

Supplementary data

for

Design, synthesis, and development of pyrazolo[1,5-*a*]pyrimidine derivatives as a novel series of selective PI3K δ inhibitors. Part II – Benzimidazole derivatives.

Mariola Stypik^{1,2*}, Stanisław Michałek^{1,2}, Nina Orłowska^{1,2}, Marcin Zagozda¹, Maciej Dziachan¹, Martyna Banach¹, Paweł Turowski¹, Paweł Gunerka¹, Daria Zdżalik-Bielecka¹, Aleksandra Stańczak¹, Urszula Kędzierska¹, Krzysztof Mulewski¹, Damian Smuga¹, Wioleta Maruszak¹, Lidia Gurba-Bryśkiewicz¹, Zbigniew Ochal², Mateusz Mach¹, Beata Zygmunt¹, Jerzy Pieczykolan¹, Krzysztof Dubiel¹, Maciej Wieczorek¹

¹ Celon Pharma S.A., R&D Centre, Marymoncka 15, 05-152 Kazuń Nowy, Poland

² Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, 00-664 Warsaw, Poland

*corresponding author: mariola.stypik@celonpharma.com

¹H NMR, ¹³C NMR and HRMS supplementary figures of the final compounds **5-9**, **11-12**, **16-38** and **40-54**

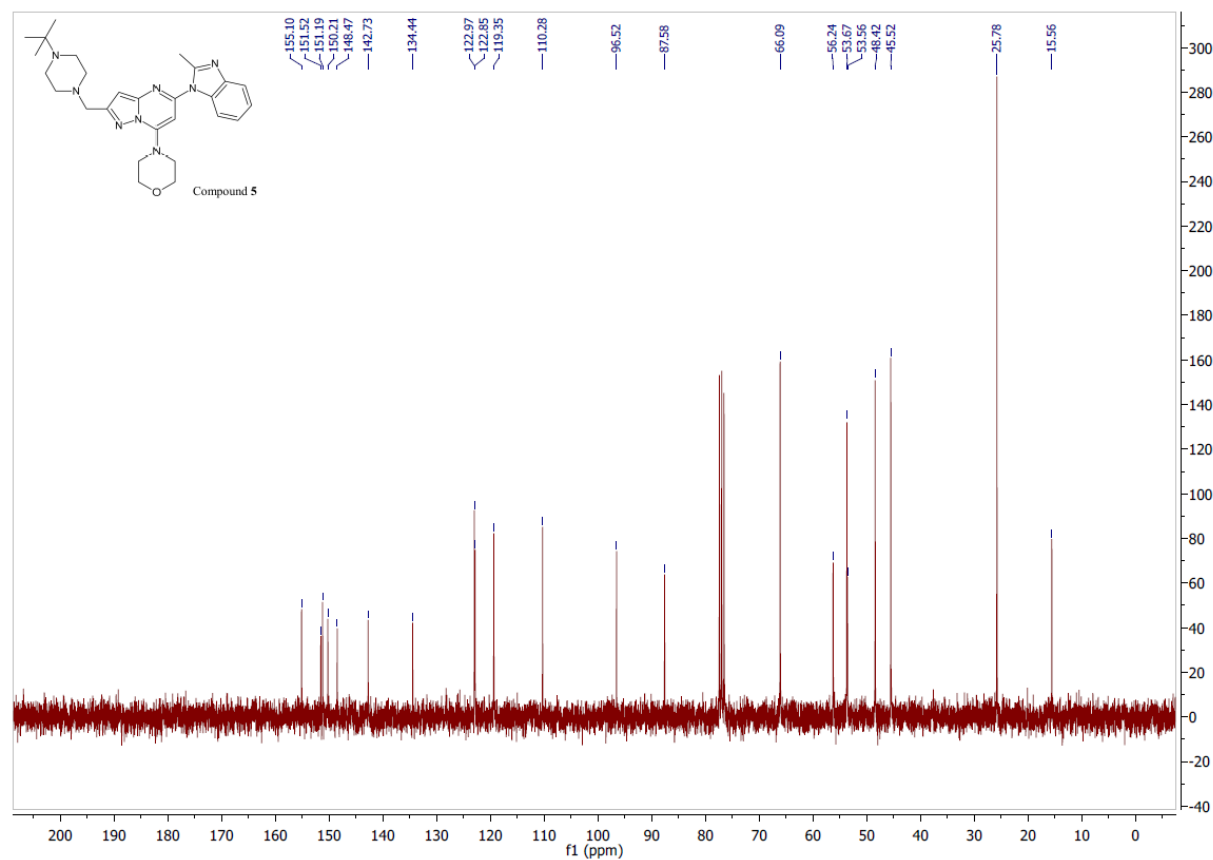
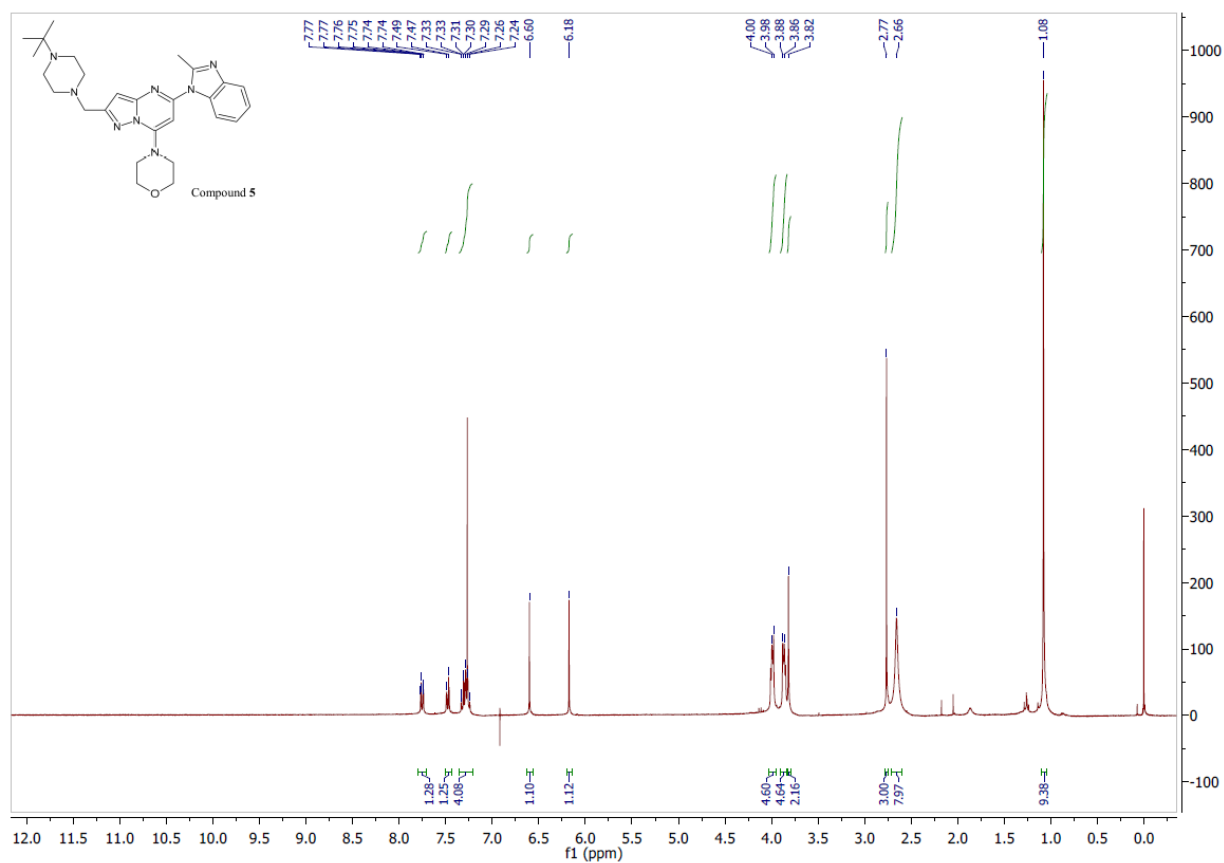
INDEX

Compound 5 ^1H NMR and ^{13}C NMR	5
Compound 5 HRMS	6
Compound 6 ^1H NMR and ^{13}C NMR	7
Compound 6 HRMS	8
Compound 7 ^1H NMR and ^{13}C NMR	9
Compound 7 HRMS	10
Compound 8 ^1H NMR and ^{13}C NMR	11
Compound 8 HRMS	12
Compound 9 ^1H NMR and ^{13}C NMR	13
Compound 9 HRMS	14
Compound 11 ^1H NMR and ^{13}C NMR	15
Compound 11 HRMS	16
Compound 12 ^1H NMR and ^{13}C NMR	17
Compound 12 HRMS	18
Compound 16 ^1H NMR and ^{13}C NMR	19
Compound 16 HRMS	20
Compound 17 ^1H NMR and ^{13}C NMR	21
Compound 17 HRMS	22
Compound 18 ^1H NMR and ^{13}C NMR	23
Compound 18 HRMS	24
Compound 19 ^1H NMR and ^{13}C NMR	25
Compound 19 HRMS	26
Compound 20 ^1H NMR and ^{13}C NMR	27
Compound 20 HRMS	28
Compound 21 ^1H NMR and ^{13}C NMR	29
Compound 21 HRMS	30
Compound 22 ^1H NMR and ^{13}C NMR	31
Compound 22 HRMS	32
Compound 23 ^1H NMR and ^{13}C NMR	33
Compound 23 HRMS	34
Compound 24 ^1H NMR and ^{13}C NMR	35
Compound 24 HRMS	36
Compound 25 ^1H NMR and ^{13}C NMR	37
Compound 25 HRMS	38
Compound 26 ^1H NMR and ^{13}C NMR	39
Compound 26 HRMS	40

Compound 27 ^1H NMR and ^{13}C NMR	41
Compound 27 HRMS	42
Compound 28 ^1H NMR and ^{13}C NMR	43
Compound 28 HRMS	44
Compound 29 ^1H NMR and ^{13}C NMR	45
Compound 29 HRMS	46
Compound 30 ^1H NMR and ^{13}C NMR	47
Compound 30 HRMS	48
Compound 31 ^1H NMR and ^{13}C NMR	49
Compound 31 HRMS	50
Compound 32 ^1H NMR and ^{13}C NMR	51
Compound 32 HRMS	52
Compound 33 ^1H NMR and ^{13}C NMR	53
Compound 33 HRMS	54
Compound 34 ^1H NMR and ^{13}C NMR	55
Compound 34 HRMS	56
Compound 35 ^1H NMR and ^{13}C NMR	57
Compound 35 HRMS	58
Compound 36 ^1H NMR and ^{13}C NMR	59
Compound 36 HRMS	60
Compound 37 ^1H NMR and ^{13}C NMR	61
Compound 37 HRMS	62
Compound 38 ^1H NMR and ^{13}C NMR	63
Compound 38 HRMS	64
Compound 40 ^1H NMR and ^{13}C NMR	65
Compound 40 HRMS	66
Compound 41 ^1H NMR and ^{13}C NMR	67
Compound 41 HRMS	68
Compound 42 ^1H NMR and ^{13}C NMR	69
Compound 42 HRMS	70
Compound 43 ^1H NMR and ^{13}C NMR	71
Compound 43 HRMS	72
Compound 44 ^1H NMR and ^{13}C NMR	73
Compound 44 HRMS	74
Compound 45 ^1H NMR and ^{13}C NMR	75
Compound 45 HRMS	76
Compound 46 ^1H NMR and ^{13}C NMR	77

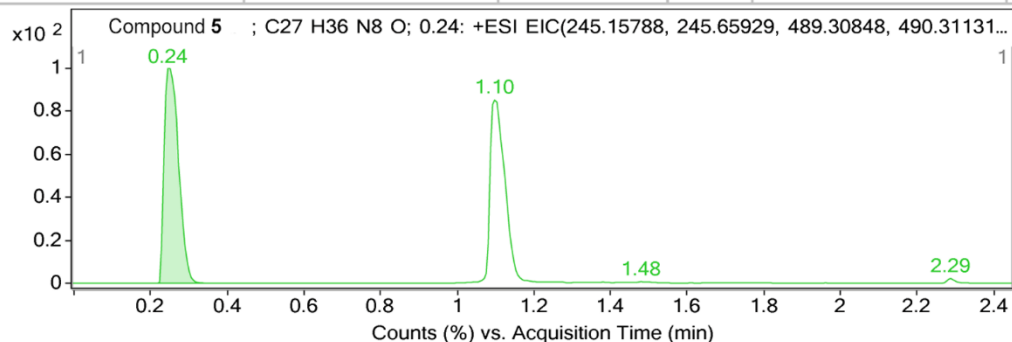
Compound 46 HRMS	78
Compound 47 ^1H NMR and ^{13}C NMR	79
Compound 47 HRMS	80
Compound 48 ^1H NMR and ^{13}C NMR	81
Compound 48 HRMS	82
Compound 49 ^1H NMR and ^{13}C NMR	83
Compound 49 HRMS	84
Compound 50 ^1H NMR and ^{13}C NMR	85
Compound 50 HRMS	86
Compound 51 ^1H NMR and ^{13}C NMR	87
Compound 51 HRMS	88
Compound 52 ^1H NMR and ^{13}C NMR	89
Compound 52 HRMS	90
Compound 53 ^1H NMR and ^{13}C NMR	91
Compound 53 HRMS	92
Compound 54 ^1H NMR and ^{13}C NMR	93
Compound 54 HRMS	94
Compound 55 ^1H NMR and ^{13}C NMR	95
Compound 55 HRMS	96
Compound 56 ^1H NMR and ^{13}C NMR	97
Compound 56 HRMS	98
Compound 57 ^1H NMR and ^{13}C NMR	99
Compound 57 HRMS	100

Compound 5

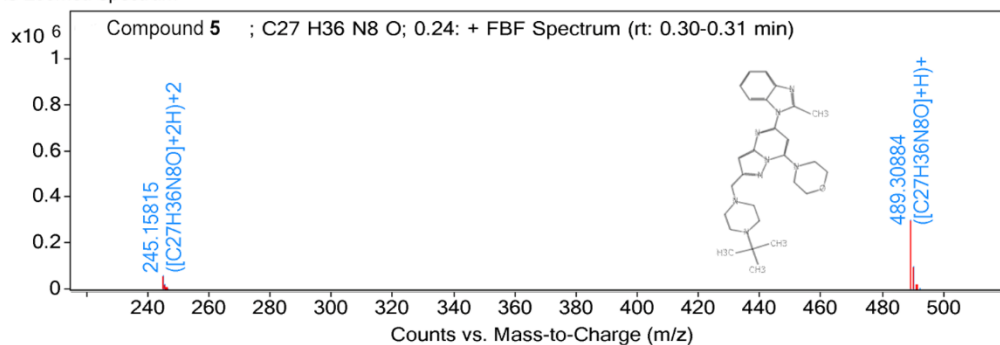


Compound 5

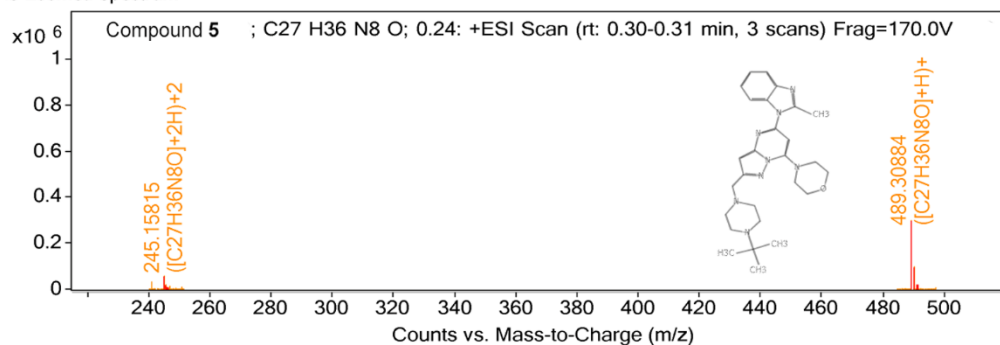
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 5	Compound 5	489.30884	0.24	Find by Formula	488.30154



MS Zoomed Spectrum



MS Zoomed Spectrum

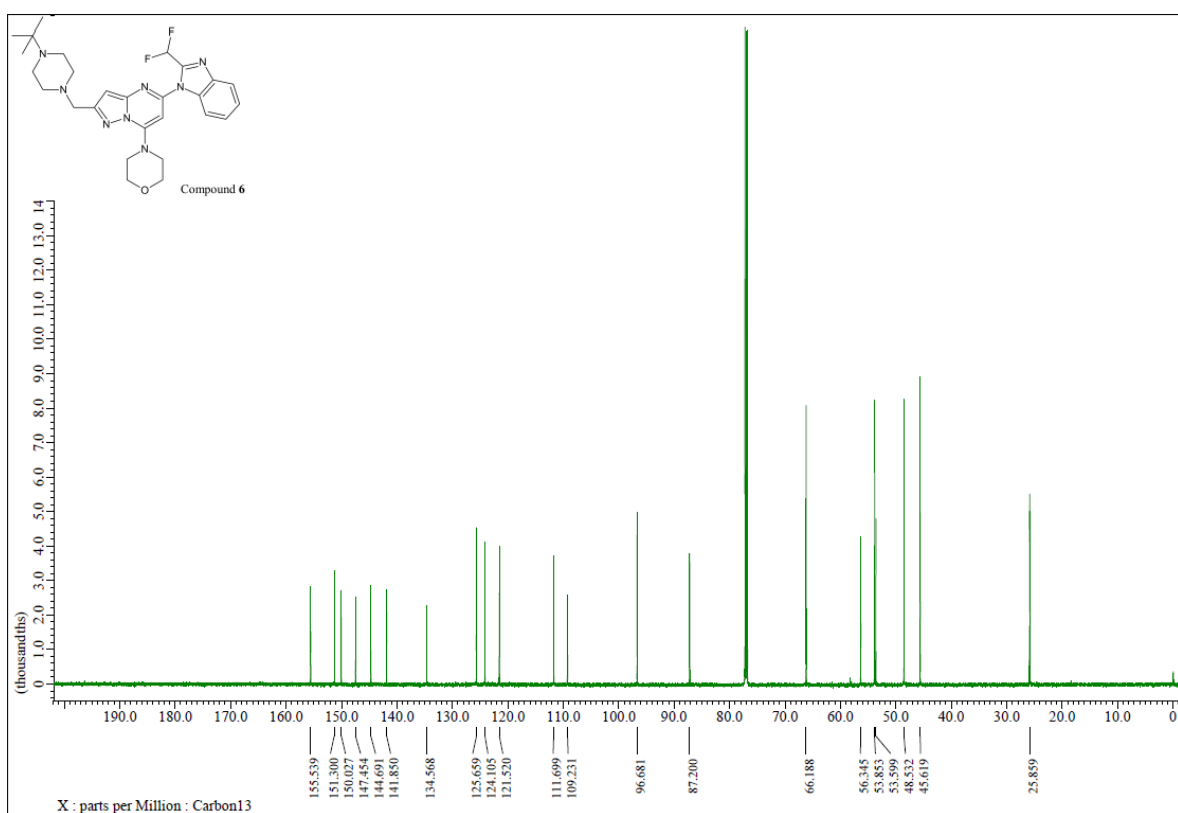
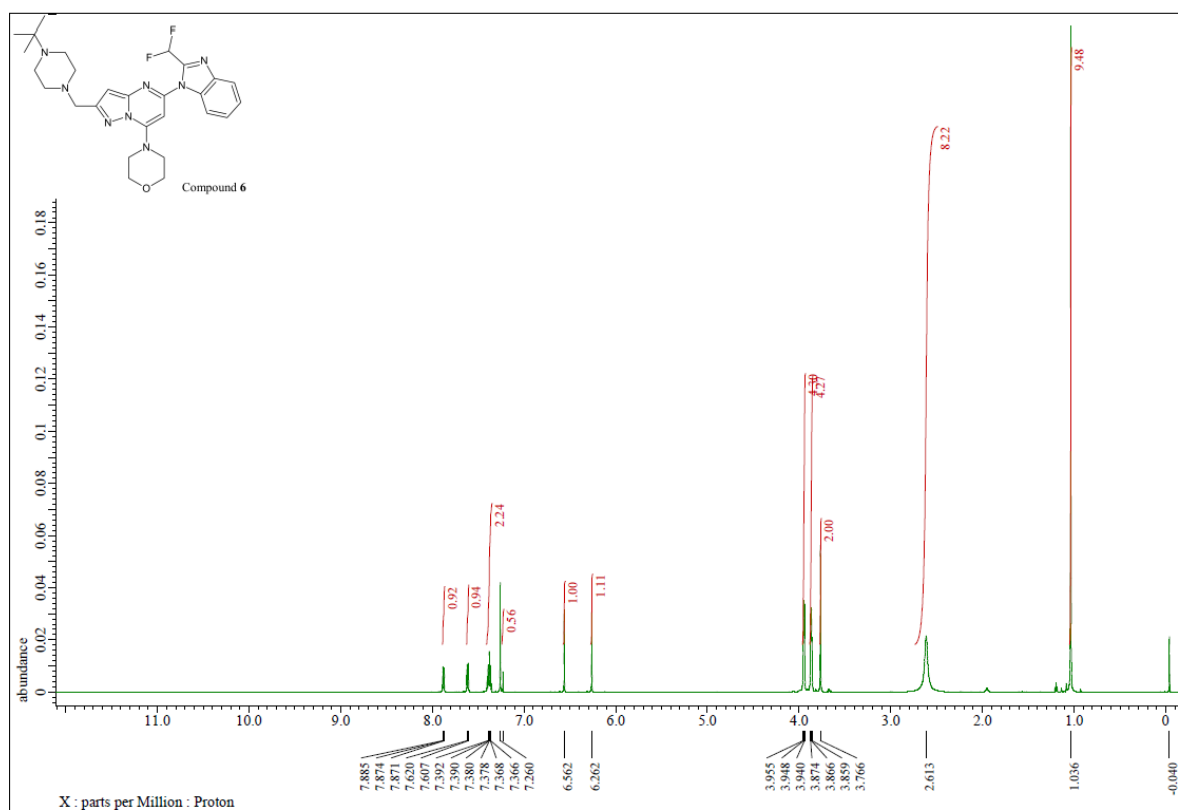


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
245.15815	245.15788	1.12	2	56190	C ₂₇ H ₃₆ N ₈ O	(M+2H)+2
245.65963	245.65929	1.38	2	18164.55	C ₂₇ H ₃₆ N ₈ O	(M+2H)+2
246.16121	246.16067	2.2	2	2663.72	C ₂₇ H ₃₆ N ₈ O	(M+2H)+2
246.66092	246.66202	-4.46	2	280.06	C ₂₇ H ₃₆ N ₈ O	(M+2H)+2
489.30884	489.30848	0.72	1	298324.84	C ₂₇ H ₃₆ N ₈ O	(M+H)+
490.31149	490.31131	0.37	1	97178.29	C ₂₇ H ₃₆ N ₈ O	(M+H)+
491.31367	491.31407	-0.81	1	14949.13	C ₂₇ H ₃₆ N ₈ O	(M+H)+
492.31654	492.31675	-0.42	1	1609.93	C ₂₇ H ₃₆ N ₈ O	(M+H)+

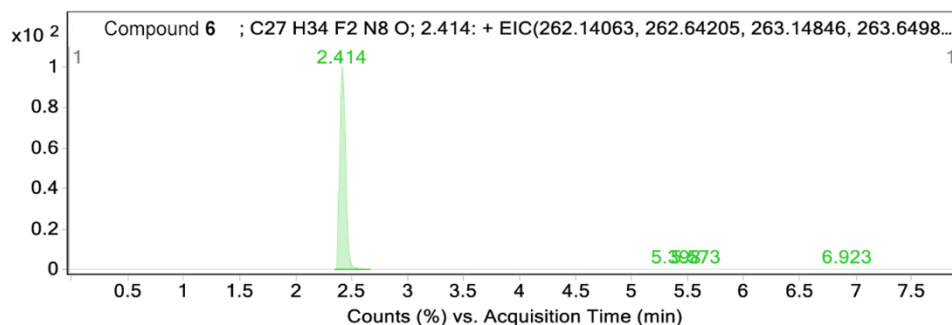
--- End Of Report ---

Compound 6

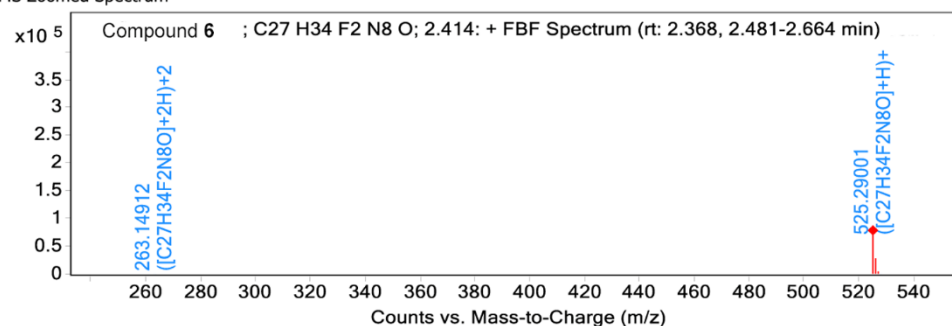


Compound 6

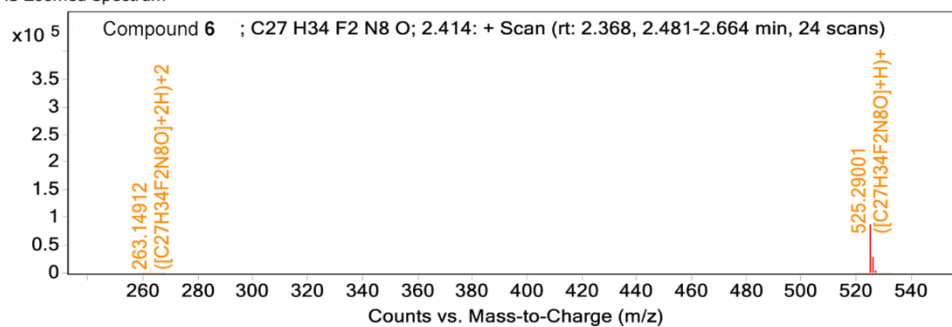
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 6	Compound 6	525.29001	2.414	Find by Formula	524.28269



MS Zoomed Spectrum



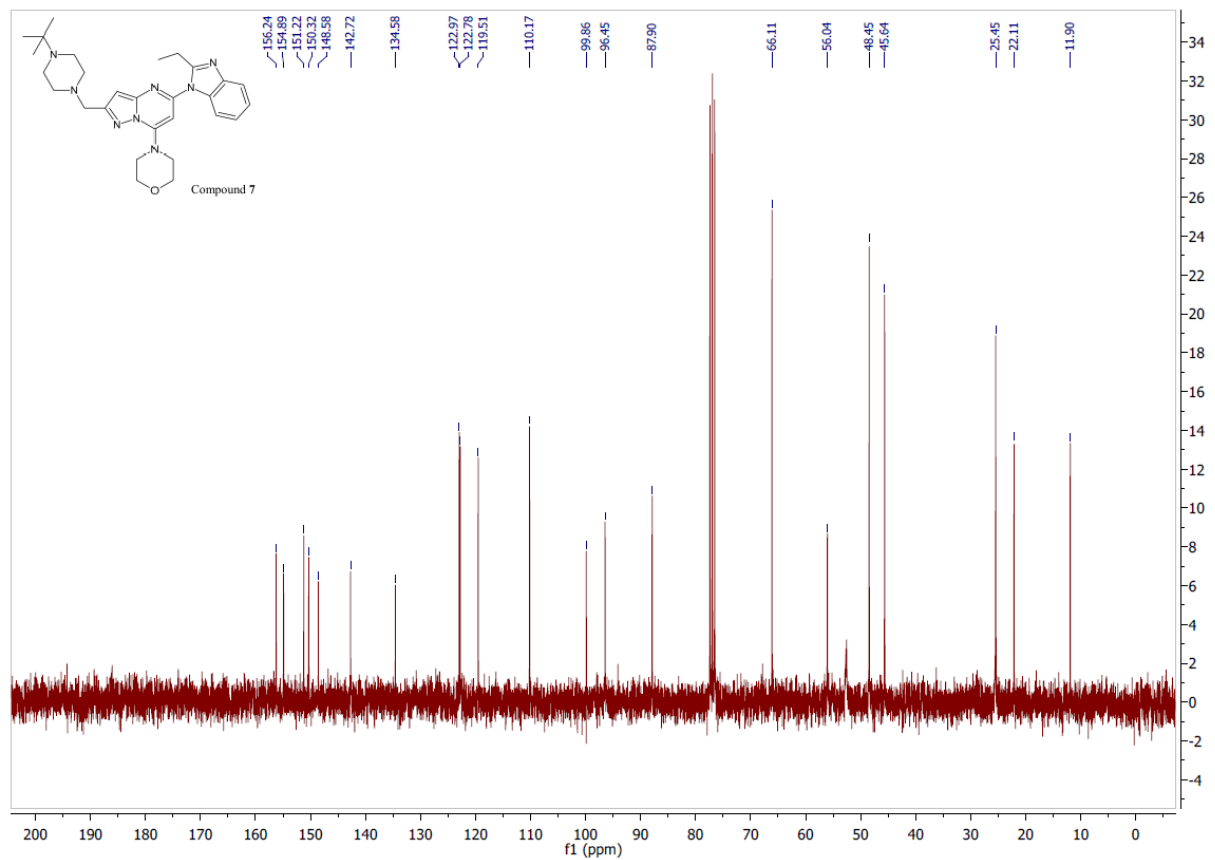
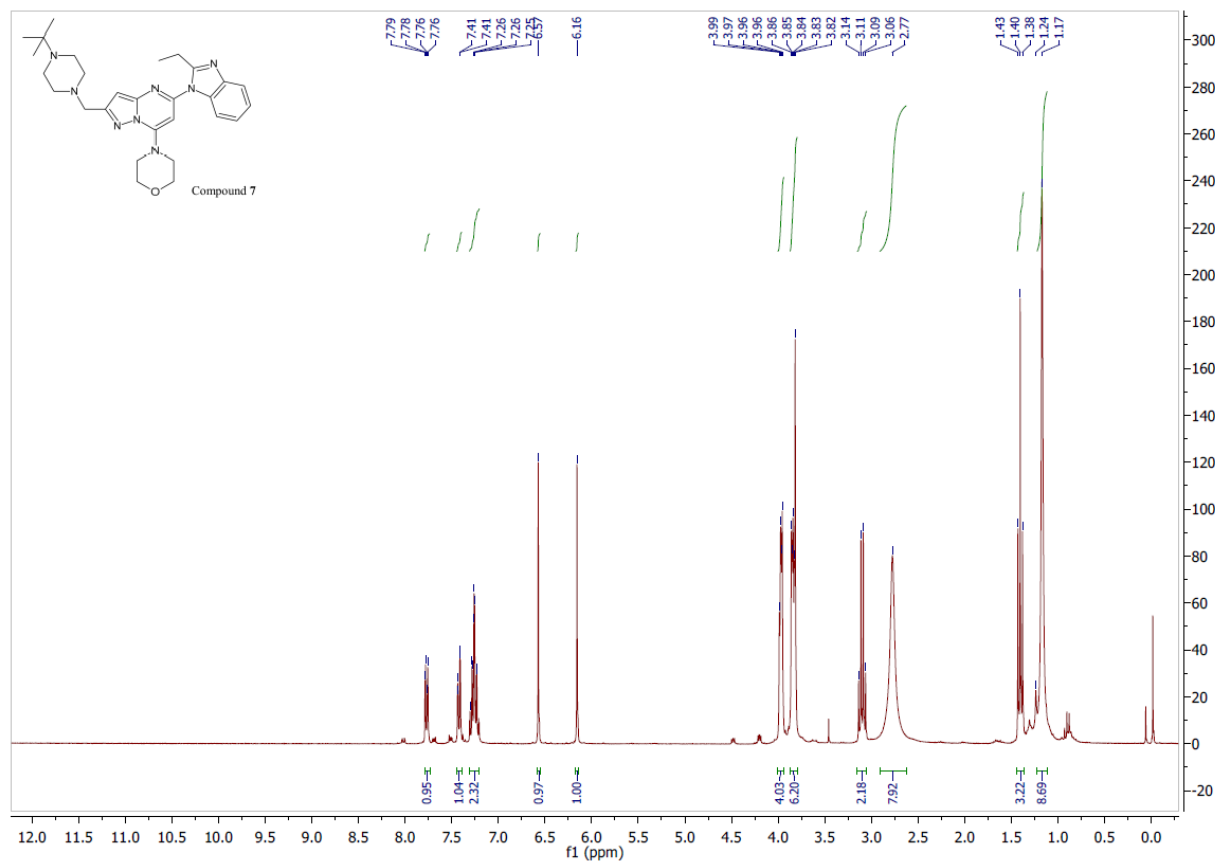
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
263.14912	263.14846	2.5	2	359.79	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+2H)+2
263.64952	263.64987	-1.32	2	96.69	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+2H)+2
524.27521	524.28182	-12.6	1	183.57	C ₂₇ H ₃₄ F ₂ N ₈ O	M+
525.29001	525.28964	0.7	1	86308.49	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+H)+
526.29271	526.29247	0.47	1	27103.87	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+H)+
527.29545	527.29522	0.45	1	3988.21	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+H)+
528.29851	528.2979	1.16	1	428.02	C ₂₇ H ₃₄ F ₂ N ₈ O	(M+H)+

Compound 7



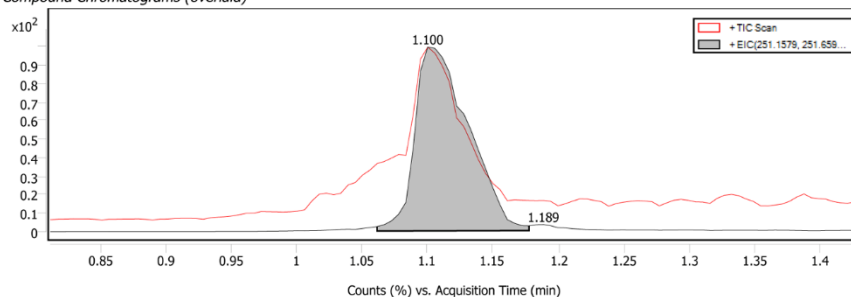
Compound 7

Compound Details

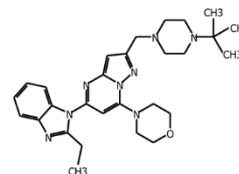
Cpd. 12: Compound 7

Table 2. Compound 7								
Name	Formula	RT	RI	Mass Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
Compound 7	C28 H38 N8 O	1.100		502.3171	0.41	FBF	99.96	FBF
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)		
(M+2H)+2	252.1661	290.1263	99.96					
(M+H)+	503.3243							

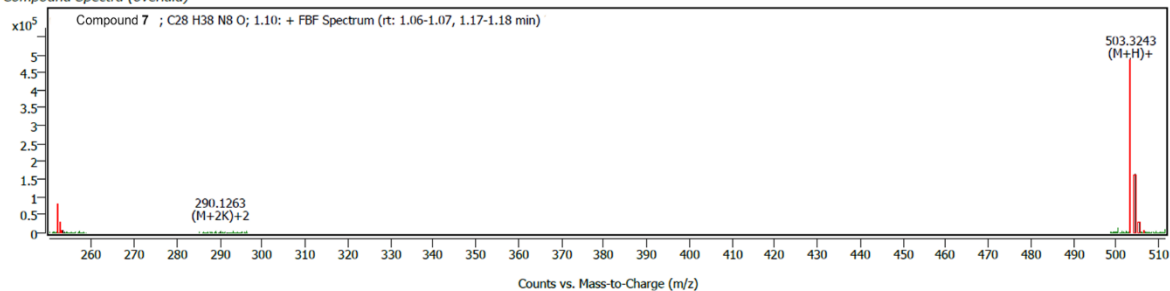
Compound Chromatograms (overlaid)



Structure



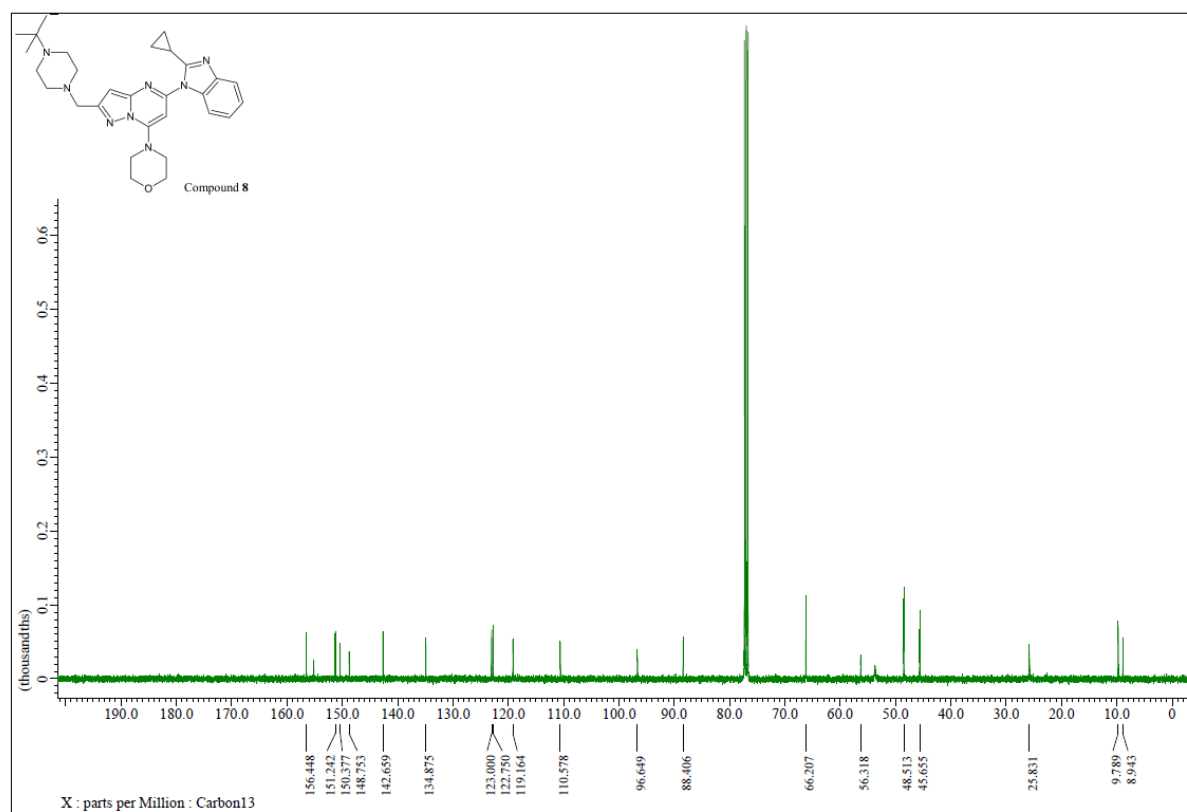
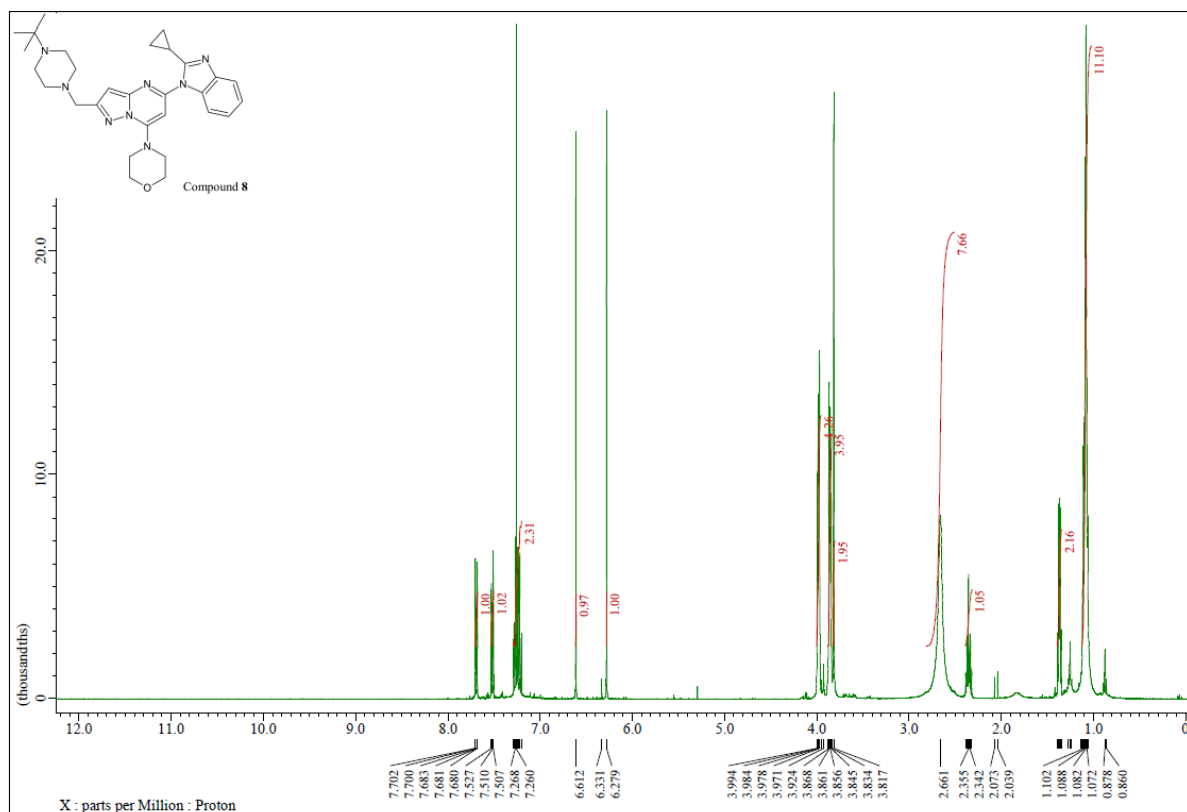
Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
Compound 7	C28 H38 N8 O	(M+2H)+2 (M+2K)+2 (M+H)+	1.100		502.3171		FBF	99.96		99.96

Compound 8



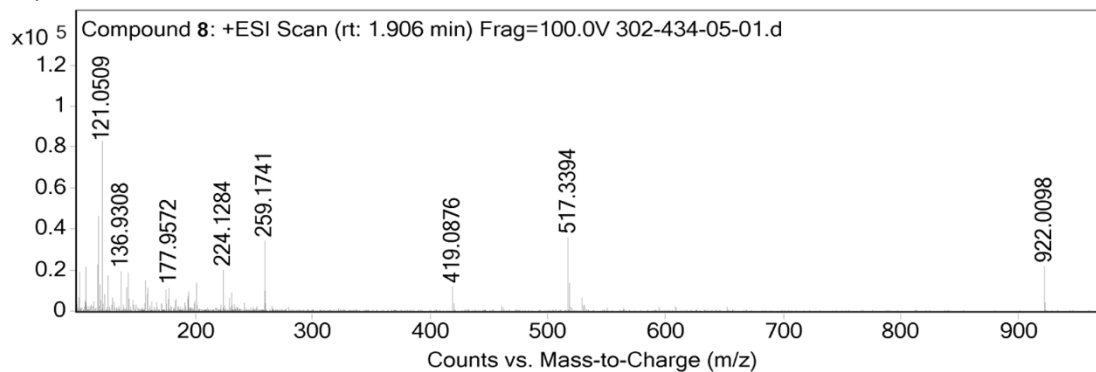
Compound 8

Compound Table

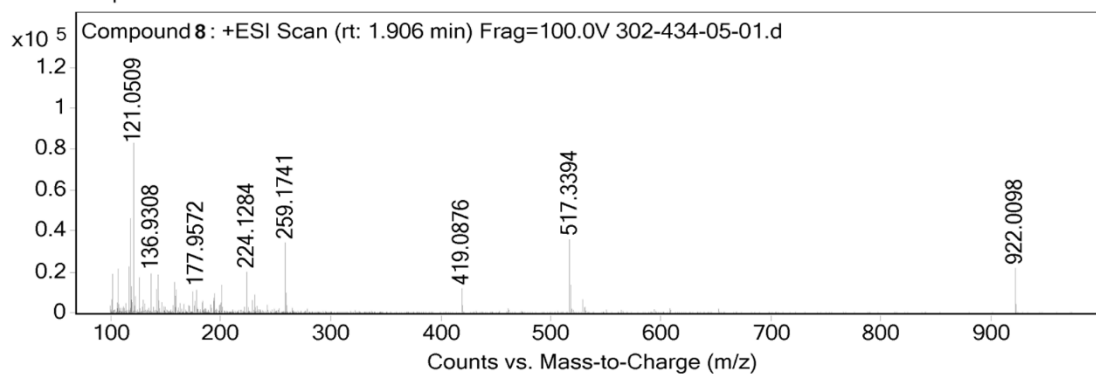
Compound Label
Compound 8

Compound Label	Algorithm
Compound 8	Spectrum Extraction

MS Spectrum



MS Zoomed Spectrum

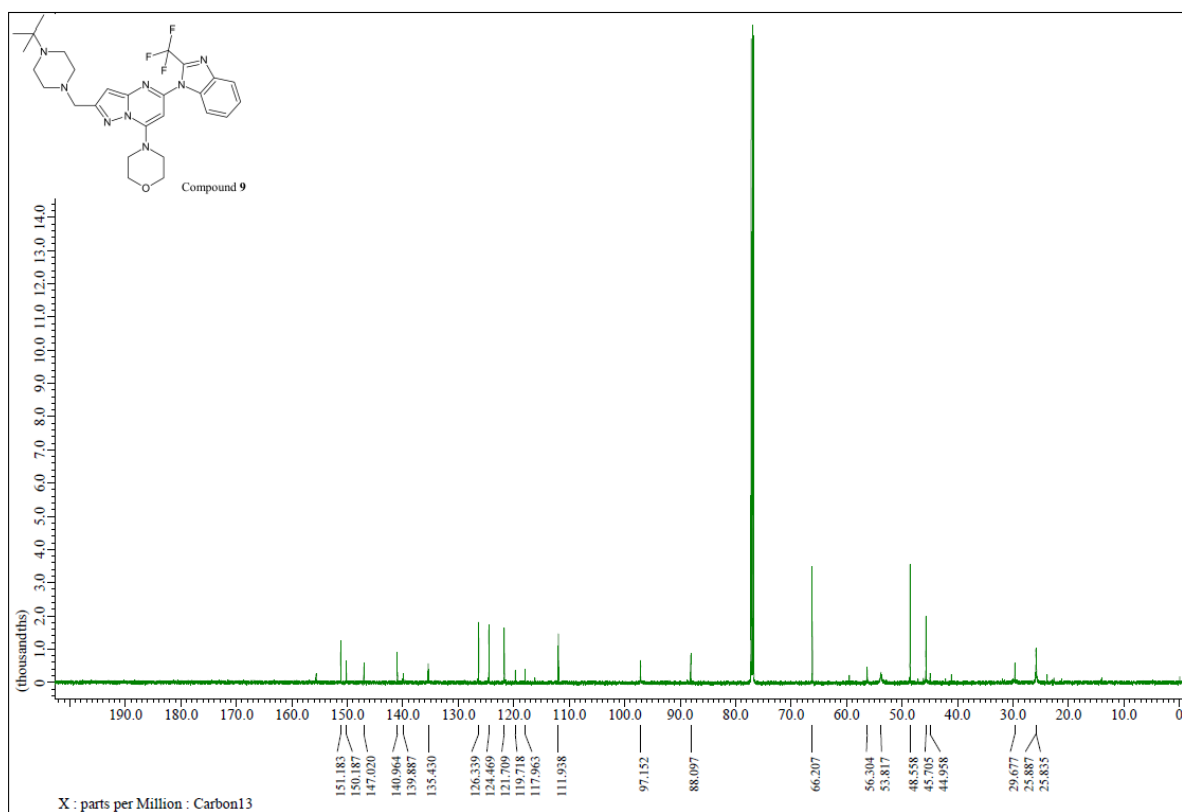
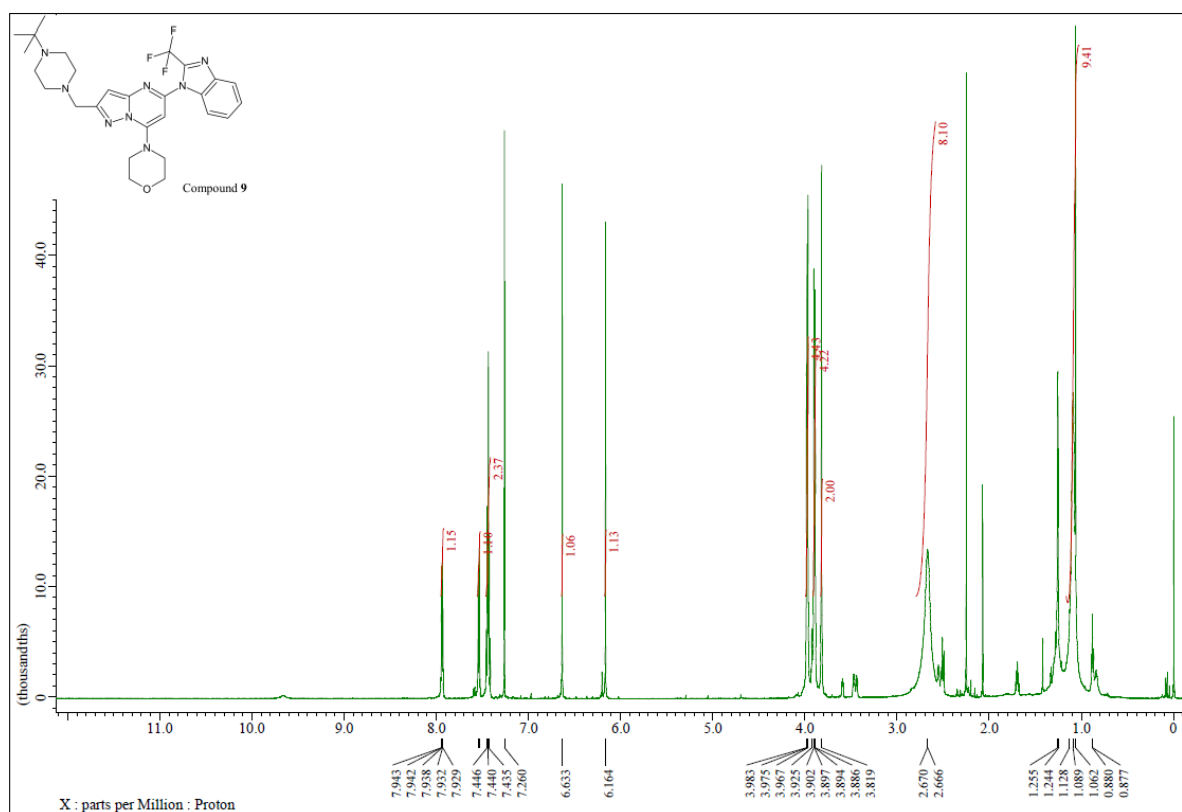


MS Spectrum Peak List

m/z	z	Abund
102.1278		18882.98
107.0437		21485.96
117.0909		22488.31
118.0865		46076.47
121.0509		82922.48
136.9308		19114.65
224.1284		19938.67
259.1741	2	34202.22
517.3394	1	35841.52
922.0098		21757.48

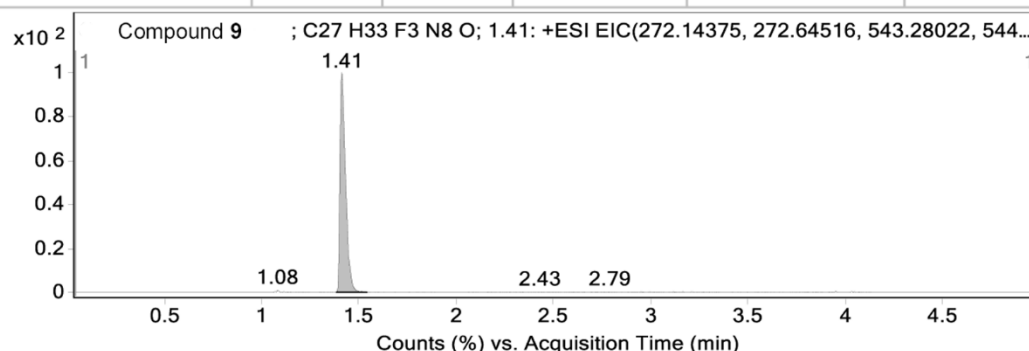
--- End Of Report ---

Compound 9

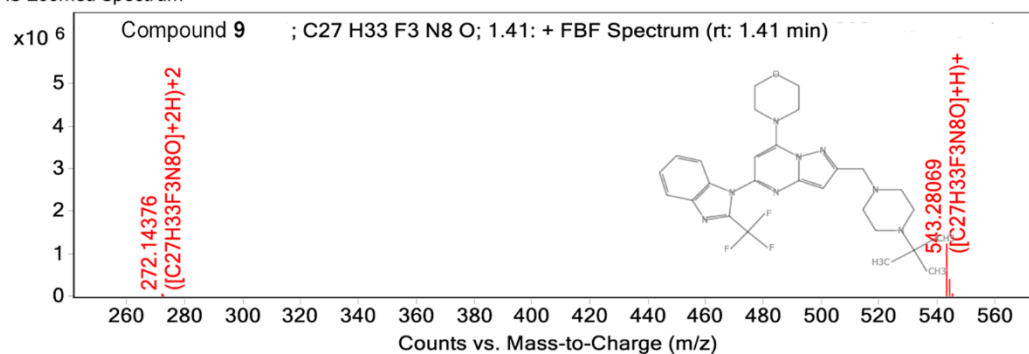


Compound 9

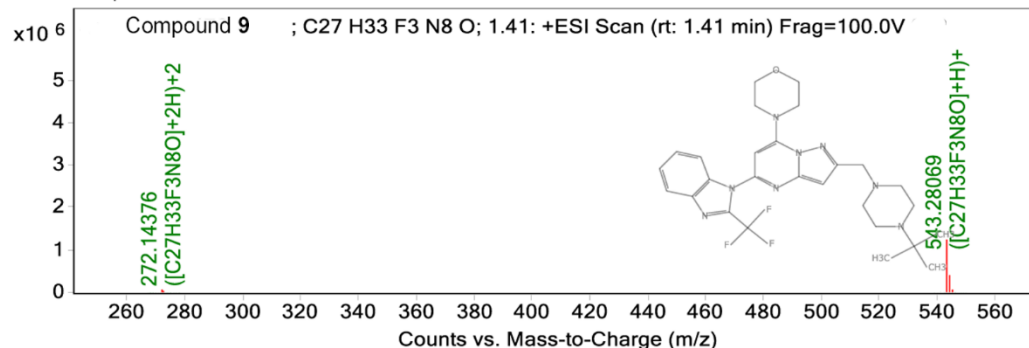
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 9	272.14376	1.41	542.27339	C27 H33 F3 N8 O	542.27294	0.83	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

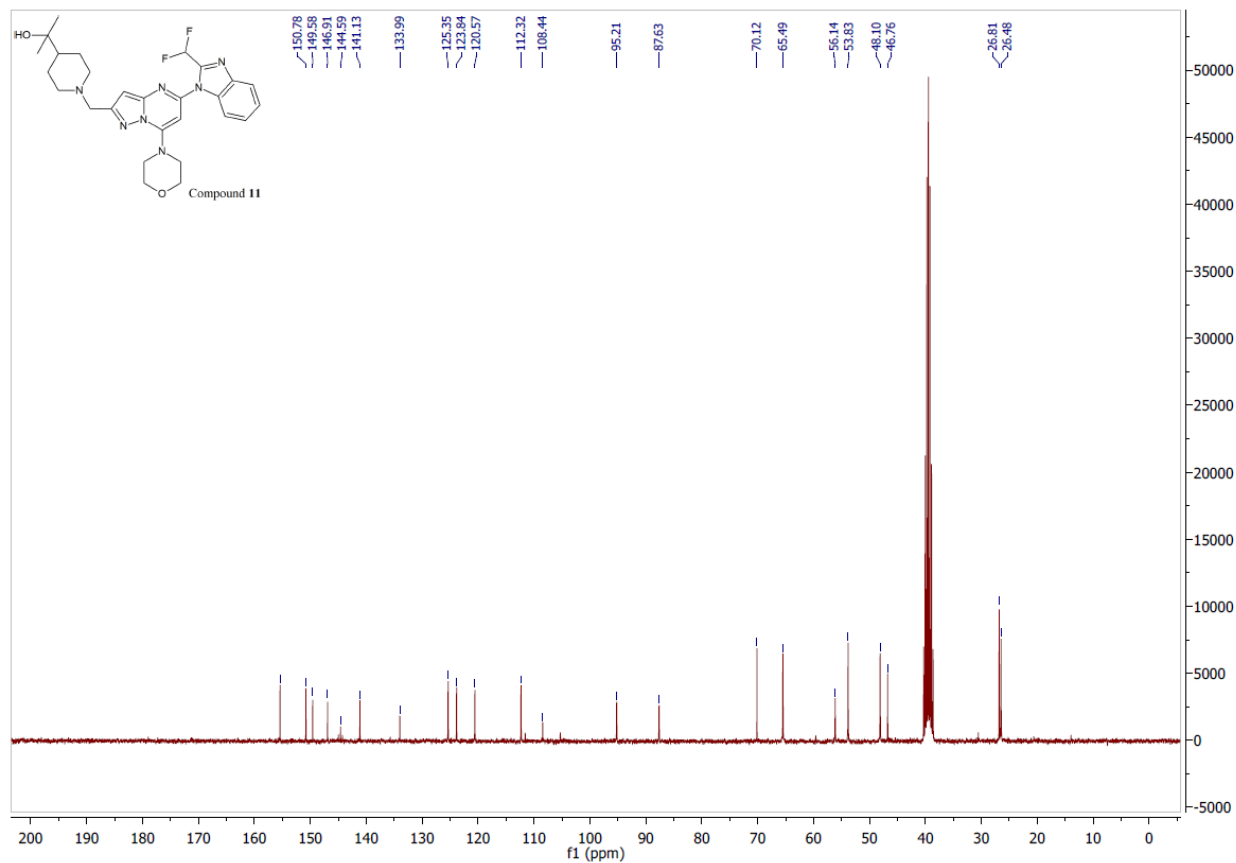
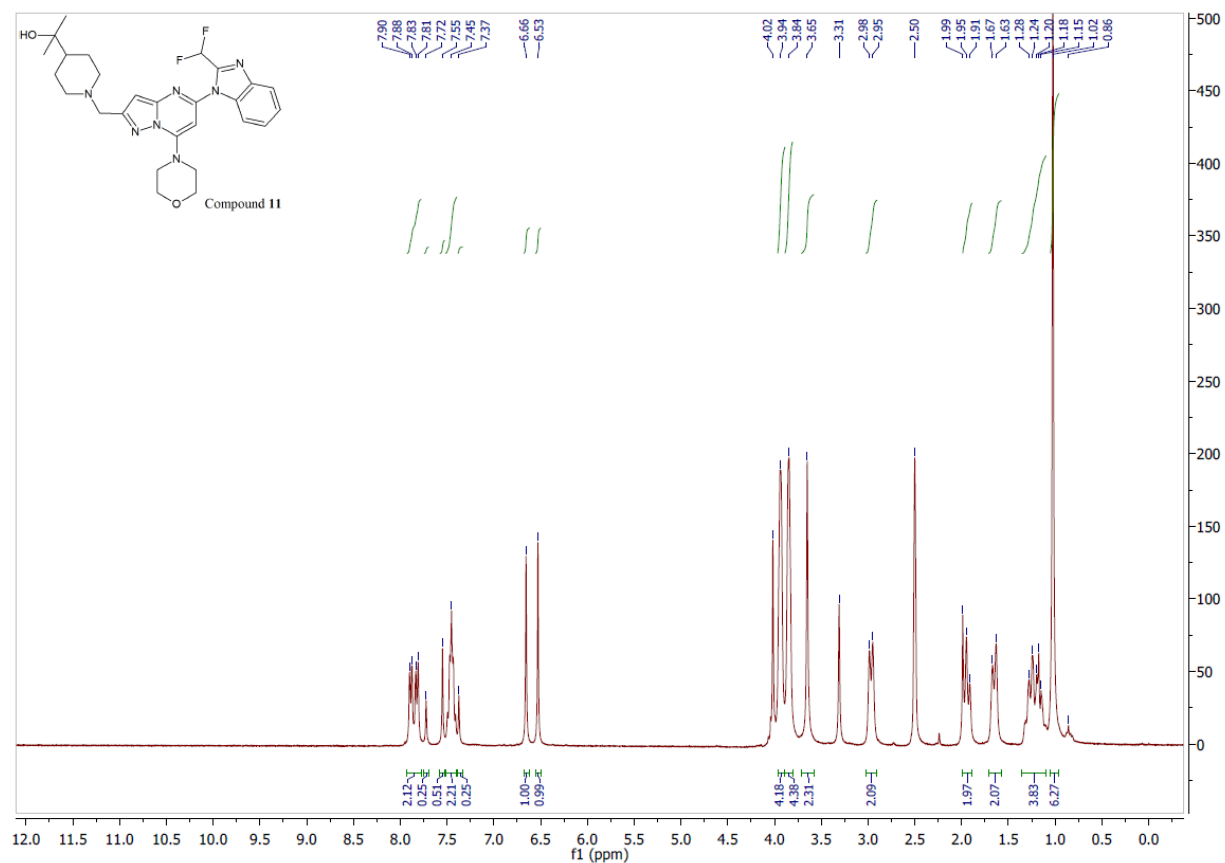


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
272.14376	2	65592.5	C27H33F3N8O	(M+2H)+2	
272.6453	2	23443.74	C27H33F3N8O	(M+2H)+2	
273.14618	2	4575.98	C27H33F3N8O	(M+2H)+2	
273.64635	2	210.29	C27H33F3N8O	(M+2H)+2	
543.28069	1	1223762.88	C27H33F3N8O	(M+H)+	
544.28358	1	331950.72	C27H33F3N8O	(M+H)+	
545.28592	1	53670.24	C27H33F3N8O	(M+H)+	
272.14376	2	65592.5	C27H33F3N8O	(M+2H)+2	0.03
272.6453	2	23443.74	C27H33F3N8O	(M+2H)+2	0.53
273.14618	2	4575.98	C27H33F3N8O	(M+2H)+2	-1.32
273.64635	2	210.29	C27H33F3N8O	(M+2H)+2	-5.59
543.28069	1	1223762.88	C27H33F3N8O	(M+H)+	0.87
544.28358	1	331950.72	C27H33F3N8O	(M+H)+	0.99
545.28592	1	53670.24	C27H33F3N8O	(M+H)+	0.23

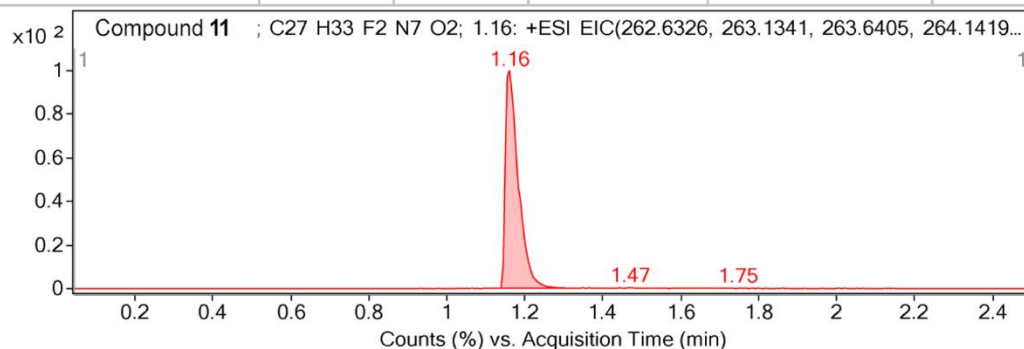
--- End Of Report ---

Compound 11

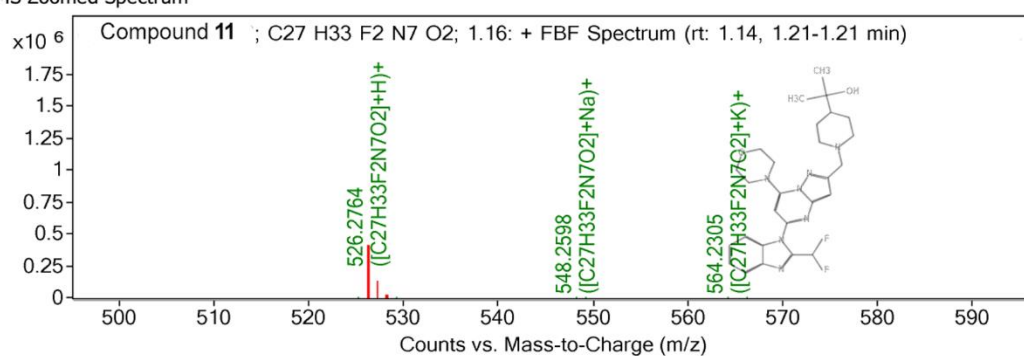


Compound 11

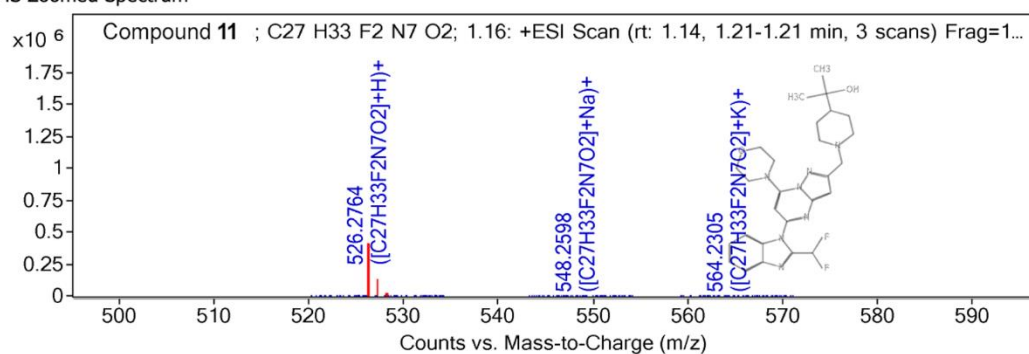
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorit
Compound 11	526.2764	1.16	525.2691	C27 H33 F2 N7 O2	525.2664	5.12	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

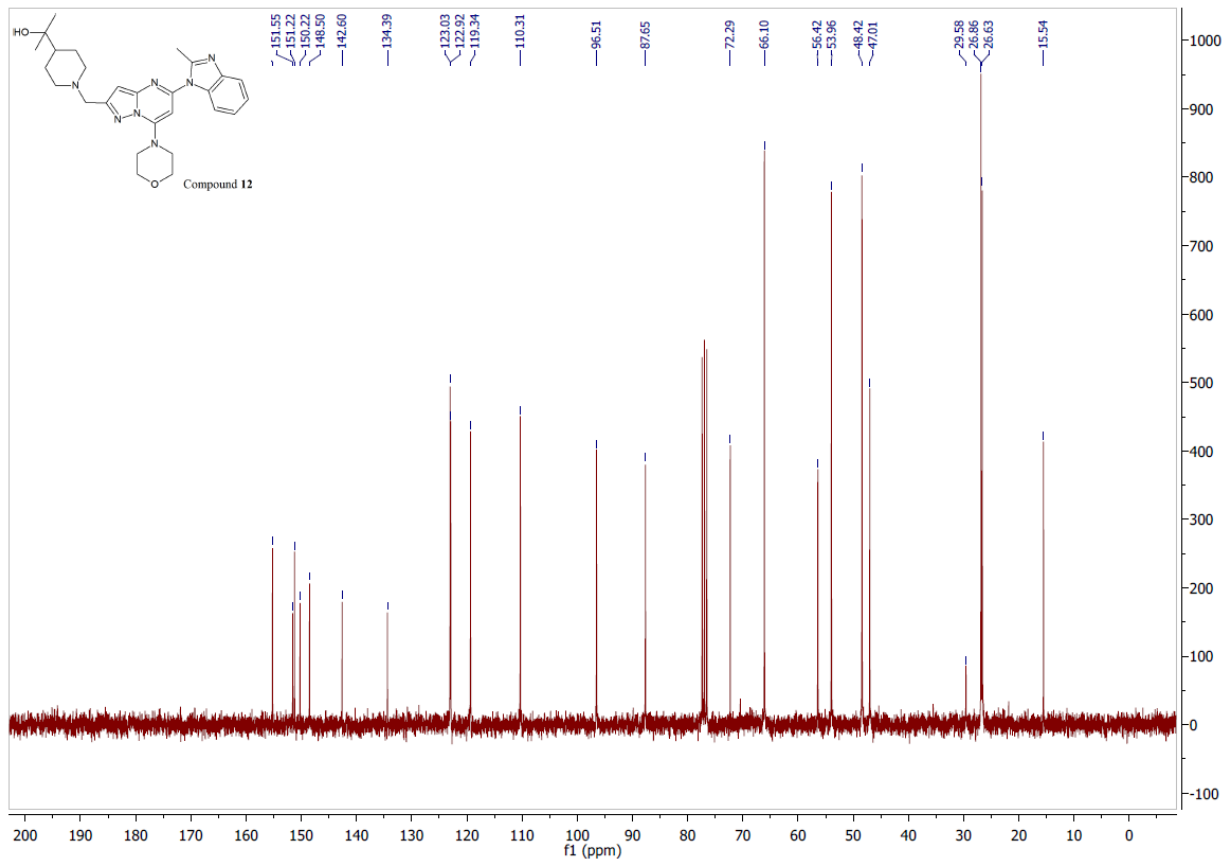
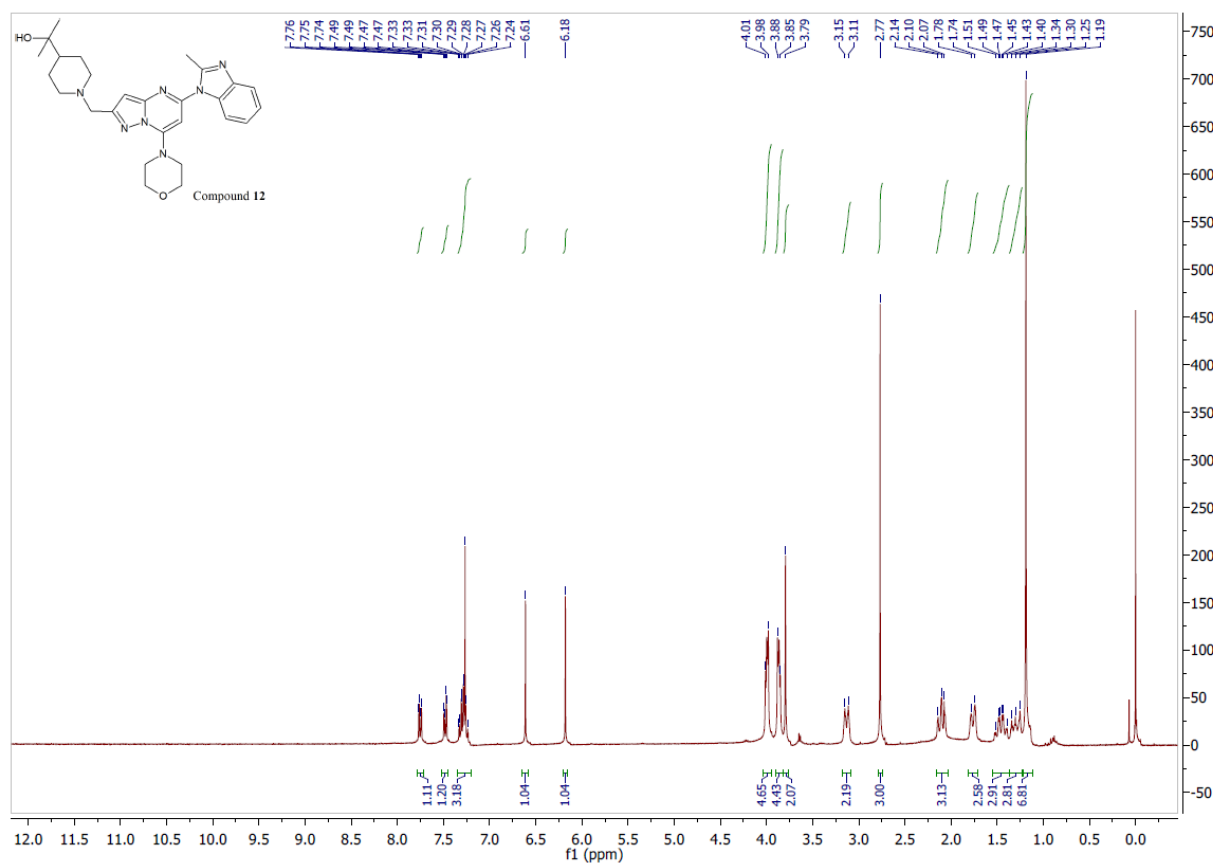


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
526.2764	1	404616.13	C27H33F2N7O2	(M+H)+	
526.2764	1	404616.13	C27H33F2N7O2	(M+H)+	5.14

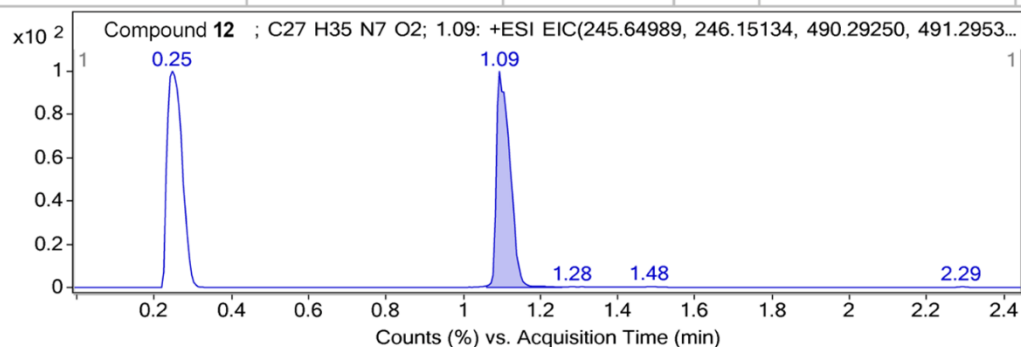
--- End Of Report ---

Compound 12

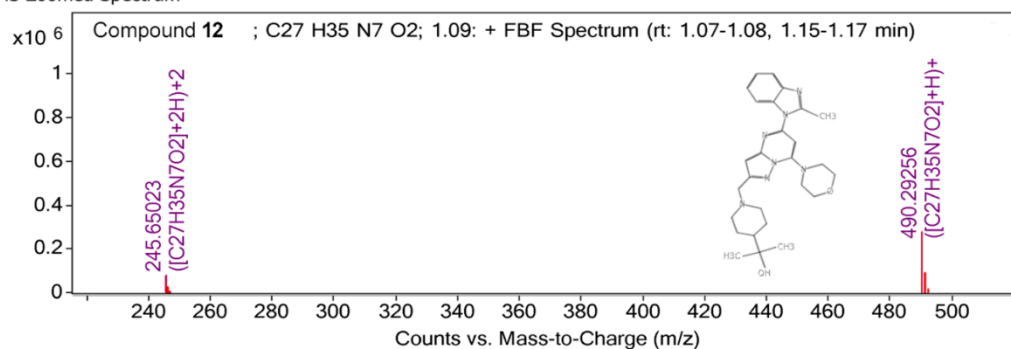


Compound 12

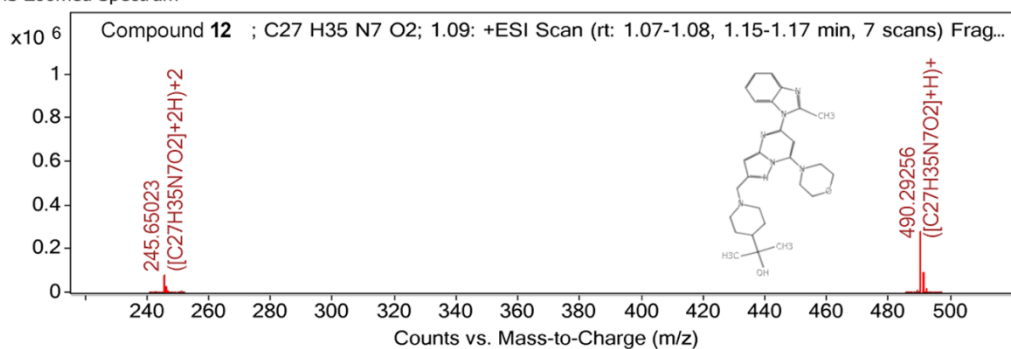
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 12	Compound 12	245.65023	1.09	Find by Formula	489.28538



MS Zoomed Spectrum



MS Zoomed Spectrum

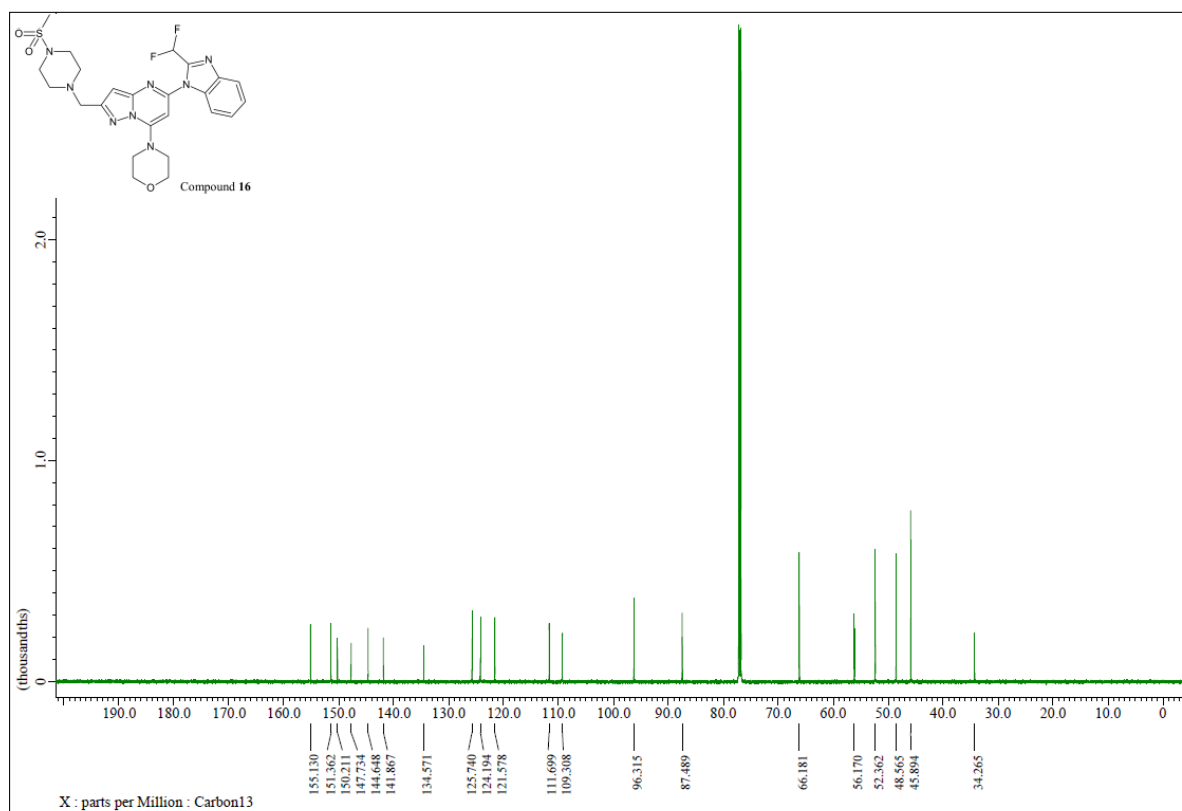
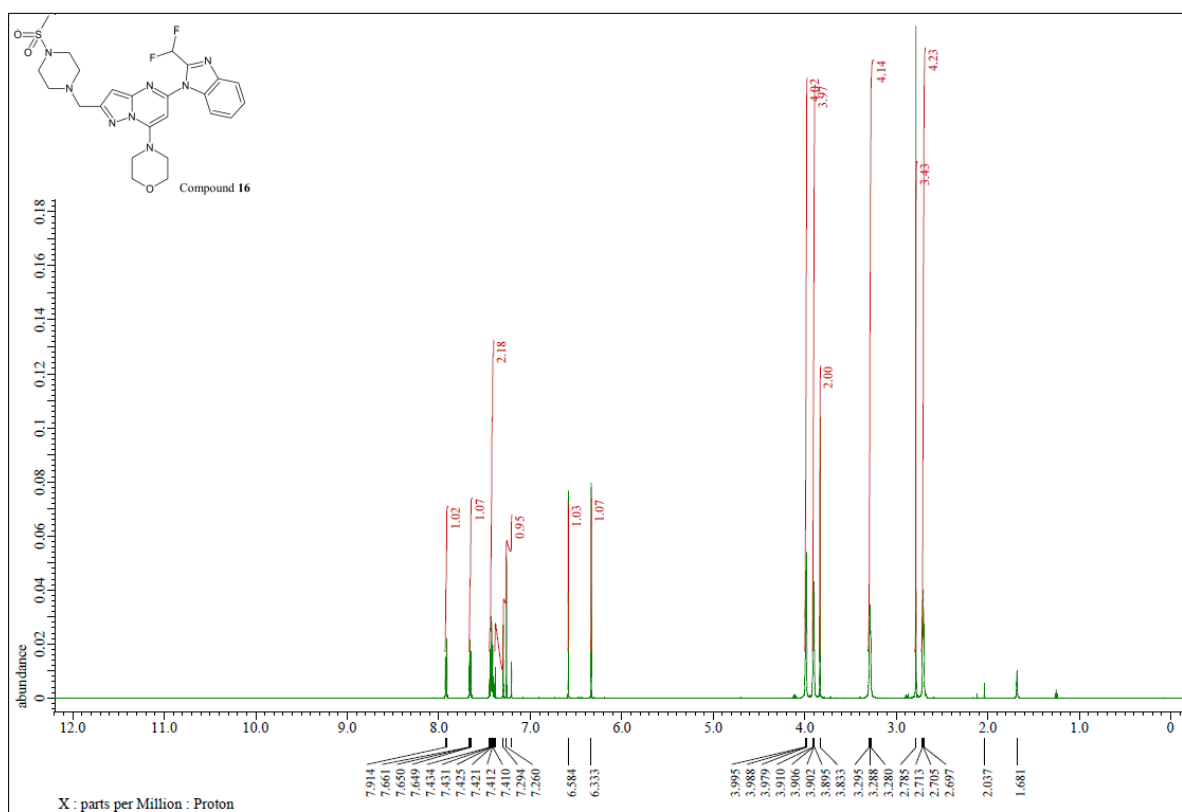


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
245.65023	245.64989	1.38	2	79116.77	C27H35N7O2	(M+2H)+2
246.15176	246.15134	1.74	2	26046.49	C27H35N7O2	(M+2H)+2
246.65239	246.65272	-1.31	2	4306.85	C27H35N7O2	(M+2H)+2
247.15487	247.15405	3.34	2	683.01	C27H35N7O2	(M+2H)+2
490.29256	490.2925	0.12	1	277845.75	C27H35N7O2	(M+H)+
491.29534	491.29539	-0.1	1	84677.91	C27H35N7O2	(M+H)+
492.29744	492.29815	-1.45	1	16256.98	C27H35N7O2	(M+H)+

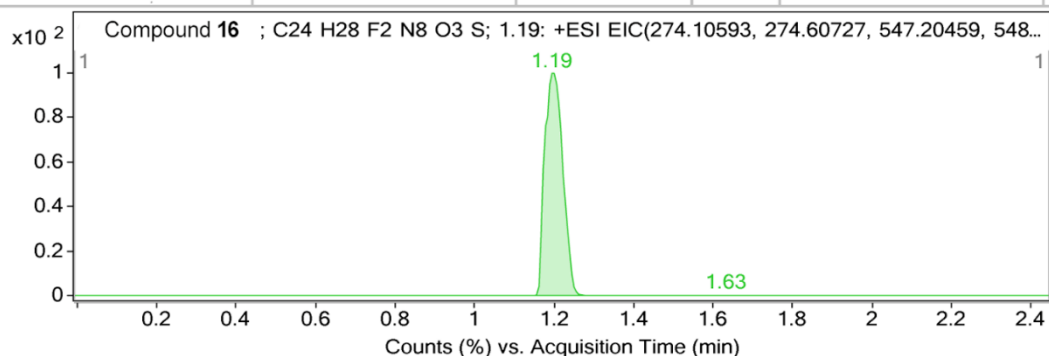
--- End Of Report ---

Compound 16

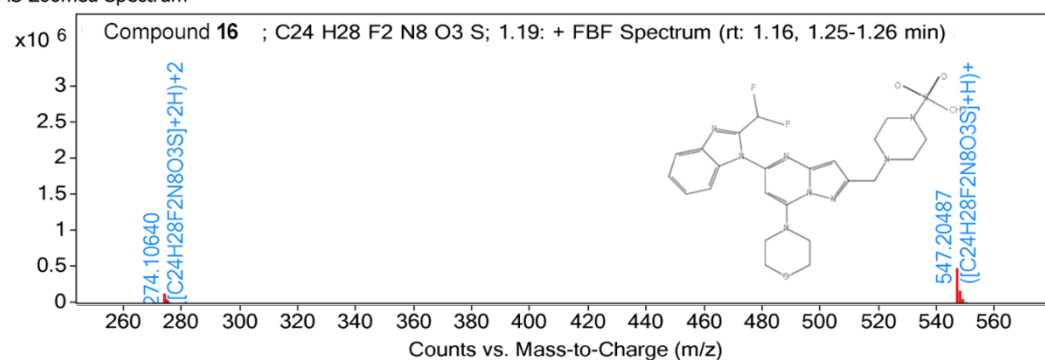


Compound 16

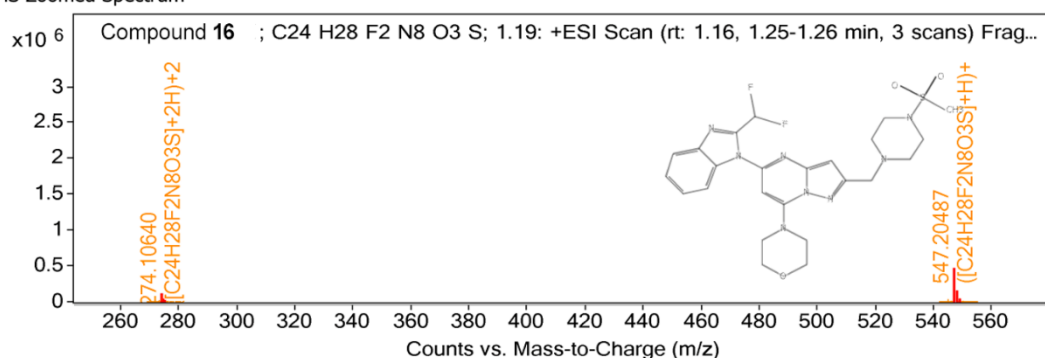
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 16	Compound 16	547.20487	1.19	Find by Formula	546.19768



MS Zoomed Spectrum



MS Zoomed Spectrum

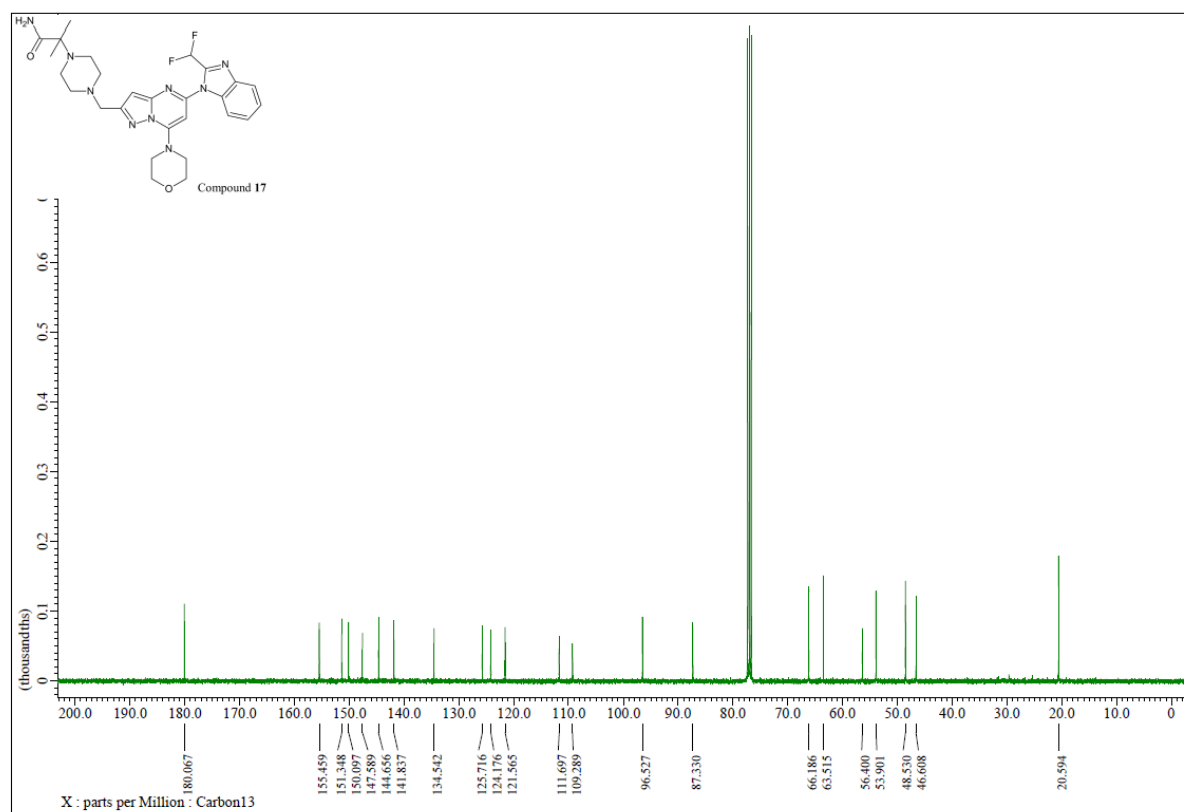
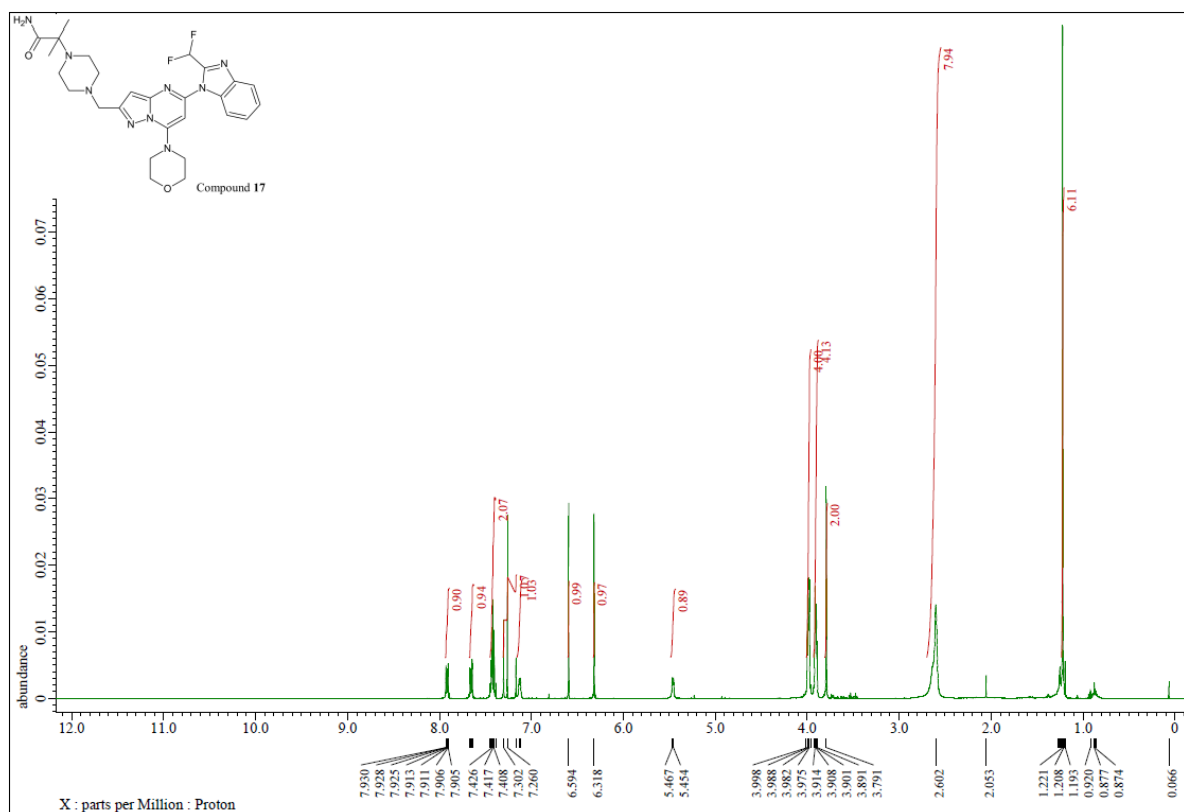


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
274.1064	274.10593	1.68	2	105049.91	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+2H)+2
274.60756	274.60727	1.04	2	33865.99	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+2H)+2
275.1073	275.10631	3.58	2	10859.48	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+2H)+2
275.60631	275.60663	-1.16	2	2302.53	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+2H)+2
547.20487	547.20459	0.52	1	465451.59	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+H)+
548.2075	548.20726	0.44	1	130005.94	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+H)+
549.20534	549.20534	-0.01	1	38941.63	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+H)+
550.20543	550.20598	-1	1	8620.2	C ₂₄ H ₂₈ F ₂ N ₈ O ₃ S	(M+H)+

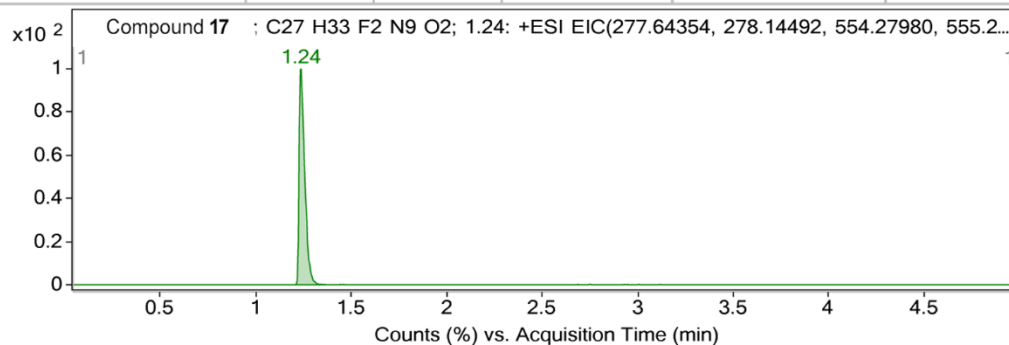
--- End Of Report ---

Compound 17

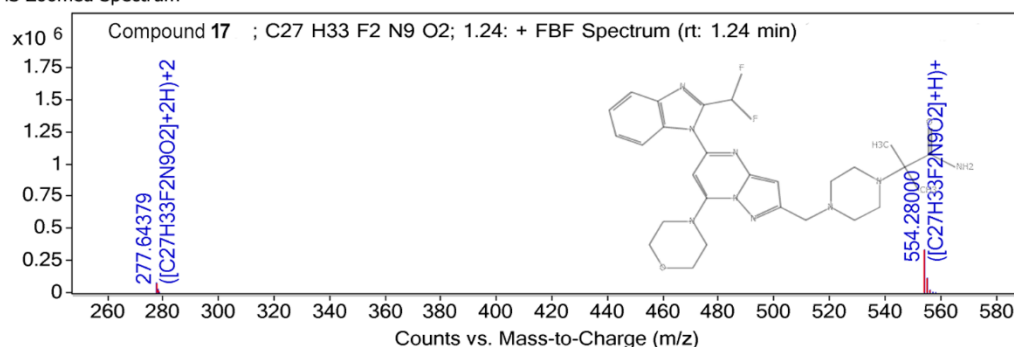


Compound 17

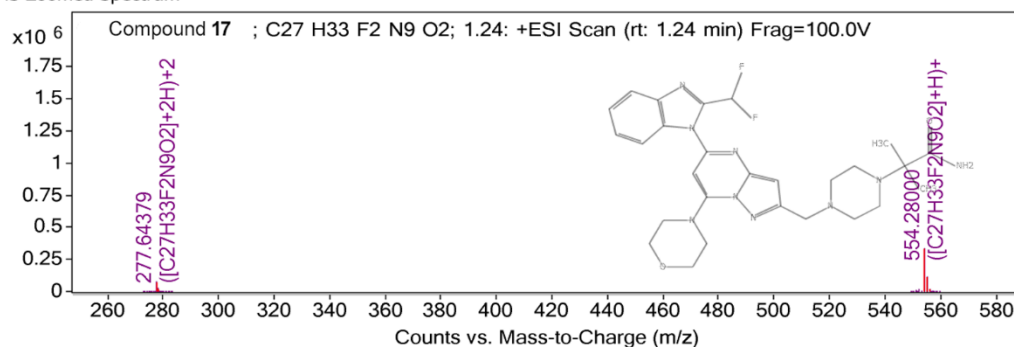
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 17	554.28	1.24	553.27265	C27 H33 F2 N9 O2	553.27253	0.23	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

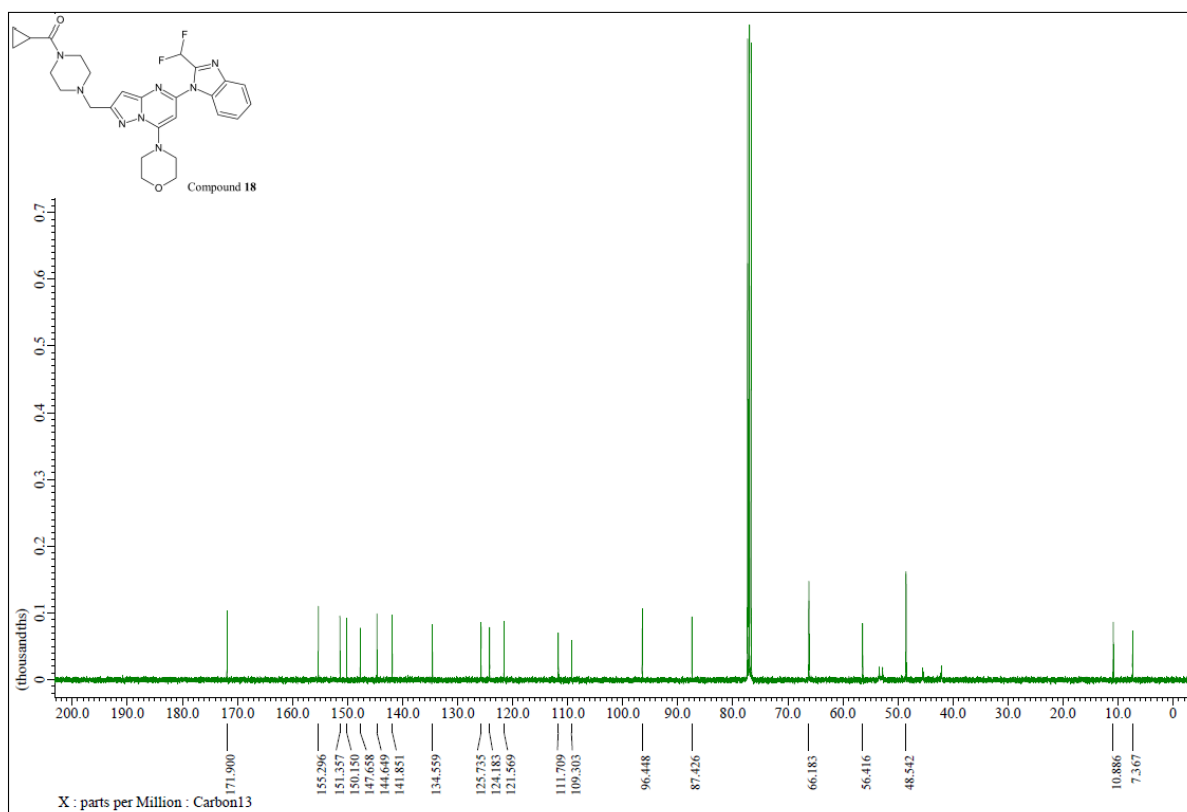
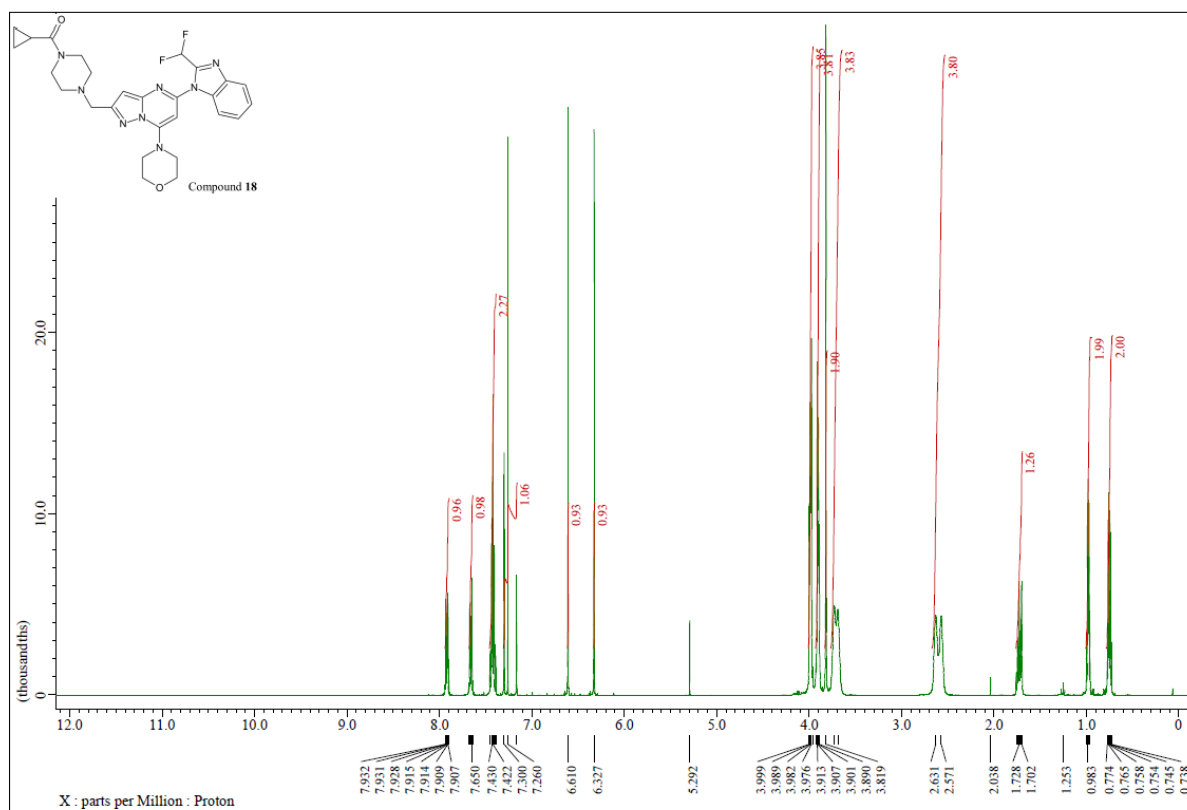


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
277.64379	2	74236.3	C27H33F2N9O2	(M+2H)+2	
278.14494	2	24665.33	C27H33F2N9O2	(M+2H)+2	
278.64678	2	3142.95	C27H33F2N9O2	(M+2H)+2	
554.28	1	331615.38	C27H33F2N9O2	(M+H)+	
555.28243	1	113299.23	C27H33F2N9O2	(M+H)+	
556.28444	1	17136.88	C27H33F2N9O2	(M+H)+	
557.28512	1	1819.13	C27H33F2N9O2	(M+H)+	
558.2883	1	234.87	C27H33F2N9O2	(M+H)+	
277.64379	2	74236.3	C27H33F2N9O2	(M+2H)+2	0.91
278.14494	2	24665.33	C27H33F2N9O2	(M+2H)+2	0.07
278.64678	2	3142.95	C27H33F2N9O2	(M+2H)+2	1.91
554.28	1	331615.38	C27H33F2N9O2	(M+H)+	0.35
555.28243	1	113299.23	C27H33F2N9O2	(M+H)+	-0.25
556.28444	1	17136.88	C27H33F2N9O2	(M+H)+	-1.38
557.28512	1	1819.13	C27H33F2N9O2	(M+H)+	-4.77
558.2883	1	234.87	C27H33F2N9O2	(M+H)+	-3.57

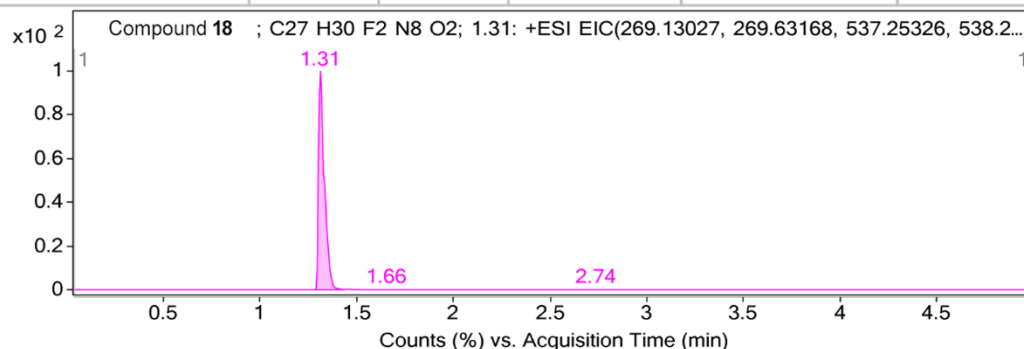
--- End Of Report ---

Compound 18

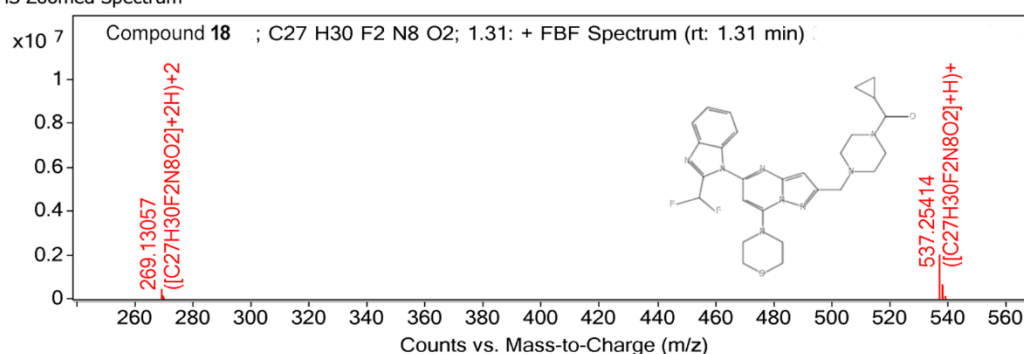


Compound 18

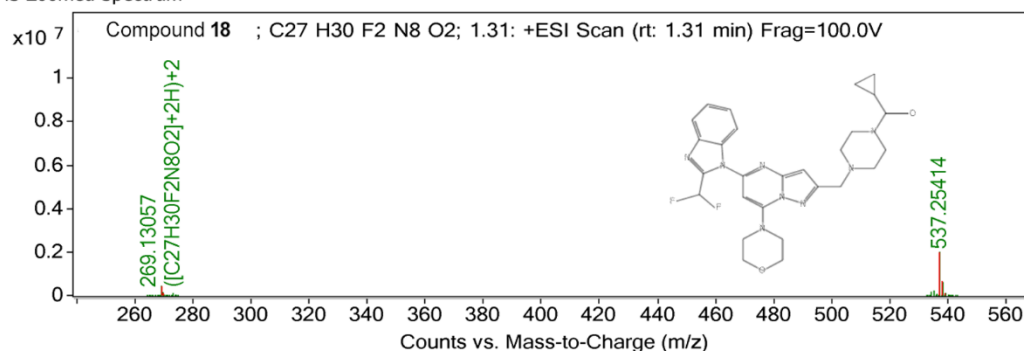
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 18	269.13057	1.31	536.24666	C27 H30 F2 N8 O2	536.24598	1.28	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

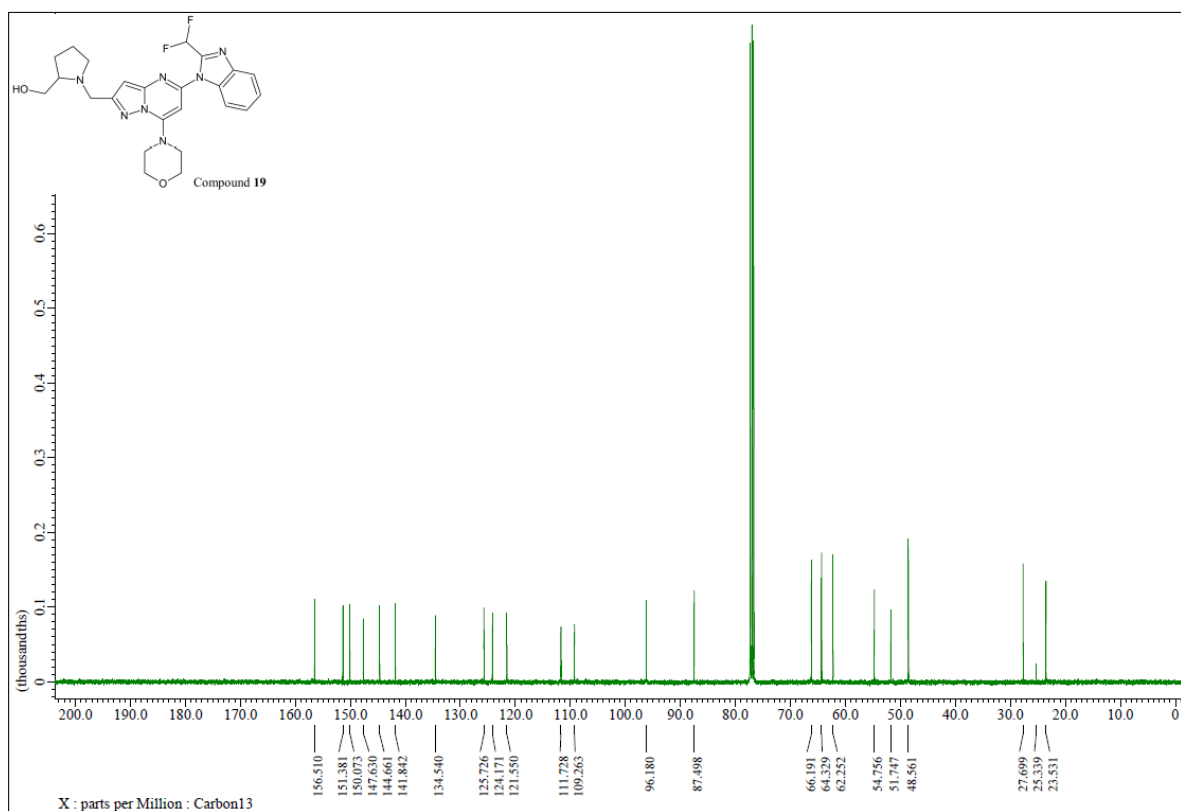
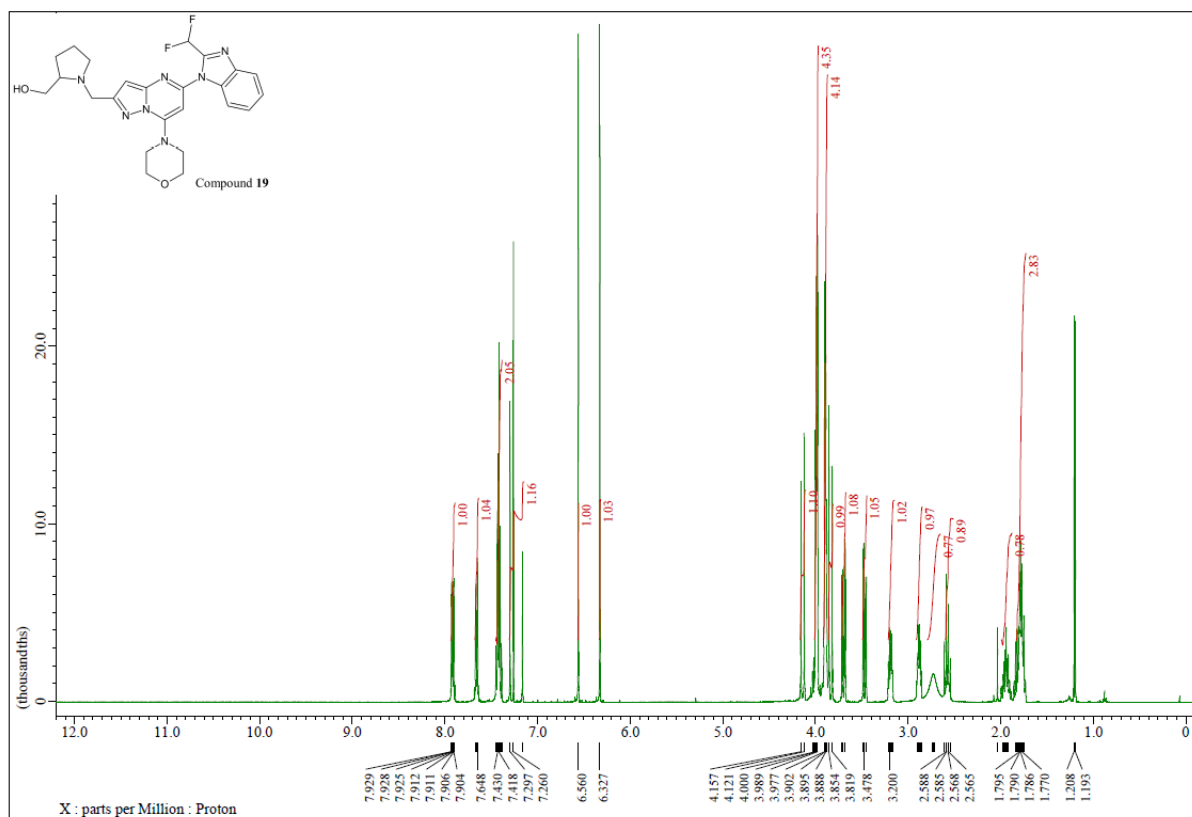


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
269.13057	2	425649.31	C27H30F2N8O2	(M+2H)+2	
269.63216	2	122896.92	C27H30F2N8O2	(M+2H)+2	
270.13329	2	19970.75	C27H30F2N8O2	(M+2H)+2	
537.25414	1	1985956.63	C27H30F2N8O2	(M+H)+	
538.25617	1	592174.13	C27H30F2N8O2	(M+H)+	
539.25893	1	86057.74	C27H30F2N8O2	(M+H)+	
269.13057	2	425649.31	C27H30F2N8O2	(M+2H)+2	1.14
269.63216	2	122896.92	C27H30F2N8O2	(M+2H)+2	1.78
270.13329	2	19970.75	C27H30F2N8O2	(M+2H)+2	0.96
537.25414	1	1985956.63	C27H30F2N8O2	(M+H)+	1.64
537.25414		1988175.75			
538.25617	1	592174.13	C27H30F2N8O2	(M+H)+	0.17
539.25893	1	86057.74	C27H30F2N8O2	(M+H)+	0.29

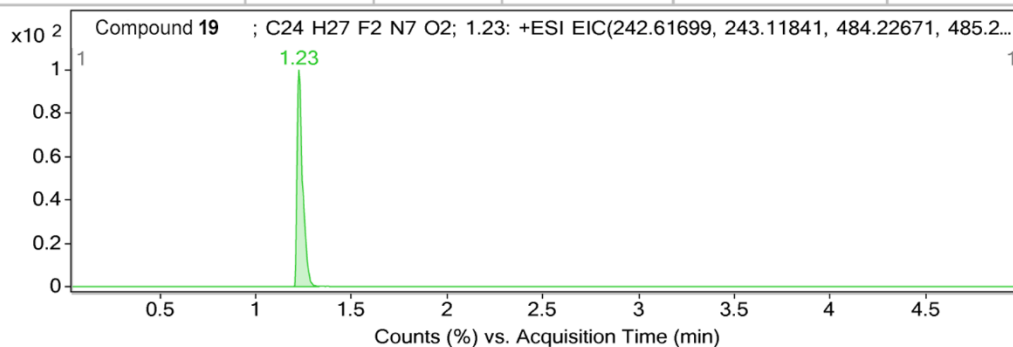
--- End Of Report ---

Compound 19

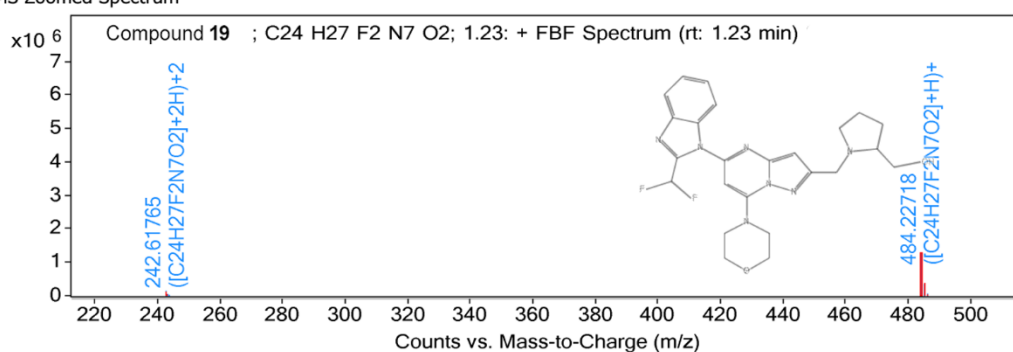


Compound 19

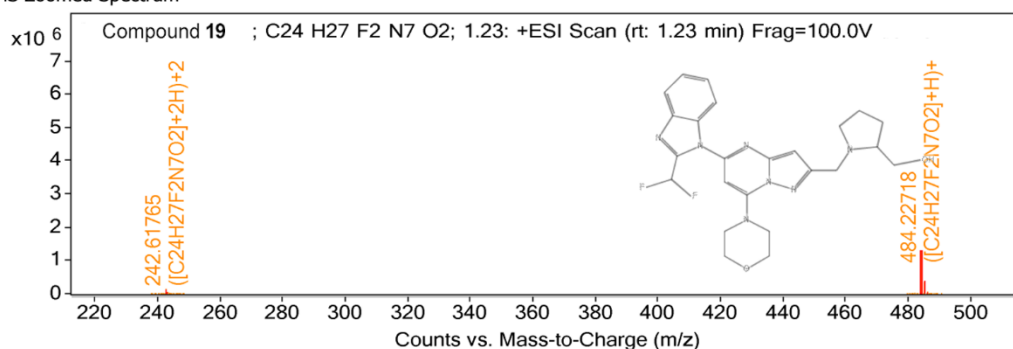
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 19	484.22718	1.23	483.21997	C24 H27 F2 N7 O2	483.21943	1.11	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

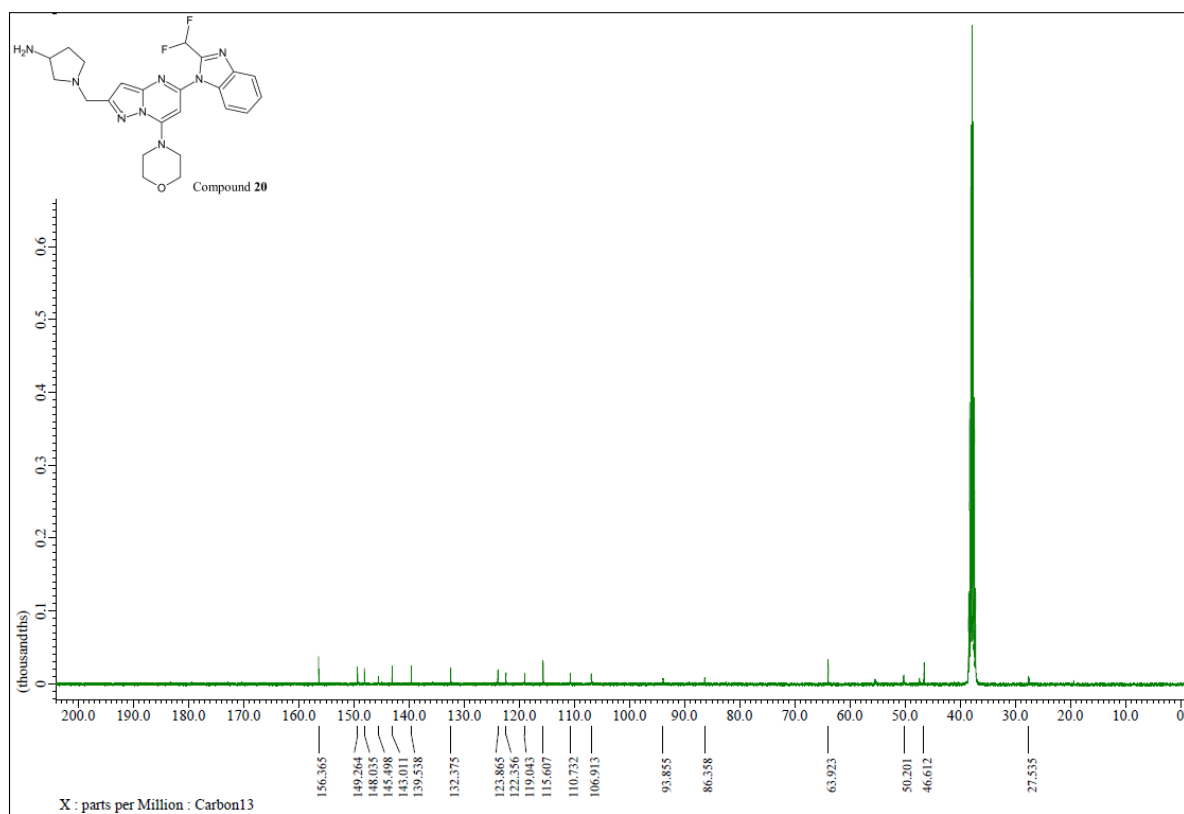
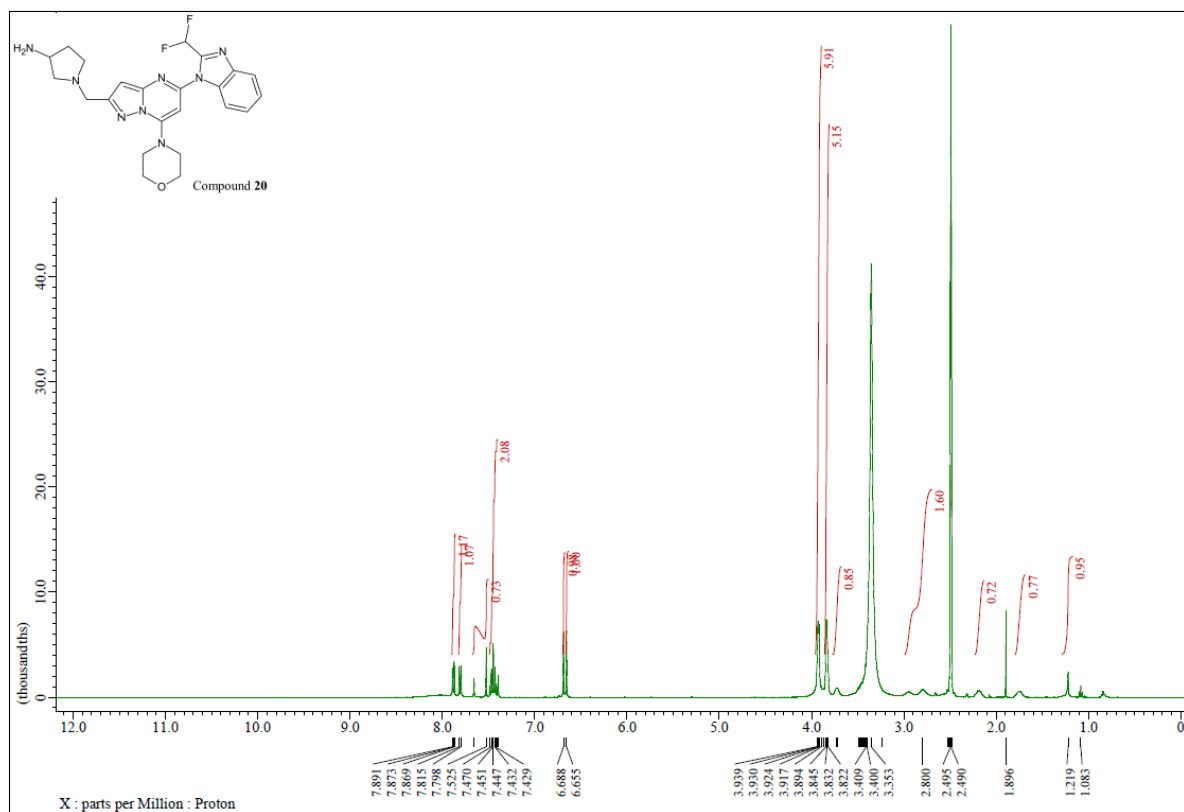


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
242.61765	2	128896.13	C24H27F2N7O2	(M+2H)+2	
243.11881	2	36127.81	C24H27F2N7O2	(M+2H)+2	
243.62073	2	7105.86	C24H27F2N7O2	(M+2H)+2	
484.22718	1	1284613.5	C24H27F2N7O2	(M+H)+	
485.23003	1	333370.47	C24H27F2N7O2	(M+H)+	
486.23205	1	49131.52	C24H27F2N7O2	(M+H)+	
242.61765	2	128896.13	C24H27F2N7O2	(M+2H)+2	2.73
243.11881	2	36127.81	C24H27F2N7O2	(M+2H)+2	1.66
243.62073	2	7105.86	C24H27F2N7O2	(M+2H)+2	4.03
484.22718	1	1284613.5	C24H27F2N7O2	(M+H)+	0.99
485.23003	1	333370.47	C24H27F2N7O2	(M+H)+	1.02
486.23205	1	49131.52	C24H27F2N7O2	(M+H)+	-0.34

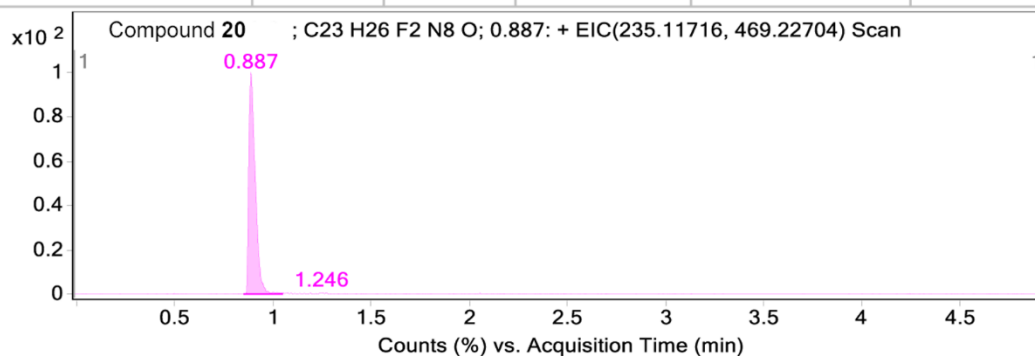
--- End Of Report ---

Compound 20

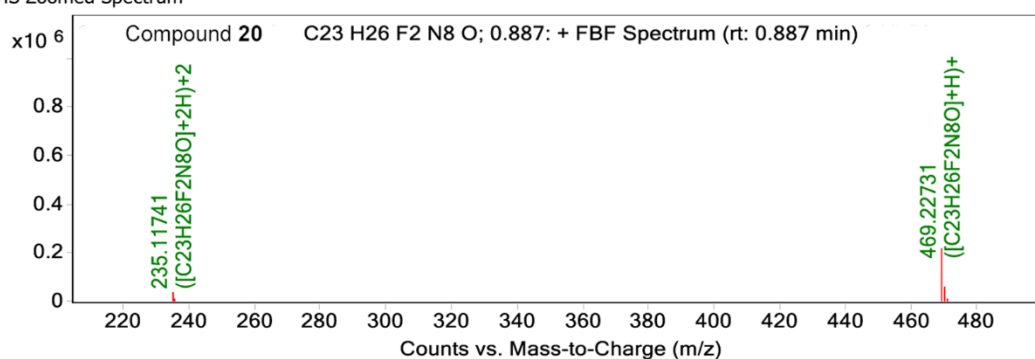


Compound 20

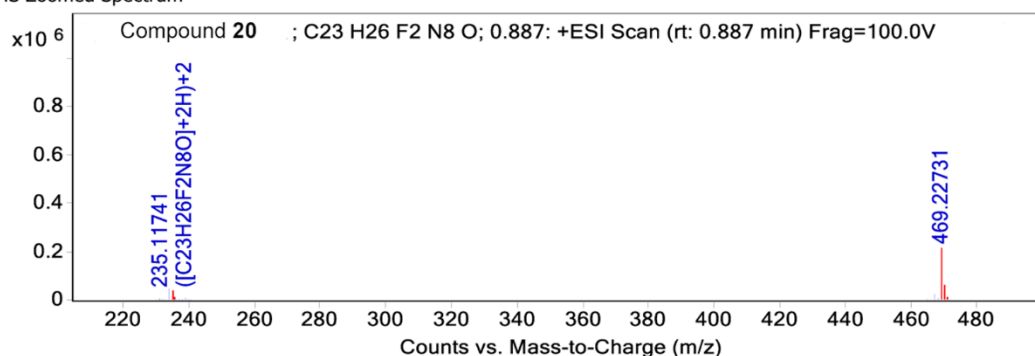
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 20	235.11741	0.887	468.22001	C23 H26 F2 N8 O	468.21976	0.54	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

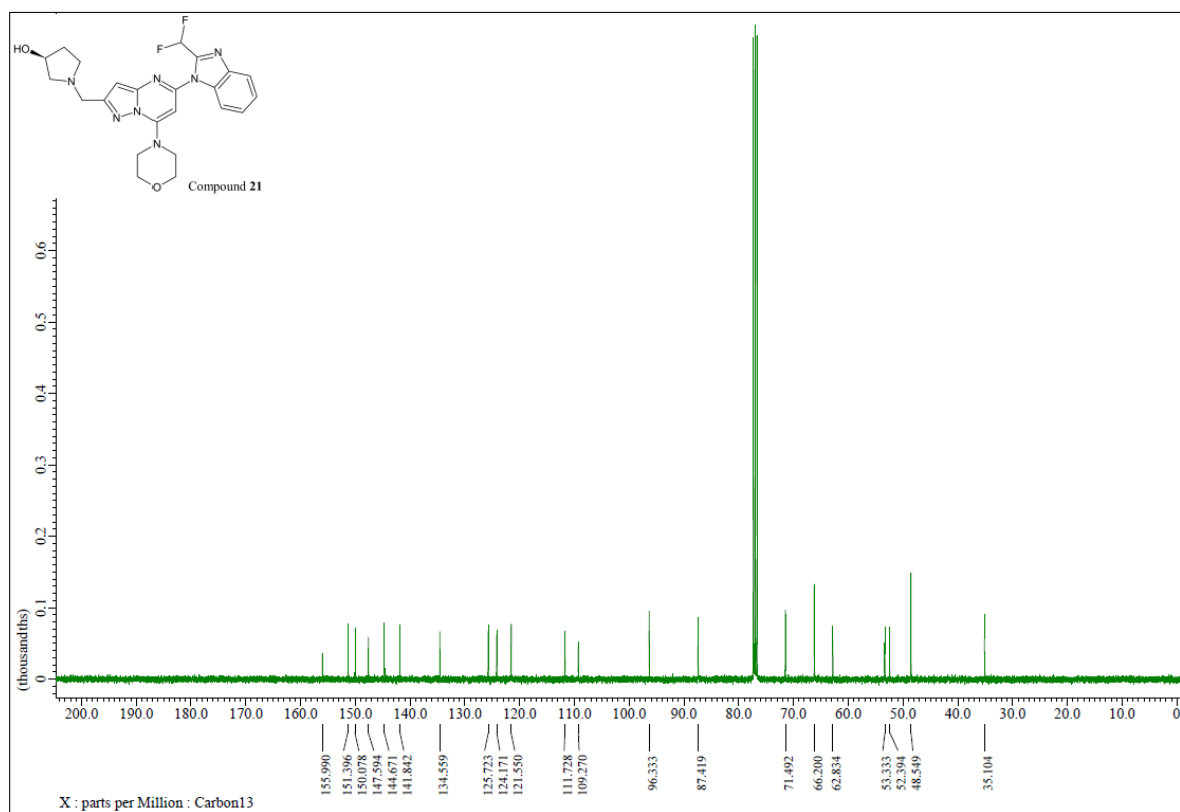
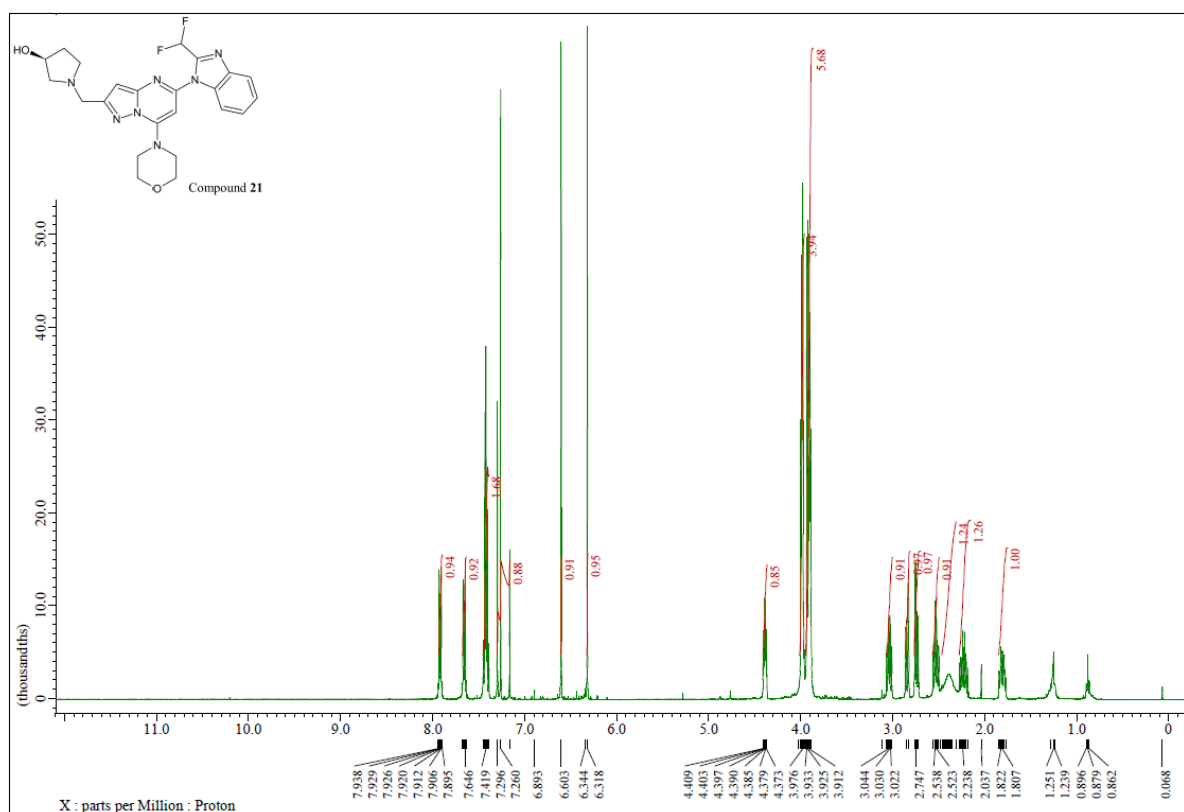


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
235.11741	2	37955.73	C23H26F2N8O	(M+2H)+2	
235.61897	2	10801.02	C23H26F2N8O	(M+2H)+2	
236.12072	2	1863.32	C23H26F2N8O	(M+2H)+2	
469.22731	1	217069.95	C23H26F2N8O	(M+H)+	
470.22977	1	53954.65	C23H26F2N8O	(M+H)+	
471.23136	1	7749.8	C23H26F2N8O	(M+H)+	
235.11741	2	37955.73	C23H26F2N8O	(M+2H)+2	1.06
235.61897	2	10801.02	C23H26F2N8O	(M+2H)+2	1.88
236.12072	2	1863.32	C23H26F2N8O	(M+2H)+2	3.7
469.22731		217402.84			0.58
469.22731	1	217069.95	C23H26F2N8O	(M+H)+	0.58
470.22977	1	53954.65	C23H26F2N8O	(M+H)+	-0.01
471.23136	1	7749.8	C23H26F2N8O	(M+H)+	-2.23

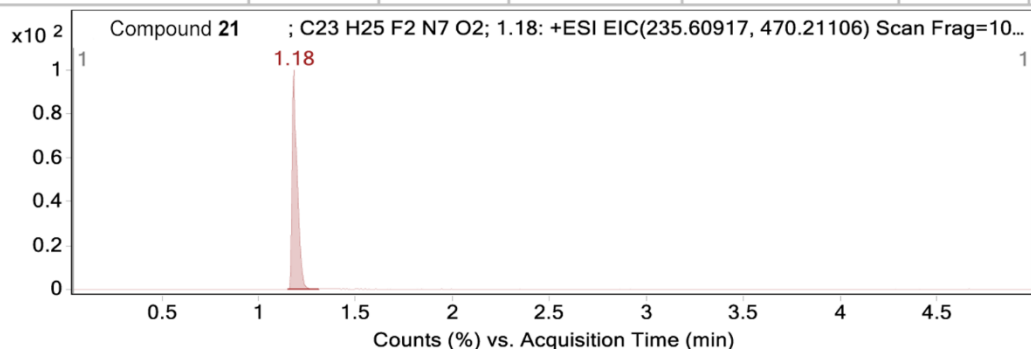
--- End Of Report ---

Compound 21

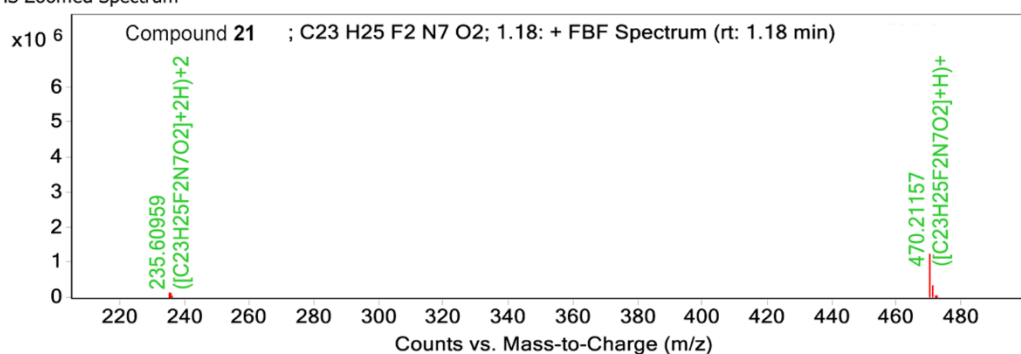


Compound 21

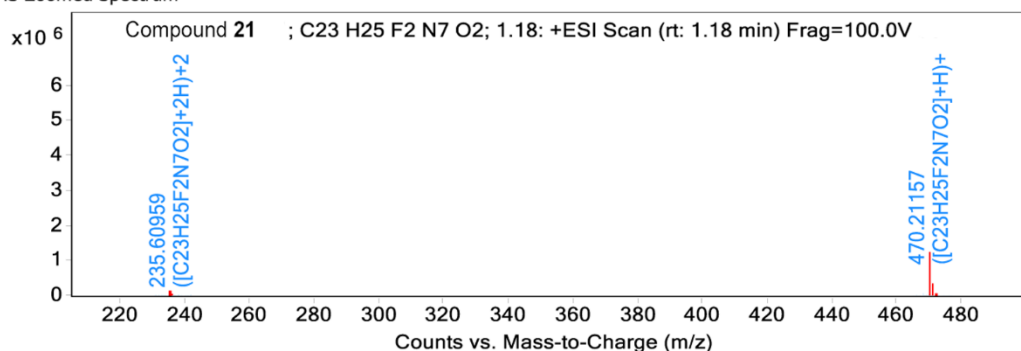
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 21	235.60959	1.18	469.20435	C23 H25 F2 N7 O2	469.20378	1.21	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

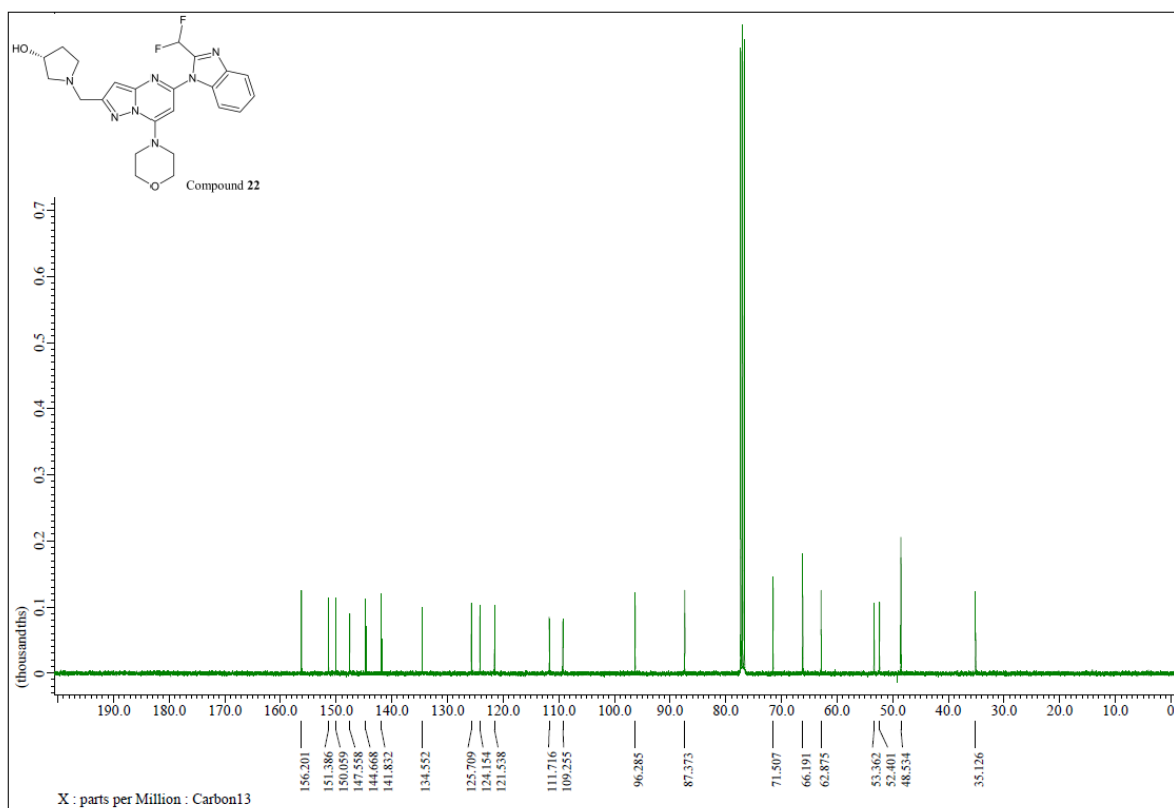
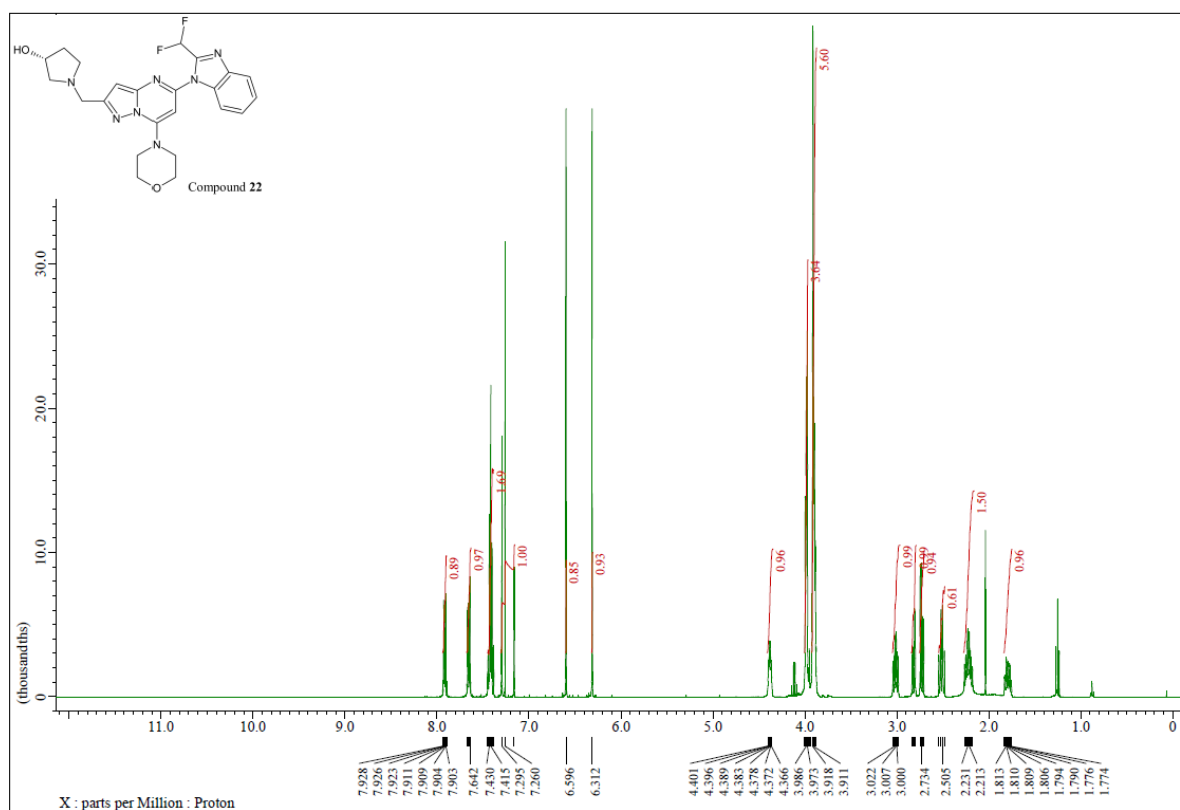


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
235.60959	2	125434.16	C23H25F2N7O2	(M+2H)+2	
236.11085	2	38404.56	C23H25F2N7O2	(M+2H)+2	
236.61302	2	4518.14	C23H25F2N7O2	(M+2H)+2	
237.11164	2	465.8	C23H25F2N7O2	(M+2H)+2	
470.21157	1	1232616.63	C23H25F2N7O2	(M+H)+	
471.21462	1	290558.94	C23H25F2N7O2	(M+H)+	
472.21628	1	40423.04	C23H25F2N7O2	(M+H)+	
235.60959	2	125434.16	C23H25F2N7O2	(M+2H)+2	1.79
236.11085	2	38404.56	C23H25F2N7O2	(M+2H)+2	1.19
236.61302	2	4518.14	C23H25F2N7O2	(M+2H)+2	4.73
237.11164	2	465.8	C23H25F2N7O2	(M+2H)+2	-6.44
470.21157	1	1232616.63	C23H25F2N7O2	(M+H)+	1.1
471.21462	1	290558.94	C23H25F2N7O2	(M+H)+	1.6
472.21628	1	40423.04	C23H25F2N7O2	(M+H)+	-0.49

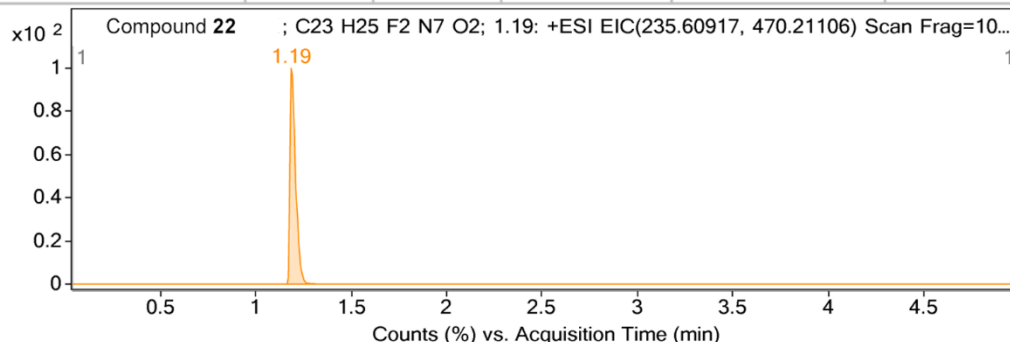
--- End Of Report ---

Compound 22

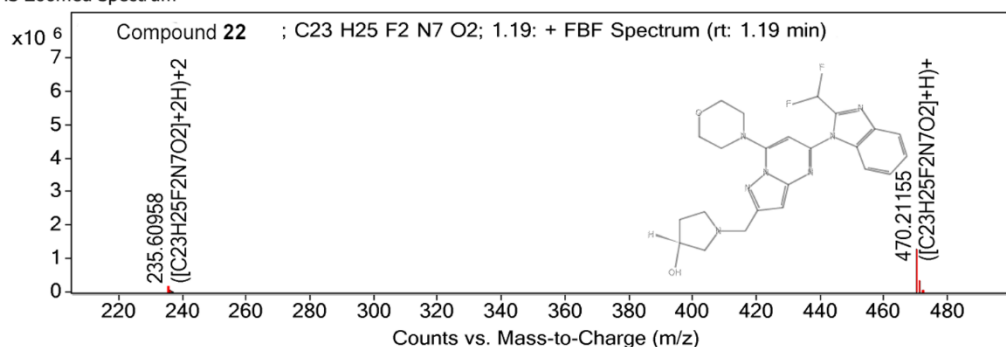


Compound 22

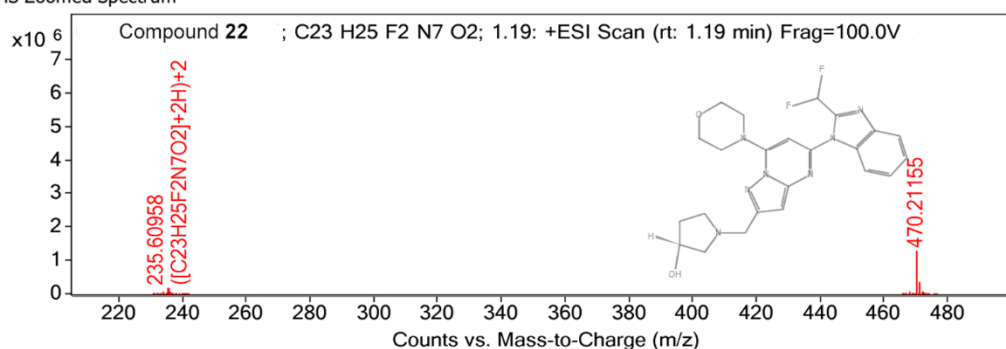
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 22	235.60958	1.19	469.20426	C23 H25 F2 N7 O2	469.20378	1.03	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

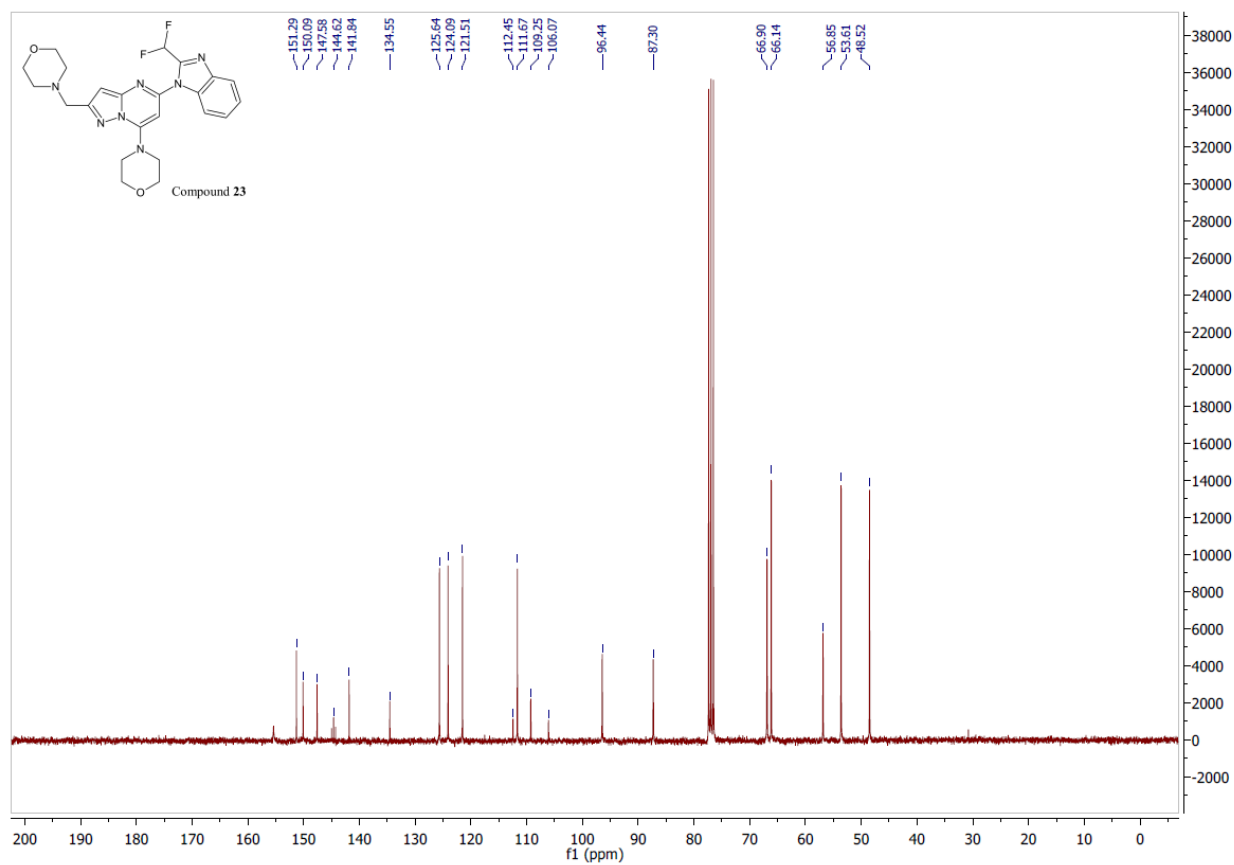
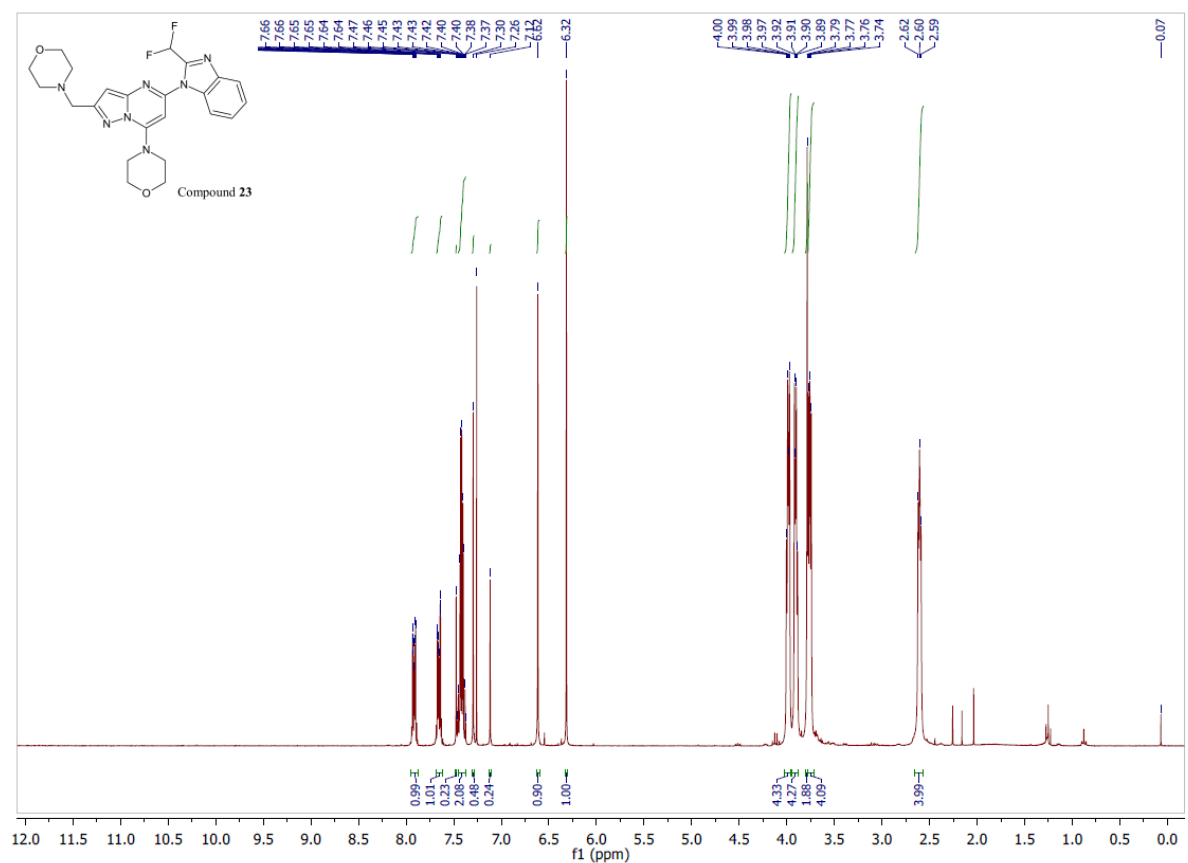


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
235.60958	2	145539.42	C23H25F2N7O2	(M+2H)+2	
236.11083	2	42062.38	C23H25F2N7O2	(M+2H)+2	
236.61221	2	5847.81	C23H25F2N7O2	(M+2H)+2	
237.11271	2	301.78	C23H25F2N7O2	(M+2H)+2	
470.21155	1	1273827.38	C23H25F2N7O2	(M+H)+	
471.21422	1	320760.09	C23H25F2N7O2	(M+H)+	
472.21647	1	44783.03	C23H25F2N7O2	(M+H)+	
235.60958	2	145539.42	C23H25F2N7O2	(M+2H)+2	1.74
236.11083	2	42062.38	C23H25F2N7O2	(M+2H)+2	1.11
236.61221	2	5847.81	C23H25F2N7O2	(M+2H)+2	1.32
237.11271	2	301.78	C23H25F2N7O2	(M+2H)+2	-1.95
470.21155	1	1273827.38	C23H25F2N7O2	(M+H)+	1.06
470.21155		1274626.38			
471.21422	1	320760.09	C23H25F2N7O2	(M+H)+	0.75
472.21647	1	44783.03	C23H25F2N7O2	(M+H)+	-0.09

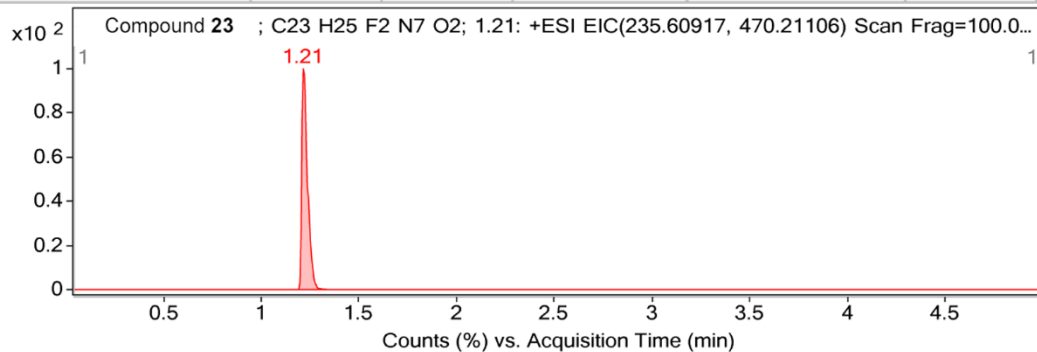
--- End Of Report ---

Compound 23

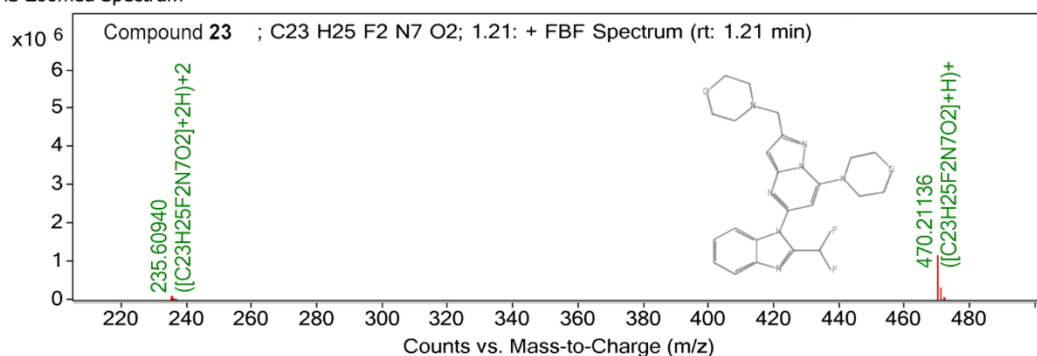


Compound 23

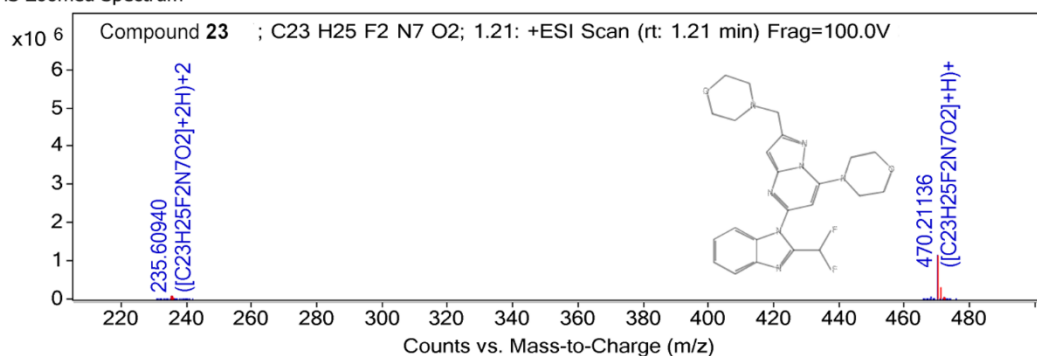
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorit
Compound 23	470.21136	1.21	469.20417	C23 H25 F2 N7 O2	469.20378	0.84	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

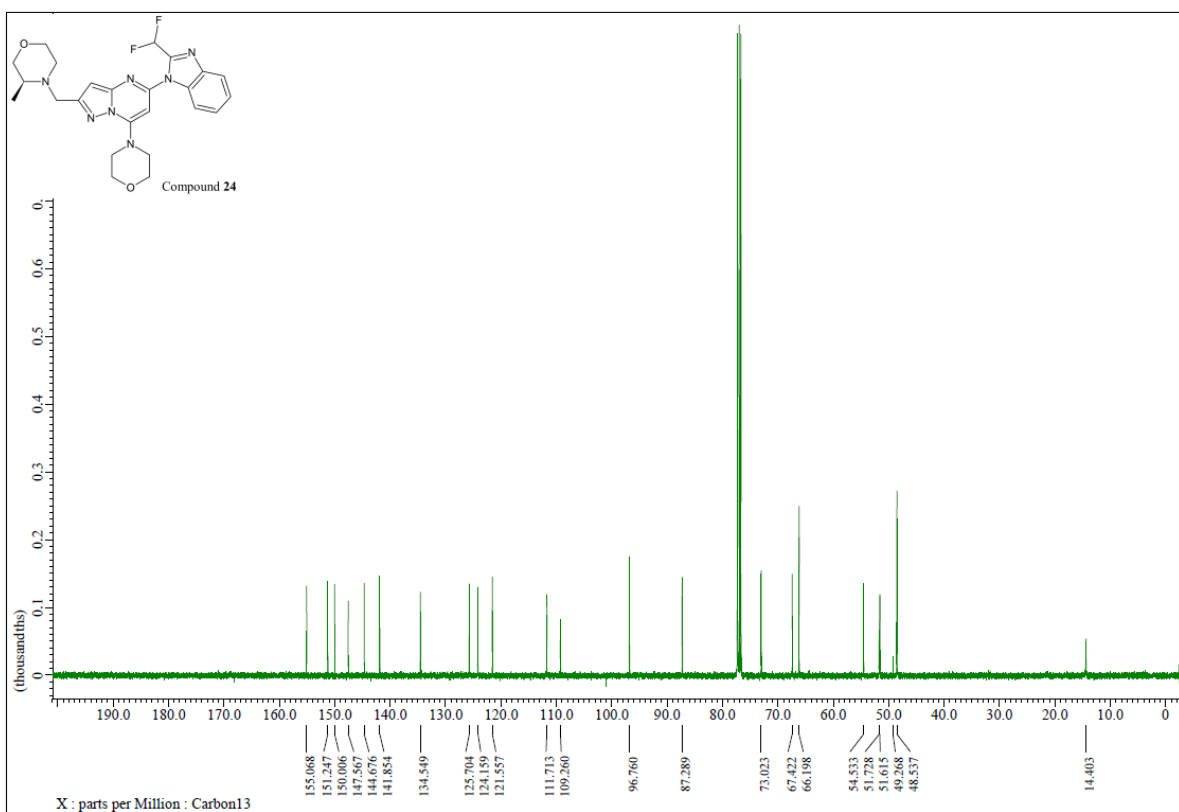
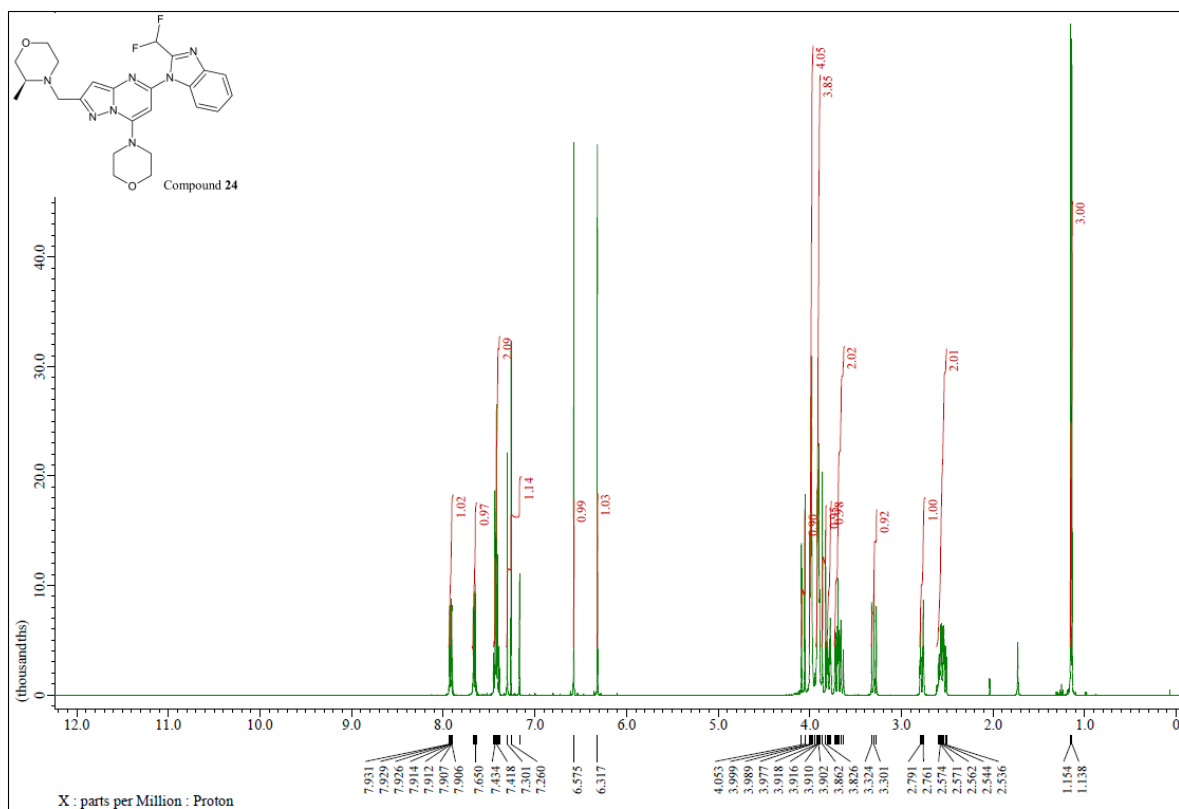


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
235.6094	2	80044.54	C23H25F2N7O2	(M+2H)+2	
236.11123	2	24413.55	C23H25F2N7O2	(M+2H)+2	
236.61164	2	3186	C23H25F2N7O2	(M+2H)+2	
237.11175	2	553.57	C23H25F2N7O2	(M+2H)+2	
470.21136	1	1140152.63	C23H25F2N7O2	(M+H)+	
471.21459	1	286698.06	C23H25F2N7O2	(M+H)+	
472.21642	1	41395.54	C23H25F2N7O2	(M+H)+	
235.6094	2	80044.54	C23H25F2N7O2	(M+2H)+2	0.99
236.11123	2	24413.55	C23H25F2N7O2	(M+2H)+2	2.78
236.61164	2	3186	C23H25F2N7O2	(M+2H)+2	-1.08
237.11175	2	553.57	C23H25F2N7O2	(M+2H)+2	-5.98
470.21136	1	1140152.63	C23H25F2N7O2	(M+H)+	0.65
471.21459	1	286698.06	C23H25F2N7O2	(M+H)+	1.53
472.21642	1	41395.54	C23H25F2N7O2	(M+H)+	-0.2

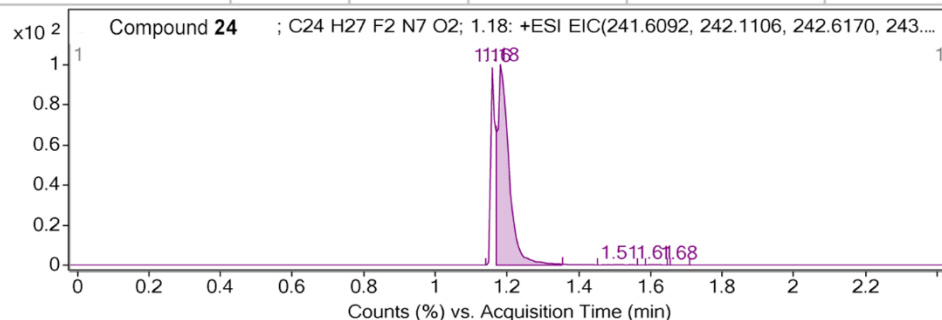
--- End Of Report ---

Compound 24

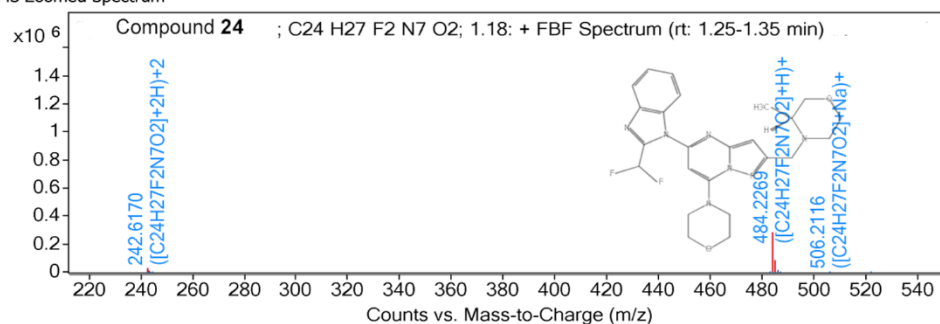


Compound 24

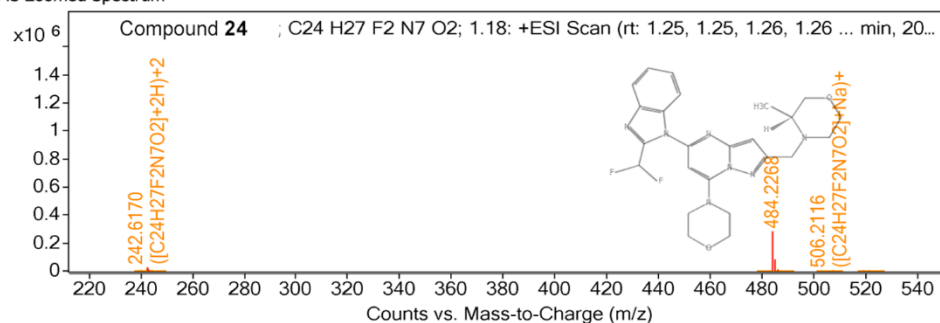
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Aloorith
Compound 24	484.2269	1.18	483.2196	C24 H27 F2 N7 O2	483.2194	0.28	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

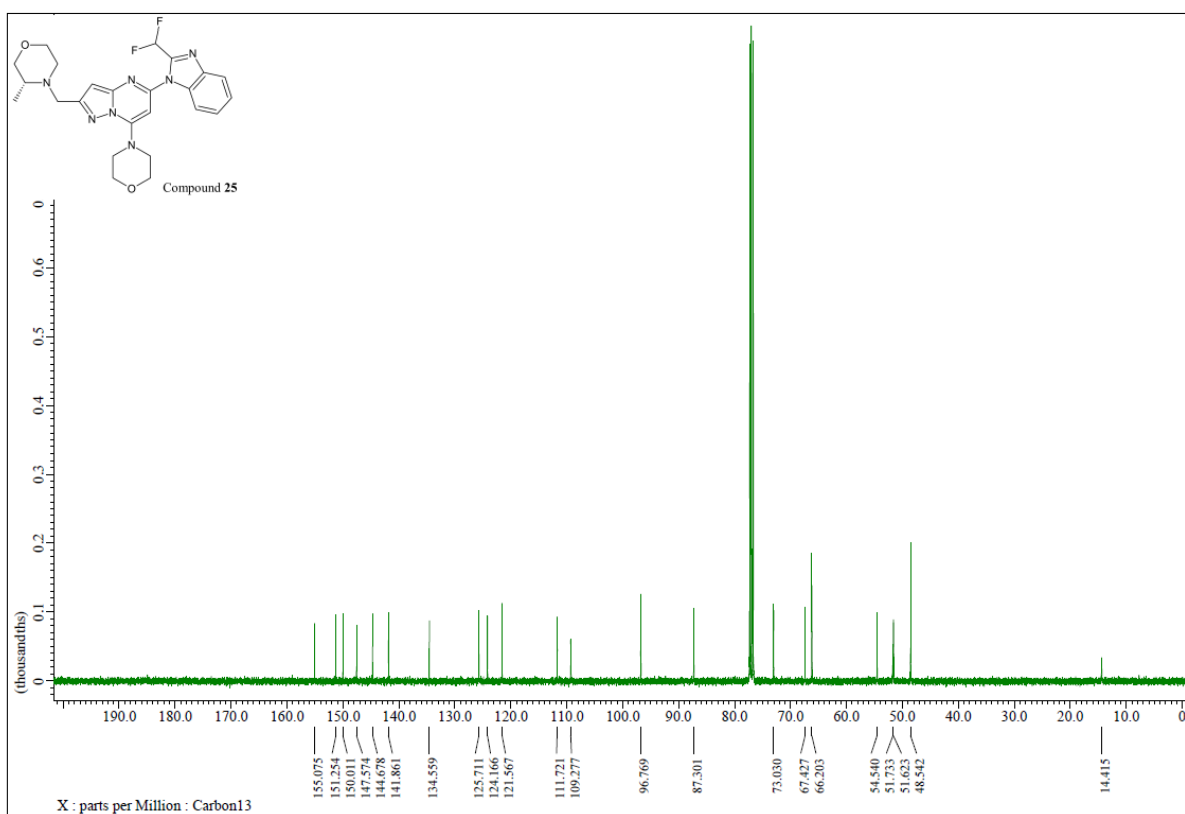
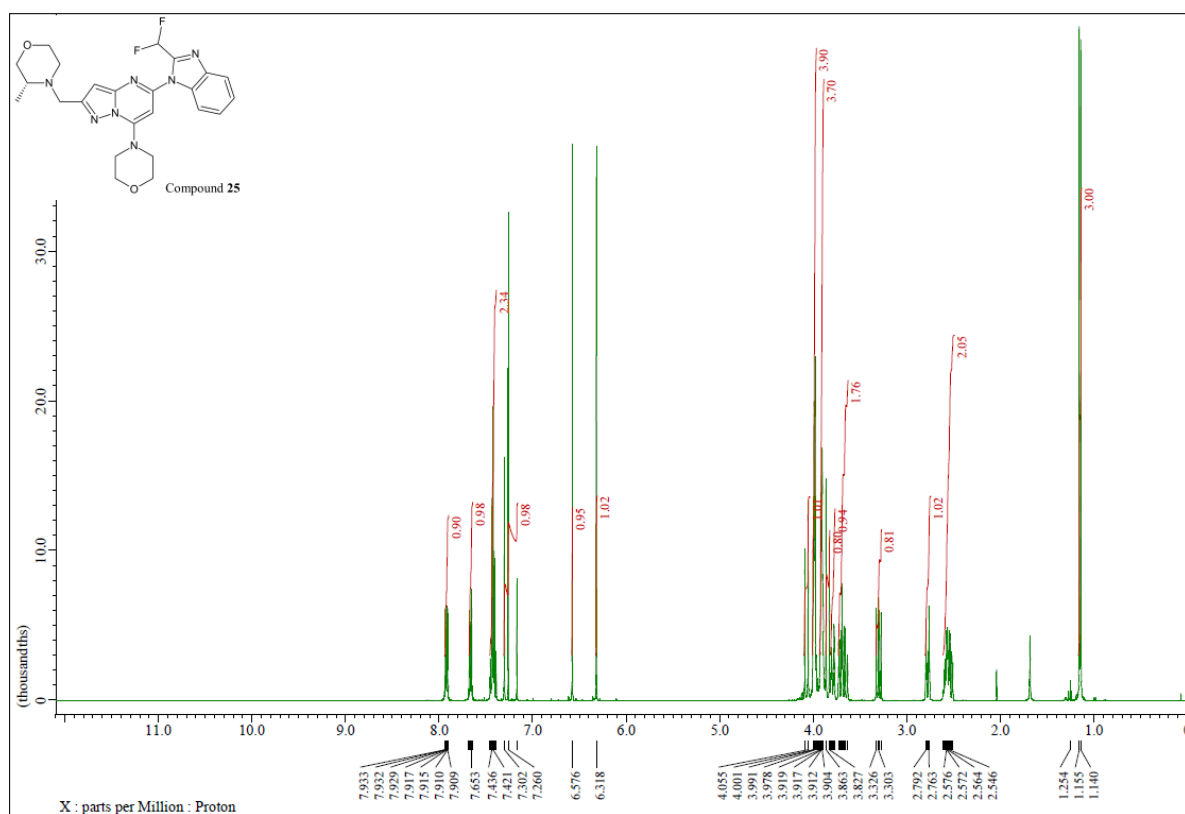


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
242.617	2	23954.76	C24H27F2N7O2	(M+2H)+2	
243.1188	2	7445.91	C24H27F2N7O2	(M+2H)+2	
243.6196	2	1176.52	C24H27F2N7O2	(M+2H)+2	
483.219	1	463.12	C24H27F2N7O2	M+	
484.2269	1	282509	C24H27F2N7O2	(M+H)+	
485.2295	1	79724.67	C24H27F2N7O2	(M+H)+	
486.2323	1	12347.87	C24H27F2N7O2	(M+H)+	
487.2351	1	1594.3	C24H27F2N7O2	(M+H)+	
506.2116	1	253.18	C24H27F2N7O2	(M+Na)+	
522.1799	1	175.05	C24H27F2N7O2	(M+K)+	
242.617	2	23954.76	C24H27F2N7O2	(M+2H)+2	0.23
243.1188	2	7445.91	C24H27F2N7O2	(M+2H)+2	1.66
243.6196	2	1176.52	C24H27F2N7O2	(M+2H)+2	-0.52
483.219	1	463.12	C24H27F2N7O2	M+	0.26
484.2269	1	282509	C24H27F2N7O2	(M+H)+	0.33
485.2295	1	79724.67	C24H27F2N7O2	(M+H)+	0.02
486.2323	1	12347.87	C24H27F2N7O2	(M+H)+	0.15
487.2351	1	1594.3	C24H27F2N7O2	(M+H)+	0.7
506.2116	1	253.18	C24H27F2N7O2	(M+Na)+	5.76
522.1799	1	175.05	C24H27F2N7O2	(M+K)+	-5.13

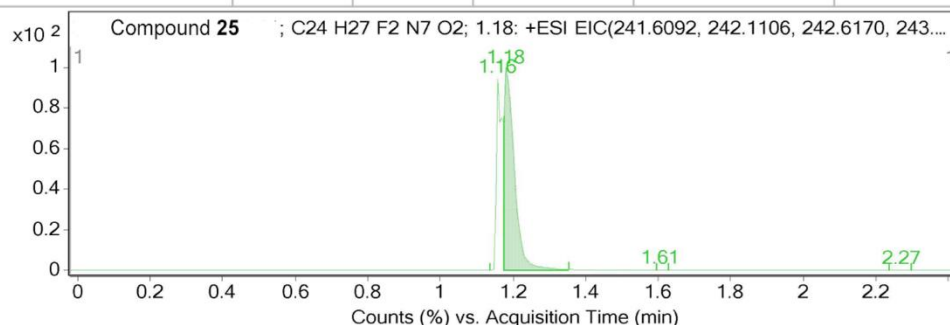
--- End Of Report ---

Compound 25

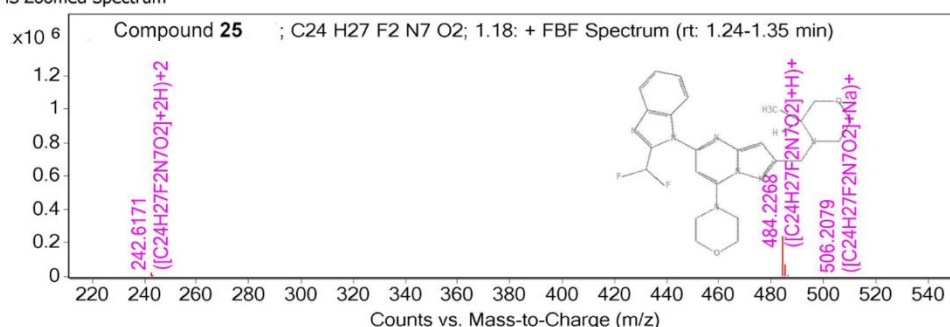


Compound 25

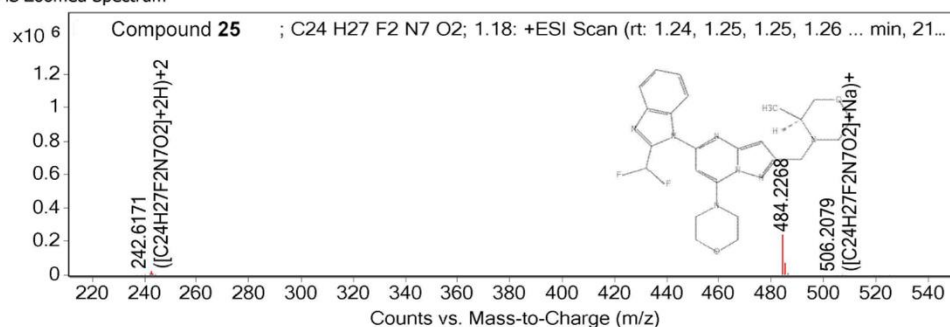
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaorith Find by Formula
Compound 25	484.2268	1.18	483.2195	C24 H27 F2 N7 O2	483.2194	0.06	



MS Zoomed Spectrum



MS Zoomed Spectrum

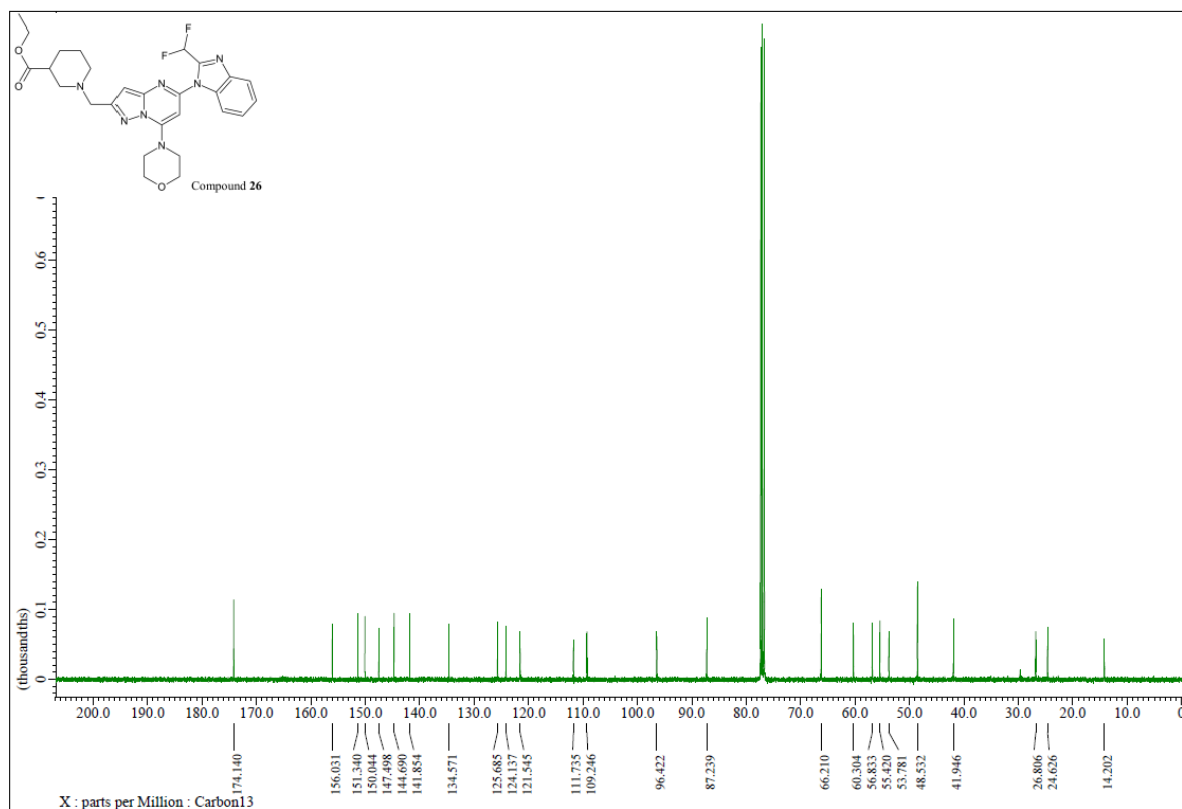
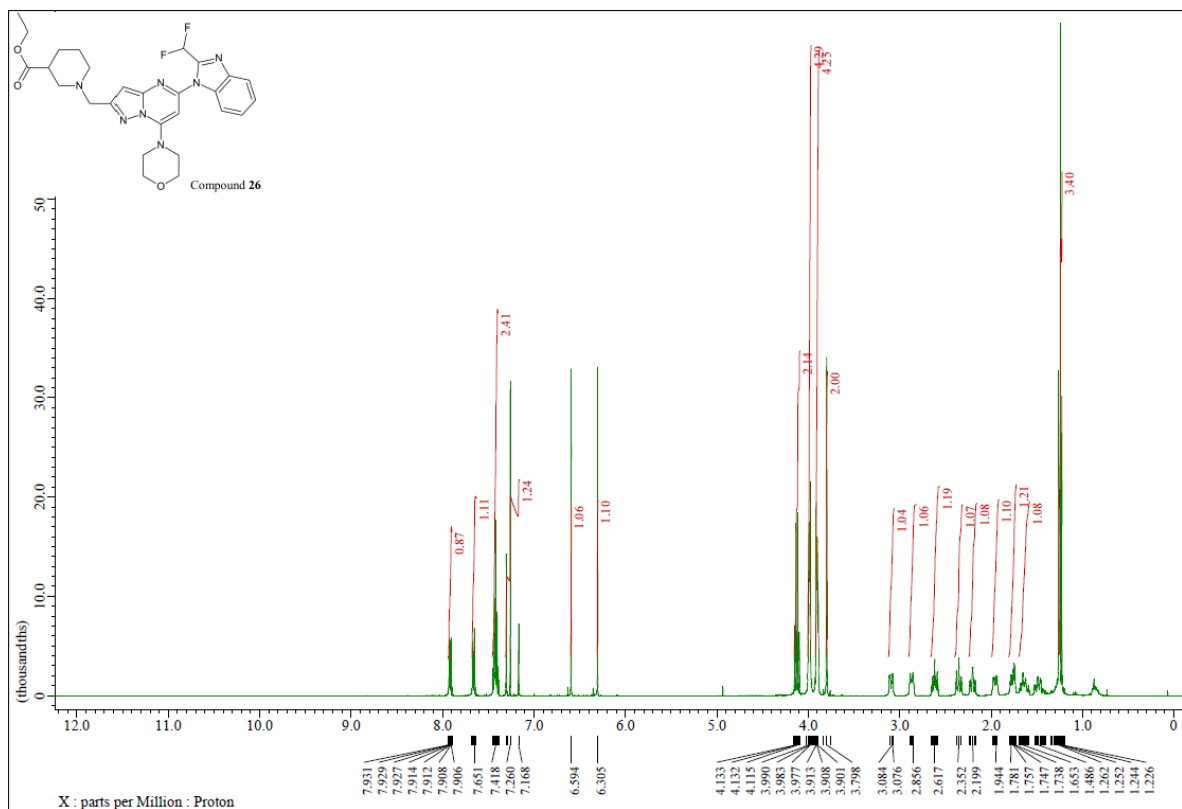


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
241.6083	2	349.53	C24H27F2N7O2	M+2	
242.6171	2	19071.85	C24H27F2N7O2	(M+2H)+2	
243.119	2	6438.57	C24H27F2N7O2	(M+2H)+2	
243.619	2	918.06	C24H27F2N7O2	(M+2H)+2	
484.2268	1	239466.45	C24H27F2N7O2	(M+H)+	
485.2293	1	67776.46	C24H27F2N7O2	(M+H)+	
486.2318	1	9900.11	C24H27F2N7O2	(M+H)+	
487.2347	1	1392.6	C24H27F2N7O2	(M+H)+	
506.2079	1	302.17	C24H27F2N7O2	(M+Na)+	
522.1879	1	143.76	C24H27F2N7O2	(M+K)+	
241.6083	2	349.53	C24H27F2N7O2	M+2	-3.76
242.6171	2	19071.85	C24H27F2N7O2	(M+2H)+2	0.44
243.119	2	6438.57	C24H27F2N7O2	(M+2H)+2	2.36
243.619	2	918.06	C24H27F2N7O2	(M+2H)+2	-2.94
484.2268	1	239466.45	C24H27F2N7O2	(M+H)+	0.15
485.2293	1	67776.46	C24H27F2N7O2	(M+H)+	-0.43
486.2318	1	9900.11	C24H27F2N7O2	(M+H)+	-0.78
487.2347	1	1392.6	C24H27F2N7O2	(M+H)+	-0.16
506.2079	1	302.17	C24H27F2N7O2	(M+Na)+	-1.49
522.1879	1	143.76	C24H27F2N7O2	(M+K)+	10.09

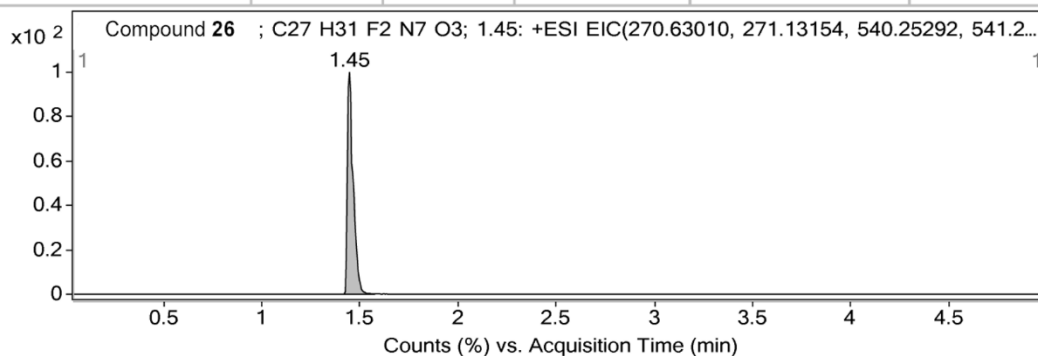
--- End Of Report ---

Compound 26

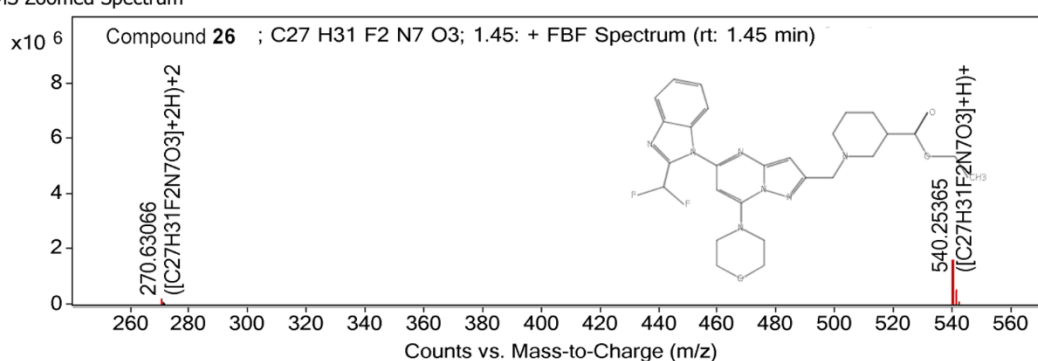


Compound 26

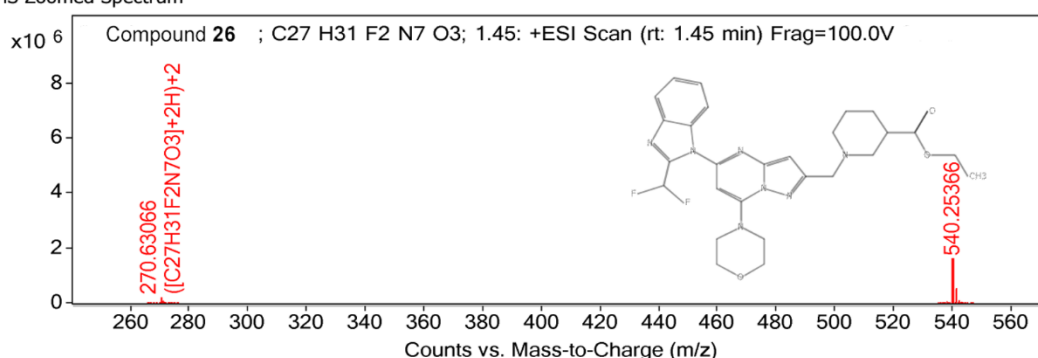
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Algorit
Compound 26	270.63066	1.45	539.24629	C27 H31 F2 N7 O3	539.24564	1.19	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

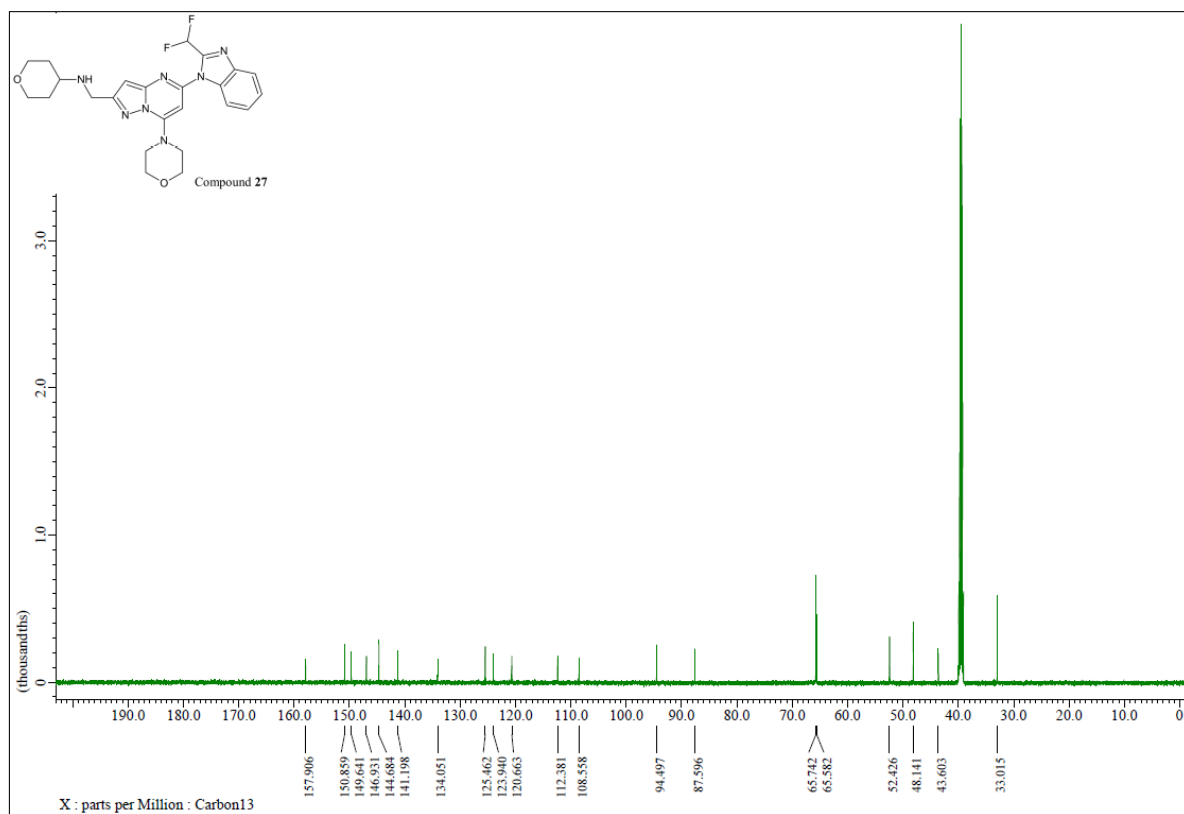
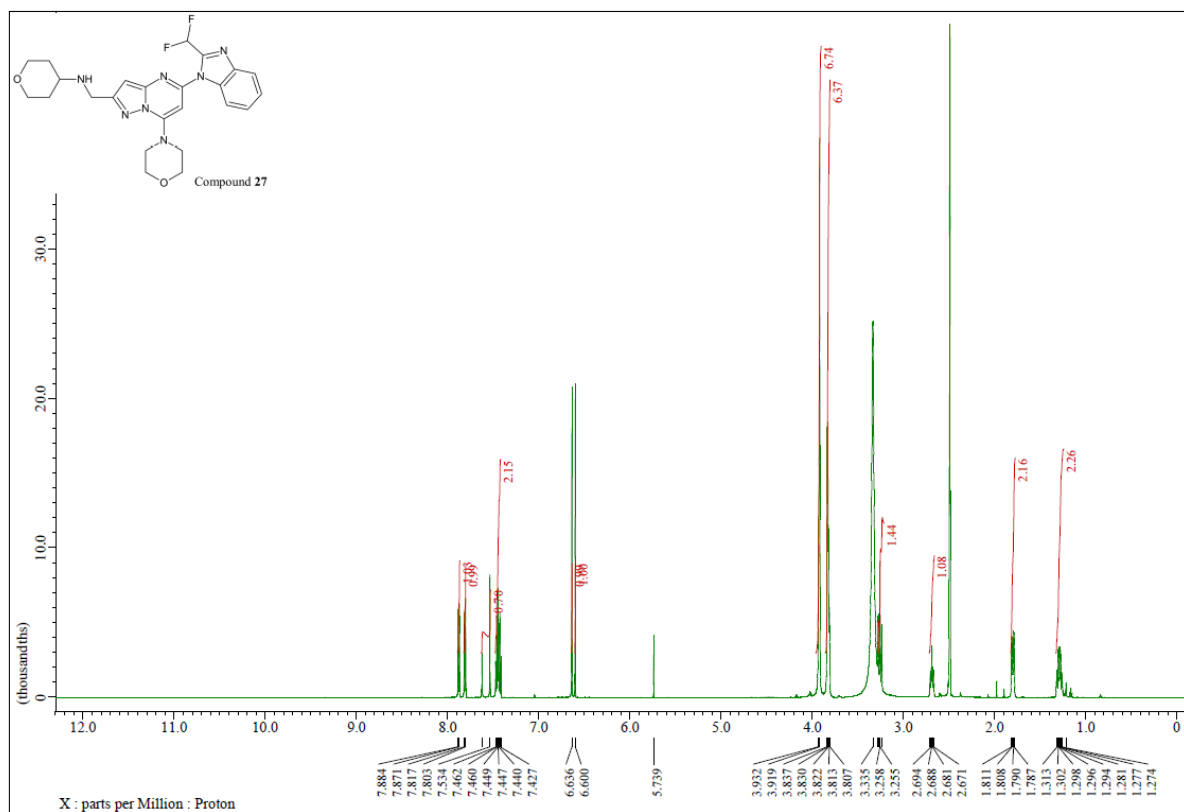


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
270.63066	2	179367.64	C27H31F2N7O3	(M+2H)+2	
271.13199	2	57800.48	C27H31F2N7O3	(M+2H)+2	
271.6328	2	10418.95	C27H31F2N7O3	(M+2H)+2	
540.25365	1	1591887.75	C27H31F2N7O3	(M+H)+	
541.25604	1	472964.91	C27H31F2N7O3	(M+H)+	
542.25858	1	77634.71	C27H31F2N7O3	(M+H)+	
270.63066	2	179367.64	C27H31F2N7O3	(M+2H)+2	2.06
271.13199	2	57800.48	C27H31F2N7O3	(M+2H)+2	1.64
271.6328	2	10418.95	C27H31F2N7O3	(M+2H)+2	-0.35
540.25365	1	1591887.75	C27H31F2N7O3	(M+H)+	1.36
540.25366		1593459.38			
541.25604	1	472964.91	C27H31F2N7O3	(M+H)+	0.43
542.25858	1	77634.71	C27H31F2N7O3	(M+H)+	0.12

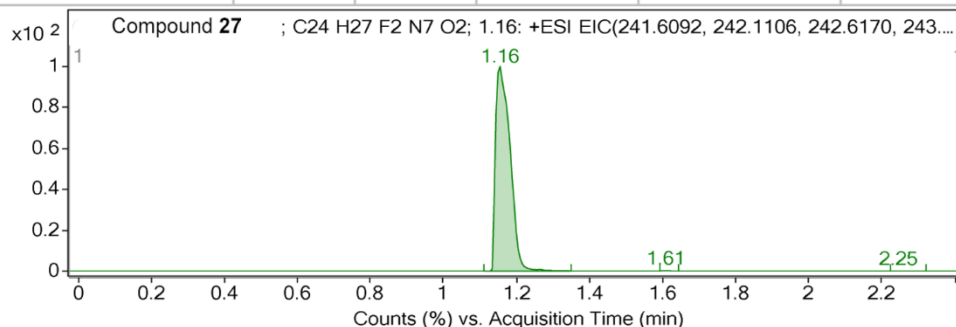
--- End Of Report ---

Compound 27

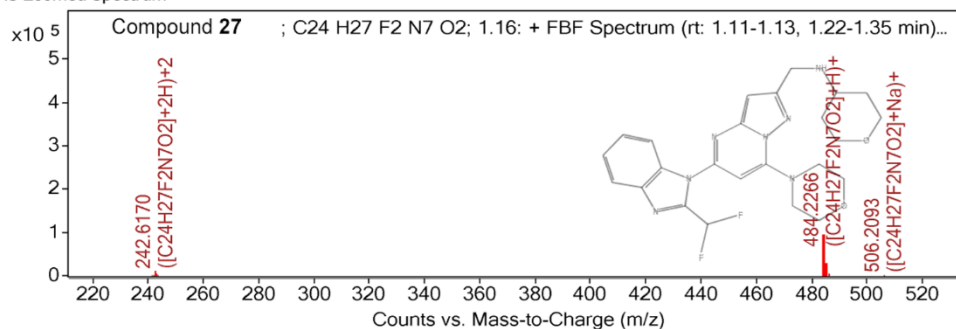


Compound 27

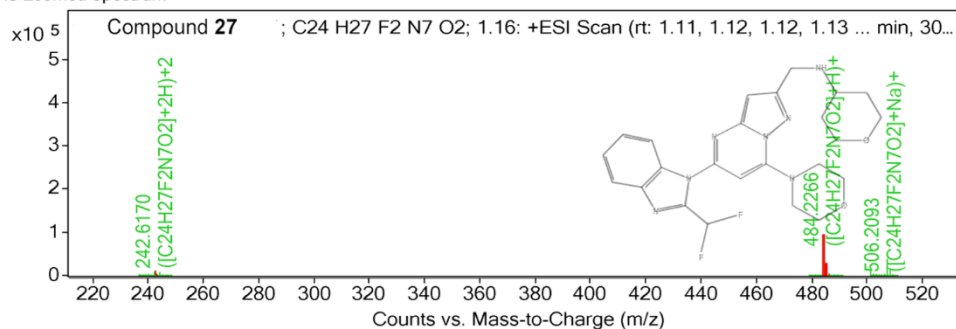
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 27	484.2266	1.16	483.2193	C24 H27 F2 N7 O2	483.2194	-0.29	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

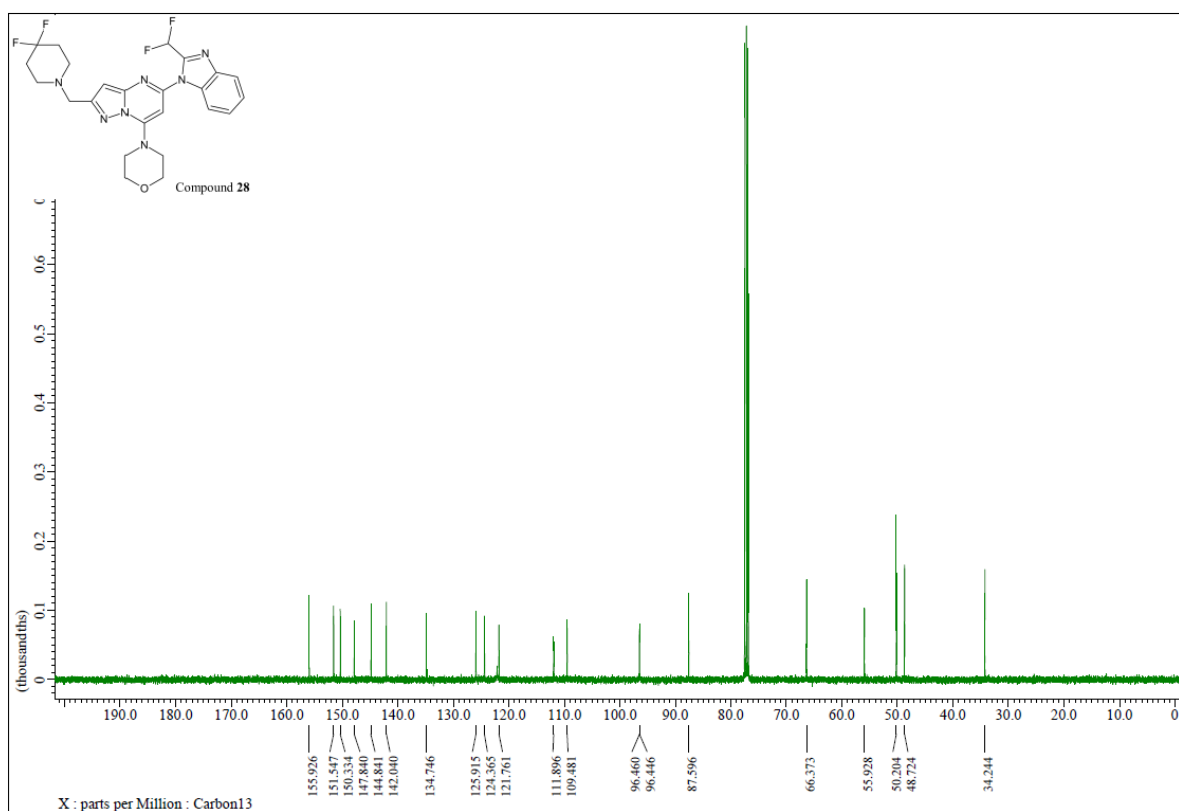
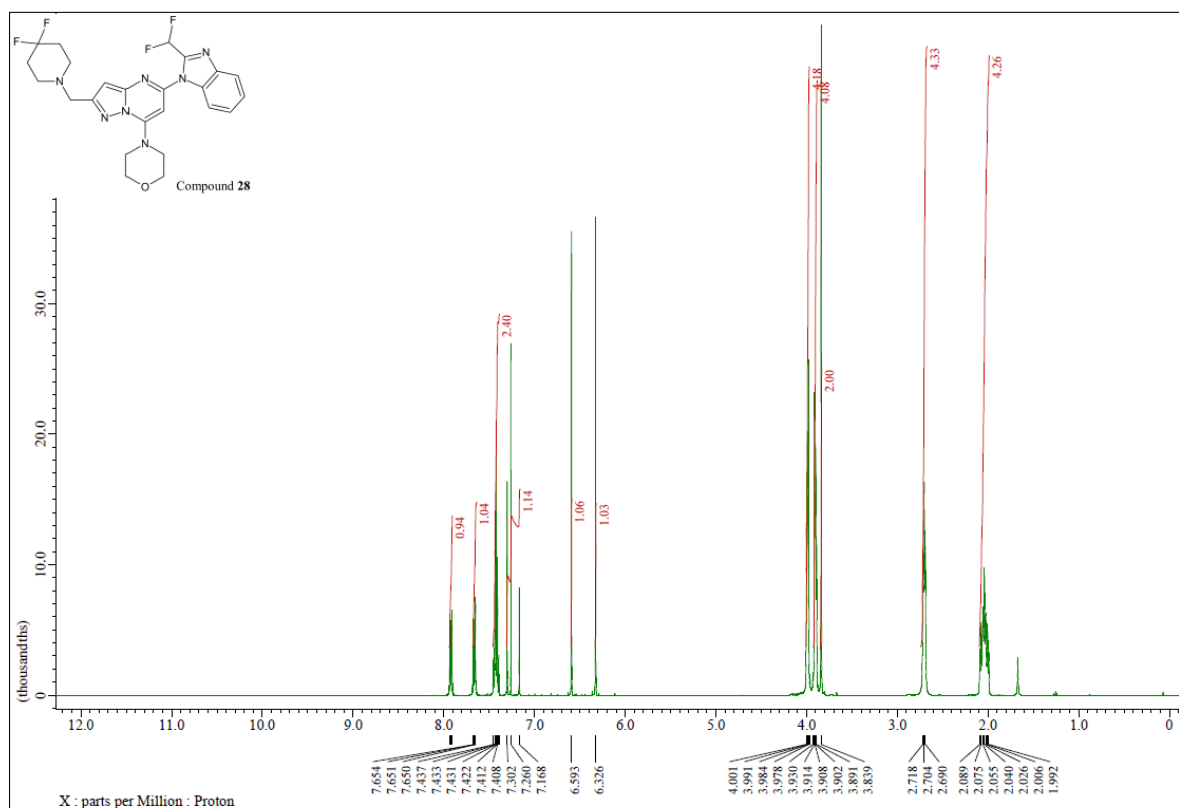


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
241.6093	2	641.2	C24H27F2N7O2	M+2	
242.1097	2	215.29	C24H27F2N7O2	M+2	
242.617	2	9418.48	C24H27F2N7O2	(M+2H)+2	
243.1191	2	3902.27	C24H27F2N7O2	(M+2H)+2	
243.6188	2	480.77	C24H27F2N7O2	(M+2H)+2	
484.2266	1	93398.47	C24H27F2N7O2	(M+H)+	
485.2292	1	26572.49	C24H27F2N7O2	(M+H)+	
486.2313	1	4498.85	C24H27F2N7O2	(M+H)+	
506.2093	1	299.24	C24H27F2N7O2	(M+Na)+	
241.6093	2	641.2	C24H27F2N7O2	M+2	0.56
242.1097	2	215.29	C24H27F2N7O2	M+2	-3.69
242.617	2	9418.48	C24H27F2N7O2	(M+2H)+2	0.19
243.1191	2	3902.27	C24H27F2N7O2	(M+2H)+2	2.77
243.6188	2	480.77	C24H27F2N7O2	(M+2H)+2	-3.99
484.2266	1	93398.47	C24H27F2N7O2	(M+H)+	-0.26
485.2292	1	26572.49	C24H27F2N7O2	(M+H)+	-0.67
486.2313	1	4498.85	C24H27F2N7O2	(M+H)+	-1.85
506.2093	1	299.24	C24H27F2N7O2	(M+Na)+	1.21

--- End Of Report ---

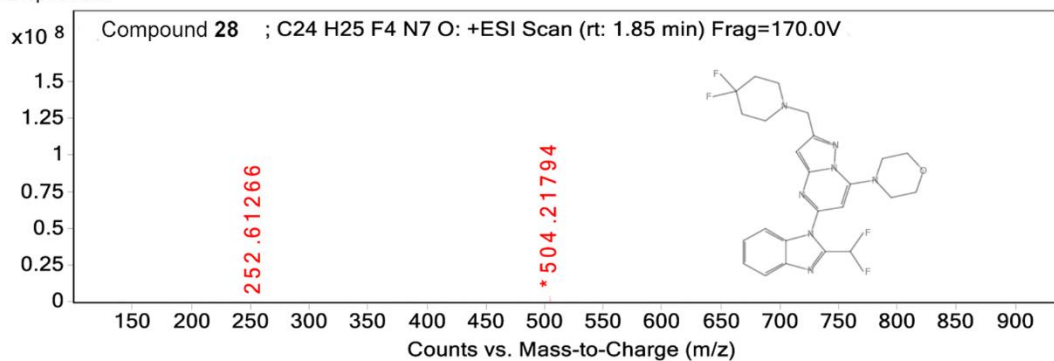
Compound 28



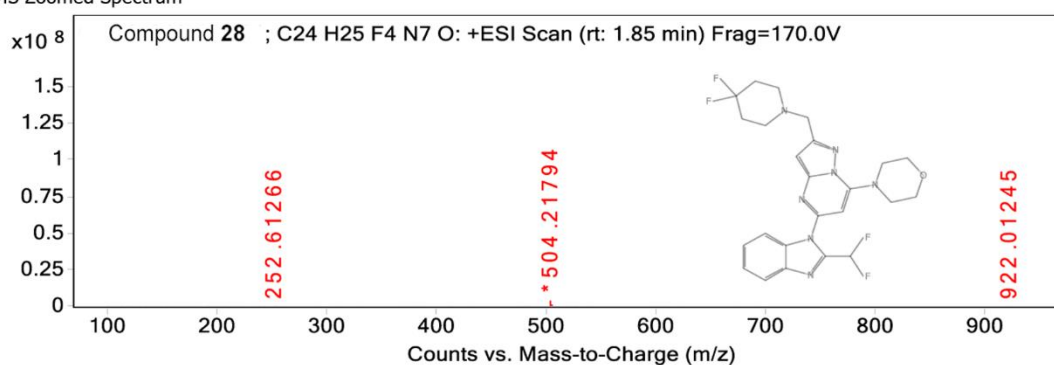
Compound 28

Compound Label	Name	Algorithm	Mass
Compound 28	Compound 28	Spectrum Extraction	503.21022

MS Spectrum



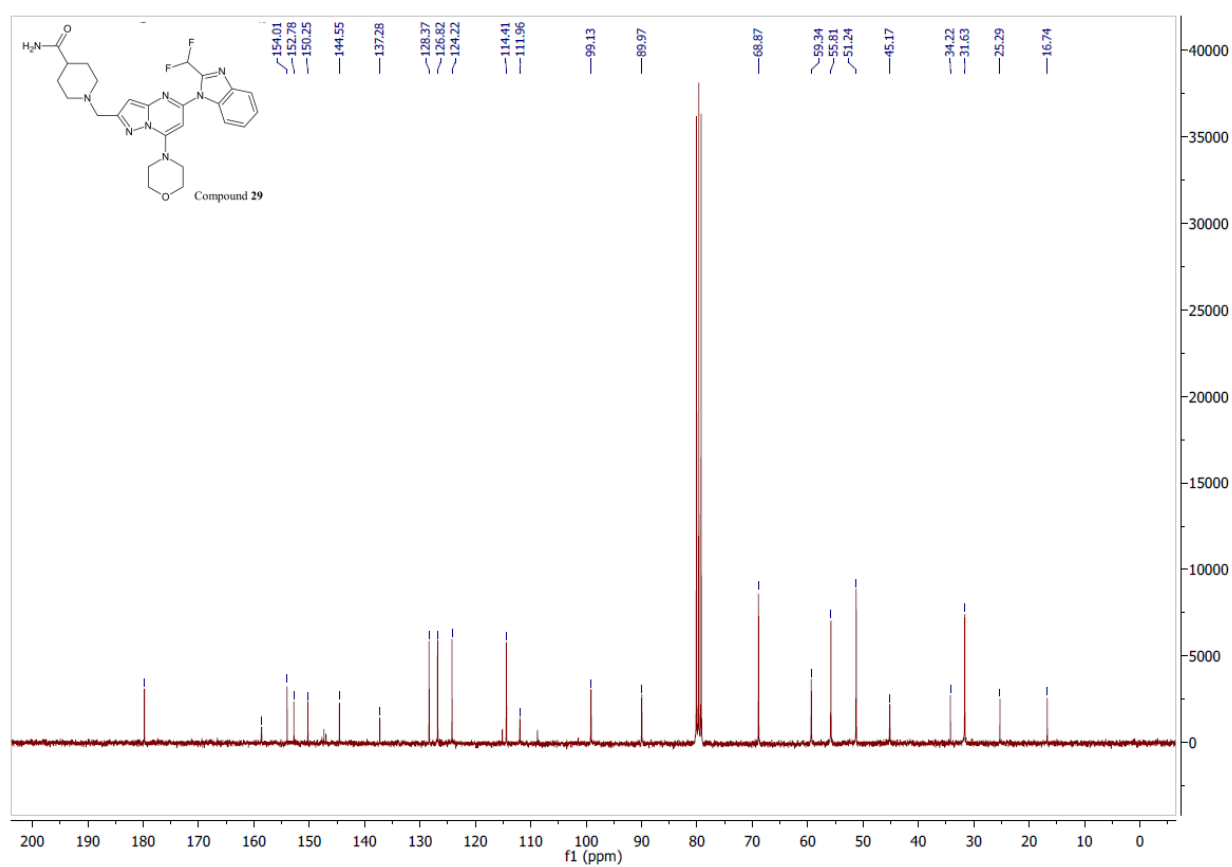
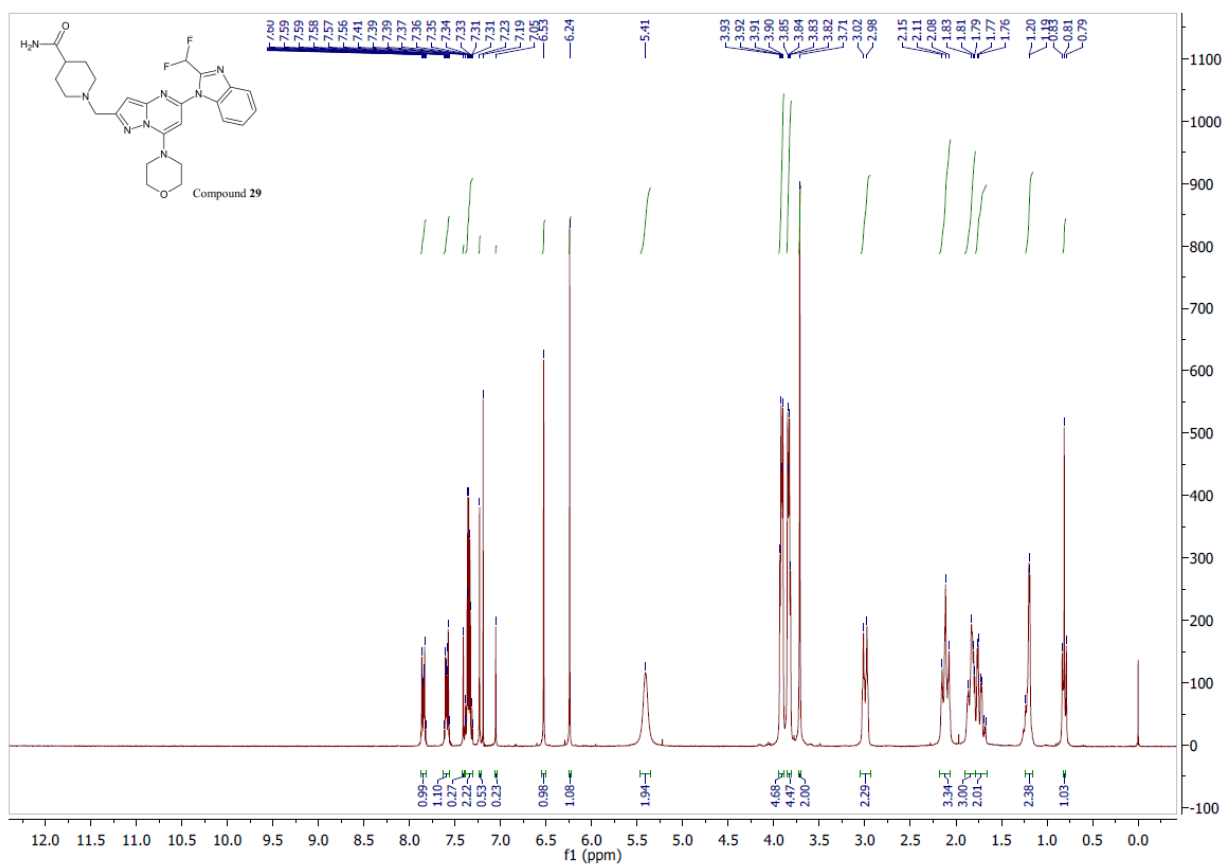
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
121.05149	98.06004	234462.98	1	107715.05	C ₅ H ₈ N O	(M+Na)+
134.0781	116.04321	155415.3	1	30413.49	C ₆ H ₆ F ₂	(M+NH ₄)+
242.60846	224.57262	80311.83	2	38307	C ₂₄ H ₁₈ F ₃ N ₅ O	(M+2(NH ₄))+2
252.61266			2	275026.94		
253.11332			2	88366.99		
502.19922	484.16292	37252.54	1	59938.18	C ₂₄ H ₂₀ F ₄ N ₆ O	(M+NH ₄)+
504.21794	504.21295	9.9	1	3615947.75		
505.21907	505.21577	6.53	1	1067767.5		
506.22162	506.21851	6.15	1	148034.56		
922.01245			1	133568.02		

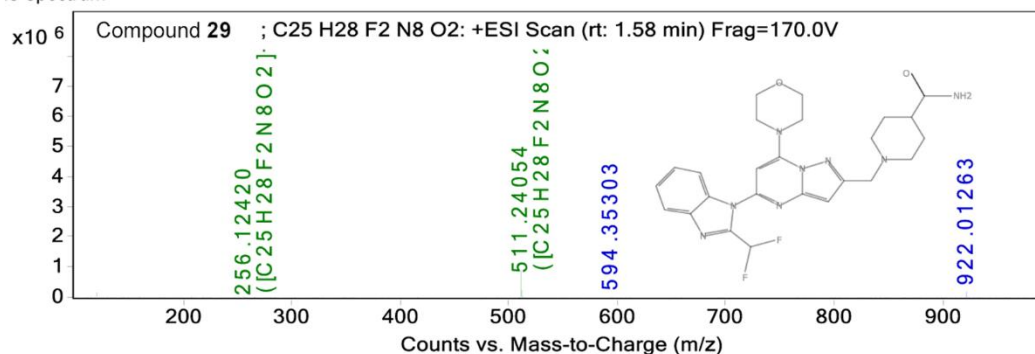
Compound 29



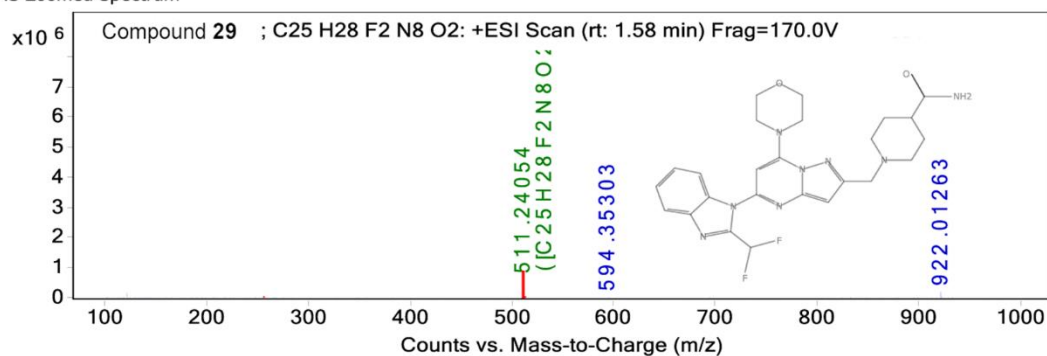
Compound 29

Compound Label	Name	Algorithm	Mass
Compound 29	Compound 29	Spectrum Extraction	510.2333

MS Spectrum



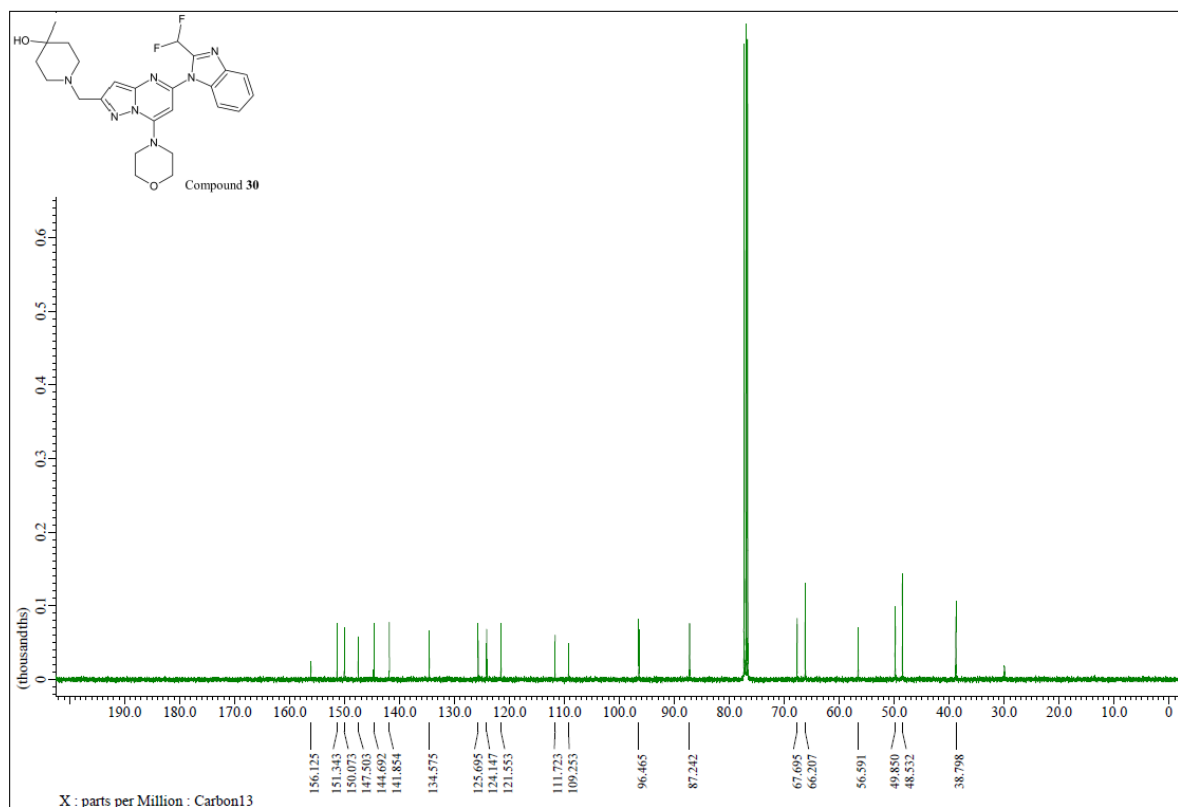
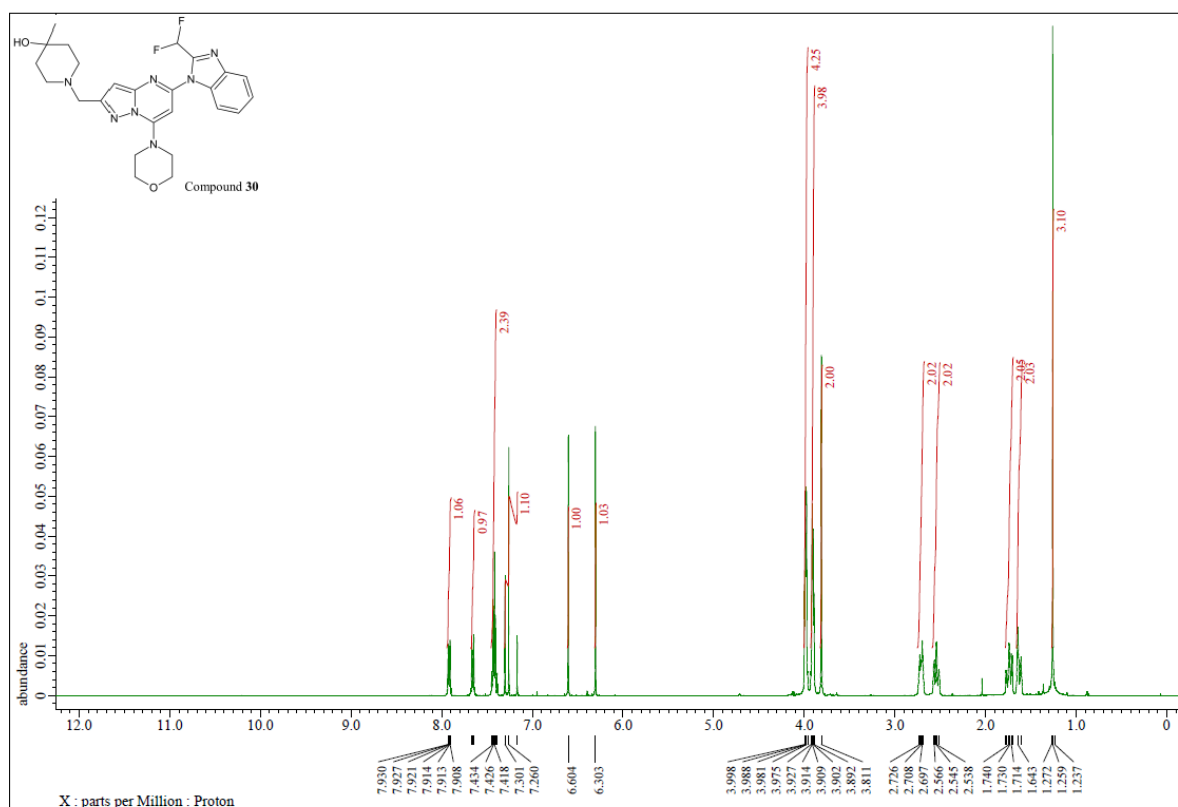
MS Zoomed Spectrum



MS Spectrum Peak List

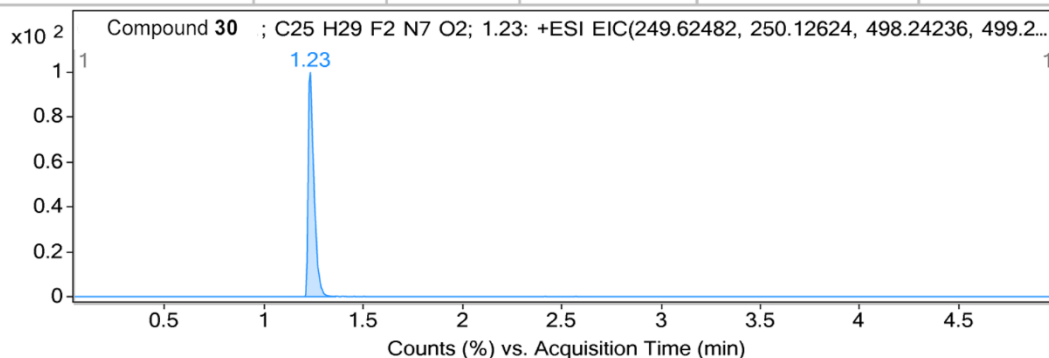
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
119.02898	96.03812	239392.99	1	15371.62	C ₃ H ₆ F ₂ O	(M+Na)+
121.05147	98.06004	234462.74	1	142227.73	C ₅ H ₈ N ₂ O	(M+Na)+
158.97415				13291.27		
194.11845	176.08318	102424.71	1	12525.6	C ₁₁ H ₁₂ O ₂	(M+NH ₄)+
256.1242	255.11462	3957.39	2	25005.71	C ₂₅ H ₂₈ F ₂ N ₈ O ₂	(M+2H)+2
511.24054	510.22978	1981	1	895150.94	C ₂₅ H ₂₈ F ₂ N ₈ O ₂	(M+H)+
512.24361	512.24039	6.28	1	231365.09	C ₂₅ H ₂₈ F ₂ N ₈ O ₂	(M+H)+
513.2455	513.24303	4.81	1	34448.2	C ₂₅ H ₂₈ F ₂ N ₈ O ₂	(M+H)+
922.01263			1	180393.22		
923.01411			1	30642.4		

Compound 30

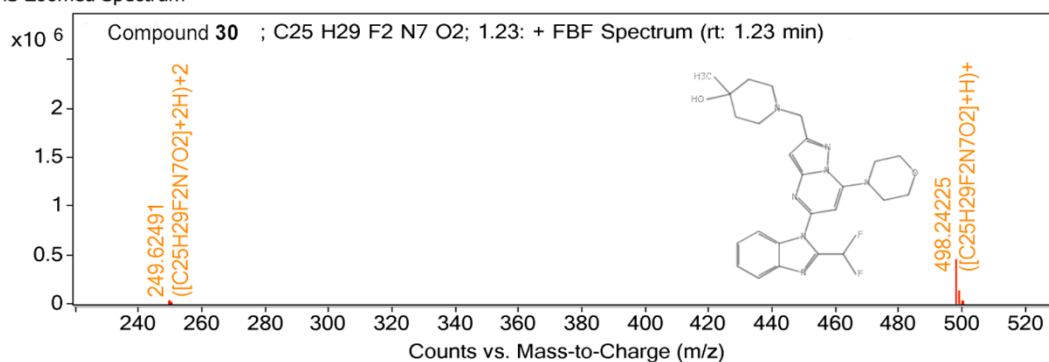


Compound 30

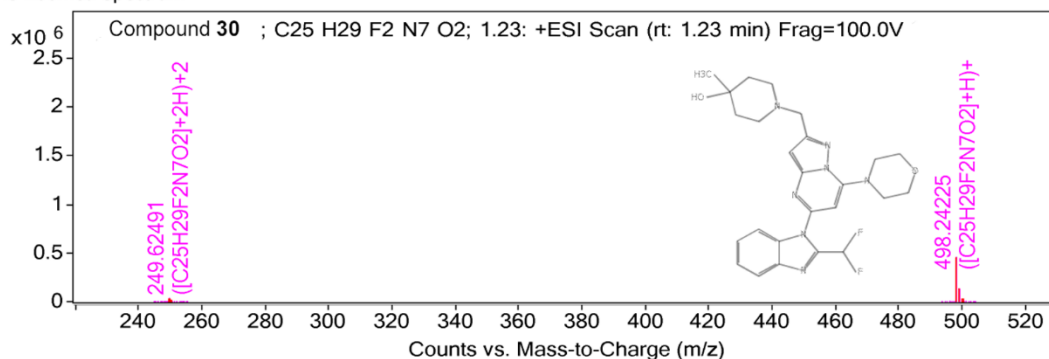
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 30	498.24225	1.23	497.23508	C25 H29 F2 N7 O2	497.23508	-0.01	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

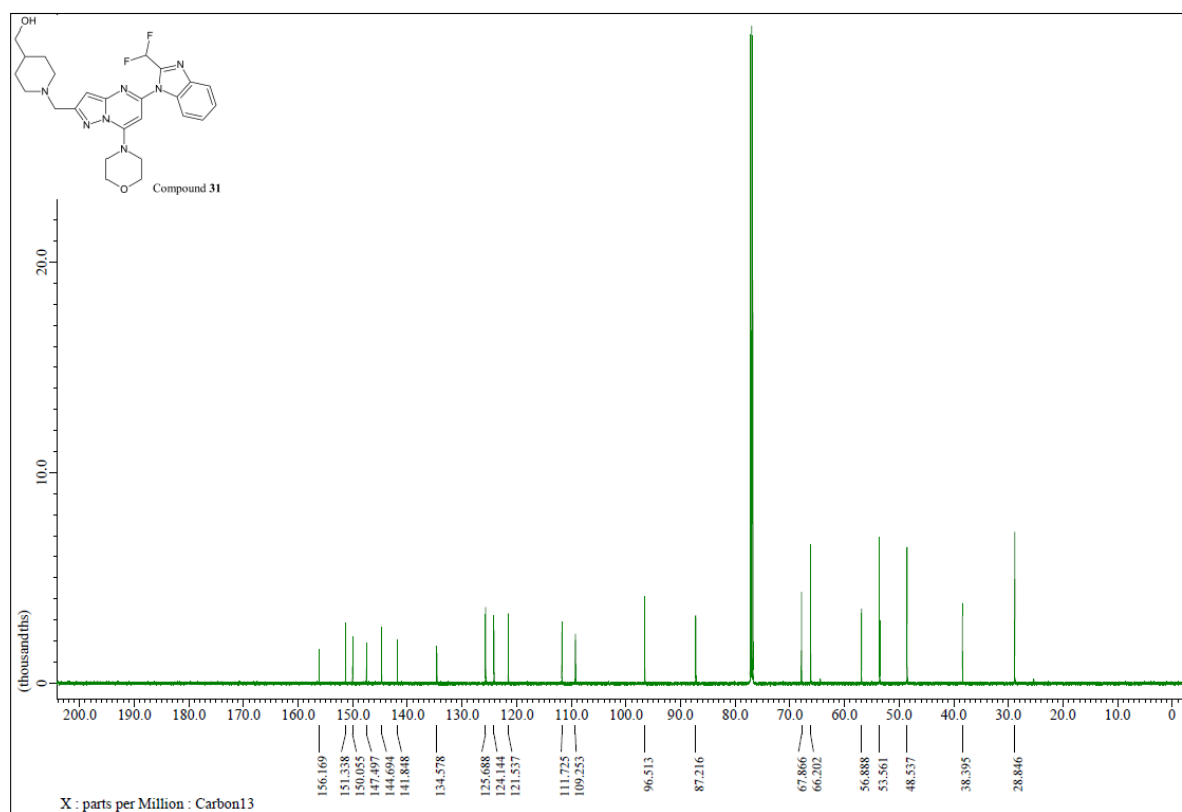
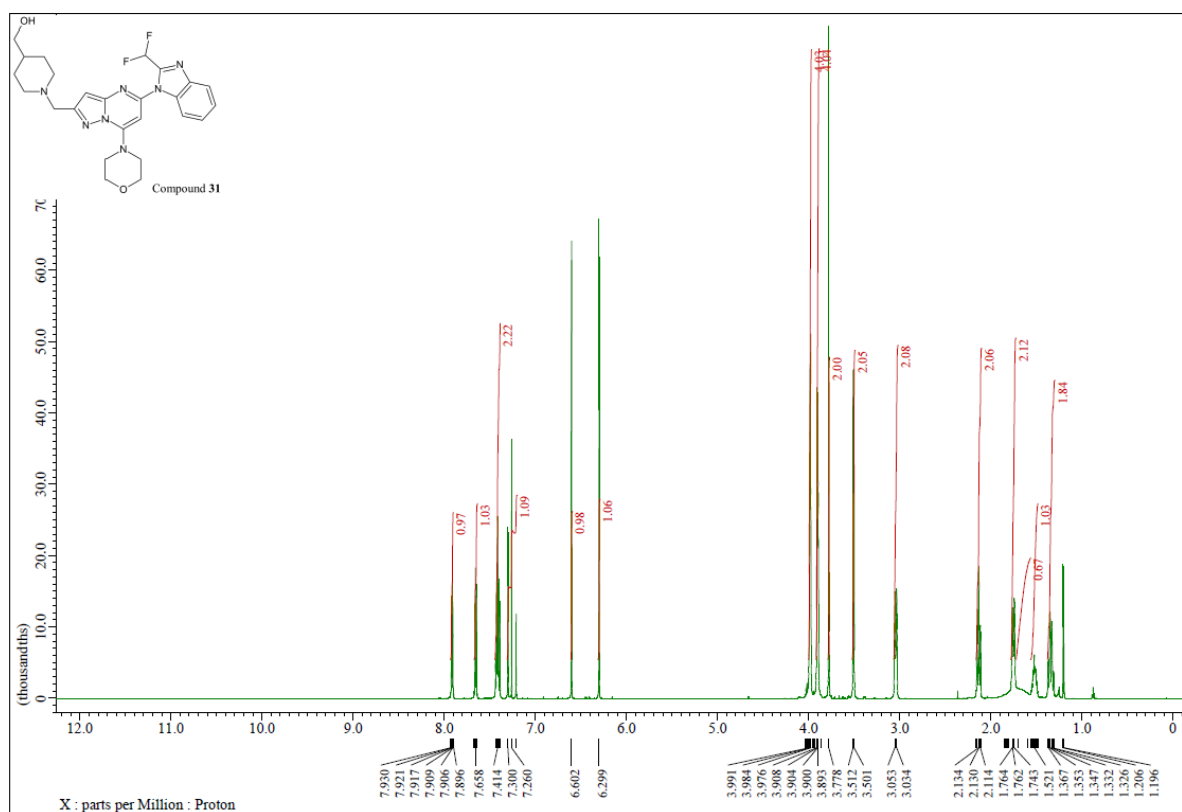


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
249.62491	2	32408.56	C25H29F2N7O2	(M+2H)+2	
250.12641	2	9351.96	C25H29F2N7O2	(M+2H)+2	
250.63006	2	1067.82	C25H29F2N7O2	(M+2H)+2	
498.24225	1	454326	C25H29F2N7O2	(M+H)+	
499.24548	1	127977.54	C25H29F2N7O2	(M+H)+	
500.24771	1	17402.12	C25H29F2N7O2	(M+H)+	
249.62491	2	32408.56	C25H29F2N7O2	(M+2H)+2	0.36
250.12641	2	9351.96	C25H29F2N7O2	(M+2H)+2	0.67
250.63006	2	1067.82	C25H29F2N7O2	(M+2H)+2	9.85
498.24225	1	454326	C25H29F2N7O2	(M+H)+	-0.21
499.24548	1	127977.54	C25H29F2N7O2	(M+H)+	0.55
500.24771	1	17402.12	C25H29F2N7O2	(M+H)+	-0.41

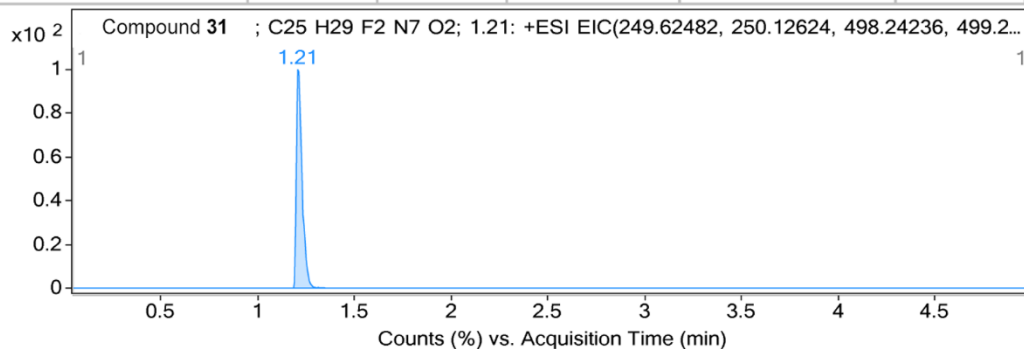
--- End Of Report ---

Compound 31

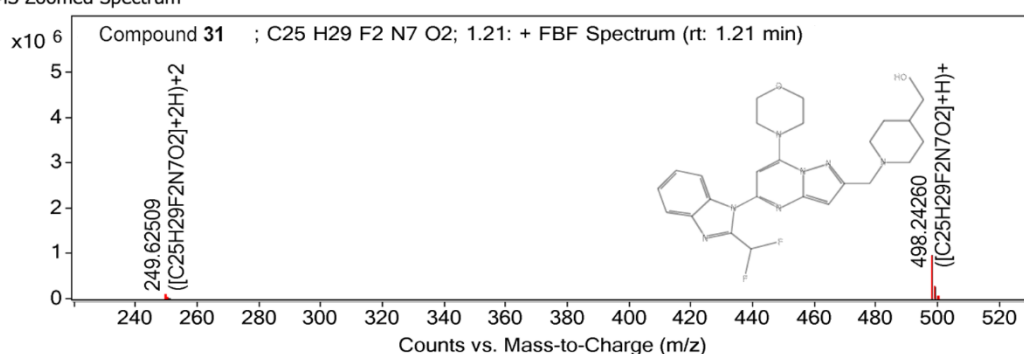


Compound 31

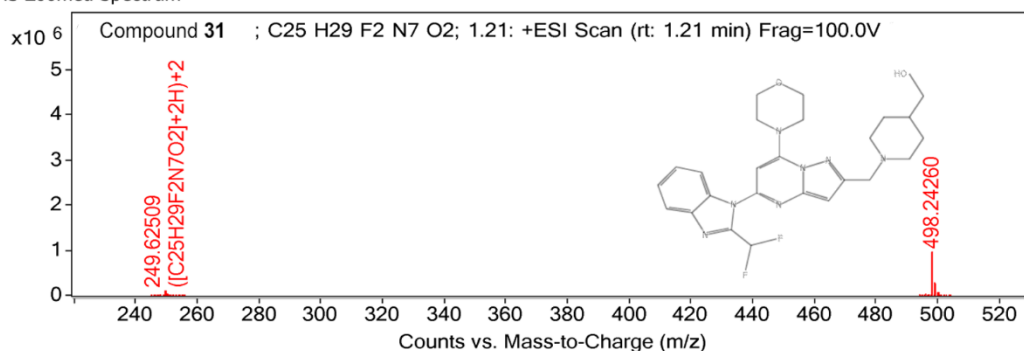
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpbs Algorit
Compound 31	249.62509	1.21	497.23538	C25 H29 F2 N7 O2	497.23508	0.6	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

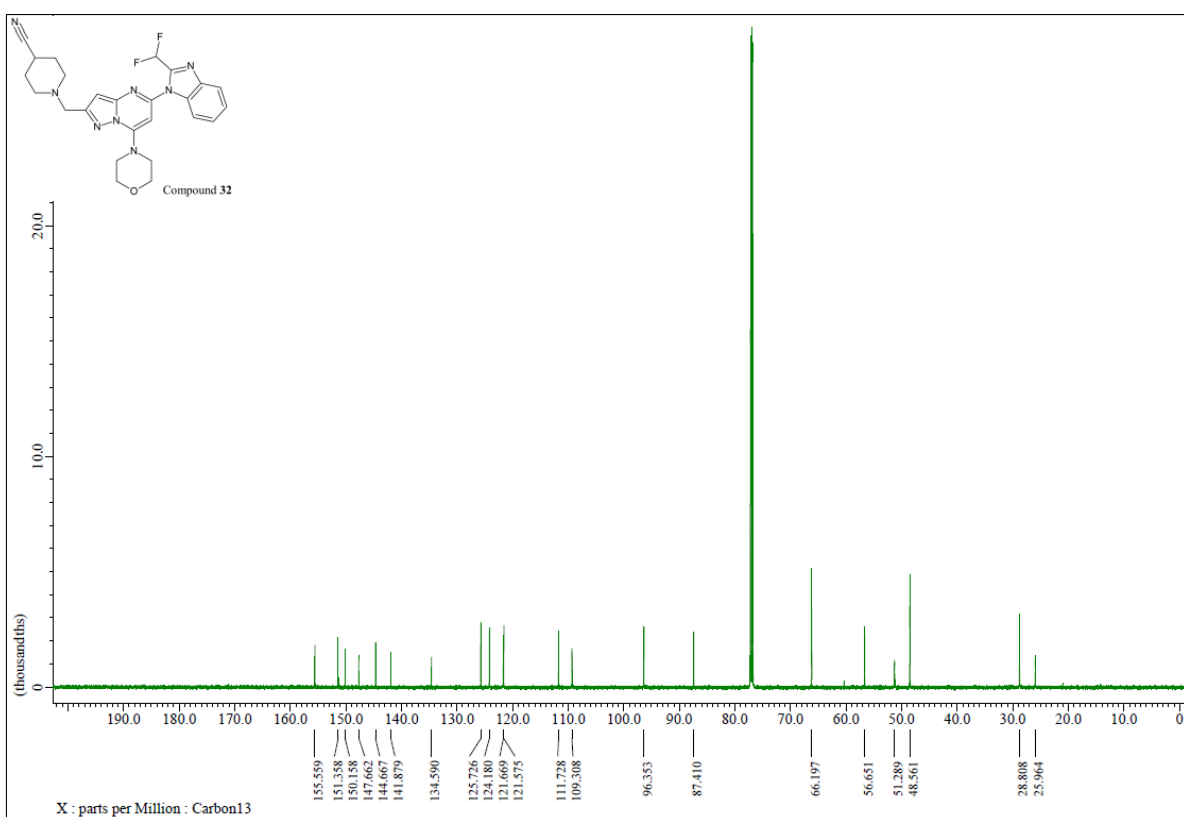
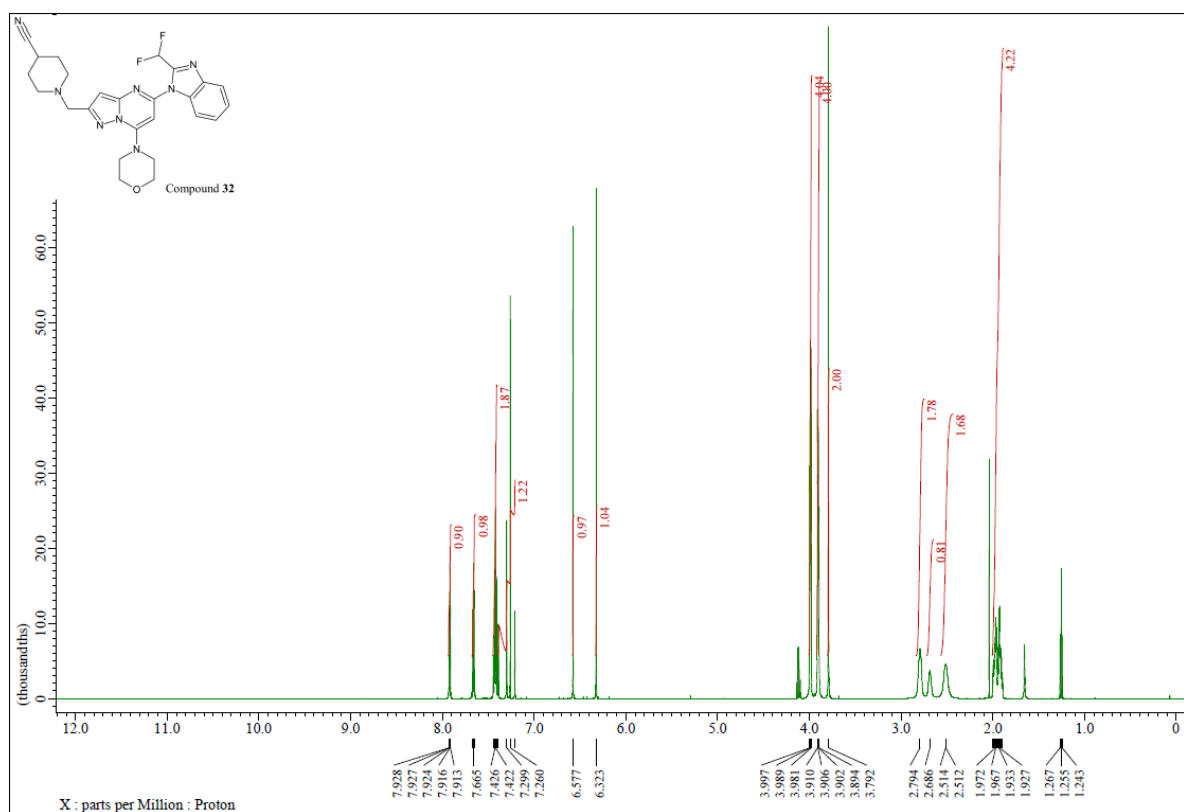


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
249.62509	2	93481.14	C25H29F2N7O2	(M+2H)+2	
250.12632	2	26983.34	C25H29F2N7O2	(M+2H)+2	
250.62759	2	4998.15	C25H29F2N7O2	(M+2H)+2	
251.12641	2	537.79	C25H29F2N7O2	(M+2H)+2	
498.2426	1	954572.56	C25H29F2N7O2	(M+H)+	
499.24579	1	250903.33	C25H29F2N7O2	(M+H)+	
500.24755	1	41231.06	C25H29F2N7O2	(M+H)+	
249.62509	2	93481.14	C25H29F2N7O2	(M+2H)+2	1.11
250.12632	2	26983.34	C25H29F2N7O2	(M+2H)+2	0.32
250.62759	2	4998.15	C25H29F2N7O2	(M+2H)+2	-0.03
251.12641	2	537.79	C25H29F2N7O2	(M+2H)+2	-9.93
498.2426		955096.81			0.48
498.2426	1	954572.56	C25H29F2N7O2	(M+H)+	0.48
499.24579	1	250903.33	C25H29F2N7O2	(M+H)+	1.16
500.24755	1	41231.06	C25H29F2N7O2	(M+H)+	-0.72

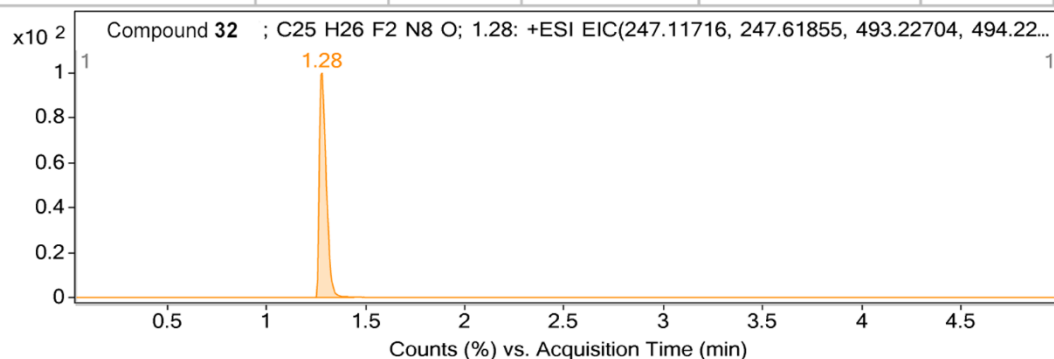
--- End Of Report ---

Compound 32

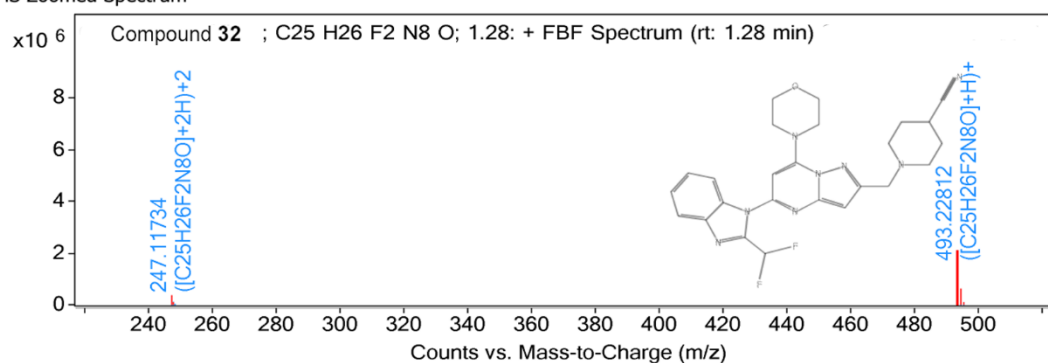


Compound 32

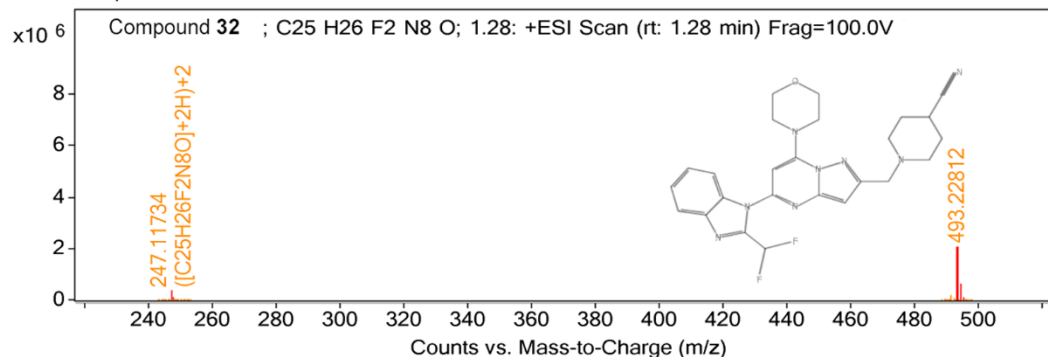
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 32	247.11734	1.28	492.22059	C25 H26 F2 N8 O	492.21976	1.67	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

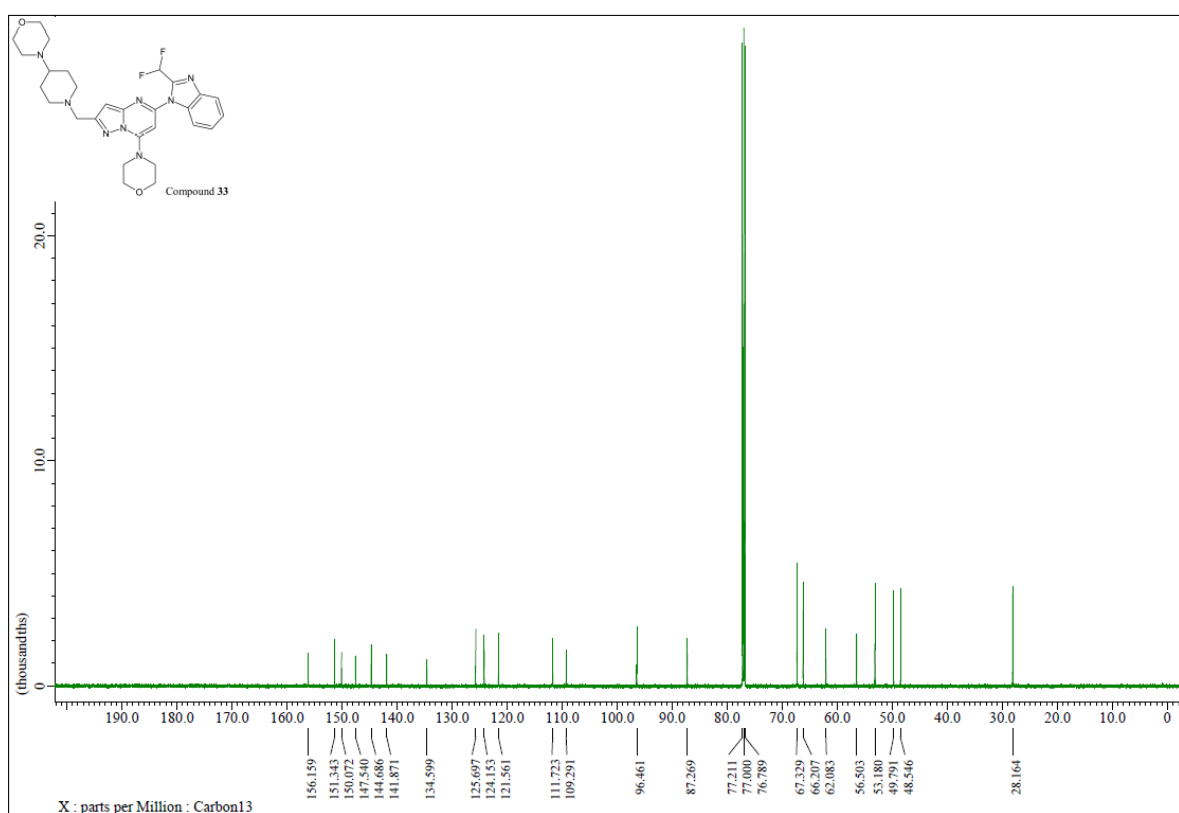
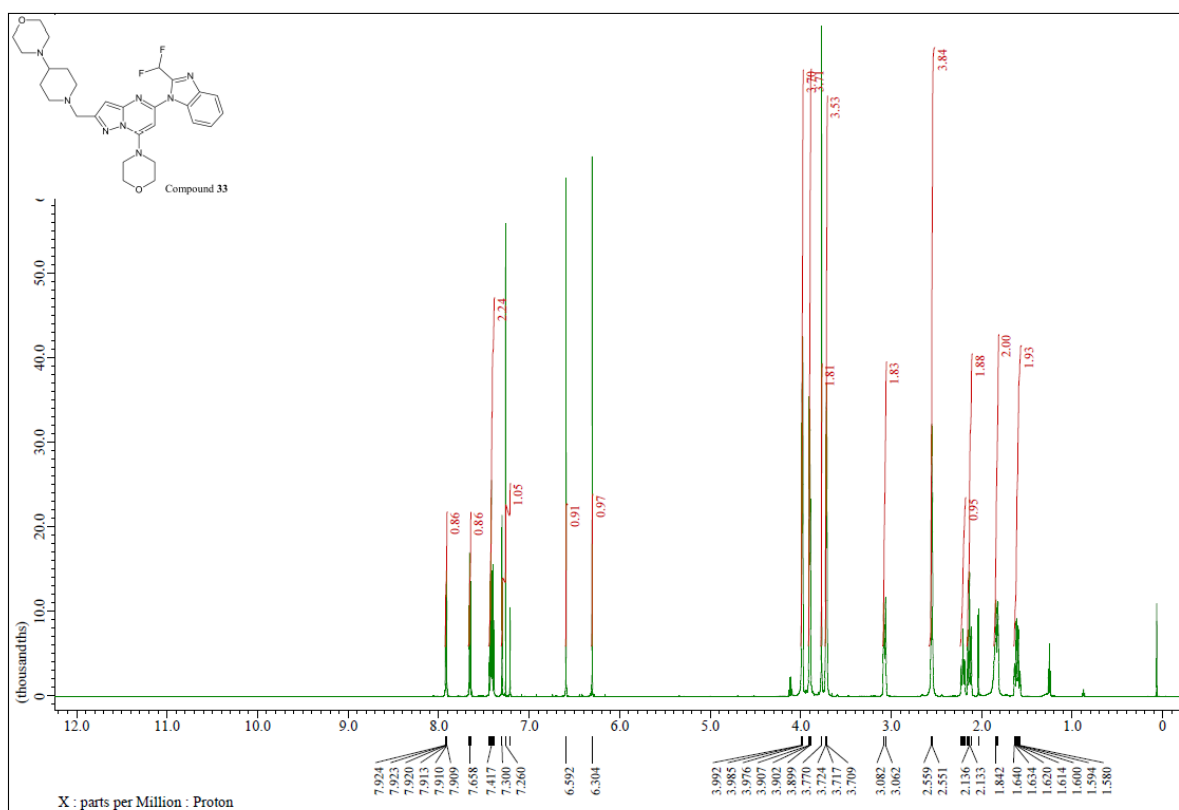


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
247.11734	2	344030.63	C25H26F2N8O	(M+2H)+2	
247.61913	2	93506.33	C25H26F2N8O	(M+2H)+2	
248.11993	2	15524.01	C25H26F2N8O	(M+2H)+2	
493.22812	1	2066621	C25H26F2N8O	(M+H)+	
494.23008	1	564287.69	C25H26F2N8O	(M+H)+	
495.23248	1	79639.52	C25H26F2N8O	(M+H)+	
247.11734	2	344030.63	C25H26F2N8O	(M+2H)+2	0.72
247.61913	2	93506.33	C25H26F2N8O	(M+2H)+2	2.36
248.11993	2	15524.01	C25H26F2N8O	(M+2H)+2	0.14
493.22812	1	2066621	C25H26F2N8O	(M+H)+	2.18
493.22812		2068672.75			
494.23008	1	564287.69	C25H26F2N8O	(M+H)+	0.52
495.23248	1	79639.52	C25H26F2N8O	(M+H)+	-0.06

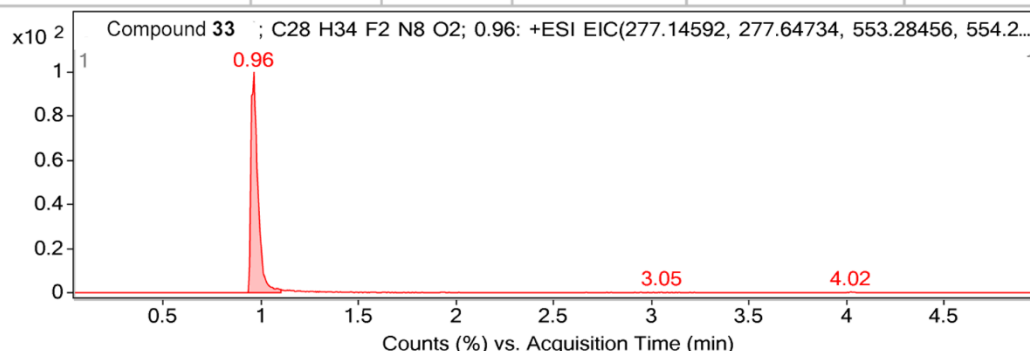
--- End Of Report ---

Compound 33

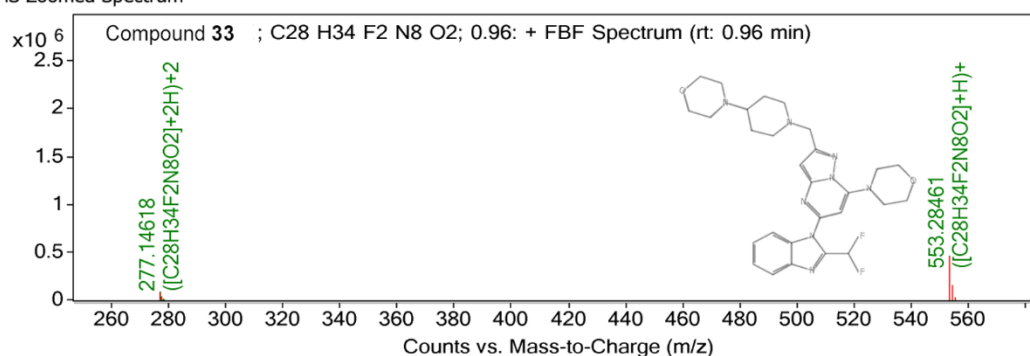


Compound 33

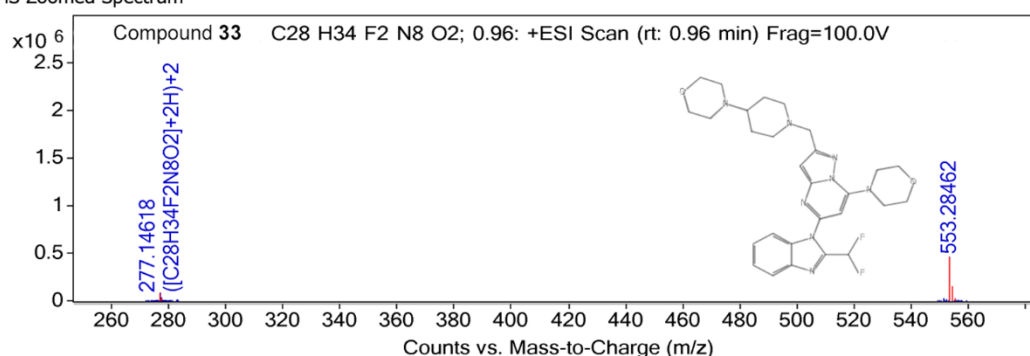
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 33	553.28461	0.96	552.27741	C28 H34 F2 N8 O2	552.27728	0.24	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

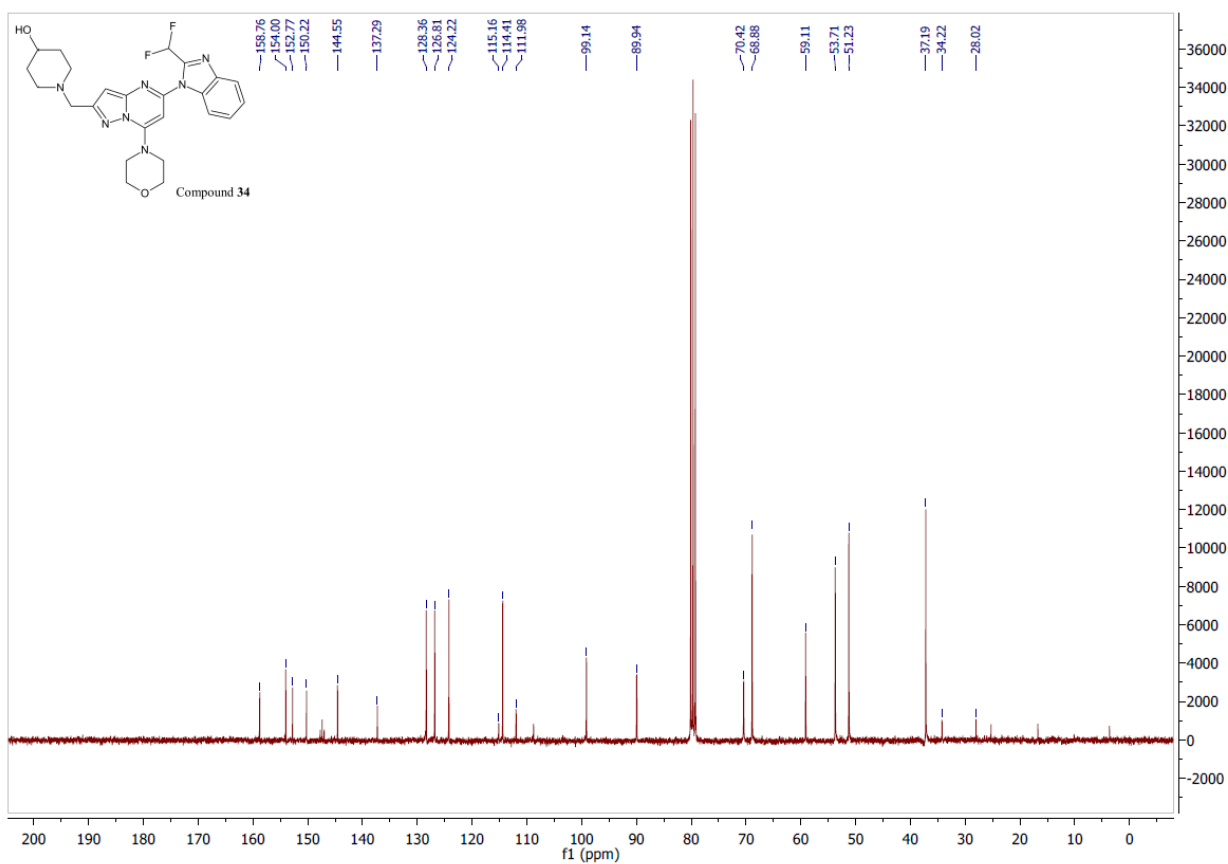
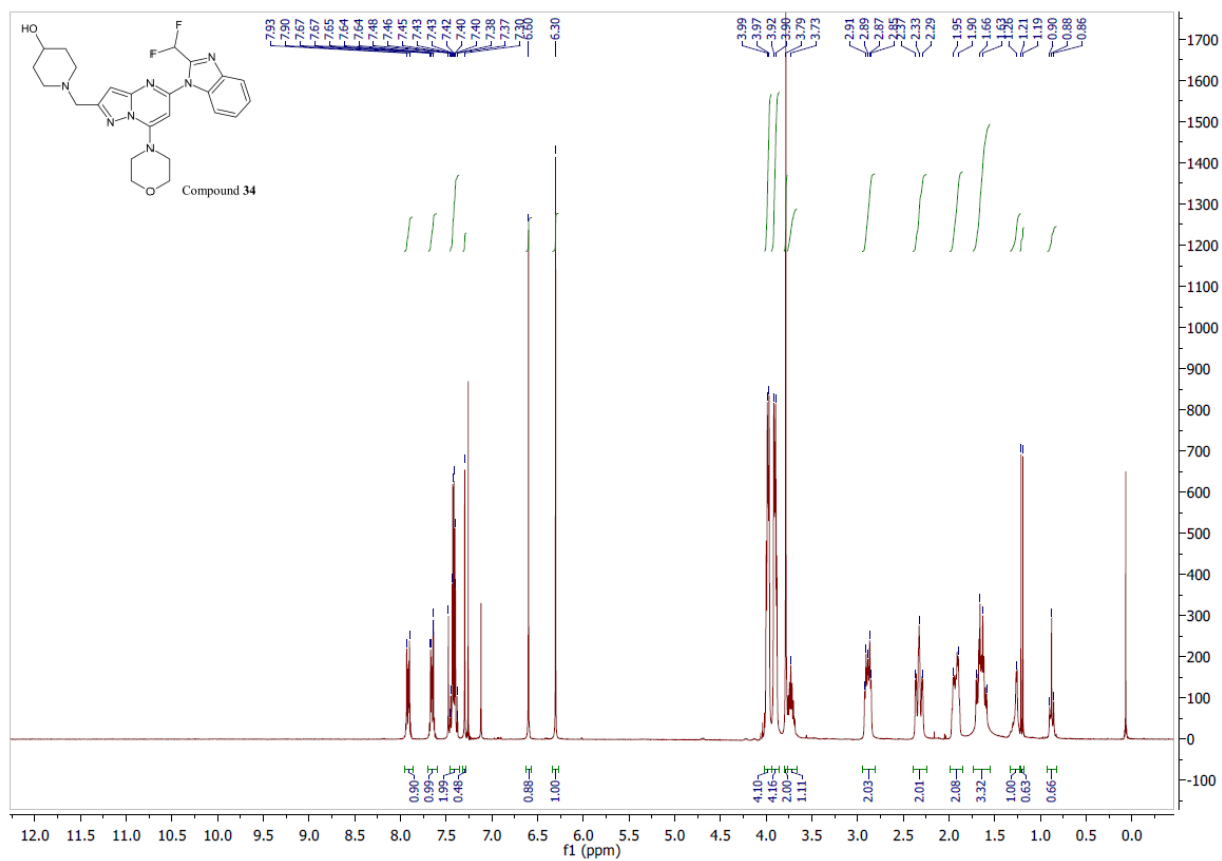


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
277.14618	2	79318.7	C28H34F2N8O2	(M+2H)+2	
277.64732	2	29703.31	C28H34F2N8O2	(M+2H)+2	
278.14977	2	5296.34	C28H34F2N8O2	(M+2H)+2	
278.65038	2	521.16	C28H34F2N8O2	(M+2H)+2	
553.28461	1	456124.09	C28H34F2N8O2	(M+H)+	
554.28756	1	135750.58	C28H34F2N8O2	(M+H)+	
555.28985	1	23141.17	C28H34F2N8O2	(M+H)+	
277.14618	2	79318.7	C28H34F2N8O2	(M+2H)+2	0.96
277.64732	2	29703.31	C28H34F2N8O2	(M+2H)+2	-0.06
278.14977	2	5296.34	C28H34F2N8O2	(M+2H)+2	3.85
278.65038	2	521.16	C28H34F2N8O2	(M+2H)+2	1.29
553.28461	1	456124.09	C28H34F2N8O2	(M+H)+	0.11
553.28462		458500.22			
554.28756	1	135750.58	C28H34F2N8O2	(M+H)+	0.29
555.28985	1	23141.17	C28H34F2N8O2	(M+H)+	-0.5

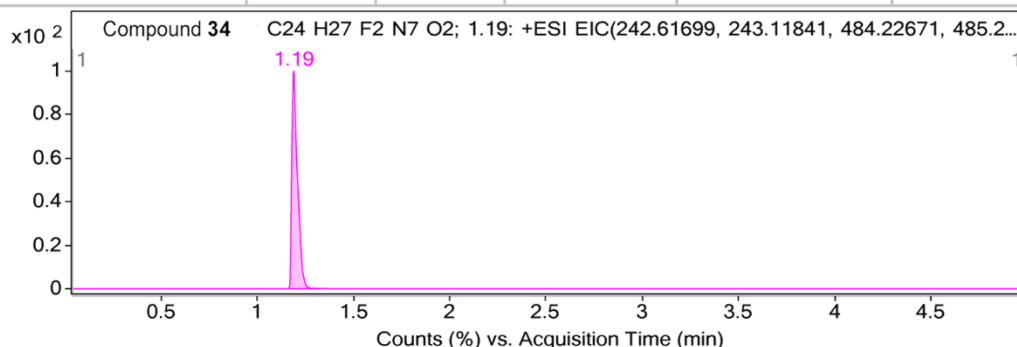
--- End Of Report ---

Compound 34

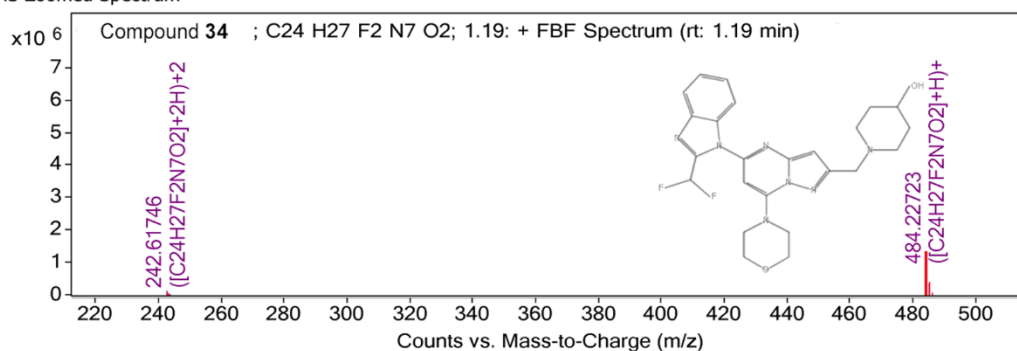


Compound 34

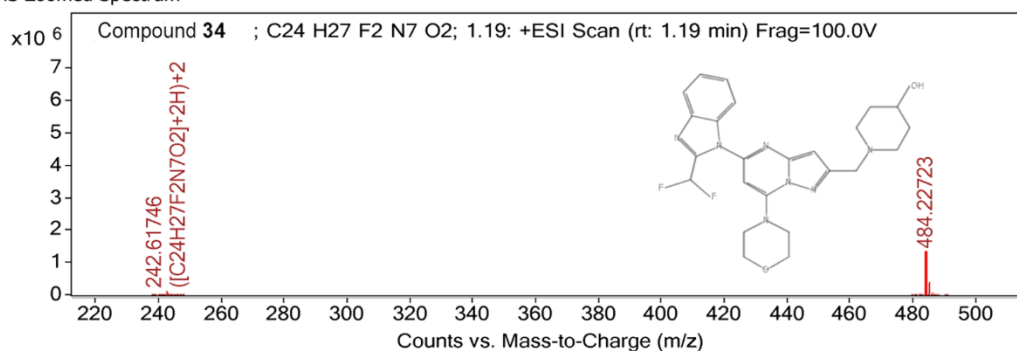
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Alaorit
Compound 34	242.61746	1.19	483.21994	C24 H27 F2 N7 O2	483.21943	1.06	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

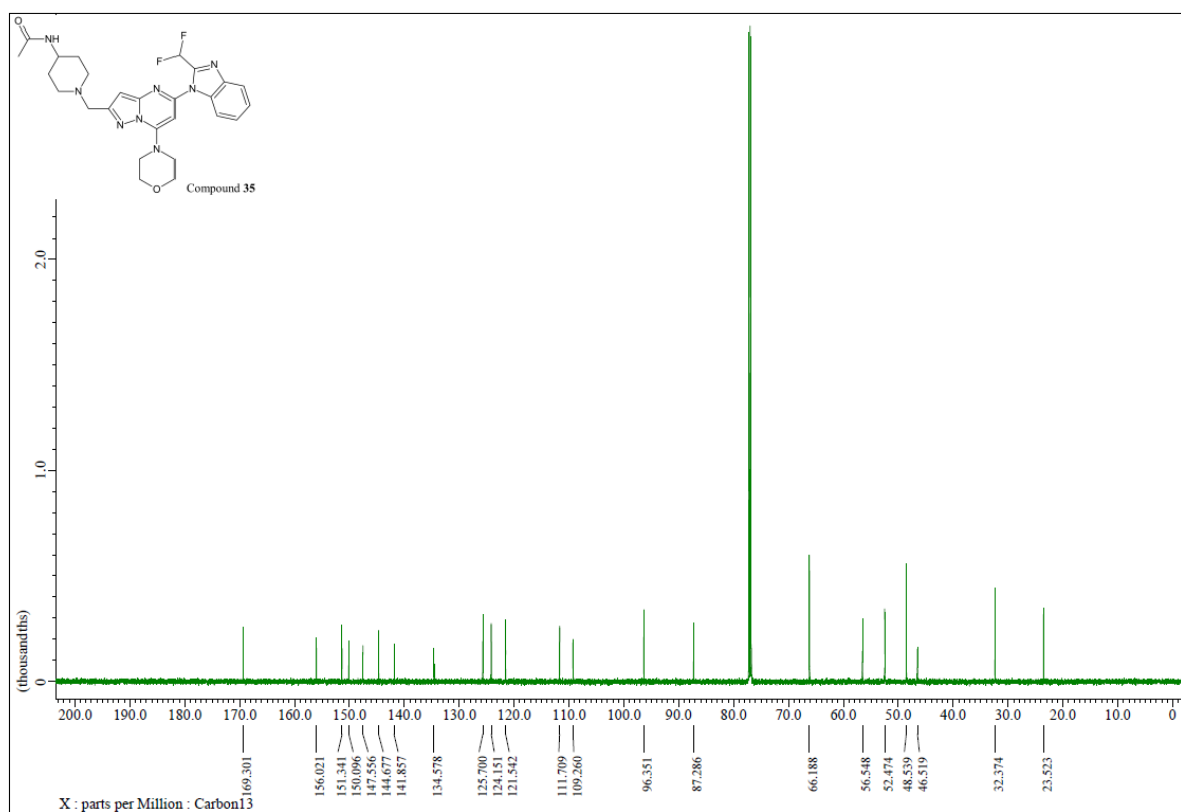
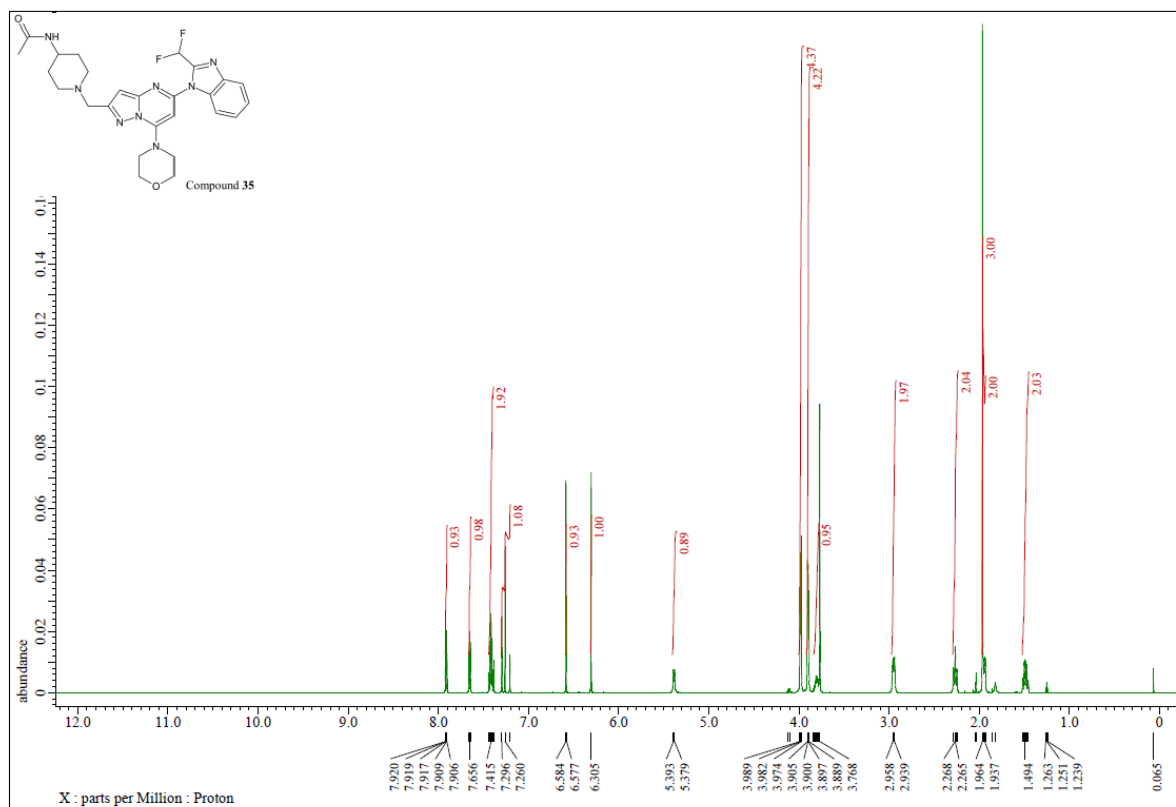


MS Spectrum Peak List

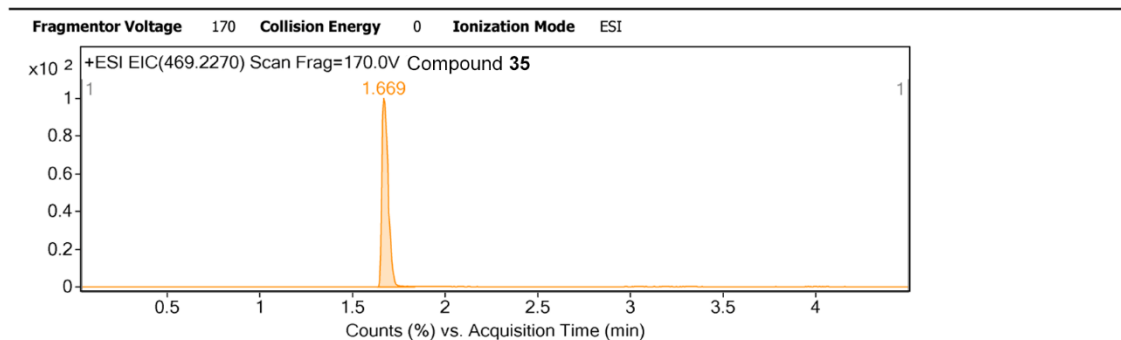
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
242.61746	2	100150.59	C24H27F2N7O2	(M+2H)+2	
243.1188	2	28050.54	C24H27F2N7O2	(M+2H)+2	
243.62017	2	4474.7	C24H27F2N7O2	(M+2H)+2	
484.22723	1	1327642.88	C24H27F2N7O2	(M+H)+	
485.22988	1	339432.13	C24H27F2N7O2	(M+H)+	
486.23245	1	46026.59	C24H27F2N7O2	(M+H)+	
242.61746	2	100150.59	C24H27F2N7O2	(M+2H)+2	1.93
243.1188	2	28050.54	C24H27F2N7O2	(M+2H)+2	1.6
243.62017	2	4474.7	C24H27F2N7O2	(M+2H)+2	1.74
484.22723	1	1327642.88	C24H27F2N7O2	(M+H)+	1.09
484.22723		1328394.5			
485.22988	1	339432.13	C24H27F2N7O2	(M+H)+	0.7
486.23245	1	46026.59	C24H27F2N7O2	(M+H)+	0.48

--- End Of Report ---

Compound 35



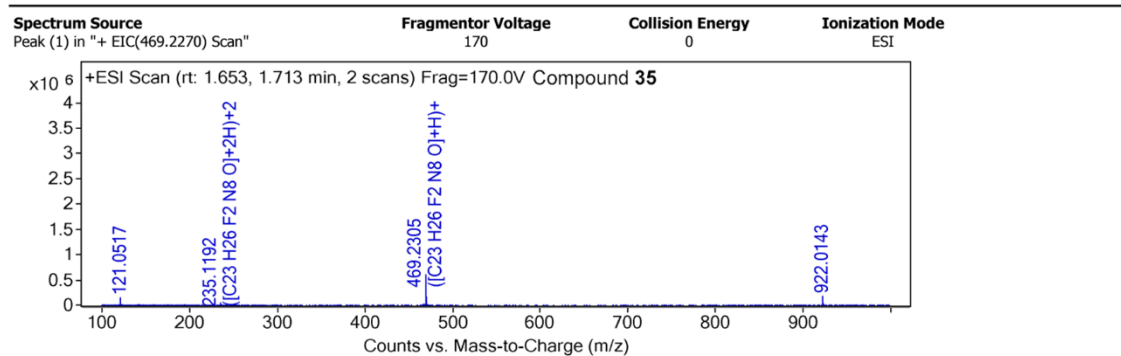
Compound 35



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.634	1.669	1.835	3781886.04	9105302.42	100

Spectra

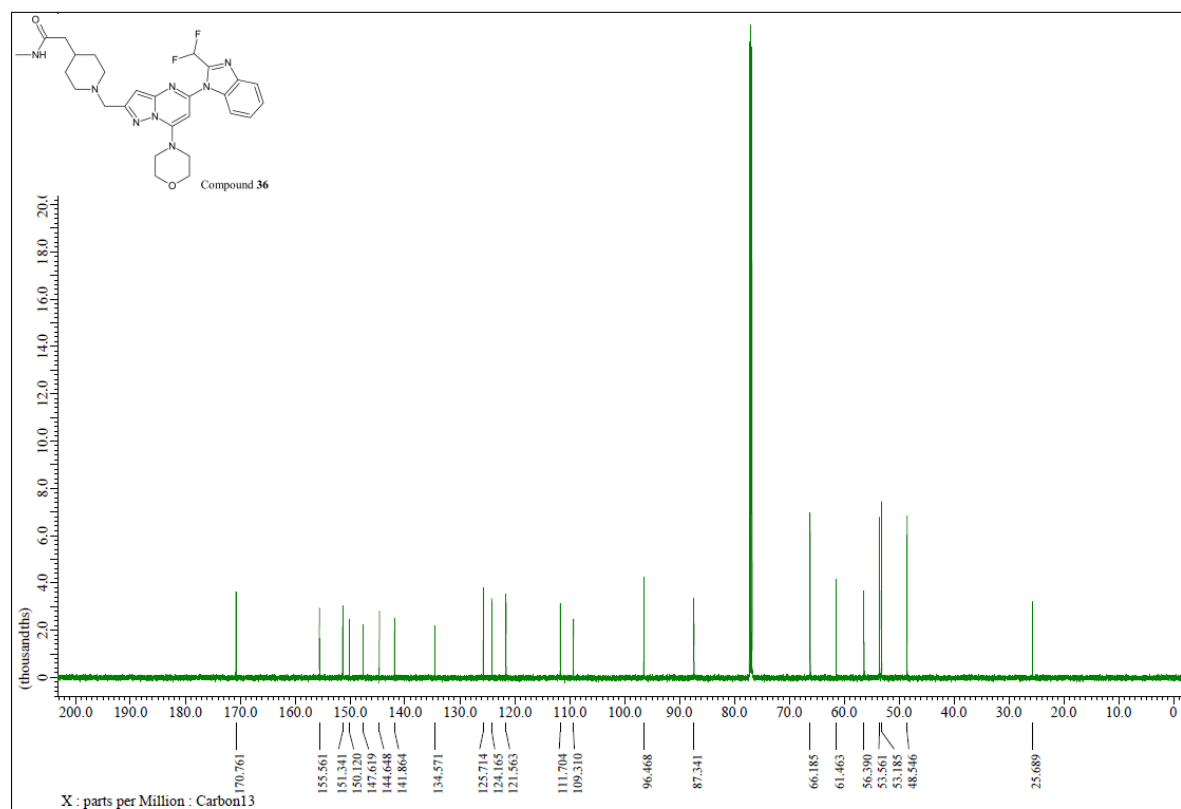
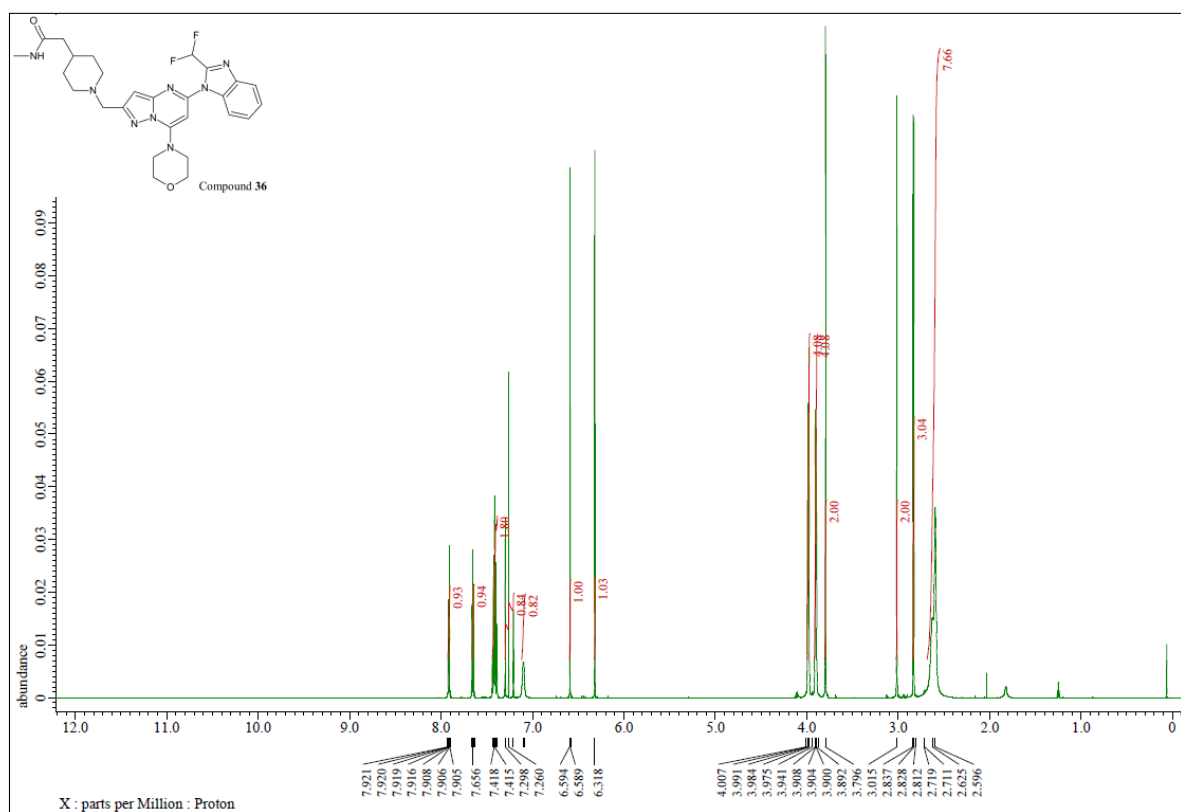


Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
469.2305	1	601001.5	Compound 35	C23 H26 F2 N8 O	(M+H)+	97.11	2

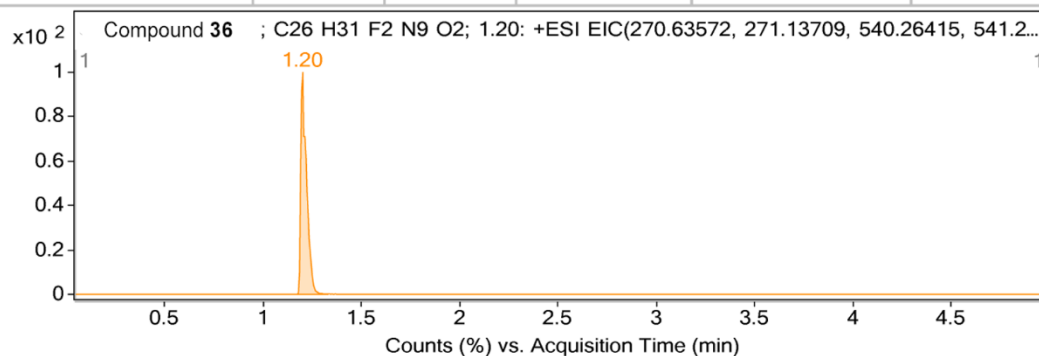
--- End Of Report ---

Compound 36

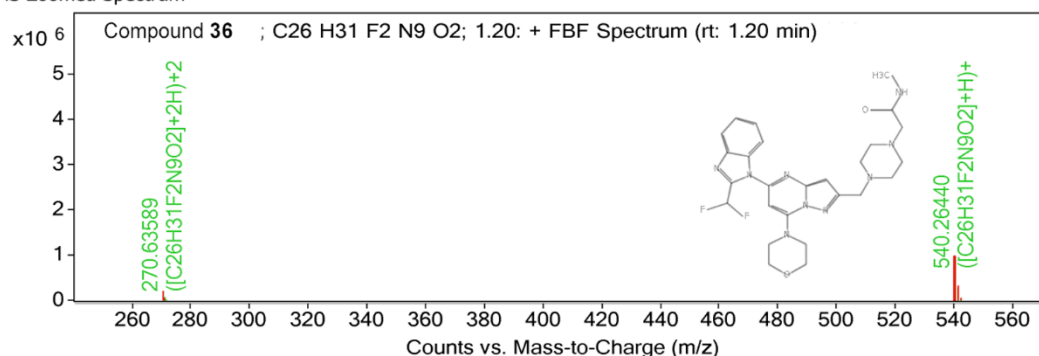


Compound 36

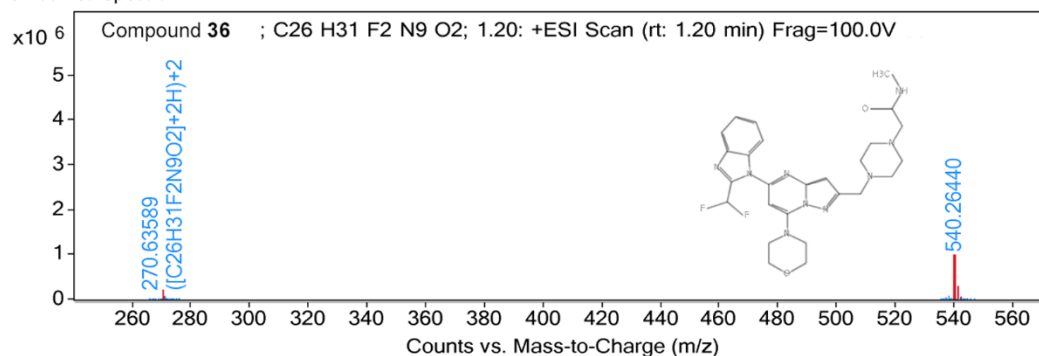
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 36	270.63589	1.2	539.2572	C26 H31 F2 N9 O2	539.25688	0.59	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

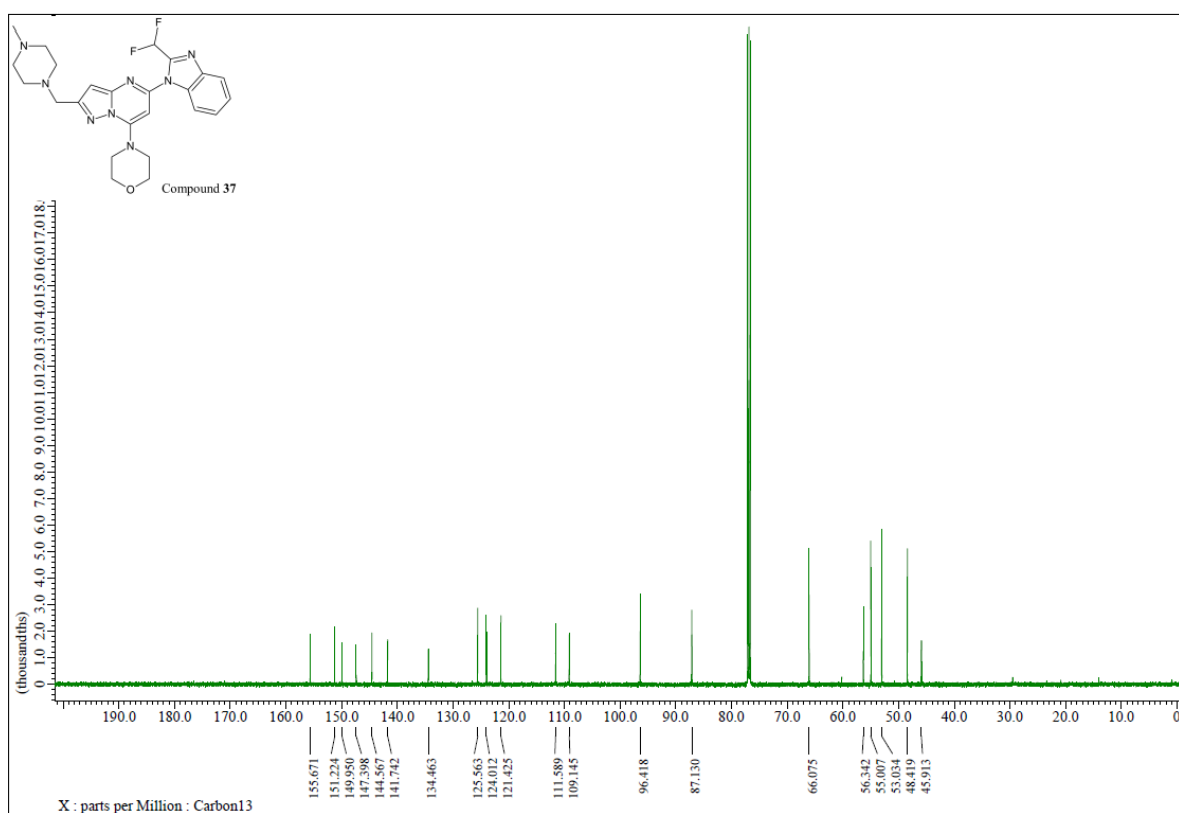
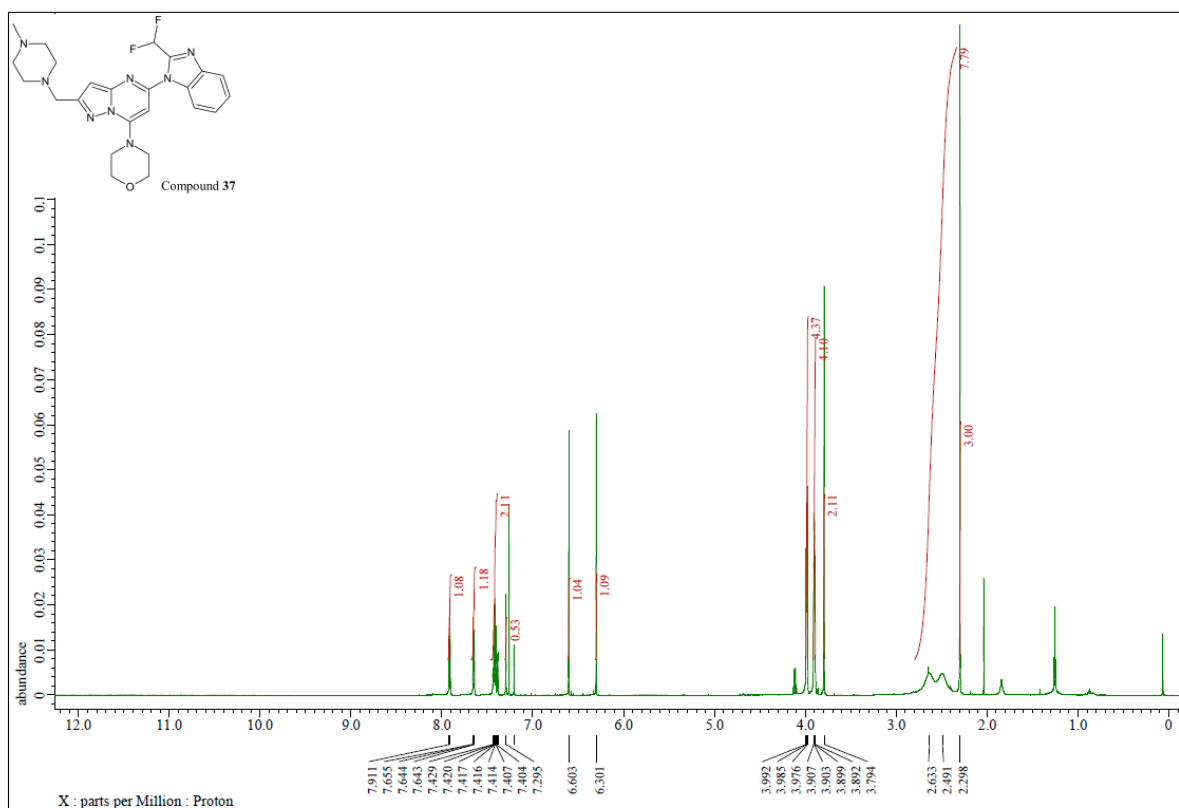


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
270.63589	2	194345.84	C26H31F2N9O2	(M+2H)+2	
271.13742	2	59180.25	C26H31F2N9O2	(M+2H)+2	
271.63847	2	11750.46	C26H31F2N9O2	(M+2H)+2	
540.2644	1	976966.31	C26H31F2N9O2	(M+H)+	
541.26743	1	275591.88	C26H31F2N9O2	(M+H)+	
542.2695	1	40836.08	C26H31F2N9O2	(M+H)+	
270.63589	2	194345.84	C26H31F2N9O2	(M+2H)+2	0.64
271.13742	2	59180.25	C26H31F2N9O2	(M+2H)+2	1.23
271.63847	2	11750.46	C26H31F2N9O2	(M+2H)+2	0.28
540.2644	1	976966.31	C26H31F2N9O2	(M+H)+	0.46
540.2644		977749.31			
541.26743	1	275591.88	C26H31F2N9O2	(M+H)+	1
542.2695	1	40836.08	C26H31F2N9O2	(M+H)+	-0.02

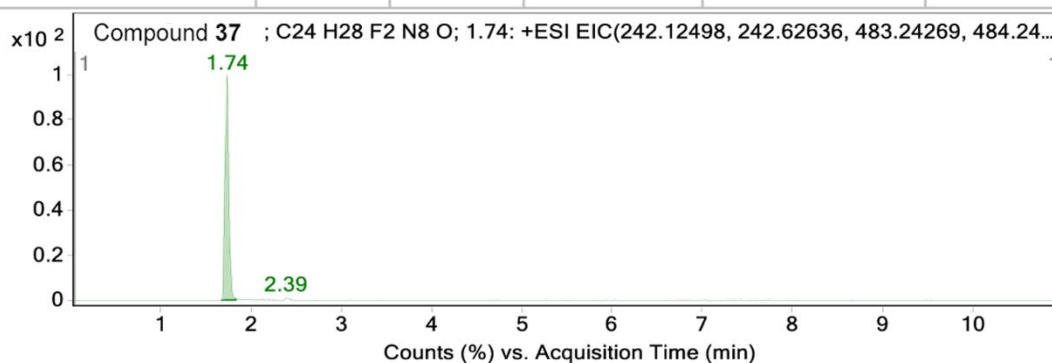
--- End Of Report ---

Compound 37

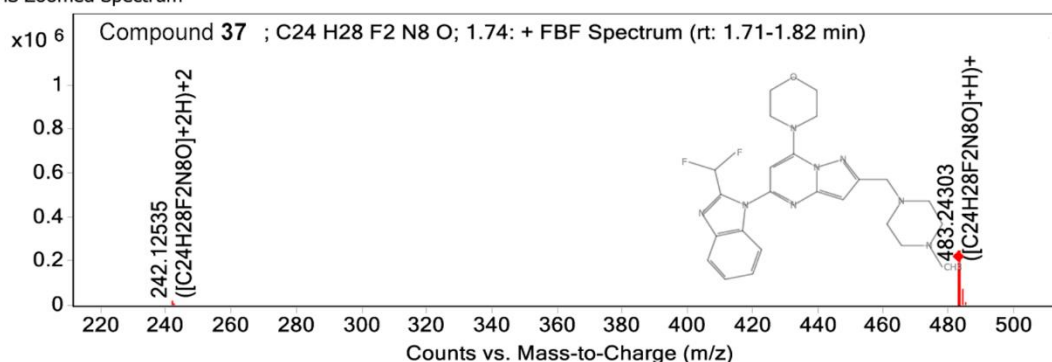


Compound 37

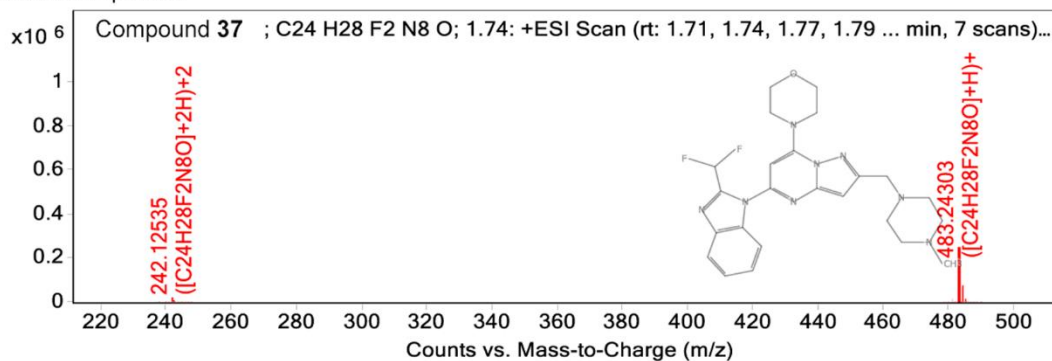
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 37	242.12535	1.74	482.23576	C ₂₄ H ₂₈ F ₂ N ₈ O	482.23541	0.72	Find by Formula



MS Zoomed Spectrum



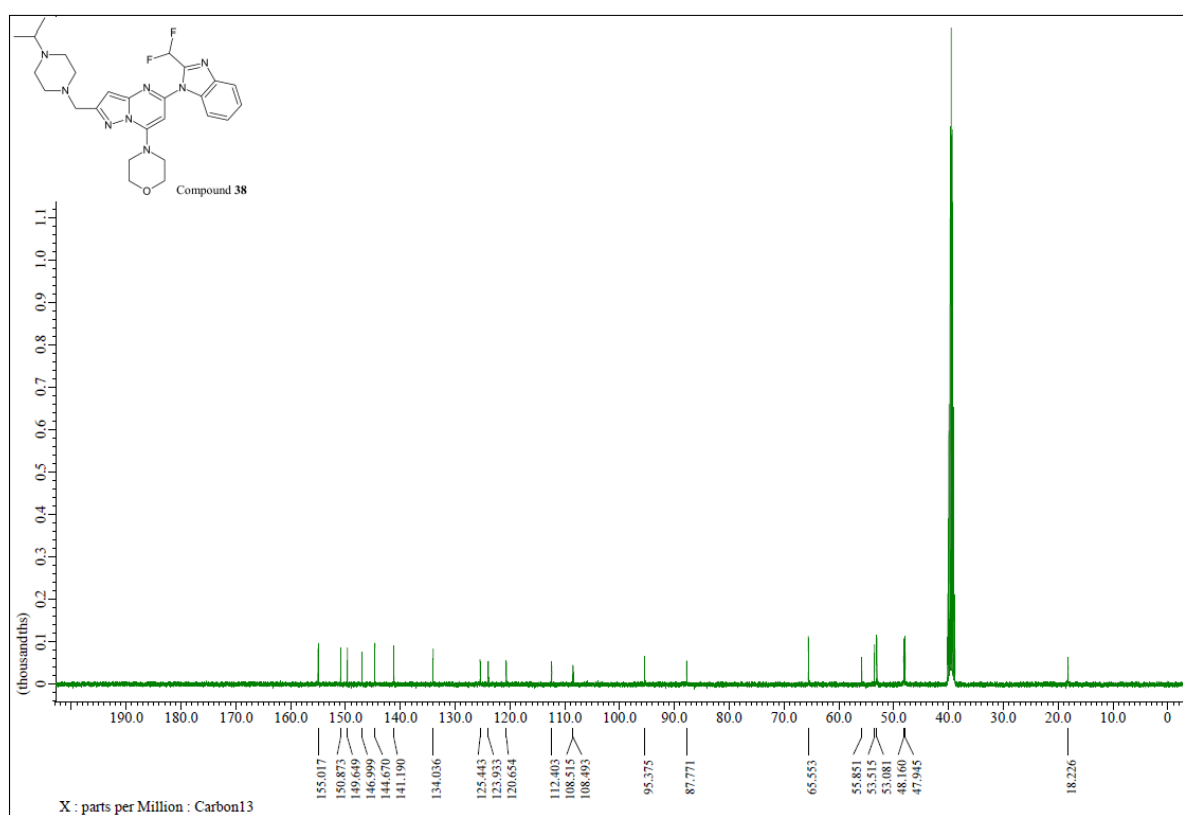
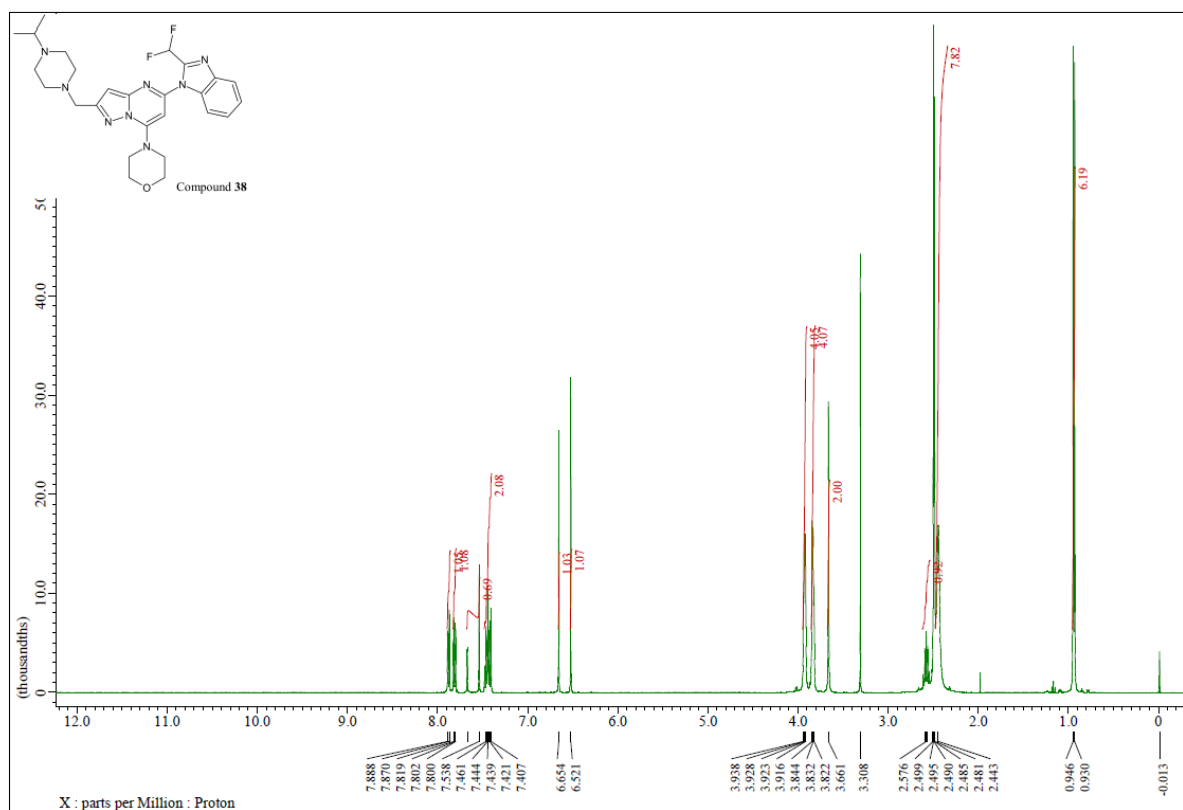
MS Zoomed Spectrum



MS Spectrum Peak List

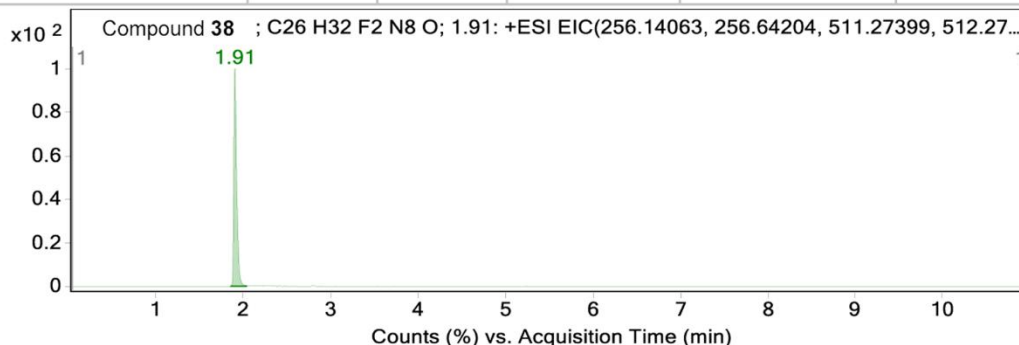
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
242.12535	2	16177.19	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	
242.62664	2	4814.55	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	
243.12655	2	892.06	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	
483.24303	1	242894.67	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	
484.24583	1	62366.9	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	
485.24787	1	8281.58	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	
242.12535	2	16177.19	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	1.5
242.62664	2	4814.55	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	1.15
243.12655	2	892.06	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+2H)+2	-4.71
483.24303	1	242894.67	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	0.7
483.24303		242894.67			
484.24583	1	62366.9	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	0.79
485.24787	1	8281.58	C ₂₄ H ₂₈ F ₂ N ₈ O	(M+H)+	-0.51

Compound 38

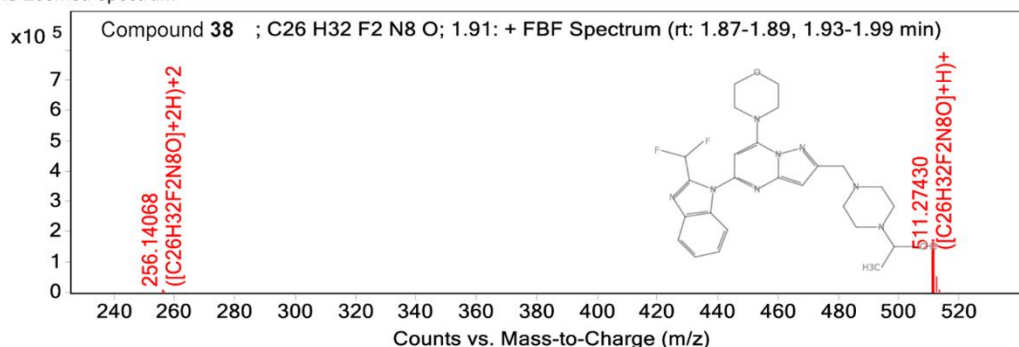


Compound 38

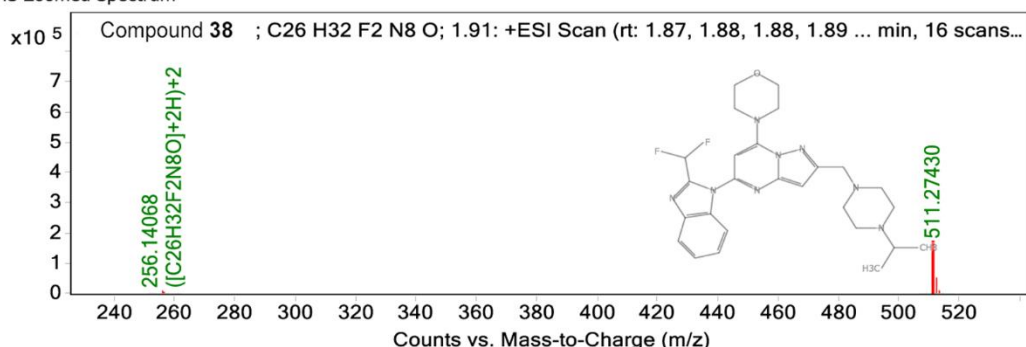
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorith
Compound 38	511.2743	1.91	510.26697	C26 H32 F2 N8 O	510.26671	0.51	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

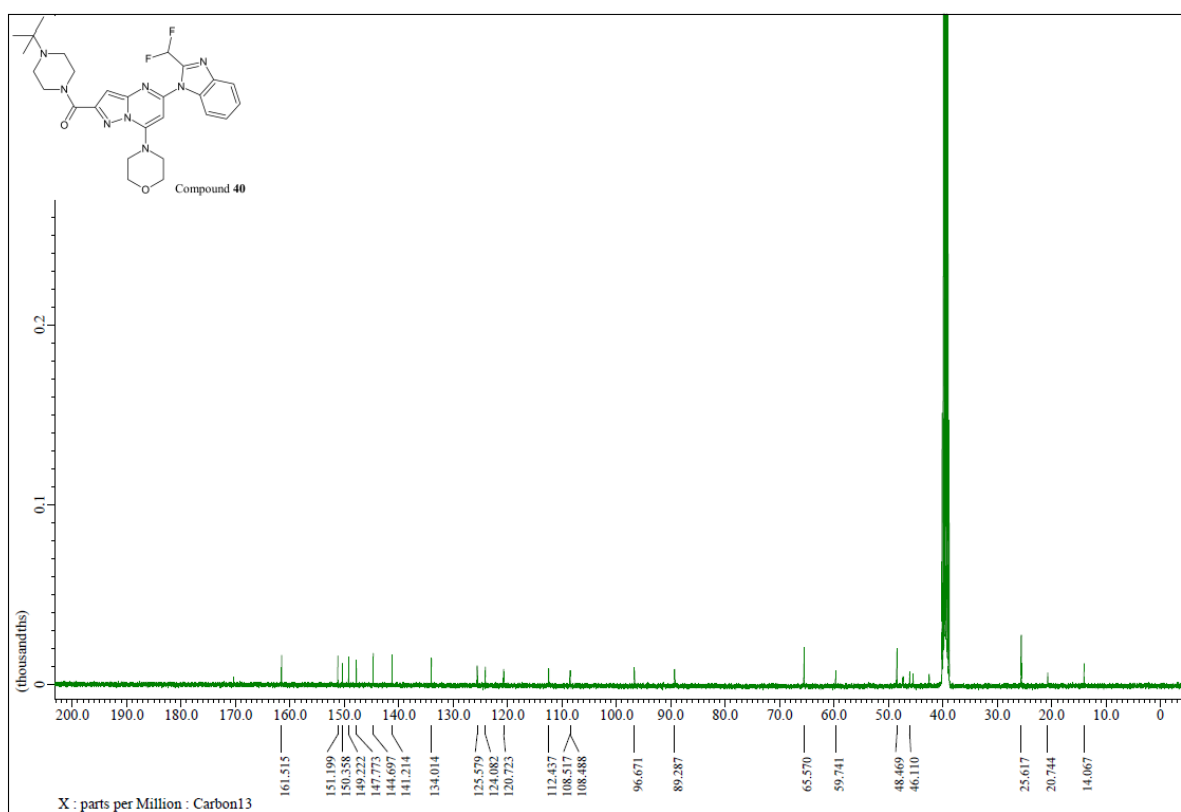
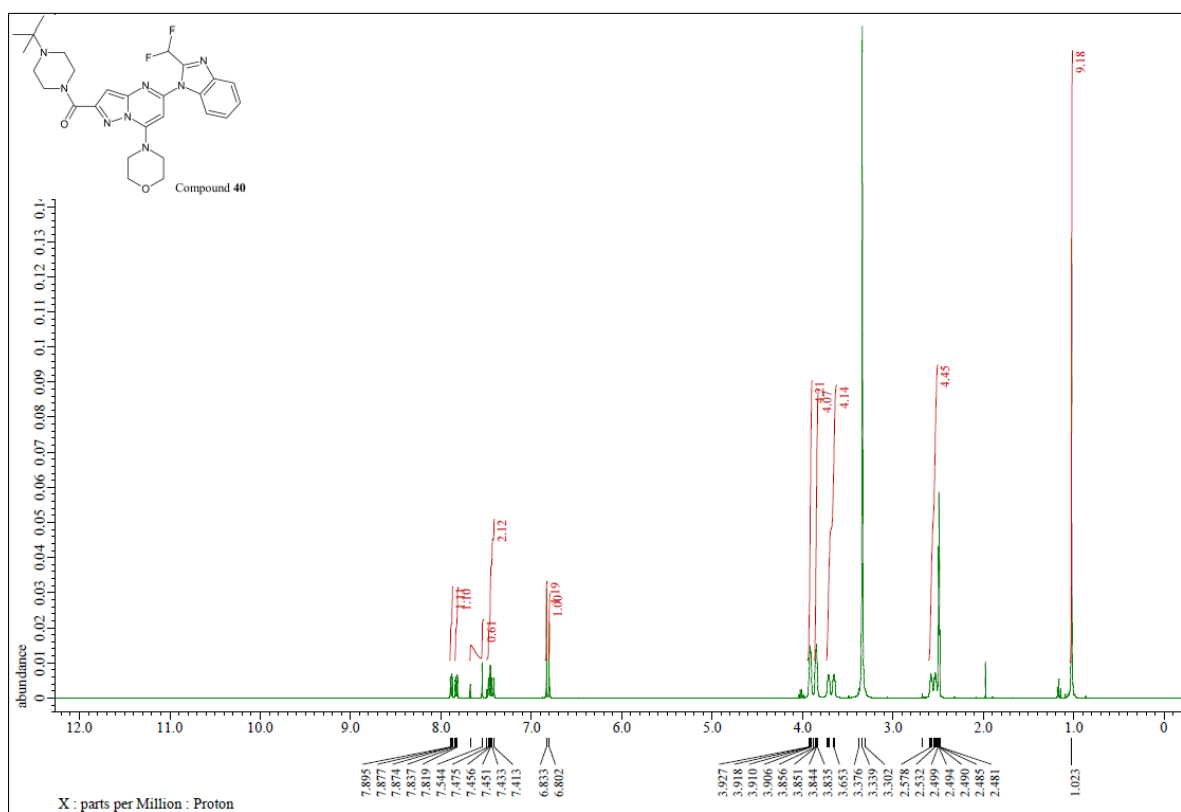


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
256.14068	2	7563.88	C26H32F2N8O	(M+2H)+2	
256.64215	2	2152.23	C26H32F2N8O	(M+2H)+2	
257.14261	2	324.73	C26H32F2N8O	(M+2H)+2	
511.2743	1	170137	C26H32F2N8O	(M+H)+	
512.27694	1	48697.73	C26H32F2N8O	(M+H)+	
513.27954	1	7568.92	C26H32F2N8O	(M+H)+	
256.14068	2	7563.88	C26H32F2N8O	(M+2H)+2	0.17
256.64215	2	2152.23	C26H32F2N8O	(M+2H)+2	0.44
257.14261	2	324.73	C26H32F2N8O	(M+2H)+2	-3.07
511.2743		170137			0.61
511.2743	1	170137	C26H32F2N8O	(M+H)+	0.61
512.27694	1	48697.73	C26H32F2N8O	(M+H)+	0.28
513.27954	1	7568.92	C26H32F2N8O	(M+H)+	0.03

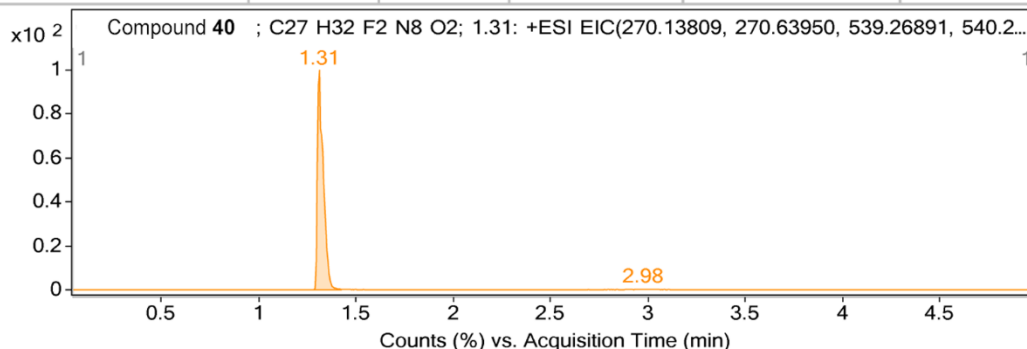
--- End Of Report ---

Compound 40

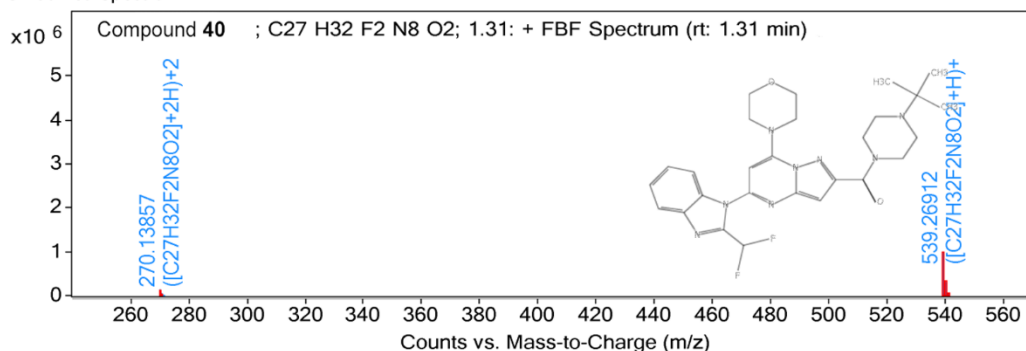


Compound 40

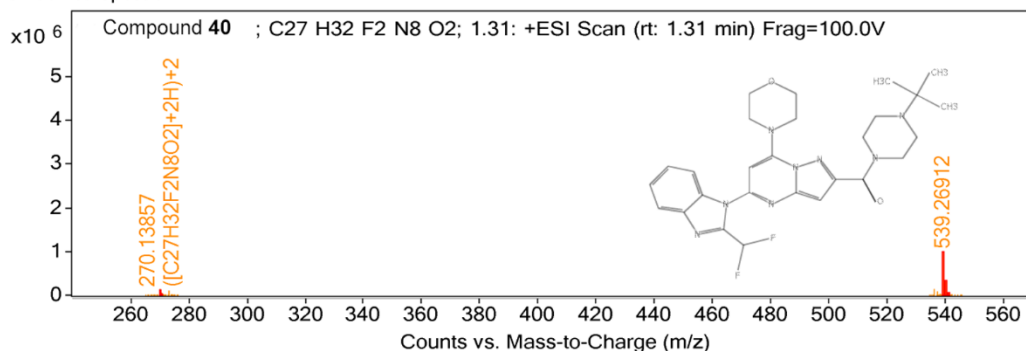
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaorit
Compound 40	539.26912	1.31	538.26195	C27 H32 F2 N8 O2	538.26163	0.6	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

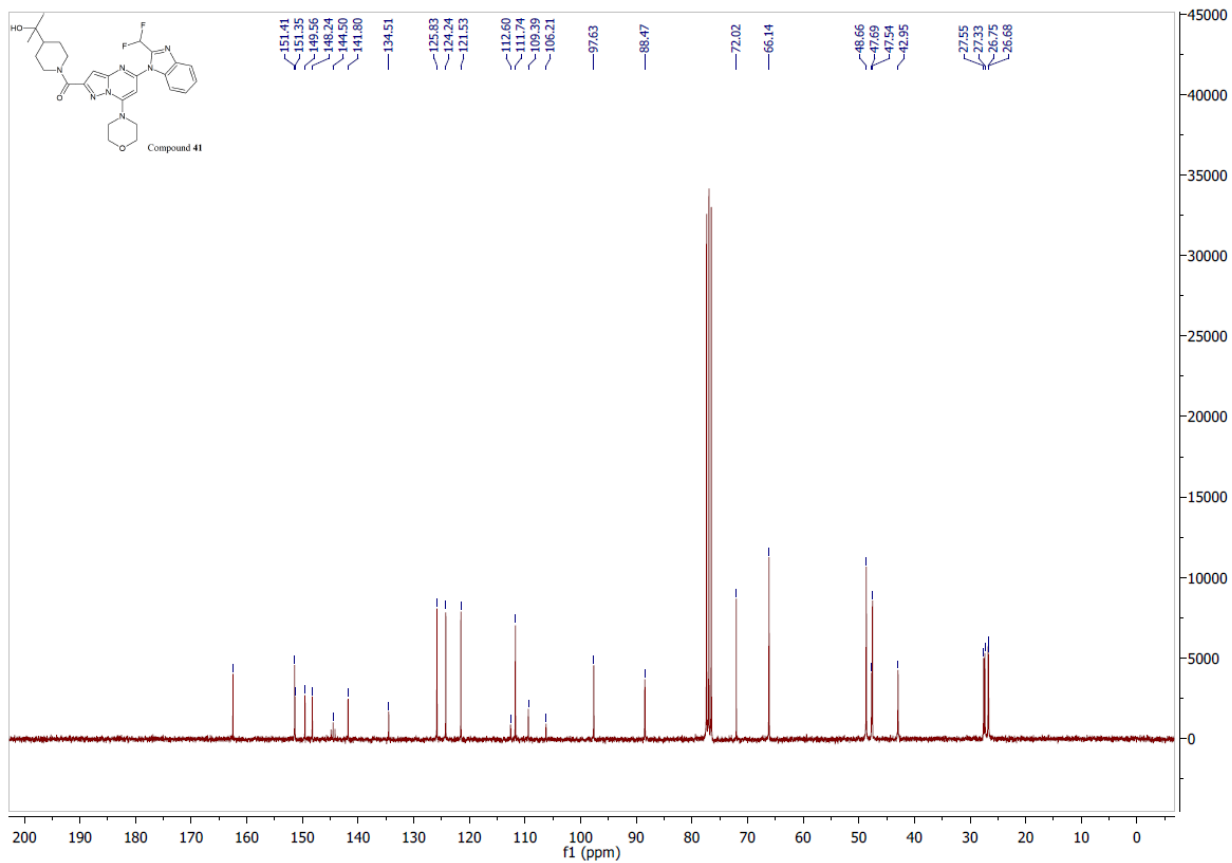
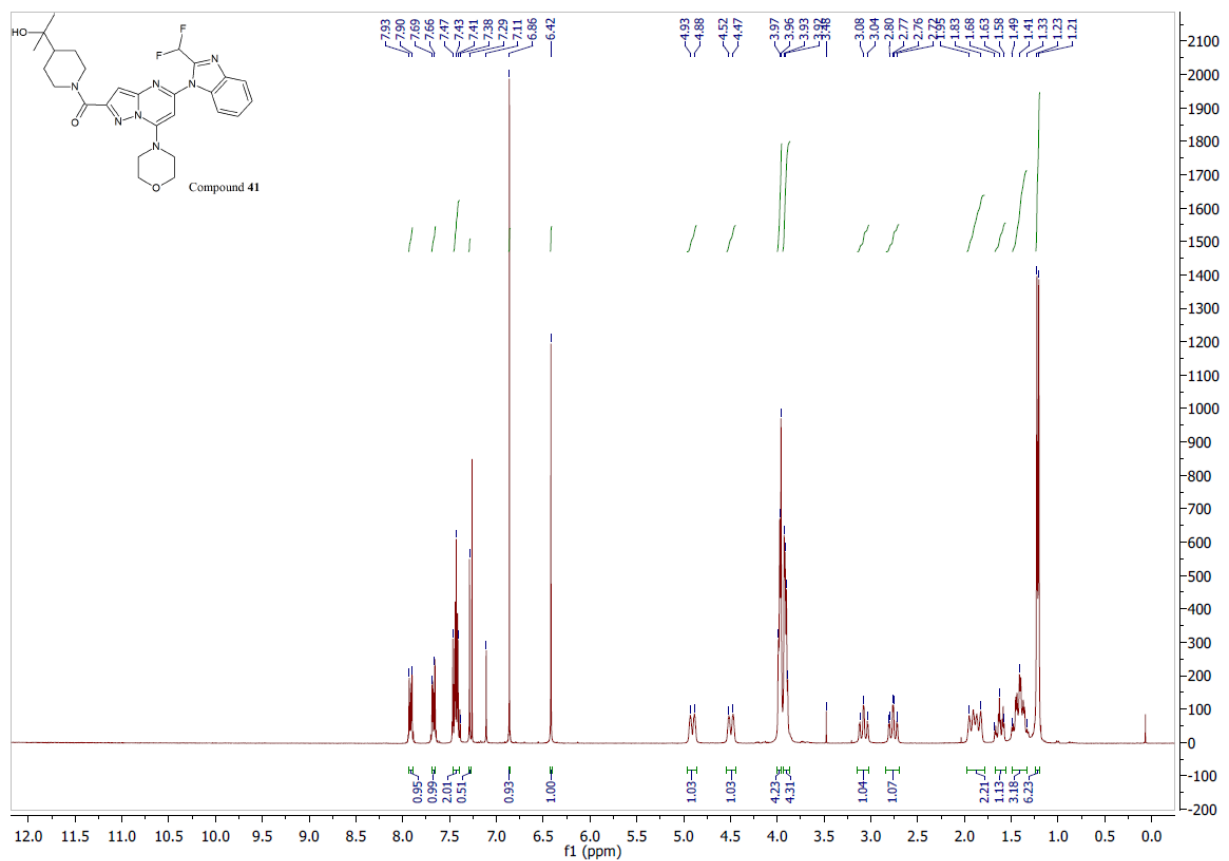


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
270.13857	2	125455.36	C27H32F2N8O2	(M+2H)+2	
270.63974	2	46195.77	C27H32F2N8O2	(M+2H)+2	
271.14284	2	8525.27	C27H32F2N8O2	(M+2H)+2	
271.64284	2	714.39	C27H32F2N8O2	(M+2H)+2	
539.26912	1	989648.63	C27H32F2N8O2	(M+H)+	
540.27212	1	296316.03	C27H32F2N8O2	(M+H)+	
541.27406	1	46140.58	C27H32F2N8O2	(M+H)+	
270.13857	2	125455.36	C27H32F2N8O2	(M+2H)+2	1.76
270.63974	2	46195.77	C27H32F2N8O2	(M+2H)+2	0.86
271.14284	2	8525.27	C27H32F2N8O2	(M+2H)+2	7.33
271.64284	2	714.39	C27H32F2N8O2	(M+2H)+2	2.5
539.26912	1	989648.63	C27H32F2N8O2	(M+H)+	0.39
539.26912		991037.31			
540.27212	1	296316.03	C27H32F2N8O2	(M+H)+	0.73
541.27406	1	46140.58	C27H32F2N8O2	(M+H)+	-0.68

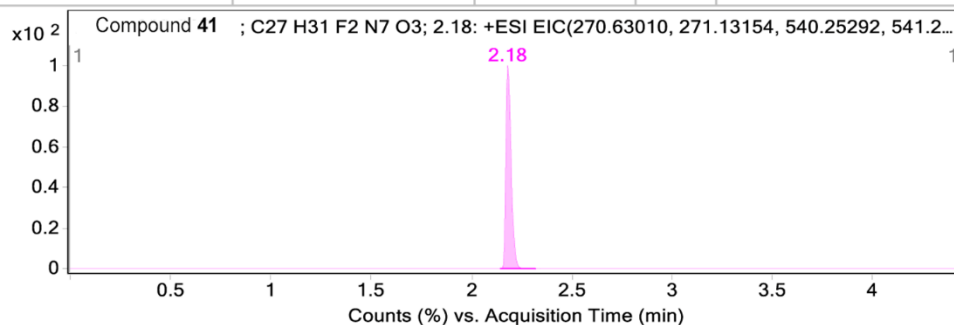
--- End Of Report ---

Compound 41

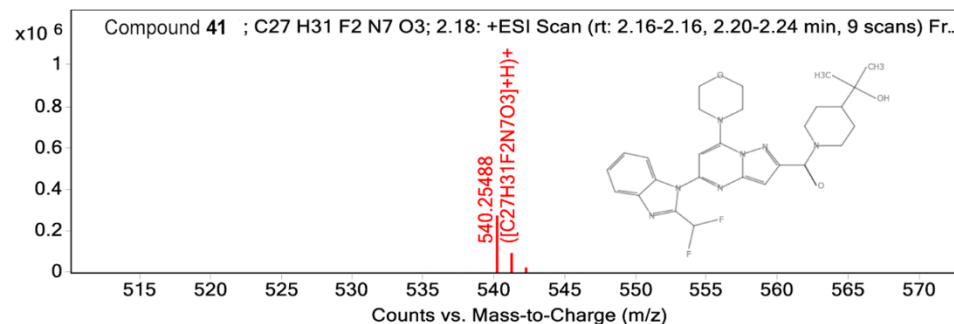
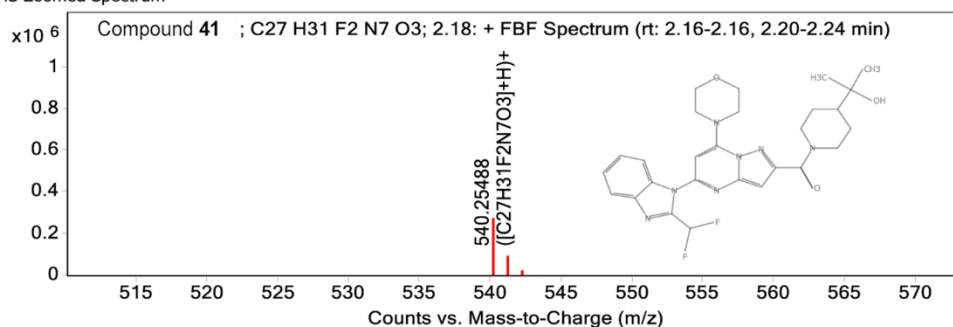


Compound 41

Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 41	Compound 41	540.25488	2.18	Find by Formula	539.24756



MS Zoomed Spectrum

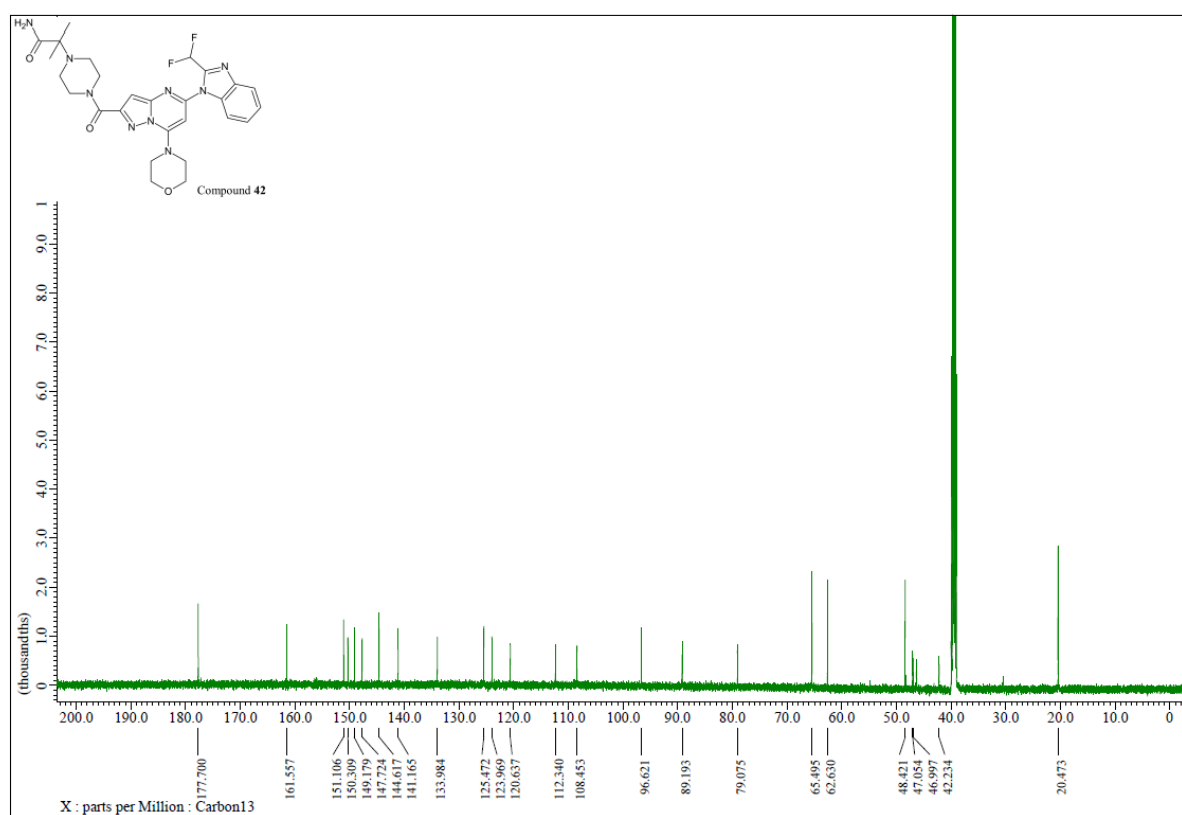
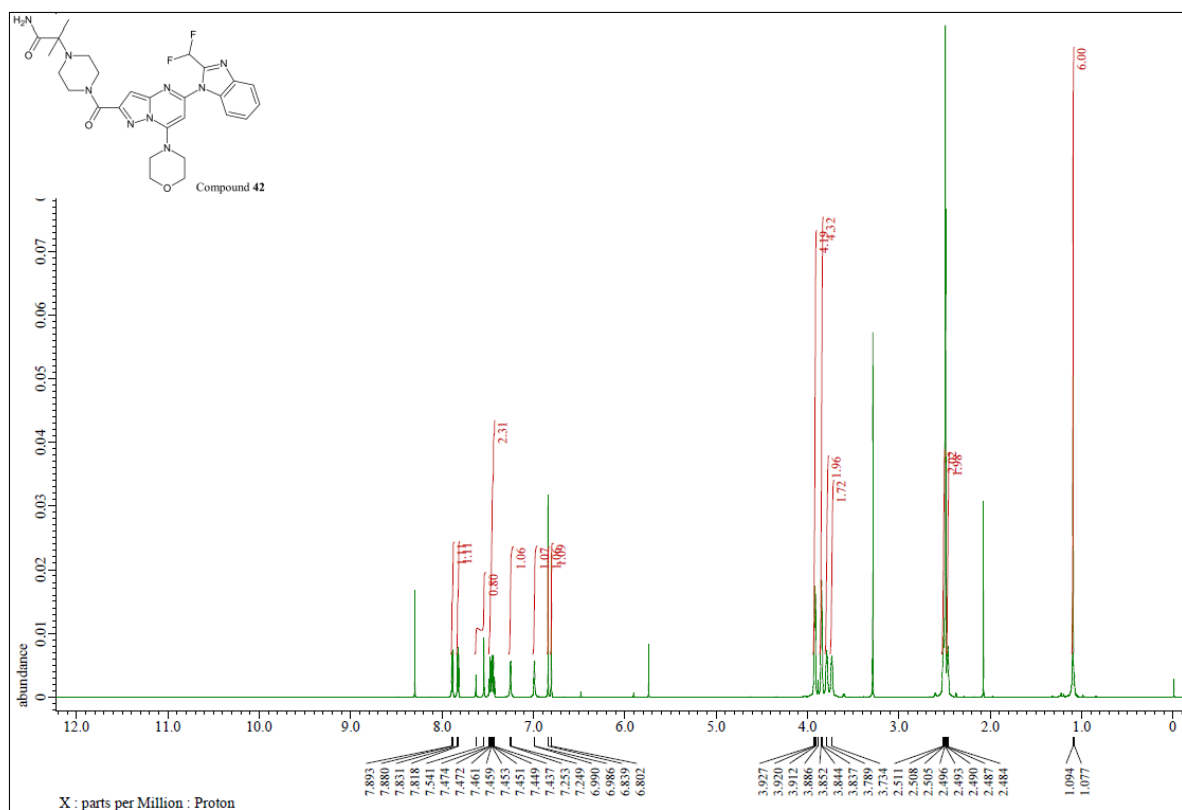


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
540.25488	540.25292	3.63	1	270345.84	C ₂₇ H ₃₁ F ₂ N ₇ O ₃	(M+H) ⁺
541.25773	541.25581	3.55	1	82090.26	C ₂₇ H ₃₁ F ₂ N ₇ O ₃	(M+H) ⁺
542.25958	542.25852	1.95	1	12735.37	C ₂₇ H ₃₁ F ₂ N ₇ O ₃	(M+H) ⁺
543.26188	543.26112	1.4	1	1682.81	C ₂₇ H ₃₁ F ₂ N ₇ O ₃	(M+H) ⁺

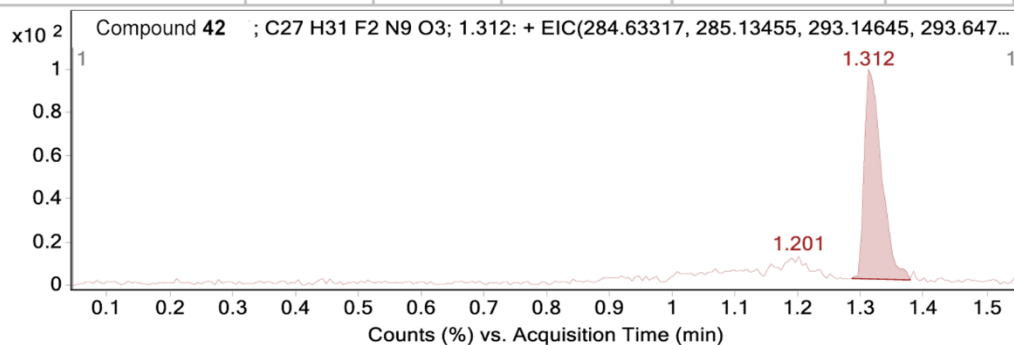
--- End Of Report ---

Compound 42

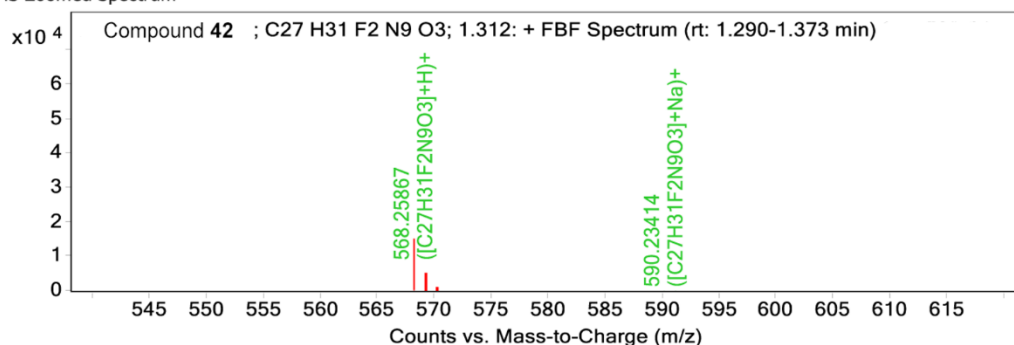


Compound 42

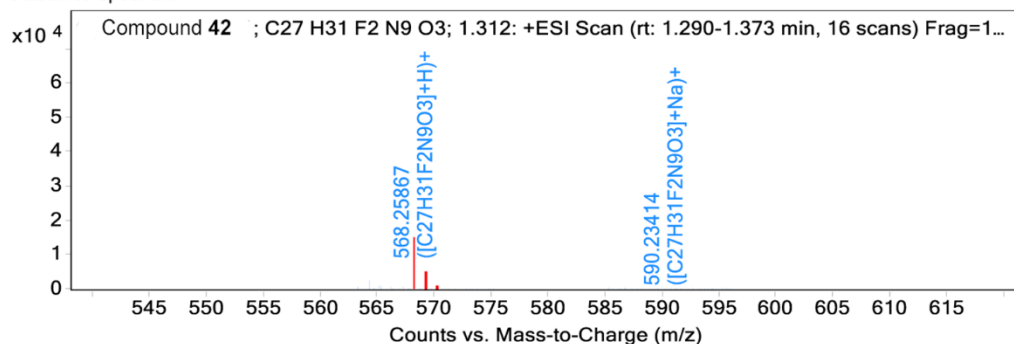
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 42	568.25867	1.312	567.25125	C27 H31 F2 N9 O3	567.25179	-0.95	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

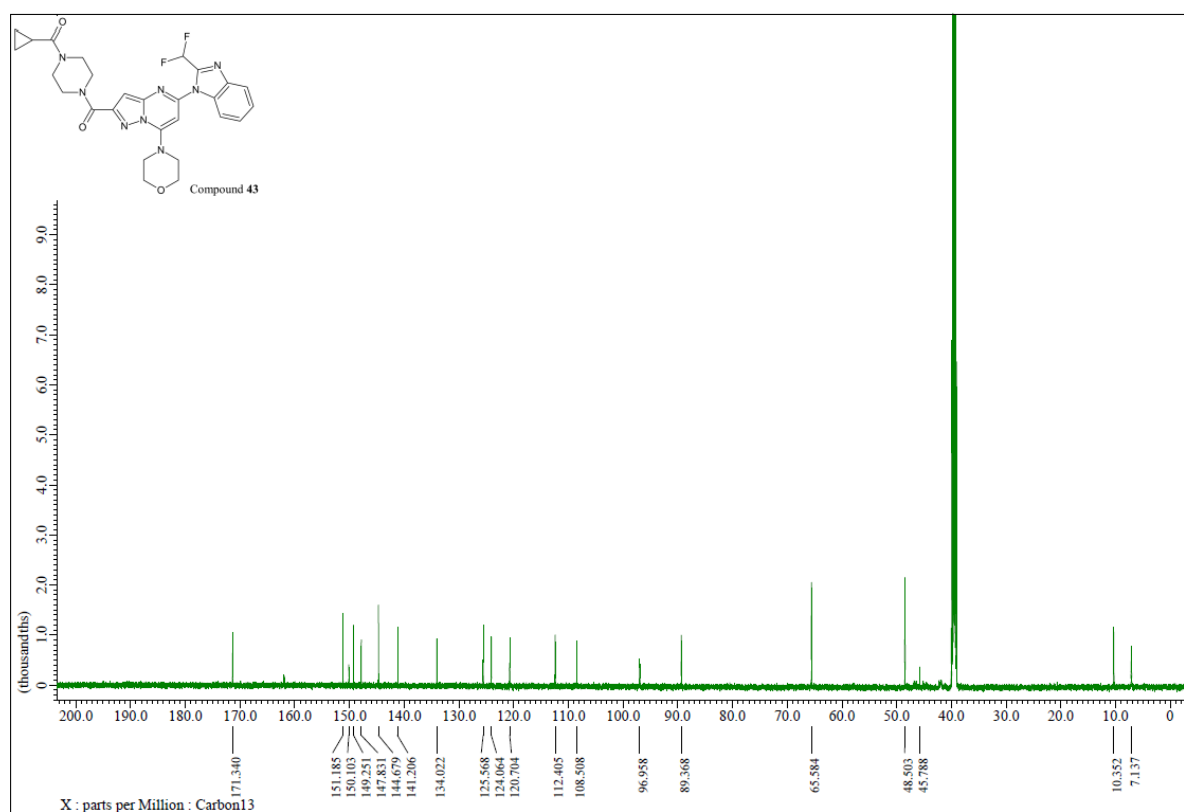
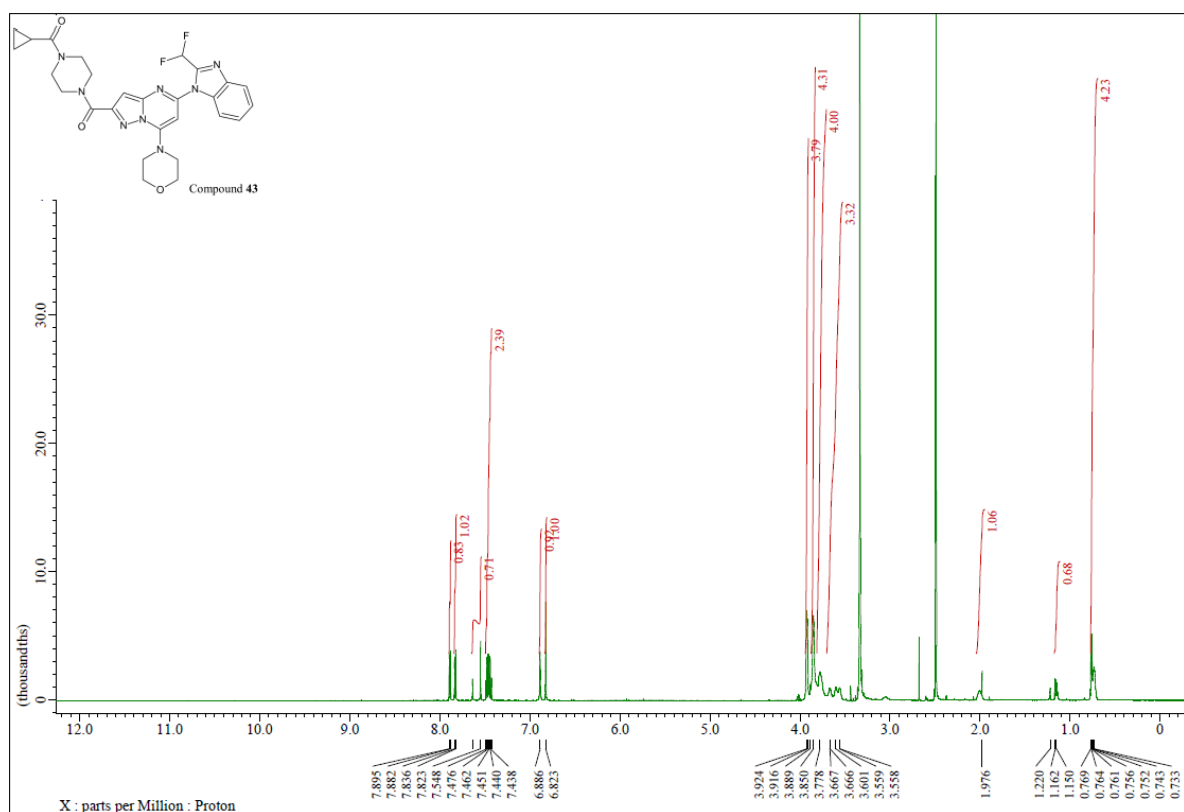


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
568.25867	1	14840.44	C27H31F2N9O3	(M+H)+	
569.26124	1	4302.48	C27H31F2N9O3	(M+H)+	
570.26212	1	858.69	C27H31F2N9O3	(M+H)+	
590.23414	1	59.04	C27H31F2N9O3	(M+Na)+	
591.24508	1	29.53	C27H31F2N9O3	(M+Na)+	
568.25867	1	14840.44	C27H31F2N9O3	(M+H)+	-0.7
569.26124	1	4302.48	C27H31F2N9O3	(M+H)+	-1.03
570.26212	1	858.69	C27H31F2N9O3	(M+H)+	-4.07
590.23414	1	59.04	C27H31F2N9O3	(M+Na)+	-11.65
591.24508	1	29.53	C27H31F2N9O3	(M+Na)+	2.21

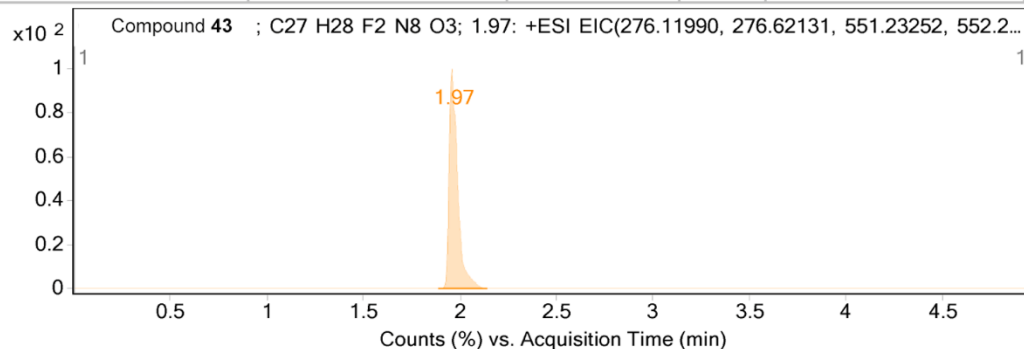
--- End Of Report ---

Compound 43

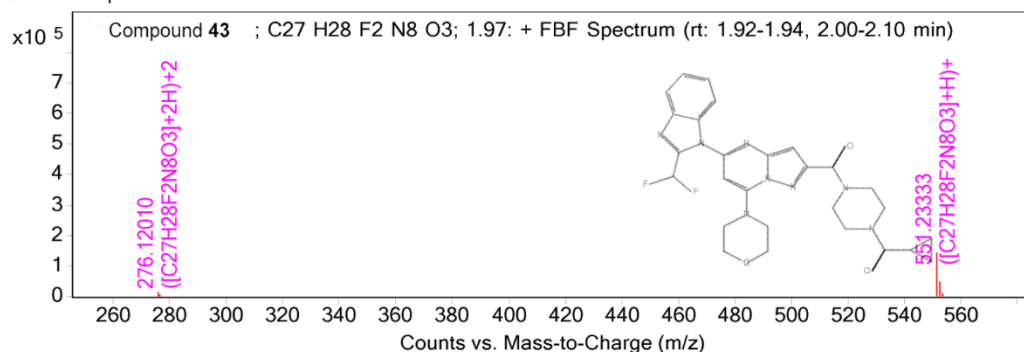


Compound 43

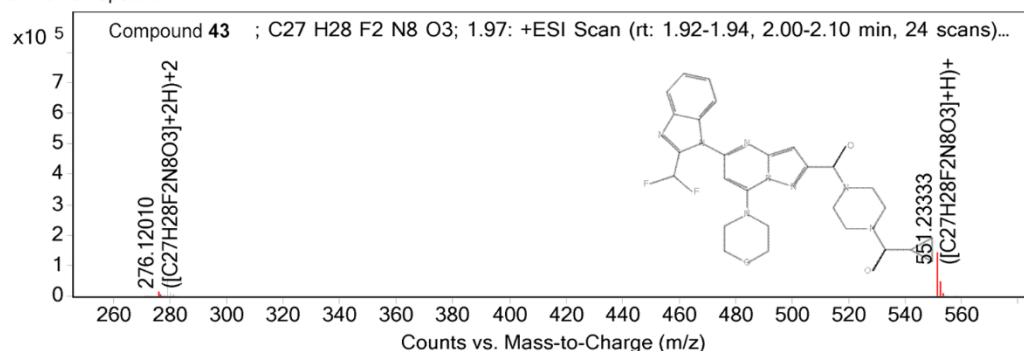
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 43	Compound 43	276.1201	1.97	Find by Formula	550.22601



MS Zoomed Spectrum



MS Zoomed Spectrum

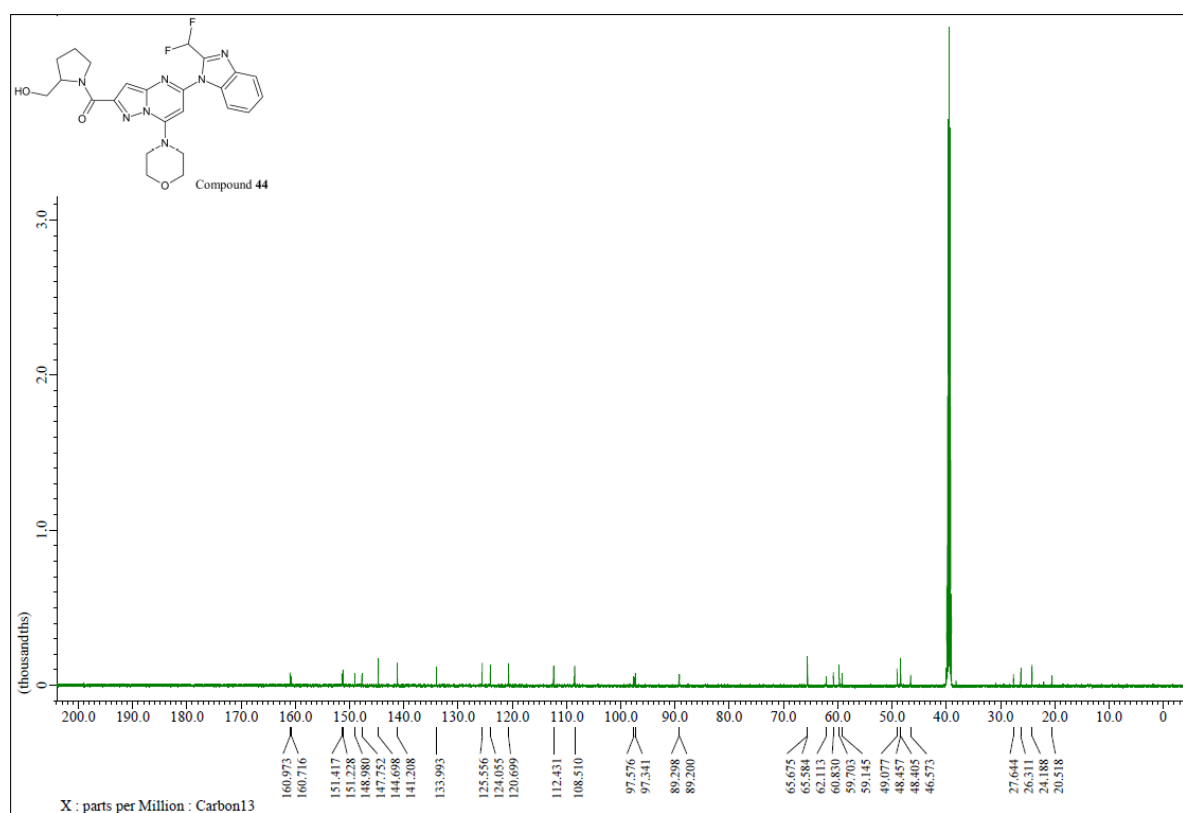
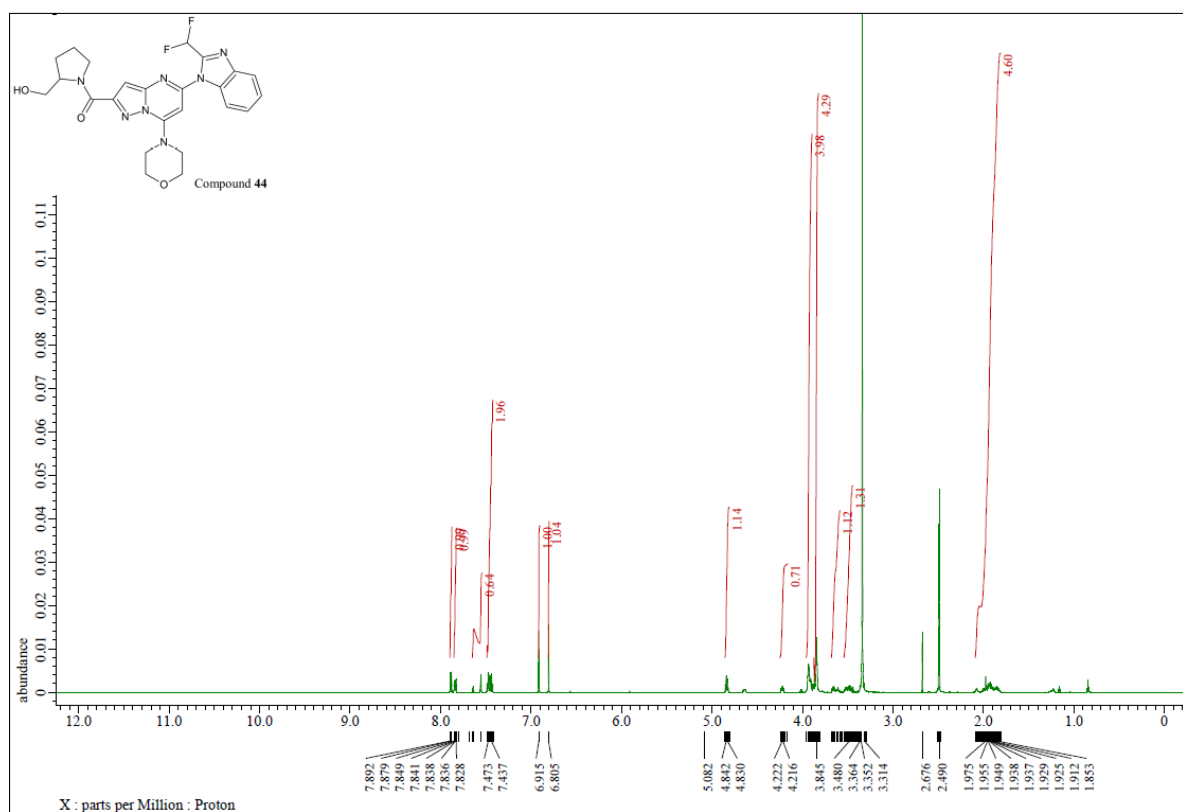


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
276.1201	276.1199	0.75	2	12256.77	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+2H)+2
276.6216	276.62131	1.04	2	3979.86	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+2H)+2
277.12341	277.12264	2.79	2	963.82	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+2H)+2
277.62135	277.62391	-9.23	2	52.08	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+2H)+2
551.23333	551.23252	1.47	1	142347.36	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+H)+
552.23614	552.23534	1.45	1	44714.86	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+H)+
553.23847	553.23799	0.85	1	7254.93	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+H)+
554.24149	554.24055	1.71	1	890.85	C ₂₇ H ₂₈ F ₂ N ₈ O ₃	(M+H)+

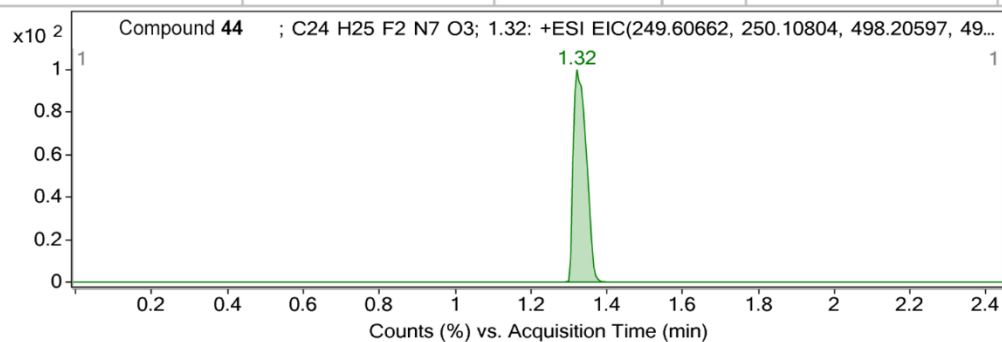
--- End Of Report ---

Compound 44

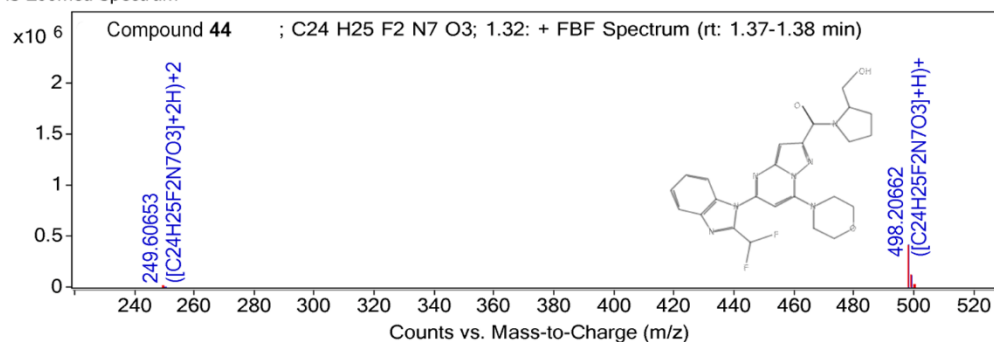


Compound 44

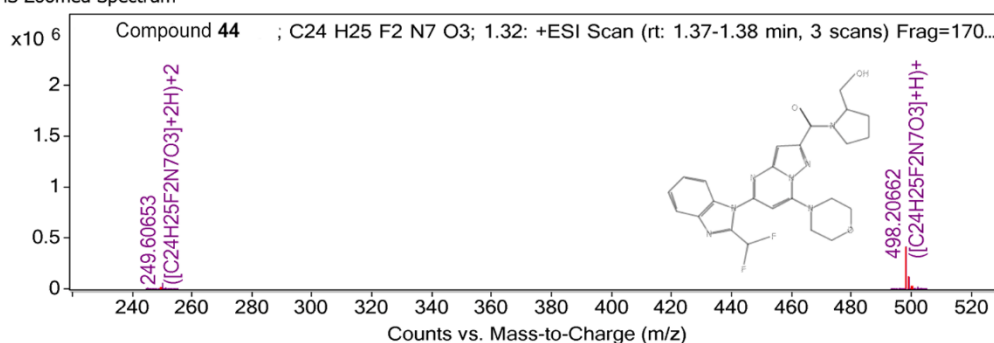
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 44	Compound 44	498.20662	1.32	Find by Formula	497.19931



MS Zoomed Spectrum



MS Zoomed Spectrum

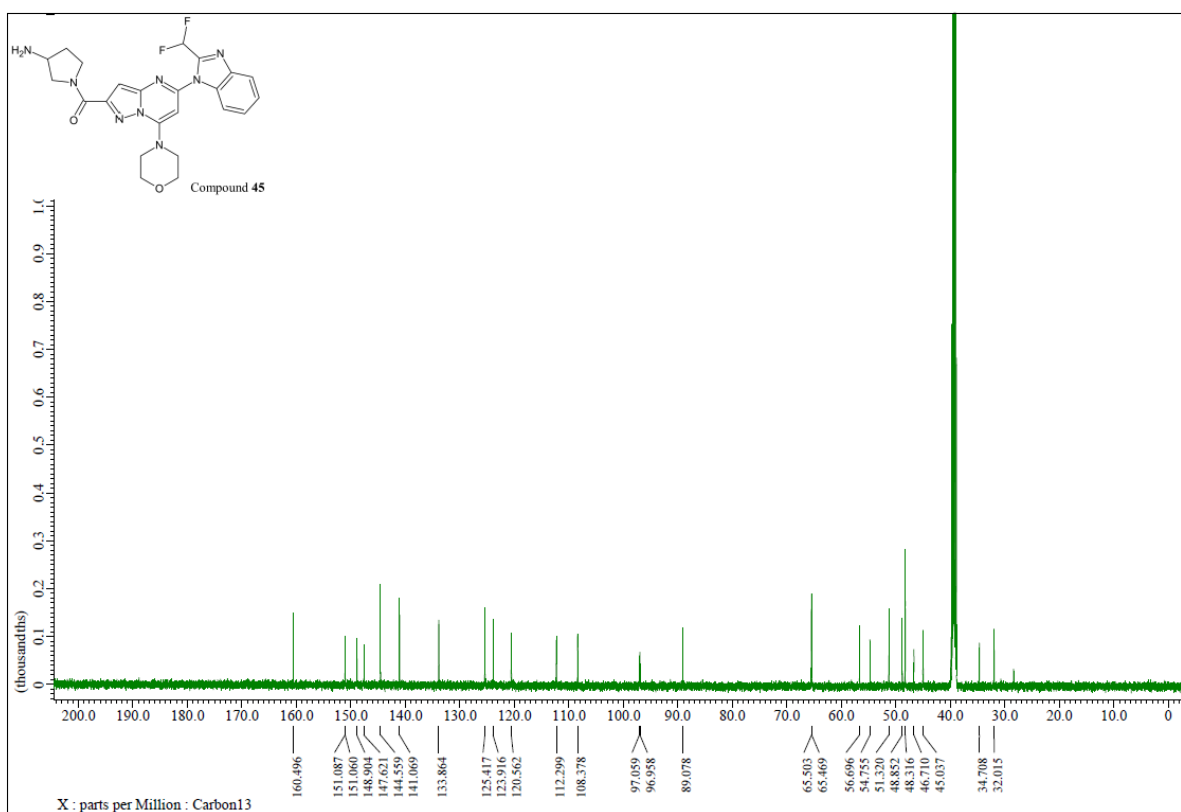
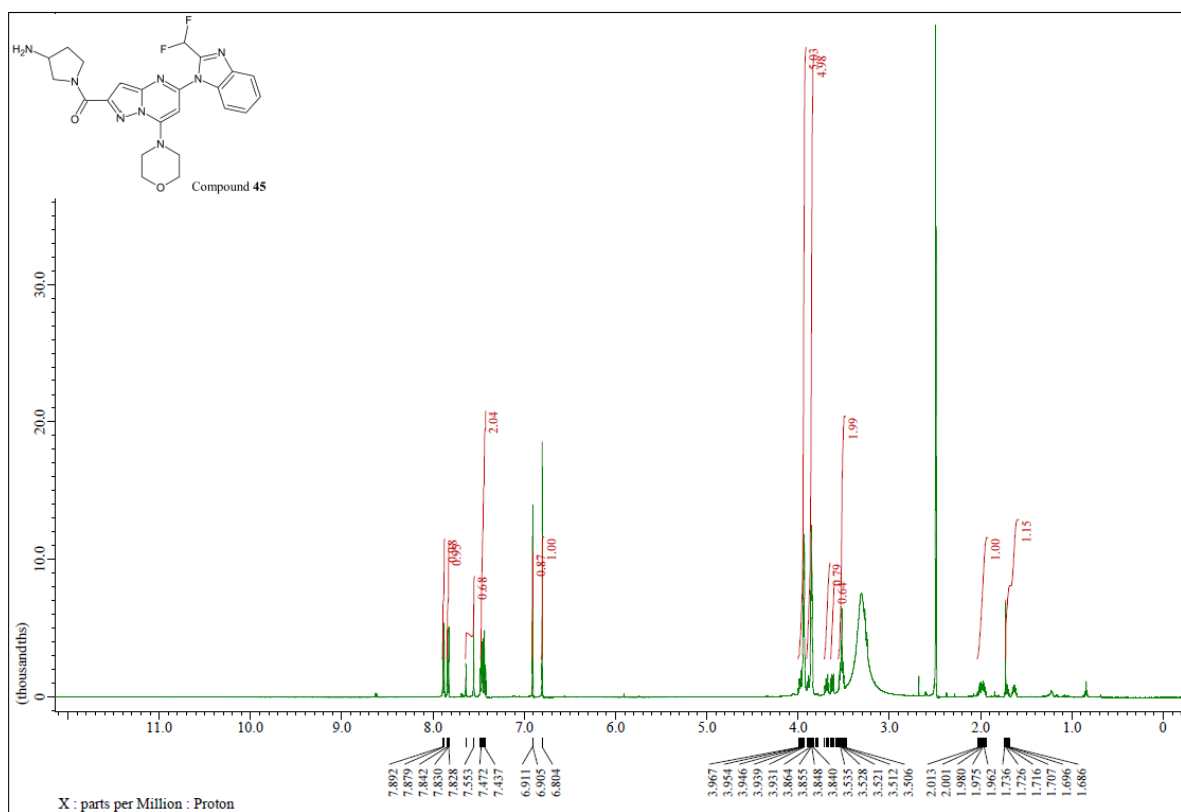


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
249.60653	249.60662	-0.37	2	7637.68	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+2H)+2
250.11133	250.10804	13.14	2	1938.11	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+2H)+2
250.60717	250.60935	-8.69	2	380.05	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+2H)+2
498.20662	498.20597	1.31	1	412028.53	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+H)+
499.20935	499.2088	1.09	1	111505.13	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+H)+
500.21156	500.21142	0.27	1	17153.88	C ₂₄ H ₂₅ F ₂ N ₇ O ₃	(M+H)+

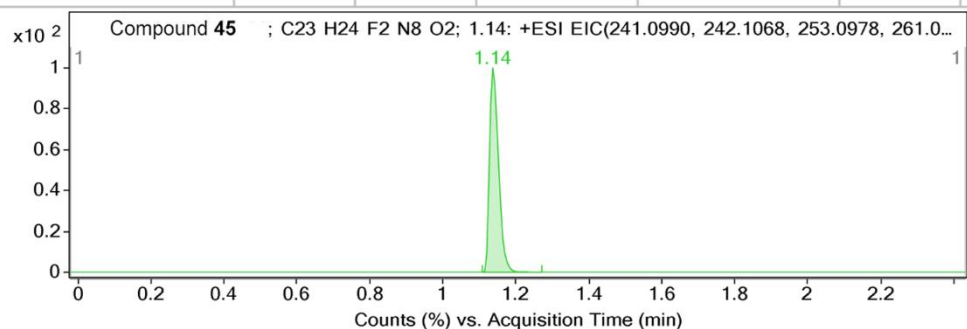
--- End Of Report ---

Compound 45

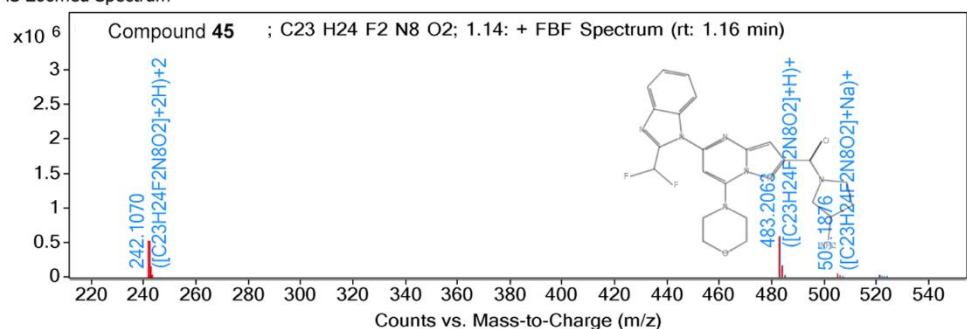


Compound 45

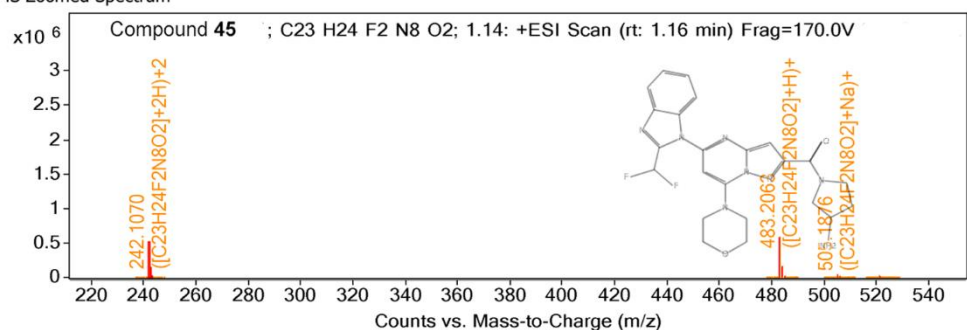
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Alaorit Find by Formula
Compound 45	505.1876	1.14	482.1996	C23 H24 F2 N8 O2	482.199	1.11	



MS Zoomed Spectrum



MS Zoomed Spectrum

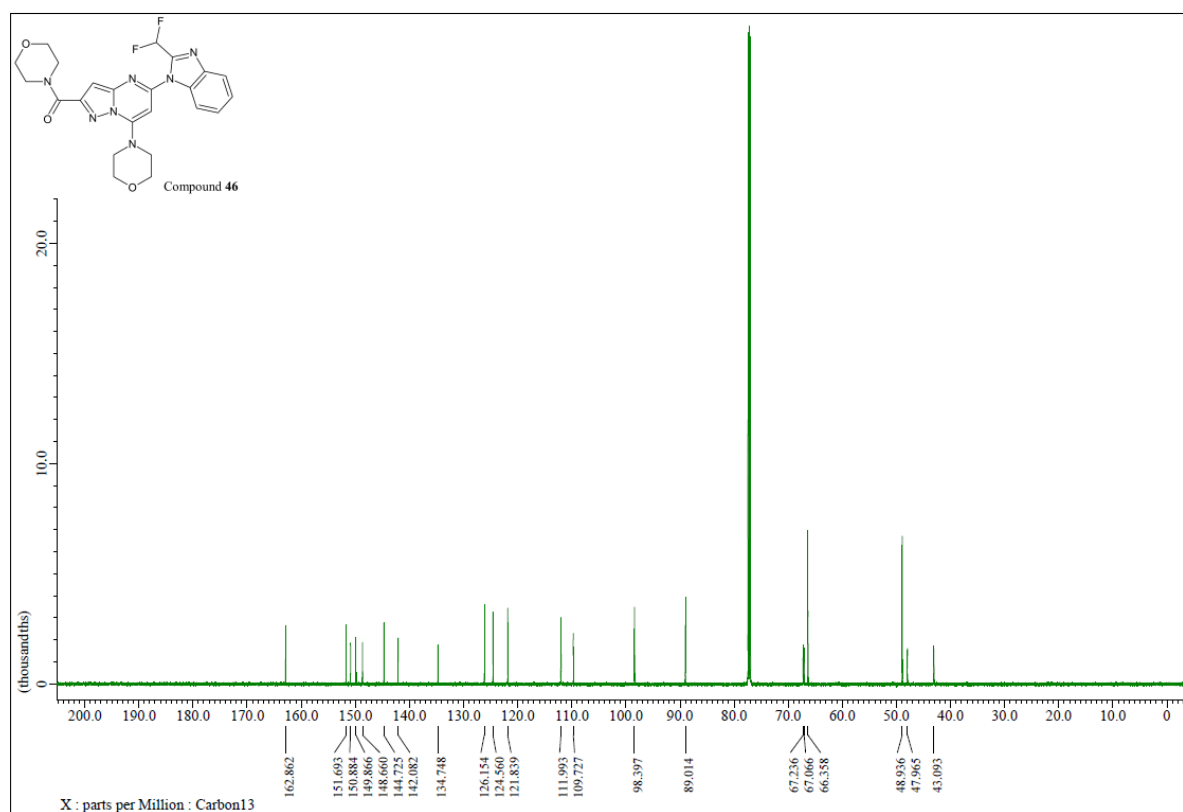
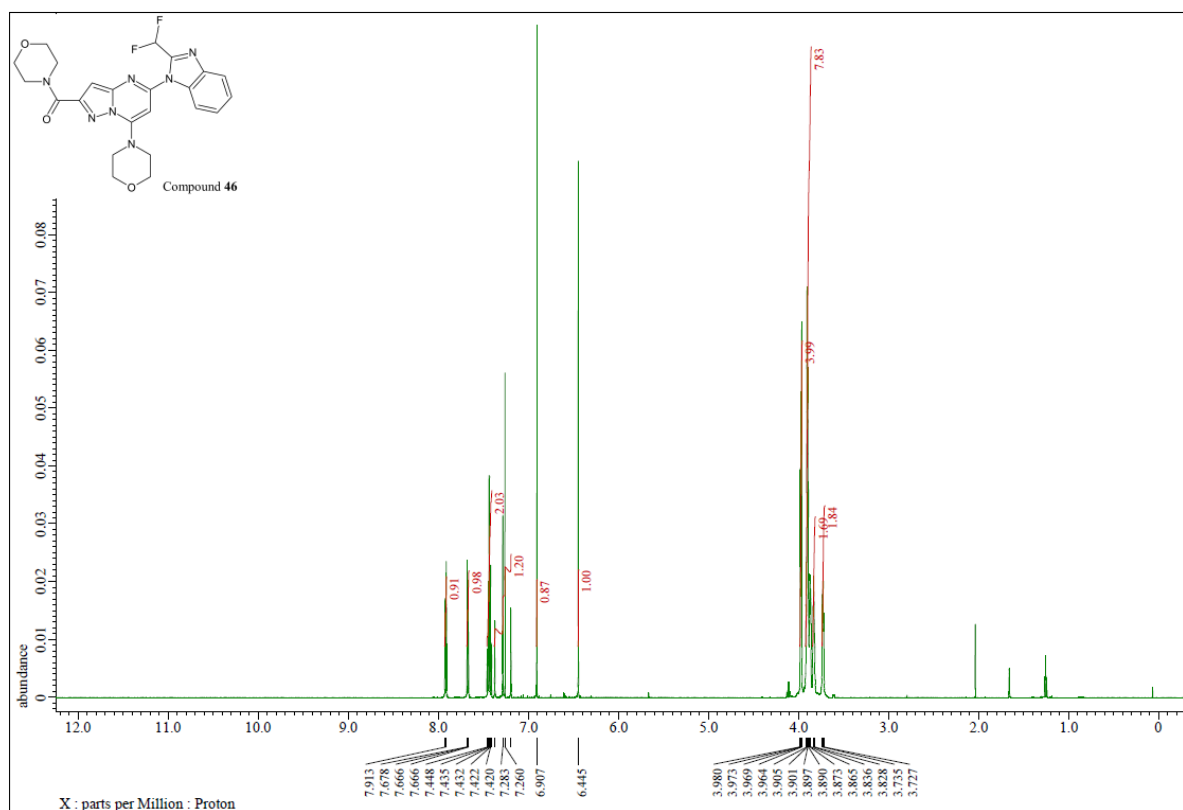


MS Spectrum Peak List

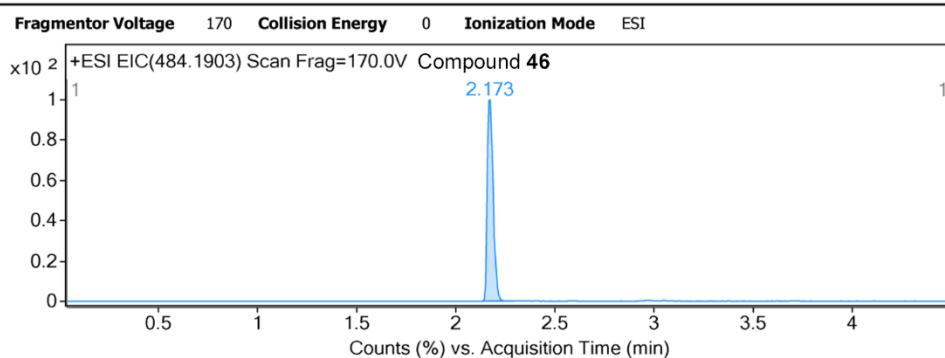
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
242.107	2	512912.66	C23H24F2N8O2	(M+2H)+2	
242.6087	2	129371.14	C23H24F2N8O2	(M+2H)+2	
243.1117	2	17811.2	C23H24F2N8O2	(M+2H)+2	
483.2063	1	585879.56	C23H24F2N8O2	(M+H)+	
484.2113	1	161792.5	C23H24F2N8O2	(M+H)+	
485.2155	1	23468.76	C23H24F2N8O2	(M+H)+	
505.1876	1	42200.06	C23H24F2N8O2	(M+Na)+	
506.1906	1	12088.44	C23H24F2N8O2	(M+Na)+	
521.1614	1	26443.12	C23H24F2N8O2	(M+K)+	
522.164	1	7111.54	C23H24F2N8O2	(M+K)+	
242.107	2	512912.66	C23H24F2N8O2	(M+2H)+2	0.88
242.6087	2	129371.14	C23H24F2N8O2	(M+2H)+2	2.24
243.1117	2	17811.2	C23H24F2N8O2	(M+2H)+2	9.44
483.2063	1	585879.56	C23H24F2N8O2	(M+H)+	-0.06
484.2113	1	161792.5	C23H24F2N8O2	(M+H)+	4.6
485.2155	1	23468.76	C23H24F2N8O2	(M+H)+	7.94
505.1876	1	42200.06	C23H24F2N8O2	(M+Na)+	-1.34
506.1906	1	12088.44	C23H24F2N8O2	(M+Na)+	-0.77
521.1614	1	26443.12	C23H24F2N8O2	(M+K)+	-1.6
522.164	1	7111.54	C23H24F2N8O2	(M+K)+	-1.83

--- End Of Report ---

Compound 46



Compound 46

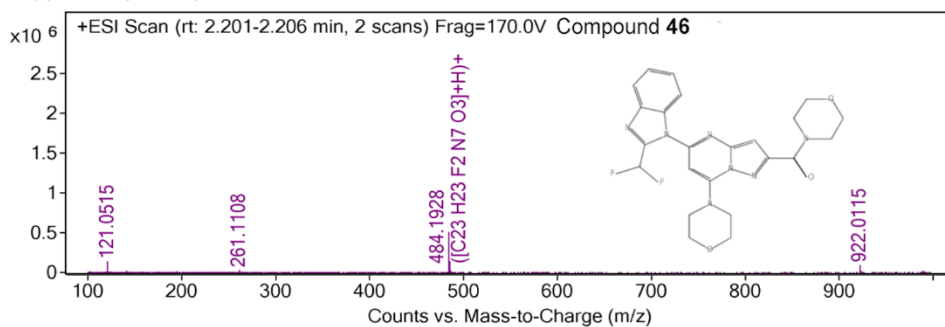


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2.135	2.173	2.295	3035891.34	6209015.39	100

Spectra

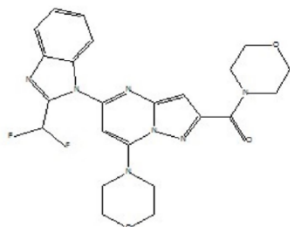
Spectrum Source Peak (1) in "+ EIC(484.1903) Scan" Fragmentor Voltage 170 Collision Energy 0 Ionization Mode ESI



Peak List

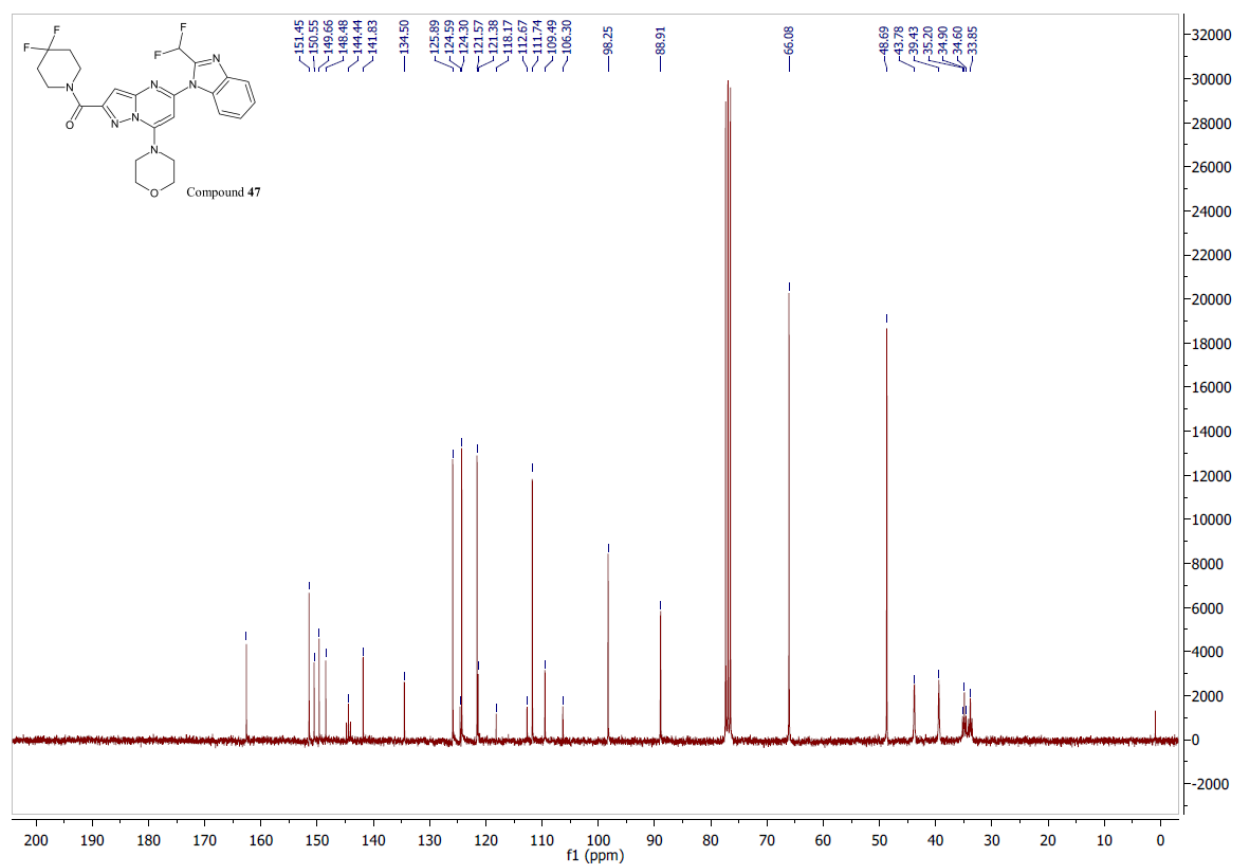
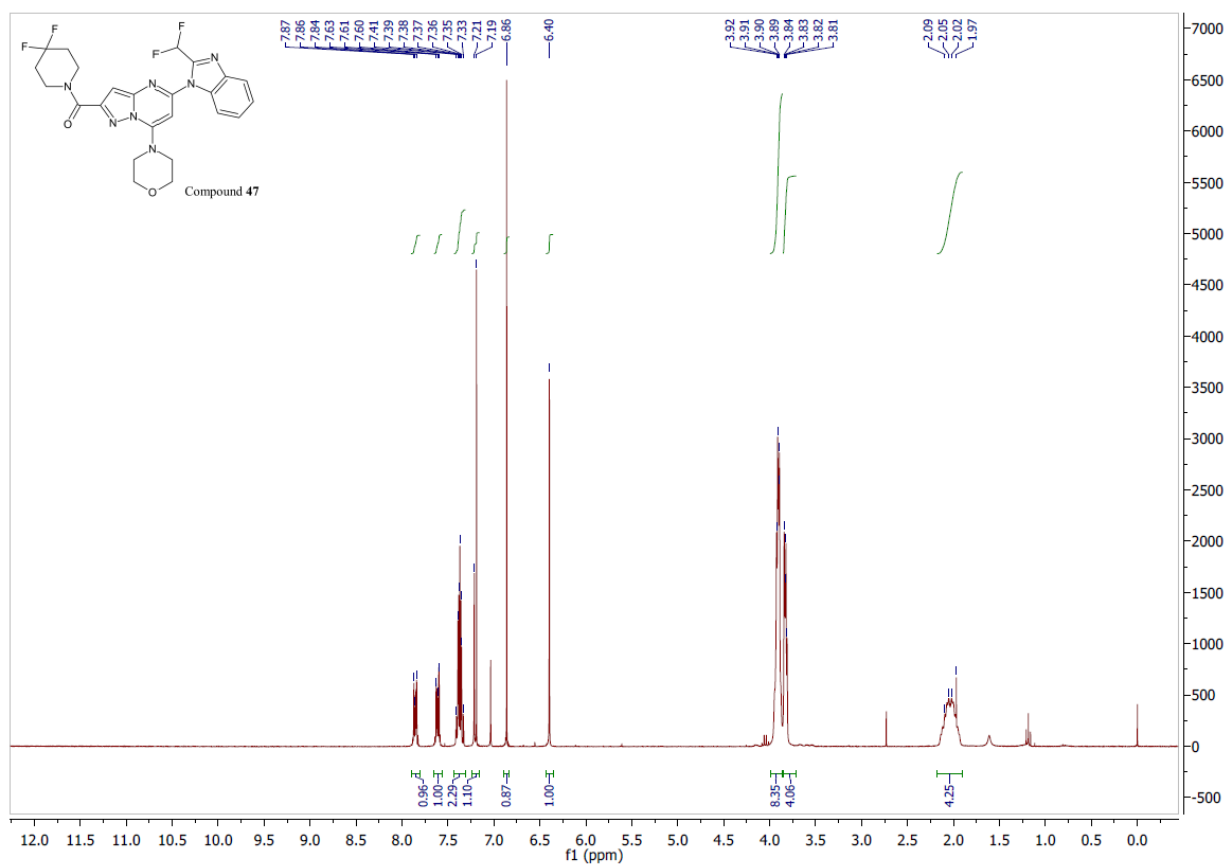
m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
484.1928	1	508306.75	Compound 46	C23 H23 F2 N7 O3	(M+H)+	98.27	1

Spectrum Structure



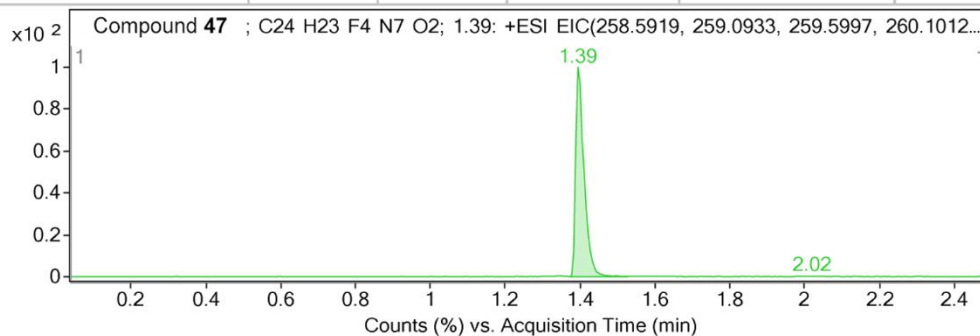
--- End Of Report ---

Compound 47

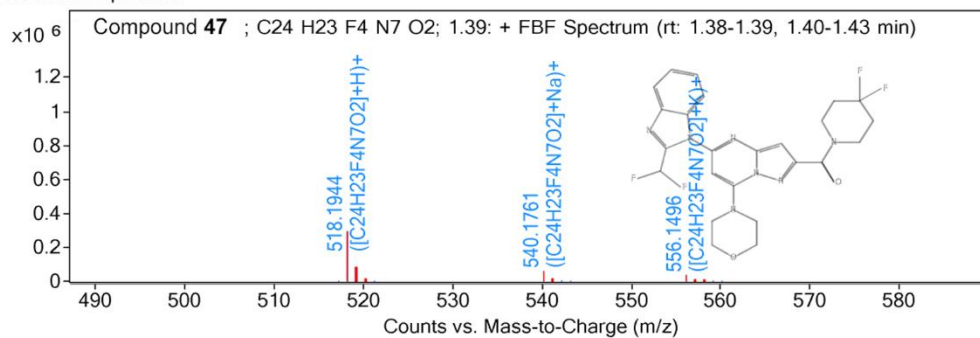


Compound 47

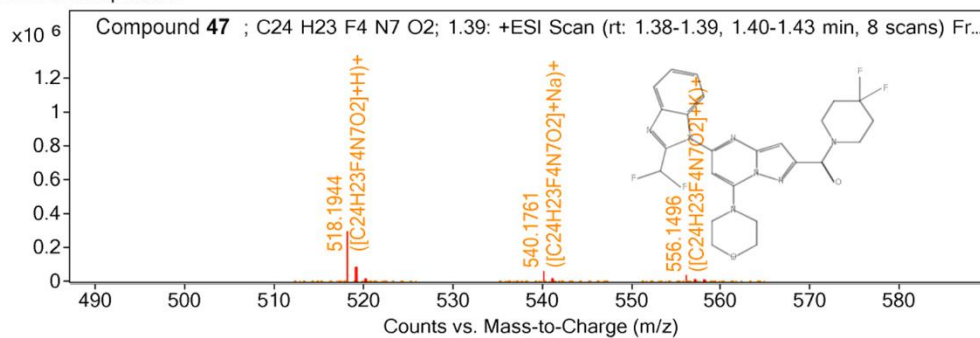
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 47	540.1761	1.39	517.187	C24 H23 F4 N7 O2	517.1849	4.06	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

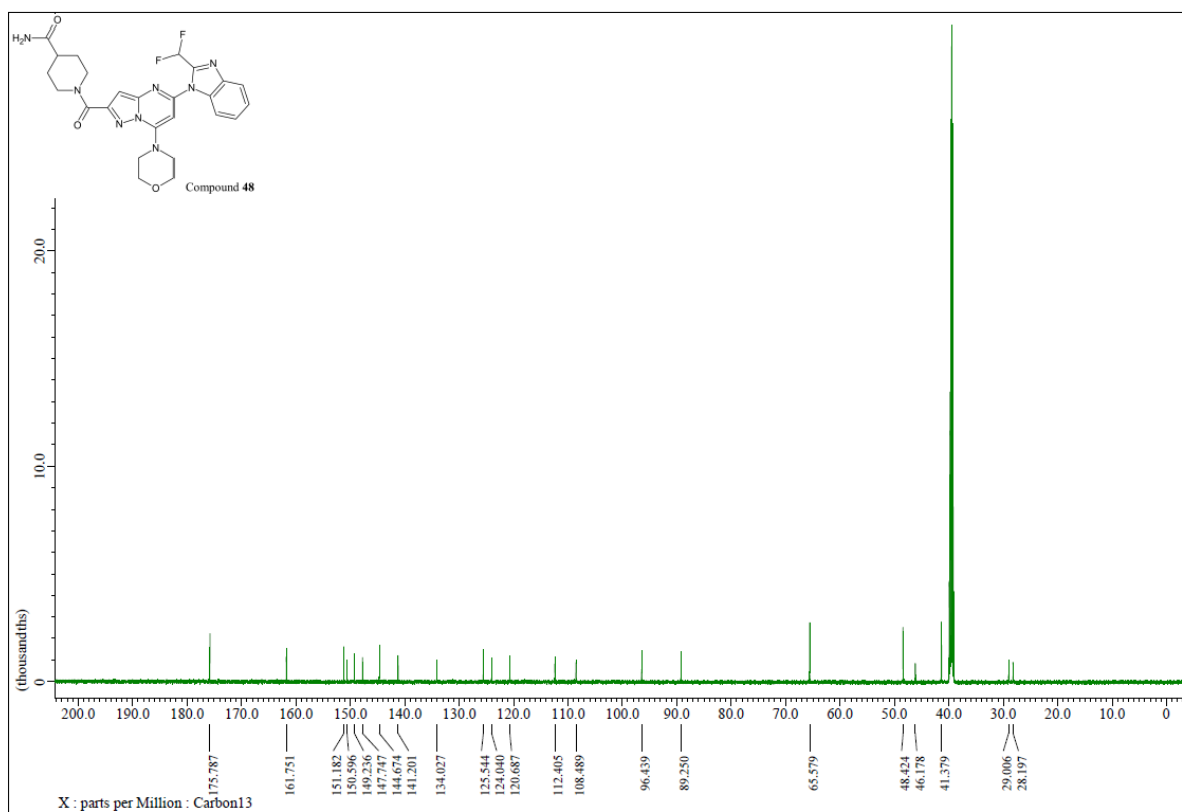
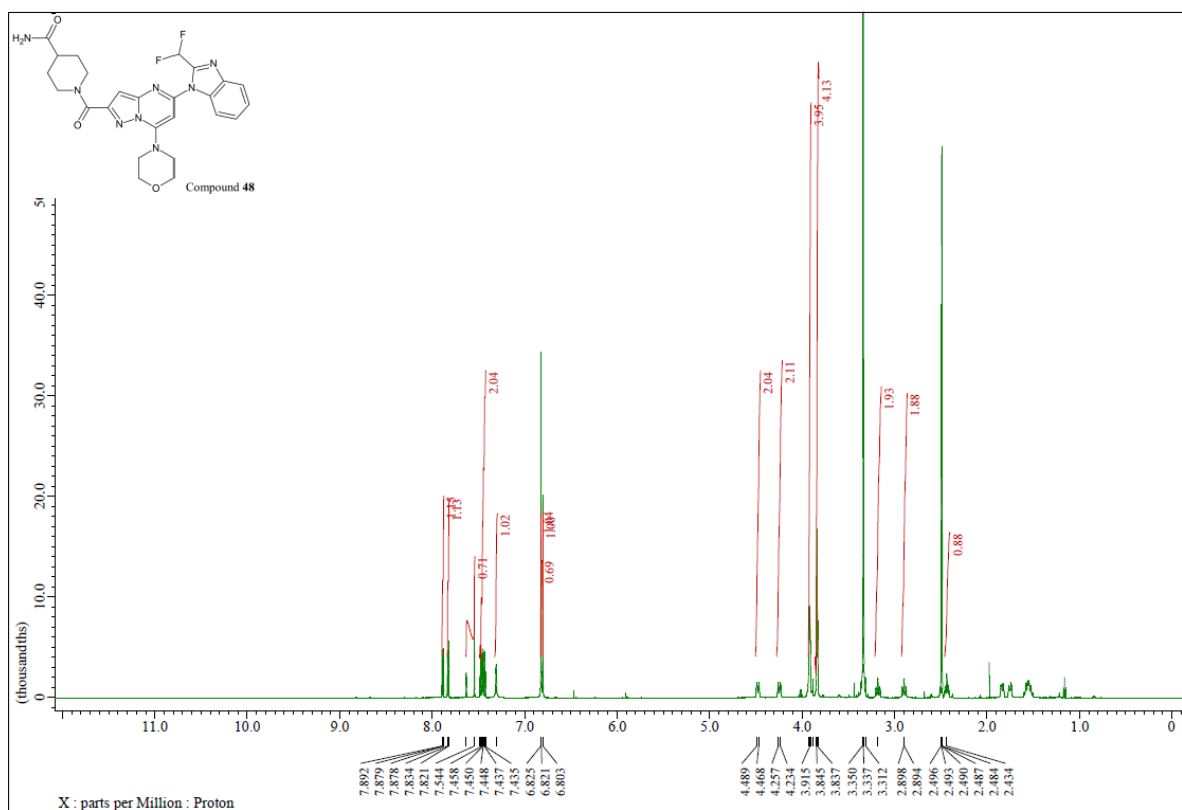


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
518.1944	1	291918.13	C24H23F4N7O2	(M+H)+	
518.1944	1	291918.13	C24H23F4N7O2	(M+H)+	4.27

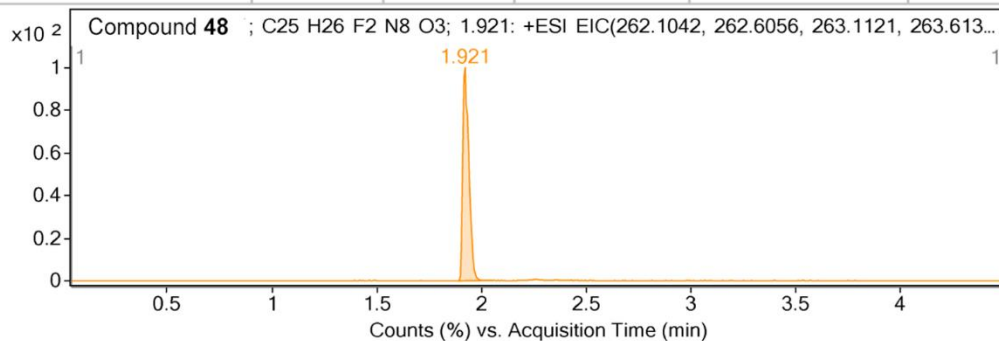
--- End Of Report ---

Compound 48

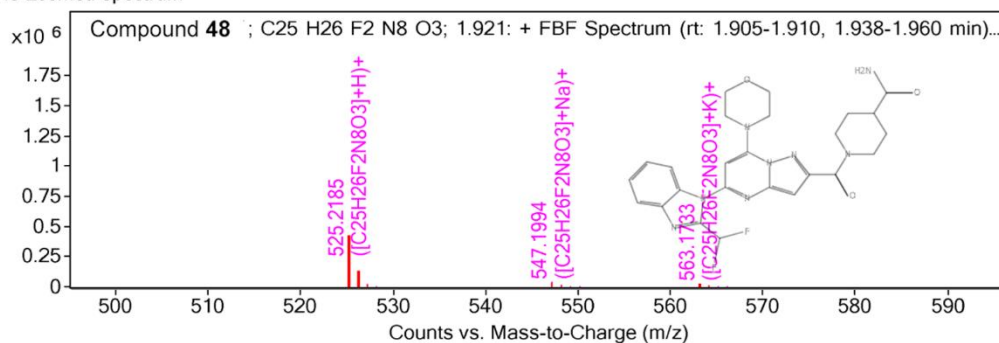


Compound 48

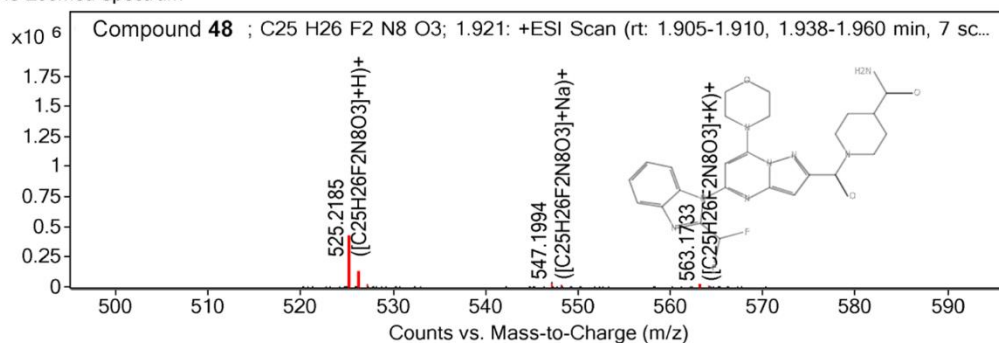
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Algorit
Compound 48	547.1994	1.921	524.2111	C25 H26 F2 N8 O3	524.2096	2.9	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

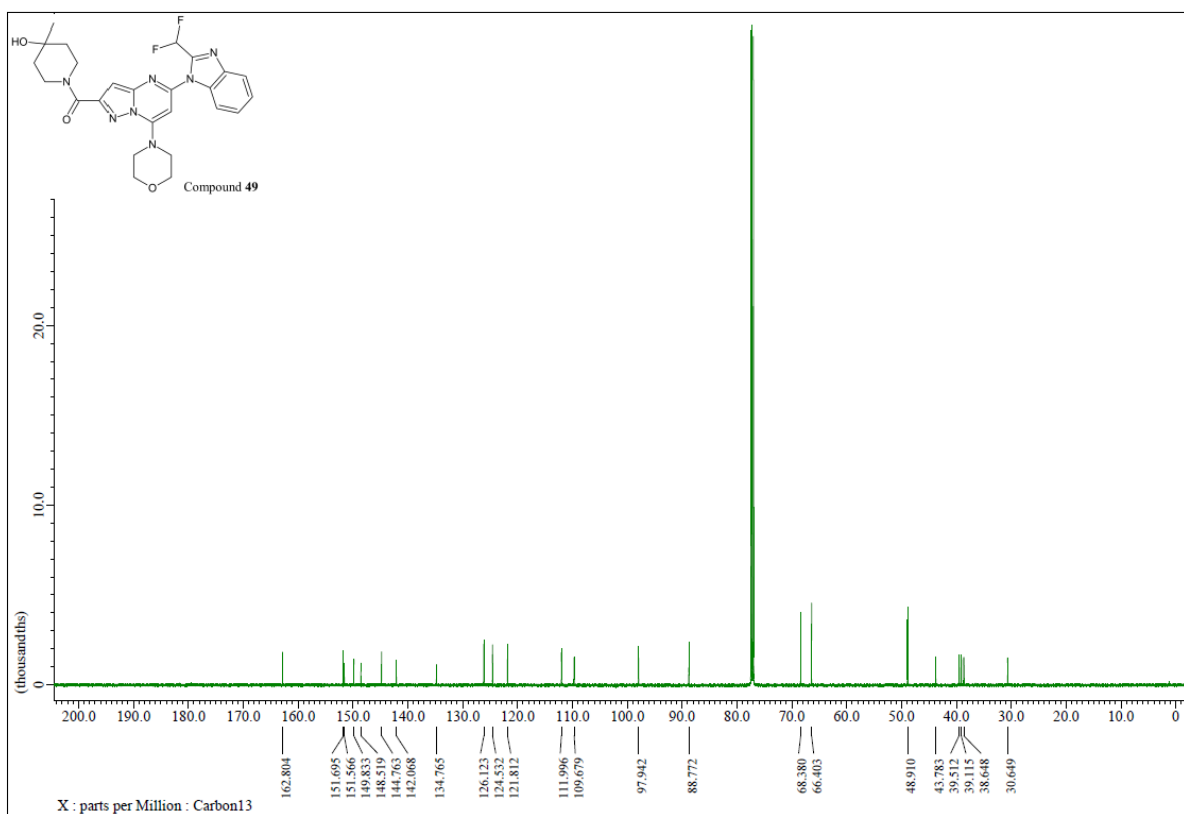
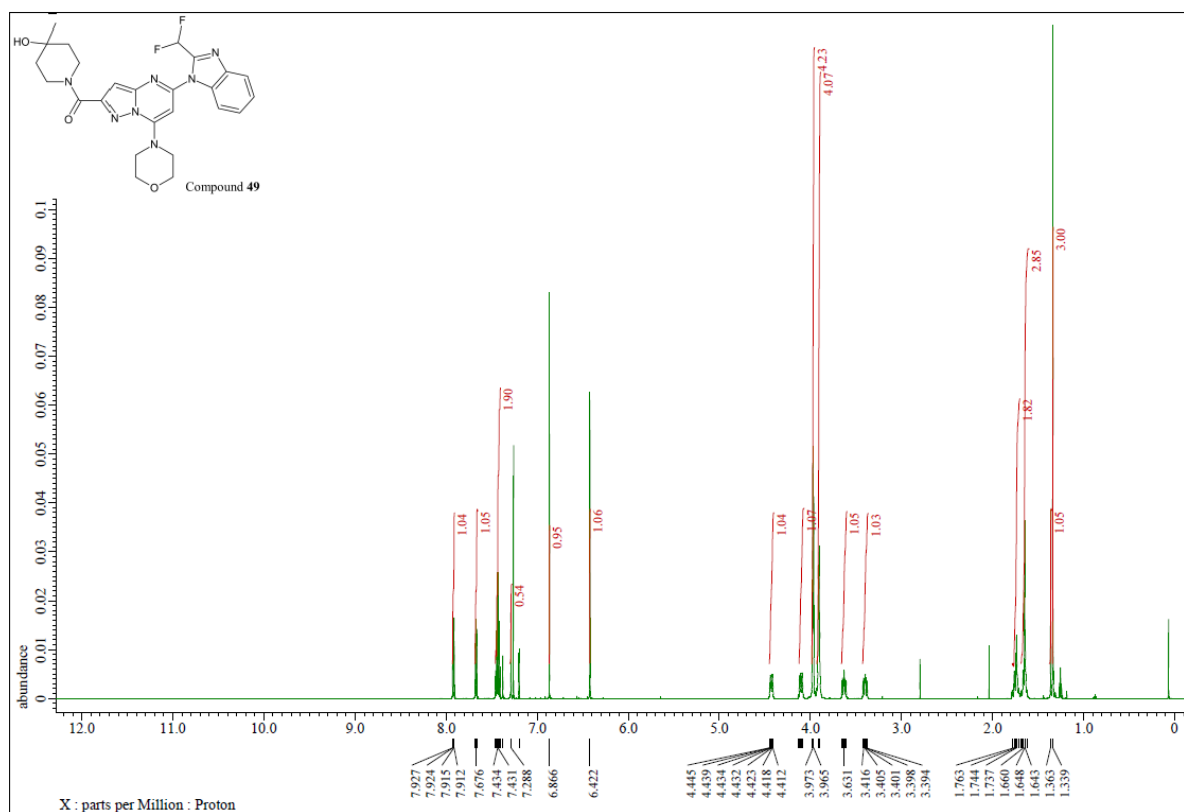


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
525.2185	1	418105.22	C25H26F2N8O3	(M+H)+	
525.2185	1	418105.22	C25H26F2N8O3	(M+H)+	3.18

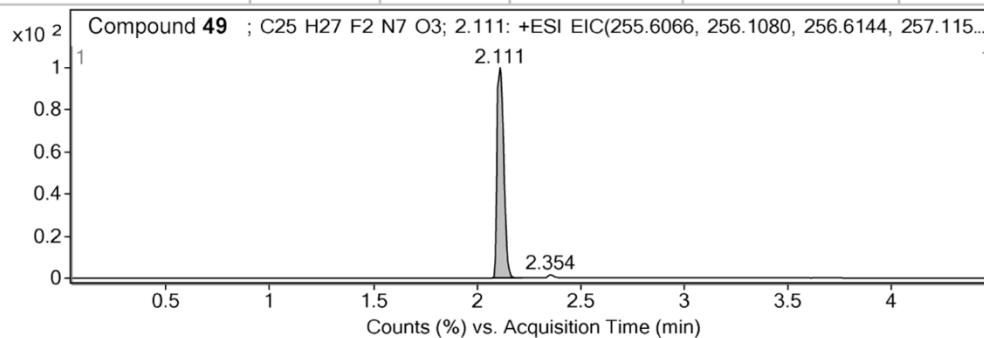
--- End Of Report ---

Compound 49

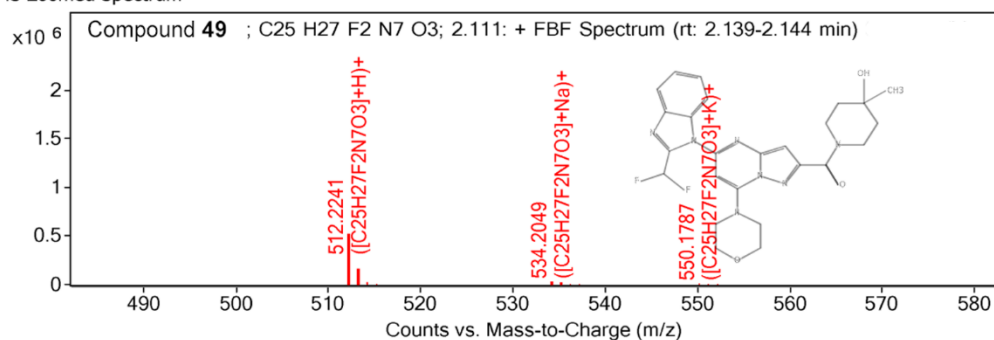


Compound 49

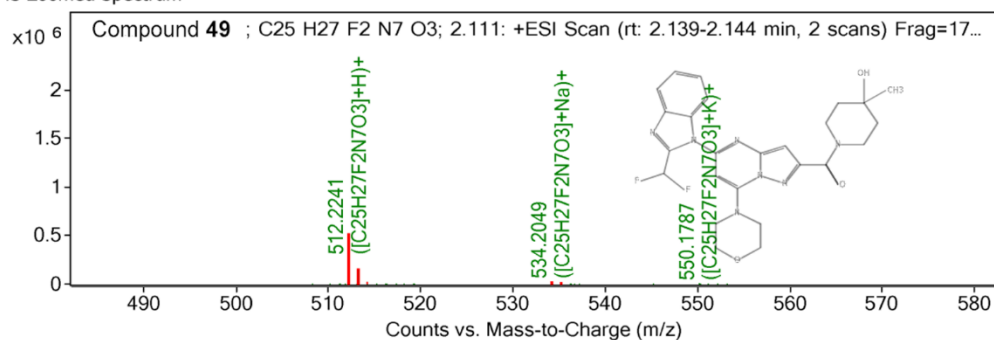
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 49	534.2049	2.111	511.2166	C25 H27 F2 N7 O3	511.2143	4.48	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

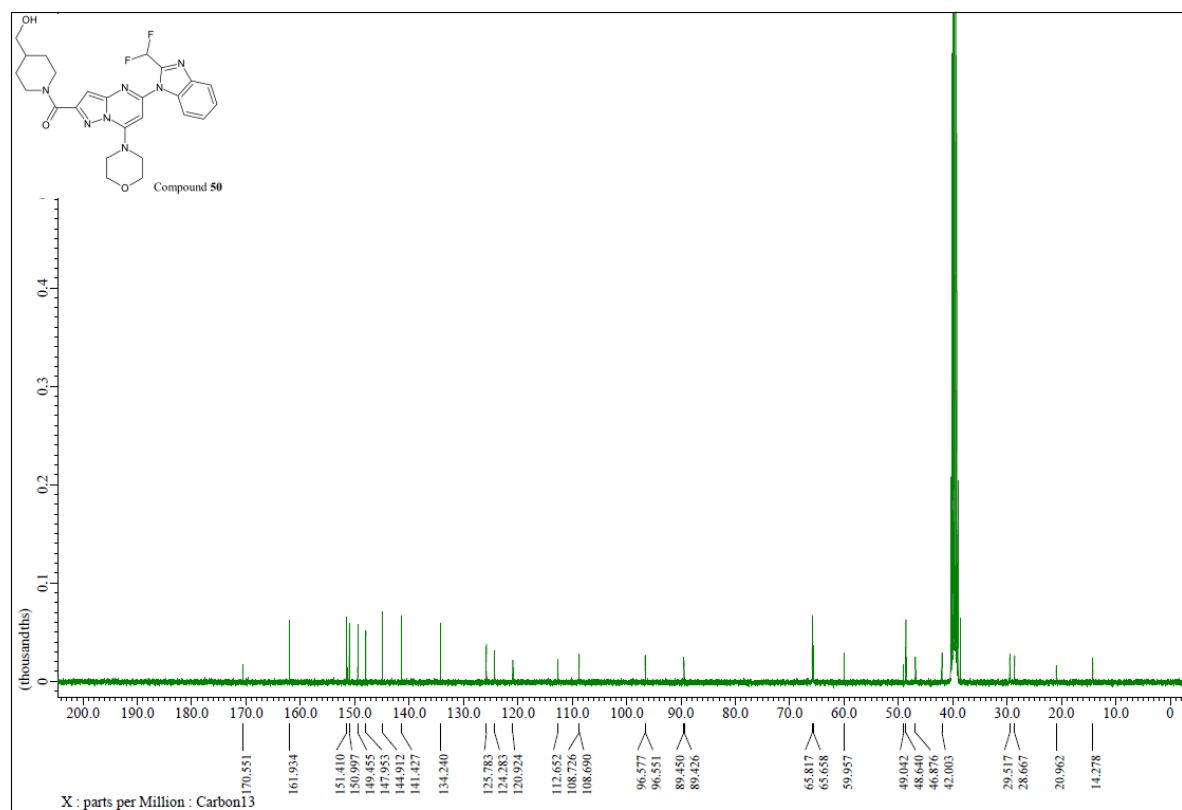
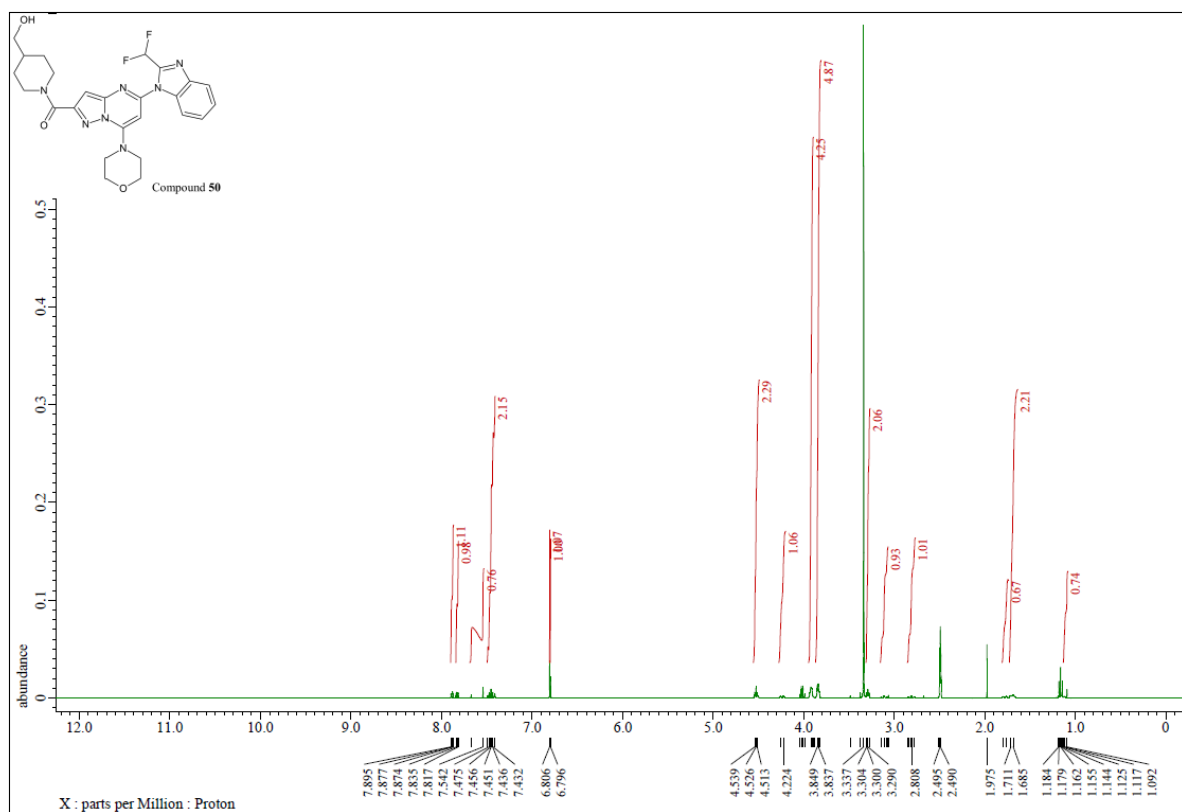


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
512.2241	1	513087.13	C25H27F2N7O3	(M+H)+	
512.2241	1	513087.13	C25H27F2N7O3	(M+H)+	4.76

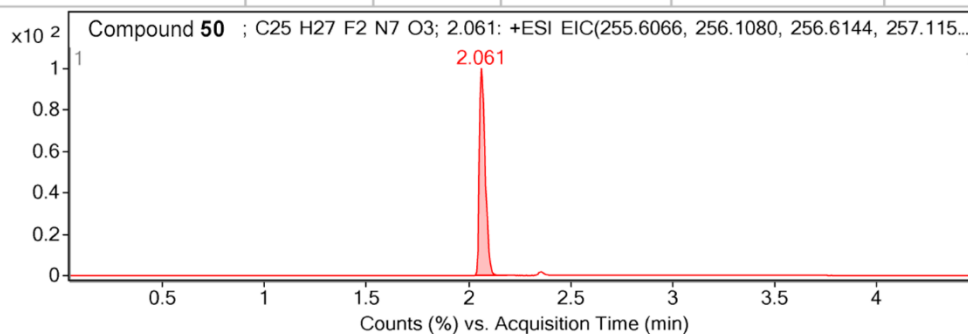
--- End Of Report ---

Compound 50

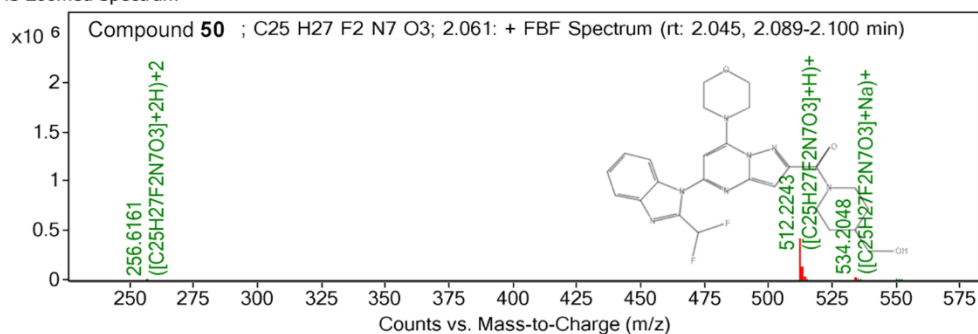


Compound 50

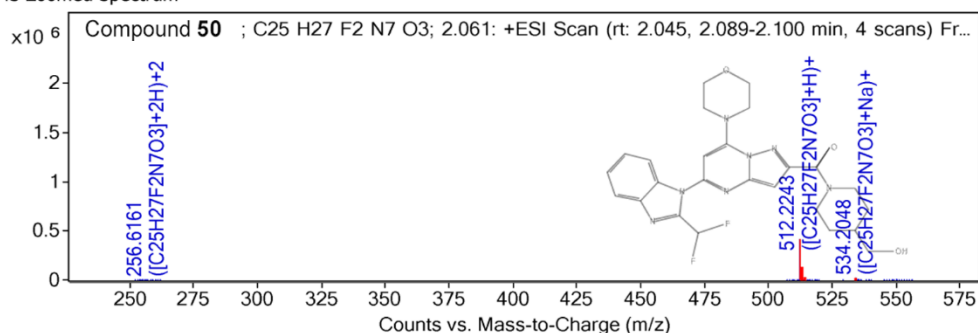
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Alaorit
Compound 50	534.2048	2.061	511.2169	C25 H27 F2 N7 O3	511.2143	4.98	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

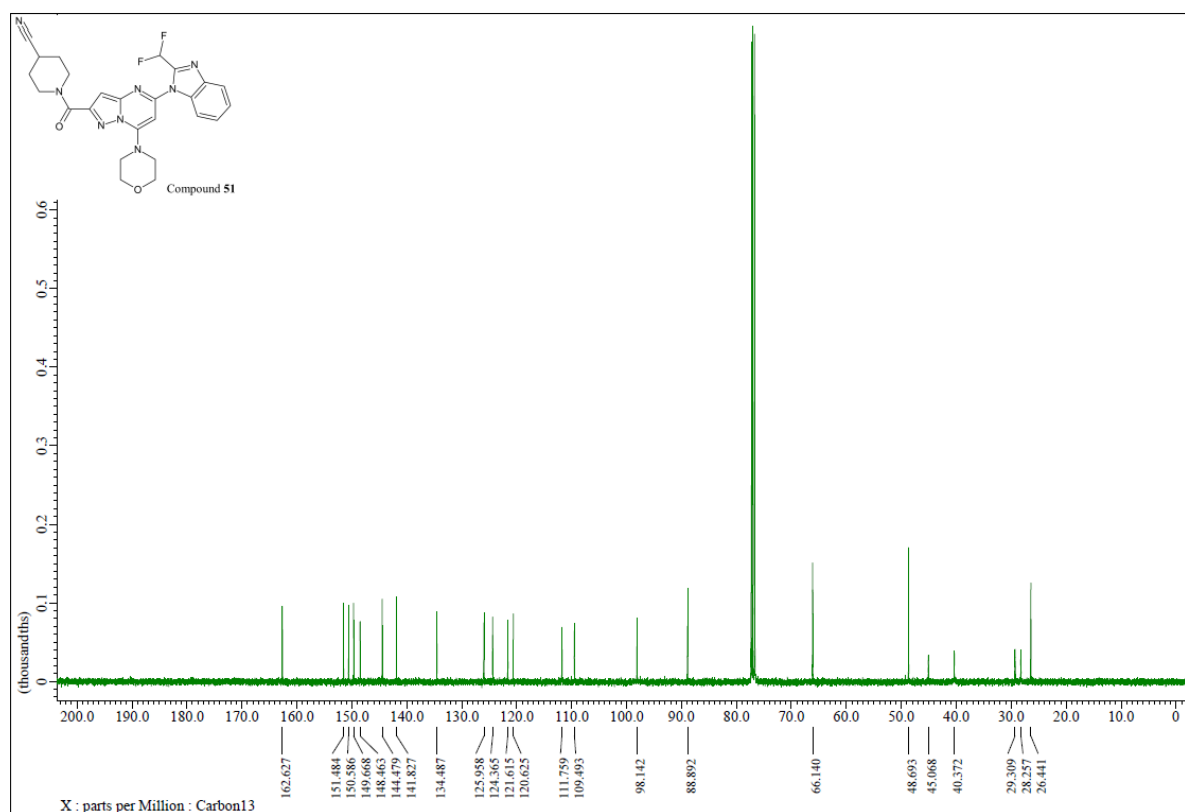
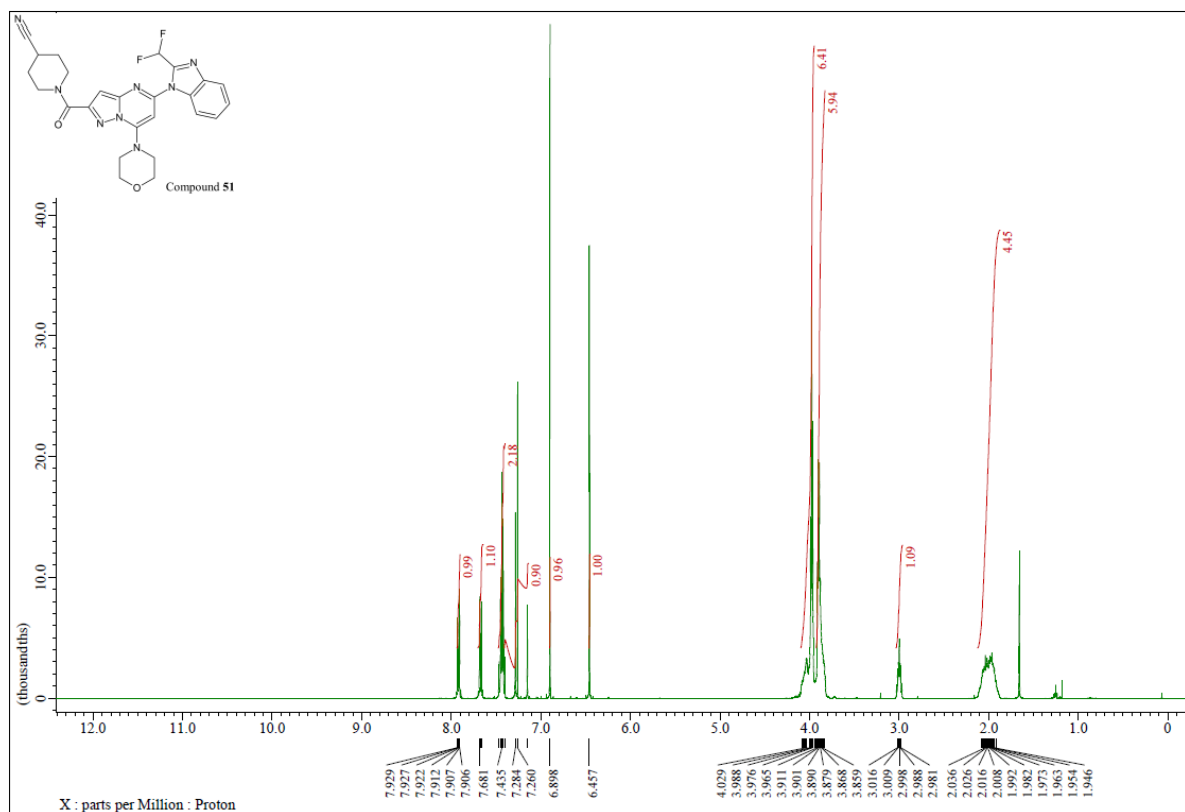


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
512.2243	1	414545.78	C25H27F2N7O3	(M+H)+	
512.2243	1	414545.78	C25H27F2N7O3	(M+H)+	5.32

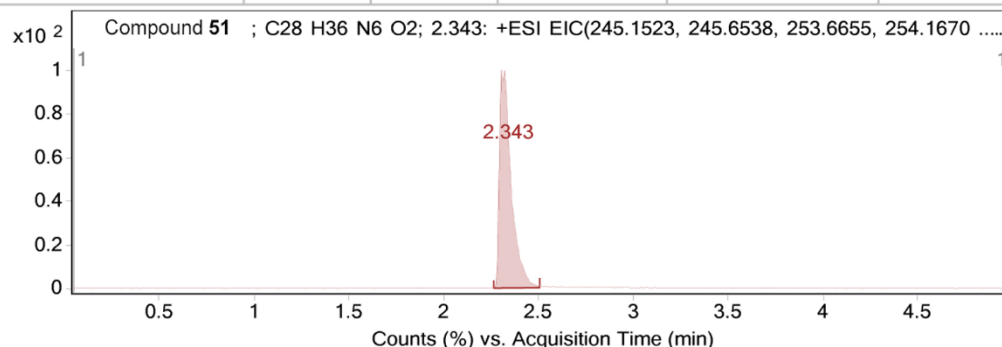
--- End Of Report ---

Compound 51

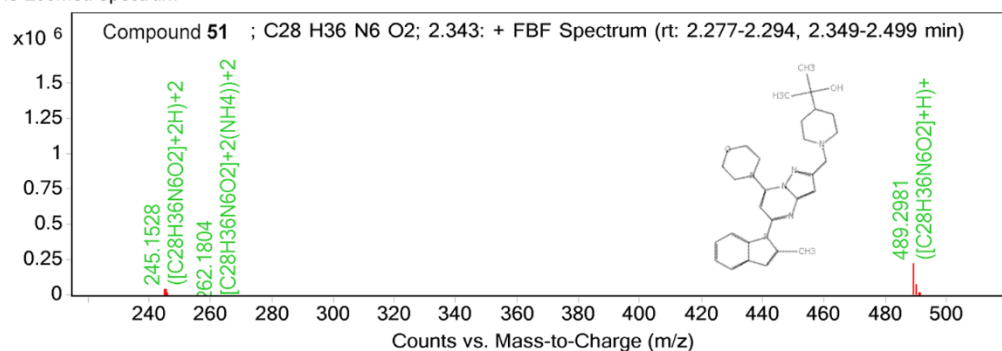


Compound 51

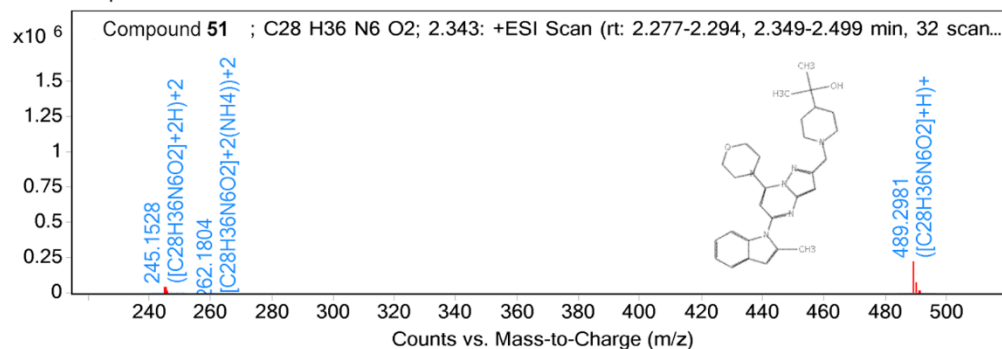
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorithm
Compound 51	245.1528	2.343	488.2908	C28 H36 N6 O2	488.29	1.65	Find by Formula



MS Zoomed Spectrum



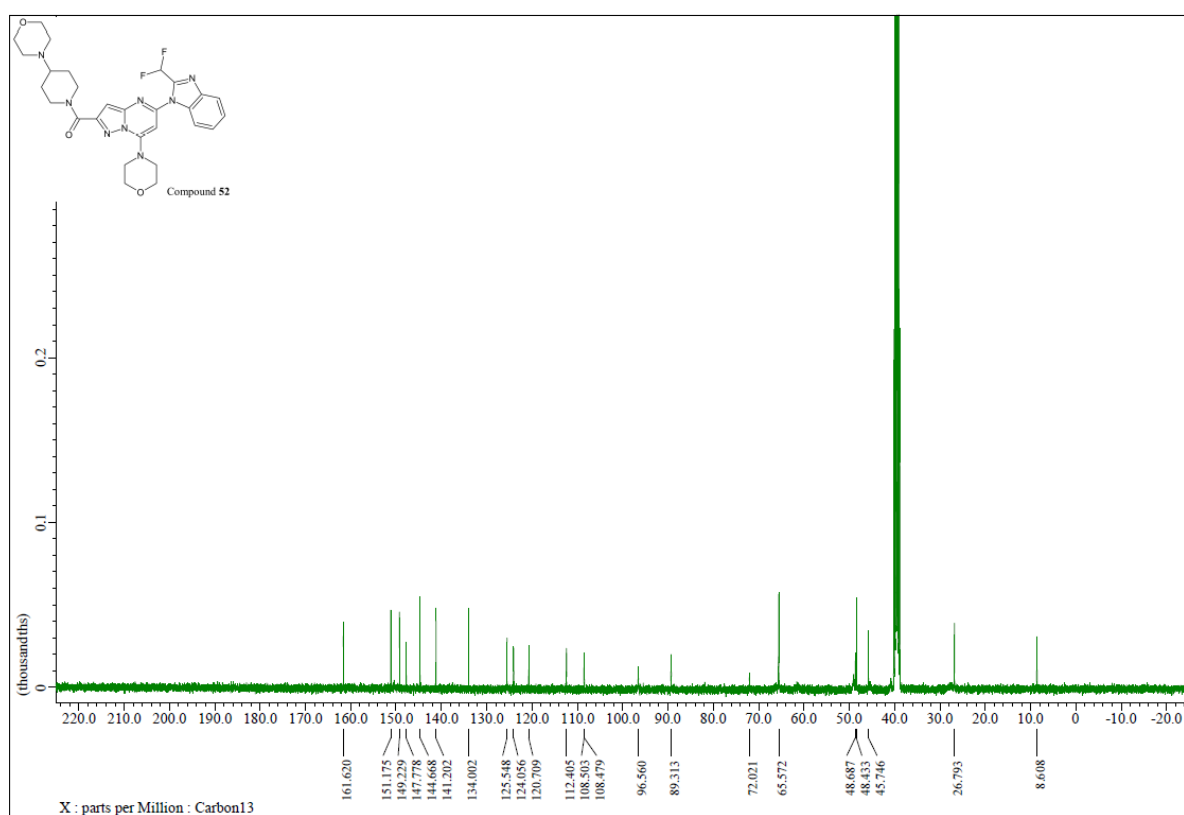
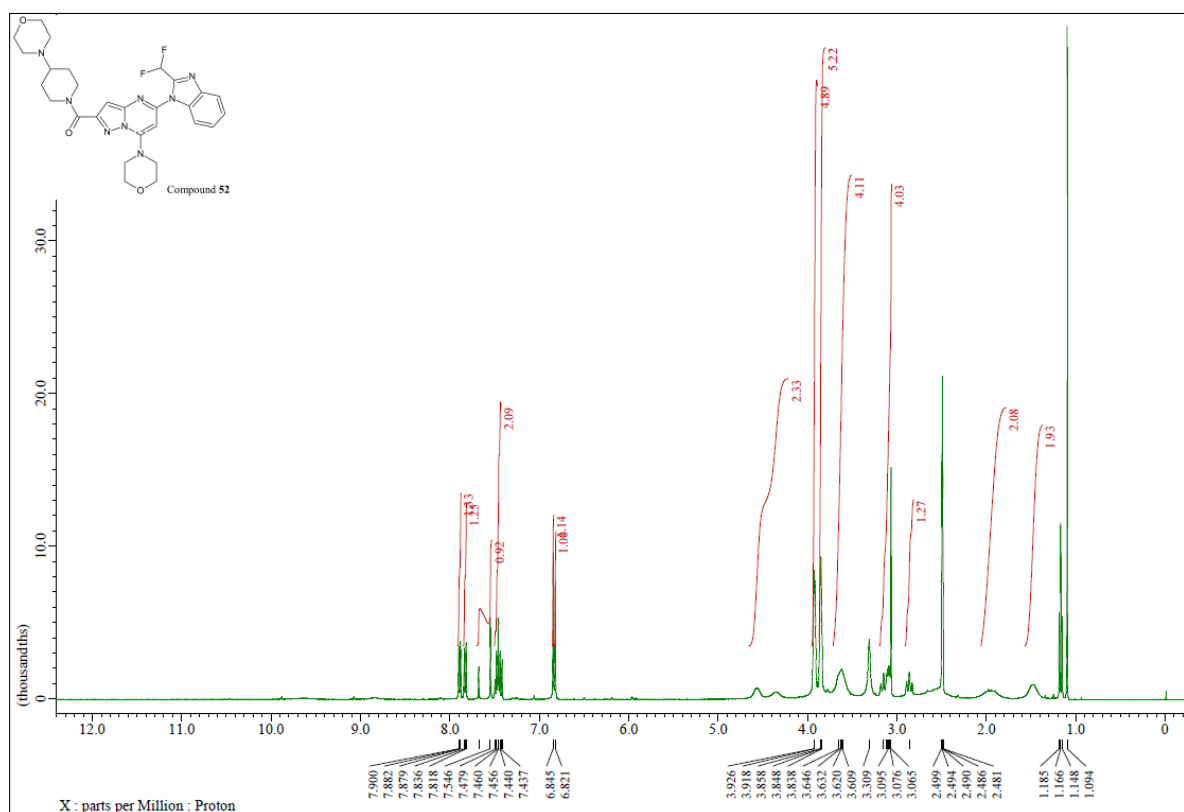
MS Zoomed Spectrum



MS Spectrum Peak List

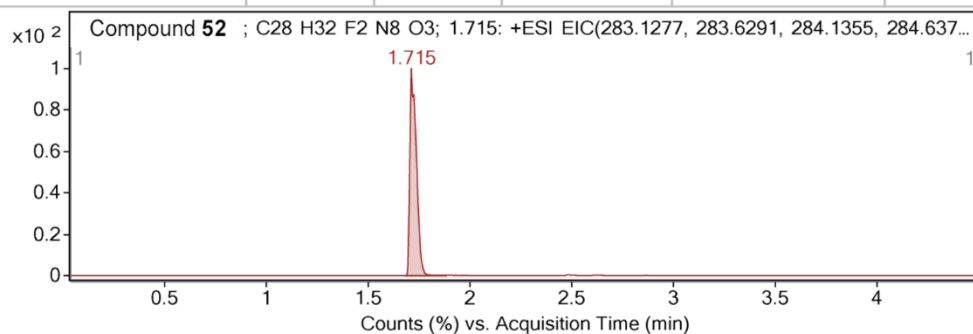
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
245.1528	2	39305.1	C28H36N6O2	(M+2H)+2	
245.6541	2	13220.31	C28H36N6O2	(M+2H)+2	
246.1556	2	2237.2	C28H36N6O2	(M+2H)+2	
246.656	2	264.83	C28H36N6O2	(M+2H)+2	
262.1804	2	2396.03	C28H36N6O2	(M+2(NH4))+2	
263.1846	2	484.19	C28H36N6O2	(M+2(NH4))+2	
489.2981	1	220426.55	C28H36N6O2	(M+H)+	
490.3008	1	64901.46	C28H36N6O2	(M+H)+	
491.3026	1	10140.32	C28H36N6O2	(M+H)+	
245.1528	2	39305.1	C28H36N6O2	(M+2H)+2	2.01
245.6541	2	13220.31	C28H36N6O2	(M+2H)+2	1.29
246.1556	2	2237.2	C28H36N6O2	(M+2H)+2	1.57
246.656	2	264.83	C28H36N6O2	(M+2H)+2	-2.37
262.1804	2	2396.03	C28H36N6O2	(M+2(NH4))+2	6
263.1846	2	484.19	C28H36N6O2	(M+2(NH4))+2	11.24
489.2981	1	220426.55	C28H36N6O2	(M+H)+	1.78
490.3008	1	64901.46	C28H36N6O2	(M+H)+	1.18

Compound 52

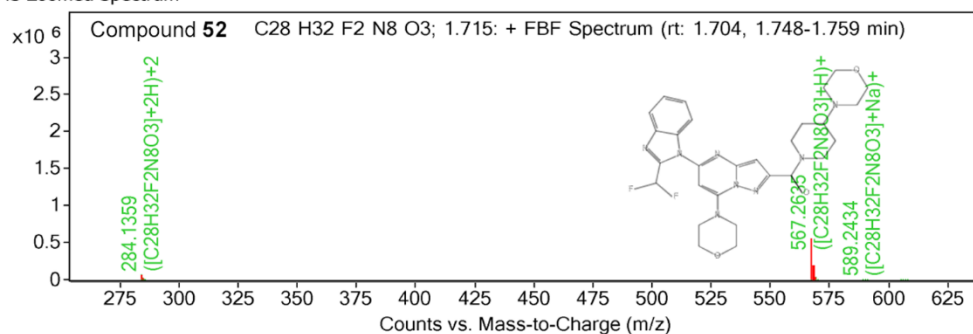


Compound 52

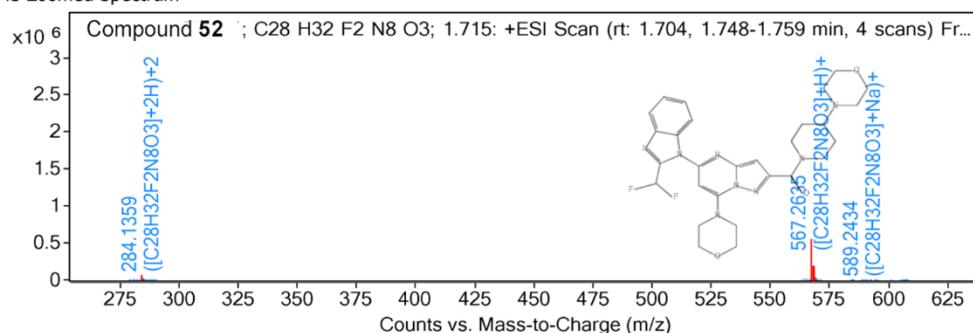
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaorit
Compound 52	567.2635	1.715	566.2563	C28 H32 F2 N8 O3	566.2565	-0.37	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

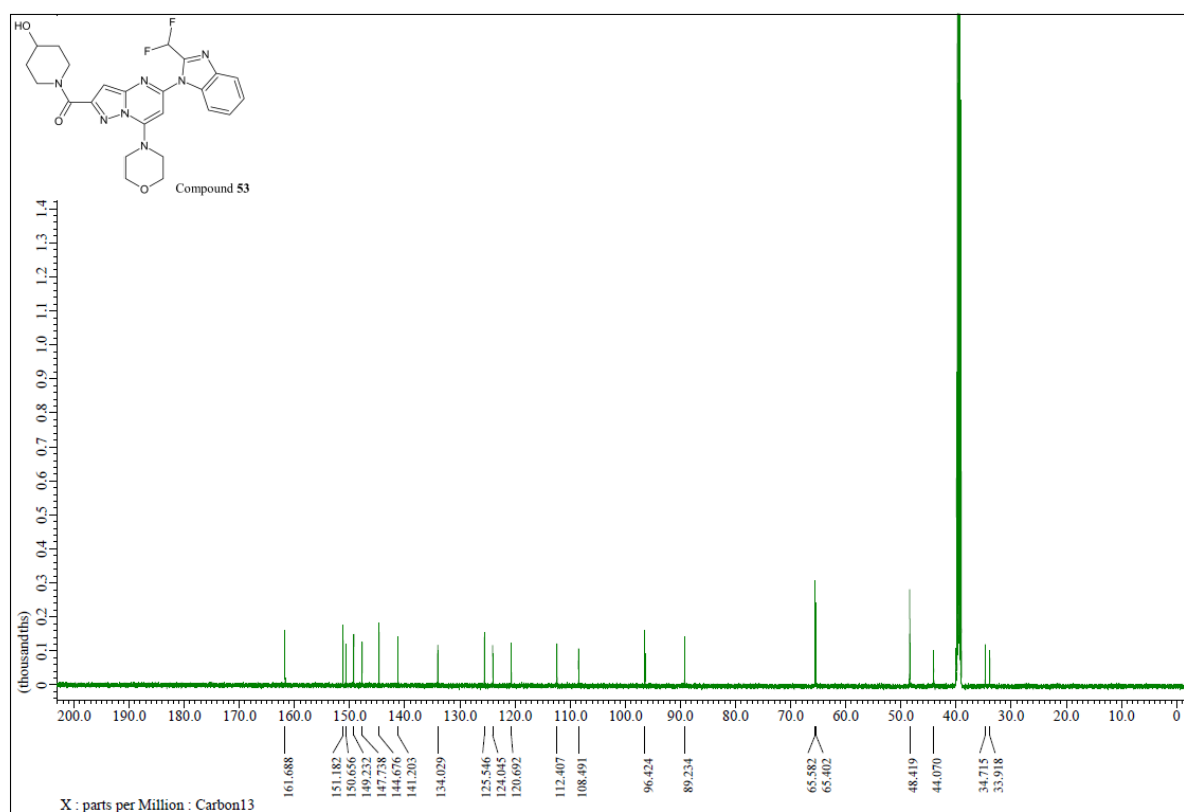
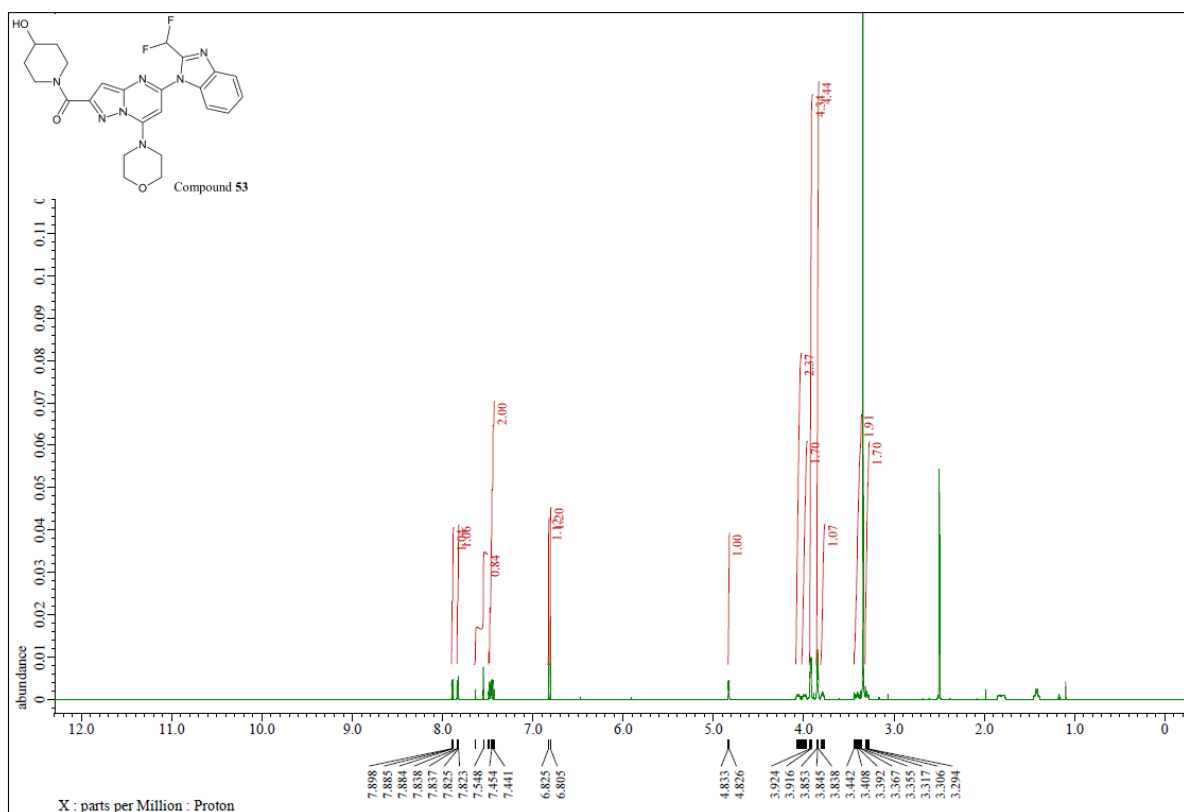


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
567.2635	1	550689.94	C28H32F2N8O3	(M+H)+	
567.2635	1	550689.94	C28H32F2N8O3	(M+H)+	-0.54

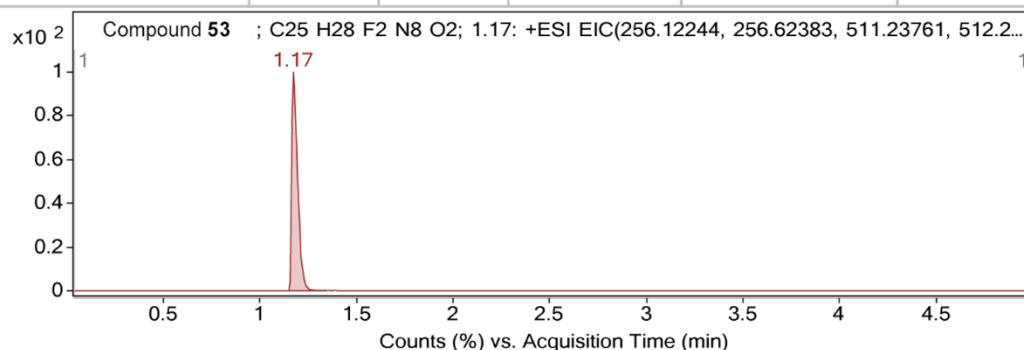
--- End Of Report ---

Compound 53

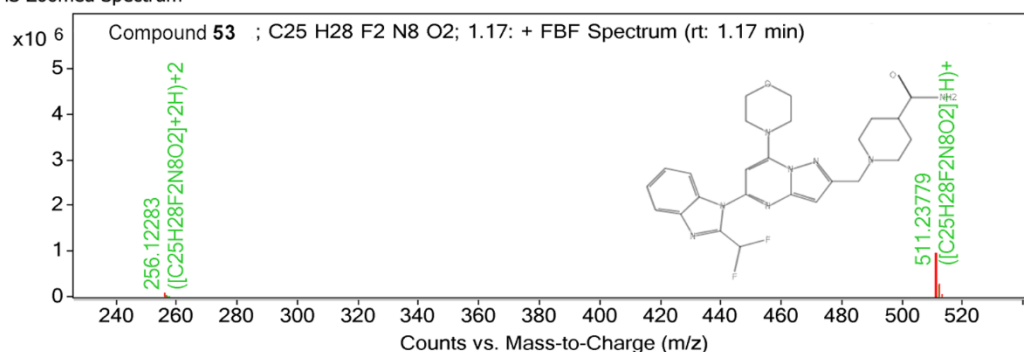


Compound 53

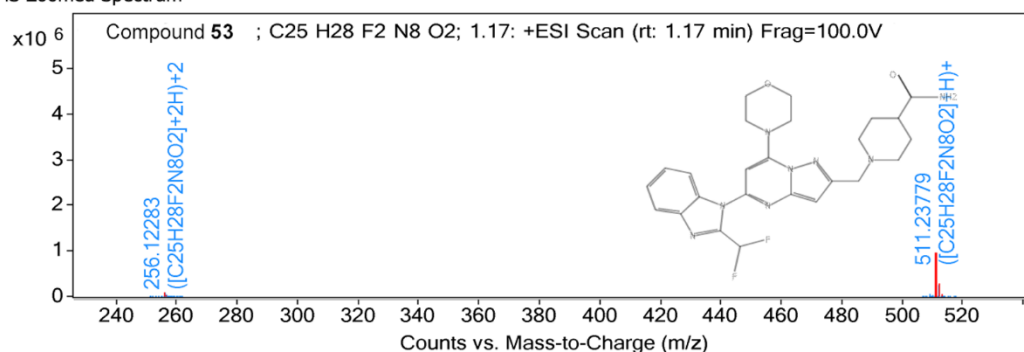
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 53	256.12283	1.17	510.23062	C25 H28 F2 N8 O2	510.23033	0.57	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

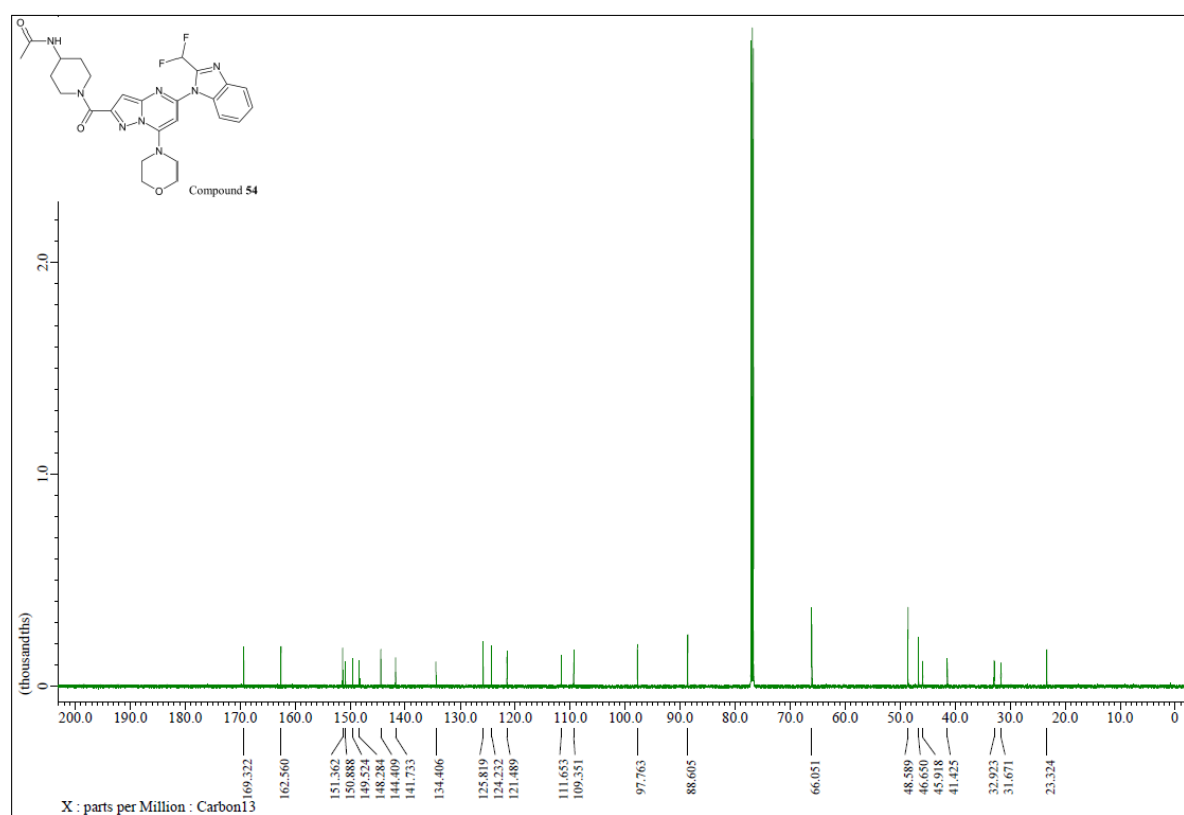
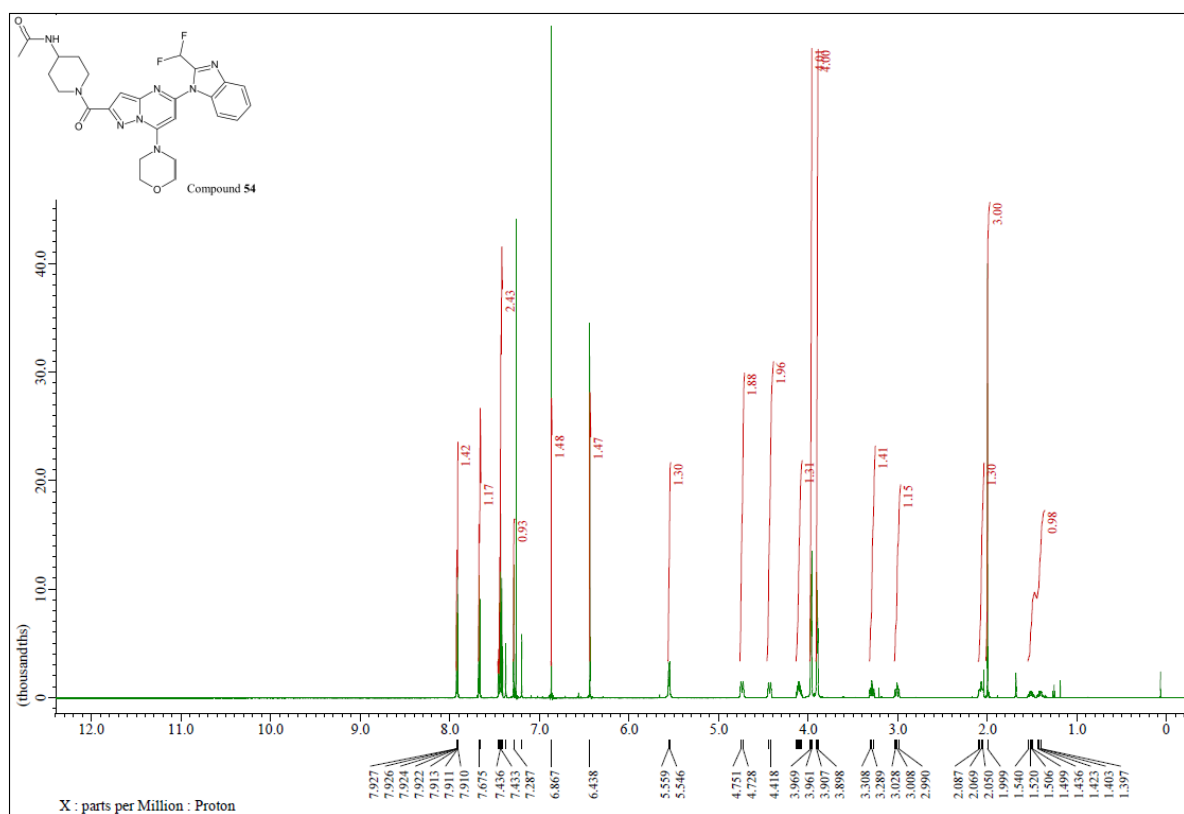


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
256.12283	2	72301.37	C25H28F2N8O2	(M+2H)+2	
256.62429	2	24112.44	C25H28F2N8O2	(M+2H)+2	
257.12683	2	2715.31	C25H28F2N8O2	(M+2H)+2	
257.6261	2	442.92	C25H28F2N8O2	(M+2H)+2	
511.23779	1	947387.88	C25H28F2N8O2	(M+H)+	
512.24099	1	244045.55	C25H28F2N8O2	(M+H)+	
513.24241	1	39640.75	C25H28F2N8O2	(M+H)+	
256.12283	2	72301.37	C25H28F2N8O2	(M+2H)+2	1.52
256.62429	2	24112.44	C25H28F2N8O2	(M+2H)+2	1.8
257.12683	2	2715.31	C25H28F2N8O2	(M+2H)+2	6.5
257.6261	2	442.92	C25H28F2N8O2	(M+2H)+2	-1.28
511.23779	1	947387.88	C25H28F2N8O2	(M+H)+	0.36
512.24099	1	244045.55	C25H28F2N8O2	(M+H)+	1.18
513.24241	1	39640.75	C25H28F2N8O2	(M+H)+	-1.22

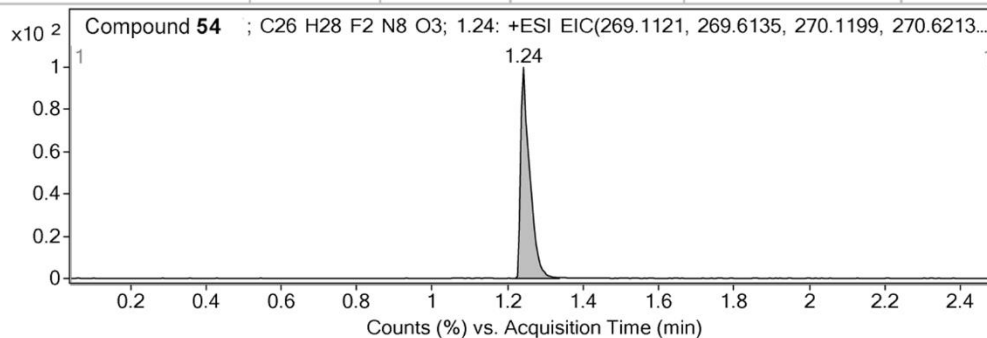
--- End Of Report ---

Compound 54

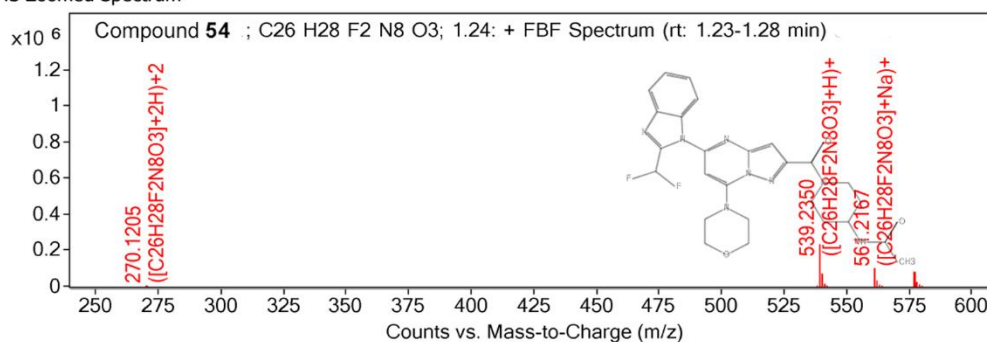


Compound 54

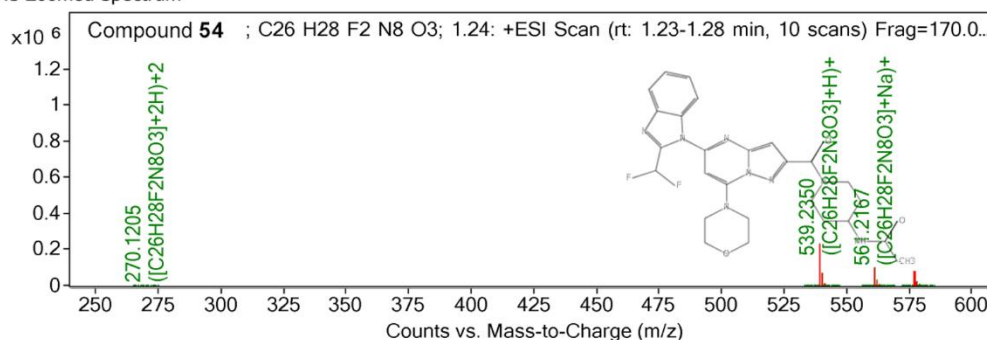
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaorit
Compound 54	561.2167	1.24	538.2275	C26 H28 F2 N8 O3	538.2252	4.19	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

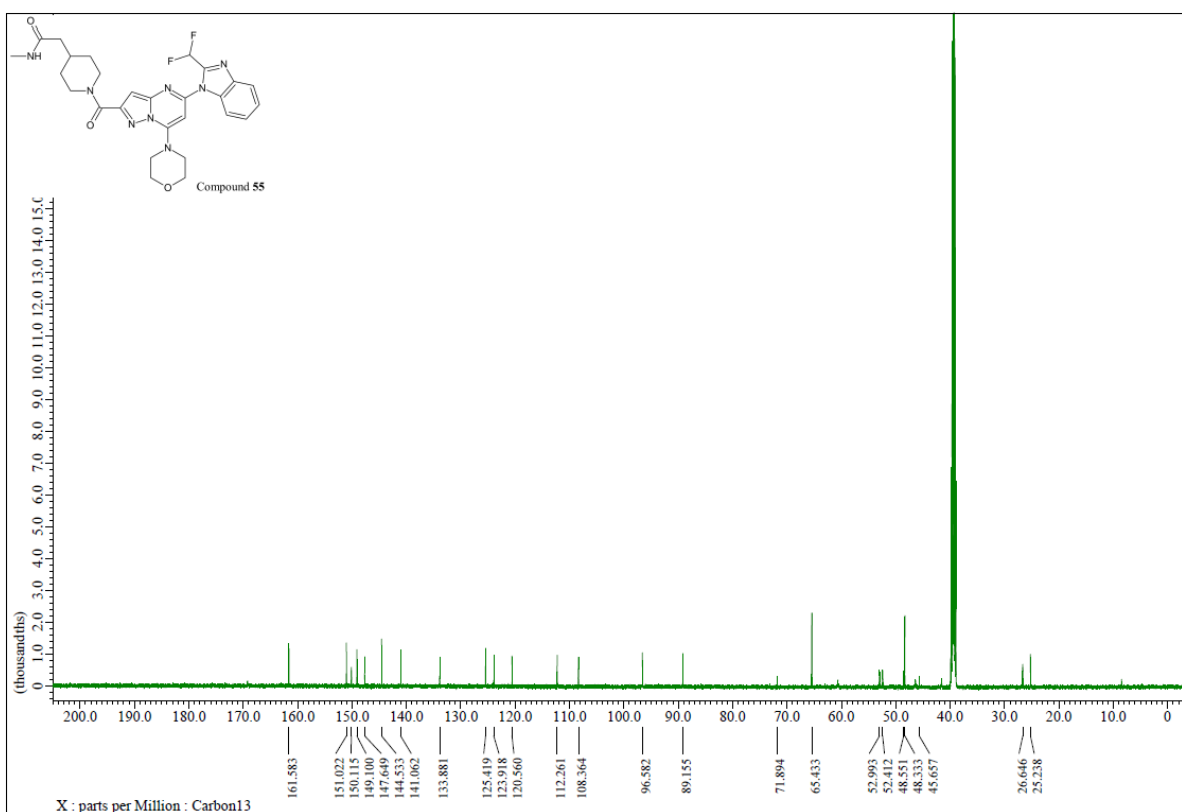
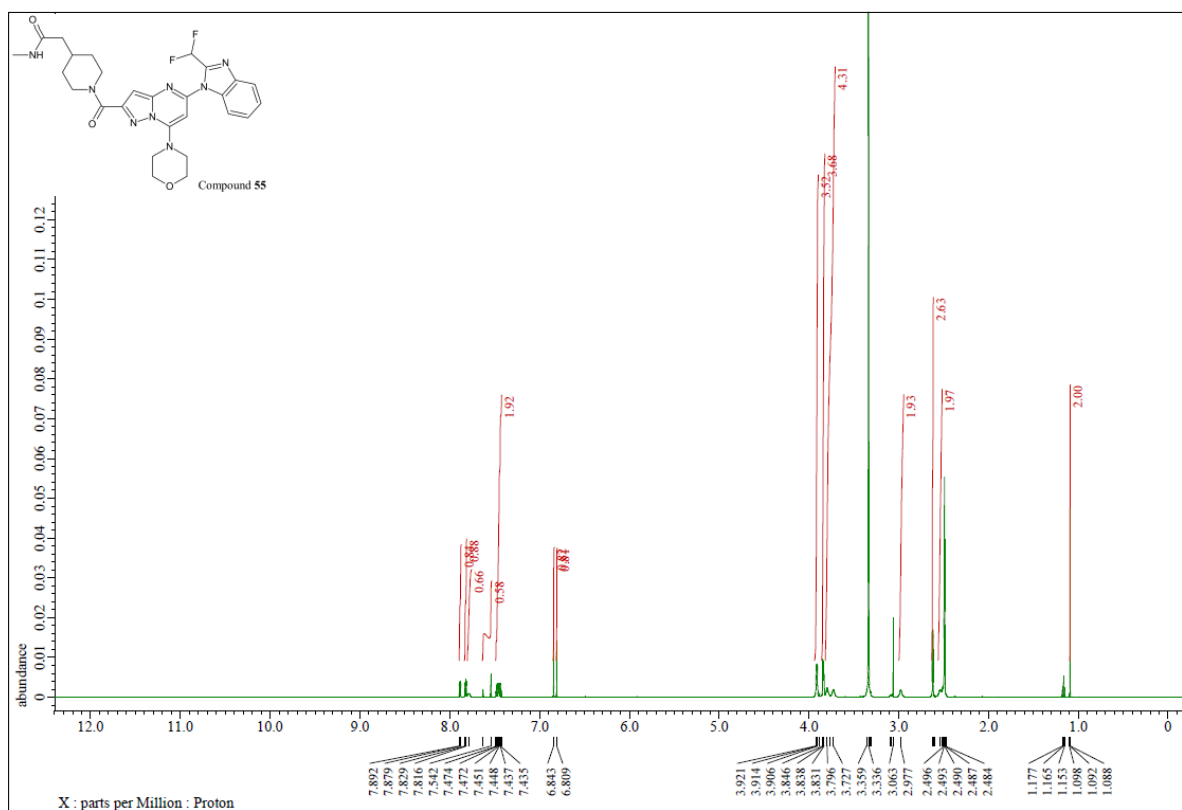


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
539.235	1	231005.8	C26H28F2N8O3	(M+H)+	
539.235	1	231005.8	C26H28F2N8O3	(M+H)+	4.65

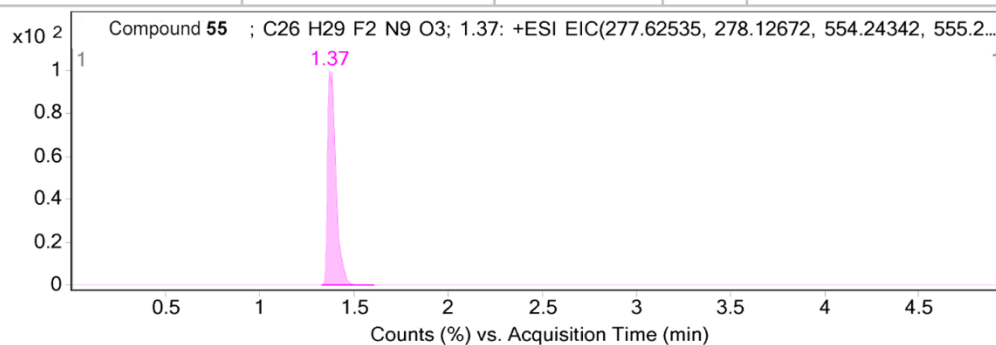
--- End Of Report ---

Compound 55

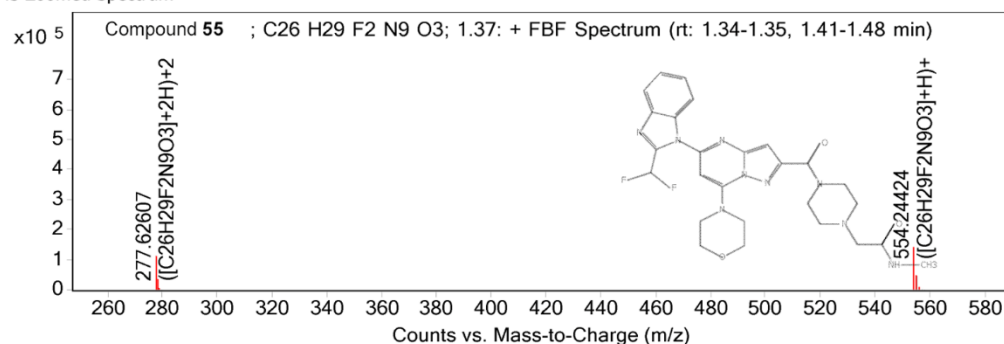


Compound 55

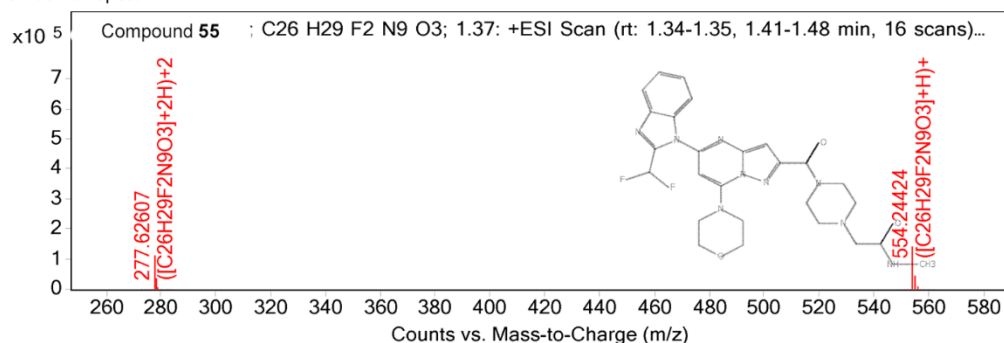
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 55	Compound 55	554.24424	1.37	Find by Formula	553.23715



MS Zoomed Spectrum



MS Zoomed Spectrum

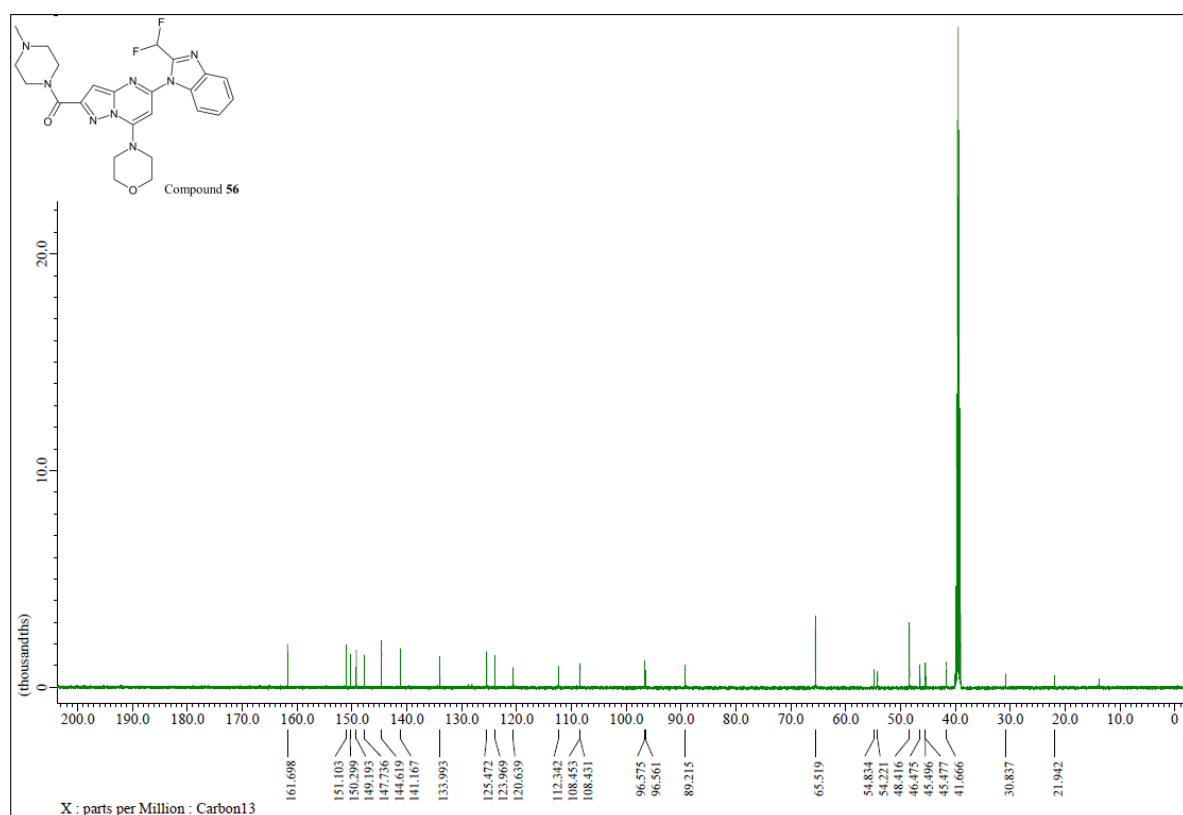
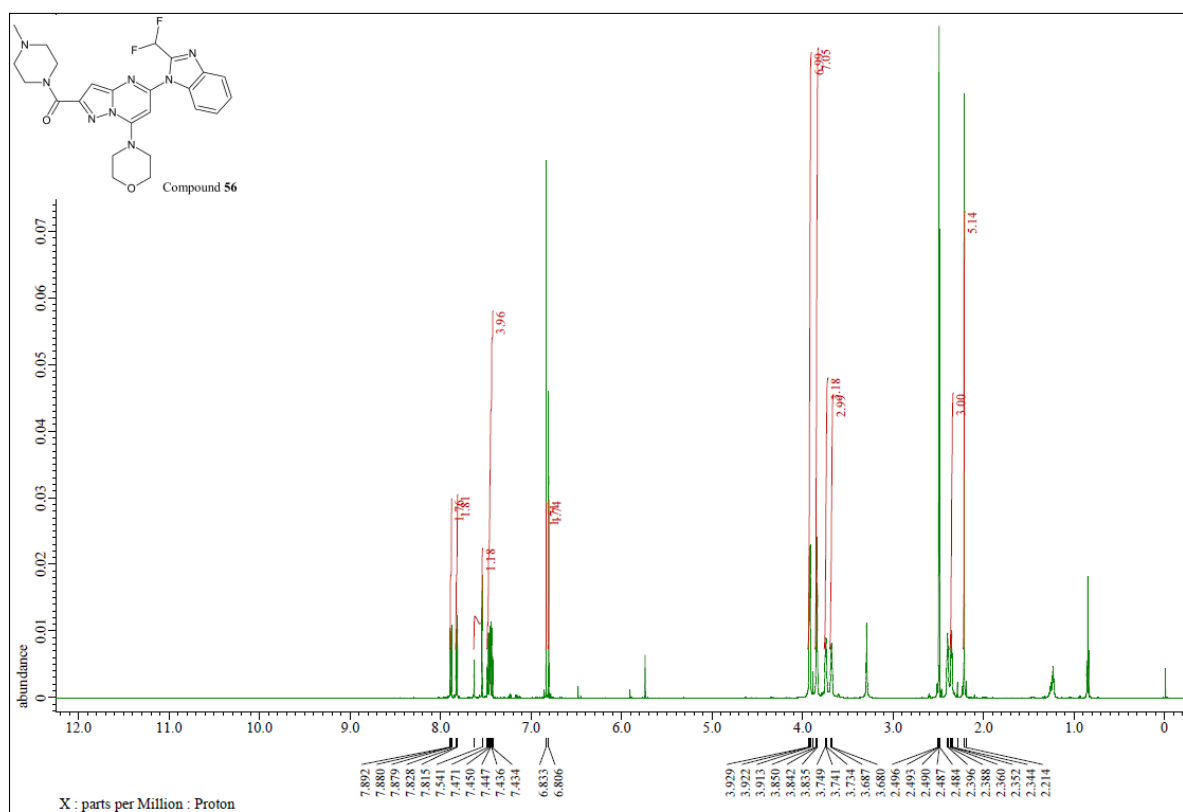


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
277.62607	277.62535	2.62	2	112238.74	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+2H)+2
278.1273	278.12672	2.09	2	35826.95	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+2H)+2
278.62837	278.62801	1.3	2	6205.88	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+2H)+2
279.12947	279.12925	0.76	2	958.56	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+2H)+2
279.62869	279.63048	-6.4	2	61.35	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+2H)+2
554.24424	554.24342	1.47	1	140783.94	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+H)+
555.24673	555.24616	1.03	1	43994.18	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+H)+
556.24896	556.24874	0.41	1	6954.29	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+H)+
557.25101	557.25123	-0.39	1	888.06	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+H)+
558.25274	558.25367	-1.68	1	85.26	C ₂₆ H ₂₉ F ₂ N ₉ O ₃	(M+H)+

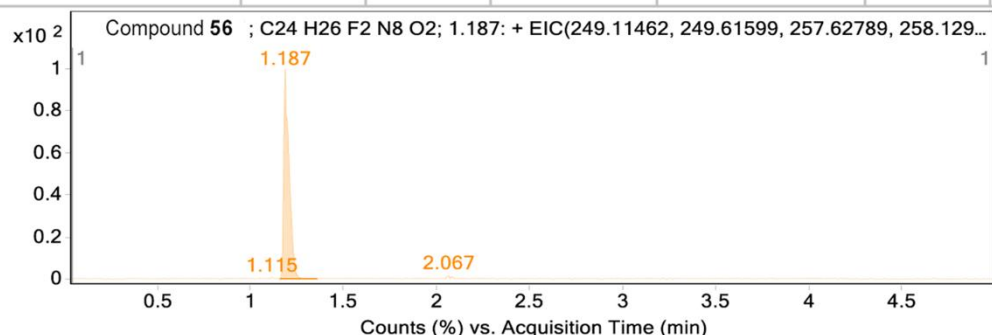
--- End Of Report ---

Compound 56

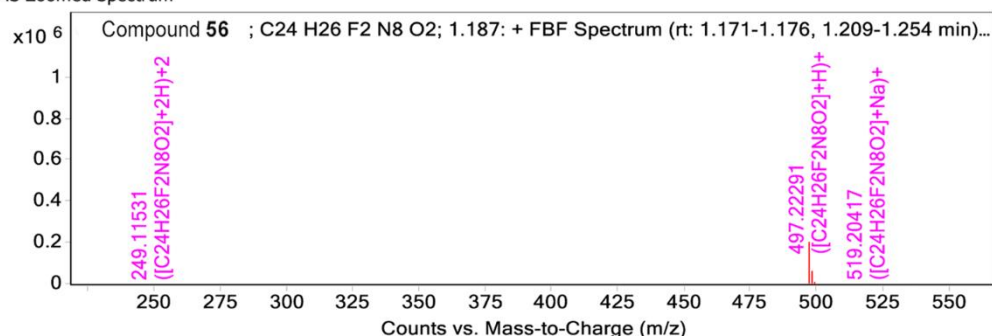


Compound 56

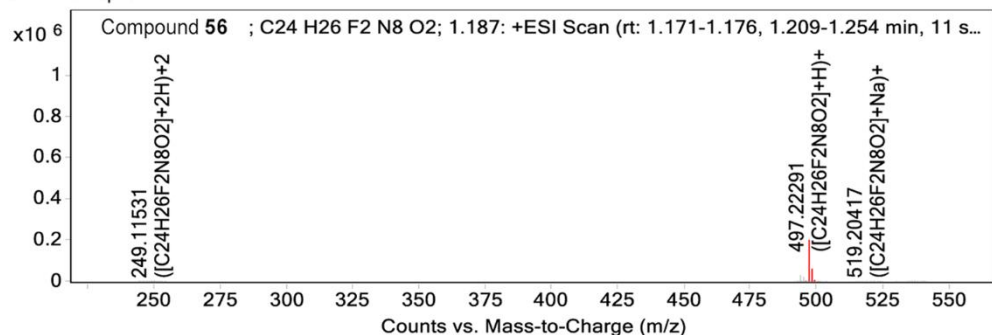
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 56	497.22291	1.187	496.21558	C24 H26 F2 N8 O2	496.21468	1.82	Find by Formula



MS Zoomed Spectrum



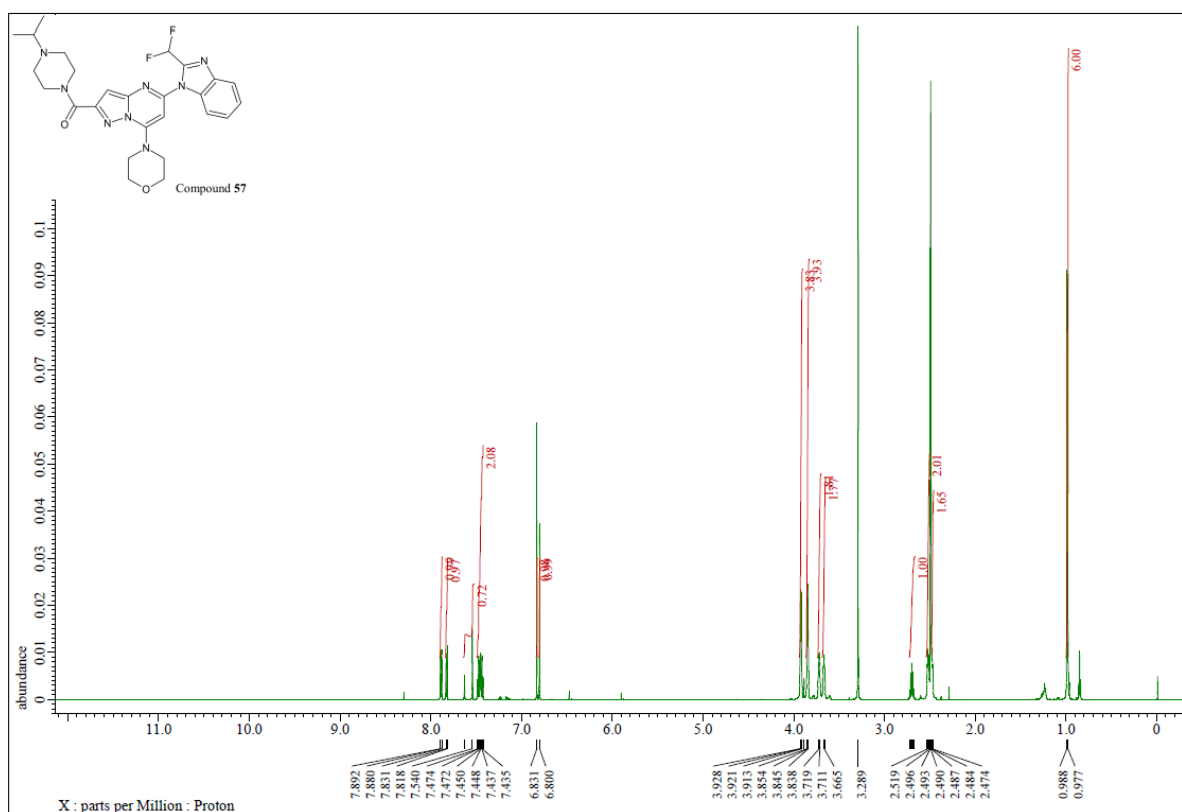
MS Zoomed Spectrum



MS Spectrum Peak List

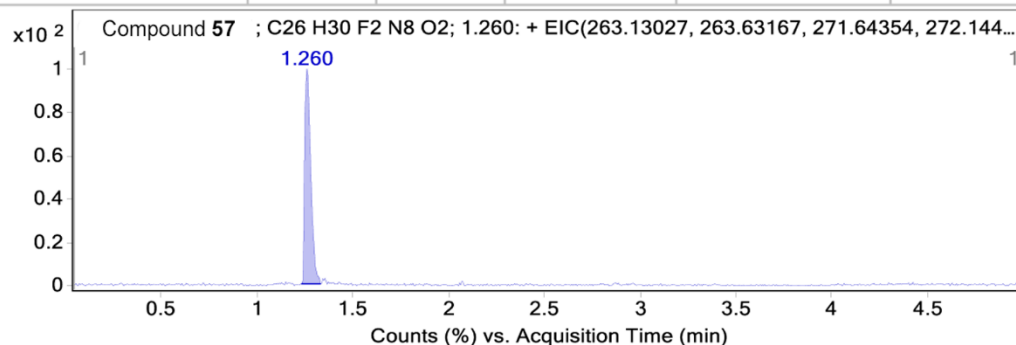
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
249.11531	2	828.16	C24H26F2N8O2	(M+2H)+2	
249.61516	2	252.8	C24H26F2N8O2	(M+2H)+2	
497.22291	1	200608.11	C24H26F2N8O2	(M+H)+	
498.22553	1	53191.16	C24H26F2N8O2	(M+H)+	
499.22792	1	7197.28	C24H26F2N8O2	(M+H)+	
519.20417	1	1904.99	C24H26F2N8O2	(M+Na)+	
520.20623	1	407.84	C24H26F2N8O2	(M+Na)+	
535.17578	1	731.13	C24H26F2N8O2	(M+K)+	
536.18331	1	308.3	C24H26F2N8O2	(M+K)+	
537.17809	1	91.6	C24H26F2N8O2	(M+K)+	
249.11531	2	828.16	C24H26F2N8O2	(M+2H)+2	2.8
249.61516	2	252.8	C24H26F2N8O2	(M+2H)+2	-3.36
497.22291	1	200608.11	C24H26F2N8O2	(M+H)+	1.92
498.22553	1	53191.16	C24H26F2N8O2	(M+H)+	1.63
499.22792	1	7197.28	C24H26F2N8O2	(M+H)+	1.18
519.20417	1	1904.99	C24H26F2N8O2	(M+Na)+	0.53
520.20623	1	407.84	C24H26F2N8O2	(M+Na)+	-0.82
535.17578	1	731.13	C24H26F2N8O2	(M+K)+	-3.85
536.18331	1	308.3	C24H26F2N8O2	(M+K)+	5.08

Compound 57

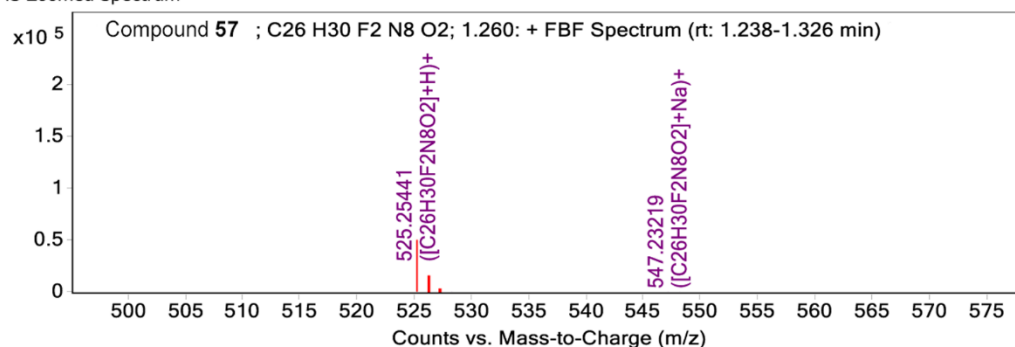


Compound 57

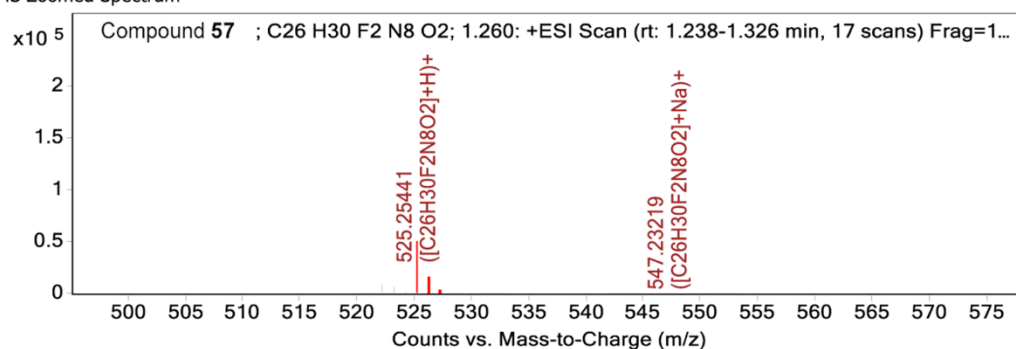
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 57	525.25441	1.26	524.24697	C26 H30 F2 N8 O2	524.24598	1.88	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
525.25441	1	49401.69	C26H30F2N8O2	(M+H)+	
526.2567	1	14426.26	C26H30F2N8O2	(M+H)+	
527.25916	1	2182.63	C26H30F2N8O2	(M+H)+	
528.25892	1	364.03	C26H30F2N8O2	(M+H)+	
547.23219	1	209.02	C26H30F2N8O2	(M+Na)+	
548.2421	1	55.47	C26H30F2N8O2	(M+Na)+	
525.25441	1	49401.69	C26H30F2N8O2	(M+H)+	2.19
526.2567	1	14426.26	C26H30F2N8O2	(M+H)+	1.21
527.25916	1	2182.63	C26H30F2N8O2	(M+H)+	0.8
528.25892	1	364.03	C26H30F2N8O2	(M+H)+	-4.53
547.23219	1	209.02	C26H30F2N8O2	(M+Na)+	-5.5
548.2421	1	55.47	C26H30F2N8O2	(M+Na)+	7.47

--- End Of Report ---