Compound Discovery Report

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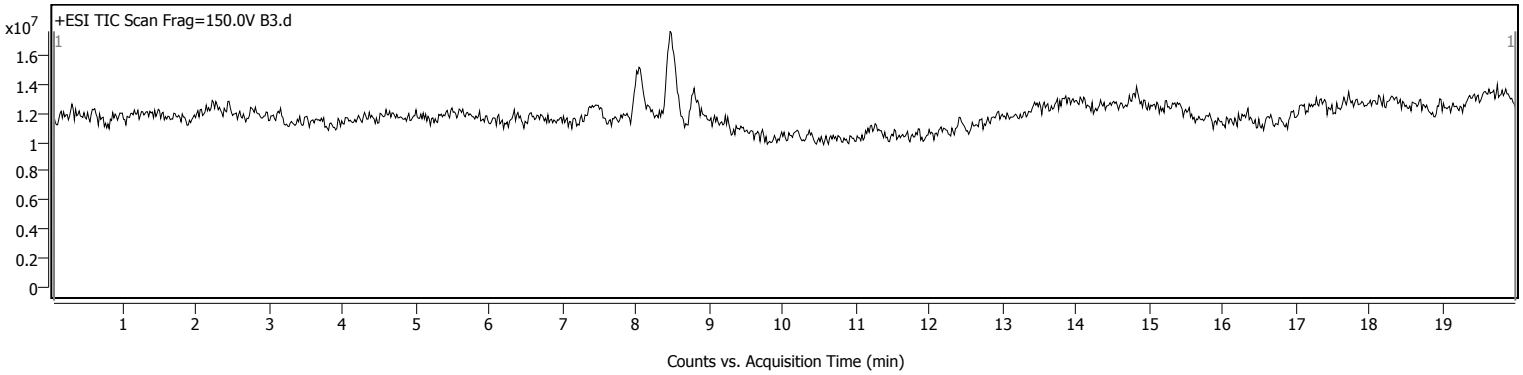
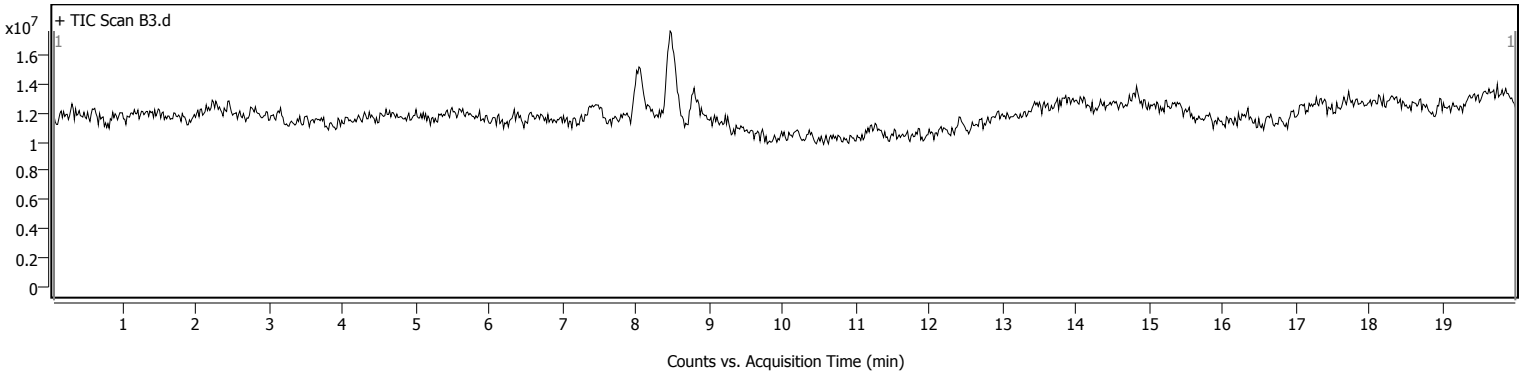
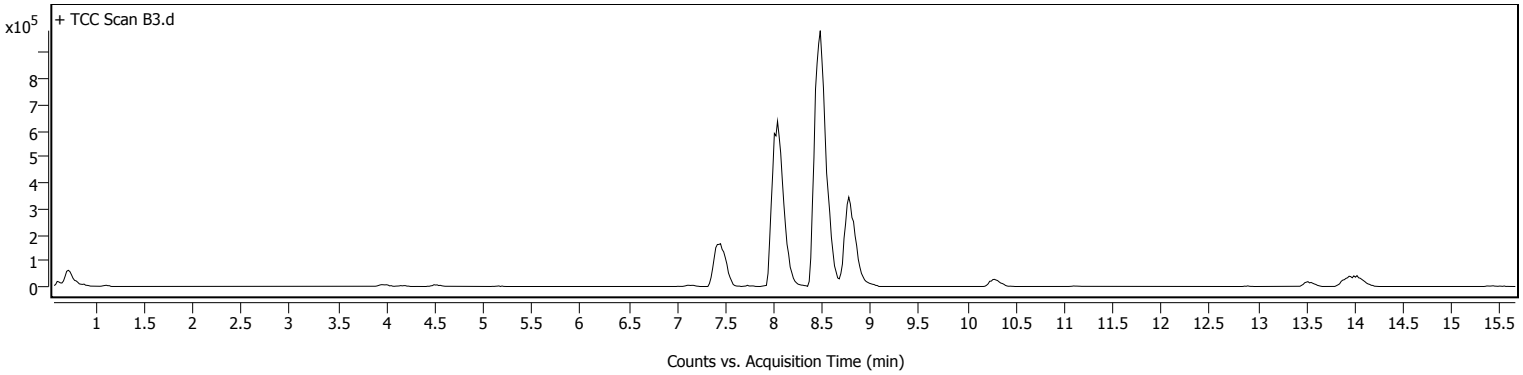
Sample Information

Name	B3	**Data File Path**	D:\MassHunter\Data\Saeed Ullah\B3.d
Sample ID		**Acq. Time (Local)**	10/3/2023 10:28:14 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-A3	**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**	49 identified (55 found)

Sample Chromatograms







Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1		C16 H31 N13 O4	0.597	469.2618		MFG	81.62			81.62	MFE
2			0.684	958.9576							MFE
3	3-Deoxyarabinohexonic acid	C6 H12 O6	0.724	180.0633	29625-79-4	DBSearch-MFG	67.24		86.87	47.61	MFE
4		C10 H18 N6 O10	0.726	382.1079		MFG	79.56			79.56	MFE
5	Cordycepin	C10 H13 N5 O3	1.105	251.1016	73-03-0	DBSearch-MFG	58.02		68.60	47.43	MFE
6	Trifluoperazine	C21 H24 F3 N3 S	3.974	407.1654	117-89-5	DBSearch	82.72		82.72		MFE
7	Cyflufenamid	C20 H17 F5 N2 O2	4.172	412.1202		DBSearch	65.65		65.65		MFE
8		C21 H39 N4 O18 S2	4.510	699.1704		MFG	89.36			89.36	MFE
9			5.161	310.0650							MFE
10		C28 H22 N O	7.136	388.1699		MFG	79.49			79.49	MFE
11		C22 H48 N3 O S2	7.430	434.3236		MFG	87.17			87.17	MFE
12		C23 H48 O8	7.438	452.3346		MFG	99.39			99.39	MFE

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Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
13		C31 H34 N6	7.444	490.2846		MFG	69.11			69.11	MFE
14	PS(18:3(9Z,12Z,15Z)/0:0)	C24 H42 N O9 P	7.447	519.2602		DBSearch	77.87		77.87		MFE
15		C24 H32 N O7	7.744	446.2178		MFG	79.00			79.00	MFE
16			8.031	547.4080							MFE
17		C28 H53 N8 O4	8.035	565.4187		MFG	99.57			99.57	MFE
18		C25 H57 N5 O7 S2	8.036	603.3706		MFG	91.51			91.51	MFE
19	16,16-dimethyl Prostaglandin E2 p-(p-acetamidobenzamido) phenyl ester	C37 H48 N2 O7	8.037	632.3453	62873-55-6	DBSearch	85.25		85.25		MFE
20	Posaconazole	C37 H42 F2 N8 O4	8.038	700.3312	171228-49-2	DBSearch	66.89		66.89		MFE
21		C50 H76 O S	8.467	724.5617		MFG	47.62			47.62	MFE
22		C48 H56 N6	8.471	716.4563		MFG	94.60			94.60	MFE
23	Calenduloside G methyl ester	C43 H68 O14	8.472	808.4600	155740-15-1	DBSearch	65.86		65.86		MFE
24		C33 H58 N16	8.474	678.5026		MFG	99.04			99.04	MFE
25	Antanapeptin C	C41 H64 N4 O8	8.476	740.4728		DBSearch	95.74		95.74		MFE
26		C44 H73 N7 O11	8.776	875.5371		MFG	92.13			92.13	MFE
27	C18 Sulfatide	C42 H81 N O11 S	8.778	807.5560		DBSearch	50.86		50.86		MFE
28		C39 H79 N6 O10	8.782	791.5857		MFG	98.78			98.78	MFE
29		C25 H20 N5 O3	8.990	438.1559		MFG	73.08			73.08	MFE
30		C42 H78 N20 O4	9.022	926.6510		MFG	63.88			63.88	MFE
31		C14 H33 N4 O	10.253	273.2658		MFG	86.31			86.31	MFE
32		C16 H37 N4 O2	10.272	317.2918		MFG	82.87			82.87	MFE
33		C18 H41 N4 O3	10.294	361.3172		MFG	74.40			74.40	MFE
34		C14 H31 N4	10.357	255.2549		MFG	70.43			70.43	MFE
35		C30 H55 N O S	11.113	477.4002		MFG	62.20			62.20	MFE
36	27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.886	438.3327	78648-95-0	DBSearch	73.50		73.50		MFE
37			13.488	1012.6845							MFE
38		C56 H86 N7 O7	13.491	968.6590		MFG	59.22			59.22	MFE
39		C50 H76 N10 O4	13.508	880.6052		MFG	59.37			59.37	MFE
40		C40 H84 N8 O4 S3	13.529	836.5776		MFG	85.57			85.57	MFE
41	PC(15:0/20:3(5Z,8Z,11Z))	C43 H81 N O8 P	13.542	770.5707		DBSearch	62.92		62.92		MFE
42		C28 H62 N15 O6	13.576	704.5011		MFG	74.47			74.47	MFE
43			13.871	1084.7402							MFE
44			13.882	1040.7155							MFE
45		C55 H92 N6 O10	13.896	996.6878		MFG	80.36			80.36	MFE
46		C55 H90 N3 O10	13.919	952.6630		MFG	94.88			94.88	MFE
47		C45 H88 N2 O11 S	13.956	864.6104		MFG	88.79			88.79	MFE
48		C44 H80 N6 O6 S	13.976	820.5860		MFG	93.50			93.50	MFE
49		C36 H74 N9 O9	14.004	776.5605		MFG	93.03			93.03	MFE
50		C48 H68 N4 O2	14.030	732.5337		MFG	82.85			82.85	MFE
51		C31 H68 N12 O S2	14.049	688.5082		MFG	82.49			82.49	MFE
52		C44 H60 N4	14.060	644.4811		MFG	64.28			64.28	MFE
53		C27 H52 N16	14.083	600.4560		MFG	67.94			67.94	MFE
54	Germanicol cinnamate	C39 H56 O2	14.105	556.4276	65883-48-9	DBSearch-MFG	60.54		60.32	60.77	MFE
55		C44 H63 N6 O2	15.443	707.5011		MFG	63.65			63.65	MFE

Compound Details

Cpd. 1: C16 H31 N13 O4

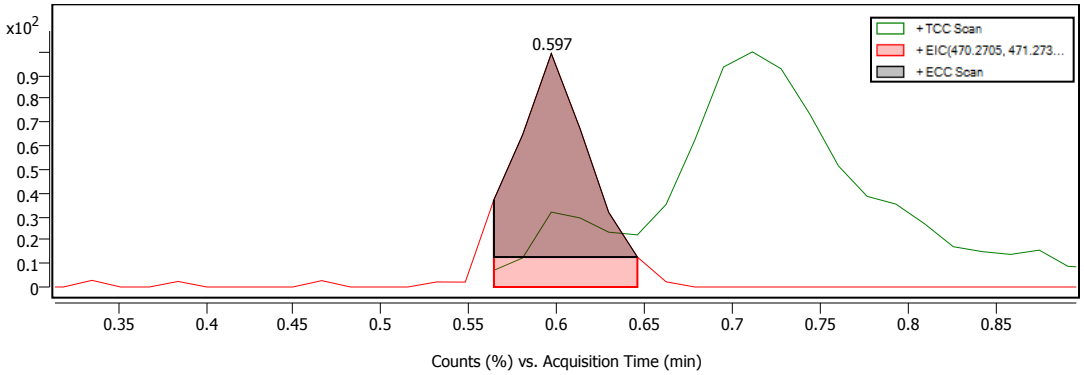
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H31 N13 O4	0.597		469.2618		MFG	81.62	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	470.2687				5	81.62	

Compound ID Table

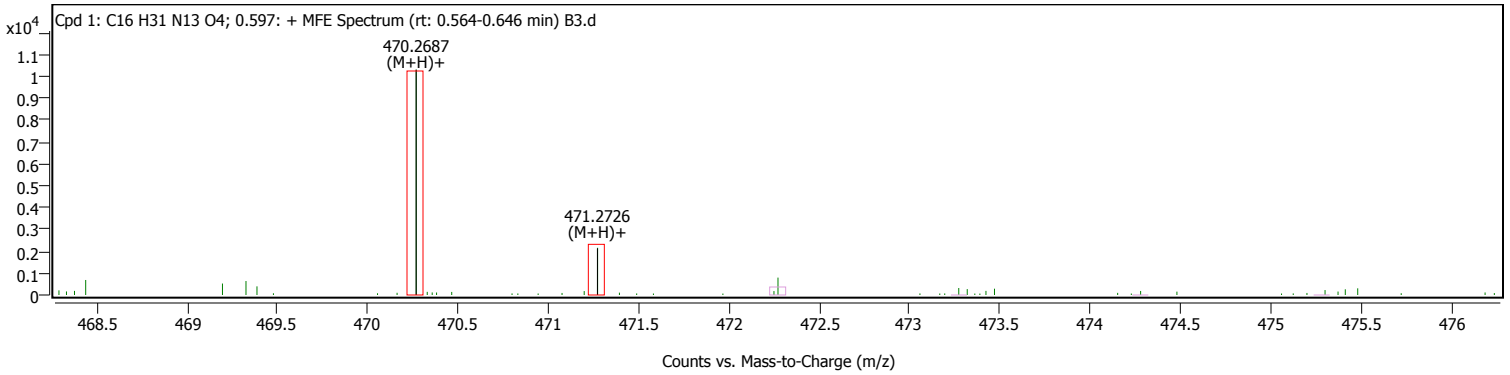
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H31 N13 O4	(M+H)+	MFG	0.597		469.2618		81.62		81.62
	C17 H37 N6 O9	(M+H)+	MFG	0.597		469.2616		81.57		81.57
	C15 H35 N9 O8	(M+H)+	MFG	0.597		469.2617		80.51		80.51
	C14 H29 N16 O3	(M+H)+	MFG	0.597		469.2618		80.04		80.04
	C18 H33 N10 O5	(M+H)+	MFG	0.597		469.2617		74.46		74.46

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)

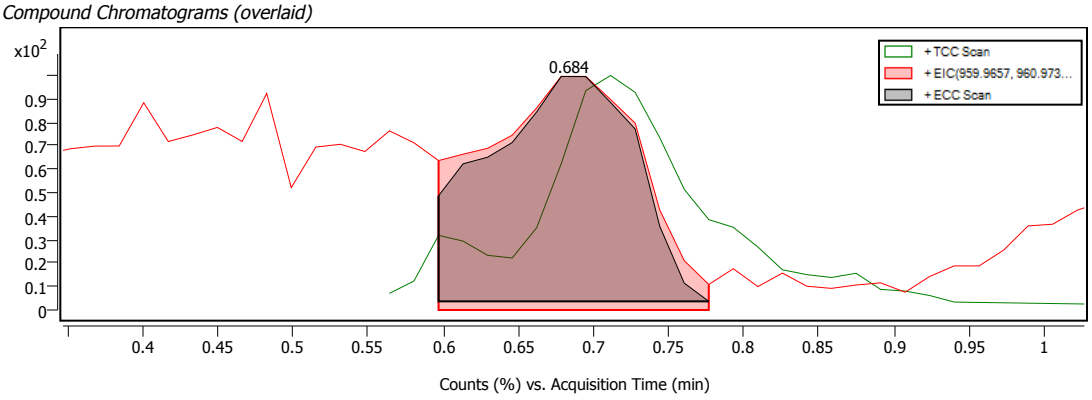


Cpd 2: 0.684

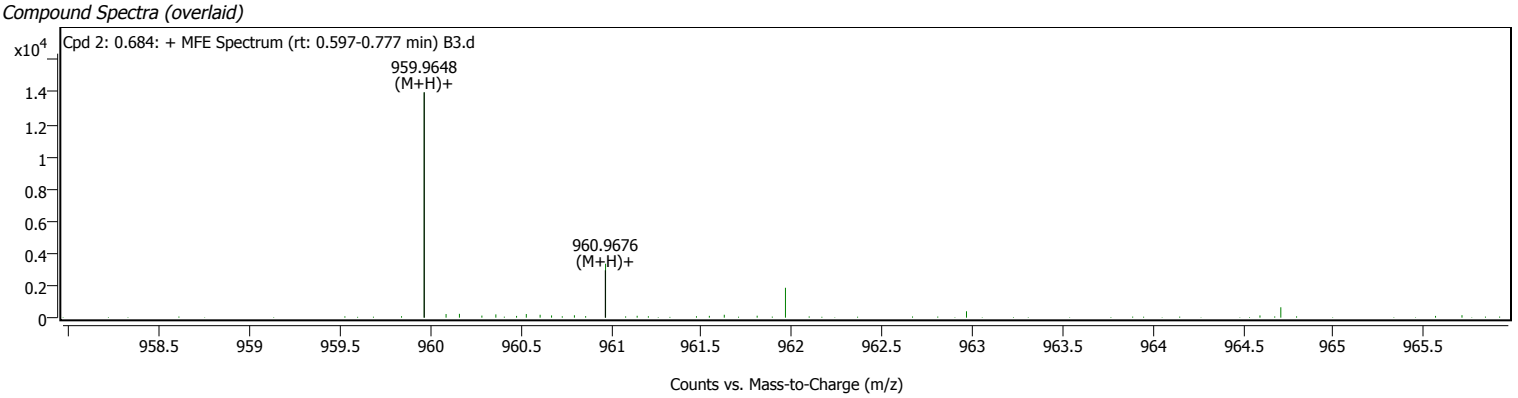
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		0.684		958.9576				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 3: 3-Deoxyarabinohexonic acid

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
3-Deoxyarabinohexonic acid	C6 H12 O6	0.724		180.0633	29625-79-4	DBSearch-MFG	67.24	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	203.0526 203.0526 203.0526		0	86.87	31	47.61	

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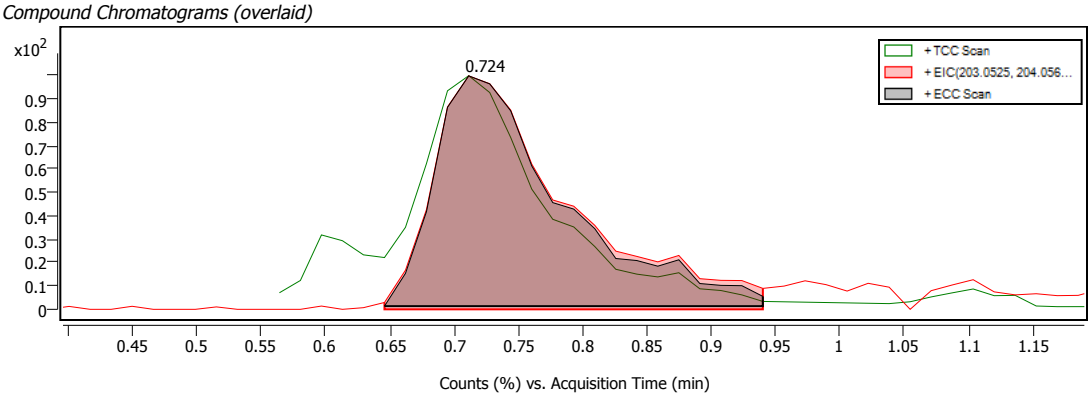
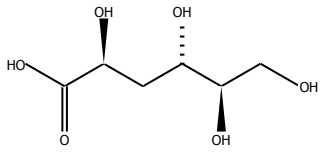
Compound ID Table

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	0.724		180.0633	29625-79-4	67.24	86.87	47.61
b-D-Galactopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	7296-64-2	67.24	86.87	47.61
D-Hamamelose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	4573-78-8	67.24	86.87	47.61
D-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	59-23-4	67.24	86.87	47.61
allo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	643-10-7	67.24	86.87	47.61
myo-Inositol	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	87-9-8	67.24	86.87	47.61
D-(+)-Mannose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	3458-28-4	67.24	86.87	47.61
b-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	492-61-5	67.24	86.87	47.61
L-(-)Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	87-79-6	67.24	86.87	47.61
α-D-Glucose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	492-62-6	67.24	86.87	47.61
D-Tagatose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	87-81-0	67.24	86.87	47.61
Sorbose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	3615-39-2	67.24	86.87	47.61
Allose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	6038-51-3	67.24	86.87	47.61
D-Fuconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633		67.24	86.87	47.61
L-Galactose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	15572-79-9	67.24	86.87	47.61
L-Rhamnonate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	6422-34-0	67.24	86.87	47.61
β-D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	53188-23-1	67.24	86.87	47.61
2-Deoxy-D-gluconate	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633		67.24	86.87	47.61
beta-D-Hamamelopyranose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633		67.24	86.87	47.61
D-Fructose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	57-48-7	67.24	86.87	47.61
L-(+)-Gulose	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	6027-89-0	67.24	86.87	47.61
1,3-Dihydroxyacetone	C6 H12 O6	(M+Na)+	DBSearch-MFG	0.724		180.0633	62147-49-3	67.24	86.87	47.61
	C7 H11 N2 O3 S	(M+H)+	MFG	0.724		203.0490		47.61		47.61
	C5 H14 N3 S2	(M+Na)+	MFG	0.724		180.0633		46.74		46.74
	C13 H5 N3	(M+H)+	MFG	0.724		203.0490		45.62		45.62
	C15 H7 O	(M+H)+	MFG	0.724		203.0490		45.36		45.36
	C7 H16 O S2	(M+Na)+	MFG	0.724		180.0633		43.74		43.74
	C12 H10 Cl N	(M+H)+	MFG	0.724		203.0490		41.36		41.36
	C4 H10 N3 O5	(M+Na)+	MFG	0.724		180.0633		40.13		40.13
	C5 H9 N5 O2 S	(M+H)+	MFG	0.724		203.0490		40.11		40.11
	C7 H8 N4 O2	(M+Na)+	MFG	0.724		180.0633		39.21		39.21

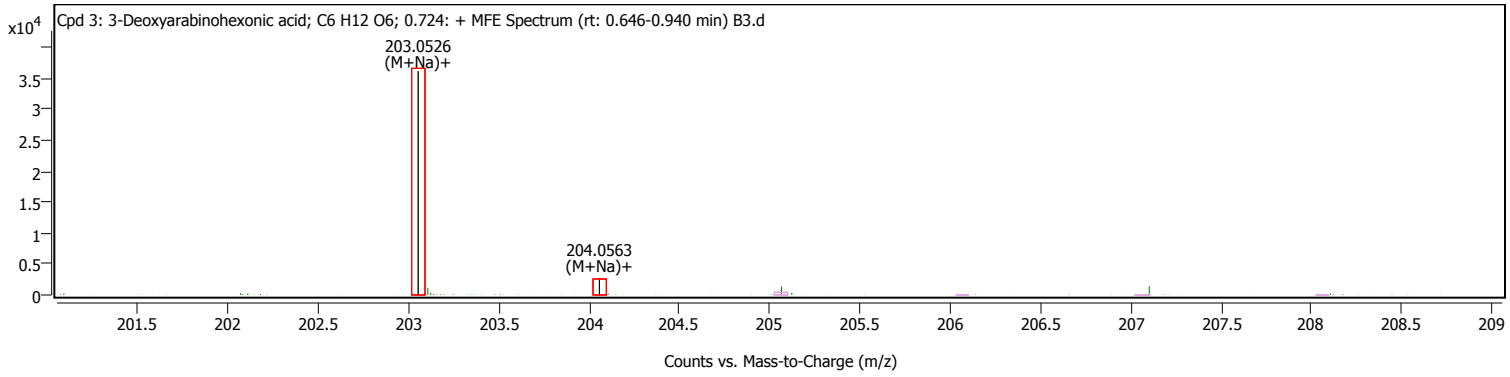
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 4: C10 H18 N6 O10

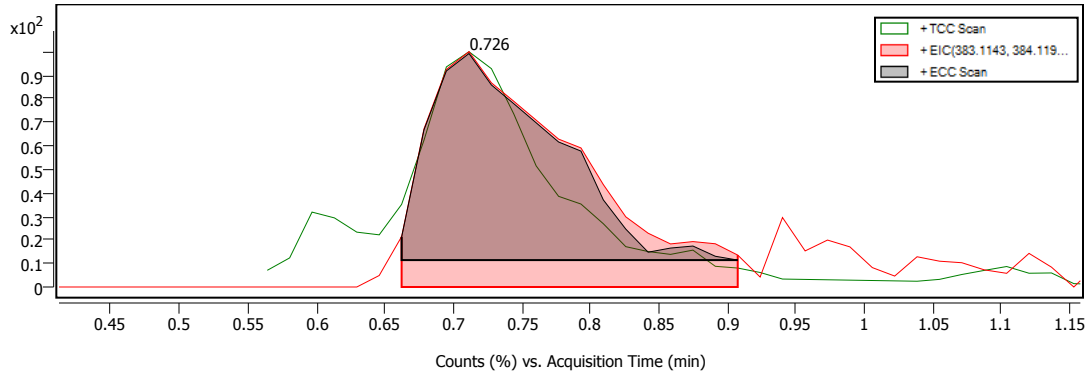
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C10 H18 N6 O10	0.726		382.1079		MFG	79.56	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	383.1149				5	79.56	

Compound ID Table

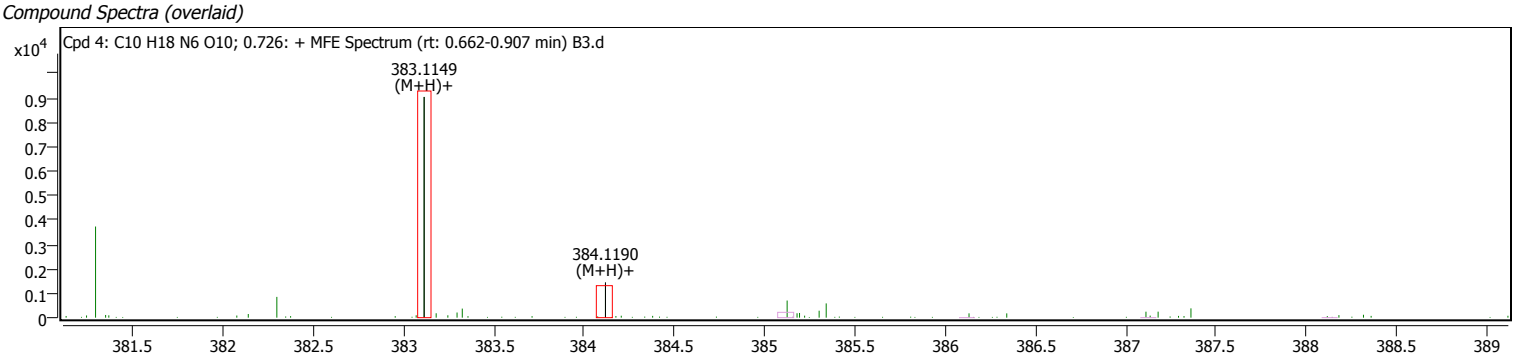
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C10 H18 N6 O10	(M+H)+	MFG	0.726		382.1079		79.56		79.56
	C11 H14 N10 O6	(M+H)+	MFG	0.726		382.1080		73.62		73.62
	C12 H20 N3 O11	(M+H)+	MFG	0.726		382.1078		72.75		72.75
	C16 H20 N3 O6 S	(M+H)+	MFG	0.726		382.1078		71.78		71.78
	C15 H14 N10 O S	(M+H)+	MFG	0.726		382.1079		70.30		70.30

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 5: Cordycepin

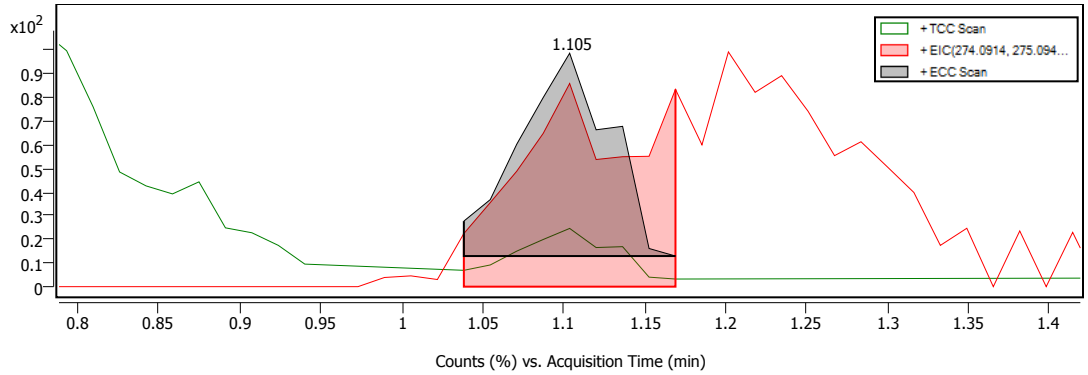
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cordycepin	C10 H13 N5 O3	1.105		251.1016	73-03-0	DBSearch-MFG	58.02	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	274.0908 274.0908 274.0908		0	68.60	12	47.43	

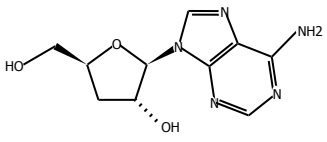
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cordycepin	C10 H13 N5 O3	(M+Na)+	DBSearch-MFG	1.105		251.1016	73-03-0	58.02	68.60	47.43
Deoxyadenosine	C10 H13 N5 O3	(M+Na)+	DBSearch-MFG	1.105		251.1016	958-09-8	58.02	68.60	47.43
5'-Deoxyadenosine	C10 H13 N5 O3	(M+Na)+	DBSearch-MFG	1.105		251.1016	4754-39-6	58.02	68.60	47.43
	C12 H18 Cl2 N3	(M+H)+	MFG	1.105		274.0876		47.54		47.54
	C12 H18 O5 S	(M+H)+	MFG	1.105		274.0876		47.54		47.54
	C11 H12 N7 S	(M+H)+	MFG	1.105		274.0876		47.54		47.54
	C10 H21 N O2 S2	(M+Na)+	MFG	1.105		251.1016		47.38		47.38
	C9 H21 Cl N O4 S	(M+H)+	MFG	1.105		274.0876		47.17		47.17
	C15 H15 Cl N2 O	(M+H)+	MFG	1.105		274.0876		47.16		47.16
	C7 H16 Cl N6 O2	(M+Na)+	MFG	1.105		251.1016		45.75		45.75
	C9 H17 N O7	(M+Na)+	MFG	1.105		251.1016		43.10		43.10
	C8 H11 N8 O2	(M+Na)+	MFG	1.105		251.1016		43.06		43.06

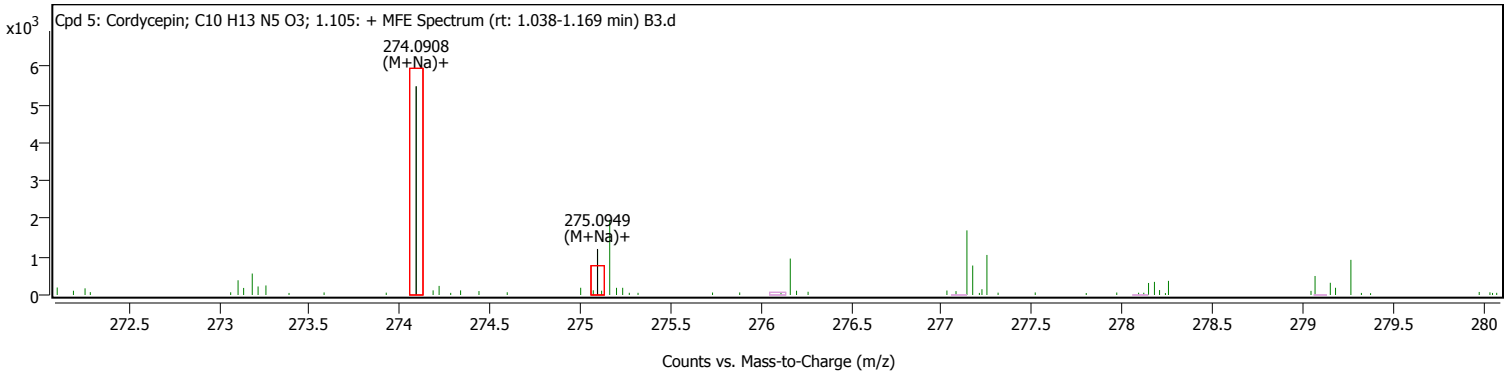
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 6: Trifluoperazine

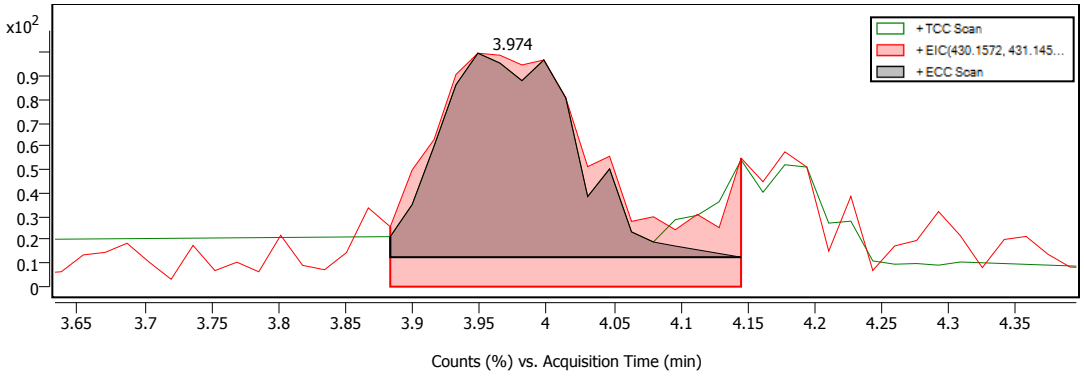
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Trifluoperazine	C21 H24 F3 N3 S	3.974		407.1654	117-89-5	DBSearch	82.72	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	430.1555 430.1555 430.1555		3	82.72	8		

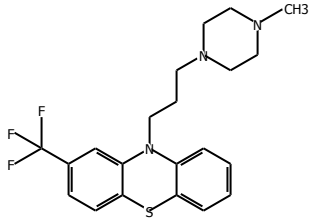
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Trifluoperazine	C21 H24 F3 N3 S	(M+Na)+	DBSearch	3.974		407.1654	117-89-5	82.72	82.72	
Cyflufenamid	C20 H17 F5 N2 O2	(M+NH4)+	DBSearch	3.974		412.1203		67.21	67.21	
	C32 H18 N2	(M+H)+	MFG	3.974		430.1456		56.96		56.96
	C19 H32 Cl3 N3	(M+Na)+	MFG	3.974		407.1663		47.59		47.59
	C15 H29 N5 O4 S2	(M+Na)+	MFG	3.974		407.1663		47.53		47.53
	C15 H21 N9 O5	(M+Na)+	MFG	3.974		407.1663		47.43		47.43
	C16 H27 N2 O10	(M+Na)+	MFG	3.974		407.1663		47.42		47.42
	C12 H32 Cl N6 O3 S2	(M+Na)+	MFG	3.974		407.1663		47.40		47.40

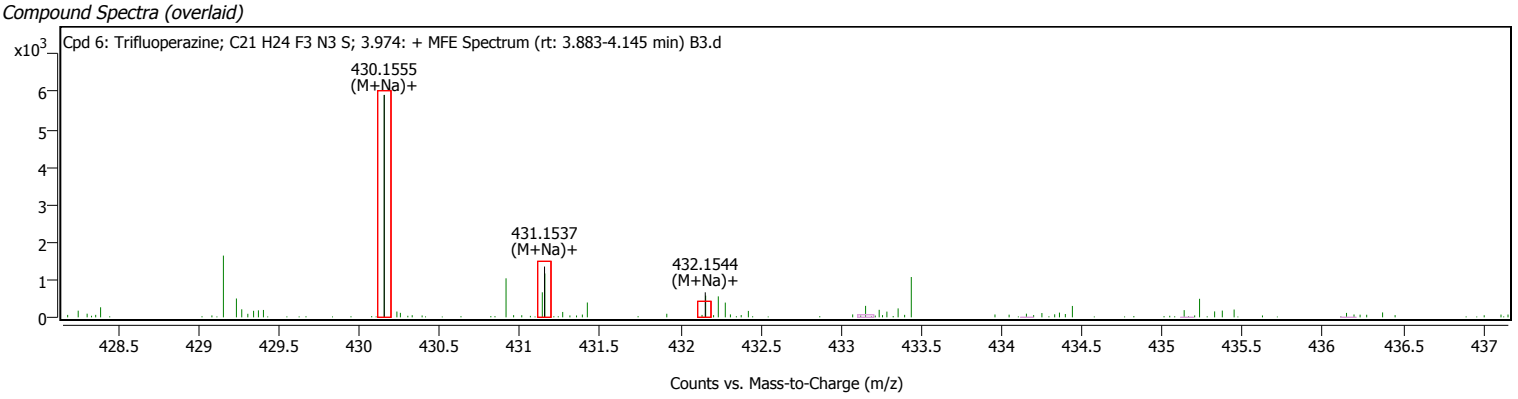
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 7: Cyflufenamid

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cyflufenamid	C20 H17 F5 N2 O2	4.172		412.1202		DBSearch	65.65	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	430.1547 430.1547 430.1547		0	65.65	12		

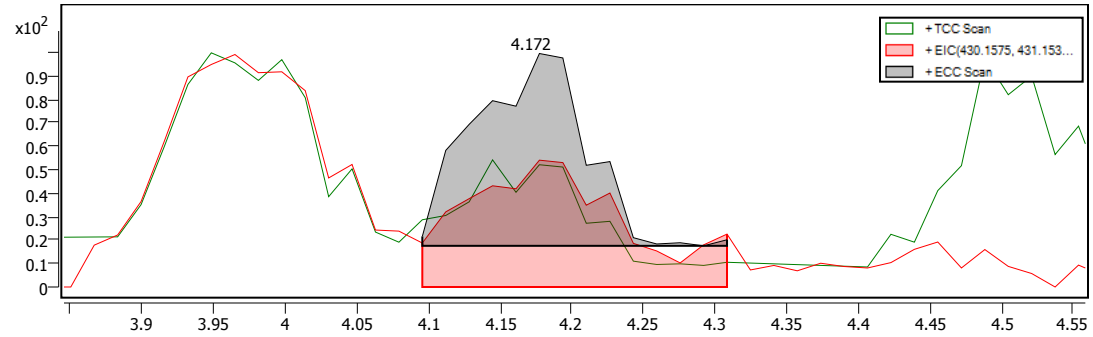
Compound Discovery Report

Agilent | Trusted Answers

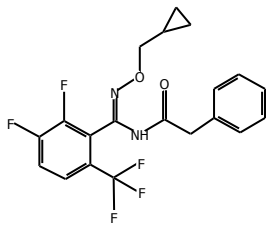
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cyflufenamid	C20 H17 F5 N2 O2	(M+NH4)+	DBSearch	4.172		412.1202		65.65	65.65	
Trifluoperazine	C21 H24 F3 N3 S	(M+Na)+	DBSearch	4.172		407.1648	117-89-5	62.66	62.66	
	C10 H25 Cl N4 O11	(M+NH4)+	MFG	4.172		412.1209		47.62		47.62
	C21 H26 Cl2 O4	(M+NH4)+	MFG	4.172		412.1209		47.61		47.61
	C26 H24 N O3 S	(M+H)+	MFG	4.172		430.1476		47.60		47.60
	C15 H31 Cl N4 O4 S2	(M+H)+	MFG	4.172		430.1476		47.60		47.60
	C19 H26 O11	(M+H)+	MFG	4.172		430.1476		47.60		47.60
	C18 H20 N7 O6	(M+H)+	MFG	4.172		430.1476		47.59		47.59
	C17 H14 N14 O	(M+H)+	MFG	4.172		430.1476		47.59		47.59
	C13 H28 N6 O S4	(M+NH4)+	MFG	4.172		412.1209		47.58		47.58
	C17 H23 Cl N5 O3 S	(M+NH4)+	MFG	4.172		412.1209		47.57		47.57
	C9 H27 Cl3 N10 S	(M+NH4)+	MFG	4.172		412.1209		47.49		47.49

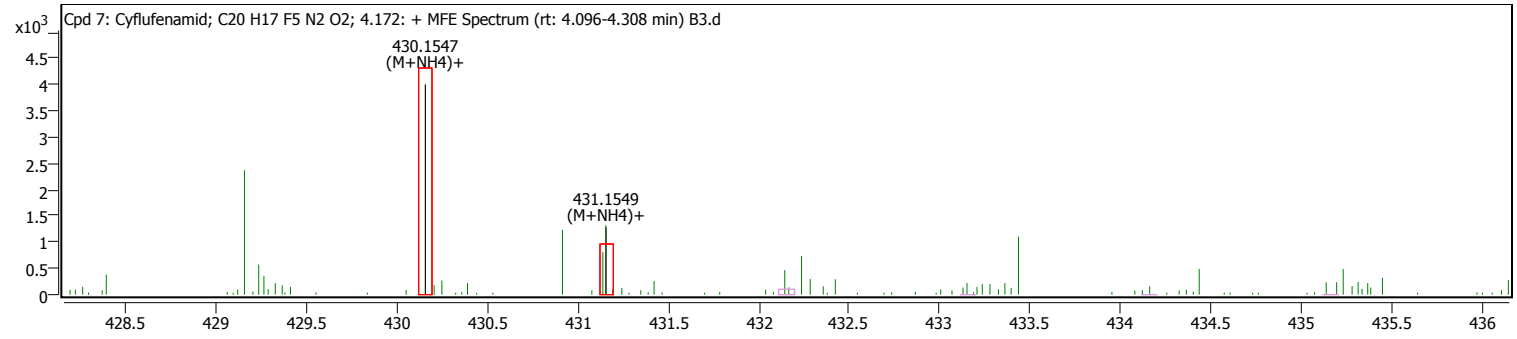
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 8: C21 H39 N4 O18 S2

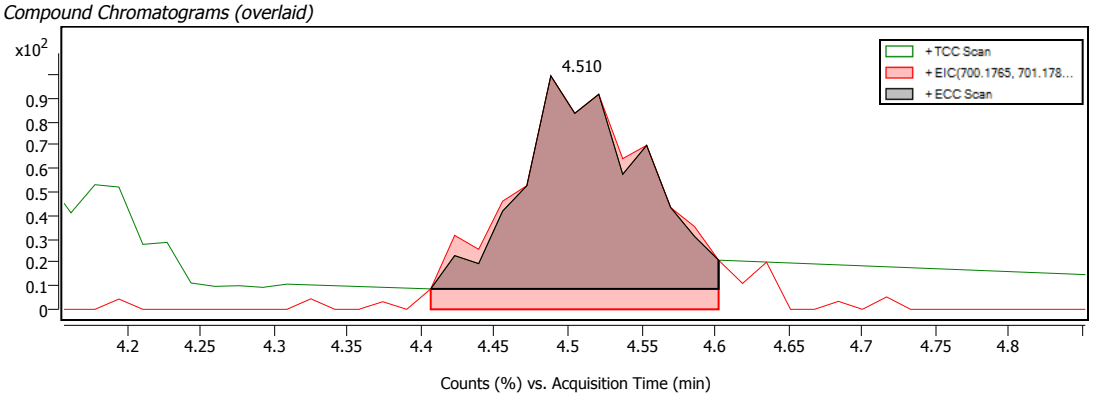
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C21 H39 N4 O18 S2	4.510		699.1704		MFG	89.36	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	700.1771				5	89.36	

Compound ID Table

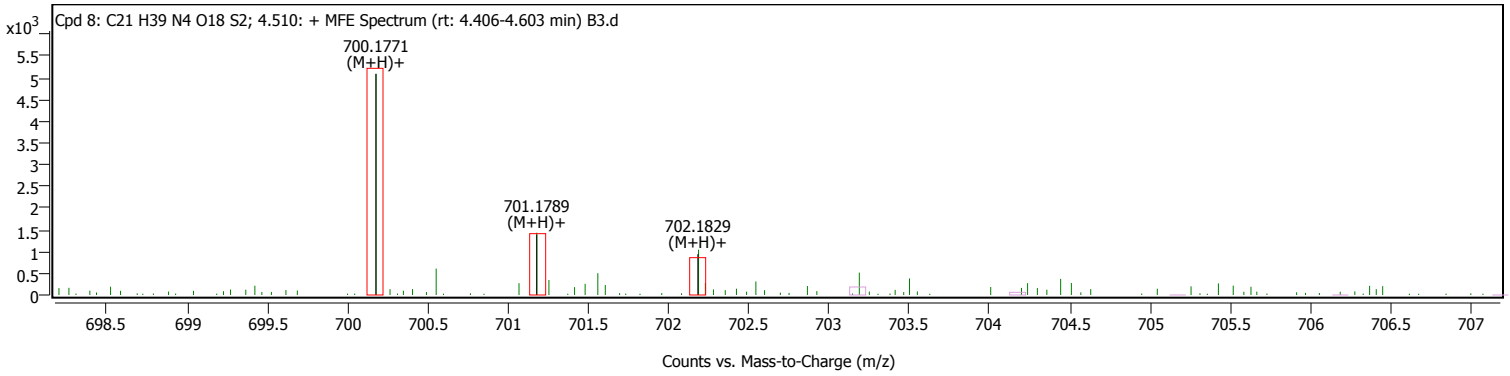
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C21 H39 N4 O18 S2	(M+H)+	MFG	4.510		699.1704		89.36		89.36
	C20 H33 N11 O13 S2	(M+H)+	MFG	4.510		699.1705		88.47		88.47
	C23 H41 N O19 S2	(M+H)+	MFG	4.510		699.1703		87.81		87.81
	C22 H35 N8 O14 S2	(M+H)+	MFG	4.510		699.1704		87.48		87.48
	C21 H29 N15 O9 S2	(M+H)+	MFG	4.510		699.1706		86.17		86.17

Compound Chromatograms (overlaid)



Structure

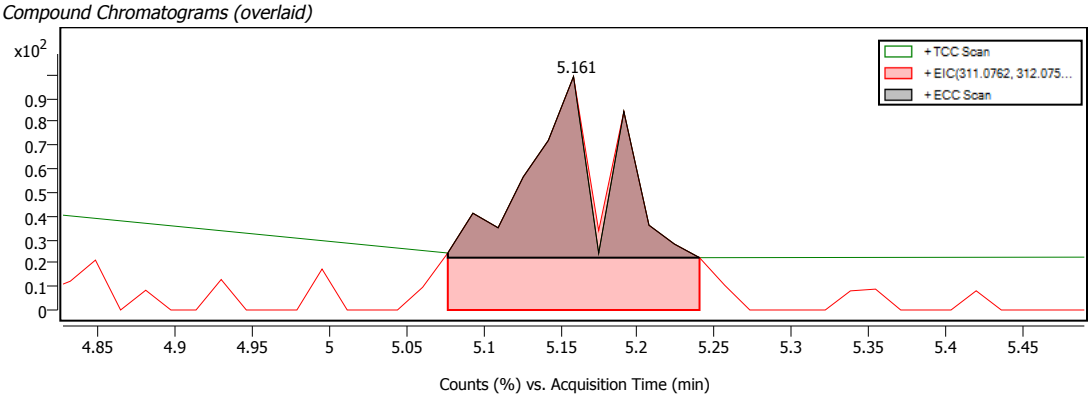
Compound Spectra (overlaid)



Cpd 9: 5.161

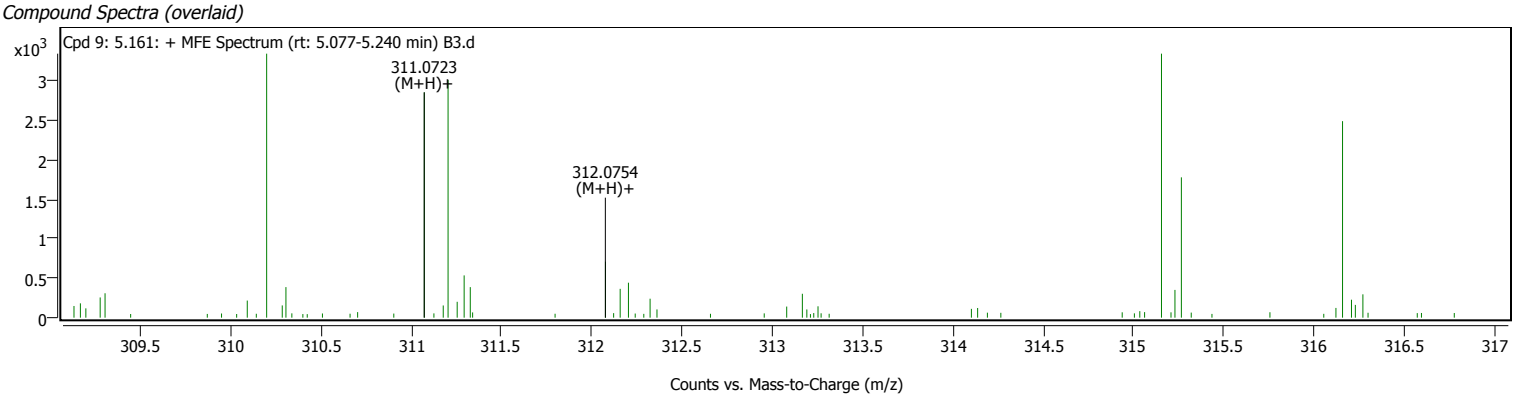
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		5.161		310.0650				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 10: C28 H22 N O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H22 N O	7.136		388.1699		MFG	79.49	MFE	

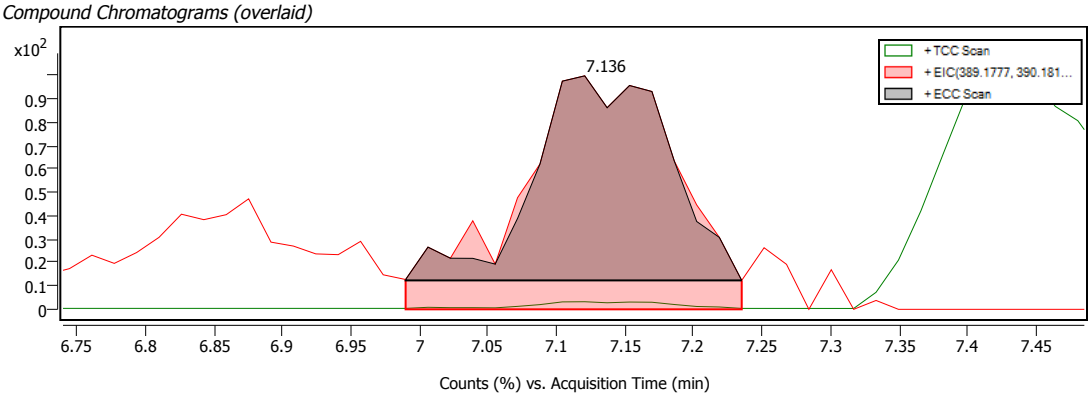
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	389.1770				22	79.49	

Compound ID Table

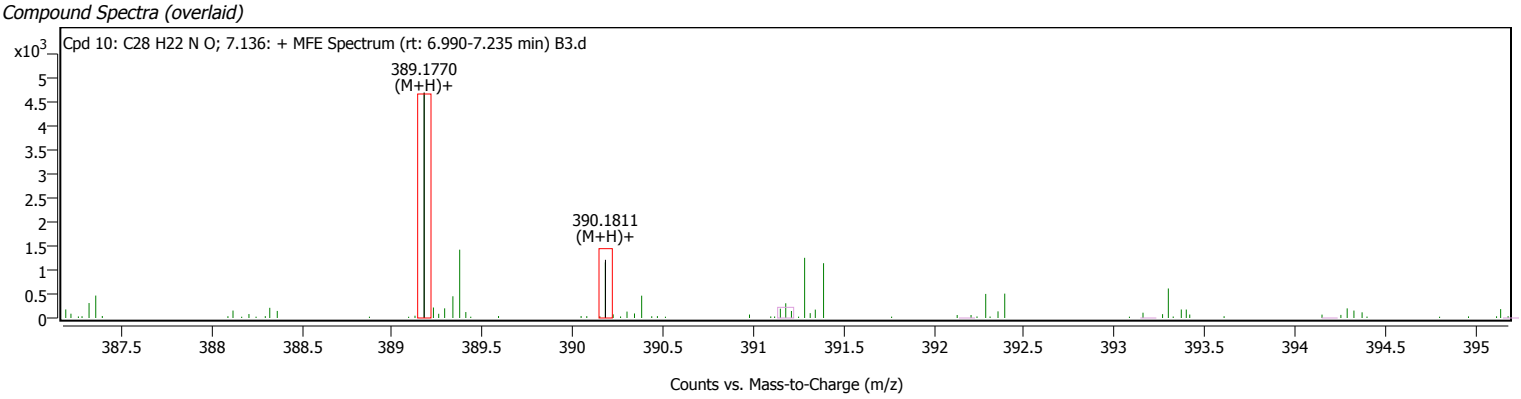
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H22 N O	(M+H)+	MFG	7.136		388.1699		79.49		79.49
	C26 H20 N4	(M+H)+	MFG	7.136		388.1699		77.63		77.63
	C13 H18 N13 O2	(M+H)+	MFG	7.136		388.1702		72.69		72.69
	C20 H26 N3 O3 S	(M+H)+	MFG	7.136		388.1700		71.46		71.46
Asn Gln Gln	C14 H24 N6 O7	(M+H)+	DBSearch-MFG	7.136		388.1700		70.68	70.60	70.75
Gln Asn Gln	C14 H24 N6 O7	(M+H)+	DBSearch-MFG	7.136		388.1700		70.68	70.60	70.75
Gln Gln Asn	C14 H24 N6 O7	(M+H)+	DBSearch-MFG	7.136		388.1700		70.68	70.60	70.75
Ser His Glu	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Ser Glu His	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
His Thr Asp	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
His Glu Ser	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Thr Asp His	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
His Ser Glu	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Asp Thr His	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Glu Ser His	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Thr His Asp	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Asp His Thr	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
Glu His Ser	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
His Asp Thr	C14 H21 N5 O7	(M+NH4)+	DBSearch	7.136		371.1435		70.55	70.55	
(1R*,2R*,4R*,8S*)-p-Menthane-1,2,8,9-tetrol 9-glucoside	C16 H30 O9	(M+Na)+	DBSearch	7.136		366.1879	402593-84-4	69.65	69.65	
(1S,2S,4R,8S)-p-Menthane-1,2,8,9-tetrol 2-glucoside	C16 H30 O9	(M+Na)+	DBSearch	7.136		366.1879	402593-52-6	69.65	69.65	
(2R,6x)-7-Methyl-3-methylene-1,2,6,7-octanetetrol 2-glucoside	C16 H30 O9	(M+Na)+	DBSearch	7.136		366.1879	219814-32-1	69.65	69.65	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 11: C22 H48 N3 O S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C22 H48 N3 O S2	7.430		434.3236		MFG	87.17	MFE	

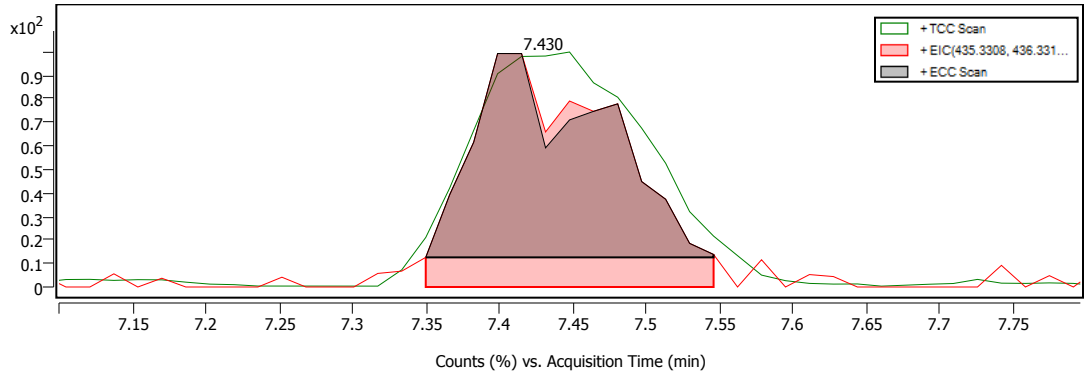
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	435.3315				5	87.17	

Compound ID Table

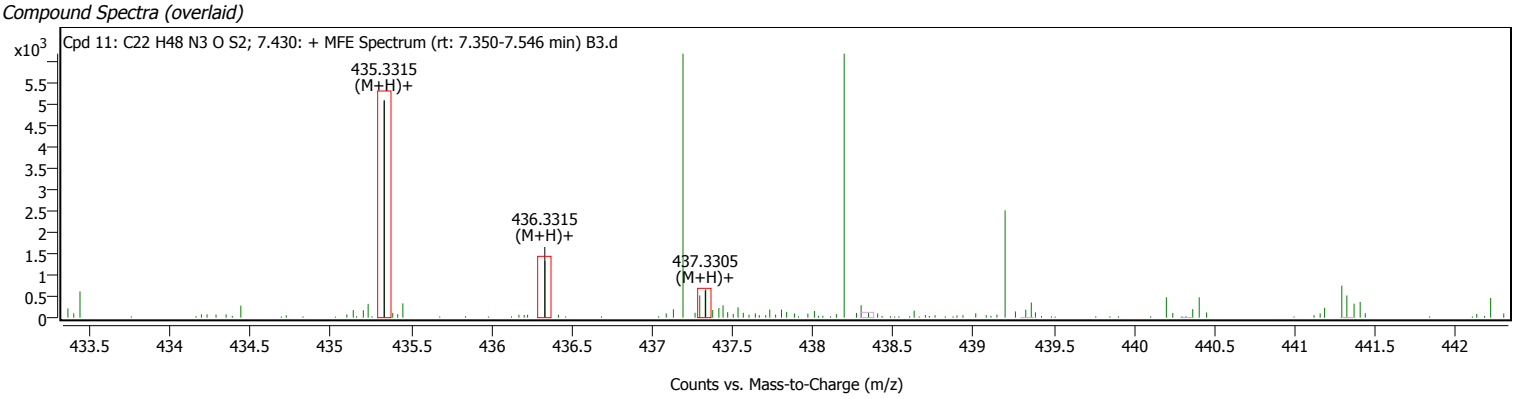
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C22 H48 N3 O S2	(M+H)+	MFG	7.430		434.3236		87.17		87.17
	C27 H46 O2 S	(M+H)+	MFG	7.430		434.3233		83.25		83.25
	C20 H46 N6 S2	(M+H)+	MFG	7.430		434.3237		83.20		83.20
	C24 H50 O2 S2	(M+H)+	MFG	7.430		434.3235		81.39		81.39
	C15 H40 N13 S	(M+H)+	MFG	7.430		434.3239		78.77		78.77

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 12: C23 H48 O8

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C23 H48 O8	7.438		452.3346		MFG	99.39	MFE	

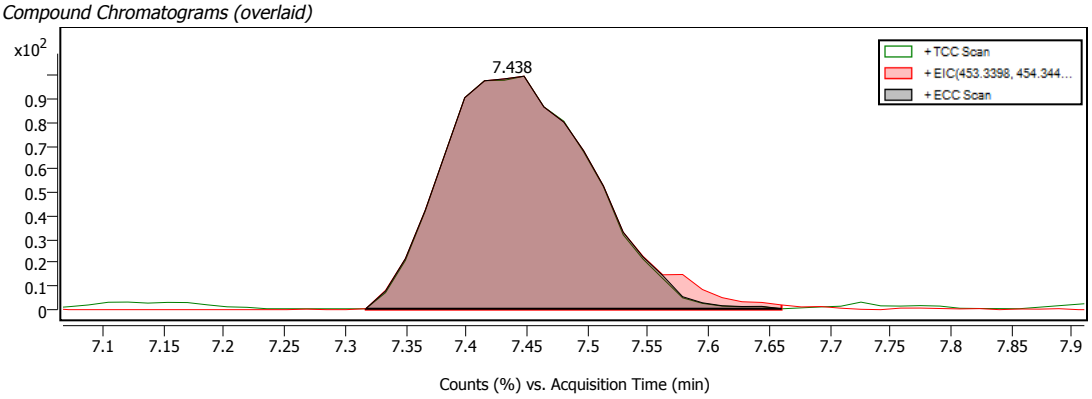
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	453.3419 475.3236				6	99.39	

Compound ID Table

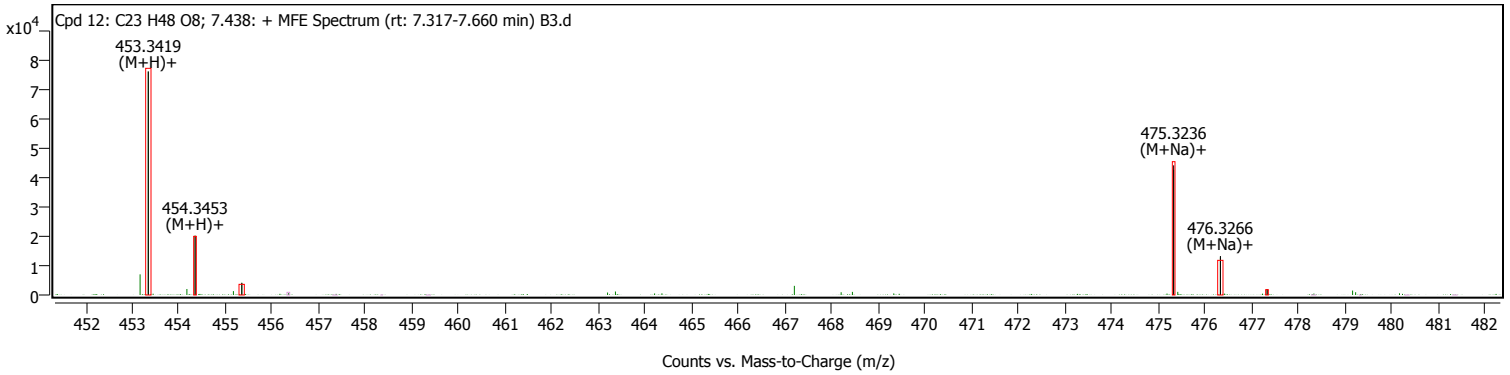
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C23 H48 O8	(M+H)+ (M+Na)+	MFG	7.438		452.3346		99.39		99.39
	C22 H42 N7 O3	(M+H)+ (M+Na)+	MFG	7.438		452.3347		98.88		98.88
	C21 H46 N3 O7	(M+H)+ (M+Na)+	MFG	7.438		452.3346		96.52		96.52
	C20 H40 N10 O2	(M+H)+ (M+Na)+	MFG	7.438		452.3348		94.98		94.98
	C24 H44 N4 O4	(M+H)+	MFG	7.438		452.3346		93.33		93.33
	C30 H46 N S	(M+Na)+	MFG	7.438		452.3344		91.73		91.73

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 13: C31 H34 N6

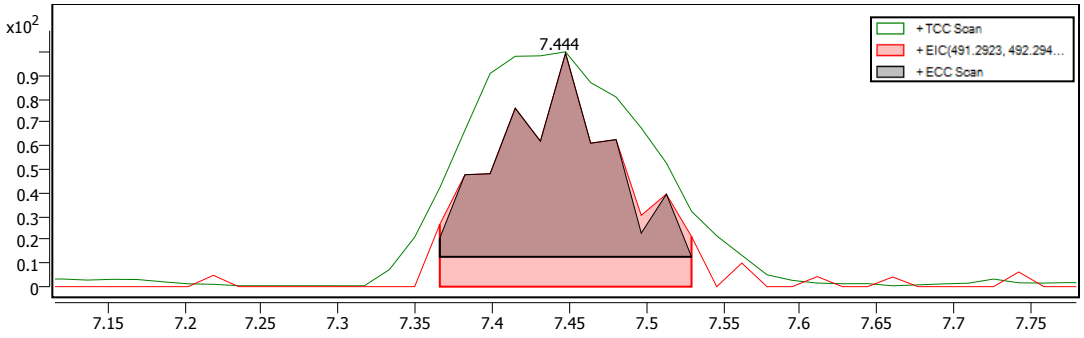
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H34 N6	7.444		490.2846		MFG	69.11	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	491.2930				5	69.11	

Compound ID Table

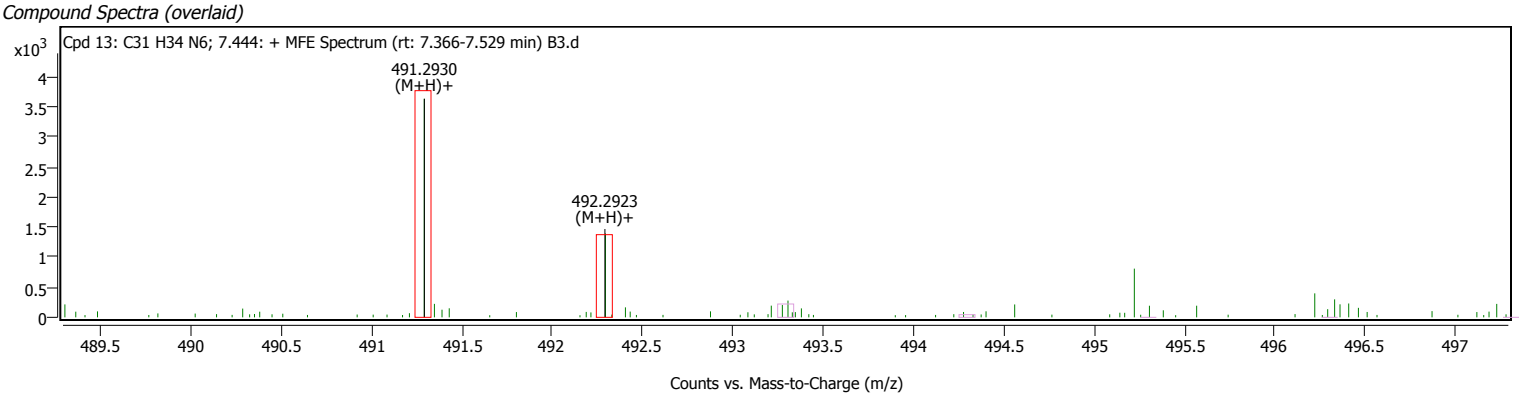
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H34 N6	(M+H)+	MFG	7.444		490.2846		69.11		69.11
	C33 H36 N3 O	(M+H)+	MFG	7.444		490.2846		65.51		65.51
	C30 H38 N2 O4	(M+H)+	MFG	7.444		490.2846		61.79		61.79
	C16 H30 N18 O	(M+H)+	MFG	7.444		490.2850		60.61		60.61
	C17 H36 N11 O6	(M+H)+	MFG	7.444		490.2848		57.54		57.54

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 14: PS(18:3(9Z,12Z,15Z)/0:0)

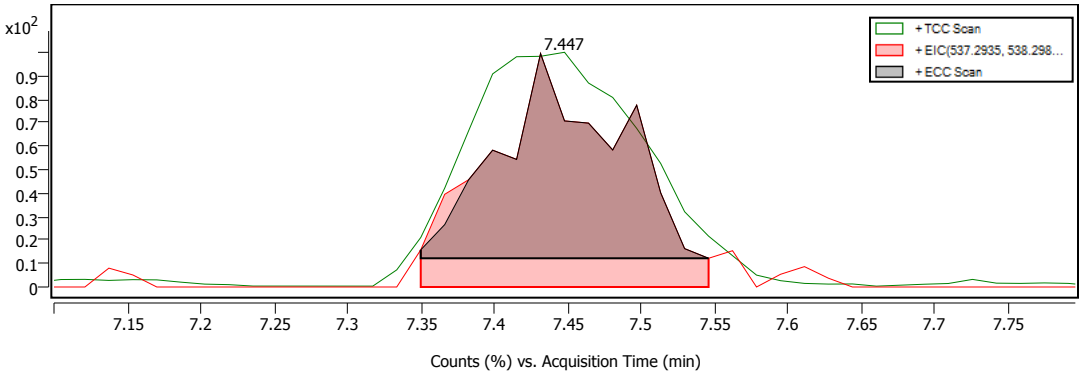
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PS(18:3(9Z,12Z,15Z)/0:0)	C24 H42 N O9 P	7.447		519.2602		DBSearch	77.87	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	537.2938 537.2938 537.2938		0	77.87	12		

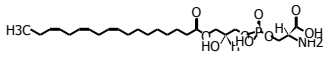
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PS(18:3(9Z,12Z,15Z)/0:0)	C24 H42 N O9 P	(M+NH4)+	DBSearch	7.447		519.2602		77.87	77.87	
PS(18:3(6Z,9Z,12Z)/0:0)	C24 H42 N O9 P	(M+NH4)+	DBSearch	7.447		519.2602		77.87	77.87	
	C24 H47 Cl2 N6 O S	(M+H)+	MFG	7.447		537.2909		47.62		47.62
	C32 H40 Cl N2 S	(M+NH4)+	MFG	7.447		519.2600		47.61		47.61
	C20 H33 N13 O2 S	(M+NH4)+	MFG	7.447		519.2600		47.61		47.61
	C21 H39 N6 O7 S	(M+NH4)+	MFG	7.447		519.2600		47.60		47.60
	C21 H47 Cl2 N5 O S2	(M+NH4)+	MFG	7.447		519.2600		47.60		47.60
	C17 H44 Cl N10 S3	(M+NH4)+	MFG	7.447		519.2600		47.60		47.60
	C16 H43 Cl2 N12 O4	(M+H)+	MFG	7.447		537.2909		47.58		47.58
	C28 H50 Cl3 N O2	(M+H)+	MFG	7.447		537.2909		47.57		47.57
	C35 H40 Cl N3	(M+H)+	MFG	7.447		537.2909		47.54		47.54
	C23 H33 N14 O2	(M+H)+	MFG	7.447		537.2909		47.52		47.52

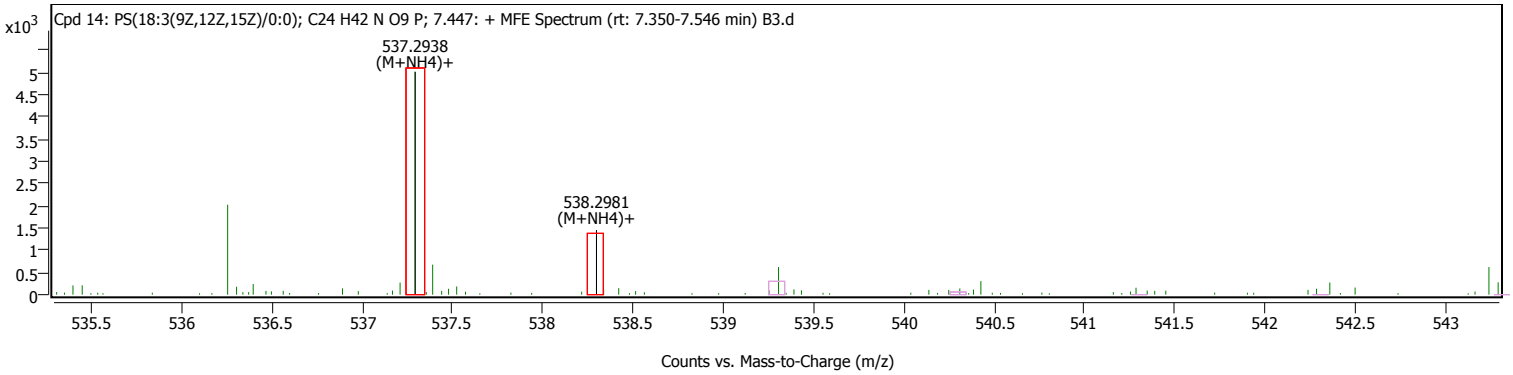
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 15: C24 H32 N O7

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C24 H32 N O7	7.744		446.2178		MFG	79.00	MFE	

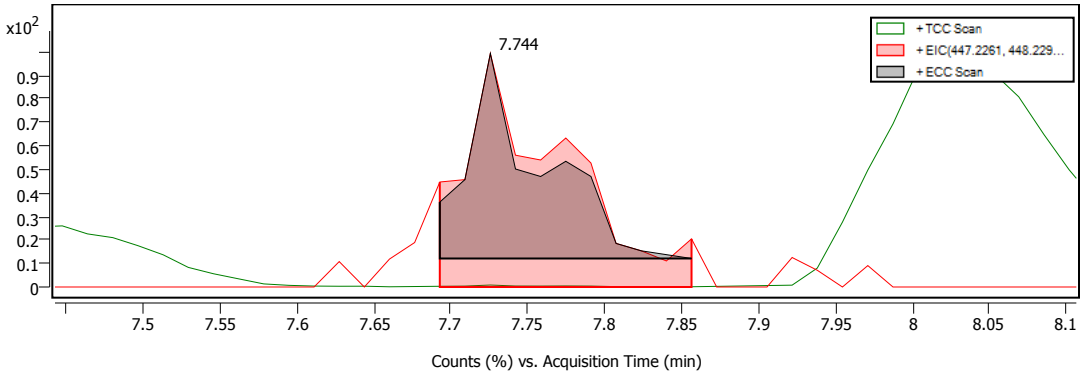
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	447.2250				22	79.00	

Compound ID Table

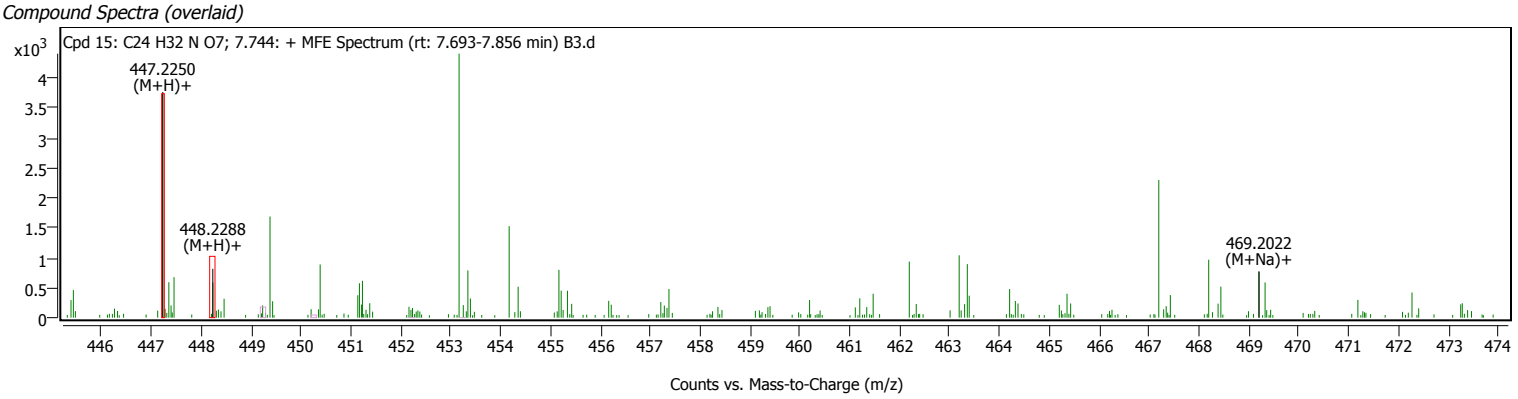
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C24 H32 N O7	(M+H)+	MFG	7.744		446.2178		79.00		79.00
	C23 H26 N8 O2	(M+H)+	MFG	7.744		446.2179		77.70		77.70
CAY10603	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179	1045792-66-2	76.55	76.60	76.49
Trp Glu Ile	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Glu Ile Trp	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Glu Trp Ile	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Glu Leu Trp	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Trp Ile Glu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Leu Trp Glu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Trp Leu Glu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Ile Trp Glu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Glu Trp Leu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Ile Glu Trp	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Leu Glu Trp	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
Trp Glu Leu	C22 H30 N4 O6	(M+H)+	DBSearch-MFG	7.744		446.2179		76.55	76.60	76.49
	C21 H24 N11 O	(M+H)+	MFG	7.744		446.2180		74.48		74.48
	C16 H26 N14 S	(M+H)+	MFG	7.744		446.2181		72.87		72.87
	C13 H27 Cl N14 O2	(M+Na)+	MFG	7.744		446.2130		47.62		47.62
	C14 H33 Cl N7 O7	(M+Na)+	MFG	7.744		446.2130		47.62		47.62
	C25 H34 Cl2 N3	(M+Na)+	MFG	7.744		446.2130		47.62		47.62
	C18 H42 N2 O2 S4	(M+Na)+	MFG	7.744		446.2130		47.60		47.60
	C22 H37 Cl N O4 S	(M+Na)+	MFG	7.744		446.2130		47.54		47.54

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

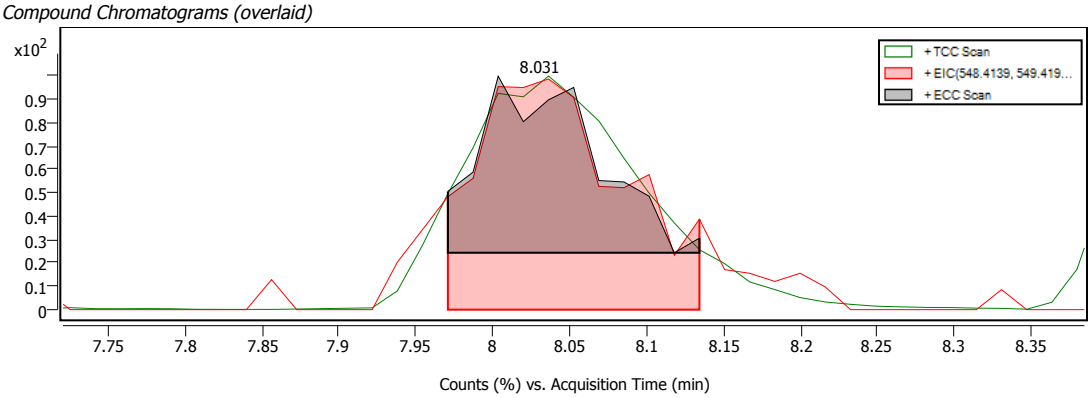


Cpd 16: 8.031

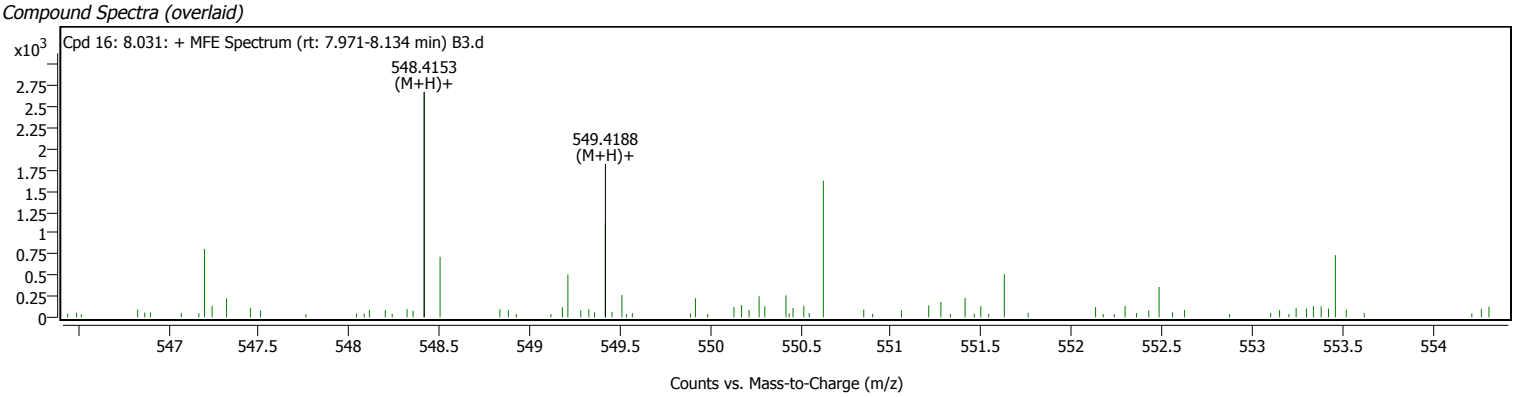
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		8.031		547.4080				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 17: C28 H53 N8 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H53 N8 O4	8.035		565.4187		MFG	99.57	MFE	

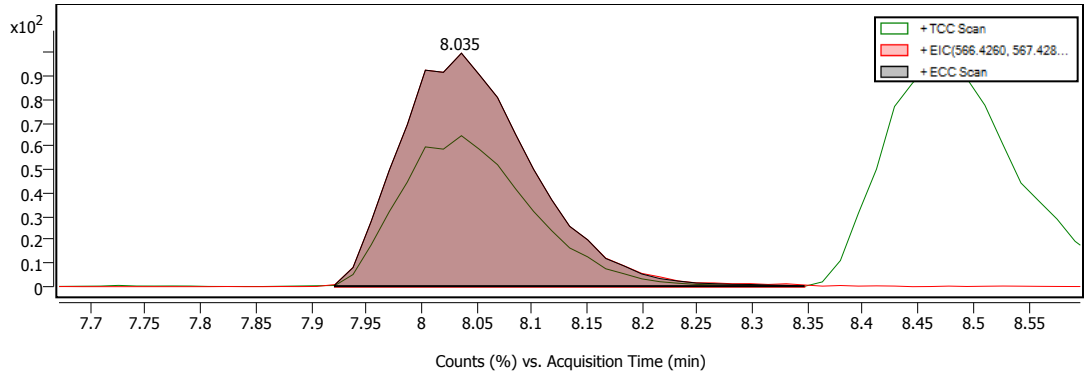
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	566.4260 588.4078				5	99.57	

Compound ID Table

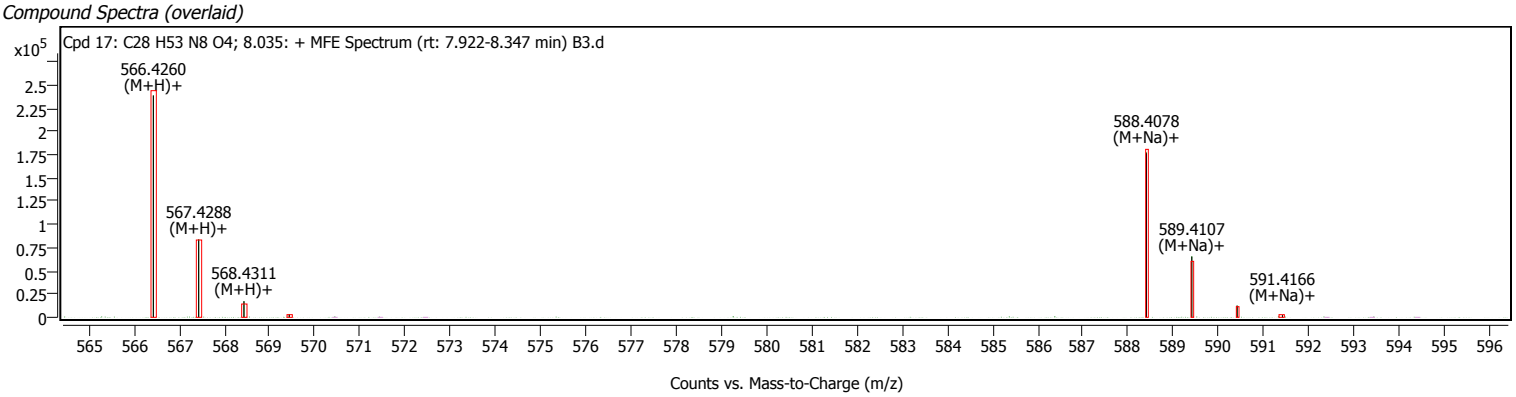
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H53 N8 O4	(M+H)+ (M+Na)+	MFG	8.035		565.4187		99.57		99.57
	C29 H59 N O9	(M+H)+ (M+Na)+	MFG	8.035		565.4185		98.60		98.60
	C26 H51 N11 O3	(M+H)+ (M+Na)+	MFG	8.035		565.4188		97.03		97.03
	C27 H57 N4 O8	(M+H)+ (M+Na)+	MFG	8.035		565.4186		96.84		96.84
	C29 H49 N12	(M+H)+ (M+Na)+	MFG	8.035		565.4187		95.42		95.42

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 18: C25 H57 N5 O7 S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C25 H57 N5 O7 S2	8.036		603.3706		MFG	91.51	MFE	

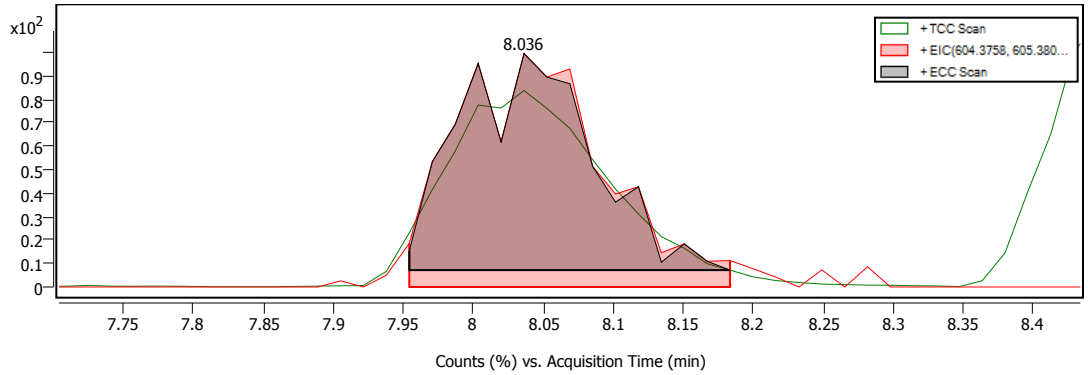
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	604.3774				5	91.51	

Compound ID Table

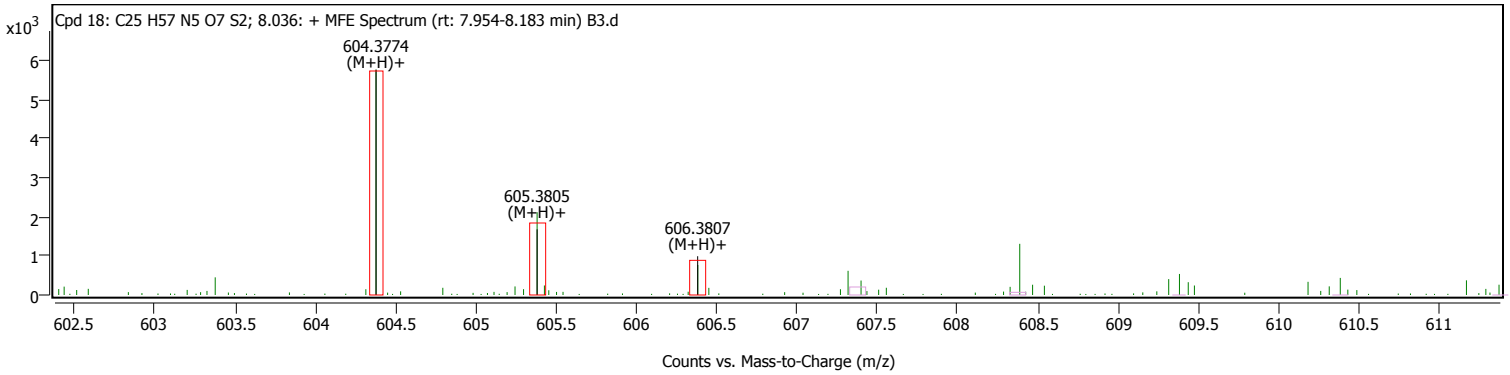
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C25 H57 N5 O7 S2	(M+H)+	MFG	8.036		603.3706		91.51		91.51
	C27 H59 N2 O8 S2	(M+H)+	MFG	8.036		603.3705		91.22		91.22
	C26 H53 N9 O3 S2	(M+H)+	MFG	8.036		603.3706		89.22		89.22
	C24 H51 N12 O2 S2	(M+H)+	MFG	8.036		603.3707		88.69		88.69
	C23 H55 N8 O6 S2	(M+H)+	MFG	8.036		603.3707		85.20		85.20

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 19: 16,16-dimethyl Prostaglandin E2 p-(p-acetamidobenzamido) phenyl ester

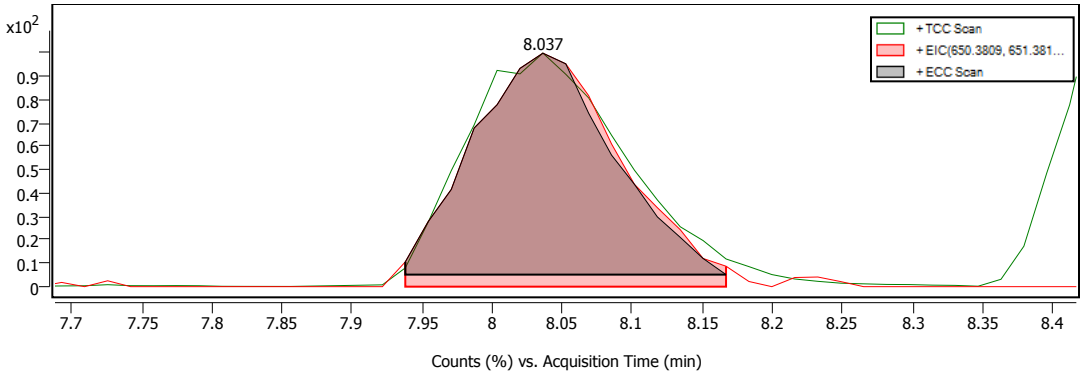
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
16,16-dimethyl Prostaglandin E2 p-(p-acetamidobenzamido) phenyl ester	C37 H48 N2 O7	8.037		632.3453	62873-55-6	DBSearch	85.25	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	650.3783 650.3783		6	85.25	11		

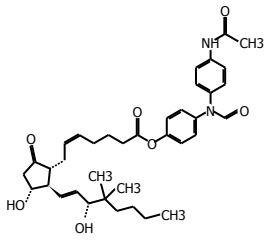
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
16,16-dimethyl Prostaglandin E2 p-(p-acetamidobenzamido) phenyl ester	C37 H48 N2 O7	(M+NH4)+	DBSearch	8.037		632.3453	62873-55-6	85.25	85.25	
	C31 H46 N12 O4	(M+H)+	MFG	8.037		650.3765		68.16		68.16
	C32 H52 N5 O9	(M+H)+	MFG	8.037		650.3763		66.78		66.78
	C32 H42 N16	(M+H)+	MFG	8.037		650.3765		65.97		65.97
	C29 H44 N15 O3	(M+H)+	MFG	8.037		650.3765		65.95		65.95
	C30 H50 N8 O8	(M+H)+	MFG	8.037		650.3764		64.79		64.79
	C28 H56 Cl2 N3 O8	(M+NH4)+	MFG	8.037		632.3445		47.62		47.62
	C27 H50 Cl2 N10 O3	(M+NH4)+	MFG	8.037		632.3445		47.62		47.62
	C28 H62 N3 O2 S5	(M+NH4)+	MFG	8.037		632.3445		47.61		47.61
	C35 H54 N O5 S2	(M+NH4)+	MFG	8.037		632.3445		47.60		47.60
	C34 H48 N8 S2	(M+NH4)+	MFG	8.037		632.3445		47.59		47.59

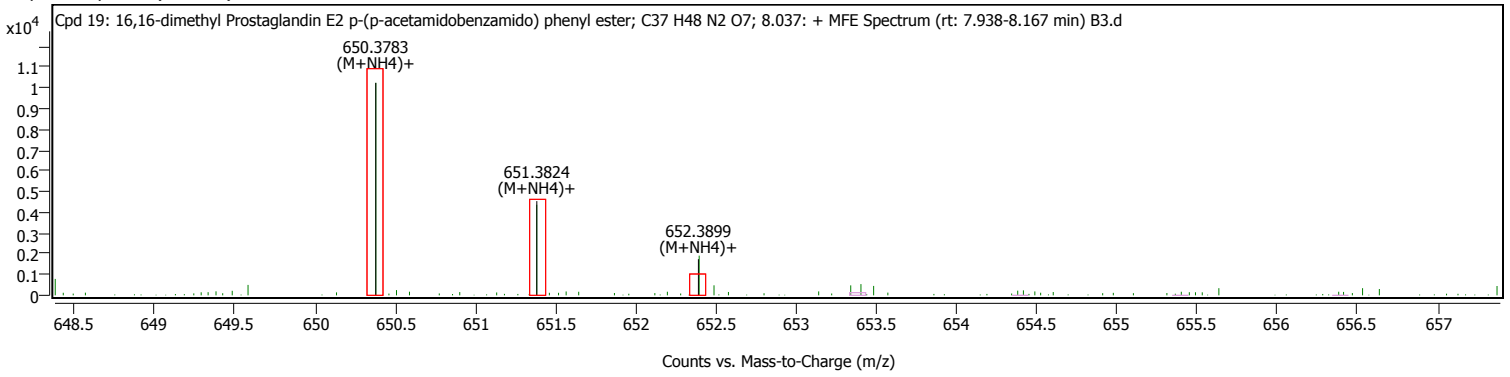
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 20: Posaconazole

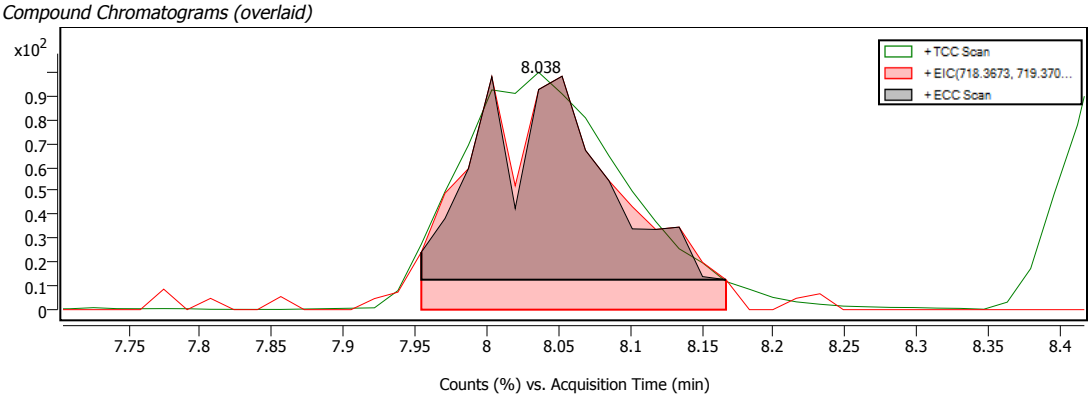
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Posaconazole	C37 H42 F2 N8 O4	8.038		700.3312	171228-49-2	DBSearch	66.89	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+NH4)+	718.3644 718.3644 718.3644		0	66.89	11		

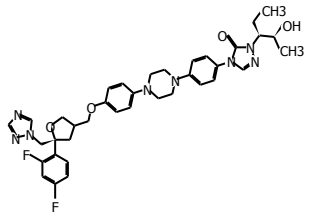
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Posaconazole	C37 H42 F2 N8 O4	(M+NH4)+	DBSearch	8.038		700.3312	171228-49-2	66.89	66.89	
	C26 H57 Cl N11 O6 S2	(M+H)+	MFG	8.038		718.3623		47.62		47.62
	C25 H51 Cl N18 O S2	(M+H)+	MFG	8.038		718.3623		47.62		47.62
	C31 H58 O18	(M+H)+	MFG	8.038		718.3623		47.62		47.62
	C30 H52 N7 O13	(M+H)+	MFG	8.038		718.3623		47.62		47.62
	C38 H64 Cl2 O4 S2	(M+H)+	MFG	8.038		718.3623		47.62		47.62
	C44 H47 Cl N3 O3	(M+NH4)+	MFG	8.038		700.3306		47.62		47.62
	C31 H34 N21	(M+NH4)+	MFG	8.038		700.3306		47.62		47.62
	C32 H40 N14 O5	(M+NH4)+	MFG	8.038		700.3306		47.62		47.62
	C41 H58 Cl2 O S2	(M+NH4)+	MFG	8.038		700.3306		47.62		47.62
	C33 H46 N7 O10	(M+NH4)+	MFG	8.038		700.3306		47.62		47.62

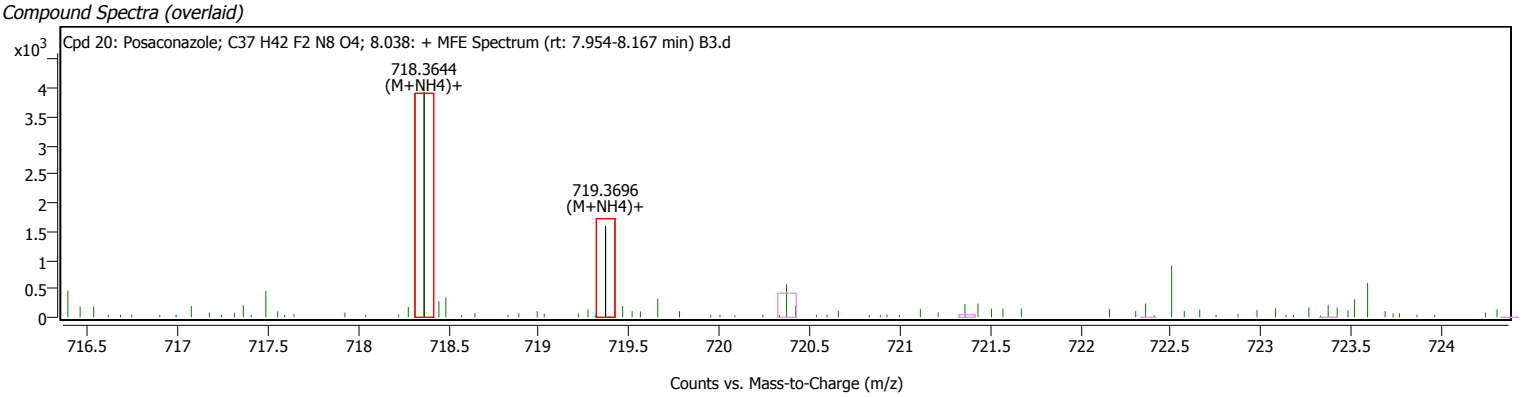
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 21: C50 H76 O S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C50 H76 O S	8.467		724.5617		MFG	47.62	MFE	

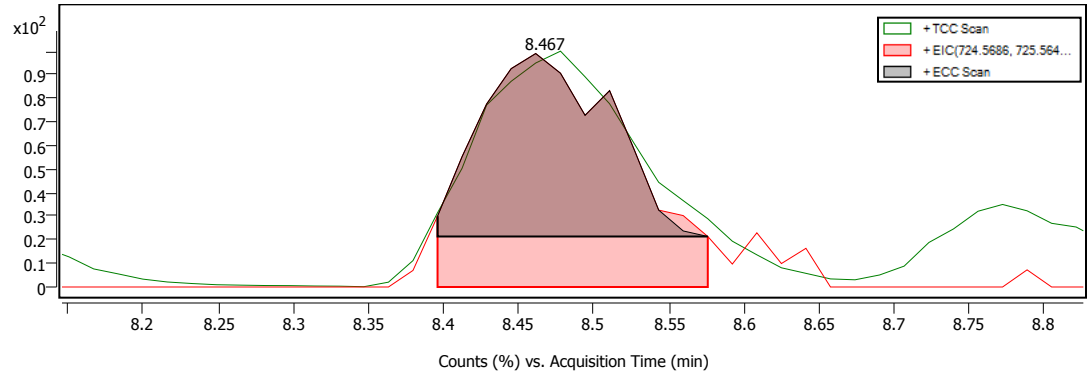
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	725.5689				12	47.62	

Compound ID Table

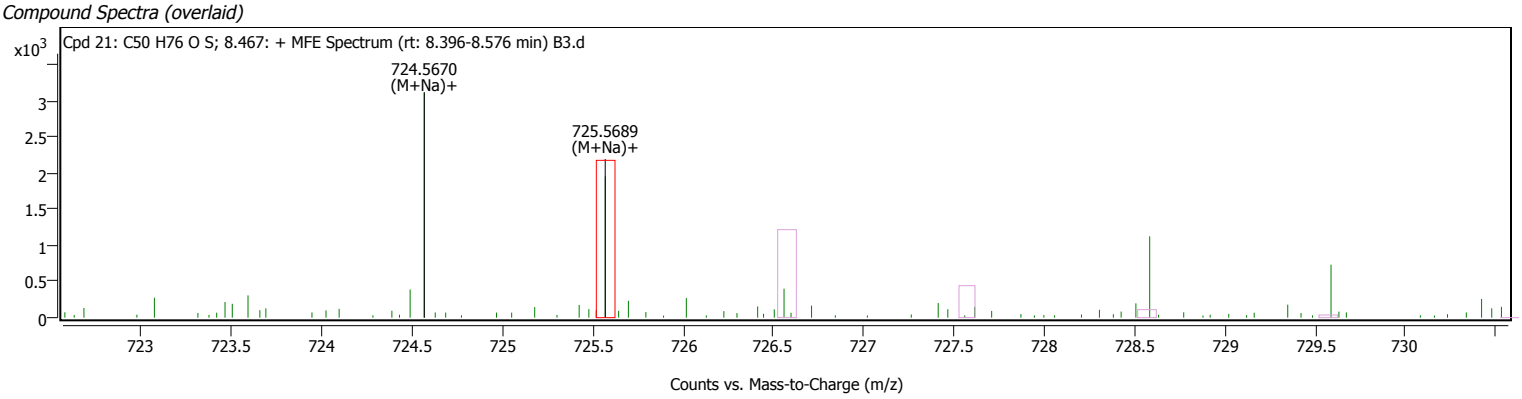
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C50 H76 O S	(M+H)+	MFG	8.467		724.5617		47.62		47.62
	C35 H69 N14 O	(M+Na)+	MFG	8.467		701.5778		47.60		47.60
	C36 H75 N7 O6	(M+Na)+	MFG	8.467		701.5778		47.60		47.60
	C39 H83 Cl N3 O2 S2	(M+H)+	MFG	8.467		724.5617		47.59		47.59
	C42 H72 N6 O4	(M+H)+	MFG	8.467		724.5617		47.58		47.58
	C44 H79 N O3 S	(M+Na)+	MFG	8.467		701.5778		47.49		47.49
	C39 H75 Cl N7 O3	(M+H)+	MFG	8.467		724.5617		47.48		47.48
	C40 H81 Cl O8	(M+H)+	MFG	8.467		724.5617		47.48		47.48
	C35 H77 N10 S2	(M+Na)+	MFG	8.467		701.5778		47.46		47.46
	C50 H73 N2	(M+Na)+	MFG	8.467		701.5778		47.43		47.43
GlcCer(d18:0/16:0)	C40 H79 N O8	(M+Na)+	DBSearch	8.467		701.5772		45.77	45.77	
GalCer(d18:0/16:0)	C40 H79 N O8	(M+Na)+	DBSearch	8.467		701.5772		45.77	45.77	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 22: C48 H56 N6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C48 H56 N6	8.471		716.4563		MFG	94.60	MFE	

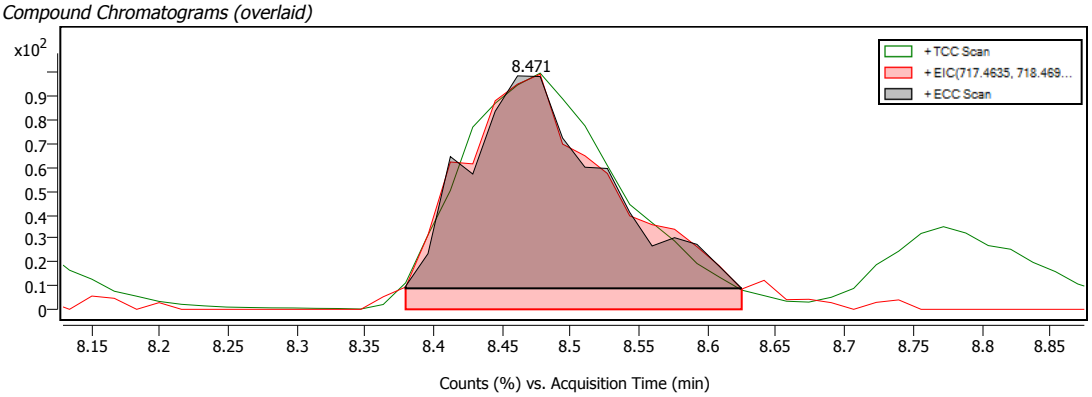
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	717.4640				5	94.60	

Compound ID Table

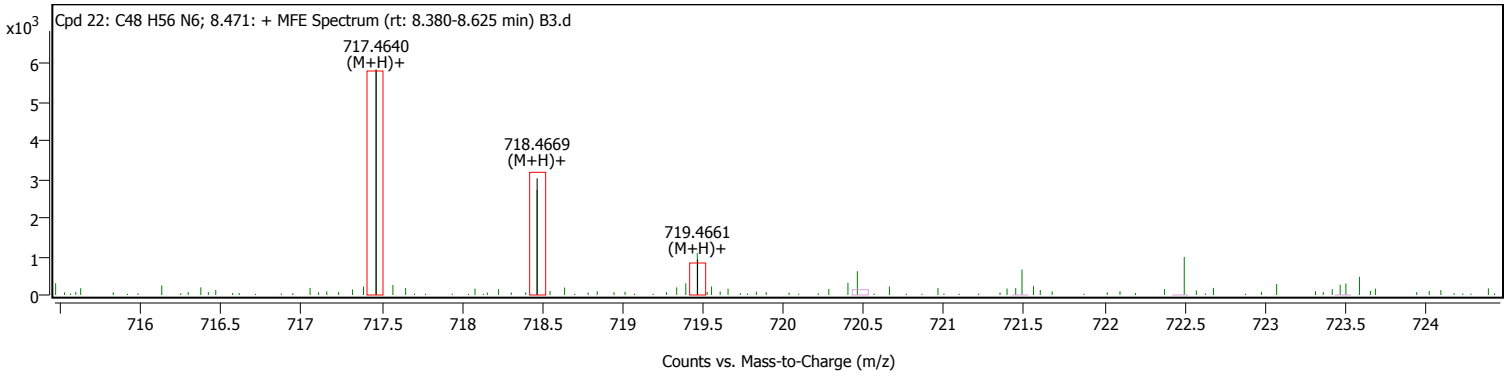
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C48 H56 N6	(M+H)+	MFG	8.471		716.4563		94.60		94.60
	C40 H60 N8 O2 S	(M+H)+	MFG	8.471		716.4566		93.93		93.93
	C42 H62 N5 O3 S	(M+H)+	MFG	8.471		716.4566		93.75		93.75
	C47 H60 N2 O4	(M+H)+	MFG	8.471		716.4562		93.60		93.60
	C41 H66 N O7 S	(M+H)+	MFG	8.471		716.4565		92.04		92.04

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 23: Calenduloside G methyl ester

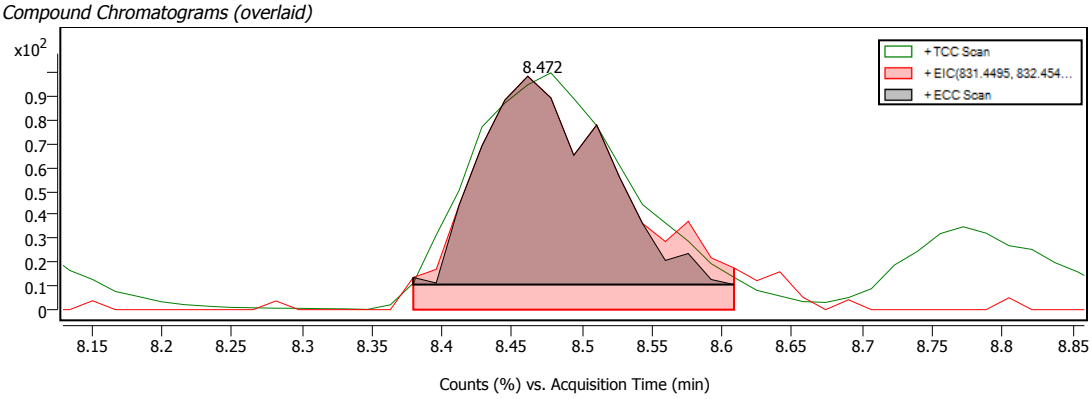
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Calenduloside G methyl ester	C43 H68 O14	8.472		808.4600	155740-15-1	DBSearch	65.86	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	831.4492 831.4492 831.4492		0	65.86	11		

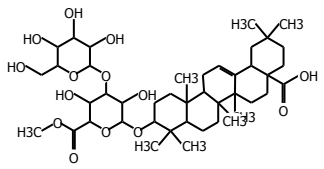
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Calenduloside G methyl ester	C43 H68 O14	(M+Na)+	DBSearch	8.472		808.4600	155740-15-1	65.86	65.86	
	C49 H63 N6 O2 S2	(M+H)+	MFG	8.472		831.4454		47.62		47.62
	C46 H74 Cl N3 S4	(M+H)+	MFG	8.472		831.4454		47.62		47.62
	C41 H72 N6 O2 S4	(M+Na)+	MFG	8.472		808.4600		47.62		47.62
	C34 H67 N14 O2 S4	(M+H)+	MFG	8.472		831.4454		47.62		47.62
	C35 H73 N7 O7 S4	(M+H)+	MFG	8.472		831.4454		47.62		47.62
	C48 H64 Cl2 N7	(M+Na)+	MFG	8.472		808.4600		47.62		47.62
	C49 H70 Cl2 O5	(M+Na)+	MFG	8.472		808.4600		47.62		47.62
	C36 H57 Cl N18 O2	(M+Na)+	MFG	8.472		808.4600		47.62		47.62
	C37 H63 Cl N11 O7	(M+Na)+	MFG	8.472		808.4600		47.62		47.62
	C30 H66 Cl3 N18 O S	(M+H)+	MFG	8.472		831.4454		47.61		47.61

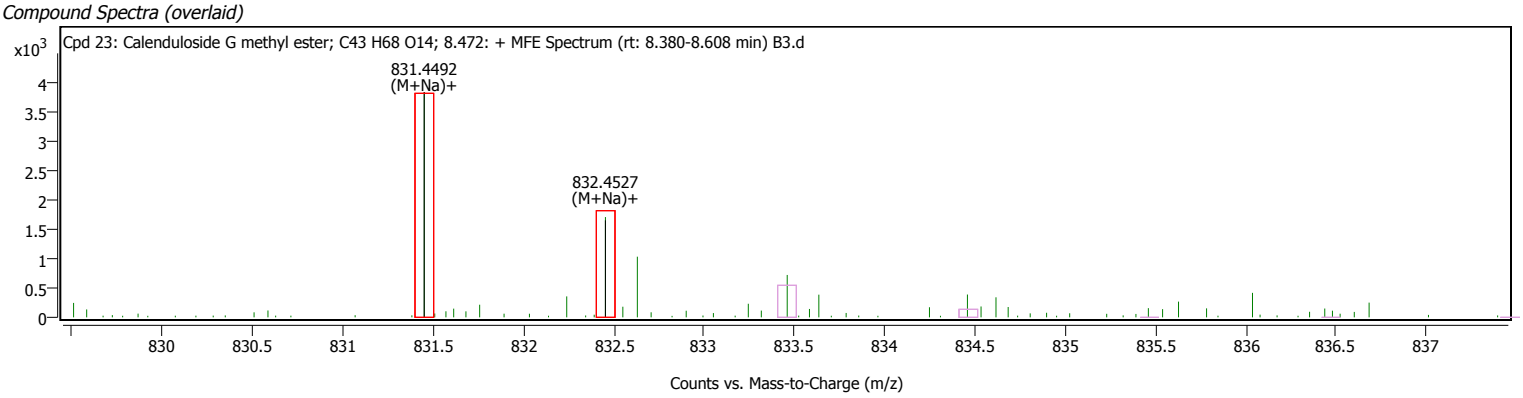
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 24: C33 H58 N16

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C33 H58 N16	8.474		678.5026		MFG	99.04	MFE	

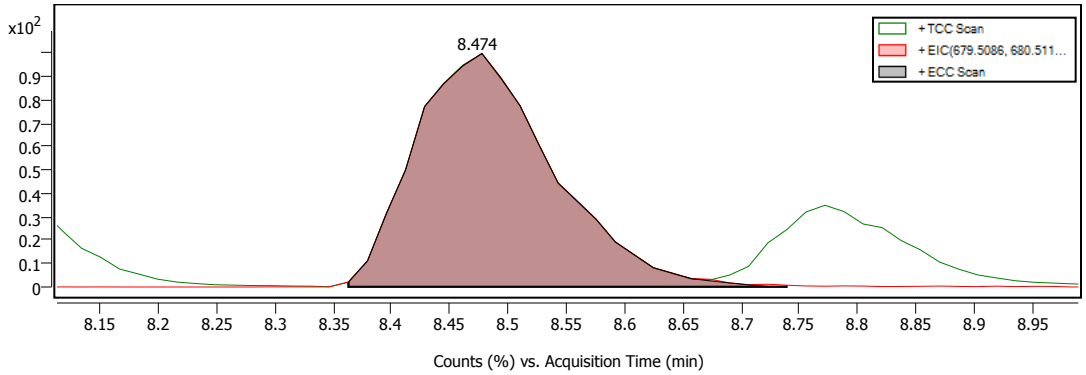
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	679.5098 701.4920				6	99.04	

Compound ID Table

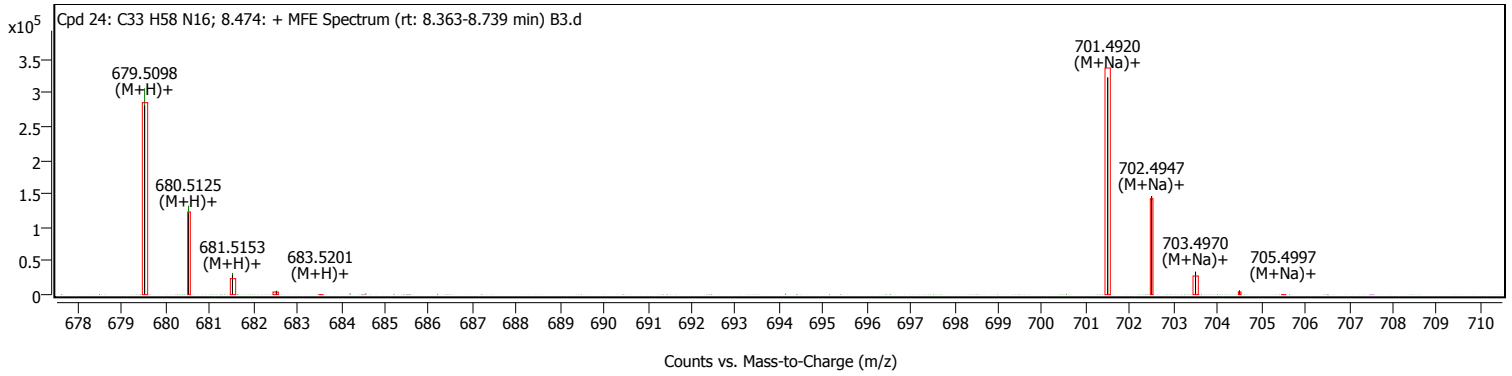
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C33 H58 N16	(M+H)+ (M+Na)+	MFG	8.474		678.5026		99.04		99.04
	C34 H64 N9 O5	(M+H)+ (M+Na)+	MFG	8.474		678.5025		99.03		99.03
	C32 H62 N12 O4	(M+H)+ (M+Na)+	MFG	8.474		678.5025		97.91		97.91
	C35 H70 N2 O10	(M+H)+ (M+Na)+	MFG	8.474		678.5023		97.90		97.90
	C33 H68 N5 O9	(M+H)+	MFG	8.474		678.5024		97.44		97.44
	C35 H60 N13 O	(M+Na)+	MFG	8.474		678.5028		96.09		96.09

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 25: Antanapeptin C

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Antanapeptin C	C41 H64 N4 O8	8.476		740.4728		DBSearch	95.74	MFE	

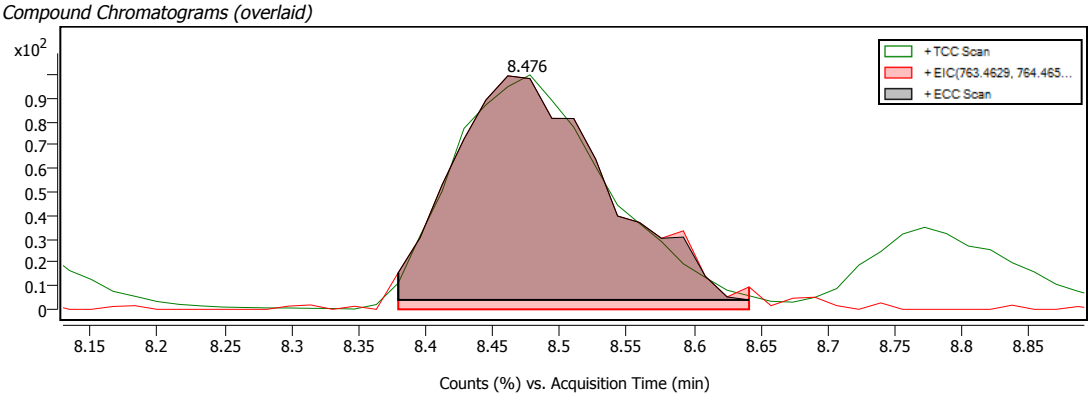
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	763.4618 763.4618		0	95.74	11		

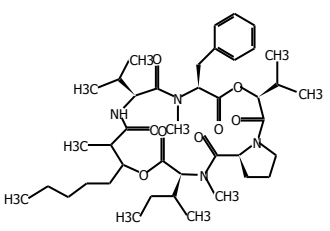
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Antanapeptin C	C41 H64 N4 O8	(M+Na)+	DBSearch	8.476		740.4728		95.74	95.74	
	C33 H53 N19 O3	(M+H)+	MFG	8.476		763.4584		71.20		71.20
	C34 H59 N12 O8	(M+H)+	MFG	8.476		763.4583		71.14		71.14
	C35 H65 N5 O13	(M+H)+	MFG	8.476		763.4582		70.69		70.69
	C35 H55 N16 O4	(M+H)+	MFG	8.476		763.4584		69.45		69.45
	C36 H61 N9 O9	(M+H)+	MFG	8.476		763.4583		69.12		69.12
	C48 H62 N5 S	(M+Na)+	MFG	8.476		740.4725		47.62		47.62
	C33 H66 N13 S3	(M+Na)+	MFG	8.476		740.4725		47.61		47.61
	C34 H72 N6 O5 S3	(M+Na)+	MFG	8.476		740.4725		47.61		47.61
	C38 H75 Cl N O6 S2	(M+Na)+	MFG	8.476		740.4725		47.60		47.60
	C37 H69 Cl N8 O S2	(M+Na)+	MFG	8.476		740.4725		47.60		47.60

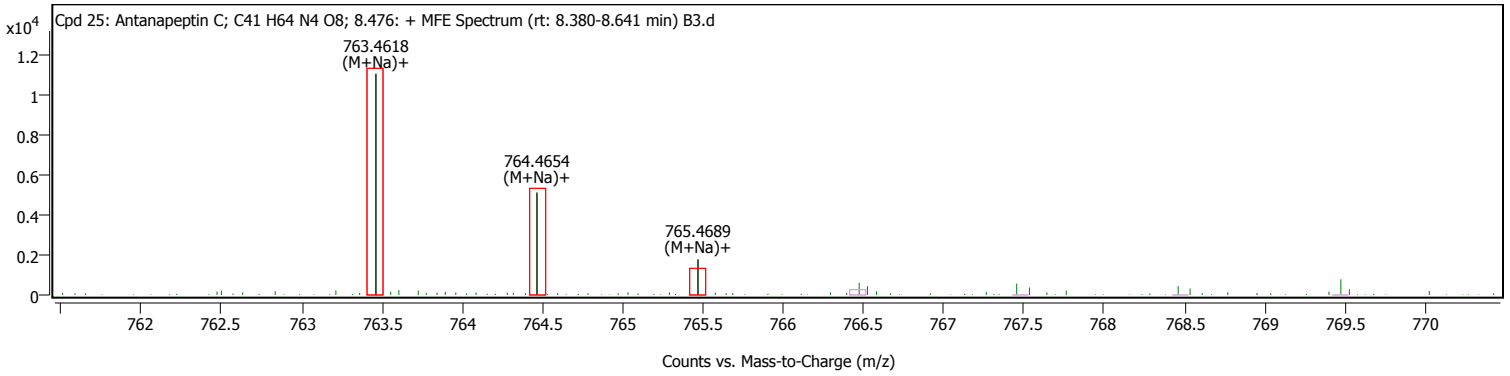
Compound Chromatograms (overlaid)

Structure





Compound Spectra (overlaid)



Cpd. 26: C44 H73 N7 O11

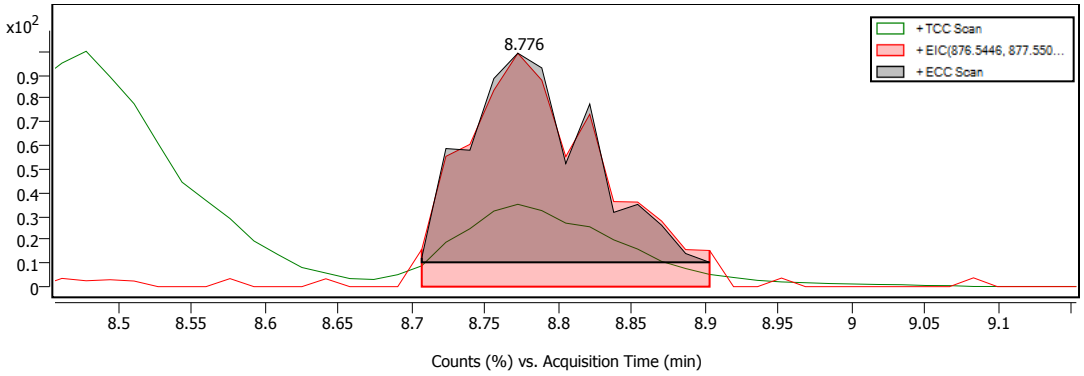
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H73 N7 O11	8.776		875.5371		MFG	92.13	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	876.5452				5	92.13	

Compound ID Table

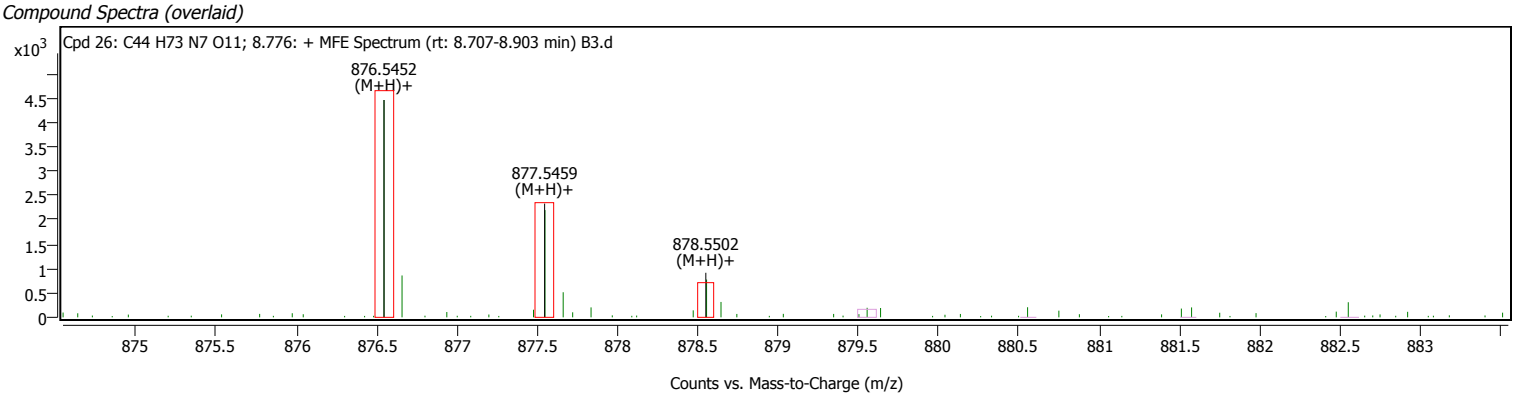
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H73 N7 O11	(M+H)+	MFG	8.776		875.5371		92.13		92.13
	C43 H67 N14 O6	(M+H)+	MFG	8.776		875.5373		92.11		92.11
	C37 H63 N24 S	(M+H)+	MFG	8.776		875.5378		91.68		91.68
	C45 H69 N11 O7	(M+H)+	MFG	8.776		875.5372		91.66		91.66
	C51 H71 N8 O3 S	(M+H)+	MFG	8.776		875.5374		91.65		91.65

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 27: C18 Sulfatide

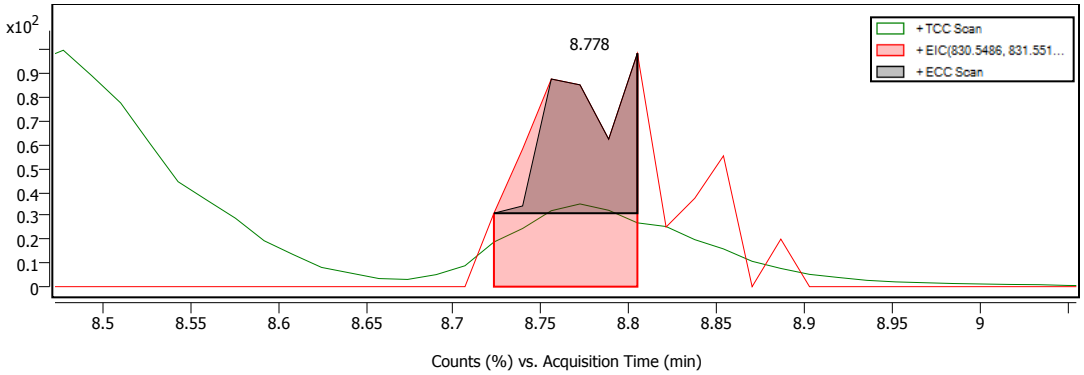
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
C18 Sulfatide	C42 H81 N O11 S	8.778		807.5560		DBSearch	50.86	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	830.5453 830.5453 830.5453		0	50.86	11		

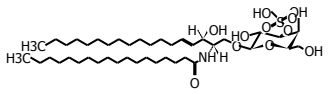
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
C18 Sulfatide	C42 H81 N O11 S	(M+Na)+	DBSearch	8.778		807.5560		50.86	50.86	
	C33 H72 Cl N16 O5	(M+Na)+	MFG	8.778		807.5561		47.62		47.62
	C32 H66 Cl N23	(M+Na)+	MFG	8.778		807.5561		47.62		47.62
	C45 H79 Cl2 N5 O3	(M+Na)+	MFG	8.778		807.5561		47.61		47.61
	C49 H75 Cl N6 O S	(M+H)+	MFG	8.778		830.5411		47.61		47.61
	C38 H82 Cl2 N9 O2 S2	(M+H)+	MFG	8.778		830.5411		47.61		47.61
	C29 H64 N23 O6	(M+H)+	MFG	8.778		830.5411		47.61		47.61
	C28 H58 N30 O	(M+H)+	MFG	8.778		830.5411		47.61		47.61
	C37 H68 N17 O3 S	(M+H)+	MFG	8.778		830.5411		47.61		47.61
	C37 H81 N11 S4	(M+Na)+	MFG	8.778		807.5561		47.60		47.60
	C41 H76 Cl N10 O2 S	(M+Na)+	MFG	8.778		807.5561		47.60		47.60

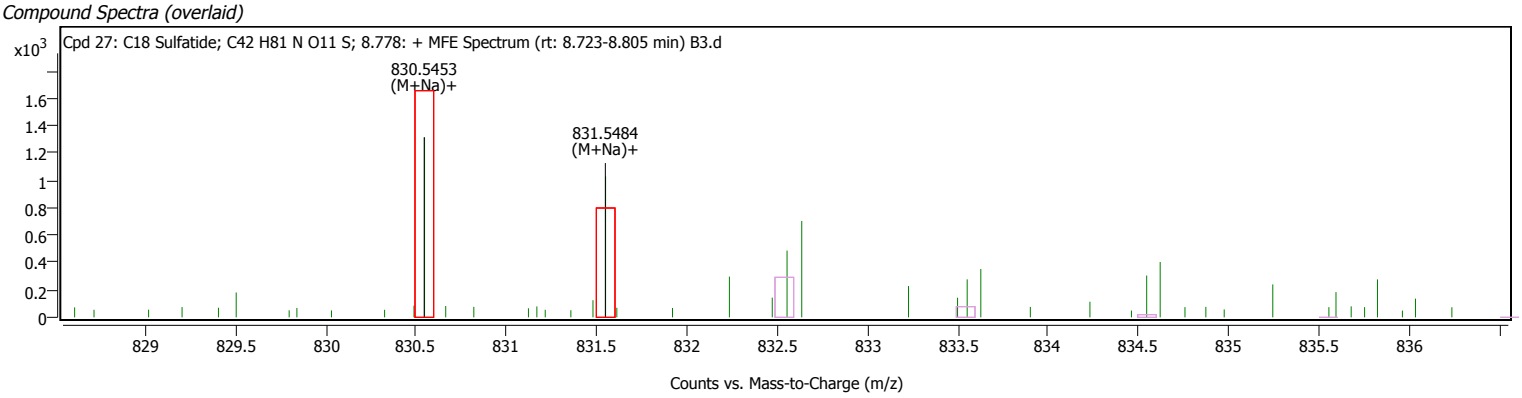
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 28: C39 H79 N6 O10

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C39 H79 N6 O10	8.782		791.5857		MFG	98.78	MFE	

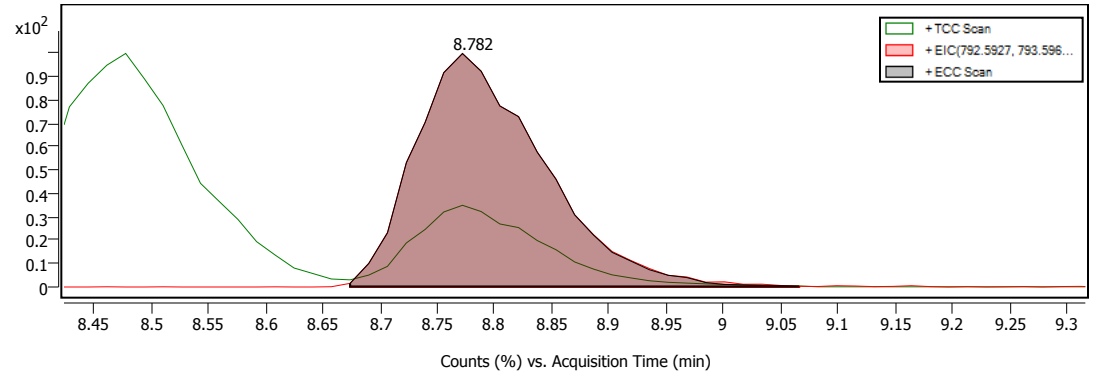
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	792.5930				16	98.78	

Compound ID Table

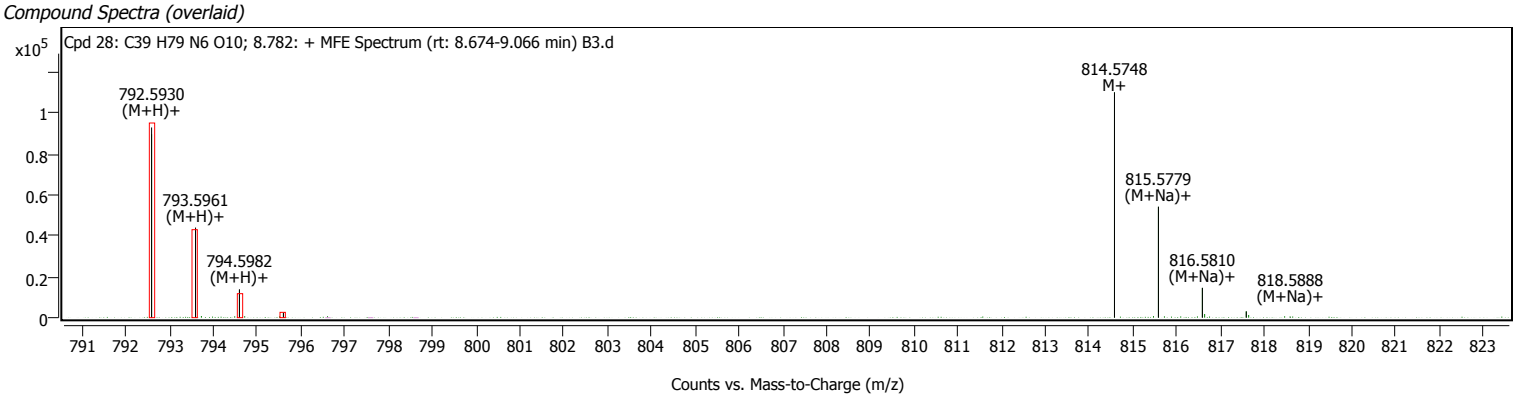
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C39 H79 N6 O10	(M+H)+	MFG	8.782		791.5857		98.78		98.78
1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C48 H81 N O7 P	M+	DBSearch	8.782		814.5752		98.74	98.74	
	C38 H73 N13 O5	(M+H)+	MFG	8.782		791.5858		98.32		98.32
	C37 H67 N20	(M+H)+	MFG	8.782		791.5860		97.04		97.04
	C40 H75 N10 O6	(M+H)+	MFG	8.782		791.5857		96.65		96.65
	C41 H81 N3 O11	(M+H)+	MFG	8.782		791.5856		96.62		96.62
	C30 H66 N25 O	(M+Na)+	MFG	8.782		792.5889		80.21		80.21
	C32 H68 N22 O2	(M+Na)+	MFG	8.782		792.5889		79.30		79.30
	C28 H64 N28	(M+Na)+	MFG	8.782		792.5890		77.06		77.06
	C35 H76 N12 O8	(M+Na)+	MFG	8.782		792.5887		75.46		75.46
	C34 H70 N19 O3	(M+Na)+	MFG	8.782		792.5888		74.34		74.34
	C38 H80 N5 O13	M+	MFG	8.782		814.5753		47.61		47.61
	C37 H74 N12 O8	M+	MFG	8.782		814.5753		47.61		47.61
	C36 H68 N19 O3	M+	MFG	8.782		814.5753		47.61		47.61
	C49 H81 Cl N O6	M+	MFG	8.782		814.5753		47.61		47.61
	C44 H72 N13 S	M+	MFG	8.782		814.5753		47.61		47.61

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 29: C25 H20 N5 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C25 H20 N5 O3	8.990		438.1559		MFG	73.08	MFE	

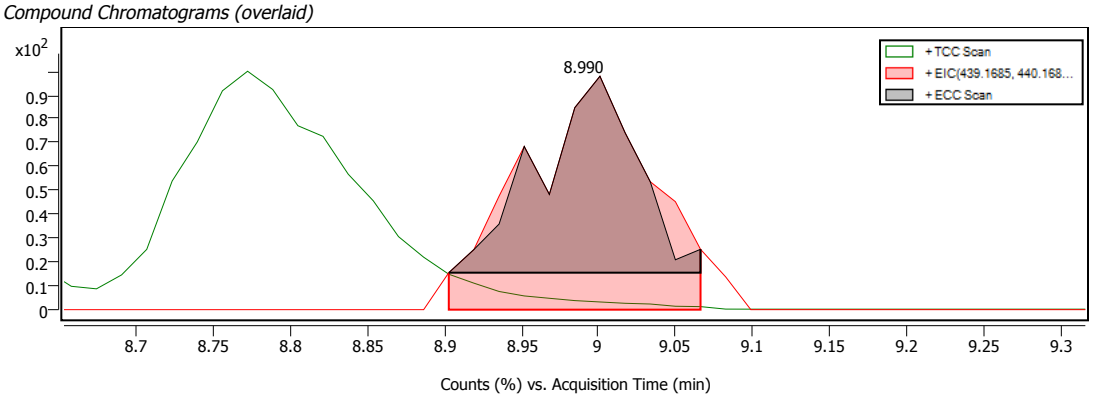
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	439.1628				9	73.08	

Compound ID Table

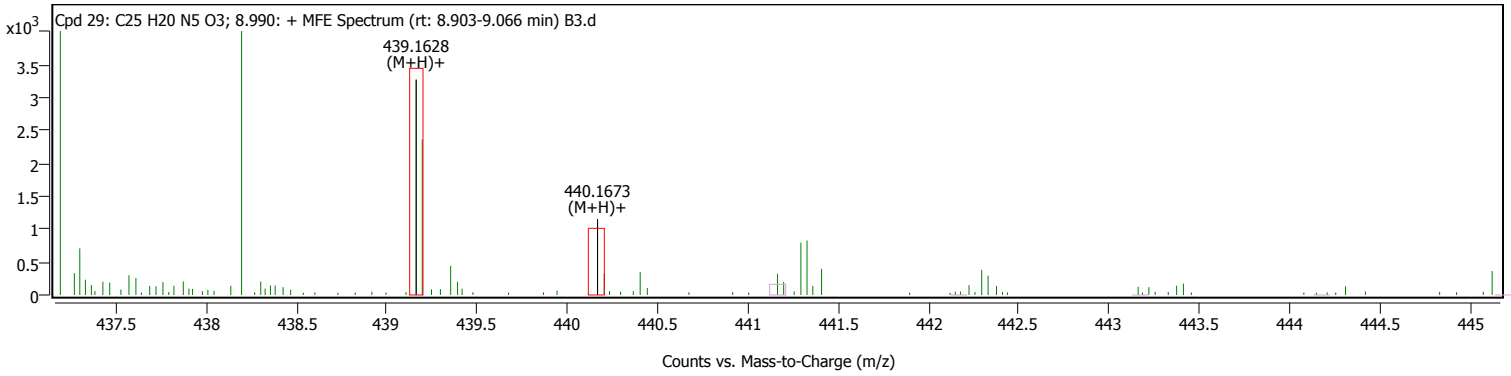
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C25 H20 N5 O3	(M+H)+	MFG	8.990		438.1559		73.08		73.08
	C23 H18 N8 O2	(M+H)+	MFG	8.990		438.1560		71.46		71.46
	C24 H24 N O7	(M+H)+	MFG	8.990		438.1558		70.12		70.12
	C27 H22 N2 O4	(M+H)+	MFG	8.990		438.1559		65.89		65.89
	C25 H28 N O2 S2	(M+H)+	MFG	8.990		438.1559		61.13		61.13
His-HoPhe-OH	C22 H22 N4 O6	(M+H)+	DBSearch	8.990		438.1559		60.42	60.42	
Losartan Metabolite (1H-Imidazole-2-propanol, 4-chloro-5-(hydroxymethyl)-a-methyl-1-[[2'-(1H-tetrazo	C22 H23 Cl N6 O2	(M+H)+	DBSearch	8.990		438.1560	141675-57-2	54.32	54.32	
Losartan Metabolite (1H-Imidazole-2,5-dimethanol, 4-chloro-a2-propyl-1-[[2'-(1H-tetrazol-5-yl)[1,1'-	C22 H23 Cl N6 O2	(M+H)+	DBSearch	8.990		438.1560	141675-59-4	54.32	54.32	
Cyproterone acetate	C24 H29 Cl O4	(M+Na)+	DBSearch	8.990		416.1739	427-51-0	52.70	52.70	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 30: C42 H78 N20 O4

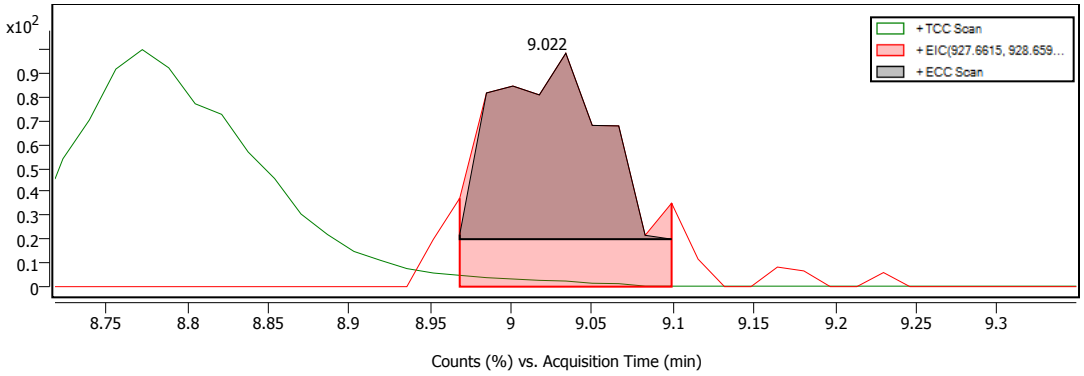
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C42 H78 N20 O4	9.022		926.6510		MFG	63.88	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	927.6581				5	63.88	

Compound ID Table

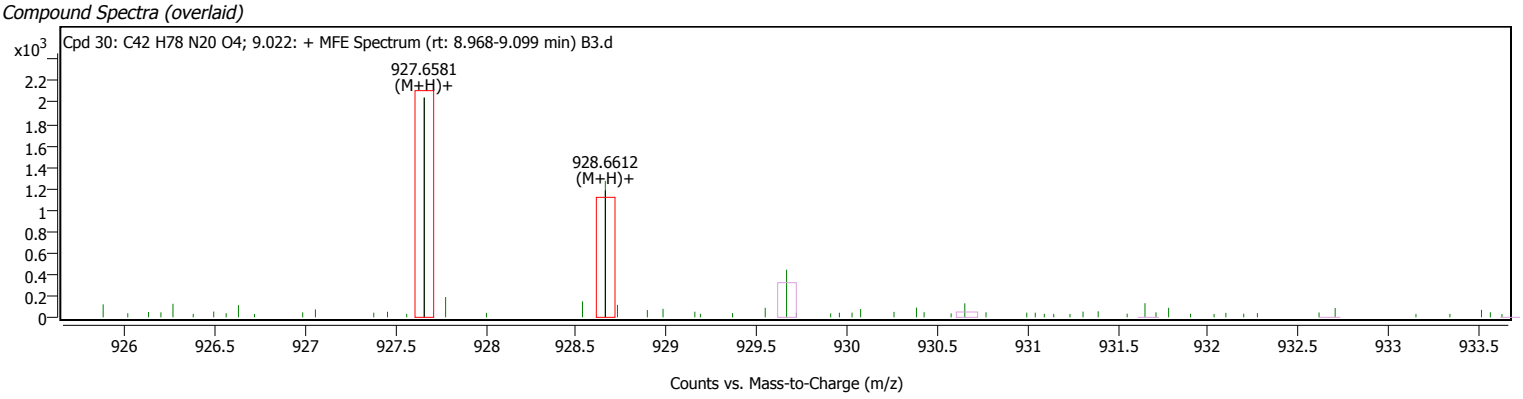
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C42 H78 N20 O4	(M+H)+	MFG	9.022		926.6510		63.88		63.88
	C40 H76 N23 O3	(M+H)+	MFG	9.022		926.6511		63.53		63.53
	C43 H84 N13 O9	(M+H)+	MFG	9.022		926.6509		63.06		63.06
	C41 H82 N16 O8	(M+H)+	MFG	9.022		926.6510		62.95		62.95
	C42 H88 N9 O13	(M+H)+	MFG	9.022		926.6509		62.38		62.38

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 31: C14 H33 N4 O

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C14 H33 N4 O	10.253		273.2658		MFG	86.31	MFE	

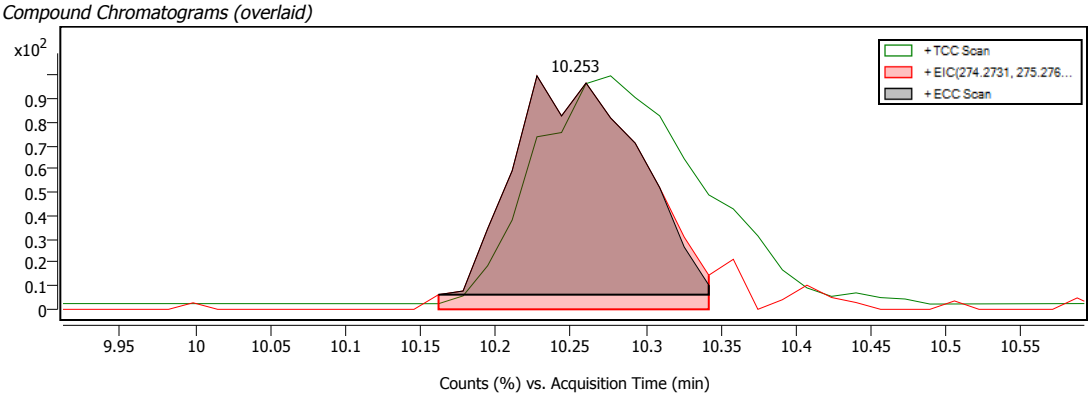
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	274.2730				34	86.31	

Compound Discovery Report

Compound ID Table

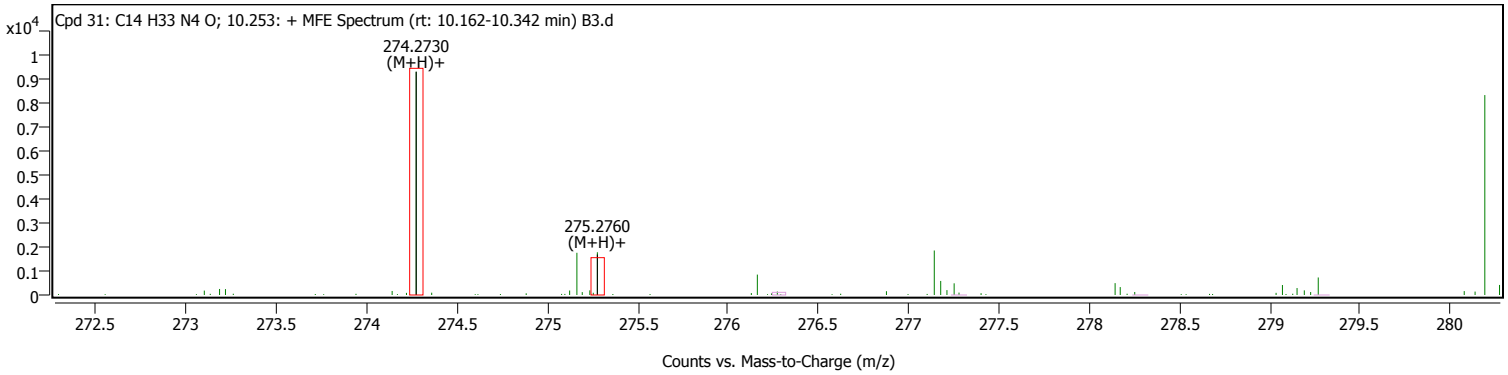
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C14 H33 N4 O	(M+H)+	MFG	10.253		273.2658		86.31		86.31
C16 Sphinganine	C16 H35 N O2	(M+H)+	DBSearch-MFG	10.253		273.2657		82.38	82.37	82.39
13,13-dimethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
Tridecanoic acid, 4,8,12-trimethyl-; 4,8,12-Trimethyltridecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
Butyl dodecanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	106-18-3	82.14	82.14	
Dodecyl butyrate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	3724-61-6	82.14	82.14	
Hexyl decanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	10448-26-7	82.14	82.14	
Octyl octanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	2306-88-9	82.14	82.14	
Dodecyl 2-methylpropanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	6624-71-1	82.14	82.14	
Palmitic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	57-10-3	82.14	82.14	
formyl 2,6,10-trimethyl-dodecanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
Isopalmitic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	4669-02-7	82.14	82.14	
2,6-Dimethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2,8-Dimethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-Hexyldecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	25354-97-6	82.14	82.14	
4,8,12-Trimethyl-tridecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
Myristic Acid ethyl ester	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392	124-06-1	82.14	82.14	
Tetradecyl acetate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
6-ethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
3-methyl-pentadecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-propyl-tridecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-hexyl-decanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
3-ethyl-3-methyl-tridecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-heptyl-nonanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
7-Methyloctyl 5-methylhexanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2,4-dimethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
3,5-dimethyl-tetradecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
4-hexyl-decanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-ethyl-2-butyl-decanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
13-methyl-pentadecanoic acid	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
14:0(10Me,13Me)	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
2-hydroxyhexadecanal	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
decyl hexanoate	C16 H32 O2	(M+NH4)+	DBSearch	10.253		256.2392		82.14	82.14	
	C12 H31 N7	(M+H)+	MFG	10.253		273.2658		75.23		75.23

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 32: C16 H37 N4 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C16 H37 N4 O2	10.272		317.2918		MFG	82.87	MFE	

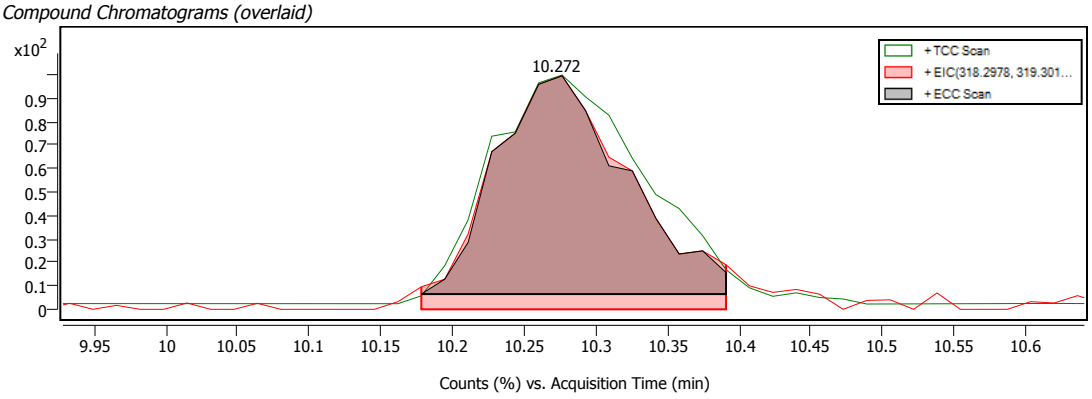
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	318.2990				31	82.87	

Compound ID Table

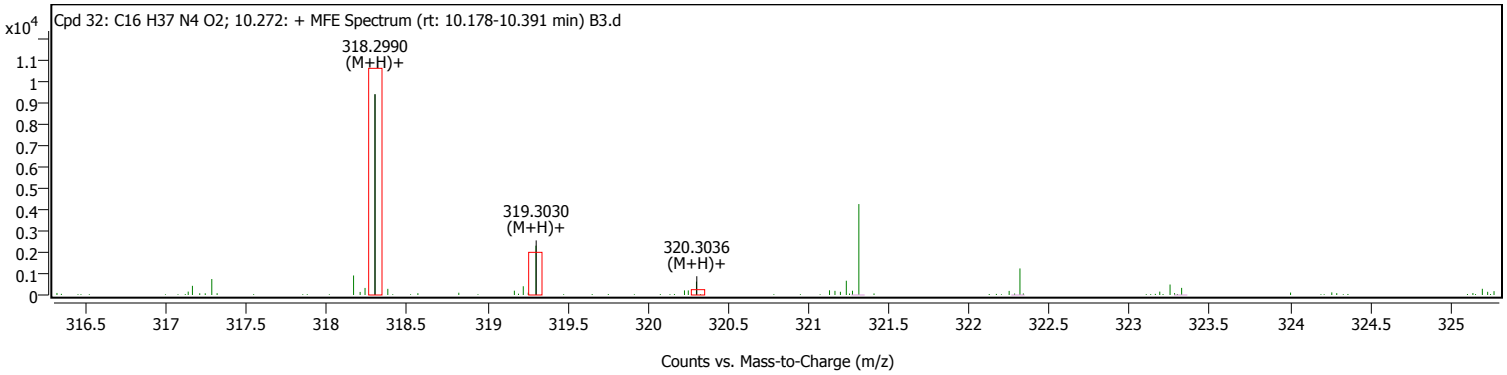
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C16 H37 N4 O2	(M+H)+	MFG	10.272		317.2918		82.87		82.87
Phytosphingosine	C18 H39 N O3	(M+H)+	DBSearch-MFG	10.272		317.2917	554-62-1	80.39	80.38	80.40
DL-9-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
3R-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
(R)-10-hydroxystearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
2S-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
2R-hydroxy-stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
13R-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-2-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652	629-22-1	80.13	80.13	
DL-3-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-4-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-5-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-6-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-7-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-8-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-10-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-11-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-12-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
DL-13-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
9-methoxy-heptadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
15-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
16-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
17-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
18-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
3-hydroxy-16-methyl-heptadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
9R-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
9S-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
12R-hydroxy-octadecanoic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
14-hydroxy stearic acid	C18 H36 O3	(M+NH4)+	DBSearch	10.272		300.2652		80.13	80.13	
	C14 H35 N7 O	(M+H)+	MFG	10.272		317.2920		71.74		71.74
	C12 H33 N10	(M+H)+	MFG	10.272		317.2921		52.55		52.55

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 33: C18 H41 N4 O3

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C18 H41 N4 O3	10.294		361.3172		MFG	74.40	MFE	

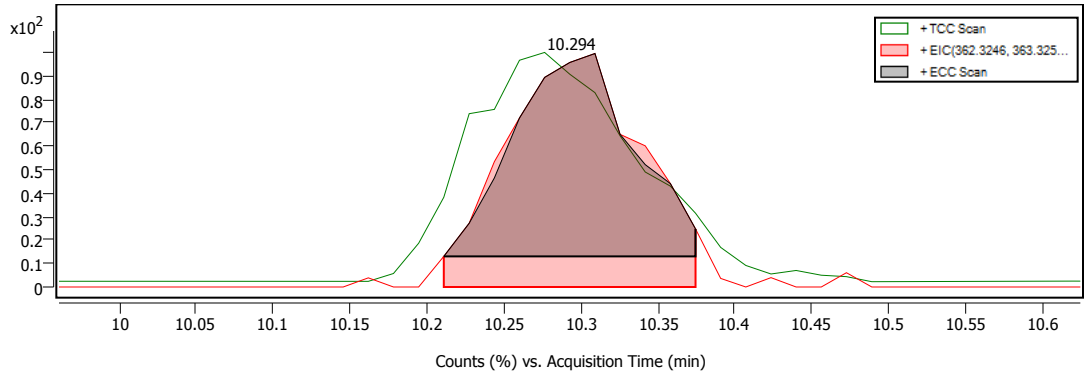
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	362.3243				5	74.40	

Compound ID Table

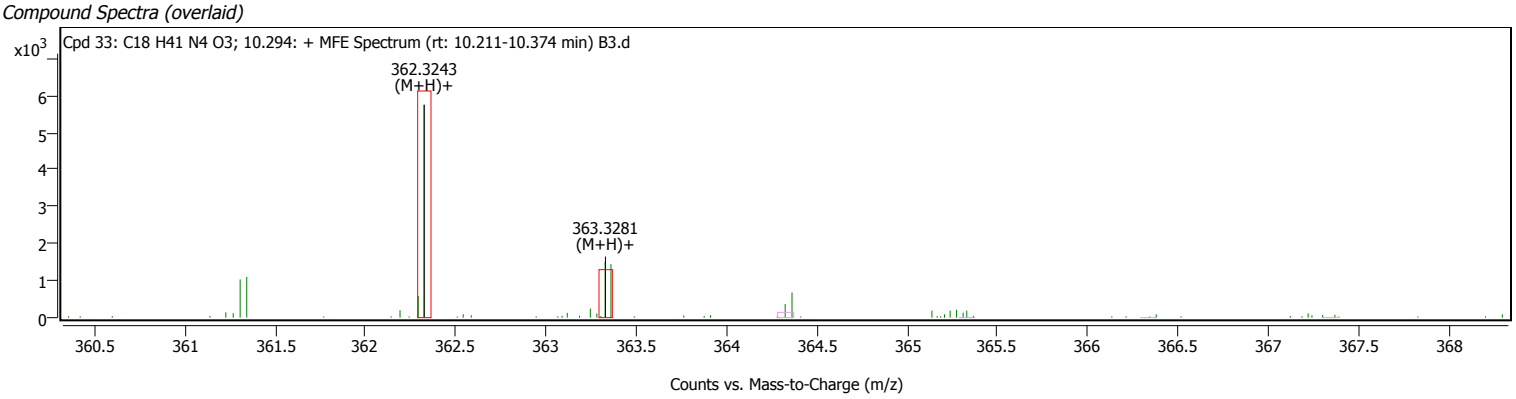
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C18 H41 N4 O3	(M+H)+	MFG	10.294		361.3172		74.40		74.40
	C16 H39 N7 O2	(M+H)+	MFG	10.294		361.3173		71.30		71.30
	C20 H43 N O4	(M+H)+	MFG	10.294		361.3172		66.64		66.64
	C21 H39 N5	(M+H)+	MFG	10.294		361.3172		58.07		58.07
	C14 H37 N10 O	(M+H)+	MFG	10.294		361.3174		57.67		57.67

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 34: C14 H31 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C14 H31 N4	10.357		255.2549		MFG	70.43	MFE	

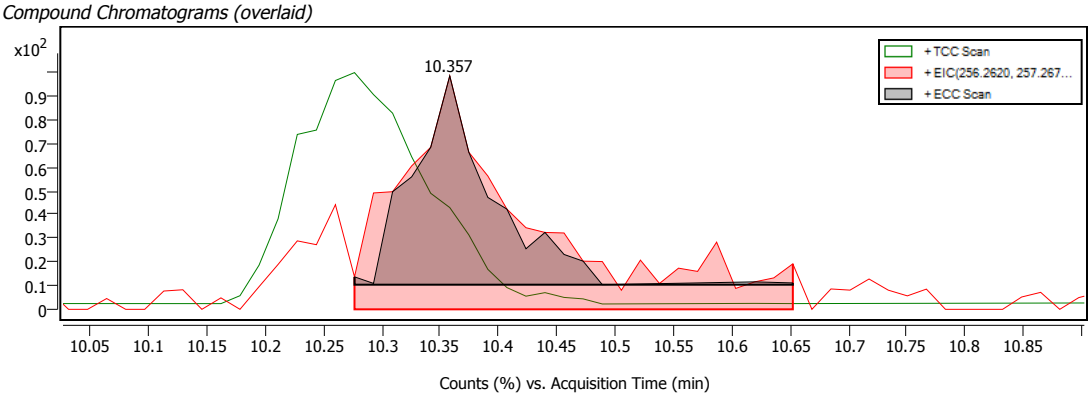
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	256.2621				2	70.43	

Compound ID Table

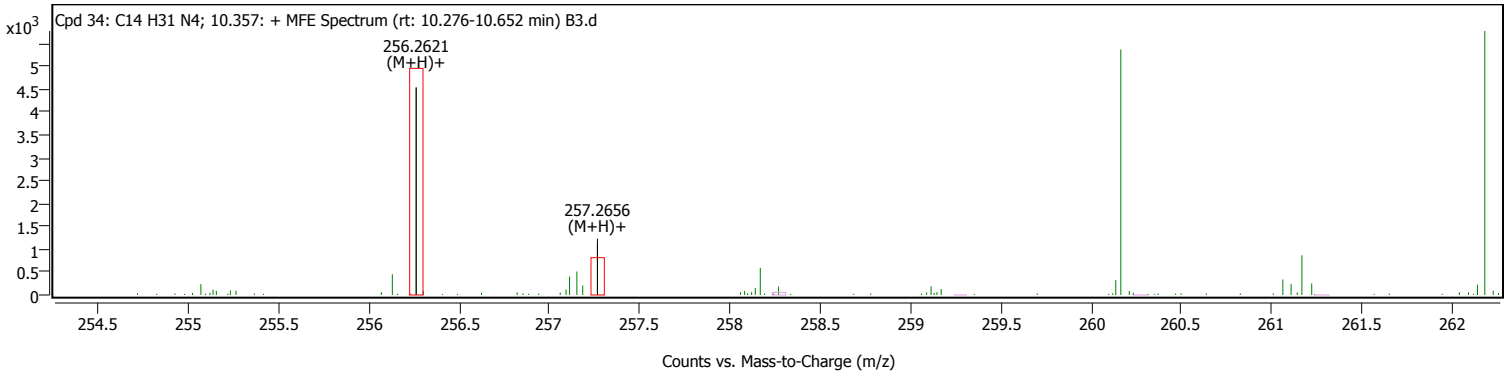
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C14 H31 N4	(M+H)+	MFG	10.357		255.2549		70.43		70.43
	C16 H33 N O	(M+H)+	MFG	10.357		255.2549		66.20		66.20

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 35: C30 H55 N O S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C30 H55 N O S	11.113		477.4002		MFG	62.20	MFE	

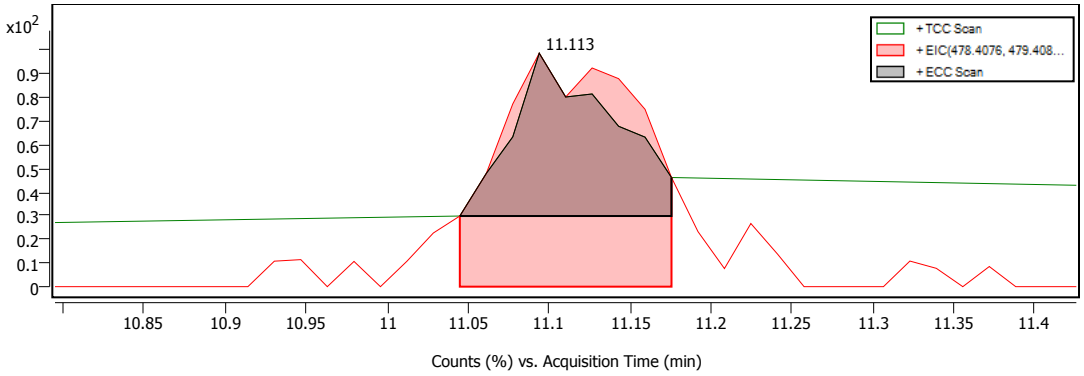
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	478.4076				5	62.20	

Compound ID Table

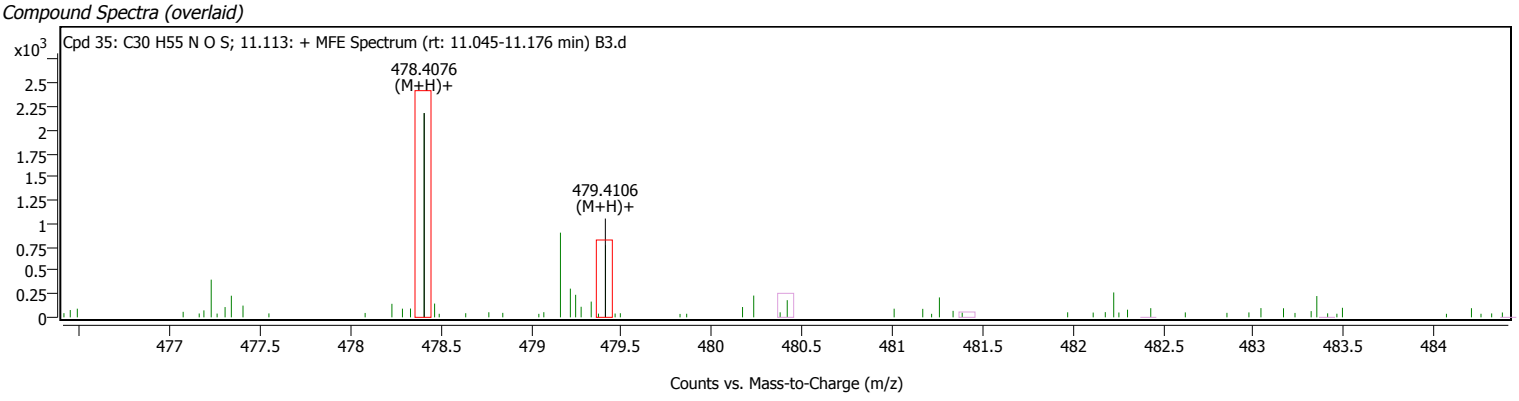
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C30 H55 N O S	(M+H)+	MFG	11.113		477.4002		62.20		62.20
	C28 H53 N4 S	(M+H)+	MFG	11.113		477.4003		59.08		59.08
	C24 H53 N4 O5	(M+H)+	MFG	11.113		477.4003		58.10		58.10
	C25 H49 N8 O	(M+H)+	MFG	11.113		477.4004		50.96		50.96
	C33 H51 N O	(M+H)+	MFG	11.113		477.4002		50.37		50.37

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 36: 27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
27-Nor-5b-cholestane-3a,7a,12a,24,25-pentol	C26 H46 O5	12.886		438.3327	78648-95-0	DBSearch	73.50	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	461.3218 461.3218 461.3218 461.3218		0	73.50	11		

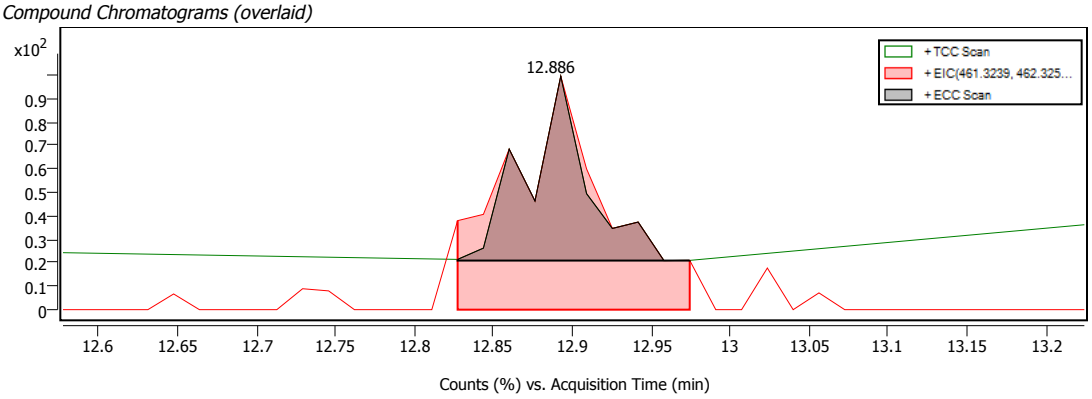
Compound Discovery Report

Agilent | Trusted Answers

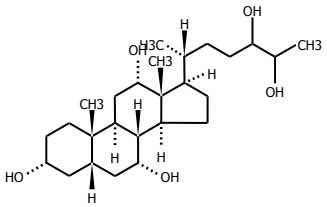
Compound ID Table

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	12.886		438.3327	78648-95-0	73.50	73.50	
	C15 H42 N12 O S	(M+Na)+	MFG	12.886		438.3325		47.62		47.62
	C25 H51 N S3	(M+H)+	MFG	12.886		461.3185		47.59		47.59
	C29 H46 Cl O2	(M+H)+	MFG	12.886		461.3185		47.56		47.56
	C17 H39 N11 O4	(M+H)+	MFG	12.886		461.3185		47.55		47.55
	C19 H45 Cl N7 O2	(M+Na)+	MFG	12.886		438.3325		47.53		47.53
	C25 H43 N5 O S	(M+H)+	MFG	12.886		461.3185		47.33		47.33
	C30 H46 S	(M+Na)+	MFG	12.886		438.3325		47.04		47.04
	C26 H49 Cl2 N O	(M+H)+	MFG	12.886		461.3185		46.69		46.69
	C24 H44 N3 O4	(M+Na)+	MFG	12.886		438.3325		46.67		46.67
	C22 H42 N6 O3	(M+Na)+	MFG	12.886		438.3325		46.55		46.55

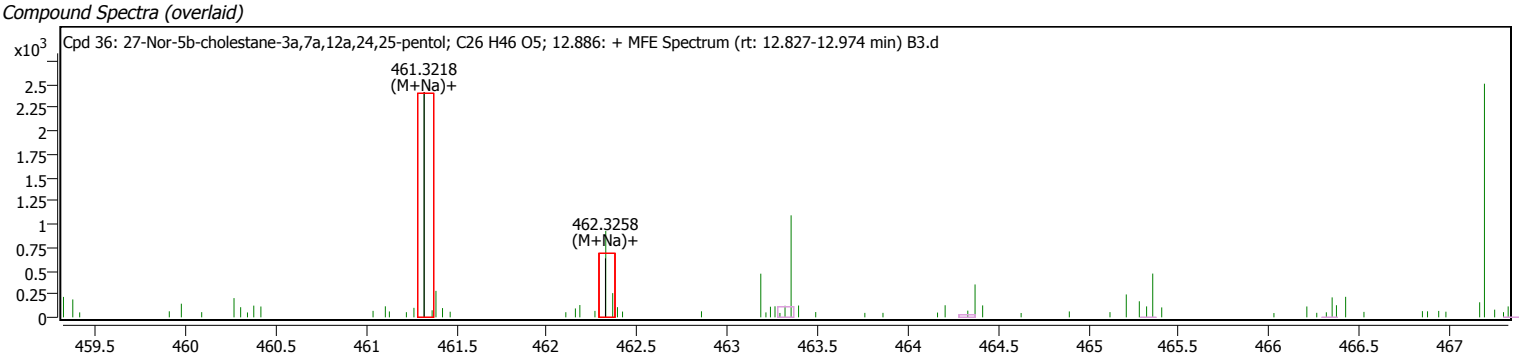
Compound Chromatograms (overlaid)



Structure



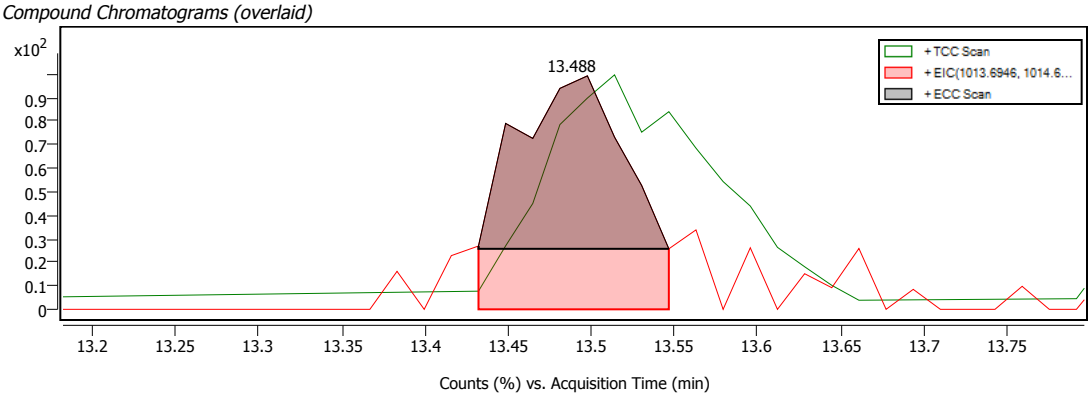
Compound Spectra (overlaid)



Cpd 37: 13.488

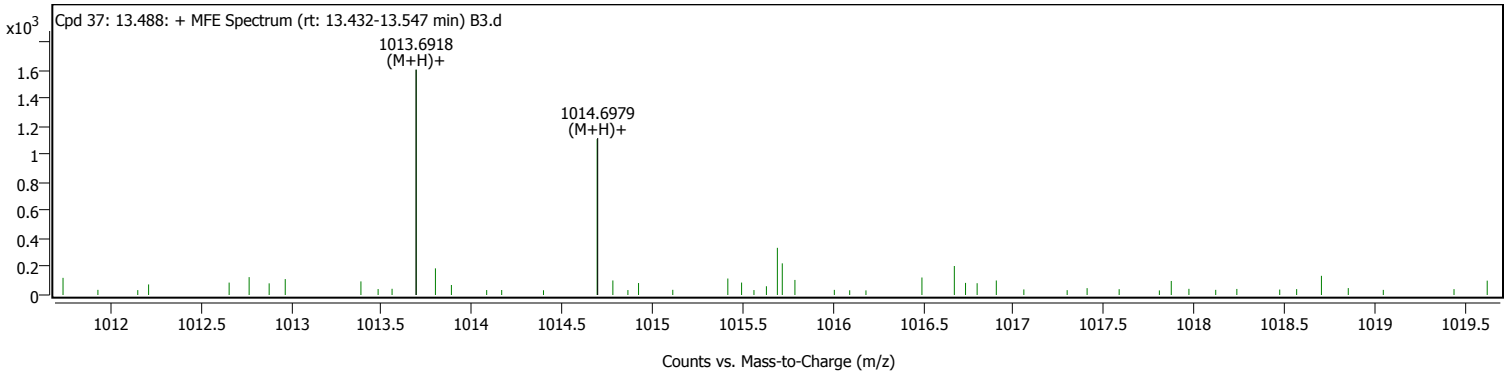
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.488		1012.6845				MFE	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 38: C56 H86 N7 O7

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C56 H86 N7 O7	13.491		968.6590		MFG	59.22	MFE	

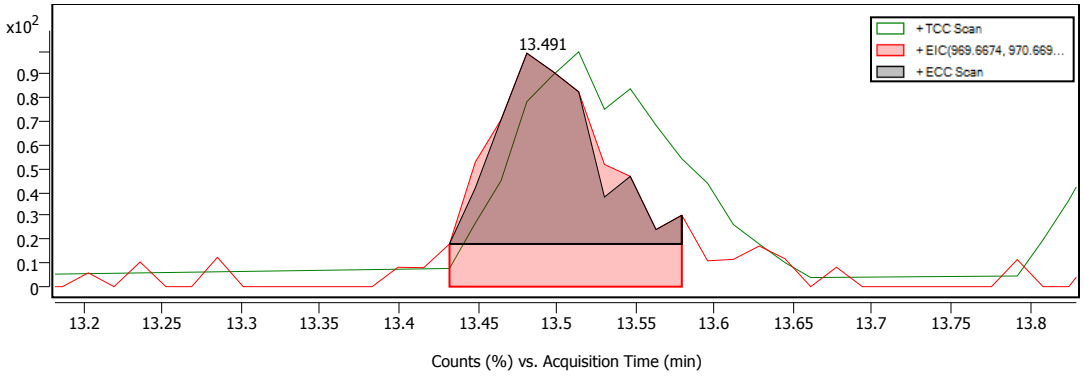
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	969.6653				5	59.22	

Compound ID Table

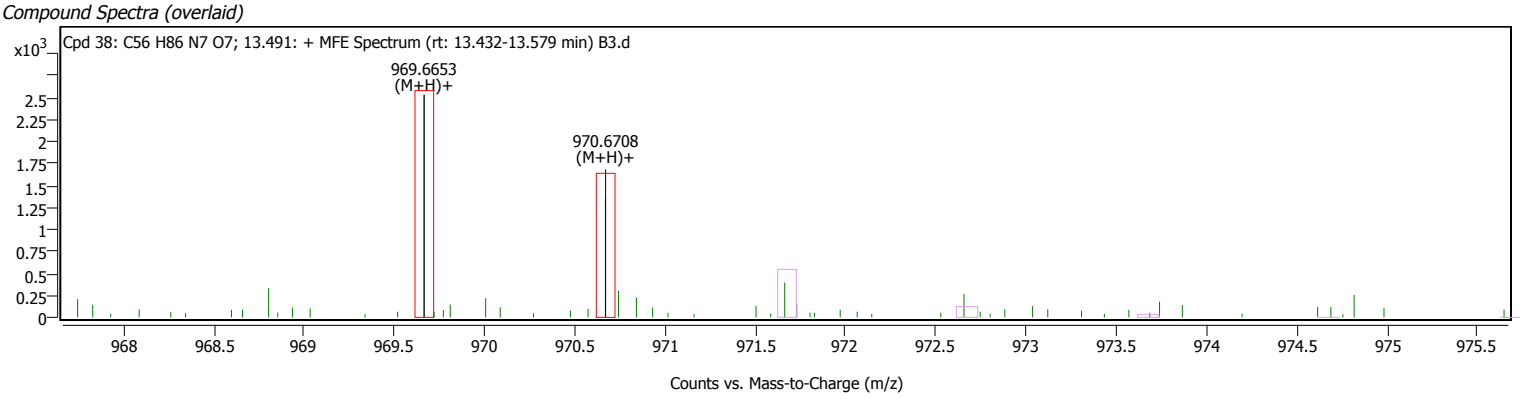
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C56 H86 N7 O7	(M+H)+	MFG	13.491		968.6590		59.22		59.22
	C55 H80 N14 O2	(M+H)+	MFG	13.491		968.6591		59.11		59.11
	C40 H76 N26 O3	(M+H)+	MFG	13.491		968.6593		58.77		58.77
	C41 H82 N19 O8	(M+H)+	MFG	13.491		968.6592		58.68		58.68
	C57 H82 N11 O3	(M+H)+	MFG	13.491		968.6590		57.96		57.96

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 39: C50 H76 N10 O4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C50 H76 N10 O4	13.508		880.6052		MFG	59.37	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	881.6113				13	59.37	

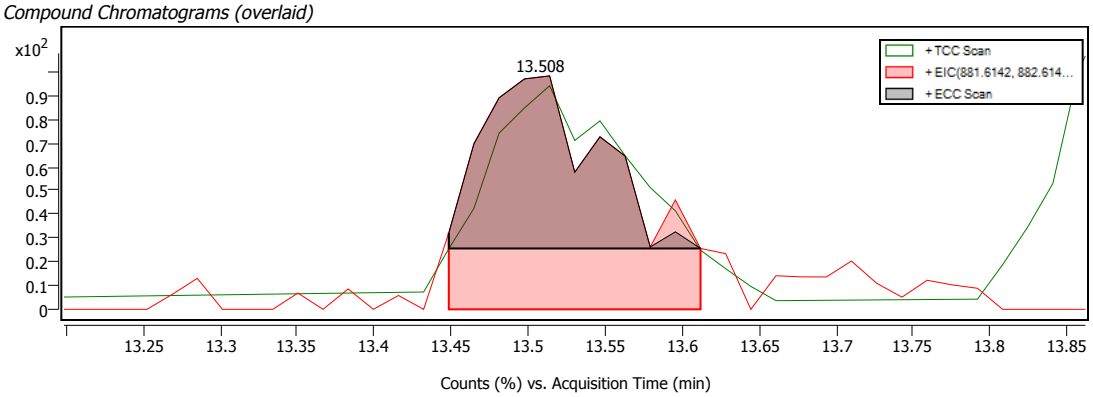
Compound Discovery Report

Compound ID Table

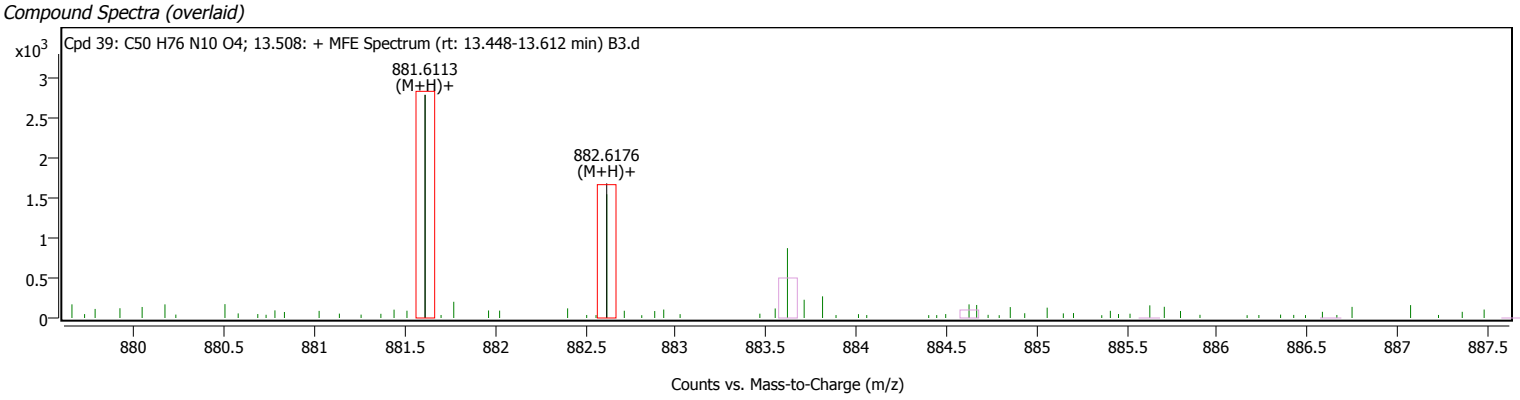
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C50 H76 N10 O4	(M+H)+	MFG	13.508		880.6052		59.37		59.37
	C51 H82 N3 O9	(M+H)+	MFG	13.508		880.6051		59.33		59.33
	C34 H66 N29	(M+H)+	MFG	13.508		880.6056		58.69		58.69
	C35 H72 N22 O5	(M+H)+	MFG	13.508		880.6055		58.23		58.23
	C51 H72 N14	(M+H)+	MFG	13.508		880.6053		58.04		58.04
PI(15:0/22:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(16:0/21:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(18:0/19:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(20:0/17:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(21:0/16:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(22:0/15:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(19:0/18:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	
PI(17:0/20:0)	C46 H89 O13 P	(M+H)+	DBSearch	13.508		880.6051		57.88	57.88	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 40: C40 H84 N8 O4 S3

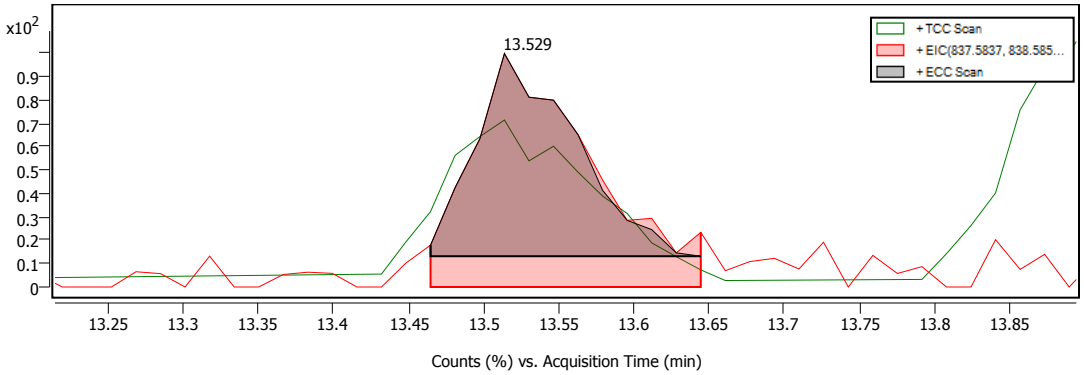
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C40 H84 N8 O4 S3	13.529		836.5776		MFG	85.57	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	837.5860				11	85.57	

Compound ID Table

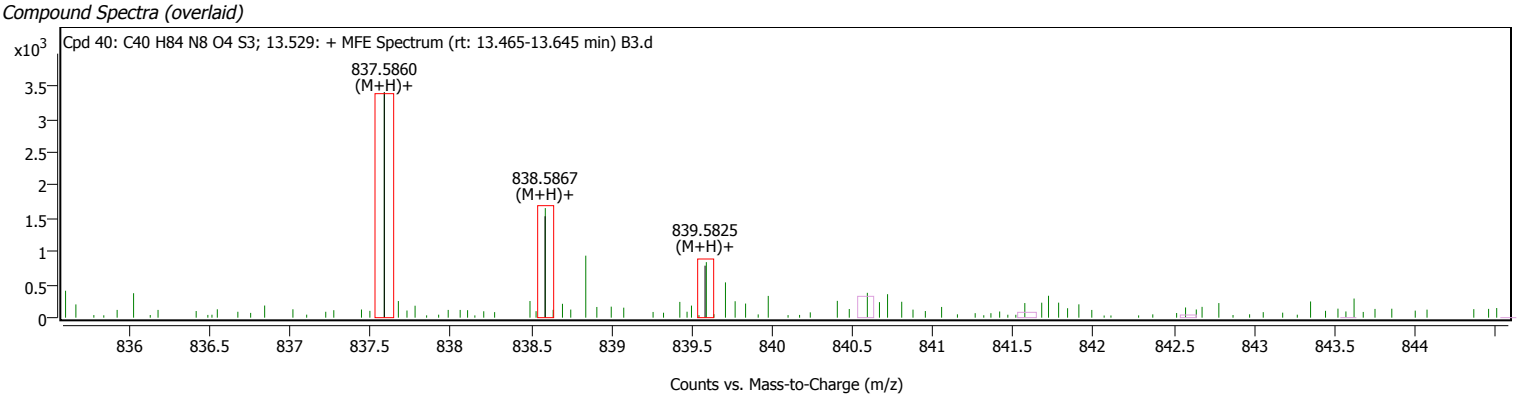
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C40 H84 N8 O4 S3	(M+H)+	MFG	13.529		836.5776		85.57		85.57
	C38 H82 N11 O3 S3	(M+H)+	MFG	13.529		836.5776		85.17		85.17
	C39 H80 N8 O9 S	(M+H)+	MFG	13.529		836.5772		83.26		83.26
	C41 H80 N12 S3	(M+H)+	MFG	13.529		836.5776		83.20		83.20
	C38 H74 N15 O4 S	(M+H)+	MFG	13.529		836.5773		83.05		83.05
PI(O-16:0/19:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	
PI(O-18:0/17:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	
PI(O-20:0/15:1(9Z))	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	
PI(P-16:0/19:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	
PI(P-18:0/17:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	
PI(P-20:0/15:0)	C44 H85 O12 P	(M+H)+	DBSearch	13.529		836.5766		73.46	73.46	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 41: PC(15:0/20:3(5Z,8Z,11Z))

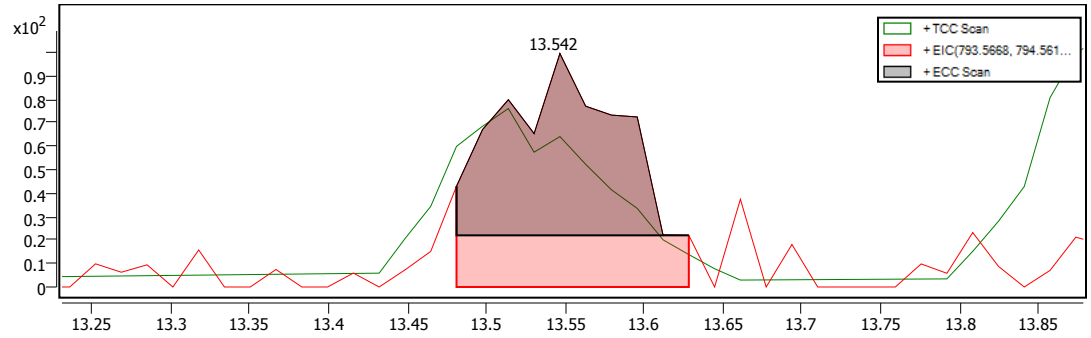
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
PC(15:0/20:3(5Z,8Z,11Z))	C43 H81 N O8 P	13.542		770.5707		DBSearch	62.92	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+Na)+	793.5608 793.5608 793.5608 793.5608		0	62.92	31		

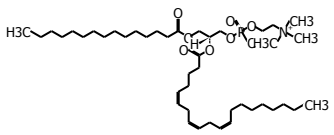
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
PC(15:0/20:3(5Z,8Z,11Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(15:0/20:3(8Z,11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(18:3(6Z,9Z,12Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(20:3(5Z,8Z,11Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(20:3(8Z,11Z,14Z)/15:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(20:2(11Z,14Z)/15:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(17:0/18:3(6Z,9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(16:0/19:3(9Z,12Z,15Z))[U]	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(18:3(9Z,12Z,15Z)/17:0)	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(15:1(9Z)/20:2(11Z,14Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(17:0/18:3(9Z,12Z,15Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(17:1(9Z)/18:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(17:2(9Z,12Z)/18:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(18:1(9Z)/17:2(9Z,12Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(18:2(9Z,12Z)/17:1(9Z))	C43 H81 N O8 P	(M+Na)+	DBSearch	13.542		770.5707		62.92	62.92	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/17:1(9Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
PC(17:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
PC(17:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C45 H79 N O8 P	(M+H)+	DBSearch	13.542		792.5526		59.86	59.86	
	C39 H83 N7 O S4	(M+H)+	MFG	13.542		793.5542		47.62		47.62
	C33 H70 N16 O5	(M+Na)+	MFG	13.542		770.5715		47.62		47.62
	C32 H64 N23	(M+Na)+	MFG	13.542		770.5715		47.62		47.62
	C47 H81 Cl2 N O4	(M+H)+	MFG	13.542		793.5542		47.62		47.62
	C45 H77 Cl N5 O3	(M+Na)+	MFG	13.542		770.5715		47.62		47.62
	C34 H68 Cl N19 O	(M+H)+	MFG	13.542		793.5542		47.61		47.61
	C35 H74 Cl N12 O6	(M+H)+	MFG	13.542		793.5542		47.61		47.61
	C41 H74 N10 O2 S	(M+Na)+	MFG	13.542		770.5715		47.60		47.60
	C42 H80 N3 O7 S	(M+Na)+	MFG	13.542		770.5715		47.59		47.59
	C43 H86 Cl N2 O2 S3	(M+H)+	MFG	13.542		793.5542		47.56		47.56

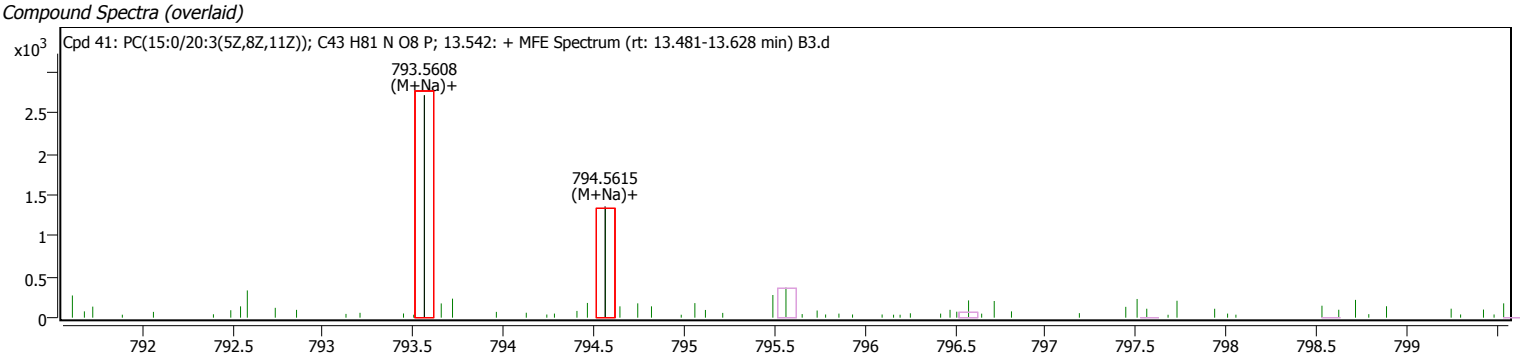
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 42: C28 H62 N15 O6

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C28 H62 N15 O6	13.576		704.5011		MFG	74.47	MFE	

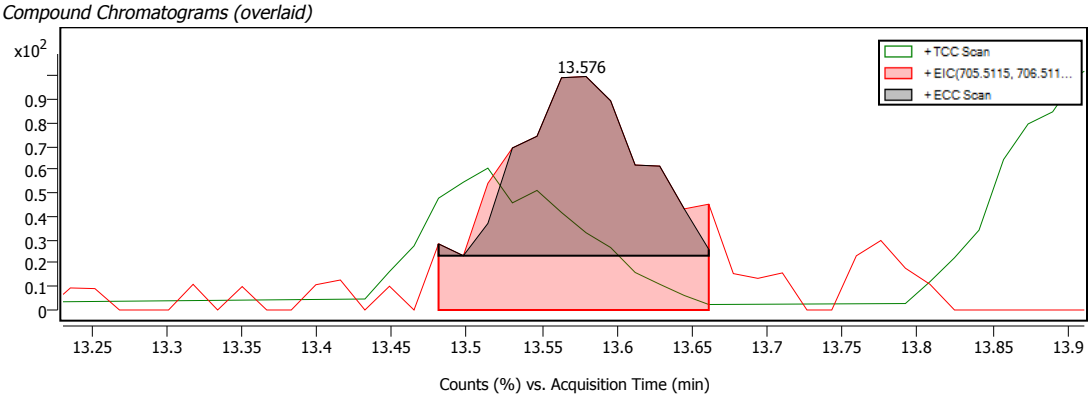
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	705.5082				7	74.47	

Compound ID Table

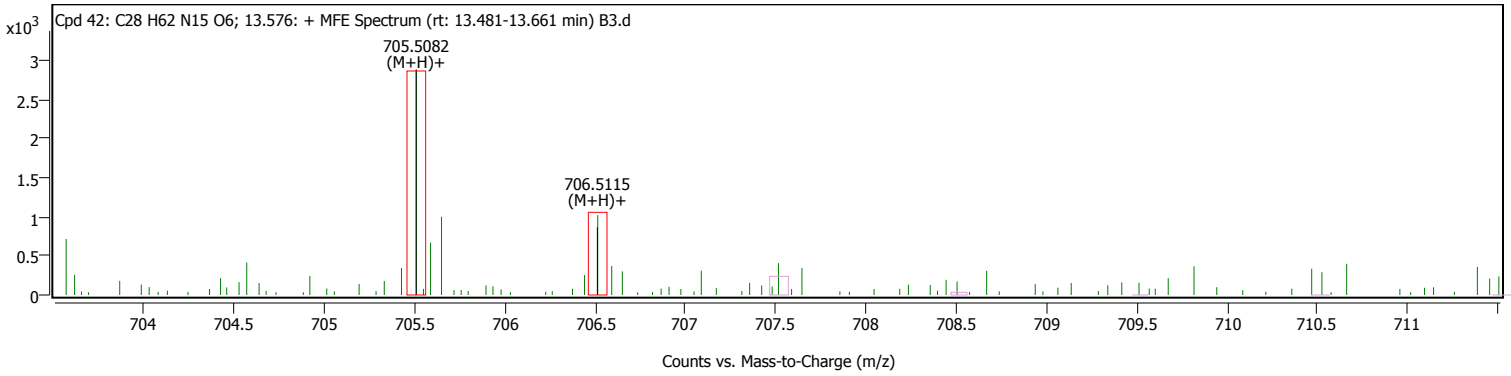
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C28 H62 N15 O6	(M+H)+	MFG	13.576		704.5011		74.47		74.47
	C27 H56 N22 O	(M+H)+	MFG	13.576		704.5012		74.05		74.05
	C30 H64 N12 O7	(M+H)+	MFG	13.576		704.5010		71.67		71.67
	C29 H58 N19 O2	(M+H)+	MFG	13.576		704.5011		71.58		71.58
	C25 H54 N25	(M+H)+	MFG	13.576		704.5012		71.49		71.49
PG(P-16:0/16:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.576		704.5009		64.99	64.99	
PG(P-18:0/14:1(9Z))	C38 H73 O9 P	(M+H)+	DBSearch	13.576		704.5009		64.99	64.99	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

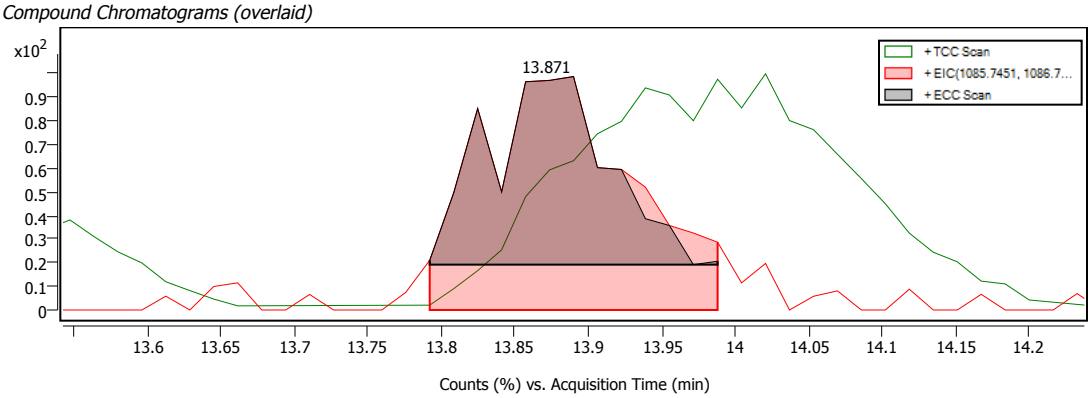


Cpd 43: 13.871

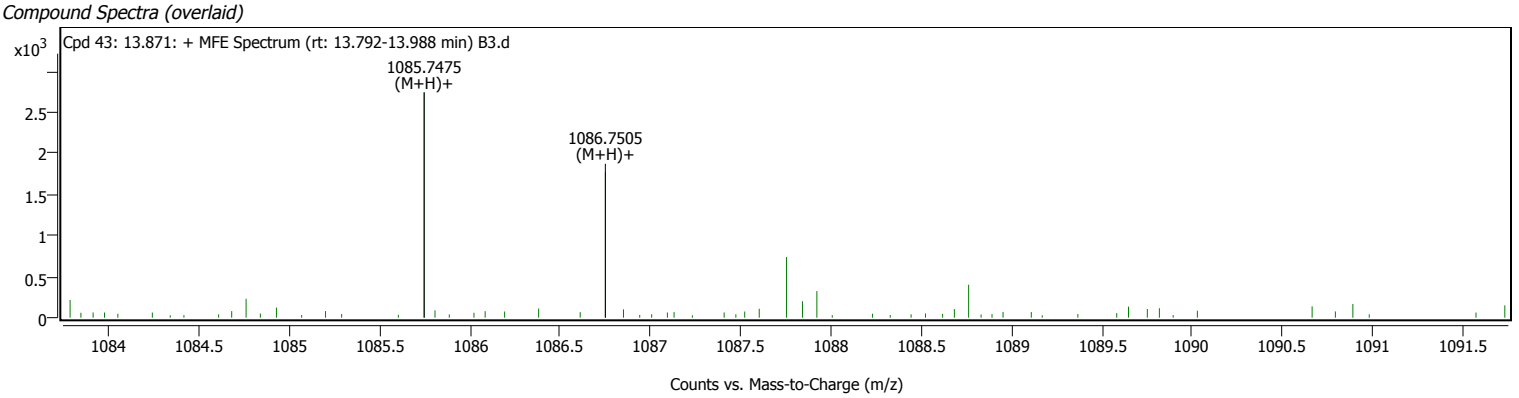
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.871		1084.7402				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

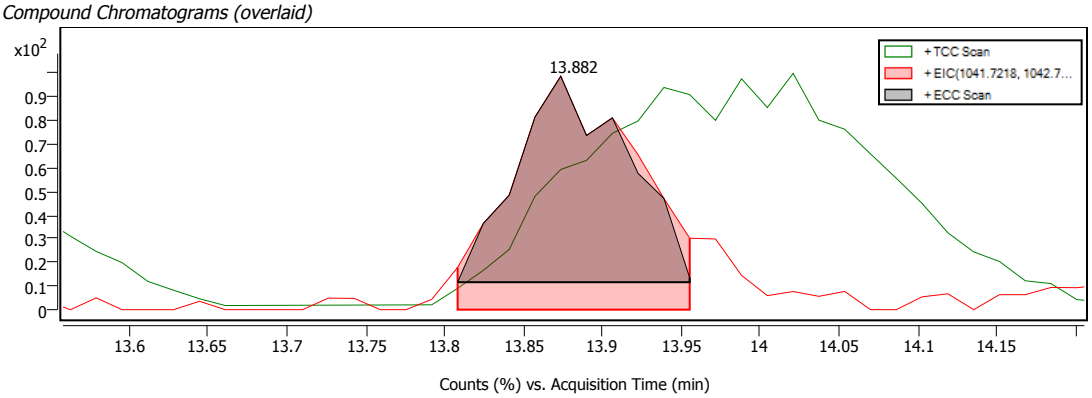


Cpd 44: 13.882

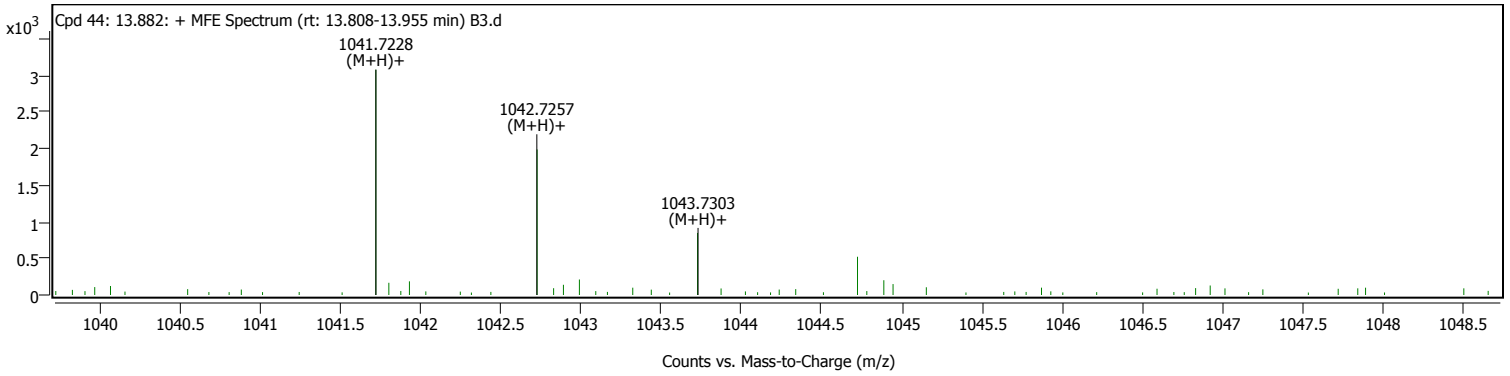
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		13.882		1040.7155				MFE	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 45: C55 H92 N6 O10

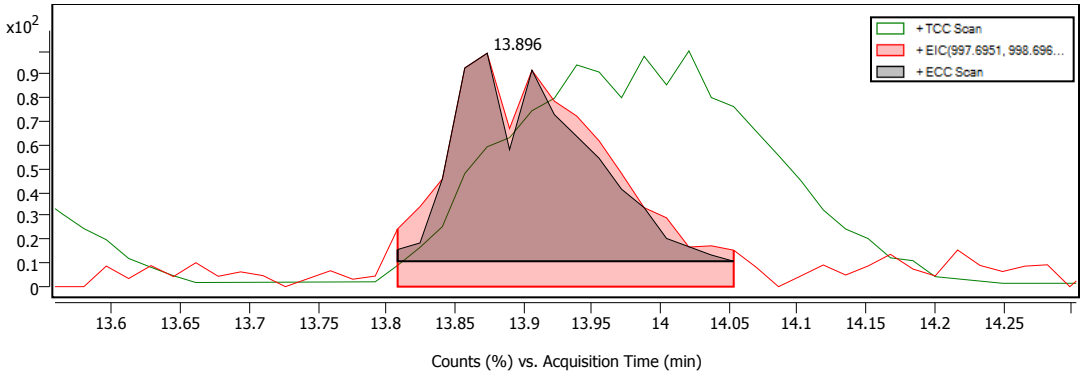
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C55 H92 N6 O10	13.896		996.6878		MFG	80.36	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	997.6929				5	80.36	

Compound ID Table

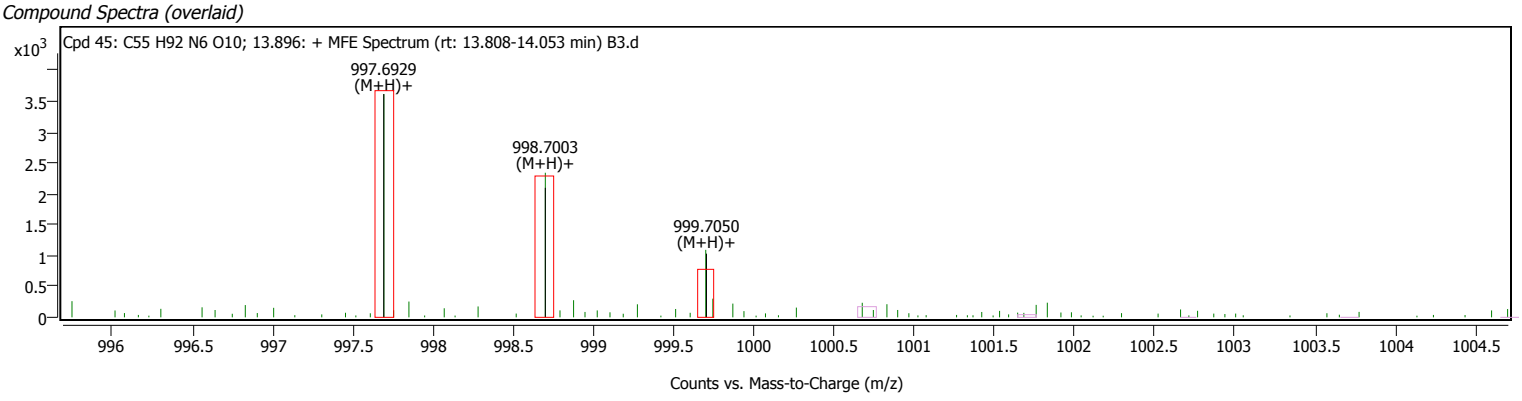
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C55 H92 N6 O10	(M+H)+	MFG	13.896		996.6878		80.36		80.36
	C49 H98 N5 O13 S	(M+H)+	MFG	13.896		996.6881		79.91		79.91
	C48 H92 N12 O8 S	(M+H)+	MFG	13.896		996.6883		79.31		79.31
	C54 H96 N2 O14	(M+H)+	MFG	13.896		996.6877		79.14		79.14
	C54 H86 N13 O5	(M+H)+	MFG	13.896		996.6880		78.66		78.66

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 46: C55 H90 N3 O10

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C55 H90 N3 O10	13.919		952.6630		MFG	94.88	MFE	

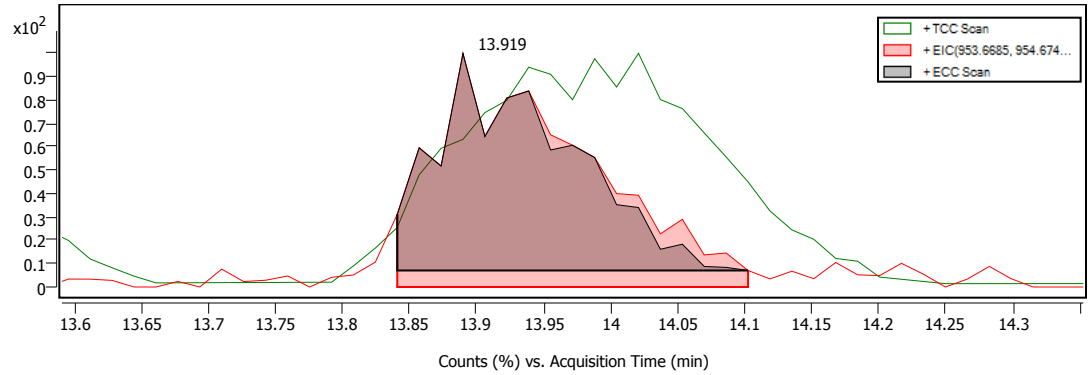
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	953.6698				5	94.88	

Compound ID Table

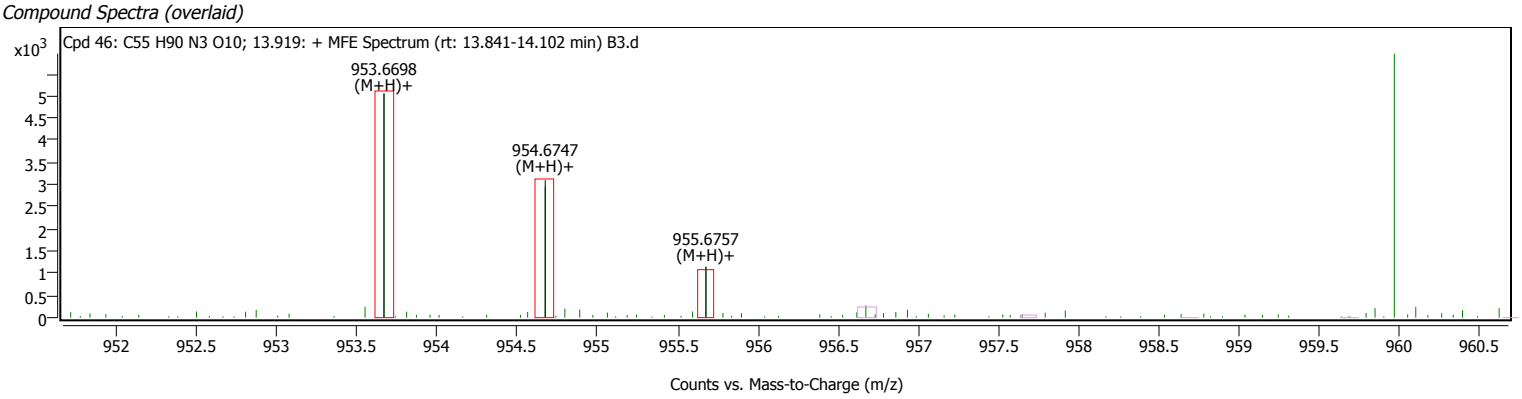
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C55 H90 N3 O10	(M+H)+	MFG	13.919		952.6630		94.88		94.88
	C54 H84 N10 O5	(M+H)+	MFG	13.919		952.6631		94.83		94.83
	C56 H86 N7 O6	(M+H)+	MFG	13.919		952.6631		94.43		94.43
	C53 H78 N17	(M+H)+	MFG	13.919		952.6633		94.38		94.38
	C55 H80 N14 O	(M+H)+	MFG	13.919		952.6632		94.37		94.37

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 47: C45 H88 N2 O11 S

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C45 H88 N2 O11 S	13.956		864.6104		MFG	88.79	MFE	

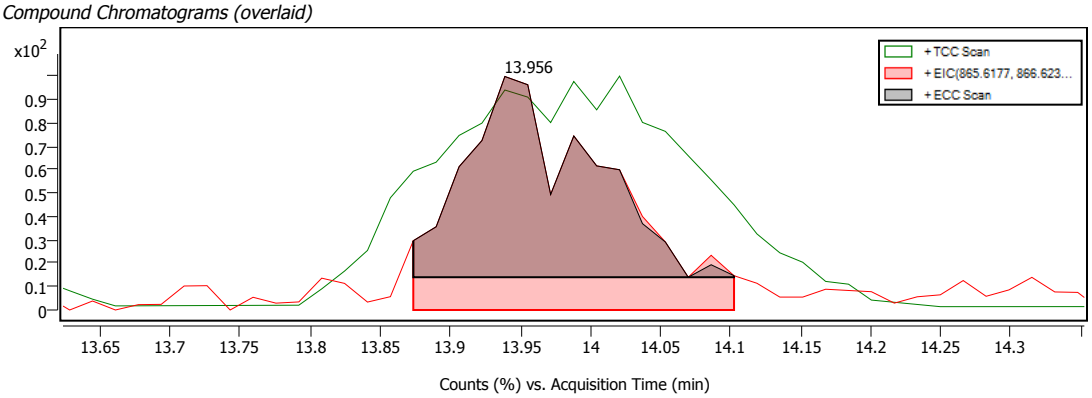
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	865.6174				10	88.79	

Compound ID Table

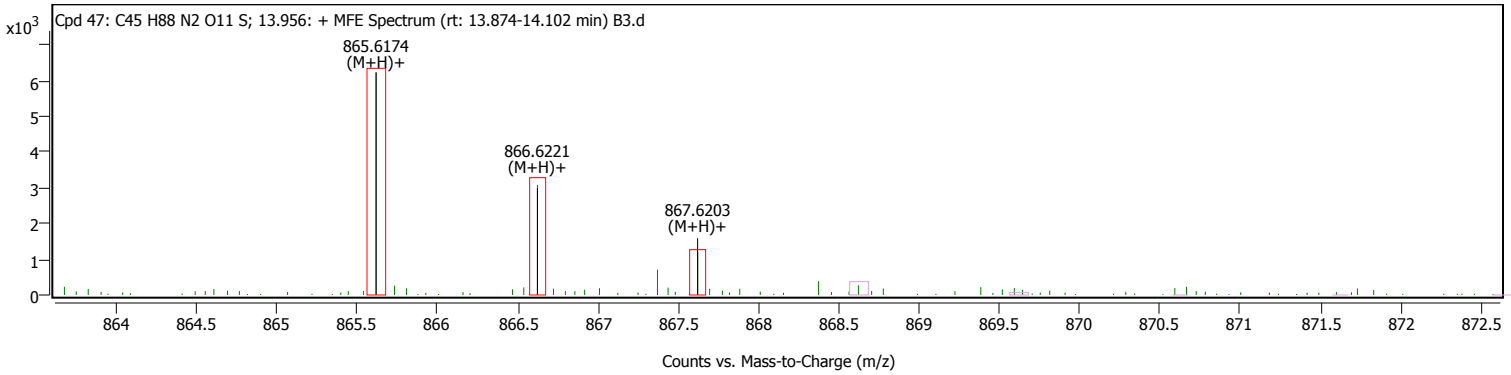
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C45 H88 N2 O11 S	(M+H)+	MFG	13.956		864.6104		88.79		88.79
	C43 H86 N5 O10 S	(M+H)+	MFG	13.956		864.6105		87.83		87.83
	C44 H82 N9 O6 S	(M+H)+	MFG	13.956		864.6106		87.75		87.75
	C44 H90 N5 O5 S3	(M+H)+	MFG	13.956		864.6109		87.31		87.31
	C52 H86 N3 O3 S2	(M+H)+	MFG	13.956		864.6106		87.04		87.04
PI(O-18:0/19:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.956		864.6100		81.61	81.61	
PI(O-20:0/17:1(9Z))	C46 H89 O12 P	(M+H)+	DBSearch	13.956		864.6100		81.61	81.61	
PI(P-16:0/21:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.956		864.6100		81.61	81.61	
PI(P-18:0/19:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.956		864.6100		81.61	81.61	
PI(P-20:0/17:0)	C46 H89 O12 P	(M+H)+	DBSearch	13.956		864.6100		81.61	81.61	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 48: C44 H80 N6 O6 S

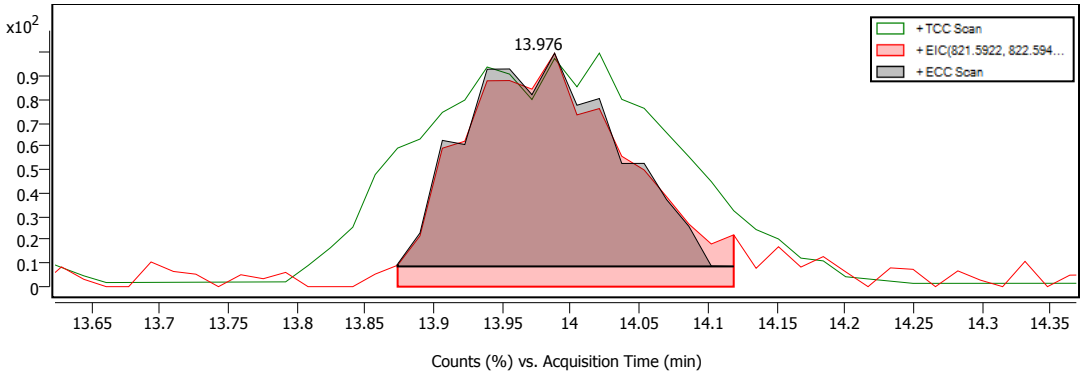
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H80 N6 O6 S	13.976		820.5860		MFG	93.50	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	821.5934				26	93.50	

Compound ID Table

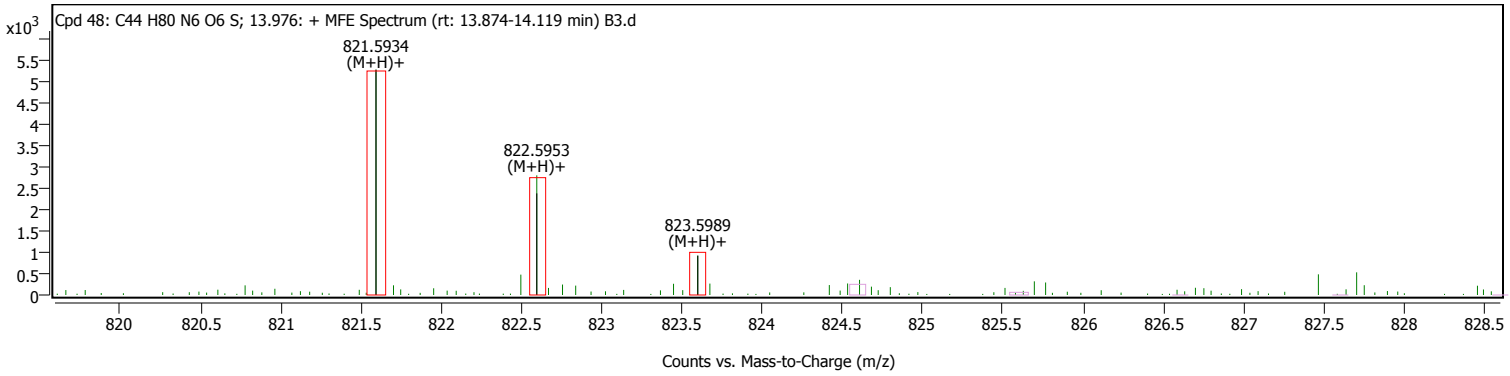
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H80 N6 O6 S	(M+H)+	MFG	13.976		820.5860		93.50		93.50
	C36 H76 N12 O9	(M+H)+	MFG	13.976		820.5859		93.36		93.36
	C43 H74 N13 O S	(M+H)+	MFG	13.976		820.5861		92.81		92.81
	C43 H84 N2 O10 S	(M+H)+	MFG	13.976		820.5859		92.60		92.60
	C35 H70 N19 O4	(M+H)+	MFG	13.976		820.5860		92.34		92.34
PC(17:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(19:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(20:5(5Z,8Z,11Z,14Z,17Z)/19:1(9Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(22:4(7Z,10Z,13Z,16Z)/17:2(9Z,12Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/17:0)	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C47 H83 N O8 P	(M+H)+	DBSearch	13.976		820.5856		92.10	92.10	
PC(18:3(9Z,12Z,15Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(18:3(6Z,9Z,12Z)/19:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(19:0/18:3(6Z,9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(20:3(8Z,11Z,14Z)/17:0)	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(22:2(13Z,16Z)/15:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(17:0/20:3(8Z,11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(15:1(9Z)/22:2(13Z,16Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(18:0/19:3(9Z,12Z,15Z))[U]	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(17:1(9Z)/20:2(11Z,14Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(19:0/18:3(9Z,12Z,15Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(19:1(9Z)/18:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(20:1(11Z)/17:2(9Z,12Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(20:2(11Z,14Z)/17:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(17:2(9Z,12Z)/20:1(11Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	
PC(18:2(9Z,12Z)/19:1(9Z))	C45 H85 N O8 P	(M+Na)+	DBSearch	13.976		798.6036		86.86	86.86	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 49: C36 H74 N9 O9

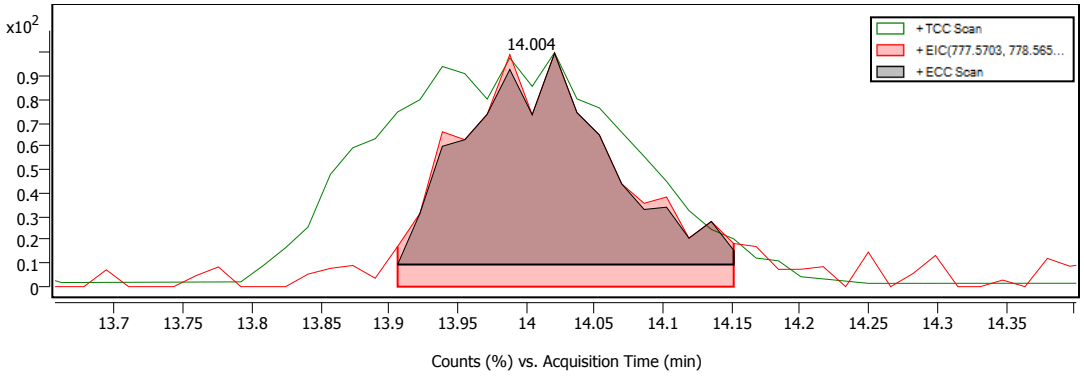
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C36 H74 N9 O9	14.004		776.5605		MFG	93.03	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	777.5681				5	93.03	

Compound ID Table

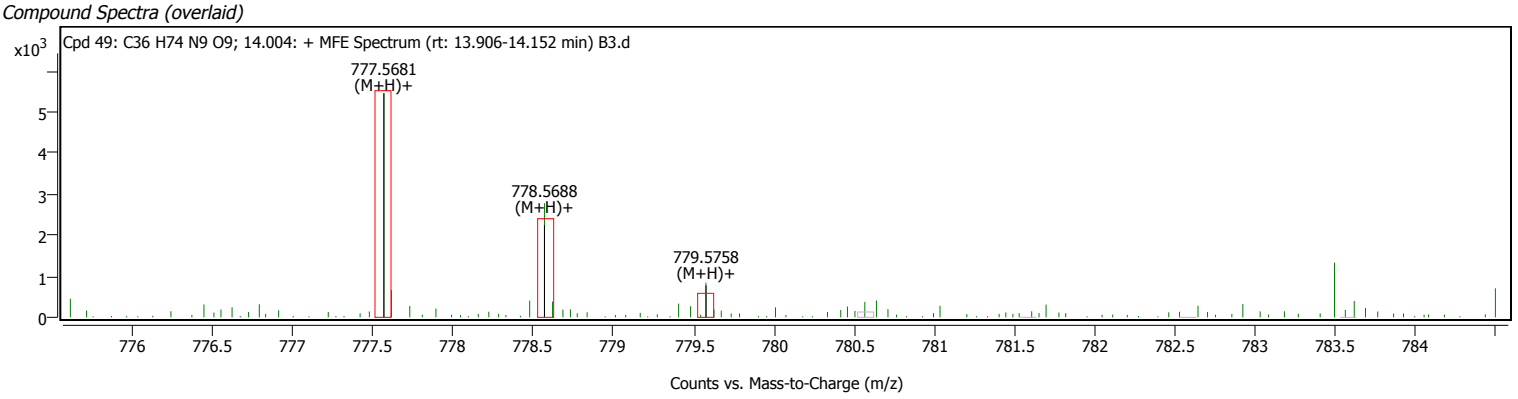
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C36 H74 N9 O9	(M+H)+	MFG	14.004		776.5605		93.03		93.03
	C34 H72 N12 O8	(M+H)+	MFG	14.004		776.5605		92.17		92.17
	C35 H68 N16 O4	(M+H)+	MFG	14.004		776.5606		91.90		91.90
	C33 H66 N19 O3	(M+H)+	MFG	14.004		776.5607		90.51		90.51
	C38 H76 N6 O10	(M+H)+	MFG	14.004		776.5604		89.11		89.11

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 50: C48 H68 N4 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C48 H68 N4 O2	14.030		732.5337		MFG	82.85	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	733.5404				9	82.85	

Compound Discovery Report

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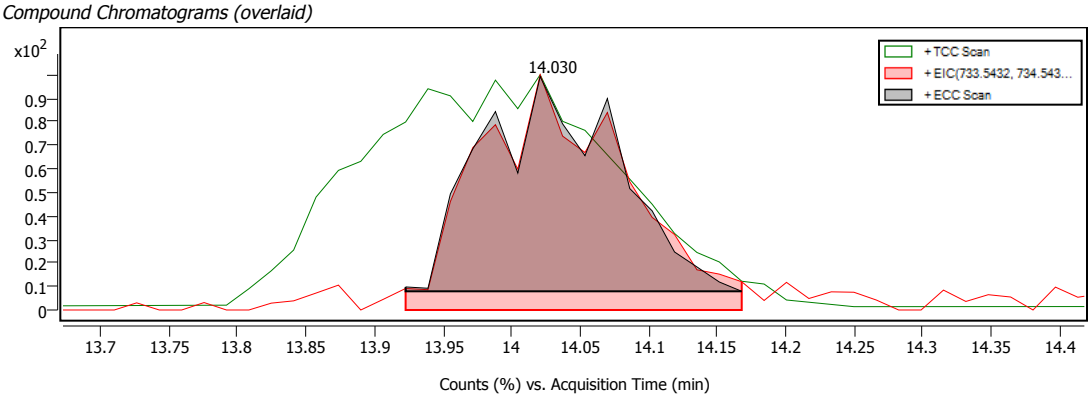
Compound ID Table

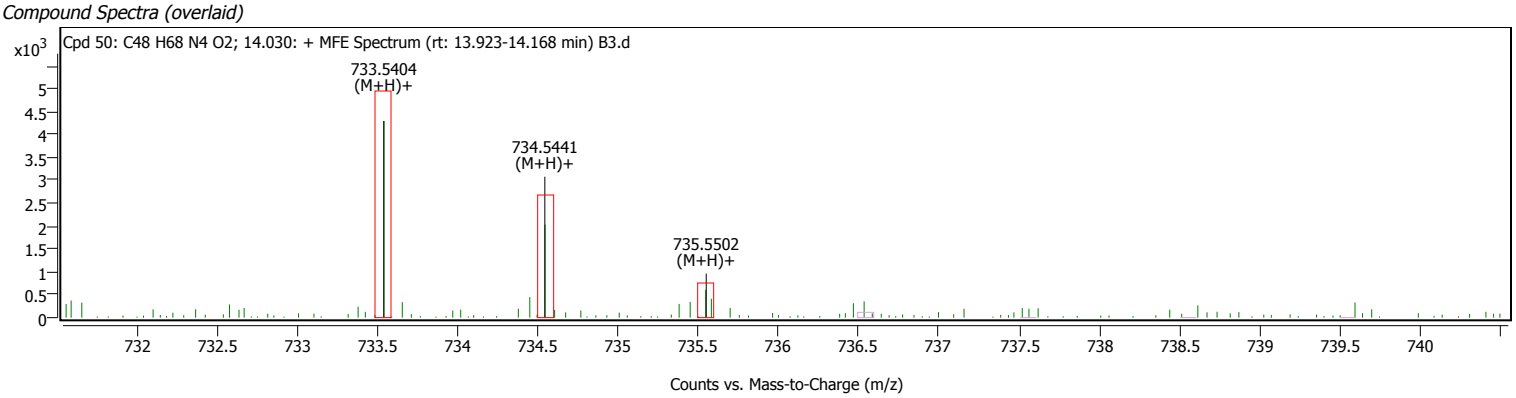
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C48 H68 N4 O2	(M+H)+	MFG	14.030		732.5337		82.85		82.85
	C46 H66 N7 O	(M+H)+	MFG	14.030		732.5338		80.73		80.73
	C47 H72 O6	(M+H)+	MFG	14.030		732.5336		80.28		80.28
	C50 H70 N O3	(M+H)+	MFG	14.030		732.5336		79.98		79.98
	C45 H70 N3 O5	(M+H)+	MFG	14.030		732.5337		74.06		74.06
PG(O-16:0/18:2(9Z,12Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.030		732.5336		63.25	63.25	
PG(P-18:0/16:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.030		732.5336		63.25	63.25	
PG(P-20:0/14:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.030		732.5336		63.25	63.25	
PG(P-16:0/18:1(9Z))	C40 H77 O9 P	(M+H)+	DBSearch	14.030		732.5336		63.25	63.25	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 51: C31 H68 N12 O S2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C31 H68 N12 O S2	14.049		688.5082		MFG	82.49	MFE	

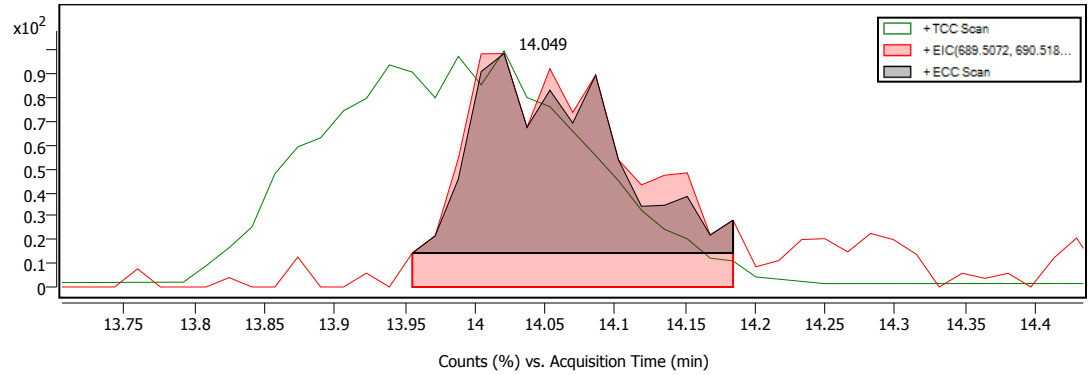
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	689.5141				52	82.49	

Compound ID Table

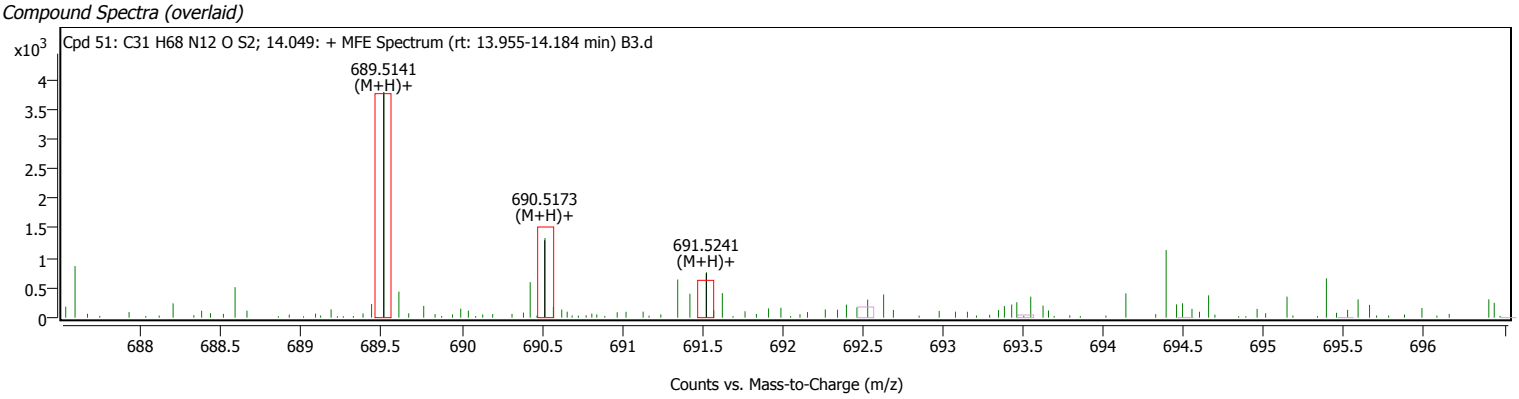
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C31 H68 N12 O S2	(M+H)+	MFG	14.049		688.5082		82.49		82.49
	C33 H70 N9 O2 S2	(M+H)+	MFG	14.049		688.5081		80.08		80.08
	C38 H76 N2 O2 S3	(M+H)+	MFG	14.049		688.5081		77.58		77.58
	C38 H68 N6 O3 S	(M+H)+	MFG	14.049		688.5078		76.95		76.95
	C30 H64 N12 O6	(M+H)+	MFG	14.049		688.5076		75.81		75.81
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(20:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C45 H68 O5	(M+H)+	DBSearch	14.049		688.5072		74.73	74.73	
PA(13:0/22:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(19:0/16:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(14:1(9Z)/21:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(17:0/18:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(21:0/14:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(20:1(11Z)/15:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(20:0/15:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(19:1(9Z)/16:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(17:1(9Z)/18:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(18:1(9Z)/17:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(15:0/20:1(11Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(16:1(9Z)/19:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(16:0/19:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(15:1(9Z)/20:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(18:0/17:1(9Z))	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
PA(22:1(11Z)/13:0)	C38 H73 O8 P	(M+H)+	DBSearch	14.049		688.5072		67.20	67.20	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(9Z,12Z,15Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(22:5(7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:2(9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:3(9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:3(8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:4(6Z,9Z,12Z,15Z)/22:3(10Z,13Z,16Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:2(9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:5(5Z,8Z,11Z,14Z,17Z)/20:2(11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:4(8Z,11Z,14Z,17Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(22:4(7Z,10Z,13Z,16Z)/18:3(6Z,9Z,12Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:2(11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	
DG(20:3(5Z,8Z,11Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	C43 H70 O5	(M+Na)+	DBSearch	14.049		666.5253		64.65	64.65	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 52: C44 H60 N4

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H60 N4	14.060		644.4811		MFG	64.28	MFE	

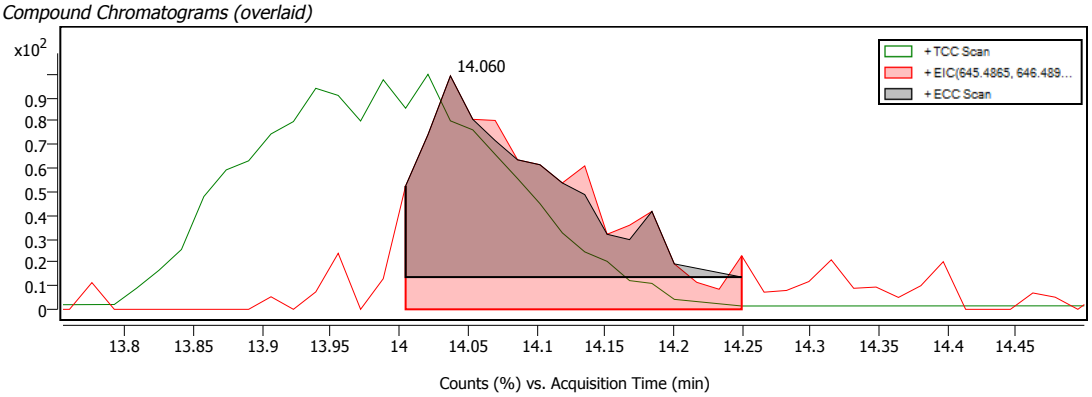
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	645.4880				8	64.28	

Compound ID Table

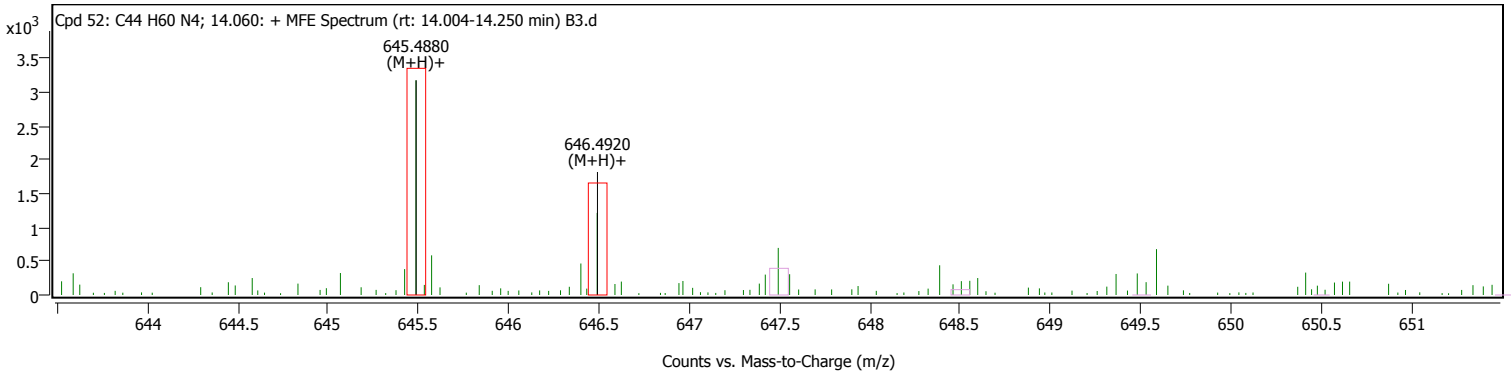
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H60 N4	(M+H)+	MFG	14.060		644.4811		64.28		64.28
	C43 H64 O4	(M+H)+	MFG	14.060		644.4810		63.81		63.81
	C36 H64 N6 O2 S	(M+H)+	MFG	14.060		644.4811		60.59		60.59
	C29 H56 N16 O	(M+H)+	MFG	14.060		644.4813		59.56		59.56
	C30 H62 N9 O6	(M+H)+	MFG	14.060		644.4812		58.87		58.87
PA(O-16:0/17:2(9Z,12Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.060		644.4810		50.73	50.73	
PA(P-16:0/17:1(9Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.060		644.4810		50.73	50.73	
PA(P-18:0/15:1(9Z))	C36 H69 O7 P	(M+H)+	DBSearch	14.060		644.4810		50.73	50.73	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 53: C27 H52 N16

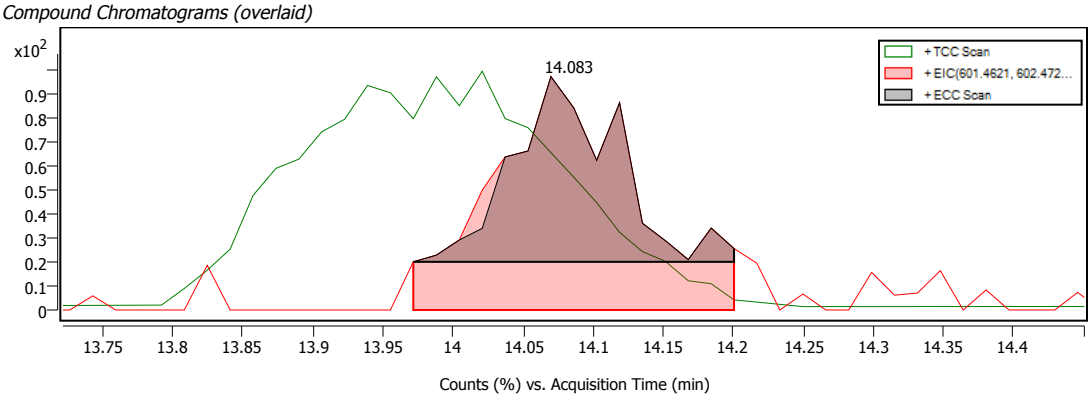
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C27 H52 N16	14.083		600.4560		MFG	67.94	MFE	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	601.4617				6	67.94	

Compound ID Table

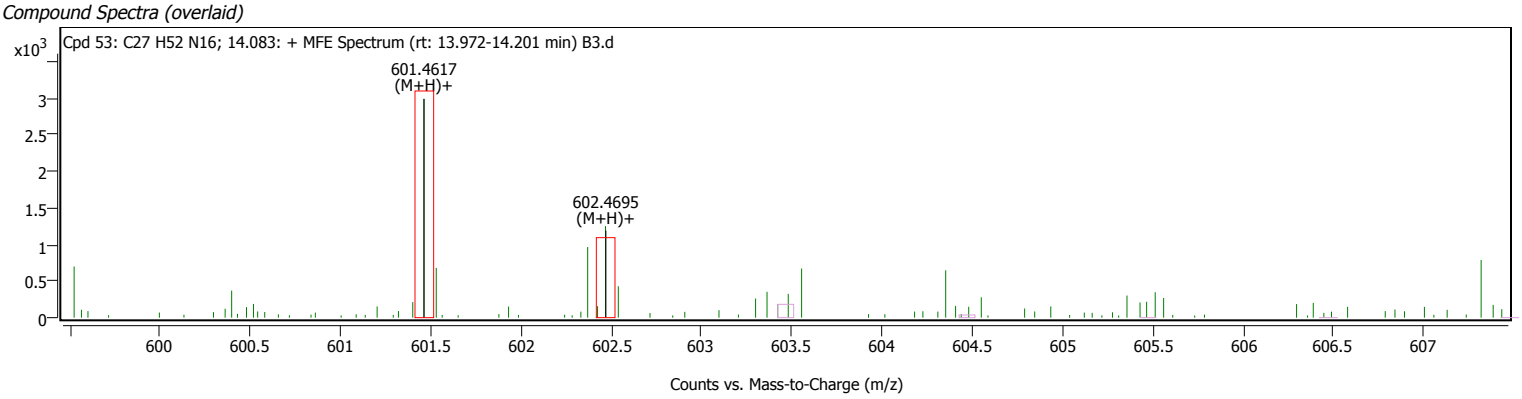
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C27 H52 N16	(M+H)+	MFG	14.083		600.4560		67.94		67.94
	C28 H58 N9 O5	(M+H)+	MFG	14.083		600.4558		65.70		65.70
	C29 H54 N13 O	(M+H)+	MFG	14.083		600.4559		64.41		64.41
	C26 H56 N12 O4	(M+H)+	MFG	14.083		600.4559		63.08		63.08
	C30 H60 N6 O6	(M+H)+	MFG	14.083		600.4558		61.85		61.85
OH-Spheroidenone	C41 H60 O3	(M+H)+	DBSearch	14.083		600.4557		61.80	61.80	

Compound Chromatograms (overlaid)



Structure

Compound Spectra (overlaid)



Cpd. 54: Germanicol cinnamate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Germanicol cinnamate	C39 H56 O2	14.105		556.4276	65883-48-9	DBSearch-MFG	60.54	MFE	

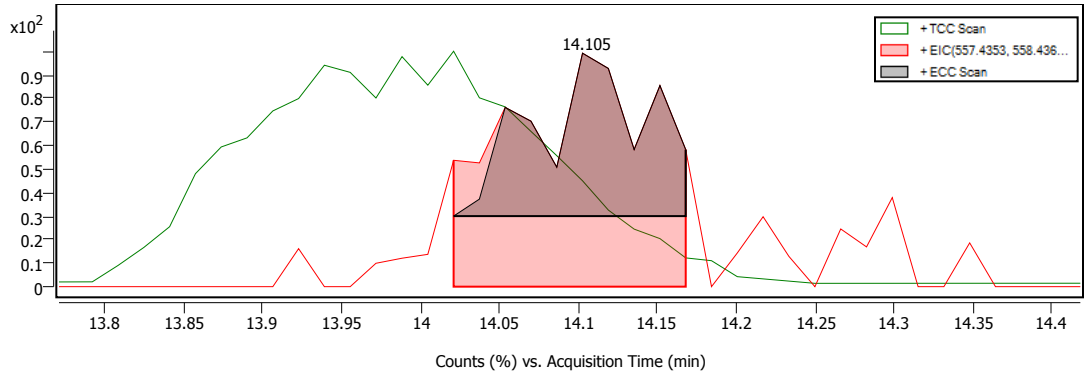
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	557.4359 557.4359 557.4359		0	60.32	5	60.77	

Compound Discovery Report

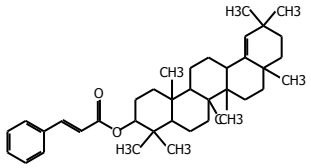
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Germanicol cinnamate	C39 H56 O2	(M+H)+	DBSearch-MFG	14.105		556.4276	65883-48-9	60.54	60.32	60.77
	C37 H54 N3 O	(M+H)+	MFG	14.105		556.4276		59.78		59.78
	C32 H56 N6 S	(M+H)+	MFG	14.105		556.4277		56.03		56.03
	C35 H52 N6	(M+H)+	MFG	14.105		556.4277		52.51		52.51
	C34 H58 N3 O S	(M+H)+	MFG	14.105		556.4277		48.08		48.08

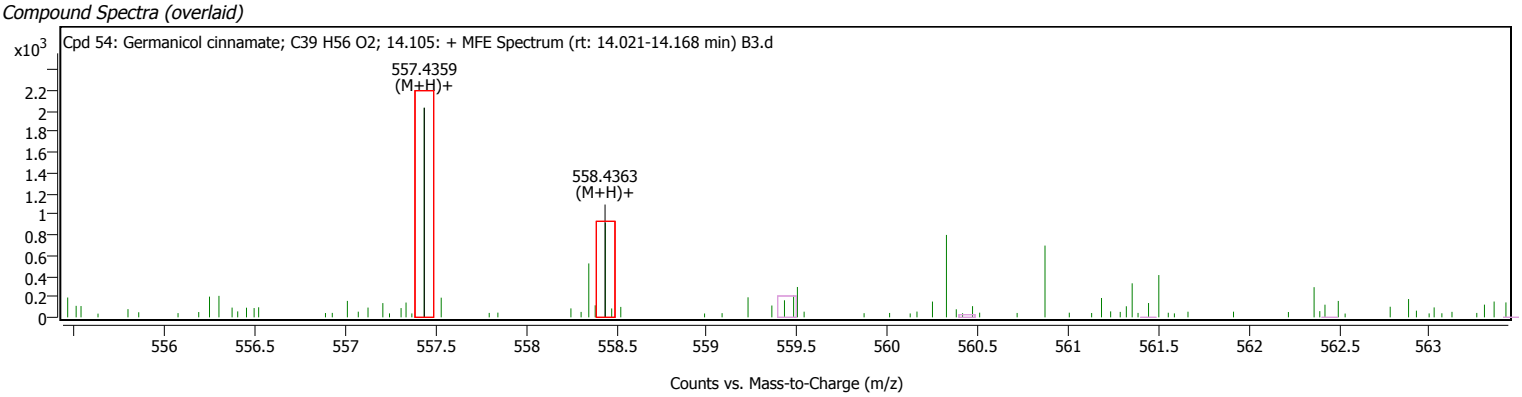
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



Cpd. 55: C44 H63 N6 O2

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
	C44 H63 N6 O2	15.443		707.5011		MFG	63.65	MFE	

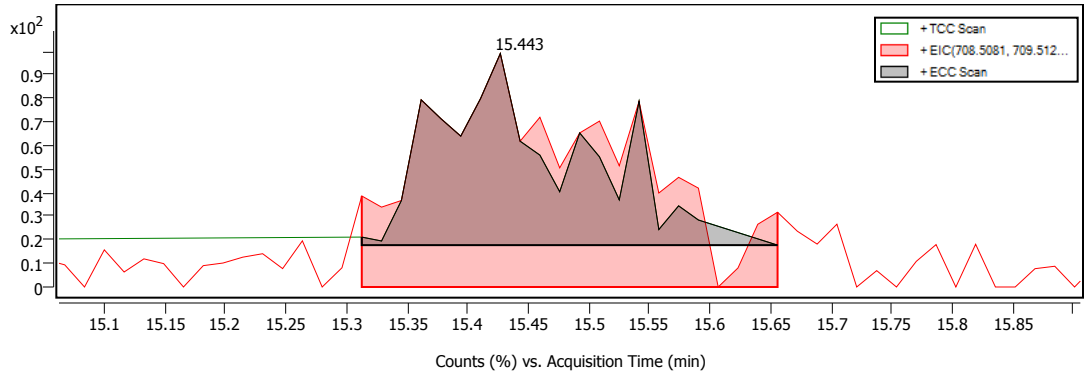
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
(M+H)+	708.5083				5	63.65	

Compound ID Table

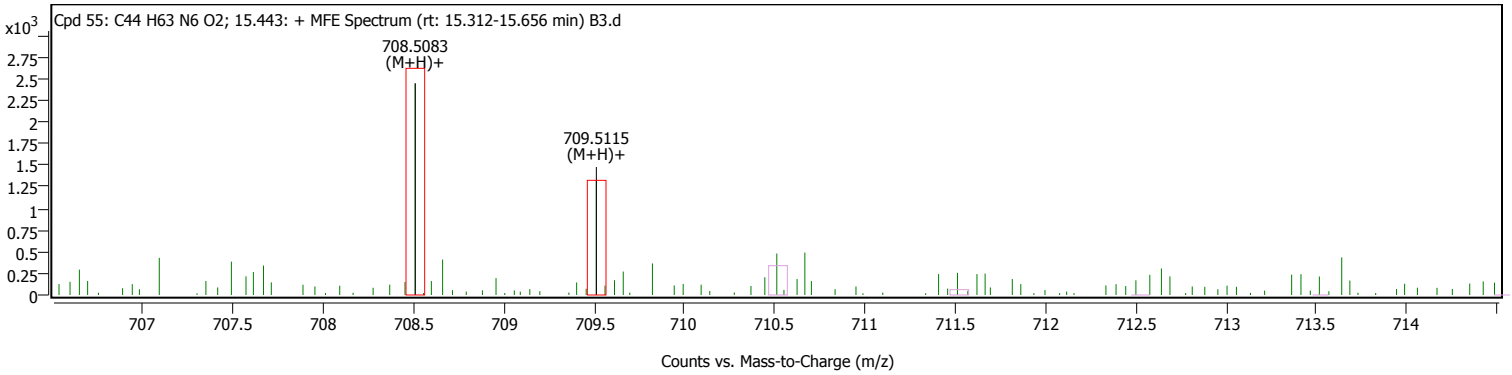
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
	C44 H63 N6 O2	(M+H)+	MFG	15.443		707.5011		63.65		63.65
	C42 H61 N9 O	(M+H)+	MFG	15.443		707.5011		61.86		61.86
	C43 H67 N2 O6	(M+H)+	MFG	15.443		707.5010		61.32		61.32
	C46 H65 N3 O3	(M+H)+	MFG	15.443		707.5010		60.31		60.31
	C37 H63 N12 S	(M+H)+	MFG	15.443		707.5012		60.18		60.18

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



MassHunter Qual 10.0
(End of Report)