	et 1 1				98.5				1.0	10 01 10 11	tieles involve involves. The first territories the involve involve the internal involves accessed
ags	Checked		Formula Annot. Sou Ann								ault Be Mass List N Mass List N MS2 Reference Area: JB10! Area: JB10! Peak Rating Peak Rating: JB10553_202503030 Multiple m No matche DDA for pr [M+H]+1 4094390 4162068 7.5 7.5
		Acetohydroxamic acid		0,78 75,03209 76,0		7	10 1		99,7	10	.,,
		Creatinine	C4 H7 N3 C Full match Full match No results Partial mat Full match	-0,35 113,0589 114,		1,342 1,03E+08	5 1		99,6	10 57.4	Single mat No matche DDA for pr [M+H]+1 1,03E+08 1,01E+08 8,4 8,4
		D-(+)-Pyroglutamic Acid	C5 H7 N O: Full match Full match No results Full match Full match	0,2 129,0426 130,	,	7	17 5		99,6	10 57,4	Multiple m No matche DDA for pr [M+H]+1 9400175 8542528 7,3 6,2
	FALSO	L-(-)-Methionine	C5 H11 N C Full match Full match No results Full match Full match	-0,26 149,051 150,			13 2			95,1	Multiple m No matche DDA for pr [M+H]+1 59182065 58736203 8,4 8,4
		L-(+)-Citrulline	CG U177 N.C. Full match Full match No results Full match Full match	0,04 175,0957 176			7 1			95,1	Single mat. No matche DDA for pr. [M+H]+1 22908237 21663172 9,5 9,5
		Acetyl-L-carnitine	C9 H17 N C Full match Full match No results Full match Full match	-1,08 203,1155 204,			10 1			68,5	Single mat. No matche DDA for pr. [M+H]+1 1,55E+08 1,53E+08 8,9 8,9
		Caffeine	C8 H10 N4 Full match Full match No results Full match Full match C9 H17 N C Full match Full match No results Full match Full match	-1,25 194,0801 195,		7	7 3			68,2	Single mat. Single mat. DDA for pr. [M+H]+1 1E+08 1,02E+08 9,5 9,5
		Acetyl-L-carnitine		-0,1 203,1157 204			10 1			67,9	Single mat(No matche DDA for pr([M+H]+1 24512950 29828226 6,7 7,3
	FALSO	Acetyl-L-carnitine	C9 H17 N C Full match Full match No results Full match Full match				10 1			67,7	Single mate No matche DDA for pre [M+H]+1 12818633 15358697 7,8 7,8
	FALSO	Valine	C5 H11 N C Full match Full match No results Full match Full match	-1,24 117,0788 118,			40 3		99	9,9	Multiple m No matche DDA for pri [M+H]+1 4,96E+08 4,89E+08 8,4 8,4
		DL-Carnitine	C7 H15 N C Full match Full match No results Full match Partial mat	-0,26 161,1052 162,			7 3			66,5	Multiple m Single mat (DDA for pr [M+H]+1 74164024 74207483 8,4 8,4
	FALSO	Lactamide	C3 H7 N O2 Full match Full match No results Not the to; Full match	0,21 89,0477 90,0	05497	1,193 42582384	19 3	0	98,9	9,9	Multiple m No matche DDA for pri [M+H]+1 42198896 42582384 7,3 8,4
	FALSO	L-Isoleucine	C6 H13 N C Full match Full match No results Not the to: 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 pri [M+H]+1 1,01E+08 88888057 5,7 6,2
	FALSO	L-Norleucine	C6 H13 N C Full match Full match No results Not the to: 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 pri [M+H]+1 4,78E+08 4,59E+08 8,4 8,4
	FALSO	L-Isoleucine	C6 H13 N C Full match Full match No results Not the tor 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
	FALSO	L-Pyroglutamic acid	C5 H7 N O: Full match Full match No results Full match Full match	0.1 129.0426 130.			17 2	0	98,6	9,9	Multiple m No matche DDA for pri [M+H]+1 18827421 8,9
		D-(-)-Glutamine	C5 H10 N2 Full match Full match No results Full match Full match	0,15 146,0692 147,			29 4	0		93,7 49,7	Multiple m No matche DDA for pre [M+H]+1 1,01E+08 8,9
		Paraxanthine	C7 H8 N4 C Full match Full match No results Full match Full match	-0.72 180.0646 181.			6 9	0		63,5 76	Multiple m No matche DDA for pr [M+H]+1 41304284 41991111 8,4 8,4
		D-(-)-Glutamine	C5 H10 N2 No match Invalid ma: No results No match No match	-280871 105.0426 106.			13 4			93,2 48,1	Multiple m No matche DDA for otl [M+H]+1 3423709 3253389 8,6 8,6
	FALSO	Kojic acid	C6 H6 O4 No match Invalid ma: No results No match No results	-16,73 142,0242 143,		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
	FALSO	Theobromine	C7 H8 N4 C Full match Full match No results Full match Full match	-0,4 180,0647 181,			6 9	0		98,9 62,5	Multiple m No matche DDA for pri [M+H]+1 19002510 20883247 7,8 8,9
	FALSO	Pipecolic acid	C6 H11 N C Full match Full match No results Full match Partial mat	0,26 129,079 130,		.,	54 4		97,8	9,9	Multiple m Multiple m DDA for pri [M+H]+1 4681244 4179992 7 5,3
								0			
		DL-Stachydrine	C7 H13 N C No match Invalid ma: No results No match No results	-223811 111,0684 144,			28 3	U	97,8	9,9	No matche No matche DDA for ot [M+H+Met] 33731160 33850351 8,4 8,4
	FALSO	Uric acid	C5 H4 N4 C Full match Full match No results Full match Full match	-0,8 168,0282 169,		-,,	4 1			92,2	Single mat(No matche DDA for pr([M+H]+1 1,45E+08 1,36E+08 8,4 8,4
	FALSO	L-Histidine	C6 H9 N3 C Full match Full match No results Full match Full match	-0,09 155,0695 156,			12 11			92,1 61,9	Multiple m No matche DDA for pri [M+H]+1 8804469 7983428 9,5 9,5
	FALSO	Uric acid	C5 H4 N4 C Full match Full match No results Full match Full match	-0,89 168,0282 169,		-,:	4 1		97,7	92	Single mat (No matche DDA for pr (M+H)+1 1,88E+08 1,9E+08 8,4 8,4
		D-(+)-Proline	C5 H9 N O7 Full match Full match No results Full match Full match	-0,06 115,0633 116,			30 2		97,5	9,9	Multiple m Single mat DDA for pr [M+H]+1 2,56E+08 2,53E+08 9,5 8,4
	FALSO	Indole-3-acetic acid	C10 H9 N C Full match Full match No results Full match Full match	-0,15 175,0633 176,			31 2		97,5	9,9	Multiple m Multiple m DDA for pri [M+H]+1 4442144 4584430 8 8
	FALSO	Triethyl phosphate	C6 H15 O4 Full match Full match No results Full match Full match	0,29 182,0709 183,	,	-,	4 1		97,2	9,9	Single mate No matche DDA for pre [M+H]+1 425105,6 448536,4 6,3 6,3
	FALSO	Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N: Full match Full match No results Full match No results	-0,74 292,0905 293,	3,0977	2,125 4,06E+08	3 1	. 0		90,6	No matche No matche DDA for pri [M+H]+1 4,06E+08 7,8
		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		98,7	No matche No matche DDA for pre [M+Na]+1 1,01E+08 7,8
		Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N. Full match Full match No results Full match No results	-1,6 292,0902 293,	3,0975	1,462 1,46E+10	3 1	0	97	98,6	No matche No matche DDA for pre [M+H]+1 1,46E+10 1,41E+10 8,4 8,4
	FALSO	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 1	0	97	58,3	Multiple m Single mat DDA for pr [M+H]+1 53041815 50972769 9,5 8,4
	FALSO	L-Pyroglutamic acid	C5 H7 N O: Full match Full match No results Full match Full match	0,21 129,0426 130,			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
	FALSO	Palmitoyl sphingomyelin	C39 H79 N. Not the to; Full match No results Full match No results	0,49 702,5679 703,			5 1		96,6	9,8	No matche No matche DDA for pri [M+H]+1 53546810 57806228 6,2 6,2
	FALSO	N3,N4-Dimethyl-L-arginine	C8 H18 N4 Full match Full match No results Partial mat Full match	0,04 202,143 203,	3.1503	1,548 7370631	8 1	. 0	96,5	98,5	Single matr No matche DDA for pr/ [M+H]+1 6749183 7370631 8,9 9,5
	FALSO	1-Aminocyclohexanecarboxylic acid	C7 H13 N C Full match Full match No results Partial mat Full match	0.22 143.0947 144.			27 2	0		55,7	Single mat Multiple m DDA for pr [M+H]+1 4590679 4278186 8 8
	FALSO	DL-α-Aminocaprylic acid	C8 H17 N C Full match Full match No results Full match Partial mat	0.32 159.126 160.	,	_,00	16 1			55,6	No matche Single mat DDA for pr [M+H]+1 1015393 1119045 7,2 8,3
		L-Tyrosine	C9 H11 N C Full match Full match No results Full match Partial mat	-0,87 181,0737 183	,	7	37 3			98,4 53,2	Multiple m Single mat DDA for pr [M+H]+1 2,18E+08 2,1E+08 9,5 9,5
		7	C5 H13 N C Full match Full match No results Partial mat Full match				17 1			9,8	
	FALSO	Choline			04,107				96,1		Single mat(No matche DDA for pri [M+H]+1 34261133 31993421 8,4 8,9
	FALSO	1-Methylhistidine	C7 H11 N3 Full match Full match No results Full match Full match	0,05 169,0851 170,		,	13 5		96,1	88	Multiple m No matche DDA for pri [M+H]+1 8508026 8275173 7,8 8,4
	FALSO	Phloroglucinol	C6 H6 O3 Full match Full match No results Partial mat Full match	-0,12 126,0317 123			24 6			87,9	Multiple m Multiple m DDA for pr [M+H]+1 47317585 4
	FALSO	7-Methylxanthine	C6 H6 N4 C Full match Full match No results Full match Full match	-0,05 166,0491 167,		.,	9 3		95,9	9,8	Multiple m No matche DDA for pri [M+H]+1 1004414 1022761 7,7 7,7
		DL-Tryptophan	C11 H12 N. Full match Full match No results Full match Partial mat	-1,08 204,0897 205,			32 4			87,6 44,6	Multiple m Multiple m DDA for pri [M+H]+1 2,63E+08 2,99E+08 9,5 9,5
		3-Acetyl-2,5-dimethylfuran		130447,2 156,0787 157,			14 9		94,7	9,7 46,2	No matche Multiple m DDA for otl [M+H]+1 10669419 10425168 4 5,1
	FALSO	DL-Homoserine	C4 H9 N O: Full match Full match No results Full match Full match	0,31 119,0583 120,			37 4	0		49,4	Multiple m No matche DDA for pri [M+H]+1 20527488 19810506 8,9 8,9
	FALSO	Maleic hydrazide	C4 H4 N2 C Full match Full match No results Partial mat Partial mat	0,27 112,0273 113,			12 3	0	94	9,7	Single mate Single mate DDA for pre [M+H]+1 1785913 1607252 7,7 7,2
	FALSO	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 mate Multiple m DDA for pre [M+H]+1 20365137 4
	FALSO	2-Mercaptoethanol	C2 H6 O S Full match Full match No results Not the to; Full match	-0,03 78,01393 79,0	02121	1,357 3,65E+08	3 1	. 0	93,8	9,7	Single mate No matche DDA for pre [M+H]+1 3,65E+08 4,6
	FALSO	NP-021074	C13 H20 O No match Invalid mas 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
	FALSO	N-Ethylglycine	C4 H9 N O. Full match Full match No results Not the tor Full match	0,04 103,0633 104,			35 8	0	93,2	9,7	Multiple m No matche DDA for pr. [M+H]+1 17995528 16561845 7,8 6,2
		DL-Arginine	C6 H14 N4 Full match Full match No results Full match Full match	-0,23 174,1116 175,			10 2	0		78,7	Multiple m No matche DDA for pri [M+H]+1 45831944 43566952 8,4 7,3
	FALSO	N,N-Dimethylaniline	C8 H11 N Full match Full match No results Partial mat Full match	0,18 121,0892 122,			46 10		93,1	9,7 48,1	Multiple m No matche DDA for pre [M+H]+1 77672731 84843803 6,2 6,2
	FALSO	Phloroglucinol	C6 H6 O3 Full match Full match No results Partial mat Full match	0,28 126,0317 12			24 7			76,9	Multiple m Multiple m DDA for pr [M+H]+1 14596962 15813251 4 4,6
	FALSO	N,N'-Diphenylguanidine	C13 H13 N. Full match Full match No results Partial mat No results	-0,21 211,1109 212,		4,936 4570455	0 3		92,3	75	No matche No matche DDA for pri [M+H]+1 4570455 4477253 8 8
		3-Methylxanthine	C6 H6 N4 C Full match Full match No results Partial mat Full match				9 3		92,2	9.6	
	FALSO	Decanovicarnitine	C17 H33 N Full match Full match No results Partial mat Full match	0,04 166,0491 167, -0.79 315.2407 316		.,	4 1			42,1	Multiple m No matche DDA for pr [M+H]+1 820202,3 841845 7,4 6,1 Single mat/ No matche DDA for pr [M+H]+1 39500046 41642668 9.5 8.4
				.,	-, -	.,					
	FALSO	L-Ergothioneine	C9 H15 N3 Full match Full match No results Full match Full match	0,16 229,0885 230,		-,	9 1			90,9	Single mat(No matche) DDA for pr([M+H]+1
	FALSO	Betaine	C5 H11 N C Full match Full match No results Partial mat Full match	-0,03 117,079 118,			40 3		91,4	9,6	Multiple m No matche DDA for pr [M+H]+1 46788134 44903028 7,8 7,8
	FALSO	Tributylamine	C12 H27 N Full match Full match No results Partial mat No results	0 185,2144 186,	, .	.,	7 4			38,8	No matche No matche DDA for pri [M+H]+1 1565873 1646698 7,7 7,7
		Acetylcholine	C7 H15 N C Full match Full match No results Partial mat Full match	0,56 145,1104 146,			32 1		90,7	9,5	Multiple m No matche DDA for pri [M+H]+1 3064911 3587324 5,3 5,3
		Acetyl-L-carnitine	C9 H17 N C Full match Full match No results Full match Full match	0,06 203,1158 204,			10 1		90,6	9,5	Single mat (No matche) DDA for pr [M+H]+1 1894972 1920311 9,1 8
		N,N-Dimethylaniline	C8 H11 N Full match Full match No results Partial mat Full match	0,12 121,0892 122,		.,	46 5		90,3	9,5	Multiple m No matche DDA for pri [M+H]+1 5878068 4545282 5,7 5,3
	FALSO	Diisobutylphthalate	C16 H22 O Full match Full match No results Full match Partial mat	-0,21 278,1518 279	9,159	0,316 3883976	27 5	0	90,1	36,9	Single mat Multiple m DDA for pr [M+H]+1 3883976 7,5
	FALSO	Palmitoylcarnitine	C23 H45 N Full match Full match No results Full match Full match	0,38 399,335 400,	,3423	7,292 1467205	2 1	. 0	90	9,5	Single mat(No matche DDA for pri [M+H]+1 1467205 1326599 6,6 8,3
	FALSO	Diphenylamine	C12 H11 N Full match Full match No results Full match Full match	-0,01 169,0892 170,			15 2	0	89,5	9,5	Multiple m No matche DDA for pre [M+H]+1 27244992 605198,8 3,5 5,8
	FALSO	L-Kynurenine	C10 H12 N. Full match Full match No results Full match Full match	-0,08 208,0848 209	9,092	3,7 10680564	19 1	. 0	88,7	85,6	Single mat(No matche DDA for pr [M+H]+1 10122170 10680564 8,4 8,4
		Crotonic acid	C4 H6 O2 No match Invalid mas No results No match No match	209336 104,0474 87,0	04409	3,221 13364449	32 1	0	88,3	9,4	Multiple m Single mat (DDA for otl [M+H-H2O 13364449 10919998 8,4 8,4
		Propionylcarnitine	C10 H19 N Full match Full match No results Full match Partial mat	-0,23 217,1314 218,		.,	5 1	. 0	88,2	35,4	Multiple m Multiple m DDA for pr [M+H]+1 5344596 5387918 8 8
		Cetrimonium	C19 H41 N Full match Full match No results Partial mat No results	0,05 283,3239 284,	,	-,	2 2		87,6	9,4 47,8	No matche No matche DDA for pri [M+H]+1 2820559 2812657 7,5 8
			C9 H7 N Full match Full match No results Not the tor Full match	1,23 129,058 130,			4 4		86,5	9,3	Multiple m No matche DDA for pr. [M+H]+1 752821,8 779551,9 6,8 7,4
		Imidazolelactic acid	C6 H8 N2 C Full match Full match No results Full match Full match	0,11 156,0535 157,			16 1	0		34,4	Multiple m No matche DDA for pr [M+H]+1 929921,5 1099284 5,5 2,3
			C13 H25 N Full match Full match No results Full match Full match	0,02 259,1784 260,			5 1	0	85,9	34,4	Single mat(No matche DDA for pri [M+H]+1 2684321 2858118 8 8
		4-Hydroxybenzaldehyde	C7 H6 O2 Full match Full match No results Partial mat Full match	0,02 259,1784 260,			10 1		84,9	9,2	Multiple m Single mat i DDA for pri [M+H]+1
		Ecgonine	C9 H15 N C Full match Full match No results Not the tor Full match				23 1			80.1	
			C6 H6 N4 C Full match Full match No results Not the tor Full match	0,13 185,1052 186,			8 2				
		1-Methyluric acid		-0,19 182,044 183,		0,0 000000,	-			33,2	Multiple m No matche DDA for pr [M+H]+1 861481,3 908038,7 8,3 8,3
			C8 H16 N2 Full match Full match No results Full match Full match	-0,05 188,1161 189,			20 6			58,8	Multiple m No matche DDA for pr [M+H]+1 3123630 3166216 8 8
		2-Aminoindan-2-carboxylic acid	C10 H11 N Full match Full match No results Partial mat Partial mat	0,02 177,079 178,			47 3		83,3	9,2	No matche Multiple m DDA for pri [M+H]+1 1228675 1252056 7,2 7,2
	FALSO	Hippuric acid	C9 H9 N O: Full match Full match No results Full match Partial mat	-0,03 179,0582 180,			27 1	. 0	83,1	9,2	Multiple m Single mat (DDA for pr [M+H]+1 2289752 2373929 7,5 7,5
	FALSO	Methyl palmitate	C17 H34 O No match Invalid ma: No results No match No match	-55501,9 255,2562 288,	3,2897	6,871 1935443	7 3	0		32,2	Single mat(No matche DDA for ot [M+H+Met 1707433 1935443 8,3 6,4
	FALSO	Methyl palmitate	C17 H34 O No match Invalid ma: No results No match No results	63001,75 287,2825 288,	3,2898	6,836 709002,9	2 3	0	83	32,2	No matche No matche DDA for pr [M+H]+1 615380 709002,9 7,4 6,8
		NP-004020	C17 H14 O No match Invalid mas No results No match No results	-20,73 314,0725 315,		1,816 1,05E+08	1 5	0		56,8	No matche No matche DDA for pri [M+H]+1 96724064 1,05E+08 4,6 5,7
			C8 H8 CI N No match Invalid ma: No results No results No results	-23,95 169,0254 170,		7 7	0 1		82,6	9,1	No matche No matche DDA for pri [M+H]+1 2849425 2976634 5,3 4,8
		Prolylleucine	C11 H20 N. Full match Full match No results Partial mat Partial mat	-0,03 228,1474 229,			6 3			9,1	Multiple m Multiple m DDA for pri [M+H]+1 8575989 8617912 7,8 7,8
			C11 H14 Cl No match Invalid ma: No results No results No results	-20,15 195,0776 196,			0 1			54,3	No matche No matche DDA for pri [M+H]+1 1543731 1562512 7,2 7,7
		1,5-Naphthalenediamine	C10 H10 N; Full match Full match No results Full match No results	0,5 158,0845 159,			19 12			52,2 65,6	No matche No matche DDA for pr [M+H]+1 526732,9 656201,3 6,3 8,5
			5°] C11 H15 N Full match Full match No results Partial mat Full match	-0,15 193,1103 194,			70 6		79,4	9	No matche no matche DDA for pro[M+H]+1
		TKK	C16 H33 N' No match Invalid ma: No results No match No results	10,63 375,2522 393			3 1			29,9	No matche No matche DDA for pro [M+NH4]+: 17463620 18370988 9,5 9,5
	FAISO				-5,200						1.00 material and material port for preprinted by 1.1700020 [10070000] [7,5] [7,5]
							1 4				
	FALSO	2-Amino-1,3,4-octadecanetriol N,N-Diisopropylethylamine (DIPEA)	C18 H39 N Full match Full match No results Full match Full match C8 H19 N Full match Full match No results Full match No results	-0,08 317,293 318, 0,24 129,1518 130,	3,3003	6,807 6200226	4 1 16 3	. 0	78,5 77,8	8,9 8,9 50,2	Single mati Single mati DDA for pri [M+H]+1 6028824 6200226 8,9 8,4 No matche No matche DDA for pri [M+H]+1 34593184 44164614 5,1 5,1

FA	ALSO	Benzothiazole	C7 H5 N S	Full match Full match No results	Full match No results	0,2	135,0143	136,0216	1,449 2	4862822	5	11	0 77,7	8,9	58,9	No matche No matche DDA for pri [M+H]+1	24862822	1682705	4	0,7
FA	ALSO	N,N-Diisopropylethylamine (DIPEA)	C8 H19 N	Full match Full match No results	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 pri [M+H]+1	4776793		5,3	
FA	ALSO	N3,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 mate No matche DDA for pre [M+H]+1	1687236	1746773	7,2	7,2
FA	ALSO .	Adenosine	C10 H13 N	Not the to: Full match No results	Full match Partial mat	0.07	267.0968	268,1041	3,299	946828	12	1	0 74,8			Multiple m Single mate DDA for pre [M+H]+1	946828	846085.3	6,1	6,6
		Methyl indole-3-acetate	C11 H11 N	Full match Full match No results	Not the tor Full match	-0.27	189.0789			2051266	29	1	0 74,7	8,7		Multiple m Multiple m DDA for pr [M+H]+1	2039385	2051266	8	8
		methyl 2-(acetylamino)-4-amino-4-oxobutar	C7 H12 N2	Full match Full match No results	Partial mat Full match	-0.16	188,0797	189,087		4090825	7	3	0 74,6	45,7	42.7		94090825	92148407	6,2	6,2
FA	ALSO	Caprolactam	C6 H11 N C	Full match Full match No results	Partial mat No results	0.35	113.0841	114.0914	4.443	806117,6	23	1	0 74,4	27		No matche No matche DDA for pre [M+H]+1	729682,3	806117.6	6,8	6,3
				Full match Full match No results		-,	129,1518	,		3168084	16	1	0 73,8	8,7		No matche No matche DDA for pre [M+H]+1	2747234		5,3	4,8
				Full match Full match No results		0.16	171,126	172 1332		1994978	20	2	0 73,6			No matche Single mati DDA for pri [M+H]+1	1895789		8.6	7,5
	_			No match Invalid mas No results					,	.8716855	3	1	0 73,5			0 1	18036861		9,5	8,4
				Not the to: Full match No results			584,2636			3664575	6	1	0 73,1	8,7		Multiple m No matche DDA for pri [M+H]+1	3424028	3664575	9.1	8,6
		bicyclo[2.2.2]oct-2-en-1-yl 4-methylbenzene					278,0938			1342137	5	1	0 71,9	25,5		No matche Single mate DDA for pre [M+H]+1	1032429		5,5	6,6
	_			Full match Full match No results			205,0739			1773973	24	2	0 71,8	42,1		Multiple m Multiple m DDA for pri [M+H]+1	1694622	1773973	7,2	7,2
				Full match Full match No results			127.0997	128.107		2300964	26	1	0 70.6	8,5		No matche No matche DDA for pri [M+H]+1	2193677	2300964	6,4	6,4
				Full match Full match No results		-,	100,0524			6710590	37	1	0 70,2				26710590		4,6	4
				No match Invalid may No results						1782541	64	1	0 70,1			No matche Multiple m DDA for pri [M+H]+1	1782541	1780556	6,6	6,6
	_	- (-) -)		Full match Full match No results			213,2456			1529381	5	1	0 68,2	8,4		No matche Single mat DDA for pr [M+H]+1	1351943	1529381	7,7	6,6
				No match Invalid ma: No results			199.0333			2735337	0	1	0 67,4	24,1		No matche Single mat DDA for pri [M+H]+1	2735337	2516788	7,7	7,5
				No match Invalid ma: No results			398,0741	,		1495208	1	1	0 67,4	24,1		No matche No matche DDA for otl [M+2H]+2	1495208		3,9	7,3
		2-(Phenylthio)-1-[4-(1H-pyrrol-1-yl)piperidin					300,1337			.8970069	3	8	0 67,4	39,2			18970069		6.2	6,2
				Full match Full match No results			75,06848			5630789	10	1	0 67,4	8,4		Multiple m No matche DDA for pri [M+H]+1	5630789	5533026	7	7,5
		2-[(3S)-1-(3,4-Difluorobenzyl)-3-pyrrolidinyl]-					314,1267			3069537	10	2	0 67,3	8,4		No matche No matche DDA for pri [M+H]+1	2523281		8	7,5
				No match Invalid ma: No results							1	4	0 65,7	8,3		No matche No matche DDA for pri [M+H]+1		3005337	7,8	7,5
							314,0726			.7521002	1	4	0 65,7				1/521002	4.475.00	7,0	6.2
				No match Invalid ma: No results			314,0726			1,17E+08	1	4		23,9		No matche No matche DDA for pri [M+H]+1		1,17E+08		6,2
				No match Invalid ma: No results			314,0725			1,5E+08	22	3	0 65	23,9		No matche No matche DDA for pri [M+H]+1	E063300	1,5E+08 5074129	7.5	5,7
				Full match Full match No results			362,2093			5074129	32	2	0 63,1	56,6		Multiple m Multiple m DDA for pri [M+H]+1	5062200	001.1220	7,5	8,6
				Not the to: Full match No results			281,1125			1170402	9	1	0 62,6	8,1		Multiple m Single mati DDA for pri [M+H]+1	1142050	1170402	7,2	7,2
				No match Invalid ma: No results		69968,43				1951352	3	6	0 61,9			No matche No matche DDA for pri [M+H]+1	1951352	202022	8,6	7.5
			C10 H18 O			118115,7		209,1172		2436344	60	4	0 60,9			Single mate Multiple m DDA for pre [M+H]+1	2436344	2038967	5,3	7,5
				Full match Full match No results		-7-	,			845965,6	9	3	0 59,4	8			802417,4	845965,6	8,5	7,7
	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			Full match Full match No results		-,	174,1005	,	-,	8221076	16	3	0 57,8	7,9	41,6	Multiple m No matche DDA for pri [M+H]+1	8221076		7,8	7,8
				Full match Full match No results			149,0511			1520644	13	2	0 57,6	23,2		Multiple m No matche DDA for pri [M+H]+1		1520644		6,1
				Full match Full match No results			196,0597	- /		502156,2	6	3	0 56,2	23			492656,2		7,4	7,9
		,		Full match Full match No results			118,0743			8669124	20	17	0 55,9	23	61,8	Single mat(Multiple m DDA for pr([M+H]+1	8669124		6,2	4,6
				Full match Full match No results			199,1209			2129271	22	1	0 55,1	22,9		Single mate Single mate DDA for pre [M+ACN+H	2129271	1096585	6,4	7,2
				Not the top Full match No results			584,2637	,		657583,3	6	1	0 54,8				657583,3	649035,9	7,9	7,9
FA				No match Invalid ma: No results			117,079		,	1431721	40	1	0 53,6	7,7			1431721		4,5	
FA	ALSO -	4-{[3-(Diethylamino)propyl]amino}-4-oxobut				0,17	228,1474	229,1547		1765610	6	2	0 53,3	36,5		Multiple m Multiple m DDA for pri [M+H]+1	1741705	1765610	7,2	5
				Full match Full match No results		-1,03		170,0963		1364549	15	2	0 52,8	7,6		Multiple m No matche DDA for pri [M+H]+1	1364549		5	
FA	ALSO			No match Invalid mas No results		-96784,7	168,0786	169,0859	6,967 8	1373112	42	1	0 52,1	22,6		Single mate Multiple m DDA for pre [M+H]+1		81373112		5,1
FA	ALSO -	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 pri [M+H]+1	1061925	1017643	7,7	7,7
FA	ALSO -	4-Acetamidobutanoic acid	C6 H11 N C	Full match Full match No results	Partial mat Full match	0,45	145,074	146,0812	1,35	1865806	29	2	0 51,1	22,5		Multiple m No matche DDA for pri [M+H]+1	393309,5	1865806	2,2	5
FA	ALSO	Cyclohexylamine	C6 H13 N	Full match Full match No results	Full match No results	0,15	99,10481	100,1121	3,505	1908042	17	1	0 50,3	22,5		No matche No matche DDA for pri [M+H]+1	1908042	1817067	7	7,2
FA	ALSO	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 pri [M+H]+1	955475,1	968928,5	8,8	8,3
FA	ALSO	Dihydrothymine	C5 H8 N2 C	Full match Full match No results	Full match Full match	0,08	128,0586	129,0659	1,381 1	7045610	19	1	0 49,8	7,5		Single mate No matche DDA for pre [M+H]+1	16407028	17045610	7,8	8,4
FA	ALSO	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 3	7409656	46	1	0 49,7	22,4		Multiple m Multiple m DDA for pri [M+H]+1		37409656		4
FA	ALSO	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 pri [M+H]+1	390967,9		4,9	
FA	ALSO	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 pri [M+H]+1	2561561	2594898	8	8
FA	ALSO	N-Acetyl-L-carnosine	C11 H16 N	Not the to: Full match No results	Full match Full match	0,12	268,1172	269,1245	1,962	1370146	12	1	0 48,5	7,4		Single mate No matche DDA for pre [M+H]+1	1248705	1370146	7,2	8,3
FA	ALSO	Guvacoline	C7 H11 N C	No results Full match No results	Not the tor Full match	-1,76	141,0787	142,0863	1,955	2143191	18	1	0 48	7,4		Single mate No matche DDA for pre [M+H]+1	1955011	2143191	7,5	7
FA	ALSO -	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 pri [M+H]+1	3175347	3276281	7	7,5
FA	ALSO	N2-[5-Phenyl-4-(trifluoromethyl)-1,3-thiazol-	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 otl [M+H]+1		6821933		5,7
FA	ALSO	Cortisone	C21 H28 O	Full match Full match No results	Full match Partial mat	0,02	360,1937	361,201	6,504	692206	17	1	0 46,7	35,2		Multiple m Multiple m DDA for pri [M+H]+1	692206	680886,7	7,9	7,9
FA	ALSO	N6,N6,N6-Trimethyl-L-lysine	C9 H20 N2	Full match Full match No results	Full match Full match	-0,2	188,1524	189,1597	1,153	1930967	5	1	0 46	22		Single mate No matche DDA for pre [M+H]+1	1930967	1870113	9,1	8,8
FA	ALSO	Trihexyphenidyl	C20 H31 N	Full match Full match No results	Full match No results	0,07	301,2406	302,2479	6,847	1115824	5	1	0 45,9	7,3		No matche No matche DDA for pre [M+H]+1	1066180	1115824	6,6	8,3
FA	ALSO .	Acetyl-β-methylcholine	C8 H17 N C	Full match Full match No results	Partial mat Partial mat	0,19	159,126	160,1332	1,959	2450027	16	1	0 43,7	21,8		No matche Single mati DDA for pri [M+H]+1	2450027	2400079	8	9,1
FA	ALSO	10-Nitrolinoleate	C18 H31 N	No match Invalid mas No results	No match No results	18481,52	331,236	332,2432	5,913	1875532	2	1	0 43	7,2		No matche No matche DDA for pri [M+H]+1	1718985	1875532	7,7	7,7
FA	ALSO -	4-tert-Butylcyclohexyl acetate	C12 H22 O	No results Full match No results	Not the tor Full match	0,35	198,1621	199,1693	1,503 2	6986552	99	1	0 42,9	7,1		Single mate Multiple m DDA for pre [M+H]+1		26986552		4
FA	ALSO	2-[(3S)-1-(3,4-Difluorobenzyl)-3-pyrrolidinyl]	C18 H16 F2	No match Invalid mas No results	No match No results	11,48	314,1267	315,134	6,919	978574,5	10	1	0 41,6	7,1		No matche No matche DDA for pri [M+H]+1	768975,1	978574,5	6,3	7,2
FA		4-[(4-chlorophenyl)sulfonyl]-3-nitrobenzoic a								2250771	0	1	0 40,9			No matche No matche DDA for pre [M+H]+1	2084433	2250771	8	4,8
FA	ALSO			Full match No results No results			161,0265	81,52054		1,44E+09	1	0	0			No matche No matche DDA for otl [M+2H]+2	1,44E+09	1,31E+09	7,3	6,7
				No results Invalid mas No results		-0,9	202,0451	203,0523		6,57E+08	3	10	0		55,4		6,57E+08	6,48E+08	9,5	8,9
			C9 H8 O2	Full match Invalid ma: No results	Full match Partial mat					2,28E+08	25	13	0		76,4	Multiple m Multiple m DDA for pre [M+NH4]+:		2,19E+08	10	9,5
	ALSO			No results No results No results			96,9841	70,0126		5,82E+08	0	0	0			No matche No matche DDA for otl [M+ACN+2		5,52E+08	7,3	5,7
		[Similar to: methyl 2-[4-ethenyl-2,6-dihydrox		No results Invalid ma: No results	No results No results		124,9789	125,9862		4,45E+08	0	1	0		52,5	No matche No matche DDA for pri [M+H]+1		4,19E+08	7,3	6,2
FA	ALSO		C4 H4 O7 F	Full match No results No results	No match No results	3,6	225,944	226,9513	1,103	2,16E+08	2	0	0			No matche No matche DDA for pre [M+H]+1	2,16E+08	2,04E+08	8,9	8,9
	ALSO			Full match No results No results			179,0372			3,13E+08	0	0	0			No matche No matche DDA for otl [M+2H]+2			7,3	7,8
	ALSO			No results No results No results			83,95242			2,35E+08	0	0	0			No matche No matche DDA for pre [M+H]+1	2,35E+08		8,4	
FA	ALSO			No results No results			176,9988	-		0446692	0	0	0			No matche No matche DDA for otl [M+2H]+2		50446692		8,4
	ALSO			No results No results No results				84,95973		2,39E+08	0	0	0			No matche No matche DDA for pri [M+H-H2O		2,39E+08		7,3
		N(3)-(4-Methoxyfumaroyl)-2,3-diaminopropi				-0,23	216,0746			1,53E+08	2	0	0			No matche No matche DDA for pri [M+H]+1	1,53E+08		8,4	8,4
				Full match No results No results			71,07351			1,13E+08	9	0	0			No matche No matche DDA for pri [M+H]+1			9,5	9,5
	ALSO	,		No results No results No results			176,9989			0348284	0	0	0			No matche No matche DDA for otl [M+2H]+2			7,3	8,4
	ALSO			No results No results No results				90,97665		1,28E+08	0	0	0			No matche No matche DDA for pri [M+H]+1			8,4	8,4
		Tris-formaminomethane		Full match No results No results			145,0491			1,46E+08	5	0	0			No matche No matche DDA for otl [M+2H]+2			7,3	6,2
				Full match No results No results			85,08915			7685895	6	0	0			Single mate No matche DDA for pre [M+H]+1			8,4	8,4
	ALSO			No results No results No results			241,9181			8377237	0	0	0			No matche No matche DDA for pri [M+H]+1			8,9	8,9
	ALSO			Full match No results No results			215,9154			5982108	3	0	0			No matche No matche DDA for pri [M+H]+1			8,4	8,4
				Full match No results No results			117,0426			2493573	14	0	0			Multiple m Single mat(DDA for pri [M+H]+1			5,9	2,3
EV				Full match No results No results			109.0014			1,18E+08	0	0	0			No matche No matche DDA for pri [M+H]+1			8,4	7,8
	ALSO				No results No results	2,00	,	80,94788		6342438	0	0	0			No matche No matche DDA for pri [M+H]+1			8,9	8,9
FA	ALSO							235,0924		3,15E+08	5	0	0			No matche No matche DDA for pri [M+H]+1	. 33-12-130		0,5	5,1
FA FA	ALSO ALSO					-0.24				-,		-						3.15F+0X		
FA FA	ALSO ALSO ALSO	glu-ser	C8 H14 N2	Full match No results No results	Full match No results				0 000	1 12F±08	0	0	0				1 1E+00	3,15E+08	7 2	
FA FA FA	ALSO ALSO ALSO ALSO	glu-ser	C8 H14 N2 C H N2 O5	Full match No results No results Full match No results No results	Full match No results No results No results	2,26	213,9103	214,9176		1,12E+08	0	0	0			No matche No matche DDA for pri [M+H]+1		1,12E+08	7,3 7.3	8,4
FA FA FA FA	ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 I C H N2 O5 I C24 H50 N	Full match No results No results Full match No results No results Full match No results No results	Full match No results No results No results Full match Full match	2,26 -0,91	213,9103 495,332	214,9176 496,3393	7,32	1,41E+08	4	0	0			No matche No matche DDA for pri [M+H]+1 Single mat(No matche DDA for pri [M+H]+1	1,41E+08	1,12E+08 1,29E+08	7,3	8,4 8,4
FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C	Full match No results No results	Full match No results No results Full match Full match No results No results	2,26 -0,91 1,75	213,9103 495,332 218,0192	214,9176 496,3393 219,0265	7,32 1,239 7	1,41E+08 1819136	4 0	-	0			No matche No matche DDA for pri [M+H]+1 Single mati No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1	1,41E+08	1,12E+08 1,29E+08 71819136		8,4 8,4 9,5
FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F	Full match No results No results	Full match No results No results Full match Full match No results No results No match No results	2,26 -0,91 1,75 4,39	213,9103 495,332 218,0192 199,9883	214,9176 496,3393 219,0265 182,9851	7,32 1,239 7 0,341 3	1,41E+08 1819136 17964855	4 0 2	0	0 0			No matche No matche DDA for pn [M+H]+1 Single match No matche DDA for pn [M+H]+1 No matche No matche DDA for pn [M+H]+1 No matche No matche DDA for pn [M+H-H2O	1,41E+08 70938899	1,12E+08 1,29E+08 71819136 37964855	7,3 8,9	8,4 8,4 9,5 9,5
FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F C3 H Cl O6 C6 C7 H5 O6 C6 C7 H5 O5 F C3 H Cl O6 C7 H5 O5 F C7 H5 O5 F	Full match No results	Full match No results No results No results Full match Full match No results No match No results No results No results	2,26 -0,91 1,75 4,39 -4,28	213,9103 495,332 218,0192 199,9883 231,8893	214,9176 496,3393 219,0265 182,9851 232,8966	7,32 1,239 7 0,341 3 1,136 3	1,41E+08 1819136 7964855 8068374	4 0 2 0	0 0 0 0	0 0 0 0			No matche No matche DDA for pri [M+H]+1 Single mat No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+12 No matche No matche DDA for pri [M+H]+1	1,41E+08 70938899 38068374	1,12E+08 1,29E+08 71819136 37964855 34752116	7,3	8,4 8,4 9,5 9,5 8,9
FA FA FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F C3 H Cl O6	Full match No results	Full match No results No results No results Full match Full match No results No results No match No results No results No results No results No results	2,26 -0,91 1,75 4,39 -4,28	213,9103 495,332 218,0192 199,9883 231,8893 99,92472	214,9176 496,3393 219,0265 182,9851 232,8966 141,9585	7,32 1,239 7 0,341 3 1,136 3 0,341 3	1,41E+08 1819136 17964855 18068374 15603509	4 0 2 0 0	0 0 0 0	0 0 0 0			No matche No matche DDA for pr [M+H]+1 Single mat No matche DDA for pr [M+H]+1 No matche No matche DDA for pr [M+ACN+H	1,41E+08 70938899 38068374	1,12E+08 1,29E+08 71819136 37964855	7,3 8,9 8,4	8,4 8,4 9,5 9,5
FA FA FA FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F C3 H Cl O6 C3 H4 N6 S	Full match No results No results	Full match No results No results No results Full match Full match No results No results No match No results	2,26 -0,91 1,75 4,39 -4,28	213,9103 495,332 218,0192 199,9883 231,8893 99,92472 156,0213	214,9176 496,3393 219,0265 182,9851 232,8966 141,9585 79,01792	7,32 1,239 7 0,341 3 1,136 3 0,341 3 0,972	1,41E+08 11819136 17964855 18068374 15603509 1,02E+08	4 0 2 0 0 0	0 0 0 0 0	0 0 0 0 0			No matche No matche DDA for pr [M+H]+1 Single mat No matche DDA for pr [M+H]+1 No matche No matche DDA for pr [M+ACN+H] No matche No matche DDA for DA for	1,41E+08 70938899 38068374	1,12E+08 1,29E+08 71819136 37964855 34752116 35603509	7,3 8,9	8,4 8,4 9,5 9,5 8,9 9,5
FA FA FA FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F C3 H Cl O6 C C7 H4 N6 S	Full match No results No results	Full match No results No results No results Full match Full match No results No match No results	2,26 -0,91 1,75 4,39 -4,28	213,9103 495,332 218,0192 199,9883 231,8893 99,92472 156,0213 78,01065	214,9176 496,3393 219,0265 182,9851 232,8966 141,9585 79,01792 79,01793	7,32 1,239 7 0,341 3 1,136 3 0,341 3 0,972 0,993	1,41E+08 '1819136 17964855 18068374 15603509 1,02E+08 1E+08	4 0 2 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0			No matche No matche DDA for pri [M+H]+1 Single mati No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+ACN+H No matche No matche DDA for pri [M+ZH]+2 No matche No matche DDA for pri [M+H]+1	1,41E+08 70938899 38068374 1,02E+08	1,12E+08 1,29E+08 71819136 37964855 34752116 35603509	7,3 8,9 8,4 6,2	8,4 8,4 9,5 9,5 8,9 9,5
FA FA FA FA FA FA FA FA FA	ALSO ALSO ALSO ALSO ALSO ALSO ALSO ALSO	glu-ser Lysolecithin	C8 H14 N2 C H N2 O5 C24 H50 N C7 H2 N6 C C7 H5 O5 F C3 H Cl O6 C C7 H4 N6 S	Full match No results No results	Full match No results No results No results Full match Full match No results No match No results	2,26 -0,91 1,75 4,39 -4,28	213,9103 495,332 218,0192 199,9883 231,8893 99,92472 156,0213 78,01065	214,9176 496,3393 219,0265 182,9851 232,8966 141,9585 79,01792	7,32 1,239 7 0,341 3 1,136 3 0,341 3 0,972 0,993	1,41E+08 11819136 17964855 18068374 15603509 1,02E+08	4 0 2 0 0 0	0 0 0 0 0	0 0 0 0 0			No matche No matche DDA for pr [M+H]+1 Single mat No matche DDA for pr [M+H]+1 No matche No matche DDA for pr [M+ACN+H] No matche No matche DDA for DA for	1,41E+08 70938899 38068374 1,02E+08	1,12E+08 1,29E+08 71819136 37964855 34752116 35603509	7,3 8,9 8,4	8,4 8,4 9,5 9,5 8,9 9,5

	Tel. III	laramania n														
FALSO	[Similar to: NP-017683; ΔMass: -562.4259 Da			No results No match No results No results Full match No results	-, -	,	383,1159		39980847		0 0	46	No matche No matche DDA for pri [M+H]+1 363 No matche No matche DDA for otl [M+2H]+2 897		9,5	9,5
FALSO	N-Carbamoyl-2,2,2-trichloroacetamide						102,9703		89764106	1	-				7,3	0.4
FALSO	Phone I and I are			No results No results No results			96,92179		42443032	0	0 0	60.4	No matche No matche DDA for pri [M+H]+1 424		9,5	8,4
FALSO				No results Full match No results			120,0808		34599633		0 0	60,4	No matche No matche DDA for otl [M+NH4]+: 338 No matche No matche DDA for pri [M+H]+1 346		9,5	9,5
FALSO FALSO				No results No results No results			362,9262		34620138	0	0 0				8,9	8,9 5,7
FALSO				No results No match No results		218,0254	130,9652 110.02		79373297 18867348	3	0 0		No matche No matche DDA for pr [M+H]+1 706 No matche No matche DDA for ot [M+2H]+2	18867348	7,8	
FALSO				No results No match No results			216.9506		62847983	1	0 0		No matche No matche DDA for pri [M+H]+1 574		8,4	9,5 8,4
FALSO				No results No results No results		.,.	430,9135		28763618	0	0 0		No matche No matche DDA for pri [M+DMSO- 287		8,9	8,9
FALSO				No results No results No results	0,0		90.50676		6703940	0	0 0		No matche No matche DDA for otl [M+2H]+2 58		9,5	8,9
FALSO				No results No match No results	-2 71		102.0339		82226748	1	0 0		No matche No matche DDA for otl [M+2H]+2 822		6.7	6,7
	4-(2-Hydroxyethyl)phenyl hydrogen sulfate					. ,	110,0199		3,97E+08	3	0 0		No matche No matche DDA for otl [M+2H]+2 3,9		6,2	5,7
FALSO	3-(4-Chlorophenyl)-3-Methoxypropyl Chloric					218,0255			19553015	6	0 0		No matche No matche DDA for ot [M+2H]+2 195		6.2	9,5
FALSO	[Similar to: EQH; \(\Delta Mass: -244.1196 \) Da]			No results No results No results			169,0584		34024938		10 0	45,8	No matche No matche DDA for pri [M+H]+1 340		9,5	9,5
FALSO				No results Full match Partial ma			82,53709		55265591	2	0 0	,.	No matche Multiple m No MS2 [M+2H1+2 552		7.3	
FALSO		C2 H5 N2 C Full match N	No results	No results No results No results			239,9666	0,989	49297987	0	0 0		No matche No matche DDA for pri [M+ACN+H 492	297987 47380703	7,8	8,4
FALSO				No results No results No results			158,9641		36314373	0	0 0		No matche No matche DDA for pre[M+H]+1 363		8,9	8,9
FALSO		C8 H12 O3 Full match N	No results	No results No match No results	-3,48	218,0254	110,02	7,377	3,18E+08	3	0 0		No matche No matche DDA for otl [M+2H]+2	3,18E+08		5,1
FALSO	Diethylpyrocarbonate	C6 H10 O5 Full match N	No results	No results Full match Full match	-0,01	162,0528	145,0496	1,247	73834250	49	0 0		Multiple m No matche DDA for pre [M+H-H2O 252	212433 73834250	9,5	5,1
FALSO		C4 H O13 F Full match N	No results	No results No match No results	-2,79	287,9147	288,922	1,072	25365367	1	0 0		No matche No matche DDA for pri [M+H]+1 253	365367 23468134	8,9	8,4
FALSO		C H3 N2 Of Full match N	No results	No results No results	2,12	231,9209	232,9282	0,995	51723142	0	0 0		No matche No matche DDA for pri [M+H]+1 498	895805 51723142	5,1	5,7
FALSO		No results N	No results	No results No results		103,996	105,0033	0,972	51569590	0	0 0		No matche No matche DDA for pre [M+H]+1 461	126481 51569590	7,3	7,3
FALSO				No results No match No results	-2,63	219,9272	220,9345	1,07	24037010	3	0 0		No matche No matche DDA for pre [M+H]+1 240	037010 22062132	8,4	8,9
FALSO		C2 H6 N2 C Full match N	No results	No results No results	3,18	122,0331	82,53712	0,974	43481716	0	0 0		No matche No matche DDA for pre [M+ACN+2	43481716		5,1
FALSO	[Similar to: 2-(4-chlorophenyl)-2-oxoethyl 2,6				-4,96	293,9316	294,9389		22934414	0	1 0	45,3	No matche No matche DDA for pre [M+H]+1 229		8,9	9,5
FALSO	3-Amino-2,3,6-trideoxy-α-L-ribo-hexopyrand						130,0863		19071582	22	0 0		No matche No matche DDA for pri [M+H-H2O 190		8,4	8,4
FALSO	C8-Carnitine			No results Full match Full match			288,2168		21184994	5	0 0		Multiple m No matche DDA for pri [M+H]+1 191		8,4	8,4
FALSO				No results No results No results			89,50669	7,584		0	0 0			3E+08 56279126	5,1	6,2
FALSO				No results Full match No results	-7.	114,0865	-,		6878409	5	0 0			878409 6596087	6,2	4,6
FALSO	EDDA			No results Full match No results	0,35	176,0798			1,17E+08	13	0 0			17E+08 90101093	6,7	4
FALSO				No results No results No results			156,1203		2,93E+08	0	0 0		No matche No matche DDA for pri [M+H]+1	2,93E+08	0.4	6,2
FALSO FALSO				No results No results No results No match No results		221,8605	,		15509102	0	0 0		No matche No matche DDA for pri [M+H]+1 155		8,4	8,4
FALSO				No results No match No metch	_	_	206,8939		17774965	1	0 0		No matche No matche DDA for pr [M+H]+1 177 Single matt No matche DDA for ot [M+2H]+2 1,5		8,4	8,4
FALSO				No results No match No match			111,0202		1,71E+08 18098696	0	0 0		No matche No matche DDA for ptr [M+H]+1 180		6,2	6,2
FALSO				No results No results No results			378,9002 89,50675		2,45E+08	0	0 0		No matche No matche DDA for otl [M+2H]+2	2,45E+08	8,9	8,9 4,6
				No results Full match No results			101,0032		48922419	1	0 0		No matche No matche DDA for pri [M+2H]+1 489		6,2	4,6
FALSO				No results Full match No results			98,51202		9722488	4	0 0		No matche No matche DDA for otl [M+2H]+2	9722488	0,2	9,5
FALSO	2-Amino-o-microbenzocinazoie			No results No match No match			111,0202		12164209	2	0 0		Single mat: No matche DDA for otl [M+2H]+2 95		9.5	9,5
FALSO	BLAH			No results Full match No results			112,8957		17052908	1	0 0		No matche No matche DDA for pri [M+H]+1 170		9.5	9,5
FALSO				No results No results No results		419,8793			15327811	0	0 0		No matche No matche DDA for pri [M+DMSO- 153		8.9	8,9
FALSO				No results No results No results		142,9895			39346691	0	0 0		No matche No matche DDA for pri [M+H]+1 393		5.1	0,5
FALSO				No results No results No results			446,8876	- 7.	14718093	0	0 0		No matche No matche DDA for otl [M+DMSO- 147		8,9	8,9
FALSO		C4 H13 N2 Full match N	No results	No results No results No results			185,0323		16848959	0	0 0		No matche No matche DDA for pri [M+H]+1	16848959	- 7	9,5
FALSO				No results No results No results	0,8	565,8812	566,8885		12249262	0	0 0		No matche No matche DDA for pre[M+H]+1 122	249262 11747883	8,9	8,4
FALSO		No results N	No results	No results No results No results		140,9513	141,9586	0,318	54404433	0	0 0		No matche No matche DDA for pre[M+H]+1 544	404433 4558261	5,1	7,5
FALSO	Citric acid	C6 H8 O7 Full match N	No results	No results Full match Partial ma	-0,28	192,027	215,0161	2,145	37169594	17	0 0		Multiple m Single mate DDA for pre [M+Na]+1 371	169594 36264946	7,8	7,8
FALSO	1-Octanesulfonyl fluoride	C8 H17 F O No results N	No results	No results Full match No results	1,37	196,0936	219,0828	1,147	6462999	1	0 0		No matche No matche DDA for pri [M+Na]+1 64	462999 5096178	9,5	9,1
FALSO		C4 H8 N O4 Full match N	No results	No results No match No results	2,75	165,0196	83,51705	0,994	33566682	4	0 0		No matche No matche No MS2 [M+2H]+2 335	566682 30519041	5,1	6,2
FALSO		C2 H N3 O2 Full match N	No results	No results No results	1,08	99,00698	100,0143	0,986	29229400	0	0 0		No matche No matche DDA for pre [M+H]+1 292	229400	6,7	
	9-Decenoylcarnitine	C17 H31 N Full match N	No results	No results Full match No results	-0,28	313,2252	314,2325	-,	15426626	1	0 0		No matche No matche DDA for pri [M+H]+1 143	357391 15426626	8,9	9,5
FALSO		C4 H N4 O7 Full match N	No results	No results No results	-0,88	309,9055	310,9128		14770823	0	0 0		No matche No matche DDA for pre [M+H]+1 147	770823 14557024	9,5	9,5
FALSO				No results No results			90,50695		6466827	0	0 0		No matche No matche DDA for otl [M+2H]+2	6466827		9,5
FALSO				No results No results		131,991			28354978	0	0 0		No matche No matche DDA for pri [M+H]+1 241		7,3	5,1
FALSO				No results No results		555,8544			9364542	0	0 0		No matche No matche DDA for otl [M+DMSO- 93		8,9	
FALSO				No results No results No results			634,8761	1,098		0	0 0		No matche No matche DDA for otl [M+2H]+2	8914071		8,9
FALSO				No results No results No results		147,9685	-7-		26716858	0	0 0		No matche No matche DDA for pri [M+H]+1 234		7,8	6,2
FALSO				No results No match No results	_	_	100,0143		28160420	1	0 0		No matche No matche DDA for otl [M+2H]+2	28160420		5,1
FALSO	[Cimilarto, marchine 12 Attack C7 7 100 7			No results No results No results			702,8634		7730766	0	0 0	44.0	No matche No matche DDA for pr [M+H]+1 77		8,9	9.4
FALSO FALSO	[Similar to: morphine-d3; ΔMass: 67.7469 Da			No results No results No results No results No results No results		355,9022 120,0648	356,9095 121,072		11704760 13234478	0	0 0	41,9	No matche No matche DDA for pr [M+H]+1 117 No matche No matche DDA for pr [M+H]+1 122		8,4 8,9	9,5
					_	_		,			0 0					
FALSO FALSO				No results No results No results No results No results No results		186,0756	94,0451 158,9614		24348737 12264697	0	0 0		No matche No matche DDA for ot [M+2H]+2 243 No matche No matche DDA for pr [M+H]+1 122		6,7 9,5	5,1 9,5
FALSO	Lysolecithin			No results Full match Full match			496,3397		35355091	4	0 0		Single mat: No matche DDA for pri [M+H]+1 243		7,3	6,2
FALSO				No results No results No results		483,3323			6425180	0	0 0		No matche No matche DDA for otl [M+2H]+2 63		8.4	9,5
FALSO				No results Full match Full match	-,	161.0688	,		3,91E+08	38	0 0		Multiple m No matche DDA for pr [M+H]+1 3,9		5.1	3,5
FALSO				No results No results No results	-,,	. ,	74,53064		20948779	0	0 0		No matche No matche No MS2 [M+2H]+2 209		6,2	6,2
FALSO				No results No match No results			156,0142		22744706	1	0 0		No matche No matche DDA for pri [M+H]+1 209		8,4	5,7
FALSO				No results No results No results			248,8706		8387629	0	0 0		No matche No matche DDA for pri [M+H]+1 83		8,4	8,9
FALSO				No results No results No results			702,8635		7559625	0	0 0		No matche No matche DDA for otl [M+2H]+2	7559625		8,9
FALSO				No results No results No results	-2,02	183,9783	184,9855	0,341	11616905	0	0 0		No matche No matche No MS2 [M+H]+1	11616905		8,4
FALSO	2-Amino-6-nitrobenzothiazole	C7 H5 N3 C Full match N	No results	No results Full match No results	-3,43	195,0096	98,51207	0,307	6627609	4	0 0		No matche No matche DDA for otl [M+2H]+2 66	627609 2298151	7,3	8,6
FALSO				No results No results No results			344,8756		21100647	0	0 0		No matche No matche DDA for pri [M+H]+1 208		4	6,7
	1-Palmitoyl-2-linoleoyl-sn-glycero-3-PC			No results Full match No results			758,5695		1,12E+08	32	0 0		No matche No matche DDA for pri [M+H]+1 760		5,7	6,2
FALSO				No results No results No results			258,8993		11062902	0	0 0		No matche No matche DDA for pri [M+H]+1 110		8,4	8,9
	Cyclopentylamine			No results Full match Full match			86,09645		29630228	6	0 0		Single mate No matche DDA for pre [M+H]+1 247		5,1	6,7
FALSO				No results No results No results			89,00834		2495405	0	0 0		No matche No matche No MS2 [M+H]+1 24		7	8
	1-Pentofuranosyl-2,4(1H,3H)-pyrimidinedion						245,0768		5662628	4	0 0		Multiple m No matche DDA for pri [M+H]+1 56		8,6	9,1
FALSO				No results Full match Partial ma			173,0921		8913437	33	0 0		Multiple m Multiple m DDA for otl [M+ACN+H 89		9,5	9,5
FALSO				No results No match No results			74,03225		18746487	2	0 0		No matche No matche DDA for otl [M+2H]+2 187		7,3	4,6
FALSO				No results No results		435,8531			7245593	0	0 0		No matche No matche DDA for ot M+DMSO- 72		8,4	9,5
FALSO				No results No results			282,905		7042454	0	0 0		No matche No matche DDA for pr [M+H-H2O 70		8,9	9,5
FALSO FALSO				No results No results No results	-3,09		88,50632		19610269	0	0 0		No matche No matche DDA for otl [M+2H]+2 No matche No matche DDA for pri [M+H]+1 198	19610269	4.6	7,3
FALSO				No results No results No results No results No results No results			88,50628 424,8969		19821951 9279839	0	0 0		No matche No matche DDA for pri [M+H]+1 198 No matche No matche DDA for otl [2M+K]+1 92		4,6 8.4	8.4
FALSO				No results No results No results			152,9471		9666543	0	0 0		No matche No matche DDA for oti [ZM+K]+1 92 No matche No matche DDA for pri [M+H]+1 96		8,4 7,8	
FALSO				No results No match No match			522,3553		68334659	5	0 0		Single mat(No matche DDA for pri [M+H]+1 521		7,8	8,9 7,3
FALSO				No results No match No match			354,1943		8797267	1	0 0		Single mat: No matche DDA for otl [M+3H]+3 87		8,4	8,4
	[Similar to: methyl 2-[4-ethenyl-2,6-dihydrox						162,9737		17935508	0	1 0	41,3	No matche No matche DDA for pri [M+H]+1	17935508	-,-	6,7
	Ethanoic anhydride			No results Full match Full match			103,039		27954508	18	0 0	-12,3	Multiple m No matche DDA for pr [M+H]+1 273		6,7	7,8
				No results Full match Full match			258,1101		4436881	3	0 0		Single mat (No matche DDA for pri [M+H]+1 44		8	8
					,	,	.,	,					- Polymony - I			

		laassaasala uu sulsuu uulsuu se		0.00							
FALSO	TEMPO	C9 H19 N C Full match No results No results			157,1467 1		7	11 0	0		No matche No matche No MS2 [M+H]+1 16145697 13249974 7,3 7,8
FALSO		No results No results No results		_	255,8135 2		-,	0 0	0		No matche No matche DDA for pri [M+H]+1 9439791 9223827 8,4 6,7
FALSO		C5 H9 Cl N. Full match No results No results C3 H2 N3 P Full match No results No results			260,0039 2		1,232 13831721	1 0	0		No matche No matche DDA for pr [M+H]+1 13391670 13831721 7,3 8,4
FALSO FALSO	Phenylac-gln-OH	C13 H16 N. Full match No results No results			110,999 1 264,111 2		0,983 16736731 4,722 7400760	1 0	0		No matche No matche DDA for pr [M+H]+1 16736731 16261382 5,7 7,8 Multiple m Multiple m DDA for pr [M+H]+1 7203945 7400760 8,4 8,9
	Benzofuran-2-carbonyl chloride	C9 H5 CLO: No results No results No results		-,	179,9973		0,3 1798508	6 0	0		No matche No matche No MS2 [M+2H]+2 1798508 8,8
FALSO	Delizoraran z carbonyi emoriac	No results No results No results			156,9875		0,981 16465062	0 0	0		No matche No matche DDA for ot [M+2H]+2 16115810 16465062 7,8 5,7
	Citric acid	C6 H8 O7 Full match No results No results			192,027			19 0	0		Multiple m Single mat(DDA for pr [M+Na]+1 29995744 30123772 7,8 7,8
FALSO		C9 H7 O P Full match No results No results			162,0237 8			3 0	0		No matche No matche DDA for ot [M+2H]+2 15720533 14525297 5,1 5,7
FALSO		C8 H4 N6 C Full match No results No results	No results No results	0,54	581,8553	582,8626	1,1 6119765	0 0	0		No matche No matche DDA for pri [M+H]+1 6017929 6119765 8,9 8,9
FALSO		No results No results No results			1299,686	650,8501	1,099 5635270	0 0	0		No matche No matche DDA for otl [M+2H]+2 5635270 5433258 8,6 8,6
FALSO		C3 H5 Cl O: Full match No results No results	No results No results	-3,51	409,8499	410,8562	1,124 4830422	0 0	0		No matche No matche DDA for otl [M+H]+1 4830422 4617532 8,6 8,6
	2-Hydroxyethyl phosphate	C2 H7 O5 F Full match No results No results			142,0036		0,983 16481762	1 0	0		No matche No matche DDA for otl [M+2H]+2 16481762 15303482 6,2 5,7
FALSO		C10 H16 N: Full match No results No results			276,0958		1,952 5290670	7 0	0		Single mat(No matche DDA for otl [M+ACN+H 5204578 5290670 7,5 8
	γ-Glu-gln	C10 H17 N. Full match No results No results		-,	275,1117 2		1,499 9926095	9 0	0		No matche No matche DDA for pri [M+H]+1 9926095 8,9
FALSO FALSO	C12-Carnitine	C5 H N4 OI Full match No results No results C19 H37 N Full match No results No results			179,9833 9 343,2722 3		0,305 1519532 6,918 8727777	0 0	0		No matche No matche No MS2 [M+H+NH4 1519532 8,3 No matche No matche DDA for pri [M+H]+1 7427797 8727777 8,4 9,5
FALSO		C28 H50 N Full match No results No results			543,3324		7,413 13908873	3 0	0		No matche No matche DDA for pr [M+H]+1 7427797 8727777 8,4 9,5 No matche No matche DDA for pr [M+H]+1 13908873 7,8
FALSO	1-aracindonoyi-sii-giycero-s-piiospiiociioiine	C4 H6 Cl2 I Full match No results No results			341,8615			0 0	0		No matche No matche DDA for pro[M+H]+1 5824351 5328207 8,4 8
FALSO	Tetrolic Acid	C4 H4 O2 Full match No results No results			84.02117 1			11 0	0		Single mat(Single mat(DDA for pr [M+H+Me(19120560 4,6
FALSO		No results No results No results			111,0107 1	112,0179		0 0	0		No matche No matche DDA for pre[M+H]+1 61654209 66067266 6,2 6,2
FALSO	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		No matche Single mat DDA for pr [M+H]+1 8306184 9777091 8,4 8,4
FALSO		C2 H4 Br Cl Full match No results No results		3,73	263,8452 2	264,8525	1,144 5819265	0 0	0		No matche No matche DDA for pri [M+H]+1 5819265 5242649 8,9 8,6
	1-71	C5 H11 N Full match No results No results			85,08917 8		2,889 25516281	6 0	0		Single mat (No matche DDA for pr [M+H]+1 25516281 22279835 5,1 6,7
FALSO	Platelet-activating factor	C26 H54 N Full match No results No results				524,371	7,124 36050639	6 0	0		No matche Multiple m DDA for pri [M+H]+1 36050639 6,7
FALSO	[Similar to: N-[1-(4-methoxyphenyl)-5-methy	No results Invalid mat No results			82,04128 1		1,504 18082503	0 4	0	71	No matche No matche DDA for ot [2M+Na]+1 18082503 5,7
FALSO FALSO		No results No results No results			110,0023 1		0,976 15136647	0 0	0		No matche No matche DDA for pri [M+H]+1 15136647 14218196 7,8 5,1
FALSO		No results No results No results No results No results No results			90,01028 2		0,976 12331925 1,099 4938340	0 0	0		No matche No matche DDA for pr [2M+K]+1 10921892 12331925 7,8 8,4 No matche No matche DDA for otl [M+2H]+2 4938340 4800017 8,6 8,6
FALSO		C H4 Br O F Full match No results No results		-0,25	237,8345 2	-,	1,143 5055138	0 0	0		No matche No matche DDA for ort [M+2/n]+2 4938340 4800017 8,6 8,6 8,6 No matche No matche DDA for pri [M+H]+1 5055138 4814135 9,1 9,1
FALSO		C2 H4 Br N Full match No results No results			273,874		1,138 5673359	0 0	0		No matche No matche DDA for pro[M+H]+1 5673359 5342252 8,4 8,6
	trans-2-Dodecenoylcarnitine	C19 H35 N Full match No results No results			341,2566			3 0	0		No matche No matche DDA for pre [M+H]+1 10349668 10924562 7,8 8,4
FALSO	Coumarone	C8 H6 O Full match Invalid ma: No results	Full match No results	0,34	118,0419 1	136,0757	3,232 6427123	6 10	0	52,3	No matche No matche DDA for pri [M+NH4]+: 6427123 5697713 8,4 8,4
FALSO		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		Single mat(Single mat(DDA for pr([M+H]+1
FALSO		C2 H Cl4 Nt Full match No results No results		-2,65	405,766		1,143 4093435	0 0	0		No matche No matche No MS2 [M+H]+1 4093435 3872335 8,6 8,6
FALSO		C6 H3 Cl O Full match No results No results			283,9029 2		1,126 4658151	0 0	0		No matche No matche No MS2 [M+H]+1 4506313 4658151 8,6 7
FALSO		C3 H5 Cl N: Full match No results No results			199,9658 2		0,0.1	0 0	0		No matche No matche No MS2 [M+ACN+H 11034456 11197713 7,8 8,4
FALSO		C H4 O2 P2 Full match No results No results			141,9408	164,93	1,114 6737043	0 0	0		No matche No matche DDA for ot [M+Na]+1 6737043 3791369 7,8 8
FALSO FALSO		No results No results No results C H2 N2 Of Full match No results No results			769,8436 7 231,9102 2		1,099 4636765 1,112 3327695	0 0	0		No matche No matche DDA for pri M+H +1 4636765 8,6 No matche No matche DDA for pri M+H +1 3327695 3169619 9,1 9,1
FALSO		C7 H11 N4 Full match No results No results		_		261,037	1,112 3327693	3 0	0		No matche No matche DDA for pri [M+H-H2O 10671974 10311111 8,9 8,9
FALSO		C5 H6 N O ⁴ Full match No results No results				88,50912	0,339 3157732	1 0	0		No matche No matche DDA for ot [M+2H]+2 3157732 9,1
FALSO		No results No results No results				770,851		0 0	0		No matche No matche DDA for oti [M+2H]+2 4885464 8,6
FALSO		C H2 Cl4 O Full match No results No results				280,8265		0 0	0		No matche No matche DDA for pri [M+H]+1 4538312 4158397 9,1 8,6
FALSO		No results No results No results	No results No results		178,0023	90,00841	0,327 4756741	0 0	0		No matche No matche DDA for ot [M+2H]+2 2429684 4756741 5,9 8
FALSO		No results No results No results			253,8164	254,8237	1,172 7701320	0 0	0		No matche No matche DDA for pre [M+H]+1 7764920 7083809 8,9 9,5
FALSO		C2 H N4 O1 Full match No results No results			349,8852		-,	0 0	0		No matche No matche DDA for pre [M+H]+1 4731438 4412086 8,6 8,6
	5-Hydroxy-2-furoic acid	C5 H4 O4 Full match No results No results		0,06	128,011		2,144 12814129	1 0	0		No matche No matche DDA for pri [M+H]+1 12710345 12814129 8,4 7,8
FALSO		C2 H7 Cl2 (Full match No results No results		0,84	289,848 2			0 0	0		No matche No matche DDA for pri [M+H]+1 4676833 4570947 8 8
FALSO FALSO		No results No results No results C4 H Cl2 O: Full match No results No results		0.01	130,967 1		0,34 3435918 1,136 5277924	0 0	0		No matche No matche DDA for ot [M+H-H2O 3435918 9,1 No matche No matche DDA for pro [M+H]+1 5277924 4740616 8 8
		C5 H7 N O4 Full match No results No results			357,8354 3 145,0376 1		1,130 3277924	2 0	0		No matche No matche DDA for pri [M+H]+1 5277924 4740616 8 Multiple m Single mati DDA for pri [M+ACN+H] 33971986 5,7
FALSO		C H N2 O P Full match No results No results			87.98304 1		0.974 13288555	0 0	0		No matche No matche DDA for ot [M+ACN+H 12892904 13288555 5,1 6,2
FALSO		No results No results No results			99,01712 8		0,975 12622085	0 0	0		No matche No matche DDA for pri [M+H-H2O 12622085 11135521 5,7 4
FALSO	[Similar to: L-(+)-Citrulline; ΔMass: 21.9942 D	C6 H15 N C Full match Invalid mas No results	No results No results	0	197,0899 1	198,0972	1,254 12754015	0 1	0	56,2	No matche No matche DDA for pri [M+H]+1 12593986 12754015 5,7 8,4
FALSO		No results No results No results	No results No results		291,1069 2	292,1142	1,442 8476717	0 0	0		No matche No matche DDA for pri [M+H]+1 8281704 8476717 8,9 6,7
FALSO		C8 H15 N2 Full match No results No results		-,	330,0466	,	7	2 0	0		No matche No matche DDA for pre [M+H]+1 8732467 6,2
FALSO		C3 H2 Cl3 I Full match No results No results		_	415,7948		-,	0 0	0		No matche No matche No MS2 [M+H]+1 4180758 3858768 8 8
FALSO		C3 H N2 O Full match No results No results				174,938	1,106 8174348	0 0	0		No matche No matche DDA for pri [M+H]+1 8174348 7557659 8,4 8,4
FALSO		No results No results No results No results No results No results			76,01284 1 87,50189 8		0,974 12204210 0,303 2515318	0 0	0		No matche No matche DDA for ot [2M+H]+1 12204210 11043779 5,7 7,8 No matche No matche No MS2 [M+H]+1 2515318 1633766 6,4 7,7
FALSO		C4 H13 N4 Full match No results No results		_				29 0	0		No matche No matche No MS2 [M+H]+1 2515318 1633766 6,4 7,7 No matche Multiple m DDA for pri [M+H]+1 2897704 8
FALSO		C4 H3 N4 C Full match No results No results			212,0675 2 491,877 4			0 0	0		No matche No matche DDA for pri [M+H]+1
FALSO		C51 H82 N/ Full match No results No results			936,5769		7,4 10442410	1 0	0		No matche Single mat (DDA for ot [M+2H]+2 10442410 9925305 8,4 7,8
FALSO		C3 H2 Cl3 (Full match No results No results			347,8066		1,142 3912509	0 0	0		No matche No matche No MS2 [M+H]+1 3912509 3834693 8,6 8,6
		H2 Cr O4 No results No results No results		-4,08	117,9353 1	159,9692	0,342 8388475	1 0	0		No matche No matche DDA for pri [M+ACN+H 8388475 6,2
	Tetraacetylethylenediamine	C10 H16 N. Full match No results No results			228,111 2		1,885 8002713	7 0	0		No matche No matche DDA for pre [M+H]+1 8002713 7835201 8,4 9,5
FALSO		No results No results No results		_	271,7875 2		1,172 7396127	0 0	0		No matche No matche DDA for pri [M+H]+1 7396127 6859111 8,9 7,3
FALSO		C3 H3 N2 C Full match No results No results			303,8887		1,073 6646334	0 0	0		No matche No matche DDA for pri [M+H]+1 6646334 6251029 7,8 8,4
	1-Linoleoyl-2-Hydroxy-sn-glycero-3-PC	C26 H50 N Full match No results No results			519,3325 5		7,356 13815336	6 0	0		Single mat Single mat DDA for pr [M+H]+1 13815336 6009566 6,7 7,8
FALSO	1-iiiioleoyi-sii-giycero-s-pnospnoetnanolami	C23 H44 N Full match No results No results C9 H28 N6 Full match No results No results			477,2855 4 426,088 2		6,92 15427754 1,498 7310074	3 0	0		No matche Single mati DDA for pri [M+H]+1 15427754 9146330 8,4 7,8 Single mati No matche DDA for pri [M+2H]+2 6783278 7310074 6,7 7,8
FALSO		C2 H Cl3 Nt Full match No results No results			399,8207			0 0	0		No matche No matche No MS2 [M+H]+1 4224678 3957149 8 8
	quinmerac	C11 H8 Cl ! No results No results No results			221,0239			5 0	0		No matche No matche No MS2 [M+H]+1 4224078 3937149 8 8 No matche No matche No MS2 [M+2H]+2 1632614 9,3
FALSO		C5 H N4 O2 Full match No results No results			179,983			0 0	0		No matche No matche DDA for pre [M+H+NH4] 3191997 8
	1-Piperideine	C5 H9 N Full match No results No results	Full match Full match	0,24	83,07352	84,0808		13 0	0		Multiple m No matche DDA for pri [M+H]+1 17658018 19229300 7,8 6,7
		C21 H37 N Full match No results No results			367,2721		-,	3 0	0		No matche Multiple m DDA for pri [M+H]+1 6077032 7051132 8,4 8,4
		C6 H11 N C Full match No results No results			129,079 1			54 0	0		Multiple m Multiple m DDA for pr [M+NH4]+: 10263122 12137184 6,7 5,7
		C6 H9 N O ⁴ Full match Invalid mas No results			159,0538 1			6 2	0	82,7	Multiple m No matche DDA for pri [M+H]+1 18055190 7,3
FALSO		C3 H7 Cl2 I Full match No results No results			425,8236		-,	0 0	0		No matche No matche No MS2 [M+H]+1 4145942 3860251 8,6 8,6
FALSO		C3 H Cl2 O Full match No results No results			391,7884		,	0 0	0		No matche No matche No MS2 [M+H]+1 3600700 8
FALSO FALSO		C4 H5 O17 Full match No results No results C2 H Cl N6 Full match No results No results			417,8727 4 477.8377			0 0	0		No matche No matche No MS2 [M+H]+1 3783235 3544616 8,6 8,6 No matche No matche No MS2 [M+DMSO- 2791313 7,5
FALSO		No results No results No results			89,02098 9	556,86 90.02826	-,	0 0	0		No matche No matche No MS2 [M+DMSO] 2791313 7,5 No matche No matche DDA for pri [M+H]+1 11444130 10092215 5,7 5,7
FALSO		C5 H3 O9 F Full match No results No results			299,8977			0 0	0		No matche No matche No MS2 [M+H]+1 2413005 9,1
FALSO		C3 H7 Cl N. Full match No results No results			233,9539 2			5 0	0		Single mat(No matche DDA for pri [M+H]+1 10458009 10699611 5,7 5,1
	Triethylene glycol	C6 H14 O4 Full match No results No results			150,0892			3 0	0		No matche No matche DDA for pri [M+Na]+1 4402322 4825392 9,1 9,1
FALSO		C3 H10 N4 Full match No results No results			180,0324			0 0	0		No matche No matche DDA for otl [M+2H]+2 11672777 5,7
FALSO		C H3 N6 Of Full match No results No results	No results No results		271,9371 2		1,074 5328314	0 0	0		No matche No matche DDA for pr [M+H]+1 5328314 5018501 8 8
		H3 O4 P No results No results No results			97,97694		1,215 15740570	1 0	0		Single mate No matche DDA for pre [M+H]+1 15740570 14842910 4 4
FALSO	pentabamate	C8 H16 N2 Full match No results No results	Full match Full match	-0,1	204,111 2	205,1183	1,481 7096646	20 0	0		Multiple m No matche DDA for pr [M+H]+1 7096646 6439135 7,8 7,8

FALCO	This was halfes	No results No results Full match No results	0.33 403 0456 404 0530	4.062 2204240	2 0		No material No material DDA forms (MATINA	2204240 2422572	0.00
FALSO FALSO		No results No results Full match No results No results No results No results No results	0,32 103,0456 104,0529 87,51355 88,52083	1,962 3384310 1 1015288	2 0 0		No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1	3384310 3132572 1015288 857058,1	8 8,6 5 3,4
FALSO		No results No results No match No results	3.71 185.949 186.9563	0,308 15634217	1 0 0			14466559 15634217	6,7 7,8
FALSO		No results No results No match No results	-2.59 277.9156 316.8788	1,111 1281640	1 0 0		No matche No matche DDA for otl [M+K]+1	1281640 1151278	8,8 7,2
FALSO		No results No results Full match Partial mat		1,96 3427847	14 0 0		Multiple m Single mat(DDA for pr [M+H]+1	3427847 3318526	8 8
FALSO		No results No results No match No results	-2,35 235,0886 236,0958	1,508 26870208	2 0 0		No matche No matche No MS2 [M+H]+1	26870208	5,1
FALSO		Invalid ma: No results Full match No results	0,37 83,03714 84,04442	0,358 50571963	6 20 0	49,6	No matche No matche DDA for pri [M+H]+1		2,9 4
FALSO	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		No matche No matche DDA for otl [M+H+Me(8 8
FALSO	C2 H Cl4 N(Full match	No results No results No results	3,25 389,7912 390,7985	1,142 3224729	0 0 0		No matche No matche No MS2 [M+H]+1	2682693 3224729	8,6
FALSO	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		Multiple m No matche DDA for pr [M+H]+1	3147192 3313026	9,1 8,6
FALSO		No results No results No results	0,99 299,8768 300,8841	1,129 3661653	0 0 0		No matche No matche DDA for pri [M+H]+1	3661653 3471252	8 8
FALSO		No results No results No results	0,84 331,8327 332,84	1,141 3435361	0 0 0		No matche No matche No MS2 [M+H]+1	3327478 3435361	8 8,6
FALSO		No results No results No results	105,9433 106,9506	1,11 7253175	0 0 0		No matche No matche DDA for pri [M+H]+1	7253175 6832726	7,8 7,8
FALSO		No results No results No results	88,00107 89,00835	0,339 2493898	0 0 0		No matche No matche DDA for pri [M+H]+1	2493898	9,1
FALSO FALSO		No results No results No results	-3,01 354,0043 355,0115	1,534 6599846	0 0 0		No matche No matche DDA for pri [M+H]+1	6599846	8,4
FALSO		No results No results No results No results No results No results No results	128,9719 129,9792	0,981 10098808	0 0 0		No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for otl [M+2H]+2	10098808 9460393 12304936 12902669	7,3 5,7
FALSO		No results No results No match No results	-2,81 590,2783 296,1464 1,49 184,0348 185,042	7,316 12902669 1,111 12259927	4 0 0			12248904 12259927	6,2 7,8 5,7 5,7
FALSO		No results No results No results No results	0,72 393,8669 394,8742	1,102 4083514	0 0 0		No matche No matche DDA for pri [M+H]+1	4083514 4056794	8,6 8,6
FALSO		No results No results No results	3,74 327,8907 328,898	0,978 7462217	0 0 0		No matche No matche No MS2 [M+H]+1	7141578 7462217	5,7 5,7
FALSO		No results No results No results	-0,05 980,6033 491,3089	7,395 7983220	0 0 0		No matche No matche DDA for otl [M+2H]+2	7983220 7733356	8,4 8,4
FALSO	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		No matche Multiple m DDA for pri [M+H-H2O	5039204 4419507	8 8
FALSO	tin(ii) 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		No matche No matche DDA for pri [M+H]+1	7001754 6585582	5,1 7,8
FALSO	C13 H2 N6 Full match	No results No results No results	-0,66 559,8644 560,8716	1,08 4352789	0 0 0		No matche No matche No MS2 [M+H]+1	4352789 4002639	8 8
FALSO		No results No results No match No results	-1,52 781,5623 782,5696	7,16 52030231	49 0 0		No matche No matche DDA for pri [M+H]+1	52030231	6,2
FALSO		No results No results No match No results	-2,89 467,3012 468,3085	6,926 8957842	5 0 0		No matche No matche DDA for pri [M+H]+1	5143749 8957842	8 8,9
FALSO	-	No results No results Full match No results	0,33 306,1064 307,1137	1,65 7439311	2 0 0		No matche No matche DDA for pri [M+H]+1	7439311 7044522	7,8 8,4
FALSO		No results No results No match No results	-1,29 781,5625 782,5698	7,272 43784322	49 0 0			43784322	5,7
FALSO FALSO		No results No results No results No results No results Full match Full match	-3,76 337,7778 338,7851 3,17 521,3498 522,3557	1,147 3226219 7,401 2932518	5 0 0		No matche No matche No MS2 [M+H]+1 Single mati No matche DDA for otl [M+H]+1	3226219 2193055 2782795 2932518	9,1 8,6 4,2 7,5
FALSO		No results No results No results No results	90,01624 91,02352	0,975 9995331	0 0 0		No matche No matche DDA for pri [M+H]+1	9995331	5,1
FALSO		No results No results No results No results	1,64 203,9497 204,957	1,07 4674244	0 0 0		No matche No matche No MS2 [M+H]+1	4674244 4331296	8 8,6
FALSO		No results No results No match No results	-3,24 206,9651 207,9724	1,194 475681,5	1 0 0			475681,5 434667	7,9 7,9
FALSO	No results	No results No results No results	809,3711 270,7976	1,173 5454052	0 0 0		No matche No matche DDA for otl [M+3H]+3	5454052	8,6
FALSO	C5 H2 N5 C Full match	No results No results No results	-2,05 178,9993 90,50694	7,582 30216323	0 0 0		No matche No matche DDA for otl [M+2H]+2	30216323 11145592	6,2 5,1
FALSO		No results No results No results	119,9736 120,9809	0,99 9804352	0 0 0		No matche No matche DDA for pri [M+H]+1	9248404 9804352	4,6 5,1
FALSO		No results No results No results	130,967 113,9637	0,304 1065488	0 0 0		No matche No matche No MS2 [M+H-H2O	1065488	8,3
FALSO		No results No results Full match Full match	0,1 188,1273 189,1346	1,229 4466616	8 0 0		Single mate Multiple m DDA for pre [M+H]+1	4364692 4466616	7,5 7,5
FALSO		No results No results No results	1247,68 624,8474	1,114 1913861	0 0 0		No matche No matche No MS2 [M+2H]+2	1913861	9,7
FALSO	1,1'-[2,6-Dimethyl-4-(3-nitrophenyl)-1,4-dihy C17 H18 N. Full match		0,09 314,1267 315,134 0.06 146,0215 147,0288	7,055 5164646	10 0 0		No matche No matche DDA for pri [M+H]+1	3997375 5164646	8,6 8
FALSO FALSO		No results No results Full match Full match No results No results No results	2.84 269.7904 270.7976	2,144 8545078 1,171 5021088	6 0 0		Multiple m No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1	8545078 8393743 5021088	7,3 8,9 7,5
FALSO		No results No results Full match No results	-3,58 195,0096 98,51205	7,381 60608138	4 0 0		No matche No matche DDA for otl [M+2H]+2		2,9 5,1
FALSO		No results No results No match No results	-4,08 611,3671 612,3744	7,461 8217571	1 0 0		No matche No matche DDA for pri [M+H]+1	5752749 8217571	6,2 8,4
FALSO		No results No results No results	-4,3 395,7378 474,76	1,142 2589920	0 0 0		No matche No matche No MS2 [M+DMSO-		8 8
FALSO	C4 H2 O13 Full match	No results No results No results	-3,85 383,8397 462,8616	1,102 3526258	0 0 0		No matche No matche DDA for otl [M+DMSO-	3526258 3490383	8,6 8,6
FALSO	No results	No results No results No results	86,98628 87,99355	0,979 8297366	0 0 0		No matche No matche DDA for pri [M+H]+1	8297366	5,1
FALSO	C2 H Cl4 P Full match	No results No results No results	4,16 195,8578 196,8651	1,168 5823920	0 0 0		No matche No matche DDA for pri [M+H]+1	5823920 5629069	8,9 6,4
FALSO		No results No results No results	-3,32 157,0165 79,51555	0,994 8220452	0 0 0		No matche No matche DDA for otl [M+2H]+2	8220452 7022212	5,7 6,2
FALSO		No results No results Full match No results	-0,02 191,0252 192,0325	1,794 5916322	1 0 0		No matche No matche DDA for pri [M+H]+1	5916322 5757167	6,2 8,4
FALSO		No results No results No results	0 892,5508 447,2827	7,411 7547466	0 0 0		No matche No matche DDA for otl [M+2H]+2	7547466 7008658	6,7 8,4
FALSO FALSO		No results No results No results No results No results No results No results	1,76 247,9917 248,999 -0.04 475,1914 238,603	1,196 3411583 1.937 2886140	0 0 0		No matche No matche DDA for pri [M+H]+1	3411583 2886140 2714277	8
FALSO		No results No results No results No results	-0,04 475,1914 238,603 1255,704 628,8591	1,081 3718970	0 0 0		No matche No matche DDA for otl [M+2H]+2 No matche No matche No MS2 [M+2H]+2	3718970	8 7,5
FALSO		No results No results No results No match	4,49 655,3934 656,4007	7,457 8018230	0 0 0		No matche Multiple m DDA for pri [M+H]+1	5521965 8018230	6,4 8,4
FALSO		No results No results No match No results	1,02 199,9304 241,9642	0,978 6623217	1 0 0		No matche No matche No MS2 [M+ACN+H	6597732 6623217	6,7 7,3
FALSO		No results No results No results	-3,71 165,0572 83,5359	0,977 7977743	0 0 0		No matche No matche No MS2 [M+2H]+2	7977743 6594971	5,1 7,3
FALSO	No results	No results No results No results	473,8263 474,8335	0,989 7652747	0 0 0		No matche No matche DDA for pri [M+H]+1	7320004 7652747	5,7 3,5
FALSO	No results	No results No results No results	361,8789 362,8861	0,994 8089065	0 0 0		No matche No matche DDA for pri [M+H]+1	7834986 8089065	4,6 5,7
FALSO	ETHYL 1-NITROSOPROLINE C7 H12 N2 Full match	No results No results Full match Partial mat	., . ,	1,611 5046765	9 0 0		Multiple m Multiple m DDA for pre [M+H]+1	5044075 5046765	8 8
FALSO		No results No results No results	0,75 217,9409 218,9482	0,979 7927857	0 0 0		No matche No matche DDA for pri [M+H]+1	7927857	6,2
FALSO		No results No results Full match Partial mat		0,992 7194900	3 0 0		No matche Single mati No MS2 [M+2H]+2	5720077 7194900	7,3 4,6
FALSO		No results No results Full match Partial mat		1,944 2772704	9 0 0		No matche Multiple m DDA for pri [M+H]+1	2772704 2662442	8 8
FALSO FALSO	1-[(8Z,11Z,14Z)-icosatrienoyl]-sn-glycero-3-p C28 H52 N Full match	No results No results Full match No results No results No results No results No results	0,1 545,3482 546,3555 0,41 567,341 568,3482	7,121 9341779 7,474 7242375	3 0 0		No matche No matche DDA for pr [M+H]+1	9341779 5145383 7242375	6.4 8.4
FALSO		No results No results No results No results	0,41 567,341 568,3482 1571,635 786,8248	1,097 2606047	0 0 0		No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for otl [M+2H]+2	2606047 2452144	6,4 8,4 8.6 8
FALSO		Invalid ma: No results Full match No results	0,46 246,0853 247,0926	1,097 2606047	4 2 0	57,6		12869103 12421495	5,7 6,2
FALSO		No results No results No results No results	1,41 222,9818 223,989	0,975 6777014	0 0 0	57,0	No matche No matche No MS2 [M+H]+1	6777014 6548210	6,2 7,3
FALSO		No results No results No results	7 7000	0,305 2478358	0 0 0			2478358	8,6
FALSO		No results No match No results		0,979 7208924	1 0 0		No matche No matche No MS2 [M+H]+1		6,7 6,2
FALSO		No results No results No results	1283,711 642,863	1,098 2164439	0 0 0		No matche No matche DDA for otl [M+2H]+2		8,6 8,6
FALSO		No results No results No results		1,143 2130818	0 0 0		No matche No matche No MS2 [M+H]+1	2130818 2024250	8,6 8,6
FALSO		No results No results No results		1,109 9645940	0 0 0		No matche No matche DDA for pri [M+NH4]+:		7,3 6,7
FALSO		No results No results No results		1,001 7745095	0 0 0		No matche No matche DDA for pri [M+H]+1	6957333 7745095	4,6 4,6
FALSO		No results No match No results		1,223 5282511	1 0 0		No matche No matche DDA for pri [M+H]+1	4996410 5282511	8,6 8,6
FALSO	4-(1,2,4-Triazol-3-ylazo)-N-benzyl-N-methyla C16 H16 Ni Full match		0,89 292,1439 293,1512 104,9968 106,0041	1,118 9550897 0,982 6737155	2 2 0 0 0	86,5	No matche No matche DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1	9550897 8172315 5997114 6737155	6,2 4 5,7 4,6
FALSO		No results No results No results No results No results No results No results		6,829 3533642	0 0 0		No matche No matche DDA for pri [M+H]+1		5,7 4,6 9,7 9,1
		No results No results Full match Partial mat		1,28 4140231	2 0 0		No matche Multiple m DDA for pri [M+H]+1	4140231	8,6
FALSO		No results No results No results No results		1,109 1707107	0 0 0		No matche No matche No MS2 [M+DMSO-		8,8
FALSO		No results No results No results		1,146 2902085	0 0 0		No matche No matche No MS2 [M+H]+1	2902085	8,6
FALSO		No results No results No results		1,078 3481647	0 0 0		No matche No matche No MS2 [M+H]+1	3481647	8
FALSO	C6 H3 N2 C Full match	No results No results No results	-2,86 371,8762 372,8834	1,076 3414786	0 0 0		No matche No matche No MS2 [M+H]+1	3414786 3193689	8 8
FALSO		No results No results No results	323,801 324,8082	1,147 2943159	0 0 0		No matche No matche No MS2 [M+H]+1		8,6 8,6
		No results No results Full match No results		1,334 3493663	1 0 0		No matche No matche DDA for pri [M+H]+1	3288652 3493663	8 8
FALSO		No results No results No results	357,8581 436,8797	1,108 1275676	0 0 0		No matche No matche No MS2 [M+DMSO-	1275676	8,8
FALSO FALSO		No results No results No results No results	397,7335 398,7408	1,148 2679584 0,308 6077252	0 0 0		No matche No matche No MS2 [M+H]+1		8,6 8,6 7,8
FALSO		No results No results No results No results No results No results No match No results		1,237 6505148	2 0 0		No matche No matche No MS2 [M+ACN+H No matche No matche DDA for pri [M+H]+1	6505148 6344499	6,2 8,4
		No results No results Full match Full match		1,157 2968460	11 0 0		Multiple m No matche No MS2 [M+H]+1	2759867 2968460	8 7,5
FALSO		No results No results No results No results	0,13 293,2203 294,2275	7,343 3857325	0 0 0		No matche No matche DDA for pri [M+H]+1	3857325	8

FALSO		C5 H6 Cl3 Full match No results No resu	ults No results No results	2,92 467,808	6 468,8149	1,134	2286996	0	0	0		No matche No matche No MS	2 [M+H]+1	2286996	2134414	8,6	8,6
FALSO		No results No results No resu	ults No results No results	313,772	1 314,7794		3064316	0	0	0		No matche No matche DDA fo	or pri [M+H]+1	3064316	2882215	9,1	8,6
FALSO		C7 H5 N3 C Full match No results No resu		-3,47 195,009			9870344	4	-	0		No matche No matche DDA fo				6,2	
FALSO		C4 H Cl4 N. Full match No results No resu			4 422,7465		1971296	0		0		No matche No matche No MS		1971296	1367695	8,6	8,3
FALSO		C6 H Cl2 O: Full match No results No resu					2051402	0		0		No matche No matche No MS			2051402		8,6
FALSO		C7 H3 Cl N(Full match No results No resu					1520045	0	0	0		No matche No matche No MS		1520045	1337910	7,7	8,8
FALSO		C11 H3 O1 Full match No results No results C5 H7 N4 C Full match No results No results		0,01 485,8 -0,85 439,863	6 486,8673		2893494 3362707	0	0	0		No matche No matche No MS No matche No matche No MS		2893494 3362707	2714973 3173760	5,9 8	3,7
FALSO		C5 H6 O3 Full match No results No resu					25477843	15	0	0		Single match No matche DDA for			25477843	0	5,1
FALSO	Cidane annyanae	No results No results No resu		387.704			3172589	0	-	0		No matche No matche DDA fo		3172589	2983934	7,5	8
FALSO		C35 H62 N: Full match No results No resu		-3.83 699.419			6922140	0	0	0		No matche Multiple m DDA fo		4859734	6922140	5,9	8,4
FALSO		C H3 Cl2 O: Full match No results No resu		.,,,			2070295	42	0	0		No matche No matche No MS		2070295		8,6	
FALSO		C7 H Cl O9 Full match No results No resu		3,28 325,879			3329882	0	0	0		No matche No matche No MS		3329882	3293292	8,6	9,1
FALSO		C7 H6 Br2 No results No results No resu		1,84 247,884	1 248,8914	1,113	1775754	3	0	0		No matche No matche DDA fo		1775754	1489558	8,8	8,8
FALSO		C35 H73 N: Full match No results No resu	ults No results No results	3,88 684,55	7 343,2858	7,159	32369620	0	0	0		No matche No matche DDA fo	or otl [M+2H]+2	32369620	30686054	5,7	5,7
FALSO		C9 H7 O3 F Full match No results No resu	ults No match No match	4,08 194,014	1 98,01431	0,299	408416,1	1	0	0		No matche Single mat No MS	2 [M+2H]+2		408416,1		8,5
FALSO	1-(Tetrahydro-2-furoyl)piperazine	C9 H16 N2 Full match No results No resu					3255076	10		0		No matche Multiple m DDA fo		2916006	3255076	8	8
FALSO		No results No results No resu			8 696,8464		3095868	0	-	0		No matche No matche No MS			2862176	8	8
FALSO		C47 H82 N! Full match No results No resu					2916221	1	0	0		No matche No matche DDA fo			2916221	8,6	8
FALSO		No results No results No resu		,	9 676,8568	7	2007785	0	0	0		No matche No matche No MS			2007785	8,6	8,6
FALSO	1-[(9Z)-hexadecenoyl]-sn-glycero-3-phospho			-0,03 493,316			8404180	0	0	0		No matche Multiple m DDA fo		8404180 954754.4	7821095 1082665	6,7	7,8
FALSO		No results			4 109,5216 3 182,9851		1082665 55893789	0	-	0	_	No matche No matche No MS No matche No matche DDA fo			55893789	6,6	8,8 5,7
FALSO		C4 H5 Cl4 I Full match No results No resu					2159627	0	0	0		No matche No matche No MS		2159627	1616034	8	7,7
FALSO		C2 H5 N O2 Full match No results No resu					4970053	10	0	0		Multiple m No matche DDA fo		4181326	4970053	7	4,8
FALSO	2-arachidonyl-sn-glycero-3-phosphoethanola				5 502,2928		13739508	5	-	0		No matche Multiple m DDA fo		13739508		7,3	7,3
FALSO	, , , , , , , , , , , , , , , , , , , ,	No results No results No resu			8 110,5217		1741042	0		0		No matche No matche No MS			1741042	,-	8,8
FALSO	L-Cysteinylglycine disulfide	C8 H15 N3 Full match No results No resu					4022448	4	-	0		No matche No matche DDA fo		4022448	3752419	7,5	6,4
FALSO		C6 H2 N2 C Full match No results No resu		-4,13 181,977			54288075	2	0	0		No matche No matche DDA fo		54288075		6,2	
FALSO		C29 H41 N! Full match No results No resu		-2,62 523,314	5 524,3218	7,486	6245885	0	0	0		No matche No matche DDA fo		4617531	6245885	5,9	8,4
FALSO	3-Hydroxy-2,2-bis(hydroxymethyl)propyl noi	C14 H28 O. Full match No results No resu	ults Full match Partial ma	t -0,27 276,193	6 277,2009	7,341	3134404	1	0	0		No matche Single mati DDA fo	or pre [M+H]+1	3134404	2718808	8	8
FALSO		C10 H4 N4 Full match No results No resu			,		1157975	0	0	0		No matche No matche No MS		1157975	1060230	8,8	8,8
FALSO		C5 H3 Br Cl Full match No results No resu		4,69 363,780			1722235	0	0	0		No matche No matche No MS		1722235	1627467	8,3	8,3
FALSO	1-arachidonoyl-sn-glycero-3-phosphocholine			0,19 543,332			5446376	3	0	0		No matche No matche DDA fo		5446376	3457440	7	6,4
FALSO		C16 H14 N Full match No results No resu		-3,58 354,106			2138709	2		0		No matche Multiple m DDA fo		2138709	2112412	8,6	8,6
FALSO		C5 H4 O2 Full match Invalid ma: No resu					5213733	6		0	67,5	Single mate No matche DDA fo		5213733		5,9	
FALSO		C6 H N2 O1 Full match No results No resu		700 0070	,	-	1269914	0		0	_	No matche No matche No MS		1269914	1002212	8,3	0.1
FALSO		No results			3 684,8438 1 330,7534	7	1893212 2908293	0	0	0		No matche No matche No MS No matche No matche DDA fo		1679842 2908293	1893212 2841453	8,3	9,1
FALSO		C7 H15 N3 Full match No results No resu					6912798	3	0	0		No matche No matche No MS			6512404	5,1	3,5
FALSO		No results No results No resu			6 710,8504		1718925	0	-	0		No matche No matche No MS		-	1718925	8,3	8,3
FALSO	glu-asp	C9 H14 N2 Full match No results No resu		0,25 262,080			6798736	5	-	0		No matche No matche DDA fo		6798736	6429320	5,7	6,2
FALSO	8.2 205	No results No results No resu	ults No results No results		6 92,52234		2176237	0	0	0		No matche No matche No MS		2176237		8,6	-,-
FALSO		C7 H6 Br Cl Full match No results No resu					1948735	0	0	0		No matche No matche No MS		1276703	1948735	7,7	8
FALSO	carglumic acid	C6 H10 N2 Full match No results No resu	ults Full match No results	0,25 190,05	9 223,0925	1,283	3182306	11	0	0		No matche No matche DDA fo	or pre [M+H+Me	3182306		8,6	
FALSO	Cystine	C6 H12 N2 Full match No results No resu	ults Full match Full match	0,05 240,023	9 241,0311	1,17	4070155	4	0	0		Single mate No matche DDA for	or pre [M+H]+1	4070155	3687840	9,1	8,6
FALSO	EDDA	C6 H12 N2 Full match No results No resu	ults Full match No results	-0,2 176,079	7 177,0869	2,011	7432640	13	0	0		No matche No matche DDA fe	or pre [M+H]+1		7432640		5,7
FALSO		C5 H Cl N2 Full match No results No resu					2326058	0	0	0		No matche No matche No MS			2219348	8,6	8,6
FALSO	(Z)-dehydrobutyrine	C4 H7 N O2 Full match No results No resu					7081408	24	-	0		Multiple m No matche DDA fo		7081408	6988444	4	2,4
FALSO		No results No results No resu			6 287,8888	-,	1246007	0	-	0		No matche No matche DDA fo			1246007		8,8
FALSO	0	C8 H14 N2 Full match No results No resu		-0,04 234,085			9235353	5	0	0		No matche No matche DDA fo			9235353		6,7
FALSO		C9 H11 N2 Full match No results No results C2 H8 CI N Full match No results No results		-0,44 591,812 0,98 222,939			2232711 2213296	0	0	0	_	No matche No matche No MS No matche No matche DDA fo			2232711	8,6	5,9
FALSO		C2 H5 Cl N; Full match No results No resu					5497329	0	-	0		No matche No matche No MS		4851798	5497329	4.8	8,6 7
FALSO		No results No results No resu			3 77,99883		1869355	0		0		No matche No matche DDA fo		708660,6	1869355	6,3	7,2
FALSO	Nefiracetam	C14 H18 N. Full match No results No resu					2505773	13	-	0		No matche Multiple m DDA fo		2385898	2505773	9,1	8,6
FALSO		No results No results No resu			7 334.915		2120490	0	0	0		No matche No matche No MS		2120490	1959400	8,6	8,6
FALSO		C2 H N2 O1 Full match No results No resu		-1,16 321,87	9 322,8868		1125406	0	0	0		No matche No matche No MS			1125406	- 7,1	8,8
FALSO	2,2'-(Decylimino)diethanol	C14 H31 N Full match Invalid mas No resu	ults Full match No results	0,01 245,235	5 246,2428	6,272	2843111	1	2	0	48,5	No matche No matche DDA fo	or pre [M+H]+1	2564829	2843111	8	8
FALSO		C2 H Cl2 N. Full match No results No resu		1,24 423,736	4 424,7436		1725721	0	0	0		No matche No matche No MS	2 [M+H]+1		1725721		8,3
FALSO		C4 H6 O2 S Full match Invalid ma: No resu				7	3561642	7		0	43,7	No matche Single mate DDA fo		3561642	3299773	8	8
FALSO		C2 H3 N2 C Full match No results No resu					5447523	0	-	0		No matche No matche DDA fo			5447523		5,3
FALSO		C4 H7 N2 C Full match No results No resu		,	5 368,8923		1801387	0	0	0		No matche No matche No MS		1801387	1267270	6,6	7,2
FALSO		No results No results No resu			8 148,9353		2523855	0	0	0		No matche No matche No MS		2523855	2276635	8	8
FALSO		C4 H2 N4 C Full match No results No results C3 H5 Cl3 C Full match No results No results		-1,1 199,965 -0,17 431,768			574266,5 1767601	0		0		No matche No matche DDA for No matche No matche No MS		1767601	574266,5 1730479	4,9 7,7	3,6 7,7
FALSO		No results No results No resu			7 432,7753 8 640.8214		954884.1	0	0	0		No matche No matche No MS		1/0/001	954884,1	7,7	8,8
FALSO		No results No results No resu			7 372,738		2374858	0	0	0		No matche No matche No MS		2374858	2191890	8	8
FALSO		C2 H2 N4 P Full match No results No resu		-4,1 143,974			29402601	1	0	0		No matche No matche DDA fo		-		5.7	5,7
FALSO		No results No results No resu			5 102,0558		5864340	0	0	0		No matche No matche DDA fo				6,2	6,2
FALSO		C52 H99 O Full match No results No resu					4960488	0	0	0		No matche No matche DDA fo				7	8
FALSO		No results No results No resu	ults No results No results		4 608,8693		1737427	0	0	0		No matche No matche No MS				8,3	8,3
FALSO		C3 H Cl2 Ol Invalid ma: No results No resu					1486532	0		0		No matche No matche No MS				7,7	7,7
FALSO	N-(3-Amino-2,6-dimethylphenyl)-2-(diethyla						6181111			0		No matche No matche DDA fo				7,8	6,2
FALSO		No results No results No resu			3 614,8187		890979	0	0	0		No matche No matche No MS			890979		8,8
FALSO		C4 H7 Cl2 I Full match No results No resu					1890254	0	0	0		No matche No matche No MS			1742403	8	7,7
FALSO		C38 H65 N Full match No results No results					2111232	0	-	0		No matche No matche DDA fo				9,1	9,1
FALSO		C38 H65 N Full match No results No results			7 322,8112		5785850 2347242	0		0		No matche No matche DDA for No matche No matche No MS				7,5 8,6	6,2 5,9
FALSO		No results No results No results No results No results No results			7 322,8112 4 110,5217		1725593	0		0		No matche No matche No MS No matche No matche No MS				8,6	7,9
FALSO		C6 H13 N3 Full match No results No resu					4427194	1	-	0		No matche No matche DDA fo				4.8	6,4
FALSO		No results No results No resu			9 446,6707		2065330	0	-	0		No matche No matche No MS				9,1	8,6
	Dihydrouridine	C9 H14 N2 Full match No results No resu					1712775	2		0		No matche No matche DDA fo				7,2	7,7
FALSO		No results No results No resu			6 98,91987		3025593	0	-	0		No matche No matche DDA fo			2948128	7,5	9,1
FALSO		C6 H10 N2 Full match No results No resu					2163265	3	0	0		No matche No matche DDA fo			2163265	7,5	9,1
FALSO		C16 H21 O Full match No results No resu	ults No results No results	0,52 308,117	9 309,1252		6985323	0	0	0		No matche No matche No MS	2 [M+H]+1	6985323	6284198	3,5	4,6
FALSO		No results No results No resu			5 83,02163		6133546	0	-	0		No matche No matche DDA fe		6133546		7,3	
FALSO		No results No results No resu			7 212,839		3557430	0		0		No matche No matche No MS		3557430		8,6	6,4
FALSO		C7 H2 N6 C Full match No results No resu					939666,9	0	0	0		No matche No matche No MS				8,3	8,5
FALSO	[Similar to: (1R,2R,5S,8S,9S,10R,11R,12S)-5,1				8 144,9921		5610042	0		0	41	No matche No matche DDA fo		5610042		4,8	5,3
FALSO		C H Cl2 O8 Full match No results No resu	ins No results No results	-2,57 305,82	2 306,8292	1,142	1564713	0	0	0		No matche No matche No MS	2 [M+H]+1	1564/13	1413632	8,3	7,7

FALSO				No results No results	-0,19 759,8148			1304428	0	0 0		No matche No n				8,8	
FALSO				No match No results	0,28 240,0958			2801857	1	0 0			natche DDA for pre [M+H]+1		2801857	8,6	8
FALSO				No results No results	-1,45 449,7478			1677338	0	0 0		No matche No n			1534113	7,7	7,7
FALSO				No results No results		109,0196		5182396	0	0 0		No matche No n			4800889	5,9	5,3
FALSO				No results No results	2,57 381,7596	,	-	2146509	0	0 0		No matche No n			2050467	8,6	7,5
FALSO				No results No results	-1,69 178,9994	90,50697		20082808	0	0 0			natche DDA for otl [M+2H]+		20082808		5,1
FALSO				No results No results	451,827	530,8489	1,101	1850460	0	0 0		No matche No n			1850335	8,3	8,3
FALSO				No results No results		692,8333	1,107	1883461	0	0 0		No matche No n			1883461		8,3
FALSO	Guanylmelamine			Full match No results	1,71 168,0875	,	-,	4112476		10 0	66,7		natche DDA for pri [M+H]+1			5,3	/
FALSO				No results No results	-1,23 339,9246		1,077	2631258	0	0 0		No matche No n			2528495	8	8
FALSO	Abdraus and a Pract According to 2 and			No results No results	137,8992		1,166	3490696	9	0 0			natche DDA for pri [M+H]+1		3360527	5,3	4,2
FALSO	thiomorpholine-3-carboxylic acid			Full match Full match	0,39 147,0355			1665189	-	0 0			natche DDA for pri [M+H]+1		1572729	7,2	8,3
FALSO	[Cimilar to 2 Undrawn 1 [2 (triffmannathul)			No results No results No results No results	0,3 712,7857 189.9047	357,4001 190,912	0,995 1,109	3195827 3436642	0	2 0	44.7	No matche No n	natche No MS2 [M+2H]+ natche DDA for pri [M+H]+1		3195827 3072176	4,2 4,8	5,3 4,8
FALSO	[Similar to: 3-Hydroxy-1-[3-(trifluoromethyl)			No match No results	3.08 316.1522	334,186		17910419	1	0 0	44,7		natche DDA for otl [M+NH4		17910419	4,0	6,2
FALSO				No results No results	0,83 164,0287			5654978	0	0 0			natche DDA for otl [M+2H]+		5654978		4.2
FALSO				No results No results	295,7931			1538302	0	0 0		No matche No n			1507150	8,3	8,3
FALSO	tyrosine O-sulfate			Full match No results	-0,17 261,0307		3,287	2207160	4	0 0			natche DDA for pri [M+H]+1		2056721	8	7,5
FALSO	tyrosine o sunate			No results No results	4,87 200,9684			789167.9	0	0 0		No matche No n			2030/21	9	7,5
FALSO				No results No results		414,7148	1,145	1370690	0	0 0		No matche No n			1283533	8,8	8,3
FALSO				No match No match	0.48 316.1077	-	1,144	5063117	2	0 0		No matche Mult			4874289	4,8	4.8
FALSO				No results No results	.,	764,8339		2090811	0	0 0		No matche No n				8	7,5
FALSO				No results No results	-3,11 249,9315		0,989	5021930	0	0 0		No matche No n		5021930	4805488	5,3	3,2
FALSO		No results	No results No results	No results No results	219,0289		7,55	35306141	0	0 0			natche DDA for otl [M+2H]+	2 35306141	7742551	5,1	6,2
FALSO	1,3-Dimethylbutylamine	C6 H15 N Full match	No results No results	Full match Full match	0,31 101,1205			42905725	15	0 0			natche DDA for pre [M+H]+1		42905725	4	5,7
FALSO				No results No results	287,7615			3101800	0	0 0		No matche No n			2943008	4,8	8
FALSO		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		No matche No n	natche No MS2 [M+H]+1	1770628	1650734	7,7	8,3
FALSO		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		No matche No n	natche No MS2 [M+H]+1		2028603	8	8
FALSO		No results	No results No results	No results No results	192,1238	193,1311	1,113	5554087	0	0 0		No matche No n	natche No MS2 [M+H]+1	5554087	5059809	5,9	5,3
FALSO				No results No results	-0,99 393,7861	394,7927	1,141	1533865	0	0 0		No matche No n	natche DDA for pro [M+H]+1		1533865		7,7
FALSO	Methylsulfonylmethane			Full match Full match	0,26 94,00887	95,01615	1,95	2837664	1	0 0			natche DDA for pri [M+H]+1		2837664	8	7,5
FALSO				No results No results		616,8564	1,097	1409587	0	0 0		No matche No n			1344181	8,3	7,7
FALSO				No results No results		668,8698	1,097	1228120	0	0 0		No matche No n				8,3	8,3
FALSO				No results No results	1,58 401,8951	402,9024	1,063	1657362	0	0 0		No matche No n			1388048	8,3	8,3
FALSO				No match No results	0,22 369,0665	,		1972295	1	0 0			natche DDA for pre [M+H]+1		1704449	8	8,3
FALSO				No results No results	4,81 217,9033			4624909	0	0 0			natche DDA for pre [M+H]+1		4624909	4,8	2,6
FALSO		140 results	140 results 140 results	No results No results		114,8939		2112972	0	0 0		No matche No n				9,1	7
FALSO				No results No results	4,89 477,7471		1,142	1320726	0	0 0		No matche No n			1231379	8,3	7,7
FALSO				No results No results	-3,27 189,0701	207,104		1858261	0	0 0		No matche No n				7,2	8,3
	9-Decenoylcarnitine			Full match No results	-0,18 313,2253		-,	2310097	1	0 0			natche DDA for pri [M+H]+1		2310097	7,5	8
FALSO	Pyrogallol			Full match Full match	0,49 126,0318	127,039		1811858	24	0 0		Multiple m Mult				7,2	
FALSO				No results No results		744,8444		1249997	0	0 0		No matche No n				8,3	
FALSO				No match No results	4,23 253,8085			1332740	1	0 0			natche DDA for pri [M+H]+1			7,2	7,7
FALSO	Phenylethyl alcohol			Full match Full match	0,09 122,0732			45006641		10 0	45,3		le mati DDA for pri [M+H]+1		23232928	5,7	4
FALSO				No results No results		752,8312	1,097	1142906	0	0 0		No matche No n			1142906 1368248	8,3	8,8
	Oleandeamitica			No results No results		742,8389	1,097		0	-		No matche No n				9.6	8,3
FALSO	Oleoylcarnitine			Full match No results	0,04 425,3505		7,328	2305457	7	0 0			natche DDA for pri [M+H]+1		2061652	8,6	7,5
FALSO	N-Nonanoylmorpholine			Full match No results No results	-0,09 227,1885			4117598 982646,8	0	0 0		No matche No n	natche DDA for pri [M+H]+1 natche No MS2 [M+2H]+		4104710 982646.8	7,5	7,5
FALSO		C2 H2 Cl N; Full match				760,8204		1577357	0	0 0			natche DDA for pri [M+H]+1		982040,8	8,8	9,3
					-0,79 341,772					-					1022202		0.2
FALSO	Diss of hydrodenium	No results	No results No results	No results No results	311,7751	312,7824	1,173	1953887	0	0 0	42.2	No matche No n	natche No MS2 [M+H]+1	1953887		8,6	8,3
FALSO	Dimethylcadmium	No results C2 H6 Cd No results	No results No results Invalid ma: No results	No results No results Full match No results	311,7751 -4,88 143,9496	312,7824 144,9569	1,173 0,306	1953887 395242,6	0	0 0 1	42,2	No matche No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1	1953887 395242,6	1822282 260244,6	8,6 8,2	8,3 7,1
FALSO FALSO	Dimethylcadmium DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match	No results Invalid ma: No results Invalid ma: No results	No results Full match Full match Full match	311,7751 -4,88 143,9496 0,06 146,1055	312,7824 144,9569 147,1128	1,173 0,306 1,164	1953887 395242,6 2155294	0 1 18	0 0 1 0 8 0	42,2 65	No matche No n No matche No n Multiple m No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1	1953887 395242,6 2155294	260244,6	8,6 8,2 7	7,1
FALSO FALSO	DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match	No results Invalid ma: No results Invalid ma: No results No results No results	No results Full match No results Full match No results No results No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885	312,7824 144,9569 147,1128 134,9958	1,173 0,306 1,164 0,967	1953887 395242,6 2155294 3922205	0 1 18 0	0 0 1 0 8 0 0 0		No matche No n No matche No n Multiple m No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1	1953887 395242,6 2155294 3304768	260244,6 3922205	8,6 8,2 7 4,2	7,1 5,3
FALSO FALSO FALSO		No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match	No results Invalid ma: No results Invalid ma: No results No results No results No results No results	No results Full match No results Full match No results No results Full match Full match Full match Full match	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216	312,7824 144,9569 147,1128 134,9958 129,0183	1,173 0,306 1,164 0,967 2,383	1953887 395242,6 2155294 3922205 7256678	0 1 18	0 0 1 0 8 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for oti [M+H-H2	1953887 395242,6 2155294 3304768 20 6896063	260244,6 3922205 7256678	8,6 8,2 7 4,2 5,7	7,1 5,3 7,3
FALSO FALSO FALSO FALSO	DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C9 H14 P2 Full match	No results No results Invalid ma No results Invalid ma No results	No results Full match Full match No results No results No results Full match Full match No match No results No match No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224	1,173 0,306 1,164 0,967 2,383 0,32	1953887 395242,6 2155294 3922205 7256678 1259932	0 1 18 0 6 3	0 0 0 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for otl [M+H-H2 natche No MS2 [M+2H]+1	1953887 395242,6 2155294 3304768 20 6896063 2 1259932	260244,6 3922205 7256678 1083387	8,6 8,2 7 4,2 5,7 4,5	7,1 5,3 7,3 8,8
FALSO FALSO FALSO	DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C9 H14 P2 Full match C4 H3 N2 C Full match	No results Invalid ma: No results Invalid ma: No results	No results Full match No results Full match No results No results Full match Full match Full match Full match	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863	1,173 0,306 1,164 0,967 2,383 0,32 1,055	1953887 395242,6 2155294 3922205 7256678	0 1 18 0	0 0 1 0 8 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for otl [M+H-H] natche No MS2 [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 0 6896063 2 1259932 1425737	260244,6 3922205 7256678	8,6 8,2 7 4,2 5,7	7,1 5,3 7,3
FALSO FALSO FALSO FALSO FALSO	DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C9 H14 P2 Full match C4 H3 N2 C Full match No results	No results No results Invalid mai No results	No results Full match No results Full match No results No results No results Full match No match No mesults No mesults No results No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972	1953887 395242,6 2155294 3922205 7256678 1259932 1425737	0 1 18 0 6 3	0 0 0 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n No matche No n No matche No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for otl [M+H-H] natche No MS2 [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 20 6896063 2 1259932 1425737 4576228	260244,6 3922205 7256678 1083387 1201043	8,6 8,2 7 4,2 5,7 4,5 8,3	7,1 5,3 7,3 8,8
FALSO FALSO FALSO FALSO FALSO FALSO	DL-Lysine	No results	No results No results Invalid ma: No results	s No results Full match No results Full match Full match No results Full match No results Full match No results Full match No results No results No results No results No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228	0 1 18 0 6 3 0	0 0 0 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for ott [M+H-H: natche No MS2 [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 0 6896063 2 1259932 1425737 4576228 2 3791663	260244,6 3922205 7256678 1083387 1201043	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8	7,1 5,3 7,3 8,8 8,8
FALSO FALSO FALSO FALSO FALSO FALSO FALSO	DL-Lysine	C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C9 H14 P2 Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match	No results Invalid max Invalid max Invalid max No results	s No results 6 Full match 10 Full match 10 Full match 11 Full match 12 Full match 13 Full match 14 Full match 15 No results 15 Full match 16 No results 17 No results 18 No match 18 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663	0 1 18 0 6 3 0 0	0 0 0 1 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for oti [M+H]+1 natche No MS2 [M+2H]+1 natche No MS2 [M+H]+1 natche DDA for oti [M+H]+1 natche DDA for oti [M+H]+1 natche DDA for pri [M+H]+1	1953887 395242,6 2155294 3304768 0 6896063 2 1259932 1425737 4576228 2 3791663	260244,6 3922205 7256678 1083387 1201043 2882505 1302971	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8	7,1 5,3 7,3 8,8 8,8 5,3
FALSO FALSO FALSO FALSO FALSO FALSO FALSO FALSO	DL-Lysine	C2 H6 Cd No results C2 H6 Cd No results C6 H14 N2 Full match C5 H6 O5 Full match C9 H14 P2 Full match No results C5 H6 N2 Full match V6 Full Match No results C5 H14 N2 Full match C7 H2 O7 F Full match	No results No results Invalid ma: No results	s No results No results Full match No results Full match Full match S No results No results Full match No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822	0 1 18 0 6 3 0 0	0 0 0 1 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ott [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 20 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3	260244,6 3922205 7256678 1083387 1201043 2882505 1302971	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7	7,1 5,3 7,3 8,8 8,8 5,3 7,7
FALSO	DL-Lysine	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C2 H2 Br CI Full match	No results No results Invalid max No results	s No results No results Full match Full match S No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276	0 1 18 0 6 3 0 0 0 5	0 0 0 1 1 0 8 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ott [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 20 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0- 895720,3 2	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3
FALSO	DL-Lysine	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C5 H3 N2 C Full match No results No results C5 H14 N2 Full match O7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N9 F Full match C2 H3 N9 F Full match C2 H3 N9 F Full match	No results No results Invalid ma. No results	s No results No results Full match No results In Ull match No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 (26907293 3937032 1507486	0 1 1 18 0 6 3 0 0 5 0 0 0 0 0 1 1 0 0	0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ot [M+2H]+1 matche DDA for ot [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+DH]+1	1953887 395242,6 2155294 3304768 20 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 3103591 1 1507486	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 7,7 8,3 4 8 7,2
FALSO	DL-lysine Acetonedicarboxylic Acid	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C3 H3 N5 Full match C4 H3 N6 Full match N6 Full match N7 Full match N8 Full match N8 Full match N9 Full match	No results No results Invalid max No results	s No results No results Full match No results Full match S Full match S No results No results S Full match Full match S No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895	0 1 18 0 6 3 0 0 0 0 5 0 0 0	0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche DDA for ort [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 476228 2 3791663 1427822 O 895720,3 2 3103591 1 1507486 5005895	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8	7,1 5,3 7,3 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2
FALSO	DL-lysine Acetonedicarboxylic Acid	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 N8 C Full match C1 H3 N9 F Full match C2 H3 N9 F Full match C2 H3 N9 F Full match C1 H3 N5 Full match No results C1 H2 N8 C Full match No results C1 H2 N8 C Full match	No results No results Invalid ma: No results	s No results No results F full match No results F full match S in Full Match S	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373	312,7824 144,9569 147,1128 134,9558 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860	0 1 18 0 6 3 0 0 0 5 0 0 0 0 1 1 0	0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n	matche No MS2	1953887 395242,6 2155294 3304768 20 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 3103591 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7
FALSO	DL-lysine Acetonedicarboxylic Acid	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C5 H3 N2 C Full match No results C5 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 NC Full match C2 H3 NC Full match C2 H3 NC Full match C3 H3 N7 P3 Full match No results No results C1 H3 N7 P3 Full match C2 H3 N5 Full match No results C4 H3 N7 P3 Full match C7 H4 N7 P3 Full match	No results No results Invalid max No results	s No results full match No results full match No results for No results for No match No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 216,0302 -2,83 411,8557 0,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635679,5	0 1 18 0 6 3 0 0 0 0 5 0 0 0 0 0 1 1 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche Mult No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for or [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 1427822 O- 895720,3 2 3103591 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8 7,7	5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8
FALSO	DL-lysine Acetonedicarboxylic Acid	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 OS Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H4 N5 N Full match C2 H4 N5 C Full match C2 H4 N7 P3 Full match C3 H2 N7 V3 Full match C4 H2 N6 C Full match C6 H2 N7 N9 Full match C6 H2 N7 N9 Full match C7 H2 N9 C Full match C7 H2 N9 C Full match C8 H2 N9 C Full match C9 H3 N9 C Full match C1 H4 N9 C Full match	No results No results Invalid max No results	s No results f Full match No results f Full match No results f No results f No results f No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512	312,7824 144,9569 147,1128 134,9958 129,0183 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 1,166 0,961 4,155 0,307	1953887 395242,6 2155294 3952205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635679,5 1050289	0 1 18 0 6 3 0 0 0 5 0 0 0 0 1 1 0	0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche Mult No matche Mult No matche No n No matche Mult No matche No n No matche Mult No matche Mult No matche Mult No matche Mult No matche No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche DDA for ort [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 tiple m DDA for pri [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 1427822 O- 895720,3 2 3103591 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8	7,1 5,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2
FALSO	DL-lysine Acetonedicarboxylic Acid	No results C2 H3 AC No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match T7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N2 Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H4 N7 Full match C2 H4 N7 Full match C2 H4 N7 E1 ull match C3 H4 N7 E1 ull match C4 H4 N7 E1 ull match C5 H4 N7 E1 ull match C5 H4 N7 E1 ull match	No results No results Invalid ma. No results	s No results No results Full match No results In Imatch No results In Imatch No results No match	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 0,70,2188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 7,492 1,162 0,961 4,155 0,307 1,305	1953887 395242,6 2155294 392205 7256678 1259932 1425737 4576228 3791663 3791663 3937032 1507486 5005895 1763860 635579,5 1050289 4522033	0 1 18 0 6 3 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ott [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+DA for pr [M+H]+1 matche No MS2 [M+DA for pr [M+H]+1 matche No MS2 [M+Na]+1 matche No MS2 [M+H]+1 matche No MS2	1953887 395242,6 2155294 3304768 00 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0-895720,3 2 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8 7,7	7,1 5,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2
FALSO	DL-lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 NC J Full match C2 H3 NC J Full match C2 H3 NC J Full match C2 H3 NF Jull match C2 H4 N9 F Jull match No results C1 H4 N0 Full match C3 H2 C4 I Match C3 H2 C4 I Match No results C3 H4 C9 H1 match No results C3 H4 C9 H1 match No results	No results No results Invalid max No results	s No results full match No results full match No results for No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719	312,7824 144,9559 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635579,5 1050289 4522033	0 1 18 0 6 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+Z]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ort [M+Z]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+DM] matche No MS2 [M+DM] matche No MS2 [M+DM] matche No MS2 [M+DM] matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 60 6896063 2 1259392 1425737 4576283 2 3791628 2 3791628 2 3103591 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8 7,7	7,1 5,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match No results C5 H6 O7 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H2 N8 Full match C2 H2 N8 C Full match C2 H3 N9 Full match No results C1 H2 N7 PF Full match C2 H3 N9 Full match C2 H3 N9 Full match No results C1 H4D N; Full match C3 H2 C1 (Invalid mat C3 H2 C1 (Invalid mat C3 H4 N9 Full match No results C3 H2 C1 (Invalid mat C3 H4 N9 Full match No results C6 H6 O3 Full match	No results No results Invalid max No results	s No results f Full match No results f Full match No results f Full match Full match s No results f Full match Full match s No results S No results S No results S No results No results S No results S No results No results S No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0241 145,1145 185,9834 448,7574 448,7574 524,3712 461,2739	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,14 7,305 1,143 0,997	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 3937032 1507486 5005895 1763860 635679,5 1050289 452033 1387882 432998	0 1 1 18 0 0 6 3 3 0 0 0 0 0 1 1 0 0 0 1 2 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche Mult No matche No n No matche Mult No matche No n No matche Mult	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche DDA for ort [M+H]+1 natche DDA for pri [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+PM] natche No MS2 [M+PM]+1 tiple m DDA for pri [M+H]+1 tiple m DDA for pri [M+H]+1 tiple m DDA for pri [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 80 22 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 3103591 1 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 4522033 1387882	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 6,4 8,3 4,8 7,7	7,1 5,3 7,3 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2 7,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N5 Full match C3 H2 C4 L3 W1 L3	No results No results Invalid ma. No results	5 No results No results Full match No results In Ull match No results No resu	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,283 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852	312,7824 144,9559 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 468,7255 127,039 2259,0392	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,14 7,305 1,143 0,997 1,143	1953887 395242,6 2155294 3922205 7256678 125993 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763869 17638	0 1 1 18 0 6 3 3 0 0 5 5 0 0 0 1 1 0 0 0 1 1 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No m No matche No m No matche No m Multiple m Multiple m Multiple mat Single	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ot [M+2H]+1 matche DDA for pri [M+H]+1 matche No MS2	1953887 395242,6 2155294 20 689603 2 125993 2 1425737 4576228 2 3791663 142782 2 895720,3 2 1507486 5005895 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 635679,5 1019256 11763862 1387882	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 4,8 8,3 4 4,2 7,7 6,8 7,2 7,5 7,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol	No results C2 H3 C2 M C2 No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H7 N9 F Full match C2 H7 N9 F Full match C2 H2 NS C Full match No results C1 H2 NS C Full match No results C1 H2 NS C Full match No results C1 H3 NF Ull match No results C3 H2 C14 (Invalid match No results C1 H4 NF Ull match No results C1 H4 NF Ull match No results C1 H4 NF Ull match No results	No results No results Invalid max No results	s No results full match No results full match No results for No results for No match for No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,402 1,166 0,961 4,155 0,307 1,14 7,305 1,143 0,997 1,871 1,143	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 6355679,5 1050289 4522033 1387882 4329938 1706941 15565026	0 1 18 0 6 6 3 0 0 0 0 1 1 0 0 0 1 1 2 0 0 0 6 6 0 0 2 4 7 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matu	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ort [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 2 3791663 2 3103591 1 1507486 5 5005895 1 1561656	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679.5 1019256 4522033 1387882 1706941 1706941	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 8,8 7,7 8,3 4 4 8 7,2 4,2 4,2 7,7 6,8 7,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol	No results C2 H6 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H2 N8 C Full match C2 H3 N8 C Full match No results C1 H2 N9 C Full match C2 H3 N9 Full match No results C1 H2 N7 P2 Full match No results C1 H49 N1 Full match C3 H2 C14 (Invalid mat C3 H4 C14 (Invalid mat C3 H4 N1 Full match No results C6 H6 O3 Full match C10 H14 N1 Full match	No results No results Invalid max No results	s No results f Full match No results f Full match No results f Full match Full match s No results f Full match Full match s No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 1,87 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 1,166 0,961 4,155 0,307 1,144 7,305 1,144 7,305 1,144 7,305 1,144 1,166	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 25907293 3937032 1507486 5005895 1050289 452203 1387882 4329938 1706941 1565026 1565026	0 1 1 18 0 0 6 3 3 0 0 0 0 1 1 1 0 0 0 1 2 2 4 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Singl No matche No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+DA for pr [M+H]+1 matche No MS2 [M+M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 20 6896053 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 3103591 1 1507486 5005895 15105289 4329938 1550266 348273,4	260244,6 3922205 7256678 1083387 1201043 2882205 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1706941 1706941 1706947	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 6.4 8.3 4,8 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 7,7 6,8 7,2 7,5 7,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2-O-Methyluridine	No results	No results No results Invalid max No results	s No results Full match No results Full match No results No results No results Full match No results No result	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 1,84 479,2833 1,87 154,0354 98,5239 0,13 26,0317 3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 480,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 0,997 1,143 1	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1753895 1050289 4522033 1387882 4329938 1706941 1706941 1565026	0 1 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 1 1 0 0 0 0 1 1 2 0 0 0 0 0 1 2 4 7 7 0 0 0 1 1 1 0 0 0 0 1 1 1 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Single	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ot [M+2H]+1 matche DDA for ot [M+2H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 30304768 30304768 304768 302 125993 1425737 4576228 2 3791663 1427822 0 895720,3 2 1507486 5005895 1561656 1050289 4329938 1565026 348273,4 7647714	260244,6 3922205 7256678 1083387 1201043 2882505 2892791 1241276 26907293 3937032 1505779 4227822 11763860 635679,5 1019256 4252033 1387882 1706941 1322179 365198,7 3478712	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 8,8 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,7 8,3 7,7 8,8 8,7 3,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol	No results C2 H3 C4 No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H6 O5 Full match C4 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 C Full match C3 H2 N5 C Full match No results C1 H2 N5 C Full match C3 H2 C4 U N8 C Full match C3 H3 N5 C Full match C3 H3 C H4 C Full match C3 H3 C H4 C Full match C3 H3 C H4 C Full match C3 H3 N5 C Full match C1 H4 N5 Full match C1 H4 C1 N5 Full match C1 H4 N5 Full match C1 H4 C1 N5 Full match	No results No results Invalid max No results	5 No results 5 Full match No results 6 No results 6 No results 7 No match No results 5 No results 7 No results 8 No results 8 No results 8 No results 8 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 29924 442,8041 588,808 317,0561 171,993	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 0,997 1,144 1,106 1,143 0,997 1,871 1,139	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 1507486 5005895 1763860 635679,5 1050289 452203 1387882 432938 1706941 1565026 365198,7 7647714 1488645	0 1 1 18 0 0 6 6 3 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matu Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 1427822 3103591 1507486 1507289 1561656 1050289 1432938 1565026 348273,4 7647714 HH 1488645 141826714 1488645 141826714 1488645 144665 144665 144665 144665	260244,6 3922205 7256678 1083387 1201043 2882205 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1706941 1706941 1706947	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 7,7 6,8 7,2 7,5 7,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2-O-Methyluridine	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C9 H3 N2 C Full match C9 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C2 H3 N3 C Full match C2 H3 N7 EVII match C3 H2 C14 (Invalid matc C3 H3 N7 P2 Full match C3 H2 C14 (Invalid matc C3 H3 N7 P2 Full match C3 H2 C14 (Invalid matc C3 H3 N7 P2 Full match C3 H2 C12 (Invalid match C3 H2 C12 (Invalid match C3 H3 C12 (Invalid match C1 H3 H3 C1 Full match C1 H4 C1 O3 No results C3 H2 C12 Full match C1 H3 C15 Full match	No results No results Invalid ma. No results	s No results No resul	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 26,01373 -3,78 184,9762 -7,97 47,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 0,02 129,9592 1,56 517,7351	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561 171,993 518,7424	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 0,997 1,871 1,134 1,106 1,376 0,306	1953887 395242,6 2155294 3922205 7256678 3922205 7256678 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 4522033 1387882 4322938 1706941 1565026 365198,7 7647714 1488645	0 1 18 0 6 3 3 0 0 5 5 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+2H]+1 matche No MS2 [M+H]+1	1953887 295242,6 2155294 20304768 20 689503 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 11050486 5005895 1561656 1050289 1565026 348273,4 7647714 1488645	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 4 8 7,2 7,7 6,8 7,2 7,5 7,7 8,3 7,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2-O-Methyluridine	No results C2 H3 C4 No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C5 H3 N2 C Full match No results C5 H3 N2 C Full match No results C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N5 Full match C3 H2 C4 V3 N5 Full match No results C4 H3 N5 Full match C3 H2 C4 C Full match C3 H2 C4 G Full match C3 H2 C4 G Full match C3 H2 C14 C Full match C3 H2 C14 C Full match C3 H2 C14 C Full match C1 H3 N5 Full match C2 H3 N5 Full match C1 H3 N5 Full match C2 H3 N5 Full match C1 H3 N5 Full match C2 H3 N5 Full match C3 H3 N5 Full match C4 H3 N5 Full match C5 H3 N5 Full match	No results No results Invalid max No results	s No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561 171,993 517,993	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 0,997 1,143 0,997 1,134 1,106 1,376 0,306 1,137	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763865 635679,5 1050289 4522033 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 1274922 1274922 1274922	0 1 1 18 0 0 6 6 0 0 0 0 1 1 0 0 0 0 0 1 1 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ort [M+H]+1 matche DDA for ort [M+H]+1 matche DDA for ort [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 2155294 2155294 2155294 2155294 2155293 2 2 3791663 1427822 2 3791663 5005895 1561656 215526 2155289 21555026 348273,4 7647714 41 1488645 11274922 1347195	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1753860 653679.5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 6,8 7,2 7,7 7,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2'-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 C4 C3 H3 C4 C4 H3 N2 C Full match C5 H3 C5 C5 H3 N2 C Full match C4 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H4 N2 Full match C7 H2 O7 F Full match C7 H2 N6 C Full match No results C1 H2 N8 C Full match No results C1 H2 N8 C Full match C3 H2 C1 H1 match No results C1 H4 N7 P3 Full match C3 H2 H4 N Full match C3 H2 H4 N Full match C1 H4 N Full match C1 H4 N Full match C1 H1 N Full match C1 H2 N Full match C1 H3 N Full match	No results No results Invalid max No results	5 No results 5 Full match No results 5 Full match Full match 5 No results 5 No results 6 No results 7 No results 7 No results 8 No results 8 No results 8 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 0,13 26,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 -0,62 597,8292	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561 171,939 518,7424 352,8082 559,83865	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 1,106 1,376 0,366 1,144 1,144 1,142	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 4576228 3791663 1427822 1427822 1427827 1507486 5005895 1763860 635679,5 1050289 4522033 1387882 4329938 1706941 1488645 1565026 365198,7 7647714 1488645 1274922 1347195 1668226	0 1 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 1 1 0 0 0 0 1 1 2 2 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Multiple m No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	3953887 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 2 1303591 1 1507486 1 1507486 1 1050289 4 4329938 4 1482934 7647714 HH 1488645 1274922 1347195 1556137	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763880 635679,2 1705941 1322179 365198,7 3478712 1431544 1431544	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2 7,5 7,7 8,3 7,7 8,7 8,7 8,7 8,7 8,7 8,7 8,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2-O-Methyluridine	No results C2 H3 Cd No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H4 N7 P2 Full match C3 H2 C14 C Invalid match No results C11 H49 N1 Full match C3 H2 C14 C Invalid match C1 H4 N5 Full match C1 H4 N5 Full match C1 H4 C10 N1 Full match C1 H4 C10 N1 Full match C1 H4 N5 Full match C1 H4 N5 Full match C1 H4 N6 Full match	No results Invalid man No results Invalid man No results No result	5 No results 5 Full match No results 5 Full match Full match 5 No results 5 No results 6 No match 5 No results 6 No results 6 No results 7 No results 7 No results 7 No results 8 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0316 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 26,01373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 47,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 0,37 204,0747	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561 171,993 518,7424 352,8082 598,865 205,082	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 0,997 1,871 1,134 1,106 1,376 0,306 1,144 1,143 1,102	1953887 395242,6 2155294 3922205 725678 3922205 725678 1259932 1425737 44576228 3791663 1427822 1241276 56907293 3937032 1507486 5005895 1763860 635679,5 1050289 4522033 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 1274952 1347195	0 1 1 18 0 6 6 3 3 0 0 5 5 0 0 0 0 1 1 0 0 0 0 1 1 2 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Multiple m Multiple m No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ott [M-2H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+P]+1 matche No MS2 [M+H]+1	1953887 295242,6 295242,6 295242,6 2155294 20 6896053 2 1259932 2 1427822 2 3791663 1 1507486 5005895 1 561656 1 1050289 1 156926 3 48273,4 7647714 1 1488645 1274922 1347195 105486137 1054865137	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7	7,1 5,3 7,3 8,8 8,8 8,8 8,7 7,7 8,3 4 8 7,2 7,7 6,8 7,7 7,7 8,3 7,7 7,7 8,3 7,7 8,3 7,7 8,3 8,5 7,7 7,7 8,8 8,8 8,7 8,7 8,7 8,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2'-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 C4 C3 H3 C4 C4 H3 N2 C Full match C5 H3 O5 C4 H3 N2 C Full match C4 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 N5 Full match C8 H3 N5 Full match C9 H3 N5 Full match C9 H3 N5 Full match No results C1 H2 N5 Full match C1 H2 N5 Full match No results C1 H4 N5 Full match C3 H2 C14 C Invalid match No results C3 H2 C14 C Invalid match C3 H2 C14 N5 Full match C3 H2 C14 N5 Full match C3 H2 C14 C Invalid match C3 H2 C14 C Invalid match C3 H2 C12 H3 N5 Full match C1 H14 N5 Full match C1 H19 N5 Full match N5 Full M18 N5 Full match N6 Full M18 N5 Full match N7 Full M18 H19	No results No results Invalid max No results	5 No results 5 Full match No results 5 Full match No results 5 No results 6 No results 5 No results 6 No results 7 No results 7 No results 7 No results 8 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 0,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 467,719 0,37 126,0317 0,37 126,0317 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 523,3639 467,719 0,37 126,0317 0,10 128,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 0,48 351,8009 -0,62 597,8292 0,37 204,0747 283,8133	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0324 442,8041 588,808 317,0561 171,993 518,7424 352,808 352,808 259,8365 205,082	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,14 7,305 1,143 1,106 1,376 0,306 1,144 1,143 1,102 1,521	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 44576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635579,5 1050289 442793 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 1274922 1347195 1668226 10448652 14400342	0 1 18 0 0 6 6 0 0 0 12 0 0 0 0 1 1 2 0 0 0 0 1 1 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matc Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+DM] matche No MS2 [M+H]+1	1953887 395242,6 2155294 309542,6 2155294 30304768 20 6896063 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 2 3103591 1 1507486 5005895 1561656 1 1050289 4 4329938 4 1565026 348273,4 7647714 H 1488645 1274922 1347195 1556137 10448652	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763880 635679,2 1705941 1322179 365198,7 3478712 1431544 1431544	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 6,8 7,2 7,5 7,7 8,3 7,7 8,7 8,7 8,7 8,7 8,7 8,7 8,7
FALSO	DL-Lysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrogallol 2'-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 CA No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C9 H14 P2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C2 H2 N3 C Full match C2 H3 N5 Full match C2 H3 N7 P2 Full match C3 H3 N7 P2 Full match No results C1 H40 N Full match C2 H4 N7 P2 Full match No results C1 H40 N Full match No results C1 H40 N Full match C1 H14 N Full match C1 H15 N Full match C7 H12 N Full match C7 H12 N Full match	No results No results Invalid ma. No results	5 No results No results Full match No results In Ull match In Ull mat	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 1,09 164,063 0,16 411,7118 -4,91 219,0289 1,87 154,0354 98,5239 1,87 154,0354 98,5239 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 1,28,4813 1,49,762 1,59 57,7351 -0,48 351,8009 1,50 577,7351	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 524,3712 468,7255 127,039 259,0924 442,8041 588,808 317,0561 171,939 518,7424 352,8082 598,8365 205,082 284,8206	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 1,106 1,376 0,991 1,144 1,143 1,106 1,376 0,306 1,144 1,143 1,106 1,376 1,144 1,143 1,102 1,521 1,142	1953887 395242,6 2155294 3922205 77256678 1259932 1425737 4576228 3791663 1427822 1241276 256907293 3937032 1507486 5005895 1763860 635679,5 1050289 452203 1387882 4322938 1766941 1565026 365198,7 7647714 1488645 1274922 1347195 11668226 110648652 1400342	0 1 18 0 0 6 6 0 0 0 1 1 0 0 0 1 1 2 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matche No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+P]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 2052942,6 2155294 20 689503,2 2 1259932 2 3791663 2 125932 2 3791663 1 1507486 5005895 1 1050289 4 329938 1 1565026 348273,4 7647714 4H 1488642 1347195 1556137 10448652	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 8,7 7,7 8,3 4 8 7,2 7,7 6,8 7,7 7,7 8,3 7,7 7,7 8,3 7,7 8,3 7,7 8,3 8,5 7,7 7,7 8,8 8,8 8,7 8,7 8,7 8,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-γ-Glutamyl-L-leucine Pyrogallol 2*-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 C4 No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 N5 Full match No results C11 H2 N1 Full match C3 H2 C14 C Invalid match C3 H2 C14 C Invalid match No results C11 H2 N5 Full match C1 H2 N5 Full match N6 results C1 H2 N5 Full match N7 results C1 H2 N5 Full match N8 results C1 H2 N5 Full match N9 results	No results No results Invalid ma. No results	5 No results 5 Full match No results 5 Full match No results 5 Full match No results 5 No results 6 No results 6 No results 7 No results 7 No results 8 No results 8 No results 8 No results 9 No results 9 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,283 1,87 154,0354 98,5239 47,7512 2,14 523,3639 467,719 47,7512 2,14 523,3639 467,719 1,56 517,7351 -0,1 258,0852 -2,17 441,7974 21,56 517,7351 -0,48 351,8009 -0,62 597,8292 -0,37 04,0747 283,8133 -2,85 523,681 -0,07 333,1787	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 409,734 110,5217 407,734 110,5217 407,734 110,5217 407,734 110,5217 407,734 110,5217 407,734 110,5217 407,734 110,5217 408,734 110,5217 408,734 117,024 1261,1445 127,039 127	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 0,997 1,871 1,134 1,106 1,376 0,366 1,144 1,143 1,102 1,521 1,142 1,152	1953887 395242,6 2155294 3922205 7256678 3922205 7256678 1259932 1425737 44576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763869 1763869 1763869 1763869 1763869 1763869 17769941 1868025 1668226 10448652 1400342 1168099	0 1 18 0 0 6 6 0 0 0 12 0 0 0 0 1 1 2 0 0 0 0 1 1 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Jingle mat Single No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ot [M+2H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+DA] matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1	1953887 395242,6 2155294 3304768 0 689603 2 1259932 1425737 4576228 2 3791663 1427822 0 895720,3 1 1507486 5005895 1561656 1050289 1565026 348273,4 7647714 H 1488645 1274922 1347195 1556137 10448562 1168099 15931594	260244,6 3922205 7256678 1020387 1201043 2882505 1302971 1241276 26907293 3937032 1763860 635679.5 1019256 452203 452203 1378782 1706941 1322179 365198,7 3478712 1431544 1256728 1668226 1400342	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7	7,1 5,3 7,3 8,8 8,8 8,8 8,7 7,7 8,3 4 8 7,2 7,7 6,8 7,7 7,7 8,3 7,7 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 7,7 8,3 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7
FALSO	DL-lysine Acetonedicarboxylic Acid L-γ-Glutamyl-L-leucine Pyrogallol 2*-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 C4 C3 H3 C4 C3 H3 C4 C4 H3 N2 C Full match C5 H3 N2 C Full match C4 H3 N2 C Full match C4 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 N2 Full match C8 H3 N5 Full match C9 H3 N5 Full match C1 H2 N2 C Full match C1 H2 N2 C Full match No results C1 H4 N5 Full match C3 H2 C14 C Invalid match C3 H2 C14 C Invalid match No results C1 H4 N5 Full match C3 H2 C14 C Invalid match C1 H4 N5 Full match C1 H4 N5 Full match C2 H1 C12 N5 Full match C3 H2 C12 F Full match C13 H3 N2 C Full match C14 H3 N5 Full match C15 H3 N2 C Full match C17 H2 N5 Full match C17 H2 N5 Full match C18 H3 N2 C Full match C18 H3 N2 C Full match C19 H3 N5 Full match	No results No results Invalid max No results	5 No results No results Full match No results In Ull match In Ull mat	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 1,09 164,063 0,16 411,7118 -4,91 219,0289 1,87 154,0354 98,5239 1,87 154,0354 98,5239 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 1,28,4813 1,49,762 1,59 57,7351 -0,48 351,8009 1,50 577,7351	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0324 442,8041 588,808 317,0561 171,993 518,7424 352,808 528,826 524,6874 332,868 332,808 524,6874 332,868 332,808 524,6874 334,186	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 1,106 1,376 0,306 1,144 1,134 1,106 1,376 0,306 1,144 1,146 1,174 1,174 1,187 1,114 1,102 1,521 1,147 1,688	1953887 395242,6 2155294 3922205 77256678 1259932 1425737 4576228 3791663 1427822 1241276 256907293 3937032 1507486 5005895 1763860 635679,5 1050289 452203 1387882 4322938 1766941 1565026 365198,7 7647714 1488645 1274922 1347195 11668226 110648652 1400342	0 1 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 1 1 0 0 0 0 1 1 2 0 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matc Single No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+P]+1 matche No MS2 [M+H]+1	1953887 395242,6 395242,6 2155294 3304768 60 6896063 2 1259932 1425737 4576228 2 3791663 1427822 3103591 1 507486 1 5005895 1561656 1 1050289 4 4329938 1 565026 348273,4 7647714 1 448645 1274922 1347195 1 1556137 10448652 1 15931594 1 15	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679.5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1256728 1668226 7472406 1400342	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 8,7 7,7 8,3 4 8 7,2 7,7 6,8 7,7 7,7 8,3 7,7 7,7 8,3 7,7 8,3 7,7 8,3 8,5 7,7 7,7 8,8 8,8 8,7 8,7 8,7 8,7
FALSO	DL-lysine Acetonedicarboxylic Acid L-γ-Glutamyl-L-leucine Pyrogallol 2*-O-Methyluridine chloromethylphosphonic acid	No results C2 H3 CA No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H4 N8 C Full match C2 H4 N8 C Full match C2 H4 N8 C Full match C3 H2 C14 G Invalid matc C3 H2 N8 C Full match C3 H2 C14 G Invalid matc C3 H3 N5 Full match C3 H3 N5 Full match C4 H3 H3 N5 Full match C7 H12 N5 Full match C1 H4 N6 Full match C1 H4 N6 Full match C1 H4 N6 Full match C1 H4 N7 Full match C1 H4 N6 Full match C1 H4 N7 Full match C1 H4 N6 Full match C3 H3 N2 C Full match C7 H12 N2 Full match C7 H12 N2 Full match C7 H12 N2 Full match C1 H12 N2 Full match C9 H14 N3 Full match	No results No results Invalid ma. No results	5 No results 5 Full match No results 5 Full match No results 5 Full match Full match 5 No results 6 No results 6 No results 7 No results 7 No results 7 No results 7 No results 8 No results 8 No results 8 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 0,13 260,1373 -3,78 184,9762 -7,97 447,7512 2,14 523,3639 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 0,37 204,0747 -0,78 38,8133 -2,85 523,681 -0,70 333,1787 -0,09 230,0903	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 127,039 259,0924 442,8041 588,808 317,0561 171,993 518,7424 352,8082 598,8365 205,082 284,8206 524,6874 334,186 231,0975	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,403 7,492 1,166 0,961 4,155 0,307 1,14 1,103 1,106 1,376 0,306 1,144 1,143 1,102 1,521 1,142 1,142 1,144 1,143 1,102 1,521 1,147 6,887 1,997	1953887 395242,6 2155294 3922205 77256678 1259932 1425737 44576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635679,5 1050289 452033 1338782 4329938 1706941 1468606 365198,7 7647714 1488645 1274922 1347195 1668226 10448652 11460342 1168099	0 1 18 0 0 6 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mati Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for ort [M+H]+1 matche DDA for pri [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+DM] matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1	395242,6 295242,6 295242,6 2155294 20 309768 20 1259932 2 1427822 2 3791663 3 102782 5 1506566 1 1507486 5 005895 1 1561656 4 1329938 1 1560269 348273,4 7647714 1 1488645 1 1274922 1 347195 1 10448652 1 168099 1 19931594 1 168089 1 1968832 1 1668832	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679.5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1256728 1668226 7472406 1400342	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 7,7 8,3 7,7 6,8 7,2 7,7 6,8 7,7 7,7 8,3 3,5 7,7
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 AV C Full match C2 H3 AV C Full match C5 H3 AV C Full match C4 H3 AV C Full match AV C Full match AV C Full match V6 H3 AV C Full match AV C Full match AV C Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 AV C Full match C2 H3 AV C Full match C2 H3 AV C Full match C3 H3 C H3 Full match C3 H3 C H3 Full match C3 H3 C H3 Full match C3 H3 AV C Full match C3 H3 AV C Full match C4 H3 C Full match C5 H4 C Full match C6 H4 C0 AV Full match C7 H3 AV C Full match C8 H3 C Full match C9 H3 H3 C Full match C1 H4 M6 Full match C1 H4 M6 Full match C1 H4 C1 Pull match C1 H4 C1 Pull match C1 H4 C1 Pull match C3 H3 C Full match C3 H3 C Full match C4 H3 N V Full match C5 H4 C1 Pull match C7 H12 C Full match C7 H12 C Full match C8 H4 C1 Pull match C9 H4 AV Full match C9 H4 R0 Full match C9 H4 R1 N Full match C9 H4 R1 N Full match C9 H4 R1 N Full match C4 H3 N Full match C4 H3 N Full match	No results No results Invalid ma. No results	5 No results No results Full match No results In Variable No results No resul	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 1,87 154,0354 98,5239 1,87 154,0354 98,5239 467,719 2,14 523,3639 467,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,15 523,3639 2,17 441,7974 2,18 31,8009 1,56 517,7351 1,91 316,0488 2,18 52,26 517,7351 1,91 316,0488 2,18 52,26 517,7351 2,19 316,0488 2,19 32,29 32,29 32,29 32,29 32,29 32,29 32,29 32,29 32,29 32,29 32,3681 2,285 523,681 2,00 333,1787 2,285 523,681 2,00 333,1787 2,00 230,0903 4,41 426,0879	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 259,0924 42,8041 588,808 317,0561 171,993 518,7424 352,8082 598,365 205,082 205,082 205,082 205,082 214,0951 214,09	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 0,997 1,143 1,098 1,376 0,306 1,144 1,143 1,102 1,144 1,147 1,887 1,908 1,855 1,908	1953887 395242,6 2155294 3922205 7725678 3922205 7725678 3791663 1427822 1241276 1241276 5005895 1763866 635679,5 1050289 452203 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 1274922 1347195 1668226 10448652 1400342 11668226 11068228	0 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 1 1 0 0 0 1 1 1 0 0 0 1 1 1 2 0 0 0 1 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+P]+1 matche No MS2 [M+P]+1 matche No MS2 [M+P]+1 matche No MS2 [M+P]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1	1953887 395242,6 2155294 215	260244,6 3922205 7256678 1083387 1201043 1201043 2882205 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,5 1019256 4522033 1387882 1706941 1332179 365198,7 3478712 1431544 1256728 1668226 7472406 1400342	8,6 8,2 7 4,2 5,7 4,5 8,3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 4 8 7,2 4,2 7,7 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 7,7 8,7 8,7 8,7 8,7 8,7 8,7
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 C4 No results C6 H14 N2 Full match C5 H3 N2 Full match No results C4 H3 N2 Full match No results C7 H2 O7 Full match C7 H3 N Full match C1 H3 N Full match C3 H2 C14 N P2 Full match C3 H2 C14 N P3 Full match C1 H3 N Full match C3 H3 N Full match C4 H3 N Full match C4 H3 N Full match	No results No results Invalid max No results	5 No results 5 Full match 5 Full match 5 Full match 5 No results 5 No results 5 No match 5 No results 6 No results 6 No results 7 No results 7 No results 7 No results 7 No results 8 No results 8 No results 8 No results 8 No results 9 No results 9 No results 10 No resu	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 1,84 479,283 1,87 154,0354 98,5239 467,719 0,37 126,0317 -0,1 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 0,37 204,0747 283,8133 -2,85 523,681 -0,09 230,0903 -0,09 230,0903 4,4 426,0879 -0,09 230,0903	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 127,039 259,0924 442,8041 588,808 317,0561 171,993 518,7424 352,8082 598,8365 205,082 284,8206 524,6874 334,186 231,0975 216,0142 230,2478 216,0142	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,144 1,130 1,167 1,144 1,145 1,167 1,144 1,146 1,177 1,177 1	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 44576228 3791663 1427822 1241276 26997293 3937032 1507486 5005895 17638695 17638695 1763869 1763869 1763869 1763869 176496 1764	0 1 1 18 0 0 6 6 0 0 0 0 1 1 1 2 0 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single mat Singl No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1	1953887 395242,6 2155294 2155294 20 689503 2 1259932 4125737 4576228 2 3791663 1427822 0 895720,3 1 1507486 5005895 1 1050289 4 4329938 4 1565026 348273,4 7647714 41488642 1168099 15931594 1468282 1168099 15931594 1468282 2 1629327 2036854	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1753860 653679.5 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544 1256728 1668226 74772406 1400342	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 7,2 4,2 7,7 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 8,7 7,7 8,3 8,7 7,7 8,3 8,7 7,7 8,3 8,7 7,7 8,3 8,7 8,7 8,7 8,7 8,7 8,7 8,7 8,7
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 C4 No results C6 H14 N2 Full match C2 H3 N2 C Full match C5 H3 N2 C Full match C6 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N5 Full match C2 H3 N6 Full match C3 H2 C14 C Invalid match C3 H2 C14 N5 Full match C3 H2 C14 N5 Full match C1 H3 H3 N5 Full match C1 H4 N6 Full match C1 H4 N6 Full match C1 H4 N6 Full match C1 H4 N7 Full match C1 H4 N8 Full match C1 H4 H3 N8 Full match C1 H4 H3 N8 Full match	No results No results Invalid ma. No results	5 No results 5 Full match No results 5 Full match No results 5 Full match Full match 5 No results 5 No results 5 No results 5 No results 6 No results 6 No results 7 No results 7 No results 7 No results 7 No results 8 No results 8 No results 8 No results 9 No results 9 No results 10 No match 10 No results 10 No match 10 No results 10 No match 10 No match 10 No match 10 No results 10 No match 10 No match 10 No match 10 No results 10 No results 10 No match 10 No results 10 No resu	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0316 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,283 1,87 154,0354 98,5239 -1,84 154,0354 47,7512 2,14 523,3639 467,719 47,7512 -2,17 441,7974 -0,17 258,0852 -2,17 441,7974 -0,17 258,0852 -2,17 441,7974 -0,18 351,8009 -0,62 597,8292 0,37 204,0747 283,8133 -0,48 351,8009 -0,62 597,8292 0,37 204,0747 283,8133 -2,85 523,681 -0,07 333,1787 -0,09 230,0903 -4,14 46,0879 0 229,2406 -3,07 215,0073 -0,14 842,7434	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 127,039 259,0924 442,8041 588,808 317,0561 171,993 518,7424 352,8082 598,8365 205,082 284,8206 524,6874 334,186 231,0975 216,0142 230,2478 216,0142	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 7,305 1,143 1,106 1,376 0,361 1,144 1,143 1,106 1,376 0,366 1,144 1,143 1,106 1,376 0,366 1,144 1,143 1,106 1,521 1,147 6,887 1,908 1,855 6,801 1,155	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 44576228 3791663 3791663 1427822 1142176 26907293 3937032 1507486 5005895 1763860 635579,5 1050289 4522033 1387882 4329938 1706941 1488645 1274922 1387882 1347195 1668226 10448652 10448652 11400342 1168099 15931594 14468283 1629327 2188137	0 1 1 18 0 0 6 6 3 0 0 0 0 0 1 1 0 0 0 0 1 1 2 0 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Multiple m No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1	1953887 395242,6 2155294 215	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 1753800 635679,5 1705941 1322179 365198,7 3478712 1431544 1226728 1668226 7472406 1400342 1352228 1590169 1153341	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 4 8 7,2 4,2 7,7 8,3 7,7 8,7 7,7 8,3 3,5 7,7 8,3 3,7 7,7 8,7 8,7 7,7 8,7 8,7 8,7 8
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 C4 No results C6 H14 N2 Full match C5 H3 N2 C Full match C6 H3 N2 C Full match C6 H3 N2 C Full match No results C5 H3 N2 C Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 C Full match C2 H3 N5 C Full match C2 H3 N5 C Full match No results C1 H4 N2 Full match No results C1 H4 N2 Full match C3 H2 C14 C Invalid match No results C1 H3 N5 Full match C3 H2 C14 C Invalid match C3 H2 C12 Full match C3 H2 C12 Full match C12 H4 N5 Full match C12 H4 N6 Full match C15 H2 N7 Full match C16 H4 N2 Full match C9 H2 N6 Full match No results	No results No results Invalid max No results	5 No results 5 Full match No results 5 Full match No results 5 Full match No results 5 No results 6 No results 6 No results 6 No results 7 No results 7 No results 8 No results 8 No results 8 No results 9 No results 9 No results 10 No results	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0316 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,283 1,87 154,0354 98,5239 -1,84 154,0354 47,7512 2,14 523,3639 467,719 47,7512 -2,17 441,7974 -0,17 258,0852 -2,17 441,7974 -0,17 258,0852 -2,17 441,7974 -0,18 351,8009 -0,62 597,8292 0,37 204,0747 283,8133 -0,48 351,8009 -0,62 597,8292 0,37 204,0747 283,8133 -2,85 523,681 -0,07 333,1787 -0,09 230,0903 -4,14 46,0879 0 229,2406 -3,07 215,0073 -0,14 842,7434	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0291 251,142 117,024 177,024 177,024 177,024 177,024 185,9834 448,7574 524,3712 468,7255 127,039 259,924 442,8041 588,808 317,0561 171,993 518,7424 352,8082 259,8084 317,0561 279,924 479,924 479,924 479,936 479,936 479,937 4	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 0,976 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,144 1,066 1,376 0,306 1,143 1,106 1,376 1,376 1,143 1,106 1,376 1,376 1,487 1,908 1,871 1,134 1,102 1,512 1,142 1,147 1,908 1,855 6,801 1,152 1,008	1953887 395242,6 2155294 3922205 7256678 3922205 725678 3922205 4425737 44576228 3791663 1427822 1241276 26907293 3937032 1507486 5005895 1763860 635679,5 1050289 4522033 1387882 4329938 17069941 1565026 365198,7 7647714 1488645 12774922 1347195 14668226 10448652 1400342 11668226 11668226 11668226 11668226 11668226 1168099 15931594 1466283 1466283 1466283 1466283	0 1 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 0 1 1 0 0 0 1 1 2 2 0 0 0 1 1 2 2 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult No matche No n	matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pri [M+H]+1 matche NO MS2 [M+H]+1 matche NO MS2 [M+H]+1 matche NO MS2 [M+H]+1	1953887 395242,6 2155294 215	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544 1256728 1668226 7472406 1400342 1352228 1590169 2188137	8.6 8.2 7 4.2 5.7 4,5 8.3 4,8 3,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7 7,7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 4 8 7,2 4,2 7,7 8,3 7,7 8,7 7,7 8,3 3,5 7,7 8,3 3,7 7,7 8,7 8,7 7,7 8,7 8,7 8,7 8
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 No results C2 H3 NO results C2 H3 N2 C Full match C3 H3 N2 C Full match No results C4 H3 N2 C Full match No results C5 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 C Full match No results C1 H4 N2 Full match C2 H3 N5 C Full match No results C1 H4 N7 P2 Full match C3 H2 K1 C Full match No results C3 H2 N4 C Full match No results C4 H4 N5 Full match No results C4 H4 N5 Full match No results C4 H4 N5 Full match C4 H2 N5 Full match C7 H12 N2 Full match C7 H13 N1 Full M13	No results No results Invalid ma. No results	5 No results 5 Full match No results 5 Full match No results 5 No results 6 No results 5 No results 5 No results 6 No results 6 No results 7 No results 7 No results 7 No results 8 No results 9 No results 9 No results 10	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7883 0,16 411,7118 -4,91 219,0289 -1,84 479,2883 1,87 154,0354 98,5239 467,719 0,37 126,0317 -0,10 258,0852 -2,17 441,7974 -0,55 587,8021 1,91 316,0488 4,02 129,9592 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 1,56 517,7351 -0,48 351,8009 -0,62 597,8292 -0,37 26,04,0747 283,8133 -2,85 523,681 -0,07 333,1787 -0,09 230,0903 4,41 426,0879 0 22,2406 -3,07 215,0073 -1,5007 -1,5007 -1,5007 -1,5007 -1,7351 -1,91 316,0488 -1,91	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 518,7424 428,041 558,808 579,836 17,0561 171,1993 518,7424 352,8082 598,8365 205,082 284,8206 524,6874 341,86 231,0975 214,0512 230,2478 216,0146 2216,	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 7,305 1,143 1,106 1,376 0,307 1,144 1,143 1,102 1,521 1,142 1,147 6,887 1,908 1,855 6,801 1,152 1,005 1,145 1,908	1953887 395242,6 2155294 3922205 7256678 1259932 1425737 44576228 3791663 1427822 1241276 26907293 3937032 15074866 635679,5 1050289 4427933 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 1274922 1400342 1168099 15931594 1468283 1629327 2188137	0 1 1 18 0 0 6 6 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matche No n No matche No n	natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche No MS2 [M+H]+1 natche DDA for ort [M+H]+1 natche No MS2 [M+H]+1 natche DDA for pri [M+H]+1 natche No MS2 [M+H]+1	1953887 395242,6 2155294 215	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 1505779 1019256 4522033 1387882 1706941 1322179 365198,7 3478712 1431544 1256728 1668226 7472406 1400342 1352228 1590169 2188137	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 8,2 4,2 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 8,5 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 7,7 8,3 8,3 8,3 8,4 8,5 8,5 8,5 8,5 8,5 8,5 8,5 8,5
FALSO	DL-tysine Acetonedicarboxylic Acid L-y-Glutamyl-L-leucine Pyrrogallol 2'-O-Methyluridine chloromethylphosphonic acid Glu-Gly THI	No results C2 H3 No results C2 H3 NO results C2 H3 N2 C Full match C3 H3 N2 C Full match No results C4 H3 N2 C Full match No results C5 H14 N2 Full match No results C5 H14 N2 Full match C7 H2 O7 F Full match C7 H2 O7 F Full match C2 H3 N5 C Full match No results C1 H4 N2 Full match C2 H3 N5 C Full match No results C1 H4 N7 P2 Full match C3 H2 K1 C Full match No results C3 H2 N4 C Full match No results C4 H4 N5 Full match No results C4 H4 N5 Full match No results C4 H4 N5 Full match C4 H2 N5 Full match C7 H12 N2 Full match C7 H13 N1 Full M13	No results No results Invalid ma. No results	5 No results 5 Full match 6 Full match 7 Full match 8 Full match 8 Full match 8 Full match 8 Full match 9 Full	311,7751 -4,88 143,9496 0,06 146,1055 2,86 133,9885 0,19 146,0216 4,86 216,0302 -2,83 411,8557 70,02188 -1,09 164,063 0,85 419,7833 0,16 411,7118 -4,91 219,0289 1,87 154,0354 98,523 467,719 2,14 523,3639 467,719 2,14 523,3639 467,719 2,14 523,3639 467,719 2,14 523,3639 467,719 2,14 523,3639 467,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,14 523,3639 47,719 2,15 63,3639 2,15 63,3639 2,15 63,3639 2,15 63,3639 2,15 63,3639 2,15 63,3639 3,1833 2,2,85 523,681 0,07 333,1787 0,09 230,0903 4,41 426,0879 0,29,2940 0,37 15,0073 0,31,215,0073	312,7824 144,9569 147,1128 134,9958 129,0183 109,0224 412,863 71,02915 83,0388 420,7956 490,734 110,5217 480,2956 177,0247 99,53117 261,1445 185,9834 448,7574 524,3712 468,7255 127,039 518,7424 428,041 558,808 579,836 17,0561 171,1993 518,7424 352,8082 598,8365 205,082 284,8206 524,6874 341,86 231,0975 214,0512 230,2478 216,0146 2216,	1,173 0,306 1,164 0,967 2,383 0,32 1,055 0,972 1,139 1,142 7,403 7,492 1,166 0,961 4,155 0,307 1,143 7,305 1,143 1,106 1,376 0,307 1,144 1,143 1,102 1,521 1,142 1,147 6,887 1,908 1,855 6,801 1,152 1,005 1,145 1,908	1953887 395242,6 2155294 3922205 7725678 3922205 7725678 392163 1427822 1425737 4576228 3791663 1427822 1241276 5005895 176386 15050289 452203 1387882 4329938 1706941 1565026 365198,7 7647714 1488645 140848652 1400342 11668226 10448652 1400342 11668226 10448652 11668226 10448652 1288137 15951594	0 1 18 0 0 6 3 3 0 0 0 5 5 0 0 0 0 0 1 1 0 0 0 1 1 1 0 0 0 1 1 1 0 0 0 0 1 1 1 1 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		No matche No n No matche No n Multiple m No n No matche No n Multiple m Mult Single matche No n No matche No n	matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+C2H]+1 matche No MS2 [M+C2H]+1 matche No MS2 [M+C2H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1 matche No MS2 [M+H]+1 matche No MS2 [M+H]+1 matche DDA for pr [M+H]+1	1953887 395242,6 2155294 215	260244,6 3922205 7256678 1083387 1201043 2882505 1302971 1241276 26907293 3937032 1505779 4227822 1763860 635679,2 1763860 1387882 1706941 1322179 365198,7 3478712 1431544 12256728 15068226 7472406 1400342 1352228 1590169 2188137 1153341 3258680	8.6 8.2 7 4.2 5.7 4.5 8.3 4.8 3.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7 7.7	7,1 5,3 7,3 8,8 8,8 8,8 5,3 7,7 8,3 4 8 8 7,2 4,2 7,7 6,8 7,2 7,5 7,7 8,3 3,5 7,7 8,3 3,5 7,7 8,3 3,5 7,7 8,7 8,7 8,7 8,7 8,7 8,7 8,7

																			_
	ALSO			sults No results No res					704,5786		7488641	0	0	0	No matche No matche No MS2 [M+H]+1		7488641		5,7
	ALSO			atch No results No res					331,0536		3747045	1	0	0	No matche No matche DDA for pri [M+H]+1		3747045		4,2
	ALSO			atch No results No res					164,0294	1,209	1533950	0	0	0	No matche No matche DDA for pri [M+H]+1	1533950		7,7	7,2
	ALSO			atch No results No res			-2,99	355,749		1,147	1293635	0	0	0	No matche No matche No MS2 [M+H]+1	1284933	1293635	8,8	8,3
	ALSO	N~5~-Isopropyl-L-ornithine		atch No results No results No results			-0,32	174,1368 1199,75		1,156 1,097	1622828 1124070	9	0	0	No matche No matche DDA for pri [M+H]+1 No matche No matche No MS2 [M+2H]+2	1579080 1076165	1622828 1124070	6,1 8,8	7,2 8,3
	ALSO			sults No results No res				728.7631		1,012	3453881	0	0	0	 No matche No matche No MS2 [M+2H]+2 No matche No matche No MS2 [M+2H]+2		3453881	4,8	4,8
		2,2'-({2-[(2-Hydroxyethyl)amino]ethyl}imino					0.00		193.1547		1532565	2	0	0	No matche No matche DDA for pri [M+H]+1	1390834	0.0000	8.3	8,3
	ALSO			atch No results No res					682.8061		579108.6	0	0	0	No matche No matche No MS2 [M+H]+1		579108,6	0,5	9
				atch No results No res			-7-	,	245,0768		1692254	8	0	0	Single mat(No matche DDA for otl [2M+Na]+:			8,3	3,9
	ALSO			atch No results No res				551,7699		1,134	1200876	0	0	0	No matche No matche No MS2 [M+H]+1		1200876	7,2	7,7
F	ALSO		C2 H3 Cl4 f Full ma	atch No results No res	ults No result:	No results	0,83	609,7287	610,7352	1,135	1165931	0	0	0	No matche No matche No MS2 [M+H]+1	1165931	1046433	7,2	8,3
F	ALSO	Xentrivalpeptide K	C40 H69 N No res	sults No results No res	ults No result	Full match	-3,97	791,5125	264,8448	1,141	1445237	0	0	0	No matche Single mate DDA for otl [M+3H]+3	1445237		7,7	
	ALSO			sults No results No res				959,6864		1,057	1088084	0	0	0	No matche No matche No MS2 [M+2H]+2	1088084		8,3	
	ALSO			atch No results No res			-,-	786,597			8188244	0	0	0	No matche No matche No MS2 [M+H]+1		8188244		6,2
	ALSO			atch No results No res			-4,61	299,8881		1,091	1304243	0	0	0	No matche No matche DDA for pri [M+H]+1	1304243		7,7	8,3
	ALSO			sults No results No results No results No results			0.27	84,50828 733.8041		0,976 1,101	2796873 1398059	0	0	0	 No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	2796873 1398059	1905226 1300396	4,2 8,3	6,4 7,7
	ALSO			sults No results No res			-0,37	429,6894			1383140	0	0	0	No matche No matche No MS2 [M+H]+1	1377182		8.8	8,8
	ALSO			atch No results No res			-0.21	972,7014		0,992	2361976	0	0	0	No matche No matche No MS2 [M+2H]+2	2361976		3,2	4,8
				atch No results No res				176,0797			9768589	13	0	0	No matche No matche DDA for pr [M+H]+1		9768589	-7/-	5,7
F	ALSO	vinylglycine	C4 H7 N O2 Full ma	atch No results No res	ults Full matcl	h 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	85735520	5,1	5,1
F	ALSO		C H3 Cl2 O! Full ma	atch No results No res	ults No result:	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	
	ALSO			sults No results No res				403,6793			1861624	0	0	0	No matche No matche No MS2 [M+H]+1	1861624	1579845	8,3	6,6
	ALSO		110.00	sults No results No res				108,0151			24953547	0	0	0	No matche No matche DDA for pri [M+H]+1	24953547		5,1	
	ALSO	γ-Glu-Ala		atch No results No res			0,16	218,0903		,	2886937	9	0	0	No matche Multiple m DDA for pr [M+H]+1	2886937		4,8	8
	ALSO			sults No results No results No results No results				1331,633 92,00806		0,993	1519008 3870870	0	0	0	No matche No matche No MS2 [M+2H]+2 No matche No matche No MS2 [M+H]+1	3870870	1519008	5,9	8,3
	ALSO			atch No results No res			0.46	826,7657		0,993	2467947	0	0	0	No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+2H]+2		2247101	5,9	2,6
	ALSO			atch No results No res				619,7575		-7	848343,8	0	0	0	No matche No matche No MS2 [M+2H]+1		765688,6	8,8	8,5
	ALSO			atch No results No res				303,2926		7,153	2753629	0	0	0	No matche No matche DDA for pri [M+H]+1	2753629		5,9	6,4
		DL-Ala-DL-Leu		sults No results No res			-,,	202,1317		1,962	1217112	6	0	0	No matche No matche No MS2 [M+H]+1		1217112		8,3
	ALSO			sults No results No res					506,6263	, -	1283327	0	0	0	No matche No matche No MS2 [M+H]+1		1283327		8,8
		DOCIGII COM C	CIOTILI I III I III	atch No results No res	uits ito resuit	, i dii iiideeii	-,	361,2101			9535105	0	0	0	No matche Single mate DDA for pre [M+H]+1	9535105		5,7	7,3
	ALSO			atch No results No res			-3,52	286,063			729984,8	2	0	0	No matche No matche No MS2 [M+H]+1	729984,8		7,9	7,9
		dimethylformamide		atch No results No res			1,05		74,06012	1,221	4847834	12	0	0	Multiple m No matche DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1		3667135	4,2	6,4
	ALSO	(25) december asid		sults No results No res			0.02	71,49484		0,993	3768934	160	0	0		3121674		5,3	3,2
	ALSO	(2E)-decenoic acid		atch No results No results No results				170,1307 189,9565			2498591 1001860	160	0	0	Multiple m Multiple m DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1	2498591 1001860	824053	8.8	7,5 7,4
		Diethyl 1,1-cyclopentanedicarboxylate		atch No results No res				,	215,1278		23699888	9	0	0	No matche Multiple m DDA for pr [M+H]+1	23699888		5,1	5,7
	ALSO	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		atch No results No res				461,7735		1.142	1167512	0	0	0	No matche No matche DDA for pri [M+H]+1	1167512	21070070	7,7	3,7
	ALSO			atch No results No res				479,8431		1,055	1097598	0	0	0	No matche No matche No MS2 [M+H]+1		1097598	- //-	5
F	ALSO		C21 H33 N Full ma	atch No results No res	ults No result:	No results	-3,41	494,1861	248,1003	1,667	4191069	0	0	0	No matche No matche DDA for otl [M+2H]+2	4191069	3643414	5,9	7
	ALSO			sults No results No res				156,1164		.,	23800652	0	0	0	No matche No matche No MS2 [M+H]+1		23800652		5,1
				atch No results No res				301,2981			2196292	4	0	0	Single mate No matche DDA for pre [M+H]+1	1725003		8,3	8
		Furaneol		atch No results No res			0,28		129,0547		11073397	31	0	0	Multiple m Multiple m DDA for pri [M+H]+1	9766773		5,1	5,7
	ALSO	Nicon Joseph Johnston	110.00	sults No results No res			0.24	1555,661			965587,4	0	0	0	No matche No matche No MS2 [M+2H]+2			8,3	8,3
	ALSO			sults No results No results No results No results			0,21		123,0805 384,8662		10712391 707816,2	25	0	0	Multiple m Single mat DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1	669183,4	707816 2	8,5	4,6 8,5
	ALSO			atch No results No res			-3.6		378,2122		3958784	0	0	0	No matche No matche DDA for pri [M+H]+1	3318679		4.8	3,7
		1-[(8Z,11Z,14Z)-icosatrienoyl]-sn-glycero-3-p					3,44		568,3394	.,	2621829	3	0	0	No matche No matche DDA for ot [M+Na]+1		3330701	5,9	3,7
	ALSO	,		atch No results No res			-1,79	601,696		1,139	1119219	0	0	0	No matche No matche No MS2 [M+H]+1		1119219		8,3
F	ALSO	N~2~-Acetyl-L-ornithine	C7 H14 N2 Full ma	atch No results No res	ults Full matcl	h Full match	0,22	174,1005	175,1078	1,419	2049523	16	0	0	Multiple m No matche DDA for pr [M+H]+1		2049523		7,5
	ALSO			atch No results No res				150,0015		0,988	3733453	0	0	0	No matche No matche DDA for pre [M+H]+1		3733453	4,2	5,3
	ALSO			atch No results No res				183,9783			21878026	0	0	0	No matche No matche No MS2 [M+H]+1	18995177		6,2	4,6
		N-(tert-Butoxycarbonyl)-L-leucine		atch No results No res					232,1544		1563923	7	0	0	Multiple m No matche DDA for pri [M+H]+1	1407917		6,6	7,2
	ALSO	4-{Methyl[(3R,4R)-4-methyl-1-propionyl-3-p		atch No results No res			-4,03		318,1912 109.0224		10578816 365377,5	3	0	0	No matche No matche DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1	10578816	365377,5	4,6	5,7 8,2
	ALSO			sults No results No res				285,7644			2374307	0	0	0	No matche No matche No MS2 [M+H]+1	2374307		5,3	7
	ALSO			atch No results No res			0,03			1,171	1522019	1	0	0	No matche No matche No MS2 [M+H]+1	2374307	1522019	3,3	7,2
	ALSO			atch No results No res			-,	385,7077			1582536	0	0	0	No matche No matche No MS2 [M+H]+1	1582536	1462955	7,2	7,2
				atch No results No res			-, -	, .	84,04446	1,006	2856504	6	0	0	No matche No matche DDA for pri [M+H]+1		2856504		7,5
		•	C23 H41 N Full ma	atch No results No res	ults No result	Full match	0,23		332,3313	7,305	3063077	0	0	0	No matche Single mate DDA for pre [M+H]+1	3014562	3063077	5,3	9,1
	ALSO			atch No results No res			0,05		479,3693	0,989	2326595	0	0	0	No matche No matche No MS2 [M+2H]+2	1926117		2,1	4,8
				atch No results No res				,	304,2119	5,083	2324946	1	0	0	No matche No matche DDA for pri [M+H]+1	2181472		8	7,5
	ALSO			atch No results No res			0,62	330,0466	,	1,799	6251453	2	0	0	No matche No matche DDA for pr [M+H]+1	6148234	6251453	3,5	5,7
	ALSO			atch No results No results No results			-,-		263,1238 704,8334	1,959 1,087	1145023 1238940	9	0	0	No matche No matche DDA for pri [M+H+Met No matche No matche No MS2 [M+ACN+N		1100911	7,7	8,3
	ALSO			atch No results No res					328.7563	1,173	1880691	0	0	0	No matche No matche No MS2 [M+ACN+N	1880691	1720809	5.5	6,1
	ALSO			atch No results No res					637,8489		1378825	0	0	0		1198698		7,2	7,2
	ALSO			atch No results No res					576,8457	1,078		0	0	0	No matche No matche No MS2 [M+H]+1	1532512		7,7	7,7
	ALSO			atch No results No res			2,19	453,6966	532,7188	1,143	984163	0	0	0	No matche No matche No MS2 [M+DMSO			8,3	7,7
	ALSO			atch No results No res					180,9039		2698836	0	0	0	No matche No matche No MS2 [M+K]+1	2697218		5,9	7,5
	ALSO			atch No results No res					596,7581		906275,1	0	0	0	No matche No matche No MS2 [M+H]+1	40000	906275,1	0.0	8,8
	ALSO			atch No results No res			0,33		424,1672	,	1066146	2	0	0	Single match No matche DDA for pri [M+H]+1	1009348		8,3	3,4
		cycloserine diketopiperazine		sults No results No results No results No results			-4 ne		309,4152 205,0923		2241499 800644,5	2	0	0	No matche No matche No MS2 [M+2H]+2 No matche No matche No MS2 [M+H]+1			2,1	5,9 4,1
				atch No results No res					91,50469		4102580	2	0	0	No matche No matche DDA for otl [M+2H]+2		020303,3	5,9	4,1
		Malathion		sults No results No res					166,0261	1,556		12	0	0	No matche Multiple m DDA for pri [M+2H]+2			4	
	ALSO			atch No results No res					306,9577		1528427	0	0	0	No matche No matche No MS2 [M+ACN+F			8,3	
F	ALSO			atch No results No res					380,7699		1384505	0	0	0	No matche No matche No MS2 [M+H]+1	1384505	1240483	7,7	5,5
		5-Chloro-4,6(1H,5H)-pyrimidinedione		atch No results No res			3,99		146,9961		2613714	4	0	0	No matche No matche DDA for pri [M+H]+1	2380168		6,4	8
	ALSO			sults No results No res					658,837		981693,6	0	0	0	No matche No matche No MS2 [M+2H]+2			8,3	8,3
	ALSO			atch No results No res			0,05		604,7906		1085759	0	0	0	No matche No matche No MS2 [M+H]+1			5	4,1
	ALSO	2.004		sults No results No res			6.11		97,51159		3570925	0	0	0	No matche No matche No MS2 [M+H]+1	3360666		5,9	4,8
	ALSO	3-DNA		atch No results No results No results			-0,19		181,1223 550,6897		26345203 919385,2	36	0	0	No matche Multiple m DDA for pr [M+H]+1 No matche No matche No MS2 [M+DMSO	883490,9	26345203	8.3	5,7 7,7
	ALSO			atch No results No res			2.28		404,8215		1211733	0	0	0	No matche No matche No MS2 [M+DMSO] No matche No matche No MS2 [M+H]+1			7,7	7,7
	ALSO			atch No results No res					279,1915		1297445	0	0	0	No matche No matche DDA for pri [M+H]+1	1152720		8,3	8,8
		ε-Caprolactone		atch No results No res					97,06482		36977256	72	0	0	Single mate Multiple m DDA for pre [M+H-H20			5,1	4,6
	ALSO		No res	sults No results No res	ults No result	No results			109,0224		25602442	0	0	0	No matche No matche DDA for pr [M+H]+1		25602442		5,1

FALSO	5-hydroxyisouric acid	C5 H4 N4 C Full matc	h No results N	No results Full match Full mat	:h 0,01	184,0233	185,0305	2,403	3882762	2	0 0		Single mate No matche DDA for p	([M+H]+1	3882762	3513151	7,5	8
FALSO		C6 H17 N1 Full matc	h No results N	No results No match No resul	ts -0,95	308,122	309,1293	1,365	1528380	2	0 0		No matche No matche DDA for p	([M+H]+1	1528380	1360628	7,7	8,3
FALSO		C6 H12 N4 Full matc	h No results N	No results No results No resul	ts 0,02	188,0732	95,04387	0,972	3523455	0	0 0		No matche No matche No MS2	[M+2H]+2	3523455	2634084	3,2	4,8
FALSO		C2 H2 O7 F Full matc	h No results N	No results No results No resul	ts 4,01	231,9006	232,9079	1,091	1142378	0	0 0		No matche No matche DDA for p	[M+H]+1	1142378	1063583	7,2	7,7
FALSO	5-Hydroxy-DL-tryptophan	C11 H12 N: Full matc	h No results N	No results Full match Partial m	at -0,19	220,0848	221,092	3,769	3114180	17	0 0		Multiple m Single mate DDA for p	[M+H]+1	3018196	3114180	4,2	7,5
FALSO		C6 H Br O S Full matc	h No results N	No results No results No resul	ts 0,68	263,8375	264,8449	1,137	1380917	0	0 0		No matche No matche DDA for p	[M+H]+1		1380917		7,7
FALSO		No result	s No results N	No results No results No resul	ts	858,7209	430,3678	0,977	2430380	0	0 0		No matche No matche No MS2	[M+2H]+2	2430380	2308064	3,2	7,5
FALSO		C33 H77 N! Full matc	h No results N	No results No match No resul	ts 0,23	759,5795	760,5868	7,139	16302260	29	0 0		No matche No matche DDA for p	[M+H]+1	16302260		5,7	
FALSO		C2 H Cl4 Ol Full matc	h No results N	No results No results No resul	ts 0,83	513,6526	592,6748	1,145	960418	0	0 0		No matche No matche No MS2	[M+DMSO	925528,2	960418	8,3	7,7
FALSO	glu-ser	C8 H14 N2 Full matc	h No results N	No results Full match No resul	ts 0,09	234,0852	235,0925	2,37	19058944	5	0 0		No matche No matche DDA for p	[M+H]+1		19058944		5,1
FALSO		C9 H3 N4 C Full matc	h No results N	No results No results No resul	ts 0,56	547,8303	548,8376	1,056	885194,9	0	0 0		No matche No matche No MS2	[M+H]+1		885194,9		8,8
FALSO	3-BHA	C11 H16 O: Full matc	h No results N	No results Full match Partial m	at -0,04	180,115	181,1223	7,204	26867992	36	0 0		No matche Multiple m DDA for p	[M+H]+1	26867992		5,1	
FALSO	Aconitic anhydride	C6 H4 O5 Full matc	h No results N	No results Full match No resul	ts 0,13	156,0059	157,0132	2,144	3262815	3	0 0		No matche No matche DDA for p	[M+H]+1	3262815	3145023	6,4	7
FALSO		C14 H2 N2 Full matc	h No results N	No results No results No resul	ts 0,8	469,8824	470,8897	1,065	1129471	0	0 0		No matche No matche No MS2	[M+H]+1	1129471	1031867	8,3	8,3
FALSO				No results No results No resul		515,7389	,		1115321	0	0 0		No matche No matche No MS2	[M+H]+1	846595,1	1115321	8,3	7,7
FALSO	[Similar to: Ethylenediaminetetraacetic acid (293,0344	, .	366013,1	7	2 0	71,6	No matche No matche DDA for p			366013,1		8,2
FALSO	CAPROYL SARCOSINE			No results Full match No resul		243,1834		6,813	2825432	2	0 0		No matche No matche DDA for p		2295570	2825432	7	7
FALSO				No results No results No resul			644,8331	1,082	1484399	0	0 0			[M+H]+1	1484399		7,7	
	-,			No results Full match Partial m			227,1278	,	27013033	14	0 0		No matche Multiple m DDA for p	-	27013033		4,6	
FALSO				No results No results No resul		361,3193			1789883	0	0 0		No matche No matche DDA for p		1643335		8,3	8,3
				No results Full match No resul		196,1576			3222058	2	0 0		No matche No matche DDA for p			3222058	8,6	8
FALSO				No results No results No resul			191,0404		1704216	0	0 0			[M+H]+1	1704216		7,7	
FALSO				No results Full match Full mat		189,1114		1,531		5	0 0		Single mate No matche DDA for p			1692087	5	3,4
FALSO FALSO				No results Full match No results No re		423,335 525,7675	424,3422	7,213	1603667	0	0 0		No matche No matche DDA for p	[M+H]+1	1603667	1567234	6,6	8,3
								1,136		-	-		No matche No matche No MS2	post-organization and the second	1505003	1033536	0.2	8,3
FALSO				No results No results No result No results No results No result		259,8902 1423,626		1,105 1,078		0	0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+2H]+2	1595092 1281470	1542050	8,3 7,7	8,3
FALSO				No results No results No result		571,8478			975131,7	0	0 0		No matche No matche No MS2	[M+2H]+2 [M+H]+1		378840.2		3 8
FALSO				No results No match No resul			352,2912		15026821	5	0 0		No matche No matche No MS2	[M+2H]+1	15026821	370040,2	8,3 4,6	3,8
				No results Full match Full mat		. ,	133.0972	1.034	2421631	11	0 0		Multiple m No matche DDA for p		23020021	2421631	7,0	7
				No results Full match No match		235.0409	,	7	910838.3	2	0 0			-	619218,6	910838.3	2,5	7,2
				No results Full match No resul		194,0919		1.104	3297633	1	0 0		No matche No matche DDA for p			2986291	5,3	4.8
				No results Full match Partial m		254,1882		7,436		26	0 0		No matche Multiple m DDA for p			4037259	5,9	7,5
FALSO				No results No match No resul		511,3274			2620198	1	0 0		No matche No matche DDA for p			2620198	8	8
FALSO				No results No results No resul	-,	369,7337	370,741	1,172	1217088	0	0 0			[M+H]+1	1217088	1178547	8,3	7,7
FALSO				No results Full match Full mat		,	75,04411	1,366	4213494	3	0 0		Single mate No matche DDA for p			1652240	4,2	3,9
FALSO	- /			No results No results No resul	,		181,0835		3727532	0	0 0		No matche No matche No MS2	[M+H]+1	3727532		4,2	6,4
FALSO				No results No results No resul			644,8331		1474848	0	0 0		No matche No matche No MS2	[M+2H]+2	0.2.002	1474848	-,-	7,7
FALSO				No results No results No resul		367.8756		1,093	1048222	0	0 0		No matche No matche No MS2	[M+H]+1	1048222		7.7	8.3
FALSO				No results No results No resul		377.205			2144860	0	0 0		No matche No matche DDA for p		1735977		8,3	8,6
FALSO				No results No results No resul		451,8465	452.8537		601984,6	0	0 0		No matche No matche No MS2	[M+H]+1	601984.6	551921.6	8,5	8,5
FALSO				No results No match No matc			496,3399		17202062	4	0 0		Single matc No matche DDA for p	[M+H]+1	17202062	, ,	5,1	
				No results Full match Full mat		180,0457	181,0529		993015,1	3	0 0		Single matc No matche No MS2	[M+H]+1	993015,1	915183,5	7,7	7,2
FALSO	·	No result	s No results N	No results No results No resul	ts	1095,661	548,8378	1,057	920823,3	0	0 0		No matche No matche No MS2	[M+2H]+2	920823,3		8,8	
FALSO	L-Proline	C5 H9 N O2 Full matc	h No results N	No results Full match Partial m	at 0,49	115,0634	133,0972	1,039	2287806	30	0 0		Multiple m Single mate DDA for or	[M+NH4]+	2287806		6,4	
FALSO	9-Nitrooleate	C18 H33 N Full matc	h No results N	No results Full match Partial m	at 0,21	327,241	328,2483	6,628	1830540	3	0 0		No matche Multiple m DDA for p	[M+H]+1	1830540	1775470	7,2	6,6
FALSO		No result	s No results N	No results No results No resul	ts	503,6231	504,6294	1,174	1083003	0	0 0		No matche No matche No MS2	[M+H]+1	1083003	974236,3	8,3	8,8
FALSO		C6 H12 Cl3 Full matc	h No results N	No results No results No resul	ts -1,72	375,9213	376,9286	1,221	1857499	0	0 0		No matche No matche No MS2	[M+H]+1	1657003	1857499	8,3	8,3
FALSO		No result	s No results N	No results No results No resul	ts	711,8132	712,8205	1,079	1337157	0	0 0		No matche No matche No MS2	[M+H]+1		1337157		7,7
FALSO		No result	No results N	No results No results No resul	ts	156,0077	157,0149	0,977	2805670	0	0 0		No matche No matche No MS2	[M+H]+1	2805670		4,8	
FALSO		C H2 Cl O5 Full matc	h No results N	No results No results No resul	ts 4,52	221,8814	222,8886	1,128	1075149	0	0 0		No matche No matche DDA for p	([M+H]+1	1075149	969263,2	7,2	7,2
				No results Full match No resul		187,079	94,54676	0,974	2013774	2	0 0		No matche No matche No MS2	[M+2H]+2	2013774	1573745	4,8	3,9
	N-Acetyl-4-chloro-D-phenylalanyl-4-chloro-D					1451,634	726,8245	1,097	895419,7	1	0 0		No matche No matche No MS2	[M+2H]+2	895419,7	723127	8,3	7,9
FALSO		C7 H16 N4 Full matc	h No results N	No results No match No matc	h -2,01	266,0515	267,0588	3,222	1201035	1	0 0		No matche Multiple m DDA for p	([M+H]+1	1132127	1201035	8,3	7,7
FALSO				No results No results No resul			300,4099	1,028	2207100	0	0 0		No matche No matche No MS2	[M+2H]+2	2207100	1032960	2,6	7,2
	N-[(2S)-4-Cyclohexyl-1-ethoxy-1-oxo-2-butar						286,2013	5,546	1431438	12	0 0		No matche No matche DDA for p			1431438	7,2	6,6
				No results Full match Partial m		194,0943	, .		26353451	97	0 0		No matche Multiple m DDA for p			26353451		4
FALSO				No results No results No mate		787,4721	,		3127848	0	0 0		No matche Single matc DDA for p				7,5	7,5
	/ / /			No results Full match Partial m		130,0743			7138633	18	0 0		No matche Single mate DDA for p		7138633	3094279	4,6	7,5
FALSO				No results No results No resul			139,0536	1,289	2711519	0	0 0		No matche No matche DDA for p			2711519	5,9	5,3
FALSO				No results No results No resul		321,9243	. ,	1,196	1105936	0	0 0		No matche No matche DDA for p		1043513	1105936	7,7	7,2
				No results Full match Full mat		87,03186	00,000	1,474		11	0 0		Single mate No matche DDA for p		7210275	5851864	5,7	5,7
FALSO				No results No results No resul		707,8016		1,114	589497	0	0 0			[M+H]+1	05005	589497	0.0	7,9
FALSO				No results No match No match		612,1521 567.332			877415,7	3	0 0		Single mate No matche DDA for or		852858	877415,7	8,3	8,3
FALSO	1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-					,	,		2248421		-					2248421		4,8
FALSO FALSO				No results No results No result No results No results No result			185,9834 236,9085	0,339 1.069	1351265 1510052	0	0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1	1510052	1351265 1455979	7,7	7,7
	3-[(2-Carboxy-2-hydroxyethyl)dithio]-L-alani						242,0152	1,803	1387304	1	0 0		No matche No matche DDA for p			1318752	7,7	8,3
FALSO	5-112-Carboxy-2-nyuroxyetnyijuitnioj-L-alani			No results No results No resul		897,5063	-		2195308	0	0 0		No matche No matche No MS2				6,4	5.0
	Hexahydropyridine			No results Full match Full mat		85,08919			1366758	6	0 0		Single match No matche No MS2				7,2	7,2
	4-[(5-Amino-4H-1,2,4-triazol-3-yl)amino]-L-p						263,1239		2276489	4	0 0		No matche No matche DDA for p		2205633		4,8	4,8
FALSO				No results No results No resul			672,7778		357929,3	0	0 0		No matche No matche No MS2		357929,3		8,2	7,6
FALSO				No results No results No resul			476,9068		1420031	0	0 0		No matche No matche No MS2	[M+H]+1	1420031		7,7	7,5
FALSO				No results No results No resul			670,6907		848405,4	0	0 0			[M+H]+1	848405,4	2231011	7,7	-,,
FALSO				No results No results No resul			647,1021		1803972	0	0 0		No matche No matche DDA for p		5.5.105,4	1803972	.,,	6.1
FALSO				No results No match No resul		335,8269			1096139	1	0 0		No matche No matche No MS2		1096139		7,7	7,7
FALSO				No results No results No resul			588,8496		575026,1	0	0 0			[M+2H]+2		350314,9	2,5	6
				No results Full match Full mat			147,0441		1354728	10	0 0			[M+H]+1		1272268	7,7	7,2
FALSO				No results No results No resul			129,0225		2865934	0	0 0		No matche No matche DDA for p			2865934	2,6	5,3
				No results Full match No resul			192,0326		2019522	1	0 0		No matche No matche DDA for p		2019522	1998258	7,5	8,6
FALSO	, , , , , , , , , , , , , , , , , , , ,			No results No results No resul			90,00841		18855216	0	0 0		No matche No matche DDA for o				5,1	
FALSO				No results No results No resul			142,9619	,	1319469	0	0 0		No matche No matche DDA for p			1319469		4,5
FALSO				No results No results No resul			168,093		1153985	0	0 0		No matche No matche No MS2	-	1153985		8,3	7,7
				No results Full match No resul			369,3511	1,443		1	0 0		No matche No matche DDA for p		950936		7,2	
FALSO				No results No results No resul			88,02318		2453611	0	0 0		No matche No matche DDA for p		2453611	1993918	4,8	5,3
	Toldimfos			No results Full match No resul			200,0832		1025033	1	0 0		No matche No matche No MS2		1025033		7,2	
FALSO				No results No results No resul			349,0178		1211685	0	0 0		No matche No matche DDA for p		693053,7	1211685	6,8	7,7
				No results Full match Full mat			141,091		39256592	7	0 0		Multiple m Multiple m DDA for p	[M+H+Me	39256592		5,1	
FALSO		C7 H12 N3 Full matc	h No results N	No results No results No resul		345,0022			23242462	0	0 0		No matche No matche DDA for p		7263639		1,8	4
FALSO				No results No results No resul			520,8617	1,107	434963	0	0 0		No matche No matche No MS2			434963		6,3
FALSO	(20R)-Cholesta-3,5-diene	C27 H44 Full matc	h No results	No results Full match No resul	ts -0,46	368,3441	369,3514	1,501	1681539	1	0 0		No matche No matche DDA for p	([M+H]+1	1681539		6,1	

	FALSO		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]+1 1162506	1058105	8,3	8,8
	FALSO		C8 H17 N P Full match	No results No results	No match No match	-2,37 189,0832	190,0905	1,479	7037419	2	0 0	Single mate No matche DDA for pre [M+	1]+1 3292243	7037419	6,4	4,6
	FALSO	Pivagabine		No results No results		-0,17 187,1208		1,904	1976800	13	0 0	Single mate No matche DDA for pre [M+			7,2	7,5
	FALSO			No results No results		73,00032		0,988	1789233	0	0 0	No matche No matche DDA for pre [M+			5,5	2,8
	FALSO			No results No results		3,87 175,9634	-7	0,994	2594067	1	0 0	No matche No matche No MS2 [M+			6,4	5,9
	FALSO			No results No results			586,7299		898899,7	0	0 0		OMSO- 898899,7		8,3	8,3
	FALSO			No results No results		-4,98 538,1765	.,	1,549	2653022	1	0 0	No matche No matche DDA for otl [M+ No matche No matche No MS2 [M+		2321816 792294.2	4,8	5,9
	FALSO			No results No results		3,04 435,8629	104,0303		930049,9 2151942	0	0 0		.,	1894605	7,7 5,3	7,4 2,6
	FALSO	Pentachloroethane								1	0 0		-		7,3	2,6
	FALSO	rentaciiloroetiiaile		No results No results No results		-0,98 199,8519 0,98 169,0165		1,168	1921216 1188762	0	0 0		H]+1 1921216 PH]+2	1188762	-/	7,7
	FALSO			No results No results			673,8481	1,086	1221949	0	0 0		2H]+2 1221949	1100/02	7,7	-,,,
	FALSO			No results No results		88.99806			867134.9	0	0 0	No matche No matche DDA for pri [M+	-	867134,9	4,1	7,7
	FALSO	Muscimol		No results No results		0,31 114,043	,	1,963	1389037	14	0 0	Multiple m Multiple m No MS2 [M+			6,6	7,2
	FALSO		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 pre [M+	H]+1 2251672	2331445	4,8	3,2
	FALSO		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+	1]+1	784755,2		7,9
	FALSO	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 mate No matche DDA for pre [M+	H]+1 5762008	5992951	6,7	6,2
	FALSO		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 otl [M+	H+Me(2413336		5,3	
	FALSO		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+	1]+1	1278822		6,1
	FALSO				Full match Partial mat	-0,09 435,2621	,	7,495	2306399	1	0 0	No matche Single mati DDA for pri [M+			7,2	7,5
	FALSO	Methyltrifluorosilane		No results No results		2,9 99,9959			17680985	1	0 0	No matche No matche DDA for pre [M+			5,1	5,1
	FALSO		110.1000.00	No results No results		- 7	88,50911	.,	18999848	0	0 0	No matche No matche DDA for pri [M+		3636086	5,1	5,9
	FALSO			No results No results		-2,57 315,8507			1053619	0	0 0	No matche No matche No MS2 [M+			6,6	7,2 4.8
	FALSO FALSO			No results No results No results			442,8782	0,984	1977315	0	0 0	No matche No matche No MS2 [M+			2,8	.,.
	FALSO	Butyl Parahydroxybenzoate			No results No results Full match Partial mat	-1,34 353,7518 0 194,0943			988473,7 1287069	97	0 0	No matche No matche No MS2 [M+ No matche Multiple m DDA for pri [M+		828612,7 1287069	8,3 8,8	7,9 7,7
	FALSO	Sury. I didniyuroxyberizoate		No results No results		-3,4 178,9961		7	996930,4	0	0 0	No matche No matche DDA for pri [M+		944376,3	8,8	7,7
	FALSO			No results No results		1209.707		1,087	1083653	0	0 0		Hl+2 1083653	1038430	7,7	7,7
	FALSO			No results No results		659,6545			761345,4	0	0 0	No matche No matche No MS2 [M+	,	744024,8	7,9	7,9
	FALSO			No results No results		-0,35 703,8257	,	1,087	1078238	0	0 0	No matche No matche No MS2 [M+		1078238		7,7
	FALSO			No results No results		2,06 333,9367	334,9439	1,223	1583066	0	0 0	No matche No matche No MS2 [M+	H]+1 1476363	1583066	6,1	6,1
	FALSO		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 otl [M+			6,1	
	FALSO		C12 H28 N Full match	No results No results	No match No results	-3,91 393,1385		1,962	971472,3	1	0 0	No matche No matche No MS2 [M+		957341,3	7,7	7,2
	FALSO		No results	No results No results	No results No results	1363,598	682,8061	1,119	599899,5	0	0 0		2H]+2 599899,5		7,4	
	FALSO			No results No results		114,9812	115,9885	0,979	1646056	0	0 0	No matche No matche DDA for pre [M+		1646056	5	4,5
	FALSO			No results No results		1,39 125,9955	,,,,,	0,973	1246389	0	0 0	No matche No matche DDA for pre [M+			3,9	4,5
	FALSO	(Z)-N-16-hydroxyhexadec-9-enoyl-L-alanine				-0,12 355,2722		6,907	1700102	0	0 0	No matche Single mate DDA for pre [M+		1700102	7,2	7,2
	FALSO			No results No results		-0,65 321,1789		6,99	8308555	2	0 0	No matche No matche DDA for pri [M+			5,7	6,2
	FALSO			No results No results		1,11 615,6737			774719,1	0	0 0	No matche No matche No MS2 [M+		377810,8	7,9	7,1
	FALSO			No results No results		-1,02 519,8346		_	433320,1	0	0 0	No matche No matche No MS2 [M+		433320,1	8,2	8,5
	FALSO			No results No results		4,68 439,7182		1,153	1072056	0	0 0	No matche No matche No MS2 [M+		968102,8	7,7	3,9
	FALSO FALSO	N-(tert-Butoxycarbonyl)-L-leucine		No results No results No results		0,69 395,8782 0.07 231.1471		1,055 3,881	787865,7 1070651	7	0 0	No matche No matche No MS2 [M+ Multiple m No matche DDA for pri [M+		723748,4 1070651	7,9 7,2	7,9
	FALSO	N-(tert-Butoxycarbonyr)-t-leucine		No results No results		1.66 187.061			991651.4	1	0 0	No matche No matche DDA for pri [M+		991651,4	7,4	8,3
	FALSO			No results No results		-4.51 178.0023		-7	19946952	0	0 0	No matche No matche DDA for otl [M+		19946952	7,4	5,1
	FALSO			No results No results		,,	562,8428		501483,4	0	0 0	No matche No matche No MS2 [M+		501483,4	5,4	4,1
	FALSO			No results No results		-0,63 222,9811		0,308		0	0 0	No matche No matche DDA for pri [M+		301103,1	5,1	-1,2
	FALSO		C16 H36 O Full match	No results No results	No results No results		290,0758	1,249	1453209	0	0 0		2H]+2 1453209	1351604	8,3	8.3
	FALSO			No results No results			236,9211	0,997	2454431	0	0 0	No matche No matche No MS2 [M+		2454431	4,2	4,8
	FALSO		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+	1]+1 1075318	1111652	8,3	8,3
	FALSO		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]+1 733136,6	750411,3	4,1	7,9
	FALSO		C3 H2 Cl2 (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+	1]+1	788903,4		7,4
	FALSO		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 pre [M+	H]+1 2754960	2837745	5,9	4,2
	FALSO	(±)-Dihydrojasmonic Acid		No results No results		-0,26 212,1412			18181060	19	0 0	Multiple m Multiple m DDA for pre [M+	H-H2O 18181060	15326967	4,6	4,6
	FALSO			No results No results			757,8098		962720,2	0	0 0		2H]+2 936865,7		4,5	5
	FALSO			No results No results		-4,83 289,8688			747031,9	1	0 0	No matche No matche DDA for pri [M+		747031,9	8,5	7,9
	FALSO FALSO			No results No results		2,47 127,0246	150,0138 88.52844		814796,8 2104216	0	0 0		Na]+1 814796,8 H]+1 770181.7	2104246	8,5	2.1
		4 nitrophonul iconomoto		No results No results		4 04 164 0229						No matche No matche DDA for pri [M+			7,9	-
	FALSO FALSO	4-nitrophenyl isocyanate 3,3-Dihydroxy-1H-1,5-benzodiazepine-2,4(3)				0,22 208,0485	05,0107		2080951 747928.3	3	0 0		,	1601449 728075,2	4,8 7,9	1,7 7,9
	FALSO	N6-SUCCINYLLYSINE		No results No results		-0.06 246.1216		3,566	,-	16	0 0	No matche No matche DDA for pri [M+	-	1110378	7,9	8,3
	FALSO	I Journal of the state of		No results No results		2.13 186.0232	,	1,205	1232982	0	0 0	No matche No matche No MS2 [M+	.,		8,3	7,7
	FALSO			No results No results		-0,35 765,7601	. ,		325226,3	0	0 0	No matche No matche No MS2 [M+		325226,3	-,-	8,2
	FALSO	Glu-Gly			Full match Partial mat	0,12 204,0747			1758973	9	0 0	No matche Single mate DDA for otl [M+		1628337	3,4	6,6
	FALSO			No results No results		163,9132	164,9205	1,092	1096971	0	0 0	No matche No matche DDA for pri [M+	H]+1 1035875	1096971	7,7	6,1
	FALSO	glu-thr			Full match Partial mat	0,04 248,1009		1,782	1470146	6	0 0	No matche Single mati DDA for pri [M+		1343197	6,6	6,6
	FALSO			No results No results		1,55 498,026	,	1,232	1611381	0	0 0	No matche No matche No MS2 [M+		1611381	7,2	8,3
	FALSO			No results No results		2,36 632,2485		7,051	1306063	0	0 0	No matche No matche No MS2 [M+		1306063	7,2	6,6
	FALSO			No results No results		1,86 177,0515	-,	1,217	1184627	0	0 0	No matche No matche No MS2 [M+			6,6	7,2
	FALSO			No results No results			88,52846		1641705	0	0 0	No matche No matche DDA for pri [M+			6,1	
		1,3-Bis[(9Z)-9-tetradecenoyloxy]-2-propanyl				-4,7 794,6387			1073817	18	0 0	No matche No matche DDA for oti [M+			6,6	7.7
	FALSO FALSO				No results No results No results No results	-1,19 559,7112			868049,5	0	0 0	No matche No matche No MS2 [M+ No matche No matche No MS2 [M+	H]+1 PH]+2 1632204	868049,5	7.2	7,7
	FALSO				No results No results No results No results	-2,07 597,2517	431,3843		1635055 2458741	0	0 0	No matche No matche No MS2 [M+ No matche No matche DDA for otl [M+			7,2 7,5	3,9
	FALSO				No results No results		603,8547		800619,7	0	0 0	No matche No matche No MS2 [M+			6,3	6,3
	FALSO				No results No results	-4,68 326,0443			1239608	0	0 0	No matche No matche No MS2 [M+		1239608	7,7	8,3
		2-(Phosphonooxy)ethyl acrylate			Not the tor No results	-4,14 196,0129			814763,9	3	0 0	No matche No matche DDA for otl [M+		814763,9	5,8	8,5
	FALSO				No results No results		574,8756	1,097		0	0 0	No matche No matche No MS2 [M+		902037		7,7
		TRIETHYLENE GLYCOLDIMETHACRYLATE			Full match Partial mat	0,22 286,1417		7,062		6	0 0	No matche Multiple m DDA for otl [M+			2,9	4,8
		C14-Carnitine	C21 H41 N Full match	No results No results	Full match No results	0,37 371,3037		7,109	1453153	3	0 0	No matche No matche DDA for pri [M+		1453153	5,5	7,2
	FALSO		C8 H15 N6 Full match	No results No results	No match No match	-1,77 354,0505		1,147	424379,7	4	0 0	No matche Multiple m No MS2 [M+	H]+1 424379,7	281817	7,9	7,6
	FALSO			No results No results		-4,42 337,8534		1,109	459601	0	0 0	No matche No matche No MS2 [M+		459601		8,5
	FALSO			No results No results		0,44 1068,656			2283628	0	0 0	No matche No matche DDA for otl [M+			5,9	7,5
		(2E,11Z)-tetradeca-2,11-dienal			Full match No results	-0,09 208,1827			2041155	16	0 0	No matche No matche DDA for pri [M+			7,5	6,4
	FALSO			No results No results			140,9618		803221,7	0	0 0	No matche No matche DDA for pri [M+	-	223672,9	2	6,5
	FALSO				No results No results		392,7063		1159516	0	0 0	No matche No matche No MS2 [M+			8,3	
	FALSO				No results No results		715,8291		981207,5	0	0 0		2H]+2 981207,5	706700.0	7,7	F 2
	FALSO	Phosphocholine			No results No results Full match Full match	0,32 183,0661	184,0734		706790,2	0	0 0	No matche No matche No MS2 [M+ Single matche No MS2 [M+		706790,2 1332071	7,9	5,2
	FALSO	i nospilotnomie		No results No results		0,03 345,0018			1332071 3426490	3	0 0	No matche No matche DDA for pri [M+			6,6	7,5
	FALSO			No results No results			104,5233		2009886	0	0 0	No matche No matche No MS2 [M+		2033431	4,2	7,3
	IALJU		INO TESUILS	THE LEGALITY IND LEGALITY	INO TESUITS INO TESUITS	103,310	107,3233	0,223	2003000	U	0 0	IN THE PROPERTY OF THE PROPERT	.,.1 2005080		7,4	
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FALSO		C5 H8 N2 C Full match	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
FALSO				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
FALSO		C16 H29 N Full match	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
FALSO		C9 H7 N5 C Full match			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
FALSO	(2E)-hexadecenoylcarnitine			Full match Partial mat	0,12 397,3193 398,3265	7,177 1609373	2	0 0	No matche Single mate DDA for pre [M+H]+1	465803,7 1609373	4,1	7,2
FALSO		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	
FALSO				No results No results	160,9623 161,9696	0,307 1308310	0	0 0	No matche No matche DDA for pre [M+H]+1	561089,6 1308310	3,6	4,5
FALSO	L-(+)-Alanine			Full match Full match	0,25 89,0477 90,05498	3,267 47017490	19	0 0	Multiple m No matche DDA for pre [M+H]+1		4	
FALSO		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
FALSO	Furfuranol	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
FALSO		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		4,2
FALSO				No match No results	3,41 314,1267 315,134	6,804 1227645	10	0 0	No matche No matche DDA for pre [M+H]+1	1170951 1227645	8,8	7,7
FALSO		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
FALSO		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
FALSO		C15 H3 N2 Full match			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
FALSO	Jasmonic acid			Full match Full match	-0,28 210,1255 211,1328	7,029 30315118	40	0 0	Multiple m DDA for pre [M+H]+1	30315118		5,1
FALSO		C3 H2 Cl N: Full match			-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
FALSO				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
FALSO		C2 H N2 O2 Full match			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
FALSO	N-Boc-L-leucine Methyl Ester			Full match Partial mat	0,09 245,1627 246,17	4,461 1223467	6	0 0	No matche Multiple m DDA for pre [M+H]+1	1121616 1223467	8,3	7,2
FALSO		C6 H12 N6 Full match			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
FALSO		140 results	140 results 140 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		7,9	7,7
FALSO		C25 H53 N: Full match			-2,41 523,3642 524,3715	6,863 18244497	6	0 0	No matche Multiple m DDA for pre [M+H]+1		5,7	
FALSO	Glutarylcarnitine	C12 H21 N Full match			-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
FALSO	Benzyl butyrate			Full match Full match	-0,11 178,0994 179,1066	7,145 17210590	95	0 0	Multiple m Multiple m DDA for otl [M+H]+1	17210590 13685985	3,5	4
FALSO		C2 H7 N4 C Full match			0,91 166,008 84,01126	0,978 1781345	0	0 0	No matche No matche DDA for otl [M+2H]+2		7,2	3,9
FALSO				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		8,3	6,6
FALSO	(3R,4R,5R,7R)-7-[(1R,2S,5S)-2,5-Dihydroxy-				0,17 284,1624 285,1697	7,094 11093125	7	0 0	No matche Multiple m DDA for otl [M+H]+1	10461666 11093125	3,5	5,7
FALSO		C8 H3 N6 C Full match			-0,94 246,0053 247,0126	0,975 1975750	6	0 0	Multiple m Single mati No MS2 [M+H]+1	1589648 1975750	4,5	2,1
FALSO		C4 H4 Br Cl Full match			-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
FALSO		C12 H8 N8 Full match			-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
FALSO	(20R)-Cholesta-3,5-diene	C27 H44 Full match			-0,04 368,3443 369,3516	0,976 2261591	1	0 0	No matche No matche No MS2 [M+H]+1	2261591		4,8
FALSO		C3 H5 N4 C Full match			-4,92 160,0142 81,01439	1 1564819	0	0 0	No matche No matche DDA for ot [M+2H]+2		5,5	
FALSO		C5 H12 N6 Full match			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
FALSO	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
FALSO		C13 H26 O Full match	No results No results	No match No match	-2,35 342,1163 343,1236	1,251 1137725	96	0 0	Multiple m No matche No MS2 [M+H]+1	1094720 1137725	4,5	6,1
FALSO	Triethylamine	C6 H15 N Full match	No results No results	Full match Full match	0,31 101,1205 102,1278	3,21 1136966	15	0 0	Multiple m No matche DDA for pre [M+H]+1	1076459 1136966	7,2	5,5
FALSO		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 otl [M+3H]+3	909055,8 831485,3	7,7	7,4
FALSO	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 otl [M+2H]+2	5899740 3041900	4	3,7
FALSO		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	
FALSO				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
FALSO	N-[2-[[2-(Ethylthio)ethyl]thio]ethyl]urea	C7 H16 N2 Full match			3,38 208,0711 209,0784	1.108 2837370	2	0 0	No matche No matche DDA for pre [M+H]+1	2837370 2510803	4,8	3,2
FALSO	[2 [[2 (2),			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
FALSO		C4 H5 Cl4 (Full match			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
FALSO				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
FALSO		C6 H N8 O4 Full match			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
FALSO		C11 H11 Br Full match			0,14 282,0004 283,0077	4,997 958833,6	0	0 0	No matche No matche DDA for pr [M+H]+1	942791 958833,6	8.3	8,3
FALSO		C4 H5 N7 C Full match			1.45 183.0507 184.058	4,856 5632733	0	0 0	No matche No matche DDA for pre [M+H]+1	5234971 5632733	4,2	2,6
FALSO		C4 H5 N7 C Full match			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
FALSO	C.C. constant	C6 H3 N5 Full match			-2,91 145,0384 146,0457	1.438 2757627	1	0 0	No matche No matche DDA for pri [M+H]+1	2757627	4,2	2,0
FALSO	6-Cyanopurine					1,438 2/3/62/	0	0 0		222077.4 398464.1	.,-	7.4
				No results No results	629,823 630,8302	, ,		-	No matche No matche No MS2 [M+H]+1	. ,,	3,8	7,4
FALSO				No results No results	1355,639 678,8265	1,114 309185,7	0	0 0	No matche No matche No MS2 [M+2H]+2		4,3	
FALSO		110.000.00		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	_
	5-Methyl-2-pyrrolidone	C5 H9 N O Full match			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
FALSO				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
FALSO		C12 H30 N! Full match			-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
FALSO				No results No results	1481,657 741,8356	1,09 843916,5	0	0 0		843916,5	7,7	
FALSO		C2 H3 Br Cl Full match			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
	Butabarbital			Full match 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
FALSO	quinolone	C9 H7 N O 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
FALSO		C2 H8 O3 F Full match			-3,89 141,9943 143,0016	0,983 2296127	0	0 0	No matche No matche DDA for pri [M+H]+1	2296127 2278335	4,8	3,2
FALSO				No results No results	738,8227 739,83	1,092 918279,4	0	0 0	No matche No matche No MS2 [M+H]+1	263189,2 918279,4	4,3	7,7
FALSO				No results No results	237,8553 238,8626	1,129 757219,9	0	0 0	No matche No matche DDA for pri [M+H]+1	757219,9 640082,3	6,8	7,4
FALSO				No results No results	519,7322 520,7394	1,14 769945,7	0	0 0	No matche No matche No MS2 [M+H]+1	769945,7		7,4
FALSO		C6 H2 Br N Full match			1,74 685,6579 686,6648	1,139 636411,9	0	0 0	No matche No matche No MS2 [M+H]+1	636411,9 552837	7,4	7,4
FALSO		C5 H Cl N2 Full match			-4,2 171,9491 172,9564	0,307 2235612	0	0 0	No matche No matche No MS2 [M+H]+1	2235612 1412752	4,8	3,9
FALSO				No results No results	503,8502 504,8575	1,091 629110,4	0	0 0	No matche No matche No MS2 [M+H]+1	622281,8 629110,4	7,4	7,4
FALSO		C6 H11 N8 Full match			1,31 258,0568 259,0641	1,099 1266462	8	0 0	No matche No matche DDA for pri [M+H]+1	1266462 1065435	7,7	8,3
FALSO		C15 H7 N4 Full match			0,24 543,8869 544,8941	1,08 1058073	0	0 0	No matche No matche No MS2 [M+H]+1		7,7	7,2
FALSO				No match No results	1,4 202,0453 203,0526	1,098 1360480	2	0 0	No matche No matche No MS2 [M+H]+1	1360480		6,1
FALSO				No match No results	-2,59 252,0972 253,1045	7,005 4498191	2	0 0	No matche No matche DDA for pri [M+H]+1		4,8	5,3
	Neopentylglycol diacrylate			Full match Partial mat	0,08 212,1049 213,1122	6,999 16287715	19	0 0	No matche Multiple m DDA for pri [M+H]+1	16287715		4,6
FALSO				No results No results	73,02313 74,03041	0,974 1554834	0	0 0	No matche No matche DDA for pri [M+H]+1		4,5	2
FALSO				No results No results	0,46 537,8699 538,8772	1,066 816659,3	0	0 0	No matche No matche No MS2 [M+H]+1		7,9	7,9
FALSO				No results No results	529,6263 608,6485	1,144 643701,5	0	0 0		590791,6 643701,5	7,4	7,4
FALSO				No results No results	1,03 440,1036 221,0591	1,96 610763,7	0	0 0	No matche No matche No MS2 [M+2H]+2		6,8	7,9
FALSO				No results No results	1247,672 624,8431	1,089 501748,5	0	0 0	No matche No matche No MS2 [M+2H]+2	501748,5		7,4
FALSO				No results No results	1361,656 681,8351	1,088 915865,2	0	0 0		839700,5 915865,2	7,7	7,7
	N-Caprylyldiethanolamine			Full match No results	0,11 217,2042 218,2115	5,507 1173663	1	0 0	No matche No matche DDA for pri [M+H]+1		7,7	7,7
	Glu-Gly			Full match Partial mat	-0,15 204,0746 187,0713	2,012 1564155	9	0 0	No matche Single mati DDA for pri [M+H-H2O			7,2
FALSO		C5 H9 Br Cl Full match	No results No results	No results No results	1,27 593,7554 672,777	1,132 687366,3	0	0 0	No matche No matche No MS2 [M+DMSO	- 687366,3		4,1
FALSO	Tritetracontan-22-one	C43 H86 O No results	No results No results	Full match No results	2,12 618,6692 619,6765	1,143 524719,5	1	0 0	No matche No matche No MS2 [M+H]+1	524719,5	7,9	
FALSO		No results	No results No results	No results No results	501,834 502,8413	1,064 703557,3	0	0 0	No matche No matche No MS2 [M+H]+1	656942,8 703557,3	4,7	1,4
	Diethylamine			Full match Full match	0,44 73,08918 74,09646	1,01 1984647	10	0 0	Single matc No matche No MS2 [M+H]+1		4,2	
FALSO				No results No results	-3,56 198,9681 199,9753	0,317 566127,8	0	0 0	No matche No matche DDA for pri [M+H]+1		7,4	7,1
FALSO				No results No results	345,7201 346,7274	1,173 970046,3	0	0 0	No matche No matche No MS2 [M+H]+1		7,7	8,3
FALSO				No results No results	0,19 1329,707 665,861	1,088 947993	0	0 0	No matche No matche No MS2 [M+2H]+2		7,7	7,7
	trans-1,2,3,4-diepoxycyclohexane			Full match Partial mat	-0,05 112,0524 113,0597	7,012 23373229	36	0 0	Multiple m Multiple m DDA for pr [M+H]+1		4,6	5,1
	1,6-Hexanediol dimethacrylate			Full match Partial mat	0,19 254,1519 255,1591	7,251 18040136	12	0 0	No matche Multiple m DDA for pr [M+H]+1		5,1	
	Ethylene brassylate			Full match Partial mat	-0,06 270,1831 271,1904	7,062 7803401	6	0 0	No matche Multiple m DDA for pr [M+H]+1		5,7	6,2
FALSO	,			No results No results	0,38 941,5327 471,7736	7,407 1959650	0	0 0	No matche No matche DDA for ot [M+2H]+2		4,8	7,5
					.,20, 0.2,2027 472,7700	, 2333030					-,,0	.,-

FALSO	THI		No results No results		0,28 230,0903			1561019	9	0 0	No matche No matche DDA for p	-	1430137		6,1	5,5
FALSO			No results No results			713,8242		626172,3	0	0 0	No matche No matche No MS2	[M+2H]+2		626172,3		8,5
FALSO		110 1000 10	No results No results			376,7322		799487,3	0	0 0	No matche No matche No MS2	[M+H]+1	799487,3	714655,9	8,5	5,8
FALSO			No results No results		112,9564	-7	0,318	3305728	0	0 0	No matche No matche No MS2	[M+H]+1	3305728		6,4	
FALSO			No results No results No results		4,41 221,8813 1,85 625,7023		1,189	1646199 717985,1	0	0 0	No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1	1646199 717985,1	1626600 599041,4	6,1 7,4	3,9 7,9
FALSO			No results No results		1,07 169,0254			2077803	0	0 0	No matche No matche DDA for p		2077803	1947193	7,4	7,5
FALSO			No results No results		-2.36 139.9885		0,341		0	0 0	No matche No matche DDA for p		2077803	1067251	7,3	7,3
			No results No results		,	337,1242		1754158	1	0 0	Single mate No matche DDA for p		1754158	1651578	7,2	6,6
FALSO			No results No results		0,71 222,0564		7,154	1524631	7	0 0	Multiple m Single mati No MS2	[M+H]+1	498480,7	1524631	4,1	5
FALSO			No results No results		1409,657			609588,1	0	0 0	No matche No matche No MS2	[M+2H]+2	272129,6	609588,1	6	6,8
FALSO	3,5-DIISOPROPYLSALICYLIC ACID	C13 H18 O Full match	No results No results	Full match Partial mat	-0,21 222,1256	255,159	7,187	18418055	36	0 0	Single mate Multiple m DDA for p	r [M+H+Me		18418055		5,1
FALSO		C7 H4 N4 C Full match	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 o	tl [M+2H]+2	8527232	3424961	5,1	6,4
FALSO			No results No results		140,9513			15451217	0	0 0	No matche No matche DDA for p		15451217		5,7	
FALSO			No results No results		1,68 277,8859	.,		683229,7	0	0 0	No matche No matche No MS2	[M+H]+1	683229,7		8,5	
FALSO			No results No results		401,7278			598985,2	0	0 0	No matche No matche No MS2	[M+H]+1	598985,2		8,5	7,9
FALSO			No results No results No results		1,48 875,5243 0.63 567,7438		7,404	1684387 574317,3	0	0 0	No matche No matche No MS2 No matche No matche No MS2	[M+2H]+2 [M+H]+1	1684387 574317,3	1546697 569136,4	6,6 7,4	6,6 7,4
FALSO			No results No results		-1,43 919,4552			1091844	0	0 0	No matche No matche DDA for o				7,4	6,6
FALSO			No results No results		335,2138		0,974		0	0 0	No matche No matche No MS2	[M+2H]+2	1040012	1720596	7,2	4,5
FALSO			No results No results		-3,57 183,0807		3,232	913900	7	0 0	No matche No matche DDA for p		913900	825843,1	8,8	7,4
FALSO			No results No results			274,8733		1052971	0	0 0	No matche No matche DDA for p		1052971		8,3	7,2
FALSO	meprobamate	C9 H18 N2 Full match	No results No results	Full match Full match	0,24 218,1267	219,134	1,958	727284,7	21	0 0	Single mate No matche DDA for p	r [M+H]+1	695428,3	727284,7	8,5	6,8
FALSO		C6 H6 Cl Nt Full match	No results No results	No match No results	-4,66 577,7725		1,121	459237,2	1	0 0	No matche No matche No MS2	[M+H]+1	388105,9	459237,2	8,2	7,9
FALSO	1-Piperideine		No results No results		0,56 83,07355			1536023	13	0 0	Multiple m No matche DDA for p		1536023		6,1	6,1
FALSO			No results No results			622,5439		556485,3	0	0 0	No matche No matche No MS2	[M+H]+1	556485,3		7,9	8,5
FALSO			No results No results		683,8051			665007,1	0	0 0	No matche No matche No MS2	[M+H]+1	531142,8		3,6	4,7
FALSO			No results No results		195,1471			875348,8	0	0 0	No matche No matche DDA for p	-		875348,8	7,4	7,2
FALSO FALSO	Methyltrifluorosilane		No results No results No results		519,5969 3.13 99.99592		1,175	789022,3 1906414	0	0 0	No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1	789022,3 1868874	754488,4 1906414	7,4 6,6	7,4 1,5
FALSO			No results No results		-2.08 347.8286	. ,	,	499284,8	0	0 0	No matche No matche No MS2	[M+DMSO		2300414	7,4	1,3
FALSO			No results No results		,	735,5943		426588,6	0	0 0	No matche No matche No MS2	[M+H]+1	426588,6		7,4	
FALSO	Palmitelaidic acid		No results No results		0,78 254,2248			50344573	36	0 0	Single mate Multiple m DDA for p			50344573		5,1
FALSO			No results No results		-0,13 229,2405			1862738	1	0 0	No matche No matche No MS2	[M+H]+1	1797739		6,1	6,6
FALSO		C6 H9 O7 F Full match	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
FALSO			No results No results		,	434,6908		674656,5	0	0 0	No matche No matche No MS2	[M+H]+1		674656,5		8,5
FALSO			No results No results		-0,06 779,8006			810450,3	0	0 0	No matche No matche No MS2	[M+H]+1	810450,3		7,4	
FALSO			No results No results		-0,28 569,7401			686516,3	0	0 0	No matche No matche No MS2	[M+H]+1	686516,3		7,4	
FALSO			No results No results		0,02 289,1525	,		911732,3	4	0 0	No matche No matche DDA for p		907321,8		7,2	6,6
FALSO FALSO			No results No results		-4,73 469,6705			544214,7	0	0 0	No matche No matche No MS2		544214,7 459986.5	515276	7,9	7,4
FALSO			No results No results No results		497,6781 1164.496		7.058	459986,5 1037718	0	0 0	No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+2H]+2	459986,5	414803,6 1037718	7,4	6,8 7,2
FALSO	Ethyl (2E.4Z)-2.4-hexadecadienoate		No results No results		1,06 280,2405			39929877	27	0 0	Multiple m Single mate DDA for p			39929877		5,1
FALSO			No results No results		-1,13 235,9515		0.986	1447667	0	0 0	No matche No matche No MS2	[M+H]+1		1447667		5
FALSO		C3 H2 N6 C Full match	No results No results	No results No results	0,9 471,8017		1,136	685849,8	0	0 0	No matche No matche No MS2	[M+H]+1	685849,8		7,4	
FALSO		C6 H6 Cl3 I Full match	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+F	784455,1	733115,5	5,8	4,7
FALSO	azidamfenicol	C11 H13 N! No results	No results No results	Full match No results	2,35 295,0924	296,0996	1,447	365737,2	7	0 0	No matche No matche DDA for p	r [M+H]+1	365737,2		4,3	
FALSO			No results No results			677,6356		522953,8	0	0 0	No matche No matche No MS2	[M+H]+1	522953,8		7,4	
FALSO			No results No results		-1,63 197,0099		7,554		0	0 0	No matche No matche No MS2	[M+2H]+2	8441568		5,7	2,1
FALSO	N-(3-Methoxyphenyl)-4-(pyrazolo[1,5-b]pyri				-4,26 318,1216		-7-	1020947	4	0 0	No matche No matche DDA for p		955710,4	1020947	7,2	8,3
FALSO	Diethylene glycol n-butyl ether		No results No results		-0,08 162,1256		0,392		17	0 0	No matche No matche DDA for p		6838397	6840645	3,5	4
FALSO	2-Nitro-5-sulfidobenzoate		No results No results		-3,85 196,9775	594,8653	0,33	527494,2 798744	0	0 0	No matche No matche No MS2	[M+2H]+2 [M+H]+1	527494,2 608043.1	798744	8,5 5,8	7,9 6,8
FALSO			No results No results		-0,97 575,695			638014,3	0	0 0	No matche No matche No MS2	[M+H]+1	008043,1	638014.3	5,6	7,4
FALSO			No results No results		.,.	460,7826	7,403	1623021	0	0 0	No matche No matche No MS2	[M+2H]+2	1623021	1598329	5,5	5,5
FALSO			No results No results		-1,16 237,0413			212143.8	1	0 0	No matche No matche No MS2	[M+2H]+2		128477,5	3,8	7,1
FALSO	3,4-DIMETHOXYBENZENEPROPANOL	C11 H16 O Full match	No results No results	Full match Partial mat		197,1172	7,064	25679277	31	0 0	No matche Multiple m DDA for p		25679277		5,1	4
FALSO		C3 H6 N P : Full match	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 p	r [M+H]+1	595570,9	543564,1	5,8	6,3
FALSO			No results No results		0,33 309,1941	310,2014	5,934	1111776	13	0 0	No matche Multiple m DDA for p	r [M+H]+1	1036958	1111776	7,7	7,7
FALSO			No results No results		-2,85 493,7215			610858,7	0	0 0	No matche No matche No MS2	[M+H]+1		610858,7		7,4
FALSO			No results No results		0.,0000.	98,01361		358981,1	0	0 0	No matche No matche No MS2	[M+H]+1	358981,1	,	6	6,5
FALSO			No results No results		0,8 131,0584		3,261	1874817	33	0 0	Multiple m Multiple m DDA for p			1874817	7,2	6,6
FALSO			No results No results		,	257,9993	-,	643140,1 478054.7	1	0 0	No matche No matche DDA for p		643140,1	570646	7,9	8,5
FALSO FALSO			No results No results No results		0,82 531,853 0,12 245,1627	532,8603 246,17	,	914476,1	6	0 0	No matche No matche No MS2 No matche Multiple m DDA for p	[M+H]+1 r: [M+H]+1	409535,7 841196,8	/	7,9 6,1	7,9 7,7
FALSO			No results No results		-1,1 487,6488			652678,9	0	0 0	No matche No matche No MS2	[M+H]+1		626699.8	7,4	7,7
FALSO			No results No results			612,8817		826234,4	0	0 0	No matche No matche No MS2	[M+H]+1	826234,4		7,4	6,8
FALSO			No results No results		-0,61 658,8365		7	572023,7	0	0 0	No matche No matche No MS2	[M+H]+1	572023,7		7,4	
FALSO			No results No results		565,665	644,6859	1,143	483373,7	0	0 0	No matche No matche No MS2	[M+DMSO	483373,7		6,8	
FALSO			No results No results			436,7698		649549,4	0	0 0	No matche No matche No MS2			649549,4		7,4
	N-(5-Aminopentanoyl)-L-α-aspartyl-L-phenyl				-2,42 1271,677			573689,5	1	0 0	No matche No matche No MS2	[M+2H]+2		573689,5		7,9
FALSO			No results No results			368,7823		609104,5	0	0 0	No matche No matche No MS2			609104,5		7,4
	(2R,3S,4E,8E)-3-Hydroxy-2-(palmitoylamino)- 5-Pentylfuran-2(5H)-one				0,36 700,5522			10533251 19839676	20	0 0	No matche No matche DDA for p				- 4	5,1
FALSO			No results No results No results No results	Full match Partial mat	-0,11 154,0994 -0.37 370.0965			908681.2	39	0 0	No matche Multiple m DDA for p No matche Single mat No MS2				5,1 6,1	3,5 7,2
			No results No results		-0,37 370,0965		, ,	2526118	2	0 0	No matche Single mati No MS2 No matche Single mati DDA for p		2203138	,	7	5,9
FALSO			No results No results		-0,14 194,1134			375250,6	0	0 0	No matche No matche No MS2		375250,6		6,5	3,3
			No results No results		0,36 286,1894			856817,6	2	0 0	No matche No matche DDA for p			856817,6	6,8	7,7
			No results No results		0,27 117,0539			984972,9	8	0 0	Single mate No matche DDA for p				5	5,2
FALSO	4-Nitropiazthiole		No results No results		1,21 180,9948	91,50468	7,42	6811846	2	0 0	No matche No matche No MS2		6811846		5,1	
FALSO			No results No results		4,7 269,1111			899008,3	5	0 0	No matche No matche No MS2				7,9	6,1
FALSO			No results No results		-0,39 133,9508			1920294	0	0 0	No matche No matche DDA for p				4,5	2,6
FALSO	5 th day 8t days to		No results No results			650,6331		554964,9	0	0 0	No matche No matche No MS2				7,4	7,4
FALSO			No results No results No results	Full match Partial mat	-0,13 220,0848			762728,8	17 4	0 0	Multiple m Single mati DDA for p No matche No matche DDA for p				7,9	7,4
FALSO			No results No results No results No results		-4,89 318,1217 561 5815	319,1289 562.588		1261924 561782,6	0	0 0	No matche No matche DDA for p No matche No matche No MS2		1132083	1261924 561782,6	7,7 7,9	7,7
FALSO			No results No results		-5,1 259,9982			1140421	7	0 0	No matche No matche No MS2	[M+H]+1	1140421		2,8	4,5
FALSO			No results No results			300,7948		600347,4	0	0 0	No matche No matche DDA for p			600347,4		5,8
	N-Acetyl-4-chloro-D-phenylalanyl-4-chloro-D				-4,34 1441,608			552266,5	1	0 0	No matche No matche No MS2			552266,5		6,8
FALSO		C23 H47 N! Full match	No results No results	No match No results	-0,42 543,3326	544,3398	7,045	10881449	3	0 0	No matche No matche No MS2	[M+H]+1		10881449		4
FALSO		C62 H98 N Full match	No results No results	No results No match	0,3 1086,681	544,348	0,984	895869,6	0	0 0	No matche Multiple m No MS2	[M+2H]+2		895869,6		5,5

FALSO		No results	No results No results	No results No results	653,7088	654,7161	1,136	542227,3	0	0 0	l l	matche No matche No MS2	[M+H]+1	542227,3		7,4	
FALSO		No results	No results No results	No results No results	1465,682	733,8484	1,088	677981,2	0	0 0	N	matche No matche No MS2	[M+2H]+2	563203,5	677981,2	3,6	7,4
FALSO	N-[(2S)-4-Cyclohexyl-1-ethoxy-1-oxo-2-butar	C15 H27 N Full match	No results No results	Not the tor No results	0,24 285,1941	286,2014	5,607	1081160	12	0 0	l l	matche No matche DDA for p	r [M+H]+1	1081160	1060607	7,7	5,5
FALSO				Full match Full match	0.67 114.0318	115.0391	1.477	20452462	15	0 0	S	ngle mate No matche No MS2	[M+H]+1	20452462		4	
FALSO	DES(PHENYLBUTOXY)PHENYLETHOXY SALME				0.14 387.241	388,2483	1.819	931332,5	1	0 0		matche Multiple m DDA for p	r [M+H]+1	875252.8	931332.5	6,6	7,7
FALSO	8,8'-Ethane-1,2-diylbis(1,3-dimethyl-3,7-dihy				-3,84 386,1436			674205,5	1	0 0		matche No matche No MS2	[M+H]+1	505586,3	674205.5	5,8	7,9
FALSO		No results	No results No results	No results No results	613,7217	614.729	1.136	552640,2	0	0 0		matche No matche No MS2	[M+H]+1	486643,5	552640.2	6,8	7,9
FALSO	Benzoylcyclohexane	C13 H16 O No results	No results No results	Full match Partial mat	0.36 188,1202	189,1275		711692,3	17	0 0		matche Single mate No MS2	[M+H]+1	711692,3		3	8.5
FALSO	, , ,			No results No results	0,49 717,6139			464353.8	0	0 0		matche No matche No MS2	[M+H]+1	464353.8		7,9	7,1
FALSO				No results No results	109,0052			448023,8	0	0 0		matche No matche DDA for o	-	329433.4		8,2	8,5
FALSO				No results No results	179.8871			853659,5	0	0 0		matche No matche No MS2	[M+H]+1	853659.5		5,5	5.8
FALSO				No results No results		168,6141		1379849	0	0 0		matche No matche No MS2	[M+H]+1	1379849	750574,4	5,5	3,0
FALSO				No results No results	0.47 425.8431			416649,8	0	0 0		matche No matche No MS2	[M+H]+1	15750-15	416649,8	3,3	8,5
FALSO				No results No results	-0.14 633.8394			550781.9	0	0 0		matche No matche DDA for p	*	550781.9	410045,8	7,9	0,5
FALSO	Decanamide			Full match No results	-0.03 171.1623			1119657	12	0 0		matche No matche No MS2	[M+H]+1	1119657	1090980	6.6	7,7
FALSO	Decariamide			No results No results	1,53 493,8308	,		301774,3	0	0 0		matche No matche No MS2	[M+H]+1	1113037	301774,3	0,0	8,2
FALSO				No results No results	0.98 675.6286			569452,6	0	0 0		matche No matche No MS2	[M+H]+1		569452,6	-	7,4
FALSO	1-ETHYL CITRATE			Full match Full match	3,2 220,059			368106.8		0 0		ultiple m No matche DDA for p		368106,8	293315,2	8,2	7,4
FALSO	1-EITHE CHRAIL			No results No results	-2,66 433,8466			637727,6	0	0 0		matche No matche No MS2	[M+H]+1	637727.6		7,9	7,0
FALSO				No results No results	1.37 529.7608			644474,8	0	0 0		matche No matche No MS2	[M+H]+1	644474,8	024021,3		7,5
FALSO				No results No results	,, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	304,7427		1795233	0	0 0		matche No matche No MS2	[M+2H]+2		C00111 7	7,4 2,3	4,7
FALSO				No results No results		580,5591		538819,1	0	0 0		matche No matche No MS2	[M+H]+1	510194.1		7,9	4,1
FALSO				No results No results	603,7838			1027230	0	0 0		matche No matche No MS2	[M+H]+1	1027230		2,8	5,2
FALSO				No results No results	2,3 265,8353	,		634076,1	0	0 0		matche No matche DDA for p		634076,1	313/02,/	7,4	3,2
FALSO				No results No results	-0,35 679,7119			607379,9	0	0 0		matche No matche No MS2	[M+H]+1	607379,9			
									-	0 0			*		202502.1	7,4	7.1
FALSO				No results No results		594,8311	1,087	710310	2	0 0		matche No matche No MS2	[M+H]+1		283502,1	2	7,1
FALSO		C9 H22 N9 Full match		No match No results No match No results	-0,82 303,1682		7,104	8879503		-		matche No matche DDA for p		8879503		4,6	
	2 Marked 2 (/25 CE) 2 7 44 1-1-1-1-1 2 2 2				1,21 166,0145		1,205	1050511	1	0 0		matche No matche No MS2	[M+H]+1	1050511	1224022	6,1	2.4
FALSO	2-Methyl-3-[(2E,6E)-3,7,11-trimethyl-2,6,10-				0,15 376,2403	189,1274	0,958	1224923 595089.2	-	0 0		matche No matche No MS2	[M+2H]+2		1224923	4,7	3,4
FALSO		C3 H Br Cl4 Full match			3,39 427,6924	-,	-,		0	0 0		matche No matche No MS2	[M+H]+1		578388,7	7,9	8,5
FALSO				No results No results	0,93 571,8377	0.2,0.0		504639,8	0	0 0		matche No matche No MS2	[M+H]+1	504639,8	439087	7,4	7,4
FALSO	an arib and an			No results No results		672,6878		471554,3	0	0 0		matche No matche No MS2	[M+H]+1	702502.5	471554,3	7.0	7,4
FALSO	meribendan	C15 H14 N Full match			-4,3 294,1216			702598,3	24	0 0		matche Multiple m No MS2	[M+H]+1	702598,3		7,9	7,4
FALSO				No results No results	- 7.	182,6298		1591279	0	0 0		matche No matche No MS2	[M+H]+1		1591279		5
FALSO				No results No results	599,6093	,.		472606,9	0	0 0		matche No matche No MS2	[M+H]+1	472606,9		7,4	
FALSO				No results No results	. ,	348,8684	1,002	1406619	0	0 0		matche No matche No MS2	[M+H]+1	1234721	1406619	4,5	3,4
FALSO				No results No results		613,8478		720474,4	0	0 0		matche No matche No MS2	[M+H]+1		720474,4	-	7,4
FALSO	2-[(2-Benzyl-1,7,7-trimethylbicyclo[2.2.1]hep				0,13 315,2563		7,009	1068035	1	0 0		matche Single mati No MS2	[M+H]+1	901832,5	1068035	7,7	5
FALSO				No results No results	. ,	749,8225	,	587028,7	0	0 0		matche No matche No MS2	[M+2H]+2			7,4	
FALSO				No match No results	-0,65 335,1945		_	10047400	1	0 0		matche No matche No MS2	[M+H]+1	10047400		4	4,6
FALSO		C15 H35 N Full match			1,38 407,2156		6,906	6495053	0	0 0		matche No matche No MS2	[M+H]+1	5863030	6495053	5,1	5,1
FALSO				No match No match	2,62 418,2945	,		795092,5	2	0 0		ngle mate No matche No MS2	[M+H]+1	748711,4	795092,5	8,5	7,9
FALSO	Hydroxyethyl imidazolidinone			Full match Partial mat	0,19 130,0743		1,591	3389687	18	0 0		matche Single mate DDA for p			3389687		4,8
FALSO		C13 H22 N Full match			-1,25 285,0962			701439,1	2	0 0		ngle mate No matche DDA for p		594882	701439,1	7,9	7,9
FALSO				No results No results		746,8141		714328,3	0	0 0		matche No matche No MS2	[M+H]+1		714328,3		6,3
FALSO				No match No results	-4,14 420,1492			653517,4	5	0 0		matche No matche No MS2	[M+H]+1	653517,4		7,4	6,8
FALSO				No match No results	-3,69 453,2856			1652623	4	0 0		matche No matche No MS2	[M+H]+1	1652623	991166,3	6,1	5,5
FALSO	Succinimide			Full match Partial mat	0,56 99,03208	,		16636010	7	0 0		matche Multiple m DDA for p		16636010		4	
FALSO	1,2-Dioxin			Full match Full match	0,43 84,02117			30162113	11	0 0		ngle mati Single mati DDA for p				4,6	
FALSO		C4 H10 Cl3 Full match			3,1 379,8829	000,000	1,195	692281	0	0 0		matche No matche No MS2	[M+H]+1	692281	665792,6	5,8	8,5
FALSO				No results No results		495,3276		1897455	0	0 0		matche No matche No MS2	[M+H]+1		1897455		
FALSO	Photo-clair And d	C18 H34 O Full match		No results No results	1203,69 -1,31 298,2504	,		505698,9 23380238	0 25	0 0		matche No matche No MS2	[M+2H]+2	23380238		8,5	
	Ricinoleic Acid						-,			-		ngle mati Multiple m DDA for p			4647000		7.7
FALSO		C12 H12 N. Full match			2,58 408,0122		2,146	1617808	0			matche No matche No MS2	[M+H]+1	1483879	1617808	7,2	7,7
FALSO				No results No results		728,6492		515063,4	-	-		matche No matche No MS2	[M+H]+1	398056,6		7,4	7,4
FALSO				No results No results	1,56 365,8592			594521,4	0	0 0		matche No matche No MS2	[M+H]+1	594521,4		7,4	7,9
FALSO				No results No results No results No results		278,8932 124.9226	1,121	546246,3 989181	0	0 0		matche No matche No MS2 matche No matche No MS2	[M+3H]+3 [M+H]+1		546246,3 989181	4.5	8,5
					-,									909439,9		4,5	7.0
FALSO				No results No results No results	0,16 420,3101			785332,5	0	0 0		matche No matche No MS2	[M+H]+1	125002.4	785332,5	7.0	7,9
FALSO FALSO	Phencyclidine			Full match No results	-0.08 243.1987	666,6069 244.206		435603,4 1135244	3	0 0				1002018		7,9 7,2	7,9 7,2
					.,					-		matche No matche DDA for p					
FALSO	Chromium(3+) tri(D-gluconate)			Full match No results	1,41 637,0928	,	_,	2699251	1	0 0		matche No matche No MS2	[M+H]+1		670274,2	3,7	8,5
FALSO	Tetrahydrobiopterin LAURIMINODIPROPIONIC ACID	C19 H15 N5 No results		Full match Full match Full match No results	0,26 241,1176	330.264	,	542399,1 1591264	5	0 0		ngle mate No matche No MS2	[M+H]+1	542399,1	1591264	7,4 6.1	7,4
FALSO	LAGMININODIFROFIGNIC ACID			No results No results	1559,601	,		841258.6	0	0 0		matche No matche DDA for po matche No matche No MS2	[M+2H]+1		841258,6	0,1	7,7
FALSO				No results No results No match No results			7		19	0 0		matche No matche No MS2	[M+2H]+2		870264,8	Е 0	
FALSO				No match No results No match No results	-0,24 235,099 -2.5 227,9947	236,1063 229.002	0.976	870264,8 1537029	2	0 0		matche No matche No MS2 matche No matche No MS2	[M+H]+1	1391430		5,8 7,2	8,3 3,4
FALSO	Phloionolic acid			Full match No results	-2,5 227,9947 -0,05 332,2563	-7		927922.3	5	0 0		matche No matche No MS2	[M+H]+1			6,6	8.3
									1	0 0			-			2.0	7.7
FALSO	N-[4-({4-[(5-Methyl-1H-pyrazol-3-yl)amino]-				2,36 450,1961			912245,4	0	0 0		matche No matche DDA for o				2,8 5	7,7 E E
FALSO				No results No results No results No results		170,8543 89,00834		1097067 9508628	0	0 0		matche No matche No MS2 matche No matche DDA for p				4	5,5
FALSO									0	0 0							5,7
FALSO				No results No results		248,8818		629745,6 286471.7	0	0 0		matche No matche DDA for p		629745,6	286471,7	7,4	7,4
FALSO				No results No results No results No results	4.4 115.9698	81,51374		1493918	0	0 0		matche No matche DDA for po matche No matche No MS2		1/02010	2864/1,/ 1411024	4,5	4,9 3,9
FALSO				No results No results No match No match	-3.02 582.248			878502,3	14	0 0		ngle mate Multiple m No MS2			1411024	5,5	3,5
FALSO				No results No results	-0,31 1339,665	,		578813,9	0	0 0		matche No matche No MS2			E70013.0	3,5	4.7
FALSO				No results No results	0,84 610,8411			667021,2	0	0 0		matche No matche No MS2				7,4	
	H-Thr(PO3H2)-OH			Full match Full match	0,84 610,8411			1669491	6	0 0				1625796			7,6 5
FALSO	II-IIII(FO3HZ)FOH			No results No results	-3,45 231,9782				0	0 0		ultiple m No matche DDA for p matche No matche DDA for p				6,1	
FALSO				No results No results No results No results	-3,45 231,9782 0,15 628,1452			1483284 650333,9	0	0 0		matche No matche DDA for p matche No matche No MS2		1421703 650333,9	1403284	6,6 7,4	6,1
FALSO				No results No results No results No results	-0,33 293,8803			710848,8	0	0 0		matche No matche DDA for p				7,4	
FALSO				No results No results No match No results	-0,33 293,8803			602185,9	2	0 0		matche No matche No MS2			602185,9	6,3	5,8
FALSO				No match No results No results No results		471,3806		949999,6	0	0 0		matche No matche No MS2			949999,6	0,3	5,8
FALSO				No results No results No results No results		91,05834		1433316	0	0 0					1433316	7,7	
FALSO				No results No results No results No results	-4,47 366,1427			647810,3	0	0 0		o matche No matche DDA for po matche No matche DDA for p				7,7	4,5 7,9
	Diethylene glycol n-butyl ether			Full match No results	0,04 162,1256			2808534	17	0 0		matche No matche DDA for p			2690414	5,3	6,4
FALSO	Dietriylerie giycor n-butyi etner			No results No results	3.6 600.2587			936241,1	0	0 0		matche No matche No MS2					8,3
FALSO				No results No results No results No results	0,21 1545,632			632080,8	0	0 0		matche No matche No MS2		1	632080,8	5,2	7,4
	5-Oxidanidyl-5-oxidanylidenenorvalylthreon				-0,09 247,093			982995,3	2	0 0		matche No matche No MS2			982995,3		7,4
FALSO	3 Salamayi 3 Osidanyildenenoi varyildireoni			No results No results	1,19 760,5825			7904862	0	0 0		matche No matche No MS2		7004963	302333,3	5.7	-,,,
FALSO				No results No results	-0,83 391,2208			12647922	0	0 0		matche No matche DDA for p			12647922	5,7 3,2	4,6
1760		CET 1134 IV FUII IIIalCII	I TO TESUITS INO TESUITS	THO LEGALES IND LEGALES	0,03 331,2208	332,2201	0,771	1204/322	3	0	, , ,		of time till±T	4515501	12041322	3,2	7,0

FALSO		C17 H11 N: Full match	No results No results	No results No results	-0.01 751.7925	752,7998	1.06 471	1434.3	0 (0		No matche No matche No MS2	[M+H]+1	471434,3	437681.2	7,4	7,9
FALSO		C11 H3 Cl4 Full match			0.17 735.6747	. ,	1,132 361		0 0	0 0		No matche No matche No MS2	[M+H]+1		361474.3		8.2
					.,,.												
FALSO		C8 H15 Cl3 Full match			-4,3 391,8953		1,22 911		-	0		No matche No matche No MS2	[M+H]+1	798061,5	911289,6		8,3
FALSO		C9 H Cl N6 Full match	No results No results	No results No results	0,74 545,8617	546,869	1,107 341	1428,7	0 (0		No matche No matche No MS2	[M+H]+1	341428,7		7,6	
FALSO	2-(6-Hydroxy-2,5,7,8-tetramethyl-3,4-dihydr	C18 H30 N No results	Invalid mas No results	Invalid mas No results	-6,02 292,2259	293,2332	1,46 315	.5924,5	1 2	2 0	76,5	No matche No matche DDA for pr	[M+H]+1	246885,3	315924,5	4,9	1,1
FALSO		C9 H7 Cl N. Full match	No results No results	No match No results	-2,05 337,9782	338.9855	1,235 12	215158	4 (0		No matche No matche No MS2	[M+H]+1	1215158		6,1	
FALSO				Full match Full match	0,29 280,2403			382926	27 (0		Multiple m Single mati No MS2	[M+H]+1		1382926		6,1
FALSO		C2 H3 N2 C Full match			2,55 259,916		1,017 14		0 0			No matche No matche No MS2	[M+H]+1		1425551		
														424245	1423331		7,2
FALSO		C4 H2 Cl3 (Full match			-,	440,7173		434315	0 (No matche No matche No MS2	[M+H]+1	434315		7,9	
FALSO		C3 H7 N3 C Full match	No results No results	No results No results	-3,5 197,01	99,51225	7,388 59	978077	0 (0		No matche No matche No MS2	[M+2H]+2		5978077		4,6
FALSO		No results	No results No results	No results No results	227,8057	228,8129	1,147 10	006102	0 (0 0		No matche No matche No MS2	[M+H]+1	984184,6	1006102	4,5	6,1
FALSO		No results	No results No results	No results No results	1207.633	604,8236	1,106 289	9979.3	0 (0		No matche No matche No MS2	[M+2H]+2		289979,3		4,9
FALSO		C3 H8 Br2 (Full match	No recults No recults	No results No results	-0.04 673.6328	674 6396	1.139 517	7202.8	0 () 0		No matche No matche No MS2	[M+H]+1	517292.8	221408,2	7,4	7,6
FALSO		C18 H26 N Full match			-4.6 351.1583	. ,	5.118 741	- /-	7 (No matche Multiple m DDA for pr					7,9
					,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	,											
FALSO		C7 H17 Cl Full match			2,16 428,0551		1,217 444		2 (No matche No matche No MS2	[M+H]+1	444425,8			7,4
FALSO		No results	No results No results	No results No results	96,52647	97,53375	1,004 12	287887	0 (0		No matche No matche No MS2	[M+H]+1	1287887	1146720	1,7	7,7
FALSO	(1S,7aR)-7-({[(2S,3R)-2-Hydroxy-2-isopropyl-	C21 H33 N Full match	No results No results	Full match No results	0,01 395,2308	396,2381	1,819 845	5854,7	1 (0 0		No matche No matche DDA for pr	[M+H]+1	794567,6	845854,7	7,9	7,2
FALSO		C3 H N4 O Full match	No results No results	No results No results	-2,04 139,9885	140.9958	0,309 7	794153	0 (0		No matche No matche DDA for pr	[M+H]+1	794153	183373,3	4,1	6,5
FALSO		C3 H6 Br Cl Full match	No results No results	No results No results	-2,41 505,7115		1,14 498		0 (0				498621,7			7,9
FALSO		C10 H3 Br (Full match			1,22 633,6473		1,143 354		0 0	0		No matche No matche No MS2	[M+H]+1	354448.7	306289,2		7,1
						318.7735			0 0			No matche No matche DDA for pr		334440,7			
FALSO				No results No results			1,171 635								635390,8		5,8
FALSO				No results No results		548,6114	1,175 440		0 (No matche No matche No MS2	[M+H]+1	440010,7			7,9
FALSO		C H3 O11 F Full match	No results No results	No results No results	3,37 315,862	316,8692	1,091 6	629198	0 (0		No matche No matche No MS2	[M+H]+1		629198		7,9
FALSO	DIHYDROXYETHYL LAURAMINE OXIDE	C16 H35 N Full match	No results No results	Full match No results	0,03 289,2617	290,269	6,822 904	4371,5	2 (0 0		No matche No matche No MS2	[M+H]+1	826721,2	904371,5	6,3	8,3
FALSO		C4 H5 N4 C Full match	No results No results	No results No results	-2,54 361,8677	384.8568	1,093 574	4634.5	0 (0		No matche No matche DDA for pr	[M+Na]+1		574634.5		7,9
FALSO		C2 H Cl N4 Full match			1,46 305,843		1,125 491		0 0	0 0		No matche No matche No MS2	[M+H]+1	491208.1	452314,4		7,4
FALSO		C11 H4 Cl Full match			-0,87 634,801		1,105 296		0 (No matche No matche No MS2	[M+ACN+N		296285,9		7,1
									-								
FALSO		C5 H14 Cl Full match			4,04 211,0845			.8535,9	27 (, ,		No matche Multiple m DDA for pr					6,8
FALSO				No results No results	451,8369			6431,9		0		No matche No matche No MS2	[M+H]+1	553441,8	576431,9		7,4
FALSO				No results No results	72,39221	73,39948	1,463 20	080298	0 (0		No matche No matche No MS2	[M+H]+1	2080298	2002852	5,9	4,8
FALSO	1-Bromo-4-chlorobutane	C4 H8 Br Cl No results	No results No results	Full match No results	3,56 169,9504	170,9577	1,065 763	3212,8	2 (0 0		No matche No matche No MS2	[M+H]+1	689732,2	763212,8	7,4	7,4
FALSO				No results No results		366,4053		308120	0 0	0 0		No matche No matche No MS2	[M+2H]+2	1219189	1308120		3,9
FALSO		C7 H21 N8 Full match			-1,17 248,1624		6,81 732		4 (No matche No matche No MS2	[M+H]+1	673864.8			6.8
														073004,8	,		-,-
FALSO	phenylsilicon	C6 H5 Si No results			-1,62 105,0159		0,98 814		1 (No matche No matche No MS2	[M+H]+1		814027,9		6,8
FALSO				No results No results	407,6738	408,6804	1,174 719		0 (0		No matche No matche DDA for pr		719600,5		7,9	
FALSO		No results	No results No results	No results No results	237,8553	238,8626	1,184 10	048486	0 (0 0		No matche No matche DDA for pr	[M+H]+1	1048486	1018636	6,1	3,4
FALSO		No results	No results No results	No results No results	1323,69	662,8523	1,071 549	9344,1	0 (0 0		No matche No matche No MS2	[M+2H]+2		549344,1		7,9
FALSO		No results	No results No results	No results No results	1549 645	775.8295	1,086 661	1979 3	0 () 0		No matche No matche No MS2	[M+2H]+2	661979 3		7,4	
FALSO		C H4 Cl N4 Full match			-4,52 329,9237	330.931	0,974 13		0 0	0 0		No matche No matche No MS2	[M+H]+1	1263002	1332584	7,2	5
FALSO				No results No results		216.8331	1,15 11		0 (No matche No matche DDA for pr		1180706	1049215		3,9
								_									
FALSO				No results No results		92,00632	0,3 339			0		No matche No matche No MS2	[M+H]+1	145597,9	339925,2	8,2	6
FALSO		C10 H2 Cl Full match			4,44 315,9792		1,195 540	0172,7	0 (0 0		No matche No matche No MS2	[M+H]+1	540172,7	511624,3	7,4	7,9
FALSO		No results	No results No results	No results No results	88,49693	89,50421	0,997 10	043406	0 (0 0		No matche No matche No MS2	[M+H]+1	901111,4	1043406	3,4	4,5
FALSO		C26 H3 Br (Full match	No results No results	No results No results	0,31 755,7319	756,7392	1,123 245	5945,3	0 (0 0		No matche No matche No MS2	[M+H]+1	245945,3	240148,8	8,2	8,2
FALSO		No results	No results No results	No results No results	594,8608	595.868	1,112 248	8906.9	0 (0		No matche No matche No MS2	[M+H]+1	248906.9		8.2	
FALSO		C23 H7 O1 Full match			0,31 679,8619		1,082 676		0 (No matche No matche No MS2	[M+H]+1	676742,8	E04762 4		6,8
) 0							
FALSO				No results No results		744,6238	1,139 453		-	, ,		No matche No matche No MS2	[M+H]+1	453229,9	408916,4		7,4
FALSO	Dimedone			Full match Full match	0,31 140,0838		1,553 168		46 (Multiple m Multiple m No MS2	[M+H]+1	16817138		4	
FALSO		No results	No results No results	No results No results	733,5874	734,5947	1,143 399	9071,7	0 (0 0		No matche No matche No MS2	[M+H]+1	380004,7	399071,7	7,1	7,4
FALSO		No results	No results No results	No results No results	579,8553	580,8626	1,105 295	5465,2	0 (0 0		No matche No matche No MS2	[M+H]+1		295465,2		4,3
FALSO		C51 H58 N Full match	No results No results	No results No results	-1,46 715,4296	716.4369	7.849 14	479419	0 (0		No matche No matche DDA for pr	[M+H]+1	1370906	1479419	7,2	7,2
FALSO				No results No results		109,5216	7,432 99	033316	0 (0		No matche No matche DDA for pr			9933316		5,1
FALSO				No results No results		696,6934	1,133 421		-) 0		No matche No matche No MS2	[M+H]+1	421374.9	3333310	7.9	3,1
 									-					- 1	752524.0		6.0
FALSO		C14 H29 N Full match			-4,53 273,1763		6,455 753			, ,		No matche No matche DDA for pr		723684,9	753521,8		6,8
FALSO	[Similar to: Ethylenediaminetetraacetic acid				-0,6 292,0125			8889,2	0 7		74,4	No matche Multiple m DDA for pr		388889,2		4,3	
FALSO		C3 H5 Br Cl Full match	No results No results	No results No results	-1,86 667,687	668,6935	1,132 414	.4206,9	0 (0 0		No matche No matche No MS2	[M+H]+1	409712,7	414206,9	7,4	7,4
FALSO		C27 H3 N2 Full match	No results No results	No results No results	-0,41 751,783	752,7902	1,117 2	231022	0 (0 0		No matche No matche No MS2	[M+H]+1		231022		8,2
FALSO		No results	No results No results	No results No results	673,8074	674,8147	1,113 237	7600,6	0 (0 0		No matche No matche No MS2	[M+H]+1	237600,6		8,2	
FALSO				No results No results		170,0411	0,969 13		0 0	0 0		No matche No matche DDA for pr	M+ACN+H	1376388	1094089	6,6	3,4
FALSO	NPYR			Full match No results	0,37 100,0637		1,213 11			0 0		No matche No matche DDA for pr		1139498			4,5
FALSO				Full match Full match			5,221 918		112				-	918770.7	1132073		-,5
	. , ,				.,	167,0703						Multiple m Multiple m DDA for pr			720562.2	7,7	7.4
FALSO		C8 H11 N4 Full match			1,98 288,0101		1,206 730		4 (No matche No matche No MS2	[M+Na]+1	702526,2	730598,9		7,4
FALSO		C26 H45 N. Full match			3,19 511,3274			313428	1 (No matche No matche No MS2	[M+H]+1	1313428		6,1	
FALSO		C42 H36 N. Full match			-1,67 648,2436	0.0,000	7,116 884		0 (No matche No matche No MS2	[M+H]+1	664692,9	884360,1	-7-	6,1
FALSO		C34 H53 N Full match	No results No results	No results No results	4,18 671,4035	672,4107	7,861 14	418433	0 (0		No matche No matche DDA for pr	[M+H]+1	1293493	1418433	7,2	7,2
FALSO	3-Oxalomalic acid	C6 H6 O8 Full match	No results No results	Full match Full match	3,4 206,007	207,0142	1,275 747	7287,3	1 (0		Single mate No matche No MS2	[M+H]+1	695620,9	747287,3	7,4	7,4
FALSO		C58 H83 N: Full match	No results No results	No results No results	-0,02 1191,553	398,1918	3,21 441	1605,3	0 (0 0		No matche No matche No MS2	[M+3H]+3	428487,9	441605,3	6,3	7,9
FALSO		C3 H6 Cl Nt Full match	No results No results	No results No results	-0,96 379,9629	380,9702	1,228 11	152877	0 (0 0		No matche No matche No MS2	[M+H]+1	1138017	1152877		7,2
FALSO		C46 H79 N' Full match			0,49 985,5588		7,394 14		0 () ^		No matche No matche No MS2				6,1	5.5
	(2S,3S,4S,5R)-3,4-Dihydroxy-2,6,10,10-tetran				-0,02 240,1362		7,073 193		10 () 0		No matche Multiple m DDA for ot					4.6
				Full match Full match	0.26 168.0284		3,208 533		4 (Single mate No matche DDA for pr					6,8
					.,	,											
				Full match No results	2,87 127,9436		0,307 762		1 (, ,		No matche No matche DDA for ot		585489,9			6,8
FALSO				No results No match	3,7 361,2102		7,031 93		0 (No matche Single mate DDA for pr			9371647		4,6
FALSO				No results No results		109,5216	7,548 98		0 (0 0		No matche No matche DDA for pr				5,1	
FALSO		C24 H37 N. Full match	No results No results	No match No match	-3,09 395,3037	396,311	7,056 983	3971,3	1 (0 0		No matche Single matc No MS2	[M+H]+1	805553,8	983971,3	4,1	5
FALSO		C12 H28 N: Full match			-0,7 345,2152		7,274 74	413839	0 0	0 0			[M+H]+1	5578313			4,6
FALSO				No results No results		702,6443	1,141 384		0 0				[M+H]+1	384611,5		7,6	
FALSO				No results No results		692,6125	1,141 304			0 0			[M+H]+1	304722,7	266192 6		7.1
	268444444																7,1
	2,6-Di-tert-butyl-4-hydroperoxy-4-methyl-2,				0,03 252,1726		7,361 93			0		No matche Multiple m DDA for pr		8036394		4,6	4
FALSO				No match No results	-3,25 261,1576		3,417 723		3 (No matche No matche DDA for pr			723233,1		6,8
FALSO		No results	No results No results	No results No results	527,6748	528,6814	1,149 392	2981,1	0 (0		No matche No matche No MS2	[M+H]+1	392981,1		7,6	
FALSO	Glutaric anhydride			Full match Full match	-2,39 114,0314	115,039	1,373 619		15 (0 0		Single mate No matche No MS2				5,8	
FALSO				No results No results	2,14 379,755		1,145 400		0 (335194,4	400030.9		7,4
FALSO				No results No results		84,95975	1,89 27		0 0			No matche No matche DDA for pr					4,8
FALSO				No results No results		767,8418	1,088 467			0				435931,8			6,3
FALSO				No match No results	-0,79 489,2072		1,961 409		1 (No matche No matche No MS2		409087,5		7,4	6
FALSO				No results No results	-1,17 457,8544	458,8617	1,108 240	0309,4	0 (0 0		No matche No matche No MS2	[M+H]+1		240309,4		8,2
FALSO	N,N-Dibutyl-2-chloroacetamide	C10 H20 Cl No results	No results No results	Full match No results	-3,66 205,1226	206,1299	1,963 550	0857,5	1 (0		No matche No matche No MS2	[M+H]+1	549213,6	550857,5	6,8	7,4
FALSO				No results No results		156,9661	0,306 723	3903,2	0 (0 0		No matche No matche No MS2	[M+H]+1	723903,2			4,7
FALSO	1,6-Dimethyl-1,6-Dinitroso-Biurea			Full match No results	1,14 204,0609		1,249 642			0		No matche No matche No MS2	[M+H]+1	565576,6			8,5
FALSO	z,z zimem, z,z ziminoso ziurea					736,6804				0 0					3.2700,3		3,3
- MLOU		ino results	ivo results NO results	No results No results	05/,0584	730,0604	1,135 4	-1U033	U (, 0		No matche No matche No MS2	[M+DMSO	410833		7,4	

														_			
FALSO			No results No results		1,79 186,0756		.,	3419236	0	-	0		No matche No matche No MS2 [M+2H]+2			4,2	4,2
FALSO		C76 H88 N Full match	No results No results	No results No results	0,28 1434,546	479,1892	6,659	813060,5	0	0	0		No matche No matche DDA for otl [M+3H]+3 8	313060,5	750029,4	6,3	4,7
FALSO		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 matche Single mate DDA for otl [M+2H]+2	1655752	1228347	6,6	5
FALSO		C4 H11 N1 Full match	No results No results	No match No results	-0,84 262,0802	263,0875	1,541	3035481	6	0	0		No matche No matche DDA for pri [M+H]+1	3035481	1492780	4,2	2,8
FALSO		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 matche No matche No MS2 [M+H]+1 8	397573,7	880153,4	8,3	5,5
FALSO		No results	No results No results	No results No results	723,7765	724,7838	1,116	251949,7	0	0	0		No matche No matche No MS2 [M+H]+1		251949,7		8,2
FALSO		No results	No results No results	No results No results	605,82	606,8273	1,114	215430,7	0	0	0		No matche No matche No MS2 [M+H]+1 2	215430,7		8,2	
FALSO	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 matche Multiple m DDA for pre [M+H]+1 1	6810881 1	7549876	3,5	4
FALSO	Guanidinosuccinic acid	C5 H9 N3 C Full match	Invalid mas No results	Full match Full match	0,21 175,0593	176,0666	1,347	702165	1	1	0	15,5	Single mate No matche DDA for pre [M+H]+1	702165	559109	7,4	7,9
FALSO		C4 H9 N Of Full match	No results No results	No results No results	1,89 167,0433	168,0506	0,981	995029,6	0	0	0		No matche No matche No MS2 [M+H]+1 6	515904,3	995029,6	5,2	3,4
FALSO		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 matche No matche No MS2 [M+H]+1 9	992042,1	1036890	5	7,7
FALSO	(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
FALSO		No results	No results No results	No results No results	85,9968	87,00407	0,339	320300,7	0	0	0		No matche No matche No MS2 [M+H]+1		320300,7		8,2
FALSO	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 matche Single mate DDA for pre [M+H]+1 1	9805963		4,6	
FALSO	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 matche Single mate DDA for pre [M+H]+1	261548,4	841659,4	7,1	2,3
FALSO		No results	No results No results	No results No results	96,96151	97,96879	0,342	542927,2	0	0	0		No matche No matche No MS2 [M+H]+1		542927,2		6,8
FALSO		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 matche No matche DDA for otl [M+2H]+2		460781,7		7,9
FALSO		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 matche No matche DDA for otl [M+2H]+2	01403,2	588088,9	6,8	6,8
FALSO	[Similar to: Ethylenediaminetetraacetic acid	C6 H5 N4 C Full match	Invalid mas No results	No results No results	1,03 291,9848	292,9921	1,425	251948,1	0	2	0	71,6	No matche No matche DDA for pri [M+H]+1	251948,1	206747	2,7	4,9
FALSO		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 matche No matche No MS2 [M+H]+1	110292,8		6,8	
FALSO		No results	No results No results	No results No results	541,8136	542,8208	1,052	362537,4	0	0	0		No matche No matche No MS2 [M+H]+1	346002,9	362537,4	7,6	7,6
FALSO	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 matche DDA for pri [M+H]+1 1	3478889 1	2433883	5,1	4,6
FALSO		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 matche No matche No MS2 [M+DMSO-	139476,8	434065,8	7,4	7,4
FALSO	[Similar to: (2R,3S,4S,5R,6S)-2-(hydroxymeth	C H2 N4 O Full match	Invalid mas No results	No results No results	-4,13 147,9698	148,9771	0,307	728248,9	0	10	0	37,4	No matche No matche DDA for pri [M+H]+1	79911,6	728248,9	5,2	4,7
FALSO	[Similar to: 3-Hydroxy-1-[3-(trifluoromethyl)	C7 H6 N6 C Full match	Invalid mas No results	No match No results	1,34 190,0606	223,0941	1,124	1492785	2	3	0	14,7	No matche No matche DDA for pri [M+H+MeC	1492785		4,5	
FALSO	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 mate No matche DDA for pre [M+H]+1	17455,3	468438,2	6,3	7,4
FALSO			No results No results		333,7404	334,7476	1,173	703199,8	0	0	0		No matche No matche No MS2 [M+H]+1	703199,8	597014,1	4,1	7,9
FALSO		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 matche No matche No MS2 [M+H]+1	334140,8	206560	5,4	7,1
FALSO		No results	No results No results	No results No results	331,8454	332,8527	1,112	282090,6	0	0	0		No matche No matche No MS2 [M+H]+1	282090,6	159253,7	7,6	7,6
FALSO		No results	No results No results	No results No results	644,6753	,	1,139	455023,5	0	0	0		No matche No matche No MS2 [M+H]+1		455023,5		7,4
FALSO	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 matche No matche No MS2 [M+H]+1		1497127		5,5
			No results No results		-0,2 243,2562		6,874	1581055	3	0	0				1581055	7,2	5
FALSO	(R)-3-hydroxybutyrylcarnitine	C11 H21 N Full match	No results No results	Full match No results	0,05 247,142		3,213	535790,6	3	0	0		No matche No matche No MS2 [M+H]+1	524413	535790,6	6,3	6,8
FALSO			No results No results		-0,58 713,7472	714,7544		234411,8	0	0	0		No matche No matche No MS2 [M+H]+1	163834,3	234411,8	7,6	8,2
FALSO		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 matche No matche No MS2 [M+H]+1	7346040		4,6	
FALSO			No results No results			438,7203		301314,4	1		0			301314,4		7,6	7,1
			No results No results		-0,05 221,0722		3,347	537177	6	0	0		No matche No matche DDA for pri [M+H]+1	537177		7,4	7,9
FALSO			No results No results		-0,83 273,9348			712443,4	0	0	0			712443,4	669531,8	7,4	4,7
FALSO			No results No results			112,5152		1262966	0	0	0			65524,6		6,8	7,2
FALSO			No results No results		-3,33 450,196			654640,9	2	-	D			80724,2		7,4	7,4
 FALSO			No results No results		-1,68 759,4558		7,841	1329019	0	-	0				1329019	7,2	7,2
 FALSO	3-Oxo-3-({5,7,9,19,23,25,27,31,33,34,35-und				-3,79 1141,719	571,8669	,	475385,4	2		0			175385,4		7,4	
 FALSO			No results No results		0,12 293,1991	. ,	6,184	1662590	11		0				1612175	6,6	7,2
FALSO			No results No results		-1,54 431,3036		6,932	956204	1	-	0		No matche Multiple m No MS2 [M+H]+1	764899	956204	7,4	6,1
FALSO	- h 1-9		No results No results		637,5104			404954,5	0		0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1		404954,5		7,9
FALSO FALSO	phenylsilicon		No results No results		-1,21 105,0159	701,6426		360761,1 373567,2	0	-	0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1		360761,1 373567,2		7,1 7,6
FALSO		110 1000	No results No results		-3.71 153.9596	195,9935		855038,5	0	-	0		No matche No matche DDA for pri [M+ACN+H		855038,5		5,5
FALSO			Invalid ma: No results		0,33 96,05755			2309491	18		0	66,2	Single mate Multiple m DDA for pri [M+ACN+H	398241		6,8	3,3
FALSO			No results No results		0,29 182,0944			793364.6	45		0	 10,2		793364,6	2303431	4,1	
FALSO	[Similar to: Ethylenediaminetetraacetic acid (2,8 291,9576		-,	227500.6	0	-	0	76.7		227500,6		4,1	
FALSO	[Similar to: Ethylenediaminetetraacetic acid		No results No results		711,6687			335290,5	0	_	0	0,7	No matche No matche No MS2 [M+H]+1		335290,5	4,5	7,6
FALSO		C9 H21 P3 Full match			4,92 222,0867	223,094		1327728	1	-	0		No matche No matche No MS2 [M+H]+1		1327728		6,6
FALSO	3,6,9-trimethyloctahydro-3,12-epoxy[1,2]dic				0,21 282,1468			13191152	22	-	0		Single mat(Multiple m DDA for pr([M+H]+1		3191152		4
FALSO			No results No results		1,9 154,0718			963823,2	0	-	0				963823,2	7,2	5
FALSO			No results No results		-0,47 614,0281			1036012	0		0			1036012		6,6	7,7
FALSO			No results No results		-2,45 651,2712			495114,3	0	-	0			128097,5		7,9	7,9
FALSO			No results No results		-3,37 476,195			464381,4	5	-	0		No matche Single mat (No MS2 [M+2H]+2		464381,4	.,5	7,9
			No results No results		0,13 128,0586			1109167	19		0			1109167		7,2	6,6
FALSO			No results No results			722,7026		288038,8	0	-	0		No matche No matche No MS2 [M+H]+1		288038.8	,,_	8,2
FALSO			No results No results		361,6952		1,144	391160	0	-	0		No matche No matche No MS2 [M+DMSO-		391160		7,1
FALSO			No results No results		-0,72 288,0846			736408,3	2		0			736408,3		7,4	7,9
			No results No results		-0,13 219,1106			627399,6	4	-	0		Single mat: No matche DDA for pri [M+H]+1	612954		7,4	6,8
				Full match Partial mat	0,18 309,1941		5,789	1005609	13		0			931068,8		5,5	7,2
FALSO			No results No results		-0,17 184,1099	167,1067		15871781	26		0		Multiple m Multiple m DDA for pre [M+H-H2O		.5871781		4
FALSO		C3 H4 N10 Full match	No results No results	No results No results	-0,08 561,819	562,8263	1,117	291283,9	0	0	0		No matche No matche No MS2 [M+H]+1 2	291283,9		5,4	
FALSO			No results No results			384,8568		559887,9	0	0	0			559887,9		7,4	
FALSO	[Similar to: 5-hydroxy-4-methoxy-5,6-dihydr				-3,77 143,9749			245539,1	1	3	0	15,8	No matche No matche DDA for pri [M+H]+1	245539,1	115847,7	8,2	8,2
FALSO		No results	No results No results	No results No results	319,8626	320,8699	1,072	694357,2	0	0	0		No matche No matche No MS2 [M+H]+1 6	88287,6	694357,2	5,8	7,4
FALSO	1-acetylimidazole	C5 H6 N2 C Full match	No results No results	Full match Full match	0,41 110,0481	111,0553		7522952	18	0	D		Multiple m Single mate DDA for otl [M+H]+1			4,6	4
FALSO		No results	No results No results	No results No results	1181,699	591,8568	1,063	278408,4	0	0	0		No matche No matche No MS2 [M+2H]+2	277990,9	278408,4	7,1	7,6
FALSO				No match No results	-4,27 315,0761			5852067	2	0	0			5852067		4,6	
FALSO				No results No results	1,67 205,9472			612016	0		0		No matche No matche DDA for pri [M+H]+1	612016	594961,1	7,4	7,4
FALSO				No results No results		83,02162		579977,8	0		0			79977,8		5,8	
FALSO				No results No results	4,12 437,7213			567694,5	0	-	0			67694,5		4,1	3,6
FALSO				No results No results	-4,36 174,0269			1191015	0		0			1082357		7,7	6,6
FALSO			No results No results		-1 176,0171			601526,2	0		0		No matche No matche DDA for pri [M+H-H2O 5			6,8	6,8
FALSO			No results No results			609,1472		2453453	0	-	0		No matche No matche No MS2 [M+H]+1 6			7,4	3,7
FALSO	U 180/20			No results No results		730,8394		408599,9	0		0		No matche No matche No MS2 [M+2H]+2		377008	7,4	7,1
	H-180/29			Full match Partial mat				448385,8	3		0		No matche Single mati No MS2 [M+H]+1 4			7,9	7,4
FALSO FALSO				No results No results		364,8085		227989,2	0		0			227989,2		7,6	8,2
	[Cimiles to 1 (1) City 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1			No results No results	106,9932			328250,9	0		0	11.6	No matche No matche No MS2 [M+H]+1		328250,9	5.3	7,1
FALSO	[Similar to: L-(+)-Citrulline; ΔMass: 0.0131 Da			No results No results No results	4,32 627,3771			734387,5 1143471	0	_	ח	1,6	No matche No matche DDA for pri [M+H]+1 No matche No matche DDA for pri [M+H]+1 S			5,2 7,7	7,4 7,2
FALSO			No results No results		-4,68 330,0466			3821000	2	-	0			3642580		4,2	4,8
			No results No results		0.17 277.1162		1,961		6		0		Multiple m No matche No MS2 [M+H]+1	450785		7,9	7,1
FALSO				No match No results	-2,38 196,0146			75665,97	1		0		No matche No matche No MS2 [M+2H]+2		75665,97	.,5	8,7
				Full match No results	-0,25 216,1547			2725408	3	-	0			2725408		4,8	3,2
FALSO			No results No results		0,38 415,8147		1,126	299363	0		0		No matche No matche No MS2 [M+H]+1	299363		8,2	
FALSO			No results No results			128,089		9108178	0		0			9108178	8527565	4,6	4,6
				No match No results	4,57 674,5367			6367058	1	0	0			6367058		4,6	
FALSO																	

FALSO			No results No results N	lo results No results No	esults 619,5395 620,54	58 1,176 384489,8	0	0 0		No matche No matche No MS2 [M+H]+1 367563,5 384489,8 7,1 7,6
FALSO				o results No results No		41 1,163 480375,2	2 0	0 0		No matche No matche No MS2 [M+H]+1 480375,2 6,3
FALSO		C2 H6 O7 F	Full match No results N	lo results No match No	esults 2,01 235,9314 236,93	87 0,344 2647152	1	0 0		No matche No matche No MS2 [M+H]+1 1855600 2647152 4,5 2,1
FALSO								0 0		No matche No matche DDA for pr [M+H]+1 1171034 1061801 2,3 4,5
FALSO		C13 H34 N	Full match No results N	o results No results No	natch 3,25 339,241 340,24	83 6,726 1021967	0	0 0		No matche Single mati DDA for pri [M+H]+1 943125,1 1021967 7,2 4,5
FALSO		C9 H N6 O	Full match No results N	o results No results No	esults -0,09 525,8357 526,8	43 1,051 307968,6	0	0 0		No matche No matche No MS2 [M+H]+1 307968,6 305707,4 7,6 7,6
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+H]+1 330709,1 174401,6 7,6 8,2
FALSO			Full match No results N					0 0		No matche No matche No MS2 [M+H]+1 947231,5 1184679 7,2 3,9
FALSO		C7 H11 N5	Full match No results N	lo results No match No	esults -2,9 261,0524 131,53	35 7,574 7269798	1	0 0		No matche No matche DDA for otl [M+2H]+2 6282045 7269798 4,6 4,6
FALSO	Furfural	C5 H4 O2	Full match No results N	o results Full match Full	match 0,48 96,02118 97,028	45 1,661 15539219	6	0 0		Single matr No matche No MS2 [M+H]+1 15539219 8033165 4 1,3
FALSO	6-(1H-Pyrrol-1-yl)norleucine	C10 H16 N	Full match No results N	o results Full match Part	al mat 0,2 196,1212 197,12	85 4,614 745095,9	9	0 0		No matche Multiple m DDA for pri [M+H]+1 721658,2 745095,9 6,8 6,8
FALSO		C10 H19 O	Full match No results N	lo results No match No	esults 4,17 234,0853 235,09	26 0,346 568333,1	. 5	0 0		No matche No matche No MS2 [M+H]+1 568333,1 6,8
FALSO	5-Oxidanidyl-5-oxidanylidenenorvalylthreon	C9 H15 N2	No results No results N	o results Full match No	esults 0,65 247,0932 248,10	05 1,45 146630,5	2	0 0		No matche No matche No MS2 [M+H]+1 146630,5 8,2
FALSO			No results No results N	o results No results No			0	0 0		No matche No matche DDA for pri [M+H]+1 315268,7 7,6
FALSO			No results No results N			7-		0 0		No matche No matche No MS2 [M+H]+1 467056 4,1
FALSO		C5 H10 Br3	Full match No results N					0 0		No matche No matche No MS2 [M+H]+1 434657,5 7,4
FALSO				lo results No results No				0 0		No matche No matche No MS2 [M+H]+1 311288,4 7,6
FALSO				o results No results No		15 1,176 389134,3	0	0 0		No matche No matche No MS2 [M+H]+1 389134,3 7,6
FALSO			No results No results N	o results No results No			0	0 0		No matche No matche No MS2 [M+2H]+2 414710,9 419943,2 7,9 7,4
FALSO		C H4 Br N2	Full match No results N	o results No results No			0	0 0		No matche No matche DDA for pri [M+H]+1 393317,4 310532,9 2,2 6,5
FALSO			Full match No results N			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		0 0		Multiple m Multiple m No MS2 [M+H]+1 460312,1 437533,1 7,4 6,3
FALSO	[Similar to: Ethylenediaminetetraacetic acid	C5 H9 O12	Invalid ma: Invalid ma: N	o results No results No	esults -5,06 291,9817 292,98			2 0	74,4	No matche No matche DDA for pri [M+H]+1 147091 162447,3 8,7 2,2
FALSO	tranexamic acid	C8 H15 N (Full match No results N	o results Full match Part	al mat 0,4 157,1103 158,11	76 1,963 711700,9	42	0 0		No matche Single mat DDA for pr [M+H]+1 711700,9 569635,5 4,7 6,8
FALSO			Full match No results N			92 1,497 13699610	3	0 0		Multiple m No matche DDA for pri [M+H]+1 13699610 4
FALSO		C2 H4 N6 (Full match No results N	o results No results No	esults -4,53 221,981 222,98	83 1,202 656505,1	. 0	0 0		No matche No matche DDA for pr [M+H]+1 656505,1 5,2
FALSO			No results No results N	o results No results No	esults 535,8287 536,8	36 1,103 154509,1	. 0	0 0		No matche No matche No MS2 [M+H]+1 154509,1 5,4
FALSO			Full match No results N					0 0		No matche No matche DDA for pri [M+H]+1 378761,1 7,6
FALSO		C11 H16 O	No results No results N					0 0		No matche Multiple m DDA for pri [M+H]+1 9834589 4
FALSO				o results No results No		, ,		0 0		No matche No matche No MS2 [M+H]+1 334994,2 317755,6 4,3 6,5
FALSO		C12 H23 N	Full match No results N			,		0 0		No matche No matche DDA for pri [M+H]+1 4660721 4,8
FALSO				o results No results No		-,,	-	0 0		No matche No matche No MS2 [M+H]+1 305249,2 7,1
FALSO		C40 H52 O	Full match No results N					0 0		No matche No matche DDA for pri [M+H]+1 1180570 1238276 5,5 6,6
FALSO			No results No results N	o results No results No	esults 629,6967 630,70	. , , .		0 0		No matche No matche No MS2 [M+H]+1 337504,5 331601,3 7,6 7,1
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+2H]+2 118287,7 537752,9 8,2 0,9
FALSO				o results No results No	,			0 0		No matche No matche No MS2 [M+H]+1 303258,2 231233,3 8,2 7,1
FALSO				o results No results No		,		0 0		No matche No matche No MS2 [M+H]+1 203858,8 4,9
FALSO	4-Aminobenzoic acid		Full match No results N			55 1,499 1784284	40	0 0		Multiple m Multiple m No MS2 [M+H]+1 467015,3 1784284 7,4 2,8
FALSO		C5 H7 N O	Full match No results N	o results Full match Full	natch 0,56 129,0427 130,049			0 0		Multiple m No matche No MS2 [M+H]+1 457613,5 5,8
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+2H]+2 5995670 6574690 5,1 3,5
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+2H]+2 406171,7 397294,2 7,9 7,4
FALSO			Full match No results N					0 0		No matche No matche DDA for pre [M+H+Met 11023745 4
FALSO			Full match No results N		7,.			0 0		No matche No matche No MS2 [M+H]+1 394222,7 243878,1 7,1 7,1
FALSO			Full match No results N					0 0		No matche No matche No MS2 [M+2H]+2 6163837 4,6
FALSO			Full match No results N				-	0 0		No matche No matche No MS2 [M+2H]+2 1544026 2089599 3,9 4,2
FALSO		C35 H78 N	Full match No results N					0 0		No matche No matche No MS2 [M+H]+1 5827302 4
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+H]+1 550076,3 524619,2 6,8 4,1
FALSO			Full match No results N					0 0		No matche Single mat No MS2 [M+2H]+2 937520,2 959460,4 6,1 5
FALSO			Full match No results N					0 0		No matche No matche No MS2 [M+H]+1 1640919 4,5
FALSO			Full match No results N					0 0		No matche Multiple m DDA for ot [M+H]+1 5256330 4932893 4,8 3,7
FALSO			Full match No results N					0 0		No matche No matche No MS2 [M+2H]+2 367901,1 6,5
FALSO			Full match No results N					0 0		Single mat (No matche No MS2 [M+H]+1 416601,8 400937,2 6,8 8,5
FALSO		C63 H114	Full match No results N					0 0		No matche No matche No MS2 [M+2H]+2 414756,9 5,2
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+H]+1 381580,2 7,1
FALSO		C2 H6 Cd	No results Invalid ma: N					1 0	42,2	No matche No matche DDA for pri [M+H]+1 528683,6 6,3
FALSO				o results No results No				0 0		No matche No matche No MS2 [M+H]+1 295570,7 343486 7,6 7,6
FALSO		C21 H40 N	Full match No results N					0 0		Multiple m No matche No MS2 [M+H]+1 743859,1 731638,9 5,2 7,9
FALSO				lo results No results No		7		0 0		No matche No matche DDA for pri [M+H]+1 5032025 5397150 4,2 3,7
			No results No results N					0 0		No matche No matche No MS2 [M+H]+1 377820,4 488108,5 7,1 4,1
FALSO			Full match No results N		,. ,			0 0		Multiple m Single mat (DDA for pr [M+H]+1 610854,8 621831,1 4,1 4,7
FALSO	,, , p		Full match No results N					0 0		Multiple m Single mati DDA for pri [M+H]+1 640183,3 581725,6 7,4 7,9
FALSO			Full match No results N			, , , , ,		0 0		No matche No matche No MS2 [M+H]+1 356594,7 298029,3 7,1 7,1
FALSO			Full match No results N					0 0		No matche No matche No MS2 [M+DMSO- 372725,1 7,6
FALSO			No results No results N			, , , , , , , , , , , , , , , , , , , ,		0 0		No matche No matche No MS2 [M+H]+1 623081,3 535054,1 7,9 4,7
FALSO			Full match No results N		.,20 2.0,0.02 200,0.	-,,,.		0 0		No matche No matche DDA for pri [M+H]+1 642183,3 6,8
FALSO			Full match No results N			. ,		0 0		No matche No matche DDA for pr [M+H]+1 1290689 1295862 5 6,6
FALSO			Full match No results N					0 0		Single mat (No matche No MS2 [M+H]+1 561262,3 587411,7 8,5 5,2
FALSO			Full match Invalid ma: N			-,		6 0	44	No matche Multiple m DDA for pr [M+H]+1 12631772 4
FALSO		C44 H86 N	Full match No results N				0	0 0		No matche No matche No MS2 [M+2H]+2 1343449 1102349 5 6,1
FALSO		C12//14		lo results No results No			0	0 0		No matche No matche No MS2 [M+H]+1 828783,4 786438,3 6,3 4,7
	(E)-3,4,5-Trimethoxycinnamic acid	C12 H14 O	Full match No results N					0 0		No matche Multiple m DDA for pri [M+H]+1 633276,3 643389,3 6,8 6,8 6,3
FALSO		C20 ! ! 4 0	No results No results N					0 0		No matche No matche No MS2 [M+H]+1 499457,6 510239,3 4,7 3,6
FALSO			Full match No results No					0 0		No matche No matche No MS2 [M+H]+1 715033,6 501050,7 3,6 4,1
	Scytovirin		No results No results No					0 0		No matche Single mat. No MS2 [M+2H]+2 404608,2 7,9
FALSO FALSO			Full match No results No					0 0		No matche No matche DDA for pri [M+H]+1 1511664 1424841 6,6 1,2 No matche No matche No MS2 [M+H]+1 447158,9 446162,4 7,4 7,4
FALSO		C1/ H10 N	Full match No results No					-		
		C5 H4 NC 4	No results No results No Full match No results No					0 0		No matche No matche No MS2 [M+H]+1 1060173 1079893 5 2,3
			Full match No results No Full match No results No					0 0		No matche No matche No MS2 [M+H]+1 1243820 1098286 6,6 5 Single mat No matche DDA for ot [M+H-H2O 875982,8 895189,8 6,6 7,2
FALSO			Full match No results N					0 0		
FALSO			Full match No results No					0 0		
FALSO								0 0		
			Full match No results No Full match No results No					0 0		
	PENTADECYLAMINE 3.4 Diaminohutanois acid							0 0		No matche Single mat DDA for pr [M+H]+1 1296289 1363367 5 4,5
FALSO	2,4-Diaminobutanoic acid muramic acid		Full match No results No		, ., ., ., ., ., .,			0 0		Single mat. Multiple m No MS2 [M+H]+1 742944,1 4,1
			Full match No results No					0 0		Single mate No matche No MS2 [M+H]+1 666560,1 694566,5 7,9 7,4 No matche No matche DDA for ot [M+2H]+2 8036803 9563508 3,5 4
FALSO			Full match No results No Full match No results No							
FALSO								0 0		No matche No matche No MS2 [M+2H]+2 741564,2 825620,5 8,5 5,2 Multiple m No matche DDA for pri [M+H]+1 14658750 4
FALSO	Cyclopentanone		Full match No results No Full match No results No					0 0		
	2-({4-[(2-Isopropoxyethoxy)methyl]phenoxy							0 0		No matche No matche DDA for ot [M+2H]+2 540961,8 570563,3 7,4 6,8
FALSO								0 0		
			Full match No results No Full match No results No					0 0		
FALSU	- (injurazinometnyjpenzene-1,2,5-tfl0)	C/ H10 N2	i un materi No results N	results Full IIIdtell Par	armaq 0,40 1/0,0092 1/1,0/0	1,024 /00051,5	, 0	0		No matche Single mat DDA for pr [M+H]+1 788051,9 762474,5 6,8 0,3

FALSO	Geranyl acetate C12	H20 O Full match No results No results	Full match Full match	0,07	196,1463	197,1536	7,344 1111481	2 81	0 ()		Single mate Multiple m DDA for pre [M+H]+1 11114812 2691070 4,6 4,8
FALSO	C15	H14 N Full match No results No results	No match No match	-4,2	310,1165	311,1238	3,723 498423,	3 6	0 ()		No matche Multiple m No MS2 [M+H]+1 452272,5 498423,3 7,9 7,9
FALSO		No results No results No results			421,6499	422,6571	1,171 476709,	6 0	0 (ו		No matche No matche No MS2 [M+H]+1 476709,6 8,5
FALSO		H37 N Full match No results No results		,		418,1933	1,721 54314		0 ()		No matche No matche No MS2 [M+H]+1 543141 516883,8 5,8 7,9
FALSO		H25 N4 Full match No results No results			268,1675		7,126 980030		0 (No matche Multiple m DDA for pri [M+H]+1 8380030 9800303 4 4,6
	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 1388673	4 22	0 ()		Single mate Multiple m DDA for pre [M+H]+1 13886734 4
FALSO		No results No results No results				641,1093	1,41 408013,		0 ()		No matche No matche No MS2 [M+H]+1 408013,5 6,3
FALSO		H3 N5 C Full match No results No results			222,9811	-,	7,058 1304911		0 (No matche No matche No MS2 [M+H]+1 13049112 5,1
FALSO	C30	H50 N Full match No results No results		1,92	517,3166	-	7,005 211385		0 (-		No matche No matche No MS2 [M+H]+1 2113853 182034,3 4,8 4,9
FALSO		No results No results No results				546,6145	1,176 33381		0 (,		No matche No matche No MS2 [M+H]+1 333813 323431,1 7,1 8,2
	2-Pyrrolidone C4 H	H7 N O Full match Invalid mas No results		-1	85,05268	,	1,487 1100181		10 (-	44,2	Single mati No matche DDA for pri [M+H]+1 11001817 10180349 4 3,5
FALSO		No results No results No results				362,8659	1,083 268549,		0 (-		No matche No matche DDA for pri [M+H]+1 268549,9 254023,9 7,1 7,6
FALSO	C2 H	H7 N2 P Full match No results No results		-1,47	122,0066		1,001 133643		0 (,		No matche No matche DDA for pri [M+H]+1 1233501 1336435 7,2 2,3
FALSO		No results No results No results			80,51334	- /	1,248 221673,		0 (No matche No matche No MS2 [M+H]+1 221673,9 5,4
FALSO		H7 P3 S Full match No results No results			223,9201		1,07 501779,		0 (No matche No matche DDA for pri [M+H]+1 468929,7 501779,4 7,9 6,8
FALSO	1	H9 N O2 Full match No results No results			127,0634		1,682 1131369		0 (,		Multiple m Multiple m No MS2 [M+H]+1 4668941 11313699 1 4
FALSO		H7 N2 C Full match No results No results				171,0166	1,172 408150,		0 ()		No matche No matche DDA for pri [M+H]+1 408150,5 403691,4 7,9 4,7
FALSO FALSO	C2 H	H4 N3 P Full match No results No results		3,/2	101,0147	102,0219 693.3321	0,984 759959,		0 0)		No matche No matche DDA for pri [M+H]+1 759959,2 675862,6 4,1 0,3 No matche No matche No MS2 [M+2H]+2 243169,9 8.2
	ec.u	No results No results No results		4.07	239.0406	,	1,098 243169,		-	,		
FALSO	5-(N,N-Dimethylcarbamimidamido)-2-oxope C8 H	H5 N7 C Full match No results No results			201,1113		0,974 924494, 3,222 498616,		0 0			No matche No matche No MS2 [M+2H]+2 924494,1 836509,8 7,2 3 No matche No matche No MS2 [M+H]+1 462349,3 498616,3 6,3 6,8
FALSO	5-(N,N-Diffiethylcarbaffilmidaffildo)-2-0x0pe C8 F	No results No results No results			1535,597		1.1 340923.		0 0			No matche No matche No MS2 [M+H]+1 402349,3 496016,3 6,3 6,8 7,6
FALSO		No results No results No results				766,8052	1,103 405506		0 0	,		No matche No matche No MS2 [M+H]+1 405506,1 225916 4,1 2,7
FALSO	(32	PH72 N: Full match No results No results		0.31	674,5368		7,074 616527			1		No matche No matche No MS2 [M+H]+1 6165270 5,1
FALSO		Br Cl N. Full match No results No results			311,7671		1,145 300885			1		No matche No matche No MS2 [M+H]+1 300885,4 270651,9 7,6 7,1
		H14 O. No results Invalid mas No results			166,0994		1.535 2567164		3 (,	54.3	Multiple m Multiple m DDA for pr [M+H-H2O 25671645 22699636 4 3,5
		6 H35 N Full match No results No results			257,2719		7,152 893129		0 (-	34,3	No matche No matche No MS2 [M+H]+1 848929,2 893129,2 6,1 4,5
FALSO	,	No results No results No results		0,03		746,7859	1,106 181658		0 0			No matche No matche No MS2 [M+H]+1 181658,3 4,3
FALSO		No results No results No results				463,0265	1,098 461447,		0 0			No matche No matche DDA for pr [M+H]+1 445912,9 461447,5 7,9 7,9
FALSO		No results No results No results				322,1874	3,241 368662		0 0	,		No matche No matche No MS2 [2M+H]+1 368662,5 7,6
	Diethyl phosphonothioate C4 H	H11 O2 Full match No results No results		-4,63		155,0283	1,956 27116		0 0	-		No matche No matche No MS2 [M+H]+1 224481,7 271167 5,4 7,6
FALSO		2 N4 O8 Full match No results No results		.,	291,9076		1,069 567360,		0 0			No matche No matche No MS2 [M+H]+1 567360,2 511353,7 7,4 7,4
		H4 O5 Full match No results No results		-,	156,0059		2,382 177470		0 0			No matche No matche No MS2 [M+H]+1 1610559 1774709 4,5 5,5
FALSO		H10 O2 Full match No results No results		0.06	126.0681	127,0754	1.452 1400484		0 0			No matche Multiple m DDA for pri [M+H]+1 403046,4 14004840 6,8 4
FALSO		H16 N5 Full match No results No results	No match No results		269,0882		1,403 349024,	4 2	0 0)		No matche No matche No MS2 [M+H]+1 349024,4 4,3
FALSO		H23 N Full match No results No results			181,1831		5,255 754483,		0 0)		Single mate Single mate DDA for pre [M+H]+1 751748,4 754483,5 6,8 6,8
FALSO		No results No results No results		.,.		601,8132	1,112 161473,		0 0			No matche No matche No MS2 [M+H]+1 114425,8 161473,2 3,8 8,2
FALSO	Cyclohexanecarboxylic anhydride C14	H22 O Full match No results No results	Full match Partial mat	-0,01	238,1569	239,1642	7,126 1000742	2 8	0 0)		No matche Multiple m No MS2 [M+H]+1 10007422 4
FALSO		H20 O Full match No results No results			236,1413		7,137 1057103		0 0)		No matche Multiple m No MS2 [M+H]+1 10571033 4,6
FALSO		No results No results No results			311,0622		1,39 452075,		0 0			No matche No matche No MS2 [M+H]+1 435299,8 452075,5 6,8 7,4
FALSO	C3 H	H5 Cl N! Full match No results No results		_	272,9659	-	1,158 343420,		0 0			No matche No matche No MS2 [M+H]+1 343420,7 323177,8 8,2 7,6
FALSO		3 Br Cl3 Full match No results No results		-1,54		776,5783	1,145 251106		0 0)		No matche No matche No MS2 [M+H]+1 251106,8 185376,3 7,6 7,6
FALSO		No results No results No results			111,9595		0,304 31686		0 0)		No matche No matche DDA for pri [M+H]+1 316866 7,6
FALSO	Neutral Red C15	H16 N Full match No results No results	Full match No match	-4,68	252,1363	253,1436	7,149 1276437	5 18	0 ()		No matche Multiple m DDA for pri [M+H]+1 12764375 12456709 4,6 4
FALSO	Furaneol C6 H	H8 O3 Full match No results No results	Full match Full match	0,4	128,0474	129,0547	1,381 642465,	9 31	0 ()		Multiple m Multiple m DDA for pri [M+H]+1 642465,9 5,8
FALSO	tert-Butyl [6-(2-aminoethyl)-2,2-dimethyl-1,: C14	H27 N Full match No results No results	Full match No results	-0,22	273,194	274,2012	7,181 150861	4 2	0 ()		No matche No matche No MS2 [M+H]+1 1508614 4,5
FALSO	C33	H48 N. Full match No results No results	No results No results	2,69	632,3326	633,3399	7,867 101763	5 0	0 ()		No matche No matche DDA for pri [M+H]+1 976536,4 1017635 6,1 6,6
FALSO		No results No results No results	No results No results		114,9569	115,9641	0,3 114310,	2 0	0 ()		No matche No matche DDA for otl [M+H]+1 114310,2 4,9
FALSO	C36	H78 N: Full match No results No results	No match No results	0,1	728,5836	729,5909	7,126 587457	7 4	0 ()		No matche No matche No MS2 [M+H]+1 4868988 5874577 3,2 4
FALSO	C32	H59 O Full match No results No results	No match No match	0,98	616,3226	617,3299	7,464 124778	7 1	0 (0		No matche Multiple m No MS2 [M+H]+1 871905,3 1247787 3,9 6,1
FALSO		No results No results No results	No results No results		622,1285	623,1357	1,512 337801,	1 0	0 ()		No matche No matche No MS2 [M+H]+1 337801,1 6
FALSO	C11	H10 N Full match No results No results	No match No match	4,02	235,0408	118,5277	7,581 211413	5 2	0 ()		No matche Multiple m DDA for ot [M+2H]+2 2114135 1837831 4,8 3,9
FALSO		No results No results No results	No results No results		1563,605	782,8096	1,087 509108,	4 0	0 (0		No matche No matche No MS2 [M+2H]+2 509108,4 7,4
FALSO	N,N-Dimethylicosan-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 ()		No matche No matche No MS2 [M+H]+1 774378,9 749801,7 5,2 6,3
FALSO		No results No results No results			285,8907	286,8979	1,059 285102,	7 0	0 ()		No matche No matche No MS2 [M+H]+1 277952,9 285102,7 7,1 8,2
FALSO	C15	H20 N: Full match No results No results	No match No match	4,17	340,1887	341,1959	7,121 962410	7 3	0 (וכ		No matche Multiple m No MS2 [M+H]+1 8970521 9624107 4,6 5,1
FALSO		No results No results No results			667,6414	,	1,139 197744,		0 ()		No matche No matche No MS2 [M+H]+1 197744,6 8,2
FALSO		H4 Cl2 Full match No results No results		-4,55	278,9395	279,9468	1,198 372698,		0 ()		No matche No matche No MS2 [M+H]+1 372698,1 361354,9 7,6 8,2
FALSO	C7 H	H5 Br Cl Full match No results No results			421,8676		1,194 376532,		0 (,		No matche No matche No MS2 [M+H]+1 249305,9 376532,6 7,6 5,4
FALSO		No results No results No results			111,5124		0,338 246250,		0 (,		No matche No matche No MS2 [M+H]+1 246250,9 7,6
FALSO		H29 N Full match No results No results		-,-	275,1919	,	6,67 423854,		0 (,		No matche No matche DDA for pri [M+H]+1 423854,1 413520 8,5 7,9
		B H36 O Full match No results No results		0,03	268,2766	203,2033	3,181 1068471	-	0 (,		Single mat(No matche DDA for pr([M+H]+1 10684710 5,1
		B H36 O Full match No results No results		-,,	268,2766	,	2,946 1234918		0 (,		Single mat(No matche DDA for pr([M+H]+1 12349185 4,6
FALSO	C2 H	H3 Br Cl Full match No results No results		1,72	605,6451	,	1,145 326376,		0 (No matche No matche No MS2 [M+H]+1 326376,5 308343,9 7,6 7,1
FALSO		No results No results No results				609,6921	1,136 22159		0 (-		No matche No matche No MS2 [M+H]+1 221596 8,2
FALSO		No results No results No results			605,563	606,5703	1,175 267351,		0 (,		No matche No matche No MS2 [M+H]+1 266266,3 267351,6 7,1 8,2
FALSO	North developed	No results No results No results		0.00	417,7018	-,	1,148 332792,		0 ()		No matche No matche No MS2 [M+H]+1 331335 332792,4 7,6 7,1
		H7 N OZ Full match No results No results		.,	125,0477	.,	1,476 2090421		0 ()		Multiple m No matche No MS2 [M+H]+1 367963,8 20904214 4,3 4
FALSO		2 Cl3 O: Full match No results No results			389,7834		1,141 336428,		0 (J		No matche No matche No MS2 [M+H]+1 329164,3 336428,2 7,6 7,1
FALSO	C32	H32 N! Full match No results No results				287,6332	7,358 170759		0 ()		No matche No matche No MS2 [M+2H]+2 1707597 4,5
FALSO		No results No results No results		_	-,	430,6887	1,147 335124,		0 (No matche No matche No MS2 [M+H]+1 298849 335124,5 7,1 4,9
FALSO	C3 H	H Br2 Cl Full match No results No results				344,7303	1,175 560483,		0 (No matche No matche No MS2 [M+H]+1 560483,2 492957,4 6,8 6,8
FALSO	2.0	No results No results No results				452,6619	1,174 344380,		0 0			No matche No matche No MS2 [M+H]+1 344380,1 307976,3 7,6 7,6
FALSO FALSO		H80 N Full match No results No results				427,7472 134.0189	7,417 929274, 1.19 358685.		0 0			No matche No matche No MS2 [M+2H]+2 929274,1 771504,6 5,5 4,1
FALSO		H8 N P : Full match No results No results		-,	,.	. ,	,		-	-		No matche No matche No MS2 [M+H]+1 358685,9 352833,5 7,1 7,6 No matche No matche No MS2 [M+H]+1 1027343 311336 7,2 0,5
		H5 Br Cl Full match No results No results H26 O Full match No results No results				296,8213 227,2006	1,135 102734 7,596 92351		0 0			
		H16 O No results No results No results		0,15		185,1173	7,596 92351 1,453 1154258		0 0			Single mat Single mat DDA for pr [M+H]+1 754065,4 923516 5,2 6,1 Multiple m Multiple m DDA for pr [M+H]+1 11542588 1339796 4 0,7
FALSO		H13 N Full match No results No results				281,0745	3,232 420074,		0 0	-		No matche No matche DDA for pri [M+H]+1 11542588 1339796 4 0,7 1 1 1 1 1 1 1 1 1
FALSO	CIO	No results No results No results			419,6529		1.159 526942		0 0			No matche No matche No MS2 [M+H]+1 526942,7 473929,5 6,3 5,2
FALSO	Call	H6 Cl N. Full match No results No results				346,881	1,159 526942,		0 0			No matche No matche No MS2 [M+H]+1 526942,7 473929,5 6,3 5,2 No matche No matche No MS2 [M+H]+1 282093,1 237985,9 7,6 7,6
FALSO	CZH	No results No results No results				770,6307	1,12 282093,		0 0	-		No matche No matche No MS2 [M+H]+1 282093,1 237985,9 7,6 7,6 No matche No matche No MS2 [M+H]+1 299068,9 215234 7,1 7,1
FALSO		No results No results No results				292,1149	1,572 484260		0 0			No matche No matche No MS2 [M+H]+1 29908,9 213234 7,1 7,1 No matche No matche No MS2 [M+H]+1 484260,1 6,8
FALSO	C40	H107 Full match No results No results				557,3485	7,366 997745,		0 0			No matche No matche No MS2 [M+H]+1 484260,1 6,8 No matche No matche No MS2 [M+2H]+2 997745,2 837448,9 5 6,1
FALSO		H2 Br2 (Full match No results No results				502,6324	1,176 386711,		0 0			No matche No matche No MS2 [M+2H]+2 997/45,2 83/448,9 5 6,1 No matche No matche No MS2 [M+H]+1 386711,4 382218,4 7,1 4,3
		6 H54 O No results No results No results				635,3778	1,098 258249		0 0			No matche Multiple m No MS2 [M+H]+1 258249,1 8,2
	N-[(2S)-4-Cyclohexyl-1-ethoxy-1-oxo-2-butar C15					286,2014	5,762 63773		0 0			No matche No matche DDA for pri [M+H]+1 538658,2 637731 6,3 5,8
FALSO		H2 N6 C Full match No results No results				380,9228	1,223 556132,		0 0			No matche No matche No MS2 [M+H]+1 517474,1 556132,1 7,9 7,9
		B H32 O. Full match No results No results				281,2475	0,317 292654,		0 0	-		Multiple m Single mat (No MS2 [M+H]+1 292654,9 6,5
		H10 N6 Full match No results No results				171,0996	1,436 126252,		0 0			No matche No matche DDA for pri [M+H]+1 126252,5 8,2
FALSO		H3 Cl N. Full match No results No results				264,8653	1,115 236791,		0 0			No matche No matche DDA for pri [M+H]+1 236791,4 217052,2 7,6 7,6
	CZT			3,20	_ 33,330	,0033	_,_15 250/91,	· ·	3			7,0

FALSO		C H Cl N2 C Full match No results No results	No results No results		441,8173 442,8246	1,123 310243,1	0 0 0		No matche No matche No MS2 [M+H]+1 310243,1 7,6
FALSO		C7 H Cl N6 Full match No results No results	No match No results	-3,95	331,9531 332,9604	1,195 323073	1 0 0		No matche No matche No MS2 [M+H]+1 323073 307852,4 7,1 8,2
FALSO	Dinitrogen trioxide	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
FALSO		C5 H16 N2 Full match No results No results	No match No match	-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
FALSO	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
FALSO		C50 H109 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
FALSO		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
FALSO		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
FALSO		C4 H8 N2 C Full match No results No results	No match 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
FALSO	[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	42.7	No matche No matche DDA for pri [M+H]+1 413683,4 8,5
FALSO		No results No results No results			517.6466 596.669	1,147 341795,5	0 0 0	- i	No matche No matche No MS2 [M+DMSO- 341795,5 7,1
FALSO		C2 H Br2 Cl Full match No results No results		1.82	459,6412 460,6475		0 0 0		No matche No matche No MS2 [M+H]+1 433306,6 434390,1 7,4 6,8
FALSO		C7 H3 N3 C Full match No results No results			256,9735 257,9808	4,738 672591,1	1 0 0		No matche No matche DDA for pr [M+H]+1 613439,4 672591,1 7,4 6,3
FALSO		C11 H25 N; Full match No results No results			300.1937 301.2011	7,039 2531956	1 0 0		No matche Multiple m DDA for otl [M+H]+1 2389142 2531956 4,8 4,8
	Phosphoric acid	H3 O4 P No results No results No results		-,-	97,97693 98,98421	1,737 12776649	1 0 0		Single mat(No matche DDA for pr([M+H]+1 12776649 4,6
FALSO		C7 H14 N C Full match No results No results			255,0503 256,0576	1.383 494704.5	5 0 0		No matche No matche No MS2 [M+H]+1 494704,5 4,7
FALSO		C8 H24 N6 Full match No results No results			268,1675 269,1747	7,339 1857403	10 0 0		No matche Multiple m No MS2 [M+H]+1 1857403 5
FALSO		C4 H11 N6 Full match No results No results			302.0369 303.0442	1.145 231648.8	2 0 0		No matche No matche No MS2 [M+H]+1 231648,8 7,6
FALSO		No results No results No results		-2,17	153,983 154,9903	7.014 8575408	0 0 0		No matche No matche No MS2 [M+H]+1 8575408 5,1
FALSO		No results No results No results			1001,744 501,8794	1,096 421527,8	0 0 0		No matche No mstche No MS2 [M+2H]+2 421527,8 5,2
	stilbamidine	C16 H16 N- Full match No results No results		-4 38	264,1363 265,1436	6,851 780108	78 0 0		Single mate Multiple m No MS2 [M+H]+1 780108 712760 4,7 4,1
		C11 H20 O No results No results No results			184,1463 185,1536		86 0 0		No matche Multiple m No MS2 [M+H]+1 5398930 4736144 5,3 4,2
		C15 H23 N! Full match No results No results			321,1801 322,1874		2 0 0		No matche No mstche No MS2 [M+H]+1 358580,6 7,1
FALSO	cocamidopropyl betaine	C19 H38 N. Full match No results No results			342,2882 343,2955	7,023 823303	1 0 0		No matche No matche DDA for pre [M+H]+1 630254,1 823303 3,6 4,7
FALSO	Cocamidopropyr became	C19 H14 N Full match No results No results			510,1005 256,0575	1,384 388241,5	1 0 0		No matche No matche No MS2 [M+2H]+2 388241,5 7,6
FALSO		C3 H Cl N4 Full match No results No results			477.8281 478.8354	1.099 451598.5	0 0 0		No matche No matche No MS2 [M+H]+1 451598,5 4,7
FALSO	methyldioctylamine	C17 H37 N Full match No results No results			255,2926 256,2999	7,161 1126870	3 0 0		No matche No matche No MS2 [M+H]+1 451596,5 4,7 No matche No matche No MS2 [M+H]+1 704056,6 1126870 2 5,5
		C17 H37 N Full match No results No results			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
FALSO		C17 H29 N Full match No results 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
FALSO	······CAIIIIIC	C6 H4 Cl N. Full match No results No results		-7-	455,8375 456,8447	1,076 493663,1	0 0 0		No matche No matche No MS2 [M+H]+1 /64/38,2 882696,5 4,7 6,6 No matche No matche No MS2 [M+H]+1 493663,1 481483,8 7,4 4,1
FALSO		No results No results No results		2,30	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
FALSO		C5 H10 N6 Full match No results No results		-3 01	218.0402 219.0475	1,268 788608,2	8 0 0		Single mat. No matche DDA for pr. [M+H]+1 788608,2 739344,7 4,7 4,1
FALSO		C4 H6 N6 C Full match No results No results		-,	186.0504 187.0577	1,522 1475201	1 0 0		No matche DDA for pr [M+H]+1 1475201 948002,5 2,8 4,5
FALSO		No results No results No results		1,02	80,51987 81,52715		0 0 0		No matche No matche DDA for pre[M+H]+1 14/5201 948002,5 2,8 4,5 No matche No matche DDA for pre[M+H]+1 153890,3 4,9
				0.05			0 0 0		
FALSO		C7 H4 O18 Full match No results No results			597,7477 598,7549	1,137 377987,4 1.139 441208.3			No matche No mstche No MS2 [M+H]+1 377987,4 6,5
FALSO		C H3 Cl2 O Full match No results No results			163,9019 164,9092 509.3482 510.3555	7	0 0 0		No matche No matche DDA for pri [M+H]+1 441208,3 417944,4 4,1 7,4 No matche No matche No MS2 [M+H]+1 2043407 3886504 3.7 4.8
FALSO		C26 H58 N Full match No results No results			,	.,			,
		C6 H6 O6 Full match No results No results		-,	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
FALSO		C4 H2 Br Cl Full match No results No results		-1,/1	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
FALSO		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 314356,8 319485,5 6,5 7,6
FALSO		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
FALSO	[Similar to: Ethylenediaminetetraacetic acid				291,9003 292,9076	1,424 178355,4	0 2 0	59,8	No matche No matche DDA for pri [M+H]+1 178355,4 4,9
FALSO		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
FALSO		C14 H28 N Full match No results No results			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
	N-[(2-Methylphenoxy)acetyl]-L-leucyl-O-[(4-	C31 H40 N No results No results No results		-2	596,2834 299,149	7,145 9414346	1 0 0		No matche No matche DDA for otl [M+2H]+2 9414346 5,1
FALSO		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
FALSO		C37 H80 Cl Full match No results No results			723,558 724,5653		0 0 0		No matche No matche No MS2 [M+H]+1 280055,2 281155,3 7,6 7,1
FALSO		C7 H6 O17 Full match No results No results			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
FALSO		C4 H N O8 Full match No results No results			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
FALSO		C7 H28 N1 Full match No results No results			410,1651 411,1724	-,	15 0 0		No matche Single mati No MS2 [M+H]+1 185808,7 4,9
FALSO		C6 H3 N5 C Full match No results No results			222,9811 223,9884	7,271 9355434	0 0 0		No matche No matche No MS2 [M+H]+1 9355434 4,6
	Palmitic Acid	C16 H32 O: Full match No results No results		0,14	256,2403 239,237	0,31 3720105	24 0 0		Single mate Multiple m No MS2 [M+H-H2O 162106,3 3720105 4,9 2,1
FALSO		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
FALSO	Phosphocreatine	C4 H10 N3 Full match No results No results		0,11	211,0358 212,0431	1,286 990819,3	1 0 0		Single matr No matche No MS2 [M+H]+1 990819,3 955565 6,6 3,9
FALSO		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
FALSO		C23 H7 N6 Full match 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
FALSO		C4 H9 N Of Full match 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
FALSO		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
FALSO		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
FALSO		No results No results No results			630,6743 631,6815		0 0 0		No matche No matche No MS2 [M+H]+1 281751,8 209733,1 7,6 7,1
FALSO		C5 H7 N8 C Full match No results No results		,	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
FALSO		C4 H4 Cl N! Full match No results No results	140 materi 140 results	0,0	236,9547 237,962	1,206 356238	1 0 0		No matche No matche No MS2 [M+H]+1 326740,1 356238 7,1 7,6
FALSO		C20 H37 N Full match No results No results		-,	435,2469 436,2542	7,354 3417942	0 0 0		No matche Single mati DDA for pri [M+H]+1 3417942 2482239 4,2 3,7
FALSO		C30 H53 O Full match No results No results		-,	572,2963 573,3035	7,477 1150917	3 0 0		No matche Multiple m No MS2 [M+H]+1 854889,4 1150917 4,5 6,6
FALSO		C18 H23 O Full match No results No results		_	318,1216 319,1289	5,658 556727,1	4 0 0		No matche No matche DDA for pri [M+H]+1 490411,9 556727,1 7,9 7,4
FALSO		C3 H6 O P2 Full match No results No results		-,-	151,9614 152,9687	0,991 627584,6	1 0 0		No matche No matche DDA for pr [M+H]+1 564856,2 627584,6 6,8 5,2
FALSO	Isariotin M	C22 H35 N Full match No results No results		-,	409,2465 410,2538	3,235 662495,9	0 0 0		No matche Single mat No MS2 [M+H]+1 620578,4 662495,9 6,3 5,2
	Chromium(3+) tri(D-gluconate)	C18 H33 Cr No results No results No results		2,24	637,0934 638,1007		1 0 0		No matche No matche No MS2 [M+H]+1 1959111 4,8
FALSO		No results No results No results			371,7239 372,7302	1,141 307736,8	0 0 0		No matche No matche No MS2 [M+H]+1 307736,8 7,1
	4-Decylaniline	C16 H27 N Full match No results No results			233,2143 234,2216		3 0 0		No matche No matche DDA for pr [M+H]+1 1248264 1150417 4,5 5
FALSO		C12 H23 Cl Full match No results No results			322,1393 323,1466		2 0 0		No matche No matche DDA for pri [M+H]+1 6910324 8540434 5,1 5,1
FALSO		C81 H103 Full match No results No results			1543,627 772,8207		0 0 0		No matche No matche No MS2 [M+2H]+2 313391,1 340152,8 7,1 3,3
FALSO		C H2 O17 S Full match No results No results			317,9005 318,9078		0 0 0		No matche No matche No MS2 [M+H]+1 353900 7,6
	1,1'-[(2-Chlorophenyl)methylene]dipiperidin	C17 H25 Cl No results Invalid mas No results			292,1715 293,1787		2 2 0	59,8	No matche No matche DDA for pri [M+H]+1 119735,3 8,2
FALSO		No results No results No results			615,7396 616,7468		0 0 0		No matche No matche No MS2 [M+H]+1 186428,4 8,2
FALSO		C5 H6 N2 C Full match No results No results			539,7891 540,7964		0 0 0		No matche No matche No MS2 [M+H]+1 307897,3 7,6
FALSO		C6 H2 Cl O: Full match No results No results			409,8409 410,8481		0 0 0		No matche No matche No MS2 [M+H]+1 440145 364382,1 6,8 7,1
FALSO		No results No results No results			443,7126 444,7199		0 0 0		No matche No matche No MS2 [M+H]+1 407900,7 338607,8 6,3 3,3
FALSO		C4 H16 N7 Full match No results No results			257,1012 258,1085		13 0 0		No matche No matche No MS2 [M+H]+1 329679,8 354367,4 7,6 7,6
	tripropylene glycol diacrylate	C15 H24 O Full match No results No results		-, -	300,1574 301,1646		14 0 0		No matche Multiple m No MS2 [M+H]+1 10114258 4,6
FALSO		C6 H3 O6 F Full match No results No results			201,9663 202,9736		0 0 0		No matche No matche No MS2 [M+H]+1 111435,2 74937,5 8,7 6,5
FALSO		No results No results No results			511,7009 512,7077		0 0 0		No matche No matche No MS2 [M+H]+1 320630,5 240264 7,1 7,1
FALSO		C2 H8 Cl2 I Full match No results No results			431,7895 510,812	, , , , , ,	1 0 0		No matche No matche No MS2 [M+DMSO- 186984,1 8,2
	Diethyleneglycol dimethacrylate	C12 H18 O Full match No results No results			242,1155 243,1228		5 0 0		No matche Multiple m DDA for pr [M+H]+1 16501378 4
	Bandrowski's base	C18 H18 N Full match No results No results		-4	318,158 319,1653		9 0 0		No matche Multiple m No MS2 [M+H]+1 437347,9 472869,9 6,8 7,4
FALSO		No results No results No results			668,793 669,8002		0 0 0		No matche No matche No MS2 [M+H]+1 118702,2 194214,2 4,3 8,2
FALSO		C60 H104 Full match No results No results		-0,03	1305,644 653,8292		0 0 0		No matche No matche No MS2 [M+2H]+2 250464,3 7,1
FALSO		No results No results No results			661,8106 662,8179		0 0 0		No matche No matche No MS2 [M+H]+1 499679,9 234660,5 0,9 7,1
FALSO		C9 H21 N P Full match No results No results			205,1143 206,1216		6 0 0		Single matr No matche No MS2 [M+H]+1 176363,7 4,9
	Dimethyl 1,4-cyclohexanedicarboxylate	C10 H16 O Full match No results No results		0,17	200,1049 201,1122		30 0 0		No matche Multiple m No MS2 [M+H]+1 386923,1 3417608 6 3,2
FALSO		No results No results No results	No results No results		1453,647 727,8309	1,068 278611,3	0 0 0		No matche No matche No MS2 [M+2H]+2 278611,3 179115,1 7,1 7,1

FALSO				No match No results	2,33 352,0286			552409,9	3	0 0				552409,9		4,7	
FALSO				No results No results	,	544,6555		289338,8	0	0 0		No matche No matche No MS2	[M+H]+1	264951,5		7,1	7,1
FALSO				No results No results	669,5938	670,601		252097,3	0	0 0			[M+H]+1	214000,3		3,3	7,6
FALSO				No match No results	2,35 551,2076		1,94	1092269	1	0 0		No matche No matche No MS2	[M+2H]+2	1092269	972893,4	5	4,5
FALSO FALSO	[Similar to: Acetyl-L-carnitine; ΔMass: 203.09 Palmitic Acid			Full match Full match	2,01 406,2063 0,21 256,2403	. ,	3,178	491471,9 9656141	24	0 0	43,1	No matche No matche DDA for oth Single match Multiple m DDA for oth		491471,9 9656141	0027402	7,4	4
FALSO	3-[(2,6-Dimethylheptanoyl)oxy]-4-(trimethyl				0,32 301,2254			427982,3	4	0 0		No matche No matche DDA for pre		419959.4		5,1 6,8	5,8
FALSO	3-[(2,0-Dimetriyineptanoyi)oxy]-4-(trimetriyi			No results No results		588,8188		235448.8	0	0 0			[M+H]+1		223194,2	7,1	7,6
FALSO	MHPG			Full match Full match	0.01 184.0736		7	1789105	27	0 0			[M+H]+1	1269542		3,9	4,5
FALSO				No match No results	-3.26 393.288	394,2952	7,005	744911	1	0 0		No matche No matche No MS2	[M+H]+1	647428,3	744911	6,3	5,2
FALSO				Full match No results	0,03 178,0565		1,486	8800213	6	0 0		No matche No matche No MS2	[M+H]+1	8800213		4	
FALSO		C H3 N O6 Full match	No results No results	No results No results	0,62 218,9158	219,923	1,133	396823,3	0	0 0		No matche No matche No MS2	[M+H]+1	391661,5	396823,3	7,1	7,4
FALSO		No results	No results No results	No results No results	582,827	583,8343	1,107	138968,6	0	0 0		No matche No matche No MS2	[M+H]+1		138968,6		4,9
FALSO		C8 H16 N4 Full match			2,25 216,1227			292156,8	3	0 0		Single mate No matche No MS2	[M+H]+1		280183,8	8,2	7,1
FALSO				No match No results	0,89 430,0351			300459,1	1	0 0		No matche No matche No MS2	[M+H]+1	291955,2		7,6	7,6
FALSO	N4-PALMITOYL CYTARABINE	C25 H43 N: Full match		No results No results	3,46 481,3169		6,932	3988572 236747.2	2	0 0		No matche No matche No MS2	[M+H]+1	1999881	3988572	2,1	5,3
FALSO				No results No match	679,495 -3 764,4113	680,5023		1111113	0	0 0		No matche No matche No MS2 No matche Single mati DDA for pro	[M+H]+1	236747,2 1107281	230818,3 1111113	7,6 6,1	7,6 6,6
FALSO				No results No results		110,5186		256825,4	0	0 0			[M+H]+1	1107201	256825.4	0,1	6,5
FALSO				No results No results	608.7077			160133,2	0	0 0		No matche No matche DDA for otl		4	160133,2		8,2
	1,3,5-Heptatriene, (E,E)-	C7 H10 Full match	No results No results	Full match No results	0,07 94,07826			9112072	13	0 0			[M+H]+1		9112072		4
FALSO	6,7-Dimethoxy-2-(1-piperazinyl)-4-quinazolir	C14 H19 N: Full match	No results No results	Full match No results	-4,54 289,1526	290,1598	3,666	421504,8	4	0 0		No matche No matche DDA for pro	[M+H]+1	379899,9	421504,8	6	6,3
FALSO	2-sec-Butyl-4-{4-[4-(4-hydroxyphenyl)-1-pipe	C22 H27 N: No results	No results No results	Full match No match	-3,02 393,2153	394,2226	1,414	312725,6	4	0 0		No matche Single mati No MS2	[M+H]+1	312725,6		7,1	
FALSO				No results No results		756,6504		208124,3	0	0 0		No matche No matche No MS2	[M+H]+1		208124,3		7,6
FALSO		C33 H59 O Full match			2,24 660,3488	,	7,456	1385083	0	0 0		No matche Multiple m No MS2	[M+H]+1	769764,7		3	5
FALSO		C27 H51 N: Full match			-2,77 545,3484			1653947	0	0 0		No matche No matche No MS2	[M+H]+1	1575368	1653947	5,5	3,4
FALSO				No results No results No match No results	-0,27 753,6445 1,17 202,0453			217910,4 952641,4	2	0 0		No matche No matche No MS2	[M+H]+1 [M+H]+1	217910,4	952641,4	7,1	7,2
FALSO		C3 H5 N6 C Full match			-1,42 347,8988	348,906		329876,7	0	0 0		No matche No matche No MS2	[M+H]+1	329876,7		2,2	6,5
FALSO				No match No results	1,63 267,0208		1,152	253878	2	0 0		No matche No matche No MS2	[M+H]+1		173936,5	7,6	7,1
FALSO				No match No results	3,38 383,082	192,5483	1,961	269667,6	1	0 0		No matche No matche No MS2	[M+2H]+2		269667,6		6,5
FALSO		No results	No results No results	No results No results	509,6133	510,6206		318484,4	0	0 0		No matche No matche No MS2	[M+H]+1	318484,4		7,6	
FALSO				No results No results		264,0826	1,52	642231	0	0 0			[M+H]+1	113954,5	642231	6	1,4
FALSO	1-Naphthylisocyanate			Full match No results	0,63 169,0529			516048,5	2	0 0		No matche No matche DDA for pro			516048,5	7,9	6,8
FALSO				No results No results		423,3776	0,958	220059	0	0 0			[M+2H]+2	220059		8,2	
FALSO FALSO				Full match Partial mat Full match No results	0,27 170,058 0,22 178,0565	171,0652	1,504 5,504	297596 4790224	32 6	0 0		Multiple m Multiple m DDA for pro No matche No matche No MS2	[M+H]+1	297596 3390145	4700224	7,1 4,8	4,8
FALSO	5,6-Dimetnyi-2-benzotniazoiamine			No results No results		94,51519		411068,5	0	0 0			[M+H]+1		411068,5	4,8	4,8
FALSO	Carvonic acid			Full match Partial mat	0.18 180.0787	181.086		1218768	95	0 0		Single mate Multiple m DDA for pre		333324	1218768	- 0	4,7
FALSO				No results No results	0,72 357,003	. ,	-,	598068,8	0	0 0		No matche No matche No MS2	[M+H]+1	361994,8		6,5	3
FALSO				Full match No results	-0,24 251,8585	252,8658		354151,4	2	0 0		No matche No matche No MS2	[M+H]+1	354151,4		7,1	
FALSO		C2 H N6 O Full match	No results No results	No results No results	3,53 377,8042			341457,4	0	0 0		No matche No matche No MS2	[M+H]+1		341457,4		7,1
FALSO		No results	No results No results	No results No results	677,7881	678,7954	1,054	219433,7	0	0 0		No matche No matche No MS2	[M+H]+1	219433,7		7,1	2,7
FALSO				No results No results	625,5308	,		273786,6	0	0 0		No matche No matche No MS2	[M+H]+1	273786,6	252384,5	7,6	7,6
FALSO				No results No results	-0,3 1137,707	569,861		120080,9	0	0 0		No matche No matche No MS2	[M+2H]+2			6,5	
FALSO		C2 H4 Cl2 1 Full match		No results No results	-2,87 439,8386			542811,4 371140,8	0	0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1	542811,4 371140.8		6,8 7,6	
FALSO				No results No results	1.46 181.0619			588384,2	0	0 0		No matche No matche DDA for pro		3/1140,8	588384,2	7,6	6.8
FALSO				No results No results	1,62 267,9177			312251,7	0	0 0		No matche No matche No MS2	[M+H]+1	312251,7		6,5	8,2
FALSO				No results No results	0.13 1007.603			699918.2	0	0 0		No matche No matche No MS2	[M+2H]+2			3	4,7
FALSO		C4 H2 N6 C Full match	No results No results	No match No results	1,25 214,0089	215,0162	3,206	534615,7	2	0 0		No matche No matche No MS2	[M+H]+1	467406,3	534615,7	4,7	4,7
FALSO	gaboxadol	C6 H8 N2 C Full match	No results No results	Full match Full match	0,07 140,0586	141,0659	1,705	734230,9	19	0 0		Single mate No matche No MS2	[M+H]+1	557737,8	734230,9	6,3	3,6
FALSO		C8 H9 Cl O: Full match	No results No results	No match No results	-2,6 233,976	234,9833	1,17	350149,6	1	0 0		No matche No matche DDA for pro	[M+H]+1	345200,1	350149,6	7,6	7,6
FALSO				No results No results	110,9611			256193,1	0	0 0		No matche No matche No MS2	[M+H]+1		256193,1		7,6
FALSO				Full match Partial mat	0,17 136,0888		6,974		70	0 0		No matche Single mati No MS2	[M+H]+1		9846555		4,6
FALSO	Betonicine			Full match Full match	0,27 159,0896 129,5185	160,0969		510350,6	28	0 0		Multiple m No matche DDA for pro		510350,6 231435.1		6,3	3,6
FALSO	(4R,9R,14R,19R)-3,10,13,20,26-Pentaazatetra			No results No results	-3.28 357.2881	,		333725,5 656666,4	2	0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1		656666.4	8,2 5,8	6,5 2,5
FALSO		C2 H6 N9 C Full match			1,72 235,0335	,		406660,1	3	0 0		No matche No matche No MS2	[M+H]+1	374889.1	,	7,6	7,4
FALSO		C4 H N10 C Full match			0,11 617,7821			147126,1	0	0 0		No matche No matche No MS2	[M+H]+1	147126,1		8,2	
FALSO				No match No results	-0,38 430,0353			443054,1	1	0 0		No matche No matche No MS2	[M+H]+1	443054,1	435449,1	7,9	7,9
FALSO		C27 H56 N: Full match			0,65 625,3465		6,69	575426,2	1	0 0		Single mate No matche No MS2	[M+H]+1	564630,7	575426,2	7,4	6,8
FALSO				No results No results	0,51 232,1074			461856,4	0	0 0		No matche No matche DDA for pro			461856,4		6,8
FALSO	Number of CO			No results No results		543,8599	,	247221,6	0	0 0		No matche No matche No MS2	[M+H]+1	247221,6		7,1	
FALSO	· · · · · · · · · · · · · · · · · · ·			No results Full match	-2,96 606,1639		1,49	163428	12	0 0			[M+H]+1	163428	07055 64	4,9	0.2
FALSO		C4 H8 N2 C Full match		No results No results	0,51 100,0637 -0.23 1317.673	101,071 659.844	1,472	1396180 285757.7	13	0 0		No matche No matche DDA for pro No matche No matche No MS2	[M+H]+1 [M+2H]+2	1990180	97855,64 285757.7	3,9	8,2 6,5
FALSO				No results No results	0,02 451,2418	,.	7,442	1614683	0	0 0			[M+H]+1	1285643		4,5	5
FALSO				No results No results	4,87 588,3063			864564,7	0	0 0		No matche No matche No MS2		-		6,8	7,2
FALSO				No results No results		706,8032		257519,4	0	0 0		No matche No matche No MS2		,-	257519,4		6,5
FALSO		C10 H12 O Full match	No results No results	No results No results	-1,75 305,9698			447335,5	0	0 0		No matche No matche No MS2	[M+H]+1		447335,5		4,1
				Full match Partial mat				23730605	31	0 0		No matche Multiple m DDA for pro				4	
FALSO				No match No match	-3,17 185,0001			684730,2	2	0 0		Single mat(No matche No MS2			684730,2	4,1	2,5
FALSO				Full match No results	-3,89 198,9932			895665,3	1	0 0		No matche No matche DDA for pro				4,7	3,9
FALSO				Full match No results No match No results	-0,35 496,1997 4,78 541,3167			258702,2 1404240	2	0 0		No matche No matche No MS2 No matche No matche No MS2	[M+2H]+2 [M+H]+1		258702,2 1404240	3.0	5,4
				Full match No results	0,14 181,0409			494262.8	7	0 0			[M+H]+1			3,9 5,2	6,8
FALSO				No results No results		652,6708	-	236805,6	0	0 0			[M+H]+1		22230,1	7,6	-,5
	Glycochenodeoxycholic acid			Full match Full match	0 449,3141			377548,2	6	0 0		Multiple m No matche No MS2		341859,9	377548,2	6	6,5
FALSO				No match No results	0,9 174,0505			530428,2	1	0 0		No matche No matche DDA for pro	[M+H]+1			7,4	7,9
FALSO				No match No results	-2,35 261,9906			2079358	1	0 0		No matche No matche No MS2	[M+H]+1	2079358	1197074	4,2	4,5
FALSO				No results No results		709,8076		137418,9	0	0 0		No matche No matche No MS2				4,9	
FALSO				No match No results	2,75 450,1961			456687,4	2	0 0			[M+2H]+2	456687,4		6,8	5,8
FALSO				No results No results		486,6965		269078,3	0	0 0			[M+H]+1	251074.0	269078,3	C.F.	7,1
FALSO FALSO				No match No results No results No results	-4,69 273,1762 1.65 196,9776			379700,4 88161,62	0	0 0			[M+H]+1	351874,3	379700,4 88161,62	6,5	7,1 6,5
				Full match Partial mat	,	- ,		998387,9	12	0 0			[M+H]+1		998387,9		7,7
	1-(1Z-octadecenyl)-2-(4Z,7Z,10Z,13Z,16Z-doc				1,11 777,5681			254198,1	11	0 0			[M+H]+1		254198,1		7,7
FALSO				No results No results	-0,29 568,8596			210505,4	0	0 0				197077,4		7,6	7,1
FALSO				Full match Partial mat				618627,7	1	0 0		No matche Single mate DDA for pre				4,7	5,8
FALSO				No results No results	-1,49 444,0791			704043,3	0	0 0		No matche No matche No MS2			704043,3	4,1	4,7

FALSO	EDDA	C6 H12 N2 Full match No results No results	Full match No results	0,37 176,0798 177,0871	-,	13 0 0		No matche No matche No MS2 [M+H]+1	2475998 2	167539	4,8 4	4,2
FALSO		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 19	91621,1	8,2 8	8,2
FALSO		No results No results No results		80,50234 81,50961	0,974 281524,1	0 0 0		No matche No matche DDA for pri [M+H]+1	281524,1		4,3	
		C16 H33 N Full match No results No results		0,23 271,2512 272,2585	7,500 1240050	7 0 0		No matche No matche No MS2 [M+H]+1		221522	5	5
		C17 H22 N Full match No results No results		-4,8 282,1831 283,1904	7-	13 0 0		No matche Multiple m No MS2 [M+H]+1		433102		4,2
FALSO		C7 H17 N2 Full match No results No results	No results No results	0,61 208,0978 209,1051	1,139 781711,2	0 0 0		No matche No matche No MS2 [M+H]+1	781711,2 68	84549,7		3,6
FALSO		C12 H32 N. Full match No results No results		2,97 373,2101 374,2174	7,03 0422343	4 0 0		No matche No matche No MS2 [M+H]+1		422949		4,6
FALSO		C H Br Cl3 Full match 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-				7,1
FALSO		No results No results No results		124,979 125,9862	-,	0 0 0		No matche No matche No MS2 [M+H]+1		80336,3		6,5
		C11 H18 O Full match No results No results		0,06 166,1358 167,1431		19 0 0		No matche Multiple m No MS2 [M+H]+1	4149217		5,3	
		C9 H12 O Full match No results No results		0,06 136,0888 137,0961		70 0 0		No matche Single mati No MS2 [M+H]+1	10094252		4	
FALSO		C15 H31 P Full match No results No results	No match No results	4,53 338,1341 339,1414	-,	3 0 0		No matche No matche No MS2 [M+H]+1	4064533		4,2	
FALSO		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		23564,8		7,1
FALSO		C4 H4 N4 C Full match 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 90	,		6,1
FALSO		No results No results No results		690,6717 691,679	-,	0 0 0		No matche No matche No MS2 [M+H]+1		89272,7		8,2
FALSO		No results No results No results		283,2591 284,2664	-,	0 0 0			22620987 22		4	4
FALSO		No results No results No results		709,6234 710,6307	-,,-	0 0 0		No matche No matche No MS2 [M+H]+1		81223,5		7,6
FALSO		No results No results No results		80,5226 81,52988	-,	0 0 0		No matche No matche DDA for pri [M+H]+1		79820,2		2,2
FALSO		No results No results No results		80,52175 81,52903	-,	0 0 0		No matche No matche DDA for pri [M+H]+1		325656		6,5
FALSO		No results No results No results		257,8038 258,811	1,145 246775,1	0 0 0		No matche No matche DDA for pri [M+H]+1	246775,1		7,1	
		C12 H19 N. Full match No results No results		0,08 285,1325 286,1398	-,	3 0 0		No matche No matche No MS2 [M+H]+1	277772 29	91571,8		5,4
	4-Chloro-N-[6,8-dibromo-2-(2-thienyl)imidaz	C18 H10 Br No results No results No results		-0,75 508,8596 509,8669	-/	1 0 0		No matche No matche No MS2 [M+H]+1	188993,2	70044.0	7,6	0.0
FALSO	- (No results No results No results		618,7129 619,7202	7	0 0 0		No matche No matche No MS2 [M+H]+1		70011,8		8,2
FALSO		C8 H12 N2 Full match No results No results		-0,12 168,0899 169,0971 -0.04 168,115 169,1223		20 0 0	47.4	Single mati Multiple m DDA for pri [M+H]+1	447895,2 64			6,3
	Massoia lactone			0,0: -00,0 -00,0	.,		47,4	Multiple m Multiple m DDA for pri [M+H]+1	7987328 10			3,5
FALSO		No results No results No results		646,649 647,6563	-,	0 0 0		No matche No matche No MS2 [M+H]+1	188367,6 23	04209,3		7,6
FALSO		C39 H71 N! Full match No results No results		-3,2 681,576 760,5988	-,,-	0 0 0		No matche No matche No MS2 [M+DMSO-		20021.1	6,5	7.1
FALSO		No results No results No results		533,6199 534,6262	-,-:	0 0 0		No matche No matche No MS2 [M+H]+1	262540,6 23	00921,1		7,1
FALSO		C3 H2 CI O: Full match No results No results		-4,05 453,7414 454,7487	-,0 0-00:0,0	0 0 0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	310578,8 189307.7 13	27102.1	7,1	7.6
		C44 H90 O No results No results No results		1,84 682,6852 683,6924	1,131 189307,7	1 0 0						7,6
	(C12 Cl10 S. No results 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 23	03120,6		3,8
FALSO		C7 H19 N1 Full match No results No results No results No results No results		-2,69 352,0947 177,0546 475,6612 476,6678	7	0 0		No matche Multiple m No MS2 [M+2H]+2 No matche No matche No MS2 [M+H]+1	685736,9	77050 2	6,8	6.5
FALSO		No results No results No results C8 H12 Cl4 Full match No results No results		,	,,,	0 0 0				07959,3		6,5
FALSO		C8 H12 Cl4 Full match No results No results C17 H27 N Full match No results No results	THO TESUIES THO TESUIES	2,1 437,8416 438,8488	-,	0 0 0		No matche No matche No MS2 [M+H]+1	301487,1 28			7,1
		C14 H27 N Full match No results No results C14 H27 N Full match No results No results		0,27 309,1941 310,2014	.,			No matche Multiple m No MS2 [M+H]+1		31946,2	-,-	6,6
FALSO				-3 273,1577 274,165	.,	5 0 0		No matche Single mati No MS2 [M+H]+1	3178873		4,2	
FALSO FALSO		C16 H26 O Full match No results No results		-2,26 298,1418 299,1491	.,			No matche Multiple m DDA for pre [M+H]+1	9623449		4,6	
		C45 H74 N! Full match No results No results No results No results No results		-2,2 779,5461 780,5534	,	0 0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	4531660 296409.8 23	22022.4	4,8	2.2
FALSO				234,8898 235,8971	1,138 296409,8	0 0 0					,	3,3
		C8 H14 N2 Full match No results No results		-1,13 232,0528 233,0601 1.45 248.0539 249.0612	3,231 626533,2	2 0 0		No matche No matche No MS2 [M+H]+1	626533,2 51		-,-	-
FALSO		C4 H9 N8 C Full match No results No results		-,,,	4,143 525730 1,121 266273.7			No matche Single mat No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1		525730		6,8
FALSO		C4 H5 Cl Ol Full match No results No results No results No results No results		-2,81 373,83 374,8373 106,9931 108,0004		4 0 0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1		16461,4 8605.24		7,6 4,9
FALSO		No results No results No results No results No results No results		685,8097 686,817	.,	0 0 0		No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	187062.3	8605,24		1,9
									, .	21252.2	6,5	4.7
FALSO	N-ethylmaleimide	No results No results No results C6 H7 N O4 Full match No results No results		71,02065 72,02792 0,55 125,0478 126,055	.,	0 0 0		No matche No matche DDA for pr [M+H]+1 Multiple m No matche No MS2 [M+H]+1	402677,1 59 22057722	91253,2	6,8 4	4,7
		C4 H4 O3 Full match No results No results		0,21 100,0161 101,0233		4 0 0		No matche No matche DDA for pre [M+H]+1	1786757 2	060122		4,8
FALSO				0,38 244,0696 245,0769		4 0 0		Multiple m No matche No MS2 [M+H]+1		59467,2		
FALSO		C9 H12 N2 Full match No results No results C8 H13 N C Full match No results No results		0,38 244,0696 245,0769		23 0 0		No matche Single mati DDA for pri [M+H]+1	747782,4 73			3,4 6,3
		C10 H22 O Full match No results No results		0,01 238,1416 239,1489		1 0 0		No matche No matche No MS2 [M+H]+1		685734		6,3
FALSO		C45 H78 O Full match No results No results		-0.71 858.4979 430.2563	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	0 0 0		No matche Single mat (No MS2 [M+2H]+2	584124 50		-	3
FALSO		No results No results No results		397,8987 398,906		0 0 0		No matche No matche No MS2 [M+H]+1		57178,3		4,3
FALSO		C40 H61 N Full match No results No results		0,49 587,4705 588,4778		0 0 0		No matche No matche No MS2 [M+H]+1		746044		4,7
FALSO		No results No results No results		609,801 610,8082		0 0 0		No matche No matche No MS2 [M+H]+1	,.	21115.4		7,1
	Glycerol	C3 H8 O3 Full match No results No results		0,31 92,04737 93,05465	1,518 314990,8	3 0 0		Single matc No matche No MS2 [M+H]+1	314990,8	21113,4	6,5	,1
FALSO		C7 H5 Cl2 (Full match No results No results		-1,26 493,8356 494,8429		0 0 0		No matche No matche No MS2 [M+H]+1	384644.2 49	7775 6		6,3
FALSO		No results No results No results		521.7292 522.7365		0 0 0		No matche No matche No MS2 [M+H]+1	246636.8	37723,0	7,6	3,3
FALSO		C4 H3 Cl O: Full match No results No results		-0.97 467.8199 468.8272	,	0 0 0		No matche No matche No MS2 [M+H]+1	150561.7		8.2	
		C18 H36 O Full match No results No results		0,07 284,2716 285,2788		34 0 0		Single mati Single mati No MS2 [M+H]+1	8641447 7	781484	4	4
FALSO		C48 H63 N Full match No results No results		1,92 731,4399 732,4472		0 0 0		No matche No matche DDA for pre [M+H]+1	691010,4 74			7,4
FALSO		No results No results No results		663.6246 664.6318		0 0 0		No matche No matche No MS2 [M+H]+1		182739		7,6
FALSO		No results No results No results		387.8501 388.8574		0 0 0		No matche No matche No MS2 [M+H]+1	376019,5 37			6,5
FALSO		C66 H105 Full match No results No results		0.34 1179.684 590.8492	1,073 376019,3	0 0 0		No matche No matche No MS2 [M+H]+1		37546.3		6,5
FALSO		No results No results No results		707.6473 708.6545	1,097 337346,3	0 0 0		No matche No matche No MS2 [M+2H]+2	189783.2		8.2	.,5
	Luteoride C	C17 H20 N. Full match No results No results		0,38 332,1374 333,1446	,	0 0 0		No matche Multiple m No MS2 [M+H]+1		441869		6,8
FALSO		C16 H31 N Full match No results No results		0,17 301,2254 302,2326	6.18 659729.8	4 0 0		No matche No matche No MS2 [M+H]+1		59729.8		4,1
FALSO	C ,	No results No results No results		693,6472 694,6545	.,	0 0 0		No matche No matche No MS2 [M+H]+1		37533.5		7,1
	Ethosuximide	C7 H11 N C Full match No results No results		0,39 141,079 142,0863		18 0 0		Single mate No matche DDA for pre [M+H]+1	1538973 1	, .		4,5
	10-Undecenoic acid	C11 H20 O No results No results No results		-0.39 184.1463 185.1535	1,002 666463,7	36 0 0		No matche Multiple m No MS2 [M+H]+1			4,1	
		C16 H33 N Full match No results No results		0,12 287,2461 288,2534	6,851 698554,9	6 0 0		No matche No matche DDA for pri [M+H]+1		98554.9		4.1
		C11 H8 I4 No results No results No results		1,99 739,6678 740,675	1,135 273215,6	1 0 0		No matche No matche No MS2 [M+H]+1				7,1
FALSO		No results No results No results		537,5672 538,5745		0 0 0		No matche No matche No MS2 [M+H]+1	318894	- /		8,2
FALSO		C H2 Br2 Cl Full match No results No results		2,07 579,6429 658,6644		0 0 0		No matche No matche No MS2 [M+DMSO-		54147,7		7,1
FALSO		C19 H25 N' Full match No results No results		1,31 351,2176 352,2249		1 0 0		No matche No matche No MS2 [M+H]+1	440659 55			7,9
FALSO		C6 H8 N9 C Full match No results No results		-0,85 253,0587 254,066	.,	4 0 0		No matche No matche No MS2 [M+H]+1	319725,1 24			7,6
		C9 H10 F2 No results No results No results		-2,09 204,0594 205,0667		1 0 0		No matche No matche No MS2 [M+H]+1	452495,2			2,5
FALSO	, , zz.z., z,z,o proparetion	No results No results No results		477,6113 478,6186		0 0 0		No matche No matche No MS2 [M+H]+1	336664,2 36			7,1
	Methohexital	C14 H18 N: Full match No results No results		0,25 262,1318 263,1391		13 0 0		No matche Multiple m DDA for pre [M+H]+1				6,3
FALSO		C42 H53 N: Full match No results No results		-1,91 709,3549 355,6847		0 0 0		No matche No matche DDA for otl [M+2H]+2				6,8
FALSO		C12 H25 N Full match No results No results		0,15 247,1606 248,1679		0 0 0		No matche No matche No MS2 [M+H]+1				7,9
FALSO		C4 H9 N2 P Full match No results No results		2,03 116,0506 117,0579		0 0 0			332253,9 38			7,1
FALSO		C5 H8 N2 C Full match No results No results		-0,81 206,0009 207,0081		1 0 0			612000,4 60			6,3
FALSO		No results No results No results		614,6973 615,7045		0 0 0		No matche No matche No MS2 [M+H]+1	188974.4 20			7,1
FALSO		C18 H18 N. Full match No results No results		3,72 340,0907 341,098		7 0 0		No matche Multiple m No MS2 [M+H]+1	327467,3 32			6,5
		C4 H11 N C Full match No results No results		0,53 105,079 106,0863		7 0 0		No matche No matche No MS2 [M+H]+1	785421,4 74			6,3
FALSO		C10 H19 N. Full match No results No results		2,71 278,0862 279,0934		3 0 0		No matche No matche DDA for pri [M+H]+1	1462530 1			5
FALSO		C4 H2 N6 C Full match No results No results		1,29 214,0089 215,0162		2 0 0		No matche No matche No MS2 [M+H]+1	545246,5 52		-	5,8
FALSO		C3 H7 N10 Full match No results No results		-1,29 342,0182 343,0254		0 0 0		No matche No matche DDA for pri [M+H]+1				3,8
		C6 H13 N3 Full match No results No results		0,23 175,0957 176,103		7 0 0		Single mat(No matche No MS2 [M+H]+1				5,2
FALSO		C3 H5 Cl N; Full match No results No results		2,55 341,8533 342,8606		0 0 0		No matche No matche DDA for pri [M+H]+1				7,1
FALSO		C34 H49 N Full match No results No results		-0,06 583,3509 584,3582		0 0 0		No matche No matche No MS2 [M+H]+1				6,8

	FALSO		C7 H26 N7 Full match No results No results	No match No results	-2,89 349,1122 350,1195	1,782 751281,8	2 0 0	No matche No matche No MS2 [M+H]+1	751281,8 699706,4	6,3 7	7,4
	FALSO		C7 H3 Cl N: Full match No results No results	No results No results	-0,95 595,7948 596,8021	1,003 697596	0 0 0	No matche No matche No MS2 [M+H]+1	697596 359601,4	5,8 6	6,5
	FALSO		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	No matche No matche No MS2 [M+H]+1	168961		8,2
	FALSO		No results No results No results		698,6616 699,6688	-,	0 0 0	No matche No matche No MS2 [M+H]+1	145270,2 192226,3		8,2
	FALSO		C59 H90 N Full match No results No results		-0,15 1040,64 521,3271	7	0 0 0	No matche No matche DDA for ot [M+2H]+2	439194,9 547090,5		6,8
	FALSO	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	Single mate No matche DDA for pre [M+H]+1	272011,7	2	4,3
	FALSO		No results No results No results		1069,732 535,8731	-,00 -00 -10,-	0 0 0	No matche No matche No MS2 [M+2H]+2	205445,1	7	7,1
			C11 H20 O No results No results No results		0,43 184,1464 185,1537		36 0 0	No matche Multiple m No MS2 [M+H]+1	166217,5		7,1
	FALSO	CUMYL-CH-MeGACLONE	C27 H30 N: No results No results No results	Full match No results	4,26 398,2375 399,2448	.,	2 0 0	No matche No matche No MS2 [M+H]+1	370127,5 419441,1	7,6 7	7,4
	FALSO	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	No matche Single mati No MS2 [M+H]+1	417088,4	4,1	
	FALSO		C6 H3 N5 C Full match No results No results		-1,55 254,9707 255,978		0 0 0	No matche No matche No MS2 [M+H]+1	224278,6 189480,8		8,2
	FALSO	Tributyl (1Z)-1-propene-1,2,3-tricarboxylate	C18 H30 O No results No results No results	Full match Partial mat	0,14 342,2043 325,201	7,311 7205497 1	12 0 0	No matche Multiple m DDA for pri [M+H-H2O	7205497	4	
	FALSO		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	No matche No matche No MS2 [M+2H]+2	89915,29	F	6,5
	FALSO		C8 H13 N1 Full match No results No results		-0,79 296,1009 297,1082		1 0 0	Single mate Multiple m No MS2 [M+H]+1	347263,5 388741,6	6,5	6
	FALSO		C8 H14 N9 Full match No results No results		1,52 331,0734 332,0807	-,	0 0 0	No matche No matche No MS2 [M+H]+1	221735,3 210120,8		7,6
		Glycerol	C3 H8 O3 Full match No results No results		0,15 92,04736 93,05463	1,562 475598,2	3 0 0	Single mate No matche No MS2 [M+H]+1	475598,2	4,1	
	FALSO		C9 H7 N Full match No results No results		0,17 129,0579 130,0652	0,010 107331,3	4 0 0	Multiple m No matche No MS2 [M+H]+1	452897,1 467534,3		6,3
	FALSO		C3 H7 N2 C Full match No results No results		-2,79 243,9383 244,9456	0,997 611062,7	1 0 0	No matche No matche No MS2 [M+H]+1	579357,1 611062,7		5,2
	FALSO		No results No results No results		645,7186 646,7258	1,15 1,52-10,5	0 0 0	No matche No matche No MS2 [M+H]+1	175240,9		8,2
	FALSO		No results No results No results		715,6357 716,643		0 0 0	No matche No matche No MS2 [M+H]+1	224230,4		7,1
	FALSO		C48 H57 N! Full match No results No results		-3,19 775,4661 776,4734	0,000,0	0 0 0	No matche No matche DDA for pri [M+H]+1	682749,9 771058,9		6,8
			C16 H24 O. Full match No results No results		0,3 296,1625 297,1697	.,	12 0 0	No matche Multiple m No MS2 [M+H]+1	7907142	4	
	FALSO		C5 H9 N O4 Full match No results No results		0,78 210,9975 212,0047	_,	1 0 0	No matche No matche No MS2 [M+H]+1	256264,1 225364,4		7,6
	FALSO		C15 H31 N Full match No results No results		4,86 389,205 390,2123	7,056 5685180	6 0 0	No matche No matche No MS2 [M+H]+1	4675021 5685180	2,6	4
	FALSO		C9 H24 Cl 1 Full match No results No results		3,2 440,0673 441,0746	1,236 679959,6	0 0 0	No matche Single mati No MS2 [M+H]+1	679959,6		4,7
		N-Butylbenzenesulfonamide	C10 H15 N No results No results No results		0,27 213,0824 214,0897	1,661 19491767	6 0 0		19491767 17084062	4	4
	FALSO		No results No results No results		767,5384 768,5457		0 0 0	No matche No matche No MS2 [M+H]+1	191590,8		7,6
	FALSO		C5 H5 N3 C Full match No results No results		-2,49 232,975 233,9822	-,	0 0 0	No matche No matche No MS2 [M+H]+1	318394,9 286956,3		7,6
	FALSO		No results No results No results		100,5015 101,5087	-,	0 0 0	No matche No matche No MS2 [M+H]+1	272156,2		6,5
	FALSO		C4 H13 N1 Full match No results No results		-3,76 294,0526 295,0599	-,	0 0 0	No matche Multiple m No MS2 [M+H]+1	244909,1 244578,6	5,4	6
	FALSO		No results No results No results	NO results into results	673,6535 674,6608		0 0 0	No matche No matche No MS2 [M+H]+1	199680,1 230521,4		7,1
		Dipivaloylmethane	C11 H20 O Full match No results No results		0,31 184,1464 185,1537	-,	36 0 0		14126721 16634065	4	4
	FALSO		No results No results No results		429,8461 430,8534	7	0 0 0	No matche No matche DDA for pri [M+H]+1	262845,8 202590,3		7,1
	FALSO		C16 H29 N Full match No results No results		0,16 363,1894 364,1967	7,207 5827495	5 0 0	No matche No matche No MS2 [M+H]+1	5404985 5827495	3,7	4
	FALSO		C5 H2 Cl N! Full match No results No results		-1,81 244,9419 245,9491		0 0 0	No matche No matche No MS2 [M+H]+1	216090,1	7,6	
	FALSO		No results No results No results		661,6933 662,7006		0 0 0	No matche No matche No MS2 [M+H]+1	224412,6 179723,4		5,4
			C4 H6 N2 Full match No results No results		1,9 82,05325 83,06042		8 0 0	No matche No matche DDA for pre [M+H]+1	549652,7	5	5,2
	FALSO		C2 H4 N3 C Full match No results No results		-2,96 164,9757 165,983	0,347 858198,4	0 0 0	No matche No matche No MS2 [M+H]+1	858198,4		5
	FALSO	p-Cresol	C7 H8 O Full match No results No results		-0,1 108,0575 109,0648	6,996 8157142	7 0 0	Multiple m DDA for pre [M+H]+1	8157142		4
	FALSO		No results No results No results		649,6896 650,6969	-,: :,-	0 0 0	No matche No matche No MS2 [M+H]+1	174313,1		8,2
	FALSO		No results No results No results		555,628 556,6353		0 0 0	No matche No matche No MS2 [M+H]+1	174647,5	8,2	
	FALSO		C8 H12 Full match No results No results		-0,04 108,0939 109,1012		1 0 0	No matche Single mati DDA for pri [M+H]+1	5160901 6504829		4,6
	FALSO		C8 H3 Cl2 (Full match No results No results		2,04 423,8646 424,8719		0 0 0	No matche No matche No MS2 [M+H]+1	336378,9	7,6	
	FALSO		C4 H8 Cl3 (Full match No results No results		1,07 509,8096 510,8169	1,210 403332,7	0 0 0	No matche No matche No MS2 [M+H]+1	403992,7 383739,3		5,4
	FALSO		C36 H57 N Full match No results No results		2,12 704,3751 705,3824	7,453 1138377	0 0 0	No matche Multiple m No MS2 [M+H]+1	767700,3 1138377	4,1	5
	FALSO		No results No results No results		713,5947 714,6019	-,	0 0 0	No matche No matche No MS2 [M+H]+1	173480,3		8,2
	FALSO		No results No results No results		109,5113 110,5186	.,	0 0 0	No matche No matche DDA for pri [M+H]+1	1126706 1428641		5,5
	FALSO		No results No results No results		191,5411 192,5484	7	0 0 0	No matche No matche No MS2 [M+H]+1	270180,3	7,1	
	FALSO		C5 H14 O8 Full match No results No results		-2,34 264,0158 265,0231	_,	0 0 0	No matche No ms2 [M+H]+1	260914,8 337669,4	6	6
	FALSO		No results No results		293,8712 294,8784	1,003 201703,2	0 0 0	No matche No matche DDA for pri [M+H]+1	264785,2 210914,3		7,1
	FALSO		C5 H8 Cl N Full match No results No results		3,67 274,9526 275,9598	-,	0 0 0	No matche No matche No MS2 [M+H]+1	267580,3 241675,8		8,2
	FALSO		No results No results No results		723,787 724,7943	_,	0 0 0	No matche No matche No MS2 [M+H]+1	181609,6 157018,8		7,1
	FALSO		C20 H25 N: Full match No results No results		0,11 419,1515 420,1588	0,100	5 0 0	No matche No matche No MS2 [M+H]+1	338768,9 370846		7,6
	FALSO		No results No results		294,2236 295,2309	.,	0 0 0	No matche No matche No MS2 [M+H]+1	444215,6		4,7
	FALSO		C6 H3 Cl O: Full match No results No results		2,28 413,8611 414,8684		0 0 0	No matche No matche No MS2 [M+H]+1	190472,2		7,6
	FALSO		C3 H3 N3 C Full match No results No results		1,93 286,8817 287,889	-,	0 0 0	No matche No ms2 [M+H]+1	95028,9		5,4
	FALSO		C7 H19 N4 Full match No results No results		4,17 238,1205 239,1278	7	15 0 0	No matche Multiple m No MS2 [M+H]+1	428411	4,7	
	FALSO		No results No results		80,52458 81,53185		0 0 0	No matche No matche DDA for pri [M+H]+1	585777,9	4,7	
	FALSO		C4 H15 N6 Full match No results No results		1,88 306,0695 307,0768	1,393 468758,3	1 0 0	No matche No matche No MS2 [M+H]+1	420074,1 468758,3		4,1
	FALSO	Diothyl phthalate	No results No results No results		1278,697 640,356	,	0 0 0	No matche No matche No MS2 [M+2H]+2	263945,2 801996 754958.8	7,1	E 2
			C12 H14 O Full match No results No results		0,12 222,0892 223,0965	,	64 0 0	No matche Multiple m No MS2 [M+H]+1			5,2
			C13 H22 O Full match No results No results		0,16 242,1519 243,1591	7,55 2507054	4 0 0	No matche Multiple m No MS2 [M+H]+1	2967854 1354176	2,1	5
	FALSO		C3 H6 N5 C Full match No results No results		1,15 238,9881 239,9954	0,342 618852,1	0 0 0	No matche No matche No MS2 [M+H]+1	618852,1	4	5,2
	FALSO FALSO	undec-10-ynoic acid	C11 H18 O Full match No results No results No results No results No results		-0,09 182,1307 183,1379 762,7852 763,7925	.,	0 0 0	No matche Multiple m DDA for pri [M+H]+1 No matche No matche No MS2 [M+H]+1	7778826 107358,5	5,4	
	FALSO		No results No results No results No results No results No results		834.4727 418.2436		0 0 0	No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+2H]+2		-	1.2
	FALSO		No results No results No results No results No results No results		834,4727 418,2436 516.8457 517.8529	.,	0 0 0	No matche No matche No MS2 [M+2H]+2 No matche No matche No MS2 [M+H]+1	5546503 2173721 274727,7 383926,3		4,2 4,3
	FALSO		C4 H6 N7 C Full match No results No results		-1.24 199.0369 200.0442	1,305 431838,4	0 0 0	No matche No matche No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	431838,4		6,8
					,		0 0 0			8.2	,,0
	FALSO	nilenrost	No results No results No results		789,6825 790,6898 0,04 391,2359 392,2432	1,128 151578,6 7 494 718279 2	8 0 0	No matche No matche No MS2 [M+H]+1		6.2	7.4
	FALSO	nileprost	C22 H33 N Full match No results No results No results No results No results		297,8717 298,879	7,494 718279,2 1,059 314648	0 0 0	No matche Multiple m No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1	314648 308726,2		7,4 7,1
	FALSO				2,98 332,1374 333,1446		0 0 0				
	FALSO		C19 H25 O Full match No results No results No results No results No results		2,98 332,1374 333,1446 276,2066 277,2139		0 0 0	No matche Multiple m No MS2 [M+H]+1 No matche No matche No MS2 [M+H]+1			7,4
		ALA-PRO	C8 H14 N2 Full match No results No results		-0,12 186,1004 187,1077		8 0 0	No matche No matche No MS2 [M+H]+1 Single mat(No matche DDA for pr([M+H]+1	203822,1		1,4 5,4
	FALSO	ALA: INU	No results No results No results		759,5936 760,6009		0 0 0	No matche No matche No MS2 [M+H]+1	203822,1		7,1
	FALSO		No results No results No results		605,6904 606,6977		0 0 0	No matche No matche No MS2 [M+H]+1	284785,2		7,1
		S-(3-oxo-3-carboxy-n-propyl)cysteine	C7 H11 N C Full match No results No results		0,05 221,0358 222,0431		1 0 0		293206,6 444011,8		5,2
	FALSO	5 (5 5% 5 carboxy ii propyrjeysteine	No results No results No results		523,8249 524,8322		0 0 0		557417,2 320772,4		6
		Myristamine oxide	C16 H35 N Full match No results No results		0,06 257,2719 258,2792		2 0 0	No matche No matche No MS2 [M+H]+1	380101.5 518601.6		5,8
			C14 H22 O Full match No results No results		-0,25 222,1619 223,1692		2 0 0 37 0 0	Single mate Multiple m DDA for pre [M+H]+1	4495397 3958862		1,5
	FALSO		C2 H2 CI N; Full match No results No results		4,35 293,8599 294,8671		0 0 0	No matche No matche No MS2 [M+H]+1	298010,6 219027,5		8,2
	FALSO		No results No results No results		664,668 665,6753		0 0 0	No matche No matche No MS2 [M+H]+1	187454,7		7,6
		meprobamate	C9 H18 N2 No results No results No results		0,14 218,1267 219,134		21 0 0	Single mat(No matche No MS2 [M+H]+1			7,1
	FALSO		No results No results No results		731,6124 732,6196	, ,	0 0 0	No matche No matche No MS2 [M+H]+1	184574,4		7,6
		Pentadecane-1-sulfonic acid	C15 H32 O No results Invalid ma: No results		1,1 292,2075 293,2148		1 2 0	No matche No matche DDA for pr [M+H]+1		6	,,,
	FALSO		C3 H Cl2 N4 Full match No results No results		0,3 655,6811 656,6884		0 0 0	No matche No matche No MS2 [M+H]+1	157745,9		7,1
	FALSO		C6 H8 N6 C Full match No results No results		1.7 180.0763 181.0835	7	0 0 0	No matche No matche DDA for pr [M+H]+1	153610,6 306672,1		4,3
	FALSO		No results No results No results		675,8219 676,8292		0 0 0	No matche No matche No MS2 [M+H]+1	334762,8		7,1
		1-{4-[(2-Ethoxyethoxylmethyllnhenoxyl-3-(ic	C17 H29 N Full match No results No results		0,25 311,2097 312,217		2 0 0	No matche Multiple m No MS2 [M+H]+1	393843,3 429794		7,4
			C10 H20 N: Full match No results No results		-0,38 216,1473 217,1546	1,96 339572,4	2 0 0	No matche Single mati No MS2 [M+H]+1	339572,4	6	
			C8 H14 O2 Full match No results No results		-0,01 142,0994 143,1067		2 0 0	No matche Single mat No MS2 [M+H]+1			4,2
		-, ···· yacc	no results		-,	.,==_ 3000.33 3			2222.0 3300733	5,5	
_											

																	_	_
FALSO		No results No results				,	739,6093	_,	177883,1		0 0			[M+H]+1	,		7,6	
	(1R,2R,6S,7S,8R,10S,11S,12R,16R,18R)-6,7-D C30 H40 O F	Full match No results	No results	Full match No	ot the top -4,38		529,2773		1114453		0 0		No matche Multiple m No MS2	[M+H]+1	743228,7		4,7	4,5
FALSO		No results No results					286,8178		227184,5	-	0 0		No matche No matche No MS2	[M+H]+1	227184,5	195511,9	7,6	7,1
FALSO		No results No results					654,6276		243634,9	-	0 0		No matche No matche No MS2	[M+H]+1		243634,9		7,1
		Full match No results					201,1848	7,338			0 0		No matche Multiple m No MS2	[M+H]+1		917076,9	4,5	3,4
	· · · · · · · · · · · · · · · · · · ·	Full match No results					146,0813	1,51			0 0		Multiple m No matche DDA for pro		92901,2		8,2	
		Full match No results					301,1184		451495,6		0 0			[M+H]+1		451495,6	6,8	7,4
		No results No results					607,1706		345874,8		0 0			[M+H]+1		293071,3	7,1	4,3
FALSO		Full match No results			, , ,		209,1536		7086157		0 0		No matche Multiple m DDA for pro		7086157		4	
FALSO		Full match No results					,		257062,2	-	0 0		No matche No matche No MS2	[M+H]+1	257062,2		7,1	7,1
FALSO		Full match No results				2 341,9223				-	0 0		No matche No matche DDA for pre			360141,7	7,1	6
FALSO		Full match No results				6 484,2438			1034483	-	0 0		No matche Multiple m No MS2	[M+H]+1			4,1	5
FALSO		Full match No results				8 262,1029			260006,6		0 0		No matche No matche No MS2	[M+H]+1	252072,5	260006,6	7,1	7,1
FALSO		No results No results				- /	765,5721		148141,7		0 0		No matche No matche No MS2	[M+H]+1	148141,7		8,2	
FALSO		Full match No results				3 1029,585		,	846563,5	-	0 0		No matche Single mati No MS2	[M+2H]+2	846563,5	810811,5	4,5	5,8
FALSO		Full match No results				6 174,0052			178016,5	-	0 0		No matche No matche No MS2	[M+H]+1		178016,5		4,3
FALSO		Full match No results				6 210,0409			287439,7		0 0		No matche No matche No MS2	[M+H]+1		287439,7	7,6	6
 FALSO		nvalid ma: No results					315,9579		265790,2	-	0 0		No matche No matche No MS2	[M+H]+1		197934,6	7,1	8,2
FALSO		No results No results				,	1 646,1023		369268,8	-	0 0		No matche No matche No MS2	[M+H]+1		369268,8	1,6	7,1
FALSO		Full match No results					248,1129		318802,2		0 0		Single mati Single mati No MS2	[M+H]+1	251723,4		7,6	6
FALSO		Full match No results					438,9809		1005041	-	0 0		No matche No matche No MS2	[M+H]+1	1005041	647945,7	5,5	6,8
		No results No results					215,1644	1,491			0 0		Single mate Multiple m No MS2	[M+H]+1	2452520	91674,9	42	7,6
FALSO		Full match No results					327,1413	6,983		-	0 0		No matche No matche No MS2	[M+H]+1		2660059	4,2	4,2
FALSO		No results No results				191,9027			483612,4	-	0 0		No matche No matche No MS2	[M+H]+1	483612,4	466871,9	4,1	3,6
FALSO		Full match No results				1 356,1836			4242171		0 0		No matche Single mati No MS2	[M+H]+1	174174	4242171	7.1	4,2
FALSO		Full match No results				5 647,6297			195239,7		0 0		No matche No matche No MS2	[M+H]+1		195239,7	7,1	8,2
FALSO		No results No results					1 568,5794		268524,1	-	0 0		No matche No matche No MS2	[M+H]+1		257237,1	7,1	7,6
FALSO		Full match No results					249,0352		419111,8		0 0		No matche No matche DDA for pro			415302,7	4,7	7,4
FALSO		Full match No results			,	497,8333			225919,6		0 0		No matche No matche DDA for pro			225919,6	7,6	7,1
FALSO		No results No results					624,7346	, .	157751,1		0 0		No matche No matche No MS2	[M+H]+1	157751,1		4,9	
FALSO		No results No results					722,6144		226539,4	-	0 0			[M+H]+1	226539,4	E12005 2	7,1	4.7
FALSO		No results No results				,	1 154,8803	,	512995,2	-	0			[M+H]+1	482365,4	512995,2	4,1	4,7
FALSO		Full match No results					1 162,0073		272261,2		0 0	70.5	No matche No matche No MS2	[M+H]+1		272261,2 127158		7,1
	Diamyrramyiphosphonate C15 1155 O. 11	to results invalid ind	. 110 1 0 3 0 1 0 3	r dir materi 14	0 (0,0.		3 293,2241	1,554				76,5	No matche No matche DDA for pro			12/158		4,9
	7 7 77	Full match No results				7 82,05319 9 151,9991	83,06046	-,,	184984,5		0 0			[M+H]+1	184984,5		6,5	
FALSO		Full match No results							324371,8		0 0		No matche No matche DDA for pro		324371,8	252042.2	4,3	7.6
FALSO		Full match No results					2 271,0415		252012,2		-		No matche No matche No MS2	[M+H]+1		252012,2	7,6	7,6
FALSO		Full match No results				4 255,0855			199653,9		0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1	199653,9	188273,3	8,2	4,9
FALSO		No results No results					110,5186	-,	72827,63		0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1	435004.0	72827,63	22	7,6
FALSO		No results No results				587,8218			136991,9		-			[M+H]+1	136991,9		8,2	
FALSO		No results No results				770,3448			161807,4	-	0		No matche No matche No MS2	[M+H]+1	161807,4	722040.0	7,6	
FALSO		Full match No results							838594,7 436358.2		0 0		No matche Single matche DDA for oth No matche No matche No MS2			723948,8	4,5	0,9
FALSO FALSO		Full match No results				3 159.0685	452,7374	4,676			0 0		Multiple m Multiple m No MS2	[M+2H]+2 [M+H]+1	575127,1	,	7,4	7,4 6,3
	_ (,					-			[5/512/,1		5,8	
FALSO FALSO		No results No results Full match No results				577,8117	7 578,819 L 556,6434		101731,1 200893,9		0 0		No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1	200893,9	101731,1	8,2	5,4
FALSO		No results No results					479,1893	6.42		-	0 0		No matche No matche No MS2	[M+3H]+3		541132	5.8	6,8
FALSO		No results No results					406.4012	0,993	664446	-	0 0		No matche No matche No MS2	[M+2H]+2	518/02,0	664446	5,8	6,3
FALSO		Full match No results					2 143,0734		343492,2		0 0		No matche No matche DDA for pro		281225,3	343492,2	7,1	7,6
		Full match No results					133,0496		661236.1	-	0 0		No matche No matche DDA for pro			343452,2	4.7	7,0
FALSO		Full match No results					252,1092	-,	771226,1	-	0 0			[M+H]+1		762820,4	4,7	5,2
		Full match No results							134046,6	-	0 0		Multiple m Multiple m DDA for pro		//1220,1	134046,6	4,7	8,2
FALSO		Full match No results				9 209.8986			284156,3		0 0		No matche No matche No MS2	[M+H]+1	284156,3	234200,8	7,6	7,1
FALSO		Full match No results				4 419,1516			352017,1	_	0 0		No matche No matche No MS2	[M+H]+1		352017,1	7,0	7,1
FALSO		Full match No results				7 447,2468			4943116		0 0		No matche No matche No MS2	[M+H]+1	4524389	4943116	4,2	3,2
		Full match No results				7 182,130					0 0		No matche Multiple m DDA for pro		4324365	9907696	4,2	4
FALSO		No results No results					5 580.6948		245080,8		0 0			[M+H]+1	245080.8		7,1	7,1
FALSO		No results No results				663.6489	,		265476.9	-	0 0		No matche No matche No MS2	[M+H]+1	243000,0	265476.9	7,1	7,1
FALSO		No results No results				1997,945	,	-	247600,9		0 0		No matche No matche No MS2	[M+3H]+3	247600.9	203470,5	7,1	-,,-
FALSO		Full match No results				4 275,8894			420081,4	-	0 0		No matche No matche No MS2	[M+H]+1	277000,9	420081.4	.,1	6,3
		No results No results				7 677.6707			185029.5		0 0		No matche No matche No MS2	[M+H]+1	185029.5	152537,2	8,2	7,1
FALSO		No results No results				601,6072	, -	,	270812,7		0 0		No matche No matche No MS2	[M+H]+1		270812,7	-,-	7,1
FALSO		Full match No results				2 641,634			148743.4	-	0 0		No matche No matche No MS2	[M+H]+1	148743.4	_,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	7,1	-,2
FALSO		Full match No results				8 500,8718			294443,1		0 0		No matche No matche No MS2	[M+H]+1		294443,1		6,5
FALSO		Full match No results				2 739,5991	740,6064		155161,3		0 0		No matche No matche No MS2	[M+H]+1		155161,3		8,2
FALSO	1-(2-deoxypentofuranosyl)-5-ethylpyrimidin C11 H16 N. F	Full match No results	No results	Full match Fu				3,439	478749,7	9	0 0		Single mate No matche No MS2	[M+H]+1	449762,2	478749,7	7,9	6,3
	(2S)-1-{[11-(3,4-Dimethyl-5-propyl-2-furyl)ur C46 H78 O					9 742,5751		-,	136346,4	9	0 0		No matche No matche No MS2	[M+H]+1		136346,4		8,2
		Full match No results				5 246,0523	3 247,0596	,	250459,5		0 0		Multiple m Multiple m No MS2	[M+H]+1	225092,4	250459,5	7,6	5,4
FALSO		Full match No results				5 292,1286			2154732	2	0 0			[M+H]+1	2154732		4,8	
FALSO		Full match No results					5 543,3402		471433,4	0	0 0		No matche No matche DDA for otl			471433,4	6,8	6,8
		Full match No results					246,1522		605435,7		0 0				599866,4		6,8	7,4
		Full match No results					737,4026		602621,2	0	0 0			[M+H]+1	542233,9	602621,2	6,8	7,4
FALSO		Full match No results					348,0705		212041,2	15	0 0			[M+H]+1		212041,2	8,2	7,6
FALSO		Full match No results					173,0784		789306,5		0 0			[M+H]+1		659921,6	3	6,8
FALSO	C12 H26 N	Full match No results	No results	No match No	o results -0,48	359,1945	360,2018	7,133	5858879	1	0 0		No matche No matche No MS2	[M+H]+1	5858879		4	
FALSO	C52 H88 N; F	Full match No results	No results	No results No	o results -0,0	7 996,6133	499,3139	7,799	442615,8	0	0 0		No matche No matche No MS2	[M+2H]+2		442615,8		6,8
FALSO		Full match No results					330,1041		181049,4	1	0 0			[M+H]+1			7,6	7,6
		Full match No results					120,0656		219601,1	37	0 0			[M+H]+1		219601,1		5,4
FALSO	N-(2-Methoxybenzyl)-2-phenylpiperidin-3-ar C19 H24 N: F						297,1962		378361,8	26	0 0			[M+H]+1	369642,2	378361,8	7,1	6,5
FALSO		Full match No results					360,3625		553394,4		0 0			[M+H]+1		553394,4	4,7	7,4
FALSO	C4 H12 N2 F	Full match No results	No results	No results No	o results -1,19	9 312,0285	313,0358		417724	0	0 0			[M+H]+1	417724	326825,7	6,8	7,1
FALSO		Full match No results					166,0533		441994,9	7	0 0			[M+H]+1		368047,6	4,1	4,9
FALSO		No results No results					786,6081		219546	0	0 0			[M+H]+1		202908,2	7,1	7,1
FALSO		Full match No results					217,0682		289176		0 0			[M+H]+1			7,6	7,1
FALSO		No results No results					746,7827		202771,5		0 0			[M+H]+1			2,2	7,1
		Full match No results					158,1176		619215,2	42	0 0		No matche Single mate DDA for pre				4,1	5,8
FALSO		No results No results					633,8381		218023,4		0 0				218023,4		7,1	
FALSO		Full match No results					484,8087		181312,4	0	0 0			[M+H]+1		159281,5	8,2	7,6
FALSO		Full match No results					756,5831		155301,3		0 0			[M+H]+1		,	7,6	
FALSO		Full match No results					266,6097		1050396	0	0 0			[M+2H]+2			4,5	
	3-MeO-PCP C18 H27 N F	Full match No results	No results	Full match No	o results 0,:	1 273,2093	3 274,2166	6,18	419576,4	5	0 0		No matche No matche No MS2	[M+H]+1	364043	419576,4	7,1	5,8

Fig. Company			
Column C	103083,1		6,5
Column C			5
Fig. Company			7,6
Prop			
Column C			7,1
Column C			
Column	5,7 7,6 212711,4		7,1
Column C			6
March Column Co			4
Prop			4,7
March Marc			
Part	5,1 195508,7 7,6	7,6	7,6
1.55	84010,36		7,1
March Marc	555217,6		4,1
April Company Compan	6,8 500356,2 3	3	5,2
Prop.	716 6,5		
Company Comp	82121,24		5,4
March Property March Pro			
March Park			
Part	1,7 210130,3 1,3		7,1
April	176062,2 5.3 459934.3 6.8		7,1
April		-,-	7,1
March 1940			3,6
PASS Million			4,7
Second Column Col	.,,		-,,,
PAGE			5,8
Accordance Acc	7		5,2
March Marc		-	5,4
Fig. Column Column C			8,2
PASS C17712 C not much the month Neuroble 10-22 S 10-22			6,5
Column C	170353		7,6
MASC State March State		6,8	5,8
Fig. 50 Cart Continue Temporary Cart Continue Te			7,6
Mapper mit mode to NAZ Minist 1975 1			7,6
Fig. 12 Fig.			
FAST 1.55 Character 1.54 February 1.54			5,4
Margin Company Compa			
PASS PASS Description for enable for sensible for s	-,	3	6,8
Mary Assign Ass	184436,3 964 269503,1 3,3	2.2	6,5
PASS No. Frontain No. Secure Security Secu			5,4
FASD CLP9 CDIF Full materials becomes to be results New results Fast Supplied Fast S			7,1
FALSD Processing Non-control Non-con	306248		4,9
FALSD No remarks No remar	599767.5		5,2
FALSO No results No resul	237987		7,1
FALSO	162335,4		7,6
FALSD Polygoline			3,9
FALSD Commanded in Cost 445 M Fall match Cost 445 M Fall m			6,8
FALSD CLTYPOWNINE CS15111 No results for results for the marking for mar	8,7 360231,9 4,9	4,9	7,1
FALSD C4-19-score	7,4 378180,4 8,2	8,2	7,6
FALSD	995 339011,8 7,6	7,6	8,2
FALSO No results September S	541963,3		6,8
FALSD No results No results	-)-		
FALSO	263635,4		7,6
FALSO	158395,8		7,6
FALSO	183461,8	_	7,6
FASD 47-ID-RIBOX-1,13-TRIBECARDIAMINE CDIF42 N Full match No results Full match No results Full match CDIF42 N Full	-,		ь
FALSO		-	8,2
FALSO CA1114A Fall mark No results No			0,2
FALSO CS114 N4 Full match No results No resu	157462,2		7,6
FALSO C1.11.11.0 Full math No results No res		6,5	3,8
FALSO 4,5-Dihydro-6-methyl-3(2H)-pyridazinone CB 180,7 c gull match No results No result	215196,9		7,6
FALSO C59 H100 F Full match No results No results No results No results No results No results C35 H3 (2.56) 1.05 (2.56)	,18 7,6		
FALSO	208597,9		7,1
FALSO C38 H756 Full match No results	2,4 7,1		
FALSO No results No resul	417434,1		6,3
FALSO 1-(1Z-octadecenyl)-2-linoleoyl-sn-glycero-3-c C41178 N No results N			2,8
FALSO FALS			
FALSO Decylamine oxide C12 H27 N Full match No results No	186820,5		6,5
FALSO No results No resul			6.5
FALSO C9 H12 N3 Full match No results			6,5
FALSO N-(2,6-dioxopiperidin-3-yl)acetamide (7 H10 N2 Full match No results No			6,5
FALSO C5 H12 Cl4 Full match No results No re			4,1
FALSO No results No re			7,6
FALSO No results No resul			
FALSO C25 H47 N Full match No results No res	209422,3		7,1
FALSO C54 H90 N; Full match No results N			3,8
FALSO 4-[Methyl[(3R,AR)-4-methyl-1-propionyl-3-p] C16 H23 N Full match No results No res	432014,3		6,8
FALSO C10 (Full match No results	0,3 4,7		
FALSO C10 H3 C1 Full match No results No res			7,1
FALSO C5 H3 Br2 (Full match No results No re			
FALSO No results No re			4,5
FALSO Tridecylamine C13 H29 N Full match No results No			7,6
FALSO No results No re			7,1
			4,1
FALSO No results 269,2804 270,2877 1,51 80267,16 0 0 No matche No matche DDA for pri [M+H]+1 80267,16			2,7
IND IESUIG INDICATUR IND IESUIG INDICATUR IN	8,2	0,2	

FALSO	Pentane-1,5-dithiol	C5 H12 S2 Full match I	No results No results	Not the top No match	3,37	136,0385	137,0458	2,705	760614,8	12	0	0		Multiple m No matche No MS	2 [M+H]+1	760614,8		4,1	
FALSO		C8 H4 Cl N Full match 1	No results No results	No results No results	4,05	290,9265	291,9338	1,158	200211,8	0	0	0		No matche No matche No MS	2 [M+H]+1	200211,8		8,2	
FALSO	y-Acetylenic gaba	C6 H9 N O2 Full match 1	No results No results	Full match Full match	0.1	127.0633	128,0706	1.855	18972733	25	0	0		Multiple m Multiple m DDA fo	or pre [M+H]+1	18972733		4	
FALSO		C33 H76 CI Full match	No results No results	No results No results			794,5493		206485,2	0	0	0		No matche No matche No MS			206485.2		7,1
FALSO		C5 H6 N2 C Full match 1					175,0342			0	0	0		No matche No matche No MS		594435.7	618378,4	6,8	4,7
FALSO				Full match No results			270,8437	1,144	195144	1	0	0		No matche No matche DDA fo		195144		7,6	7.
FALSO				No results No results			364,1352		204217,7	0	0	0		No matche No matche No MS			200299.9	5,4	6,5
FALSO		C3 H N O9 Full match 1					227.9445		255990,1	0	0	0		No matche No matche No MS		255990,1	252469,7	7.6	7,6
FALSO		C6 H5 Cl Nt Full match 1					261.0127		244167,8	2	0	0		No matche No matche No MS		233330,1	244167,8	7,0	7,6
						,					0	0							
FALSO				No results No results			115,9641		190721,2	0	0	-		No matche No matche DDA fo		2405040	190721,2	7.4	6,5
FALSO				No results No results		,	136,9696		310594,8	0	0	0		No matche No matche No MS		310594,8	303515,2	7,1	6,5
FALSO		C23 H6 N2 Full match 1				358,0367			339440,8	2	0	0		No matche Single mati No MS			339440,8		4,9
FALSO		C4 H8 N2 C Full match 1				100,0637	- /-		75461,24	13	0	0		No matche No matche No MS			75461,24		5,4
FALSO		C6 H12 Cl Full match				367,9506				0	0	0		No matche No matche No MS			327275,4	4,3	3,3
FALSO				No results No results			749,6381		145135,9	0	0	0		No matche No matche No MS		145135,9		7,6	
FALSO	CHOLESTERYL ARACHIDATE	C47 H84 O. No results					681,6512			5	0	0		No matche No matche No MS			177500,8		7,1
FALSO				No results No results	- 1	638,6632	639,6705	1,137	162344,3	0	0	0		No matche No matche No MS	2 [M+H]+1		162344,3		7,6
FALSO		No results 1	No results No results	No results No results		73,96813	74,9754	0,96	238425,3	0	0	0		No matche No matche No MS	2 [M+H]+1		238425,3		7,1
FALSO	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		Multiple m No matche DDA fo	or pre [M+H]+1		180525,6		7,1
FALSO	Nicotinamide	C6 H6 N2 C Full match 1	No results No results	Full match Full match	0,29	122,0481	123,0553	2,523	1616961	11	0	0		Single mate No matche No MS	2 [M+H]+1	1616961	1472835	5	4,5
FALSO	Methyl 2,6-di-O-stearoyl-α-D-glucopyranosic	C43 H82 O No results 1	No results No results	Full match No results	-4,92	726,5974	727,6047	1,142	137783,4	7	0	0		No matche No matche No MS	2 [M+H]+1	131729,7	137783,4	7,6	7,1
FALSO		No results 1	No results No results	No results No results		487,6388	488,646	1,15	134696,2	0	0	0		No matche No matche No MS	2 [M+H]+1	134696,2		7,6	
FALSO		No results 1	No results No results	No results No results		735,6282	736,6355	1,136	178284,8	0	0	0		No matche No matche No MS	2 [M+H]+1		178284,8		6,5
FALSO		No results 1	No results No results	No results No results		775.8004	776,8077	1,092	186821,6	0	0	0		No matche No matche No MS	2 [M+H]+1	186821,6		7,1	
FALSO	Metalaxyl	C15 H21 N Full match N					280,1548		303891,3	21	0	0		No matche Multiple m No MS		,	303891,3		4,9
FALSO		C2 H7 O17 Full match 1					396,8968		337336,2	0	0	0		No matche No matche No MS		337336.2	333831	4.3	4,9
FALSO		C41 H58 N: Full match 1				687,4137			529372,4	2	0	0		No matche Multiple m DDA fo		449604,4	529372.4	7,4	6,8
FALSO				No results No results		245,7767	246,784		293694,5	0	0	0		No matche No matche No MS		293694,5		4,9	-,-
 FALSO		C6 H17 N4 Full match N					193,1222		229412,5	74	0	0		No matche Multiple m No MS				6,5	
FALSO	(10E,17E)-3,25-Dioxa-11,14,17,31-tetraazate						415,2116		475532.8	12	0	0		No matche Multiple m No MS			461485.7	4,7	6,8
FALSO	(100,170, 3,23 Dioxa 11,14,17,31-tetfdd2dte			No results No results			204,9185		148103.8	0	0	0		No matche No matche No MS			701403,7	7,6	0,0
 	Thalassospiramide R2								438543.6	0	0	0		No matche Single mati DDA fo			438543.6	7,0	5.8
FALSO	Thalassospiramide B2	C50 H79 N Full match No results					501,7916		438543,6 154895.6		0	0				•			5,8
FALSO				No results No results			637,6948 700.6027	,	, .	0	0	-		No matche No matche No MS		150000	154895,6	7.0	8,2
FALSO				No results No results		,			150393,8	0	0	0		No matche No matche No MS		150393,8		7,6	
FALSO		C30 H57 N: Full match					749,4087		929086,6	1	0	0		No matche No matche No MS			929086,6		5,5
FALSO		C6 H6 N2 C Full match					139,0503		390525,5	33	0	0		Multiple m Single mate No MS		339102,5	390525,5	7,6	3,3
FALSO		C9 H10 O3 Full match I			0,26	166,063	167,0703	1,537		112	3	0	54,3	Multiple m Multiple m DDA fo	or pro [M+H]+1	6413414	6551961	3,5	4
FALSO		C41 H65 O Full match					781,4288	8,101	580951	3	0	0		No matche No matche No MS		516655,9	580951	6,8	6,8
FALSO		C42 H86 N: Full match					397,3326	7,176	2826293	0	0	0		No matche No matche No MS	2 [M+2H]+2	2826293		4,2	
FALSO	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		Multiple m No matche DDA fo	or pre [M+H]+1		6784657		4
FALSO		C2 H3 N3 C Full match 1	No results No results	No results No results	-2,33	132,9943	134,0016	0,973	686234,1	0	0	0		No matche No matche No MS	2 [M+H]+1	218962	686234,1	6,5	0,9
FALSO		C H3 Br2 Cl Full match 1	No results No results	No results No results	3,24	559,5838	560,5911	1,175	212366,5	0	0	0		No matche No matche No MS	2 [M+H]+1	212366,5		8,2	
FALSO		C7 H15 O3 Full match 1	No results No results	No match No match	1,74	240,0238	241,0311	1,371	180019,4	5	0	0		Single mate No matche No MS	2 [M+H]+1	180019,4		6,5	
FALSO		C8 H20 N8 Full match 1	No results No results	No match No match	-0,72	354,108	355,1153	6,881	1635873	1	0	0		No matche Multiple m No MS	2 [M+H]+1	1635873		4,5	
FALSO	N-Acetyl-L-aspartic acid	C6 H9 N O5 Full match 1	No results No results	Full match Full match	0	175,0481	176,0554	1,981	461203,8	9	0	0		Multiple m No matche No MS	2 [M+H]+1	396377,6	461203,8	5,2	3,6
FALSO		No results 1	No results No results	No results No results		373,7201	374,7274	1,15	191401	0	0	0		No matche No matche No MS		191401		7,1	
FALSO				No results No results			469,8456		355657,9	0	0	0		No matche No matche No MS			355657.9	6,5	7,6
FALSO				No results No results			666,7424		206005,8	0	0	0		No matche No matche No MS		206005.8		7,1	
FALSO				No results No results			632,7237	1,134	168972	0	0	0		No matche No matche No MS		200003,0	168972	7,1	7,6
FALSO	afegostat	C6 H13 N C Full match 1					148.0969		592890,7	22	0	0		No matche No matche No MS		592890,7	492281.3	5.8	5,8
FALSO		C8 H Cl3 N4 Full match 1			-,-	,	498,8046		268696,2	0	0	0		No matche No matche No MS			239389	7,1	6,5
					0,48						0	0					239369		0,5
FALSO FALSO				No results No results			72,01008		131776,2	0	0	0		No matche No matche DDA fo		131776,2		7,6	
				No results No results		1520,625	761,32		190335,3	0	0	0		No matche No matche No MS		190335,3		7,1	
FALSO		C2 H3 Br N Full match 1			0,31	624,6617			159566,8	0	0	0		No matche No matche No MS			159566,8		7,6
FALSO				No results No results			328,8922		184362,8	0	0	0		No matche No matche No MS			184362,8		7,1
FALSO		C36 H71 N. Full match					742,5368		160996,2	39	0	0		No matche No matche No MS				7,1	
FALSO				No results No results		.,	420,9005			0	0	0		No matche No matche No MS			148306,8	7,1	7,6
 FALSO		C15 H13 N Full match					240,1019		281375,3	24	0	0		Single mate Multiple m No MS		279436,8		7,6	7,6
FALSO		C16 H35 N Full match N					242,2842		322758,9	6	0	0		No matche No matche No MS			322758,9		4,9
FALSO		C5 H9 O6 F Full match					99,01371	7,231		3	0	0		No matche No matche DDA fo		4045275	249806,1	3,7	6,5
 FALSO	[Similar to: N3,N4-Dimethyl-L-arginine; ΔMas						203,0526		269679,8	2	1	0	42,3	No matche No matche DDA fo			269679,8		6,5
FALSO		C17 H18 N. Full match					299,1391		409407,4	10	0	0		No matche Single mati No MS	2 [M+H]+1	360162,5	409407,4	6,5	6,8
FALSO	2-(4-Boc-piperazino)acetic acid	C11 H20 N: Full match	No results No results	Full match Partial mat	-,	,	245,1496	3,51	526216,3	7	0	0		No matche Multiple m No MS	2 [M+H]+1		349906,1	6,3	5,4
FALSO		C2 H4 N6 C Full match			_,-,		398,8613	1,197	201922	0	0	0		No matche No matche No MS		201922		7,6	
FALSO		C61 H110 Full match			-0,1	1307,714	654,8641	1,068	159705,8	0	0	0		No matche No matche No MS	2 [M+2H]+2	2	159705,8		8,2
FALSO	PYRIDOXAMINE	C8 H12 N2 Full match	No results No results	Full match Full match	0,26	168,0899	169,0972	3,778	391566,6	20	0	0		Single mate Multiple m DDA fo			391566,6		6,5
FALSO		No results 1	No results No results	No results No results		670,8408	671,8481	1,094	152898	0	0	0		No matche No matche No MS	2 [M+H]+1	152898	143352,5	7,1	7,6
FALSO		No results 1	No results No results	No results No results		697,6196	698,6268	1,143	131134,9	0	0	0		No matche No matche No MS	2 [M+H]+1	131134,9		7,1	
FALSO		No results 1	No results No results	No results No results		719,6522	720,6595	1,133	156240,8	0	0	0		No matche No matche No MS	2 [M+H]+1	156240,8		7,1	
FALSO	Skatole	C9 H9 N Full match N	No results No results	Full match Full match	0,85	131,0736	132,0809	4,13	233664,6	21	0	0		Multiple m No matche DDA fo	or pre [M+H]+1		233664,6		8,2
FALSO		No results 1	No results No results	No results No results			674,7059		133345,7	0	0	0		No matche No matche No MS			133345,7		7,6
FALSO		C9 H3 N6 C Full match	No results No results	No match No results	2,27	367,9031	368,9104		218116,1	1	0	0		No matche No matche No MS				7,1	
FALSO		C5 H7 N7 C Full match					182,0788		275878,2	1	0	0		No matche No matche DDA fo			275878,2	7,6	7,6
		C6 H12 N2 Full match N					145,0971		377159,8	13	0	0		Single mate No matche DDA fo				4,3	6,5
FALSO		C8 H17 N C Full match					256,1026		316429	0	0	0		No matche No matche No MS			316429		6
FALSO		C32 H76 CI Full match					716,5341		179977,7	0	0	0		No matche No matche No MS				7,1	
FALSO		C7 H22 Cl f Full match f					402,0516		152355,2	0	0	0		No matche No matche No MS			129663.8	4,9	7,6
FALSO		C11 H25 N Full match					282,1198		1263113	9	0	0		Multiple m Single mati No MS			1263113	.,5	5
FALSO				No results No results			747,5966		136270,8	0	0	0		No matche No matche No MS			136270,8		7,6
	Geranyl butyrate	C14 H24 O. Full match					225,1849		5053370	41	0	0		No matche Multiple m No MS			5053370		4,8
									1193067		0	0						0,7	
		C5 H11 N C Full match N					102,0914			31	-	-		Multiple m Single mate DDA for No matche No matche No MS					6,5
FALSO		C66 H79 N Full match 1					348,1911		323520,2	1	0	0						3,8	5,4
	amfepentorex	C15 H25 N Full match N			-7.5		220,206		756342,4	3	0	0		No matche No matche No MS			/52416,6	4,1	4,7
FALSO				No results No results			468,6364		228304,9	0	0	0		No matche No matche No MS		228304,9	450650	7,6	7.0
FALSO				No results No results			566,8283		159659,4	0	0	0		No matche No matche DDA fo			159659,4	7,6	7,1
FALSO				No results No results			591,7412		131989,9	0	0	0		No matche No matche No MS		131989,9		7,1	8,2
FALSO		C27 H34 O Full match					455,2251		3950514	1	0	0		No matche No matche No MS		3111258		4,8	4,2
FALSO		C5 H13 N3 Full match					228,0301		344997,7	0	0	0		No matche No matche No MS		313449,7		7,1	6,5
		C9 H16 N4 No results N					229,1294		236428,1	3	0	0		Single mate Single mate No MS			236428,1		4,9
		C12 H23 N Full match N					214,1801	6,955	843516	4	0	0		No matche No matche DDA fo		820032,5	843516	4,1	4,5
FALSO		C13 H25 N: Full match	No results No results	No results No results	-4,23	299,1945	300,2018	4,225	286443	0	0	0		No matche No matche No MS	2 [M+H]+1		286443		6,5

	ethylene adipate	C8 H12 O4 Full match No results No results		-7-	172,0735 173,080	. ,,	35 0 0	No matche Multiple m DDA for pri [M+H]+1 74320,29 368779,1 8,2 0,5
FALSO		C4 H12 N3 Full match No results No results			181,0619 182,069	.,	0 0 0	No matche No matche No MS2 [M+H]+1 283351,9 7,6
FALSO		No results No results No results			531,3165 532,323		0 0 0	No matche No matche No MS2 [M+H]+1 99737,15 4,9
FALSO		C6 H9 N4 P Full match No results No results		-0,69	230,0039 231,011		1 0 0	No matche No matche DDA for pri [M+H]+1 326422,5 343366,7 7,1 4,3
FALSO FALSO	N (2 I/C Chlore 2 I/2 method: 4 /4 method:	No results No results No results 1 C25 H27 Cl No results No results No results		2.75	667,8313 668,838 494,1852 495,192		0 0 0	No matche No matche No MS2 [M+H]+1 165853,7 7,1 No matche No matche No MS2 [M+H]+1 341401,1 4,3
FALSO	N-{3-[(3-CHI010-2-{[2-Hethoxy-4-(4-Hethyl-	No results No results No results		_	684.6168 685.624		0 0 0	No matche No matche No MS2 [M+H]+1 341401,1 4,3 No matche No matche No MS2 [M+H]+1 149185,9 7,1
FALSO		No results No results No results			489,6366 490,643		0 0 0	No matche No matche No MS2 [M+H]+1 161480,7 7,1
FALSO		No results No results No results			607,7081 608,715		0 0 0	No matche No matche No MS2 [M+H]+1 145392,2 8,2
FALSO		C5 H9 N3 C Full match No results No results		-0,85	335,0082 336,015	4 1,148 108948,8	1 0 0	No matche No matche No MS2 [M+H]+1 108948,8 8,2
FALSO		No results No results No results	No results No results		1259,644 630,829	4 1,061 142386,7	0 0 0	No matche No matche No MS2 [M+2H]+2 142386,7 7,1
FALSO	Cyclopentenone	C5 H6 O Full match No results No results	Full match No results	0,65	82,04192 83,0491	9 1,783 8589948	9 0 0	No matche No matche DDA for pri [M+H]+1 8589948 4
FALSO		No results No results No results			191,0871 192,094	.,	0 0 0	No matche No matche No MS2 [M+H]+1 96081,06 6
FALSO		No results No results No results			1279,693 640,853		0 0 0	No matche No matche No MS2 [M+2H]+2 214111 6,5
FALSO FALSO		No results No results No results C7 H8 Cl3 I Full match No results No results			349,2101 350,217 336,8982 337,905		0 0 0	No matche No matche No MS2 [M+H]+1 2210250 4,2 No matche No matche No MS2 [M+H]+1 221377,1 7,1
FALSO		No results No results No results		-3,/3	550,8386 551,845		0 0 0	No matche No matche No MS2 [M+H]+1 221577,1 7,1 No matche No matche No MS2 [M+H]+1 143208,8 7,1
	N-Crotonyl-g-Ethylaminobutyric Acid Diethy	C14 H26 N. Full match No results No results		0.26	254,1995 255,206		1 0 0	No matche No matche No MS2 [M+H]+1 572977,7 5,8
FALSO	, , ,	C3 H12 N6 Full match No results No results		-,	196,0736 197,080		89 0 0	Multiple m Multiple m No MS2 [M+H]+1 118684 7,1
FALSO	(2E)-2-Cyano-N-(ethylcarbamoyl)-2-(methox	C7 H10 N4 Full match No results No results	Full match Full match	0,15	198,0753 199,082	6 3,333 463495,5	6 0 0	Single mati No matche DDA for pri [M+H]+1 432863,5 463495,5 6,3 5,2
FALSO		C85 H179 Full match No results No results		-0,03	1413,296 707,655		0 0 0	No matche No matche No MS2 [M+2H]+2 128736,5 7,1
	Dyphylline	C10 H14 N Full match No results No results		-4,93	254,1003 255,107		10 0 0	Multiple m Single mat (No MS2 [M+H]+1 227407,5 261984,7 7,1 7,1
FALSO		No results No results No results			581,7465 582,753		0 0 0	No matche No matche DDA for pr [M+H]+1 140418,2 7,6
FALSO FALSO	(1Z,5Z)-1,5-Cyclooctadiene	C8 H12 Full match No results No results No results No results No results		0,11	108,0939 109,101 1551,599 776,806		0 0 0	No matche Single mati No MS2 [M+H]+1 10421699 4 No matche No matche No MS2 [M+2H]+2 194852,3 6,5
FALSO		No results No results No results			198,1189 199,126		0 0 0	No matche No matche No MS2 [M+2H]+2 194852,3 6,5 No matche No matche DDA for pri [M+H]+1 2445489 4,8
FALSO		C5 H8 N Of Full match No results No results		1.51	193,0143 97,5144		0 0 0	No matche No matche No MS2 [M+2H]+2 442476,1 4,1
FALSO		C3 H11 N6 Full match No results No results			354,0178 355,025		3 0 0	No matche No matche DDA for pri [M+H]+1 874731,7 2344517 5,5 1
FALSO		No results No results No results	No results No results		704,6076 705,614		0 0 0	No matche No matche No MS2 [M+H]+1 117715,4 7,1
FALSO	Caffeine	C8 H10 N4 Full match No results No results		0,21	194,0804 195,087		7 0 0	Single mati Single mati No MS2 [M+H]+1 336488,9 6
FALSO		No results No results No results			721,5825 722,589		0 0 0	No matche No matche No MS2 [M+H]+1 107881,9 8,2
FALSO		No results No results No results			658,6081 659,615		0 0 0	No matche No ms2 [M+H]+1 142694 7,6
	Mesitol	C9 H12 O Full match No results No results C10 H7 N C Full match No results No results			136,0889 137,096	7	70 0 0	No matche Single mat (No MS2 [M+H]+1 136623,6 6,5
FALSO FALSO	Kynurenic acid 2,3-dinor-8-epi-prostaglandin F2α	C10 H7 N C Full match No results No results C18 H30 O: Full match No results No results		0,14	189,0426 190,049 326,2094 327,216	3 1,110 1,1321,1	19 0 0	Multiple m Multiple m No MS2 [M+H]+1 456269,3 471924,1 6,3 4,7 No matche Multiple m No MS2 [M+H]+1 3488405 3648842 3,7 4,2
FALSO		C5 H7 N O2 No results No results No results			145.0198 146.027		3 0 0	Single mat(No matche No MS2 [M+H]+1 383008 405866,9 3,8 5,2
FALSO	3-ETHTE-2-THIOXO-4-OXAZOLIDINONE	C37 H80 Ni Full match No results No results		-1.6	730,569 731,576		0 0 0	No matche Single mati No MS2 [M+H]+1 148307,6 7,6
FALSO		No results No results No results		-/-	1245,371 623,692		0 0 0	No matche No matche No MS2 [M+2H]+2 177489,1 7,1
FALSO		C6 H3 N O Full match No results No results	No results No results	0,69	105,0215 106,028		0 0 0	No matche No matche No MS2 [M+H]+1 122524,2 84577,14 0,5 5,4
FALSO		No results No results No results	No results No results		79,53243 80,539	7 0,973 128351,1	0 0 0	No matche No mS2 [M+H]+1 128351,1 4,3
FALSO	N-boc-1-azacyclopentan-2-one	C9 H15 N C Full match No results No results		0,01	185,1052 186,112		23 0 0	Multiple m No matche No MS2 [M+H]+1 612506,7 484150,3 4,7 5,2
FALSO	2,6-Dimethylquinoline	C11 H11 N Full match No results No results		-,	157,0892 158,096		26 0 0	No matche No matche DDA for pri [M+H]+1 1360771 1328972 3,9 5
FALSO		C17 H30 O Full match No results No results		-2,5			11 0 0	No matche Multiple m DDA for pri [M+H]+1 7253694 4
FALSO FALSO	4-(1-Carboxyethyl)-3-hydroxy-2-(3-methyl-2 EDDA	C20 H26 O Full match No results No results C6 H12 N2 Full match No results No results			426,1527 427,1 176,0798 177,087		1 0 0 13 0 0	No matche Multiple m No MS2 [M+H]+1 347230,4 513013 7,6 5,8 No matche No matche No MS2 [M+H]+1 224712,6 269638,1 7,1 4,3
FALSO		C10 H17 N Full match No results No results			247,0878 248,095		1 0 0	No matche No matche No MS2 [M+H]+1 224712,6 269638,1 7,1 4,3 No matche No matche No MS2 [M+H]+1 268940,1 259879,4 7,6 7,6
FALSO		C5 H6 N9 C Full match No results No results			239,0431 240,050		9 0 0	No matche No matche No MS2 [M+H]+1 548389,3 523891,1 5,2 5,8
FALSO		No results No results No results	No results No results		535,5698 536,57		0 0 0	No matche No matche No MS2 [M+H]+1 241049 7,6
FALSO		No results No results No results	No results No results		1459,595 730,804	9 1,055 170072,4	0 0 0	No matche No matche No MS2 [M+2H]+2 170072,4 4,3
FALSO		C4 H9 Br N Full match No results No results	No results No results	0,93	534,866 535,873	2 1,093 196586,3	0 0 0	No matche No matche No MS2 [M+H]+1 196586,3 7,1
FALSO		No results No results No results			653,4847 654,49		0 0 0	No matche No matche No MS2 [M+H]+1 173683,8 181910,8 7,1 7,1
FALSO		No results No results No results			1595,638 798,826		0 0 0	No matche No matche No MS2 [M+2H]+2 187745,7 7,6
FALSO FALSO		No results No results No results C4 H8 N6 C Full match No results No results			83,90404 84,9113		0 0 0	No matche No matche DDA for pr [M+H]+1 283698,8 333219 4,3 4,9 No matche No matche No MS2 [M+H]+1 303904.2 283571.7 3.8 4.3
FALSO		C2 H6 Cl2 I Full match No results No results		-1.69	220,0562 221,063 284,896 285,903		0 0 0	No matche No matche No MS2 [M+H]+1 303904,2 283571,7 3,8 4,3 No matche No matche No MS2 [M+H]+1 212415,3 7,1
FALSO		No results No results No results		-,	134,9698 135,977		0 0 0	No matche No matche No MS2 [M+H]+1 130150,9 129377,1 7,6 7,6
FALSO		No results No results No results			117,0641 118,071		0 0 0	No matche No matche DDA for pri [M+H]+1 154088,4 7,6
FALSO		No results No results No results	No results No results		640,7038 641,711		0 0 0	No matche No matche No MS2 [M+H]+1 154680,5 7,1
FALSO		C12 H22 N Full match No results No results	No match No results	3,82	259,117 260,124	2 1,65 416659,2	12 0 0	No matche No mS2 [M+H]+1 376918,2 416659,2 7,1 6,3
FALSO		No results No results No results			770,7736 771,780		0 0 0	No matche No matche No MS2 [M+H]+1 196673,2 4,9
FALSO	2,2'-(Hexadecylimino)diethanol	C20 H43 N Full match No results No results		-,	329,3293 330,336		1 0 0	No matche No matche No MS2 [M+H]+1 358611,4 6
FALSO		C4 H3 Cl Nt Full match No results No results	140 materi 140 results	0,47	249,95 250,957		1 0 0	No matche No matche No MS2 [M+H]+1 238235,2 230350,7 7,1 7,6
FALSO FALSO		C5 H16 N5 Full match No results No results No results No results No results		2,34	273,0845 274,091 1537.61 769.812	7	1 0 0	No matche No matche No MS2 [M+H]+1 321219,9 4,9 No matche No matche No MS2 [M+2H]+2 131849,5 7,6
FALSO	12-Aminolauric Acid	C12 H25 N Full match No results No results		0.08	215,1886 216,195		10 0 0	No matche No matche No MS2 [M+2h]+2 131849,3 7,6 7,6 7,6 7,6 7,6 7,6 7,6 7,6 7,6 7,6
FALSO		No results No results No results		,,,,	656,6789 657,686	,	0 0 0	No matche No matche No MS2 [M+H]+1 131840,1 7,1
FALSO		C2 H7 O14 Full match No results No results		1,5	317,9299 318,937		2 0 0	No matche No matche No MS2 [M+H]+1 233199,4 7,1
FALSO		No results No results No results	No results No results		88,49949 89,5067	7 0,959 162258	0 0 0	No matche No matche No MS2 [M+H]+1 162258 4,3
FALSO		No results No results No results			112,0238 113,031		0 0 0	No matche No matche No MS2 [M+H]+1 102719,2 7,6
FALSO		No results No results No results			681,7902 682,797		0 0 0	No matche No matche No MS2 [M+H]+1 143820,9 7,1
FALSO		No results No results No results			1262,724 632,369		0 0 0	No matche No matche No MS2 [M+2H]+2 272007,1 6,5
FALSO	5-Indolol	C13 H17 P Full match No results No results C8 H7 N O Full match No results No results			236,0797 237,08 133,0528 134,060		7 0 0 20 0 0	Multiple m Single mati DDA for pri [M+H]+1 336231,9 371067,2 4,3 6,5 Multiple m Multiple m DDA for pri [M+H]+1 343566,8 324983,4 6,5 7,6
FALSO	J-IIIGOIDI	C H3 Br2 Cl Full match No results No results			427,6842 428,691		0 0 0	Multiple m Multiple m DDA for pri [M+H]+1 343566,8 324983,4 6,5 7,6 No matche No matche No MS2 [M+H]+1 183531 184479,7 7,1 7,6
FALSO		No results No results No results			179,6068 180,614		0 0 0	No matche No matche No MS2 [M+H]+1 155331 184479,7 7,1 7,6
FALSO		C9 H19 N4 Full match No results No results			294,108 295,115		3 0 0	No matche No matche No MS2 [M+H]+1 748316,4 912439,7 4,7 4,5
FALSO		No results No results No results	No results No results		674,8112 675,818	5 1,065 152578,7	0 0 0	No matche No mS2 [M+H]+1 152578,7 7,1
FALSO		C2 H N7 O1 Full match No results No results			408,9049 409,912		0 0 0	No matche No matche No MS2 [M+H]+1 146556,6 4,3
FALSO		C2 H8 Br Cl Full match No results No results			715,6153 716,622		0 0 0	No matche No matche No MS2 [M+H]+1 138425,9 7,6
FALSO		C13 H13 N Full match No results No results			311,1231 312,130		3 0 0	No matche Single mat (No MS2 [M+H]+1 235194,2 7,6
FALSO FALSO		C10 H25 N- Full match No results No results		4,15	280,1676 281,174		21 0 0 0 0 0	No matche Multiple m No MS2 [M+H]+1 282596,8 5,4
FALSO		No results No results No results C19 H38 N. Full match No results No results		-0.94	715,57 716,577 387,247 388,254		0 0 0	No matche No matche No MS2 [M+H]+1 127291,5 7,6 No matche No matche No MS2 [M+H]+1 303169,4 6
FALSO		No results No results No results			387,247 388,254 558,8266 559,833		0 0 0	No matche No matche No MS2 [M+H]+1 303169,4 6 No matche No matche No MS2 [M+H]+1 274853,7 180994,7 0 7,1
	Solvent Green 3	C28 H22 N. No results No results No results			418,17 419,177		7 0 0	No matche No matche No MS2 [M+H]+1 2/4853,7 180994,7 0 7,1 No matche No matche No MS2 [M+H]+1 156477,5 4,9
	Heptenal	C7 H12 O Full match No results No results			112,0889 113,096		51 0 0	No matche Single mat. No MS2 [M+H]+1 649406,2 553877,5 4,1 6,3
FALSO		C26 H41 Cl Full match No results No results			433,2673 434,274		0 0 0	No matche Single mat (No MS2 [M+H]+1 3691076 4,2
FALSO		C8 H13 N4 Full match No results No results		-3,33	196,0871 197,094		2 0 0	No matche No matche DDA for pri [M+H]+1 257069 6
FALSO		C7 H11 N7 Full match No results No results			225,098 226,105		0 0 0	No matche No matche No MS2 [M+H]+1 148543,1 6,5
FALSO		C3 H Cl2 N Full match No results No results			481,8234 482,830		0 0 0	No matche No matche No MS2 [M+H]+1 229563,6 7,1
FALSO		C18 H35 N Full match No results No results	No results No results	3,97	343,2208 344,22	8 4,395 336680,1	0 0 0	No matche No matche No MS2 [M+H]+1 336680,1 5,4

FALSO			atch No results No res			-,	,	322,0769	-, -	342282,3	7	0	0	No matche No matche No MS2			342282,3		5,4
FALSO			atch No results No res			4,41	546,2117			449702,8	1	0	0	No matche Multiple m No MS2		449702,8		5,8	4,1
FALSO			ults No results No res				700,5925	,		127979,5	0	0	0	No matche No matche No MS2	[M+H]+1		127979,5		7,6
FALSO			ults No results No res				609,6838			141558,6	0	0	0	No matche No matche No MS2	[M+H]+1		141558,6		7,1
FALSO FALSO	Benzaldehyde		atch No results No res			0,21	106,0419 117,0659		3,682	2211094 88846,21	0	0	0	Multiple m No matche No MS2 No matche No matche DDA for			1714479 88846.21	4,2	3,9 4,9
FALSO			ults No results No res				690.8592			158386,1	0	0	0	No matche No matche DDA 101		158386.1	00040,21	7.6	4,9
FALSO			ults No results No res				705.6072	,		133711,8	0	0	0	No matche No matche No MS2		133711,8		7,0	
	Glutaric acid		atch No results No res			-0.27		133.0495		163436.1	23	0	0	Multiple m No matche No MS2			163436,1	,,_	7,1
FALSO			atch No results No res			-3.24	304.0785	305,0857	3,591	280028.1	5	0	0	No matche No matche No MS2			280028,1		7,6
FALSO	Lipovelutibol A	C38 H69 N No res	ults No results No res	ults No results	Full match	4,54	783,5142	784,5214	1,145	157678,5	0	0	0	No matche Single mati No MS2	[M+H]+1		157678,5		7,1
FALSO		No res	ults No results No res	ults No results	No results		623,6838	624,6911	1,135	134138,9	0	0	0	No matche No matche No MS2	[M+H]+1		134138,9		7,6
FALSO		C7 H16 O5 Full ma	atch No results No res	ults No match	No results	-2,74	242,0466	243,0539	0,982	135386,5	6	0	0	No matche No matche No MS2	[M+H]+1		135386,5		4,3
FALSO			atch No results No res			-0,5	449,3717			408058,7	0	0	0	No matche No matche No MS2	[M+H]+1	400154,6		6,8	7,4
FALSO			ults No results No res				580,8171			98441,26	0	0	0	No matche No matche No MS2			98441,26		4,9
FALSO			atch No results No res				428,1068		1,92		1	0	0	No matche Single mati No MS2		432049	,	7,4	4,9
FALSO			atch No results No res atch No results No res			-0,91 0.64	359,8946 195,041			261726,7 143833,2	2	0	0	No matche No matche No MS2 No matche No matche No MS2		259809,3 143833,2	261726,7	7,1 7,1	6
FALSO			atch No results No res			-,		645,1272	1,151	207548	0	0	0	No matche No matche No MS2		207548		7,1	
FALSO			ults No results No res			0,43	239.1733		3,784		0	0	0	No matche No matche No MS2		207340	381743	7,1	4,9
FALSO			atch No results No res			3.53		334.1399	4,569		13	0	0	No matche No matche No MS2			245908		7,6
FALSO		No res	ults No results No res	ults No results	No results		679,3253	680,3326	1,083	221154,1	0	0	0	No matche No matche No MS2	[M+H]+1		221154,1		6
FALSO		C45 H74 N Full ma	atch No results No res	ults No results	No results	-1,13	714,5916	715,5989	1,146	162814,7	0	0	0	No matche No matche No MS2	[M+H]+1	162814,7		7,1	
FALSO			atch No results No res			3,88	403,8923			206300,7	0	0	0	No matche No matche No MS2			206300,7		7,1
FALSO			ults No results No res				525,5875	,		238838,7	0	0	0	No matche No matche No MS2	[M+H]+1	238838,7	192986,4	4,3	7,6
FALSO			atch No results No res			-3,49	264,0017			331355,9	1	0	0	No matche No matche DDA for		331355,9	220262 =	7,1	
FALSO FALSO			ults No results No res atch No results No res			2.54	611,8331 408,0121			229262,5 642396,2	0	0	0	No matche No matche No MS2 No matche No matche No MS2	[M+H]+1 [M+H]+1		229262,5 642396,2		4,7
			atch No results No res				288,1111			302342,2	6	0	0	No matche Multiple m No MS2			302342,2	7,1	4,7
FALSO			ults No results No res			5,23	613,585			156652,3	0	0	0	No matche No matche No MS2		156652,3	JULU 12,2	7,1	.,,5
	3-Methylglutarylcarnitine		atch No results No res			0,22	289,1526			1155071	4	0	0	No matche No matche No MS2	[M+H]+1	1155071	1018887	3,4	4,5
			atch No results No res				123,0797		7,452	68977,25	13	0	0	No matche No matche No MS2		68977,25		8,2	
FALSO		C2 H7 N2 P Full ma	atch No results No res	ults No match	No results	-3,19	183,9537		0,31	744716,8	1	0	0	No matche No matche No MS2		744716,8		4,1	
FALSO			atch No results No res				431,2732		4,664	300947	1	0	0	No matche No matche No MS2		269408,7	300947	6	5,4
FALSO			atch No results No res			-2,41	169,082		7,135		3	0	0	No matche No matche DDA for		8752416		4	
FALSO	N-Acetyl-L-aspartic acid		atch No results No res			0,49		176,0554		386488,8	9	0	0	Multiple m No matche No MS2			386488,8		4,9
FALSO			ults No results No res					711,7814		119191,3	0	0	0	No matche No matche No MS2		119191,3		7,6	
FALSO FALSO	Erucamide		atch No results No res			0,16	423,7563	338,3418 424.7636		693783,5 185891,5	0	0	0	No matche No matche No MS2 No matche No matche No MS2	[M+H]+1	185891.5	693783,5	7.1	7,4
FALSO			atch No results No res			3 68		410.9167		270440,5	1	0	0	No matche No matche No MS2			270440,5	7,1	6,5
FALSO			atch No results No res			-,	181.0357			185837,7	0	0	0	No matche No matche No MS2			270440,3	6,5	0,5
			ults No results No res			.,==		246.1448		181760,6	9	0	0	No matche No matche No MS2	[M+H]+1		181760.6	0,5	7,6
			ults No results No res			4,23	247,0887	248,096		148336,2	2	0	0	No matche No matche No MS2	[M+H]+1	148336,2		6	
FALSO		No res	ults No results No res	ults No results	No results		383,7489	384,7561	1,143	174291,1	0	0	0	No matche No matche No MS2	[M+H]+1		174291,1		7,1
FALSO		C4 H Br Cl I Full ma	atch No results No res	ults No results	No results	-4,15	471,687	472,6943	1,18	314713,1	0	0	0	No matche No matche No MS2	[M+H]+1	314713,1	272392,3	4,3	4,3
FALSO			ults No results No res					108,5219	0,98		0	0	0	No matche No matche No MS2			323556		4,3
FALSO			ults No results No res					132,0826		200862,3	0	0	0	No matche No matche DDA for		200862,3		4,9	
FALSO			ults No results No res			2.40	769,5372			144964,5	0 4	0	0	No matche No matche No MS2		144964,5	256245.6	7,6	-
FALSO			atch No results No res			2,49		204,0895 324.8007		256245,6 161837.1	0	0	0	No matche Multiple m No MS2 No matche No matche No MS2	[M+2H]+2 [M+H]+1		161837.1		7,1
FALSO			atch No results No res			1.46	,	226,0379	-,	146233,6	1	0	0	No matche No matche No MS2	[M+H]+1		146233,6		8,2
FALSO			atch No results No res				230,0539			297257,5	0	0	0	No matche No matche No MS2		297257,5	140233,0	7,1	0,2
FALSO			atch No results No res				603,5662			158968,3	0	0	0	No matche No matche No MS2	[M+H]+1		158968,3	.,_	7,1
FALSO		C3 H Cl2 N Full ma	atch No results No res	ults No results	No results	-0,1	280,8977	281,905	1,166	183045,3	0	0	0	No matche No matche No MS2	[M+H]+1	183045,3		8,2	
FALSO		No res	ults No results No res	ults No results	No results		145,0457	146,0529	1,384	196015,1	0	0	0	No matche No matche No MS2	[M+H]+1	196015,1		6,5	
			atch No results No res				197,0801			263678,8	11	0	0	Single mate No matche No MS2		235058,6	263678,8	3,8	7,6
FALSO			atch No results No res			4,55		313,0183	1,166	210646	0	0	0	No matche No matche No MS2		210646		4,9	
FALSO			ults No results No res				. ,	738,5662	1,141		0	0	0	No matche No matche No MS2			131861		7,6
FALSO			atch No results No res			4,57		197,1285		300750,3	9	0	0	No matche Multiple m No MS2		287967,6		6	4,9
FALSO FALSO			ults No results No res atch No results No res			3 80	80,50539 339 8954	81,51266 340.9027		120034,2 166090,6	0	0	0	No matche No matche DDA for No matche No matche No MS2	pr([M+H]+1 [M+H]+1		120034,2 166090,6		6,5 7,6
FALSO			ults No results No res			3,03	409,6703	,	1,195	186617	0	0	0	No matche No matche No MS2	[M+H]+1		186617		8,2
FALSO	sulfacarbamide		atch No results No res			4.59	,.	216,0447	_,	424192,4	3	0	0	No matche No matche No MS2		407305,5		7,4	5,8
FALSO			atch No results No res				70,04189			222879,3	13	0	0	No matche No matche No MS2	[M+H]+1		222879,3	-,-	6,5
FALSO		C H3 Cl N5 Full ma	atch No results No res	ults No results	No results	2,2	340,8535	341,8608		184065,7	0	0	0	No matche No matche No MS2	[M+H]+1	184065,7	181365,5	4,3	7,6
FALSO	n-butyl methacrylate		atch No results No res			0,13	142,0994		7,21	2405368	98	0	0	No matche Single mati No MS2		2405368		4,8	
FALSO			ults No results No res				528,8794	,	1,093	186373	0	0	0	No matche No matche No MS2		186373		6,5	
FALSO			ults No results No res					738,5892		165889,5	0	0	0	No matche No matche No MS2			165889,5		7,1
	Dibenzylamine		ults No results No res			0,03		198,1277	-,	363214,6	16	0	0	No matche No matche No MS2		363214,6	102050.2	6	0.2
FALSO FALSO			ults No results No res atch No results No res			0.10		630,6394 373,9165		102656,3 158559,7	0	0	0	No matche No matche No MS2 No matche No matche No MS2			102656,3	7,1	8,2
FALSO			ults No results No res			0,18		742,6498		110705,2	0	0	0	No matche No matche No MS2				8,2	
FALSO			atch No results No res			2.88		226,1054		403042,8	0	0	0	No matche No matche No MS2			403042,8	3,2	5,2
			atch No results No res					211,1441		294465,3	10	0	0	No matche Multiple m No MS2			294465,3		6,5
FALSO		C3 H9 Cl N4 Full ma	atch No results No res	ults No results	No results			328,9989		203745,5	0	0	0	No matche No matche No MS2				4,9	
FALSO			atch No results No res					220,1177		200978,4	4	0	0	Single mate No matche No MS2			200978,4		6
	1-{[2-(4-Chlorophenyl)-4,4-dimethyl-1-cyclol							319,1946		1432221	2	0	0	No matche No matche No MS2		1432221		4,5	
	4-{Methyl[(3R,4R)-4-methyl-1-propionyl-3-pi							318,1913		536583,4	3	0	0	No matche No matche No MS2			536583,4		6,3
	1-Boc-4-Cyanopiperidine		atch No results No res					211,1442		333951,4	10	0	0	No matche Multiple m No MS2			333951,4		8,2
FALSO FALSO			atch No results No res			-0,08		331,9319 232,8071		150163,3 283387,9	0	0	0	No matche No matche No MS2 No matche No matche DDA for			150163,3	7,1	7,6
FALSO			atch No results No res			0.26		328,2306		283387,9	0	0	0	No matche No matche No MS2			291212,8	7,1	6,5
FALSO			ults No results No res			5,20		350,7217		255148,1	0	0	0	No matche No matche No MS2		255148,1		7,1	3,3
FALSO	Leu-Leu		atch No results No res			0,15	244,1787			274172,7	11	0	0	Single mate No matche No MS2			274172,7	7,1	7,1
			ults No results No res					454,0935		269265,8	0	0	0	No matche Single mati No MS2				7,1	7,1
FALSO			atch No results No res					384,2745	6,662	312093	1	0	0	No matche Single mati No MS2		312093		7,1	
FALSO			ults No results No res					494,6466		151948,2	0	0	0	No matche No matche No MS2			151948,2		7,6
FALSO			atch No results No res					716,3297		209285,5	0	0	0	No matche Single mati No MS2			209285,5		7,1
	· ·		atch No results No res					186,0762		541093,9	5	0	0	No matche Multiple m No MS2			427467.0	4,7	4.7
	EDDA		atch No results No res			0,04	176,0797			437497,2	13	0	0	No matche No matche No MS2			437497,2	7.1	4,7
FALSO		No res	ults No results No res	uits INO results	INO TESUITS		433,0805	436,6878	1,1/6	208008,8	0	U	0	No matche No matche No MS2	[[IVI+H]+1	208008,8		7,1	

FALSO		No results No resu	ults 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]+2	157966,1		7,1	
FALSO	1	No results No resi	ults 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]+1	115752,5		8,2	
FALSO Triallyl phosphite	C9 H15 O3 I	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 pro	[M+H]+1		137053,7		4,3
FALSO	1	No results No resu	ults 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]+2	165216,4		7,1	
FALSO	C3 H4 N4 C	Full match No resi	ults 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]+1	62374,88		8,2	
FALSO	1	No results No resu	ults 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]+1		101668,1		8,2
FALSO	C3 H6 N4 C	Full match No resi	ults 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]+2	795525,6		4,7	
FALSO	C5 H N6 P	Full match No resi	ults 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 pro	[M+H]+1		252278,6		6,5
FALSO Boc-Gly-ONp	C13 H16 N	No results No resu	ults No results	Full match Full match	0,96	296,1011	297,1084	1,573	78071,36	12	0	0		Single mate Multiple m No MS2	[M+H]+1	78071,36		4,9	
FALSO		No results No resi	ults 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]+2		182882,2		7,1
FALSO Dibenzylhydroxylamine	C14 H15 N	Full match No resi	ults 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]+1		282940,1		6
FALSO	C8 H22 Br I I	Full match No resi	ults 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]+1	331263,9		4,3	
FALSO	1	No results No resu	ults 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]+1		219575,4		5,4
FALSO	C9 H15 N6 I	Full match No resi	ults 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]+1	530687,1		4,1	
FALSO	C11 H21 CI I	Full match No resi	ults 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]+2	130084,1		6	
FALSO	C44 H81 N	Full match No resi	ults 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]+1		131337,4		7,1
FALSO	1	No results No resu	ults 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]+2	186476,8		7,1	
FALSO	C3 H2 CI N! I	Full match No resi	ults 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]+1		178109,2		7,1
FALSO	C14 H39 N	Full match No resi	ults 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]+1		2834697		4,2
FALSO (2-Dodecen-1-yl)succinic anhydride	C16 H26 O	Full match No resi	ults 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]+1	2078939		4,2	
FALSO slaframine	C10 H18 N	Full match No resi	ults 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]+1		541879,4		7,4
FALSO	C28 H41 N	Full match No resi	ults 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]+1		424056,9		6,8
FALSO chlorphthalidone	C8 H3 CI O: I	No results No resi	ults 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]+1		134505,4		4,3