Target Compound Screening Report

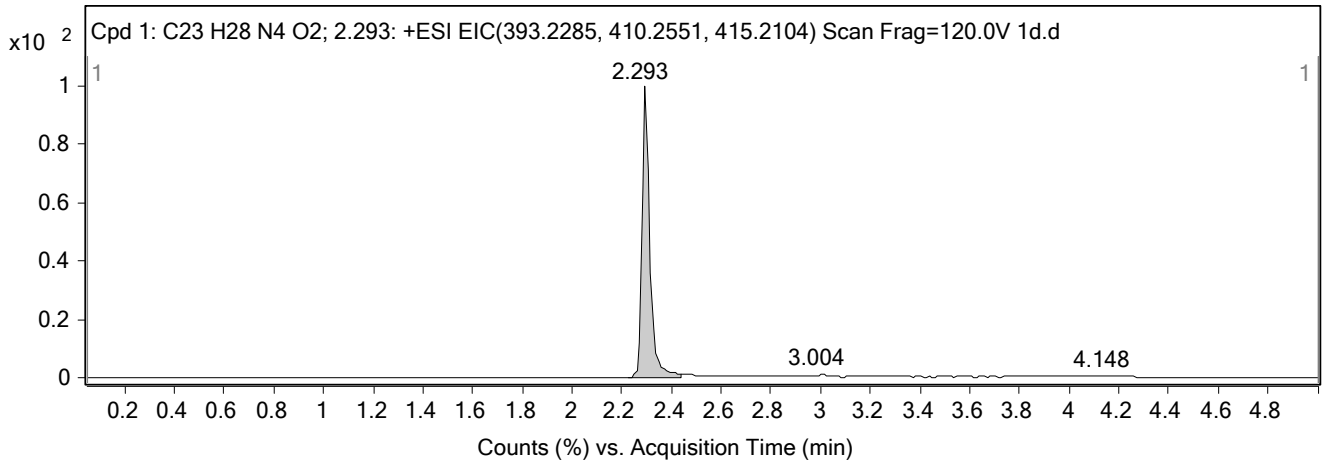
Data File	1d.d	**Sample Name**	H3475346
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:13:35 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H28N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:13:35 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H28 N4 O2; 2.293	92.3	-2.2	C23 H28 N4 O2	2.293	392.2212	392.2204

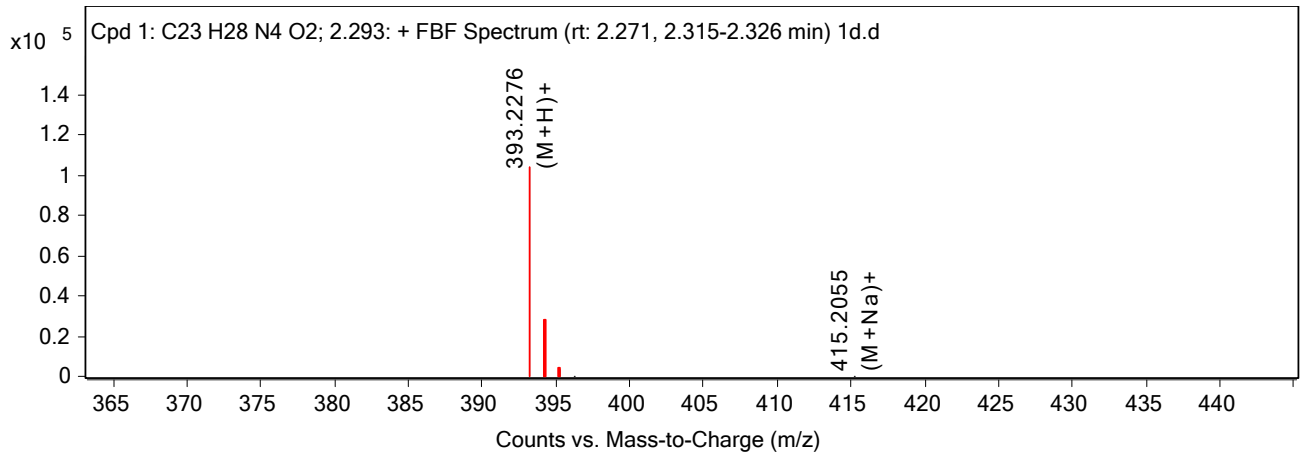
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
393.2276	2.293	392.2204	C23 H28 N4 O2	392.2212	-2.2	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

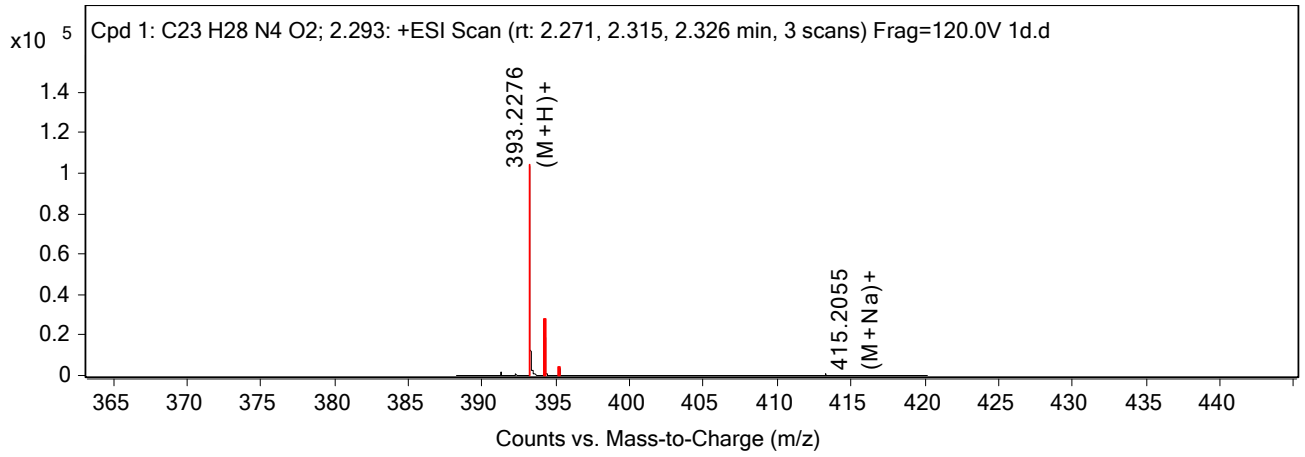
Agilent Technologies



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
393.2276	1	104005.23	(M+H)+
394.2306	1	21882.24	(M+H)+
395.2344	1	3139.41	(M+H)+
396.2407	1	366.21	(M+H)+
415.2055	1	137.82	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
393.2276	1	104005.24	(M+H)+	2.25
393.2276		104005.24		
394.2306	1	21882.24	(M+H)+	2.4
395.2344	1	3139.41	(M+H)+	-0.09
396.2407	1	366.21	(M+H)+	-9.15
415.2055	1	137.82	(M+Na)+	11.81

--- End Of Report ---

Target Compound Screening Report

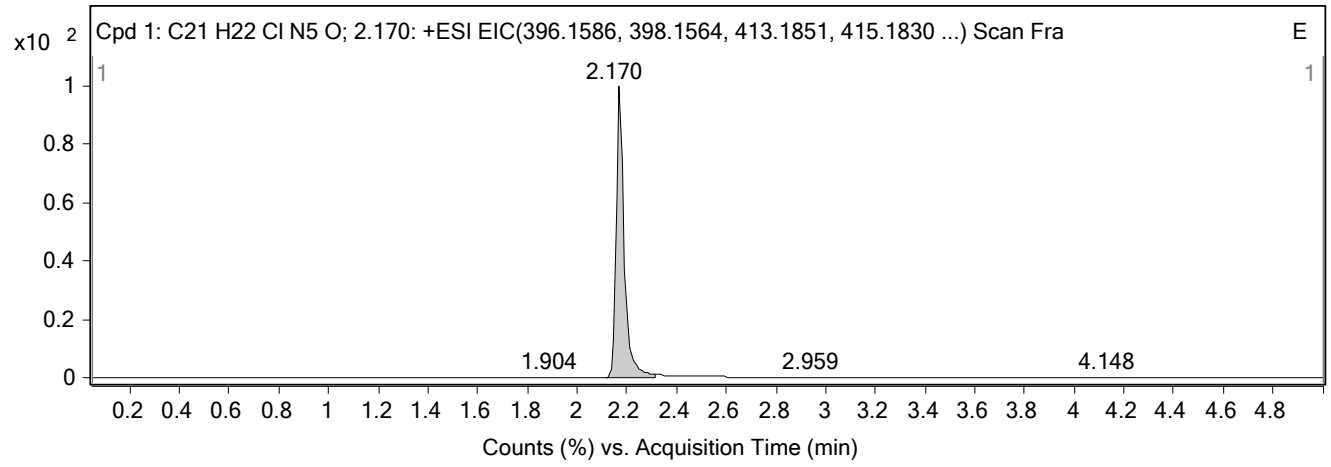
Data File	1-2.d	**Sample Name**	H1682149
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/27/2021 3:34:45 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H22ClN5O	**Stream Name**	LC 1
Acquisition Time (Local)	9/27/2021 3:34:45 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

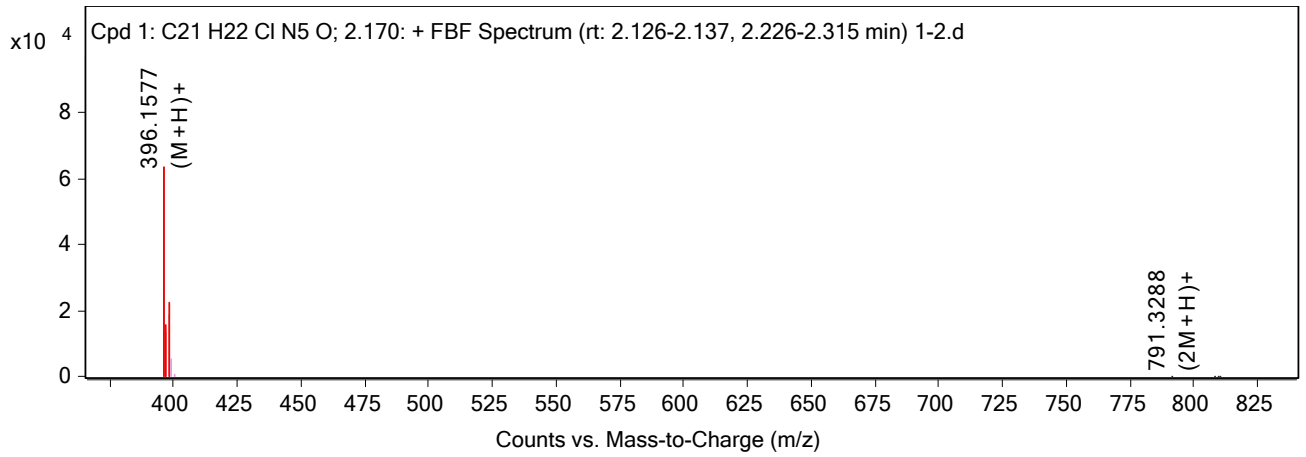
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H22 Cl N5 O; 2.170	88.55	-2.1	C21 H22 Cl N5 O	2.17	395.1513	395.1505

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
396.1577	2.17	395.1505	C21 H22 Cl N5 O	395.1513	-2.1	Find By Formula	

Compound Chromatograms



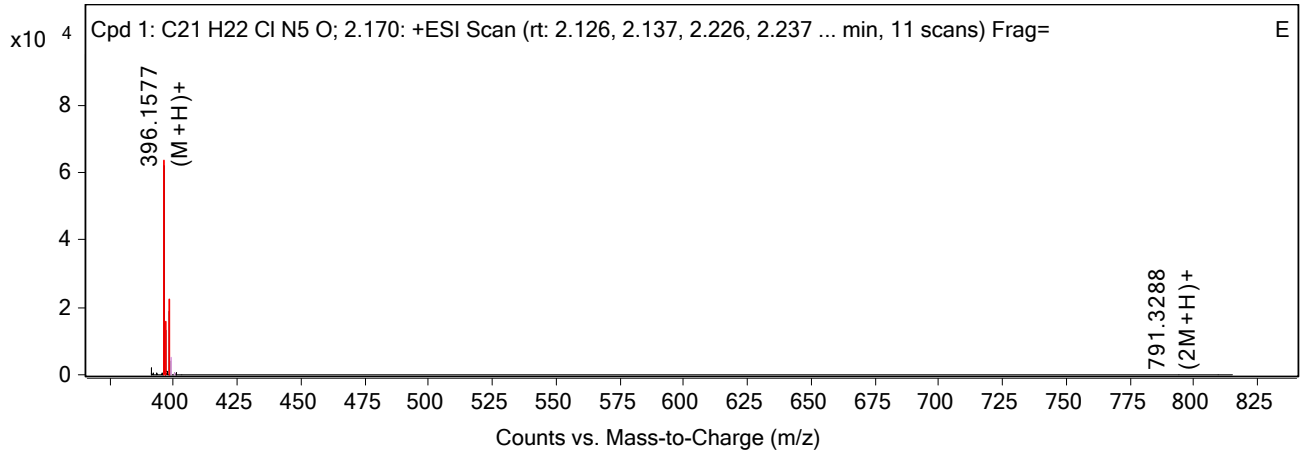
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
396.1577	1	63387.52	(M+H)+
397.1606	1	13470.55	(M+H)+
398.1555	1	19009.04	(M+H)+
791.3288	1	73.93	(2M+H)+
808.3489	1	70.82	(2M+NH4)+
809.3484	1	61.28	(2M+NH4)+
810.3558	1	64.69	(2M+NH4)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
396.1577	1	63387.52	(M+H)+	2.2
397.1606	1	13470.55	(M+H)+	2.25
398.1555	1	19009.05	(M+H)+	2.19
791.3288	1	73.93	(2M+H)+	-23.93
808.3489	1	70.82	(2M+NH4)+	-15.48
809.3484	1	61.28	(2M+NH4)+	-11.24
810.3558	1	64.69	(2M+NH4)+	-25.8

--- End Of Report ---

Target Compound Screening Report

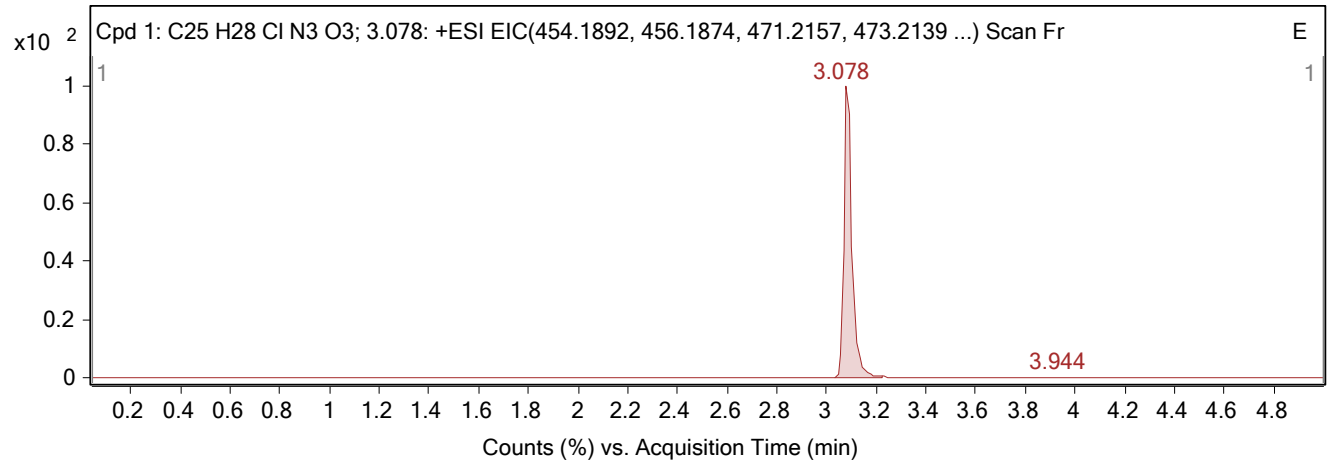
Data File	38.d	**Sample Name**	H1661315
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:42:07 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28ClN3O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:42:07 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 Cl N3 O3; 3.078	98.25	-1.51	C25 H28 Cl N3 O3	3.078	453.1819	453.1812

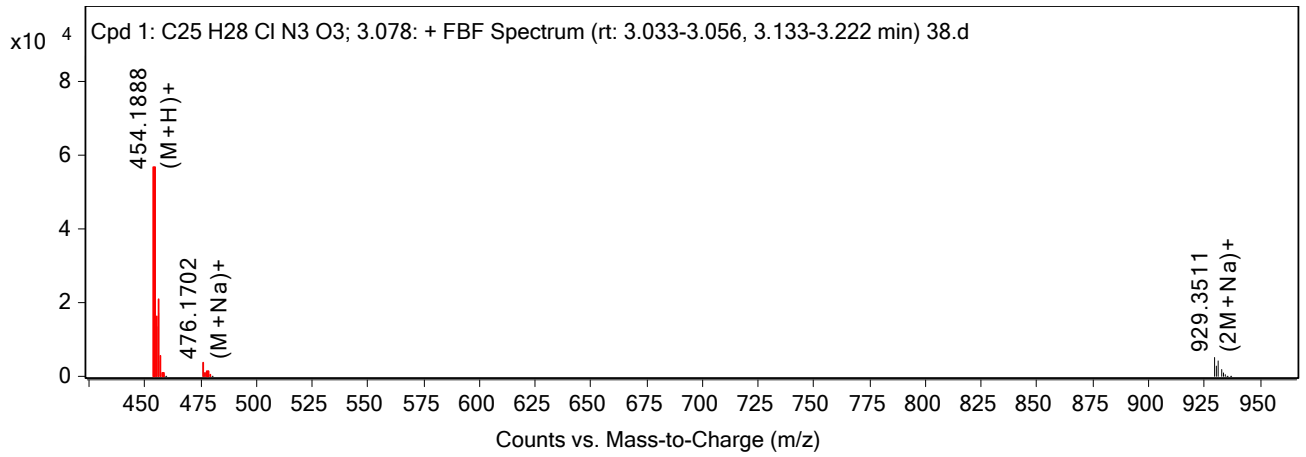
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
929.3511	3.078	453.1812	C25 H28 Cl N3 O3	453.1819	-1.51	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

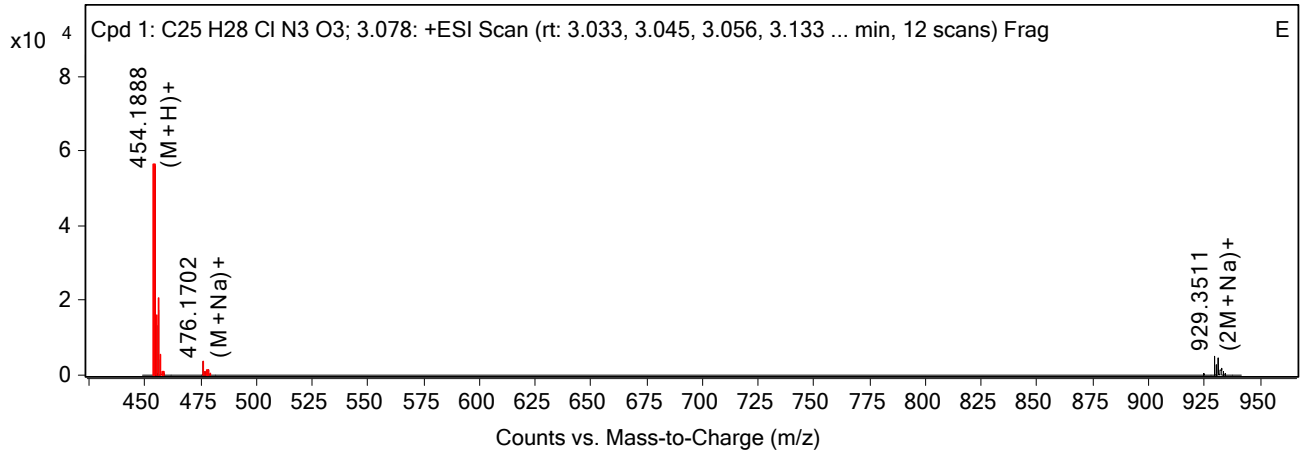
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
454.1888	1	56691.43	(M+H)+
455.1918	1	13385.82	(M+H)+
456.1866	1	17465.06	(M+H)+
457.1889	1	4220.61	(M+H)+
476.1702	1	3684.23	(M+Na)+
478.1689	1	1243.53	(M+Na)+
929.3511	1	5299.29	(2M+Na)+
930.3554	1	2960.56	(2M+Na)+
931.3509	1	4426.38	(2M+Na)+
932.3529	1	2082.41	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
454.1888	1	56691.44	(M+H)+	0.88
455.1918	1	13385.82	(M+H)+	1.21
456.1866	1	17465.06	(M+H)+	1.6
457.1889	1	4220.61	(M+H)+	2
476.1702	1	3684.23	(M+Na)+	1.98
478.1689	1	1243.53	(M+Na)+	0.94
929.3511	1	5299.29	(2M+Na)+	2.06
930.3554	1	2960.56	(2M+Na)+	0.89
931.3509	1	4426.38	(2M+Na)+	1.21
932.3529	1	2082.41	(2M+Na)+	1.22

--- End Of Report ---

Target Compound Screening Report

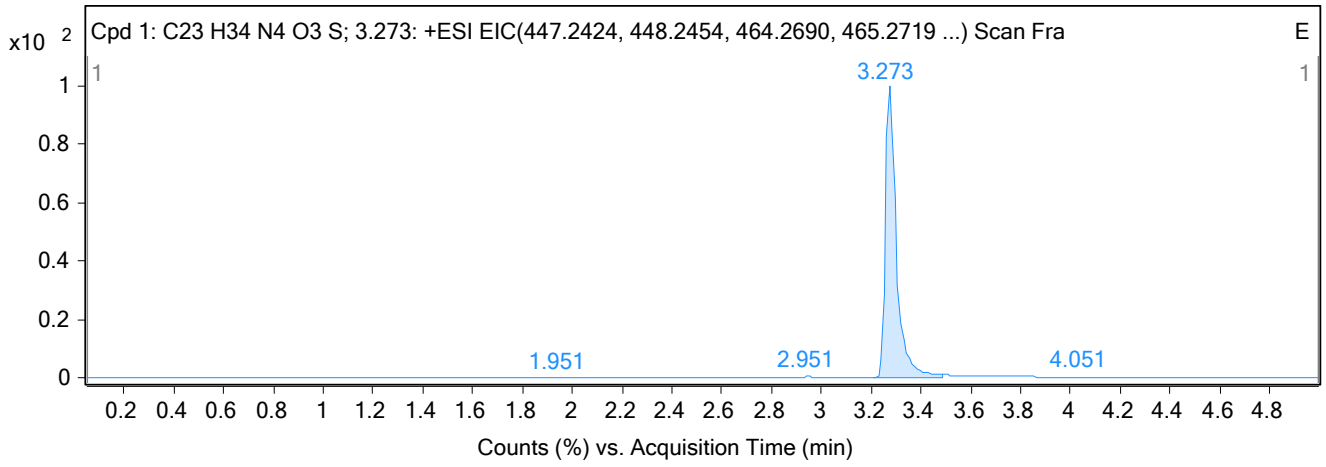
Data File	29.d	**Sample Name**	H1657343
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:52:08 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H34N4O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:52:08 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

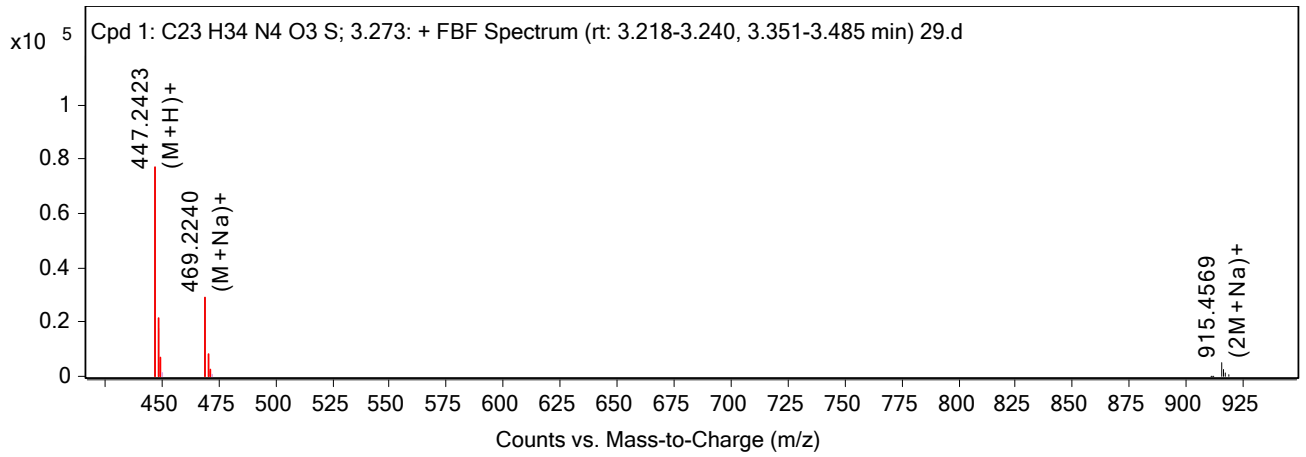
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H34 N4 O3 S; 3.273	97.6	-0.89	C23 H34 N4 O3 S	3.273	446.2352	446.2348

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
469.224	3.273	446.2348	C23 H34 N4 O3 S	446.2352	-0.89	Find By Formula	

Compound Chromatograms



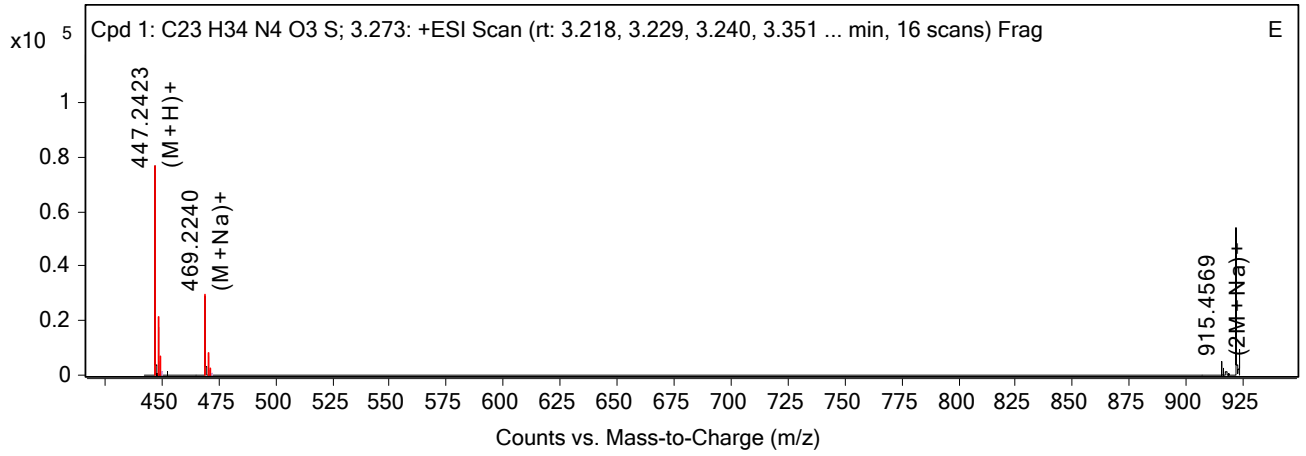
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2423	1	76902.98	(M+H)+
448.2451	1	17573.74	(M+H)+
449.2438	1	5033.54	(M+H)+
469.224	1	29269.54	(M+Na)+
470.2267	1	7093.01	(M+Na)+
471.2248	1	2186.25	(M+Na)+
915.4569	1	5167.22	(2M+Na)+
916.4596	1	2807.54	(2M+Na)+
917.459	1	1271.82	(2M+Na)+
918.4616	1	423.02	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2423	1	76902.98	(M+H)+	0.41
448.2451	1	17573.74	(M+H)+	0.59
449.2438	1	5033.54	(M+H)+	-1.64
469.224	1	29269.54	(M+Na)+	0.74
470.2267	1	7093.01	(M+Na)+	1.26
471.2248	1	2186.25	(M+Na)+	0.49
915.4569	1	5167.22	(2M+Na)+	2.85
916.4596	1	2807.54	(2M+Na)+	3.13
917.459	1	1271.82	(2M+Na)+	3.05
918.4616	1	423.02	(2M+Na)+	0.78

--- End Of Report ---

Target Compound Screening Report

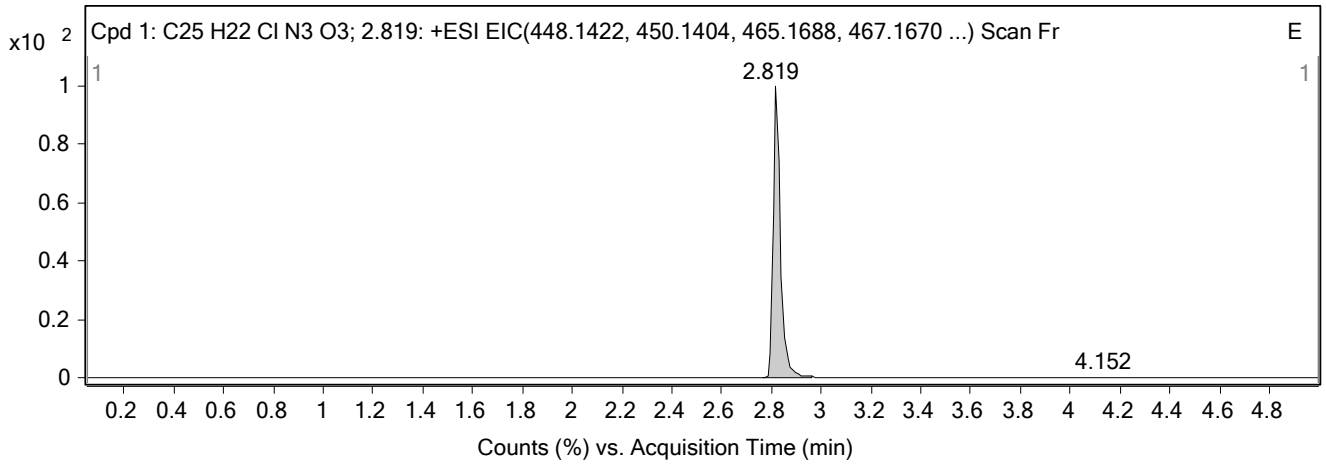
Data File	43.d	**Sample Name**	H1661310
Sample Type	Sample	**Position**	P1-E7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:09:53 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H22ClN3O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:09:53 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H22 Cl N3 O3; 2.819	95.45	-1.18	C25 H22 Cl N3 O3	2.819	447.135	447.1344

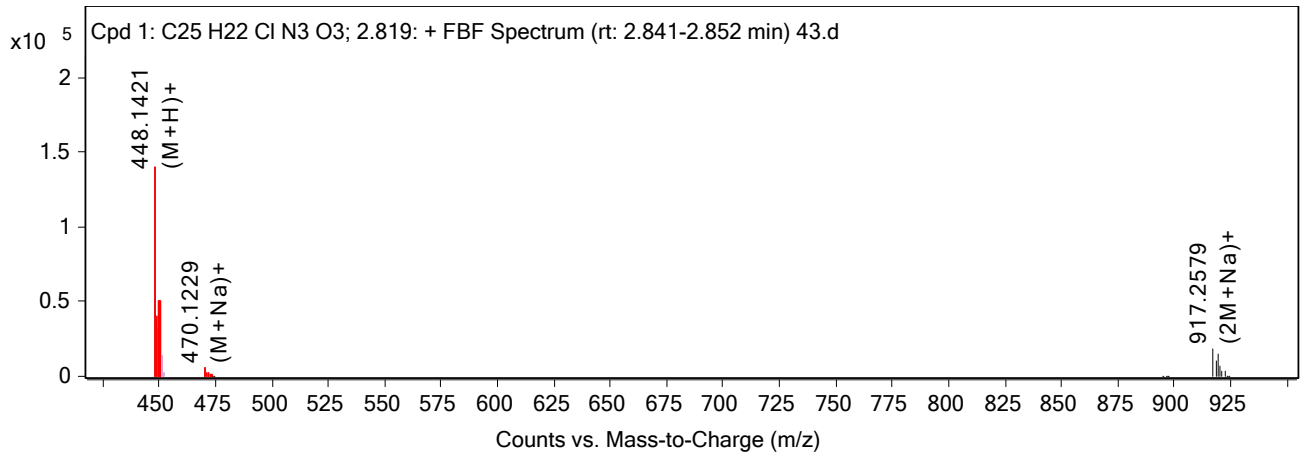
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
470.1229	2.819	447.1344	C25 H22 Cl N3 O3	447.135	-1.18	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

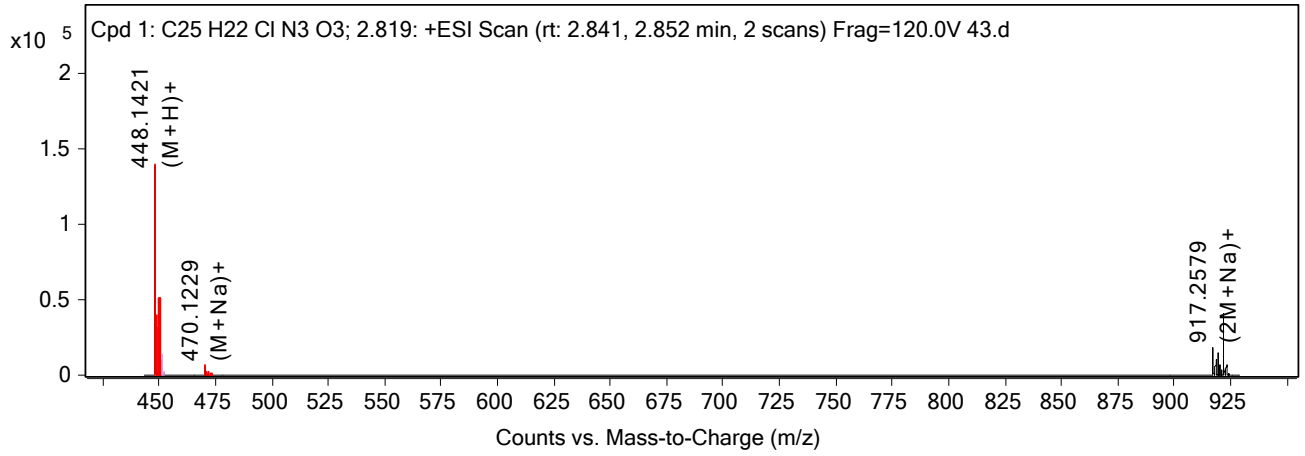
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
448.1421	1	139812.81	(M+H)+
449.1456	1	31859.01	(M+H)+
450.1405	1	40511.06	(M+H)+
470.1229	1	6258.92	(M+Na)+
917.2579	1	18521.58	(2M+Na)+
918.2601	1	10081.4	(2M+Na)+
919.2567	1	14537.28	(2M+Na)+
920.2583	1	6679.98	(2M+Na)+
921.2569	1	3461.63	(2M+Na)+
922.249	1	3013.06	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
448.1421	1	139812.82	(M+H)+	0.24
449.1456	1	31859.01	(M+H)+	-0.46
450.1405	1	40511.06	(M+H)+	-0.14
470.1229	1	6258.92	(M+Na)+	2.83
917.2579	1	18521.58	(2M+Na)+	1.42
918.2601	1	10081.4	(2M+Na)+	2.38
919.2567	1	14537.28	(2M+Na)+	1.57
920.2583	1	6679.98	(2M+Na)+	2.02
921.2569	1	3461.63	(2M+Na)+	1.49
922.249	1	3013.06	(2M+Na)+	10.94

--- End Of Report ---

Target Compound Screening Report

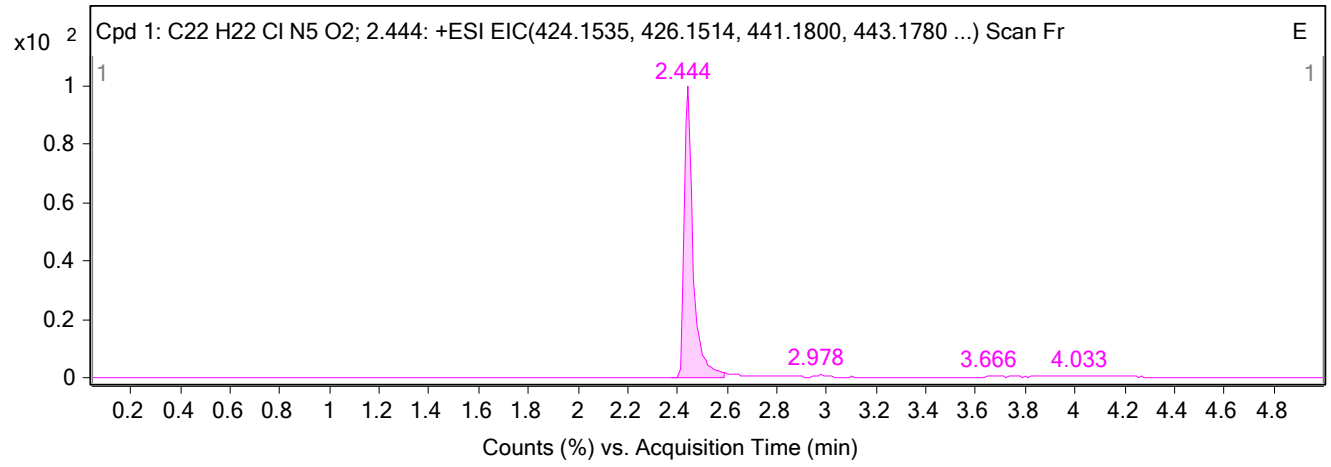
Data File	42.d	**Sample Name**	H1660424
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:04:20 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H22ClN5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:04:20 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

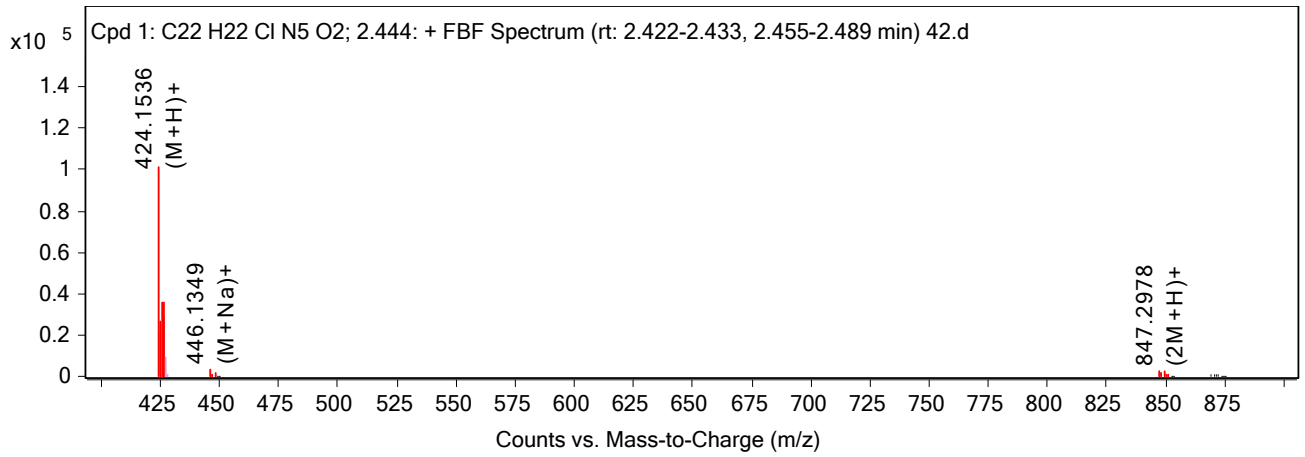
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H22 Cl N5 O2; 2.444	98.96	-0.2	C22 H22 Cl N5 O2	2.444	423.1462	423.1461

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
446.1349	2.444	423.1461	C22 H22 Cl N5 O2	423.1462	-0.2	Find By Formula	

Compound Chromatograms



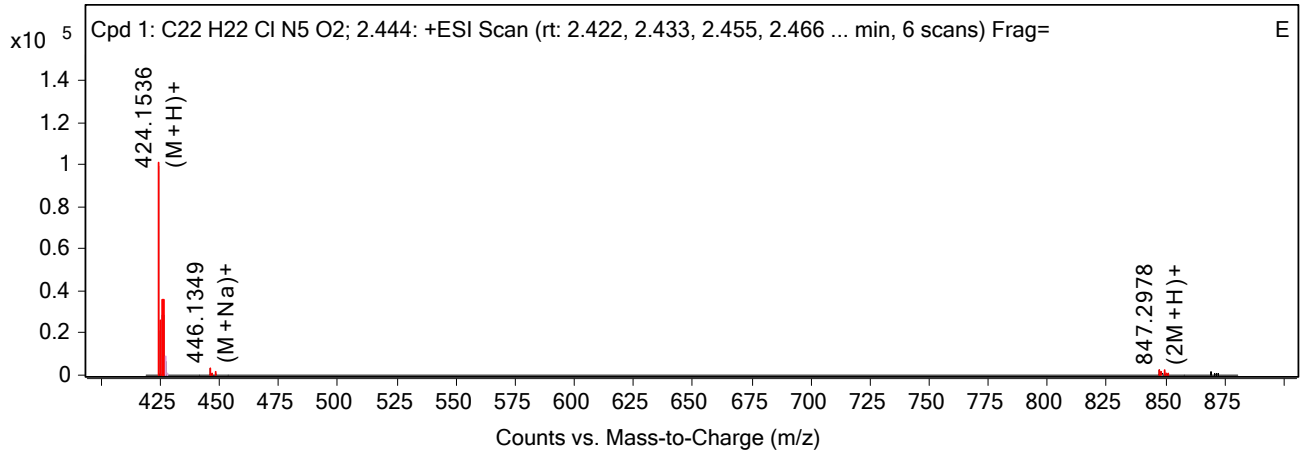
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
424.1536	1	100979.1	(M+H)+
425.1563	1	21348.81	(M+H)+
426.1514	1	29342.94	(M+H)+
446.1349	1	3525.93	(M+Na)+
448.1321	1	1187.77	(M+Na)+
847.2978	1	2807.32	(2M+H)+
848.3023	1	1451.27	(2M+H)+
849.2975	1	2021	(2M+H)+
869.2792	1	1281.22	(2M+Na)+
871.2787	1	979.23	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
424.1536	1	100979.1	(M+H)+	-0.19
425.1563	1	21348.81	(M+H)+	0.19
426.1514	1	29342.94	(M+H)+	-0.08
446.1349	1	3525.93	(M+Na)+	1.2
448.1321	1	1187.77	(M+Na)+	2.8
847.2978	1	2807.32	(2M+H)+	2.27
848.3023	1	1451.27	(2M+H)+	0.43
849.2975	1	2021	(2M+H)+	0.98
869.2792	1	1281.22	(2M+Na)+	2.77
871.2787	1	979.23	(2M+Na)+	1.81

--- End Of Report ---

Target Compound Screening Report

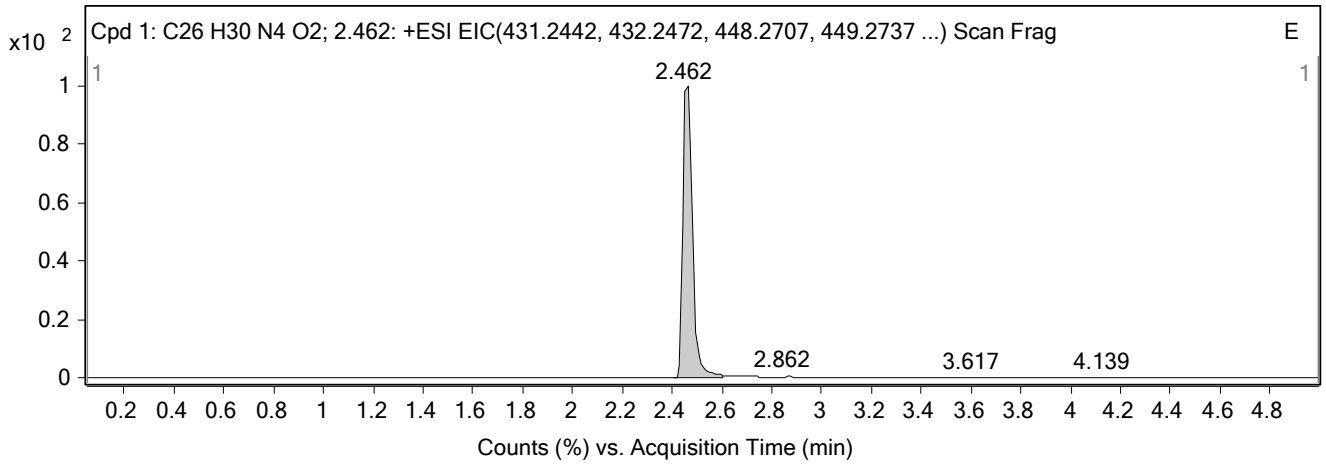
Data File	11.d	**Sample Name**	H3472156
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 6:35:19 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 6:35:19 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

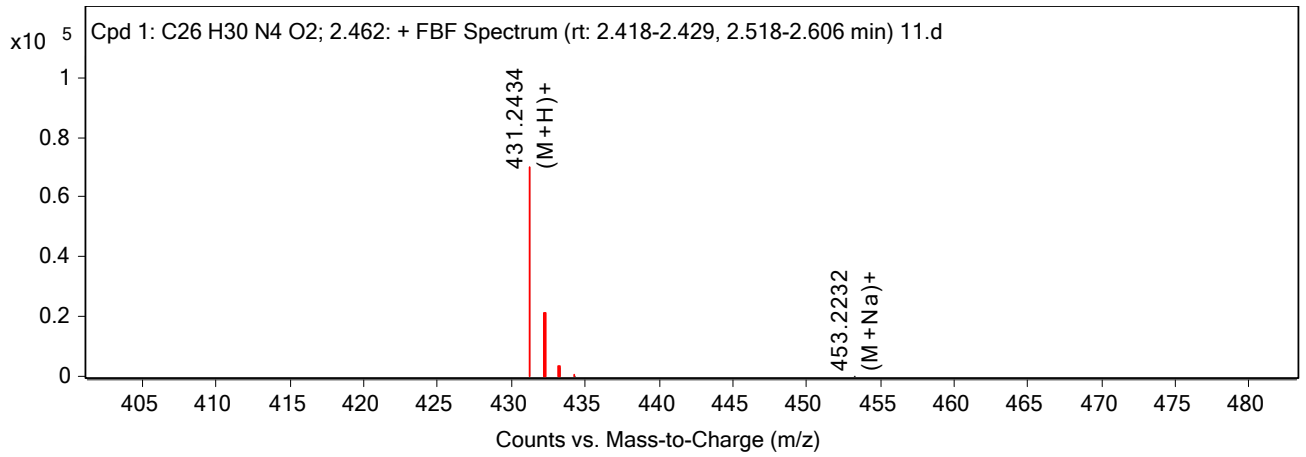
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O2; 2.462	95.67	-1.8	C26 H30 N4 O2	2.462	430.2369	430.2361

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
431.2434	2.462	430.2361	C26 H30 N4 O2	430.2369	-1.8	Find By Formula	

Compound Chromatograms



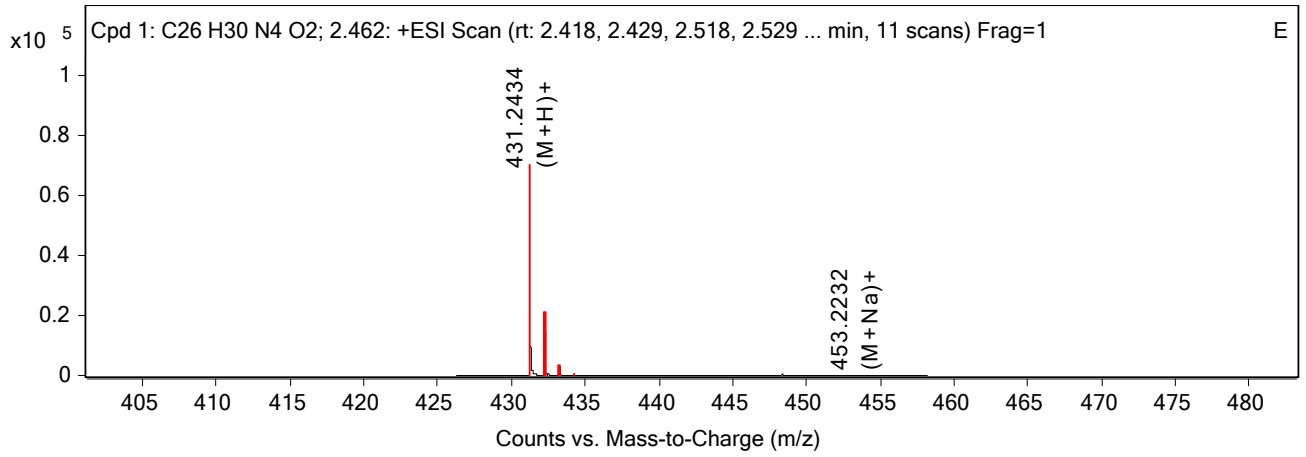
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
431.2434	1	69930.02	(M+H)+
432.2464	1	18001.77	(M+H)+
433.249	1	2654.52	(M+H)+
434.2493	1	306.15	(M+H)+
453.2232	1	132.72	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
431.2434	1	69930.02	(M+H)+	1.69
432.2464	1	18001.77	(M+H)+	1.91
433.249	1	2654.52	(M+H)+	2.68
434.2493	1	306.15	(M+H)+	8.43
453.2232	1	132.72	(M+Na)+	6.43

--- End Of Report ---

Target Compound Screening Report

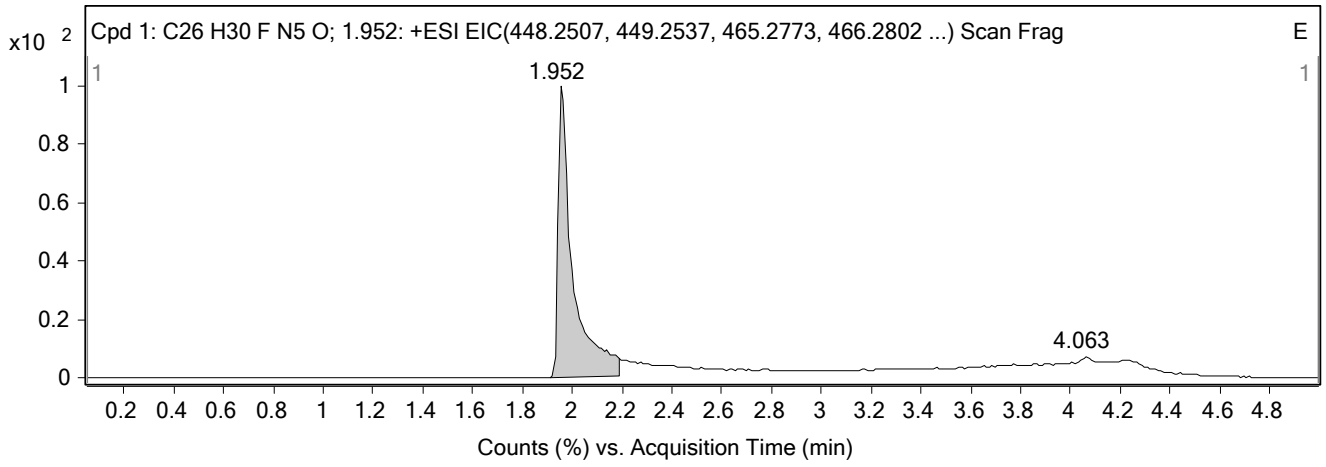
Data File	22.d	**Sample Name**	H1666494
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:13:15 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30FN5O	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:13:15 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

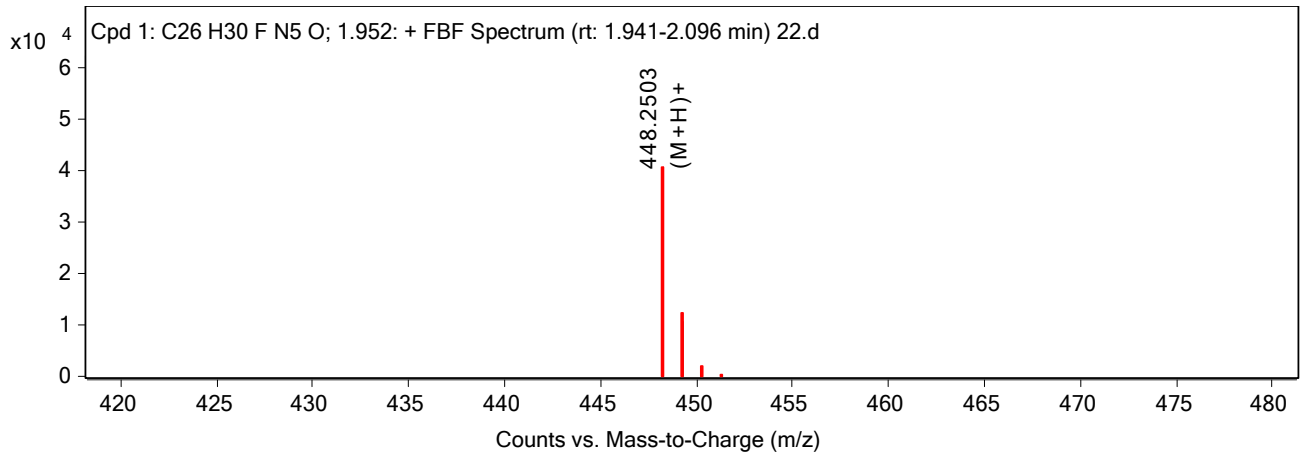
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 F N5 O; 1.952	97.05	-0.96	C26 H30 F N5 O	1.952	447.2434	447.243

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
448.2503	1.952	447.243	C26 H30 F N5 O	447.2434	-0.96	Find By Formula	

Compound Chromatograms



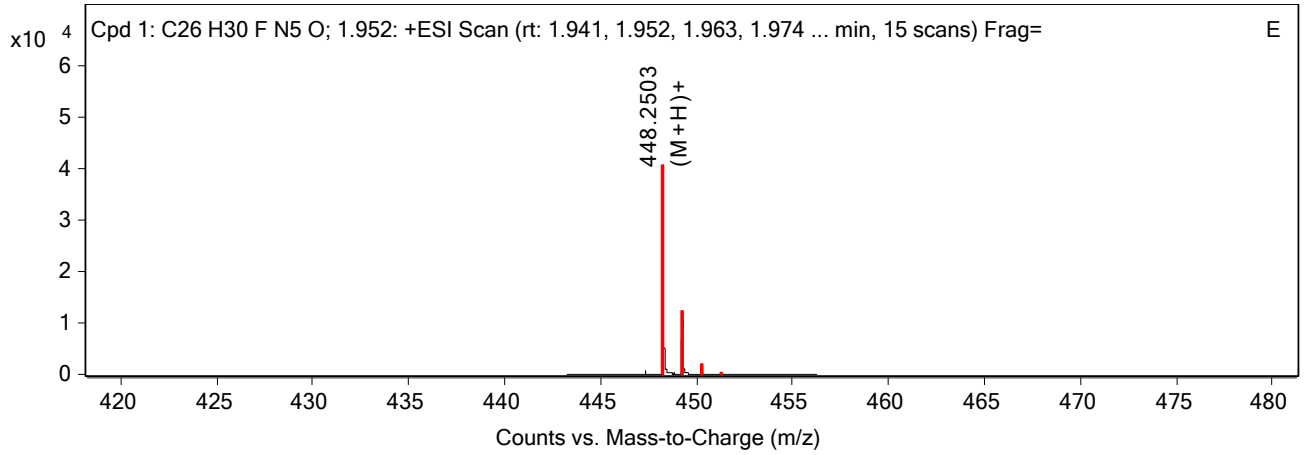
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
448.2503	1	40752.52	(M+H)+
449.2532	1	10668.18	(M+H)+
450.2559	1	1490.55	(M+H)+
451.2574	1	165.26	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
448.2503	1	40752.52	(M+H)+	0.86
448.2503		40752.52		
449.2532	1	10668.18	(M+H)+	1.19
450.2559	1	1490.55	(M+H)+	1.65
451.2574	1	165.26	(M+H)+	4.55

--- End Of Report ---

Target Compound Screening Report

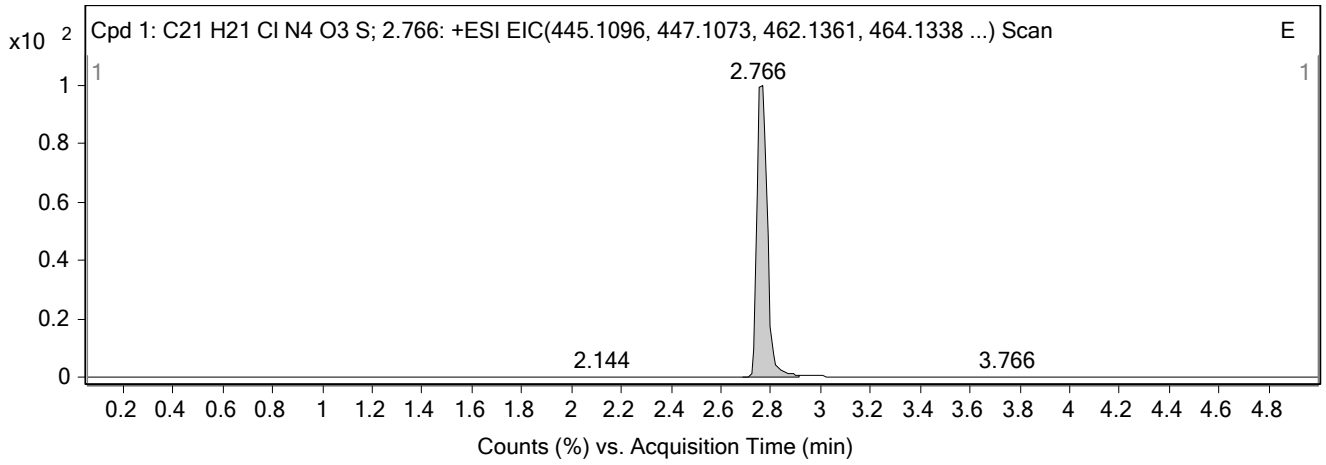
Data File	10.d	**Sample Name**	H3464504
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 6:29:46 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H21ClN4O3S	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 6:29:46 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

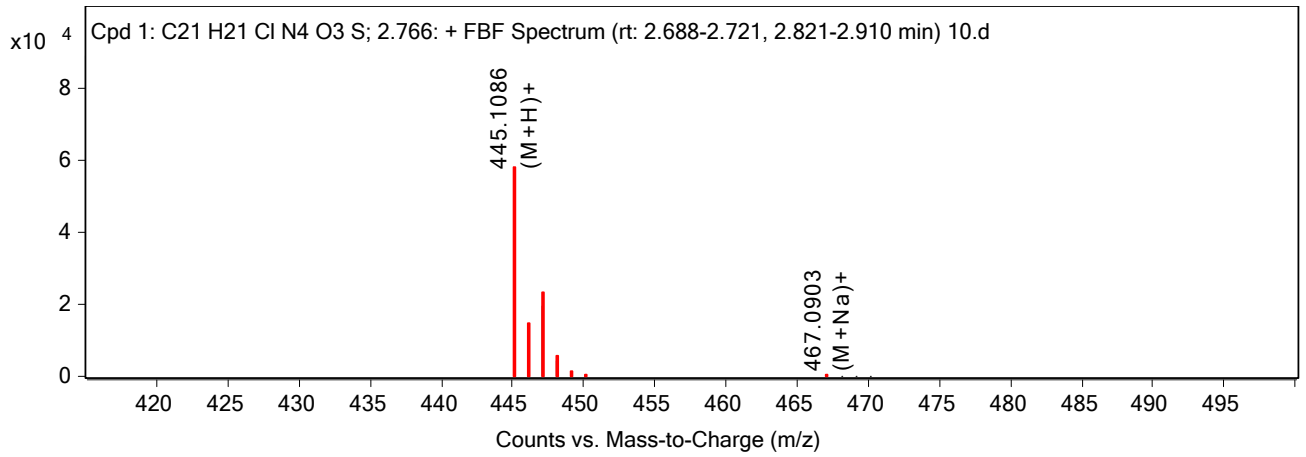
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H21 Cl N4 O3 S; 2.766	94.84	-2.01	C21 H21 Cl N4 O3 S	2.766	444.1023	444.1014

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
445.1086	2.766	444.1014	C21 H21 Cl N4 O3 S	444.1023	-2.01	Find By Formula	

Compound Chromatograms



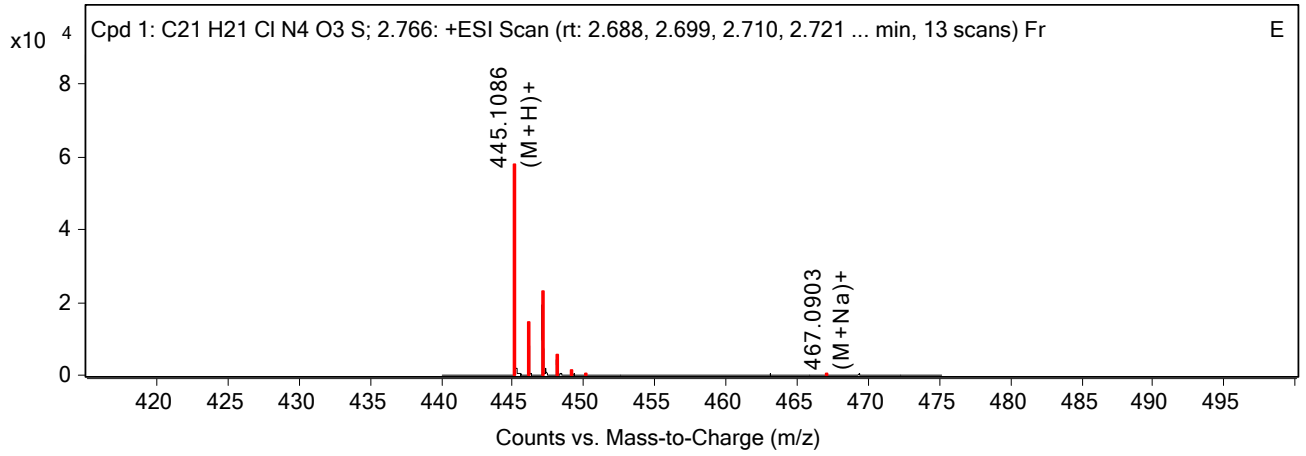
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
445.1086	1	57880.9	(M+H)+
446.1117	1	12194	(M+H)+
447.1063	1	19513.03	(M+H)+
448.1088	1	4306.13	(M+H)+
449.1072	1	1151.96	(M+H)+
450.1085	1	220.05	(M+H)+
467.0903	1	381.84	(M+Na)+
468.0949	1	111.9	(M+Na)+
469.0875	1	178.43	(M+Na)+
470.0909	1	56.46	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
445.1086	1	57880.9	(M+H)+	2.07
446.1117	1	12194	(M+H)+	1.72
447.1063	1	19513.03	(M+H)+	2.07
448.1088	1	4306.13	(M+H)+	2.14
449.1072	1	1151.96	(M+H)+	0
450.1085	1	220.05	(M+H)+	-0.87
467.0903	1	381.84	(M+Na)+	2.62
468.0949	1	111.9	(M+Na)+	-1.12
469.0875	1	178.43	(M+Na)+	3.67
470.0909	1	56.46	(M+Na)+	1.57

--- End Of Report ---

Target Compound Screening Report

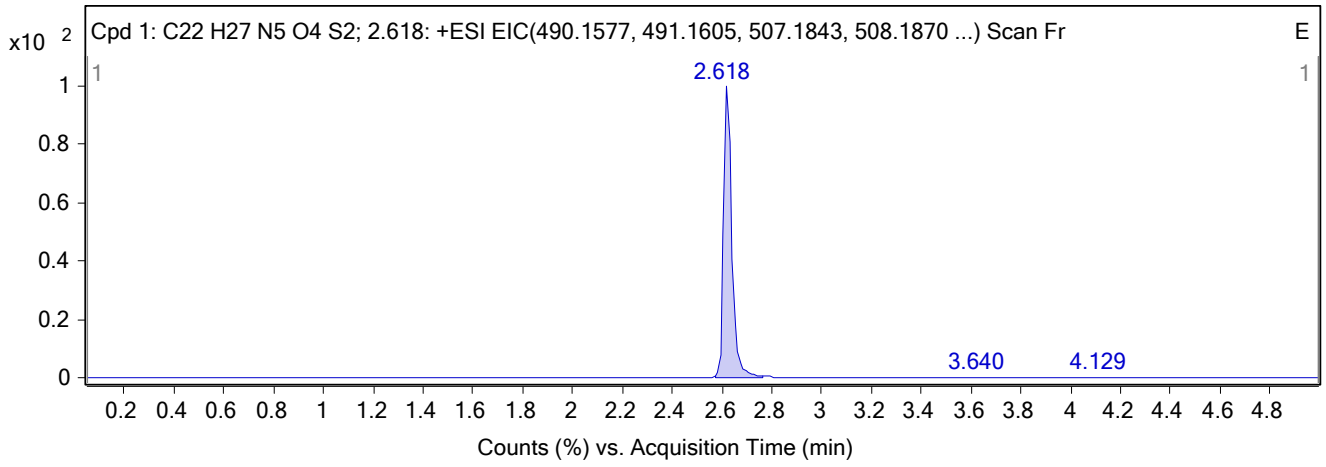
Data File	25.d	**Sample Name**	H1657378
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:29:56 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H27N5O4S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:29:56 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

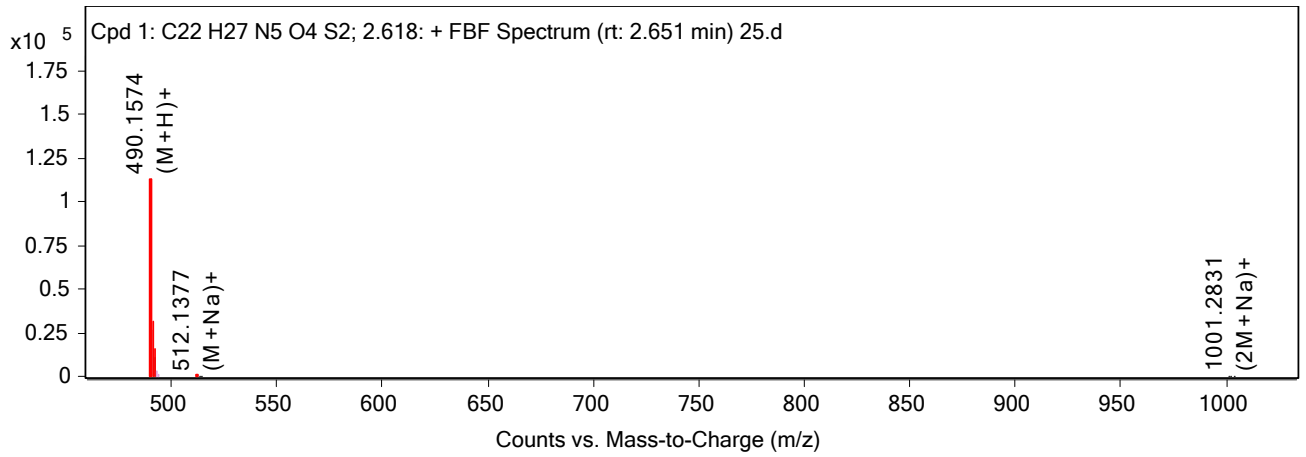
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H27 N5 O4 S2; 2.618	94.49	-1.07	C22 H27 N5 O4 S2	2.618	489.1504	489.1499

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
490.1574	2.618	489.1499	C22 H27 N5 O4 S2	489.1504	-1.07	Find By Formula	

Compound Chromatograms



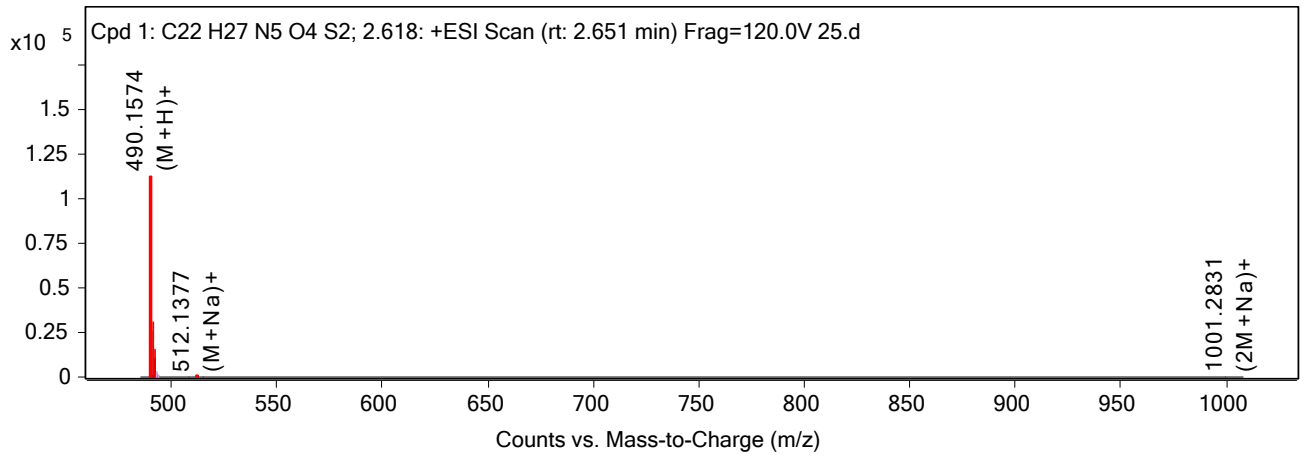
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
490.1574	1	113003.87	(M+H)+
491.1598	1	26144.04	(M+H)+
492.1556	1	11181.79	(M+H)+
512.1377	1	890.04	(M+Na)+
513.1442	1	331.03	(M+Na)+
514.1262	1	173.09	(M+Na)+
1001.2831	1	134.64	(2M+Na)+
1002.2734	1	99.56	(2M+Na)+
1003.2684	1	49.13	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
490.1574	1	113003.87	(M+H)+	0.74
491.1598	1	26144.04	(M+H)+	1.45
492.1556	1	11181.79	(M+H)+	2.3
512.1377	1	890.04	(M+Na)+	3.91
513.1442	1	331.03	(M+Na)+	-3.55
514.1262	1	173.09	(M+Na)+	24.16
1001.2831	1	134.64	(2M+Na)+	7.03
1002.2734	1	99.56	(2M+Na)+	19.43
1003.2684	1	49.13	(2M+Na)+	22.04

--- End Of Report ---

Target Compound Screening Report

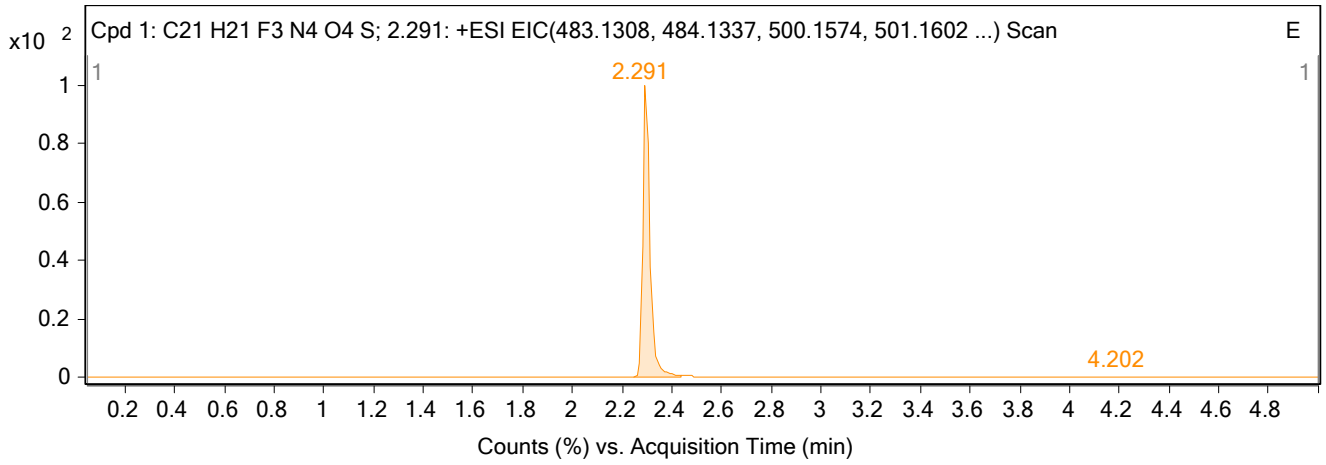
Data File	30.d	**Sample Name**	H1660632
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:57:42 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H21F3N4O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:57:42 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

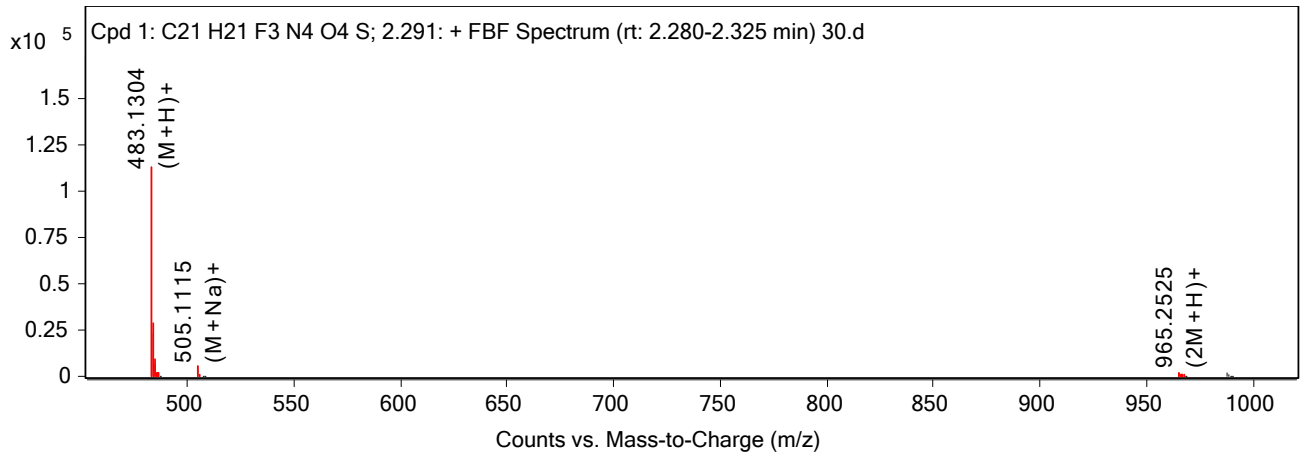
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H21 F3 N4 O4 S; 2.291	98.11	-1.17	C21 H21 F3 N4 O4 S	2.291	482.1236	482.123

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
505.1115	2.291	482.123	C21 H21 F3 N4 O4 S	482.1236	-1.17	Find By Formula	

Compound Chromatograms



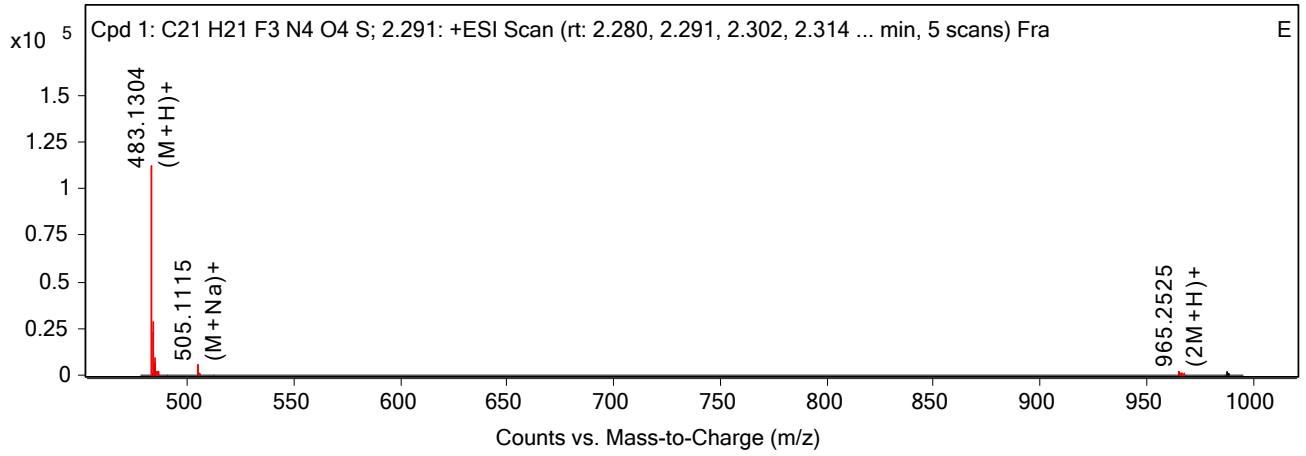
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
483.1304	1	112535.14	(M+H)+
484.1331	1	22723.8	(M+H)+
485.1302	1	6765.78	(M+H)+
486.1314	1	1226.17	(M+H)+
505.1115	1	5266.39	(M+Na)+
506.1152	1	1266.26	(M+Na)+
965.2525	1	2162.13	(2M+H)+
966.2584	1	973.14	(2M+H)+
987.2346	1	1853.45	(2M+Na)+
988.2376	1	959.07	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
483.1304	1	112535.14	(M+H)+	0.88
484.1331	1	22723.8	(M+H)+	1.33
485.1302	1	6765.78	(M+H)+	1.96
486.1314	1	1226.17	(M+H)+	1.93
505.1115	1	5266.39	(M+Na)+	2.62
506.1152	1	1266.26	(M+Na)+	0.94
965.2525	1	2162.13	(2M+H)+	2.02
966.2584	1	973.14	(2M+H)+	-1.14
987.2346	1	1853.45	(2M+Na)+	1.74
988.2376	1	959.07	(2M+Na)+	1.65

--- End Of Report ---

Target Compound Screening Report

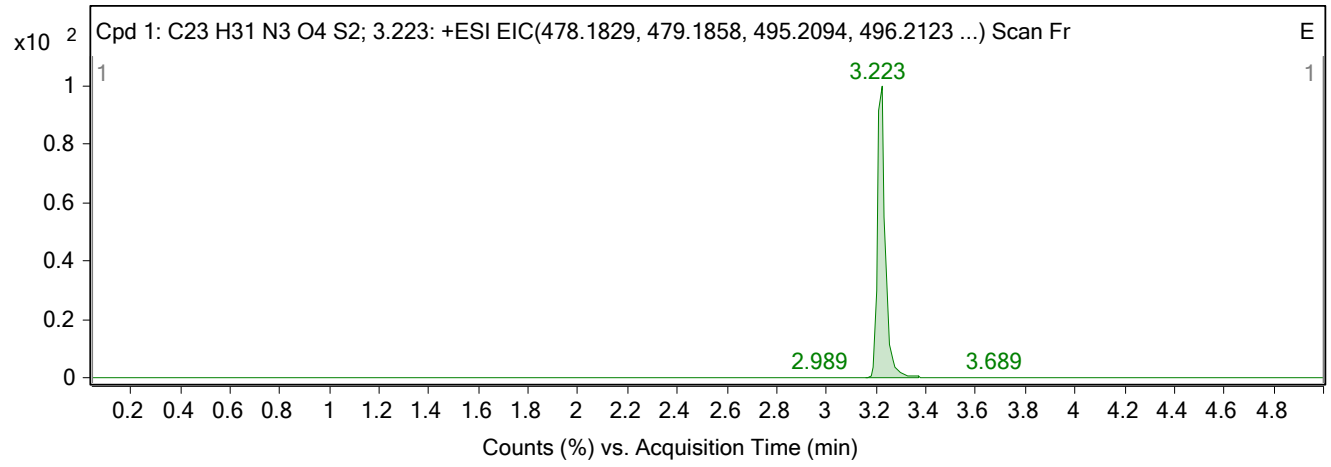
Data File	47.d	**Sample Name**	H1660622
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:32:02 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H31N3O4S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:32:02 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

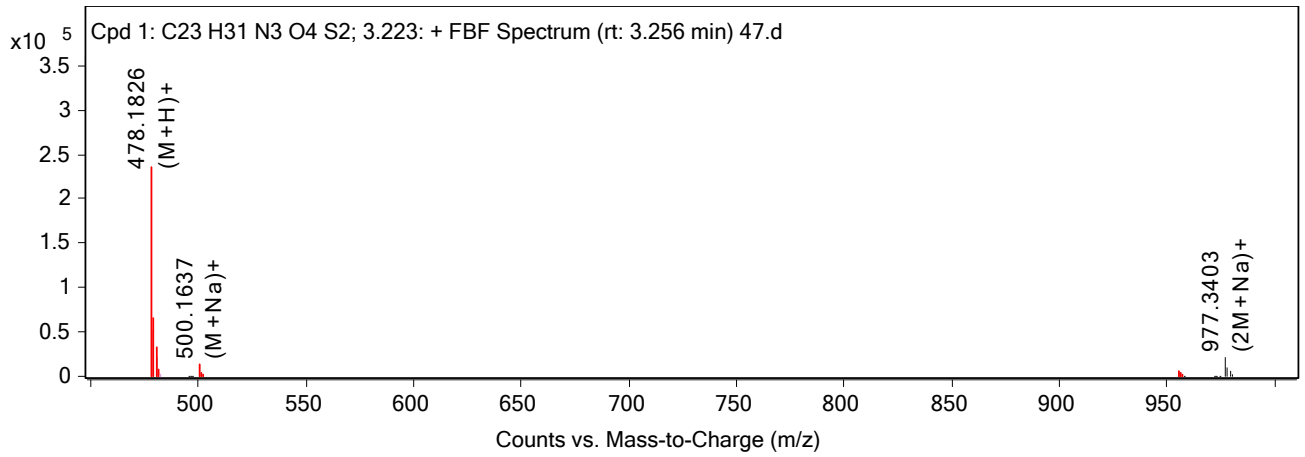
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H31 N3 O4 S2; 3.223	95.2	-0.87	C23 H31 N3 O4 S2	3.223	477.1756	477.1752

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
955.3579	3.223	477.1752	C23 H31 N3 O4 S2	477.1756	-0.87	Find By Formula	

Compound Chromatograms



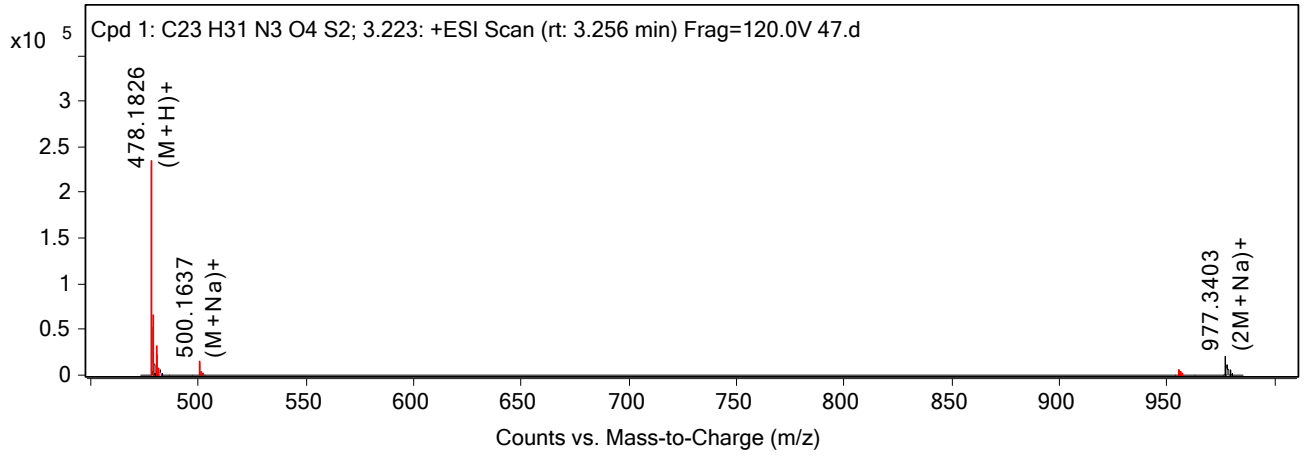
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
478.1826	1	235155.36	(M+H)+
479.1853	1	52884.65	(M+H)+
480.1813	1	22050.39	(M+H)+
481.1844	1	4296.08	(M+H)+
500.1637	1	14220.31	(M+Na)+
501.1666	1	3545.12	(M+Na)+
955.3579	1	5968.19	(2M+H)+
977.3403	1	21600.68	(2M+Na)+
978.3414	1	10595.62	(2M+Na)+
979.339	1	6303.5	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
478.1826	1	235155.36	(M+H)+	0.48
479.1853	1	52884.65	(M+H)+	1.06
480.1813	1	22050.39	(M+H)+	1.49
481.1844	1	4296.08	(M+H)+	-1.99
500.1637	1	14220.31	(M+Na)+	2.18
501.1666	1	3545.12	(M+Na)+	2.33
955.3579	1	5968.19	(2M+H)+	0.6
977.3403	1	21600.68	(2M+Na)+	0.17
978.3414	1	10595.62	(2M+Na)+	1.99
979.339	1	6303.5	(2M+Na)+	2.04

--- End Of Report ---

Target Compound Screening Report

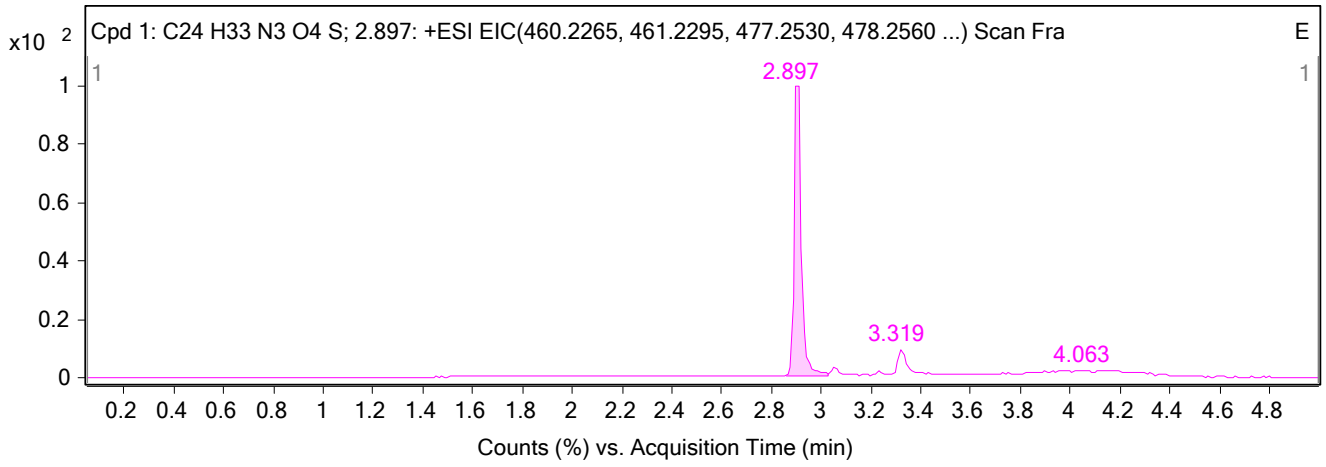
Data File	44.d	**Sample Name**	N953274$2
Sample Type	Sample	**Position**	P1-E8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 10:52:05 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H33N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 10:52:05 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

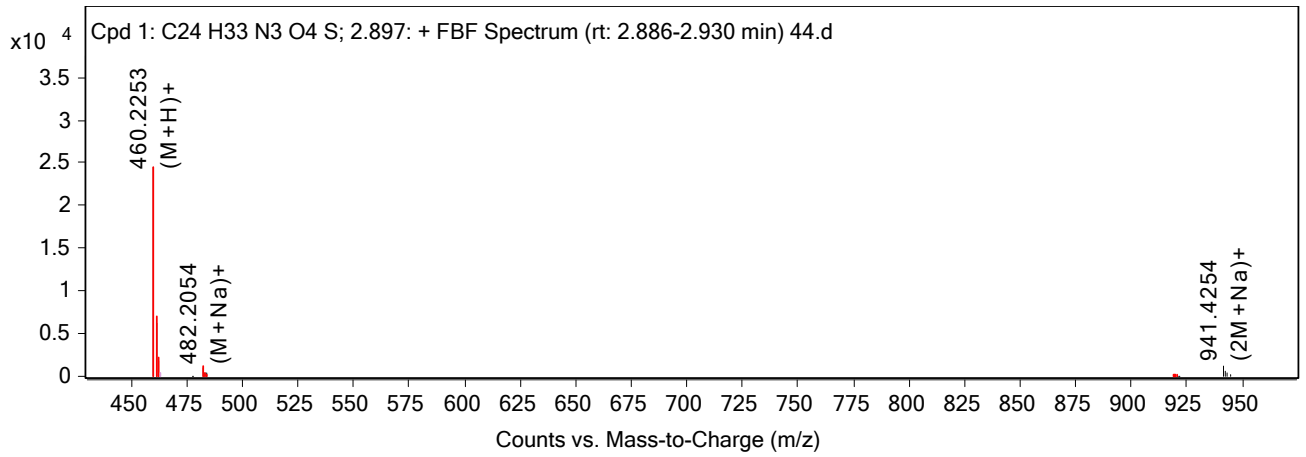
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H33 N3 O4 S; 2.897	97.85	-2.62	C24 H33 N3 O4 S	2.897	459.2192	459.218

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
941.4254	2.897	459.218	C24 H33 N3 O4 S	459.2192	-2.62	Find By Formula	

Compound Chromatograms



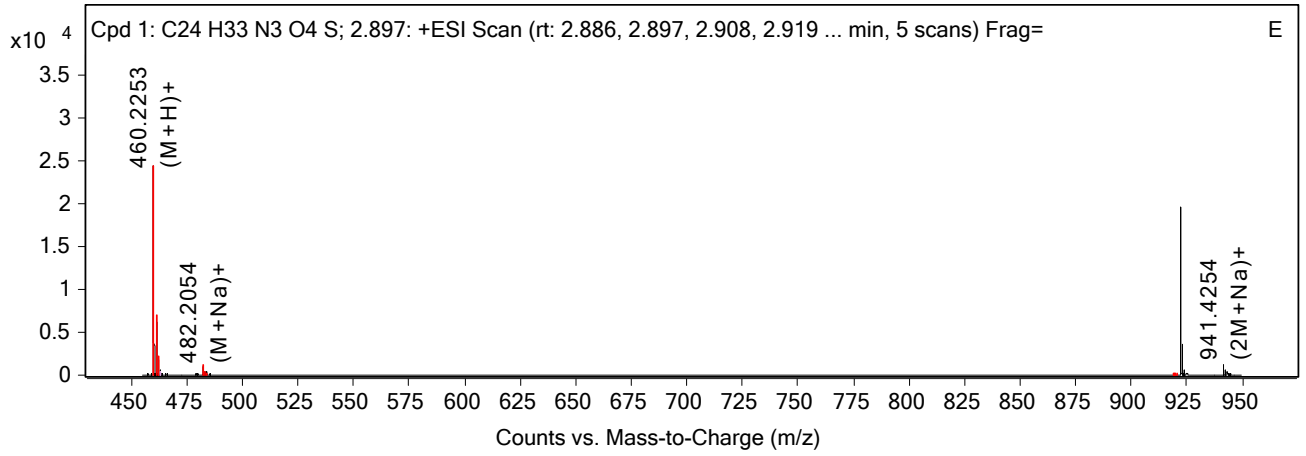
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
460.2253	1	24467.78	(M+H)+
461.2286	1	6231.39	(M+H)+
462.2262	1	1853.54	(M+H)+
482.2054	1	953.12	(M+Na)+
483.2103	1	332.37	(M+Na)+
484.2093	1	360.64	(M+Na)+
919.4441	1	213.1	(2M+H)+
941.4254	1	1232.33	(2M+Na)+
942.4287	1	683.17	(2M+Na)+
943.4281	1	322.18	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
460.2253	1	24467.78	(M+H)+	2.46
461.2286	1	6231.39	(M+H)+	1.98
462.2262	1	1853.54	(M+H)+	2.56
482.2054	1	953.12	(M+Na)+	6.12
483.2103	1	332.37	(M+Na)+	2.31
484.2093	1	360.64	(M+Na)+	-0.05
919.4441	1	213.1	(2M+H)+	1.65
941.4254	1	1232.33	(2M+Na)+	2.31
942.4287	1	683.17	(2M+Na)+	2.09
943.4281	1	322.18	(2M+Na)+	2.05

--- End Of Report ---

Target Compound Screening Report

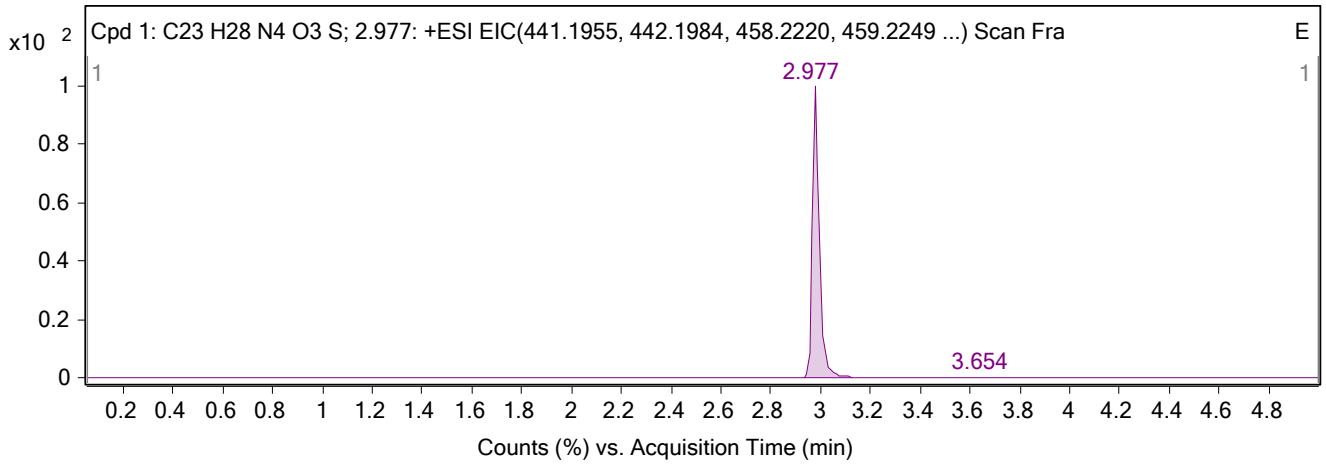
Data File	37.d	**Sample Name**	H1660662
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:36:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H28N4O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:36:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

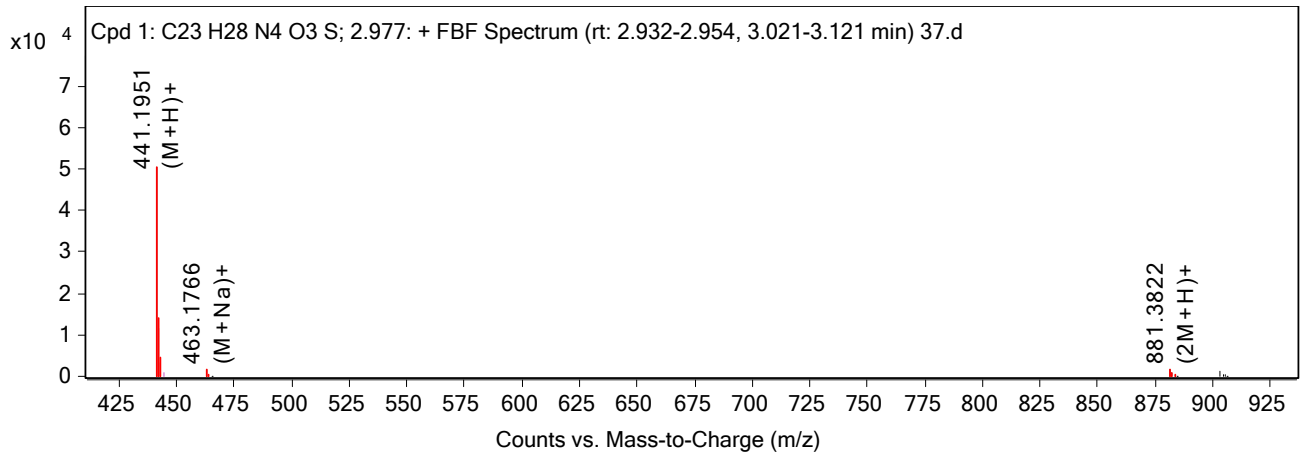
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H28 N4 O3 S; 2.977	97.98	-0.89	C23 H28 N4 O3 S	2.977	440.1882	440.1878

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
881.3822	2.977	440.1878	C23 H28 N4 O3 S	440.1882	-0.89	Find By Formula	

Compound Chromatograms



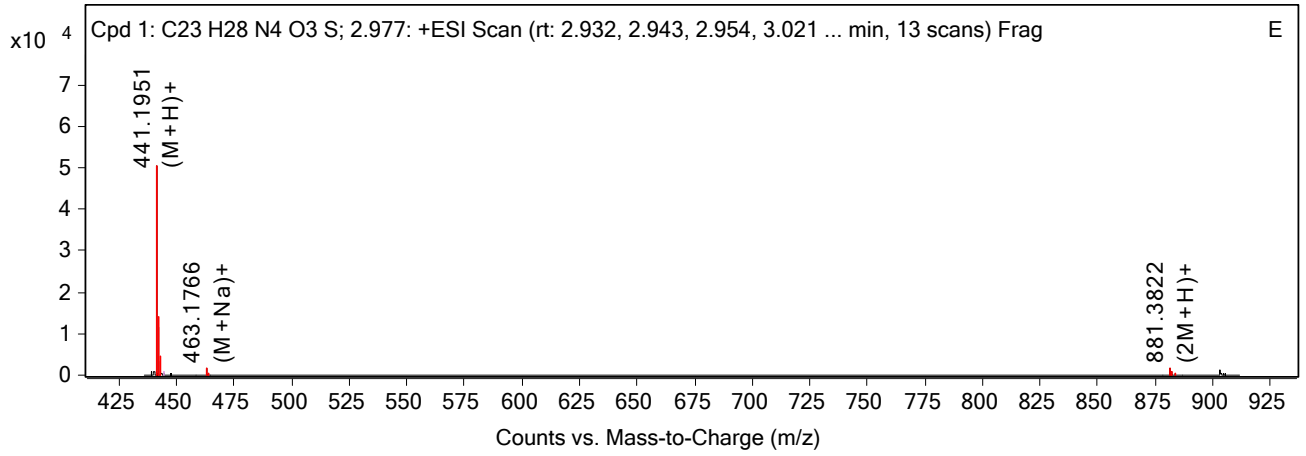
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
441.1951	1	50384.77	(M+H)+
442.1982	1	11759	(M+H)+
443.1962	1	3186.91	(M+H)+
463.1766	1	1729.45	(M+Na)+
464.1804	1	514.03	(M+Na)+
881.3822	1	1739.52	(2M+H)+
882.3858	1	992.88	(2M+H)+
883.3847	1	431.51	(2M+H)+
903.364	1	1085.37	(2M+Na)+
904.367	1	589.18	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
441.1951	1	50384.77	(M+H)+	0.77
442.1982	1	11759	(M+H)+	0.45
443.1962	1	3186.91	(M+H)+	-0.27
463.1766	1	1729.45	(M+Na)+	1.83
464.1804	1	514.03	(M+Na)+	0.05
881.3822	1	1739.52	(2M+H)+	1.7
882.3858	1	992.88	(2M+H)+	1.01
883.3847	1	431.51	(2M+H)+	1.39
903.364	1	1085.37	(2M+Na)+	1.87
904.367	1	589.18	(2M+Na)+	1.71

--- End Of Report ---

Target Compound Screening Report

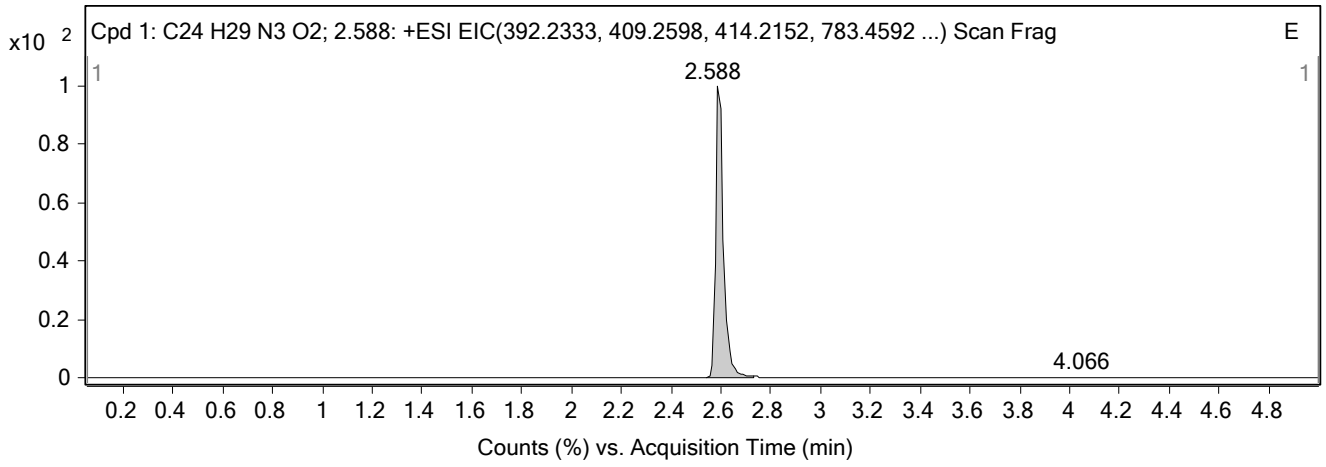
Data File	44.d	**Sample Name**	H1657338
Sample Type	Sample	**Position**	P1-E8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:15:28 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H29N3O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:15:28 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

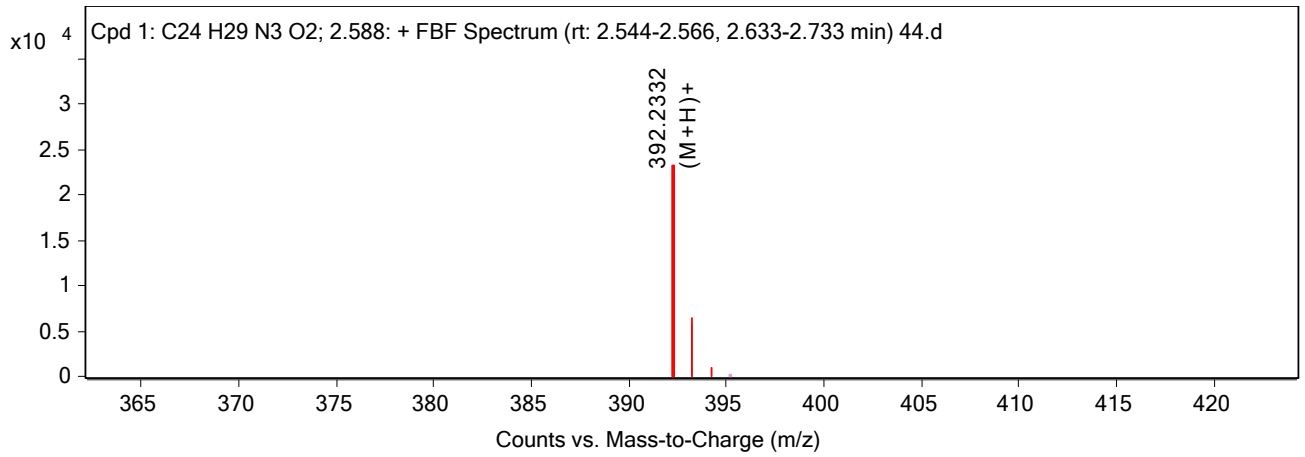
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H29 N3 O2; 2.588	97.89	-0.19	C24 H29 N3 O2	2.588	391.226	391.2259

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
392.2332	2.588	391.2259	C24 H29 N3 O2	391.226	-0.19	Find By Formula	

Compound Chromatograms



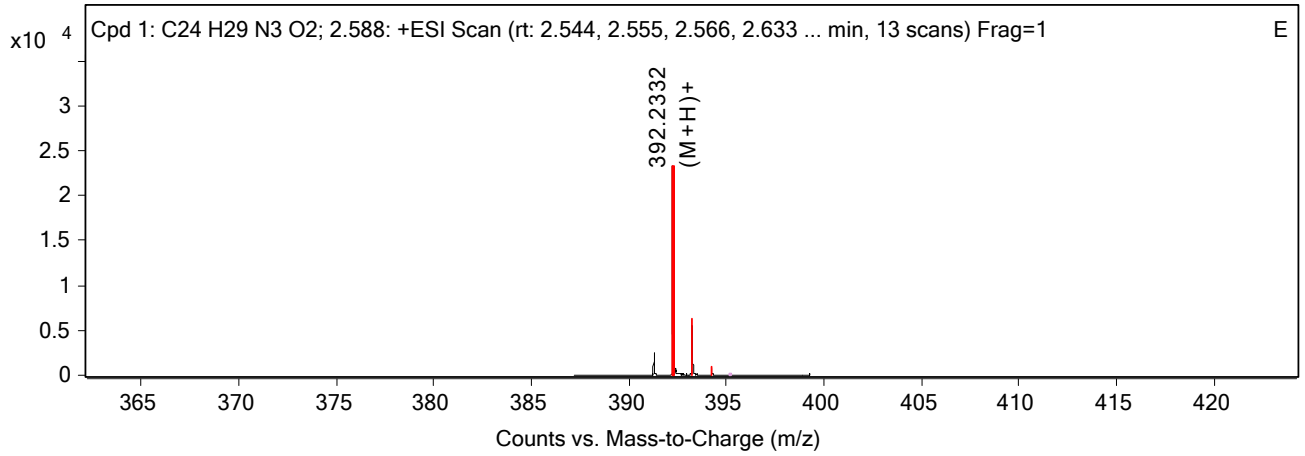
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
392.2332	1	23266.55	(M+H)+
393.2364	1	5583.1	(M+H)+
394.2386	1	866.02	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
392.2332	1	23266.55	(M+H)+	0.14
392.2332		23266.55		
393.2364	1	5583.1	(M+H)+	0.09
394.2386	1	866.02	(M+H)+	1.94

--- End Of Report ---

Target Compound Screening Report

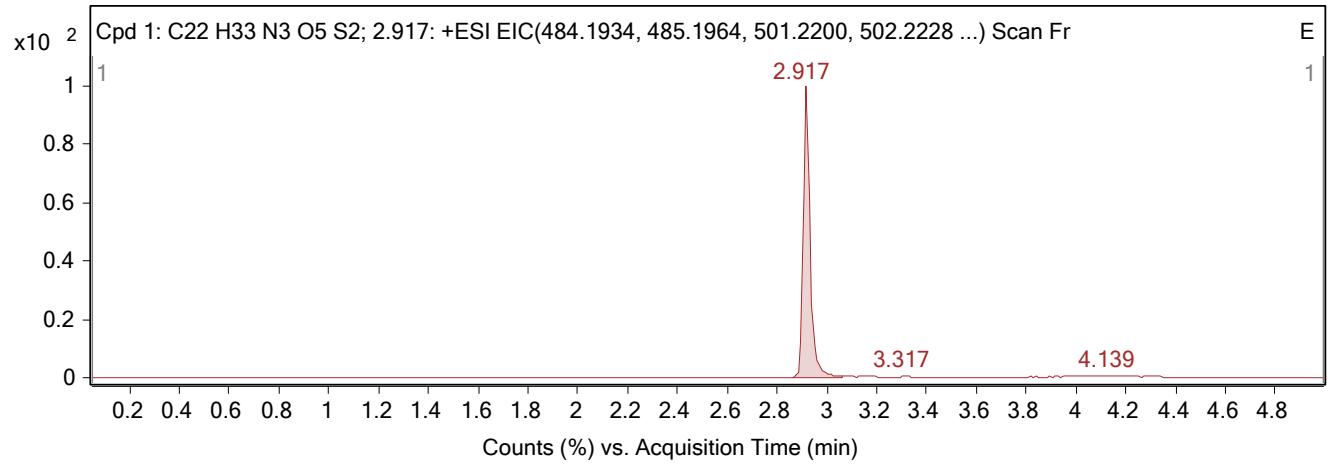
Data File	34.d	**Sample Name**	H2974295
Sample Type	Sample	**Position**	P1-D7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:23:38 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:23:38 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

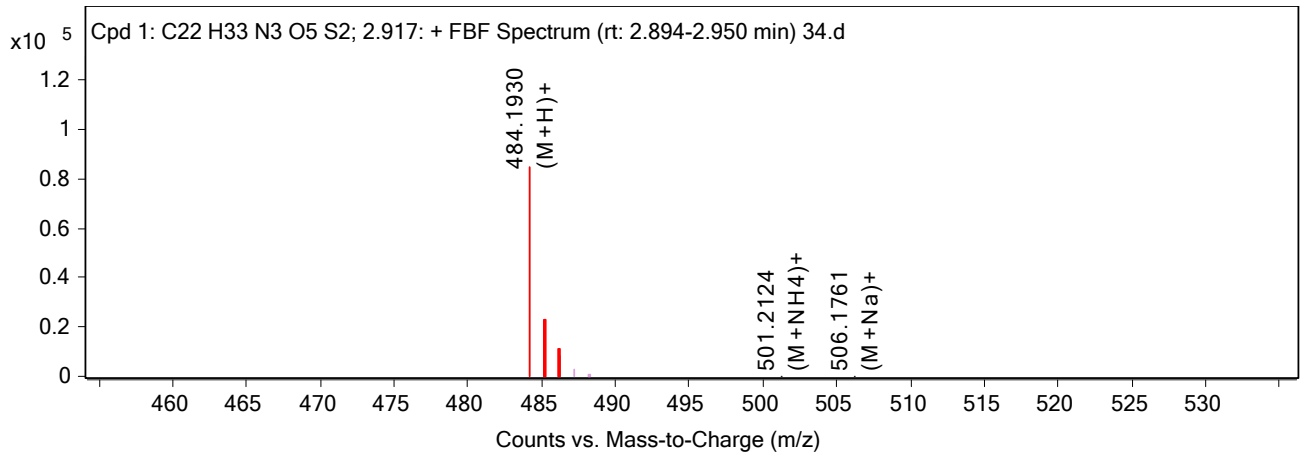
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O5 S2; 2.917	94.1	-1.22	C22 H33 N3 O5 S2	2.917	483.1862	483.1856

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
484.193	2.917	483.1856	C22 H33 N3 O5 S2	483.1862	-1.22	Find By Formula	

Compound Chromatograms



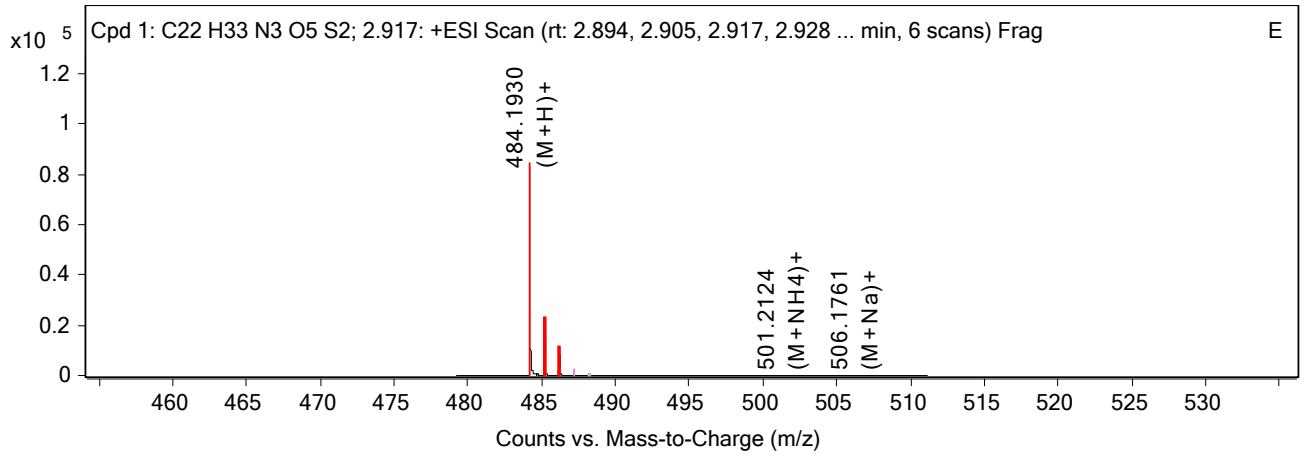
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
484.193	1	84677.05	(M+H)+
485.1952	1	18926.76	(M+H)+
486.1919	1	8357.12	(M+H)+
501.2124	1	51.01	(M+NH4)+
506.1761	1	114.2	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
484.193	1	84677.04	(M+H)+	0.97
484.193		84677.04		
485.1952	1	18926.76	(M+H)+	2.31
486.1919	1	8357.12	(M+H)+	1.21
501.2124	1	51.01	(M+NH4)+	15.16
506.1761	1	114.2	(M+Na)+	-1.44

--- End Of Report ---

Target Compound Screening Report

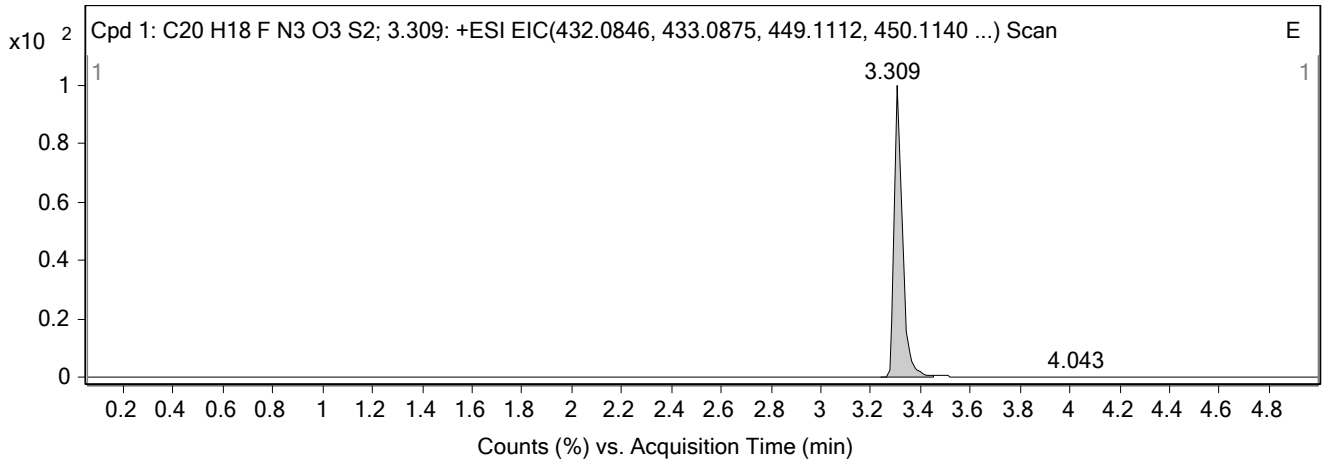
Data File	21.d	**Sample Name**	H2045012
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:07:42 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H18FN3O3S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:07:42 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H18 F N3 O3 S2; 3.309	97.57	-1.11	C20 H18 F N3 O3 S2	3.309	431.0774	431.0769

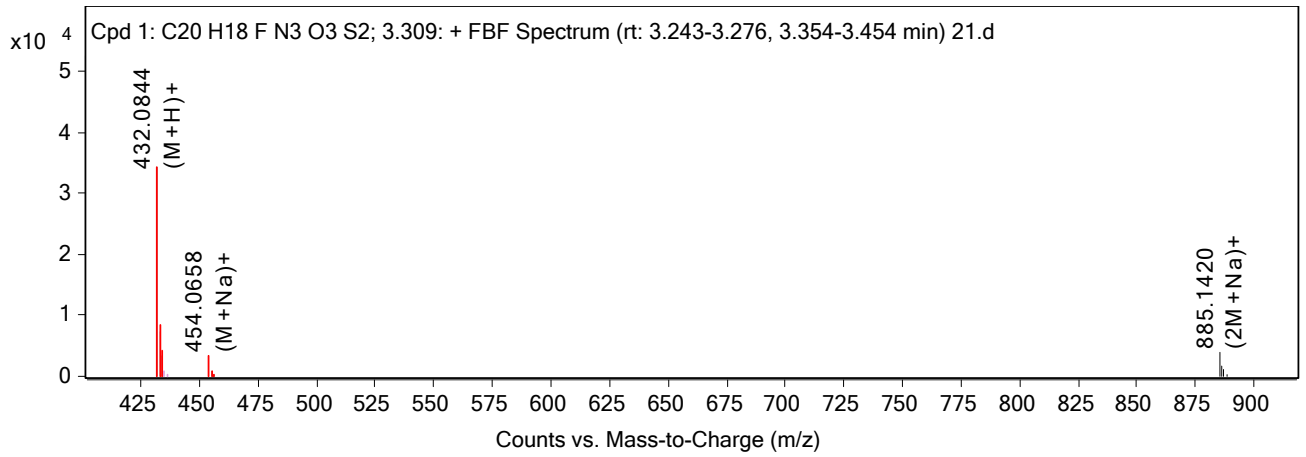
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
454.0658	3.309	431.0769	C20 H18 F N3 O3 S2	431.0774	-1.11	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

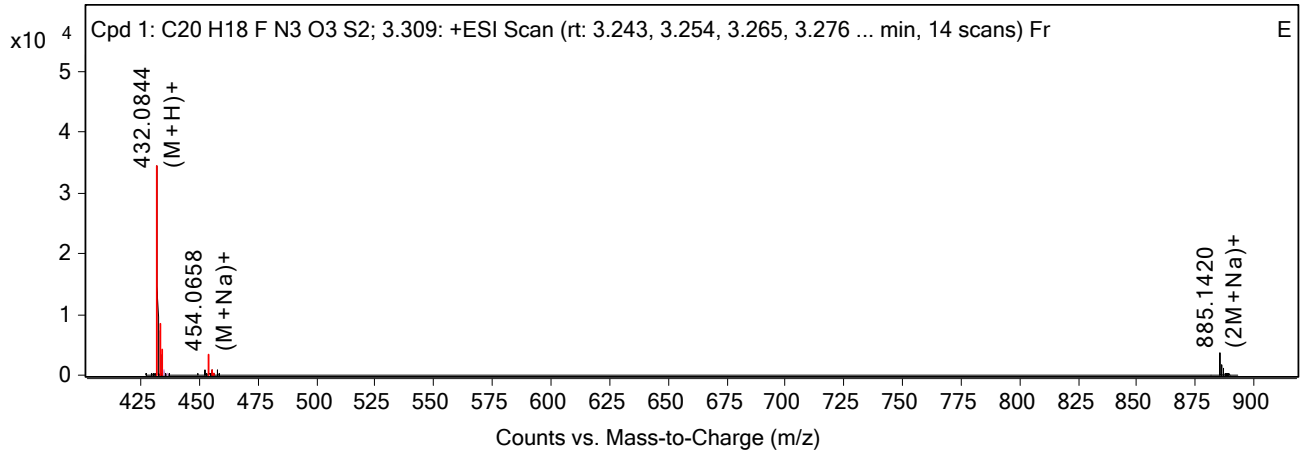
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
432.0844	1	34400.64	(M+H)+
433.0873	1	7304.68	(M+H)+
434.0827	1	3295.85	(M+H)+
454.0658	1	3357.05	(M+Na)+
455.0689	1	790.06	(M+Na)+
456.064	1	380.87	(M+Na)+
885.142	1	3822.59	(2M+Na)+
886.1445	1	1829.54	(2M+Na)+
887.1423	1	1081.26	(2M+Na)+
888.1441	1	387.19	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
432.0844	1	34400.64	(M+H)+	0.51
433.0873	1	7304.68	(M+H)+	0.41
434.0827	1	3295.85	(M+H)+	0.97
454.0658	1	3357.05	(M+Na)+	1.74
455.0689	1	790.06	(M+Na)+	1.19
456.064	1	380.87	(M+Na)+	2.33
885.142	1	3822.59	(2M+Na)+	2.15
886.1445	1	1829.54	(2M+Na)+	2.58
887.1423	1	1081.26	(2M+Na)+	1.74
888.1441	1	387.19	(2M+Na)+	0.77

--- End Of Report ---

Target Compound Screening Report

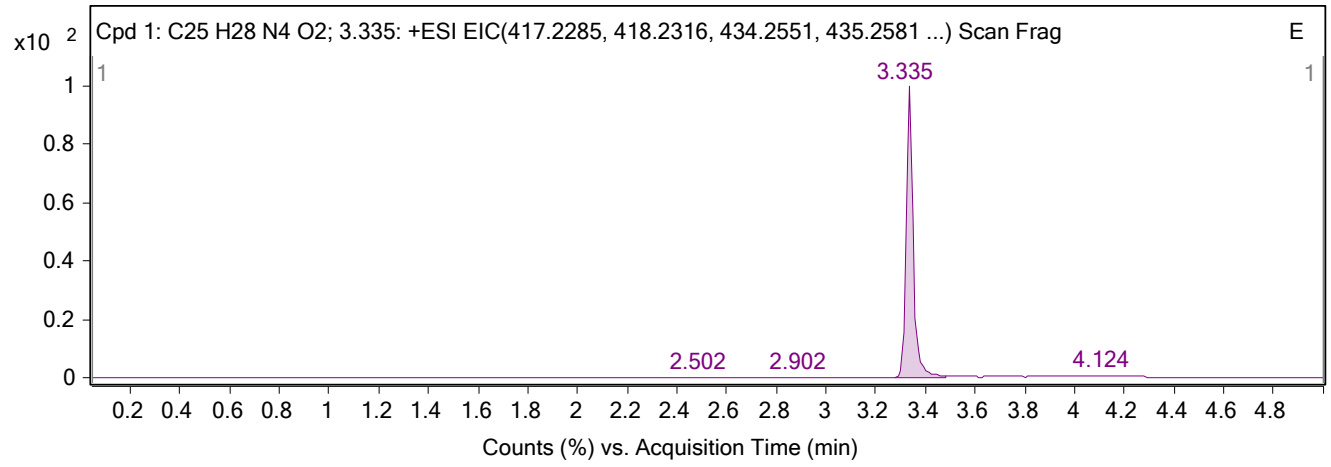
Data File	19.d	**Sample Name**	H2982866
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:58:47 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:58:47 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O2; 3.335	95.49	-1.47	C25 H28 N4 O2	3.335	416.2212	416.2206

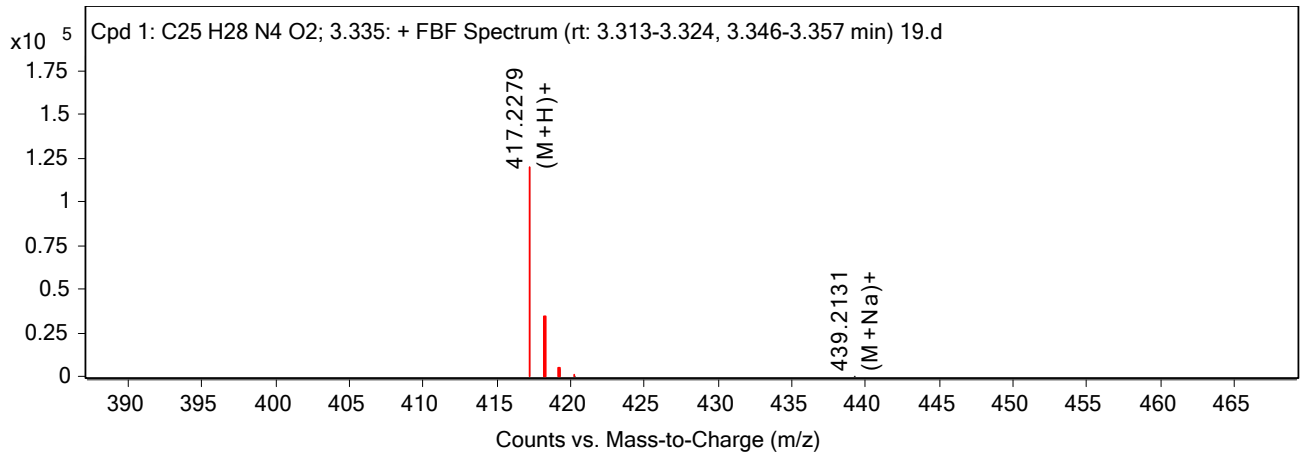
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
417.2279	3.335	416.2206	C25 H28 N4 O2	416.2212	-1.47	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

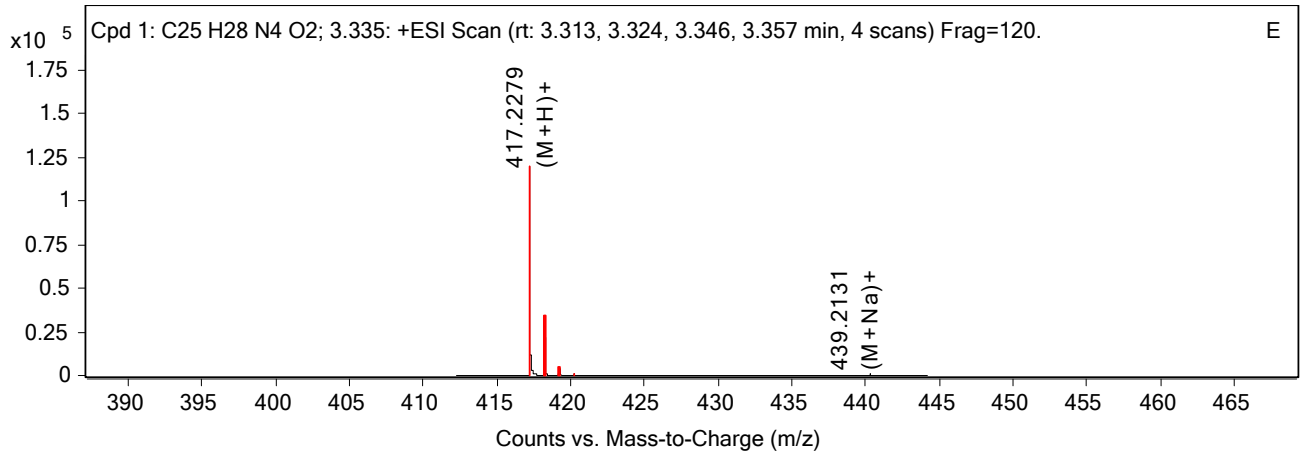
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
417.2279	1	119662.51	(M+H)+
418.2308	1	28702.96	(M+H)+
419.2344	1	3767.42	(M+H)+
420.2377	1	500.54	(M+H)+
439.2131	1	388.25	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
417.2279	1	119662.51	(M+H)+	1.45
417.2279		119662.51		
418.2308	1	28702.96	(M+H)+	1.84
419.2344	1	3767.42	(M+H)+	0.13
420.2377	1	500.54	(M+H)+	-1.05
439.2131	1	388.25	(M+Na)+	-5.96

--- End Of Report ---

Target Compound Screening Report

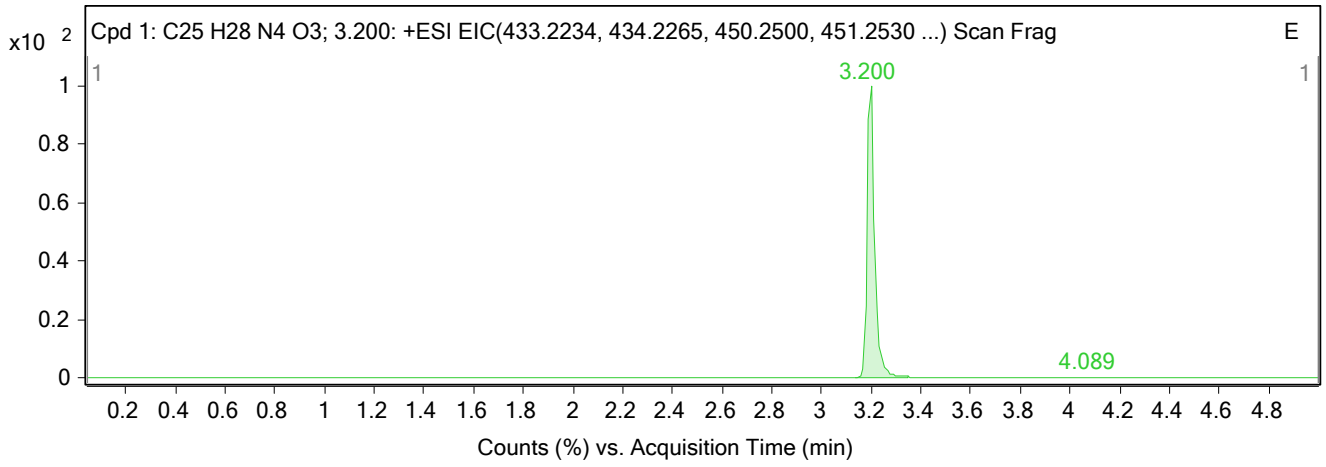
Data File	21.d	**Sample Name**	H2997945
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:39:01 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:39:01 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

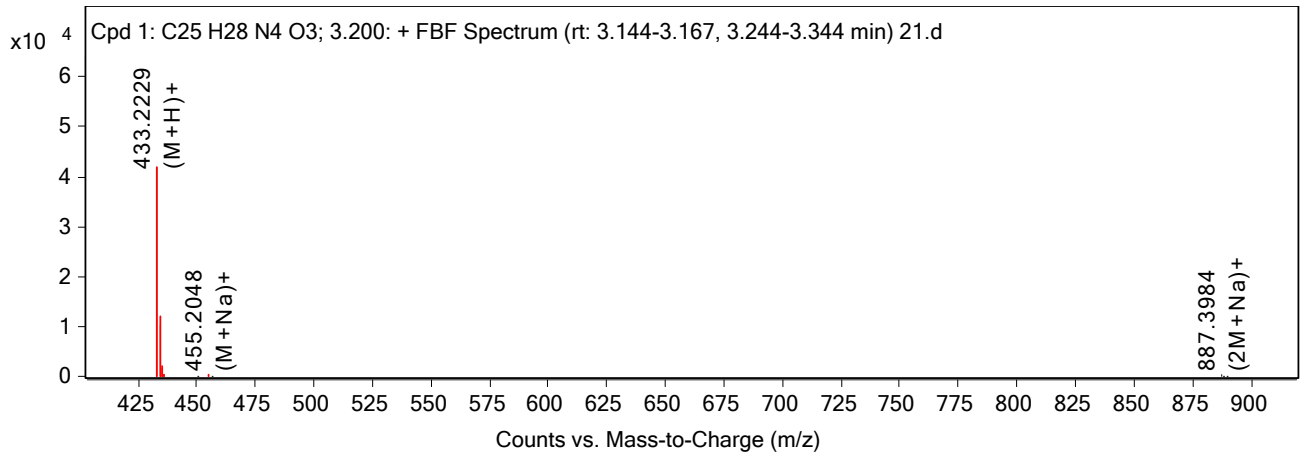
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O3; 3.200	96.43	-1.55	C25 H28 N4 O3	3.2	432.2161	432.2155

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
433.2229	3.2	432.2155	C25 H28 N4 O3	432.2161	-1.55	Find By Formula	

Compound Chromatograms



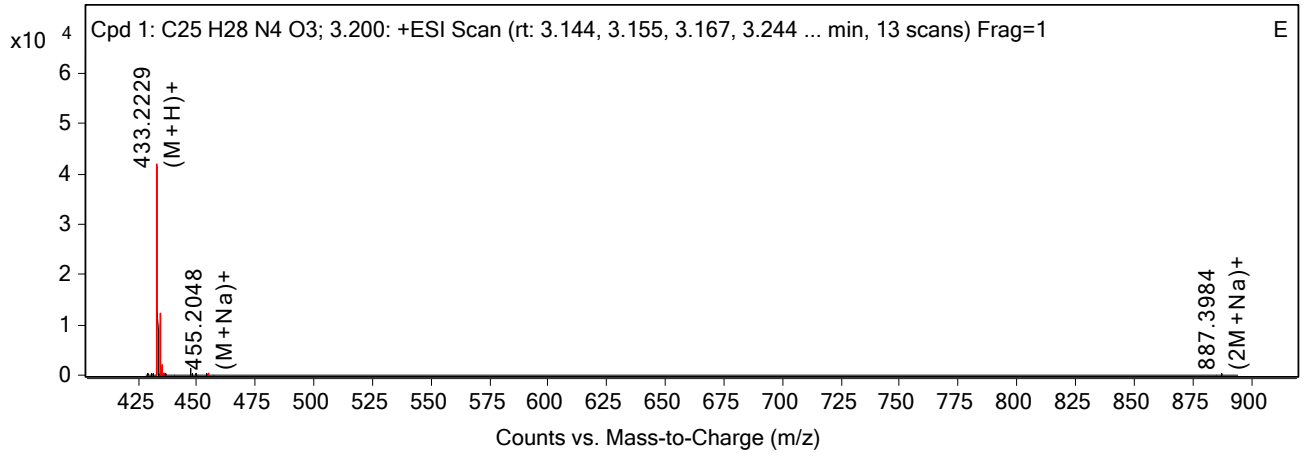
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
433.2229	1	41853.31	(M+H)+
434.2259	1	10243.66	(M+H)+
435.2297	1	1611.19	(M+H)+
436.2348	1	222.14	(M+H)+
450.2549	1	82.17	(M+NH4)+
455.2048	1	236.3	(M+Na)+
456.2093	1	94.59	(M+Na)+
887.3984	1	308.2	(2M+Na)+
888.4057	1	163.63	(2M+Na)+
889.4008	1	85.32	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
433.2229	1	41853.31	(M+H)+	1.08
434.2259	1	10243.66	(M+H)+	1.41
435.2297	1	1611.19	(M+H)+	-0.85
436.2348	1	222.14	(M+H)+	-6.39
450.2549	1	82.17	(M+NH4)+	-10.98
455.2048	1	236.3	(M+Na)+	1.33
456.2093	1	94.59	(M+Na)+	-1.81
887.3984	1	308.2	(2M+Na)+	26.01
888.4057	1	163.62	(2M+Na)+	21.27
889.4008	1	85.32	(2M+Na)+	29.98

--- End Of Report ---

Target Compound Screening Report

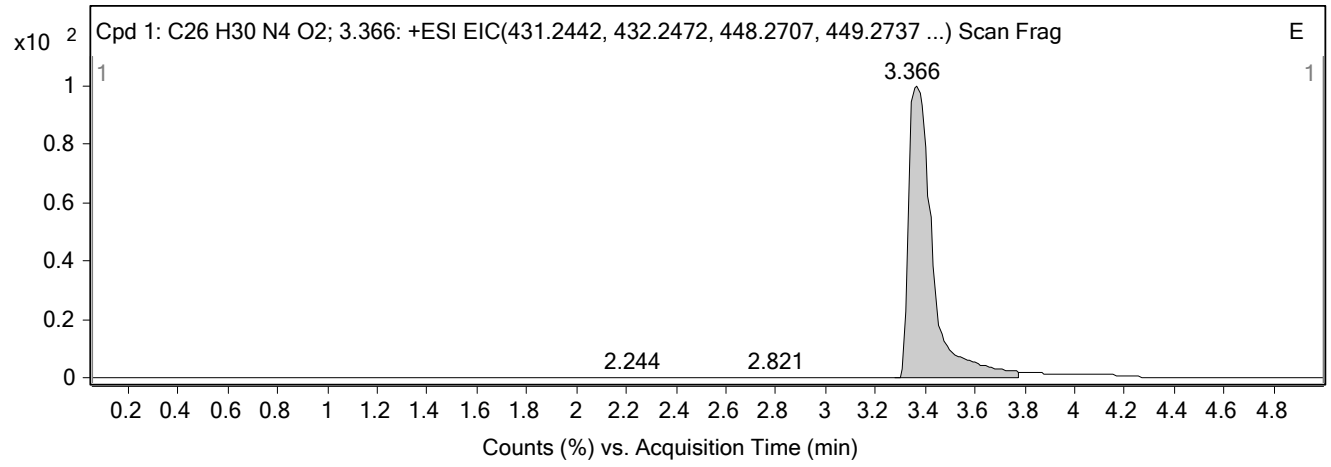
Data File	8.d	**Sample Name**	H2980200
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 5:20:40 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 5:20:40 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

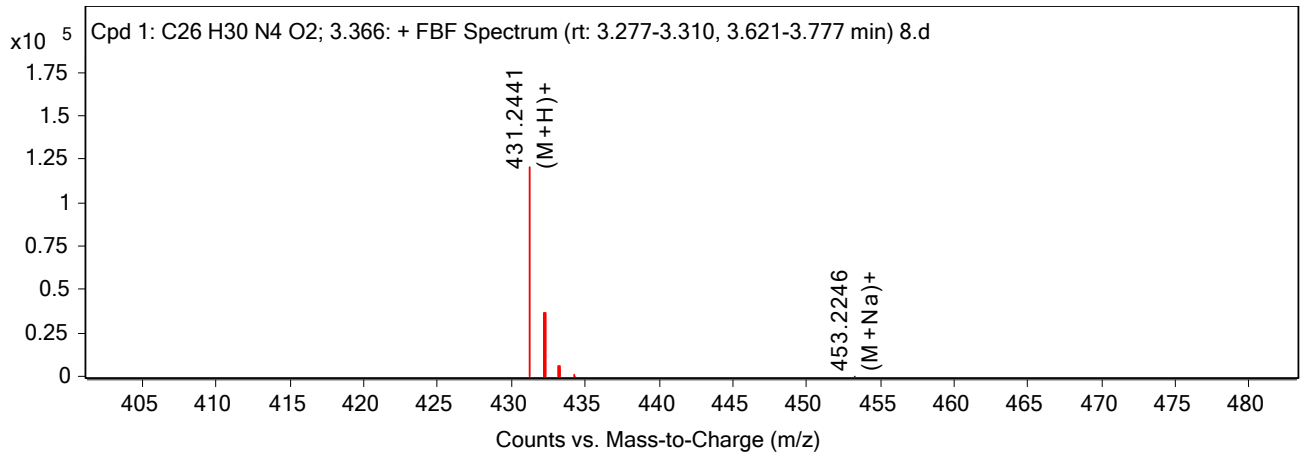
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O2; 3.366	96.29	-0.18	C26 H30 N4 O2	3.366	430.2369	430.2368

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
431.2441	3.366	430.2368	C26 H30 N4 O2	430.2369	-0.18	Find By Formula	

Compound Chromatograms



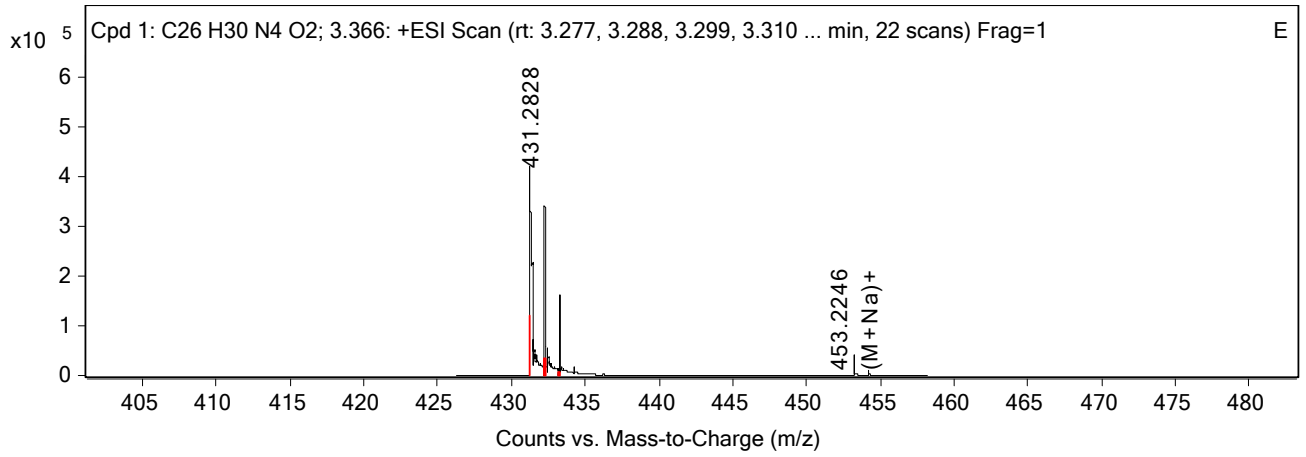
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
431.2441	1	120421.3	(M+H)+
432.247	1	30368.74	(M+H)+
433.2499	1	4328.82	(M+H)+
434.253	1	510.33	(M+H)+
453.2246	1	388.85	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
431.2441	1	120421.31	(M+H)+	0.04
431.2828		420432.04		
432.247	1	30368.74	(M+H)+	0.65
433.2499	1	4328.82	(M+H)+	0.56
434.253	1	510.33	(M+H)+	-0.14
453.2246	1	388.85	(M+Na)+	3.27

--- End Of Report ---

Target Compound Screening Report

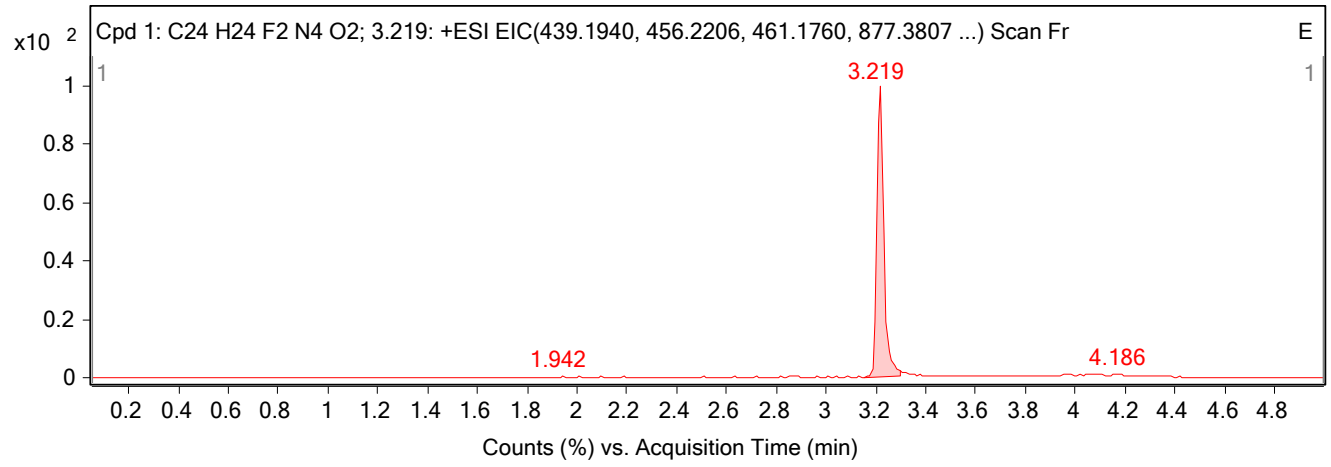
Data File	5-2.d	**Sample Name**	H2978807
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:32:29 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H24F2N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:32:29 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

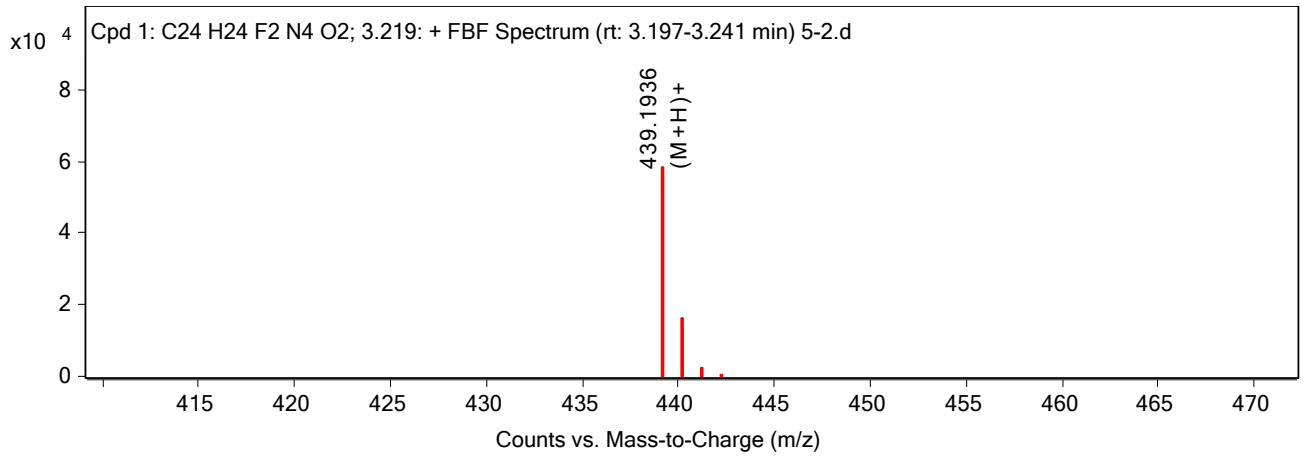
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H24 F2 N4 O2; 3.219	96.12	-1.2	C24 H24 F2 N4 O2	3.219	438.1867	438.1862

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
439.1936	3.219	438.1862	C24 H24 F2 N4 O2	438.1867	-1.2	Find By Formula	

Compound Chromatograms



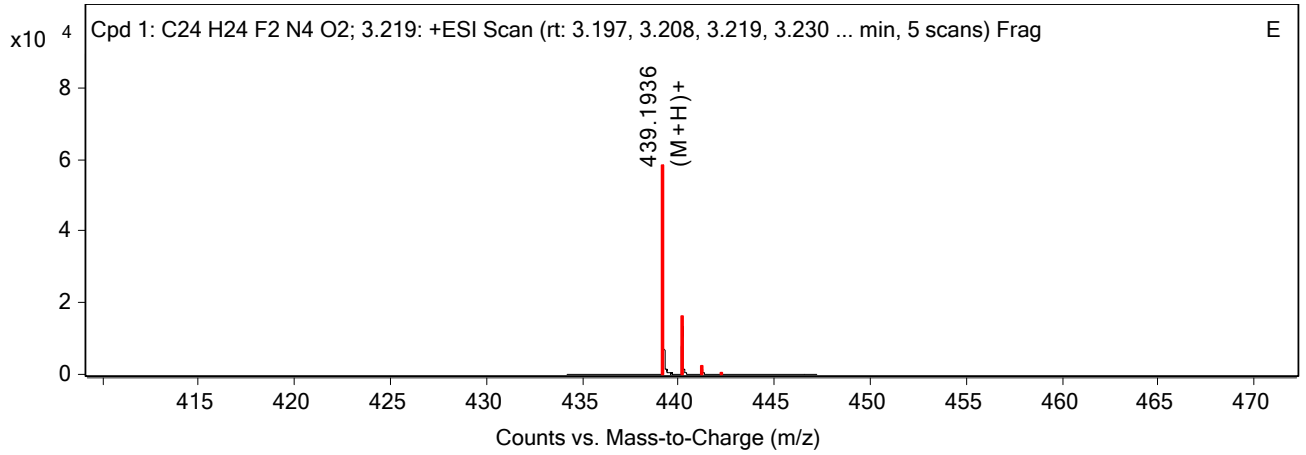
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
439.1936	1	58360.18	(M+H)+
440.1962	1	13594.51	(M+H)+
441.1992	1	1912.09	(M+H)+
442.2042	1	225.78	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
439.1936	1	58360.18	(M+H)+	1
439.1936		58360.18		
440.1962	1	13594.51	(M+H)+	2.05
441.1992	1	1912.09	(M+H)+	1.59
442.2042	1	225.78	(M+H)+	-3.39

--- End Of Report ---

Target Compound Screening Report

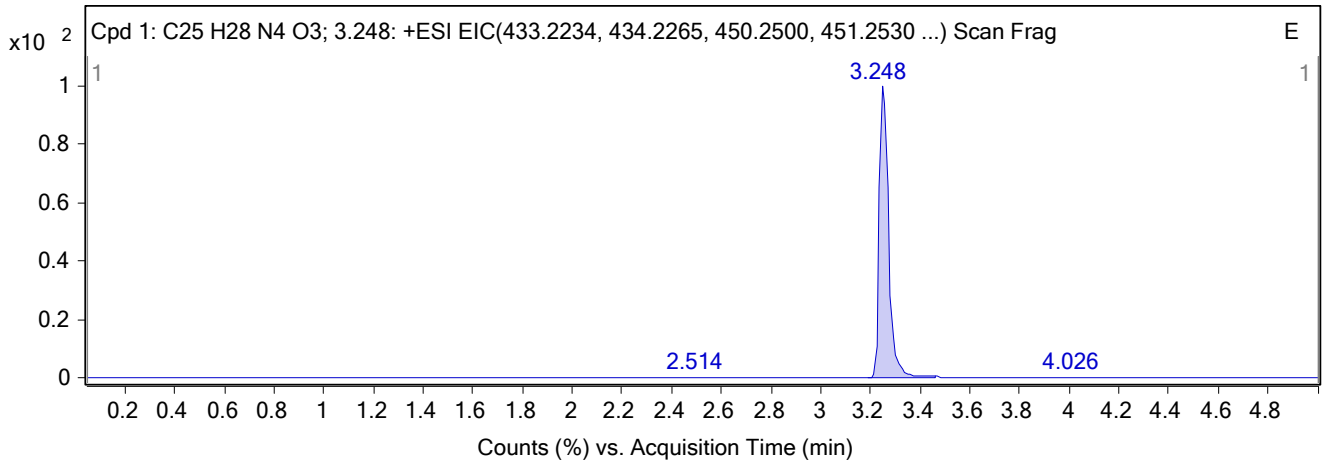
Data File	50.d	**Sample Name**	H2977660
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:20:08 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:20:08 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

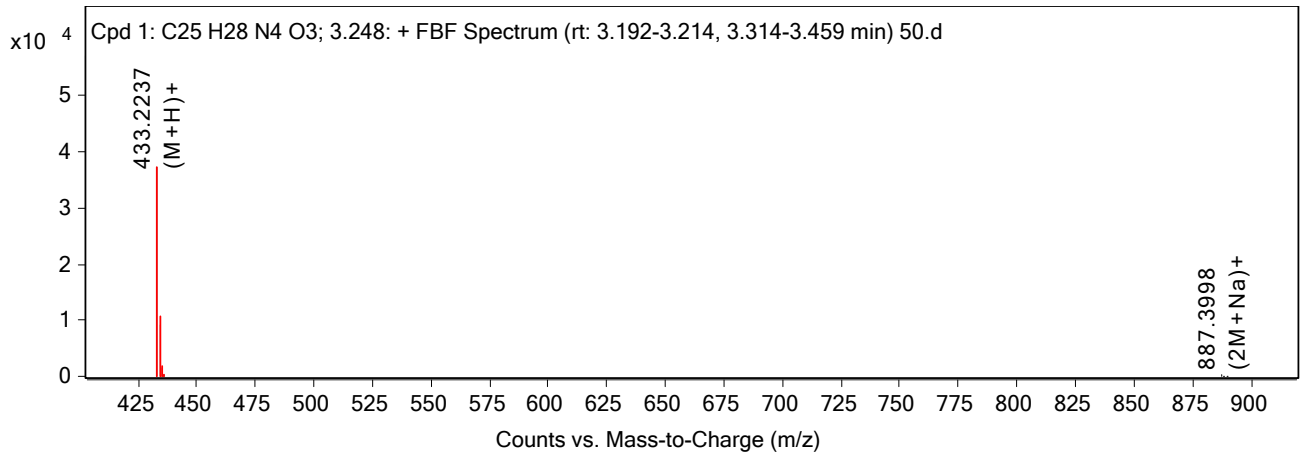
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O3; 3.248	96.44	0.11	C25 H28 N4 O3	3.248	432.2161	432.2162

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
433.2237	3.248	432.2162	C25 H28 N4 O3	432.2161	0.11	Find By Formula	

Compound Chromatograms



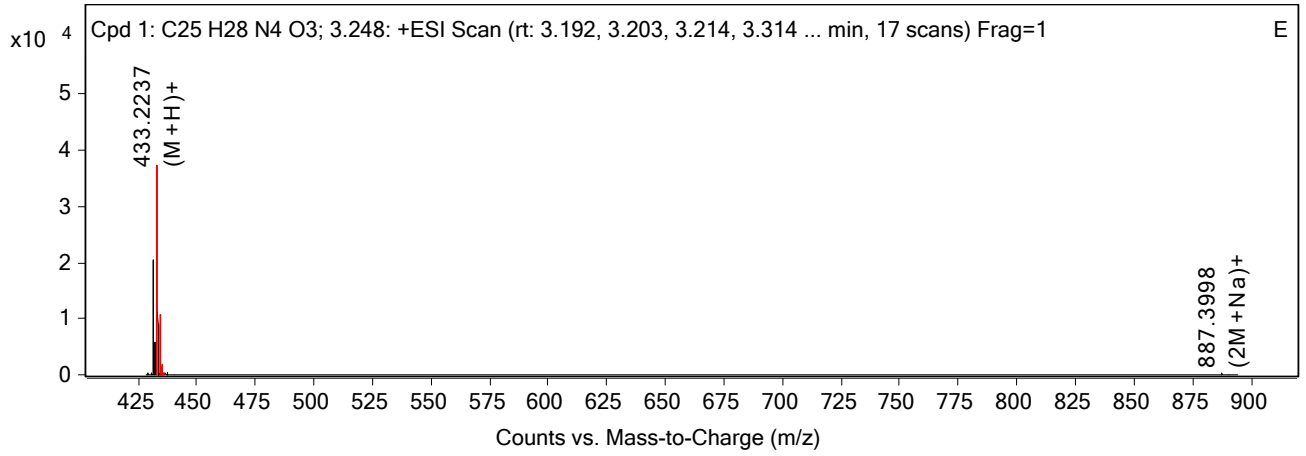
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
433.2237	1	37225.01	(M+H)+
434.2268	1	9077.53	(M+H)+
435.2293	1	1457.09	(M+H)+
436.2341	1	214.63	(M+H)+
887.3998	1	326.1	(2M+Na)+
888.404	1	161.14	(2M+Na)+
889.4015	1	96.45	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
433.2237	1	37225.01	(M+H)+	-0.76
434.2268	1	9077.53	(M+H)+	-0.62
435.2293	1	1457.09	(M+H)+	-0.03
436.2341	1	214.63	(M+H)+	-4.79
887.3998	1	326.1	(2M+Na)+	24.43
888.404	1	161.14	(2M+Na)+	23.17
889.4015	1	96.45	(2M+Na)+	29.23

--- End Of Report ---

Target Compound Screening Report

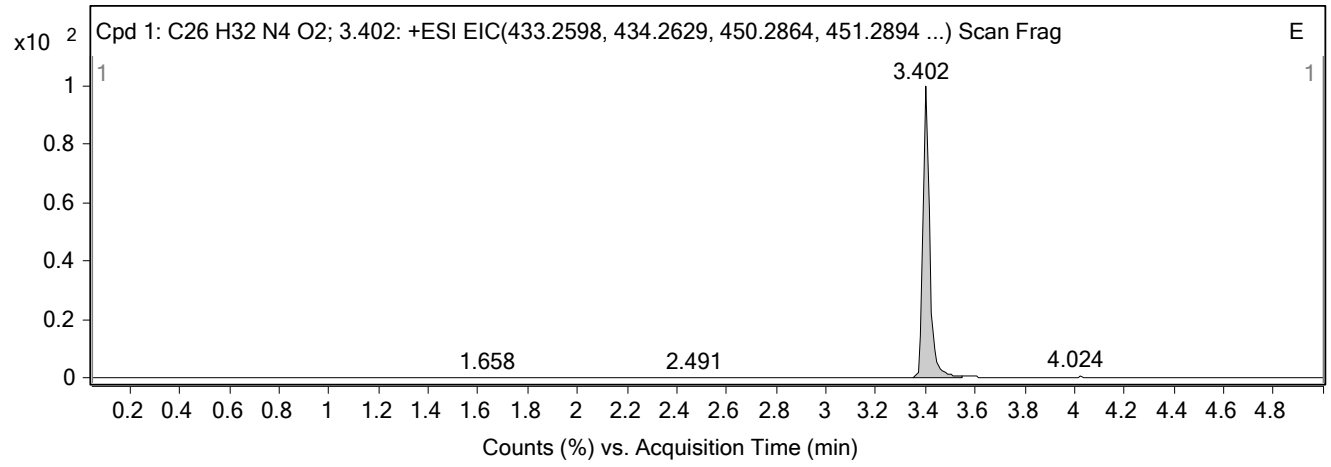
Data File	40.d	**Sample Name**	H2982094
Sample Type	Sample	**Position**	P1-E4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:51:17 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H32N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:51:17 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

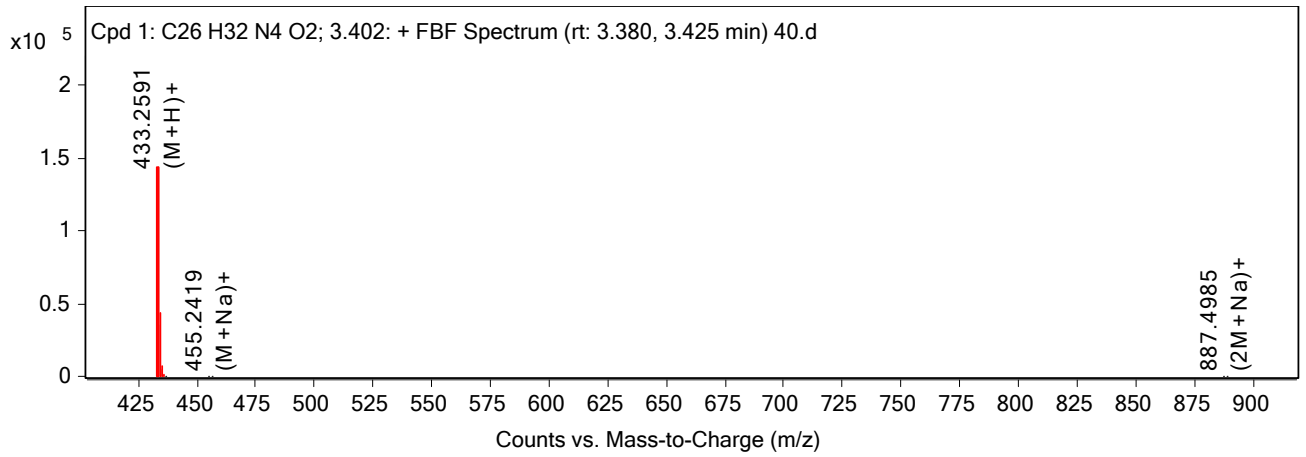
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H32 N4 O2; 3.402	95.34	-1.51	C26 H32 N4 O2	3.402	432.2525	432.2519

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
433.2591	3.402	432.2519	C26 H32 N4 O2	432.2525	-1.51	Find By Formula	

Compound Chromatograms



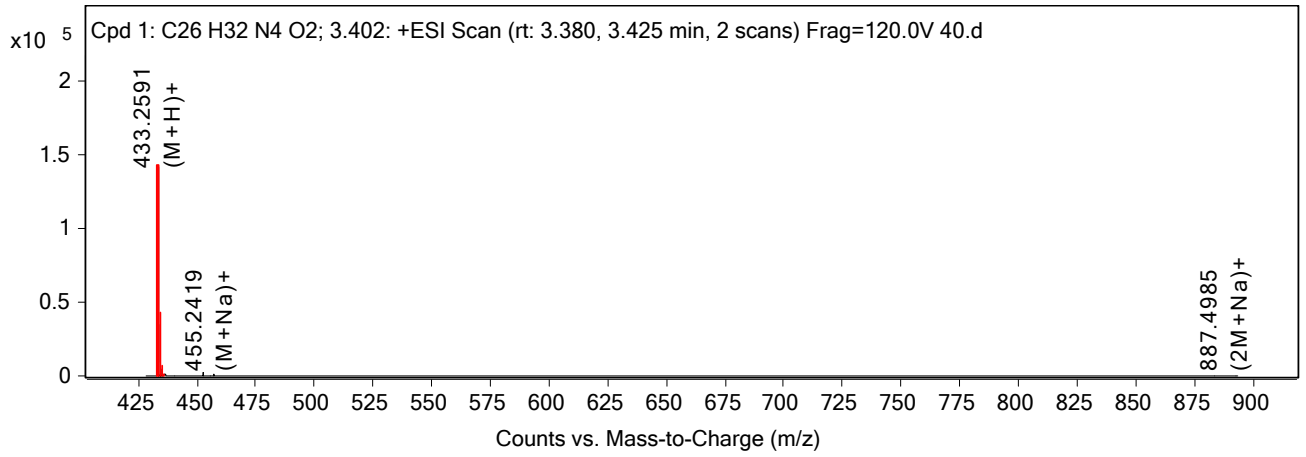
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
433.2591	1	143286.47	(M+H)+
434.262	1	35737.59	(M+H)+
435.2664	1	5114.85	(M+H)+
436.2735	1	623.79	(M+H)+
455.2419	1	402.62	(M+Na)+
456.244	1	215.25	(M+Na)+
887.4985	1	59.47	(2M+Na)+
888.4915	1	44.03	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
433.2591	1	143286.46	(M+H)+	1.52
433.2591		143286.46		
434.262	1	35737.59	(M+H)+	2.1
435.2664	1	5114.85	(M+H)+	-1.39
436.2735	1	623.79	(M+H)+	-11.26
455.2419	1	402.62	(M+Na)+	-0.34
456.244	1	215.25	(M+Na)+	1.88
887.4985	1	59.47	(2M+Na)+	-4.76
888.4915	1	44.03	(2M+Na)+	6.54

--- End Of Report ---

Target Compound Screening Report

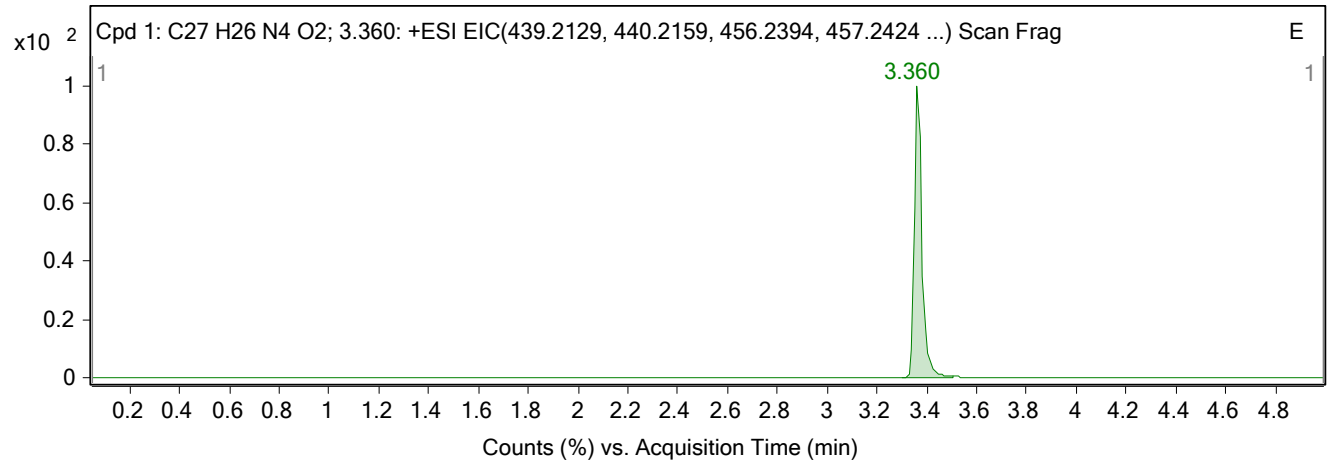
Data File	25.d	**Sample Name**	H2976997
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:01:16 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C27H26N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:01:16 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

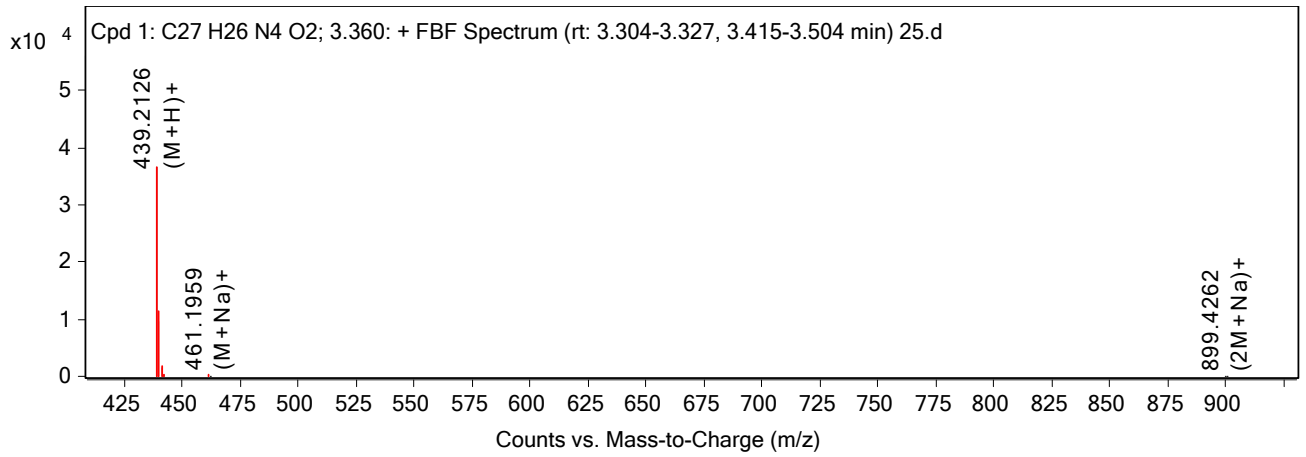
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C27 H26 N4 O2; 3.360	96.9	-0.35	C27 H26 N4 O2	3.36	438.2056	438.2054

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
439.2126	3.36	438.2054	C27 H26 N4 O2	438.2056	-0.35	Find By Formula	

Compound Chromatograms



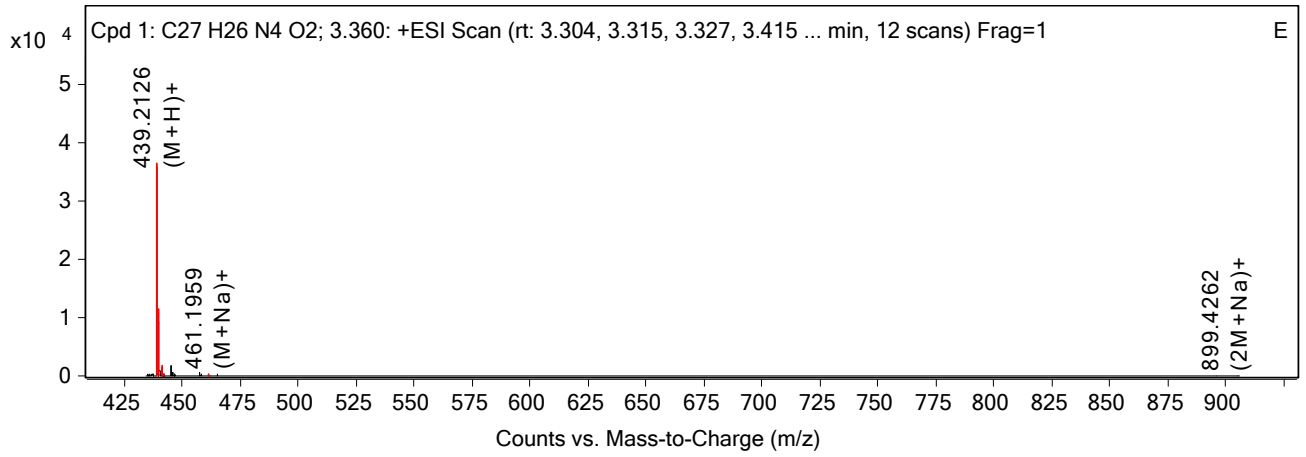
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
439.2126	1	36512.76	(M+H)+
440.2157	1	9708.31	(M+H)+
441.2184	1	1520.41	(M+H)+
442.2188	1	185.88	(M+H)+
461.1959	1	387.07	(M+Na)+
462.2024	1	143.77	(M+Na)+
899.4262	1	77.54	(2M+Na)+
900.4336	1	45.83	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
439.2126	1	36512.76	(M+H)+	0.53
440.2157	1	9708.31	(M+H)+	0.53
441.2184	1	1520.41	(M+H)+	0.96
442.2188	1	185.88	(M+H)+	6.48
461.1959	1	387.07	(M+Na)+	-2.3
462.2024	1	143.77	(M+Na)+	-9.66
899.4262	1	77.54	(2M+Na)+	-28.77
900.4336	1	45.83	(2M+Na)+	-33.45

--- End Of Report ---

Target Compound Screening Report

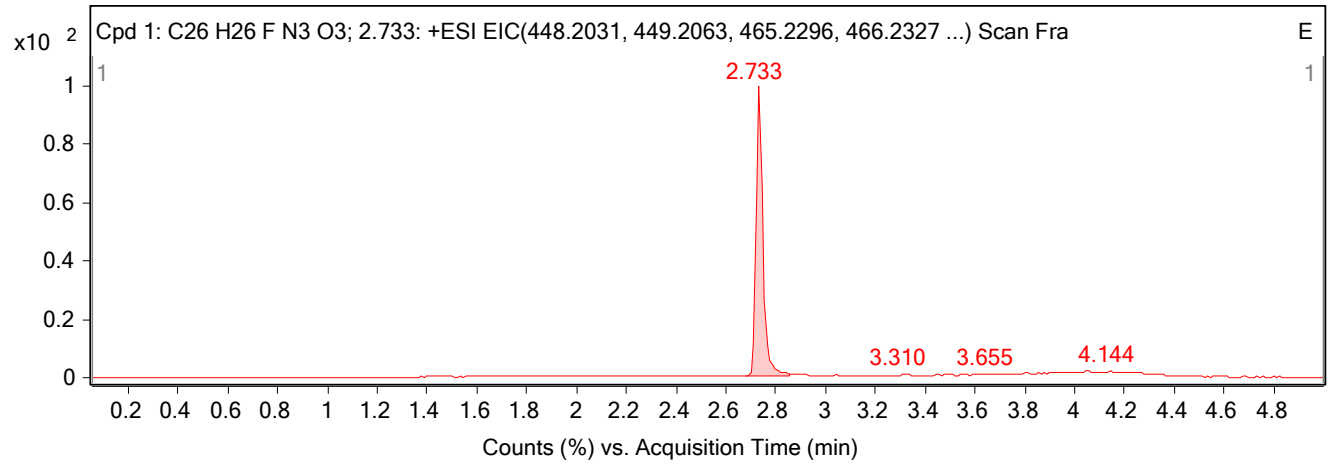
Data File	46.d	**Sample Name**	p211701$2
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 11:03:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H26FN3O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 11:03:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H26 F N3 O3; 2.733	97.53	-2.21	C26 H26 F N3 O3	2.733	447.1958	447.1948

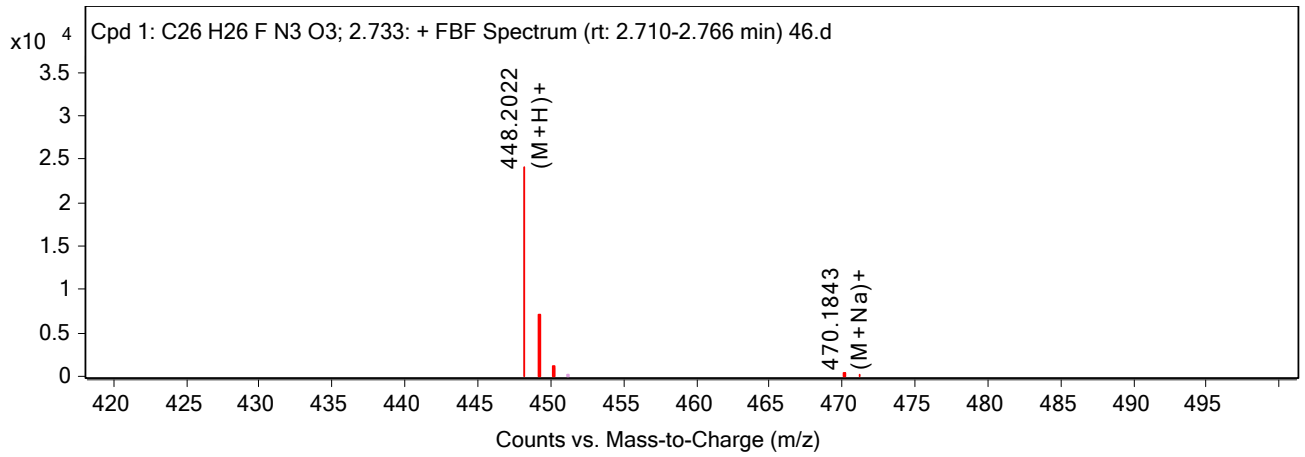
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
448.2022	2.733	447.1948	C26 H26 F N3 O3	447.1958	-2.21	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

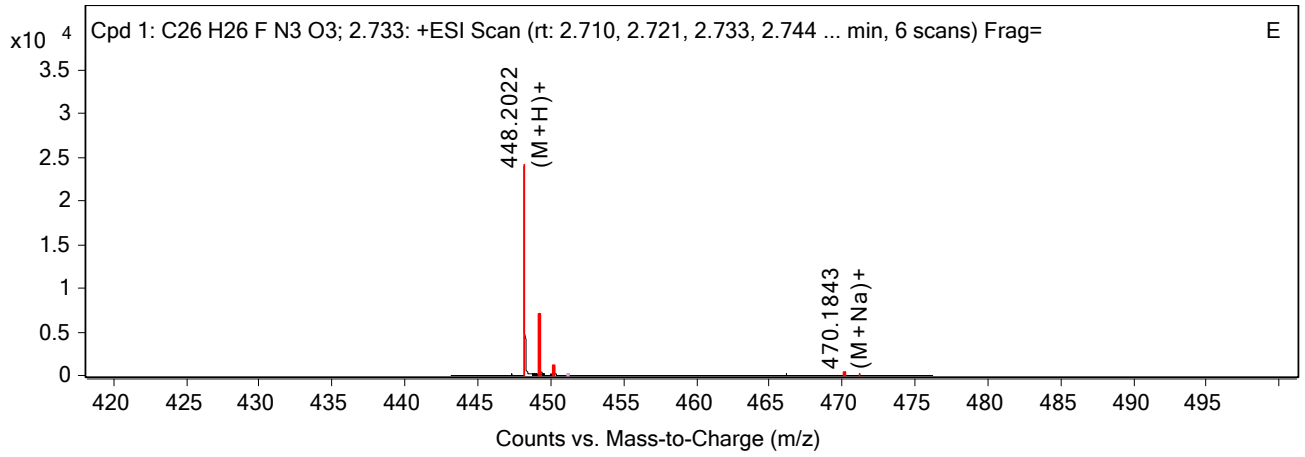
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
448.2022	1	24051.2	(M+H)+
449.205	1	6419.56	(M+H)+
450.2086	1	1003.35	(M+H)+
470.1843	1	350.11	(M+Na)+
471.1823	1	113.31	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
448.2022	1	24051.2	(M+H)+	2.05
448.2022		24051.2		
449.205	1	6419.56	(M+H)+	2.75
450.2086	1	1003.35	(M+H)+	1.28
470.1843	1	350.11	(M+Na)+	1.55
471.1823	1	113.31	(M+Na)+	12.52

--- End Of Report ---

Target Compound Screening Report

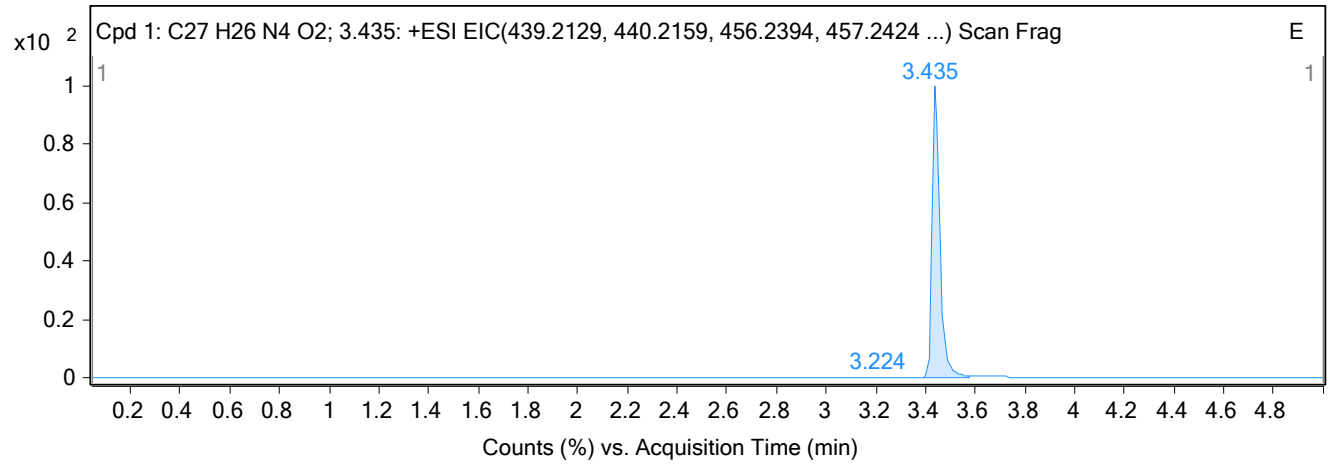
Data File	30.d	**Sample Name**	H2977004
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:29:02 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C27H26N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:29:02 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

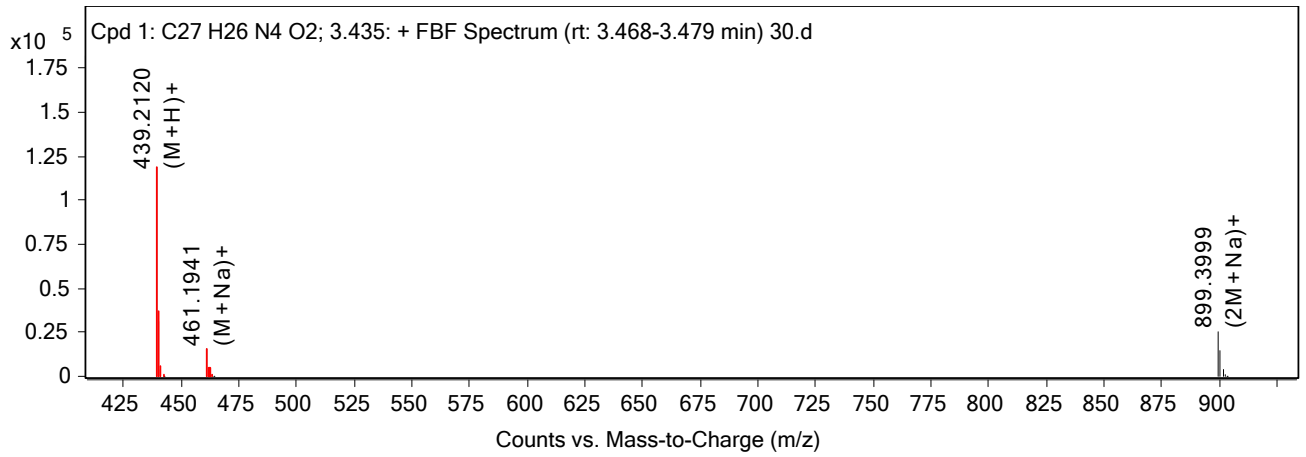
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C27 H26 N4 O2; 3.435	97.5	-2.24	C27 H26 N4 O2	3.435	438.2056	438.2046

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
899.3999	3.435	438.2046	C27 H26 N4 O2	438.2056	-2.24	Find By Formula	

Compound Chromatograms



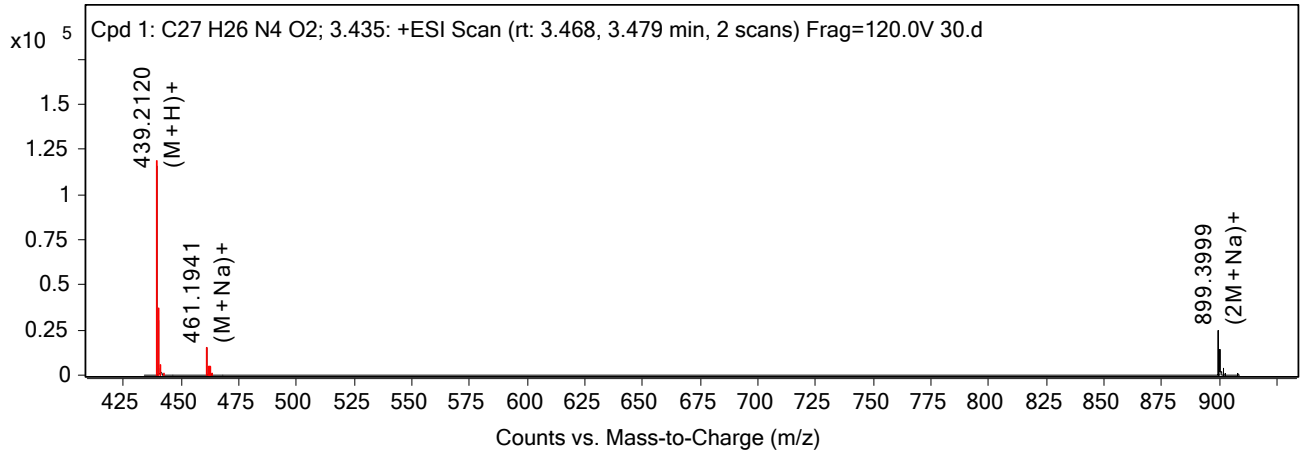
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
439.212	1	118738.65	(M+H)+
440.215	1	30928.34	(M+H)+
441.2181	1	4228.78	(M+H)+
461.1941	1	15278.77	(M+Na)+
462.196	1	4237.02	(M+Na)+
463.1983	1	792.37	(M+Na)+
899.3999	1	25191.49	(2M+Na)+
900.4017	1	14736.32	(2M+Na)+
901.4032	1	4326.79	(2M+Na)+
902.406	1	1160.61	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
439.212	1	118738.65	(M+H)+	2
440.215	1	30928.34	(M+H)+	2.16
441.2181	1	4228.78	(M+H)+	1.68
461.1941	1	15278.77	(M+Na)+	1.56
462.196	1	4237.02	(M+Na)+	4.13
463.1983	1	792.37	(M+Na)+	5.34
899.3999	1	25191.49	(2M+Na)+	0.54
900.4017	1	14736.32	(2M+Na)+	1.96
901.4032	1	4326.79	(2M+Na)+	3.6
902.406	1	1160.61	(2M+Na)+	3.8

--- End Of Report ---

Target Compound Screening Report

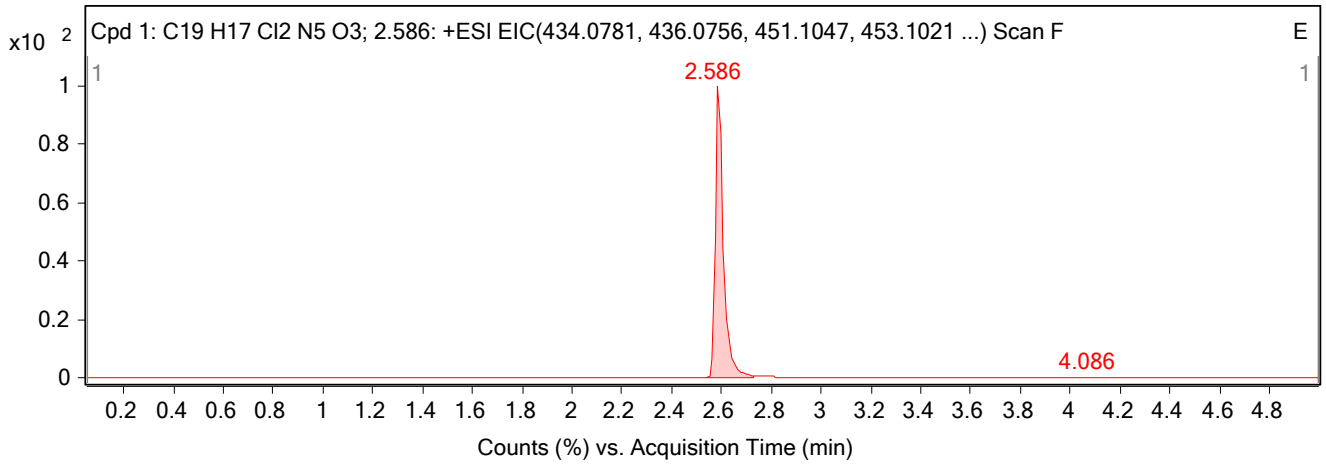
Data File	46.d	**Sample Name**	H1661306
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:26:31 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C19H17Cl2N5O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:26:31 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

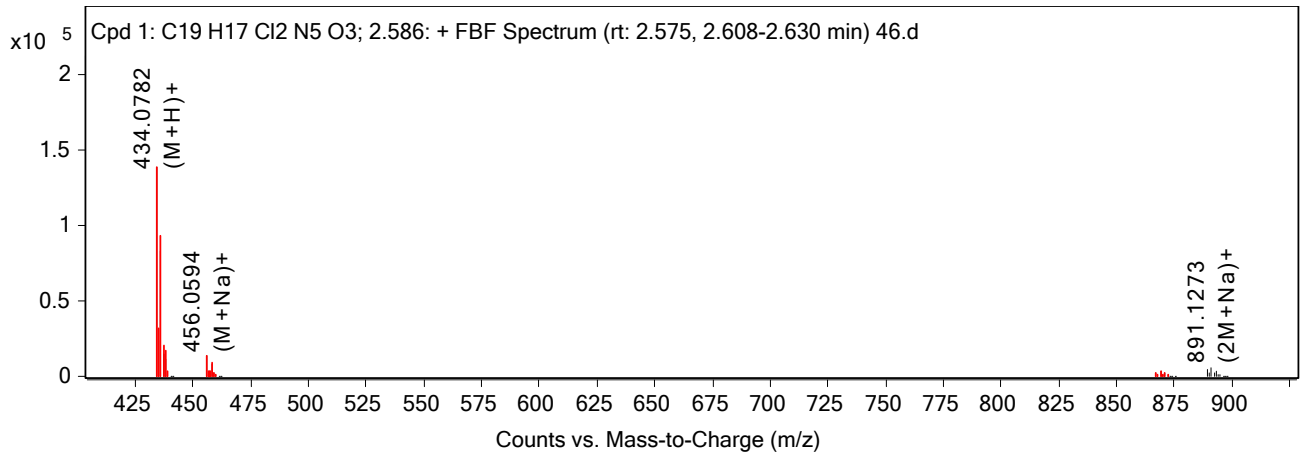
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H17 Cl2 N5 O3; 2.586	97.95	-0.67	C19 H17 Cl2 N5 O3	2.586	433.0708	433.0706

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
891.1273	2.586	433.0706	C19 H17 Cl2 N5 O3	433.0708	-0.67	Find By Formula	

Compound Chromatograms



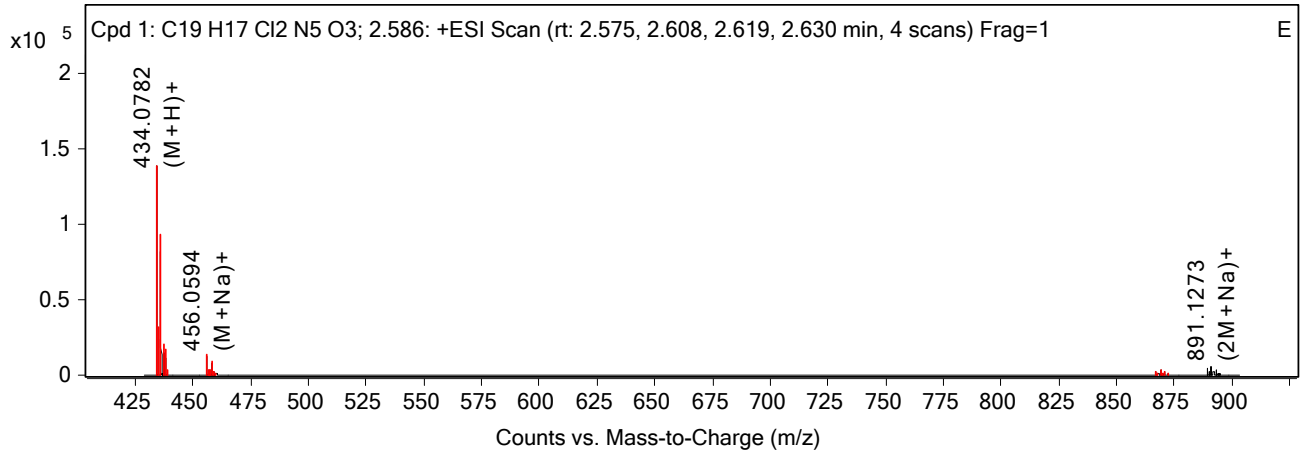
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
434.0782	1	138737.61	(M+H)+
435.0807	1	24407.09	(M+H)+
436.0756	1	83734.3	(M+H)+
437.0779	1	15014.28	(M+H)+
438.0734	1	11507.3	(M+H)+
456.0594	1	13263.06	(M+Na)+
458.0569	1	7998.1	(M+Na)+
869.1443	1	3375.26	(2M+H)+
889.1287	1	4089.35	(2M+Na)+
891.1273	1	5900.84	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
434.0782	1	138737.61	(M+H)+	-0.15
435.0807	1	24407.09	(M+H)+	0.67
436.0756	1	83734.3	(M+H)+	-0.13
437.0779	1	15014.28	(M+H)+	0.7
438.0734	1	11507.3	(M+H)+	0.39
456.0594	1	13263.06	(M+Na)+	1.44
458.0569	1	7998.1	(M+Na)+	1.36
869.1443	1	3375.26	(2M+H)+	2.72
889.1287	1	4089.35	(2M+Na)+	2.46
891.1273	1	5900.84	(2M+Na)+	1.47

--- End Of Report ---

Target Compound Screening Report

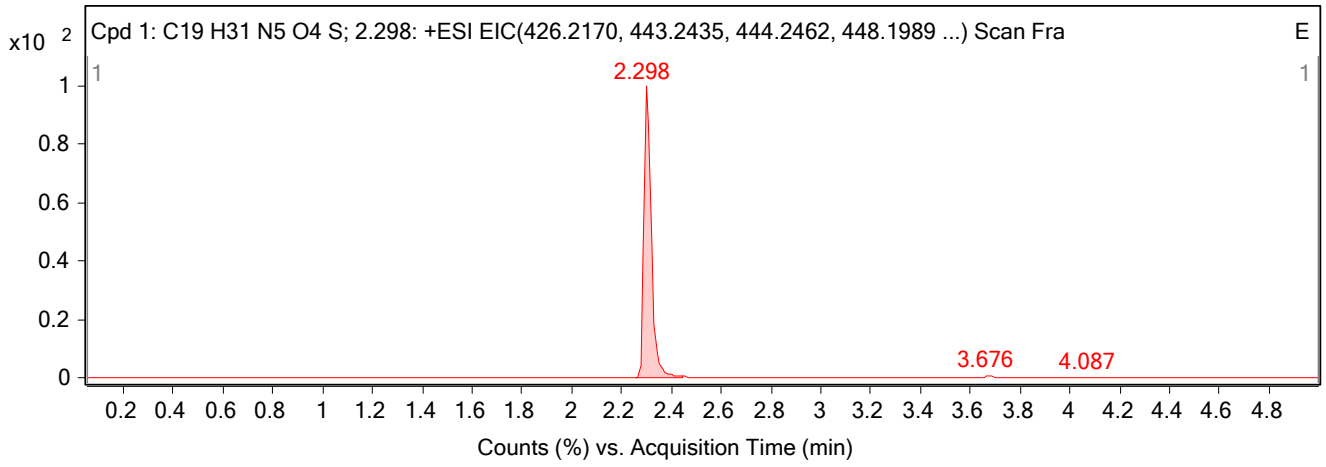
Data File	34.d	**Sample Name**	H1660633
Sample Type	Sample	**Position**	P1-D7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:19:56 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C19H31N5O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:19:56 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

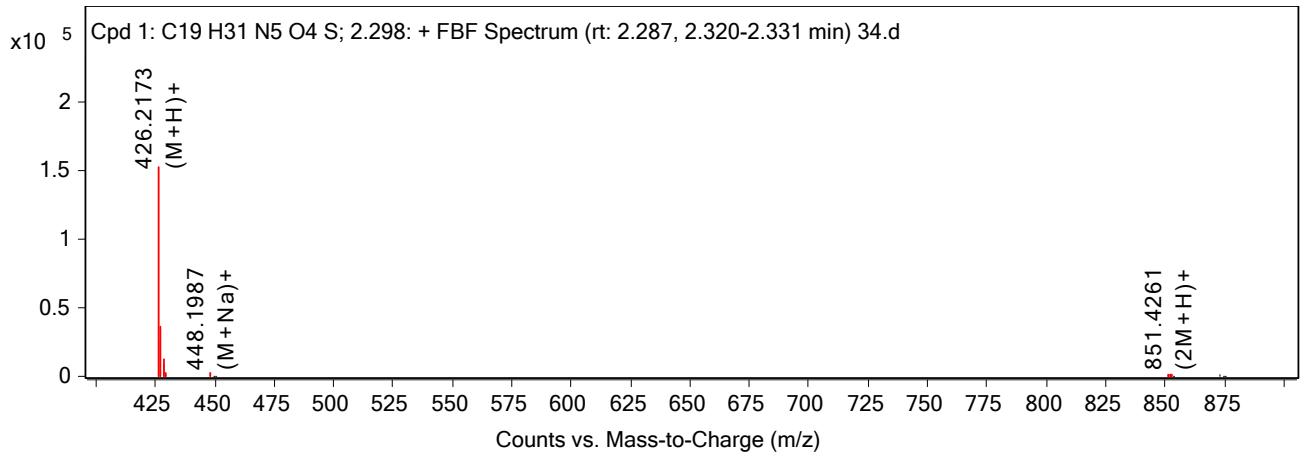
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H31 N5 O4 S; 2.298	97.93	0.77	C19 H31 N5 O4 S	2.298	425.2097	425.21

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
448.1987	2.298	425.21	C19 H31 N5 O4 S	425.2097	0.77	Find By Formula	

Compound Chromatograms



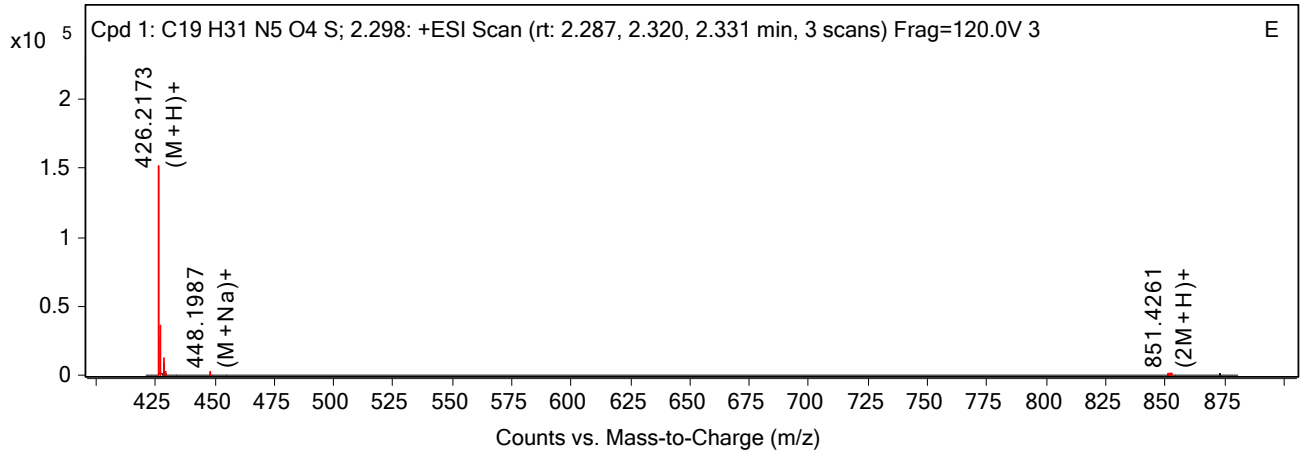
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
426.2173	1	152303.09	(M+H)+
427.22	1	27819.89	(M+H)+
428.2172	1	8336.16	(M+H)+
429.2201	1	1441.47	(M+H)+
448.1987	1	2499.93	(M+Na)+
449.2008	1	634.84	(M+Na)+
851.4261	1	1635.89	(2M+H)+
852.4288	1	836.76	(2M+H)+
873.4081	1	1021.73	(2M+Na)+
874.408	1	486.63	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
426.2173	1	152303.09	(M+H)+	-0.88
427.22	1	27819.89	(M+H)+	-0.7
428.2172	1	8336.16	(M+H)+	-0.72
429.2201	1	1441.47	(M+H)+	-4.52
448.1987	1	2499.93	(M+Na)+	0.33
449.2008	1	634.84	(M+Na)+	1.87
851.4261	1	1635.89	(2M+H)+	0.64
852.4288	1	836.76	(2M+H)+	0.73
873.4081	1	1021.73	(2M+Na)+	0.54
874.408	1	486.63	(2M+Na)+	3.8

--- End Of Report ---

Target Compound Screening Report

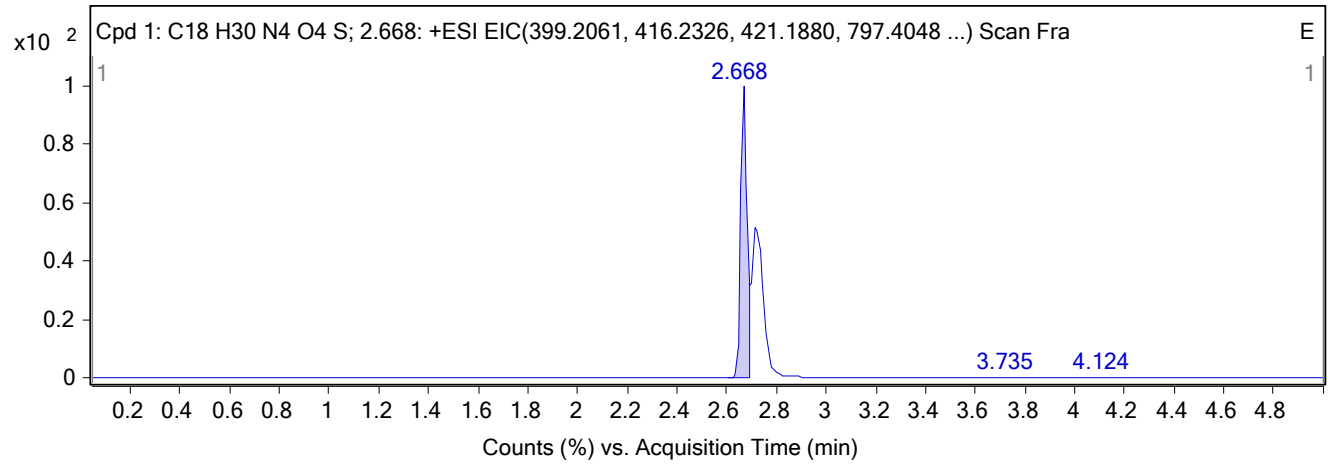
Data File	48.d	**Sample Name**	H1663678
Sample Type	Sample	**Position**	P1-F3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:37:34 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C18H30N4O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:37:34 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

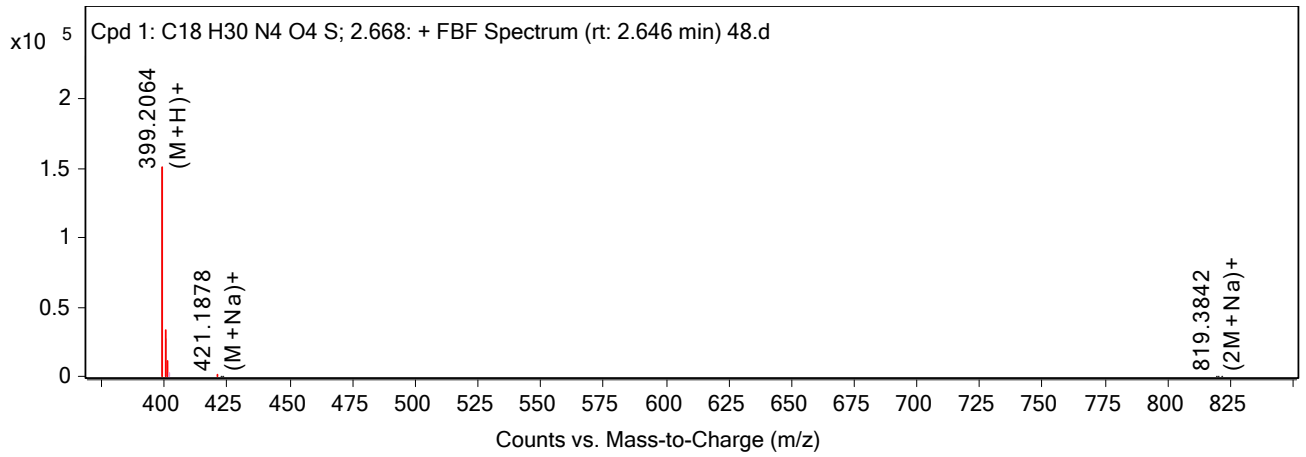
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C18 H30 N4 O4 S; 2.668	95.33	0.85	C18 H30 N4 O4 S	2.668	398.1988	398.1991

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
399.2064	2.668	398.1991	C18 H30 N4 O4 S	398.1988	0.85	Find By Formula	

Compound Chromatograms



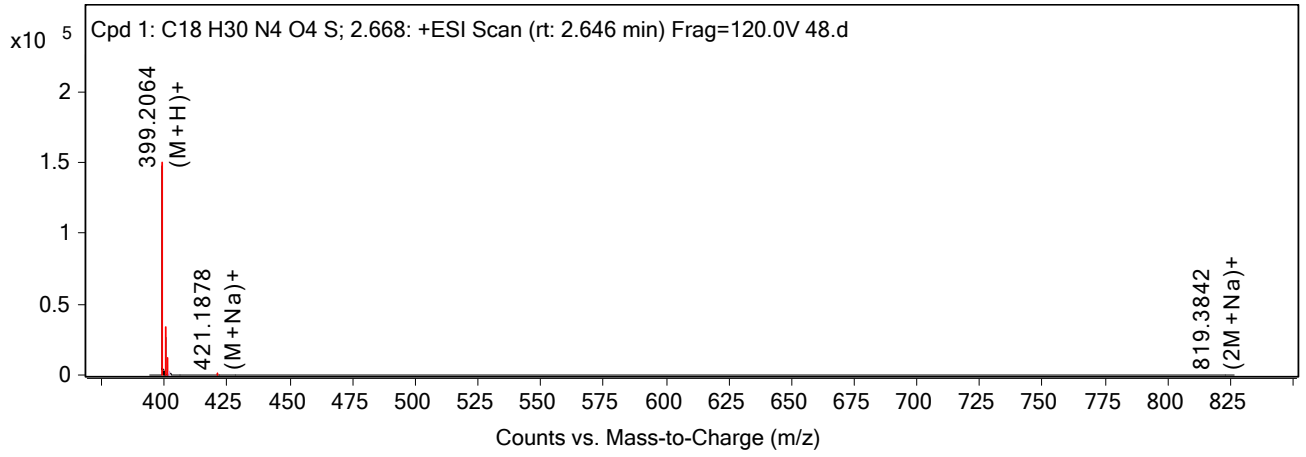
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
399.2064	1	150441.56	(M+H)+
400.2094	1	26965.12	(M+H)+
401.2059	1	7613.94	(M+H)+
421.1878	1	1081.75	(M+Na)+
422.1976	1	212.13	(M+Na)+
423.1797	1	220.29	(M+Na)+
819.3842	1	574.72	(2M+Na)+
820.3819	1	388	(2M+Na)+
821.3729	1	143.67	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
399.2064	1	150441.55	(M+H)+	-0.94
400.2094	1	26965.12	(M+H)+	-1.21
401.2059	1	7613.94	(M+H)+	-0.32
421.1878	1	1081.75	(M+Na)+	0.56
422.1976	1	212.13	(M+Na)+	-16.04
423.1797	1	220.29	(M+Na)+	19.1
819.3842	1	574.72	(2M+Na)+	3.17
820.3819	1	388	(2M+Na)+	9.41
821.3729	1	143.67	(2M+Na)+	18.35

--- End Of Report ---

Target Compound Screening Report

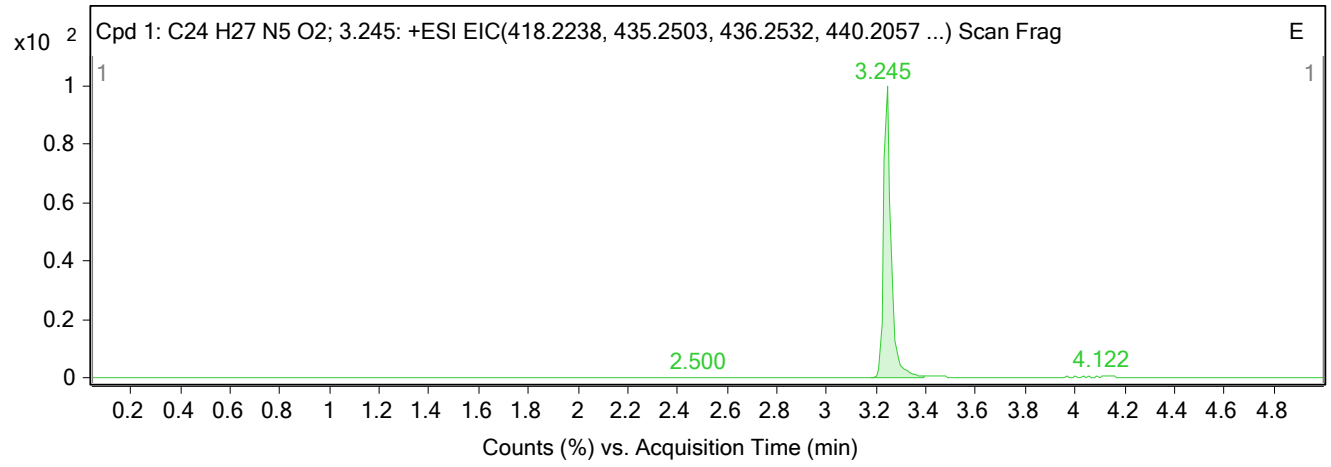
Data File	35.d	**Sample Name**	H2980916
Sample Type	Sample	**Position**	P1-D8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:29:13 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H27N5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:29:13 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

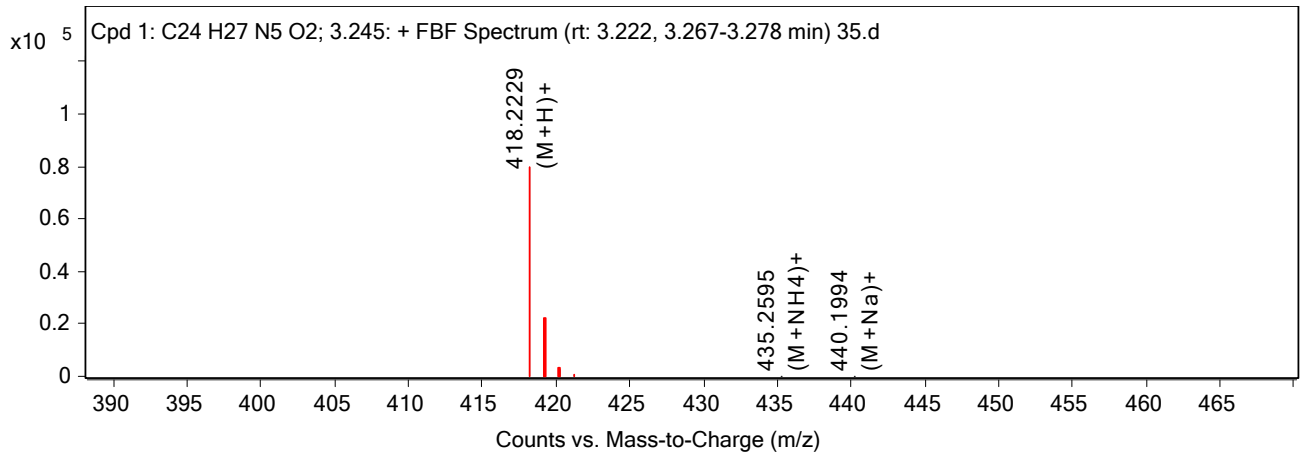
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H27 N5 O2; 3.245	95.03	-1.92	C24 H27 N5 O2	3.245	417.2165	417.2157

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
418.2229	3.245	417.2157	C24 H27 N5 O2	417.2165	-1.92	Find By Formula	

Compound Chromatograms



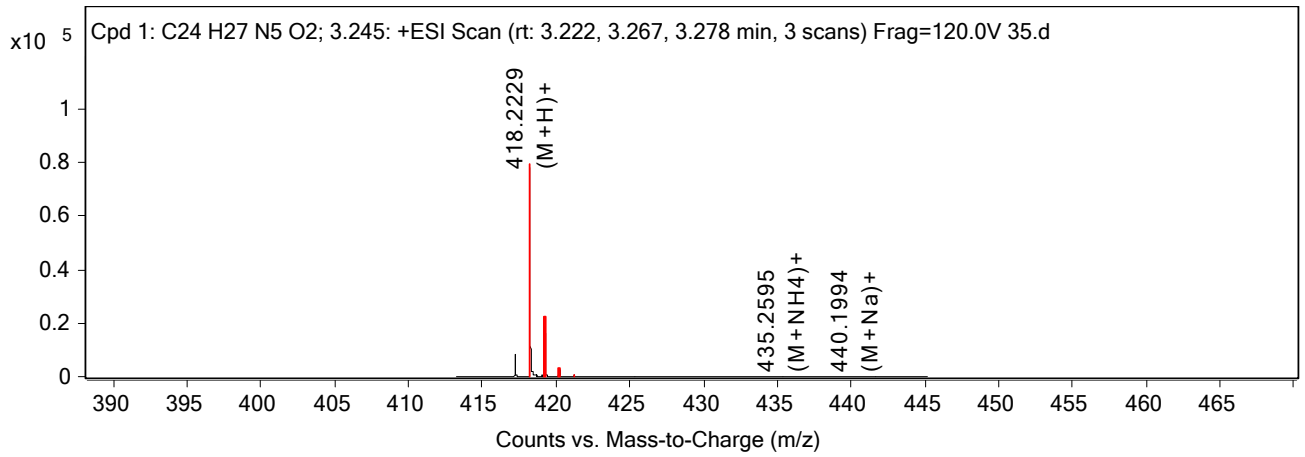
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
418.2229	1	79623.73	(M+H)+
419.2261	1	18527.39	(M+H)+
420.2298	1	2614.28	(M+H)+
421.2323	1	404.32	(M+H)+
435.2595	1	119.75	(M+NH4)+
440.1994	1	190.34	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
418.2229	1	79623.72	(M+H)+	2.12
418.2229		79623.72		
419.2261	1	18527.39	(M+H)+	1.46
420.2298	1	2614.28	(M+H)+	-0.6
421.2323	1	404.32	(M+H)+	-0.15
435.2595	1	119.75	(M+NH4)+	-21.08
440.1994	1	190.34	(M+Na)+	14.25

--- End Of Report ---

Target Compound Screening Report

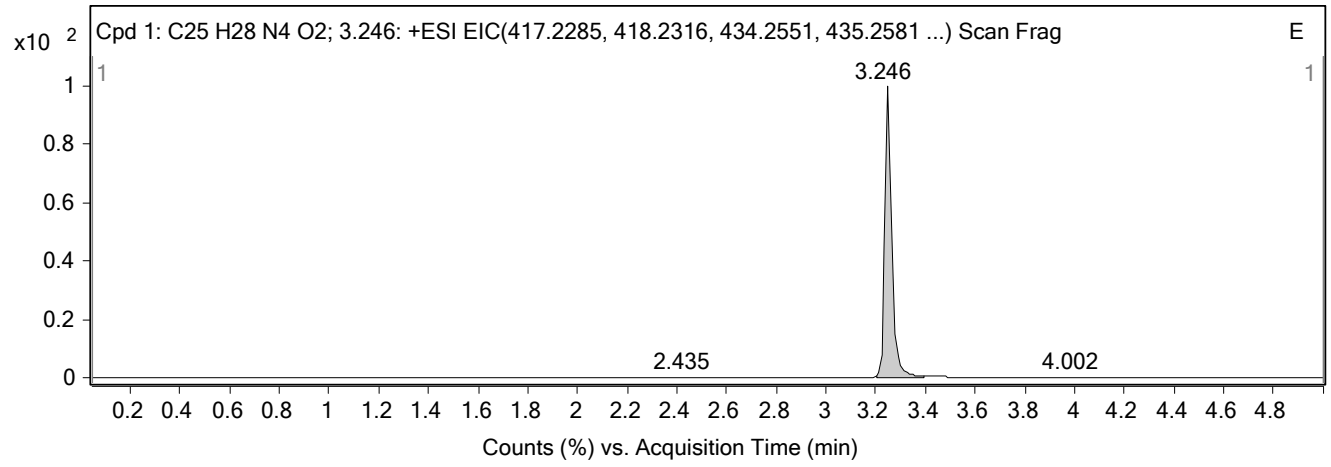
Data File	29-3.d	**Sample Name**	H2976996
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:54:26 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:54:26 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O2; 3.246	94.5	0.42	C25 H28 N4 O2	3.246	416.2212	416.2214

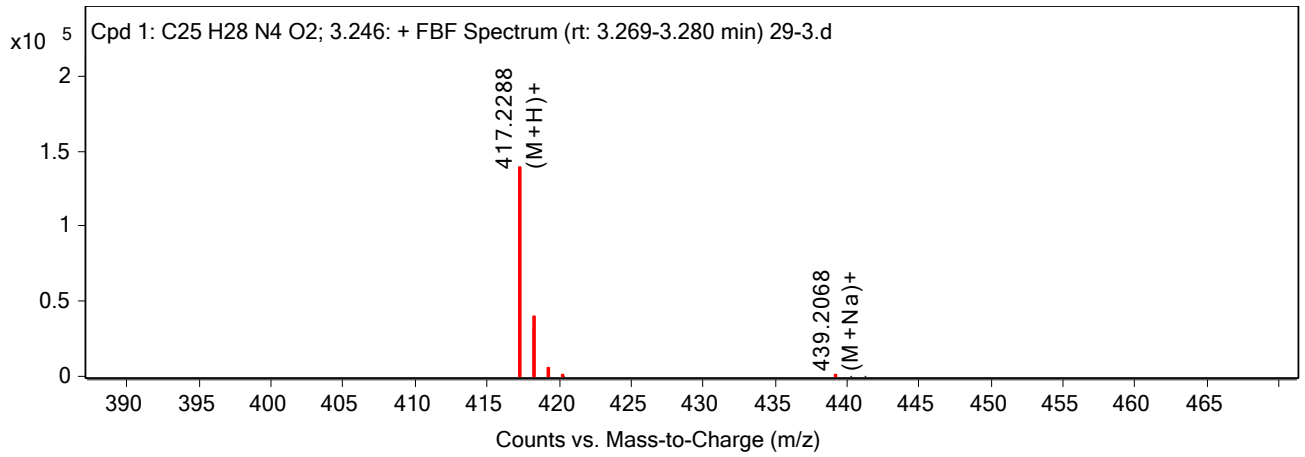
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
417.2288	3.246	416.2214	C25 H28 N4 O2	416.2212	0.42	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

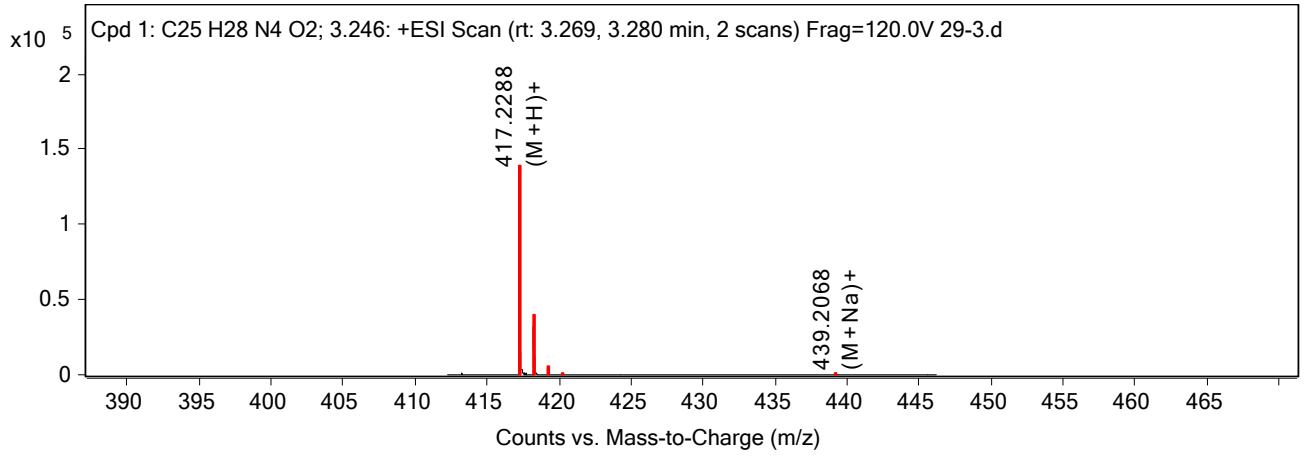
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
417.2288	1	139169.81	(M+H)+
418.2316	1	32177.25	(M+H)+
419.234	1	4238.26	(M+H)+
420.2404	1	446.89	(M+H)+
439.2068	1	952.57	(M+Na)+
440.2081	1	293.52	(M+Na)+
441.2135	1	91	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
417.2288	1	139169.81	(M+H)+	-0.6
418.2316	1	32177.25	(M+H)+	-0.14
419.234	1	4238.26	(M+H)+	1.13
420.2404	1	446.89	(M+H)+	-7.64
439.2068	1	952.57	(M+Na)+	8.22
440.2081	1	293.52	(M+Na)+	12.27
441.2135	1	91	(M+Na)+	6.54

--- End Of Report ---

Target Compound Screening Report

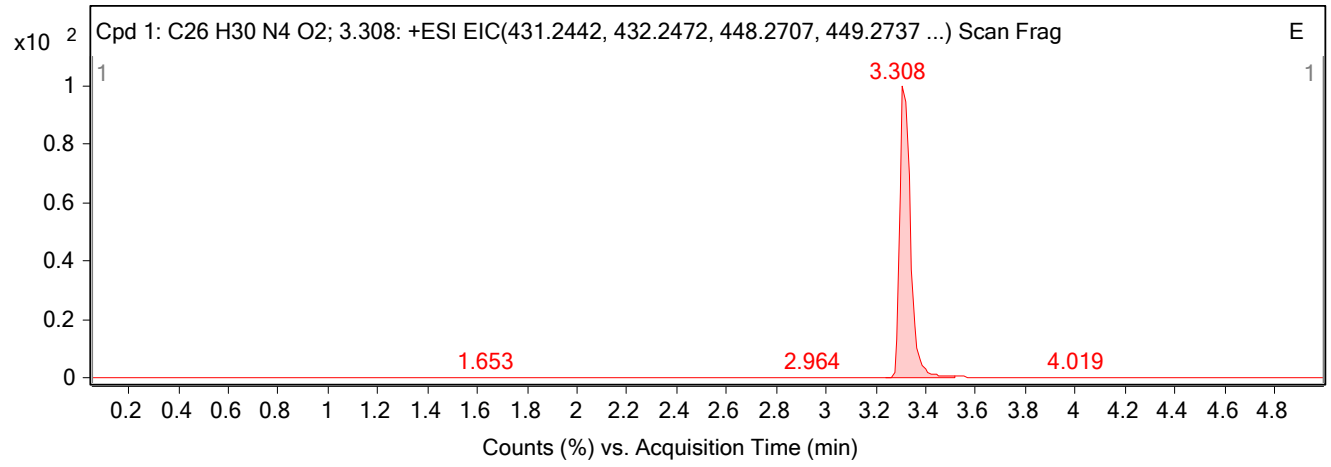
Data File	37.d	**Sample Name**	H2978811
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:07:55 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:07:55 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

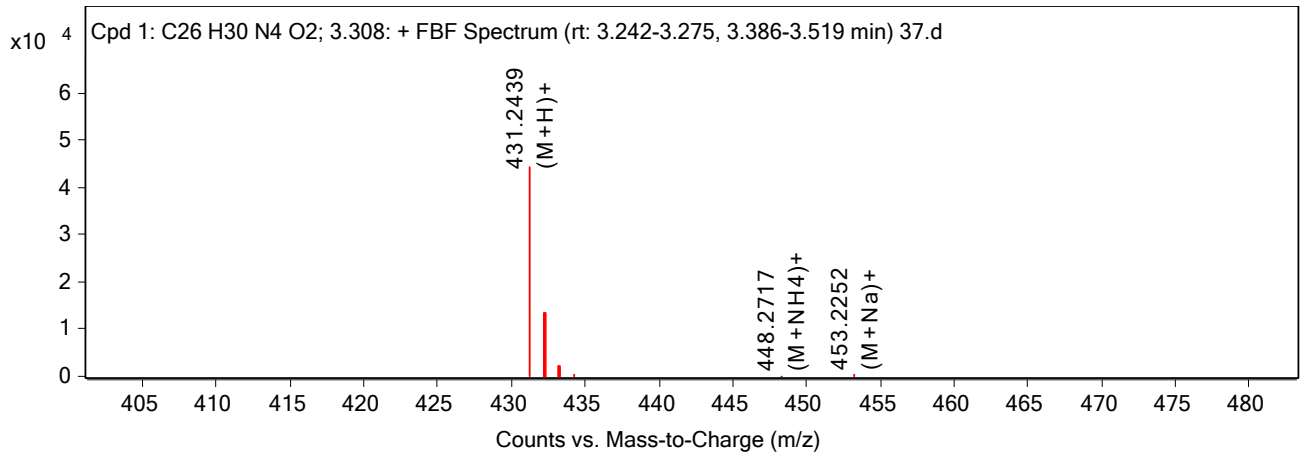
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O2; 3.308	97.06	-0.5	C26 H30 N4 O2	3.308	430.2369	430.2367

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
431.2439	3.308	430.2367	C26 H30 N4 O2	430.2369	-0.5	Find By Formula	

Compound Chromatograms



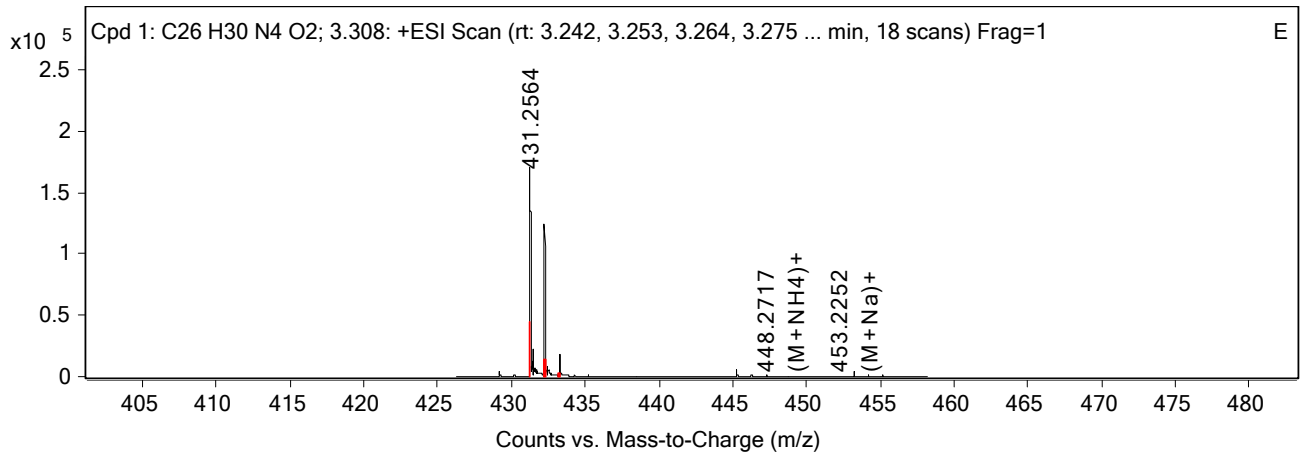
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
431.2439	1	44286.14	(M+H)+
432.2469	1	11408.54	(M+H)+
433.25	1	1690.88	(M+H)+
434.2538	1	224.21	(M+H)+
448.2717	1	130.71	(M+NH4)+
453.2252	1	378.63	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
431.2439	1	44286.14	(M+H)+	0.47
431.2564		170359.95		
432.2469	1	11408.54	(M+H)+	0.67
433.25	1	1690.88	(M+H)+	0.35
434.2538	1	224.21	(M+H)+	-1.98
448.2717	1	130.71	(M+NH4)+	-2.27
453.2252	1	378.63	(M+Na)+	1.89

--- End Of Report ---

Target Compound Screening Report

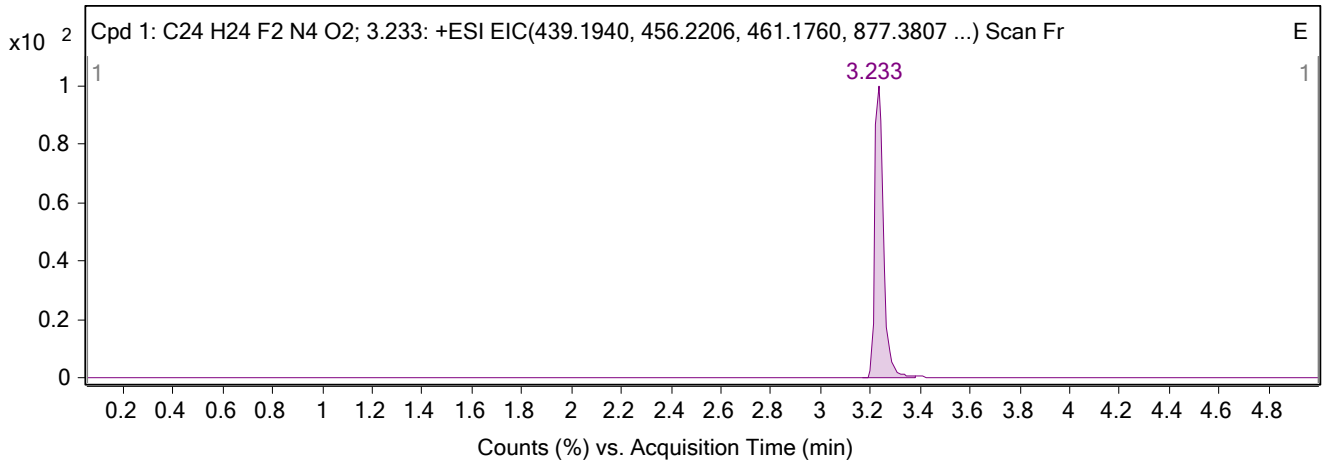
Data File	27.d	**Sample Name**	H2976999
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:12:23 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H24F2N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:12:23 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

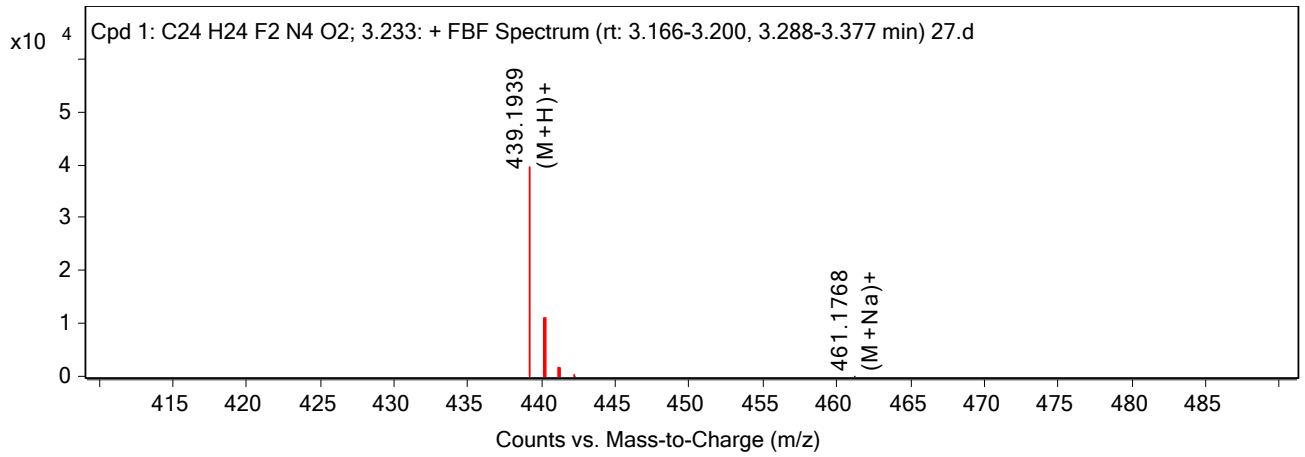
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H24 F2 N4 O2; 3.233	96.58	-0.23	C24 H24 F2 N4 O2	3.233	438.1867	438.1866

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
439.1939	3.233	438.1866	C24 H24 F2 N4 O2	438.1867	-0.23	Find By Formula	

Compound Chromatograms



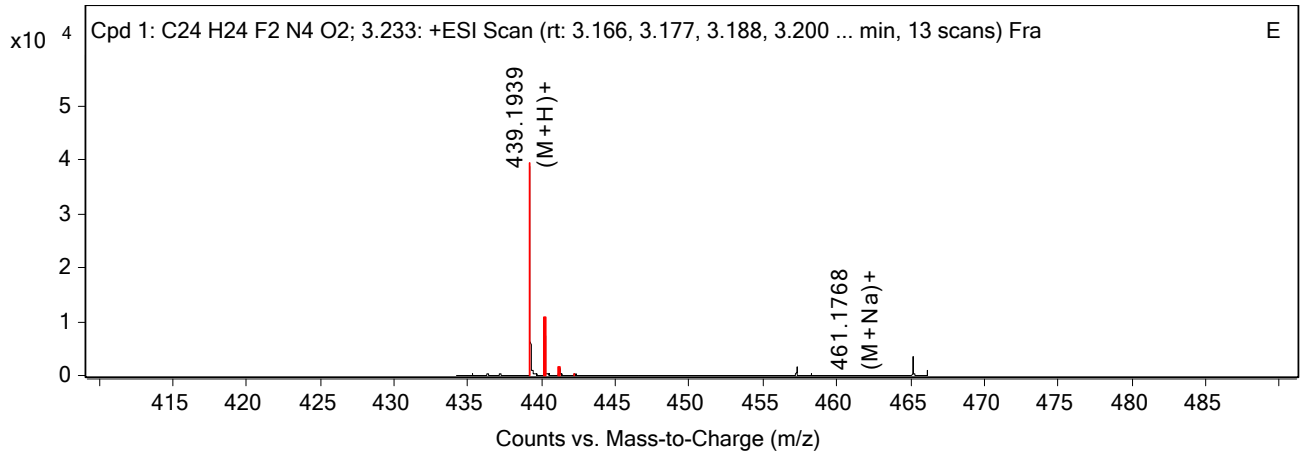
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
439.1939	1	39488.62	(M+H)+
440.1969	1	9223.66	(M+H)+
441.2007	1	1331.97	(M+H)+
442.201	1	180.49	(M+H)+
461.1768	1	90.23	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
439.1939	1	39488.62	(M+H)+	0.23
440.1969	1	9223.66	(M+H)+	0.45
441.2007	1	1331.97	(M+H)+	-1.85
442.201	1	180.49	(M+H)+	3.77
461.1768	1	90.23	(M+Na)+	-1.77

--- End Of Report ---

Target Compound Screening Report

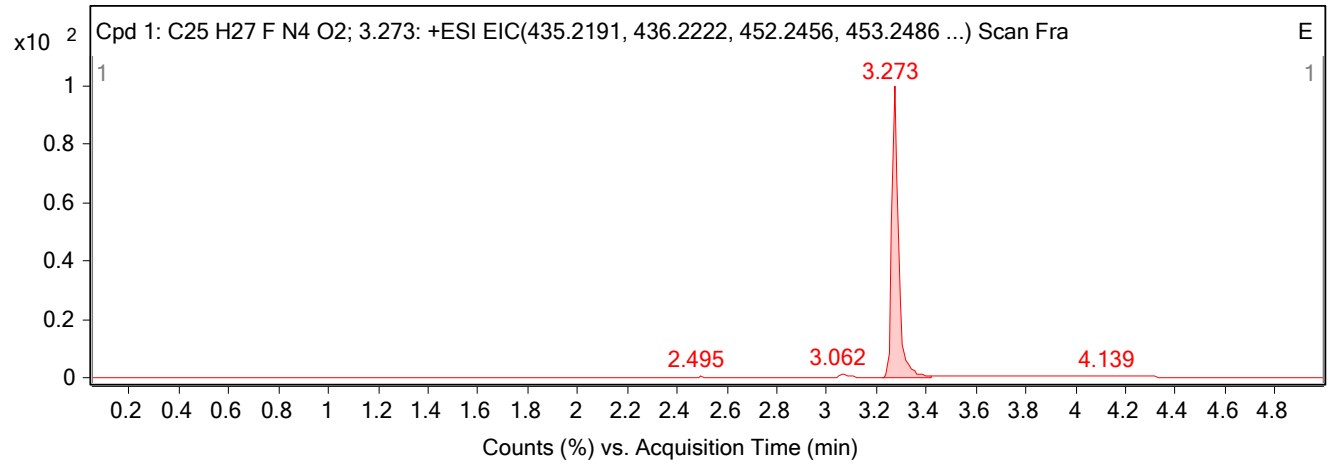
Data File	15.d	**Sample Name**	H2982407
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:42:15 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H27FN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:42:15 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

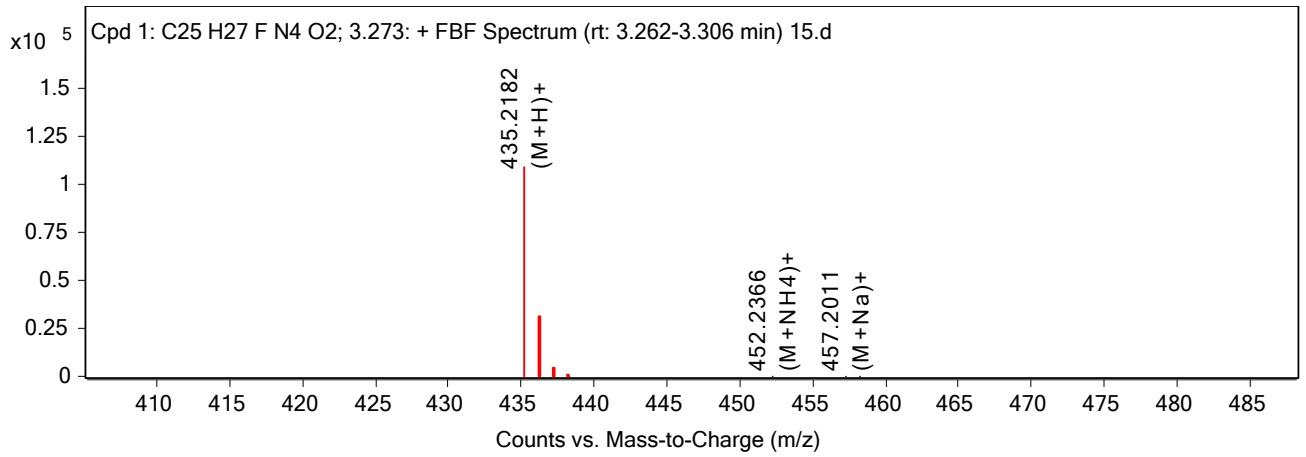
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H27 F N4 O2; 3.273	94.41	-2.01	C25 H27 F N4 O2	3.273	434.2118	434.2109

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
435.2182	3.273	434.2109	C25 H27 F N4 O2	434.2118	-2.01	Find By Formula	

Compound Chromatograms



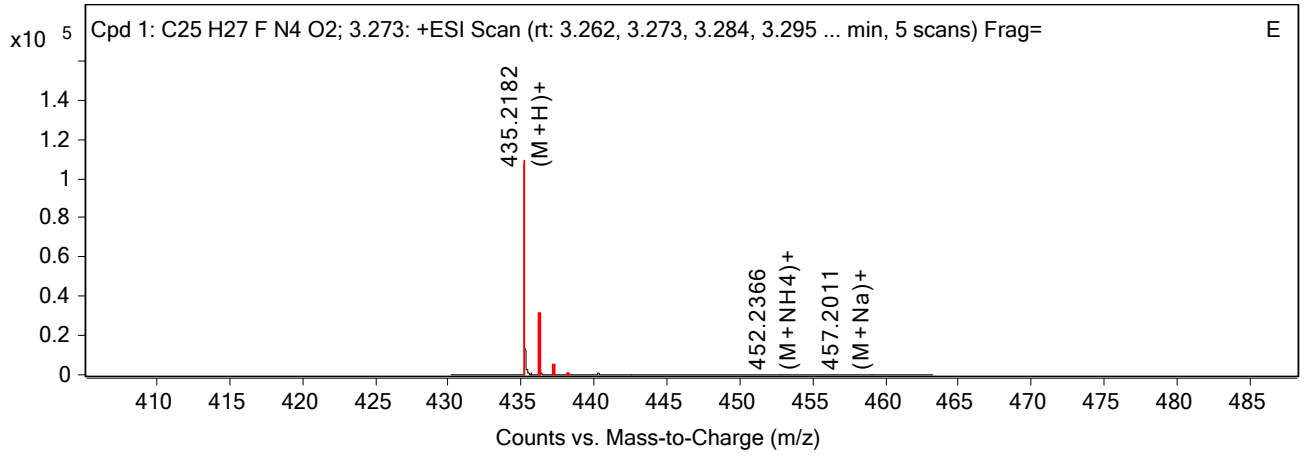
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
435.2182	1	108911.49	(M+H)+
436.2214	1	25626.43	(M+H)+
437.2231	1	3456.38	(M+H)+
438.2285	1	402.54	(M+H)+
452.2366	1	152.4	(M+NH4)+
457.2011	1	279.1	(M+Na)+
458.1971	1	102.73	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
435.2182	1	108911.49	(M+H)+	1.95
435.2182		108911.49		
436.2214	1	25626.43	(M+H)+	1.81
437.2231	1	3456.38	(M+H)+	4.36
438.2285	1	402.54	(M+H)+	-1.51
452.2366	1	152.4	(M+NH4)+	20
457.2011	1	279.1	(M+Na)+	-0.15
458.1971	1	102.73	(M+Na)+	15.34

--- End Of Report ---

Target Compound Screening Report

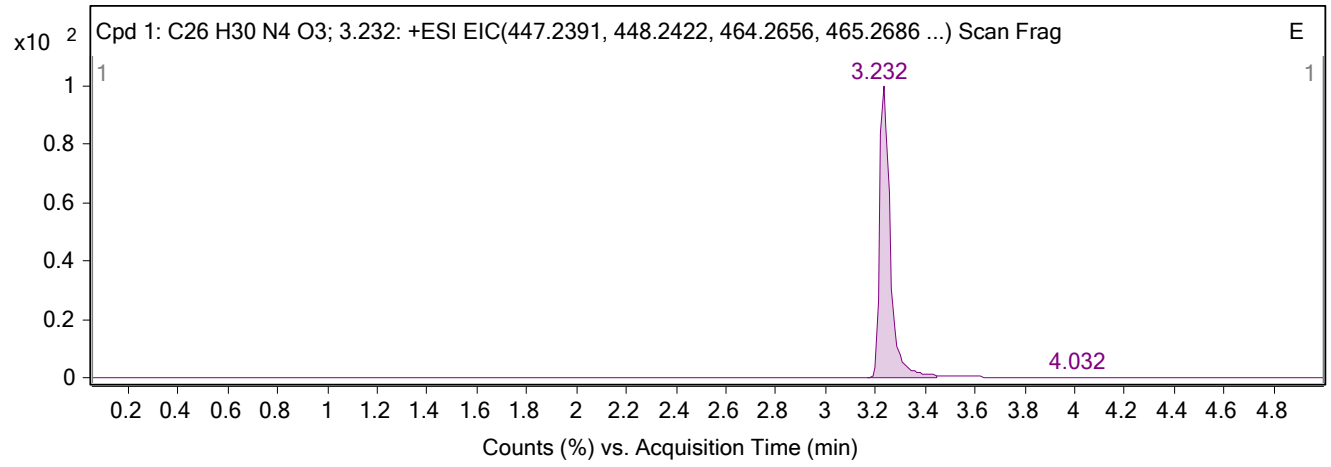
Data File	51.d	**Sample Name**	H2978812
Sample Type	Sample	**Position**	P1-F6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:25:41 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:25:41 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

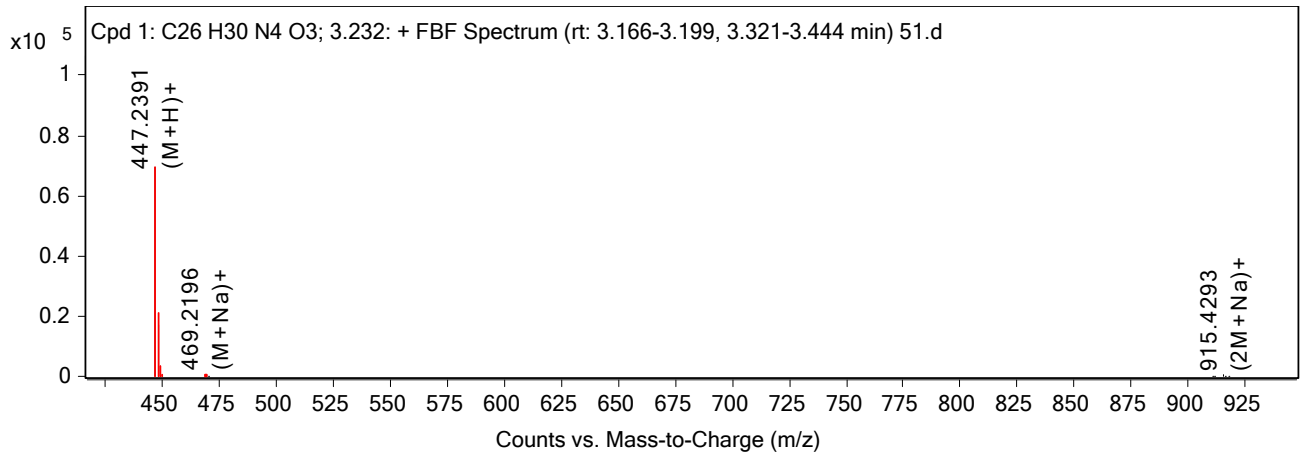
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O3; 3.232	95.15	-0.89	C26 H30 N4 O3	3.232	446.2318	446.2314

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2391	3.232	446.2314	C26 H30 N4 O3	446.2318	-0.89	Find By Formula	

Compound Chromatograms



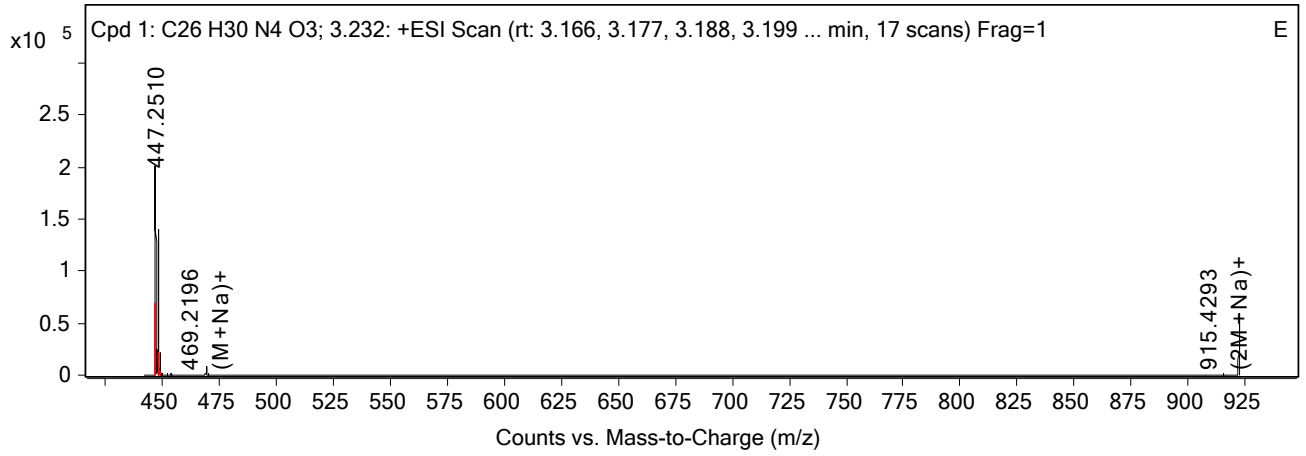
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2391	1	69393.39	(M+H)+
448.2418	1	17151.14	(M+H)+
449.243	1	3168.75	(M+H)+
450.2426	1	493.79	(M+H)+
469.2196	1	639.33	(M+Na)+
470.2214	1	236.99	(M+Na)+
910.4736	1	84.03	(2M+NH4)+
915.4293	1	428.8	(2M+Na)+
916.4323	1	222.98	(2M+Na)+
917.4314	1	113.23	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2391	1	69393.39	(M+H)+	-0.03
448.2418	1	17151.14	(M+H)+	0.75
449.243	1	3168.75	(M+H)+	4.34
450.2426	1	493.79	(M+H)+	11.35
469.2196	1	639.33	(M+Na)+	2.93
470.2214	1	236.99	(M+Na)+	5.66
910.4736	1	84.03	(2M+NH4)+	26.2
915.4293	1	428.8	(2M+Na)+	25.67
916.4323	1	222.98	(2M+Na)+	25.7
917.4314	1	113.23	(2M+Na)+	29.92

--- End Of Report ---

Target Compound Screening Report

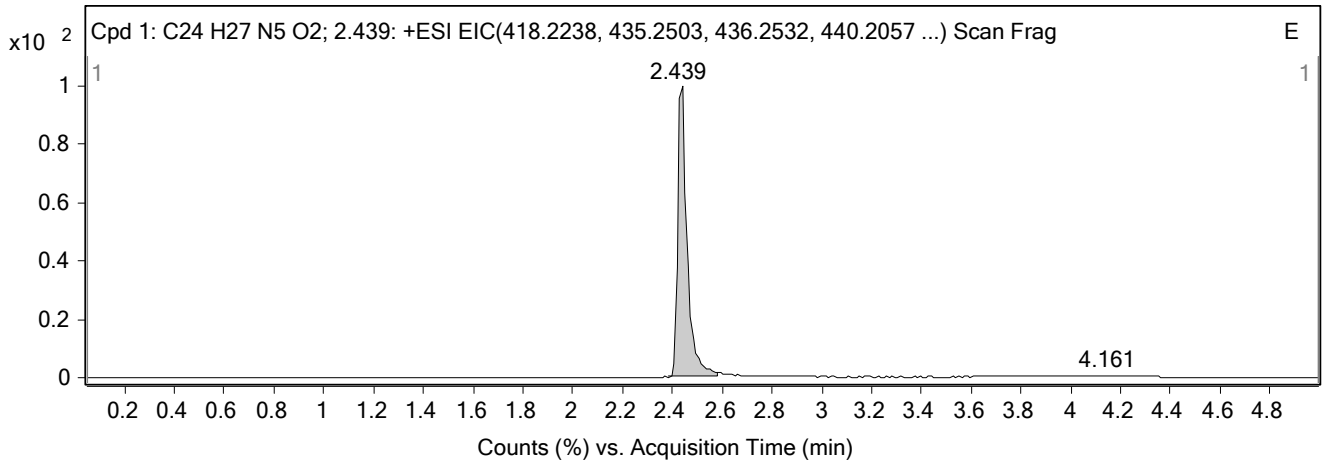
Data File	23.d	**Sample Name**	H2997284
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:50:08 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H27N5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:50:08 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

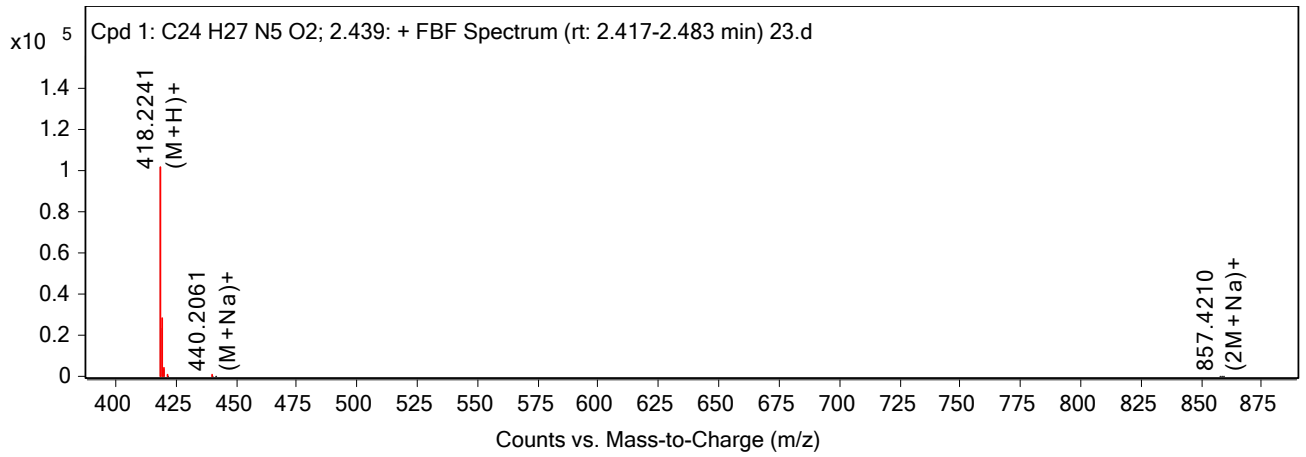
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H27 N5 O2; 2.439	95.42	0.87	C24 H27 N5 O2	2.439	417.2165	417.2168

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
418.2241	2.439	417.2168	C24 H27 N5 O2	417.2165	0.87	Find By Formula	

Compound Chromatograms



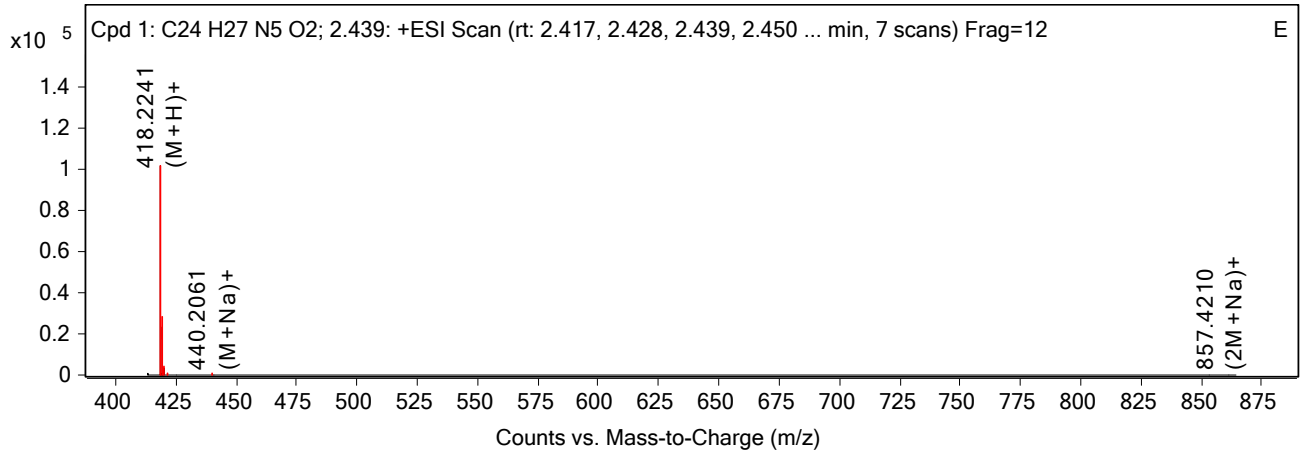
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
418.2241	1	101648.93	(M+H)+
419.2271	1	23430.54	(M+H)+
420.2294	1	3136.55	(M+H)+
421.2344	1	327.74	(M+H)+
440.2061	1	439	(M+Na)+
441.2091	1	174.28	(M+Na)+
857.421	1	130.35	(2M+Na)+
858.4236	1	94.52	(2M+Na)+
859.4354	1	43.05	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
418.2241	1	101648.93	(M+H)+	-0.89
419.2271	1	23430.54	(M+H)+	-0.88
420.2294	1	3136.55	(M+H)+	0.31
421.2344	1	327.74	(M+H)+	-5.23
440.2061	1	439	(M+Na)+	-0.85
441.2091	1	174.28	(M+Na)+	-1.03
857.421	1	130.35	(2M+Na)+	1.38
858.4236	1	94.52	(2M+Na)+	1.8
859.4354	1	43.05	(2M+Na)+	-8.54

--- End Of Report ---

Target Compound Screening Report

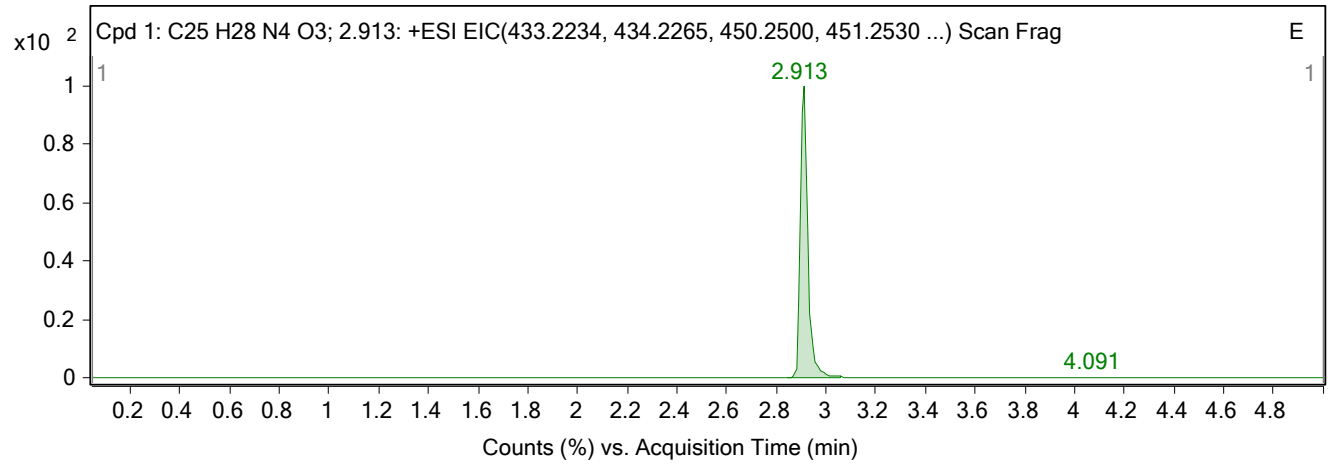
Data File	35.d	**Sample Name**	H3002224
Sample Type	Sample	**Position**	P1-D8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:25:29 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:25:29 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

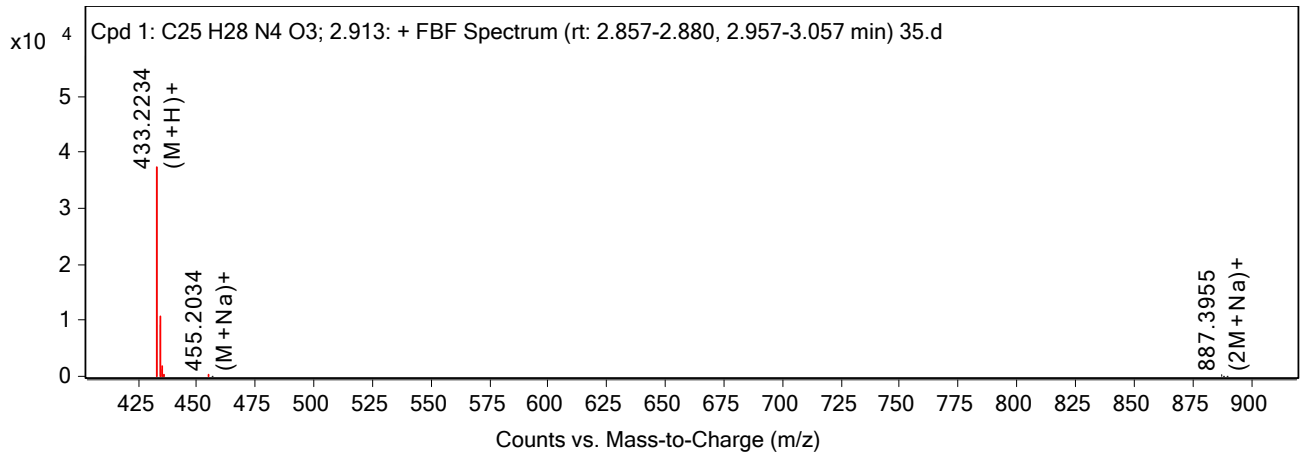
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O3; 2.913	96.85	-0.56	C25 H28 N4 O3	2.913	432.2161	432.2159

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
433.2234	2.913	432.2159	C25 H28 N4 O3	432.2161	-0.56	Find By Formula	

Compound Chromatograms



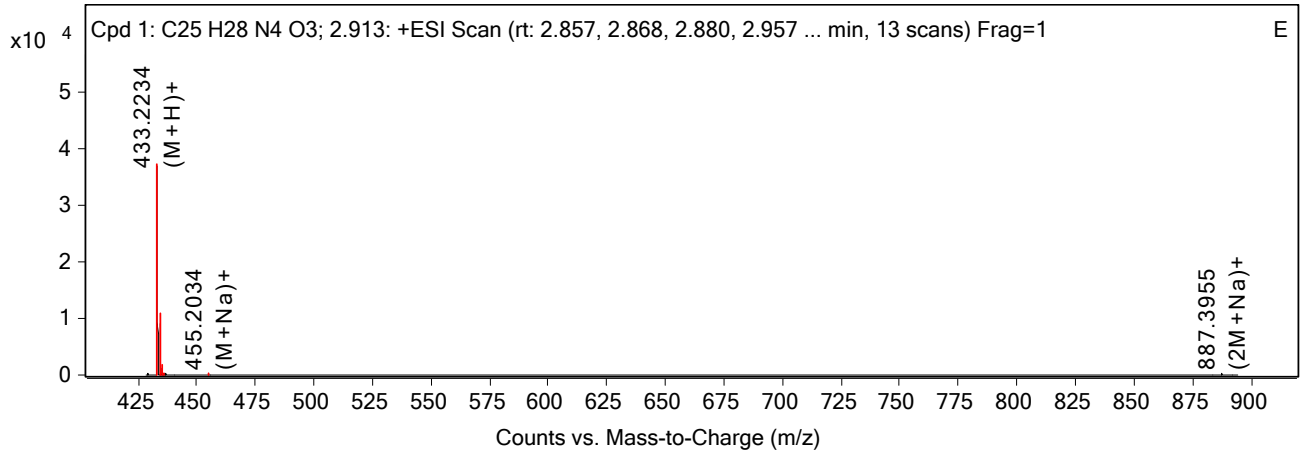
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
433.2234	1	37314.74	(M+H)+
434.2262	1	9180.93	(M+H)+
435.2296	1	1338.14	(M+H)+
436.2362	1	178.25	(M+H)+
455.2034	1	173.94	(M+Na)+
456.2136	1	57.19	(M+Na)+
887.3955	1	214	(2M+Na)+
888.403	1	110.96	(2M+Na)+
889.397	1	72.45	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
433.2234	1	37314.74	(M+H)+	0.01
433.2234		37314.74		
434.2262	1	9180.93	(M+H)+	0.67
435.2296	1	1338.14	(M+H)+	-0.74
436.2362	1	178.25	(M+H)+	-9.59
455.2034	1	173.94	(M+Na)+	4.32
456.2136	1	57.19	(M+Na)+	-11.34
887.3955	1	214	(2M+Na)+	29.25
888.403	1	110.96	(2M+Na)+	24.3
889.397	1	72.45	(2M+Na)+	34.32

--- End Of Report ---

Target Compound Screening Report

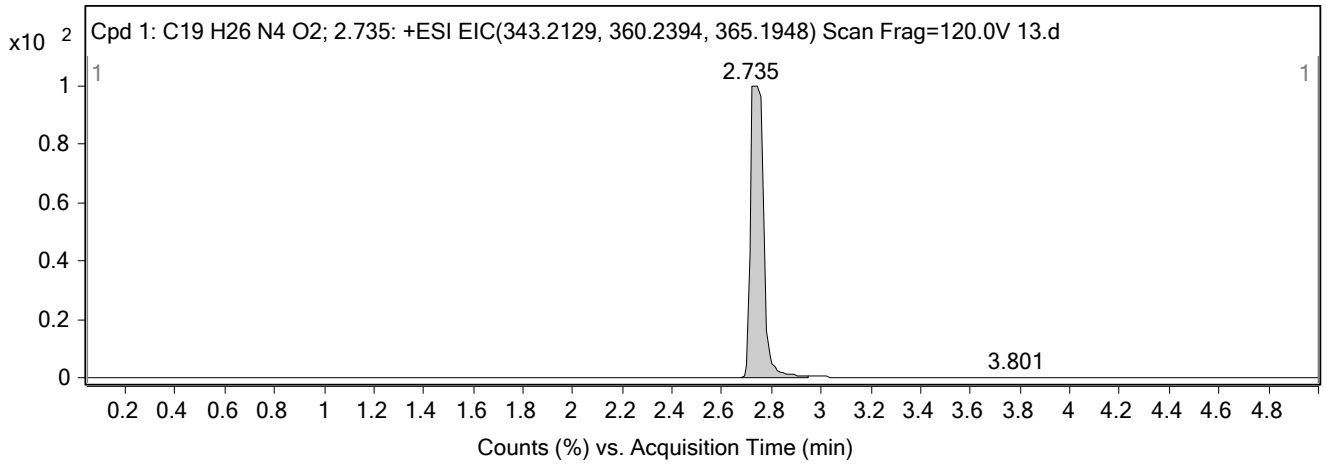
Data File	13.d	**Sample Name**	H3468064
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 6:46:36 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C19H26N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 6:46:36 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H26 N4 O2; 2.735	96.49	-1.81	C19 H26 N4 O2	2.735	342.2056	342.205

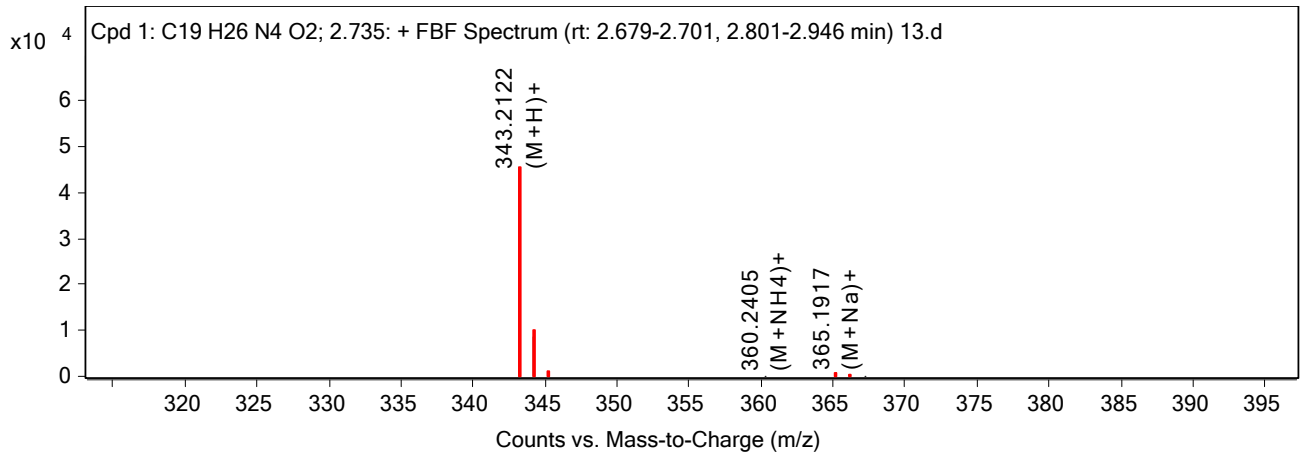
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
343.2122	2.735	342.205	C19 H26 N4 O2	342.2056	-1.81	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

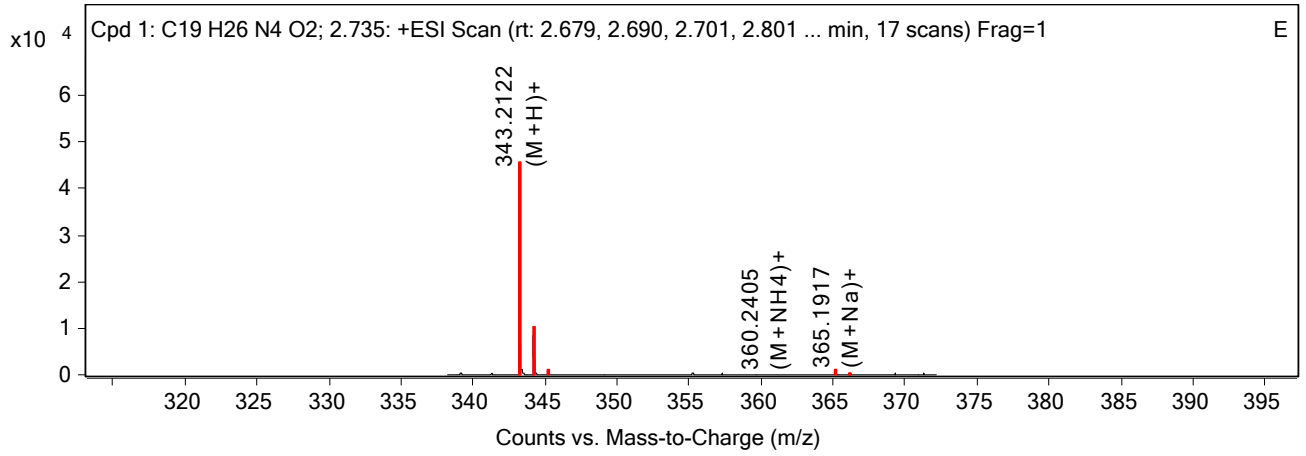
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
343.2122	1	45520.04	(M+H)+
344.2155	1	8649.44	(M+H)+
345.2183	1	1147.63	(M+H)+
360.2405	1	72.71	(M+NH4)+
365.1917	1	734.84	(M+Na)+
366.1916	1	225.31	(M+Na)+
367.2008	1	193.96	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
343.2122	1	45520.04	(M+H)+	1.8
344.2155	1	8649.44	(M+H)+	1.02
345.2183	1	1147.63	(M+H)+	0.78
360.2405	1	72.71	(M+NH4)+	-3.12
365.1917	1	734.84	(M+Na)+	8.53
366.1916	1	225.31	(M+Na)+	16.86
367.2008	1	193.96	(M+Na)+	-0.95

--- End Of Report ---

Target Compound Screening Report

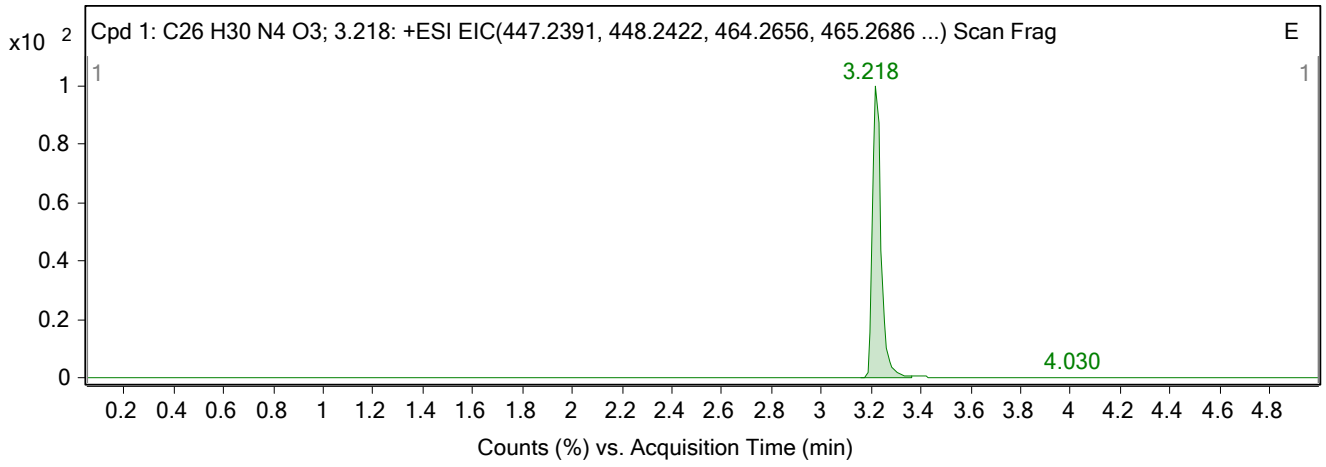
Data File	41.d	**Sample Name**	H2976529
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:30:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:30:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

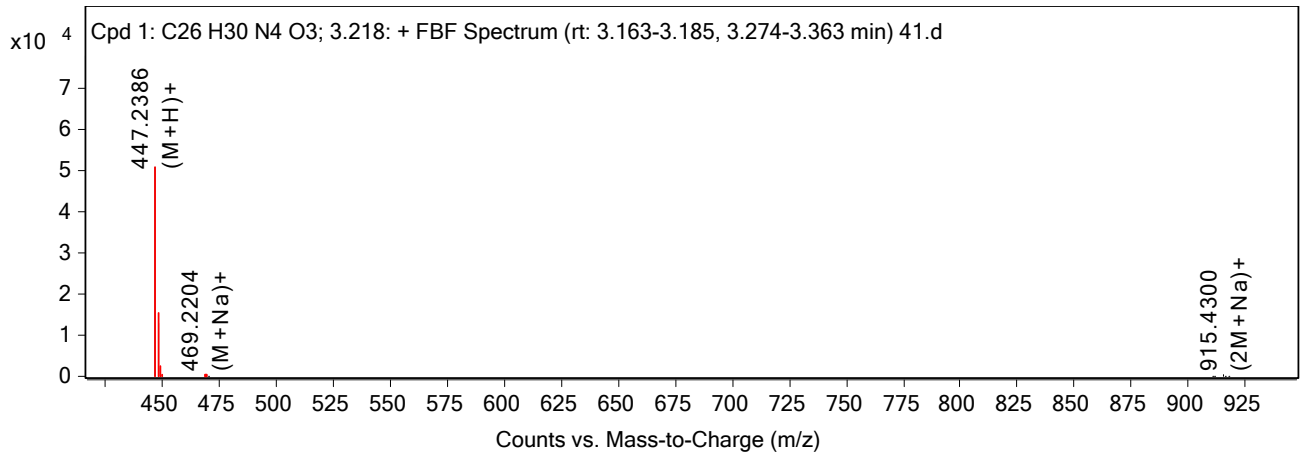
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O3; 3.218	96.59	-1.84	C26 H30 N4 O3	3.218	446.2318	446.231

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2386	3.218	446.231	C26 H30 N4 O3	446.2318	-1.84	Find By Formula	

Compound Chromatograms



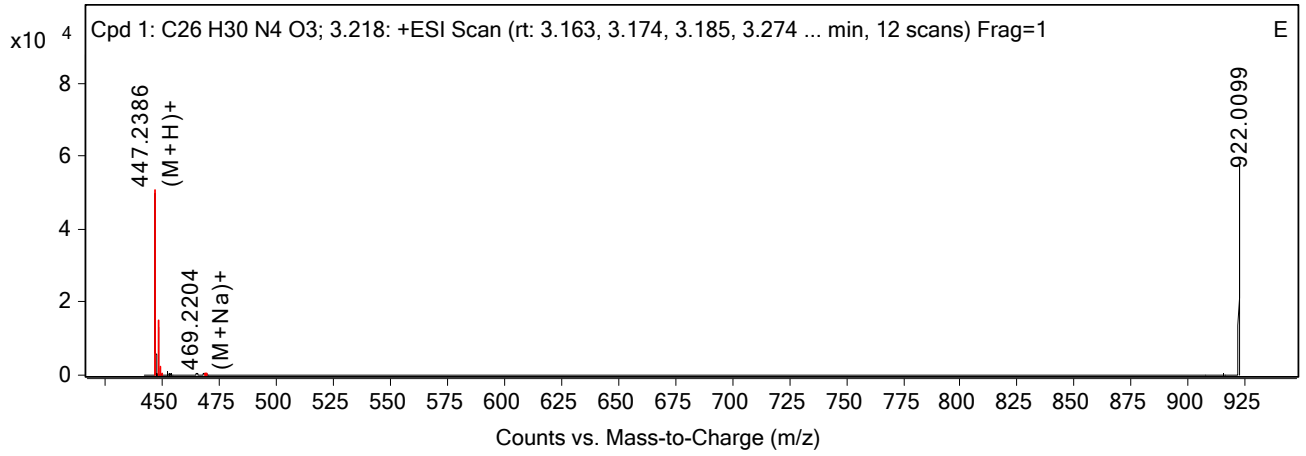
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2386	1	50610.57	(M+H)+
448.2415	1	12972.39	(M+H)+
449.2446	1	2010.11	(M+H)+
450.2427	1	279.11	(M+H)+
469.2204	1	338.14	(M+Na)+
470.2219	1	123.81	(M+Na)+
910.4753	1	85.89	(2M+NH4)+
915.43	1	373.4	(2M+Na)+
916.4323	1	187.86	(2M+Na)+
917.4275	1	110.44	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2386	1	50610.57	(M+H)+	1.09
448.2415	1	12972.39	(M+H)+	1.37
449.2446	1	2010.11	(M+H)+	0.9
450.2427	1	279.11	(M+H)+	11.18
469.2204	1	338.14	(M+Na)+	1.36
470.2219	1	123.81	(M+Na)+	4.73
910.4753	1	85.89	(2M+NH4)+	24.31
915.43	1	373.4	(2M+Na)+	24.94
916.4323	1	187.86	(2M+Na)+	25.79
917.4275	1	110.44	(2M+Na)+	34.16

--- End Of Report ---

Target Compound Screening Report

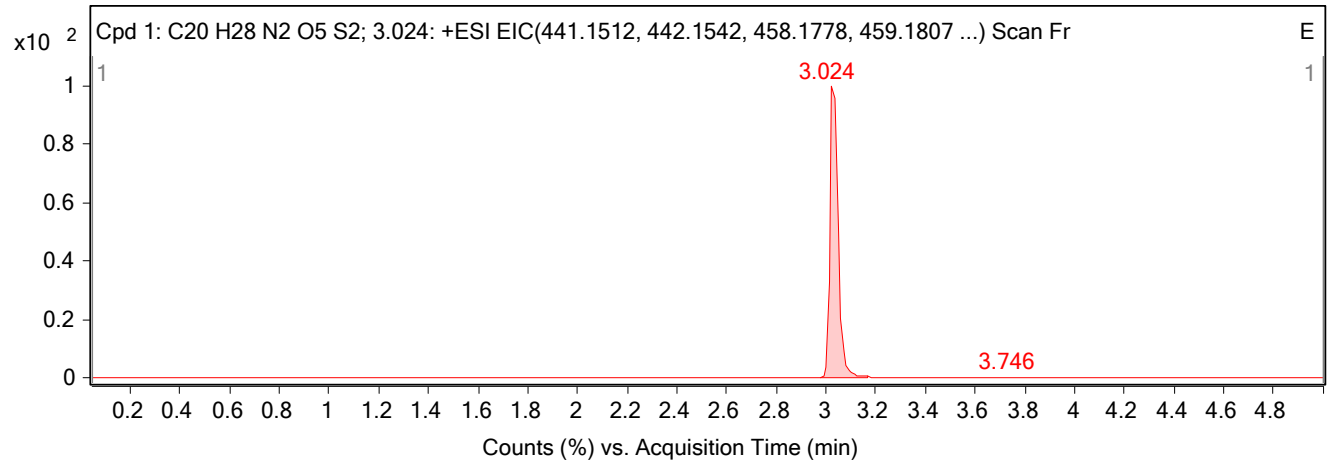
Data File	13.d	**Sample Name**	H2980129
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 12:23:09 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 12:23:09 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

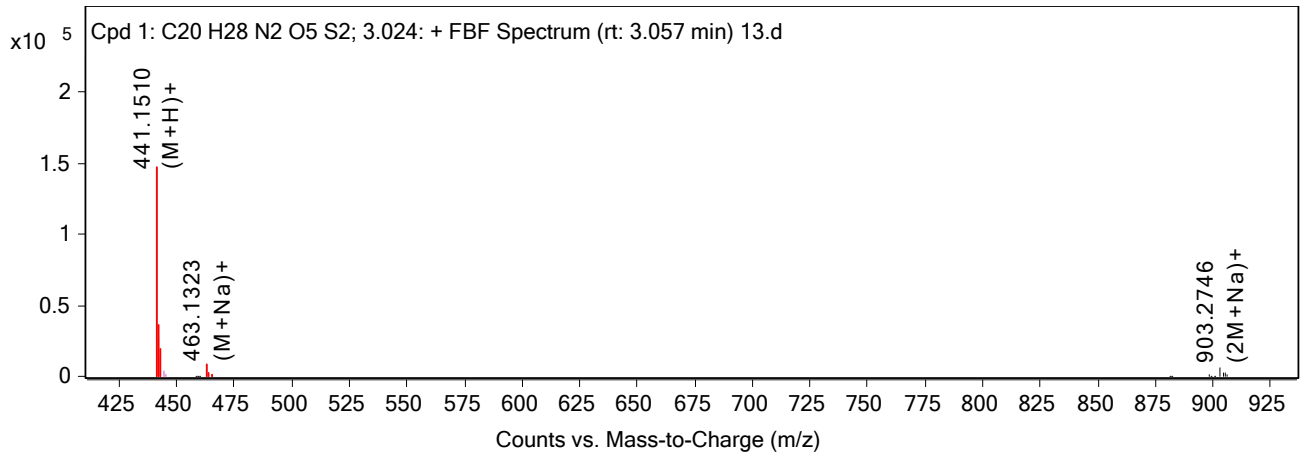
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O5 S2; 3.024	96.73	-0.7	C20 H28 N2 O5 S2	3.024	440.144	440.1437

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
463.1323	3.024	440.1437	C20 H28 N2 O5 S2	440.144	-0.7	Find By Formula	

Compound Chromatograms



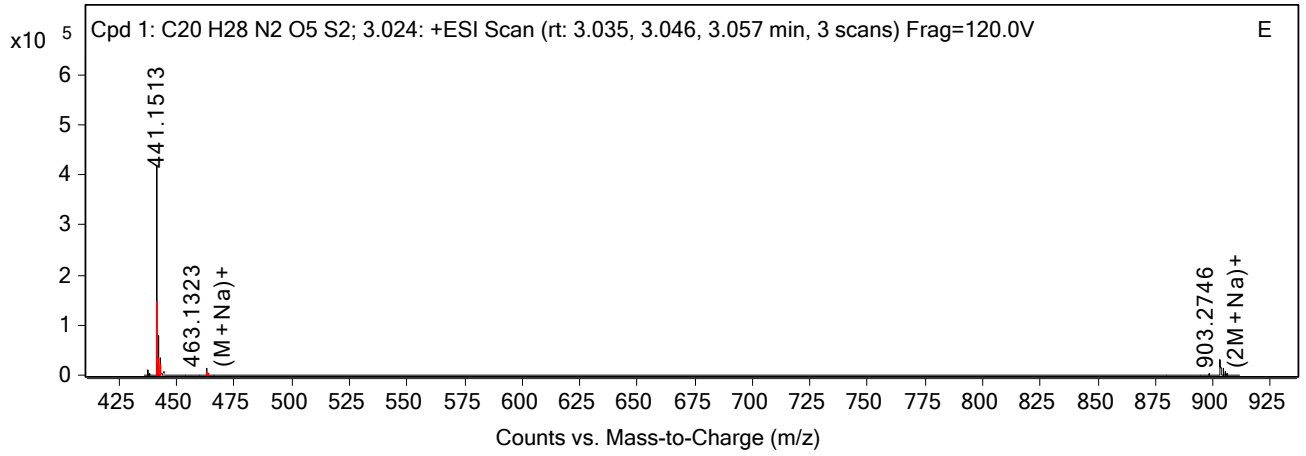
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
441.151	1	146924.36	(M+H)+
442.1547	1	28280.64	(M+H)+
443.1495	1	13634.68	(M+H)+
463.1323	1	7949.02	(M+Na)+
464.1344	1	1902.66	(M+Na)+
465.1319	1	941.89	(M+Na)+
903.2746	1	6345.11	(2M+Na)+
904.2804	1	3035.1	(2M+Na)+
905.2749	1	2238.02	(2M+Na)+
906.2766	1	689.22	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
441.151	1	146924.36	(M+H)+	0.51
442.1547	1	28280.64	(M+H)+	-1.16
443.1495	1	13634.68	(M+H)+	1.03
463.1323	1	7949.02	(M+Na)+	1.97
464.1344	1	1902.66	(M+Na)+	3.76
465.1319	1	941.89	(M+Na)+	0.12
903.2746	1	6345.11	(2M+Na)+	2.81
904.2804	1	3035.1	(2M+Na)+	-0.38
905.2749	1	2238.02	(2M+Na)+	2.56
906.2766	1	689.22	(2M+Na)+	1.93

--- End Of Report ---

Target Compound Screening Report

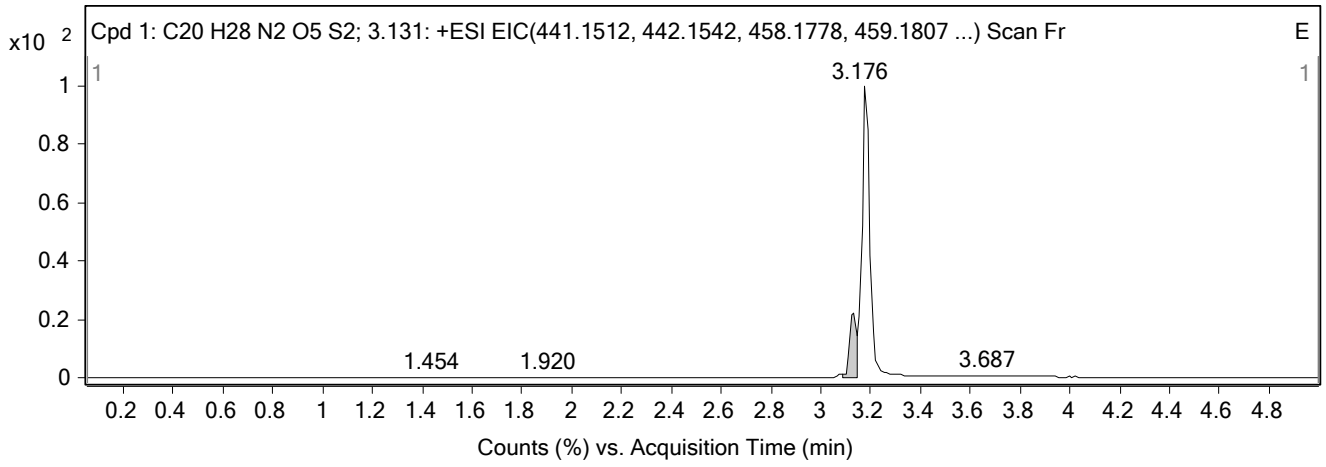
Data File	1e.d	**Sample Name**	H3475361
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/8/2021 9:39:00 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/8/2021 9:39:00 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

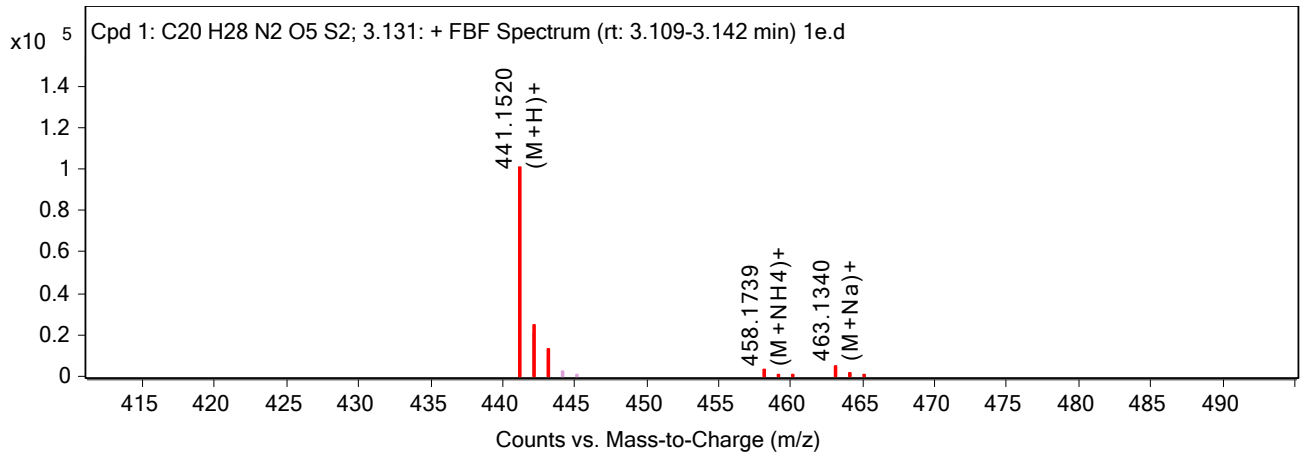
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O5 S2; 3.131	94.12	1.25	C20 H28 N2 O5 S2	3.131	440.144	440.1445

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
441.152	3.131	440.1445	C20 H28 N2 O5 S2	440.144	1.25	Find By Formula	

Compound Chromatograms



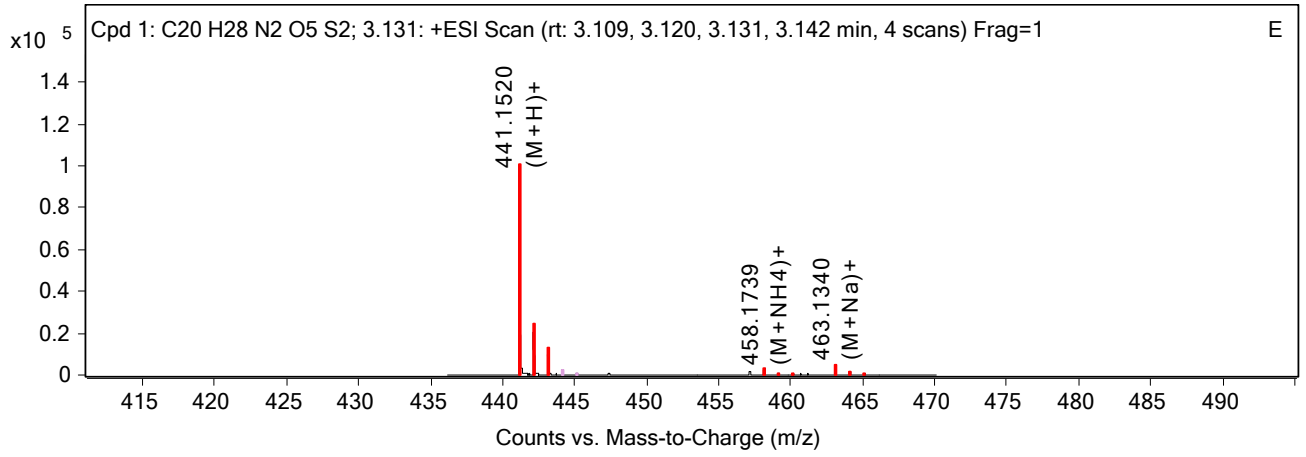
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
441.152	1	100866.29	(M+H)+
442.1545	1	20527.08	(M+H)+
443.1511	1	9943.68	(M+H)+
458.1739	1	3113.27	(M+NH4)+
459.174	1	812.08	(M+NH4)+
460.1649	1	552	(M+NH4)+
463.134	1	5133.08	(M+Na)+
464.1377	1	1344.4	(M+Na)+
465.1361	1	765.3	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
441.152	1	100866.29	(M+H)+	-1.7
442.1545	1	20527.08	(M+H)+	-0.66
443.1511	1	9943.68	(M+H)+	-2.63
458.1739	1	3113.27	(M+NH4)+	8.54
459.174	1	812.08	(M+NH4)+	14.44
460.1649	1	552	(M+NH4)+	25.31
463.134	1	5133.08	(M+Na)+	-1.81
464.1377	1	1344.4	(M+Na)+	-3.43
465.1361	1	765.3	(M+Na)+	-9.11

--- End Of Report ---

Target Compound Screening Report

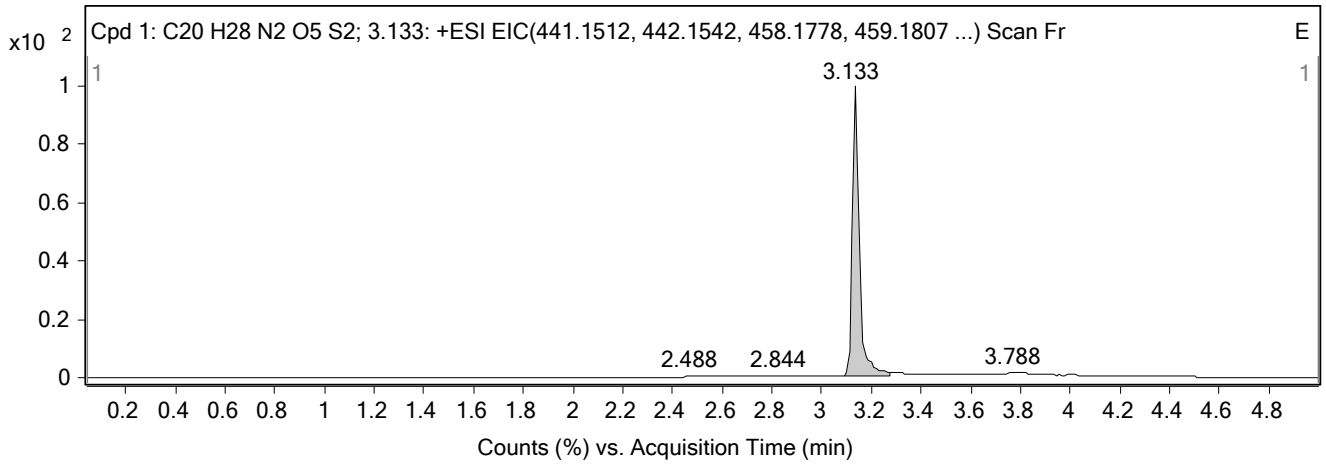
Data File	2.d	**Sample Name**	H3475364
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 4:47:21 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 4:47:21 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O5 S2; 3.133	90.61	2.86	C20 H28 N2 O5 S2	3.133	440.144	440.1452

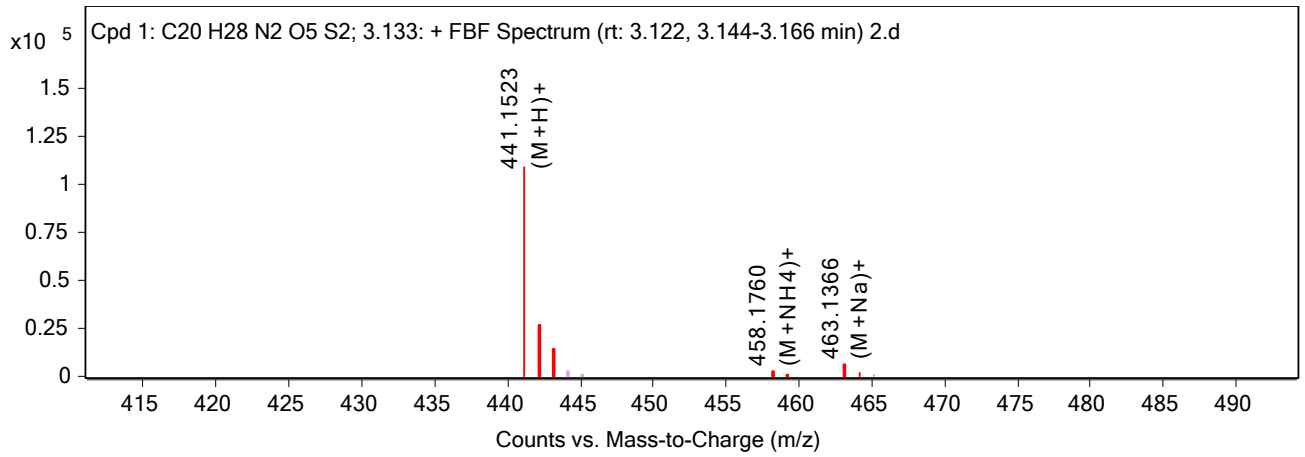
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
441.1523	3.133	440.1452	C20 H28 N2 O5 S2	440.144	2.86	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

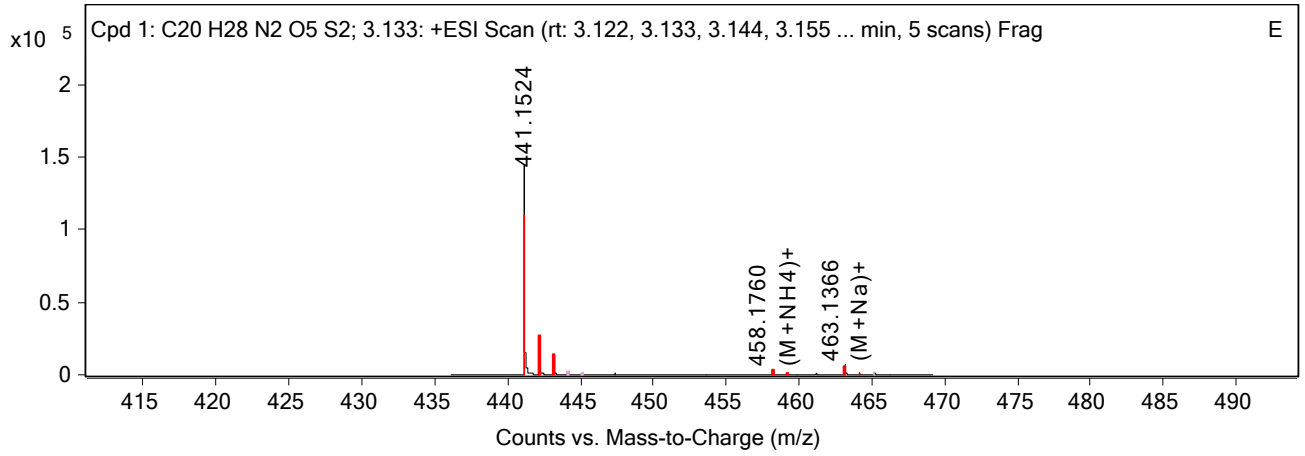
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
441.1523	1	109257.45	(M+H)+
442.1555	1	21399.08	(M+H)+
443.1523	1	10442.96	(M+H)+
458.176	1	2902.92	(M+NH4)+
459.1787	1	859.51	(M+NH4)+
463.1366	1	6463.25	(M+Na)+
464.1418	1	1621.39	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
441.1523	1	109257.44	(M+H)+	-2.4
441.1524		143903.64		
442.1555	1	21399.08	(M+H)+	-2.99
443.1523	1	10442.96	(M+H)+	-5.17
458.176	1	2902.92	(M+NH4)+	3.82
459.1787	1	859.51	(M+NH4)+	4.31
463.1366	1	6463.25	(M+Na)+	-7.37
464.1418	1	1621.39	(M+Na)+	-12.29

--- End Of Report ---

Target Compound Screening Report

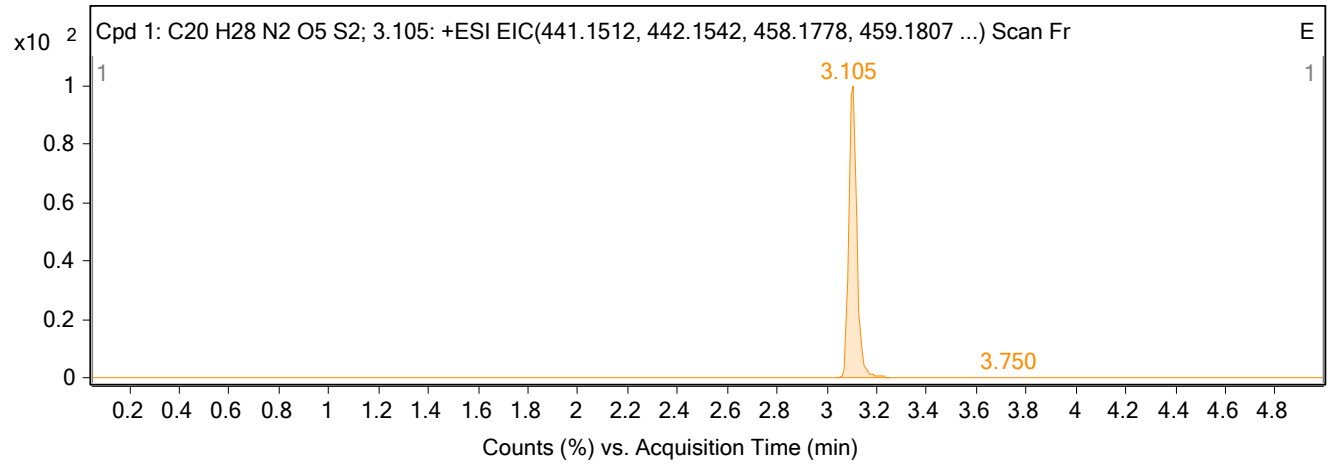
Data File	31.d	**Sample Name**	H2979259
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:34:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:34:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

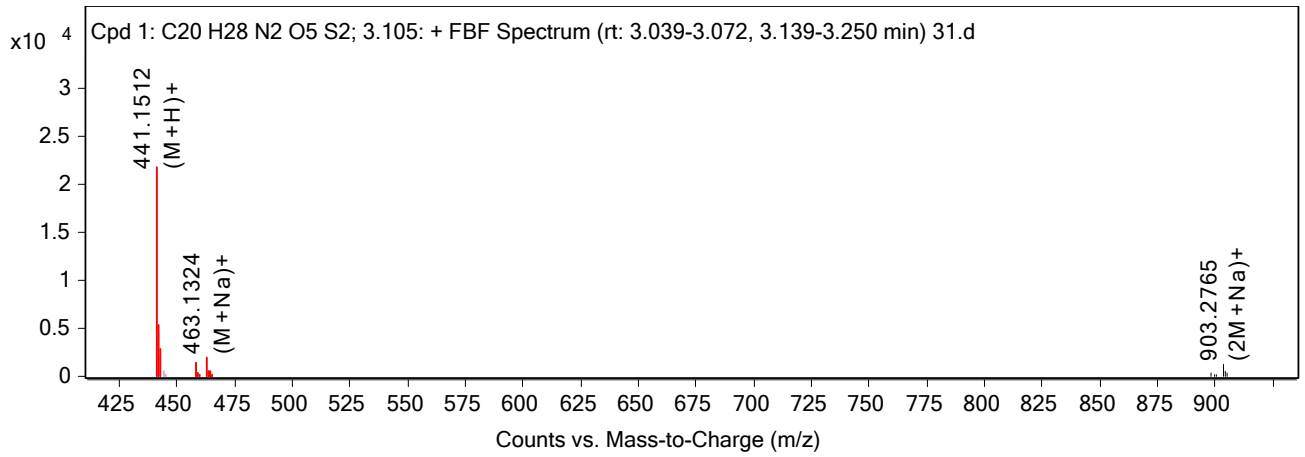
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O5 S2; 3.105	97.6	-0.76	C20 H28 N2 O5 S2	3.105	440.144	440.1436

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
463.1324	3.105	440.1436	C20 H28 N2 O5 S2	440.144	-0.76	Find By Formula	

Compound Chromatograms



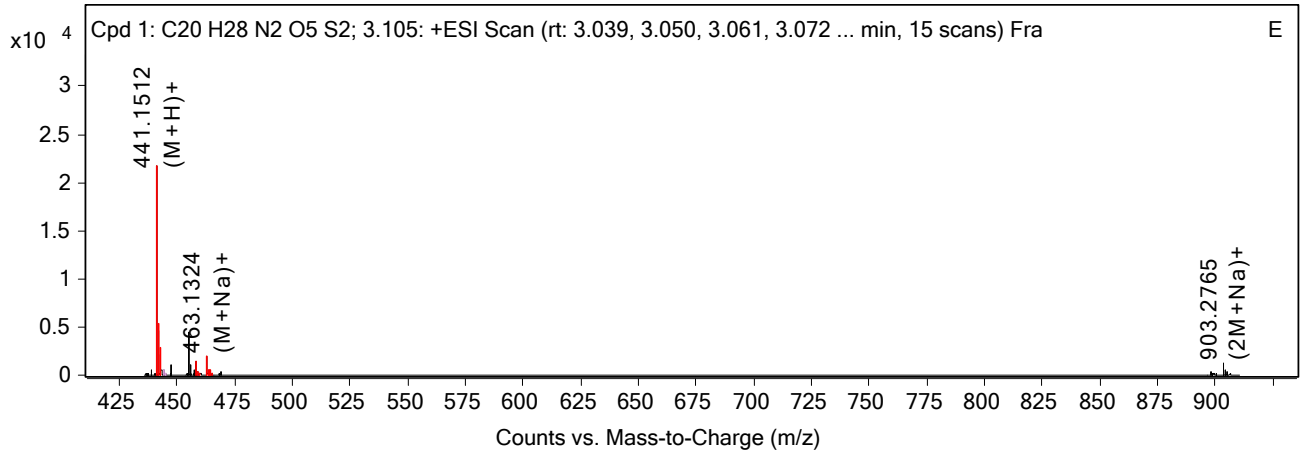
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
441.1512	1	21739.97	(M+H)+
442.1539	1	4615.2	(M+H)+
443.1504	1	2208.88	(M+H)+
458.1759	1	1486.77	(M+NH4)+
463.1324	1	1914.03	(M+Na)+
464.1356	1	452.92	(M+Na)+
898.3196	1	438.8	(2M+NH4)+
903.2765	1	1221.36	(2M+Na)+
904.2777	1	572.66	(2M+Na)+
905.2738	1	391.82	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
441.1512	1	21739.98	(M+H)+	0.01
442.1539	1	4615.2	(M+H)+	0.67
443.1504	1	2208.88	(M+H)+	-0.92
458.1759	1	1486.77	(M+NH4)+	4.17
463.1324	1	1914.03	(M+Na)+	1.77
464.1356	1	452.92	(M+Na)+	1.23
898.3196	1	438.8	(2M+NH4)+	2.43
903.2765	1	1221.36	(2M+Na)+	0.75
904.2777	1	572.66	(2M+Na)+	2.66
905.2738	1	391.82	(2M+Na)+	3.84

--- End Of Report ---

Target Compound Screening Report

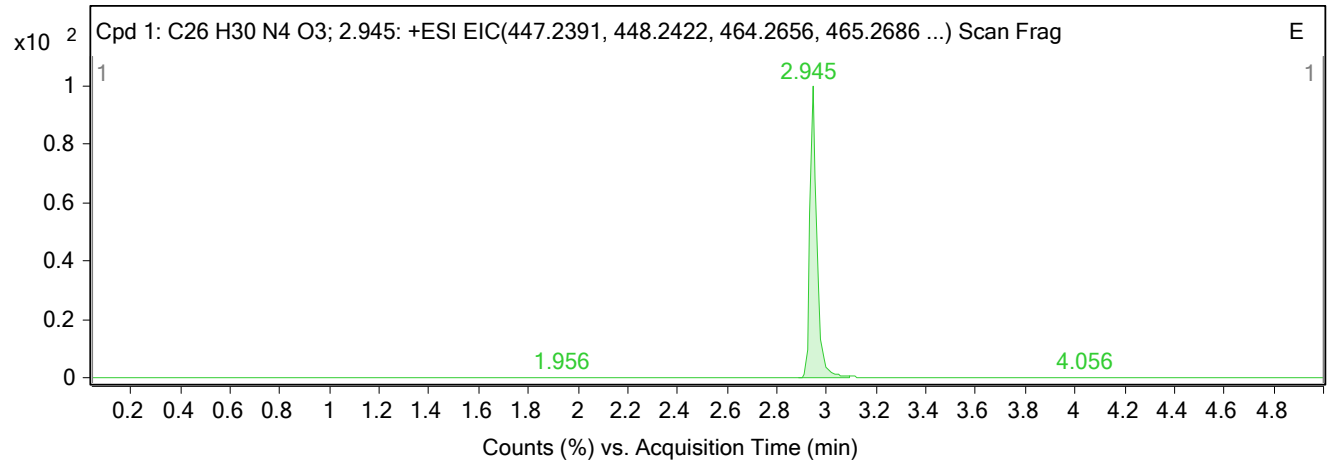
Data File	28.d	**Sample Name**	H2976537
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:46:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:46:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

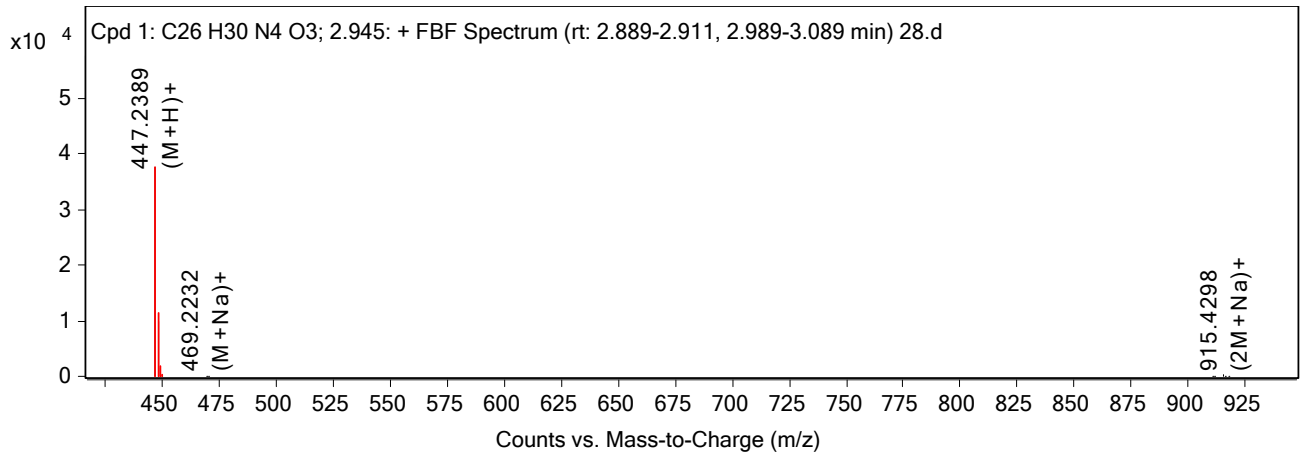
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O3; 2.945	97.65	-1	C26 H30 N4 O3	2.945	446.2318	446.2313

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2389	2.945	446.2313	C26 H30 N4 O3	446.2318	-1	Find By Formula	

Compound Chromatograms



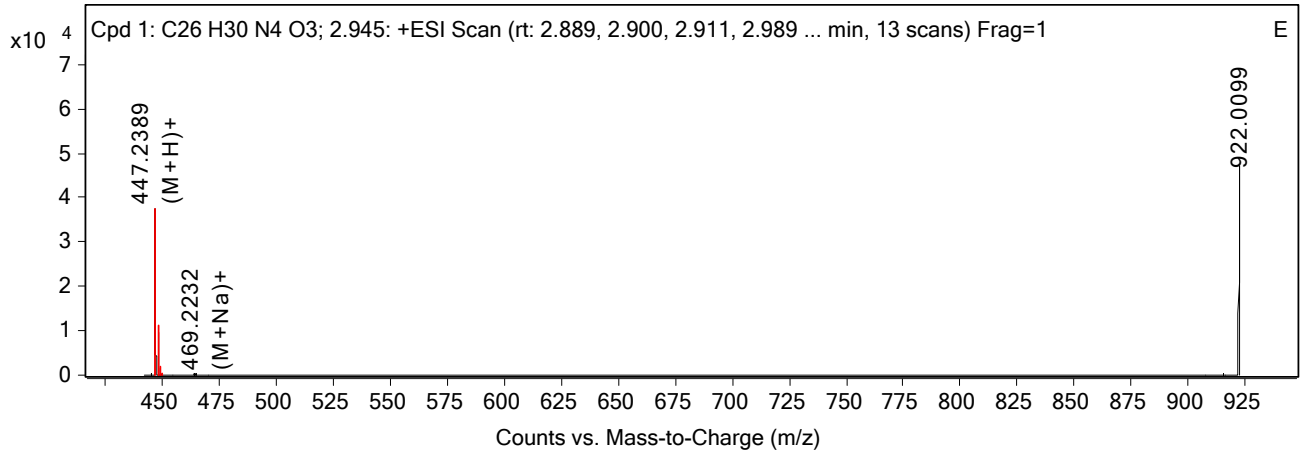
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2389	1	37493.01	(M+H)+
448.2419	1	9841.59	(M+H)+
449.2446	1	1650.6	(M+H)+
450.2459	1	220.41	(M+H)+
469.2232	1	100.21	(M+Na)+
910.4793	1	72.39	(2M+NH4)+
911.4782	1	59.38	(2M+NH4)+
915.4298	1	279.26	(2M+Na)+
916.4382	1	141.54	(2M+Na)+
917.4322	1	75.55	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2389	1	37493.01	(M+H)+	0.31
448.2419	1	9841.59	(M+H)+	0.64
449.2446	1	1650.6	(M+H)+	0.86
450.2459	1	220.41	(M+H)+	4.07
469.2232	1	100.21	(M+Na)+	-4.68
910.4793	1	72.39	(2M+NH4)+	19.88
911.4782	1	59.38	(2M+NH4)+	24.42
915.4298	1	279.26	(2M+Na)+	25.07
916.4382	1	141.54	(2M+Na)+	19.27
917.4322	1	75.55	(2M+Na)+	29.05

--- End Of Report ---

Target Compound Screening Report

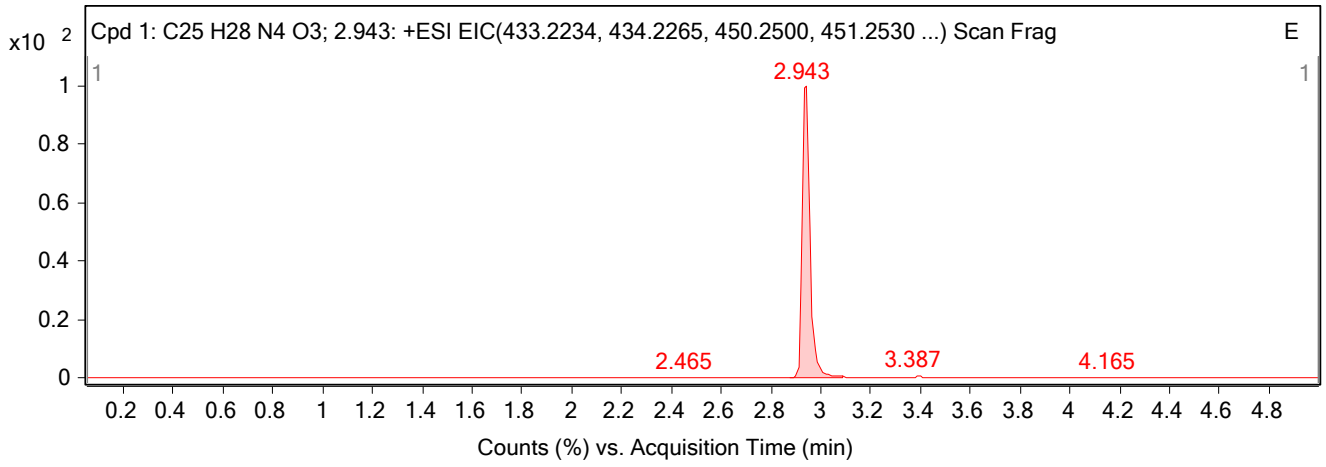
Data File	23.d	**Sample Name**	H2977003
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:18:48 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:18:48 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

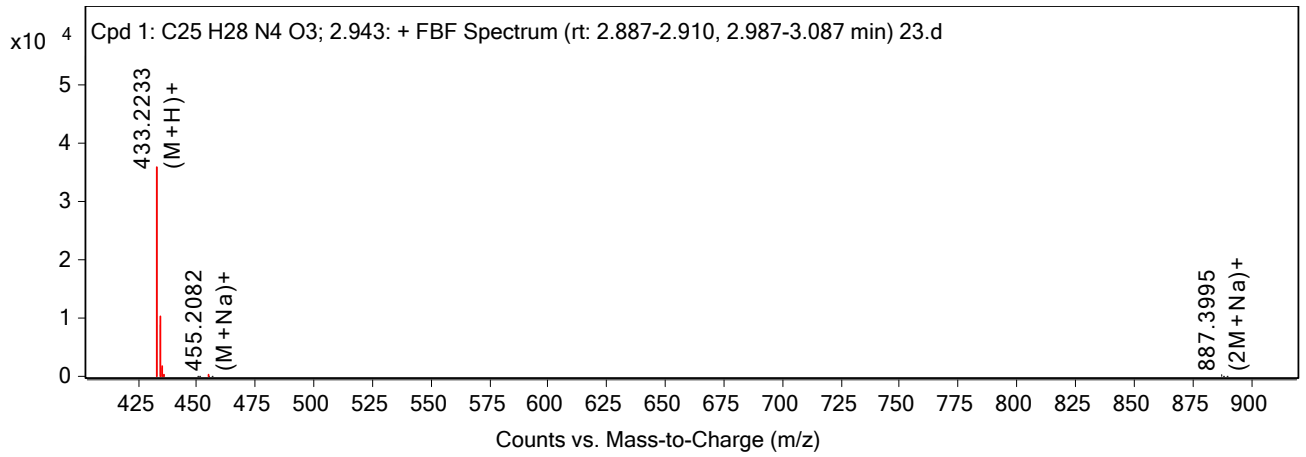
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O3; 2.943	97.28	-0.8	C25 H28 N4 O3	2.943	432.2161	432.2158

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
433.2233	2.943	432.2158	C25 H28 N4 O3	432.2161	-0.8	Find By Formula	

Compound Chromatograms



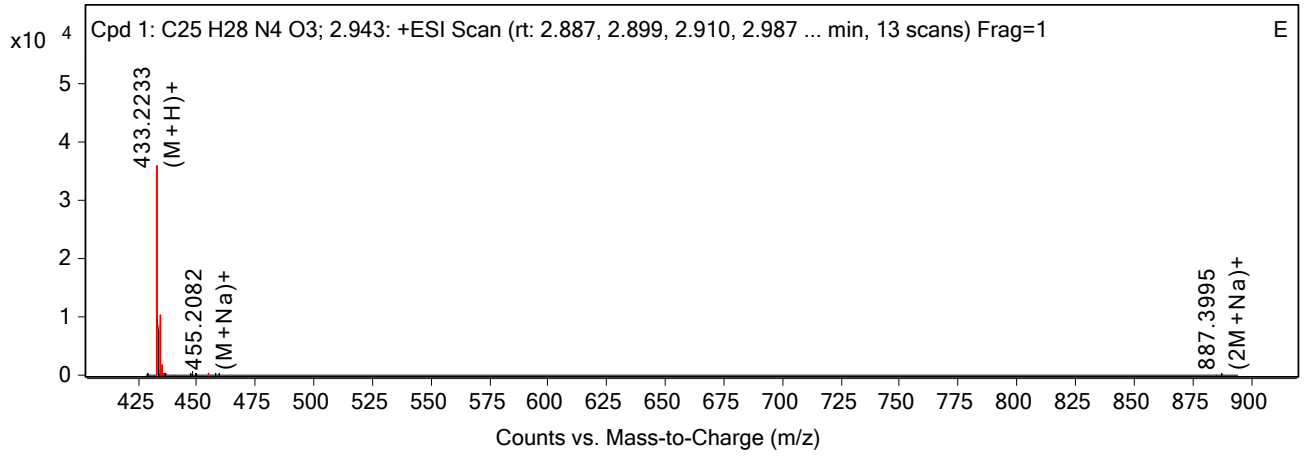
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
433.2233	1	35905.52	(M+H)+
434.226	1	8955.73	(M+H)+
435.2296	1	1381.28	(M+H)+
436.2346	1	173.45	(M+H)+
450.2425	1	84.85	(M+NH4)+
455.2082	1	160.31	(M+Na)+
456.2073	1	66.24	(M+Na)+
887.3995	1	209.48	(2M+Na)+
888.4008	1	121.57	(2M+Na)+
889.3989	1	57.07	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
433.2233	1	35905.52	(M+H)+	0.2
434.226	1	8955.73	(M+H)+	1.03
435.2296	1	1381.28	(M+H)+	-0.73
436.2346	1	173.45	(M+H)+	-5.97
450.2425	1	84.85	(M+NH4)+	16.5
455.2082	1	160.31	(M+Na)+	-6.24
456.2073	1	66.24	(M+Na)+	2.58
887.3995	1	209.48	(2M+Na)+	24.75
888.4008	1	121.57	(2M+Na)+	26.76
889.3989	1	57.07	(2M+Na)+	32.17

--- End Of Report ---

Target Compound Screening Report

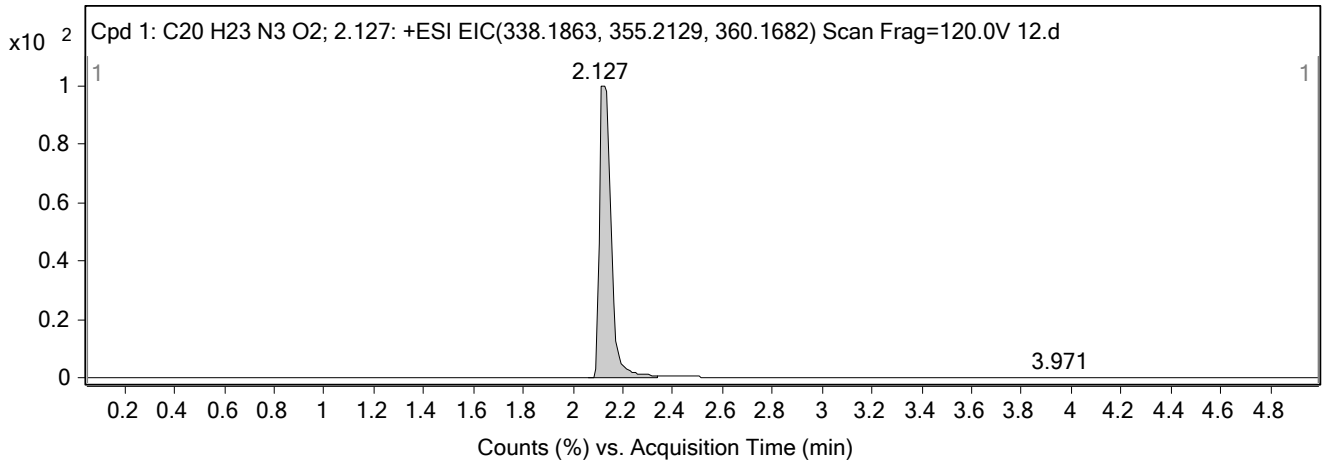
Data File	12.d	**Sample Name**	H3468887
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 6:40:51 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H23N3O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 6:40:51 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

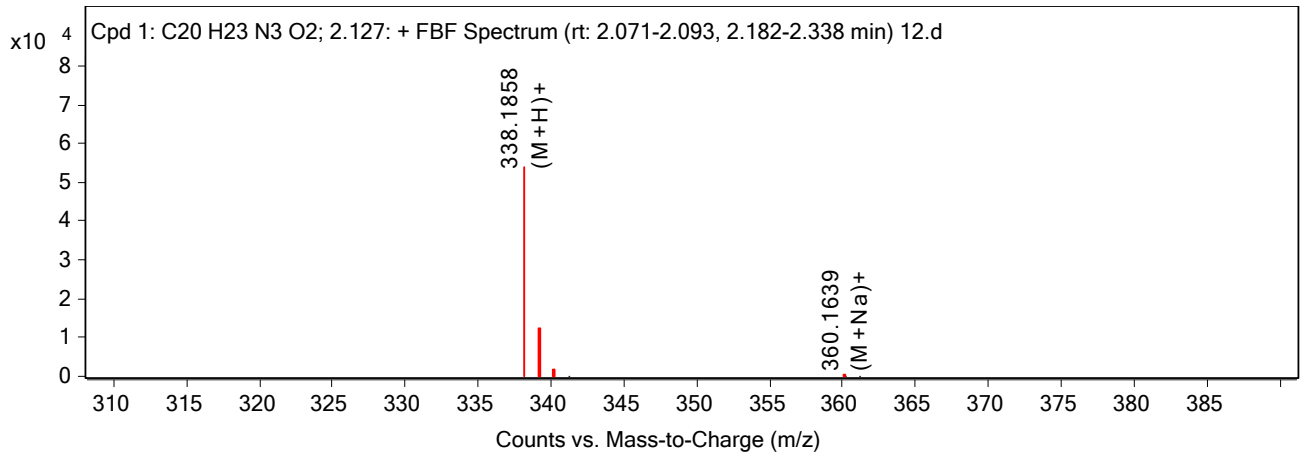
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H23 N3 O2; 2.127	95.79	-1.59	C20 H23 N3 O2	2.127	337.179	337.1785

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
338.1858	2.127	337.1785	C20 H23 N3 O2	337.179	-1.59	Find By Formula	

Compound Chromatograms



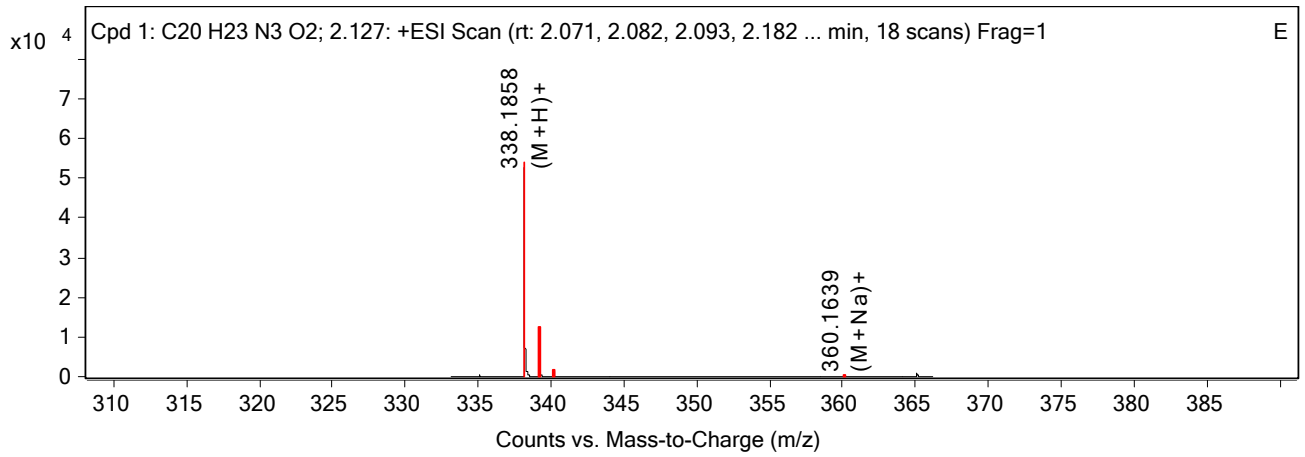
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
338.1858	1	53812.58	(M+H)+
339.1888	1	10257.24	(M+H)+
340.1927	1	1356.2	(M+H)+
341.195	1	171.49	(M+H)+
360.1639	1	224.11	(M+Na)+
361.1625	1	81.62	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
338.1858	1	53812.58	(M+H)+	1.55
339.1888	1	10257.24	(M+H)+	1.74
340.1927	1	1356.2	(M+H)+	-1.44
341.195	1	171.49	(M+H)+	-0.4
360.1639	1	224.11	(M+Na)+	12.06
361.1625	1	81.62	(M+Na)+	24.49

--- End Of Report ---

Target Compound Screening Report

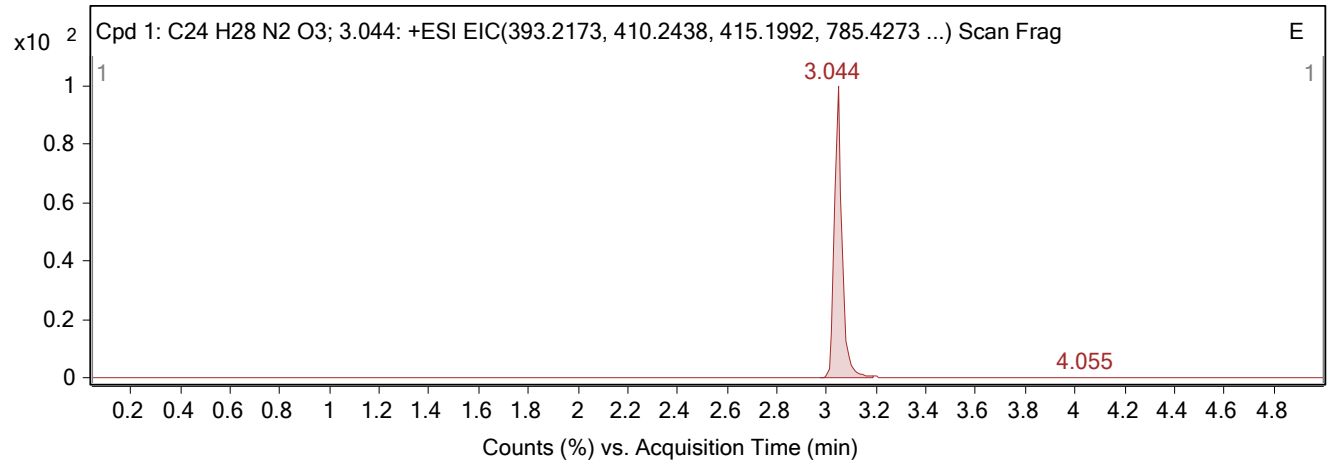
Data File	27.d	**Sample Name**	H1657372
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:41:04 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H28N2O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:41:04 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

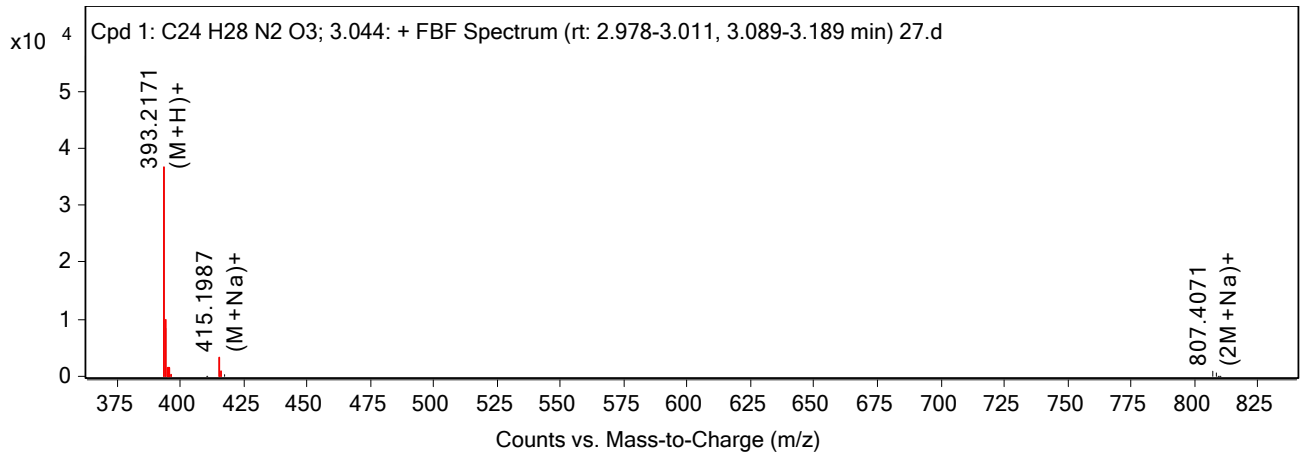
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H28 N2 O3; 3.044	96.35	-0.23	C24 H28 N2 O3	3.044	392.21	392.2099

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
393.2171	3.044	392.2099	C24 H28 N2 O3	392.21	-0.23	Find By Formula	

Compound Chromatograms



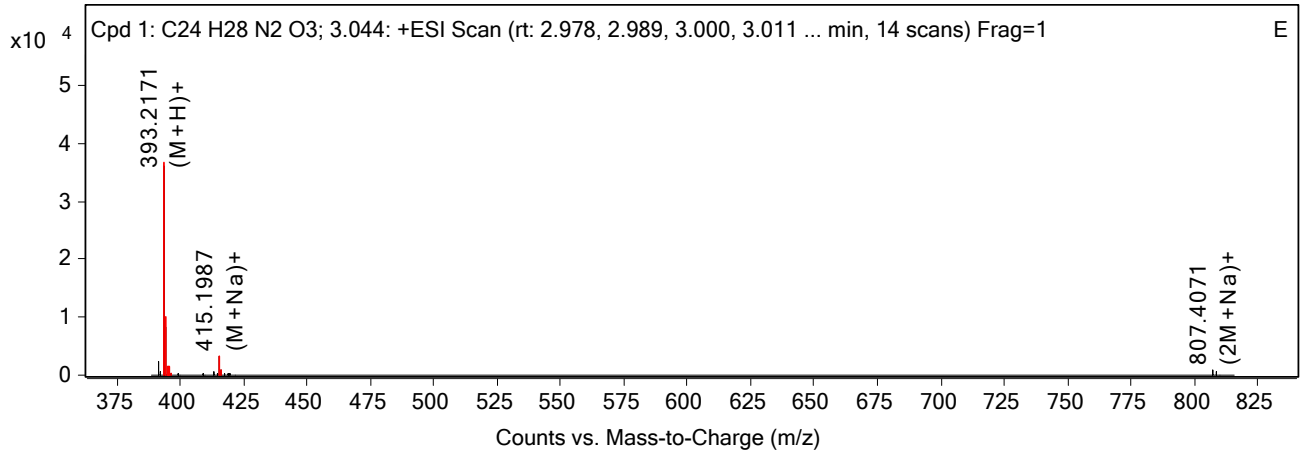
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
393.2171	1	36613.93	(M+H)+
394.2206	1	8316.89	(M+H)+
395.2251	1	1384.62	(M+H)+
396.2279	1	185.92	(M+H)+
415.1987	1	3364.81	(M+Na)+
416.2019	1	863.39	(M+Na)+
417.2159	1	198.55	(M+Na)+
807.4071	1	994.68	(2M+Na)+
808.4094	1	523.7	(2M+Na)+
809.4151	1	165.51	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
393.2171	1	36613.93	(M+H)+	0.32
394.2206	1	8316.89	(M+H)+	-0.28
395.2251	1	1384.62	(M+H)+	-4.31
396.2279	1	185.92	(M+H)+	-4.36
415.1987	1	3364.81	(M+Na)+	1.24
416.2019	1	863.39	(M+Na)+	1.19
417.2159	1	198.55	(M+Na)+	-25.38
807.4071	1	994.68	(2M+Na)+	2.58
808.4094	1	523.7	(2M+Na)+	3.76
809.4151	1	165.51	(2M+Na)+	0.42

--- End Of Report ---

Target Compound Screening Report

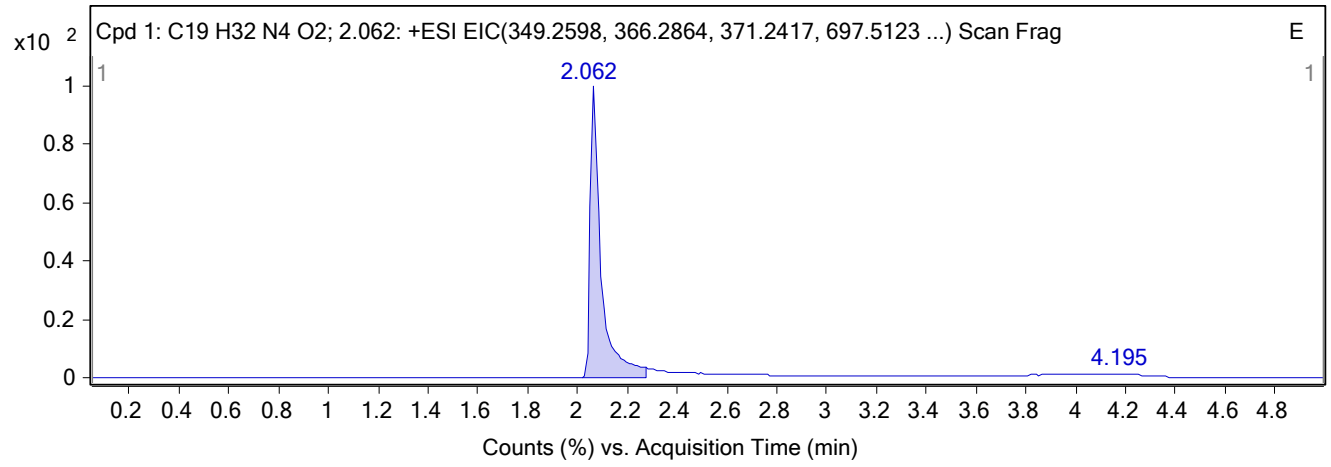
Data File	36.d	**Sample Name**	H3003309
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:31:04 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C19H32N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:31:04 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

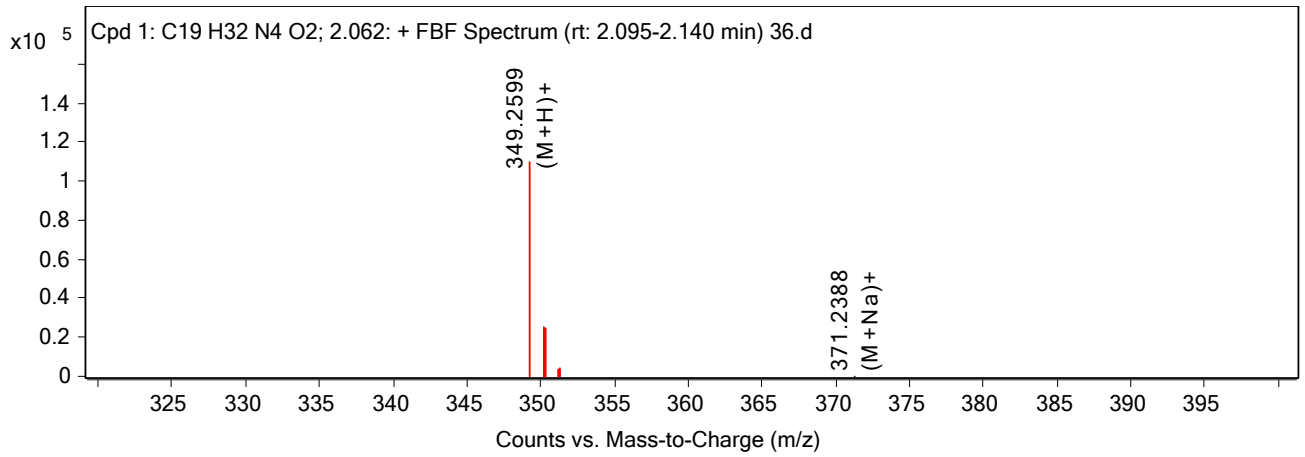
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C19 H32 N4 O2; 2.062	97.34	1.1	C19 H32 N4 O2	2.062	348.2525	348.2529

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
349.2599	2.062	348.2529	C19 H32 N4 O2	348.2525	1.1	Find By Formula	

Compound Chromatograms



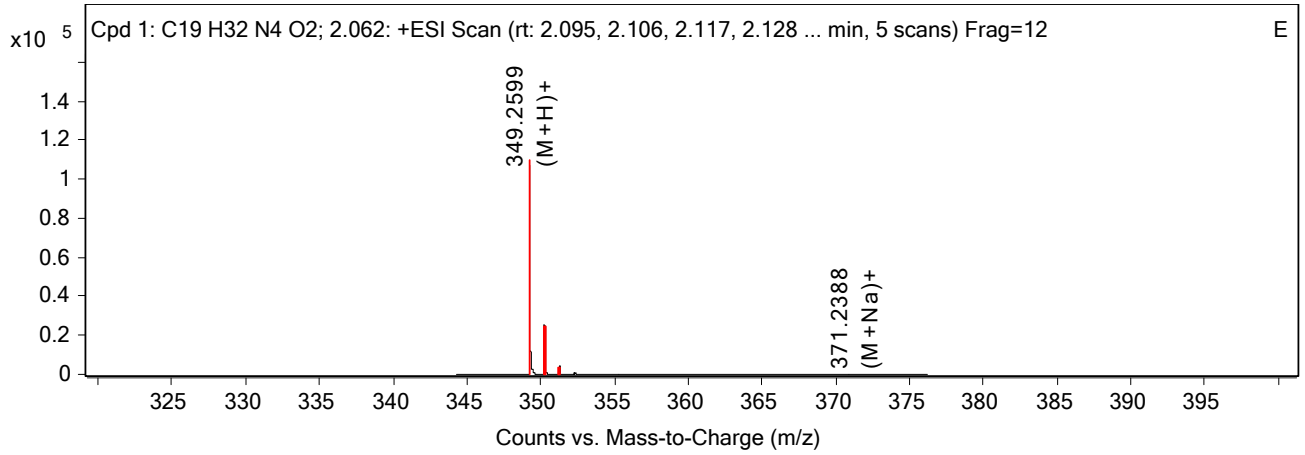
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
349.2599	1	106952.05	(M+H)+
350.2638	1	25956.21	(M+H)+
351.2692	1	4830.54	(M+H)+
371.2388	1	81.6	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
349.2599	1	106952.06	(M+H)+	-0.29
350.2638	1	25956.21	(M+H)+	-2.72
351.2692	1	4830.54	(M+H)+	-10.44
371.2388	1	81.6	(M+Na)+	8.07

--- End Of Report ---

Target Compound Screening Report

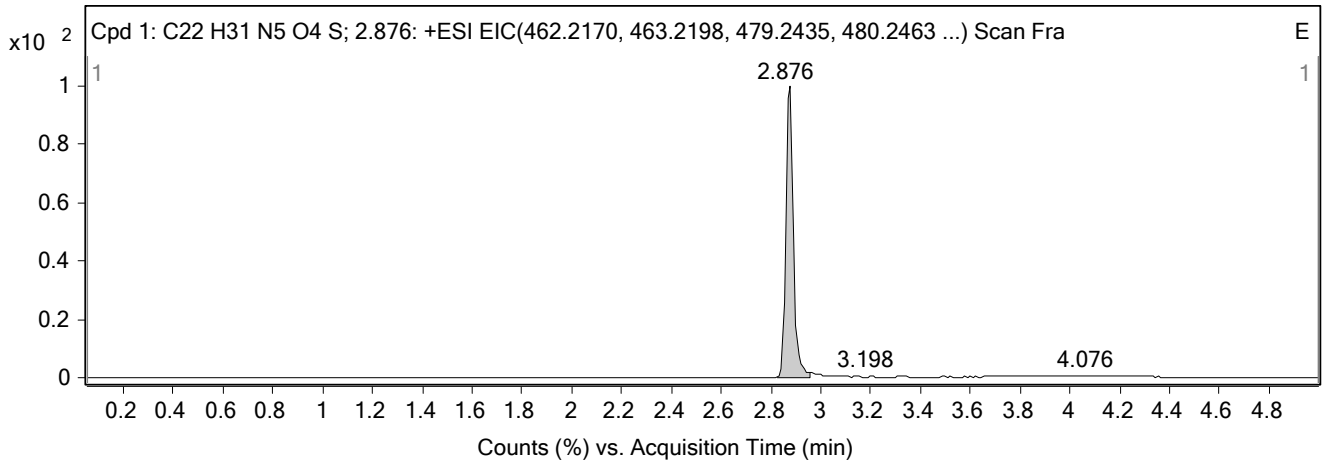
Data File	45.d	**Sample Name**	P212016$3
Sample Type	Sample	**Position**	P1-E9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 10:57:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H31N5O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 10:57:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

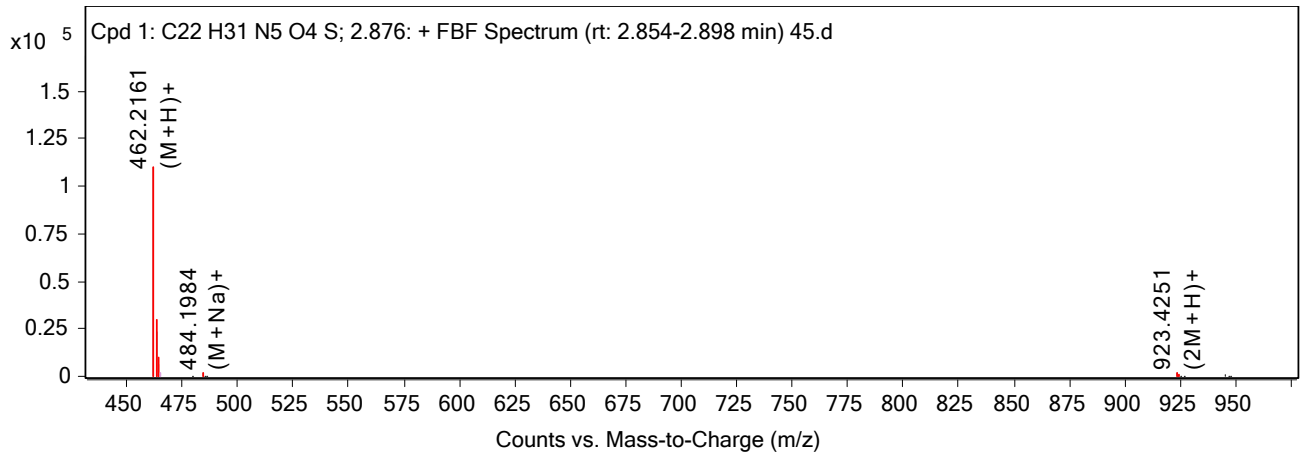
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H31 N5 O4 S; 2.876	98.54	-2.19	C22 H31 N5 O4 S	2.876	461.2097	461.2087

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
484.1984	2.876	461.2087	C22 H31 N5 O4 S	461.2097	-2.19	Find By Formula	

Compound Chromatograms



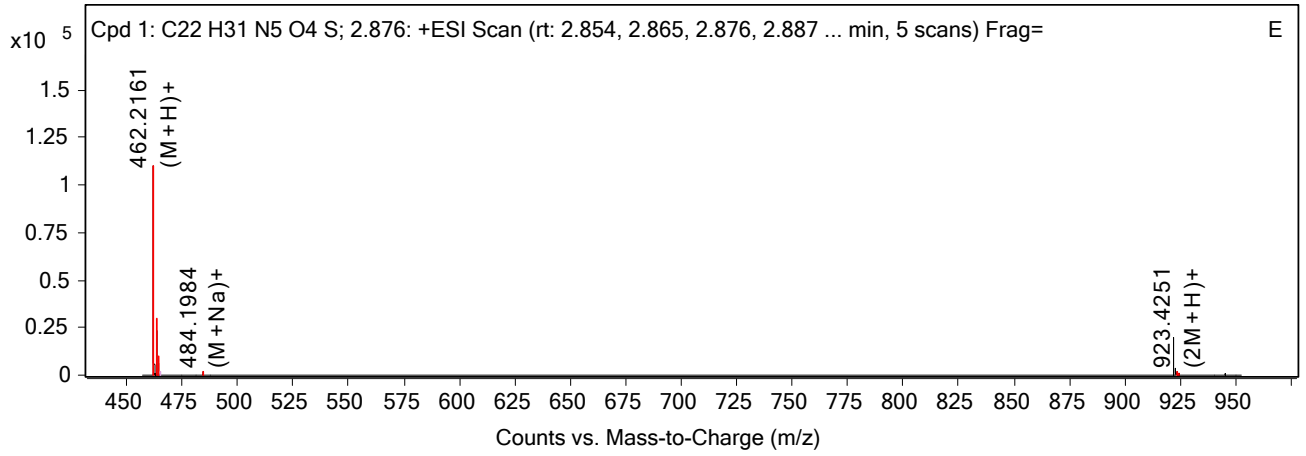
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
462.2161	1	109836.17	(M+H)+
463.2184	1	23548.04	(M+H)+
464.2164	1	6614.05	(M+H)+
484.1984	1	1576.03	(M+Na)+
485.2013	1	428.61	(M+Na)+
923.4251	1	1474.52	(2M+H)+
924.4266	1	809.8	(2M+H)+
925.4284	1	386.22	(2M+H)+
945.4049	1	611.88	(2M+Na)+
946.4081	1	349.49	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
462.2161	1	109836.17	(M+H)+	1.9
463.2184	1	23548.04	(M+H)+	2.99
464.2164	1	6614.05	(M+H)+	2.32
484.1984	1	1576.03	(M+Na)+	1.12
485.2013	1	428.61	(M+Na)+	1.03
923.4251	1	1474.52	(2M+H)+	1.63
924.4266	1	809.8	(2M+H)+	3.14
925.4284	1	386.22	(2M+H)+	0.29
945.4049	1	611.88	(2M+Na)+	3.84
946.4081	1	349.49	(2M+Na)+	3.5

--- End Of Report ---

Target Compound Screening Report

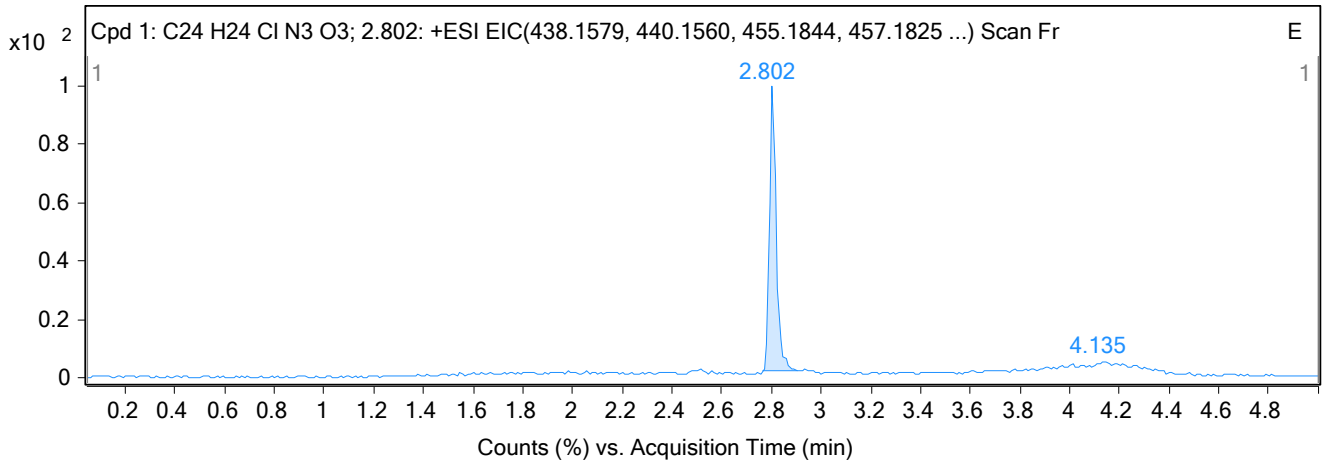
Data File	47.d	**Sample Name**	p212021$4
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 11:08:37 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H24ClN3O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 11:08:37 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

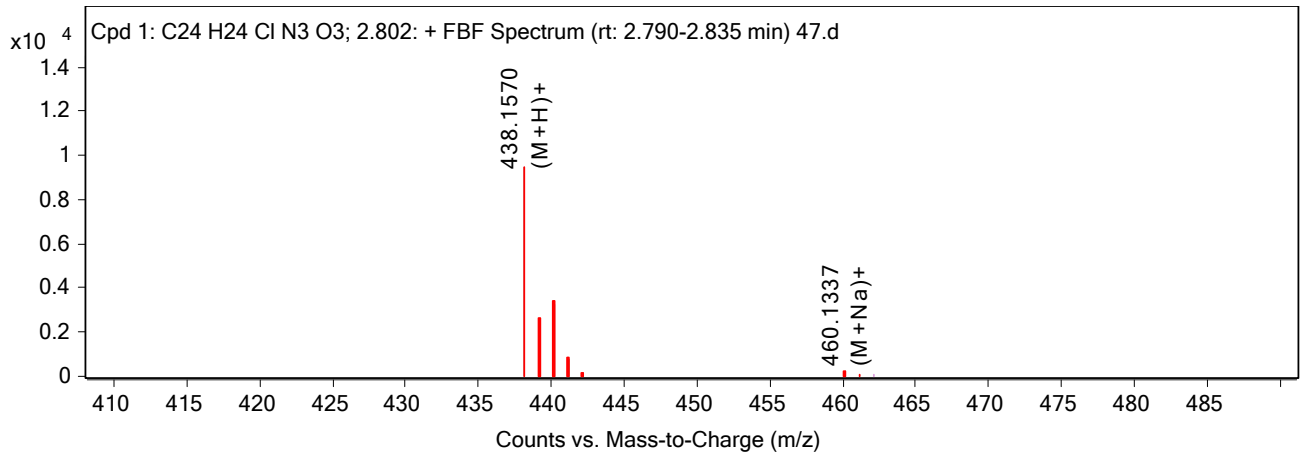
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H24 Cl N3 O3; 2.802	98.79	-2.19	C24 H24 Cl N3 O3	2.802	437.1506	437.1497

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
438.157	2.802	437.1497	C24 H24 Cl N3 O3	437.1506	-2.19	Find By Formula	

Compound Chromatograms



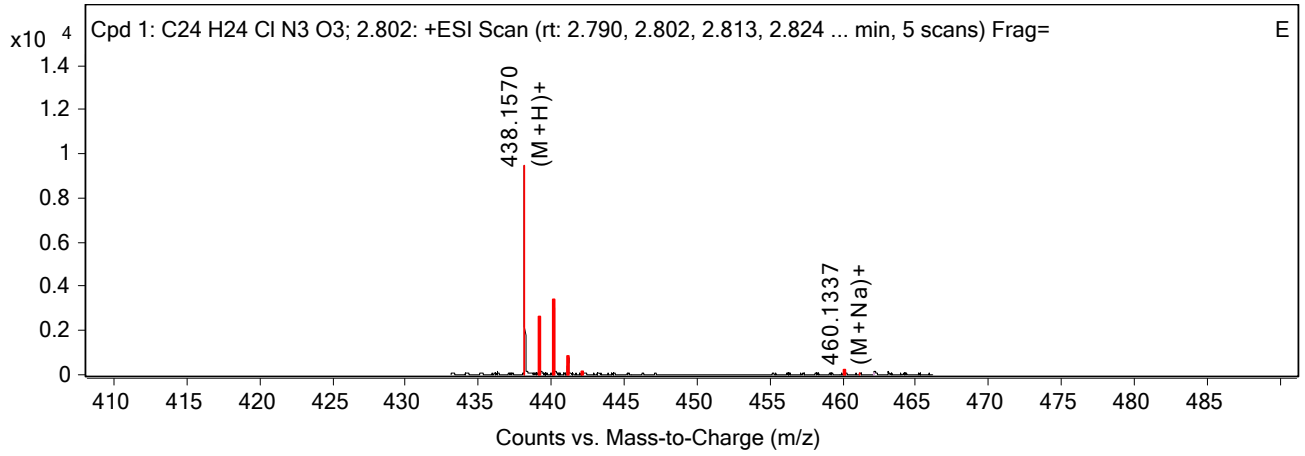
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
438.157	1	9480.1	(M+H)+
439.1601	1	2500.31	(M+H)+
440.1554	1	3298.95	(M+H)+
441.1581	1	780.43	(M+H)+
442.1594	1	178.69	(M+H)+
460.1337	1	246.35	(M+Na)+
461.138	1	90.97	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
438.157	1	9480.1	(M+H)+	2.15
439.1601	1	2500.31	(M+H)+	2.17
440.1554	1	3298.95	(M+H)+	1.33
441.1581	1	780.43	(M+H)+	0.87
442.1594	1	178.69	(M+H)+	4.02
460.1337	1	246.35	(M+Na)+	13.28
461.138	1	90.97	(M+Na)+	10.7

--- End Of Report ---

Target Compound Screening Report

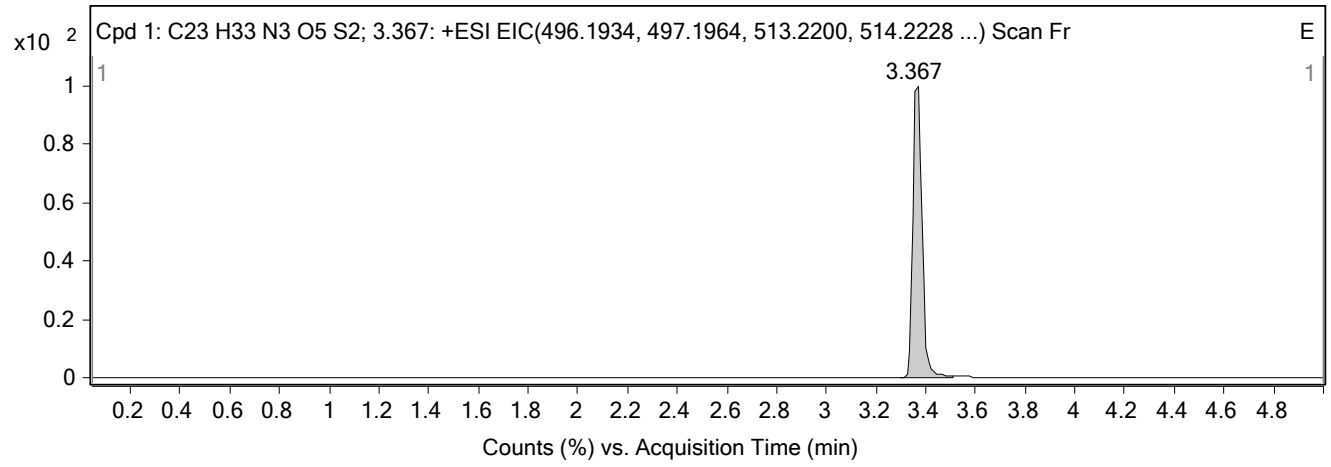
Data File	3.d	**Sample Name**	H3464500
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 5:50:51 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H33N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 5:50:51 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

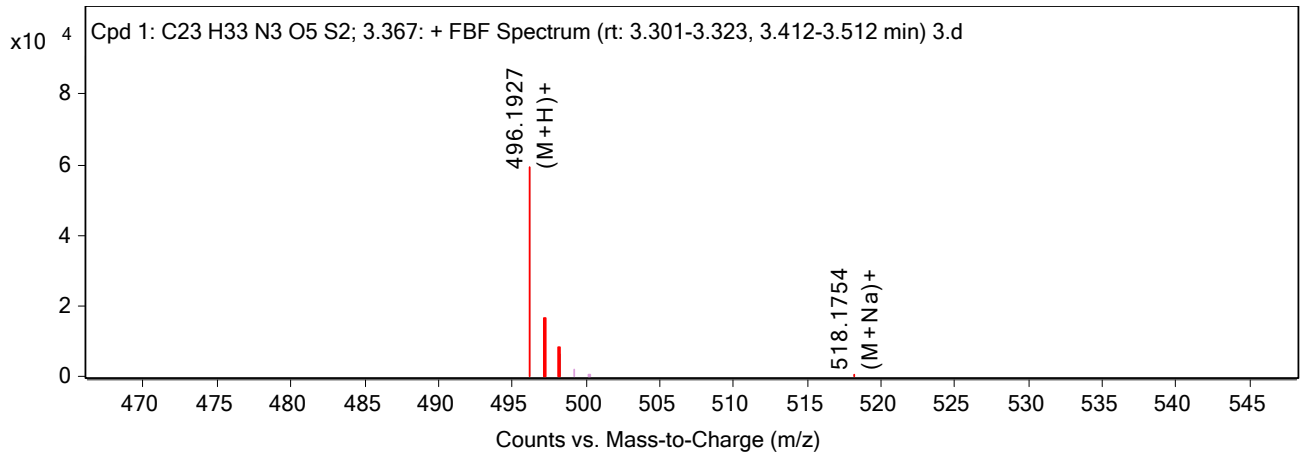
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H33 N3 O5 S2; 3.367	93.7	-1.6	C23 H33 N3 O5 S2	3.367	495.1862	495.1854

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
496.1927	3.367	495.1854	C23 H33 N3 O5 S2	495.1862	-1.6	Find By Formula	

Compound Chromatograms



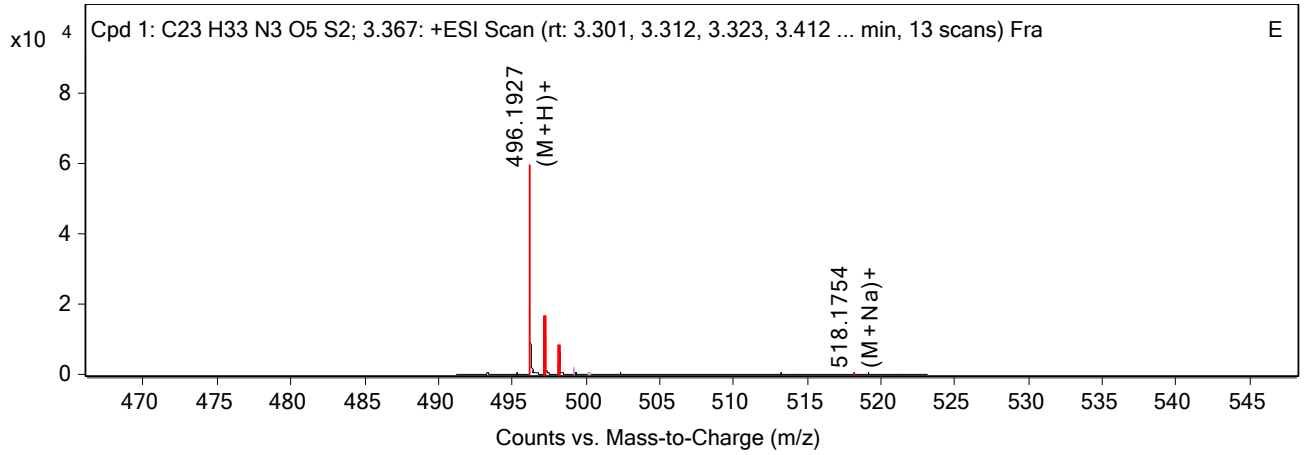
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
496.1927	1	59378.1	(M+H)+
497.1954	1	13925.82	(M+H)+
498.1919	1	6276.47	(M+H)+
518.1754	1	617.86	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
496.1927	1	59378.1	(M+H)+	1.54
497.1954	1	13925.82	(M+H)+	1.9
498.1919	1	6276.47	(M+H)+	1.55
518.1754	1	617.86	(M+Na)+	-0.08

--- End Of Report ---

Target Compound Screening Report

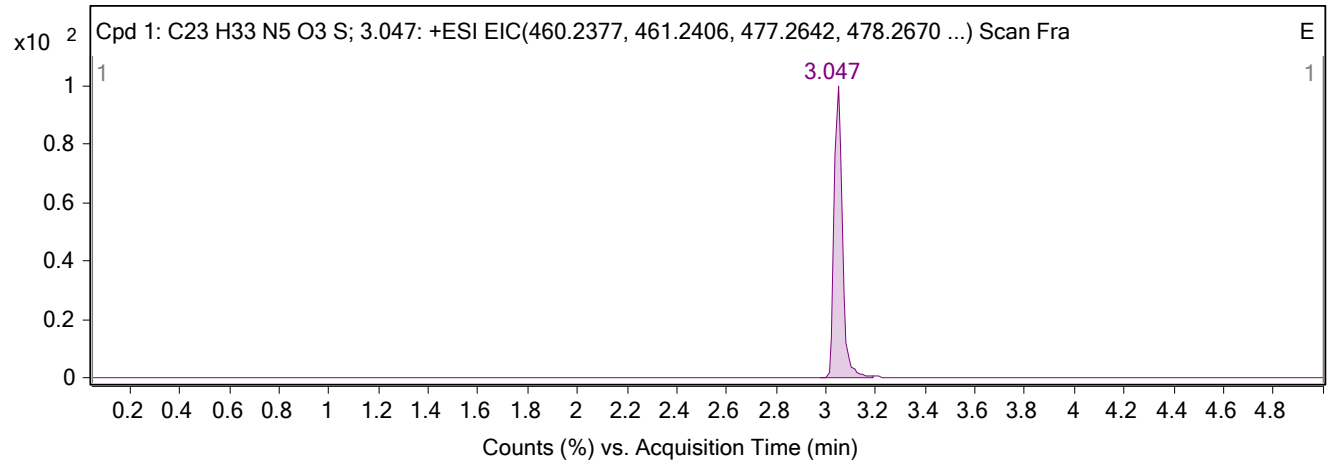
Data File	31.d	**Sample Name**	H2373341
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 9:40:08 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H33N5O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 9:40:08 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

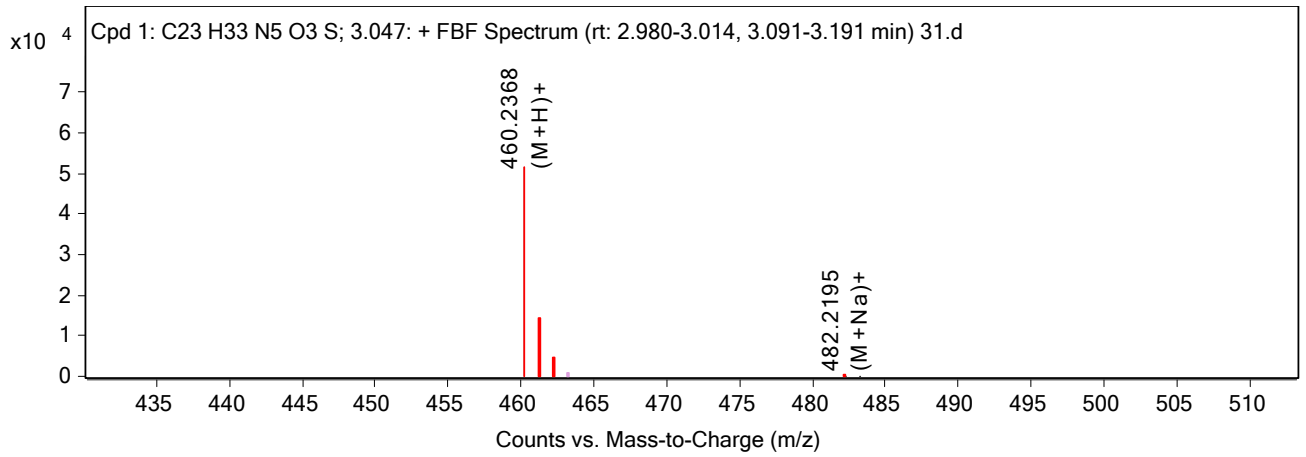
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H33 N5 O3 S; 3.047	94.69	-2.05	C23 H33 N5 O3 S	3.047	459.2304	459.2295

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
460.2368	3.047	459.2295	C23 H33 N5 O3 S	459.2304	-2.05	Find By Formula	

Compound Chromatograms



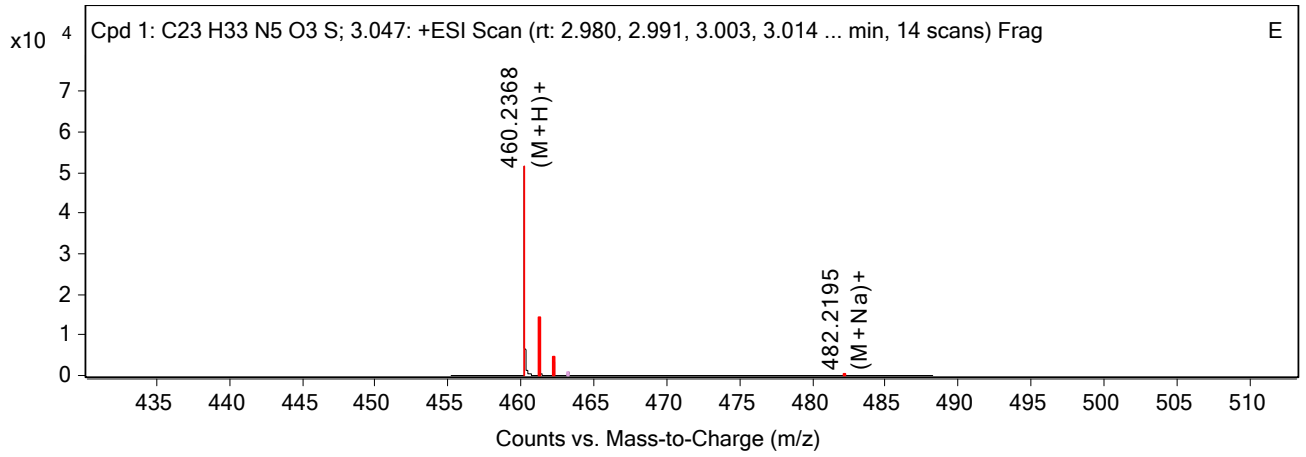
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
460.2368	1	51431.06	(M+H)+
461.2394	1	11898.45	(M+H)+
462.2374	1	3297.47	(M+H)+
482.2195	1	206.4	(M+Na)+
483.2333	1	92.87	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
460.2368	1	51431.06	(M+H)+	2
460.2368		51431.06		
461.2394	1	11898.45	(M+H)+	2.51
462.2374	1	3297.47	(M+H)+	1.97
482.2195	1	206.4	(M+Na)+	0.17
483.2333	1	92.87	(M+Na)+	-22.42

--- End Of Report ---

Target Compound Screening Report

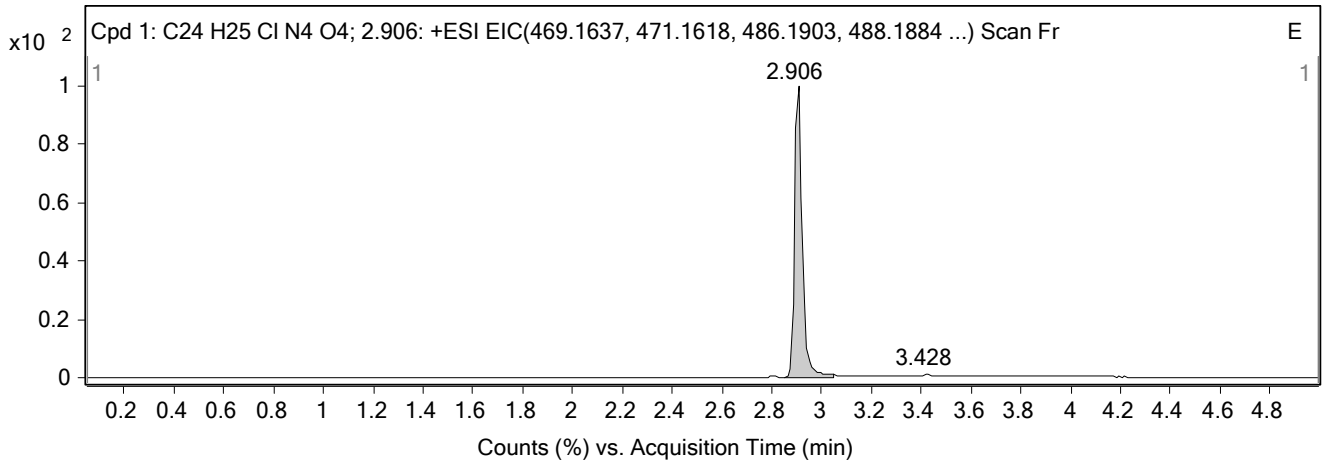
Data File	6d.d	**Sample Name**	H2055790
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:41:09 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H25ClN4O4	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:41:09 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

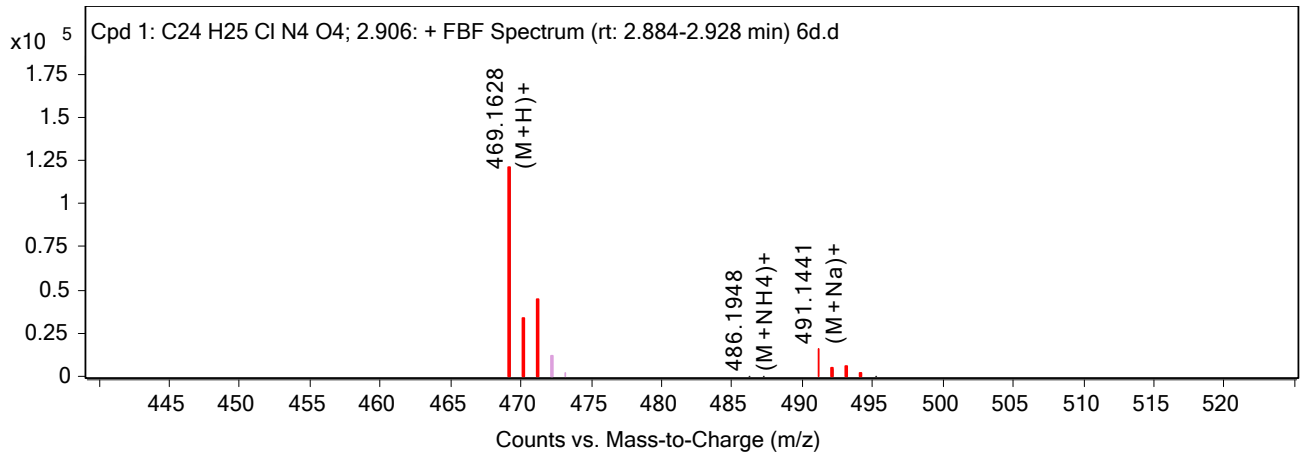
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H25 Cl N4 O4; 2.906	94.2	-2.15	C24 H25 Cl N4 O4	2.906	468.1564	468.1554

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
491.1441	2.906	468.1554	C24 H25 Cl N4 O4	468.1564	-2.15	Find By Formula	

Compound Chromatograms



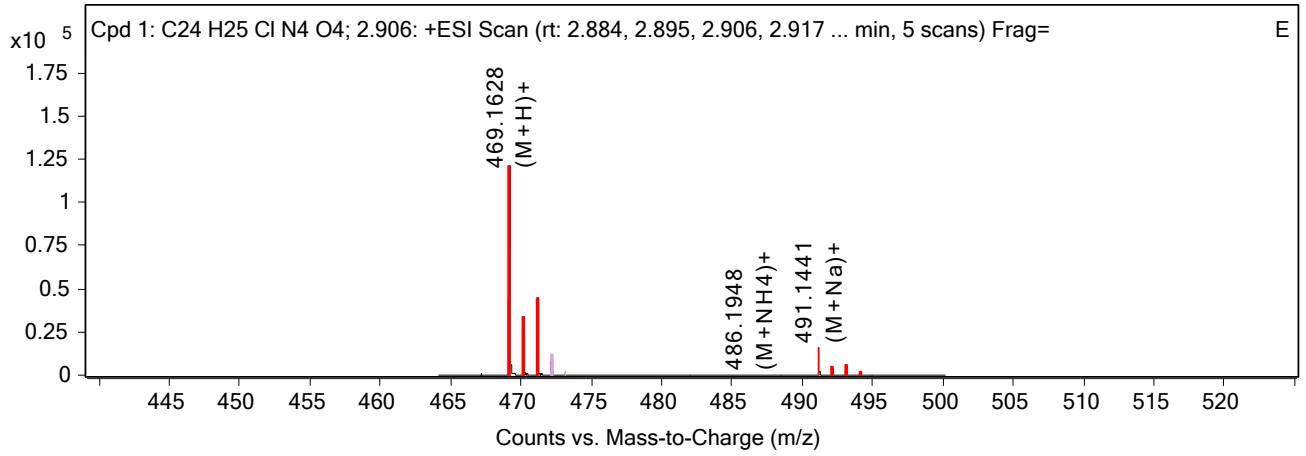
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
469.1628	1	120879.06	(M+H)+
470.1655	1	26882.93	(M+H)+
471.1611	1	35642.86	(M+H)+
486.1948	1	67.61	(M+NH4)+
487.1987	1	41.27	(M+NH4)+
491.1441	1	16138.39	(M+Na)+
492.1477	1	4173.06	(M+Na)+
493.1423	1	5251.41	(M+Na)+
494.1447	1	1381.58	(M+Na)+
495.1498	1	240.35	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
469.1628	1	120879.06	(M+H)+	1.97
470.1655	1	26882.93	(M+H)+	2.73
471.1611	1	35642.86	(M+H)+	1.64
486.1948	1	67.61	(M+NH4)+	-9.33
487.1987	1	41.27	(M+NH4)+	-11.15
491.1441	1	16138.39	(M+Na)+	3.23
492.1477	1	4173.06	(M+Na)+	2.02
493.1423	1	5251.41	(M+Na)+	2.93
494.1447	1	1381.58	(M+Na)+	3.07
495.1498	1	240.35	(M+Na)+	-2.01

--- End Of Report ---

Target Compound Screening Report

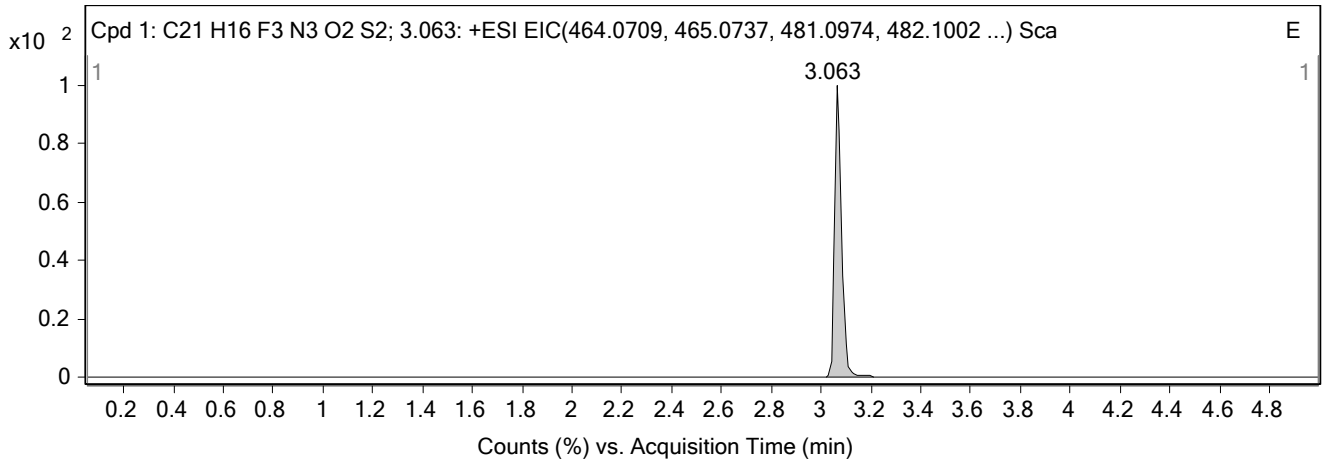
Data File	2.d	**Sample Name**	H3464498
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 5:45:16 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H16F3N3O2S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 5:45:16 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

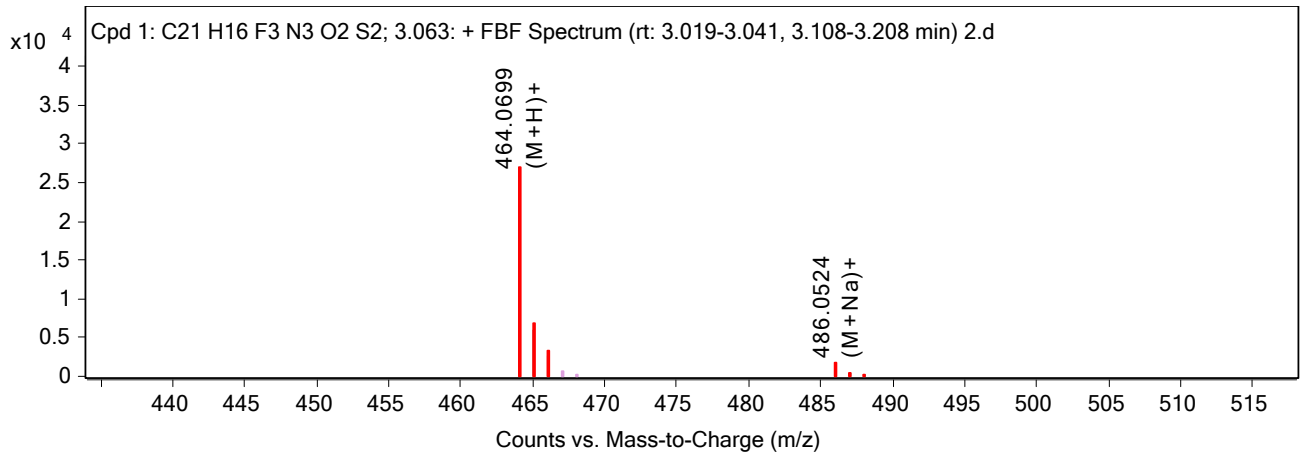
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H16 F3 N3 O2 S2; 3.063	94.17	-2.03	C21 H16 F3 N3 O2 S2	3.063	463.0636	463.0627

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
464.0699	3.063	463.0627	C21 H16 F3 N3 O2 S2	463.0636	-2.03	Find By Formula	

Compound Chromatograms



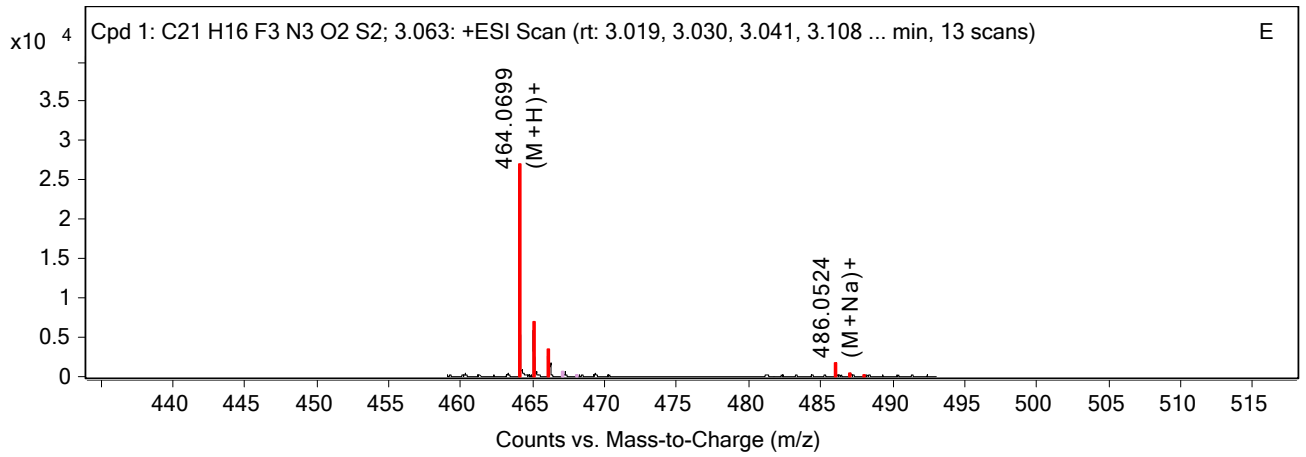
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
464.0699	1	27014.93	(M+H)+
465.0729	1	5908.43	(M+H)+
466.0683	1	2680.69	(M+H)+
486.0524	1	1820.18	(M+Na)+
487.0536	1	480.81	(M+Na)+
488.0529	1	229.43	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
464.0699	1	27014.93	(M+H)+	2.12
465.0729	1	5908.43	(M+H)+	1.75
466.0683	1	2680.69	(M+H)+	2.44
486.0524	1	1820.18	(M+Na)+	0.82
487.0536	1	480.81	(M+Na)+	4.3
488.0529	1	229.43	(M+Na)+	-3

--- End Of Report ---

Target Compound Screening Report

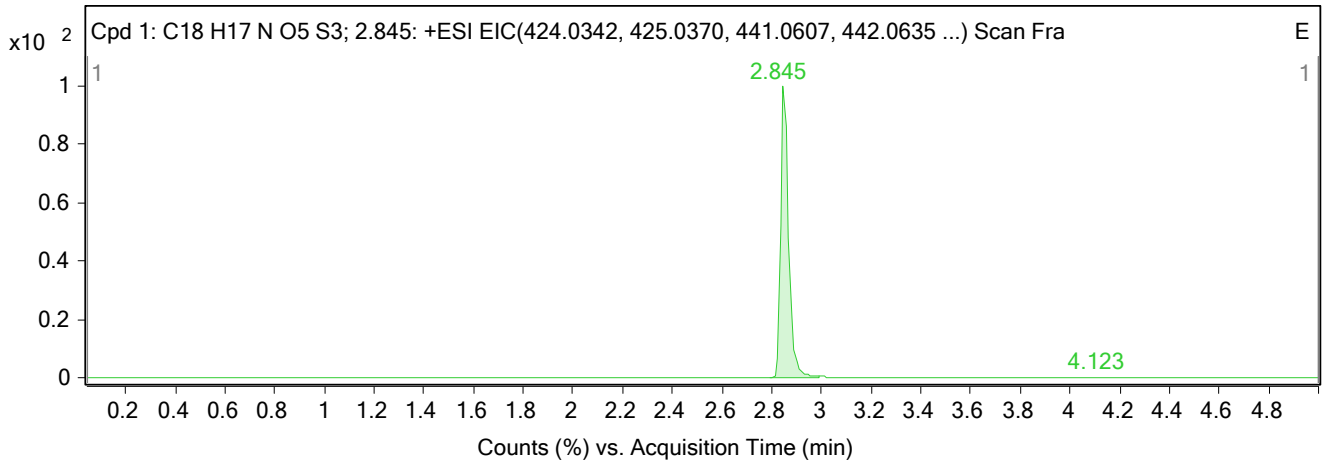
Data File	51.d	**Sample Name**	H2049812
Sample Type	Sample	**Position**	P1-F6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:54:14 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C18H17NO5S3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:54:14 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

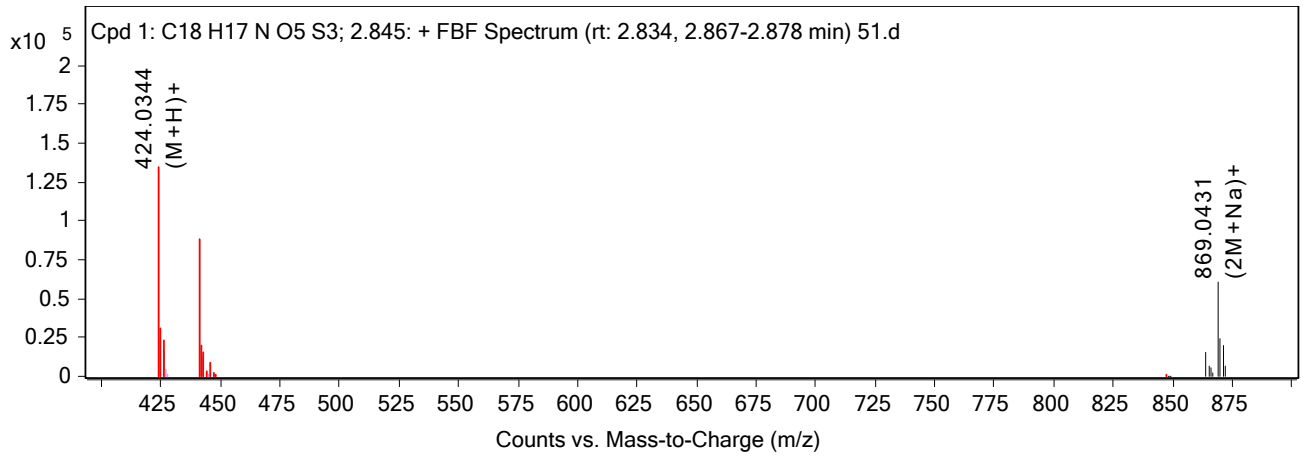
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C18 H17 N O5 S3; 2.845	96.87	-0.14	C18 H17 N O5 S3	2.845	423.0269	423.0268

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
446.0163	2.845	423.0268	C18 H17 N O5 S3	423.0269	-0.14	Find By Formula	

Compound Chromatograms



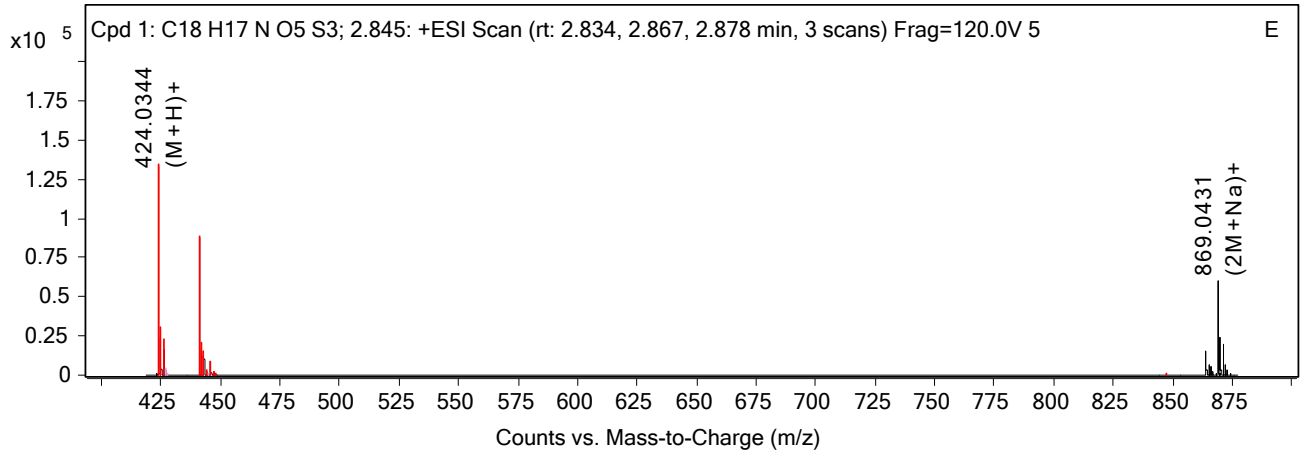
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
424.0344	1	134384.28	(M+H)+
425.0368	1	24419.9	(M+H)+
426.032	1	16798.2	(M+H)+
441.0609	1	88163.88	(M+NH4)+
442.0632	1	16869.2	(M+NH4)+
443.0583	1	11711.34	(M+NH4)+
864.0865	1	15663.35	(2M+NH4)+
869.0431	1	60359.11	(2M+Na)+
870.0459	1	23990.24	(2M+Na)+
871.0414	1	19461.12	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
424.0344	1	134384.28	(M+H)+	-0.46
425.0368	1	24419.9	(M+H)+	0.44
426.032	1	16798.2	(M+H)+	-0.18
441.0609	1	88163.88	(M+NH4)+	-0.4
442.0632	1	16869.2	(M+NH4)+	0.59
443.0583	1	11711.34	(M+NH4)+	0.28
864.0865	1	15663.35	(2M+NH4)+	1.23
869.0431	1	60359.11	(2M+Na)+	-0.14
870.0459	1	23990.24	(2M+Na)+	-0.02
871.0414	1	19461.12	(2M+Na)+	0.49

--- End Of Report ---

Target Compound Screening Report

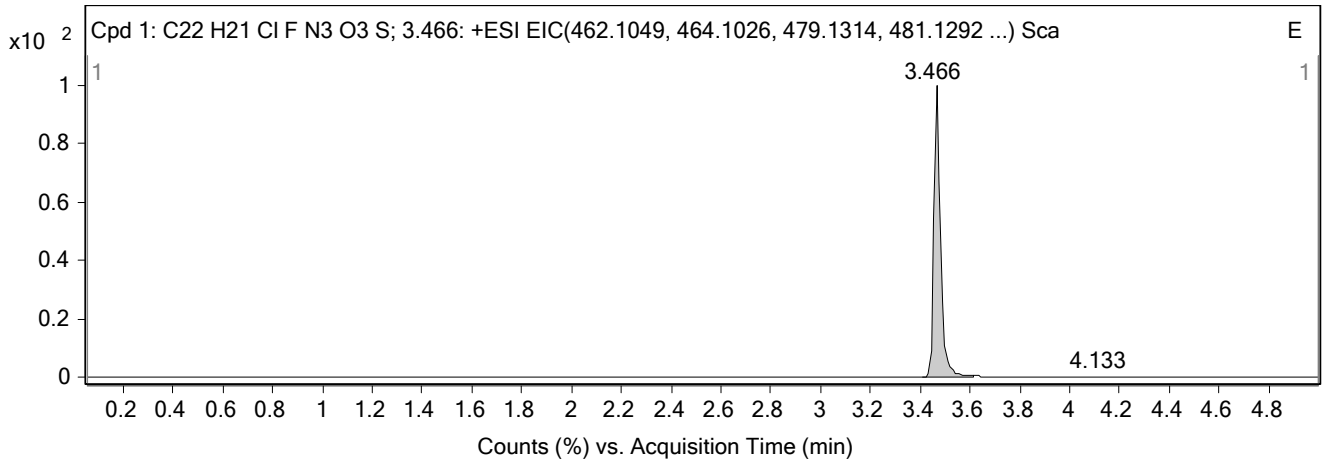
Data File	1-2.d	**Sample Name**	H2045014
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 11:15:03 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H21ClFN3O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 11:15:03 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

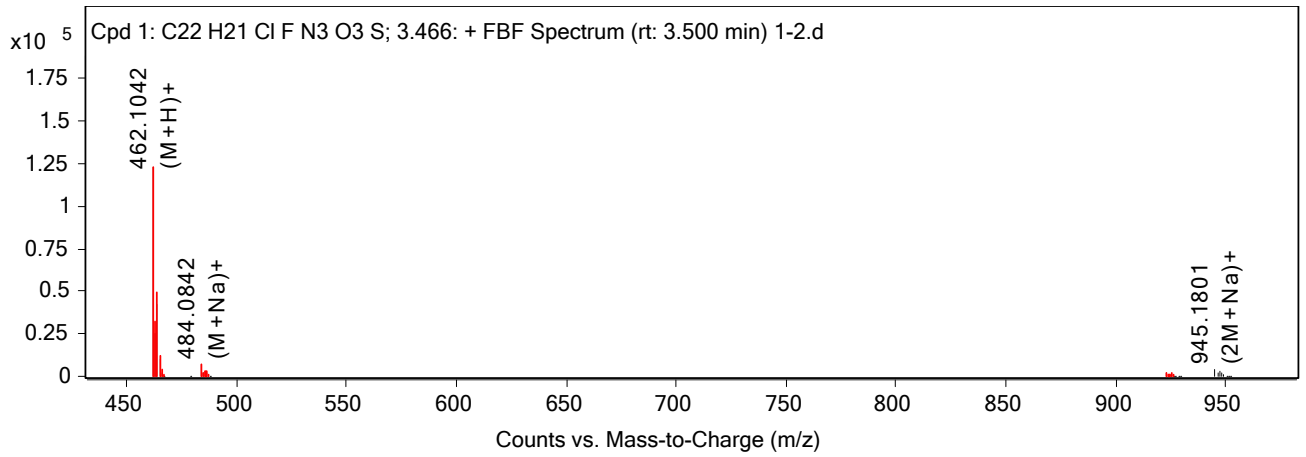
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H21 Cl F N3 O3 S; 3.466	95.94	-2.1	C22 H21 Cl F N3 O3 S	3.466	461.0976	461.0967

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
462.1042	3.466	461.0967	C22 H21 Cl F N3 O3 S	461.0976	-2.1	Find By Formula	

Compound Chromatograms



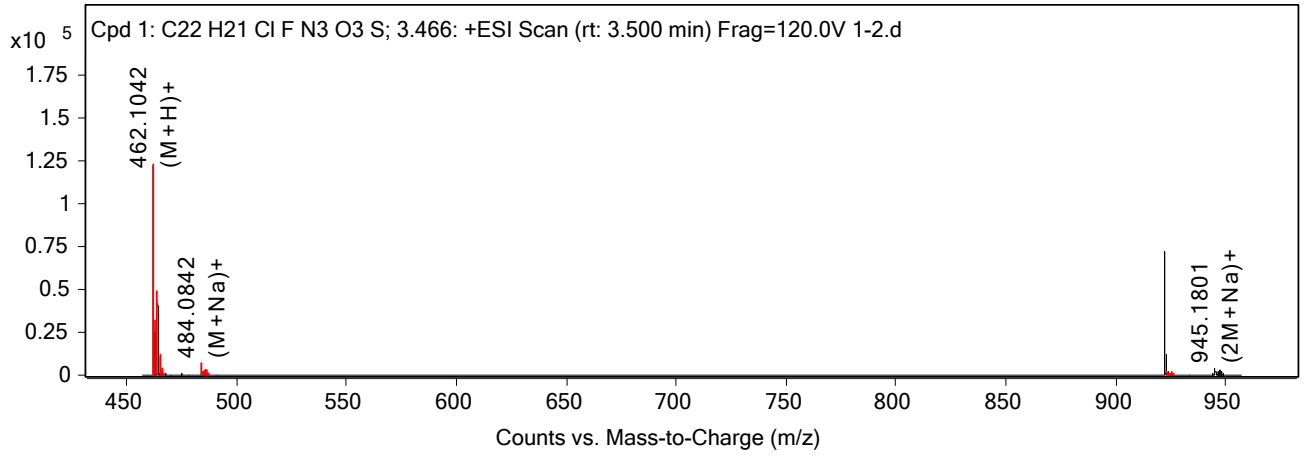
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
462.1042	1	122704.11	(M+H)+
463.107	1	25532.82	(M+H)+
464.1019	1	42062.22	(M+H)+
465.1042	1	9807.51	(M+H)+
466.1024	1	2356.21	(M+H)+
484.0842	1	7318.45	(M+Na)+
486.0845	1	2551.92	(M+Na)+
945.1801	1	4078.53	(2M+Na)+
946.1871	1	1949.31	(2M+Na)+
947.1822	1	3323.41	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
462.1042	1	122704.11	(M+H)+	1.47
463.107	1	25532.82	(M+H)+	2
464.1019	1	42062.22	(M+H)+	1.65
465.1042	1	9807.51	(M+H)+	2.09
466.1024	1	2356.21	(M+H)+	0.82
484.0842	1	7318.45	(M+Na)+	5.42
486.0845	1	2551.92	(M+Na)+	0.12
945.1801	1	4078.53	(2M+Na)+	4.65
946.1871	1	1949.31	(2M+Na)+	0.35
947.1822	1	3323.41	(2M+Na)+	0.7

--- End Of Report ---

Target Compound Screening Report

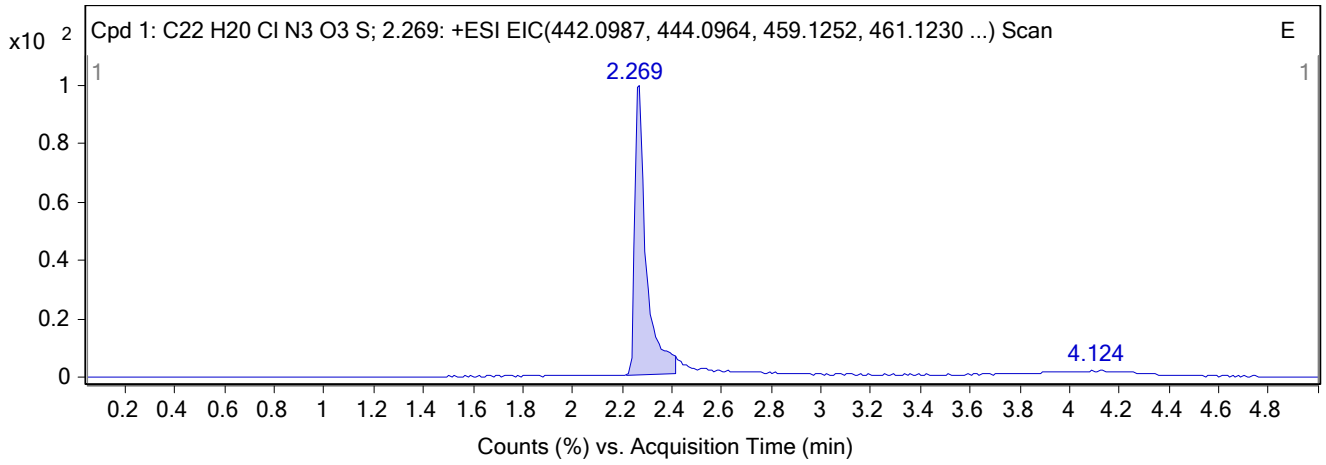
Data File	30.d	**Sample Name**	H2045019
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 9:34:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H20ClN3O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 9:34:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

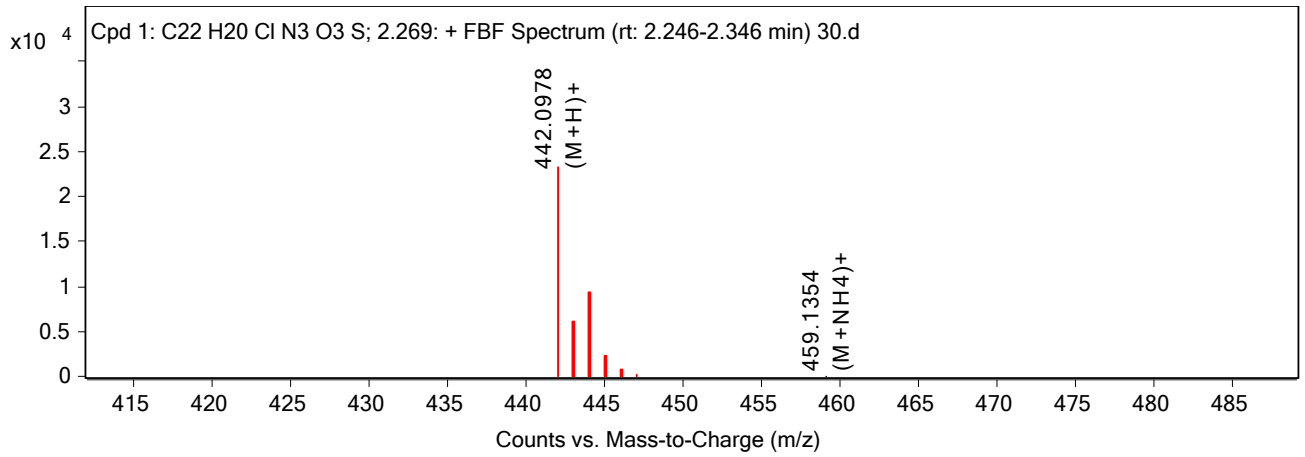
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H20 Cl N3 O3 S; 2.269	97.2	-1.99	C22 H20 Cl N3 O3 S	2.269	441.0914	441.0905

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
442.0978	2.269	441.0905	C22 H20 Cl N3 O3 S	441.0914	-1.99	Find By Formula	

Compound Chromatograms



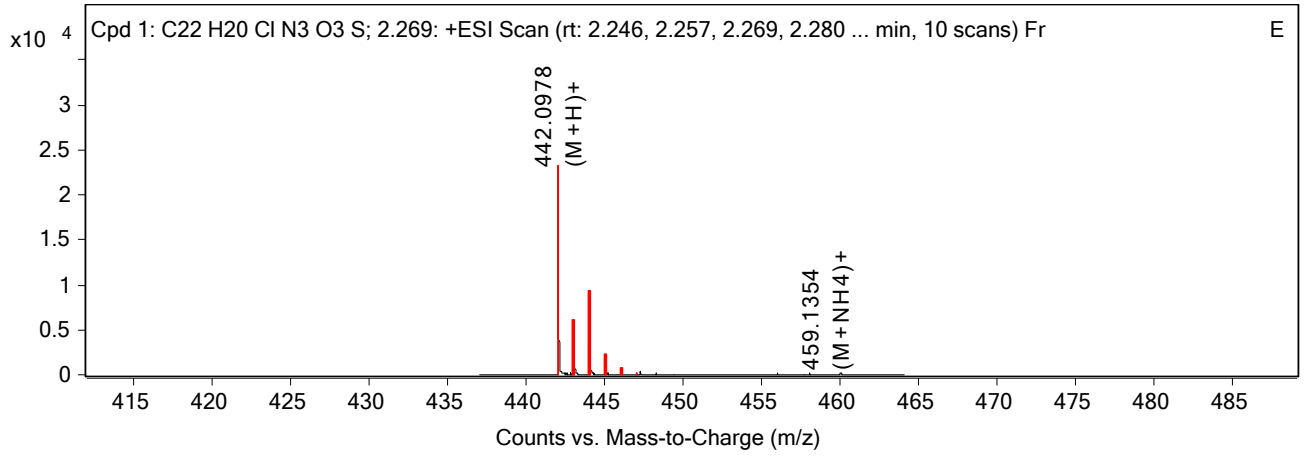
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
442.0978	1	23221.43	(M+H)+
443.1008	1	5174.75	(M+H)+
444.0954	1	8345.08	(M+H)+
445.0981	1	1935.73	(M+H)+
446.0958	1	566.65	(M+H)+
447.0971	1	159.72	(M+H)+
459.1354	1	60.08	(M+NH4)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
442.0978	1	23221.43	(M+H)+	1.97
443.1008	1	5174.75	(M+H)+	1.98
444.0954	1	8345.08	(M+H)+	2.3
445.0981	1	1935.73	(M+H)+	1.81
446.0958	1	566.65	(M+H)+	1.6
447.0971	1	159.72	(M+H)+	0.71
459.1354	1	60.08	(M+NH4)+	-22.24

--- End Of Report ---

Target Compound Screening Report

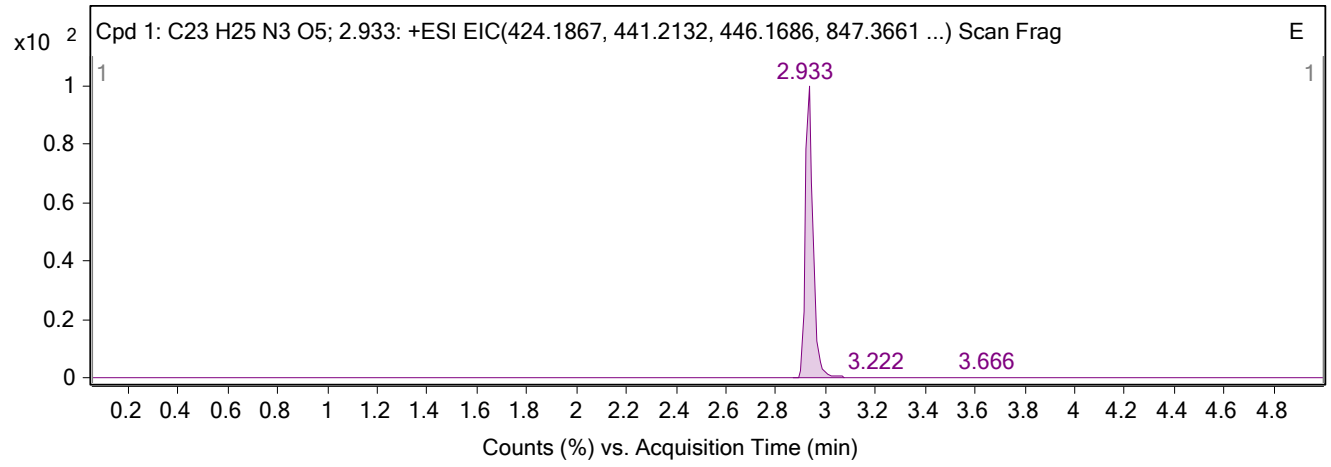
Data File	49.d	**Sample Name**	H2382810
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:43:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H25N3O5	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:43:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

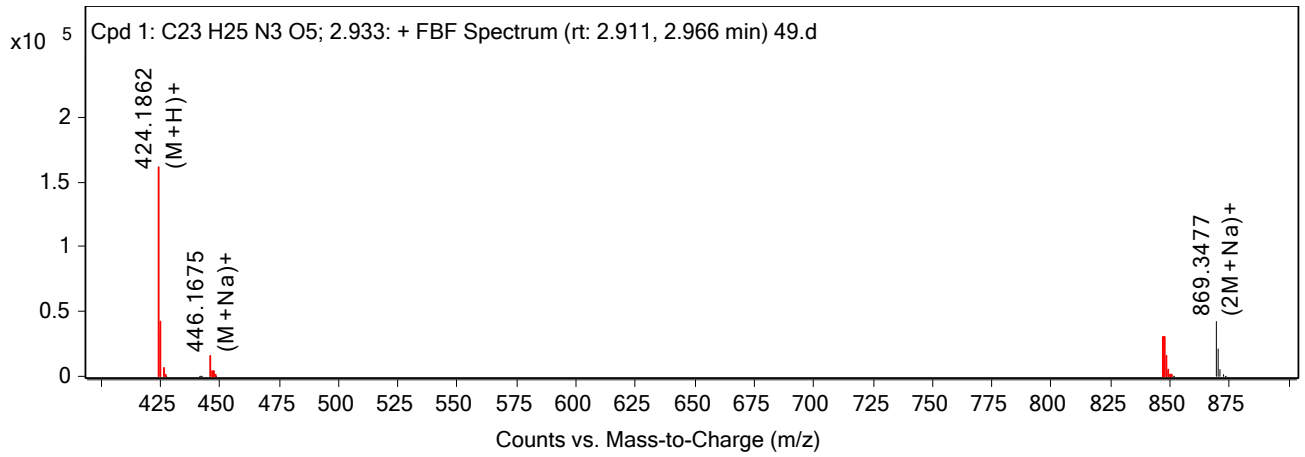
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H25 N3 O5; 2.933	99.02	-1.38	C23 H25 N3 O5	2.933	423.1794	423.1788

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
869.3477	2.933	423.1788	C23 H25 N3 O5	423.1794	-1.38	Find By Formula	

Compound Chromatograms



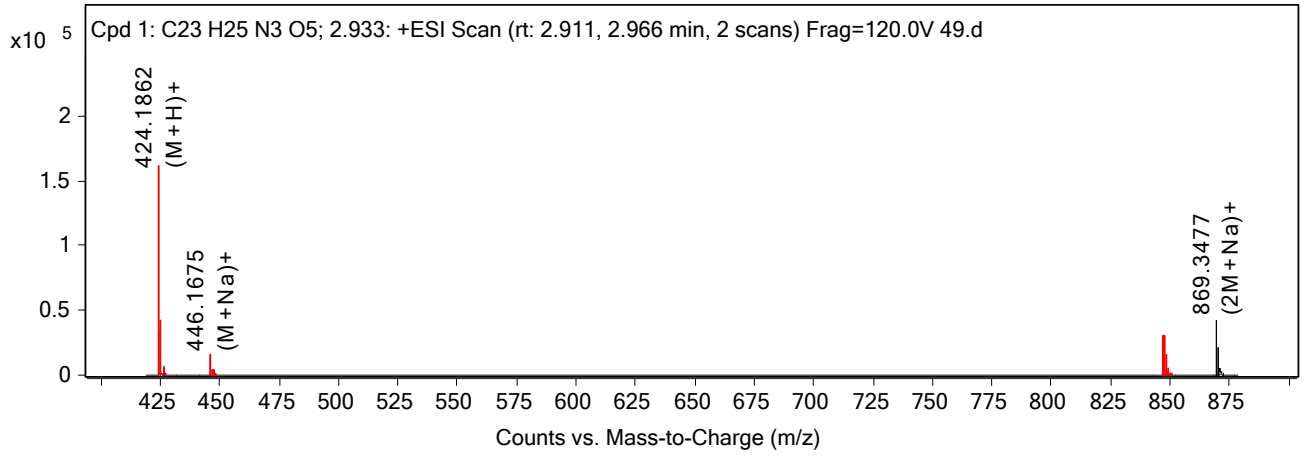
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
424.1862	1	161157.53	(M+H)+
425.1893	1	34475.91	(M+H)+
426.1918	1	5216.42	(M+H)+
446.1675	1	15690.04	(M+Na)+
847.3659	1	29870.93	(2M+H)+
848.3686	1	14771.41	(2M+H)+
849.3696	1	4186.91	(2M+H)+
869.3477	1	42831.88	(2M+Na)+
870.3507	1	21448.79	(2M+Na)+
871.352	1	5994.26	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
424.1862	1	161157.54	(M+H)+	1.17
425.1893	1	34475.91	(M+H)+	1.27
426.1918	1	5216.42	(M+H)+	1.68
446.1675	1	15690.04	(M+Na)+	2.52
847.3659	1	29870.93	(2M+H)+	0.25
848.3686	1	14771.41	(2M+H)+	0.77
849.3696	1	4186.91	(2M+H)+	2.97
869.3477	1	42831.88	(2M+Na)+	0.43
870.3507	1	21448.79	(2M+Na)+	0.59
871.352	1	5994.26	(2M+Na)+	2.36

--- End Of Report ---

Target Compound Screening Report

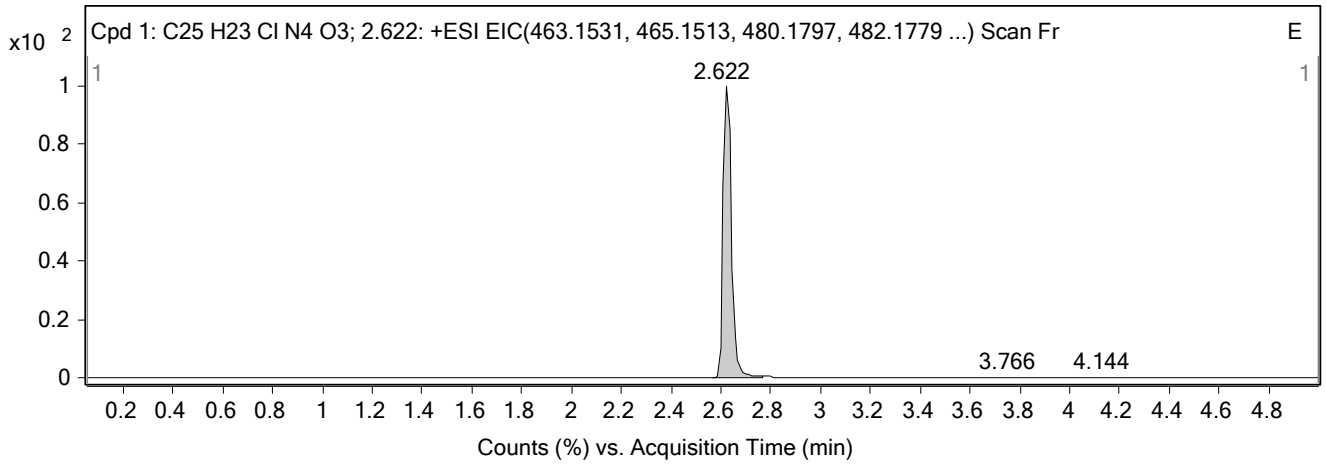
Data File	9.d	**Sample Name**	T8793466
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 6:24:12 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H23ClN4O3	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 6:24:12 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H23 Cl N4 O3; 2.622	94.96	-2.02	C25 H23 Cl N4 O3	2.622	462.1459	462.1449

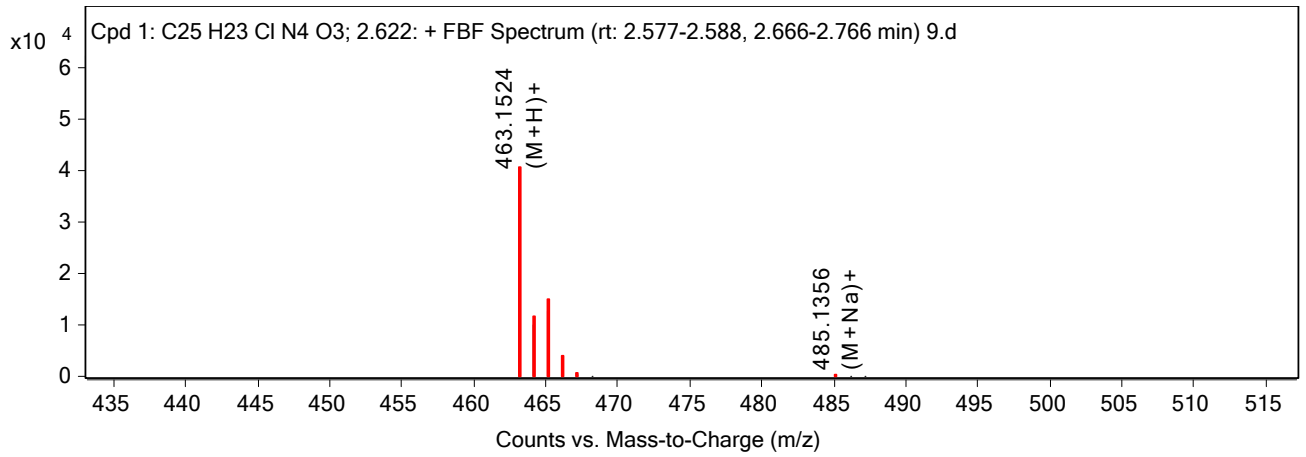
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
463.1524	2.622	462.1449	C25 H23 Cl N4 O3	462.1459	-2.02	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

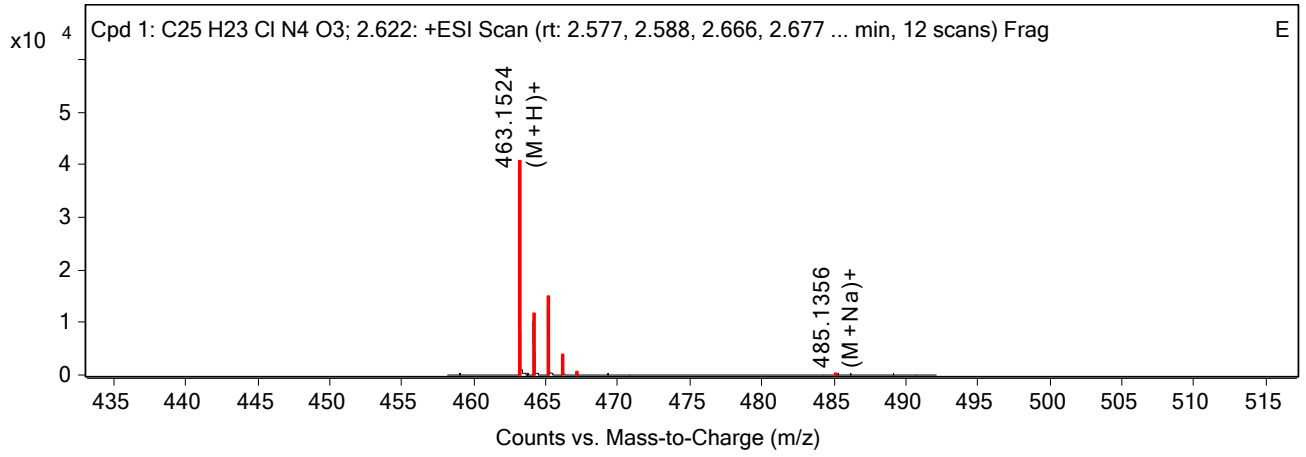
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
463.1524	1	40632.36	(M+H)+
464.1548	1	10089.17	(M+H)+
465.1501	1	12766.08	(M+H)+
466.1523	1	3113.97	(M+H)+
467.1557	1	451.45	(M+H)+
468.1586	1	101.58	(M+H)+
485.1356	1	381.55	(M+Na)+
486.134	1	185.47	(M+Na)+
487.1337	1	157.38	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
463.1524	1	40632.36	(M+H)+	1.53
464.1548	1	10089.17	(M+H)+	2.98
465.1501	1	12766.08	(M+H)+	2.58
466.1523	1	3113.97	(M+H)+	3.12
467.1557	1	451.45	(M+H)+	1.3
468.1586	1	101.58	(M+H)+	0.7
485.1356	1	381.55	(M+Na)+	-1.01
486.134	1	185.47	(M+Na)+	8.51
487.1337	1	157.38	(M+Na)+	-0.88

--- End Of Report ---

Target Compound Screening Report

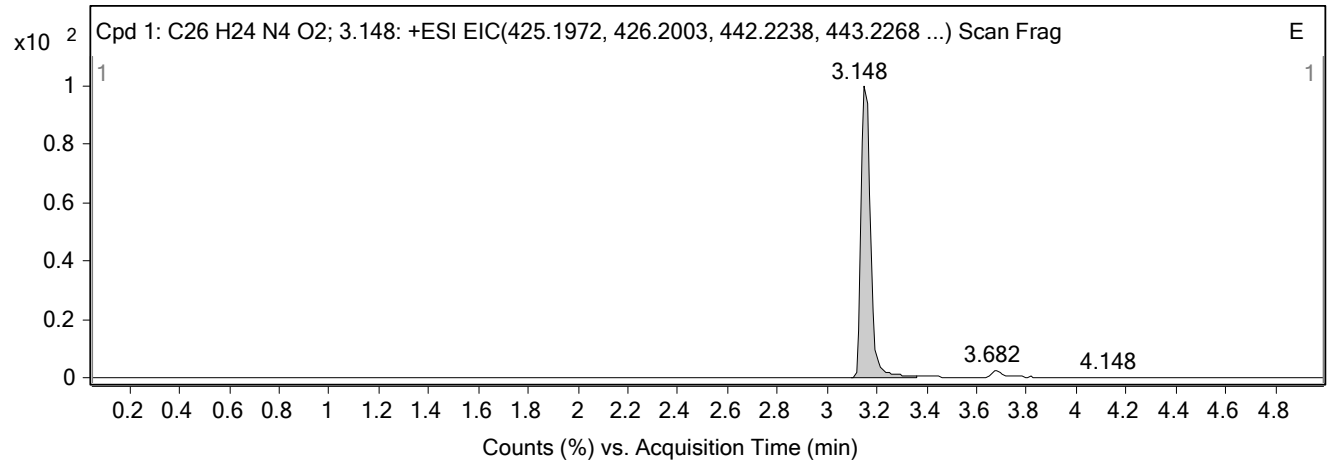
Data File	1.d	**Sample Name**	H3467611
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/5/2021 5:39:45 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H24N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/5/2021 5:39:45 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H24 N4 O2; 3.148	92.6	-0.74	C26 H24 N4 O2	3.148	424.1899	424.1896

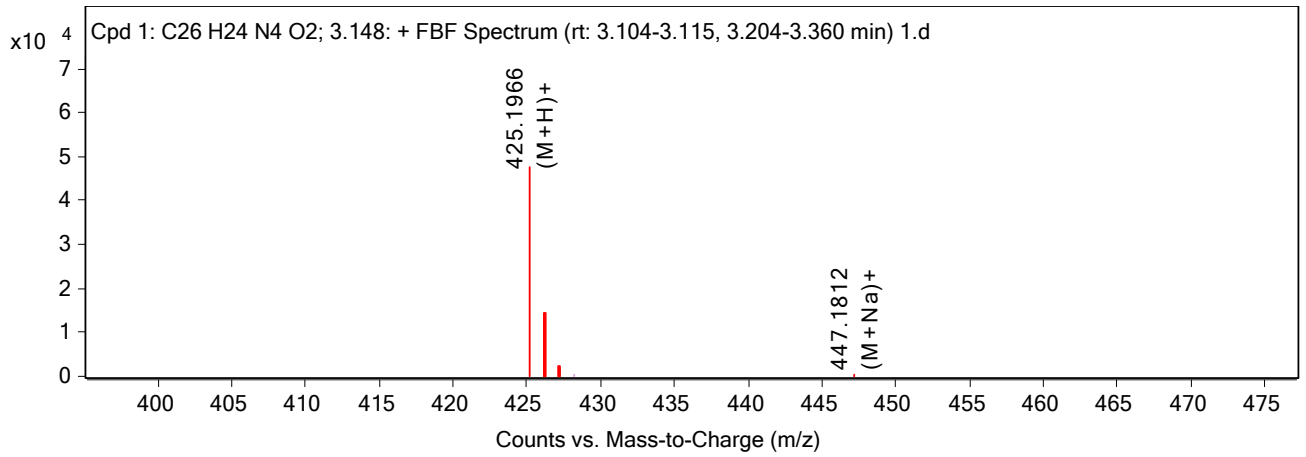
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
425.1966	3.148	424.1896	C26 H24 N4 O2	424.1899	-0.74	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

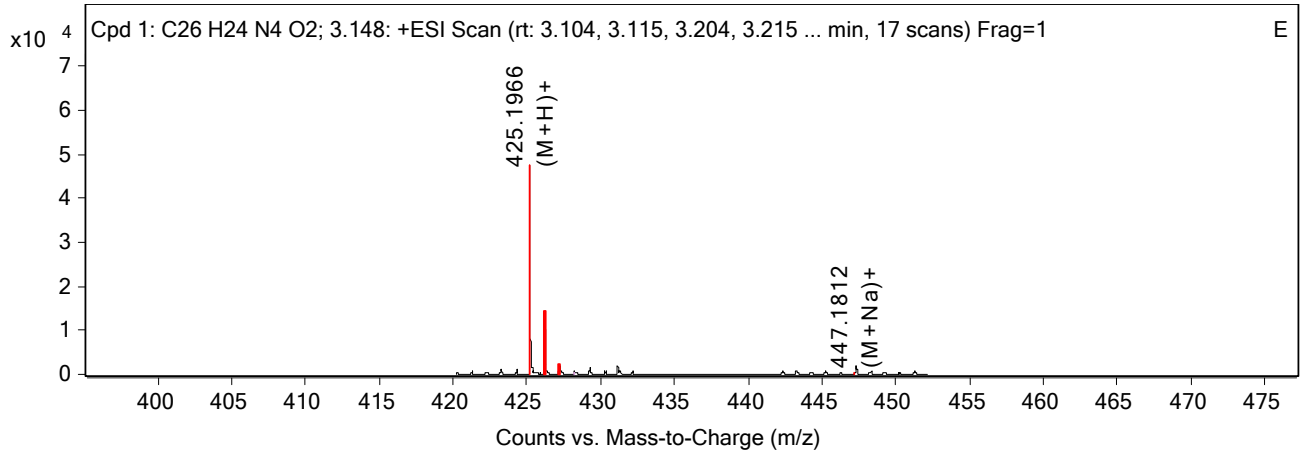
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
425.1966	1	47685	(M+H)+
426.1997	1	12483.08	(M+H)+
427.2112	1	2150.48	(M+H)+
447.1812	1	556.71	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
425.1966	1	47685	(M+H)+	1.51
426.1997	1	12483.07	(M+H)+	1.38
427.2112	1	2150.48	(M+H)+	-18.69
447.1812	1	556.71	(M+Na)+	-4.48

--- End Of Report ---

Target Compound Screening Report

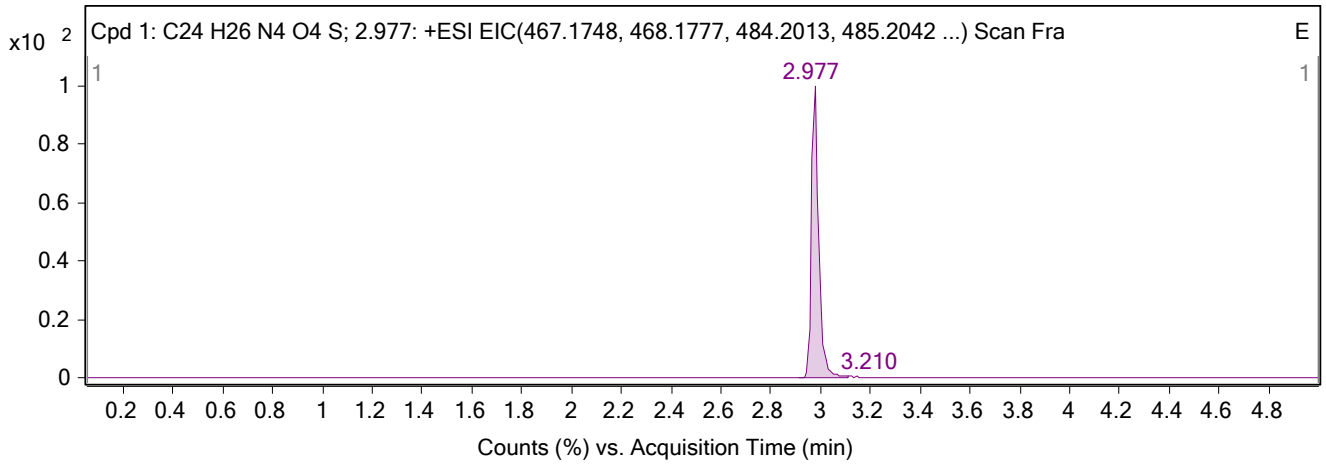
Data File	19.d	**Sample Name**	H2994757
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:27:54 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H26N4O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:27:54 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

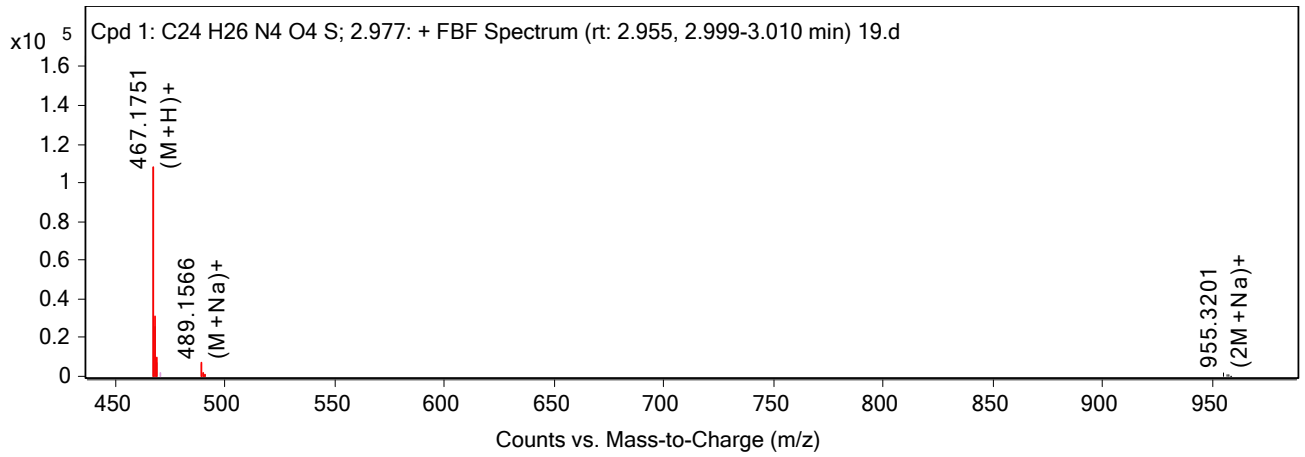
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H26 N4 O4 S; 2.977	98.29	0.51	C24 H26 N4 O4 S	2.977	466.1675	466.1677

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
489.1566	2.977	466.1677	C24 H26 N4 O4 S	466.1675	0.51	Find By Formula	

Compound Chromatograms



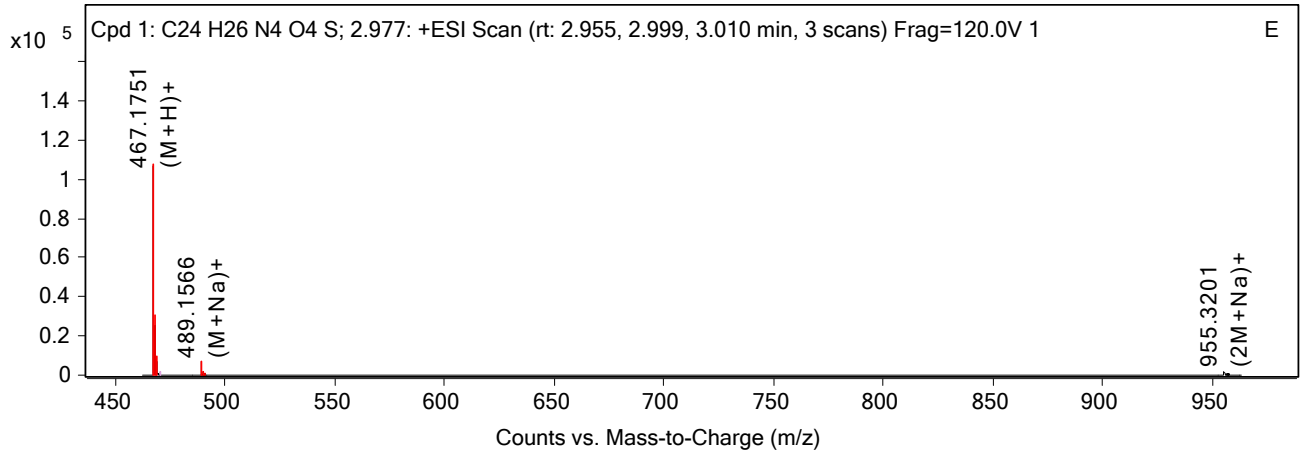
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
467.1751	1	107970.35	(M+H)+
468.1781	1	25957.75	(M+H)+
469.1752	1	6925.37	(M+H)+
489.1566	1	6698.95	(M+Na)+
490.1607	1	1962.07	(M+Na)+
491.1565	1	610.57	(M+Na)+
955.3201	1	2034.22	(2M+Na)+
956.3252	1	1190.13	(2M+Na)+
957.3235	1	500.47	(2M+Na)+
958.3208	1	172.4	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
467.1751	1	107970.35	(M+H)+	-0.84
468.1781	1	25957.75	(M+H)+	-0.82
469.1752	1	6925.37	(M+H)+	1.01
489.1566	1	6698.95	(M+Na)+	0.12
490.1607	1	1962.07	(M+Na)+	-2.08
491.1565	1	610.57	(M+Na)+	2.27
955.3201	1	2034.22	(2M+Na)+	4.24
956.3252	1	1190.13	(2M+Na)+	2.02
957.3235	1	500.47	(2M+Na)+	3.24
958.3208	1	172.4	(2M+Na)+	6.63

--- End Of Report ---

Target Compound Screening Report

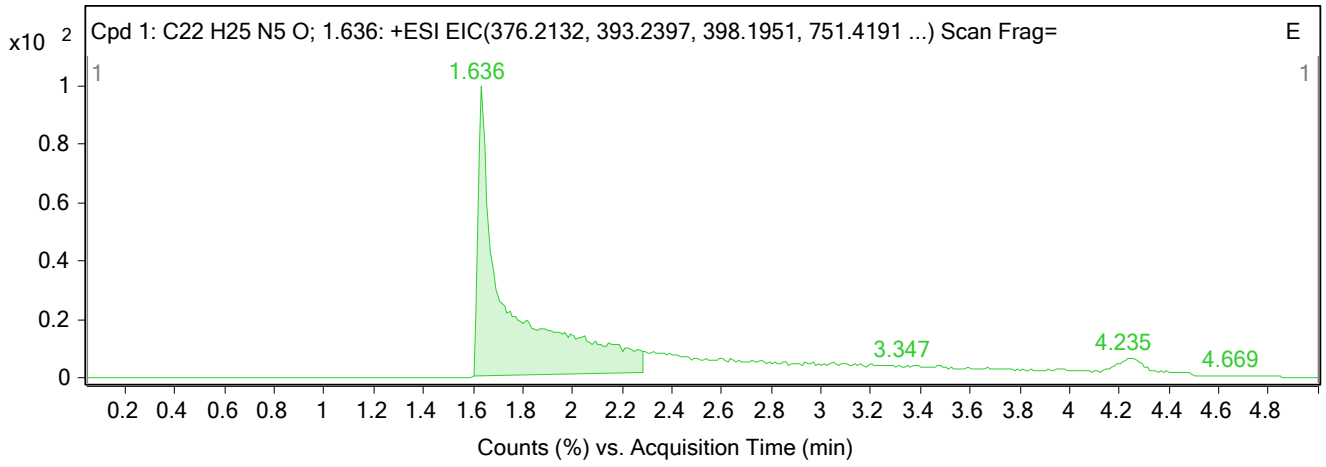
Data File	39.d	**Sample Name**	H2045144
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:47:38 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H25N5O	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:47:38 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

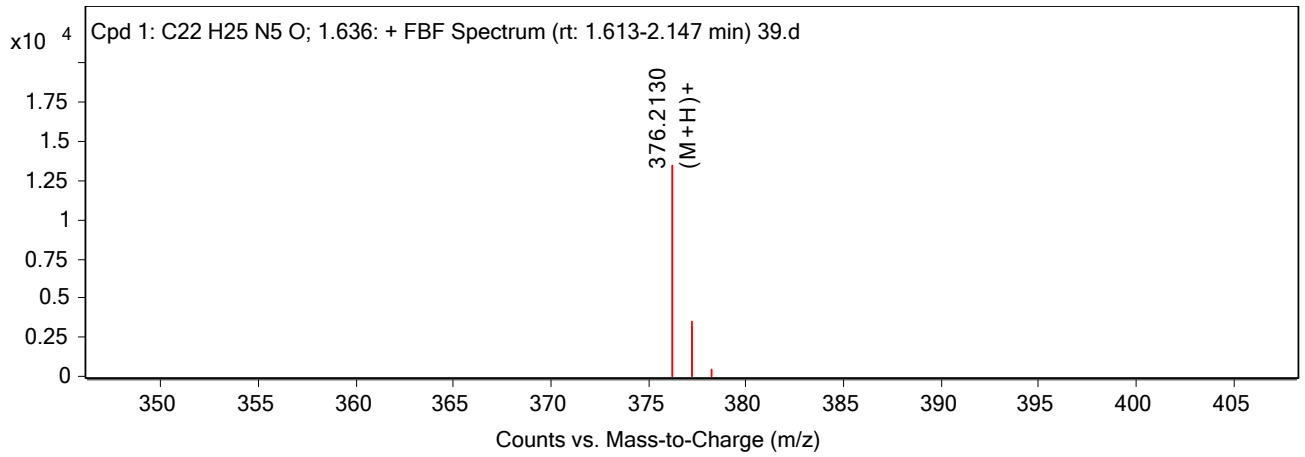
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H25 N5 O; 1.636	98.93	-0.46	C22 H25 N5 O	1.636	375.2059	375.2057

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
376.213	1.636	375.2057	C22 H25 N5 O	375.2059	-0.46	Find By Formula	

Compound Chromatograms



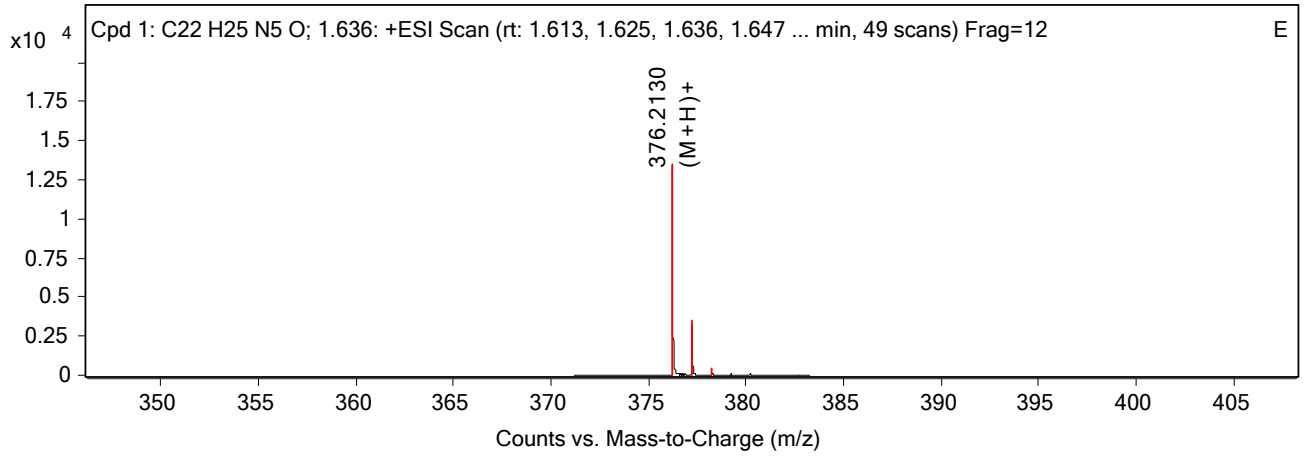
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
376.213	1	13482.71	(M+H)+
377.216	1	3183.78	(M+H)+
378.2191	1	450.68	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
376.213	1	13482.71	(M+H)+	0.48
377.216	1	3183.78	(M+H)+	0.47
378.2191	1	450.68	(M+H)+	-0.28

--- End Of Report ---

Target Compound Screening Report

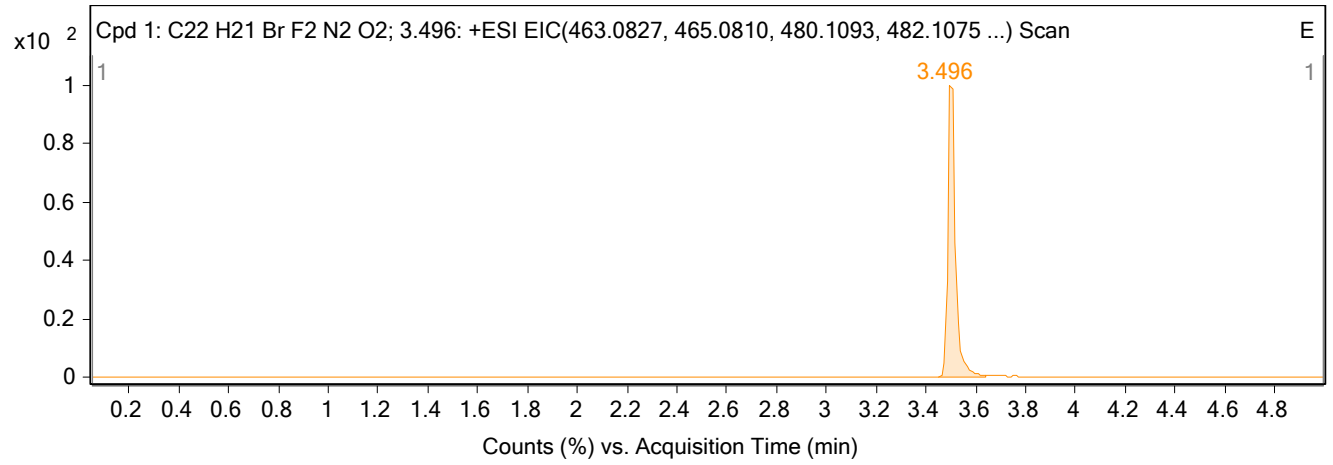
Data File	41.d	**Sample Name**	H2055735
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:58:46 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H21BrF2N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:58:46 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

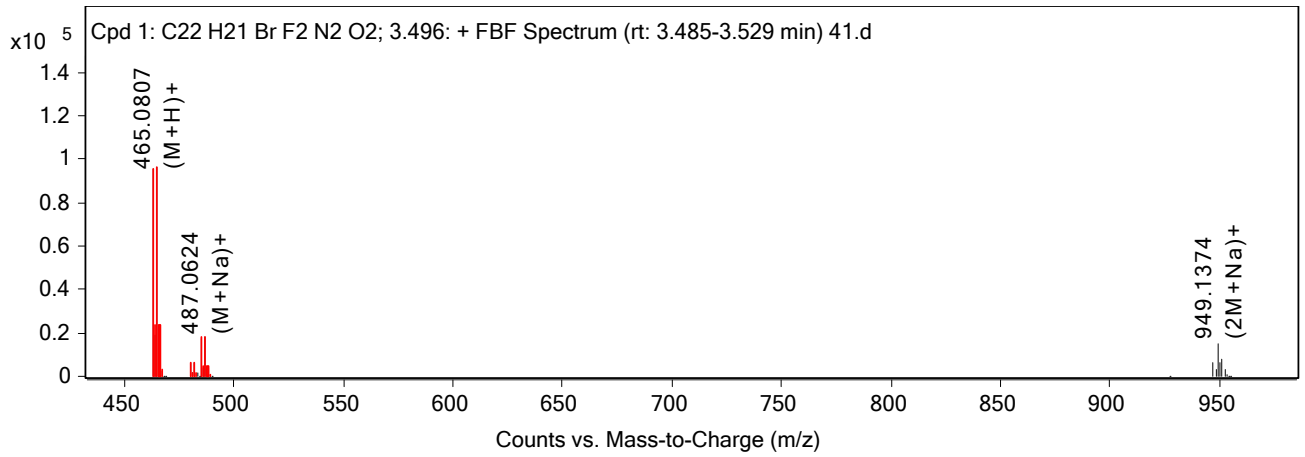
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H21 Br F2 N2 O2; 3.496	98.65	-1.09	C22 H21 Br F2 N2 O2	3.496	462.0754	462.0749

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
480.1085	3.496	462.0749	C22 H21 Br F2 N2 O2	462.0754	-1.09	Find By Formula	

Compound Chromatograms



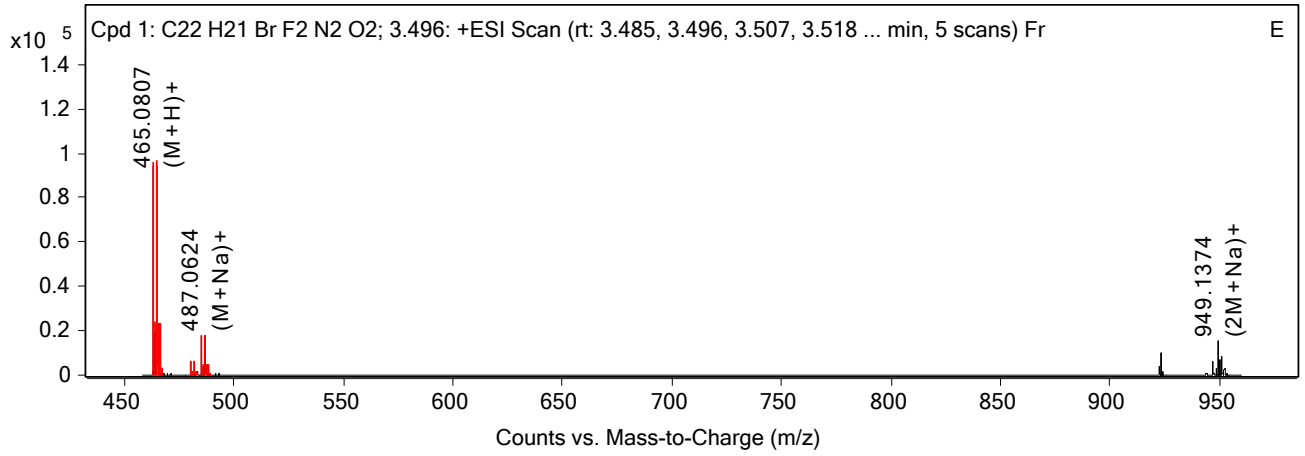
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
463.0825	1	95661.08	(M+H)+
464.0853	1	19336.82	(M+H)+
465.0807	1	96250.91	(M+H)+
466.0835	1	19235.23	(M+H)+
485.0643	1	17581.22	(M+Na)+
487.0624	1	17974.75	(M+Na)+
947.1382	1	6660.32	(2M+Na)+
949.1374	1	15211.95	(2M+Na)+
950.1403	1	6763.01	(2M+Na)+
951.1362	1	8327.4	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
463.0825	1	95661.08	(M+H)+	0.56
464.0853	1	19336.82	(M+H)+	1.28
465.0807	1	96250.91	(M+H)+	0.44
466.0835	1	19235.23	(M+H)+	0.96
485.0643	1	17581.22	(M+Na)+	0.74
487.0624	1	17974.75	(M+Na)+	0.93
947.1382	1	6660.32	(2M+Na)+	2.07
949.1374	1	15211.95	(2M+Na)+	1.22
950.1403	1	6763.01	(2M+Na)+	1.2
951.1362	1	8327.4	(2M+Na)+	1.73

--- End Of Report ---

Target Compound Screening Report

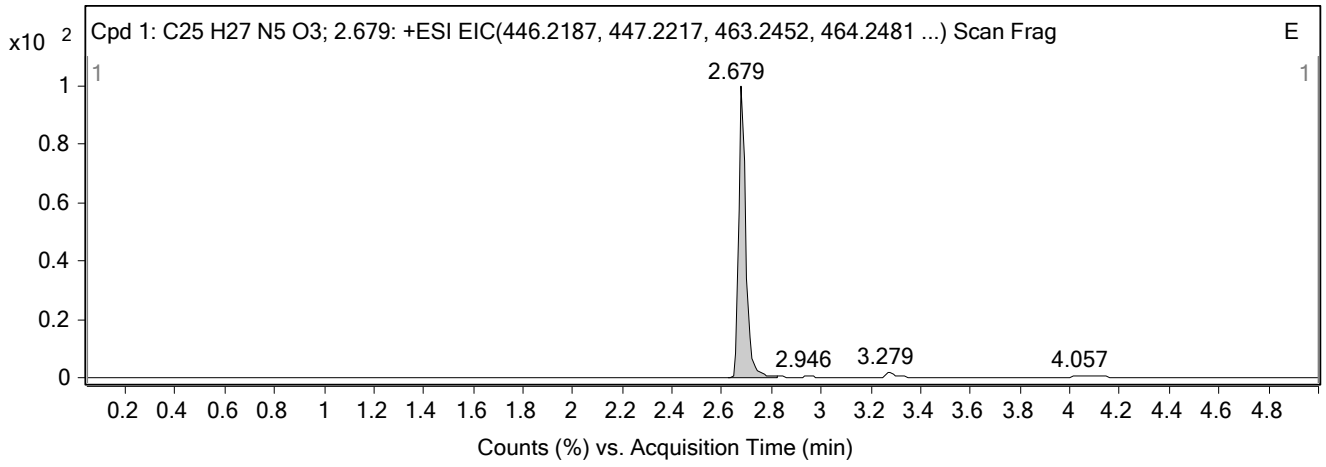
Data File	31.d	**Sample Name**	H2993319
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:03:14 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H27N5O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:03:14 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H27 N5 O3; 2.679	98.39	-0.74	C25 H27 N5 O3	2.679	445.2114	445.2111

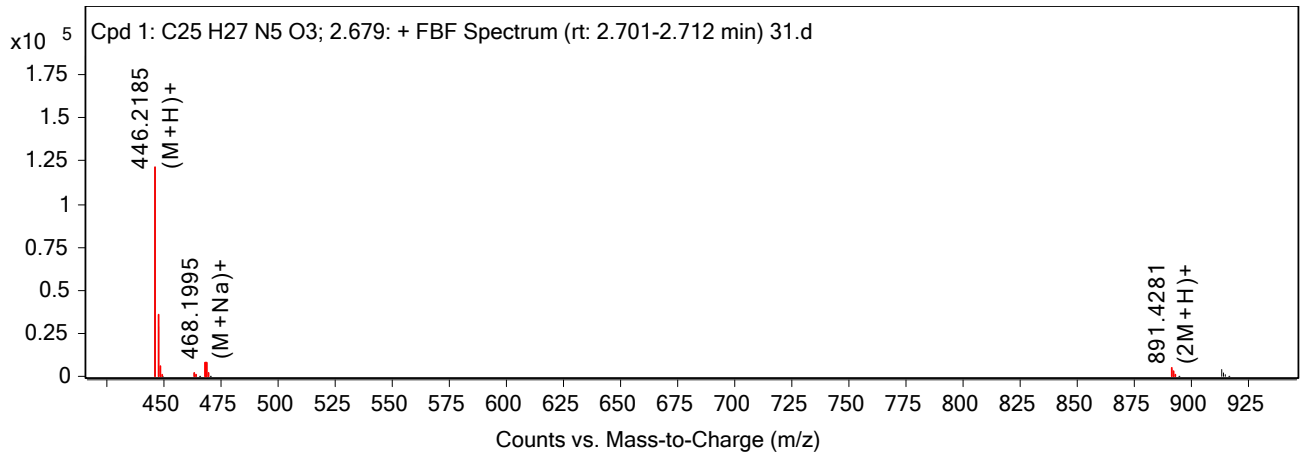
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
468.1995	2.679	445.2111	C25 H27 N5 O3	445.2114	-0.74	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

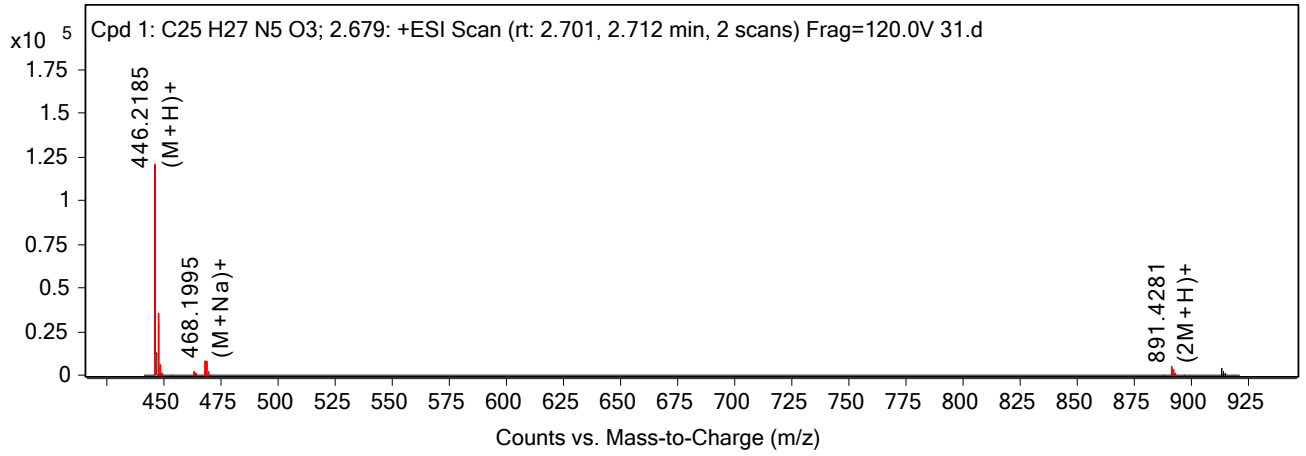
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
446.2185	1	121327.05	(M+H)+
447.2215	1	29422.94	(M+H)+
448.2238	1	4552.7	(M+H)+
463.2454	1	1940.01	(M+NH4)+
468.1995	1	7803.28	(M+Na)+
469.2023	1	2275.27	(M+Na)+
891.4281	1	4480.26	(2M+H)+
892.4305	1	2783.43	(2M+H)+
913.4101	1	3938.07	(2M+Na)+
914.4136	1	2408.93	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
446.2185	1	121327.05	(M+H)+	0.36
447.2215	1	29422.94	(M+H)+	0.4
448.2238	1	4552.7	(M+H)+	1.4
463.2454	1	1940.01	(M+NH4)+	-0.32
468.1995	1	7803.28	(M+Na)+	2.36
469.2023	1	2275.27	(M+Na)+	2.8
891.4281	1	4480.26	(2M+H)+	2.16
892.4305	1	2783.43	(2M+H)+	2.9
913.4101	1	3938.07	(2M+Na)+	2.13
914.4136	1	2408.93	(2M+Na)+	1.55

--- End Of Report ---

Target Compound Screening Report

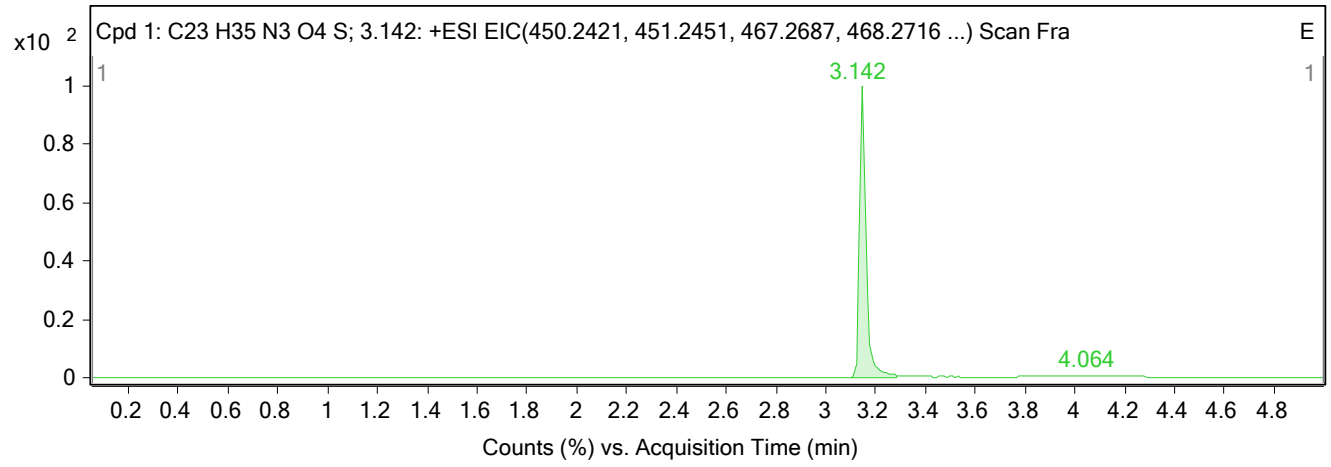
Data File	33.d	**Sample Name**	H2371467
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 9:51:13 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H35N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 9:51:13 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

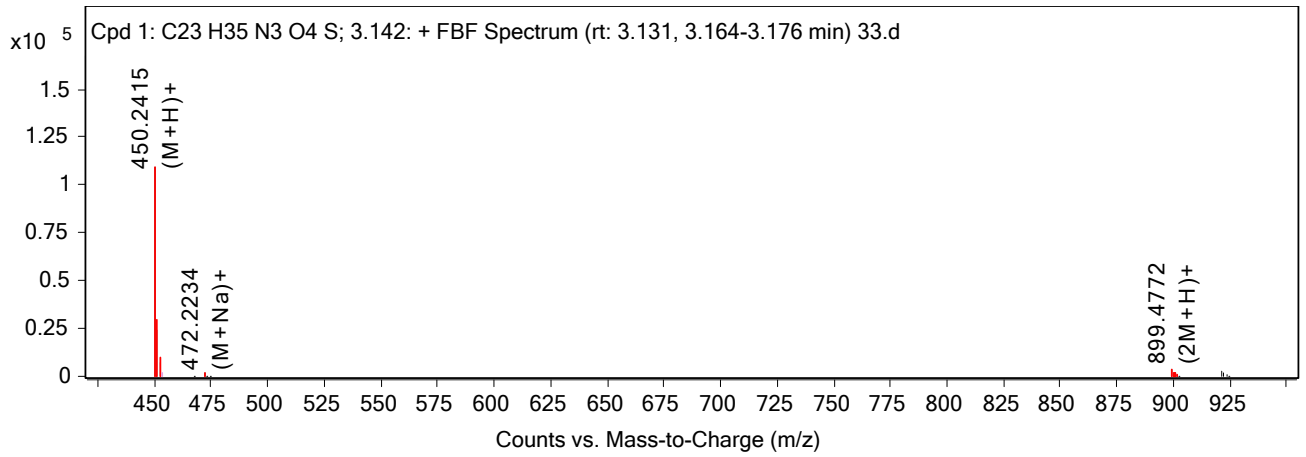
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H35 N3 O4 S; 3.142	94.7	-1.45	C23 H35 N3 O4 S	3.142	449.2348	449.2342

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
921.4577	3.142	449.2342	C23 H35 N3 O4 S	449.2348	-1.45	Find By Formula	

Compound Chromatograms



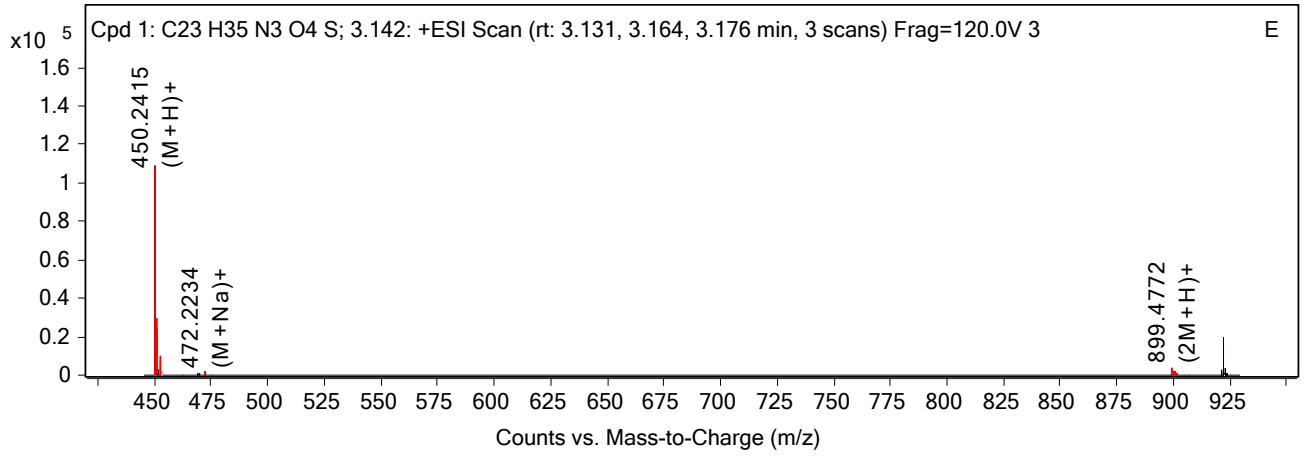
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
450.2415	1	109077.75	(M+H)+
451.2447	1	23920.62	(M+H)+
452.2422	1	6867.6	(M+H)+
472.2234	1	1495.51	(M+Na)+
899.4772	1	3723.46	(2M+H)+
900.4768	1	2180.31	(2M+H)+
901.4786	1	833.61	(2M+H)+
921.4577	1	2949.56	(2M+Na)+
922.4607	1	1879.11	(2M+Na)+
923.4594	1	907.71	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
450.2415	1	109077.75	(M+H)+	1.42
451.2447	1	23920.62	(M+H)+	0.87
452.2422	1	6867.6	(M+H)+	1.49
472.2234	1	1495.51	(M+Na)+	1.47
899.4772	1	3723.46	(2M+H)+	-0.32
900.4768	1	2180.31	(2M+H)+	3.55
901.4786	1	833.61	(2M+H)+	0.74
921.4577	1	2949.56	(2M+Na)+	1.33
922.4607	1	1879.11	(2M+Na)+	1.32
923.4594	1	907.71	(2M+Na)+	1.89

--- End Of Report ---

Target Compound Screening Report

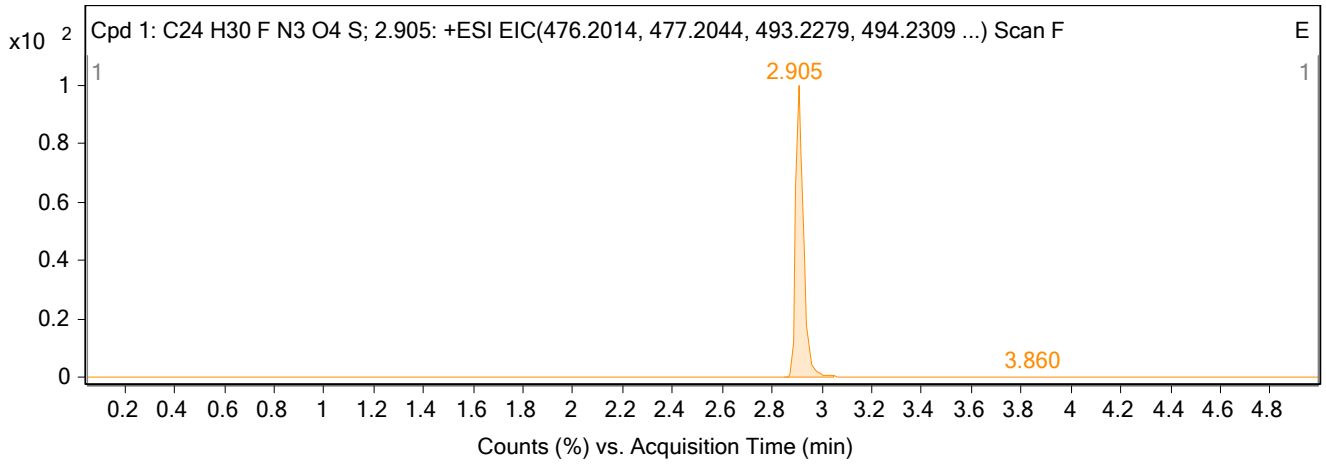
Data File	20.d	**Sample Name**	H2047760
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:02:07 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H30FN3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:02:07 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

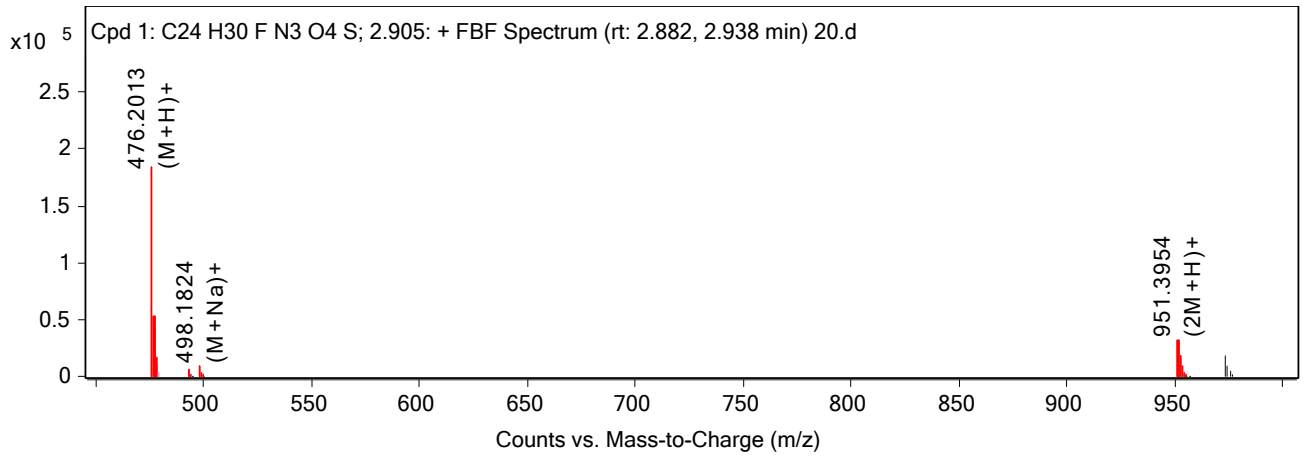
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H30 F N3 O4 S; 2.905	98.96	-0.51	C24 H30 F N3 O4 S	2.905	475.1941	475.1939

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
951.3954	2.905	475.1939	C24 H30 F N3 O4 S	475.1941	-0.51	Find By Formula	

Compound Chromatograms



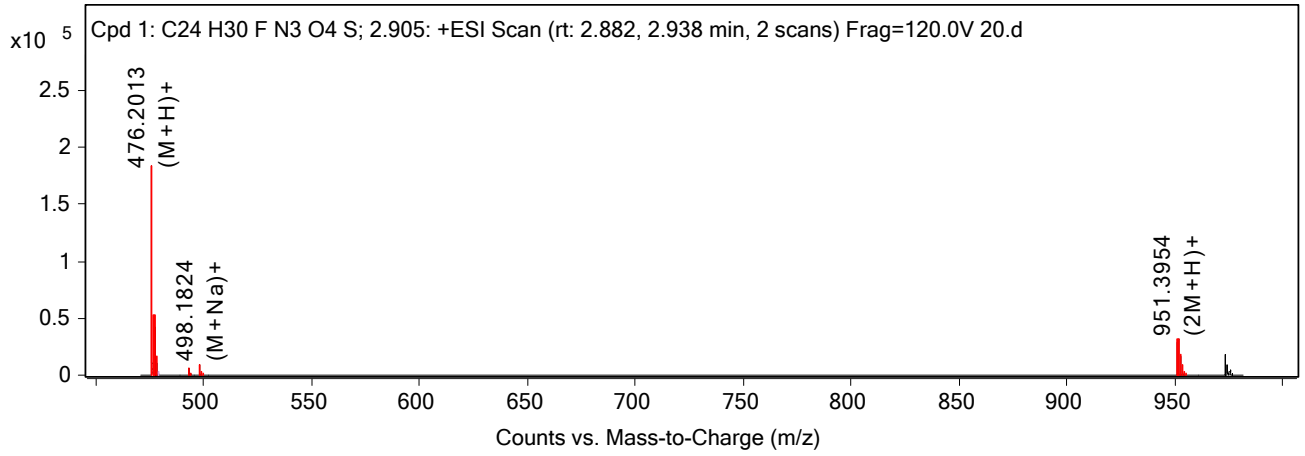
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
476.2013	1	183757.03	(M+H)+
477.2044	1	42242.05	(M+H)+
478.2023	1	11093.78	(M+H)+
493.2275	1	6156.96	(M+NH4)+
498.1824	1	8637.63	(M+Na)+
951.3954	1	31510.93	(2M+H)+
952.3983	1	16768.66	(2M+H)+
953.3961	1	7423.25	(2M+H)+
973.377	1	18011.31	(2M+Na)+
974.3802	1	9275.56	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
476.2013	1	183757.03	(M+H)+	0.24
477.2044	1	42242.05	(M+H)+	0.11
478.2023	1	11093.78	(M+H)+	-0.06
493.2275	1	6156.96	(M+NH4)+	0.8
498.1824	1	8637.63	(M+Na)+	1.78
951.3954	1	31510.93	(2M+H)+	0.06
952.3983	1	16768.66	(2M+H)+	0.19
953.3961	1	7423.25	(2M+H)+	1.9
973.377	1	18011.31	(2M+Na)+	0.49
974.3802	1	9275.56	(2M+Na)+	0.29

--- End Of Report ---

Target Compound Screening Report

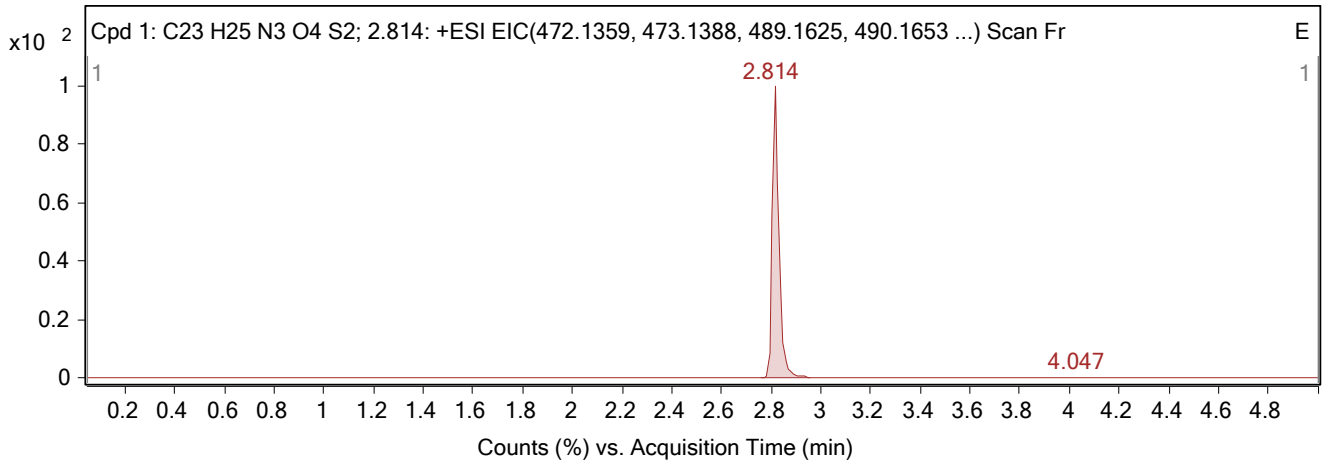
Data File	50.d	**Sample Name**	H2046077
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:48:41 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H25N3O4S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:48:41 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H25 N3 O4 S2; 2.814	94.48	-0.69	C23 H25 N3 O4 S2	2.814	471.1286	471.1283

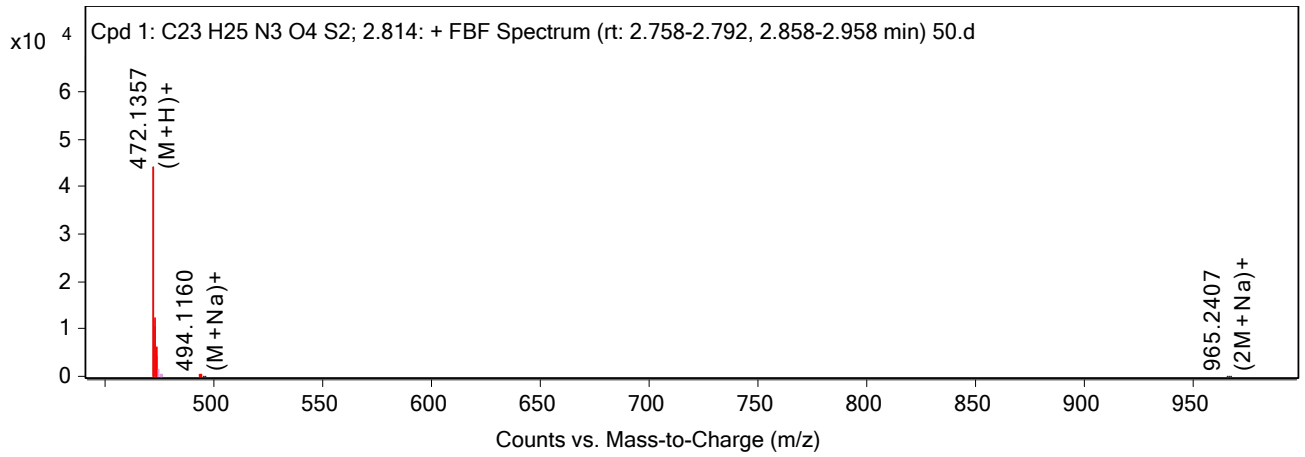
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
472.1357	2.814	471.1283	C23 H25 N3 O4 S2	471.1286	-0.69	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

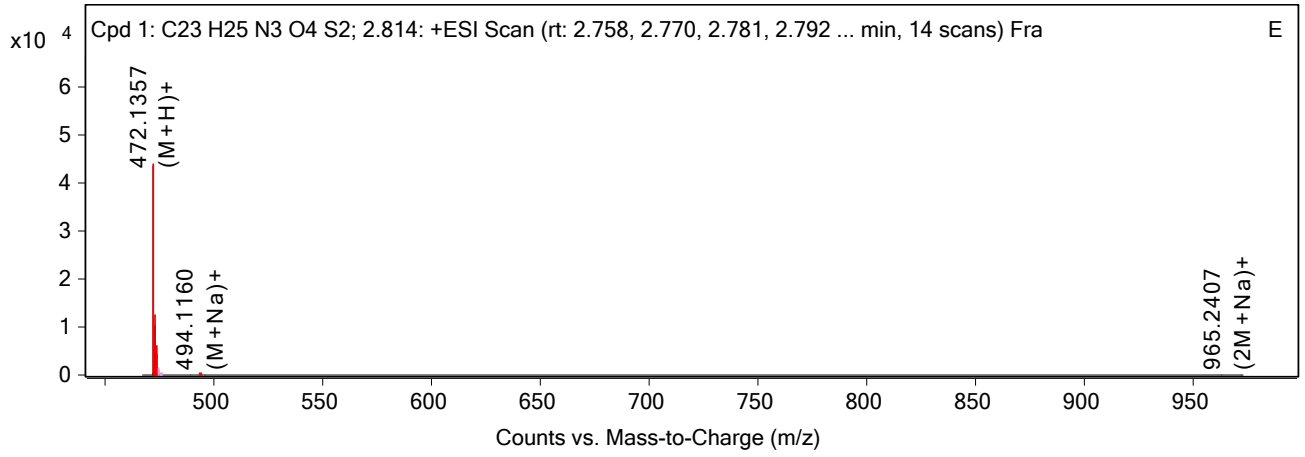
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
472.1357	1	44067.86	(M+H)+
473.1382	1	10352.43	(M+H)+
474.1348	1	4278.93	(M+H)+
494.116	1	262.46	(M+Na)+
495.1256	1	73.94	(M+Na)+
496.1186	1	36.66	(M+Na)+
965.2407	1	88.1	(2M+Na)+
966.2558	1	50.06	(2M+Na)+
967.2301	1	34.63	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
472.1357	1	44067.86	(M+H)+	0.51
473.1382	1	10352.43	(M+H)+	1.38
474.1348	1	4278.93	(M+H)+	0.57
494.116	1	262.46	(M+Na)+	3.83
495.1256	1	73.94	(M+Na)+	-9.7
496.1186	1	36.66	(M+Na)+	-3.35
965.2407	1	88.1	(2M+Na)+	5.99
966.2558	1	50.06	(2M+Na)+	-6.55
967.2301	1	34.63	(2M+Na)+	17.58

--- End Of Report ---

Target Compound Screening Report

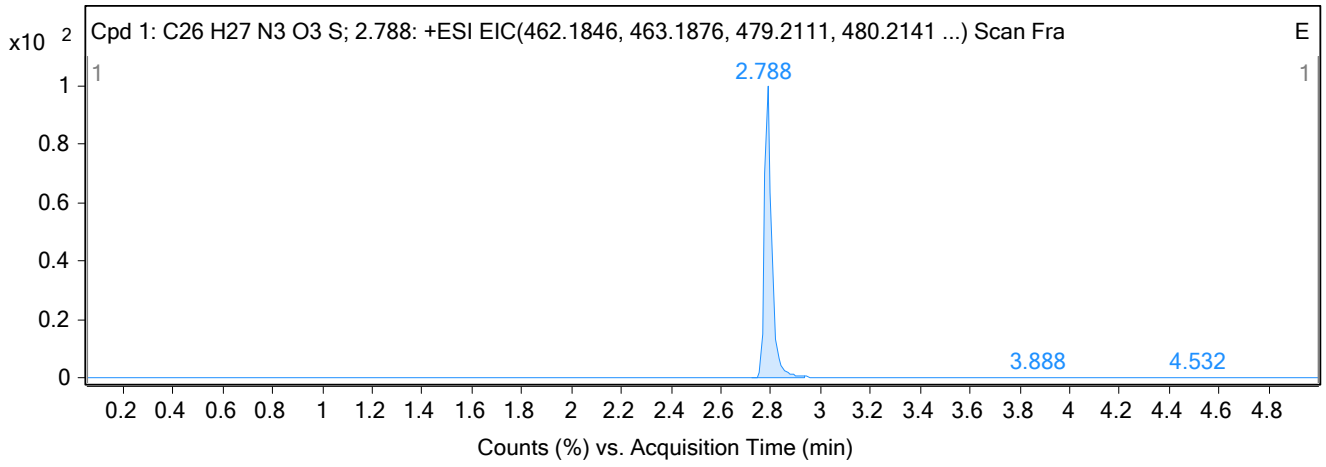
Data File	19.d	**Sample Name**	H2046366
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 12:56:34 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H27N3O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 12:56:34 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

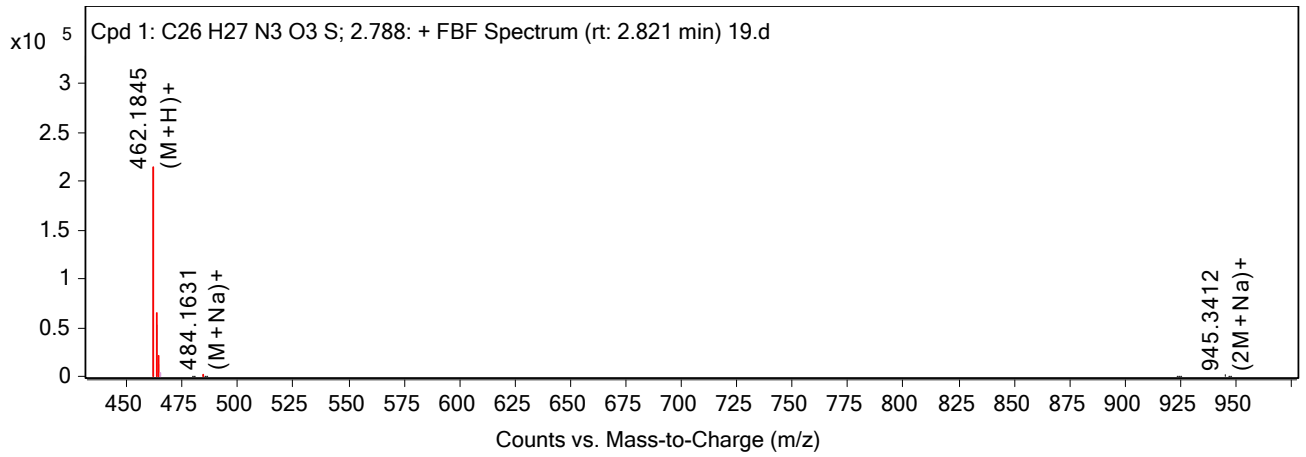
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H27 N3 O3 S; 2.788	94.16	-0.3	C26 H27 N3 O3 S	2.788	461.1773	461.1772

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
462.1845	2.788	461.1772	C26 H27 N3 O3 S	461.1773	-0.3	Find By Formula	

Compound Chromatograms



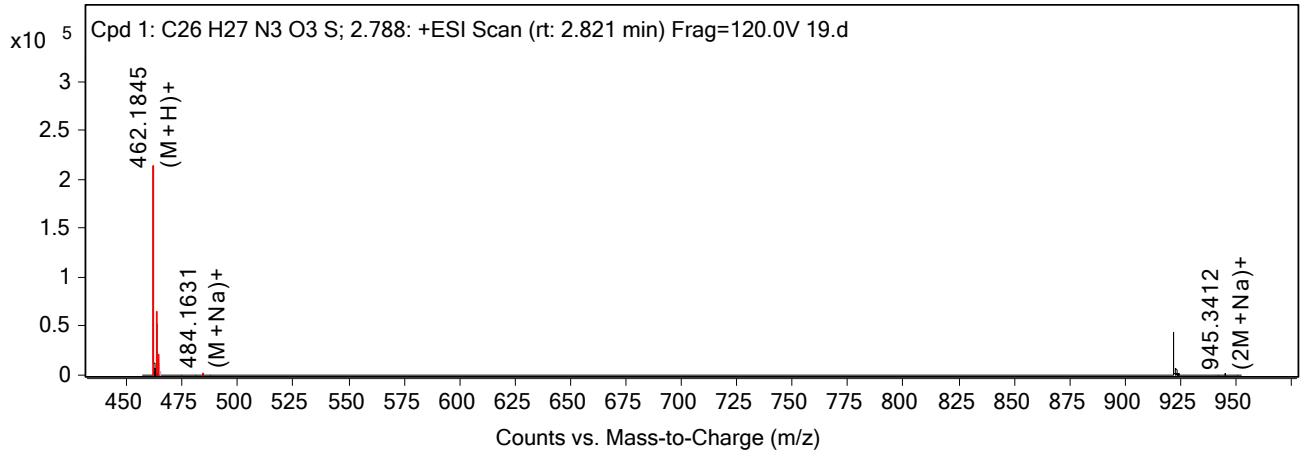
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
462.1845	1	213768.16	(M+H)+
463.1873	1	52947	(M+H)+
464.1869	1	13057.43	(M+H)+
484.1631	1	2486.48	(M+Na)+
485.1707	1	749.21	(M+Na)+
923.3571	1	773.71	(2M+H)+
924.364	1	346.76	(2M+H)+
945.3412	1	1074.07	(2M+Na)+
946.3448	1	862	(2M+Na)+
947.3494	1	354.9	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
462.1845	1	213768.16	(M+H)+	0.21
463.1873	1	52947	(M+H)+	0.74
464.1869	1	13057.43	(M+H)+	-2.42
484.1631	1	2486.48	(M+Na)+	7.03
485.1707	1	749.21	(M+Na)+	-2.2
923.3571	1	773.71	(2M+H)+	5.16
924.364	1	346.76	(2M+H)+	1.05
945.3412	1	1074.07	(2M+Na)+	2.76
946.3448	1	862	(2M+Na)+	2.17
947.3494	1	354.9	(2M+Na)+	-2.93

--- End Of Report ---

Target Compound Screening Report

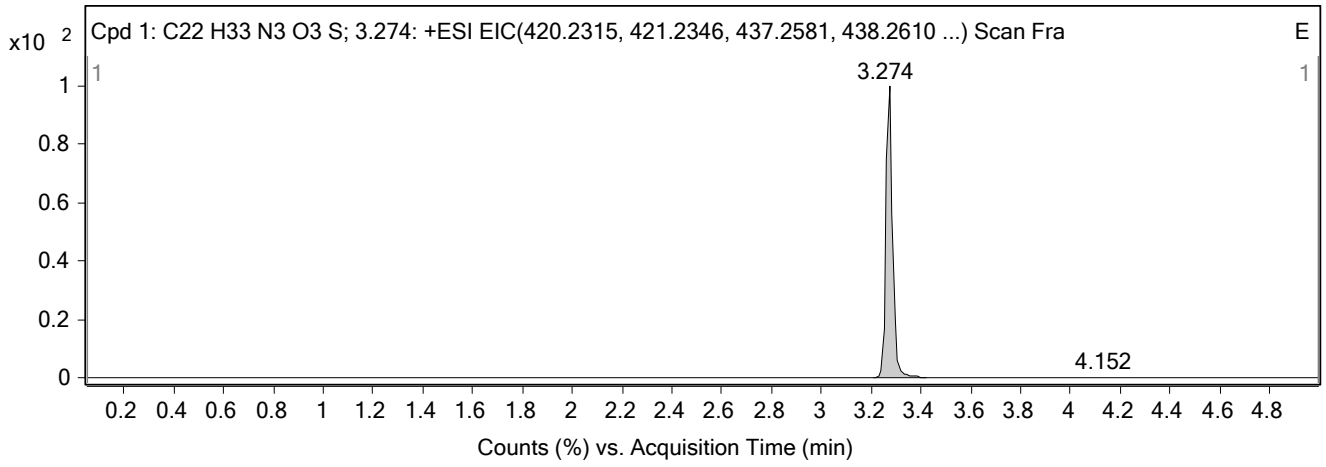
Data File	7d.d	**Sample Name**	H3460666
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:46:40 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O3S	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:46:40 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

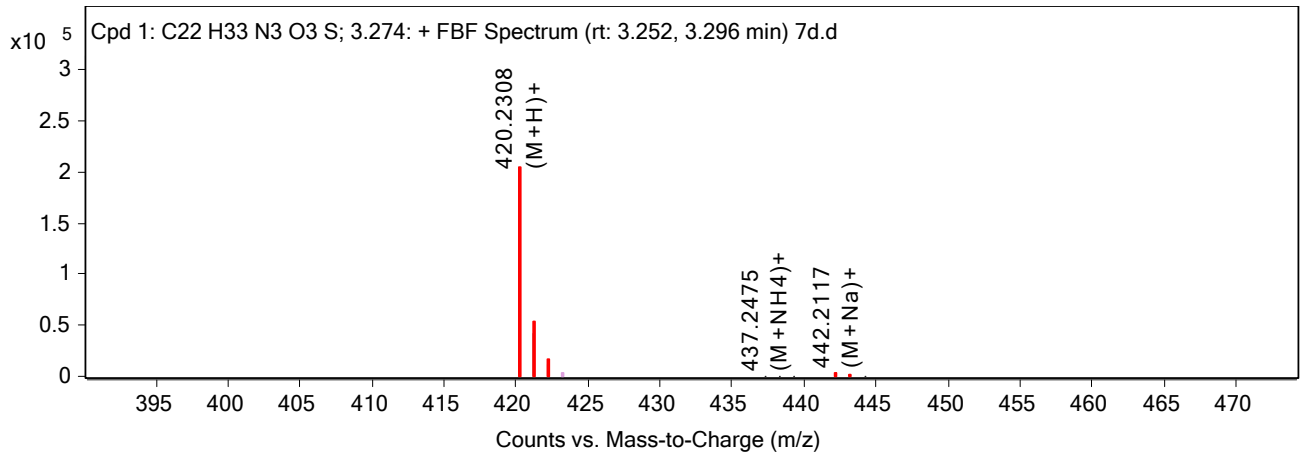
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O3 S; 3.274	92.49	-1.74	C22 H33 N3 O3 S	3.274	419.2243	419.2235

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
420.2308	3.274	419.2235	C22 H33 N3 O3 S	419.2243	-1.74	Find By Formula	

Compound Chromatograms



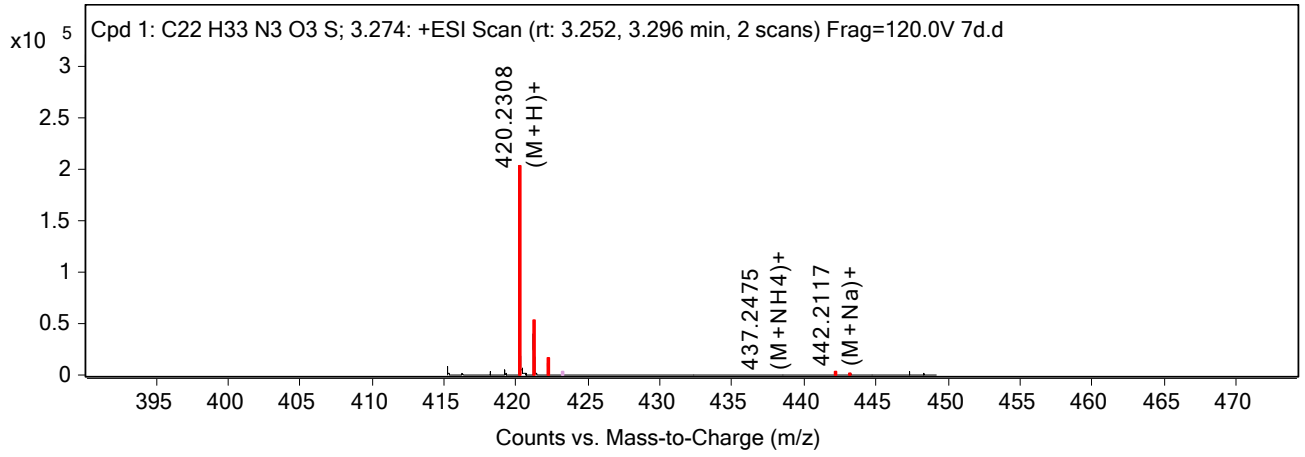
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
420.2308	1	204366.73	(M+H)+
421.2342	1	41619	(M+H)+
422.2315	1	11469.81	(M+H)+
437.2475	1	326.11	(M+NH4)+
438.2338	1	173.4	(M+NH4)+
439.2523	1	90.66	(M+NH4)+
442.2117	1	3758.43	(M+Na)+
443.2173	1	998.78	(M+Na)+
444.2163	1	321.71	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
420.2308	1	204366.73	(M+H)+	1.83
420.2308		204366.73		
421.2342	1	41619	(M+H)+	0.92
422.2315	1	11469.81	(M+H)+	1.13
437.2475	1	326.11	(M+NH4)+	24.13
438.2338	1	173.4	(M+NH4)+	62.07
439.2523	1	90.66	(M+NH4)+	14.23
442.2117	1	3758.43	(M+Na)+	4.09
443.2173	1	998.78	(M+Na)+	-1.83
444.2163	1	321.71	(M+Na)+	-5.35

--- End Of Report ---

Target Compound Screening Report

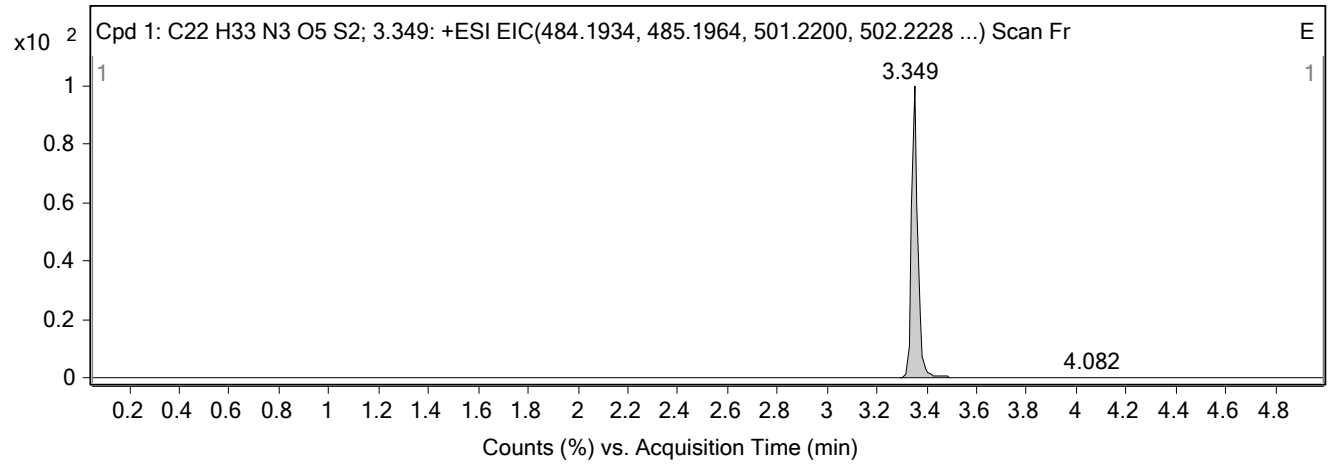
Data File	2d.d	**Sample Name**	H3475358
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:19:06 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:19:06 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

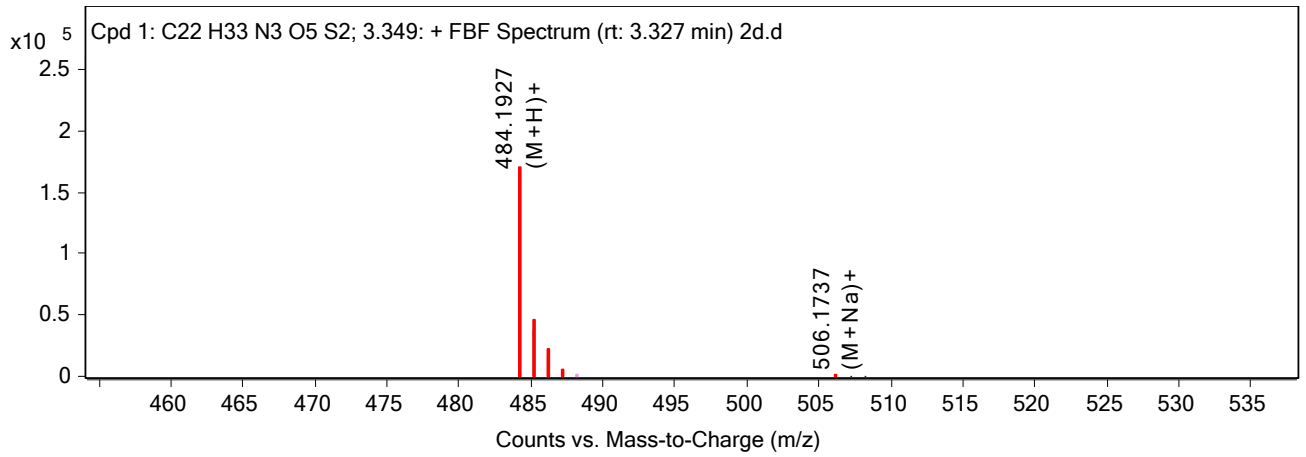
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O5 S2; 3.349	94.01	-1.64	C22 H33 N3 O5 S2	3.349	483.1862	483.1854

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
484.1927	3.349	483.1854	C22 H33 N3 O5 S2	483.1862	-1.64	Find By Formula	

Compound Chromatograms



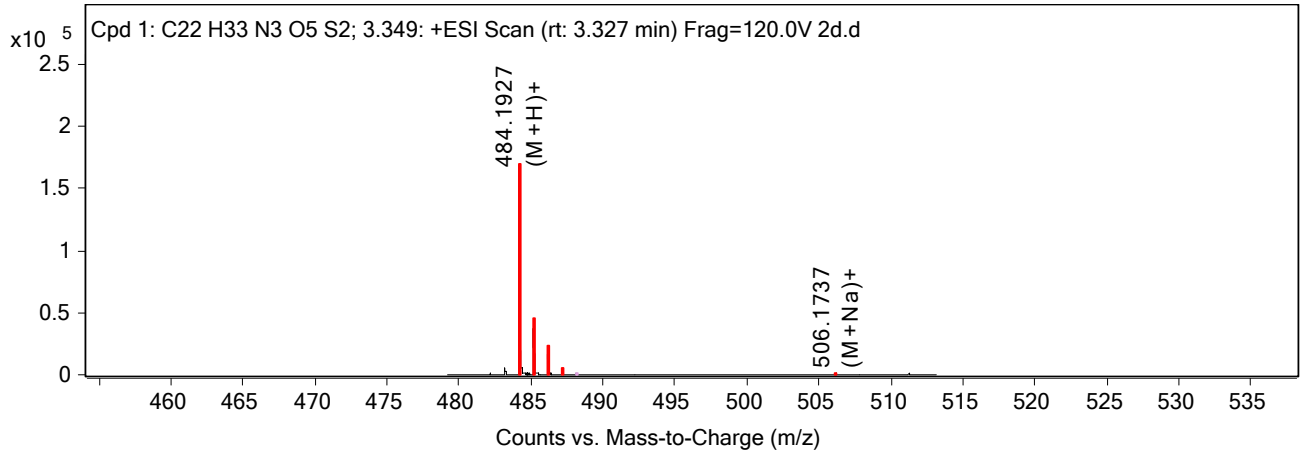
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
484.1927	1	170076.86	(M+H)+
485.1954	1	37749.28	(M+H)+
486.1918	1	16337.28	(M+H)+
487.1946	1	3302.68	(M+H)+
506.1737	1	1570.67	(M+Na)+
507.1764	1	565.41	(M+Na)+
508.1751	1	269.02	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
484.1927	1	170076.85	(M+H)+	1.61
485.1954	1	37749.28	(M+H)+	1.97
486.1918	1	16337.28	(M+H)+	1.52
487.1946	1	3302.68	(M+H)+	-1.18
506.1737	1	1570.67	(M+Na)+	3.34
507.1764	1	565.41	(M+Na)+	3.7
508.1751	1	269.02	(M+Na)+	-1.35

--- End Of Report ---

Target Compound Screening Report

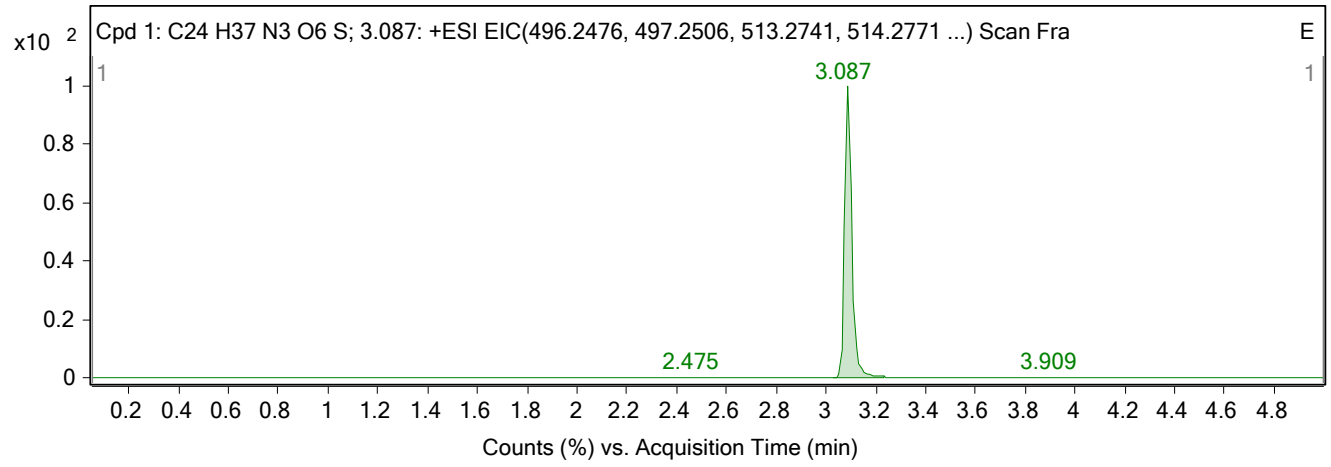
Data File	37.d	**Sample Name**	H2973905
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 10:13:22 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H37N3O6S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 10:13:22 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

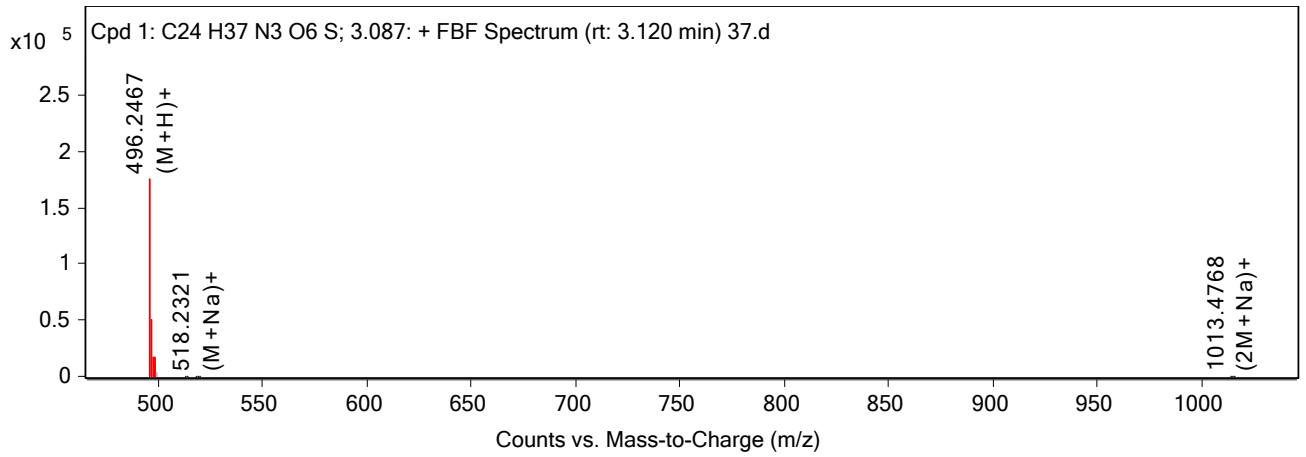
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H37 N3 O6 S; 3.087	93.8	-1.69	C24 H37 N3 O6 S	3.087	495.2403	495.2395

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
496.2467	3.087	495.2395	C24 H37 N3 O6 S	495.2403	-1.69	Find By Formula	

Compound Chromatograms



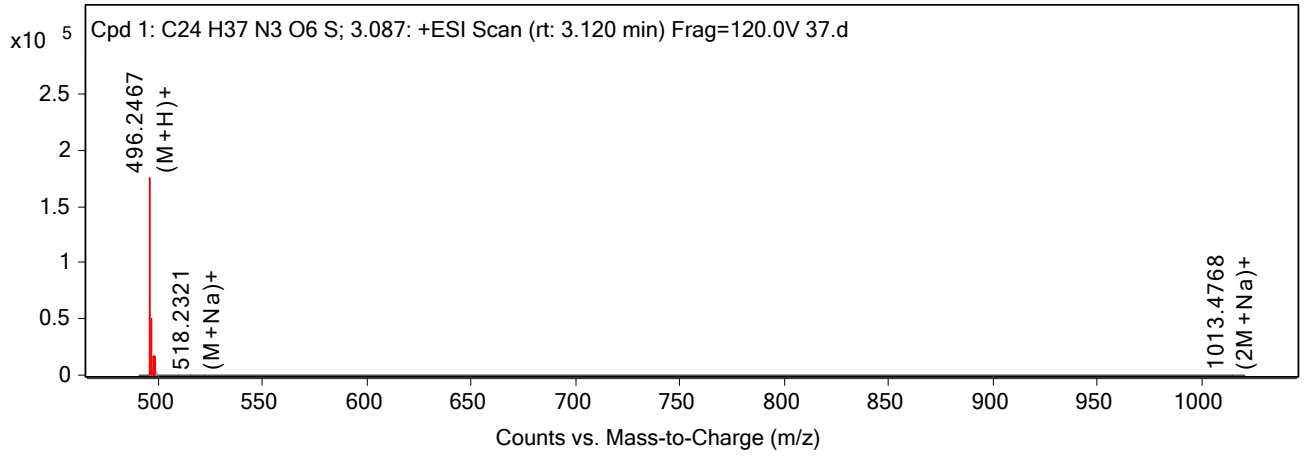
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
496.2467	1	175581.97	(M+H)+
497.2499	1	40440.36	(M+H)+
498.2476	1	11332.53	(M+H)+
513.2682	1	71.01	(M+NH4)+
518.2321	1	219	(M+Na)+
519.2321	1	105.88	(M+Na)+
520.2288	1	106.21	(M+Na)+
1013.4768	1	149.45	(2M+Na)+
1014.4632	1	101.8	(2M+Na)+
1015.4687	1	72.32	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
496.2467	1	175581.97	(M+H)+	1.7
497.2499	1	40440.36	(M+H)+	1.49
498.2476	1	11332.53	(M+H)+	2.04
513.2682	1	71.01	(M+NH4)+	11.65
518.2321	1	219	(M+Na)+	-4.93
519.2321	1	105.88	(M+Na)+	0.92
520.2288	1	106.21	(M+Na)+	3.5
1013.4768	1	149.45	(2M+Na)+	-6.89
1014.4632	1	101.8	(2M+Na)+	9.55
1015.4687	1	72.32	(2M+Na)+	3.63

--- End Of Report ---

Target Compound Screening Report

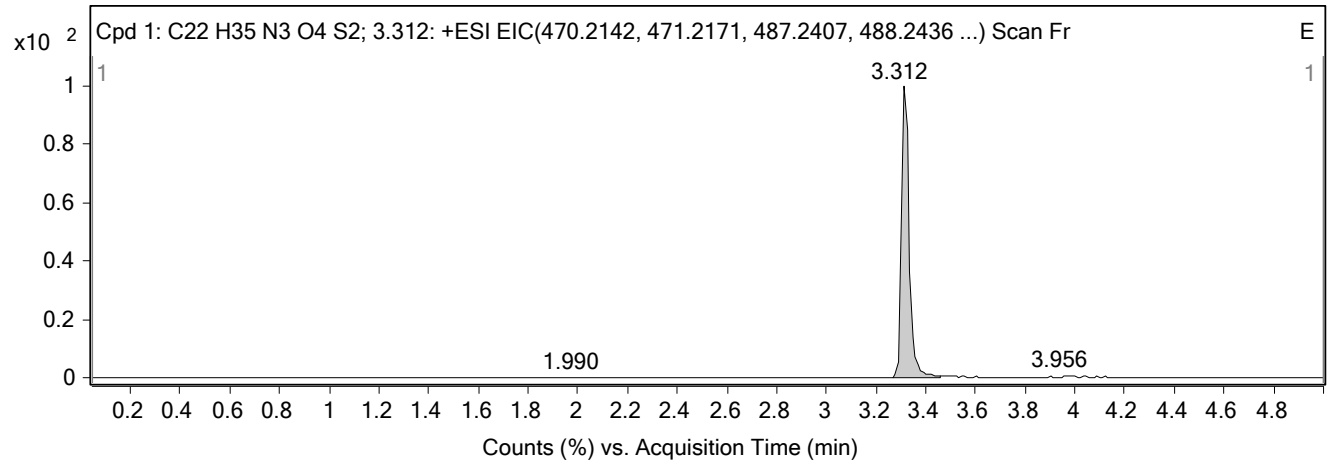
Data File	26.d	**Sample Name**	H2980920
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 12:56:03 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H35N3O4S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 12:56:03 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

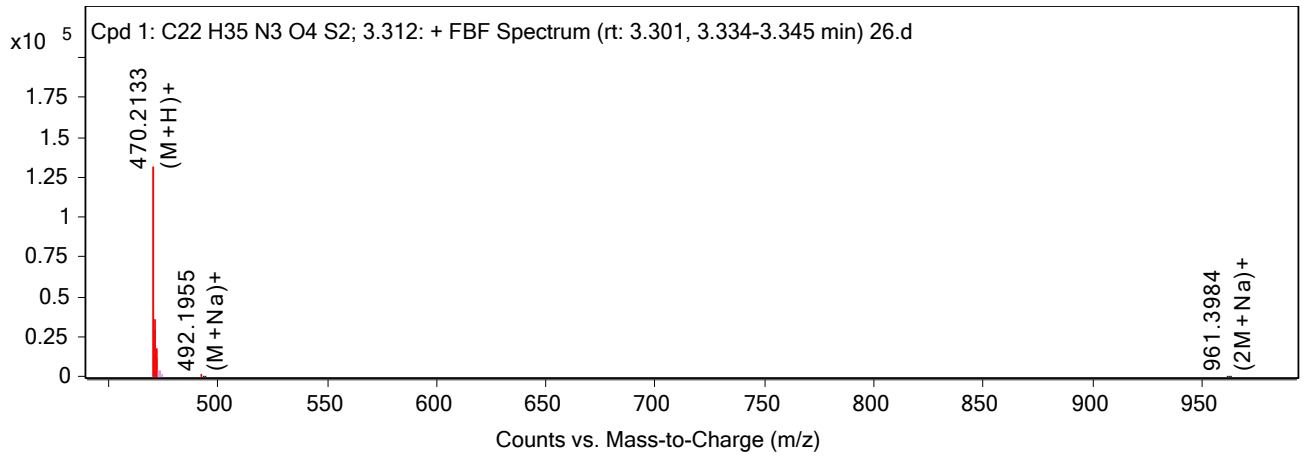
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H35 N3 O4 S2; 3.312	93.34	-1.8	C22 H35 N3 O4 S2	3.312	469.2069	469.2061

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
470.2133	3.312	469.2061	C22 H35 N3 O4 S2	469.2069	-1.8	Find By Formula	

Compound Chromatograms



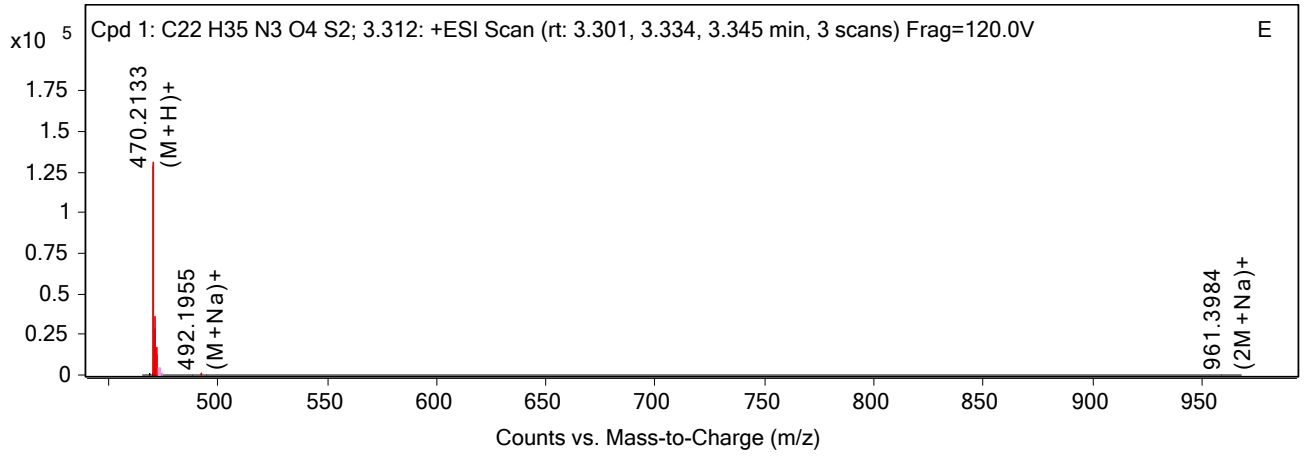
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
470.2133	1	131060.13	(M+H)+
471.2163	1	28710.51	(M+H)+
472.2124	1	12437.16	(M+H)+
492.1955	1	673.54	(M+Na)+
493.1949	1	198.54	(M+Na)+
494.1928	1	132.02	(M+Na)+
961.3984	1	374.8	(2M+Na)+
962.4011	1	283.33	(2M+Na)+
963.3979	1	148.47	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
470.2133	1	131060.13	(M+H)+	1.79
470.2133		131060.13		
471.2163	1	28710.51	(M+H)+	1.62
472.2124	1	12437.16	(M+H)+	1.61
492.1955	1	673.54	(M+Na)+	1.35
493.1949	1	198.54	(M+Na)+	8.33
494.1928	1	132.02	(M+Na)+	4.54
961.3984	1	374.8	(2M+Na)+	4.78
962.4011	1	283.33	(2M+Na)+	5.02
963.3979	1	148.47	(2M+Na)+	5.81

--- End Of Report ---

Target Compound Screening Report

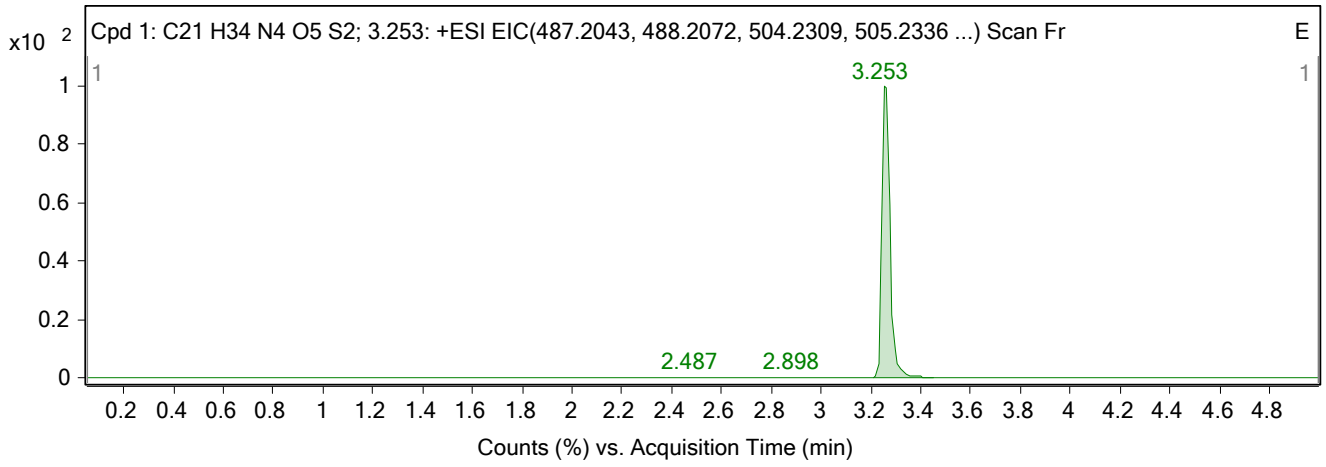
Data File	24.d	**Sample Name**	H2979293
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:24:21 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H34N4O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:24:21 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H34 N4 O5 S2; 3.253	96.55	-0.86	C21 H34 N4 O5 S2	3.253	486.1971	486.1966

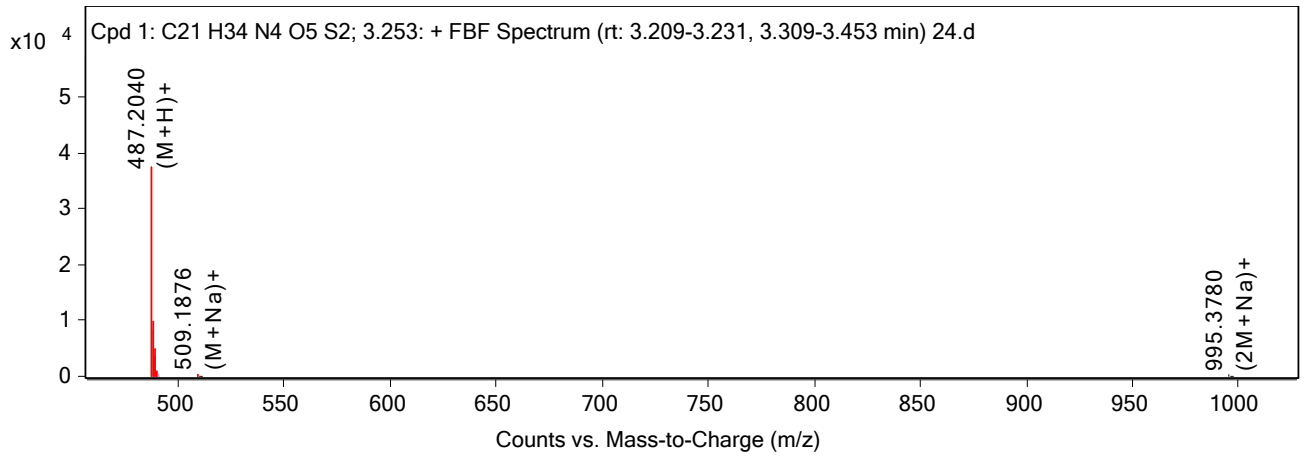
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
487.204	3.253	486.1966	C21 H34 N4 O5 S2	486.1971	-0.86	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

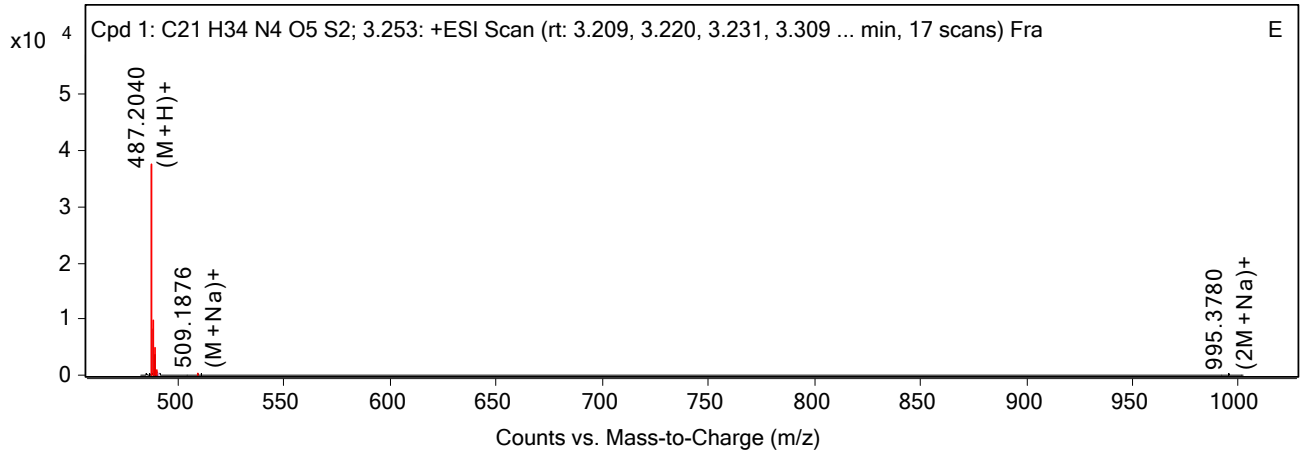
Agilent Technologies



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
487.204	1	37433.84	(M+H)+
488.2067	1	8314.08	(M+H)+
489.2027	1	3823.58	(M+H)+
490.2051	1	779.89	(M+H)+
509.1876	1	384.59	(M+Na)+
510.1874	1	118.66	(M+Na)+
511.1823	1	74.27	(M+Na)+
995.378	1	199.17	(2M+Na)+
996.3823	1	110.39	(2M+Na)+
997.3771	1	81.27	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
487.204	1	37433.84	(M+H)+	0.77
488.2067	1	8314.08	(M+H)+	0.89
489.2027	1	3823.58	(M+H)+	1.16
490.2051	1	779.89	(M+H)+	-0.73
509.1876	1	384.59	(M+Na)+	-2.55
510.1874	1	118.66	(M+Na)+	3.41
511.1823	1	74.27	(M+Na)+	5.75
995.378	1	199.17	(2M+Na)+	5.35
996.3823	1	110.39	(2M+Na)+	3.92
997.3771	1	81.27	(2M+Na)+	6.54

--- End Of Report ---

Target Compound Screening Report

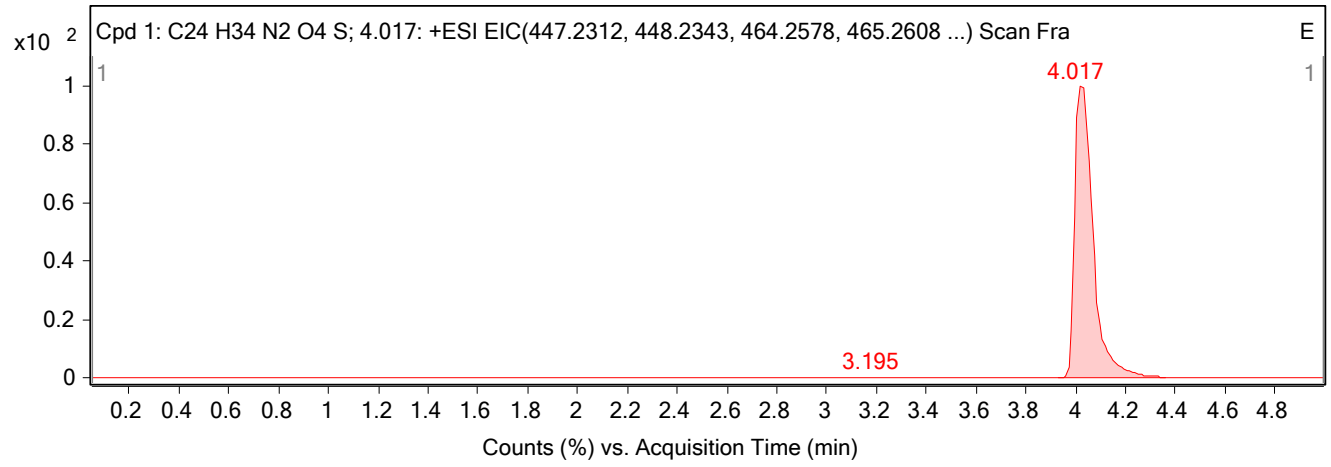
Data File	34.d	**Sample Name**	H2974027
Sample Type	Sample	**Position**	P1-D7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:51:17 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H34N2O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:51:17 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

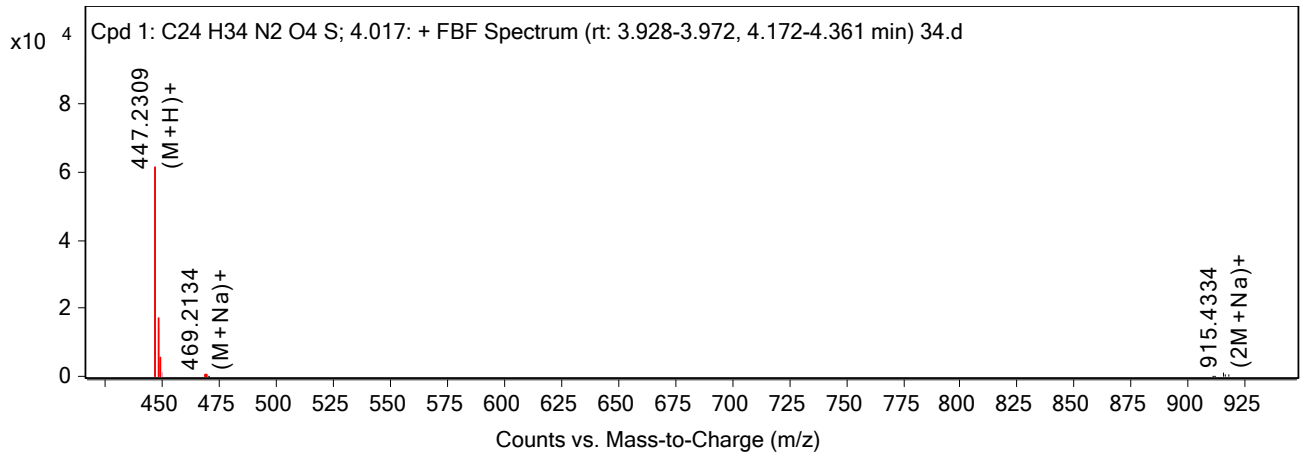
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H34 N2 O4 S; 4.017	95.8	-0.98	C24 H34 N2 O4 S	4.017	446.2239	446.2235

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2309	4.017	446.2235	C24 H34 N2 O4 S	446.2239	-0.98	Find By Formula	

Compound Chromatograms



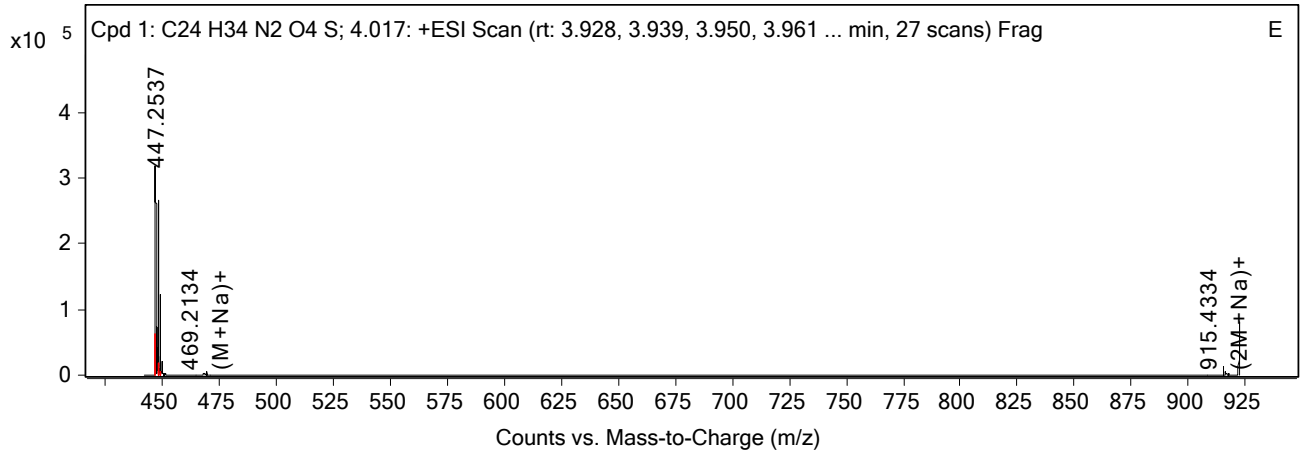
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2309	1	61369.73	(M+H)+
448.2339	1	14351.24	(M+H)+
449.2321	1	4019.23	(M+H)+
469.2134	1	581.71	(M+Na)+
470.2176	1	206.88	(M+Na)+
910.4791	1	126.47	(2M+NH4)+
911.4812	1	93.63	(2M+NH4)+
915.4334	1	1136.11	(2M+Na)+
916.4329	1	574.46	(2M+Na)+
917.4309	1	334.96	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2309	1	61369.72	(M+H)+	0.67
448.2339	1	14351.24	(M+H)+	1
449.2321	1	4019.23	(M+H)+	-0.07
469.2134	1	581.71	(M+Na)+	-0.49
470.2176	1	206.88	(M+Na)+	-2.87
910.4791	1	126.47	(2M+NH4)+	2.83
911.4812	1	93.63	(2M+NH4)+	3.94
915.4334	1	1136.11	(2M+Na)+	4.05
916.4329	1	574.46	(2M+Na)+	7.93
917.4309	1	334.96	(2M+Na)+	9.53

--- End Of Report ---

Target Compound Screening Report

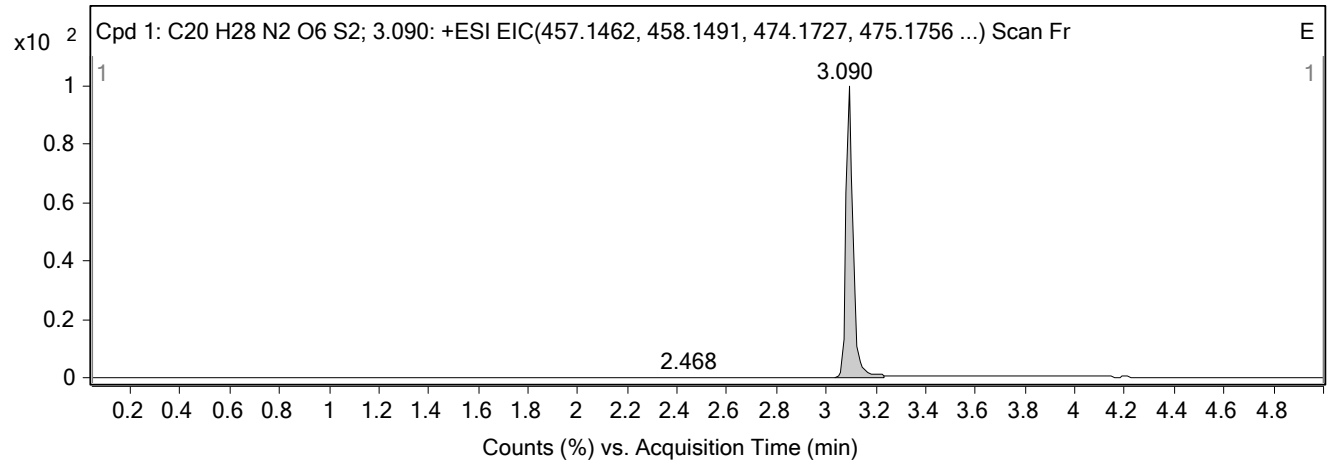
Data File	3.d	**Sample Name**	H3475368
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 4:53:01 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 4:53:01 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

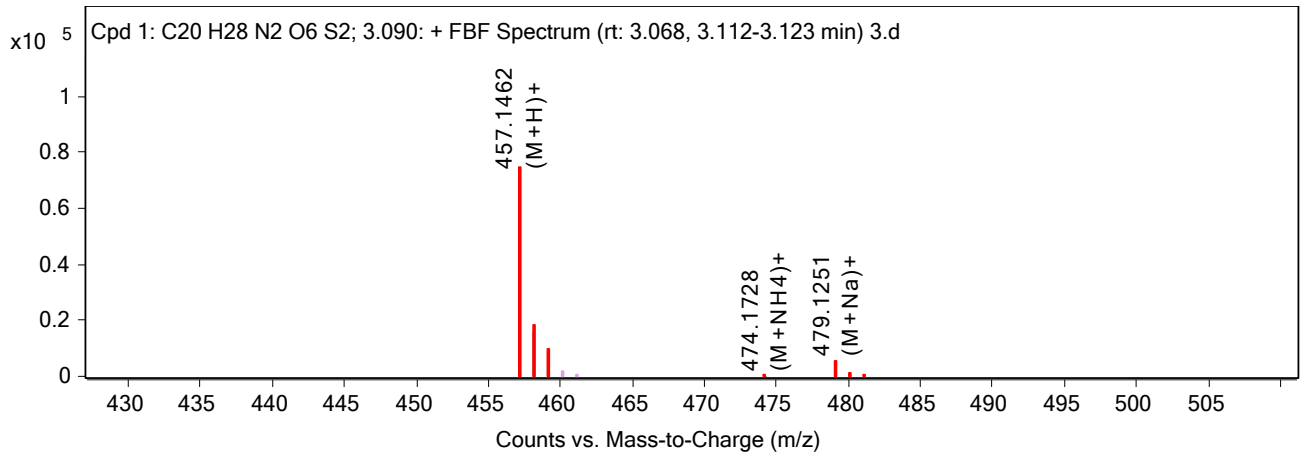
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O6 S2; 3.090	95.38	0.1	C20 H28 N2 O6 S2	3.09	456.1389	456.1389

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
457.1462	3.09	456.1389	C20 H28 N2 O6 S2	456.1389	0.1	Find By Formula	

Compound Chromatograms



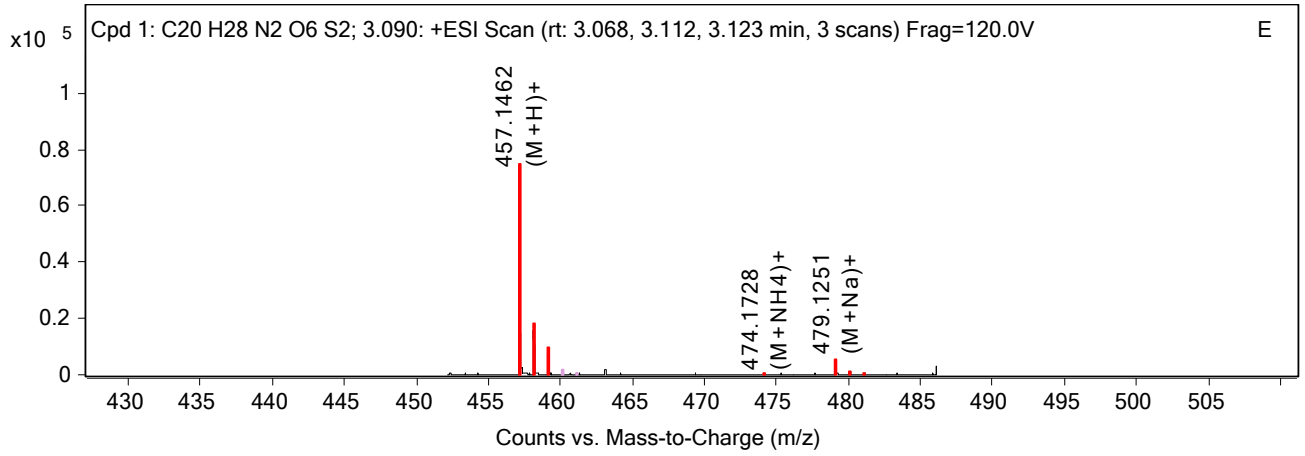
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
457.1462	1	74601.09	(M+H)+
458.1501	1	16153.98	(M+H)+
459.1456	1	7511.37	(M+H)+
474.1728	1	308.01	(M+NH4)+
479.1251	1	5550.54	(M+Na)+
480.1286	1	1382.03	(M+Na)+
481.1261	1	692.15	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
457.1462	1	74601.09	(M+H)+	-0.12
457.1462		74601.09		
458.1501	1	16153.98	(M+H)+	-2.22
459.1456	1	7511.37	(M+H)+	-1.3
474.1728	1	308.01	(M+NH4)+	-0.2
479.1251	1	5550.54	(M+Na)+	6.19
480.1286	1	1382.03	(M+Na)+	5.07
481.1261	1	692.15	(M+Na)+	1.61

--- End Of Report ---

Target Compound Screening Report

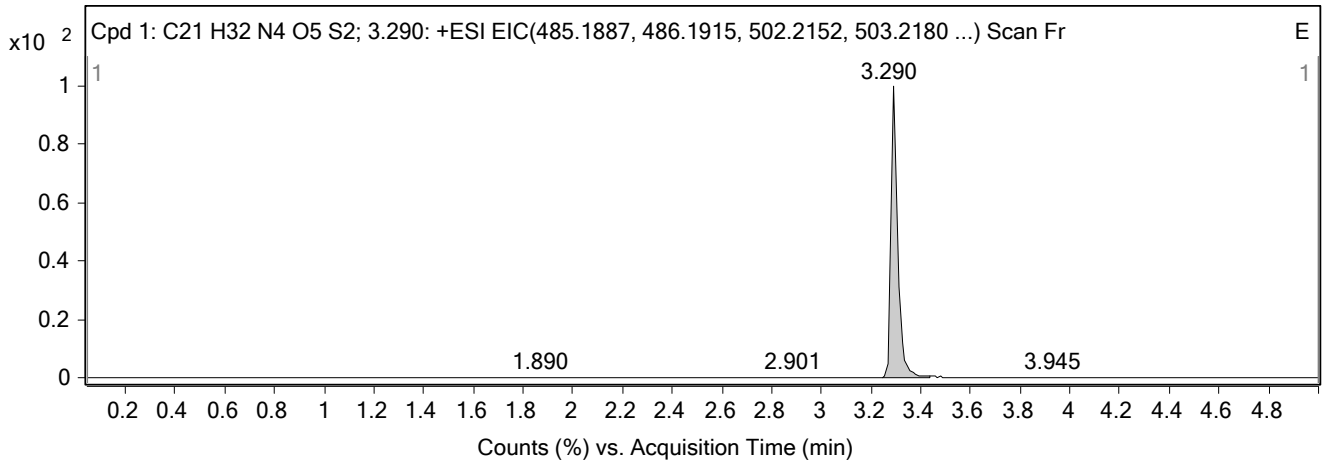
Data File	36.d	**Sample Name**	H2980849
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:34:44 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H32N4O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:34:44 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

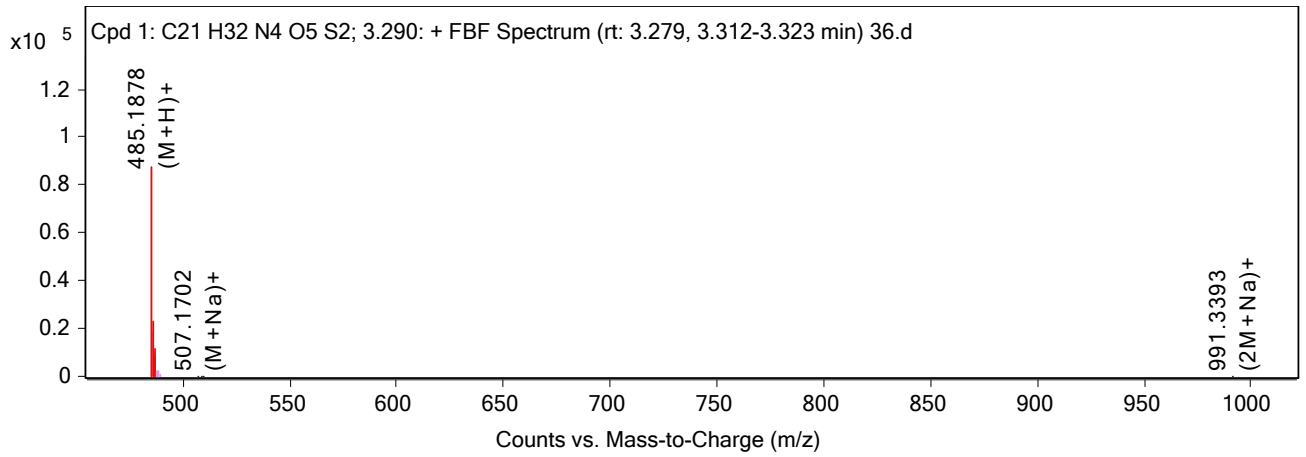
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H32 N4 O5 S2; 3.290	93.13	-2.01	C21 H32 N4 O5 S2	3.29	484.1814	484.1804

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
485.1878	3.29	484.1804	C21 H32 N4 O5 S2	484.1814	-2.01	Find By Formula	

Compound Chromatograms



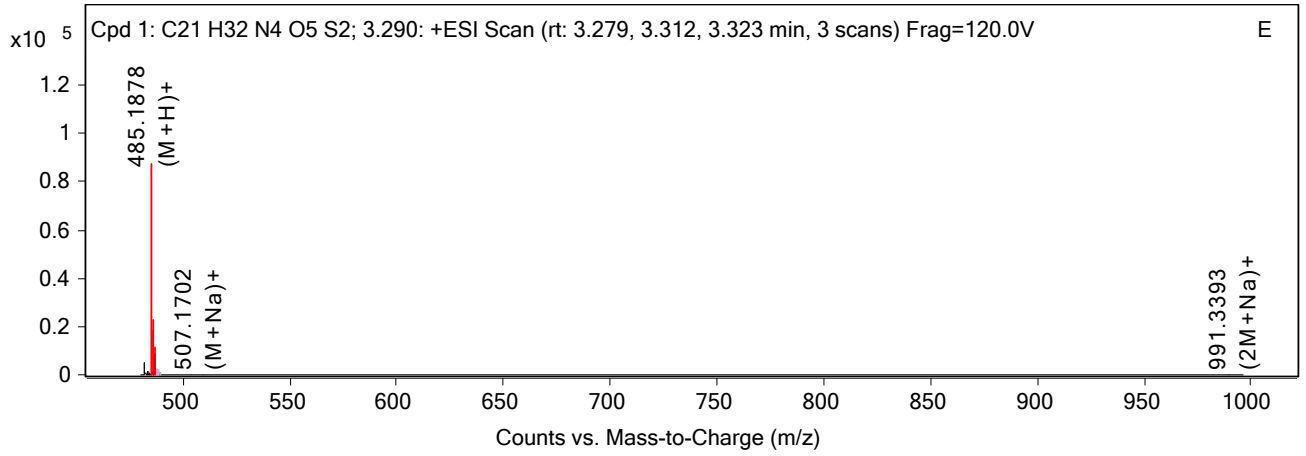
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
485.1878	1	87304.8	(M+H)+
486.1903	1	18475.08	(M+H)+
487.1868	1	8468.09	(M+H)+
507.1702	1	297.74	(M+Na)+
508.1712	1	120.28	(M+Na)+
509.1778	1	76.17	(M+Na)+
991.3393	1	76.63	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
485.1878	1	87304.81	(M+H)+	1.93
486.1903	1	18475.08	(M+H)+	2.49
487.1868	1	8468.09	(M+H)+	1.61
507.1702	1	297.74	(M+Na)+	0.84
508.1712	1	120.28	(M+Na)+	4.42
509.1778	1	76.17	(M+Na)+	-16.21
991.3393	1	76.63	(2M+Na)+	12.86

--- End Of Report ---

Target Compound Screening Report

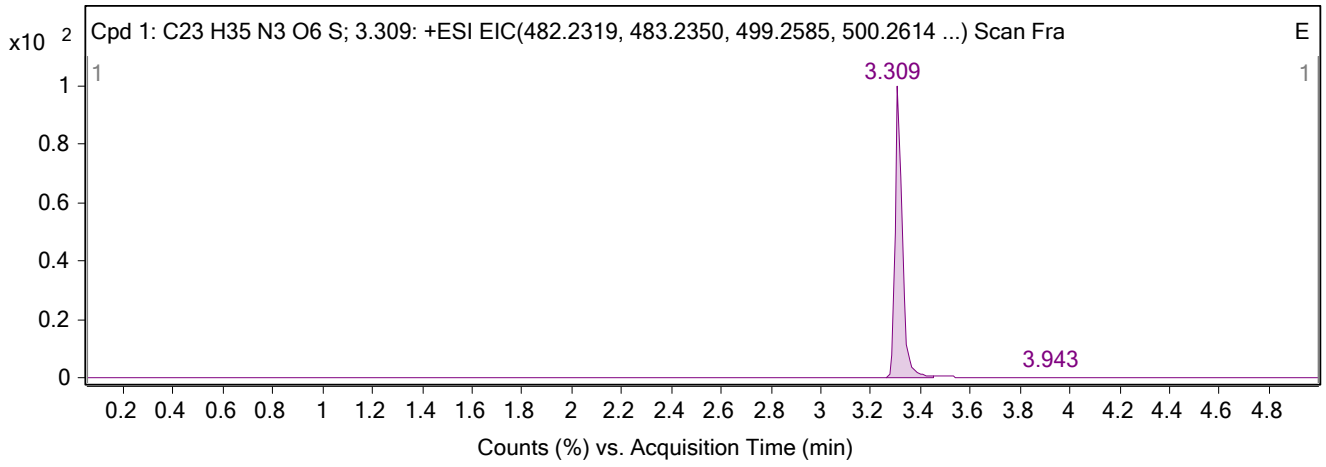
Data File	32.d	**Sample Name**	T8733239
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:18:07 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H35N3O6S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:18:07 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

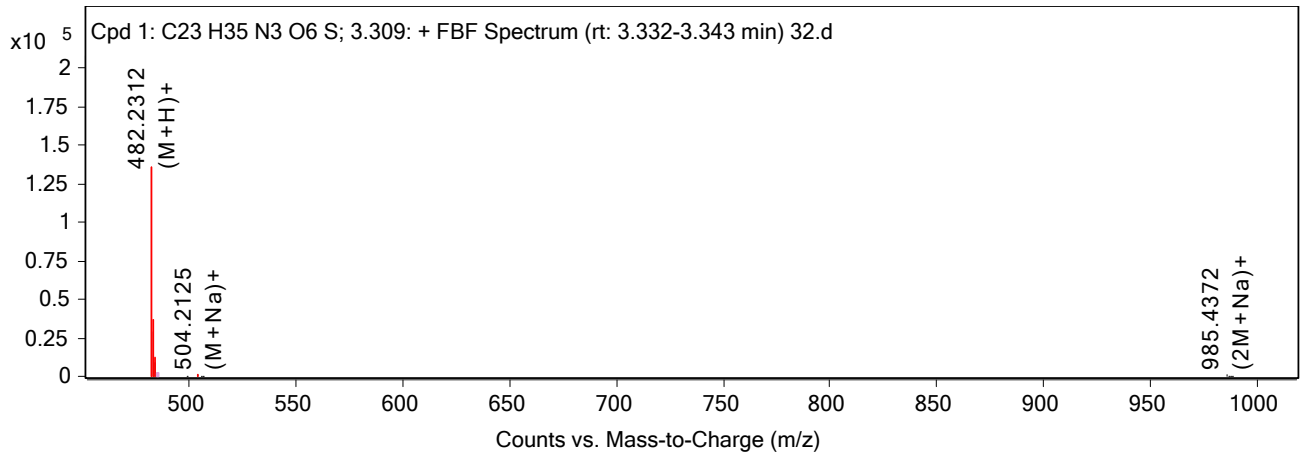
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H35 N3 O6 S; 3.309	95.89	-1.49	C23 H35 N3 O6 S	3.309	481.2247	481.2239

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
985.4372	3.309	481.2239	C23 H35 N3 O6 S	481.2247	-1.49	Find By Formula	

Compound Chromatograms



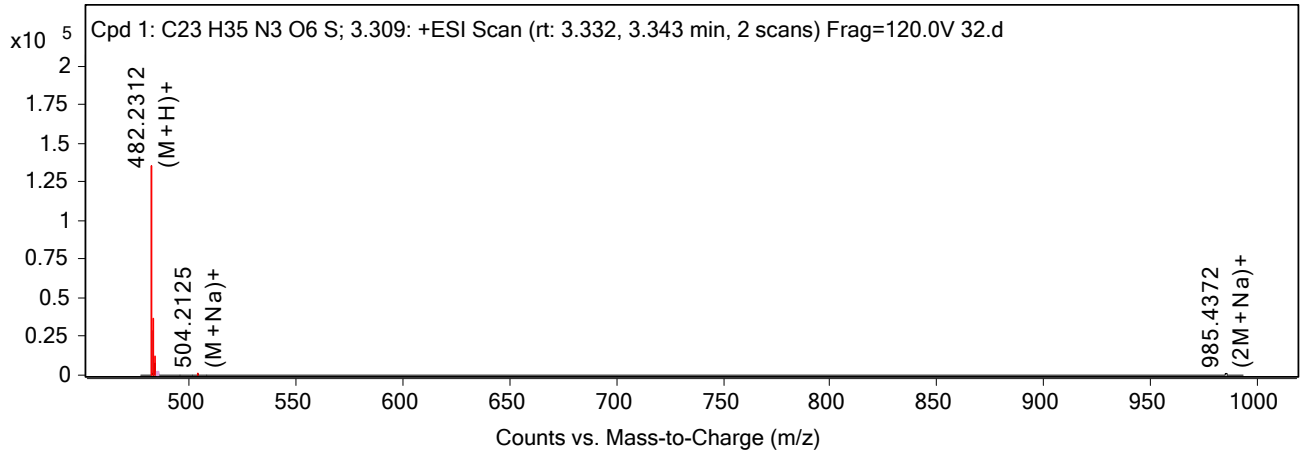
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
482.2312	1	135358.25	(M+H)+
483.2344	1	29481.96	(M+H)+
484.2324	1	8417.35	(M+H)+
504.2125	1	1516.25	(M+Na)+
505.2206	1	418.9	(M+Na)+
506.2149	1	159.62	(M+Na)+
985.4372	1	1226.35	(2M+Na)+
986.4396	1	608.97	(2M+Na)+
987.4422	1	341.59	(2M+Na)+
988.4445	1	111.44	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
482.2312	1	135358.25	(M+H)+	1.62
483.2344	1	29481.96	(M+H)+	1.22
484.2324	1	8417.35	(M+H)+	0.82
504.2125	1	1516.25	(M+Na)+	2.77
505.2206	1	418.9	(M+Na)+	-7.32
506.2149	1	159.62	(M+Na)+	-0.27
985.4372	1	1226.35	(2M+Na)+	1.32
986.4396	1	608.97	(2M+Na)+	1.98
987.4422	1	341.59	(2M+Na)+	-1.31
988.4445	1	111.44	(2M+Na)+	-2.8

--- End Of Report ---

Target Compound Screening Report

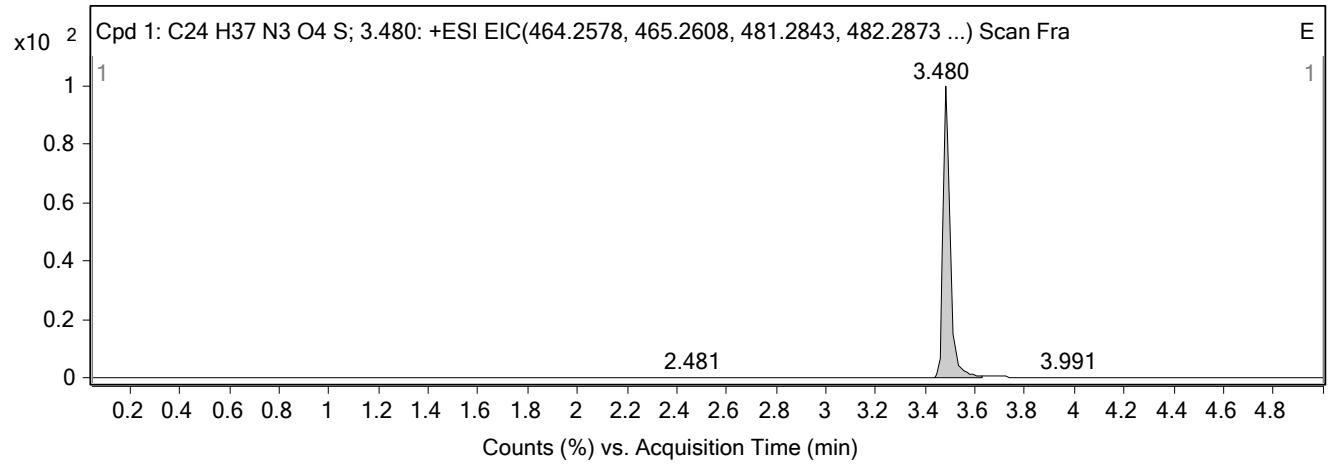
Data File	39.d	**Sample Name**	H2974329
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:45:47 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H37N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:45:47 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

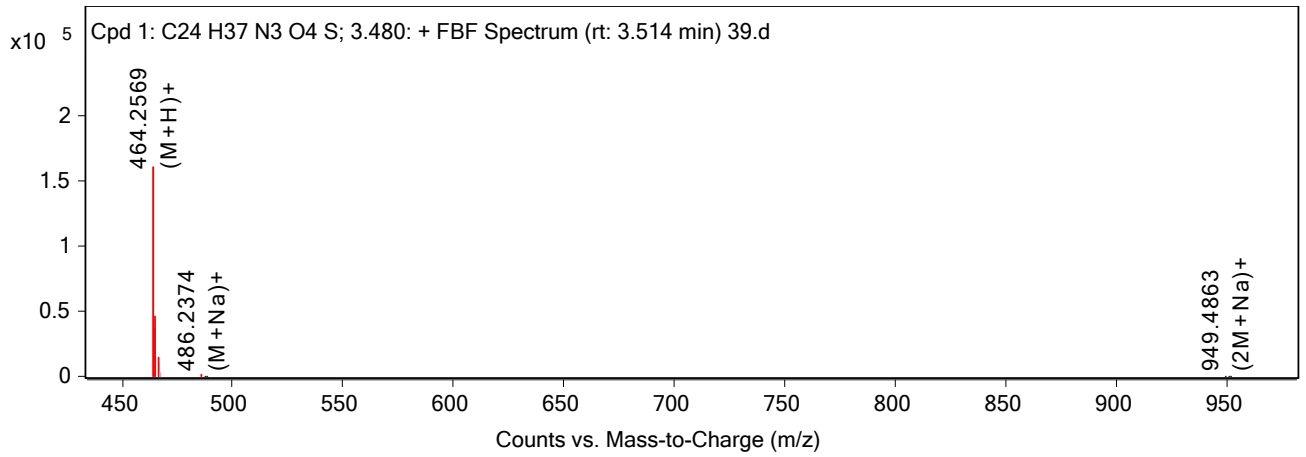
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H37 N3 O4 S; 3.480	94.15	-1.88	C24 H37 N3 O4 S	3.48	463.2505	463.2496

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
464.2569	3.48	463.2496	C24 H37 N3 O4 S	463.2505	-1.88	Find By Formula	

Compound Chromatograms



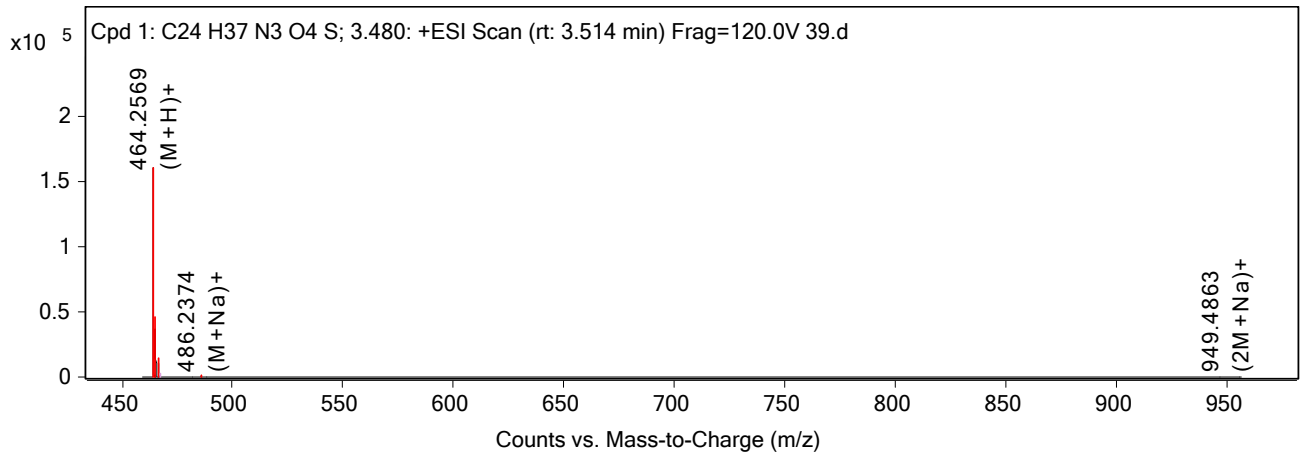
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
464.2569	1	160267.63	(M+H)+
465.2601	1	37092.69	(M+H)+
466.2582	1	10078	(M+H)+
486.2374	1	1213.17	(M+Na)+
487.2437	1	379.01	(M+Na)+
488.227	1	177.41	(M+Na)+
949.4863	1	342.37	(2M+Na)+
950.4861	1	270.4	(2M+Na)+
951.4788	1	108.56	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
464.2569	1	160267.63	(M+H)+	1.92
464.2569		160267.63		
465.2601	1	37092.69	(M+H)+	1.45
466.2582	1	10078	(M+H)+	0.99
486.2374	1	1213.17	(M+Na)+	4.78
487.2437	1	379.01	(M+Na)+	-1.98
488.227	1	177.41	(M+Na)+	27.9
949.4863	1	342.37	(2M+Na)+	4.09
950.4861	1	270.4	(2M+Na)+	7.54
951.4788	1	108.56	(2M+Na)+	14.59

--- End Of Report ---

Target Compound Screening Report

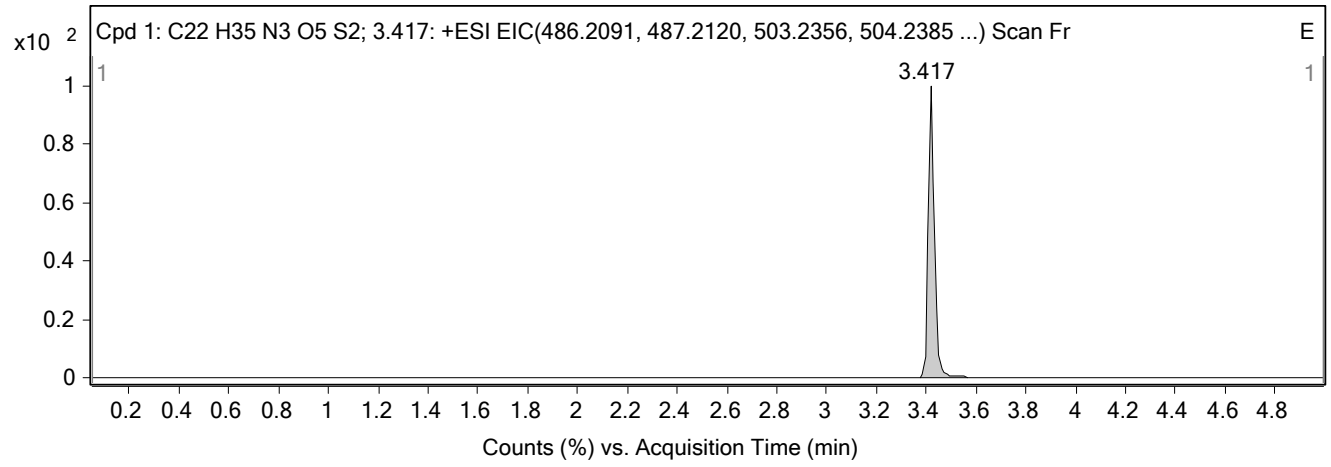
Data File	5d.d	**Sample Name**	H3475348
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:35:38 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H35N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:35:38 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H35 N3 O5 S2; 3.417	94.61	-1.57	C22 H35 N3 O5 S2	3.417	485.2018	485.201

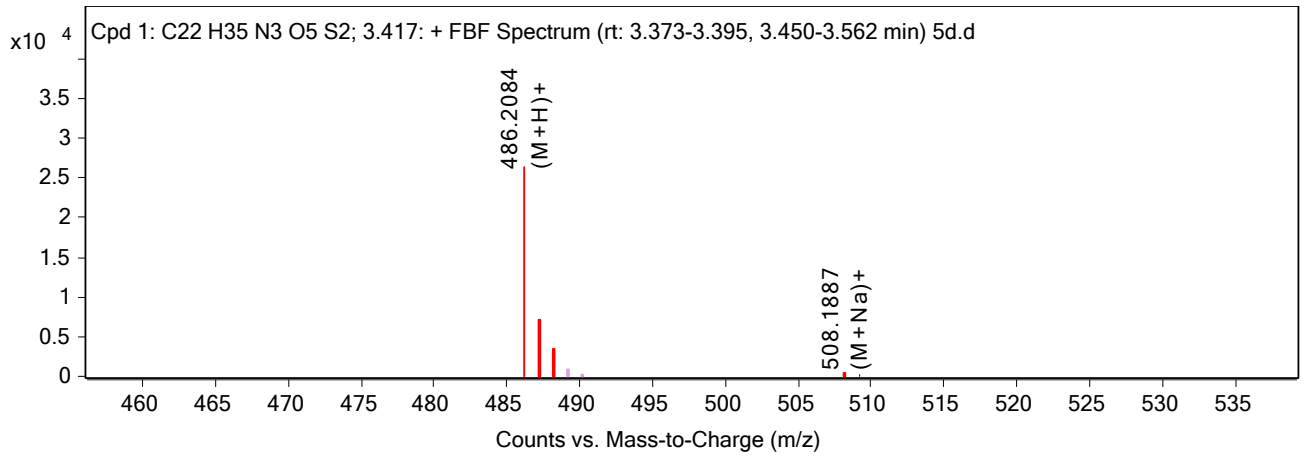
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
486.2084	3.417	485.201	C22 H35 N3 O5 S2	485.2018	-1.57	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

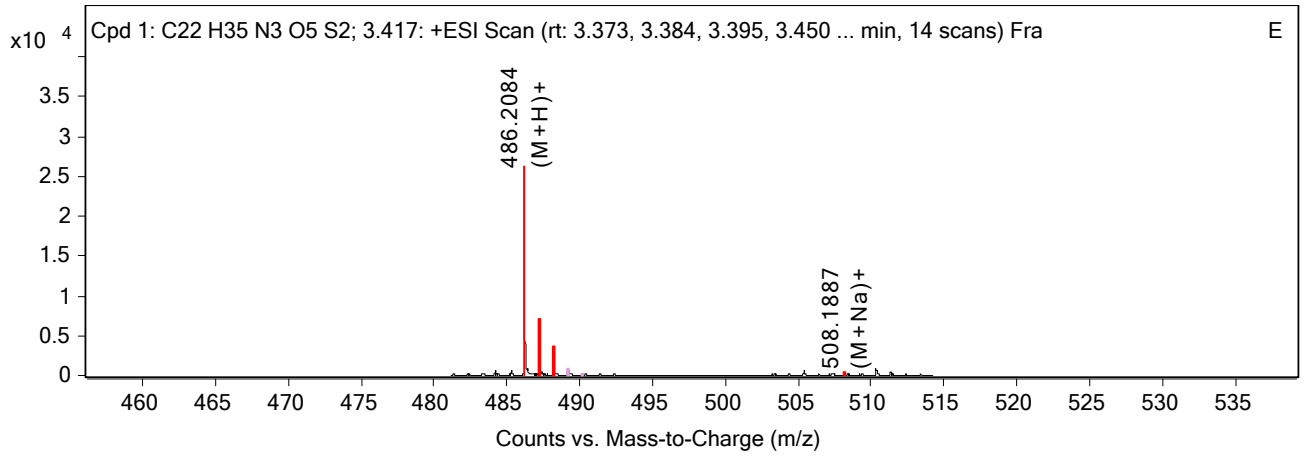
Agilent Technologies



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
486.2084	1	26351.47	(M+H)+
487.2112	1	6152.42	(M+H)+
488.2072	1	2743.54	(M+H)+
508.1887	1	301.12	(M+Na)+
509.196	1	142.46	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
486.2084	1	26351.47	(M+H)+	1.49
487.2112	1	6152.42	(M+H)+	1.68
488.2072	1	2743.54	(M+H)+	2
508.1887	1	301.12	(M+Na)+	4.56
509.196	1	142.46	(M+Na)+	-4.03

--- End Of Report ---

Target Compound Screening Report

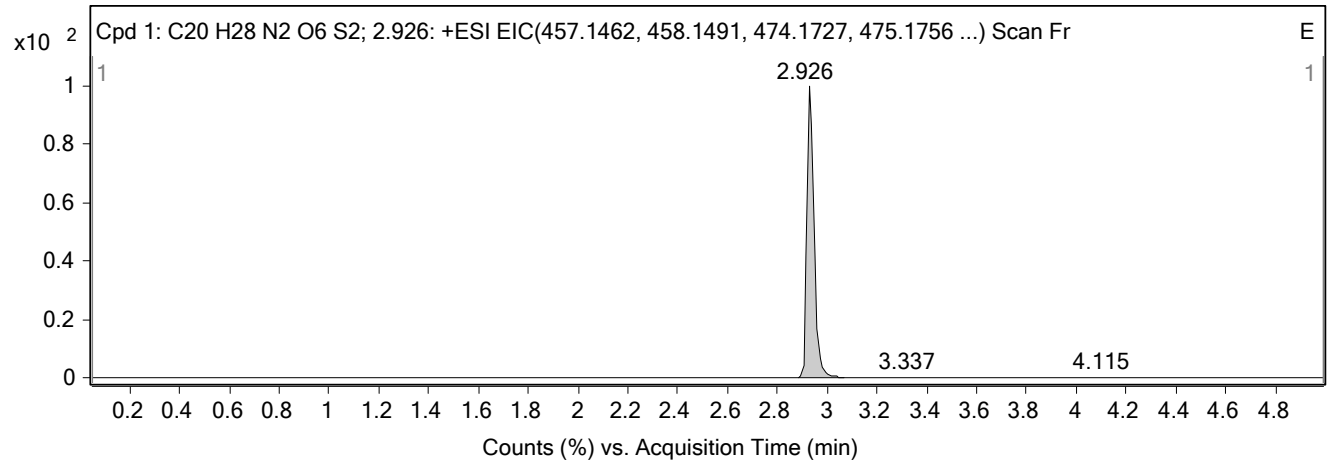
Data File	47.d	**Sample Name**	H2979253
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:03:26 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C20H28N2O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:03:26 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

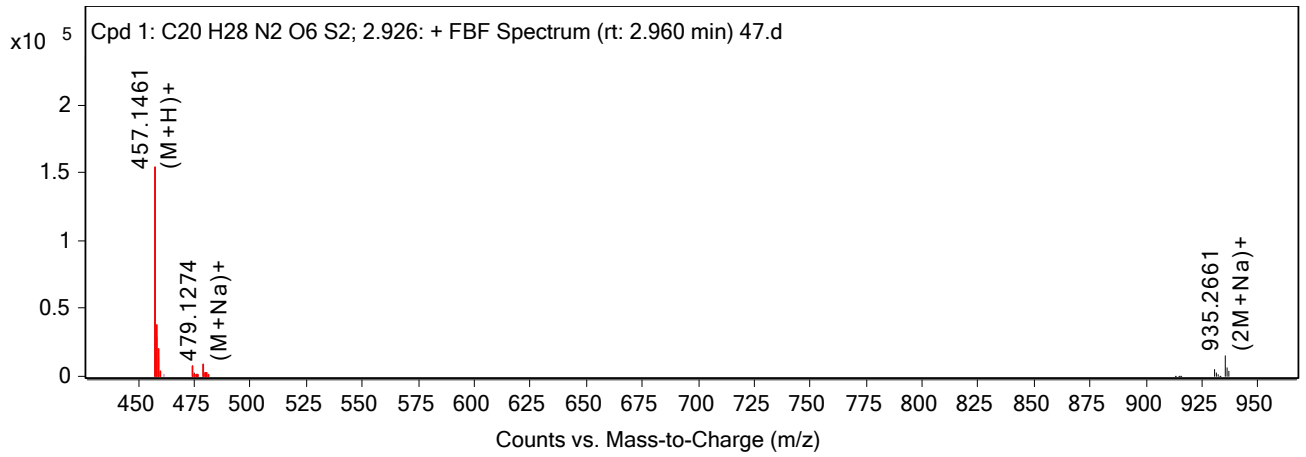
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C20 H28 N2 O6 S2; 2.926	94.44	-0.94	C20 H28 N2 O6 S2	2.926	456.1389	456.1384

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
479.1274	2.926	456.1384	C20 H28 N2 O6 S2	456.1389	-0.94	Find By Formula	

Compound Chromatograms



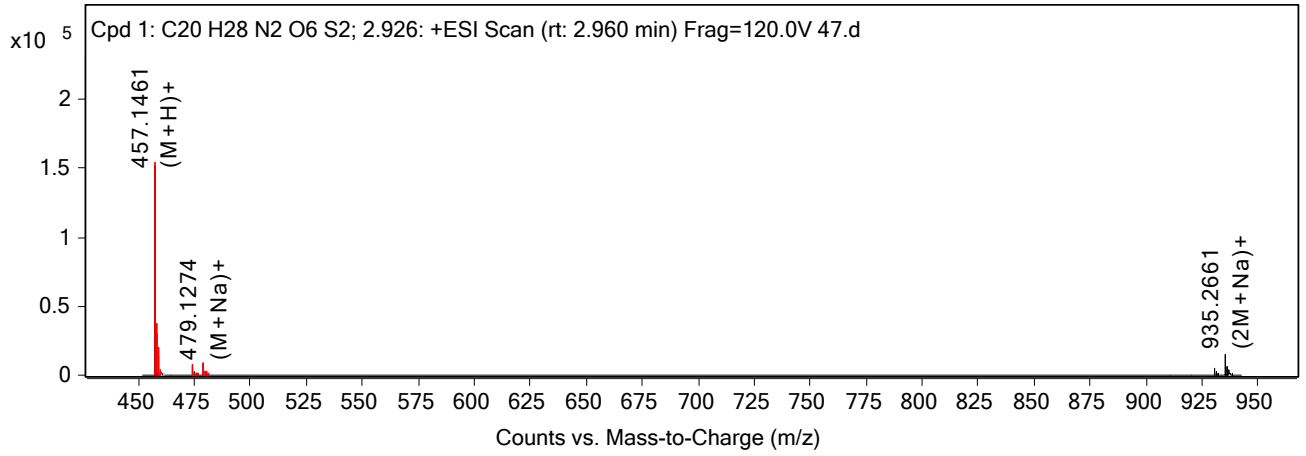
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
457.1461	1	153992.41	(M+H)+
458.1491	1	29544.45	(M+H)+
459.1451	1	13558.98	(M+H)+
460.1463	1	2550.44	(M+H)+
474.1715	1	7301.85	(M+NH4)+
479.1274	1	8310.12	(M+Na)+
930.3097	1	5279.98	(2M+NH4)+
935.2661	1	15471.37	(2M+Na)+
936.2678	1	6327.08	(2M+Na)+
937.2641	1	3897.15	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
457.1461	1	153992.41	(M+H)+	0.2
458.1491	1	29544.45	(M+H)+	-0.03
459.1451	1	13558.98	(M+H)+	-0.17
460.1463	1	2550.44	(M+H)+	1.17
474.1715	1	7301.85	(M+NH4)+	2.54
479.1274	1	8310.12	(M+Na)+	1.36
930.3097	1	5279.98	(2M+NH4)+	1.99
935.2661	1	15471.37	(2M+Na)+	0.94
936.2678	1	6327.08	(2M+Na)+	2.26
937.2641	1	3897.15	(2M+Na)+	3.25

--- End Of Report ---

Target Compound Screening Report

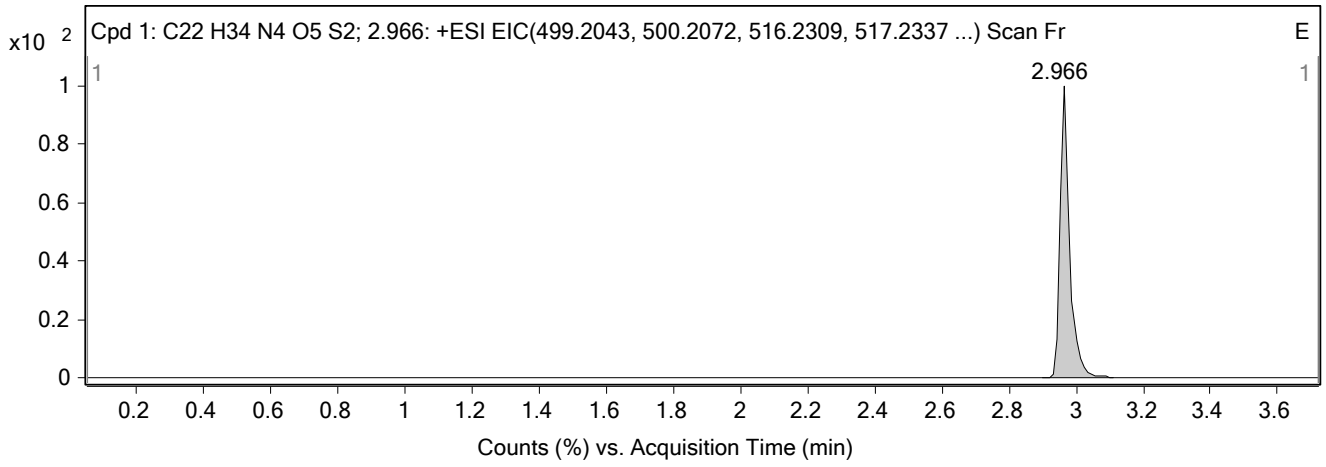
Data File	54.d	**Sample Name**	H2974331
Sample Type	Sample	**Position**	P1-F9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:42:22 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H34N4O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:42:22 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H34 N4 O5 S2; 2.966	94.49	-0.87	C22 H34 N4 O5 S2	2.966	498.1971	498.1966

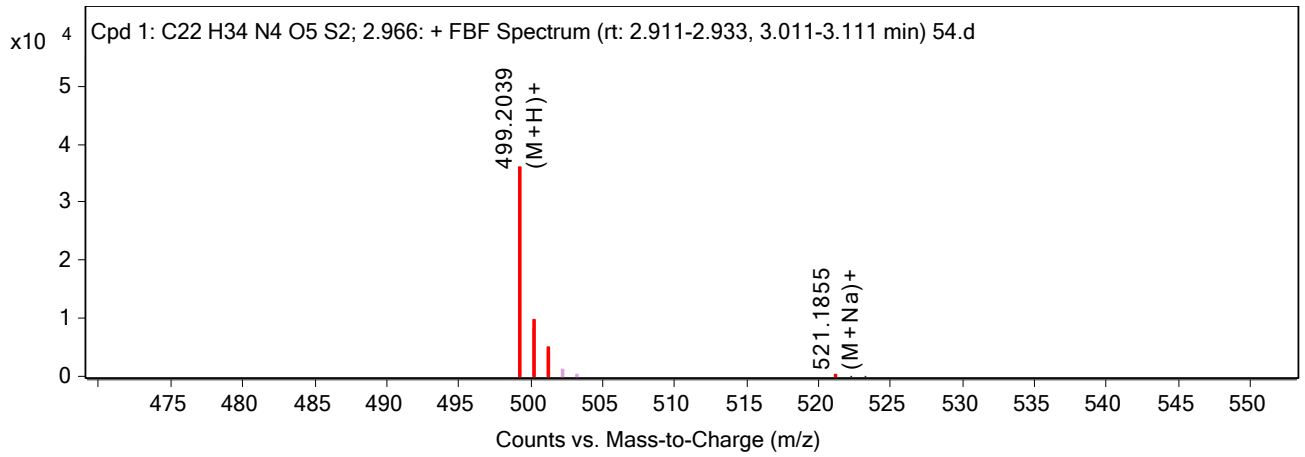
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
499.2039	2.966	498.1966	C22 H34 N4 O5 S2	498.1971	-0.87	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

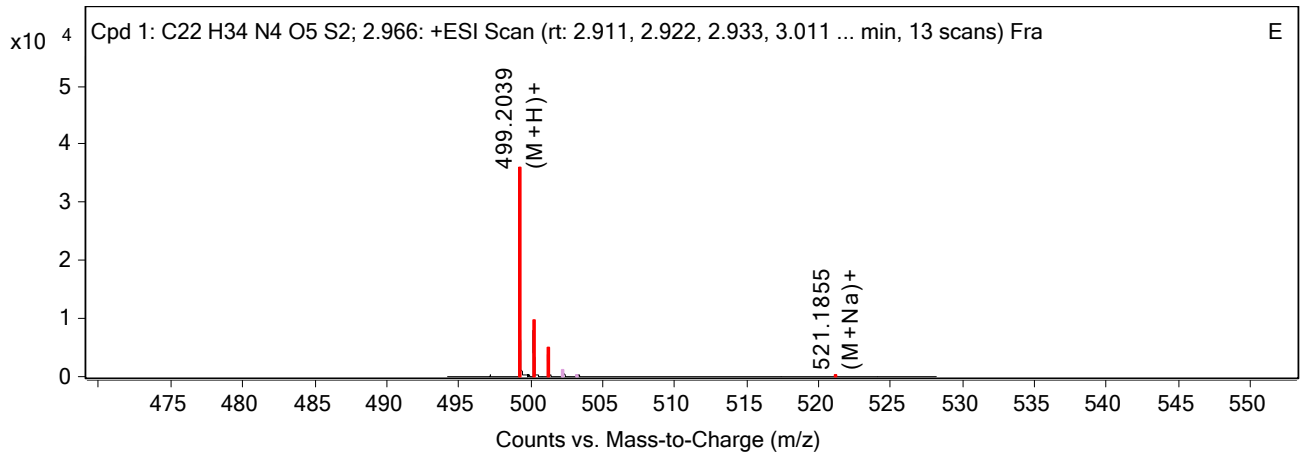
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
499.2039	1	35993.04	(M+H)+
500.2065	1	8148.3	(M+H)+
501.2034	1	3798.41	(M+H)+
521.1855	1	426.13	(M+Na)+
522.188	1	112.24	(M+Na)+
523.1963	1	73.62	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
499.2039	1	35993.04	(M+H)+	0.88
500.2065	1	8148.3	(M+H)+	1.35
501.2034	1	3798.41	(M+H)+	-0.02
521.1855	1	426.13	(M+Na)+	1.44
522.188	1	112.24	(M+Na)+	2.16
523.1963	1	73.62	(M+Na)+	-20.96

--- End Of Report ---

Target Compound Screening Report

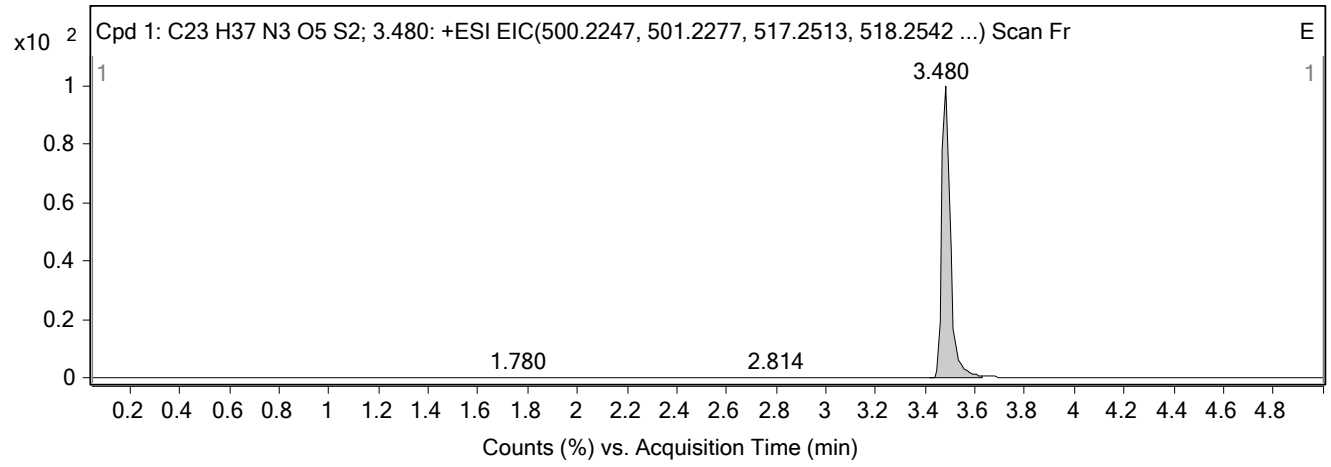
Data File	11.d	**Sample Name**	H2981847
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:07:04 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H37N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:07:04 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

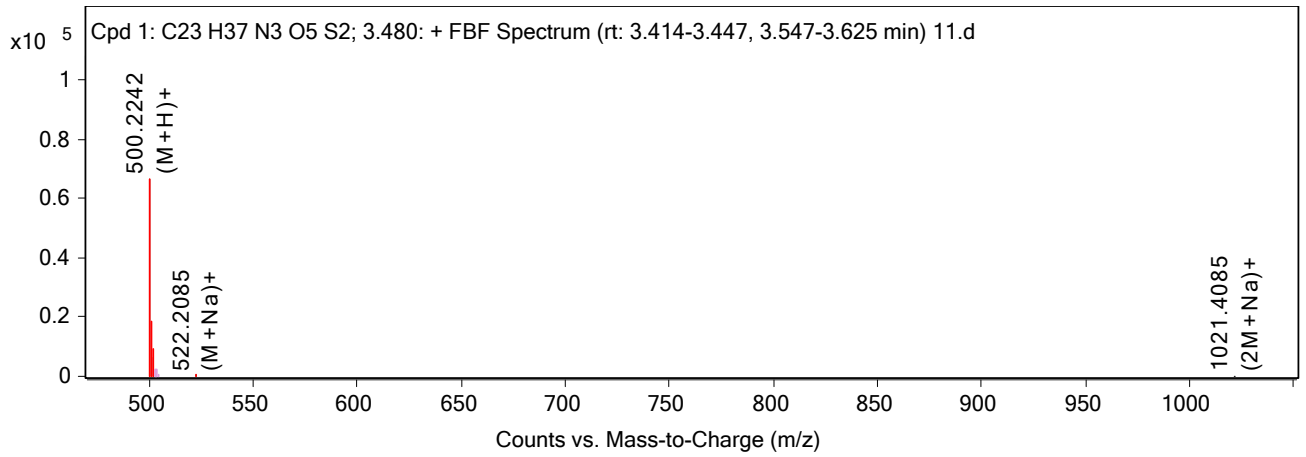
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H37 N3 O5 S2; 3.480	94.07	-1.1	C23 H37 N3 O5 S2	3.48	499.2175	499.2169

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.2242	3.48	499.2169	C23 H37 N3 O5 S2	499.2175	-1.1	Find By Formula	

Compound Chromatograms



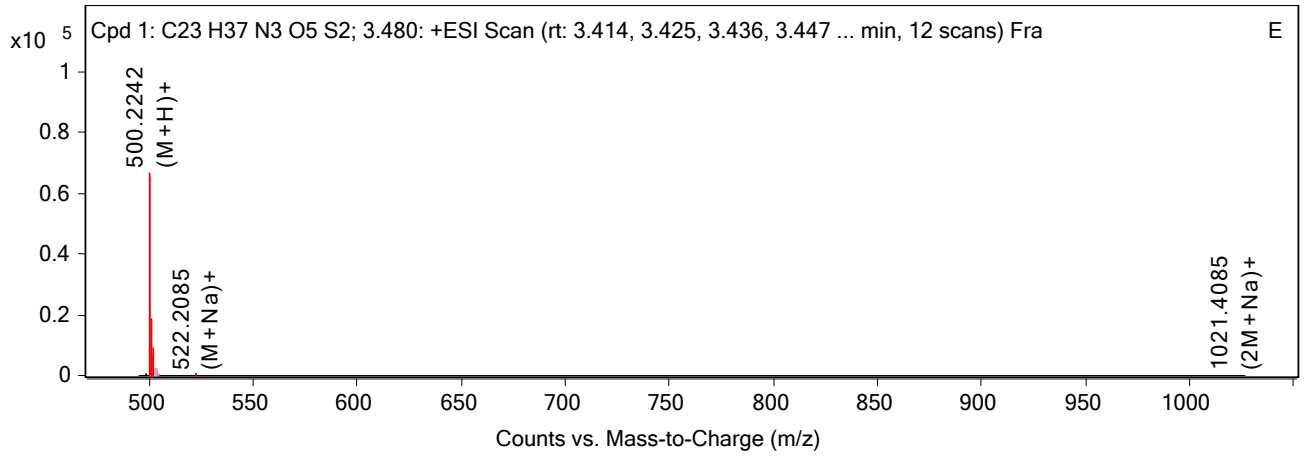
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.2242	1	66565.27	(M+H)+
501.227	1	15513.76	(M+H)+
502.2238	1	6664.13	(M+H)+
522.2085	1	412.17	(M+Na)+
1021.4085	1	59.4	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.2242	1	66565.27	(M+H)+	1.09
501.227	1	15513.76	(M+H)+	1.41
502.2238	1	6664.13	(M+H)+	0.4
522.2085	1	412.17	(M+Na)+	-3.56
1021.4085	1	59.4	(2M+Na)+	15.33

--- End Of Report ---

Target Compound Screening Report

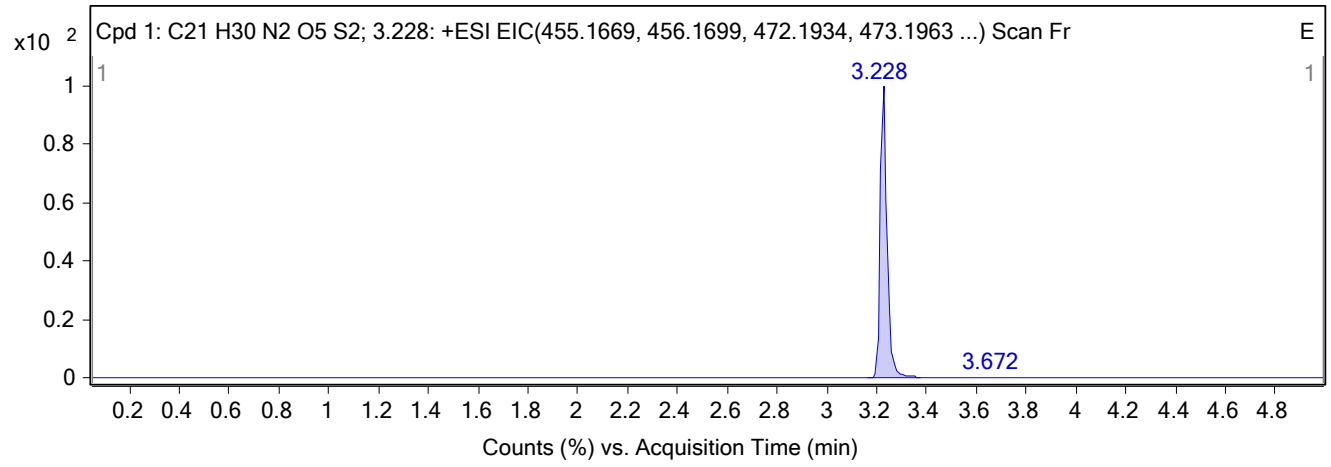
Data File	26.d	**Sample Name**	H2979255
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:06:49 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H30N2O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:06:49 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

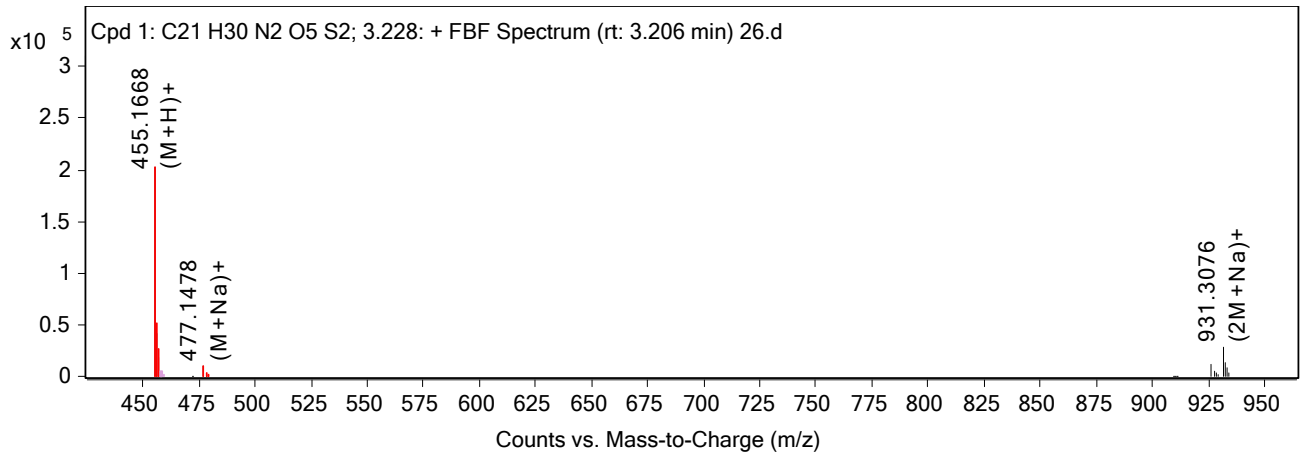
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H30 N2 O5 S2; 3.228	96.96	-0.66	C21 H30 N2 O5 S2	3.228	454.1596	454.1593

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
477.1478	3.228	454.1593	C21 H30 N2 O5 S2	454.1596	-0.66	Find By Formula	

Compound Chromatograms



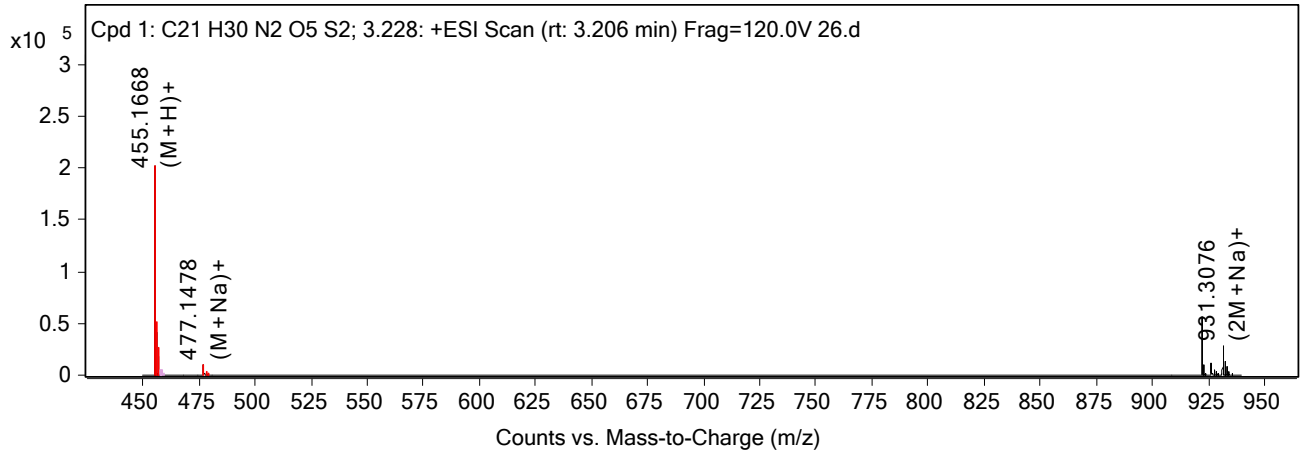
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
455.1668	1	202255.66	(M+H)+
456.1692	1	41929.46	(M+H)+
457.1664	1	17927.61	(M+H)+
477.1478	1	10232.1	(M+Na)+
926.3523	1	11084.71	(2M+NH4)+
927.354	1	5344.25	(2M+NH4)+
928.3508	1	3687.02	(2M+NH4)+
931.3076	1	28910	(2M+Na)+
932.311	1	13106.23	(2M+Na)+
933.3094	1	7915.01	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
455.1668	1	202255.66	(M+H)+	0.16
456.1692	1	41929.46	(M+H)+	1.43
457.1664	1	17927.61	(M+H)+	-1.37
477.1478	1	10232.1	(M+Na)+	2.22
926.3523	1	11084.71	(2M+NH4)+	0.83
927.354	1	5344.25	(2M+NH4)+	2.15
928.3508	1	3687.02	(2M+NH4)+	2.77
931.3076	1	28910	(2M+Na)+	0.88
932.311	1	13106.23	(2M+Na)+	0.44
933.3094	1	7915.01	(2M+Na)+	-0.71

--- End Of Report ---

Target Compound Screening Report

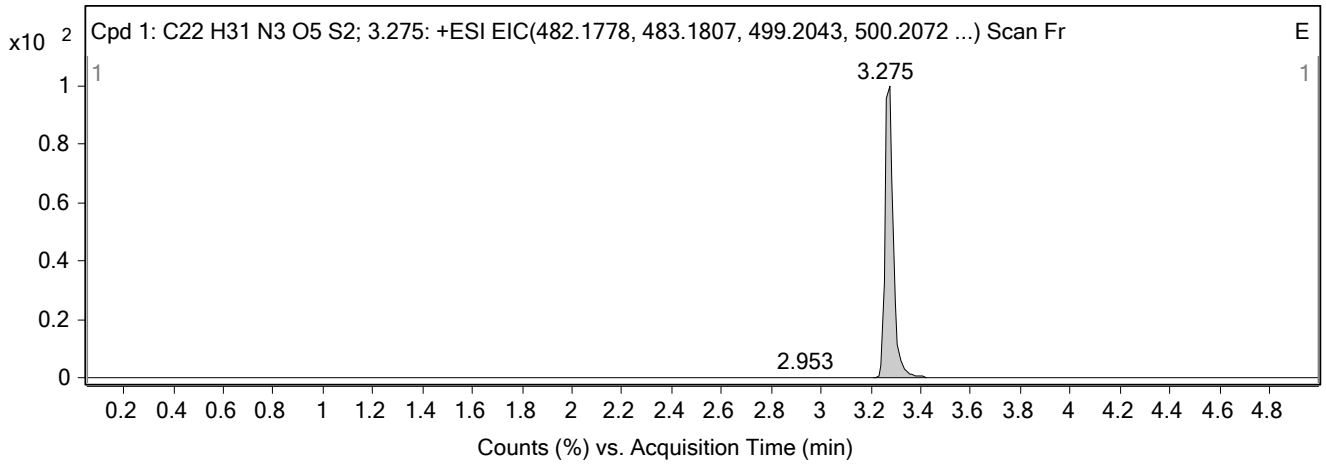
Data File	45.d	**Sample Name**	H2979248
Sample Type	Sample	**Position**	P1-E9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 3:21:00 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H31N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 3:21:00 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

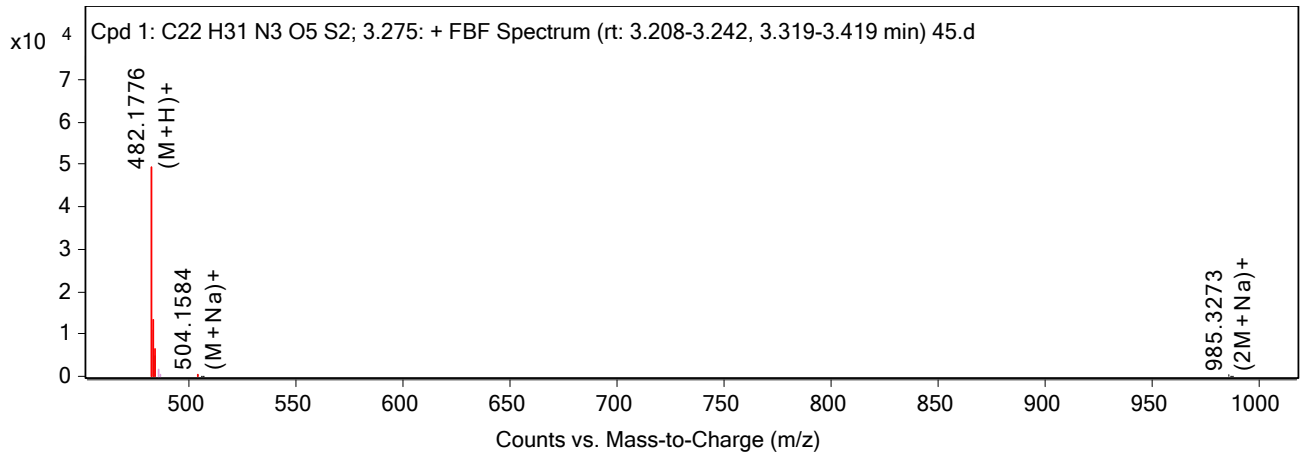
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H31 N3 O5 S2; 3.275	94.3	-0.62	C22 H31 N3 O5 S2	3.275	481.1705	481.1702

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
482.1776	3.275	481.1702	C22 H31 N3 O5 S2	481.1705	-0.62	Find By Formula	

Compound Chromatograms



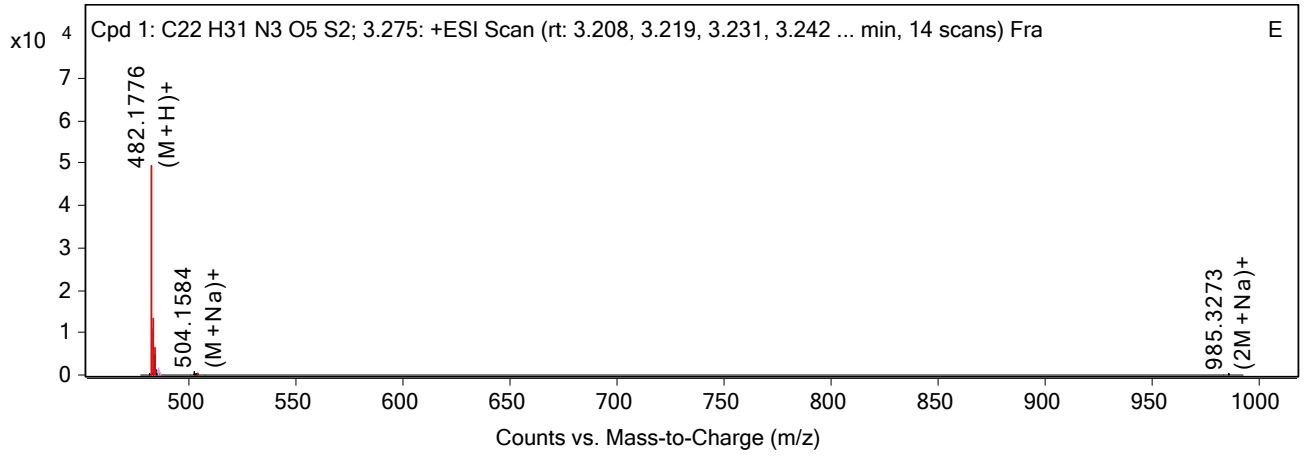
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
482.1776	1	49314.06	(M+H)+
483.1804	1	10892.37	(M+H)+
484.1762	1	4877.44	(M+H)+
504.1584	1	560.66	(M+Na)+
505.1602	1	153.51	(M+Na)+
506.1607	1	92.28	(M+Na)+
985.3273	1	227	(2M+Na)+
986.328	1	122.96	(2M+Na)+
987.3223	1	85.73	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
482.1776	1	49314.06	(M+H)+	0.42
483.1804	1	10892.37	(M+H)+	0.69
484.1762	1	4877.44	(M+H)+	1.34
504.1584	1	560.66	(M+Na)+	2.69
505.1602	1	153.51	(M+Na)+	4.82
506.1607	1	92.28	(M+Na)+	-3.83
985.3273	1	227	(2M+Na)+	3.04
986.328	1	122.96	(2M+Na)+	5.2
987.3223	1	85.73	(2M+Na)+	8.56

--- End Of Report ---

Target Compound Screening Report

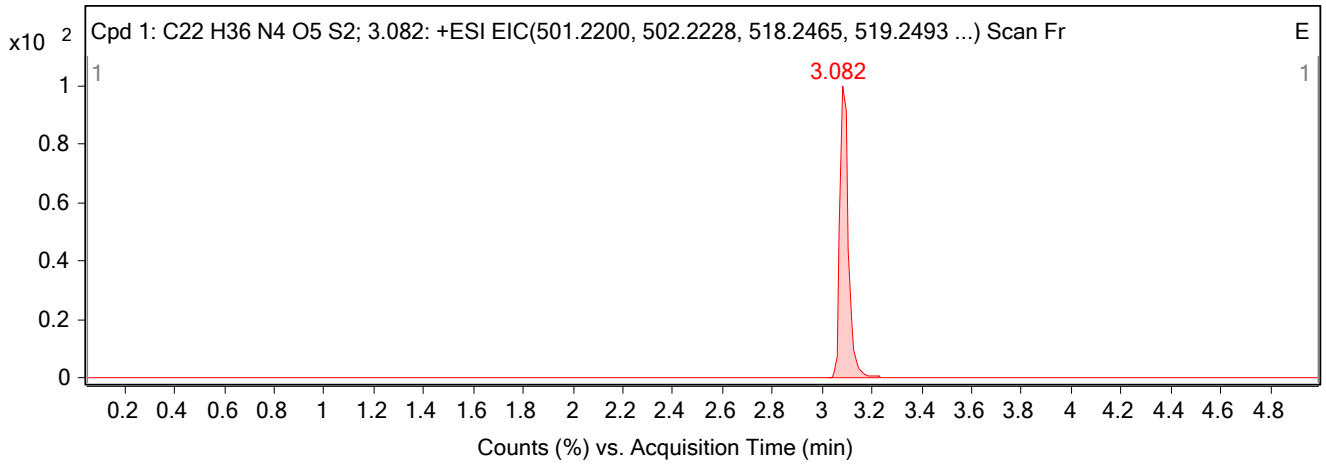
Data File	40.d	**Sample Name**	H2974330
Sample Type	Sample	**Position**	P1-E4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:24:33 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H36N4O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:24:33 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

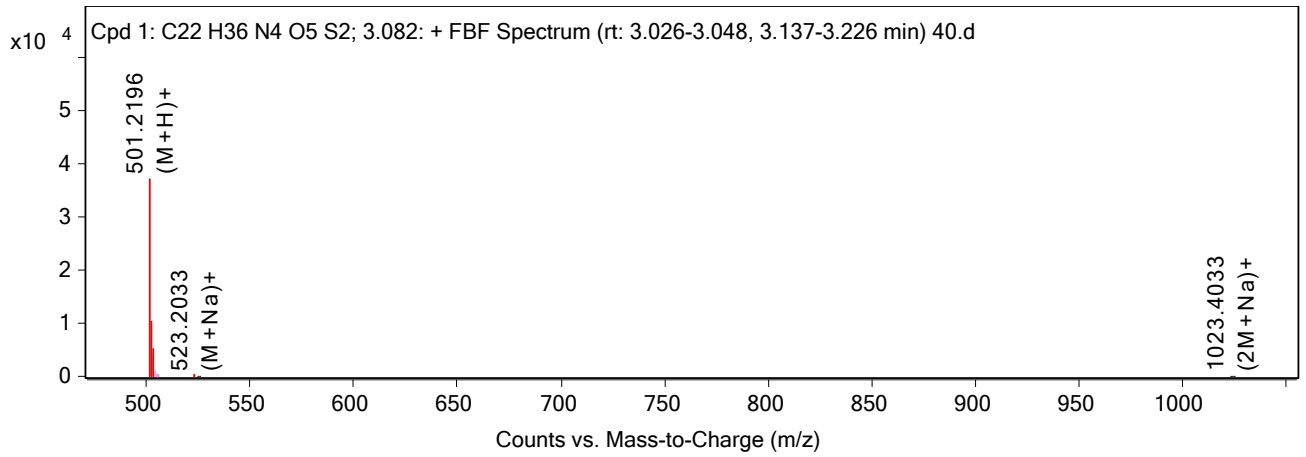
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H36 N4 O5 S2; 3.082	95.17	-0.85	C22 H36 N4 O5 S2	3.082	500.2127	500.2123

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
501.2196	3.082	500.2123	C22 H36 N4 O5 S2	500.2127	-0.85	Find By Formula	

Compound Chromatograms



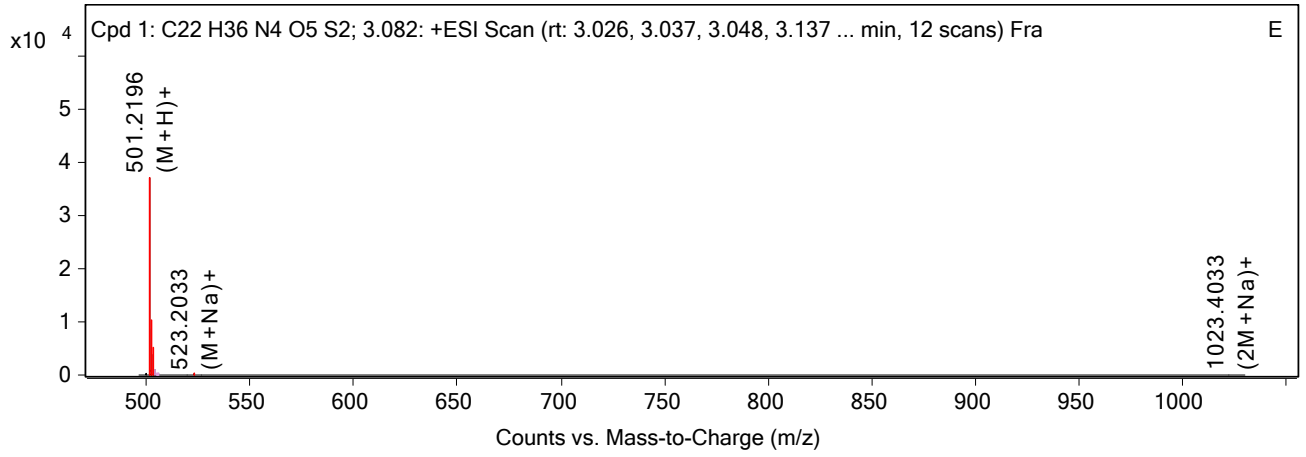
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
501.2196	1	37159	(M+H)+
502.2225	1	8667.16	(M+H)+
503.2185	1	3795.55	(M+H)+
523.2033	1	313.92	(M+Na)+
524.2044	1	101.09	(M+Na)+
525.2014	1	49.72	(M+Na)+
1023.4033	1	128.47	(2M+Na)+
1024.4123	1	76.24	(2M+Na)+
1025.4111	1	51.31	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
501.2196	1	37159	(M+H)+	0.79
502.2225	1	8667.16	(M+H)+	0.71
503.2185	1	3795.55	(M+H)+	1.1
523.2033	1	313.92	(M+Na)+	-2.68
524.2044	1	101.09	(M+Na)+	0.8
525.2014	1	49.72	(M+Na)+	-0.68
1023.4033	1	128.47	(2M+Na)+	11.07
1024.4123	1	76.24	(2M+Na)+	5.04
1025.4111	1	51.31	(2M+Na)+	3.94

--- End Of Report ---

Target Compound Screening Report

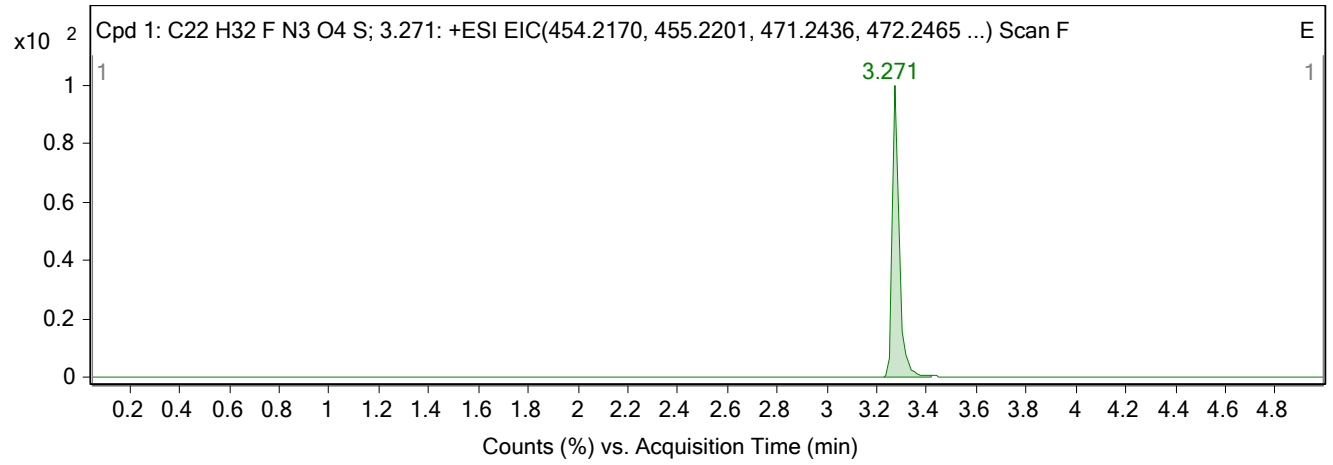
Data File	35.d	**Sample Name**	H2979306
Sample Type	Sample	**Position**	P1-D8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:56:49 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H32FN3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:56:49 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

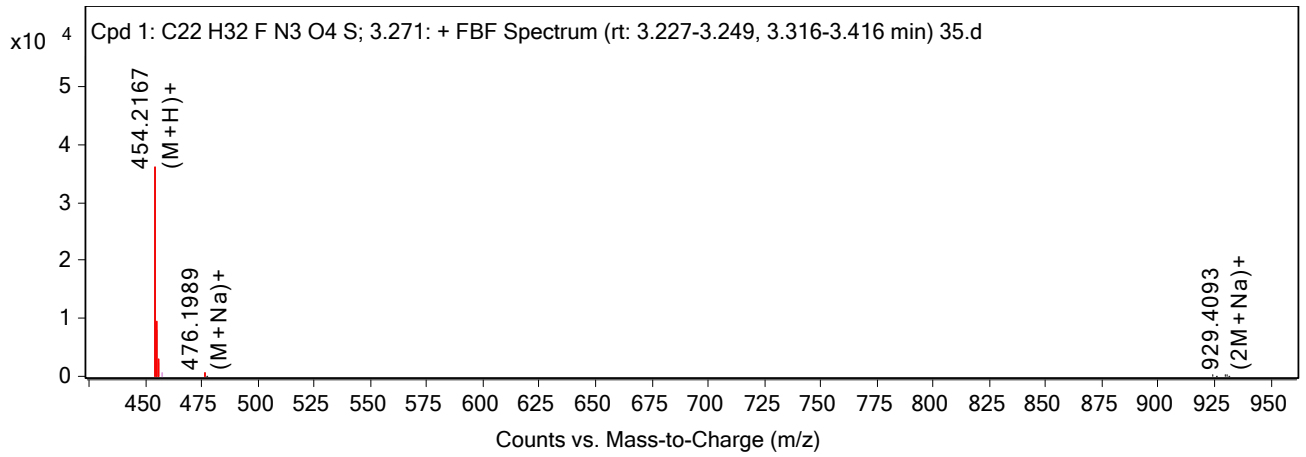
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H32 F N3 O4 S; 3.271	96.57	-0.29	C22 H32 F N3 O4 S	3.271	453.2098	453.2096

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
454.2167	3.271	453.2096	C22 H32 F N3 O4 S	453.2098	-0.29	Find By Formula	

Compound Chromatograms



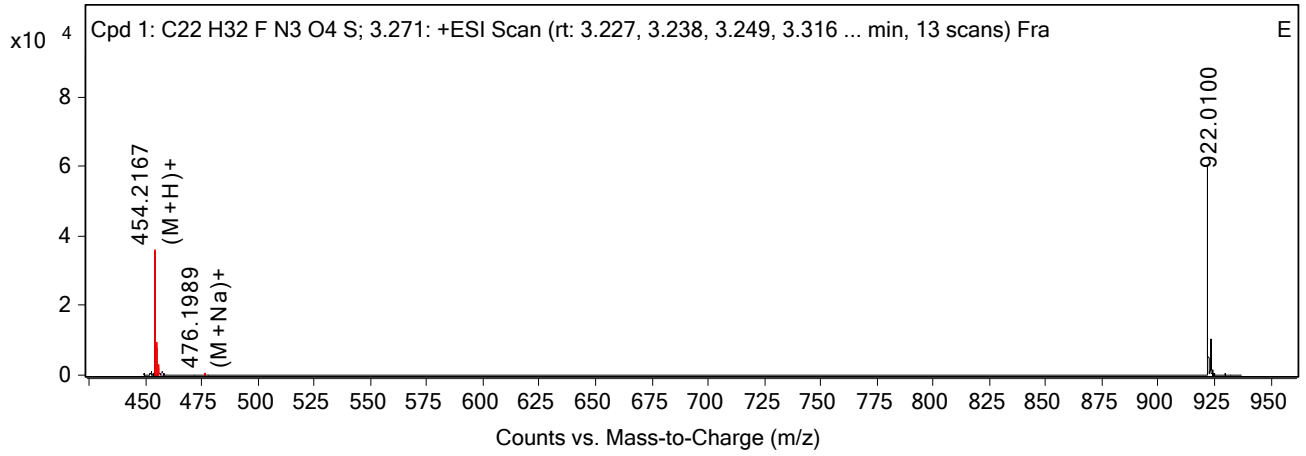
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
454.2167	1	36111.81	(M+H)+
455.2196	1	8070.88	(M+H)+
456.2171	1	2248.47	(M+H)+
476.1989	1	533.9	(M+Na)+
477.2039	1	145.14	(M+Na)+
924.4786	1	226.52	(2M+NH4)+
925.4775	1	154.61	(2M+NH4)+
929.4093	1	332.05	(2M+Na)+
930.4129	1	209.89	(2M+Na)+
931.4089	1	113.38	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
454.2167	1	36111.81	(M+H)+	0.68
455.2196	1	8070.88	(M+H)+	0.96
456.2171	1	2248.47	(M+H)+	0.96
476.1989	1	533.9	(M+Na)+	0.17
477.2039	1	145.14	(M+Na)+	-3.89
924.4786	1	226.52	(2M+NH4)+	-27.37
925.4775	1	154.61	(2M+NH4)+	-22.91
929.4093	1	332.05	(2M+Na)+	-0.63
930.4129	1	209.89	(2M+Na)+	-1.18
931.4089	1	113.38	(2M+Na)+	2.08

--- End Of Report ---

Target Compound Screening Report

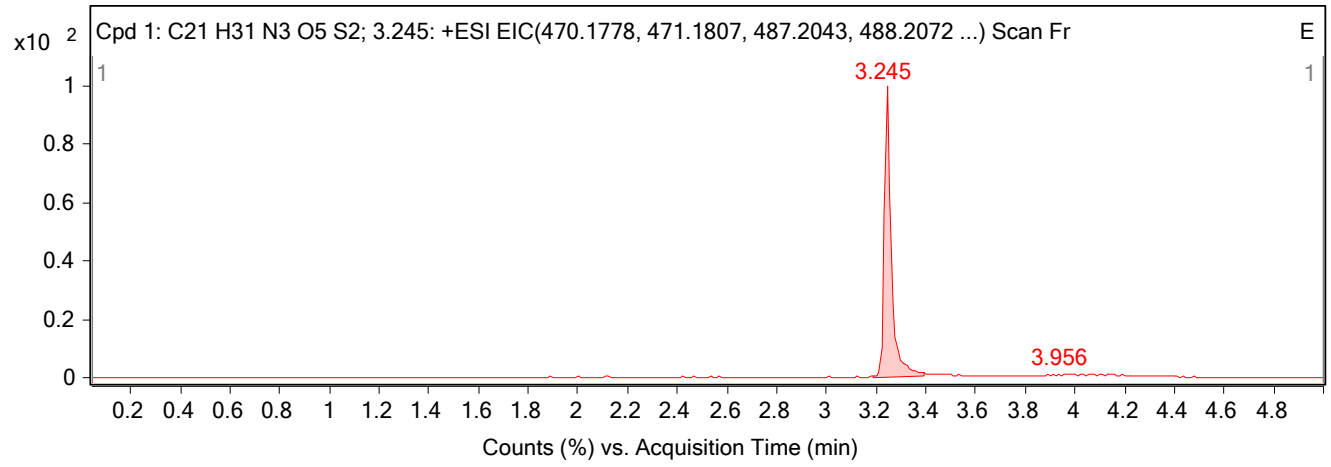
Data File	9-2.d	**Sample Name**	H2981848
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:54:33 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H31N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:54:33 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

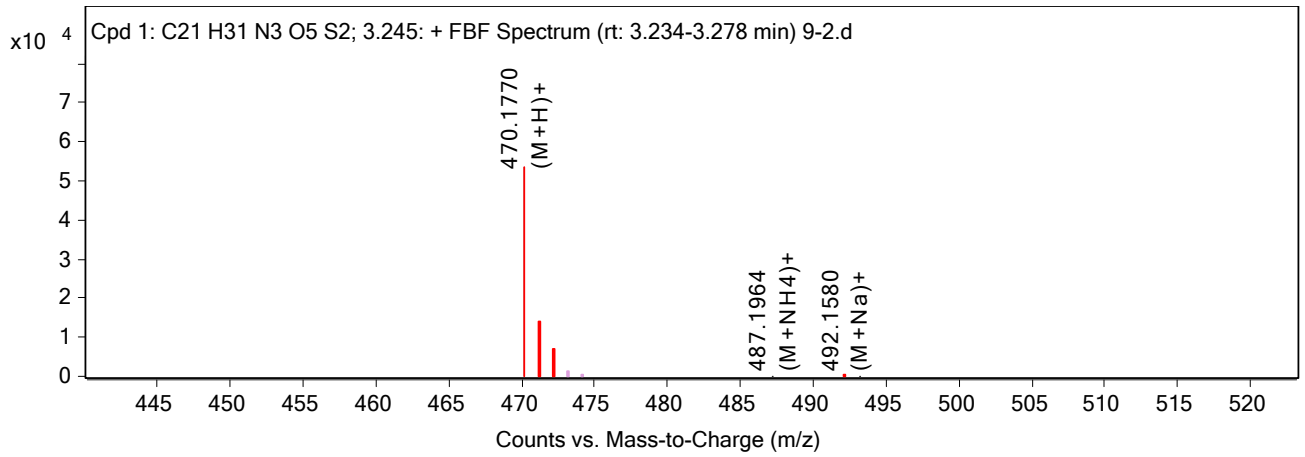
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H31 N3 O5 S2; 3.245	94.61	-1.93	C21 H31 N3 O5 S2	3.245	469.1705	469.1696

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
470.177	3.245	469.1696	C21 H31 N3 O5 S2	469.1705	-1.93	Find By Formula	

Compound Chromatograms



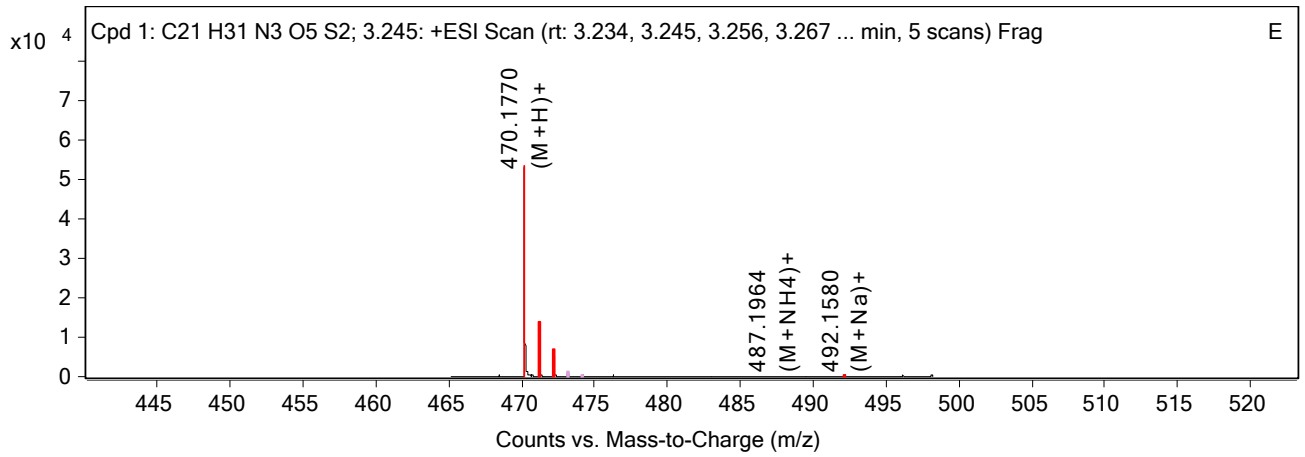
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
470.177	1	53450.74	(M+H)+
471.1796	1	11702.55	(M+H)+
472.1754	1	5371.45	(M+H)+
487.1964	1	63.23	(M+NH4)+
492.158	1	360.29	(M+Na)+
493.1669	1	126.41	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
470.177	1	53450.74	(M+H)+	1.74
471.1796	1	11702.55	(M+H)+	2.33
472.1754	1	5371.45	(M+H)+	2.77
487.1964	1	63.23	(M+NH4)+	16.26
492.158	1	360.29	(M+Na)+	3.51
493.1669	1	126.41	(M+Na)+	-8.6

--- End Of Report ---

Target Compound Screening Report

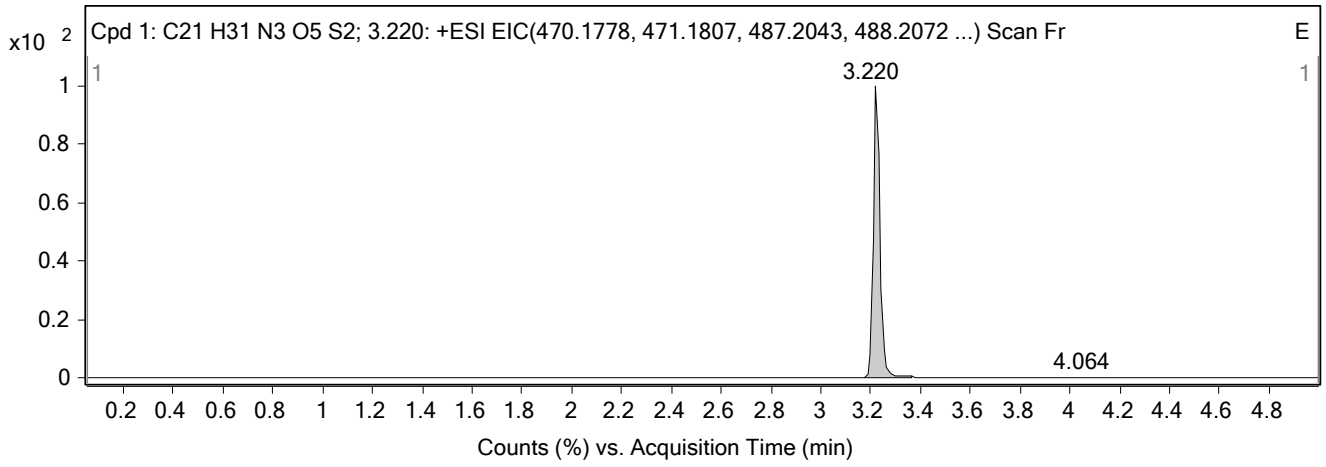
Data File	3d.d	**Sample Name**	H3472157
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:24:37 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H31N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:24:37 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H31 N3 O5 S2; 3.220	95.19	-1.75	C21 H31 N3 O5 S2	3.22	469.1705	469.1697

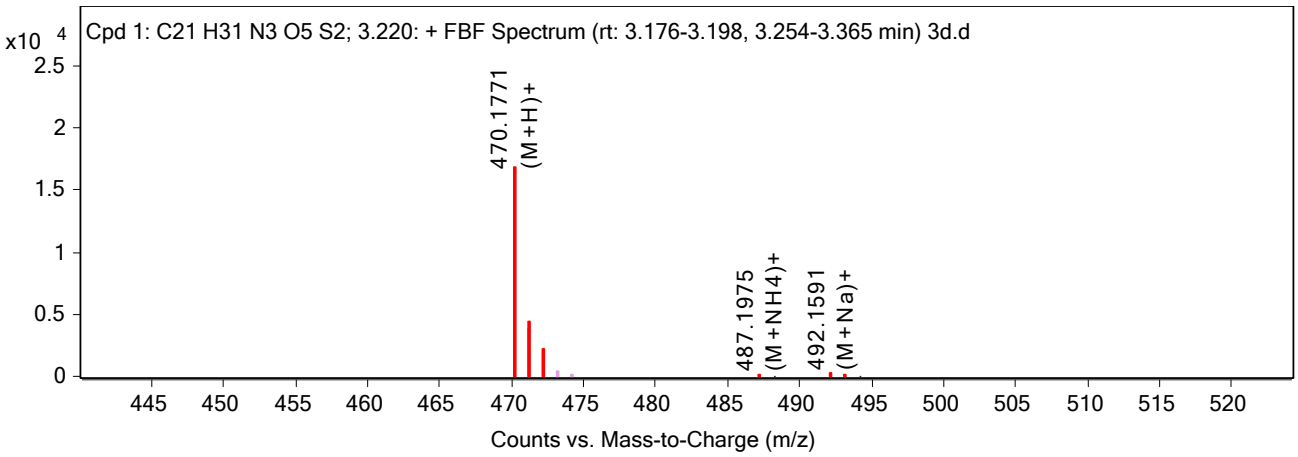
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
470.1771	3.22	469.1697	C21 H31 N3 O5 S2	469.1705	-1.75	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

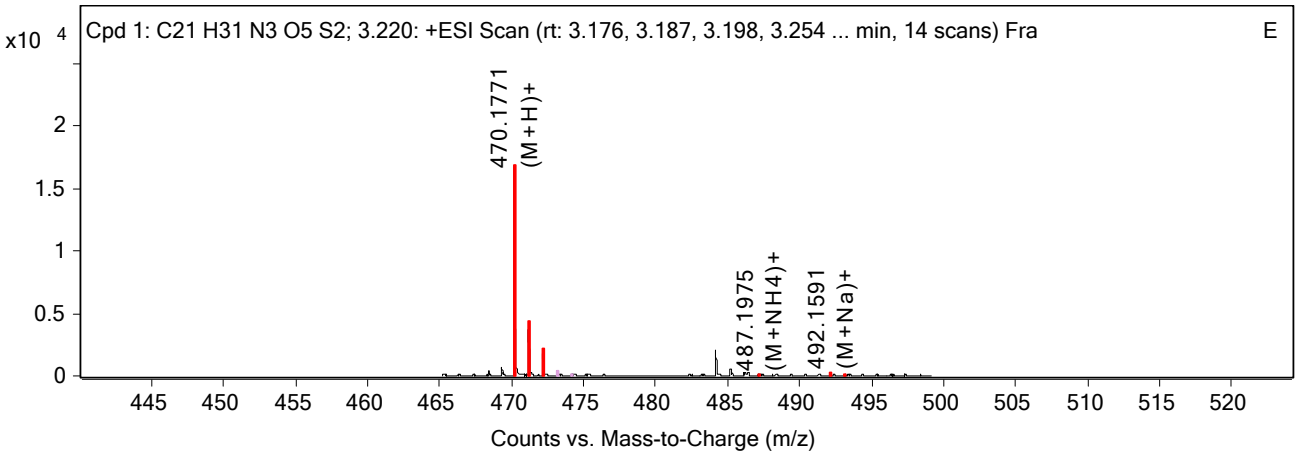
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
470.1771	1	16850.59	(M+H)+
471.1795	1	3815.82	(M+H)+
472.1765	1	1832.47	(M+H)+
487.1975	1	114.57	(M+NH4)+
488.191	1	75.1	(M+NH4)+
492.1591	1	225.58	(M+Na)+
493.1634	1	85	(M+Na)+
494.1609	1	68.33	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
470.1771	1	16850.59	(M+H)+	1.55
471.1795	1	3815.82	(M+H)+	2.41
472.1765	1	1832.47	(M+H)+	0.49
487.1975	1	114.57	(M+NH4)+	14.06
488.191	1	75.1	(M+NH4)+	33.09
492.1591	1	225.58	(M+Na)+	1.19
493.1634	1	85	(M+Na)+	-1.52
494.1609	1	68.33	(M+Na)+	-4.51

--- End Of Report ---

Target Compound Screening Report

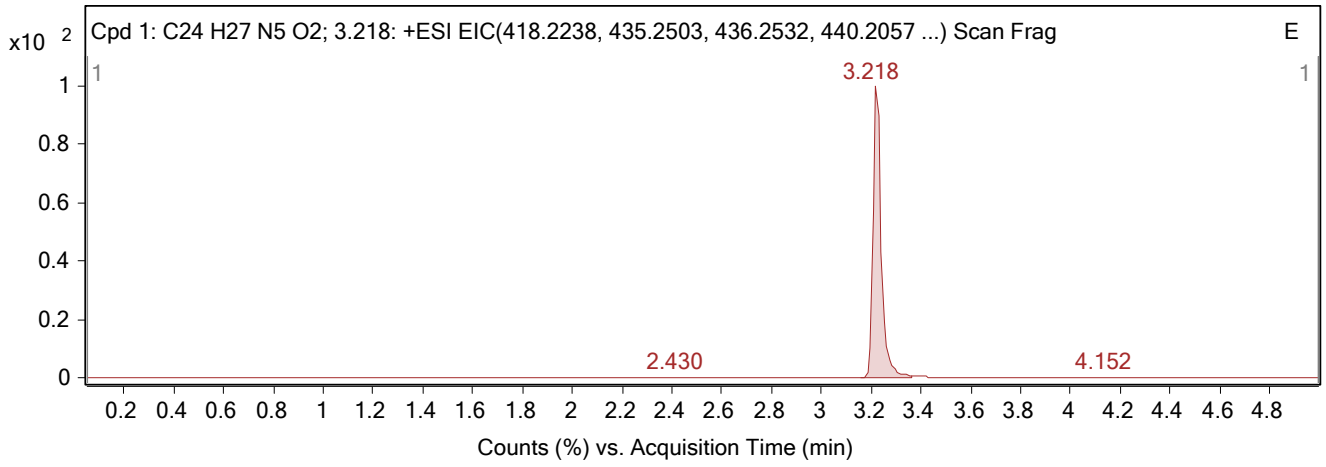
Data File	28.d	**Sample Name**	H2977006
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:17:56 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H27N5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:17:56 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

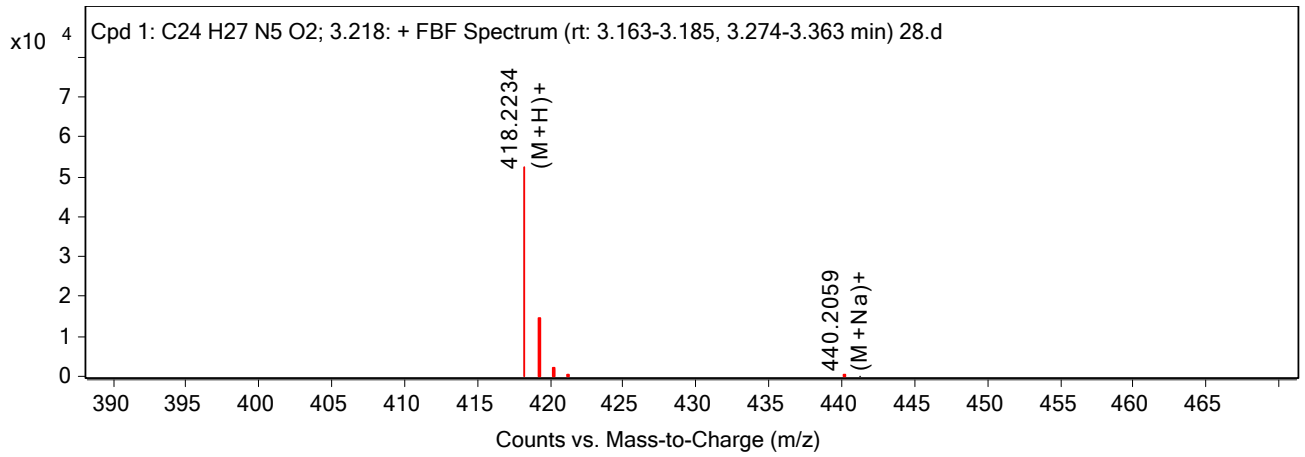
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H27 N5 O2; 3.218	95.35	-0.62	C24 H27 N5 O2	3.218	417.2165	417.2162

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
418.2234	3.218	417.2162	C24 H27 N5 O2	417.2165	-0.62	Find By Formula	

Compound Chromatograms



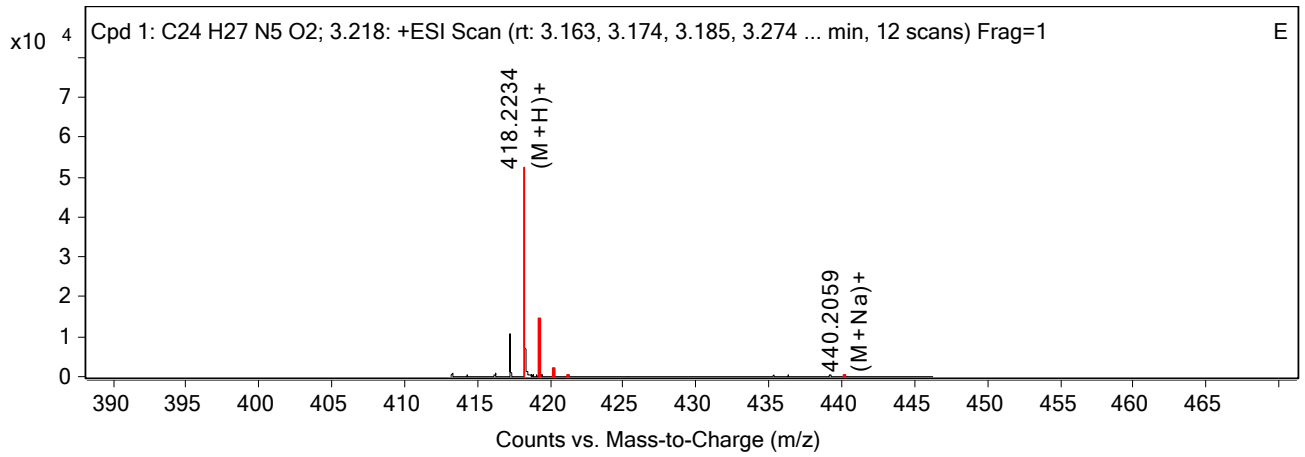
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
418.2234	1	52399.58	(M+H)+
419.2266	1	12055.75	(M+H)+
420.2296	1	1757.9	(M+H)+
421.235	1	256.69	(M+H)+
440.2059	1	345.36	(M+Na)+
441.2142	1	118.75	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
418.2234	1	52399.58	(M+H)+	0.79
418.2234		52399.58		
419.2266	1	12055.75	(M+H)+	0.32
420.2296	1	1757.9	(M+H)+	-0.14
421.235	1	256.69	(M+H)+	-6.54
440.2059	1	345.36	(M+Na)+	-0.49
441.2142	1	118.75	(M+Na)+	-12.52

--- End Of Report ---

Target Compound Screening Report

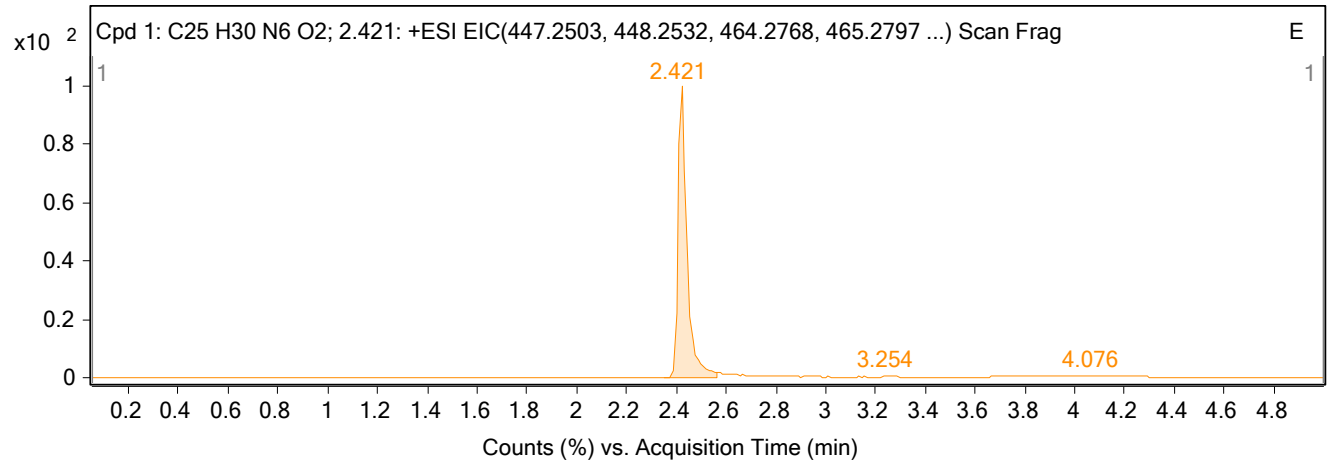
Data File	10.d	**Sample Name**	H2980296
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 7:43:52 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H30N6O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 7:43:52 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

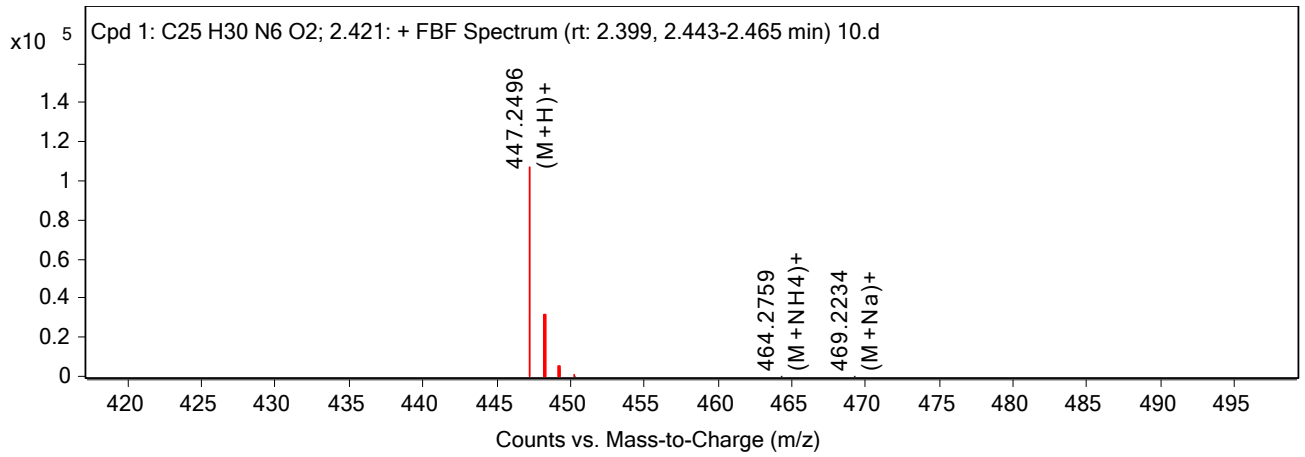
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H30 N6 O2; 2.421	94.39	-1.65	C25 H30 N6 O2	2.421	446.243	446.2423

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2496	2.421	446.2423	C25 H30 N6 O2	446.243	-1.65	Find By Formula	

Compound Chromatograms



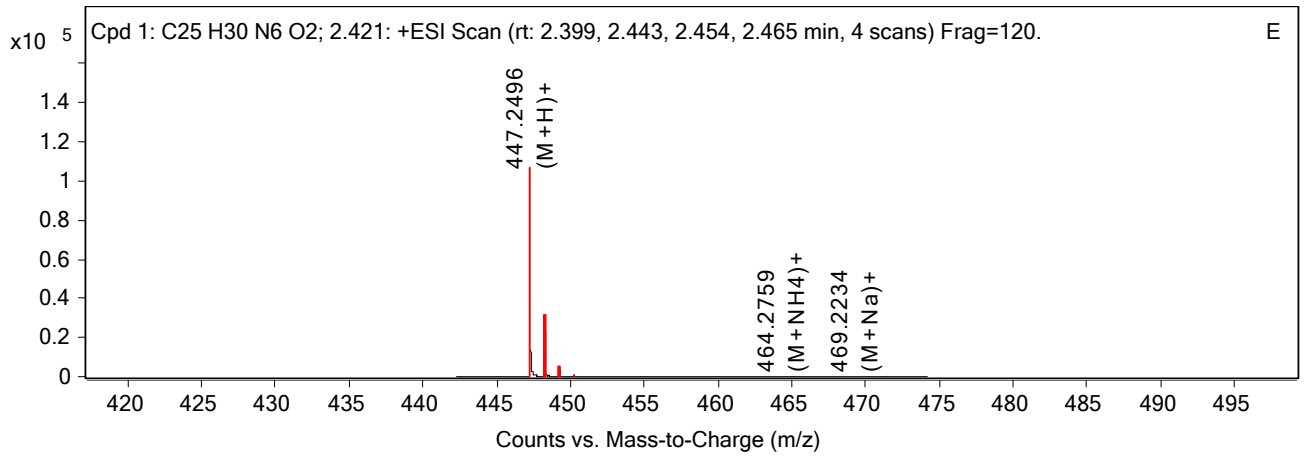
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2496	1	106848.6	(M+H)+
448.2525	1	25685.4	(M+H)+
449.2547	1	3613.69	(M+H)+
450.2597	1	449.02	(M+H)+
464.2759	1	55.67	(M+NH4)+
469.2234	1	97.72	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2496	1	106848.6	(M+H)+	1.59
447.2496		106848.6		
448.2525	1	25685.4	(M+H)+	1.68
449.2547	1	3613.69	(M+H)+	2.93
450.2597	1	449.02	(M+H)+	-2.32
464.2759	1	55.67	(M+NH4)+	1.95
469.2234	1	97.72	(M+Na)+	18.79

--- End Of Report ---

Target Compound Screening Report

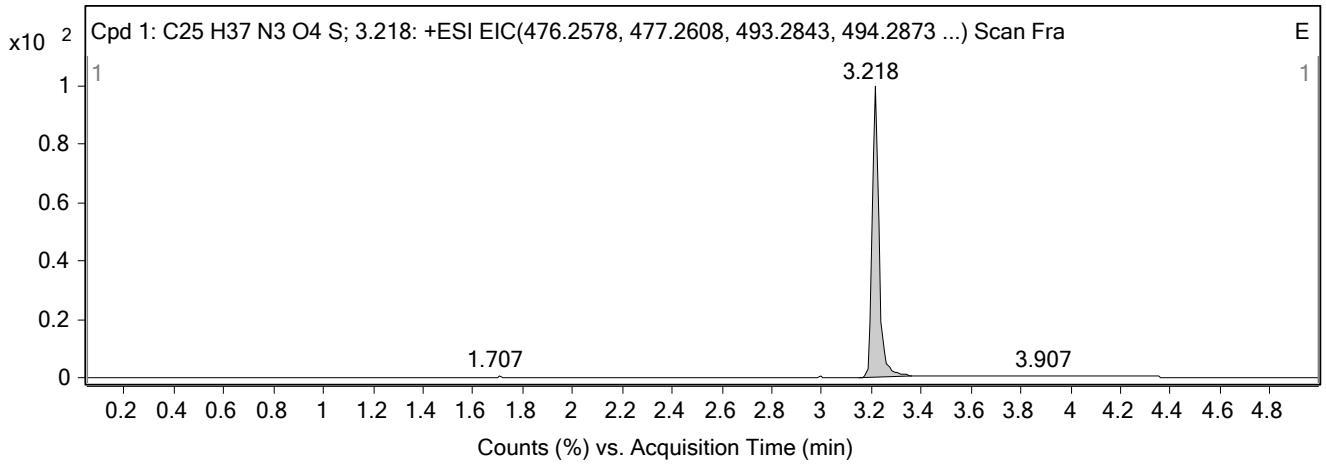
Data File	2-3.d	**Sample Name**	H2980680
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:12:53 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H37N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:12:53 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

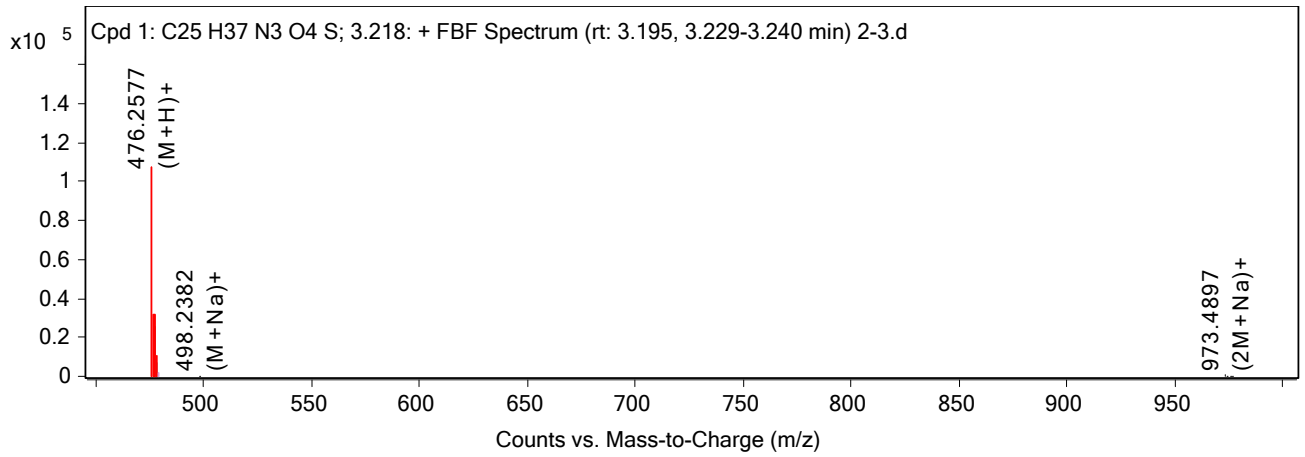
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H37 N3 O4 S; 3.218	94.16	-0.27	C25 H37 N3 O4 S	3.218	475.2505	475.2504

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
476.2577	3.218	475.2504	C25 H37 N3 O4 S	475.2505	-0.27	Find By Formula	

Compound Chromatograms



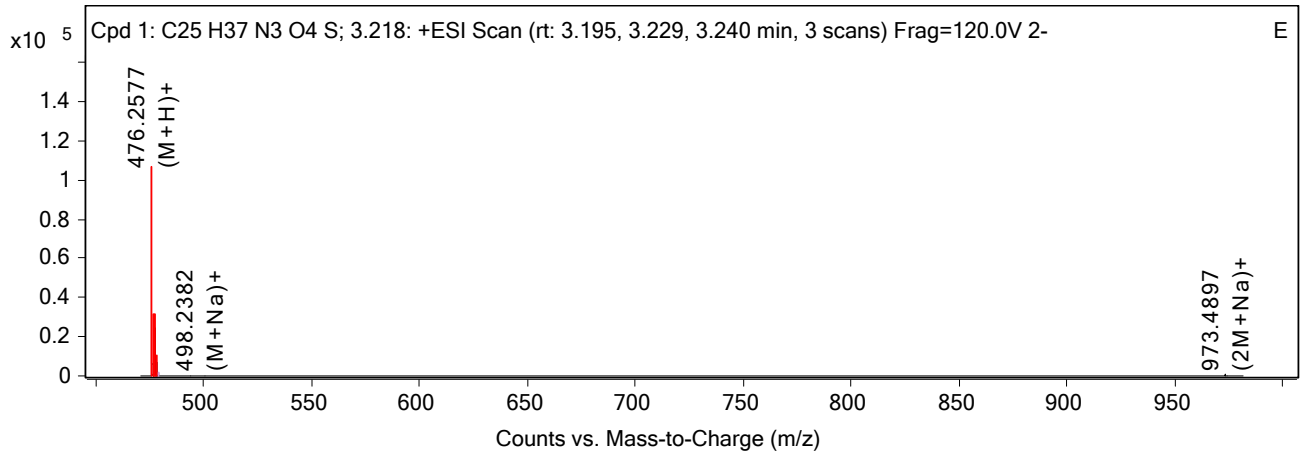
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
476.2577	1	107156.63	(M+H)+
477.2607	1	25236.92	(M+H)+
478.2574	1	7331.12	(M+H)+
498.2382	1	421	(M+Na)+
973.4897	1	593.72	(2M+Na)+
974.4931	1	361.82	(2M+Na)+
975.4877	1	216.34	(2M+Na)+
976.4883	1	78.12	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
476.2577	1	107156.63	(M+H)+	0.05
476.2577		107156.63		
477.2607	1	25236.92	(M+H)+	0.2
478.2574	1	7331.12	(M+H)+	3.02
498.2382	1	421	(M+Na)+	3.03
973.4897	1	593.72	(2M+Na)+	0.49
974.4931	1	361.82	(2M+Na)+	0.12
975.4877	1	216.34	(2M+Na)+	5.29
976.4883	1	78.12	(2M+Na)+	5.34

--- End Of Report ---

Target Compound Screening Report

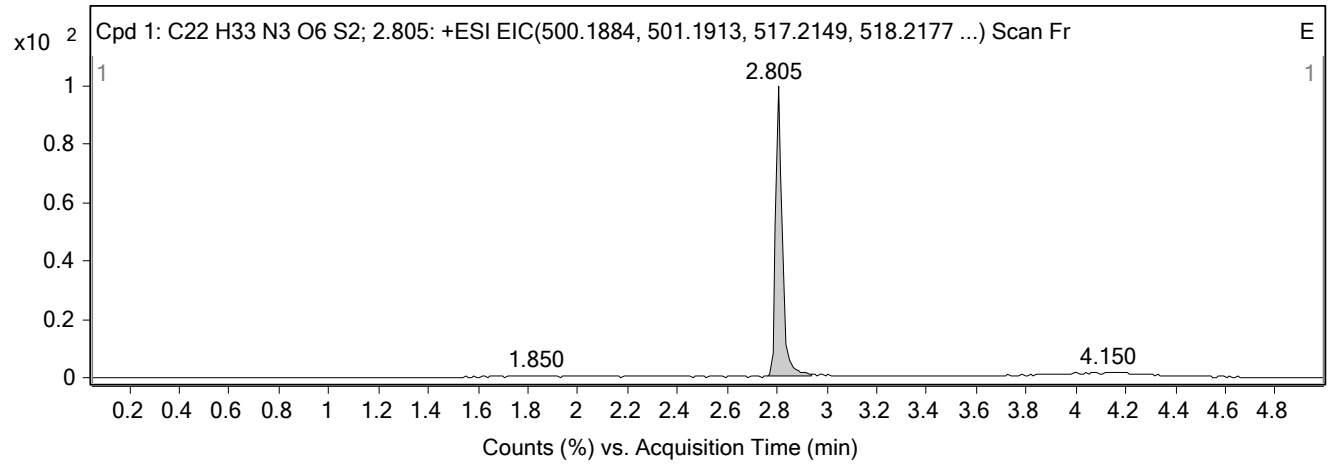
Data File	7-2.d	**Sample Name**	H2980682
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:43:32 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:43:32 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O6 S2; 2.805	94.93	-2.01	C22 H33 N3 O6 S2	2.805	499.1811	499.1801

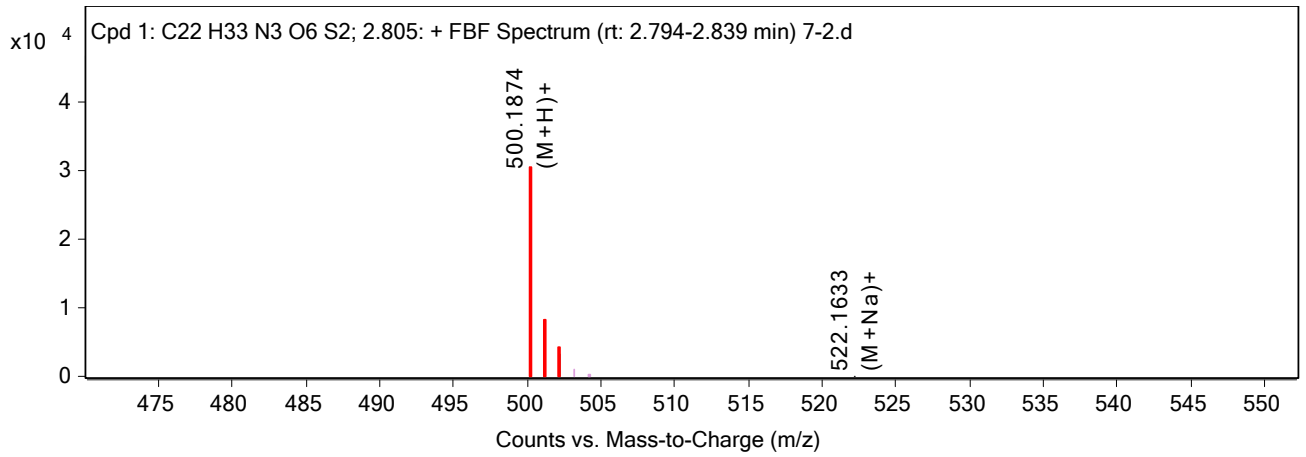
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.1874	2.805	499.1801	C22 H33 N3 O6 S2	499.1811	-2.01	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

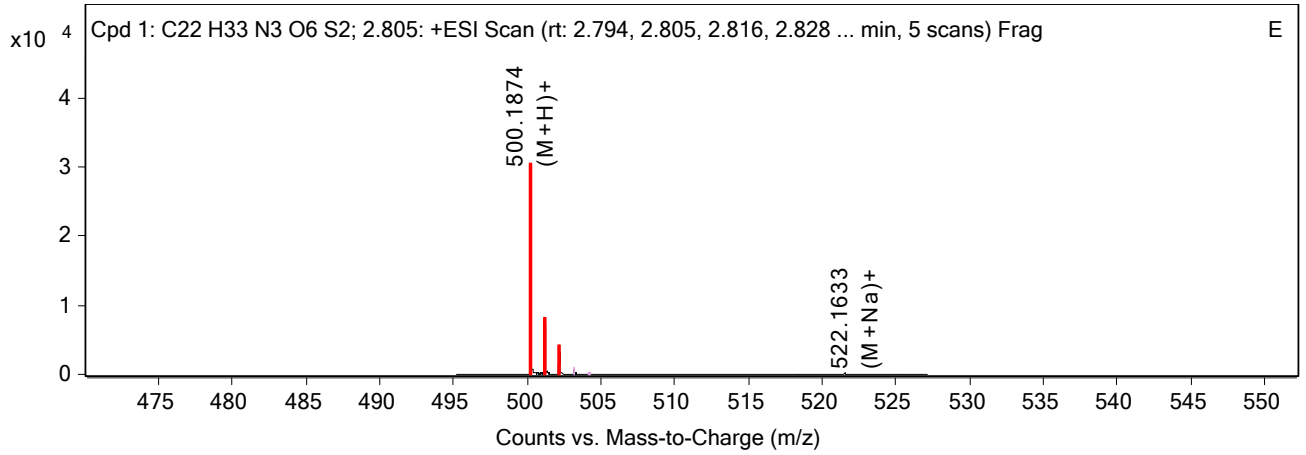
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.1874	1	30444.02	(M+H)+
501.1904	1	7132.11	(M+H)+
502.1861	1	3246.71	(M+H)+
522.1633	1	76.33	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.1874	1	30444.02	(M+H)+	1.98
501.1904	1	7132.11	(M+H)+	1.64
502.1861	1	3246.71	(M+H)+	2.72
522.1633	1	76.33	(M+Na)+	13.33

--- End Of Report ---

Target Compound Screening Report

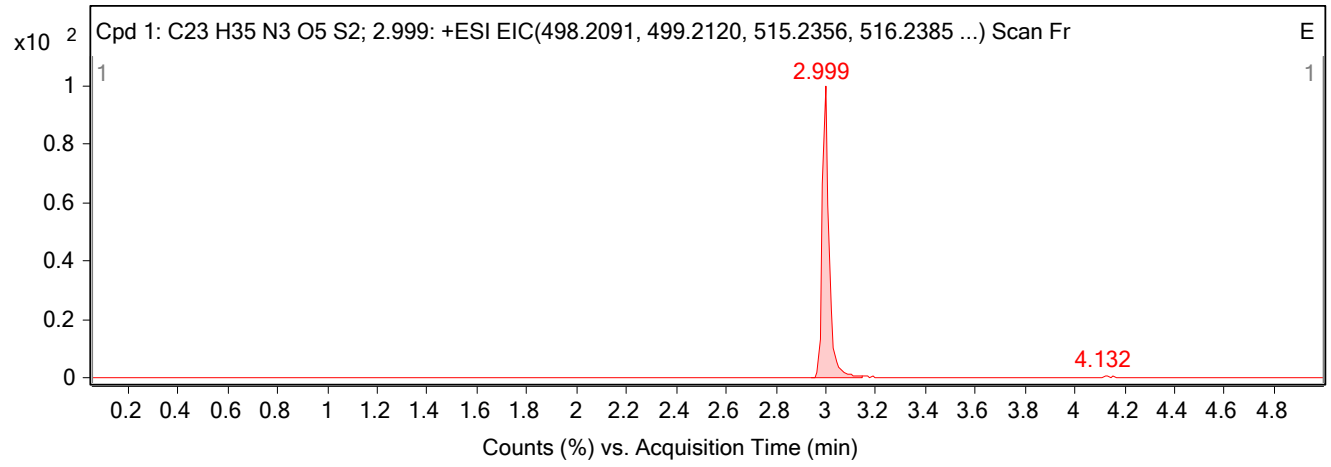
Data File	41.d	**Sample Name**	H2975461
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:56:49 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H35N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:56:49 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H35 N3 O5 S2; 2.999	93.55	-1.69	C23 H35 N3 O5 S2	2.999	497.2018	497.201

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
498.2083	2.999	497.201	C23 H35 N3 O5 S2	497.2018	-1.69	Find By Formula	

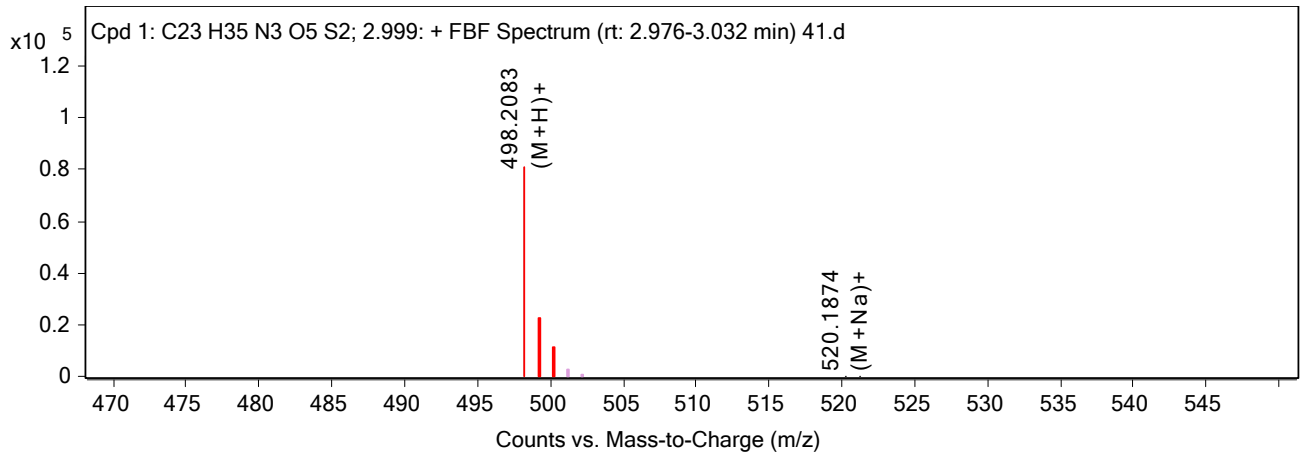
Compound Chromatograms



MS Zoomed Spectrum

Agilent Technologies

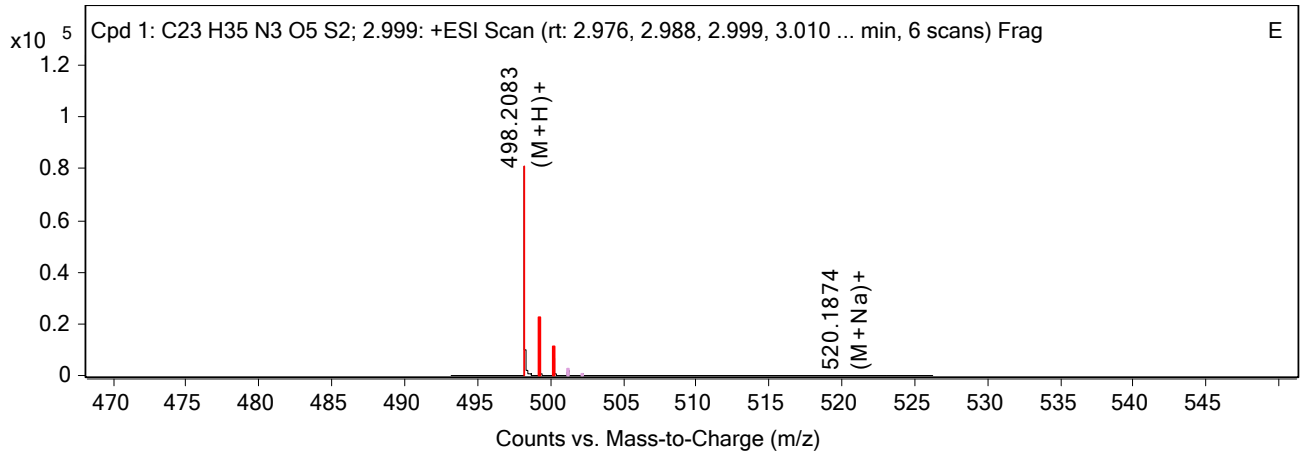
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
498.2083	1	80827.17	(M+H)+
499.2113	1	18751.76	(M+H)+
500.2069	1	8079.76	(M+H)+
520.1874	1	135.68	(M+Na)+
521.2053	1	51.07	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
498.2083	1	80827.17	(M+H)+	1.65
499.2113	1	18751.76	(M+H)+	1.37
500.2069	1	8079.76	(M+H)+	2.83
520.1874	1	135.68	(M+Na)+	7.02
521.2053	1	51.07	(M+Na)+	-21.83

--- End Of Report ---

Target Compound Screening Report

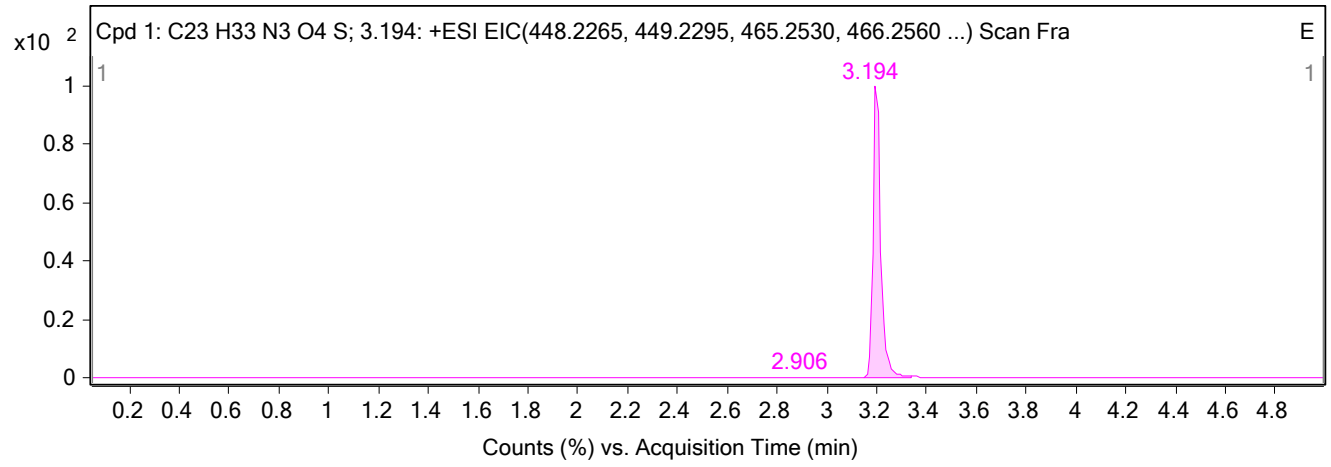
Data File	32.d	**Sample Name**	H2975746
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:40:09 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H33N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:40:09 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

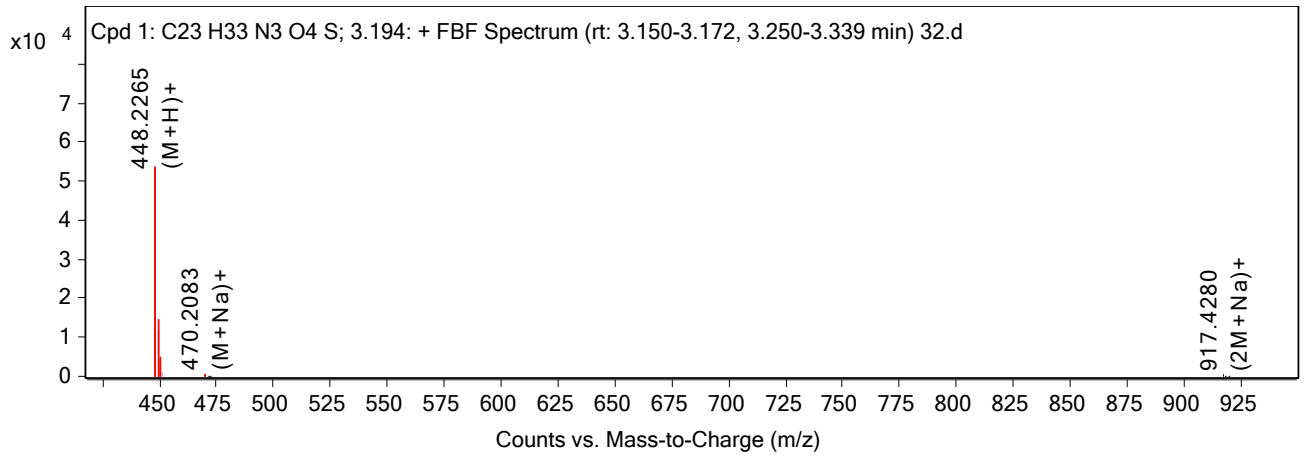
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H33 N3 O4 S; 3.194	95.71	0.05	C23 H33 N3 O4 S	3.194	447.2192	447.2192

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
448.2265	3.194	447.2192	C23 H33 N3 O4 S	447.2192	0.05	Find By Formula	

Compound Chromatograms



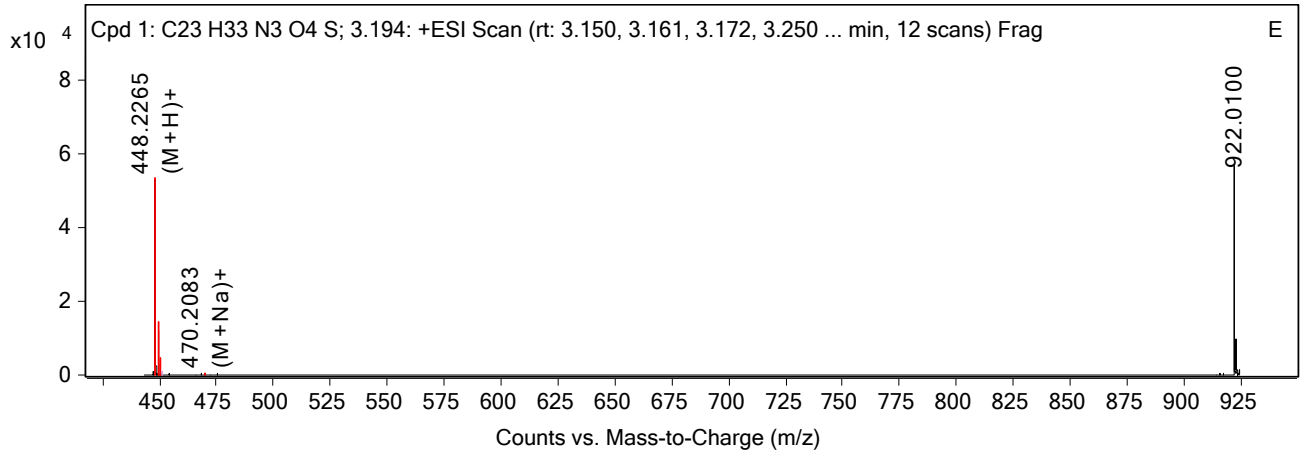
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
448.2265	1	53485.56	(M+H)+
449.2297	1	12059.64	(M+H)+
450.227	1	3421.13	(M+H)+
470.2083	1	490.2	(M+Na)+
471.2135	1	161.3	(M+Na)+
472.2058	1	66.25	(M+Na)+
917.428	1	326.45	(2M+Na)+
918.4279	1	179.22	(2M+Na)+
919.4261	1	97.73	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
448.2265	1	53485.56	(M+H)+	-0.01
449.2297	1	12059.64	(M+H)+	-0.45
450.227	1	3421.13	(M+H)+	0.3
470.2083	1	490.2	(M+Na)+	0.17
471.2135	1	161.3	(M+Na)+	-4.34
472.2058	1	66.25	(M+Na)+	7.06
917.428	1	326.45	(2M+Na)+	-0.41
918.4279	1	179.22	(2M+Na)+	2.95
919.4261	1	97.73	(2M+Na)+	4.13
922.01		57476.34		

--- End Of Report ---

Target Compound Screening Report

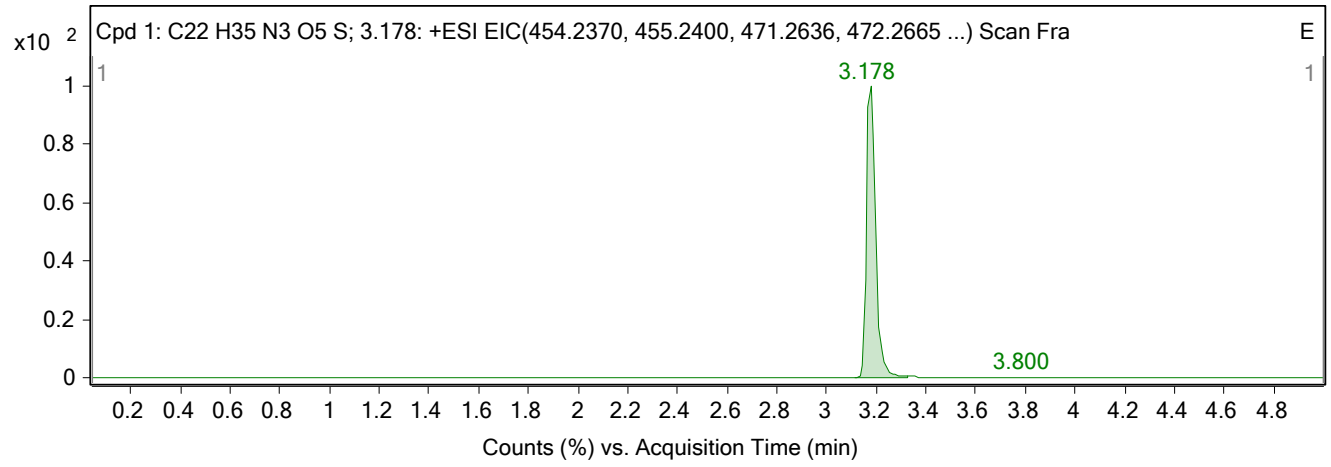
Data File	49.d	**Sample Name**	H2975884
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:14:33 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H35N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:14:33 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

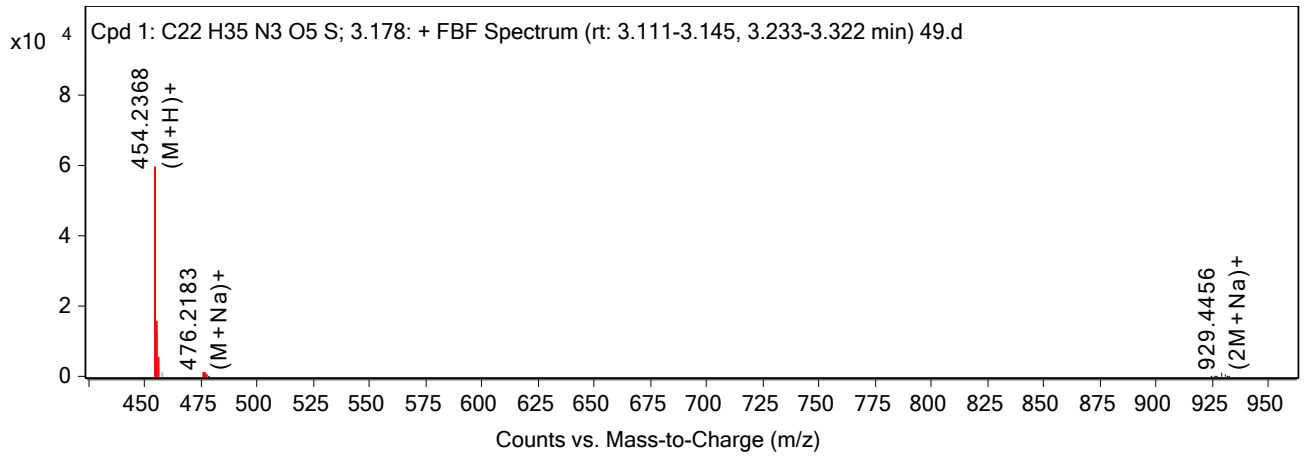
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H35 N3 O5 S; 3.178	95.71	-0.56	C22 H35 N3 O5 S	3.178	453.2297	453.2295

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
454.2368	3.178	453.2295	C22 H35 N3 O5 S	453.2297	-0.56	Find By Formula	

Compound Chromatograms



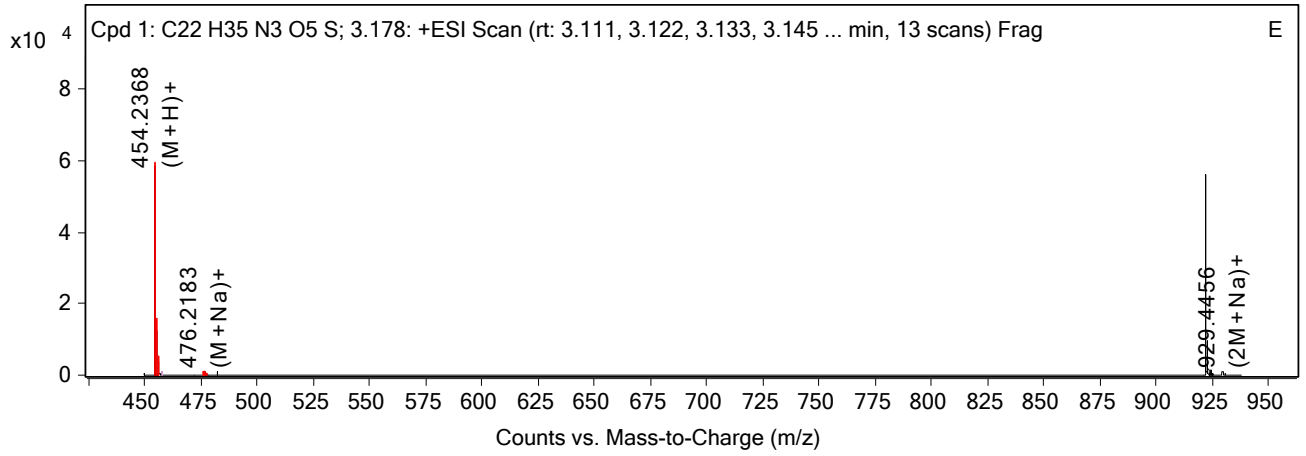
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
454.2368	1	59559.87	(M+H)+
455.2398	1	12940.12	(M+H)+
456.2371	1	3714.34	(M+H)+
476.2183	1	937.71	(M+Na)+
477.2253	1	279.42	(M+Na)+
924.4896	1	205.17	(2M+NH4)+
925.5076	1	144.6	(2M+NH4)+
929.4456	1	952.87	(2M+Na)+
930.4483	1	483.57	(2M+Na)+
931.4456	1	255.81	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
454.2368	1	59559.87	(M+H)+	0.43
455.2398	1	12940.12	(M+H)+	0.57
456.2371	1	3714.34	(M+H)+	1.2
476.2183	1	937.71	(M+Na)+	1.39
477.2253	1	279.42	(M+Na)+	-6.9
924.4896	1	205.17	(2M+NH4)+	4.05
925.5076	1	144.6	(2M+NH4)+	-12.24
929.4456	1	952.87	(2M+Na)+	3.32
930.4483	1	483.57	(2M+Na)+	3.72
931.4456	1	255.81	(2M+Na)+	5.61

--- End Of Report ---

Target Compound Screening Report

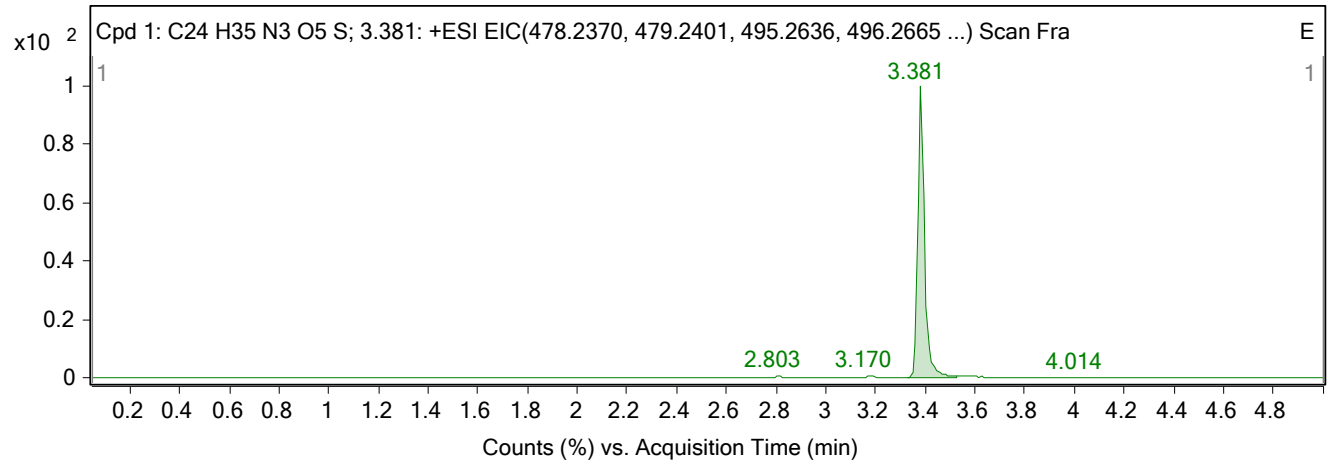
Data File	17.d	**Sample Name**	H2978618
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:47:46 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H35N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:47:46 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

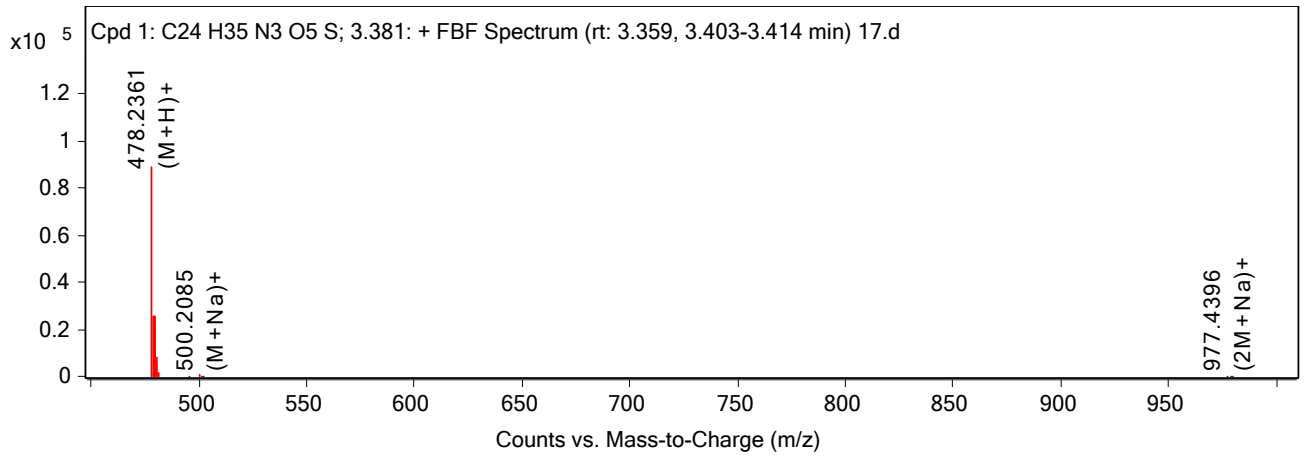
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H35 N3 O5 S; 3.381	94.62	-2.24	C24 H35 N3 O5 S	3.381	477.2297	477.2287

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
478.2361	3.381	477.2287	C24 H35 N3 O5 S	477.2297	-2.24	Find By Formula	

Compound Chromatograms



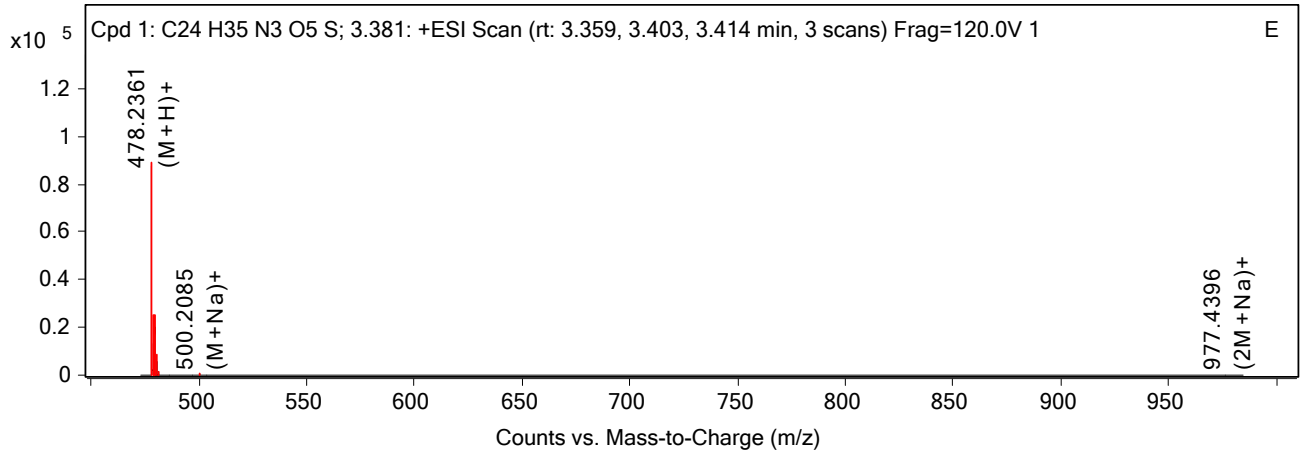
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
478.2361	1	88689.67	(M+H)+
479.2389	1	20597.17	(M+H)+
480.2368	1	6105.07	(M+H)+
481.2393	1	1207.81	(M+H)+
495.2572	1	82.39	(M+NH4)+
500.2085	1	465.48	(M+Na)+
501.2184	1	163.59	(M+Na)+
502.2081	1	111.49	(M+Na)+
977.4396	1	194.1	(2M+Na)+
978.4271	1	121.06	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
478.2361	1	88689.67	(M+H)+	1.93
479.2389	1	20597.17	(M+H)+	2.44
480.2368	1	6105.07	(M+H)+	2.57
481.2393	1	1207.81	(M+H)+	-0.39
495.2572	1	82.39	(M+NH4)+	12.76
500.2085	1	465.48	(M+Na)+	20.89
501.2184	1	163.59	(M+Na)+	7.27
502.2081	1	111.49	(M+Na)+	23.65
977.4396	1	194.1	(2M+Na)+	9.27
978.4271	1	121.06	(2M+Na)+	25.15

--- End Of Report ---

Target Compound Screening Report

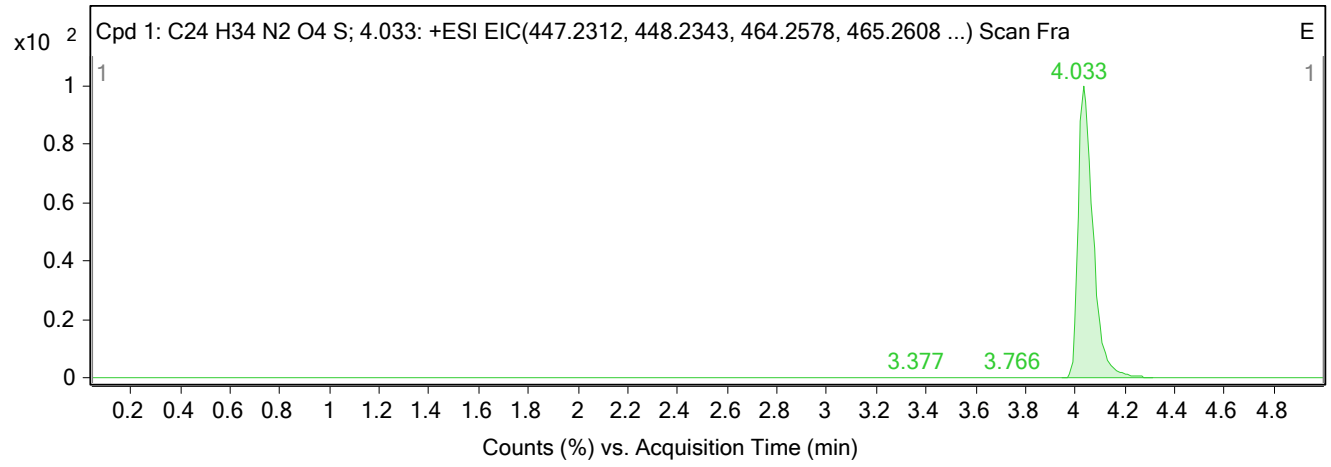
Data File	18.d	**Sample Name**	H2975412
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 12:51:02 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H34N2O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 12:51:02 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

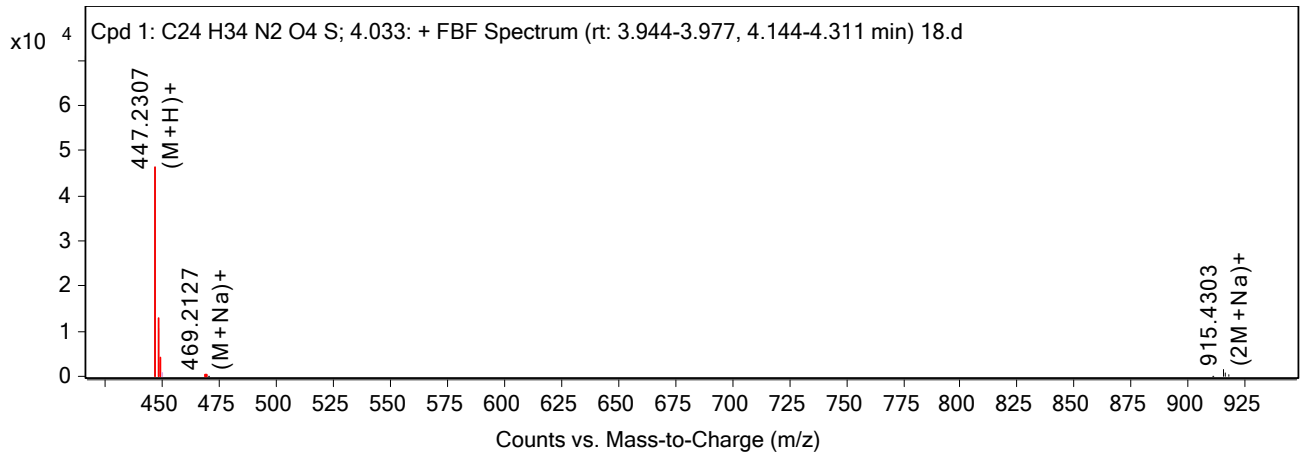
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H34 N2 O4 S; 4.033	95.83	-1.61	C24 H34 N2 O4 S	4.033	446.2239	446.2232

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
447.2307	4.033	446.2232	C24 H34 N2 O4 S	446.2239	-1.61	Find By Formula	

Compound Chromatograms



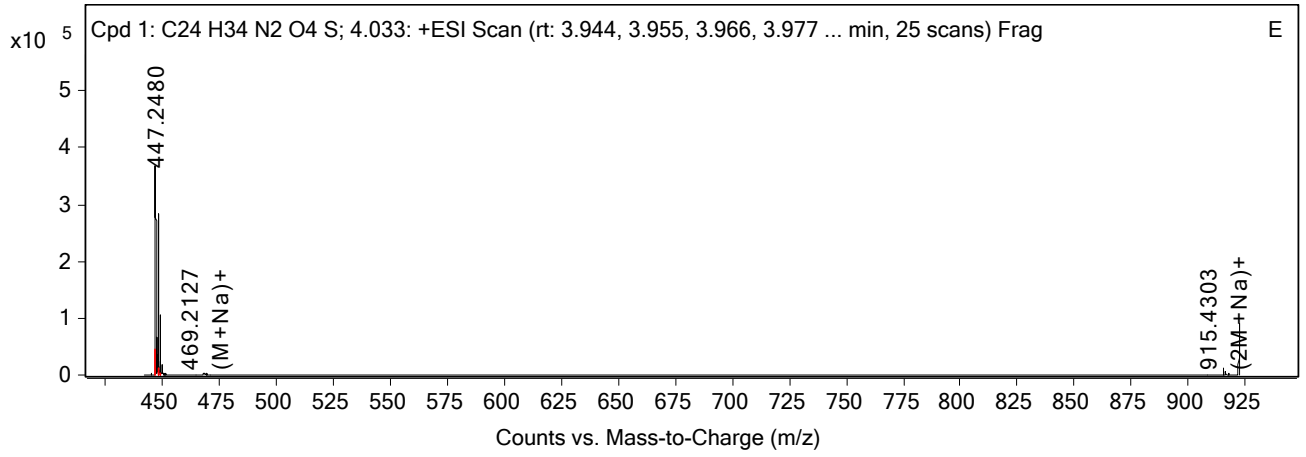
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
447.2307	1	46334.3	(M+H)+
448.2338	1	10819.21	(M+H)+
449.2324	1	3232.21	(M+H)+
469.2127	1	504.06	(M+Na)+
470.2174	1	181.63	(M+Na)+
910.4763	1	138.28	(2M+NH4)+
915.4303	1	1436.42	(2M+Na)+
916.4334	1	669.26	(2M+Na)+
917.4325	1	372.45	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
447.2307	1	46334.3	(M+H)+	1.1
447.248		367723.65		
448.2338	1	10819.21	(M+H)+	1.22
449.2324	1	3232.21	(M+H)+	-0.53
469.2127	1	504.06	(M+Na)+	1.05
470.2174	1	181.63	(M+Na)+	-2.4
910.4763	1	138.28	(2M+NH4)+	5.95
915.4303	1	1436.42	(2M+Na)+	7.37
916.4334	1	669.26	(2M+Na)+	7.45
917.4325	1	372.45	(2M+Na)+	7.71

--- End Of Report ---

Target Compound Screening Report

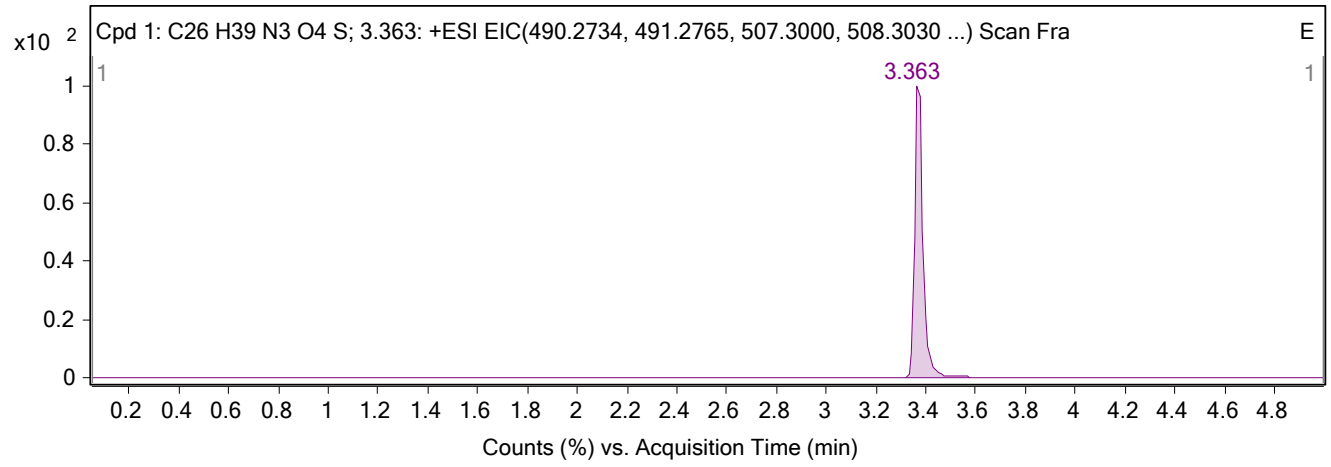
Data File	43.d	**Sample Name**	H2975748
Sample Type	Sample	**Position**	P1-E7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:41:13 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H39N3O4S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:41:13 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

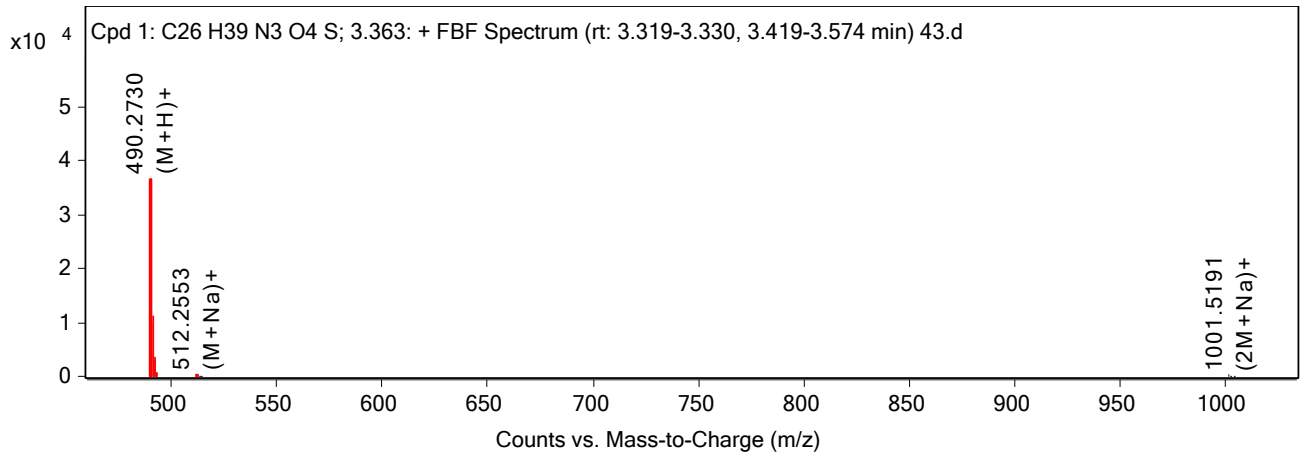
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H39 N3 O4 S; 3.363	97.56	-0.83	C26 H39 N3 O4 S	3.363	489.2661	489.2657

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
490.273	3.363	489.2657	C26 H39 N3 O4 S	489.2661	-0.83	Find By Formula	

Compound Chromatograms



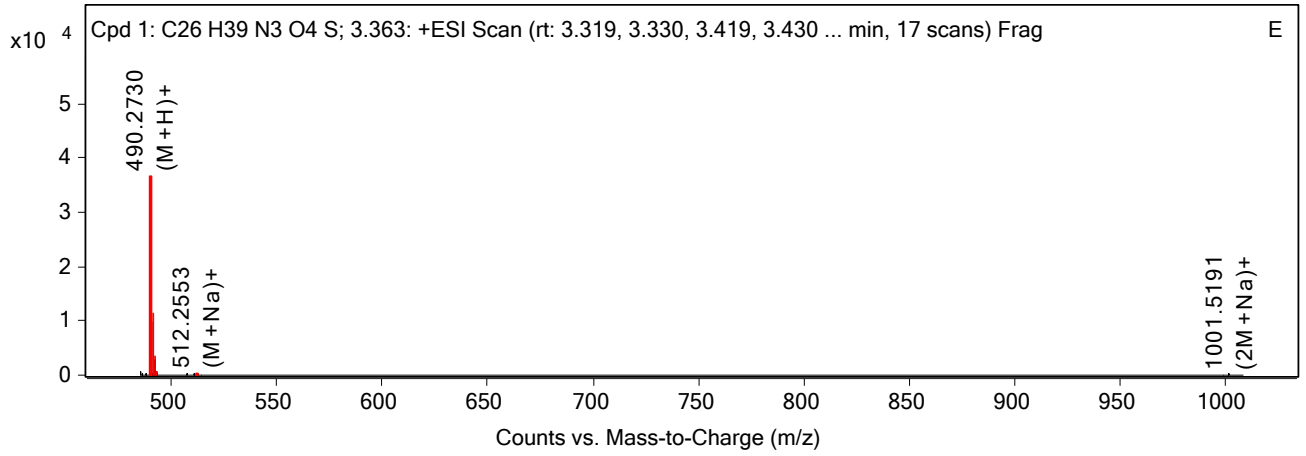
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
490.273	1	36668.31	(M+H)+
491.276	1	9851.04	(M+H)+
492.2742	1	2798.04	(M+H)+
493.2757	1	568.28	(M+H)+
512.2553	1	336	(M+Na)+
513.2621	1	137.9	(M+Na)+
514.2697	1	62.76	(M+Na)+
1001.5191	1	244.91	(2M+Na)+
1002.5223	1	152.96	(2M+Na)+
1003.5219	1	79.04	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
490.273	1	36668.31	(M+H)+	0.83
491.276	1	9851.04	(M+H)+	0.99
492.2742	1	2798.04	(M+H)+	0.93
493.2757	1	568.28	(M+H)+	-0.28
512.2553	1	336	(M+Na)+	0.02
513.2621	1	137.9	(M+Na)+	-7.2
514.2697	1	62.76	(M+Na)+	-25.4
1001.5191	1	244.91	(2M+Na)+	2.37
1002.5223	1	152.96	(2M+Na)+	2.27
1003.5219	1	79.04	(2M+Na)+	2.43

--- End Of Report ---

Target Compound Screening Report

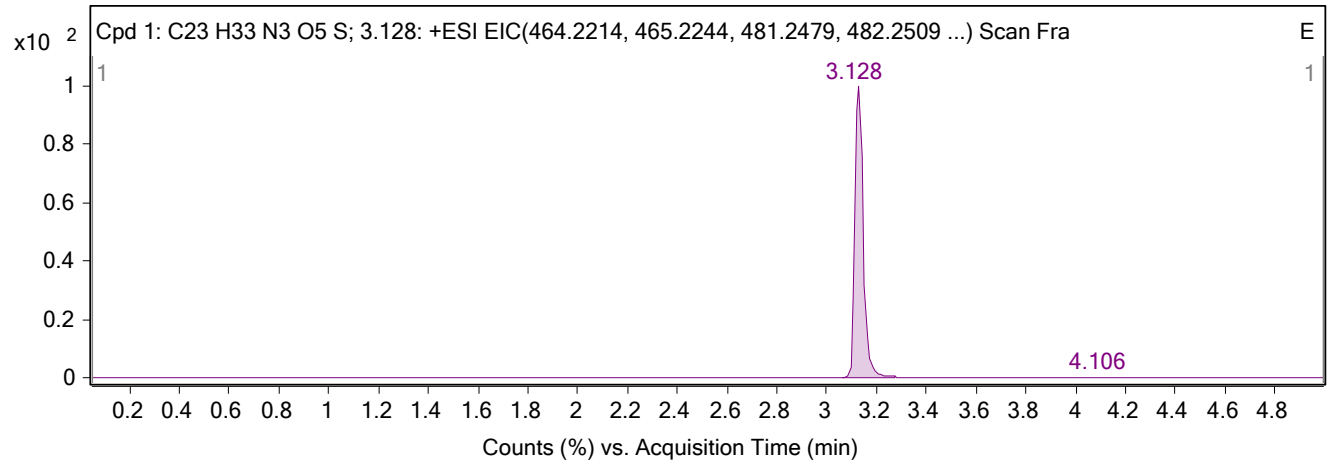
Data File	14.d	**Sample Name**	H2983149
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:00:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H33N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:00:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

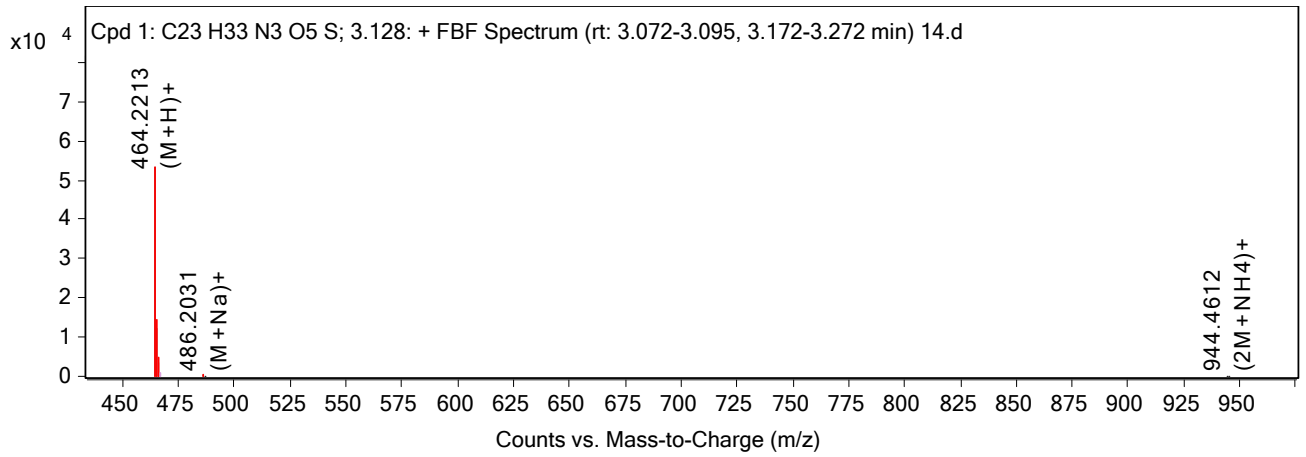
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H33 N3 O5 S; 3.128	96.16	-0.32	C23 H33 N3 O5 S	3.128	463.2141	463.2139

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
464.2213	3.128	463.2139	C23 H33 N3 O5 S	463.2141	-0.32	Find By Formula	

Compound Chromatograms



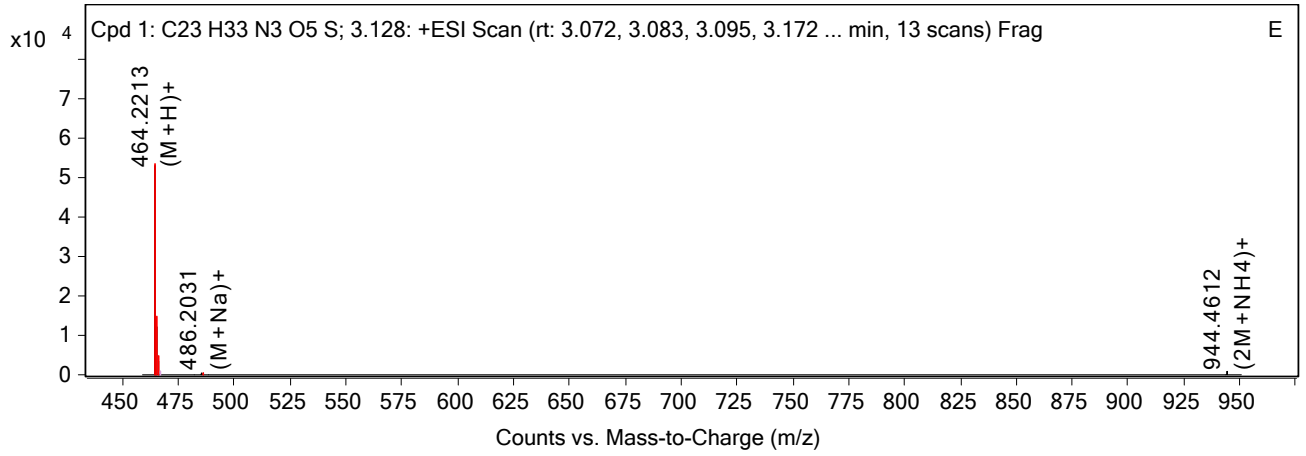
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
464.2213	1	53203.98	(M+H)+
465.2241	1	12226.22	(M+H)+
466.2222	1	3522.03	(M+H)+
486.2031	1	273.43	(M+Na)+
487.2065	1	92.74	(M+Na)+
944.4612	1	83.1	(2M+NH4)+
945.4492	1	60.15	(2M+NH4)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
464.2213	1	53203.98	(M+H)+	0.22
465.2241	1	12226.22	(M+H)+	0.66
466.2222	1	3522.03	(M+H)+	-0.05
486.2031	1	273.43	(M+Na)+	0.46
487.2065	1	92.74	(M+Na)+	-0.3
944.4612	1	83.1	(2M+NH4)+	0.87
945.4492	1	60.15	(2M+NH4)+	16.72

--- End Of Report ---

Target Compound Screening Report

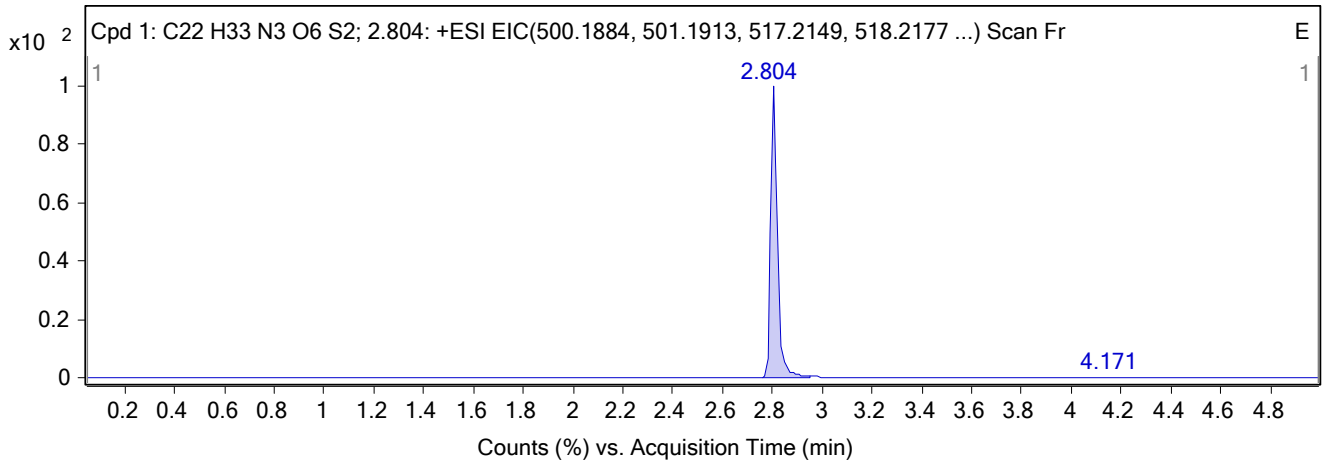
Data File	38.d	**Sample Name**	H2974256
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 10:18:53 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 10:18:53 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

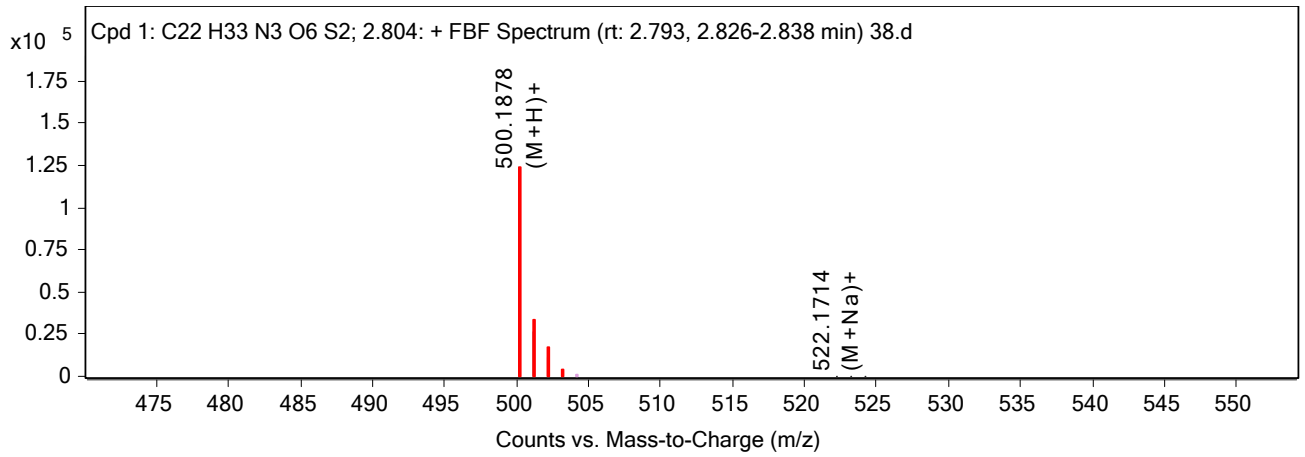
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O6 S2; 2.804	93.69	-1.37	C22 H33 N3 O6 S2	2.804	499.1811	499.1804

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.1878	2.804	499.1804	C22 H33 N3 O6 S2	499.1811	-1.37	Find By Formula	

Compound Chromatograms



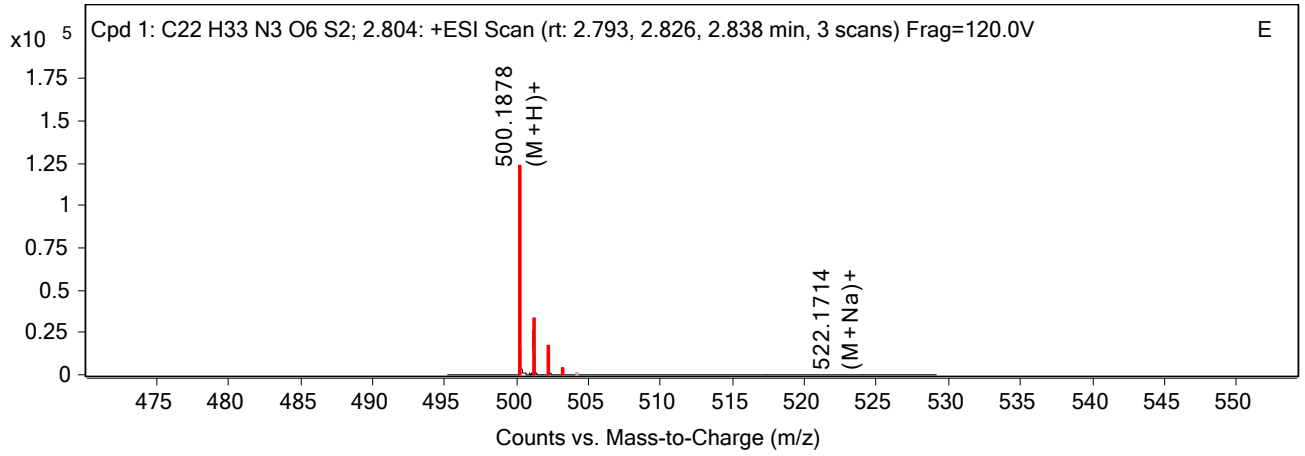
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.1878	1	123840.36	(M+H)+
501.1902	1	26936.81	(M+H)+
502.1871	1	11476.67	(M+H)+
503.1866	1	2343.6	(M+H)+
522.1714	1	209.94	(M+Na)+
523.162	1	60.13	(M+Na)+
524.1746	1	54.33	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.1878	1	123840.36	(M+H)+	1.18
501.1902	1	26936.81	(M+H)+	2.13
502.1871	1	11476.67	(M+H)+	0.87
503.1866	1	2343.6	(M+H)+	5.03
522.1714	1	209.94	(M+Na)+	-2.08
523.162	1	60.13	(M+Na)+	21.34
524.1746	1	54.33	(M+Na)+	-9.93

--- End Of Report ---

Target Compound Screening Report

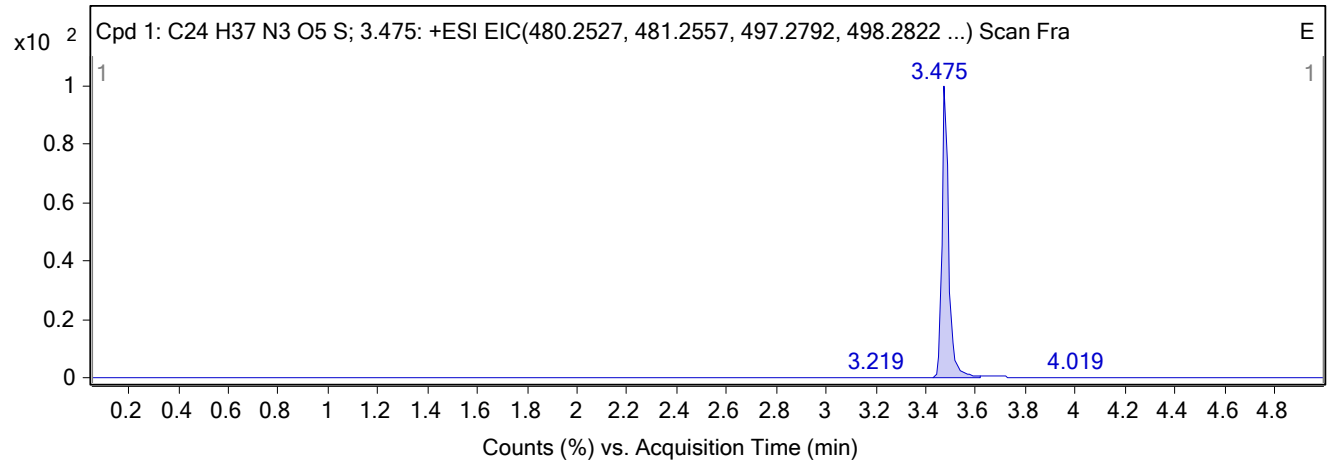
Data File	18.d	**Sample Name**	H2978617
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:53:16 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H37N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:53:16 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

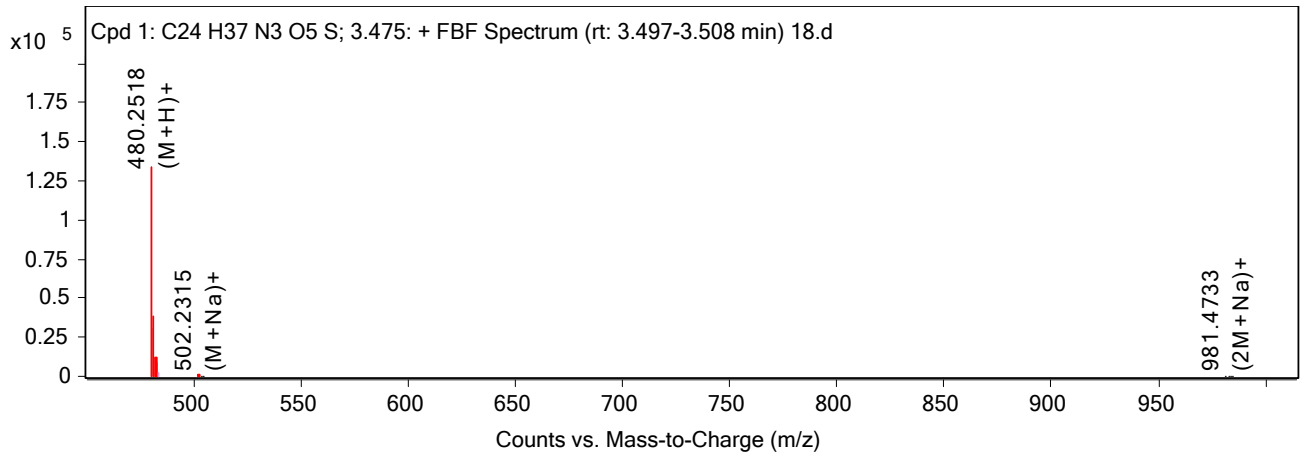
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H37 N3 O5 S; 3.475	93.48	-2.08	C24 H37 N3 O5 S	3.475	479.2454	479.2444

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
480.2518	3.475	479.2444	C24 H37 N3 O5 S	479.2454	-2.08	Find By Formula	

Compound Chromatograms



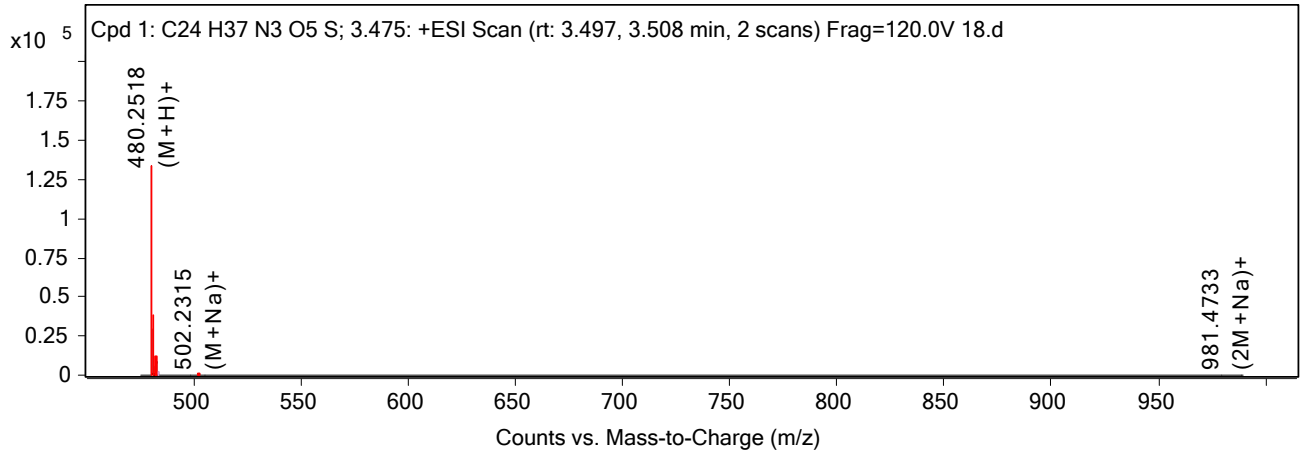
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
480.2518	1	133490.31	(M+H)+
481.2543	1	30563.98	(M+H)+
482.253	1	8695.6	(M+H)+
502.2315	1	735.07	(M+Na)+
503.2363	1	271.08	(M+Na)+
504.2317	1	138.13	(M+Na)+
981.4733	1	356.76	(2M+Na)+
982.4793	1	161.28	(2M+Na)+
983.4922	1	125.2	(2M+Na)+
984.4884	1	50.44	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
480.2518	1	133490.32	(M+H)+	1.89
481.2543	1	30563.98	(M+H)+	2.89
482.253	1	8695.6	(M+H)+	1.37
502.2315	1	735.07	(M+Na)+	6.17
503.2363	1	271.08	(M+Na)+	2.72
504.2317	1	138.13	(M+Na)+	7.66
981.4733	1	356.76	(2M+Na)+	6.79
982.4793	1	161.28	(2M+Na)+	3.83
983.4922	1	125.2	(2M+Na)+	-9.84
984.4884	1	50.44	(2M+Na)+	-5.27

--- End Of Report ---

Target Compound Screening Report

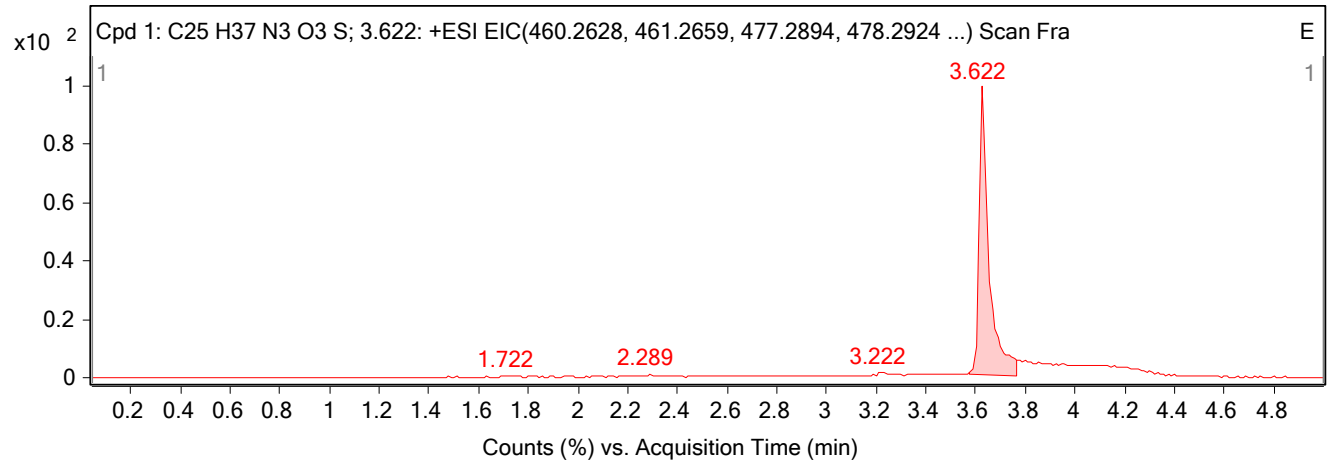
Data File	45-2.d	**Sample Name**	H2975887
Sample Type	Sample	**Position**	P1-E9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 7:09:18 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H37N3O3S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 7:09:18 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

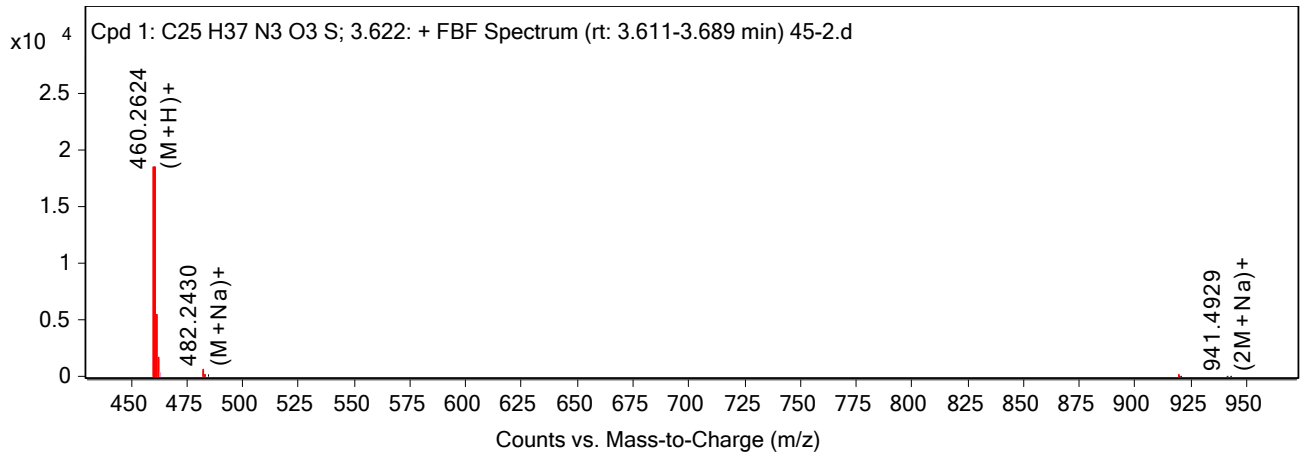
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H37 N3 O3 S; 3.622	95.71	0.38	C25 H37 N3 O3 S	3.622	459.2556	459.2557

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
460.2624	3.622	459.2557	C25 H37 N3 O3 S	459.2556	0.38	Find By Formula	

Compound Chromatograms



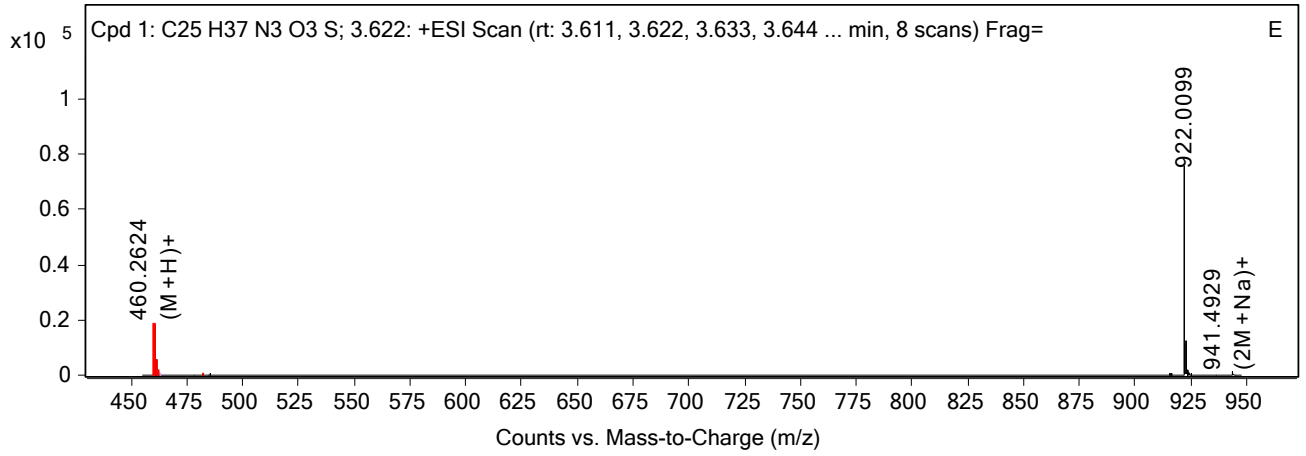
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
460.2624	1	18515.07	(M+H)+
461.2674	1	5413.6	(M+H)+
462.267	1	1583.75	(M+H)+
482.243	1	529.74	(M+Na)+
483.2504	1	221.37	(M+Na)+
484.2488	1	91.77	(M+Na)+
919.5129	1	81.81	(2M+H)+
920.5311	1	56.76	(2M+H)+
941.4929	1	82.33	(2M+Na)+
942.4981	1	46.69	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
460.2624	1	18515.07	(M+H)+	0.91
461.2674	1	5413.6	(M+H)+	-3.32
462.267	1	1583.75	(M+H)+	-6.88
482.243	1	529.74	(M+Na)+	3.65
483.2504	1	221.37	(M+Na)+	-5.28
484.2488	1	91.77	(M+Na)+	-6.21
919.5129	1	81.81	(2M+H)+	5.98
920.5311	1	56.76	(2M+H)+	-10.46
941.4929	1	82.33	(2M+Na)+	7.89
942.4981	1	46.69	(2M+Na)+	5.64

--- End Of Report ---

Target Compound Screening Report

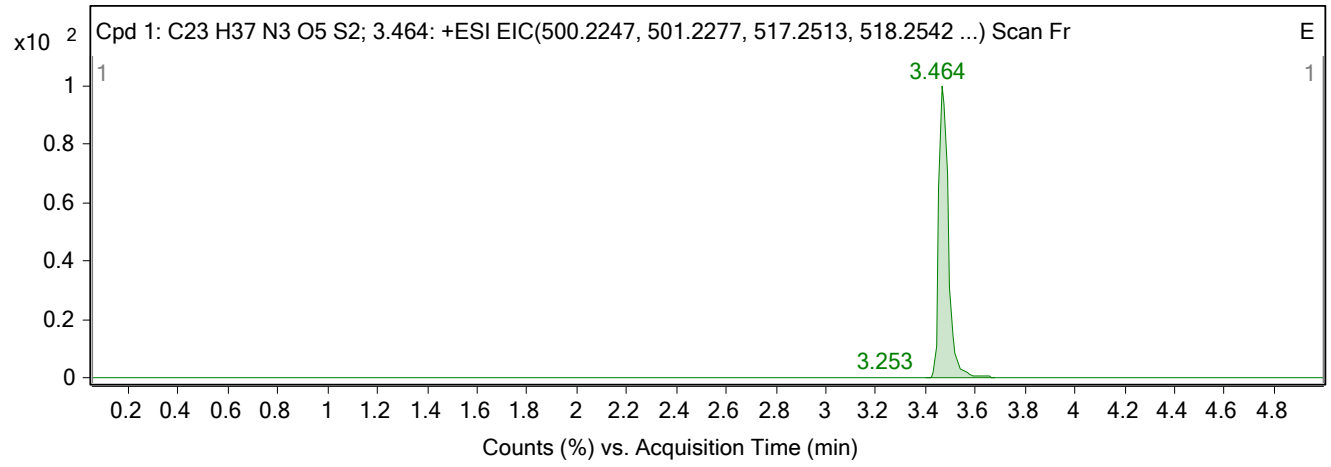
Data File	14.d	**Sample Name**	H2979256
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 12:28:43 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H37N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 12:28:43 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

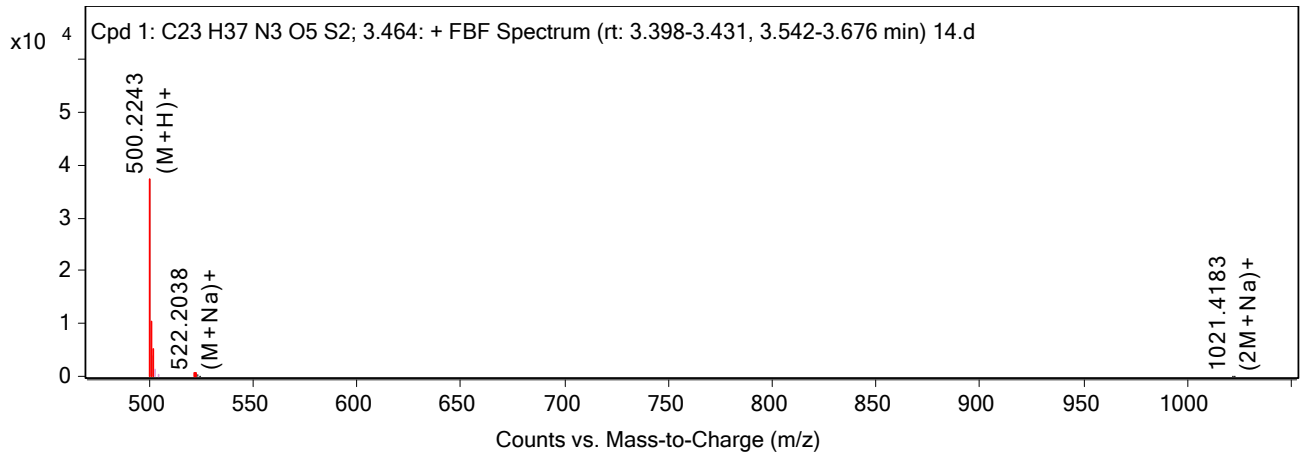
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H37 N3 O5 S2; 3.464	95.11	-1.08	C23 H37 N3 O5 S2	3.464	499.2175	499.2169

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.2243	3.464	499.2169	C23 H37 N3 O5 S2	499.2175	-1.08	Find By Formula	

Compound Chromatograms



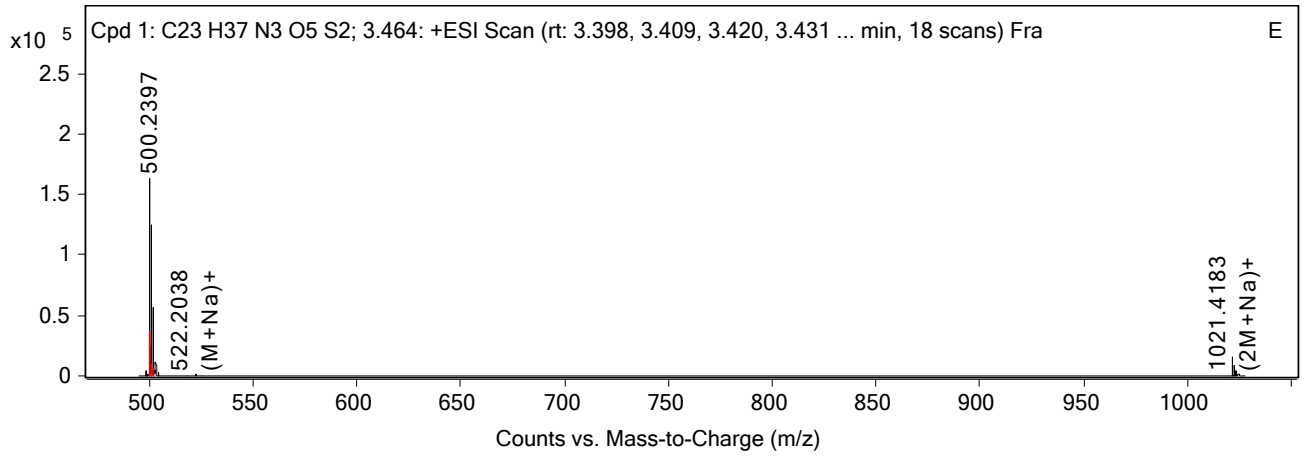
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.2243	1	37452.68	(M+H)+
501.2271	1	9076.02	(M+H)+
502.2229	1	3887.74	(M+H)+
522.2038	1	485.65	(M+Na)+
523.2167	1	187.5	(M+Na)+
524.2092	1	97.48	(M+Na)+
1021.4183	1	134.94	(2M+Na)+
1022.423	1	90.12	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.2243	1	37452.68	(M+H)+	0.94
500.2397		163906.14		
501.2271	1	9076.02	(M+H)+	1.14
502.2229	1	3887.74	(M+H)+	2.07
522.2038	1	485.65	(M+Na)+	5.61
523.2167	1	187.5	(M+Na)+	-13.48
524.2092	1	97.48	(M+Na)+	-6.36
1021.4183	1	134.94	(2M+Na)+	5.73
1022.423	1	90.12	(2M+Na)+	4.01

--- End Of Report ---

Target Compound Screening Report

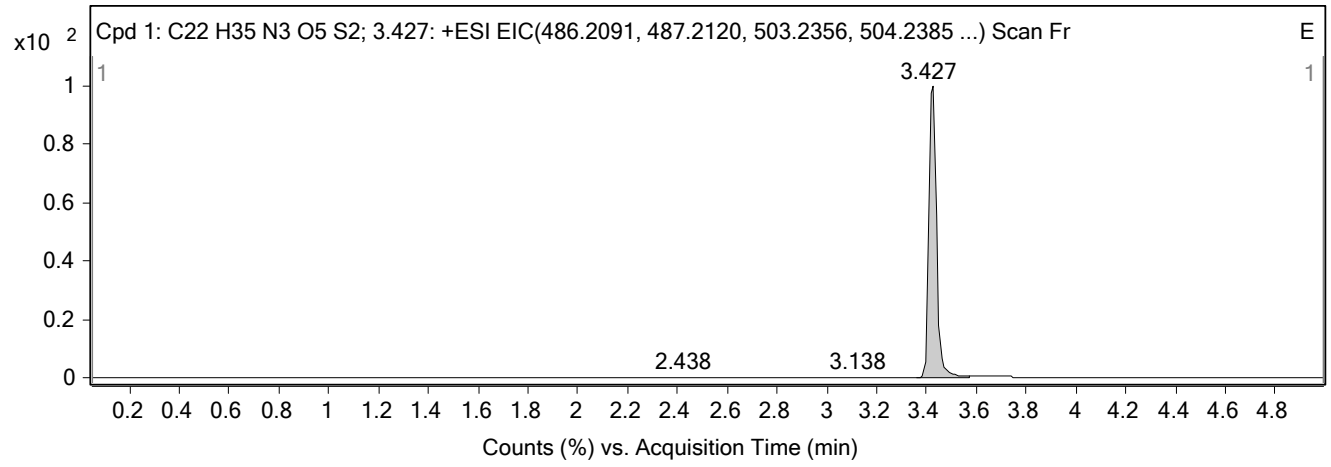
Data File	4.d	**Sample Name**	H3475353
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 4:58:33 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H35N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 4:58:33 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

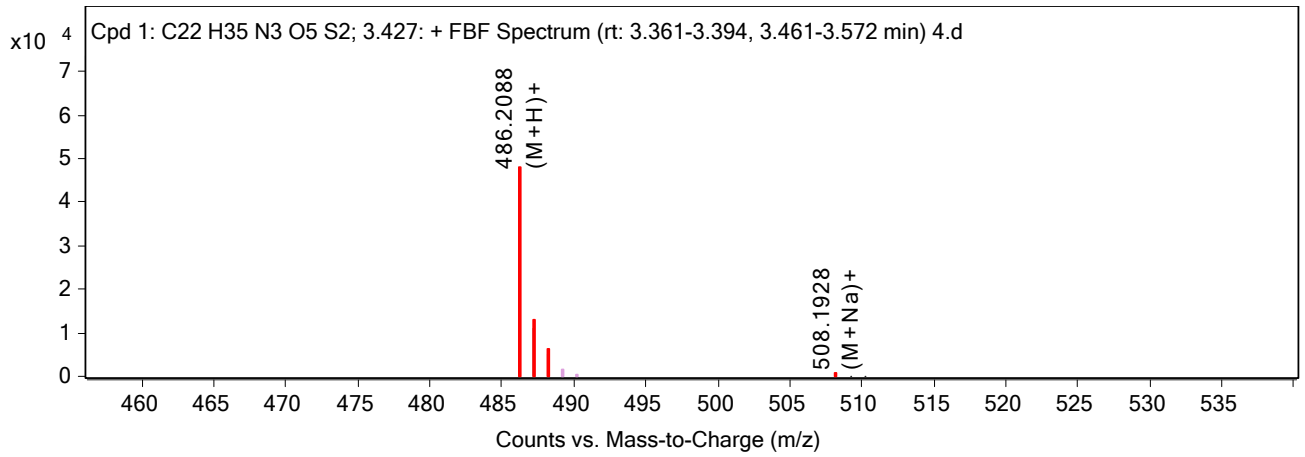
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H35 N3 O5 S2; 3.427	94.49	-0.71	C22 H35 N3 O5 S2	3.427	485.2018	485.2015

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
486.2088	3.427	485.2015	C22 H35 N3 O5 S2	485.2018	-0.71	Find By Formula	

Compound Chromatograms



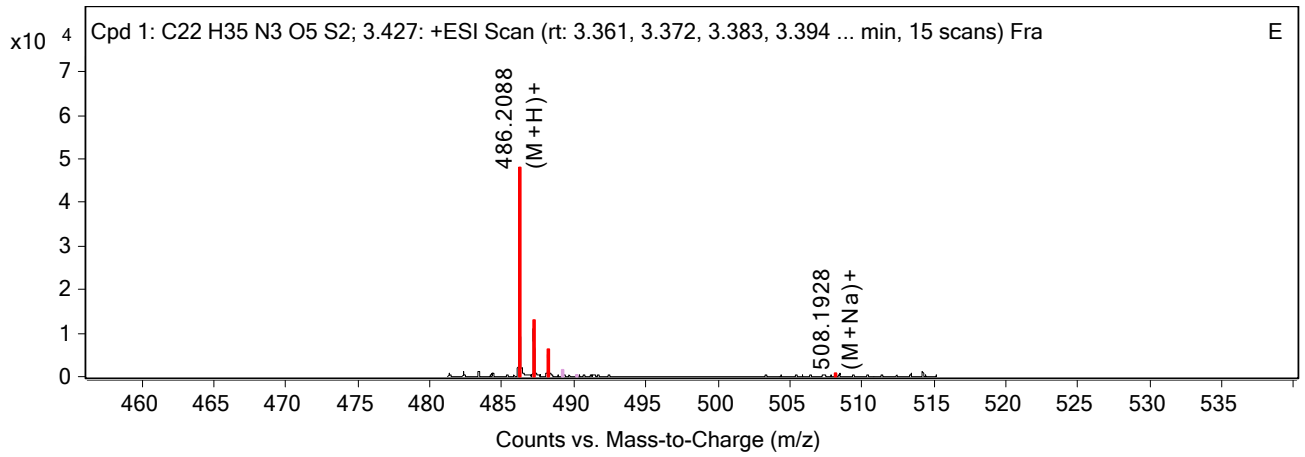
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
486.2088	1	47996.16	(M+H)+
487.2119	1	10956.43	(M+H)+
488.2065	1	5002.01	(M+H)+
508.1928	1	497.22	(M+Na)+
509.1965	1	200.94	(M+Na)+
510.1937	1	153.01	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
486.2088	1	47996.16	(M+H)+	0.63
486.209		47996.16		
487.2119	1	10956.43	(M+H)+	0.3
488.2065	1	5002.01	(M+H)+	3.34
508.1928	1	497.22	(M+Na)+	-3.5
509.1965	1	200.94	(M+Na)+	-4.99
510.1937	1	153.01	(M+Na)+	-7.1

--- End Of Report ---

Target Compound Screening Report

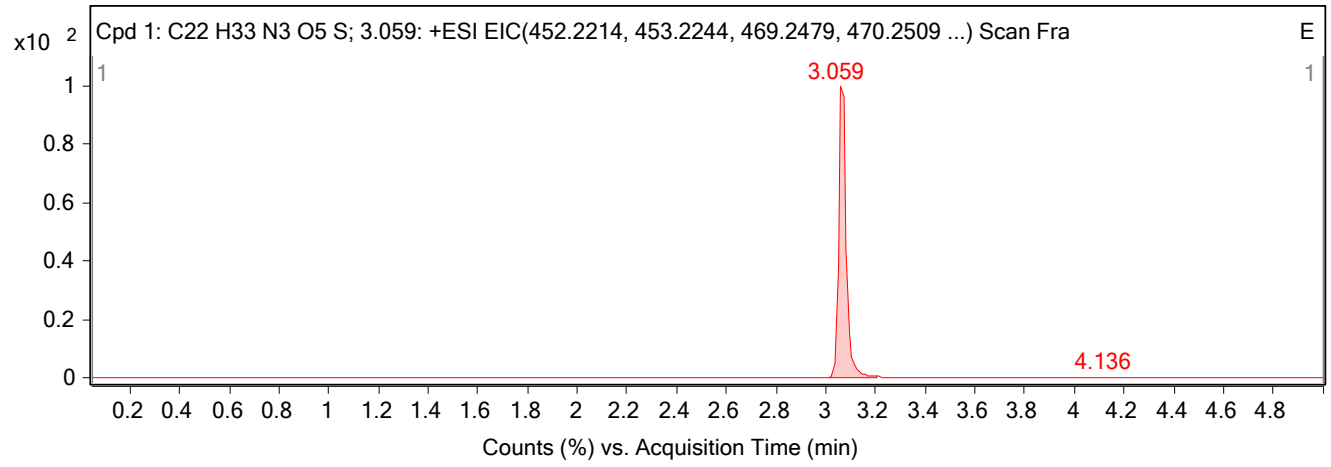
Data File	13.d	**Sample Name**	H2983886
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:23:48 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:23:48 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

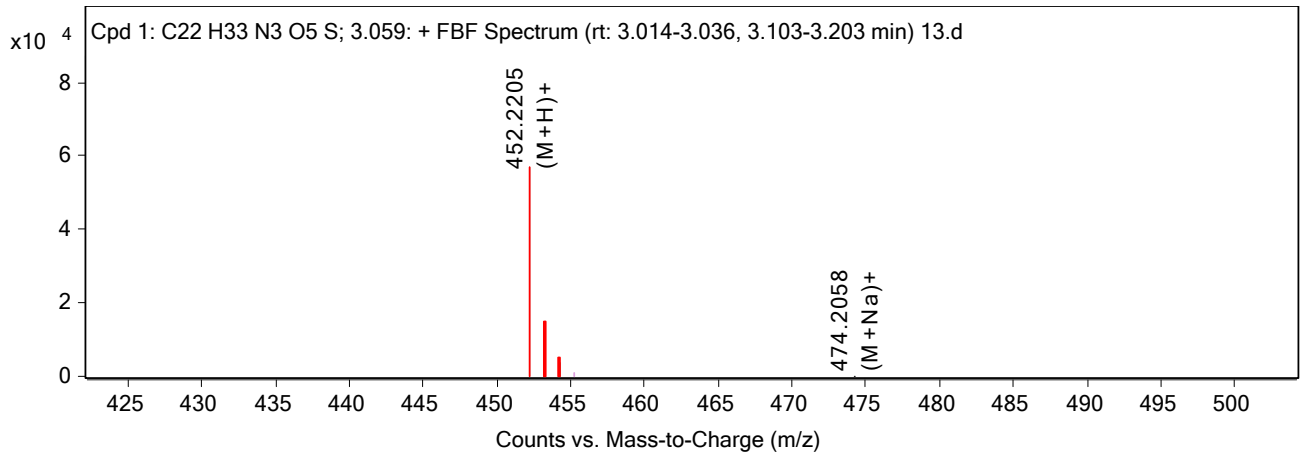
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O5 S; 3.059	94.72	-1.87	C22 H33 N3 O5 S	3.059	451.2141	451.2132

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
452.2205	3.059	451.2132	C22 H33 N3 O5 S	451.2141	-1.87	Find By Formula	

Compound Chromatograms



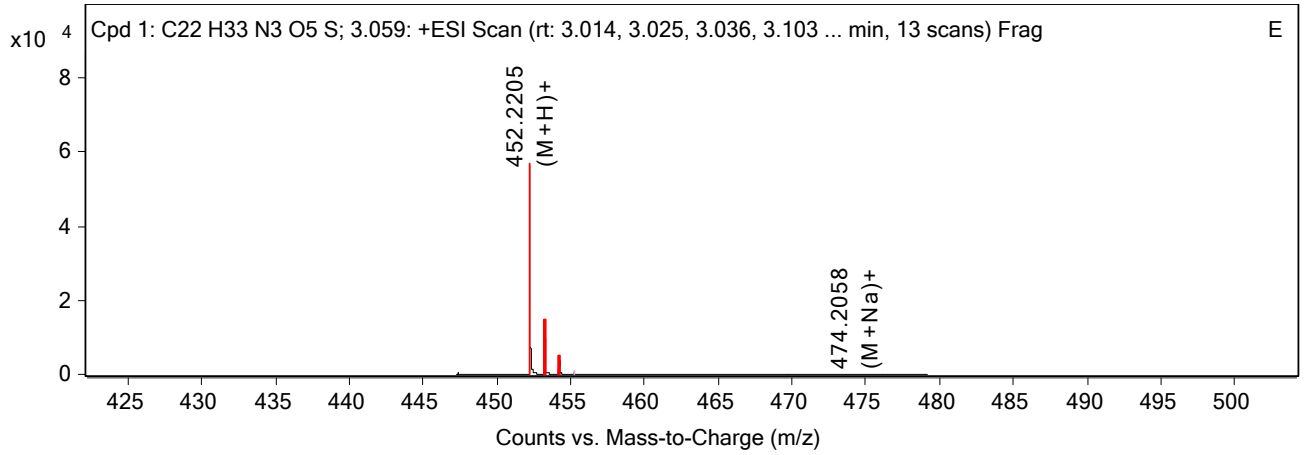
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
452.2205	1	56862.88	(M+H)+
453.2235	1	12157.67	(M+H)+
454.2215	1	3679.68	(M+H)+
474.2058	1	129.32	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
452.2205	1	56862.88	(M+H)+	1.93
452.2205		56862.88		
453.2235	1	12157.67	(M+H)+	1.89
454.2215	1	3679.68	(M+H)+	1.12
474.2058	1	129.32	(M+Na)+	-5.26

--- End Of Report ---

Target Compound Screening Report

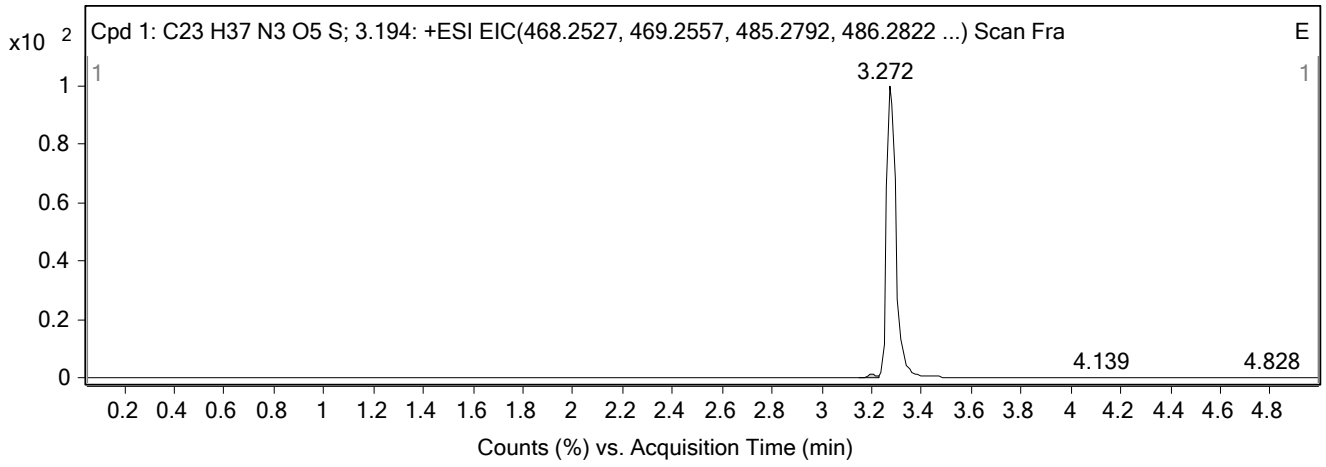
Data File	44.d	**Sample Name**	H2974264
Sample Type	Sample	**Position**	P1-E8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:46:48 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H37N3O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:46:48 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

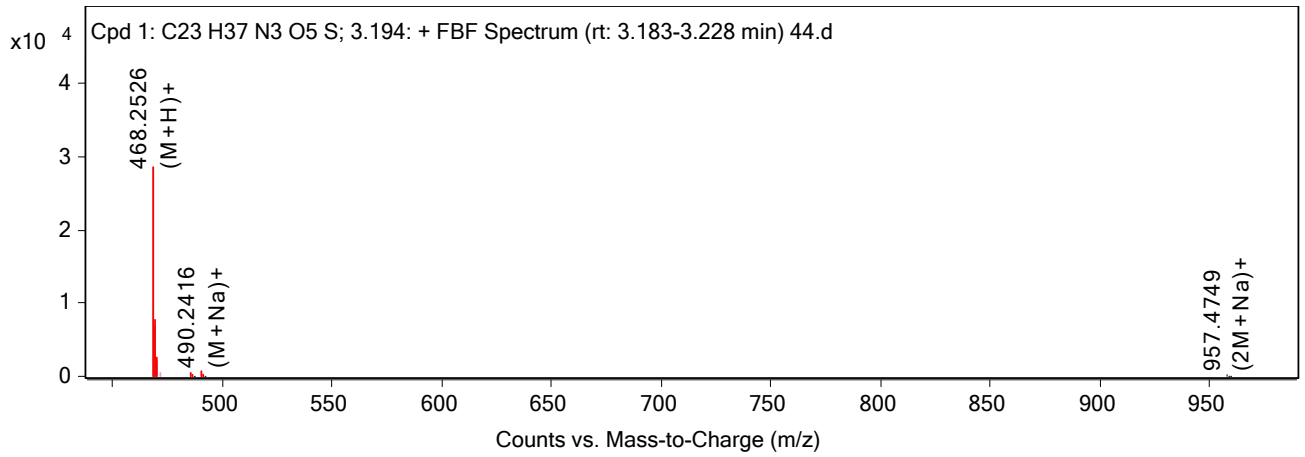
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H37 N3 O5 S; 3.194	97.49	0.84	C23 H37 N3 O5 S	3.194	467.2454	467.2458

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
468.2526	3.194	467.2458	C23 H37 N3 O5 S	467.2454	0.84	Find By Formula	

Compound Chromatograms



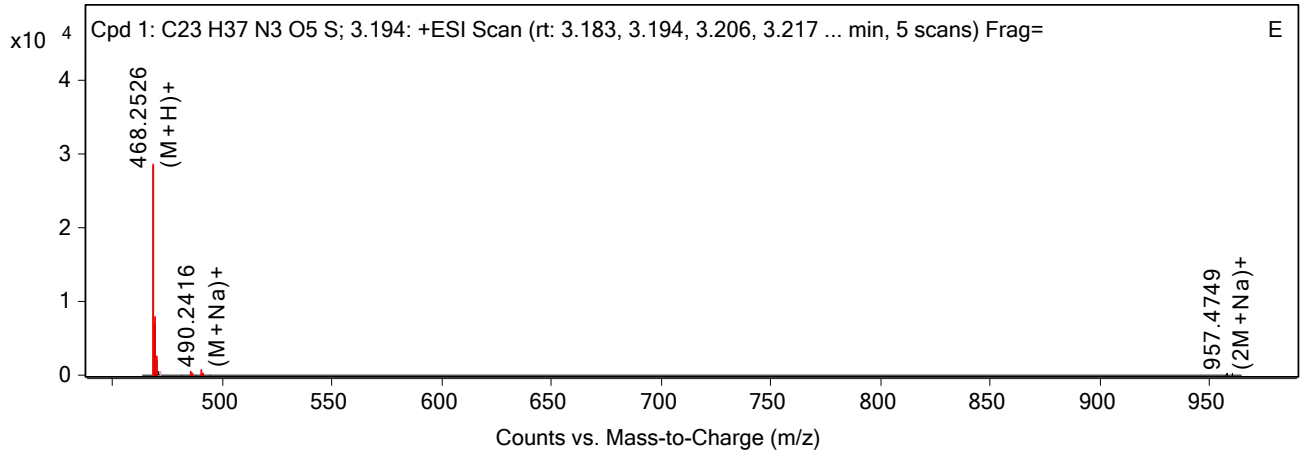
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
468.2526	1	28551.13	(M+H)+
469.2559	1	6902.61	(M+H)+
470.2543	1	2032.03	(M+H)+
485.2911	1	400.46	(M+NH4)+
486.2976	1	138.08	(M+NH4)+
490.2416	1	617.12	(M+Na)+
491.2456	1	212.52	(M+Na)+
957.4749	1	223.38	(2M+Na)+
958.4819	1	129.79	(2M+Na)+
959.4764	1	88.41	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
468.2526	1	28551.13	(M+H)+	0.08
469.2559	1	6902.61	(M+H)+	-0.38
470.2543	1	2032.03	(M+H)+	-1.79
485.2911	1	400.46	(M+NH4)+	-24.4
486.2976	1	138.08	(M+NH4)+	-31.8
490.2416	1	617.12	(M+Na)+	-14.18
491.2456	1	212.52	(M+Na)+	-16.18
957.4749	1	223.38	(2M+Na)+	5.3
958.4819	1	129.79	(2M+Na)+	1.15
959.4764	1	88.41	(2M+Na)+	6.2

--- End Of Report ---

Target Compound Screening Report

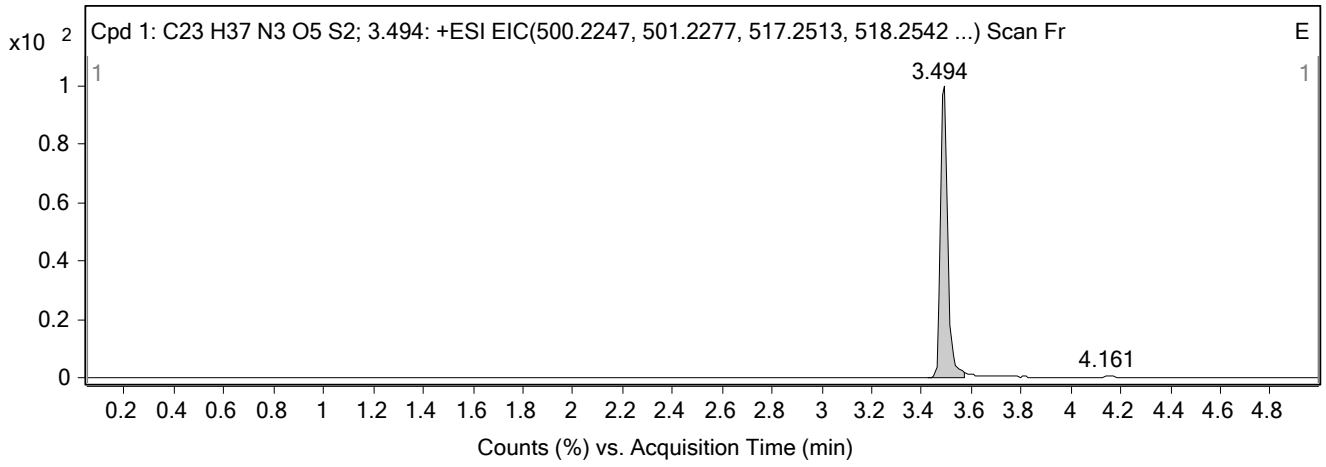
Data File	4d.d	**Sample Name**	H3472162
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 9:30:08 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H37N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 9:30:08 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

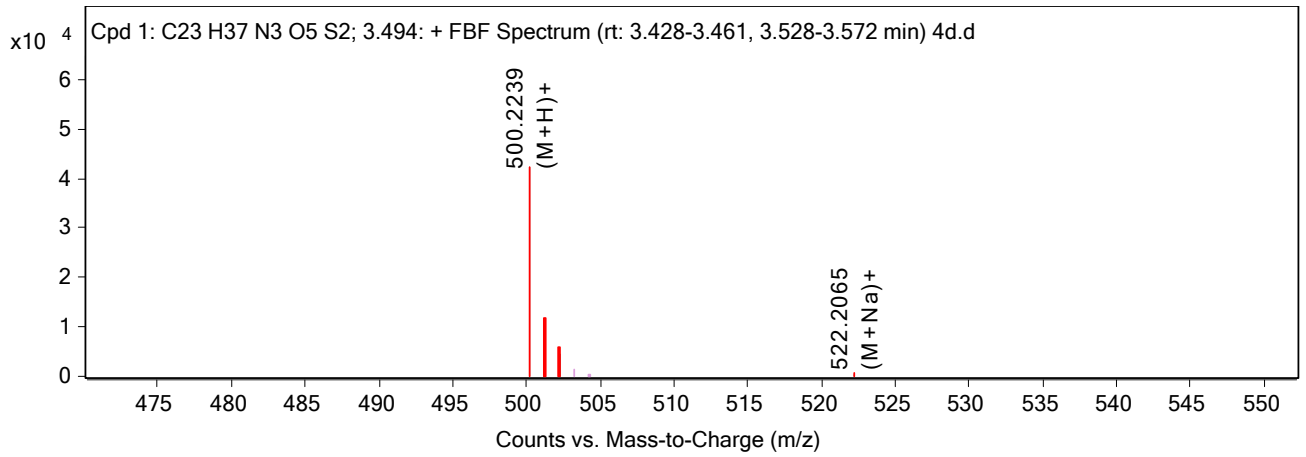
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H37 N3 O5 S2; 3.494	94.5	-1.65	C23 H37 N3 O5 S2	3.494	499.2175	499.2166

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.2239	3.494	499.2166	C23 H37 N3 O5 S2	499.2175	-1.65	Find By Formula	

Compound Chromatograms



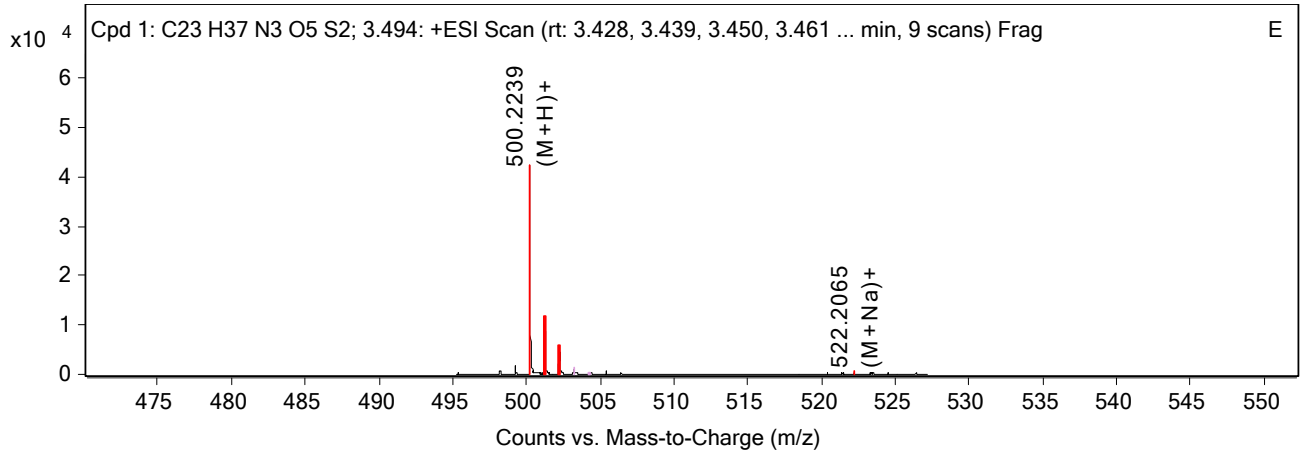
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.2239	1	42343.1	(M+H)+
501.2267	1	10346.71	(M+H)+
502.2234	1	4595.75	(M+H)+
522.2065	1	534.55	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.2239	1	42343.1	(M+H)+	1.64
500.2239		42343.1		
501.2267	1	10346.71	(M+H)+	1.99
502.2234	1	4595.75	(M+H)+	1.13
522.2065	1	534.55	(M+Na)+	0.38

--- End Of Report ---

Target Compound Screening Report

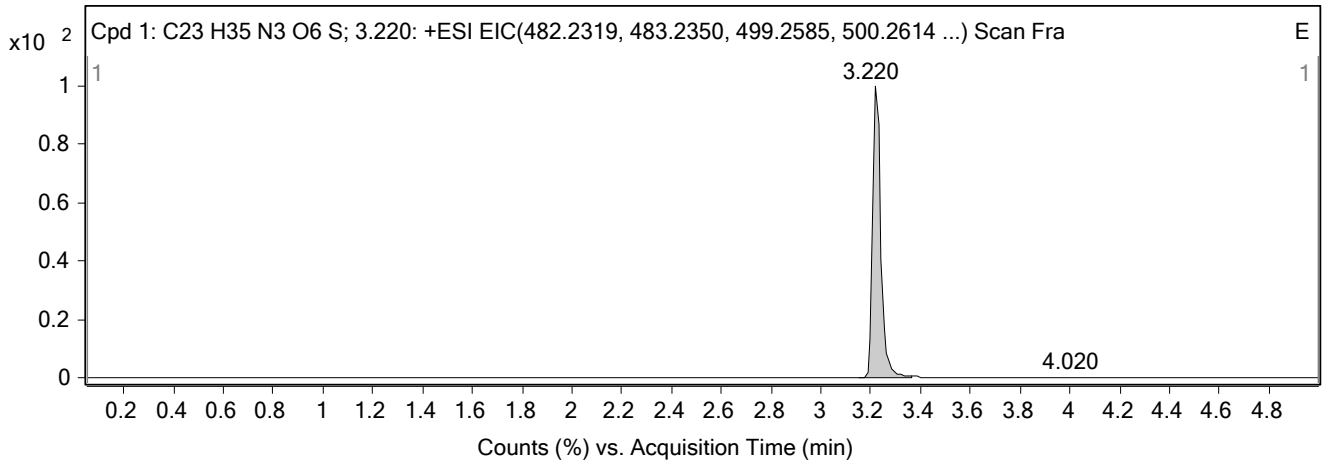
Data File	46.d	**Sample Name**	H2978088
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:57:54 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H35N3O6S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:57:54 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H35 N3 O6 S; 3.220	95.84	-0.99	C23 H35 N3 O6 S	3.22	481.2247	481.2242

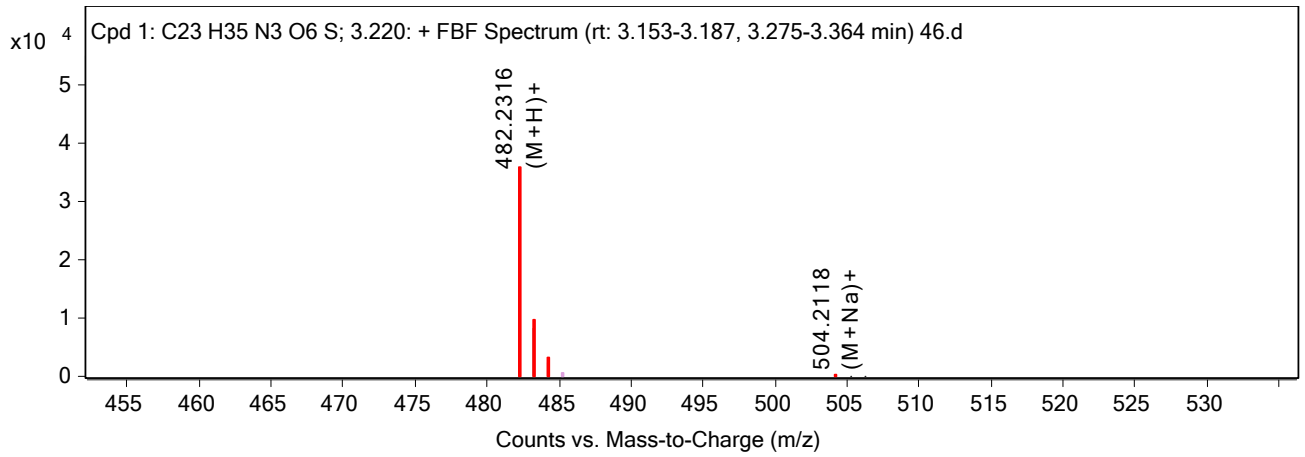
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
482.2316	3.22	481.2242	C23 H35 N3 O6 S	481.2247	-0.99	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

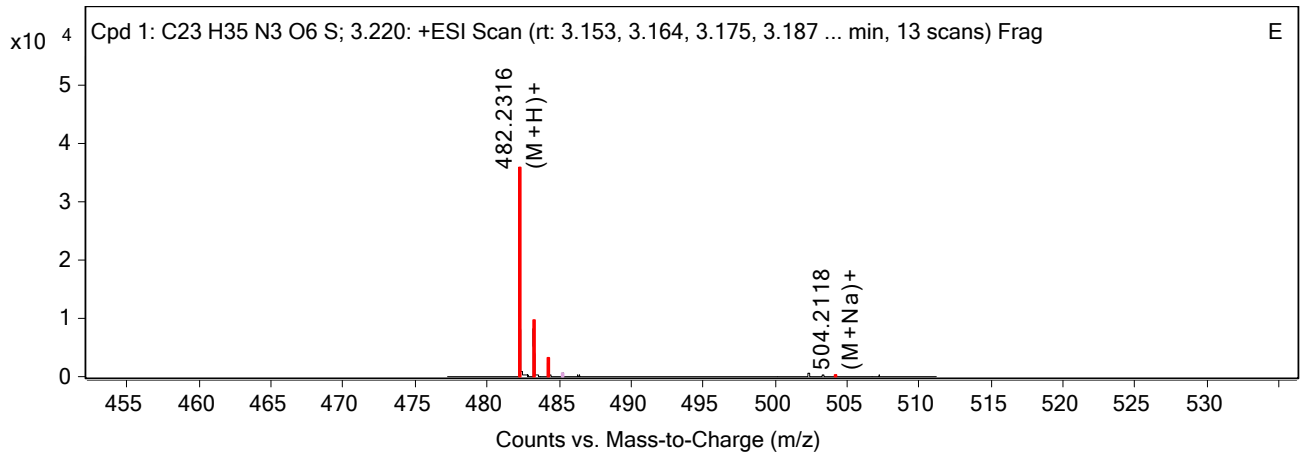
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
482.2316	1	35857.57	(M+H)+
483.2341	1	8224.68	(M+H)+
484.2321	1	2504.68	(M+H)+
504.2118	1	377.79	(M+Na)+
505.2176	1	111.58	(M+Na)+
506.2122	1	60.43	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
482.2316	1	35857.57	(M+H)+	0.73
483.2341	1	8224.68	(M+H)+	1.76
484.2321	1	2504.68	(M+H)+	1.55
504.2118	1	377.79	(M+Na)+	4.17
505.2176	1	111.58	(M+Na)+	-1.43
506.2122	1	60.43	(M+Na)+	5.1

--- End Of Report ---

Target Compound Screening Report

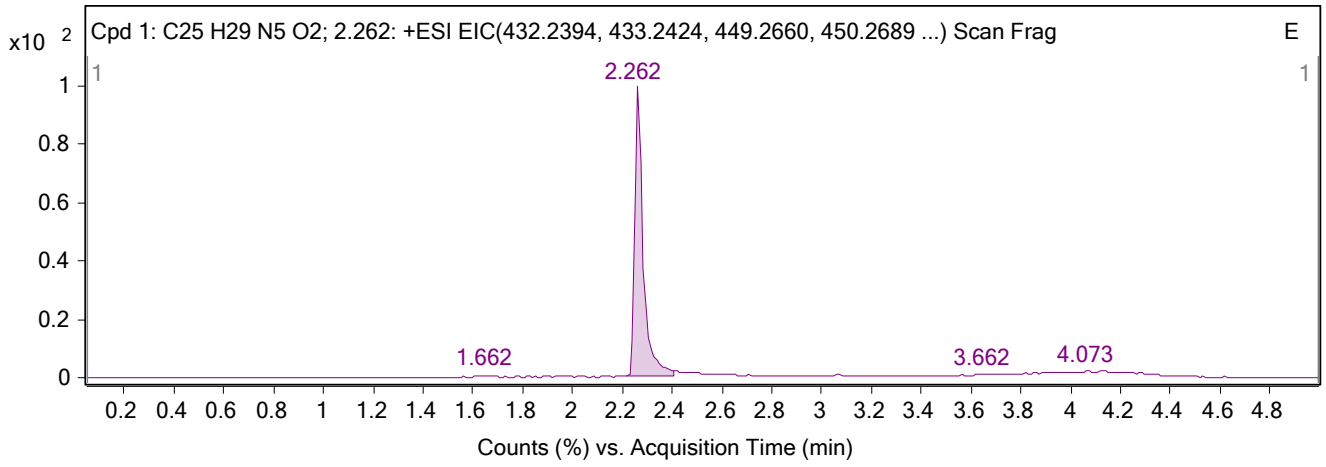
Data File	16.d	**Sample Name**	H2982867
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 8:17:01 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H29N5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 8:17:01 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

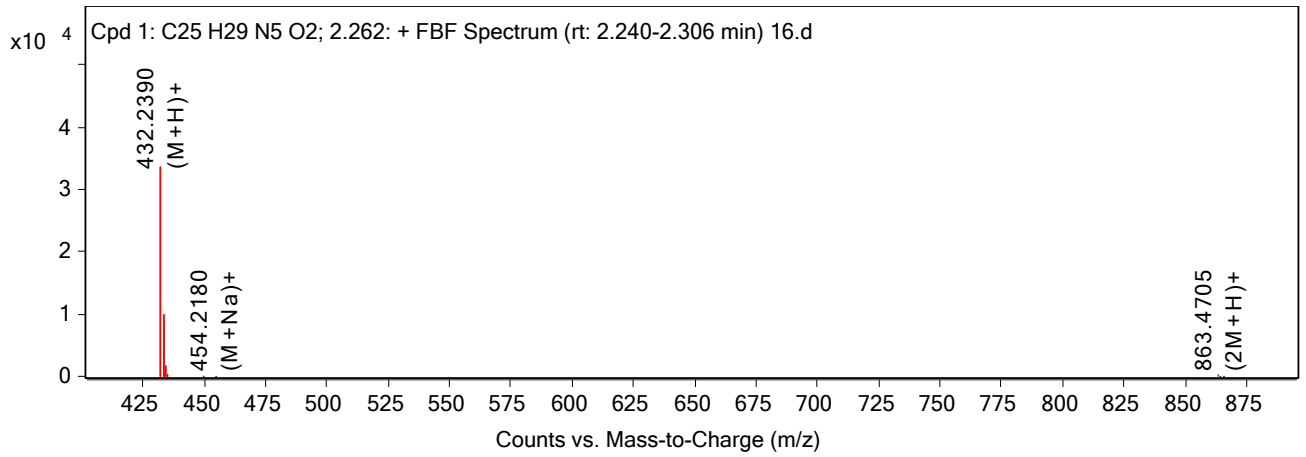
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H29 N5 O2; 2.262	98.06	-1.19	C25 H29 N5 O2	2.262	431.2321	431.2316

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
432.239	2.262	431.2316	C25 H29 N5 O2	431.2321	-1.19	Find By Formula	

Compound Chromatograms



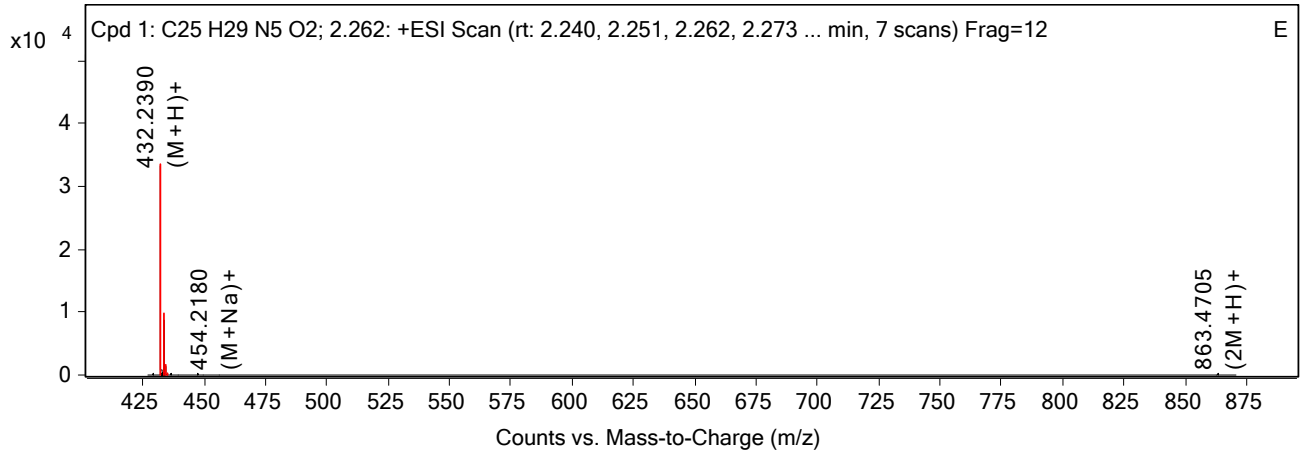
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
432.239	1	33493.14	(M+H)+
433.2416	1	8780.1	(M+H)+
434.2443	1	1325.06	(M+H)+
435.243	1	164.88	(M+H)+
449.2789	1	51.55	(M+NH4)+
454.218	1	73.46	(M+Na)+
863.4705	1	168.2	(2M+H)+
864.4691	1	111.16	(2M+H)+
865.4632	1	41.85	(2M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
432.239	1	33493.14	(M+H)+	0.88
433.2416	1	8780.1	(M+H)+	1.85
434.2443	1	1325.06	(M+H)+	2.2
435.243	1	164.88	(M+H)+	11.26
449.2789	1	51.55	(M+NH4)+	-28.89
454.218	1	73.46	(M+Na)+	7.35
863.4705	1	168.2	(2M+H)+	1.23
864.4691	1	111.16	(2M+H)+	6.26
865.4632	1	41.85	(2M+H)+	16.43

--- End Of Report ---

Target Compound Screening Report

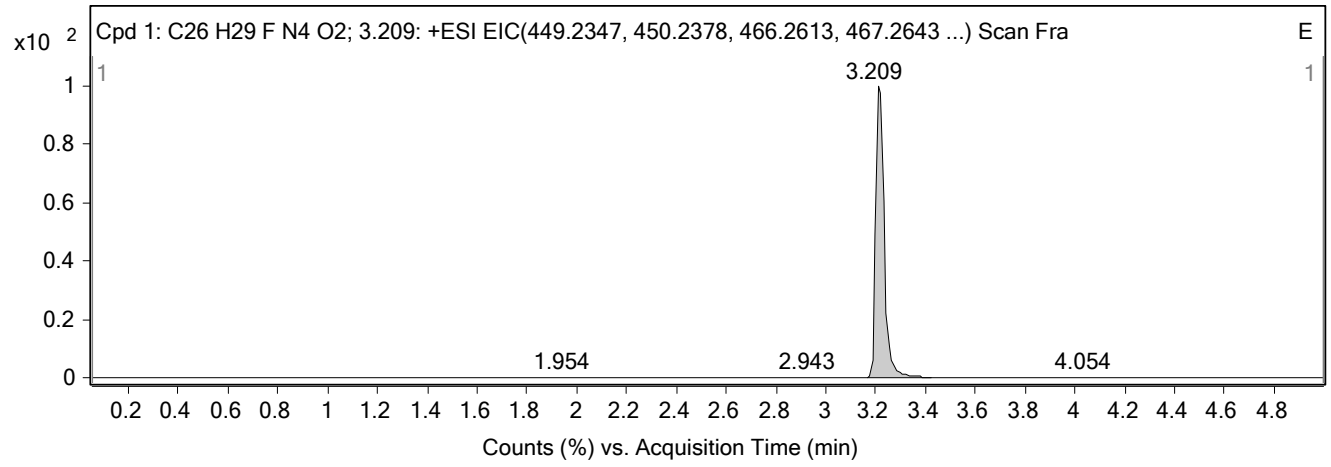
Data File	32.d	**Sample Name**	H2989503
Sample Type	Sample	**Position**	P1-D5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:08:49 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H29FN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:08:49 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

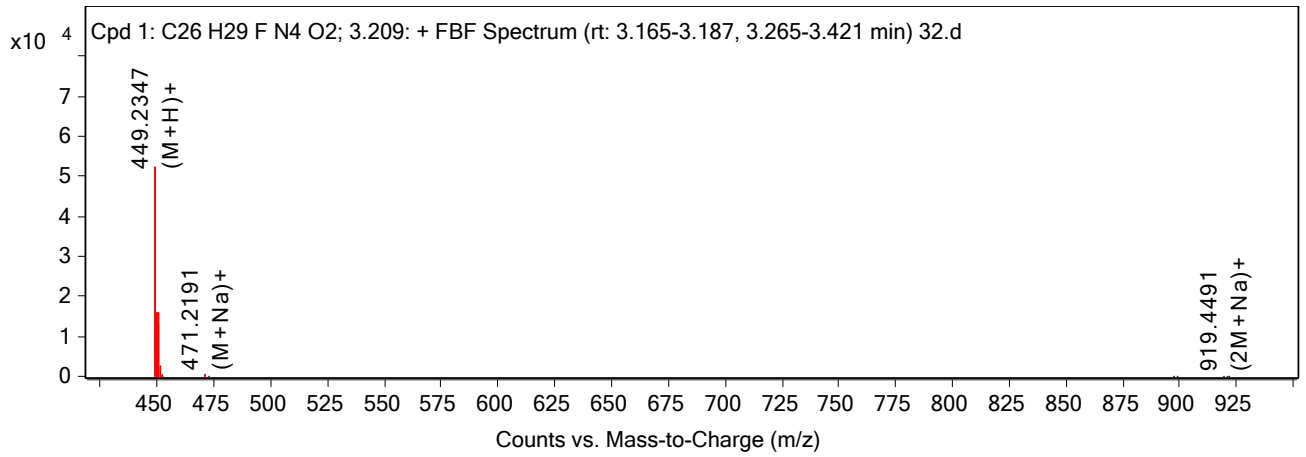
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H29 F N4 O2; 3.209	95.72	0.17	C26 H29 F N4 O2	3.209	448.2275	448.2275

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
449.2347	3.209	448.2275	C26 H29 F N4 O2	448.2275	0.17	Find By Formula	

Compound Chromatograms



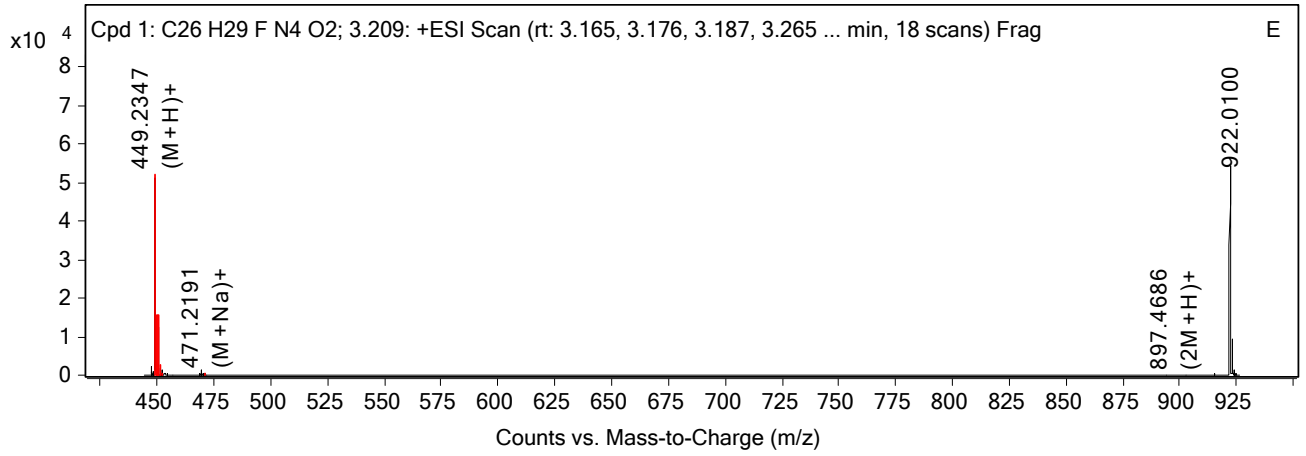
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
449.2347	1	52173.42	(M+H)+
450.238	1	12927.57	(M+H)+
451.2407	1	1914.88	(M+H)+
452.2447	1	215.11	(M+H)+
471.2191	1	557.43	(M+Na)+
472.2188	1	191.02	(M+Na)+
897.4686	1	58.16	(2M+H)+
919.4491	1	114.36	(2M+Na)+
920.4449	1	70.03	(2M+Na)+
921.4706	1	45.97	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
449.2347	1	52173.42	(M+H)+	0.01
450.238	1	12927.57	(M+H)+	-0.36
451.2407	1	1914.88	(M+H)+	-0.02
452.2447	1	215.11	(M+H)+	-2.61
471.2191	1	557.43	(M+Na)+	-5.16
472.2188	1	191.02	(M+Na)+	1.98
897.4686	1	58.16	(2M+H)+	-7.1
919.4491	1	114.36	(2M+Na)+	-5.38
920.4449	1	70.03	(2M+Na)+	2.5
921.4706	1	45.97	(2M+Na)+	-22.18

--- End Of Report ---

Target Compound Screening Report

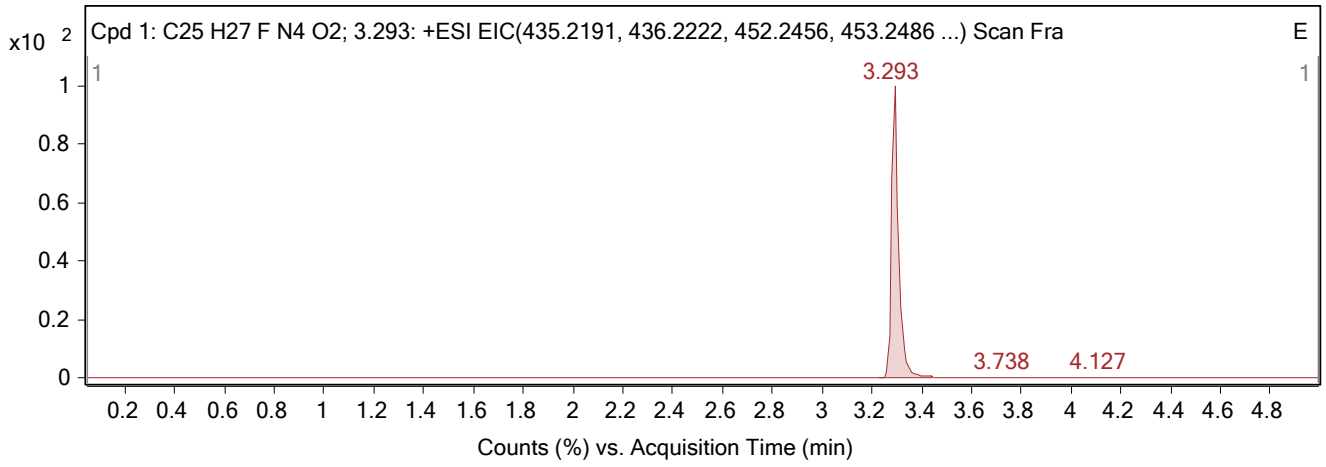
Data File	17.d	**Sample Name**	H2993387
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 12:45:27 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H27FN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 12:45:27 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H27 F N4 O2; 3.293	95.78	-0.89	C25 H27 F N4 O2	3.293	434.2118	434.2114

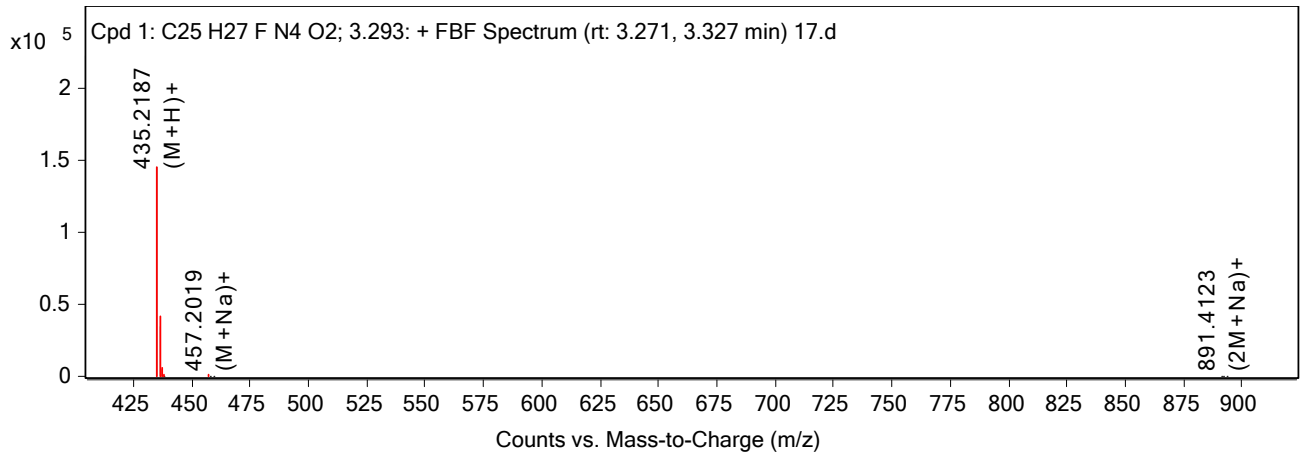
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
435.2187	3.293	434.2114	C25 H27 F N4 O2	434.2118	-0.89	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

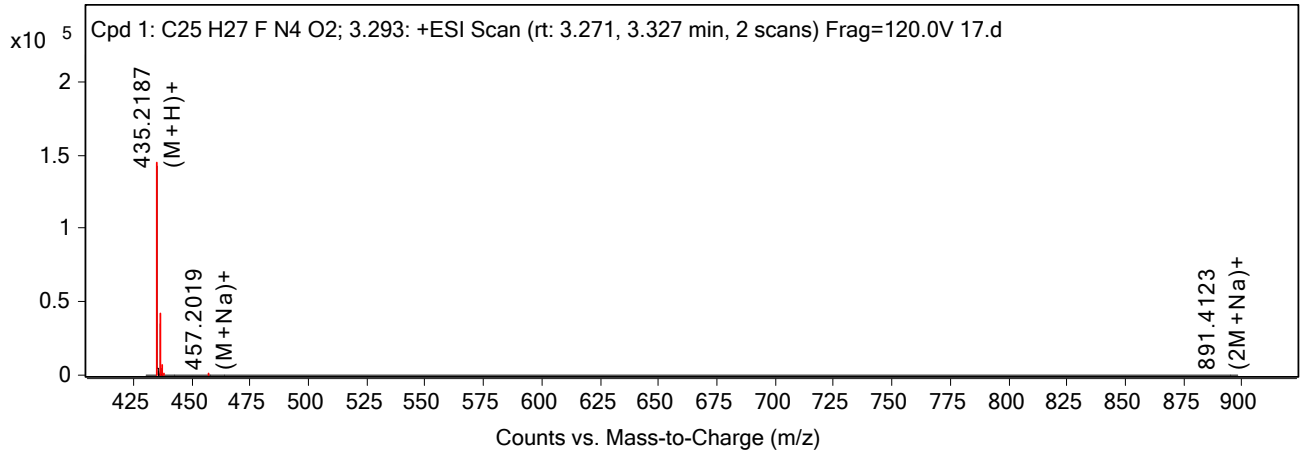
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
435.2187	1	145181.56	(M+H)+
436.2217	1	34741.37	(M+H)+
437.2241	1	5084.26	(M+H)+
438.2291	1	553.21	(M+H)+
457.2019	1	1024.52	(M+Na)+
458.2073	1	329.13	(M+Na)+
459.2	1	170.66	(M+Na)+
891.4123	1	410.09	(2M+Na)+
892.4141	1	237.74	(2M+Na)+
893.4205	1	89.01	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
435.2187	1	145181.57	(M+H)+	0.85
436.2217	1	34741.37	(M+H)+	0.97
437.2241	1	5084.26	(M+H)+	2.14
438.2291	1	553.21	(M+H)+	-3.02
457.2019	1	1024.52	(M+Na)+	-1.89
458.2073	1	329.13	(M+Na)+	-6.89
459.2	1	170.66	(M+Na)+	15.14
891.4123	1	410.09	(2M+Na)+	0.59
892.4141	1	237.74	(2M+Na)+	2.02
893.4205	1	89.01	(2M+Na)+	-1.85

--- End Of Report ---

Target Compound Screening Report

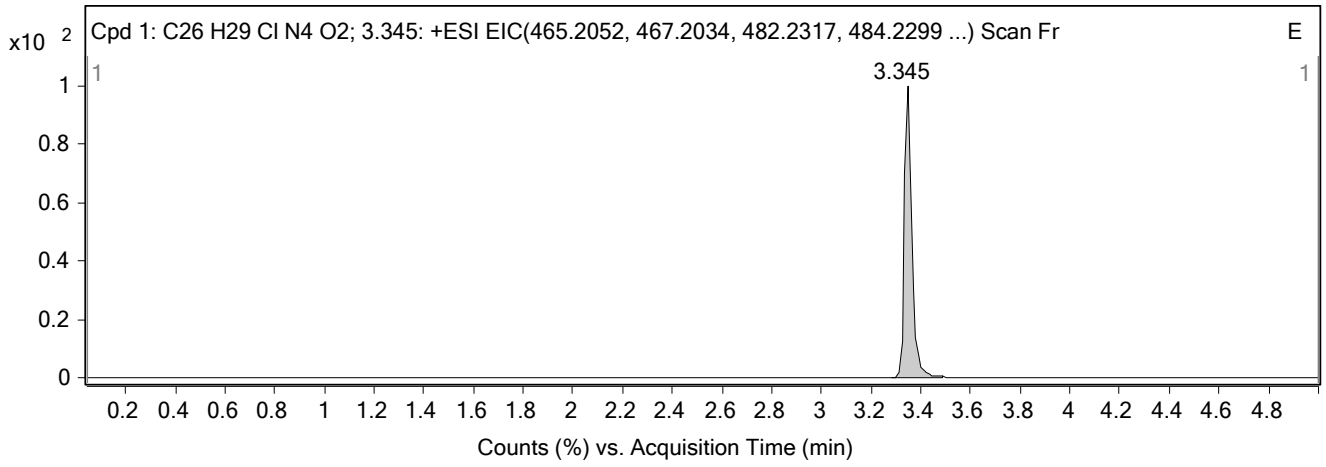
Data File	53.d	**Sample Name**	H2978522
Sample Type	Sample	**Position**	P1-F8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:36:48 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H29ClN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:36:48 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

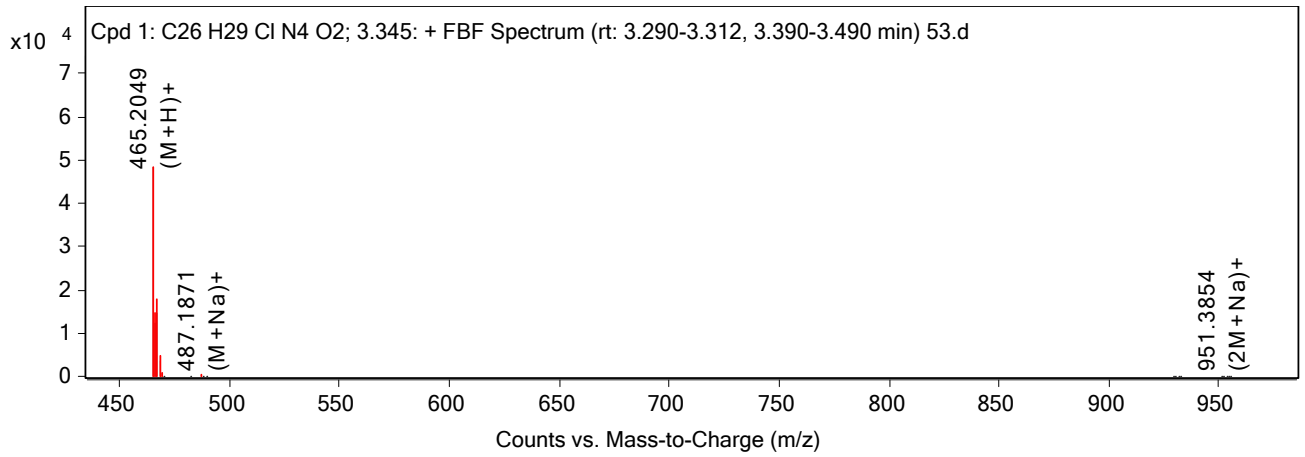
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H29 Cl N4 O2; 3.345	96.17	-0.59	C26 H29 Cl N4 O2	3.345	464.1979	464.1976

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
465.2049	3.345	464.1976	C26 H29 Cl N4 O2	464.1979	-0.59	Find By Formula	

Compound Chromatograms



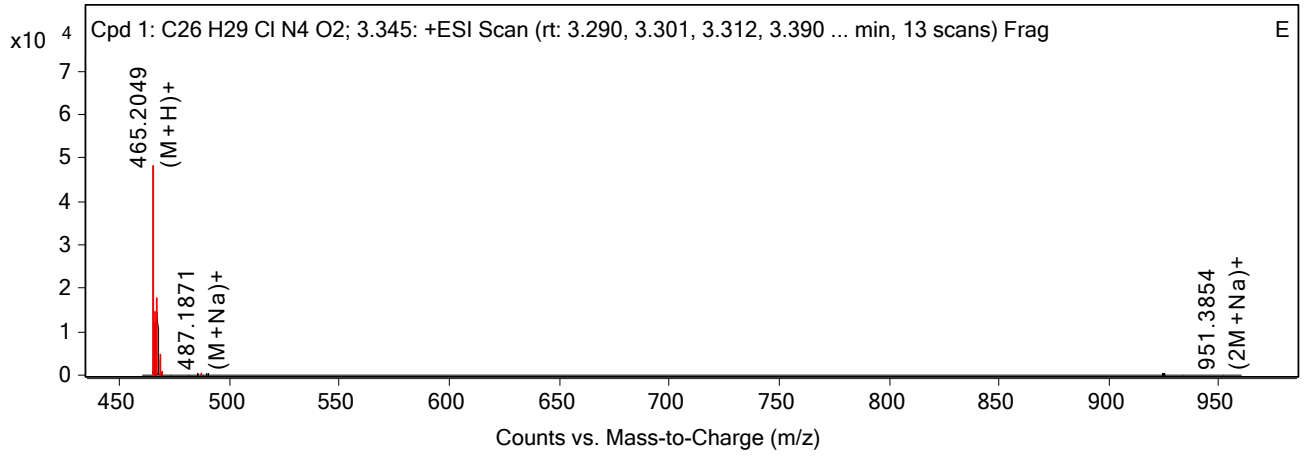
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
465.2049	1	48285.03	(M+H)+
466.2079	1	12146.15	(M+H)+
467.2032	1	14817.45	(M+H)+
468.2056	1	3632.82	(M+H)+
469.2065	1	821.98	(M+H)+
470.2117	1	147.86	(M+H)+
482.2333	1	186.77	(M+NH4)+
487.1871	1	393.65	(M+Na)+
488.1882	1	146.62	(M+Na)+
489.1835	1	137.55	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
465.2049	1	48285.03	(M+H)+	0.65
466.2079	1	12146.15	(M+H)+	0.84
467.2032	1	14817.45	(M+H)+	0.32
468.2056	1	3632.82	(M+H)+	0.44
469.2065	1	821.98	(M+H)+	4.11
470.2117	1	147.86	(M+H)+	-1.13
482.2333	1	186.77	(M+NH4)+	-3.2
487.1871	1	393.65	(M+Na)+	-0.05
488.1882	1	146.62	(M+Na)+	4.12
489.1835	1	137.55	(M+Na)+	3.75

--- End Of Report ---

Target Compound Screening Report

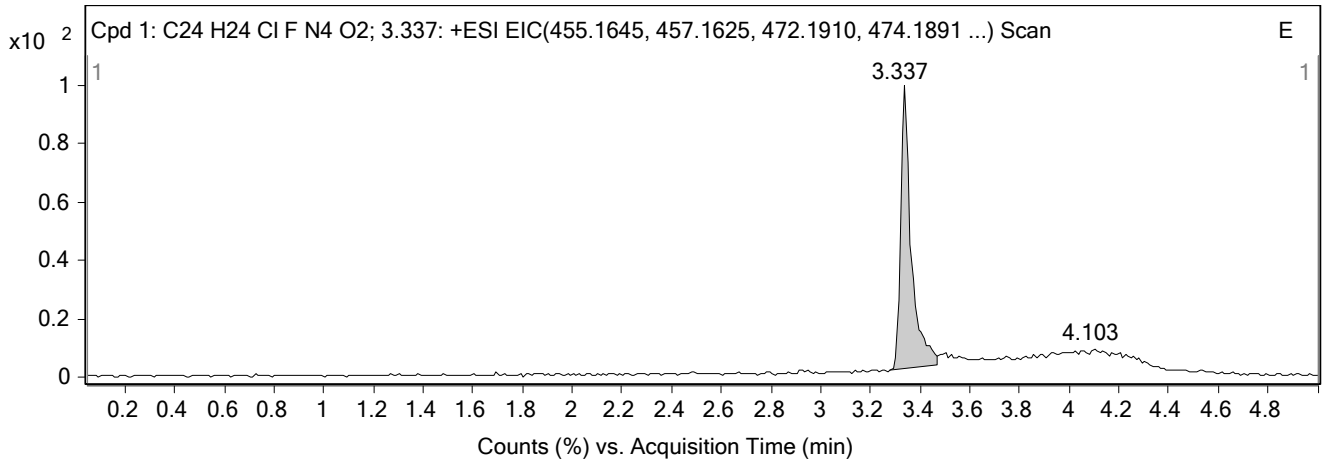
Data File	36-2.d	**Sample Name**	H2977891
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 7:00:54 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H24ClFN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 7:00:54 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

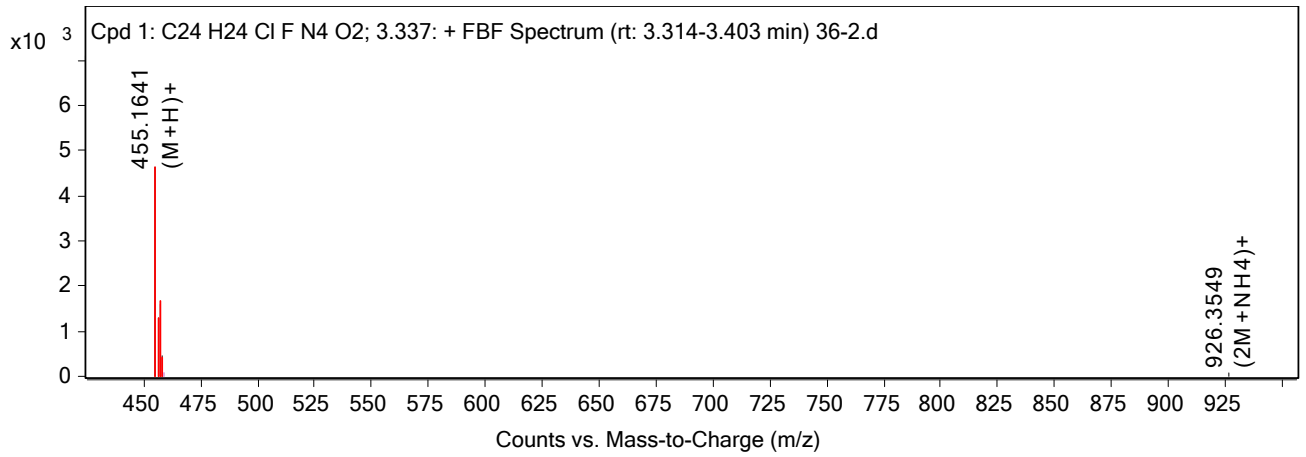
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H24 Cl F N4 O2; 3.337	99.03	-0.49	C24 H24 Cl F N4 O2	3.337	454.1572	454.157

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
455.1641	3.337	454.157	C24 H24 Cl F N4 O2	454.1572	-0.49	Find By Formula	

Compound Chromatograms



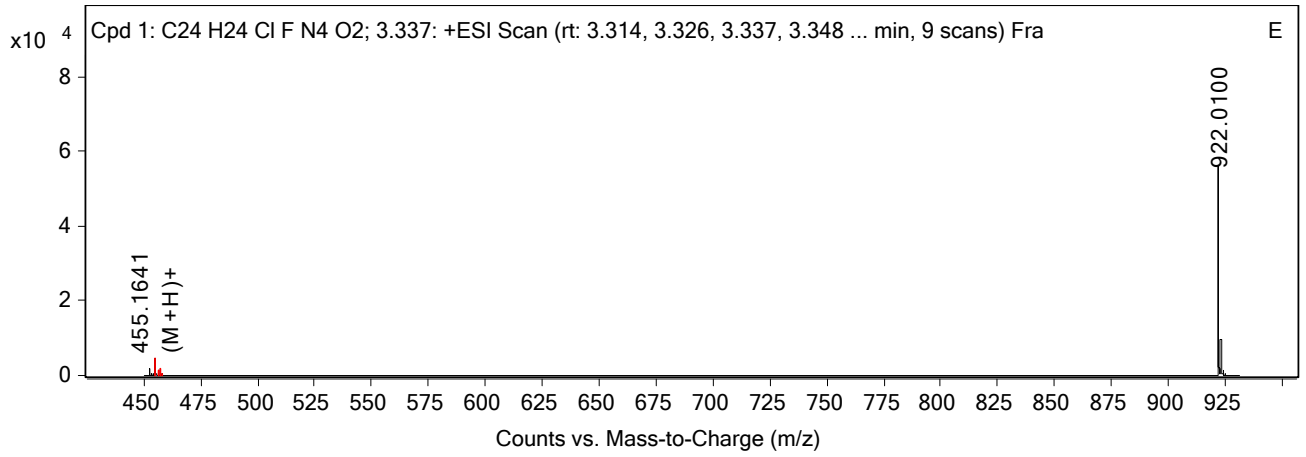
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
455.1641	1	4650.45	(M+H)+
456.1671	1	1298.14	(M+H)+
457.1622	1	1591.19	(M+H)+
458.1661	1	476.68	(M+H)+
926.3549	1	79.96	(2M+NH4)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
455.1641	1	4650.45	(M+H)+	0.81
456.1671	1	1298.14	(M+H)+	0.94
457.1622	1	1591.19	(M+H)+	0.79
458.1661	1	476.68	(M+H)+	-2.39
922.01		55953.79		
926.3549	1	79.96	(2M+NH4)+	-7.23

--- End Of Report ---

Target Compound Screening Report

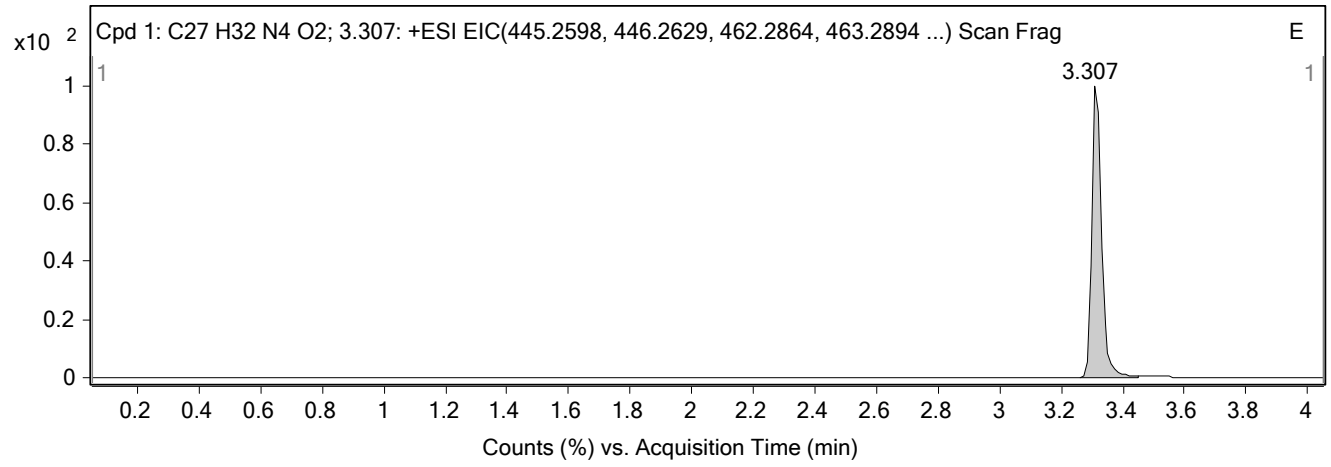
Data File	52-3.d	**Sample Name**	H2978196
Sample Type	Sample	**Position**	P1-F7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 7:28:57 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C27H32N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 7:28:57 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

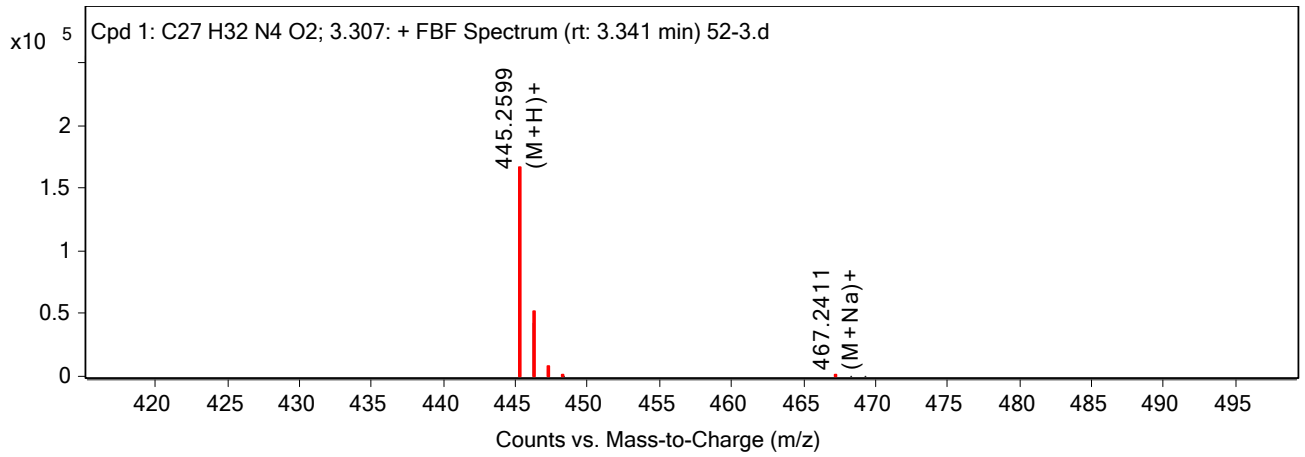
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C27 H32 N4 O2; 3.307	94.83	0.19	C27 H32 N4 O2	3.307	444.2525	444.2526

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
445.2599	3.307	444.2526	C27 H32 N4 O2	444.2525	0.19	Find By Formula	

Compound Chromatograms



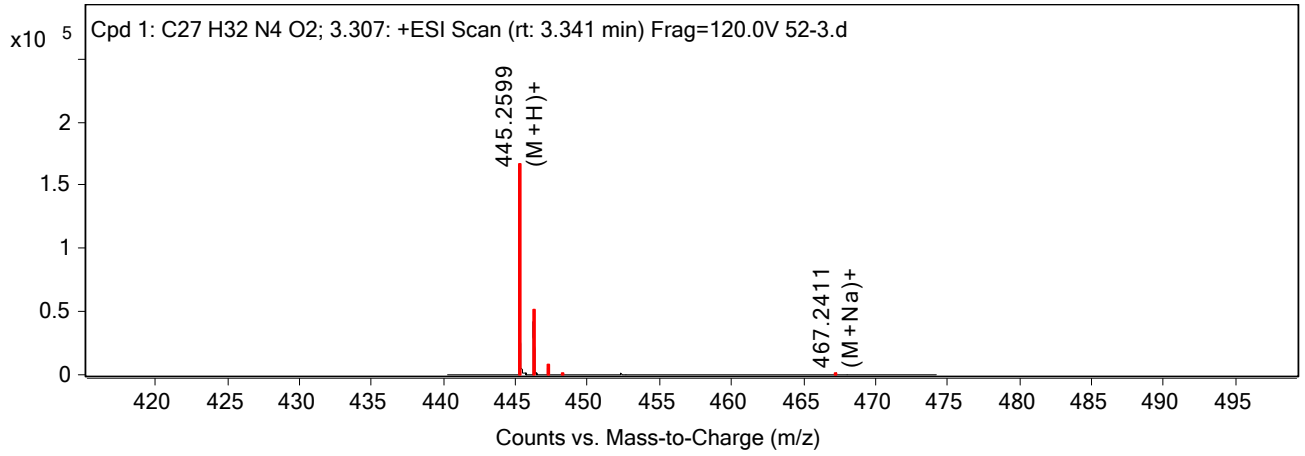
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
445.2599	1	166385.94	(M+H)+
446.2627	1	42192	(M+H)+
447.2671	1	5743.2	(M+H)+
448.2706	1	661.12	(M+H)+
467.2411	1	1554.64	(M+Na)+
468.2461	1	639	(M+Na)+
469.2318	1	122.98	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
445.2599	1	166385.95	(M+H)+	-0.25
445.2599		166385.95		
446.2627	1	42192	(M+H)+	0.38
447.2671	1	5743.2	(M+H)+	-2.95
448.2706	1	661.12	(M+H)+	-4.28
467.2411	1	1554.64	(M+Na)+	1.45
468.2461	1	639	(M+Na)+	-2.78
469.2318	1	122.98	(M+Na)+	33.97

--- End Of Report ---

Target Compound Screening Report

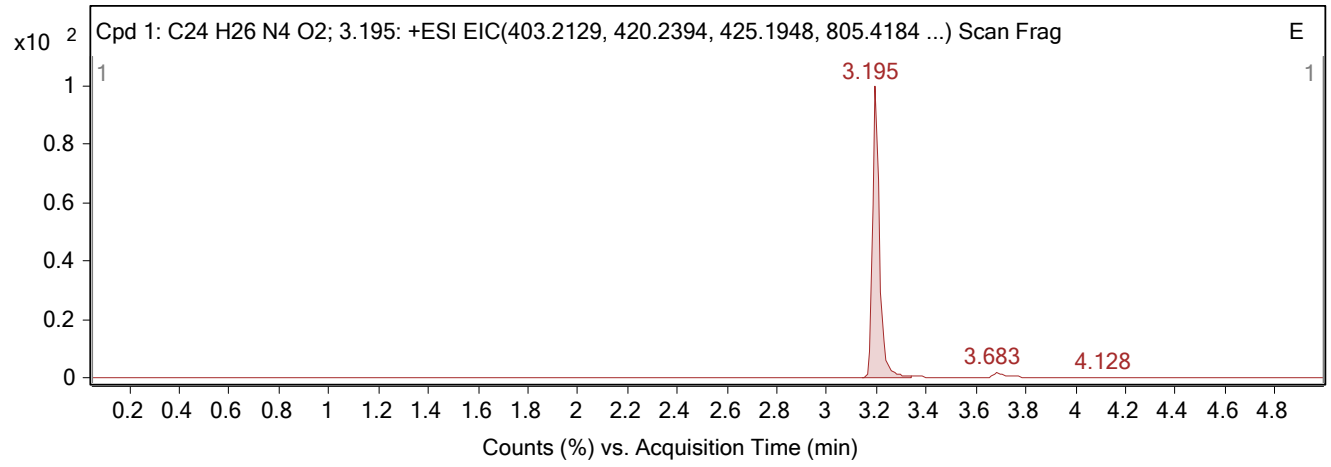
Data File	20.d	**Sample Name**	H2998372
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:33:27 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H26N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:33:27 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

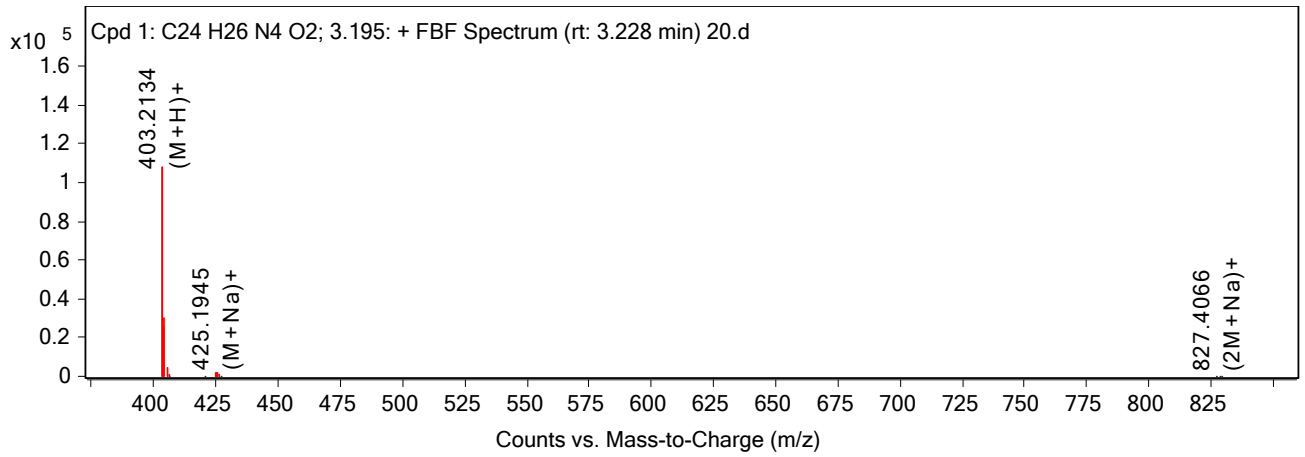
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H26 N4 O2; 3.195	97.01	1.07	C24 H26 N4 O2	3.195	402.2056	402.206

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
403.2134	3.195	402.206	C24 H26 N4 O2	402.2056	1.07	Find By Formula	

Compound Chromatograms



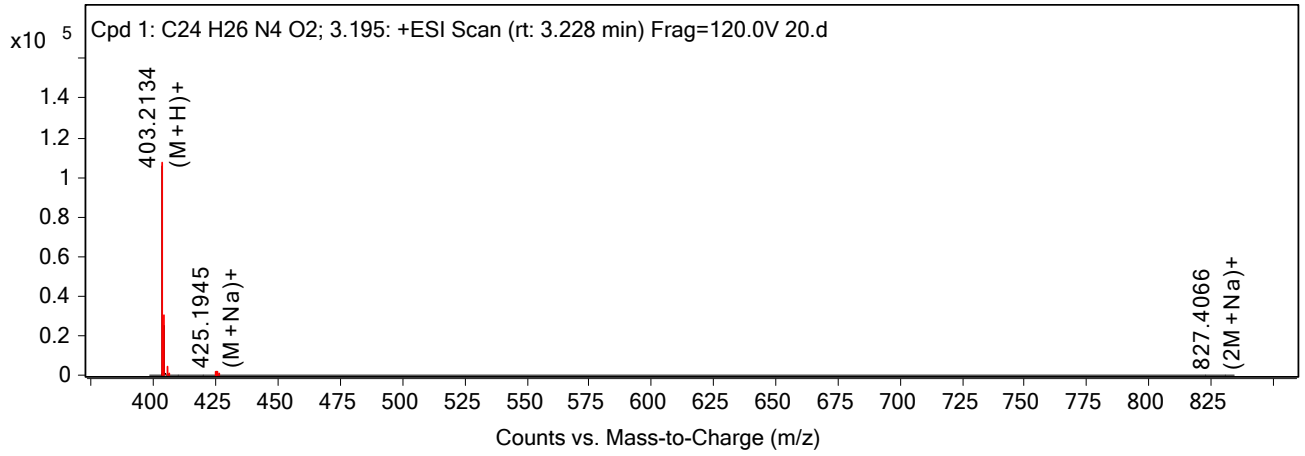
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
403.2134	1	107794.27	(M+H)+
404.2161	1	25771.5	(M+H)+
405.2184	1	3237.43	(M+H)+
406.2187	1	487.92	(M+H)+
420.2431	1	83.33	(M+NH4)+
425.1945	1	1552.36	(M+Na)+
426.1977	1	561.53	(M+Na)+
427.1932	1	90.89	(M+Na)+
827.4066	1	332.78	(2M+Na)+
828.4058	1	257.46	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
403.2134	1	107794.27	(M+H)+	-1.28
404.2161	1	25771.5	(M+H)+	-0.42
405.2184	1	3237.43	(M+H)+	0.86
406.2187	1	487.92	(M+H)+	6.91
420.2431	1	83.33	(M+NH4)+	-8.86
425.1945	1	1552.36	(M+Na)+	0.62
426.1977	1	561.53	(M+Na)+	0.42
427.1932	1	90.89	(M+Na)+	17.48
827.4066	1	332.78	(2M+Na)+	-7.5
828.4058	1	257.46	(2M+Na)+	-2.88

--- End Of Report ---

Target Compound Screening Report

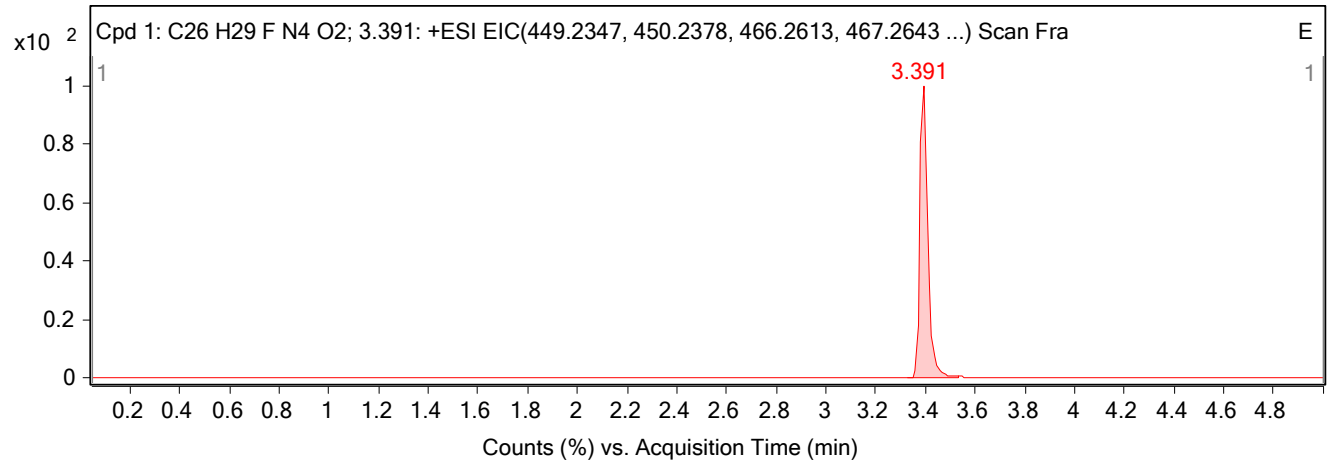
Data File	48.d	**Sample Name**	H2977001
Sample Type	Sample	**Position**	P1-F3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 6:09:01 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H29FN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 6:09:01 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

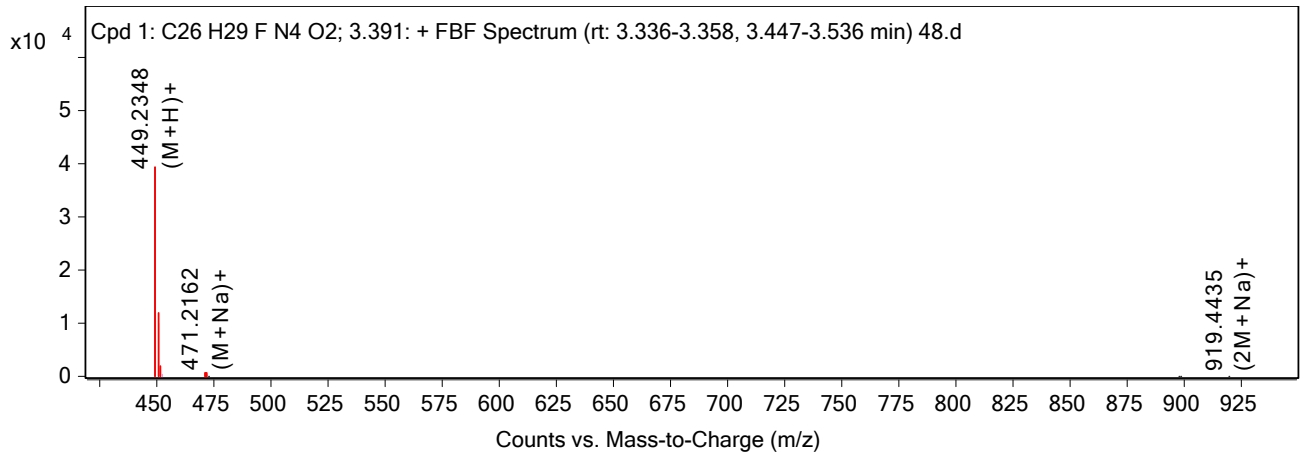
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H29 F N4 O2; 3.391	97.26	0.21	C26 H29 F N4 O2	3.391	448.2275	448.2275

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
449.2348	3.391	448.2275	C26 H29 F N4 O2	448.2275	0.21	Find By Formula	

Compound Chromatograms



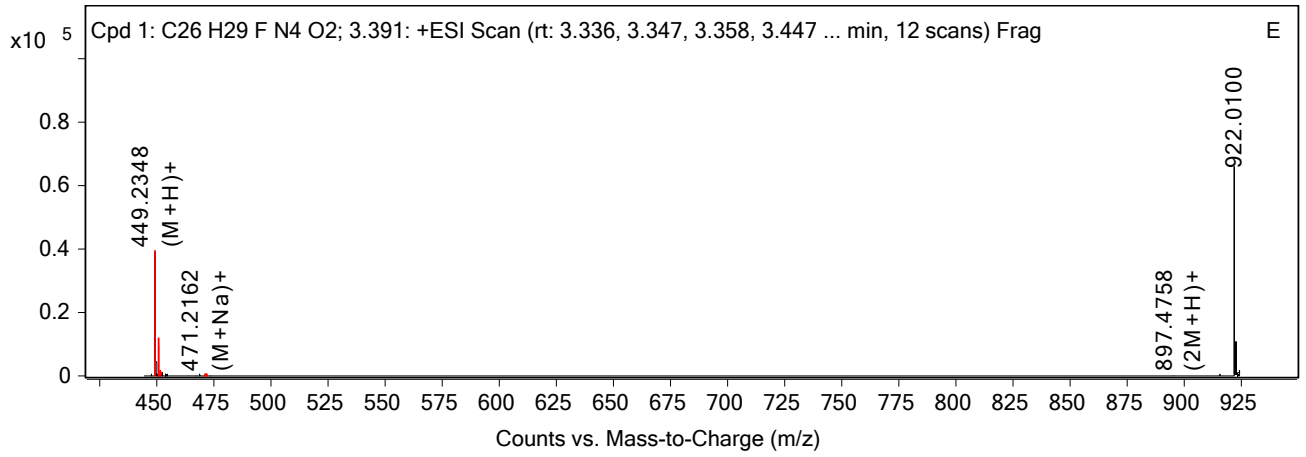
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
449.2348	1	39302.29	(M+H)+
450.2378	1	10142.3	(M+H)+
451.2414	1	1546.89	(M+H)+
471.2162	1	481.15	(M+Na)+
472.2168	1	153.97	(M+Na)+
897.4758	1	74.67	(2M+H)+
898.454	1	33.05	(2M+H)+
919.4435	1	90.67	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
449.2348	1	39302.29	(M+H)+	-0.23
450.2378	1	10142.3	(M+H)+	0.01
451.2414	1	1546.89	(M+H)+	-1.52
471.2162	1	481.15	(M+Na)+	0.96
472.2168	1	153.97	(M+Na)+	6.19
897.4758	1	74.67	(2M+H)+	-15.12
898.454	1	33.05	(2M+H)+	12.54
919.4435	1	90.67	(2M+Na)+	0.7
922.01		65807.62		

--- End Of Report ---

Target Compound Screening Report

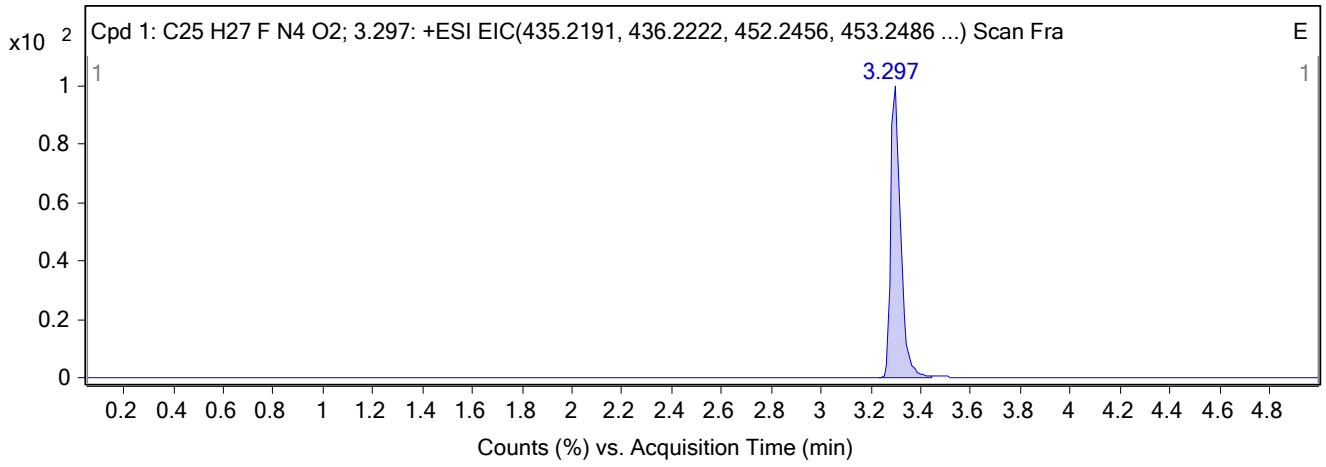
Data File	42.d	**Sample Name**	H2976534
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:35:40 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H27FN4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:35:40 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

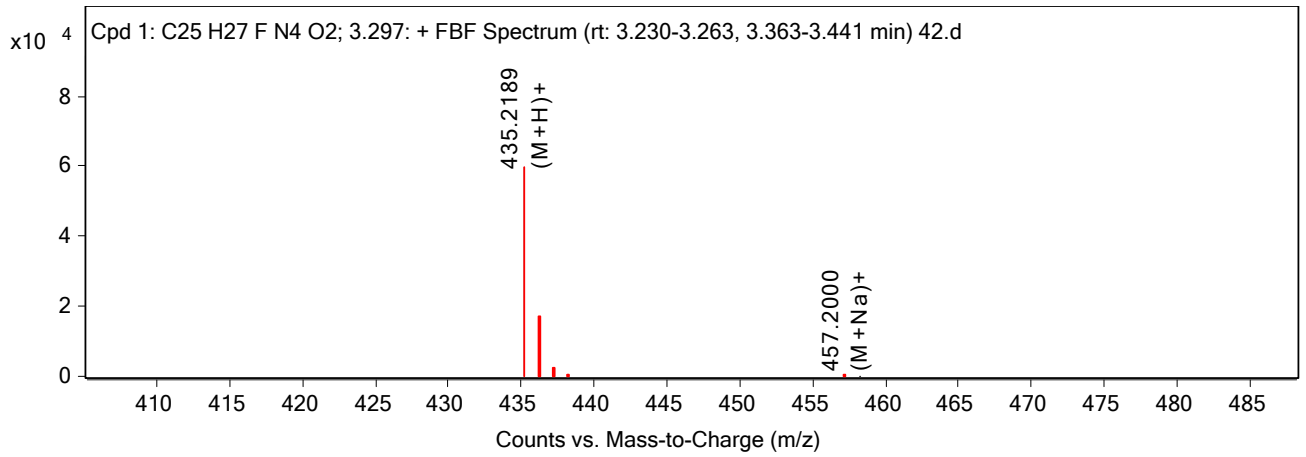
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H27 F N4 O2; 3.297	95.89	-0.25	C25 H27 F N4 O2	3.297	434.2118	434.2117

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
435.2189	3.297	434.2117	C25 H27 F N4 O2	434.2118	-0.25	Find By Formula	

Compound Chromatograms



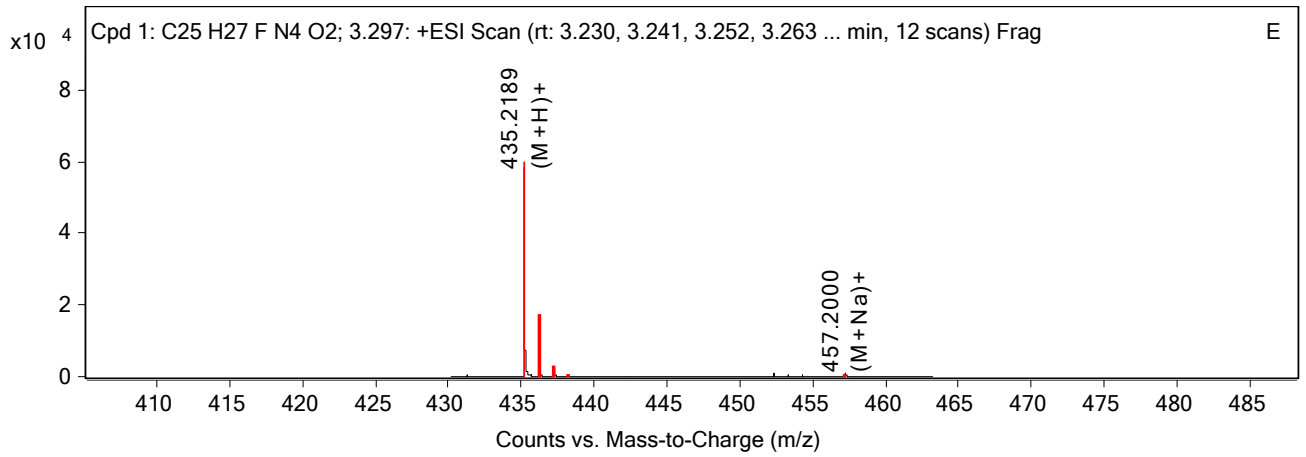
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
435.2189	1	59655.84	(M+H)+
436.2221	1	14278.27	(M+H)+
437.2251	1	2291.54	(M+H)+
438.2289	1	292.88	(M+H)+
457.2	1	321.46	(M+Na)+
458.2053	1	105.95	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
435.2189	1	59655.84	(M+H)+	0.3
436.2221	1	14278.27	(M+H)+	0.11
437.2251	1	2291.54	(M+H)+	-0.15
438.2289	1	292.88	(M+H)+	-2.57
457.2	1	321.46	(M+Na)+	2.15
458.2053	1	105.95	(M+Na)+	-2.72

--- End Of Report ---

Target Compound Screening Report

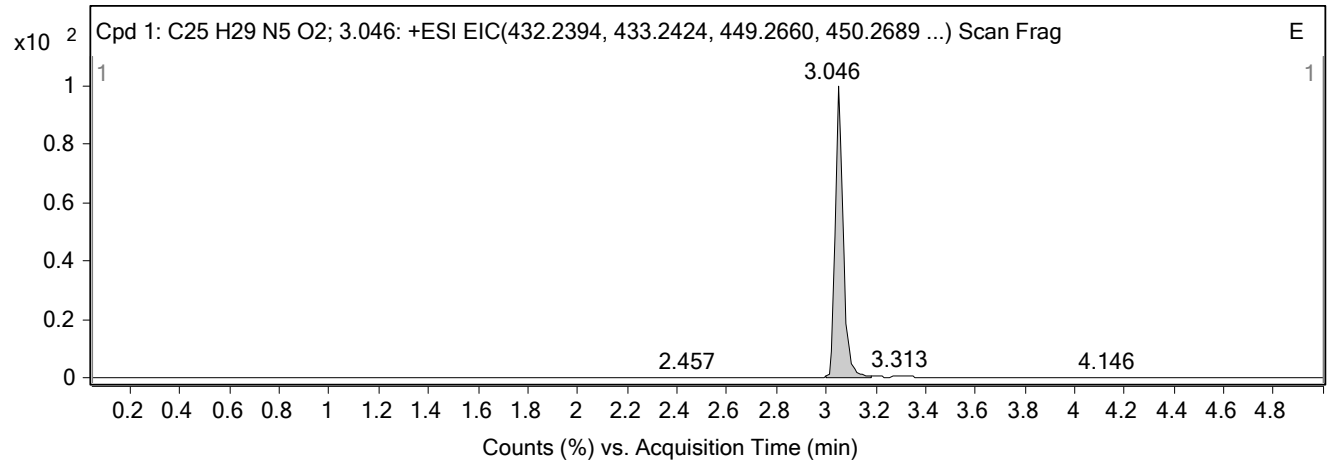
Data File	38.d	**Sample Name**	H2978886
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:13:26 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H29N5O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:13:26 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

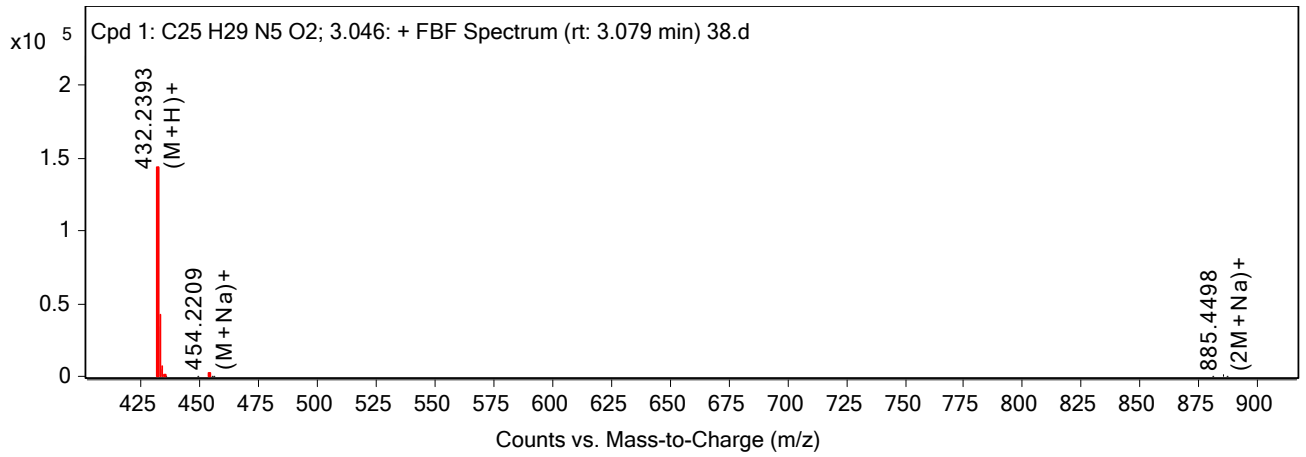
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H29 N5 O2; 3.046	95.06	-0.36	C25 H29 N5 O2	3.046	431.2321	431.232

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
432.2393	3.046	431.232	C25 H29 N5 O2	431.2321	-0.36	Find By Formula	

Compound Chromatograms



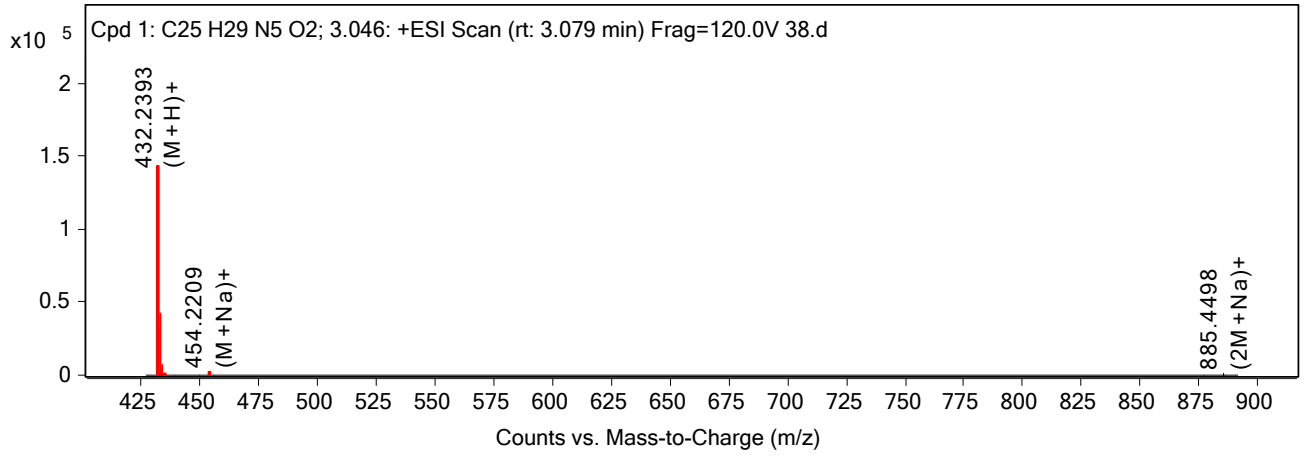
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
432.2393	1	143589.5	(M+H)+
433.2423	1	34081.01	(M+H)+
434.2449	1	4774.8	(M+H)+
435.2461	1	498.31	(M+H)+
454.2209	1	1831.04	(M+Na)+
455.22	1	561.48	(M+Na)+
456.2174	1	136	(M+Na)+
880.4958	1	66.17	(2M+NH4)+
885.4498	1	670.12	(2M+Na)+
886.4526	1	361.27	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
432.2393	1	143589.51	(M+H)+	0.25
433.2423	1	34081.01	(M+H)+	0.13
434.2449	1	4774.8	(M+H)+	0.7
435.2461	1	498.31	(M+H)+	4.13
454.2209	1	1831.04	(M+Na)+	1.08
455.22	1	561.48	(M+Na)+	9.45
456.2174	1	136	(M+Na)+	21.33
880.4958	1	66.17	(2M+NH4)+	2.61
885.4498	1	670.12	(2M+Na)+	4.18
886.4526	1	361.28	(2M+Na)+	4.41

--- End Of Report ---

Target Compound Screening Report

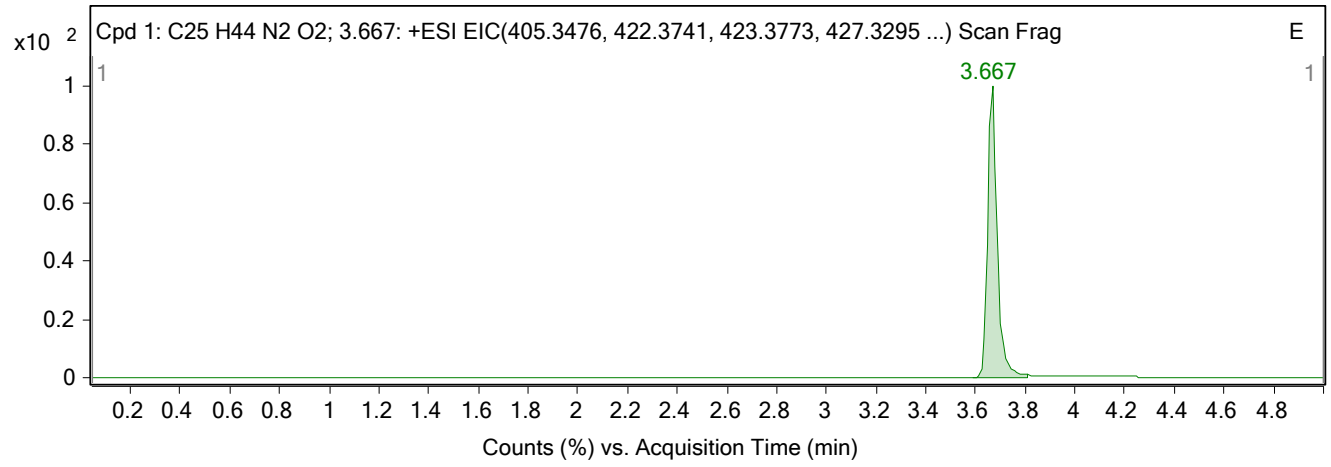
Data File	28.d	**Sample Name**	H3007333
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:07:04 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H44N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:07:04 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

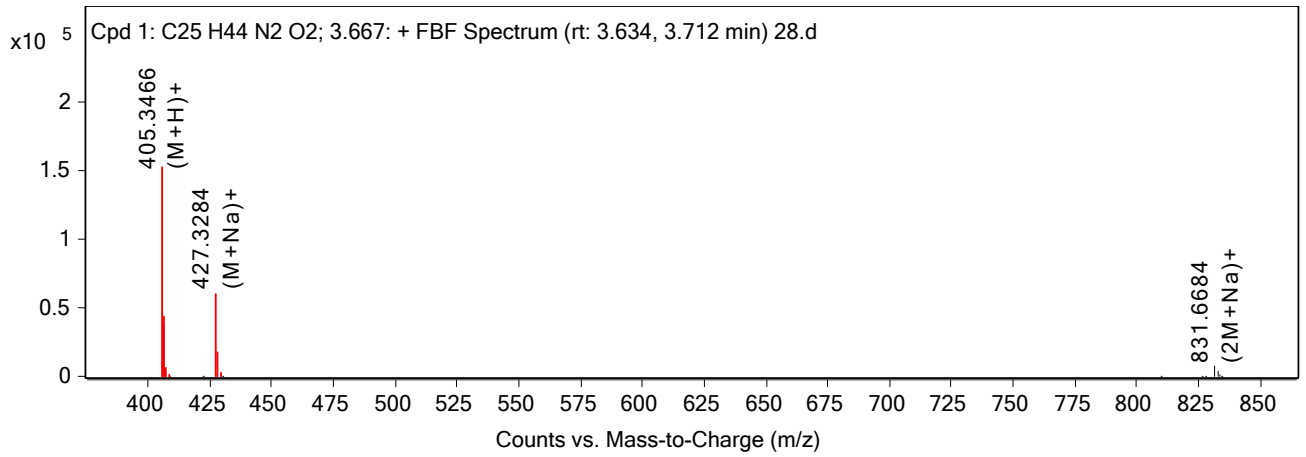
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H44 N2 O2; 3.667	94.6	-2.92	C25 H44 N2 O2	3.667	404.3403	404.3391

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
405.3466	3.667	404.3391	C25 H44 N2 O2	404.3403	-2.92	Find By Formula	

Compound Chromatograms



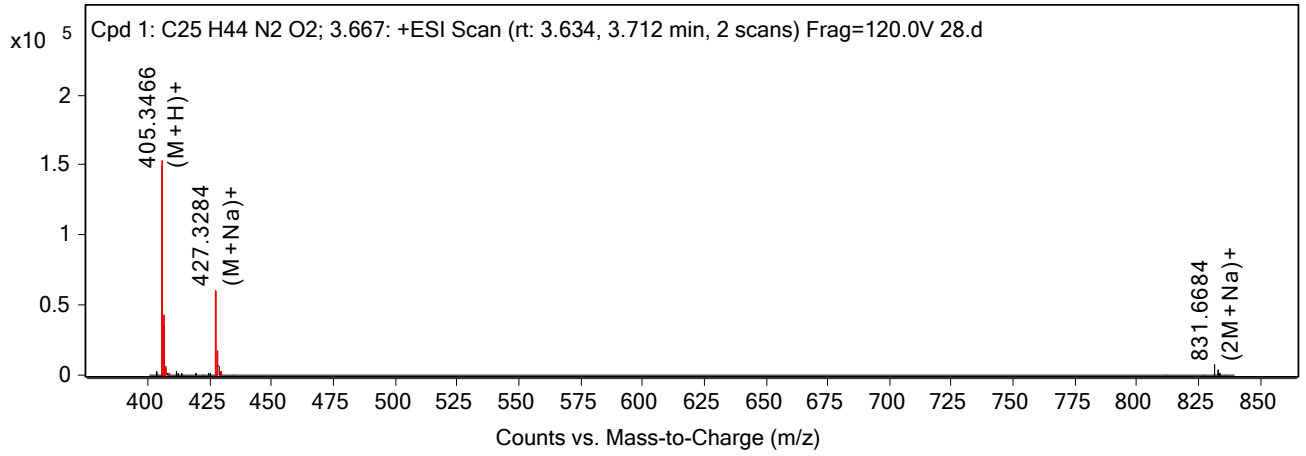
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
405.3466	1	152406.67	(M+H)+
406.3496	1	35746.78	(M+H)+
407.3522	1	5145.98	(M+H)+
408.3508	1	602.08	(M+H)+
427.3284	1	60534.8	(M+Na)+
428.3315	1	14707.77	(M+Na)+
429.3317	1	2699.94	(M+Na)+
831.6684	1	7108.09	(2M+Na)+
832.6707	1	4067.8	(2M+Na)+
833.6686	1	1243.77	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
405.3466	1	152406.66	(M+H)+	2.3
406.3496	1	35746.78	(M+H)+	2.96
407.3522	1	5145.98	(M+H)+	4.01
408.3508	1	602.08	(M+H)+	14.44
427.3284	1	60534.8	(M+Na)+	2.66
428.3315	1	14707.77	(M+Na)+	3
429.3317	1	2699.94	(M+Na)+	9.57
831.6684	1	7108.09	(2M+Na)+	1.65
832.6707	1	4067.8	(2M+Na)+	2.76
833.6686	1	1243.77	(2M+Na)+	9.04

--- End Of Report ---

Target Compound Screening Report

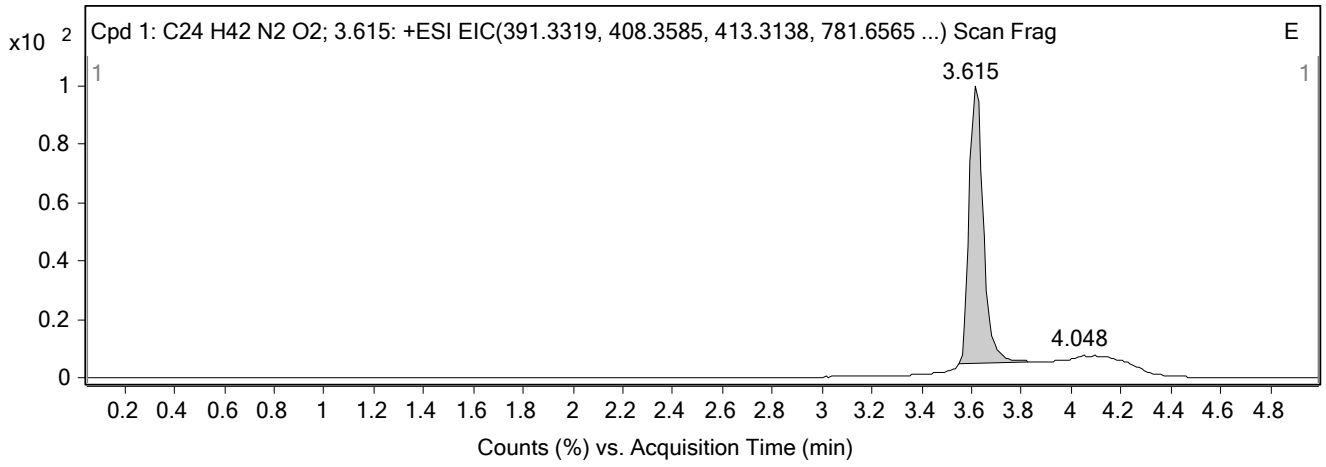
Data File	15-a3.d	**Sample Name**	H2986297
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 5:53:18 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 5:53:18 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

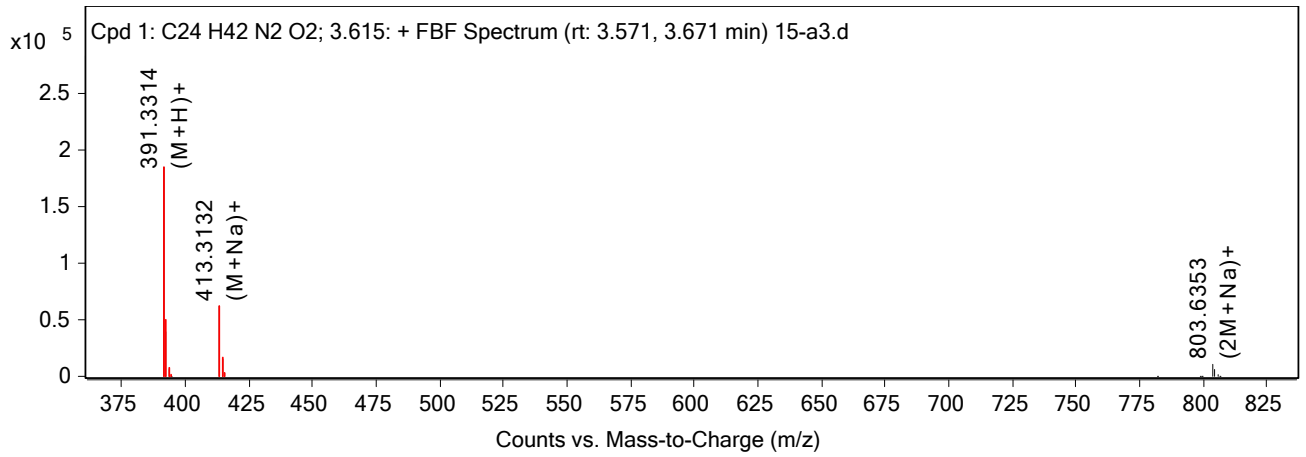
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.615	98.05	-1.81	C24 H42 N2 O2	3.615	390.3246	390.3239

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
413.3132	3.615	390.3239	C24 H42 N2 O2	390.3246	-1.81	Find By Formula	

Compound Chromatograms



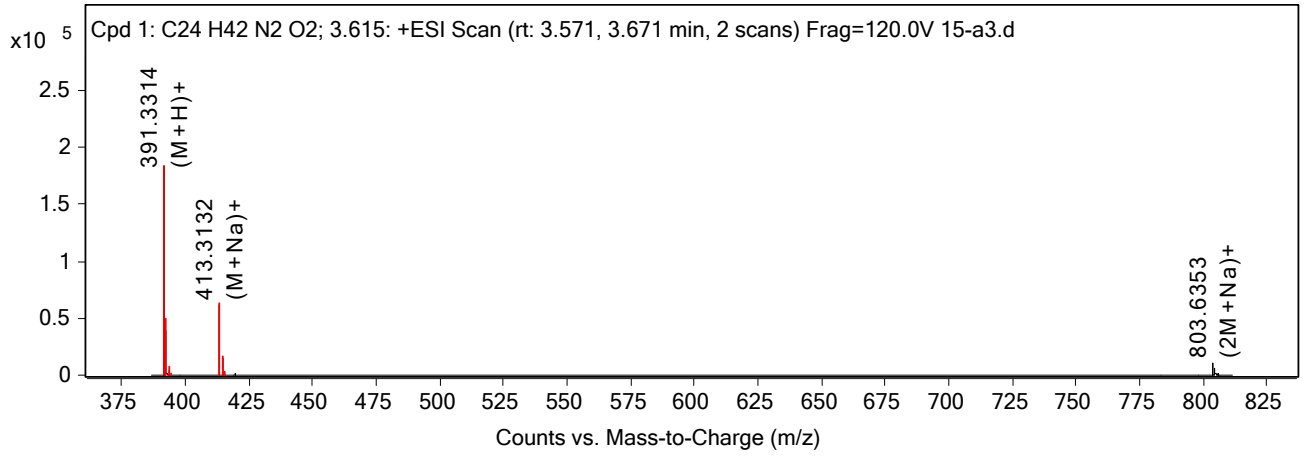
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3314	1	183993.78	(M+H)+
392.3345	1	39800.55	(M+H)+
393.3377	1	5452.61	(M+H)+
394.3343	1	682.64	(M+H)+
413.3132	1	62638.36	(M+Na)+
414.3163	1	15422.1	(M+Na)+
415.3187	1	2553.1	(M+Na)+
803.6353	1	10966.41	(2M+Na)+
804.6397	1	5701.53	(2M+Na)+
805.6421	1	1610.93	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3314	1	183993.78	(M+H)+	1.19
392.3345	1	39800.55	(M+H)+	1.56
393.3377	1	5452.61	(M+H)+	1.02
394.3343	1	682.64	(M+H)+	17.03
413.3132	1	62638.36	(M+Na)+	1.67
414.3163	1	15422.1	(M+Na)+	1.81
415.3187	1	2553.1	(M+Na)+	3.27
803.6353	1	10966.4	(2M+Na)+	3.91
804.6397	1	5701.53	(2M+Na)+	2.45
805.6421	1	1610.93	(2M+Na)+	3.41

--- End Of Report ---

Target Compound Screening Report

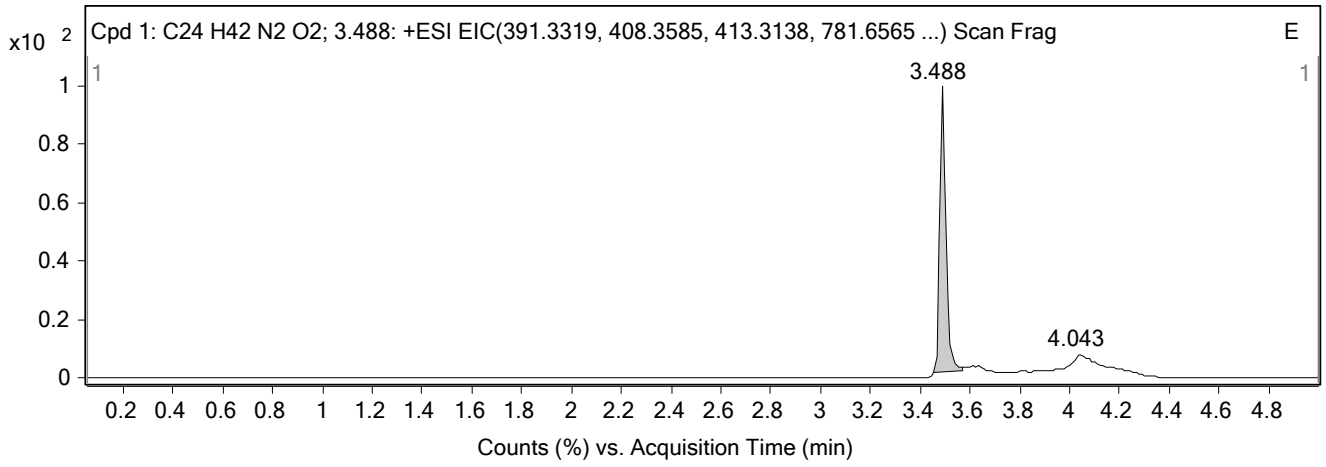
Data File	22.d	**Sample Name**	H2990768
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 12:15:20 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 12:15:20 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

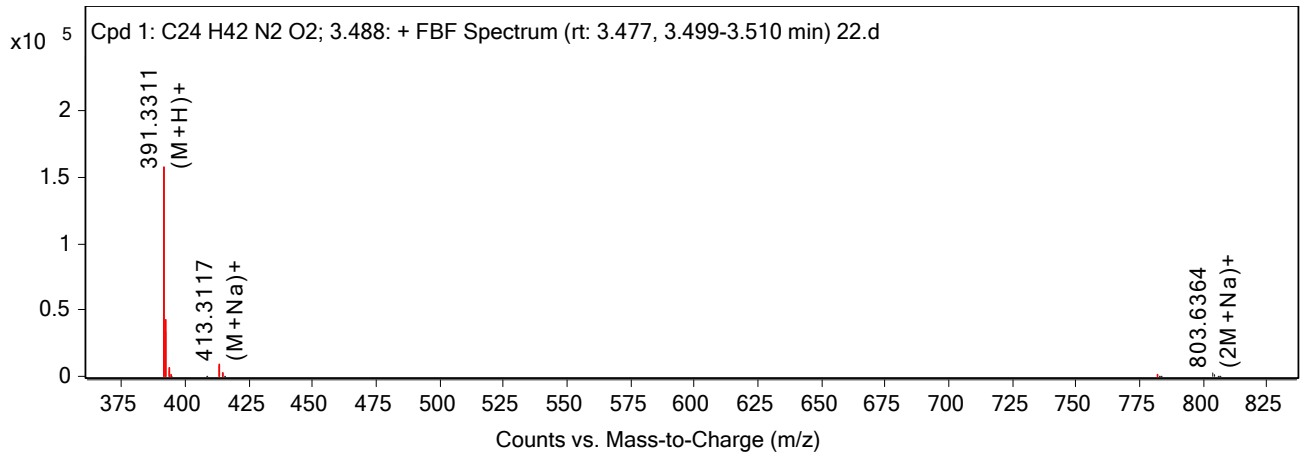
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.488	94.87	-2.42	C24 H42 N2 O2	3.488	390.3246	390.3237

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
803.6364	3.488	390.3237	C24 H42 N2 O2	390.3246	-2.42	Find By Formula	

Compound Chromatograms



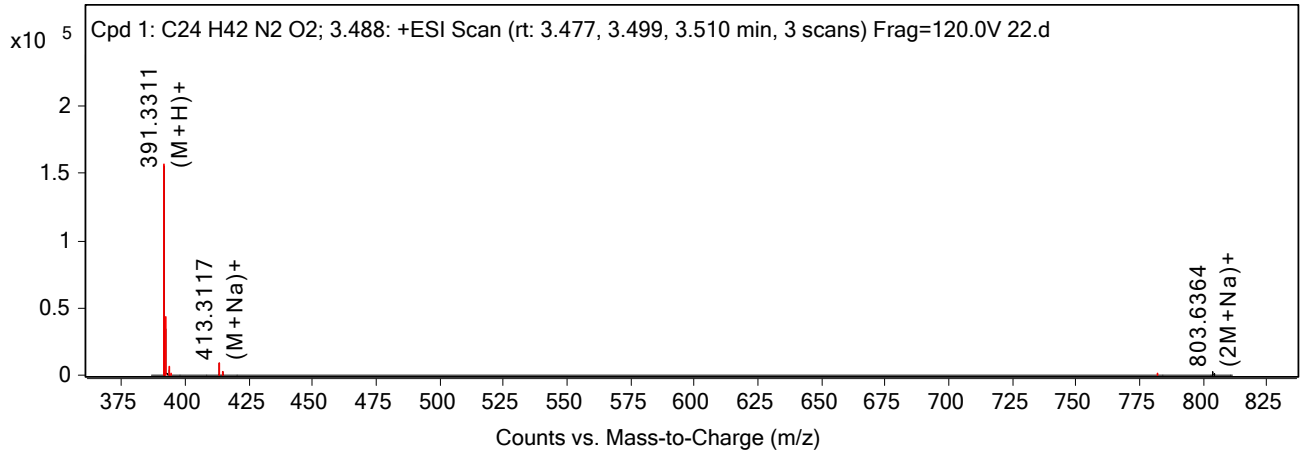
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3311	1	157186.2	(M+H)+
392.3343	1	34222.82	(M+H)+
393.3367	1	4374.26	(M+H)+
394.3365	1	581.23	(M+H)+
413.3117	1	8389.9	(M+Na)+
414.3157	1	2212.25	(M+Na)+
415.3139	1	561.18	(M+Na)+
781.6537	1	848.04	(2M+H)+
803.6364	1	2707.53	(2M+Na)+
804.6401	1	1508.45	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3311	1	157186.2	(M+H)+	2.05
392.3343	1	34222.83	(M+H)+	2.13
393.3367	1	4374.26	(M+H)+	3.68
394.3365	1	581.23	(M+H)+	11.37
413.3117	1	8389.9	(M+Na)+	5.14
414.3157	1	2212.25	(M+Na)+	3.3
415.3139	1	561.18	(M+Na)+	14.79
781.6537	1	848.04	(2M+H)+	3.65
803.6364	1	2707.53	(2M+Na)+	2.56
804.6401	1	1508.45	(2M+Na)+	2.05

--- End Of Report ---

Target Compound Screening Report

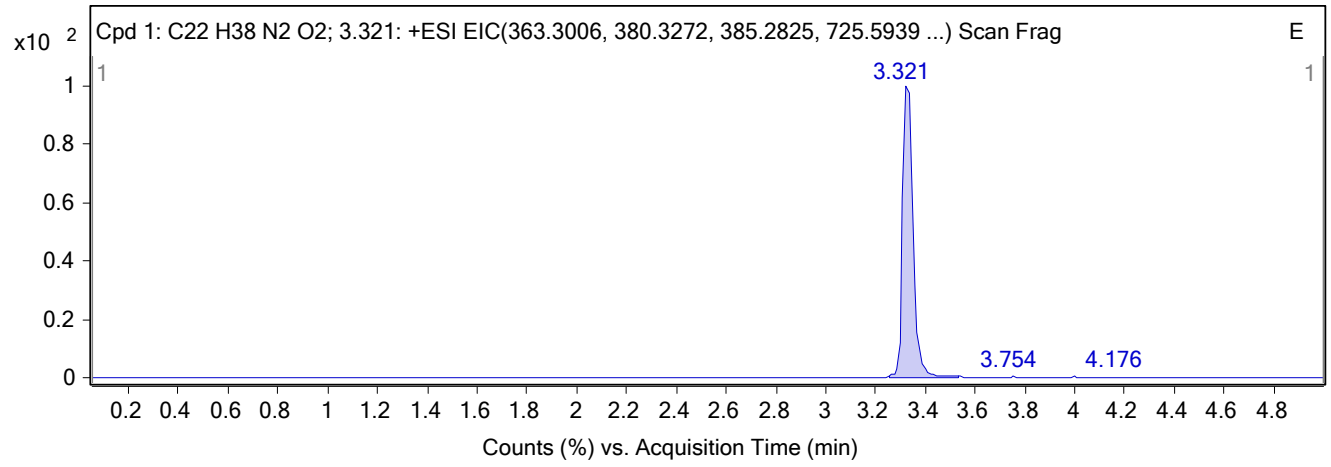
Data File	18.d	**Sample Name**	H2987841
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:22:21 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H38N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:22:21 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

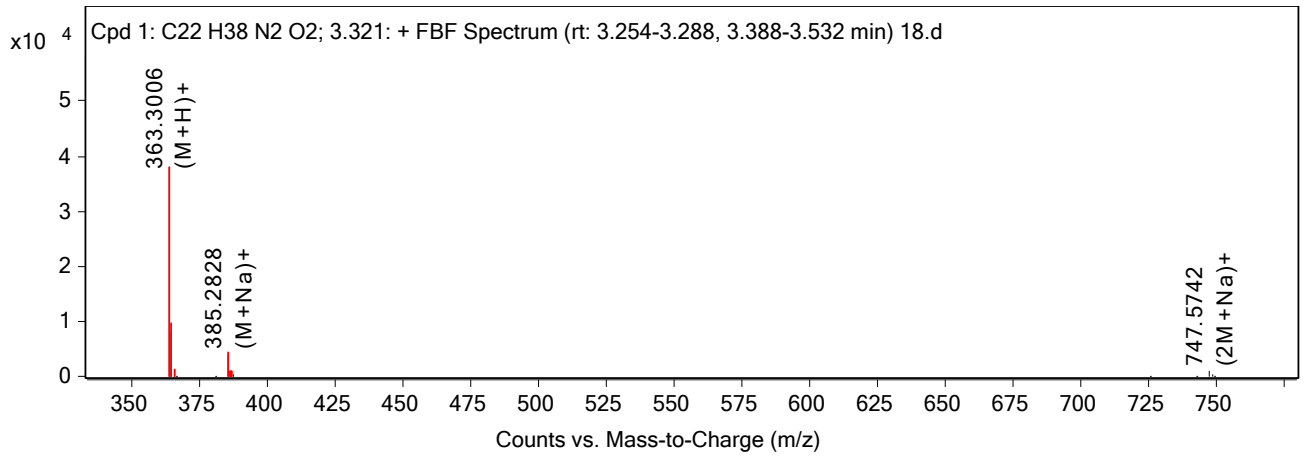
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H38 N2 O2; 3.321	97.7	-0.34	C22 H38 N2 O2	3.321	362.2933	362.2932

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
363.3006	3.321	362.2932	C22 H38 N2 O2	362.2933	-0.34	Find By Formula	

Compound Chromatograms



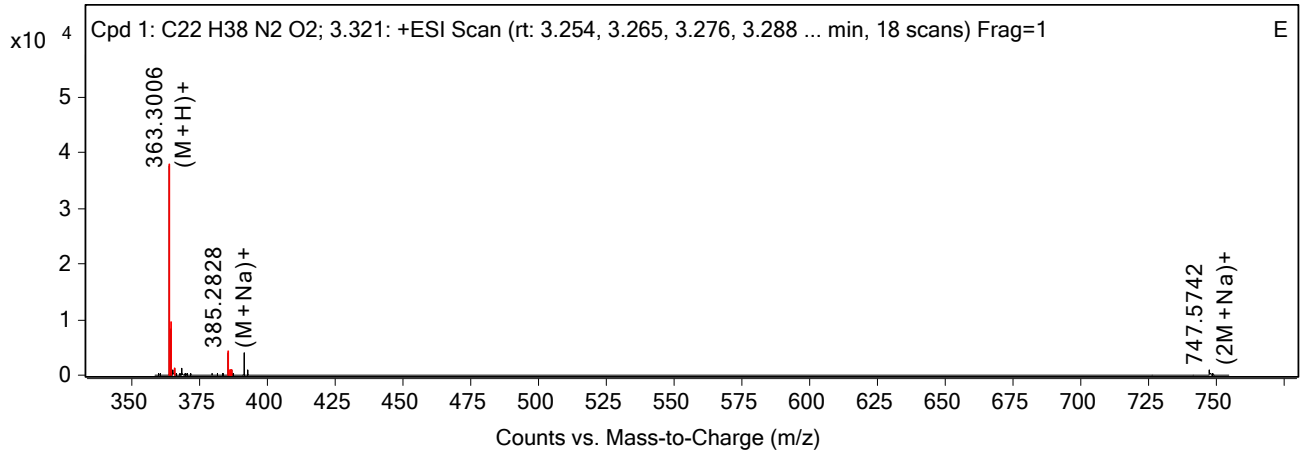
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
363.3006	1	37950.66	(M+H)+
364.3039	1	8242.74	(M+H)+
365.3048	1	1183.07	(M+H)+
366.3031	1	167.22	(M+H)+
385.2828	1	4117.02	(M+Na)+
386.286	1	1048.16	(M+Na)+
387.2843	1	236.5	(M+Na)+
747.5742	1	944.49	(2M+Na)+
748.578	1	475.91	(2M+Na)+
749.5795	1	162.14	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
363.3006	1	37950.66	(M+H)+	-0.12
364.3039	1	8242.74	(M+H)+	-0.08
365.3048	1	1183.07	(M+H)+	5.48
366.3031	1	167.22	(M+H)+	17.71
385.2828	1	4117.02	(M+Na)+	-0.66
386.286	1	1048.16	(M+Na)+	-0.48
387.2843	1	236.5	(M+Na)+	11.49
747.5742	1	944.49	(2M+Na)+	2.18
748.578	1	475.91	(2M+Na)+	1.41
749.5795	1	162.14	(2M+Na)+	3.54

--- End Of Report ---

Target Compound Screening Report

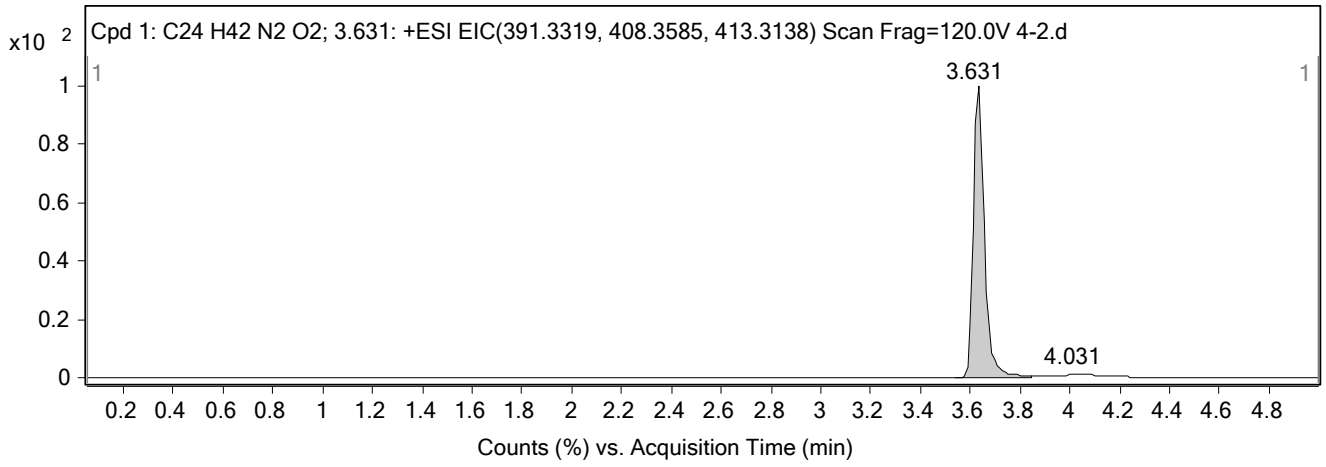
Data File	4-2.d	**Sample Name**	H2980753
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:26:58 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:26:58 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

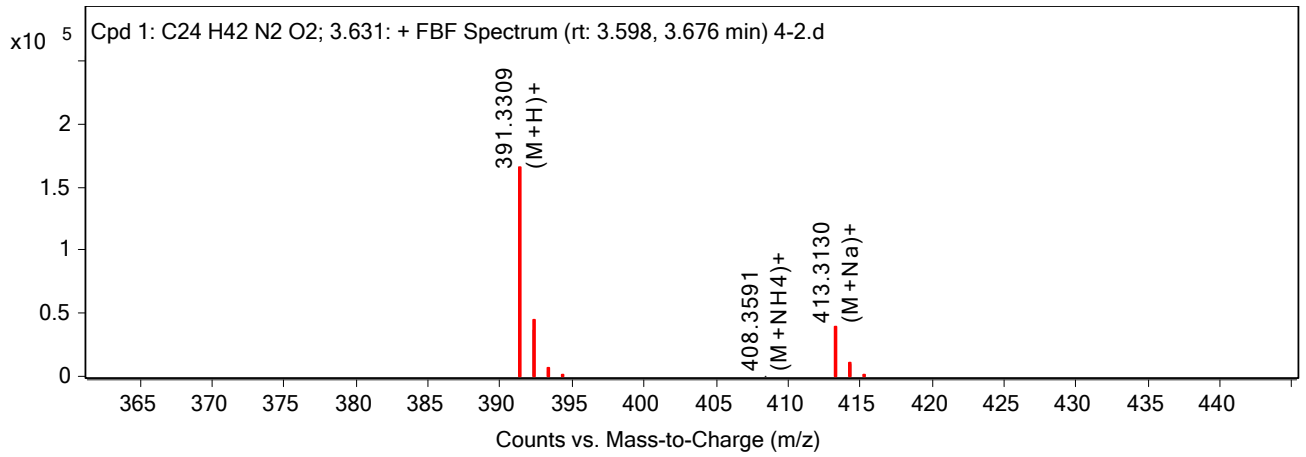
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.631	95.36	-2.58	C24 H42 N2 O2	3.631	390.3246	390.3236

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
413.313	3.631	390.3236	C24 H42 N2 O2	390.3246	-2.58	Find By Formula	

Compound Chromatograms



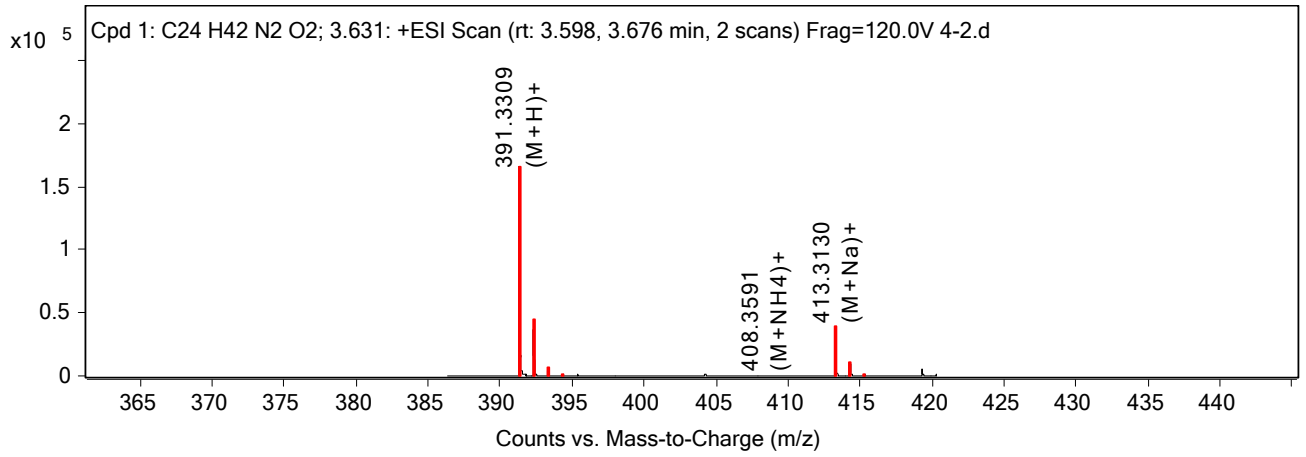
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3309	1	165707.5	(M+H)+
392.3338	1	37082.18	(M+H)+
393.3377	1	4610.06	(M+H)+
394.3359	1	735.86	(M+H)+
408.3591	1	184.18	(M+NH4)+
413.313	1	38906.3	(M+Na)+
414.3159	1	9269.09	(M+Na)+
415.3208	1	1666.13	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3309	1	165707.5	(M+H)+	2.48
391.3309		165707.5		
392.3338	1	37082.17	(M+H)+	3.47
393.3377	1	4610.06	(M+H)+	1.24
394.3359	1	735.86	(M+H)+	12.93
408.3591	1	184.18	(M+NH4)+	-1.56
413.313	1	38906.31	(M+Na)+	2.05
414.3159	1	9269.09	(M+Na)+	2.79
415.3208	1	1666.13	(M+Na)+	-1.75

--- End Of Report ---

Target Compound Screening Report

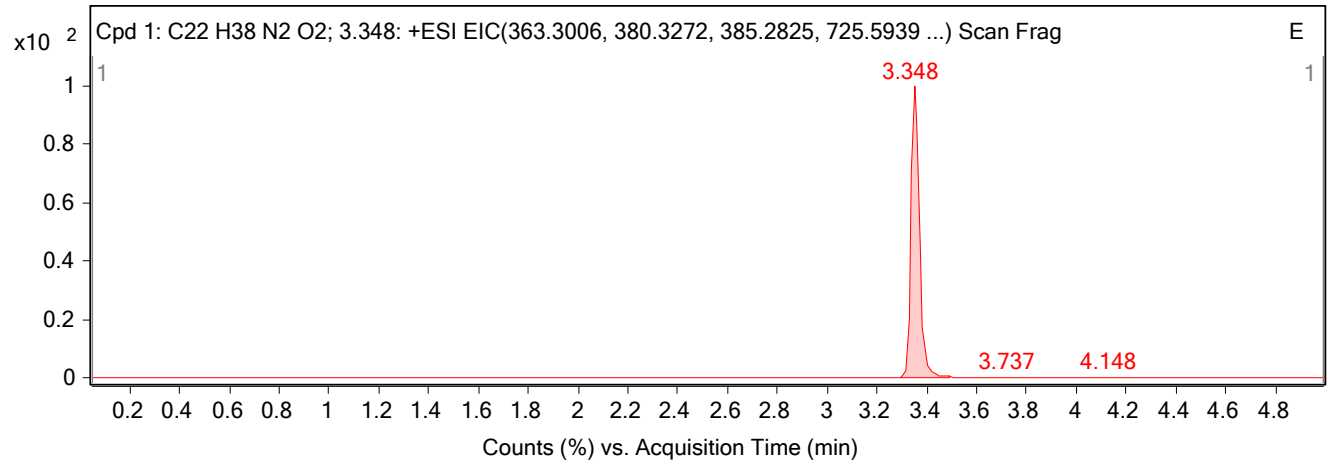
Data File	16.d	**Sample Name**	H2986293
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:11:13 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H38N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:11:13 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

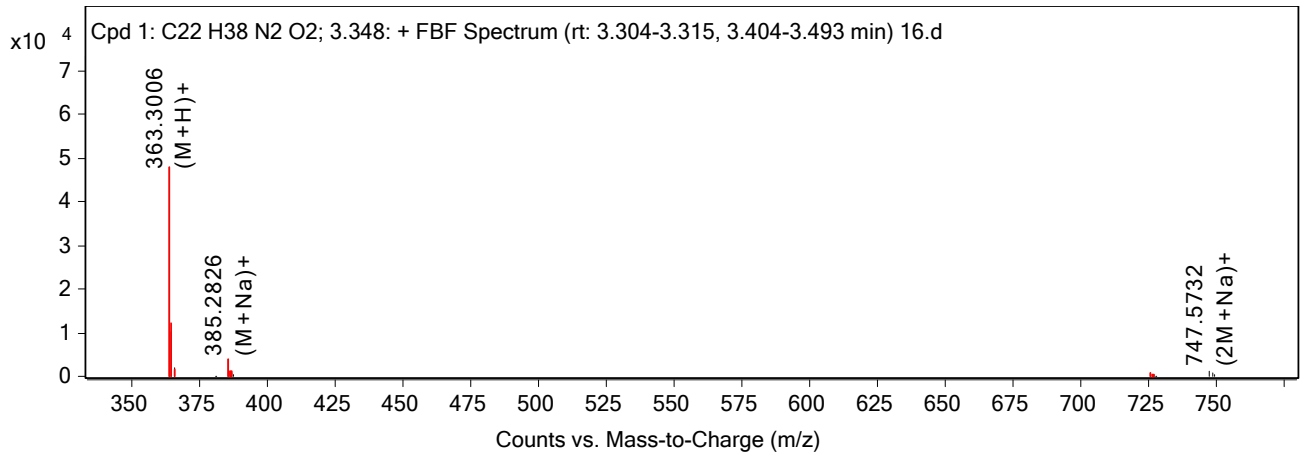
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H38 N2 O2; 3.348	97.21	-0.25	C22 H38 N2 O2	3.348	362.2933	362.2932

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
363.3006	3.348	362.2932	C22 H38 N2 O2	362.2933	-0.25	Find By Formula	

Compound Chromatograms



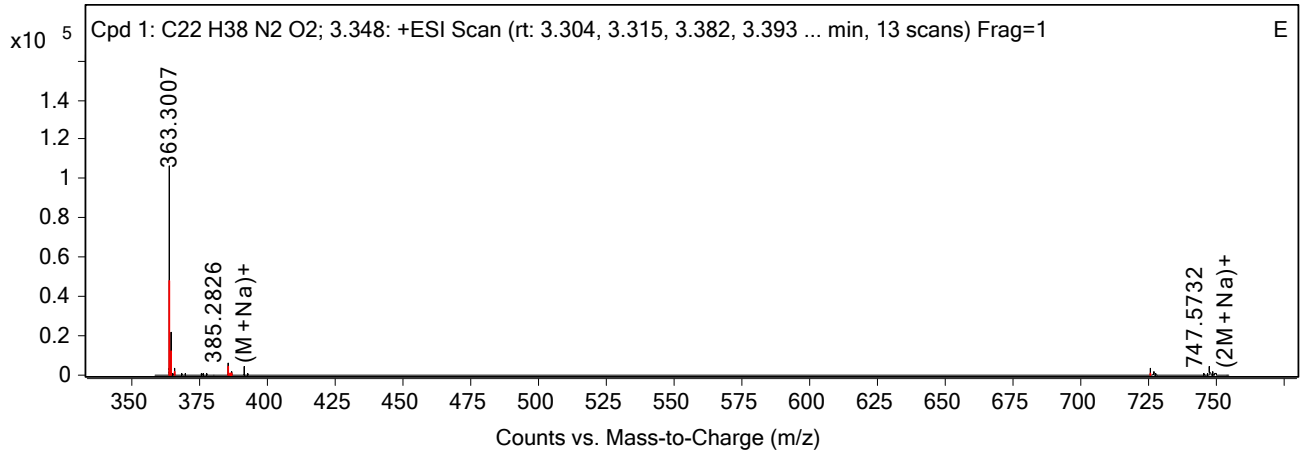
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
363.3006	1	47887.86	(M+H)+
364.3038	1	10303.15	(M+H)+
365.3085	1	1855.27	(M+H)+
385.2826	1	3929.68	(M+Na)+
386.2868	1	970.68	(M+Na)+
387.2885	1	288.41	(M+Na)+
725.5925	1	741.21	(2M+H)+
726.5945	1	454.63	(2M+H)+
747.5732	1	1264.37	(2M+Na)+
748.5762	1	629.96	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
363.3006	1	47887.85	(M+H)+	-0.04
364.3038	1	10303.15	(M+H)+	0.17
365.3085	1	1855.27	(M+H)+	-4.8
385.2826	1	3929.68	(M+Na)+	-0.26
386.2868	1	970.68	(M+Na)+	-2.78
387.2885	1	288.41	(M+Na)+	0.62
725.5925	1	741.21	(2M+H)+	2.02
726.5945	1	454.63	(2M+H)+	3.61
747.5732	1	1264.37	(2M+Na)+	3.58
748.5762	1	629.96	(2M+Na)+	3.85

--- End Of Report ---

Target Compound Screening Report

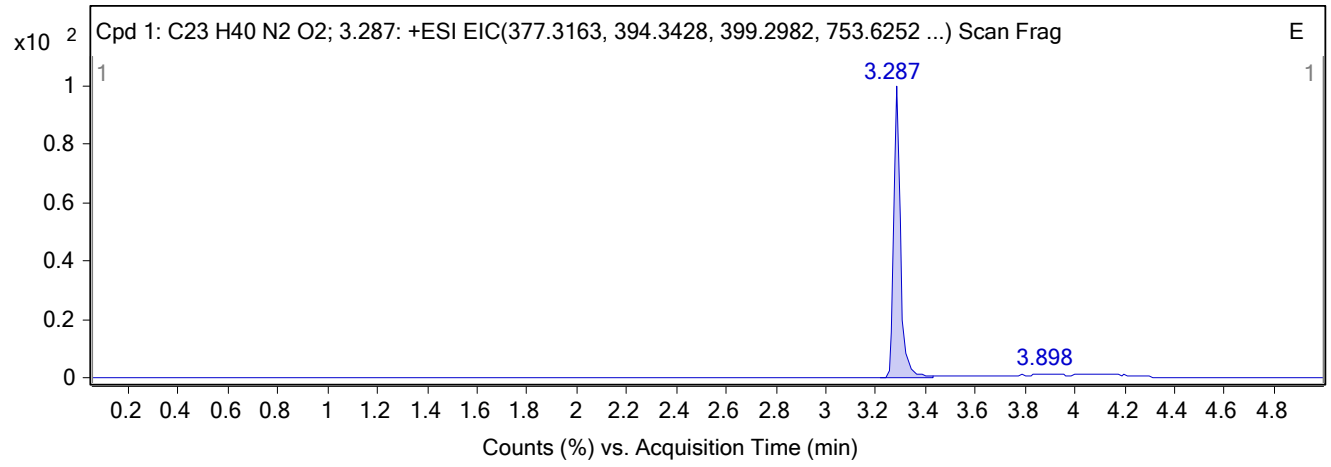
Data File	24.d	**Sample Name**	H2987842
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 12:45:00 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H40N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 12:45:00 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

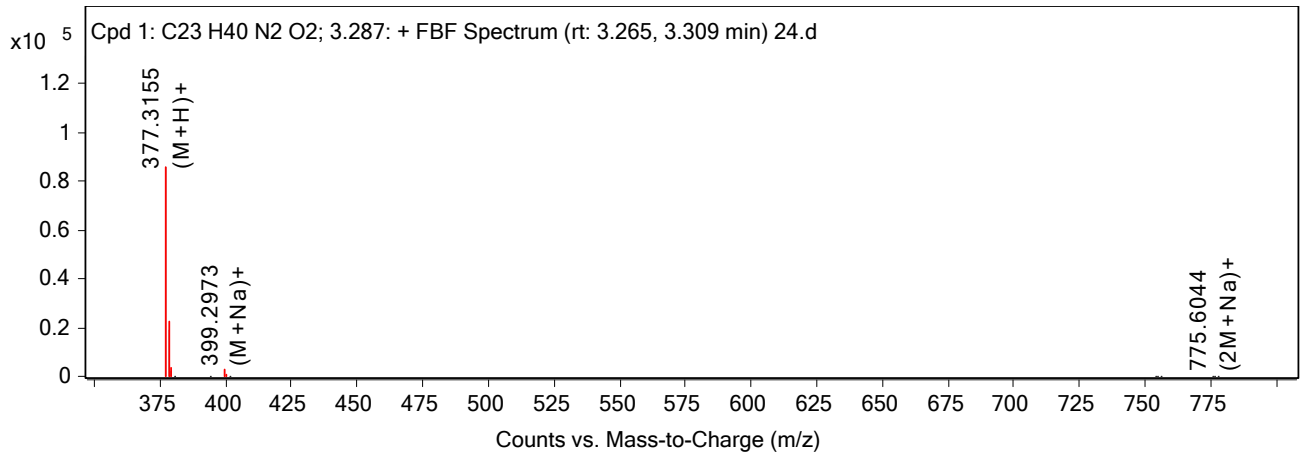
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H40 N2 O2; 3.287	96.01	-2.23	C23 H40 N2 O2	3.287	376.309	376.3081

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
377.3155	3.287	376.3081	C23 H40 N2 O2	376.309	-2.23	Find By Formula	

Compound Chromatograms



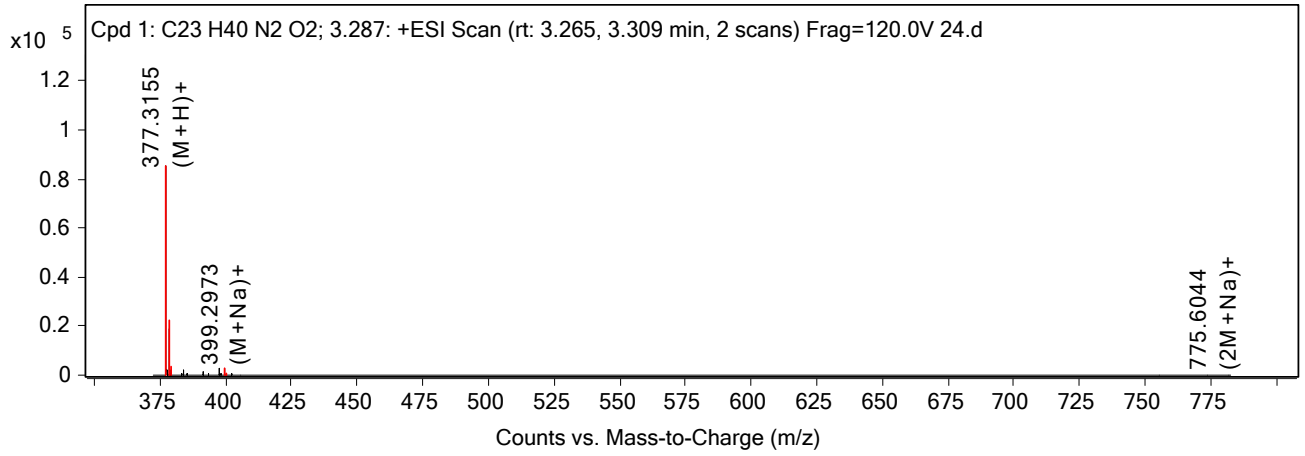
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
377.3155	1	85542.08	(M+H)+
378.3188	1	18818.13	(M+H)+
379.3219	1	2489.17	(M+H)+
380.3247	1	245.07	(M+H)+
399.2973	1	2521.12	(M+Na)+
400.2993	1	815.44	(M+Na)+
401.2943	1	218.01	(M+Na)+
753.6175	1	162.61	(2M+H)+
775.6044	1	384.5	(2M+Na)+
776.6032	1	205.69	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
377.3155	1	85542.08	(M+H)+	2.08
378.3188	1	18818.13	(M+H)+	1.95
379.3219	1	2489.17	(M+H)+	1.63
380.3247	1	245.07	(M+H)+	1.64
399.2973	1	2521.12	(M+Na)+	2.23
400.2993	1	815.44	(M+Na)+	5.27
401.2943	1	218.01	(M+Na)+	25.13
753.6175	1	162.61	(2M+H)+	10.31
775.6044	1	384.5	(2M+Na)+	3.62
776.6032	1	205.69	(2M+Na)+	9.34

--- End Of Report ---

Target Compound Screening Report

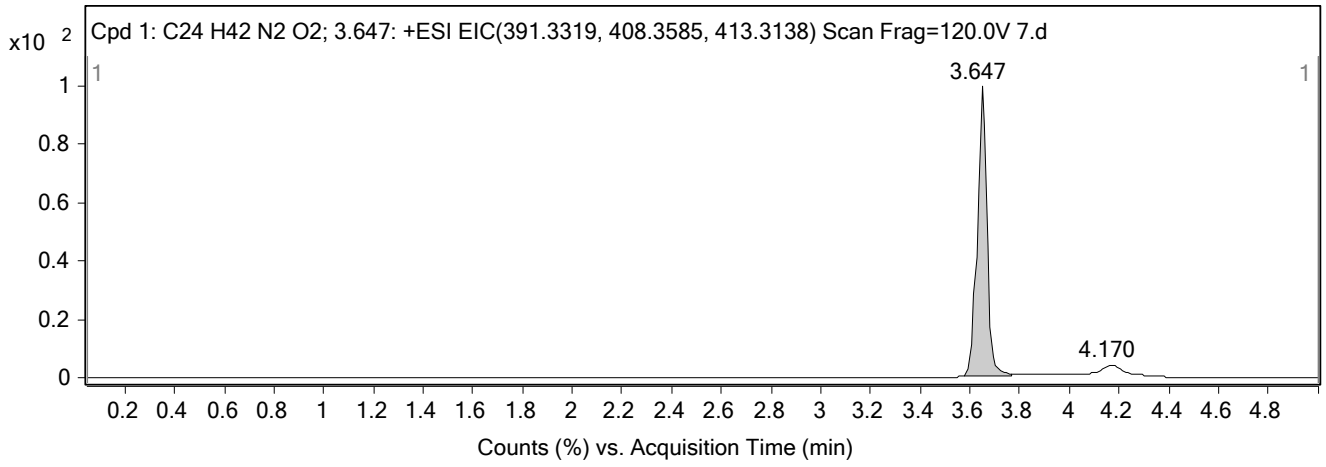
Data File	7.d	**Sample Name**	H2990491
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/7/2021 5:15:06 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/7/2021 5:15:06 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.647	95.34	-0.75	C24 H42 N2 O2	3.647	390.3246	390.3243

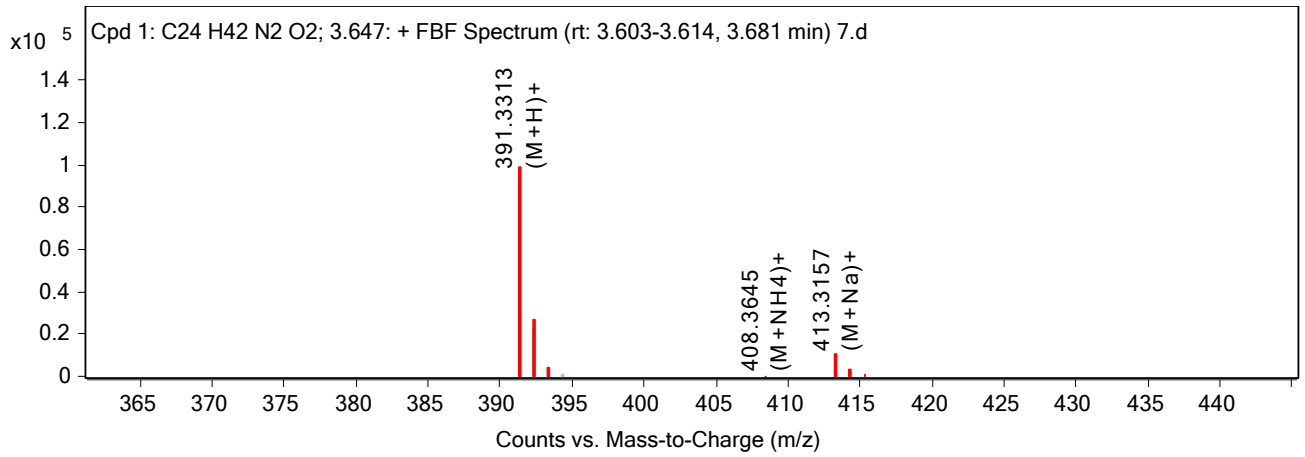
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
391.3313	3.647	390.3243	C24 H42 N2 O2	390.3246	-0.75	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

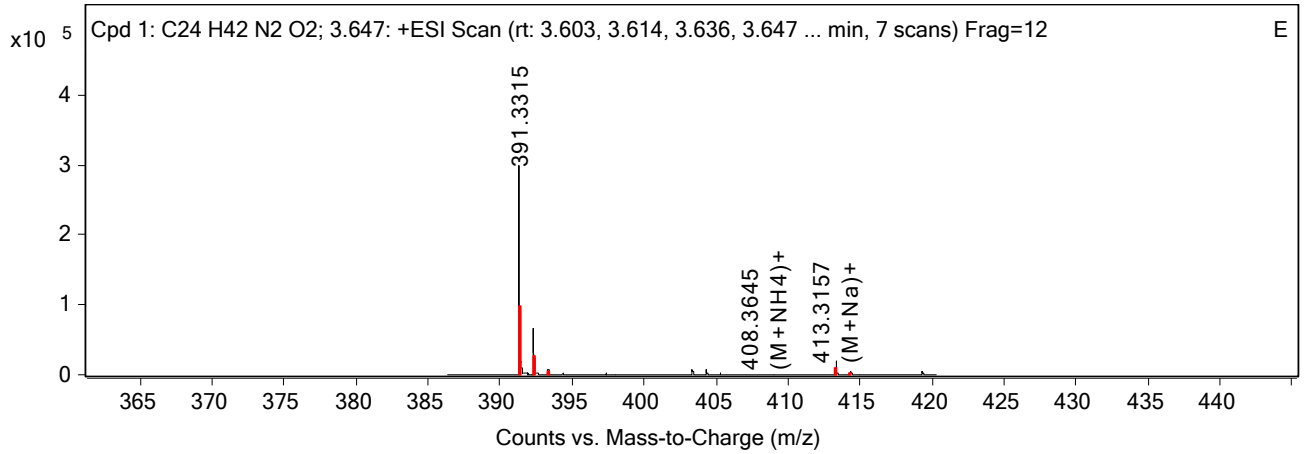
Agilent Technologies



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3313	1	98789.72	(M+H)+
392.3346	1	22481.72	(M+H)+
393.3358	1	3314.95	(M+H)+
408.3645	1	225.44	(M+NH4)+
413.3157	1	10243.92	(M+Na)+
414.3238	1	2865.45	(M+Na)+
415.3151	1	793.69	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3313	1	98789.72	(M+H)+	1.43
391.3315		298853.51		
392.3346	1	22481.72	(M+H)+	1.45
393.3358	1	3314.95	(M+H)+	6.06
408.3645	1	225.44	(M+NH4)+	-14.85
413.3157	1	10243.93	(M+Na)+	-4.48
414.3238	1	2865.45	(M+Na)+	-16.1
415.3151	1	793.69	(M+Na)+	11.94

--- End Of Report ---

Target Compound Screening Report

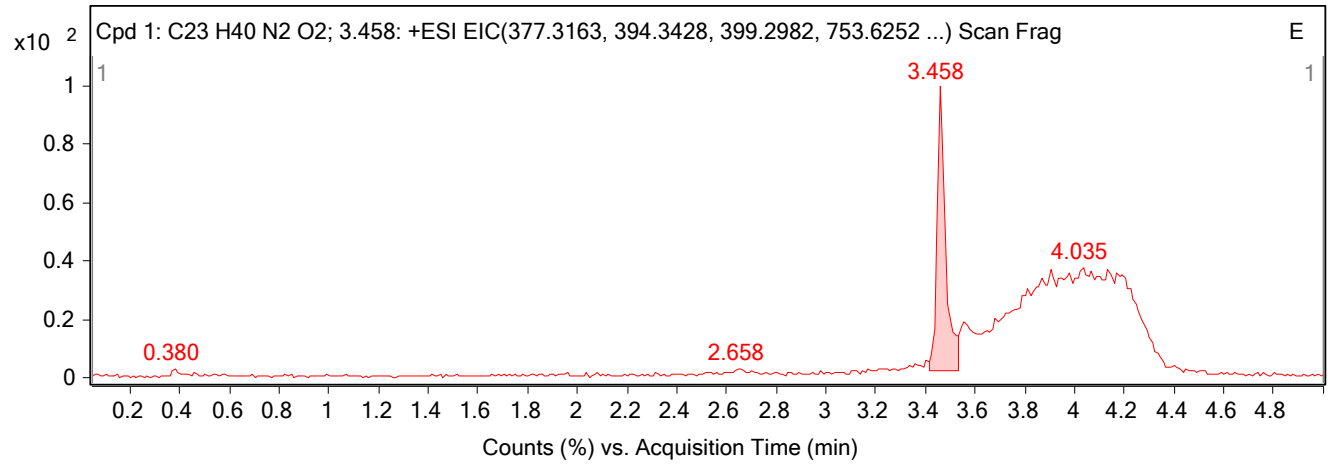
Data File	16-5.d	**Sample Name**	H2986295
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 4:33:24 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H40N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 4:33:24 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

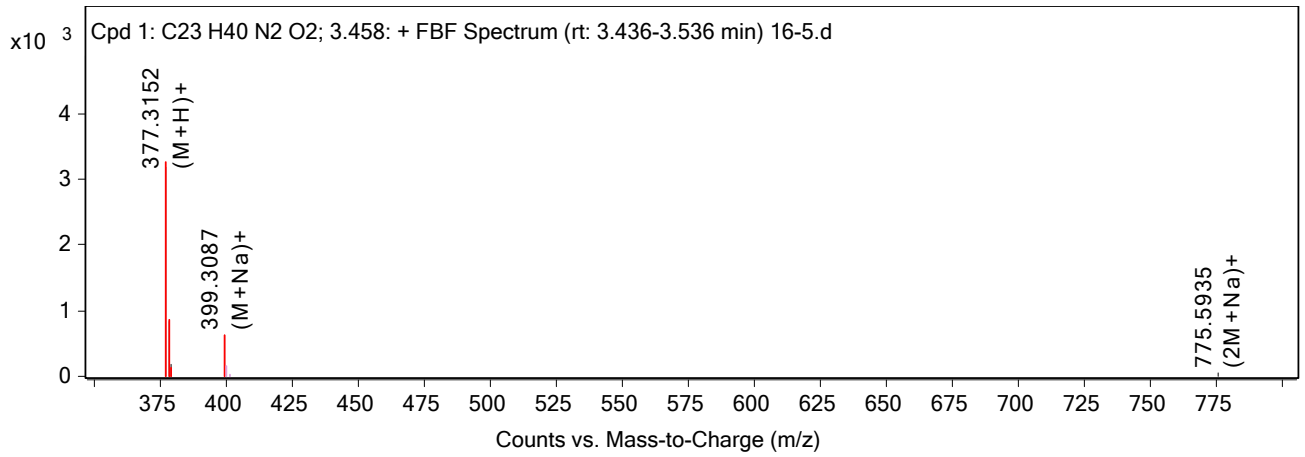
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H40 N2 O2; 3.458	96.06	0.65	C23 H40 N2 O2	3.458	376.309	376.3092

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
377.3152	3.458	376.3092	C23 H40 N2 O2	376.309	0.65	Find By Formula	

Compound Chromatograms



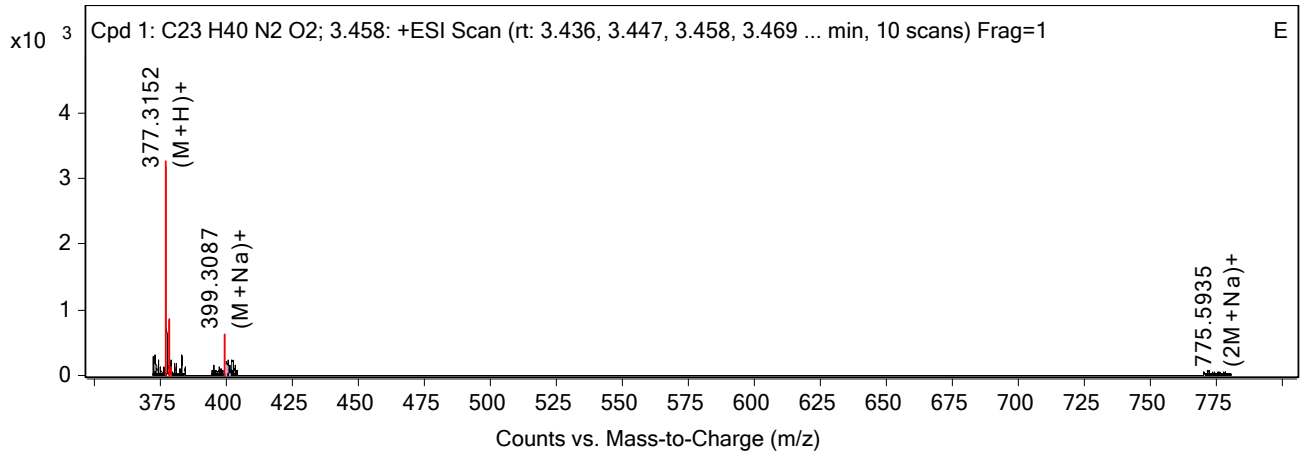
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
377.3152	1	3200.99	(M+H)+
378.319	1	845.65	(M+H)+
379.3186	1	190.26	(M+H)+
399.3087	1	633.02	(M+Na)+
775.5935	1	62.1	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
377.3152	1	3200.99	(M+H)+	2.86
378.319	1	845.65	(M+H)+	1.22
379.3186	1	190.26	(M+H)+	10.19
399.3087	1	633.02	(M+Na)+	-26.25
775.5935	1	62.1	(2M+Na)+	17.6

--- End Of Report ---

Target Compound Screening Report

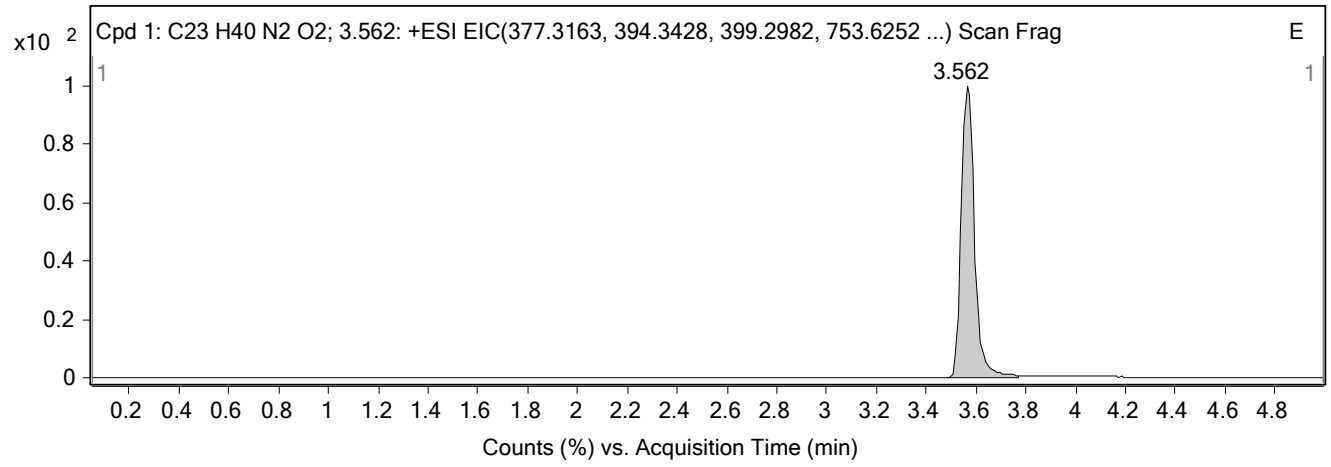
Data File	15.d	**Sample Name**	H2987844
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:05:40 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H40N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:05:40 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

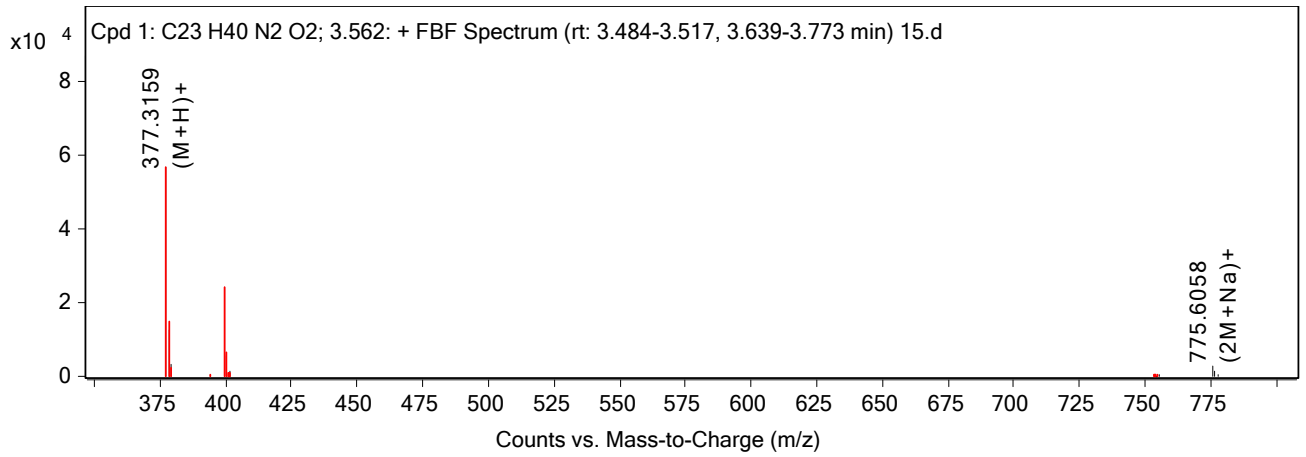
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H40 N2 O2; 3.562	93.82	-0.95	C23 H40 N2 O2	3.562	376.309	376.3086

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
377.3159	3.562	376.3086	C23 H40 N2 O2	376.309	-0.95	Find By Formula	

Compound Chromatograms



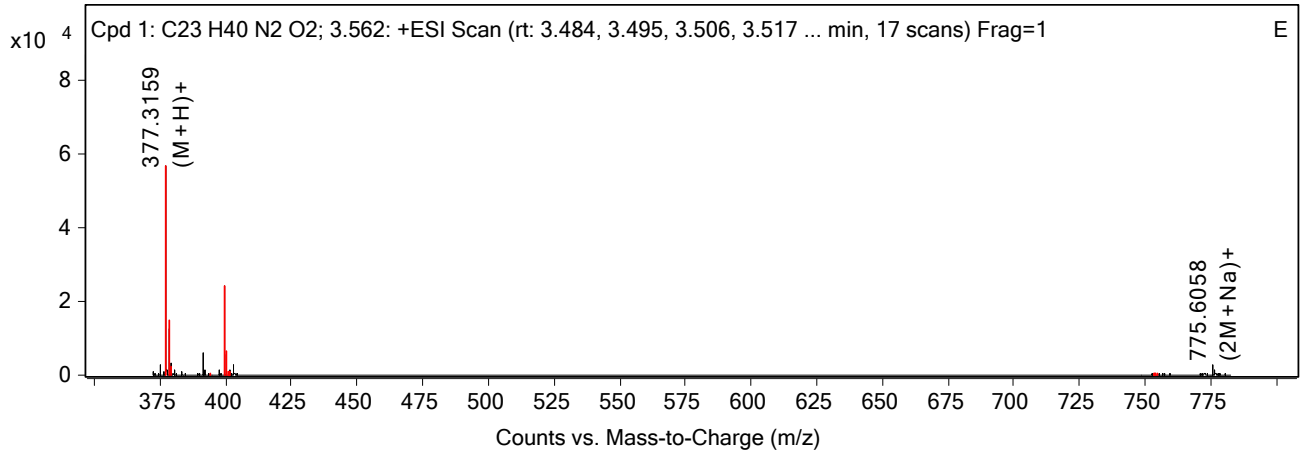
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
377.3159	1	56735.79	(M+H)+
378.3192	1	12484.55	(M+H)+
379.3266	1	3094.38	(M+H)+
399.298	1	24281.5	(M+Na)+
400.301	1	5641.24	(M+Na)+
401.3096	1	1526.26	(M+Na)+
754.6242	1	302.18	(2M+H)+
775.6058	1	2665.99	(2M+Na)+
776.6059	1	1493.38	(2M+Na)+
777.6086	1	613.83	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
377.3159	1	56735.79	(M+H)+	0.95
378.3192	1	12484.55	(M+H)+	0.83
379.3266	1	3094.38	(M+H)+	-10.91
399.298	1	24281.5	(M+Na)+	0.59
400.301	1	5641.24	(M+Na)+	0.98
401.3096	1	1526.26	(M+Na)+	-13
754.6242	1	302.18	(2M+H)+	5.7
775.6058	1	2665.99	(2M+Na)+	1.77
776.6059	1	1493.38	(2M+Na)+	5.8
777.6086	1	613.83	(2M+Na)+	6.26

--- End Of Report ---

Target Compound Screening Report

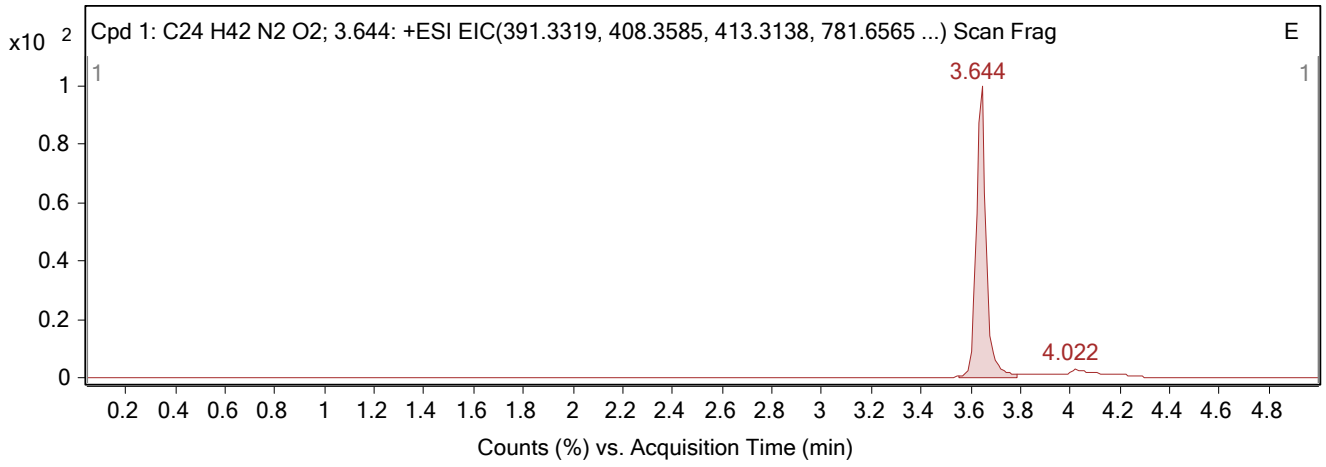
Data File	20.d	**Sample Name**	H2986947
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 12:04:18 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 12:04:18 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

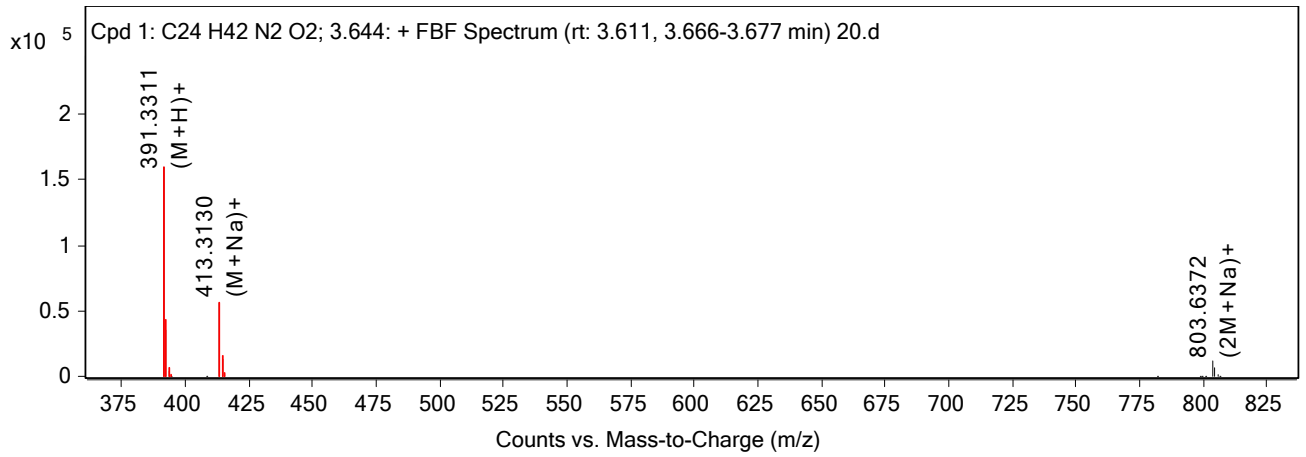
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.644	98.34	-2.49	C24 H42 N2 O2	3.644	390.3246	390.3237

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
803.6372	3.644	390.3237	C24 H42 N2 O2	390.3246	-2.49	Find By Formula	

Compound Chromatograms



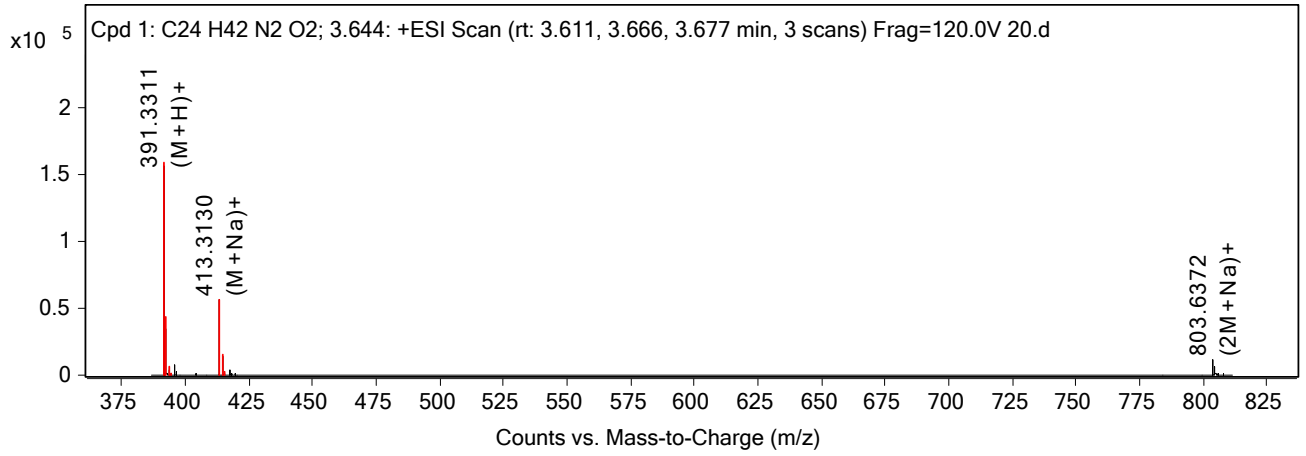
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3311	1	159283.53	(M+H)+
392.3341	1	35164.73	(M+H)+
393.3372	1	4554.9	(M+H)+
394.3383	1	643.87	(M+H)+
413.313	1	56289.82	(M+Na)+
414.3157	1	13612.59	(M+Na)+
415.319	1	1899.72	(M+Na)+
803.6372	1	11544.44	(2M+Na)+
804.6397	1	6031.28	(2M+Na)+
805.6432	1	1734.36	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3311	1	159283.54	(M+H)+	2.16
392.3341	1	35164.73	(M+H)+	2.65
393.3372	1	4554.9	(M+H)+	2.31
394.3383	1	643.87	(M+H)+	6.98
413.313	1	56289.82	(M+Na)+	2.07
414.3157	1	13612.59	(M+Na)+	3.31
415.319	1	1899.72	(M+Na)+	2.7
803.6372	1	11544.44	(2M+Na)+	1.55
804.6397	1	6031.28	(2M+Na)+	2.51
805.6432	1	1734.36	(2M+Na)+	2.07

--- End Of Report ---

Target Compound Screening Report

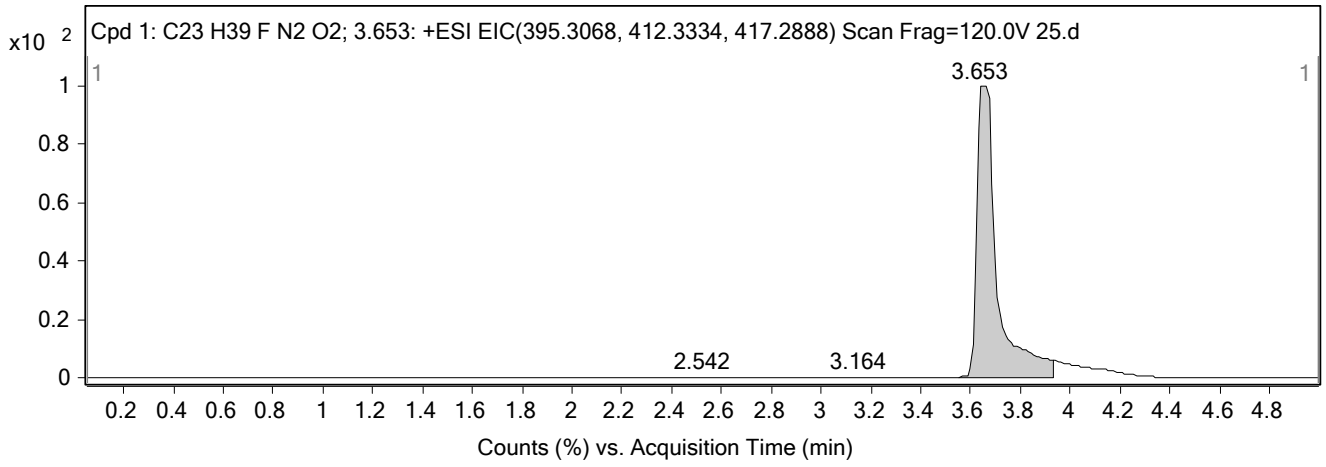
Data File	25.d	**Sample Name**	H3486837
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	10/8/2021 3:28:52 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H39FN2O2	**Stream Name**	LC 1
Acquisition Time (Local)	10/8/2021 3:28:52 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H39 F N2 O2; 3.653	86.75	-1.63	C23 H39 F N2 O2	3.653	394.2996	394.2989

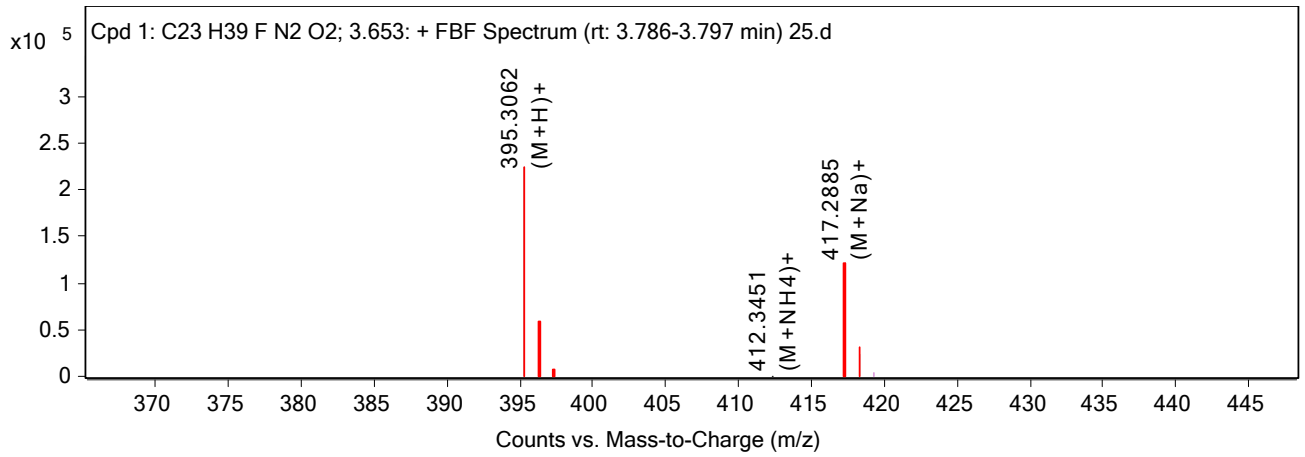
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
395.3062	3.653	394.2989	C23 H39 F N2 O2	394.2996	-1.63	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

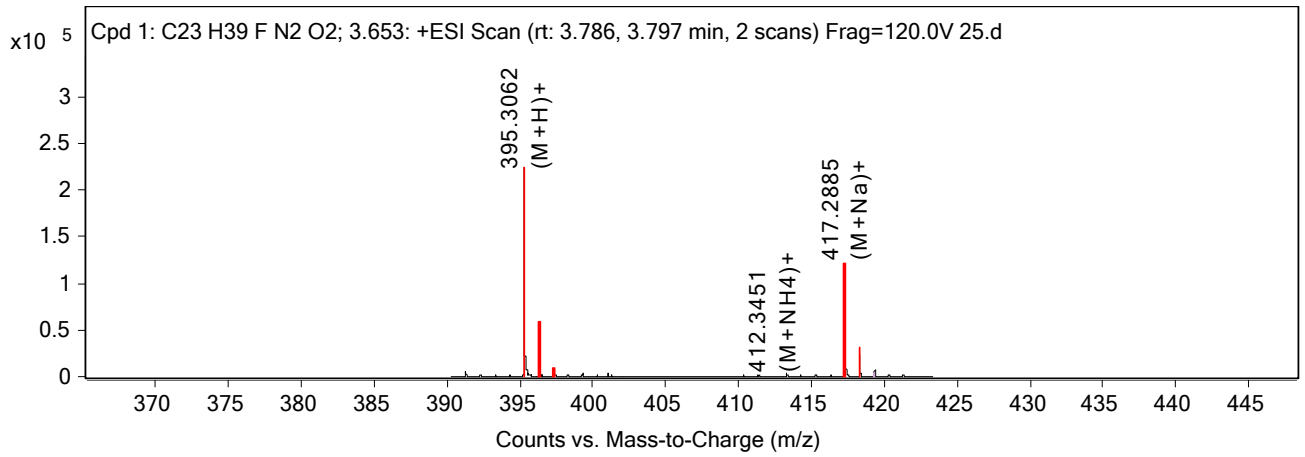
Agilent Technologies



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
395.3062	1	223752.03	(M+H)+
396.3098	1	46393.2	(M+H)+
397.3007	1	7963.53	(M+H)+
412.3451	1	486.37	(M+NH4)+
417.2885	1	120792.13	(M+Na)+
418.2925	1	24671.84	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
395.3062	1	223752.03	(M+H)+	1.6
395.3062		223752.03		
396.3098	1	46393.2	(M+H)+	0.64
397.3007	1	7963.53	(M+H)+	31.09
412.3451	1	486.37	(M+NH4)+	-28.48
417.2885	1	120792.13	(M+Na)+	0.78
418.2925	1	24671.84	(M+Na)+	-1.16

--- End Of Report ---

Target Compound Screening Report

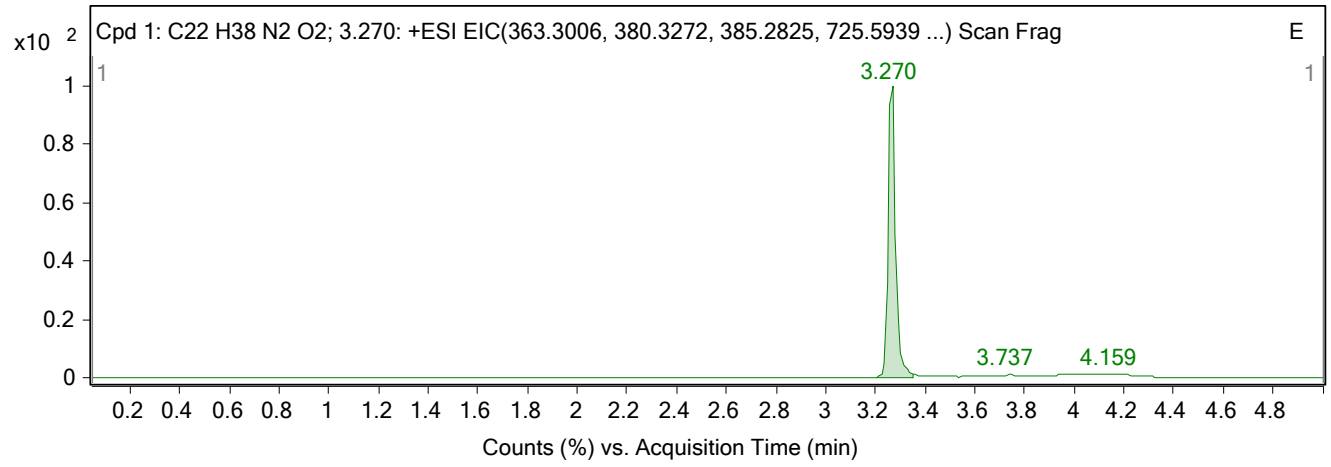
Data File	17.d	**Sample Name**	H2987845
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:16:48 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H38N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:16:48 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

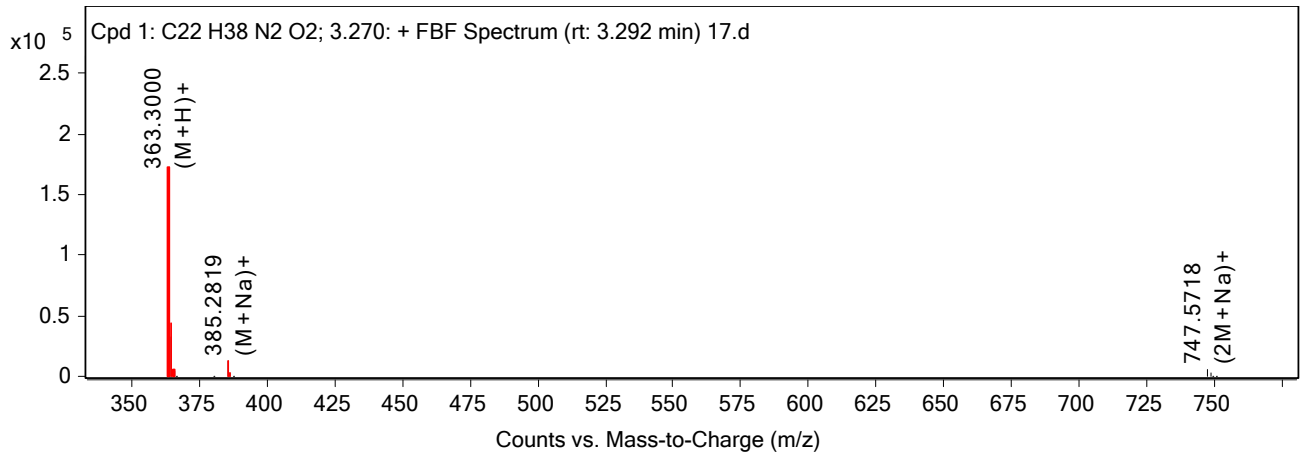
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H38 N2 O2; 3.270	98.01	-1.99	C22 H38 N2 O2	3.27	362.2933	362.2926

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
385.2819	3.27	362.2926	C22 H38 N2 O2	362.2933	-1.99	Find By Formula	

Compound Chromatograms



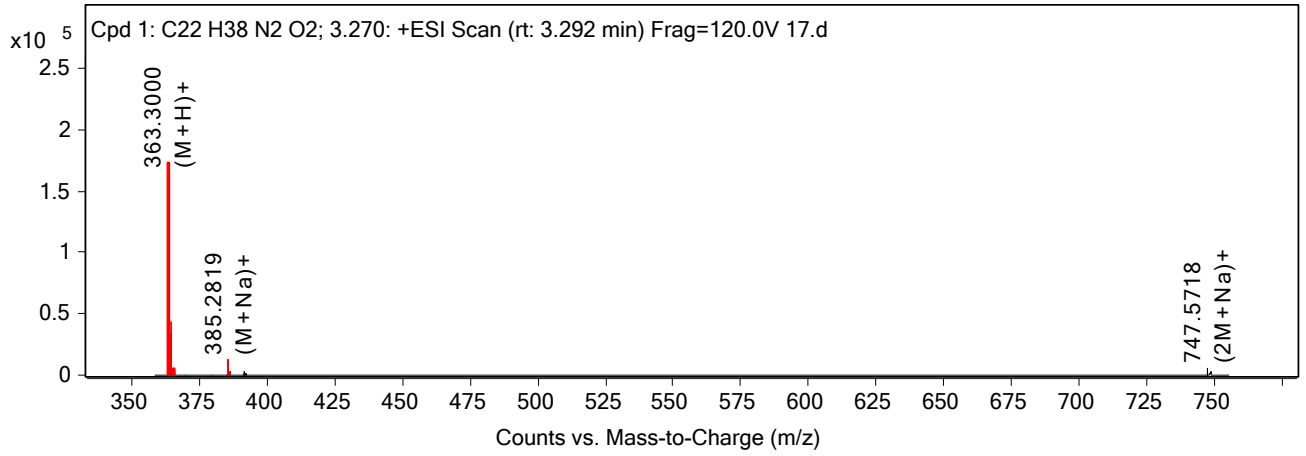
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
363.3	1	172473.55	(M+H)+
364.3035	1	33215.32	(M+H)+
365.3066	1	4170.14	(M+H)+
366.3097	1	516	(M+H)+
385.2819	1	13034.42	(M+Na)+
386.2849	1	3121.38	(M+Na)+
387.2853	1	586.75	(M+Na)+
747.5718	1	5772.5	(2M+Na)+
748.5763	1	2706.85	(2M+Na)+
749.5754	1	770.83	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
363.3	1	172473.55	(M+H)+	1.75
364.3035	1	33215.32	(M+H)+	0.78
365.3066	1	4170.14	(M+H)+	0.56
366.3097	1	516	(M+H)+	-0.21
385.2819	1	13034.42	(M+Na)+	1.73
386.2849	1	3121.38	(M+Na)+	2.2
387.2853	1	586.75	(M+Na)+	8.82
747.5718	1	5772.5	(2M+Na)+	5.5
748.5763	1	2706.85	(2M+Na)+	3.8
749.5754	1	770.83	(2M+Na)+	9.01

--- End Of Report ---

Target Compound Screening Report

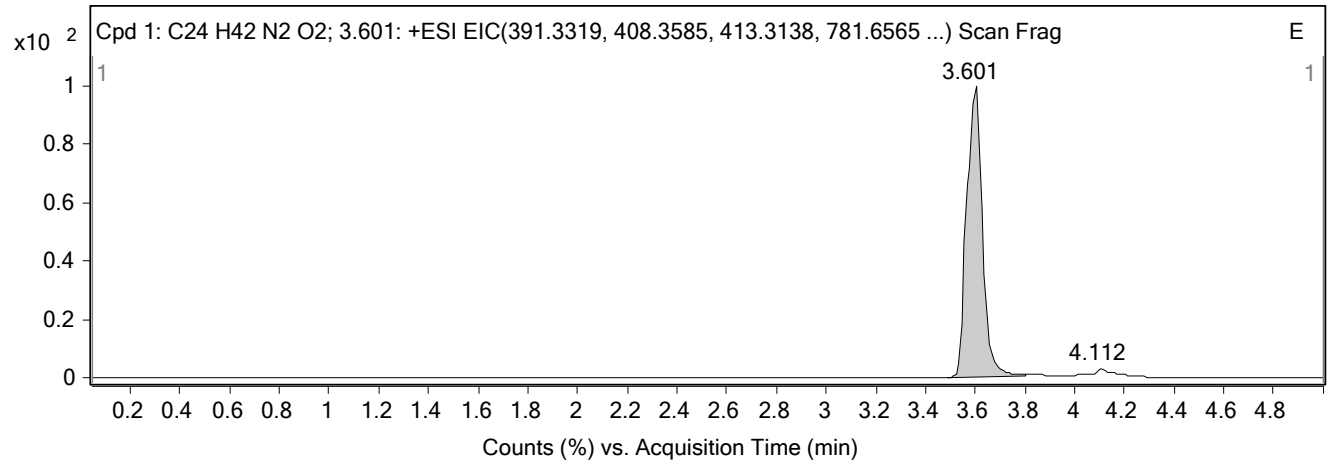
Data File	21-7.d	**Sample Name**	H2986949
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 5:50:21 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H42N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 5:50:21 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

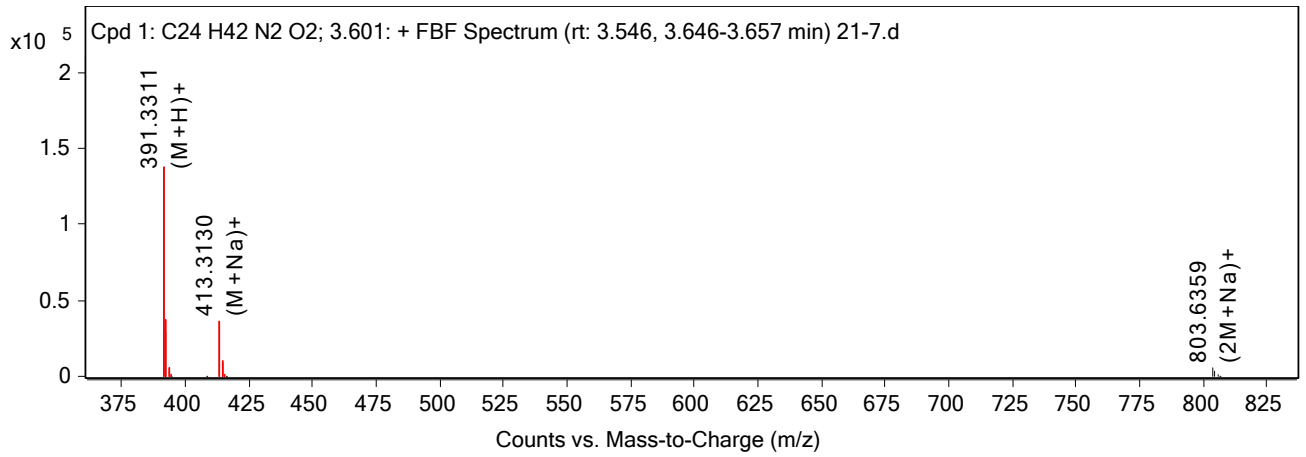
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H42 N2 O2; 3.601	95.7	-2.38	C24 H42 N2 O2	3.601	390.3246	390.3237

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
413.313	3.601	390.3237	C24 H42 N2 O2	390.3246	-2.38	Find By Formula	

Compound Chromatograms



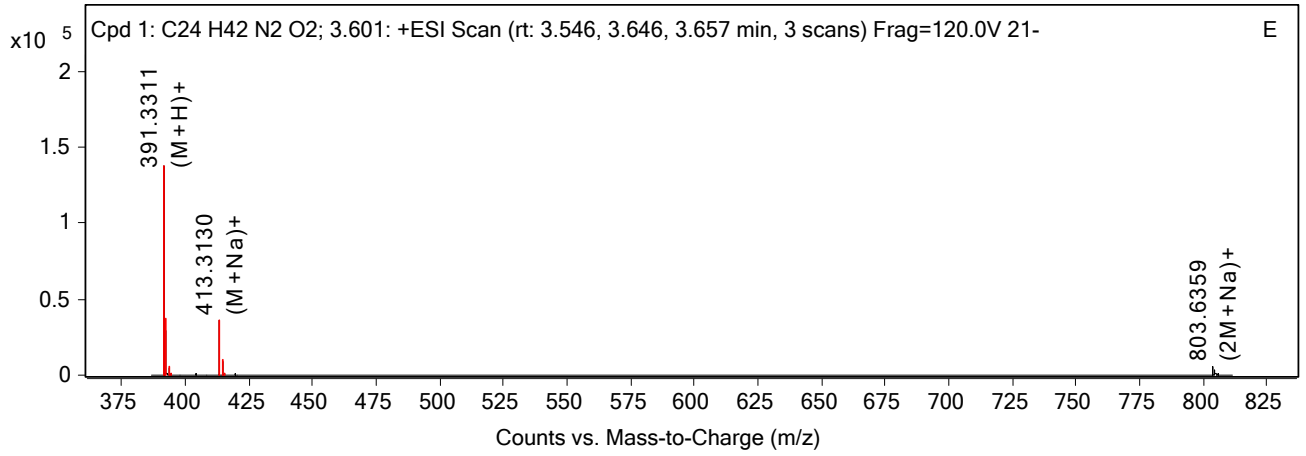
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
391.3311	1	137549.02	(M+H)+
392.3345	1	29926.91	(M+H)+
393.3381	1	4325.33	(M+H)+
394.3363	1	604.7	(M+H)+
413.313	1	36632.86	(M+Na)+
414.3161	1	8643.9	(M+Na)+
415.3173	1	1623.49	(M+Na)+
803.6359	1	5816.76	(2M+Na)+
804.6381	1	3272.98	(2M+Na)+
805.6389	1	972.12	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
391.3311	1	137549.02	(M+H)+	1.99
392.3345	1	29926.91	(M+H)+	1.76
393.3381	1	4325.33	(M+H)+	0.26
394.3363	1	604.7	(M+H)+	11.89
413.313	1	36632.85	(M+Na)+	2.12
414.3161	1	8643.9	(M+Na)+	2.46
415.3173	1	1623.49	(M+Na)+	6.63
803.6359	1	5816.76	(2M+Na)+	3.23
804.6381	1	3272.98	(2M+Na)+	4.53
805.6389	1	972.12	(2M+Na)+	7.36

--- End Of Report ---

Target Compound Screening Report

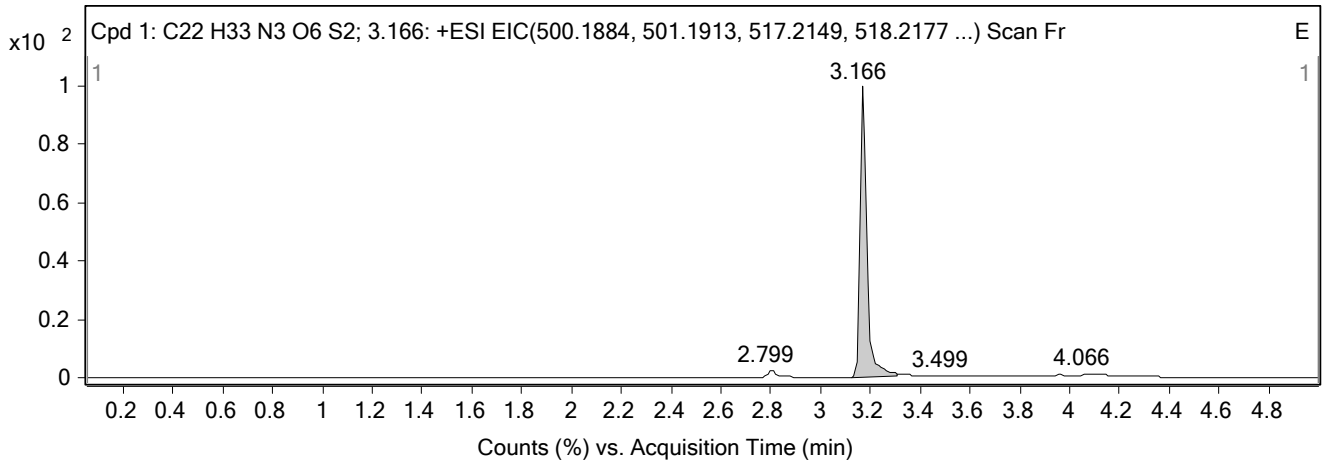
Data File	14.d	**Sample Name**	H2981663
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:36:43 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H33N3O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:36:43 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

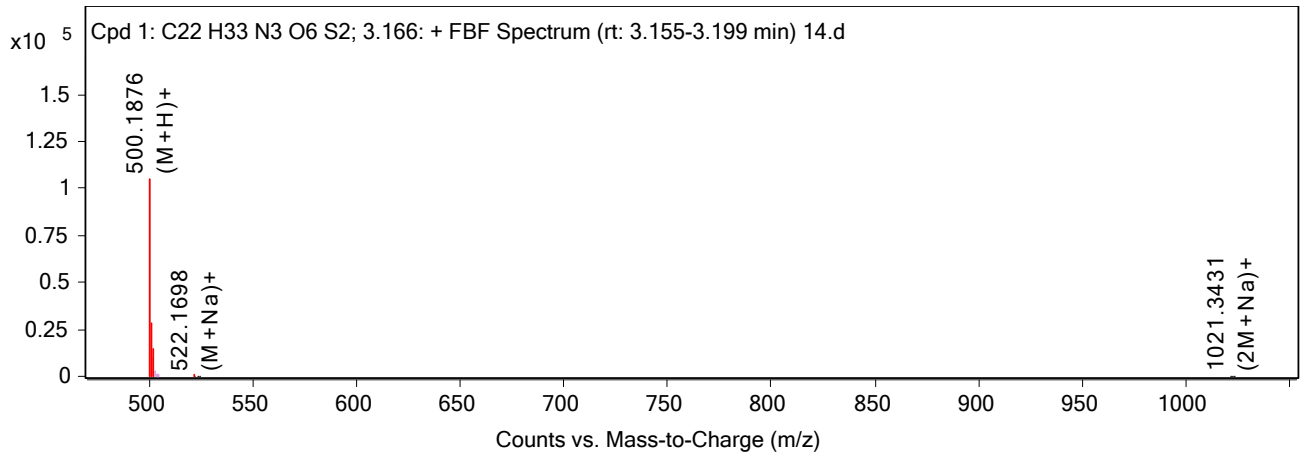
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H33 N3 O6 S2; 3.166	92.89	-1.44	C22 H33 N3 O6 S2	3.166	499.1811	499.1804

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
500.1876	3.166	499.1804	C22 H33 N3 O6 S2	499.1811	-1.44	Find By Formula	

Compound Chromatograms



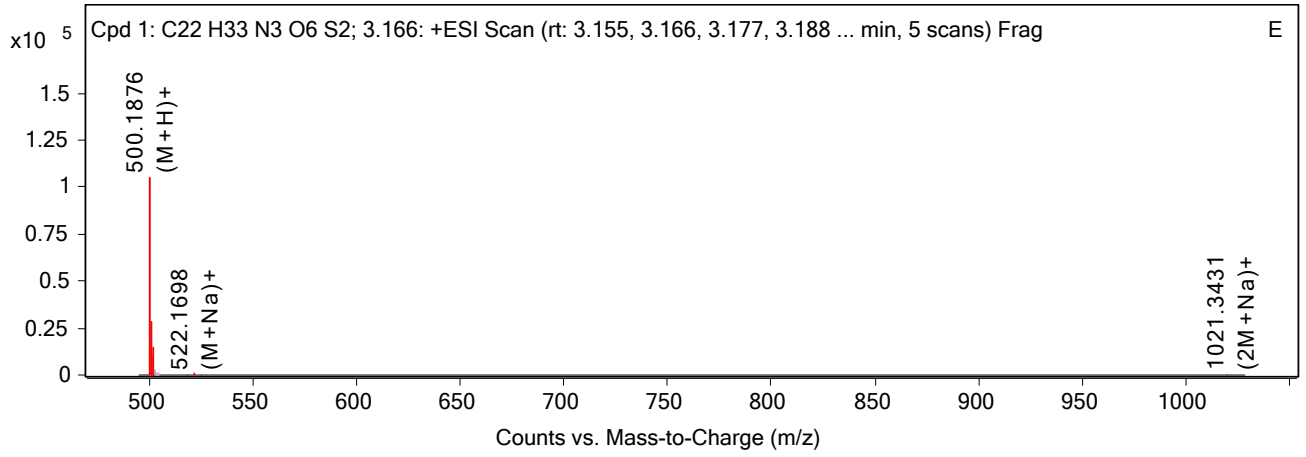
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
500.1876	1	105141.89	(M+H)+
501.1907	1	22892.09	(M+H)+
502.1867	1	9947.18	(M+H)+
522.1698	1	468.63	(M+Na)+
523.17	1	170.03	(M+Na)+
524.1723	1	104.2	(M+Na)+
1021.3431	1	99.38	(2M+Na)+
1022.3423	1	46.02	(2M+Na)+
1023.3538	1	64.88	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
500.1876	1	105141.89	(M+H)+	1.48
501.1907	1	22892.09	(M+H)+	1.09
502.1867	1	9947.18	(M+H)+	1.55
522.1698	1	468.63	(M+Na)+	0.9
523.17	1	170.03	(M+Na)+	6.18
524.1723	1	104.2	(M+Na)+	-5.51
1021.3431	1	99.38	(2M+Na)+	8.13
1022.3423	1	46.02	(2M+Na)+	11.74
1023.3538	1	64.88	(2M+Na)+	-1.8

--- End Of Report ---

Target Compound Screening Report

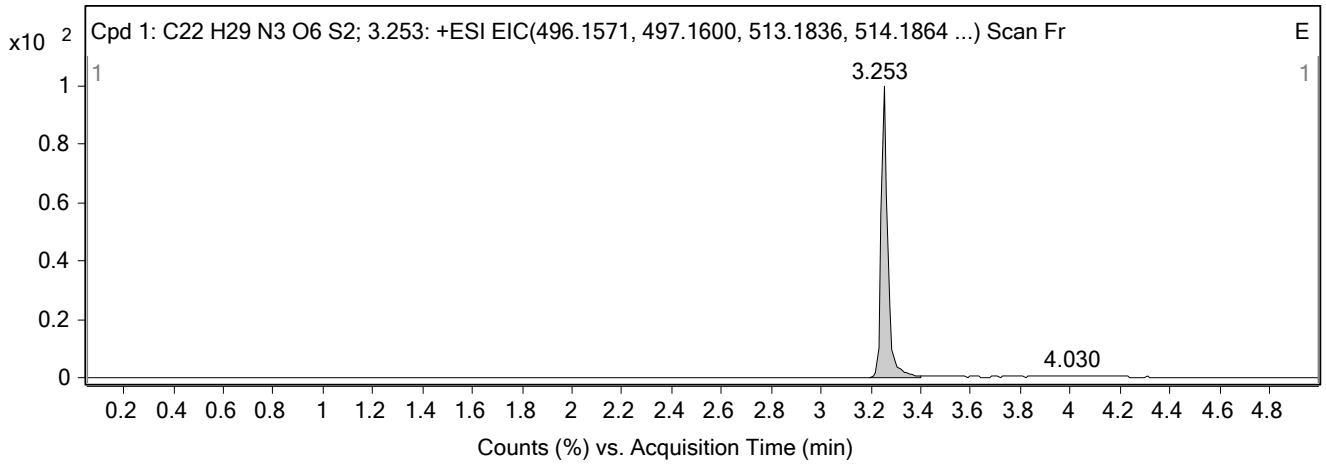
Data File	3-2.d	**Sample Name**	H2979258
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:21:27 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H29N3O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:21:27 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

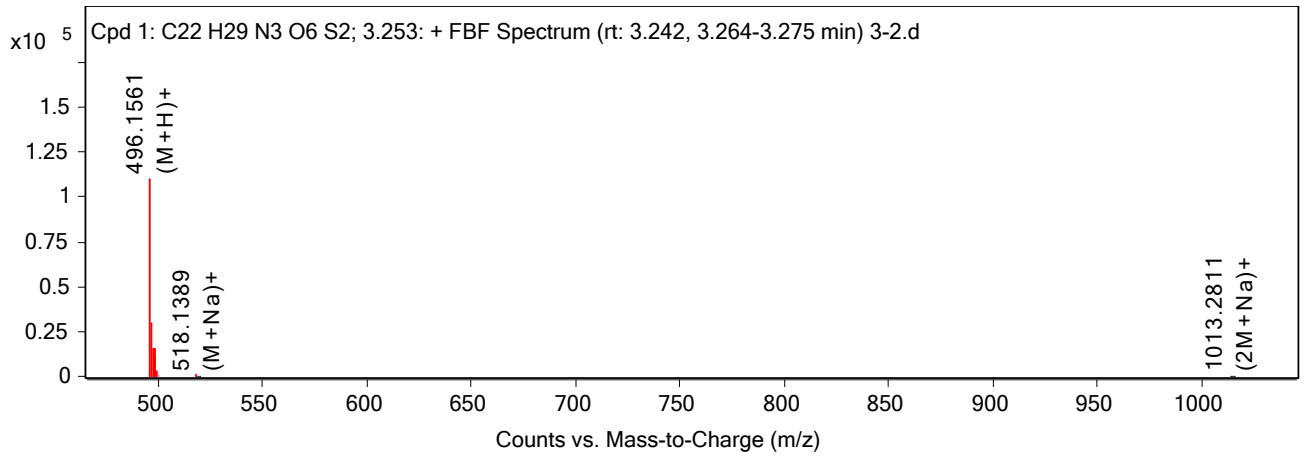
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H29 N3 O6 S2; 3.253	94.76	-1.96	C22 H29 N3 O6 S2	3.253	495.1498	495.1488

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
496.1561	3.253	495.1488	C22 H29 N3 O6 S2	495.1498	-1.96	Find By Formula	

Compound Chromatograms



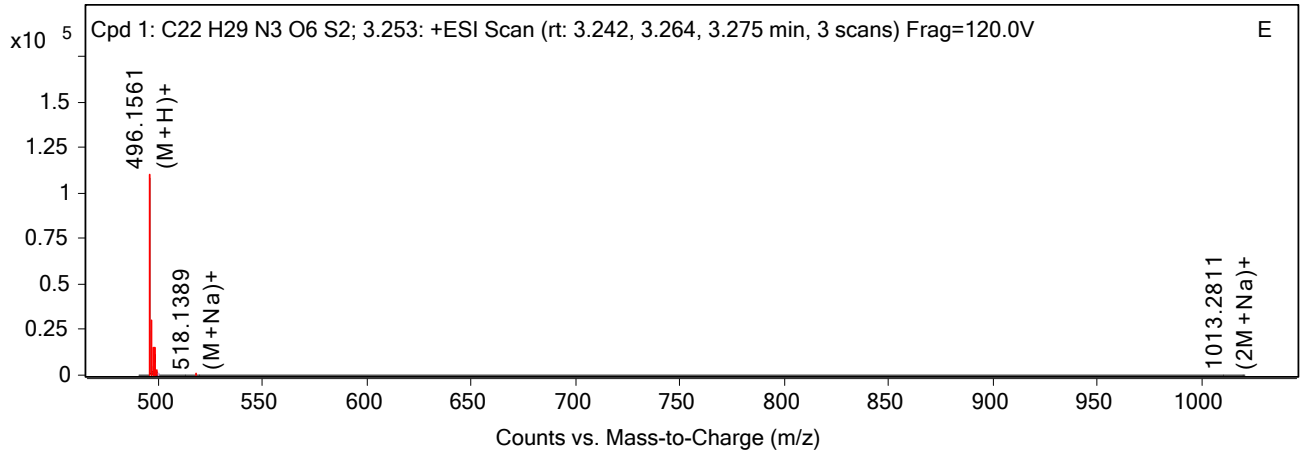
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
496.1561	1	110150.62	(M+H)+
497.1587	1	24613.67	(M+H)+
498.1555	1	11038.03	(M+H)+
499.1577	1	2068.2	(M+H)+
518.1389	1	509.4	(M+Na)+
519.1377	1	189.34	(M+Na)+
520.138	1	117.31	(M+Na)+
1013.2811	1	61.45	(2M+Na)+
1014.2847	1	34.38	(2M+Na)+
1015.2895	1	27.02	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
496.1561	1	110150.62	(M+H)+	1.89
497.1587	1	24613.67	(M+H)+	2.63
498.1555	1	11038.03	(M+H)+	1.4
499.1577	1	2068.2	(M+H)+	0.08
518.1389	1	509.4	(M+Na)+	0.11
519.1377	1	189.34	(M+Na)+	8.13
520.138	1	117.31	(M+Na)+	0.25
1013.2811	1	61.45	(2M+Na)+	7.58
1014.2847	1	34.38	(2M+Na)+	6.92
1015.2895	1	27.02	(2M+Na)+	-0.14

--- End Of Report ---

Target Compound Screening Report

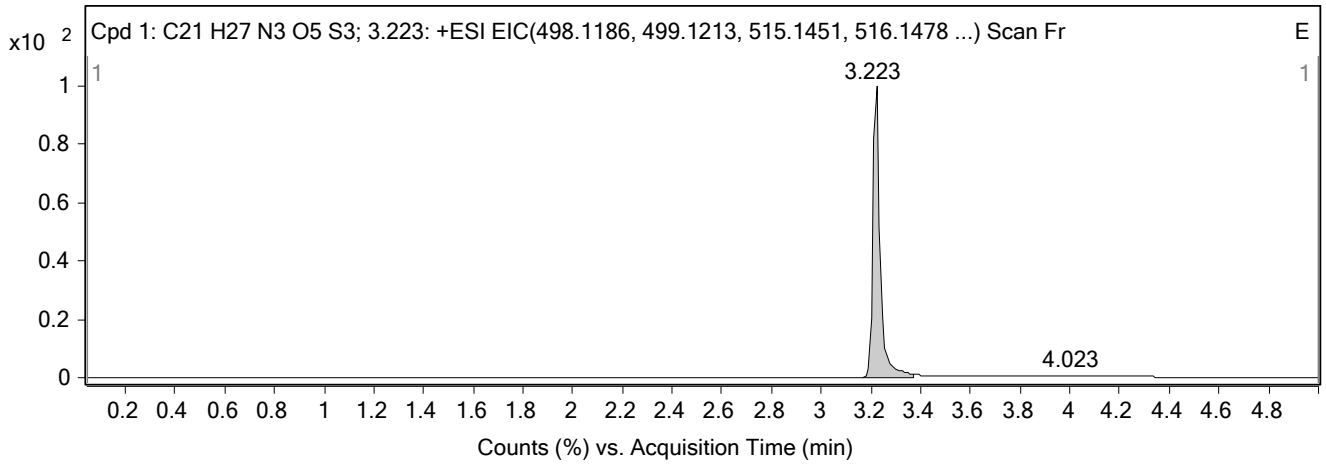
Data File	8-2.d	**Sample Name**	H2982698
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:49:03 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H27N3O5S3	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:49:03 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

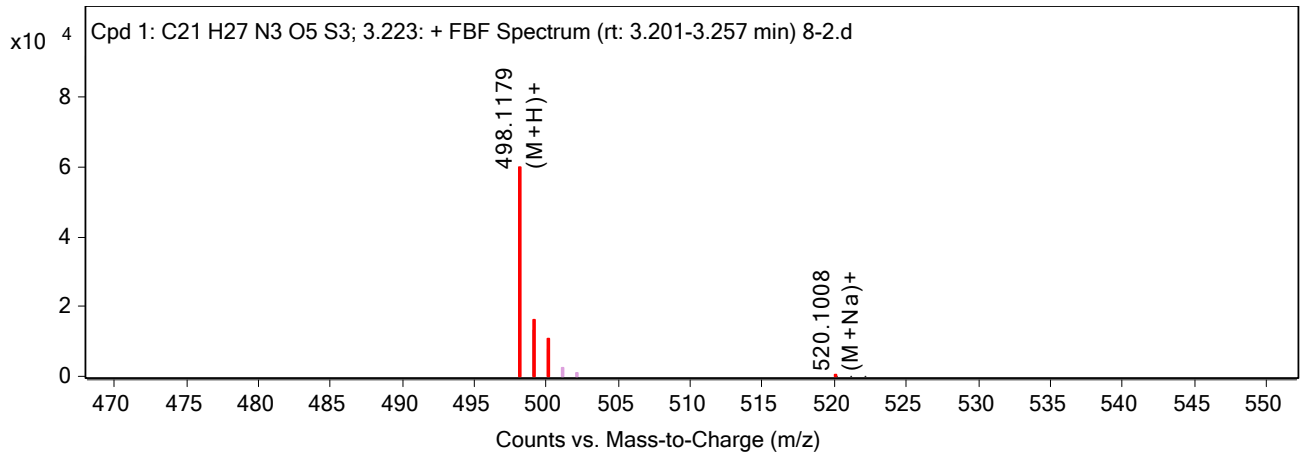
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H27 N3 O5 S3; 3.223	93.17	-1.24	C21 H27 N3 O5 S3	3.223	497.1113	497.1107

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
498.1179	3.223	497.1107	C21 H27 N3 O5 S3	497.1113	-1.24	Find By Formula	

Compound Chromatograms



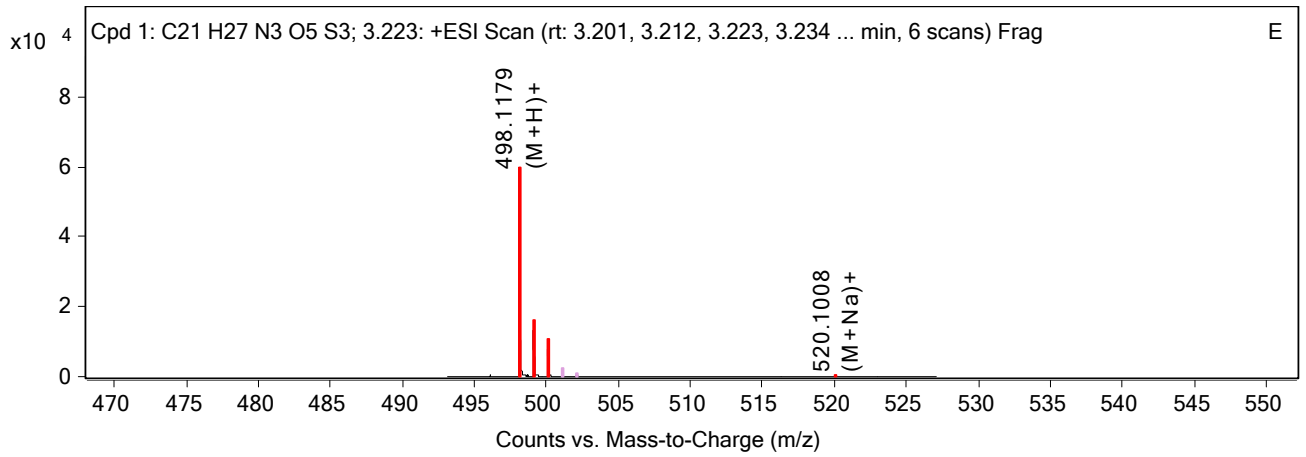
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
498.1179	1	59932.77	(M+H)+
499.1207	1	13306.17	(M+H)+
500.116	1	8061.89	(M+H)+
520.1008	1	268.57	(M+Na)+
521.1039	1	78.68	(M+Na)+
522.1112	1	61.78	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
498.1179	1	59932.77	(M+H)+	1.23
498.1179		59932.77		
499.1207	1	13306.17	(M+H)+	1.29
500.116	1	8061.89	(M+H)+	1.48
520.1008	1	268.57	(M+Na)+	-0.51
521.1039	1	78.68	(M+Na)+	-1.23
522.1112	1	61.78	(M+Na)+	-24.1

--- End Of Report ---

Target Compound Screening Report

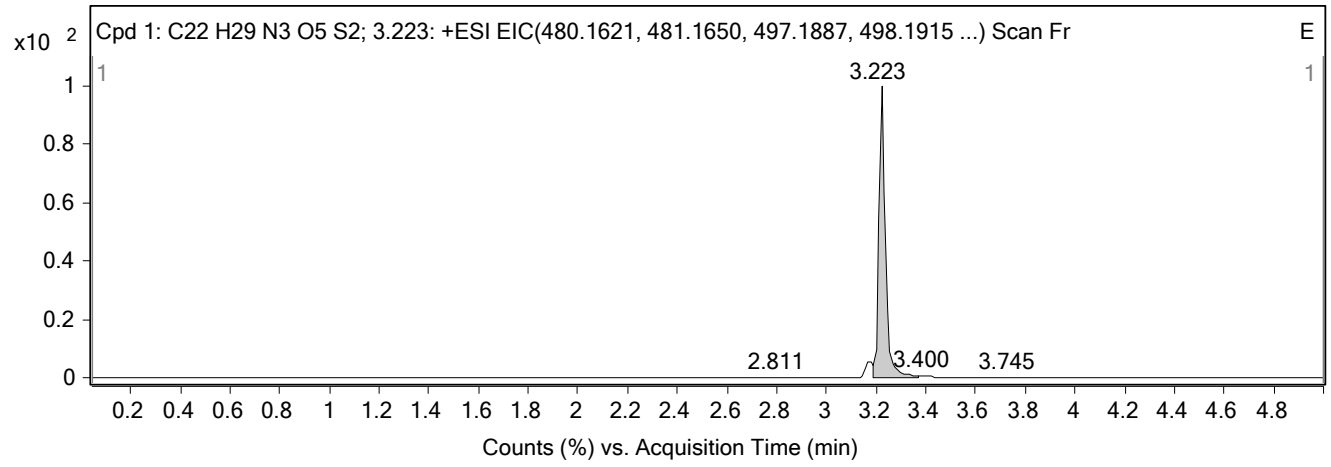
Data File	12-2.d	**Sample Name**	H2981205
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 11:31:11 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H29N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 11:31:11 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

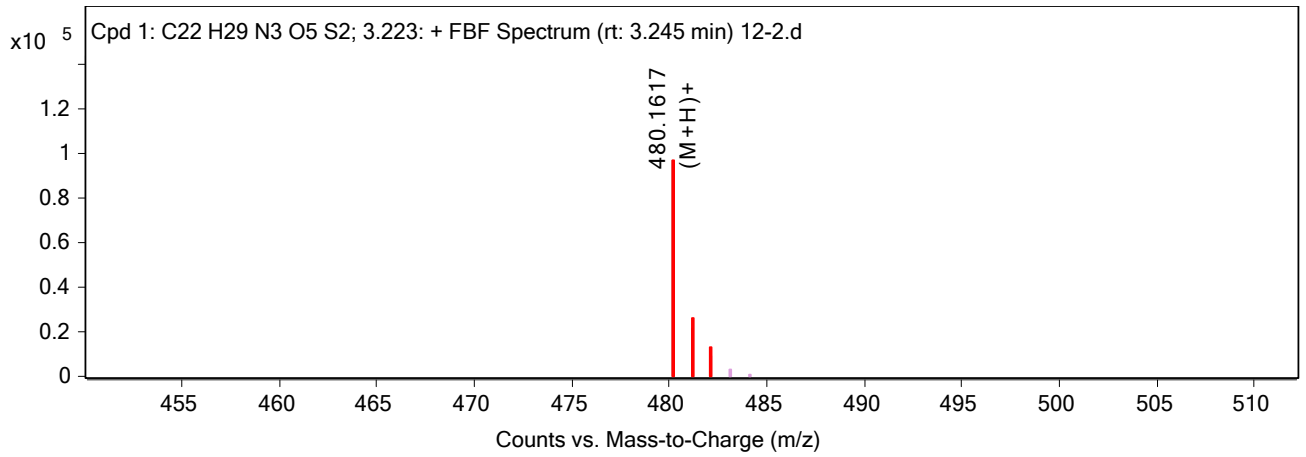
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H29 N3 O5 S2; 3.223	94.44	-1.02	C22 H29 N3 O5 S2	3.223	479.1549	479.1544

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
480.1617	3.223	479.1544	C22 H29 N3 O5 S2	479.1549	-1.02	Find By Formula	

Compound Chromatograms



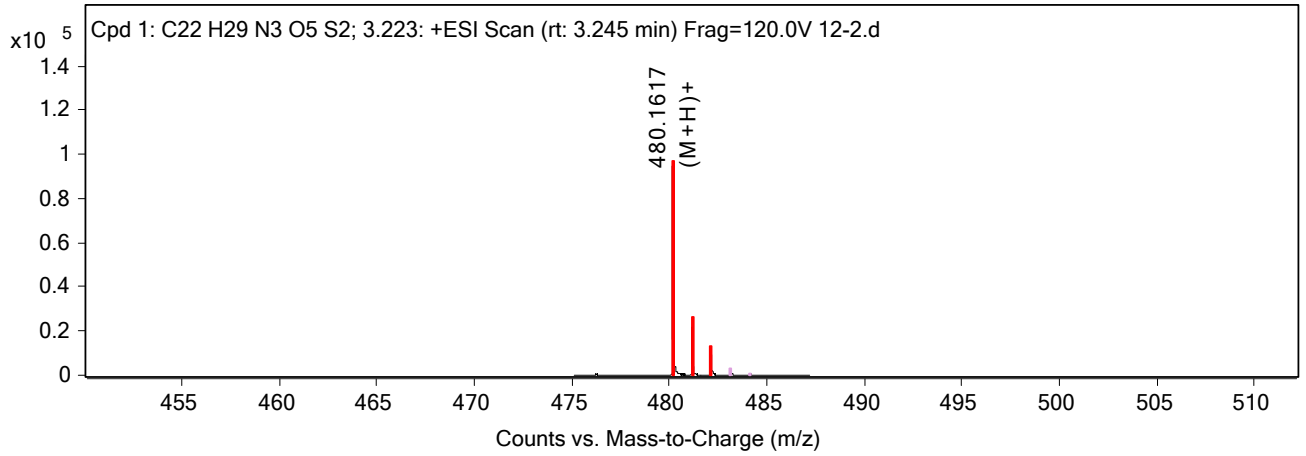
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
480.1617	1	96713.21	(M+H)+
481.1644	1	21765.28	(M+H)+
482.161	1	9451.3	(M+H)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
480.1617	1	96713.21	(M+H)+	0.98
480.1617		96713.21		
481.1644	1	21765.27	(M+H)+	1.44
482.161	1	9451.3	(M+H)+	0.35

--- End Of Report ---

Target Compound Screening Report

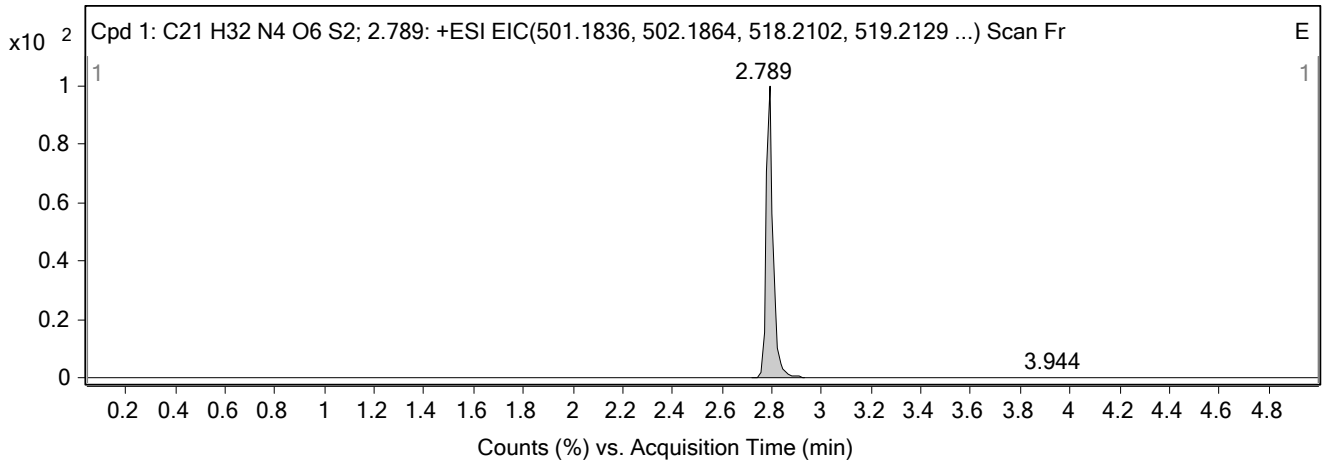
Data File	1.d	**Sample Name**	H2981851
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 6:16:20 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H32N4O6S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 6:16:20 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

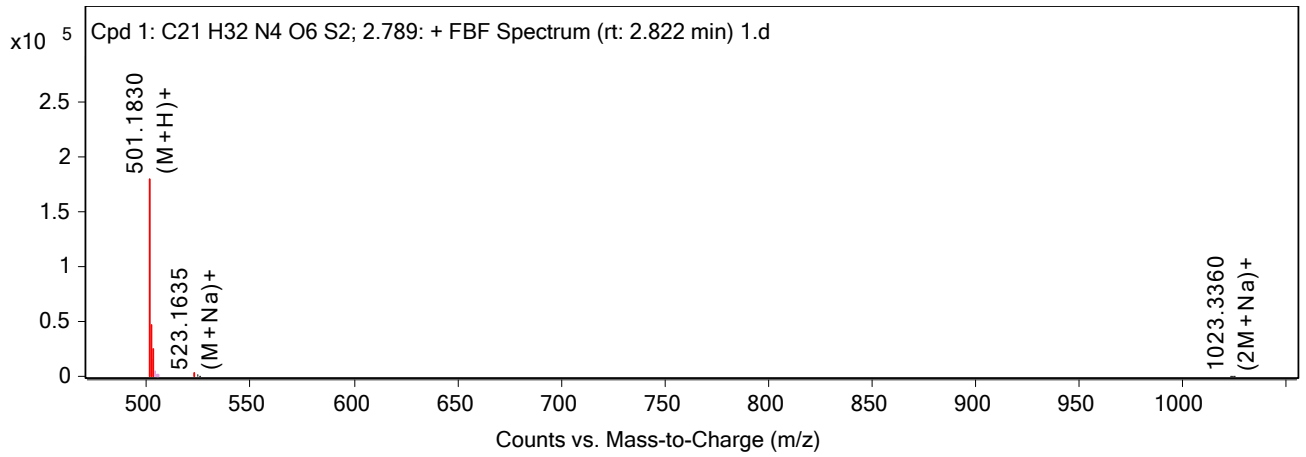
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H32 N4 O6 S2; 2.789	92.88	-1.13	C21 H32 N4 O6 S2	2.789	500.1763	500.1758

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
501.183	2.789	500.1758	C21 H32 N4 O6 S2	500.1763	-1.13	Find By Formula	

Compound Chromatograms



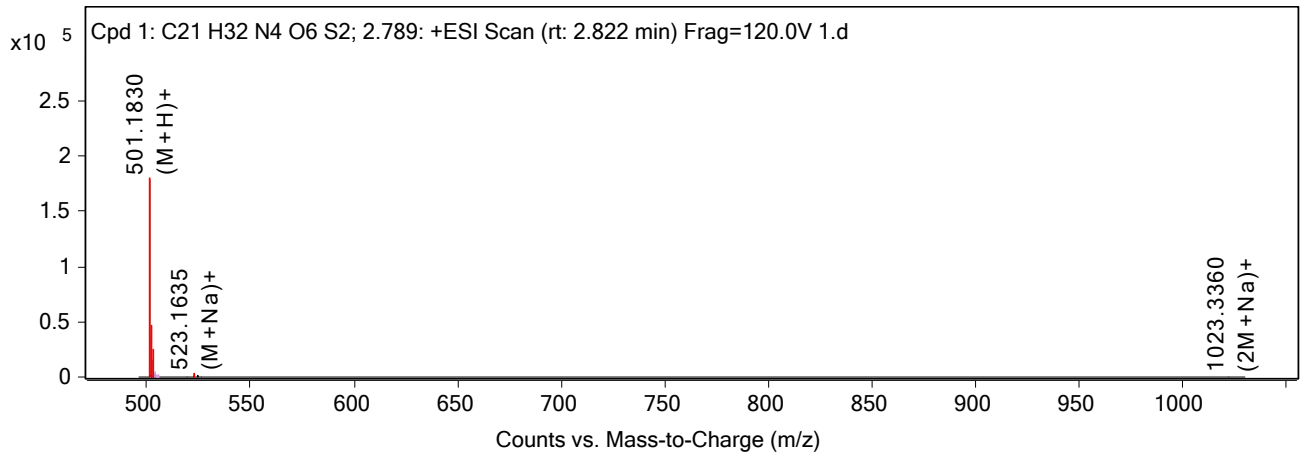
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
501.183	1	179483.88	(M+H)+
502.1862	1	38143.91	(M+H)+
503.1821	1	16147.53	(M+H)+
523.1635	1	2475.8	(M+Na)+
524.1696	1	933.39	(M+Na)+
525.1558	1	347.65	(M+Na)+
1023.336	1	573.57	(2M+Na)+
1024.3397	1	297.71	(2M+Na)+
1025.332	1	180.2	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
501.183	1	179483.88	(M+H)+	1.18
502.1862	1	38143.91	(M+H)+	0.37
503.1821	1	16147.53	(M+H)+	0.94
523.1635	1	2475.8	(M+Na)+	3.86
524.1696	1	933.39	(M+Na)+	-2.42
525.1558	1	347.65	(M+Na)+	16.7
1023.336	1	573.57	(2M+Na)+	5.7
1024.3397	1	297.71	(2M+Na)+	4.9
1025.332	1	180.2	(2M+Na)+	9.97

--- End Of Report ---

Target Compound Screening Report

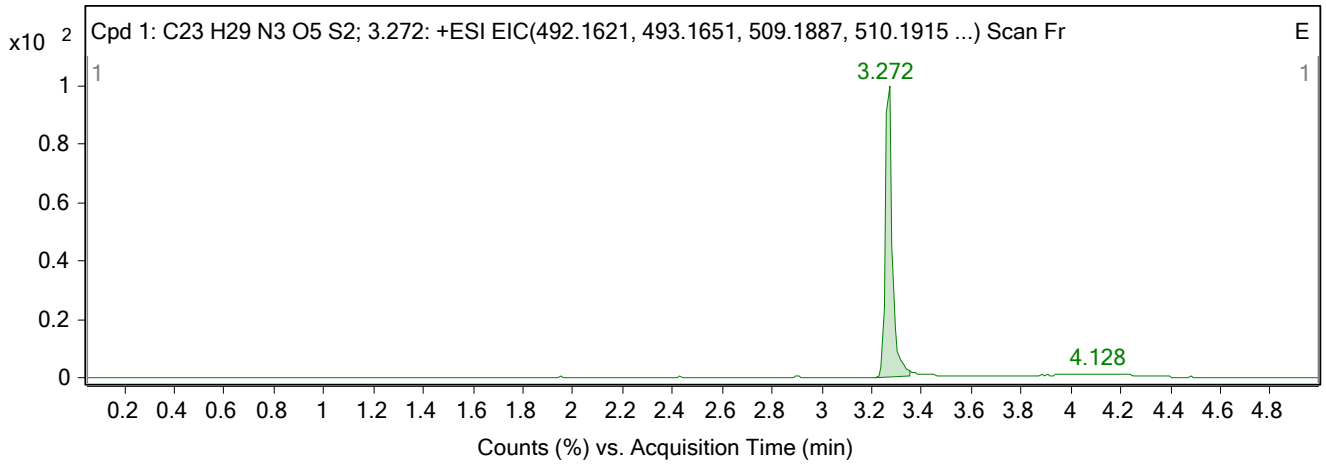
Data File	6-2.d	**Sample Name**	H2980128
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 10:38:00 AM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H29N3O5S2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 10:38:00 AM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H29 N3 O5 S2; 3.272	94.09	-2.11	C23 H29 N3 O5 S2	3.272	491.1549	491.1538

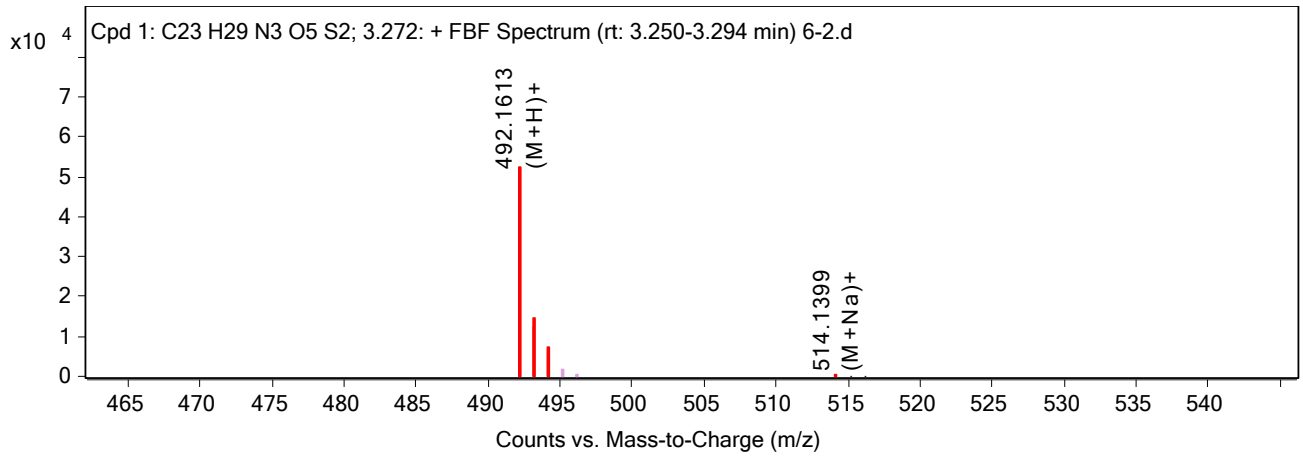
Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
492.1613	3.272	491.1538	C23 H29 N3 O5 S2	491.1549	-2.11	Find By Formula	

Compound Chromatograms



MS Zoomed Spectrum

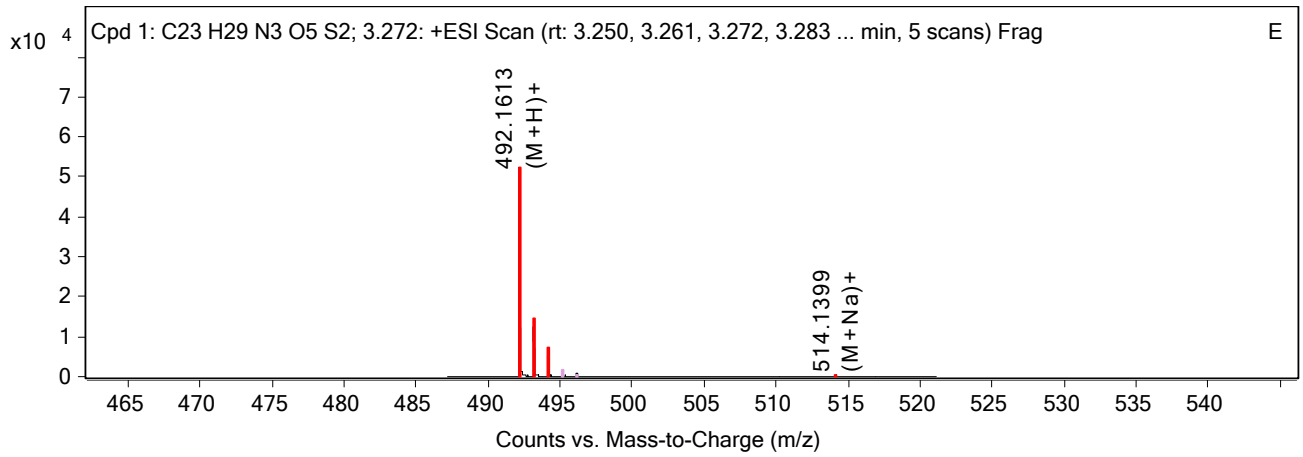
Target Compound Screening Report



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
492.1613	1	52308.46	(M+H)+
493.1636	1	12494.91	(M+H)+
494.1601	1	5416.83	(M+H)+
514.1399	1	261.42	(M+Na)+
515.1414	1	113.3	(M+Na)+
516.1404	1	69.64	(M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
492.1613	1	52308.46	(M+H)+	1.8
492.1613		52308.46		
493.1636	1	12494.91	(M+H)+	2.99
494.1601	1	5416.83	(M+H)+	2.46
514.1399	1	261.42	(M+Na)+	8.12
515.1414	1	113.3	(M+Na)+	10.87
516.1404	1	69.64	(M+Na)+	5.67

--- End Of Report ---

Target Compound Screening Report

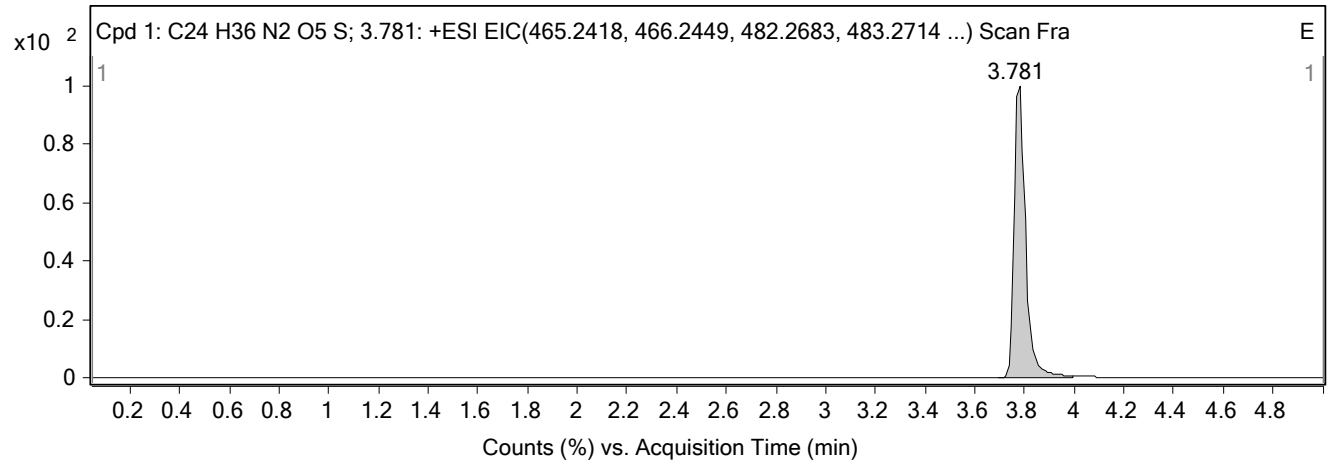
Data File	39.d	**Sample Name**	H2974026
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 5:18:58 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H36N2O5S	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 5:18:58 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

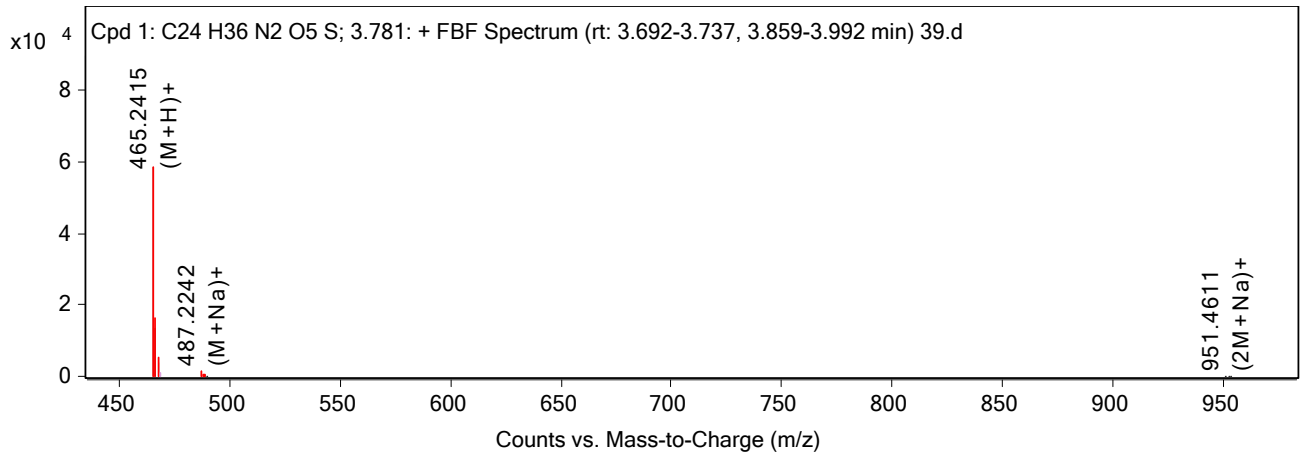
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H36 N2 O5 S; 3.781	96.79	-0.4	C24 H36 N2 O5 S	3.781	464.2345	464.2343

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
487.2242	3.781	464.2343	C24 H36 N2 O5 S	464.2345	-0.4	Find By Formula	

Compound Chromatograms



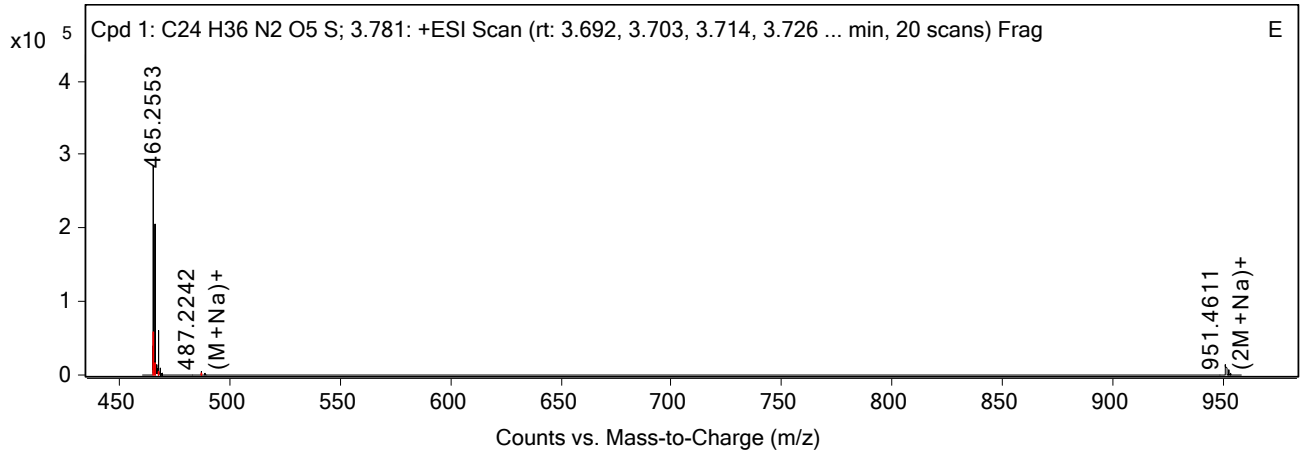
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
465.2415	1	58522.44	(M+H)+
466.2445	1	13513.19	(M+H)+
467.2435	1	4099.84	(M+H)+
487.2242	1	1585.76	(M+Na)+
488.2264	1	485.3	(M+Na)+
489.2247	1	183.57	(M+Na)+
951.4611	1	159.12	(2M+Na)+
952.4589	1	109.36	(2M+Na)+
953.4572	1	80.07	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
465.2415	1	58522.44	(M+H)+	0.48
465.2553		284031.68		
466.2445	1	13513.19	(M+H)+	0.8
467.2435	1	4099.84	(M+H)+	-1.46
487.2242	1	1585.76	(M+Na)+	-1.02
488.2264	1	485.3	(M+Na)+	0.87
489.2247	1	183.57	(M+Na)+	-0.01
951.4611	1	159.12	(2M+Na)+	-3.09
952.4589	1	109.36	(2M+Na)+	2.6
953.4572	1	80.07	(2M+Na)+	3.71

--- End Of Report ---

Target Compound Screening Report

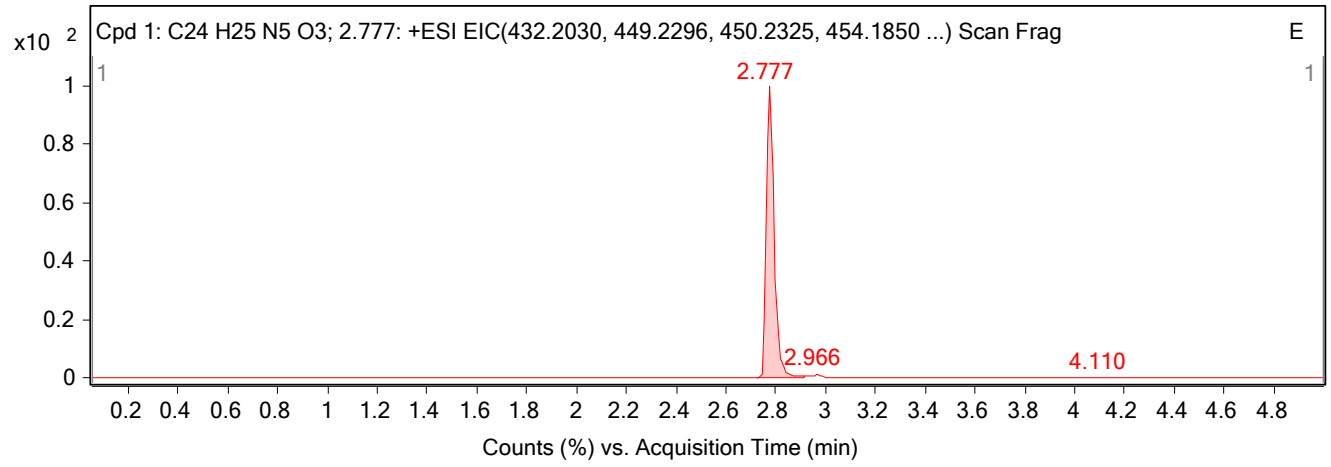
Data File	24.d	**Sample Name**	H3000295
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:55:41 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H25N5O3	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:55:41 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

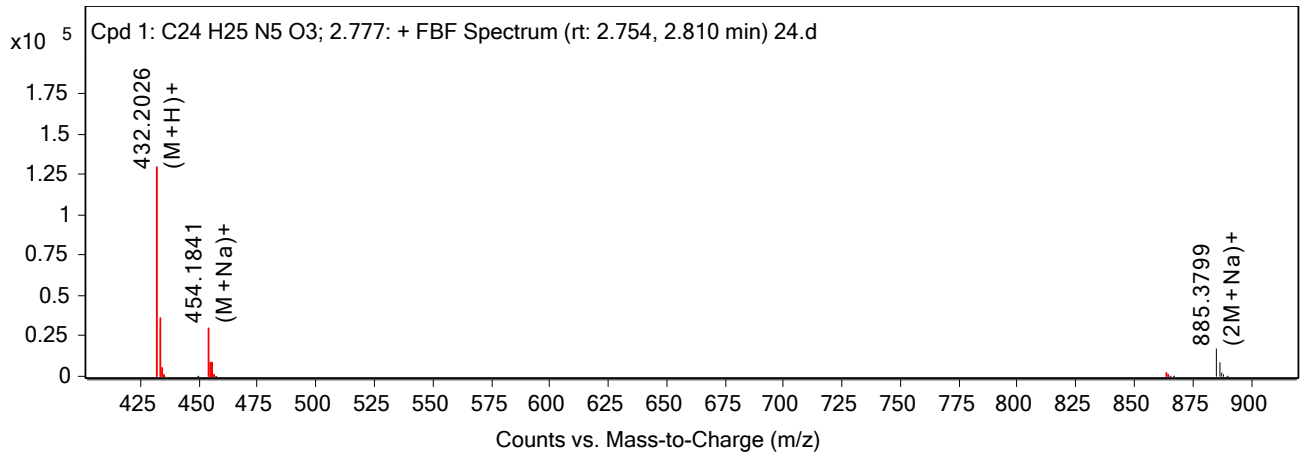
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H25 N5 O3; 2.777	98.45	-1.3	C24 H25 N5 O3	2.777	431.1957	431.1952

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
454.1841	2.777	431.1952	C24 H25 N5 O3	431.1957	-1.3	Find By Formula	

Compound Chromatograms



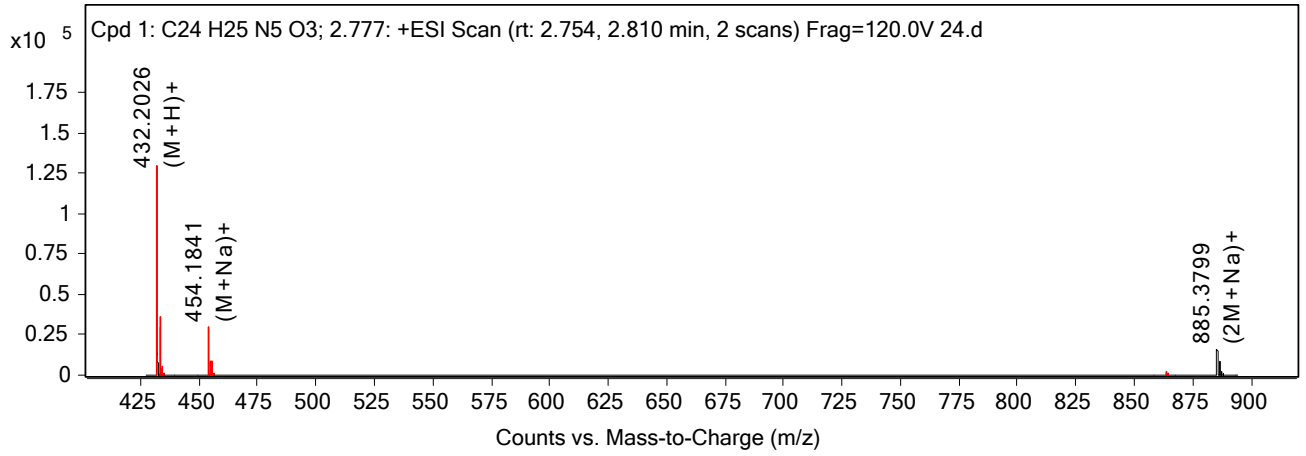
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
432.2026	1	129515.03	(M+H)+
433.2055	1	30015.54	(M+H)+
434.2084	1	4094.67	(M+H)+
454.1841	1	30002.59	(M+Na)+
455.188	1	7843.45	(M+Na)+
863.3957	1	2510.33	(2M+H)+
864.3998	1	1447.51	(2M+H)+
885.3799	1	16570.65	(2M+Na)+
886.3822	1	8850.51	(2M+Na)+
887.389	1	2685.03	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
432.2026	1	129515.03	(M+H)+	1.05
433.2055	1	30015.54	(M+H)+	1.11
434.2084	1	4094.67	(M+H)+	0.67
454.1841	1	30002.59	(M+Na)+	1.8
455.188	1	7843.45	(M+Na)+	-0.08
863.3957	1	2510.33	(2M+H)+	3.59
864.3998	1	1447.51	(2M+H)+	2.21
885.3799	1	16570.65	(2M+Na)+	0.87
886.3822	1	8850.51	(2M+Na)+	1.65
887.389	1	2685.03	(2M+Na)+	-2.79

--- End Of Report ---

Target Compound Screening Report

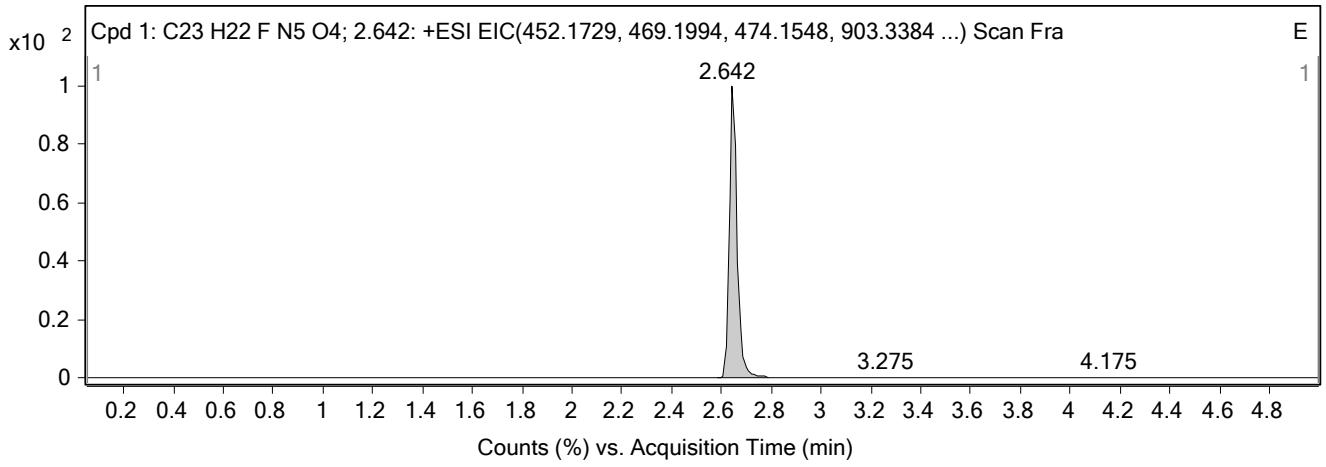
Data File	33.d	**Sample Name**	H2990793
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 2:14:21 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H22FN5O4	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 2:14:21 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

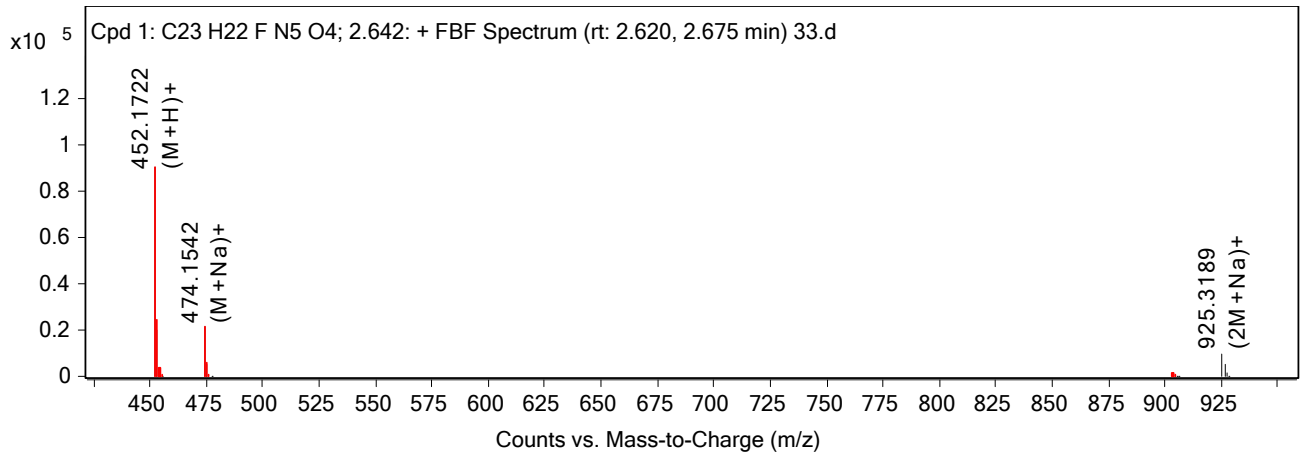
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H22 F N5 O4; 2.642	99.22	-1.86	C23 H22 F N5 O4	2.642	451.1656	451.1647

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
474.1542	2.642	451.1647	C23 H22 F N5 O4	451.1656	-1.86	Find By Formula	

Compound Chromatograms



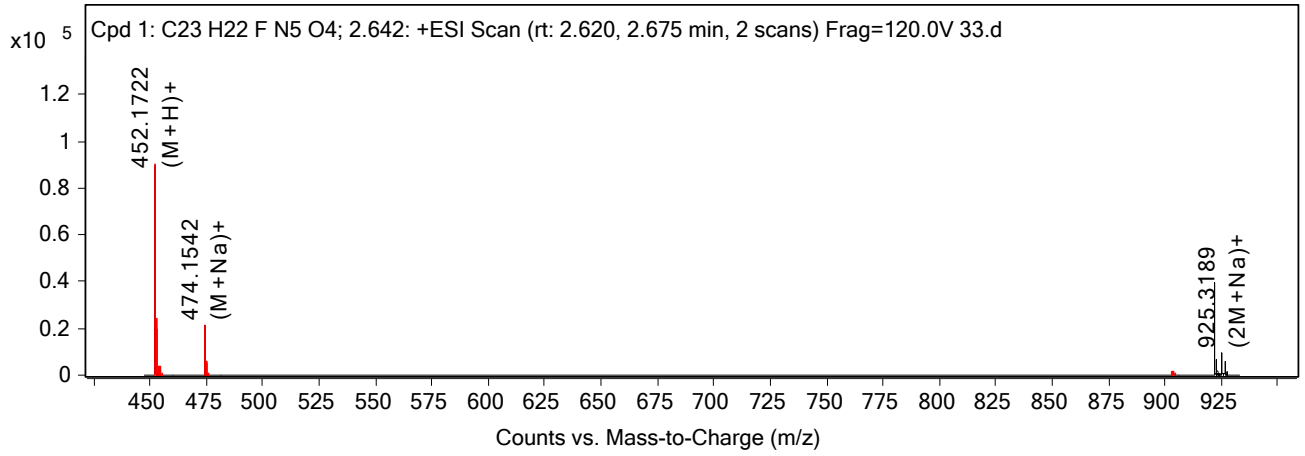
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
452.1722	1	90265.47	(M+H)+
453.1748	1	19805.79	(M+H)+
454.1774	1	3108.79	(M+H)+
474.1542	1	21409.36	(M+Na)+
475.1574	1	5457.98	(M+Na)+
476.1605	1	898.78	(M+Na)+
903.3347	1	1608.19	(2M+H)+
925.3189	1	9933.19	(2M+Na)+
926.3214	1	5580.23	(2M+Na)+
927.325	1	1516.13	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
452.1722	1	90265.47	(M+H)+	1.44
453.1748	1	19805.79	(M+H)+	2.3
454.1774	1	3108.79	(M+H)+	2.23
474.1542	1	21409.36	(M+Na)+	1.34
475.1574	1	5457.98	(M+Na)+	0.8
476.1605	1	898.78	(M+Na)+	-0.14
903.3347	1	1608.19	(2M+H)+	4.14
925.3189	1	9933.19	(2M+Na)+	1.55
926.3214	1	5580.23	(2M+Na)+	2.06
927.325	1	1516.13	(2M+Na)+	1.19

--- End Of Report ---

Target Compound Screening Report

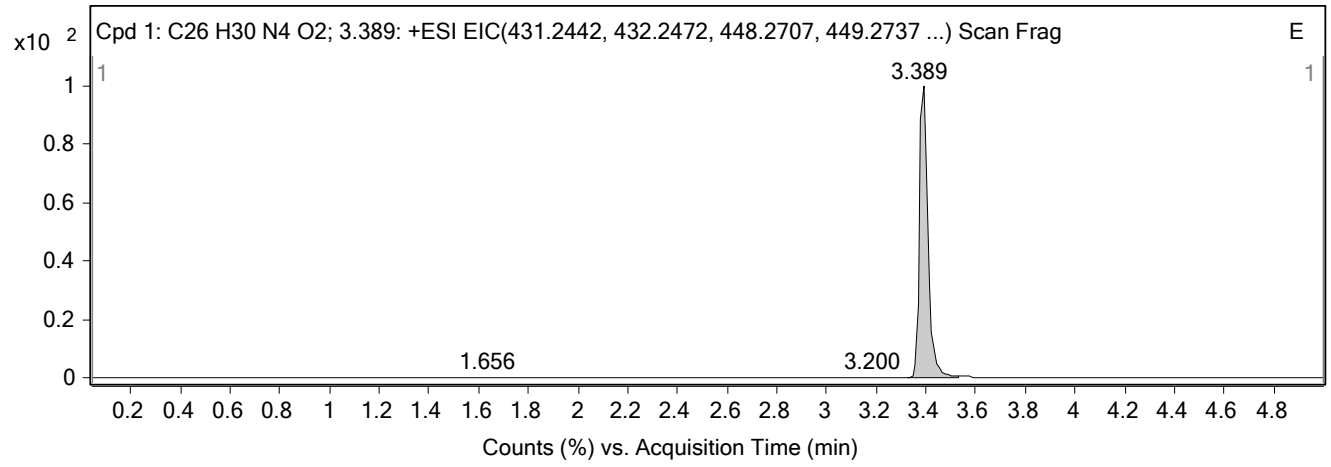
Data File	33.d	**Sample Name**	H2976998
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 4:45:42 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C26H30N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 4:45:42 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

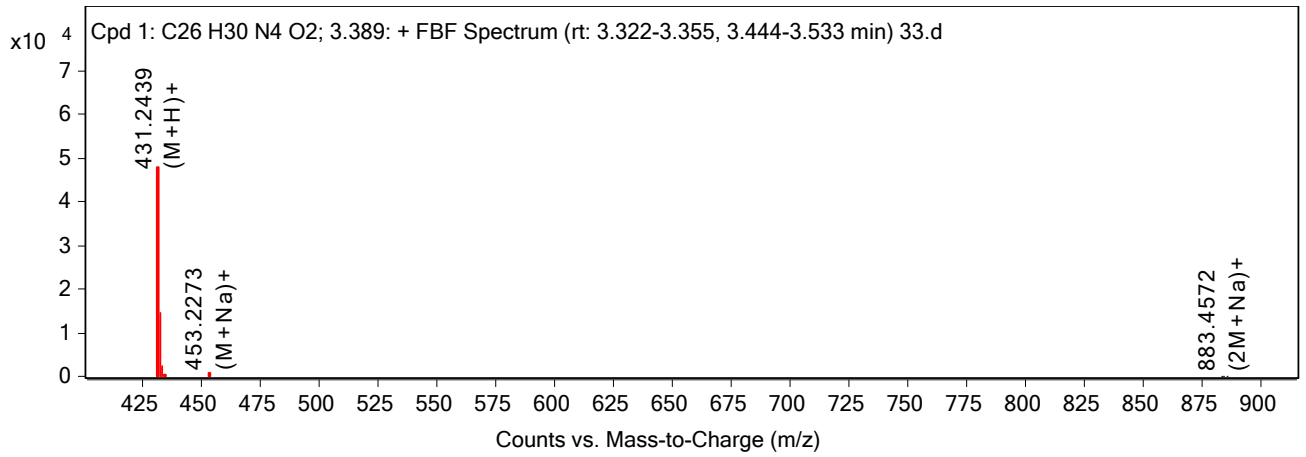
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C26 H30 N4 O2; 3.389	97.37	-0.62	C26 H30 N4 O2	3.389	430.2369	430.2366

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
431.2439	3.389	430.2366	C26 H30 N4 O2	430.2369	-0.62	Find By Formula	

Compound Chromatograms



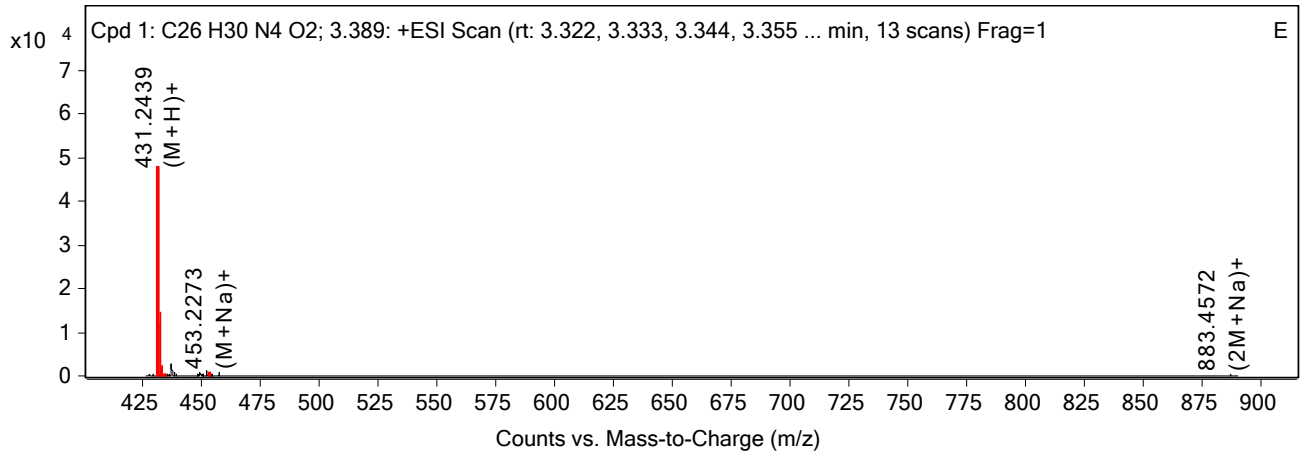
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
431.2439	1	47804.26	(M+H)+
432.247	1	12436.5	(M+H)+
433.2498	1	1944.15	(M+H)+
434.2525	1	259.19	(M+H)+
453.2273	1	590.08	(M+Na)+
883.4572	1	213.24	(2M+Na)+
884.4626	1	122.24	(2M+Na)+
885.468	1	66.55	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
431.2439	1	47804.26	(M+H)+	0.59
431.2439		47804.26		
432.247	1	12436.5	(M+H)+	0.5
433.2498	1	1944.15	(M+H)+	0.84
434.2525	1	259.19	(M+H)+	1.1
453.2273	1	590.08	(M+Na)+	-2.67
883.4572	1	213.24	(2M+Na)+	6.55
884.4626	1	122.24	(2M+Na)+	3.93
885.468	1	66.55	(2M+Na)+	1.22

--- End Of Report ---

Target Compound Screening Report

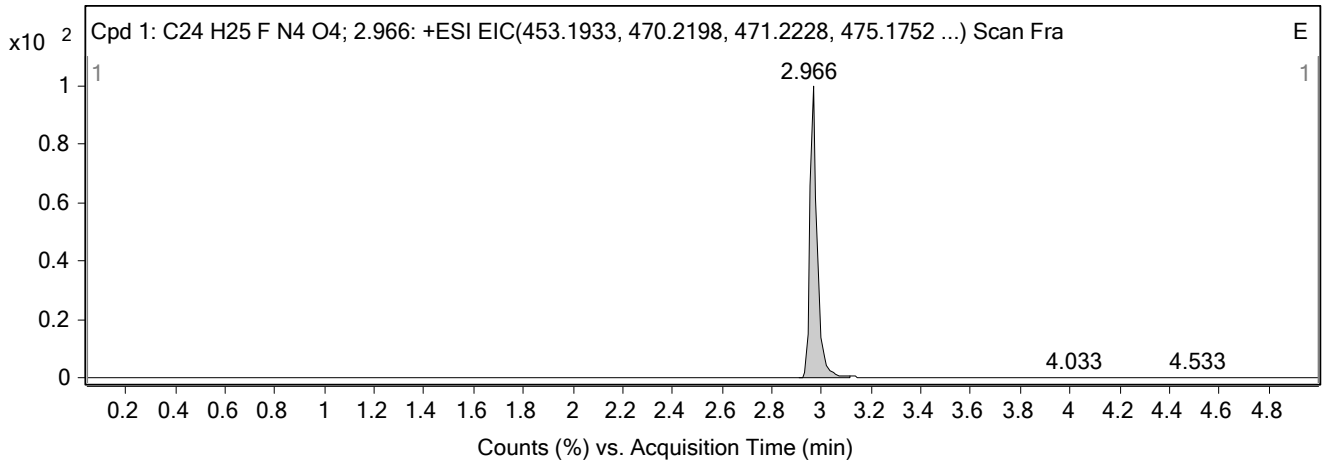
Data File	22.d	**Sample Name**	H2997982
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/22/2021 3:44:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C24H25FN4O4	**Stream Name**	LC 1
Acquisition Time (Local)	9/22/2021 3:44:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

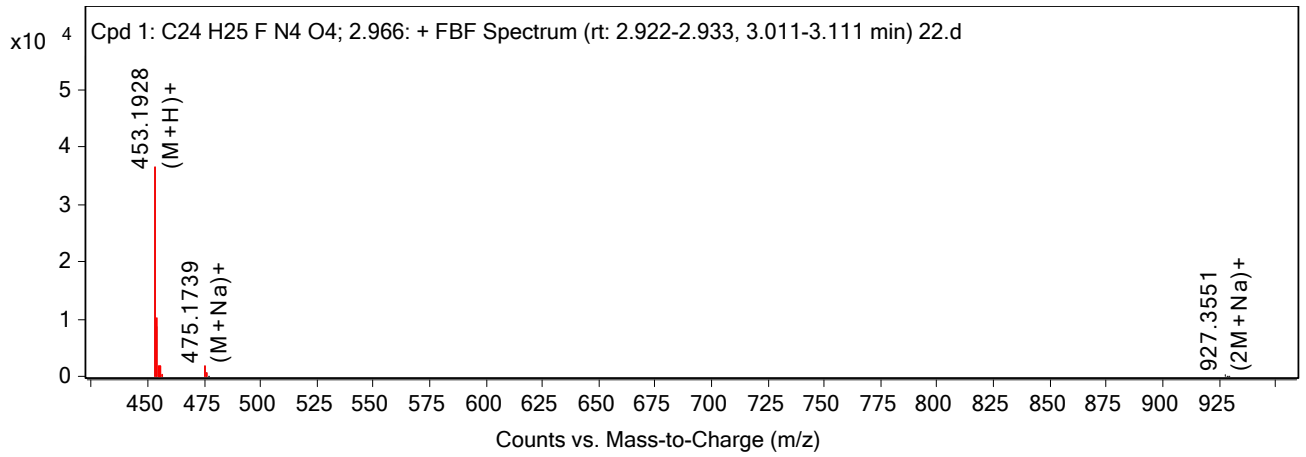
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H25 F N4 O4; 2.966	97.37	-0.93	C24 H25 F N4 O4	2.966	452.186	452.1856

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
475.1739	2.966	452.1856	C24 H25 F N4 O4	452.186	-0.93	Find By Formula	

Compound Chromatograms



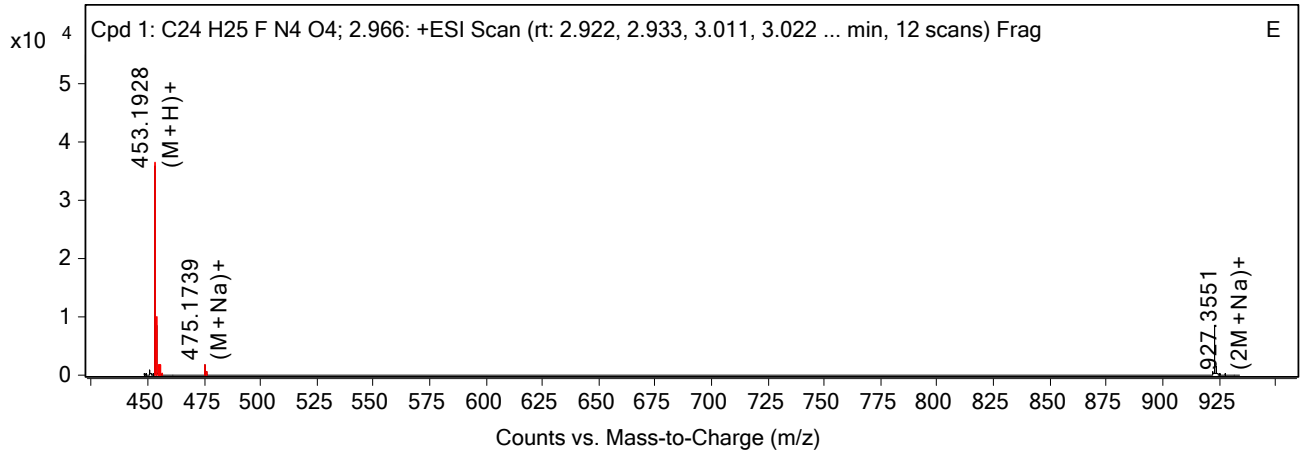
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
453.1928	1	36475.39	(M+H)+
454.1961	1	8699.07	(M+H)+
455.1992	1	1415.51	(M+H)+
456.2026	1	168.28	(M+H)+
475.1739	1	1792.66	(M+Na)+
476.1782	1	519.44	(M+Na)+
477.1807	1	108.92	(M+Na)+
927.3551	1	258.7	(2M+Na)+
928.3622	1	147.77	(2M+Na)+
929.3845	1	60.49	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
453.1928	1	36475.4	(M+H)+	0.97
454.1961	1	8699.07	(M+H)+	0.51
455.1992	1	1415.51	(M+H)+	-0.37
456.2026	1	168.28	(M+H)+	-2.07
475.1739	1	1792.66	(M+Na)+	2.83
476.1782	1	519.44	(M+Na)+	0.09
477.1807	1	108.92	(M+Na)+	0.48
927.3551	1	258.7	(2M+Na)+	6.62
928.3622	1	147.77	(2M+Na)+	2.24
929.3845	1	60.49	(2M+Na)+	-18.68

--- End Of Report ---

Target Compound Screening Report

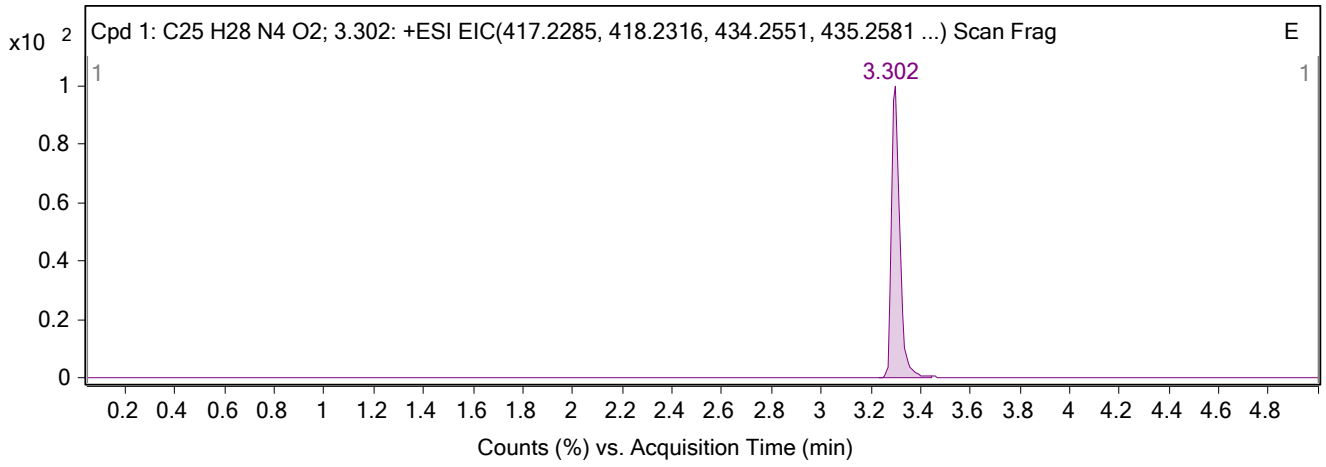
Data File	26.d	**Sample Name**	H2977667
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 1:35:29 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C25H28N4O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 1:35:29 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

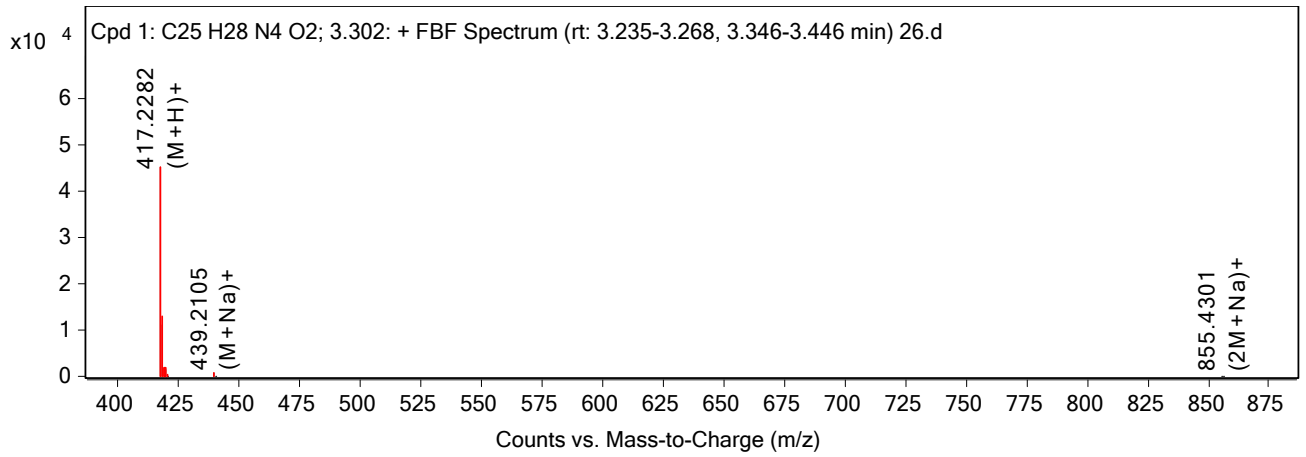
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C25 H28 N4 O2; 3.302	96.35	-0.64	C25 H28 N4 O2	3.302	416.2212	416.221

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
417.2282	3.302	416.221	C25 H28 N4 O2	416.2212	-0.64	Find By Formula	

Compound Chromatograms



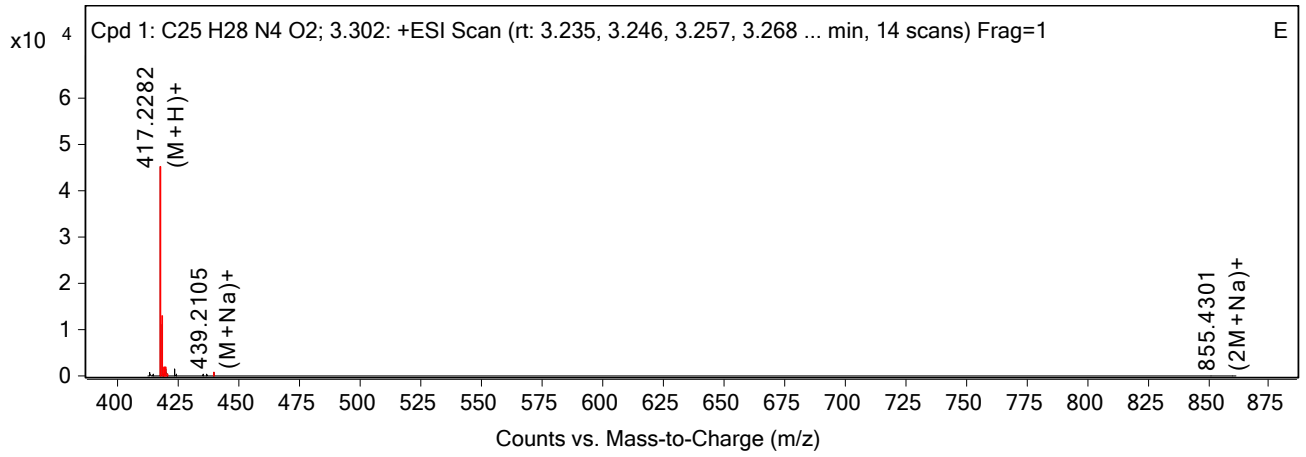
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
417.2282	1	45228.46	(M+H)+
418.2312	1	10977.14	(M+H)+
419.2349	1	1663.48	(M+H)+
420.236	1	191.55	(M+H)+
439.2105	1	627.68	(M+Na)+
440.2163	1	176.59	(M+Na)+
855.4301	1	163.33	(2M+Na)+
856.4348	1	105.99	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
417.2282	1	45228.46	(M+H)+	0.65
418.2312	1	10977.14	(M+H)+	0.92
419.2349	1	1663.48	(M+H)+	-0.97
420.236	1	191.55	(M+H)+	2.87
439.2105	1	627.68	(M+Na)+	-0.18
440.2163	1	176.59	(M+Na)+	-6.31
855.4301	1	163.33	(2M+Na)+	1.81
856.4348	1	105.99	(2M+Na)+	-0.02

--- End Of Report ---

Target Compound Screening Report

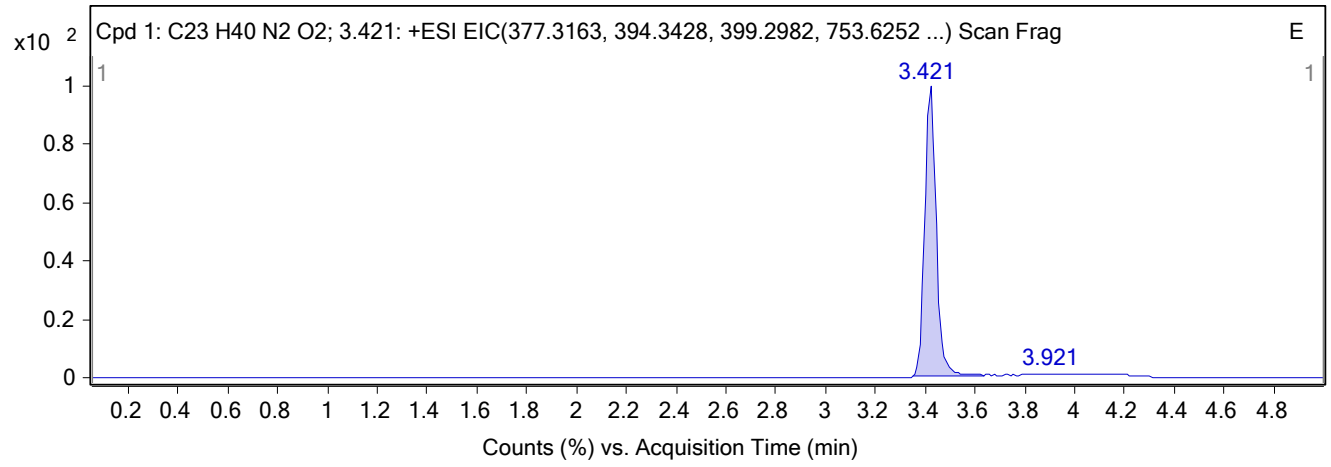
Data File	29.d	**Sample Name**	H2986300
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 1:12:35 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C23H40N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 1:12:35 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

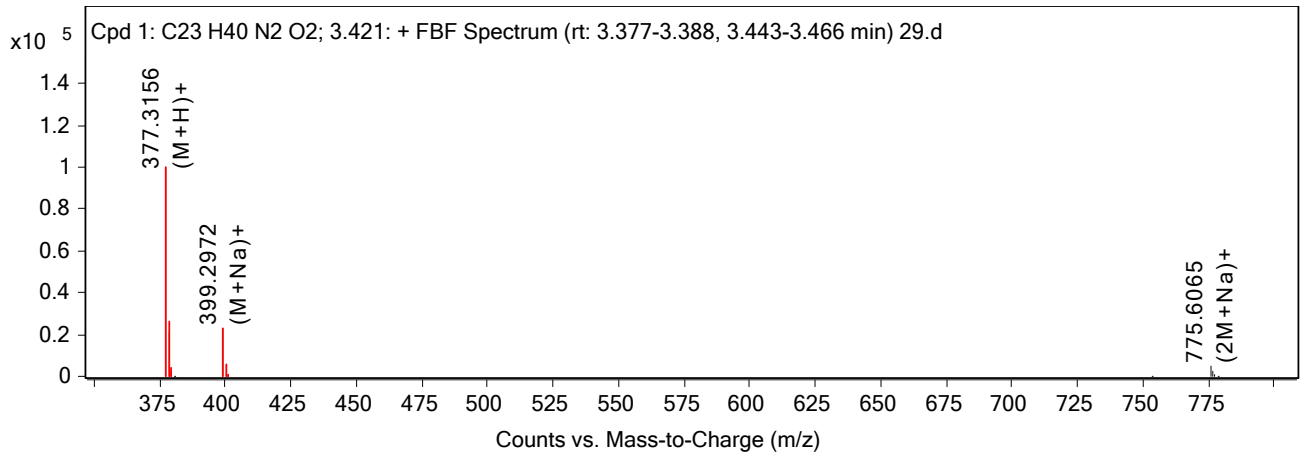
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C23 H40 N2 O2; 3.421	97.46	-2.03	C23 H40 N2 O2	3.421	376.309	376.3082

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
775.6065	3.421	376.3082	C23 H40 N2 O2	376.309	-2.03	Find By Formula	

Compound Chromatograms



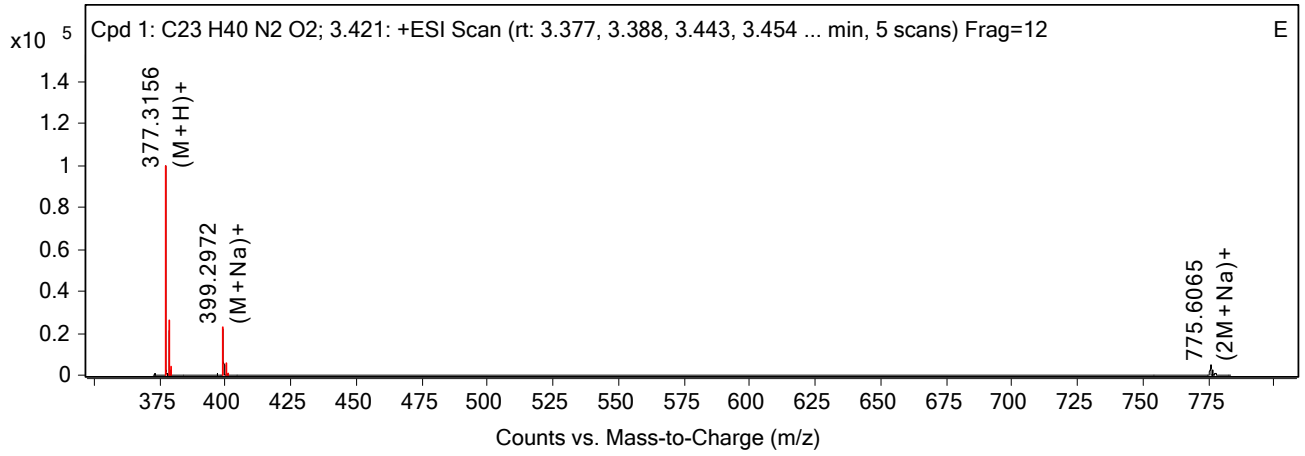
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
377.3156	1	99809.05	(M+H)+
378.3186	1	21266.61	(M+H)+
379.3217	1	2699.36	(M+H)+
380.3181	1	354.17	(M+H)+
399.2972	1	22646.62	(M+Na)+
400.301	1	5160.78	(M+Na)+
401.3018	1	799.57	(M+Na)+
775.6065	1	4701.25	(2M+Na)+
776.6088	1	2407.88	(2M+Na)+
777.611	1	537.13	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
377.3156	1	99809.05	(M+H)+	1.72
378.3186	1	21266.61	(M+H)+	2.31
379.3217	1	2699.36	(M+H)+	1.92
380.3181	1	354.17	(M+H)+	18.81
399.2972	1	22646.62	(M+Na)+	2.38
400.301	1	5160.78	(M+Na)+	0.99
401.3018	1	799.57	(M+Na)+	6.47
775.6065	1	4701.25	(2M+Na)+	0.9
776.6088	1	2407.88	(2M+Na)+	2.12
777.611	1	537.13	(2M+Na)+	3.21

--- End Of Report ---

Target Compound Screening Report

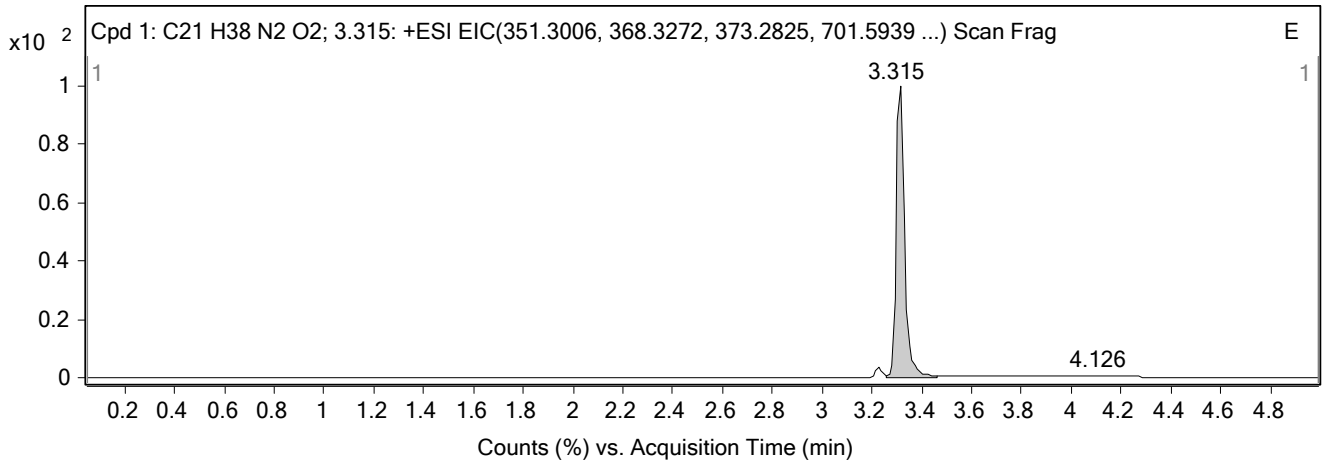
Data File	25.d	**Sample Name**	H2990769
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/24/2021 12:50:32 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C21H38N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/24/2021 12:50:32 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

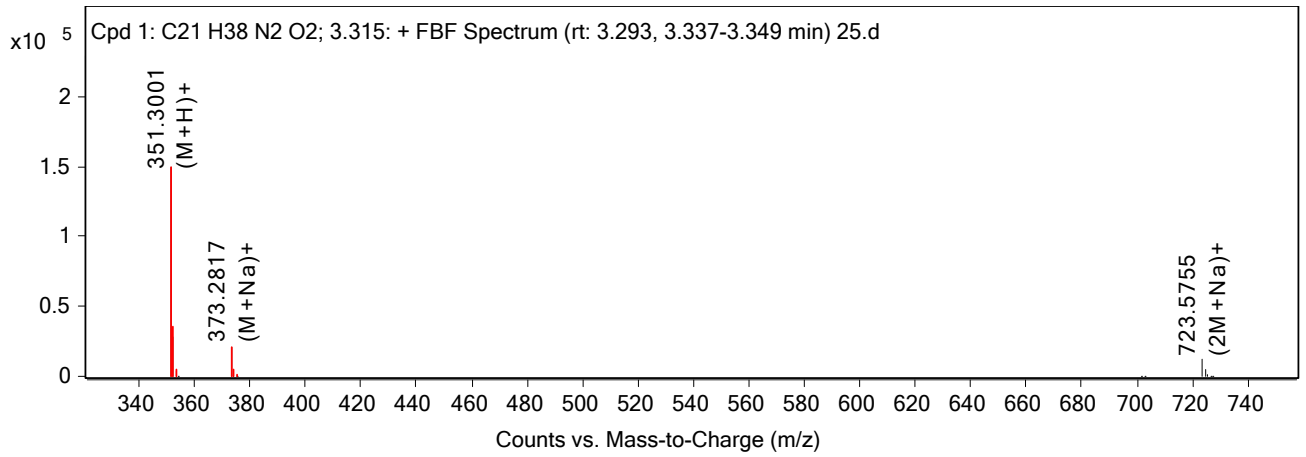
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C21 H38 N2 O2; 3.315	98.41	-1.19	C21 H38 N2 O2	3.315	350.2933	350.2929

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
723.5755	3.315	350.2929	C21 H38 N2 O2	350.2933	-1.19	Find By Formula	

Compound Chromatograms



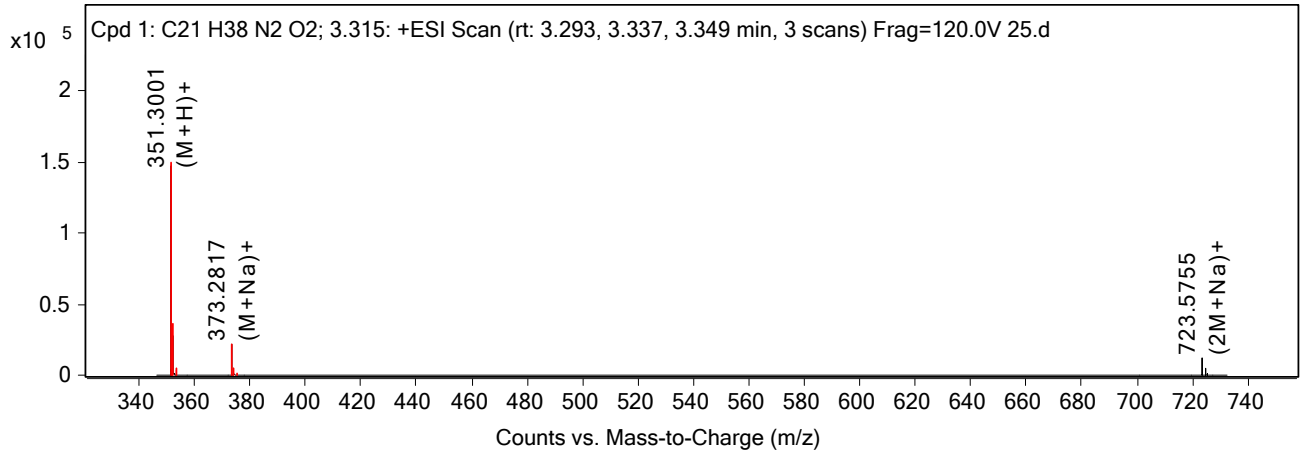
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
351.3001	1	149143.94	(M+H)+
352.3041	1	27999.71	(M+H)+
353.3077	1	3514.03	(M+H)+
354.3111	1	400.44	(M+H)+
373.2817	1	21229.28	(M+Na)+
374.2854	1	4681.22	(M+Na)+
375.2865	1	673.8	(M+Na)+
723.5755	1	11723.36	(2M+Na)+
724.5777	1	5218.04	(2M+Na)+
725.5812	1	1314.22	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
351.3001	1	149143.94	(M+H)+	1.36
352.3041	1	27999.71	(M+H)+	-0.84
353.3077	1	3514.03	(M+H)+	-2.75
354.3111	1	400.44	(M+H)+	-4.32
373.2817	1	21229.28	(M+Na)+	2.15
374.2854	1	4681.22	(M+Na)+	1
375.2865	1	673.8	(M+Na)+	5.73
723.5755	1	11723.36	(2M+Na)+	0.5
724.5777	1	5218.04	(2M+Na)+	1.98
725.5812	1	1314.22	(2M+Na)+	1.27

--- End Of Report ---

Target Compound Screening Report

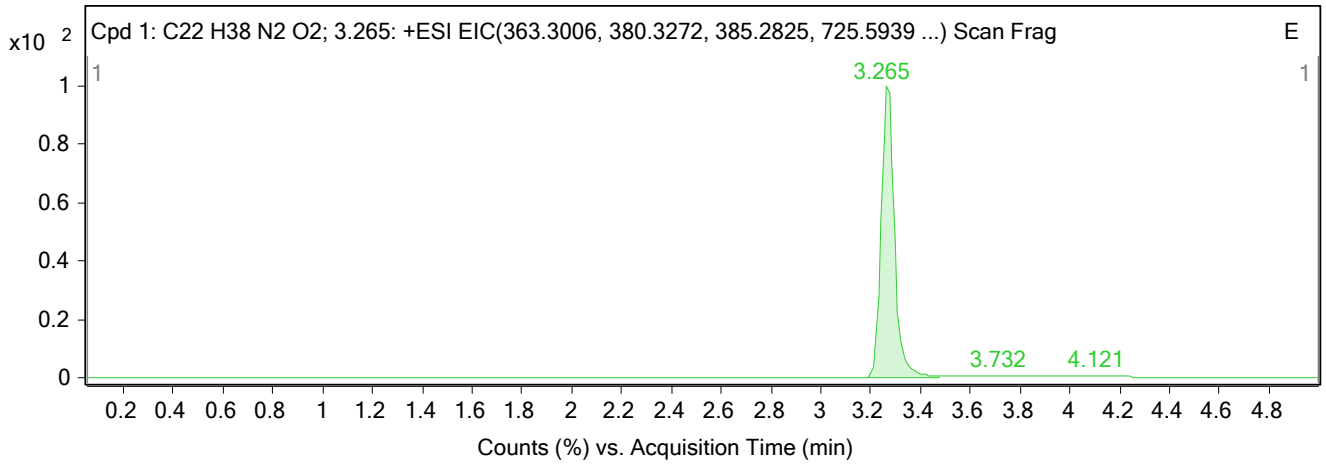
Data File	23.d	**Sample Name**	H2990770
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	Denis V.Bylina
Acq Method	Fast_Gradient_HRMS_pos_Lock_08272019.m	**Acquired Time**	9/23/2021 8:55:47 PM (UTC+03:00)
IRM Calibration Status	Success	**DA Method**	1.m
Comment			
Sample Group		**Info.**	Agilent 6224 TOF LC/MS
MFC	C22H38N2O2	**Stream Name**	LC 1
Acquisition Time (Local)	9/23/2021 8:55:47 PM (UTC+03:00)	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)
TOF Driver Version	8.00.00	**TOF Firmware Version**	8.643
Tune Mass Range Max.	1700		

Compound Table

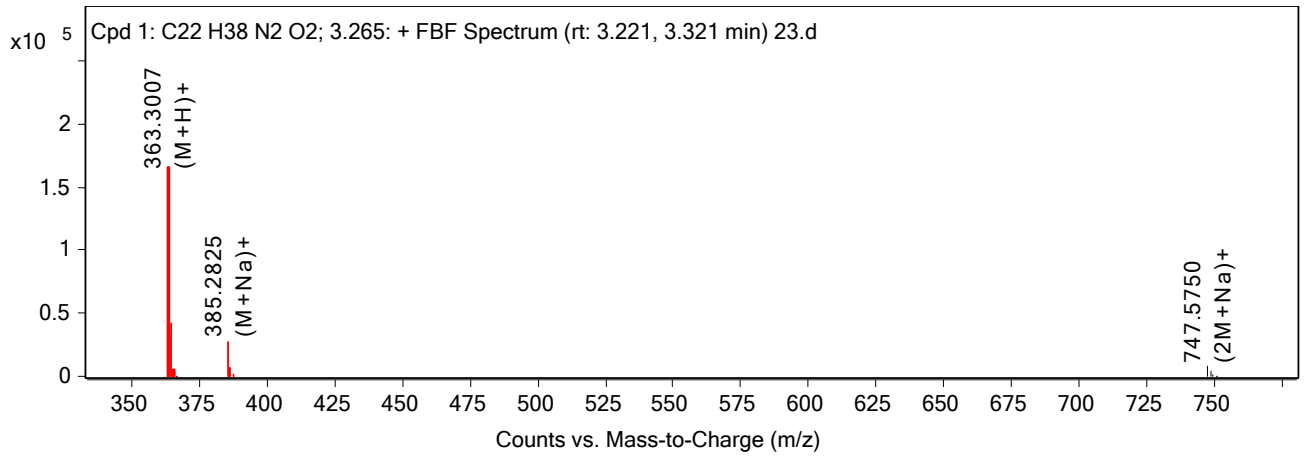
Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C22 H38 N2 O2; 3.265	99.72	-0.15	C22 H38 N2 O2	3.265	362.2933	362.2933

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
385.2825	3.265	362.2933	C22 H38 N2 O2	362.2933	-0.15	Find By Formula	

Compound Chromatograms



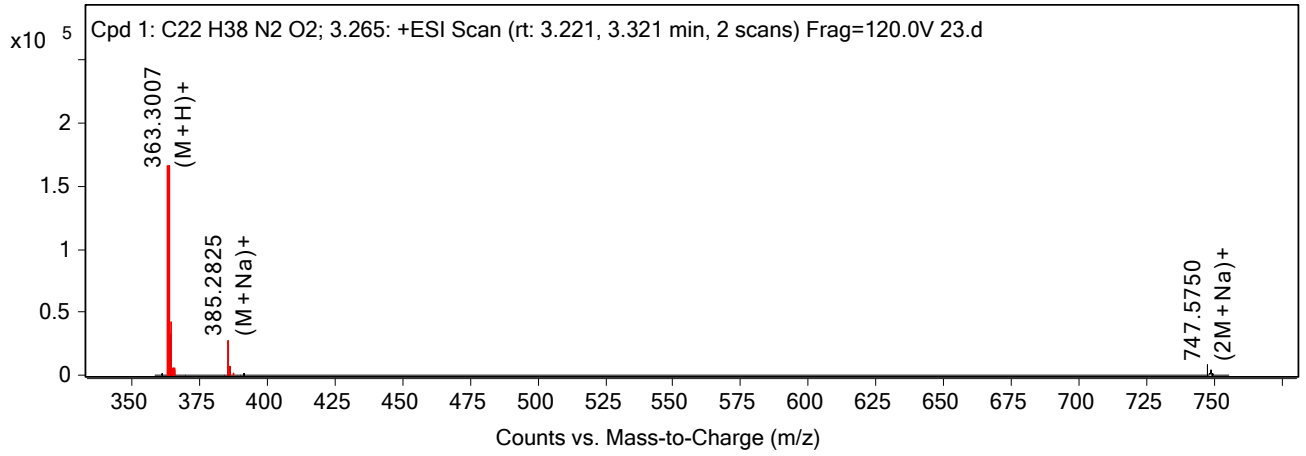
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope
363.3007	1	165753.05	(M+H)+
364.3035	1	32806.52	(M+H)+
365.3071	1	3868.58	(M+H)+
366.3047	1	416.89	(M+H)+
385.2825	1	27447.09	(M+Na)+
386.2858	1	6593.94	(M+Na)+
387.2892	1	1026.03	(M+Na)+
747.575	1	7863.71	(2M+Na)+
748.5766	1	3904.6	(2M+Na)+
749.5785	1	1055.03	(2M+Na)+

MS Zoomed Spectrum



MS Spectrum Peak List

Obs. *m/z*	Charge	Abund	Ion/Isotope	Tgt Mass Error (ppm)
363.3007	1	165753.05	(M+H)+	-0.35
364.3035	1	32806.52	(M+H)+	1.04
365.3071	1	3868.58	(M+H)+	-0.88
366.3047	1	416.89	(M+H)+	13.29
385.2825	1	27447.09	(M+Na)+	0
386.2858	1	6593.94	(M+Na)+	-0.03
387.2892	1	1026.03	(M+Na)+	-1.16
747.575	1	7863.71	(2M+Na)+	1.14
748.5766	1	3904.6	(2M+Na)+	3.28
749.5785	1	1055.03	(2M+Na)+	4.95

--- End Of Report ---