281	1,141	610858,7	0	0	0	No matche	No matche	No MS2	[M+H]+1		610858,7		7,4
FALSE			No results	No results	No results	No results</																		

FALSE				No results	No results	No results	No results	No results	653,7088	654,7161	1,136	542227,3	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	542227,3		7,4			
FALSE				No results	No results	No results	No results	No results	1465,682	733,8484	1,088	677981,2	0	0	0	No matche	No matche	No MS2	[M+2H] <sup>+</sup>	563203,5	677981,2	3,6	7,4		
FALSE	N-[[2S]-4-Cyclohexyl-1-ethoxy-1-oxo-2-butanoic acid]	C15 H27 N	Full match	No results	No results	No results	Not the top	No results	0,24	285,1941	286,2014	5,607	1081160	12	0	0	No matche	No matche	DDA for pr	[M+H] <sup>+</sup>	1081160	1060607	7,7	5,5	
FALSE	Glutaric anhydride	C5 H6 O3	Full match	No results	No results	No results	Full match	Full match	0,67	114,0318	115,0391	1,477	20452462	15	0	0	Single mat	No matche	No MS2	[M+H] <sup>+</sup>	20452462		4		
FALSE	DES(PHENYLBUTOXY)PHENYLETHOXY SALME	C23 H33 N	Full match	No results	No results	Full match	Partial mat		0,14	387,241	388,2483	1,819	931332,5	1	0	0	No matche	Multiple m	DDA for pr	[M+H] <sup>+</sup>	875252,8	931332,5	6,6	7,7	
FALSE	8,8'-Ethane-1,2-diylbis(1,3-dimethyl-3,7-dihydro-2H-benzofuran-2-one)	C16 H18 N	No results	No results	No results	Full match	No results	No results	-3,84	386,1436	387,1509	1,511	674205,5	1	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	505586,3	674205,5	5,8	7,9	
FALSE			No results	No results	No results	No results	No results	No results		613,7217	614,729	1,136	552640,2	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	486643,5	552640,2	6,8	7,9	
FALSE	Benzocyclohexane	C13 H16 O	No results	No results	No results	Full match	Partial mat		0,36	188,1202	189,1275	1,011	711692,3	17	0	0	No matche	Single mat	No MS2	[M+H] <sup>+</sup>	711692,3	441070,6	3	8,5	
FALSE		C14 H14 N4	Full match	No results	No results	No results	No results	No results	0,49	717,6139	718,6204	1,142	464353,8	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	464353,8	394288,9	7,9	7,1	
FALSE			No results	No results	No results	No results	No results	No results		109,0052	110,0125	1,963	448023,8	0	0	0	No matche	No matche	DDA for ot	[M+H] <sup>+</sup>	329433,4	448023,8	8,2	8,5	
FALSE			No results	No results	No results	No results	No results	No results		179,8871	180,8944	1,092	853659,5	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	853659,5	750974,4	5,5	5,8	
FALSE			No results	No results	No results	No results	No results	No results		167,6068	168,6141	0,973	1379849	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1379849		5,5		
FALSE		C5 H15 Cl2	Full match	No results	No results	No results	No results	No results	0,47	425,8431	426,8503	1,119	416649,8	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		416649,8		8,5	
FALSE		C3 H10 Br	Full match	No results	No results	No results	No results	No results	-0,14	633,8394	634,8467	1,075	550781,9	0	0	0	No matche	No matche	DDA for pr	[M+H] <sup>+</sup>	550781,9		7,9		
FALSE	Decanamide	C10 H21 N	Full match	No results	No results	No results	Full match	No results	-0,03	171,1623	172,1696	7,422	1119657	12	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1119657	1090980	6,6	7,7	
FALSE		C4 H11 Cl2	Full match	No results	No results	No results	No results	No results	1,53	493,8308	494,838	1,117	301774,3	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		301774,3		8,2	
FALSE		C5 H Br Cl	Full match	No results	No results	No results	No results	No results	0,98	675,6286	676,6359	1,141	569452,6	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		569452,6		7,4	
FALSE	1-ETHYL CITRATE	C8 H12 O7	Full match	No results	No results	Full match	Full match		3,2	220,059	221,0663	1,146	368106,8	5	0	0	Multiple m	No matche	DDA for pr	[M+H] <sup>+</sup>	368106,8	293315,2	8,2	7,6	
FALSE		C7 H O16 F	Full match	No results	No results	No results	No results	No results	-2,66	433,8466	434,8539	1,065	637727,6	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	637727,6	624021,5	7,9	7,9	
FALSE		C3 H Cl N2	Full match	No results	No results	No results	No results	No results	1,37	529,7608	530,7674	1,139	644474,8	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		644474,8		7,4	
FALSE			No results	No results	No results	No results	No results	No results		607,4709	304,7427	1,148	1795233	0	0	0	No matche	No matche	No MS2	[M+2H] <sup>+</sup>	1795233	608111,7	2,3	4,7	
FALSE			No results	No results	No results	No results	No results	No results		579,5523	580,5591	1,174	538819,1	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	510194,1	538819,1	7,9	4,1	
FALSE			No results	No results	No results	No results	No results	No results		603,7838	604,7911	0,977	1027230	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1027230	513702,7	2,8	5,2	
FALSE		C2 H2 Cl O	Full match	No results	No results	No results	No results	No results	2,3	265,8353	266,8426	1,142	634076,1	0	0	0	No matche	No matche	DDA for pr	[M+H] <sup>+</sup>		634076,1		7,4	
FALSE		C6 H Cl2 N	Full match	No results	No results	No results	No results	No results	-0,35	679,7119	680,7192	1,134	607379,9	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	607379,9		7,4		
FALSE			No results	No results	No results	No results	No results	No results		593,8239	594,8311	1,087	710310	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		710310	283502,1	2	7,1
FALSE		C9 H22 N9	Full match	No results	No results	No match	No results	No results	-0,82	303,1682	304,1755	7,104	8879503	2	0	0	No matche	No matche	DDA for pr	[M+H] <sup>+</sup>	8879503		4,6		
FALSE		C3 H7 N2 Cl	Full match	No results	No results	No match	No results	No results	1,21	166,0145	167,0218	1,205	1050511	2	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1050511		6,1		
FALSE	2-Methyl-3-[(2E,6E)-3,7,11-trimethyl-2,6,10-octadecatrien-1-yl]propanoic acid	C26 H32 O	No results	No results	No results	Full match	No results	No results	0,15	376,2403	189,1274	0,958	1224923	1	0	0	No matche	No matche	No MS2	[M+2H] <sup>+</sup>	521455,8	1224923	4,7	3,4	
FALSE		C3 H Br Cl4	Full match	No results	No results	No results	No results	No results	3,39	427,6924	428,6997	1,174	595089,2	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	595089,2	578388,7	7,9	8,5	
FALSE		C5 H3 N8 C	Full match	No results	No results	No results	No results	No results	0,93	571,8377	572,845	1,09	504639,8	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	504639,8	439087	7,4	7,4	
FALSE			No results	No results	No results	No results	No results	No results		671,6813	672,6878	1,138	471554,3	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		471554,3		7,4	
FALSE	meribendan	C15 H14 N	Full match	No results	No results	No results	Not the top	No match	-4,3	294,1216	295,1289	4,327	702598,3	24	0	0	No matche	Multiple m	No MS2	[M+H] <sup>+</sup>	702598,3	699491,4	7,9	7,4	
FALSE			No results	No results	No results	No results	No results	No results		181,6226	182,6298	0,971	1591279	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		1591279		5	
FALSE			No results	No results	No results	No results	No results	No results		599,6093	600,6166	1,148	472606,9	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	472606,9		7,4		
FALSE			No results	No results	No results	No results	No results	No results		347,8612	348,8684	1,002	1406619	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1234721	1406619	4,5	3,4	
FALSE			No results	No results	No results	No results	No results	No results		612,8405	613,8478	1,086	720474,4	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		720474,4		7,4	
FALSE	2-[[2-Benzyl-1,7,7-trimethylbicyclo[2.2.2]hept-2-ylidene]ethyl]propanoic acid	C21 H33 N	Full match	No results	No results	Full match	Partial mat		0,13	315,2563	316,2635	7,009	1068035	1	0	0	No matche	Single mat	No MS2	[M+H] <sup>+</sup>	901832,5	1068035	7,7	5	
FALSE			No results	No results	No results	No results	No results	No results		1497,63	749,8225	1,089	587028,7	0	0	0	No matche	No matche	No MS2	[M+2H] <sup>+</sup>	587028,7		7,4		
FALSE		C10 H26 N	Full match	No results	No results	No match	No results	No results	-0,65	335,1945	336,2018	7,038	10047400	1	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	10047400	7469738	4	4,6	
FALSE		C15 H35 N	Full match	No results	No results	No results	No results	No results	1,38	407,2156	408,2228	6,906	6495053	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	5863030	6495053	5,1	5,1	
FALSE		C17 H39 N	Full match	No results	No results	No match	No match	No match	2,62	418,2945	419,3017	7,397	795092,5	2	0	0	Single mat	No matche	No MS2	[M+H] <sup>+</sup>	748711,4	795092,5	8,5	7,9	
FALSE	Hydroxyethyl imidazolidinone	C5 H10 N2	Full match	No results	No results	Full match	Partial mat		0,19	130,0743	131,0815	1,591	3389687	18	0	0	No matche	Single mat	DDA for pr	[M+H] <sup>+</sup>		3389687		4,8	
FALSE		C13 H22 N	Full match	No results	No results	No results	No match	No match	-1,25	285,0962	308,0854	3,686	701439,1	2	0	0	Single mat	No matche	DDA for pr	[M+Na] <sup>+</sup>	594882	701439,1	7,9	7,9	
FALSE			No results	No results	No results	No results	No results	No results		745,8068	746,8141	1,087	714328,3	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		714328,3		6,3	
FALSE		C13 H29 N	Full match	No results	No results	No match	No results	No results	-4,14	420,1492	421,1564	1,381	653517,4	5	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	653517,4	635553,3	7,4	6,8	
FALSE		C20 H43 N	Full match	No results	No results	No match	No results	No results	-3,69	453,2856	454,2929	7,319	1652623	4	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1652623	991166,3	6,1	5,5	
FALSE	Succinimide	C4 H5 N O2	Full match	No results	No results	Full match	Partial mat		0,56	99,03208	100,0394	1,957	16636010	7	0	0	No matche	Multiple m	DDA for pr	[M+H] <sup>+</sup>		16636010		4	
FALSE	1,2-Dioxin	C4 H4 O2	Full match	No results	No results	Full match	Full match		0,43	84,02117	85,02844	3,149	30162113	11	0	0	Single mat	Single mat	DDA for pr	[M+H] <sup>+</sup>	30162113		4,6		
FALSE		C4 H10 Cl3	Full match	No results	No results	No results	No results	No results	3,1	379,8829	380,8902	1,195	692281	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	692281	665792,6	5,8	8,5	
FALSE			No results	No results	No results	No results	No results	No results		494,3203	495,3276	7,177	1897455	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		1897455		7	
FALSE			No results	No results	No results	No results	No results	No results		1203,69	602,8522	1,072	505698,9	0	0	0	No matche	No matche	No MS2	[M+2H] <sup>+</sup>	505698,9		8,5		
FALSE	Ricinoleic Acid	C18 H34 O	Full match	No results	No results	Full match	Full match		-1,31	298,2504	299,2576	1,608	23380238	25	0	0	Single mat	Multiple m	DDA for pr	[M+H] <sup>+</sup>		23380238		4	
FALSE		C12 H12 N	Full match	No results	No results	No results	No results	No results	2,58	408,0122	409,0194	2,146	1617808	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	1483879	1617808	7,2	7,7	
FALSE			No results	No results	No results	No results	No results	No results		727,6419	728,6492	1,139	515063,4	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	398056,6	515063,4	7,4	7,4	
FALSE		C8 H2 Cl N	Full match	No results	No results	No results	No results	No results	1,56	365,8592	366,8664	1,061	594521,4	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	594521,4	518199,5	7,4	7,9	
FALSE			No results	No results	No results	No results	No results	No results		833,6578	278,8932	1,121	546246,3	0	0	0	No matche	No matche	No MS2	[M+3H] <sup>+</sup>		546246,3		8,5	
FALSE			No results	No results	No results	No results	No results	No results		123,9154	124,9226	1,105	989181	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>	969439,9	989181	4,5	5	
FALSE		C23 H40 N	Full match	No results	No results	No results	No results	No results	0,16	420,3101	421,3174	7,394	785332,5	0	0	0	No matche	No matche	No MS2	[M+H] <sup>+</sup>		785332,5		7,9	
FALSE			No results	No results	No results	No results	No results	No results		587,5848	666,6069	1,146	435603,4	0	0	0	No matche	No matche	No MS2	[M+DMSO]	435603,4	413109,5	7,9</		

FALSE		C17 H11 N	Full match	No results	No results	No results	No results	-0.01	751,7925	752,7998	1,06	471434,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	471434,3	437681,2	7,4	7,9	
FALSE		C11 H13 Cl4	Full match	No results	No results	No results	No results	0,17	735,6747	736,682	1,132	361474,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	361474,3	361474,3	8,2		
FALSE		C8 H15 Cl3	Full match	No results	No results	No results	No results	-4,3	391,8953	392,9026	1,22	911289,6	0	0	0	No matche	No matche	No MS2	[M+H]+1	798061,5	911289,6	8,5	8,3	
FALSE		C9 H Cl N6	Full match	No results	No results	No results	No results	0,74	545,8617	546,869	1,107	341428,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	341428,7		7,6		
FALSE	2-6-Hydroxy-2,5,7,8-tetramethyl-3,4-dihydr	C18 H30 N	No results	Invalid ma	No results	Invalid ma	No results	-6,02	292,2259	293,2332	1,46	315924,5	1	2	0	No matche	No matche	DDA for pri	[M+H]+1	246885,3	315924,5	4,9	1,1	
FALSE		C9 H7 Cl N	Full match	No results	No results	No match	No results	-2,05	337,9782	338,9855	1,235	1215158	4	0	0	No matche	No matche	No MS2	[M+H]+1	1215158		6,1		
FALSE	Linoelaidic Acid	C18 H32 O	Full match	No results	No results	Full match	Full match	0,29	280,2403	281,2476	1,238	1382926	27	0	0	Multiple m	Single mati	No MS2	[M+H]+1		1382926		6,1	
FALSE		C2 H3 N2 C	Full match	No results	No results	No results	No results	2,55	259,916	260,9233	1,017	1425551	0	0	0	No matche	No matche	No MS2	[M+H]+1		1425551		7,2	
FALSE		C4 H2 Cl3 C	Full match	No results	No results	No results	No results	-3,17	439,71	440,7173	1,145	434315	0	0	0	No matche	No matche	No MS2	[M+H]+1	434315		7,9		
FALSE		C3 H7 N3 C	Full match	No results	No results	No results	No results	-3,5	197,01	99,51225	7,388	5978077	0	0	0	No matche	No matche	No MS2	[M+2H]+2		5978077		4,6	
FALSE			No results	No results	No results	No results	No results		227,8057	228,8129	1,147	1006102	0	0	0	No matche	No matche	No MS2	[M+H]+1	984184,6	1006102	4,5	6,1	
FALSE			No results	No results	No results	No results	No results		1207,633	604,8236	1,106	289979,3	0	0	0	No matche	No matche	No MS2	[M+2H]+2		289979,3		4,9	
FALSE		C3 H8 Br2 C	Full match	No results	No results	No results	No results	-0,04	673,6328	674,6396	1,139	517292,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	517292,8	221408,2	7,4	7,6	
FALSE		C18 H26 N	Full match	No results	No results	No match	No match	-4,6	351,1583	352,1656	5,118	741019,2	7	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	714633,5	741019,2	7,9	7,9	
FALSE		C7 H17 Cl	Full match	No results	No results	No results	No results	2,16	428,0551	429,0624	1,217	444425,8	2	0	0	No matche	No matche	No MS2	[M+H]+1	444425,8	403658,1	7,9	7,4	
FALSE			No results	No results	No results	No results	No results		96,52647	97,53375	1,004	1287887	0	0	0	No matche	No matche	No MS2	[M+H]+1	1287887	1146720	1,7	7,7	
FALSE	(15,7aR)-7-(((25,3R)-2-Hydroxy-2-isopropyl-	C21 H33 N	Full match	No results	No results	Full match	No results	0,01	395,2308	396,2381	1,819	845854,7	1	0	0	No matche	No matche	DDA for pri	[M+H]+1	794567,6	845854,7	7,9	7,2	
FALSE		C3 H N4 O	Full match	No results	No results	No results	No results	-2,04	139,9885	140,9958	0,309	794153	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	794153	133373,3	4,1	6,5	
FALSE		C3 H6 Br Cl	Full match	No results	No results	No results	No results	-2,41	505,7115	584,7335	1,14	498621,7	0	0	0	No matche	No matche	No MS2	[M+DMSO]	498621,7	460121,8	7,4	7,9	
FALSE		C10 H3 Br C	Full match	No results	No results	No results	No results	1,22	633,6473	634,6546	1,143	354448,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	354448,7	360289,2	7,1	7,1	
FALSE			No results	No results	No results	No results	No results		317,7663	318,7735	1,171	635390,8	0	0	0	No matche	No matche	DDA for pri	[M+H]+1		635390,8		5,8	
FALSE			No results	No results	No results	No results	No results		547,6041	548,6114	1,175	440010,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	440010,7	411168,3	8,5	7,9	
FALSE		C H3 O11 F	Full match	No results	No results	No results	No results	3,37	315,862	316,8692	1,091	629198	0	0	0	No matche	No matche	No MS2	[M+H]+1		629198		7,9	
FALSE	DIHYDROXYETHYL LAURAMINE OXIDE	C16 H35 N	Full match	No results	No results	Full match	No results	0,03	289,2617	290,269	6,822	904371,5	2	0	0	No matche	No matche	No MS2	[M+H]+1	826721,2	904371,5	6,3	8,3	
FALSE		C4 H5 N4 C	Full match	No results	No results	No results	No results	-2,54	361,8677	384,8568	1,093	574634,5	0	0	0	No matche	No matche	DDA for pri	[M+Na]+1		574634,5		7,9	
FALSE		C2 H Cl N4	Full match	No results	No results	No results	No results	1,46	305,843	306,85	1,125	491208,1	0	0	0	No matche	No matche	No MS2	[M+H]+1	491208,1	452314,4	7,9	7,4	
FALSE		C11 H4 Cl F	Full match	No results	No results	No results	No results	-0,87	634,801	698,8177	1,105	296285,9	0	0	0	No matche	No matche	No MS2	[M+ACN+N		296285,9		7,1	
FALSE		C5 H14 Cl F	Full match	No results	No results	No match	No match	4,04	211,0845	212,0917	3,448	718535,9	27	0	0	No matche	Multiple m	DDA for pri	[M+H]+1	663678,7	718535,9	6,8	6,8	
FALSE			No results	No results	No results	No results	No results		451,8369	452,8442	1,096	576431,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	553441,8	576431,9	7,4	7,4	
FALSE			No results	No results	No results	No results	No results		72,39221	73,39948	1,463	2080298	0	0	0	No matche	No matche	No MS2	[M+H]+1	2080298	2002852	5,9	4,8	
FALSE	1-Bromo-4-chlorobutane	C4 H8 Br Cl	No results	No results	No results	Full match	No results	3,56	169,9504	170,9577	1,065	763212,8	2	0	0	No matche	No matche	No MS2	[M+H]+1	689732,2	763212,8	7,4	7,4	
FALSE			No results	No results	No results	No results	No results		730,7961	366,4053	0,984	1308120	0	0	0	No matche	No matche	No MS2	[M+2H]+2	1219189	1308120	7,2	3,9	
FALSE		C7 H21 N8	Full match	No results	No results	No match	No result	-1,17	248,1624	249,1697	6,81	732269,2	4	0	0	No matche	No matche	No MS2	[M+H]+1	673864,8	732269,2	6,8	6,8	
FALSE	phenylisilicon	C6 H5 Si	No results	No results	No results	Full match	No results	-1,62	105,0159	106,0232	0,98	814027,9	1	0	0	No matche	No matche	No MS2	[M+H]+1		814027,9		6,8	
FALSE			No results	No results	No results	No results	No results		407,6738	408,6804	1,174	719600,5	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	719600,5		7,9		
FALSE			No results	No results	No results	No results	No results		237,8553	238,8626	1,184	1048486	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1048486	1018636	6,1	3,4	
FALSE			No results	No results	No results	No results	No results		1323,69	662,8523	1,071	549344,1	0	0	0	No matche	No matche	No MS2	[M+2H]+2		549344,1		7,9	
FALSE			No results	No results	No results	No results	No results		1549,645	775,8295	1,086	661979,3	0	0	0	No matche	No matche	No MS2	[M+2H]+2	661979,3		7,4		
FALSE		C H4 Cl N4	Full match	No results	No results	No results	No results	-4,52	329,9237	330,931	0,974	1332584	0	0	0	No matche	No matche	No MS2	[M+H]+1	1263002	1332584	7,2	5	
FALSE			No results	No results	No results	No results	No results		215,8259	216,8331	1,15	1180706	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1180706	1049215	6,1	3,9	
FALSE			No results	No results	No results	No results	No results		90,99905	92,00632	0,3	339925,2	0	0	0	No matche	No matche	No MS2	[M+H]+1	145597,9	339925,2	8,2	6	
FALSE		C10 H2 Cl F	Full match	No results	No results	No results	No results	4,44	315,9792	316,9865	1,195	540172,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	540172,7	511624,3	7,4	7,9	
FALSE			No results	No results	No results	No results	No results		88,49693	89,50421	0,997	1043406	0	0	0	No matche	No matche	No MS2	[M+H]+1	901111,4	1043406	3,4	4,5	
FALSE		C26 H3 Br C	Full match	No results	No results	No results	No results	0,31	755,7319	756,7392	1,123	245945,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	245945,3	240148,8	8,2	8,2	
FALSE			No results	No results	No results	No results	No results		594,8608	595,868	1,112	248906,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	248906,9		8,2		
FALSE		C23 H7 O1	Full match	No results	No results	No results	No results	0,31	679,8619	680,8692	1,082	676742,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	676742,8	584762,4	7,4	6,8	
FALSE			No results	No results	No results	No results	No results		743,6165	744,6238	1,139	453229,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	453229,9	408916,4	7,4	7,4	
FALSE	Dimedone	C8 H12 O2	Full match	No results	No results	Full match	Full match	0,31	140,0838	141,0911	1,553	16817138	46	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	16817138		4		
FALSE			No results	No results	No results	No results	No results		733,5874	734,5947	1,143	399071,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	380004,7	399071,7	7,1	7,4	
FALSE			No results	No results	No results	No results	No results		579,8553	580,8626	1,105	295465,2	0	0	0	No matche	No matche	No MS2	[M+H]+1		295465,2		4,3	
FALSE		C51 H58 N	Full match	No results	No results	No results	No results	-1,46	715,4296	716,4369	7,849	1479419	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	1370906	1479419	7,2	7,2	
FALSE			No results	No results	No results	No results	No results		108,5143	109,5216	7,432	9933316	0	0	0	No matche	No matche	DDA for pri	[M+H]+1		9933316		5,1	
FALSE			No results	No results	No results	No results	No results		695,6861	696,6934	1,133	421374,9	0	0	0	No matche	No matche	No MS2	[M+H]+1		421374,9		7,9	
FALSE		C14 H29 N	Full match	No results	No results	No match	No results	-4,53	273,1763	274,1836	6,455	753521,8	1	0	0	No matche	No matche	DDA for pri	[M+H]+1	723684,9	753521,8	7,4	6,8	
FALSE	[Similar to: Ethylenediaminetetraacetic acid	C7 H10 N4	Full match	Invalid ma	No results	No results	No match	-0,6	292,0125	293,0197	1,457	388889,2	0	2	0	No matche	Multiple m	DDA for pri	[M+H]+1		388889,2		4,3	
FALSE		C3 H5 Br Cl	Full match	No results	No results	No results	No results	-1,86	667,687	668,6935	1,132	414206,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	409712,7	414206,9	7,4	7,4	
FALSE		C27 H3 N2	Full match	No results	No results	No results	No results	-0,41	751,783	752,7902	1,117	231022	0	0	0	No matche	No matche	No MS2	[M+H]+1		231022		8,2	
FALSE			No results	No results	No results	No results	No results		673,8074	674,8147	1,113	237600,6	0	0	0	No matche	No matche	No MS2	[M+H]+1	237600,6		8,2		
FALSE			No results	No results	No results	No results	No results		128,0073	170,0411	0,969	1376388	0	0	0	No matche	No matche	DDA for pri	[M+ACN+H		1094089		6,6	3,4
FALSE	NPYR	C4 H8 N2 C	Full match	No results	No results	Full match	No results	0,37	100,0637	101,071	1,213	1139498	13	0	0	No matche	No matche	DDA for pri	[M+H]+1	1139498	1132675	5,5	4,5	
FALSE	Ethylparaben	C9 H10 O3	Full match	No results	No results	Full match	Full match	-0,12	166,063	167,0703	5,221	918770,7	112	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1	918770,7		7,7		
FALSE		C8 H11 N4	Full match	No results	No results	No match	No results	1,98	288,0101	310,9993	1,206	730598,9	4	0	0	No matche	No matche	No MS2	[M+Na]+1	702526,2	730598,9	6,8	7,4	
FALSE		C26 H45 N	Full match	No results	No results	No match	No results	3,19	511,3274	512,3347	6,955	1313428	1	0	0	No matche	No matche	No MS2	[M+H]+1	1313428		6,1		
FALSE</																								



FALSE		C6 H10 N4	Full match	No results	No results	No results	No results	1.79	186,0756	94,04509	0.319	3419236	0	0	0	No match	No match	No MS2	[M+2H]+2	3419236	2231185	4,2	4,2	
FALSE		C76 H88 N10	Full match	No results	No results	No results	No results	0.28	1434,546	479,1892	6.659	813060,5	0	0	0	No match	No match	DDA for ort	[M+3H]+3	813060,5	7500249	6,3	4,7	
FALSE		C7 H6 N10	Full match	No results	No results	No match	No match	4.73	422,0009	212,0077	2.141	1655752	1	0	0	No match	Single mat	DDA for ort	[M+2H]+2	1655752	1228347	6,6	5	
FALSE		C4 H11 N11	Full match	No results	No results	No results	No results	-0.84	262,0802	263,0875	1.541	3035481	6	0	0	No match	No match	DDA for pri	[M+H]+1	3035481	1492780	4,2	2,8	
FALSE		C4 H9 N6 C	Full match	No results	No results	No match	No results	-1.38	204,0522	205,0595	1.243	897573,7	1	0	0	No match	No match	No MS2	[M+H]+1	897573,7	880153,4	8,3	5,5	
FALSE				No results	No results	No results	No results		723,7765	724,7838	1.116	251949,7	0	0	0	No match	No match	No MS2	[M+H]+1		251949,7		8,2	
FALSE				No results	No results	No results	No results		605,82	606,8273	1.114	215430,7	0	0	0	No match	No match	No MS2	[M+H]+1			8,2		
FALSE	6-Methoxyelemicin	C13 H18 O	Full match	No results	No results	Full match	Partial mat	0.23	238,1206	239,1278	7.049	17549876	15	0	0	No match	Multiple m	DDA for pri	[M+H]+1	16810881	17549876	3,5	4	
FALSE	Guanidininosuccinic acid	C19 H33 C	Full match	Invalid ma	No results	Full match	Full match	0.21	175,0593	176,0666	1.347	702165	1	1	0	Single mat	No match	DDA for pri	[M+H]+1	702165	559109	7,4	7,9	
FALSE		C4 H9 N O6	Full match	No results	No results	No results	No results	1.89	167,0433	168,0506	0.981	995029,6	0	0	0	No match	No match	No MS2	[M+H]+1	615904,3	995029,6	5,2	3,4	
FALSE		C4 H7 N O5	Full match	No results	No results	No match	No results	0.5	242,9521	243,9594	0.981	1036890	1	0	0	No match	No match	No MS2	[M+H]+1	992042,1	1036890	5	7,7	
FALSE	[9E,11E]-13-Hydroperoxy-9,11-octadecadien	C18 H32 O	Full match	No results	No results	Full match	Full match	0.15	312,2301	313,2374	7.504	1782769	25	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	1456489	1782769	6,1	5,5	
FALSE				No results	No results	No results	No results		85,9968	87,00407	0.339	320300,7	0	0	0	No match	No match	No MS2	[M+H]+1		320300,7		8,2	
FALSE	5-Methyl-3-isoxazolamine	C4 H6 N2 C	Full match	No results	No results	Full match	Partial mat	0.71	98,04808	99,05536	1.63	19805963	10	0	0	No match	Single mat	DDA for pri	[M+H]+1	19805963		4,6		
FALSE	N-(2,6-dioxopiperidin-3-yl)acetamide	C7 H10 N2	Full match	No results	No results	Full match	Partial mat	0.72	170,0693	171,0765	1.477	841659,4	6	0	0	No match	Single mat	DDA for pri	[M+H]+1	261548,4	841659,4	7,1	2,3	
FALSE				No results	No results	No results	No results		96,96151	97,96879	0.342	542927,2	0	0	0	No match	No match	No MS2	[M+H]+1		542927,2		6,8	
FALSE		C7 H4 N4 C	Full match	No results	No results	No match	No results	3.17	224,0189	113,0167	0.341	460781,7	1	0	0	No match	No match	DDA for ort	[M+2H]+2		460781,7		7,9	
FALSE		C19 H43 N	Full match	No results	No results	No results	No results	-4.12	505,2648	253,6397	3.729	601403,2	0	0	0	No match	No match	DDA for ort	[M+2H]+2	601403,2	588088,9	6,8	6,8	
FALSE	[Similar to: Ethylenediaminetetraacetic acid]	C6 H5 N4 C	Full match	Invalid ma	No results	No results	No results	1.03	291,9848	292,9921	1.425	251948,1	0	2	0	No match	No match	DDA for pri	[M+H]+1	251948,1	206747	2,7	4,9	
FALSE		C4 H8 P2	Full match	No results	No results	No results	No results	3.06	118,0105	119,0178	1.958	410292,8	0	0	0	No match	No match	No MS2	[M+H]+1	410292,8		6,8		
FALSE				No results	No results	No results	No results		541,8136	542,8208	1.052	362537,4	0	0	0	No match	No match	No MS2	[M+H]+1	346002,9	362537,4	7,6	7,6	
FALSE	Ethanoic anhydride	C4 H6 O3	Full match	No results	No results	Full match	Full match	0.03	102,0317	103,039	2.827	13478889	18	0	0	Multiple m	No match	DDA for pri	[M+H]+1	13478889	12433883	5,1	4,6	
FALSE		C2 H4 Br Cl	Full match	No results	No results	No results	No results	3.82	511,6554	590,6772	1.144	439476,8	0	0	0	No match	No match	No MS2	[M+DMSO-	439476,8	434065,8	7,4	7,4	
FALSE	[Similar to: [2R,3S,4S,5R,6S]-2-(hydroxymeth	C H2 N4 O	Full match	Invalid ma	No results	No results	No results	-4.13	147,9698	148,9771	0.307	728248,9	0	10	0	No match	No match	DDA for pri	[M+H]+1	579911,6	728248,9	5,2	4,7	
FALSE	[Similar to: 3-hydroxy-1-[3-(trifluoromethyl)	C7 H6 N6 C	Full match	Invalid ma	No results	No match	No results	1.34	190,0606	223,0941	1.124	1492785	2	3	0	No match	No match	DDA for pri	[M+H+MeC	1492785		4,5		
FALSE	Dehydroglycine	C2 H3 N O2	Full match	No results	No results	Full match	Full match	0.94	73,01645	74,02372	1.927	517455,3	1	0	0	Single mat	No match	DDA for pri	[M+H]+1	517455,3	468438,2	6,3	7,4	
FALSE				No results	No results	No results	No results		333,7404	334,7476	1.173	703199,8	0	0	0	No match	No match	No MS2	[M+H]+1	703199,8	597014,1	4,1	7,9	
FALSE		C5 H Br Cl3	Full match	No results	No results	No results	No results	1.77	369,7267	370,7331	1.144	334140,8	0	0	0	No match	No match	No MS2	[M+H]+1	334140,8	206560	5,4	7,1	
FALSE				No results	No results	No results	No results		331,8454	332,8527	1.112	282090,6	0	0	0	No match	No match	No MS2	[M+H]+1	282090,6	159253,7	7,6	7,6	
FALSE				No results	No results	No results	No results		644,6753	645,6826	1.139	455023,3	0	0	0	No match	No match	No MS2	[M+H]+1		455023,5		7,4	
FALSE	TEMPO	C9 H19 N C	Full match	No results	No results	Full match	No results	0.03	157,1467	158,154	7.507	1497127	11	0	0	No match	No match	No MS2	[M+H]+1		1497127		5,5	
FALSE	Laurixamine	C15 H33 N	Full match	No results	No results	Full match	No results	-0.2	243,2562	244,2634	6.874	1581055	3	0	0	No match	No match	DDA for pri	[M+H]+1	1306589	1581055	7,2	5	
FALSE	(R)-3-hydroxybutyrylcarnitine	C11 H21 N	Full match	No results	No results	Full match	No results	0.05	247,142	248,1493	3.213	535790,6	3	0	0	No match	No match	No MS2	[M+H]+1	524413	535790,6	6,3	6,8	
FALSE		C3 H4 Cl3	Full match	No results	No results	No results	No results	-0.58	713,7472	714,7544	1.121	234411,8	0	0	0	No match	No match	No MS2	[M+H]+1	163834,3	234411,8	7,6	8,2	
FALSE		C12 H28 N	Full match	No results	No results	No results	No results	-0.47	377,2051	378,2124	7.214	7346040	0	0	0	No match	No match	No MS2	[M+H]+1	7346040		4,6		
FALSE		C6 H4 Cl4 F	Full match	No results	No results	No match	No results	-3.7	437,713	438,7203	1.146	301314,4	1	0	0	No match	No match	No MS2	[M+H]+1	301314,4	275578,6	7,6	7,1	
FALSE	N-Acetyl-S-(3-hydroxypropyl)-L-cysteine	C8 H15 N C	Full match	No results	No results	Full match	No results	-0.05	221,0722	222,0794	3.347	537177	6	0	0	No match	No match	DDA for pri	[M+H]+1	537177	532166,9	7,4	7,9	
FALSE		C8 H5 O5 F	Full match	No results	No results	No results	No results	-0.83	273,9348	274,942	1.074	712443,4	0	0	0	No match	No match	DDA for pri	[M+H]+1	712443,4	669531,8	7,4	4,7	
FALSE		C6 H11 N C	Full match	No results	No results	No results	No results	-2.28	223,0158	112,5152	0.97	1262966	0	0	0	No match	No match	No MS2	[M+2H]+2	565524,6	1262966	6,8	7,2	
FALSE	β-Alanyl-L-histidyl-L-seryl-L-histidine	C18 H26 N	Full match	No results	No results	Full match	No results	-3.33	450,196	226,1053	1.881	654640,9	2	0	0	No match	No match	DDA for ort	[M+2H]+2	580724,2	654640,9	7,4	7,4	
FALSE		C43 H61 N	Full match	No results	No results	No results	No match	-1.68	759,4558	760,4631	7.841	1329019	0	0	0	No match	Single mat	DDA for pri	[M+H]+1	1161028	1329019	7,2	7,2	
FALSE	3-Oxo-3-(5,7,9,19,23,25,27,31,33,34,35-and	C59 H103 F	No results	No results	No results	Full match	Full match	-3.79	1141,719	571,8669	1.088	475385,4	2	0	0	No match	Multiple m	No MS2	[M+2H]+2		475385,4		7,4	
FALSE	Nonivamide	C17 H27 N	Full match	No results	No results	Full match	Full match	0.12	293,1991	294,2064	6.184	1662590	11	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1	1662590	1612175	6,6	7,2	
FALSE		C19 H41 N	Full match	No results	No results	No match	No match	-1.54	431,3036	432,3109	6.932	956204	1	0	0	No match	Multiple m	No MS2	[M+H]+1	764899	956204	7,4	6,1	
FALSE				No results	No results	No results	No results		637,5104	638,5177	1.174	404954,5	0	0	0	No match	No match	No MS2	[M+H]+1		404954,5		7,9	
FALSE	phenylsilicon	C6 H5 Si	No results	No results	No results	Full match	No results	-1.21	105,0159	106,0232	0.943	360761,1	1	0	0	No match	No match	No MS2	[M+H]+1		360761,1		7,1	
FALSE				No results	No results	No results	No results		700,6354	701,6426	1.138	373567,2	0	0	0	No match	No match	No MS2	[M+H]+1		373567,2		7,6	
FALSE		C H3 N2 O2	Full match	No results	No results	No results	No results	-3.71	153,9596	195,9935	0.342	855038,5	0	0	0	No match	No match	DDA for pri	[M+ACN+H		855038,5		5,5	
FALSE	cyclohexenone	C6 H8 O	Full match	Invalid ma	No results	Full match	Full match	0.33	96,05755	97,06482	1.438	2309491	18	10	0	Single mat	Multiple m	DDA for pri	[M+H]+1	398241	2309491	6,8	1	
FALSE	mephenesin	C10 H14 O	No results	No results	No results	Full match	Full match	0.29	182,0944	183,1016	1.019	793364,6	45	0	0	Multiple m	Multiple m	No MS2	[M+H]+1		793364,6		4,1	
FALSE	[Similar to: Ethylenediaminetetraacetic acid]	C7 H7 N2 C	Full match	Invalid ma	No results	No results	No results	2,8	291,9576	292,9649	1,49	227500,6	0	2	0	No match	No match	DDA for pri	[M+H]+1	227500,6		4,9		
FALSE				No results	No results	No results	No results		711,6687	712,6757	1,135	335290,5	0	0	0	No match	No match	No MS2	[M+H]+1			335290,5		7,6
FALSE	3,6,9-trimethyloctahydro-3,12-epoxy[1,2]dic	C15 H22 O	Full match	No results	No results	Full match	Partial mat	0.21	282,1468	283,1541	7.022	13191152	22	0	0	No match	No match	No MS2	[M+H]+1			1327728		6,6
FALSE		C3 H6 N8	Full match	No results	No results	No results	No results	1,9	154,0718	177,0611	1,092	963823,2	0	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1			13191152		4
FALSE		C27 H19 O	Full match	No results	No results	No results	No results	-0.47	614,0281	308,0213	2,147	1036012	0	0	0	No match	No match	DDA for ort	[M+2H]+2	1036012	943070,2	6,6	7,7	
FALSE		C22 H46 N	Full match	No results	No results	No results	No results	-2.45	651,2712	326,6429	1,961	495114,3	0	0	0	No match	Single mat	No MS2	[M+2H]+2	428097,5	495114,3	7,9	7,9	
FALSE		C15 H32 N	Full match	No results	No results	No match	No match	-3.37	476,195	239,1048	1,938	464381,4	5	0	0	No match	Single mat	No MS2	[M+2H]+2		464381,4		7,9	
FALSE	Dihydrothymine	C5 H8 N2 C	Full match	No results	No results	Full match	Full match	0.13	128,0586	129,0659	3.395	1109167	19	0	0	Single mat	No match	No MS2	[M+H]+1	1109167	1023687	7,2	6,6	
FALSE				No results	No results	No results	No results		721,6954	722,7026	1,131	288038,8	0	0	0	No match	No match	No MS2	[M+H]+1		288038,8		8,2	
FALSE				No results	No results	No results	No results		361,6952	440,7174	1,144	391160	0	0	0	No match	No match	No MS2	[M+DMSO-		391160		7,1	
FALSE		C7 H13 N8	Full match	No results	No results	No match	No match	-0.72	288,0846	289,0919	1,246	736408,3	2	0	0	No match	Single mat	No MS2	[M+H]+1	736408,3	686326,9	7,4	7,9	
FALSE	D-PANTOTHENIC ACID	C9 H17 N C	Full match	No results	No results	Full match	Full match	-0.13	219,1106	22														

FALSE			No results	No results	No results	No results	No results	619,5395	620,5468	1,176	384489,8	0	0	0			No match	No match	No MS2	[M+H]+1	367563,5	384489,8	7,1	7,6		
FALSE			No results	No results	No results	No results	No results	573,6069	574,6141	1,163	480375,2	0	0	0			No match	No match	No MS2	[M+H]+1	480375,2		6,3			
FALSE			C2 H6 O7 F	Full match	No results	No results	No match	No results	2,01	235,9314	236,9387	0,344	2647152	1	0	0		No match	No match	No MS2	[M+H]+1	1855600	2647152	4,5	2,1	
FALSE			3-(2H-Tetrazol-5-ylhydrazono)-2,4-pentanedione	C6 H8 N6 C	Full match	No results	No results	Full match	No results	1,71	196,0712	197,0785	1,107	1171034	1	0	0		No match	No match	DDA for pri	[M+H]+1	1171034	1061801	2,3	4,5
FALSE				C13 H34 N	Full match	No results	No results	No results	No match	3,25	339,241	340,2483	6,726	1021967	0	0	0		No match	Single mat	DDA for pri	[M+H]+1	943125,1	1021967	7,2	4,5
FALSE				C9 H N6 O	Full match	No results	No results	No results	No results	-0,09	525,8357	526,843	1,051	307968,6	0	0	0		No match	No match	No MS2	[M+H]+1	307968,6	305707,4	7,6	7,6
FALSE					No results	No results	No results	No results	No results		719,6987	720,706	1,131	330709,1	0	0	0		No match	No match	No MS2	[M+H]+1	330709,1	174401,6	7,6	8,2
FALSE				C5 H10 O1	Full match	No results	No results	No match	No results	1,18	230,0277	231,0349	0,978	1184679	1	0	0		No match	No match	No MS2	[M+H]+1	947231,5	1184679	7,2	3,9
FALSE				C7 H11 N5	Full match	No results	No results	No match	No results	-2,9	261,0524	131,5335	7,574	7269798	1	0	0		No match	No match	DDA for ori	[M+2H]+2	6282045	7269798	4,6	4,6
FALSE			Furfural	C5 H4 O2	Full match	No results	No results	Full match	Full match	0,48	96,02118	97,02845	1,661	15539219	6	0	0		Single mat	No match	No MS2	[M+H]+1	15539219	8033165	4	1,3
FALSE			6-(1H-Pyrrrol-1-yl)norleucine	C10 H16 N	Full match	No results	No results	Full match	Partial mat	0,2	196,1212	197,1285	4,614	745095,9	9	0	0		No match	Multiple m	DDA for pri	[M+H]+1	721658,2	745095,9	6,8	6,8
FALSE				C10 H19 O	Full match	No results	No results	No match	No results	4,17	234,0853	235,0926	0,346	568333,1	5	0	0		No match	No match	No MS2	[M+H]+1		568333,1		6,8
FALSE			5-Oxidaniidyl-5-oxidanilydenenorvalylthreonine	C9 H15 N2	No results	No results	No results	Full match	No results	0,65	247,0932	248,1005	1,45	146630,5	2	0	0		No match	No match	No MS2	[M+H]+1		146630,5		8,2
FALSE					No results	No results	No results	No results	No results		313,7645	314,7717	1,146	315268,7	0	0	0		No match	No match	DDA for pri	[M+H]+1	315268,7		7,6	
FALSE					No results	No results	No results	No results	No results		599,8441	600,8514	1,072	467056	0	0	0		No match	No match	No MS2	[M+H]+1		467056		4,1
FALSE				C5 H10 Br3	Full match	No results	No results	No results	No results	-0,17	641,6817	642,689	1,138	434657,5	0	0	0		No match	No match	No MS2	[M+H]+1		434657,5		7,4
FALSE					No results	No results	No results	No results	No results		731,7256	732,7329	1,125	311288,4	0	0	0		No match	No match	No MS2	[M+H]+1		311288,4		7,6
FALSE					No results	No results	No results	No results	No results		639,5077	640,515	1,176	389134,3	0	0	0		No match	No match	No MS2	[M+H]+1				
FALSE					No results	No results	No results	No results	No results		1587,609	794,8117	1,097	419943,2	0	0	0		No match	No match	No MS2	[M+H]+1	389134,3		7,6	
FALSE				C4 H4 Br N2	Full match	No results	No results	No results	No results	3,55	279,84	280,8472	1,134	393317,4	0	0	0		No match	No match	No MS2	[M+2H]+2	414710,9	419943,2	7,9	7,4
FALSE			p-Nitrophenol butyrate	C10 H11 N	Full match	No results	No results	Full match	Full match	0,53	209,0689	210,0762	1,965	460312,1	31	0	0		No match	No match	DDA for pri	[M+H]+1	393317,4	310532,9	2,2	6,5
FALSE			[Similar to: Ethylenediaminetetraacetic acid]tranexamic acid	C5 H9 O12	Invalid mat	No results	No results	No results	No results	-5,06	291,9817	292,989	1,424	162447,3	0	2	0	74,4	Multiple m	Multiple m	No MS2	[M+H]+1	460312,1	437533,1	7,4	6,3
FALSE				C8 H15 N C	Full match	No results	No results	Full match	Partial mat	0,4	157,1103	158,1176	1,963	711700,9	42	0	0		No match	No match	DDA for pri	[M+H]+1	147091	162447,3	8,7	2,2
FALSE			Benzaldehyde	C7 H6 O	Full match	No results	No results	Full match	Full match	0,43	106,0419	107,0492	1,497	13699610	3	0	0		No match	Single mat	DDA for pri	[M+H]+1	711700,9	569635,5	4,7	6,8
FALSE				C2 H4 N6 C	Full match	No results	No results	No results	No results	-4,53	221,981	222,9883	1,202	656505,1	0	0	0		Multiple m	No match	DDA for pri	[M+H]+1		13699610		4
FALSE					No results	No results	No results	No results	No results		535,8287	536,836	1,103	154509,1	0	0	0		No match	No match	DDA for pri	[M+H]+1	656505,1		5,2	
FALSE					No results	No results	No results	No results	No results										No match	No match	No MS2	[M+H]+1		154509,1		5,4
FALSE				C5 H8 Cl2 F	Full match	No results	No results	No results	No results	-1,85	357,856	358,8633	1,121	378761,1	0	0	0		No match	No match	DDA for pri	[M+H]+1	378761,1		7,6	
FALSE			3,4-DIMETHOXYBENZENEPROPANOL	C11 H16 O	No results	No results	No results	Full match	Partial mat	0,14	196,11	197,1173	1,447	9834589	31	0	0		No match	Multiple m	DDA for pri	[M+H]+1		9834589		4
FALSE					No results	No results	No results	No results	No results		548,8339	549,8412	1,105	334994,2	0	0	0		No match	No match	No MS2	[M+H]+1	334994,2	317755,6	4,3	6,5
FALSE			Icaridin	C12 H23 N	Full match	No results	No results	Full match	No results	-0,23	229,1677	230,175	6,893	4660721	11	0	0		No match	No match	DDA for pri	[M+H]+1	4660721		4,8	
FALSE					No results	No results	No results	No results	No results		626,8127	627,82	1,114	305249,2	0	0	0		No match	No match	No MS2	[M+H]+1		305249,2		7,1
FALSE				C40 H52 O	Full match	No results	No results	No match	No results	-3,48	676,3588	677,3661	7,863	1238276	1	0	0		No match	No match	DDA for pri	[M+H]+1	1180570	1238276	5,5	6,6
FALSE					No results	No results	No results	No results	No results		629,6967	630,704	1,137	337504,5	0	0	0		No match	No match	No MS2	[M+H]+1	337504,5	331601,3	7,6	7,1
FALSE					No results	No results	No results	No results	No results		1447,634	724,8241	1,091	537752,9	0	0	0		No match	No match	No MS2	[M+2H]+2	118287,7	537752,9	8,2	0,9
FALSE					No results	No results	No results	No results	No results		707,8132	708,8205	1,095	303258,2	0	0	0		No match	No match	No MS2	[M+H]+1	303258,2	231233,3	8,2	7,1
FALSE					No results	No results	No results	No results	No results		644,7198	645,7271	1,126	203858,8	0	0	0		No match	No match	No MS2	[M+H]+1	203858,8		4,9	
FALSE			4-Aminobenzoic acid	C7 H7 N O2	Full match	No results	No results	Full match	Full match	0,15	137,0477	138,055	1,499	1784284	40	0	0		Multiple m	Multiple m	No MS2	[M+H]+1	467015,3	1784284	7,4	2,8
FALSE			L-Proglutamic acid	C5 H7 N O2	Full match	No results	No results	Full match	Full match	0,56	129,0427	130,0499	1,39	457613,5	17	0	0		Multiple m	No match	No MS2	[M+H]+1	457613,5		5,8	
FALSE					No results	No results	No results	No results	No results		838,5036	420,2591	7,319	6574690	0	0	0		No match	No match	No MS2	[M+2H]+2	5995670	6574690	5,1	3,5
FALSE					No results	No results	No results	No results	No results		1475,639	738,8269	1,076	406171,7	0	0	0		No match	No match	No MS2	[M+2H]+2	406171,7	397294,2	7,9	7,4
FALSE				C8 H25 N7	Full match	No results	No results	No match	No results	-1,97	335,1683	348,2017	7,025	11023745	3	0	0		No match	No match	DDA for pri	[M+H+MeC]		11023745		4
FALSE				C2 H Br3 Cl	Full match	No results	No results	No results	No results	-2,62	635,5135	636,5207	1,177	394222,7	0	0	0		No match	No match	No MS2	[M+H]+1	394222,7	243878,1	7,1	7,1
FALSE				C30 H74 N	Full match	No results	No results	No results	No results	1,43	812,4848	407,2497	7,117	6163837	0	0	0		No match	No match	No MS2	[M+2H]+2		6163837		4,6
FALSE				C30 H40 N	Full match	No results	No results	No results	No results	-2,91	590,2783	296,1464	7,058	2089599	0	0	0		No match	No match	No MS2	[M+2H]+2	1544026	2089599	3,9	4,2
FALSE				C35 H78 N	Full match	No results	No results	No match	No results	-0,43	755,5469	756,5541	7,131	5827302	36	0	0		No match	No match	No MS2	[M+H]+1		5827302		4
FALSE					No results	No results	No results	No results	No results		459,6871	460,6938	1,152	550076,3	0	0	0		No match	No match	No MS2	[M+H]+1	550076,3	524619,2	6,8	4,1
FALSE				C39 H73 N	Full match	No results	No results	No results	No match	2,3	831,4981	416,7563	7,423	959460,4	0	0	0		No match	Single mat	No MS2	[M+2H]+2	937520,2	959460,4	6,1	5
FALSE				C2 H2 N4 C	Full match	No results	No results	No match	No results	-3,7	175,9647	176,9719	0,31	1640919	1	0	0		No match	No match	No MS2	[M+H]+1		1640919		4,5
FALSE			TRIALLYL PENTAERYTHRITOL	C14 H24 O	Full match	No results	No results	Full match	Partial mat	-0,12	256,1674	257,1747	7,193	5256330	14	0	0		No match	Multiple m	DDA for ori	[M+H]+1	5256330	4932893	4,8	3,7
FALSE				C6 H9 N2 C	Full match	No results	No results	No results	No results	4,73	236,0209	119,0178	1,968	367901,1	0	0	0		No match	No match	No MS2	[M+2H]+2		367901,1		6,5
FALSE			Xanthine	C5 H4 N4 C	Full match	No results	No results	Full match	Full match	0,15	152,0335	153,0407	3,242	416601,8	4	0	0		Single mat	No match	No MS2	[M+H]+1	416601,8	400937,2	6,8	8,5
FALSE				C63 H114 F	Full match	No results	No results	No results	No results	-0,12	1509,603	755,809	1,108	414756,9	0	0	0		No match	No match	No MS2	[M+2H]+2	414756,9		5,2	
FALSE					No results	No results	No results	No results	No results		585,6335	586,6403	1,149	381580,2	0	0	0		No match	No match	No MS2	[M+H]+1		381580,2		7,1
FALSE			Dimethylcadmium	C2 H6 Cd	No results	Invalid mat	No results	Full match	No results	-4,91	143,9496	144,9569	0,339	528683,6	1	1	0	42,2	No match	No match	DDA for pri	[M+H]+1		528683,6		6,3
FALSE					No results	No results	No results	No results	No results		639,8255	640,8328	1,094	343486	0	0	0		No match	No match	No MS2	[M+H]+1	295570,7	343486	7,6	7,6
FALSE				C21 H40 N	Full match	No results	No results	No match	No match	-0,32	449,3143	450,3216	7,253	743859,1	6	0	0		Multiple m	No match	No MS2	[M+H]+1	743859,1	731638,9	5,2	7,9
FALSE					No results	No results	No results	No results	No results		111,5123	112,5196	7,59	5397150	0	0	0		No match	No match	DDA for pri	[M+H]+1	5032025	5397150	4,2	3,7
FALSE			e-(γ-Glutamyl)-lysine	C11 H21 N	No results	No results	No results	Full match	No results	-0,84	275,1479	276,1552	1,39	488108,5	6	0	0		No match	No match	No MS2	[M+H]+1	377820,4	488108,5	7,1	4,1
FALSE			DL-Glutamic acid	C5 H9 N O4	Full match	No results	No results	Full match	Full match	0,04	147,0532	148,0604	1,876	621831,1	31	0	0									

FALSE	Geranyl acetate	C12 H20 O	Full match	No results	No results	Full match	Full match	0,07	196,1463	197,1536	7,344	11114812	81	0	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1	11114812	2691070	4,6	4,8
FALSE		C15 H14 N	Full match	No results	No results	No match	No match	-4,2	100,1165	311,1238	3,723	498423,3	6	0	0	0	No match	Multiple m	No MS2	[M+H]+1	452272,5	498423,3	7,9	7,9
FALSE			No results	No results	No results	No results	No results		421,6499	422,6571	1,171	476709,6	0	0	0	0	No match	No match	No MS2	[M+H]+1		476709,6		8,5
FALSE		C16 H37 N	Full match	No results	No results	No results	No results	-1,68	417,1861	418,1933	1,721	543141	2	0	0	0	No match	No match	No MS2	[M+H]+1	543141	516883,8	5,8	7,9
FALSE		C9 H25 N4	Full match	No results	No results	No match	No match	3,98	268,1675	269,1748	7,126	9800303	10	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	8380030	9800303	4	4,6
FALSE	3,6,9-trimethyloctahydro-3,12-epoxy[1,2]dic	C15 H22 O	Full match	No results	No results	Full match	Full match	0,19	282,1468	283,1541	7,133	13886734	22	0	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1	13886734		4	
FALSE			No results	No results	No results	No results	No results		640,102	641,1093	1,41	408013,5	0	0	0	0	No match	No match	No MS2	[M+H]+1		408013,5		6,3
FALSE		C6 H3 N5 C	Full match	No results	No results	No results	No results	-0,77	222,9811	223,9884	7,058	13049112	0	0	0	0	No match	No match	No MS2	[M+H]+1		13049112		5,1
FALSE		C30 H50 N	Full match	No results	No results	No match	No results	1,92	517,3166	518,3239	7,005	2113853	5	0	0	0	No match	No match	No MS2	[M+H]+1	2113853	182034,3	4,8	4,9
FALSE			No results	No results	No results	No results	No results		545,6073	546,6145	1,176	333813	0	0	0	0	No match	No match	No MS2	[M+H]+1	333813	323431,1	7,1	8,2
FALSE	2-Pyrrolidone	C4 H7 N O	Full match	Invalid ma	No results	Full match	Full match	-1	85,05268	86,05996	1,487	11001817	12	10	0	0	Single mat	No match	DDA for pri	[M+H]+1	11001817	10180349	4	3,5
FALSE			No results	No results	No results	No results	No results		361,8586	362,8659	1,083	268549,9	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	268549,9	254023,9	7,1	7,6
FALSE		C2 H7 N2 P	Full match	No results	No results	No results	No results	-1,47	122,0066	123,0139	1,001	1336435	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	1233501	1336435	7,2	2,3
FALSE			No results	No results	No results	No results	No results		80,51334	81,52061	1,248	221673,9	0	0	0	0	No match	No match	No MS2	[M+H]+1	221673,9		5,4	
FALSE		C5 H7 P3 S	Full match	No results	No results	No match	No results	-0,45	223,9201	224,9274	1,07	501779,4	3	0	0	0	No match	No match	DDA for pri	[M+H]+1	468929,7	501779,4	7,9	6,8
FALSE	γ-Acetylenic gaba	C6 H9 N O2	Full match	No results	No results	Full match	Full match	0,41	127,0634	128,0707	1,682	11313699	25	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	4668941	11313699	1	4
FALSE		C2 H7 N2 C	Full match	No results	No results	No match	No results	0,62	170,0094	171,0166	1,172	408150,5	3	0	0	0	No match	No match	DDA for pri	[M+H]+1	408150,5	403691,4	7,9	4,7
FALSE		C2 H4 N3 P	Full match	No results	No results	No results	No results	3,72	101,0147	102,0219	0,984	79959,2	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	759959,2	675862,6	4,1	0,3
FALSE			No results	No results	No results	No results	No results		1384,65	693,3321	1,098	243169,9	0	0	0	0	No match	No match	No MS2	[M+2H]+2	243169,9		8,2	
FALSE		C6 H5 N7 C	Full match	No results	No results	No match	No results	1,07	239,0406	120,5276	0,974	924494,1	2	0	0	0	No match	No match	No MS2	[M+2H]+2	924494,1	836509,8	7,2	3
FALSE	5-(N,N-Dimethylcarbamimidamido)-2-oxope	C8 H15 N3	Full match	No results	No results	Full match	No results	-0,13	201,1113	202,1186	3,222	498616,3	1	0	0	0	No match	No match	No MS2	[M+H]+1	462349,3	498616,3	6,3	6,8
FALSE			No results	No results	No results	No results	No results		1535,597	768,8055	1,1	340923,3	0	0	0	0	No match	No match	No MS2	[M+2H]+2	340923,3		7,6	
FALSE			No results	No results	No results	No results	No results		765,7979	766,8052	1,103	405506,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	405506,1	225916	4,1	2,7
FALSE		C32 H72 N	Full match	No results	No results	No match	No results	0,31	674,5368	675,5441	7,074	6165270	1	0	0	0	No match	No match	No MS2	[M+H]+1		6165270		5,1
FALSE		C1 H8 Cl N	Full match	No results	No results	No results	No results	1,67	311,7671	312,7744	1,145	300885,4	0	0	0	0	No match	No match	No MS2	[M+H]+1	300885,4	270651,9	7,6	7,1
FALSE	6-Amyl-α-pyrone	C10 H14 O	No results	Invalid ma	No results	Full match	Partial mat	0,25	166,0994	149,0961	1,535	25671645	110	3	0	0	Multiple m	Multiple m	DDA for pri	[M+H+H20	25671645	22699636	4	3,5
FALSE	Myristamine oxide	C16 H35 N	Full match	No results	No results	Full match	No results	-0,05	257,2719	258,2791	7,152	893129,2	2	0	0	0	No match	No match	No MS2	[M+H]+1	848929,2	893129,2	6,1	4,5
FALSE			No results	No results	No results	No results	No results		745,7786	746,7859	1,106	181658,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		181658,3		4,3
FALSE			No results	No results	No results	No results	No results		462,0192	463,0265	1,098	461447,5	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	445912,9	461447,5	7,9	7,9
FALSE			No results	No results	No results	No results	No results		160,5901	322,1874	3,241	368662,5	0	0	0	0	No match	No match	No MS2	[2M+H]+1		368662,5		7,6
FALSE	Diethyl phosphonothioate	C4 H11 O2	Full match	No results	No results	Full match	No results	-4,63	154,021	155,0283	1,956	271167	1	0	0	0	No match	No match	No MS2	[M+H]+1	224481,7	271167	5,4	7,6
FALSE		C H2 N4 O	Full match	No results	No results	No results	No results	2,48	291,9076	292,9149	1,069	567360,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	567360,2	511353,7	7,4	7,4
FALSE	2,5-Furandicarboxylic acid	C6 H4 O5	Full match	No results	No results	Full match	No results	0,23	156,0059	157,0132	2,382	1774709	3	0	0	0	No match	No match	No MS2	[M+H]+1	1610559	1774709	4,5	5,5
FALSE	1-Cyclohexenecarboxylic Acid	C7 H10 O2	Full match	No results	No results	Full match	Partial mat	0,06	126,0681	127,0754	1,452	14004840	43	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	403046,4	14004840	6,8	4
FALSE	C6 H16 N5	Full match	No results	No results	No results	No match	No results	-2,57	269,0882	270,0955	1,403	349024,4	2	0	0	0	No match	No match	No MS2	[M+H]+1		349024,4		4,3
FALSE	Dicyclohexylamine	C12 H23 N	Full match	No results	No results	Full match	Full match	0,02	181,1831	182,1903	5,255	754483,5	7	0	0	0	Single mat	Single mat	DDA for pri	[M+H]+1	751748,4	754483,5	6,8	6,8
FALSE			No results	No results	No results	No results	No results		600,806	601,8132	1,112	161473,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	114425,8	161473,2	3,8	8,2
FALSE	Cyclohexanecarboxylic anhydride	C14 H22 O	Full match	No results	No results	Full match	Partial mat	-0,01	238,1569	239,1642	7,126	10007422	8	0	0	0	No match	Multiple m	No MS2	[M+H]+1	10007422		4	
FALSE	Heptylparaben	C14 H20 O	Full match	No results	No results	Full match	Partial mat	0,03	236,1413	237,1485	7,137	10571033	13	0	0	0	No match	Multiple m	No MS2	[M+H]+1		10571033		4,6
FALSE			No results	No results	No results	No results	No results		311,0622	312,0691	1,39	452075,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	435299,8	452075,5	6,8	7,4
FALSE		C3 H5 Cl N	Full match	No results	No results	No results	No results	-2,56	272,9659	273,9732	1,158	343420,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	343420,7	323177,8	8,2	7,6
FALSE		C H3 Br Cl3	Full match	No results	No results	No results	No results	-1,54	775,571	776,5783	1,145	251106,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	251106,8	185376,3	7,6	7,6
FALSE			No results	No results	No results	No results	No results		111,9595	112,9668	0,304	316866	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		316866		7,6
FALSE	Neutral Red	C15 H16 N	Full match	No results	No results	Full match	No match	-4,68	252,1363	253,1436	7,149	12764375	18	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	12764375	12456609	4,6	4
FALSE	Furaneol	C6 H8 O3	Full match	No results	No results	Full match	Full match	0,4	128,0474	129,0547	1,381	642465,9	31	0	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1	642465,9		5,8	
FALSE	tert-Butyl [6-(2-aminoethyl)-2,2-dimethyl-1,3	C14 H27 N	Full match	No results	No results	Full match	No results	-0,22	273,194	274,2012	7,181	1508614	2	0	0	0	No match	No match	No MS2	[M+H]+1		1508614		4,5
FALSE		C33 H48 N	Full match	No results	No results	No results	No results	2,69	632,3326	633,3399	7,867	1017635	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	976536,4	1017635	6,1	6,6
FALSE			No results	No results	No results	No results	No results		114,9569	115,9641	0,3	114310,2	0	0	0	0	No match	No match	DDA for otl	[M+H]+1		114310,2		4,9
FALSE		C36 H78 N	Full match	No results	No results	No match	No results	0,1	728,5836	729,5909	7,126	5874577	4	0	0	0	No match	No match	No MS2	[M+H]+1	4868988	5874577	3,2	4
FALSE		C32 H59 O	Full match	No results	No results	No match	No match	0,98	616,3226	617,3299	7,464	1247787	1	0	0	0	No match	Multiple m	No MS2	[M+H]+1	871905,3	1247787	3,9	6,1
FALSE			No results	No results	No results	No results	No results		622,1285	623,1357	1,512	337801,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	337801,1		6	
FALSE		C11 H10 N	Full match	No results	No results	No match	No match	4,02	235,0408	118,5277	7,581	2114135	2	0	0	0	No match	Multiple m	DDA for otl	[M+2H]+2	2114135	1837831	4,8	3,9
FALSE			No results	No results	No results	No results	No results		1563,605	782,8096	1,087	509108,4	0	0	0	0	No match	No match	No MS2	[M+2H]+2		509108,4		7,4
FALSE	N,N-Dimethylcosan-1-amine	C22 H47 N	Full match	No results	No results	Full match	No results	0,24	325,3709	326,3782	7,371	774378,9	1	0	0	0	No match	No match	No MS2	[M+H]+1	774378,9	749801,7	5,2	6,3
FALSE			No results	No results	No results	No results	No results		285,8907	286,8979	1,059	285102,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	277952,9	285102,7	7,1	8,2
FALSE		C15 H20 N	Full match	No results	No results	No match	No match	4,17	340,1887	341,1959	7,121	9624107	3	0	0	0	No match	Multiple m	No MS2	[M+H]+1	8970521	9624107	4,6	5,1
FALSE			No results	No results	No results	No results	No results		667,6414	668,6487	1,139	197744,6	0	0	0	0	No match	No match	No MS2	[M+H]+1		197744,6		8,2
FALSE		C12 H4 Cl2	Full match	No results	No results	No match	No results	-4,55	278,9395	279,9468	1,198	372698,1	3	0	0	0	No match	No match	No MS2	[M+H]+1	372698,1	361354,9	7,6	8,2
FALSE		C7 H5 Br Cl	Full match	No results	No results	No results	No results	1,94	421,8676	422,8749	1,194	376532,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	249305,9	376532,6	7,6	5,4
FALSE			No results	No results	No results	No results	No results		111,5124	112,5196	0,338	246250,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		246250,9		7,6
FALSE		C14 H29 N	Full match	No results	No results	No results	No results	0,1	275,1919	276,1992	6,67													



FALSE		C H C1 N2 C	Full match	No results	No results	No results	No results	3,1	441,8173	442,8246	1,123	310243,1	0	0	0		No matche	No matche	No MS2	[M+H]+1	310243,1	7,6		
FALSE	Dinitrogen trioxide	C7 H C1 N6	Full match	No results	No results	No results	No results	-3,95	331,9531	332,9604	1,195	323073,1	1	0	0		No matche	No matche	No MS2	[M+H]+1	323073,1	307852,4	7,1	8,2
FALSE		N2 O3	No results	No results	No results	Full match	No results	2,51	75,99108	76,99836	0,983	802815	1	0	0		No matche	No matche	No MS2	[M+H]+1	802815	731031,4	2,5	4,1
FALSE		C5 H16 N2	Full match	No results	No results	No match	No results	-2,29	230,058	231,0653	1,052	611853,2	22	0	0		Multiple m	Multiple m	No MS2	[M+H]+1		611853,2		7,4
FALSE	laurylbetaine	C16 H33 N	Full match	No results	No results	Full match	No results	0,06	271,2512	272,2584	6,925	1191484	7	0	0		No matche	No matche	No MS2	[M+H]+1	796628,9	1191484	5,2	3,9
FALSE		C50 H109 F	Full match	No results	No results	No results	No results	0,14	1113,712	557,8632	1,061	254336,1	0	0	0		No matche	No matche	No MS2	[M+2H]+2		254336,1		7,1
FALSE			No results	No results	No results	No results	No results		671,8036	672,8109	1,106	184449	0	0	0		No matche	No matche	No MS2	[M+H]+1		184449		4,9
FALSE			No results	No results	No results	No results	No results		1488,677	745,3458	1,093	363349,2	0	0	0		No matche	No matche	No MS2	[M+2H]+2		363349,2		7,1
FALSE		C4 H8 N2 C	Full match	No results	No results	No results	No results	-1,6	178,0058	179,0131	1,96	798633,1	2	0	0		No matche	No matche	No MS2	[M+H]+1	771372,6	798633,1	4,7	6,8
FALSE	[Similar to: Acetyl-L-carnitine; ΔMass: -0,012]		No results	Invalid ma	No results	No results	No results		203,1031	204,1104	1,878	413683,4	0	1	0		No matche	No matche	DDA for pri	[M+H]+1		413683,4		8,5
FALSE			No results	No results	No results	No results	No results		517,6466	596,6609	1,147	341795,5	0	0	0		No matche	No matche	No MS2	[M+DMSO]	341795,5		7,1	
FALSE		C2 H Br2 Cl	Full match	No results	No results	No results	No results	1,82	459,6412	460,6475	1,16	434390,1	0	0	0		No matche	No matche	No MS2	[M+H]+1	433306,6	434390,1	7,4	6,8
FALSE		C7 H3 N3 C	Full match	No results	No results	No results	No results	-2,94	256,9735	257,9808	4,738	672591,1	1	0	0		No matche	No matche	DDA for pri	[M+H]+1	613439,4	672591,1	7,4	6,3
FALSE		C11 H25 N	Full match	No results	No results	No match	No match	-0,84	300,1937	301,2011	7,039	2531956	1	0	0		No matche	Multiple m	DDA for ott	[M+H]+1	2389142	2531956	4,8	4,8
FALSE	Phosphoric acid	H3 O4 P	No results	No results	No results	Full match	Full match	0,36	97,97693	98,98421	1,737	12776649	1	0	0		Single mat	No matche	DDA for pri	[M+H]+1	12776649		4,6	
FALSE		C7 H14 N C	Full match	No results	No results	No match	No results	-1,99	255,0503	256,0576	1,383	494704,5	5	0	0		No matche	No matche	No MS2	[M+H]+1		494704,5		4,7
FALSE		C8 H24 N6	Full match	No results	No results	No match	No match	-2,53	268,1675	269,1747	7,339	1857403	10	0	0		No matche	Multiple m	No MS2	[M+H]+1	1857403		5	
FALSE		C4 H11 N6	Full match	No results	No results	No match	No results	-2,17	302,0369	303,0442	1,145	231648,8	2	0	0		No matche	No matche	No MS2	[M+H]+1		231648,8		7,6
FALSE			No results	No results	No results	No results	No results		153,983	154,9903	7,014	8575408	0	0	0		No matche	No matche	No MS2	[M+H]+1		8575408		5,1
FALSE			No results	No results	No results	No results	No results		1001,744	501,8794	1,096	421527,8	0	0	0		No matche	No matche	No MS2	[M+2H]+2		421527,8		5,2
FALSE	stilbamidine	C16 H16 N	Full match	No results	No results	Not the top	No match	-4,38	264,1363	265,1436	6,851	780108	78	0	0		Single mat	Multiple m	No MS2	[M+H]+1	780108	121260	4,7	4,1
FALSE	10-Undecenoic acid	C11 H20 O	No results	No results	No results	Full match	Partial mat	-0,16	184,1463	185,1536	7,126	5398930	86	0	0		No matche	Multiple m	No MS2	[M+H]+1	5398930	4736144	5,3	4,2
FALSE	ARG-PHE	C15 H23 N	Full match	No results	No results	Full match	No results	-0,09	321,1801	322,1874	3,246	358580,6	2	0	0		No matche	No matche	No MS2	[M+H]+1	358580,6		7,1	
FALSE	cocamidopropyl betaine	C19 H38 N	Full match	No results	No results	Full match	No results	-0,07	342,2882	343,2955	7,023	823303	1	0	0		No matche	No matche	DDA for pri	[M+H]+1	630254,1	823303	3,6	4,7
FALSE		C19 H14 N	Full match	No results	No results	No match	No results	1,75	510,1005	256,0575	1,384	388241,5	1	0	0		No matche	No matche	No MS2	[M+2H]+2		388241,5		7,6
FALSE		C3 H C1 N4	Full match	No results	No results	No results	No results	1,97	477,8281	478,8354	1,099	451598,5	0	0	0		No matche	No matche	No MS2	[M+H]+1	451598,5		4,7	
FALSE	methyldioctylamine	C17 H37 N	Full match	No results	No results	Full match	No results	-0,01	255,2926	256,2999	7,161	1126870	3	0	0		No matche	No matche	No MS2	[M+H]+1	704056,6	1126870	2	5,5
FALSE	3-[[2,6-dimethylheptanoyl]oxy]-4-(trimethyl	C16 H31 N	Full match	No results	No results	Full match	No results	0,32	301,2254	302,2327	6,319	557770	4	0	0		No matche	No matche	DDA for pri	[M+H]+1	514292,1	557770	7,9	7,4
FALSE	Trimexiline	C17 H29 N	Full match	No results	No results	Full match	No results	-0,01	247,23	248,2373	7,11	882696,5	2	0	0		No matche	No matche	No MS2	[M+H]+1	764738,2	882696,5	4,7	6,6
FALSE		C6 H4 C1 N	Full match	No results	No results	No results	No results	-2,56	455,8375	456,8447	1,076	493663,1	0	0	0		No matche	No matche	No MS2	[M+H]+1	493663,1	481483,8	7,4	4,1
FALSE			No results	No results	No results	No results	No results		90,99756	92,00484	0,301	118867,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	89194,65	118867,8	6	6,5
FALSE		C5 H10 N6	Full match	No results	No results	No match	No match	-3,01	218,0402	219,0475	1,268	788608,2	8	0	0		Single mat	No matche	DDA for pri	[M+H]+1	788608,2	739344,7	4,7	4,1
FALSE		C4 H6 N6 C	Full match	No results	No results	No match	No results	1,62	186,0504	187,0577	1,522	1475201	1	0	0		No matche	No matche	DDA for pri	[M+H]+1	1475201	948002,5	2,8	4,5
FALSE			No results	No results	No results	No results	No results		80,51987	81,52715	1,031	153890,3	0	0	0		No matche	No matche	DDA for pri	[M+H]+1	153890,3		4,9	
FALSE		C7 H4 O18	Full match	No results	No results	No results	No results	0,05	597,7477	598,7549	1,137	377987,4	0	0	0		No matche	No matche	No MS2	[M+H]+1	377987,4		6,5	
FALSE		C H3 C12 O	Full match	No results	No results	No results	No results	-0,23	163,9019	164,9092	1,139	441208,3	0	0	0		No matche	No matche	DDA for pri	[M+H]+1	441208,3	417944,4	4,1	7,4
FALSE		C26 H58 N	Full match	No results	No results	No match	No results	-4,12	509,3482	510,3555	7,205	3886504	5	0	0		No matche	No matche	No MS2	[M+H]+1	2043407	3886504	3,7	4,8
FALSE	DEHYDROASCORBIC ACID	C6 H6 O6	Full match	No results	No results	Full match	Full match	0,03	174,0164	175,0237	1,777	603425	11	0	0		Multiple m	No matche	DDA for pri	[M+H]+1	592661,9	603425	5,8	4,1
FALSE		C4 H2 Br C	Full match	No results	No results	No results	No results	-1,71	749,5624	750,5697	1,143	241362,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	183732,8	241362,6	7,1	7,6
FALSE			No results	No results	No results	No results	No results		597,9939	599,0012	1,095	319485,5	0	0	0		No matche	No matche	No MS2	[M+H]+1	313455,8	319485,5	6,5	7,6
FALSE			No results	No results	No results	No results	No results		151,5772	152,5845	1,462	297420,3	0	0	0		No matche	No matche	No MS2	[M+H]+1		297420,3		7,1
FALSE	[Similar to: Ethylenediaminetetraacetic acid]		No results	Invalid ma	No results	No results	No results		291,9003	292,9076	1,424	178355,4	0	2	0		No matche	No matche	No MS2	[M+H]+1	178355,4		4,9	
FALSE			No results	No results	No results	No results	No results		199,1767	200,184	1,439	120925,7	0	0	0		No matche	No matche	No MS2	[M+H]+1		120925,7		8,2
FALSE		C14 H28 N	Full match	No results	No results	No match	No results	4,37	384,1761	385,1834	7,079	2958340	2	0	0		No matche	No matche	No MS2	[M+H]+1	2250783	2958340	4,2	4,8
FALSE	N-[[2-Methylphenoxy]acetyl]-L-leucyl-O-(4-	C31 H40 N	No results	No results	No results	Full match	No results	-2	596,2834	299,149	7,145	9414346	1	0	0		No matche	No matche	DDA for ott	[M+2H]+2		9414346		5,1
FALSE			No results	No results	No results	No results	No results		599,7624	600,7697	1,125	162631	0	0	0		No matche	No matche	No MS2	[M+H]+1	162631		8,2	
FALSE		C37 H80 Cl	Full match	No results	No results	No results	No results	-1,36	723,558	724,5653	1,147	281155,3	0	0	0		No matche	No matche	No MS2	[M+H]+1	280055,2	281155,3	7,6	7,1
FALSE		H6 O17	Full match	No results	No results	No results	No results	-0,83	519,8238	520,8311	1,094	406253,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	406253,6	348962,6	7,4	7,1
FALSE		C4 H N O8	Full match	No results	No results	No match	No results	-0,19	190,9702	191,9775	1,191	372228,1	2	0	0		No matche	No matche	No MS2	[M+H]+1	372228,1	347098,6	7,6	7,1
FALSE		C7 H28 N1	Full match	No results	No results	No match	No match	-4,3	410,1651	411,1724	1,49	185808,7	15	0	0		No matche	Single mat	No MS2	[M+H]+1	185808,7		4,9	
FALSE		C6 H3 N5 C	Full match	No results	No results	No results	No results	-0,63	222,9811	223,9884	7,271	9355434	0	0	0		No matche	No matche	No MS2	[M+H]+1	9355434		4,6	
FALSE	Palmitic Acid	C16 H32 O	Full match	No results	No results	Full match	Full match	0,14	256,2403	239,237	0,31	3720105	24	0	0		Single mat	Multiple m	No MS2	[M+H-H2O]	162106,3	3720105	4,9	2,1
FALSE			No results	No results	No results	No results	No results		503,7499	504,7572	1,14	339664,1	0	0	0		No matche	No matche	No MS2	[M+H]+1	316008,4	339664,1	7,1	7,1
FALSE	Phosphocreatine	C4 H10 N3	Full match	No results	No results	Full match	Full match	0,11	211,0358	212,0431	1,286	990819,3	1	0	0		Single mat	No matche	No MS2	[M+H]+1	990819,3	955565	6,6	3,9
FALSE			No results	No results	No results	No results	No results		385,7536	386,7609	1,149	428580,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	428580,6		7,4	
FALSE		C23 H7 N6	Full match	No results	No results	No results	No results	-0,76	747,8491	748,8564	1,084	428927,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	385049,6	428927,8	7,1	3,6
FALSE		C18 H N O6	Full match	No results	No results	No results	No results	1,91	167,0433	168,0506	1,027	320116,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	320116,6		6	
FALSE			No results	No results	No results	No results	No results		714,6379	715,6452	1,139	217345,2	0	0	0		No matche	No matche	No MS2	[M+H]+1	217345,2		7,6	
FALSE			No results	No results	No results	No results	No results		577,5559	578,5621	1,175	360802,5	0	0	0		No matche	No matche	No MS2	[M+H]+1	360802,5	359686,6	7,1	4,3
FALSE			No results	No results	No results	No results	No results		630,6743	631,6815	1,137	281751,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	281751,8	209733,1	7,6	7,1
FALSE		C5 H7 N8 C	Full match	No results	No results	No match	No results	1,66	258,0205	259,0278	1,198	371177,4	6	0	0		No matche	No matche	No MS2	[M+H]+1	371177,4	307163,5	7,6	7,1
FALSE		C4 H4 C1 N	Full match	No results	No results	No match	No results	0,6	236,9547	237,962	1,206	356238	1	0	0		No matche	No matche	No MS2	[M+H]+1				

FALSE			C11 H12 O	Full match	No results	No results	No results	No results	No results	2,33	352,0286	353,0359	1,35	552409,9	3	0	0	0	No match	No match	No MS2	[M+H]+1	552409,9		4,7	
FALSE				No results	No results	No results	No results	No results	No results		543,6491	544,6555	1,146	289338,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	264951,5	289338,8	7,1	7,1
FALSE				No results	No results	No results	No results	No results	No results		669,5938	670,601	1,146	252097,3	0	0	0	0	No match	No match	No MS2	[M+H]+1	214000,3	252097,3	3,3	7,6
FALSE			C24 H35 N	Full match	No results	No results	No results	No match	No results	2,35	551,2076	576,6111	1,94	1092269	1	0	0	0	No match	No match	No MS2	[M+2H]+2	1092269	972893,4	5	4,5
FALSE	[Similar to: Acetyl-L-carnitine; ΔMass: 203.09]		C18 H35 N	Full match	Invalid mat	No results	No match	No results	No results	2,01	406,2063	204,1104	1,878	491471,9	1	1	0	0	No match	No match	DDA for ori	[M+2H]+2	491471,9		7,4	
FALSE			Palmitic Acid	Full match	No results	No results	Full match	Full match		0,21	256,2403	257,2475	3,178	9656141	24	0	0	0	Single mat	Multiple m	DDA for ori	[M+H]+1	9656141	8027483	5,1	4
FALSE			C16 H32 O	Full match	No results	No results	Full match	Full match	No results	0,32	301,2254	302,2327	6,12	427982,3	4	0	0	0	No match	No match	DDA for pri	[M+H]+1	419959,4	427982,3	6,8	5,8
FALSE				No results	No results	No results	No results	No results	No results		587,8115	588,8188	1,091	235448,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	235448,8	223194,2	7,1	7,6
FALSE		MHPG	C9 H12 O4	Full match	No results	No results	Full match	Full match		0,01	184,0736	185,0808	6,381	1789105	27	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	1269542	1789105	3,9	4,5
FALSE			C24 H35 N	Full match	No results	No results	No match	No results	No results	-3,26	393,288	394,2952	7,005	744911	1	0	0	0	No match	No match	No MS2	[M+H]+1	647428,3	744911	6,3	5,2
FALSE		5,6-Dimethyl-2-benzothiazolamine	C9 H10 N2	Full match	No results	No results	Full match	No results	No results	0,03	178,0565	179,0638	1,486	8800213	6	0	0	0	No match	No match	No MS2	[M+H]+1	8800213		4	
FALSE			C H3 N O6	Full match	No results	No results	No results	No results	No results	0,62	218,9158	219,923	1,133	396823,3	0	0	0	0	No match	No match	No MS2	[M+H]+1	391661,5	396823,3	7,1	7,4
FALSE				No results	No results	No results	No results	No results	No results		582,827	583,8343	1,107	138968,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	138968,6			4,9
FALSE		ACETYL ARGININE	C8 H16 N4	Full match	No results	No results	Full match	Full match		2,25	216,1227	217,1294	1,962	292156,8	3	0	0	0	Single mat	No match	No MS2	[M+H]+1	292156,8	280183,8	8,2	7,1
FALSE			C13 H21 O	Full match	No results	No results	No match	No results	No results	0,89	430,0351	431,0424	1,961	300459,1	1	0	0	0	No match	No match	No MS2	[M+H]+1	291955,2	300459,1	7,6	7,6
FALSE		N4-PALMITOYL CYTARABINE	C25 H43 N	Full match	No results	No results	Full match	No results	No results	3,46	481,3169	482,3241	6,932	3988572	2	0	0	0	No match	No match	No MS2	[M+H]+1	1999881	3988572	2,1	5,3
FALSE				No results	No results	No results	No results	No results	No results		679,495	680,5023	1,174	236747,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	236747,2	230818,3	7,6	7,6
FALSE			C44 H60 O	Full match	No results	No results	No results	No match	No results	-3	764,4113	765,4186	7,844	1111113	0	0	0	0	No match	Single mat	DDA for pri	[M+H]+1	1107281	1111113	6,1	6,6
FALSE				No results	No results	No results	No results	No results	No results		109,5113	110,5186	0,339	256825,4	0	0	0	0	No match	No match	No MS2	[M+H]+1		256825,4		6,5
FALSE				No results	No results	No results	No results	No results	No results		608,7077	650,742	1,128	160133,2	0	0	0	0	No match	No match	DDA for ori	[M+ACN+H]		160133,2		8,2
FALSE		1,3,5-Heptatriene, (E,E)-	C7 H10	Full match	No results	No results	Full match	No results	No results	0,07	94,07826	95,08553	7,071	9112072	13	0	0	0	No match	No match	No MS2	[M+H]+1		9112072		4
FALSE		6,7-Dimethoxy-2-(1-piperazinyl)-4-quinazolinol	C14 H19 N	Full match	No results	No results	Full match	No results	No results	-4,54	289,1526	290,1598	3,666	421504,8	4	0	0	0	No match	No match	DDA for pri	[M+H]+1	379899,9	421504,8	6	6,3
FALSE		2-sec-Butyl-4-[4-[4-(4-hydroxyphenyl)-1-pi	C22 H27 N	No results	No results	No results	Full match	No match	No results	-3,02	393,2153	394,2226	1,414	312725,6	4	0	0	0	No match	Single mat	No MS2	[M+H]+1	312725,6		7,1	
FALSE				No results	No results	No results	No results	No results	No results		755,6431	756,6504	1,133	208124,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		208124,3		7,6
FALSE			C33 H59 O	Full match	No results	No results	No results	No match	No results	2,24	660,3488	661,3561	7,456	1385083	0	0	0	0	No match	Multiple m	No MS2	[M+H]+1	769764,7	1385083	3	5
FALSE			C27 H51 N	Full match	No results	No results	No results	No results	No results	-2,77	545,3484	546,3556	6,913	1653947	3	0	0	0	No match	No match	No MS2	[M+H]+1	1575368	1653947	5,5	3,4
FALSE			C43 H88 N	Full match	No results	No results	No results	No results	No results	-0,27	753,6445	754,6518	1,137	217910,4	0	0	0	0	No match	No match	No MS2	[M+H]+1	217910,4		7,1	
FALSE			C4 H6 N6 C	Full match	No results	No results	No match	No results	No results	1,17	202,0453	203,0526	2,012	952641,4	2	0	0	0	No match	No match	No MS2	[M+H]+1		952641,4		7,2
FALSE			C3 H5 N6 C	Full match	No results	No results	No results	No results	No results	-1,42	347,8988	348,906	1,032	329876,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	329876,7	202276,8	2,2	6,5
FALSE			C5 H12 N5	Full match	No results	No results	No match	No results	No results	1,63	267,0208	268,0281	1,152	253878	2	0	0	0	No match	No match	No MS2	[M+H]+1	253878	173936,5	7,6	7,1
FALSE			C24 H9 N5	Full match	No results	No results	No match	No results	No results	3,38	383,082	192,5483	1,961	269667,6	1	0	0	0	No match	No match	No MS2	[M+2H]+2		269667,6		6,5
FALSE				No results	No results	No results	No results	No results	No results		509,6133	510,6206	1,177	318484,4	0	0	0	0	No match	No match	No MS2	[M+H]+1	318484,4		7,6	
FALSE				No results	No results	No results	No results	No results	No results		263,0753	264,0826	1,52	642231	0	0	0	0	No match	No match	No MS2	[M+H]+1	113954,5	642231	6	1,4
FALSE		1-Naphthylisocyanate	C11 H7 N	Full match	No results	No results	Full match	No results	No results	0,63	169,0529	202,0864	4,124	516048,5	2	0	0	0	No match	No match	DDA for pri	[M+H+MeC]	406059,9	516048,5	7,9	6,8
FALSE				No results	No results	No results	No results	No results	No results		844,7406	423,3776	0,958	220059	0	0	0	0	No match	No match	No MS2	[M+2H]+2		220059		8,2
FALSE		3,4-Dihydroxyphenylglycol	C8 H10 O4	Full match	No results	No results	Full match	Partial mat	No results	0,27	170,058	171,0652	1,504	297596	32	0	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1		297596		7,1
FALSE		5,6-Dimethyl-2-benzothiazolamine	C9 H10 N2	No results	No results	No results	Full match	No results	No results	0,22	178,0565	179,0638	5,504	4790224	6	0	0	0	No match	No match	No MS2	[M+H]+1	3390145	4790224	4,8	4,8
FALSE				No results	No results	No results	No results	No results	No results		93,50792	94,51519	1,974	411068,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	359524	411068,5	6	4,7
FALSE		Carvonic acid	C10 H12 O	Full match	No results	No results	Full match	Partial mat	No results	0,18	180,0787	181,086	5,54	1218768	95	0	0	0	Single mat	Multiple m	DDA for pri	[M+H]+1		1218768		4,5
FALSE			C5 H11 N C	Full match	No results	No results	No results	No results	No results	0,72	357,003	358,0102	1,541	598068,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	361994,8	598068,8	6,5	3
FALSE		2,4-Dibromo-1-fluorobenzene	C6 H3 Br2	No results	No results	No results	Full match	No results	No results	-0,24	251,8585	252,8658	1,136	354151,4	2	0	0	0	No match	No match	No MS2	[M+H]+1	354151,4		7,1	
FALSE			C2 H N6 O	Full match	No results	No results	No results	No results	No results	3,53	377,8042	378,8114	1,138	341457,4	0	0	0	0	No match	No match	No MS2	[M+H]+1		341457,4		7,1
FALSE				No results	No results	No results	No results	No results	No results		677,7881	678,7954	1,054	219433,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	219433,7	186095,5	7,1	2,7
FALSE				No results	No results	No results	No results	No results	No results		625,5308	626,5381	1,176	273786,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	273786,6	252384,5	7,6	7,6
FALSE			C56 H107	Full match	No results	No results	No results	No results	No results	-0,3	1137,707	569,861	1,114	120080,9	0	0	0	0	No match	No match	No MS2	[M+2H]+2		120080,9		6,5
FALSE				No results	No results	No results	No results	No results	No results		111,5079	112,5152	1,016	542811,4	0	0	0	0	No match	No match	No MS2	[M+H]+1		542811,4		6,8
FALSE			C2 H4 Cl2	Full match	No results	No results	No results	No results	No results	-2,87	439,8386	440,8459	1,197	371140,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		371140,8		7,6
FALSE			C4 H12 N3	Full match	No results	No results	No results	No results	No results	1,46	181,0619	182,0692	4,189	588384,2	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		588384,2		6,8
FALSE			C H N8 O P	Full match	No results	No results	No results	No results	No results	1,62	267,9177	268,925	1,057	312251,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	312251,7	273814,8	6,5	8,2
FALSE			C55 H87 N	Full match	No results	No results	No results	No results	No results	0,13	1007,603	504,8088	7,389	699918,2	0	0	0	0	No match	No match	No MS2	[M+2H]+2	699918,2	687684,2	3	4,7
FALSE			C4 H2 N6 C	Full match	No results	No results	No match	No results	No results	1,25	214,0089	215,0162	3,206	534615,7	2	0	0	0	No match	No match	No MS2	[M+H]+1	467406,3	534615,7	4,7	4,7
FALSE		gaboxadol	C6 H8 N2 C	Full match	No results	No results	Full match	Full match	No results	0,07	140,0586	141,0659	1,705	734230,9	19	0	0	0	Single mat	No match	No MS2	[M+H]+1	557737,8	734230,9	6,3	3,6
FALSE			C8 H9 Cl O	Full match	No results	No results	No match	No results	No results	-2,6	233,976	234,9833	1,17	350149,6	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	345200,1	350149,6	7,6	7,6
FALSE				No results	No results	No results	No results	No results	No results		110,9611	111,9684	0,34	256193,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		256193,1		7,6
FALSE		Mesitol	C9 H12 O	Full match	No results	No results	Full match	Partial mat	No results	0,17	136,0888	137,0961	6,974	9846555	70	0	0	0	No match	Single mat	No MS2	[M+H]+1		9846555		4,6
FALSE		Betonidine	C7 H13 N C	Full match	No results	No results	Full match	Full match	No results	0,27	159,0896	160,0969	1,326	510350,6	28	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1	510350,6	488517,6	6,3	3,6
FALSE				No results	No results	No results	No results	No results	No results		129,5185	130,5258	1,97	333725,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	231435,1	333725,5	8,2	6,5
FALSE		(4R,9R,14R,19R)-3,10,13,20,26-Pentaazatetrin	C21 H35 N	Full match	No results	No results	Full match	No results	No results	-3,28	357,2881	358,2954	6,983	656666,4	2	0	0	0	No match	No match	No MS2	[M+H]+1	507059	656666,4	5,8	

FALSE	EDDA		C6 H12 N2	Full match	No results	No results	No results	Full match	No results	0,37	176,0798	177,0871	3,255	2475998	13	0	0		No matche	No matche	No MS2	[M+H]+1	2475998	2167539	4,8	4,2
FALSE				No results	No results	No results	No results	No results	No results		631,5659	632,5732	1,16	246193,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	246193,6	191621,1	8,2	8,2
FALSE				No results	No results	No results	No results	No results	No results		80,50234	81,50961	0,974	281524,1	0	0	0		No matche	No matche	DDA for pr	[M+H]+1	281524,1		4,3	
FALSE	laurylbetaine		C16 H33 N	Full match	No results	No results	No results	Full match	No results	0,23	271,2512	272,2585	7,366	1240696	7	0	0		No matche	No matche	No MS2	[M+H]+1	1240696	1221552	5	5
FALSE	6-(4-Methylpiperazin-1-yl)-4-(o-tolyl)pyridin-		C17 H22 N	Full match	No results	No results	Not the top	No match		-4,8	282,1831	283,1904	7,314	2433102	13	0	0		No matche	Multiple m	No MS2	[M+H]+1		2433102		4,2
FALSE			C7 H17 N2	Full match	No results	No results	No results	No results	No results	0,61	208,0978	209,1051	1,139	781171,2	0	0	0		No matche	No matche	No MS2	[M+H]+1	781711,2	684549,7	5,2	3,6
FALSE			C12 H32 N	Full match	No results	No results	No match	No results	No results	2,97	373,2101	374,2174	7,03	6422949	4	0	0		No matche	No matche	No MS2	[M+H]+1	5900179	6422949	4,6	4,6
FALSE			C18 H Br Cl3	Full match	No results	No results	No results	No results	No results	-3,33	495,6814	574,7034	1,143	287796,6	0	0	0		No matche	No matche	No MS2	[M+DMSO]	249739,6	287796,6	7,1	7,1
FALSE				No results	No results	No results	No results	No results	No results		124,979	125,9862	1,158	280336,3	0	0	0		No matche	No matche	No MS2	[M+H]+1		280336,3		6,5
FALSE	Dihydroajmone		C11 H18 O	Full match	No results	No results	Full match	Partial mat		0,06	166,1358	167,1431	7,158	4149217	49	0	0		No matche	Multiple m	No MS2	[M+H]+1	4149217		5,3	
FALSE	Mesitol		C9 H12 O	Full match	No results	No results	Full match	Partial mat		0,06	136,0888	137,0961	7,153	10094252	70	0	0		No matche	Single mati	No MS2	[M+H]+1	10094252		4	
FALSE			C15 H31 P	Full match	No results	No results	No match	No results	No results	4,53	338,1341	339,1414	6,877	4064533	3	0	0		No matche	No matche	No MS2	[M+H]+1	4064533		4,2	
FALSE				No results	No results	No results	No results	No results	No results		567,8514	568,8587	1,071	323564,8	0	0	0		No matche	No matche	No MS2	[M+H]+1		323564,8		7,1
FALSE			C4 H4 N4 C	Full match	No results	No results	No results	No results	No results	0,33	140,0335	141,0408	2,404	916535,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	916535,8	902397,3	6,1	6,1
FALSE				No results	No results	No results	No results	No results	No results		690,6717	691,679	1,131	189272,7	0	0	0		No matche	No matche	No MS2	[M+H]+1		189272,7		8,2
FALSE				No results	No results	No results	No results	No results	No results		283,2591	284,2664	1,735	22620987	0	0	0		No matche	No matche	DDA for pr	[M+H]+1	22620987	22499529	4	4
FALSE				No results	No results	No results	No results	No results	No results		709,6234	710,6307	1,14	189952,5	0	0	0		No matche	No matche	No MS2	[M+H]+1	189952,5	181223,5	7,6	7,6
FALSE				No results	No results	No results	No results	No results	No results		80,5226	81,52988	1,029	256118,4	0	0	0		No matche	No matche	DDA for pr	[M+H]+1	256118,4	1798220	7,1	2,2
FALSE				No results	No results	No results	No results	No results	No results		80,52175	81,52903	0,955	325656	0	0	0		No matche	No matche	DDA for pr	[M+H]+1		325656		6,5
FALSE				No results	No results	No results	No results	No results	No results		257,8038	258,811	1,145	246775,1	0	0	0		No matche	No matche	DDA for pr	[M+H]+1	246775,1		7,1	
FALSE	HC blue 2		C12 H19 N	Full match	No results	No results	Full match	No results	No results	0,08	285,1325	286,1398	1,96	291571,8	3	0	0		No matche	No matche	No MS2	[M+H]+1	277772	291571,8	4,9	5,4
FALSE	4-Chloro-N-[6,8-dibromo-2-(2-thienyl)imidaz		C18 H10 Br	No results	No results	No results	Full match	No results	No results	-0,75	508,8596	509,8669	1,1	188993,2	1	0	0		No matche	No matche	No MS2	[M+H]+1	188993,2		7,6	
FALSE				No results	No results	No results	No results	No results	No results		618,7129	619,7202	1,132	170011,8	0	0	0		No matche	No matche	No MS2	[M+H]+1		170011,8		8,2
FALSE	5-[2-Methyl-2-propanyl)-2,4-pyrimidinediol		C8 H12 N2	Full match	No results	No results	Full match	Partial mat		-0,12	168,0899	169,0971	2,315	647646,8	20	0	0		Single mati	Multiple m	DDA for pr	[M+H]+1	447895,2	647646,8	6,8	6,3
FALSE	Massoia lactone		C10 H16 O	Full match	Invalid ma	No results	Full match	Partial mat		-0,04	168,115	169,1223	7,239	10216242	126	2	0	47,4	Multiple m	Multiple m	DDA for pr	[M+H]+1	7987328	10216242	5,1	3,5
FALSE				No results	No results	No results	No results	No results	No results		646,649	647,6563	1,139	234269,3	0	0	0		No matche	No matche	No MS2	[M+H]+1	188367,6	234269,3	7,1	7,6
FALSE			C39 H71 N	Full match	No results	No results	No results	No results	No results	-3,2	681,576	760,5988	1,144	218056,1	0	0	0		No matche	No matche	No MS2	[M+DMSO]	218056,1		6,5	
FALSE				No results	No results	No results	No results	No results	No results		533,6199	534,6262	1,146	262540,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	262540,6	230921,1	7,1	7,1
FALSE			C3 H2 Cl O	Full match	No results	No results	No results	No results	No results	-4,05	453,7414	454,7487	1,145	310578,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	310578,8		7,1	
FALSE	PEG-3 OCTATRIACONTANYL ETHER		C44 H90 O	No results	No results	No results	Full match	No results	No results	1,84	682,6852	683,6924	1,131	189307,7	1	0	0		No matche	No matche	No MS2	[M+H]+1	189307,7	137192,1	6,5	7,6
FALSE	Bis(pentachlorophenyl) disulfide		C12 Cl10 S	No results	No results	No results	Full match	No results	No results	2,05	557,6338	558,6408	1,161	239362,7	1	0	0		No matche	No matche	No MS2	[M+H]+1	239362,7	233120,6	8,2	3,8
FALSE			C7 H19 N1	Full match	No results	No results	No match	No match		-2,69	352,0947	177,0546	7,37	685736,9	19	0	0		No matche	Multiple m	No MS2	[M+2H]+2	685736,9		6,8	
FALSE				No results	No results	No results	No results	No results	No results		475,6612	476,6678	1,147	307959,3	0	0	0		No matche	No matche	No MS2	[M+H]+1		307959,3		6,5
FALSE			C8 H12 Cl4	Full match	No results	No results	No results	No results	No results	2,1	437,8416	438,8488	1,196	301487,1	0	0	0		No matche	No matche	No MS2	[M+H]+1	301487,1	281284,7	7,1	7,1
FALSE	METIPRANOLOL		C17 H27 N	Full match	No results	No results	Full match	Partial mat		0,27	309,1941	310,2014	6,28	881946,2	13	0	0		No matche	Multiple m	No MS2	[M+H]+1	762512,1	881946,2	5,8	6,6
FALSE			C14 H27 N	Full match	No results	No results	No match	No match		-3	273,1577	274,165	5,886	317887,3	5	0	0		No matche	Single mati	No MS2	[M+H]+1	317887,3		4,2	
FALSE			C16 H26 O	Full match	No results	No results	No match	No match		-2,26	298,1418	299,1491	7,143	9623449	17	0	0		No matche	Multiple m	DDA for pr	[M+H]+1	9623449		4,6	
FALSE			C45 H74 N	Full match	No results	No results	No match	No results	No results	-2,2	779,5461	780,5534	7,278	4531660	54	0	0		No matche	No matche	No MS2	[M+H]+1	4531660		4,8	
FALSE				No results	No results	No results	No results	No results	No results		234,8898	235,8971	1,138	296409,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	296409,8	232033,1	7,1	3,3
FALSE			C8 H14 N2	Full match	No results	No results	No match	No results	No results	-1,13	232,0528	233,0601	3,231	626533,2	7	0	0		No matche	No matche	No MS2	[M+H]+1	626533,2	515011,7	4,1	3
FALSE			C4 H9 N8 C	Full match	No results	No results	No match	No match		1,45	248,0539	249,0612	4,143	525730	2	0	0		No matche	Single mati	No MS2	[M+H]+1	458787,5	525730	3,6	6,8
FALSE			C4 H5 Cl O	Full match	No results	No results	No match	No results	No results	-2,81	373,83	374,8373	1,121	266273,7	4	0	0		No matche	No matche	No MS2	[M+H]+1	266273,7	216461,4	7,6	7,6
FALSE				No results	No results	No results	No results	No results	No results		106,9931	108,0004	0,3	98605,24	0	0	0		No matche	No matche	No MS2	[M+H]+1		98605,24		4,9
FALSE				No results	No results	No results	No results	No results	No results		685,8097	686,817	1,114	187062,3	0	0	0		No matche	No matche	No MS2	[M+H]+1	187062,3		6,5	
FALSE				No results	No results	No results	No results	No results	No results		71,02065	72,02792	0,983	591253,2	0	0	0		No matche	No matche	DDA for pr	[M+H]+1	402677,1	591253,2	6,8	4,7
FALSE	N-ethylmaleimide		C6 H7 N O	Full match	No results	No results	Full match	Full match		0,55	125,0478	126,055	1,654	22057722	24	0	0		Multiple m	No matche	No MS2	[M+H]+1	22057722		4	
FALSE	Succinic anhydride		C4 H4 O3	Full match	No results	No results	Full match	No results	No results	0,21	100,0161	101,0233	3,126	2960133	4	0	0		No matche	No matche	DDA for pr	[M+H]+1	1786757	2960133	4,5	4,8
FALSE	1-Pentofuranosyl-2,4(1H,3H)-pyrimidinedior		C9 H12 N2	Full match	No results	No results	Full match	Full match		0,38	244,0696	245,0769	2,212	969467,2	4	0	0		Multiple m	No matche	No MS2	[M+H]+1	930788,8	969467,2	5	3,4
FALSE	ARECOLINE		C8 H13 N C	Full match	No results	No results	Full match	Partial mat		0,15	155,0947	156,1019	4,827	747782,4	23	0	0		No matche	Single mati	DDA for pr	[M+H]+1	747782,4	739686,8	5,8	6,3
FALSE	2,3,4,6-Tetra-O-methyl-D-galactitol		C10 H22 O	Full match	No results	No results	Full match	No results	No results	0,01	238,1416	239,1489	4,028	729120,2	1	0	0		No matche	No matche	No MS2	[M+H]+1	729120,2	685734	3	6,3
FALSE			C45 H78 O	Full match	No results	No results	No results	No match	No results	-0,71	858,4979	430,2563	7,414	584124	0	0	0		No matche	Single mati	No MS2	[M+2H]+2	584124	501166,5	4,1	3
FALSE				No results	No results	No results	No results	No results	No results		397,8987	398,906	0,972	267178,3	0	0	0		No matche	No matche	No MS2	[M+H]+1		267178,3		4,3
FALSE			C40 H61 N	Full match	No results	No results	No results	No results	No results	0,49	587,4705	588,4778	7,435	746044	0	0	0		No matche	No matche	No MS2	[M+H]+1	641099,9	746044	4,7	4,7
FALSE				No results	No results	No results	No results	No results	No results		609,801	610,8082	1,051	221115,4	0	0	0		No matche	No matche	No MS2	[M+H]+1		221115,4		7,1
FALSE	Glycerol		C3 H8 O3	Full match	No results	No results	Full match	Full match		0,31	92,04737	93,05465	1,518	314990,8	3	0	0		Single mati	No matche	No MS2	[M+H]+1	314990,8		6,5	
FALSE	10-Undecenoic acid		C7 H5 Cl2	Full match	No results	No results	No results	No results	No results	-1,26	493,8356	494,8429	1,219	497725,6	0	0	0		No matche	No matche	No MS2	[M+H]+1	384644,2	497725,6	7,1	6,3
FALSE				No results	No results	No results	No results	No results	No results		521,7292	522,7365	1,146	246636,8	0	0	0		No matche	No matche	No MS2	[M+H]+1	246636,8		7,6	
FALSE			C4 H3 Cl O	Full match	No results	No results	No results	No results	No results	-0,97	467,8199	468,8272	1,111	150561,7	0	0	0		No matche	No matche	No MS2	[M+H]+1	150561,7		8,2	
FALSE	Stearic acid		C18 H36 O	Full match	No results	No results	Full match	Full match		0,07	284,2716	285,2788	3,176	8641447	34	0	0		Single mati	Single mati	No MS2					



FALSE		C7 H26 N7	Full match	No results	No results	No results	No results	-2.89	349,1122	350,1195	1,782	751281,8	2	0	0	0	No matche	No matche	No MS2	[M+H]+1	751281,8	699706,4	6,3	7,4
FALSE		C7 H32 C1 N	Full match	No results	No results	No results	No results	-0.95	595,7948	596,8021	1,003	697596,0	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	697596,0	359601,4	5,8	6,5
FALSE		C39 H81 N	Full match	No results	No results	No results	No results	-2.58	623,6135	624,6208	1,145	168961	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	168961			8,2
FALSE			No results	No results	No results	No results	No results		698,6616	699,6688	1,136	192226,3	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	145270,2	192226,3	7,6	8,2
FALSE		C59 H90 N	Full match	No results	No results	No results	No results	-0.15	1040,64	521,3271	7,794	547090,5	0	0	0	0	No matche	No matche	DDA for ot	[M+2H]+2	439194,9	547090,5	6,8	6,8
FALSE	Phosphoric acid	H3 O4 P	No results	No results	No results	Full match	Full match	0,36	97,97693	98,98421	1,522	272011,7	1	0	0	0	Single mat	No matche	DDA for pr	[M+H]+1		272011,7		4,3
FALSE			No results	No results	No results	No results	No results		1069,732	535,8731	1,09	205445,1	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2		205445,1		7,1
FALSE	10-Undecenoic acid	C11 H20 O	No results	No results	No results	Full match	Partial mat	0,43	184,1464	185,1537	1,509	166217,5	86	0	0	0	No matche	Multiple m	No MS2	[M+H]+1		166217,5		7,1
FALSE	CUMYL-CH-MeGACLONE	C27 H30 N	No results	No results	No results	Full match	No results	4,26	398,2375	399,2448	7,395	419441,1	2	0	0	0	No matche	No matche	No MS2	[M+H]+1	370127,5	419441,1	7,6	7,4
FALSE	Dimetofrine	C11 H17 N	Full match	No results	No results	Full match	Partial mat	-2,36	227,1152	228,1225	1,346	417088,4	3	0	0	0	No matche	Single mat	No MS2	[M+H]+1	417088,4		4,1	
FALSE		C6 H3 N5 C	Full match	No results	No results	No results	No results	-1,55	254,9707	255,978	1,149	224278,6	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	224278,6	189480,8	7,6	8,2
FALSE	Tributyl (1Z)-1-propene-1,2,3-tricarboxylate	C18 H34 O	No results	No results	No results	Full match	Partial mat	0,14	342,2043	325,201	7,311	720549,7	12	0	0	0	No matche	Multiple m	DDA for pr	[M+H+H2O]	7205497		4	
FALSE		C4 H4 N5 P	Full match	No results	No results	No results	No results	-3,25	184,9919	93,50323	0,3	89915,29	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2		89915,29		6,5
FALSE		C8 H13 N1	Full match	No results	No results	No results	No match	-0,79	296,1009	297,1082	1,944	388741,6	11	0	0	0	Single mat	Multiple m	No MS2	[M+H]+1	347263,5	388741,6	6,5	6
FALSE		C8 H14 N9	Full match	No results	No results	No results	No results	1,52	331,0734	332,0807	1,206	221735,3	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	221735,3	210120,8	7,6	7,6
FALSE	Glycerol	C3 H8 O3	Full match	No results	No results	Full match	Full match	0,15	92,04736	93,05463	1,562	475598,2	3	0	0	0	Single mat	No matche	No MS2	[M+H]+1	475598,2		4,1	
FALSE	leucocline	C9 H7 N	Full match	No results	No results	Full match	Full match	0,17	129,0579	130,0652	6,018	467534,3	4	0	0	0	Multiple m	No matche	No MS2	[M+H]+1	452897,1	467534,3	6,8	6,3
FALSE		C3 H7 N2 C	Full match	No results	No results	No match	No results	-2,79	243,9383	244,9456	0,997	611062,7	1	0	0	0	No matche	No matche	No MS2	[M+H]+1	579357,1	611062,7	1,4	5,2
FALSE			No results	No results	No results	No results	No results		645,7186	646,7258	1,13	175240,9	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		175240,9		8,2
FALSE			No results	No results	No results	No results	No results		715,6357	716,643	1,137	224230,4	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		224230,4		7,1
FALSE		C48 H57 N	Full match	No results	No results	No results	No results	-3,19	775,4661	776,4734	8,1	771058,9	0	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	682749,9	771058,9	7,4	6,8
FALSE	4-Hydroxy-5-methoxy-4-[2-methyl-3-(3-met	C16 H24 O	Full match	No results	No results	Full match	Partial mat	0,3	296,1625	297,1697	7,187	7907142	12	0	0	0	No matche	Multiple m	No MS2	[M+H]+1		7907142		4
FALSE		C5 H9 N O4	Full match	No results	No results	Invalid mat	No results	0,78	210,9975	212,0047	1,957	256264,1	1	0	0	0	No matche	No matche	No MS2	[M+H]+1	256264,1	225364,4	8,2	7,6
FALSE		C15 H31 N	Full match	No results	No results	No match	No results	4,86	389,205	390,2123	7,056	5685180	6	0	0	0	No matche	No matche	No MS2	[M+H]+1	4675021	5685180	2,6	4
FALSE		C9 H24 Cl	Full match	No results	No results	No results	No match	3,2	440,0673	441,0746	1,236	679959,6	0	0	0	0	No matche	Single mat	No MS2	[M+H]+1		679959,6		4,7
FALSE	N-Butylbenzenesulfonamide	C10 H15 N	No results	No results	No results	Full match	Full match	0,27	213,0824	214,0897	1,661	19491767	6	0	0	0	No matche	Single mat	DDA for pr	[M+H]+1	19491767	17084062	4	4
FALSE			No results	No results	No results	No results	No results		767,5384	768,5457	1,142	191590,8	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		191590,8		7,6
FALSE		C5 H5 N3 C	Full match	No results	No results	No results	No results	-2,49	232,975	233,9822	1,962	318394,9	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	318394,9	286956,3	4,3	7,6
FALSE			No results	No results	No results	No results	No results		100,5015	101,5087	0,339	272156,2	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		272156,2		6,5
FALSE		C4 H13 N1	Full match	No results	No results	No results	No match	-3,76	294,0526	295,0599	1,961	244909,1	0	0	0	0	No matche	Multiple m	No MS2	[M+H]+1	244909,1	244578,6	5,4	6
FALSE			No results	No results	No results	No results	No results		673,6535	674,6608	1,138	230521,4	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	199680,1	230521,4	7,1	7,1
FALSE	Dipivaloylmethane	C11 H20 O	Full match	No results	No results	Full match	Partial mat	0,31	184,1464	185,1537	1,643	16634065	86	0	0	0	No matche	Multiple m	DDA for pr	[M+H]+1	14126721	16634065	4	4
FALSE			No results	No results	No results	No results	No results		429,8461	430,8534	1,085	262845,8	0	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	262845,8	202590,3	7,1	7,1
FALSE		C16 H29 N	Full match	No results	No results	No match	No results	0,16	363,1894	364,1967	7,207	5827495	5	0	0	0	No matche	No matche	No MS2	[M+H]+1	5404985	5827495	3,7	4
FALSE		C5 H2 Cl N	Full match	No results	No results	No results	No results	-1,81	244,9419	245,9491	1,153	216090,1	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		216090,1		7,6
FALSE			No results	No results	No results	No results	No results		661,6933	662,7006	1,132	224412,6	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	224412,6	179723,4	7,1	5,4
FALSE	1,2-Dihydropyrimidine	C4 H6 N2	Full match	No results	No results	Full match	No results	1,9	82,05325	83,06042	1,377	549652,7	8	0	0	0	No matche	No matche	DDA for pr	[M+H]+1		549652,7		5
FALSE		C2 H4 N3 C	Full match	No results	No results	No results	No results	-2,96	164,9757	165,983	0,347	858198,4	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		858198,4		5,2
FALSE	p-Cresol	C7 H8 O	Full match	No results	No results	Full match	Full match	-0,1	108,0575	109,0648	6,996	8157142	7	0	0	0	Multiple m	Multiple m	DDA for pr	[M+H]+1		8157142		8
FALSE			No results	No results	No results	No results	No results		649,6896	650,6969	1,133	174313,1	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		174313,1		4,2
FALSE			No results	No results	No results	No results	No results		555,628	556,6353	1,147	174647,5	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		174647,5		8,2
FALSE	(1Z,5Z)-1,5-Cyclooctadiene	C8 H12	Full match	No results	No results	Full match	Partial mat	-0,04	108,0939	109,1012	7,148	6504829	11	0	0	0	No matche	Single mat	DDA for pr	[M+H]+1	5160901	6504829	1	4,6
FALSE		C8 H3 Cl2	Full match	No results	No results	No results	No results	2,04	423,8646	424,8719	1,194	336378,9	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		336378,9		7,6
FALSE		C4 H8 Cl3	Full match	No results	No results	No results	No results	1,07	509,8096	510,8169	1,218	403992,7	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	403992,7	383739,3	6,3	5,4
FALSE		C36 H57 N	Full match	No results	No results	No results	No match	2,12	704,3751	705,3824	7,453	1138377	0	0	0	0	No matche	Multiple m	No MS2	[M+H]+1	767700,3	1138377	4,1	5
FALSE			No results	No results	No results	No results	No results		713,5947	714,6019	1,138	173480,3	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		173480,3		8,2
FALSE			No results	No results	No results	No results	No results		109,5113	110,5186	7,574	1428641	0	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	1126706	1428641	7,2	5,5
FALSE			No results	No results	No results	No results	No results		191,5411	192,5484	1,953	270180,3	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		270180,3		7,1
FALSE		C5 H14 O8	Full match	No results	No results	No results	No results	-2,34	264,0158	265,0231	1,957	337669,4	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	260914,8	337669,4	6	6
FALSE			No results	No results	No results	No results	No results		293,8712	294,8784	1,083	264785,2	0	0	0	0	No matche	No matche	DDA for pr	[M+H]+1	264785,2	210914,3	7,1	7,1
FALSE		C5 H8 Cl N	Full match	No results	No results	No results	No results	3,67	274,9526	275,9598	1,161	267580,3	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	267580,3	241675,8	7,6	8,2
FALSE			No results	No results	No results	No results	No results		723,787	724,7943	1,093	181609,6	0	0	0	0	No matche	No matche	No MS2	[M+H]+1	181609,6	157018,8	7,6	7,1
FALSE		C20 H25 N	Full match	No results	No results	No match	No results	0,11	419,1515	420,1588	5,791	370846	5	0	0	0	No matche	No matche	No MS2	[M+H]+1	338768,9	370846	7,1	7,6
FALSE			No results	No results	No results	No results	No results		294,2236	295,2309	7,341	444215,6	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		444215,6		4,7
FALSE		C6 H3 Cl O	Full match	No results	No results	No results	No results	2,28	413,8611	414,8684	1,115	190472,2	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		190472,2		7,6
FALSE		C3 H3 N3 C	Full match	No results	No results	No results	No results	1,93	286,8817	287,889	0,305	95028,9	0	0	0	0	No matche	No matche	No MS2	[M+H]+1		95028,9		5,4
FALSE		C7 H19 N4	Full match	No results	No results	No match	No match	4,17	238,1205	239,1278	1,009	428411	15	0	0	0	No matche	Multiple m	No MS2	[M+H]+1		428411		4,7
FALSE			No results	No results	No results	No results	No results		80,52458	81,53185	0,978	585777,9	0	0	0	0	No matche	No matche	DDA for pr	[M+H]+1		585777,9		4,7
FALSE		C4 H15 N6	Full match	No results	No results	No match	No results	1,88	306,0695	307,0768	1,393	468758,3	1	0	0	0	No matche	No matche	No MS2	[M+H]+1	420074,1	468758,3	4,1	4,1
FALSE			No results	No results	No results	No results	No results		1278,697	640,356	1,088	263945,2	0	0	0	0	No matche	No matche	No MS2	[M+2H]+2		263945,2		7,1
FALSE	Diethyl phthalate	C12 H14 O	Full match	No results	No results	Full match	Partial mat	0,12	222,0892	223,0965	7,368	801996	64	0	0	0	No matche	Multiple m	No MS2	[M+H]+1	801996	754958,8	5,2	5,2
FALSE	2-Isoacpryloyl-3																							

FALSE				No results	No results	No results	No results	No results	738,602	739,6093	1,145	177883,1		0	0	0	No matche	No matche	No MS2	[M+H]+1	177883,1		7,6		
FALSE	(1R,2R,6S,7S,8R,10S,11S,12R,16R,18R)-6,7-D	C30 H40 O	Full match	No results	No results	No results	Full match	Not the top	-4,38	528,27	529,2773	7,486	1114453		2	0	0	No matche	Multiple m	No MS2	[M+H]+1	743228,7	1114453	4,7	4,5
FALSE				No results	No results	No results	No results	No results		285,8105	286,8178	1,144	227184,5		0	0	0	No matche	No matche	No MS2	[M+H]+1	227184,5	195511,9	7,6	7,1
FALSE				No results	No results	No results	No results	No results		653,6204	654,6276	1,144	243634,9		0	0	0	No matche	No matche	No MS2	[M+H]+1		243634,9		7,1
FALSE	Lauric acid	C12 H24 O	Full match	No results	No results	Full match	Partial mat		-0,52	200,1775	201,1848	7,338	1154028		44	0	0	No matche	Multiple m	No MS2	[M+H]+1	1154028	917076,9	4,5	3,4
FALSE	Ethyl NN-Dimethyloxamate	C6 H11 N C	Full match	No results	No results	Full match	Full match		0,57	145,074	146,0813	1,51	92901,2		29	0	0	Multiple m	No matche	DDA for pri	[M+H]+1	92901,2		8,2	
FALSE	NPPB	C16 H16 N	Full match	No results	No results	Full match	Partial mat		0,22	300,1111	301,1184	4,979	451495,6		7	0	0	No matche	Multiple m	No MS2	[M+H]+1	395551,7	451495,6	6,8	7,4
FALSE	Naphthacemycin C2	C33 H31 Cl	No results	No results	No results	No results	Full match		-3,84	606,1633	607,1706	1,377	345874,8		0	0	0	No matche	Single mat	No MS2	[M+H]+1	345874,8	293071,3	7,1	4,3
FALSE		C7 H21 N4	Full match	No results	No results	No match	No match		4,87	208,1463	209,1536	7,357	7086157		42	0	0	No matche	Multiple m	DDA for pri	[M+H]+1			4	
FALSE		C3 H Br Cl	Full match	No results	No results	No results	No results		1,88	485,651	486,6583	1,175	257062,2		0	0	0	No matche	No matche	No MS2	[M+H]+1	257062,2	188072,5	7,1	7,1
FALSE		C7 H N6 O5	Full match	No results	No results	No results	No results		0,42	341,9223	342,9296	1,078	360141,7		0	0	0	No matche	No matche	DDA for pri	[M+H]+1	339858,3	360141,7	7,1	6
FALSE		C23 H36 N	Full match	No results	No results	No match	No match		3,46	484,2438	485,251	7,498	1034483		4	0	0	No matche	Multiple m	No MS2	[M+H]+1	774092,2	1034483	4,1	5
FALSE		C15 H20 P2	Full match	No results	No results	No results	No results		-4,38	262,1029	263,1102	3,21	260006,6		1	0	0	No matche	No matche	No MS2	[M+H]+1	252072,5	260006,6	7,1	7,1
FALSE				No results	No results	No results	No results			764,5649	765,5721	1,144	148141,7		0	0	0	No matche	No matche	No MS2	[M+H]+1	148141,7		8,2	
FALSE		C59 H88 N	Full match	No results	No results	No results	No results		-0,33	1029,585	515,7997	7,393	846563,5		0	0	0	No matche	Single mat	No MS2	[M+2H]+2	846563,5	810811,5	4,5	5,8
FALSE		C2 H3 N6 C	Full match	No results	No results	No results	No results		-1,66	174,0052	175,0125	0,306	178016,5		0	0	0	No matche	No matche	No MS2	[M+H]+1		178016,5		4,3
FALSE		C5 H11 N2	Full match	No results	No results	No results	No results		1,46	210,0409	211,0481	1,235	287439,7		0	0	0	No matche	No matche	No MS2	[M+H]+1	277477,1	287439,7	7,6	6
FALSE		C11 H7 Cl	Invalid ma	No results	No results	No results	No results		-5,07	314,9506	315,9579	1,159	265790,2		0	0	0	No matche	No matche	No MS2	[M+H]+1	265790,2	197934,6	7,1	8,2
FALSE				No results	No results	No results	No results			645,0951	646,1023	1,551	369268,8		0	0	0	No matche	No matche	No MS2	[M+H]+1	365521,1	369268,8	1,6	7,1
FALSE		C5 H14 N9	Full match	No results	No results	No results	No match		-1,06	247,1056	248,1129	1,896	318802,2		4	0	0	Single mat	Single mat	No MS2	[M+H]+1	251723,4	318802,2	7,6	6
FALSE		C13 H10 O	Full match	No results	No results	No results	No results		-1,03	437,9736	438,9809	2,143	1005041		0	0	0	No matche	No matche	No MS2	[M+H]+1	1005041	647945,7	5,5	6,8
FALSE	Caproic anhydride	C12 H22 O	No results	No results	No results	Full match	Full match		0,92	214,1571	215,1644	1,491	91674,9		27	0	0	Single mat	Multiple m	No MS2	[M+H]+1		91674,9		7,6
FALSE		C20 H24 P2	Full match	No results	No results	No results	No results		-3,86	326,1341	327,1413	6,983	2660059		3	0	0	No matche	No matche	No MS2	[M+H]+1	2453630	2660059	4,2	4,2
FALSE				No results	No results	No results	No results			191,9027	192,91	1,105	483612,4		0	0	0	No matche	No matche	No MS2	[M+H]+1	483612,4	466871,9	4,1	3,6
FALSE		C11 H28 N	Full match	No results	No results	No match	No match		-1,71	356,1836	357,1909	6,969	4242171		4	0	0	No matche	Single mat	No MS2	[M+H]+1		4242171		4,2
FALSE		C2 H3 Br2	Full match	No results	No results	No results	No results		2,65	647,6297	648,6359	1,142	195239,7		0	0	0	No matche	No matche	No MS2	[M+H]+1	174171	195239,7	7,1	8,2
FALSE				No results	No results	No results	No results			567,5721	568,5794	1,175	268524,1		0	0	0	No matche	No matche	No MS2	[M+H]+1	268524,1	257237,1	7,1	7,6
FALSE		C7 H8 N2 C	Full match	No results	No results	No match	No results		-0,41	248,028	249,0352	1,139	419111,8		4	0	0	No matche	No matche	DDA for pri	[M+H]+1	419111,8	415302,7	4,7	7,4
FALSE		C9 H4 N6 C	Full match	No results	No results	No results	No results		2,11	497,8333	498,8405	1,084	225919,6		0	0	0	No matche	No matche	DDA for pri	[M+H]+1	166824	225919,6	7,6	7,1
FALSE				No results	No results	No results	No results			623,7273	624,7346	1,129	157751,1		0	0	0	No matche	No matche	No MS2	[M+H]+1	157751,1		4,9	
FALSE				No results	No results	No results	No results			721,6071	722,6144	1,145	226539,4		0	0	0	No matche	No matche	No MS2	[M+H]+1	226539,4		7,1	
FALSE				No results	No results	No results	No results			153,8731	154,8803	1,155	512995,2		0	0	0	No matche	No matche	No MS2	[M+H]+1	482365,4	512995,2	4,1	4,7
FALSE		C2 H3 N5 C	Full match	No results	No results	No results	No results		-4,24	161,0001	162,0073	0,955	27261,2		0	0	0	No matche	No matche	No MS2	[M+H]+1		27261,2		7,1
FALSE	Diamyl Amylphosphonate	C15 H33 O	No results	Invalid ma	No results	Full match	No results		0,39	292,2168	293,2241	1,554	127158		1	2	0	No matche	No matche	DDA for pri	[M+H]+1		127158		4,9
FALSE	1,2-Dihydropyrimidine	C4 H6 N2	Full match	No results	No results	Full match	No results		1,07	82,05319	83,06046	0,308	184984,5		8	0	0	No matche	No matche	No MS2	[M+H]+1	184984,5		6,5	
FALSE		C2 H5 N2 C	Full match	No results	No results	No results	No results		2,49	151,9991	153,0064	0,99	324371,8		0	0	0	No matche	No matche	DDA for pri	[M+H]+1	324371,8		4,3	
FALSE		C9 H13 N4	Full match	No results	No results	No results	No results		-4,16	270,0342	271,0415	3,957	252012,2		2	0	0	No matche	No matche	No MS2	[M+H]+1	206431,6	252012,2	7,6	7,6
FALSE		C4 H14 N7	Full match	No results	No results	No match	No results		4,14	255,0855	256,0928	1,957	199653,9		1	0	0	No matche	No matche	No MS2	[M+H]+1	199653,9	188273,3	8,2	4,9
FALSE				No results	No results	No results	No results			109,5113	110,5186	0,305	72827,63		0	0	0	No matche	No matche	No MS2	[M+H]+1		72827,63		7,6
FALSE				No results	No results	No results	No results			587,8218	588,829	1,112	136991,9		0	0	0	No matche	No matche	No MS2	[M+H]+1	136991,9		8,2	
FALSE				No results	No results	No results	No results			770,3448	771,3521	1,098	161807,4		0	0	0	No matche	No matche	No MS2	[M+H]+1	161807,4		7,6	
FALSE		C4 H15 N1	Full match	No results	No results	No results	No match		4,64	266,1129	267,1202	1,119	838594,7		4	0	0	No matche	Single mat	DDA for ori	[M+H]+1	838594,7	723948,8	4,5	0,9
FALSE		C52 H75 N	Full match	No results	No results	No match	No results		-1,07	903,4603	452,7374	4,676	436358,2		2	0	0	No matche	No matche	No MS2	[M+2H]+2	409487,6	436358,2	7,4	7,4
FALSE	1-(1H-Indol-3-yl)ethanone	C10 H9 N C	Full match	No results	No results	Full match	Full match		0,63	159,0685	160,0758	4,134	579670		48	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	575127,1	579670	5,8	6,3
FALSE				No results	No results	No results	No results			577,8117	578,819	1,107	101731,1		0	0	0	No matche	No matche	No MS2	[M+H]+1		101731,1		5,4
FALSE		C3 H Br Cl3	Full match	No results	No results	No results	No results		-4,91	555,6361	556,6434	1,165	200893,9		0	0	0	No matche	No matche	No MS2	[M+H]+1	200893,9		8,2	
FALSE				No results	No results	No results	No results			1434,546	479,1893	6,42	541132		0	0	0	No matche	No matche	No MS2	[M+3H]+3	518702,6	541132	5,8	6,8
FALSE				No results	No results	No results	No results			810,7879	406,4012	0,993	664446		0	0	0	No matche	No matche	No MS2	[M+2H]+2		664446		6,3
FALSE		C6 H11 N2	Full match	No results	No results	No results	No results		1,21	142,0662	143,0734	4,133	343492,2		4	0	0	No matche	No matche	DDA for pri	[M+H]+1	281225,3	343492,2	7,1	7,6
FALSE	Succinic anhydride	C4 H4 O3	Full match	No results	No results	Full match	No results		0,75	100,0161	133,0496	1,249	661236,1		4	0	0	No matche	No matche	DDA for pri	[M+H+MeC]	661236,1		4,7	
FALSE		C10 H23 N	Full match	No results	No results	No match	No match		-3,08	251,1019	252,1092	3,358	771226,1		8	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	771226,1	762820,4	4,7	5,2
FALSE	dimethyl itaconate	C7 H10 O4	Full match	No results	No results	Full match	Full match		0,39	158,058	159,0653	1,51	134046,6		24	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1		134046,6		8,2
FALSE		C H4 Cl O4	Full match	No results	No results	No results	No results		3,99	209,8986	210,9058	1,123	284156,3		1	0	0	No matche	No matche	No MS2	[M+H]+1	284156,3	234200,8	7,6	7,1
FALSE		C18 H30 N	Full match	No results	No results	No match	No results		-3,74	419,1516	420,1589	5,9	352017,1		5	0	0	No matche	No matche	No MS2	[M+H]+1	295595,6	352017,1	7,1	7,6
FALSE		C26 H33 N	Full match	No results	No results	No match	No results		2,57	447,2468	448,2541	7,321	4943116		1	0	0	No matche	No matche	No MS2	[M+H]+1	4524389	4943116	4,2	3,2
FALSE	undec-10-ynoic acid	C11 H18 O	Full match	No results	No results	Full match	Partial mat		-0,07	182,1307	183,138	7,095	9907696		46	0	0	No matche	Multiple m	DDA for pri	[M+H]+1		9907696		4
FALSE				No results	No results	No results	No results			579,6875	580,6948	1,145	245080,8		0	0	0	No matche	No matche	No MS2	[M+H]+1	245080,8	202609,4	7,1	7,1
FALSE				No results	No results	No results	No results			663,6489	664,6562	1,141	265476,9		0	0	0	No matche	No matche	No MS2	[M+H]+1		265476,9		7,1
FALSE				No results	No results	No results	No results			1997,945	666,9888	1,098	247600,9		0	0	0	No matche	No matche	No MS2	[M+3H]+3	247600,9		7,1	
FALSE		C3 H2 O9 F	Full match	No results	No results	No results	No results		-0,34	275,8894	276,8967	0,34	420081,4		0	0	0	No matche	No matche	No MS2	[M+H]+1		420081,4		6,3
FALSE	Ceramide (d18:1/26:0)	C44 H87 N	No results	No results	No results	Full match	No results		3,17	677,6707	678,678														

FALSE	EDDA		C6 H12 N2	Full match	No results	No results	Full match	No results	0.39	176,0798	177,0871	0.306	103083,1	13	0	0	No matche	No matche	No MS2	[M+H]+1		103083,1		6,5
FALSE	Dodecylethanol amide		C14 H29 N	Full match	No results	No results	Full match	No results	0.06	243,2198	244,2271	6.366	1176891	3	0	0	No matche	No matche	DDA for pri	[M+H]+1	1043548	1176891	4,5	5
FALSE			C7 H6 N2 F	Full match	No results	No results	No results	No results	2.62	180,0011	181,0084	1.321	330127,8	1	0	0	No matche	No matche	No MS2	[M+H]+1	330127,8	327588,2	7,6	7,6
FALSE				No results	No results	No results	No results	No results		645,2974	646,3047	0.978	107400,4	0	0	0	No matche	No matche	No MS2	[M+H]+1	107400,4		4,9	
FALSE			C7 H4 O	Full match	No results	No results	No results	No results	0.26	104,0262	105,0335	4.83	392036,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	392036,8	357160,6	6	7,1
FALSE				No results	No results	No results	No results	No results		749,7781	750,7854	1.112	125763,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	125763,5		7,6	
FALSE			C H Cl4 N2	Full match	No results	No results	No results	No results	-0.31	321,7953	322,8033	1.143	178935,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	178935,7		7,6	
FALSE				No results	No results	No results	No results	No results		683,5703	684,5776	1.145	212711,4	0	0	0	No matche	No matche	No MS2	[M+H]+1		212711,4		7,1
FALSE				No results	No results	No results	No results	No results		243,7795	244,7868	1.15	265010,3	0	0	0	No matche	No matche	No MS2	[M+H]+1		265010,3	7,6	6
FALSE	n-butyl methacrylate		C8 H14 O2	Full match	Invalid ma	No results	Full match	Partial mat	0.05	142,0994	143,1067	1.546	6001657	98	3	0	No matche	Single mati	DDA for pri	[M+H]+1	2899772	6001657	3,2	4
FALSE			C6 H8 N8 C	Full match	No results	No results	No match	No results	0.49	256,067	257,0743	1.365	428482,9	5	0	0	No matche	No matche	No MS2	[M+H]+1	396763,2	428482,9	7,4	4,7
FALSE				No results	No results	No results	No results	No results		1361,288	681,6511	1.139	148105,3	0	0	0	No matche	No matche	No MS2	[M+2H]+2	148105,3		7,6	
FALSE				No results	No results	No results	No results	No results		797,4096	798,4168	1.175	195508,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	168195,1	195508,7	7,6	7,6
FALSE				No results	No results	No results	No results	No results		76,49314	77,50042	0.303	84010,36	0	0	0	No matche	No matche	No MS2	[M+H]+1		84010,36		7,1
FALSE			C47 H82 O	Full match	No results	No results	No results	No results	-0.69	902,5241	452,2694	7.401	555217,6	0	0	0	No matche	No matche	No MS2	[M+2H]+2		555217,6		4,1
FALSE			C40 H79 N	Full match	No results	No results	No results	No match	-2.95	788,4885	395,2515	6.745	644306,8	0	0	0	No matche	Single mati	No MS2	[M+2H]+2	644306,8	500356,2	3	5,2
FALSE				No results	No results	No results	No results	No results		283,2595	284,2666	1.176	305716	0	0	0	No matche	No matche	No MS2	[M+H]+1	305716		6,5	
FALSE	5-Oxidanylid-5-oxidanylideneorvalylthreon		C9 H15 N2	No results	No results	No results	Full match	No results	0.47	247,0931	248,1004	1.502	82121,24	2	0	0	No matche	No matche	No MS2	[M+H]+1		82121,24		5,4
FALSE			C7 H15 Br I	Full match	No results	No results	No match	No results	-4.25	346,0109	347,0182	1.383	360261,4	2	0	0	No matche	No matche	No MS2	[M+H]+1	360261,4		7,6	
FALSE			C5 H Br Cl I	Full match	No results	No results	No results	No results	-0.53	665,7087	666,7159	1.13	161097,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	161097,5		7,6	
FALSE				No results	No results	No results	No results	No results		225,8837	226,891	1.082	216436,9	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	196411,7	216436,9	4,3	7,1
FALSE				No results	No results	No results	No results	No results		779,6544	780,6617	1.136	176062,2	0	0	0	No matche	No matche	No MS2	[M+H]+1		176062,2		7,1
FALSE			C2 H2 Br Cl	Full match	No results	No results	No results	No results	-2.64	301,7383	302,7456	1.169	464285,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	464285,3	459934,3	6,8	2
FALSE			C12 H30 N	Full match	No results	No results	No results	No results	2.5	475,1916	476,1989	1.813	439213,5	0	0	0	No matche	No matche	No MS2	[M+H]+1	439213,5	347748,2	7,4	7,1
FALSE	2-morpholinoacetic acid		C6 H11 N C	Full match	No results	No results	Full match	Full match	0.32	145,0739	146,0812	1.24	471933,2	29	0	0	Multiple m	No matche	No MS2	[M+H]+1	471933,2	396040,5	6,8	3,6
FALSE	3-AB		C7 H8 N2 C	Full match	No results	No results	Full match	Full match	0.21	136,0637	137,071	1.332	563753,4	22	0	0	Multiple m	No matche	No MS2	[M+H]+1	563753,4	537940,7	2,5	4,7
FALSE			C3 H5 Cl4 F	Full match	No results	No results	No results	No results	-1.01	637,6635	638,6708	1.144	125503	0	0	0	No matche	No matche	No MS2	[M+H]+1	125503		7,1	
FALSE	POBN		C10 H14 N	Full match	No results	No results	Full match	Full match	0.21	194,1056	195,1128	4.181	554881,8	37	0	0	Single mati	Single mati	No MS2	[M+H]+1	554881,8	506901	6,3	5,8
FALSE			C18 H24 N	Full match	No results	No results	No results	No matche	-2.38	332,1373	333,1446	6.153	442573,9	0	0	0	No matche	Multiple m	No MS2	[M+H]+1	391063,2	442573,9	7,1	5,2
FALSE			C8 H12 Cl F	Full match	No results	No results	No results	No results	-1.95	250,0269	251,0342	1.963	292807,8	0	0	0	No matche	No matche	No MS2	[M+H]+1	283288,3	292807,8	7,6	5,4
FALSE	2-Methoxy-6-nitrobenzonitrile		C8 H6 N2 C	Full match	No results	No results	Full match	No results	-0.41	178,0378	179,0451	1.961	205664	2	0	0	No matche	No matche	No MS2	[M+H]+1	205664	187414,7	7,6	8,2
FALSE			C5 H13 N6	Full match	No results	No results	No match	No match	4.3	236,0797	237,087	4.129	418138,9	7	0	0	Multiple m	Single mati	DDA for pri	[M+H]+1	418138,9	372974,7	5,2	6,5
FALSE	N-[3-[(4aS,7aS)-2-amino-4H,4aH,5H,7H-furo		C18 H16 F2	No results	No results	No results	Full match	No match	-3.74	390,0947	391,102	1.248	170353	12	0	0	No matche	Multiple m	No MS2	[M+H]+1		170353		7,6
FALSE			C37 H57 O	Full match	No results	No results	No match	No results	0.22	692,3691	693,3764	8.11	553771,3	1	0	0	No matche	No matche	No MS2	[M+H]+1	477939,6	553771,3	6,8	5,8
FALSE	locetamic acid		C12 H13 I3	No results	No results	No results	Full match	No results	-4.09	613,8035	614,8108	1.097	185718,1	2	0	0	No matche	No matche	No MS2	[M+H]+1	185718,1	179387,8	7,6	7,6
FALSE				No results	No results	No results	No results	No results		695,4691	696,4764	1.176	218924,9	0	0	0	No matche	No matche	No MS2	[M+H]+1	218924,9	193886,6	7,1	7,6
FALSE			C H Cl2 N4	Full match	No results	No results	No results	No results	0.03	233,8935	234,9008	1.127	196671,8	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	196671,8		7,1	
FALSE	N(1)-acetylspemidine		C18 H21 N3	No results	No results	No results	Full match	Full match	-0.55	187,1684	188,1756	1.155	194604,6	2	0	0	Multiple m	No matche	No MS2	[M+H]+1	194604,6	191607,8	6,5	5,4
FALSE				No results	No results	No results	No results	No results		647,6922	648,6995	1.139	173992,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	173992,7		7,6	
FALSE	8,8'-Ethane-1,2-diylbis(1,3-dimethyl-3,7-dihy		C16 H18 N	No results	No results	No results	Full match	No result	-4.34	386,1434	387,1507	1.592	620399,1	1	0	0	No matche	No matche	No MS2	[M+H]+1	620399,1	416083	3	6,8
FALSE	[Similar to: (1R,2R,5S,8S,9S,10R,11R,12S)-5,1		C2 H2 N4 F	Full match	Invalid ma	No results	No match	No results	-4.16	143,9749	144,9822	0.337	184436,3	1	1	0	No matche	No matche	DDA for pri	[M+H]+1		184436,3		6,5
FALSE				No results	No results	No results	No results	No results		111,0159	112,0232	1.022	269503,1	0	0	0	No matche	No matche	DDA for pri	[M+H]+1	186964	269503,1	3,3	5,4
FALSE	β-Alanyl-L-histidyl-D-lyeryl-L-histidine		C18 H26 N	No results	No results	No results	Full match	No results	-2.4	450,1965	451,2037	1.543	506906,2	2	0	0	No matche	No matche	No MS2	[M+H]+1	206775,9	506906,2	7,1	2
FALSE				No results	No results	No results	No results	No results		595,5258	596,5331	1.177	247927,3	0	0	0	No matche	No matche	No MS2	[M+H]+1	247927,3	155893	7,1	7,1
FALSE			C4 H2 O10	Full match	No results	No results	No results	No results	-0.21	303,8843	304,8916	0.34	306248	0	0	0	No matche	No matche	No MS2	[M+H]+1		306248		4,9
FALSE	hymecromone		C10 H8 O3	Full match	No results	No results	Full match	Full match	0.03	176,0474	177,0546	7.367	599767,5	23	0	0	Multiple m	Multiple m	No MS2	[M+H]+1		599767,5		5,2
FALSE				No results	No results	No results	No results	No results		655,7988	656,806	1.093	237987	0	0	0	No matche	No matche	No MS2	[M+H]+1		237987		7,1
FALSE				No results	No results	No results	No results	No results		652,6622	653,6694	1.135	162335,4	0	0	0	No matche	No matche	No MS2	[M+H]+1		162335,4		7,6
FALSE			C11 H28 N	Full match	No results	No results	No match	No match	-1.79	356,1836	357,1908	7.159	593987,1	4	0	0	No matche	Single mati	No MS2	[M+H]+1	593987,1	1738683	5,1	3,9
FALSE	Pivagabine		C9 H17 N C	No results	No results	No results	Full match	Full match	0.14	187,1209	188,1282	1.815	465938,9	14	0	0	Single mati	No matche	No MS2	[M+H]+1	465938,9	411155,9	1,4	6,8
FALSE			C9 H19 N6	Full match	No results	No results	No match	No results	2.82	370,1012	371,1085	1.925	360231,9	1	0	0	No matche	No matche	No MS2	[M+H]+1	324428,7	360231,9	4,9	7,1
FALSE	Neomastoidin A		C25 H45 N	Full match	No results	No results	No results	Full match	0.11	455,3247	456,332	6.831	378180,4	0	0	0	No matche	Single mati	No MS2	[M+H]+1	367957,4	378180,4	8,2	7,6
FALSE	DL-Thyroxine		C15 H11 I4	No results	No results	No results	Full match	Full match	0.29	776,6869	777,6942	6.587	339011,8	29	0	0	Single mati	No matche	No MS2	[M+H]+1	336995	339011,8	7,6	8,2
FALSE	L-(-)-Leucine		C6 H13 N C	Full match	No results	No results	Full match	Full match	0.53	131,0947	132,102	1.013	541963,3	52	0	0	Multiple m	No matche	No MS2	[M+H]+1		541963,3		6,8
FALSE			C42 H85 N	Full match	No results	No results	No results	No results	0.19	691,6705	692,6777	1.136	220595,4	0	0	0	No matche	No matche	No MS2	[M+H]+1	220595,4		6,5	
FALSE				No results	No results	No results	No results	No results		393,696	394,7033	1.173	263635,4	0	0	0	No matche	No matche	No MS2	[M+H]+1		263635,4		7,6
FALSE				No results	No results	No results	No results	No results		495,8523	496,8596	1.025	158395,8	0	0	0	No matche	No matche	No MS2	[M+H]+1		158395,8		7,6
FALSE				No results	No results	No results	No results	No results		711,5774	712,585	1.147	183461,8	0	0	0	No matche	No matche	No MS2	[M+H]+1		183461,8		7,6
FALSE				No results	No results	No results	No results	No results		181,8948	182,902	1.119	551758,7	0	0	0	No matche	No matche	No MS2	[M+H]+1	551758,7	185888,7	3,6	6
FALSE				No results	No results	No results	No results	No results		679,6227	680,6299	1.145	199735	0	0	0	No matche	No matche	No MS2	[M+H]+1		199735		7,1
FALSE	4,7,10-TRIOXA-1,13-TRIDECANEDIAMINE		C10 H24 N	Full match	No results	No results	Full match	No results	0.29	220,1788	221,186	1.31	282811,2	2	0	0	No matche	No matche	No MS2	[M+H]+1	241184,8	282811,2	7,6	8,2
FALSE	2,4-Nonadien-1-al		C9 H14 O	Full match	Invalid ma	No results	Full match	Full match																



FALSE	Pentane-1,5-dithiol	C5 H12 S2	Full match	No results	No results	Not the top	No match	3,37	136,0385	137,0458	2,705	760614,8	12	0	0	0	Multiple m	No match	No MS2	[M+H]+1	760614,8	4,1	
FALSE		C8 H4 Cl N	Full match	No results	No results	No results	No results	4,05	290,9265	291,9338	1,158	200211,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	200211,8	8,2	
FALSE	γ-Acetylenic gaba	C6 H9 N O2	Full match	No results	No results	Full match	Full match	0,1	127,0633	128,0706	1,855	18972733	25	0	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1	18972733	4	
FALSE		C33 H76 Cl	Full match	No results	No results	No results	No results	2,11	793,542	794,5493	1,139	206485,2	0	0	0	0	No match	No match	No MS2	[M+H]+1		206485,2	7,1
FALSE		C5 H6 N2 C	Full match	No results	No results	No results	No results	-4,41	174,0269	175,0342	4,755	618378,4	0	0	0	0	No match	No match	No MS2	[M+H]+1	594435,7	618378,4	6,8
FALSE	holmium chloride	C13 Ho	No results	No results	No results	Full match	No results	1,29	269,8372	270,8437	1,144	195144	1	0	0	0	No match	No match	DDA for pri	[M+H]+1	195144		7,6
FALSE			No results	No results	No results	No results	No results		363,1279	364,1352	1,965	204217,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	204217,7	200299,9	5,4
FALSE		C3 H N O9	Full match	No results	No results	No results	No results	-0,09	226,9372	227,9445	1,172	255990,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	255990,1	252469,7	7,6
FALSE		C6 H5 Cl N	Full match	No results	No results	No match	No results	-2,66	260,0054	261,0127	3,956	244167,8	2	0	0	0	No match	No match	No MS2	[M+H]+1		244167,8	7,6
FALSE			No results	No results	No results	No results	No results		114,9568	115,9641	0,34	190721,2	0	0	0	0	No match	No match	DDA for pri	[M+H]+1		190721,2	6,5
FALSE			No results	No results	No results	No results	No results		135,9623	136,9696	1,064	310594,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	310594,8	303515,2	7,1
FALSE		C23 H6 N2	Full match	No results	No results	No match	No match	-3,11	358,0367	359,044	1,338	339440,8	2	0	0	0	No match	Single mat	No MS2	[M+H]+1		339440,8	4,9
FALSE	NPYR	C4 H8 N2 C	Full match	No results	No results	Full match	No results	0,14	100,0637	101,071	1,502	75461,24	13	0	0	0	No match	No match	No MS2	[M+H]+1		75461,24	5,4
FALSE		C6 H12 Cl	Full match	No results	No results	No results	No results	3	367,9506	368,9579	1,202	393835,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	393835,6	327275,4	4,3
FALSE			No results	No results	No results	No results	No results		748,6309	749,6381	1,134	145135,9	0	0	0	0	No match	No match	No MS2	[M+H]+1	145135,9		7,6
FALSE	CHOLESTERYL ARACHIDATE	C47 H84 O	No results	No results	No results	Full match	No results	-4,74	680,6439	681,6512	1,14	177500,8	5	0	0	0	No match	No match	No MS2	[M+H]+1		177500,8	7,1
FALSE			No results	No results	No results	No results	No results		638,6632	639,6705	1,137	162344,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		162344,3	7,6
FALSE			No results	No results	No results	No results	No results		73,96813	74,9754	0,96	238425,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		238425,3	7,1
FALSE	Diethyl (E)-azodicarboxylate	C6 H10 N2	Full match	No results	No results	Full match	Full match	-0,08	174,064	175,0713	1,408	180525,6	14	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1		180525,6	7,1
FALSE	Nicotinamide	C6 H6 N2 C	Full match	No results	No results	Full match	Full match	0,29	122,0481	123,0553	2,523	1616961	11	0	0	0	Single mat	No match	No MS2	[M+H]+1	1616961	1472835	5
FALSE	Methyl 2,6-di-O-stearoyl-α-D-glucopyranoside	C43 H82 O	No results	No results	No results	Full match	No results	-4,92	726,5974	727,6047	1,142	137783,4	7	0	0	0	No match	No match	No MS2	[M+H]+1	131729,7	137783,4	7,6
FALSE			No results	No results	No results	No results	No results		487,6388	488,646	1,15	134696,2	0	0	0	0	No match	No match	No MS2	[M+H]+1		134696,2	7,6
FALSE			No results	No results	No results	No results	No results		735,6282	736,6355	1,136	178284,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		178284,8	6,5
FALSE			No results	No results	No results	No results	No results		775,8004	776,8077	1,092	186821,6	0	0	0	0	No match	No match	No MS2	[M+H]+1	186821,6		7,1
FALSE	Metalaxyl	C15 H21 N	Full match	No results	No results	Full match	Partial mat	1,61	279,1475	280,1548	4,704	303891,3	21	0	0	0	No match	Multiple m	No MS2	[M+H]+1		303891,3	
FALSE		C2 H7 O17	Full match	No results	No results	No results	No results	-0,28	395,8895	396,8968	1,223	33736,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	337336,2	333831	4,3
FALSE		C41 H58 N	Full match	No results	No results	No match	No match	-4,06	687,4137	688,421	8,109	529372,4	2	0	0	0	No match	Multiple m	DDA for pri	[M+H]+1	449604,4	529372,4	7,4
FALSE			No results	No results	No results	No results	No results		245,7767	246,784	1,151	293694,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	293694,5		4,9
FALSE		C6 H17 N4	Full match	No results	No results	No match	No match	4,94	192,115	193,1222	1,395	229412,5	74	0	0	0	No match	Multiple m	No MS2	[M+H]+1		229412,5	6,5
FALSE	(10E,17E)-3,25-Dioxia-11,14,17,31-tetraazate	C25 H26 N	Full match	No results	No results	Not the top	No match	-3,15	414,2043	415,2116	7,421	475532,8	12	0	0	0	No match	Multiple m	No MS2	[M+H]+1	475532,8	461485,7	4,7
FALSE			No results	No results	No results	No results	No results		203,9112	204,9185	1,109	148103,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		148103,8	7,6
FALSE	Thalassospiramide B2	C50 H79 N	Full match	No results	No results	No results	Full match	0,2	1001,569	501,7916	7,802	438543,6	0	0	0	0	No match	Single mat	DDA for ori	[M+2H]+2		438543,6	5,8
FALSE			No results	No results	No results	No results	No results		636,6875	637,6948	1,133	154895,6	0	0	0	0	No match	No match	No MS2	[M+H]+1		154895,6	8,2
FALSE			No results	No results	No results	No results	No results		699,5954	700,6027	1,145	150393,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	150393,8		7,6
FALSE		C30 H57 N	Full match	No results	No results	No match	No results	2,33	748,4014	749,4087	7,441	929086,6	1	0	0	0	No match	No match	No MS2	[M+H]+1		929086,6	5,5
FALSE	4-Nitroaniline	C6 H6 N2 C	Full match	No results	No results	Full match	Full match	0,36	138,043	139,0503	1,994	390525,5	33	0	0	0	Multiple m	Single mat	No MS2	[M+H]+1	339102,5	390525,5	7,6
FALSE	3-Hydroxy-3-phenylpropanoic acid	C9 H10 O3	Full match	Invalid ma	No results	Full match	Partial mat	0,26	166,063	167,0703	1,537	6551961	112	3	0	0	Multiple m	Multiple m	DDA for pri	[M+H]+1	6413414	6551961	3,5
FALSE		C41 H65 O	Full match	No results	No results	No match	No results	0,2	780,4215	781,4288	8,101	580951	3	0	0	0	No match	No match	No MS2	[M+H]+1	516655,9	580951	6,8
FALSE		C42 H86 N	Full match	No results	No results	No results	No results	-0,69	792,6507	397,3326	7,176	2826293	0	0	0	0	No match	No match	No MS2	[M+2H]+2	2826293		4,2
FALSE	Diethylpyrocarbonate	C6 H10 O5	Full match	No results	No results	Full match	Full match	0,22	162,0529	163,0601	3,176	6784657	49	0	0	0	Multiple m	No match	DDA for pri	[M+H]+1		6784657	4
FALSE		C2 H3 N3 C	Full match	No results	No results	No results	No results	-2,33	132,9943	134,0016	0,973	686234,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	218962	686234,1	6,5
FALSE		C H3 Br2 Cl	Full match	No results	No results	No results	No results	3,24	559,5838	560,5911	1,175	212366,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	212366,5		8,2
FALSE		C7 H15 O3	Full match	No results	No results	No match	No match	1,74	240,0238	241,0311	1,371	180019,4	5	0	0	0	Single mat	No match	No MS2	[M+H]+1	180019,4		6,5
FALSE		C8 H20 N8	Full match	No results	No results	No match	No match	-0,72	354,108	355,1153	6,881	1635873	1	0	0	0	No match	Multiple m	No MS2	[M+H]+1		1635873	4,5
FALSE	N-Acetyl-L-aspartic acid	C6 H9 N O5	Full match	No results	No results	Full match	Full match	0	175,0481	176,0554	1,981	461203,8	9	0	0	0	Multiple m	No match	No MS2	[M+H]+1	396377,6	461203,8	5,2
FALSE			No results	No results	No results	No results	No results		373,7201	374,7274	1,15	191401	0	0	0	0	No match	No match	No MS2	[M+H]+1		191401	7,1
FALSE			No results	No results	No results	No results	No results		1406,515	469,8456	6,294	355657,9	0	0	0	0	No match	No match	No MS2	[M+3H]+3	331280,4	355657,9	6,5
FALSE			No results	No results	No results	No results	No results		665,7352	666,7424	1,133	206005,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		206005,8	7,1
FALSE			No results	No results	No results	No results	No results		631,7164	632,7237	1,134	168972	0	0	0	0	No match	No match	No MS2	[M+H]+1		168972	7,6
FALSE	afegostat	C6 H13 N C	Full match	No results	No results	Full match	No results	0,2	147,0896	148,0969	2,231	592890,7	22	0	0	0	No match	No match	No MS2	[M+H]+1	592890,7	492281,3	5,8
FALSE		C8 H Cl3 N	Full match	No results	No results	No results	No results	0,48	497,7974	498,8046	1,199	268696,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	268696,2	239389	7,1
FALSE			No results	No results	No results	No results	No results		71,0028	72,01008	0,943	131776,2	0	0	0	0	No match	No match	DDA for pri	[M+H]+1	131776,2		7,6
FALSE			No results	No results	No results	No results	No results		1520,625	761,32	1,097	190335,3	0	0	0	0	No match	No match	No MS2	[M+2H]+2		190335,3	7,1
FALSE		C2 H3 Br N	Full match	No results	No results	No results	No results	0,31	624,6617	625,669	1,139	159566,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		159566,8	7,6
FALSE			No results	No results	No results	No results	No results		327,885	328,8922	0,341	184362,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		184362,8	7,1
FALSE		C36 H71 N	Full match	No results	No results	No match	No results	-0,48	741,5295	742,5368	1,148	160996,2	39	0	0	0	No match	No match	No MS2	[M+H]+1	160996,2		7,1
FALSE			No results	No results	No results	No results	No results		419,8932	420,9005	1,058	148306,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	141371,3	148306,8	7,1
FALSE	Hydroxyacetylaminofluorene	C15 H13 N	Full match	No results	No results	Full match	Full match	0,04	239,0946	240,1019	3,789	281375,3	24	0	0	0	Single mat	Multiple m	No MS2	[M+H]+1	279436,8	281375,3	7,6
FALSE	HAD	C16 H35 N	Full match	No results	No results	Full match	No results	0,06	241,277	242,2842	7,119	322758,9	6	0	0	0	No match	No match	No MS2	[M+H]+1		322758,9	4,9
FALSE	2-(Phosphonoxy)ethyl acrylate	C5 H9 O6 F	Full match	No results	No results	Not the top	No results	-4,14	196,0129	99,01371	7,231	4045275	3	0	0	0	No match	No match	DDA for ori	[M+2H]+2	4045275	249806,1	3,7
FALSE	[Similar to: N3,N4-Dimethyl-L-arginine; ΔMas]	C4 H6 N6 C	Full match	Invalid ma	No results	No match	No results	1,33	202,0453	203,0526	1,547	269679,8	2	1	0	0	No match	No match	DDA for pri	[M+H]+1		269679,8	6,5
FALSE	diphoxazide	C17 H18 N	Full match	No results	No results	Full match	Partial mat	0,17	298,1318	299,1391	6,402	409407,4	10	0	0	0	No match	Single mat	No MS2	[M+H]+1	360162,5	409407,4	6,5
FALSE	2-(4-Boc-piperazino)acetic acid	C11 H20 N	Full match	No results	No results	Full match	Partial mat	0,04	244,1423	245,1496	3,51	526216,3	7	0	0	0	No match	Multiple m	No MS2	[M+H]+1	526216,3	349906,1	6,3
FALSE		C2 H4 N6 C	Full match	No results	No results	No results	No results	-2,63	397,854	398,8613	1,197												

FALSE	ethylene adipate	C8 H12 O4	Full match	No results	No results	Full match	Partial match	-0,31	172,0735	173,0808	1,554	368779,1	35	0	0	0	No match	Multiple m DDA for pr	[M+H]+1	74320,29	368779,1	8,2	0,5		
FALSE		C4 H12 N3	Full match	No results	No results	No results	No results	1,37	181,0619	182,0692	3,956	283351,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		283351,9	7,6		
FALSE			No results	No results	No results	No results	No results		531,3165	532,3238	1,004	99737,15	0	0	0	0	No match	No match	No MS2	[M+H]+1		99737,15	4,9		
FALSE		C6 H9 N4 F	Full match	No results	No results	No results	No results	-0,69	230,0039	231,0111	1,347	343366,7	1	0	0	0	No match	No match	DDA for pr	[M+H]+1	326422,5	343366,7	7,1	4,3	
FALSE			No results	No results	No results	No results	No results		667,8313	668,8386	1,091	165853,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	165853,7		7,1		
FALSE	N-[3-[[5-Chloro-2-[(2-methoxy-4-(4-methyl-2,3-dinor-8-epi-prostaglandin F2α)-3-ethoxymethyl]-2-thioxo-4-oxa-2,4-diazepin-5-ylideneamino)propyl]amino]propanoate	C25 H27 Cl	No results	No results	No results	Full match	No results	3,75	494,1852	495,1924	1,399	341401,1	3	0	0	0	No match	No match	No MS2	[M+H]+1	341401,1		4,3		
FALSE			No results	No results	No results	No results	No results		684,6168	685,6241	1,142	149185,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		149185,9	7,1		
FALSE			No results	No results	No results	No results	No results		489,6366	490,6438	1,147	161480,7	0	0	0	0	No match	No match	No MS2	[M+H]+1		161480,7	7,1		
FALSE			No results	No results	No results	No results	No results		607,7081	608,7154	1,135	145392,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	145392,2		8,2		
FALSE		C5 H9 N3 C	Full match	No results	No results	No match	No results	-0,85	335,0082	336,0154	1,148	108948,8	1	0	0	0	No match	No match	No MS2	[M+H]+1		108948,8	8,2		
FALSE			No results	No results	No results	No results	No results		1259,644	630,8294	1,061	142386,7	0	0	0	0	No match	No match	No MS2	[M+2H]+2		142386,7	7,1		
FALSE	Cyclopentenone	C5 H6 O	Full match	No results	No results	Full match	No results	0,65	82,04192	83,04919	1,783	8589948	9	0	0	0	No match	No match	DDA for pr	[M+H]+1	8589948		4		
FALSE			No results	No results	No results	No results	No results		191,0871	192,0944	0,968	96081,06	0	0	0	0	No match	No match	No MS2	[M+H]+1	96081,06		6		
FALSE			No results	No results	No results	No results	No results		1279,693	640,8536	1,083	214111	0	0	0	0	No match	No match	No MS2	[M+2H]+2		214111	6,5		
FALSE			No results	No results	No results	No results	No results		349,2101	350,2174	7,024	2210250	0	0	0	0	No match	No match	No MS2	[M+H]+1		2210250	4,2		
FALSE		C7 H8 Cl3 F	Full match	No results	No results	No results	No results	-3,75	336,8982	337,9054	1,196	221377,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		221377,1	7,1		
FALSE			No results	No results	No results	No results	No results		550,8386	551,8459	1,055	143208,8	0	0	0	0	No match	No match	No MS2	[M+H]+1		143208,8	7,1		
FALSE	N-Crotonyl-α-ethylaminobutyric Acid Diethyl	C14 H26 N	Full match	No results	No results	Full match	No results	0,26	254,1995	255,2068	7,631	572977,7	1	0	0	0	No match	No match	No MS2	[M+H]+1		572977,7	5,8		
FALSE		C3 H12 N6	Full match	No results	No results	No match	No match	-3,47	196,0736	197,0808	1,411	118684	89	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	118684				
FALSE	(2E)-2-Cyano-N-(ethylcarbamoyl)-2-(methoxycarbonyl)-N-methyl-N-(2-methyl-2-oxo-1,2,3,4-tetrahydro-2H-pyridin-4-yl)acetamide	C17 H18 N4	Full match	No results	No results	Full match	Full match	0,15	198,0753	199,0826	3,333	463495,5	6	0	0	0	Single mat	No match	DDA for pr	[M+H]+1	432863,5	463495,5	6,3	5,2	
FALSE		C8 H5 H179 F	Full match	No results	No results	No results	No results	-0,03	1413,296	707,6553	1,133	128736,5	0	0	0	0	No match	No match	No MS2	[M+2H]+2		128736,5	7,1		
FALSE	Dyphylline	C10 H14 N4	Full match	No results	No results	Full match	No match	-4,93	254,1003	255,1075	1,349	261984,7	10	0	0	0	Multiple m	Single mat	No MS2	[M+H]+1	227407,5	261984,7	7,1	7,1	
FALSE			No results	No results	No results	No results	No results		581,7465	582,7537	1,131	140418,2	0	0	0	0	No match	No match	DDA for pr	[M+H]+1		140418,2	7,6		
FALSE	(1Z,5Z)-1,5-Cyclooctadiene	C8 H12	Full match	No results	No results	Full match	Partial match	0,11	108,0939	109,1012	1,856	10421699	11	0	0	0	No match	Single mat	No MS2	[M+H]+1	10421699		4		
FALSE			No results	No results	No results	No results	No results		1551,599	776,8066	1,088	194852,3	0	0	0	0	No match	No match	No MS2	[M+2H]+2		194852,3	6,5		
FALSE			No results	No results	No results	No results	No results		198,1189	199,1262	4,5	2445489	0	0	0	0	No match	No match	DDA for pr	[M+H]+1		2445489	4,8		
FALSE		C5 H8 N O5	Full match	No results	No results	No results	No results	1,51	193,0143	97,51443	0,309	442476,1	0	0	0	0	No match	No match	No MS2	[M+2H]+2	442476,1		4,1		
FALSE		C3 H11 N6	Full match	No results	No results	No match	No results	1,61	354,0178	355,0251	1,884	2344517	3	0	0	0	No match	No match	DDA for pr	[M+H]+1	874731,7	2344517	5,5	1	
FALSE			No results	No results	No results	No results	No results		704,6076	705,6149	1,142	117715,4	0	0	0	0	No match	No match	No MS2	[M+H]+1		117715,4	7,1		
FALSE	Caffeine	C8 H10 N4	Full match	No results	No results	Full match	Full match	0,21	194,0804	195,0877	1,387	336488,9	7	0	0	0	Single mat	Single mat	No MS2	[M+H]+1	336488,9		6		
FALSE			No results	No results	No results	No results	No results		721,5825	722,5898	1,141	107881,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		107881,9	8,2		
FALSE			No results	No results	No results	No results	No results		658,6081	659,6154	1,145	142694	0	0	0	0	No match	No match	No MS2	[M+H]+1		142694	7,6		
FALSE	Mesitol	C9 H12 O	Full match	No results	No results	Full match	Partial match	0,4	136,0889	137,0962	1,563	136623,6	70	0	0	0	No match	Single mat	No MS2	[M+H]+1	136623,6		6,5		
FALSE	Kynurenic acid	C10 H7 N C	Full match	No results	No results	Full match	Full match	0,14	189,0426	190,0499	4,418	471924,1	19	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	456269,3	471924,1	6,3	4,7	
FALSE	2,3-dinor-8-epi-prostaglandin F2α	C18 H30 O	Full match	No results	No results	Full match	Partial match	0,13	326,2094	327,2166	7,222	3648842	2	0	0	0	Multiple m	Multiple m	No MS2	[M+H]+1	3488405	3648842	3,7	4,2	
FALSE	3-ETHYL-2-THIOXO-4-OKAZOLIDINONE	C5 H7 N O2	No results	No results	No results	Full match	Full match	0,3	145,0198	146,0271	1,794	405866,9	3	0	0	0	Single mat	No match	No MS2	[M+H]+1	383008	405866,9	3,8	5,2	
FALSE		C37 H80 N	Full match	No results	No results	No results	No match	-1,6	730,569	731,5763	1,143	148307,6	0	0	0	0	No match	Single mat	No MS2	[M+H]+1		148307,6	7,6		
FALSE			No results	No results	No results	No results	No results		1245,371	623,6929	1,138	177489,1	0	0	0	0	No match	No match	No MS2	[M+2H]+2		177489,1	7,1		
FALSE		C6 H3 N O	Full match	No results	No results	No results	No results	0,69	105,0215	106,0288	1,007	122524,2	0	0	0	0	No match	No match	No MS2	[M+H]+1	122524,2	84577,14	0,5	5,4	
FALSE			No results	No results	No results	No results	No results		79,53243	80,5397	0,973	128351,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		128351,1	4,3		
FALSE	N-boc-1-azacyclopentan-2-one	C9 H15 N C	Full match	No results	No results	Full match	Full match	0,01	185,1052	186,1125	3,629	612506,7	23	0	0	0	Multiple m	No match	No MS2	[M+H]+1	612506,7	484150,3	4,7	5,2	
FALSE	2,6-Dimethylquinoline	C11 H11 N	Full match	No results	No results	Full match	No results	0,16	157,0892	158,0965	4,306	136077,1	26	0	0	0	No match	No match	DDA for pr	[M+H]+1	136077,1	1328972	3,9	5	
FALSE		C17 H30 O	Full match	No results	No results	No match	No match	-2,5	314,173	315,1803	7,145	7253694	11	0	0	0	No match	Multiple m	DDA for pr	[M+H]+1		7253694	4		
FALSE	4-(1-Carboxyethyl)-3-hydroxy-2-(3-methyl-2-oxo-1,2,3,4-tetrahydro-2H-pyridin-4-yl)acetamide	C20 H26 O	Full match	No results	No results	Full match	Partial match	0,3	426,1527	427,16	6,796	513013	1	0	0	0	No match	Multiple m	No MS2	[M+H]+1	347230,4	513013	7,6	5,8	
FALSE	EDDA	C6 H12 N2	Full match	No results	No results	Full match	No results	0,55	176,0798	177,0871	1,236	269638,1	13	0	0	0	No match	No match	No MS2	[M+H]+1	224712,6	269638,1	7,1	4,3	
FALSE		C10 H17 N	Full match	No results	No results	No match	No results	-0,05	247,0878	248,0951	3,837	268940,1	1	0	0	0	No match	No match	No MS2	[M+H]+1	268940,1	259879,4	7,6	7,6	
FALSE		C5 H6 N C	Full match	No results	No results	No match	No results	-1	239,0431	240,0503	3,24	548389,3	9	0	0	0	No match	No match	No MS2	[M+H]+1	548389,3	523891,1	5,2	5,8	
FALSE			No results	No results	No results	No results	No results		535,5698	536,577	1,174	241049	0	0	0	0	No match	No match	No MS2	[M+H]+1		241049	7,6		
FALSE			No results	No results	No results	No results	No results		1459,595	730,8049	1,055	170072,4	0	0	0	0	No match	No match	No MS2	[M+2H]+2		170072,4	4,3		
FALSE		C4 H9 Br N	Full match	No results	No results	No results	No results	0,93	534,866	535,8732	1,093	196586,3	0	0	0	0	No match	No match	No MS2	[M+H]+1	196586,3		7,1		
FALSE			No results	No results	No results	No results	No results		653,4847	654,492	1,177	181910,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	173683,8	181910,8	7,1	7,1	
FALSE			No results	No results	No results	No results	No results		1595,638	798,8261	1,072	187745,7	0	0	0	0	No match	No match	No MS2	[M+2H]+2		187745,7	7,6		
FALSE			No results	No results	No results	No results	No results		83,90404	84,91131	1,142	333219	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	283698,8	333219	4,3	4,9	
FALSE		C4 H8 N6 C	Full match	No results	No results	No match	No results	2,57	220,0562	221,0635	1,243	303904,2	4	0	0	0	No match	No match	No MS2	[M+H]+1	303904,2	283571,7	3,8	4,3	
FALSE		C2 H6 Cl2 F	Full match	No results	No results	No results	No results	-1,69	284,896	285,9033	1,173	212415,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		212415,3	7,1		
FALSE			No results	No results	No results	No results	No results		134,9698	135,9771	1,153	130150,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		130150,9	129377,1	7,6	7,6
FALSE			No results	No results	No results	No results	No results		117,0641	118,0714	1,827	154088,4	0	0	0	0	No match	No match	DDA for pr	[M+H]+1		154088,4	7,6		
FALSE			No results	No results	No results	No results	No results		640,7038	641,7111	1,135	154680,5	0	0	0	0	No match	No match	No MS2	[M+H]+1		154680,5		7,1	
FALSE		C12 H22 N	Full match	No results	No results	No results	No results	3,82	259,117	260,1242	1,65	416659,2	12	0	0	0	No match	No match	No MS2	[M+H]+1	376918,2	416659,2	7,1	6,3	
FALSE			No results	No results	No results	No results	No results		770,7736	771,7809	1,109	196673,2	0	0	0	0	No match	No match	No MS2	[M+H]+1		196673,2	4,9	6	
FALSE	2,2'-(Hexadecylimino)diethanol	C20 H43 N	Full match	No results	No results	Full match	No results	-0,33	329,3293	330,3366	7,184	358611,4	1	0	0	0	No match	No match	No MS2	[M+H]+1		358611,4		6,3	
FALSE		C4 H3 Cl N	Full match	No results	No results	No match	No results	0,47	249,95	250,9572	1,169	238235,2	1	0	0	0	No match	No match	No MS2	[M+H]+1	238235,2	230350,7	7,1	7,6	
FALSE		C5 H16 N5	Full match	No results	No results	No match	No results	2,34	273,0845	274,0917	1,634														

FALSE		C8 H23 Cl	Full match	No results	No results	No match	No results	1,35	321,0696	322,0769	3,245	342282,3	7	0	0	0	No match	No match	No MS2	[M+H]+1	342282,3		5,4	
FALSE		C12 H34 N	Full match	No results	No results	No match	No results	4,41	546,2117	547,219	7,35	449702,8	1	0	0	0	No match	Multiple m	No MS2	[M+H]+1	449702,8	425990,6	5,8	4,1
FALSE			No results	No results	No results	No results	No results		700,5925	701,5998	1,14	127979,5	0	0	0	0	No match	No match	No MS2	[M+H]+1		127979,5		7,6
FALSE			No results	No results	No results	No results	No results		609,6838	610,691	1,136	141558,6	0	0	0	0	No match	No match	No MS2	[M+H]+1		141558,6		7,1
FALSE	Benzaldehyde	C7 H6 O	Full match	No results	No results	Full match	Full match	0,21	106,0419	107,0492	3,682	2211094	3	0	0	0	Multiple m	No match	No MS2	[M+H]+1	2211094	1714479	4,2	3,9
FALSE			No results	No results	No results	No results	No results		117,0659	118,0732	1,825	88846,21	0	0	0	0	No match	No match	DDA for pr	[M+H]+1		88846,21		4,9
FALSE			No results	No results	No results	No results	No results		690,8592	691,8665	1,091	158386,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	158386,1		7,6	
FALSE			No results	No results	No results	No results	No results		705,6072	706,6145	1,143	133711,8	0	0	0	0	No match	No match	No MS2	[M+H]+1	133711,8		7,1	
FALSE	Glutaric acid	C5 H8 O4	Full match	No results	No results	Full match	Full match	-0,27	132,0422	133,0495	1,539	163436,1	23	0	0	0	Multiple m	No match	No MS2	[M+H]+1		163436,1		7,1
FALSE		C12 H16 O	Full match	No results	No results	No match	No results	-3,24	304,0785	305,0857	3,591	280028,1	5	0	0	0	No match	No match	No MS2	[M+H]+1		280028,1		7,6
FALSE	Lipovelutibol A	C38 H69 N	No results	No results	No results	No results	Full match	4,54	783,5142	784,5214	1,145	157678,5	0	0	0	0	No match	Single mat	No MS2	[M+H]+1		157678,5		7,1
FALSE			No results	No results	No results	No results	No results		623,6838	624,6911	1,135	134138,9	0	0	0	0	No match	No match	No MS2	[M+H]+1		134138,9		7,6
FALSE		C7 H16 O5	Full match	No results	No results	No match	No results	-2,74	242,0466	243,0539	0,982	135386,5	6	0	0	0	No match	No match	No MS2	[M+H]+1		135386,5		4,3
FALSE		C19 H48 N	Full match	No results	No results	No results	No results	-0,5	449,3717	450,379	6,837	408058,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	400154,6	408058,7	6,8	7,4
FALSE			No results	No results	No results	No results	No results		980,8171	981,8244	0,983	98441,26	0	0	0	0	No match	No match	No MS2	[M+H]+1		98441,26		4,9
FALSE		C29 H16 O	Full match	No results	No results	No match	No match	4,61	428,1068	429,1141	1,92	432049	1	0	0	0	No match	Single mat	No MS2	[M+H]+1	432049	391857,1	7,4	4,9
FALSE		C5 H3 N2 C	Full match	No results	No results	No results	No results	-0,91	359,8946	360,9019	1,078	261726,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	259809,3	261726,7	7,1	6
FALSE		C4 H10 N3	Full match	No results	No results	No match	No results	0,64	195,041	196,0483	1,151	143833,2	2	0	0	0	No match	No match	No MS2	[M+H]+1		143833,2		7,1
FALSE		C17 H29 N	Full match	No results	No results	No results	No results	0,45	644,1199	645,1272	1,371	207548	0	0	0	0	No match	No match	No MS2	[M+H]+1		207548		7,1
FALSE			No results	No results	No results	No results	No results		239,1733	240,1806	3,784	381743	0	0	0	0	No match	No match	No MS2	[M+H]+1		381743		4,9
FALSE		C10 H20 N	Full match	No results	No results	No match	No results	3,53	333,1326	334,1399	4,569	245908	13	0	0	0	No match	No match	No MS2	[M+H]+1		245908		7,6
FALSE			No results	No results	No results	No results	No results		679,3253	680,3326	1,083	221154,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		221154,1		6
FALSE		C45 H74 N	Full match	No results	No results	No results	No results	-1,13	714,5916	715,5989	1,146	162814,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	162814,7		7,1	
FALSE		C3 H10 N4	Full match	No results	No results	No results	No results	3,88	403,8923	404,8996	1,063	206300,7	0	0	0	0	No match	No match	No MS2	[M+H]+1		206300,7		7,1
FALSE			No results	No results	No results	No results	No results		525,5875	526,5947	1,175	238838,7	0	0	0	0	No match	No match	No MS2	[M+H]+1	238838,7	192986,4	4,3	7,6
FALSE		C3 H10 Cl	Full match	No results	No results	No results	No results	-3,49	264,0017	265,009	1,157	331355,9	1	0	0	0	No match	No match	DDA for pr	[M+H]+1		331355,9		7,1
FALSE			No results	No results	No results	No results	No results		611,8331	612,8404	1,102	229262,5	0	0	0	0	No match	No match	No MS2	[M+H]+1		229262,5		6
FALSE		C12 H12 N	Full match	No results	No results	No results	No results	2,54	408,0121	409,0194	2,351	642396,2	0	0	0	0	No match	No match	No MS2	[M+H]+1		642396,2		4,7
FALSE	APAZIQUONE	C15 H16 N	Full match	No results	No results	Full match	Partial mat	0,23	288,1111	289,1184	4,714	302342,2	6	0	0	0	No match	Multiple m	No MS2	[M+H]+1	277275,3	302342,2	7,1	4,9
FALSE			No results	No results	No results	No results	No results		613,585	614,5922	1,147	156652,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		156652,3		7,1
FALSE	3-Methylglutarylcarnitine	C13 H23 N	Full match	No results	No results	Not the top	No results	0,22	289,1526	290,1599	5,021	115507,1	4	0	0	0	No match	No match	No MS2	[M+H]+1	115507,1	1018887	3,4	4,5
FALSE	Di(2-cyanoethyl)amine	C6 H9 N3	Full match	No results	No results	Full match	No results	0,17	123,0797	124,0869	7,452	68977,25	13	0	0	0	No match	No match	No MS2	[M+H]+1		68977,25		8,2
FALSE		C2 H7 N2 P	Full match	No results	No results	No match	No results	-3,19	183,9537	184,961	0,31	744716,8	1	0	0	0	No match	No match	No MS2	[M+H]+1		744716,8		4,1
FALSE		C13 H38 N	Full match	No results	No results	No match	No results	-0,47	431,2732	432,2804	4,664	300947	1	0	0	0	No match	No match	No MS2	[M+H]+1	269408,7	300947	6	5,4
FALSE		C3 H7 N9	Full match	No results	No results	No match	No results	-2,41	169,082	170,0893	7,135	8752416	3	0	0	0	No match	No match	DDA for pr	[M+H]+1		8752416		4
FALSE	N-Acetyl-L-aspartic acid	C6 H9 N O5	Full match	No results	No results	Full match	Full match	0,49	175,0482	176,0554	0,346	386488,8	9	0	0	0	Multiple m	No match	No MS2	[M+H]+1		386488,8		4,9
FALSE			No results	No results	No results	No results	No results		710,7741	711,7814	1,116	119191,3	0	0	0	0	No match	No match	No MS2	[M+H]+1	119191,3		7,6	
FALSE	Erucamide	C22 H43 N	Full match	No results	No results	Full match	No results	0,16	337,3345	338,3418	7,791	693783,5	4	0	0	0	No match	No match	No MS2	[M+H]+1		693783,5		7,4
FALSE			No results	No results	No results	No results	No results		423,7563	424,7636	1,135	185891,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	185891,5		7,1	
FALSE		C5 H N8 O5	Full match	No results	No results	No match	No results	3,68	409,9094	410,9167	1,074	270440,5	1	0	0	0	No match	No match	No MS2	[M+H]+1		270440,5		6,5
FALSE		C2 H8 N5 C	Full match	No results	No results	No results	No results	-4,15	181,0357	91,52514	0,953	185837,7	0	0	0	0	No match	No match	No MS2	[M+2H]+2	185837,7		6,5	
FALSE	Leu-Gly-Gly	C10 H19 N	No results	No results	No results	Full match	No results	0,02	245,1376	246,1448	1,96	181760,6	9	0	0	0	No match	No match	No MS2	[M+H]+1		181760,6		7,6
FALSE	7-Chloro-4-piperazin-1-yl-quinoline	C13 H14 Cl	No results	No results	No results	Full match	No results	4,23	247,0887	248,096	1,958	148336,2	2	0	0	0	No match	No match	No MS2	[M+H]+1	148336,2		6	
FALSE			No results	No results	No results	No results	No results		383,7489	384,7561	1,143	174291,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		174291,1		7,1
FALSE		C4 H Br Cl	Full match	No results	No results	No results	No results	-4,15	471,687	472,6943	1,18	314713,1	0	0	0	0	No match	No match	No MS2	[M+H]+1	314713,1	272392,3	4,3	4,3
FALSE			No results	No results	No results	No results	No results		107,5146	108,5219	0,98	323556	0	0	0	0	No match	No match	No MS2	[M+H]+1		323556		4,3
FALSE			No results	No results	No results	No results	No results		131,0753	132,0826	3,24	200862,3	0	0	0	0	No match	No match	DDA for pr	[M+H]+1	200862,3		4,9	
FALSE			No results	No results	No results	No results	No results		769,5372	770,5445	1,148	144964,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	144964,5		7,6	
FALSE		C13 H32 N	Full match	No results	No results	No match	No match	2,49	406,1644	204,0895	4,137	256245,6	4	0	0	0	No match	Multiple m	No MS2	[M+2H]+2		256245,6		6
FALSE			No results	No results	No results	No results	No results		323,7934	324,8007	1,141	161837,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		161837,1		7,1
FALSE		C8 H8 N3 C	Full match	No results	No results	No match	No results	1,46	225,0307	226,0379	1,961	146233,6	1	0	0	0	No match	No match	No MS2	[M+H]+1		146233,6		8,2
FALSE		C8 H10 N2	Full match	No results	No results	No results	No results	0,04	230,0539	231,0612	2,009	297257,5	0	0	0	0	No match	No match	No MS2	[M+H]+1	297257,5		7,1	
FALSE		C H2 Br2 Cl	Full match	No results	No results	No results	No results	-3,72	603,5662	604,5735	1,178	158968,3	0	0	0	0	No match	No match	No MS2	[M+H]+1				7,1
FALSE		C3 H Cl2 N	Full match	No results	No results	No results	No results	-0,1	280,8977	281,905	1,166	183045,3	0	0	0	0	No match	No match	No MS2	[M+H]+1		183045,3		8,2
FALSE			No results	No results	No results	No results	No results		145,0457	146,0529	1,384	196015,1	0	0	0	0	No match	No match	No MS2	[M+H]+1		196015,1		6,5
FALSE	N-Acetyl-L-histidine	C8 H11 N3	Full match	No results	No results	Full match	Full match	0,16	197,0801	198,0874	1,703	263678,8	11	0	0	0	Single mat	No match	No MS2	[M+H]+1	235058,6	263678,8	3,8	7,6
FALSE		C6 H13 Cl	Full match	No results	No results	No results	No results	4,55	312,011	313,0183	1,166	210646	0	0	0	0	No match	No match	No MS2	[M+H]+1		210646		4,9
FALSE			No results	No results	No results	No results	No results		737,5589	738,5662	1,141	131861	0	0	0	0	No match	No match	No MS2	[M+H]+1		131861		7,6
FALSE		C5 H17 Cl	Full match	No results	No results	No match	No match	4,57	196,1212	197,1285	4,216	300750,3	9	0	0	0	No match	Multiple m	No MS2	[M+H]+1	287967,6	300750,3	6	4,9
FALSE			No results	No results	No results	No results	No results		80,50539	81,51266	0,948	120034,2	0	0	0	0	No match	No match	DDA for pr	[M+H]+1		120034,2		6,5
FALSE		C8 H3 Cl O	Full match	No results	No results	No results	No results	3,89	339,8954	340,9027	1,195	166090,6	0	0	0	0	No match	No match	No MS2	[M+H]+1		166090,6		7,6
FALSE	sulfacarbamide		No results	No results	No results	No results	No results		409,6703	410,6776	1,171	186617	0	0	0	0	No match	No match	No MS2	[M+H]+1		186617		8,2
FALSE		C7 H9 N3 C	Full match	No results	No results	Full match	No results	4,59	215,0375	216,0447	3,39	424192,4	3	0	0	0	No match	No match	No MS2	[M+H]+1	407305,5	424192,4	7,4	5,8
FALSE	Vinylloxirane	C4 H6 O	Full match	No results	No results	Full match	No results	0,43	70,04189	71,04917	1,547	222879,3												



	FALSO			No results	No results	No results	No results	No results		989,6821	495,8483	1,031	157966,1	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2	157966,1		7,1	
	FALSO			No results	No results	No results	No results	No results		117,5261	118,5334	1,025	115752,5	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1	115752,5		8,2	
	FALSO	Triallyl phosphite	C9 H15 O3	Full match	Invalid ma	No results	Full match	No results	2,28	202,0763	203,0836	1,228	137053,7	1	10	0		55,4	No matche	No matche	DDA for pri	[M+H] <sup>+</sup> 1		137053,7		4,3
	FALSO			No results	No results	No results	No results	No results		1148,74	575,3771	1,096	165216,4	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2	165216,4		7,1	
	FALSO		C3 H4 N4 C	Full match	No results	No results	No match	No results	2,05	223,9856	224,9929	1	62374,88	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1	62374,88		8,2	
	FALSO			No results	No results	No results	No results	No results		603,7372	604,7445	1,132	101668,1	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		101668,1		8,2
	FALSO		C3 H6 N4 C	Full match	No results	No results	No match	No results	0,11	226,0186	114,0166	7,549	795525,6	1	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2	795525,6		4,7	
	FALSO		C5 H N6 P	Full match	No results	No results	No results	No results	-1,12	175,9998	177,0071	1,358	252278,6	0	0	0			No matche	No matche	DDA for pri	[M+H] <sup>+</sup> 1		252278,6		6,5
	FALSO	Boc-Gly-ONp	C13 H16 N	No results	No results	No results	Full match	Full match	0,96	296,1011	297,1084	1,573	78071,36	12	0	0			Single matr	Multiple m	No MS2	[M+H] <sup>+</sup> 1	78071,36		4,9	
	FALSO			No results	No results	No results	No results	No results		1313,73	657,8724	1,086	182882,2	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2		182882,2		7,1
	FALSO	Dibenzylhydroxylamine	C14 H15 N	Full match	No results	No results	Full match	Partial mat	0,26	213,1154	214,1227	5,568	282940,1	13	0	0			No matche	Multiple m	No MS2	[M+H] <sup>+</sup> 1		282940,1		6
	FALSO		C8 H22 Br f	Full match	No results	No results	No results	No results	-1,64	513,9999	515,0072	1,24	331263,9	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1	331263,9		4,3	
	FALSO			No results	No results	No results	No results	No results		235,6007	236,608	7,397	219575,4	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		219575,4		5,4
	FALSO		C9 H15 N6	Full match	No results	No results	No results	No results	3,39	428,0179	429,0252	2,127	530687,1	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1	530687,1		4,1	
	FALSO		C11 H21 Cl	Full match	No results	No results	No results	No results	-2,7	348,0104	175,0125	0,304	130084,1	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2	130084,1		6	
	FALSO		C44 H81 N	Full match	No results	No results	No results	No results	-0,65	696,6194	697,6267	1,138	131337,4	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		131337,4		7,1
	FALSO			No results	No results	No results	No results	No results		1575,638	788,8261	1,096	186476,8	0	0	0			No matche	No matche	No MS2	[M+2H] <sup>+</sup> 2	186476,8		7,1	
	FALSO		C3 H2 Cl N	Full match	No results	No results	No results	No results	0,46	206,9441	207,9514	1,189	178109,2	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		178109,2		7,1
	FALSO		C14 H39 N	Full match	No results	No results	No results	No results	-4,03	463,2418	464,2491	7,036	2834697	0	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		2834697		4,2
	FALSO	(2-Dodecen-1-yl)succinic anhydride	C16 H26 O	Full match	No results	No results	Full match	Full match	0,32	266,1883	267,1956	7,349	2078939	18	0	0			Multiple m	Multiple m	No MS2	[M+H] <sup>+</sup> 1	2078939		4,2	
	FALSO	slaframine	C10 H18 N	Full match	No results	No results	Full match	Partial mat	0,15	198,1369	199,1441	7,632	541879,4	6	0	0			No matche	Multiple m	No MS2	[M+H] <sup>+</sup> 1		541879,4		7,4
	FALSO		C28 H41 N	Full match	No results	No results	No match	No results	4,65	539,3245	540,3318	7,87	424056,9	1	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		424056,9		6,8
	FALSO	chlorphthalidone	C8 H3 Cl O	No results	No results	No results	Full match	No results	4,59	181,9779	182,9852	0,971	134505,4	2	0	0			No matche	No matche	No MS2	[M+H] <sup>+</sup> 1		134505,4		4,3