Compound Discovery Report

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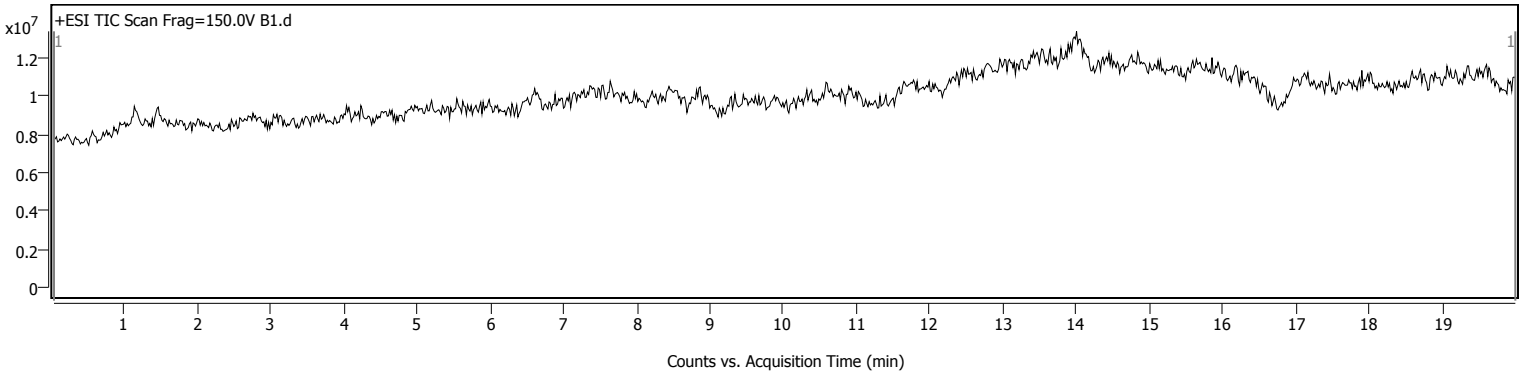
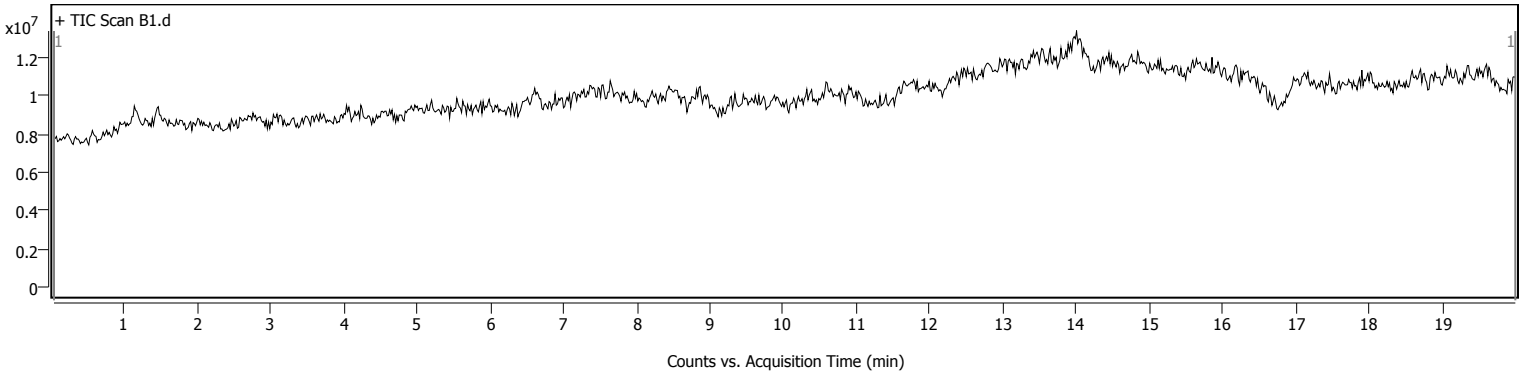
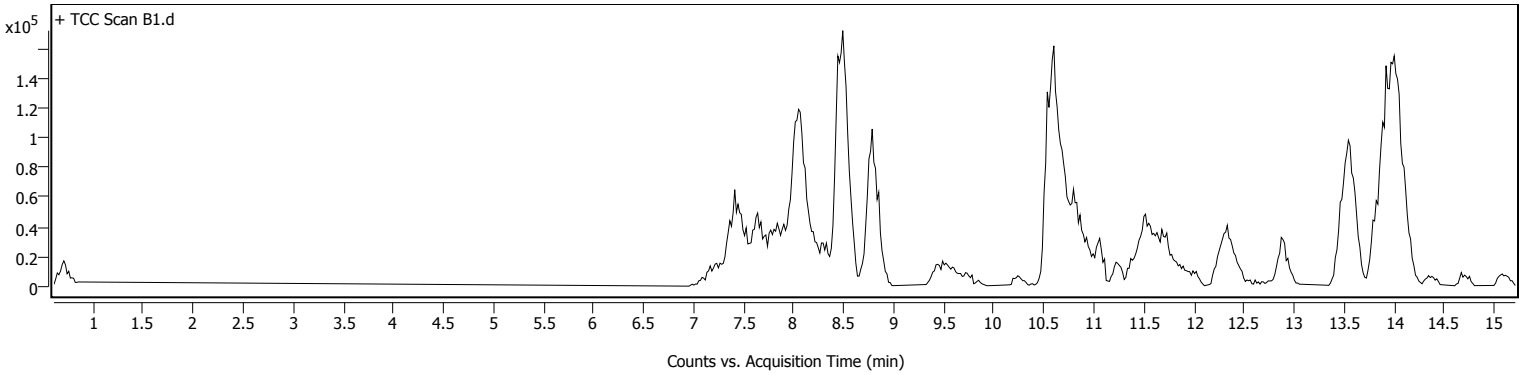
Sample Information

Name	B1	**Data File Path**	D:\MassHunter\Data\Saeed Ullah\B1.d
Sample ID		**Acq. Time (Local)**	10/3/2023 9:46:26 AM (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	P1-A1	**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**	87 identified (114 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	0.706	180.0640	29625-79-4	DBSearch-MFG	65.39		85.11	45.67	MFE
2		C18 H35 N18 O	7.219	519.3241		MFG	75.47			75.47	MFE
3	5β-Cyprinolsulfate	C27 H48 O8 S	7.347	532.3072		DBSearch-MFG	56.50		65.43	47.56	MFE
4		C23 H48 O8	7.386	452.3350		MFG	97.00			97.00	MFE
5		C29 H46 O3 S	7.387	474.3171		MFG	86.85			86.85	MFE
6		C28 H53 N O8 S	7.427	563.3495		MFG	96.26			96.26	MFE
7		C20 H36 N17 O2	7.442	546.3237		MFG	82.86			82.86	MFE
8		C22 H47 N11 O8	7.559	593.3610		MFG	77.12			77.12	MFE
9		C30 H54 O9 S	7.619	590.3496		MFG	94.90			94.90	MFE
10		C24 H50 N9 O12	7.796	656.3579		MFG	90.83			90.83	MFE
11		C26 H59 N4 O14	7.798	651.4020		MFG	96.26			96.26	MFE
12		C25 H55 N14 O9	7.951	695.4282		MFG	96.94			96.94	MFE

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
13		C34 H58 N3 O10 S	7.960	700.3838		MFG	95.05			95.05	MFE
14		C28 H53 N8 O4	8.044	565.4184		MFG	98.56			98.56	MFE
15		C35 H63 N8 O7 S	8.096	739.4539		MFG	96.43			96.43	MFE
16	Ophiopogonin C'	C39 H62 O12	8.098	722.4274	19057-67-1	DBSearch	56.58		56.58		MFE
17	Pitheduloside A	C41 H66 O13	8.221	766.4540	78285-89-9	DBSearch	67.68		67.68		MFE
18	PE(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C43 H72 N O8 P	8.224	761.4987		DBSearch	93.83		93.83		MFE
19		C38 H58 N17 O3 S	8.329	832.4628		MFG	95.12			95.12	MFE
20		C31 H67 N14 O12	8.333	827.5064		MFG	95.98			95.98	MFE
21		C31 H52 N30 O2	8.433	876.4882		MFG	71.02			71.02	MFE
22	PS(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H80 N O10 P	8.436	849.5505		DBSearch	77.23		77.23		MFE
23		C47 H71 N4 O2	8.481	723.5581		MFG	61.59			61.59	MFE
24		C32 H62 N12 O4	8.482	678.5023		MFG	98.50			98.50	MFE
25		C52 H101 N3 S3	8.487	863.7152		MFG	85.25			85.25	MFE
26	Hebevinoside XIII	C49 H76 O16	8.513	920.5123	138995-52-5	DBSearch	57.33		57.33		MFE
27	Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	C47 H78 O16	8.534	898.5303		DBSearch	62.47		62.47		MFE
28		C35 H67 N28 O5	8.619	959.5851		MFG	63.80			63.80	MFE
29		C47 H66 O3	8.750	678.5021		MFG	95.32			95.32	MFE
30		C40 H O25 S3	8.777	976.7975		MFG	78.95			78.95	MFE
31	1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	8.790	814.5751		DBSearch	98.53		98.53		MFE
32	Halaminol A	C14 H29 N O	9.513	227.2242		DBSearch-MFG	82.71		82.69	82.72	MFE
33		C12 H29 N4	9.835	229.2395		MFG	71.88			71.88	MFE
34		C20 H26 N16 O5	10.240	570.2269		MFG	79.04			79.04	MFE
35		C19 H22 N16 O4	10.487	538.2007		MFG	81.23			81.23	MFE
36		C36 H63 N14 O S2	10.553	771.4753		MFG	89.69			89.69	MFE
37		C33 H42 N3 O9 S	10.571	656.2633		MFG	89.54			89.54	MFE
38		C39 H63 N21 O4	10.582	889.5379		MFG	58.57			58.57	MFE
39		C14 H31 N4	10.601	255.2551		MFG	98.61			98.61	MFE
40		C30 H55 N O S	10.769	477.4002		MFG	61.40			61.40	MFE
41			10.779	433.3754							MFE
42		C28 H48 N5 O18	10.835	742.2996		MFG	92.35			92.35	MFE
43		C33 H50 N9 O16	11.056	828.3371		MFG	97.08			97.08	MFE
44		C37 H63 N7 O19	11.231	909.4187		MFG	65.31			65.31	MFE
45		C34 H48 N19 O12	11.236	914.3730		MFG	96.59			96.59	MFE
46			11.369	995.4517							MFE
47			11.378	1000.4100							MFE
48			11.520	1086.4457							MFE
49		C16 H35 N4	11.532	283.2863		MFG	98.70			98.70	MFE
50			11.631	1172.4820							MFE
51	Austrobailignan 7	C20 H22 O5	11.701	342.1456	55890-25-0	DBSearch	79.18		79.18		MFE
52			11.731	1258.5178							MFE
53			11.819	1344.5532							MFE
54			11.896	1430.5916							MFE
55		C35 H63 N13 O	11.994	681.5279		MFG	72.05			72.05	MFE
56		C19 H24 N12	12.005	420.2242		MFG	77.66			77.66	MFE
57		C35 H61 N10 O2	12.017	653.4985		MFG	65.91			65.91	MFE
58			12.282	370.2679							MFE
59		C22 H50 N2 O10	12.317	502.3466		MFG	85.62			85.62	MFE
60		C22 H52 N5 O10	12.317	546.3716		MFG	82.39			82.39	MFE
61		C19 H40 N9 O4	12.318	458.3204		MFG	83.04			83.04	MFE
62		C22 H44 N19 O	12.322	590.3981		MFG	79.13			79.13	MFE
63		C41 H54 N4 O2	12.323	634.4250		MFG	66.07			66.07	MFE
64			12.452	304.2366							MFE
65		C24 H38 N16	12.584	550.3461		MFG	69.05			69.05	MFE
66		C19 H40 N9 O3	12.768	442.3251		MFG	83.96			83.96	MFE
67		C31 H40 O	12.818	428.3087		MFG	62.56			62.56	MFE
68		C26 H46 N9 O4	12.884	548.3670		MFG	77.06			77.06	MFE
69	Petromyzonol	C24 H42 O4	12.885	394.3068	28979-29-5	DBSearch	68.32		68.32		MFE
70	PC(O-16:0/0:0)[U]	C24 H53 N O6 P	12.887	482.3595		DBSearch	70.29		70.29		MFE
71	27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.895	438.3324	78648-95-0	DBSearch	64.90		64.90		MFE
72		C43 H39 Cl3 N3 O3 S	13.397	782.1778		MFG	47.62			47.62	MFE
73			13.445	1188.7883							MFE
74			13.451	1232.8136							MFE
75			13.454	1144.7597							MFE
76	35S-Methylokadaic acid 7-hexadecanoate	C61 H100 O14	13.474	1056.7104		DBSearch	92.96		92.96		MFE
77			13.487	1012.6854							MFE
78		C57 H92 O12	13.506	968.6584		MFG	94.38			94.38	MFE
79		C53 H76 N14 O	13.511	924.6318		MFG	91.09			91.09	MFE
80		C51 H72 N14	13.527	880.6063		MFG	97.22			97.22	MFE
81		C43 H74 N13 O2 S	13.534	836.5805		MFG	95.38			95.38	MFE
82		C48 H70 N7 O3	13.548	792.5543		MFG	63.98			63.98	MFE
83		C48 H68 N4 O3	13.559	748.5289		MFG	87.52			87.52	MFE
84		C31 H68 N12 O2 S2	13.569	704.5027		MFG	85.17			85.17	MFE
85		C44 H68 S2	13.586	660.4763		MFG	85.03			85.03	MFE
86		C52 H42 N2 S5	13.592	854.1946		MFG	73.41			73.41	MFE
87		C42 H56 N4	13.601	616.4512		MFG	67.46			67.46	MFE
88		C24 H52 N12 O4	13.611	572.4234		MFG	77.95			77.95	MFE
89		C37 H52 O2	13.615	528.3984		MFG	64.33			64.33	MFE
90			13.775	1414.9132							MFE
91			13.795	928.2144							MFE

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
92			13.811	1260.8447							MFE
93			13.816	1282.8336							MFE
94			13.828	1216.8190							MFE
95			13.846	1172.7928							MFE
96			13.863	1128.7661							MFE
97			13.881	1084.7395							MFE
98			13.898	1040.7150							MFE
99		C56 H88 N10 O6	13.916	996.6892		MFG	98.67			98.67	MFE
100		C55 H90 N3 O10	13.929	952.6627		MFG	95.06			95.06	MFE
101		C53 H86 N3 O9	13.952	908.6370		MFG	96.79			96.79	MFE
102		C39 H86 N5 O15	13.966	864.6113		MFG	97.36			97.36	MFE
103		C43 H84 N2 O10 S	13.984	820.5858		MFG	92.39			92.39	MFE
104		C34 H72 N12 O8	14.003	776.5596		MFG	94.71			94.71	MFE
105		C32 H68 N12 O7	14.026	732.5339		MFG	87.71			87.71	MFE
106		C30 H64 N12 O6	14.042	688.5071		MFG	92.99			92.99	MFE
107		C44 H60 N4	14.064	644.4815		MFG	95.82			95.82	MFE
108			14.065	1002.2336							MFE
109	OH-Spheroidenone	C41 H60 O3	14.093	600.4546		DBSearch-MFG	94.64		94.64	94.64	MFE
110		C32 H56 N6 S	14.121	556.4290		MFG	93.42			93.42	MFE
111		C37 H52 O	14.141	512.4024		MFG	69.46			69.46	MFE
112			14.366	1076.2524							MFE
113			14.699	1151.2724							MFE
114			15.089	1224.2884							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	0.706		180.0640	29625-79-4	DBSearch-MFG	65.39	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	203.0533 203.0533 203.0533		0	85.11	33	45.67	

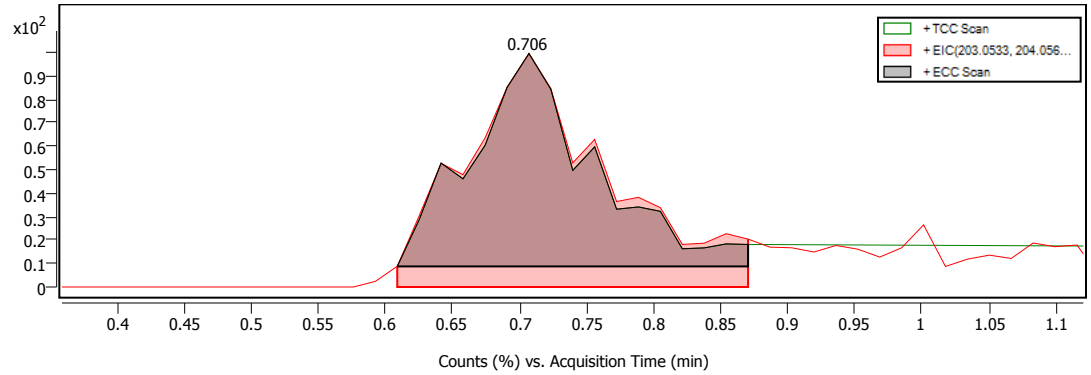
Compound ID Table

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	0.706		180.0640	29625-79-4	65.39	85.11	45.67
D-Fuconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640		65.39	85.11	45.67
L-Rhamnonate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	6422-34-0	65.39	85.11	45.67
D-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	59-23-4	65.39	85.11	45.67
allo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	643-10-7	65.39	85.11	45.67
myo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	87-9-8	65.39	85.11	45.67
D-(+)-Mannose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	3458-28-4	65.39	85.11	45.67
b-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	492-61-5	65.39	85.11	45.67
L-(-)Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	87-79-6	65.39	85.11	45.67
α-D-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	492-62-6	65.39	85.11	45.67
D-Tagatose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	87-81-0	65.39	85.11	45.67
Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	3615-39-2	65.39	85.11	45.67
Allose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	6038-51-3	65.39	85.11	45.67
L-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	15572-79-9	65.39	85.11	45.67
b-D-Galactopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	7296-64-2	65.39	85.11	45.67
D-Hamamelose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	4573-78-8	65.39	85.11	45.67
β-D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	53188-23-1	65.39	85.11	45.67
2-Deoxy-D-gluconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640		65.39	85.11	45.67
beta-D-Hamamelopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640		65.39	85.11	45.67
D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	57-48-7	65.39	85.11	45.67
L-(+)-Gulose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	6027-89-0	65.39	85.11	45.67
1,3-Dihydroxyacetone	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.706		180.0640	62147-49-3	65.39	85.11	45.67
Theophylline	C7 H8 N4 O2	(M+Na)+	DBSearch-MFG	0.706		180.0640	58-55-9	64.37	83.40	45.33
Theobromine	C7 H8 N4 O2	(M+Na)+	DBSearch-MFG	0.706		180.0640	83-67-0	64.37	83.40	45.33
Paraxanthine	C7 H8 N4 O2	(M+Na)+	DBSearch-MFG	0.706		180.0640	611-59-6	64.37	83.40	45.33
	C7 H11 N2 O3 S	(M+H)+	MFG	0.706		203.0490		47.61		47.61
	C7 H16 O S2	(M+Na)+	MFG	0.706		180.0640		47.37		47.37
	C13 H5 N3	(M+H)+	MFG	0.706		203.0490		45.63		45.63
	C15 H7 O	(M+H)+	MFG	0.706		203.0490		45.36		45.36
	C5 H14 N3 S2	(M+Na)+	MFG	0.706		180.0640		41.97		41.97
	C12 H10 Cl N	(M+H)+	MFG	0.706		203.0490		41.36		41.36
	C4 H11 Cl N5 O	(M+Na)+	MFG	0.706		180.0640		41.30		41.30
	C5 H9 N5 O2 S	(M+H)+	MFG	0.706		203.0490		40.11		40.11

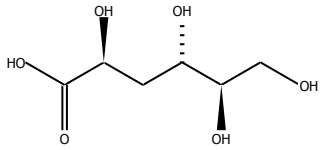
Compound Discovery Report

Agilent | Trusted Answers

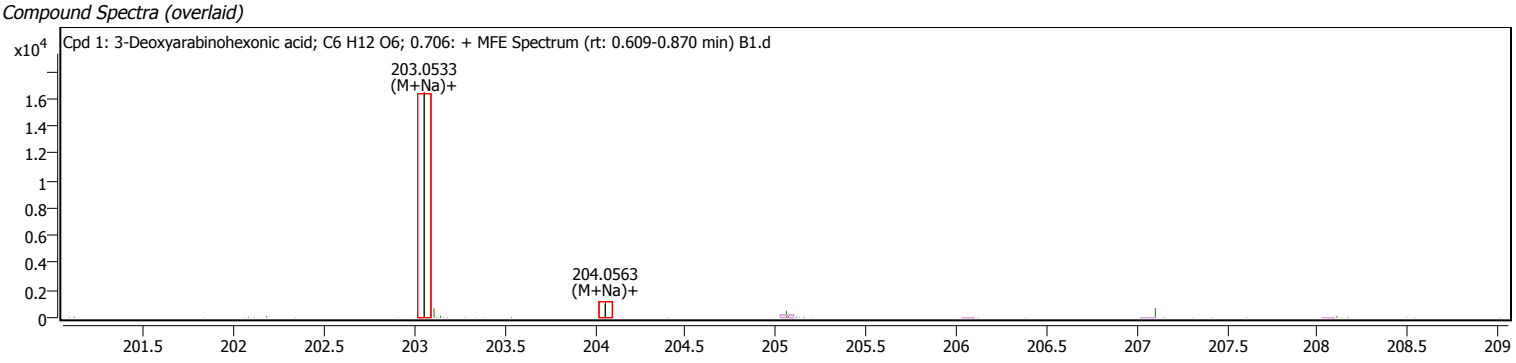
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 2: C18 H35 N18 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C18 H35 N18 O	7.219		519.3241		MFG	75.47	MFE	

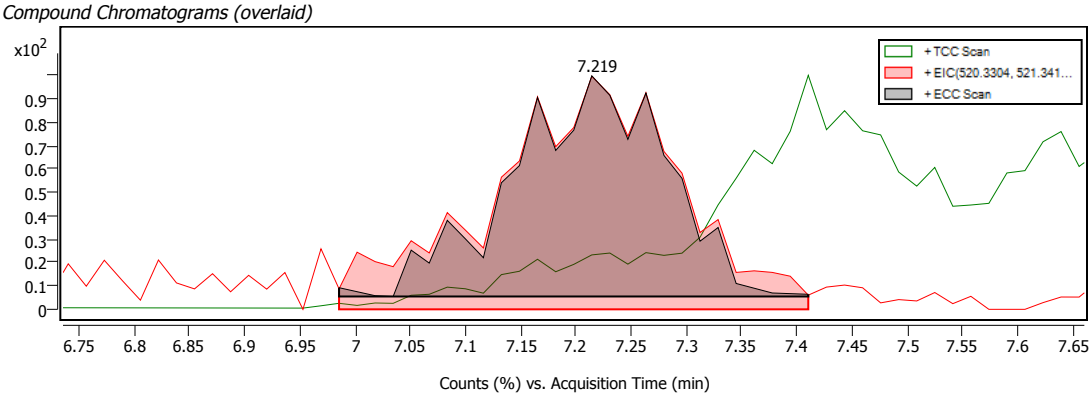
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	520.3308				5	75.47	

Compound ID Table

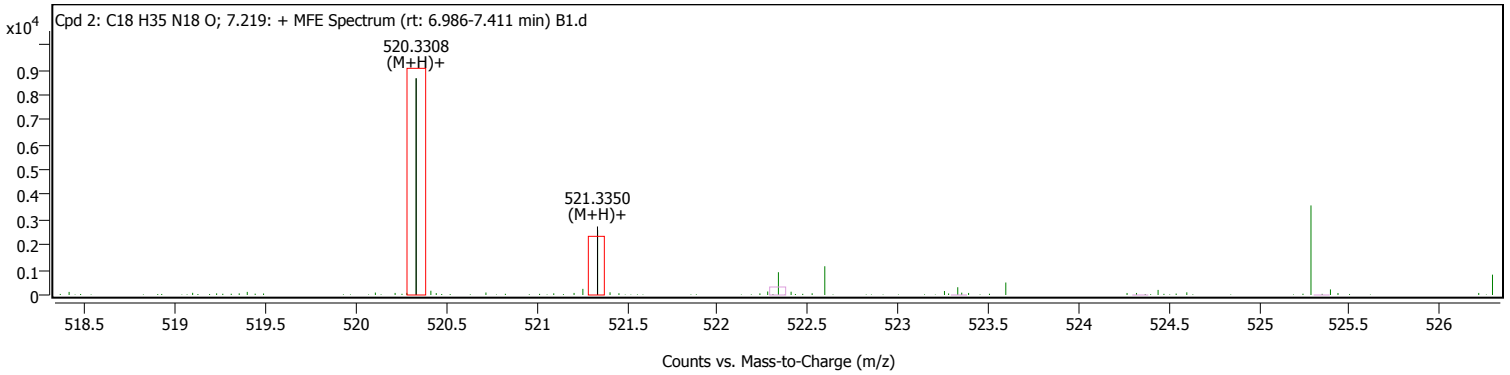
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C18 H35 N18 O	(M+H)+	MFG	7.219		519.3241		75.47		75.47
	C33 H39 N6	(M+H)+	MFG	7.219		519.3238		75.21		75.21
	C19 H41 N11 O6	(M+H)+	MFG	7.219		519.3239		73.42		73.42
	C20 H37 N15 O2	(M+H)+	MFG	7.219		519.3240		72.85		72.85
	C32 H43 N2 O4	(M+H)+	MFG	7.219		519.3237		72.85		72.85

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 3: 5β-Cyprinolsulfate

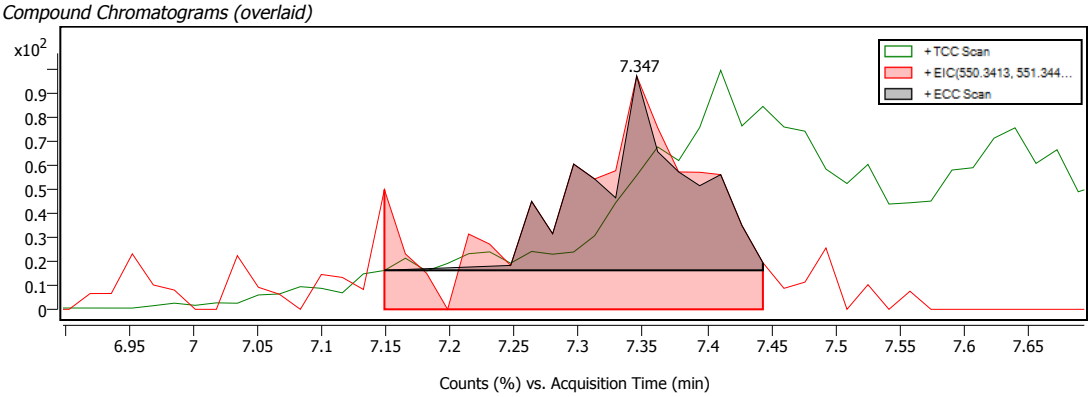
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
5β-Cyprinolsulfate	C27 H48 O8 S	7.347		532.3072		DBSearch-MFG	56.50	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	550.3410 550.3410 550.3410 550.3410		0	65.43	10	47.56	

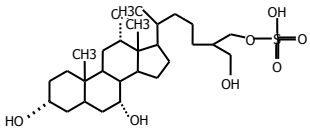
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
5β-Cyprinolsulfate	C27 H48 O8 S	(M+NH4)+	DBSearch-MFG	7.347		532.3072		56.50	65.43	47.56
	C34 H46 N S2	(M+NH4)+	MFG	7.347		532.3072		47.62		47.62
	C19 H50 N9 S4	(M+NH4)+	MFG	7.347		532.3072		47.62		47.62
	C18 H48 Cl2 N12 O3	(M+H)+	MFG	7.347		550.3350		47.61		47.61
	C30 H55 Cl3 N O	(M+H)+	MFG	7.347		550.3350		47.61		47.61
	C27 H48 Cl2 N3 O3	(M+NH4)+	MFG	7.347		532.3072		47.60		47.60
	C15 H41 Cl N14 O5	(M+NH4)+	MFG	7.347		532.3072		47.59		47.59
	C26 H52 Cl2 N6 S	(M+H)+	MFG	7.347		550.3350		47.59		47.59
	C26 H52 N3 O5 S2	(M+H)+	MFG	7.347		550.3350		47.58		47.58
	C25 H46 N10 S2	(M+H)+	MFG	7.347		550.3350		47.57		47.57

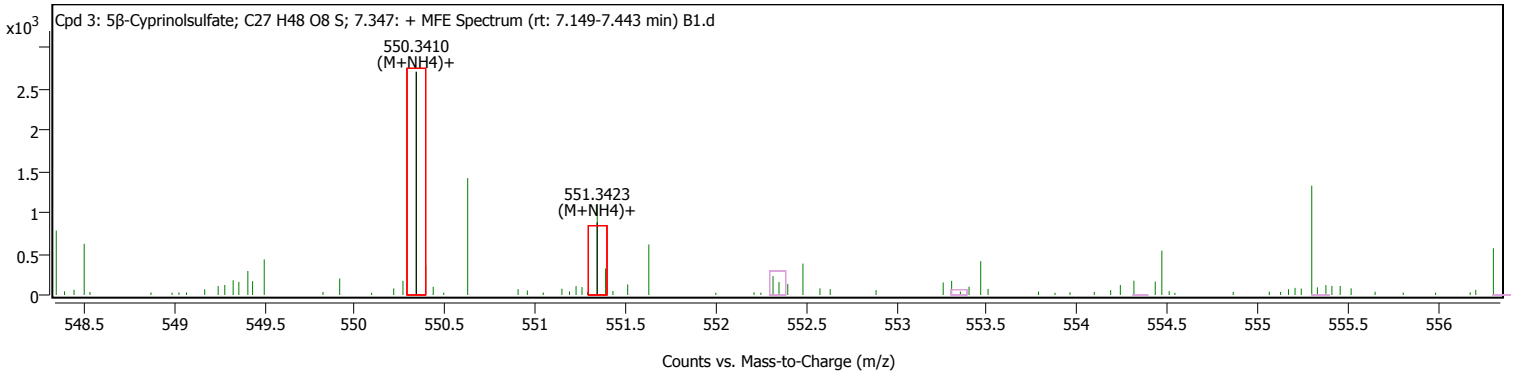
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 4: C23 H48 O8

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C23 H48 O8	7.386		452.3350		MFG	97.00	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	453.3421				5	97.00	

Compound Discovery Report

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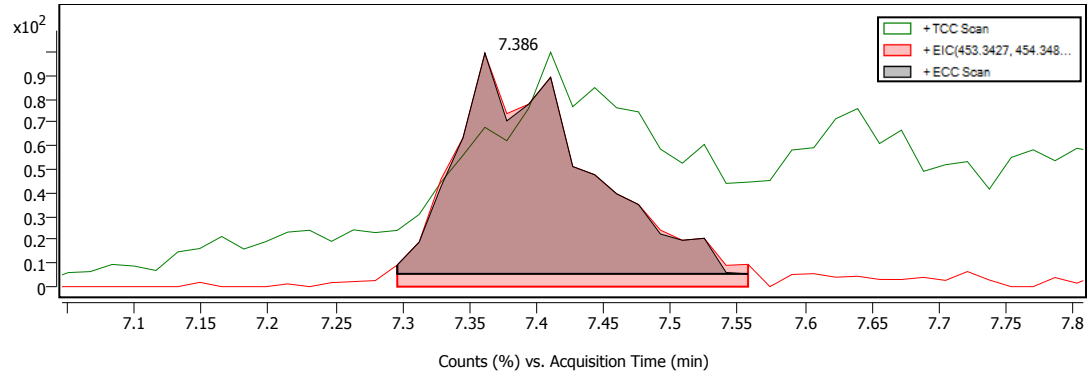
Compound ID Table

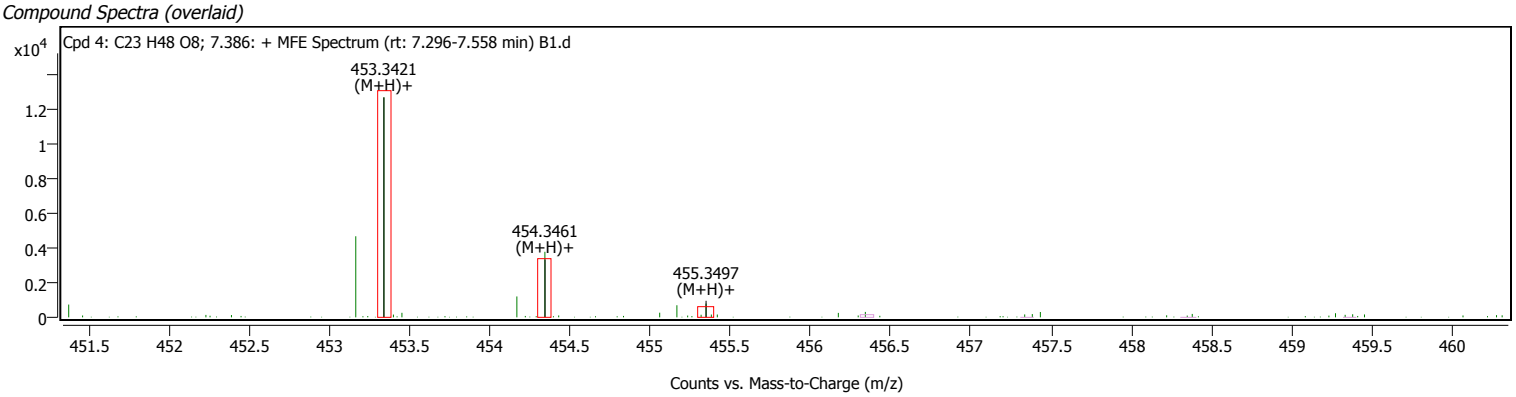
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C23 H48 O8	(M+H)+	MFG	7.386		452.3350		97.00		97.00
	C22 H42 N7 O3	(M+H)+	MFG	7.386		452.3351		94.04		94.04
	C24 H44 N4 O4	(M+H)+	MFG	7.386		452.3351		91.98		91.98
	C21 H46 N3 O7	(M+H)+	MFG	7.386		452.3351		90.66		90.66
	C20 H40 N10 O2	(M+H)+	MFG	7.386		452.3352		86.57		86.57

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 5: C29 H46 O3 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C29 H46 O3 S	7.387		474.3171		MFG	86.85	MFE	

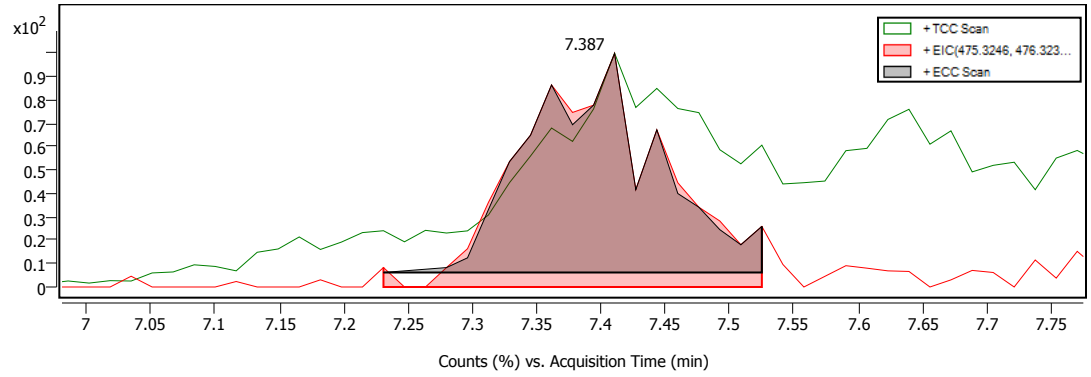
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	475.3235				5	86.85	

Compound ID Table

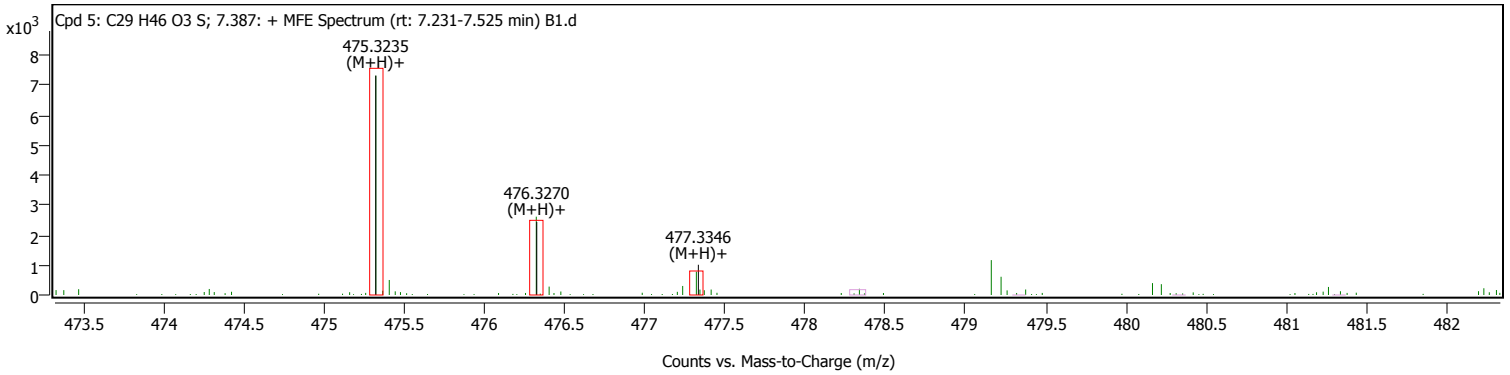
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C29 H46 O3 S	(M+H)+	MFG	7.387		474.3171		86.85		86.85
	C22 H46 N6 O S2	(M+H)+	MFG	7.387		474.3175		83.76		83.76
	C24 H48 N3 O2 S2	(M+H)+	MFG	7.387		474.3174		81.29		81.29
	C35 H40 N	(M+H)+	MFG	7.387		474.3166		80.87		80.87
	C27 H44 N3 O2 S	(M+H)+	MFG	7.387		474.3172		79.81		79.81

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 6: C28 H53 N O8 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H53 N O8 S	7.427		563.3495		MFG	96.26	MFE	

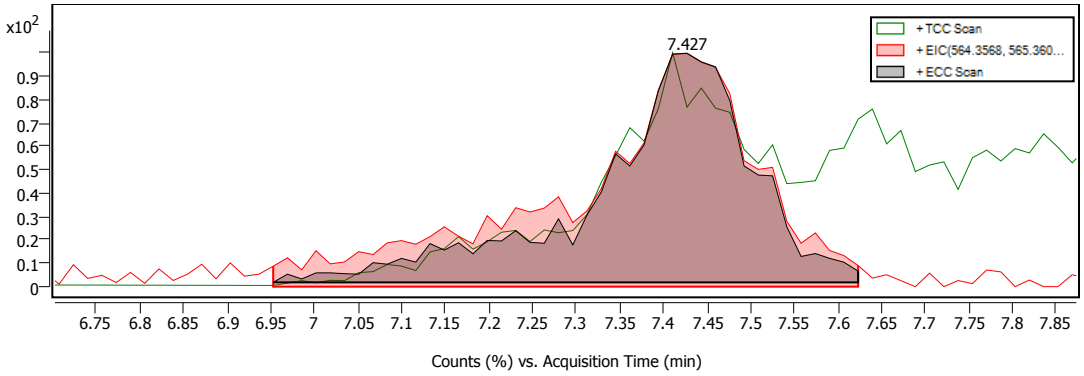
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	564.3566				5	96.26	

Compound ID Table

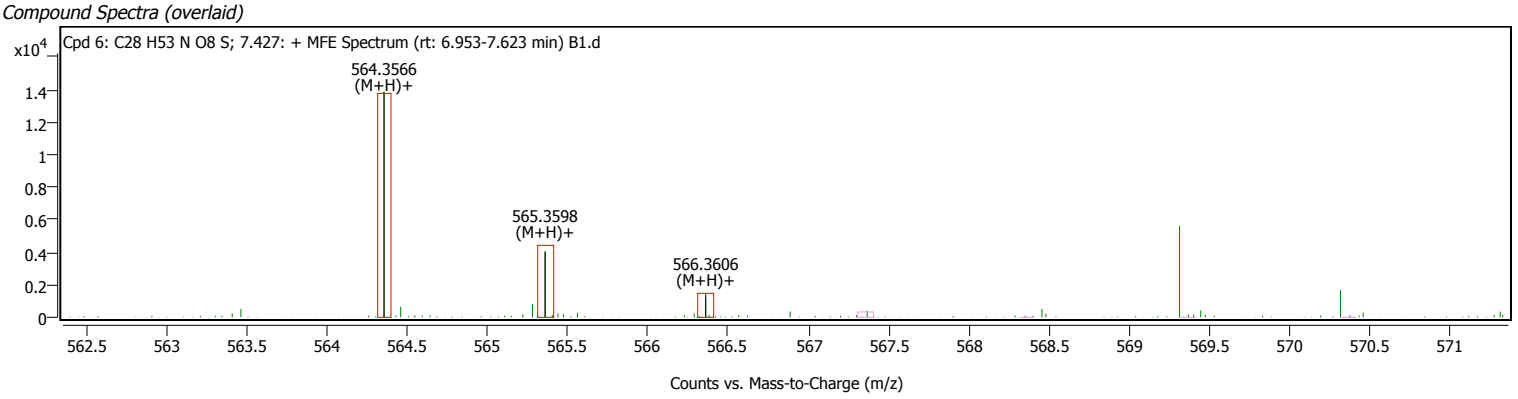
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H53 N O8 S	(M+H)+	MFG	7.427		563.3495		96.26		96.26
	C27 H47 N8 O3 S	(M+H)+	MFG	7.427		563.3496		94.25		94.25
	C20 H49 N7 O11	(M+H)+	MFG	7.427		563.3494		92.88		92.88
	C29 H49 N5 O4 S	(M+H)+	MFG	7.427		563.3496		92.58		92.58
	C22 H51 N4 O12	(M+H)+	MFG	7.427		563.3493		92.42		92.42

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 7: C20 H36 N17 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C20 H36 N17 O2	7.442		546.3237		MFG	82.86	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	569.3129				10	82.86	

Compound Discovery Report

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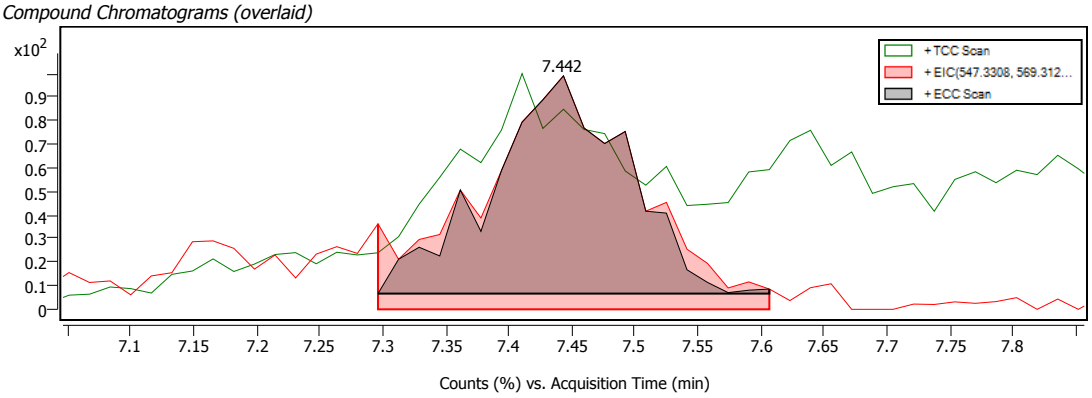
Compound ID Table

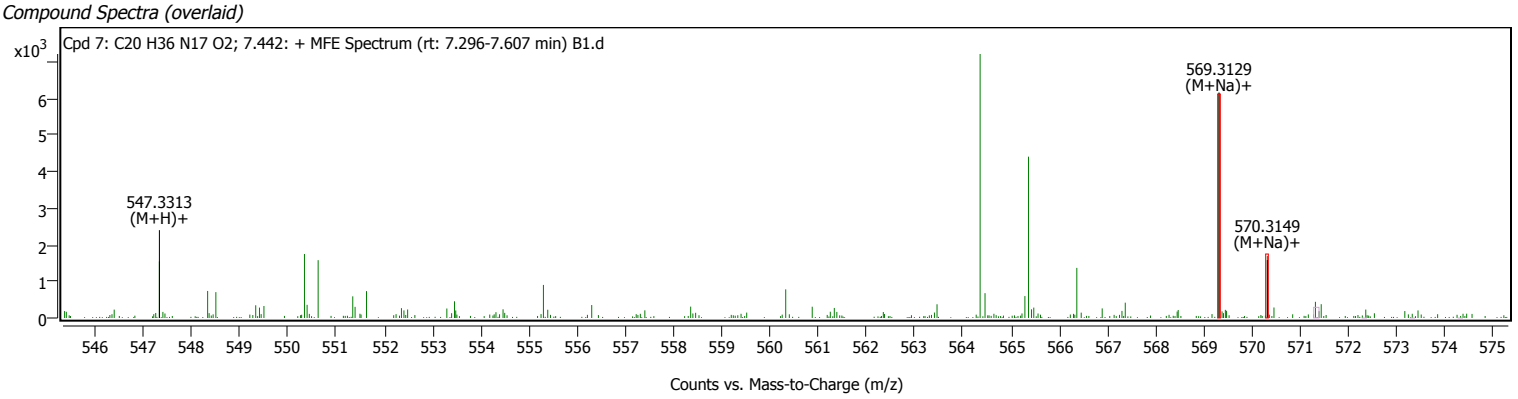
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C20 H36 N17 O2	(M+Na)+	MFG	7.442		546.3237		82.86		82.86
	C21 H42 N10 O7	(M+Na)+	MFG	7.442		546.3235		81.37		81.37
	C18 H34 N20 O	(M+Na)+	MFG	7.442		546.3237		81.26		81.26
	C19 H40 N13 O6	(M+Na)+	MFG	7.442		546.3236		80.22		80.22
	C22 H48 N3 O12	(M+Na)+	MFG	7.442		546.3234		78.63		78.63
	C29 H46 N4 O4 S	(M+H)+	MFG	7.442		546.3241		47.61		47.61
	C30 H52 Cl2 O4	(M+H)+	MFG	7.442		546.3241		47.54		47.54
	C17 H39 Cl N18 O	(M+H)+	MFG	7.442		546.3241		47.53		47.53
	C18 H45 Cl N11 O6	(M+H)+	MFG	7.442		546.3241		47.53		47.53
	C17 H47 Cl N14 S2	(M+H)+	MFG	7.442		546.3241		47.50		47.50

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 8: C22 H47 N11 O8

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H47 N11 O8	7.559		593.3610		MFG	77.12	MFE	

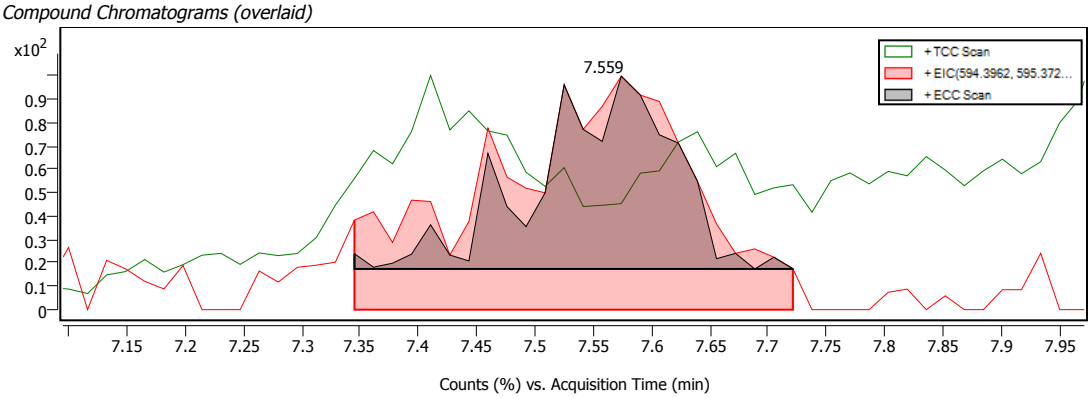
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	594.3678				5	77.12	

Compound ID Table

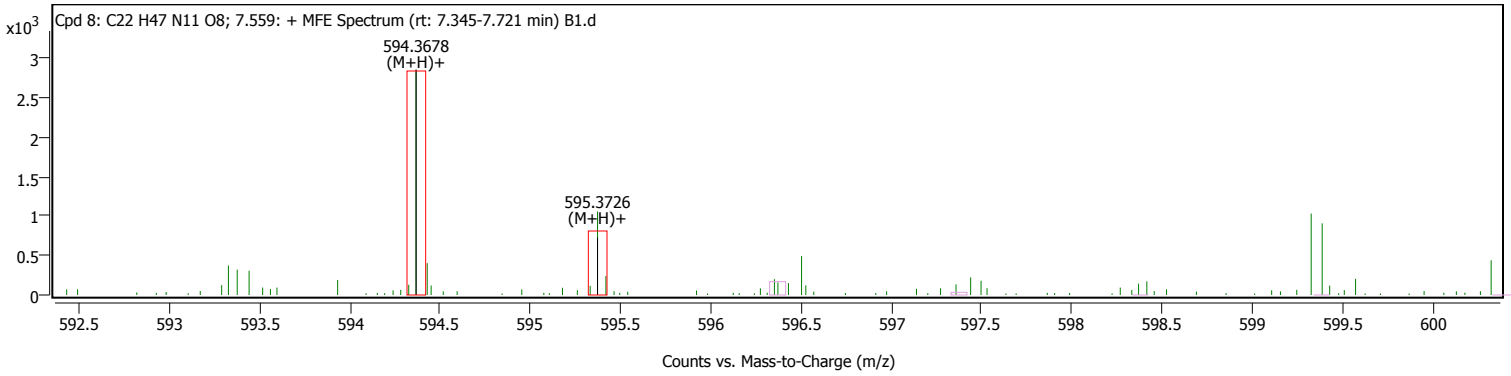
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H47 N11 O8	(M+H)+	MFG	7.559		593.3610		77.12		77.12
	C23 H53 N4 O13	(M+H)+	MFG	7.559		593.3609		76.99		76.99
	C21 H41 N18 O3	(M+H)+	MFG	7.559		593.3611		76.54		76.54
	C21 H51 N7 O12	(M+H)+	MFG	7.559		593.3609		74.37		74.37
	C20 H45 N14 O7	(M+H)+	MFG	7.559		593.3611		74.24		74.24

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 9: C30 H54 O9 S

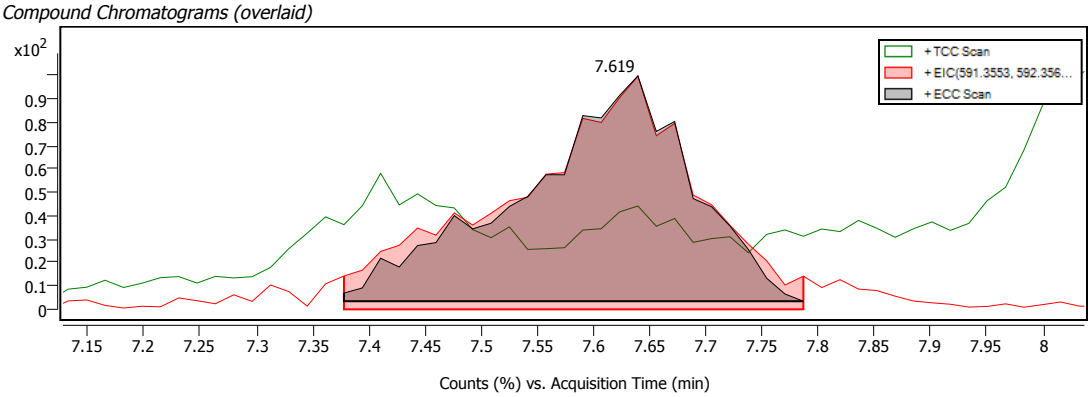
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C30 H54 O9 S	7.619		590.3496		MFG	94.90	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	608.3834				13	94.90	

Compound ID Table

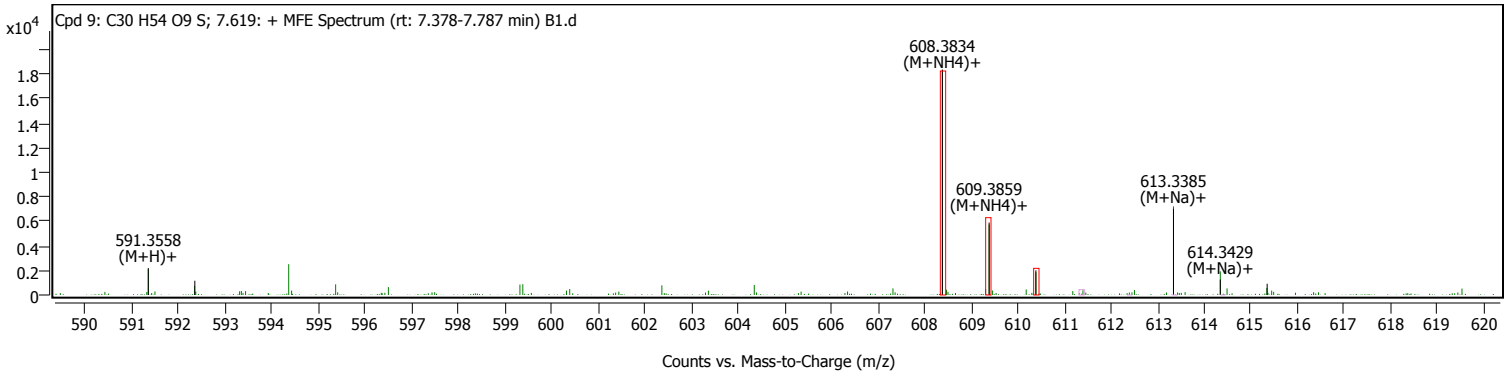
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C30 H54 O9 S	(M+NH4)+	MFG	7.619		590.3496		94.90		94.90
	C23 H46 N10 O8	(M+NH4)+ (M+Na)+	MFG	7.619		590.3495		94.19		94.19
	C31 H50 N4 O5 S	(M+NH4)+	MFG	7.619		590.3496		94.03		94.03
	C24 H52 N3 O13	(M+NH4)+ (M+Na)+	MFG	7.619		590.3494		93.96		93.96
	C29 H48 N7 O4 S	(M+NH4)+	MFG	7.619		590.3497		93.76		93.76
	C22 H50 N6 O12	(M+Na)+	MFG	7.619		590.3498		72.98		72.98
	C23 H54 N6 O7 S2	(M+Na)+	MFG	7.619		590.3504		72.43		72.43
	C25 H56 N3 O8 S2	(M+Na)+	MFG	7.619		590.3503		72.21		72.21
	C33 H40 N11	(M+H)+	MFG	7.619		590.3470		58.35		58.35
	C34 H46 N4 O5	(M+H)+	MFG	7.619		590.3468		56.37		56.37
	C35 H42 N8 O	(M+H)+	MFG	7.619		590.3469		55.79		55.79
	C36 H48 N O6	(M+H)+	MFG	7.619		590.3468		53.21		53.21
	C32 H44 N7 O4	(M+H)+	MFG	7.619		590.3469		53.04		53.04

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 10: C24 H50 N9 O12

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C24 H50 N9 O12	7.796		656.3579		MFG	90.83	MFE	

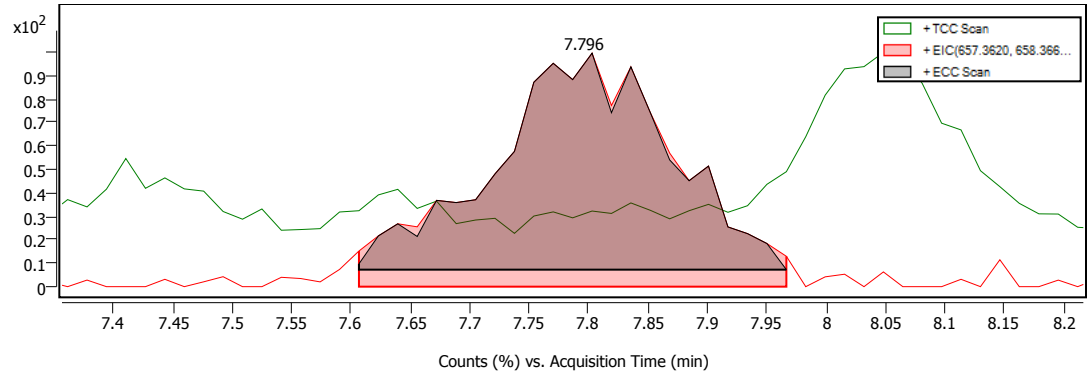
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	657.3652				5	90.83	

Compound ID Table

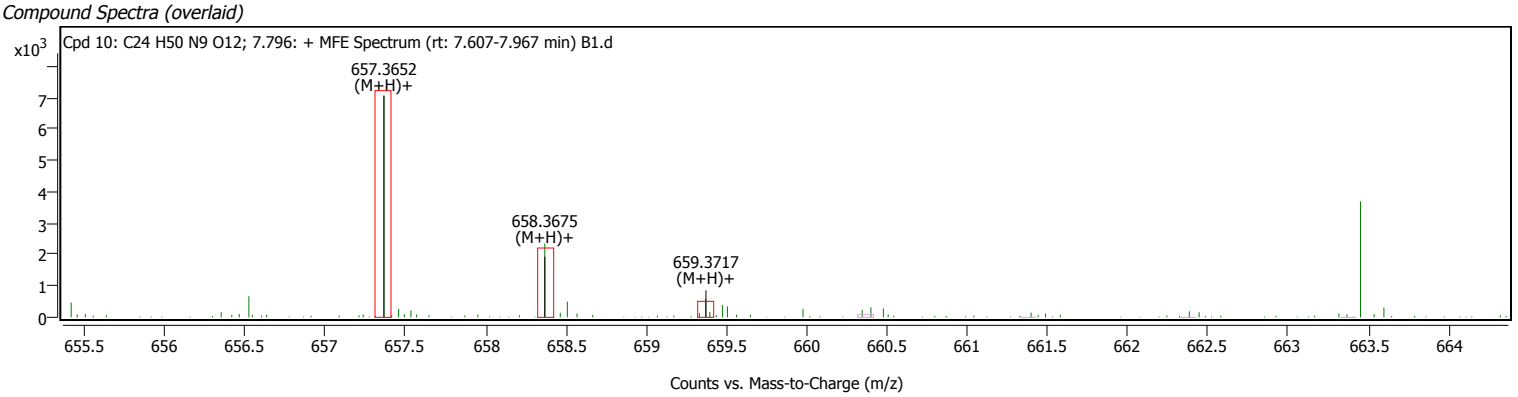
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C24 H50 N9 O12	(M+H)+	MFG	7.796		656.3579		90.83		90.83
	C23 H54 N5 O16	(M+H)+	MFG	7.796		656.3579		90.42		90.42
	C26 H52 N6 O13	(M+H)+	MFG	7.796		656.3579		88.04		88.04
	C23 H44 N16 O7	(M+H)+	MFG	7.796		656.3581		87.61		87.61
	C22 H48 N12 O11	(M+H)+	MFG	7.796		656.3580		87.44		87.44

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 11: C26 H59 N4 O14

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C26 H59 N4 O14	7.798		651.4020		MFG	96.26	MFE	

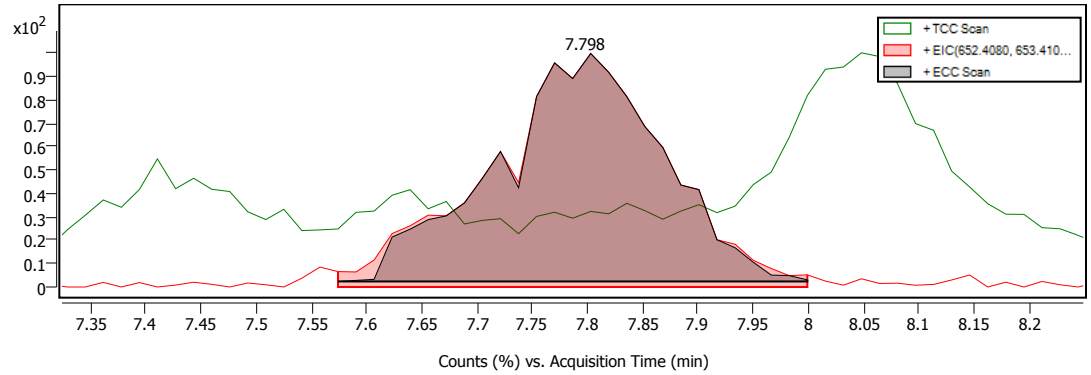
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	652.4088				5	96.26	

Compound ID Table

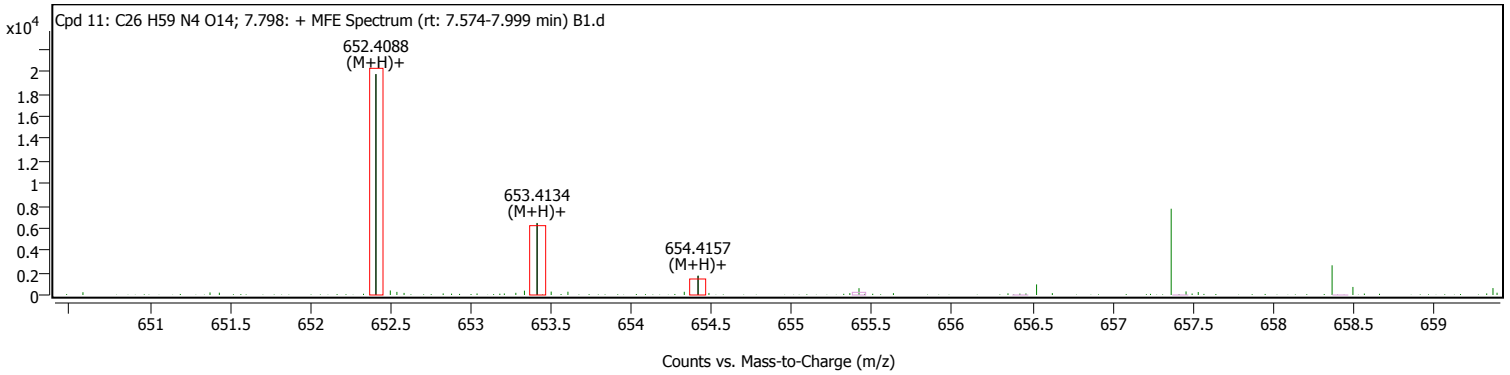
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C26 H59 N4 O14	(M+H)+	MFG	7.798		651.4020		96.26		96.26
	C25 H53 N11 O9	(M+H)+	MFG	7.798		651.4021		95.50		95.50
	C23 H51 N14 O8	(M+H)+	MFG	7.798		651.4022		93.93		93.93
	C24 H47 N18 O4	(M+H)+	MFG	7.798		651.4023		93.54		93.54
	C22 H45 N21 O3	(M+H)+	MFG	7.798		651.4023		91.30		91.30

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 12: C25 H55 N14 O9

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C25 H55 N14 O9	7.951		695.4282		MFG	96.94	MFE	

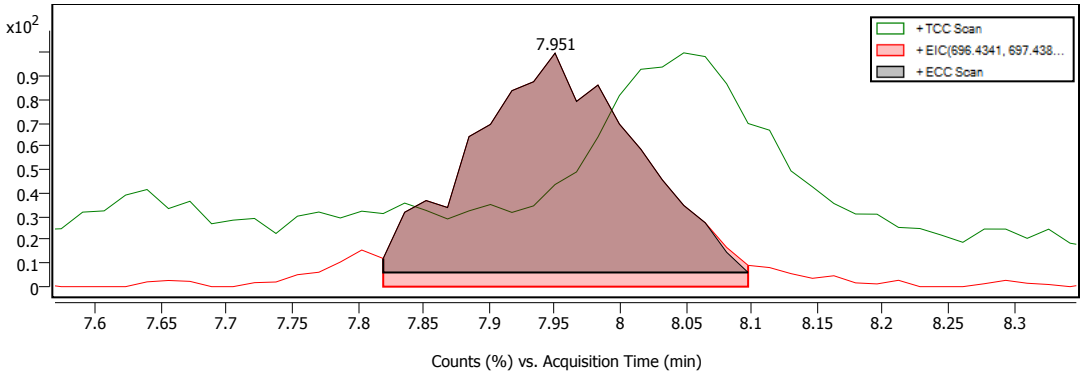
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	696.4356				5	96.94	

Compound ID Table

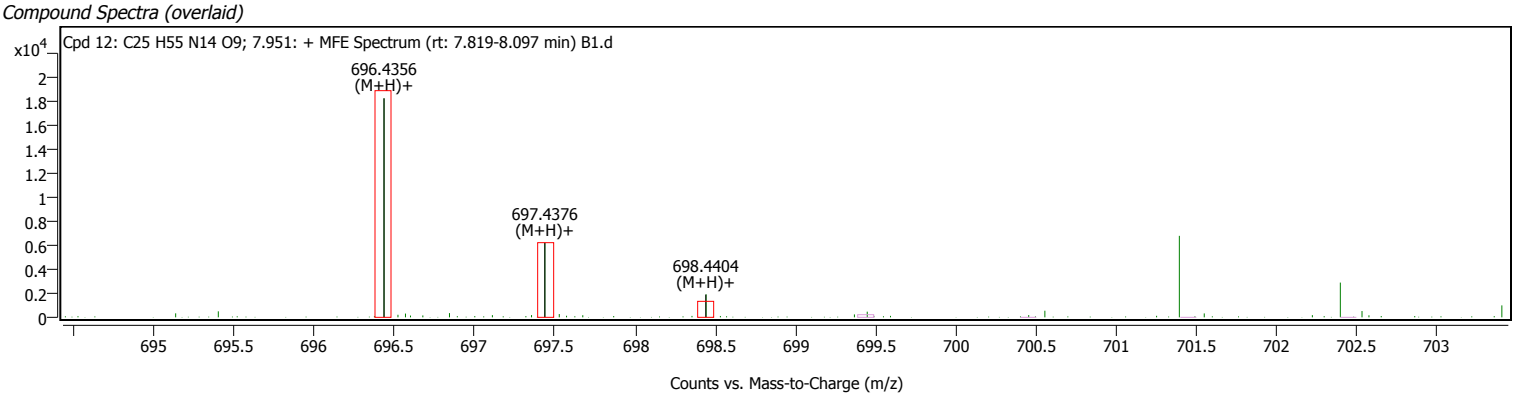
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C25 H55 N14 O9	(M+H)+	MFG	7.951		695.4282		96.94		96.94
	C27 H57 N11 O10	(M+H)+	MFG	7.951		695.4281		96.78		96.78
	C28 H63 N4 O15	(M+H)+	MFG	7.951		695.4280		96.24		96.24
	C26 H51 N18 O5	(M+H)+	MFG	7.951		695.4283		96.14		96.14
	C24 H49 N21 O4	(M+H)+	MFG	7.951		695.4284		95.62		95.62

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 13: C34 H58 N3 O10 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H58 N3 O10 S	7.960		700.3838		MFG	95.05	MFE	

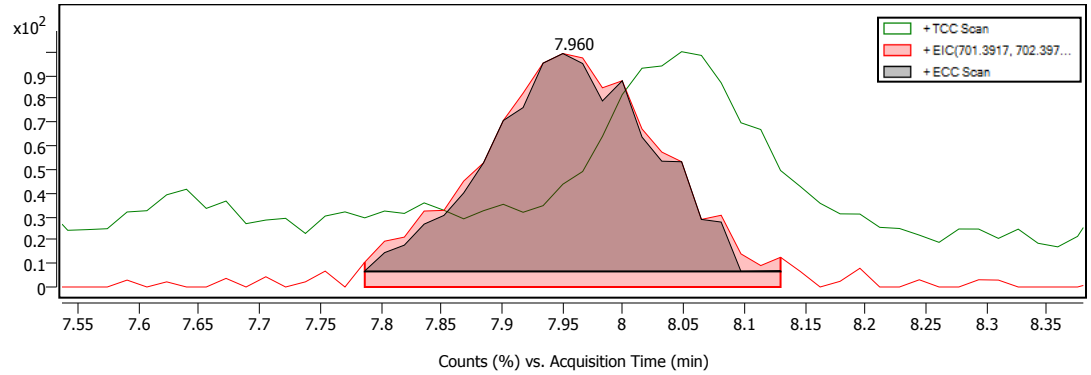
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	701.3910				5	95.05	

Compound ID Table

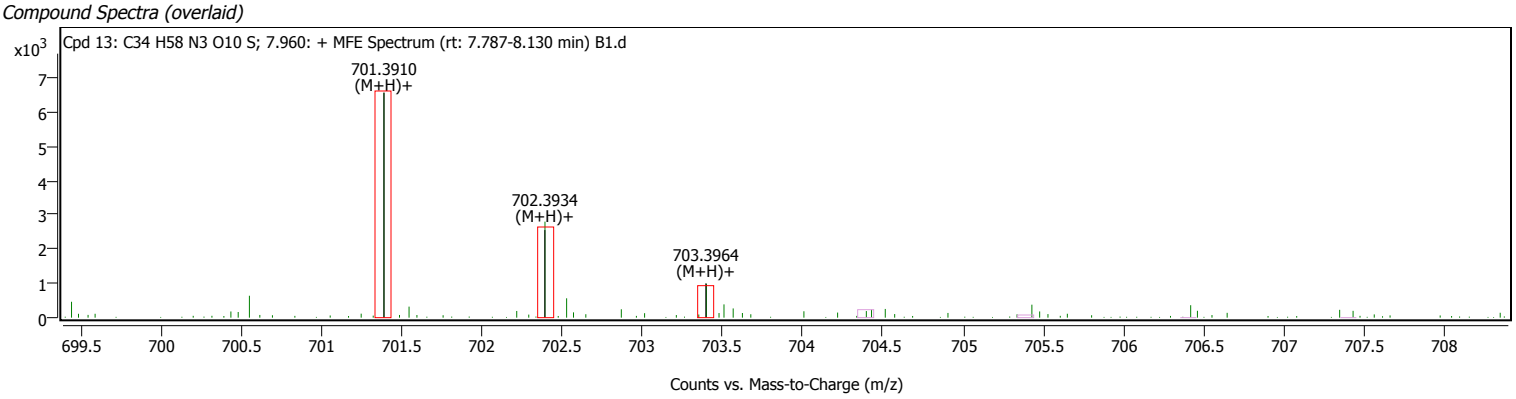
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H58 N3 O10 S	(M+H)+	MFG	7.960		700.3838		95.05		95.05
	C33 H52 N10 O5 S	(M+H)+	MFG	7.960		700.3840		94.68		94.68
	C32 H56 N6 O9 S	(M+H)+	MFG	7.960		700.3839		93.71		93.71
	C32 H46 N17 S	(M+H)+	MFG	7.960		700.3841		93.42		93.42
	C31 H50 N13 O4 S	(M+H)+	MFG	7.960		700.3841		92.72		92.72

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 14: C28 H53 N8 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H53 N8 O4	8.044		565.4184		MFG	98.56	MFE	

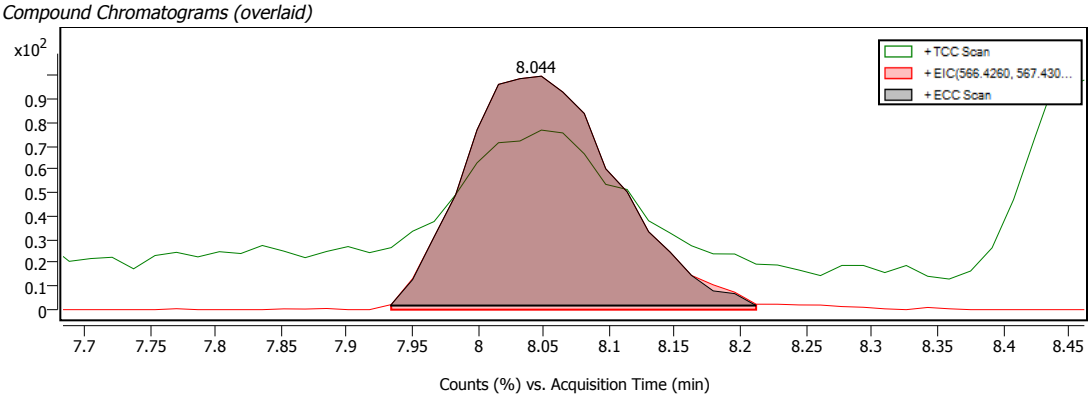
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	566.4255 588.4076				6	98.56	

Compound ID Table

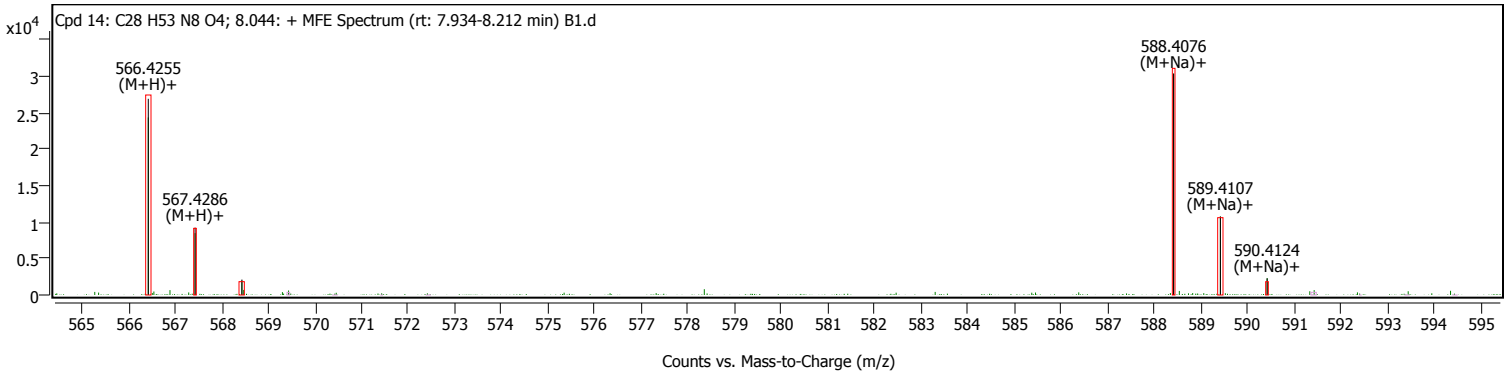
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H53 N8 O4	(M+H)+ (M+Na)+	MFG	8.044		565.4184		98.56		98.56
	C29 H59 N O9	(M+H)+ (M+Na)+	MFG	8.044		565.4182		97.72		97.72
	C26 H51 N11 O3	(M+H)+ (M+Na)+	MFG	8.044		565.4185		97.28		97.28
	C27 H57 N4 O8	(M+H)+ (M+Na)+	MFG	8.044		565.4183		97.23		97.23
	C29 H49 N12	(M+Na)+	MFG	8.044		565.4184		93.73		93.73
	C30 H55 N5 O5	(M+H)+	MFG	8.044		565.4183		92.19		92.19

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 15: C35 H63 N8 O7 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C35 H63 N8 O7 S	8.096		739.4539		MFG	96.43	MFE	

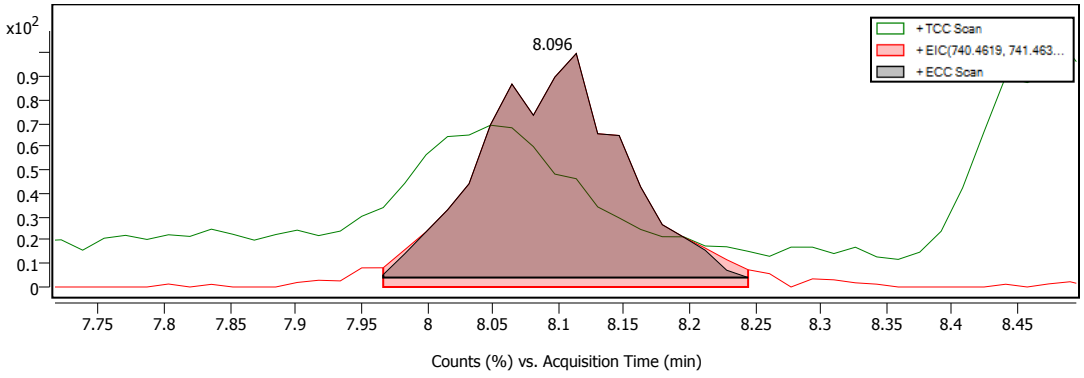
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	740.4612				9	96.43	

Compound ID Table

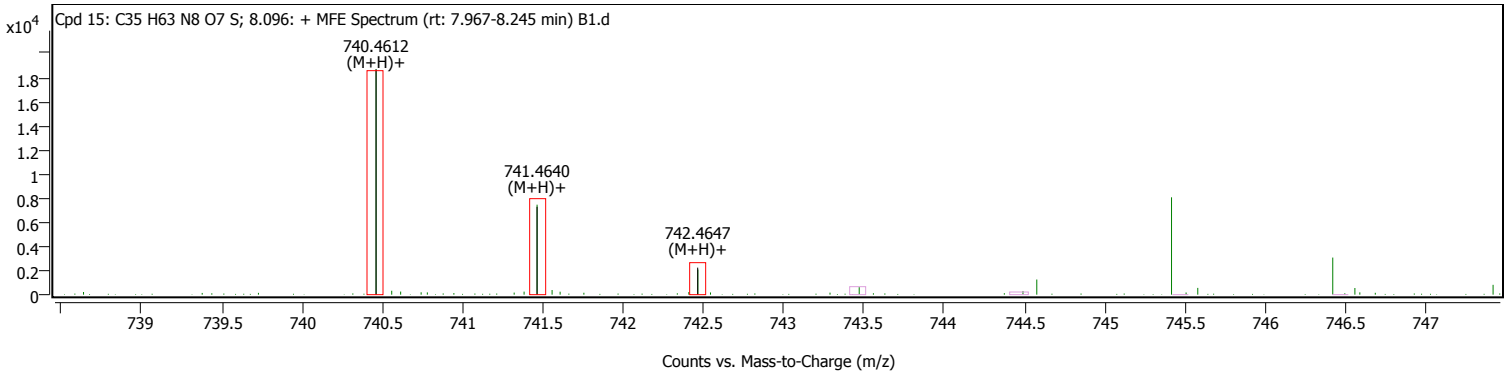
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C35 H63 N8 O7 S	(M+H)+	MFG	8.096		739.4539		96.43		96.43
	C34 H57 N15 O2 S	(M+H)+	MFG	8.096		739.4541		96.23		96.23
	C36 H69 N O12 S	(M+H)+	MFG	8.096		739.4538		95.79		95.79
	C27 H59 N14 O10	(M+H)+	MFG	8.096		739.4539		95.63		95.63
	C26 H53 N21 O5	(M+H)+	MFG	8.096		739.4540		95.57		95.57
Lycoperoside D	C39 H65 N O12	(M+H)+	DBSearch	8.096		739.4535	81037-16-3	86.18	86.18	
Yamogenin 3-O-neohesperidoside	C39 H62 O12	(M+NH4)+	DBSearch	8.096		722.4270	110996-52-6	85.91	85.91	
Ophiopogonin B	C39 H62 O12	(M+NH4)+	DBSearch	8.096		722.4270	38971-41-4	85.91	85.91	
Ophiopogonin C'	C39 H62 O12	(M+NH4)+	DBSearch	8.096		722.4270	19057-67-1	85.91	85.91	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 16: Ophiopogonin C'

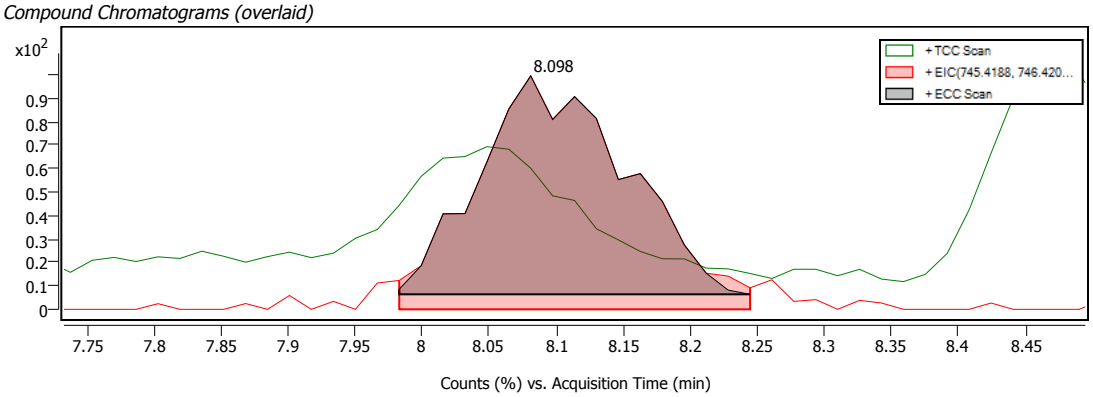
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Ophiopogonin C'	C39 H62 O12	8.098		722.4274	19057-67-1	DBSearch	56.58	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	745.4163 745.4163 745.4163		0	56.58	13		

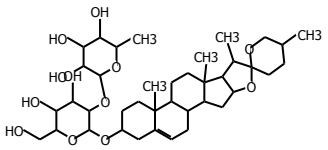
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Ophiopogonin C'	C39 H62 O12	(M+Na)+	DBSearch	8.098		722.4274	19057-67-1	56.58	56.58	
Yamogenin 3-O-neohesperidoside	C39 H62 O12	(M+Na)+	DBSearch	8.098		722.4274	110996-52-6	56.58	56.58	
Ophiopogonin B	C39 H62 O12	(M+Na)+	DBSearch	8.098		722.4274	38971-41-4	56.58	56.58	
	C30 H65 N8 O7 S3	(M+H)+	MFG	8.098		745.4138		47.62		47.62
	C29 H59 N15 O2 S3	(M+H)+	MFG	8.098		745.4138		47.62		47.62
	C41 H66 Cl N4 S3	(M+H)+	MFG	8.098		745.4138		47.62		47.62
	C35 H68 N3 O6 S3	(M+Na)+	MFG	8.098		722.4271		47.62		47.62
	C45 H61 O7 S	(M+H)+	MFG	8.098		745.4138		47.62		47.62
	C34 H62 N10 O S3	(M+Na)+	MFG	8.098		722.4271		47.62		47.62
	C44 H55 N7 O2 S	(M+H)+	MFG	8.098		745.4138		47.62		47.62
	C39 H71 Cl3 N O2 S	(M+Na)+	MFG	8.098		722.4271		47.62		47.62
	C49 H58 N2 O S	(M+Na)+	MFG	8.098		722.4271		47.61		47.61
	C31 H67 Cl3 N7 O5	(M+Na)+	MFG	8.098		722.4271		47.60		47.60

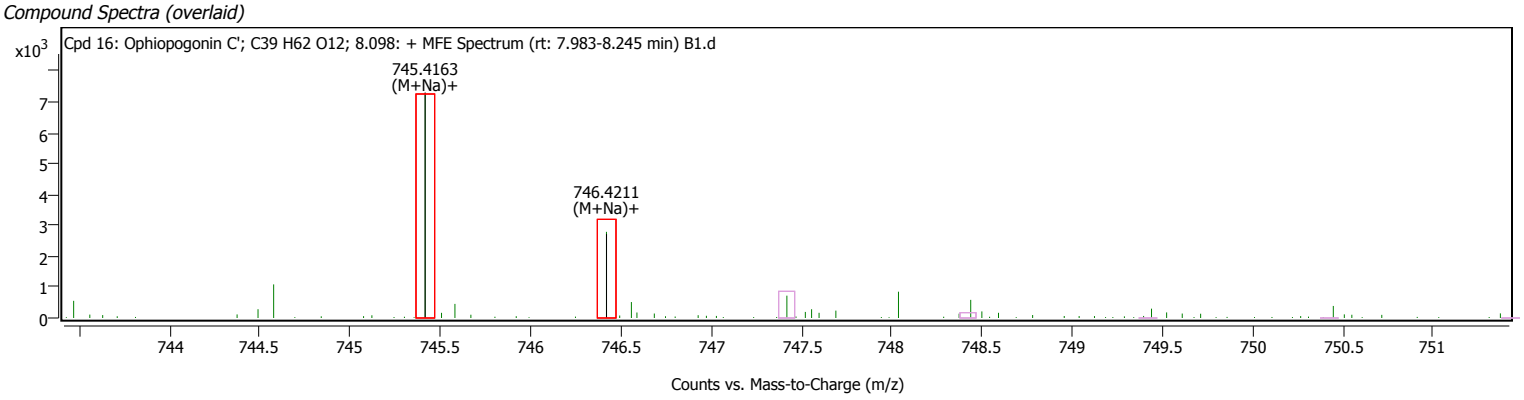
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 17: Pitheduloside A

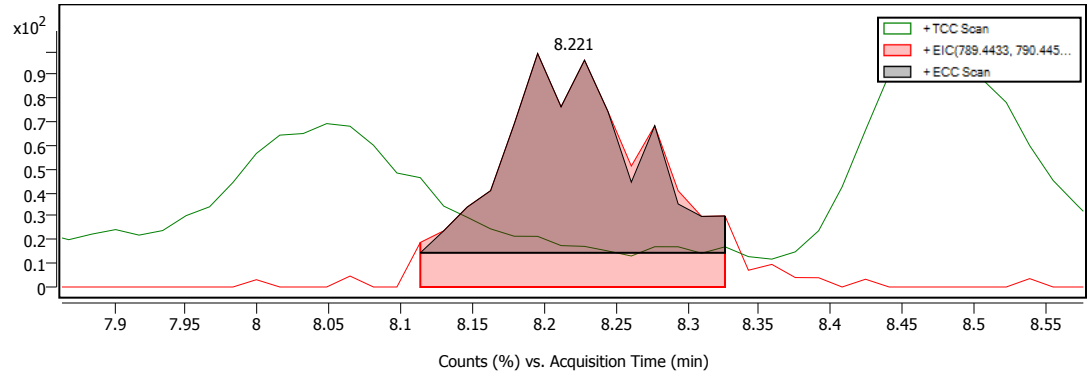
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Pitheduloside A	C41 H66 O13	8.221		766.4540	78285-89-9	DBSearch	67.68	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	789.4431 789.4431 789.4431		0	67.68	18		

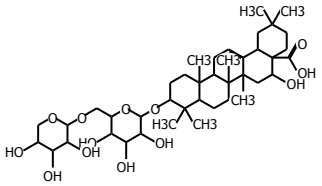
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Pitheduloside A	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540	78285-89-9	67.68	67.68	
28-Glucosylsiaresinolate 3-arabinoside	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540	356785-71-2	67.68	67.68	
Soyasaponin IV	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540	108906-97-4	67.68	67.68	
Akeboside Std	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540		67.68	67.68	
Tautomycin	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540	109946-35-2	67.68	67.68	
Cauloside C	C41 H66 O13	(M+Na)+	DBSearch	8.221		766.4540	20853-58-1	67.68	67.68	
	C37 H49 N20 O	(M+H)+	MFG	8.221		789.4397		66.92		66.92
	C38 H55 N13 O6	(M+H)+	MFG	8.221		789.4396		66.35		66.35
PA(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H67 O8 P	(M+Na)+	DBSearch	8.221		766.4540		65.84	65.84	
PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H67 O8 P	(M+Na)+	DBSearch	8.221		766.4540		65.84	65.84	
	C39 H61 N6 O11	(M+H)+	MFG	8.221		789.4395		65.70		65.70
	C35 H47 N23	(M+H)+	MFG	8.221		789.4398		65.62		65.62
	C36 H53 N16 O5	(M+H)+	MFG	8.221		789.4397		65.22		65.22
	C45 H68 N O5 S2	(M+Na)+	MFG	8.221		766.4539		47.62		47.62
	C29 H66 N16 S4	(M+Na)+	MFG	8.221		766.4539		47.62		47.62
	C44 H62 N8 S2	(M+Na)+	MFG	8.221		766.4539		47.62		47.62
	C59 H58	(M+Na)+	MFG	8.221		766.4539		47.62		47.62
	C37 H64 Cl2 N10 O3	(M+Na)+	MFG	8.221		766.4539		47.61		47.61

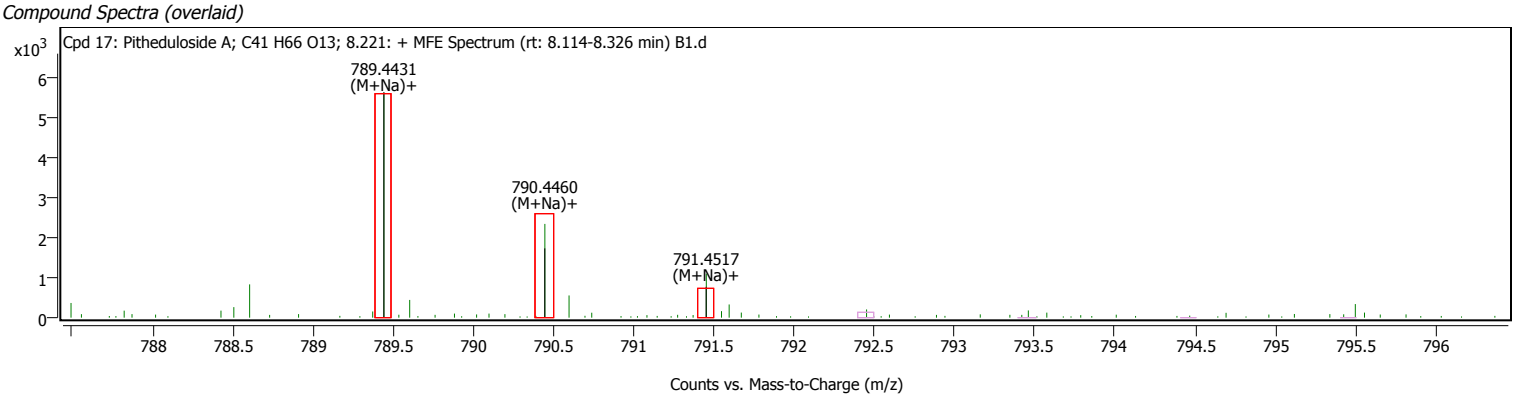
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 18: PE(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PE(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C43 H72 N O8 P	8.224		761.4987		DBSearch	93.83	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	784.4885 784.4885 784.4885 784.4885		0	93.83	31		

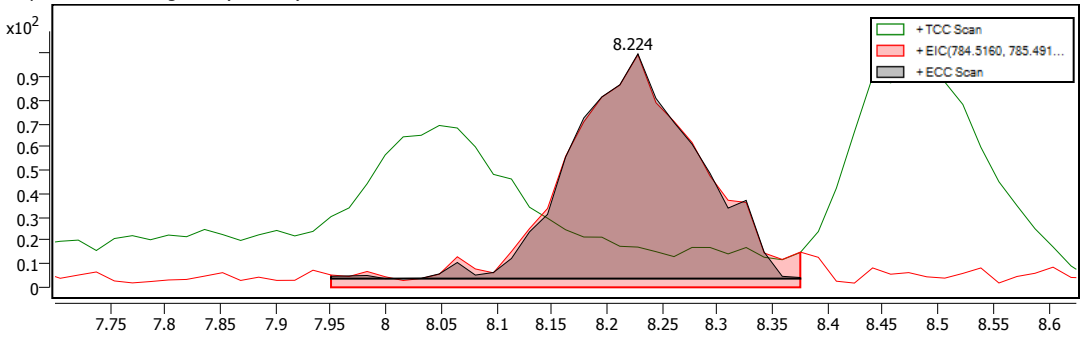
Compound Discovery Report

Agilent | Trusted Answers

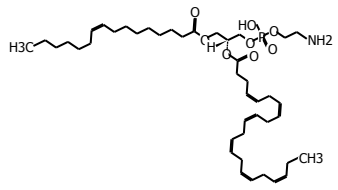
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PE(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:3(6Z,9Z,12Z)/20:4(8Z,11Z,14Z,17Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(20:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:4(6Z,9Z,12Z,15Z)/20:3(8Z,11Z,14Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:3(9Z,12Z,15Z)/20:4(8Z,11Z,14Z,17Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:3(9Z,12Z,15Z)/20:4(5Z,8Z,11Z,14Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:3(6Z,9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	C43 H72 N O8 P	(M+Na)+	DBSearch	8.224		761.4987		93.83	93.83	
PE(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H70 N O8 P	(M+H)+	DBSearch	8.224		783.4806		83.22	83.22	
PE(20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H70 N O8 P	(M+H)+	DBSearch	8.224		783.4806		83.22	83.22	
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C45 H70 N O8 P	(M+H)+	DBSearch	8.224		783.4806		83.22	83.22	
PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H67 O8 P	(M+NH4)+	DBSearch	8.224		766.4541		82.92	82.92	
PA(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H67 O8 P	(M+NH4)+	DBSearch	8.224		766.4541		82.92	82.92	
	C37 H66 N7 O11	(M+H)+	MFG	8.224		784.4829		68.01		68.01
	C36 H60 N14 O6	(M+H)+	MFG	8.224		784.4830		68.00		68.00
	C38 H62 N11 O7	(M+H)+	MFG	8.224		784.4830		67.78		67.78
	C37 H56 N18 O2	(M+H)+	MFG	8.224		784.4831		67.75		67.75
	C38 H72 O16	(M+H)+	MFG	8.224		784.4828		67.69		67.69
	C31 H67 N15 O3 S2	(M+Na)+	MFG	8.224		761.4993		47.62		47.62
	C36 H76 Cl3 N6 O4	(M+Na)+	MFG	8.224		761.4993		47.62		47.62
	C43 H74 Cl N4 O S2	(M+Na)+	MFG	8.224		761.4993		47.61		47.61
	C47 H69 O8	(M+Na)+	MFG	8.224		761.4993		47.61		47.61
	C46 H63 N7 O3	(M+Na)+	MFG	8.224		761.4993		47.61		47.61

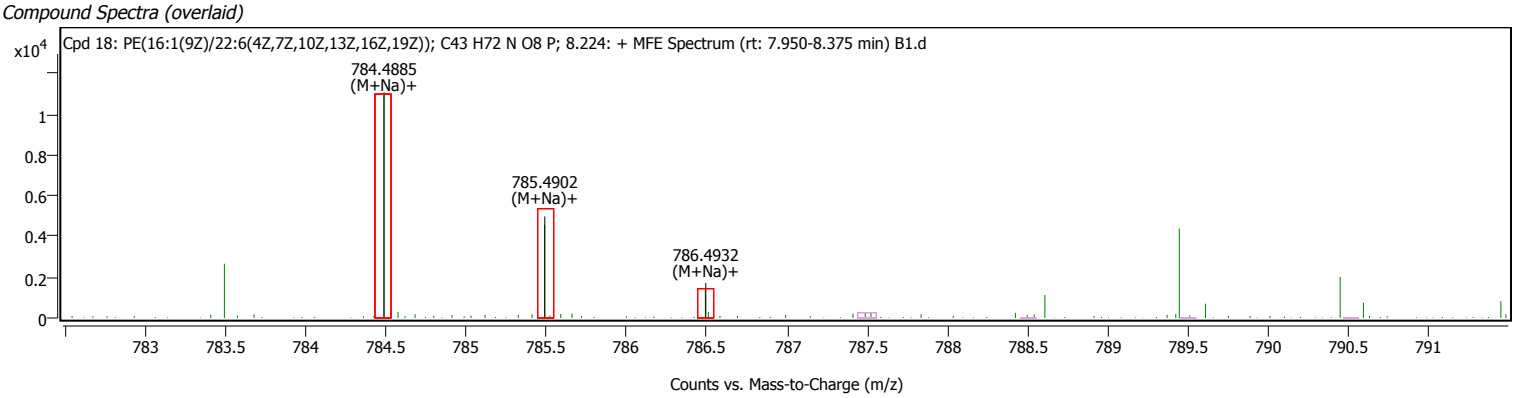
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 19: C38 H58 N17 O3 S

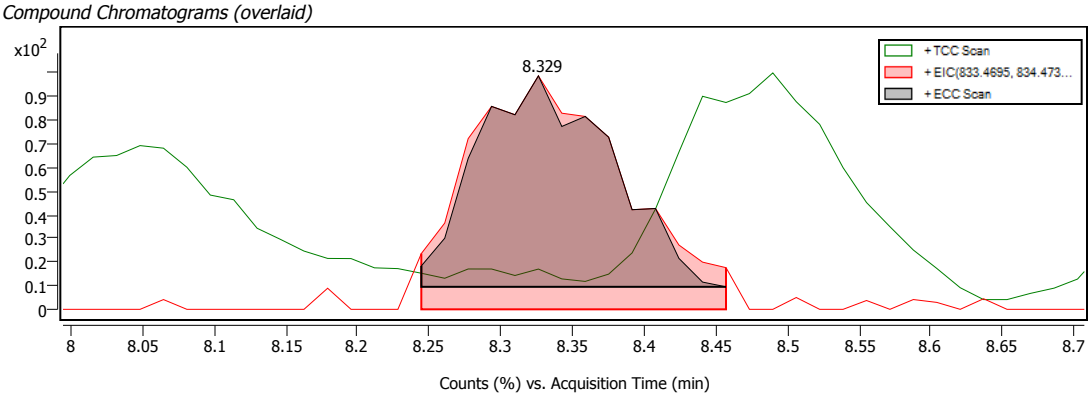
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C38 H58 N17 O3 S	8.329		832.4628		MFG	95.12	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	833.4699				5	95.12	

Compound ID Table

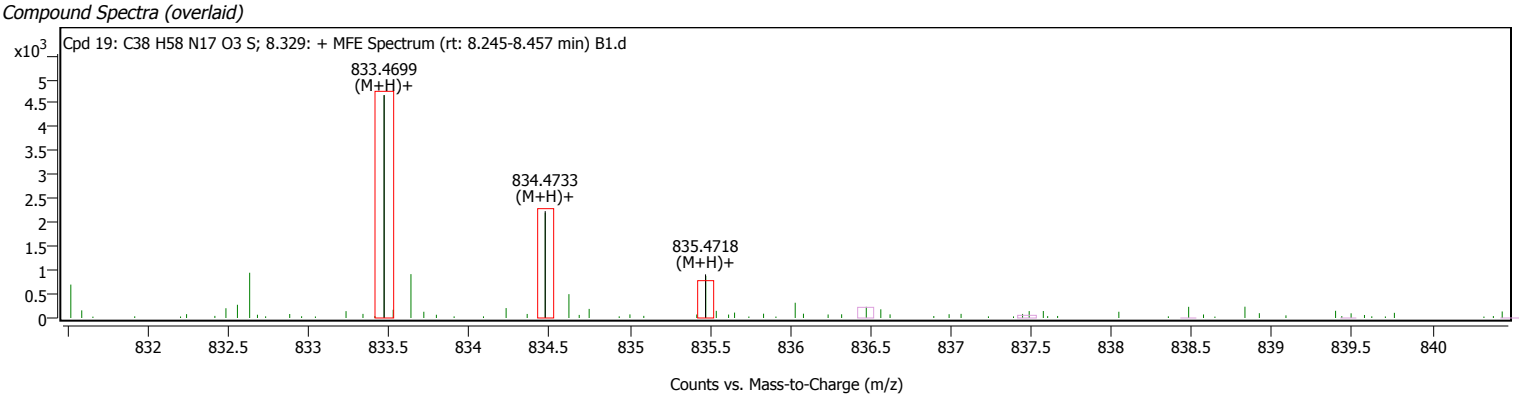
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C38 H58 N17 O3 S	(M+H)+	MFG	8.329		832.4628		95.12		95.12
	C39 H64 N10 O8 S	(M+H)+	MFG	8.329		832.4627		94.98		94.98
	C40 H70 N3 O13 S	(M+H)+	MFG	8.329		832.4625		94.27		94.27
	C37 H62 N13 O7 S	(M+H)+	MFG	8.329		832.4627		93.40		93.40
	C38 H68 N6 O12 S	(M+H)+	MFG	8.329		832.4626		93.15		93.15

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 20: C31 H67 N14 O12

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H67 N14 O12	8.333		827.5064		MFG	95.98	MFE	

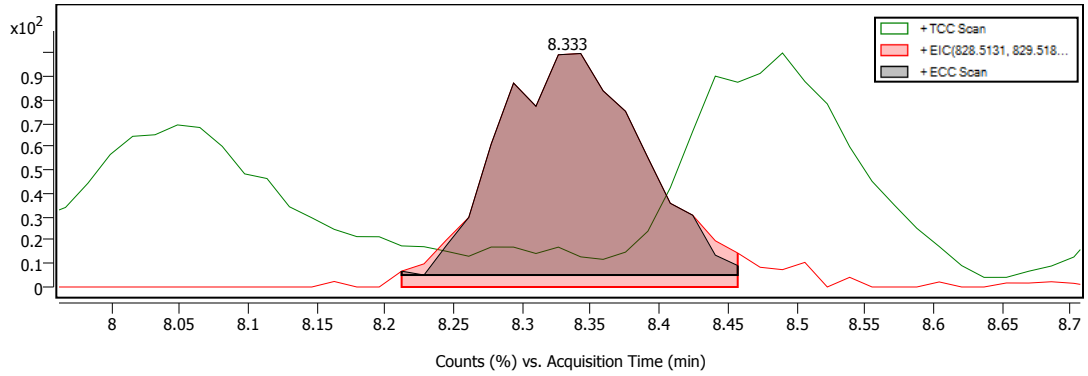
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	828.5142				7	95.98	

Compound ID Table

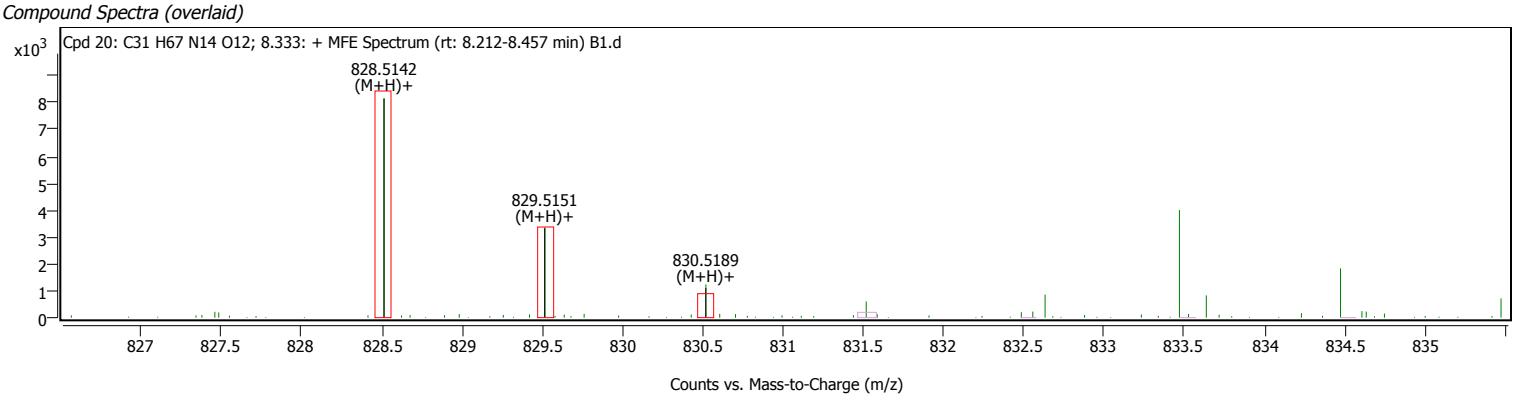
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H67 N14 O12	(M+H)+	MFG	8.333		827.5064		95.98		95.98
	C30 H61 N21 O7	(M+H)+	MFG	8.333		827.5066		95.71		95.71
	C29 H55 N28 O2	(M+H)+	MFG	8.333		827.5067		94.56		94.56
	C32 H63 N18 O8	(M+H)+	MFG	8.333		827.5065		94.55		94.55
	C33 H69 N11 O13	(M+H)+	MFG	8.333		827.5063		94.37		94.37
Mycobactin S	C44 H69 N5 O10	(M+H)+	DBSearch	8.333		827.5062	26769-11-9	87.54	87.54	
Goyaglycoside g	C43 H70 O14	(M+NH4)+	DBSearch	8.333		810.4796	333333-14-5	83.46	83.46	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 21: C31 H52 N30 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H52 N30 O2	8.433		876.4882		MFG	71.02	MFE	

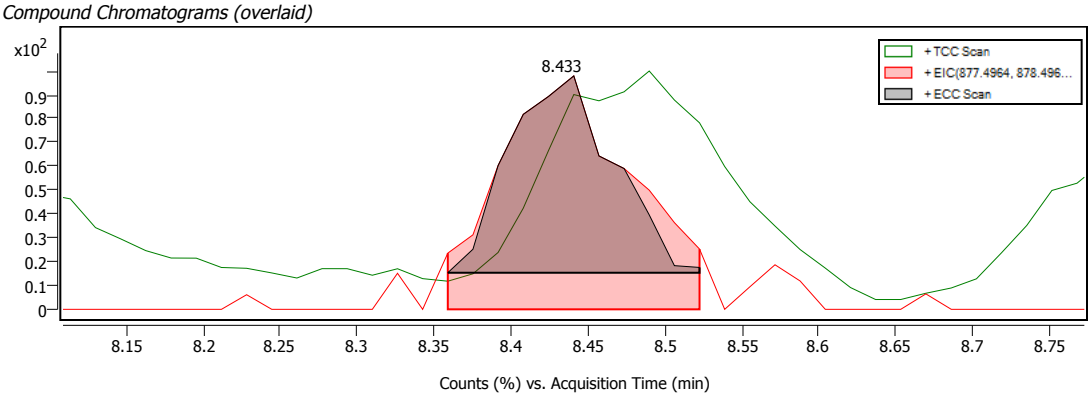
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	877.4957				8	71.02	

Compound ID Table

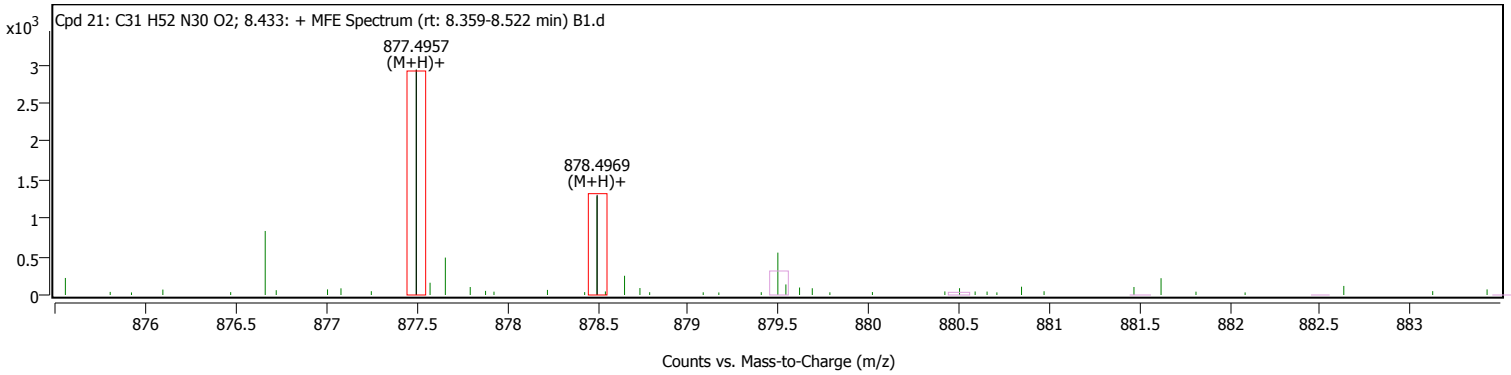
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H52 N30 O2	(M+H)+	MFG	8.433		876.4882		71.02		71.02
	C30 H56 N26 O6	(M+H)+	MFG	8.433		876.4882		70.18		70.18
	C32 H58 N23 O7	(M+H)+	MFG	8.433		876.4881		69.12		69.12
	C31 H62 N19 O11	(M+H)+	MFG	8.433		876.4881		68.30		68.30
	C33 H64 N16 O12	(M+H)+	MFG	8.433		876.4880		67.06		67.06
Pectenotoxin 2 secoacid	C47 H72 O15	(M+H)+	DBSearch	8.433		876.4878	212502-87-9	62.48	62.48	
Avermectin B2b	C47 H72 O15	(M+H)+	DBSearch	8.433		876.4878		62.48	62.48	
(3b,21b)-12-Oleanene-3,21,28-triol 28-[arabinosyl-(1->3)-arabinosyl-(1->3)-arabinoside]	C45 H74 O15	(M+Na)+	DBSearch	8.433		854.5058	243468-98-6	54.96	54.96	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



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

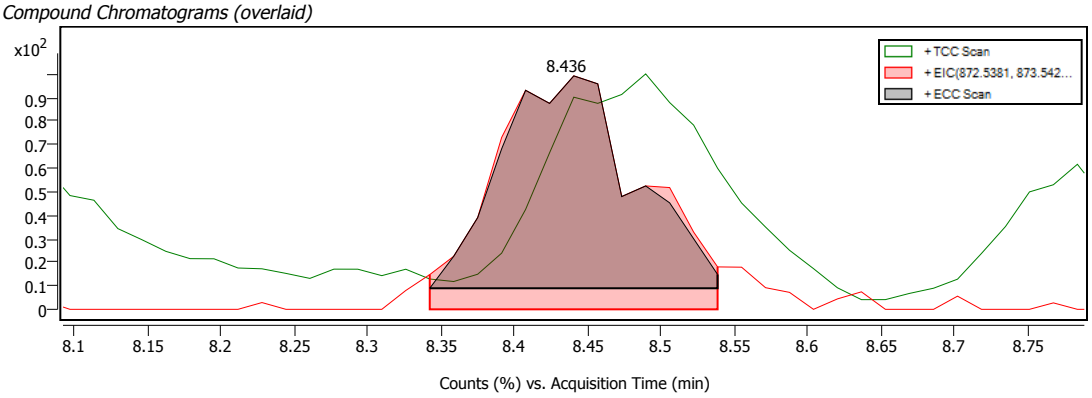
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PS(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H80 N O10 P	8.436		849.5505		DBSearch	77.23	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	872.5407 872.5407 872.5407		0	77.23	13		

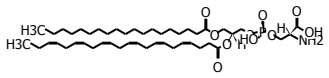
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PS(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H80 N O10 P	(M+Na)+	DBSearch	8.436		849.5505		77.23	77.23	
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/19:0)	C47 H80 N O10 P	(M+Na)+	DBSearch	8.436		849.5505		77.23	77.23	
(3b,21b)-12-Oleanene-3,21,28-triol 28-[arabinosyl-(1->3)-arabinosyl-(1->3)-arabinoside]	C45 H74 O15	(M+NH4)+	DBSearch	8.436		854.5059	243468-98-6	71.32	71.32	
	C39 H62 N21 O3	(M+H)+	MFG	8.436		872.5348		64.88		64.88
	C40 H68 N14 O8	(M+H)+	MFG	8.436		872.5347		64.09		64.09
	C41 H64 N18 O4	(M+H)+	MFG	8.436		872.5347		63.64		63.64
	C41 H74 N7 O13	(M+H)+	MFG	8.436		872.5345		63.30		63.30
	C54 H66 N9 O2	(M+H)+	MFG	8.436		872.5346		62.59		62.59
	C43 H87 N5 O S5	(M+Na)+	MFG	8.436		849.5514		47.62		47.62
	C38 H72 Cl N17 O S	(M+Na)+	MFG	8.436		849.5514		47.62		47.62
	C39 H78 Cl N10 O6 S	(M+Na)+	MFG	8.436		849.5514		47.62		47.62
	C40 H84 Cl N3 O11 S	(M+Na)+	MFG	8.436		849.5514		47.61		47.61
	C39 H86 Cl3 N9 S2	(M+Na)+	MFG	8.436		849.5514		47.60		47.60

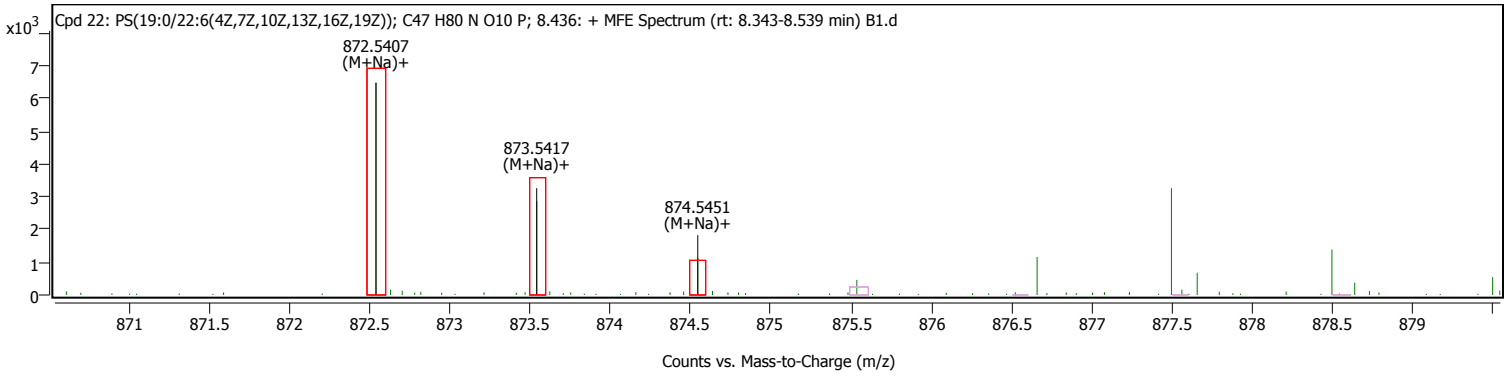
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 23: C47 H71 N4 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C47 H71 N4 O2	8.481		723.5581		MFG	61.59	MFE	

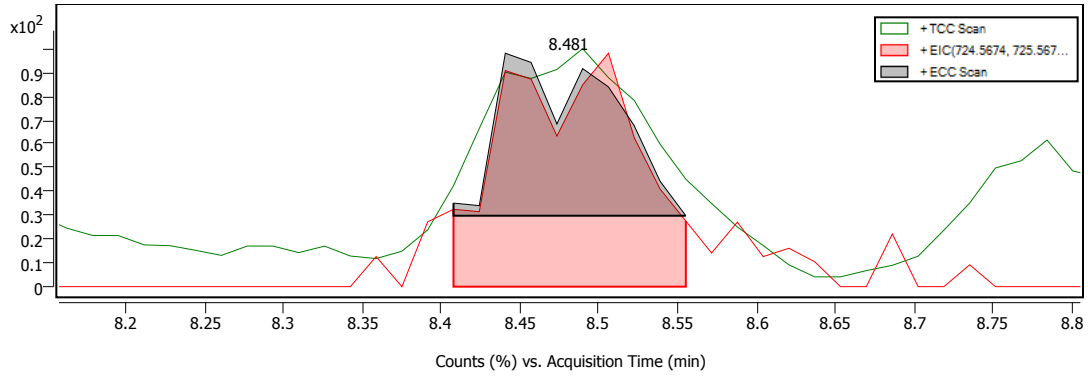
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	724.5660				5	61.59	

Compound ID Table

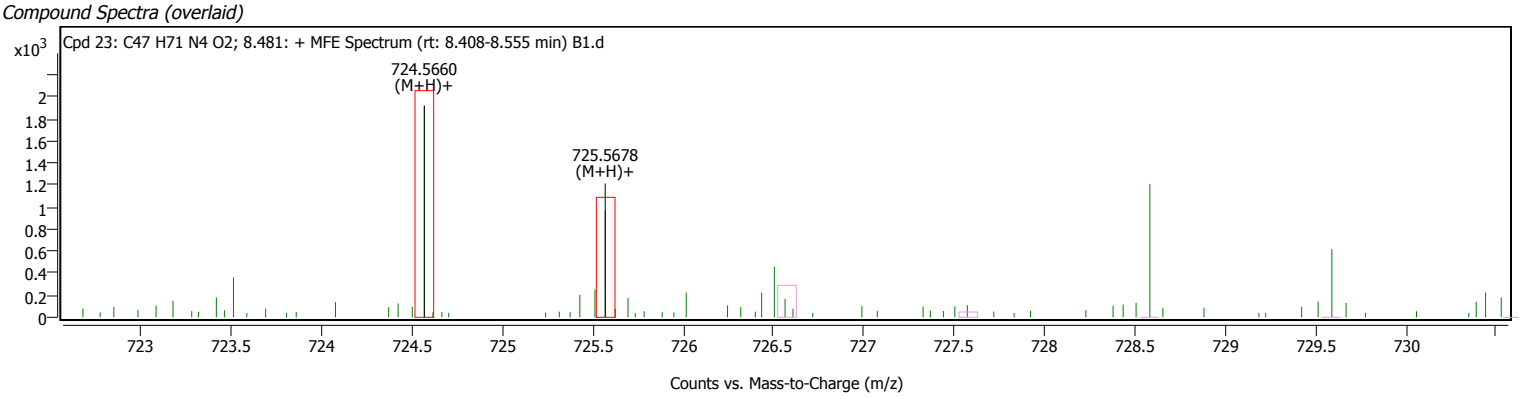
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C47 H71 N4 O2	(M+H)+	MFG	8.481		723.5581		61.59		61.59
	C49 H73 N O3	(M+H)+	MFG	8.481		723.5581		60.38		60.38
	C34 H69 N13 O4	(M+H)+	MFG	8.481		723.5584		59.05		59.05
	C45 H69 N7 O	(M+H)+	MFG	8.481		723.5582		57.93		57.93
	C46 H75 O6	(M+H)+	MFG	8.481		723.5581		57.32		57.32

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 24: C32 H62 N12 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H62 N12 O4	8.482		678.5023		MFG	98.50	MFE	

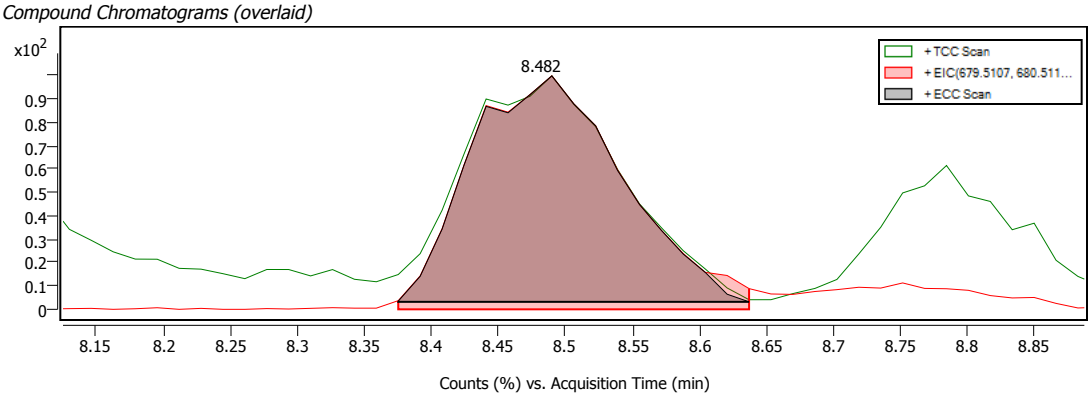
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	679.5091 701.4916				6	98.50	

Compound ID Table

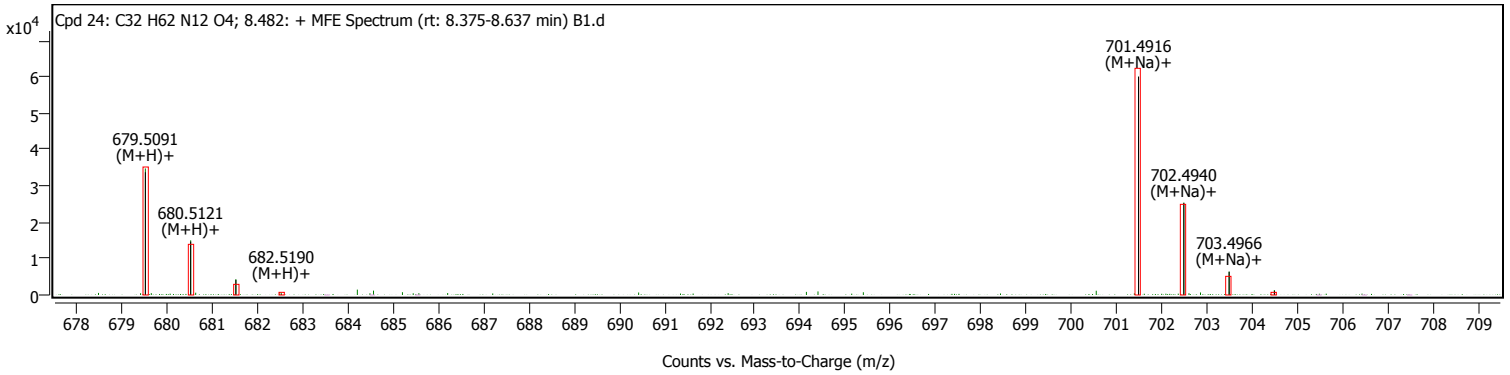
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H62 N12 O4	(M+H)+ (M+Na)+	MFG	8.482		678.5023		98.50		98.50
	C33 H58 N16	(M+H)+ (M+Na)+	MFG	8.482		678.5024		98.46		98.46
	C34 H64 N9 O5	(M+H)+ (M+Na)+	MFG	8.482		678.5022		98.43		98.43
	C33 H68 N5 O9	(M+H)+ (M+Na)+	MFG	8.482		678.5021		97.99		97.99
	C35 H70 N2 O10	(M+Na)+	MFG	8.482		678.5021		97.34		97.34
	C40 H66 N6 O S	(M+H)+	MFG	8.482		678.5019		96.78		96.78

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 25: C52 H101 N3 S3

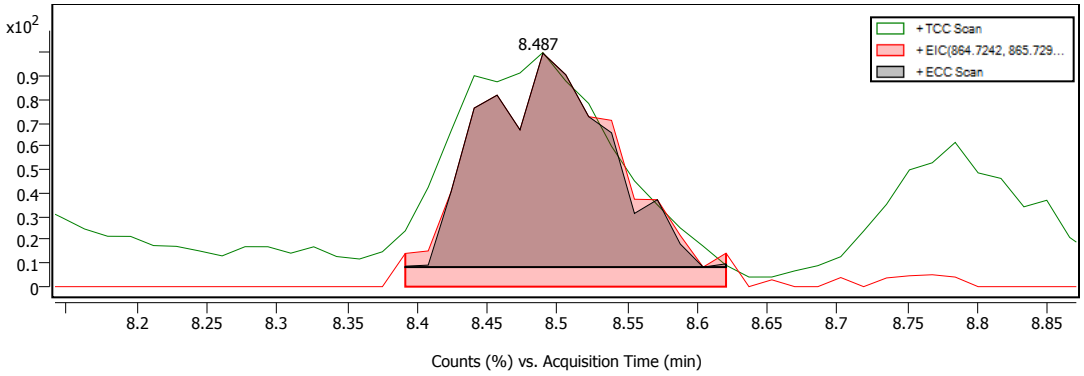
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C52 H101 N3 S3	8.487		863.7152		MFG	85.25	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	864.7219				5	85.25	

Compound ID Table

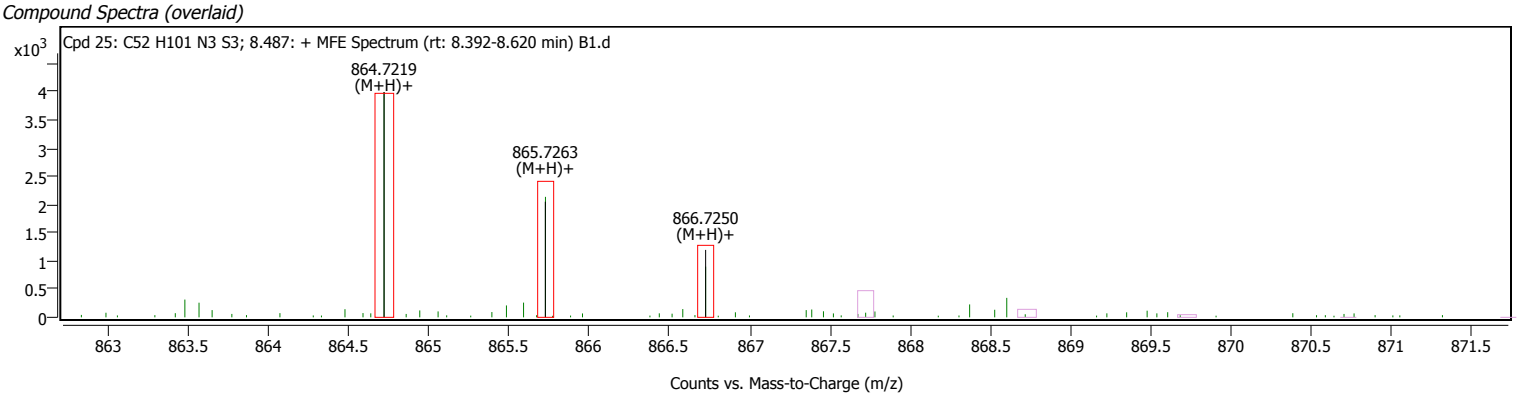
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C52 H101 N3 S3	(M+H)+	MFG	8.487		863.7152		85.25		85.25
	C51 H97 N3 O5 S	(M+H)+	MFG	8.487		863.7148		84.32		84.32
	C46 H99 N6 O4 S2	(M+H)+	MFG	8.487		863.7151		84.10		84.10
	C57 H99 O S2	(M+H)+	MFG	8.487		863.7149		83.80		83.80
	C50 H91 N10 S	(M+H)+	MFG	8.487		863.7149		83.20		83.20

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 26: Hebevinoside XIII

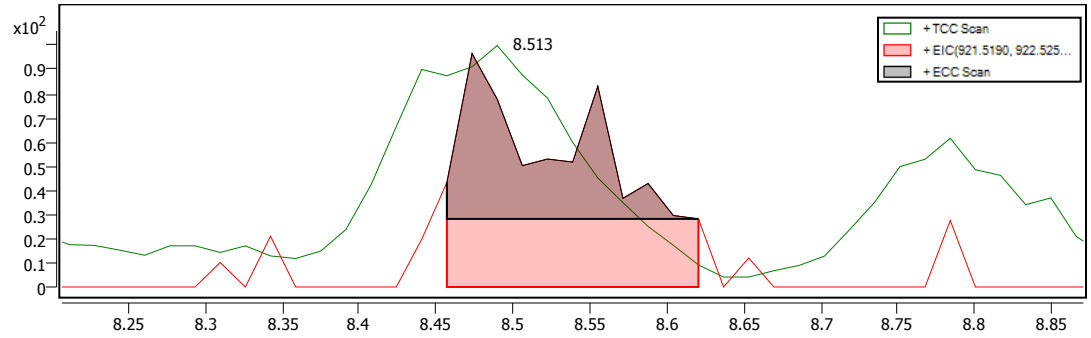
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Hebevinoside XIII	C49 H76 O16	8.513		920.5123	138995-52-5	DBSearch	57.33	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	921.5205 921.5205 921.5205		0	57.33	3		

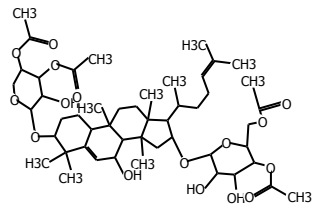
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Hebevinoside XIII	C49 H76 O16	(M+H)+	DBSearch	8.513		920.5123	138995-52-5	57.33		57.33
Melilotoside C	C47 H78 O16	(M+Na)+	DBSearch	8.513		898.5304	170678-03-2	56.46		56.46
Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	C47 H78 O16	(M+Na)+	DBSearch	8.513		898.5304		56.46		56.46

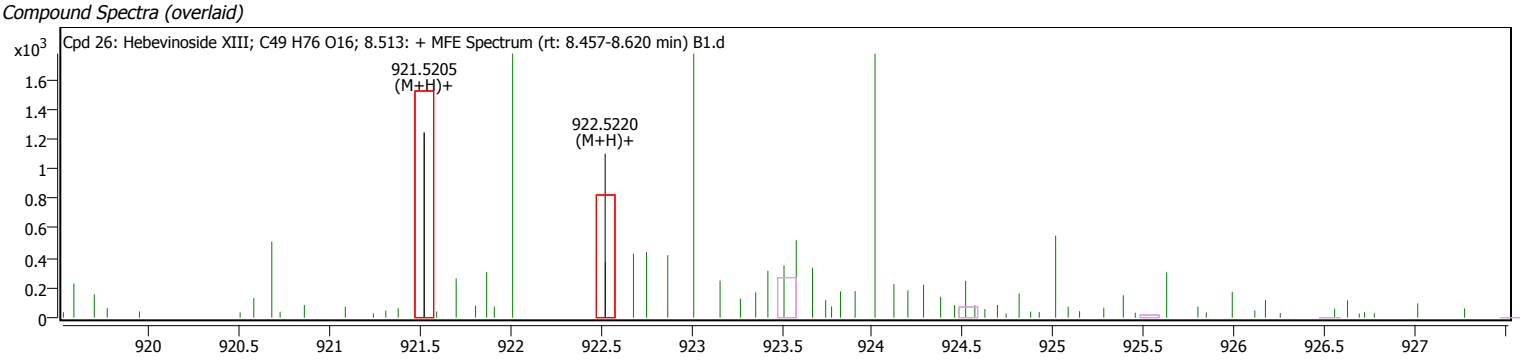
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 27: Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]

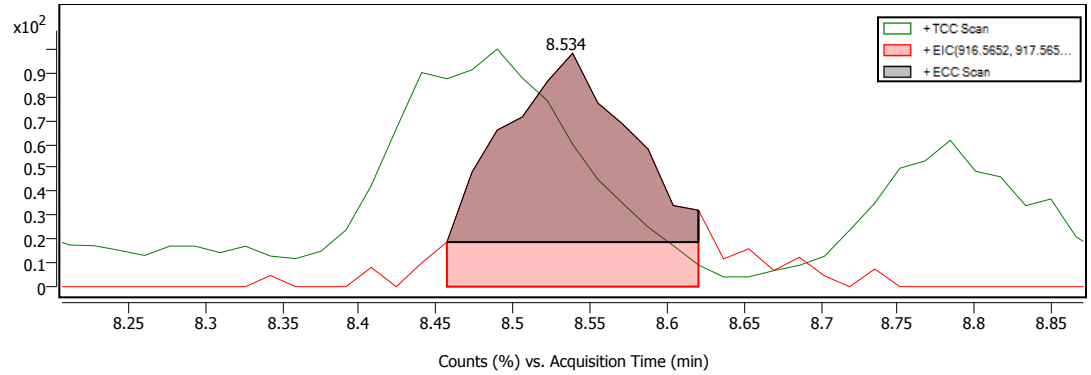
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	C47 H78 O16	8.534		898.5303		DBSearch	62.47	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	916.5640 916.5640 916.5640		0	62.47	12		

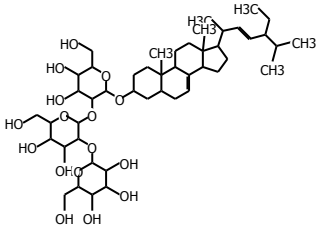
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	C47 H78 O16	(M+NH4)+	DBSearch	8.534		898.5303		62.47	62.47	
Melilotoside C	C47 H78 O16	(M+NH4)+	DBSearch	8.534		898.5303	170678-03-2	62.47	62.47	
	C47 H76 Cl2 N10 O S	(M+NH4)+	MFG	8.534		898.5301		47.62		47.62
	C48 H82 Cl2 N3 O6 S	(M+NH4)+	MFG	8.534		898.5301		47.62		47.62
	C35 H69 Cl N21 O3 S	(M+NH4)+	MFG	8.534		898.5301		47.62		47.62
	C36 H75 Cl N14 O8 S	(M+NH4)+	MFG	8.534		898.5301		47.62		47.62
	C37 H81 Cl N7 O13 S	(M+NH4)+	MFG	8.534		898.5301		47.62		47.62
	C39 H83 Cl N11 O7 S2	(M+H)+	MFG	8.534		916.5607		47.62		47.62
	C38 H77 Cl N18 O2 S2	(M+H)+	MFG	8.534		916.5607		47.62		47.62
	C44 H84 O19	(M+H)+	MFG	8.534		916.5607		47.62		47.62
	C43 H78 N7 O14	(M+H)+	MFG	8.534		916.5607		47.62		47.62
	C51 H90 Cl2 O5 S2	(M+H)+	MFG	8.534		916.5607		47.62		47.62

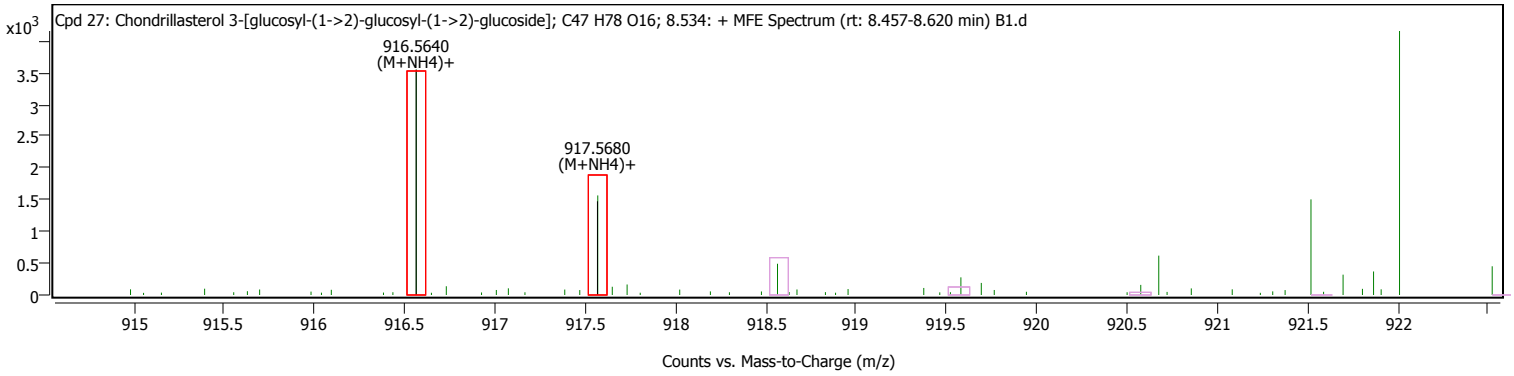
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 28: C35 H67 N28 O5

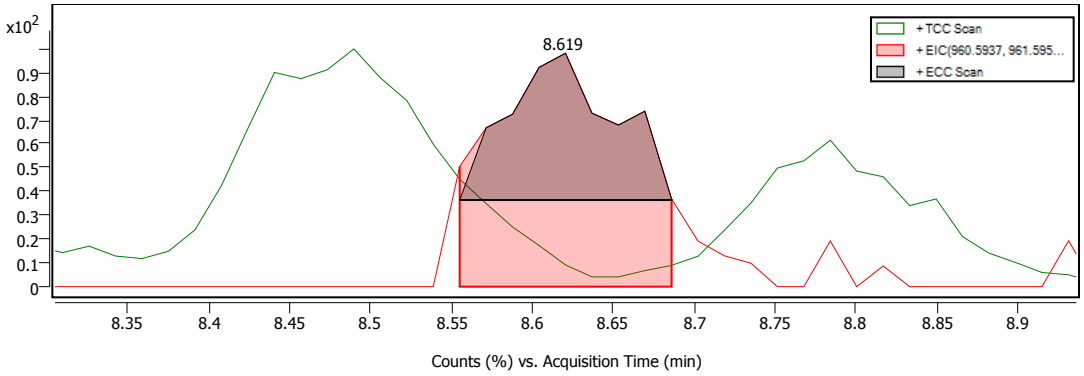
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C35 H67 N28 O5	8.619		959.5851		MFG	63.80	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	960.5921				5	63.80	

Compound ID Table

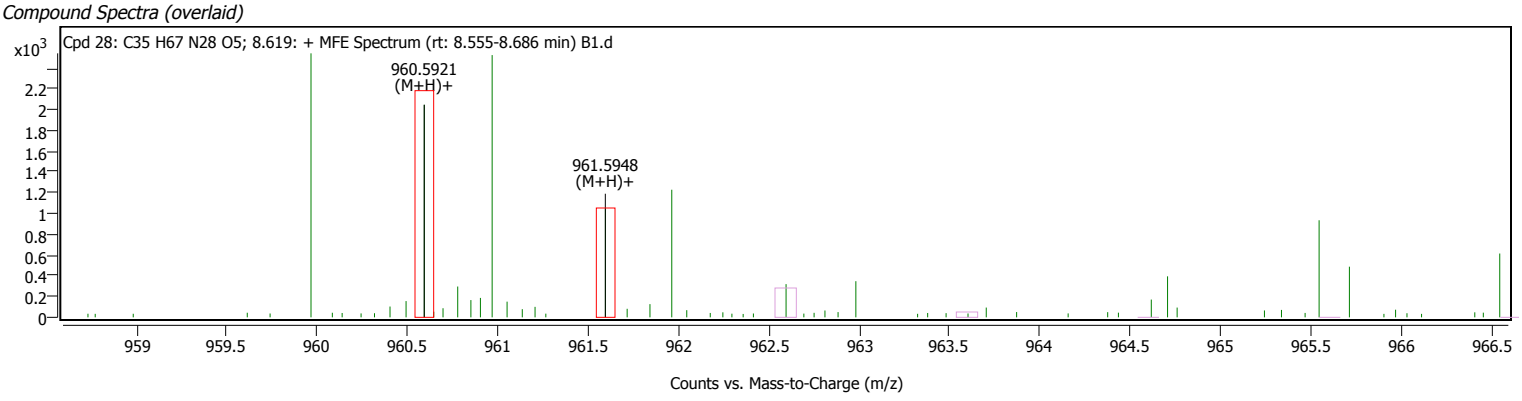
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C35 H67 N28 O5	(M+H)+	MFG	8.619		959.5851		63.80		63.80
	C36 H73 N21 O10	(M+H)+	MFG	8.619		959.5849		62.99		62.99
	C50 H71 N16 O4	(M+H)+	MFG	8.619		959.5848		62.74		62.74
	C37 H69 N25 O6	(M+H)+	MFG	8.619		959.5850		62.35		62.35
	C51 H77 N9 O9	(M+H)+	MFG	8.619		959.5847		62.32		62.32

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 29: C47 H66 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C47 H66 O3	8.750		678.5021		MFG	95.32	MFE	

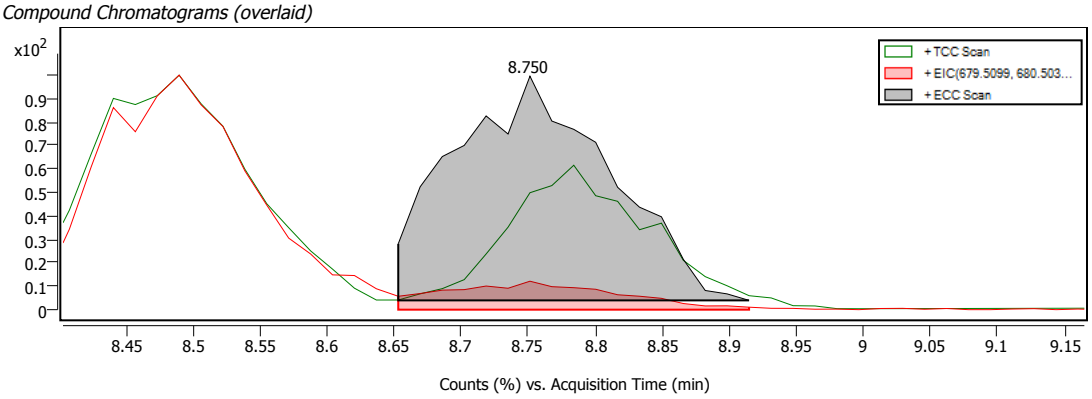
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	679.5091 701.4910				8	95.32	

Compound ID Table

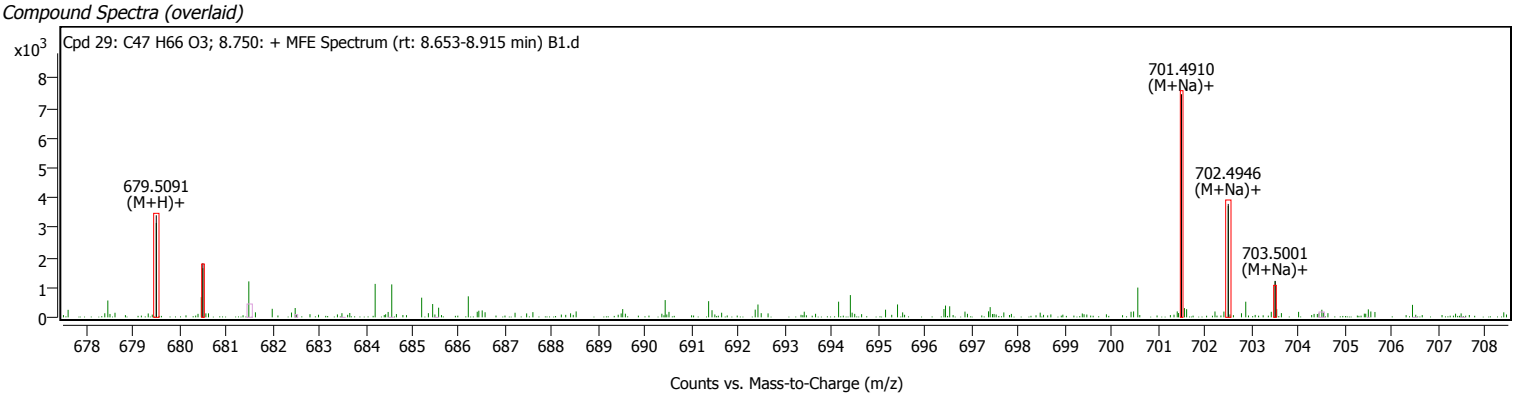
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C47 H66 O3	(M+H)+ (M+Na)+	MFG	8.750		678.5021		95.32		95.32
	C50 H64 N	(M+Na)+	MFG	8.750		678.5021		91.62		91.62
	C42 H68 N3 O2 S	(M+Na)+	MFG	8.750		678.5024		89.45		89.45
	C45 H64 N3 O2	(M+H)+ (M+Na)+	MFG	8.750		678.5021		89.18		89.18
	C40 H66 N6 O S	(M+Na)+	MFG	8.750		678.5025		88.93		88.93
	C30 H60 N15 O3	(M+H)+	MFG	8.750		678.5007		59.97		59.97
	C32 H62 N12 O4	(M+H)+	MFG	8.750		678.5007		58.62		58.62
	C31 H66 N8 O8	(M+H)+	MFG	8.750		678.5006		57.98		57.98

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 30: C40 H O25 S3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C40 H O25 S3	8.777		976.7975		MFG	78.95	MFE	

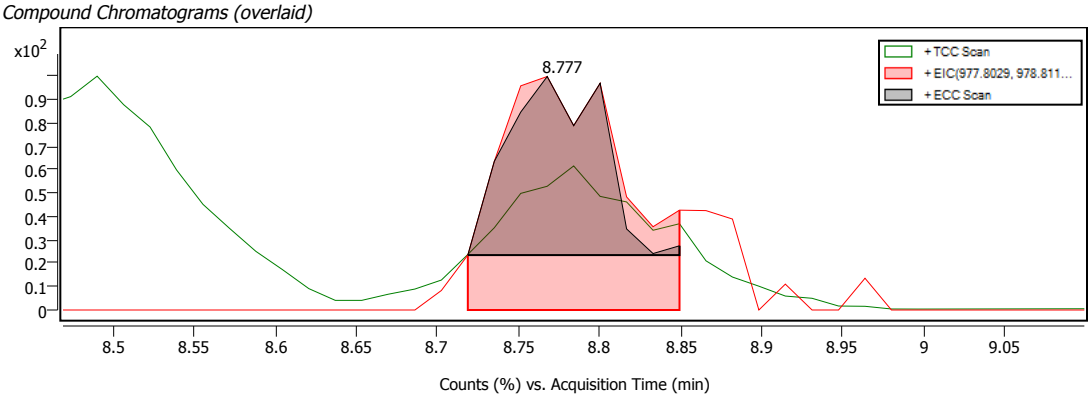
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	977.8044				5	78.95	

Compound ID Table

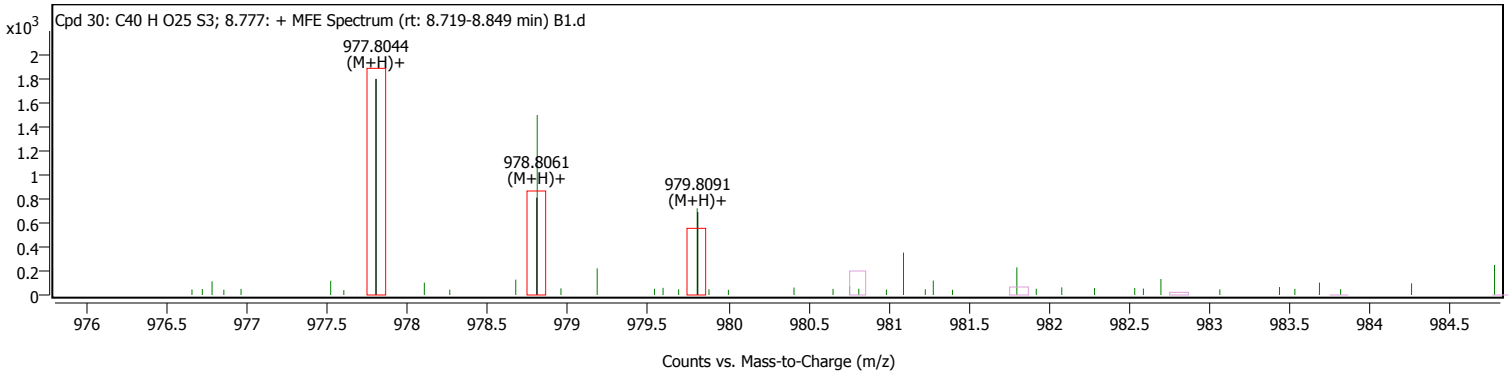
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C40 H O25 S3	(M+H)+	MFG	8.777		976.7975		78.95		78.95
	C35 H3 N3 O24 S4	(M+H)+	MFG	8.777		976.7978		78.58		78.58
	C41 H5 O20 S5	(M+H)+	MFG	8.777		976.7978		78.27		78.27
	C32 H5 N2 O27 S4	(M+H)+	MFG	8.777		976.7978		77.03		77.03
	C39 H3 N3 O19 S5	(M+H)+	MFG	8.777		976.7979		76.74		76.74

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 31: 1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine

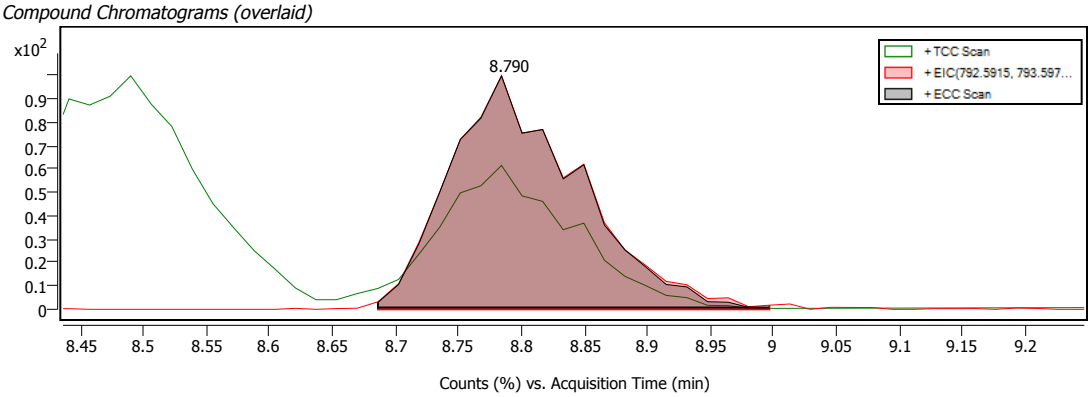
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	8.790		814.5751		DBSearch	98.53	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
M+	814.5748 814.5748 814.5748		0	98.53	16		

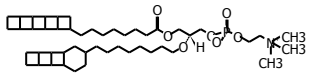
Compound ID Table

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	8.790		814.5751		98.53	98.53	
	C53 H77 N O4	(M+H)+	MFG	8.790		791.5852		98.29		98.29
	C51 H75 N4 O3	(M+H)+	MFG	8.790		791.5853		96.54		96.54
	C54 H73 N5	(M+H)+	MFG	8.790		791.5853		95.42		95.42
	C37 H67 N20	(M+H)+	MFG	8.790		791.5857		93.20		93.20
	C38 H73 N13 O5	(M+H)+	MFG	8.790		791.5855		92.90		92.90
	C30 H66 N25 O	(M+Na)+	MFG	8.790		792.5888		85.93		85.93
	C32 H68 N22 O2	(M+Na)+	MFG	8.790		792.5887		84.06		84.06
	C28 H64 N28	(M+Na)+	MFG	8.790		792.5888		83.65		83.65
	C35 H76 N12 O8	(M+Na)+	MFG	8.790		792.5886		79.01		79.01
	C34 H70 N19 O3	(M+Na)+	MFG	8.790		792.5887		78.22		78.22
	C38 H80 N5 O13	M+	MFG	8.790		814.5753		47.62		47.62
	C37 H74 N12 O8	M+	MFG	8.790		814.5753		47.62		47.62
	C36 H68 N19 O3	M+	MFG	8.790		814.5753		47.61		47.61
	C49 H81 Cl N O6	M+	MFG	8.790		814.5753		47.61		47.61
	C48 H75 Cl N8 O	M+	MFG	8.790		814.5753		47.61		47.61

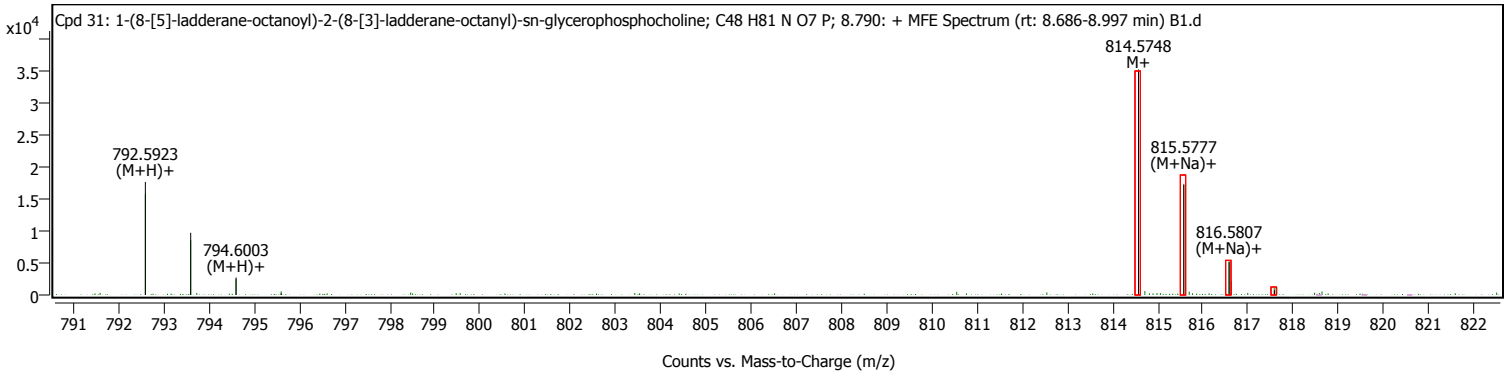
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Compound Discovery Report

Agilent | Trusted Answers

Cpd. 32: Halaminol A

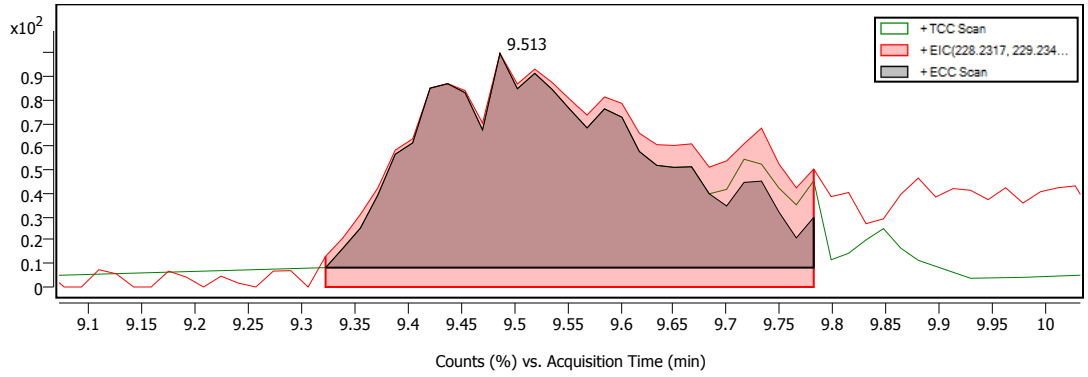
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Halaminol A	C14 H29 N O	9.513		227.2242		DBSearch-MFG	82.71	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	228.2316 228.2316 228.2316		0	82.69	31	82.72	

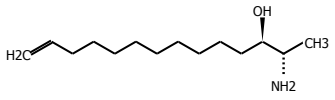
Compound ID Table

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	9.513		227.2242		82.71	82.69	82.72
1-Tetradecen-3-one	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
11Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
3-methyl-6-(1-methyl-ethyl)-3,9-decadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9S-(2-cyclopentenyl)-1-nonanol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9R-(2-cyclopentenyl)-1-nonanol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
11E,13-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
10E,12E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
8E,10E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
8Z,10E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9Z,11E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9Z,12E-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
10Z,12Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9Z,11Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9Z,12Z-Tetradecadien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
11E-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
7-Ethyl-4E-dodecen-6-one	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
5Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
7Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9Z-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
5-Tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
3-methyl-6-(1-methyl-ethyl)-deca-3,9-dien-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9S-(2-cyclopentenyl)-nonan-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9R-(2-cyclopentenyl)-nonan-1-ol	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
2-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
7-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
9-tetradecenal	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
7E-Tetradecen-2-one	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
7Z-Tetradecen-2-one	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
1,13-Tetradecadien-3-one	C14 H26 O	(M+NH4)+	DBSearch	9.513		210.1977		82.58	82.58	
	C12 H27 N4	(M+H)+	MFG	9.513		227.2243		81.27		81.27

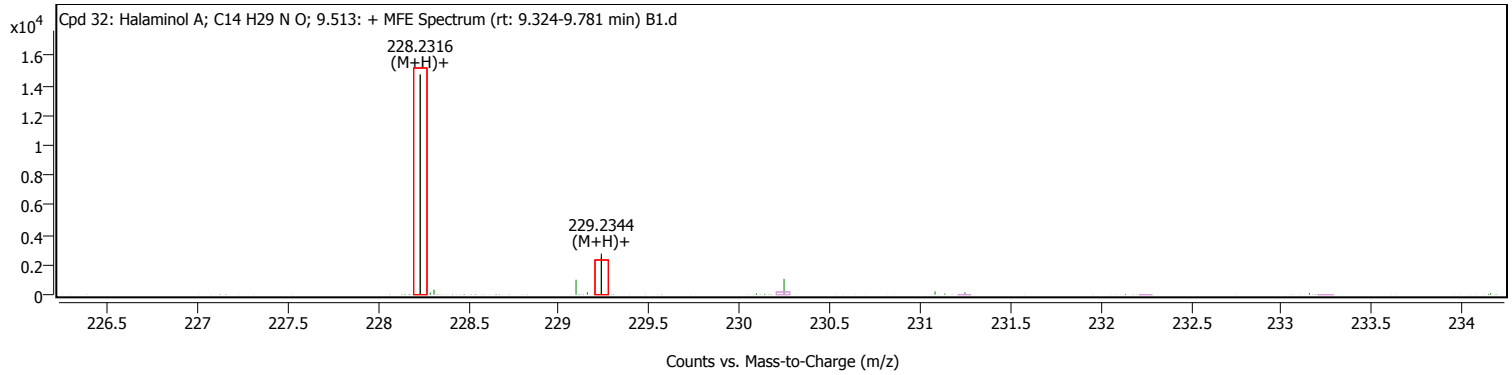
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 33: C12 H29 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C12 H29 N4	9.835		229.2395		MFG	71.88	MFE	

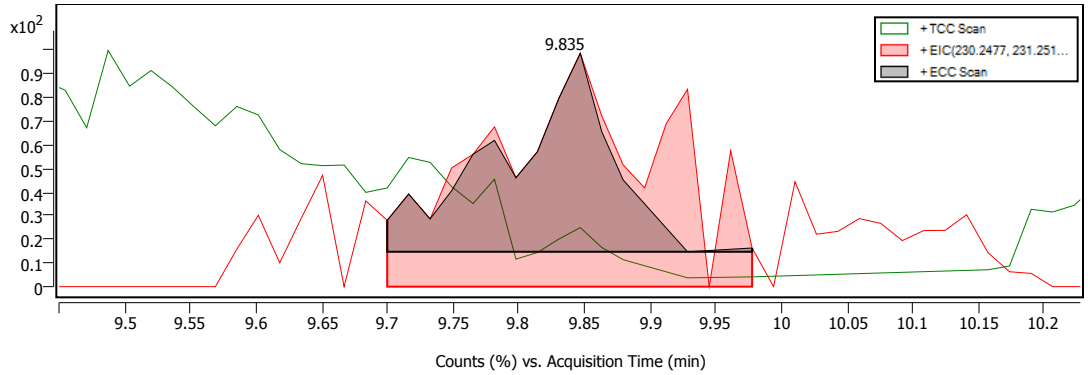
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	230.2464				2	71.88	

Compound ID Table

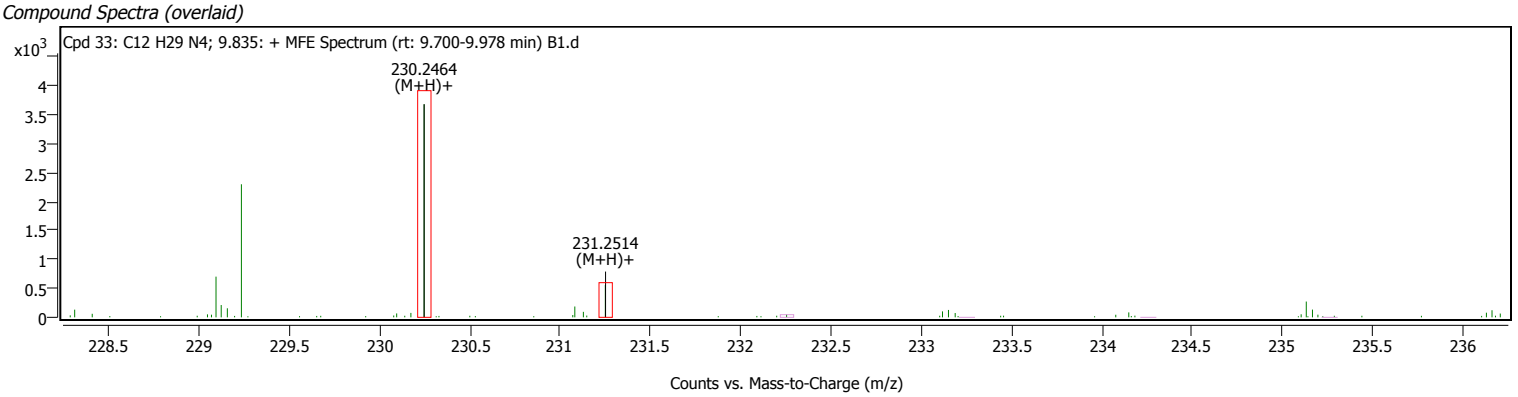
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C12 H29 N4	(M+H)+	MFG	9.835		229.2395		71.88		71.88
	C14 H31 N O	(M+H)+	MFG	9.835		229.2395		71.15		71.15

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 34: C20 H26 N16 O5

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C20 H26 N16 O5	10.240		570.2269		MFG	79.04	MFE	

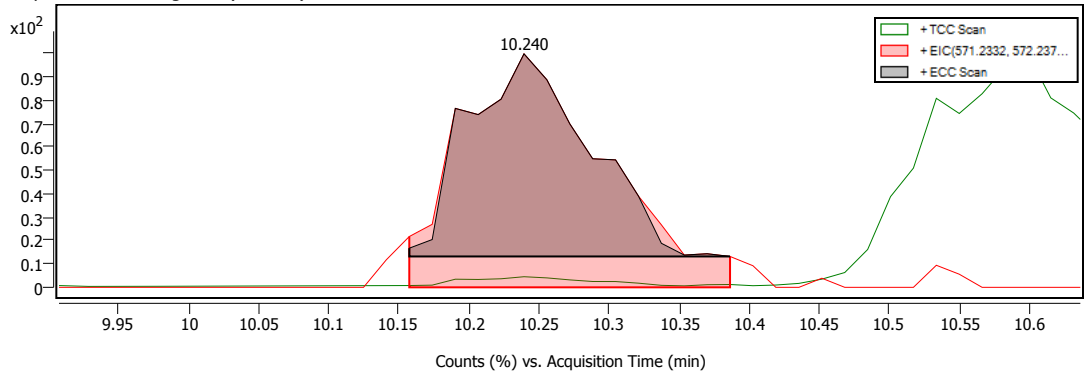
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	571.2343				6	79.04	

Compound ID Table

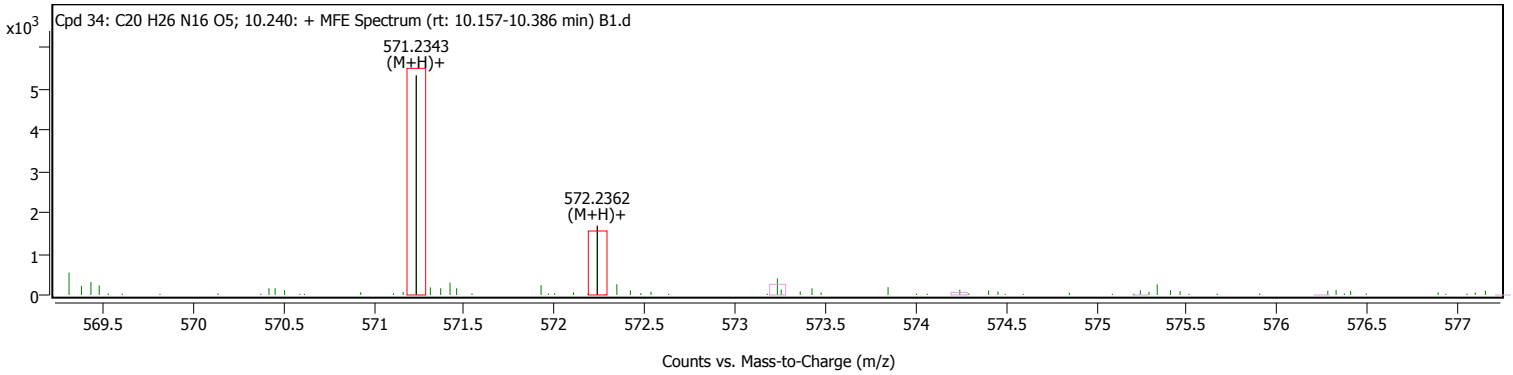
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C20 H26 N16 O5	(M+H)+	MFG	10.240		570.2269		79.04		79.04
	C21 H22 N20 O	(M+H)+	MFG	10.240		570.2270		77.77		77.77
	C18 H24 N19 O4	(M+H)+	MFG	10.240		570.2270		76.39		76.39
	C21 H32 N9 O10	(M+H)+	MFG	10.240		570.2268		75.45		75.45
	C22 H28 N13 O6	(M+H)+	MFG	10.240		570.2269		74.47		74.47
PKC 412	C35 H30 N4 O4	(M+H)+	DBSearch	10.240		570.2267	120685-11-2	72.38	72.38	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 35: C19 H22 N16 O4

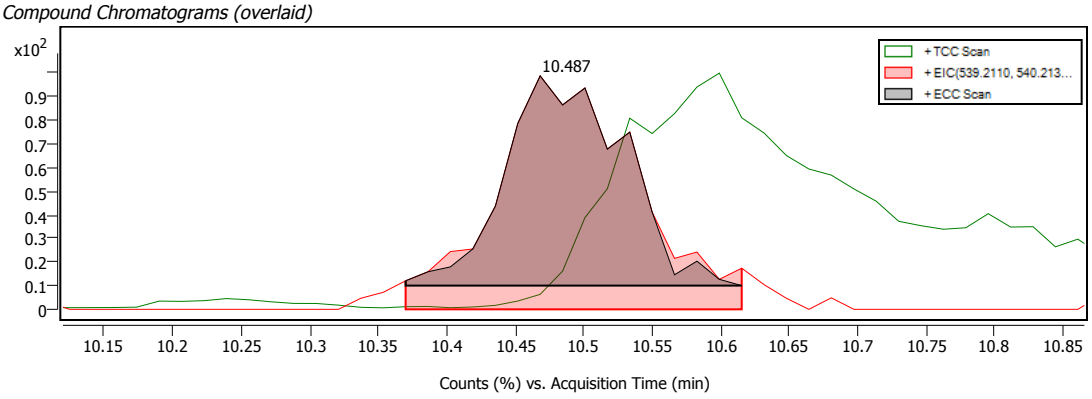
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C19 H22 N16 O4	10.487		538.2007		MFG	81.23	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	539.2078				7	81.23	

Compound ID Table

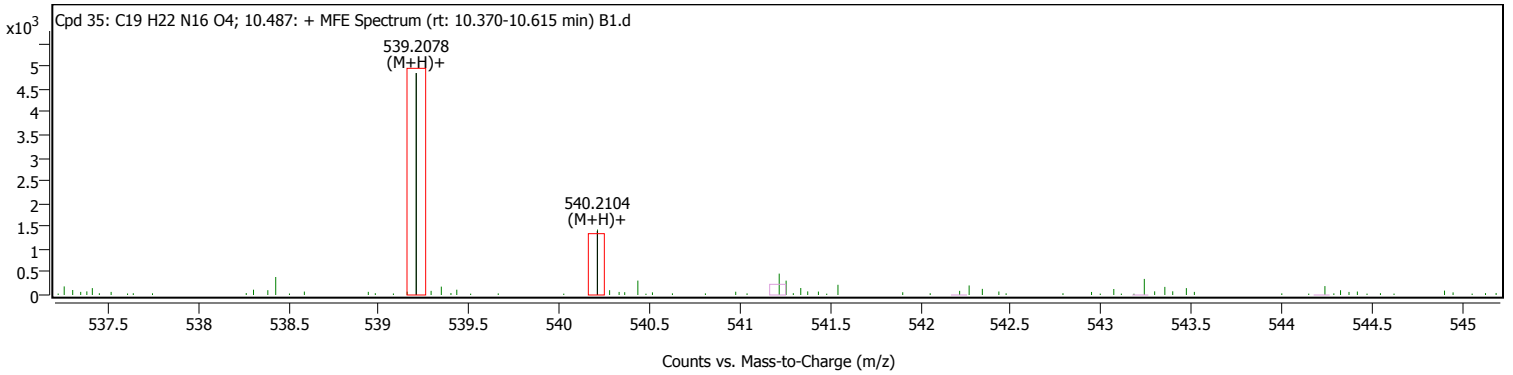
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C19 H22 N16 O4	(M+H)+	MFG	10.487		538.2007		81.23		81.23
	C20 H28 N9 O9	(M+H)+	MFG	10.487		538.2005		78.35		78.35
	C18 H26 N12 O8	(M+H)+	MFG	10.487		538.2006		76.49		76.49
	C21 H24 N13 O5	(M+H)+	MFG	10.487		538.2006		76.07		76.07
	C21 H34 N2 O14	(M+H)+	MFG	10.487		538.2004		74.54		74.54
8-trans-[2-(6-Benzoyloxy-4-hydroxy-2-methoxy-3-methylphenyl)ethenyl]-5-methoxyflavan-7-ol	C33 H30 O7	(M+H)+	DBSearch	10.487		538.2004		71.28	71.28	
Asticolorin A	C33 H30 O7	(M+H)+	DBSearch	10.487		538.2004	93376-70-6	71.28	71.28	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 36: C36 H63 N14 O S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C36 H63 N14 O S2	10.553		771.4753		MFG	89.69	MFE	

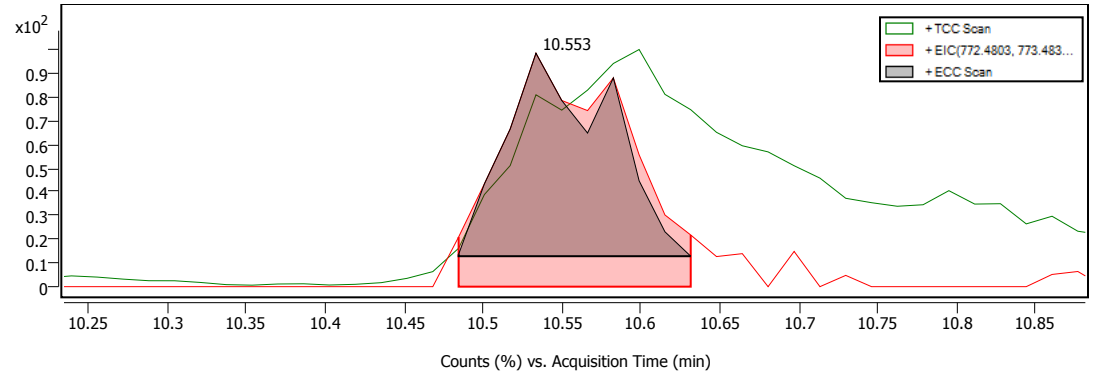
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	772.4834				5	89.69	

Compound ID Table

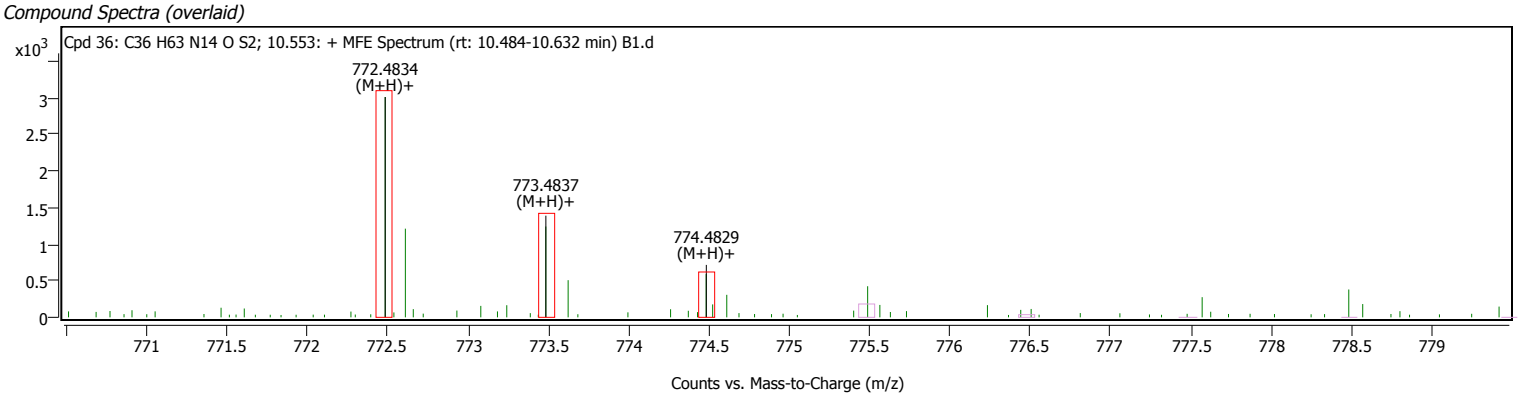
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C36 H63 N14 O S2	(M+H)+	MFG	10.553		771.4753		89.69		89.69
	C37 H69 N7 O6 S2	(M+H)+	MFG	10.553		771.4752		88.87		88.87
	C38 H65 N11 O2 S2	(M+H)+	MFG	10.553		771.4752		87.77		87.77
	C38 H75 O11 S2	(M+H)+	MFG	10.553		771.4750		87.57		87.57
	C34 H61 N17 S2	(M+H)+	MFG	10.553		771.4754		86.67		86.67

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 37: C33 H42 N3 O9 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H42 N3 O9 S	10.571		656.2633		MFG	89.54	MFE	

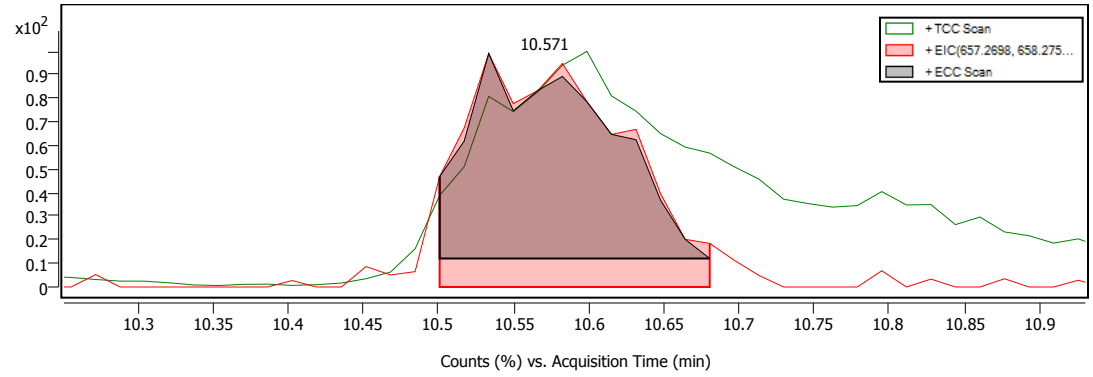
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	657.2702				5	89.54	

Compound ID Table

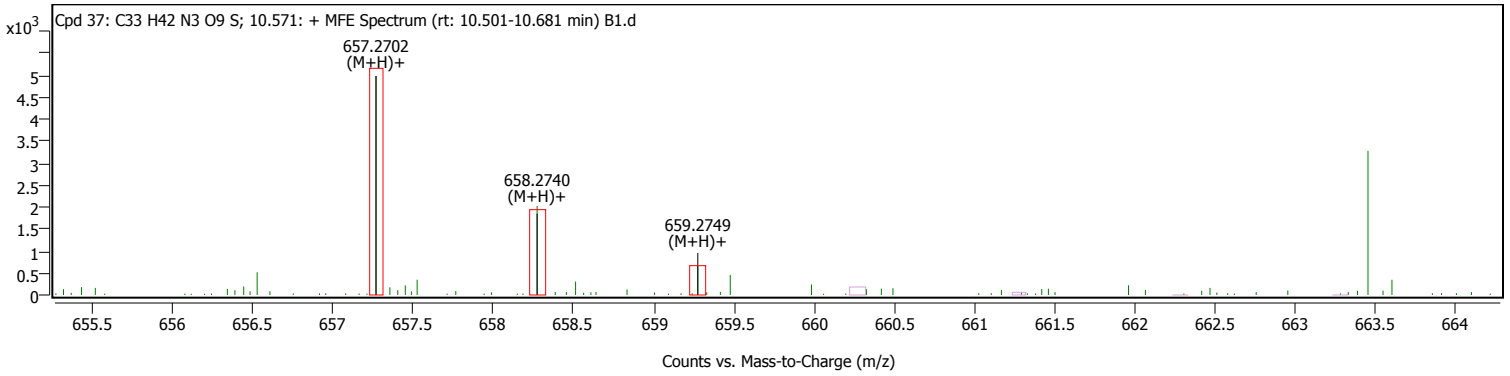
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H42 N3 O9 S	(M+H)+	MFG	10.571		656.2633		89.54		89.54
	C39 H44 O5 S2	(M+H)+	MFG	10.571		656.2634		89.33		89.33
	C31 H40 N6 O8 S	(M+H)+	MFG	10.571		656.2634		89.05		89.05
	C32 H44 N6 O3 S3	(M+H)+	MFG	10.571		656.2638		87.52		87.52
	C32 H36 N10 O4 S	(M+H)+	MFG	10.571		656.2635		87.44		87.44

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 38: C39 H63 N21 O4

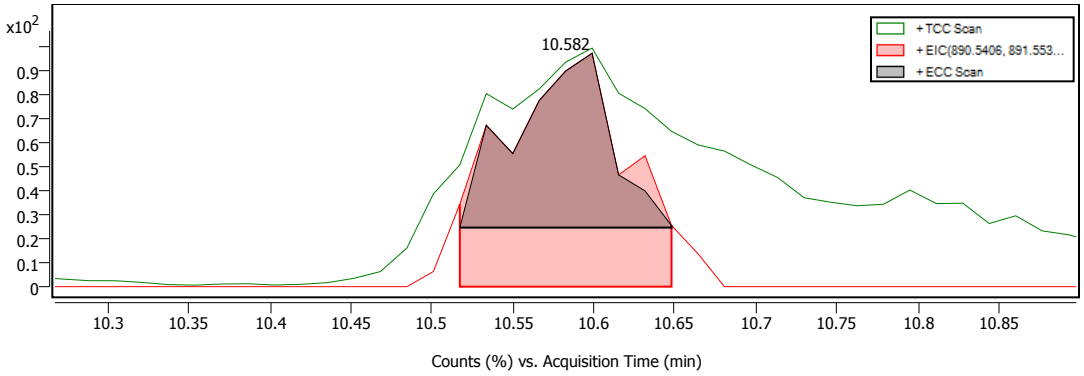
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C39 H63 N21 O4	10.582		889.5379		MFG	58.57	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	890.5431				5	58.57	

Compound ID Table

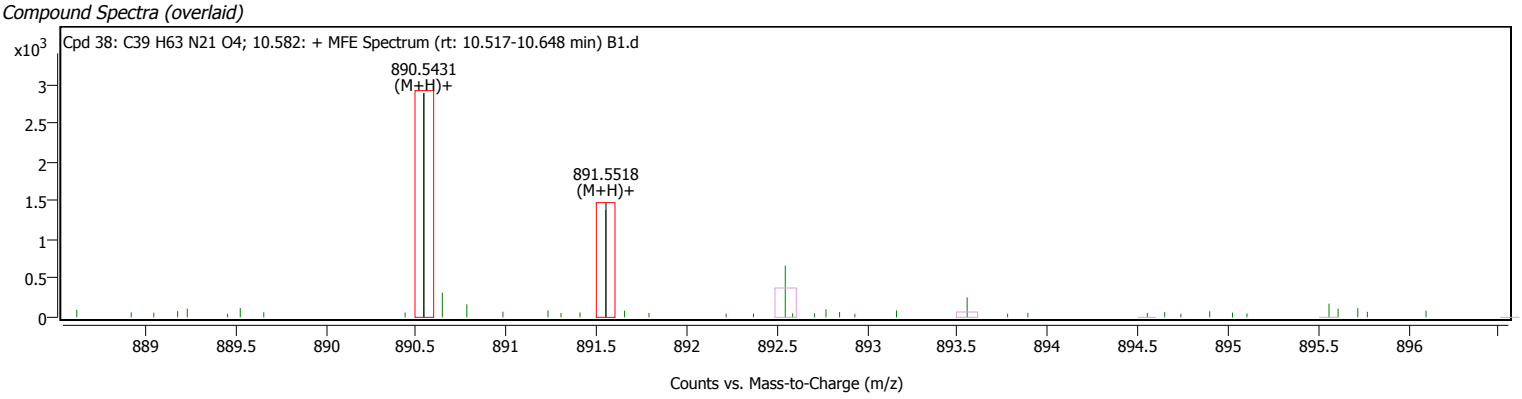
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C39 H63 N21 O4	(M+H)+	MFG	10.582		889.5379		58.57		58.57
	C40 H69 N14 O9	(M+H)+	MFG	10.582		889.5378		57.95		57.95
	C41 H75 N7 O14	(M+H)+	MFG	10.582		889.5377		57.42		57.42
	C42 H81 O19	(M+H)+	MFG	10.582		889.5376		57.00		57.00
	C37 H61 N24 O3	(M+H)+	MFG	10.582		889.5380		55.20		55.20

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 39: C14 H31 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C14 H31 N4	10.601		255.2551		MFG	98.61	MFE	

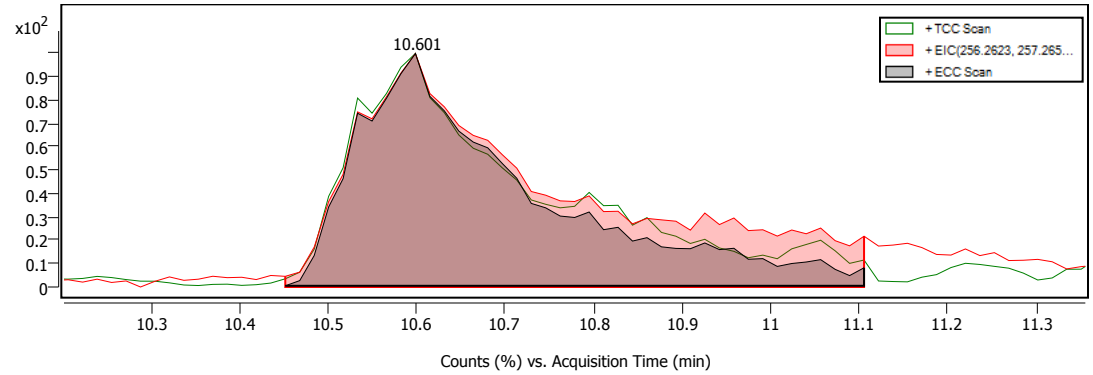
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	256.2623				2	98.61	

Compound ID Table

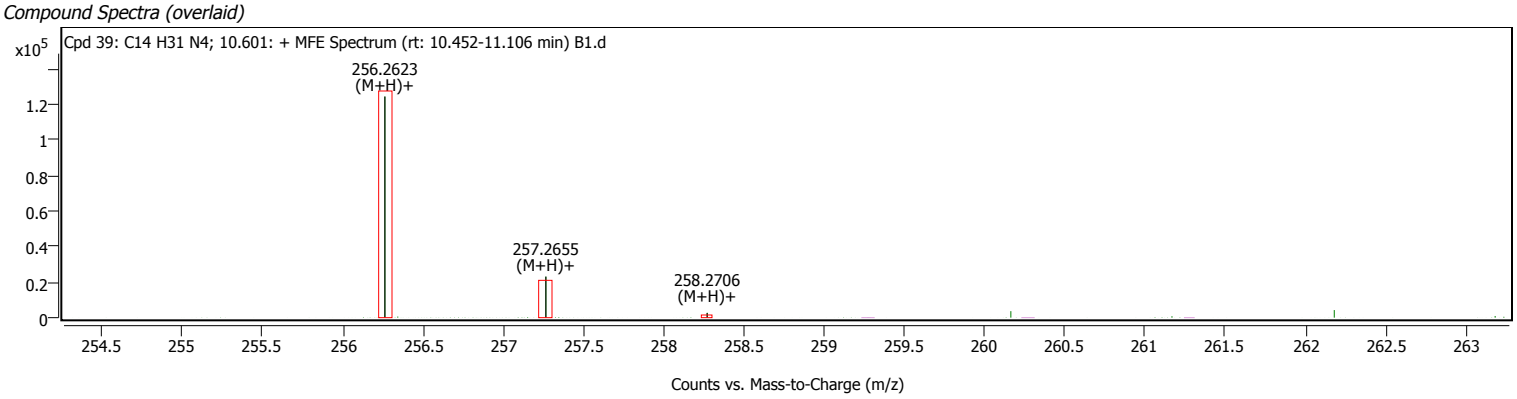
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C14 H31 N4	(M+H)+	MFG	10.601		255.2551		98.61		98.61
Palmitic amide	C16 H33 N O	(M+H)+	DBSearch-MFG	10.601		255.2550	629-54-9	94.31	94.30	94.32

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 40: C30 H55 N O S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C30 H55 N O S	10.769		477.4002		MFG	61.40	MFE	

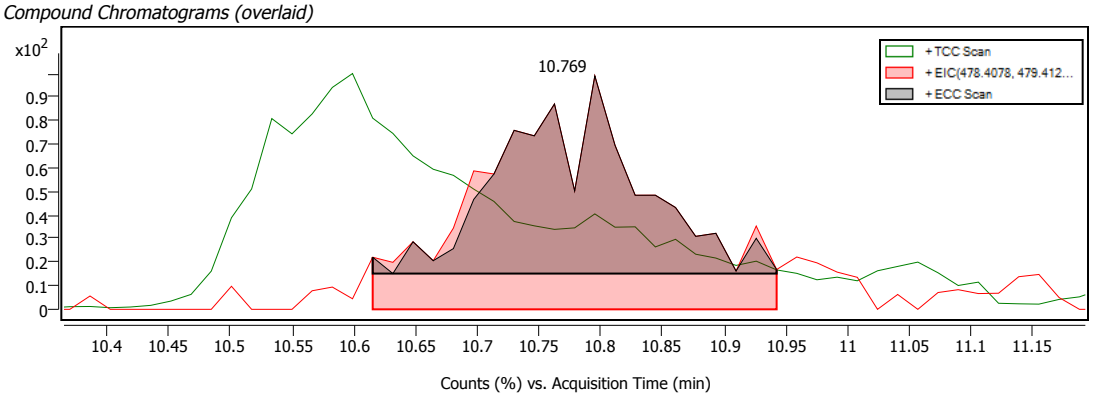
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	478.4076				5	61.40	

Compound ID Table

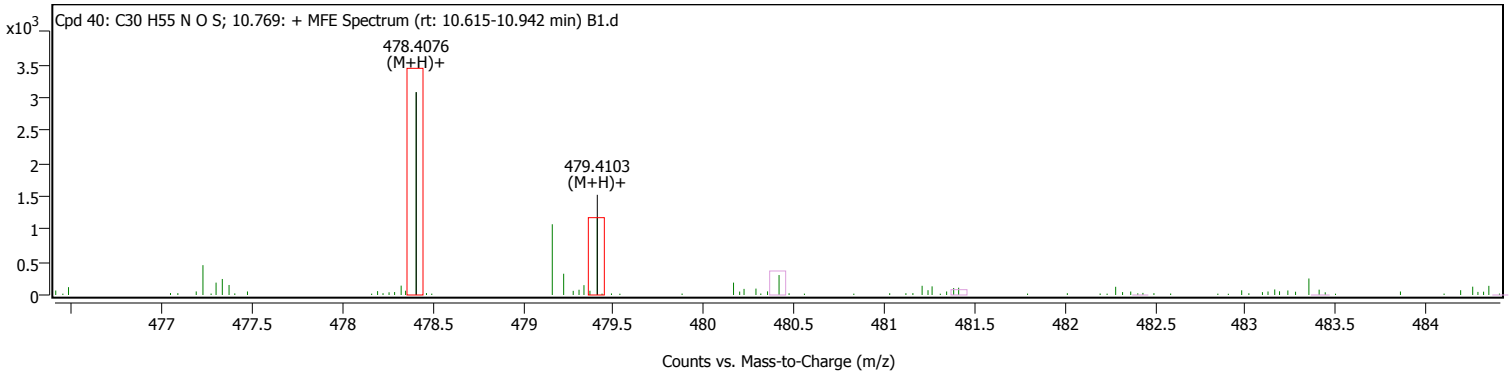
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C30 H55 N O S	(M+H)+	MFG	10.769		477.4002		61.40		61.40
	C28 H53 N4 S	(M+H)+	MFG	10.769		477.4002		58.85		58.85
	C25 H49 N8 O	(M+H)+	MFG	10.769		477.4003		49.86		49.86
	C33 H51 N O	(M+H)+	MFG	10.769		477.4001		49.62		49.62
	C26 H55 N O6	(M+H)+	MFG	10.769		477.4001		46.84		46.84

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

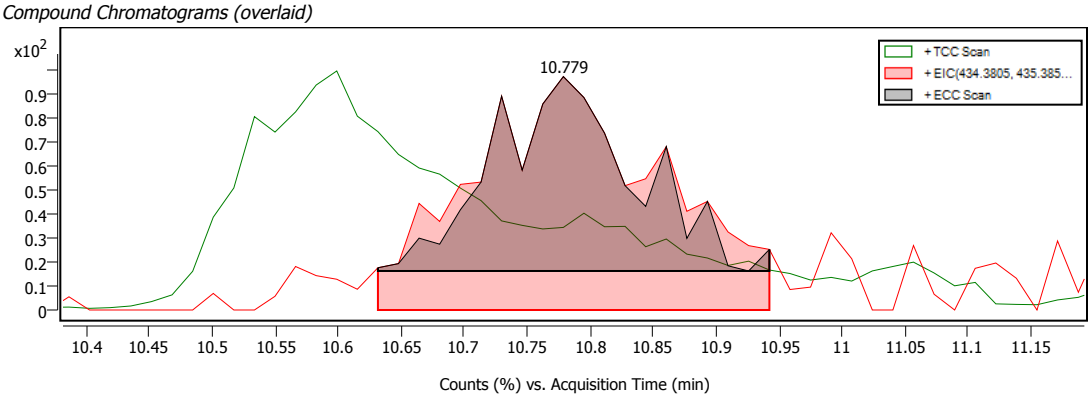


Cpd 41: 10.779

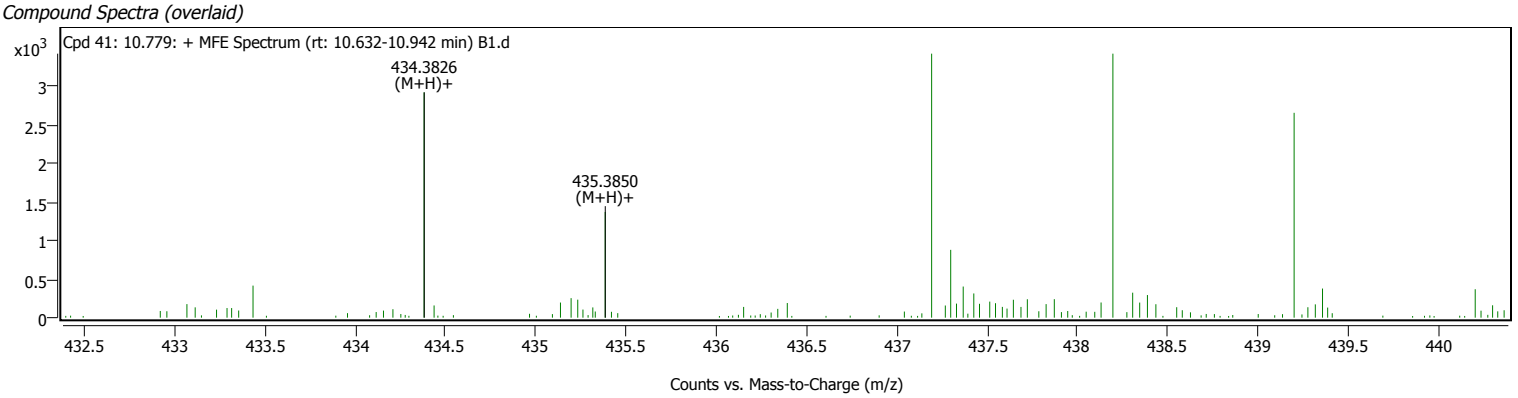
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		10.779		433.3754				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 42: C28 H48 N5 O18

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H48 N5 O18	10.835		742.2996		MFG	92.35	MFE	

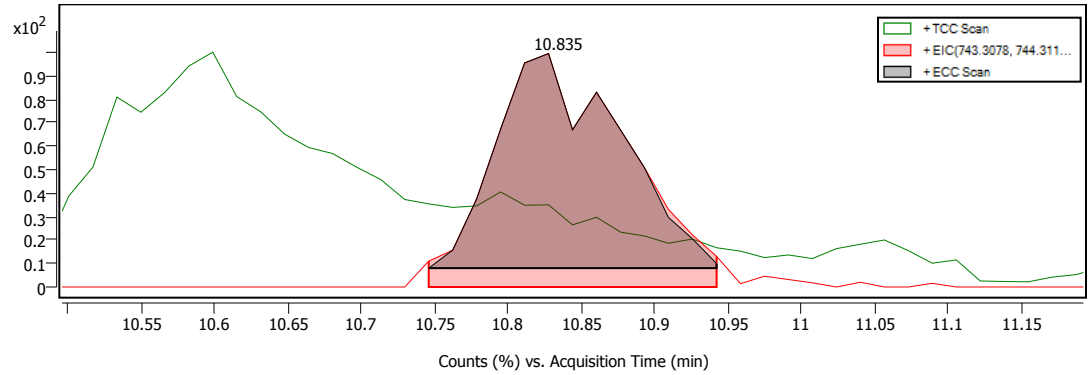
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	743.3066				7	92.35	

Compound ID Table

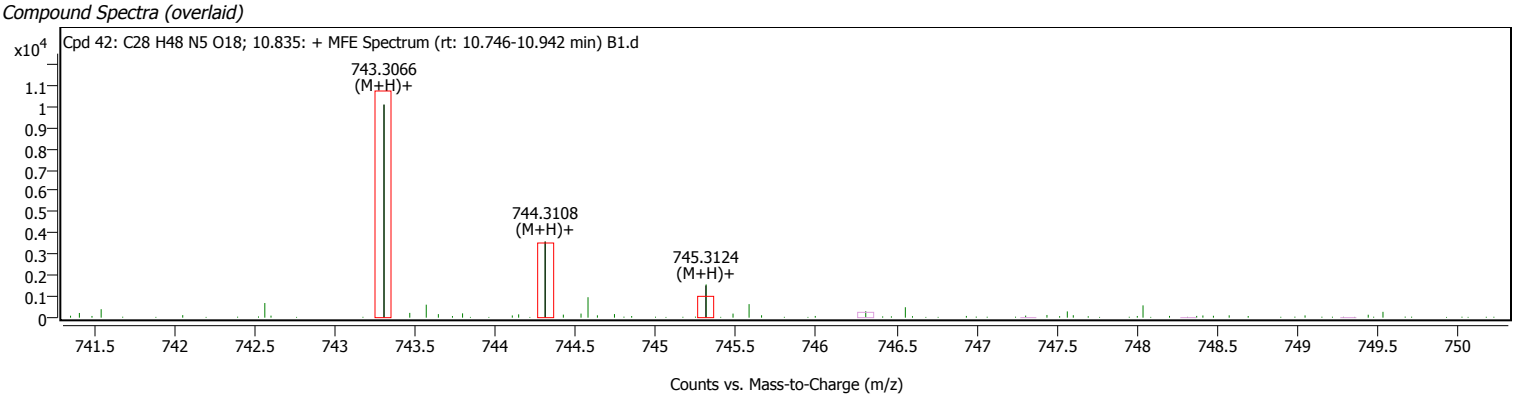
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H48 N5 O18	(M+H)+	MFG	10.835		742.2996		92.35		92.35
	C35 H46 N6 O10 S	(M+H)+	MFG	10.835		742.2999		91.96		91.96
	C30 H50 N2 O19	(M+H)+	MFG	10.835		742.2996		91.67		91.67
	C34 H50 N2 O14 S	(M+H)+	MFG	10.835		742.2999		91.04		91.04
	C27 H42 N12 O13	(M+H)+	MFG	10.835		742.2998		90.44		90.44
Neoarctin A	C42 H46 O12	(M+H)+	DBSearch	10.835		742.2995		87.23	87.23	
Neoarctin B	C42 H46 O12	(M+H)+	DBSearch	10.835		742.2995		87.23	87.23	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 43: C33 H50 N9 O16

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H50 N9 O16	11.056		828.3371		MFG	97.08	MFE	

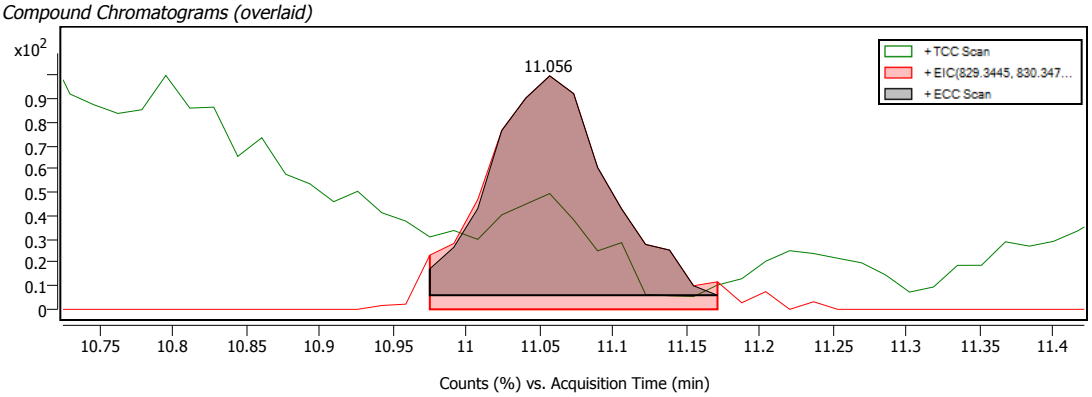
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	829.3446				5	97.08	

Compound ID Table

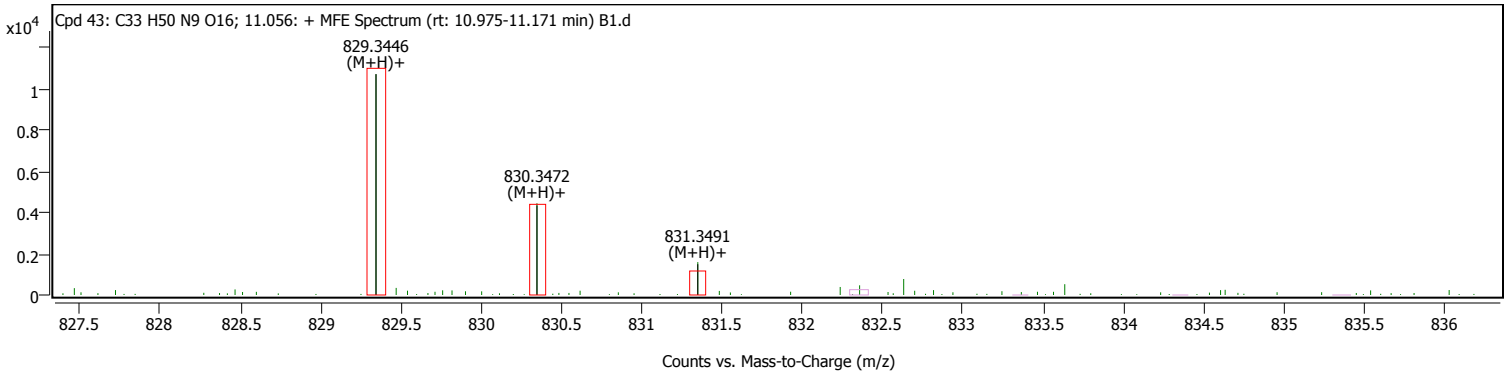
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H50 N9 O16	(M+H)+	MFG	11.056		828.3371		97.08		97.08
	C32 H44 N16 O11	(M+H)+	MFG	11.056		828.3373		96.71		96.71
	C34 H56 N2 O21	(M+H)+	MFG	11.056		828.3370		96.60		96.60
	C31 H48 N12 O15	(M+H)+	MFG	11.056		828.3372		95.71		95.71
	C32 H54 N5 O20	(M+H)+	MFG	11.056		828.3371		95.67		95.67

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 44: C37 H63 N7 O19

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H63 N7 O19	11.231		909.4187		MFG	65.31	MFE	

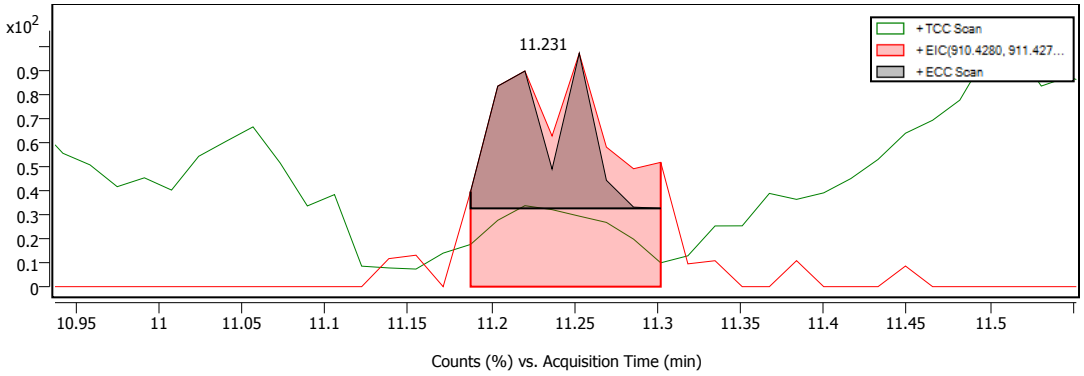
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	910.4254				5	65.31	

Compound ID Table

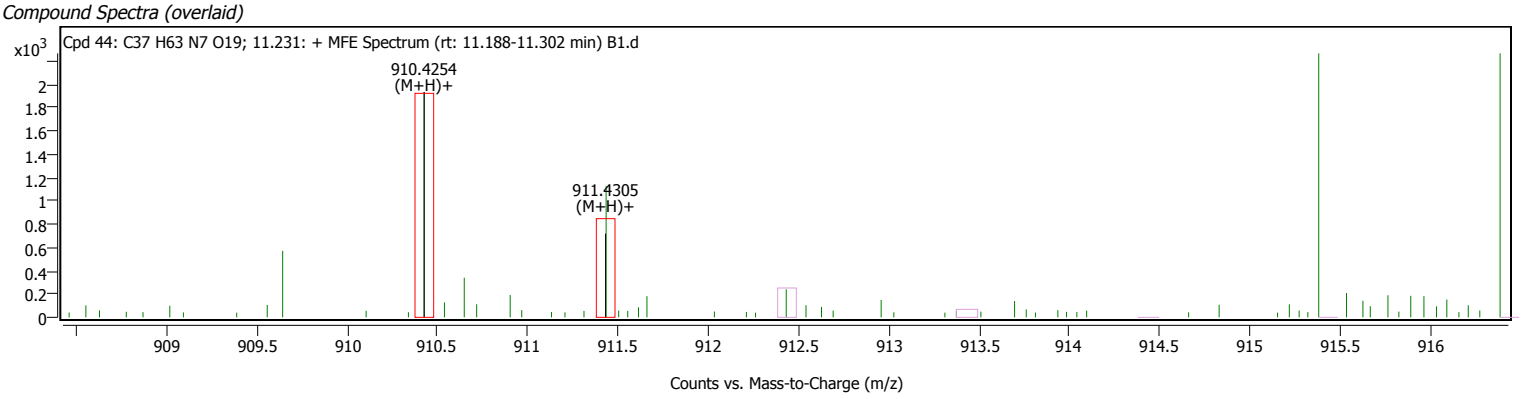
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H63 N7 O19	(M+H)+	MFG	11.231		909.4187		65.31		65.31
	C36 H57 N14 O14	(M+H)+	MFG	11.231		909.4188		65.26		65.26
	C38 H69 O24	(M+H)+	MFG	11.231		909.4186		65.20		65.20
	C35 H51 N21 O9	(M+H)+	MFG	11.231		909.4189		65.04		65.04
	C38 H59 N11 O15	(M+H)+	MFG	11.231		909.4187		65.01		65.01

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 45: C34 H48 N19 O12

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H48 N19 O12	11.236		914.3730		MFG	96.59	MFE	

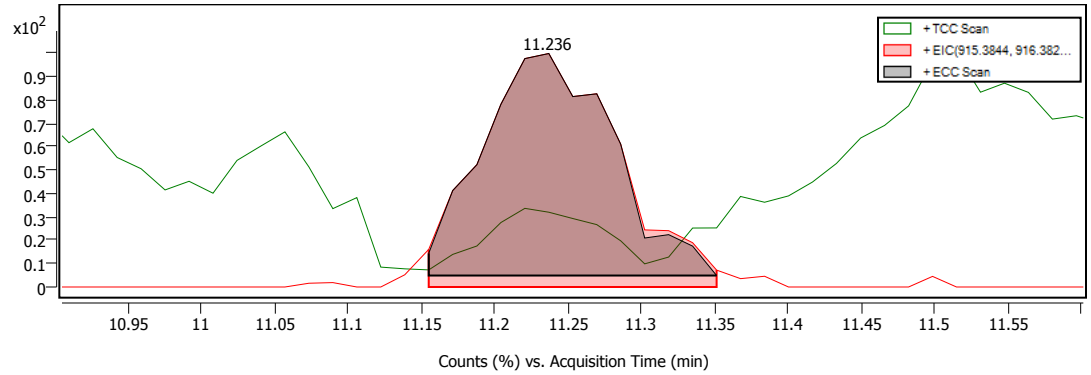
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	915.3800				5	96.59	

Compound ID Table

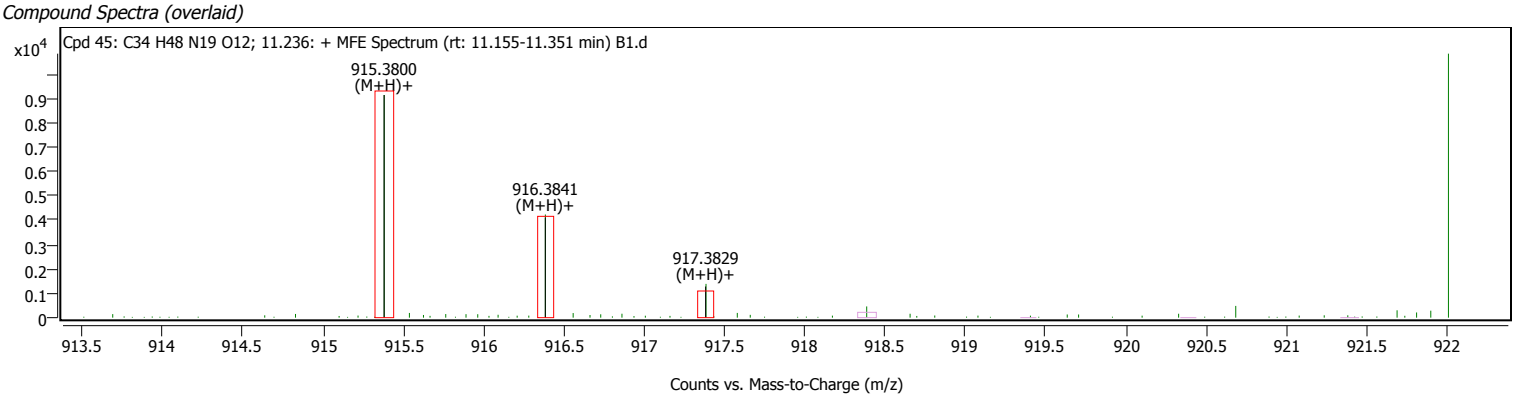
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H48 N19 O12	(M+H)+	MFG	11.236		914.3730		96.59		96.59
	C35 H54 N12 O17	(M+H)+	MFG	11.236		914.3729		96.27		96.27
	C33 H42 N26 O7	(M+H)+	MFG	11.236		914.3731		96.24		96.24
	C36 H60 N5 O22	(M+H)+	MFG	11.236		914.3727		95.30		95.30
	C33 H52 N15 O16	(M+H)+	MFG	11.236		914.3729		94.29		94.29

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

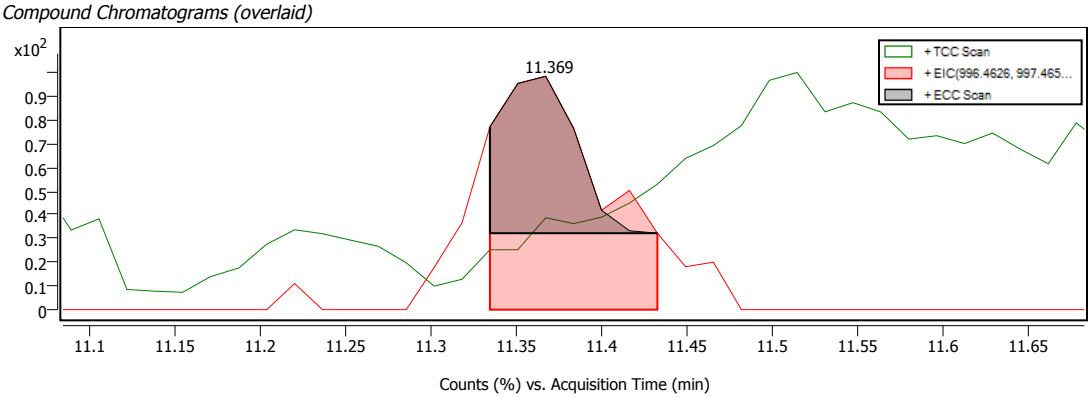


Cpd 46: 11.369

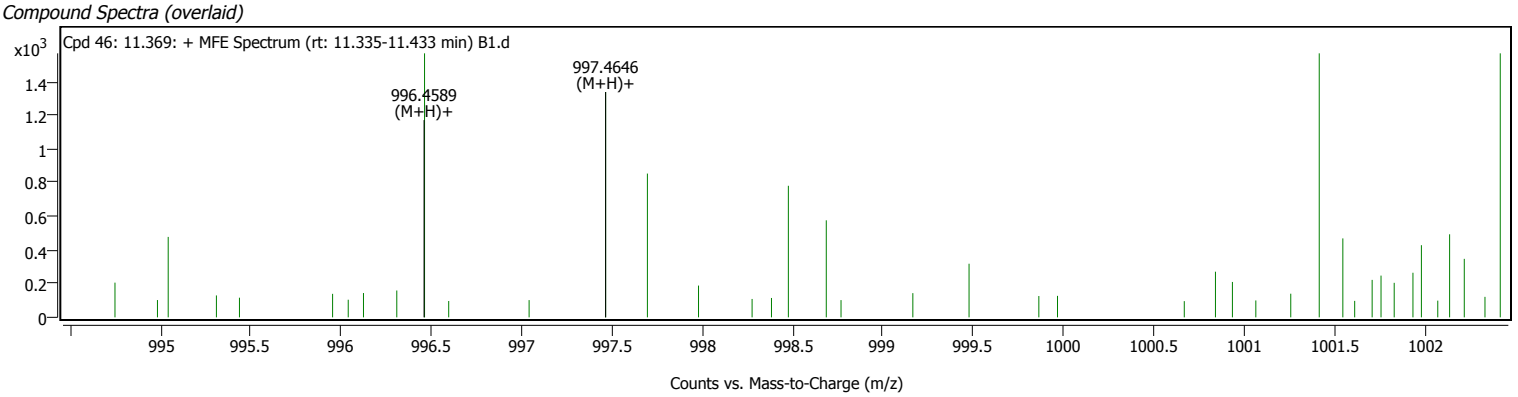
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.369		995.4517				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

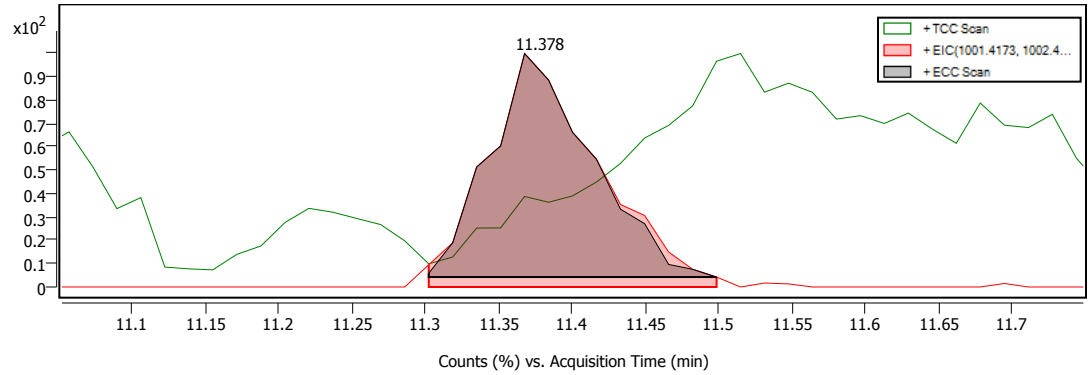


Cpd 47: 11.378

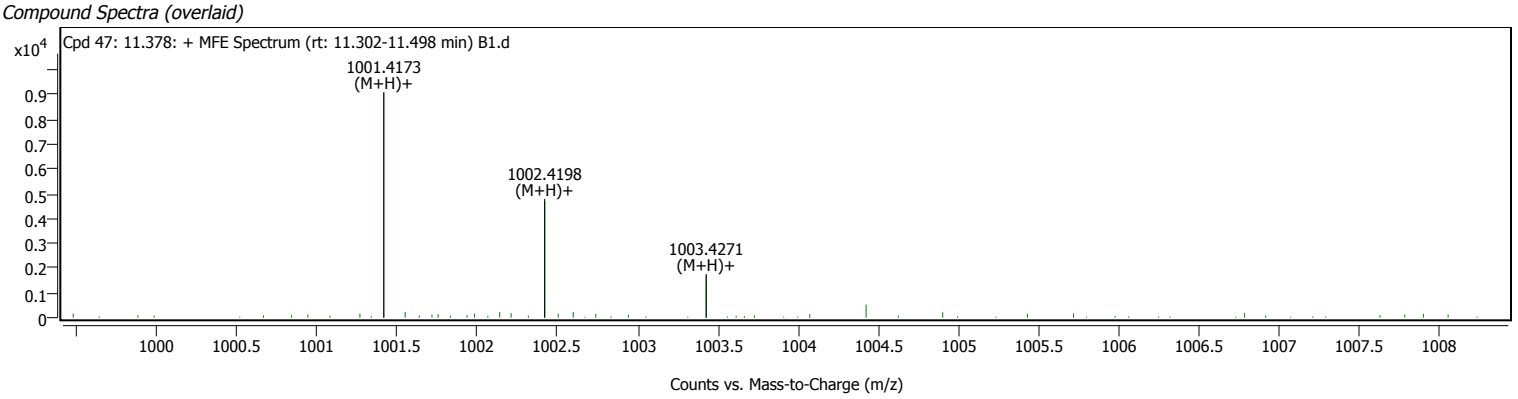
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.378		1000.4100				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

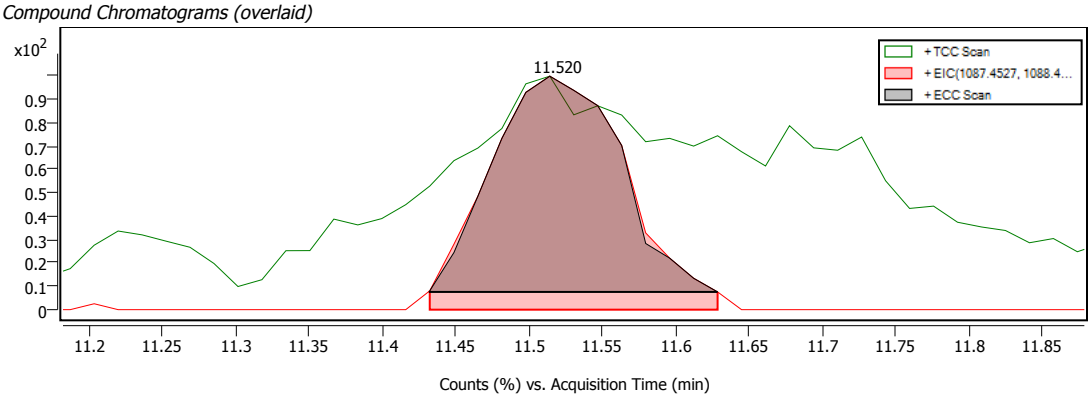


Cpd 48: 11.520

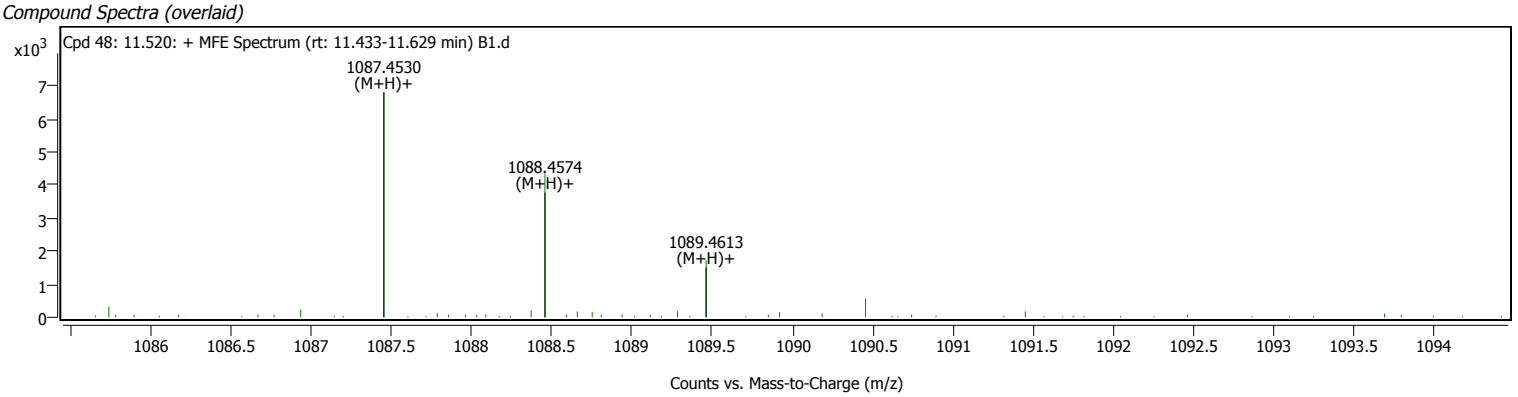
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.520		1086.4457				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 49: C16 H35 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H35 N4	11.532		283.2863		MFG	98.70	MFE	

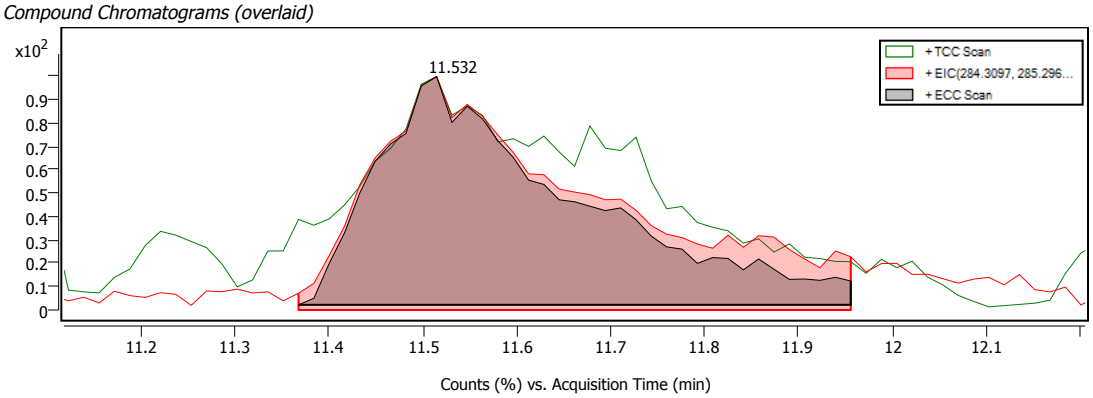
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	284.2935				21	98.70	

Compound ID Table

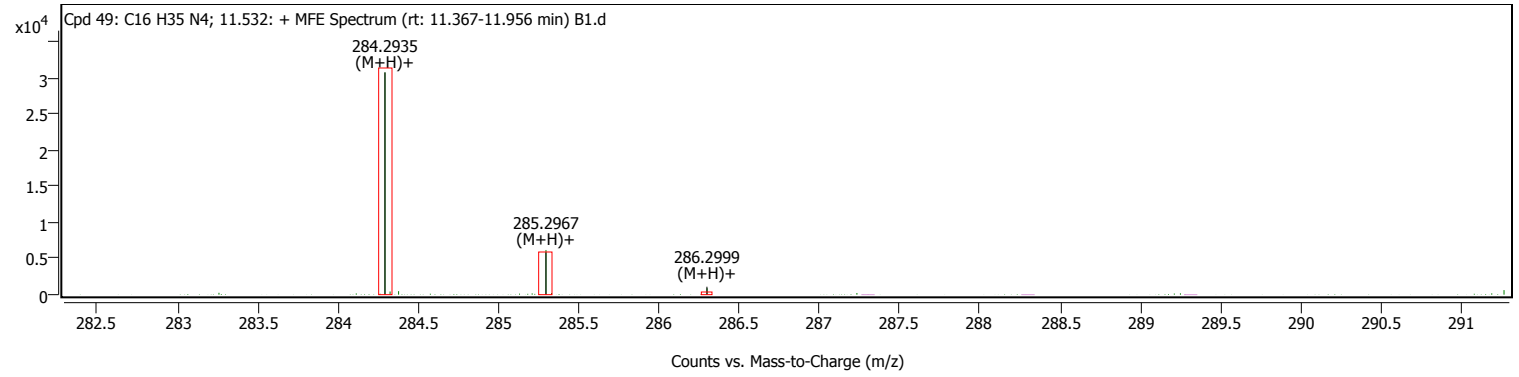
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H35 N4	(M+H)+	MFG	11.532		283.2863		98.70		98.70
Stearamide	C18 H37 N O	(M+H)+	DBSearch-MFG	11.532		283.2862	124-26-5	93.12	93.11	93.13
11-octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
2-Tetradecylcyclobutanone	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597	35493-47-1	92.82	92.82	
7Z-Octadecen-11-one	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
3Z,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
3E,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
2E,13Z-octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
2Z,13Z-Octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
9,12-Octadecadien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
13E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
11Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
2E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
6,7-Epoxy-9Z-octadecene	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
13Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
9Z-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
octadecan-3Z,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
octadecan-3E,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
octadecan-2E,13Z-dien-1-ol	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
9-octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	
14E-Octadecenal	C18 H34 O	(M+NH4)+	DBSearch	11.532		266.2597		92.82	92.82	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

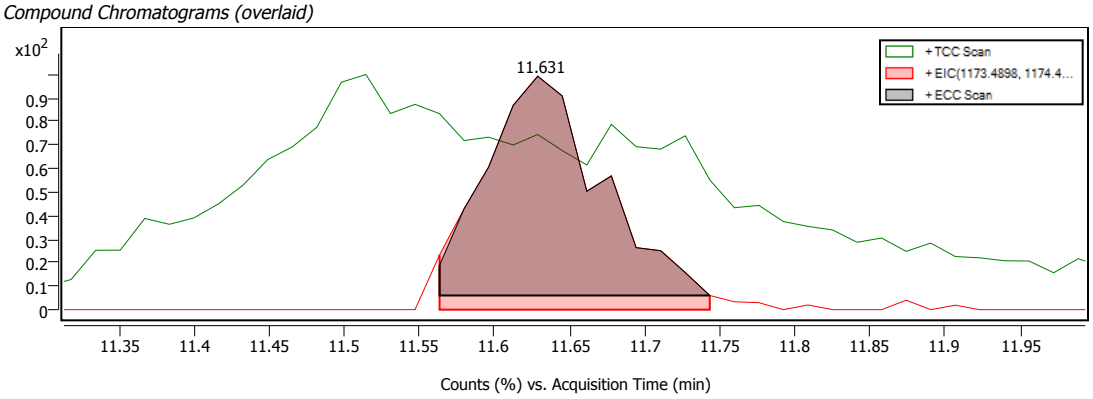


Cpd 50: 11.631

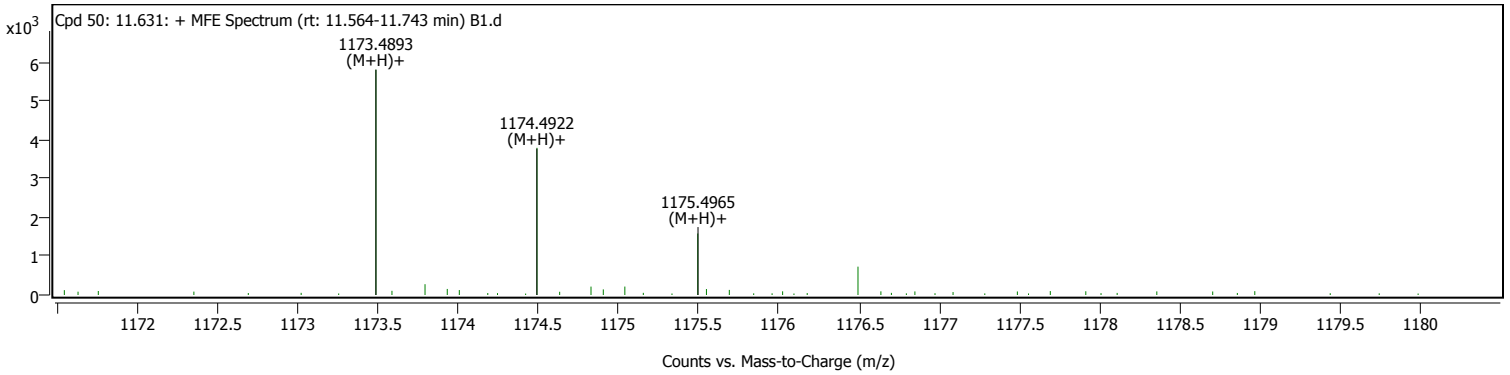
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.631		1172.4820				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 51: Austrobailignan 7

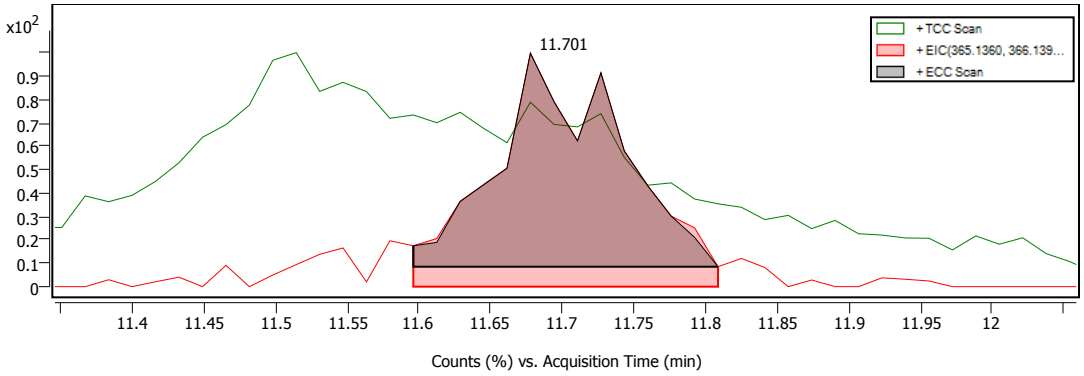
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Austrobailignan 7	C20 H22 O5	11.701		342.1456	55890-25-0	DBSearch	79.18	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	365.1348 365.1348 365.1348		0	79.18	17		

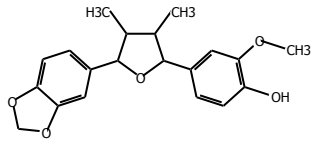
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Austrobailignan 7	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456	55890-25-0	79.18	79.18	
Brosimacutin C	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456		79.18	79.18	
Phaseollidin hydrate	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456		79.18	79.18	
Deoxymiroestrol	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456		79.18	79.18	
1,2,3,4-Tetrahydro-1-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]-7-methoxy-2,6-naphthalenediol	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456	163811-77-6	79.18	79.18	
7-Hydroxyaustrobailignan 5	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456		79.18	79.18	
Hydroxygaleon	C20 H22 O5	(M+Na)+	DBSearch	11.701		342.1456	61576-09-8	79.18	79.18	
	C11 H28 N5 O S3	(M+Na)+	MFG	11.701		342.1456		47.62		47.62
	C23 H22 Cl O2	(M+H)+	MFG	11.701		365.1308		47.61		47.61
	C11 H15 N11 O4	(M+H)+	MFG	11.701		365.1308		47.61		47.61
	C12 H21 N4 O9	(M+H)+	MFG	11.701		365.1308		47.60		47.60
	C8 H26 Cl N8 O2 S2	(M+H)+	MFG	11.701		365.1308		47.60		47.60
	C15 H31 Cl O2 S2	(M+Na)+	MFG	11.701		342.1456		47.49		47.49
	C19 H27 N S3	(M+H)+	MFG	11.701		365.1308		47.48		47.48
	C18 H20 N3 O4	(M+Na)+	MFG	11.701		342.1456		47.46		47.46
	C15 H23 Cl N4 O3	(M+Na)+	MFG	11.701		342.1456		47.43		47.43
	C11 H20 N9 O2 S	(M+Na)+	MFG	11.701		342.1456		47.02		47.02

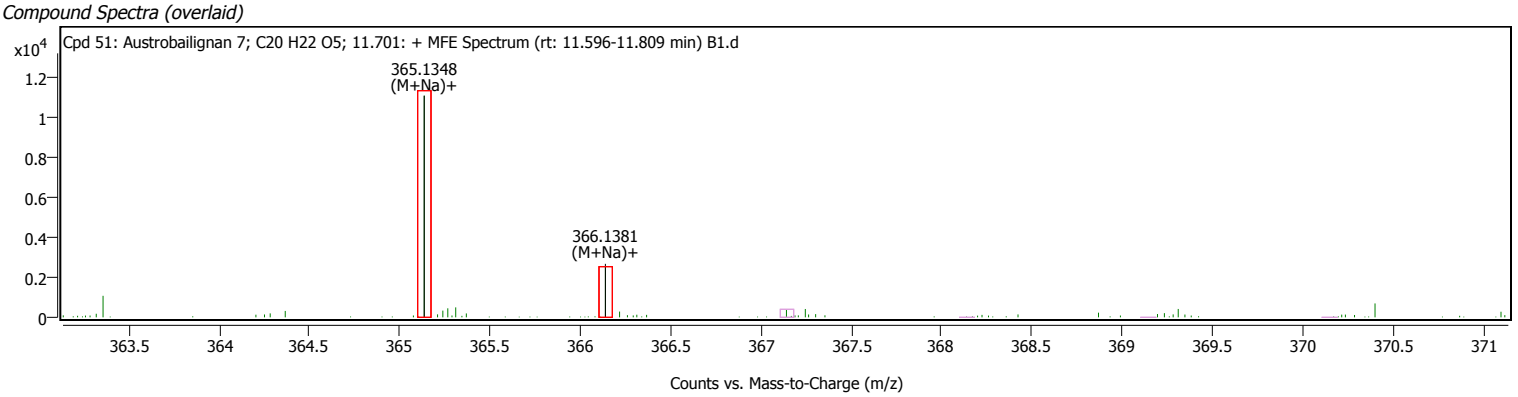
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)

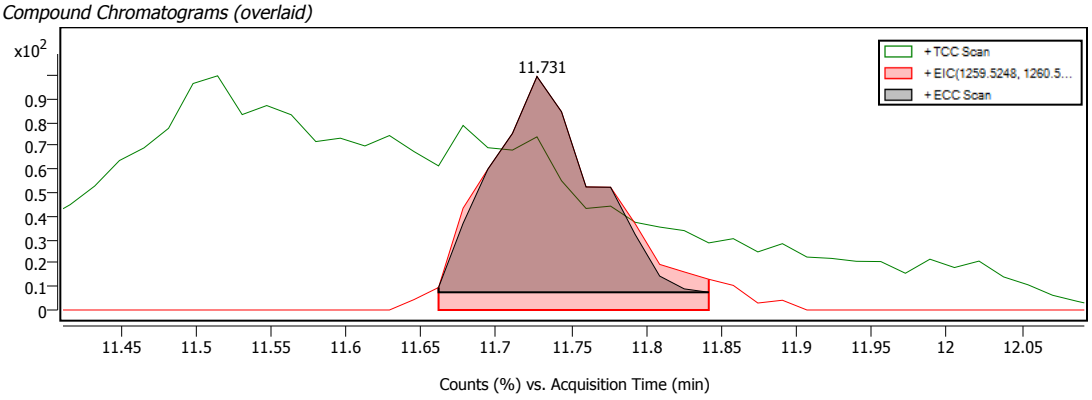


Cpd 52: 11.731

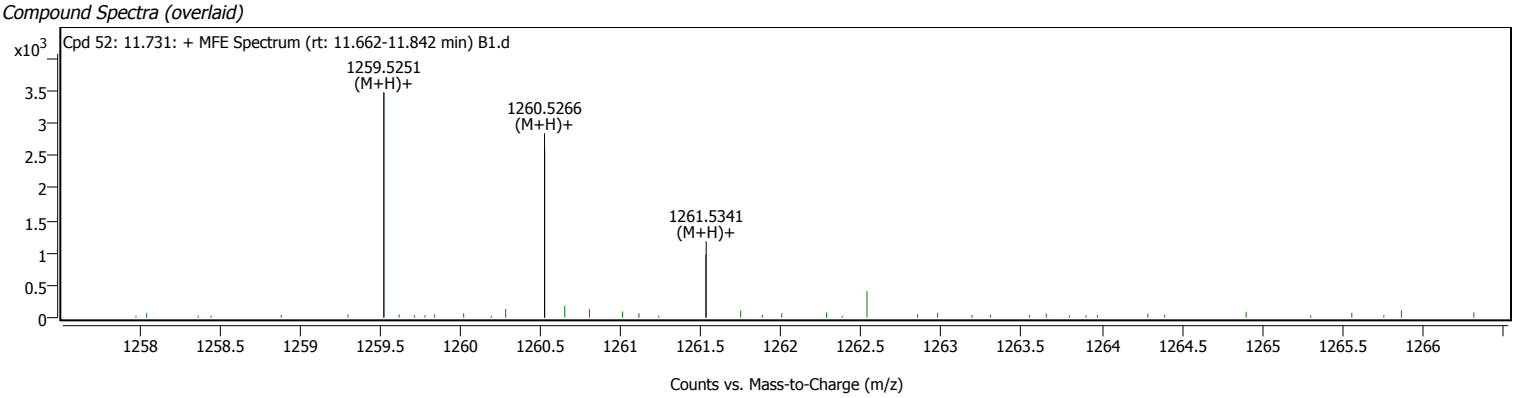
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.731		1258.5178				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

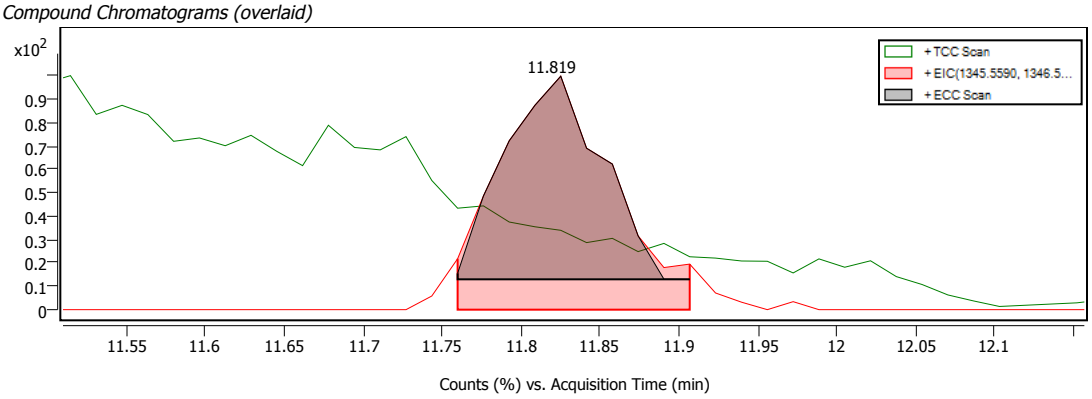


Cpd 53: 11.819

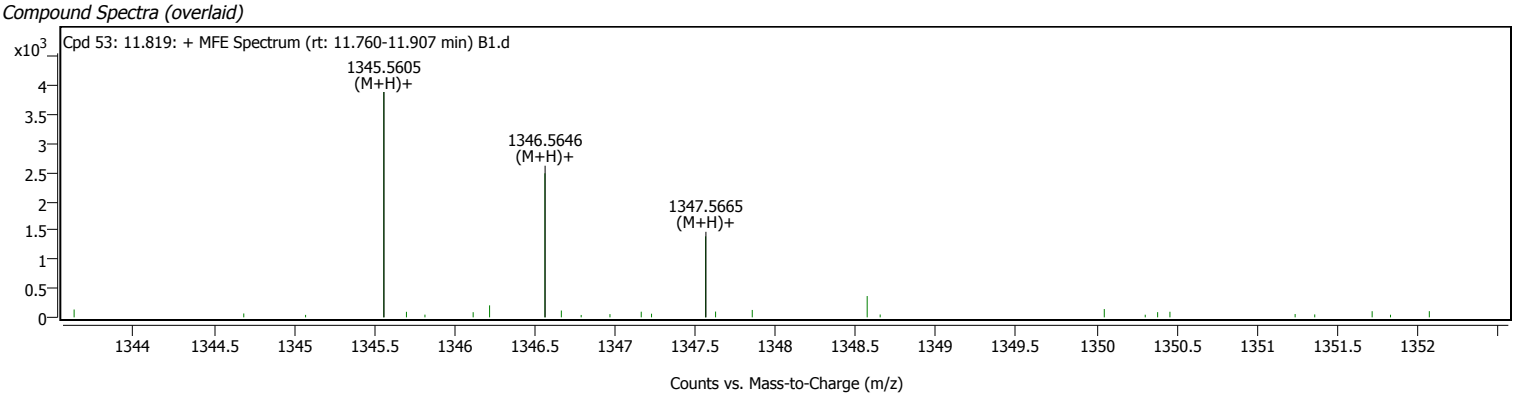
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.819		1344.5532				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

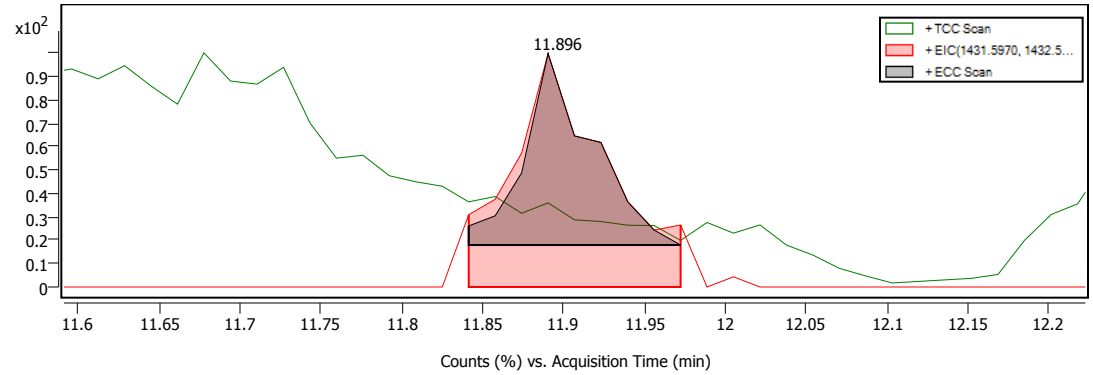


Cpd 54: 11.896

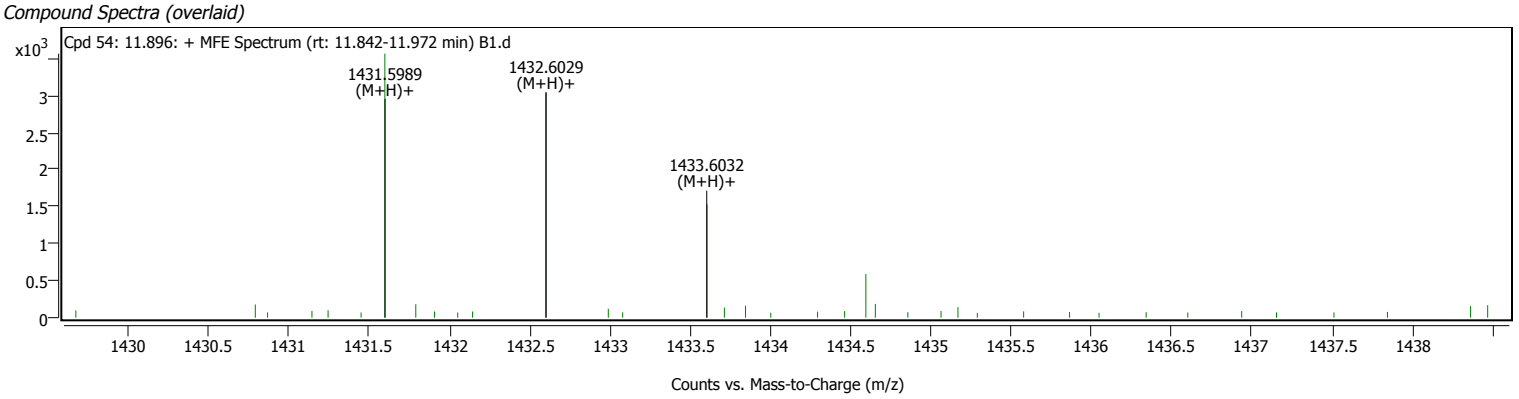
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		11.896		1430.5916				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 55: C35 H63 N13 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C35 H63 N13 O	11.994		681.5279		MFG	72.05	MFE	

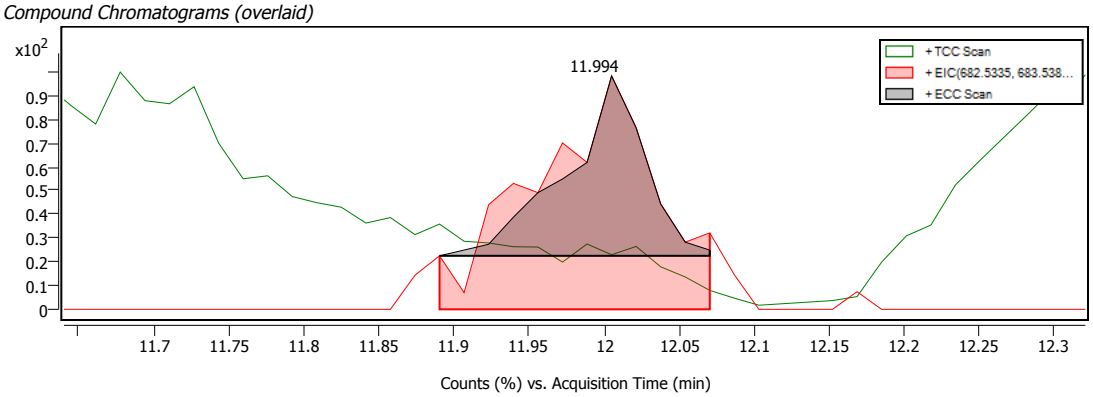
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	682.5355				5	72.05	

Compound ID Table

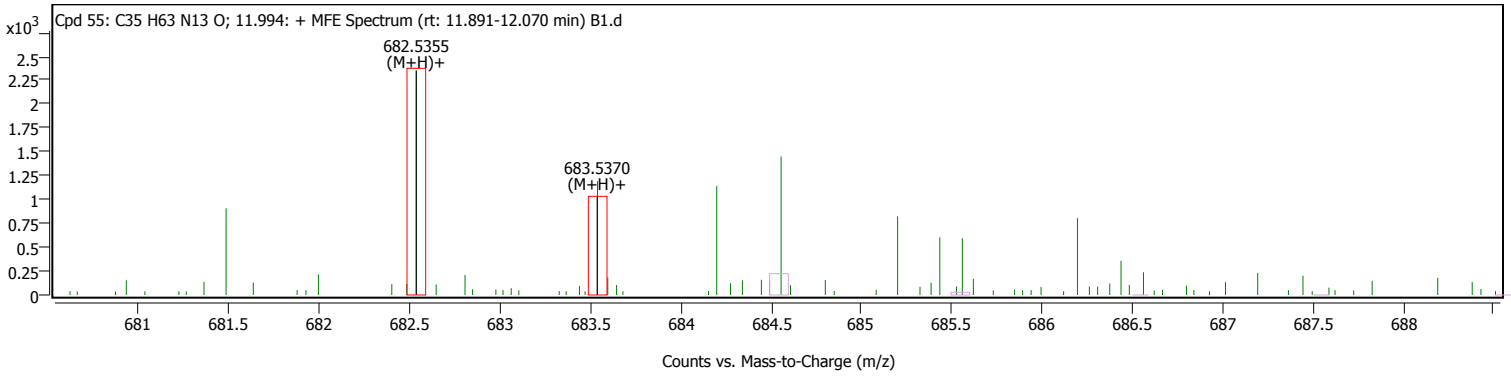
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C35 H63 N13 O	(M+H)+	MFG	11.994		681.5279		72.05		72.05
	C33 H61 N16	(M+H)+	MFG	11.994		681.5279		70.17		70.17
	C36 H69 N6 O6	(M+H)+	MFG	11.994		681.5278		69.73		69.73
	C37 H65 N10 O2	(M+H)+	MFG	11.994		681.5278		68.47		68.47
	C34 H67 N9 O5	(M+H)+	MFG	11.994		681.5278		68.16		68.16

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 56: C19 H24 N12

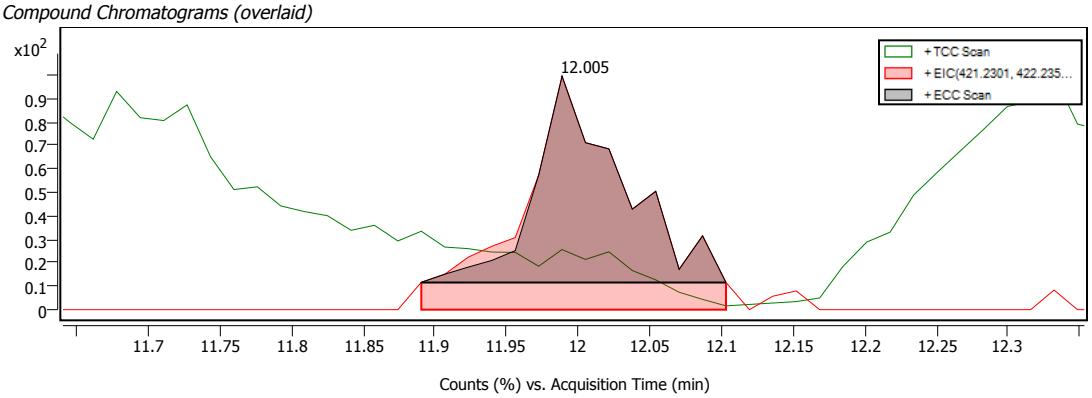
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C19 H24 N12	12.005		420.2242		MFG	77.66	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	421.2310				8	77.66	

Compound ID Table

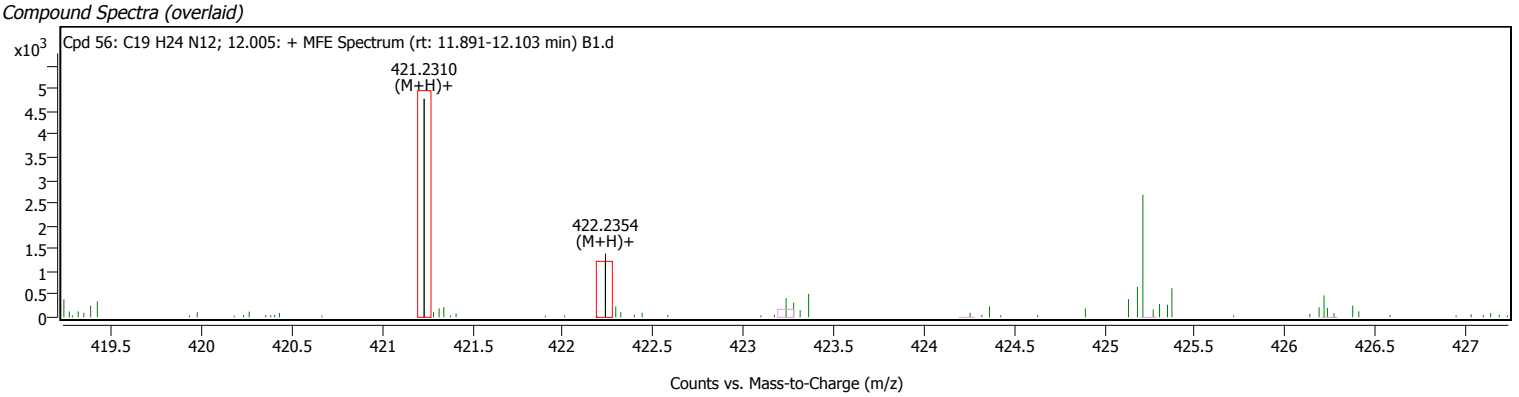
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C19 H24 N12	(M+H)+	MFG	12.005		420.2242		77.66		77.66
	C20 H30 N5 O5	(M+H)+	MFG	12.005		420.2241		75.62		75.62
His His Lys	C18 H28 N8 O4	(M+H)+	DBSearch-MFG	12.005		420.2242		72.80	72.71	72.88
Lys His His	C18 H28 N8 O4	(M+H)+	DBSearch-MFG	12.005		420.2242		72.80	72.71	72.88
His Lys His	C18 H28 N8 O4	(M+H)+	DBSearch-MFG	12.005		420.2242		72.80	72.71	72.88
	C21 H26 N9 O	(M+H)+	MFG	12.005		420.2242		71.64		71.64
	C19 H34 N O9	(M+H)+	MFG	12.005		420.2240		71.62		71.62
Tris(butoxyethyl)phosphate	C18 H39 O7 P	(M+Na)+	DBSearch	12.005		398.2420	78-51-3	66.66	66.66	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 57: C35 H61 N10 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C35 H61 N10 O2	12.017		653.4985		MFG	65.91	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	654.5047				5	65.91	

Compound Discovery Report

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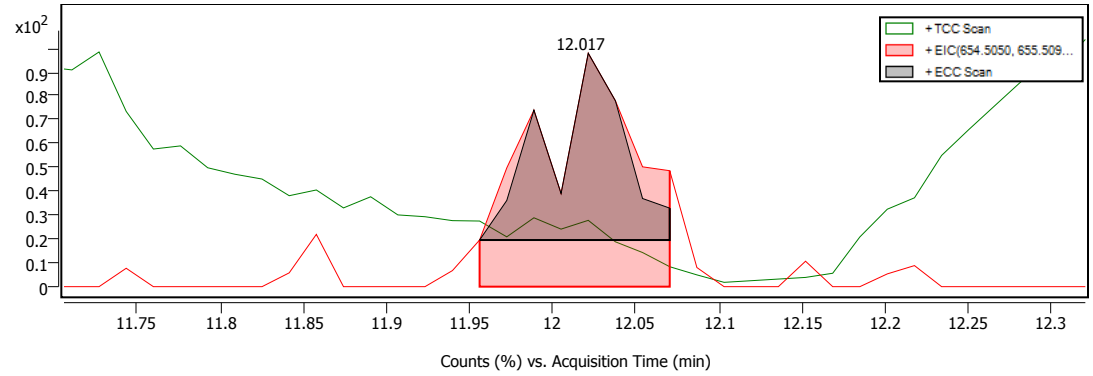
Compound ID Table

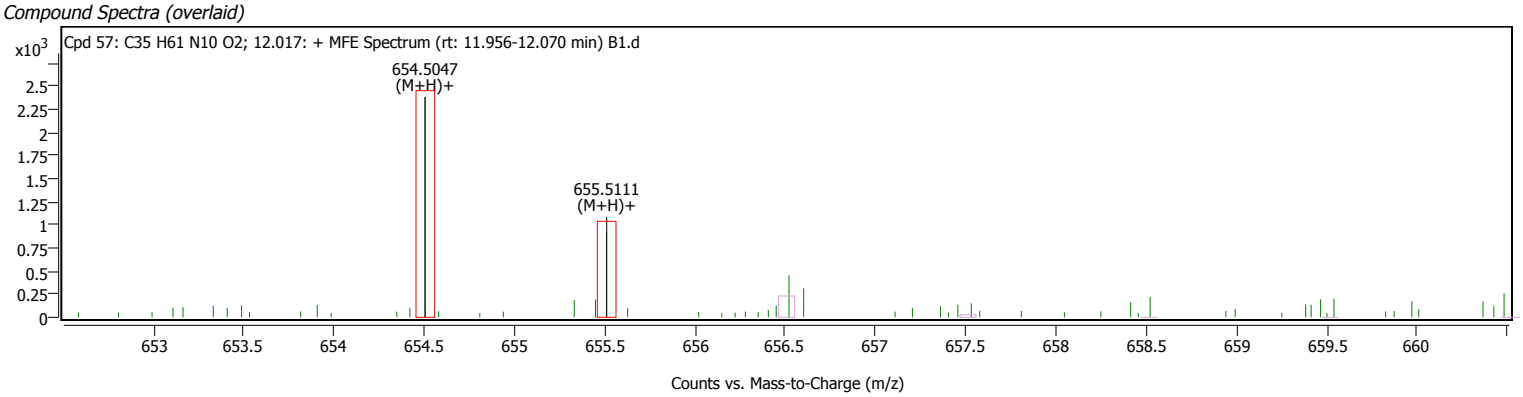
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C35 H61 N10 O2	(M+H)+	MFG	12.017		653.4985		65.91		65.91
	C37 H63 N7 O3	(M+H)+	MFG	12.017		653.4985		65.60		65.60
	C36 H67 N3 O7	(M+H)+	MFG	12.017		653.4984		64.97		64.97
	C38 H69 O8	(M+H)+	MFG	12.017		653.4984		64.32		64.32
	C33 H59 N13 O	(M+H)+	MFG	12.017		653.4986		60.64		60.64

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

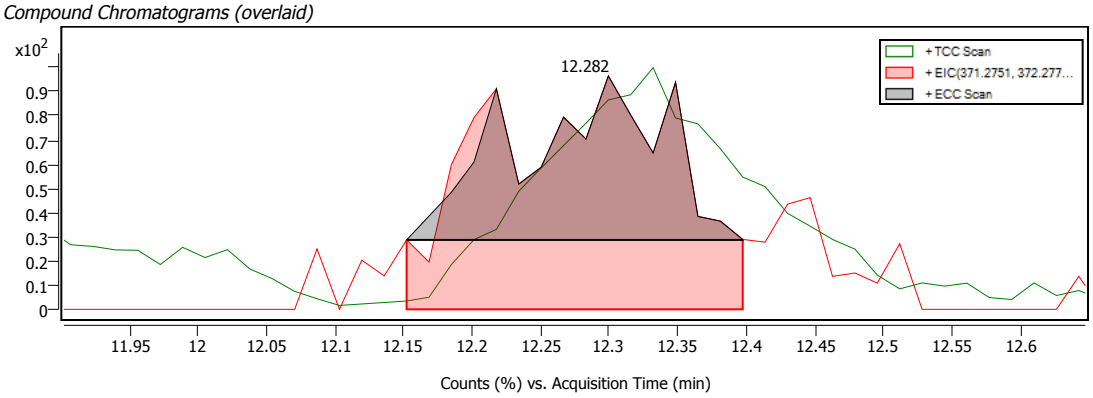


Cpd 58: 12.282

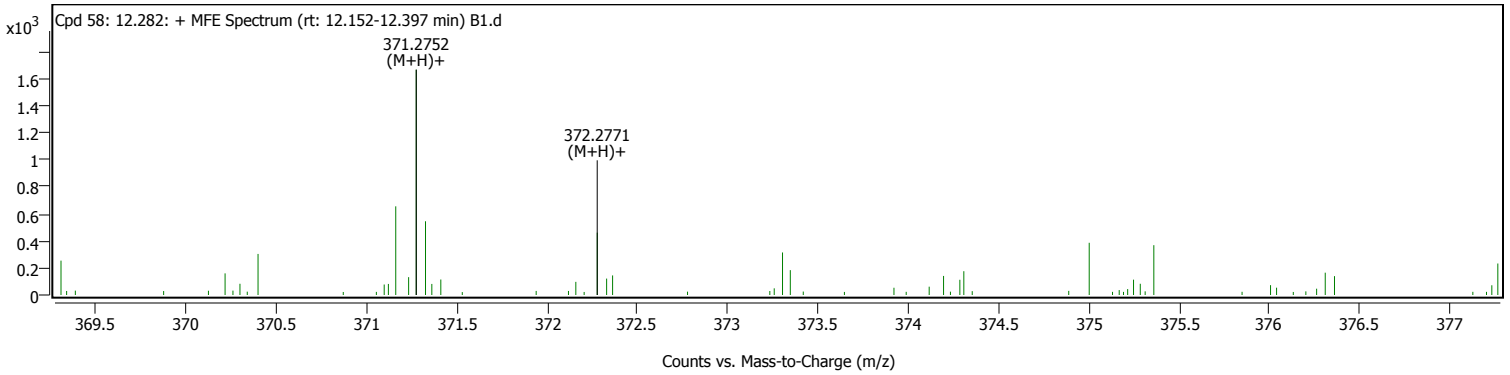
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		12.282		370.2679				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 59: C22 H50 N2 O10

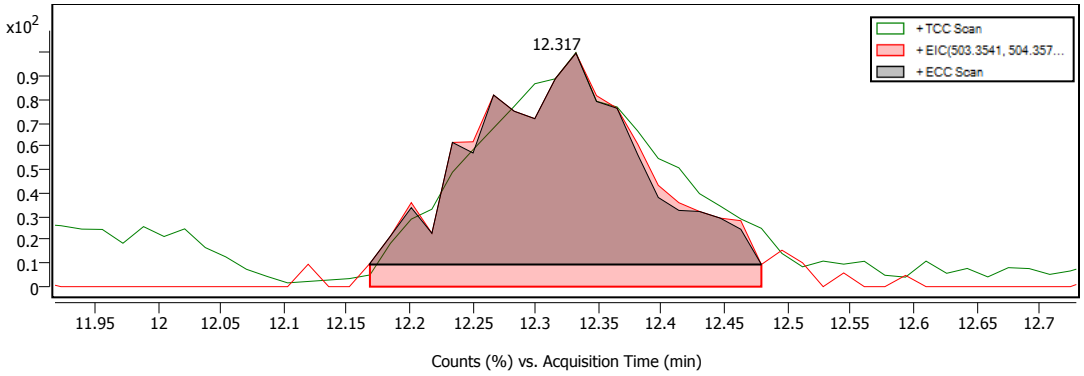
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H50 N2 O10	12.317		502.3466		MFG	85.62	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	503.3538				5	85.62	

Compound ID Table

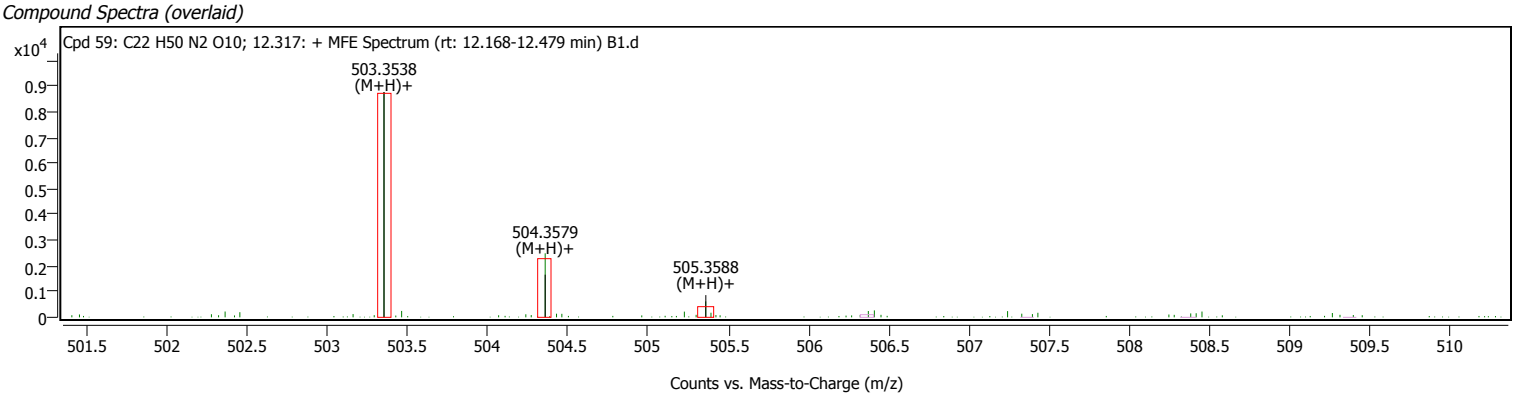
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H50 N2 O10	(M+H)+	MFG	12.317		502.3466		85.62		85.62
	C20 H48 N5 O9	(M+H)+	MFG	12.317		502.3467		81.90		81.90
	C16 H46 N12 O4 S	(M+H)+	MFG	12.317		502.3472		81.49		81.49
	C21 H44 N9 O5	(M+H)+	MFG	12.317		502.3467		81.44		81.44
	C23 H46 N6 O6	(M+H)+	MFG	12.317		502.3467		78.17		78.17

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 60: C22 H52 N5 O10

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H52 N5 O10	12.317		546.3716		MFG	82.39	MFE	

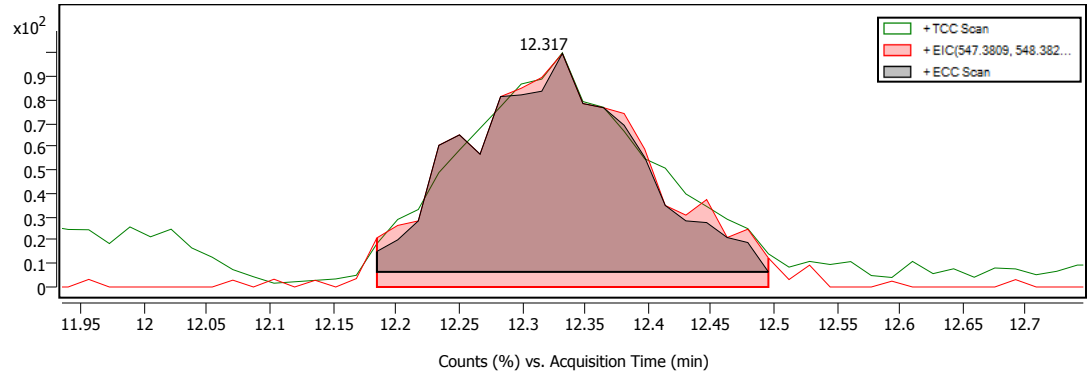
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	547.3787				5	82.39	

Compound ID Table

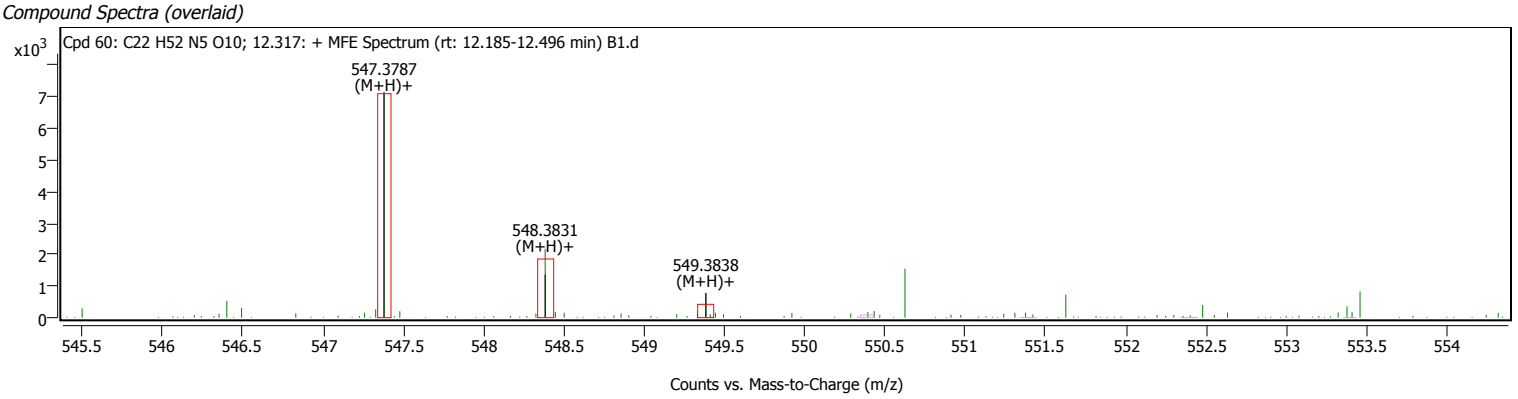
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H52 N5 O10	(M+H)+	MFG	12.317		546.3716		82.39		82.39
	C20 H50 N8 O9	(M+H)+	MFG	12.317		546.3716		78.24		78.24
	C21 H46 N12 O5	(M+H)+	MFG	12.317		546.3717		78.19		78.19
	C23 H48 N9 O6	(M+H)+	MFG	12.317		546.3716		76.04		76.04
	C22 H50 N12 S2	(M+H)+	MFG	12.317		546.3722		75.14		75.14

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 61: C19 H40 N9 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C19 H40 N9 O4	12.318		458.3204		MFG	83.04	MFE	

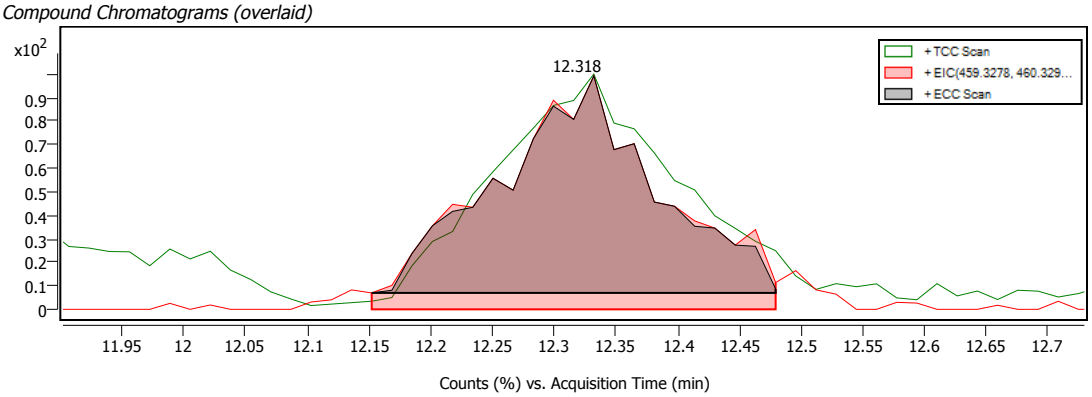
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	459.3273				5	83.04	

Compound ID Table

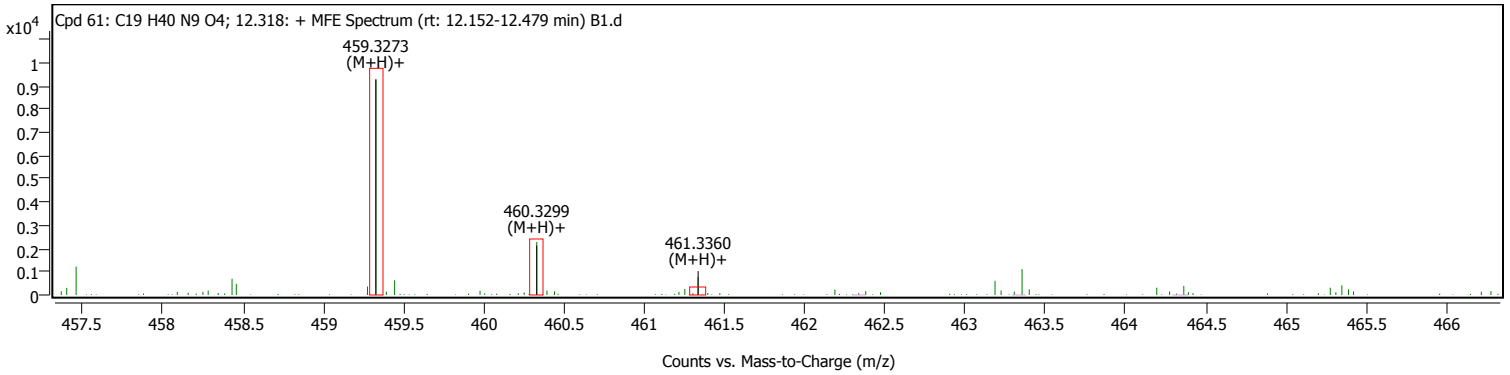
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C19 H40 N9 O4	(M+H)+	MFG	12.318		458.3204		83.04		83.04
	C14 H42 N12 O3 S	(M+H)+	MFG	12.318		458.3210		81.93		81.93
	C18 H44 N5 O8	(M+H)+	MFG	12.318		458.3203		81.51		81.51
	C22 H46 N6 S2	(M+H)+	MFG	12.318		458.3209		79.99		79.99
	C21 H42 N6 O5	(M+H)+	MFG	12.318		458.3203		79.80		79.80

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 62: C22 H44 N19 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H44 N19 O	12.322		590.3981		MFG	79.13	MFE	

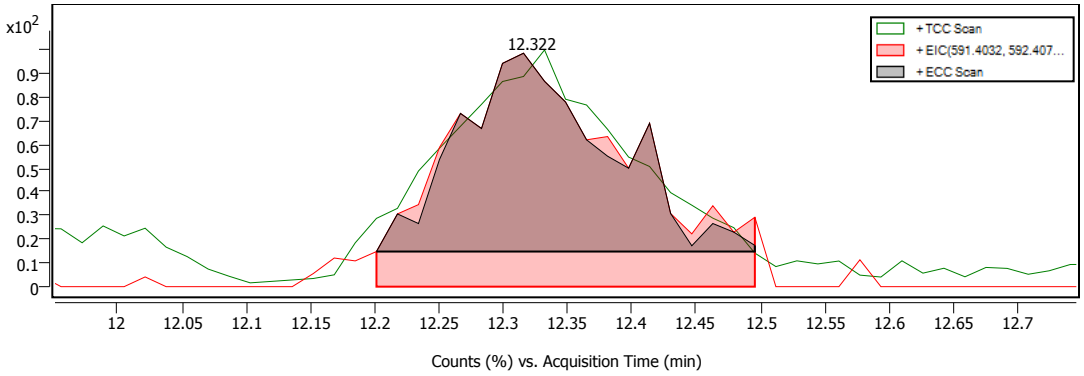
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	591.4055				5	79.13	

Compound ID Table

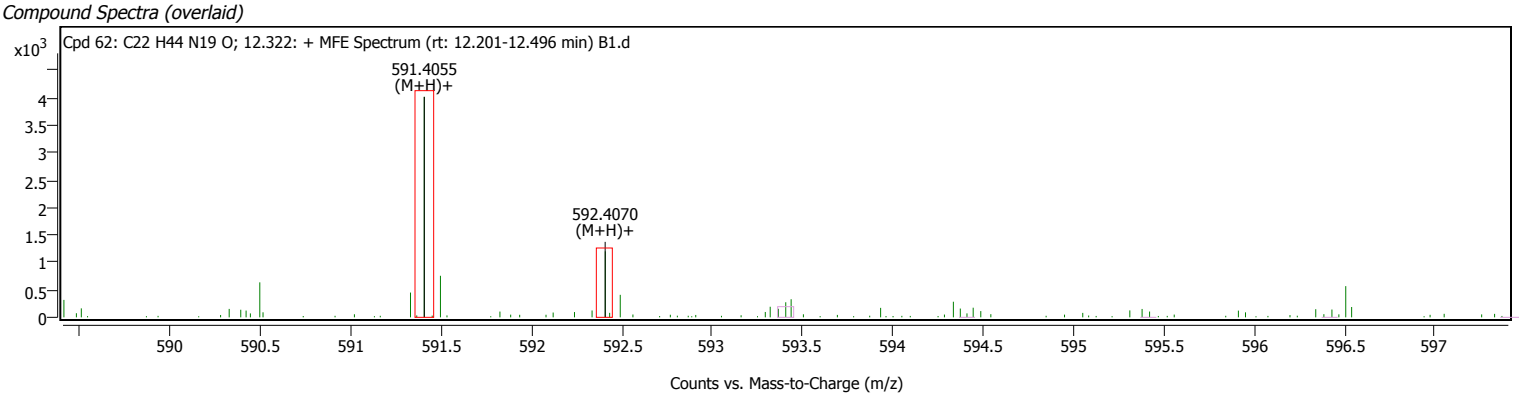
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H44 N19 O	(M+H)+	MFG	12.322		590.3981		79.13		79.13
	C24 H46 N16 O2	(M+H)+	MFG	12.322		590.3980		77.60		77.60
	C23 H50 N12 O6	(M+H)+	MFG	12.322		590.3979		75.95		75.95
	C25 H52 N9 O7	(M+H)+	MFG	12.322		590.3979		73.91		73.91
	C20 H42 N22	(M+H)+	MFG	12.322		590.3981		73.88		73.88

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 63: C41 H54 N4 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C41 H54 N4 O2	12.323		634.4250		MFG	66.07	MFE	

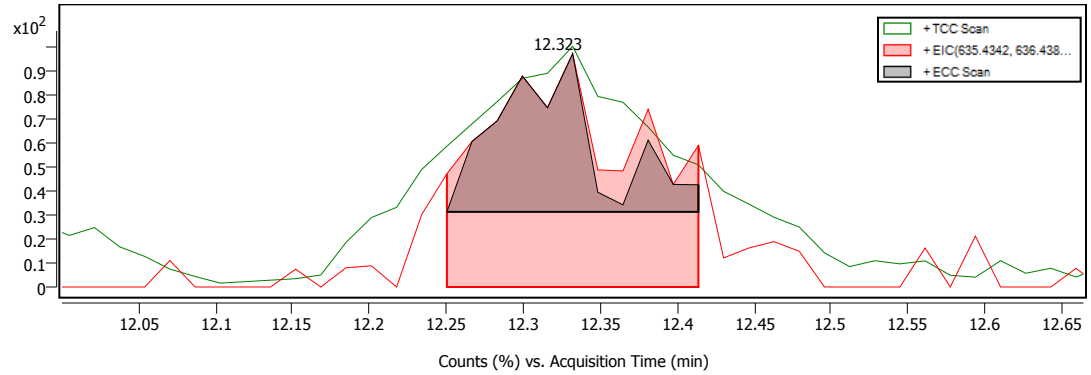
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	635.4313				5	66.07	

Compound ID Table

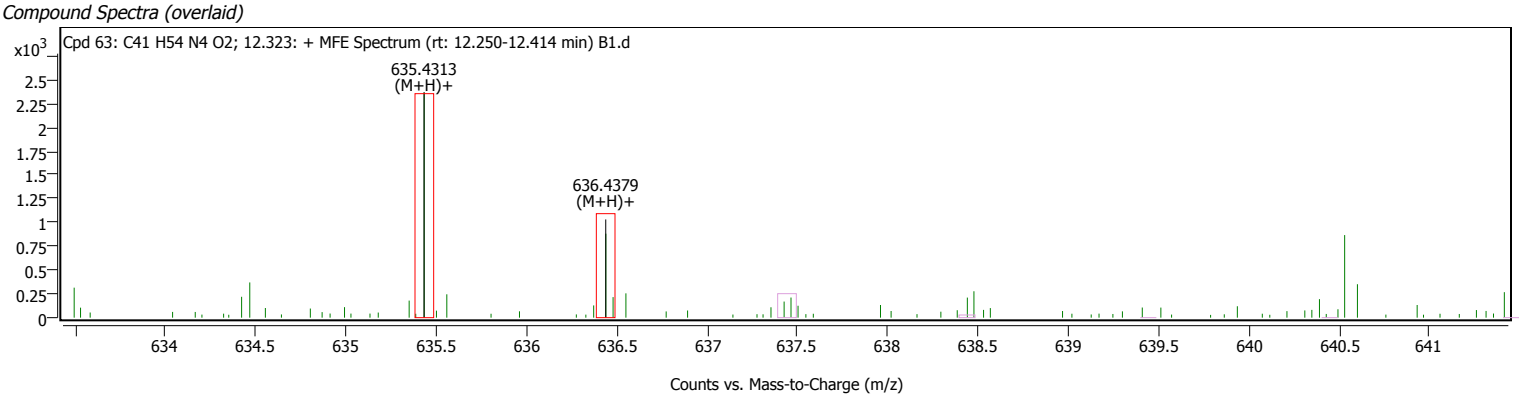
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C41 H54 N4 O2	(M+H)+	MFG	12.323		634.4250		66.07		66.07
	C43 H56 N O3	(M+H)+	MFG	12.323		634.4250		64.00		64.00
	C26 H50 N16 O3	(M+H)+	MFG	12.323		634.4253		63.66		63.66
	C39 H52 N7 O	(M+H)+	MFG	12.323		634.4251		62.40		62.40
	C40 H58 O6	(M+H)+	MFG	12.323		634.4250		62.26		62.26

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

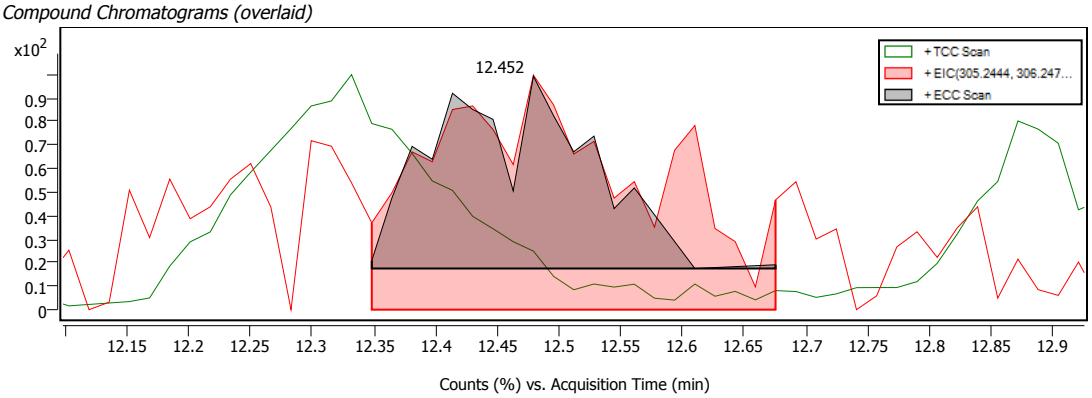


Cpd 64: 12.452

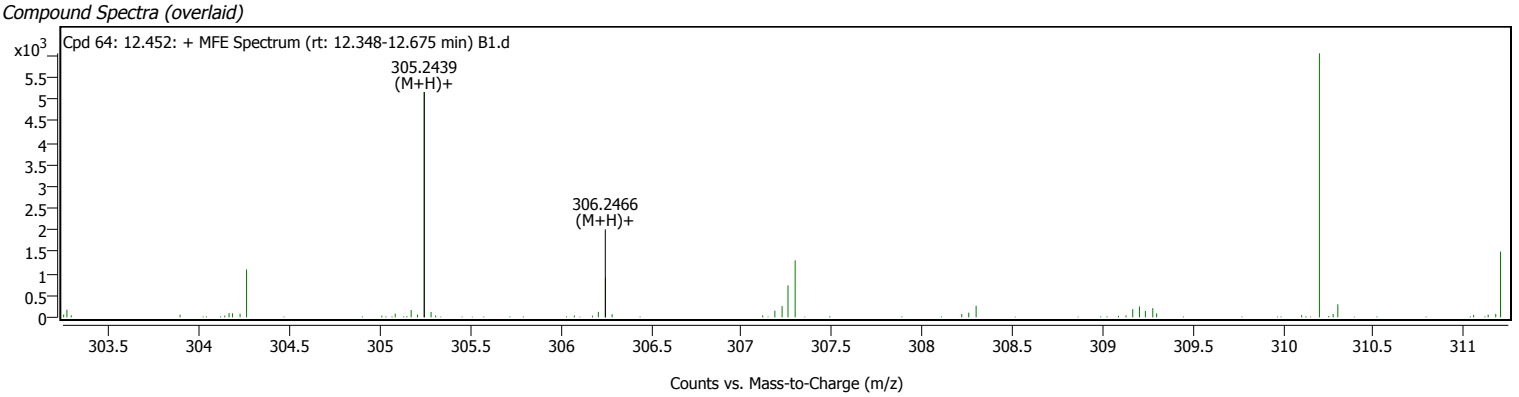
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		12.452		304.2366				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 65: C24 H38 N16

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C24 H38 N16	12.584		550.3461		MFG	69.05	MFE	

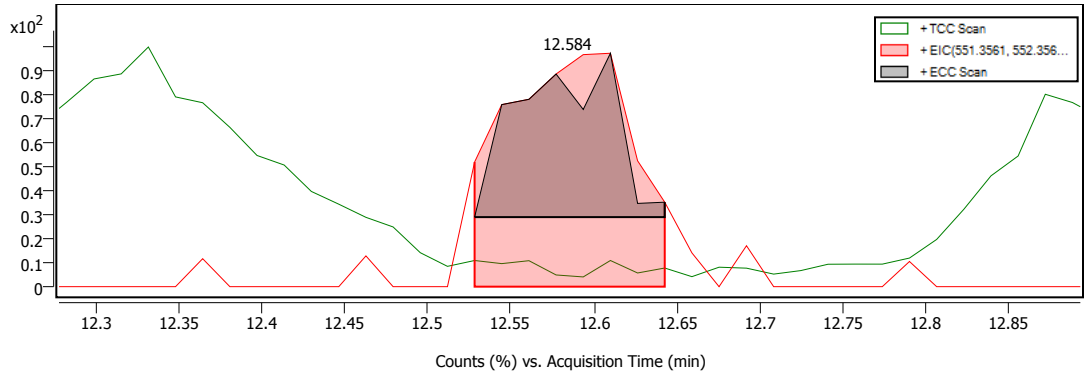
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	551.3523				5	69.05	

Compound ID Table

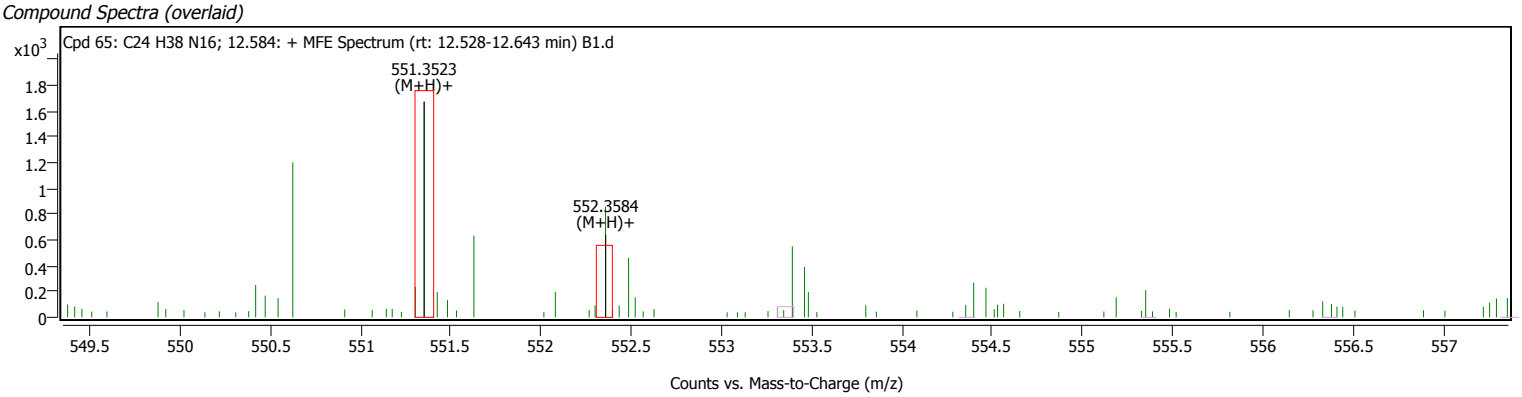
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C24 H38 N16	(M+H)+	MFG	12.584		550.3461		69.05		69.05
	C38 H46 O3	(M+H)+	MFG	12.584		550.3458		68.12		68.12
	C25 H44 N9 O5	(M+H)+	MFG	12.584		550.3460		66.81		66.81
	C23 H42 N12 O4	(M+H)+	MFG	12.584		550.3460		64.85		64.85
	C26 H50 N2 O10	(M+H)+	MFG	12.584		550.3458		64.82		64.82

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 66: C19 H40 N9 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C19 H40 N9 O3	12.768		442.3251		MFG	83.96	MFE	

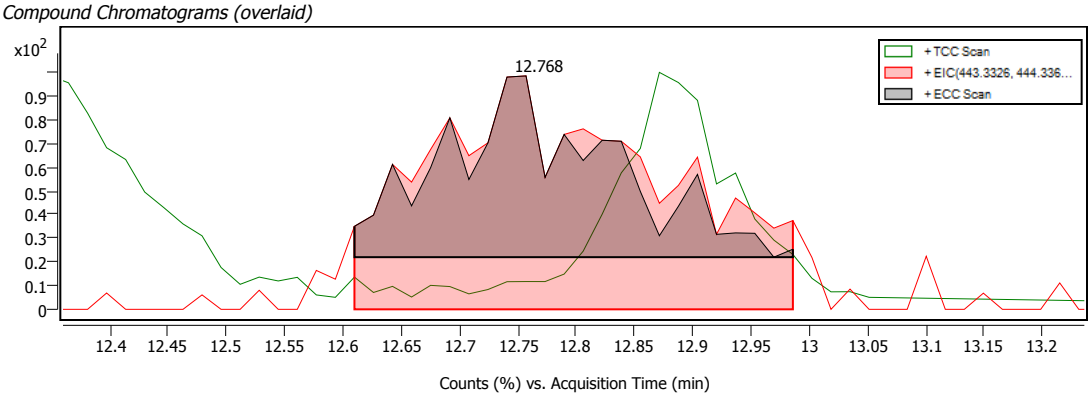
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	443.3323				6	83.96	

Compound ID Table

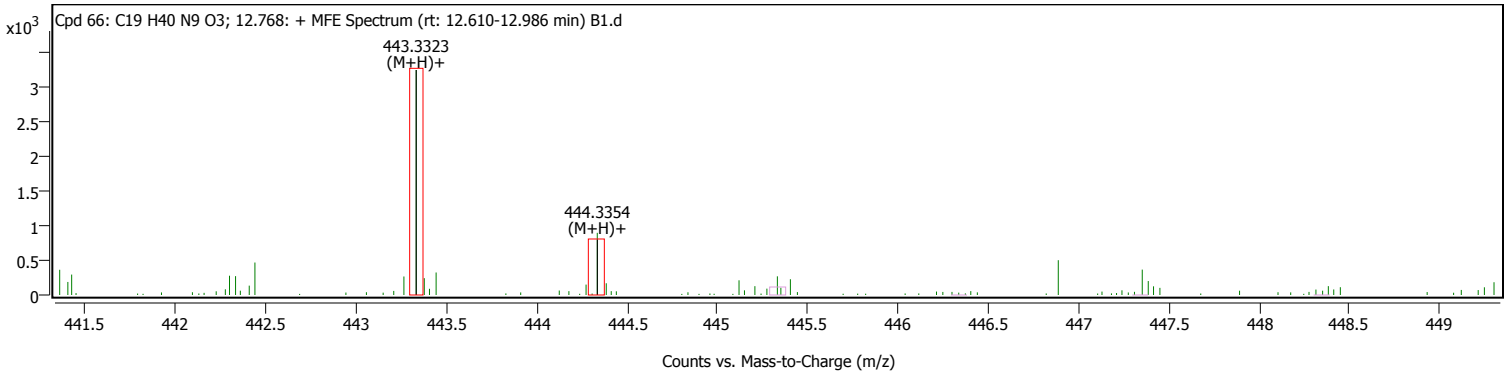
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C19 H40 N9 O3	(M+H)+	MFG	12.768		442.3251		83.96		83.96
	C20 H46 N2 O8	(M+H)+	MFG	12.768		442.3250		81.66		81.66
	C17 H38 N12 O2	(M+H)+	MFG	12.768		442.3252		80.87		80.87
	C18 H44 N5 O7	(M+H)+	MFG	12.768		442.3251		79.50		79.50
	C21 H42 N6 O4	(M+H)+	MFG	12.768		442.3251		77.52		77.52
(all-E)-6'-Apo-y-caroten-6'-al	C32 H42 O	(M+H)+	DBSearch	12.768		442.3250	22255-36-3	67.97	67.97	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 67: C31 H40 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H40 O	12.818		428.3087		MFG	62.56	MFE	

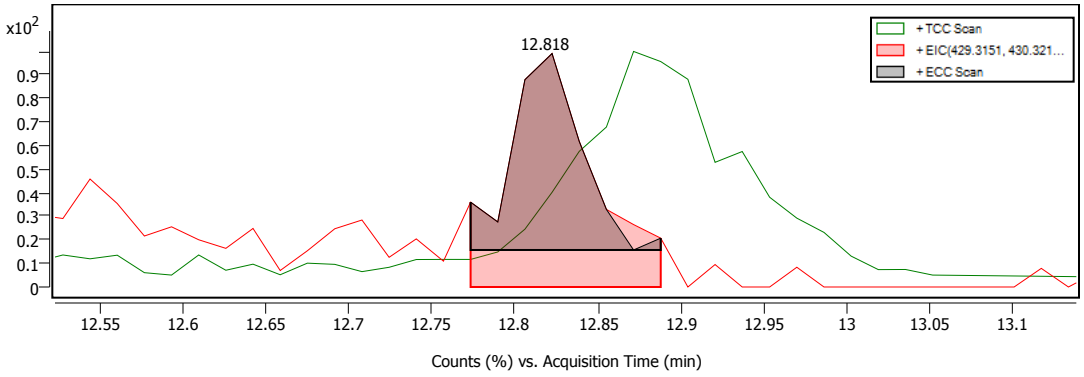
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	429.3155				3	62.56	

Compound ID Table

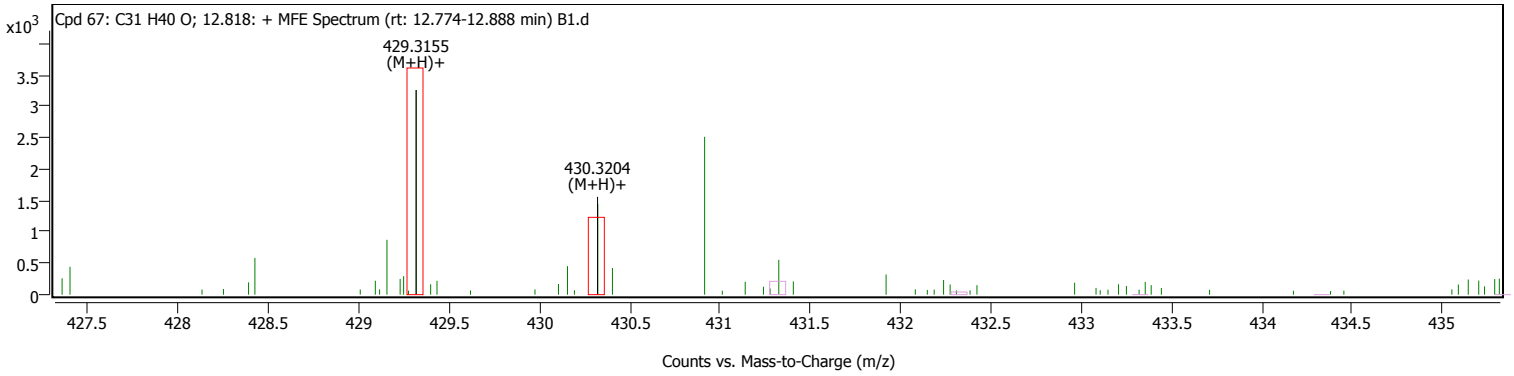
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H40 O	(M+H)+	MFG	12.818		428.3087		62.56		62.56
	C29 H38 N3	(M+H)+	MFG	12.818		428.3088		52.29		52.29
	C28 H44 O S	(M+H)+	MFG	12.818		428.3088		45.98		45.98

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 68: C26 H46 N9 O4

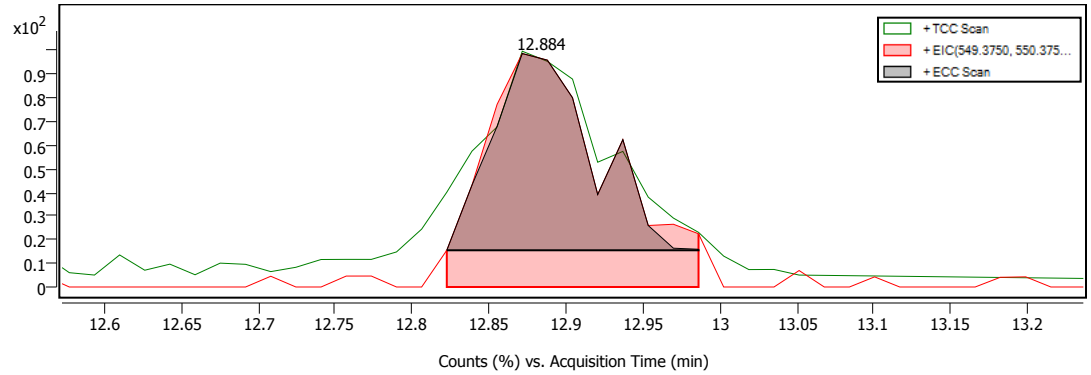
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C26 H46 N9 O4	12.884		548.3670		MFG	77.06	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	549.3745				5	77.06	

Compound ID Table

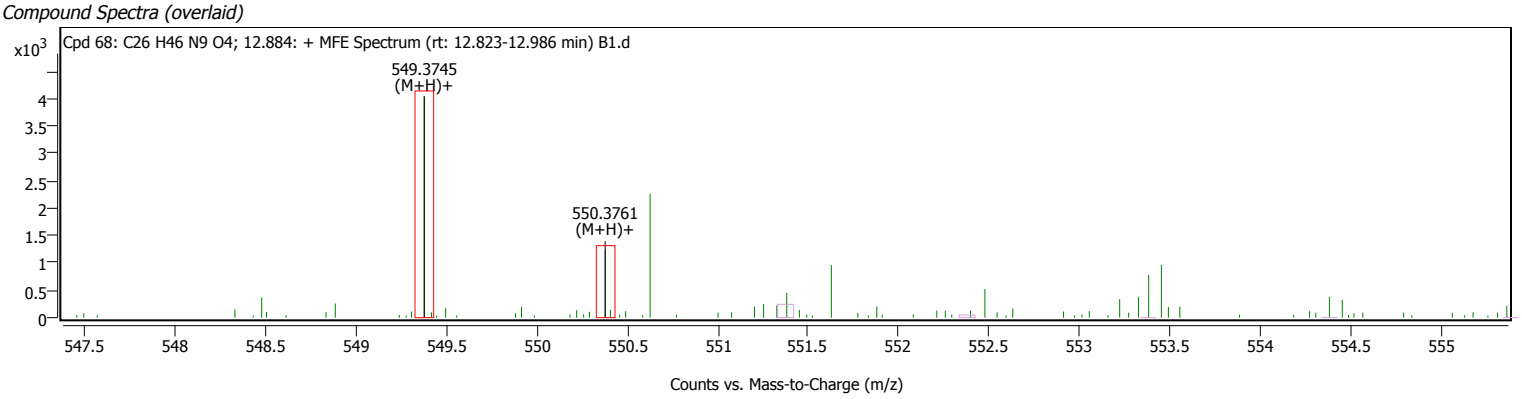
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C26 H46 N9 O4	(M+H)+	MFG	12.884		548.3670		77.06		77.06
	C24 H44 N12 O3	(M+H)+	MFG	12.884		548.3670		75.52		75.52
	C27 H42 N13	(M+H)+	MFG	12.884		548.3670		74.99		74.99
	C27 H52 N2 O9	(M+H)+	MFG	12.884		548.3668		73.20		73.20
	C25 H50 N5 O8	(M+H)+	MFG	12.884		548.3669		72.24		72.24

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 69: Petromyzonol

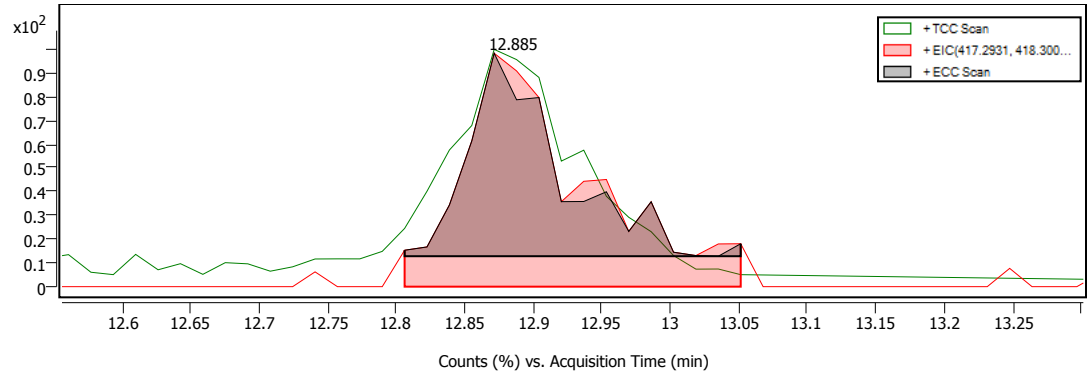
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Petromyzonol	C24 H42 O4	12.885		394.3068	28979-29-5	DBSearch	68.32	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	417.2956 417.2956 417.2956		2	68.32	15		

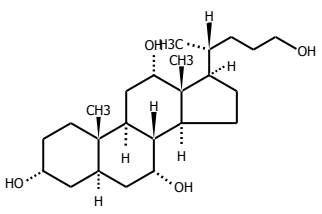
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Petromyzonol	C24 H42 O4	(M+Na)+	DBSearch	12.885		394.3068	28979-29-5	68.32	68.32	
5β-Cholane-3α,7α,12α,24-tetrol	C24 H42 O4	(M+Na)+	DBSearch	12.885		394.3068		68.32	68.32	
5β-Cholane-3α,7α,23,24-tetrol	C24 H42 O4	(M+Na)+	DBSearch	12.885		394.3068		68.32	68.32	
5beta-Cholane-3alpha,7alpha,12alpha,24-tetrol	C24 H42 O4	(M+Na)+	DBSearch	12.885		394.3068		68.32	68.32	
5beta-Cholane-3alpha,7alpha,23,24-tetrol	C24 H42 O4	(M+Na)+	DBSearch	12.885		394.3068		68.32	68.32	
	C13 H38 N12 S	(M+Na)+	MFG	12.885		394.3064		47.61		47.61
	C17 H37 N8 O4	(M+H)+	MFG	12.885		417.2935		47.48		47.48
	C17 H41 Cl N7 O	(M+Na)+	MFG	12.885		394.3064		47.46		47.46
	C25 H41 N2 O S	(M+H)+	MFG	12.885		417.2935		47.18		47.18
	C22 H40 N3 O3	(M+Na)+	MFG	12.885		394.3064		46.70		46.70
	C12 H38 Cl N12 O2	(M+H)+	MFG	12.885		417.2935		46.66		46.66
	C24 H45 Cl2 N	(M+H)+	MFG	12.885		417.2935		46.61		46.61
	C20 H38 N6 O2	(M+Na)+	MFG	12.885		394.3064		46.26		46.26
	C22 H44 Cl N3 S	(M+H)+	MFG	12.885		417.2935		45.60		45.60
	C19 H43 Cl N4 O2	(M+Na)+	MFG	12.885		394.3064		44.69		44.69

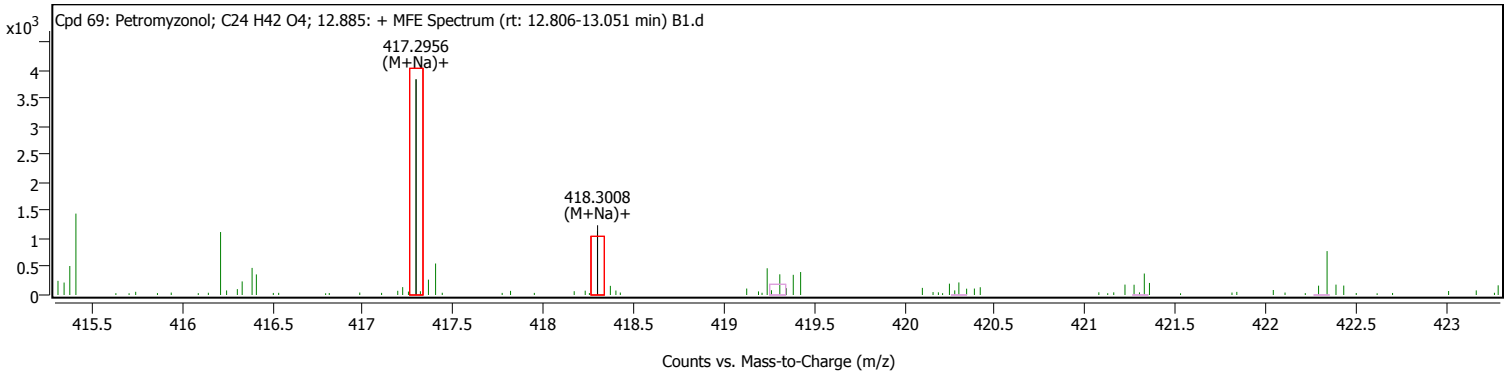
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 70: PC(O-16:0/0:0)[U]

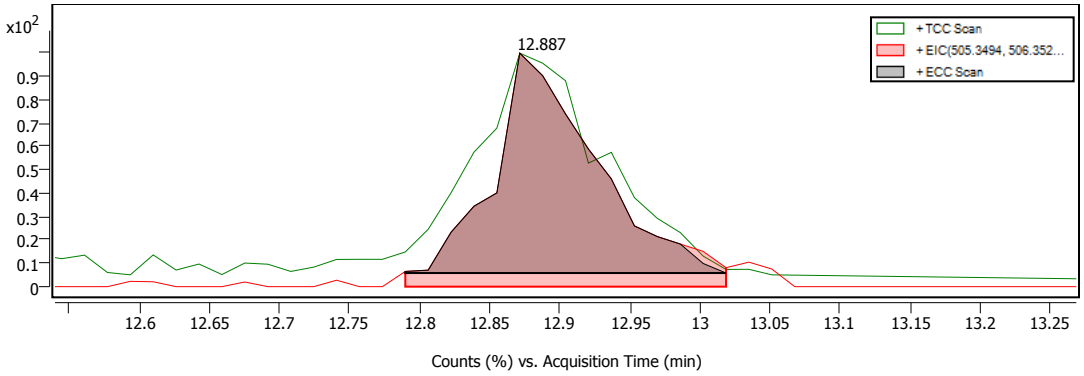
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(O-16:0/0:0)[U]	C24 H53 N O6 P	12.887		482.3595		DBSearch	70.29	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	505.3489 505.3489 505.3489 505.3489		0	70.29	17		

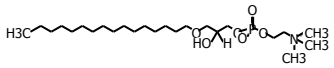
Compound ID Table

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	12.887		482.3595		70.29	70.29	
Lyso-PAF C-16	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595	52691-62-0	70.29	70.29	
PC(O-15:0/O-1:0)[U]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595		70.29	70.29	
PC(O-8:0/O-8:0)	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595		70.29	70.29	
PC(O-8:0/O-8:0)[U]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595		70.29	70.29	
PC(O-16:0/0:0)	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595		70.29	70.29	
PC(O-16:0/0:0)[S]	C24 H53 N O6 P	(M+Na)+	DBSearch	12.887		482.3595		70.29	70.29	
	C22 H48 Cl N9 S	(M+H)+	MFG	12.887		505.3442		47.62		47.62
	C23 H51 Cl N4 O4	(M+Na)+	MFG	12.887		482.3597		47.52		47.52
	C26 H51 Cl2 N4 O	(M+H)+	MFG	12.887		505.3442		47.52		47.52
	C26 H48 N3 O5	(M+Na)+	MFG	12.887		482.3597		47.47		47.47
	C25 H42 N10	(M+Na)+	MFG	12.887		482.3597		47.47		47.47
	C27 H55 N O S3	(M+H)+	MFG	12.887		505.3442		47.35		47.35
	C19 H48 N9 O3 S	(M+Na)+	MFG	12.887		482.3597		47.26		47.26
	C26 H51 N O6 S	(M+H)+	MFG	12.887		505.3442		47.10		47.10
	C25 H45 N8 O S	(M+H)+	MFG	12.887		505.3442		47.09		47.09
	C27 H52 N3 S2	(M+Na)+	MFG	12.887		482.3597		46.89		46.89

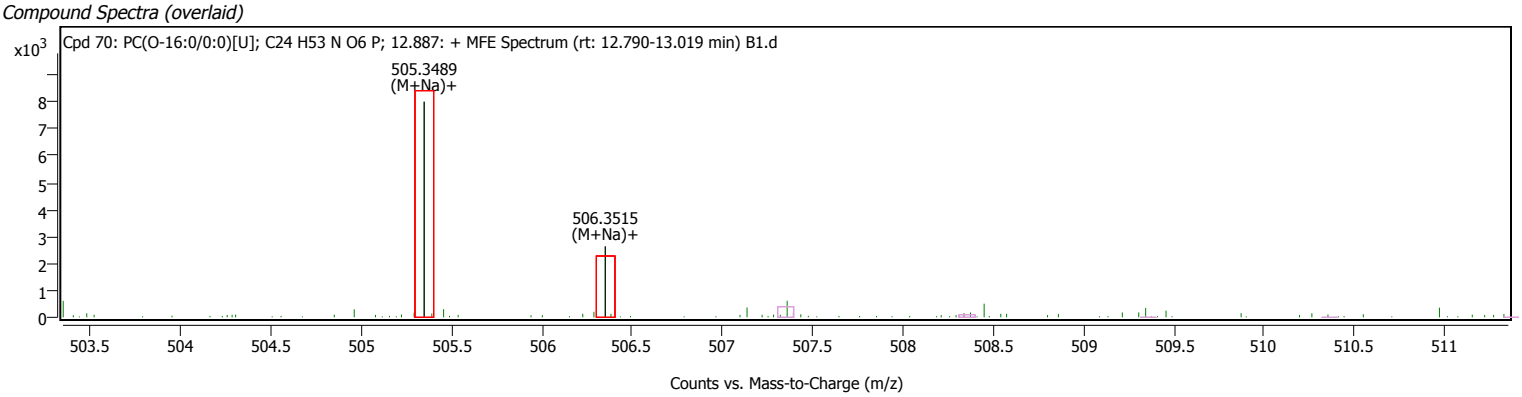
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 71: 27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol

Compound Discovery Report

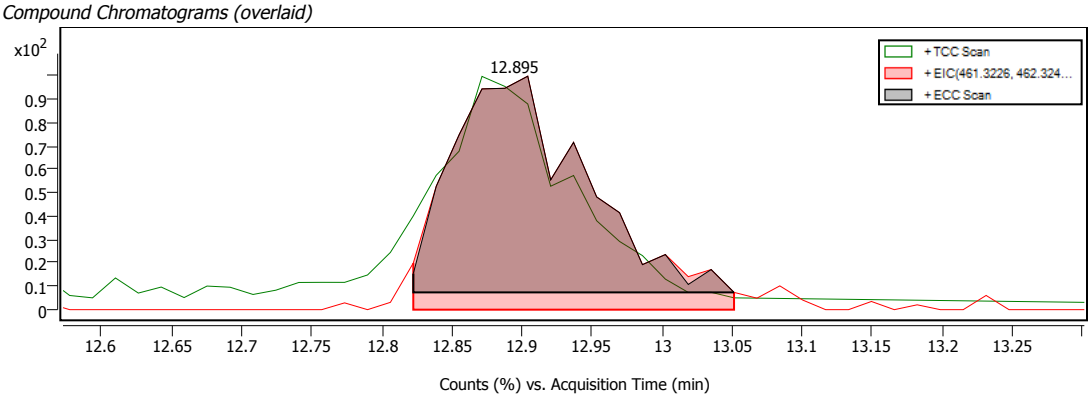
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.895		438.3324	78648-95-0	DBSearch	64.90	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	461.3220 461.3220 461.3220 461.3220		0	64.90	11		

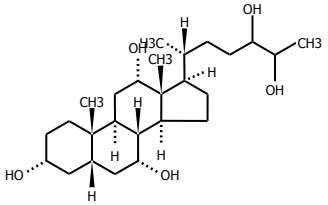
Compound ID Table

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	12.895		438.3324	78648-95-0	64.90	64.90	
	C30 H41 N2 O2	(M+H)+	MFG	12.895		461.3167		47.61		47.61
	C15 H42 N12 O S	(M+Na)+	MFG	12.895		438.3327		47.51		47.51
	C19 H45 Cl N7 O2	(M+Na)+	MFG	12.895		438.3327		47.22		47.22
	C24 H44 N3 O4	(M+Na)+	MFG	12.895		438.3327		47.19		47.19
	C27 H44 Cl N3 O	(M+H)+	MFG	12.895		461.3167		46.94		46.94
	C15 H37 N14 O3	(M+H)+	MFG	12.895		461.3167		46.91		46.91
	C22 H45 N4 O4 S	(M+H)+	MFG	12.895		461.3167		46.84		46.84
	C30 H46 S	(M+Na)+	MFG	12.895		438.3327		46.44		46.44
	C23 H41 N8 S	(M+H)+	MFG	12.895		461.3167		46.37		46.37
	C22 H42 N6 O3	(M+Na)+	MFG	12.895		438.3327		45.79		45.79

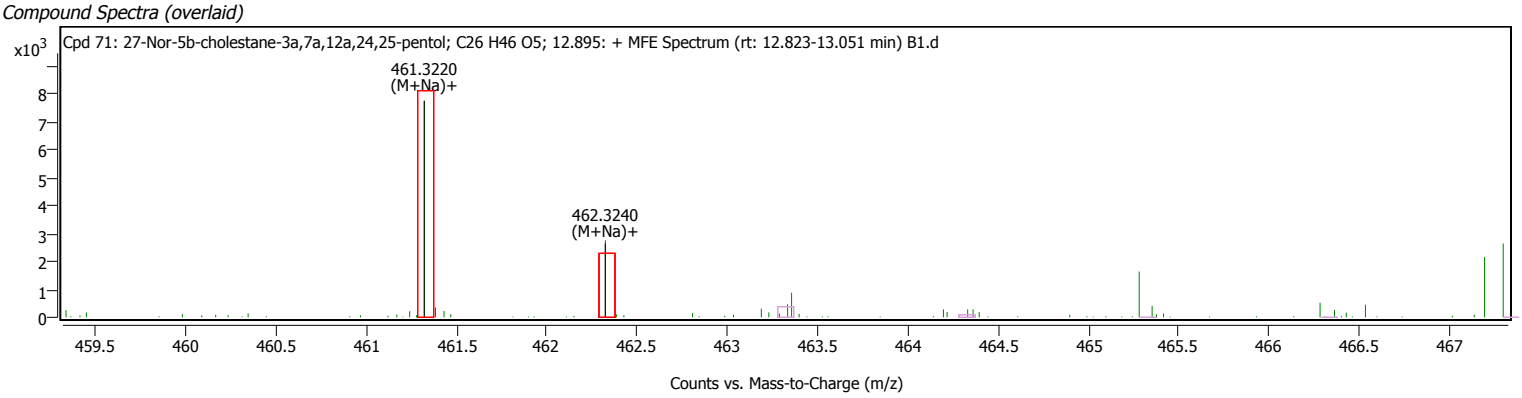
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 72: C43 H39 Cl3 N3 O3 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C43 H39 Cl3 N3 O3 S	13.397		782.1778		MFG	47.62	MFE	

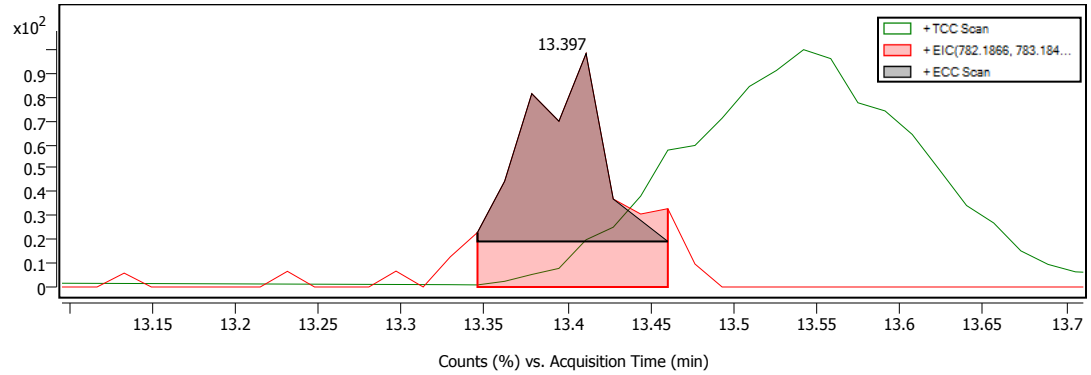
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	783.1851				11	47.62	

Compound ID Table

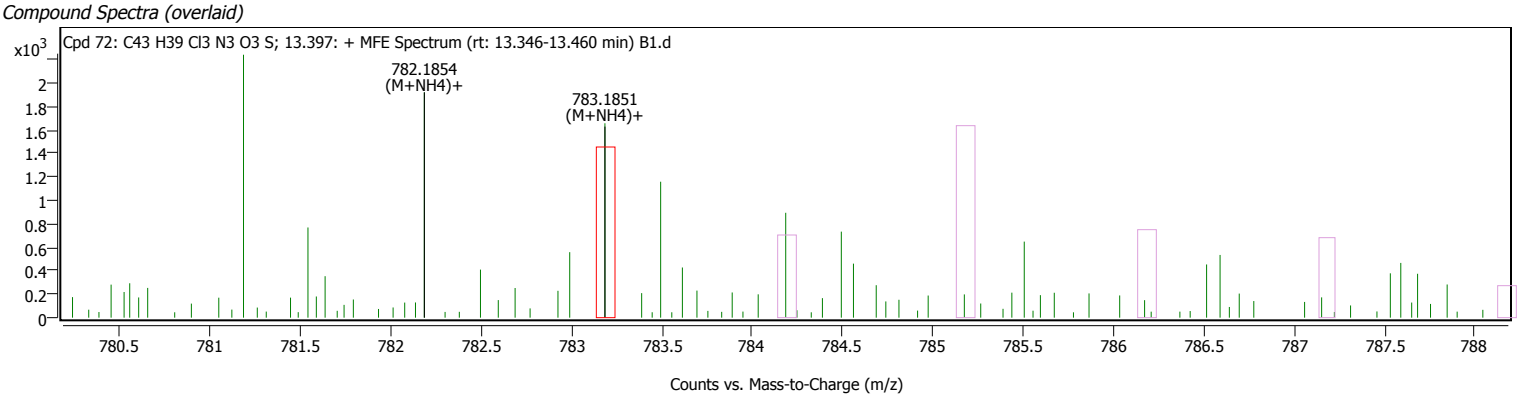
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C43 H39 Cl3 N3 O3 S	(M+H)+	MFG	13.397		782.1778		47.62		47.62
	C52 H21 Cl N6	(M+NH4)+	MFG	13.397		764.1516		47.62		47.62
	C30 H26 Cl2 N21 S	(M+H)+	MFG	13.397		782.1778		47.62		47.62
	C31 H32 Cl2 N14 O5 S	(M+H)+	MFG	13.397		782.1778		47.62		47.62
	C32 H38 Cl2 N7 O10 S	(M+H)+	MFG	13.397		782.1778		47.62		47.62
	C33 H44 Cl2 O15 S	(M+H)+	MFG	13.397		782.1778		47.62		47.62
	C41 H20 N10 O7	(M+NH4)+	MFG	13.397		764.1516		47.62		47.62
	C42 H26 N3 O12	(M+NH4)+	MFG	13.397		764.1516		47.62		47.62
	C37 H25 Cl N14 S2	(M+NH4)+	MFG	13.397		764.1516		47.62		47.62
	C38 H31 Cl N7 O5 S2	(M+NH4)+	MFG	13.397		764.1516		47.62		47.62
Fast green FCF aluminium salt	C37 H36 N2 O10 S3	(M+NH4)+	DBSearch	13.397		764.1500		44.66	44.66	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

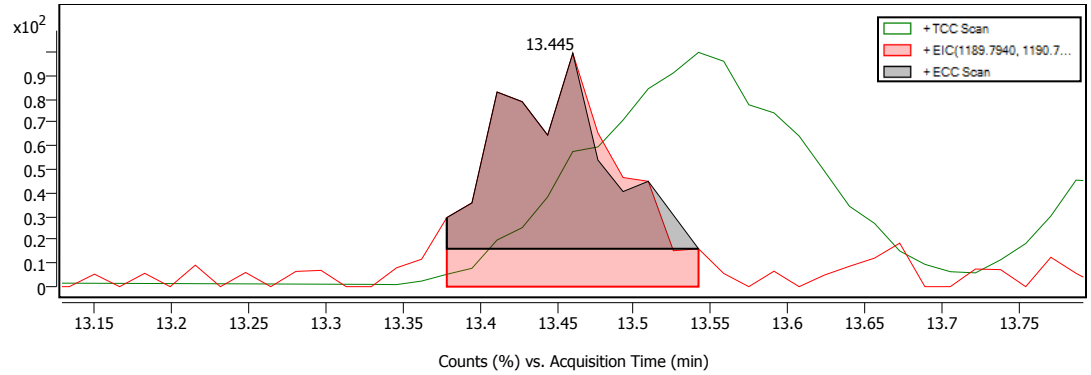


Cpd 73: 13.445

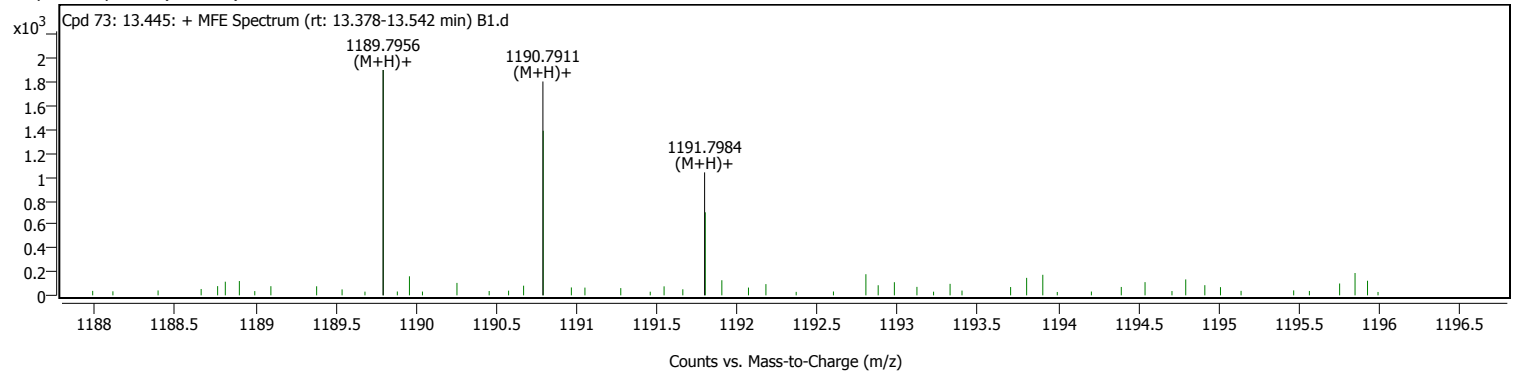
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.445		1188.7883				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

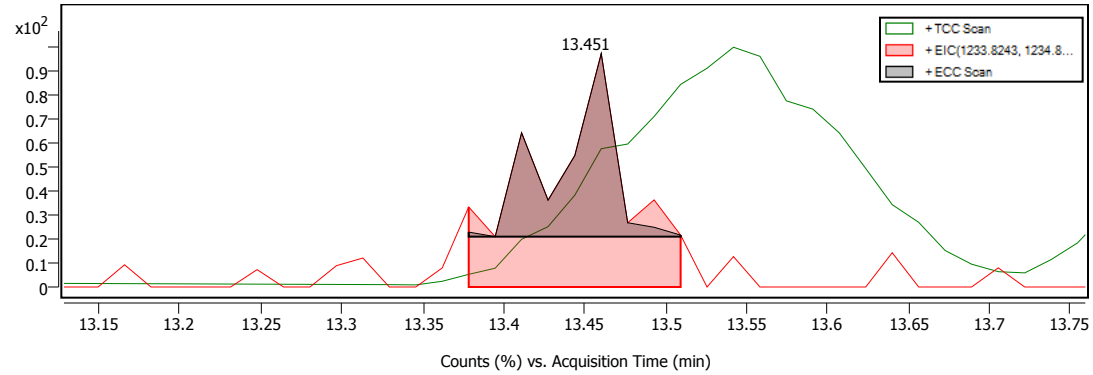


Cpd 74: 13.451

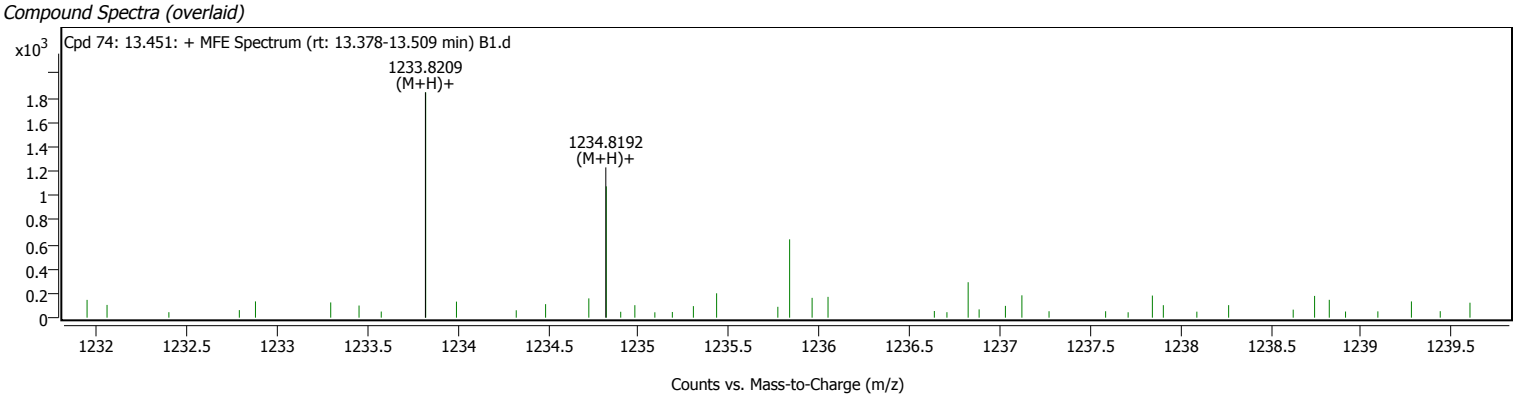
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.451		1232.8136				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

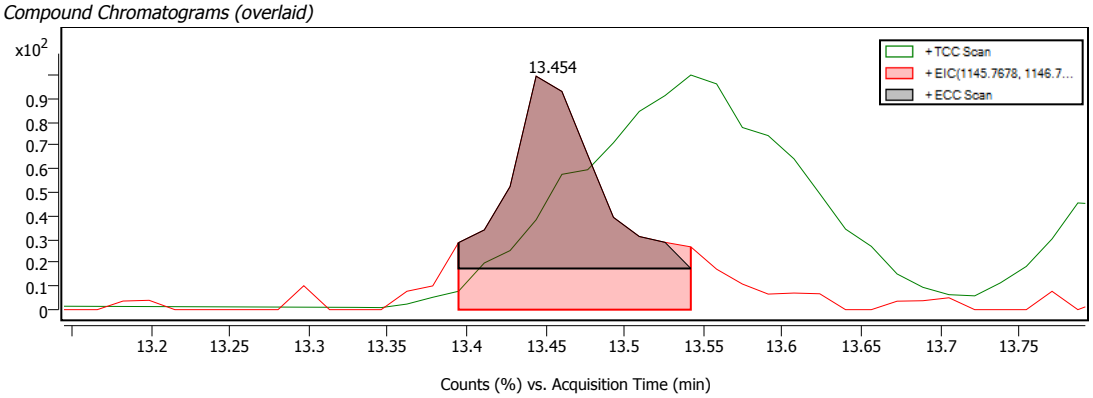


Cpd 75: 13.454

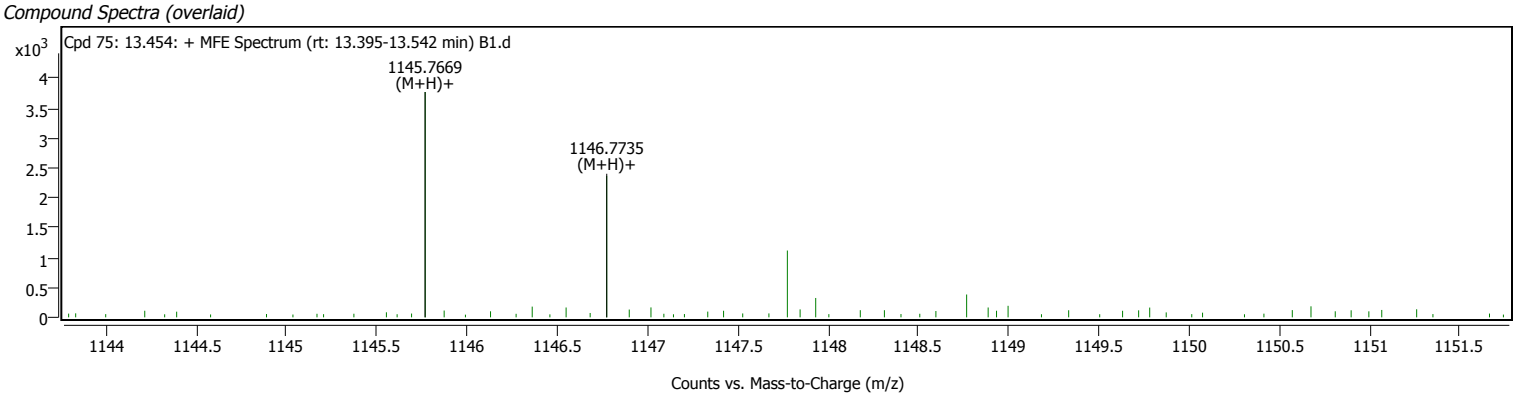
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.454		1144.7597				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 76: 35S-Methylokadaic acid 7-hexadecanoate

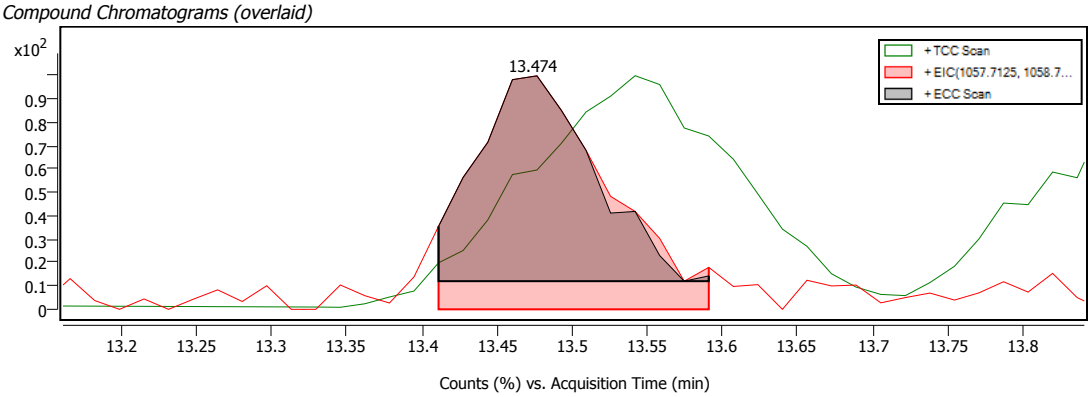
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
35S-Methylokadaic acid 7-hexadecanoate	C61 H100 O14	13.474		1056.7104		DBSearch	92.96	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	1057.7179 1057.7179 1057.7179		0	92.96	1		

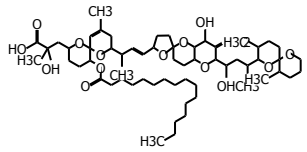
Compound ID Table

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	13.474		1056.7104		92.96	92.96	

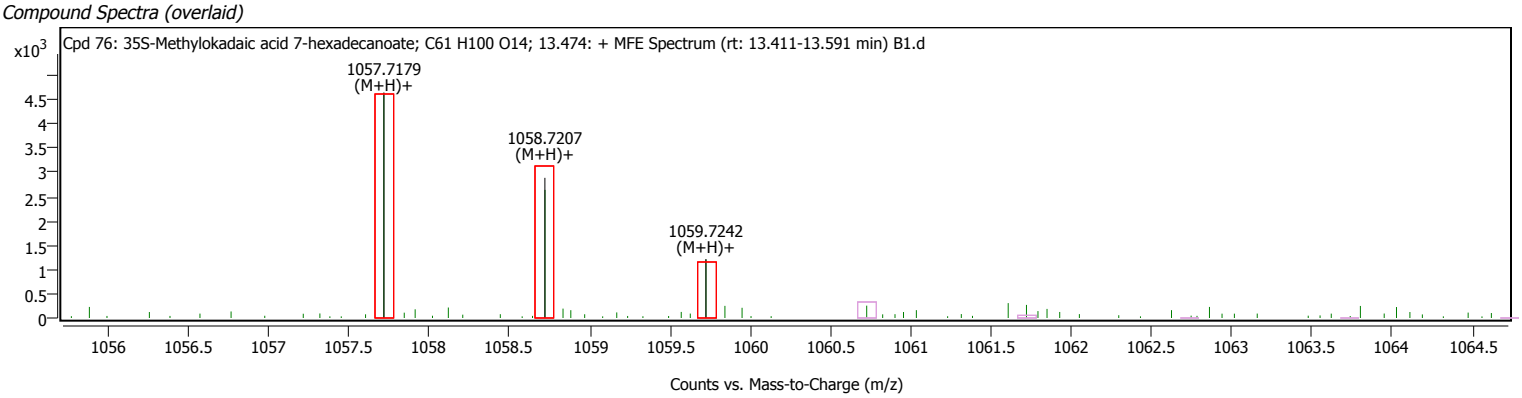
Compound Chromatograms (overlaid)



Structure



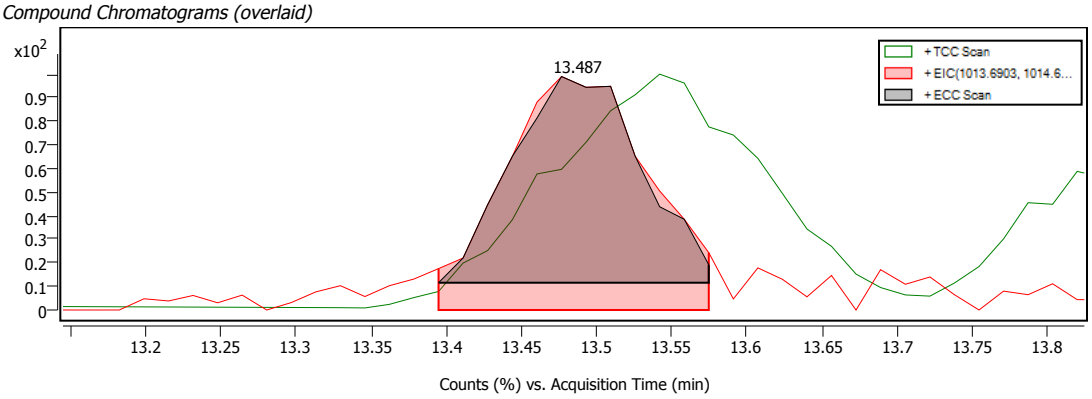
Compound Spectra (overlaid)



Cpd 77: 13.487

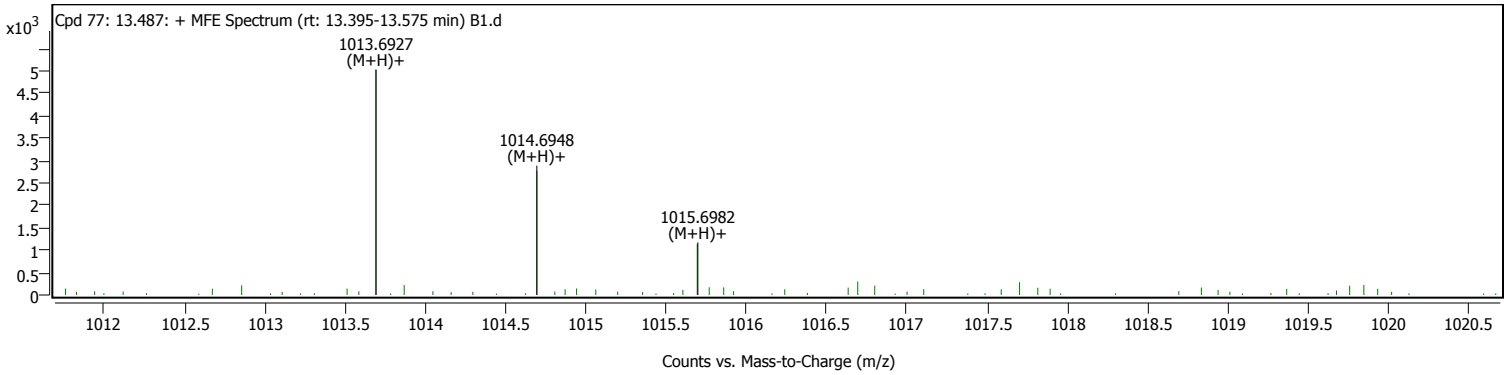
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.487		1012.6854				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 78: C57 H92 O12

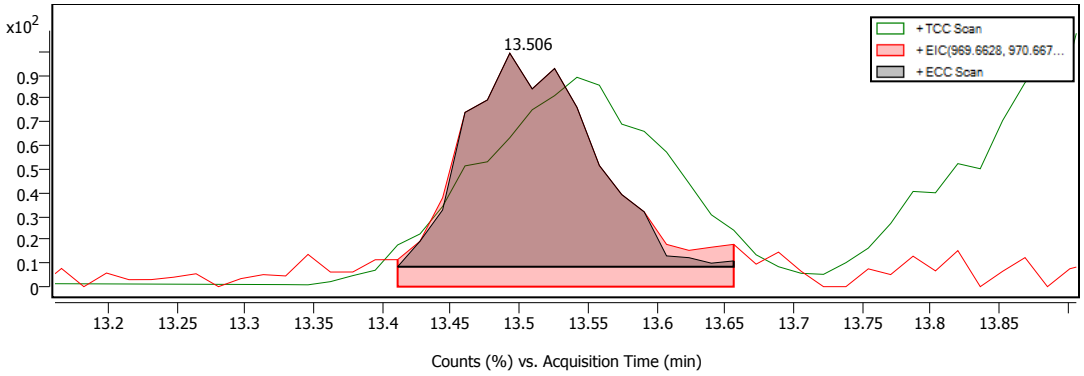
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C57 H92 O12	13.506		968.6584		MFG	94.38	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	969.6655				5	94.38	

Compound ID Table

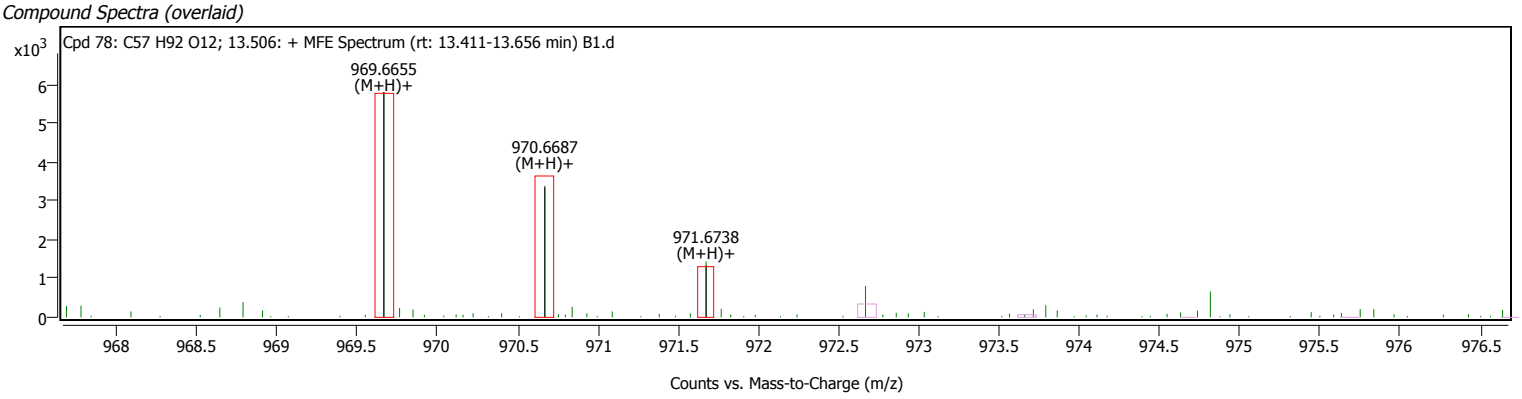
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C57 H92 O12	(M+H)+	MFG	13.506		968.6584		94.38		94.38
	C56 H86 N7 O7	(M+H)+	MFG	13.506		968.6585		94.04		94.04
	C55 H90 N3 O11	(M+H)+	MFG	13.506		968.6585		93.85		93.85
	C55 H80 N14 O2	(M+H)+	MFG	13.506		968.6587		93.31		93.31
	C54 H84 N10 O6	(M+H)+	MFG	13.506		968.6586		93.13		93.13

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 79: C53 H76 N14 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C53 H76 N14 O	13.511		924.6318		MFG	91.09	MFE	

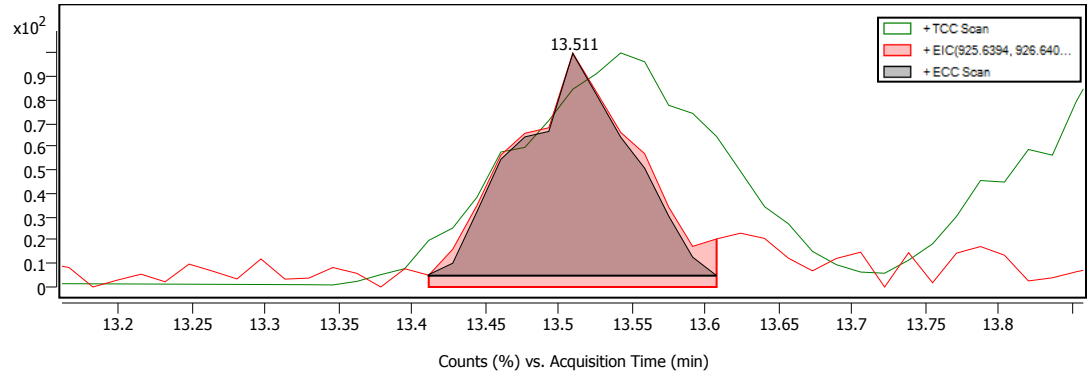
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	925.6389				5	91.09	

Compound ID Table

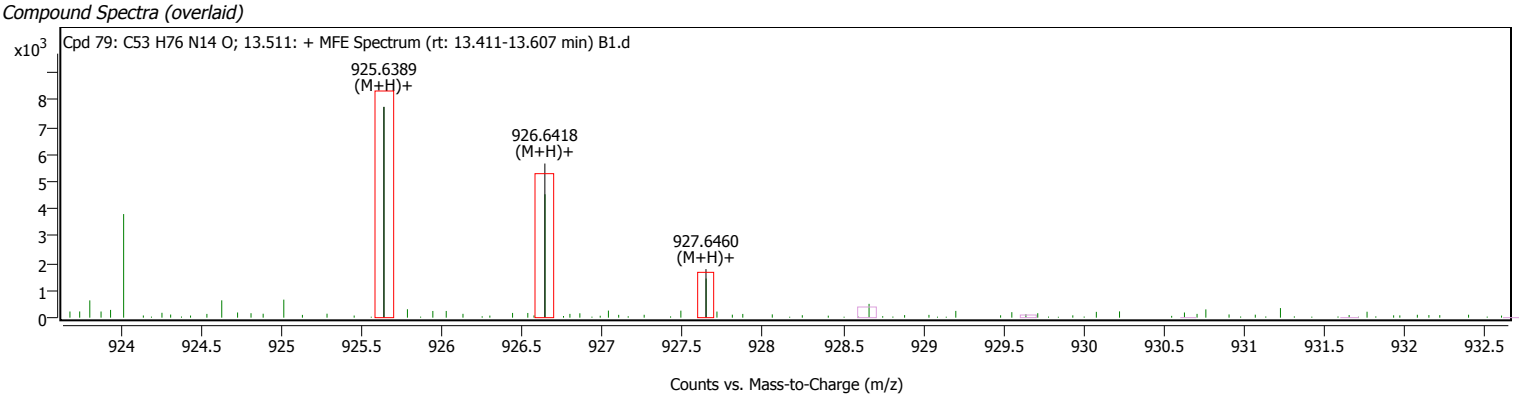
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C53 H76 N14 O	(M+H)+	MFG	13.511		924.6318		91.09		91.09
	C51 H74 N17	(M+H)+	MFG	13.511		924.6318		90.88		90.88
	C52 H80 N10 O5	(M+H)+	MFG	13.511		924.6317		89.50		89.50
	C54 H82 N7 O6	(M+H)+	MFG	13.511		924.6316		89.24		89.24
	C53 H86 N3 O10	(M+H)+	MFG	13.511		924.6316		87.88		87.88

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 80: C51 H72 N14

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C51 H72 N14	13.527		880.6063		MFG	97.22	MFE	

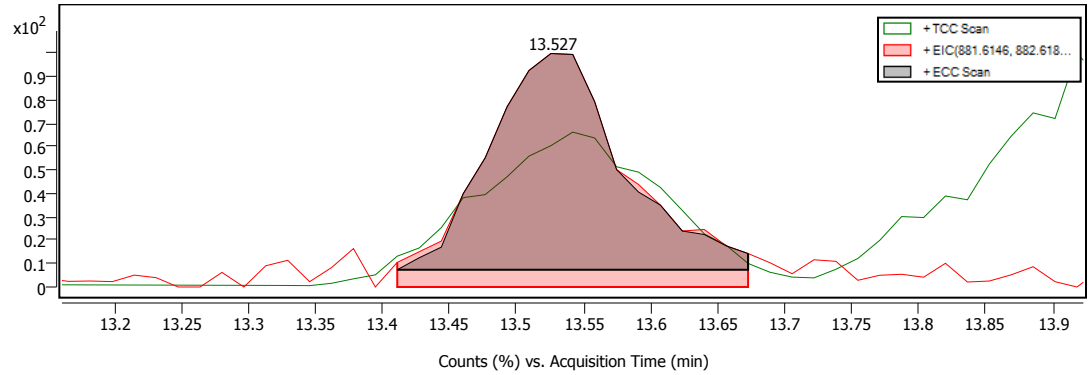
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	881.6134				13	97.22	

Compound ID Table

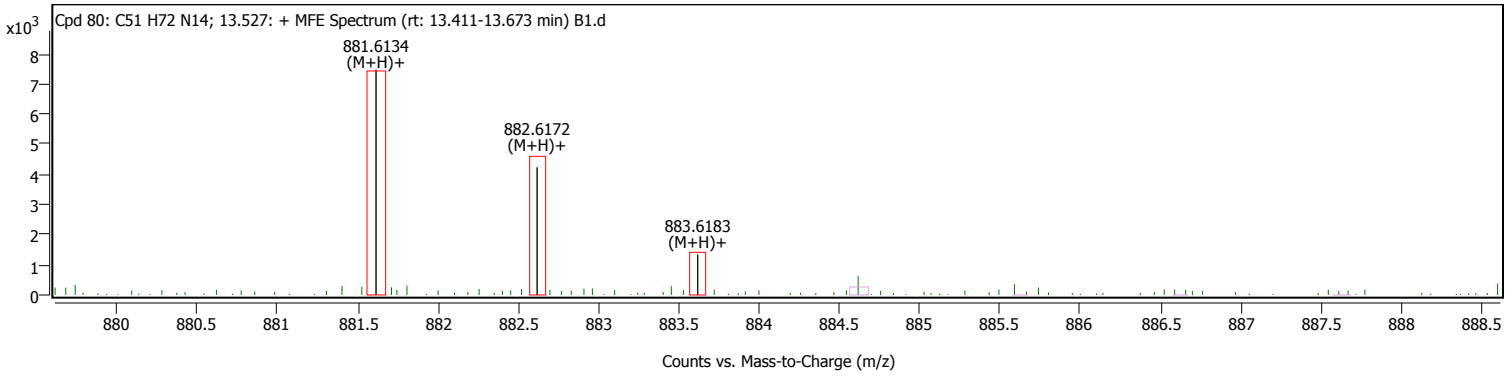
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C51 H72 N14	(M+H)+	MFG	13.527		880.6063		97.22		97.22
	C52 H78 N7 O5	(M+H)+	MFG	13.527		880.6062		97.08		97.08
	C53 H84 O10	(M+H)+	MFG	13.527		880.6061		96.46		96.46
	C50 H76 N10 O4	(M+H)+	MFG	13.527		880.6063		96.12		96.12
	C51 H82 N3 O9	(M+H)+	MFG	13.527		880.6061		95.89		95.89
PI(15:0/22:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(16:0/21:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(18:0/19:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(20:0/17:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(21:0/16:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(22:0/15:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(19:0/18:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	
PI(17:0/20:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.527		880.6061		90.34	90.34	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 81: C43 H74 N13 O2 S

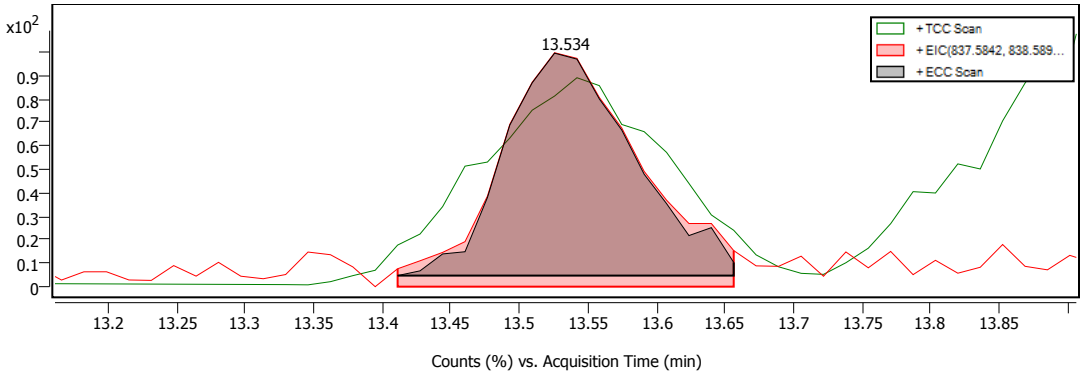
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C43 H74 N13 O2 S	13.534		836.5805		MFG	95.38	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	837.5881				11	95.38	

Compound ID Table

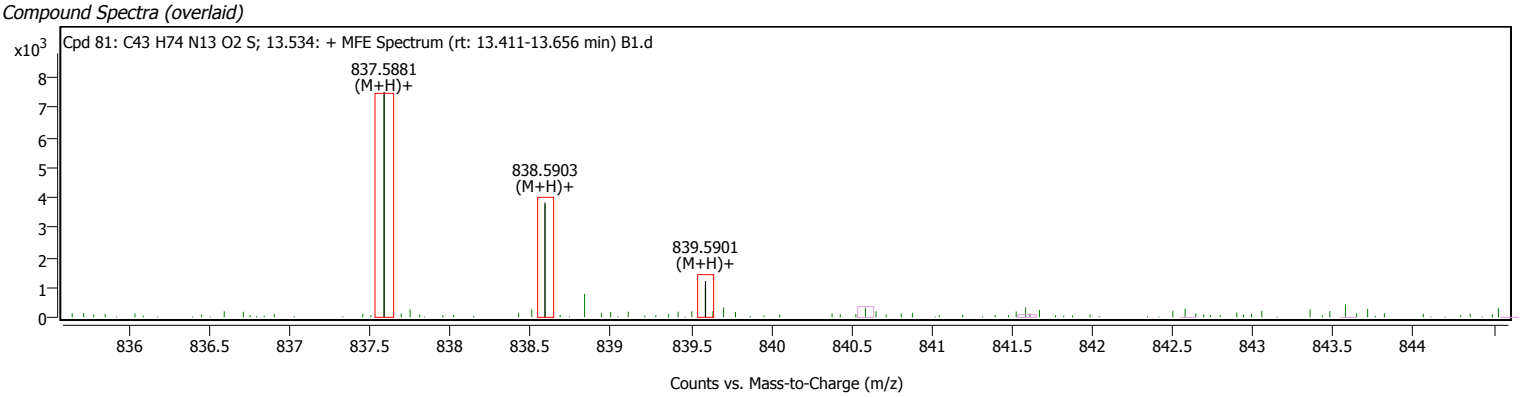
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C43 H74 N13 O2 S	(M+H)+	MFG	13.534		836.5805		95.38		95.38
	C41 H72 N16 O S	(M+H)+	MFG	13.534		836.5806		95.01		95.01
	C34 H64 N26	(M+H)+	MFG	13.534		836.5806		94.31		94.31
	C42 H78 N9 O6 S	(M+H)+	MFG	13.534		836.5805		93.83		93.83
	C44 H80 N6 O7 S	(M+H)+	MFG	13.534		836.5804		93.80		93.80
PI(O-16:0/19:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	
PI(O-18:0/17:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	
PI(O-20:0/15:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	
PI(P-16:0/19:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	
PI(P-18:0/17:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	
PI(P-20:0/15:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.534		836.5800		88.84	88.84	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 82: C48 H70 N7 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C48 H70 N7 O3	13.548		792.5543		MFG	63.98	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	793.5616				26	63.98	

Compound Discovery Report

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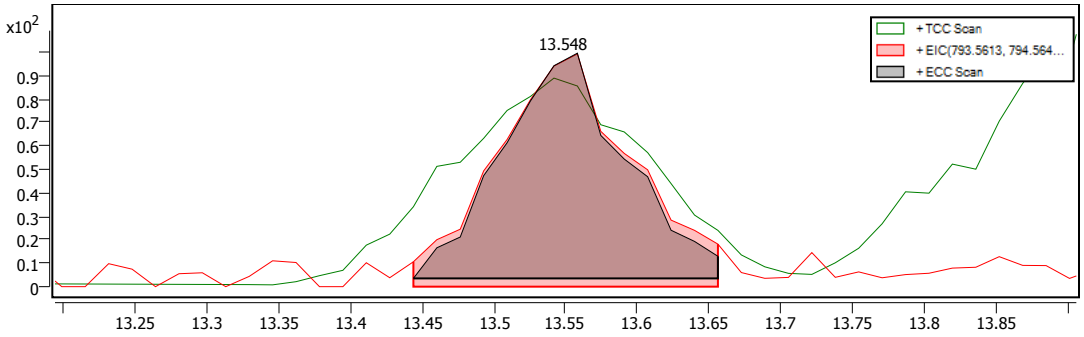
Compound ID Table

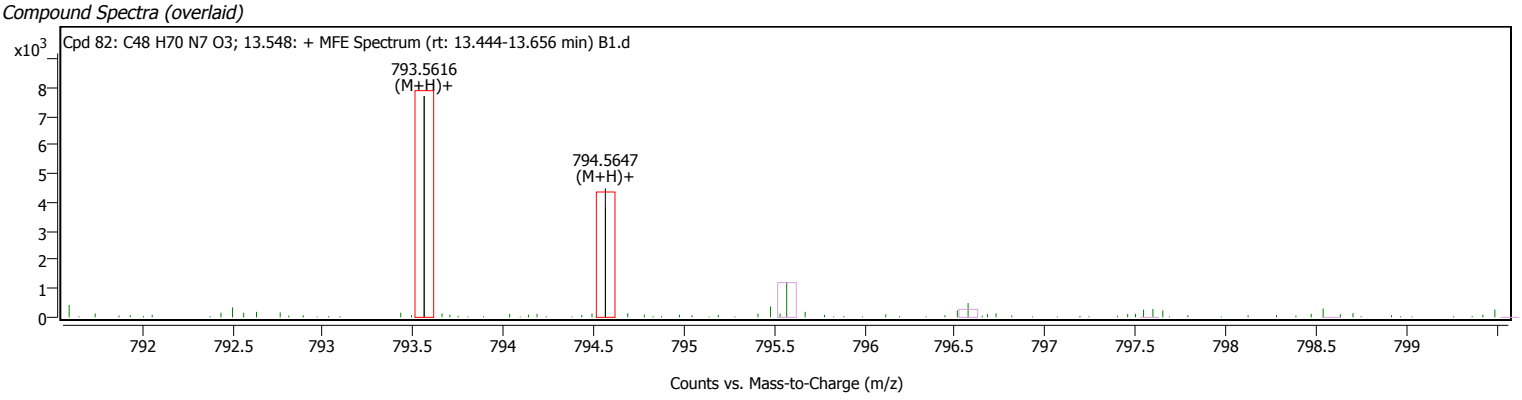
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C48 H70 N7 O3	(M+H)+	MFG	13.548		792.5543		63.98		63.98
	C49 H76 O8	(M+H)+	MFG	13.548		792.5542		63.25		63.25
	C33 H66 N19 O4	(M+H)+	MFG	13.548		792.5545		63.01		63.01
PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
PC(17:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
PC(17:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/17:1(9Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.548		792.5542		62.90	62.90	
	C34 H62 N23	(M+H)+	MFG	13.548		792.5546		62.36		62.36
	C50 H72 N4 O4	(M+H)+	MFG	13.548		792.5542		62.28		62.28
PC(17:0/18:3(6Z,9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(15:1(9Z)/20:2(11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(17:0/18:3(9Z,12Z,15Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(20:2(11Z,14Z)/15:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(16:0/19:3(9Z,12Z,15Z))[U]	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(17:1(9Z)/18:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(17:2(9Z,12Z)/18:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(18:1(9Z)/17:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(18:2(9Z,12Z)/17:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(20:3(8Z,11Z,14Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(20:3(5Z,8Z,11Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(15:0/20:3(8Z,11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(15:0/20:3(5Z,8Z,11Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(18:3(6Z,9Z,12Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	
PC(18:3(9Z,12Z,15Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.548		770.5722		57.09	57.09	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 83: C48 H68 N4 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C48 H68 N4 O3	13.559		748.5289		MFG	87.52	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	749.5355				24	87.52	

Compound Discovery Report

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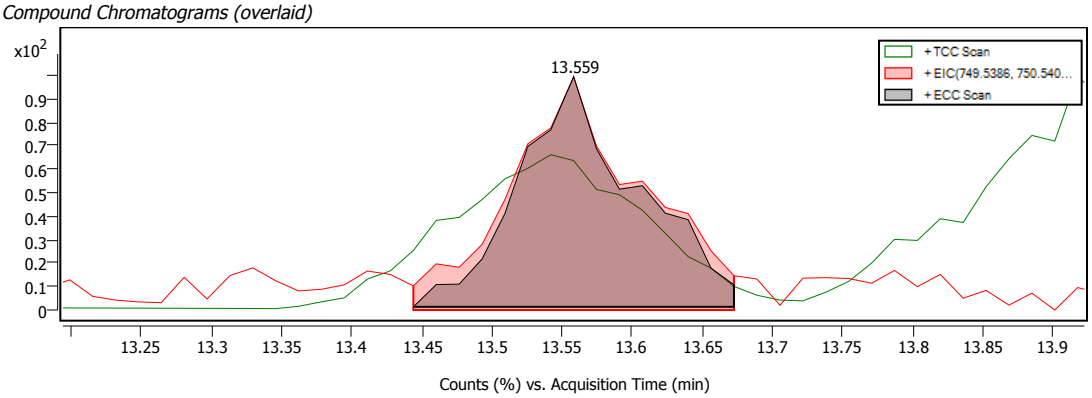
Compound ID Table

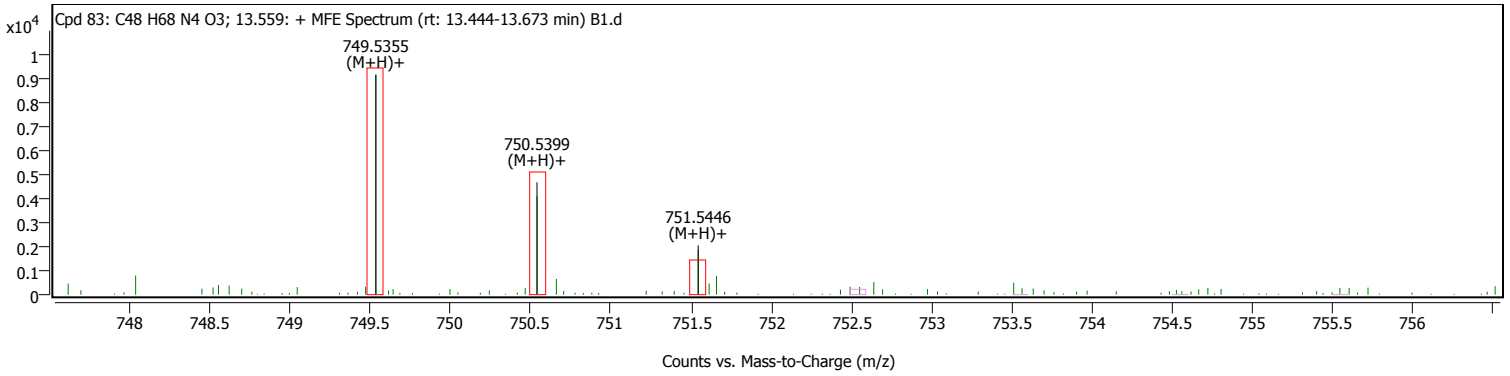
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C48 H68 N4 O3	(M+H)+	MFG	13.559		748.5289		87.52		87.52
	C47 H72 O7	(M+H)+	MFG	13.559		748.5288		87.30		87.30
	C42 H74 N3 O6 S	(M+H)+	MFG	13.559		748.5293		86.74		86.74
	C41 H68 N10 O S	(M+H)+	MFG	13.559		748.5294		86.04		86.04
	C48 H76 O2 S2	(M+H)+	MFG	13.559		748.5294		85.27		85.27
PG(15:0/19:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(18:0/16:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(18:1(11Z)/16:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(18:1(9Z)/16:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(16:0/18:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
LBPA(16:0/18:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(14:1(9Z)/20:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(12:0/22:1(11Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(14:0/20:1(11Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(15:1(9Z)/19:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(22:1(11Z)/12:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(17:0/17:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(17:1(9Z)/17:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(19:0/15:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(19:1(9Z)/15:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(20:0/14:1(9Z))	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(20:1(11Z)/14:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(16:0/18:1(9Z))[U]	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	
PG(16:1(9Z)/18:0)	C40 H77 O10 P	(M+H)+	DBSearch	13.559		748.5288		72.30	72.30	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 84: C31 H68 N12 O2 S2

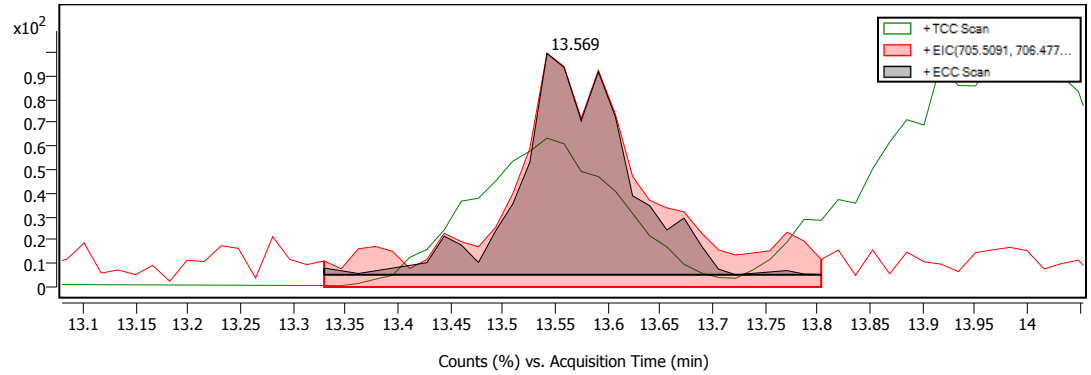
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H68 N12 O2 S2	13.569		704.5027		MFG	85.17	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	705.5092				7	85.17	

Compound ID Table

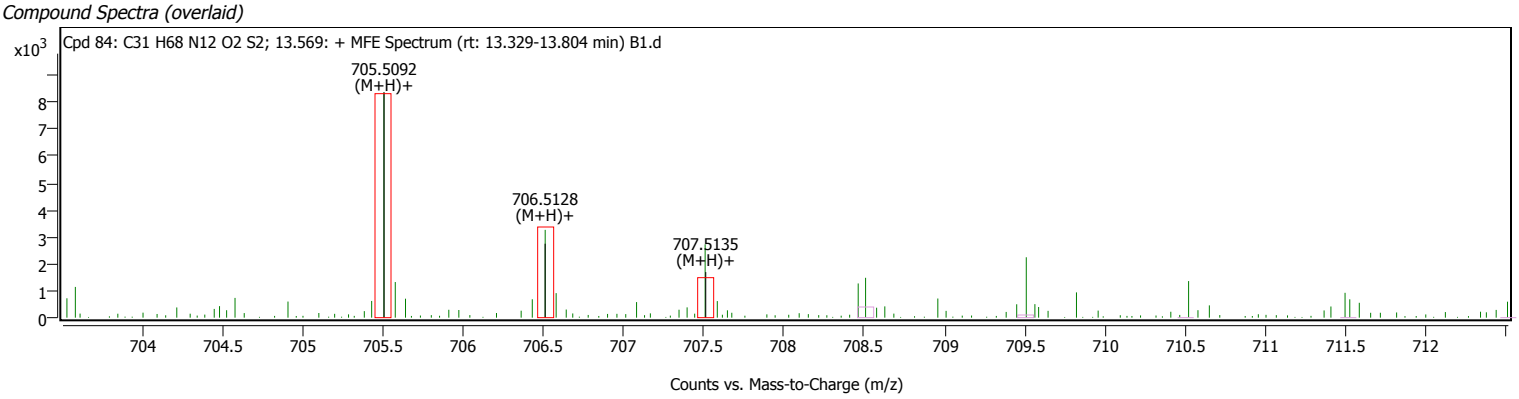
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H68 N12 O2 S2	(M+H)+	MFG	13.569		704.5027		85.17		85.17
	C38 H76 N2 O3 S3	(M+H)+	MFG	13.569		704.5025		82.44		82.44
	C37 H72 N2 O8 S	(M+H)+	MFG	13.569		704.5022		81.65		81.65
	C33 H70 N9 O3 S2	(M+H)+	MFG	13.569		704.5026		81.40		81.40
	C38 H68 N6 O4 S	(M+H)+	MFG	13.569		704.5022		81.10		81.10
PG(P-16:0/16:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.569		704.5017		70.32	70.32	
PG(P-18:0/14:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.569		704.5017		70.32	70.32	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 85: C44 H68 S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H68 S2	13.586		660.4763		MFG	85.03	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	661.4829				38	85.03	

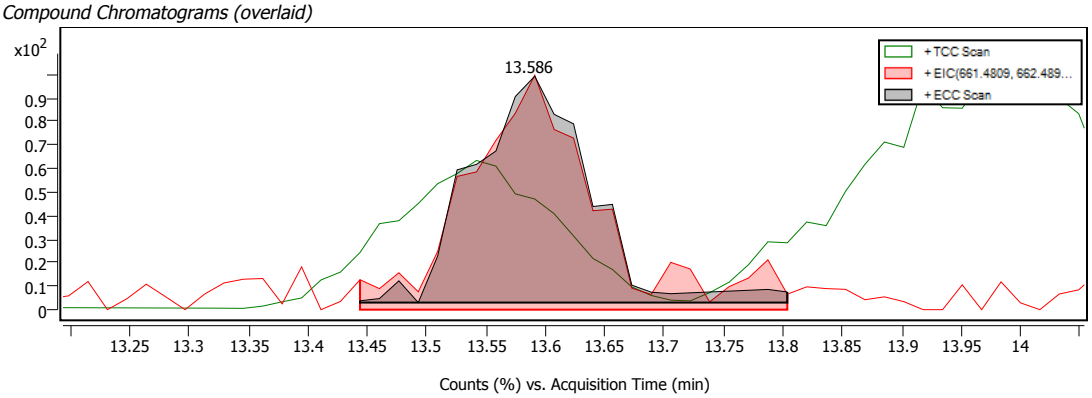
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

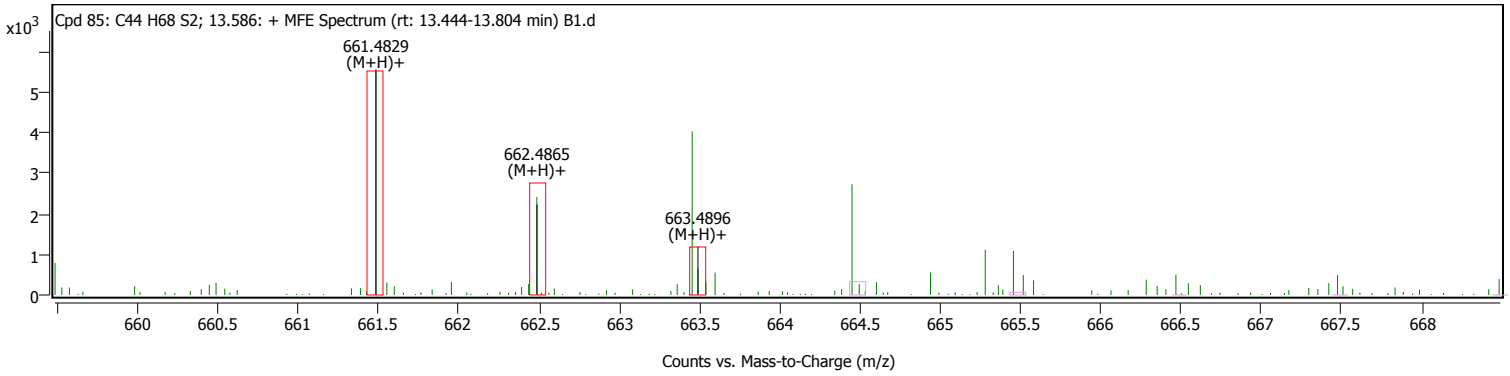
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H68 S2	(M+H)+	MFG	13.586		660.4763		85.03		85.03
	C36 H64 N6 O3 S	(M+H)+	MFG	13.586		660.4763		84.78		84.78
	C29 H64 N12 O S2	(M+H)+	MFG	13.586		660.4768		84.78		84.78
	C36 H72 N2 O2 S3	(M+H)+	MFG	13.586		660.4766		84.21		84.21
	C38 H66 N3 O4 S	(M+H)+	MFG	13.586		660.4762		83.56		83.56
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.586		660.4757		81.74	81.74	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.586		660.4757		81.74	81.74	
DG(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C43 H64 O5	(M+H)+	DBSearch	13.586		660.4757		81.74	81.74	
PA(16:0/17:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(15:1(9Z)/18:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(19:1(9Z)/14:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(20:1(11Z)/13:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(13:0/20:1(11Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(14:1(9Z)/19:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(15:0/18:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(14:0/19:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(16:1(9Z)/17:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(17:1(9Z)/16:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(18:0/15:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(18:1(9Z)/15:0)	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(19:0/14:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
PA(17:0/16:1(9Z))	C36 H69 O8 P	(M+H)+	DBSearch	13.586		660.4757		72.88	72.88	
DG(20:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:3(6Z,9Z,12Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:3(6Z,9Z,12Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:3(9Z,12Z,15Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:4(6Z,9Z,12Z,15Z)/20:3(8Z,11Z,14Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(18:3(9Z,12Z,15Z)/20:4(5Z,8Z,11Z,14Z)/0:0)[iso2]	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)/0:0)	C41 H66 O5	(M+Na)+	DBSearch	13.586		638.4937		72.06	72.06	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 86: C52 H42 N2 S5

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C52 H42 N2 S5	13.592		854.1946		MFG	73.41	MFE	

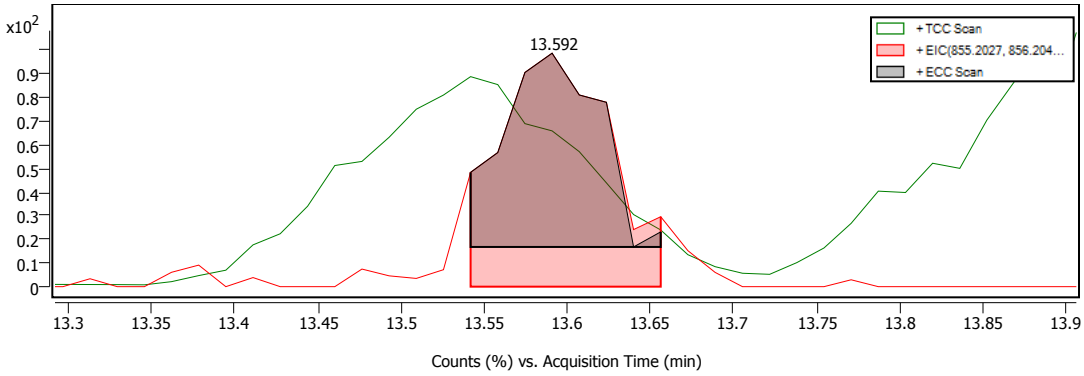
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	855.2027				5	73.41	

Compound ID Table

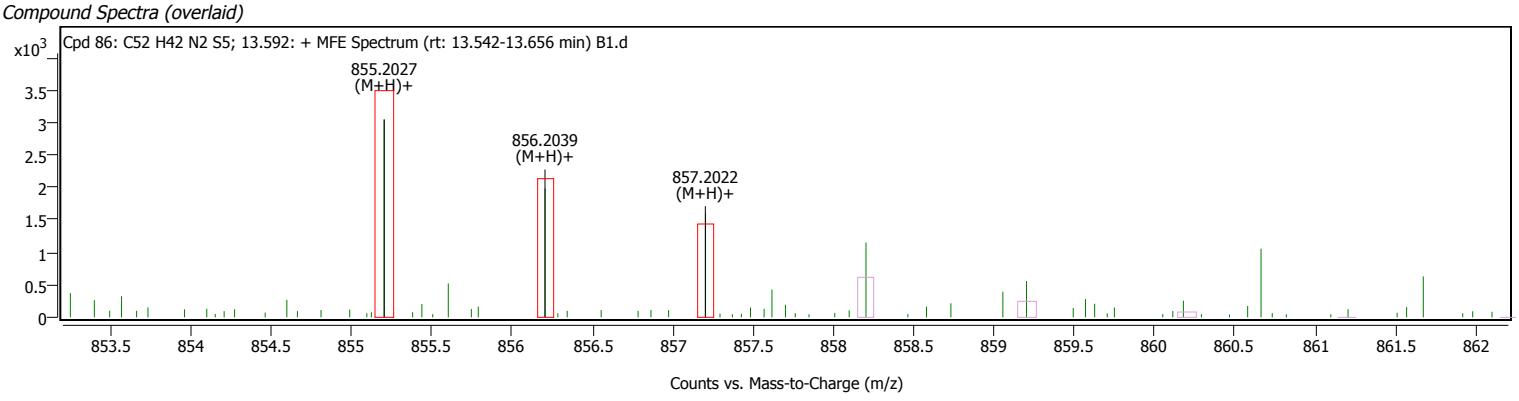
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C52 H42 N2 S5	(M+H)+	MFG	13.592		854.1946		73.41		73.41
	C44 H38 N8 O3 S4	(M+H)+	MFG	13.592		854.1947		73.22		73.22
	C50 H32 N9 S3	(M+H)+	MFG	13.592		854.1944		73.07		73.07
	C45 H44 N O8 S4	(M+H)+	MFG	13.592		854.1946		72.48		72.48
	C51 H38 N2 O5 S3	(M+H)+	MFG	13.592		854.1943		72.47		72.47

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 87: C42 H56 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C42 H56 N4	13.601		616.4512		MFG	67.46	MFE	

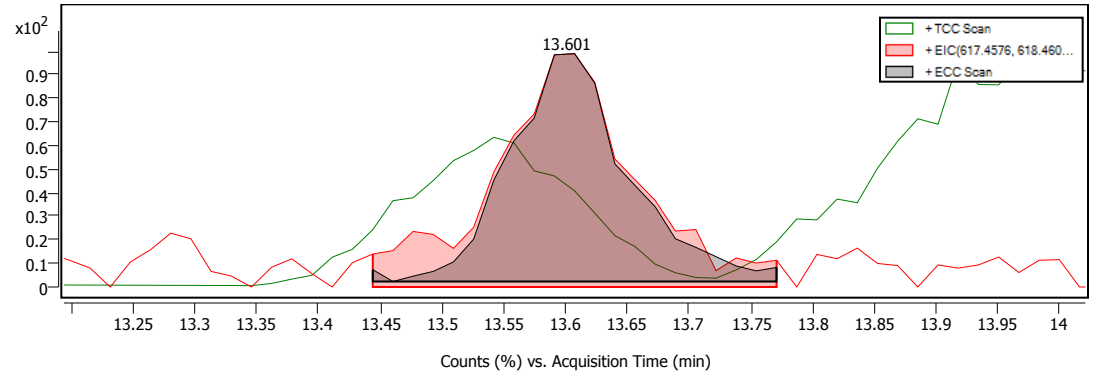
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	617.4578				6	67.46	

Compound ID Table

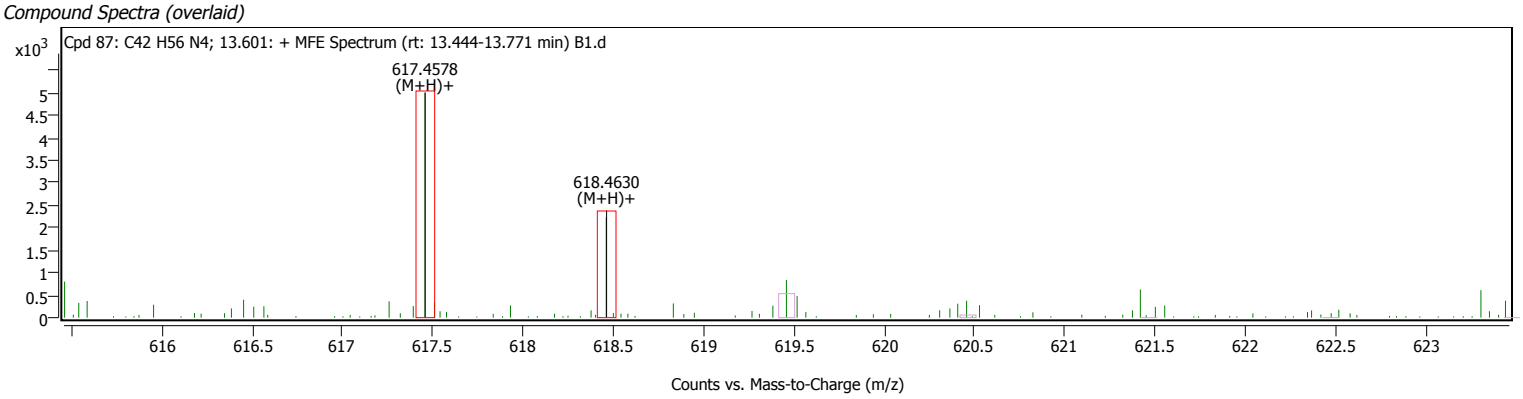
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C42 H56 N4	(M+H)+	MFG	13.601		616.4512		67.46		67.46
	C44 H58 N O	(M+H)+	MFG	13.601		616.4511		66.87		66.87
	C27 H52 N16 O	(M+H)+	MFG	13.601		616.4514		63.14		63.14
	C29 H54 N13 O2	(M+H)+	MFG	13.601		616.4514		62.85		62.85
	C28 H58 N9 O6	(M+H)+	MFG	13.601		616.4513		62.33		62.33
Oryzanol C	C41 H60 O4	(M+H)+	DBSearch	13.601		616.4511		61.50	61.50	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 88: C24 H52 N12 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C24 H52 N12 O4	13.611		572.4234		MFG	77.95	MFE	

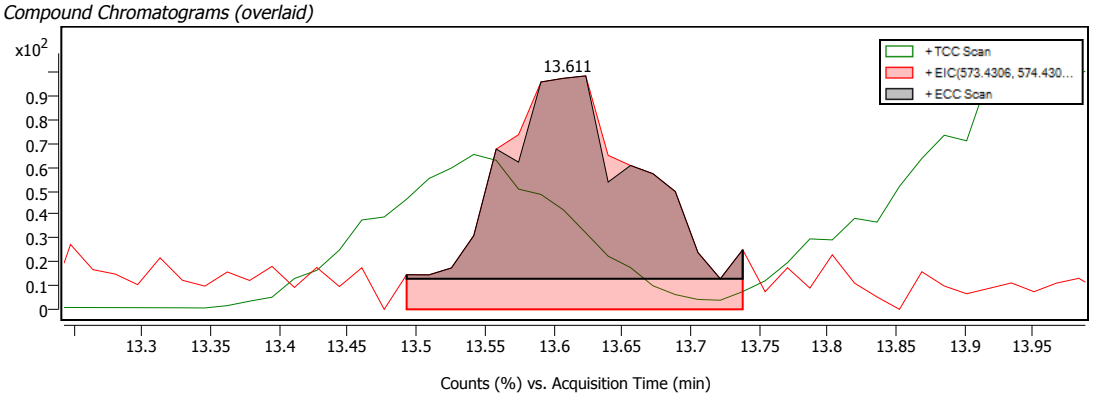
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	573.4311				5	77.95	

Compound ID Table

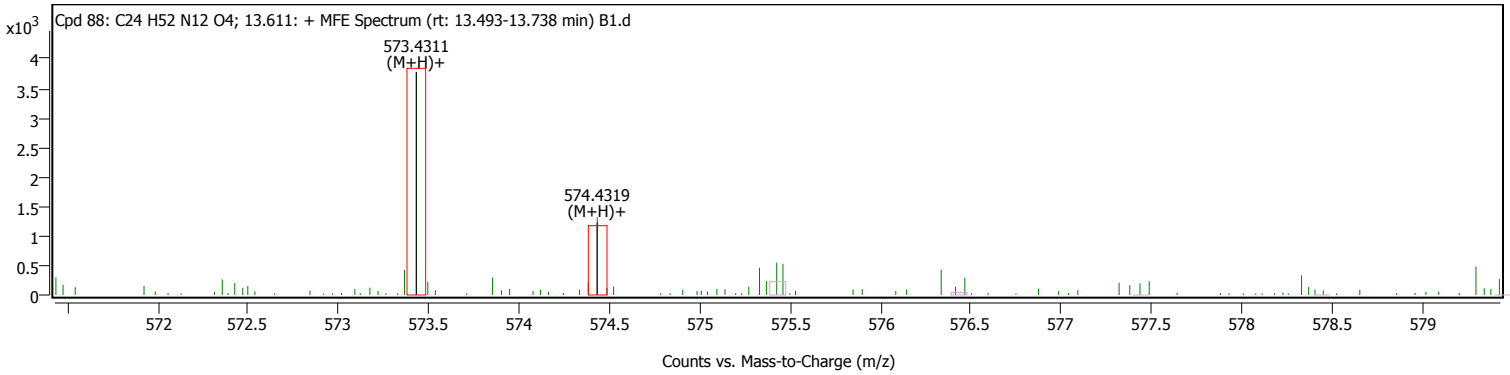
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C24 H52 N12 O4	(M+H)+	MFG	13.611		572.4234		77.95		77.95
	C25 H48 N16	(M+H)+	MFG	13.611		572.4234		76.68		76.68
	C22 H50 N15 O3	(M+H)+	MFG	13.611		572.4234		75.61		75.61
	C26 H54 N9 O5	(M+H)+	MFG	13.611		572.4233		73.29		73.29
	C20 H48 N18 O2	(M+H)+	MFG	13.611		572.4235		67.36		67.36

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 89: C37 H52 O2

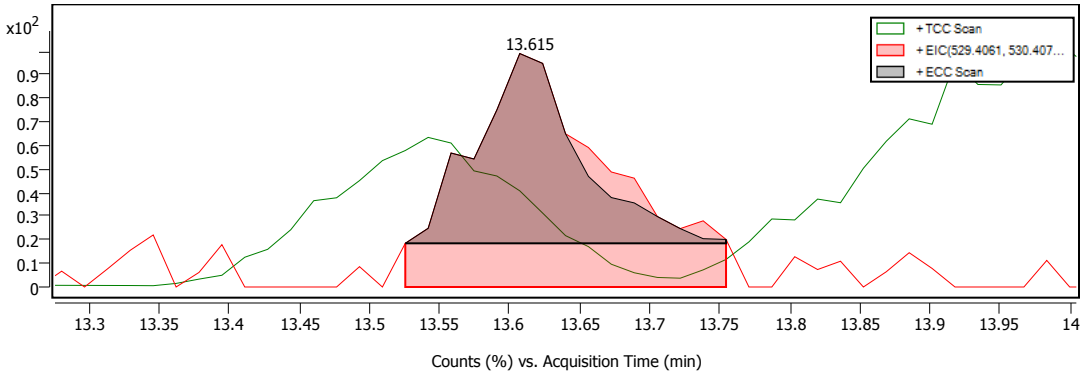
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H52 O2	13.615		528.3984		MFG	64.33	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	529.4053				6	64.33	

Compound ID Table

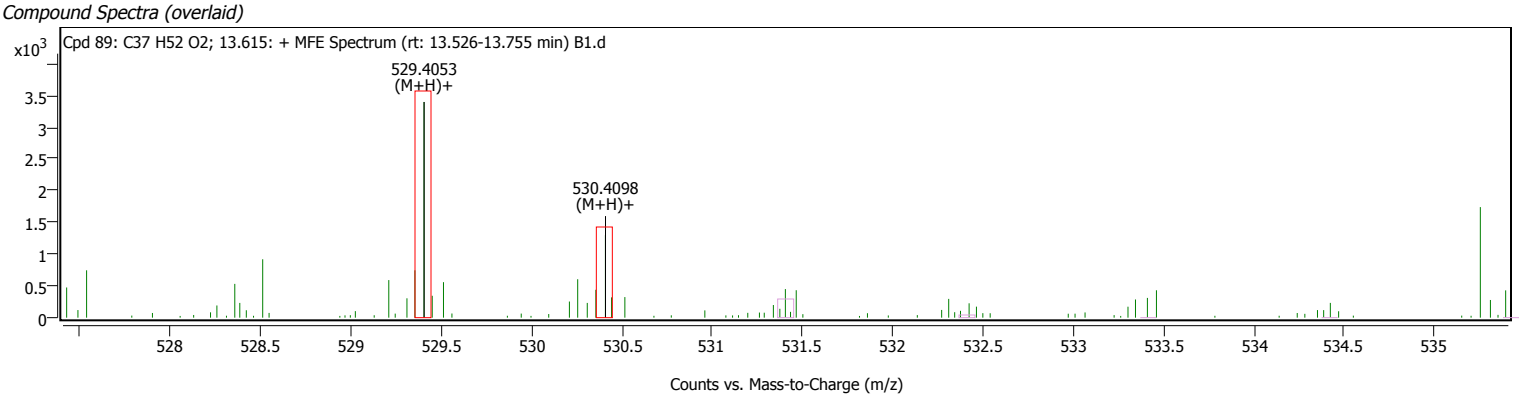
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H52 O2	(M+H)+	MFG	13.615		528.3984		64.33		64.33
	C32 H54 N3 O S	(M+H)+	MFG	13.615		528.3985		62.17		62.17
	C24 H50 N9 O4	(M+H)+	MFG	13.615		528.3986		61.23		61.23
	C25 H46 N13	(M+H)+	MFG	13.615		528.3987		60.16		60.16
	C30 H52 N6 S	(M+H)+	MFG	13.615		528.3985		59.39		59.39
PAF C-16-d4	C26 H51 D4 N O7 P	(M+H)+	DBSearch	13.615		528.3984		56.32	56.32	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)

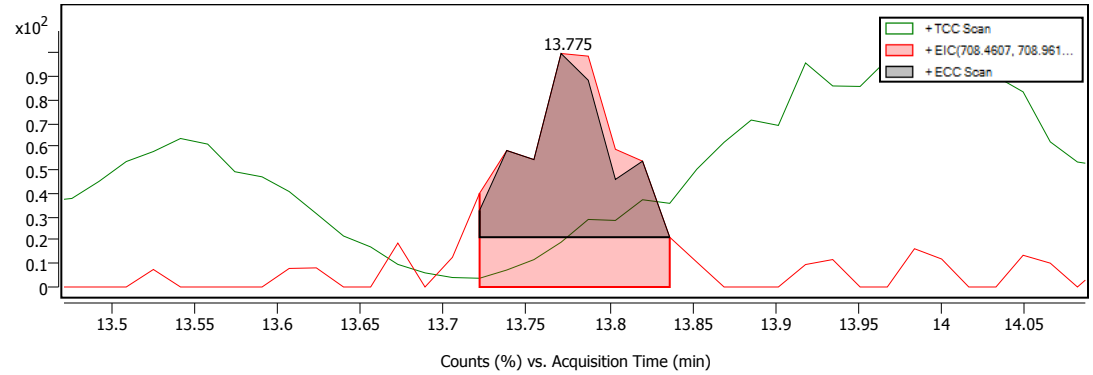


Cpd 90: 13.775

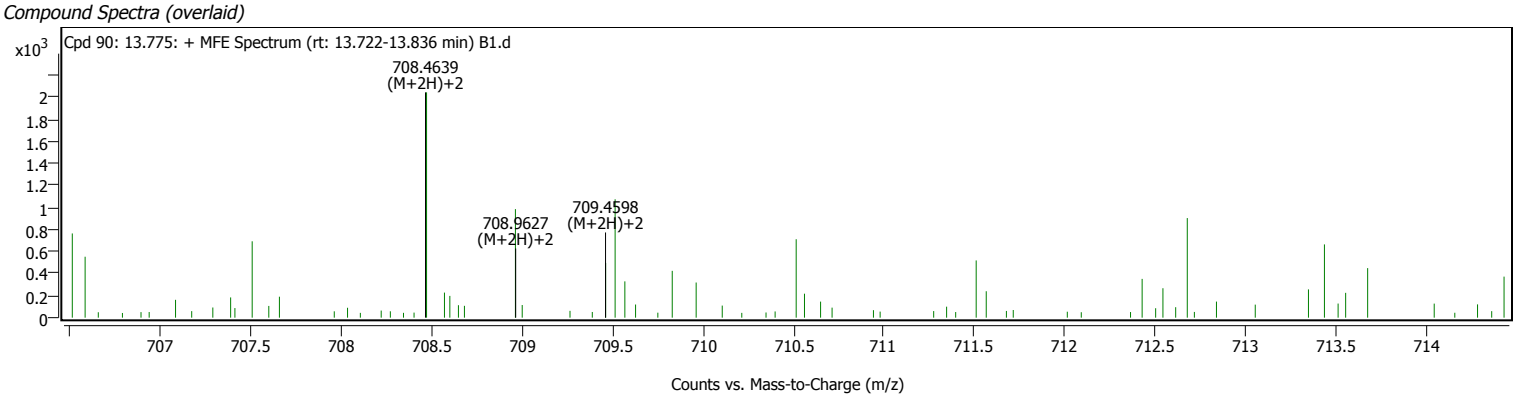
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.775		1414.9132				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

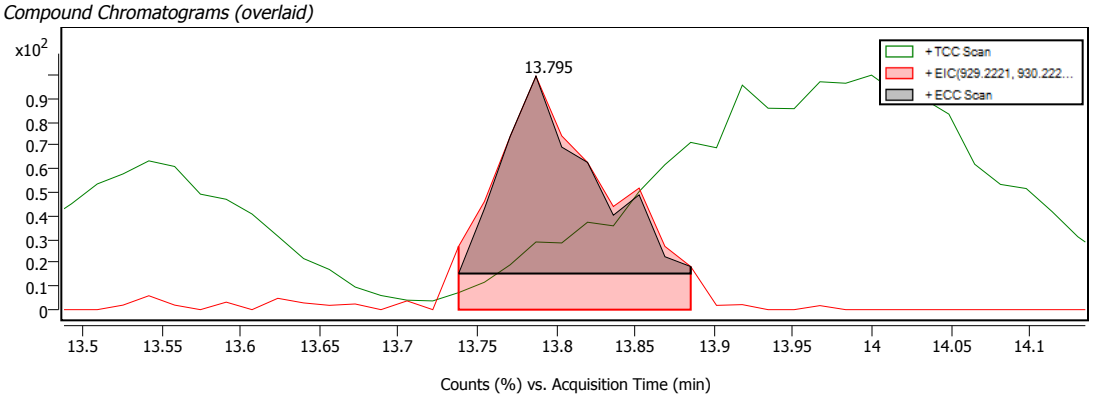


Cpd 91: 13.795

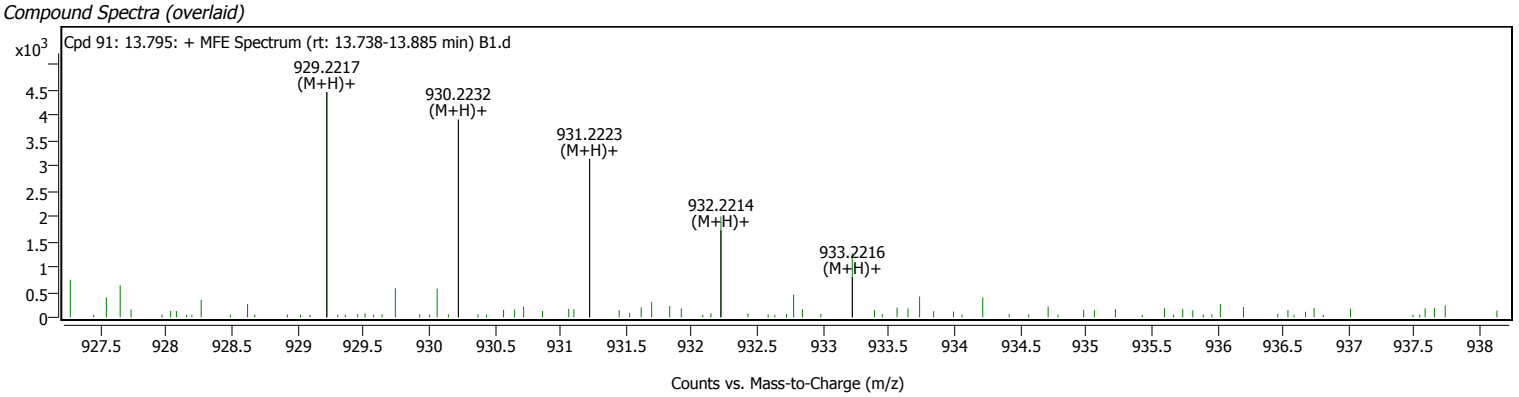
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.795		928.2144				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

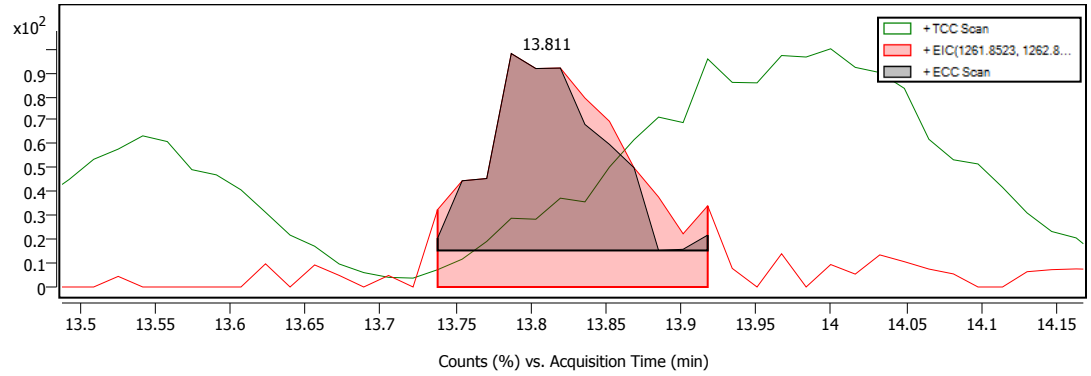


Cpd 92: 13.811

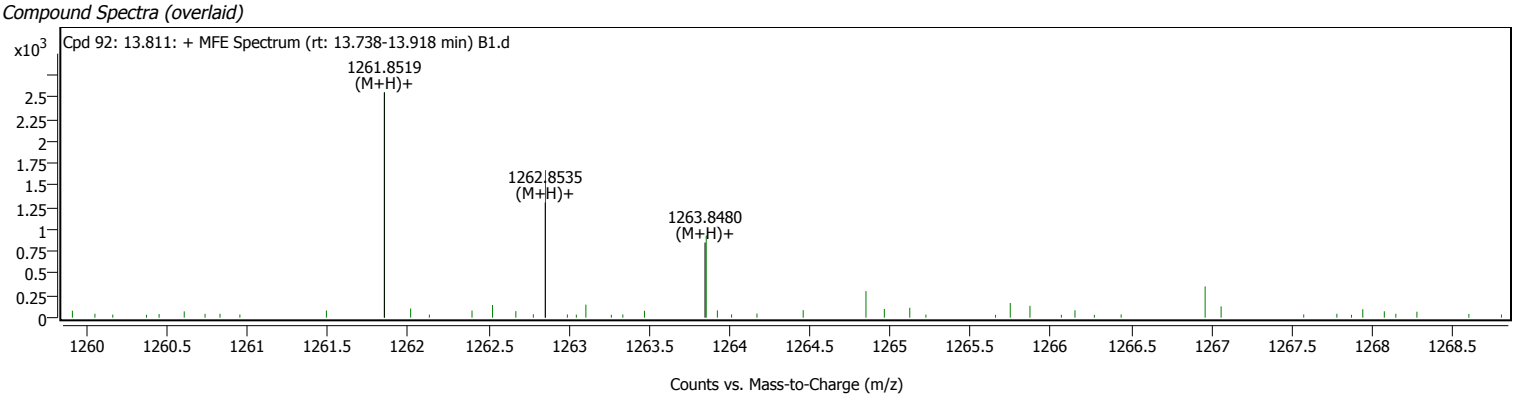
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.811		1260.8447				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

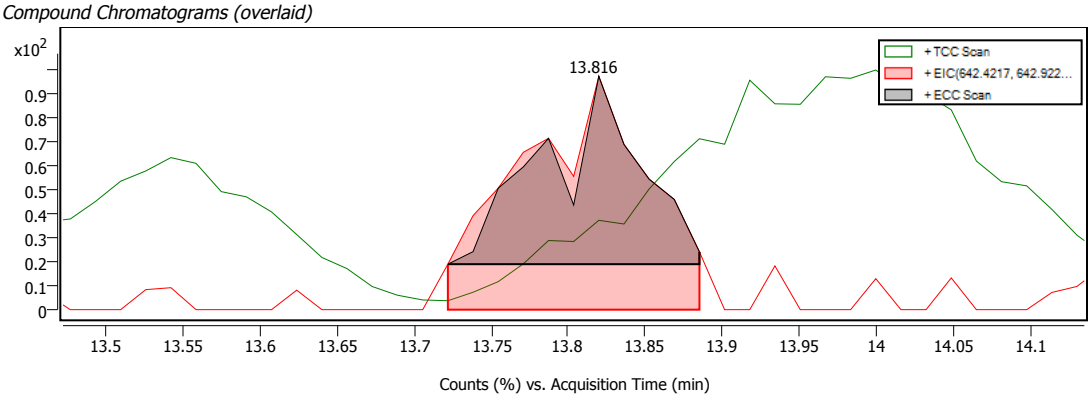


Cpd 93: 13.816

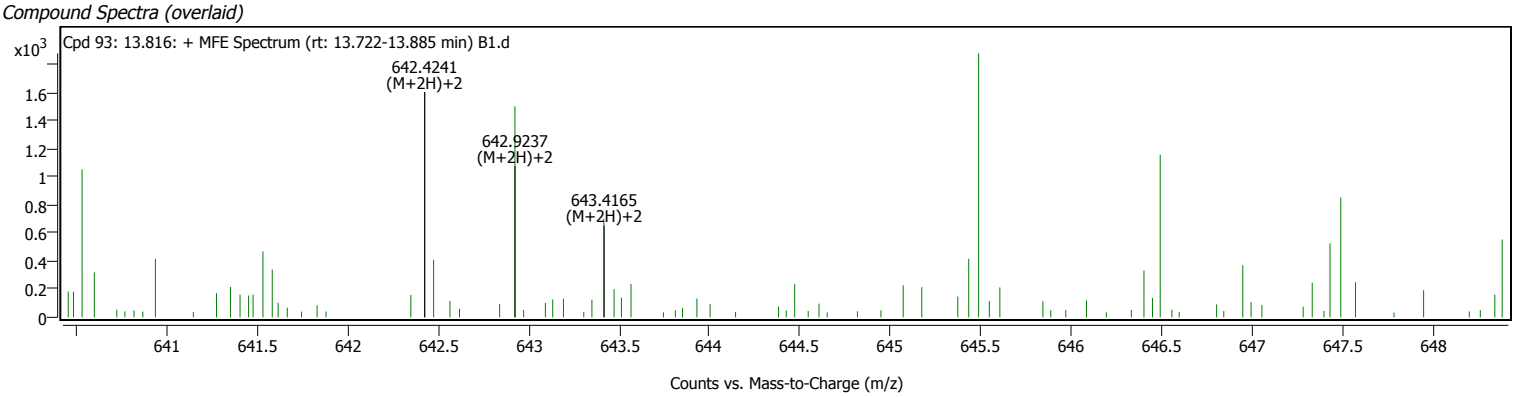
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.816		1282.8336				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

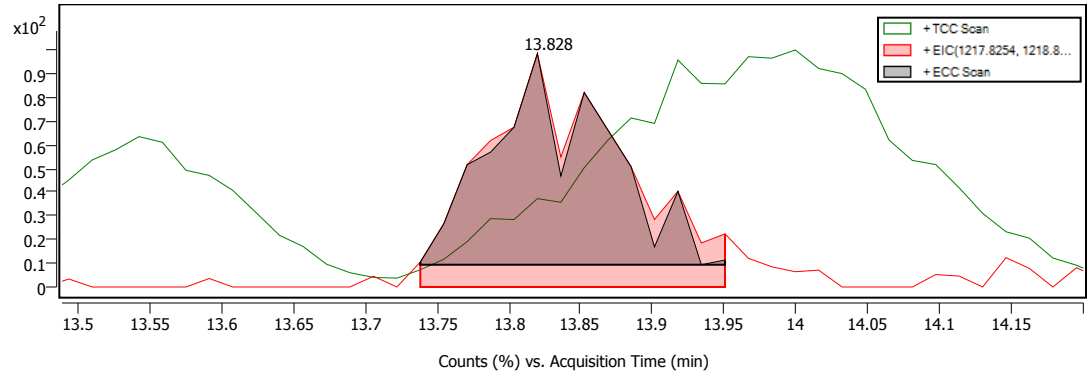


Cpd 94: 13.828

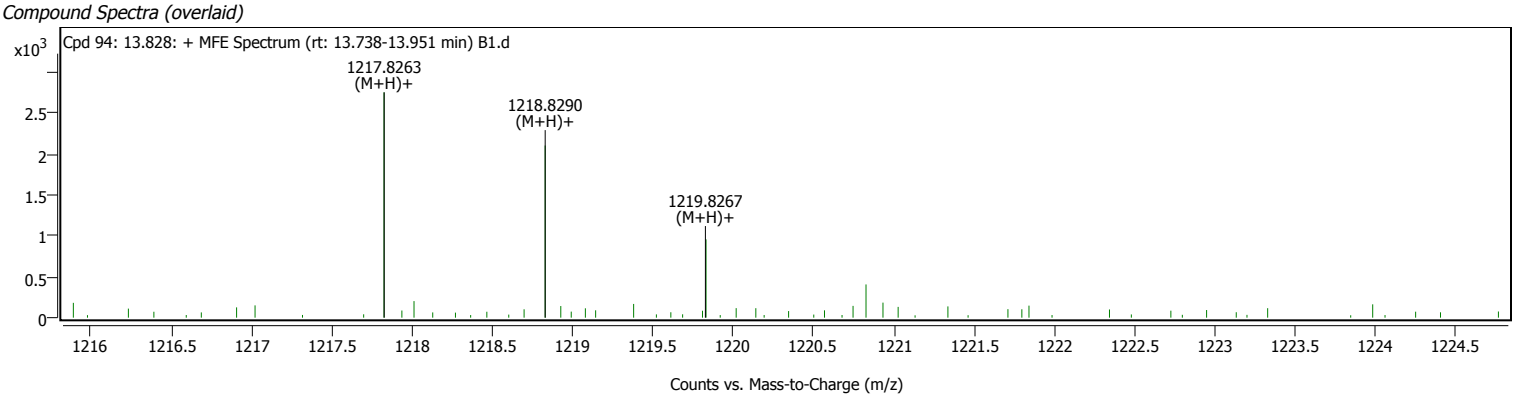
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.828		1216.8190				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

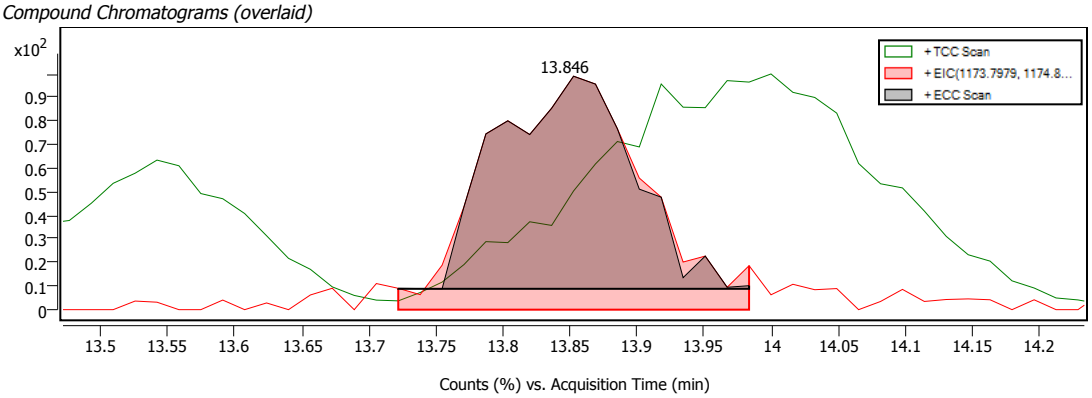


Cpd 95: 13.846

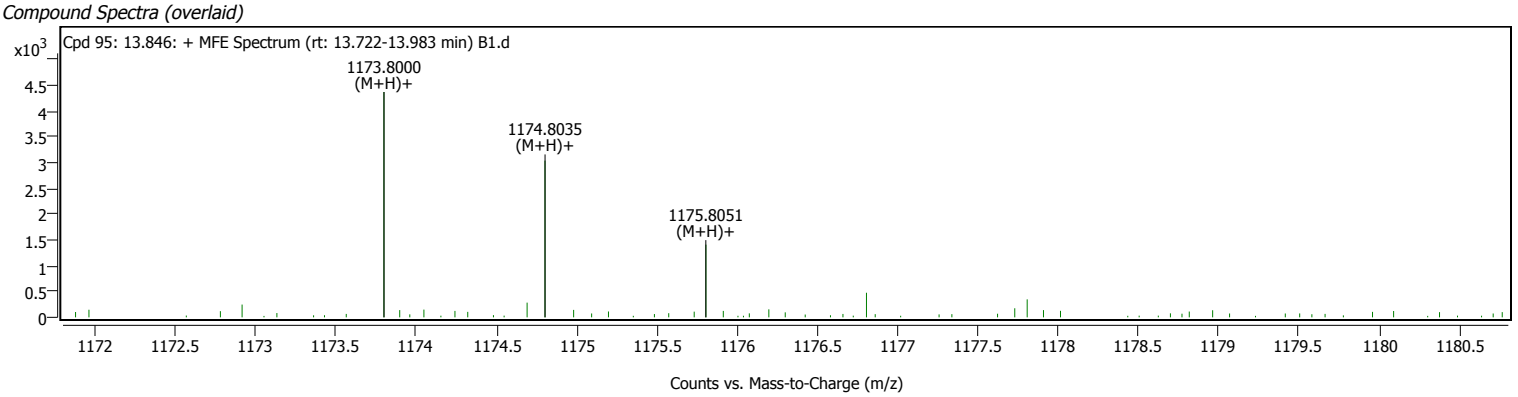
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.846		1172.7928				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

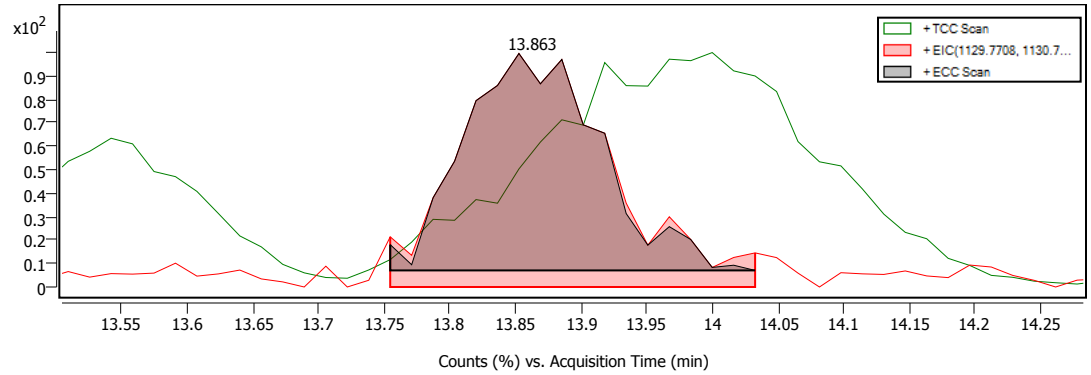


Cpd 96: 13.863

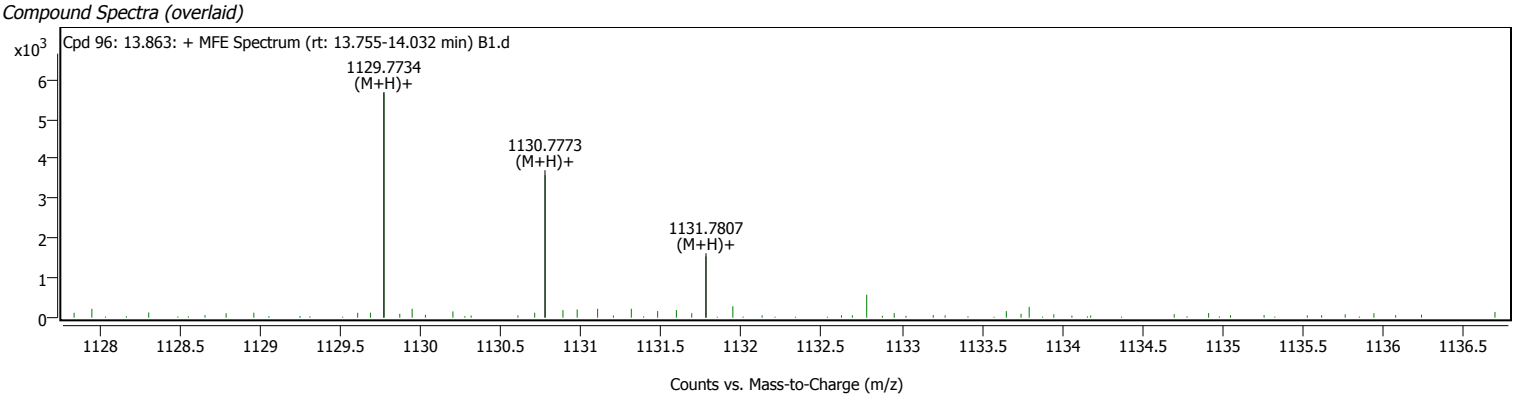
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.863		1128.7661				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

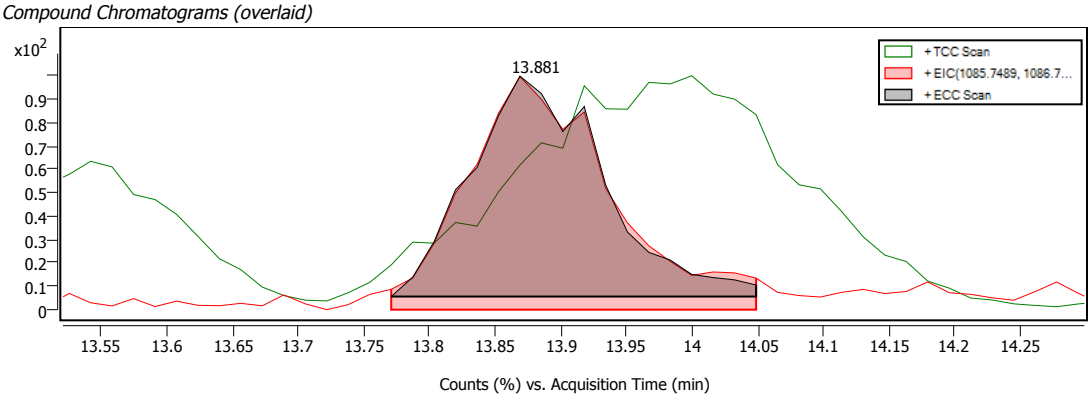


Cpd 97: 13.881

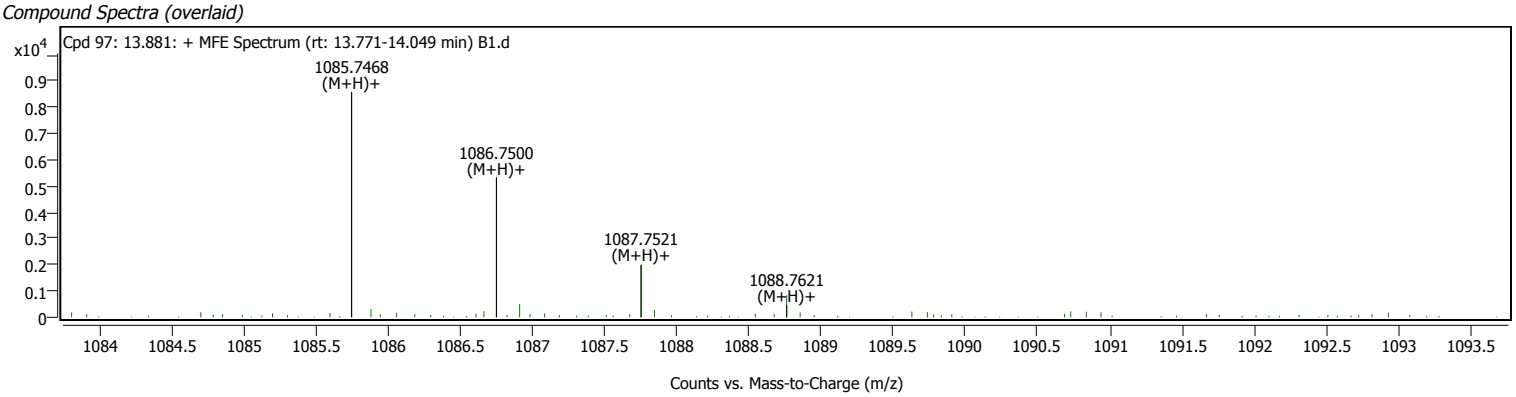
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.881		1084.7395				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

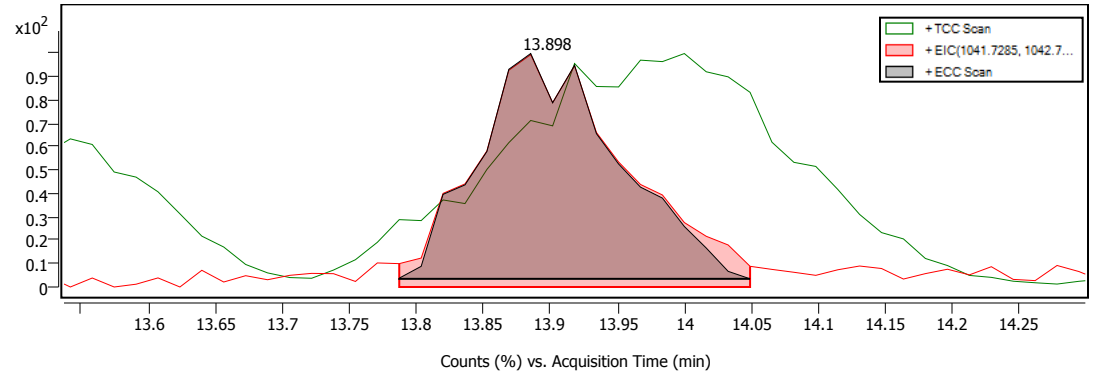


Cpd 98: 13.898

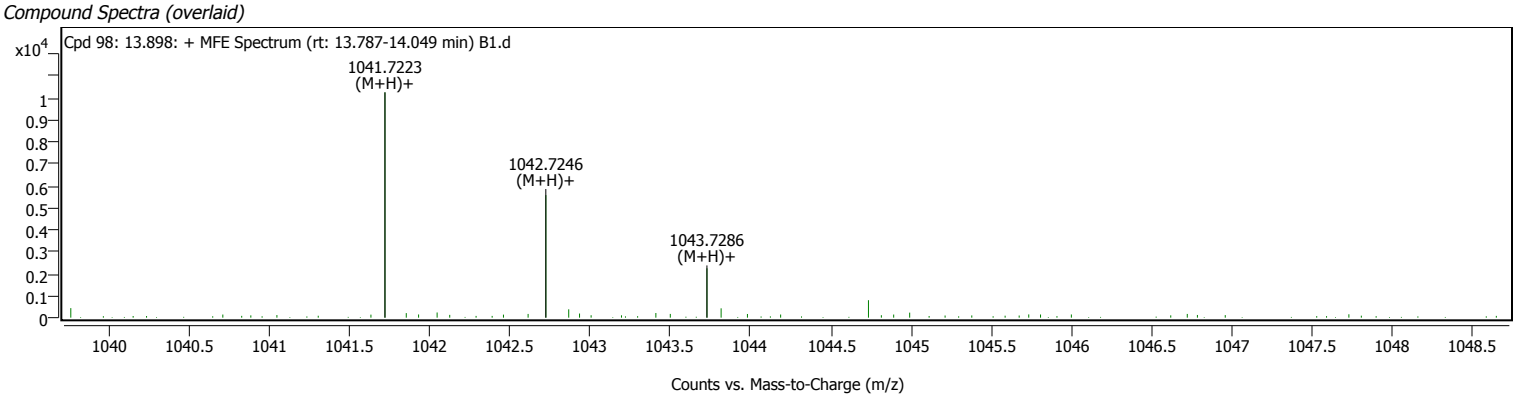
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.898		1040.7150				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 99: C56 H88 N10 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C56 H88 N10 O6	13.916		996.6892		MFG	98.67	MFE	

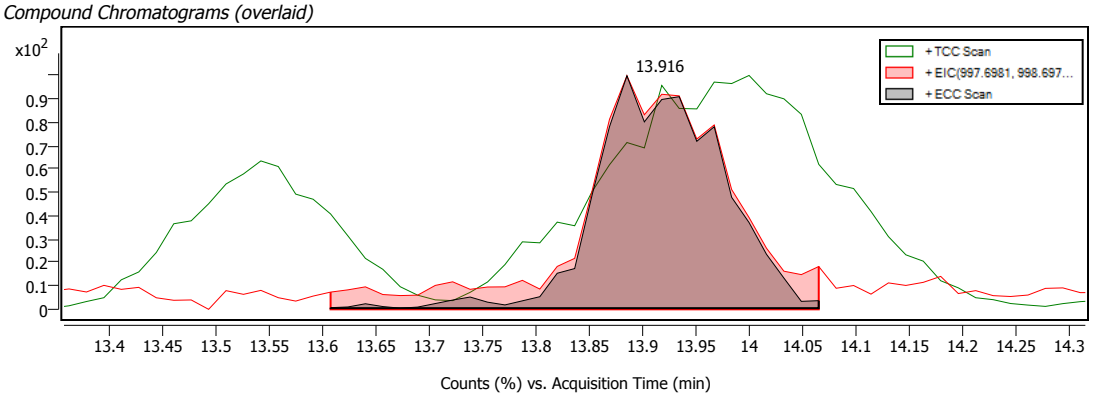
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	997.6962				5	98.67	

Compound ID Table

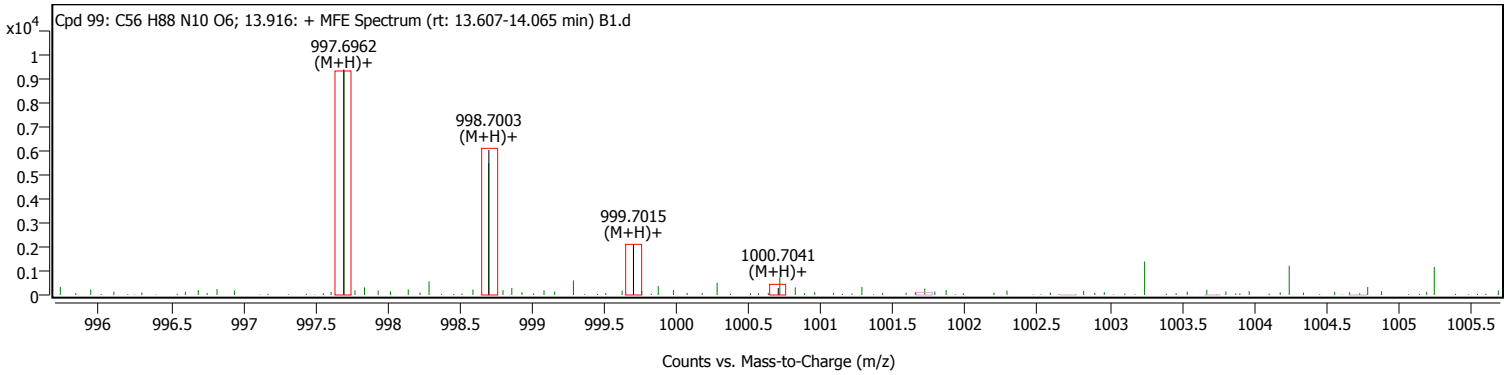
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C56 H88 N10 O6	(M+H)+	MFG	13.916		996.6892		98.67		98.67
	C55 H82 N17 O	(M+H)+	MFG	13.916		996.6893		98.54		98.54
	C57 H94 N3 O11	(M+H)+	MFG	13.916		996.6890		98.34		98.34
	C57 H84 N14 O2	(M+H)+	MFG	13.916		996.6892		97.98		97.98
	C58 H90 N7 O7	(M+H)+	MFG	13.916		996.6891		97.73		97.73

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 100: C55 H90 N3 O10

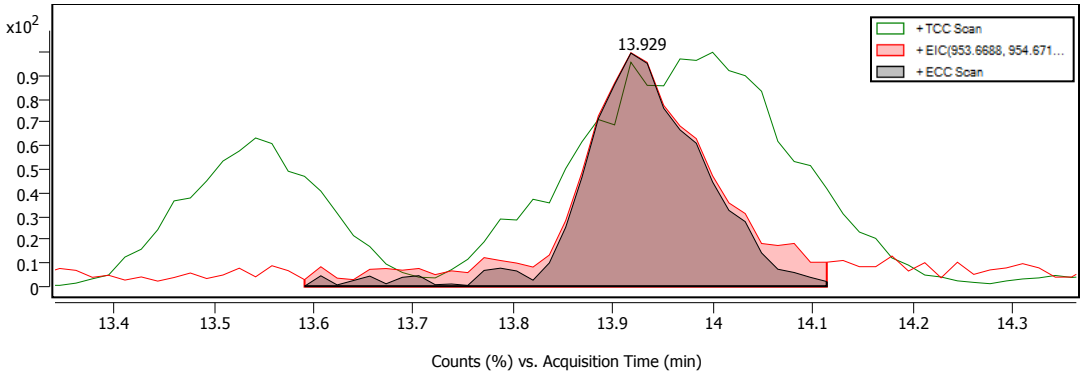
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C55 H90 N3 O10	13.929		952.6627		MFG	95.06	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	953.6696				5	95.06	

Compound ID Table

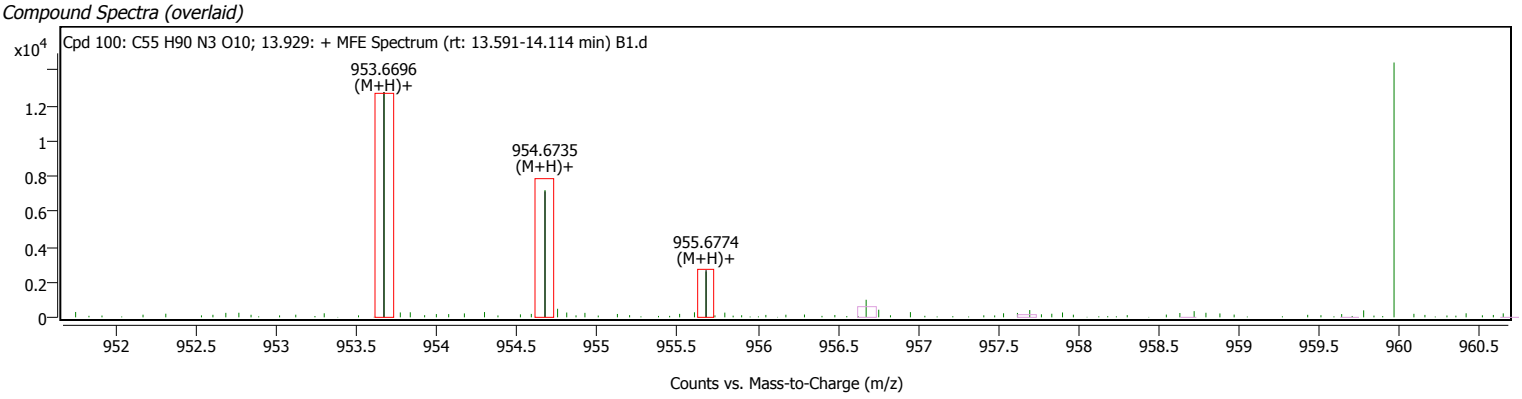
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C55 H90 N3 O10	(M+H)+	MFG	13.929		952.6627		95.06		95.06
	C54 H84 N10 O5	(M+H)+	MFG	13.929		952.6628		94.29		94.29
	C53 H88 N6 O9	(M+H)+	MFG	13.929		952.6628		93.29		93.29
	C57 H92 O11	(M+H)+	MFG	13.929		952.6627		93.26		93.26
	C53 H78 N17	(M+H)+	MFG	13.929		952.6630		93.11		93.11

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 101: C53 H86 N3 O9

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C53 H86 N3 O9	13.952		908.6370		MFG	96.79	MFE	

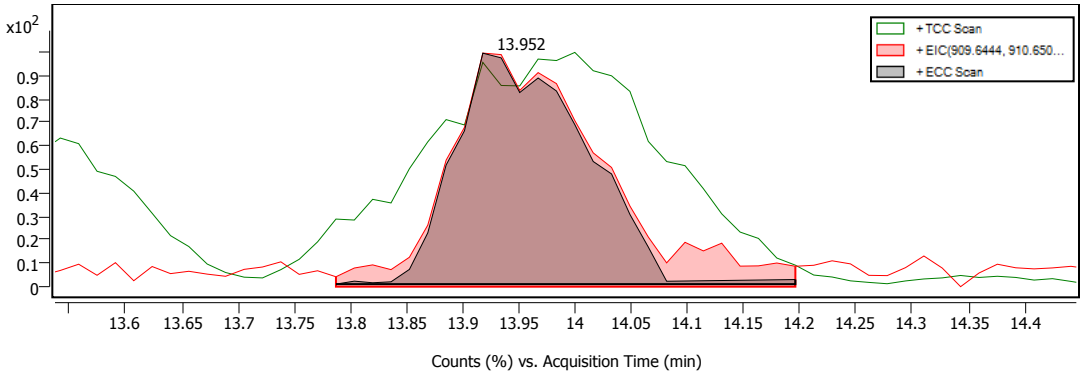
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	909.6442				11	96.79	

Compound ID Table

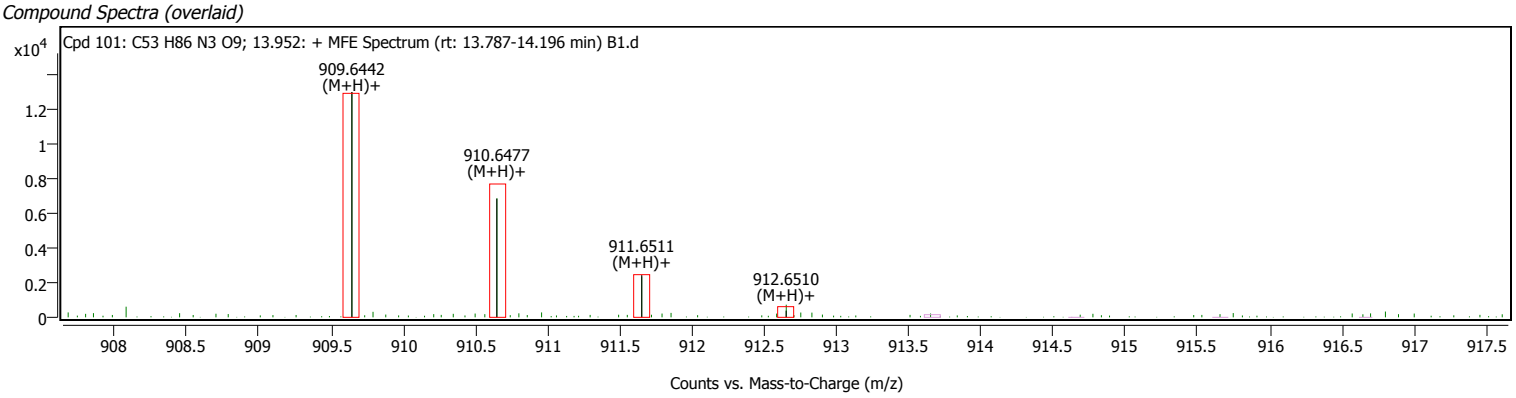
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C53 H86 N3 O9	(M+H)+	MFG	13.952		908.6370		96.79		96.79
	C46 H86 N9 O7 S	(M+H)+	MFG	13.952		908.6375		96.63		96.63
PI(17:0/22:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
PI(18:0/21:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
PI(19:0/20:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
PI(20:0/19:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
PI(22:0/17:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
PI(21:0/18:0)	C48 H93 O13 P	(M+H)+	DBSearch	13.952		908.6370		96.56	96.56	
	C47 H92 N2 O12 S	(M+H)+	MFG	13.952		908.6373		96.44		96.44
	C45 H80 N16 O2 S	(M+H)+	MFG	13.952		908.6376		96.26		96.26
	C55 H88 O10	(M+H)+	MFG	13.952		908.6370		96.10		96.10

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 102: C39 H86 N5 O15

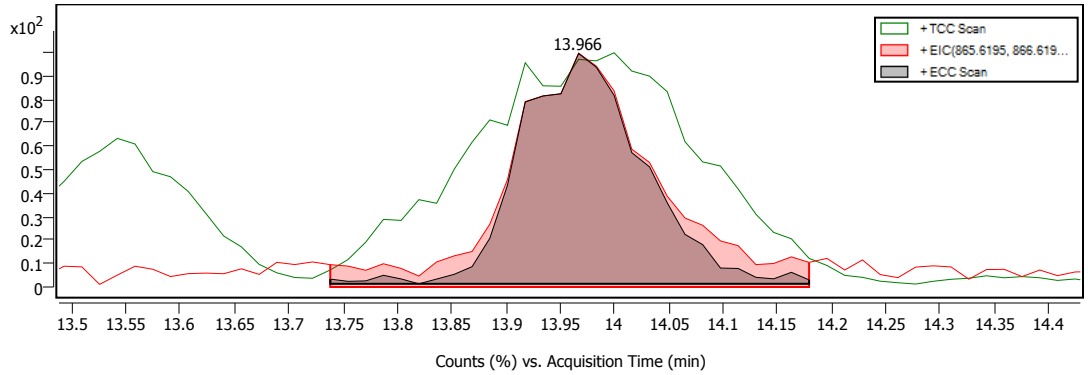
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C39 H86 N5 O15	13.966		864.6113		MFG	97.36	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	865.6185				10	97.36	

Compound ID Table

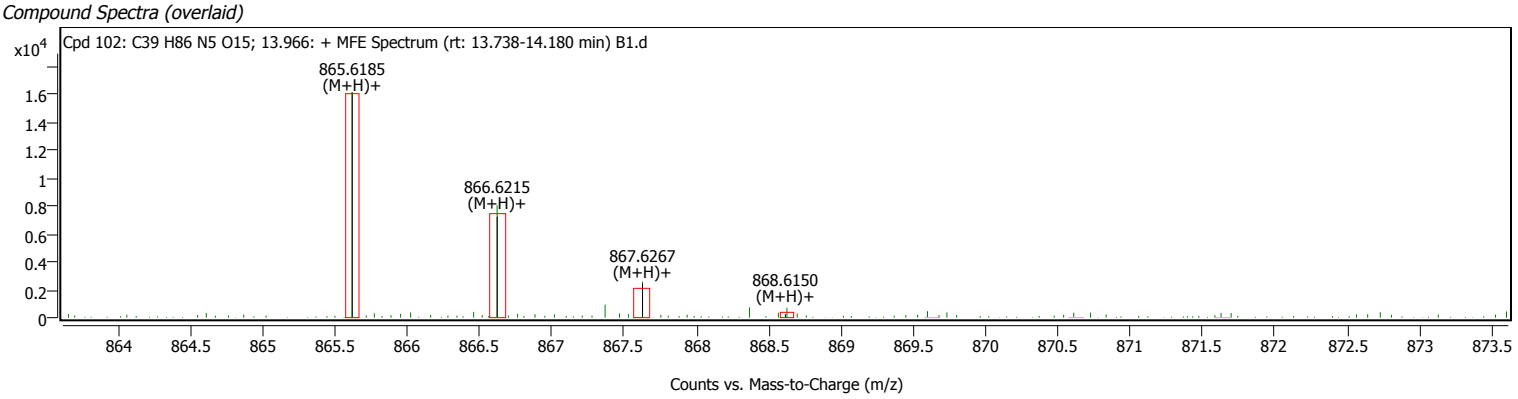
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C39 H86 N5 O15	(M+H)+	MFG	13.966		864.6113		97.36		97.36
	C38 H80 N12 O10	(M+H)+	MFG	13.966		864.6114		96.52		96.52
	C36 H78 N15 O9	(M+H)+	MFG	13.966		864.6115		95.80		95.80
	C37 H74 N19 O5	(M+H)+	MFG	13.966		864.6116		94.92		94.92
	C35 H72 N22 O4	(M+H)+	MFG	13.966		864.6116		93.72		93.72
PI(O-18:0/19:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.966		864.6111		92.50	92.50	
PI(O-20:0/17:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.966		864.6111		92.50	92.50	
PI(P-16:0/21:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.966		864.6111		92.50	92.50	
PI(P-18:0/19:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.966		864.6111		92.50	92.50	
PI(P-20:0/17:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.966		864.6111		92.50	92.50	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 103: C43 H84 N2 O10 S

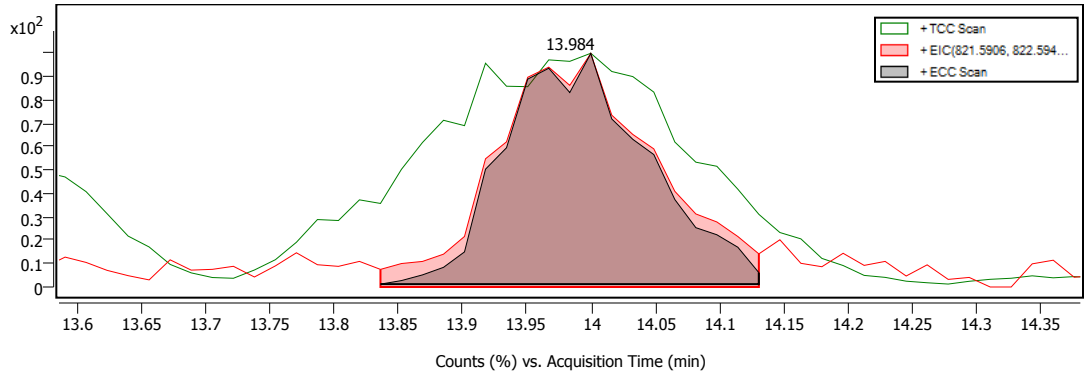
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C43 H84 N2 O10 S	13.984		820.5858		MFG	92.39	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	821.5925				26	92.39	

Compound ID Table

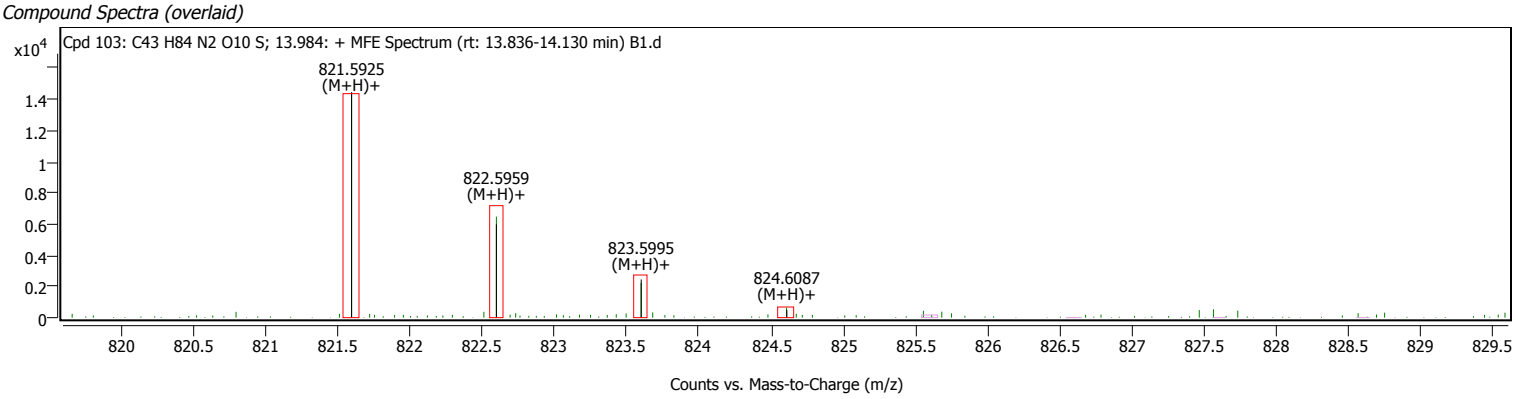
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C43 H84 N2 O10 S	(M+H)+	MFG	13.984		820.5858		92.39		92.39
	C37 H80 N12 O4 S2	(M+H)+	MFG	13.984		820.5863		91.96		91.96
	C36 H76 N12 O9	(M+H)+	MFG	13.984		820.5857		91.88		91.88
	C44 H80 N6 O6 S	(M+H)+	MFG	13.984		820.5859		91.39		91.39
	C42 H78 N9 O5 S	(M+H)+	MFG	13.984		820.5860		89.99		89.99
PC(17:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(19:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/19:1(9Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(22:4(7Z,10Z,13Z,16Z)/17:2(9Z,12Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/17:0)	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.984		820.5854		88.66	88.66	
PC(18:3(9Z,12Z,15Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(18:3(6Z,9Z,12Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(19:0/18:3(6Z,9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(20:3(8Z,11Z,14Z)/17:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(22:2(13Z,16Z)/15:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(17:0/20:3(8Z,11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(15:1(9Z)/22:2(13Z,16Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(18:0/19:3(9Z,12Z,15Z))[U]	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(17:1(9Z)/20:2(11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(19:0/18:3(9Z,12Z,15Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(19:1(9Z)/18:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(20:1(11Z)/17:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(20:2(11Z,14Z)/17:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(17:2(9Z,12Z)/20:1(11Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	
PC(18:2(9Z,12Z)/19:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.984		798.6035		84.75	84.75	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 104: C34 H72 N12 O8

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C34 H72 N12 O8	14.003		776.5596		MFG	94.71	MFE	

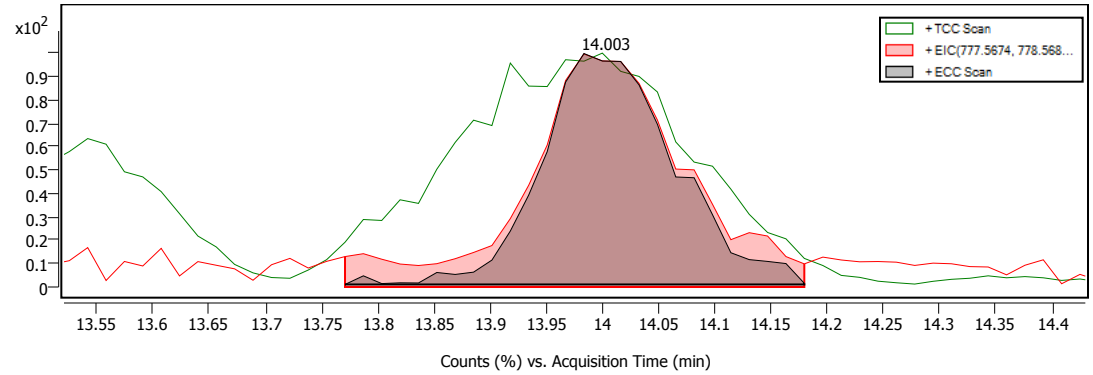
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	777.5664				27	94.71	

Compound ID Table

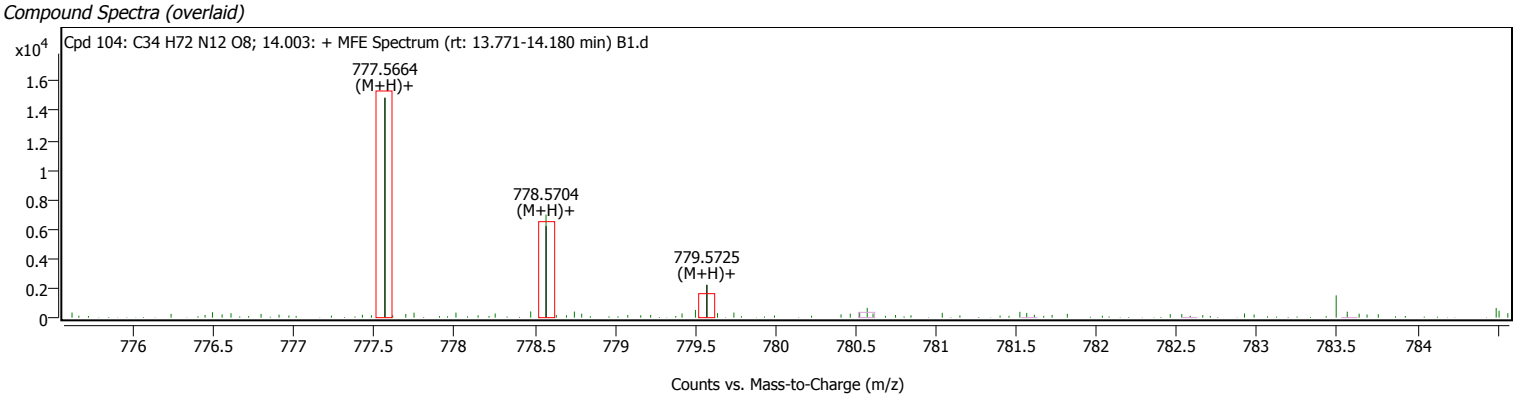
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C34 H72 N12 O8	(M+H)+	MFG	14.003		776.5596		94.71		94.71
	C36 H74 N9 O9	(M+H)+	MFG	14.003		776.5595		92.82		92.82
	C33 H66 N19 O3	(M+H)+	MFG	14.003		776.5597		92.71		92.71
	C41 H80 N2 O9 S	(M+H)+	MFG	14.003		776.5596		92.50		92.50
	C42 H76 N6 O5 S	(M+H)+	MFG	14.003		776.5597		92.45		92.45
PG(17:0/19:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(18:1(11Z)/18:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(18:1(9Z)/18:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(18:0/18:1(9Z))[U]	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(16:1(9Z)/20:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(18:0/18:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
1-Stearoyl-2-Oleoyl-sn-Glycero-3-[Phospho-rac-(1-glycerol)]	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(14:0/22:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(14:1(9Z)/22:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(15:1(9Z)/21:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(19:0/17:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(17:1(9Z)/19:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(19:1(9Z)/17:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(20:0/16:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(20:1(11Z)/16:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(21:0/15:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(22:0/14:1(9Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(22:1(11Z)/14:0)	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(16:0/20:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PG(18:0/18:1(11Z))	C42 H81 O10 P	(M+H)+	DBSearch	14.003		776.5593		88.19	88.19	
PC(O-15:0/20:4(5Z,8Z,11Z,14Z))	C43 H81 N O7 P	(M+Na)+	DBSearch	14.003		754.5773		88.04	88.04	
PC(O-15:0/20:4(5Z,8Z,11Z,14Z))[U]	C43 H81 N O7 P	(M+Na)+	DBSearch	14.003		754.5773		88.04	88.04	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 105: C32 H68 N12 O7

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H68 N12 O7	14.026		732.5339		MFG	87.71	MFE	

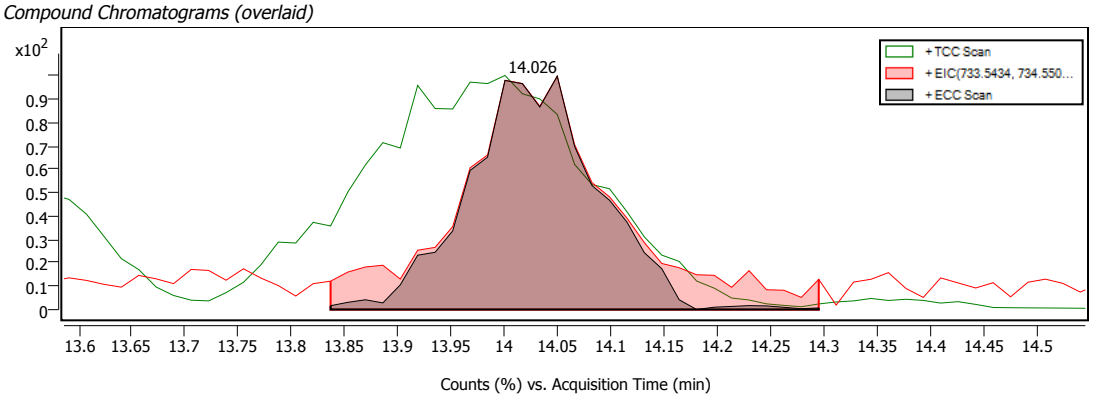
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	733.5407				9	87.71	

Compound ID Table

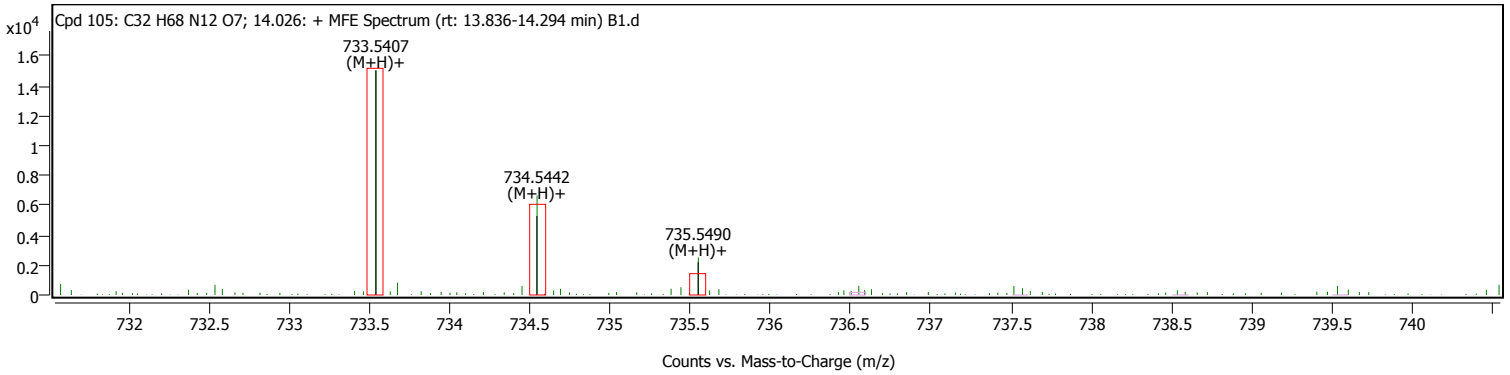
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H68 N12 O7	(M+H)+	MFG	14.026		732.5339		87.71		87.71
	C34 H70 N9 O8	(M+H)+	MFG	14.026		732.5338		87.22		87.22
	C33 H72 N12 O2 S2	(M+H)+	MFG	14.026		732.5344		85.33		85.33
	C33 H64 N16 O3	(M+H)+	MFG	14.026		732.5339		84.28		84.28
	C31 H62 N19 O2	(M+H)+	MFG	14.026		732.5340		84.08		84.08
PG(O-16:0/18:2(9Z,12Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.026		732.5336		76.97	76.97	
PG(P-18:0/16:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.026		732.5336		76.97	76.97	
PG(P-20:0/14:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.026		732.5336		76.97	76.97	
PG(P-16:0/18:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.026		732.5336		76.97	76.97	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 106: C30 H64 N12 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C30 H64 N12 O6	14.042		688.5071		MFG	92.99	MFE	

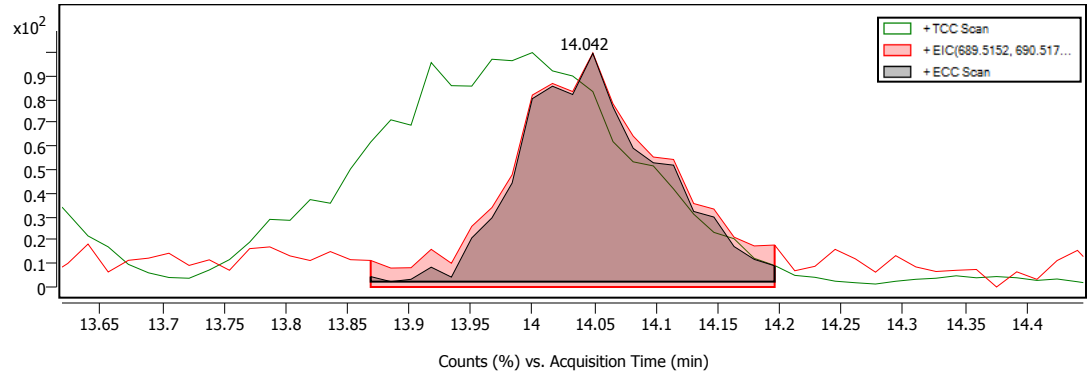
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	689.5141				52	92.99	

Compound ID Table

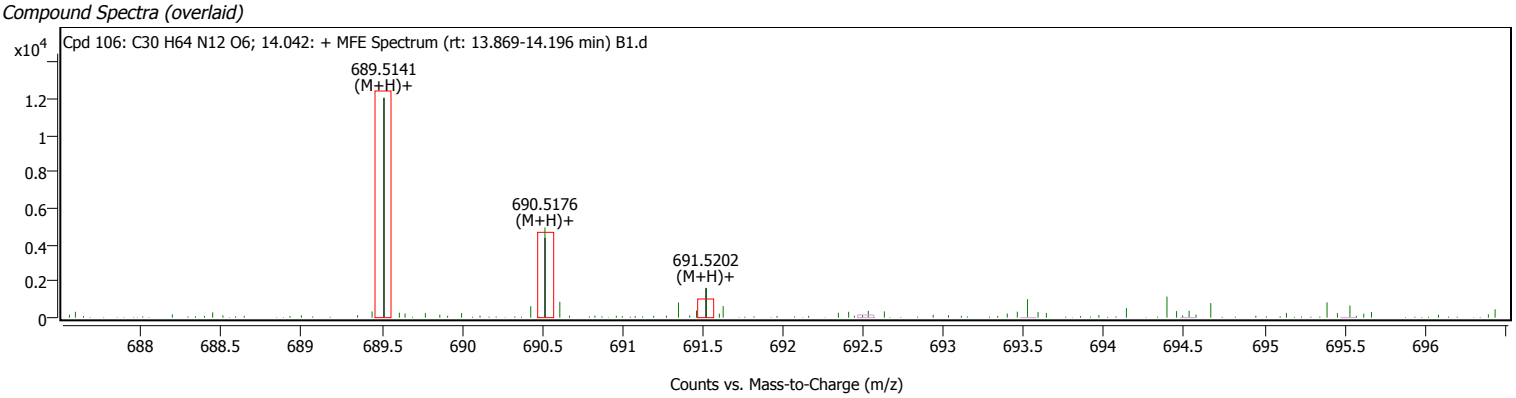
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C30 H64 N12 O6	(M+H)+	MFG	14.042		688.5071		92.99		92.99
	C37 H72 N2 O7 S	(M+H)+	MFG	14.042		688.5072		91.25		91.25
	C38 H68 N6 O3 S	(M+H)+	MFG	14.042		688.5072		90.67		90.67
	C32 H66 N9 O7	(M+H)+	MFG	14.042		688.5070		90.64		90.64
	C29 H58 N19 O	(M+H)+	MFG	14.042		688.5073		90.17		90.17
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(20:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.042		688.5068		86.33	86.33	
PA(13:0/22:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(19:0/16:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(14:1(9Z)/21:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(17:0/18:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(21:0/14:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(20:1(11Z)/15:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(20:0/15:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(19:1(9Z)/16:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(17:1(9Z)/18:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(18:1(9Z)/17:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(15:0/20:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(16:1(9Z)/19:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(16:0/19:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(15:1(9Z)/20:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(18:0/17:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
PA(22:1(11Z)/13:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.042		688.5068		84.81	84.81	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(9Z,12Z,15Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:2(9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:3(9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:3(8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:4(6Z,9Z,12Z,15Z)/22:3(10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:2(9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/20:2(11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(6Z,9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:2(11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	
DG(20:3(5Z,8Z,11Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.042		666.5249		79.63	79.63	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 107: C44 H60 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H60 N4	14.064		644.4815		MFG	95.82	MFE	

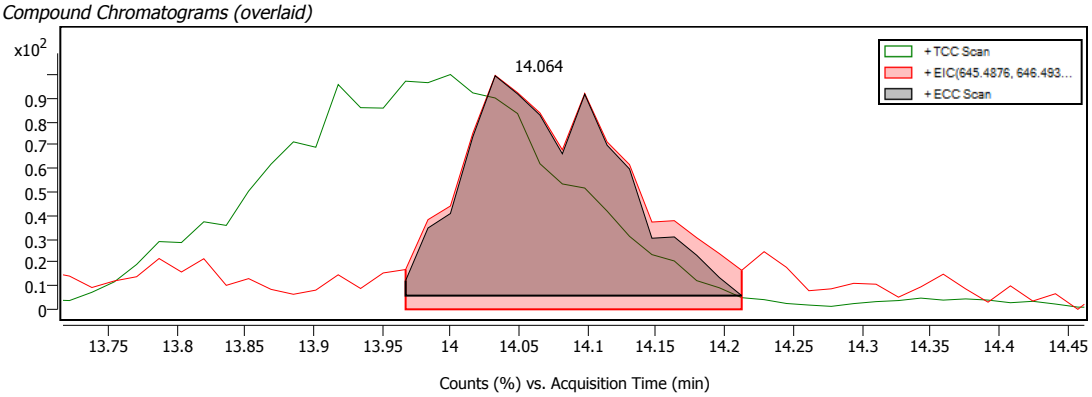
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	645.4888				5	95.82	

Compound ID Table

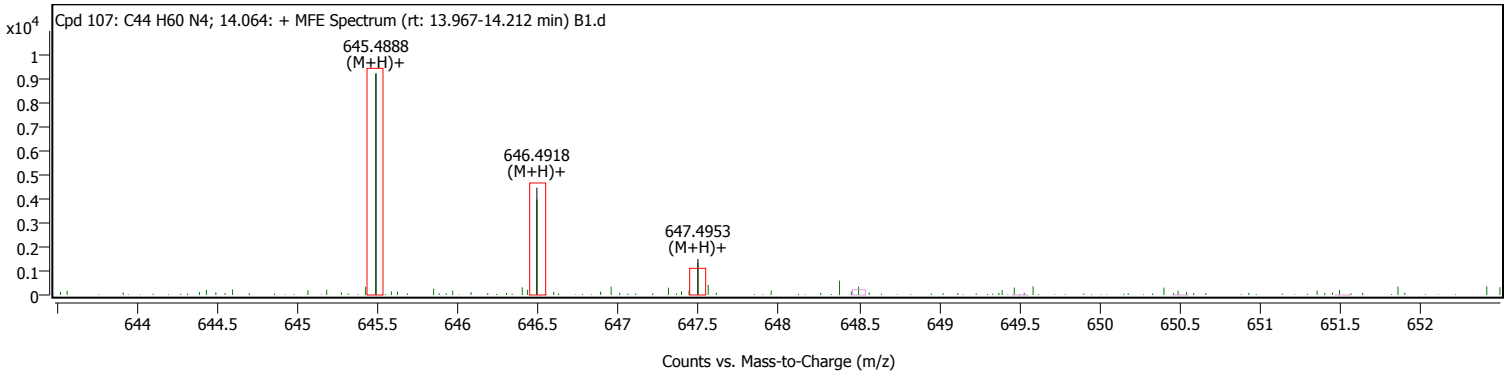
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H60 N4	(M+H)+	MFG	14.064		644.4815		95.82		95.82
	C43 H64 O4	(M+H)+	MFG	14.064		644.4814		94.68		94.68
	C46 H62 N O	(M+H)+	MFG	14.064		644.4814		91.92		91.92
	C38 H66 N3 O3 S	(M+H)+	MFG	14.064		644.4818		91.58		91.58
	C36 H64 N6 O2 S	(M+H)+	MFG	14.064		644.4819		90.11		90.11

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

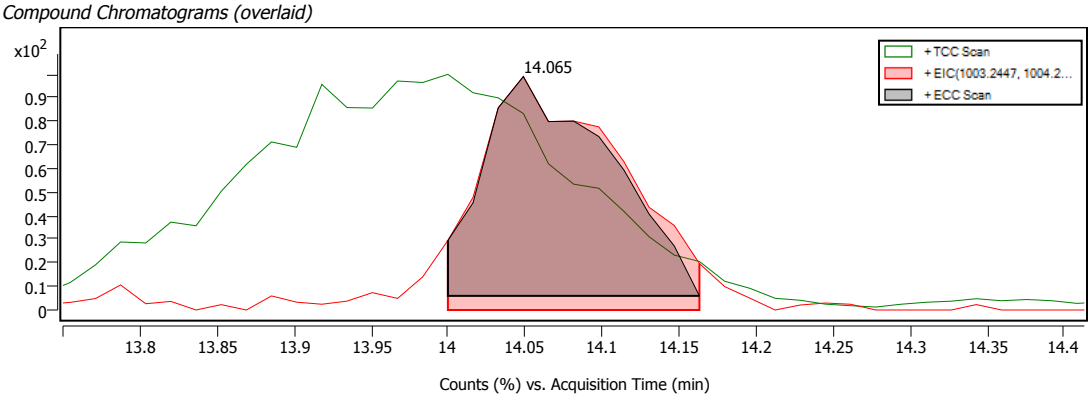


Cpd 108: 14.065

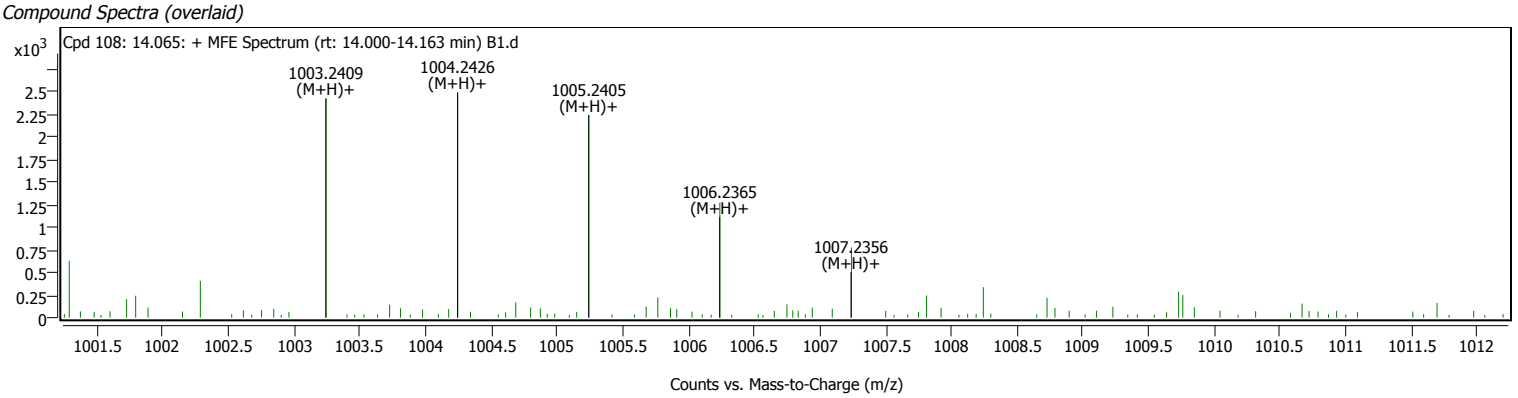
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.065		1002.2336				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 109: OH-Spheroidenone

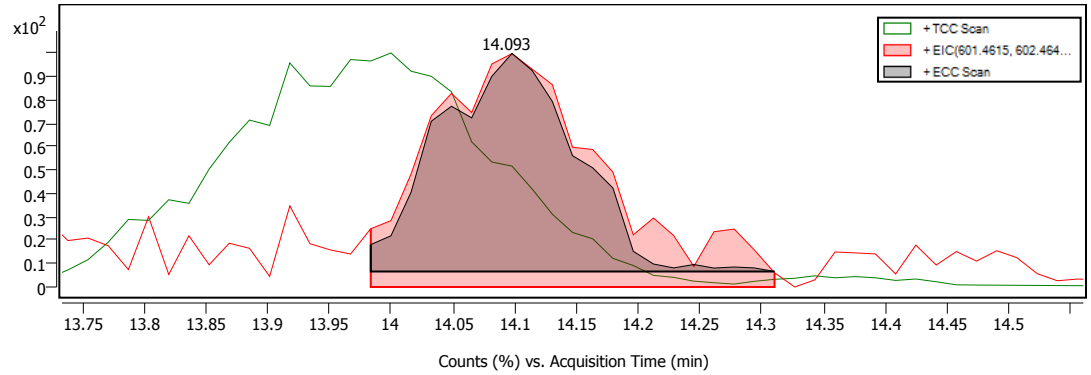
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
OH-Spheroidenone	C41 H60 O3	14.093		600.4546		DBSearch-MFG	94.64	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	601.4620 601.4620 601.4620 601.4620		0	94.64	5	94.64	

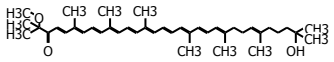
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
OH-Spheroidenone	C41 H60 O3	(M+H)+	DBSearch-MFG	14.093		600.4546		94.64	94.64	94.64
	C34 H60 N6 O S	(M+H)+	MFG	14.093		600.4551		92.04		92.04
	C36 H62 N3 O2 S	(M+H)+	MFG	14.093		600.4550		90.91		90.91
	C39 H58 N3 O2	(M+H)+	MFG	14.093		600.4546		89.50		89.50
	C33 H64 N2 O5 S	(M+H)+	MFG	14.093		600.4550		86.78		86.78

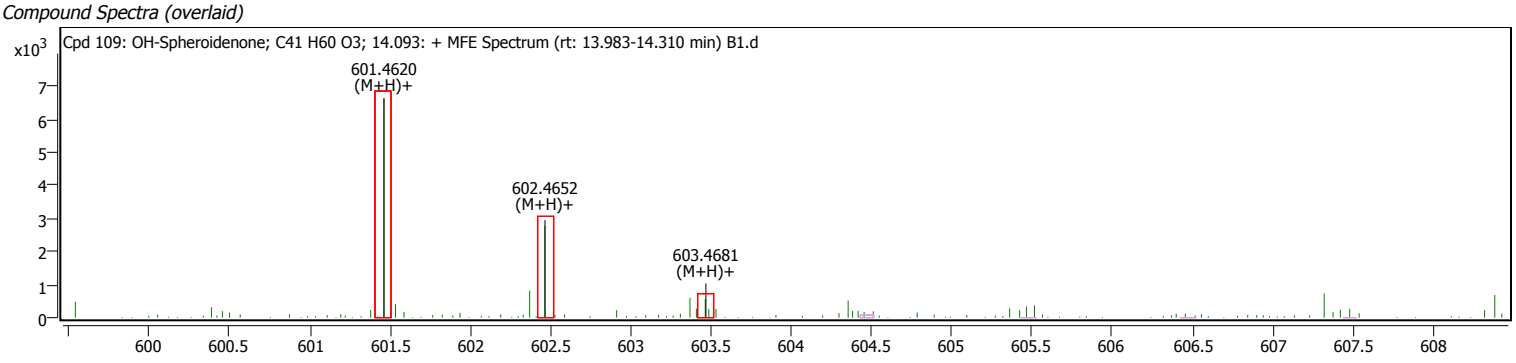
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 110: C32 H56 N6 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C32 H56 N6 S	14.121		556.4290		MFG	93.42	MFE	

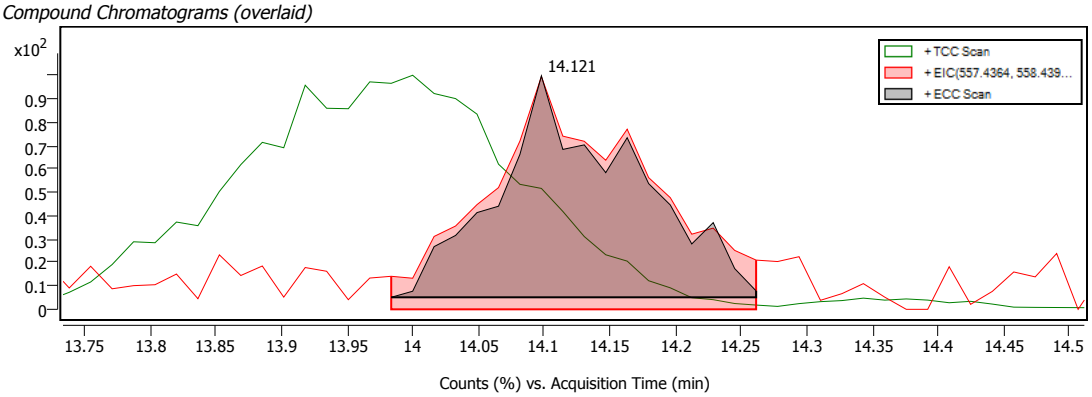
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	557.4359				5	93.42	

Compound ID Table

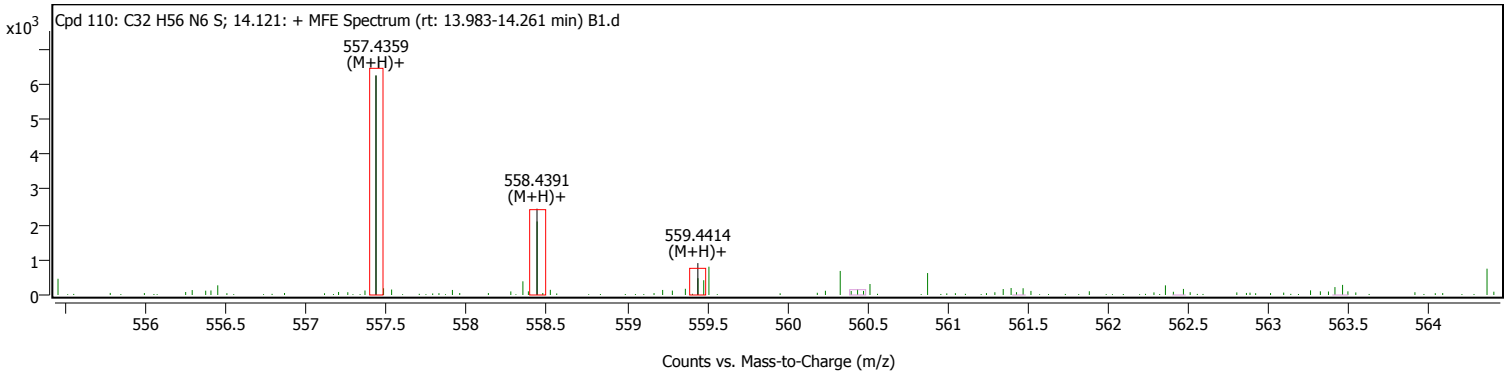
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C32 H56 N6 S	(M+H)+	MFG	14.121		556.4290		93.42		93.42
	C34 H58 N3 O S	(M+H)+	MFG	14.121		556.4290		92.47		92.47
Germanicol cinnamate	C39 H56 O2	(M+H)+	DBSearch-MFG	14.121		556.4285	65883-48-9	91.54	91.56	91.52
	C31 H60 N2 O4 S	(M+H)+	MFG	14.121		556.4290		88.48		88.48
	C37 H54 N3 O	(M+H)+	MFG	14.121		556.4286		85.93		85.93

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 111: C37 H52 O

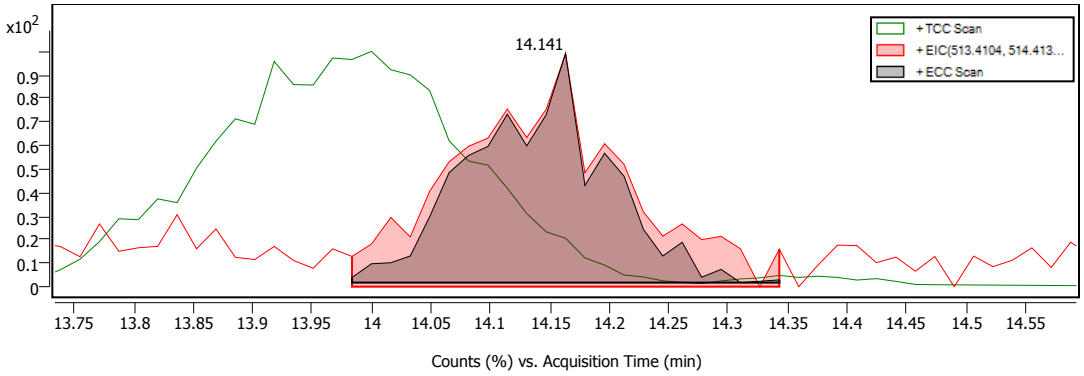
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C37 H52 O	14.141		512.4024		MFG	69.46	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	513.4097				5	69.46	

Compound ID Table

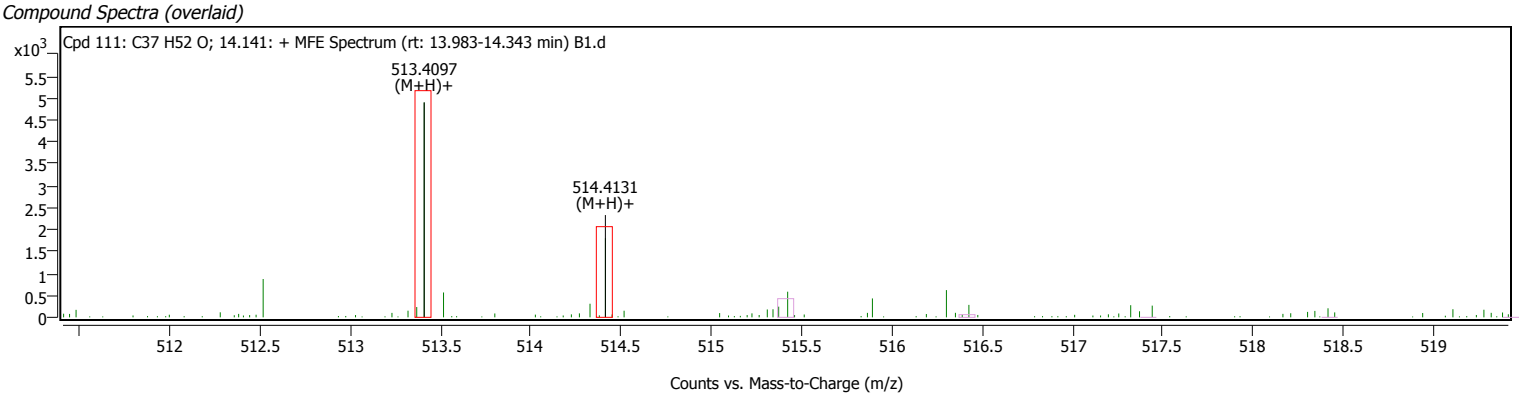
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C37 H52 O	(M+H)+	MFG	14.141		512.4024		69.46		69.46
	C35 H50 N3	(M+H)+	MFG	14.141		512.4025		62.59		62.59
	C22 H48 N12 O2	(M+H)+	MFG	14.141		512.4027		61.72		61.72
	C23 H54 N5 O7	(M+H)+	MFG	14.141		512.4026		61.46		61.46
	C24 H50 N9 O3	(M+H)+	MFG	14.141		512.4027		61.00		61.00

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)

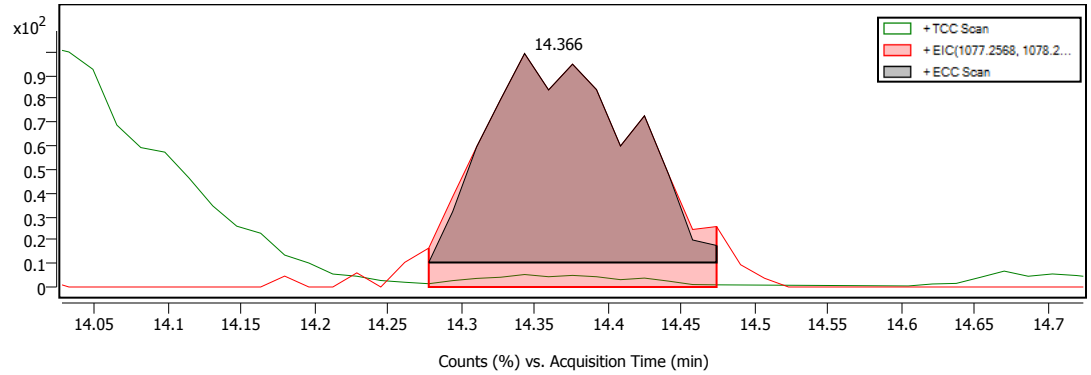


Cpd 112: 14.366

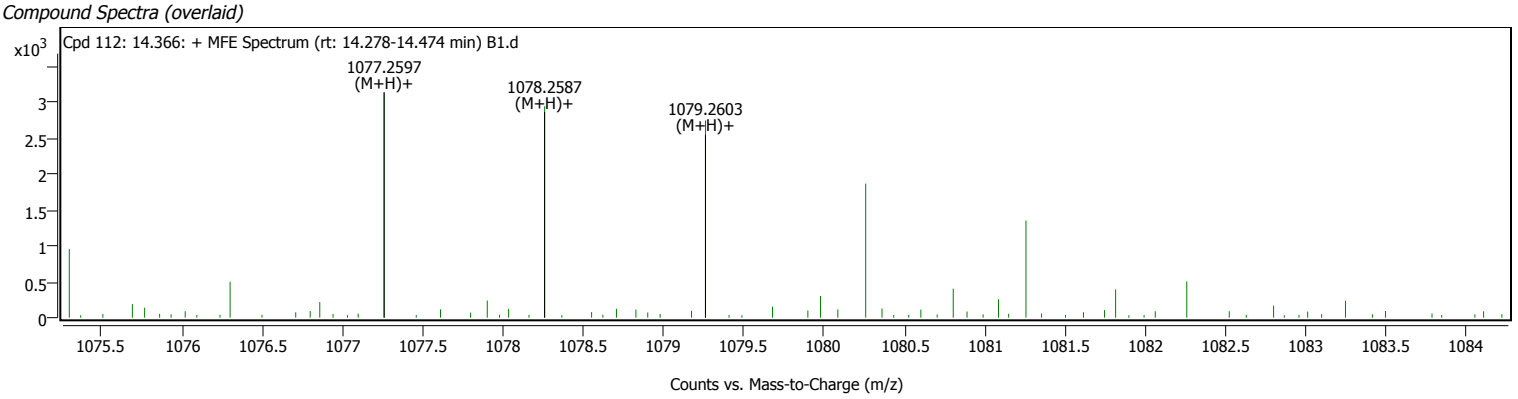
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.366		1076.2524				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

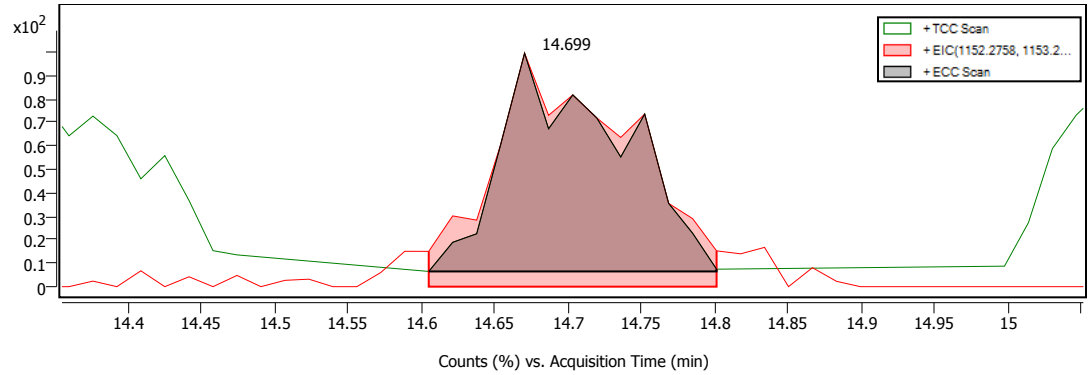


Cpd 113: 14.699

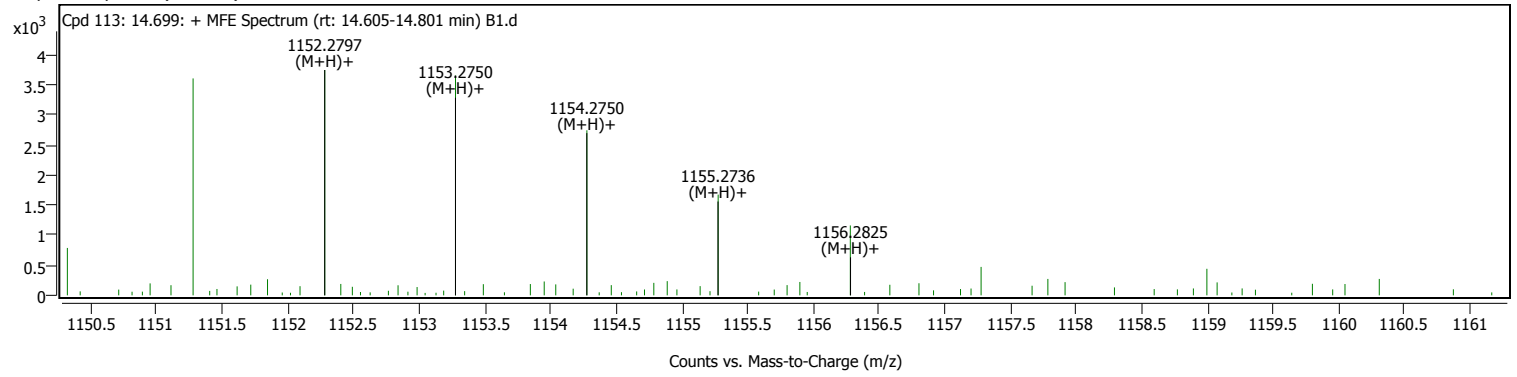
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		14.699		1151.2724				MFE	

Compound Chromatograms (overlaid)

Structure



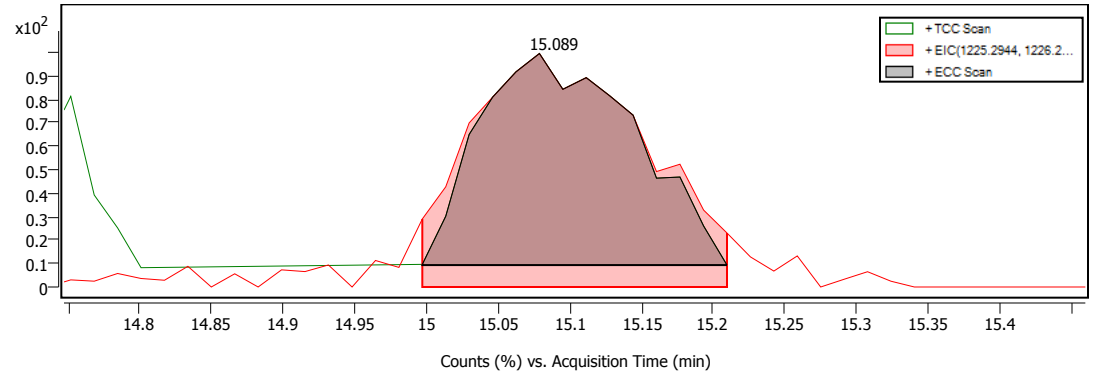
Compound Spectra (overlaid)



Cpd 114: 15.089

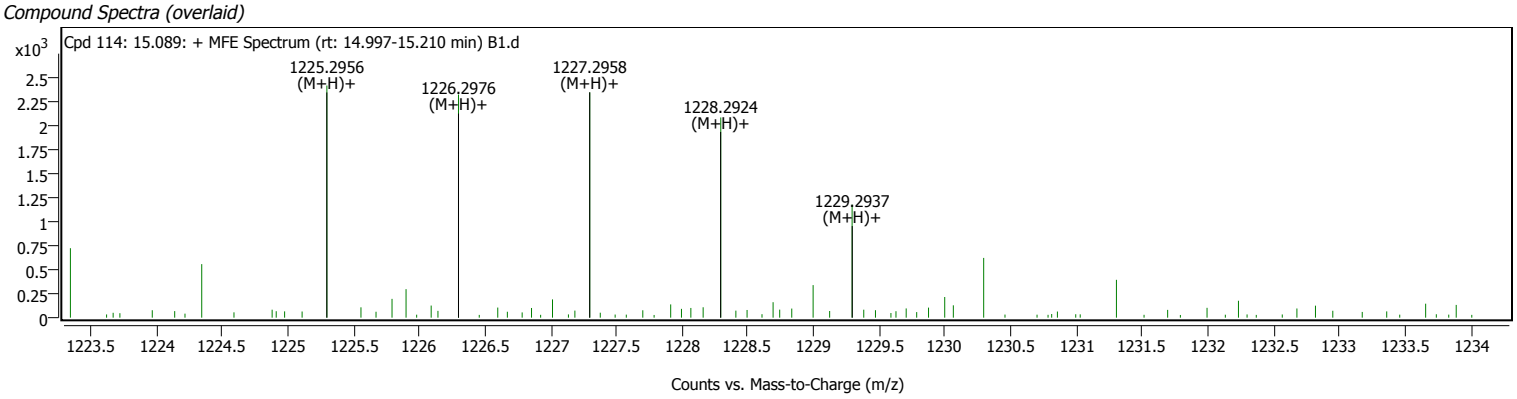
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		15.089		1224.2884				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



MassHunter Qual 10.0
(End of Report)