Compound Discovery Report

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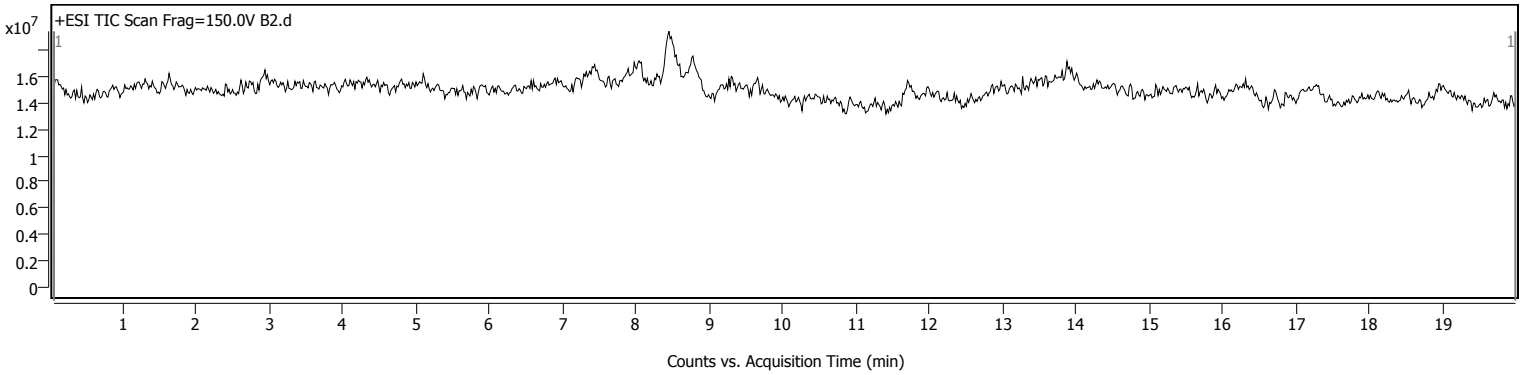
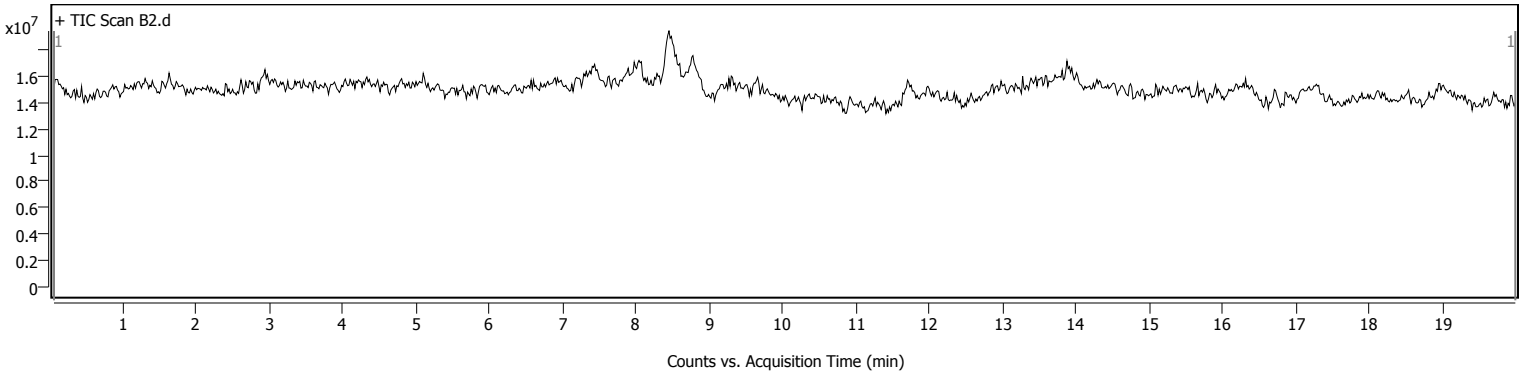
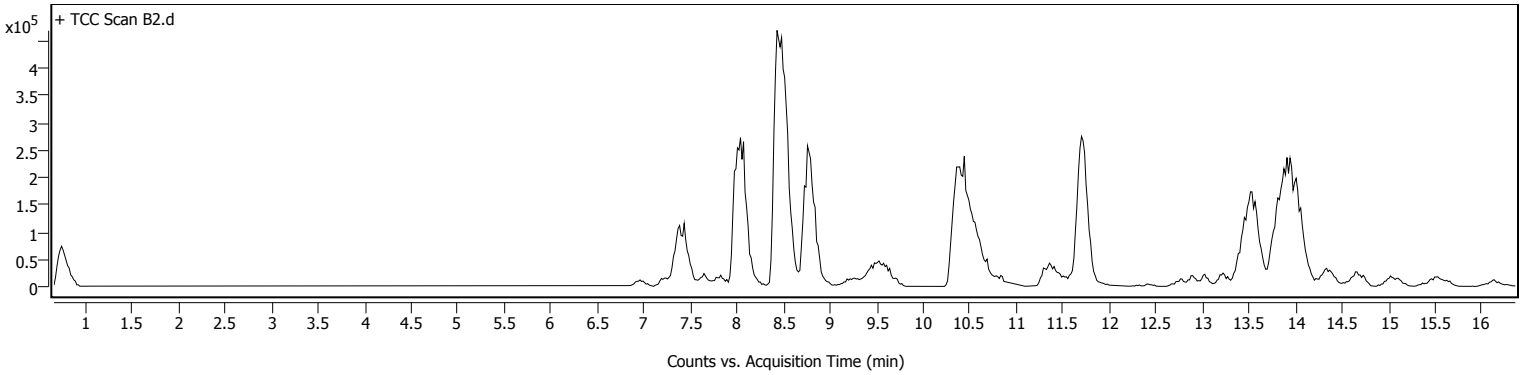
Sample Information

Name	B2	**Data File Path**	D:\MassHunter\Data\Saeed Ullah\B2.d
Sample ID		**Acq. Time (Local)**	10/9/2023 12:57:49 PM (UTC+08:00)
Instrument	Instrument 1	**Method Path (Acq)**	D:\MassHunter\Methods\Training Method 210822.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.1 SP1)
Inj. Vol. (ul)	1	**IRM Status**	Success
Position	P1A3	**Method Path (DA)**	D:\MassHunter\Methods\10.0\Default-LCMS.m
Plate Pos.		**Target Source Path**	D:\MassHunter\PCDL\default.csv;D:\MassHunter\PCDL\Metlin_Metabolites_AM_PCDL.cdb;D:\MassHunter\PCDL\Pesticide_Example.cdb;D:\MassHunter\PCDL\Metlin_AM_PCDL.cdb;D:\MassHunter\PCDL\Metlin_AMRT_PCDL.cdb;D:\MassHunter\PCDL\Metlin_Lipids_AM_PCDL.cdb
Operator		**Result Summary**	78 identified (117 found)

Sample Chromatograms







Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1	3-Deoxyarabinohexonic acid	C6 H12 O6	0.748	180.0635	29625-79-4	DBSearch-MFG	71.07		94.55	47.58	MFE
2		C18 H22 O7 S	0.753	382.1080		MFG	91.84			91.84	MFE
3			0.756	1123.0449							MFE
4		C33 H26 N4 O	0.850	494.2105		MFG	77.48			77.48	MFE
5		C16 H28 N17	6.949	458.2715		MFG	73.66			73.66	MFE
6	Arg Gln Arg	C17 H34 N10 O5	6.961	458.2707		DBSearch	76.76		76.76		MFE
7		C33 H39 N6	7.228	519.3241		MFG	84.34			84.34	MFE
8		C32 H36 N4 O3	7.233	524.2783		MFG	66.86			66.86	MFE
9		C22 H42 N7 O3	7.389	452.3346		MFG	99.39			99.39	MFE
10	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	C28 H32 O16	7.424	624.1679		DBSearch	60.31		60.31		MFE
11		C22 H51 N4 O12	7.448	563.3498		MFG	97.18			97.18	MFE

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
12	Ceanothine E	C34 H40 N4 O4	7.457	568.3052	23926-98-9	DBSearch-MFG	75.32		75.35	75.30	MFE
13		C33 H38 N8	7.466	546.3221		MFG	66.24			66.24	MFE
14		C20 H34 N23 O	7.648	612.3320		MFG	74.58			74.58	MFE
15		C22 H53 N7 O12	7.651	607.3756		MFG	95.86			95.86	MFE
16		C37 H42 N11 O	7.818	656.3579		MFG	72.30			72.30	MFE
17		C32 H61 N O10 S	7.824	651.4020		MFG	95.54			95.54	MFE
18		C26 H59 N14 O4 S2	7.977	695.4281		MFG	83.29			83.29	MFE
19		C27 H40 N24	7.987	700.3860		MFG	68.71			68.71	MFE
20		C28 H53 N8 O4	8.031	565.4185		MFG	99.10			99.10	MFE
21		C41 H57 N9 O4	8.101	739.4536		MFG	67.90			67.90	MFE
22		C34 H75 N4 O18	8.350	827.5082		MFG	58.25			58.25	MFE
23	GalCer(d18:0/26:0)	C50 H99 N O8	8.451	841.7340		DBSearch	79.42		79.42		MFE
24		C33 H58 N16	8.464	678.5024		MFG	98.61			98.61	MFE
25	1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	8.773	814.5753		DBSearch	99.40		99.40		MFE
26			8.784	829.5427							MFE
27			9.020	926.6502							MFE
28		C47 H67 N13	9.135	813.5635		MFG	58.26			58.26	MFE
29	Halaminol A	C14 H29 N O	9.267	227.2243		DBSearch-MFG	83.81		83.80	83.82	MFE
30		C14 H33 N4 O	9.425	273.2652		MFG	80.51			80.51	MFE
31		C37 H68 N5 O	9.444	598.5421		MFG	71.89			71.89	MFE
32		C16 H37 N4 O2	9.495	317.2913		MFG	83.38			83.38	MFE
33		C37 H38 N11 O2	9.538	668.3210		MFG	65.26			65.26	MFE
34		C18 H41 N4 O3	9.563	361.3177		MFG	90.74			90.74	MFE
35	(+/-)-2-methyl-5,8,11,14-all-cis-tricosatetraenoyl-2'-fluoroethylamine	C26 H44 F N O	9.608	405.3421		DBSearch	74.00		74.00		MFE
36		C24 H38 N23 O4	9.638	712.3475		MFG	75.07			75.07	MFE
37		C30 H65 Cl N5 O	10.385	546.4863		MFG	77.35			77.35	MFE
38		C34 H64 N10 O7	10.390	724.4956		MFG	97.02			97.02	MFE
39	Palmitic amide	C16 H33 N O	10.419	255.2555	629-54-9	DBSearch	97.74		97.74		MFE
40		C16 H35 N4 O	11.307	299.2813		MFG	47.41			47.41	MFE
41		C16 H35 N4	11.375	283.2866		MFG	98.02			98.02	MFE
42		C36 H36 N9 O7	11.704	706.2735		MFG	98.71			98.71	MFE
43	Austrobailignan 7	C20 H22 O5	11.707	342.1458	55890-25-0	DBSearch	97.17		97.17		MFE
44		C27 H44 N3 O S	12.313	458.3207		MFG	55.56			55.56	MFE
45		C26 H28 O S4	12.434	484.1026		MFG	81.25			81.25	MFE
46		C44 H52 N11	12.671	734.4402		MFG	62.50			62.50	MFE
47			12.734	1242.7618							MFE
48		C36 H70 N29 O3	12.757	956.6210		MFG	61.76			61.76	MFE
49		C31 H28 N O3 S3	12.773	558.1223		MFG	77.80			77.80	MFE
50	PC(O-16:0/0:0)[U]	C24 H53 N O6 P	12.884	482.3591		DBSearch	54.81		54.81		MFE
51		C20 H34 N9 O	12.884	416.2887		MFG	61.99			61.99	MFE
52	27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.885	438.3327	78648-95-0	DBSearch	66.50		66.50		MFE
53			13.020	632.1413							MFE
54		C34 H15 N17 O3	13.208	709.1549		MFG	56.30			56.30	MFE
55		C37 H23 Cl N10 O4	13.209	706.1590		MFG	69.74			69.74	MFE
56		C53 H31 Cl N O2 S	13.374	780.1768		MFG	90.95			90.95	MFE
57			13.380	1430.9001							MFE
58			13.380	775.2238							MFE
59			13.399	1342.8475							MFE
60			13.401	1386.8691							MFE
61			13.416	1210.7722							MFE
62			13.424	1188.7863							MFE
63			13.442	1144.7628							MFE
64			13.451	1100.7357							MFE
65	35S-Methylokadaic acid 7-hexadecanoate	C61 H100 O14	13.459	1056.7092		DBSearch	92.04		92.04		MFE
66			13.473	1012.6838							MFE
67		C55 H80 N14 O2	13.483	968.6585		MFG	95.94			95.94	MFE
68		C46 H86 N9 O8 S	13.500	924.6322		MFG	93.78			93.78	MFE
69		C37 H74 N19 O6	13.506	880.6066		MFG	96.92			96.92	MFE
70		C43 H84 N2 O11 S	13.521	836.5799		MFG	95.53			95.53	MFE
71	PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H79 N O8 P	13.531	792.5544		DBSearch	96.60		96.60		MFE
72		C40 H72 N6 O5 S	13.544	748.5282		MFG	94.70			94.70	MFE
73		C38 H68 N6 O4 S	13.562	704.5019		MFG	96.75			96.75	MFE
74		C36 H64 N6 O3 S	13.572	660.4756		MFG	93.74			93.74	MFE
75			13.573	854.1975							MFE
76			13.574	849.2413							MFE
77		C37 H31 N17 O3 S3	13.575	857.1944		MFG	77.71			77.71	MFE
78		C25 H50 N19	13.581	616.4501		MFG	72.94			72.94	MFE
79		C32 H64 N2 S3	13.594	572.4236		MFG	86.30			86.30	MFE
80		C32 H58 N19 O	13.632	724.5075		MFG	70.14			70.14	MFE
81			13.723	1458.9332							MFE
82			13.737	1414.9102							MFE
83			13.761	1370.8764							MFE
84			13.763	1326.8618							MFE
85		C41 H22 N23 O6	13.764	932.2128		MFG	62.96			62.96	MFE
86			13.766	928.2151							MFE
87			13.772	1282.8295							MFE
88			13.786	1304.8698							MFE
89			13.786	1238.8016							MFE
90			13.790	1260.8457							MFE

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
91			13.799	1216.8188							MFE
92			13.815	1172.7933							MFE
93			13.825	1128.7668							MFE
94			13.846	1084.7410							MFE
95			13.863	1040.7150							MFE
96		C57 H94 N3 O11	13.881	996.6896		MFG	98.47			98.47	MFE
97		C55 H90 N3 O10	13.900	952.6627		MFG	98.85			98.85	MFE
98		C53 H86 N3 O9	13.918	908.6367		MFG	98.73			98.73	MFE
99		C51 H82 N3 O8	13.939	864.6107		MFG	98.25			98.25	MFE
100	PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H83 N O8 P	13.958	820.5845		DBSearch	97.43		97.43		MFE
101	PC(O-15:0/20:4(5Z,8Z,11Z,14Z))[U]	C43 H81 N O7 P	13.984	754.5779		DBSearch	89.13		89.13		MFE
102		C47 H72 O6	14.000	732.5335		MFG	94.21			94.21	MFE
103		C38 H68 N6 O3 S	14.025	688.5072		MFG	94.70			94.70	MFE
104			14.041	1005.2306							MFE
105			14.043	1002.2333							MFE
106		C28 H60 N12 O5	14.046	644.4813		MFG	91.74			91.74	MFE
107		C26 H54 N9 O4	14.091	556.4295		MFG	79.42			79.42	MFE
108		C22 H48 N12 O2	14.108	512.4029		MFG	76.34			76.34	MFE
109			14.326	1076.2519							MFE
110	Retinoyl CoA	C41 H62 N7 O17 P3 S	14.338	1049.3121	81295-48-9	DBSearch	58.49		58.49		MFE
111	TG(10:0/10:0/10:0)	C33 H62 O6	14.376	554.4519	621-71-6	DBSearch	56.11		56.11		MFE
112			14.664	1150.2707							MFE
113			15.044	1225.2887							MFE
114			15.047	1228.2868							MFE
115			15.364	707.5001							MFE
116			15.529	1298.3082							MFE
117			16.145	1372.3259							MFE

Compound Details

Cpd. 1: 3-Deoxyarabinohexonic acid

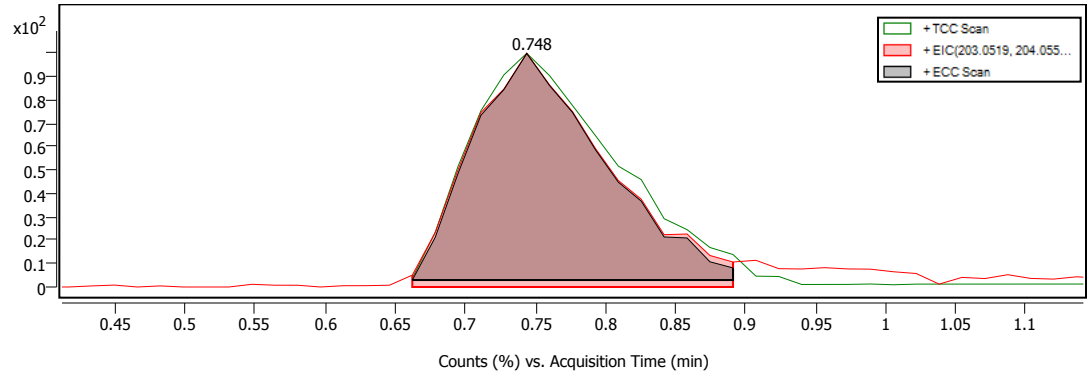
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
3-Deoxyarabinohexonic acid	C6 H12 O6	0.748		180.0635	29625-79-4	DBSearch-MFG	71.07	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	203.0527 203.0527 203.0527		0	94.55	26	47.58	

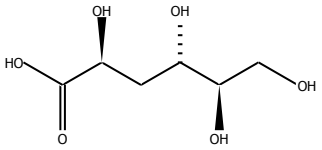
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
3-Deoxyarabinohexonic acid	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	29625-79-4	71.07	94.55	47.58
b-D-Galactopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	7296-64-2	71.07	94.55	47.58
D-Fuconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635		71.07	94.55	47.58
D-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	59-23-4	71.07	94.55	47.58
allo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	643-10-7	71.07	94.55	47.58
myo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	87-9-8	71.07	94.55	47.58
D-(+)-Mannose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	3458-28-4	71.07	94.55	47.58
b-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	492-61-5	71.07	94.55	47.58
L-(-)Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	87-79-6	71.07	94.55	47.58
α-D-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	492-62-6	71.07	94.55	47.58
D-Tagatose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	87-81-0	71.07	94.55	47.58
Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	3615-39-2	71.07	94.55	47.58
Allose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	6038-51-3	71.07	94.55	47.58
L-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	15572-79-9	71.07	94.55	47.58
D-Hamamelose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	4573-78-8	71.07	94.55	47.58
L-Rhamnonate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	6422-34-0	71.07	94.55	47.58
β-D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	53188-23-1	71.07	94.55	47.58
2-Deoxy-D-gluconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635		71.07	94.55	47.58
beta-D-Hamamelopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635		71.07	94.55	47.58
D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	57-48-7	71.07	94.55	47.58
L-(+)-Gulose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	6027-89-0	71.07	94.55	47.58
1,3-Dihydroxyacetone	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.748		180.0635	62147-49-3	71.07	94.55	47.58
	C5 H14 N3 S2	(M+Na)+	MFG	0.748		180.0635		46.10		46.10
	C7 H16 O S2	(M+Na)+	MFG	0.748		180.0635		44.77		44.77
	C7 H8 N4 O2	(M+Na)+	MFG	0.748		180.0635		40.65		40.65
	C4 H10 N3 O5	(M+Na)+	MFG	0.748		180.0635		38.66		38.66

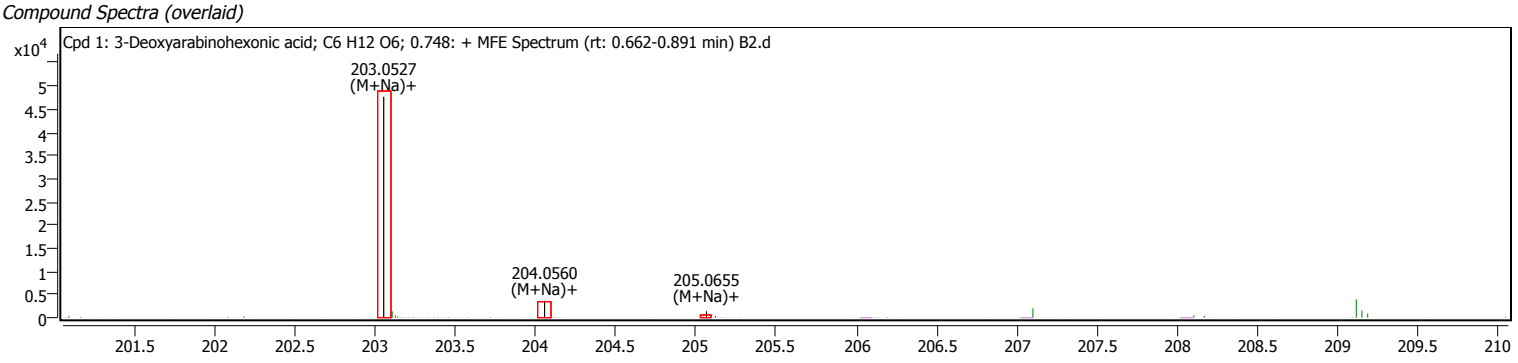
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 2: C18 H22 O7 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C18 H22 O7 S	0.753		382.1080		MFG	91.84	MFE	

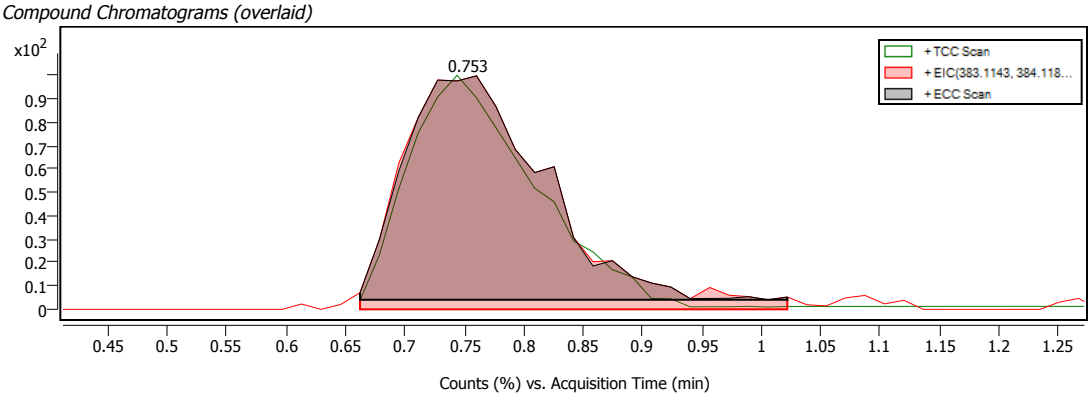
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	383.1150				5	91.84	

Compound ID Table

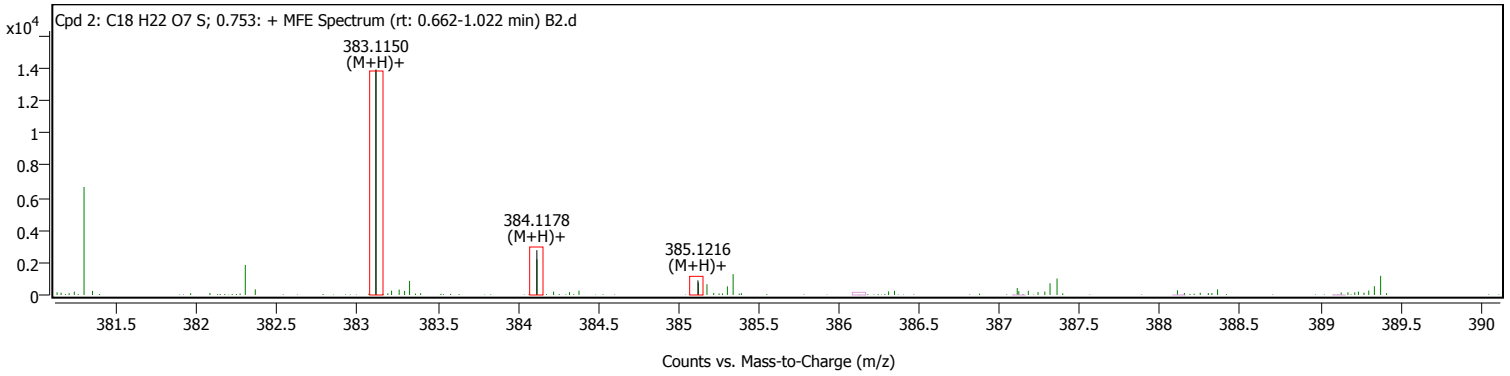
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C18 H22 O7 S	(M+H)+	MFG	0.753		382.1080		91.84		91.84
	C17 H16 N7 O2 S	(M+H)+	MFG	0.753		382.1082		91.54		91.54
	C16 H20 N3 O6 S	(M+H)+	MFG	0.753		382.1081		91.11		91.11
	C24 H16 N O4	(M+H)+	MFG	0.753		382.1077		89.43		89.43
	C15 H14 N10 O S	(M+H)+	MFG	0.753		382.1083		89.28		89.28

Compound Chromatograms (overlaid)

Structure



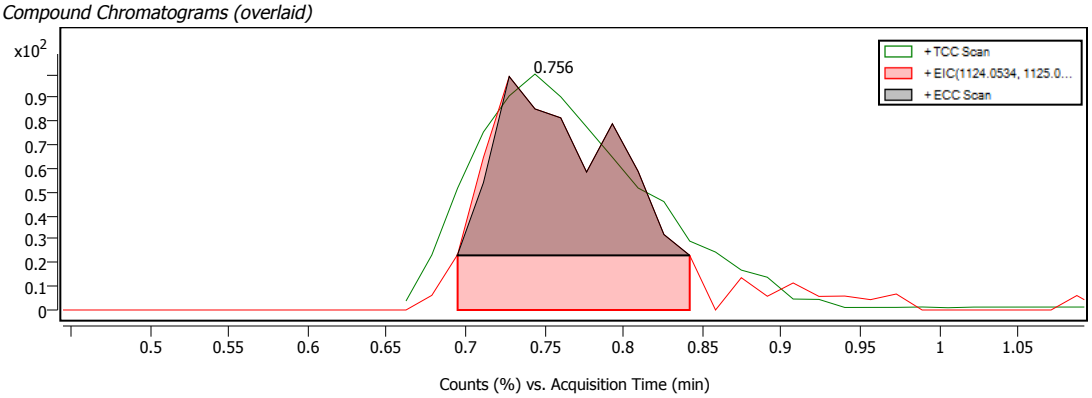
Compound Spectra (overlaid)



Cpd 3: 0.756

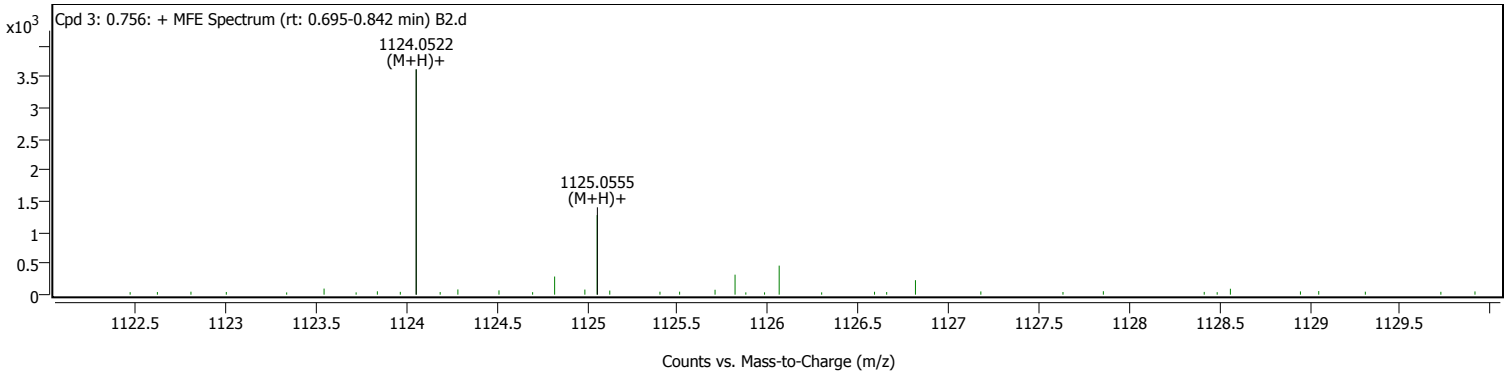
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		0.756		1123.0449				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 4: C33 H26 N4 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H26 N4 O	0.850		494.2105		MFG	77.48	MFE	

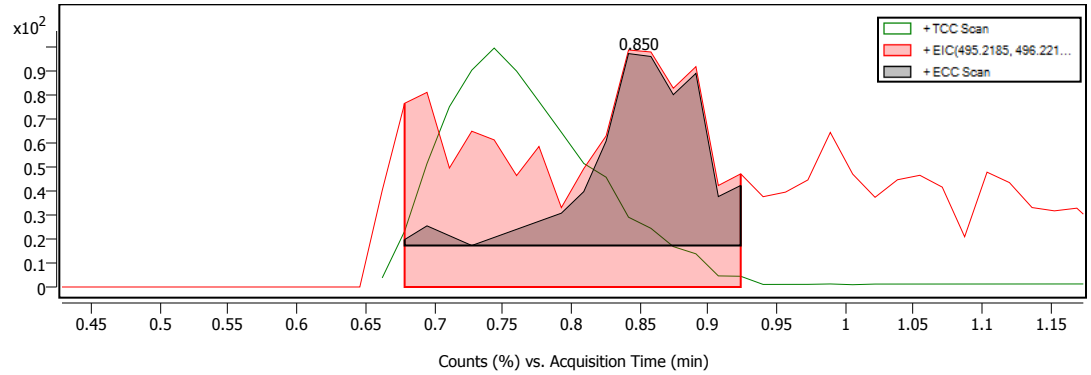
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	495.2175				8	77.48	

Compound ID Table

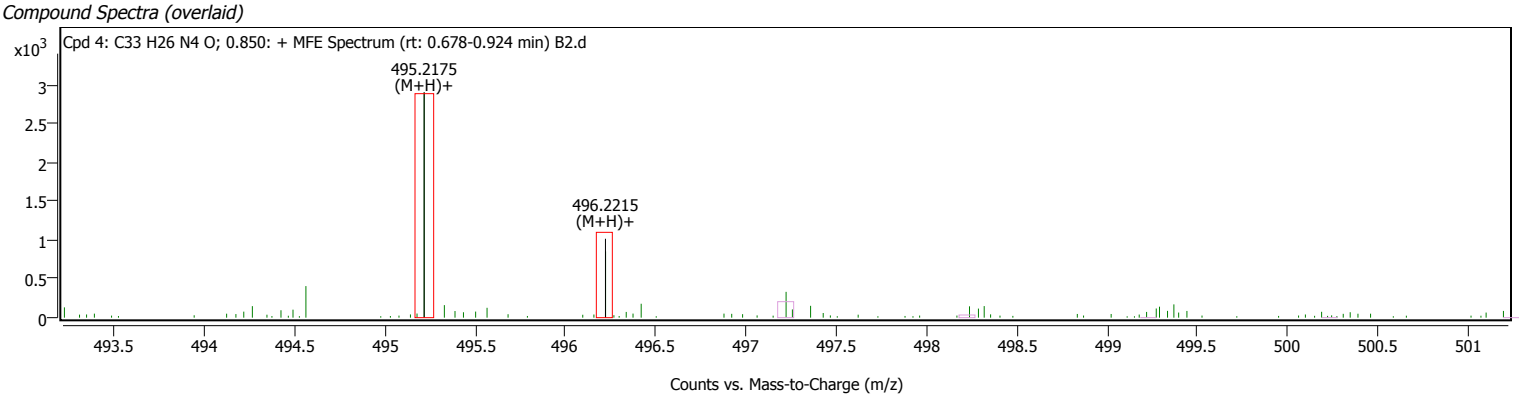
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H26 N4 O	(M+H)+	MFG	0.850		494.2105		77.48		77.48
	C31 H24 N7	(M+H)+	MFG	0.850		494.2105		75.48		75.48
	C32 H30 O5	(M+H)+	MFG	0.850		494.2104		74.87		74.87
	C35 H28 N O2	(M+H)+	MFG	0.850		494.2104		71.53		71.53
Diflorasone diacetate	C26 H32 F2 O7	(M+H)+	DBSearch	0.850		494.2104	33564-31-7	70.71	70.71	
Fluocinonide	C26 H32 F2 O7	(M+H)+	DBSearch	0.850		494.2104	356-12-7	70.71	70.71	
	C18 H22 N16 O2	(M+H)+	MFG	0.850		494.2108		68.99		68.99
BAY-u9773	C27 H36 O5 S	(M+Na)+	DBSearch	0.850		472.2285	154978-38-8	66.97	66.97	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 5: C16 H28 N17

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H28 N17	6.949		458.2715		MFG	73.66	MFE	

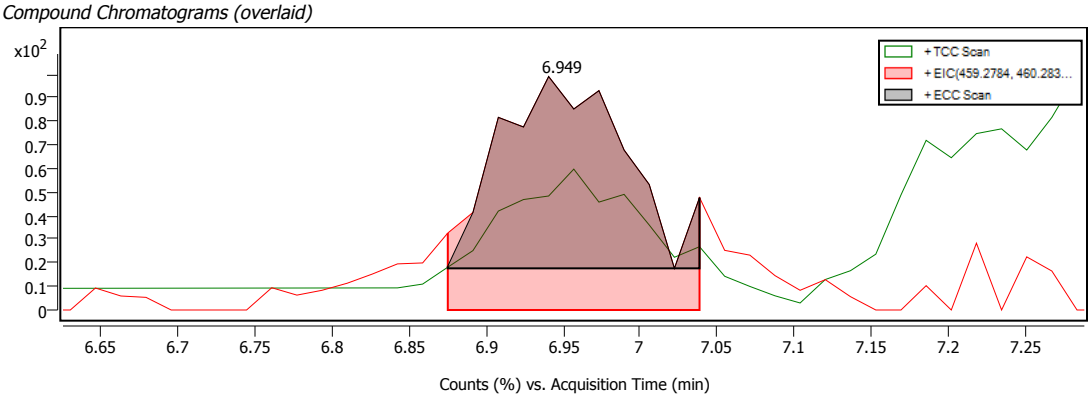
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	481.2589				7	73.66	

Compound ID Table

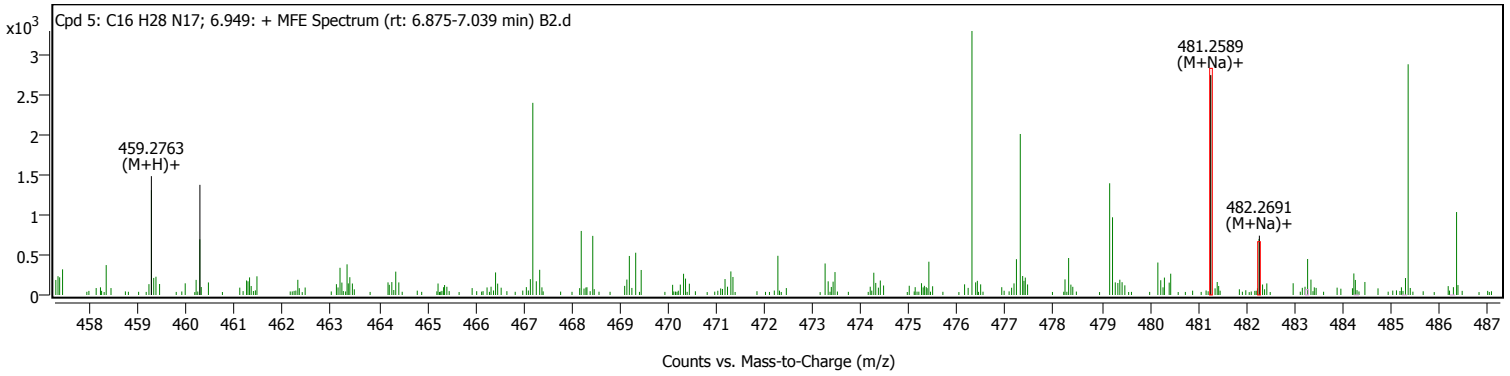
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H28 N17	(M+Na)+	MFG	6.949		458.2715		73.66		73.66
	C18 H30 N14 O	(M+Na)+	MFG	6.949		458.2714		70.79		70.79
Arg Arg Gln	C17 H34 N10 O5	(M+Na)+	DBSearch-MFG	6.949		458.2714		70.48	70.39	70.56
Gln Arg Arg	C17 H34 N10 O5	(M+Na)+	DBSearch-MFG	6.949		458.2714		70.48	70.39	70.56
Arg Gln Arg	C17 H34 N10 O5	(M+Na)+	DBSearch-MFG	6.949		458.2714		70.48	70.39	70.56
	C19 H36 N7 O6	(M+Na)+	MFG	6.949		458.2713		67.19		67.19
	C18 H40 N3 O10	(M+Na)+	MFG	6.949		458.2712		67.05		67.05

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 6: Arg Gln Arg

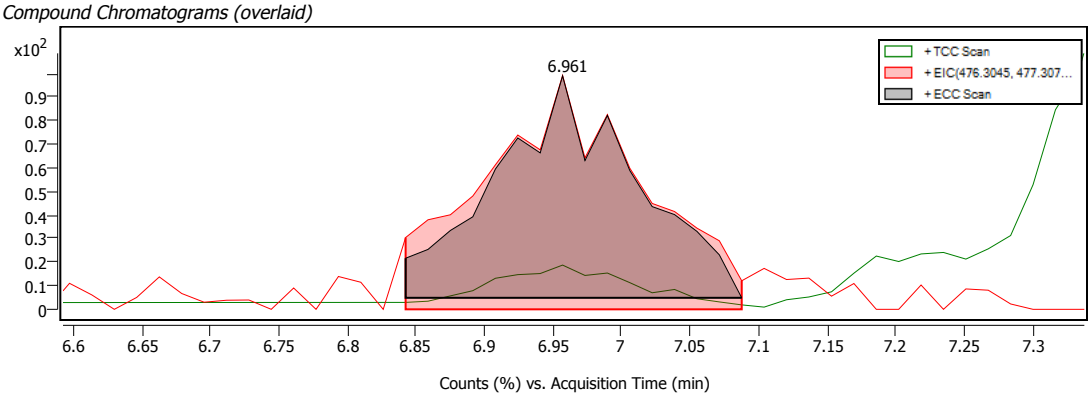
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Arg Gln Arg	C17 H34 N10 O5	6.961		458.2707		DBSearch	76.76	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	476.3044 476.3044		0	76.76	13		

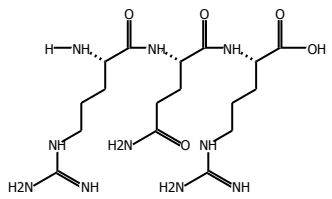
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Arg Gln Arg	C17 H34 N10 O5	(M+NH4)+	DBSearch	6.961		458.2707		76.76	76.76	
Arg Arg Gln	C17 H34 N10 O5	(M+NH4)+	DBSearch	6.961		458.2707		76.76	76.76	
Gln Arg Arg	C17 H34 N10 O5	(M+NH4)+	DBSearch	6.961		458.2707		76.76	76.76	
	C12 H35 Cl N14 O3	(M+NH4)+	MFG	6.961		458.2706		47.61		47.61
	C24 H42 Cl2 N3 O	(M+NH4)+	MFG	6.961		458.2706		47.61		47.61
	C20 H39 Cl N8 S	(M+NH4)+	MFG	6.961		458.2706		47.59		47.59
	C21 H45 Cl N O5 S	(M+NH4)+	MFG	6.961		458.2706		47.58		47.58
	C25 H40 N4 O5	(M+H)+	MFG	6.961		476.3000		47.55		47.55
	C24 H34 N11	(M+H)+	MFG	6.961		476.3000		47.55		47.55
	C22 H43 Cl N5 O4	(M+H)+	MFG	6.961		476.3000		47.41		47.41
	C17 H42 N6 O4 S2	(M+NH4)+	MFG	6.961		458.2706		47.39		47.39
	C18 H40 N10 O3 S	(M+H)+	MFG	6.961		476.3000		47.06		47.06
	C17 H44 Cl2 N9 O2	(M+H)+	MFG	6.961		476.3000		46.98		46.98

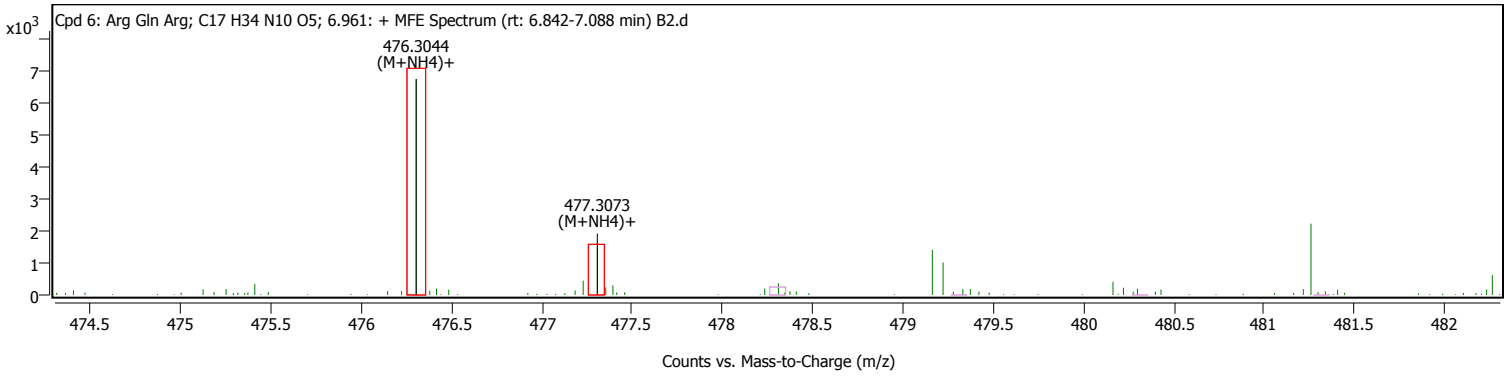
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 7: C33 H39 N6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H39 N6	7.228		519.3241		MFG	84.34	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	520.3312				5	84.34	

Compound Discovery Report

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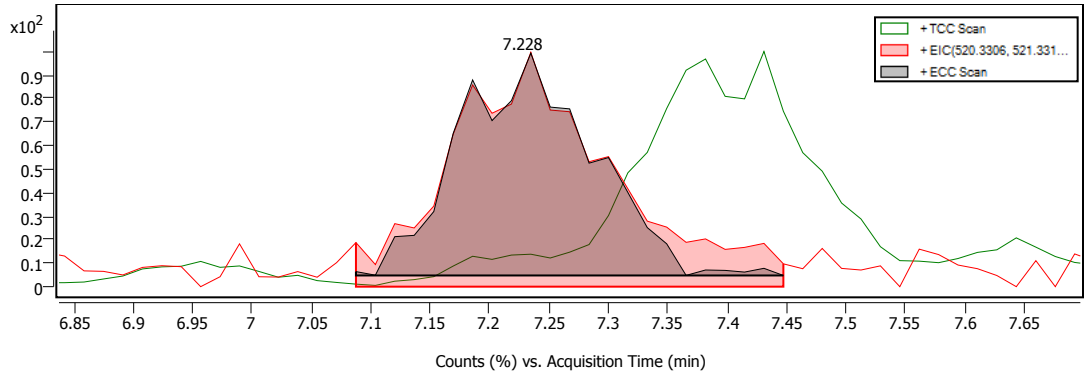
Compound ID Table

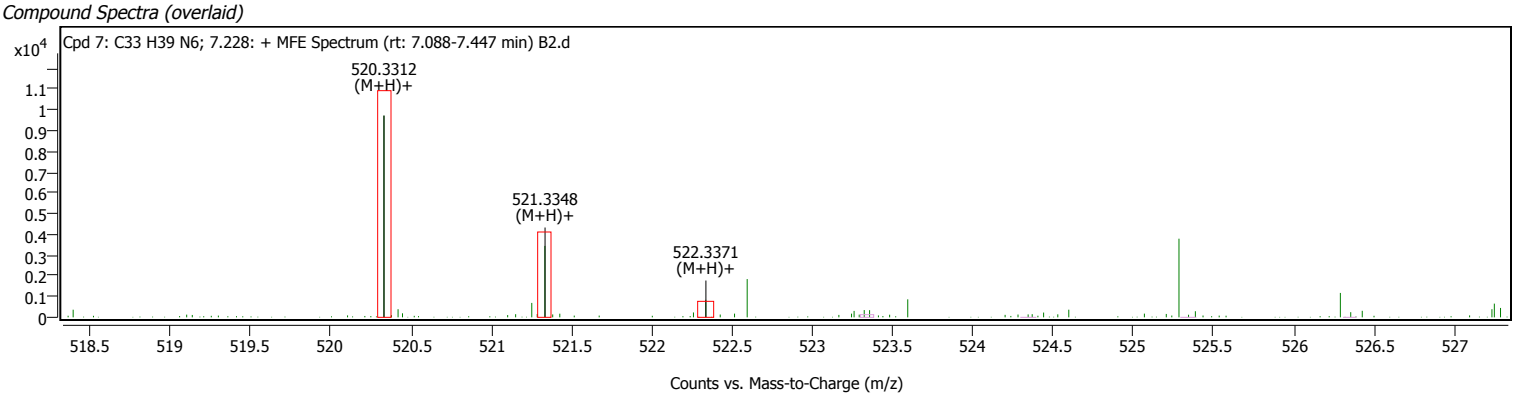
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H39 N6	(M+H)+	MFG	7.228		519.3241		84.34		84.34
	C35 H41 N3 O	(M+H)+	MFG	7.228		519.3240		84.21		84.21
	C29 H47 N2 O4 S	(M+H)+	MFG	7.228		519.3245		78.93		78.93
	C27 H45 N5 O3 S	(M+H)+	MFG	7.228		519.3246		78.83		78.83
	C32 H43 N2 O4	(M+H)+	MFG	7.228		519.3240		78.70		78.70

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 8: C32 H36 N4 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H36 N4 O3	7.233		524.2783		MFG	66.86	MFE	

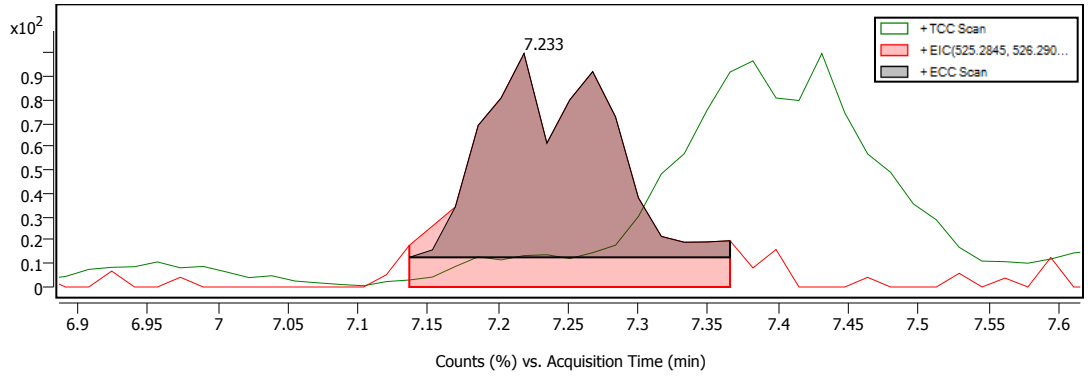
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	525.2849				5	66.86	

Compound ID Table

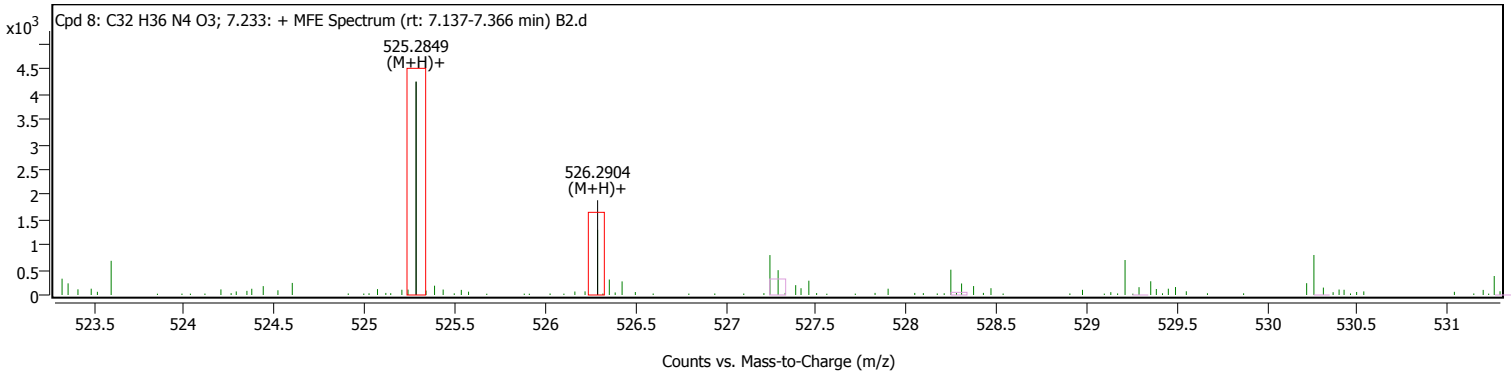
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H36 N4 O3	(M+H)+	MFG	7.233		524.2783		66.86		66.86
	C30 H34 N7 O2	(M+H)+	MFG	7.233		524.2784		64.49		64.49
	C31 H40 O7	(M+H)+	MFG	7.233		524.2782		63.78		63.78
	C34 H38 N O4	(M+H)+	MFG	7.233		524.2783		61.81		61.81
	C32 H44 O2 S2	(M+H)+	MFG	7.233		524.2783		58.05		58.05

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 9: C22 H42 N7 O3

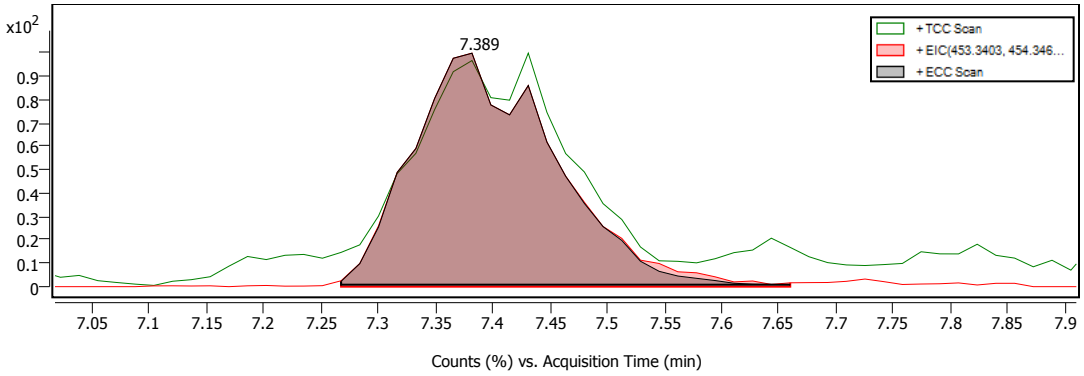
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H42 N7 O3	7.389		452.3346		MFG	99.39	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	453.3418 475.3236				5	99.39	

Compound ID Table

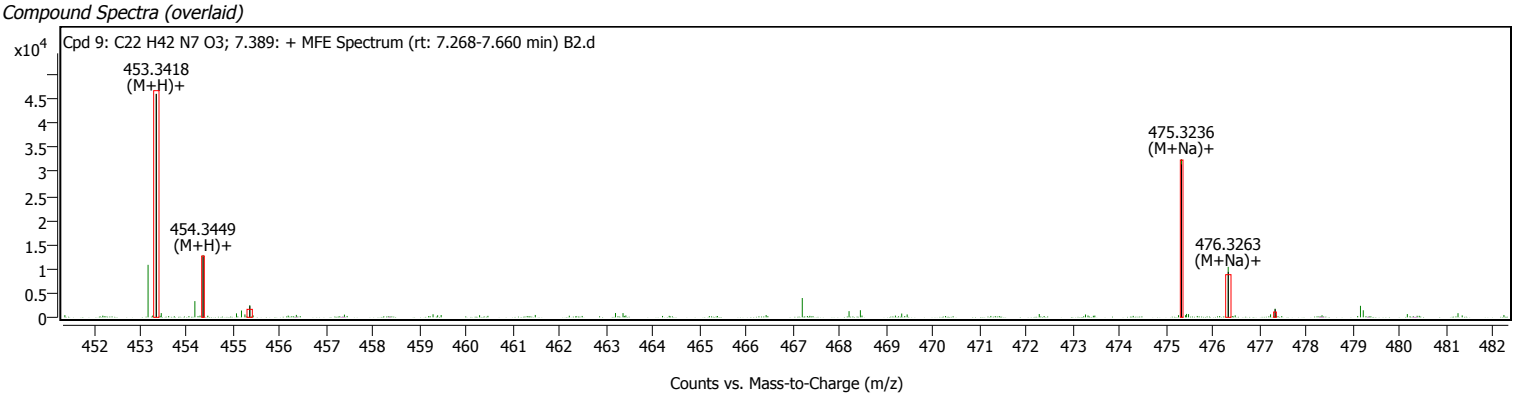
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H42 N7 O3	(M+H)+ (M+Na)+	MFG	7.389		452.3346		99.39		99.39
	C23 H48 O8	(M+H)+ (M+Na)+	MFG	7.389		452.3344		98.78		98.78
	C21 H46 N3 O7	(M+H)+ (M+Na)+	MFG	7.389		452.3345		96.59		96.59
	C20 H40 N10 O2	(M+H)+ (M+Na)+	MFG	7.389		452.3347		96.13		96.13
	C24 H44 N4 O4	(M+H)+ (M+Na)+	MFG	7.389		452.3345		93.26		93.26

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 10: Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	C28 H32 O16	7.424		624.1679		DBSearch	60.31	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	647.1566 647.1566 647.1566		0	60.31	75		

Compound ID Table

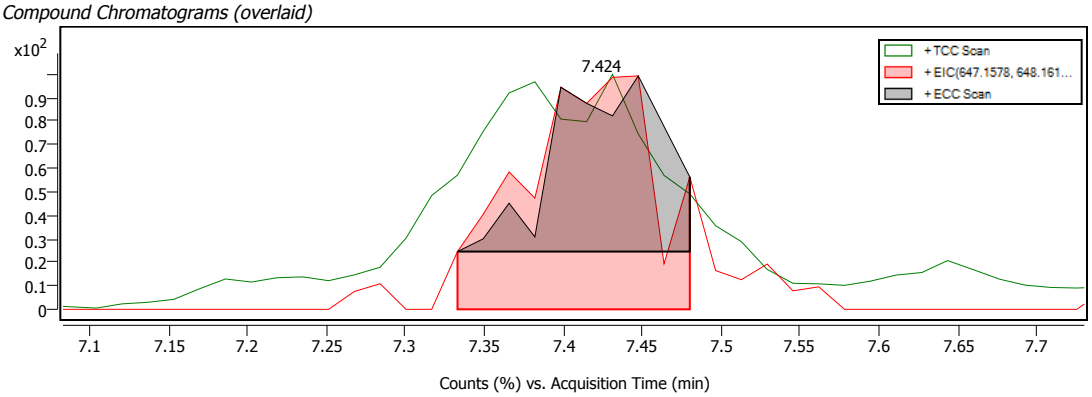
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-glucoside 4'-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	28289-13-6	60.31	60.31	
Scoparin 6''-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-glucoside-7-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-galactoside-7-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-rhamnosyl-(1->2)-galactoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Kaempferide 3,7-diglucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
6,8-Di-C-glucopyranosyldiosmetin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isoscutellarein 4'-methyl ether 7-allosyl-(1->2)-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
6-C-Rhamnopyranosylrhamnetin 3-O-glucopyranoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Swertiajaponin 3'-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Luteoayamenin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
6-C-Arabinopyranosyl-8-C-glucopyranosyltricin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
6-C-Glucopyranosyl-8-C-arabinopyranosyltricin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Luteolin 4'-methyl ether 7-sophoroside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Tricetin 7-methyl ether 3'-glucoside-5'-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Tamarixetin 3-neohesperidoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isoscoparin 2''-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-glucoside-4'-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
3,8-Di-C-glucopyranosyldiosmetin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Luteolin 3'-methyl ether 7,4'-diglucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Keioside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	107740-46-5	60.31	60.31	
3,8-Diglucosyldiosmetin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	97218-32-1	60.31	60.31	
6,8-Diglucosyldiosmetin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	98813-28-6	60.31	60.31	
Sexangularetin 3-glucoside 7-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	47850-51-1	60.31	60.31	
Pasternoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	10576-85-9	60.31	60.31	
Isorhamnetin 3-O-[b-L-rhamnofuranosyl-(1->6)-D-glucopyranoside]	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	37138-79-7	60.31	60.31	
Calendoflavoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	55033-90-4	60.31	60.31	
Scoparin 2''-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	124902-15-4	60.31	60.31	
Isorhamnetin 4'-neohesperidoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Crosatoside A	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679	139742-27-1	60.31	60.31	
Isorhamnetin 3-robinobioside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Tamarixetin 7-rutinoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Narcissin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-neohesperidoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Stellarin 2	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Scoparin 2''-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
6-Methoxykaempferol 3-robinobioside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnetin 3-robinobioside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Luteolin 3'-methyl ether 5,4'-diglucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnetin 3-galactoside-3'-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Patuletin 3,7-dirhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Myricetin 3,4'-dimethyl ether 7-rhamnoside-3'-xyloside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Quercetin 3,4'-dimethyl ether 7-alpha-L-Arabinofuranosyl-(1->6)-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Myricetin 7-methyl ether 3,4'-di-O-alpha-L-rhamnopyranoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnazin 3-xylosyl-(1->2)-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnazin 3-glucosyl-(1->5)-alpha-L-arabinofuranoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnetin 3-rutinoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnetin 3-neohesperidoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Subulin	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnocitrin 3-galactoside-4'-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnocitrin 3-glucosyl-(1->2)-galactoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Rhamnocitrin 3,4'-diglucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isoscoparin 4'-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isorhamnetin 3-rhamnoside-7-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Sexangularetin 3-rhamnoside-7-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Sexangularetin 3-glucoside-7-rhamnoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Sexangularetin 3-rutinoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Isoscoparin 7-O-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Tamarixetin 3-robinobioside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Sexangularetin 3-neohesperidoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Luteolin 3'-methyl ether 7-allosyl-(1->2)-glucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	

Compound Discovery Report

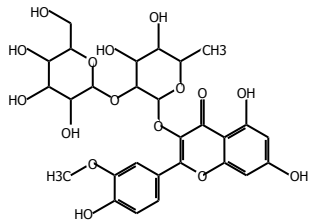
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Luteolin 3'-methyl ether 7-mannosyl-(1->2)-alloside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Chrysoeriol 7-O-8-C-bisglucoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
Knoutinoside	C28 H32 O16	(M+Na)+	DBSearch	7.424		624.1679		60.31	60.31	
	C17 H34 N15 O S5	(M+Na)+	MFG	7.424		624.1674		47.62		47.62
	C33 H36 O6 S3	(M+Na)+	MFG	7.424		624.1674		47.62		47.62
	C18 H40 N8 O6 S5	(M+Na)+	MFG	7.424		624.1674		47.62		47.62
	C32 H30 N7 O S3	(M+Na)+	MFG	7.424		624.1674		47.62		47.62
	C43 H29 Cl2 O2	(M+H)+	MFG	7.424		647.1544		47.61		47.61
	C31 H22 Cl N11 O4	(M+H)+	MFG	7.424		647.1544		47.61		47.61
	C32 H28 Cl N4 O9	(M+H)+	MFG	7.424		647.1544		47.61		47.61
	C17 H40 Cl3 N11 O3 S3	(M+H)+	MFG	7.424		647.1544		47.61		47.61
	C14 H39 Cl3 N12 O5 S2	(M+Na)+	MFG	7.424		624.1674		47.61		47.61
	C28 H33 Cl2 N8 O2 S2	(M+H)+	MFG	7.424		647.1544		47.61		47.61

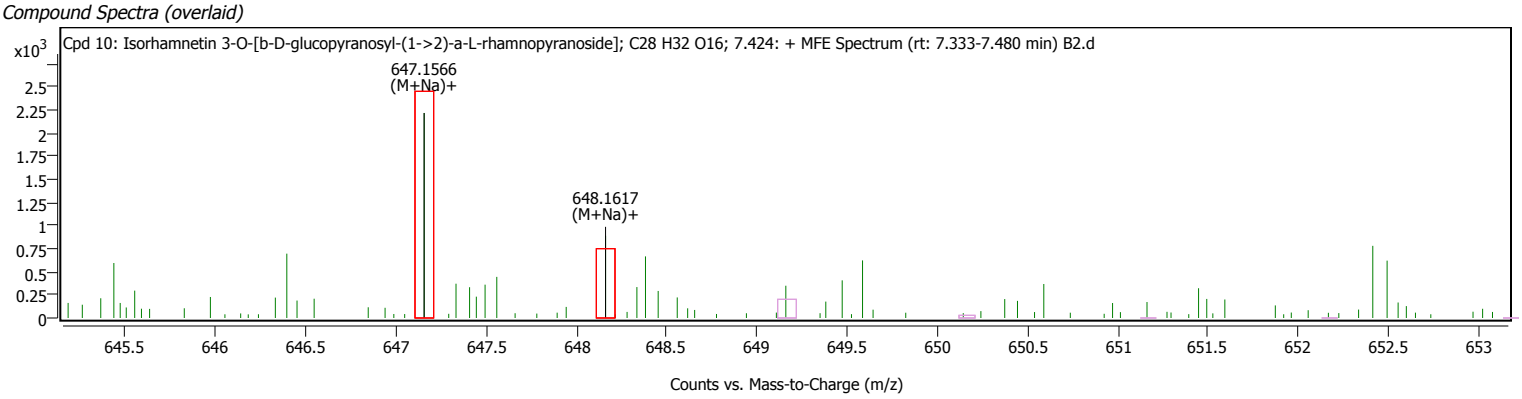
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 11: C22 H51 N4 O12

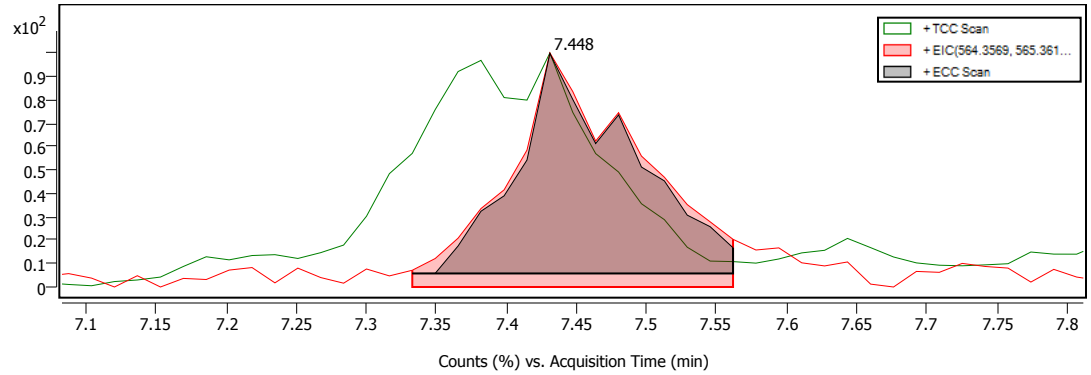
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H51 N4 O12	7.448		563.3498		MFG	97.18	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	564.3570				5	97.18	

Compound ID Table

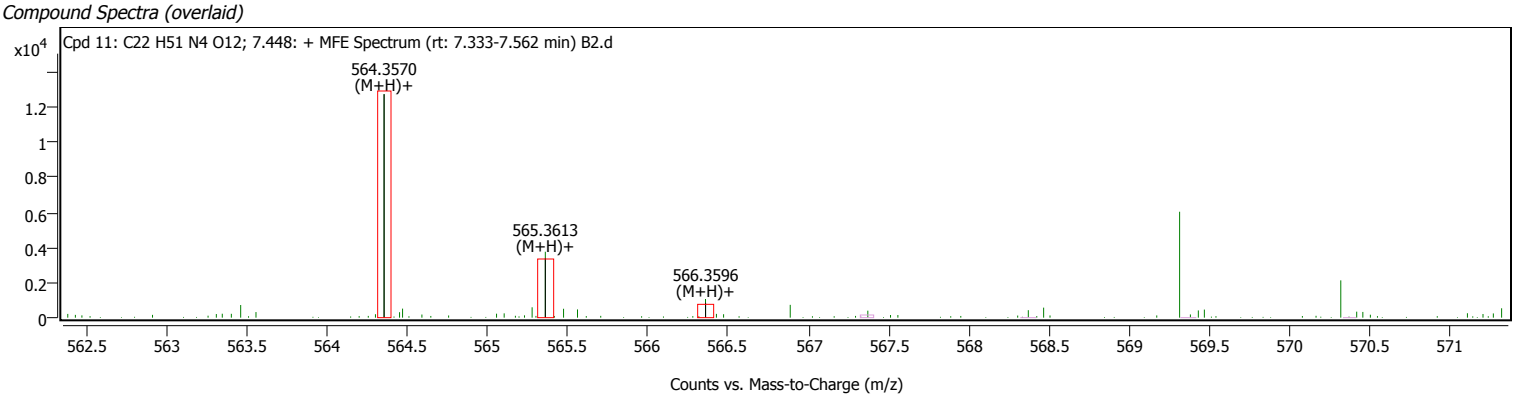
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H51 N4 O12	(M+H)+	MFG	7.448		563.3498		97.18		97.18
	C21 H45 N11 O7	(M+H)+	MFG	7.448		563.3500		96.15		96.15
	C20 H49 N7 O11	(M+H)+	MFG	7.448		563.3499		95.45		95.45
	C20 H39 N18 O2	(M+H)+	MFG	7.448		563.3501		94.01		94.01
	C19 H43 N14 O6	(M+H)+	MFG	7.448		563.3501		93.81		93.81

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 12: Ceanothine E

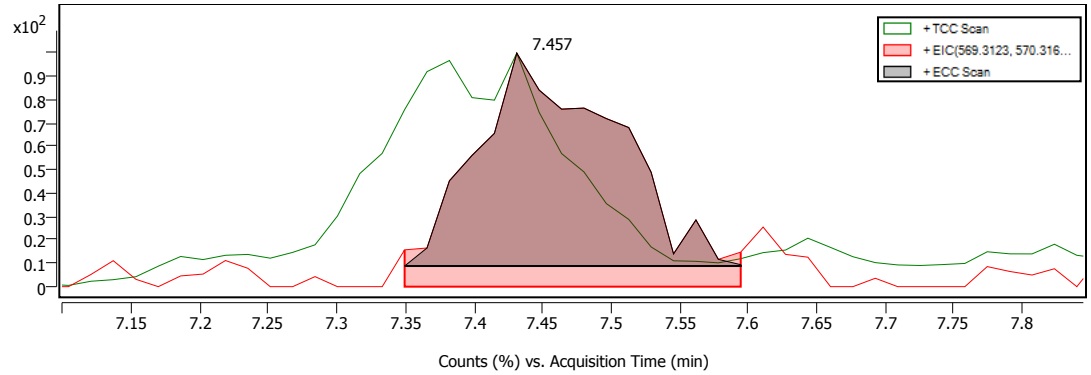
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Ceanothine E	C34 H40 N4 O4	7.457		568.3052	23926-98-9	DBSearch-MFG	75.32	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	569.3123 569.3123 569.3123		0	75.35	9	75.30	

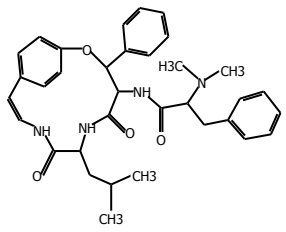
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Ceanothine E	C34 H40 N4 O4	(M+H)+	DBSearch-MFG	7.457		568.3052	23926-98-9	75.32	75.35	75.30
Protoporphyrinogen IX	C34 H40 N4 O4	(M+H)+	DBSearch-MFG	7.457		568.3052	7412-77-3	75.32	75.35	75.30
Adouetine Y	C34 H40 N4 O4	(M+H)+	DBSearch-MFG	7.457		568.3052	19542-38-2	75.32	75.35	75.30
Crenatine A	C34 H40 N4 O4	(M+H)+	DBSearch-MFG	7.457		568.3052	52801-20-4	75.32	75.35	75.30
	C18 H30 N23	(M+H)+	MFG	7.457		568.3057		73.44		73.44
	C35 H36 N8	(M+H)+	MFG	7.457		568.3053		72.67		72.67
	C20 H32 N20 O	(M+H)+	MFG	7.457		568.3056		72.46		72.46
	C36 H42 N O5	(M+H)+	MFG	7.457		568.3052		72.09		72.09
5-Oxoavermectin "1b" aglycone	C33 H44 O8	(M+H)+	DBSearch	7.457		568.3052		71.32	71.32	

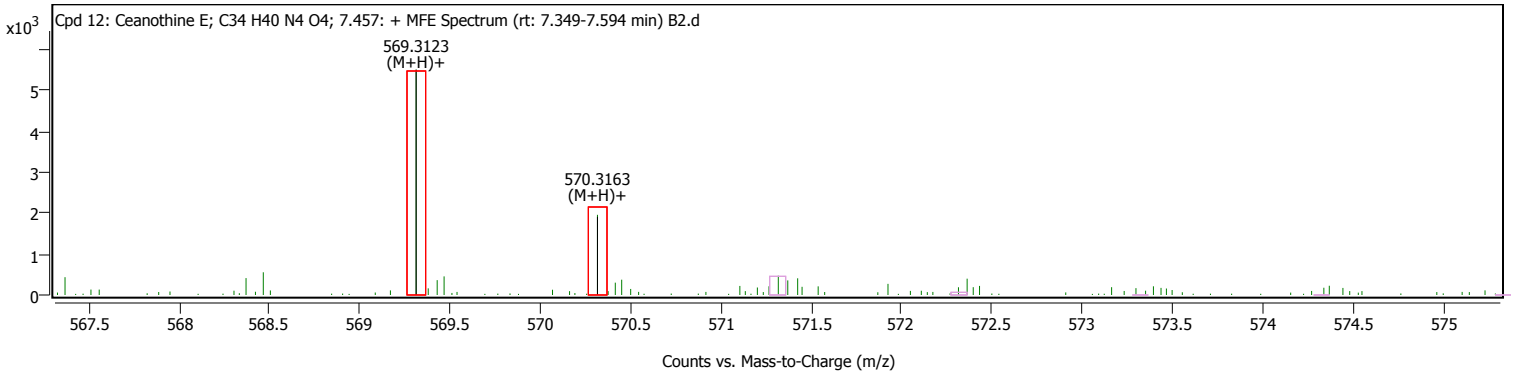
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 13: C33 H38 N8

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H38 N8	7.466		546.3221		MFG	66.24	MFE	

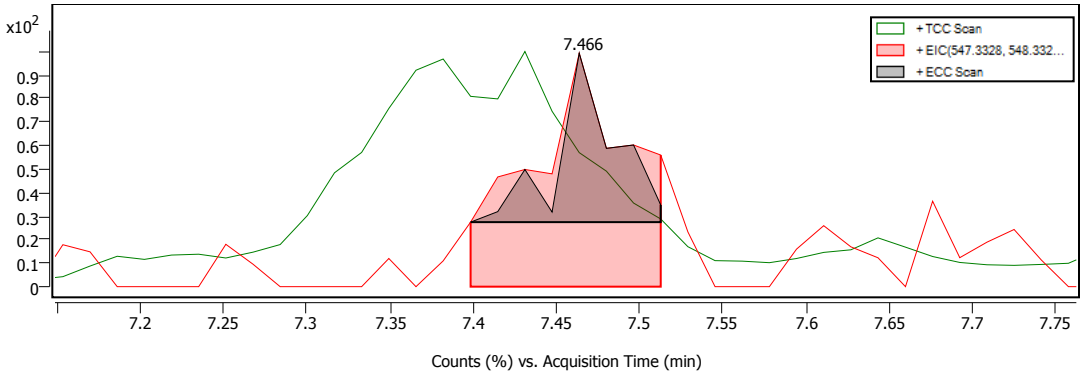
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	547.3298				5	66.24	

Compound ID Table

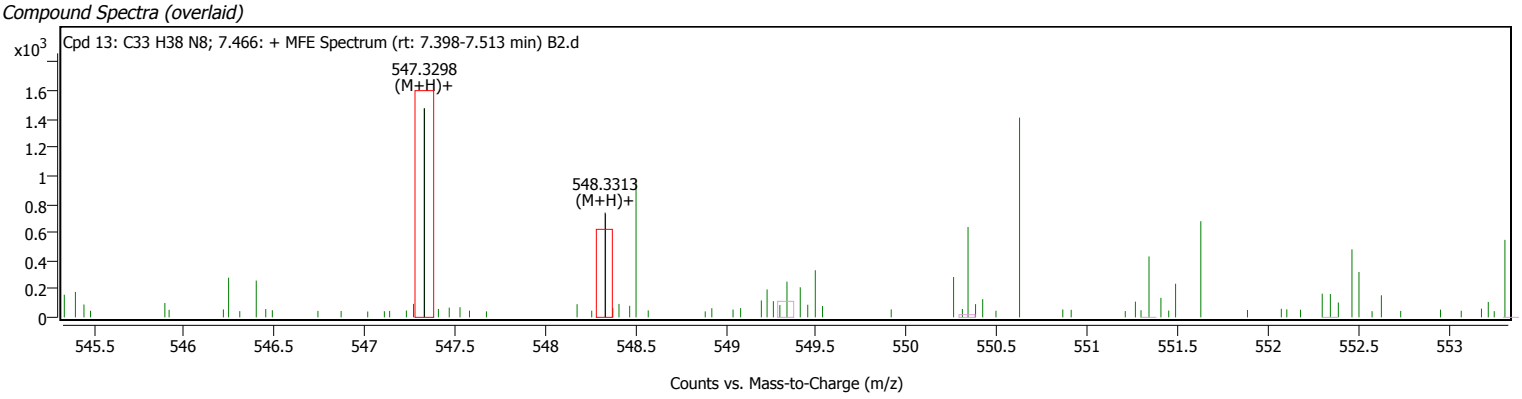
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H38 N8	(M+H)+	MFG	7.466		546.3221		66.24		66.24
	C34 H44 N O5	(M+H)+	MFG	7.466		546.3219		63.61		63.61
	C35 H40 N5 O	(M+H)+	MFG	7.466		546.3220		63.27		63.27
	C32 H42 N4 O4	(M+H)+	MFG	7.466		546.3220		60.18		60.18
	C27 H44 N7 O3 S	(M+H)+	MFG	7.466		546.3221		59.53		59.53

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 14: C20 H34 N23 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C20 H34 N23 O	7.648		612.3320		MFG	74.58	MFE	

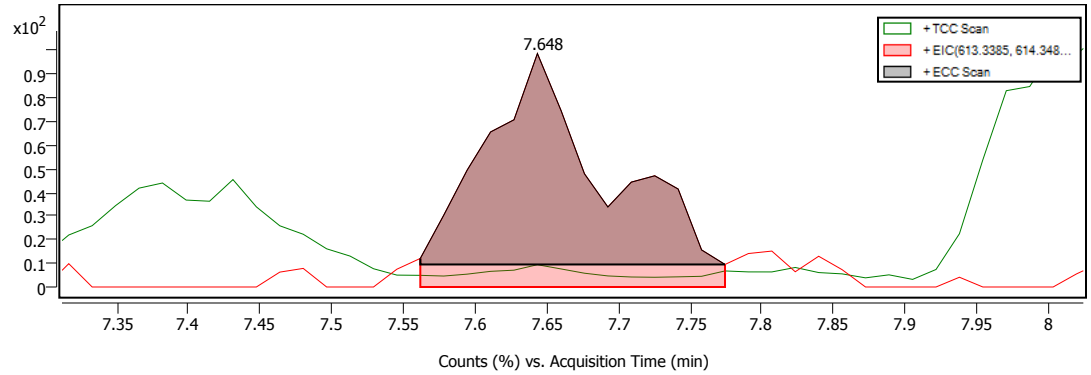
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	613.3386				5	74.58	

Compound ID Table

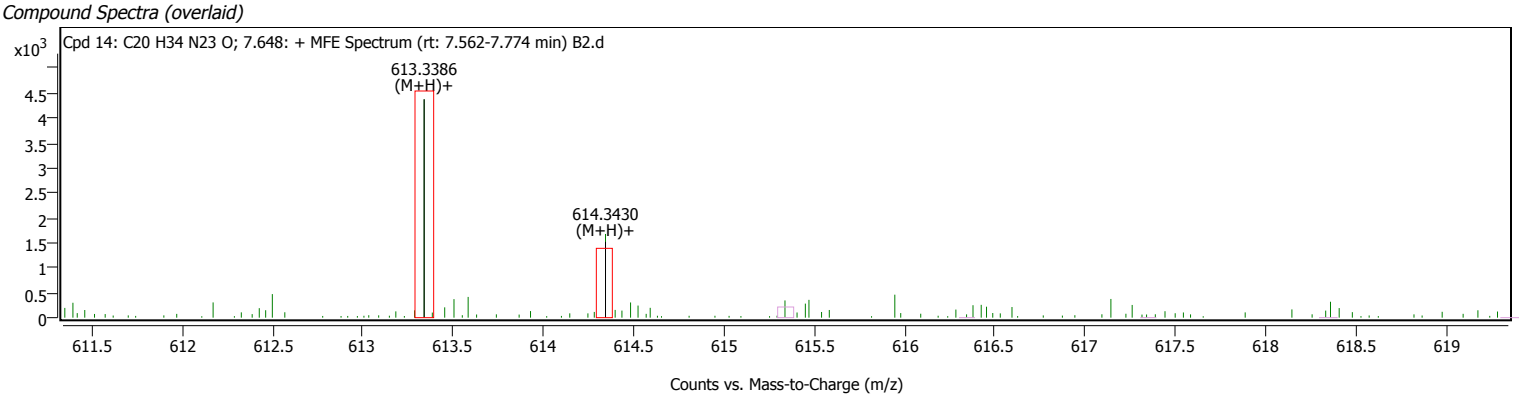
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C20 H34 N23 O	(M+H)+	MFG	7.648		612.3320		74.58		74.58
	C22 H36 N20 O2	(M+H)+	MFG	7.648		612.3319		73.78		73.78
	C21 H40 N16 O6	(M+H)+	MFG	7.648		612.3319		72.73		72.73
	C36 H44 N4 O5	(M+H)+	MFG	7.648		612.3316		72.15		72.15
	C35 H38 N11	(M+H)+	MFG	7.648		612.3317		71.81		71.81

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 15: C22 H53 N7 O12

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H53 N7 O12	7.651		607.3756		MFG	95.86	MFE	

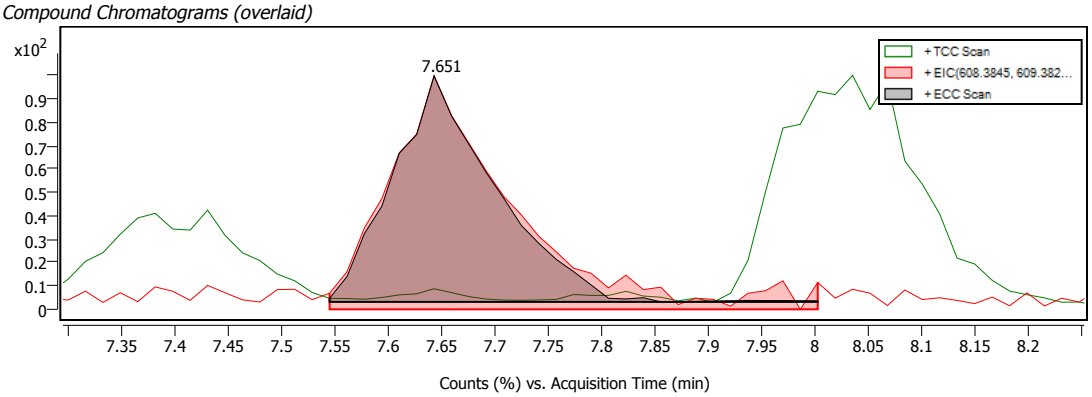
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	608.3829				5	95.86	

Compound ID Table

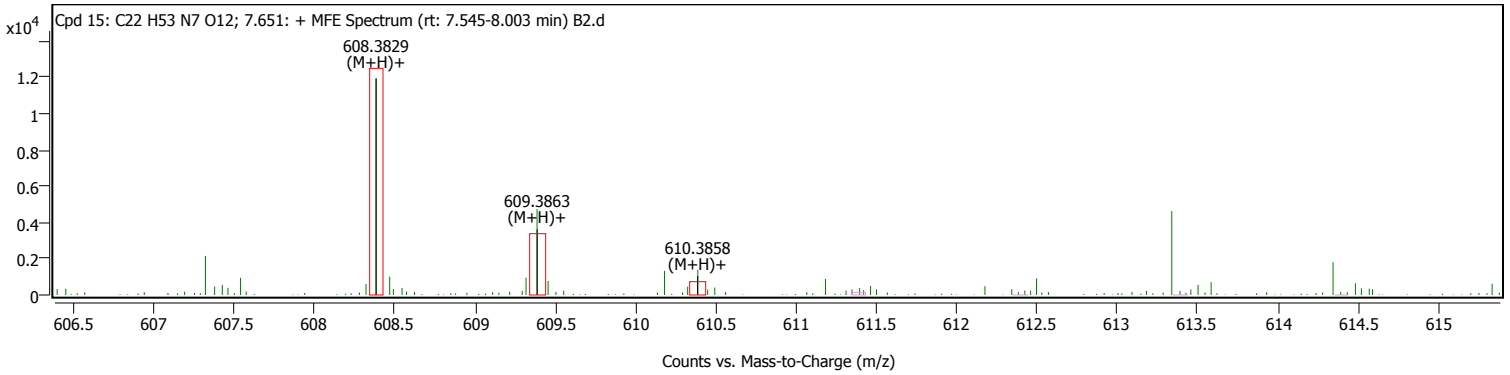
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H53 N7 O12	(M+H)+	MFG	7.651		607.3756		95.86		95.86
	C30 H57 N O9 S	(M+H)+	MFG	7.651		607.3757		95.66		95.66
	C23 H49 N11 O8	(M+H)+	MFG	7.651		607.3757		95.47		95.47
	C21 H47 N14 O7	(M+H)+	MFG	7.651		607.3758		95.44		95.44
	C24 H55 N4 O13	(M+H)+	MFG	7.651		607.3755		95.23		95.23

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 16: C37 H42 N11 O

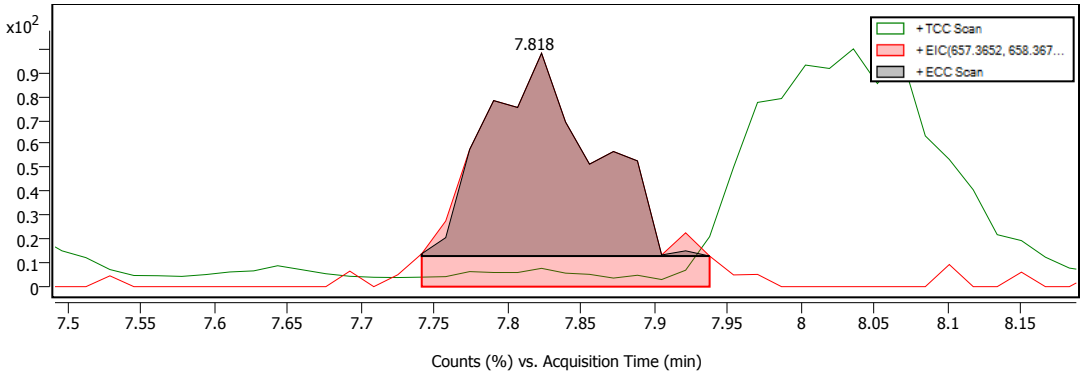
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H42 N11 O	7.818		656.3579		MFG	72.30	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	657.3649				5	72.30	

Compound ID Table

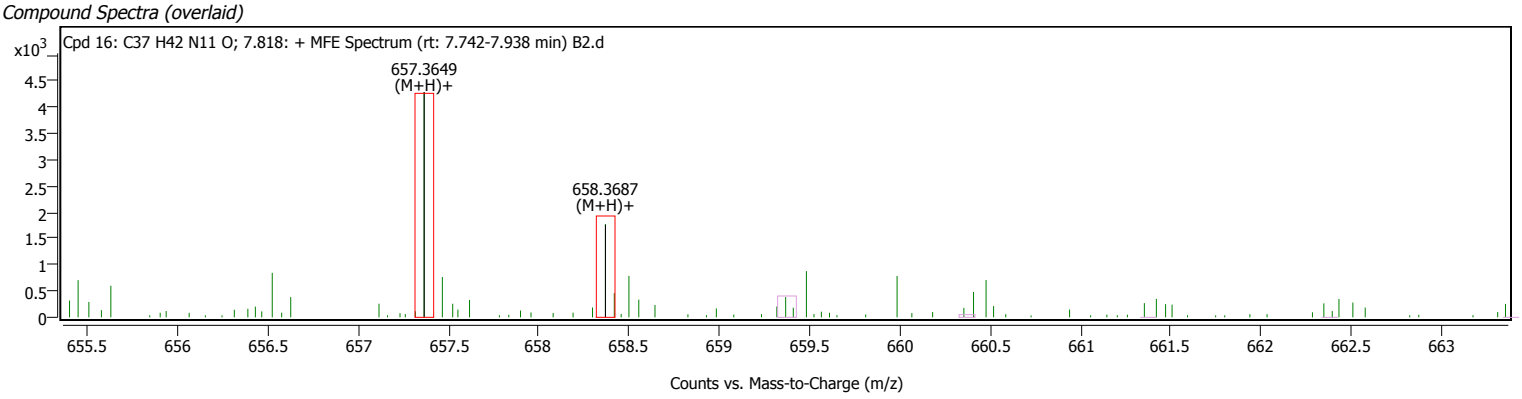
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H42 N11 O	(M+H)+	MFG	7.818		656.3579		72.30		72.30
	C38 H48 N4 O6	(M+H)+	MFG	7.818		656.3578		71.53		71.53
	C39 H44 N8 O2	(M+H)+	MFG	7.818		656.3579		70.75		70.75
	C22 H38 N23 O2	(M+H)+	MFG	7.818		656.3582		69.89		69.89
	C40 H50 N O7	(M+H)+	MFG	7.818		656.3578		69.65		69.65

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 17: C32 H61 N O10 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H61 N O10 S	7.824		651.4020		MFG	95.54	MFE	

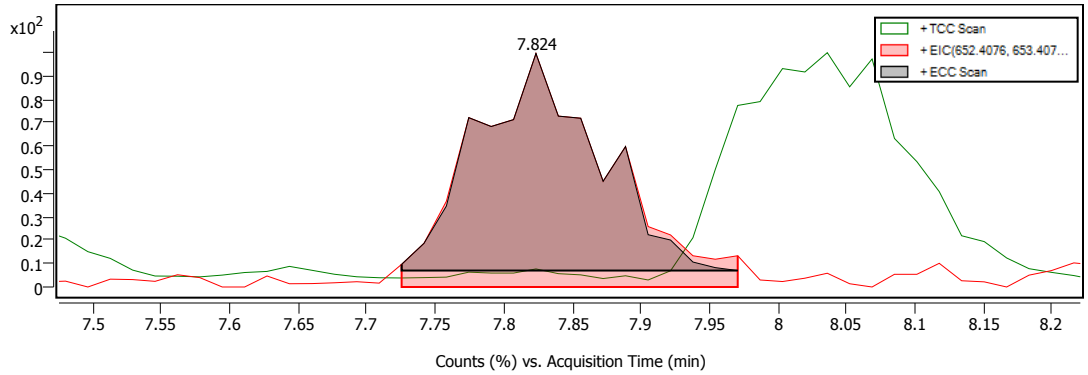
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	652.4090				5	95.54	

Compound ID Table

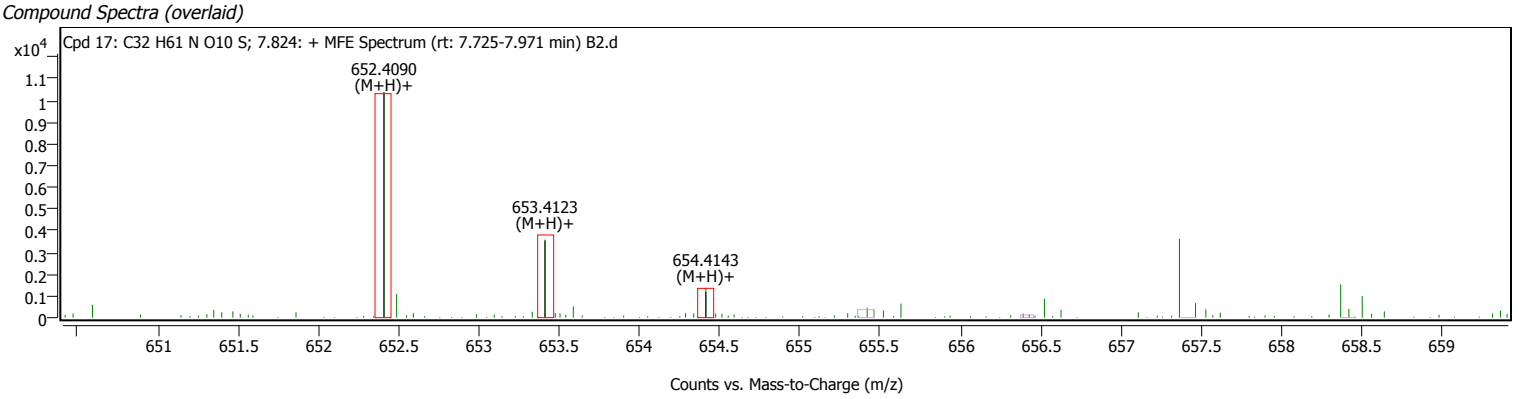
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H61 N O10 S	(M+H)+	MFG	7.824		651.4020		95.54		95.54
	C31 H55 N8 O5 S	(M+H)+	MFG	7.824		651.4021		94.63		94.63
	C25 H53 N11 O9	(M+H)+	MFG	7.824		651.4019		94.03		94.03
	C26 H59 N4 O14	(M+H)+	MFG	7.824		651.4018		93.95		93.95
	C33 H57 N5 O6 S	(M+H)+	MFG	7.824		651.4020		93.41		93.41

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 18: C26 H59 N14 O4 S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C26 H59 N14 O4 S2	7.977		695.4281		MFG	83.29	MFE	

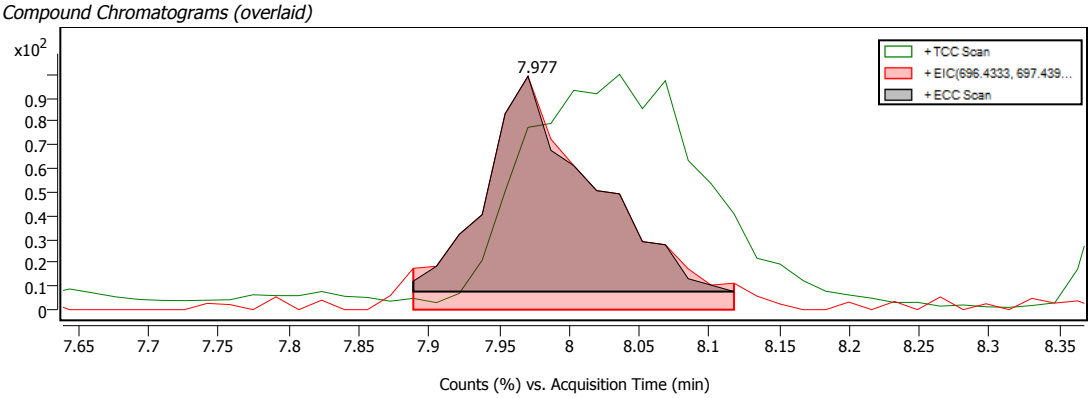
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	696.4347				6	83.29	

Compound ID Table

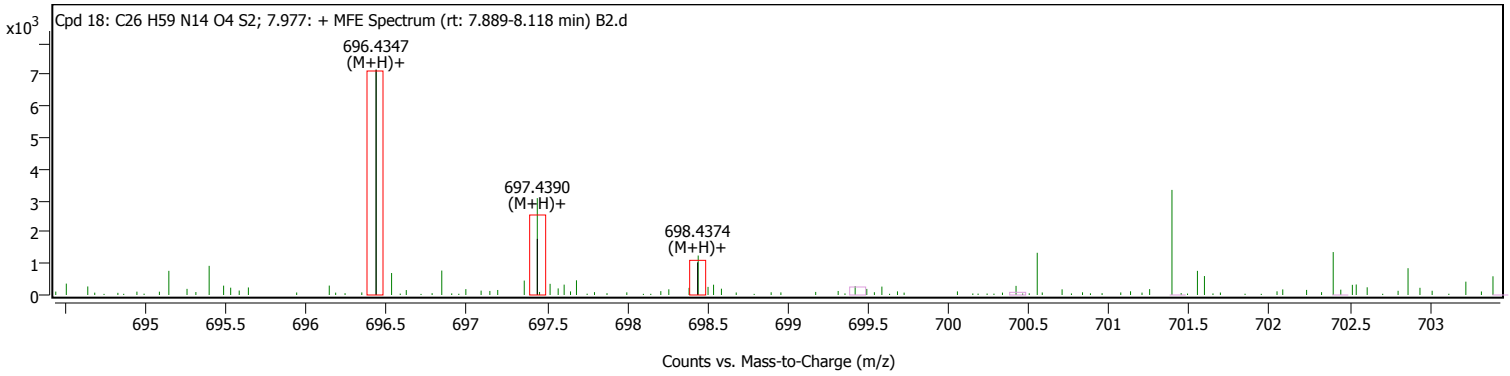
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C26 H59 N14 O4 S2	(M+H)+	MFG	7.977		695.4281		83.29		83.29
	C24 H57 N17 O3 S2	(M+H)+	MFG	7.977		695.4282		82.78		82.78
	C34 H65 N O11 S	(M+H)+	MFG	7.977		695.4276		81.15		81.15
	C32 H63 N4 O10 S	(M+H)+	MFG	7.977		695.4277		80.22		80.22
	C33 H59 N8 O6 S	(M+H)+	MFG	7.977		695.4277		78.84		78.84
Mycinamicin IV	C37 H61 N O11	(M+H)+	DBSearch	7.977		695.4272	73684-71-6	64.26	64.26	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 19: C27 H40 N24

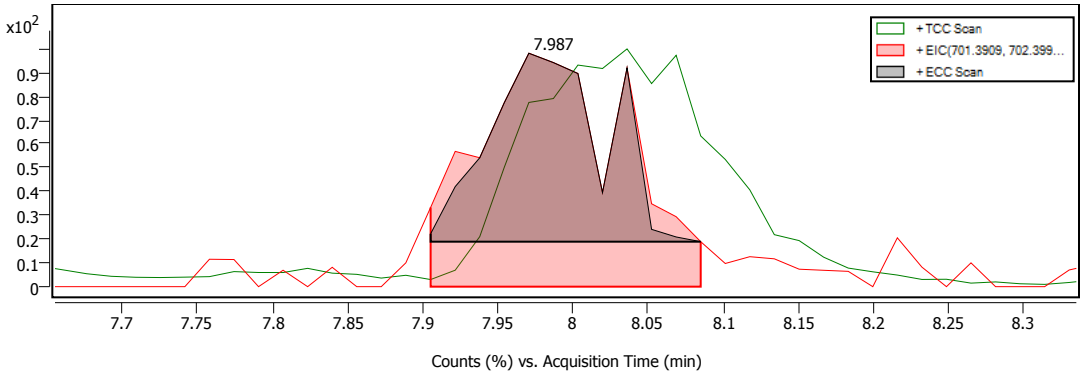
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C27 H40 N24	7.987		700.3860		MFG	68.71	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	701.3923				5	68.71	

Compound ID Table

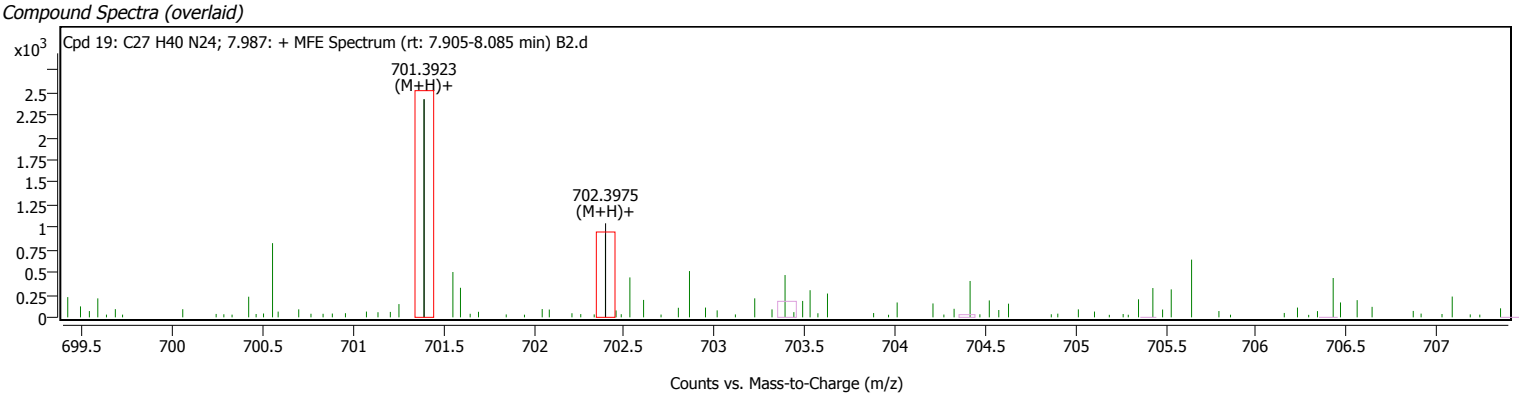
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C27 H40 N24	(M+H)+	MFG	7.987		700.3860		68.71		68.71
	C41 H48 N8 O3	(M+H)+	MFG	7.987		700.3857		67.17		67.17
	C26 H44 N20 O4	(M+H)+	MFG	7.987		700.3859		67.00		67.00
	C42 H54 N O8	(M+H)+	MFG	7.987		700.3856		67.00		67.00
	C28 H46 N17 O5	(M+H)+	MFG	7.987		700.3859		66.83		66.83

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 20: C28 H53 N8 O4

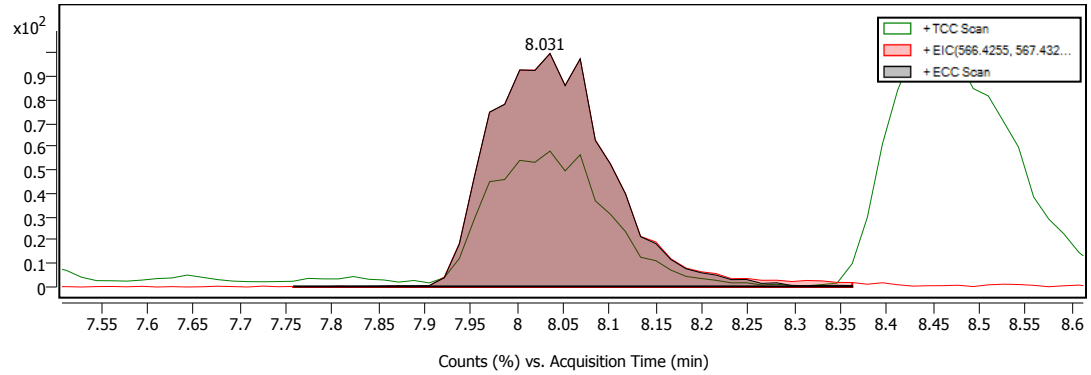
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H53 N8 O4	8.031		565.4185		MFG	99.10	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	566.4254 588.4077				6	99.10	

Compound ID Table

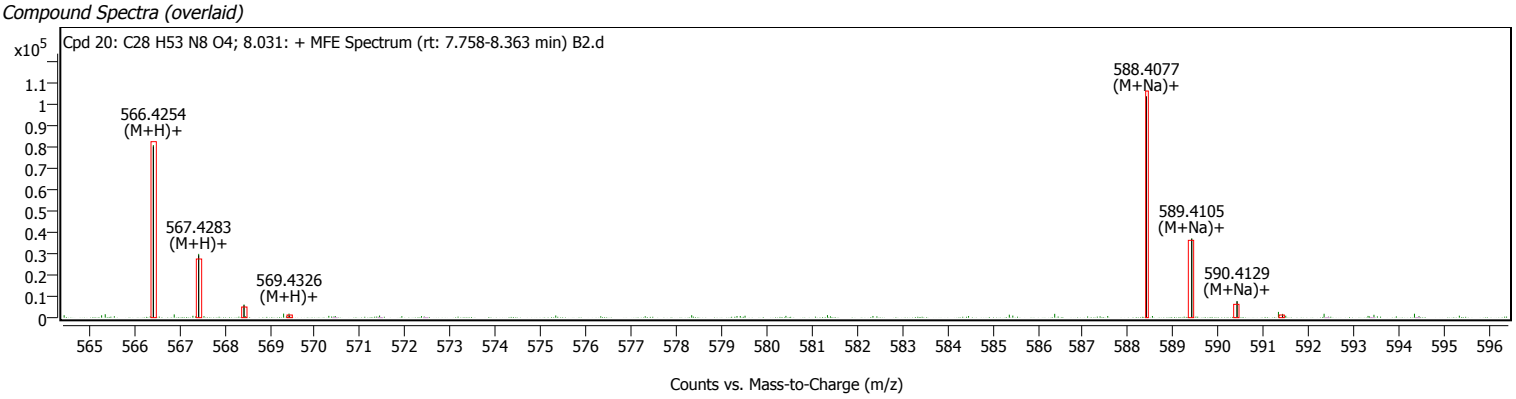
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H53 N8 O4	(M+H)+ (M+Na)+	MFG	8.031		565.4185		99.10		99.10
	C29 H59 N O9	(M+H)+ (M+Na)+	MFG	8.031		565.4183		97.74		97.74
	C26 H51 N11 O3	(M+H)+ (M+Na)+	MFG	8.031		565.4185		97.46		97.46
	C27 H57 N4 O8	(M+H)+ (M+Na)+	MFG	8.031		565.4184		96.86		96.86
	C29 H49 N12	(M+Na)+	MFG	8.031		565.4185		94.47		94.47
	C34 H55 N5 S	(M+H)+	MFG	8.031		565.4183		92.22		92.22

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 21: C41 H57 N9 O4

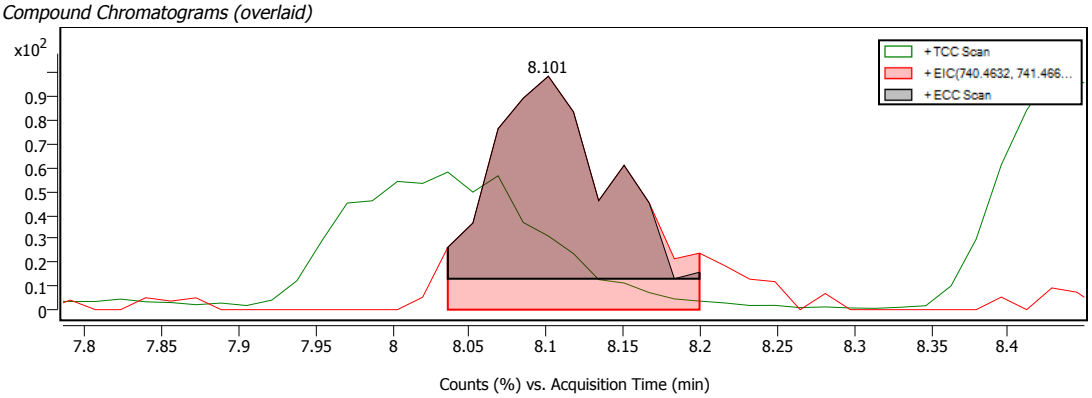
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C41 H57 N9 O4	8.101		739.4536		MFG	67.90	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	740.4604				9	67.90	

Compound ID Table

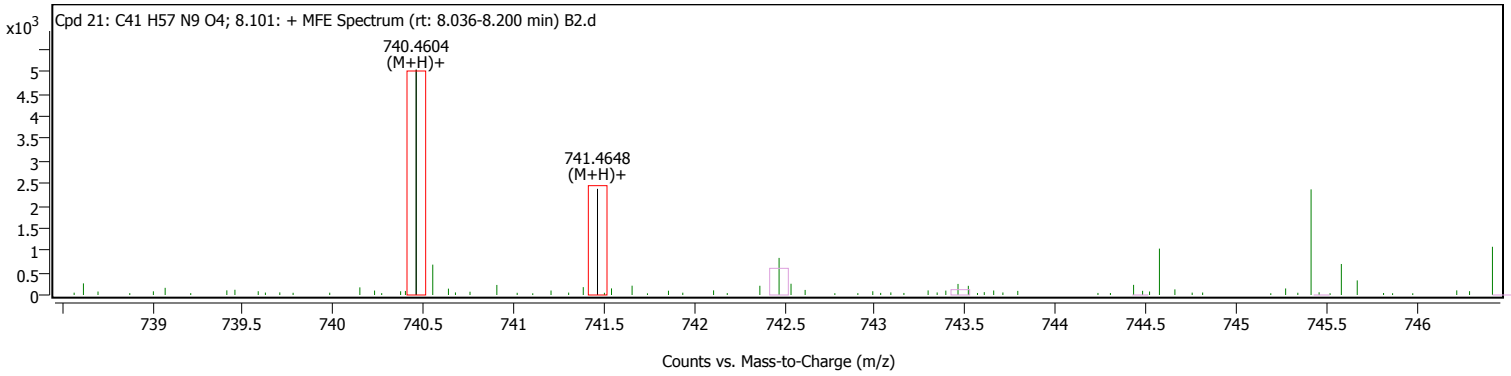
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C41 H57 N9 O4	(M+H)+	MFG	8.101		739.4536		67.90		67.90
	C42 H63 N2 O9	(M+H)+	MFG	8.101		739.4535		67.16		67.16
	C42 H53 N13	(M+H)+	MFG	8.101		739.4536		66.60		66.60
	C25 H47 N28	(M+H)+	MFG	8.101		739.4540		66.51		66.51
	C43 H59 N6 O5	(M+H)+	MFG	8.101		739.4535		65.73		65.73
Lycoperoside D	C39 H65 N O12	(M+H)+	DBSearch	8.101		739.4535	81037-16-3	57.40	57.40	
Yamogenin 3-O-neohesperidoside	C39 H62 O12	(M+NH4)+	DBSearch	8.101		722.4269	110996-52-6	57.14	57.14	
Ophiopogonin B	C39 H62 O12	(M+NH4)+	DBSearch	8.101		722.4269	38971-41-4	57.14	57.14	
Ophiopogonin C'	C39 H62 O12	(M+NH4)+	DBSearch	8.101		722.4269	19057-67-1	57.14	57.14	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 22: C34 H75 N4 O18

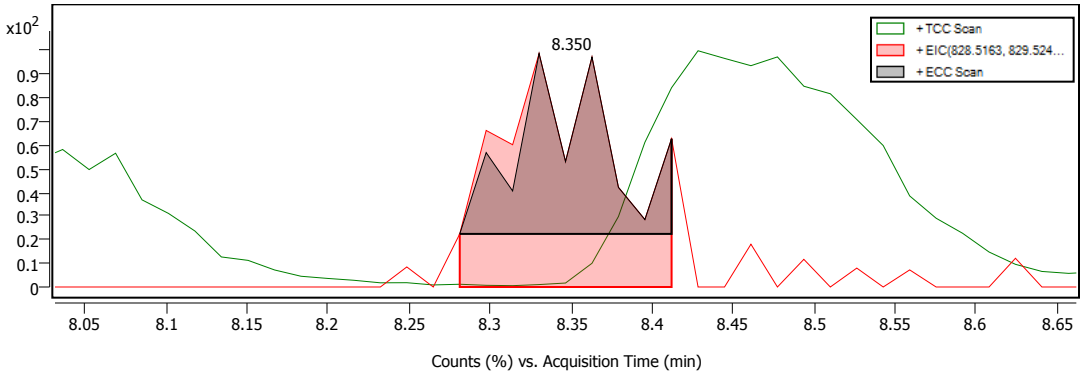
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H75 N4 O18	8.350		827.5082		MFG	58.25	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	828.5139				6	58.25	

Compound ID Table

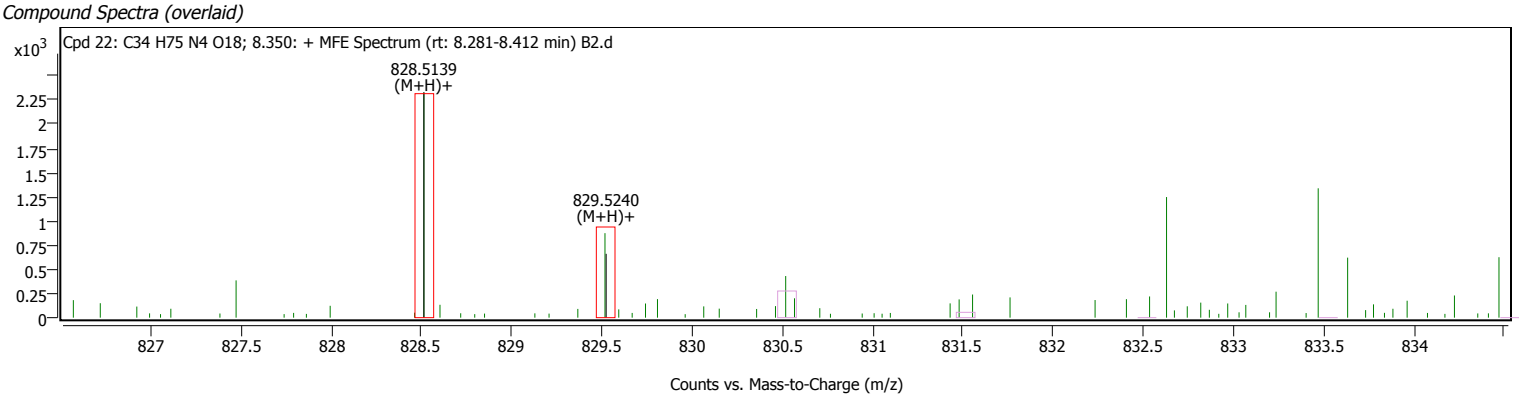
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H75 N4 O18	(M+H)+	MFG	8.350		827.5082		58.25		58.25
	C33 H69 N11 O13	(M+H)+	MFG	8.350		827.5083		57.81		57.81
	C32 H63 N18 O8	(M+H)+	MFG	8.350		827.5084		57.25		57.25
	C35 H71 N8 O14	(M+H)+	MFG	8.350		827.5082		56.64		56.64
	C31 H57 N25 O3	(M+H)+	MFG	8.350		827.5084		56.58		56.58
Mycobactin S	C44 H69 N5 O10	(M+H)+	DBSearch	8.350		827.5082	26769-11-9	40.34	40.34	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 23: GalCer(d18:0/26:0)

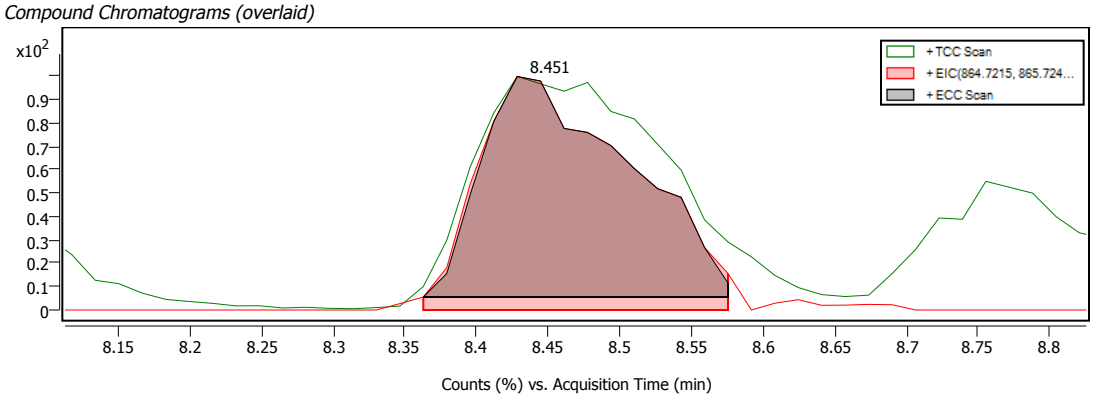
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
GalCer(d18:0/26:0)	C50 H99 N O8	8.451		841.7340		DBSearch	79.42	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	864.7233 864.7233 864.7233		0	79.42	9		

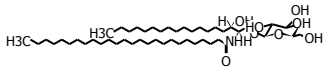
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
GalCer(d18:0/26:0)	C50 H99 N O8	(M+Na)+	DBSearch	8.451		841.7340		79.42	79.42	
GlcCer(d18:0/26:0)	C50 H99 N O8	(M+Na)+	DBSearch	8.451		841.7340		79.42	79.42	
	C38 H84 N22 O	(M+H)+	MFG	8.451		864.7193		60.07		60.07
	C40 H86 N19 O2	(M+H)+	MFG	8.451		864.7193		56.33		56.33
	C28 H Cl3 O19 S3	(M+Na)+	MFG	8.451		841.7341		47.60		47.60
	C45 H97 N10 S2	(M+Na)+	MFG	8.451		841.7341		47.58		47.58
	C60 H93 N2	(M+Na)+	MFG	8.451		841.7341		47.57		47.57
	C45 H89 N14 O	(M+Na)+	MFG	8.451		841.7341		47.54		47.54
	C46 H95 N7 O6	(M+Na)+	MFG	8.451		841.7341		47.54		47.54

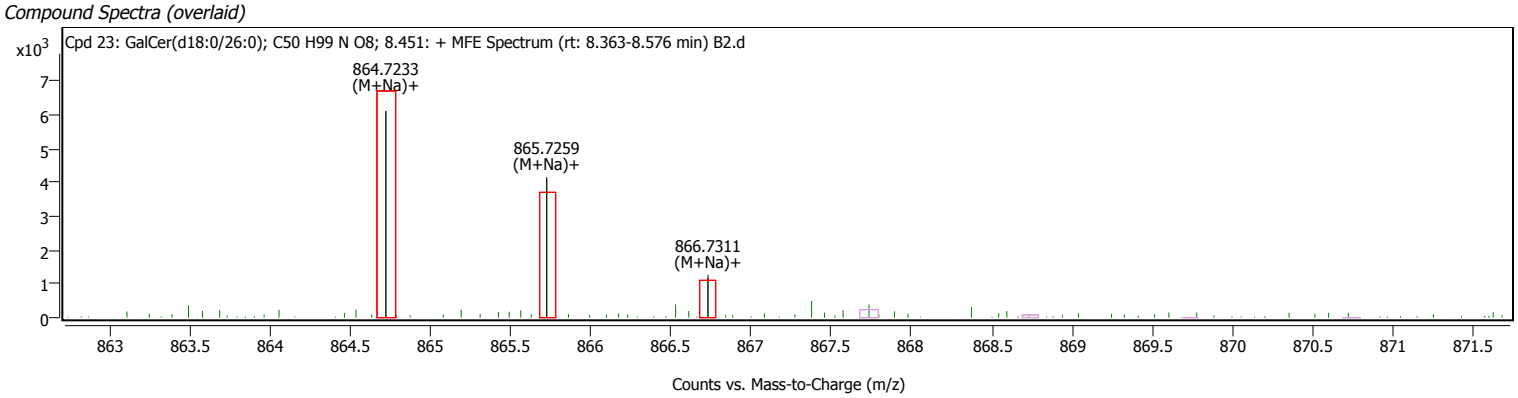
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 24: C33 H58 N16

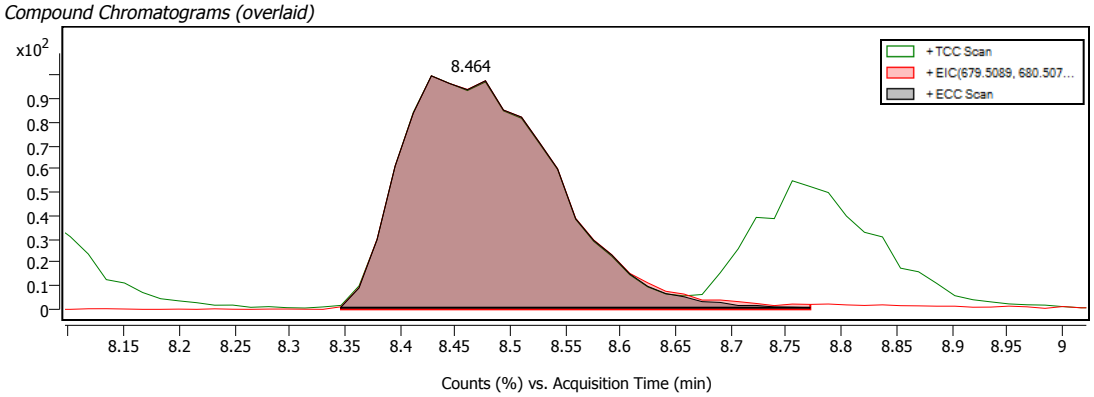
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H58 N16	8.464		678.5024		MFG	98.61	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	679.5091 701.4915				5	98.61	

Compound ID Table

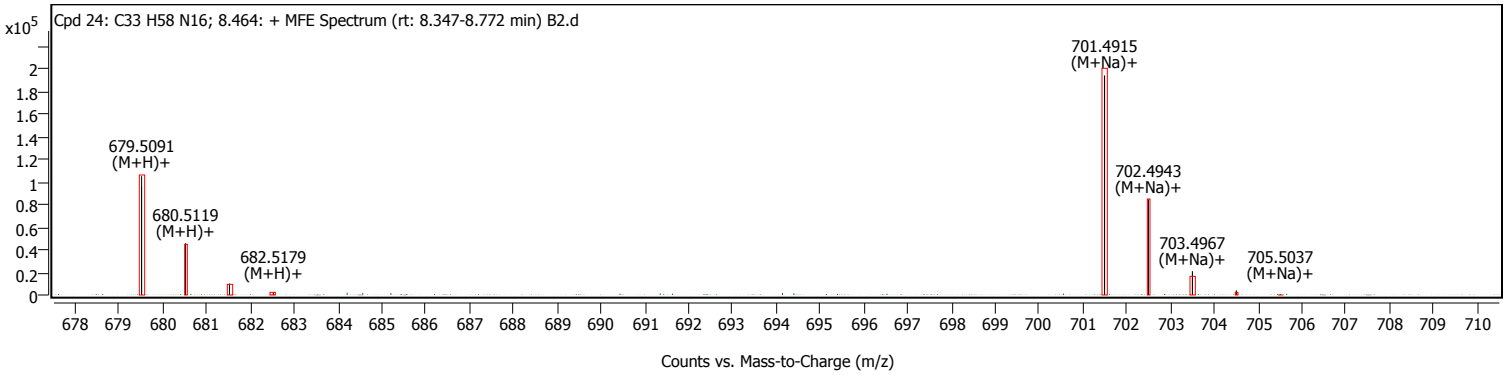
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H58 N16	(M+H)+ (M+Na)+	MFG	8.464		678.5024		98.61		98.61
	C32 H62 N12 O4	(M+H)+ (M+Na)+	MFG	8.464		678.5019		98.61		98.61
	C34 H64 N9 O5	(M+H)+ (M+Na)+	MFG	8.464		678.5022		98.37		98.37
	C33 H68 N5 O9	(M+H)+ (M+Na)+	MFG	8.464		678.5022		97.34		97.34
	C35 H70 N2 O10	(M+H)+ (M+Na)+	MFG	8.464		678.5021		97.06		97.06

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 25: 1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine

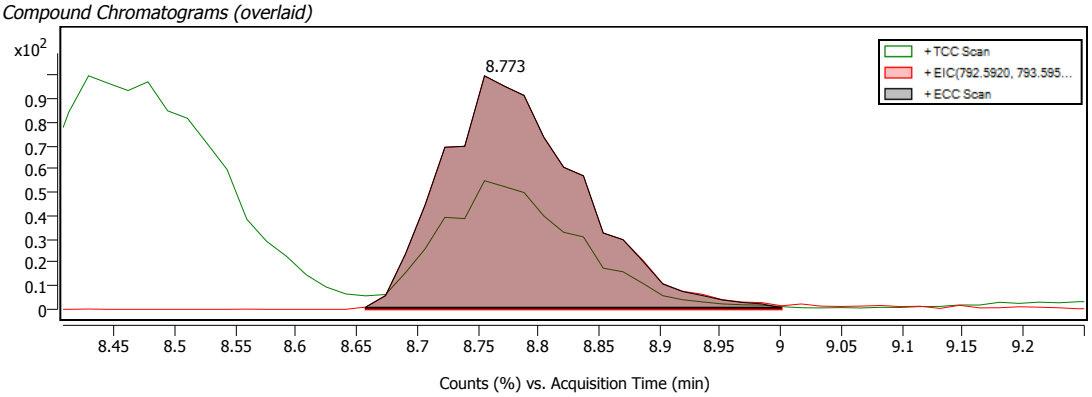
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	8.773		814.5753		DBSearch	99.40	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
M+	814.5748 814.5748 814.5748		0	99.40	16		

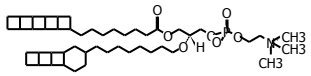
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	M+	DBSearch	8.773		814.5753		99.40	99.40	
	C38 H73 N13 O5	(M+H)+	MFG	8.773		791.5854		98.88		98.88
	C37 H67 N20	(M+H)+	MFG	8.773		791.5856		98.77		98.77
	C39 H79 N6 O10	(M+H)+	MFG	8.773		791.5853		98.14		98.14
	C36 H71 N16 O4	(M+H)+	MFG	8.773		791.5855		96.95		96.95
	C37 H77 N9 O9	(M+H)+	MFG	8.773		791.5853		96.75		96.75
	C30 H66 N25 O	(M+Na)+	MFG	8.773		792.5891		78.23		78.23
	C32 H68 N22 O2	(M+Na)+	MFG	8.773		792.5890		78.04		78.04
	C35 H76 N12 O8	(M+Na)+	MFG	8.773		792.5889		75.26		75.26
	C28 H64 N28	(M+Na)+	MFG	8.773		792.5892		74.41		74.41
	C34 H70 N19 O3	(M+Na)+	MFG	8.773		792.5890		73.74		73.74
	C44 H72 N13 S	M+	MFG	8.773		814.5754		47.61		47.61
	C45 H78 N6 O5 S	M+	MFG	8.773		814.5754		47.61		47.61
	C42 H89 Cl N3 O3 S3	M+	MFG	8.773		814.5754		47.61		47.61
	C38 H80 N5 O13	M+	MFG	8.773		814.5754		47.61		47.61
	C37 H74 N12 O8	M+	MFG	8.773		814.5754		47.61		47.61

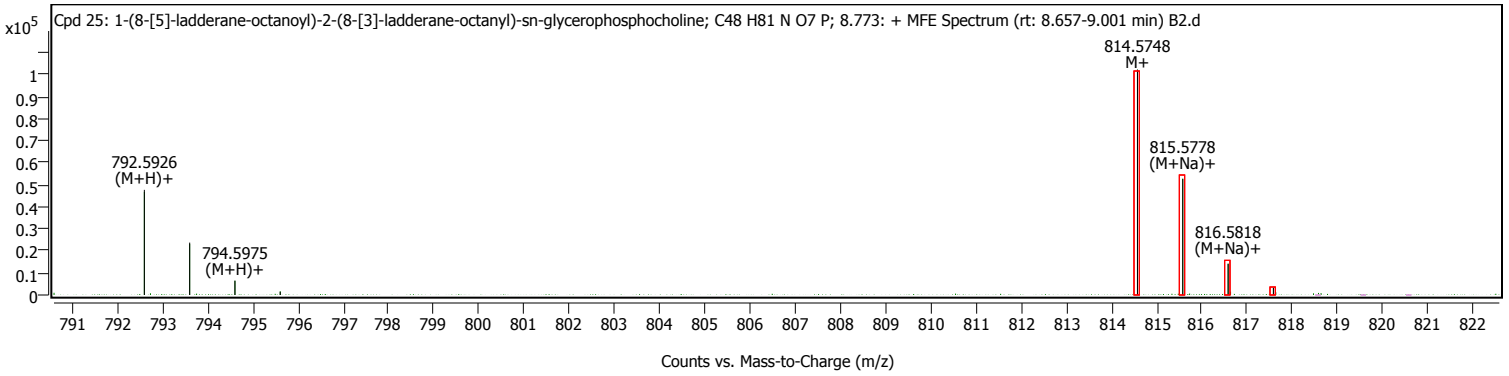
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)

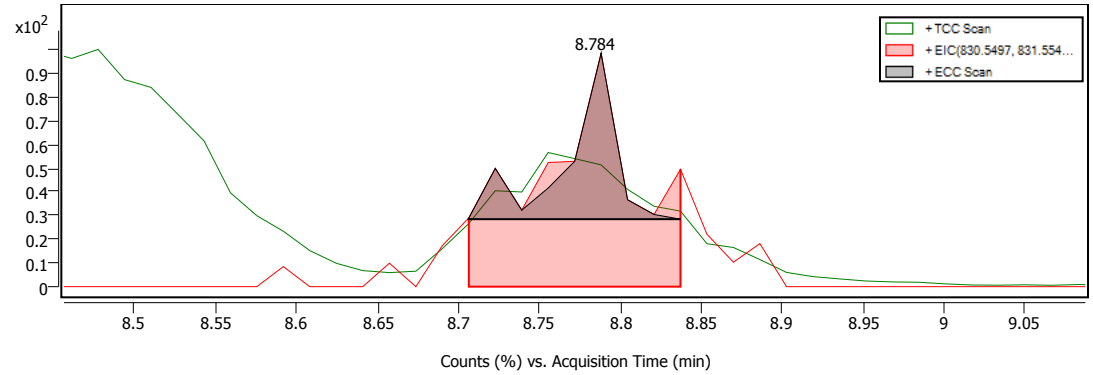


Cpd 26: 8.784

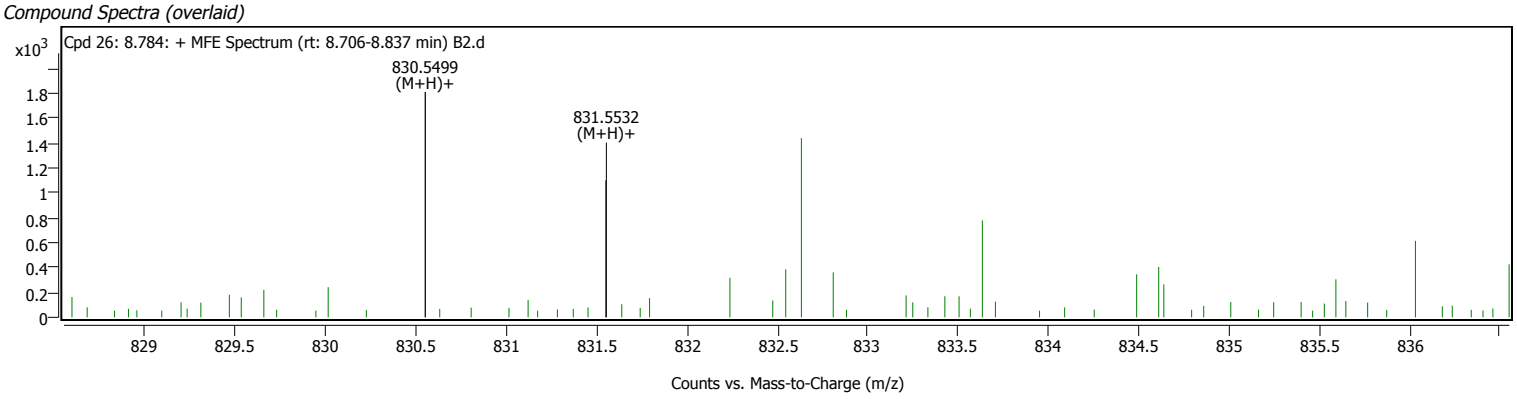
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		8.784		829.5427				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

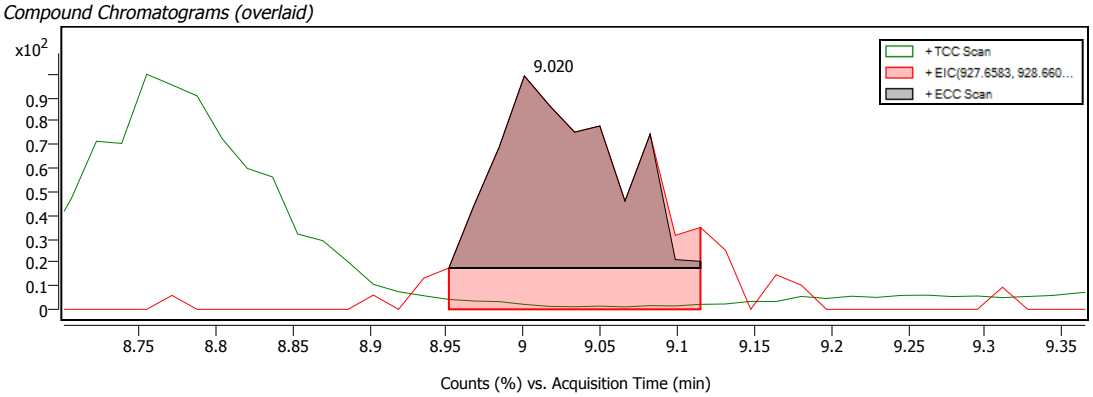


Cpd 27: 9.020

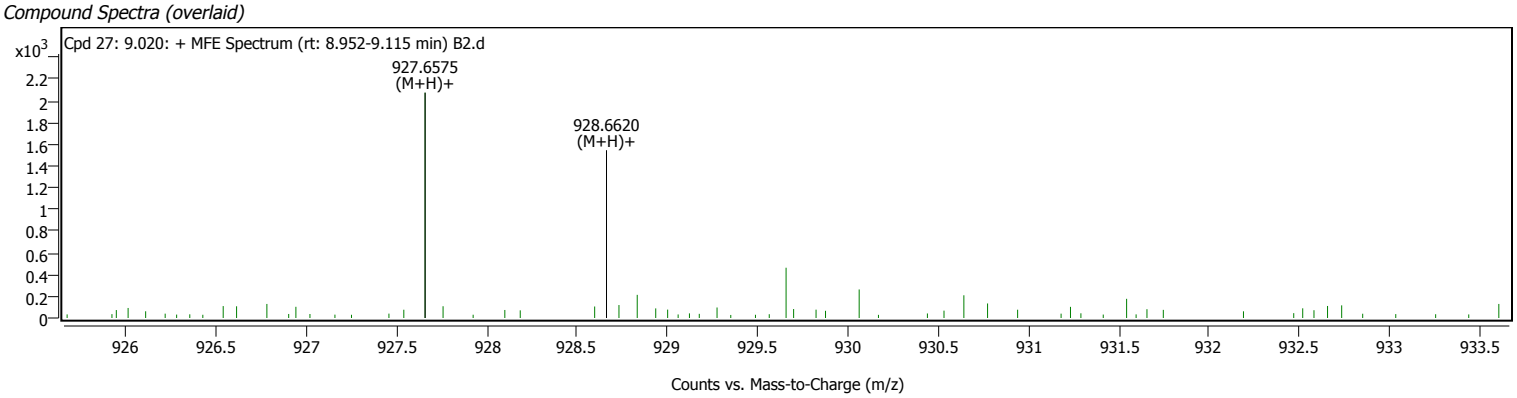
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		9.020		926.6502				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 28: C47 H67 N13

Compound Discovery Report

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C47 H67 N13	9.135		813.5635		MFG	58.26	MFE	

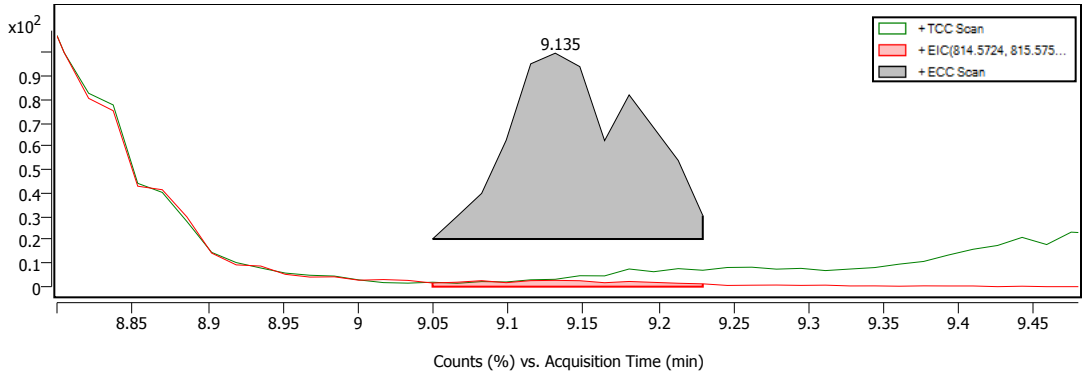
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	814.5698				5	58.26	

Compound ID Table

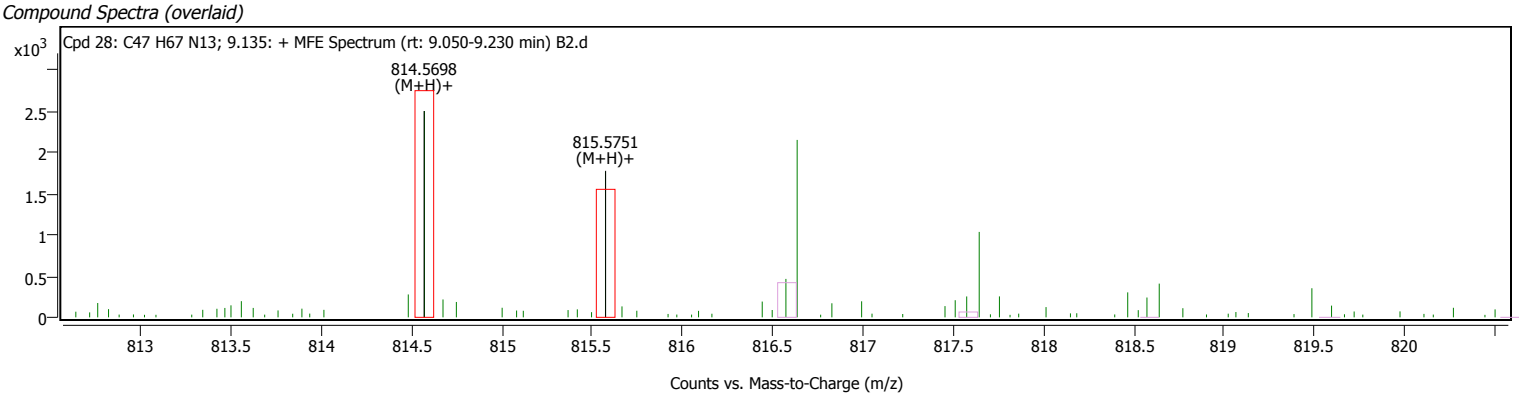
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C47 H67 N13	(M+H)+	MFG	9.135		813.5635		58.26		58.26
	C49 H69 N10 O	(M+H)+	MFG	9.135		813.5635		54.27		54.27
	C51 H71 N7 O2	(M+H)+	MFG	9.135		813.5634		47.25		47.25
	C57 H71 N3 O	(M+H)+	MFG	9.135		813.5633		46.69		46.69
	C53 H73 N4 O3	(M+H)+	MFG	9.135		813.5634		38.82		38.82

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 29: Halaminol A

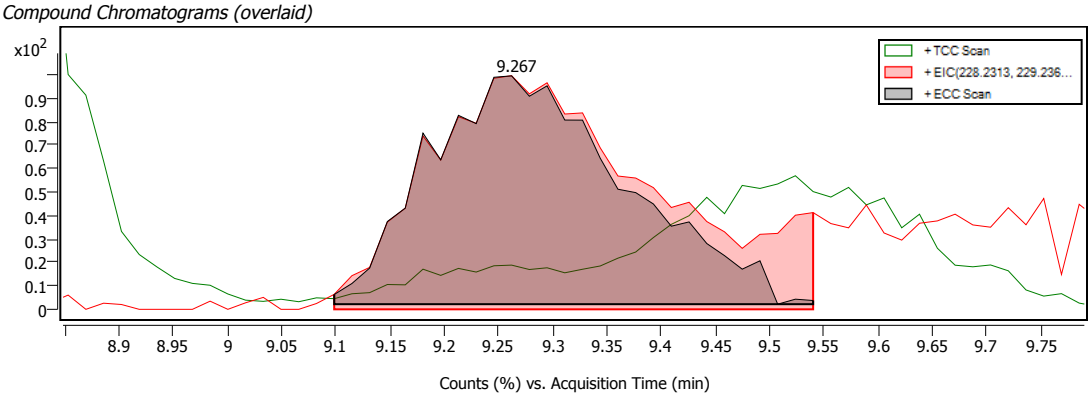
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Halaminol A	C14 H29 N O	9.267		227.2243		DBSearch-MFG	83.81	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	228.2316 228.2316 228.2316		0	83.80	31	83.82	

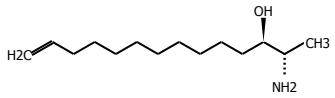
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Halaminol A	C14 H29 N O	(M+H)+	DBSearch-MFG	9.267		227.2243		83.81	83.80	83.82
1-Tetradecen-3-one	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
11Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
3-methyl-6-(1-methyl-ethyl)-3,9-decadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9S-(2-cyclopentenyl)-1-nonanol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9R-(2-cyclopentenyl)-1-nonanol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
11E,13-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
10E,12E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
8E,10E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
8Z,10E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9Z,11E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9Z,12E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
10Z,12Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9Z,11Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9Z,12Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
11E-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
7-Ethyl-4E-dodecen-6-one	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
5Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
7Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
5-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
3-methyl-6-(1-methyl-ethyl)-deca-3,9-dien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9S-(2-cyclopentenyl)-nonan-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9R-(2-cyclopentenyl)-nonan-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
2-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
7-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
9-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
7E-Tetradecen-2-one	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
7Z-Tetradecen-2-one	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
1,13-Tetradecadien-3-one	C14 H26 O	(M+NH4)+	DBSearch	9.267		210.1978		83.70	83.70	
	C12 H27 N4	(M+H)+	MFG	9.267		227.2244		81.03		81.03

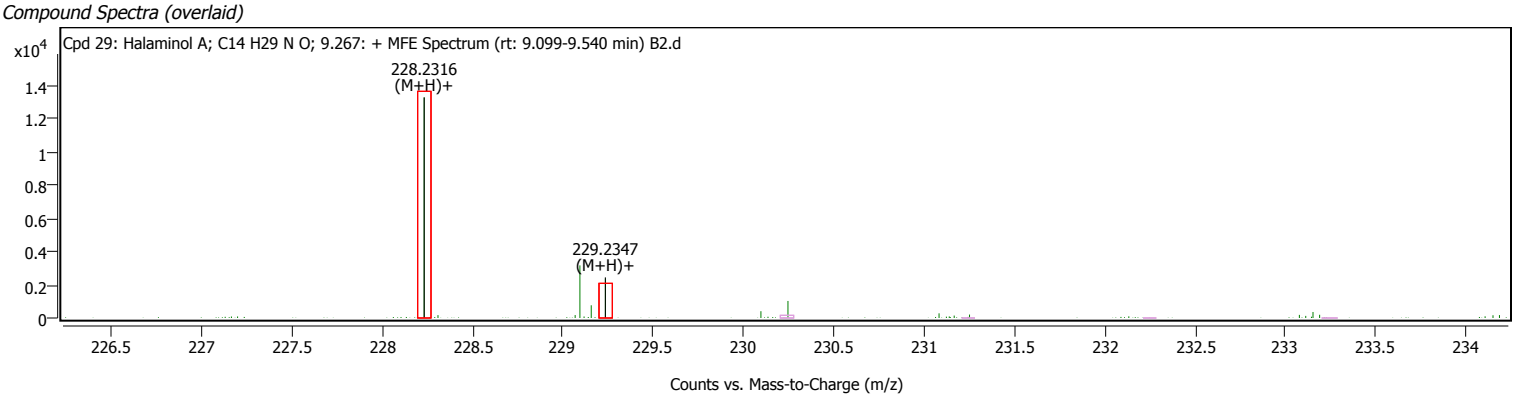
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 30: C14 H33 N4 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C14 H33 N4 O	9.425		273.2652		MFG	80.51	MFE	

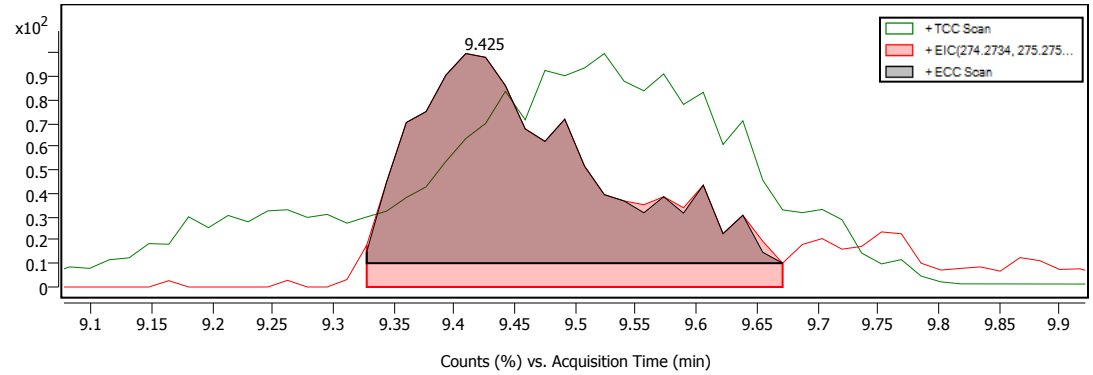
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	274.2724				4	80.51	

Compound ID Table

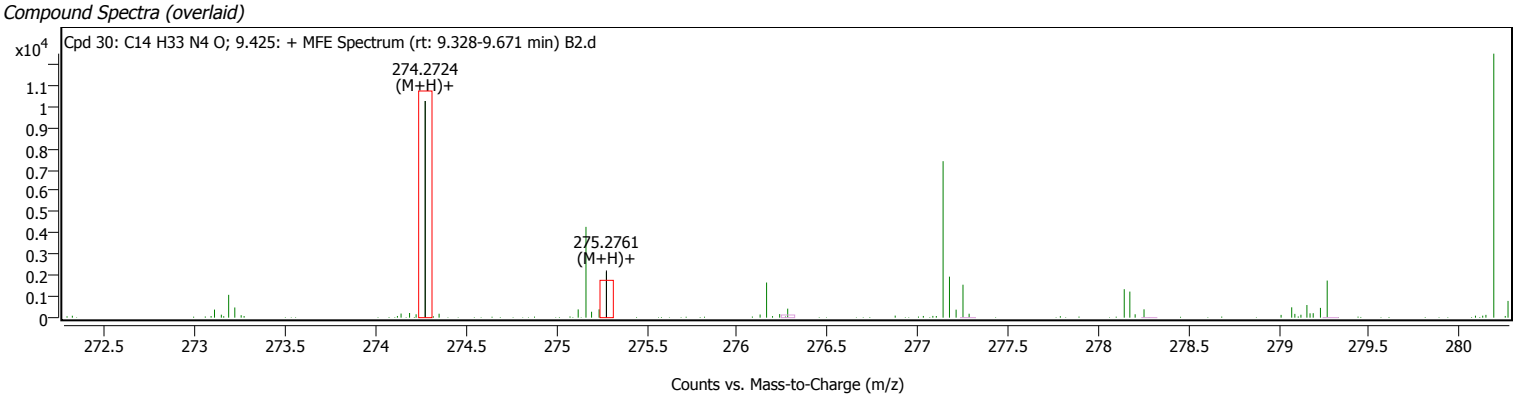
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C14 H33 N4 O	(M+H)+	MFG	9.425		273.2652		80.51		80.51
	C16 H35 N O2	(M+H)+	MFG	9.425		273.2652		74.04		74.04
	C12 H31 N7	(M+H)+	MFG	9.425		273.2653		71.89		71.89
	C17 H37 S	(M+H)+	MFG	9.425		273.2652		45.36		45.36

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 31: C37 H68 N5 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H68 N5 O	9.444		598.5421		MFG	71.89	MFE	

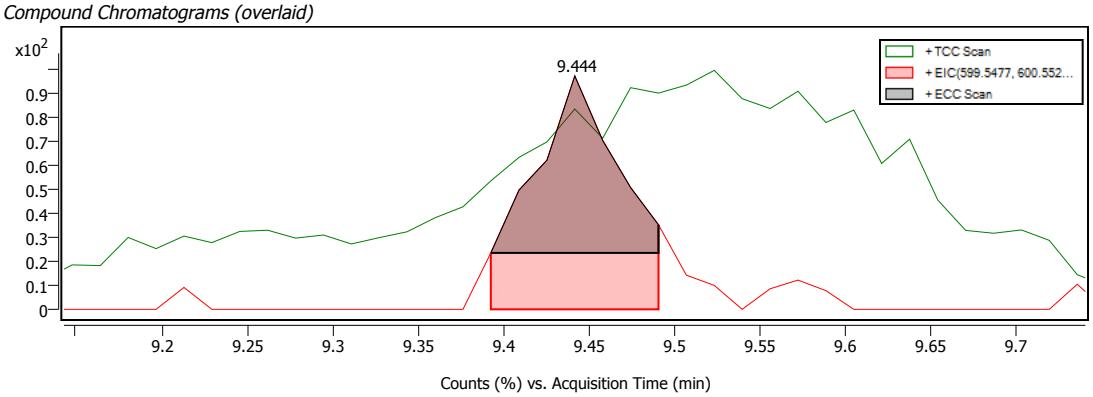
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	599.5493				5	71.89	

Compound ID Table

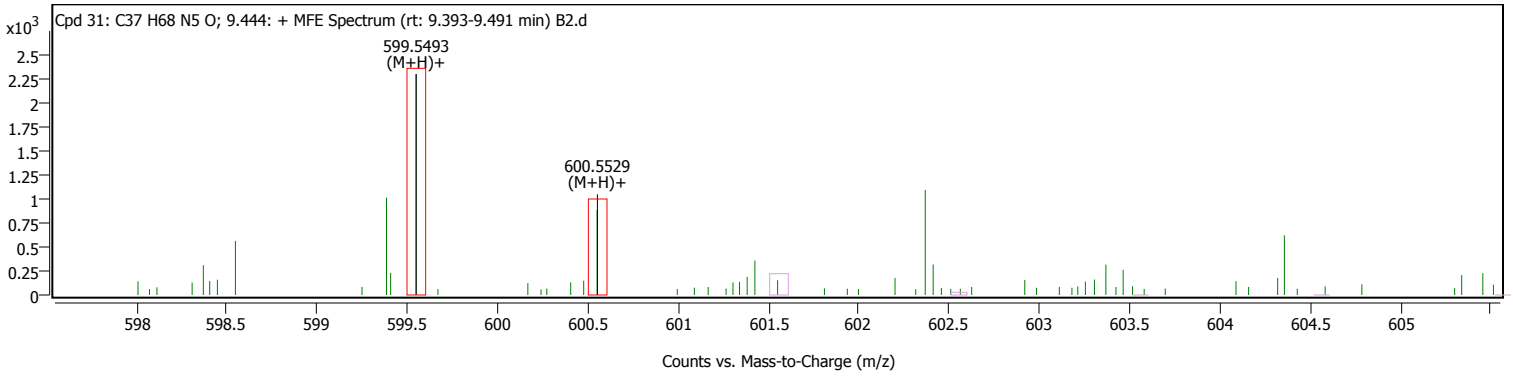
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H68 N5 O	(M+H)+	MFG	9.444		598.5421		71.89		71.89
	C35 H66 N8	(M+H)+	MFG	9.444		598.5422		70.10		70.10
	C36 H72 N O5	(M+H)+	MFG	9.444		598.5421		68.71		68.71
	C39 H70 N2 O2	(M+H)+	MFG	9.444		598.5421		67.29		67.29
	C34 H70 N4 O4	(M+H)+	MFG	9.444		598.5421		61.62		61.62

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 32: C16 H37 N4 O2

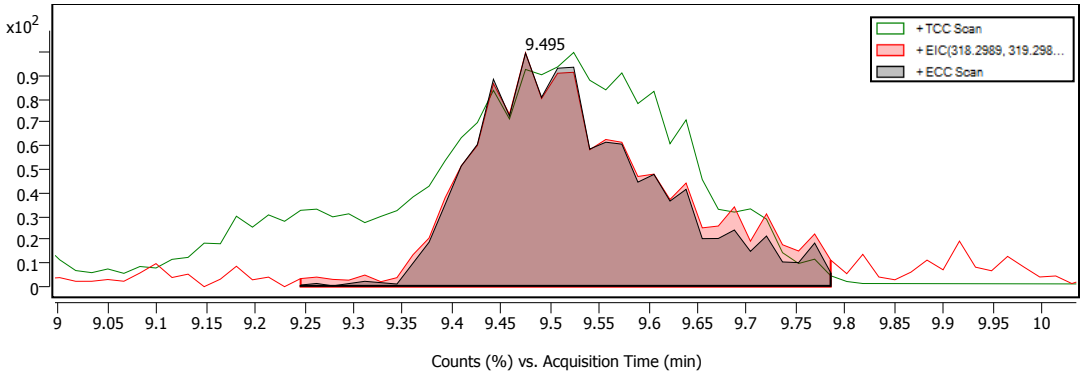
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H37 N4 O2	9.495		317.2913		MFG	83.38	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	318.2987 340.2803				5	83.38	

Compound ID Table

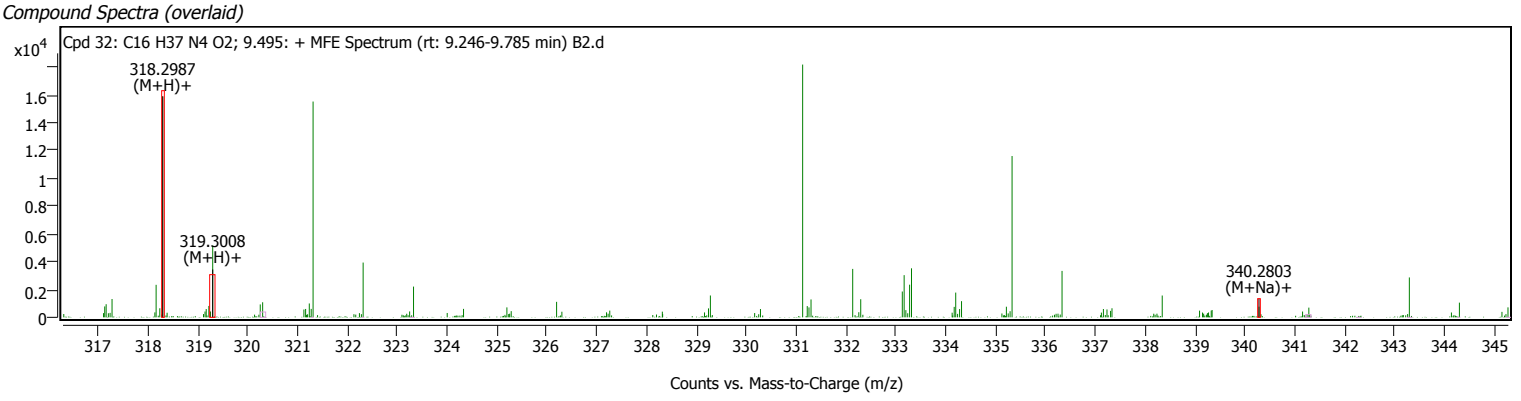
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H37 N4 O2	(M+H)+ (M+Na)+	MFG	9.495		317.2913		83.38		83.38
	C14 H35 N7 O	(M+H)+ (M+Na)+	MFG	9.495		317.2913		80.09		80.09
	C18 H39 N O3	(M+H)+ (M+Na)+	MFG	9.495		317.2912		73.86		73.86
	C12 H33 N10	(M+H)+ (M+Na)+	MFG	9.495		317.2914		65.78		65.78
	C19 H41 O S	(M+H)+	MFG	9.495		317.2912		48.29		48.29

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 33: C37 H38 N11 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H38 N11 O2	9.538		668.3210		MFG	65.26	MFE	

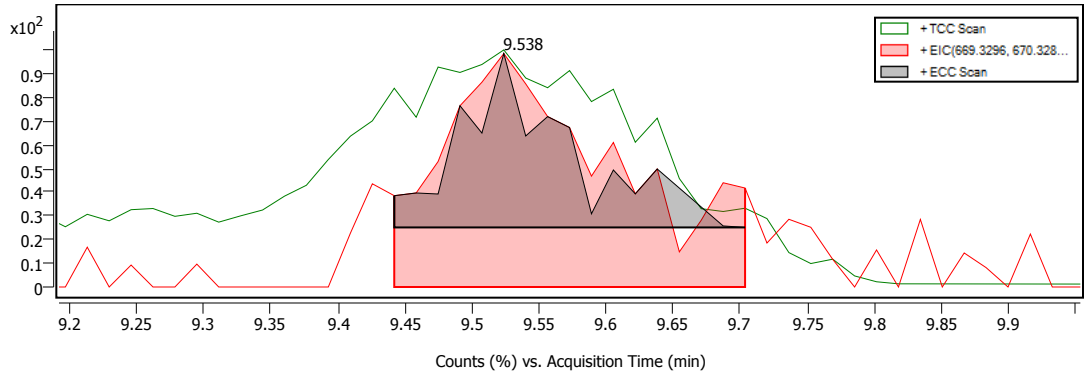
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	669.3298				5	65.26	

Compound ID Table

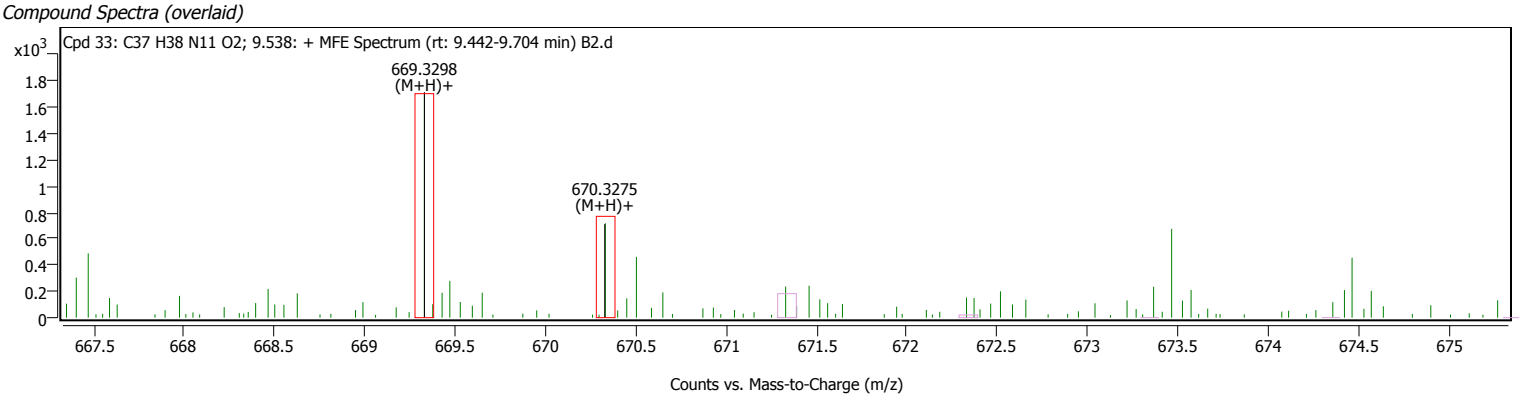
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H38 N11 O2	(M+H)+	MFG	9.538		668.3210		65.26		65.26
	C22 H34 N23 O3	(M+H)+	MFG	9.538		668.3213		65.19		65.19
	C38 H44 N4 O7	(M+H)+	MFG	9.538		668.3209		63.53		63.53
	C24 H36 N20 O4	(M+H)+	MFG	9.538		668.3213		61.84		61.84
	C23 H40 N16 O8	(M+H)+	MFG	9.538		668.3212		61.79		61.79

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 34: C18 H41 N4 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C18 H41 N4 O3	9.563		361.3177		MFG	90.74	MFE	

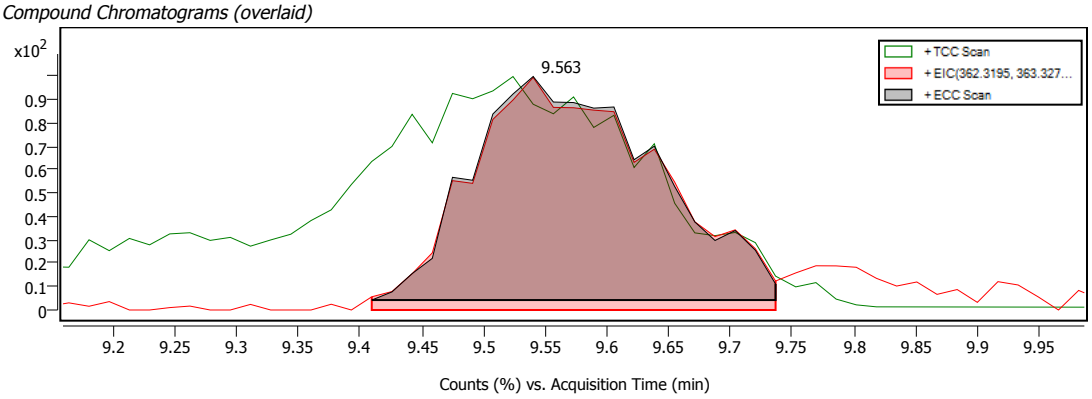
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	362.3248 384.3052				7	90.74	

Compound ID Table

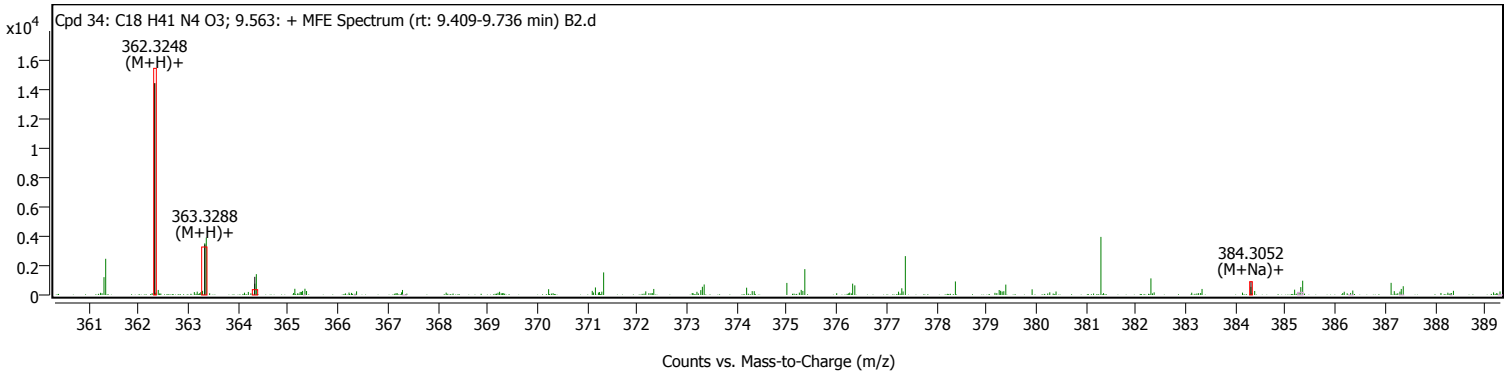
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C18 H41 N4 O3	(M+H)+ (M+Na)+	MFG	9.563		361.3177		90.74		90.74
	C20 H43 N O4	(M+H)+	MFG	9.563		361.3176		85.98		85.98
	C16 H39 N7 O2	(M+H)+ (M+Na)+	MFG	9.563		361.3178		83.34		83.34
	C21 H39 N5	(M+H)+	MFG	9.563		361.3177		71.86		71.86
	C14 H37 N10 O	(M+H)+ (M+Na)+	MFG	9.563		361.3179		66.59		66.59
	C21 H45 O2 S	(M+Na)+	MFG	9.563		361.3160		37.99		37.99
	C12 H35 N13	(M+Na)+	MFG	9.563		361.3160		36.31		36.31

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 35: (+/-)-2-methyl-5,8,11,14-all-cis-tricosatetraenoyl-2'-fluoroethylamine

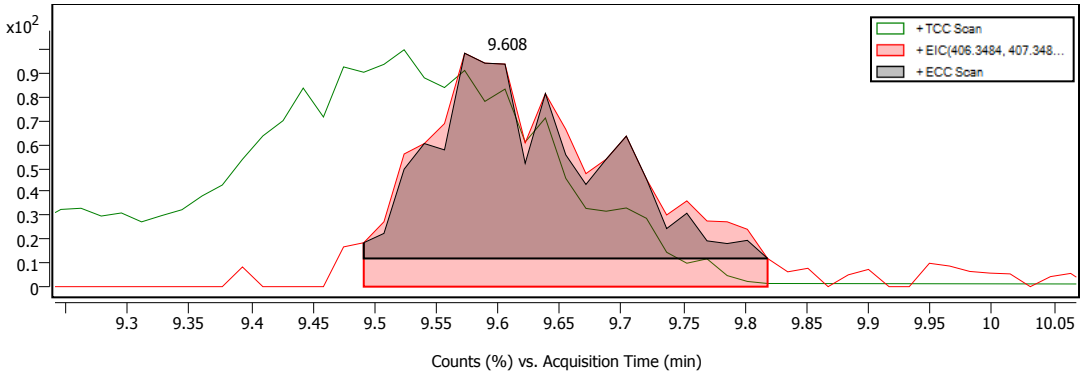
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
(+/-)-2-methyl-5,8,11,14-all-cis-tricosatetraenoyl-2'-fluoroethylamine	C26 H44 F N O	9.608		405.3421		DBSearch	74.00	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	406.3497 406.3497 406.3497		0	74.00	11		

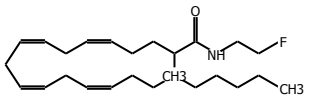
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
(+/-)-2-methyl-5,8,11,14-all-cis-tricosatetraenoyl-2'-fluoroethylamine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
(±)N-(2-fluro-ethyl)-2,16-dimethyl-5Z,8Z,11Z,14Z-docosatetraenoyl amine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
(±)N-(2-fluro-ethyl)-2,17-dimethyl-5Z,8Z,11Z,14Z-docosatetraenoyl amine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
(±)N-(2-fluro-ethyl)-2-methyl-5Z,8Z,11Z,14Z-tricosatetraenoyl amine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
(+/-)-2,16,-dimethyl-5,8,11,14-all-cis-docosatetraenoyl-2'-fluoroethylamine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
(+/-)-2,17,-dimethyl-5,8,11,14-all-cis-docosatetraenoyl-2'-fluoroethylamine	C26 H44 F N O	(M+H)+	DBSearch	9.608		405.3421		74.00	74.00	
	C18 H43 N7 O3	(M+H)+	MFG	9.608		405.3422		71.16		71.16
	C16 H41 N10 O2	(M+H)+	MFG	9.608		405.3423		68.46		68.46
	C26 H47 N S	(M+H)+	MFG	9.608		405.3421		68.46		68.46
	C29 H43 N	(M+H)+	MFG	9.608		405.3421		65.70		65.70
	C20 H45 N4 O4	(M+H)+	MFG	9.608		405.3422		63.96		63.96

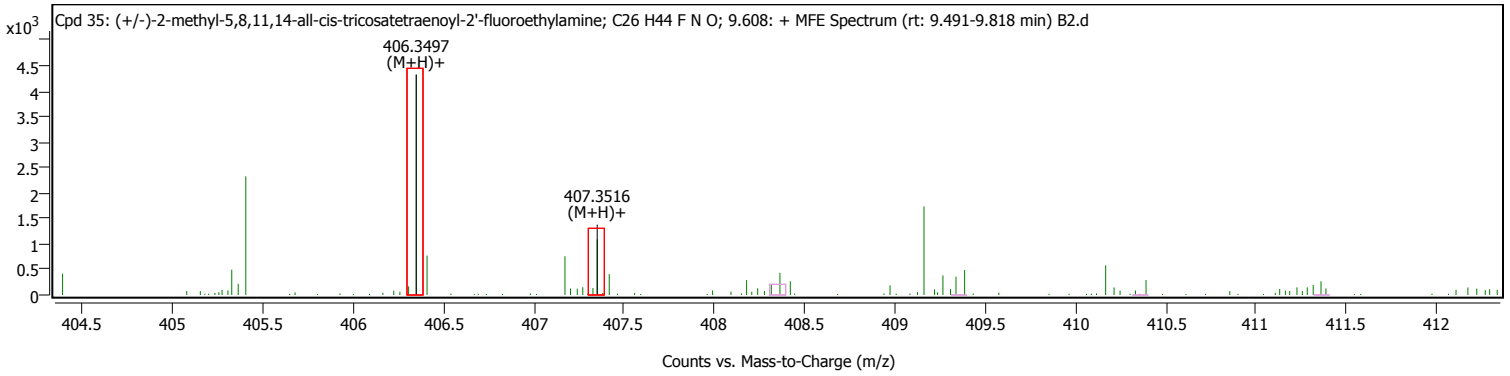
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 36: C24 H38 N23 O4

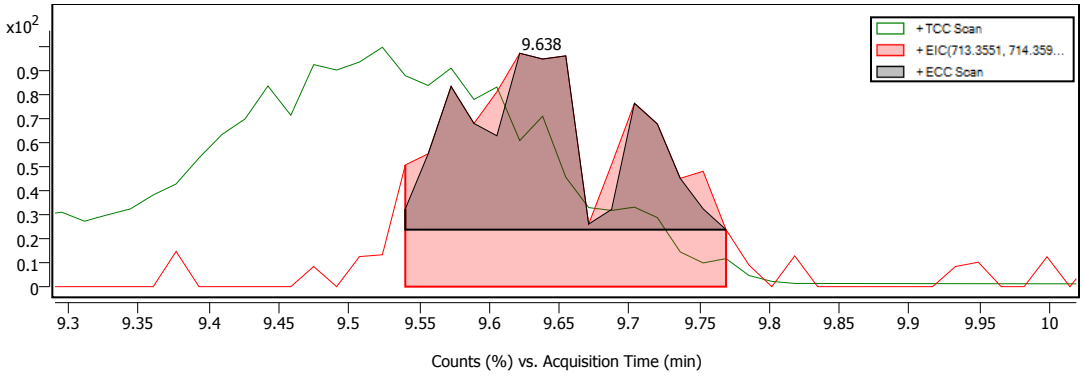
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C24 H38 N23 O4	9.638		712.3475		MFG	75.07	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	713.3541				5	75.07	

Compound ID Table

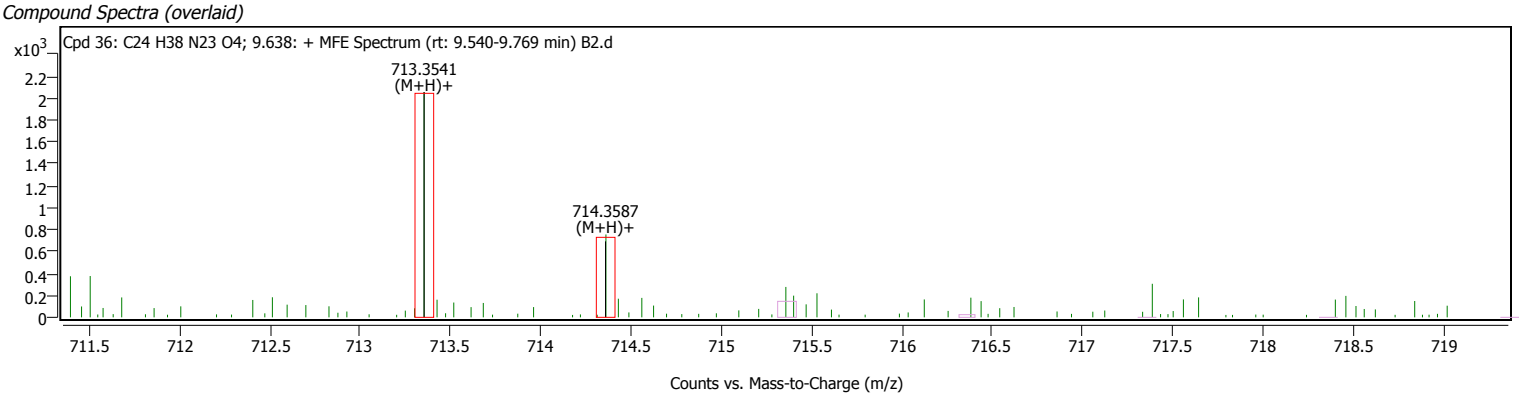
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C24 H38 N23 O4	(M+H)+	MFG	9.638		712.3475		75.07		75.07
	C25 H44 N16 O9	(M+H)+	MFG	9.638		712.3474		73.93		73.93
	C23 H42 N19 O8	(M+H)+	MFG	9.638		712.3475		72.63		72.63
	C26 H50 N9 O14	(M+H)+	MFG	9.638		712.3473		72.45		72.45
	C25 H34 N27	(M+H)+	MFG	9.638		712.3475		72.08		72.08

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 37: C30 H65 Cl N5 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C30 H65 Cl N5 O	10.385		546.4863		MFG	77.35	MFE	

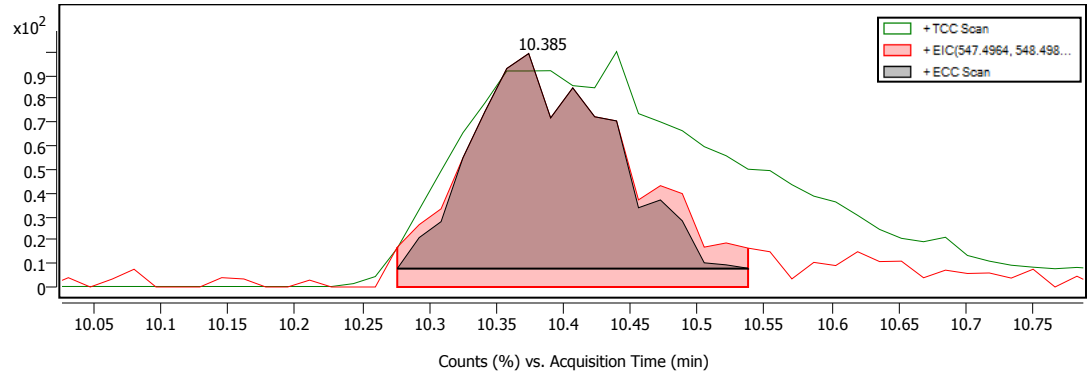
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	547.4937				3	77.35	

Compound ID Table

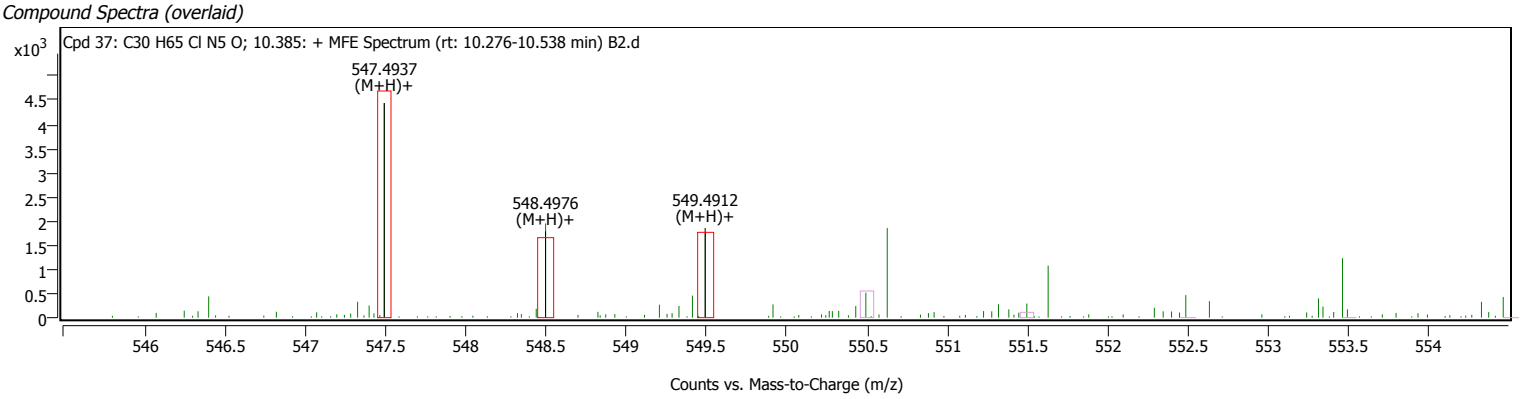
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C30 H65 Cl N5 O	(M+H)+	MFG	10.385		546.4863		77.35		77.35
	C33 H69 Cl N S	(M+H)+	MFG	10.385		546.4863		70.52		70.52
	C32 H67 Cl N2 O2	(M+H)+	MFG	10.385		546.4863		68.12		68.12

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 38: C34 H64 N10 O7

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H64 N10 O7	10.390		724.4956		MFG	97.02	MFE	

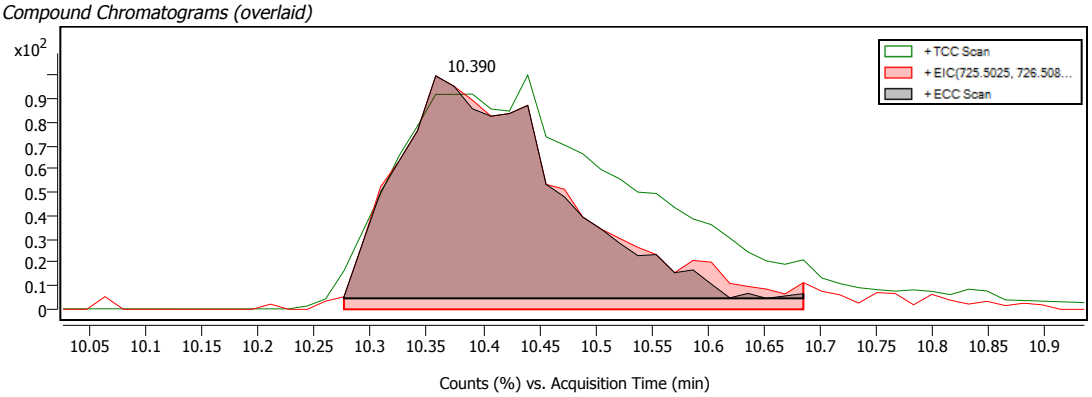
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	725.5030				5	97.02	

Compound ID Table

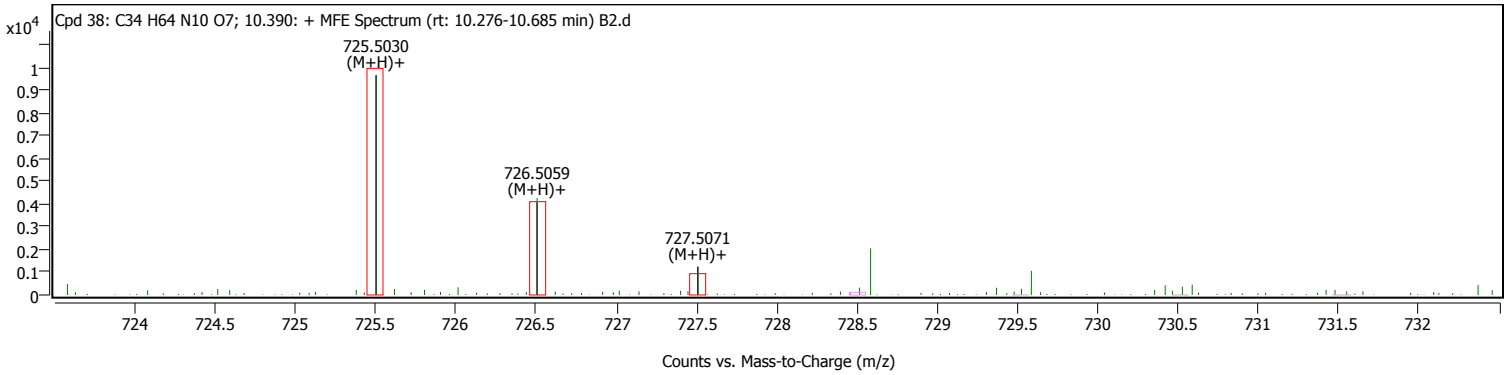
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H64 N10 O7	(M+H)+	MFG	10.390		724.4956		97.02		97.02
	C33 H58 N17 O2	(M+H)+	MFG	10.390		724.4958		96.68		96.68
	C35 H70 N3 O12	(M+H)+	MFG	10.390		724.4955		96.48		96.48
	C33 H68 N6 O11	(M+H)+	MFG	10.390		724.4955		95.17		95.17
	C32 H62 N13 O6	(M+H)+	MFG	10.390		724.4957		95.16		95.16

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 39: Palmitic amide

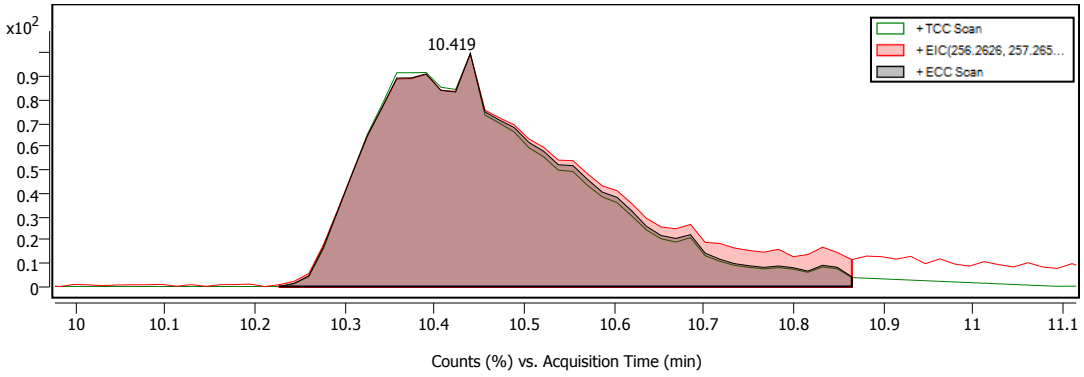
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Palmitic amide	C16 H33 N O	10.419		255.2555	629-54-9	DBSearch	97.74	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	256.2628 256.2628 256.2628		0	97.74	36		

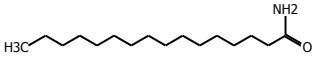
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Palmitic amide	C16 H33 N O	(M+H)+	DBSearch	10.419		255.2555	629-54-9	97.74	97.74	
3-Methylcyclopentadecanone	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289	541-91-3	71.55	97.62	45.48
4E,6Z-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
7,11-hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
6E,11Z-hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
6Z,11Z-hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
1,3-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11E,13E-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11E,13Z-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11Z,13E-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
cis-11-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289	53939-28-9	71.55	97.62	45.48
7Z,11E-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11Z,13Z-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
10E,12E-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
2Z-1-hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
Bombykol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
(±)-2-Dodecylcyclobutanone	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
10-propyl-5,9-tridecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
7Z,11Z-Hexadecadien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
10E-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
10Z-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
12Z-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
7Z-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
9Z-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
10-propyl-trideca-5,9-dien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
hexadeca-7,11-dien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
hexadecan-6E,11Z-dien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
hexadecan-6Z,11Z-dien-1-ol	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
1-Hexadecen-3-one	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
7-hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
9-hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11-hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
11Z-Hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
2-hexadecenal	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
1,15-Hexadecadien-3-one	C16 H30 O	(M+NH4)+	DBSearch-MFG	10.419		238.2289		71.55	97.62	45.48
	C14 H28 N3	(M+NH4)+	MFG	10.419		238.2289		46.16		46.16

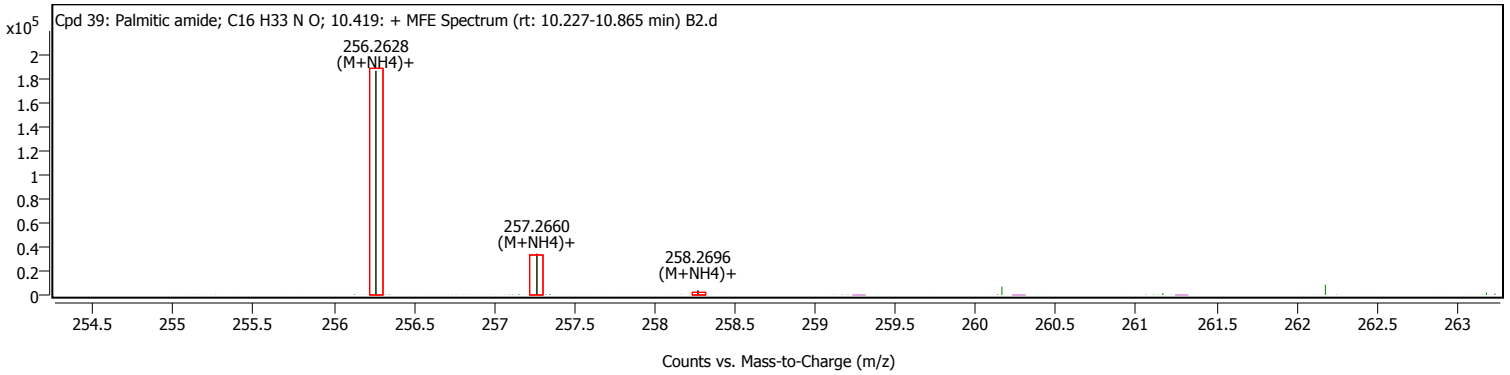
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 40: C16 H35 N4 O

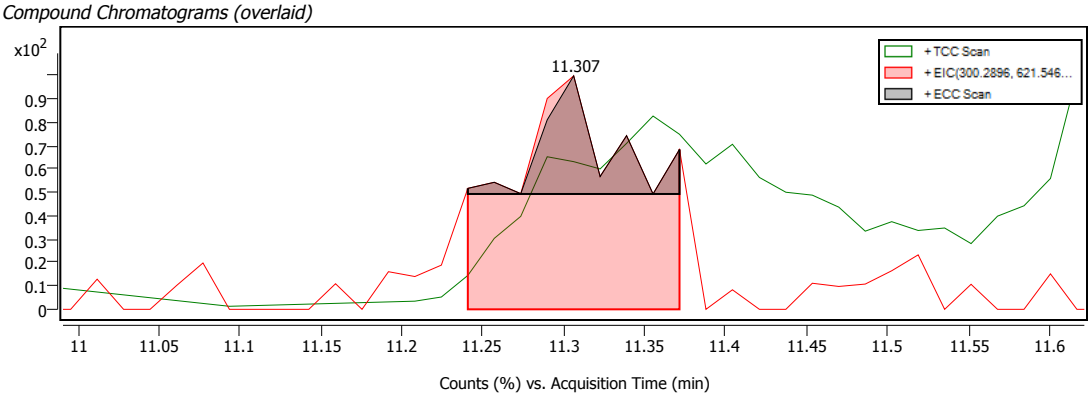
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H35 N4 O	11.307		299.2813		MFG	47.41	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	300.2886				13	47.41	

Compound ID Table

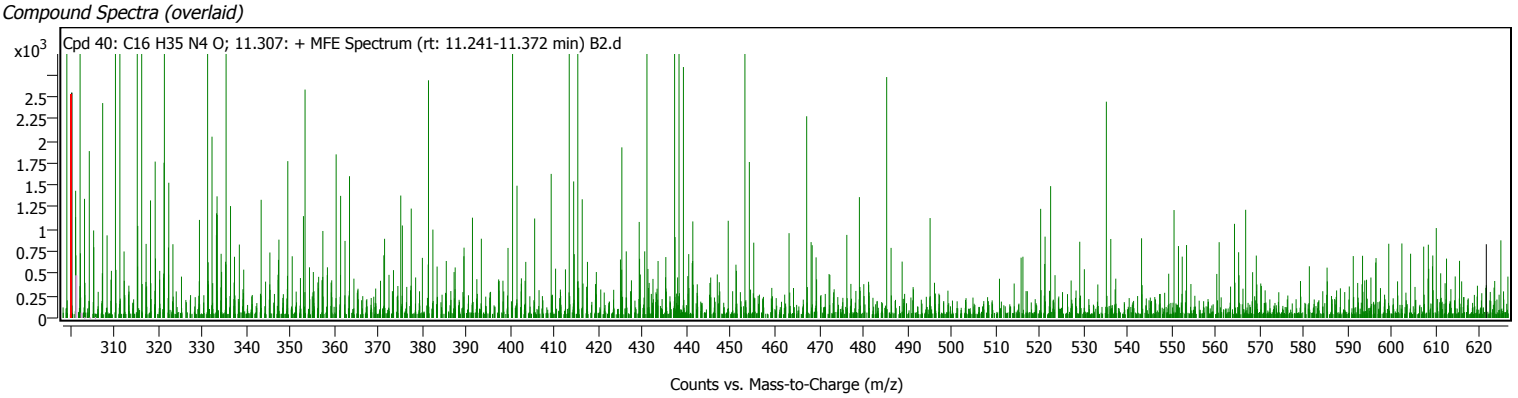
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H35 N4 O	(M+H)+	MFG	11.307		299.2813		47.41		47.41
L-threo-Sphingosine C-18	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813	25695-95-8	43.55	43.54	43.55
2R-aminooctadec-4Z-ene-1,3S-diol	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
5-hydroxy,3E-sphingosine	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
(8Z,d18:1) sphingosine	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
12-amino-octadecanoic acid	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
2-amino-octadecanoic acid	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
Sphingosine	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813	123-78-4	43.55	43.54	43.55
3-ketosphinganine	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813	16105-69-4	43.55	43.54	43.55
Palmitoyl Ethanolamide	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813	544-31-0	43.55	43.54	43.55
Palmitoyl-EA	C18 H37 N O2	(M+H)+	DBSearch-MFG	11.307		299.2813		43.55	43.54	43.55
	C14 H33 N7	(M+H)+ (2M+Na)+	MFG	11.307		299.2776		41.09		41.09
	C19 H39 S	(2M+Na)+	MFG	11.307		299.2801		36.06		36.06

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 41: C16 H35 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H35 N4	11.375		283.2866		MFG	98.02	MFE	

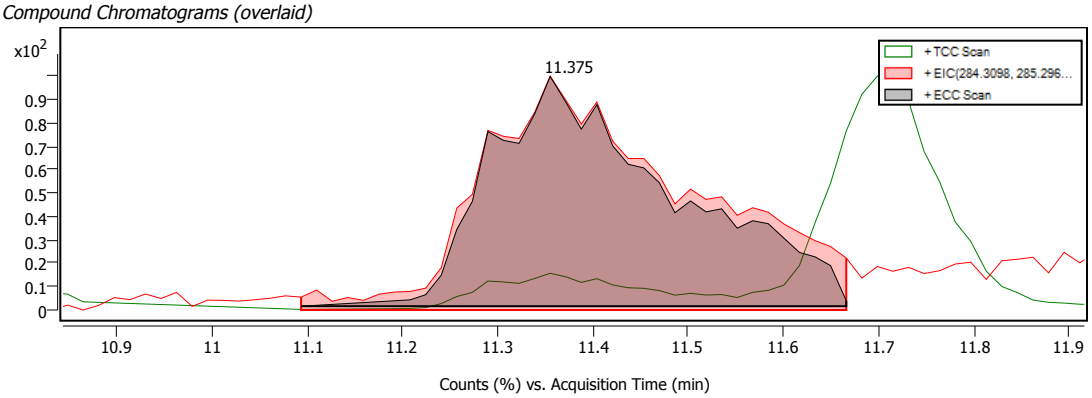
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	284.2937				21	98.02	

Compound ID Table

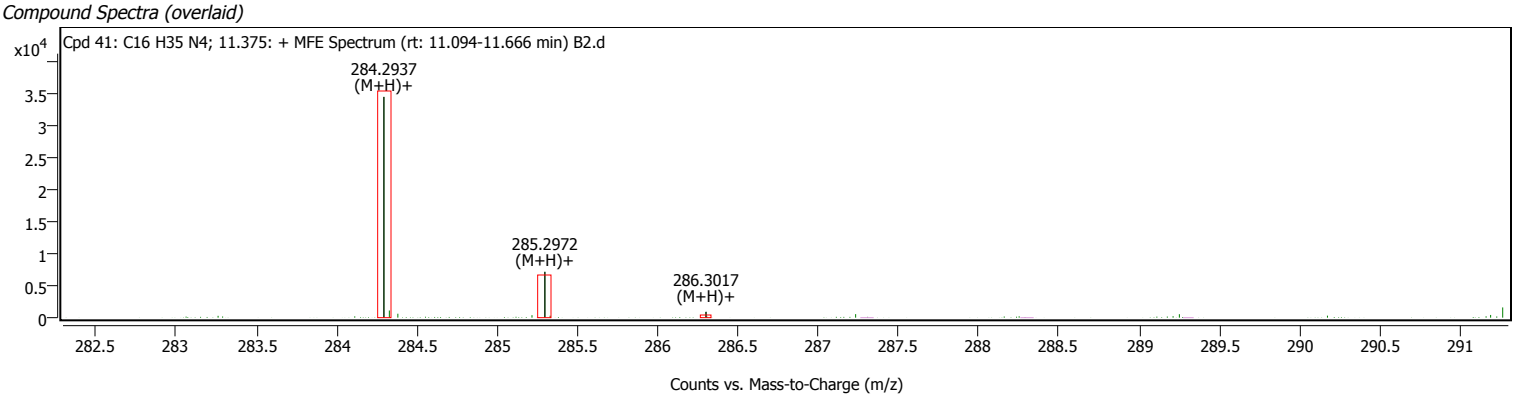
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H35 N4	(M+H)+	MFG	11.375		283.2866		98.02		98.02
Stearamide	C18 H37 N O	(M+H)+	DBSearch-MFG	11.375		283.2865	124-26-5	96.06	96.05	96.07
11-octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
2-Tetradecylcyclobutanone	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600	35493-47-1	95.86	95.86	
7Z-Octadecen-11-one	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
3Z,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
3E,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
2E,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
2Z,13Z-Octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
9,12-Octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
13E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
11Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
2E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
6,7-Epoxy-9Z-octadecene	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
13Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
9Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
octadecan-3Z,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
octadecan-3E,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
octadecan-2E,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
9-octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	
14E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.375		266.2600		95.86	95.86	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 42: C36 H36 N9 O7

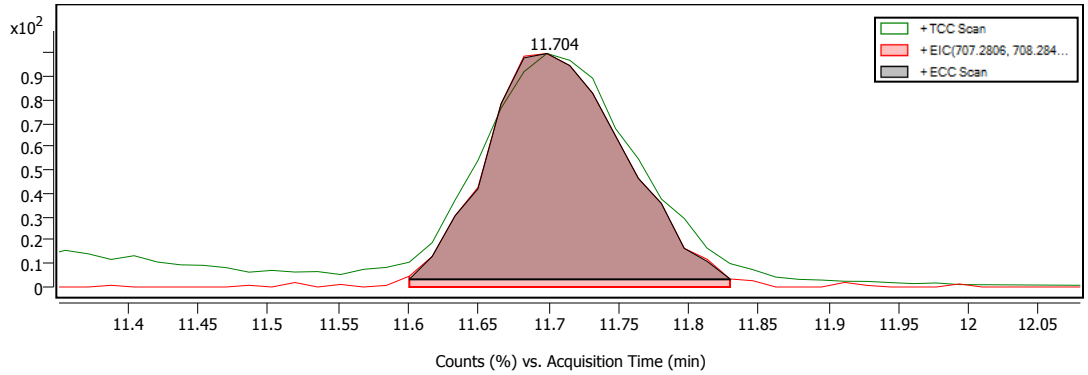
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C36 H36 N9 O7	11.704		706.2735		MFG	98.71	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	707.2806				5	98.71	

Compound ID Table

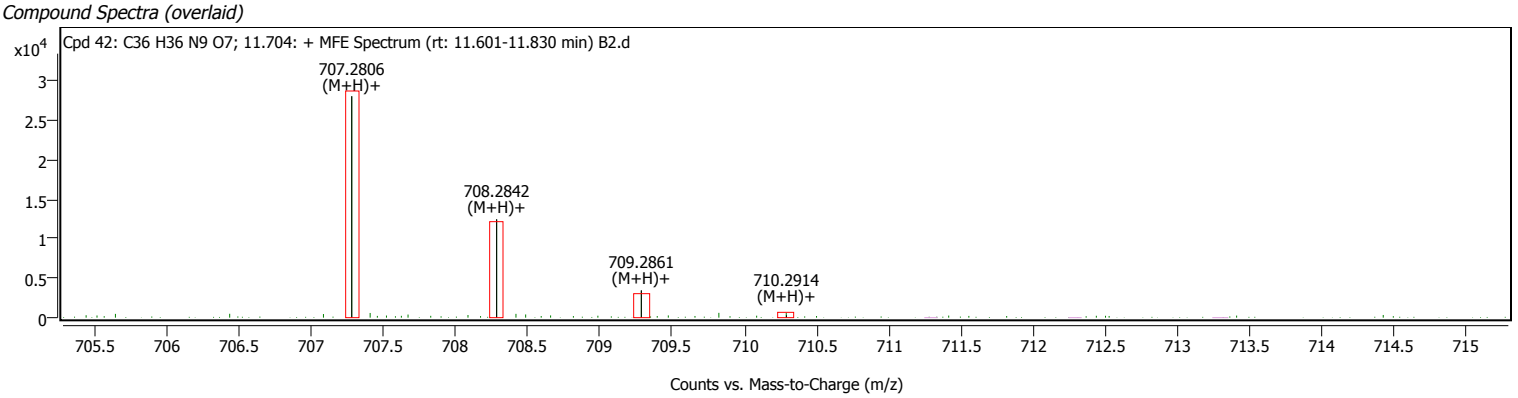
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C36 H36 N9 O7	(M+H)+	MFG	11.704		706.2735		98.71		98.71
	C37 H42 N2 O12	(M+H)+	MFG	11.704		706.2734		98.26		98.26
	C35 H30 N16 O2	(M+H)+	MFG	11.704		706.2737		98.19		98.19
	C35 H40 N5 O11	(M+H)+	MFG	11.704		706.2734		96.40		96.40
	C34 H34 N12 O6	(M+H)+	MFG	11.704		706.2736		96.24		96.24

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 43: Austrobailignan 7

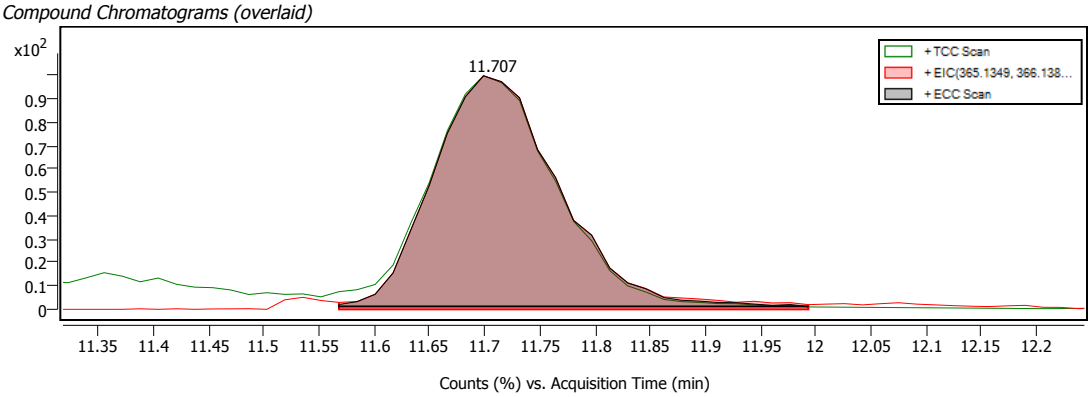
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Austrobailignan 7	C20 H22 O5	11.707		342.1458	55890-25-0	DBSearch	97.17	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	365.1351 365.1351 365.1351		0	97.17	17		

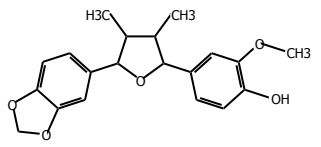
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Austrobailignan 7	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458	55890-25-0	97.17	97.17	
Brosimacutin C	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458		97.17	97.17	
Phaseollidin hydrate	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458		97.17	97.17	
Deoxymiroestrol	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458		97.17	97.17	
1,2,3,4-Tetrahydro-1-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]-7-methoxy-2,6-naphthalenediol	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458	163811-77-6	97.17	97.17	
7-Hydroxyaustrobailignan 5	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458		97.17	97.17	
Hydroxygaleon	C20 H22 O5	(M+Na)+	DBSearch	11.707		342.1458	61576-09-8	97.17	97.17	
	C11 H15 N11 O4	(M+H)+	MFG	11.707		365.1311		85.80		85.80
	C12 H21 N4 O9	(M+H)+	MFG	11.707		365.1310		84.02		84.02
	C13 H17 N8 O5	(M+H)+	MFG	11.707		365.1311		82.41		82.41
	C14 H23 N O10	(M+H)+	MFG	11.707		365.1309		79.07		79.07
	C10 H19 N7 O8	(M+H)+	MFG	11.707		365.1311		76.89		76.89
	C15 H23 Cl N4 O3	(M+Na)+	MFG	11.707		342.1458		47.62		47.62
	C11 H20 N9 O2 S	(M+Na)+	MFG	11.707		342.1458		47.48		47.48
	C12 H26 N2 O7 S	(M+Na)+	MFG	11.707		342.1458		47.47		47.47
	C11 H28 N5 O S3	(M+Na)+	MFG	11.707		342.1458		47.44		47.44
	C15 H31 Cl O2 S2	(M+Na)+	MFG	11.707		342.1458		47.05		47.05

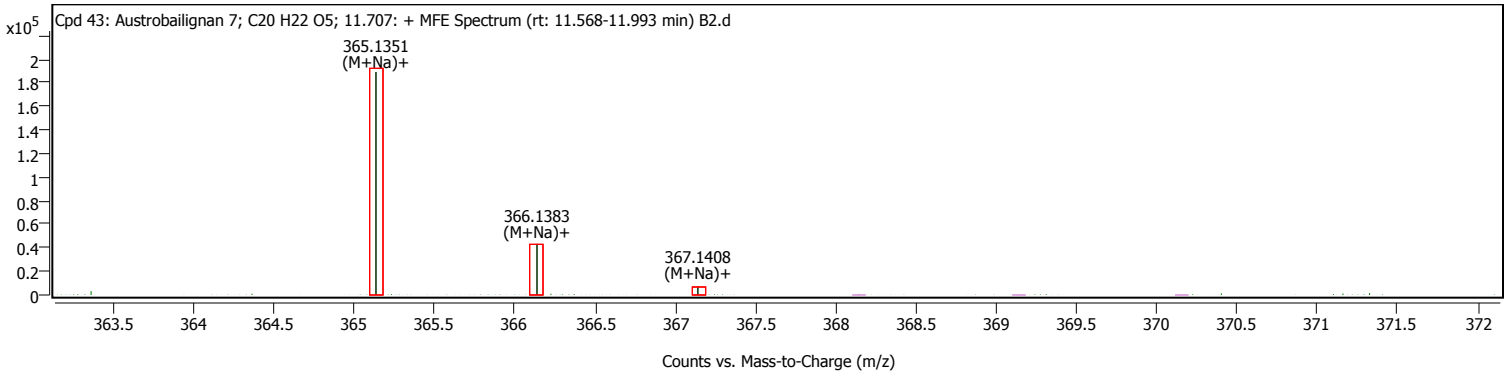
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 44: C27 H44 N3 O S

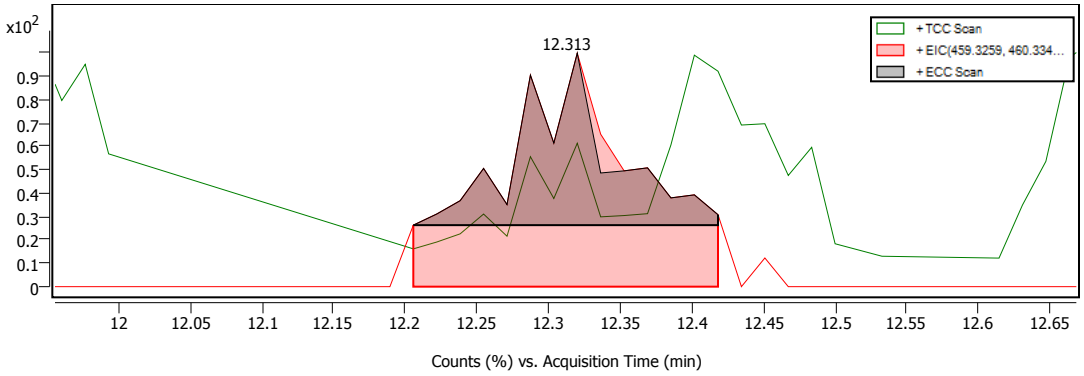
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C27 H44 N3 O S	12.313		458.3207		MFG	55.56	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	459.3263				5	55.56	

Compound ID Table

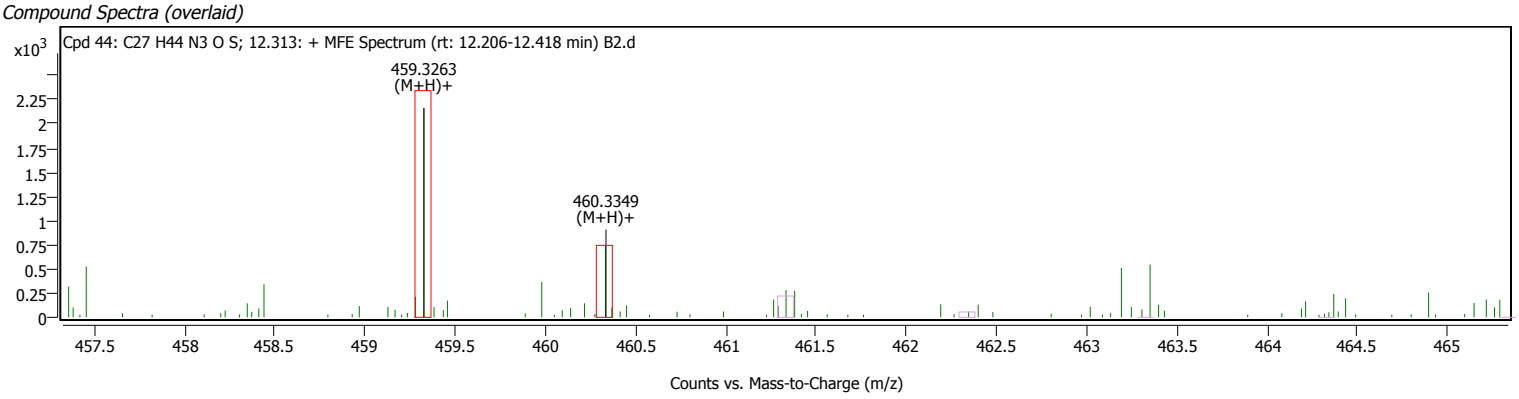
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C27 H44 N3 O S	(M+H)+	MFG	12.313		458.3207		55.56		55.56
	C32 H42 O2	(M+H)+	MFG	12.313		458.3206		55.01		55.01
	C20 H36 N13	(M+H)+	MFG	12.313		458.3209		54.93		54.93
	C19 H40 N9 O4	(M+H)+	MFG	12.313		458.3208		53.23		53.23
	C21 H42 N6 O5	(M+H)+	MFG	12.313		458.3207		52.69		52.69

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 45: C26 H28 O S4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C26 H28 O S4	12.434		484.1026		MFG	81.25	MFE	

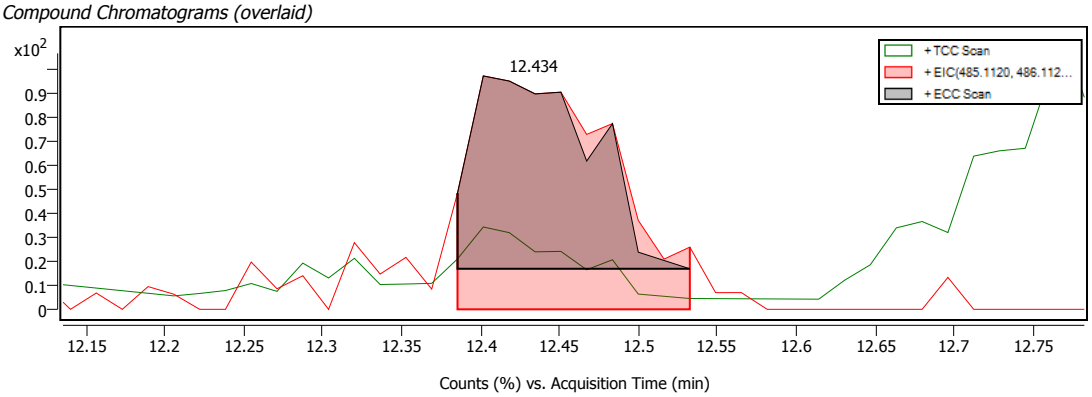
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	485.1104				7	81.25	

Compound ID Table

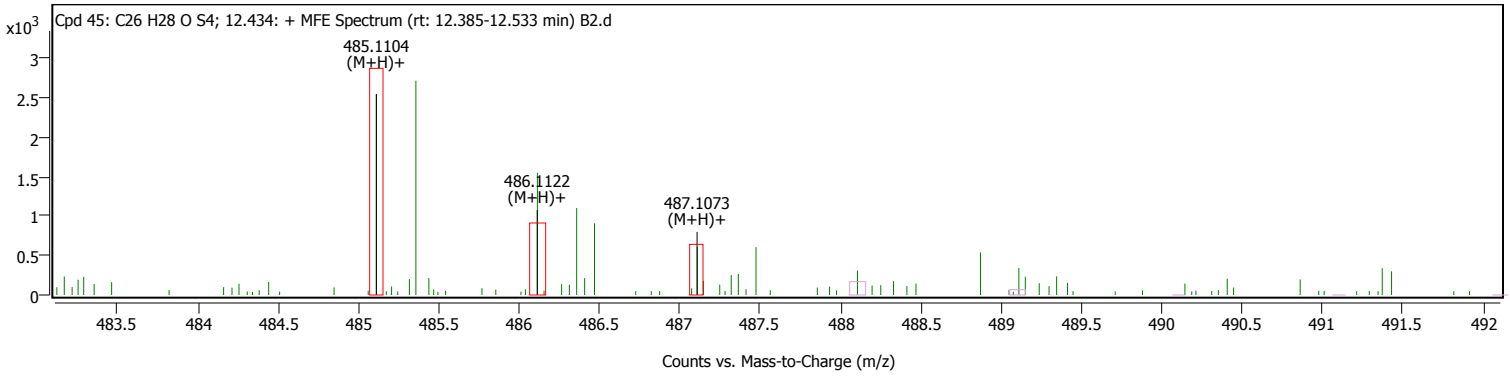
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C26 H28 O S4	(M+H)+	MFG	12.434		484.1026		81.25		81.25
	C19 H20 N10 S3	(M+H)+	MFG	12.434		484.1029		76.50		76.50
	C36 H17 Cl	(M+H)+	MFG	12.434		484.1024		75.70		75.70
	C21 H30 N3 S5	(M+H)+	MFG	12.434		484.1029		75.58		75.58
	C24 H26 N3 S4	(M+H)+	MFG	12.434		484.1028		74.71		74.71
Tyr-Phe4Cl-OH	C24 H21 Cl N2 O7	(M+H)+	DBSearch	12.434		484.1026		69.94	69.94	
Phe4Cl-TyrMe-OH	C24 H21 Cl N2 O7	(M+H)+	DBSearch	12.434		484.1026		69.94	69.94	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 46: C44 H52 N11

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H52 N11	12.671		734.4402		MFG	62.50	MFE	

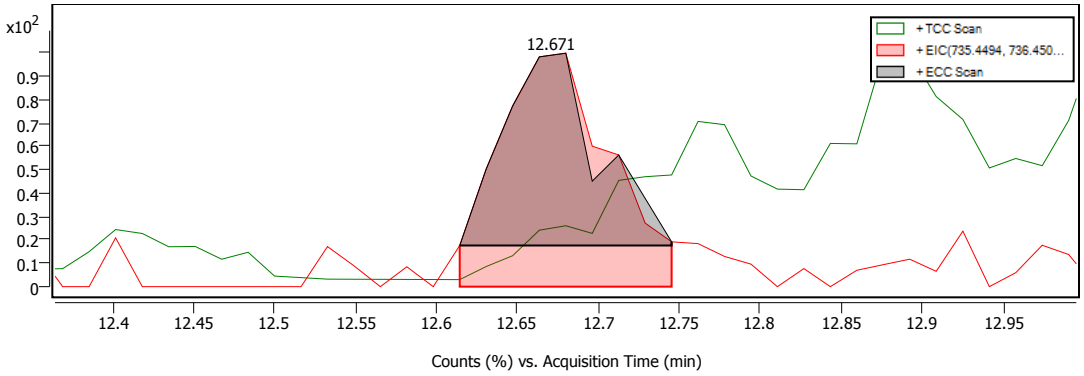
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	735.4466				5	62.50	

Compound ID Table

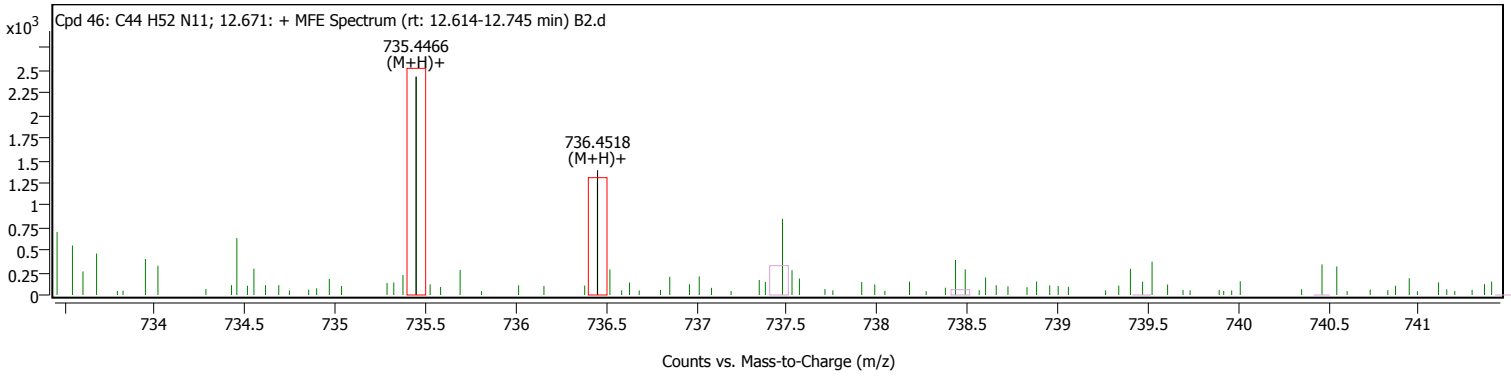
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H52 N11	(M+H)+	MFG	12.671		734.4402		62.50		62.50
	C45 H58 N4 O5	(M+H)+	MFG	12.671		734.4400		61.85		61.85
	C43 H56 N7 O4	(M+H)+	MFG	12.671		734.4401		61.76		61.76
	C44 H62 O9	(M+H)+	MFG	12.671		734.4400		61.53		61.53
	C51 H60 N O S	(M+H)+	MFG	12.671		734.4400		59.29		59.29

Compound Chromatograms (overlaid)

Structure



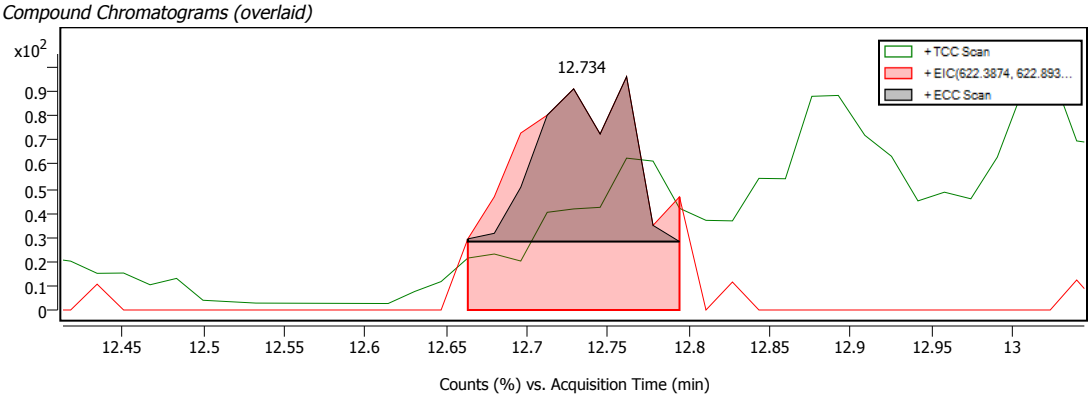
Compound Spectra (overlaid)



Cpd 47: 12.734

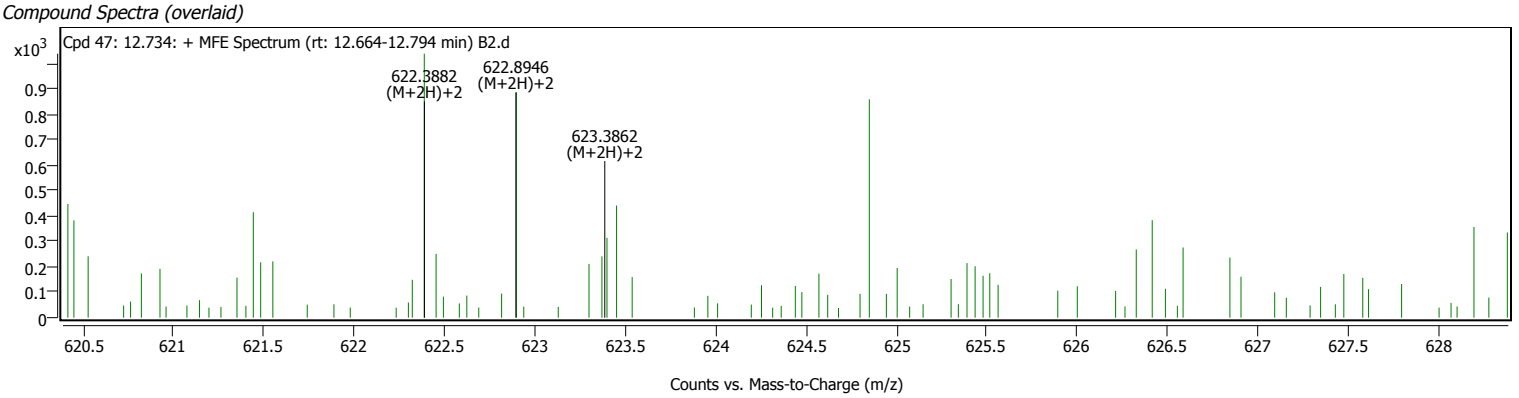
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		12.734		1242.7618				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 48: C36 H70 N29 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C36 H70 N29 O3	12.757		956.6210		MFG	61.76	MFE	

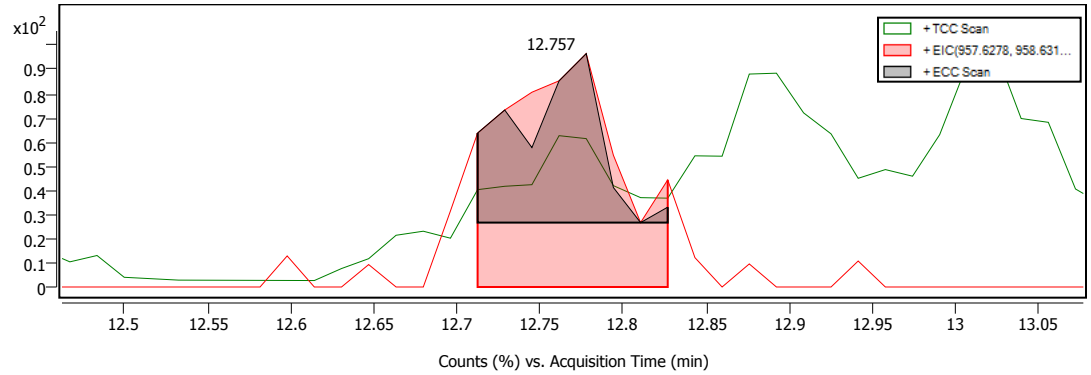
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	957.6298				5	61.76	

Compound ID Table

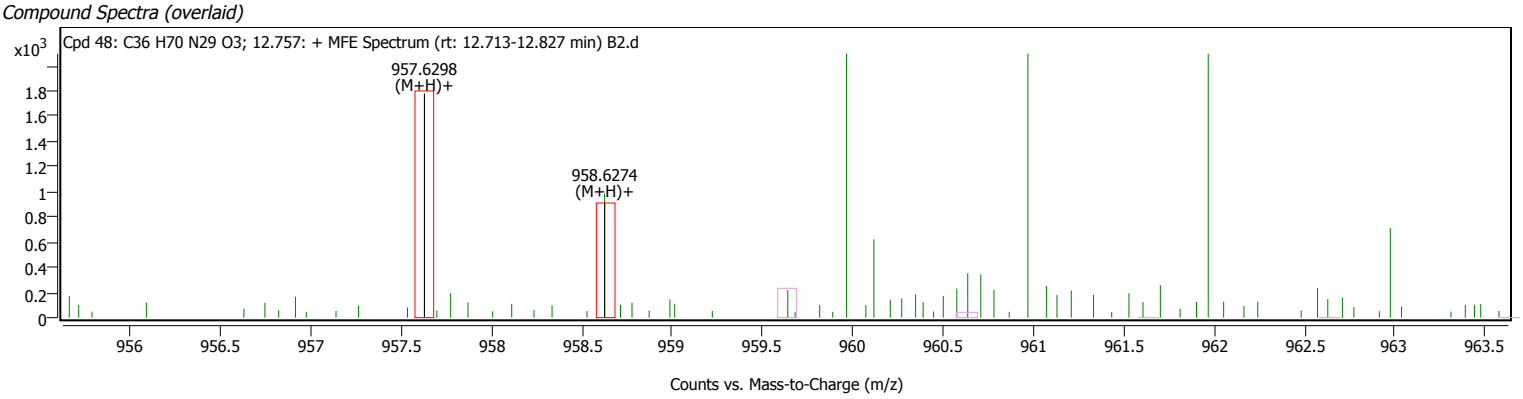
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C36 H70 N29 O3	(M+H)+	MFG	12.757		956.6210		61.76		61.76
	C35 H74 N25 O7	(M+H)+	MFG	12.757		956.6210		60.77		60.77
	C37 H76 N22 O8	(M+H)+	MFG	12.757		956.6209		60.06		60.06
	C36 H80 N18 O12	(M+H)+	MFG	12.757		956.6209		59.24		59.24
	C38 H82 N15 O13	(M+H)+	MFG	12.757		956.6208		58.38		58.38

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 49: C31 H28 N O3 S3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H28 N O3 S3	12.773		558.1223		MFG	77.80	MFE	

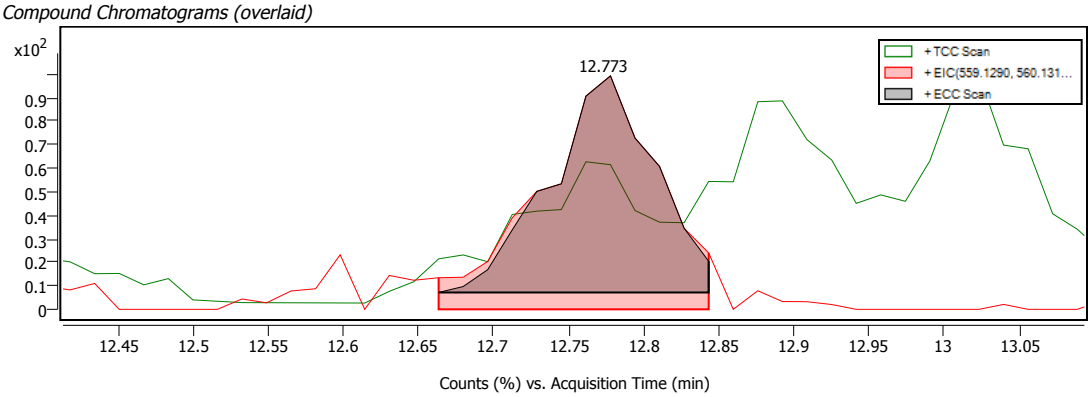
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	559.1297				5	77.80	

Compound ID Table

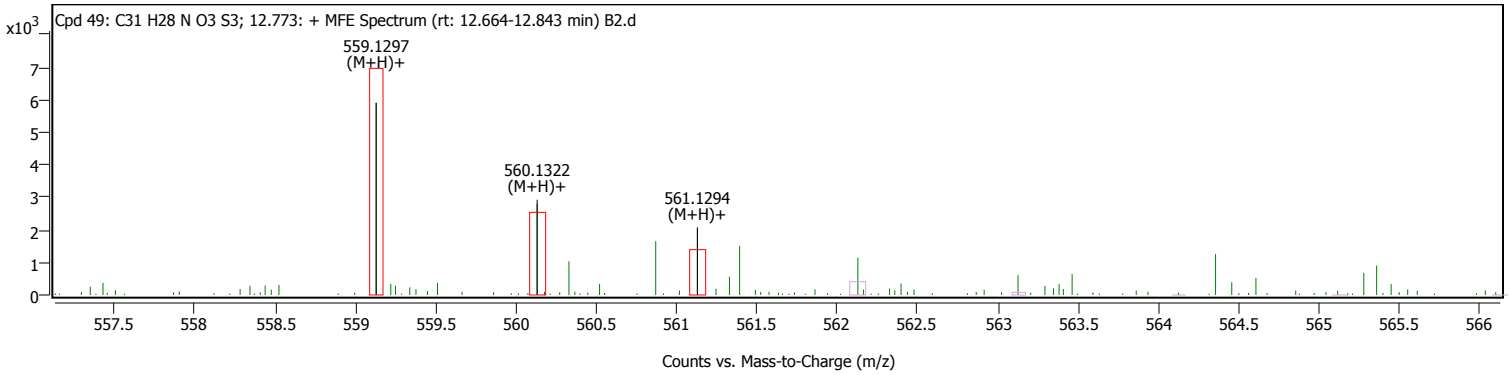
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H28 N O3 S3	(M+H)+	MFG	12.773		558.1223		77.80		77.80
	C29 H26 N4 O2 S3	(M+H)+	MFG	12.773		558.1224		77.53		77.53
	C37 H22 N2 S2	(M+H)+	MFG	12.773		558.1220		77.25		77.25
	C29 H34 O S5	(M+H)+	MFG	12.773		558.1226		76.00		76.00
	C23 H32 N3 O5 S4	(M+H)+	MFG	12.773		558.1227		75.26		75.26

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 50: PC(O-16:0/0:0)[U]

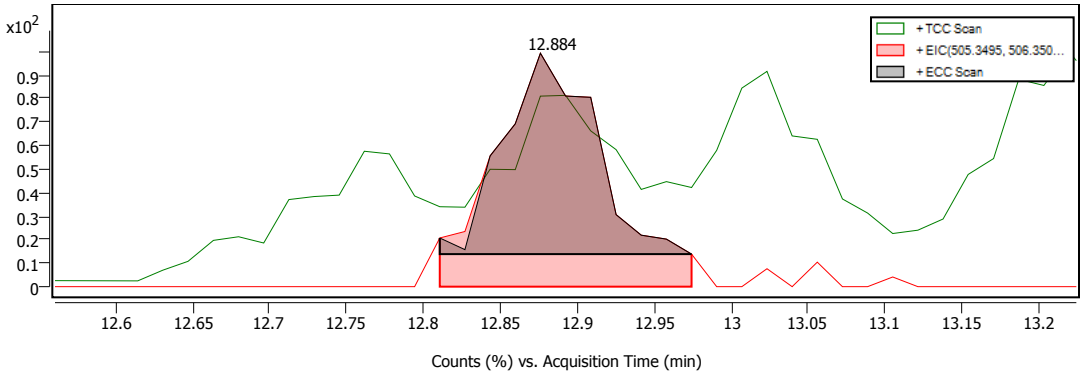
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(O-16:0/0:0)[U]	C24 H53 N O6 P	12.884		482.3591		DBSearch	54.81	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	505.3490 505.3490 505.3490 505.3490		0	54.81	17		

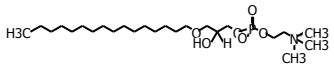
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PC(O-16:0/0:0)[U]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
Lyso-PAF C-16	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591	52691-62-0	54.81	54.81	
PC(O-15:0/O-1:0)[U]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
PC(O-8:0/O-8:0)	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
PC(O-8:0/O-8:0)[U]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
PC(O-16:0/0:0)	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
PC(O-16:0/0:0)[S]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.884		482.3591		54.81	54.81	
	C24 H49 Cl2 N7	(M+H)+	MFG	12.884		505.3427		47.61		47.61
	C23 H51 Cl N4 O4	(M+Na)+	MFG	12.884		482.3598		47.61		47.61
	C19 H48 N9 O3 S	(M+Na)+	MFG	12.884		482.3598		47.46		47.46
	C32 H45 N2 O3	(M+H)+	MFG	12.884		505.3427		47.44		47.44
	C24 H49 N4 O5 S	(M+H)+	MFG	12.884		505.3427		47.37		47.37
	C23 H43 N11 S	(M+H)+	MFG	12.884		505.3427		47.36		47.36
	C26 H48 N3 O5	(M+Na)+	MFG	12.884		482.3598		47.28		47.28
	C25 H42 N10	(M+Na)+	MFG	12.884		482.3598		47.28		47.28
	C27 H52 N3 S2	(M+Na)+	MFG	12.884		482.3598		47.18		47.18
	C25 H53 N4 S3	(M+H)+	MFG	12.884		505.3427		47.08		47.08

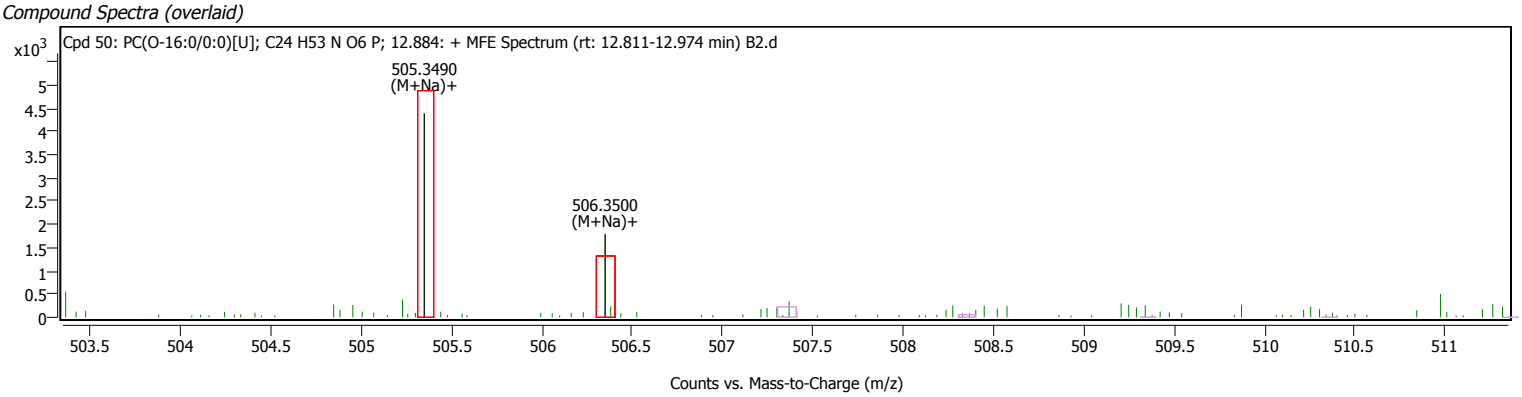
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 51: C20 H34 N9 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C20 H34 N9 O	12.884		416.2887		MFG	61.99	MFE	

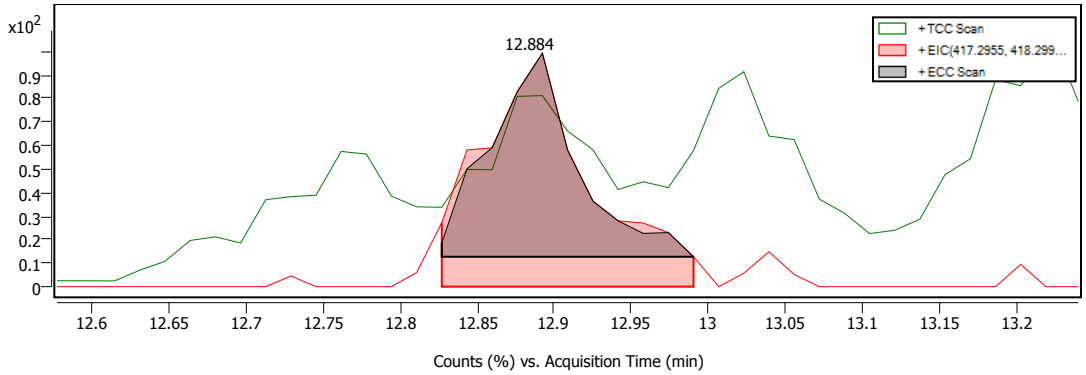
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	417.2953				5	61.99	

Compound ID Table

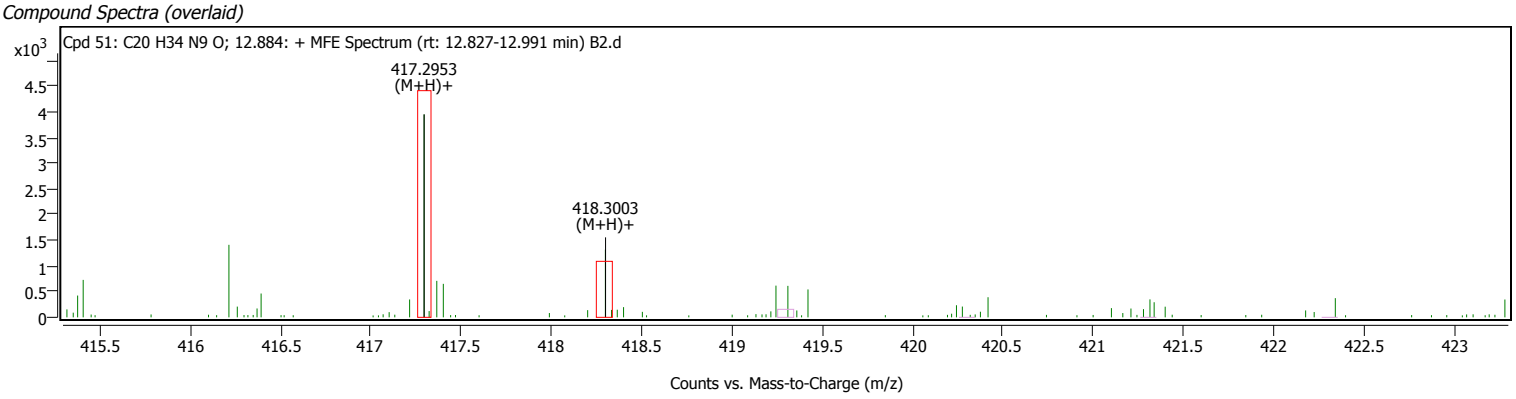
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C20 H34 N9 O	(M+H)+	MFG	12.884		416.2887		61.99		61.99
	C21 H40 N2 O6	(M+H)+	MFG	12.884		416.2886		61.75		61.75
	C22 H36 N6 O2	(M+H)+	MFG	12.884		416.2887		59.76		59.76
	C22 H44 N2 O S2	(M+H)+	MFG	12.884		416.2886		55.84		55.84
	C19 H38 N5 O5	(M+H)+	MFG	12.884		416.2887		55.63		55.63

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 52: 27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol

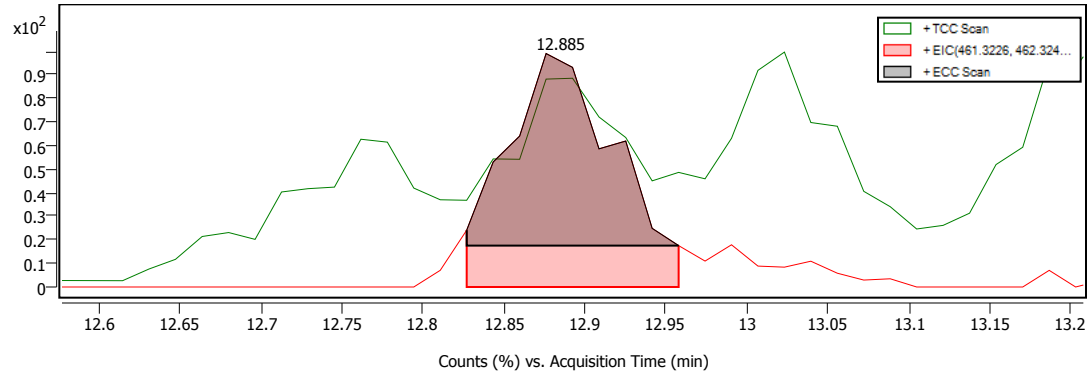
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.885		438.3327	78648-95-0	DBSearch	66.50	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	461.3222 461.3222 461.3222 461.3222		0	66.50	11		

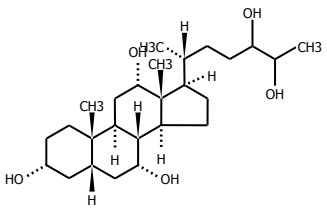
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	(M+Na)+	DBSearch	12.885		438.3327	78648-95-0	66.50	66.50	
	C15 H37 N14 O3	(M+H)+	MFG	12.885		461.3174		47.61		47.61
	C27 H44 Cl N3 O	(M+H)+	MFG	12.885		461.3174		47.61		47.61
	C23 H41 N8 S	(M+H)+	MFG	12.885		461.3174		47.58		47.58
	C24 H47 N O5 S	(M+H)+	MFG	12.885		461.3174		47.58		47.58
	C24 H44 N3 O4	(M+Na)+	MFG	12.885		438.3330		47.51		47.51
	C24 H47 Cl2 N4	(M+H)+	MFG	12.885		461.3174		47.22		47.22
	C15 H42 N12 O S	(M+Na)+	MFG	12.885		438.3330		47.18		47.18
	C19 H45 Cl N7 O2	(M+Na)+	MFG	12.885		438.3330		46.71		46.71
	C21 H47 Cl N4 O3	(M+Na)+	MFG	12.885		438.3330		46.50		46.50
	C17 H44 N9 O2 S	(M+Na)+	MFG	12.885		438.3330		45.80		45.80

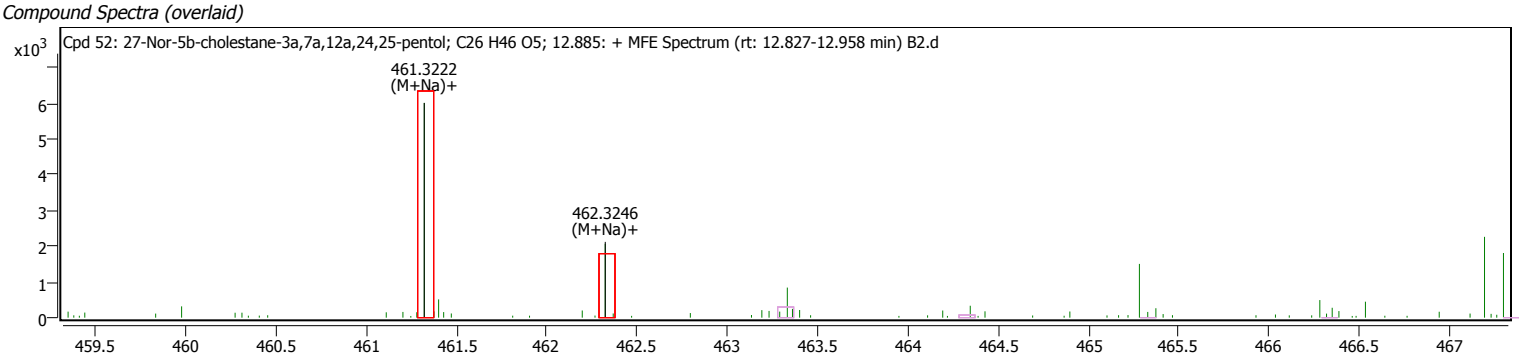
Compound Chromatograms (overlaid)



Structure



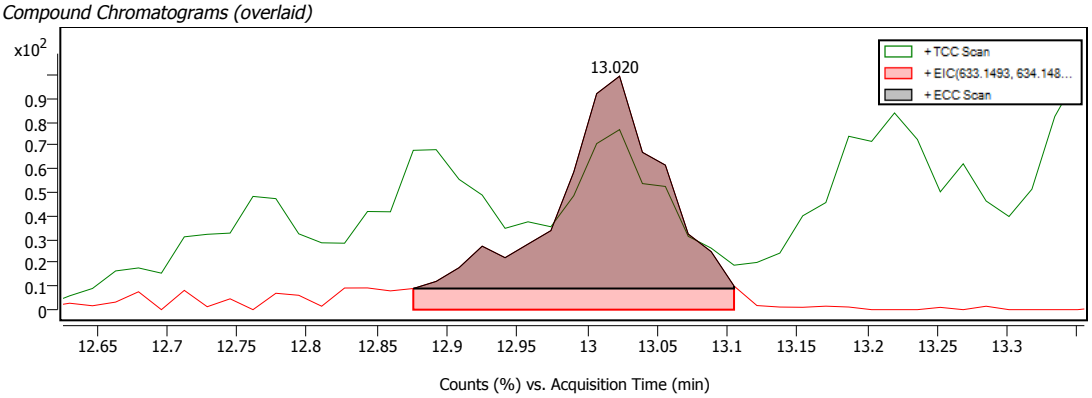
Compound Spectra (overlaid)



Cpd 53: 13.020

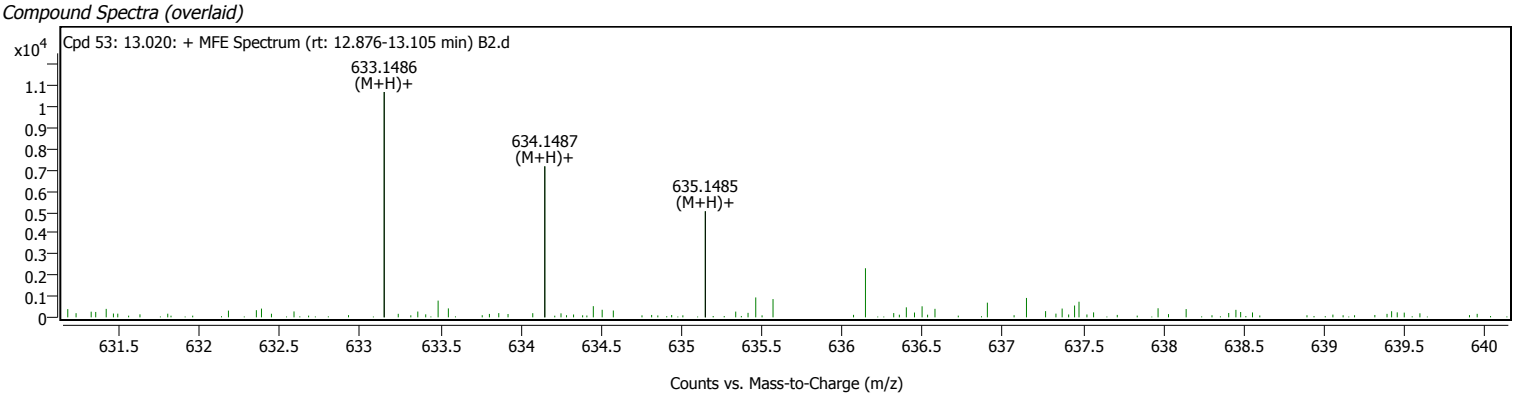
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.020		632.1413				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 54: C34 H15 N17 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H15 N17 O3	13.208		709.1549		MFG	56.30	MFE	

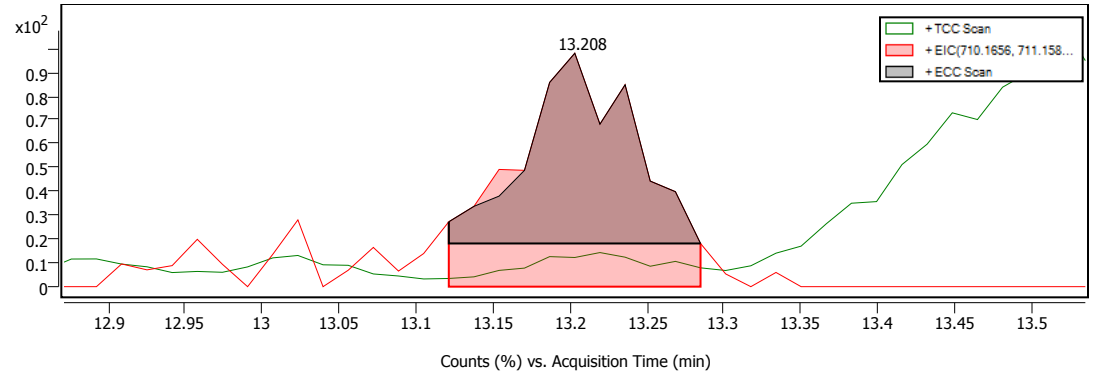
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	710.1638				5	56.30	

Compound ID Table

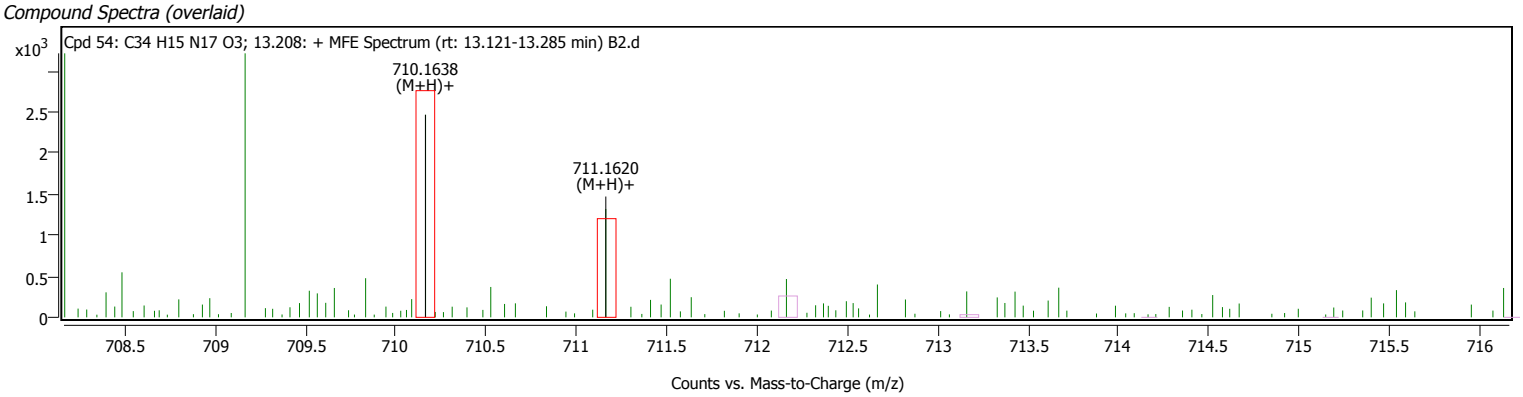
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H15 N17 O3	(M+H)+	MFG	13.208		709.1549		56.30		56.30
	C49 H19 N5 O2	(M+H)+	MFG	13.208		709.1547		55.97		55.97
	C51 H21 N2 O3	(M+H)+	MFG	13.208		709.1546		55.83		55.83
	C36 H17 N14 O4	(M+H)+	MFG	13.208		709.1549		55.54		55.54
	C35 H21 N10 O8	(M+H)+	MFG	13.208		709.1548		55.05		55.05

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 55: C37 H23 Cl N10 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H23 Cl N10 O4	13.209		706.1590		MFG	69.74	MFE	

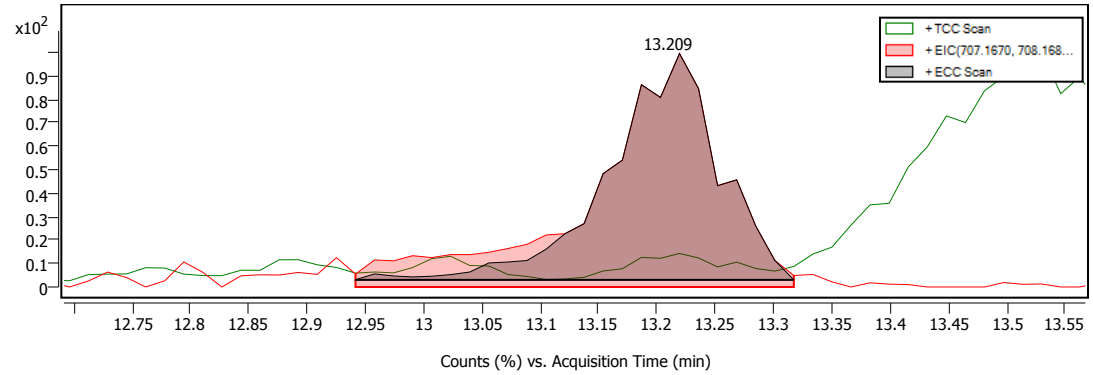
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	707.1672				5	69.74	

Compound ID Table

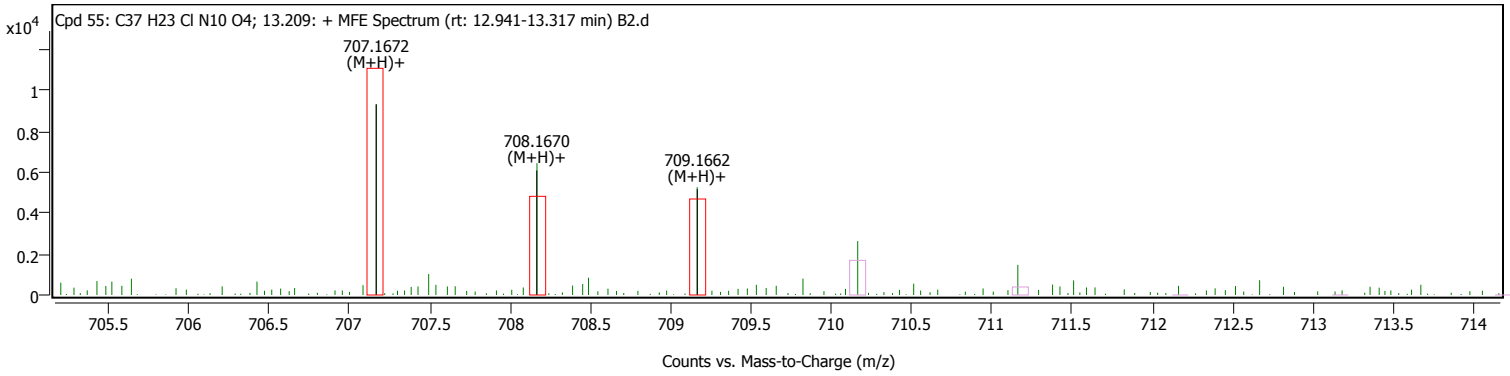
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H23 Cl N10 O4	(M+H)+	MFG	13.209		706.1590		69.74		69.74
	C45 H27 Cl N4 O S	(M+H)+	MFG	13.209		706.1588		68.84		68.84
	C43 H25 Cl N7 S	(M+H)+	MFG	13.209		706.1589		68.69		68.69
	C38 H29 Cl N3 O9	(M+H)+	MFG	13.209		706.1588		68.62		68.62
	C37 H31 Cl N6 O3 S2	(M+H)+	MFG	13.209		706.1591		68.60		68.60

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 56: C53 H31 Cl N O2 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C53 H31 Cl N O2 S	13.374		780.1768		MFG	90.95	MFE	

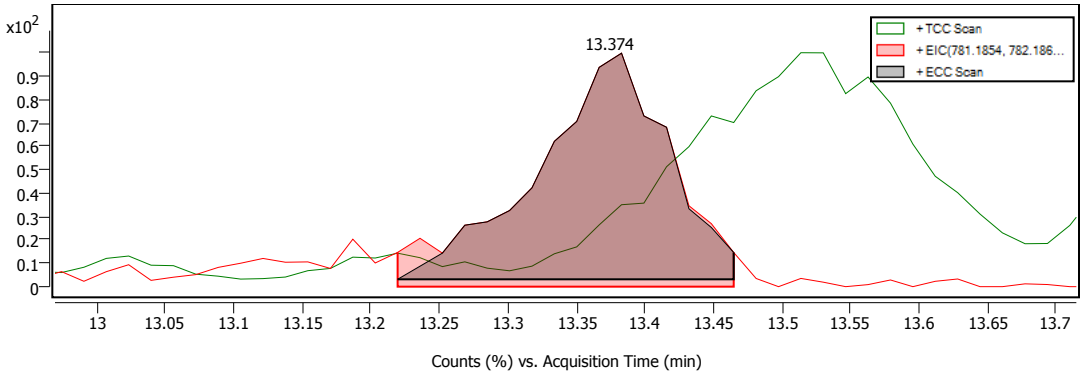
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	781.1857				5	90.95	

Compound ID Table

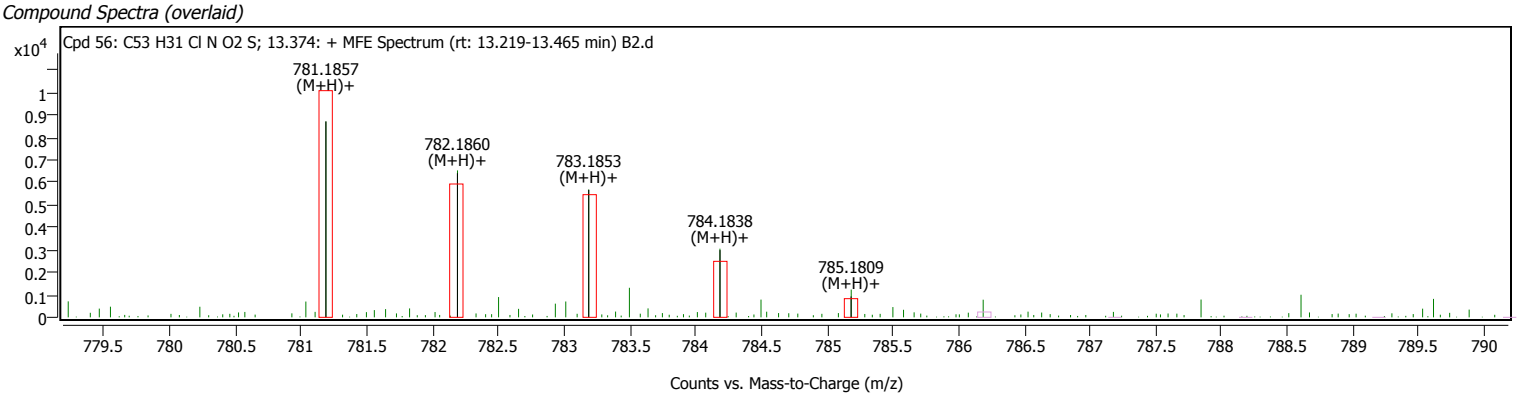
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C53 H31 Cl N O2 S	(M+H)+	MFG	13.374		780.1768		90.95		90.95
	C46 H31 Cl N7 S2	(M+H)+	MFG	13.374		780.1773		88.08		88.08
	C46 H23 Cl N11 O	(M+H)+	MFG	13.374		780.1770		87.12		87.12
	C48 H33 Cl N4 O S2	(M+H)+	MFG	13.374		780.1772		86.86		86.86
	C51 H29 Cl N4 O S	(M+H)+	MFG	13.374		780.1770		86.75		86.75

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

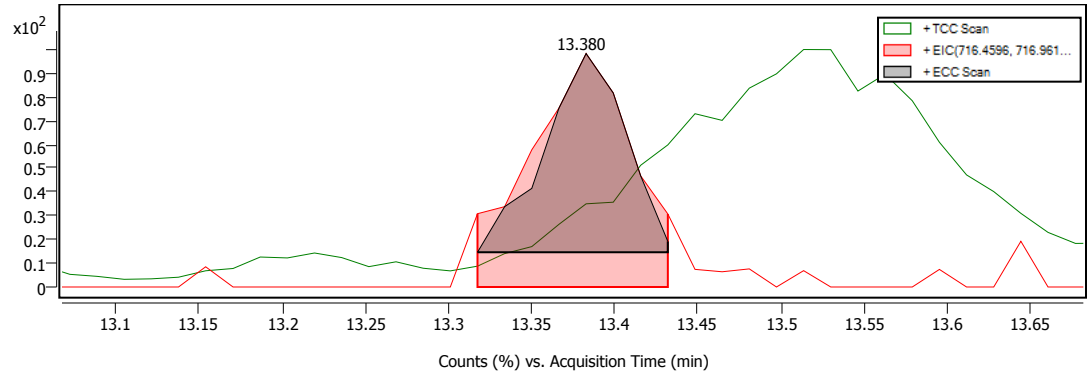


Cpd 57: 13.380

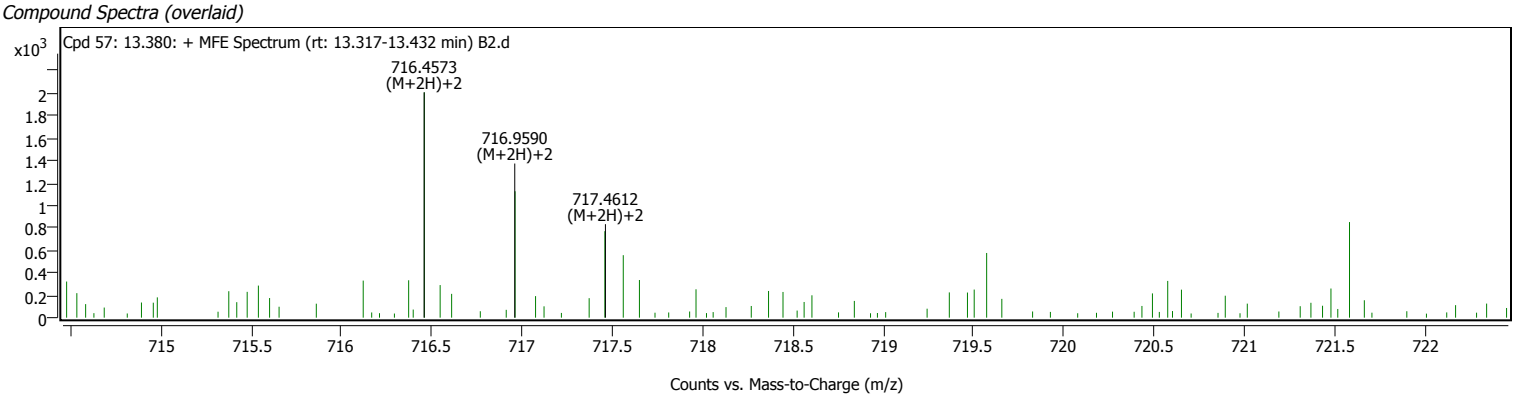
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.380		1430.9001				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

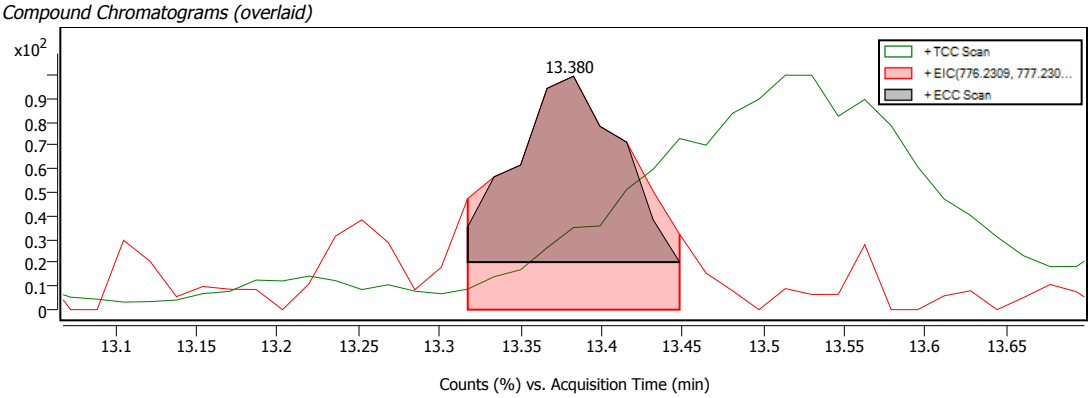


Cpd 58: 13.380

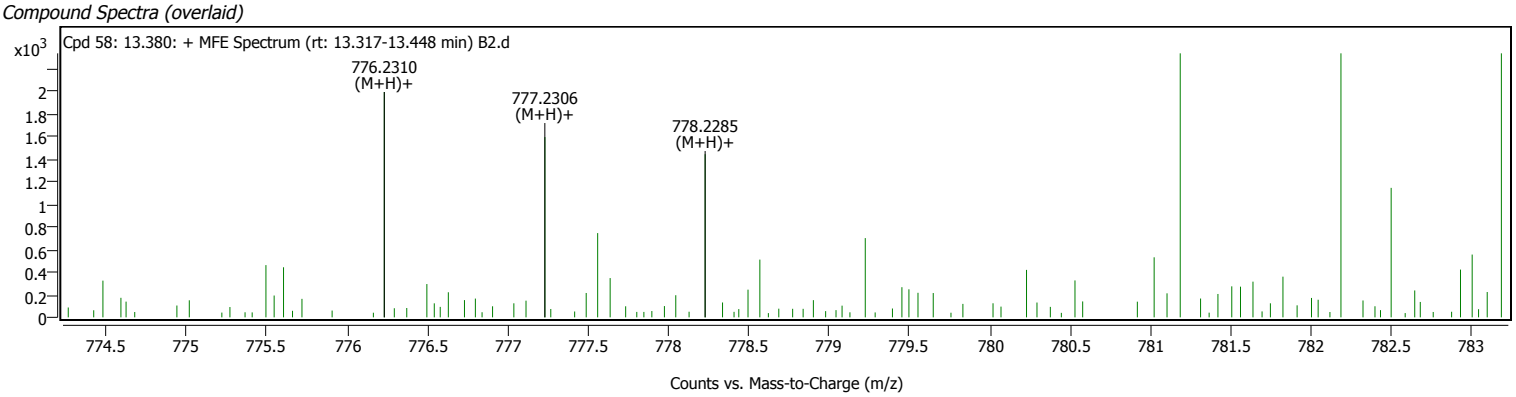
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.380		775.2238				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

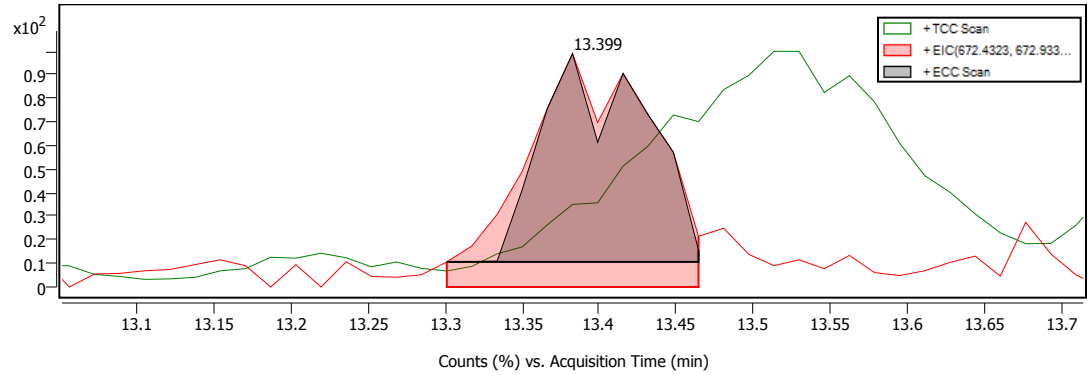


Cpd 59: 13.399

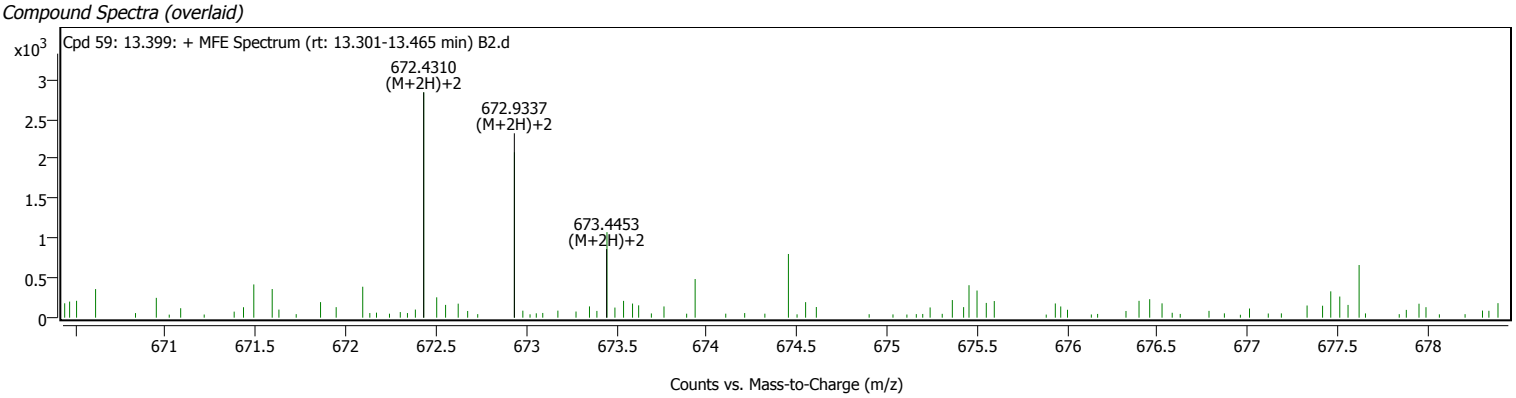
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.399		1342.8475				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

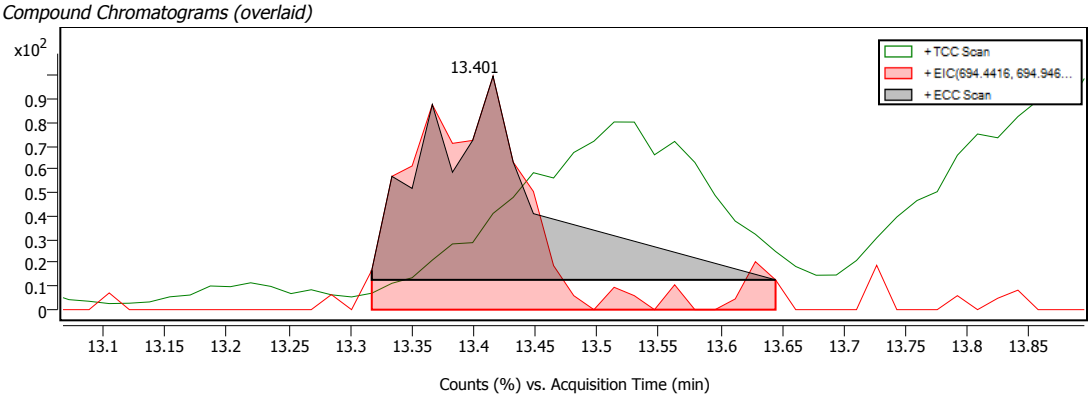


Cpd 60: 13.401

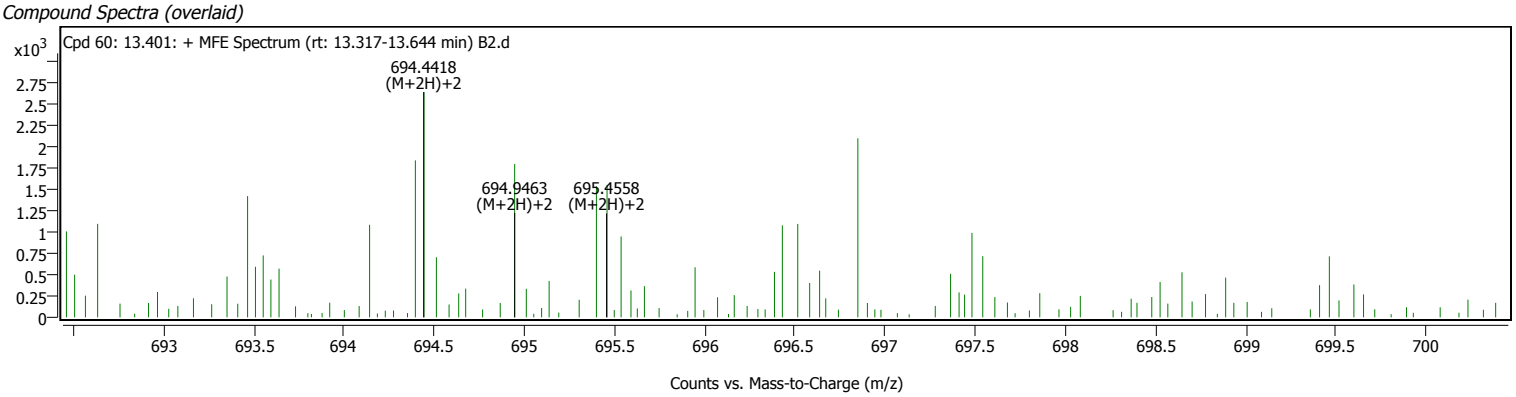
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.401		1386.8691				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

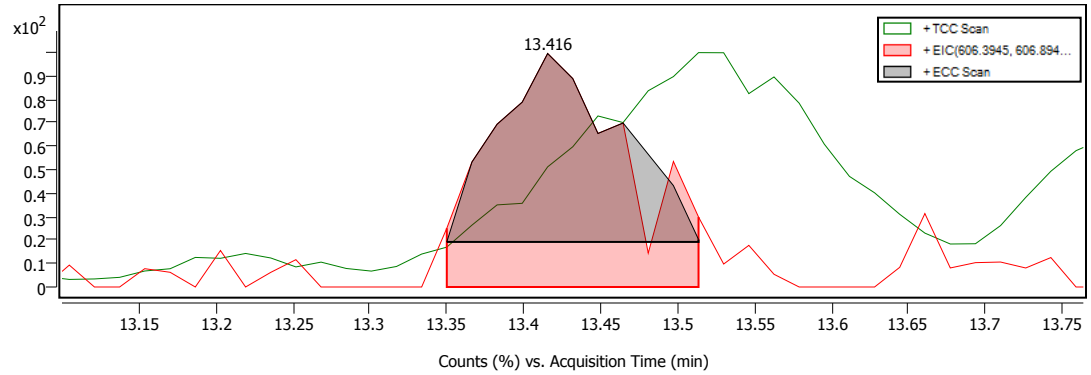


Cpd 61: 13.416

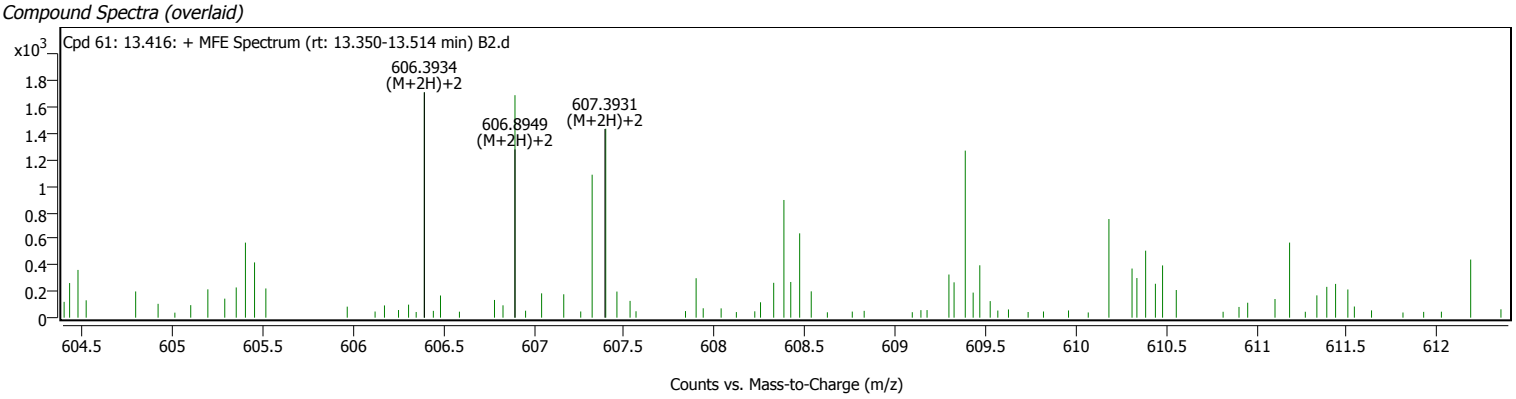
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.416		1210.7722				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

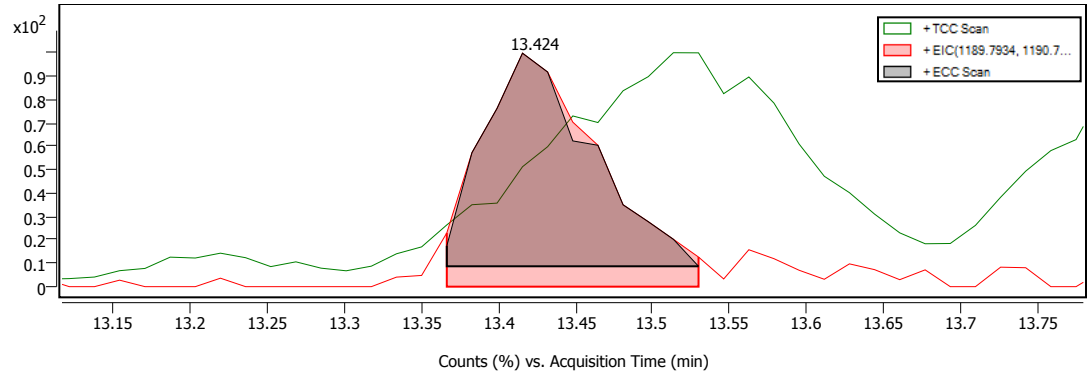


Cpd 62: 13.424

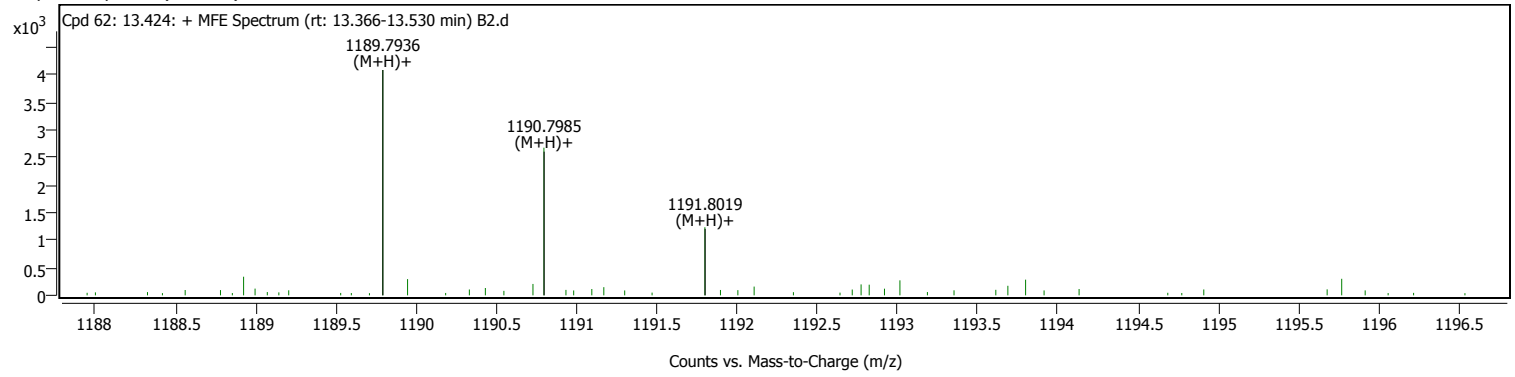
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.424		1188.7863				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

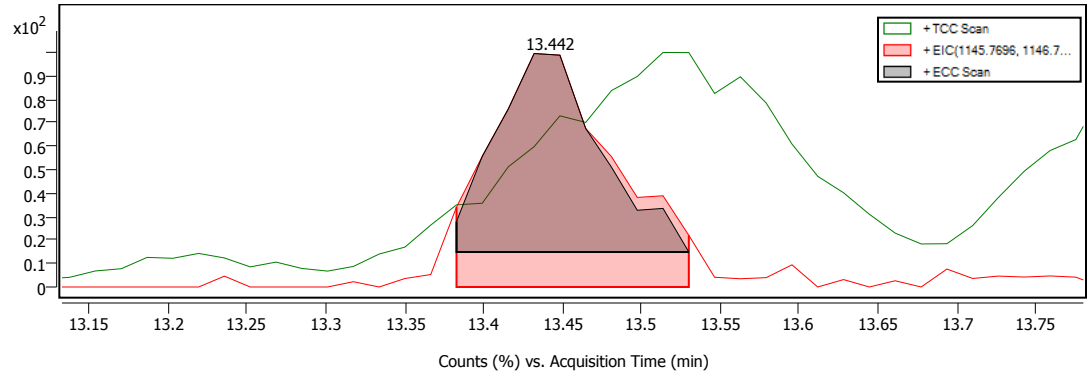


Cpd 63: 13.442

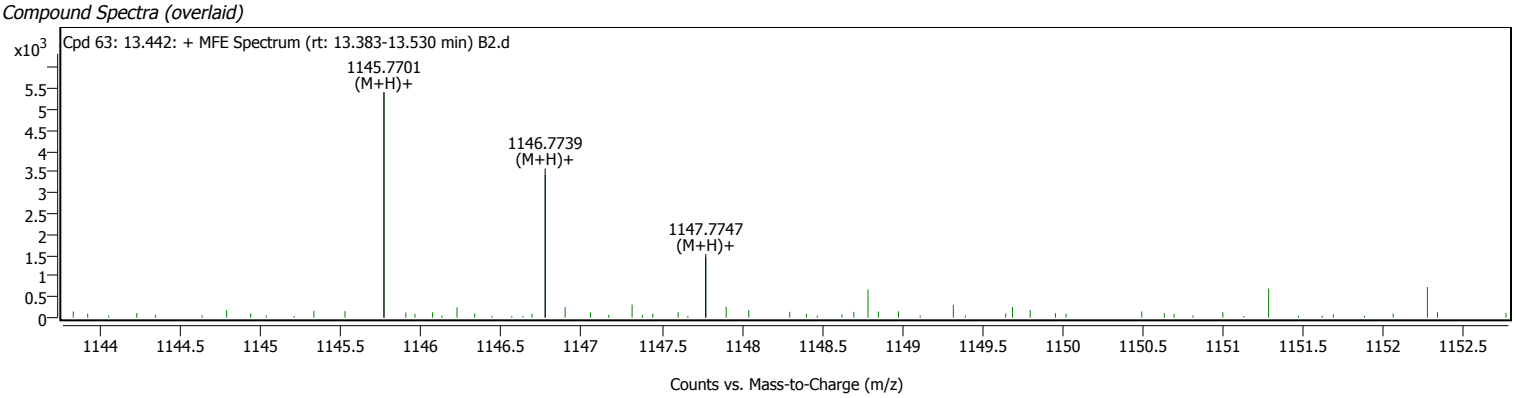
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.442		1144.7628				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

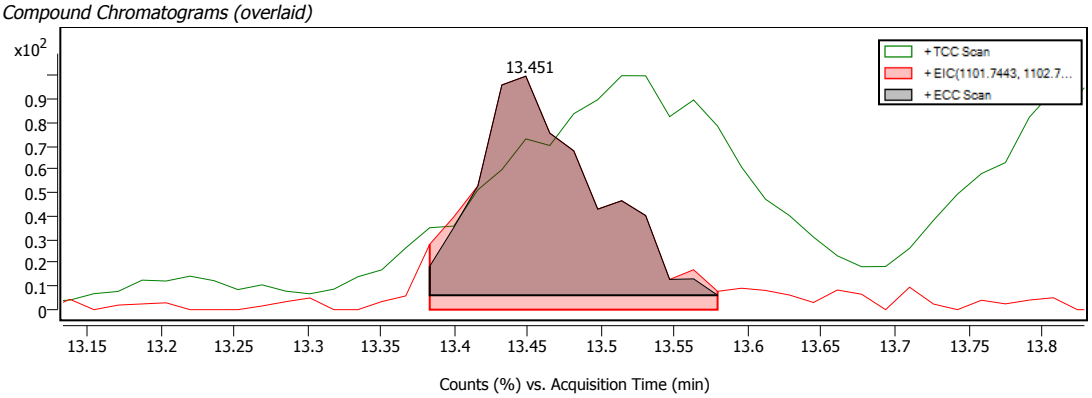


Cpd 64: 13.451

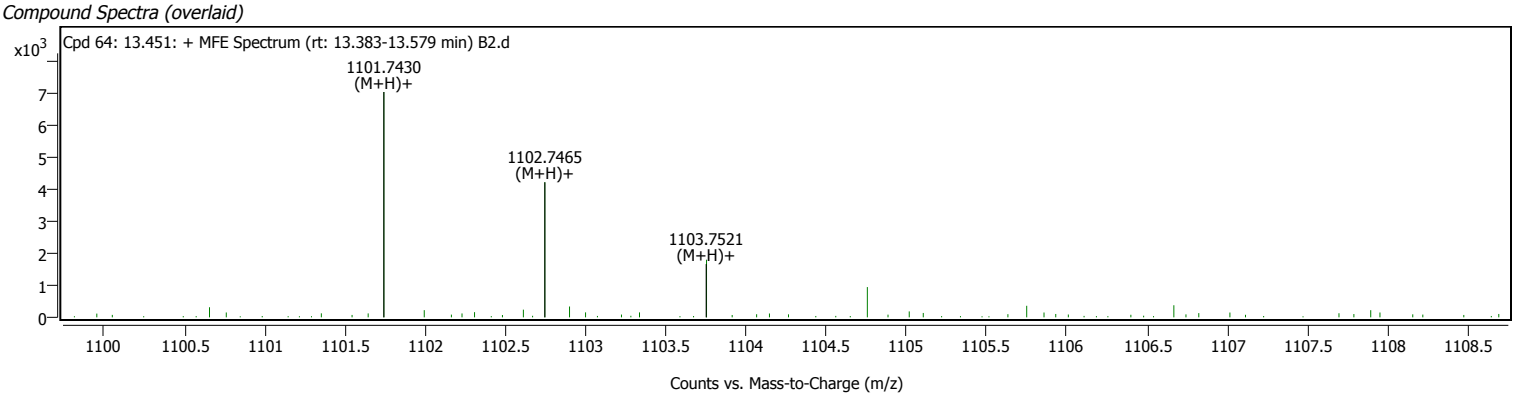
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.451		1100.7357				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 65: 35S-Methylokadaic acid 7-hexadecanoate

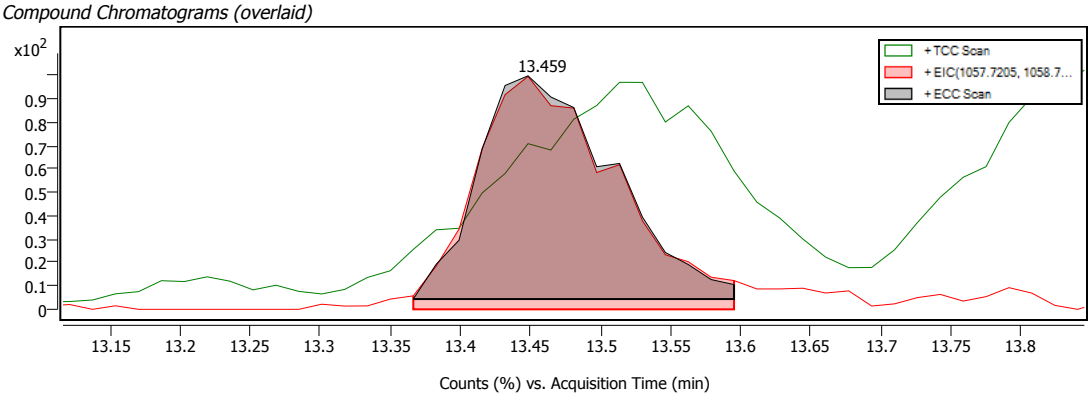
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
35S-Methylokadaic acid 7-hexadecanoate	C61 H100 O14	13.459		1056.7092		DBSearch	92.04	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	1057.7164 1057.7164 1057.7164		0	92.04	1		

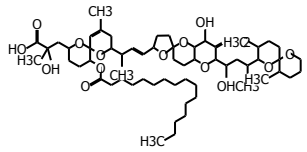
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
35S-Methylokadaic acid 7-hexadecanoate	C61 H100 O14	(M+H)+	DBSearch	13.459		1056.7092		92.04	92.04	

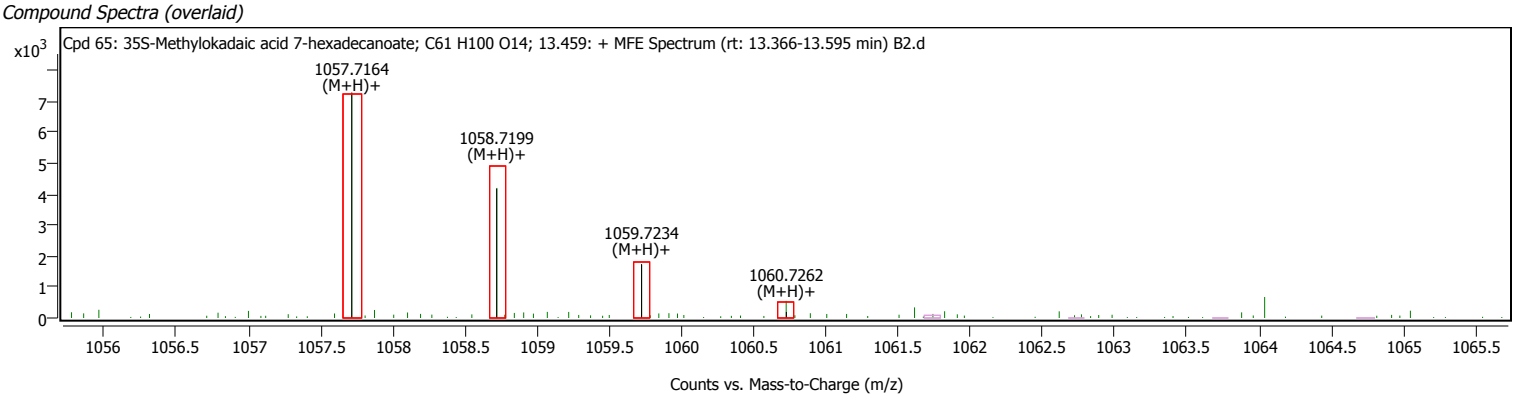
Compound Chromatograms (overlaid)



Structure



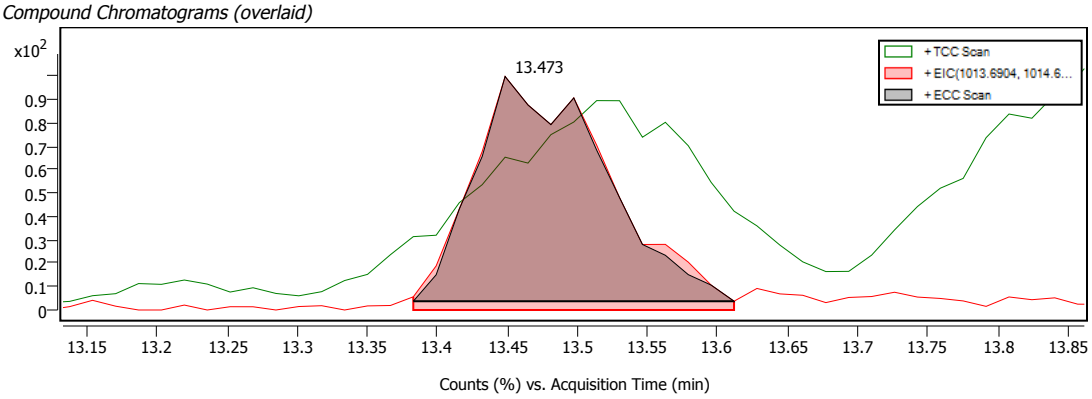
Compound Spectra (overlaid)



Cpd 66: 13.473

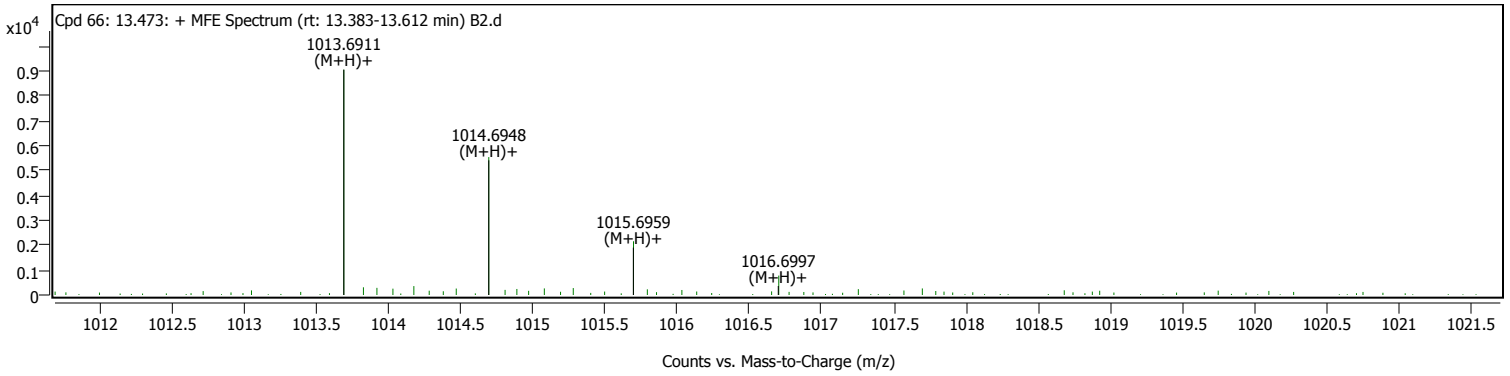
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.473		1012.6838				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 67: C55 H80 N14 O2

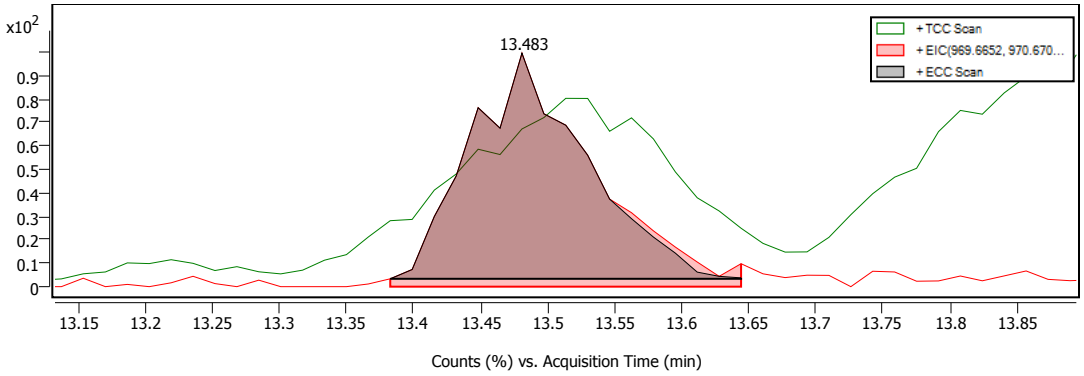
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C55 H80 N14 O2	13.483		968.6585		MFG	95.94	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	969.6655				5	95.94	

Compound ID Table

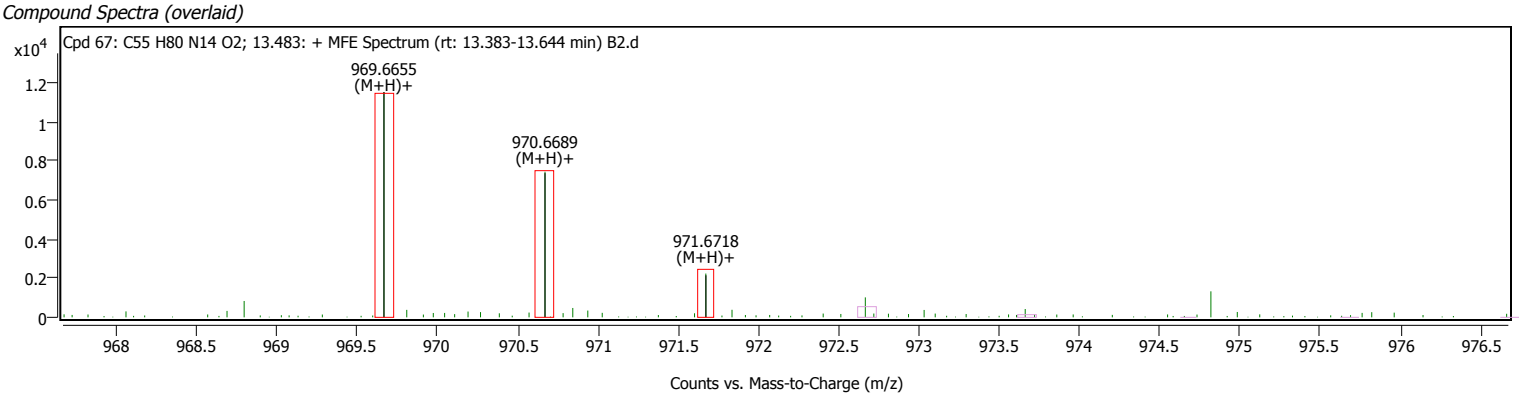
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C55 H80 N14 O2	(M+H)+	MFG	13.483		968.6585		95.94		95.94
	C53 H78 N17 O	(M+H)+	MFG	13.483		968.6585		95.62		95.62
	C54 H84 N10 O6	(M+H)+	MFG	13.483		968.6584		94.80		94.80
	C56 H86 N7 O7	(M+H)+	MFG	13.483		968.6583		94.79		94.79
	C55 H90 N3 O11	(M+H)+	MFG	13.483		968.6583		93.62		93.62

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 68: C46 H86 N9 O8 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C46 H86 N9 O8 S	13.500		924.6322		MFG	93.78	MFE	

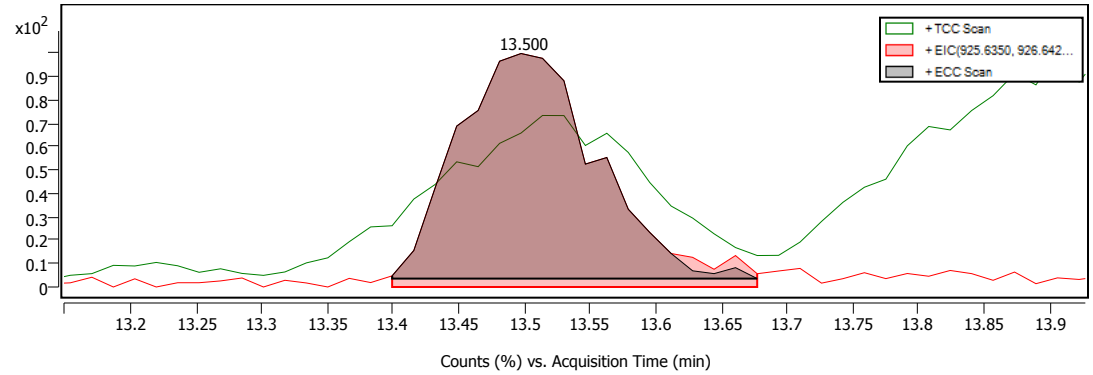
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	925.6391				5	93.78	

Compound ID Table

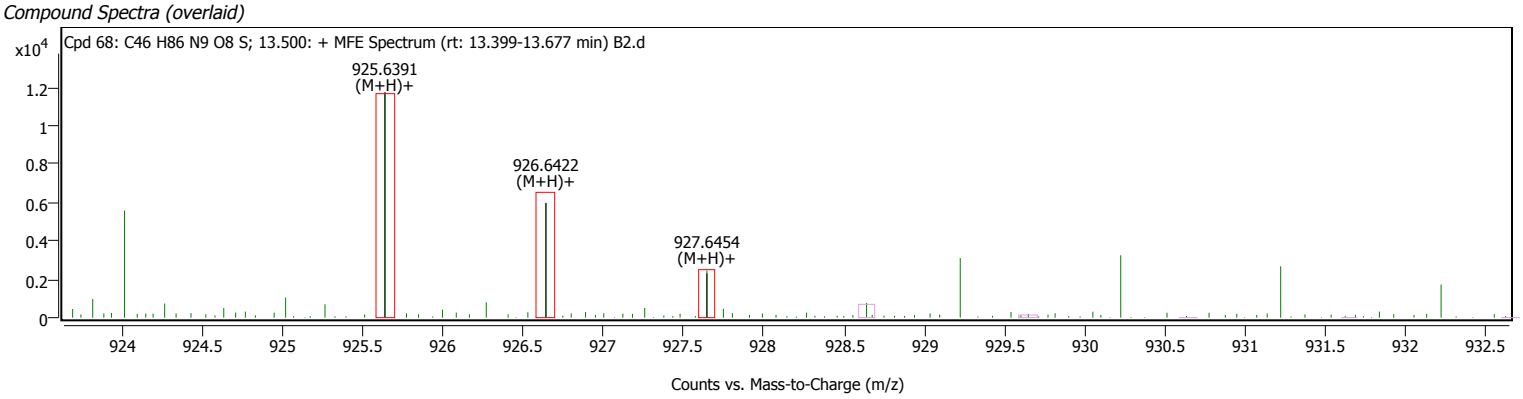
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C46 H86 N9 O8 S	(M+H)+	MFG	13.500		924.6322		93.78		93.78
	C47 H92 N2 O13 S	(M+H)+	MFG	13.500		924.6320		93.63		93.63
	C53 H86 N3 O10	(M+H)+	MFG	13.500		924.6318		93.50		93.50
	C45 H80 N16 O3 S	(M+H)+	MFG	13.500		924.6323		93.46		93.46
	C38 H82 N15 O11	(M+H)+	MFG	13.500		924.6321		93.37		93.37

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 69: C37 H74 N19 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H74 N19 O6	13.506		880.6066		MFG	96.92	MFE	

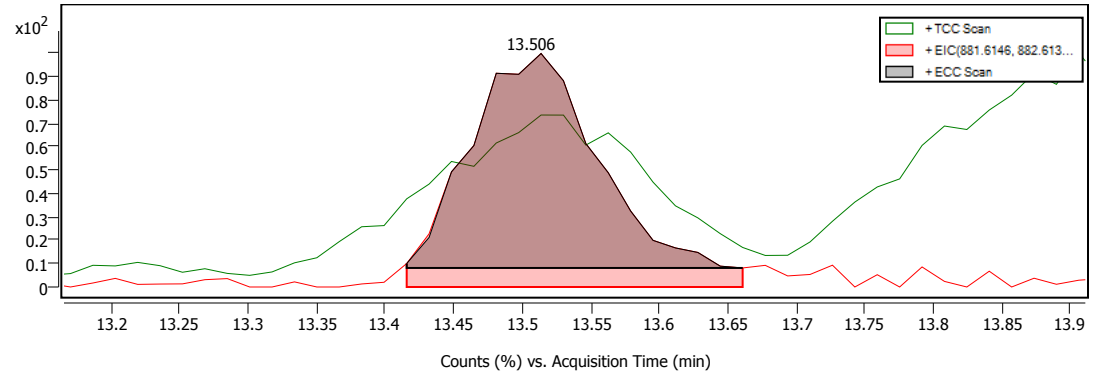
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	881.6137				13	96.92	

Compound ID Table

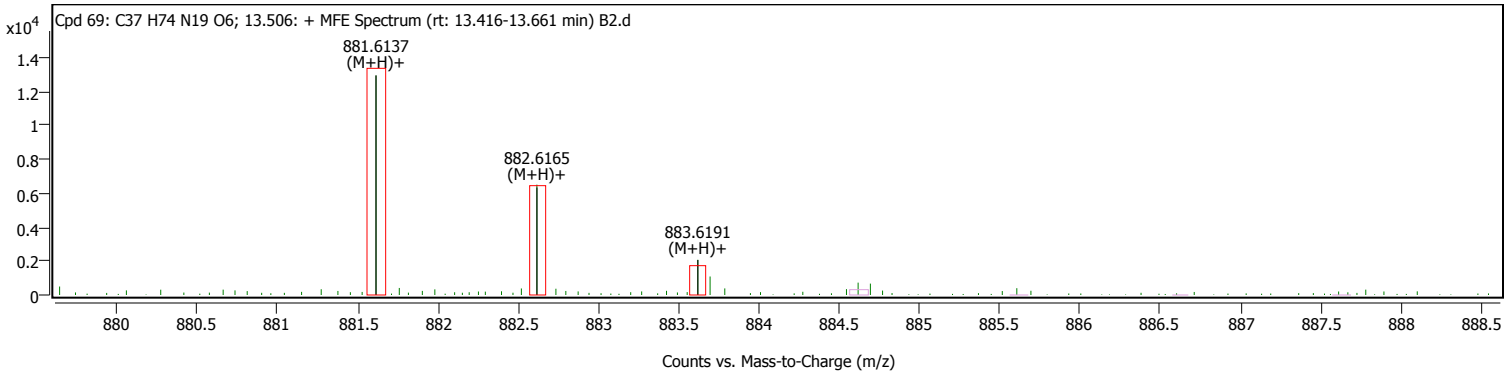
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H74 N19 O6	(M+H)+	MFG	13.506		880.6066		96.92		96.92
	C38 H80 N12 O11	(M+H)+	MFG	13.506		880.6064		96.74		96.74
	C36 H68 N26 O	(M+H)+	MFG	13.506		880.6067		96.36		96.36
	C39 H86 N5 O16	(M+H)+	MFG	13.506		880.6063		95.86		95.86
	C36 H78 N15 O10	(M+H)+	MFG	13.506		880.6065		95.52		95.52
PI(15:0/22:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(16:0/21:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(18:0/19:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(20:0/17:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(21:0/16:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(22:0/15:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(19:0/18:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	
PI(17:0/20:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.506		880.6062		93.34	93.34	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 70: C43 H84 N2 O11 S

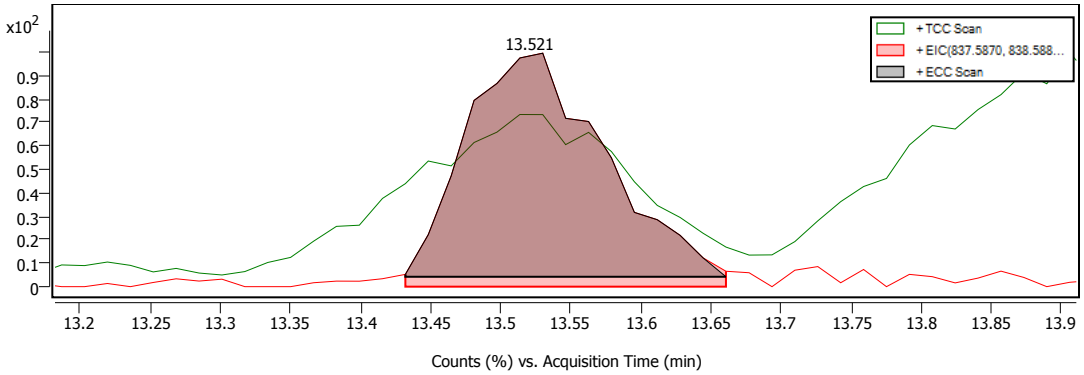
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C43 H84 N2 O11 S	13.521		836.5799		MFG	95.53	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	837.5871				11	95.53	

Compound ID Table

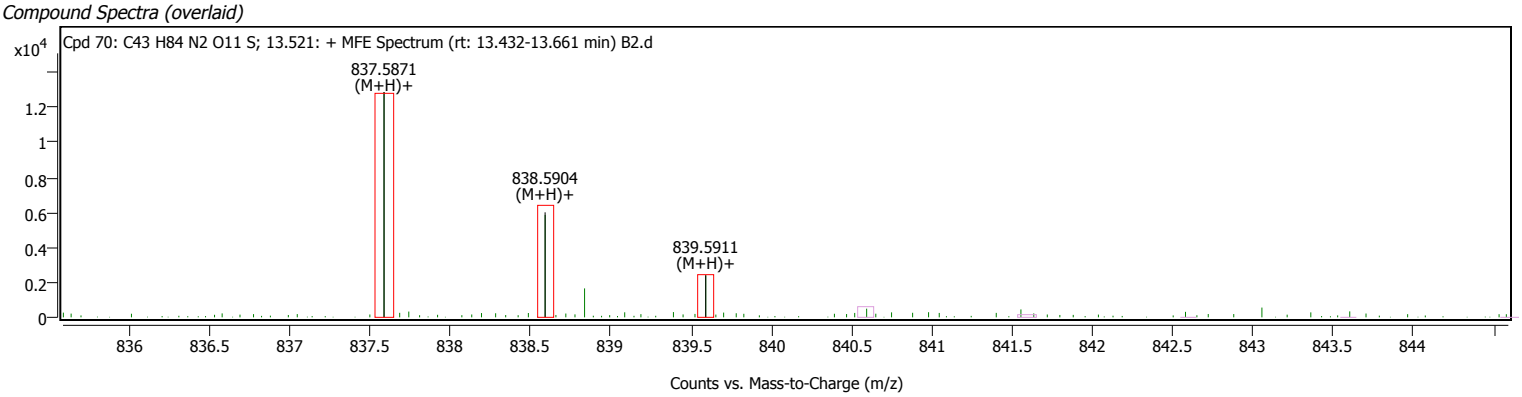
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C43 H84 N2 O11 S	(M+H)+	MFG	13.521		836.5799		95.53		95.53
	C42 H78 N9 O6 S	(M+H)+	MFG	13.521		836.5800		95.23		95.23
	C41 H72 N16 O S	(M+H)+	MFG	13.521		836.5802		94.36		94.36
	C44 H80 N6 O7 S	(M+H)+	MFG	13.521		836.5799		94.10		94.10
	C43 H74 N13 O2 S	(M+H)+	MFG	13.521		836.5801		93.70		93.70
PI(O-16:0/19:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	
PI(O-18:0/17:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	
PI(O-20:0/15:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	
PI(P-16:0/19:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	
PI(P-18:0/17:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	
PI(P-20:0/15:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.521		836.5795		90.48	90.48	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 71: PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

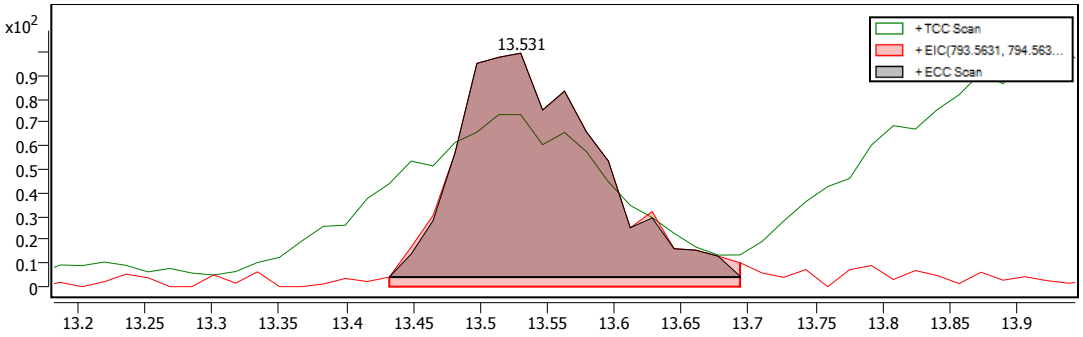
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H79 N O8 P	13.531		792.5544		DBSearch	96.60	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	793.5618 793.5618 793.5618 793.5618		0	96.60	26		

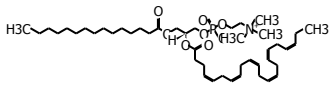
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
PC(17:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
PC(17:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/17:1(9Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.531		792.5544		96.60	96.60	
	C49 H76 O8	(M+H)+	MFG	13.531		792.5544		95.35		95.35
	C48 H70 N7 O3	(M+H)+	MFG	13.531		792.5545		94.19		94.19
	C41 H70 N13 O S	(M+H)+	MFG	13.531		792.5549		93.87		93.87
	C42 H76 N6 O6 S	(M+H)+	MFG	13.531		792.5548		93.86		93.86
	C50 H72 N4 O4	(M+H)+	MFG	13.531		792.5544		92.95		92.95
PC(17:0/18:3(9Z,12Z,15Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(17:0/18:3(6Z,9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(17:1(9Z)/18:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(18:3(9Z,12Z,15Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(20:2(11Z,14Z)/15:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(16:0/19:3(9Z,12Z,15Z))[U]	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(17:2(9Z,12Z)/18:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(18:1(9Z)/17:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(18:2(9Z,12Z)/17:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(18:3(6Z,9Z,12Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(20:3(8Z,11Z,14Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(20:3(5Z,8Z,11Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(15:0/20:3(8Z,11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(15:0/20:3(5Z,8Z,11Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	
PC(15:1(9Z)/20:2(11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.531		770.5724		89.68	89.68	

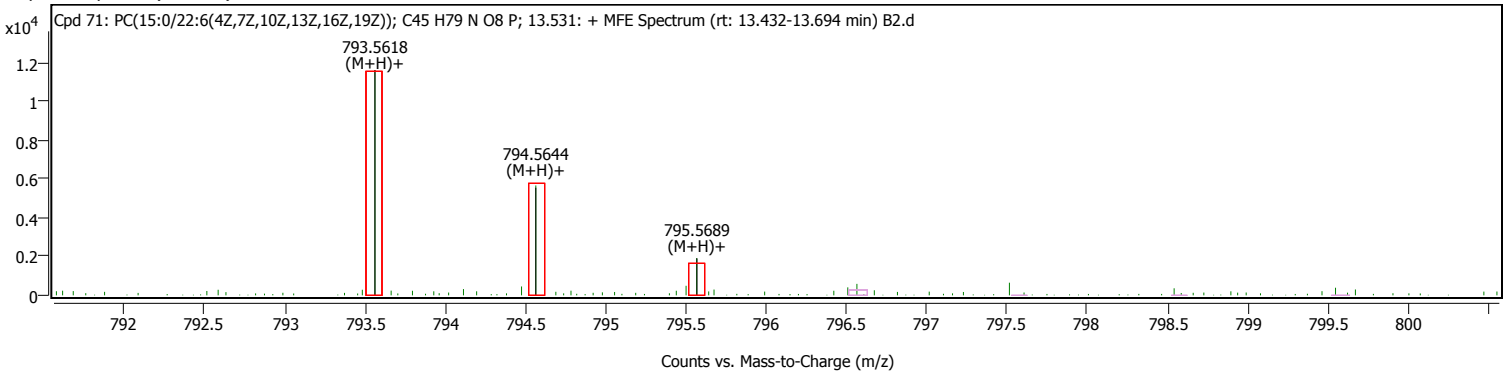
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 72: C40 H72 N6 O5 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C40 H72 N6 O5 S	13.544		748.5282		MFG	94.70	MFE	

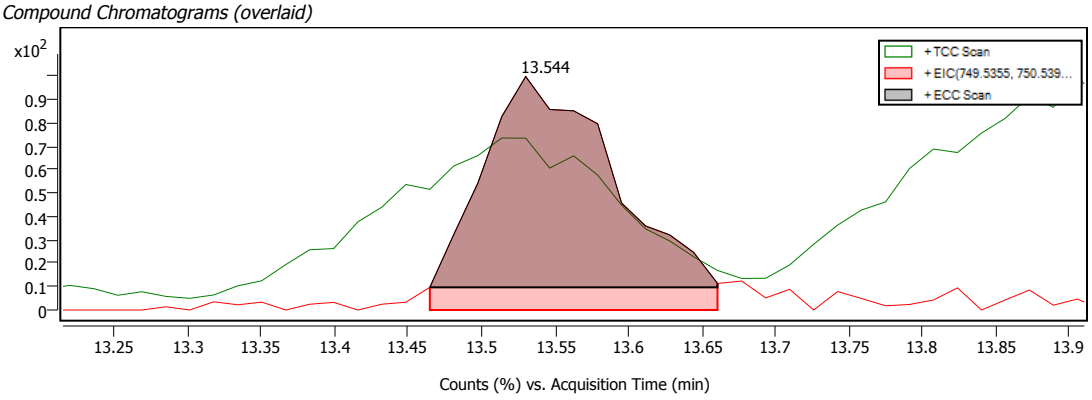
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	749.5353				24	94.70	

Compound ID Table

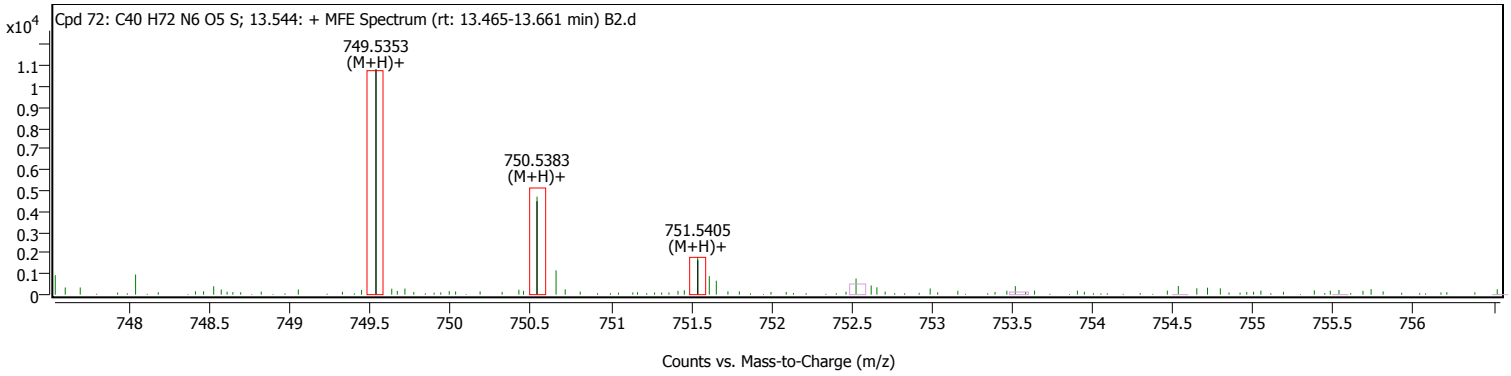
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C40 H72 N6 O5 S	(M+H)+	MFG	13.544		748.5282		94.70		94.70
	C39 H76 N2 O9 S	(M+H)+	MFG	13.544		748.5281		94.62		94.62
	C32 H68 N12 O8	(M+H)+	MFG	13.544		748.5281		93.93		93.93
	C38 H70 N9 O4 S	(M+H)+	MFG	13.544		748.5283		93.63		93.63
	C39 H66 N13 S	(M+H)+	MFG	13.544		748.5283		93.57		93.57
PG(15:0/19:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(18:0/16:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(18:1(11Z)/16:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(18:1(9Z)/16:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(16:0/18:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
LBPA(16:0/18:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(14:1(9Z)/20:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(12:0/22:1(11Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(14:0/20:1(11Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(15:1(9Z)/19:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(22:1(11Z)/12:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(17:0/17:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(17:1(9Z)/17:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(19:0/15:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(19:1(9Z)/15:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(20:0/14:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(20:1(11Z)/14:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(16:0/18:1(9Z))[U]	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	
PG(16:1(9Z)/18:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.544		748.5278		88.50	88.50	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 73: C38 H68 N6 O4 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C38 H68 N6 O4 S	13.562		704.5019		MFG	96.75	MFE	

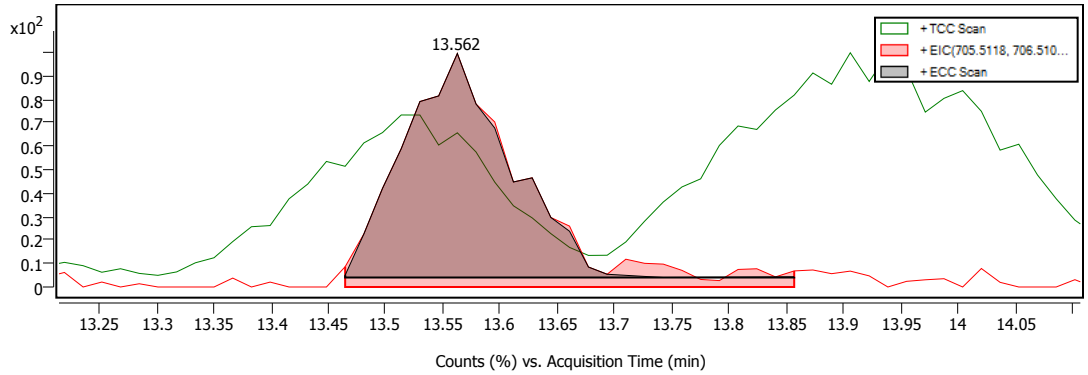
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	705.5095				7	96.75	

Compound ID Table

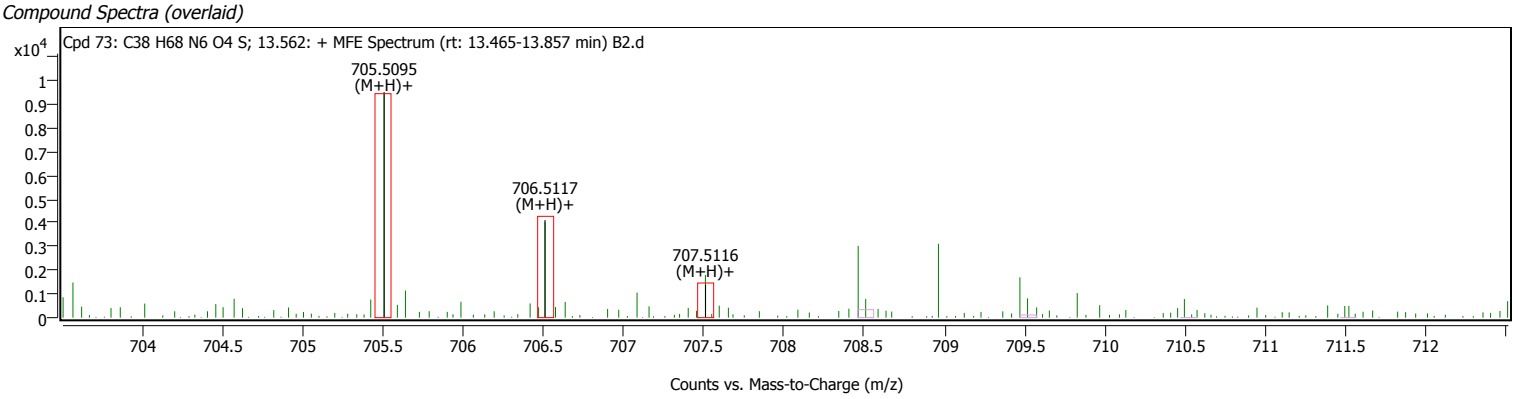
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C38 H68 N6 O4 S	(M+H)+	MFG	13.562		704.5019		96.75		96.75
	C36 H66 N9 O3 S	(M+H)+	MFG	13.562		704.5020		95.86		95.86
	C37 H72 N2 O8 S	(M+H)+	MFG	13.562		704.5018		95.06		95.06
	C39 H64 N10 S	(M+H)+	MFG	13.562		704.5020		93.26		93.26
	C40 H70 N3 O5 S	(M+H)+	MFG	13.562		704.5018		92.16		92.16
PG(P-16:0/16:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.562		704.5015		85.57	85.57	
PG(P-18:0/14:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.562		704.5015		85.57	85.57	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 74: C36 H64 N6 O3 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C36 H64 N6 O3 S	13.572		660.4756		MFG	93.74	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	661.4830				38	93.74	

Compound Discovery Report

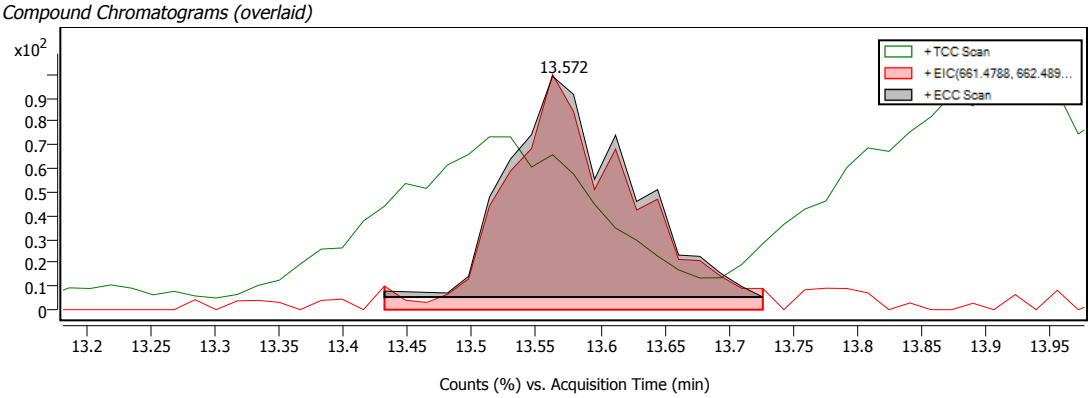
Agilent | Trusted Answers

Compound ID Table

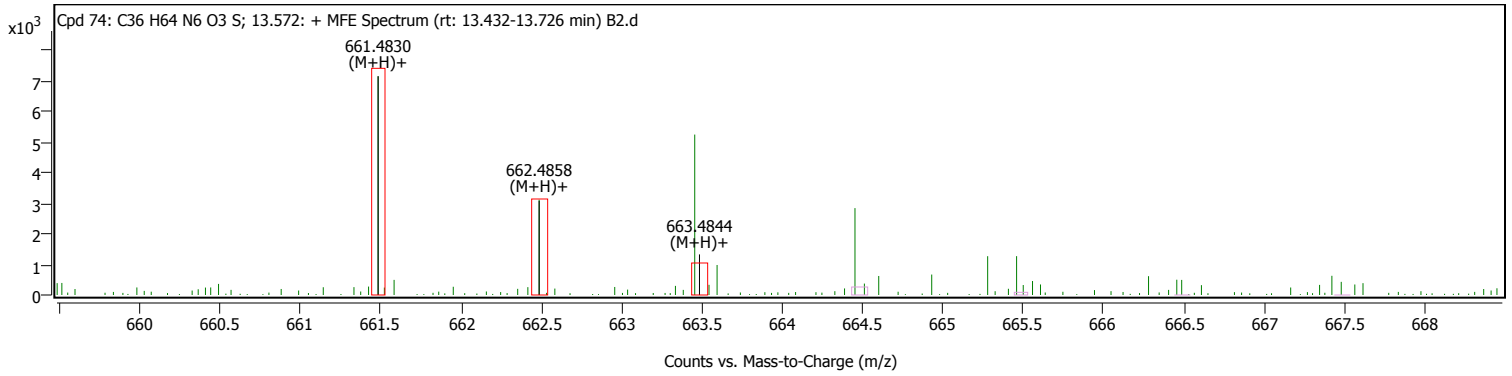
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C36 H64 N6 O3 S	(M+H)+	MFG	13.572		660.4756		93.74		93.74
	C35 H68 N2 O7 S	(M+H)+	MFG	13.572		660.4755		92.75		92.75
	C34 H62 N9 O2 S	(M+H)+	MFG	13.572		660.4756		92.55		92.55
	C44 H68 S2	(M+H)+	MFG	13.572		660.4756		92.28		92.28
	C29 H64 N12 O S2	(M+H)+	MFG	13.572		660.4760		91.70		91.70
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.572		660.4750		84.15	84.15	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.572		660.4750		84.15	84.15	
DG(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.572		660.4750		84.15	84.15	
DG(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:3(6Z,9Z,12Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:3(6Z,9Z,12Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:3(9Z,12Z,15Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:4(6Z,9Z,12Z,15Z)/20:3(8Z,11Z,14Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(20:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:3(9Z,12Z,15Z)/20:4(5Z,8Z,11Z,14Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
DG(18:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.572		638.4931		78.35	78.35	
PA(20:1(11Z)/13:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(18:1(9Z)/15:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(19:1(9Z)/14:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(15:1(9Z)/18:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(13:0/20:1(11Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(14:0/19:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(14:1(9Z)/19:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(15:0/18:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(17:1(9Z)/16:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(16:1(9Z)/17:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(17:0/16:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(18:0/15:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(16:0/17:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	
PA(19:0/14:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.572		660.4750		77.96	77.96	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

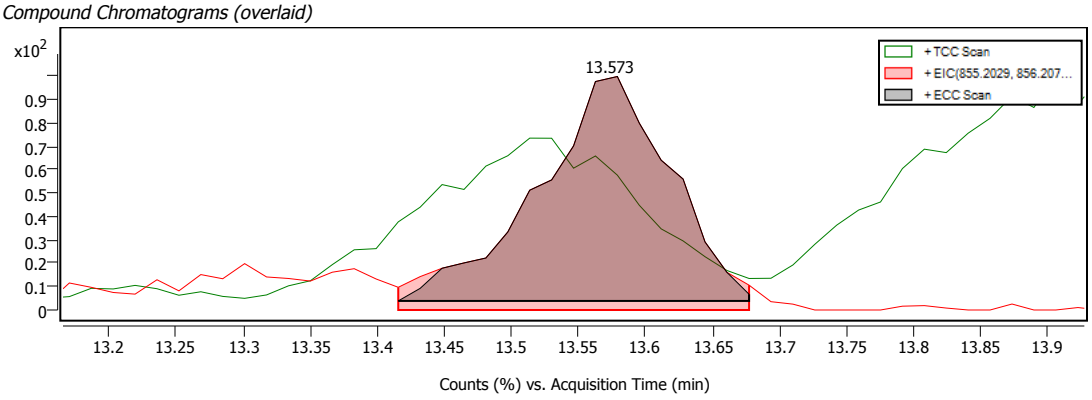


Cpd 75: 13.573

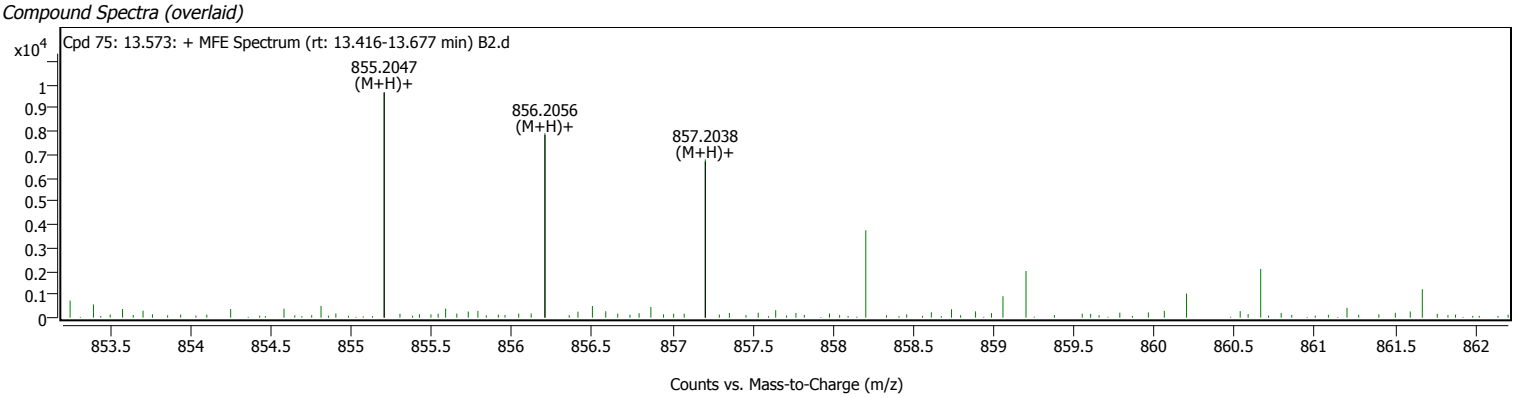
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.573		854.1975				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

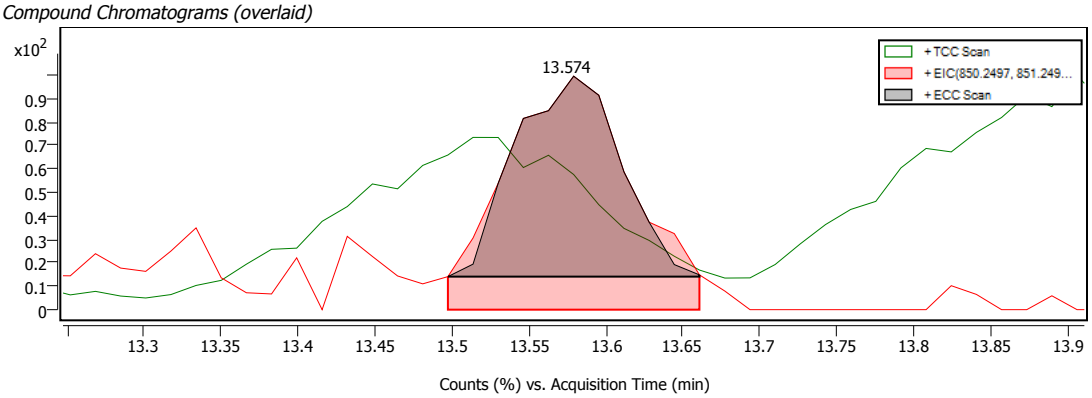


Cpd 76: 13.574

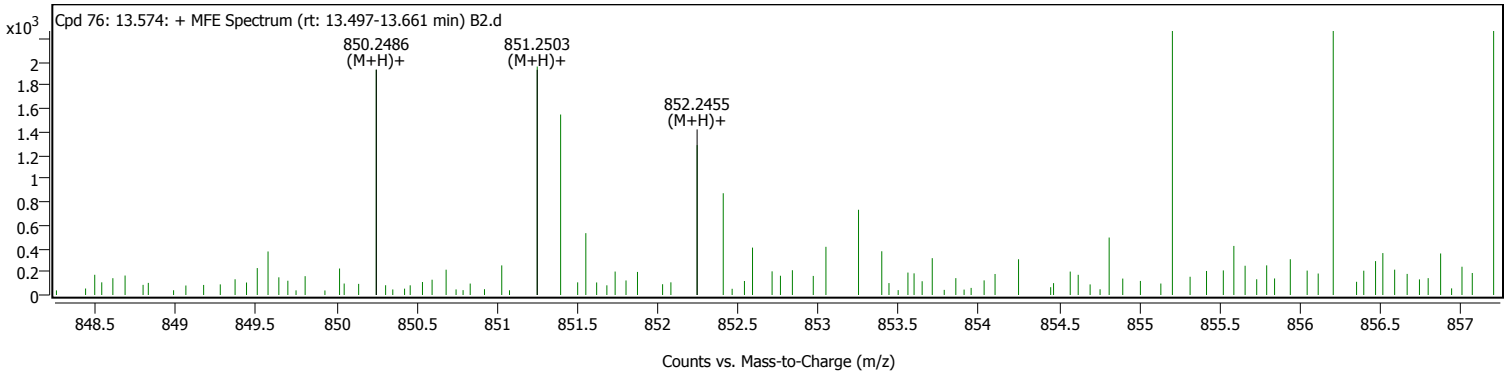
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.574		849.2413				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 77: C37 H31 N17 O3 S3

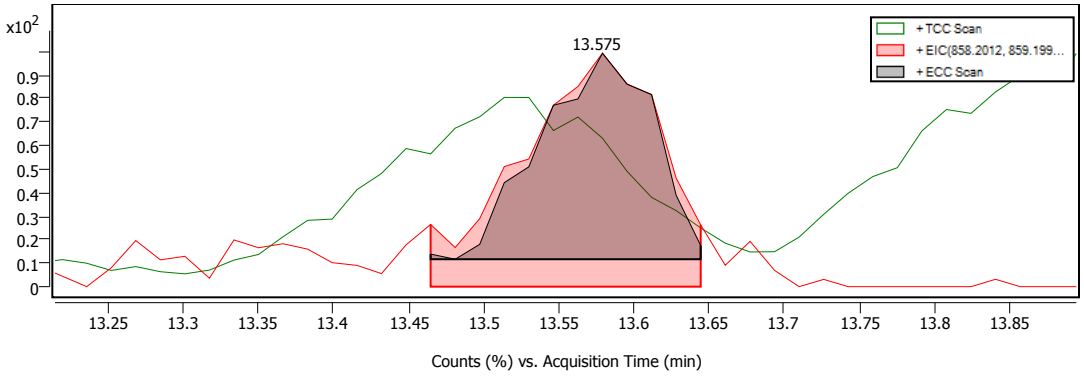
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H31 N17 O3 S3	13.575		857.1944		MFG	77.71	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	858.2034				5	77.71	

Compound ID Table

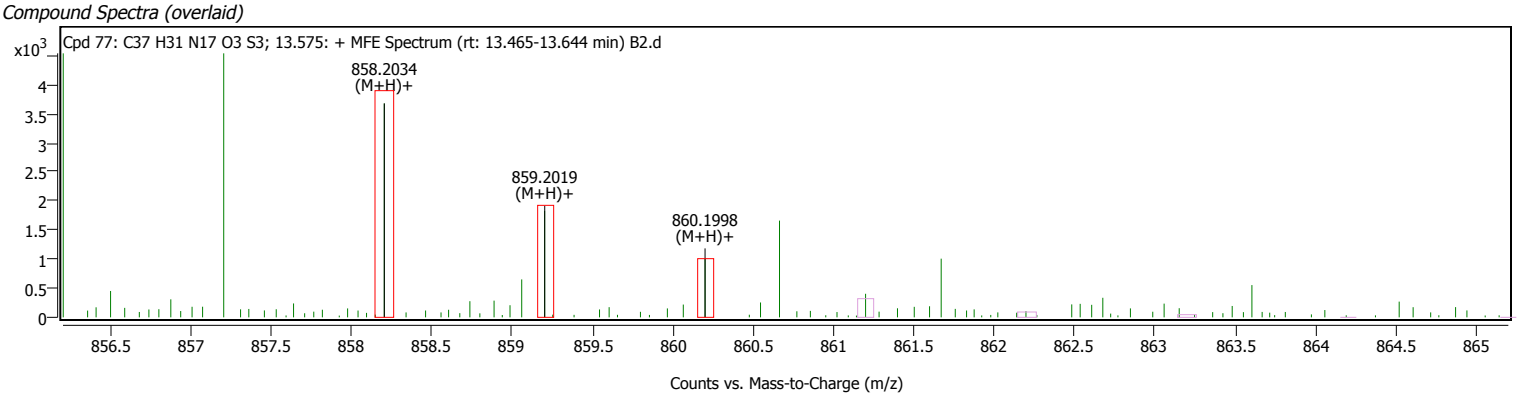
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H31 N17 O3 S3	(M+H)+	MFG	13.575		857.1944		77.71		77.71
	C30 H31 N23 O S4	(M+H)+	MFG	13.575		857.1948		76.71		76.71
	C38 H37 N10 O8 S3	(M+H)+	MFG	13.575		857.1943		76.02		76.02
	C37 H39 N13 O2 S5	(M+H)+	MFG	13.575		857.1946		75.91		75.91
	C45 H35 N11 S4	(M+H)+	MFG	13.575		857.1943		74.92		74.92

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 78: C25 H50 N19

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C25 H50 N19	13.581		616.4501		MFG	72.94	MFE	

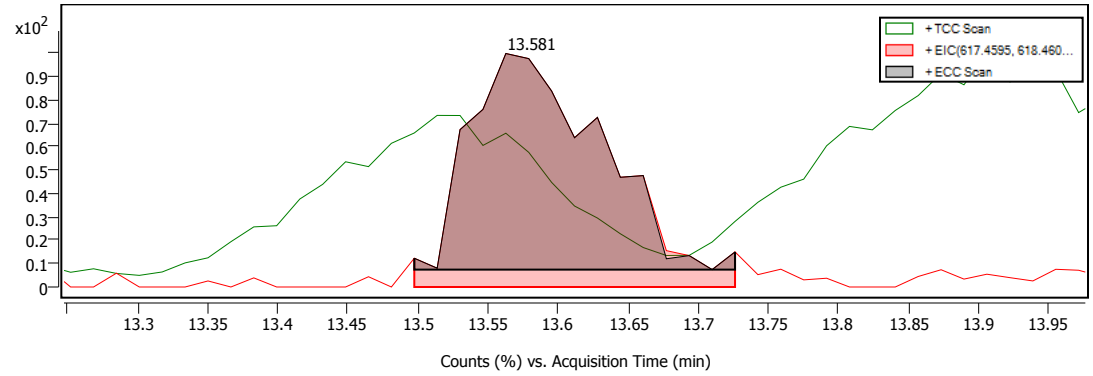
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	617.4569				6	72.94	

Compound ID Table

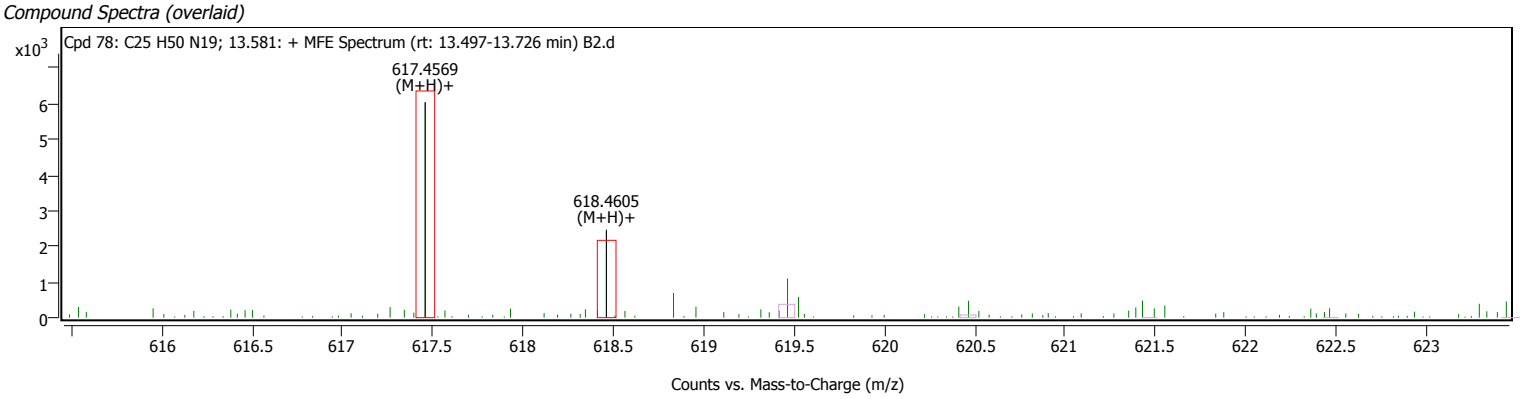
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C25 H50 N19	(M+H)+	MFG	13.581		616.4501		72.94		72.94
	C27 H52 N16 O	(M+H)+	MFG	13.581		616.4500		72.21		72.21
Oryzanol C	C41 H60 O4	(M+H)+	DBSearch-MFG	13.581		616.4497		71.22	71.19	71.24
	C26 H56 N12 O5	(M+H)+	MFG	13.581		616.4499		71.02		71.02
	C42 H56 N4	(M+H)+	MFG	13.581		616.4497		70.38		70.38
PA(P-16:0/15:1(9Z))	C34 H65 O7 P	(M+H)+	DBSearch	13.581		616.4497		60.69	60.69	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 79: C32 H64 N2 S3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H64 N2 S3	13.594		572.4236		MFG	86.30	MFE	

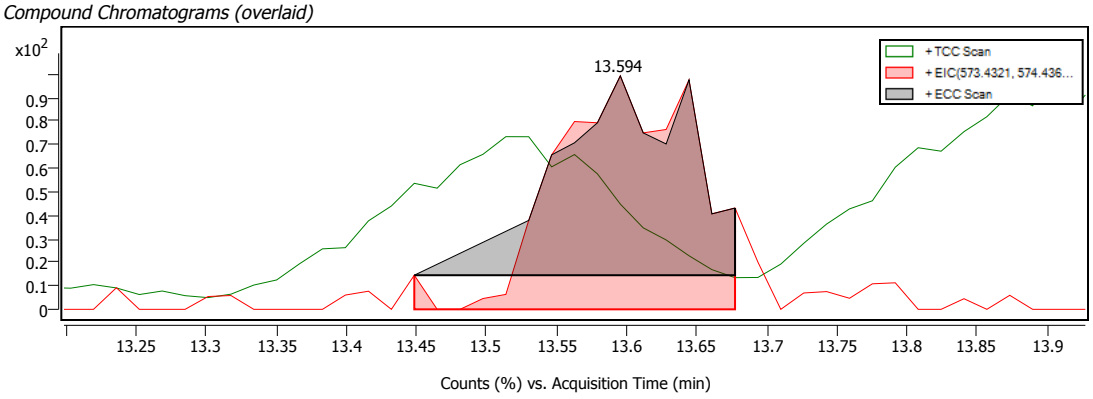
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	573.4314				5	86.30	

Compound ID Table

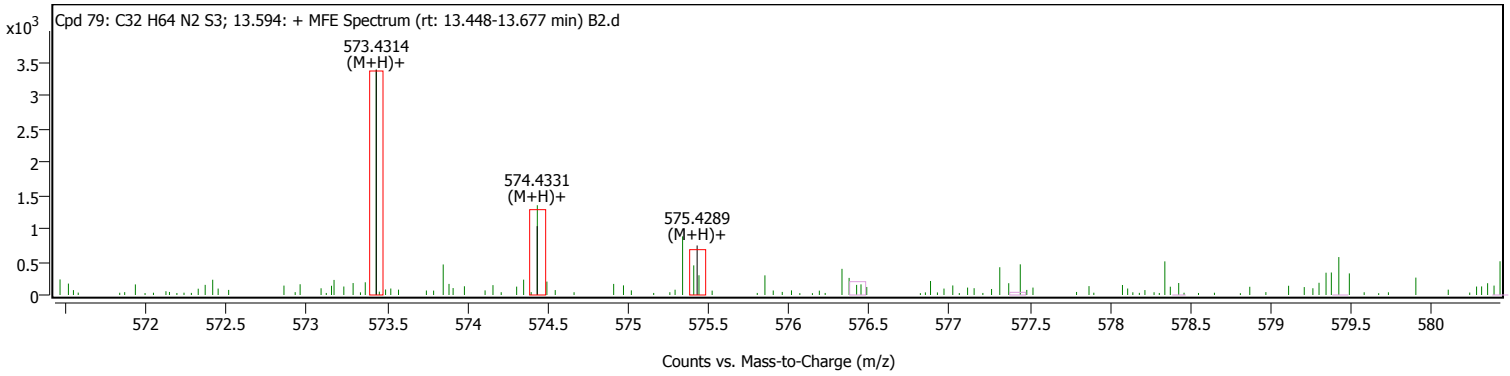
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H64 N2 S3	(M+H)+	MFG	13.594		572.4236		86.30		86.30
	C27 H58 N9 S2	(M+H)+	MFG	13.594		572.4237		78.39		78.39
	C36 H59 Cl N O2	(M+H)+	MFG	13.594		572.4236		74.47		74.47
	C29 H59 Cl N7 S	(M+H)+	MFG	13.594		572.4238		74.00		74.00
	C31 H60 N2 O5 S	(M+H)+	MFG	13.594		572.4232		73.15		73.15

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 80: C32 H58 N19 O

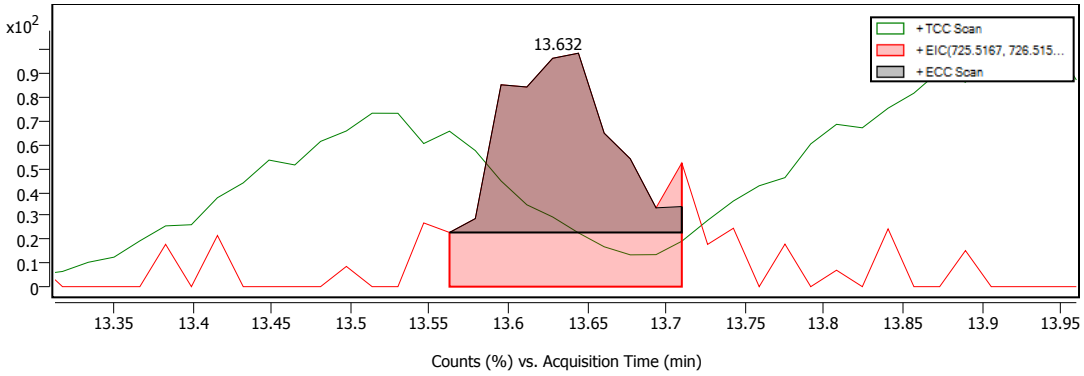
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H58 N19 O	13.632		724.5075		MFG	70.14	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	725.5154				5	70.14	

Compound ID Table

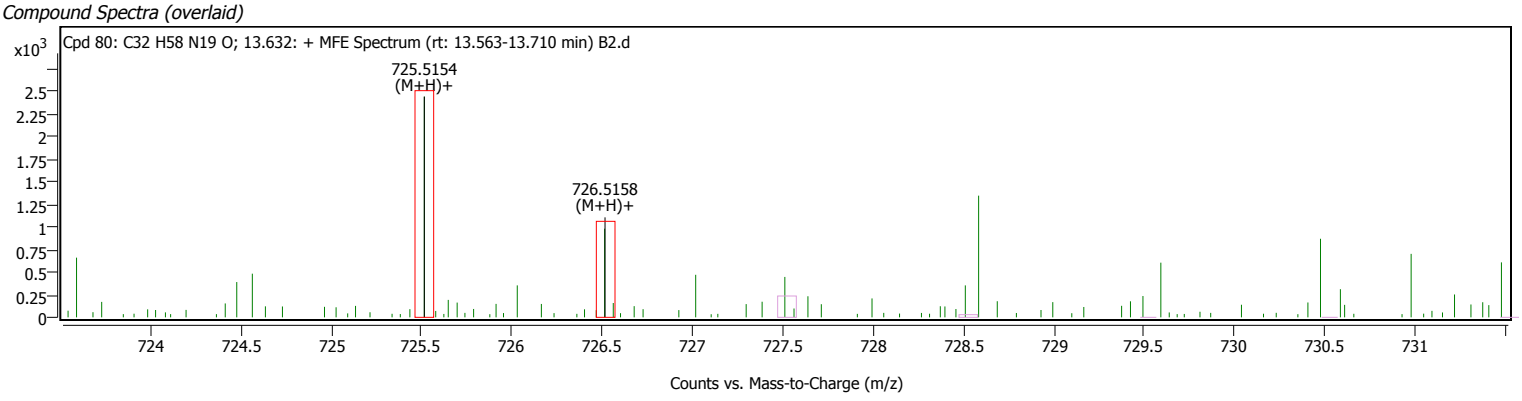
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H58 N19 O	(M+H)+	MFG	13.632		724.5075		70.14		70.14
	C34 H60 N16 O2	(M+H)+	MFG	13.632		724.5075		68.12		68.12
	C33 H64 N12 O6	(M+H)+	MFG	13.632		724.5074		67.60		67.60
	C30 H56 N22	(M+H)+	MFG	13.632		724.5076		67.09		67.09
	C35 H66 N9 O7	(M+H)+	MFG	13.632		724.5074		65.31		65.31

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)

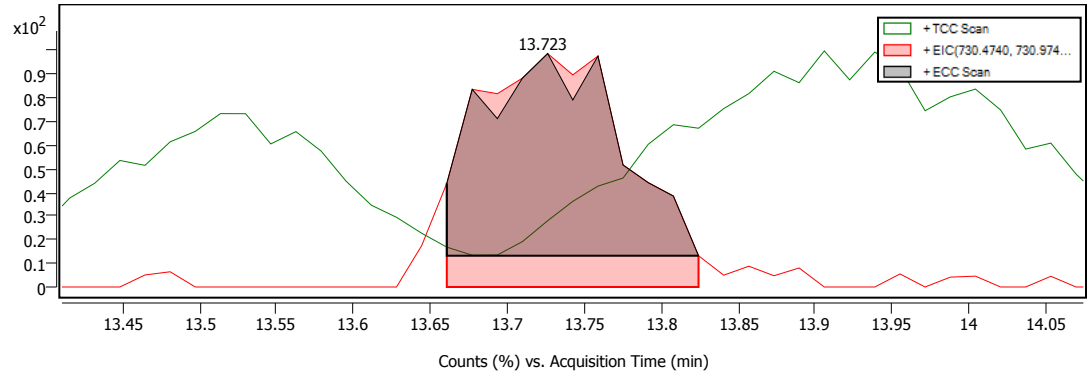


Cpd 81: 13.723

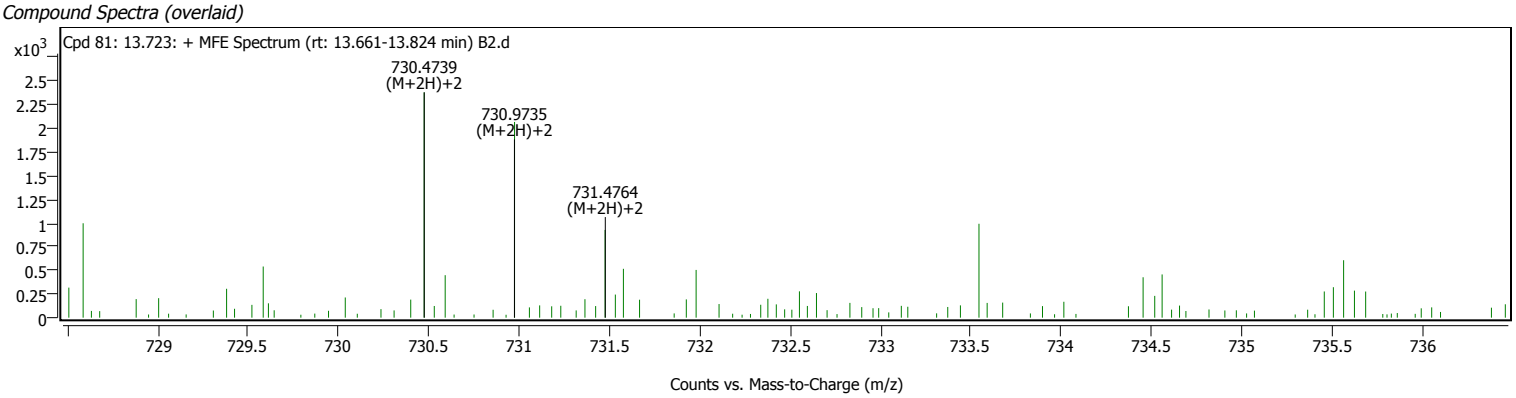
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.723		1458.9332				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

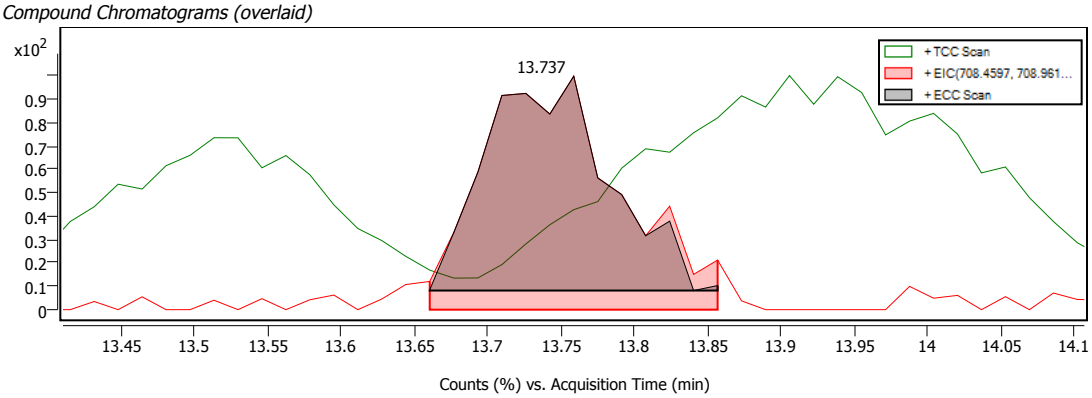


Cpd 82: 13.737

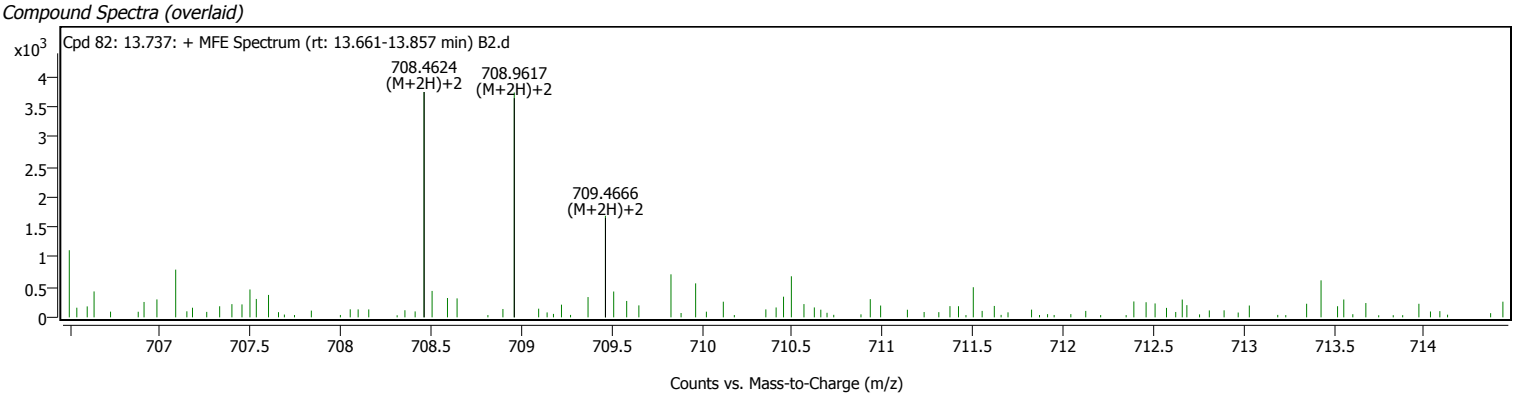
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.737		1414.9102				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

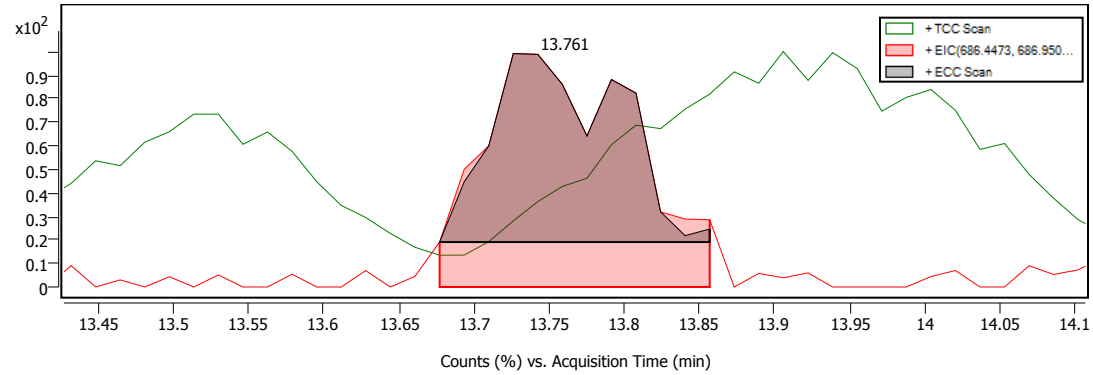


Cpd 83: 13.761

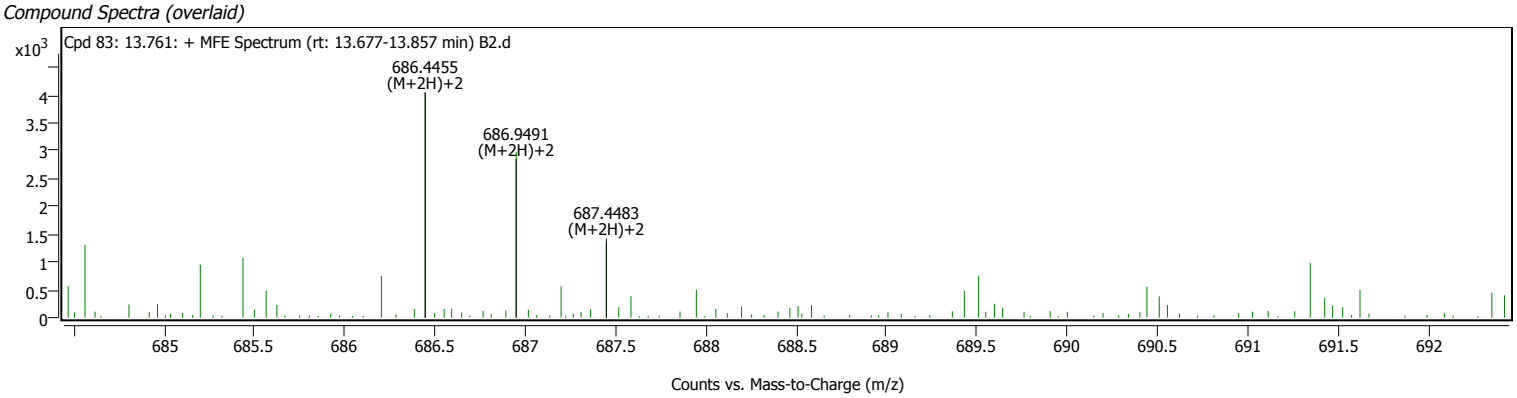
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.761		1370.8764				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

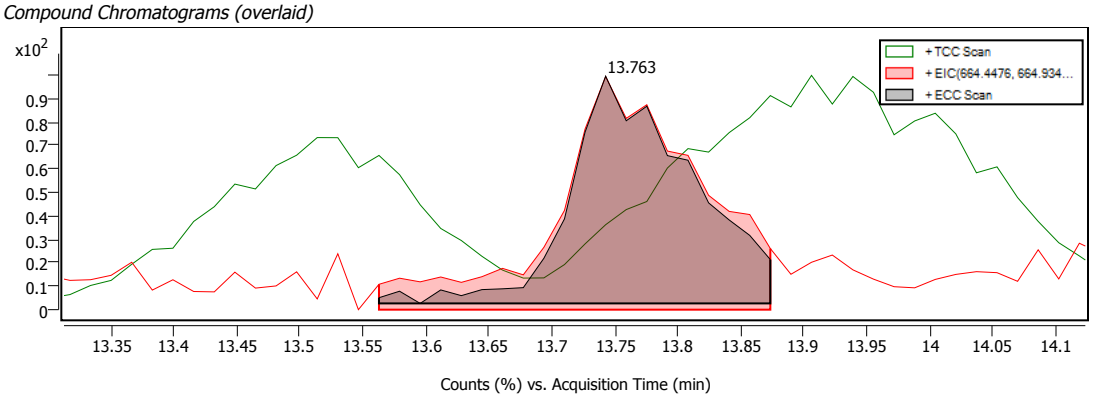


Cpd 84: 13.763

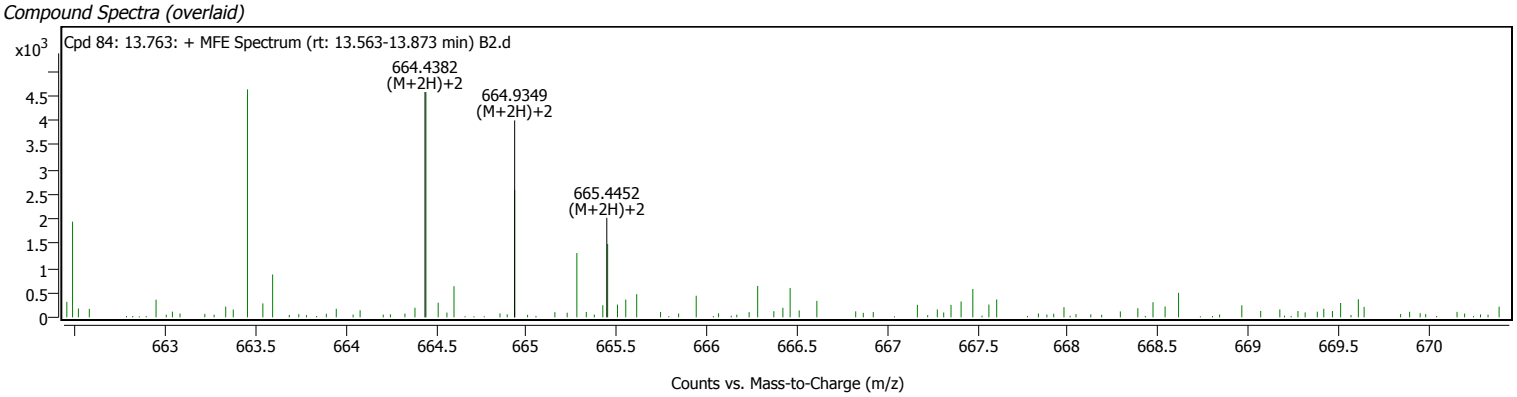
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.763		1326.8618				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 85: C41 H22 N23 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C41 H22 N23 O6	13.764		932.2128		MFG	62.96	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	933.2201				11	62.96	

Compound Discovery Report

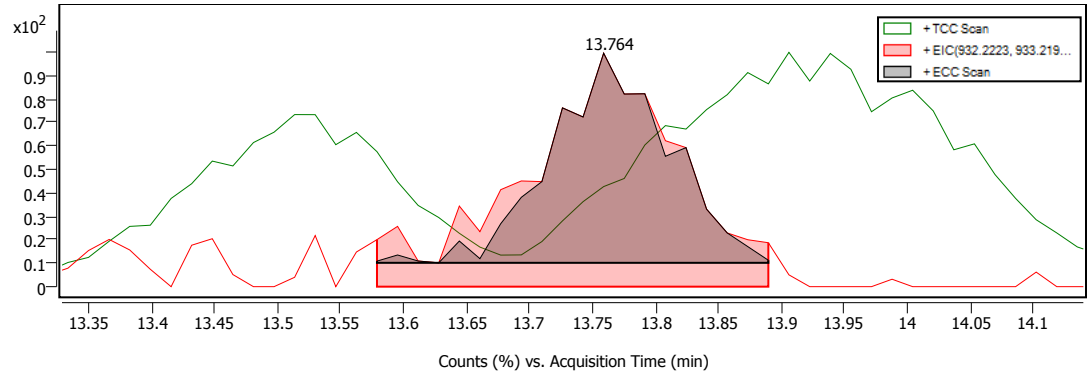
Agilent | Trusted Answers

Compound ID Table

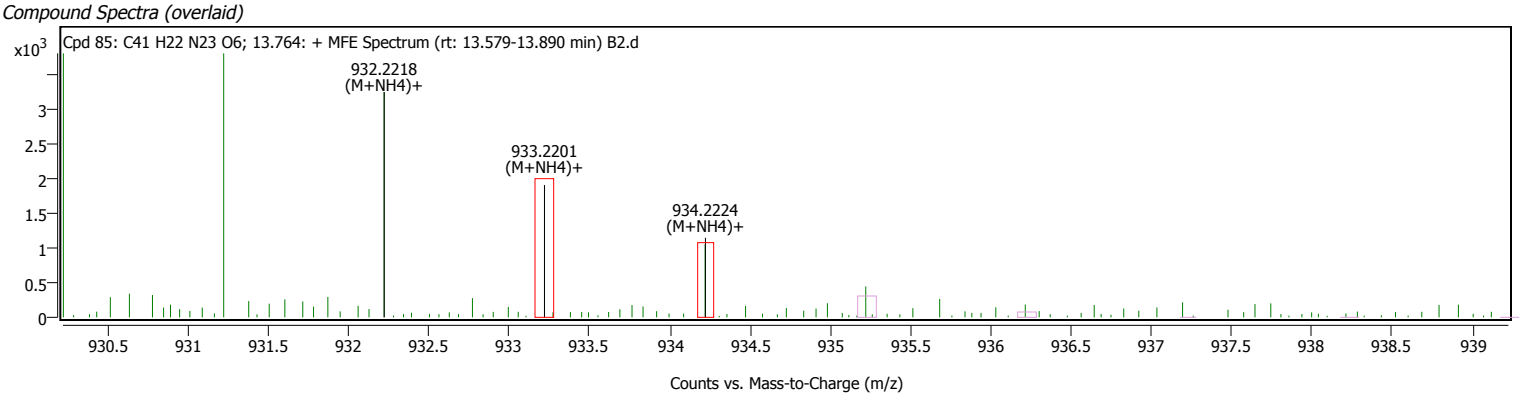
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C41 H22 N23 O6	(M+H)+	MFG	13.764		932.2128		62.96		62.96
β-Phenylalanoyl-CoA	C30 H45 N8 O17 P3 S	(M+NH4)+	DBSearch	13.764		914.1863		62.86	62.86	
	C42 H28 N16 O11	(M+H)+	MFG	13.764		932.2127		62.29		62.29
	C43 H34 N9 O16	(M+H)+	MFG	13.764		932.2126		61.62		61.62
	C57 H22 N15 O	(M+H)+	MFG	13.764		932.2126		61.27		61.27
	C44 H40 N2 O21	(M+H)+	MFG	13.764		932.2125		60.93		60.93
	C28 H50 O29 S2	(M+NH4)+	MFG	13.764		914.1879		47.62		47.62
	C27 H44 N7 O24 S2	(M+NH4)+	MFG	13.764		914.1879		47.62		47.62
	C35 H56 Cl2 O15 S4	(M+NH4)+	MFG	13.764		914.1879		47.62		47.62
	C28 H29 Cl3 N26 O5	(M+NH4)+	MFG	13.764		914.1879		47.62		47.62
	C34 H50 Cl2 N7 O10 S4	(M+NH4)+	MFG	13.764		914.1879		47.62		47.62

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

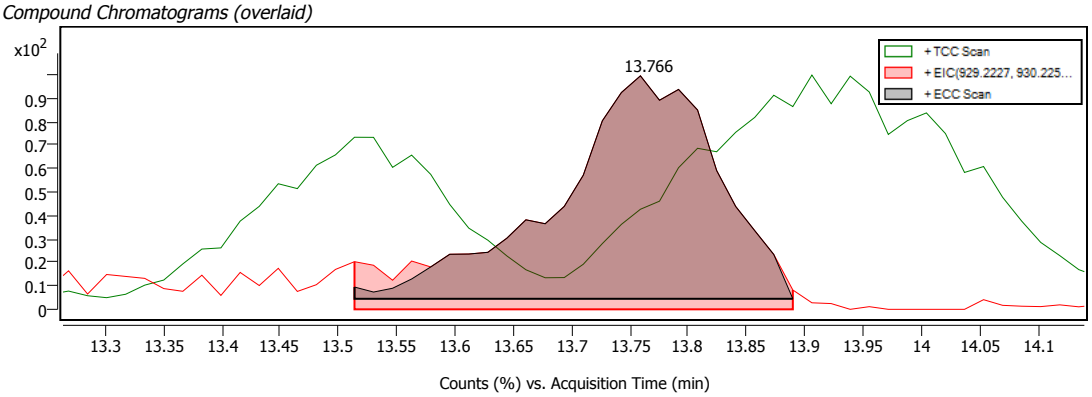


Cpd 86: 13.766

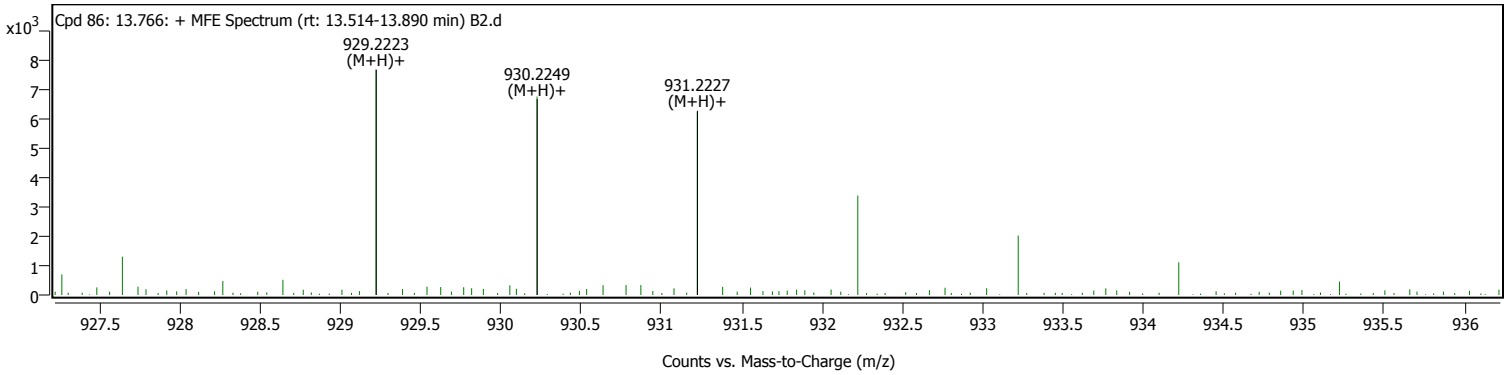
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.766		928.2151				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

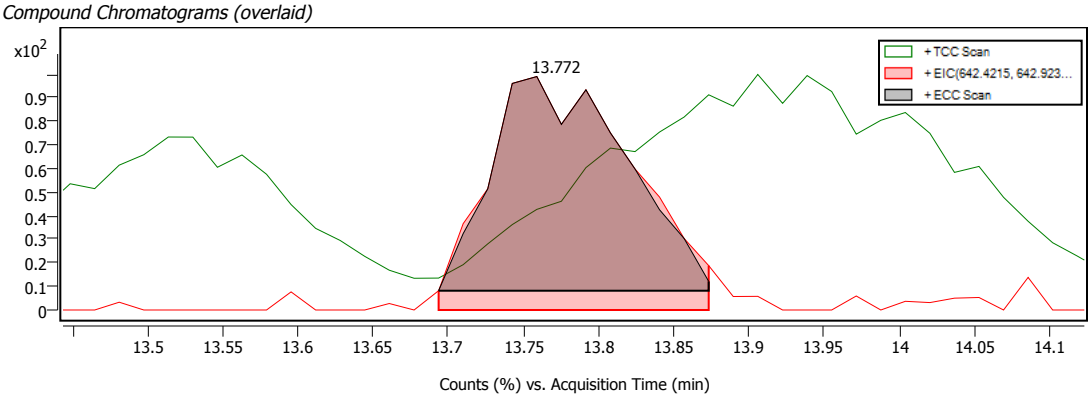


Cpd 87: 13.772

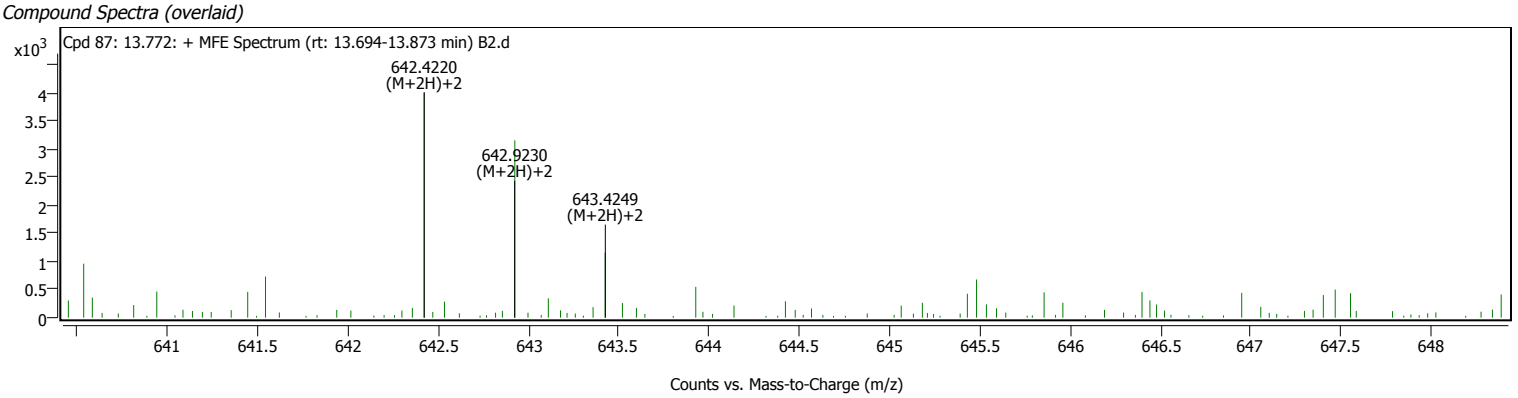
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.772		1282.8295				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

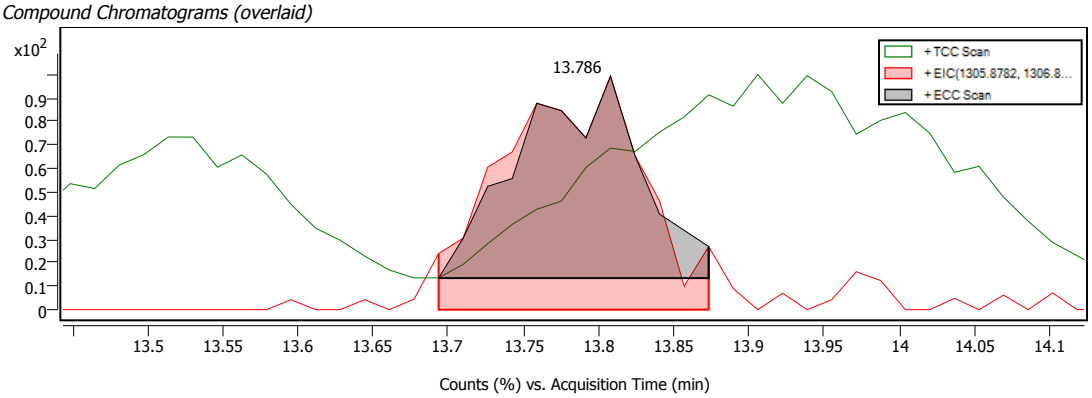


Cpd 88: 13.786

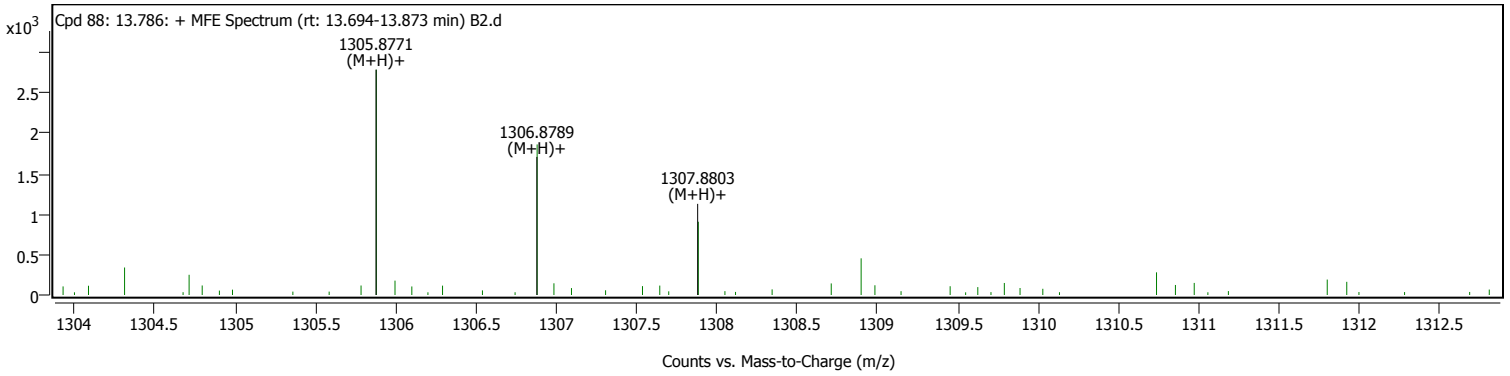
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.786		1304.8698				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

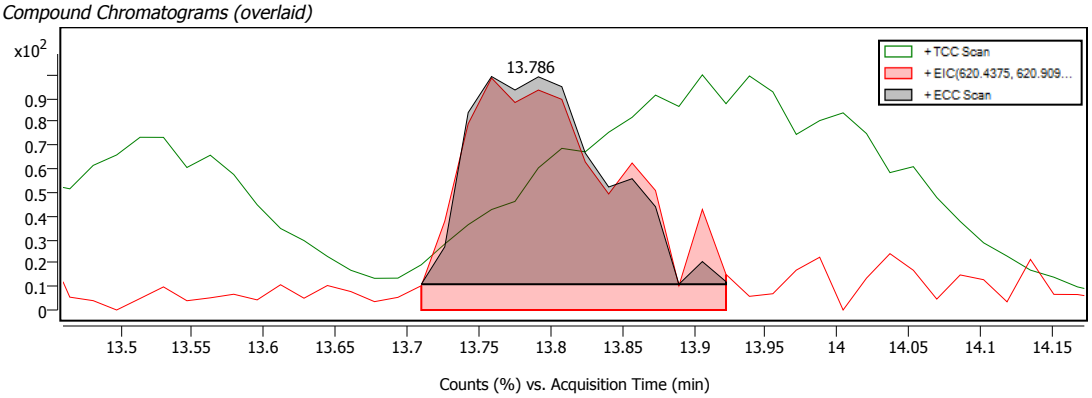


Cpd 89: 13.786

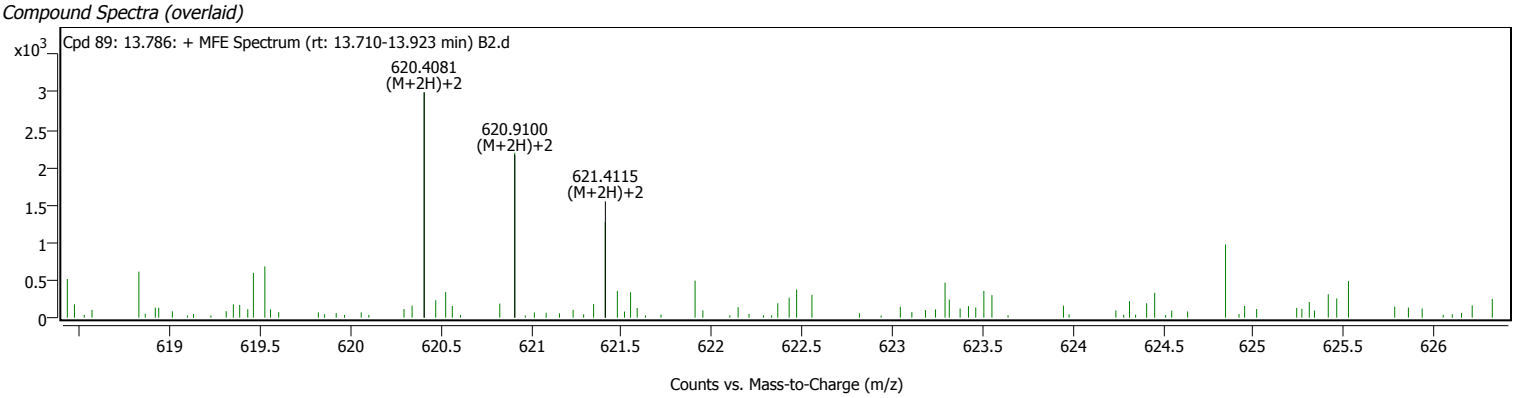
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.786		1238.8016				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

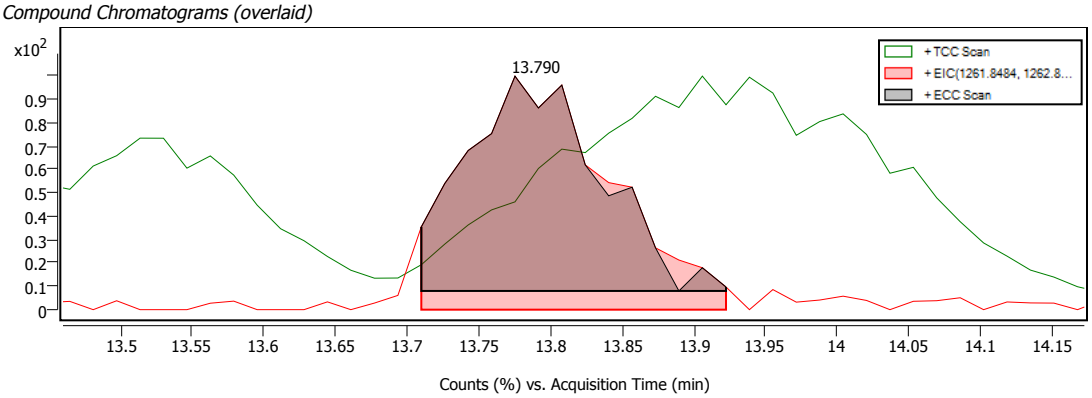


Cpd 90: 13.790

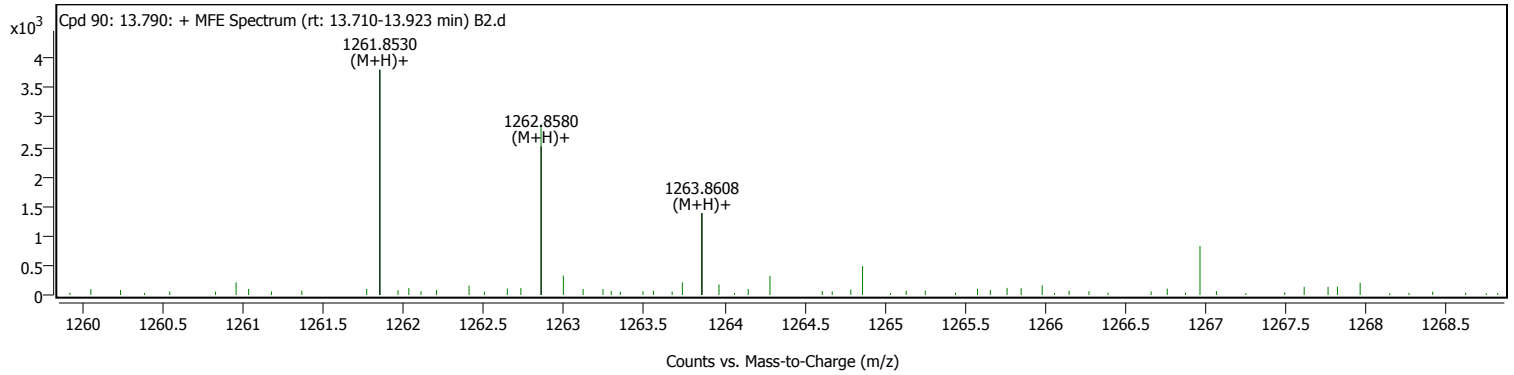
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.790		1260.8457				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

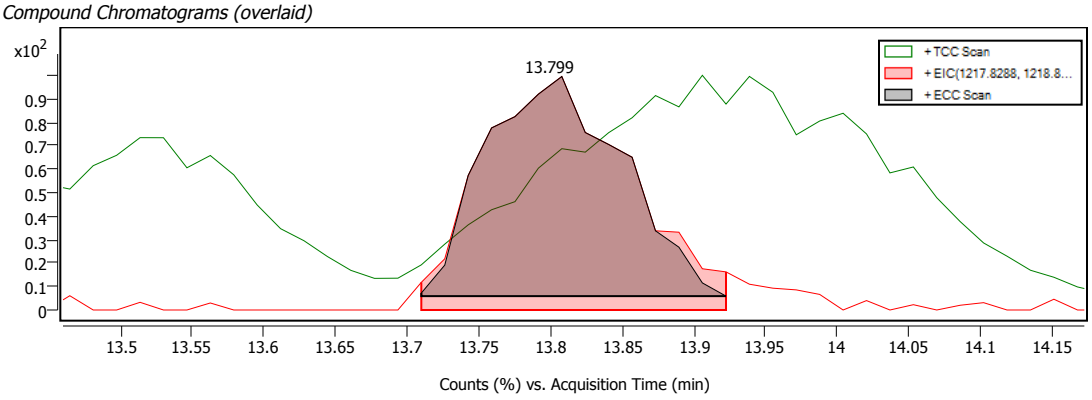


Cpd 91: 13.799

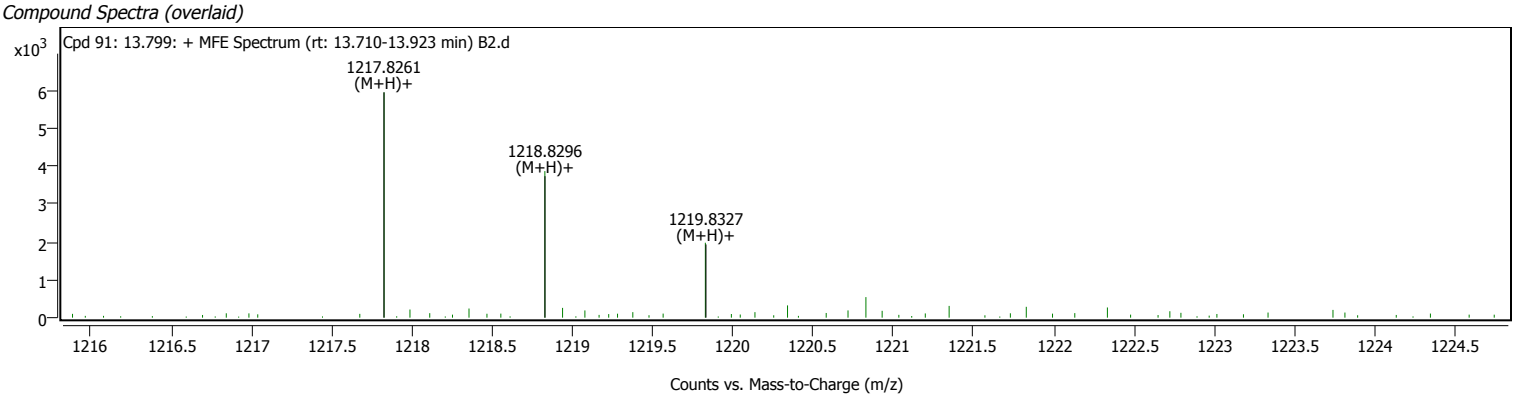
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.799		1216.8188				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

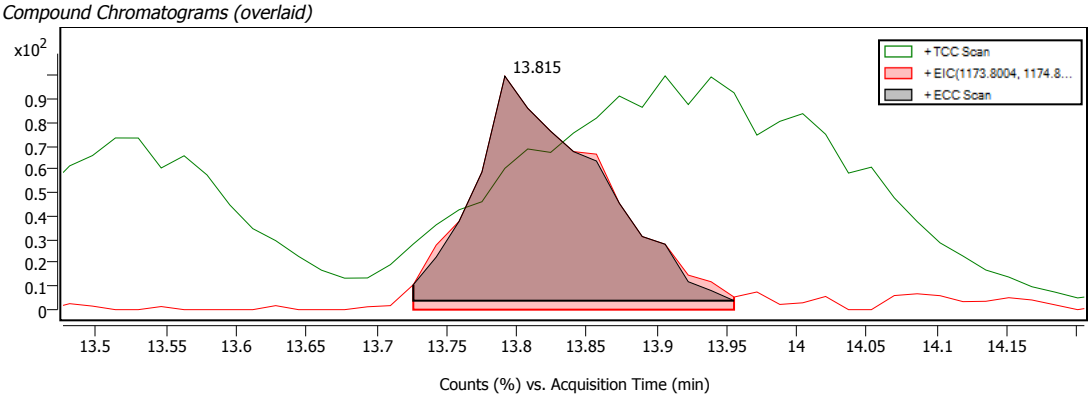


Cpd 92: 13.815

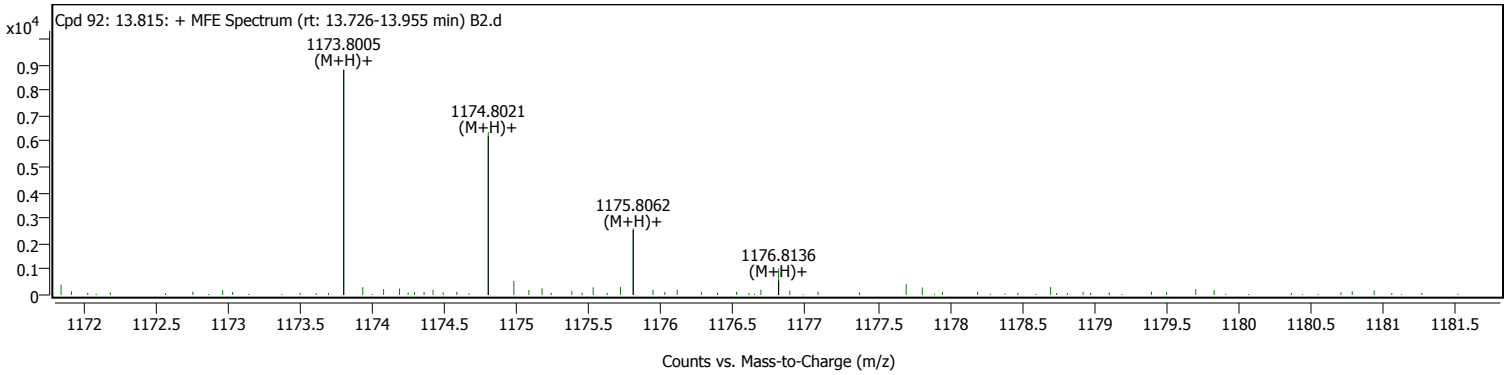
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.815		1172.7933				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

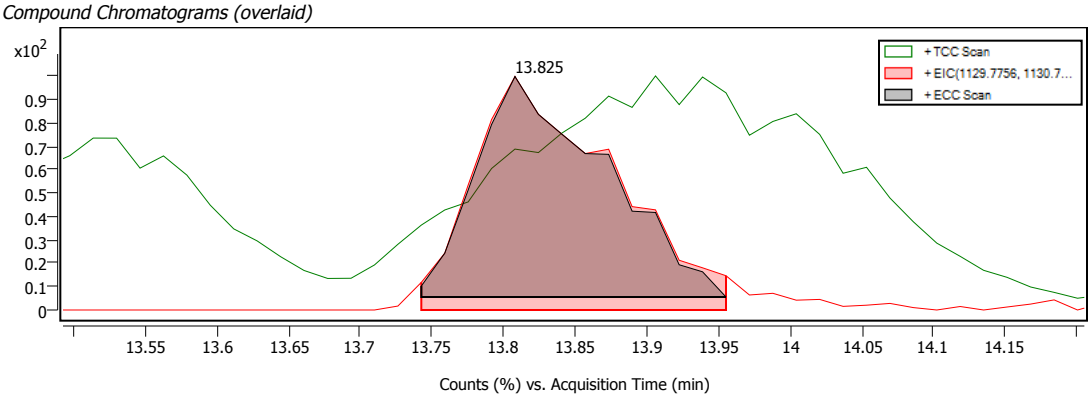


Cpd 93: 13.825

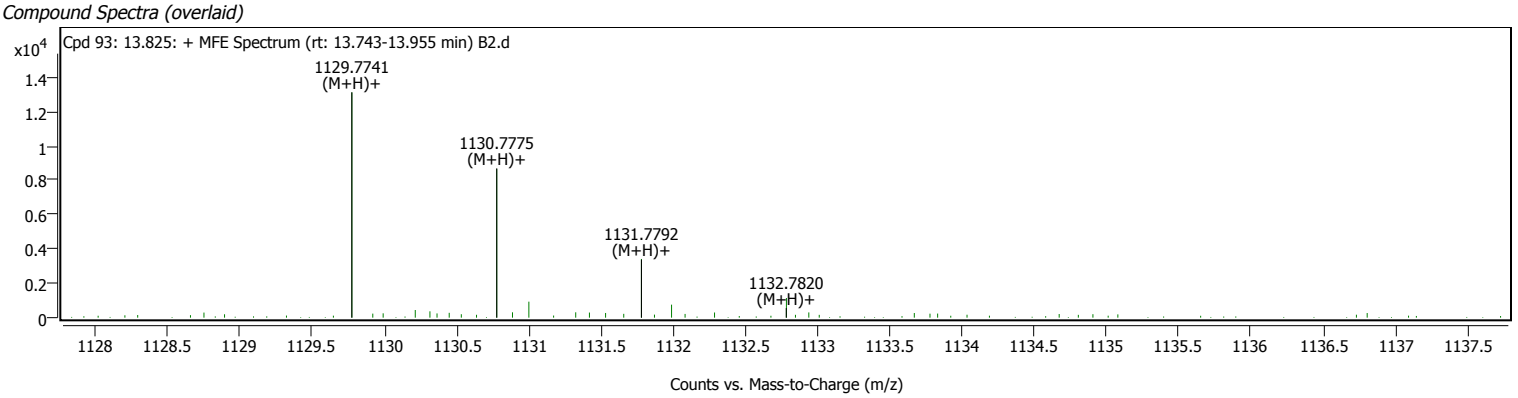
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.825		1128.7668				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

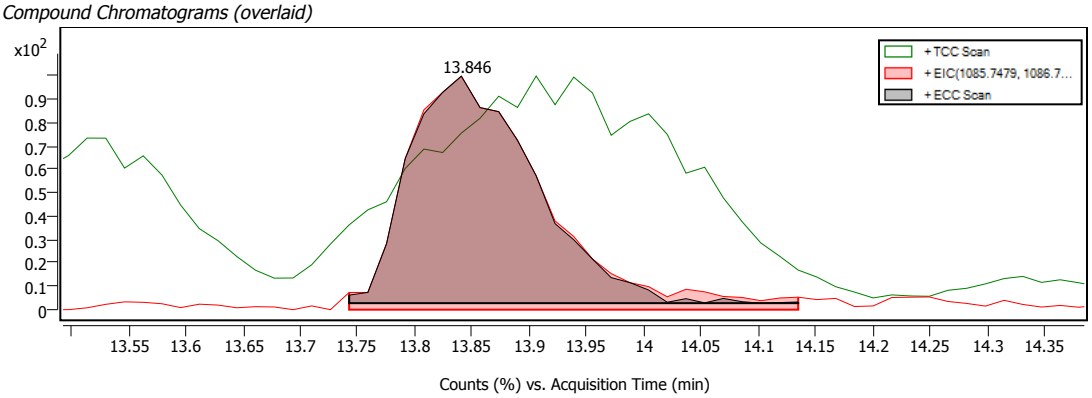


Cpd 94: 13.846

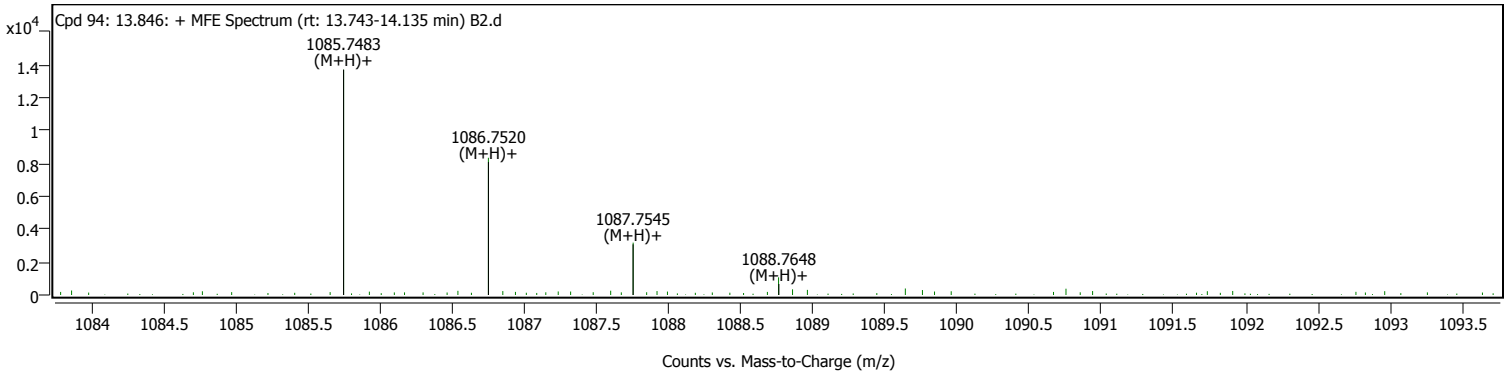
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.846		1084.7410				MFE	

Compound Chromatograms (overlaid)

Structure



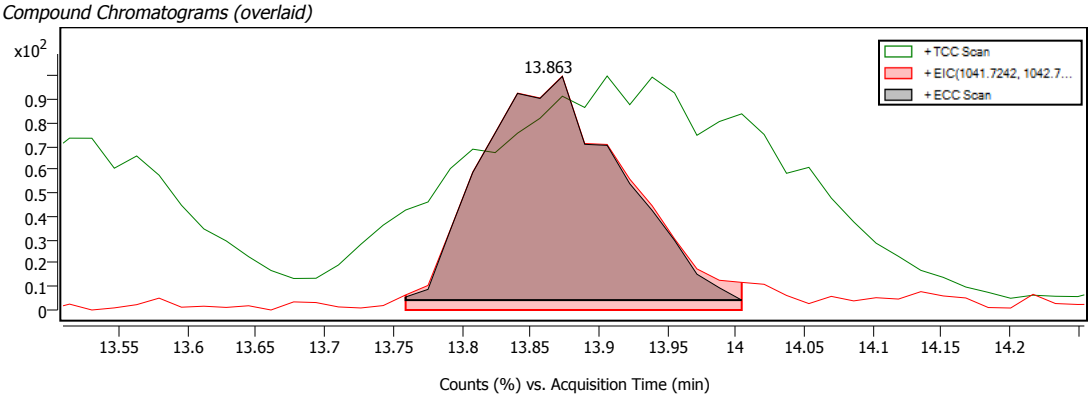
Compound Spectra (overlaid)



Cpd 95: 13.863

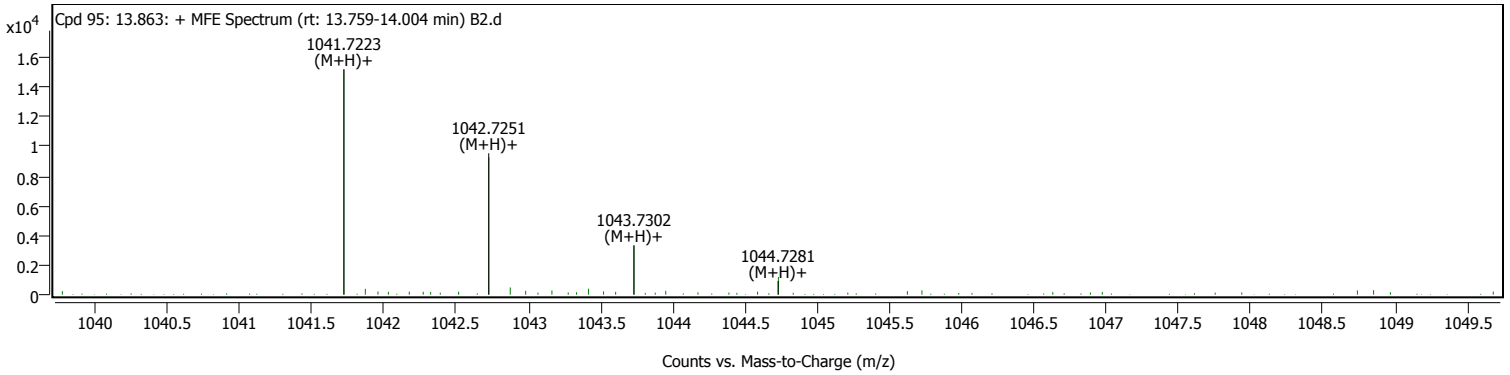
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.863		1040.7150				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 96: C57 H94 N3 O11

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C57 H94 N3 O11	13.881		996.6896		MFG	98.47	MFE	

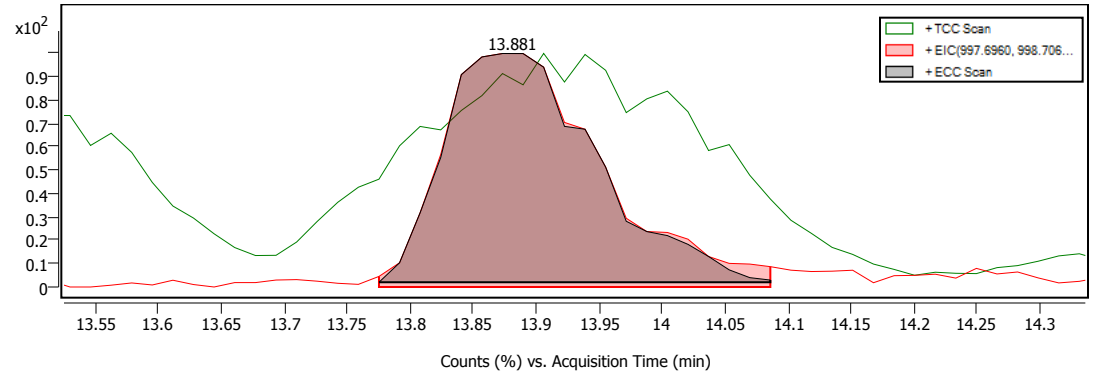
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	997.6972				5	98.47	

Compound ID Table

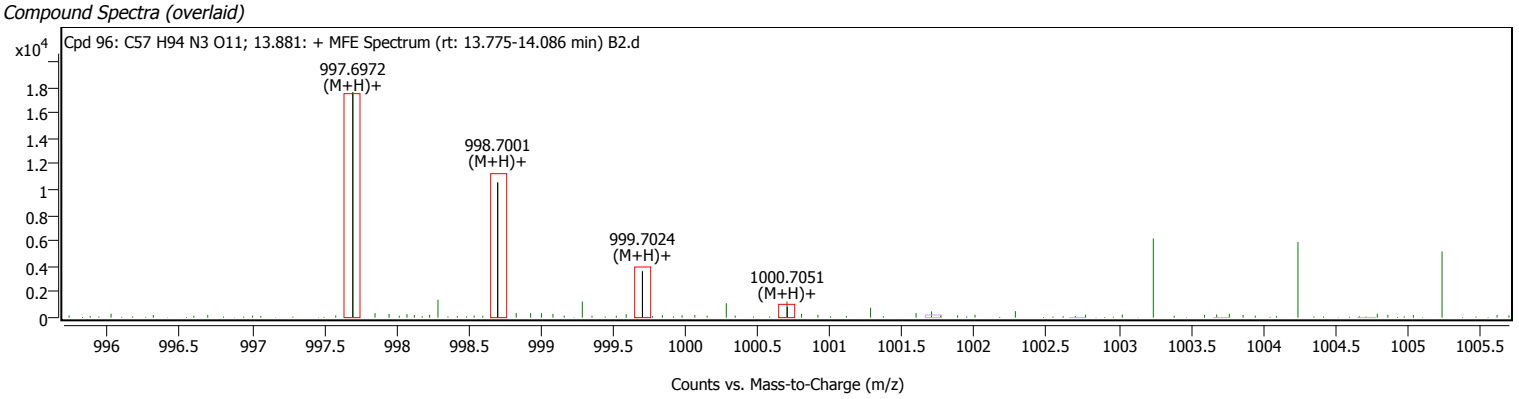
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C57 H94 N3 O11	(M+H)+	MFG	13.881		996.6896		98.47		98.47
	C59 H96 O12	(M+H)+	MFG	13.881		996.6896		98.14		98.14
	C58 H90 N7 O7	(M+H)+	MFG	13.881		996.6897		98.01		98.01
	C56 H88 N10 O6	(M+H)+	MFG	13.881		996.6898		97.96		97.96
	C50 H84 N20 S	(M+H)+	MFG	13.881		996.6903		97.82		97.82

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 97: C55 H90 N3 O10

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C55 H90 N3 O10	13.900		952.6627		MFG	98.85	MFE	

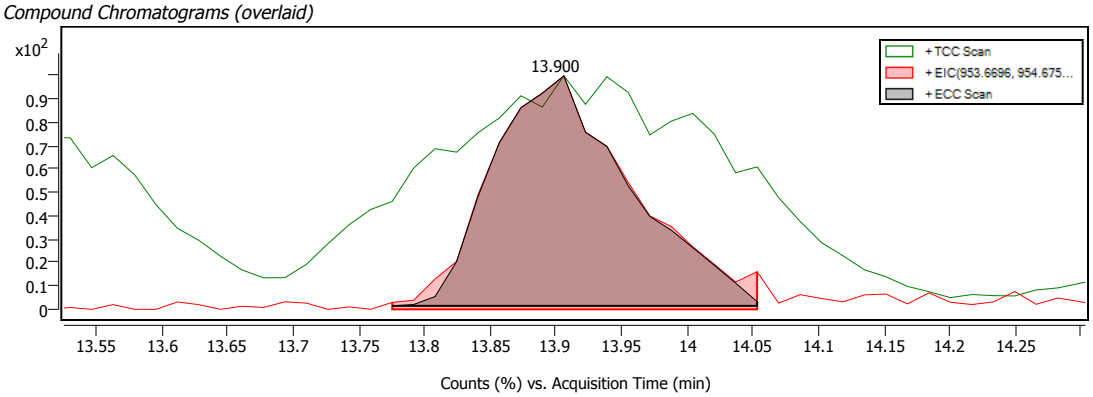
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	953.6700				5	98.85	

Compound ID Table

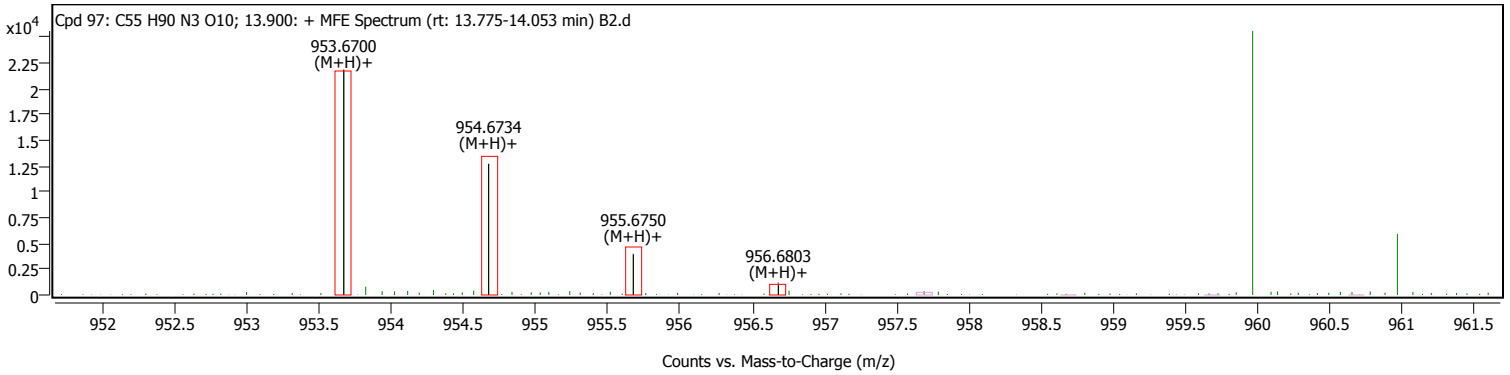
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C55 H90 N3 O10	(M+H)+	MFG	13.900		952.6627		98.85		98.85
	C54 H84 N10 O5	(M+H)+	MFG	13.900		952.6628		98.64		98.64
	C53 H78 N17	(M+H)+	MFG	13.900		952.6629		97.92		97.92
	C53 H88 N6 O9	(M+H)+	MFG	13.900		952.6627		97.53		97.53
	C47 H84 N16 O3 S	(M+H)+	MFG	13.900		952.6633		97.21		97.21

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 98: C53 H86 N3 O9

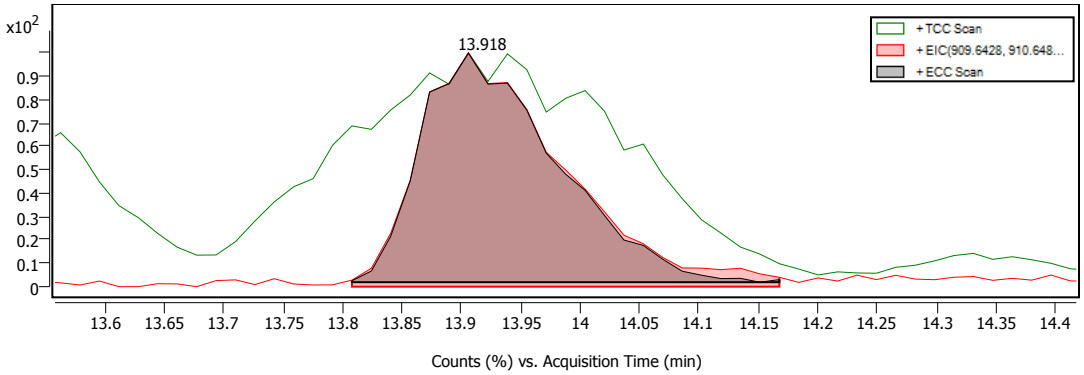
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C53 H86 N3 O9	13.918		908.6367		MFG	98.73	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	909.6443				11	98.73	

Compound ID Table

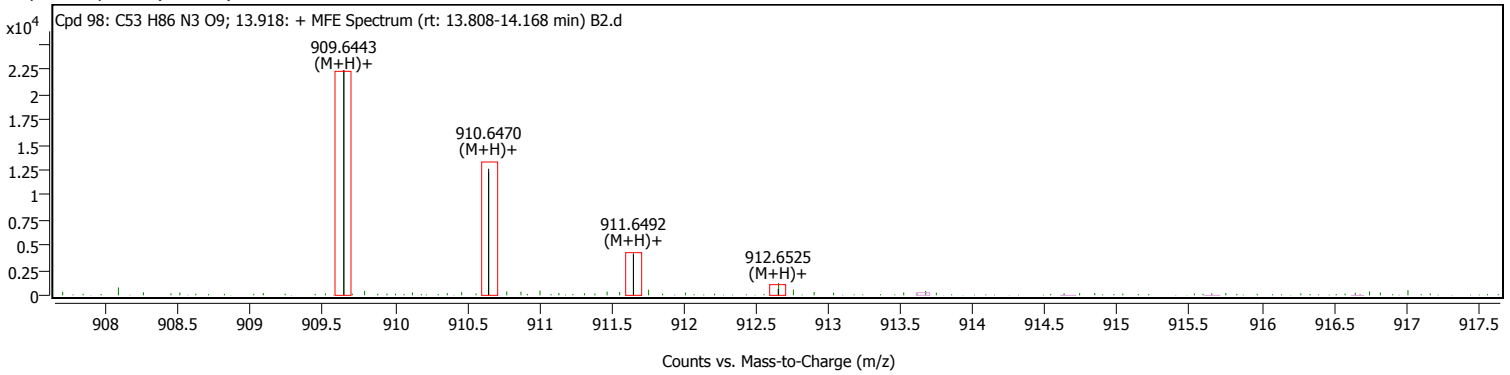
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C53 H86 N3 O9	(M+H)+	MFG	13.918		908.6367		98.73		98.73
	C52 H80 N10 O4	(M+H)+	MFG	13.918		908.6368		98.46		98.46
	C45 H80 N16 O2 S	(M+H)+	MFG	13.918		908.6373		97.67		97.67
	C54 H82 N7 O5	(M+H)+	MFG	13.918		908.6368		97.20		97.20
	C55 H88 O10	(M+H)+	MFG	13.918		908.6366		97.07		97.07
PI(17:0/22:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	
PI(18:0/21:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	
PI(19:0/20:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	
PI(20:0/19:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	
PI(22:0/17:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	
PI(21:0/18:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.918		908.6366		96.78	96.78	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 99: C51 H82 N3 O8

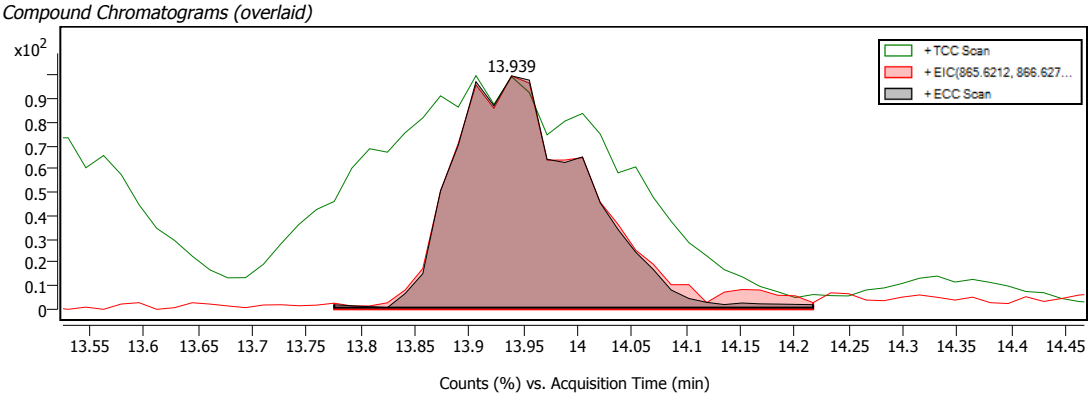
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C51 H82 N3 O8	13.939		864.6107		MFG	98.25	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	865.6179				10	98.25	

Compound ID Table

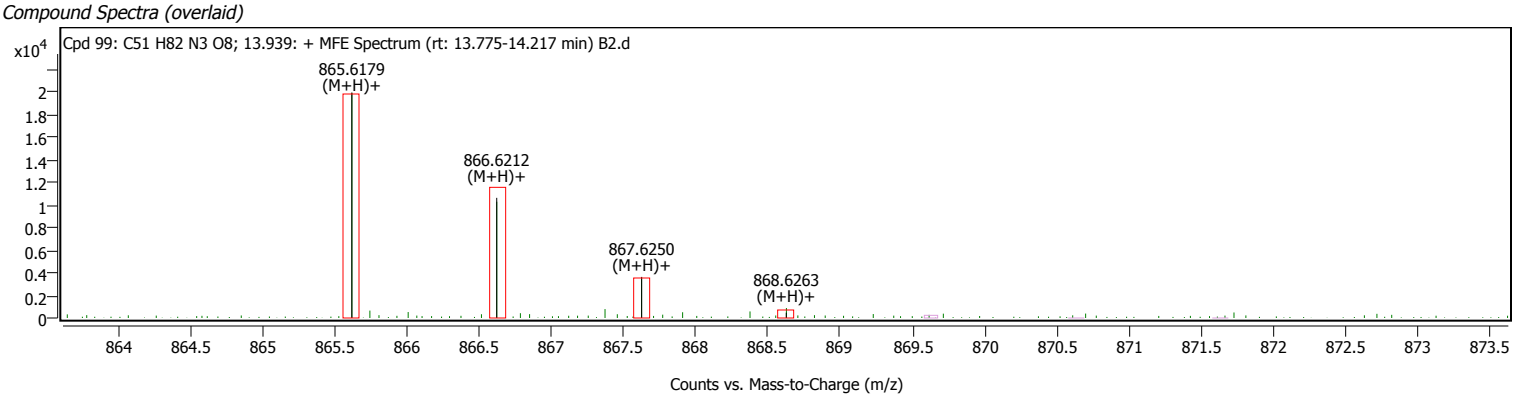
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C51 H82 N3 O8	(M+H)+	MFG	13.939		864.6107		98.25		98.25
	C53 H84 O9	(M+H)+	MFG	13.939		864.6106		97.43		97.43
	C50 H76 N10 O3	(M+H)+	MFG	13.939		864.6108		97.03		97.03
	C52 H78 N7 O4	(M+H)+	MFG	13.939		864.6108		96.68		96.68
PI(O-18:0/19:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.939		864.6106		96.19	96.19	
PI(O-20:0/17:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.939		864.6106		96.19	96.19	
PI(P-16:0/21:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.939		864.6106		96.19	96.19	
PI(P-18:0/19:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.939		864.6106		96.19	96.19	
PI(P-20:0/17:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.939		864.6106		96.19	96.19	
	C43 H76 N16 O S	(M+H)+	MFG	13.939		864.6113		95.73		95.73

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 100: PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

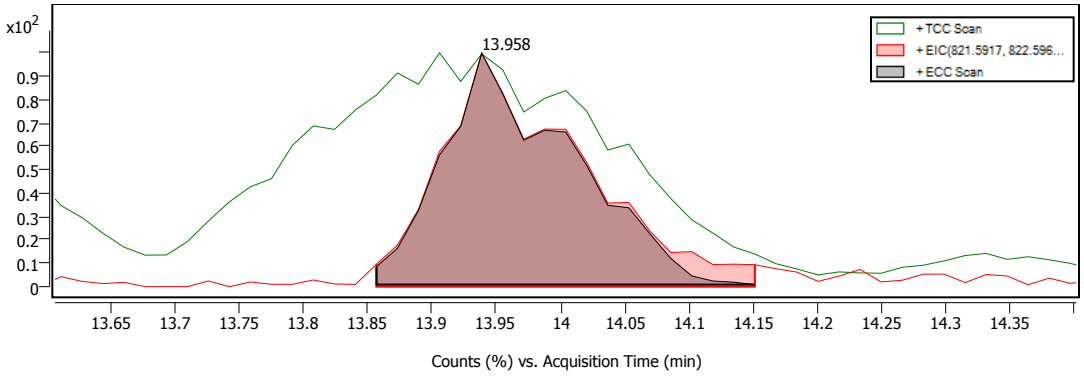
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H83 N O8 P	13.958		820.5845		DBSearch	97.43	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	821.5920 821.5920 821.5920		0	97.43	26		

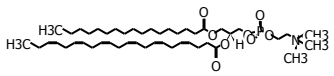
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(17:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(19:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/19:1(9Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(22:4(7Z,10Z,13Z,16Z)/17:2(9Z,12Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/17:0)	C47 H83 N O8 P	(M+H)+	DBSearch	13.958		820.5845		97.43	97.43	
PC(18:2(9Z,12Z)/19:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(17:1(9Z)/20:2(11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(18:0/19:3(9Z,12Z,15Z))[U]	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(15:1(9Z)/22:2(13Z,16Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(17:0/20:3(8Z,11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(22:2(13Z,16Z)/15:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(20:3(8Z,11Z,14Z)/17:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(18:3(6Z,9Z,12Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(18:3(9Z,12Z,15Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(19:0/18:3(6Z,9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(19:0/18:3(9Z,12Z,15Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(19:1(9Z)/18:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(20:1(11Z)/17:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(20:2(11Z,14Z)/17:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
PC(17:2(9Z,12Z)/20:1(11Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.958		798.6026		97.33	97.33	
	C35 H70 N19 O4	(M+H)+	MFG	13.958		820.5850		97.04		97.04
	C49 H78 N3 O7	(M+H)+	MFG	13.958		820.5846		96.83		96.83
	C36 H76 N12 O9	(M+H)+	MFG	13.958		820.5848		96.77		96.77
	C34 H74 N15 O8	(M+H)+	MFG	13.958		820.5849		96.55		96.55
	C41 H72 N16 S	(M+H)+	MFG	13.958		820.5851		96.29		96.29

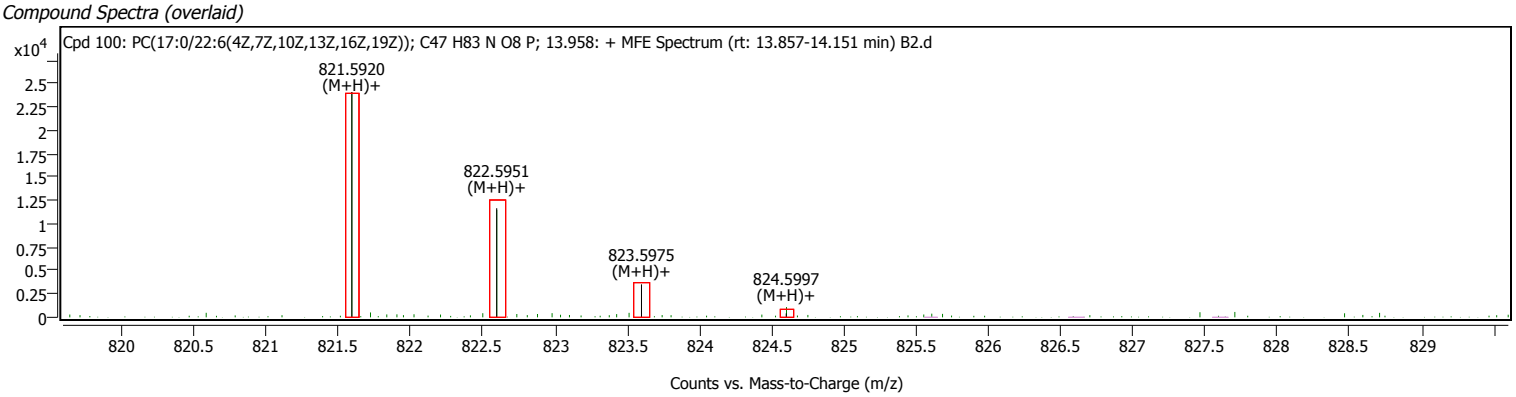
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 101: PC(O-15:0/20:4(5Z,8Z,11Z,14Z))[U]

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(O-15:0/20:4(5Z,8Z,11Z,14Z))[U]	C43 H81 N O7 P	13.984		754.5779		DBSearch	89.13	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	777.5673 777.5673 777.5673		0	89.13	32		

Compound Discovery Report

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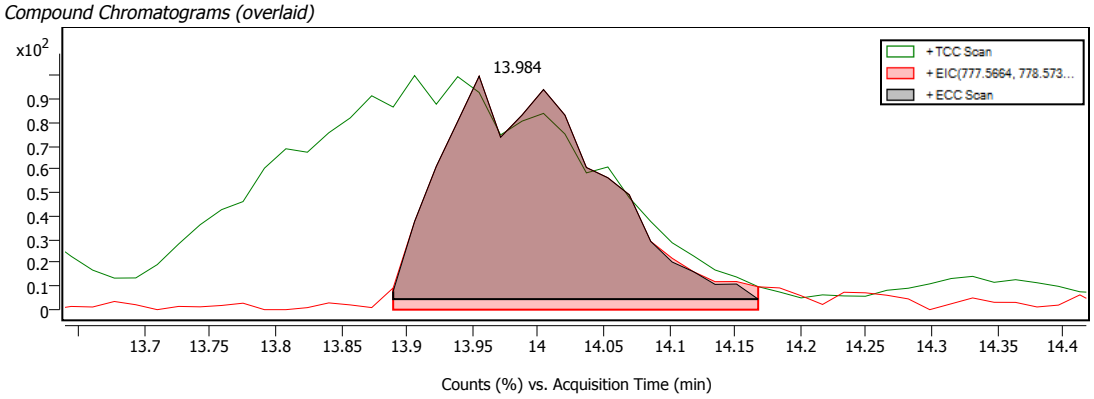
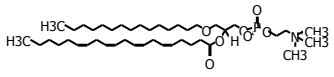
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PC(O-15:0/20:4(5Z,8Z,11Z,14Z))[U]	C43 H81 N O7 P	(M+Na)+	DBSearch	13.984		754.5779		89.13	89.13	
PC(O-15:0/20:4(5Z,8Z,11Z,14Z))	C43 H81 N O7 P	(M+Na)+	DBSearch	13.984		754.5779		89.13	89.13	
PG(18:0/18:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(20:0/16:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(18:1(11Z)/18:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(18:1(9Z)/18:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(18:0/18:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
1-Stearoyl-2-Oleoyl-sn-Glycero-3-[Phospho-rac-(1-glycerol)]	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(14:0/22:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(14:1(9Z)/22:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(15:1(9Z)/21:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(16:1(9Z)/20:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(17:0/19:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(17:1(9Z)/19:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(19:0/17:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(19:1(9Z)/17:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(20:1(11Z)/16:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(21:0/15:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(22:0/14:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(22:1(11Z)/14:0)	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(16:0/20:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
PG(18:0/18:1(9Z))[U]	C42 H81 O10 P	(M+H)+	DBSearch	13.984		776.5599		88.06	88.06	
	C27 H61 N28	(M+H)+	MFG	13.984		777.5633		70.58		70.58
	C29 H63 N25 O	(M+H)+	MFG	13.984		777.5633		66.51		66.51
	C36 H71 N15 O2 S	(M+H)+	MFG	13.984		777.5631		61.92		61.92
	C35 H75 N11 O6 S	(M+H)+	MFG	13.984		777.5631		61.91		61.91
	C34 H69 N18 O S	(M+H)+	MFG	13.984		777.5632		61.86		61.86
	C43 H76 N7 O2 S	(M+Na)+	MFG	13.984		754.5781		47.62		47.62
	C44 H82 O7 S	(M+Na)+	MFG	13.984		754.5781		47.62		47.62
	C36 H78 N6 O10	(M+Na)+	MFG	13.984		754.5781		47.59		47.59
	C35 H72 N13 O5	(M+Na)+	MFG	13.984		754.5781		47.59		47.59
	C34 H66 N20	(M+Na)+	MFG	13.984		754.5781		47.59		47.59

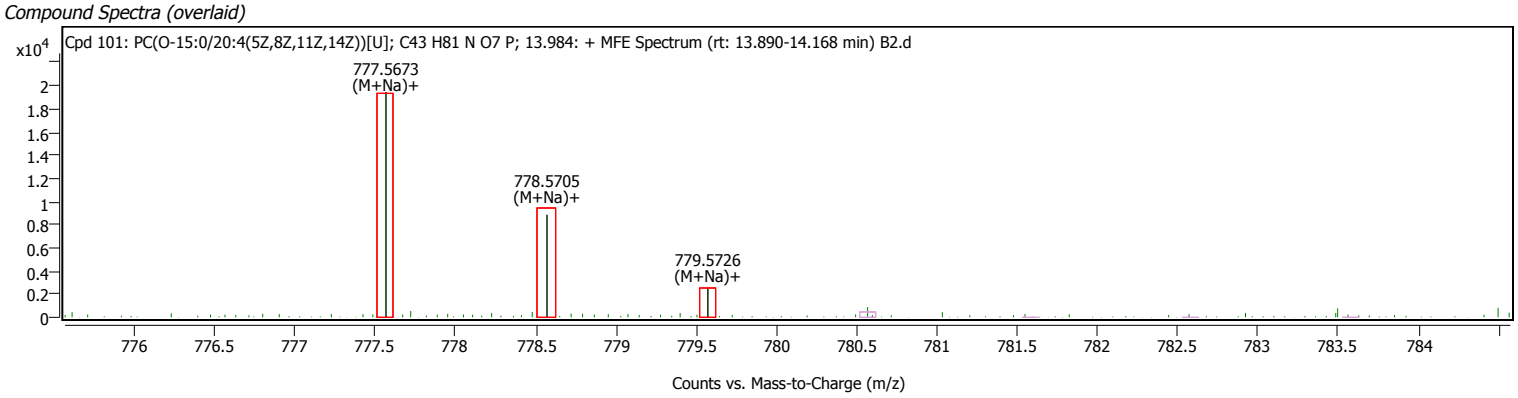
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 102: C47 H72 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C47 H72 O6	14.000		732.5335		MFG	94.21	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	733.5407				9	94.21	

Compound Discovery Report

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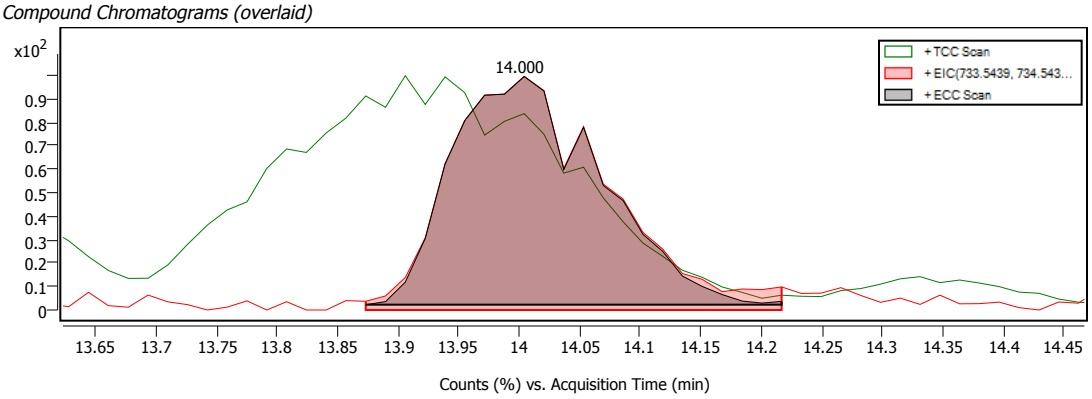
Compound ID Table

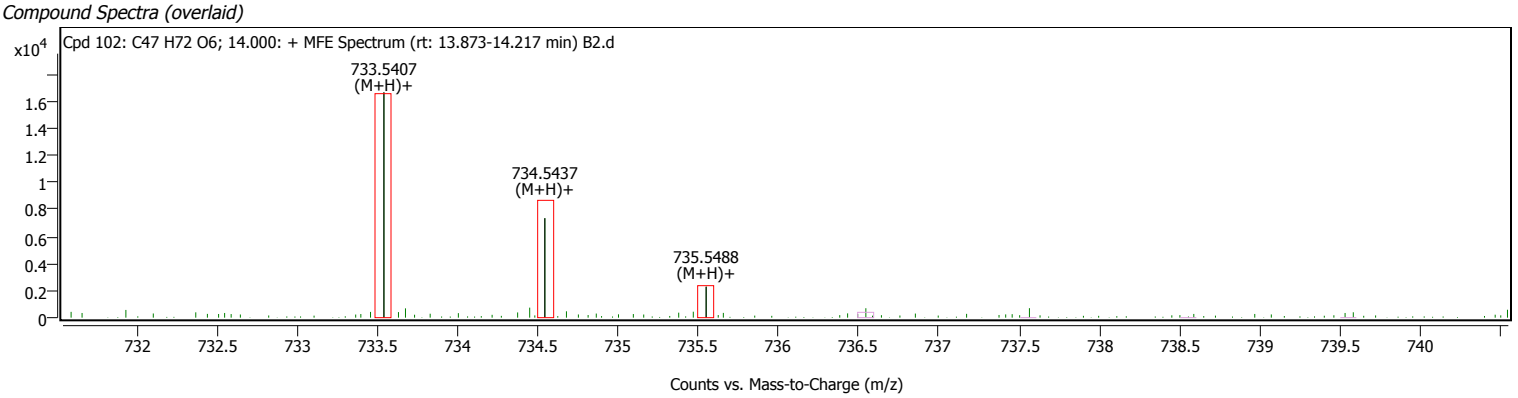
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C47 H72 O6	(M+H)+	MFG	14.000		732.5335		94.21		94.21
	C34 H70 N9 O8	(M+H)+	MFG	14.000		732.5337		93.85		93.85
	C32 H68 N12 O7	(M+H)+	MFG	14.000		732.5338		93.63		93.63
	C33 H64 N16 O3	(M+H)+	MFG	14.000		732.5338		93.39		93.39
	C31 H62 N19 O2	(M+H)+	MFG	14.000		732.5339		92.53		92.53
PG(O-16:0/18:2(9Z,12Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.000		732.5335		87.37	87.37	
PG(P-18:0/16:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.000		732.5335		87.37	87.37	
PG(P-20:0/14:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.000		732.5335		87.37	87.37	
PG(P-16:0/18:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.000		732.5335		87.37	87.37	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 103: C38 H68 N6 O3 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C38 H68 N6 O3 S	14.025		688.5072		MFG	94.70	MFE	

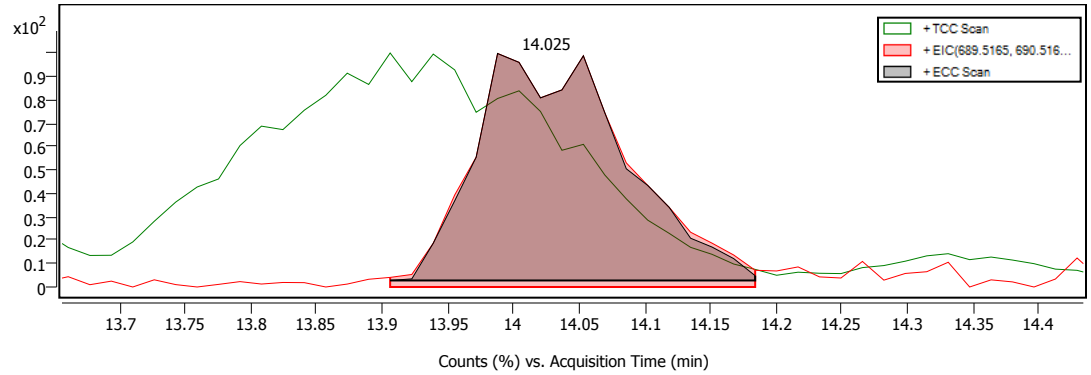
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	689.5143				52	94.70	

Compound ID Table

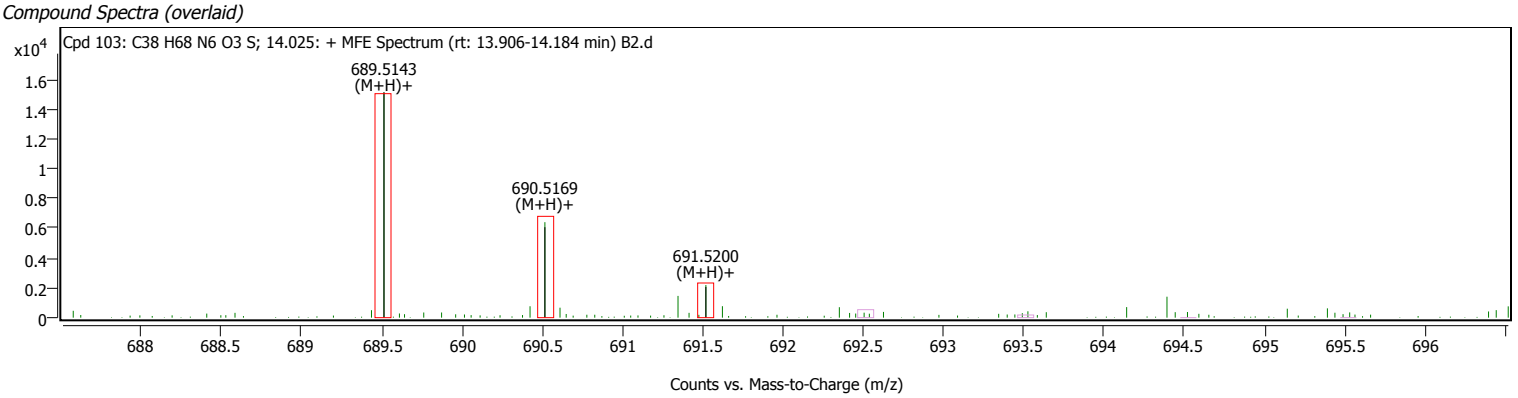
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C38 H68 N6 O3 S	(M+H)+	MFG	14.025		688.5072		94.70		94.70
	C30 H64 N12 O6	(M+H)+	MFG	14.025		688.5070		94.46		94.46
	C37 H72 N2 O7 S	(M+H)+	MFG	14.025		688.5071		93.93		93.93
	C29 H58 N19 O	(M+H)+	MFG	14.025		688.5072		93.21		93.21
	C36 H66 N9 O2 S	(M+H)+	MFG	14.025		688.5072		93.09		93.09
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(20:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.025		688.5067		91.56	91.56	
PA(13:0/22:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(19:0/16:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(14:1(9Z)/21:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(17:0/18:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(21:0/14:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(20:1(11Z)/15:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(20:0/15:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(19:1(9Z)/16:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(17:1(9Z)/18:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(18:1(9Z)/17:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(15:0/20:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(16:1(9Z)/19:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(16:0/19:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(15:1(9Z)/20:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(18:0/17:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
PA(22:1(11Z)/13:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.025		688.5067		88.34	88.34	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(9Z,12Z,15Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:2(9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:3(9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:3(8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:4(6Z,9Z,12Z,15Z)/22:3(10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:2(9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/20:2(11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(6Z,9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:2(11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	
DG(20:3(5Z,8Z,11Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.025		666.5248		85.13	85.13	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

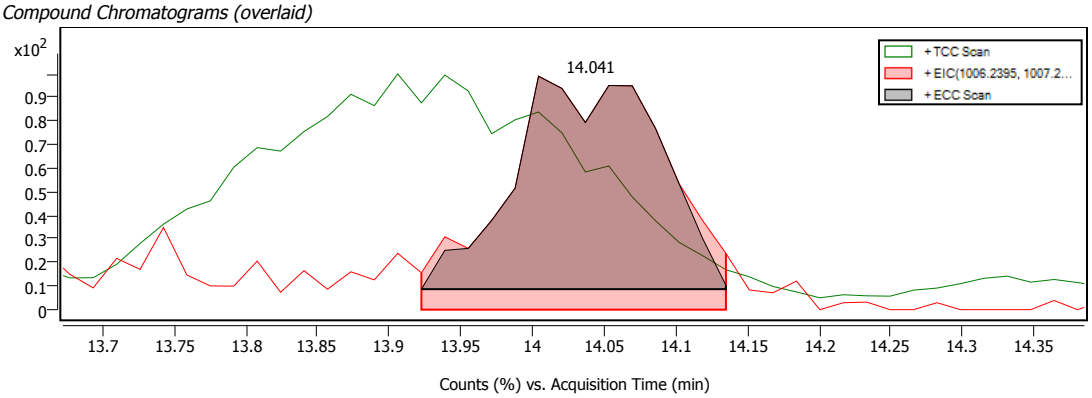


Cpd 104: 14.041

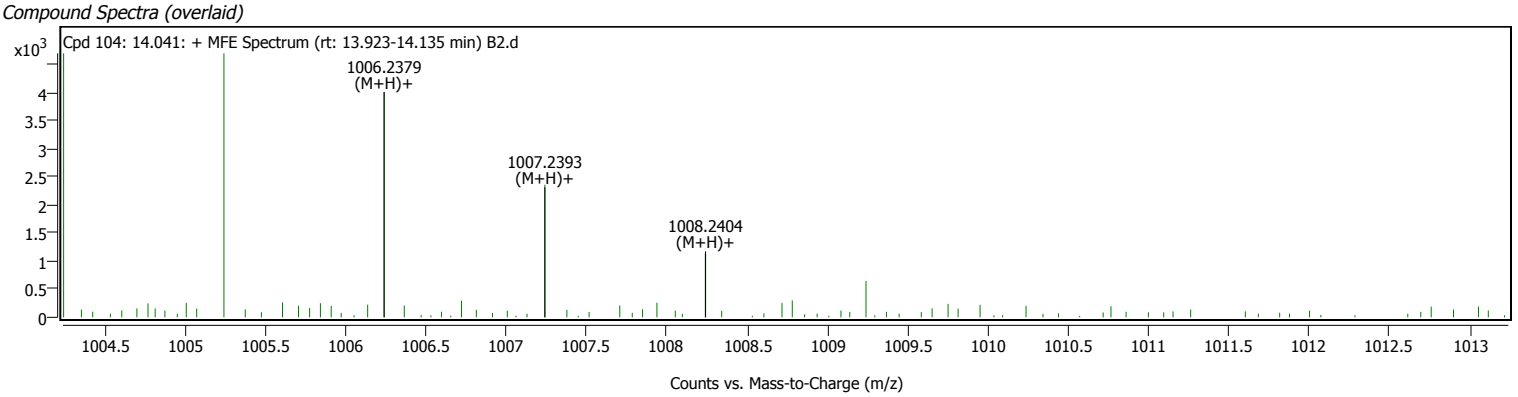
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.041		1005.2306				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

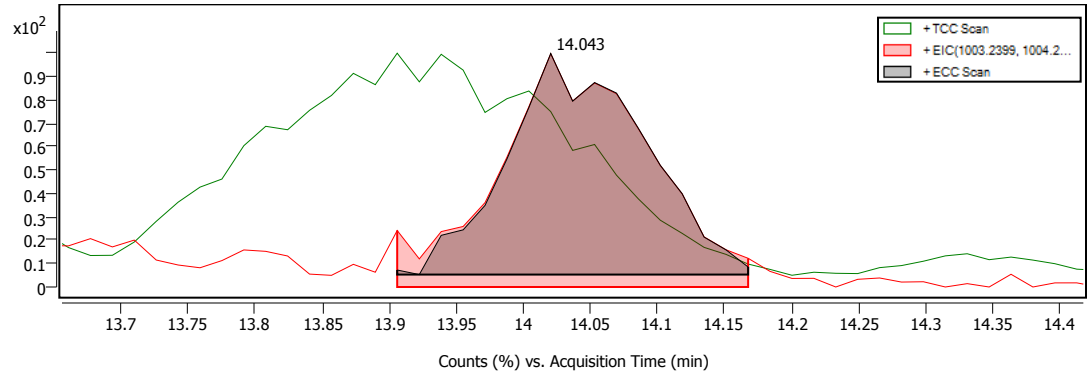


Cpd 105: 14.043

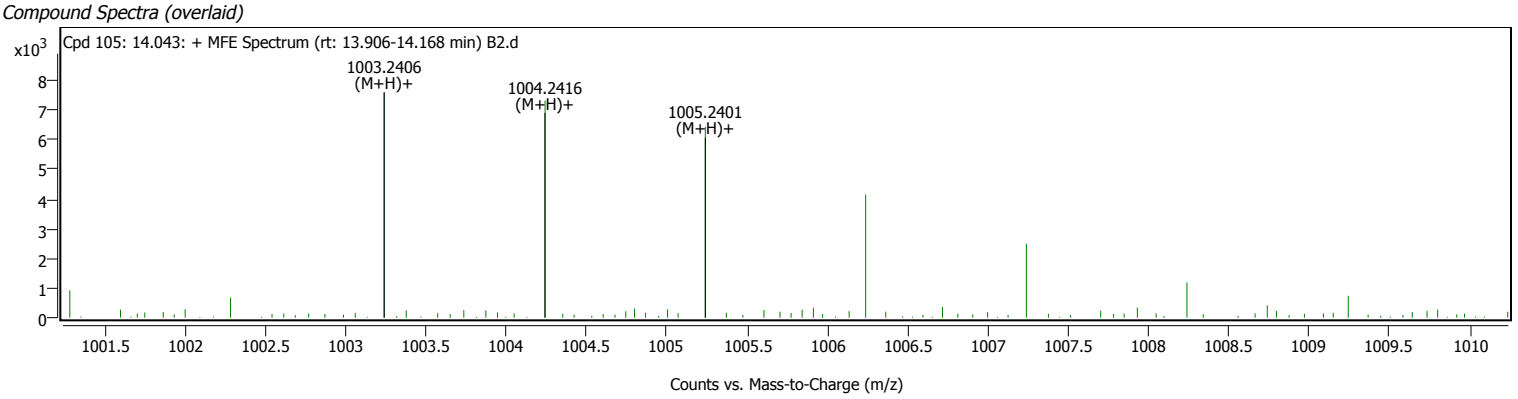
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.043		1002.2333				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 106: C28 H60 N12 O5

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H60 N12 O5	14.046		644.4813		MFG	91.74	MFE	

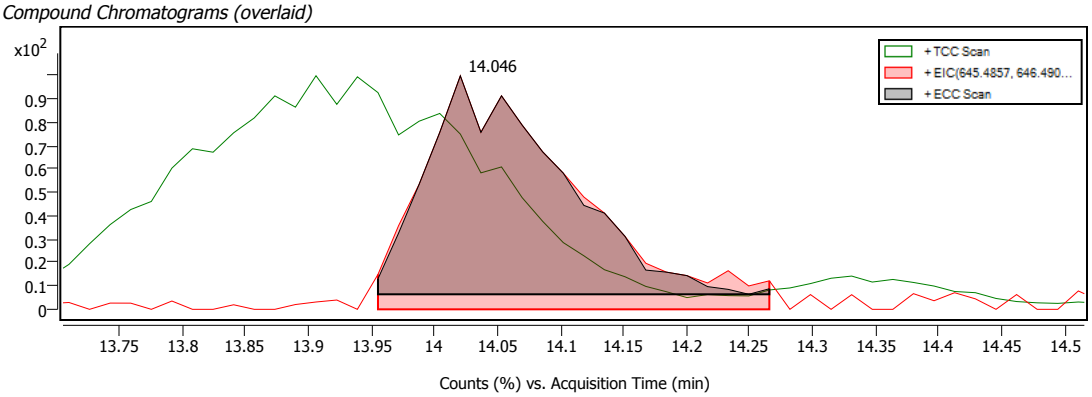
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	645.4883				8	91.74	

Compound ID Table

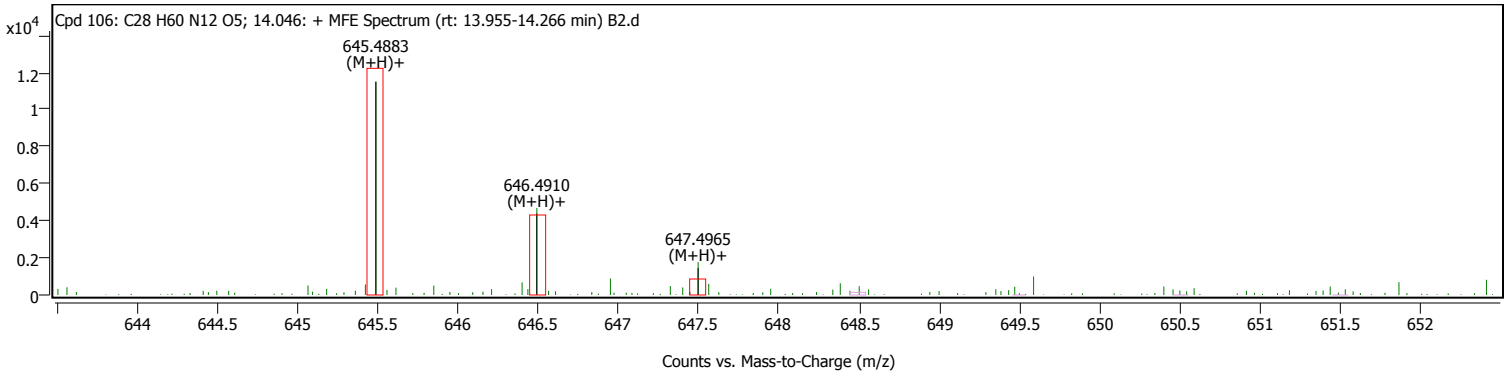
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H60 N12 O5	(M+H)+	MFG	14.046		644.4813		91.74		91.74
	C30 H62 N9 O6	(M+H)+	MFG	14.046		644.4812		91.60		91.60
	C36 H64 N6 O2 S	(M+H)+	MFG	14.046		644.4814		91.20		91.20
	C43 H64 O4	(M+H)+	MFG	14.046		644.4810		90.27		90.27
	C29 H56 N16 O	(M+H)+	MFG	14.046		644.4814		90.06		90.06
PA(O-16:0/17:2(9Z,12Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.046		644.4810		84.03	84.03	
PA(P-16:0/17:1(9Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.046		644.4810		84.03	84.03	
PA(P-18:0/15:1(9Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.046		644.4810		84.03	84.03	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 107: C26 H54 N9 O4

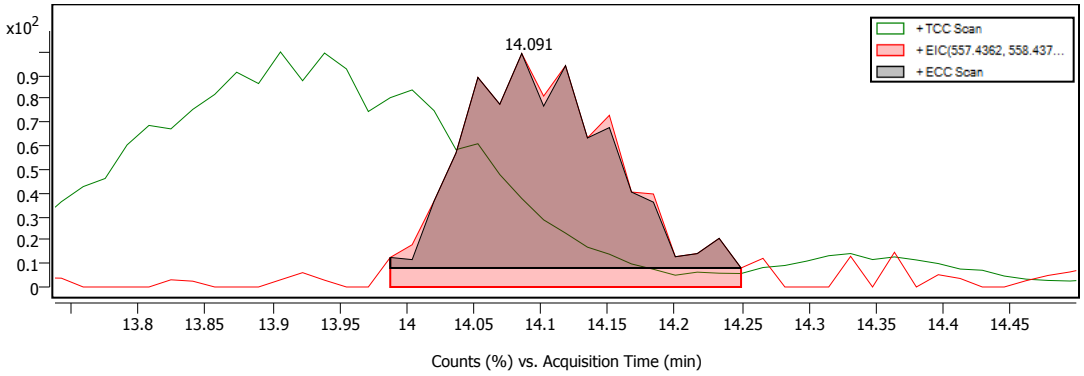
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C26 H54 N9 O4	14.091		556.4295		MFG	79.42	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	557.4367				6	79.42	

Compound ID Table

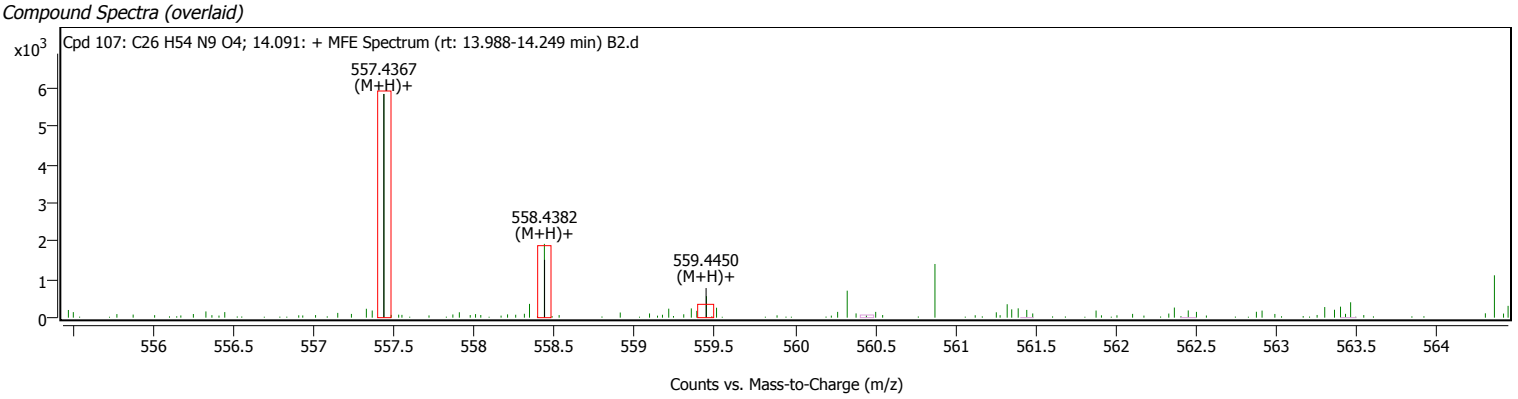
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C26 H54 N9 O4	(M+H)+	MFG	14.091		556.4295		79.42		79.42
	C24 H52 N12 O3	(M+H)+	MFG	14.091		556.4296		77.78		77.78
	C28 H56 N6 O5	(M+H)+	MFG	14.091		556.4294		73.86		73.86
	C34 H58 N3 O S	(M+H)+	MFG	14.091		556.4297		73.78		73.78
	C32 H56 N6 S	(M+H)+	MFG	14.091		556.4298		73.00		73.00
Germanicol cinnamate	C39 H56 O2	(M+H)+	DBSearch	14.091		556.4292	65883-48-9	70.73	70.73	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 108: C22 H48 N12 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H48 N12 O2	14.108		512.4029		MFG	76.34	MFE	

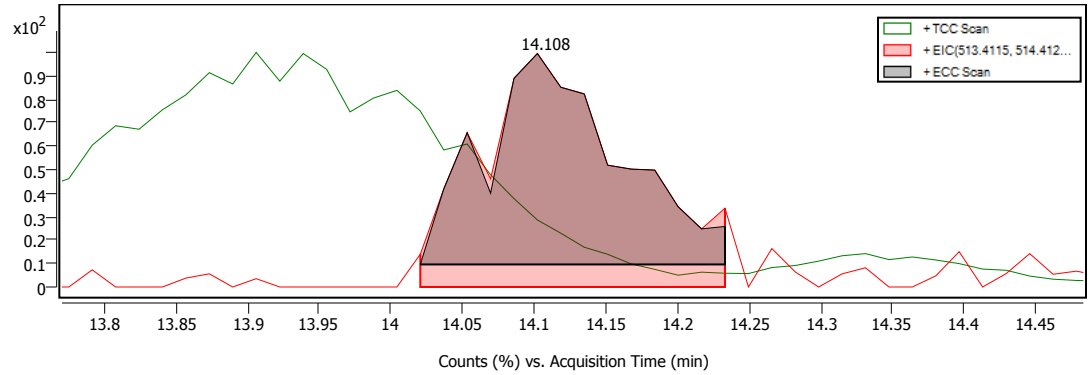
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	513.4101				5	76.34	

Compound ID Table

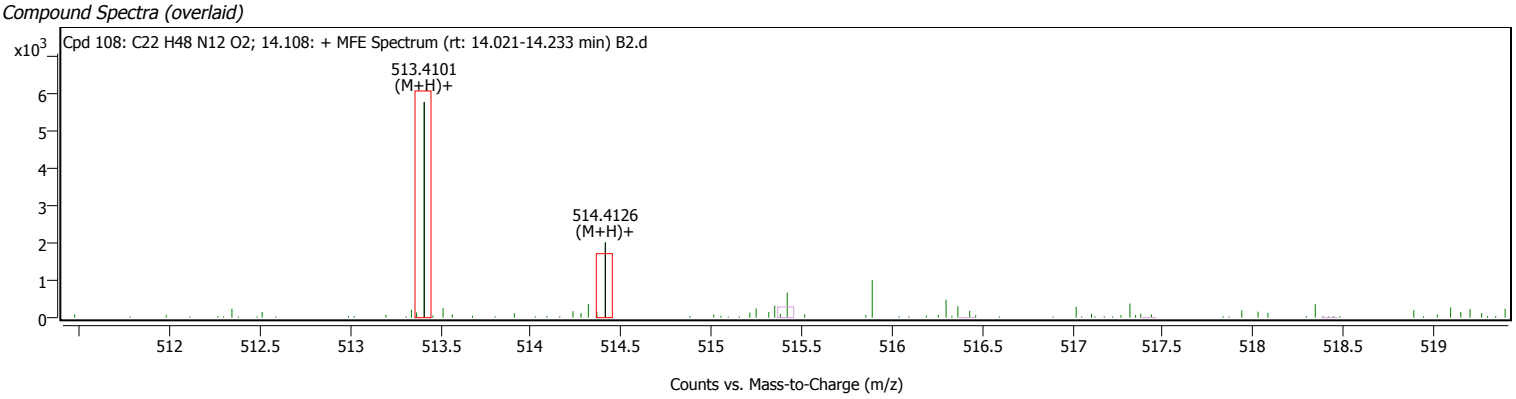
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H48 N12 O2	(M+H)+	MFG	14.108		512.4029		76.34		76.34
	C24 H50 N9 O3	(M+H)+	MFG	14.108		512.4028		76.02		76.02
	C37 H52 O	(M+H)+	MFG	14.108		512.4026		73.45		73.45
	C23 H54 N5 O7	(M+H)+	MFG	14.108		512.4027		73.26		73.26
	C20 H46 N15 O	(M+H)+	MFG	14.108		512.4029		68.81		68.81

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

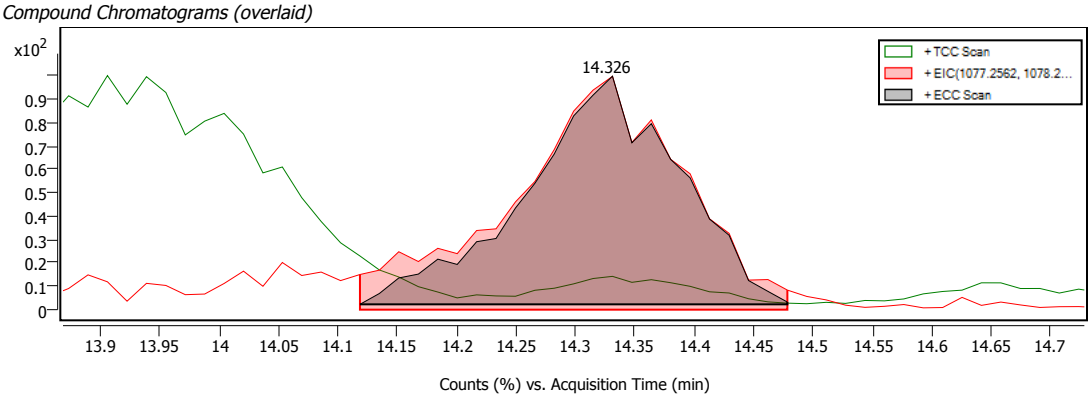


Cpd 109: 14.326

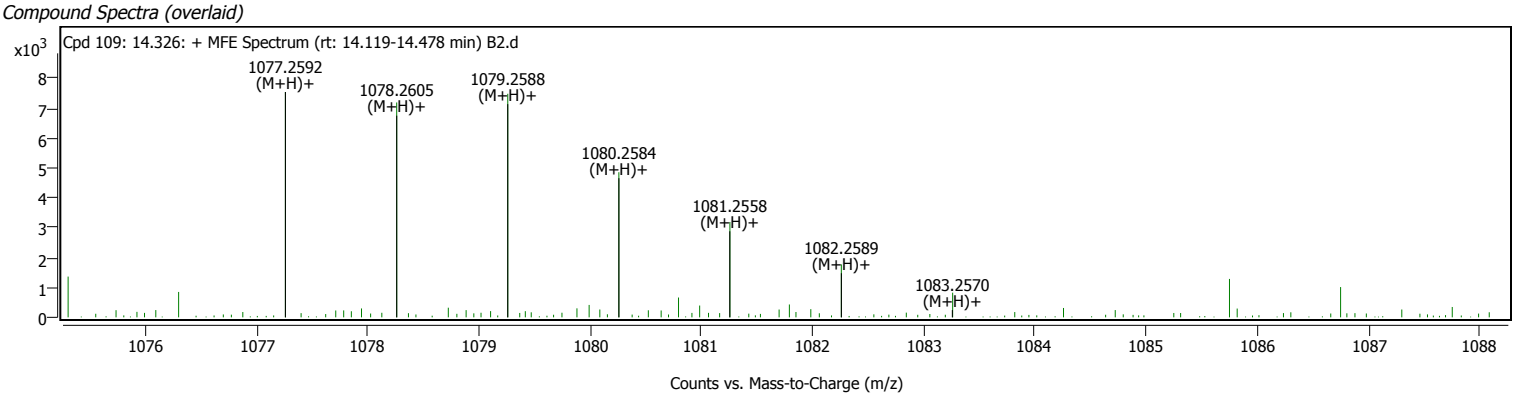
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.326		1076.2519				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 110: Retinoyl CoA

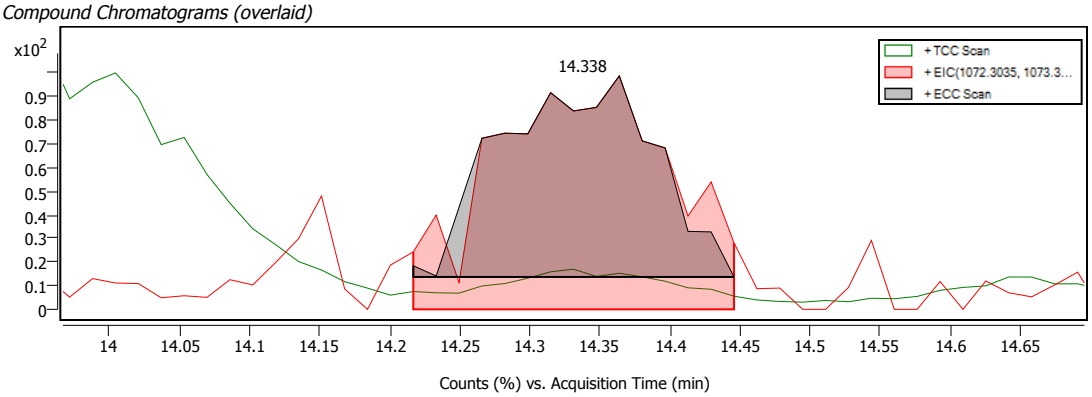
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Retinoyl CoA	C41 H62 N7 O17 P3 S	14.338		1049.3121	81295-48-9	DBSearch	58.49	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	1072.3056 1072.3056 1072.3056		0	58.49	1		

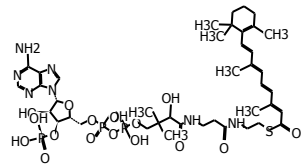
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Retinoyl CoA	C41 H62 N7 O17 P3 S	(M+Na)+	DBSearch	14.338		1049.3121	81295-48-9	58.49	58.49	

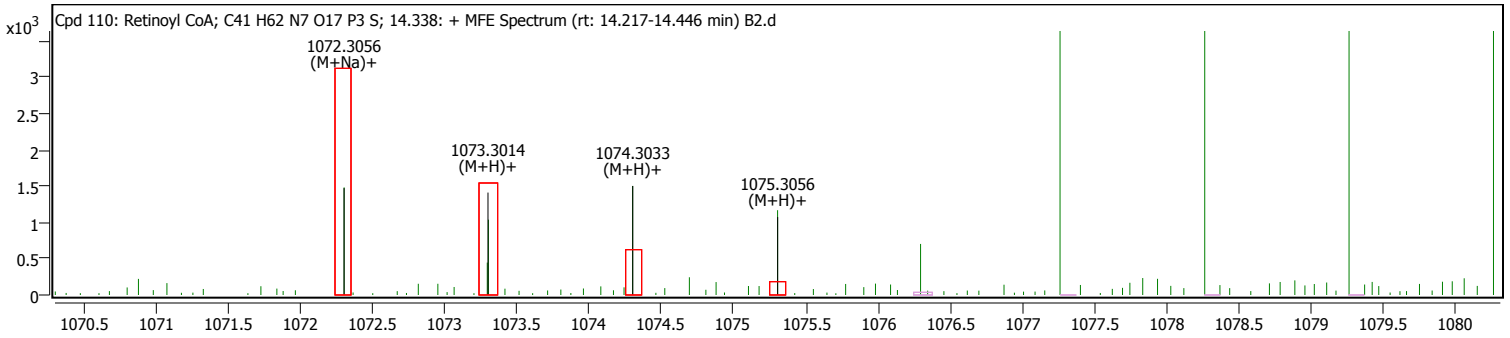
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 111: TG(10:0/10:0/10:0)

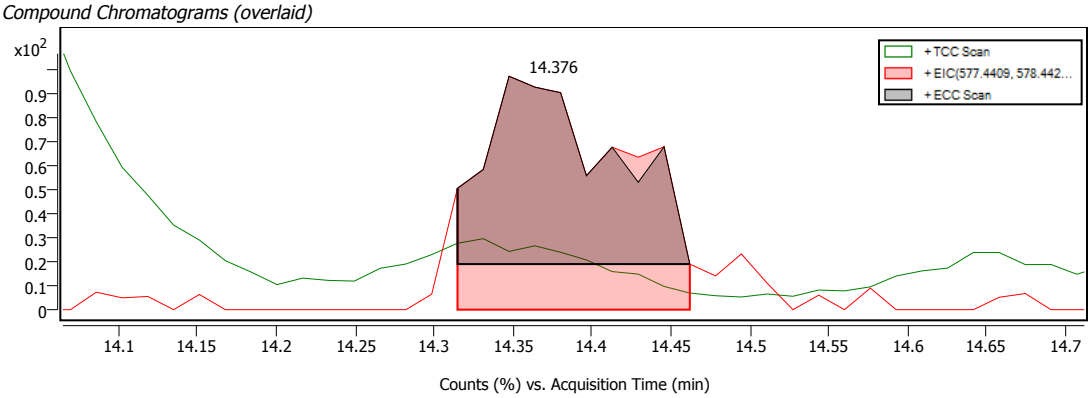
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
TG(10:0/10:0/10:0)	C33 H62 O6	14.376		554.4519	621-71-6	DBSearch	56.11	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	577.4416 577.4416 577.4416 577.4416		0	56.11	11		

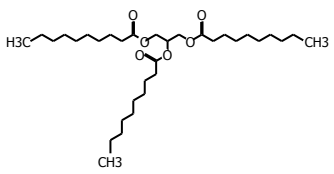
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
TG(10:0/10:0/10:0)	C33 H62 O6	(M+Na)+	DBSearch	14.376		554.4519	621-71-6	56.11	56.11	
	C28 H55 N11 S	(M+H)+	MFG	14.376		577.4362		47.61		47.61
	C29 H61 N4 O5 S	(M+H)+	MFG	14.376		577.4362		47.61		47.61
	C20 H51 N17 O3	(M+H)+	MFG	14.376		577.4362		47.59		47.59
	C32 H58 Cl N6 O	(M+H)+	MFG	14.376		577.4362		47.59		47.59
	C34 H65 Cl N S	(M+Na)+	MFG	14.376		554.4524		47.55		47.55
	C37 H62 O S	(M+Na)+	MFG	14.376		554.4524		47.48		47.48
	C29 H61 Cl2 N7	(M+H)+	MFG	14.376		577.4362		47.41		47.41
	C29 H58 N6 O4	(M+Na)+	MFG	14.376		554.4524		47.24		47.24
	C30 H54 N10	(M+Na)+	MFG	14.376		554.4524		46.32		46.32
	C31 H60 N3 O5	(M+Na)+	MFG	14.376		554.4524		46.31		46.31

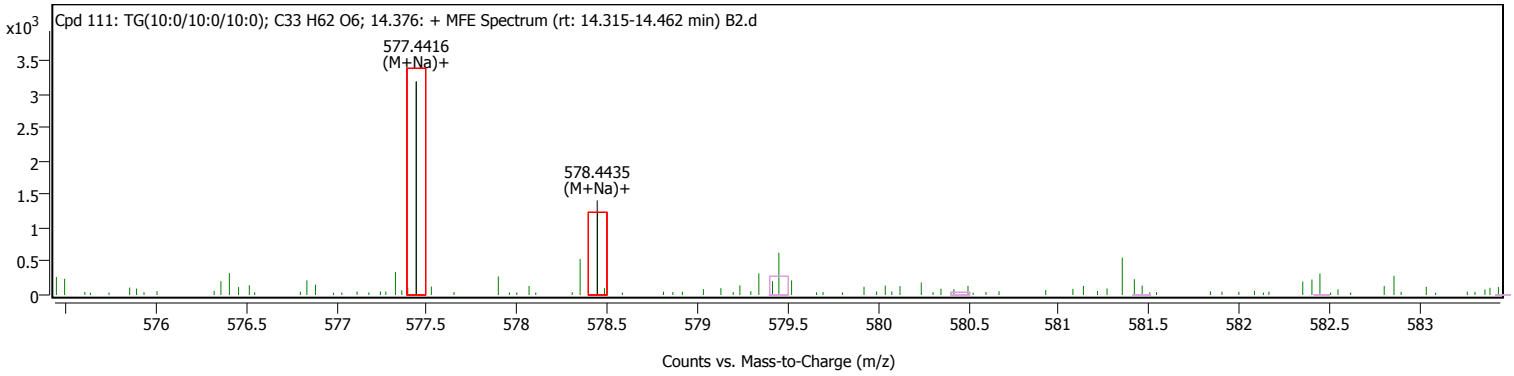
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)

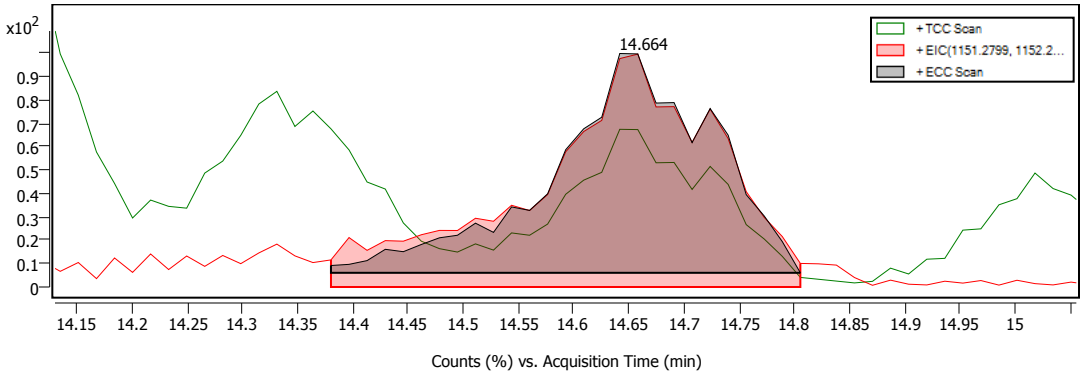


Cpd 112: 14.664

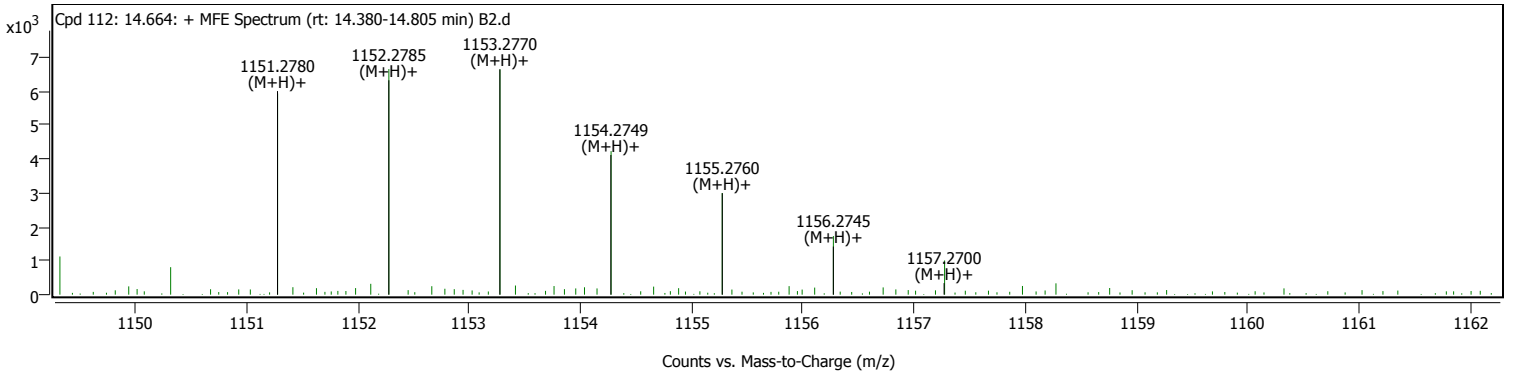
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.664		1150.2707				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

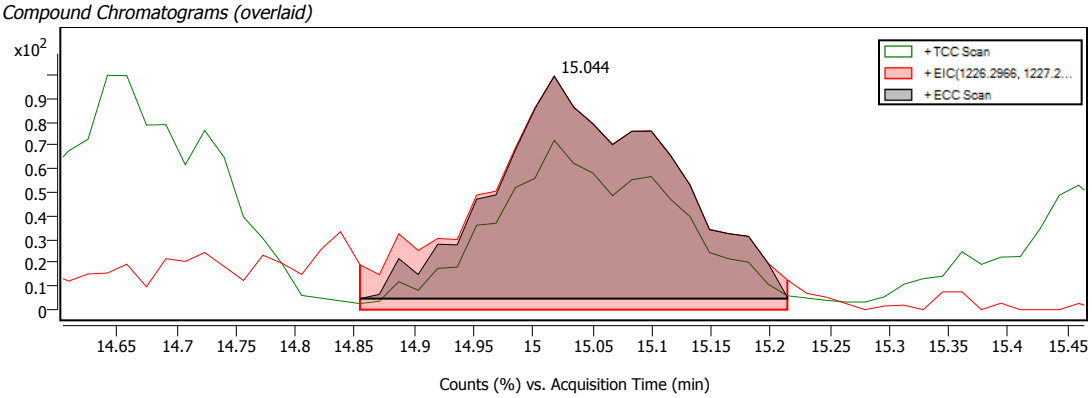


Cpd 113: 15.044

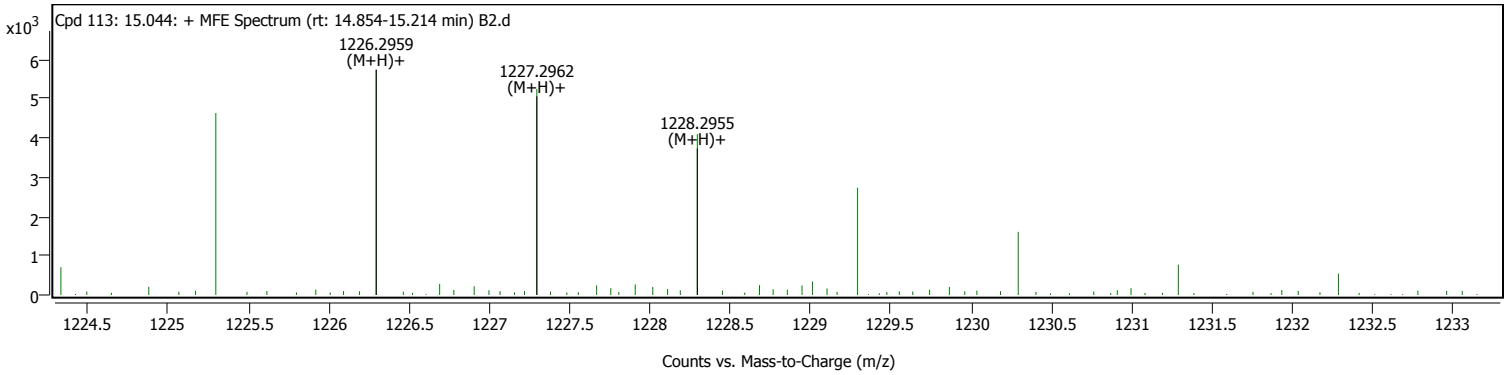
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		15.044		1225.2887				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

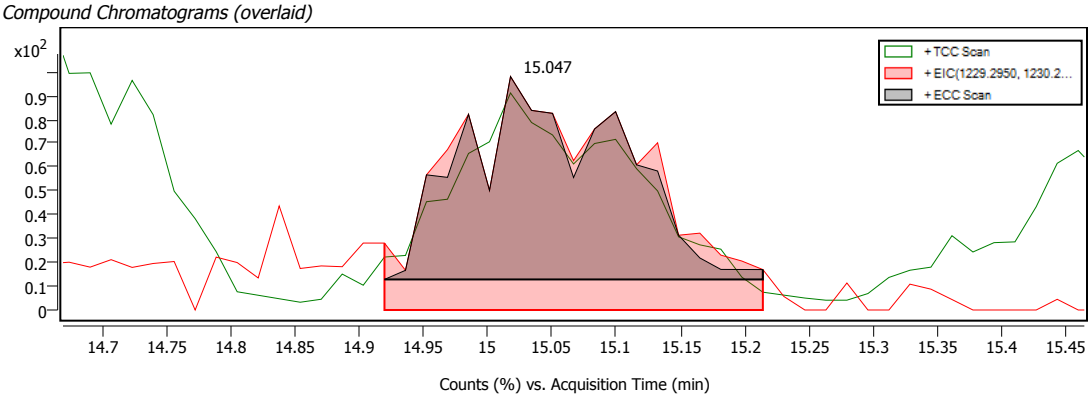


Cpd 114: 15.047

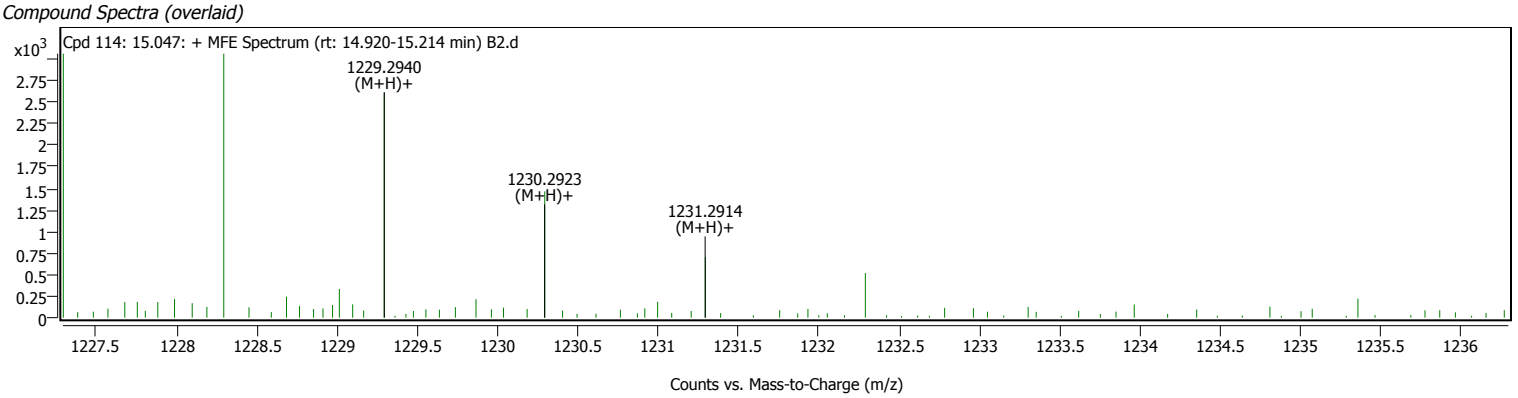
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		15.047		1228.2868				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

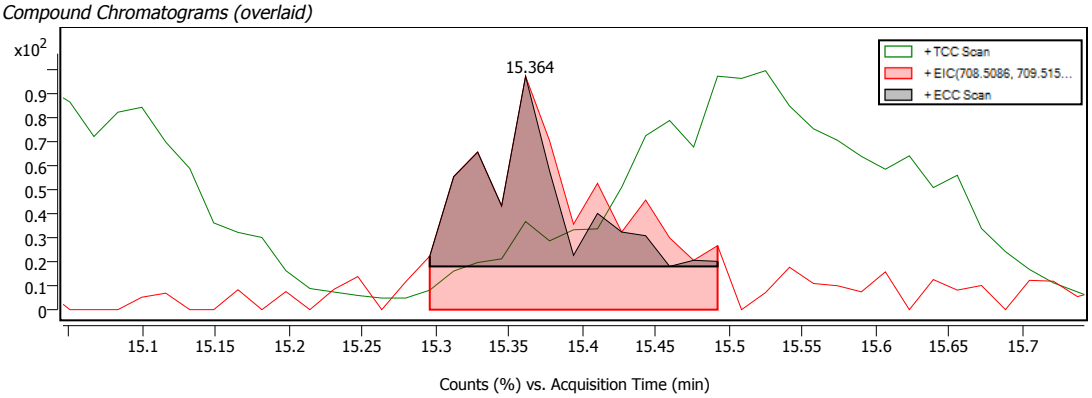


Cpd 115: 15.364

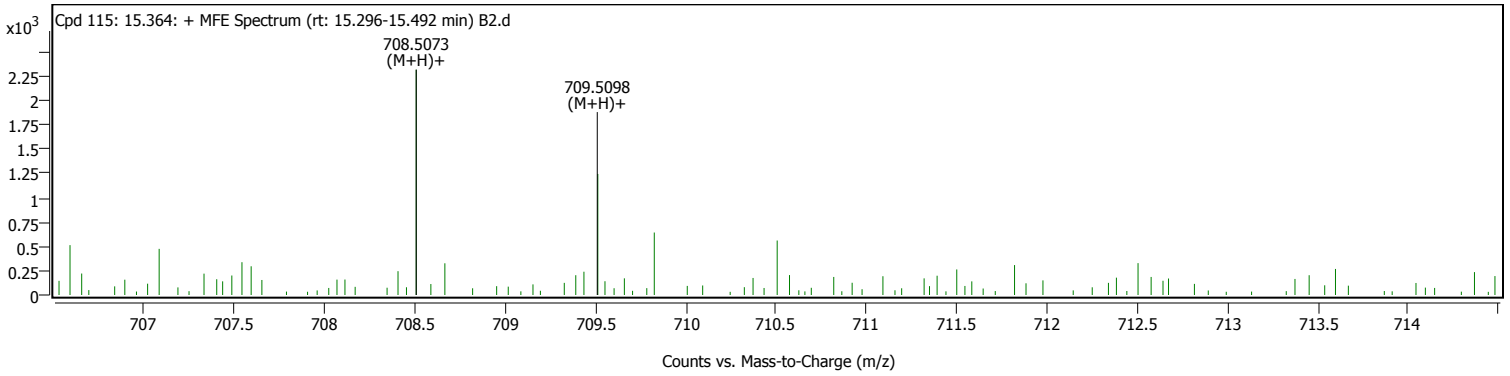
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		15.364		707.5001				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

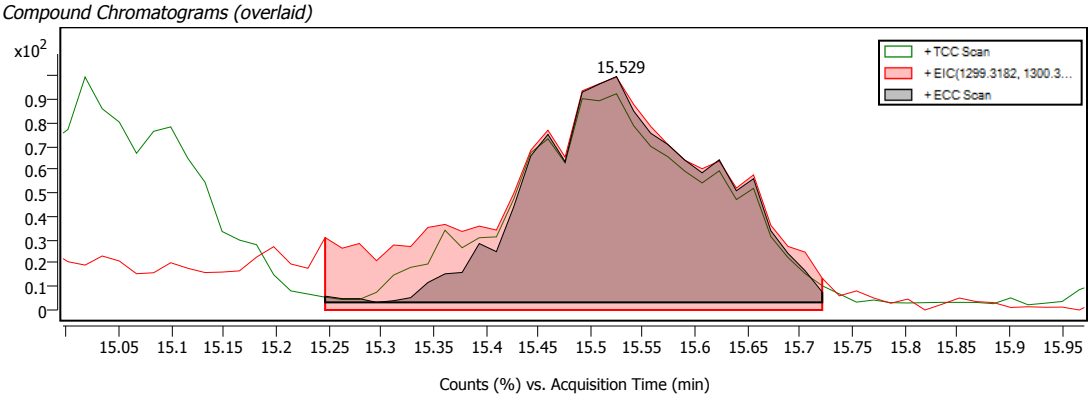


Cpd 116: 15.529

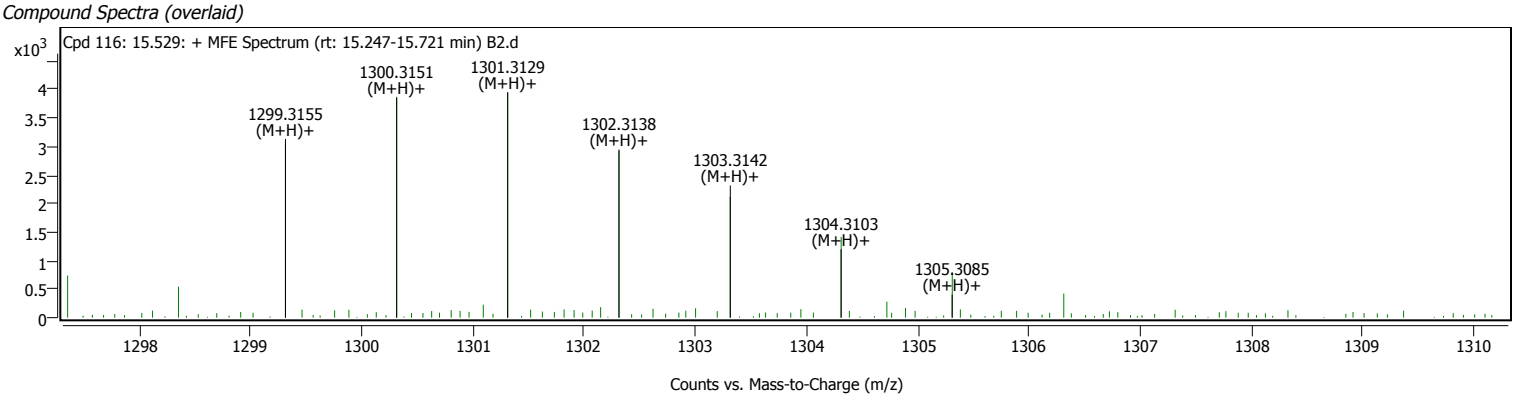
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		15.529		1298.3082				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

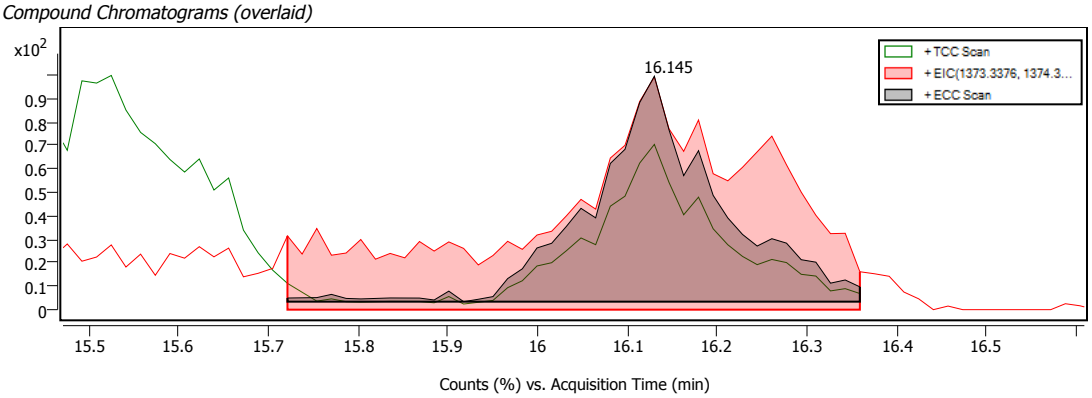


Cpd 117: 16.145

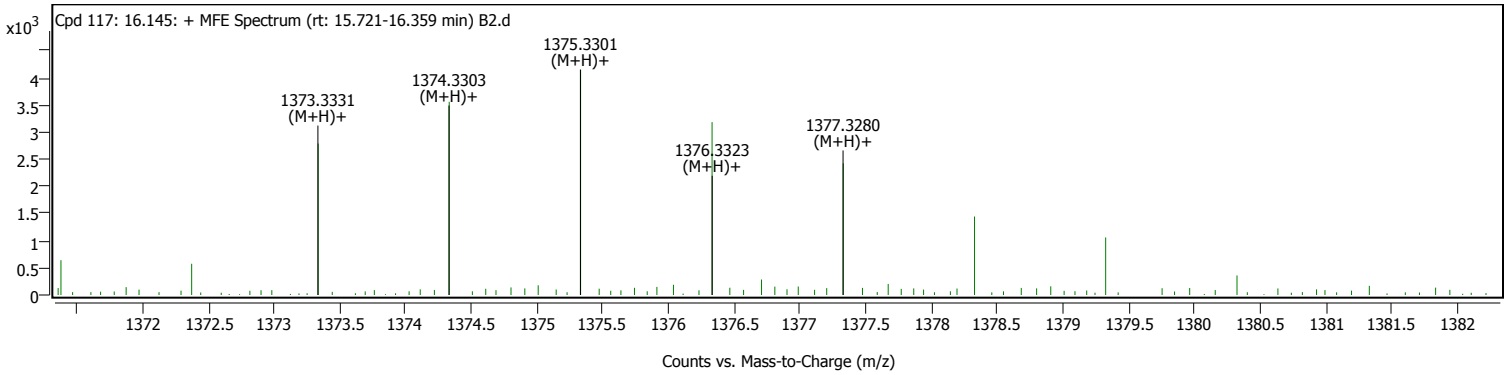
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		16.145		1372.3259				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



MassHunter Qual 10.0
(End of Report)