

Supplementary data

for

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

Mariola Stypik^{1,2*}, Marcin Zagozda¹, Stanisław Michałek^{1,2}, Barbara Dymek¹, Daria Zdżalik-Bielecka¹, Maciej Dziachan¹, Nina Orłowska^{1,2}, Paweł Gunerka¹, Paweł Turowski¹, Joanna Hucz-Kalitowska¹, Aleksandra Stańczak¹, Paulina Stańczak¹, Krzysztof Mulewski¹, Damian Smuga¹, Filip Stefaniak¹, Lidia Gurba-Bryśkiewicz¹, Arkadiusz Leniak¹, Zbigniew Ochal², Mateusz Mach¹, Karolina Dzwonek¹, Monika Lamparska-Przybysz¹, Krzysztof Dubiel¹, Maciej Wieczorek¹

¹ Celon Pharma S.A. ul. Marymoncka 15, 05-152 Kązuoł Nowy, Poland

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

*corresponding author: mariola.stypik@celonpharma.com

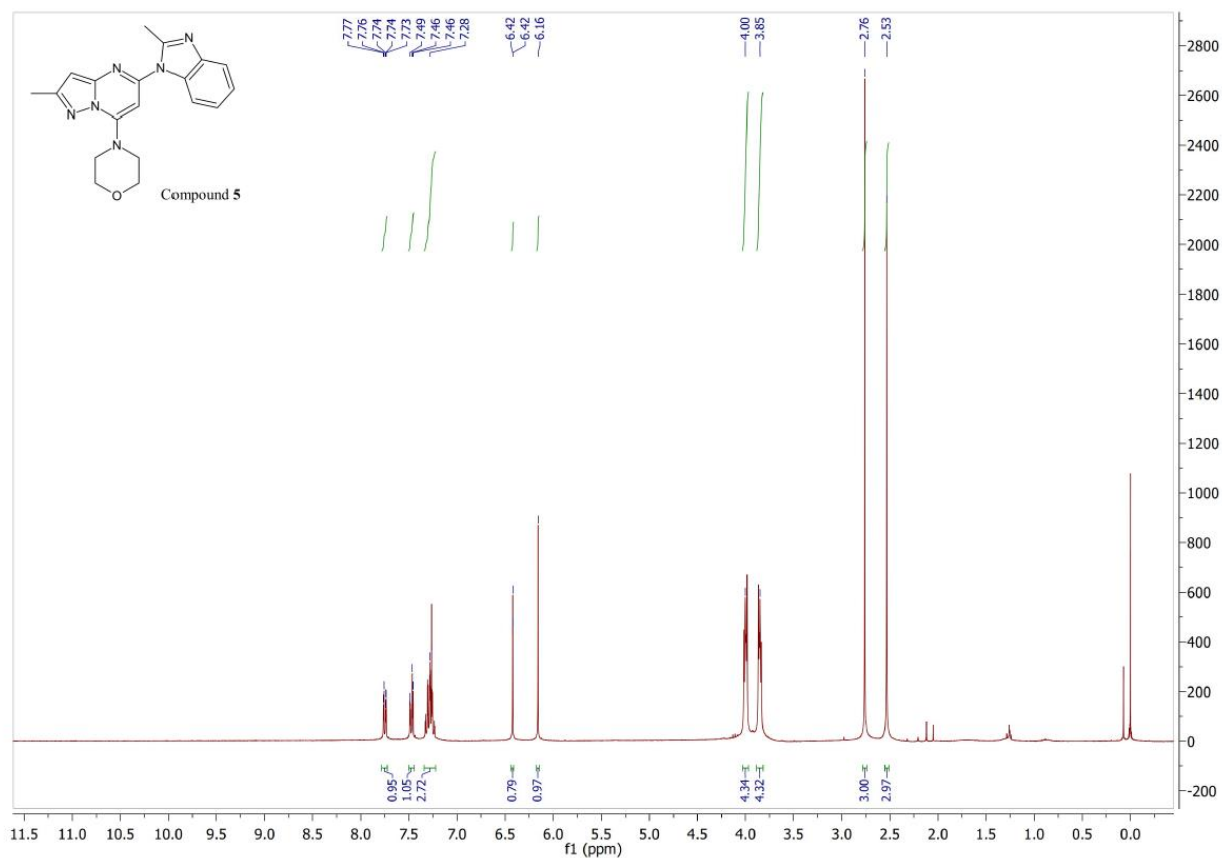
¹H NMR, ¹³C NMR and HRMS supplementary figures of the final compounds **5-13**, **23-45**, **49-51** and **53-55**

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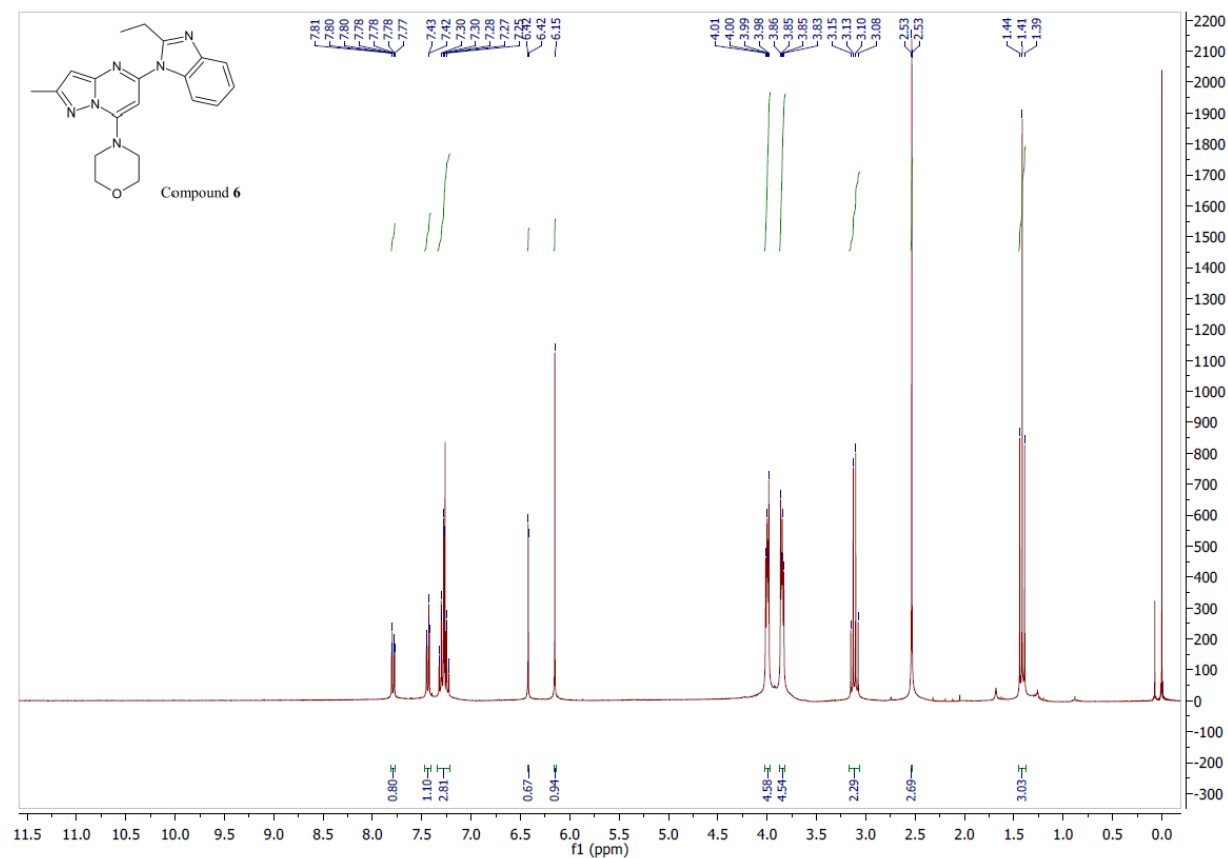
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Compound 54 ^1H NMR and ^{13}C NMR	60
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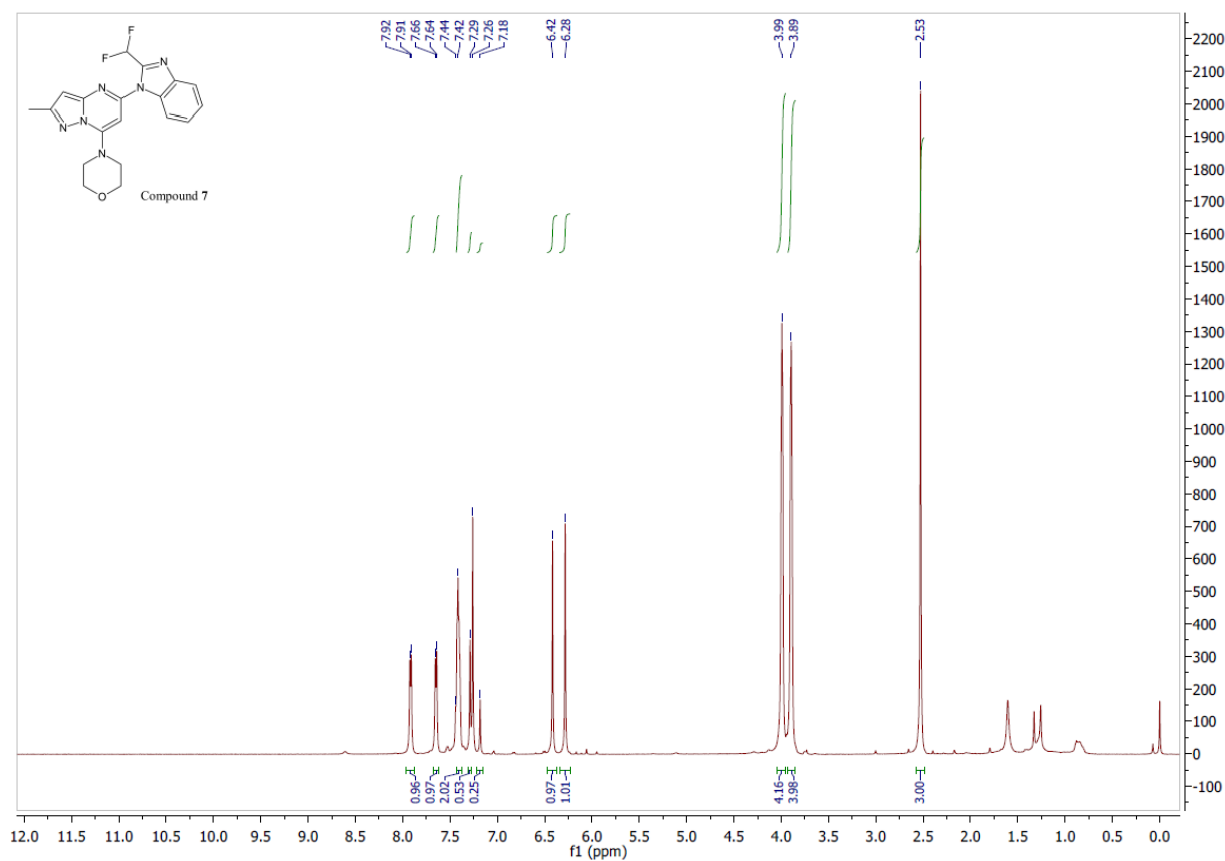
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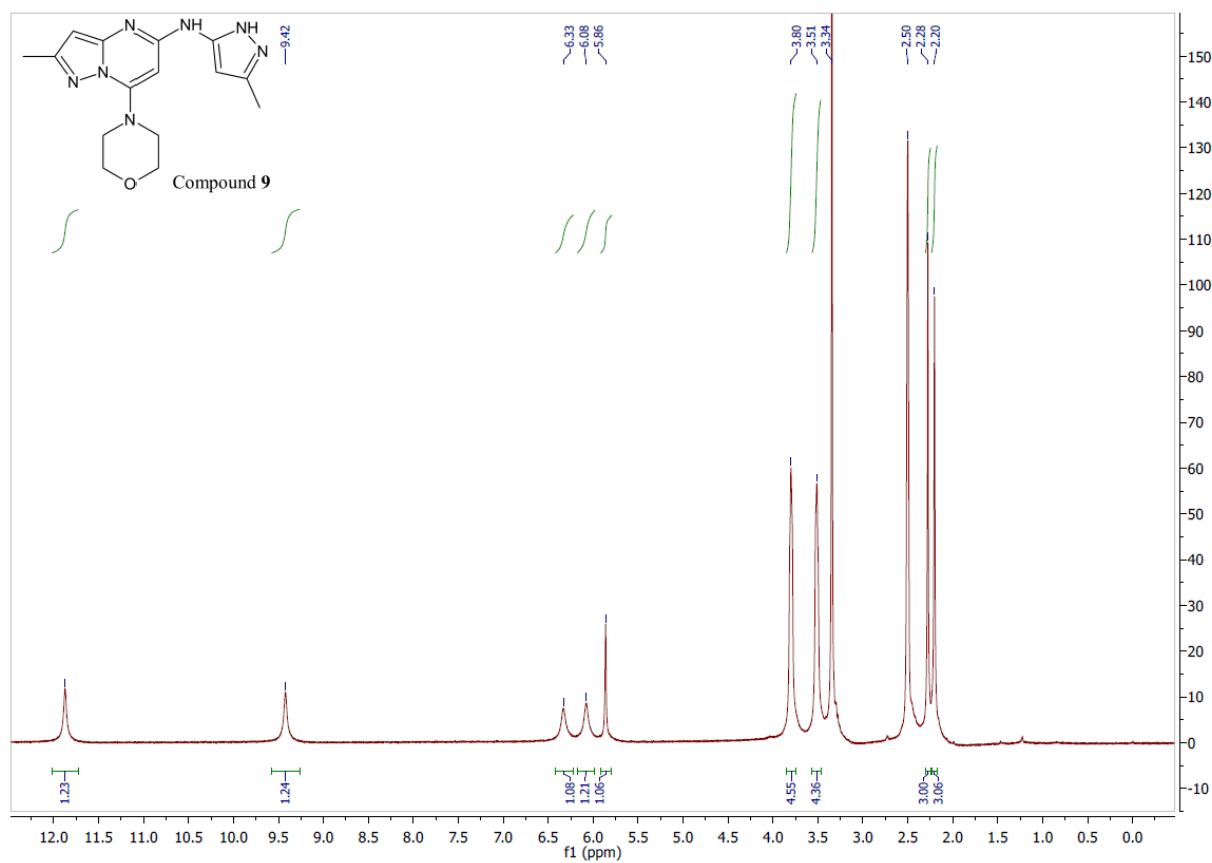
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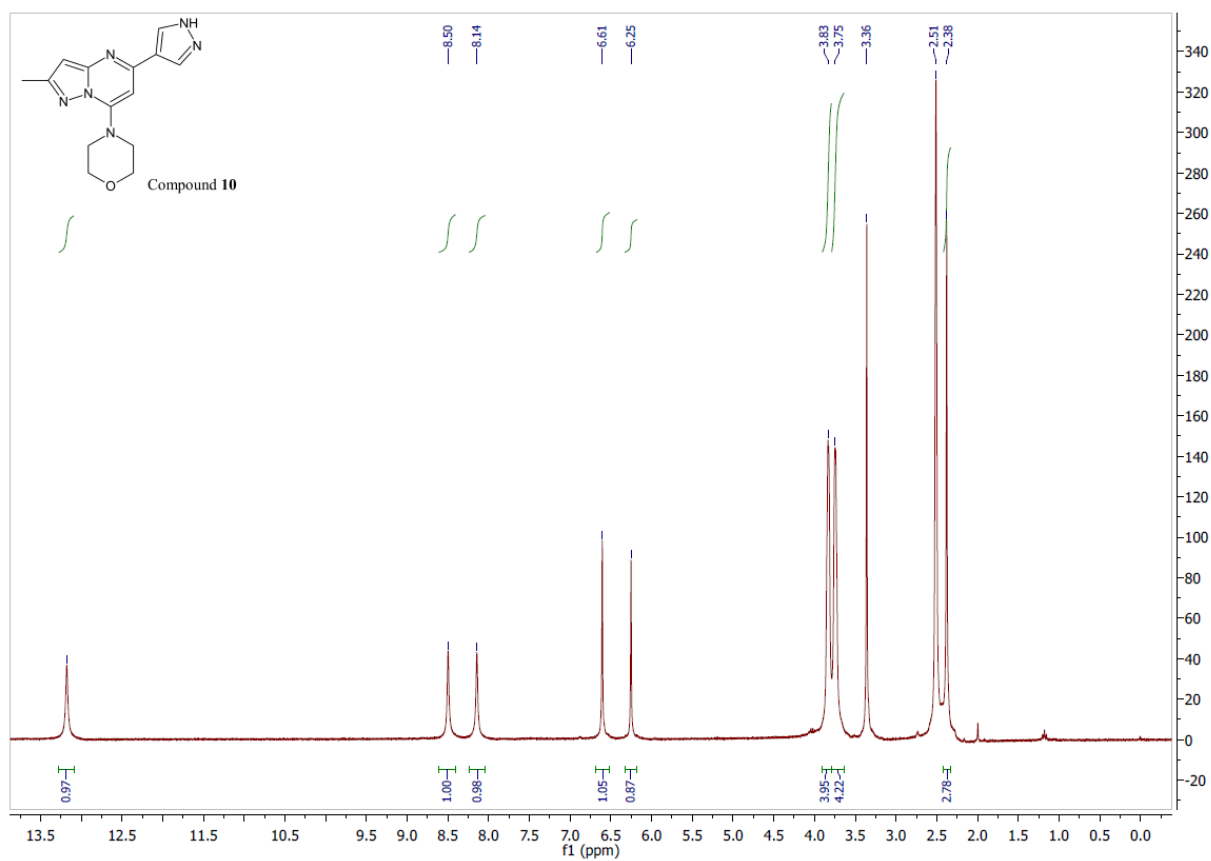
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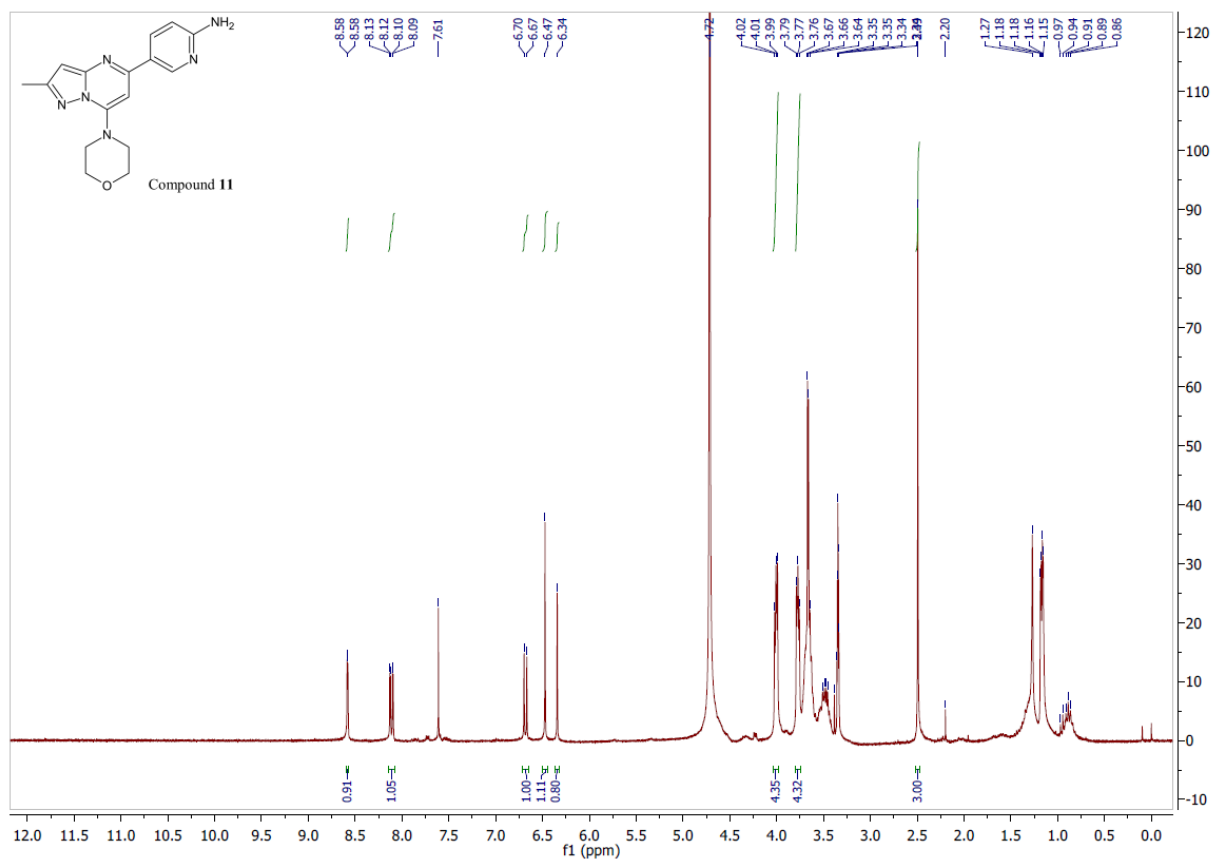
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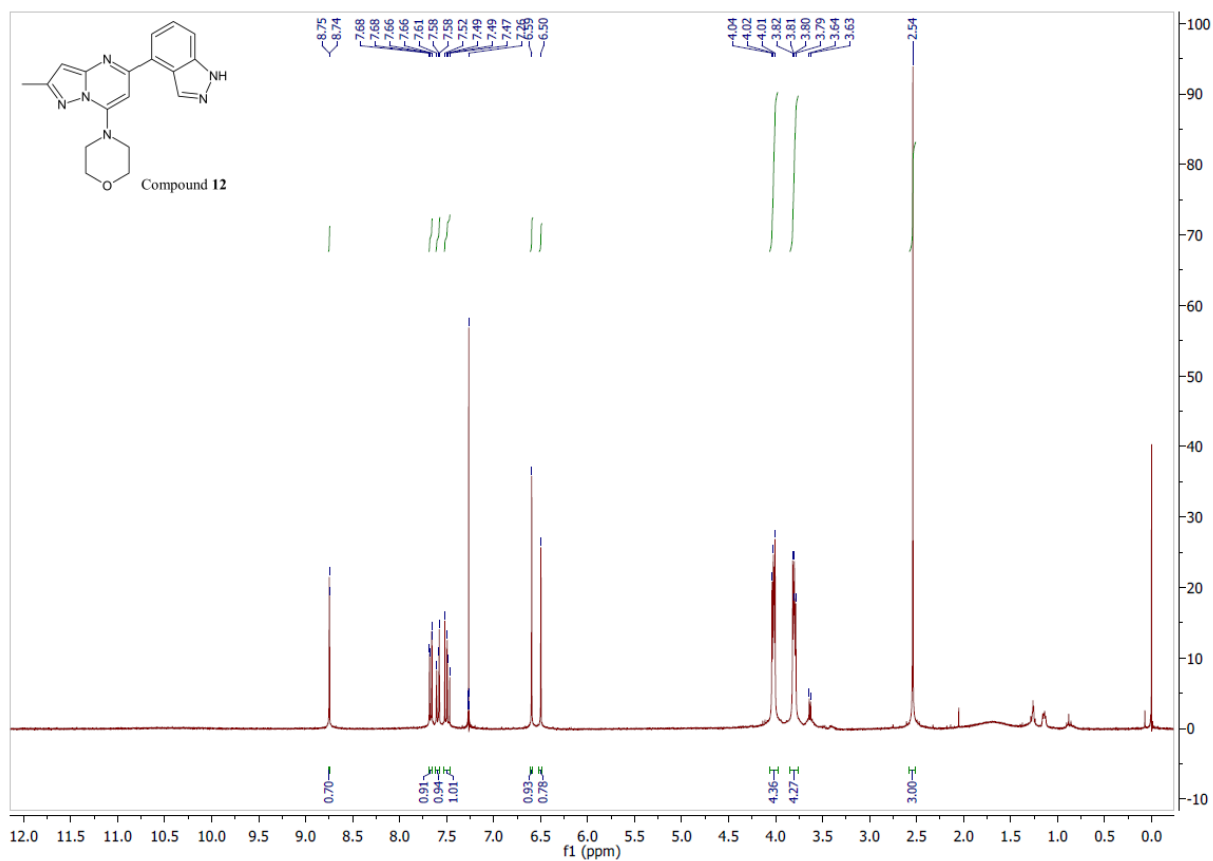
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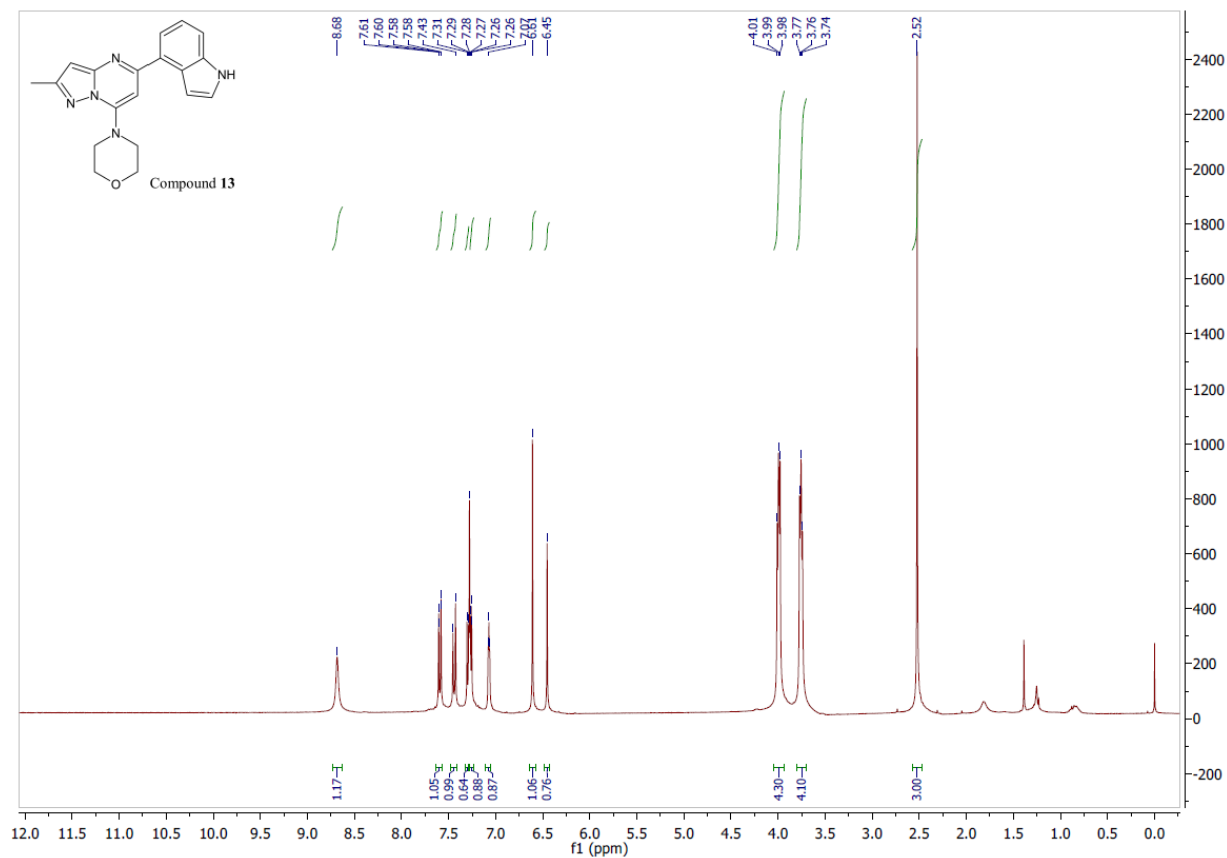
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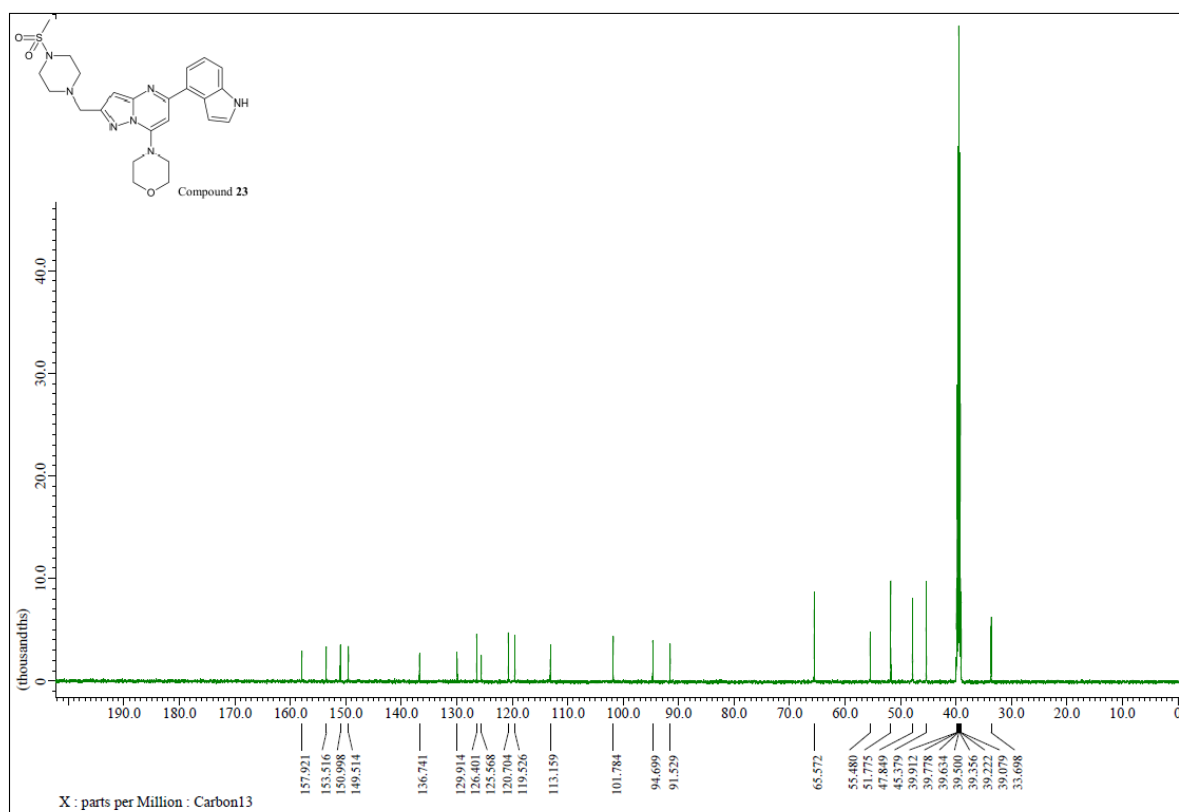
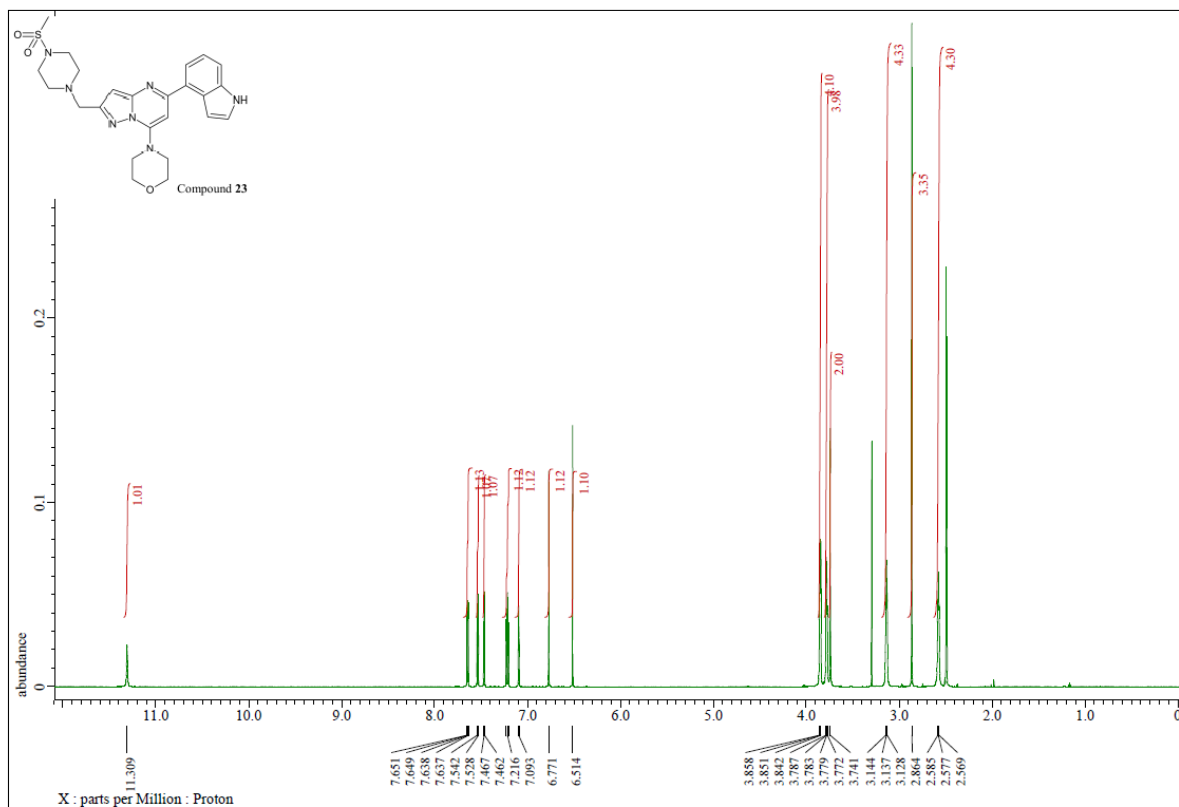
Compound 12



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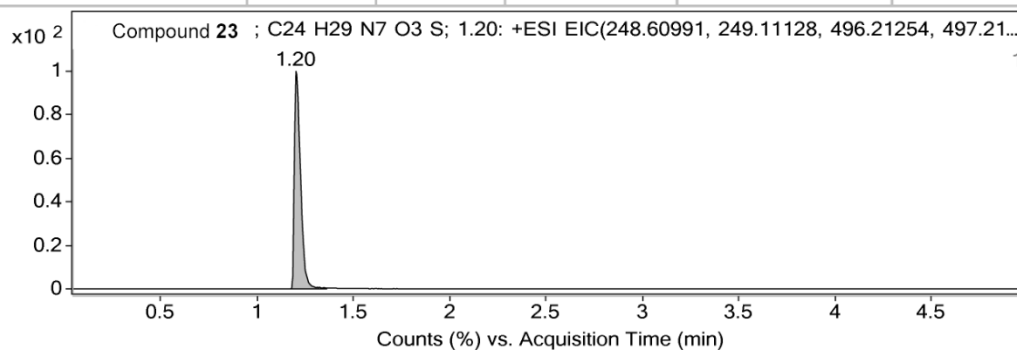


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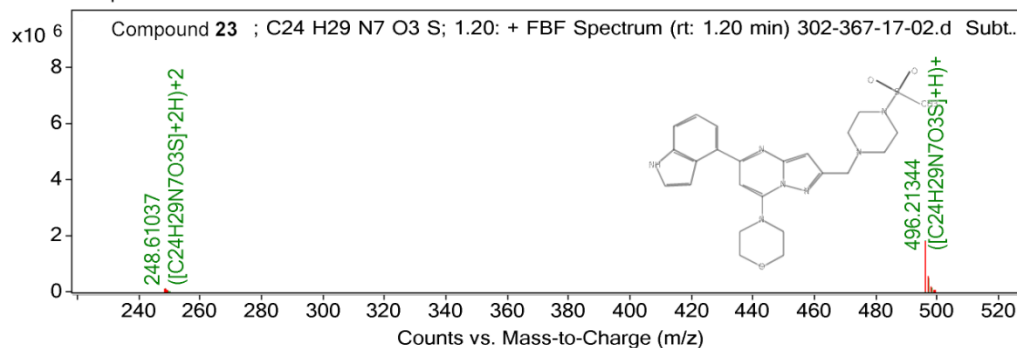


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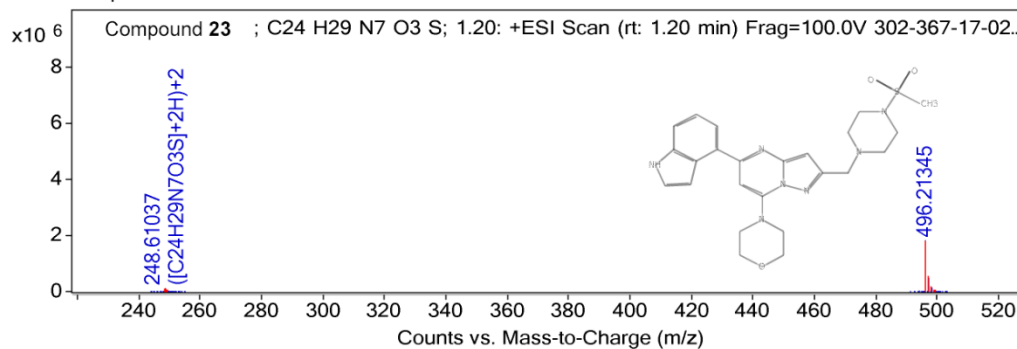
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpbs Alaoirit
Compound 23	248.61037	1.2	495.2061	C24 H29 N7 O3 S	495.20526	1.69	Find by Formula



MS Zoomed Spectrum



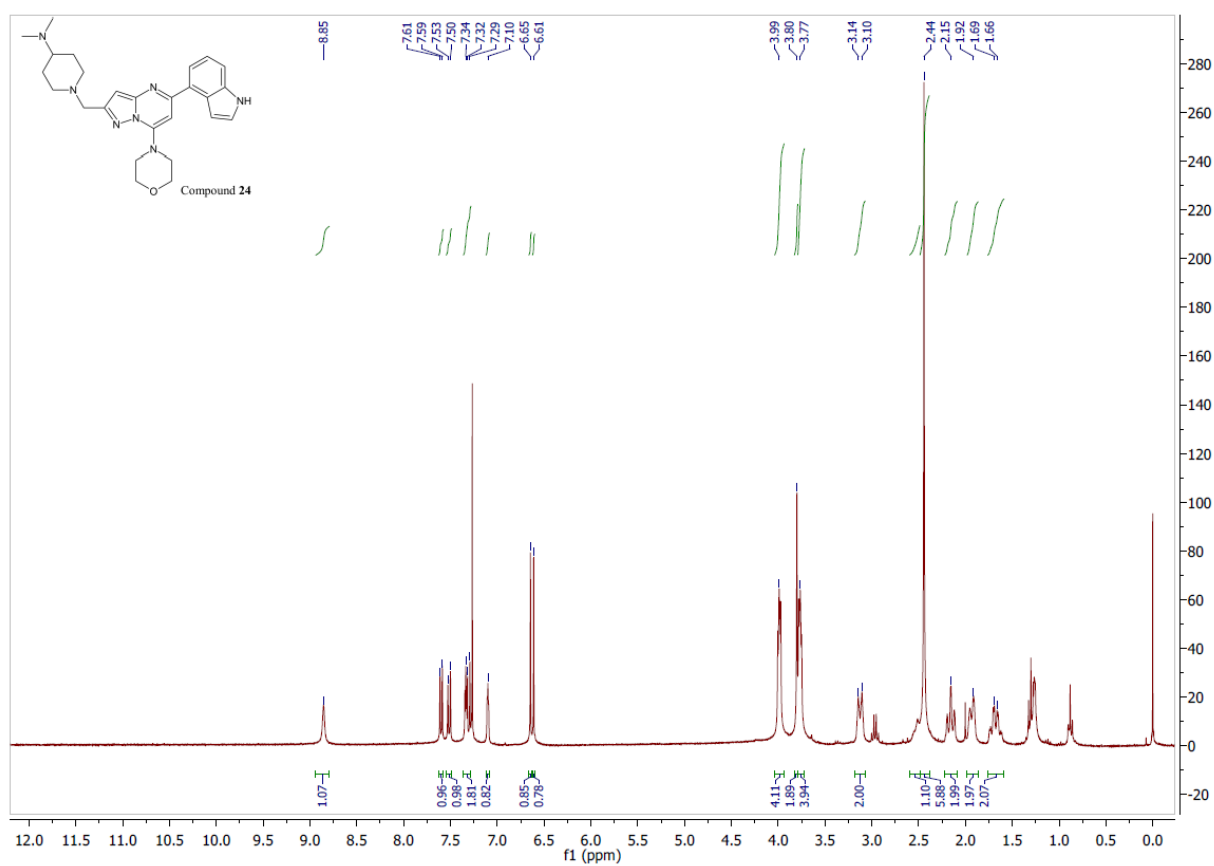
MS Zoomed Spectrum



MS Spectrum Peak List

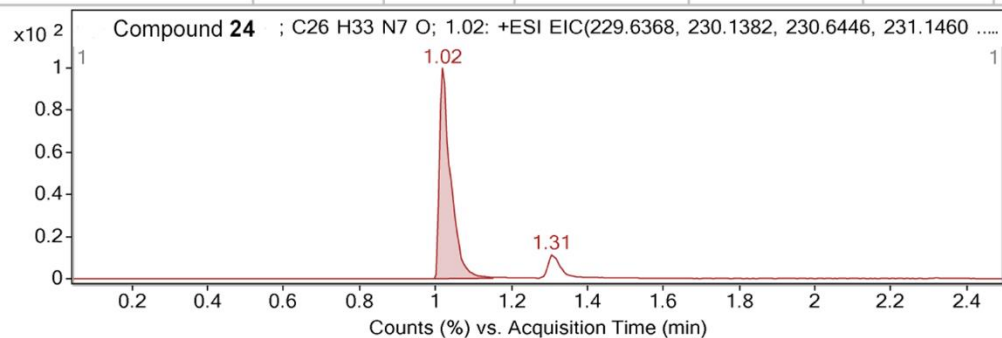
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
248.61037	2	102185.98	C24H29N7O3S	(M+2H)+2	
249.11171	2	27759.85	C24H29N7O3S	(M+2H)+2	
249.6106	2	9742.93	C24H29N7O3S	(M+2H)+2	
250.11214	2	2644.55	C24H29N7O3S	(M+2H)+2	
496.21344	1	1807565	C24H29N7O3S	(M+H)+	
497.2157	1	473910.06	C24H29N7O3S	(M+H)+	
498.21467	1	127993.41	C24H29N7O3S	(M+H)+	
499.21422	1	21856.06	C24H29N7O3S	(M+H)+	
248.61037	2	102185.98	C24H29N7O3S	(M+2H)+2	1.85
249.11171	2	27759.85	C24H29N7O3S	(M+2H)+2	1.72
249.6106	2	9742.93	C24H29N7O3S	(M+2H)+2	1.25
250.11214	2	2644.55	C24H29N7O3S	(M+2H)+2	5.99
496.21344	1	1807565	C24H29N7O3S	(M+H)+	1.83
496.21345		1811059.88			
497.2157	1	473910.06	C24H29N7O3S	(M+H)+	0.84
498.21467	1	127993.41	C24H29N7O3S	(M+H)+	2.74
499.21422	1	21856.06	C24H29N7O3S	(M+H)+	0.44

Compound 24

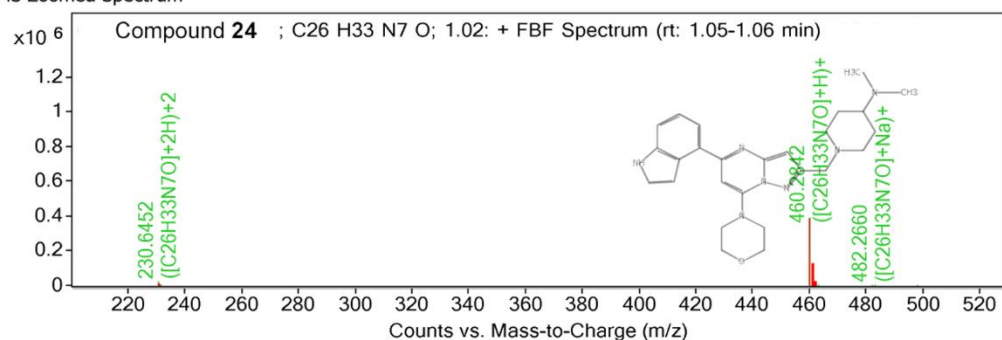


Compound 24

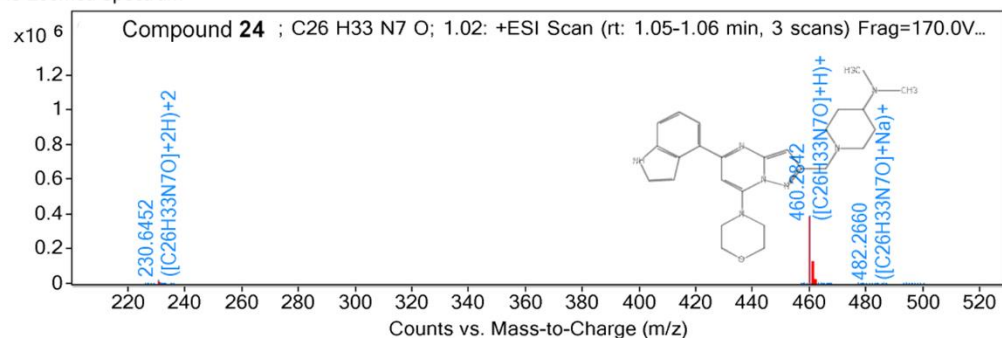
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 24	460.2842	1.02	459.2768	C26 H33 N7 O	459.2747	4.76	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

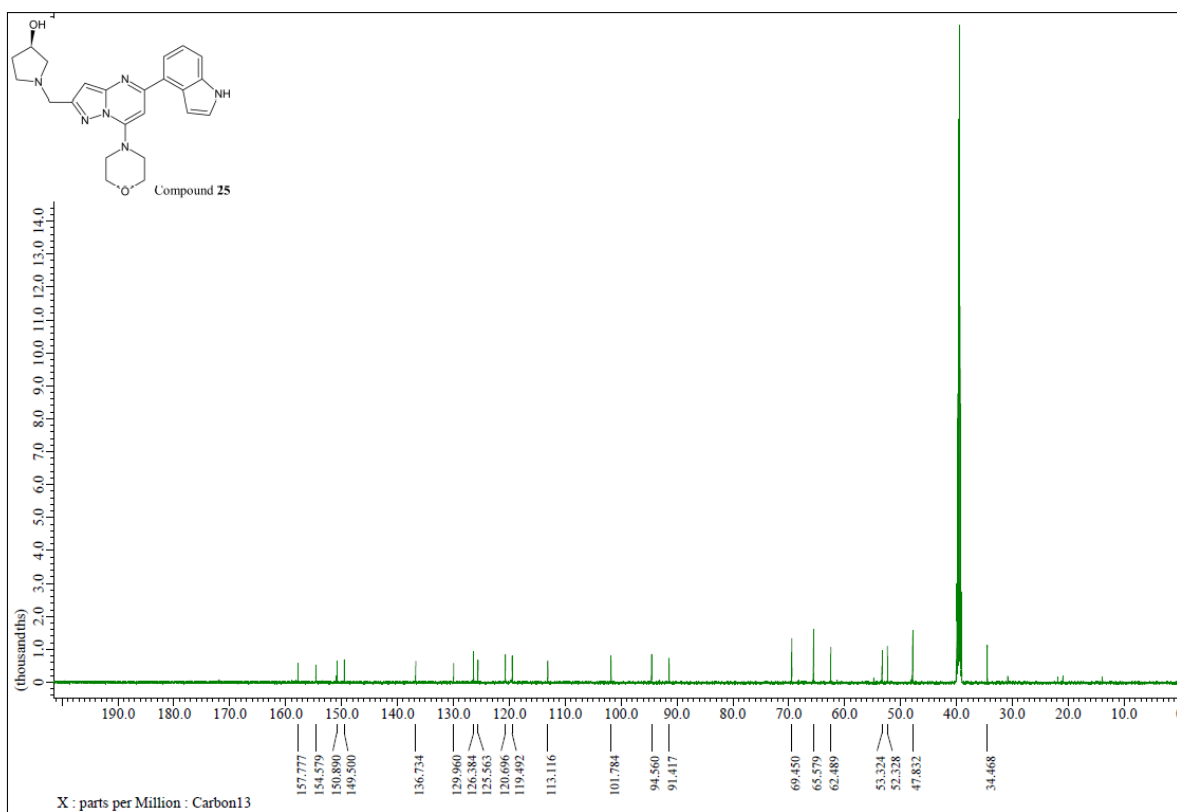
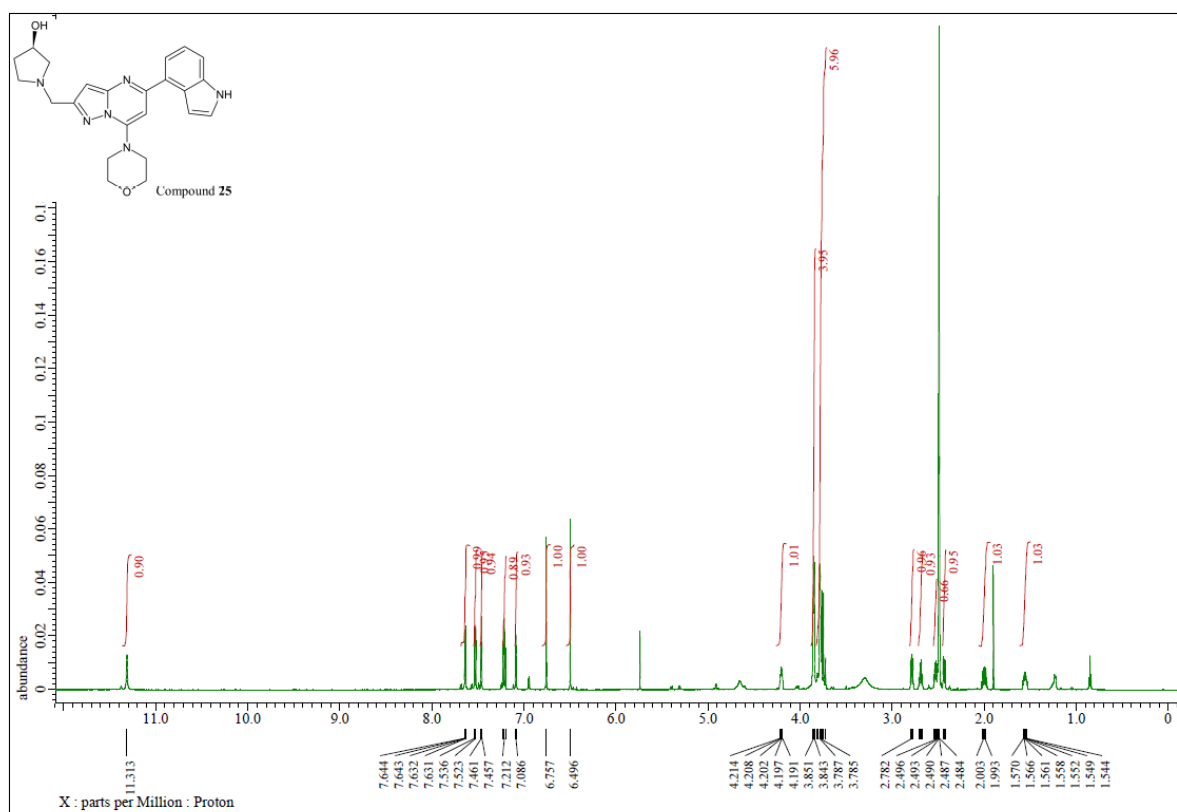


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
460.2842	1	387752.75	C26H33N7O	(M+H)+	
460.2842	1	387752.75	C26H33N7O	(M+H)+	5

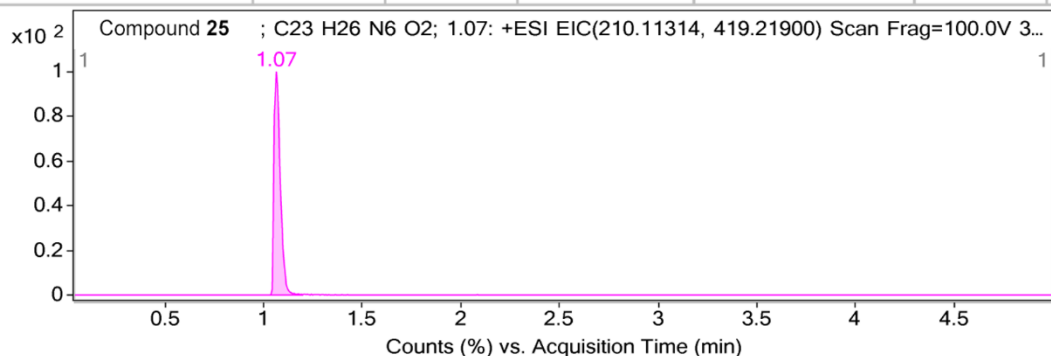
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Compound 25

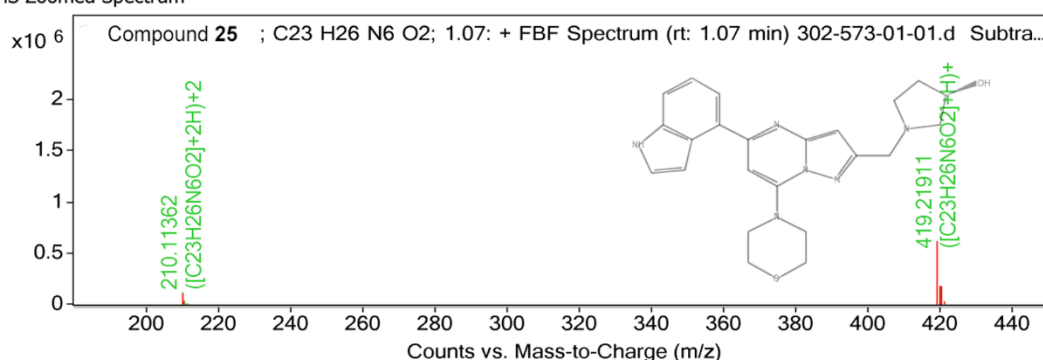


Compound 25

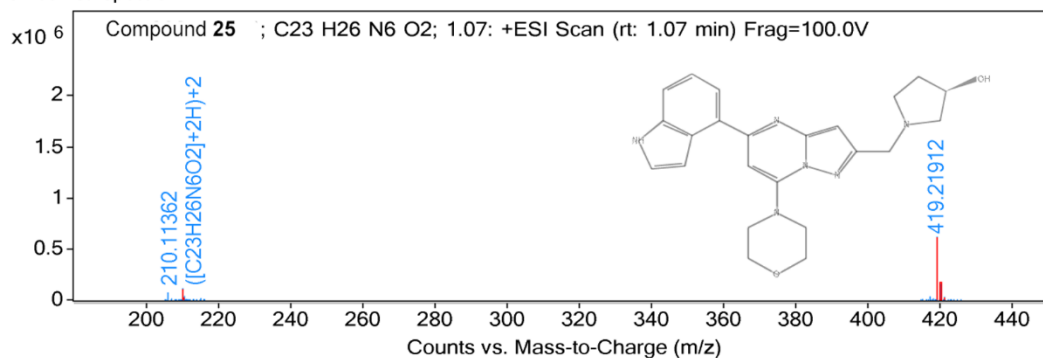
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Algorit
Compound 25	419.21911	1.07	418.21196	C23 H26 N6 O2	418.21172	0.57	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

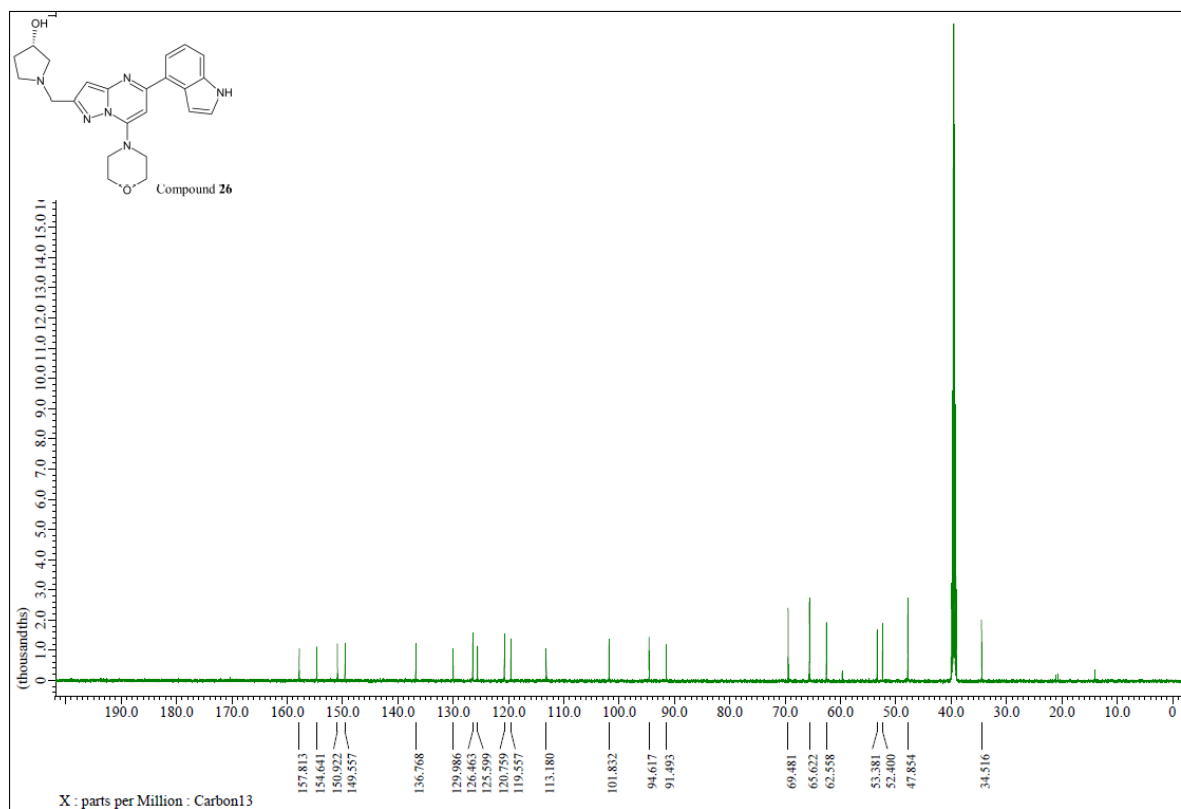
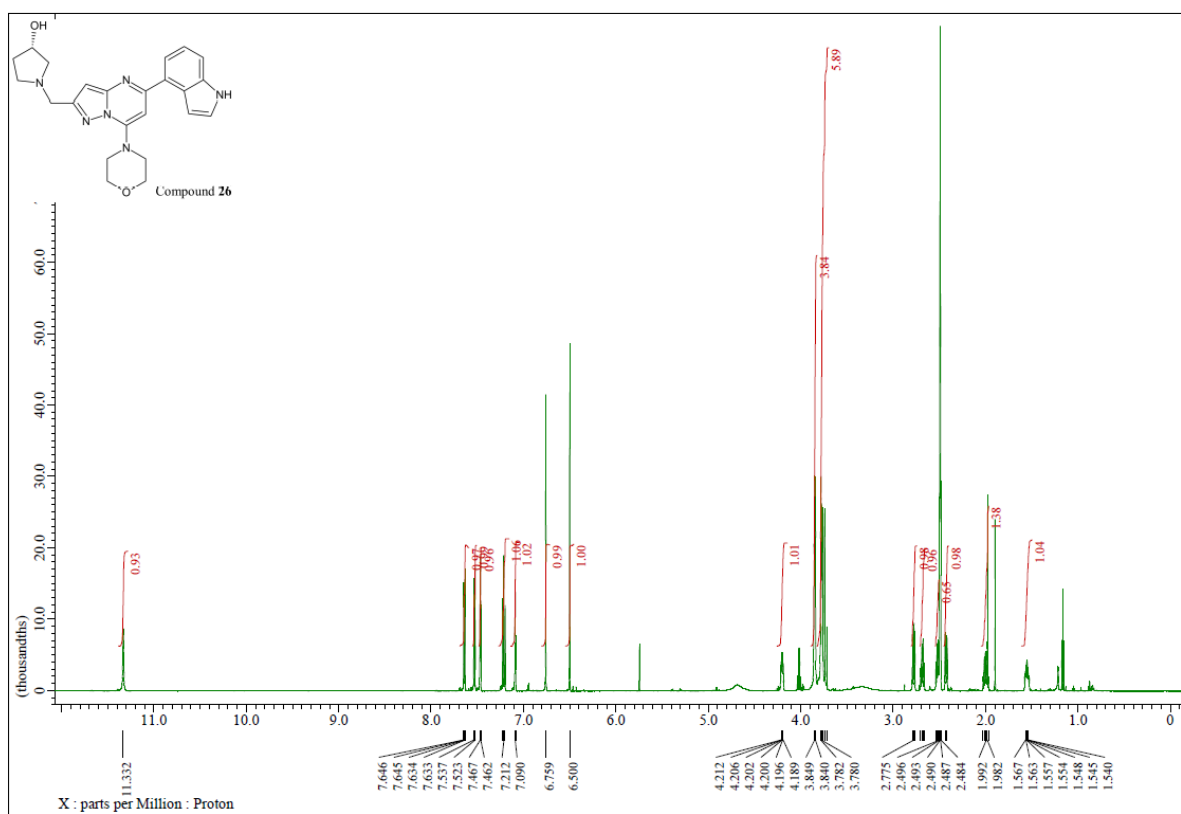


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
210.11362	2	107105.88	C23H26N6O2	(M+2H)+2	
210.61466	2	33089.72	C23H26N6O2	(M+2H)+2	
211.11704	2	4649.13	C23H26N6O2	(M+2H)+2	
211.61535	2	736.03	C23H26N6O2	(M+2H)+2	
419.21911	1	612612	C23H26N6O2	(M+H)+	
420.22217	1	149687.05	C23H26N6O2	(M+H)+	
421.2243	1	22332.43	C23H26N6O2	(M+H)+	
210.11362	2	107105.88	C23H26N6O2	(M+2H)+2	2.31
210.61466	2	33089.72	C23H26N6O2	(M+2H)+2	0.38
211.11704	2	4649.13	C23H26N6O2	(M+2H)+2	5.23
211.61535	2	736.03	C23H26N6O2	(M+2H)+2	-8.95
419.21911	1	612612	C23H26N6O2	(M+H)+	0.27
419.21912		613355.75			
420.22217	1	149687.05	C23H26N6O2	(M+H)+	0.68
421.2243	1	22332.43	C23H26N6O2	(M+H)+	-0.71

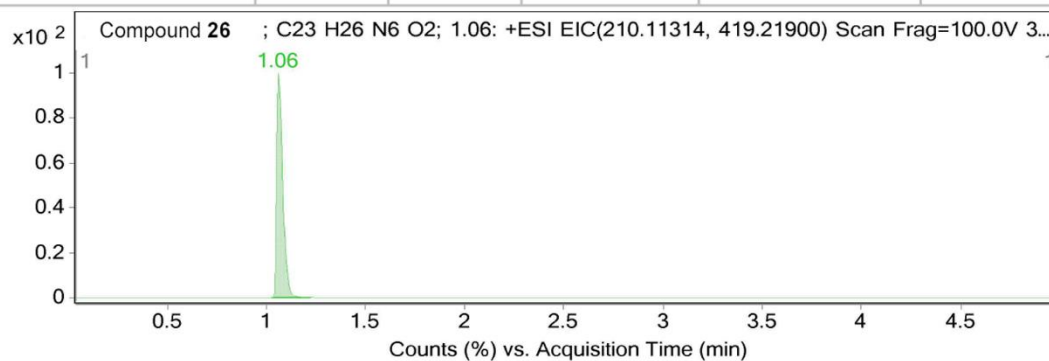
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Compound 26

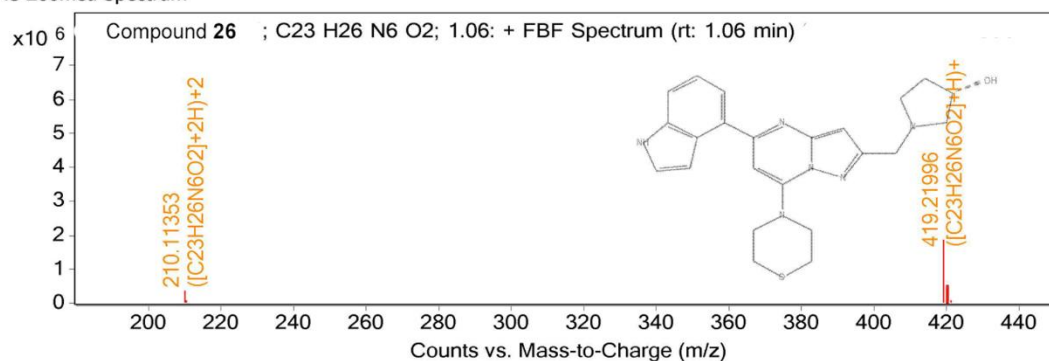


Compound 26

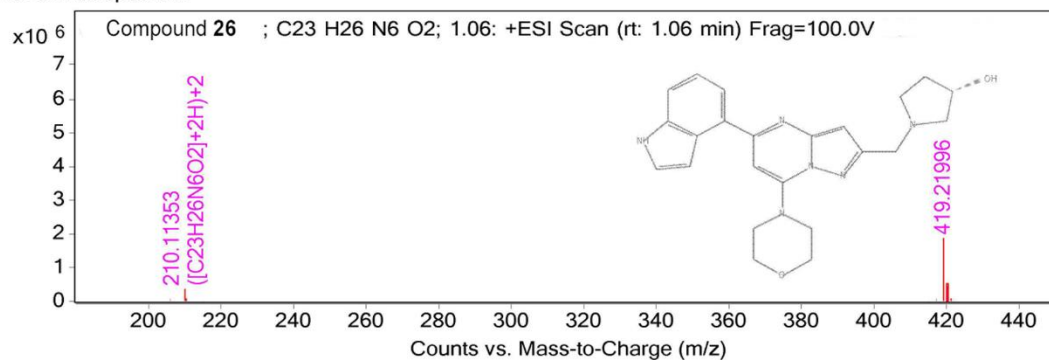
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorit
Compound 26	210.11353	1.06	418.21255	C23 H26 N6 O2	418.21172	1.98	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

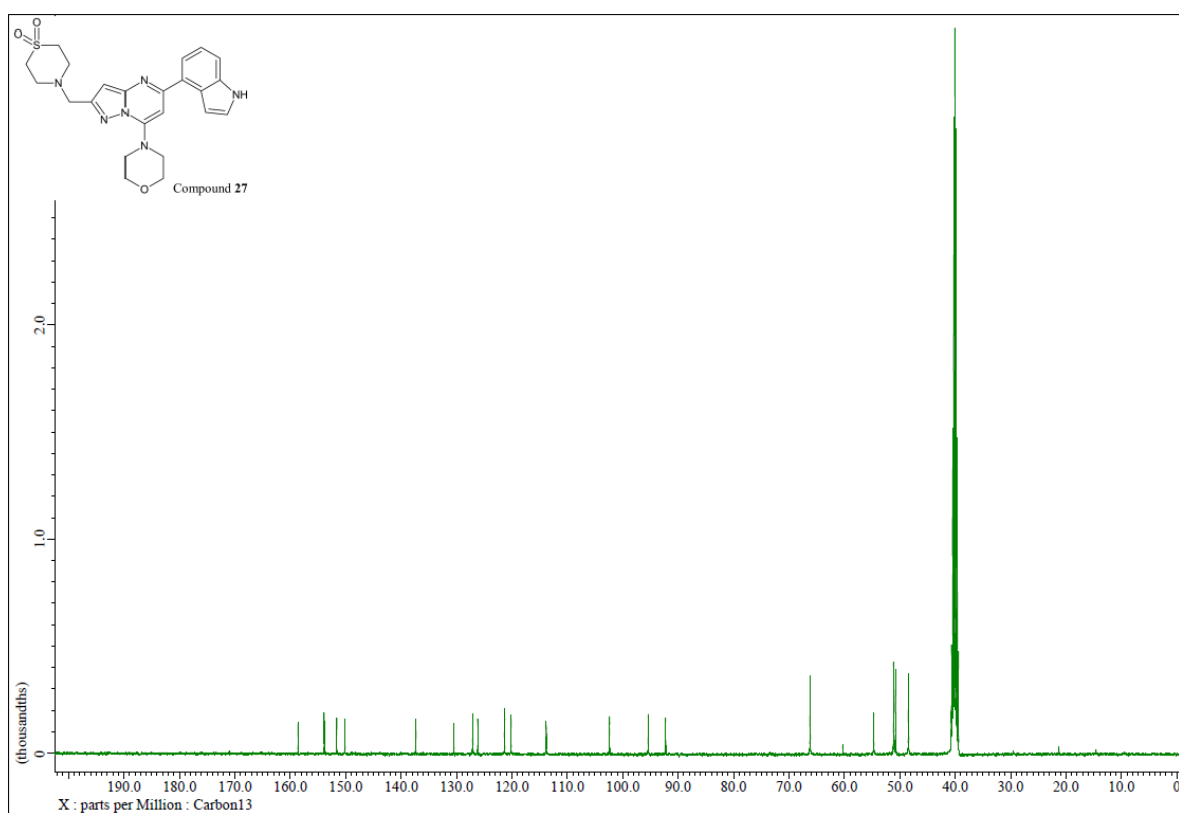
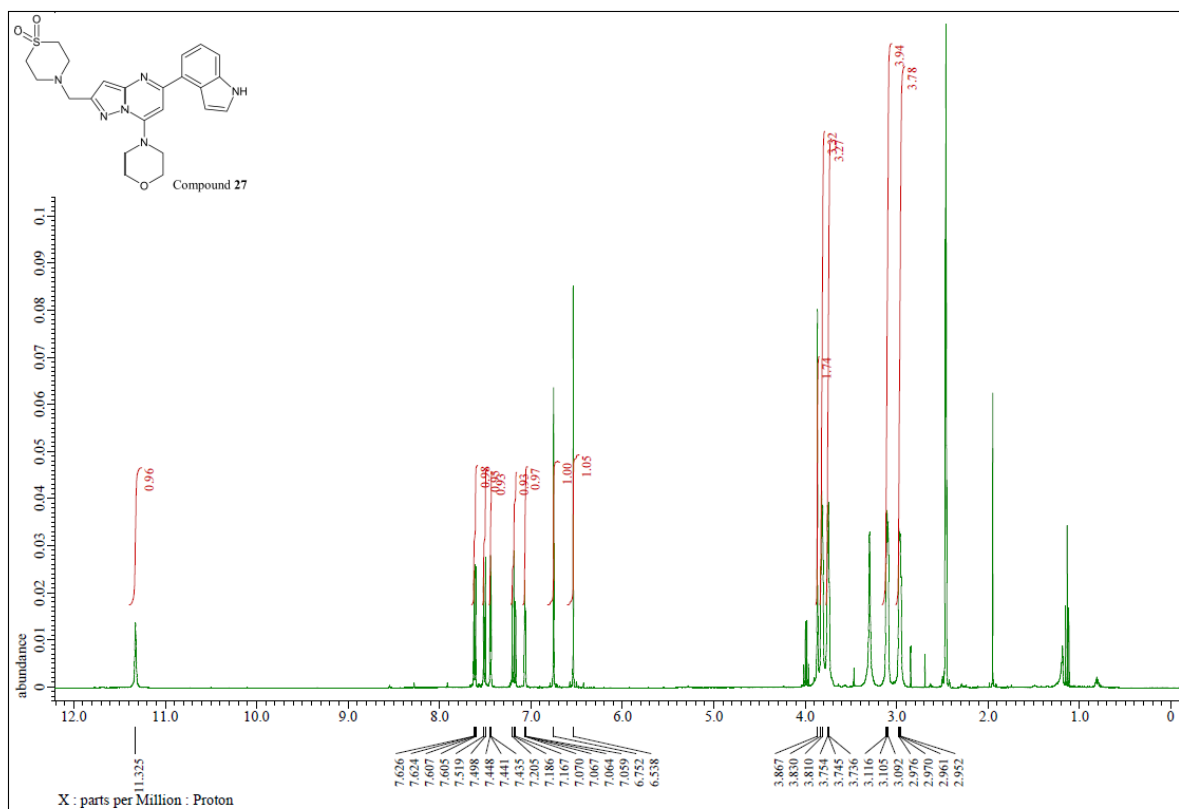


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
210.11353	2	350755.53	C23H26N6O2	(M+2H)+2	
210.61496	2	90613.7	C23H26N6O2	(M+2H)+2	
211.11719	2	12392.01	C23H26N6O2	(M+2H)+2	
419.21996	1	1863211.5	C23H26N6O2	(M+H)+	
420.22229	1	447282	C23H26N6O2	(M+H)+	
421.2245	1	65189.49	C23H26N6O2	(M+H)+	
210.11353	2	350755.53	C23H26N6O2	(M+2H)+2	1.86
210.61496	2	90613.7	C23H26N6O2	(M+2H)+2	1.81
211.11719	2	12392.01	C23H26N6O2	(M+2H)+2	5.92
419.21996	1	1863211.5	C23H26N6O2	(M+H)+	2.29
419.21996		1864620.63			
420.22229	1	447282	C23H26N6O2	(M+H)+	0.97
421.2245	1	65189.49	C23H26N6O2	(M+H)+	-0.23

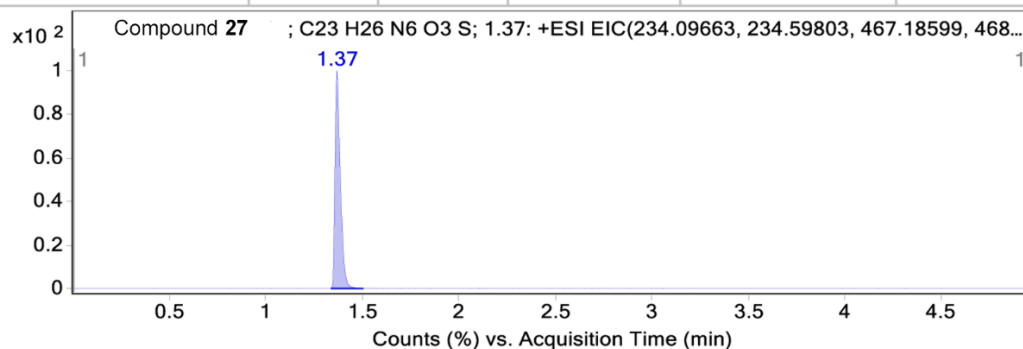
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Compound 27

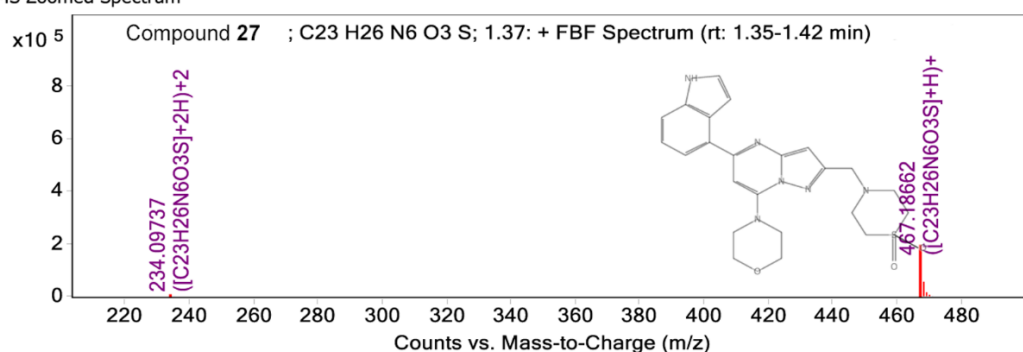


Compound 27

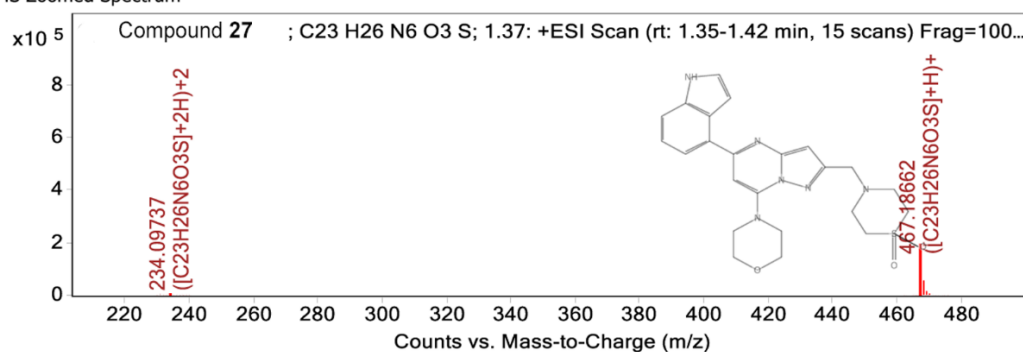
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorit
Compound 27	467.18662	1.37	466.17936	C23 H26 N6 O3 S	466.17871	1.4	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

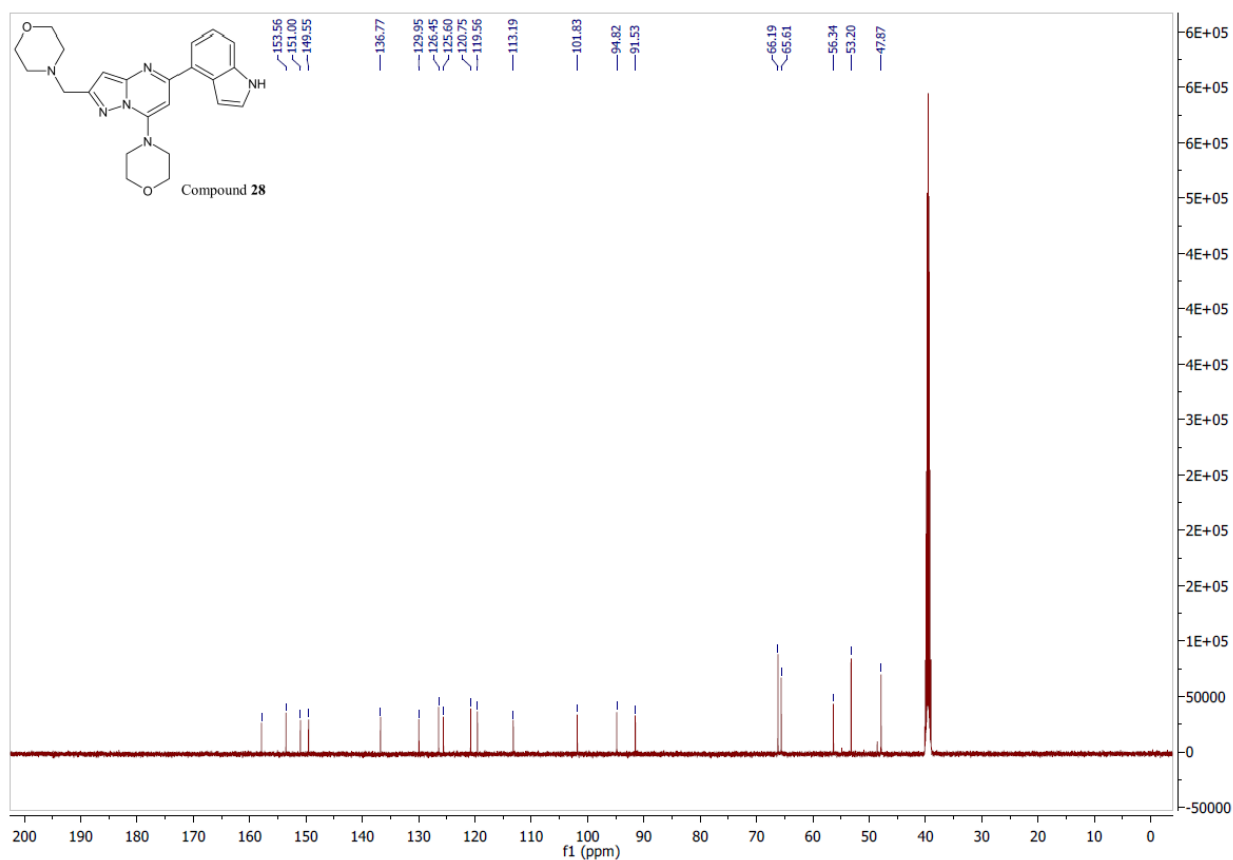
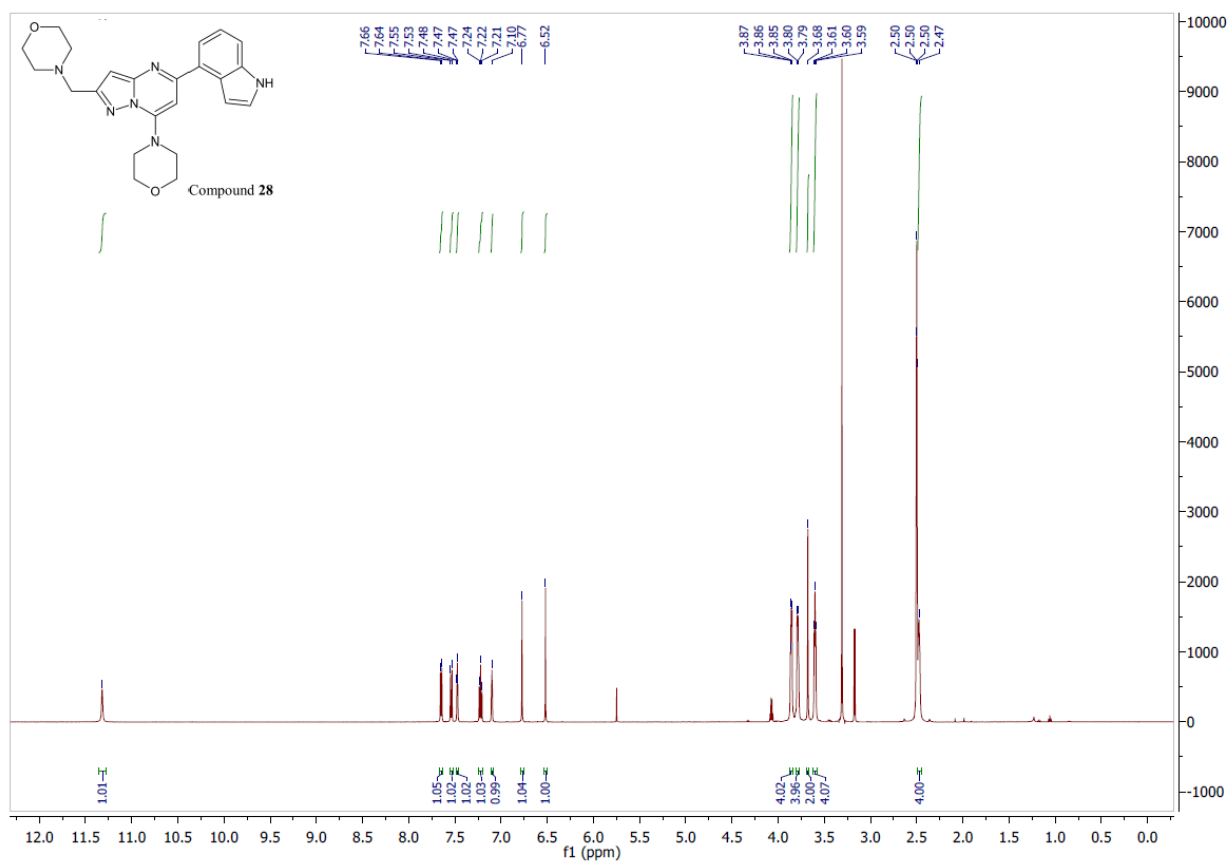


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
234.09737	2	4366.86	C23H26N6O3S	(M+2H)+2	
234.59878	2	1087.41	C23H26N6O3S	(M+2H)+2	
235.09806	2	303.18	C23H26N6O3S	(M+2H)+2	
235.59344	2	49.08	C23H26N6O3S	(M+2H)+2	
467.18662	1	192986.59	C23H26N6O3S	(M+H)+	
468.1894	1	54429.01	C23H26N6O3S	(M+H)+	
469.18746	1	14103.24	C23H26N6O3S	(M+H)+	
470.18826	1	2630.32	C23H26N6O3S	(M+H)+	
471.18539	1	698.5	C23H26N6O3S	(M+H)+	
234.09737	2	4366.86	C23H26N6O3S	(M+2H)+2	3.17
234.59878	2	1087.41	C23H26N6O3S	(M+2H)+2	3.2
235.09806	2	303.18	C23H26N6O3S	(M+2H)+2	4.83
235.59344	2	49.08	C23H26N6O3S	(M+2H)+2	-16.47
467.18662	1	192986.59	C23H26N6O3S	(M+H)+	1.35
468.1894	1	54429.01	C23H26N6O3S	(M+H)+	1.32
469.18746	1	14103.24	C23H26N6O3S	(M+H)+	1.89
470.18826	1	2630.32	C23H26N6O3S	(M+H)+	1.9
471.18539	1	698.5	C23H26N6O3S	(M+H)+	-7.1

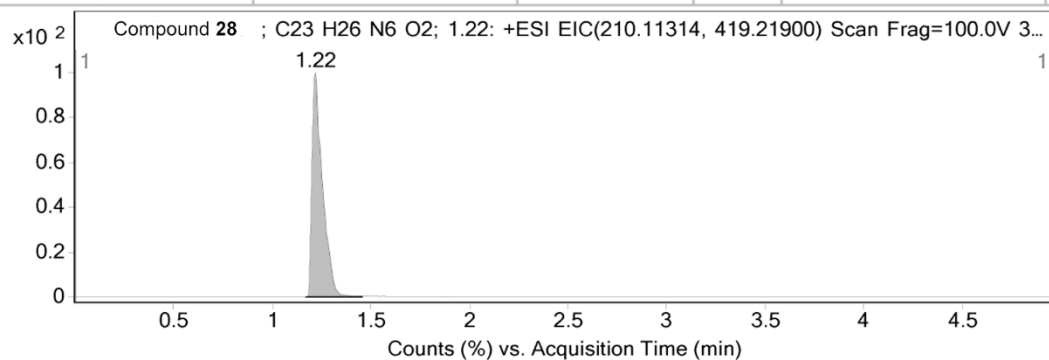
--- End Of Report ---

Compound 28

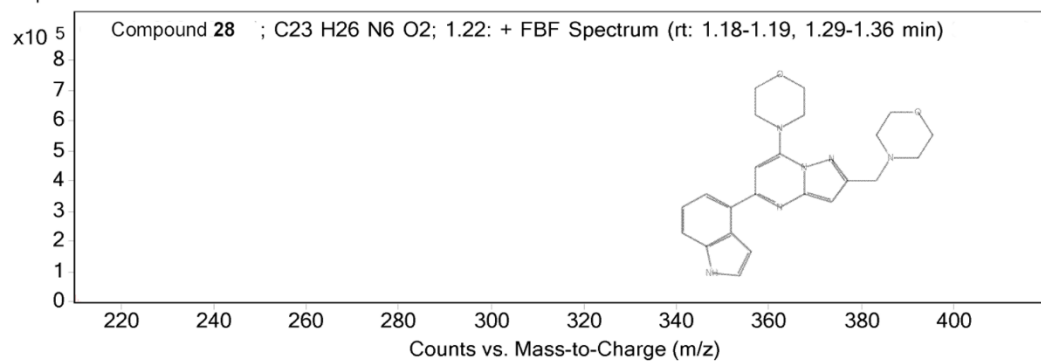


Compound 28

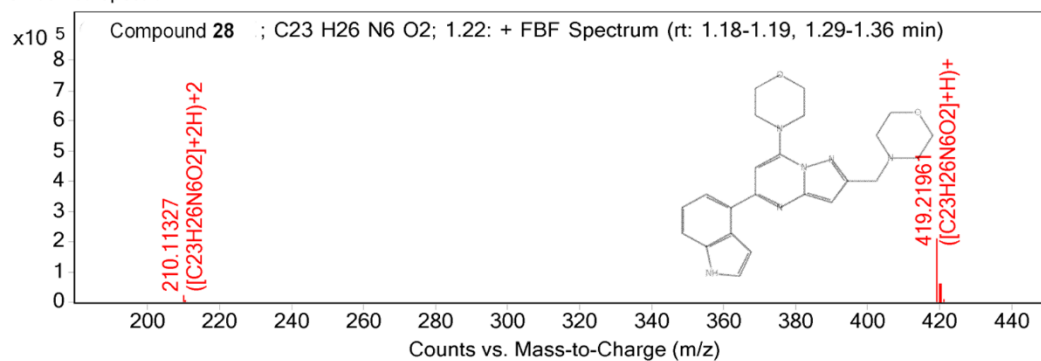
Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 28	Compound 28	419.21961	1.22	Find by Formula	418.21231



MS Spectrum



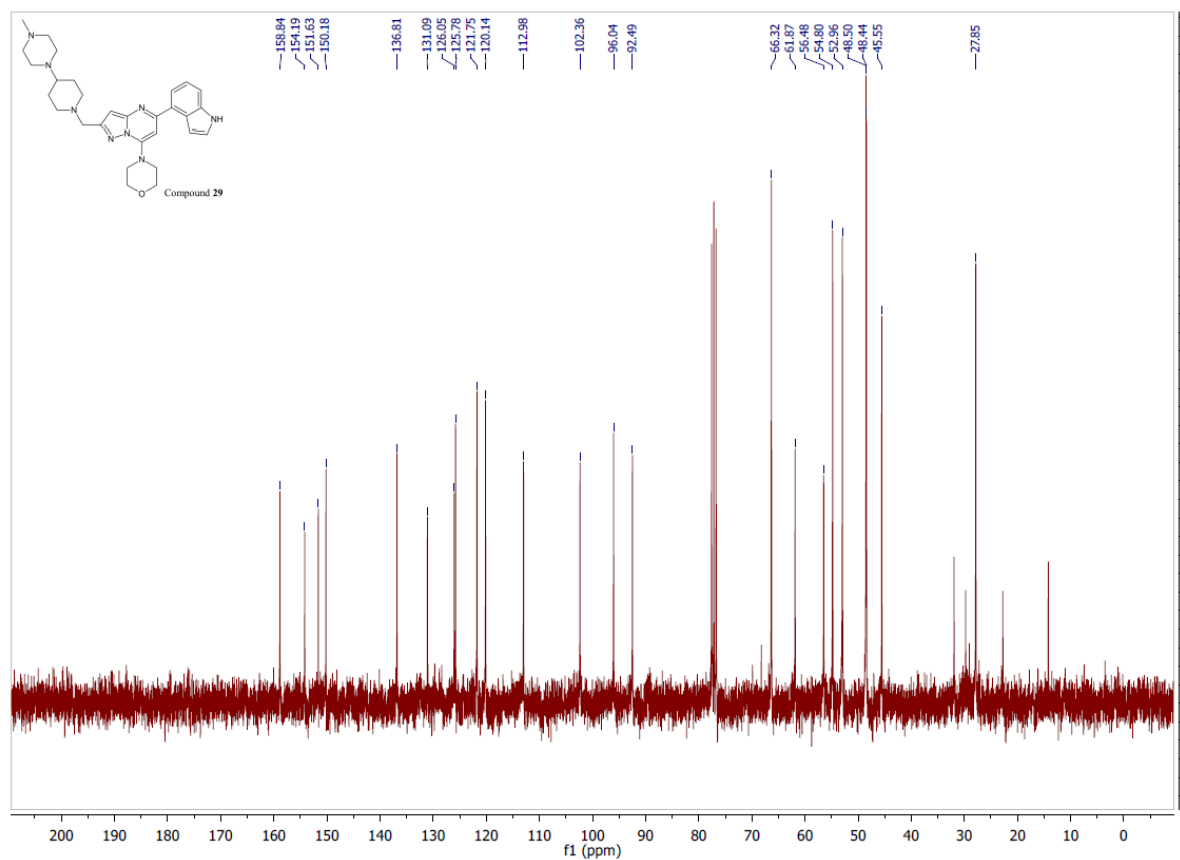
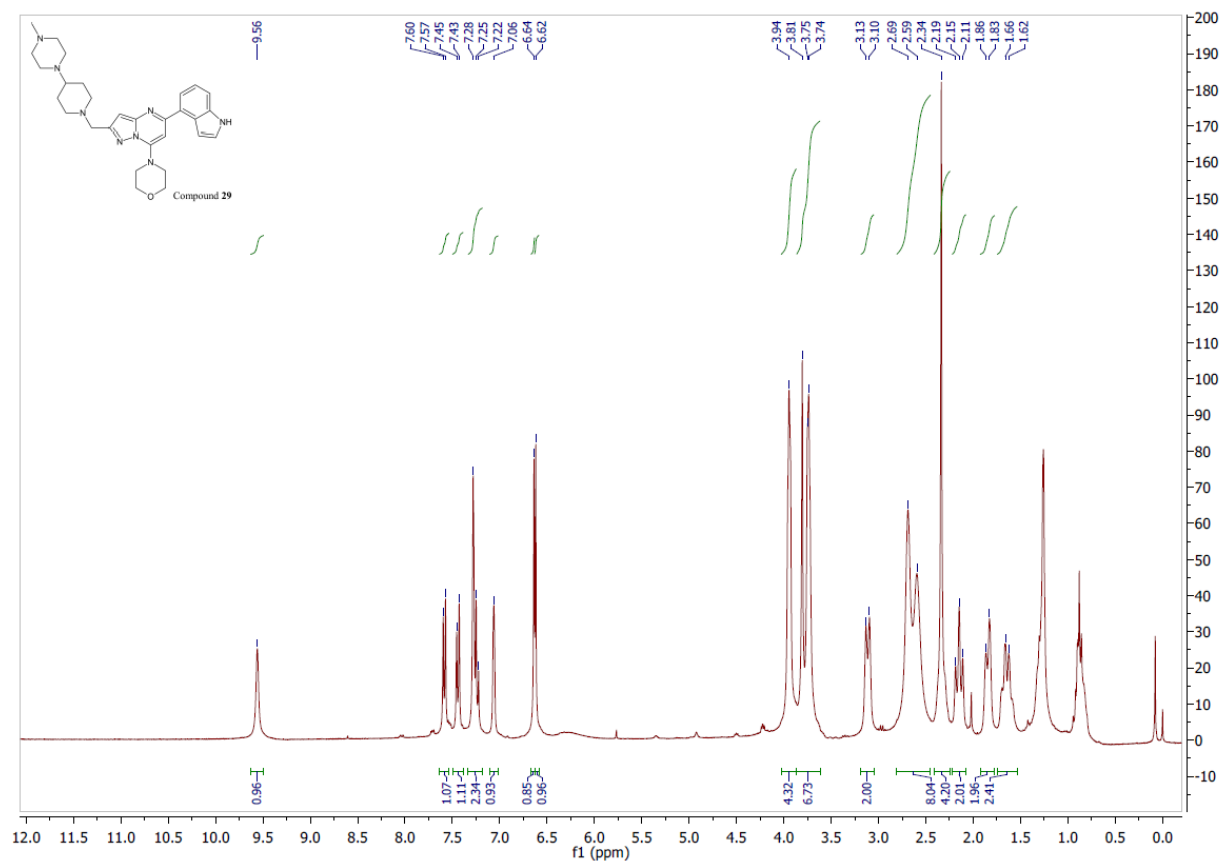
MS Zoomed Spectrum



MS Spectrum Peak List

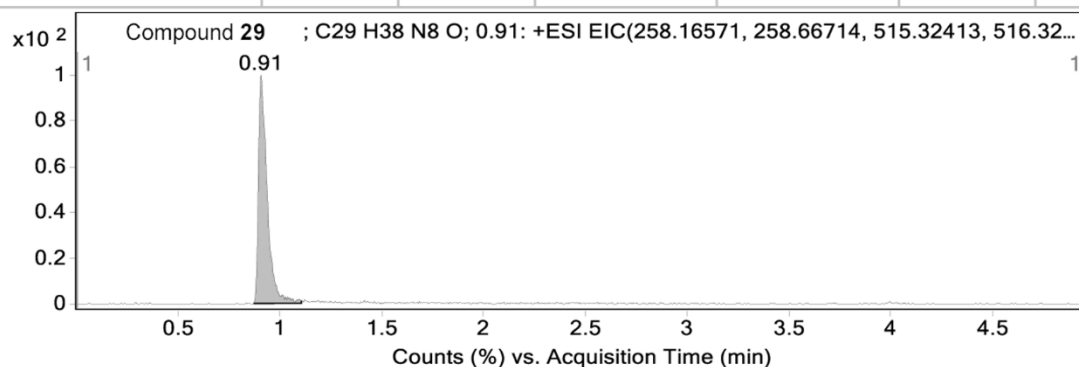
m/z	z	Abund	Formula	Ion
210.11327	2	21627.81	C ₂₃ H ₂₆ N ₆ O ₂	(M+2H)+2
210.6148	2	6590.59	C ₂₃ H ₂₆ N ₆ O ₂	(M+2H)+2
211.11612	2	1038.7	C ₂₃ H ₂₆ N ₆ O ₂	(M+2H)+2
419.21961	1	208915.36	C ₂₃ H ₂₆ N ₆ O ₂	(M+H)+
420.22254	1	53420.48	C ₂₃ H ₂₆ N ₆ O ₂	(M+H)+

Compound 29

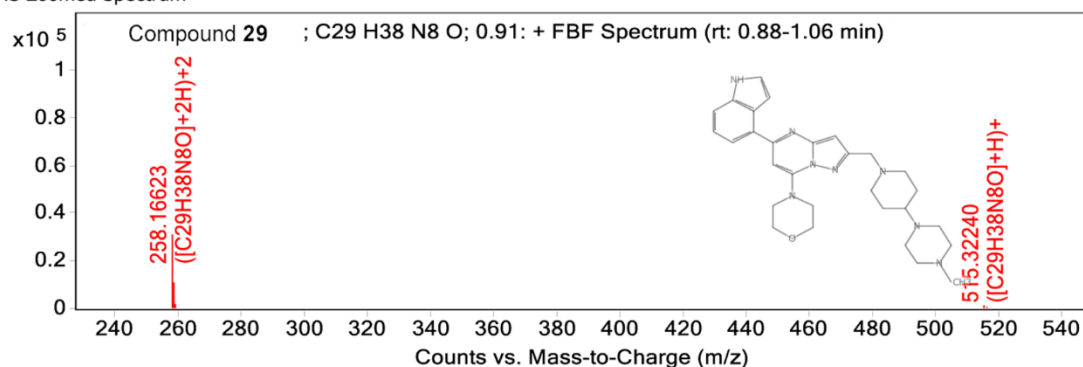


Compound 29

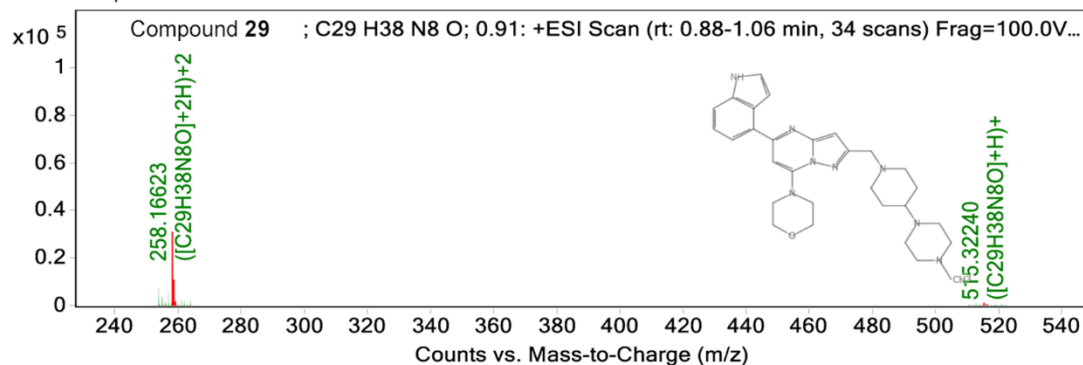
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 29	258.16623	0.91	514.31764	C29 H38 N8 O	514.31686	1.51	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

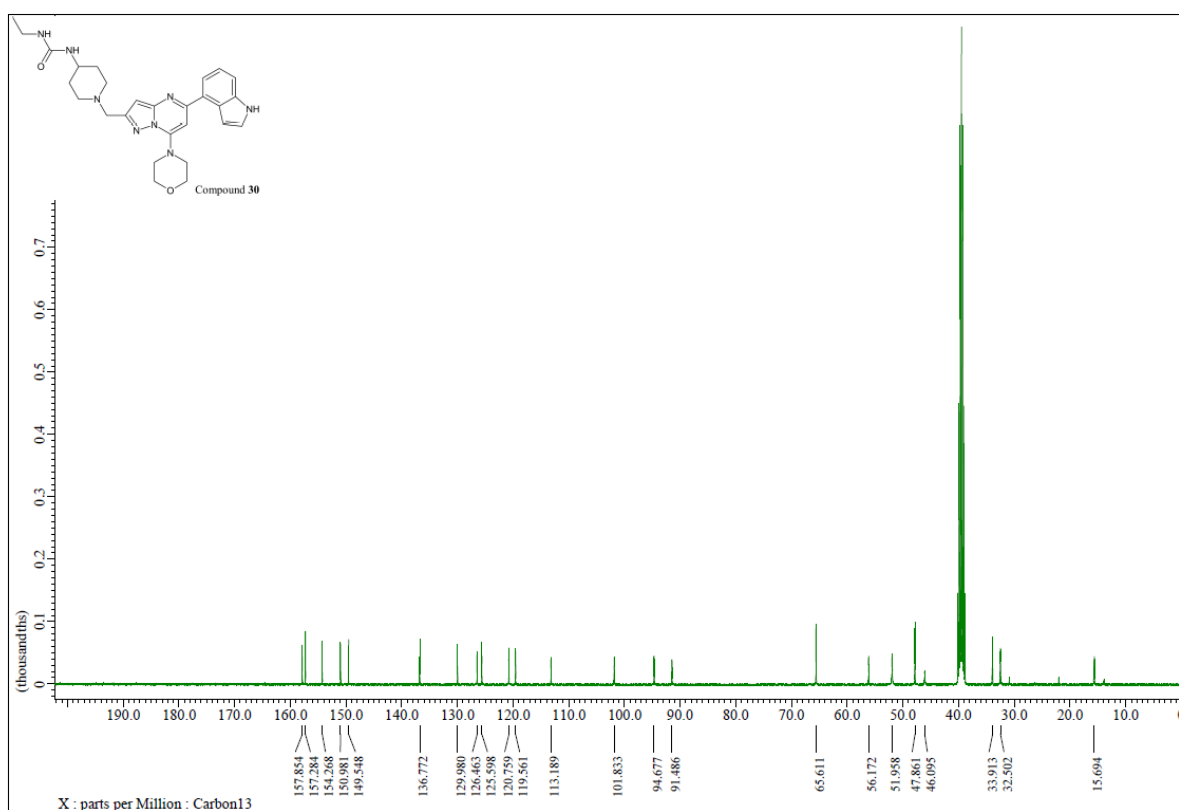
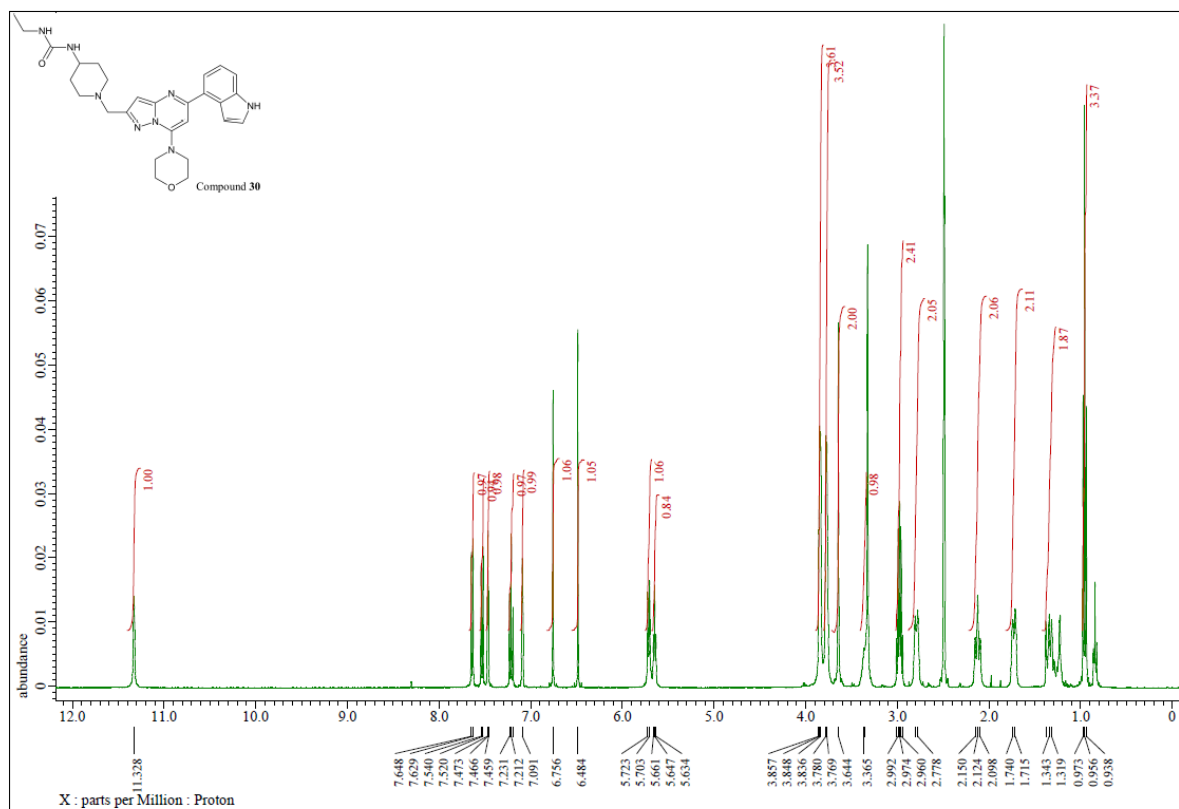


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
258.16623	2	30690.7	C29H38N8O	(M+2H)+2	
258.66762	2	10530.33	C29H38N8O	(M+2H)+2	
259.16777	2	2840.49	C29H38N8O	(M+2H)+2	
259.66954	2	271.58	C29H38N8O	(M+2H)+2	
515.3224	1	978.89	C29H38N8O	(M+H)+	
516.32472	1	341.54	C29H38N8O	(M+H)+	
517.32756	1	45.86	C29H38N8O	(M+H)+	
258.16623	2	30690.7	C29H38N8O	(M+2H)+2	2.05
258.66762	2	10530.33	C29H38N8O	(M+2H)+2	1.87
259.16777	2	2840.49	C29H38N8O	(M+2H)+2	-2.93
259.66954	2	271.58	C29H38N8O	(M+2H)+2	-1.38
515.3224	1	978.89	C29H38N8O	(M+H)+	-3.37
516.32472	1	341.54	C29H38N8O	(M+H)+	-4.42
517.32756	1	45.86	C29H38N8O	(M+H)+	-4.31

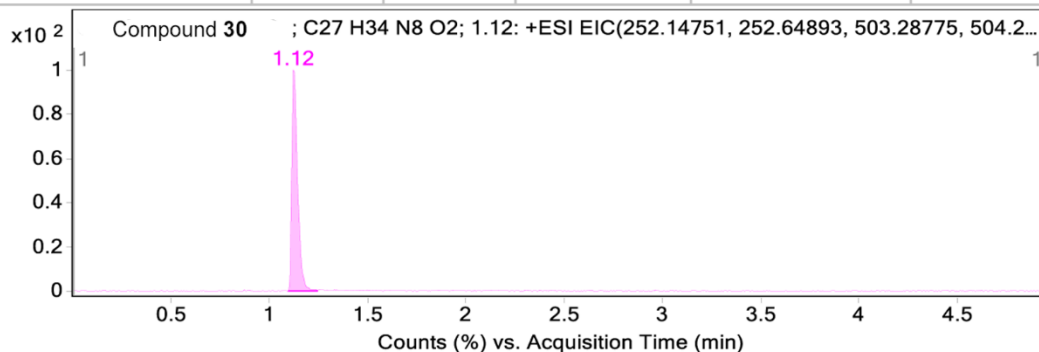
--- End Of Report ---

Compound 30

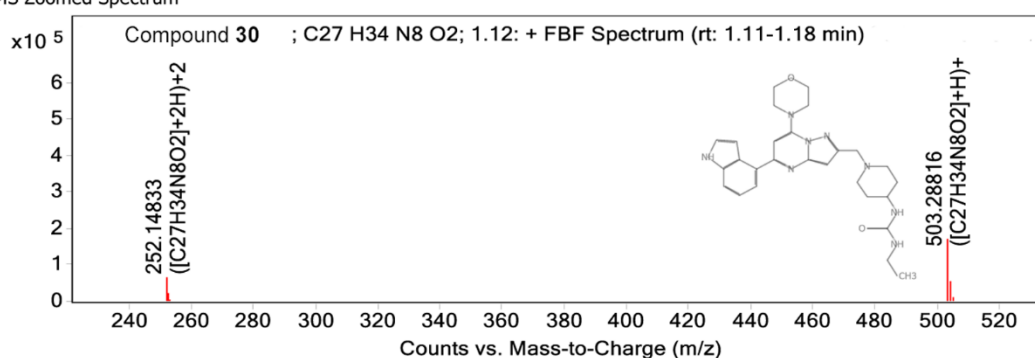


Compound 30

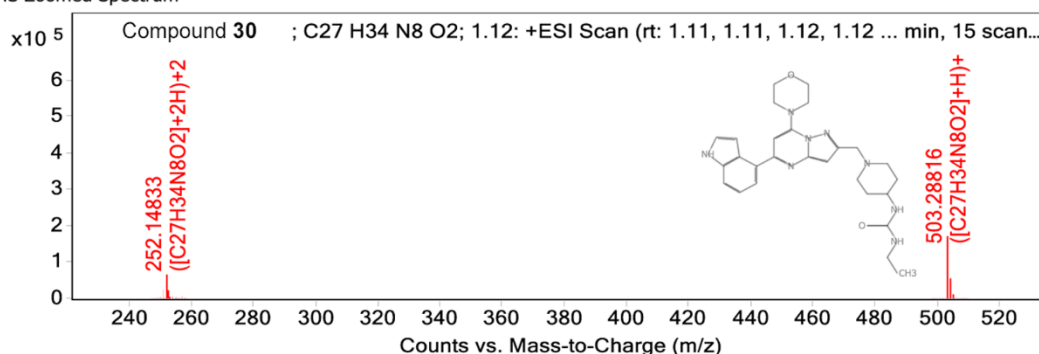
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaorith
Compound 30	503.28816	1.12	502.28111	C27 H34 N8 O2	502.28047	1.26	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

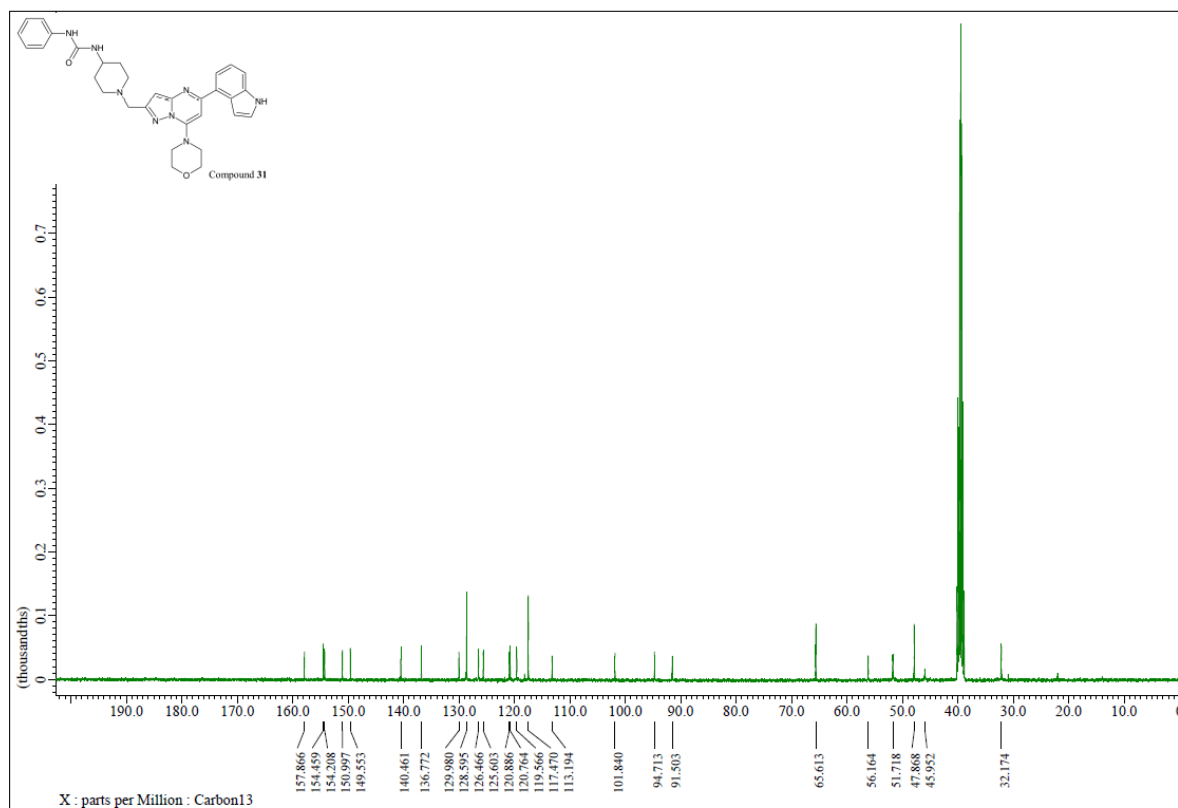
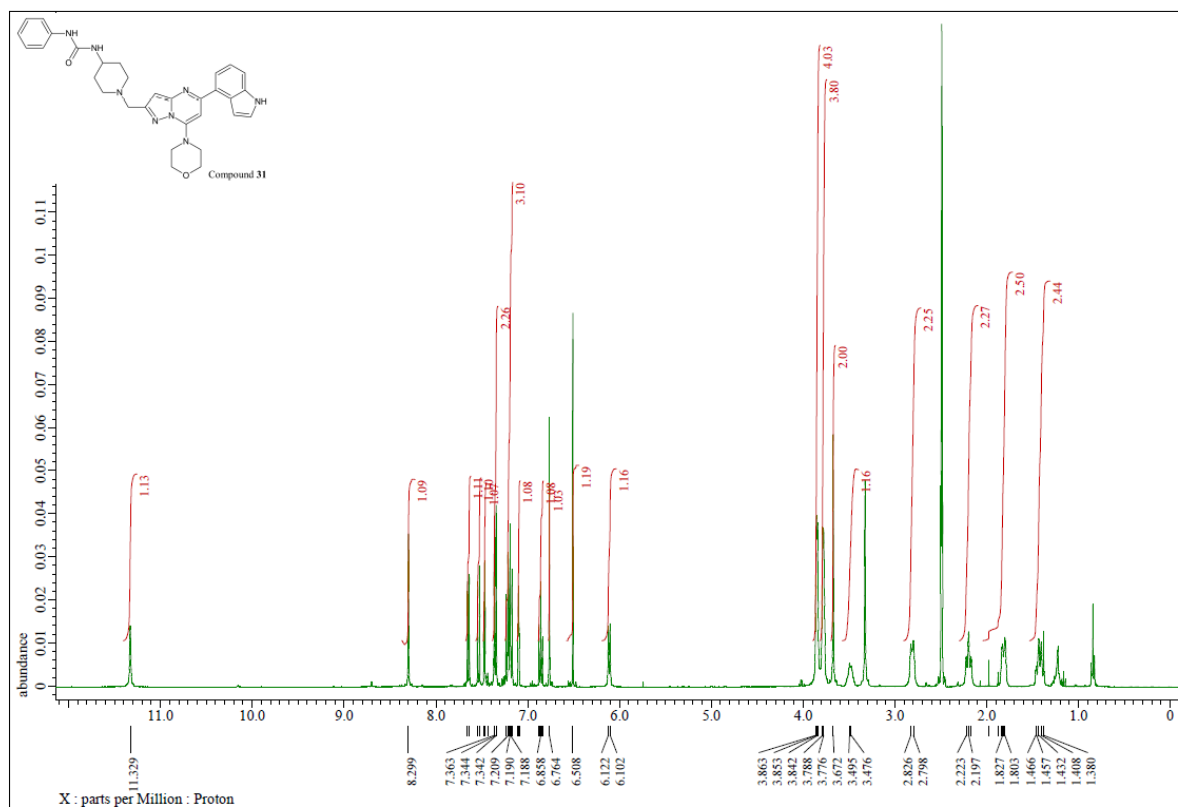


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
252.14833	2	64928.3	C27H34N8O2	(M+2H)+2	
252.64947	2	21703.73	C27H34N8O2	(M+2H)+2	
253.14989	2	4265.57	C27H34N8O2	(M+2H)+2	
253.6516	2	378.26	C27H34N8O2	(M+2H)+2	
503.28816	1	170039.05	C27H34N8O2	(M+H)+	
504.29073	1	51172.18	C27H34N8O2	(M+H)+	
505.29311	1	8059.46	C27H34N8O2	(M+H)+	
252.14833	2	64928.3	C27H34N8O2	(M+2H)+2	3.26
252.64947	2	21703.73	C27H34N8O2	(M+2H)+2	2.17
253.14989	2	4265.57	C27H34N8O2	(M+2H)+2	-1.55
253.6516	2	378.26	C27H34N8O2	(M+2H)+2	0.07
503.28816	1	170039.05	C27H34N8O2	(M+H)+	0.81
504.29073	1	51172.18	C27H34N8O2	(M+H)+	0.3
505.29311	1	8059.46	C27H34N8O2	(M+H)+	-0.34

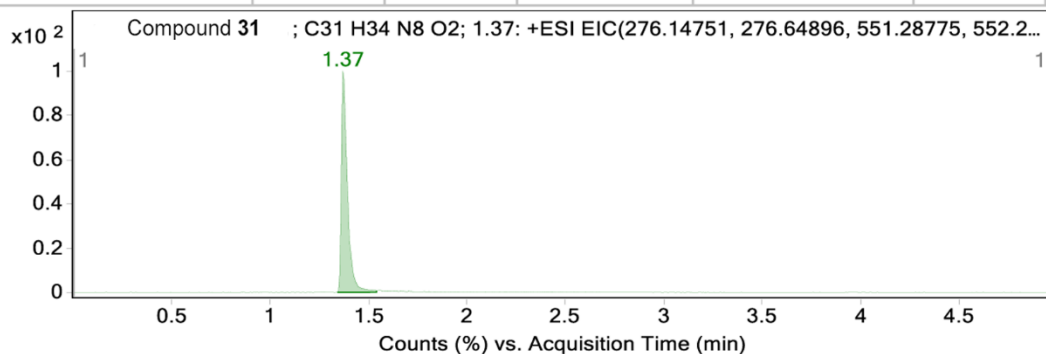
--- End Of Report ---

Compound 31

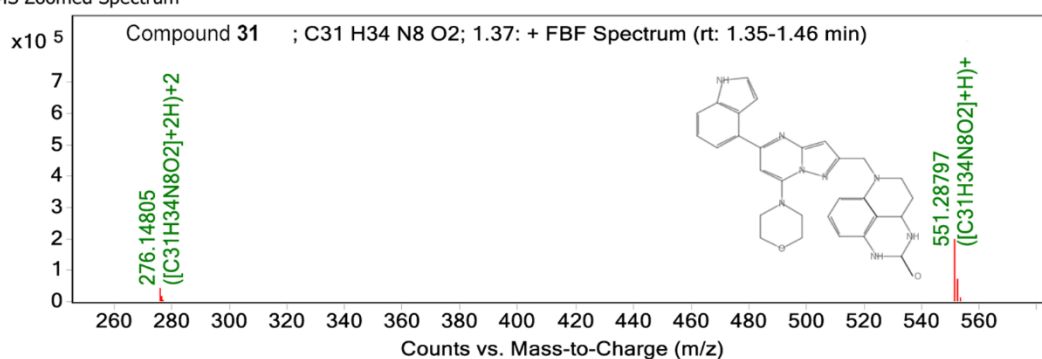


Compound 31

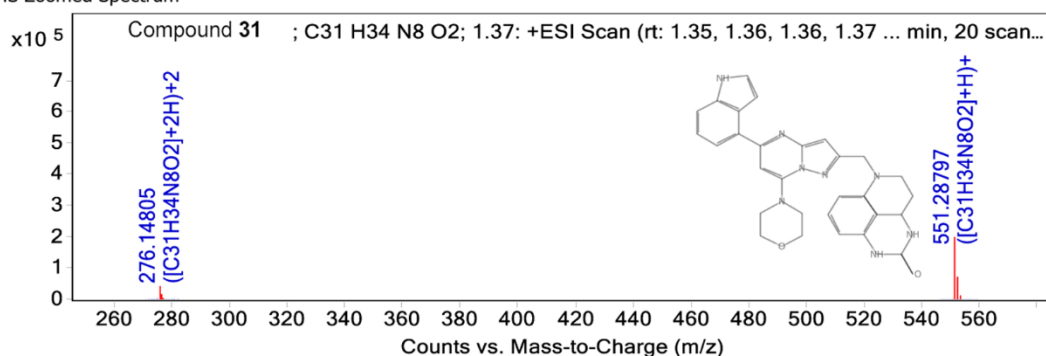
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 31	551.28797	1.37	550.28084	C31 H34 N8 O2	550.28047	0.66	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

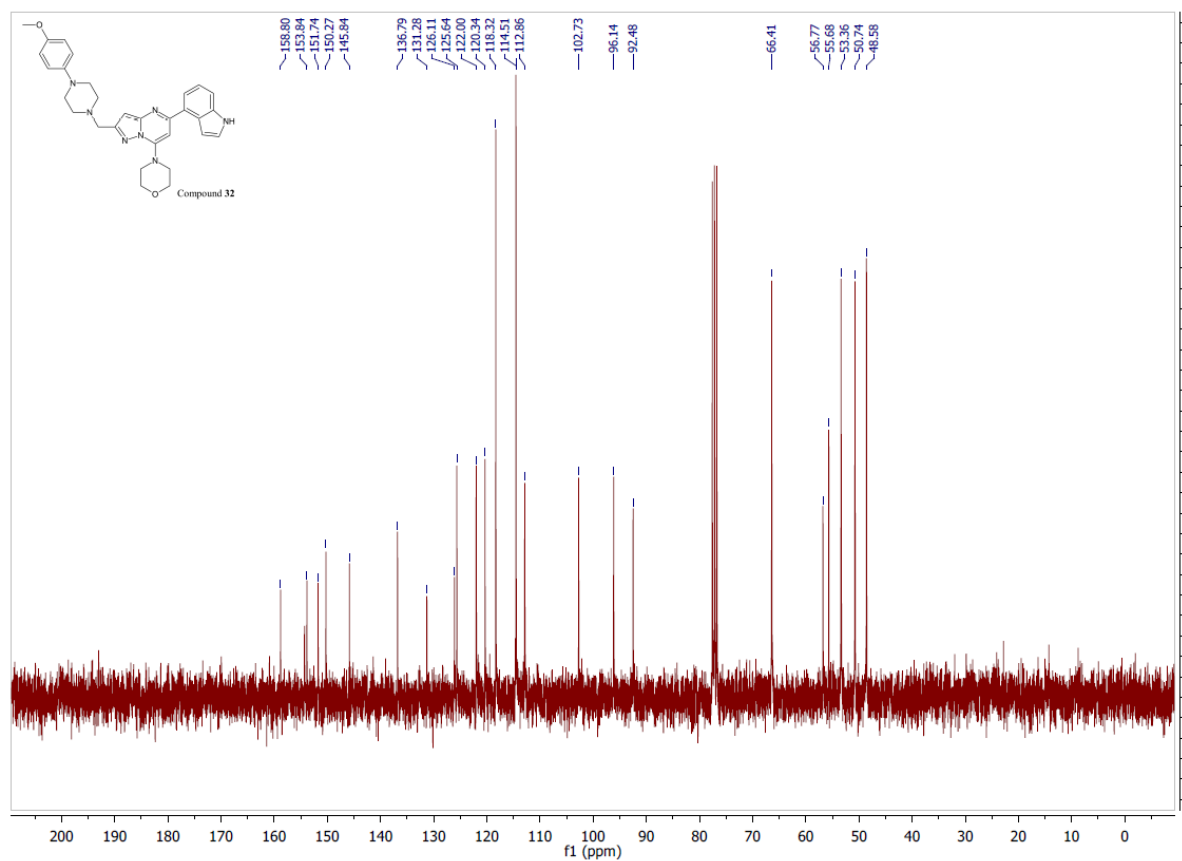
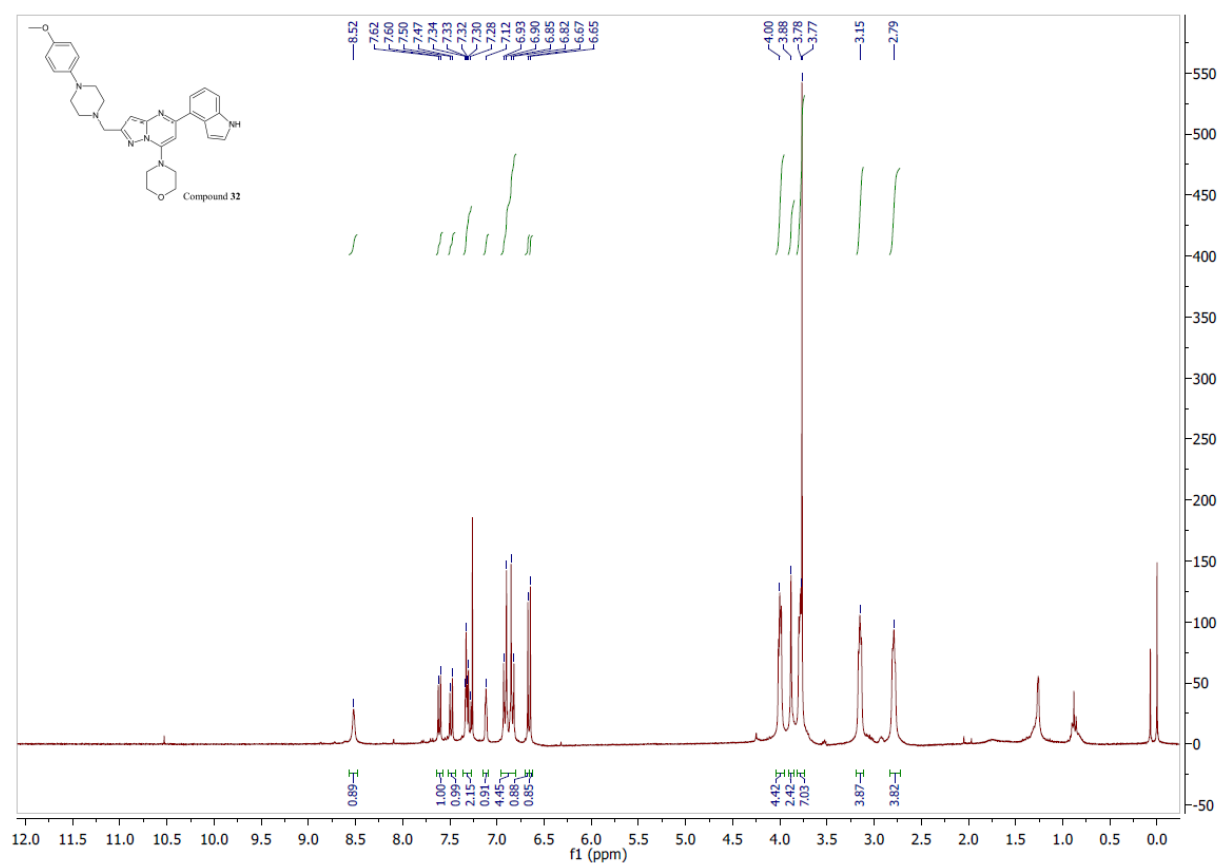


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
276.14805	2	40949.66	C31H34N8O2	(M+2H)+2	
276.64942	2	15629.86	C31H34N8O2	(M+2H)+2	
277.15073	2	3435.34	C31H34N8O2	(M+2H)+2	
277.65147	2	351.9	C31H34N8O2	(M+2H)+2	
551.28797	1	197852.61	C31H34N8O2	(M+H)+	
552.29099	1	69000.93	C31H34N8O2	(M+H)+	
553.29311	1	12470.17	C31H34N8O2	(M+H)+	
554.29584	1	1658.46	C31H34N8O2	(M+H)+	
276.14805	2	40949.66	C31H34N8O2	(M+2H)+2	1.94
276.64942	2	15629.86	C31H34N8O2	(M+2H)+2	1.67
277.15073	2	3435.34	C31H34N8O2	(M+2H)+2	1.39
277.65147	2	351.9	C31H34N8O2	(M+2H)+2	-0.83
551.28797	1	197852.61	C31H34N8O2	(M+H)+	0.4
552.29099	1	69000.93	C31H34N8O2	(M+H)+	0.64
553.29311	1	12470.17	C31H34N8O2	(M+H)+	-0.57
554.29584	1	1658.46	C31H34N8O2	(M+H)+	-0.52

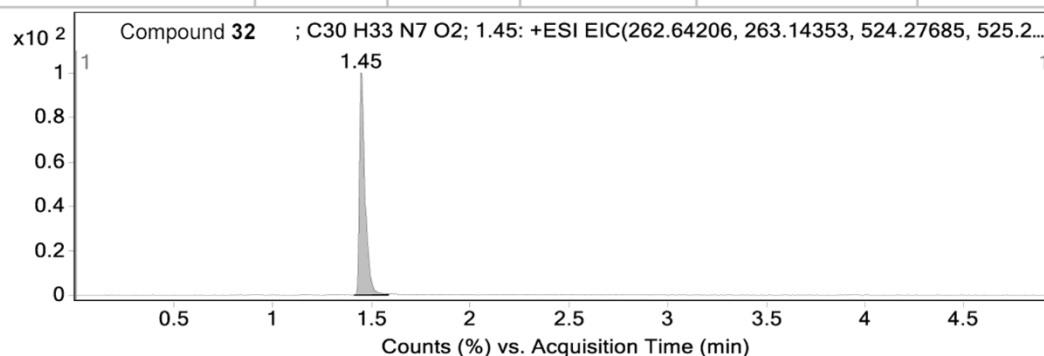
--- End Of Report ---

Compound 32

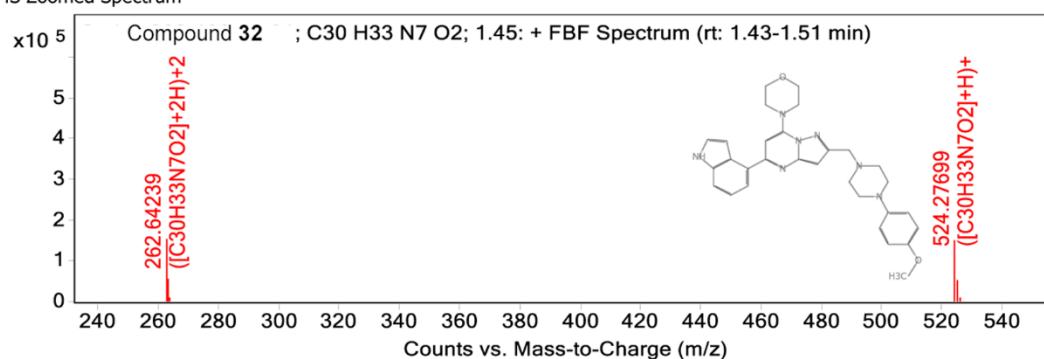


Compound 32

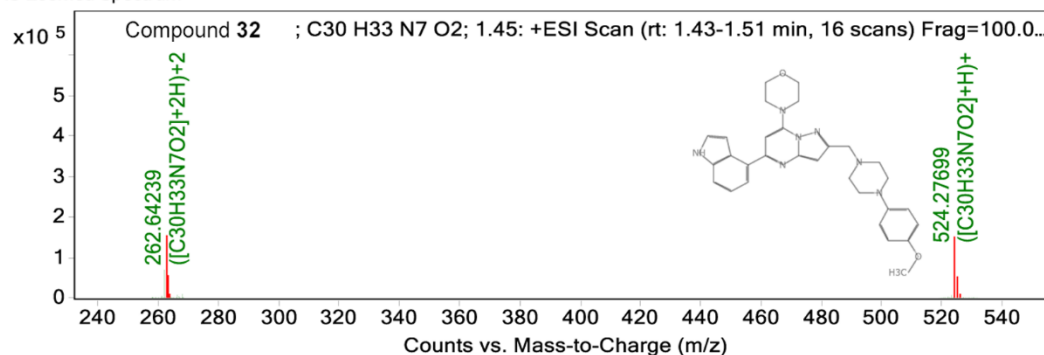
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpsds Alaoirith Find by Formula
Compound 32	524.27699	1.45	523.26996	C30 H33 N7 O2	523.26957	0.75	



MS Zoomed Spectrum



MS Zoomed Spectrum

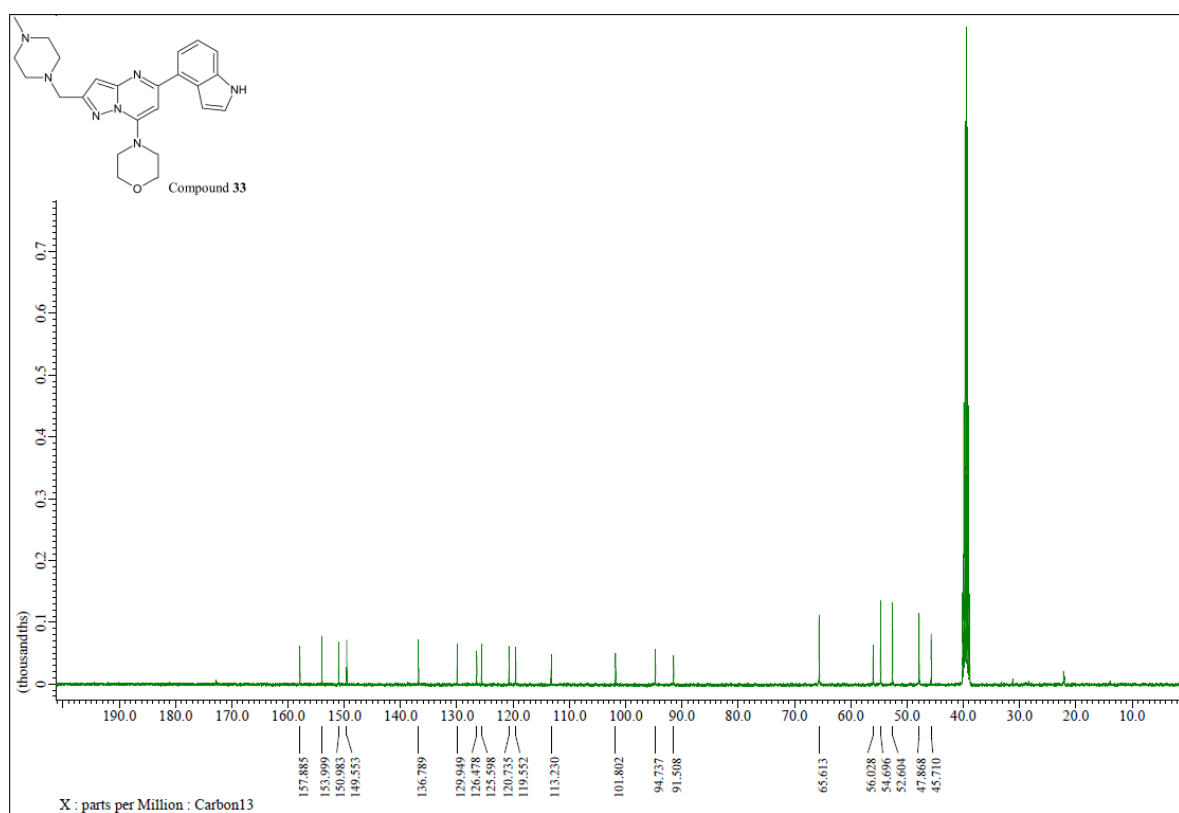
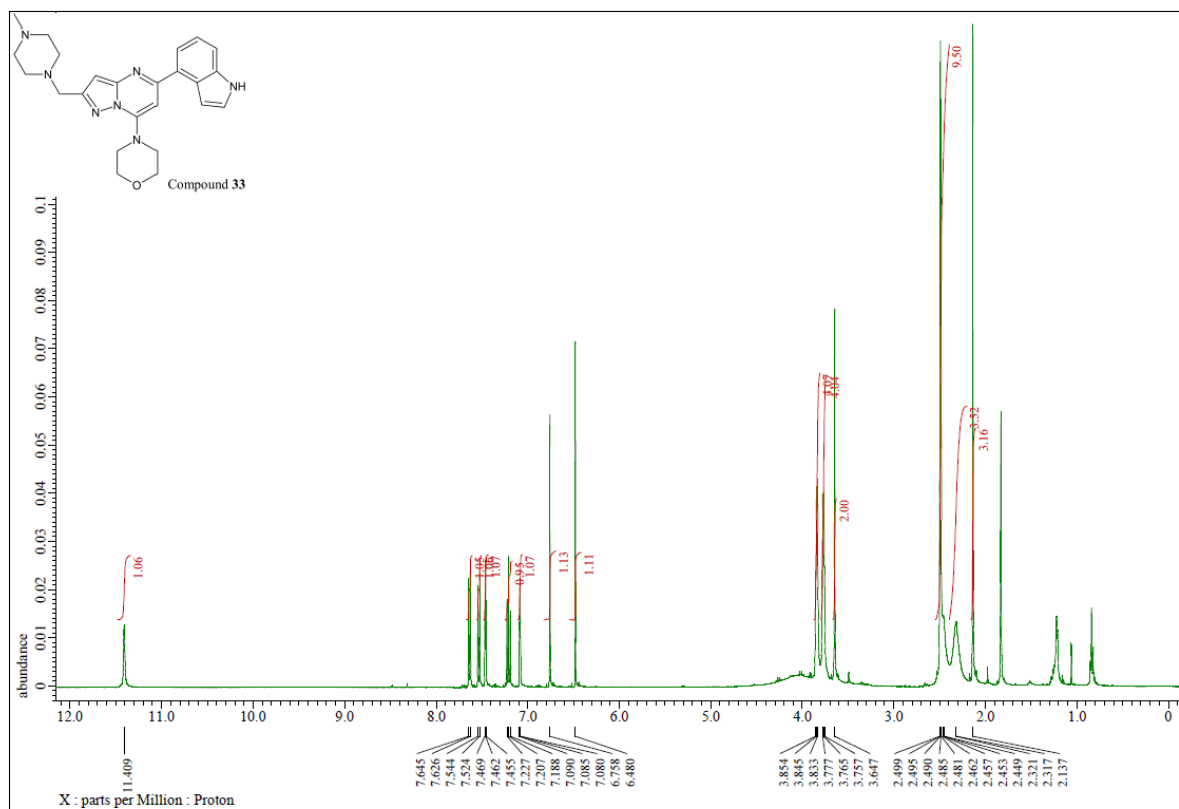


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
262.64239	2	153431.98	C30H33N7O2	(M+2H)+2	
263.14403	2	49281.49	C30H33N7O2	(M+2H)+2	
263.64525	2	8827.74	C30H33N7O2	(M+2H)+2	
524.27699	1	149768.55	C30H33N7O2	(M+H)+	
525.27966	1	50773.94	C30H33N7O2	(M+H)+	
526.28195	1	8617.05	C30H33N7O2	(M+H)+	
527.28537	1	1117.81	C30H33N7O2	(M+H)+	
262.64239	2	153431.98	C30H33N7O2	(M+2H)+2	1.25
263.14403	2	49281.49	C30H33N7O2	(M+2H)+2	1.89
263.64525	2	8827.74	C30H33N7O2	(M+2H)+2	1.18
524.27699	1	149768.55	C30H33N7O2	(M+H)+	0.28
525.27966	1	50773.94	C30H33N7O2	(M+H)+	-0.24
526.28195	1	8617.05	C30H33N7O2	(M+H)+	-1.24
527.28537	1	1117.81	C30H33N7O2	(M+H)+	0.08

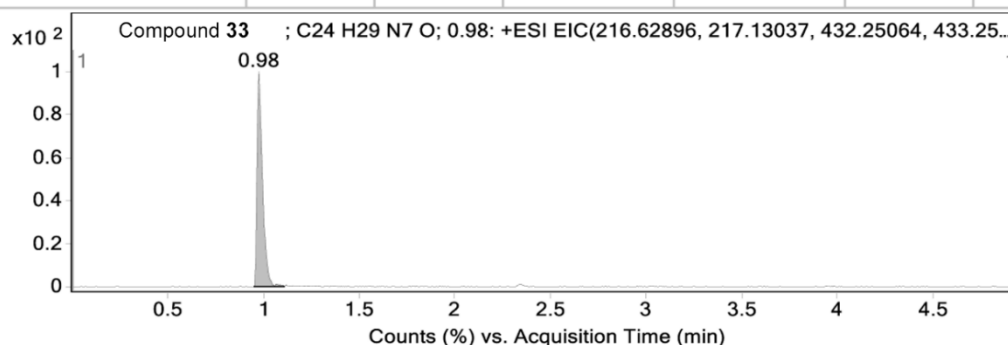
--- End Of Report ---

Compound 33

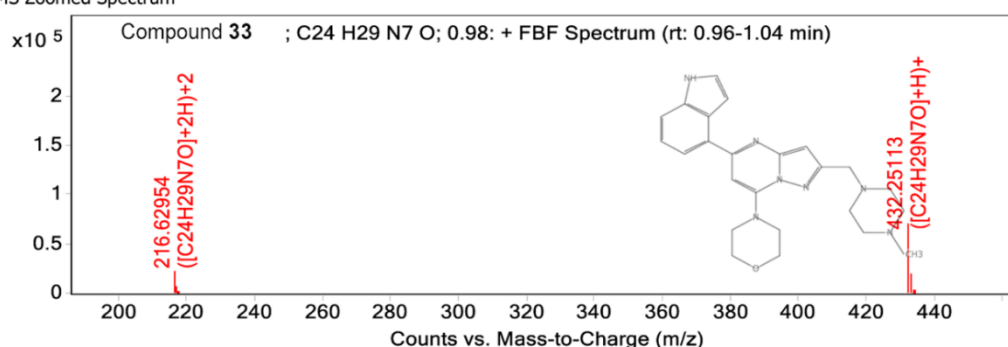


Compound 33

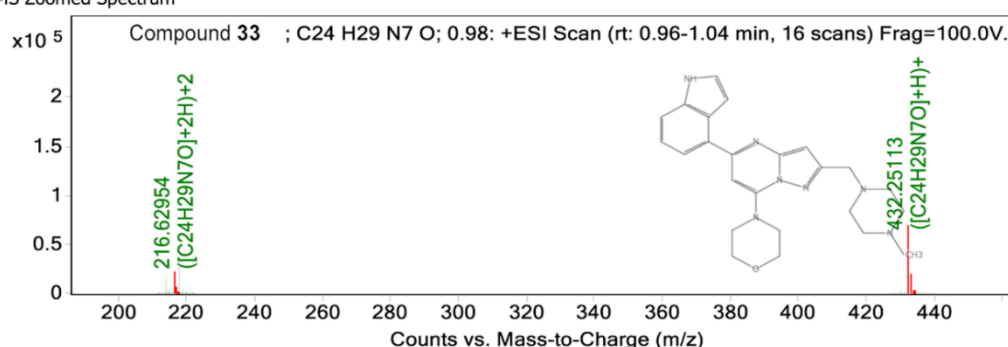
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Algorith
Compound 33	432.25113	0.98	431.24397	C24 H29 N7 O	431.24336	1.43	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

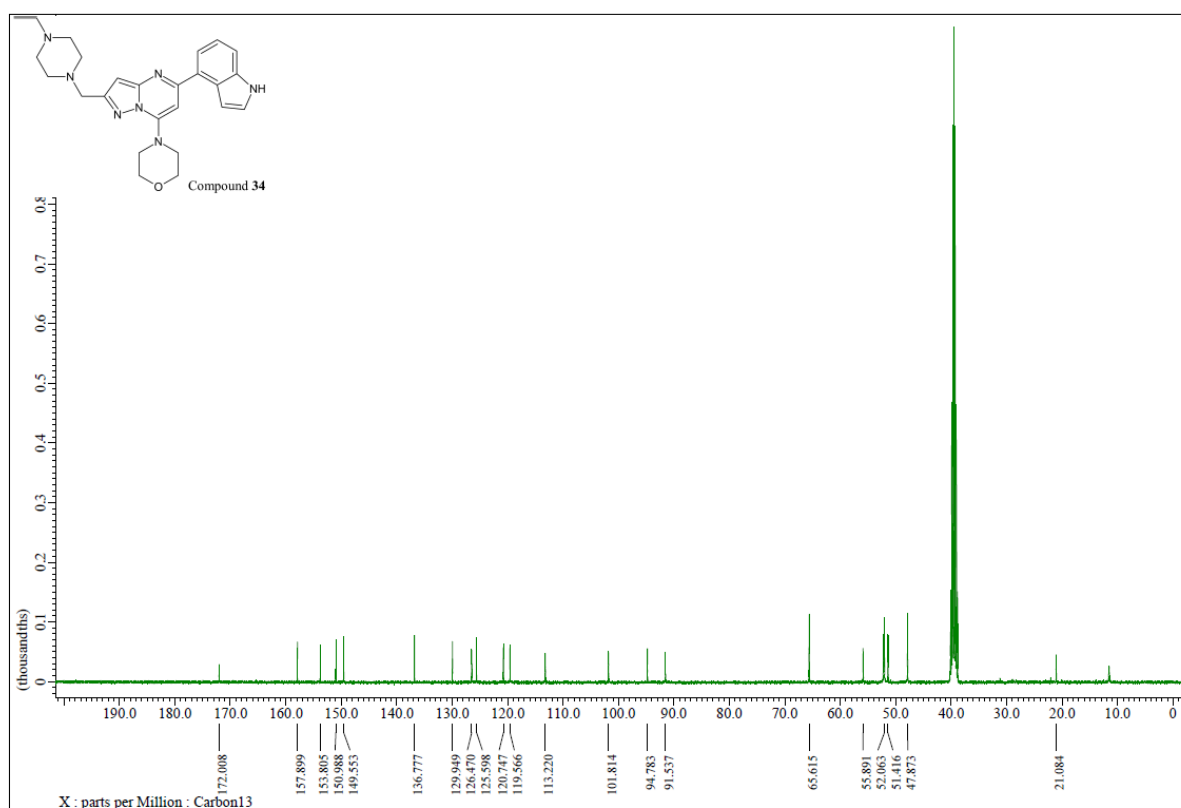
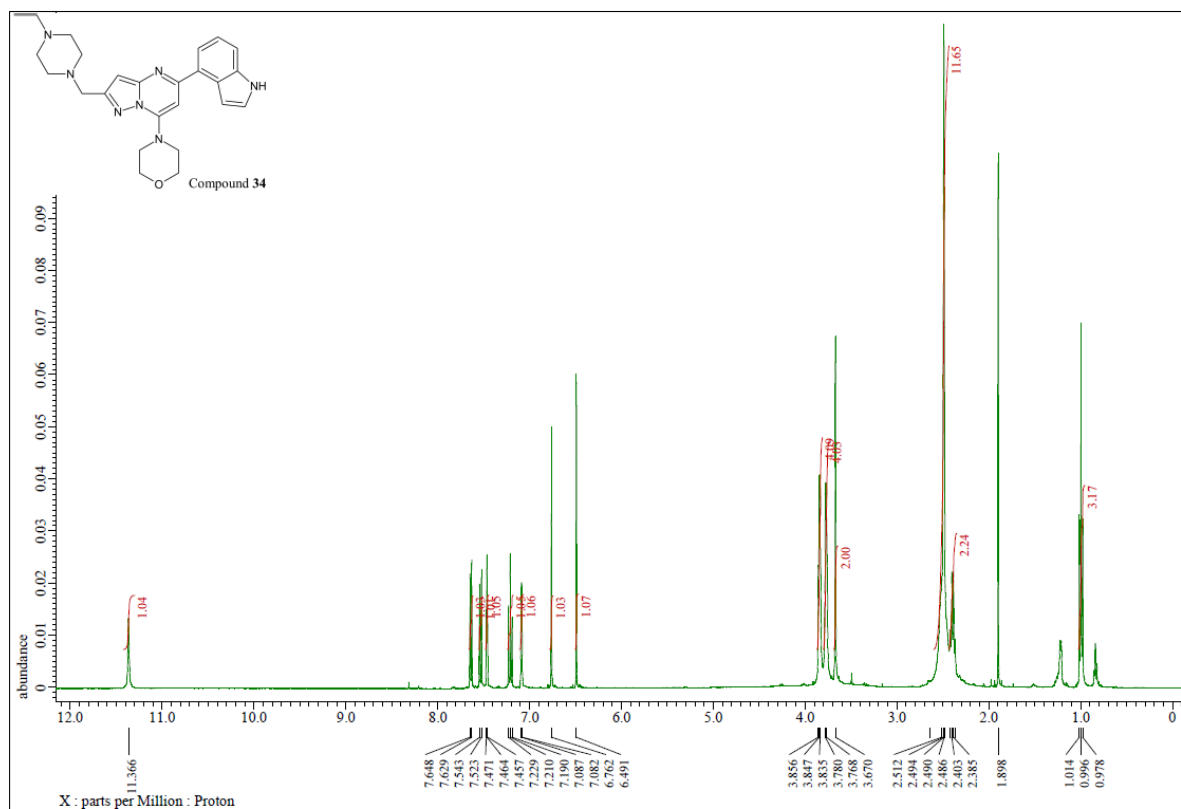


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
216.62954	2	21711.37	C24H29N7O	(M+2H)+2	
217.13078	2	6384.77	C24H29N7O	(M+2H)+2	
217.63214	2	939.34	C24H29N7O	(M+2H)+2	
432.25113	1	69948.29	C24H29N7O	(M+H)+	
433.25391	1	19650.1	C24H29N7O	(M+H)+	
434.2564	1	2730.67	C24H29N7O	(M+H)+	
435.25842	1	318.43	C24H29N7O	(M+H)+	
216.62954	2	21711.37	C24H29N7O	(M+2H)+2	2.7
217.13078	2	6384.77	C24H29N7O	(M+2H)+2	1.86
217.63214	2	939.34	C24H29N7O	(M+2H)+2	1.83
432.25113	1	69948.29	C24H29N7O	(M+H)+	1.14
433.25391	1	19650.1	C24H29N7O	(M+H)+	1.02
434.2564	1	2730.67	C24H29N7O	(M+H)+	0.44
435.25842	1	318.43	C24H29N7O	(M+H)+	-1.03

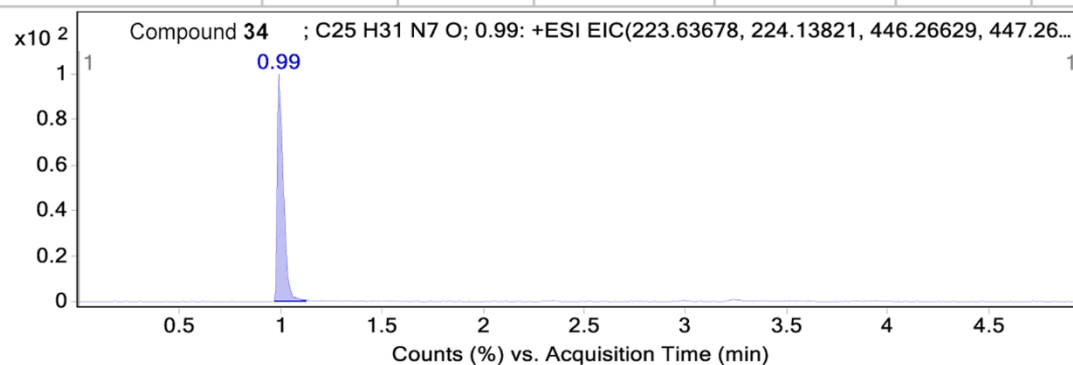
--- End Of Report ---

Compound 34

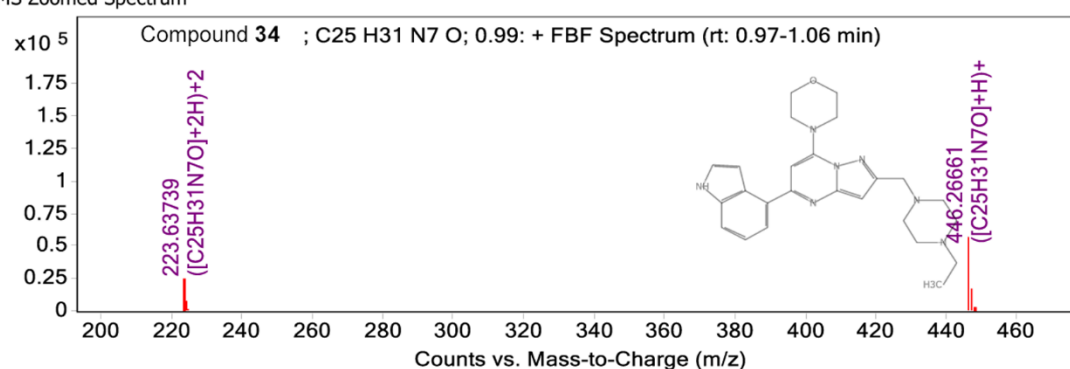


Compound 34

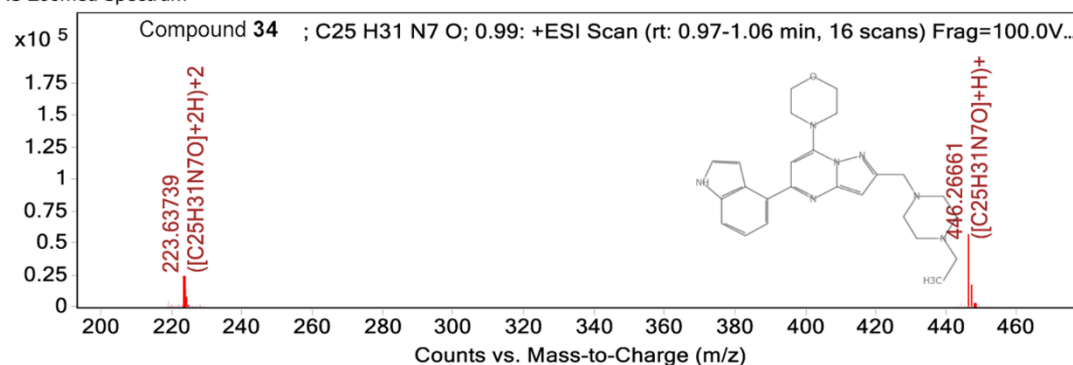
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 34	446.26661	0.99	445.25954	C25 H31 N7 O	445.25901	1.19	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

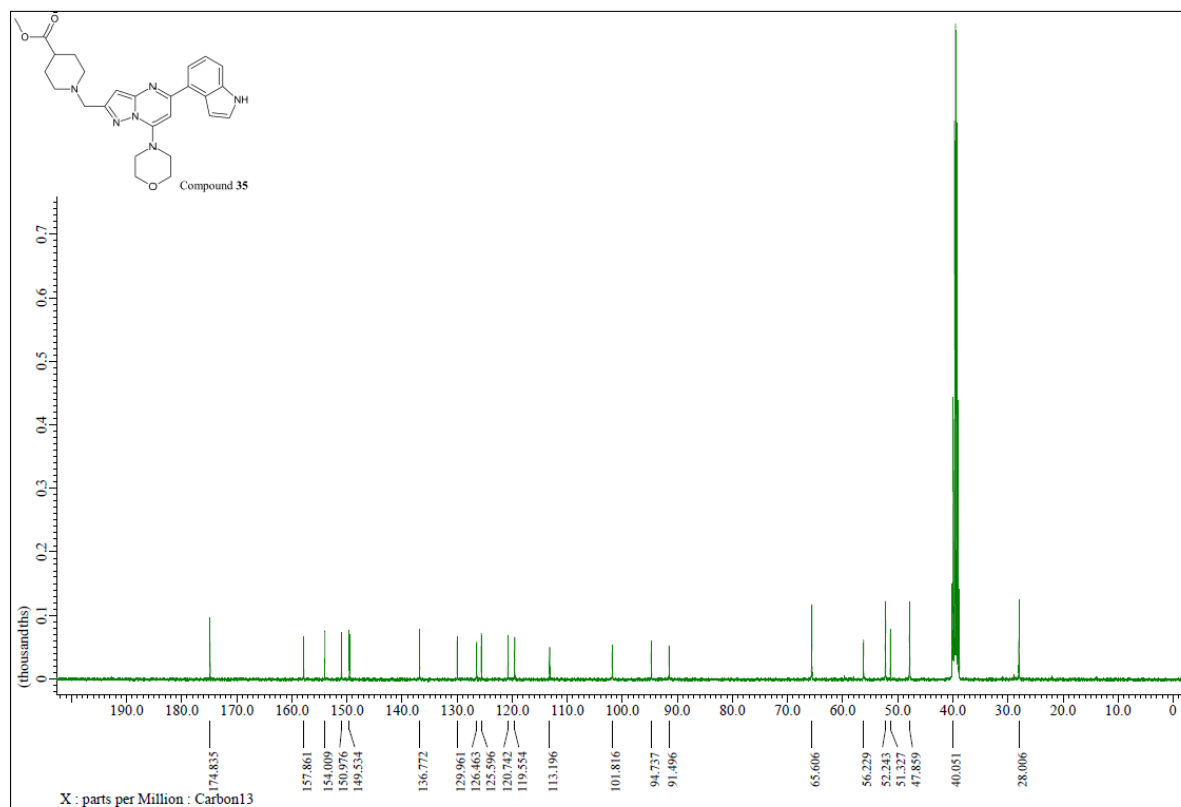
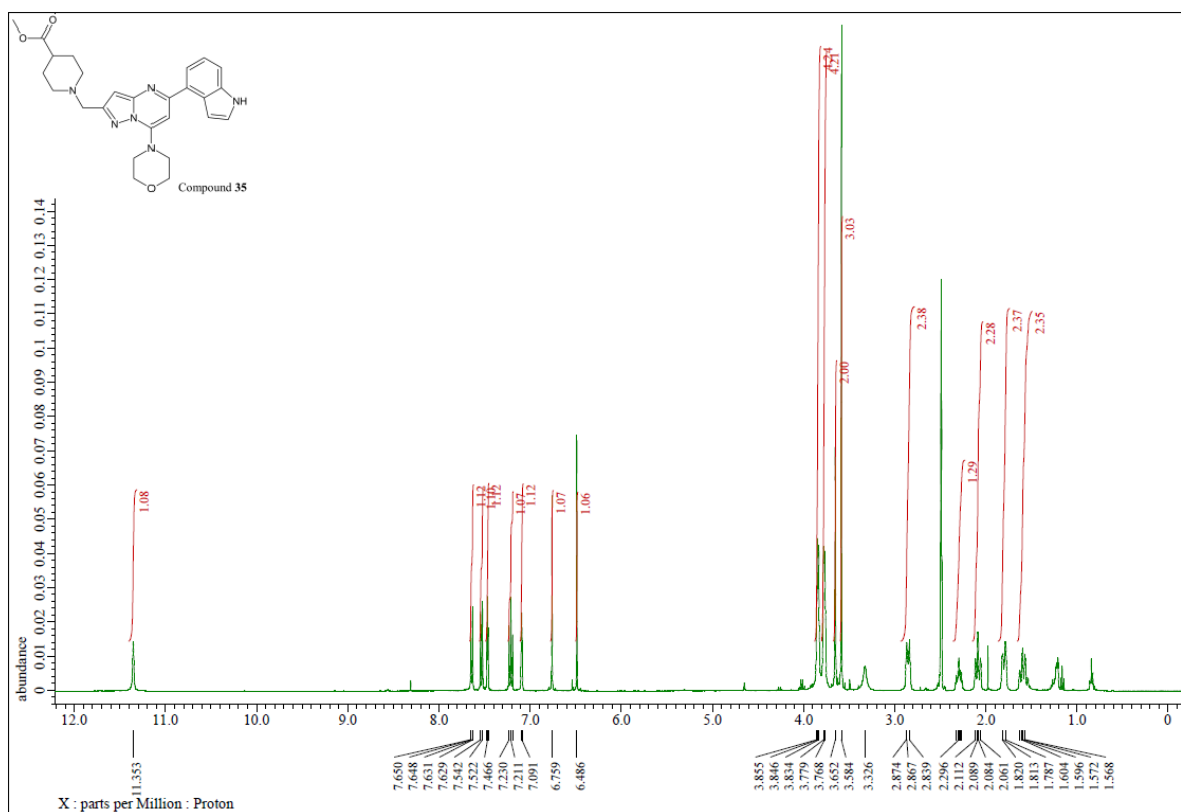


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
223.63739	2	23763.25	C25H31N7O	(M+2H)+2	
224.6402	2	1095.98	C25H31N7O	(M+2H)+2	
446.26661	1	56774.48	C25H31N7O	(M+H)+	
447.26924	1	15807.67	C25H31N7O	(M+H)+	
448.27271	1	2984.79	C25H31N7O	(M+H)+	
223.63739	2	23763.25	C25H31N7O	(M+2H)+2	2.74
224.6402	2	1095.98	C25H31N7O	(M+2H)+2	2.7
446.26661	1	56774.48	C25H31N7O	(M+H)+	0.74
447.26924	1	15807.67	C25H31N7O	(M+H)+	0.22
448.27271	1	2984.79	C25H31N7O	(M+H)+	1.8

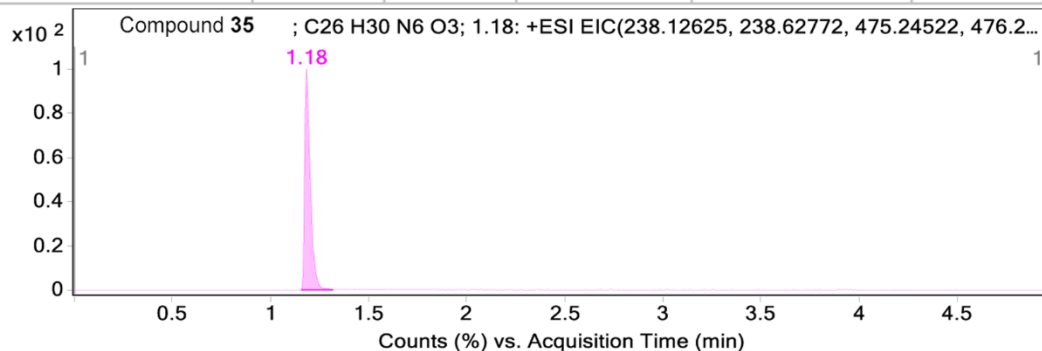
--- End Of Report ---

Compound 35

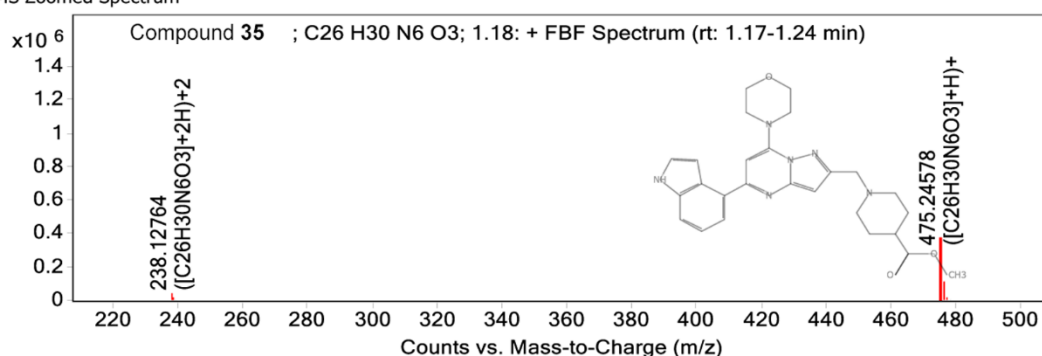


Compound 35

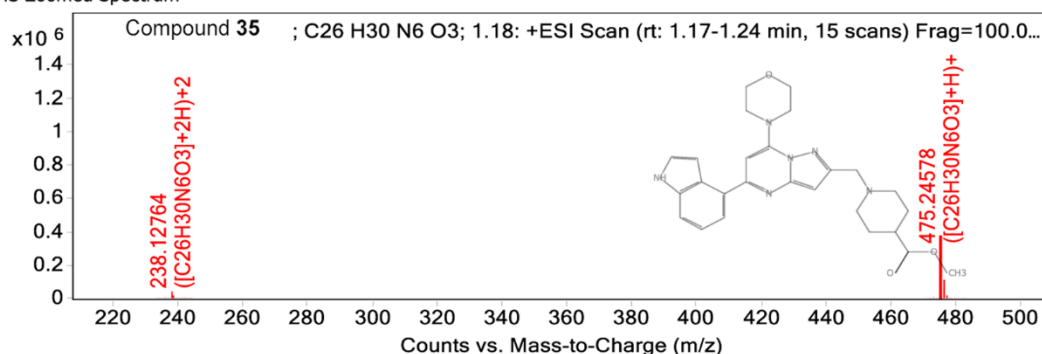
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 35	475.24578	1.18	474.23875	C26 H30 N6 O3	474.23794	1.71	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

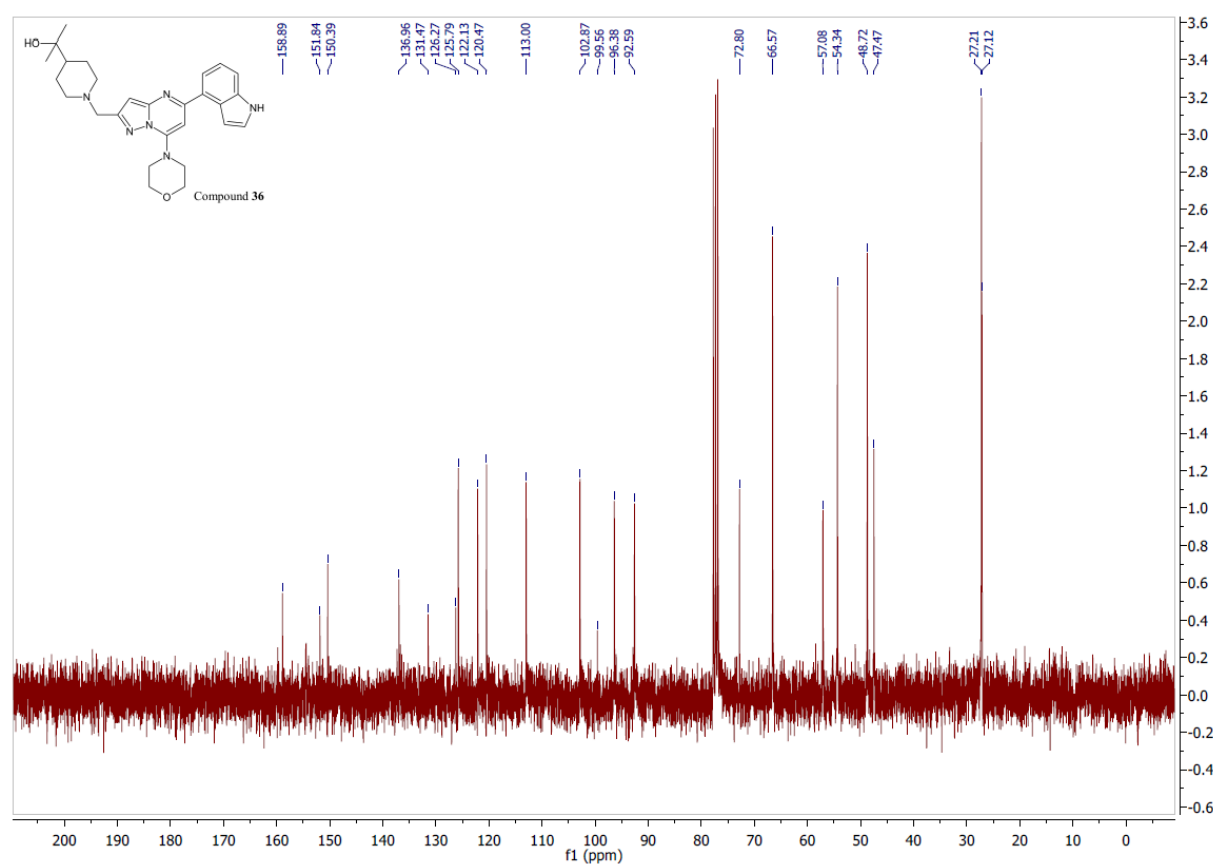
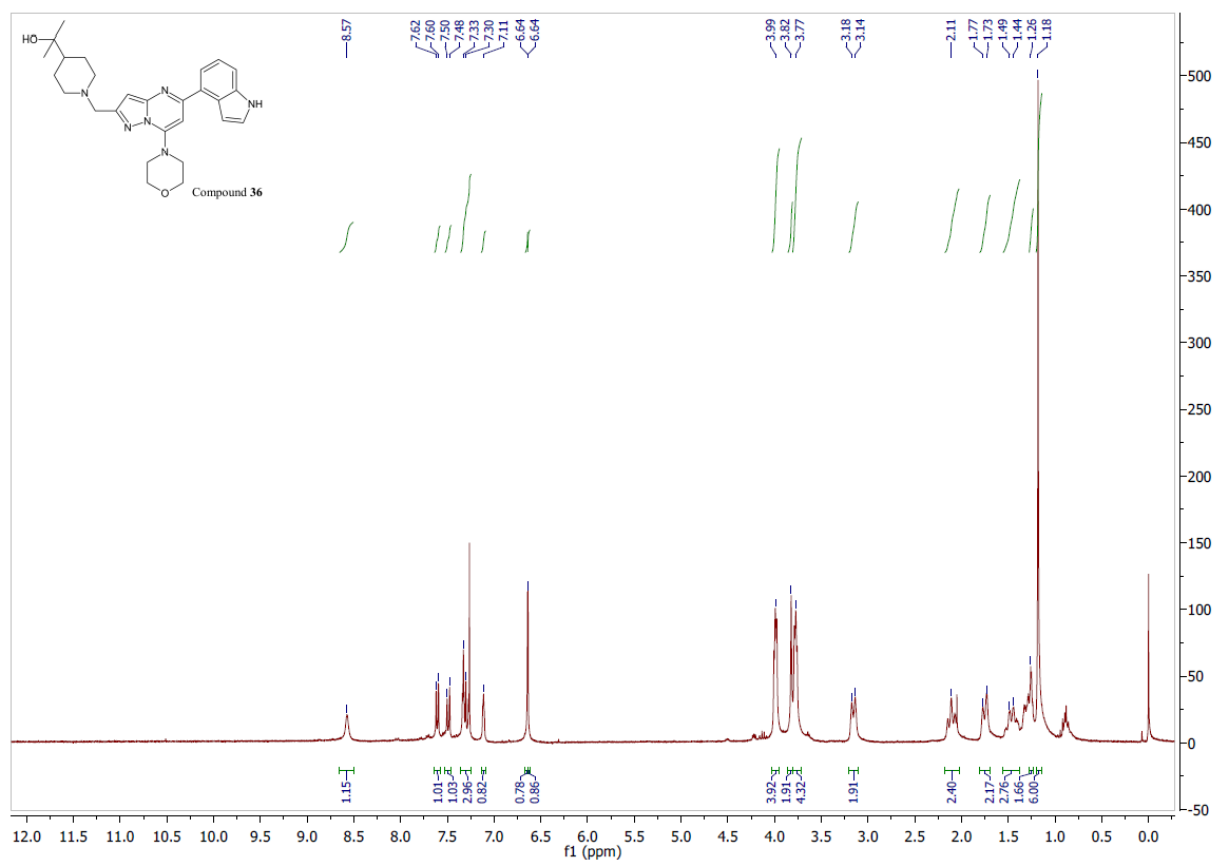


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.12764	2	39287.81	C26H30N6O3	(M+2H)+2	
238.62889	2	12270.96	C26H30N6O3	(M+2H)+2	
239.13084	2	1943.22	C26H30N6O3	(M+2H)+2	
239.62934	2	274.5	C26H30N6O3	(M+2H)+2	
475.24578	1	370502.28	C26H30N6O3	(M+H)+	
476.24896	1	106459.38	C26H30N6O3	(M+H)+	
477.25109	1	17094.23	C26H30N6O3	(M+H)+	
478.25404	1	2155.16	C26H30N6O3	(M+H)+	
238.12764	2	39287.81	C26H30N6O3	(M+2H)+2	5.87
238.62889	2	12270.96	C26H30N6O3	(M+2H)+2	4.91
239.13084	2	1943.22	C26H30N6O3	(M+2H)+2	7.36
239.62934	2	274.5	C26H30N6O3	(M+2H)+2	-4.42
475.24578	1	370502.28	C26H30N6O3	(M+H)+	1.19
476.24896	1	106459.38	C26H30N6O3	(M+H)+	1.69
477.25109	1	17094.23	C26H30N6O3	(M+H)+	0.41
478.25404	1	2155.16	C26H30N6O3	(M+H)+	1.11

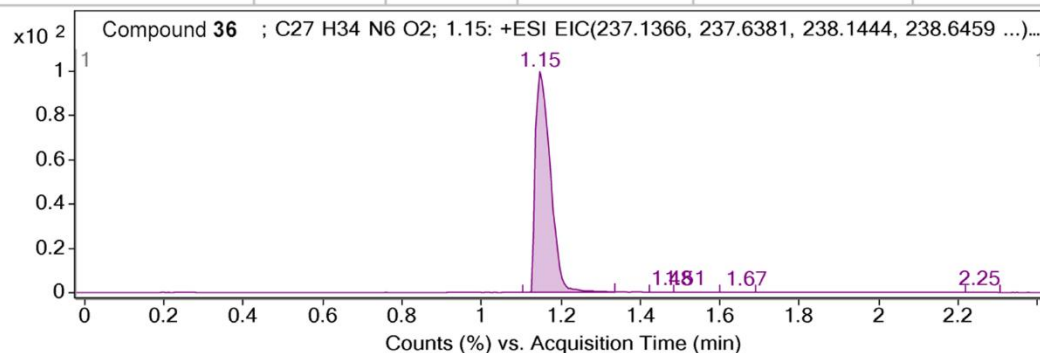
--- End Of Report ---

Compound 36

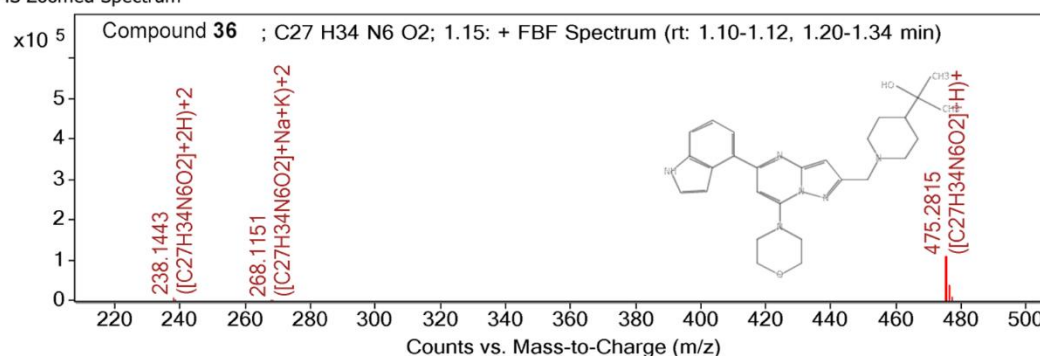


Compound 36

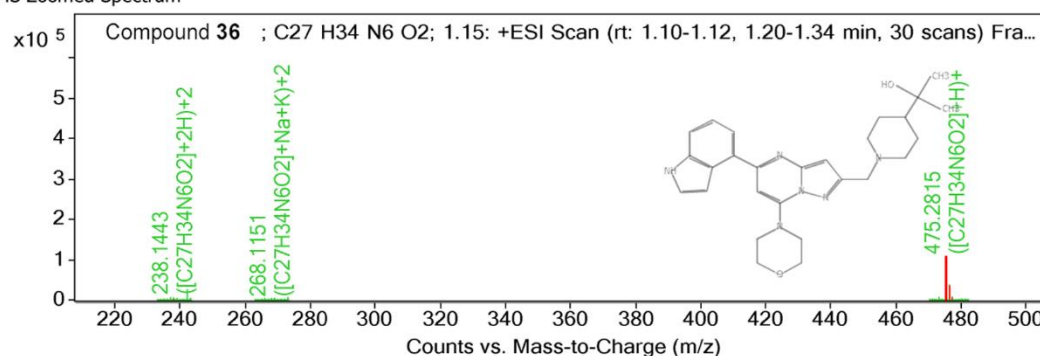
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 36	475.2815	1.15	474.2752	C27 H34 N6 O2	474.2743	1.85	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

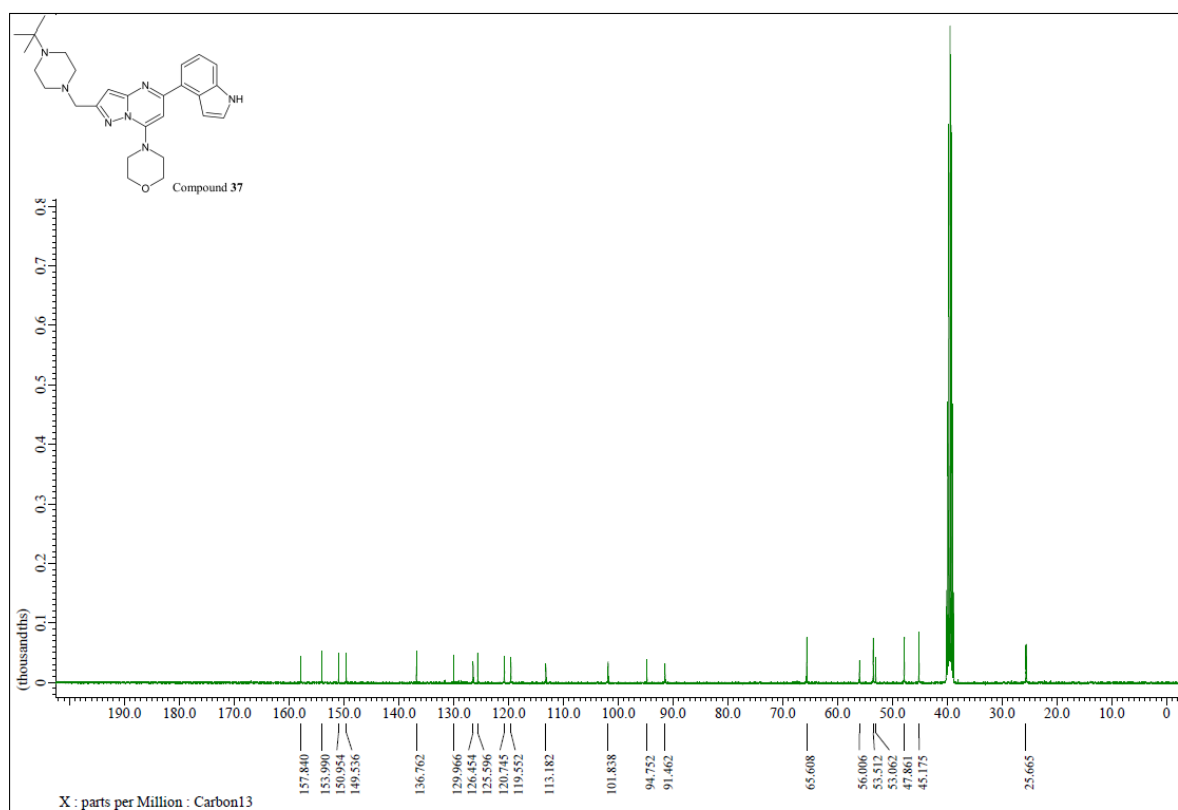
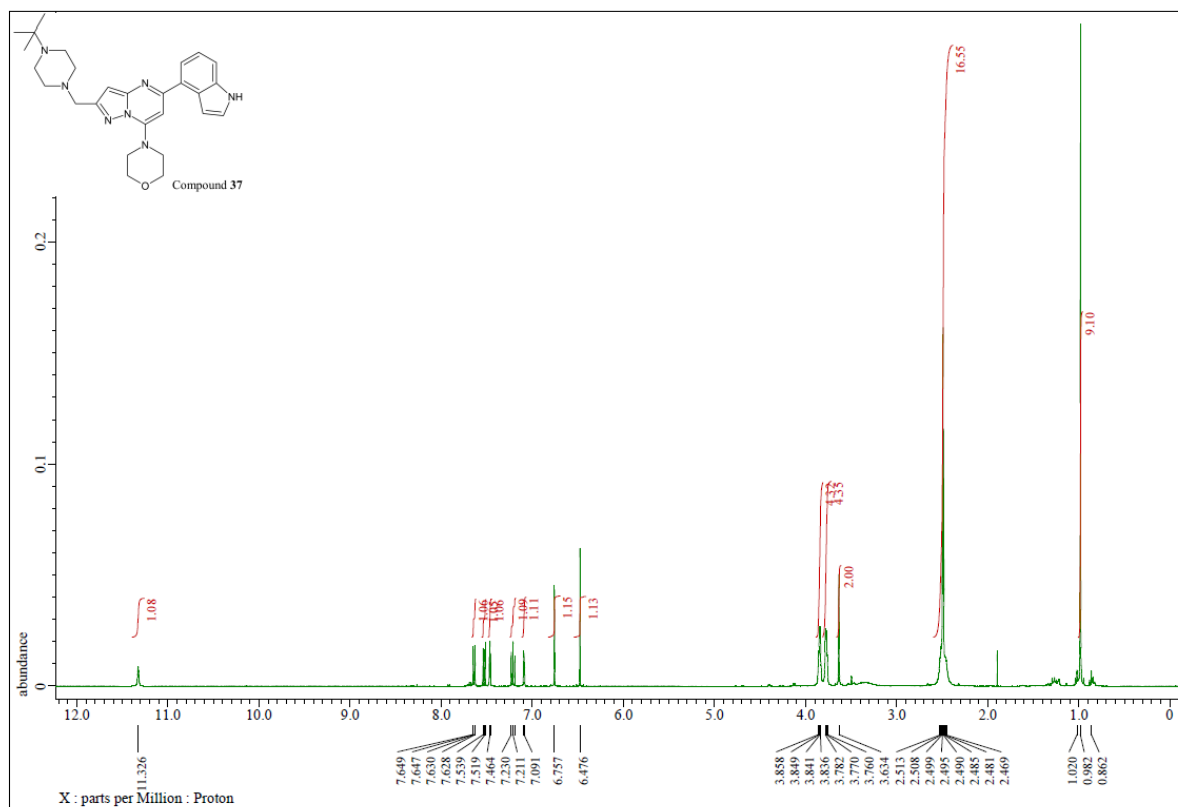


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.1443	2	4850.05	C27H34N6O2	(M+2H)+2	
238.6462	2	1098.49	C27H34N6O2	(M+2H)+2	
268.1151	2	173.99	C27H34N6O2	(M+Na+K)+2	
268.6137	2	18.68	C27H34N6O2	(M+Na+K)+2	
475.2815	1	104772.1	C27H34N6O2	(M+H)+	
476.288	1	36473.09	C27H34N6O2	(M+H)+	
477.29	1	7399.36	C27H34N6O2	(M+H)+	
238.1443	2	4850.05	C27H34N6O2	(M+2H)+2	-0.54
238.6462	2	1098.49	C27H34N6O2	(M+2H)+2	1.15
268.1151	2	173.99	C27H34N6O2	(M+Na+K)+2	6.37
268.6137	2	18.68	C27H34N6O2	(M+Na+K)+2	-4.18
475.2815	1	104772.1	C27H34N6O2	(M+H)+	-0.18
476.288	1	36473.09	C27H34N6O2	(M+H)+	7.21
477.29	1	7399.36	C27H34N6O2	(M+H)+	5.4

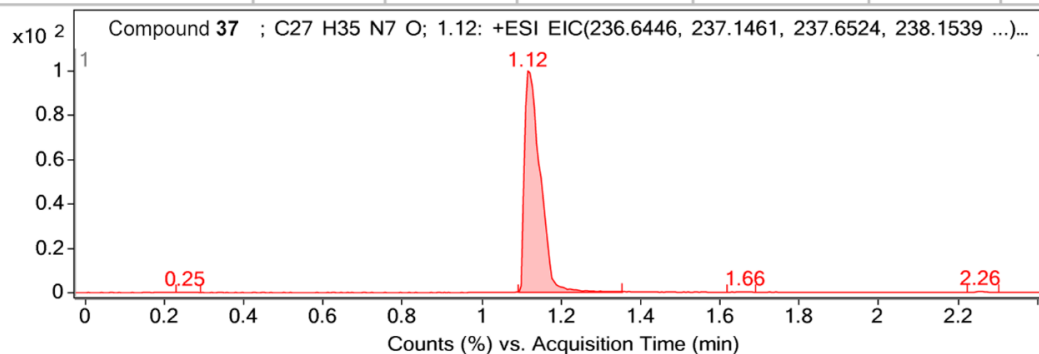
--- End Of Report ---

Compound 37

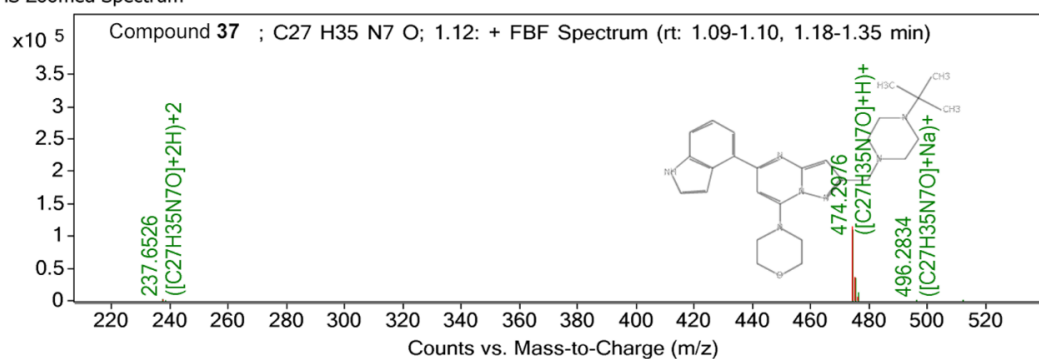


Compound 37

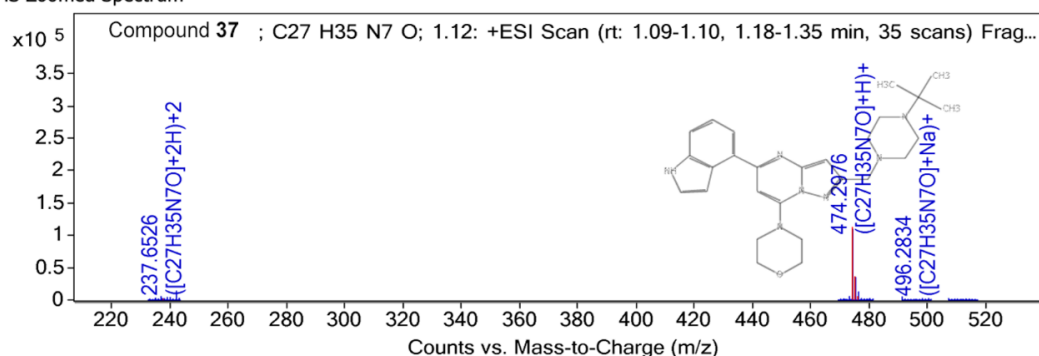
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Algorith
Compound 37	474.2976	1.12	473.2904	C27 H35 N7 O	473.2903	0.1	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

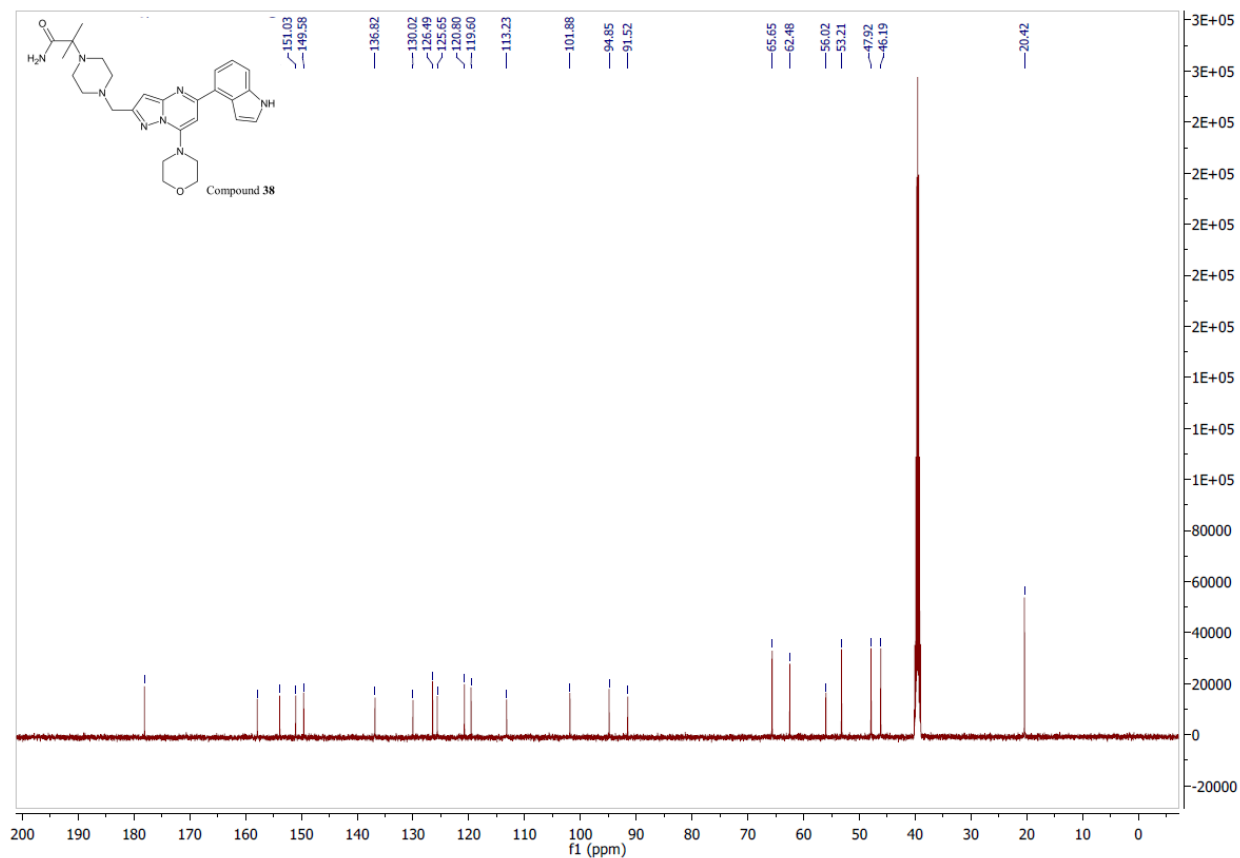
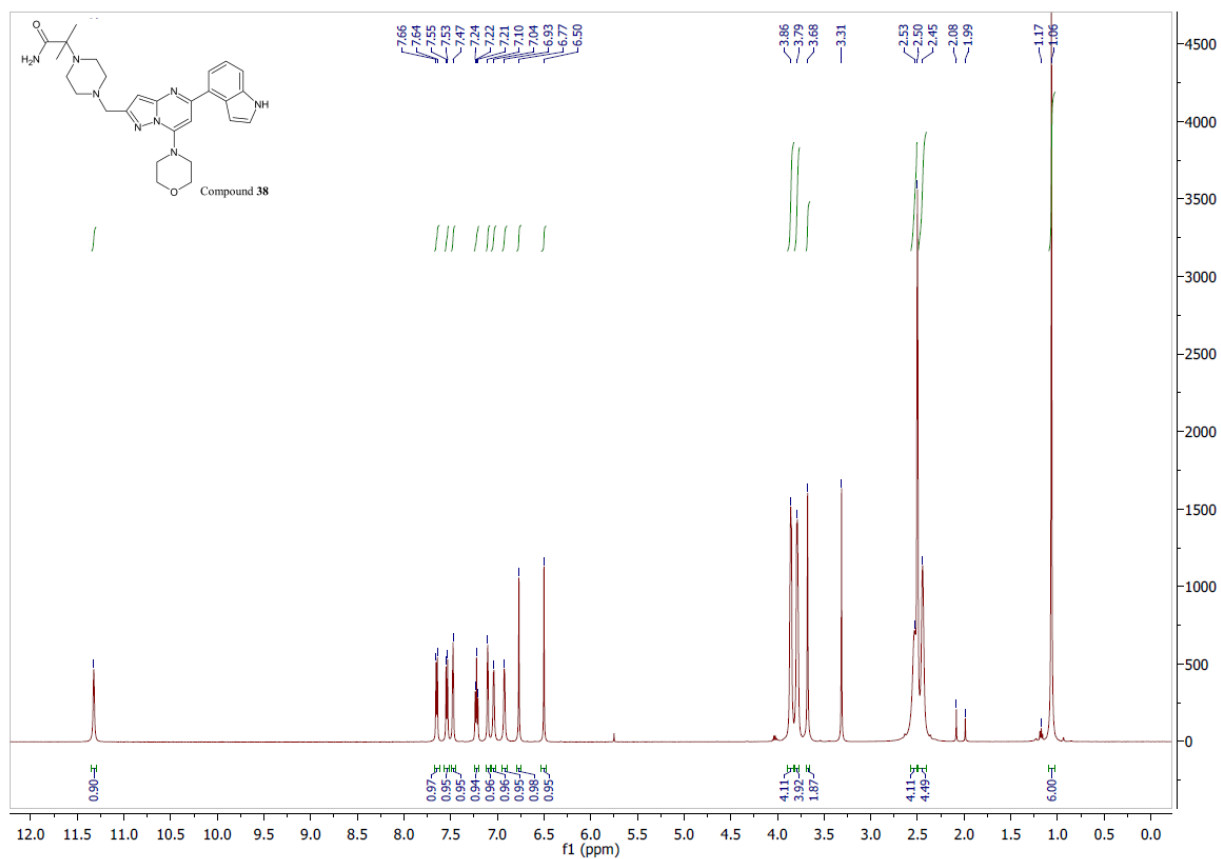


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
237.6526	2	1976.24	C27H35N7O	(M+2H)+2	
238.655	2	91.48	C27H35N7O	(M+2H)+2	
474.2976	1	109334.64	C27H35N7O	(M+H)+	
475.3002	1	34766.21	C27H35N7O	(M+H)+	
476.3044	1	12225.21	C27H35N7O	(M+H)+	
496.2834	1	461.95	C27H35N7O	(M+Na)+	
512.2544	1	408.88	C27H35N7O	(M+K)+	
237.6526	2	1976.24	C27H35N7O	(M+2H)+2	0.59
238.655	2	91.48	C27H35N7O	(M+2H)+2	-1
474.2976	1	109334.64	C27H35N7O	(M+H)+	0.02
475.3002	1	34766.21	C27H35N7O	(M+H)+	-0.58
476.3044	1	12225.21	C27H35N7O	(M+H)+	2.33
496.2834	1	461.95	C27H35N7O	(M+Na)+	7.8
512.2544	1	408.88	C27H35N7O	(M+K)+	1.88

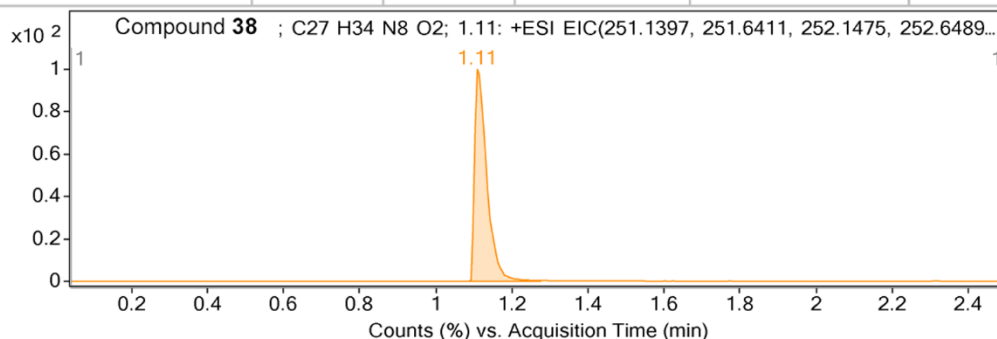
--- End Of Report ---

Compound 38

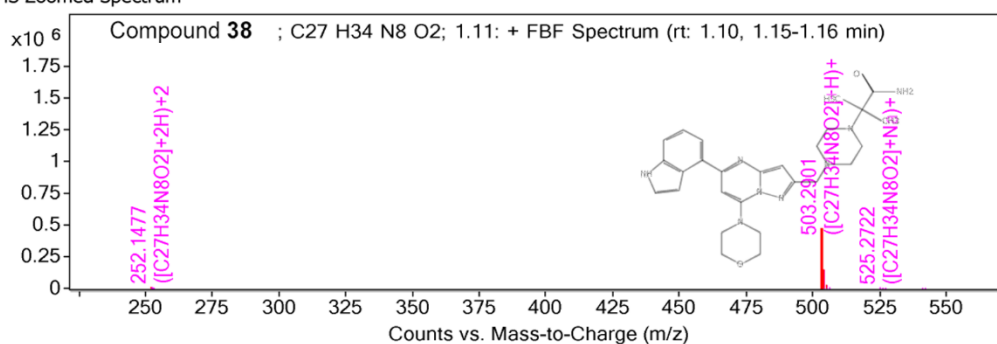


Compound 38

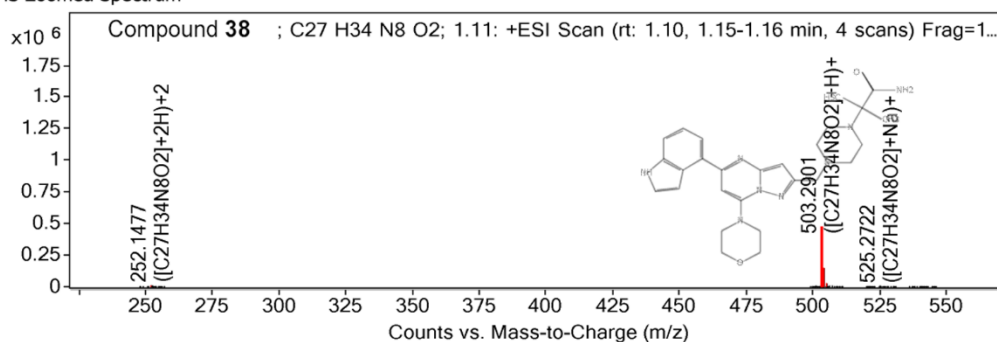
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaoirith
Compound 38	525.2722	1.11	502.2828	C27 H34 N8 O2	502.2805	4.69	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

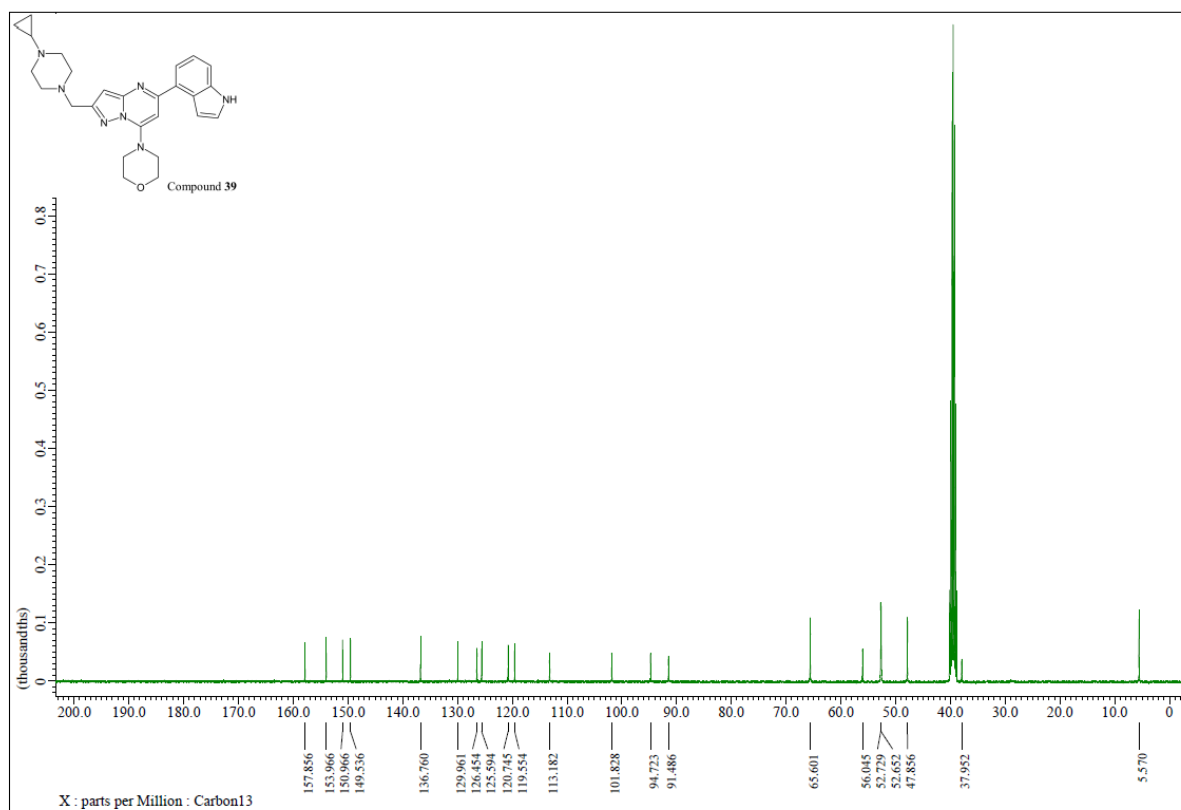
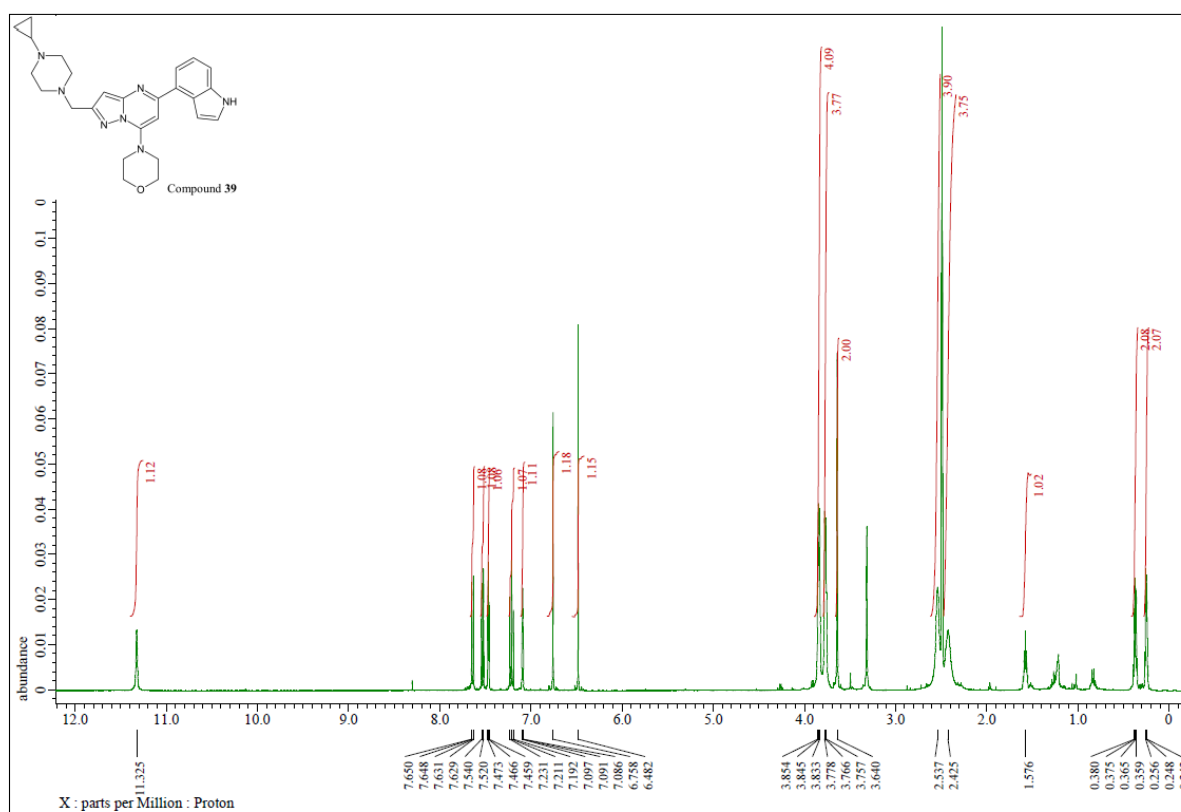


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
503.2901	1	469024.59	C27H34N8O2	(M+H)+	
503.2901	1	469024.59	C27H34N8O2	(M+H)+	4.59

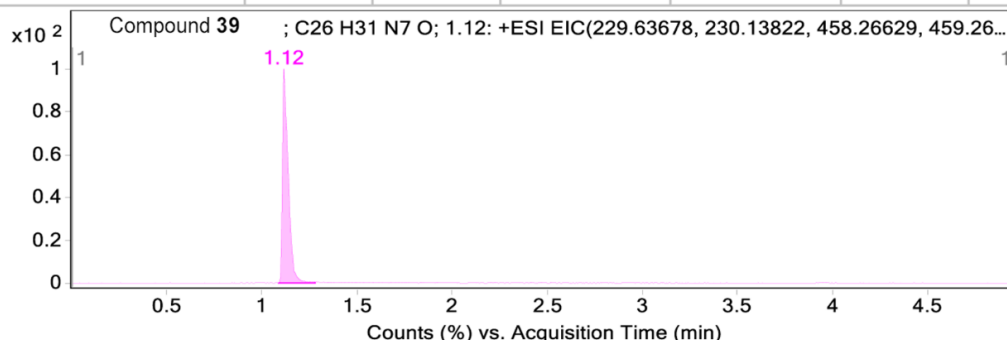
--- End Of Report ---

Compound 39

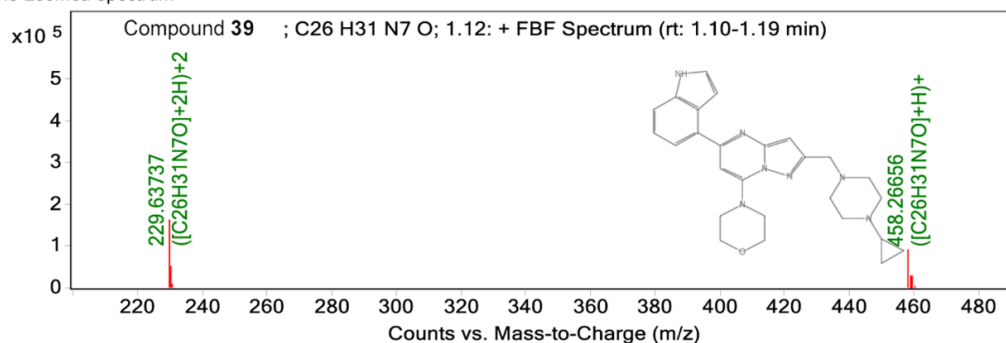


Compound 39

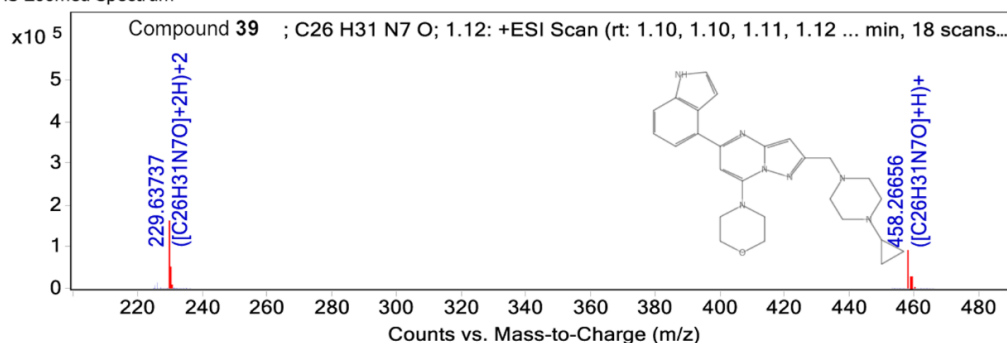
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 39	458.26656	1.12	457.2599	C26 H31 N7 O	457.25901	1.94	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

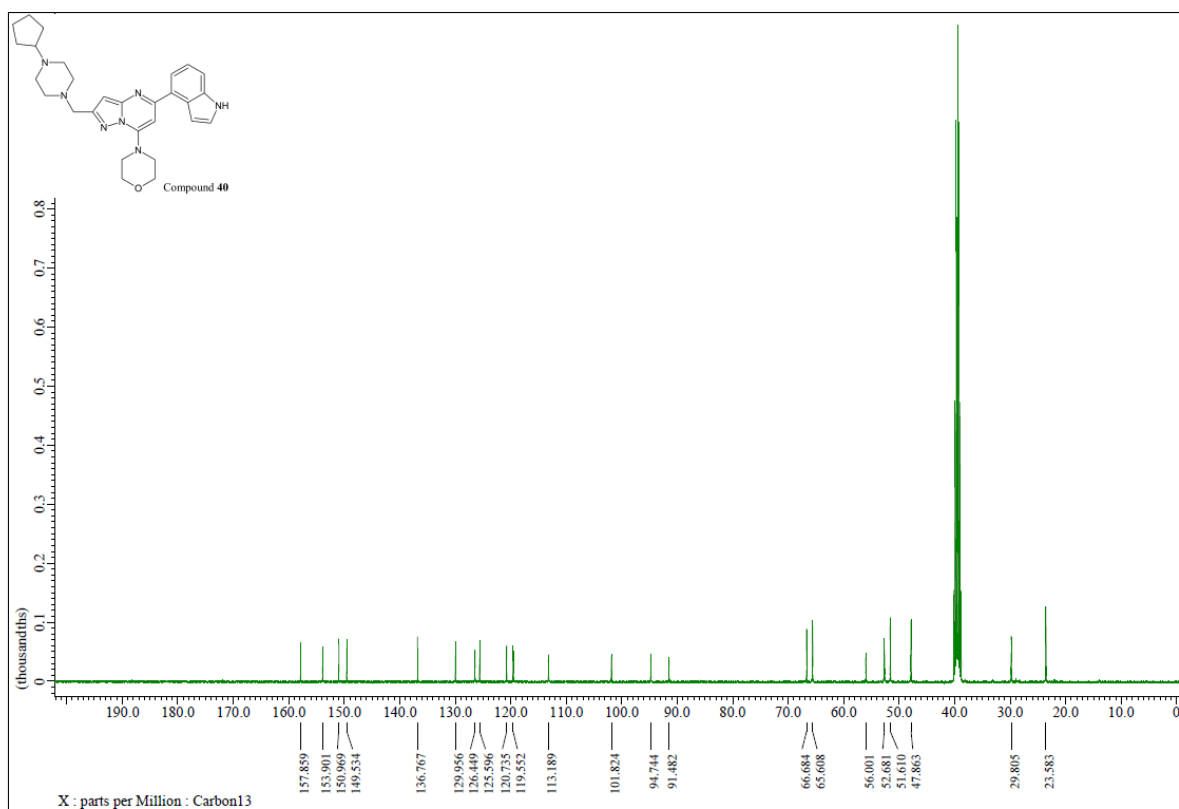
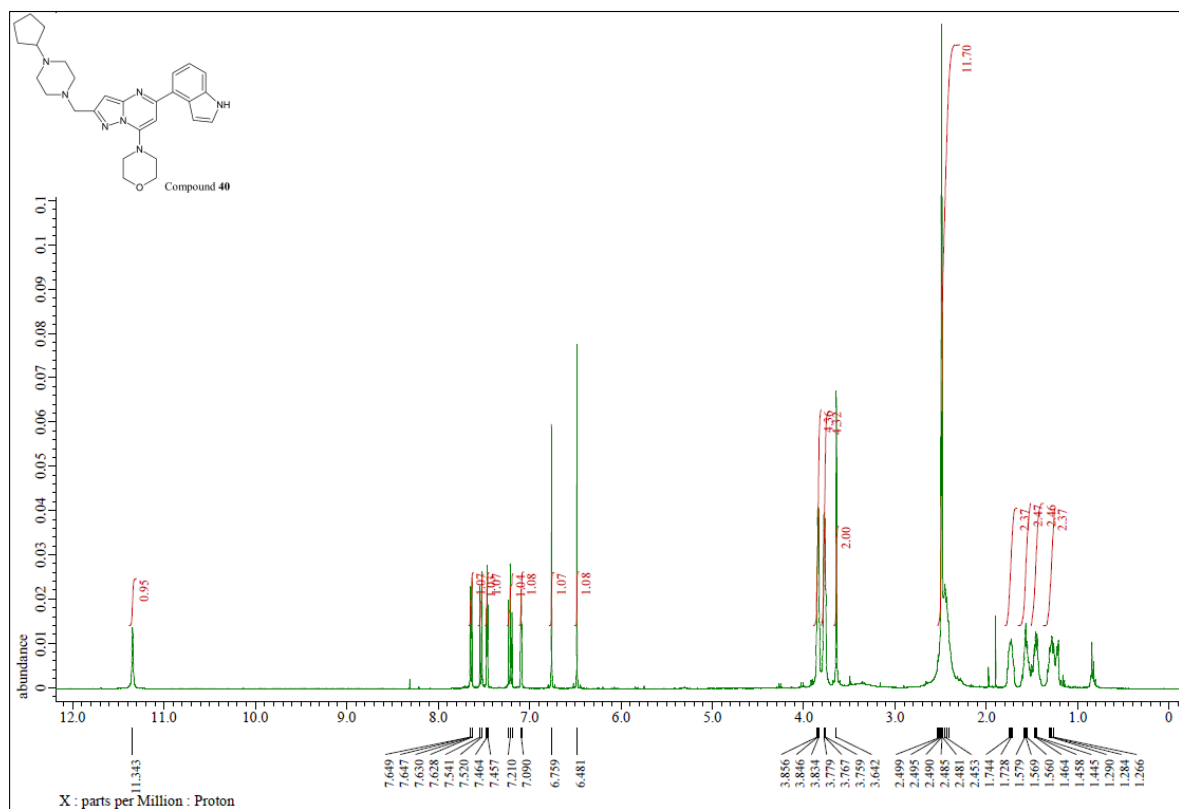


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
229.63737	2	163876.17	C26H31N7O	(M+2H)+2	
230.139	2	49603.69	C26H31N7O	(M+2H)+2	
230.64031	2	7768.41	C26H31N7O	(M+2H)+2	
231.13724	2	993.14	C26H31N7O	(M+2H)+2	
458.26656	1	90851.98	C26H31N7O	(M+H)+	
459.26935	1	28360.6	C26H31N7O	(M+H)+	
460.27201	1	4396.89	C26H31N7O	(M+H)+	
461.27623	1	511.48	C26H31N7O	(M+H)+	
229.63737	2	163876.17	C26H31N7O	(M+2H)+2	2.58
230.139	2	49603.69	C26H31N7O	(M+2H)+2	3.41
230.64031	2	7768.41	C26H31N7O	(M+2H)+2	3.05
231.13724	2	993.14	C26H31N7O	(M+2H)+2	-16.14
458.26656	1	90851.98	C26H31N7O	(M+H)+	0.6
459.26935	1	28360.6	C26H31N7O	(M+H)+	0.41
460.27201	1	4396.89	C26H31N7O	(M+H)+	0.14
461.27623	1	511.48	C26H31N7O	(M+H)+	3.4

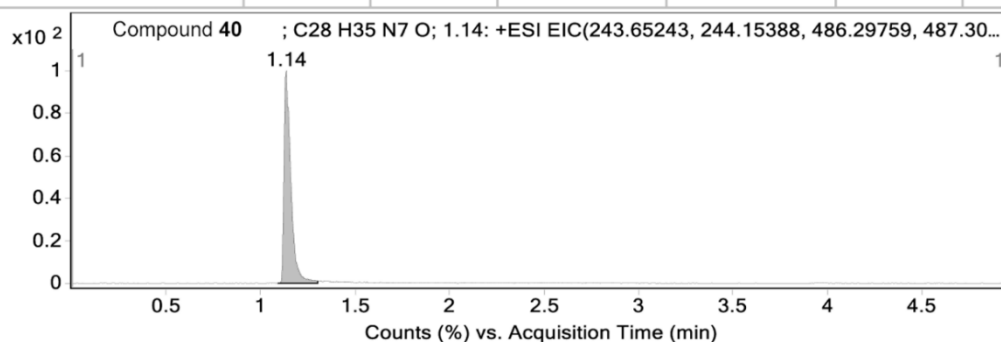
--- End Of Report ---

Compound 40

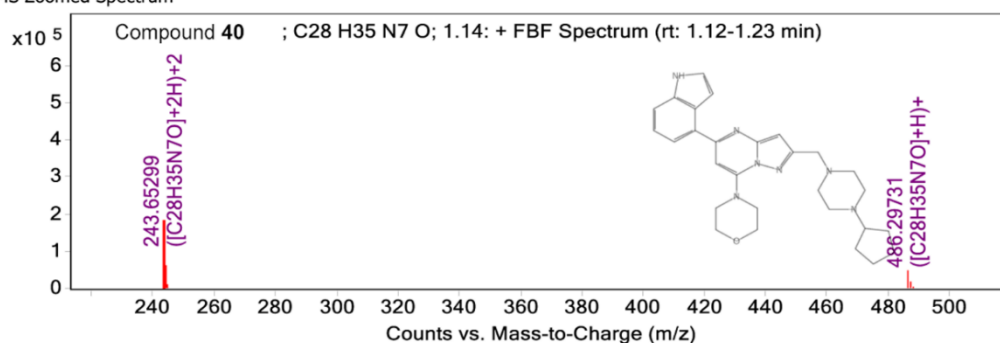


Compound 40

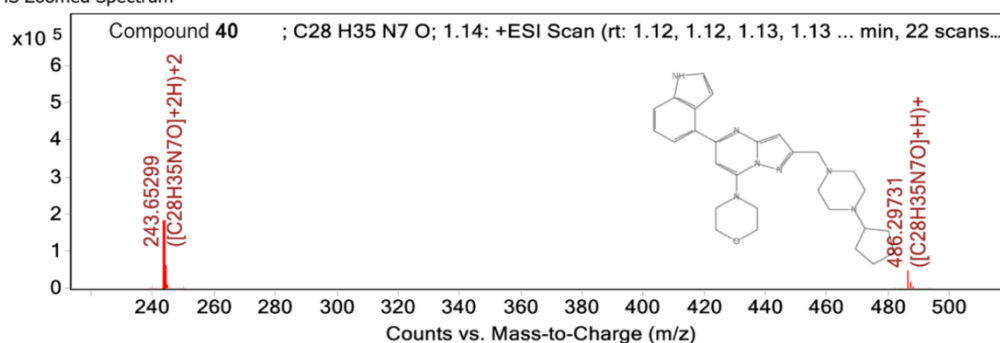
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 40	486.29731	1.14	485.29115	C28 H35 N7 O	485.29031	1.73	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

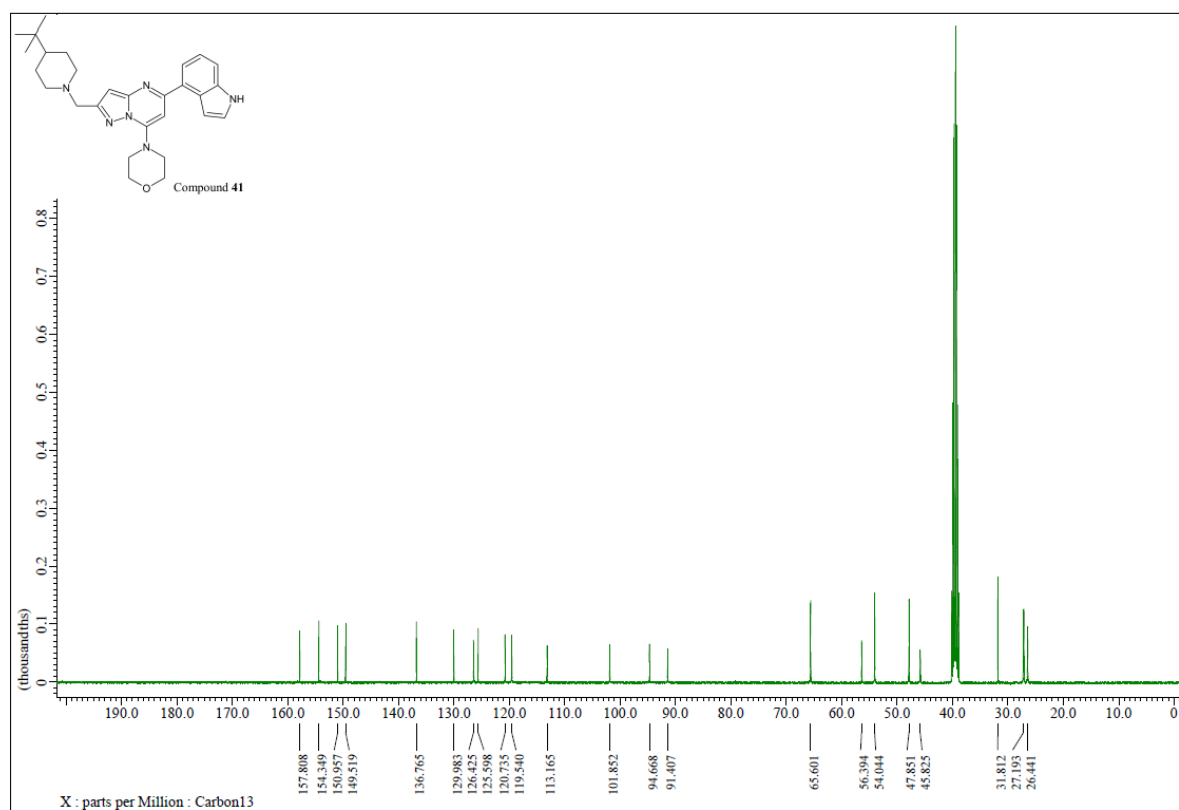
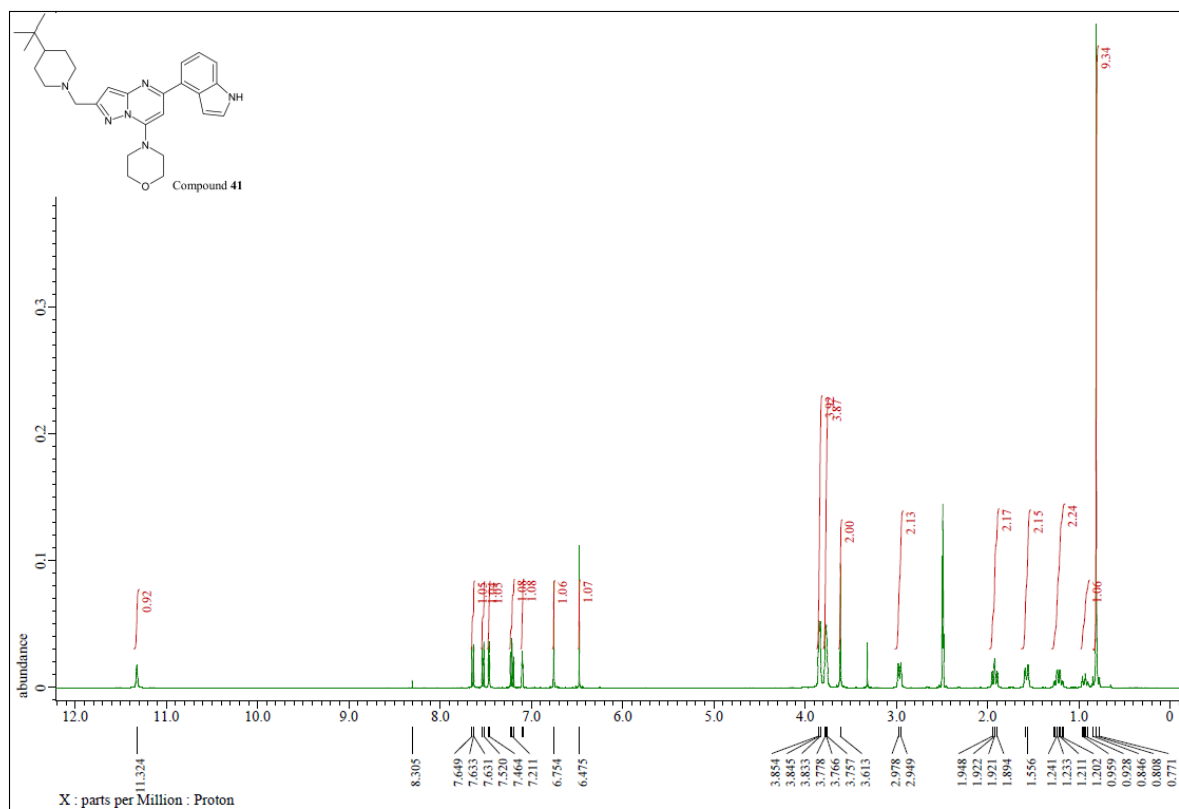


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
243.65299	2	183132.14	C28H35N7O	(M+2H)+2	
244.1546	2	57179.7	C28H35N7O	(M+2H)+2	
244.65581	2	9451.18	C28H35N7O	(M+2H)+2	
245.1542	2	1692.28	C28H35N7O	(M+2H)+2	
486.29731	1	47318.36	C28H35N7O	(M+H)+	
487.30016	1	15779.74	C28H35N7O	(M+H)+	
488.30307	1	2791.22	C28H35N7O	(M+H)+	
489.30436	1	349.8	C28H35N7O	(M+H)+	
243.65299	2	183132.14	C28H35N7O	(M+2H)+2	2.28
244.1546	2	57179.7	C28H35N7O	(M+2H)+2	2.95
244.65581	2	9451.18	C28H35N7O	(M+2H)+2	2.07
245.1542	2	1692.28	C28H35N7O	(M+2H)+2	-10.14
486.29731	1	47318.36	C28H35N7O	(M+H)+	-0.57
487.30016	1	15779.74	C28H35N7O	(M+H)+	-0.68
488.30307	1	2791.22	C28H35N7O	(M+H)+	-0.53
489.30436	1	349.8	C28H35N7O	(M+H)+	-3.52

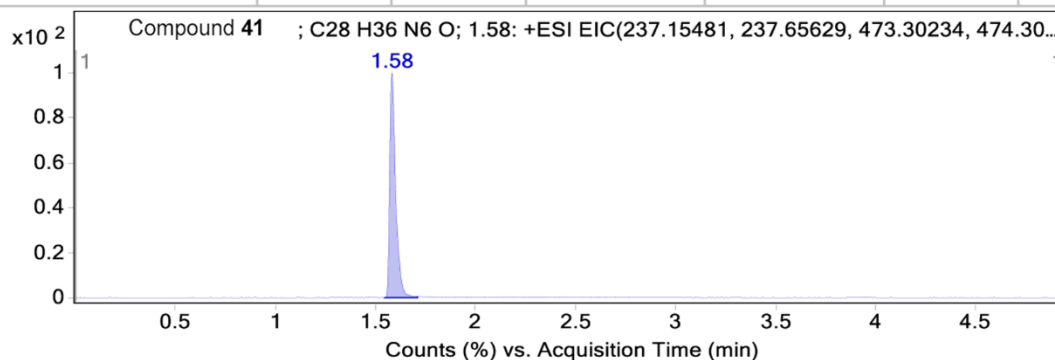
--- End Of Report ---

Compound 41

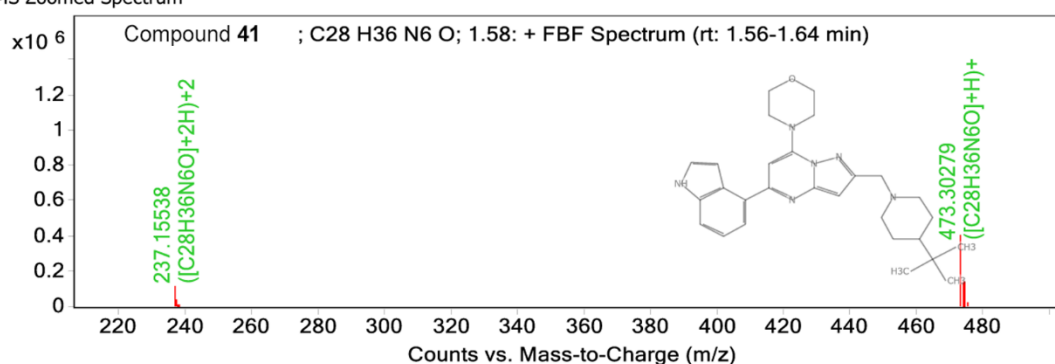


Compound 41

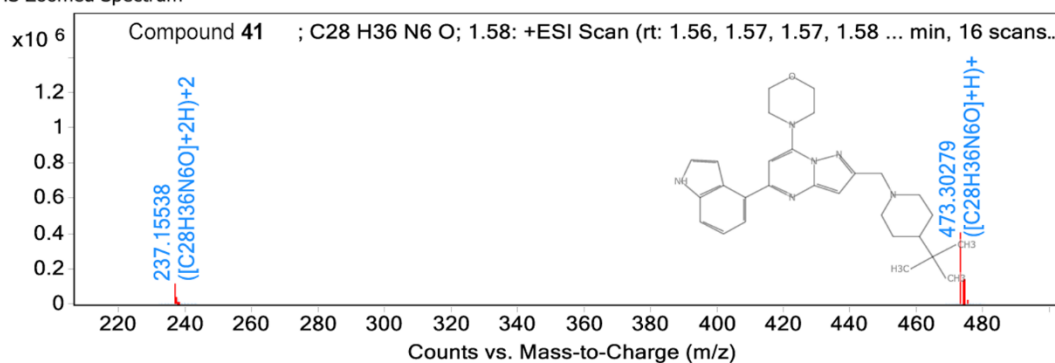
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 41	237.15538	1.58	472.29562	C28 H36 N6 O	472.29506	1.18	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

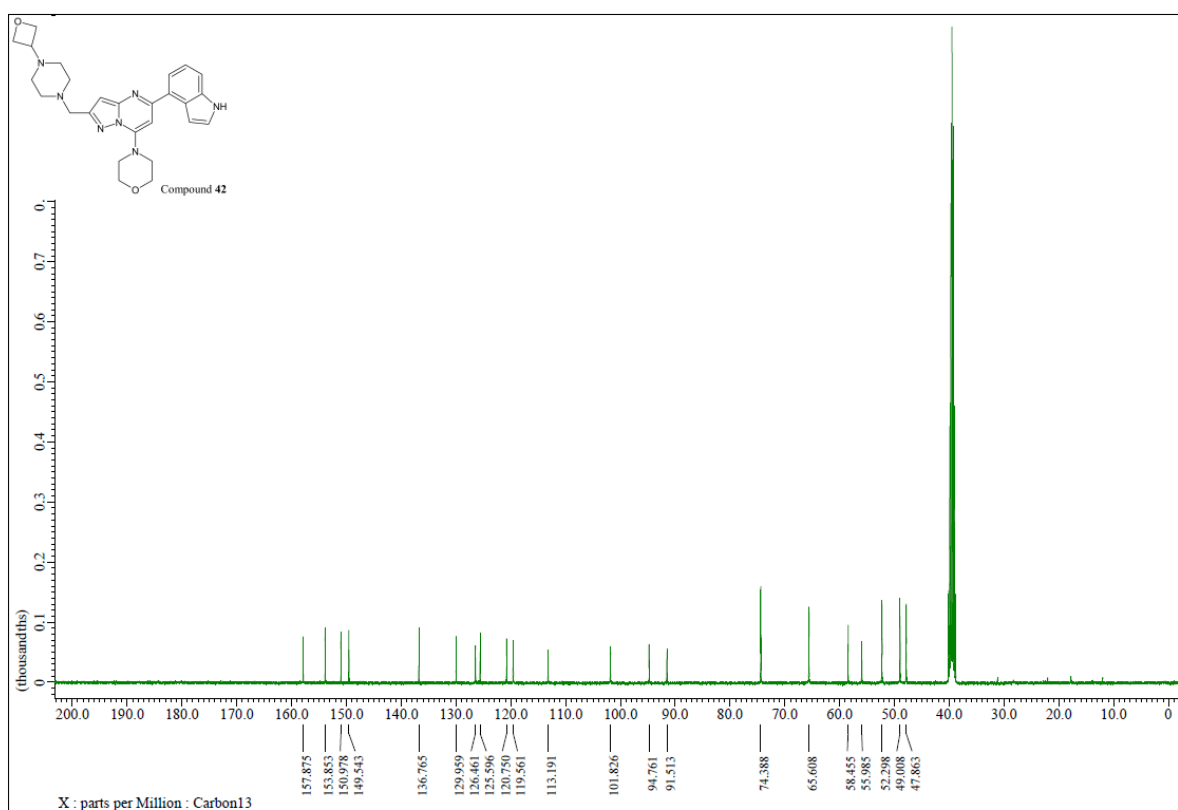
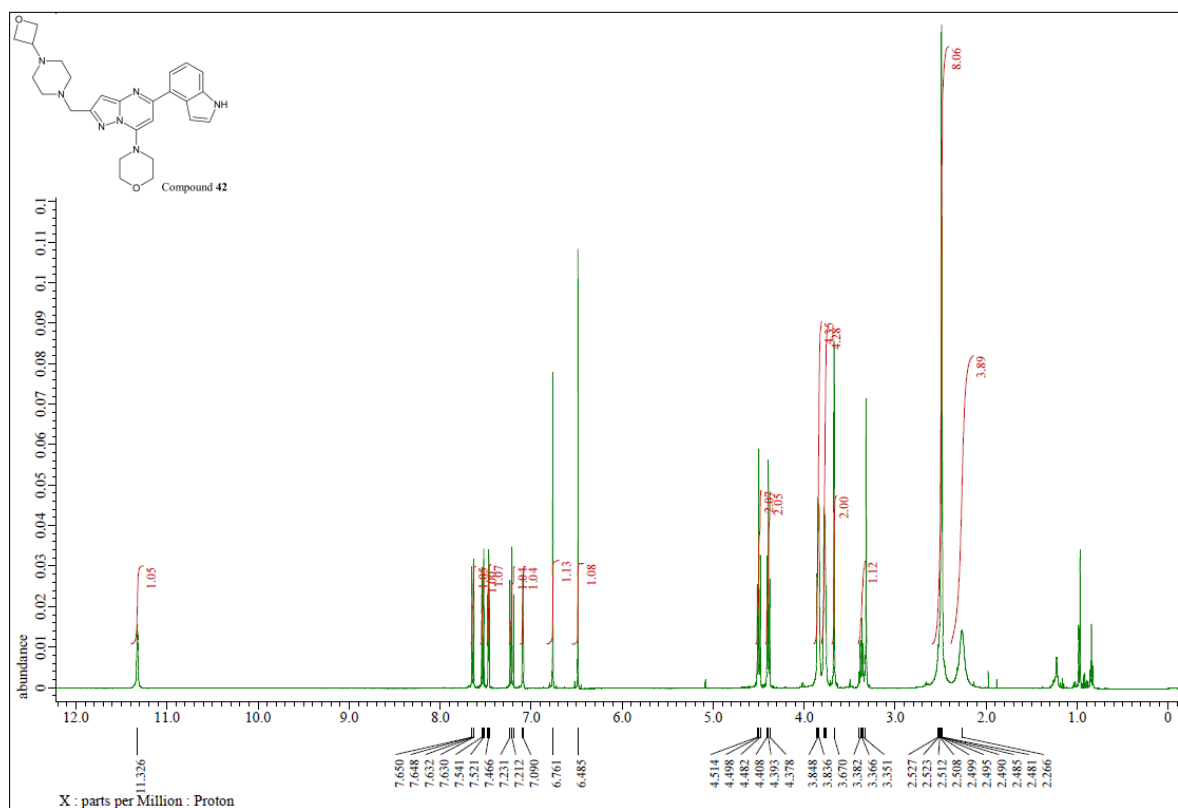


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
237.15538	2	111387.02	C28H36N6O	(M+2H)+2	
237.65676	2	36742.8	C28H36N6O	(M+2H)+2	
238.15755	2	6752.31	C28H36N6O	(M+2H)+2	
238.65771	2	829.94	C28H36N6O	(M+2H)+2	
473.30279	1	407145.97	C28H36N6O	(M+H)+	
474.30575	1	121042.59	C28H36N6O	(M+H)+	
475.30801	1	19658.06	C28H36N6O	(M+H)+	
237.15538	2	111387.02	C28H36N6O	(M+2H)+2	2.42
237.65676	2	36742.8	C28H36N6O	(M+2H)+2	1.97
238.15755	2	6752.31	C28H36N6O	(M+2H)+2	-0.8
238.65771	2	829.94	C28H36N6O	(M+2H)+2	-6.03
473.30279	1	407145.97	C28H36N6O	(M+H)+	0.96
474.30575	1	121042.59	C28H36N6O	(M+H)+	0.94
475.30801	1	19658.06	C28H36N6O	(M+H)+	-0.41

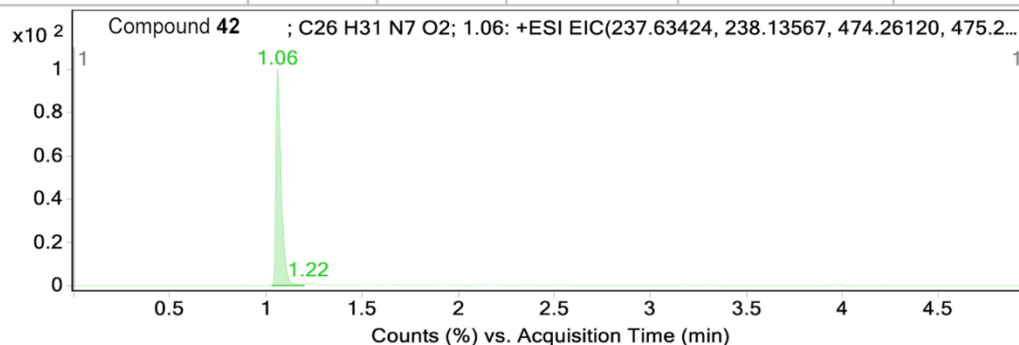
--- End Of Report ---

Compound 42

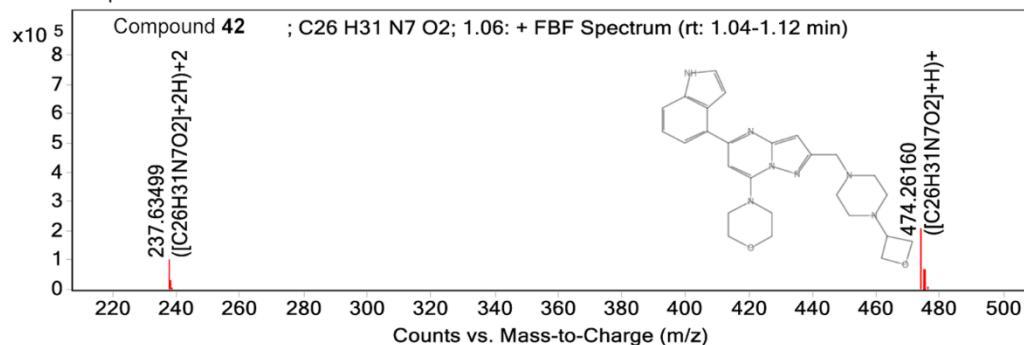


Compound 42

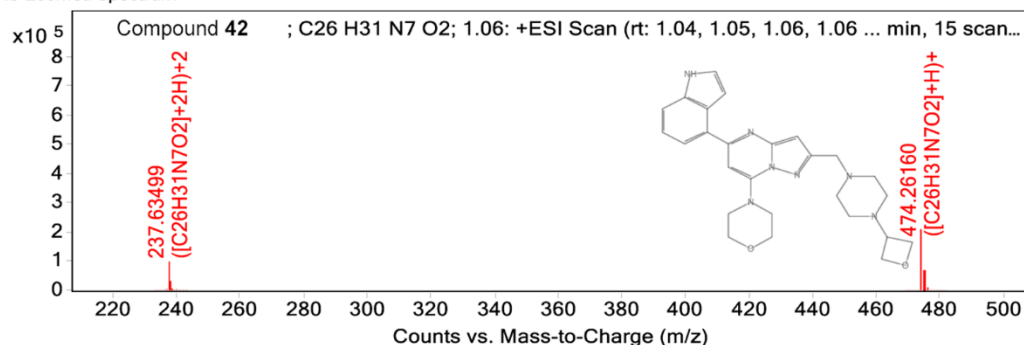
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaoirith
Compound 42	474.2616	1.06	473.25456	C26 H31 N7 O2	473.25392	1.35	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

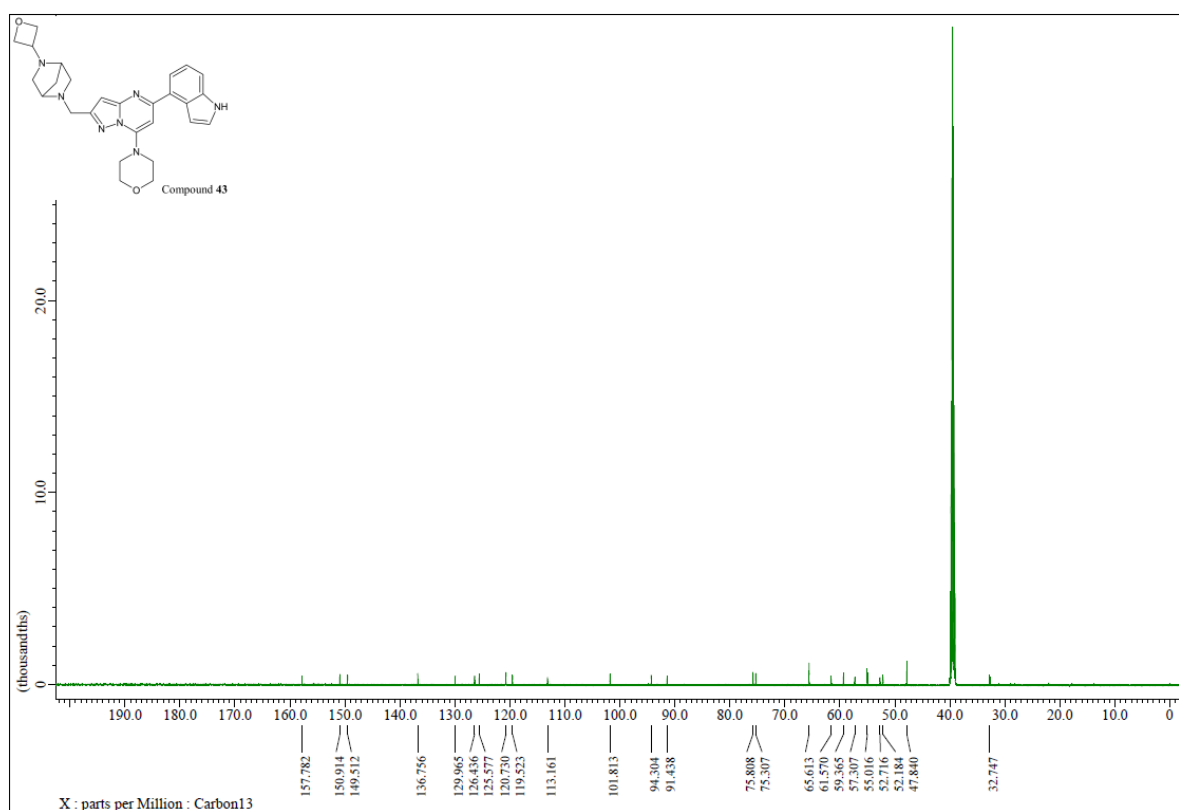
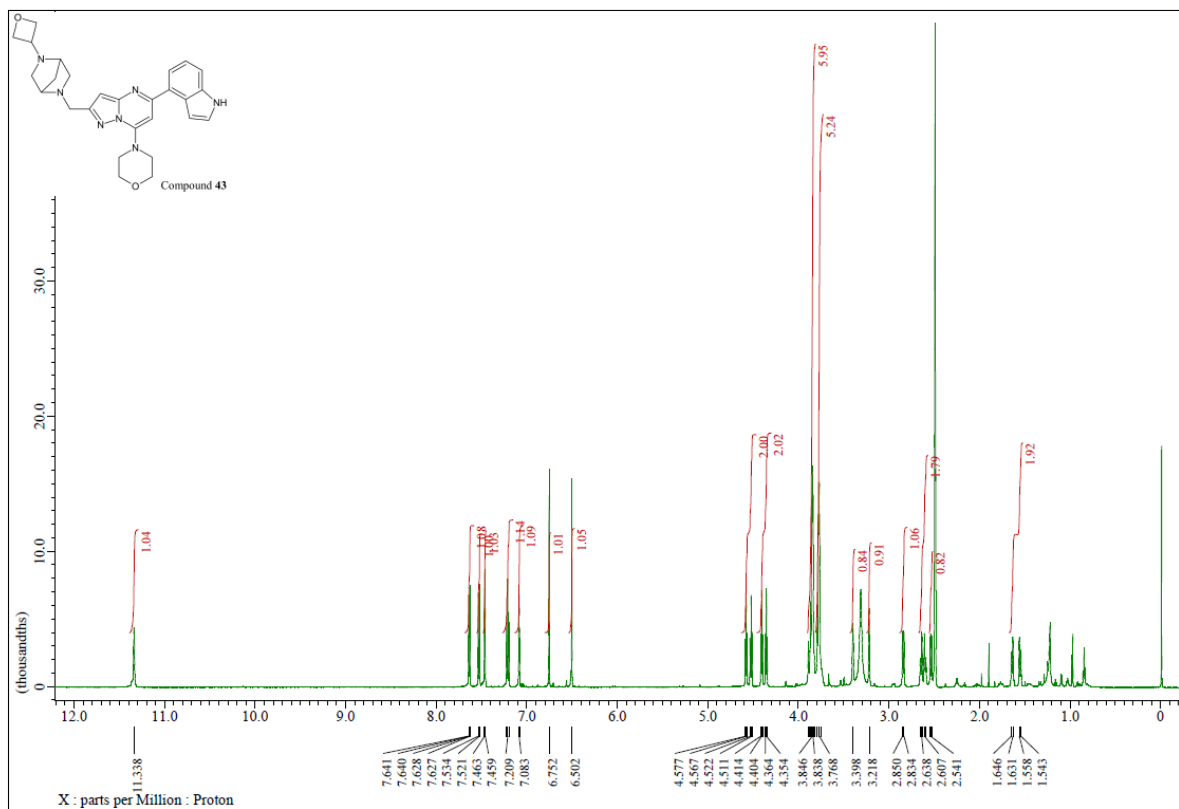


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
237.63499	2	99213.34	C26H31N7O2	(M+2H)+2	
238.13576	2	31857.8	C26H31N7O2	(M+2H)+2	
238.63738	2	4981.81	C26H31N7O2	(M+2H)+2	
474.2616	1	207817.77	C26H31N7O2	(M+H)+	
475.26443	1	63939.76	C26H31N7O2	(M+H)+	
476.267	1	9934.29	C26H31N7O2	(M+H)+	
477.27038	1	1159.53	C26H31N7O2	(M+H)+	
237.63499	2	99213.34	C26H31N7O2	(M+2H)+2	3.16
238.13576	2	31857.8	C26H31N7O2	(M+2H)+2	0.35
238.63738	2	4981.81	C26H31N7O2	(M+2H)+2	1.42
474.2616	1	207817.77	C26H31N7O2	(M+H)+	0.84
475.26443	1	63939.76	C26H31N7O2	(M+H)+	0.75
476.267	1	9934.29	C26H31N7O2	(M+H)+	0.42
477.27038	1	1159.53	C26H31N7O2	(M+H)+	1.96

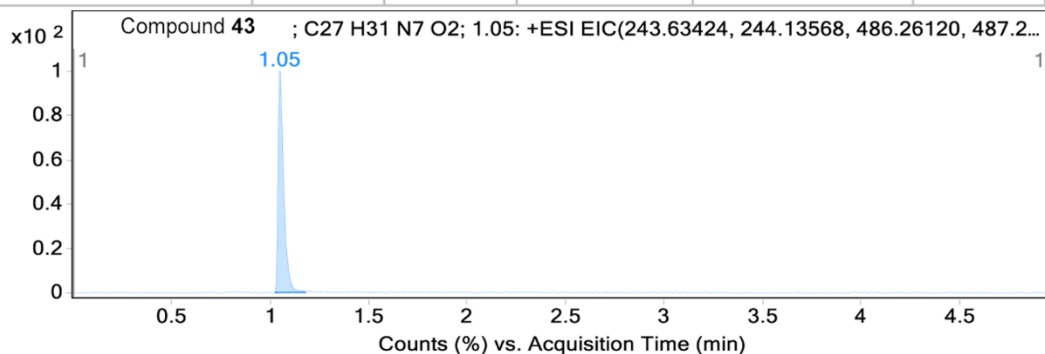
--- End Of Report ---

Compound 43

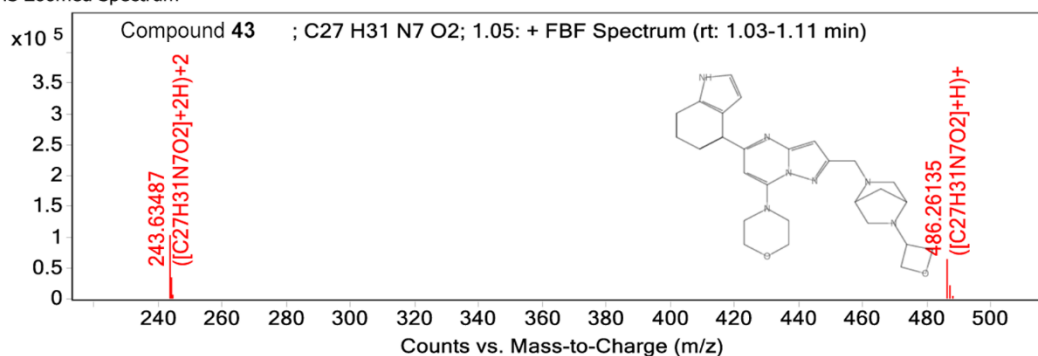


Compound 43

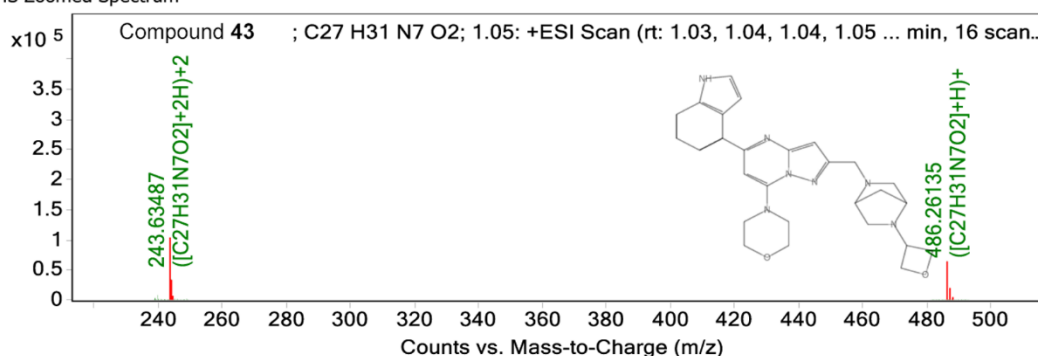
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 43	486.26135	1.05	485.25477	C27 H31 N7 O2	485.25392	1.74	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

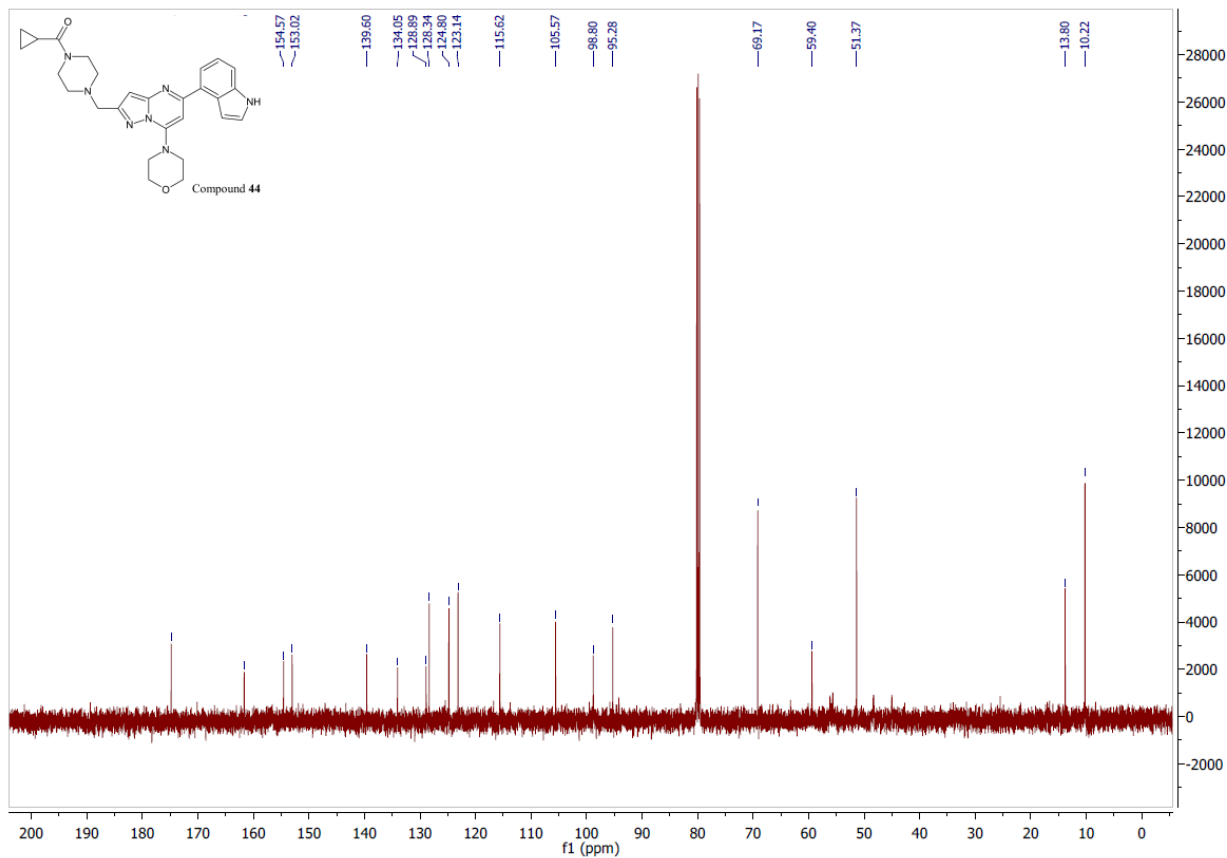
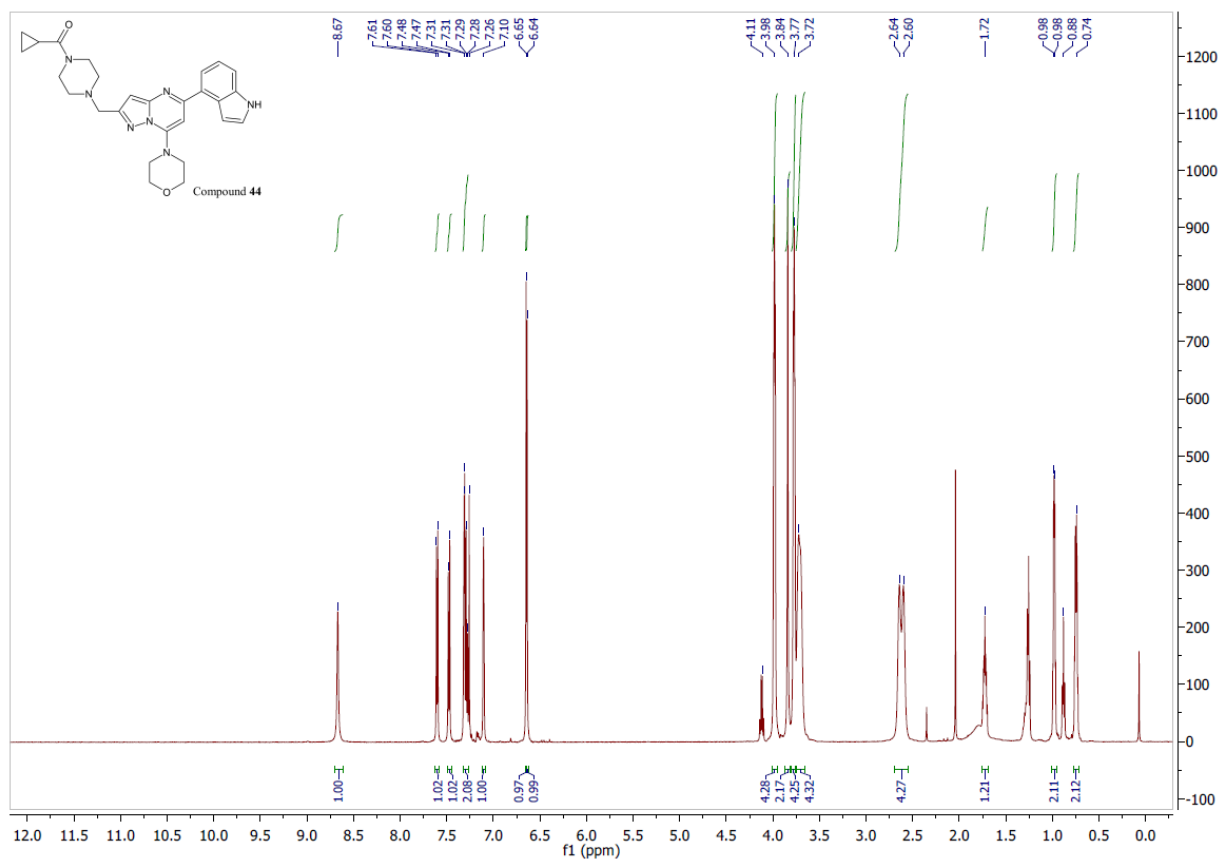


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
243.63487	2	102960.16	C27H31N7O2	(M+2H)+2	
244.13647	2	34634.86	C27H31N7O2	(M+2H)+2	
244.63749	2	5934.04	C27H31N7O2	(M+2H)+2	
486.26135	1	64416.76	C27H31N7O2	(M+H)+	
487.26383	1	19490.92	C27H31N7O2	(M+H)+	
488.2669	1	3146.05	C27H31N7O2	(M+H)+	
243.63487	2	102960.16	C27H31N7O2	(M+2H)+2	2.6
244.13647	2	34634.86	C27H31N7O2	(M+2H)+2	3.23
244.63749	2	5934.04	C27H31N7O2	(M+2H)+2	1.75
486.26135	1	64416.76	C27H31N7O2	(M+H)+	0.31
487.26383	1	19490.92	C27H31N7O2	(M+H)+	-0.53
488.2669	1	3146.05	C27H31N7O2	(M+H)+	0.12

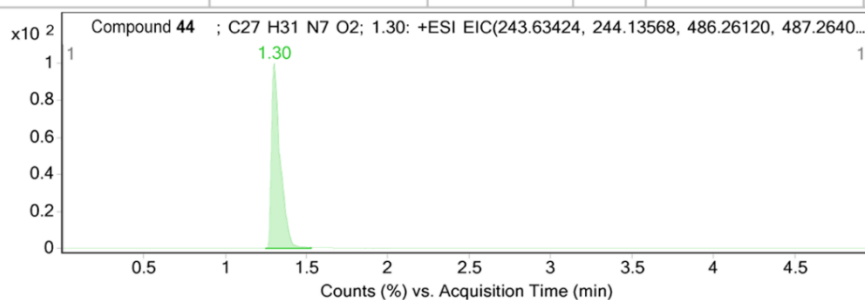
--- End Of Report ---

Compound 44

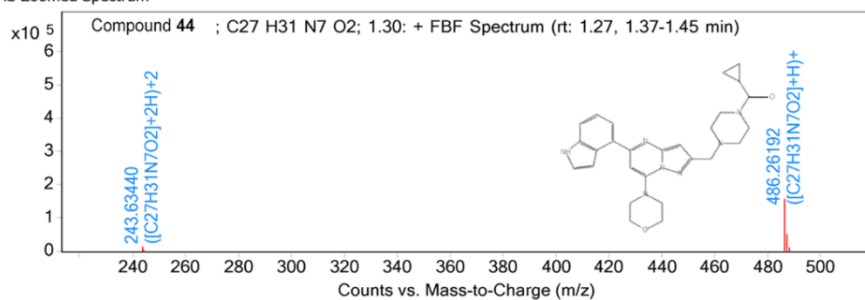


Compound 44

Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 44	Compound 44	243.6344	1.3	Find by Formula	485.25457



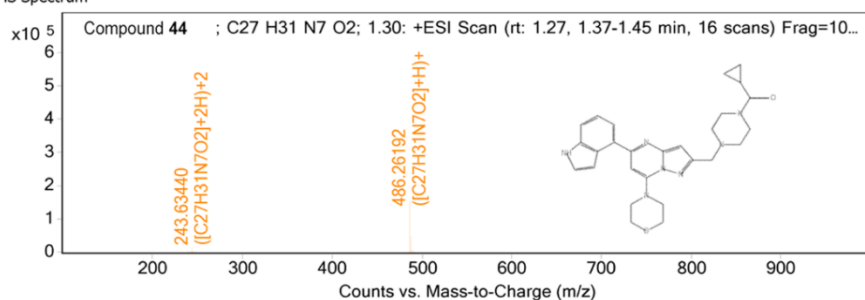
MS Zoomed Spectrum



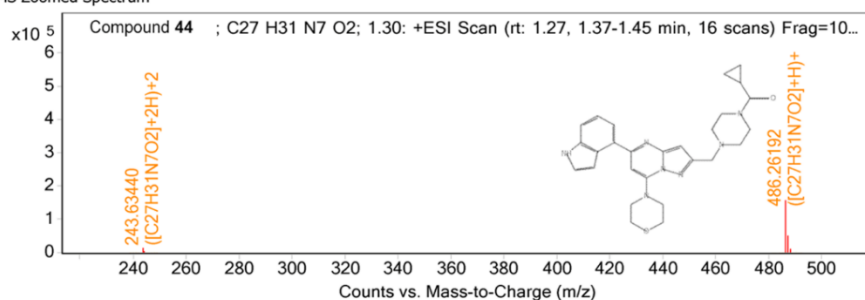
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
243.6344	2	12024.05	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
244.13608	2	3727.14	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
244.63743	2	671.81	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
486.26192	1	156276.28	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺
487.26456	1	46874.78	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺
488.26754	1	7930.26	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺

MS Spectrum



MS Zoomed Spectrum

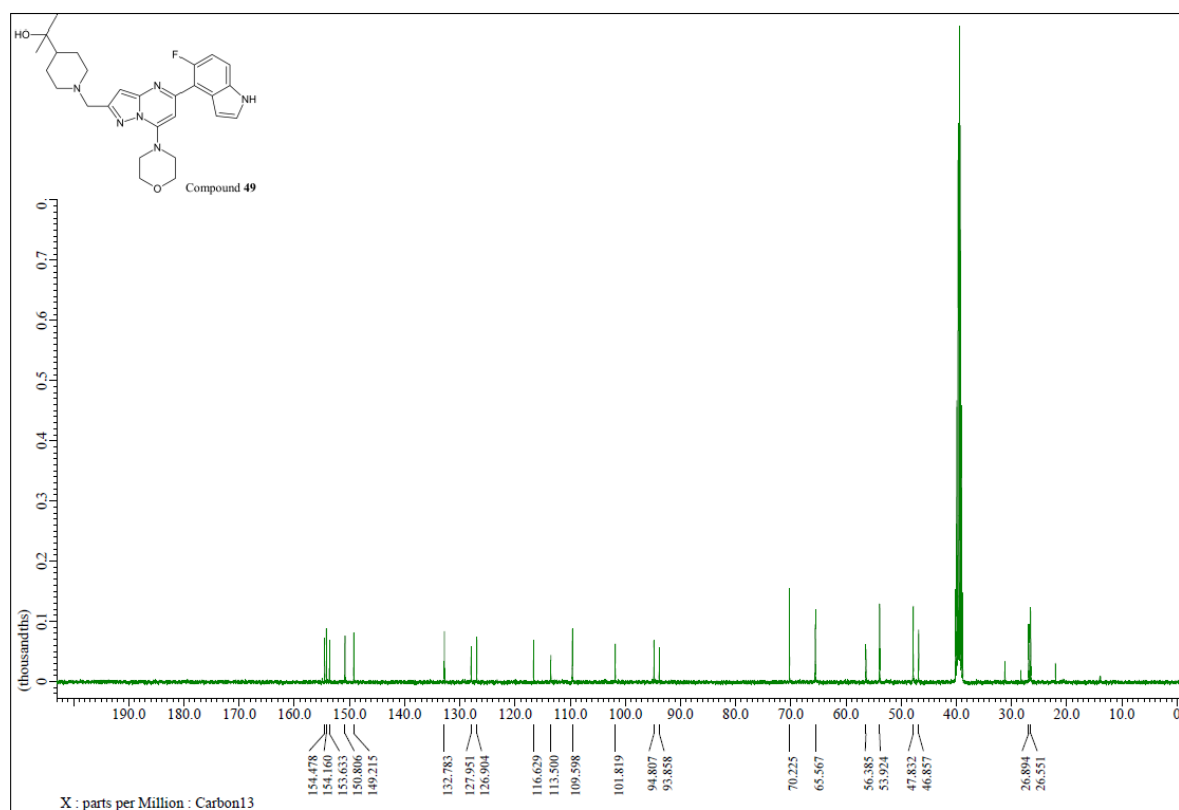
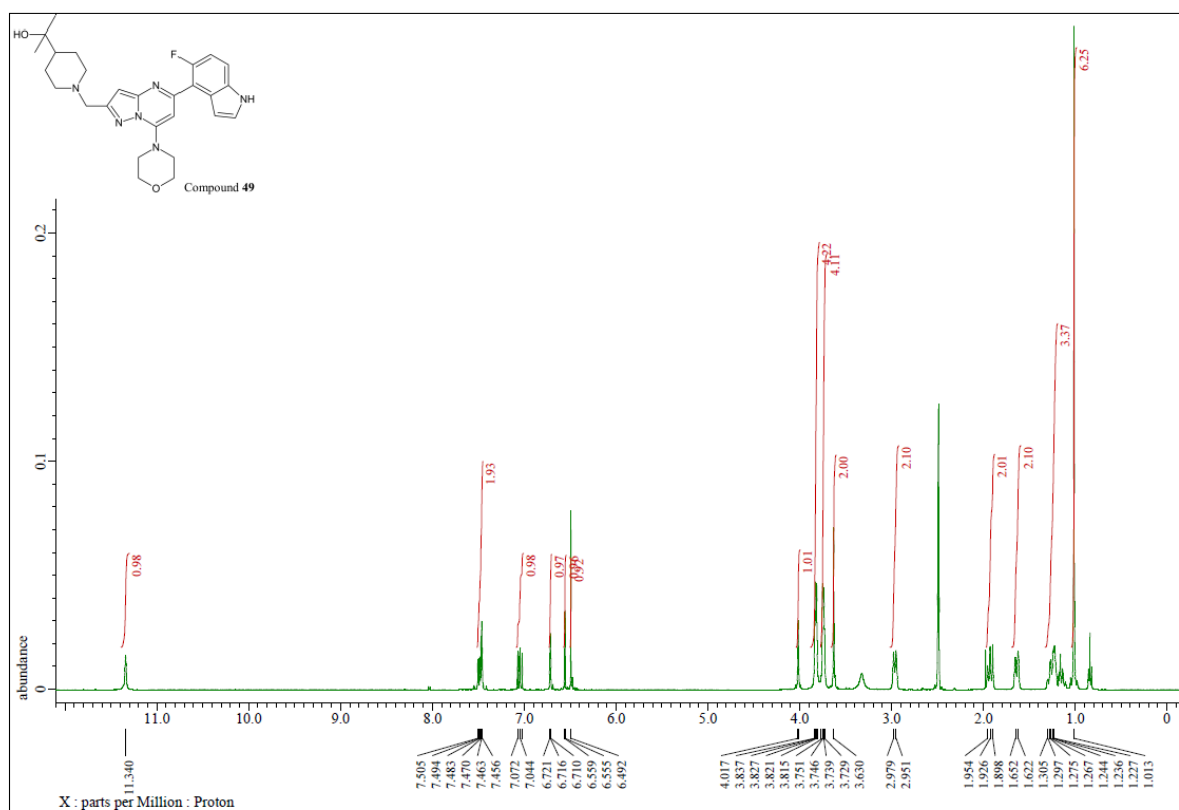


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
243.6344	243.63424	0.68	2	12024.05	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
244.13608	244.13568	1.62	2	3727.14	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
244.63743	244.63706	1.52	2	671.81	C ₂₇ H ₃₁ N ₇ O ₂	(M+2H) ²⁺
486.26192	486.2612	1.49	1	156276.28	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺
487.26456	487.26409	0.97	1	46874.78	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺
488.26754	488.26684	1.43	1	7930.26	C ₂₇ H ₃₁ N ₇ O ₂	(M+H) ⁺

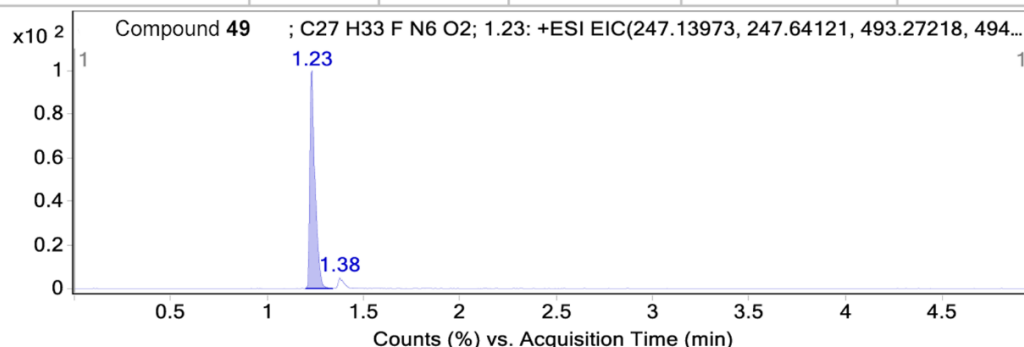
--- End Of Report ---

Compound 49

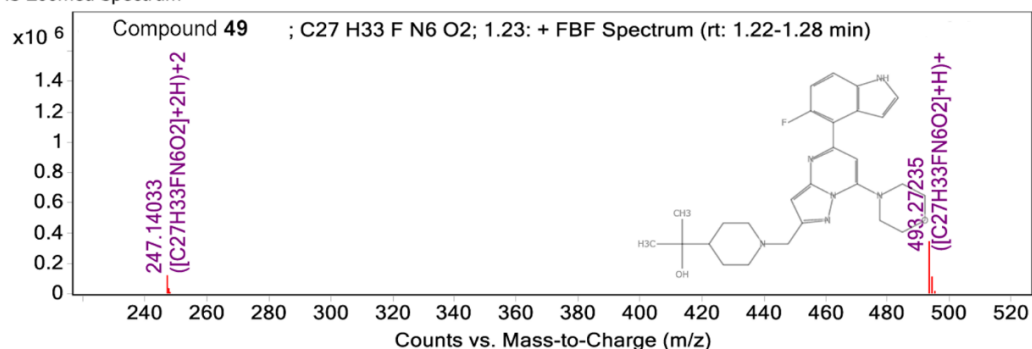


Compound 49

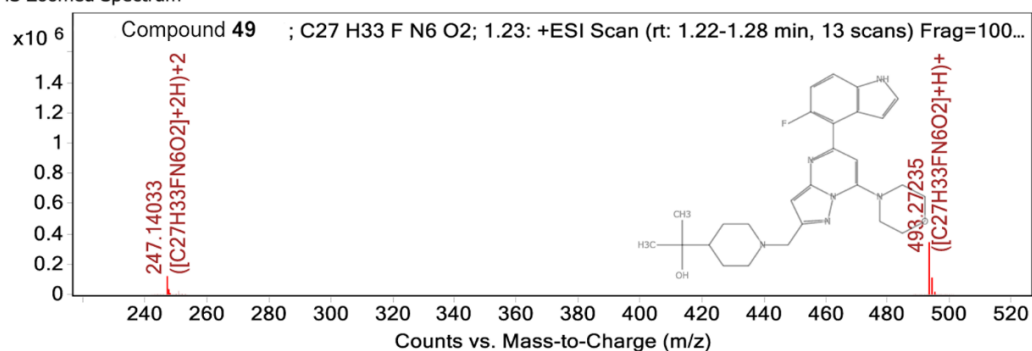
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd's Alao rit
Compound 49	493.27235	1.23	492.26532	C27 H33 F N6 O2	492.2649	0.86	Find by Formula



MS Zoomed Spectrum



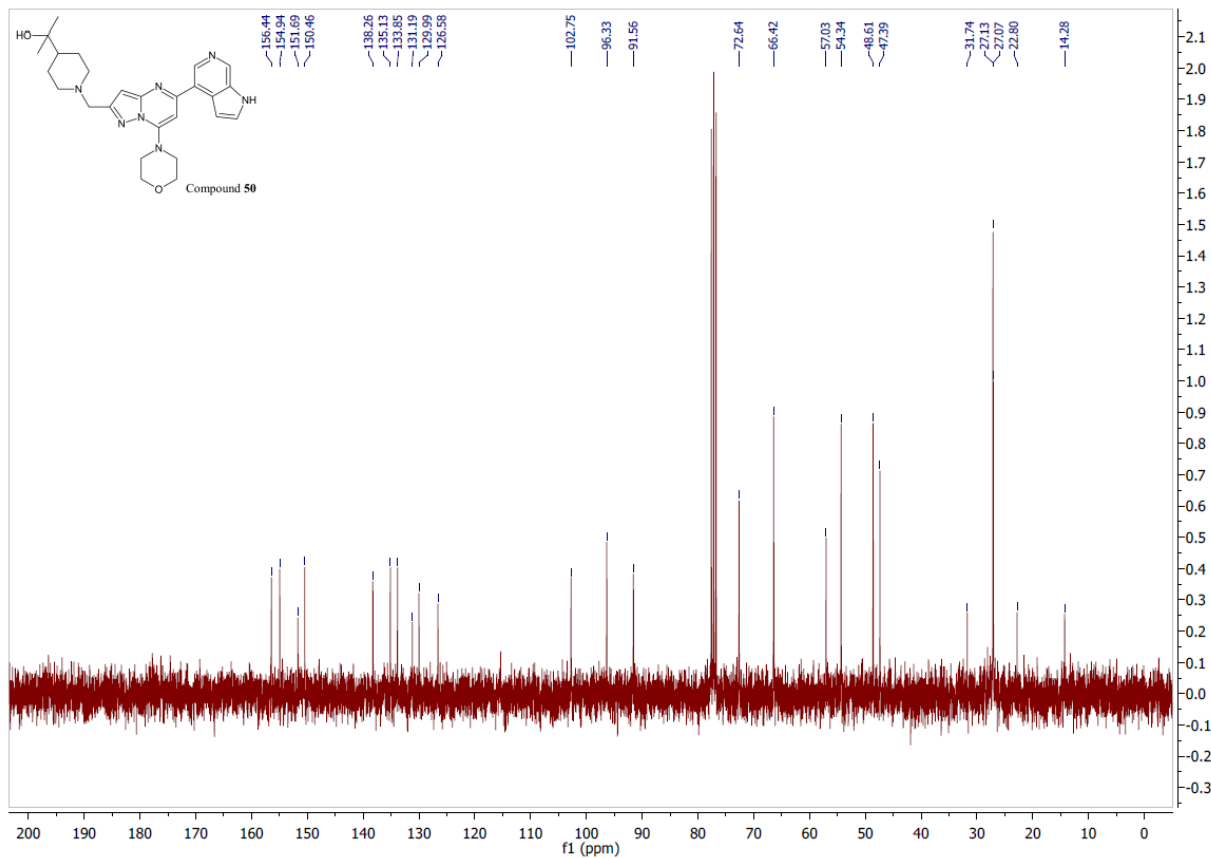
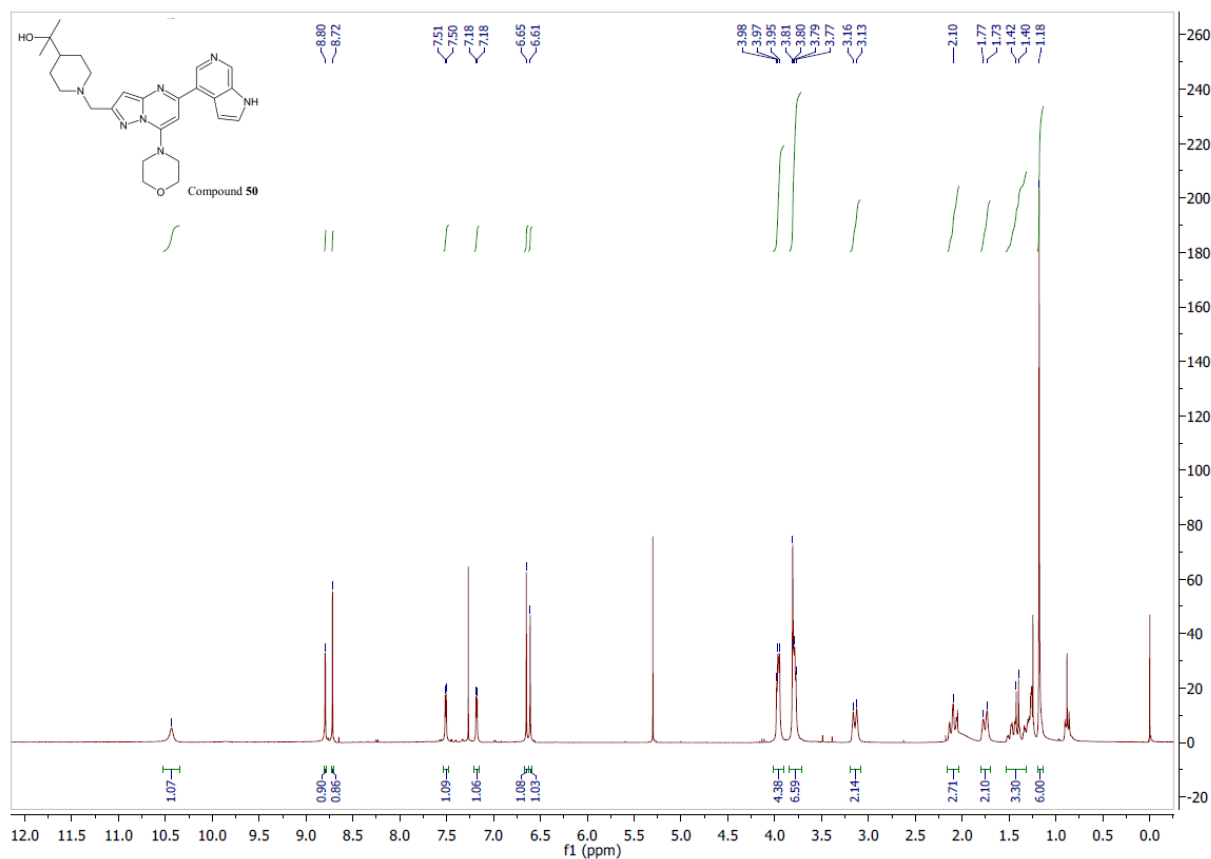
MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
247.14033	2	115650.79	C27H33FN6O2	(M+2H)+2	
247.64167	2	39414.14	C27H33FN6O2	(M+2H)+2	
248.14313	2	6640.41	C27H33FN6O2	(M+2H)+2	
248.64393	2	647.28	C27H33FN6O2	(M+2H)+2	
493.27235	1	340789.47	C27H33FN6O2	(M+H)+	
494.27539	1	101668.37	C27H33FN6O2	(M+H)+	
495.27769	1	16018.31	C27H33FN6O2	(M+H)+	
496.28007	1	2014.64	C27H33FN6O2	(M+H)+	
247.14033	2	115650.79	C27H33FN6O2	(M+2H)+2	2.45
247.64167	2	39414.14	C27H33FN6O2	(M+2H)+2	1.86
248.14313	2	6640.41	C27H33FN6O2	(M+2H)+2	2.09
248.64393	2	647.28	C27H33FN6O2	(M+2H)+2	-0.15
493.27235	1	340789.47	C27H33FN6O2	(M+H)+	0.35
494.27539	1	101668.37	C27H33FN6O2	(M+H)+	0.51
495.27769	1	16018.31	C27H33FN6O2	(M+H)+	-0.52
496.28007	1	2014.64	C27H33FN6O2	(M+H)+	-1.18

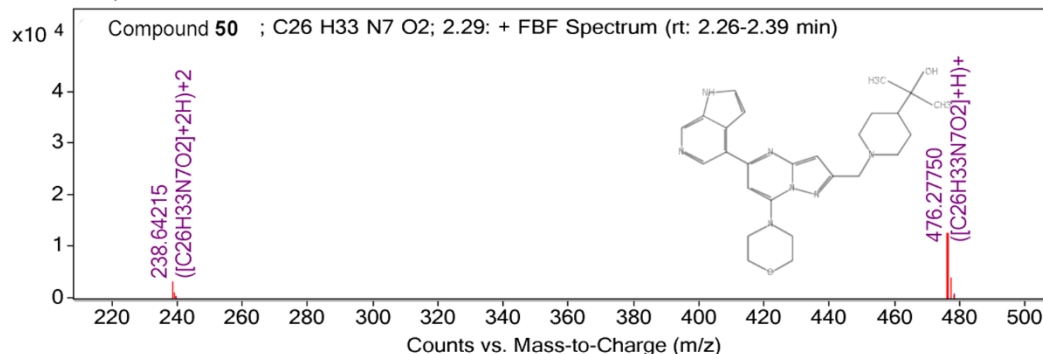
Compound 50



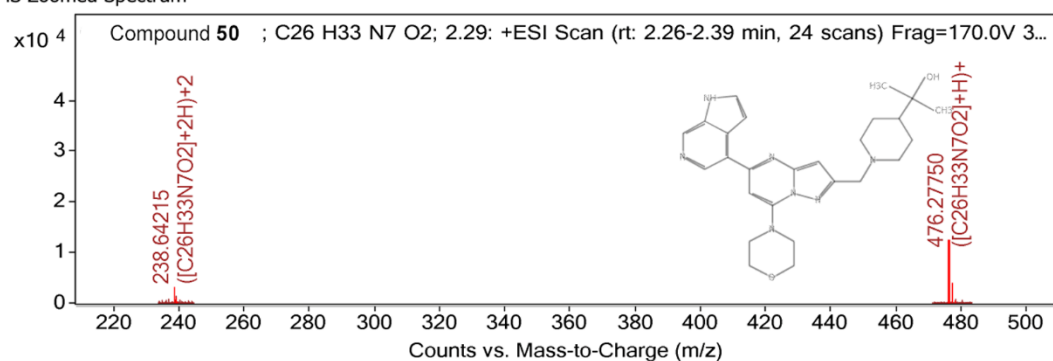
Compound 50

Compound Label	Name	m/z	RT	Algorithm	Mass
Compound 50	Compound 50	476.2775	2.29	Find by Formula	475.27003

MS Zoomed Spectrum



MS Zoomed Spectrum

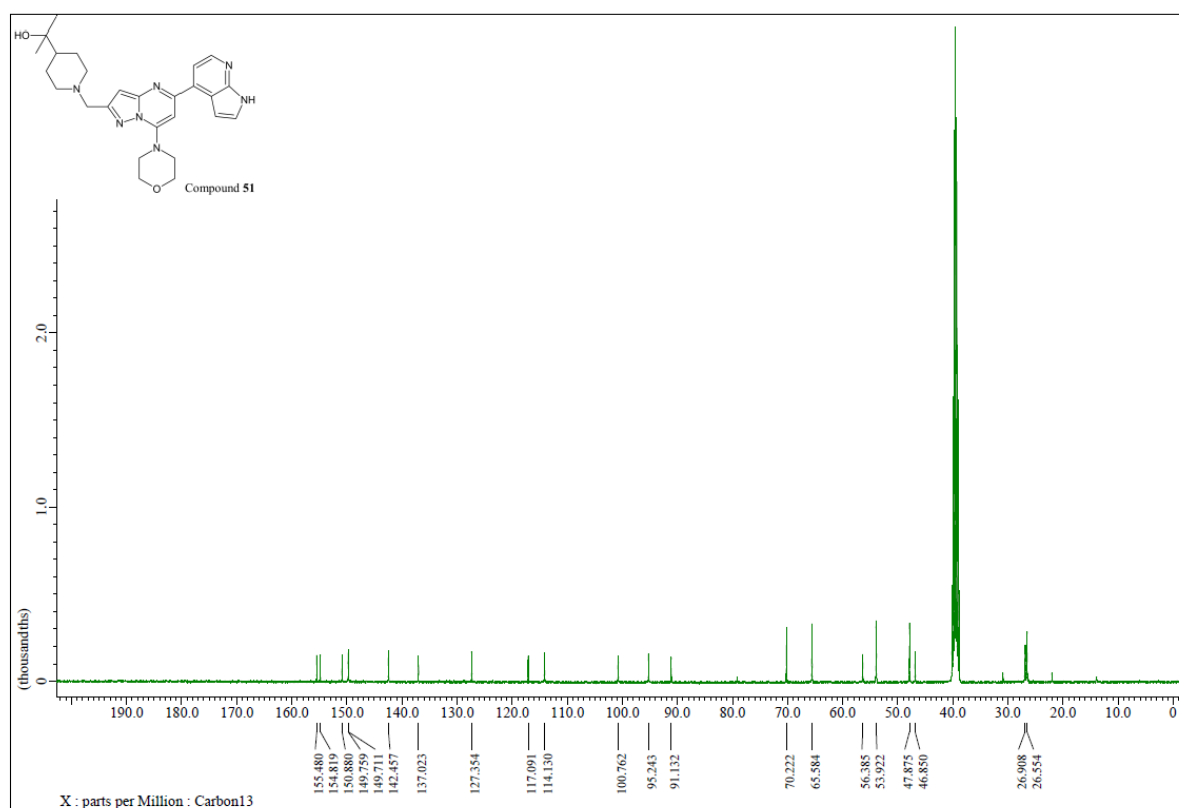
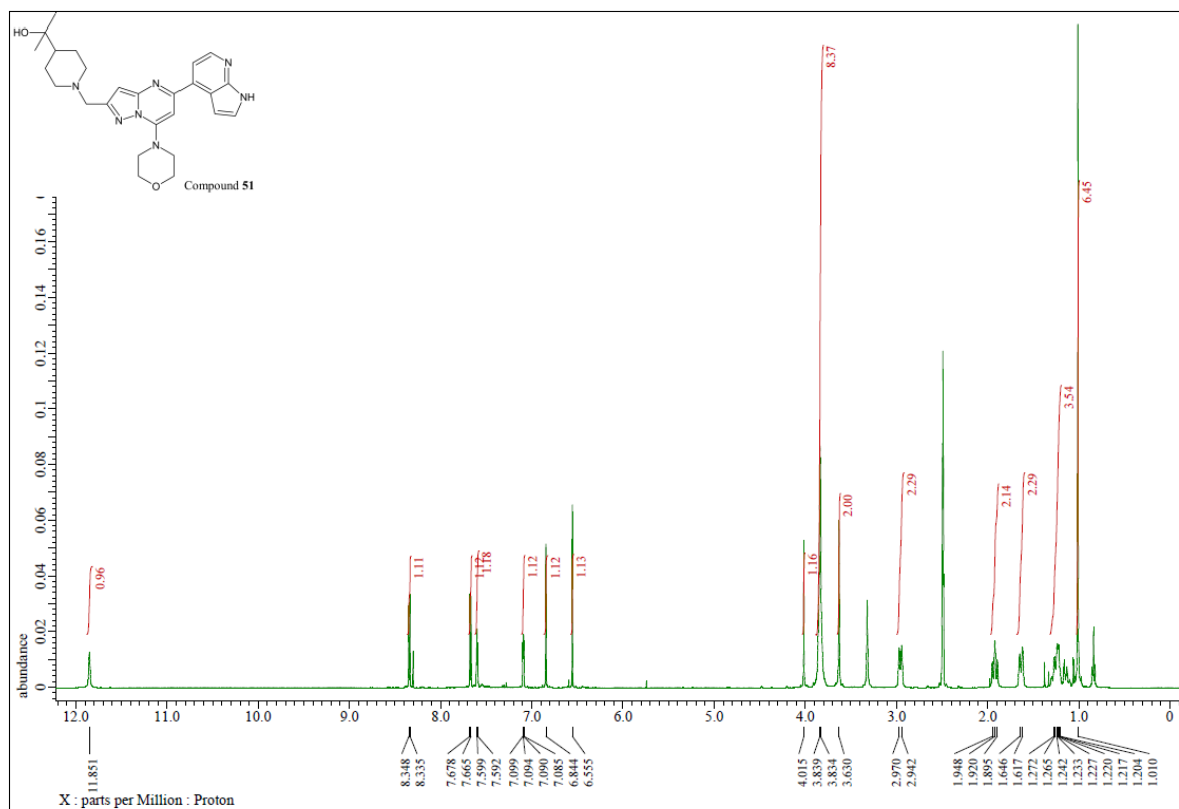


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
238.64215	238.64206	0.37	2	3046.57	C ₂₆ H ₃₃ N ₇ O ₂	(M+2H)+2
239.6443	239.64487	-2.37	2	280.47	C ₂₆ H ₃₃ N ₇ O ₂	(M+2H)+2
476.2775	476.27685	1.37	1	12351.18	C ₂₆ H ₃₃ N ₇ O ₂	(M+H)+
477.28005	477.27972	0.68	1	3493.83	C ₂₆ H ₃₃ N ₇ O ₂	(M+H)+
478.28194	478.28246	-1.1	1	760.19	C ₂₆ H ₃₃ N ₇ O ₂	(M+H)+

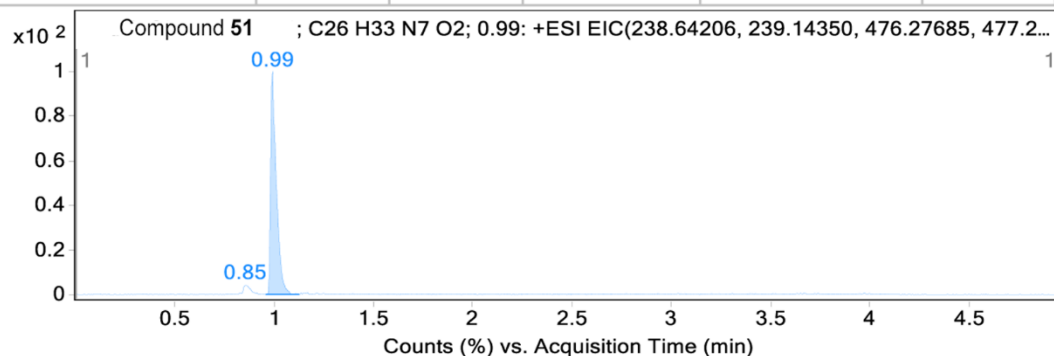
--- End Of Report ---

Compound 51

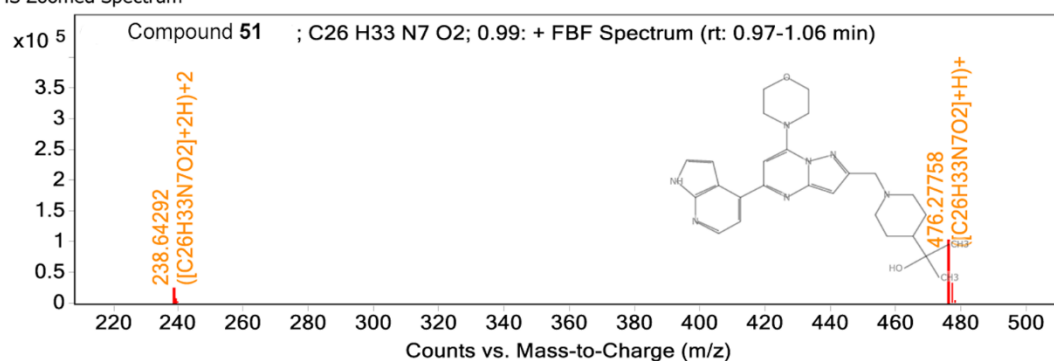


Compound 51

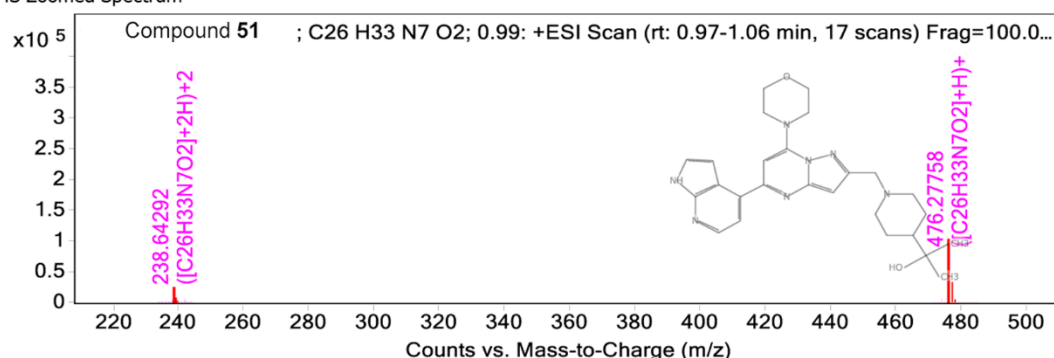
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorith
Compound 51	476.27758	0.99	475.27041	C26 H33 N7 O2	475.26957	1.76	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

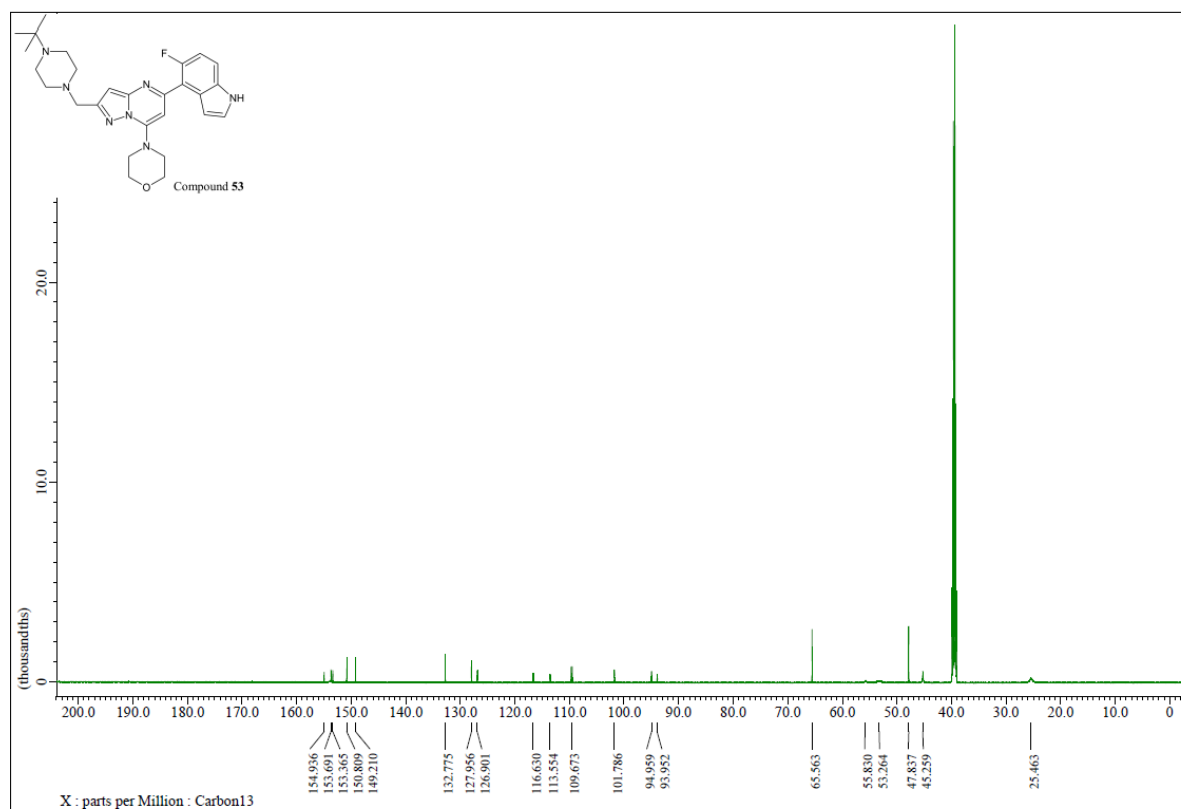
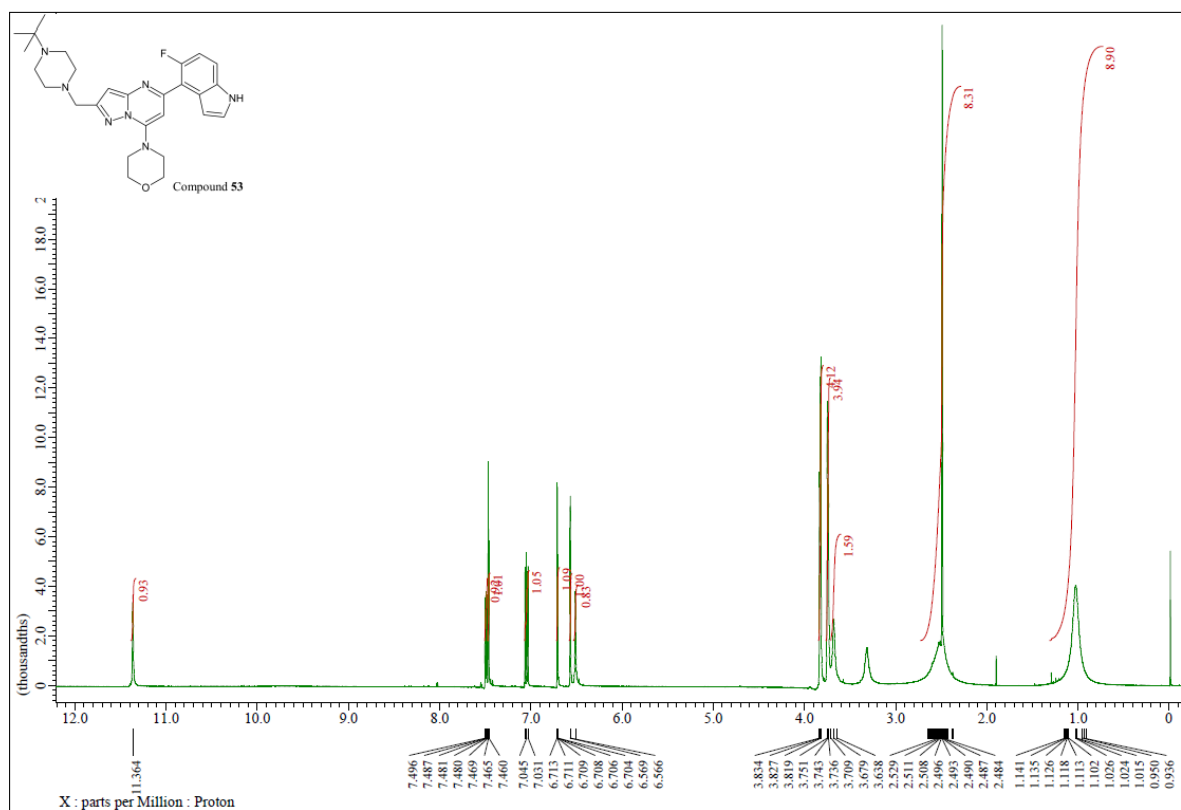


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.64292	2	23357.19	C26H33N7O2	(M+2H)+2	
239.14466	2	7984.02	C26H33N7O2	(M+2H)+2	
239.64525	2	1242.2	C26H33N7O2	(M+2H)+2	
476.27758	1	101934.38	C26H33N7O2	(M+H)+	
477.28003	1	32395.08	C26H33N7O2	(M+H)+	
478.28266	1	4780.62	C26H33N7O2	(M+H)+	
479.28502	1	601.29	C26H33N7O2	(M+H)+	
480.28589	1	75.69	C26H33N7O2	(M+H)+	
238.64292	2	23357.19	C26H33N7O2	(M+2H)+2	3.58
239.14466	2	7984.02	C26H33N7O2	(M+2H)+2	4.84
239.64525	2	1242.2	C26H33N7O2	(M+2H)+2	1.57
476.27758	1	101934.38	C26H33N7O2	(M+H)+	1.53
477.28003	1	32395.08	C26H33N7O2	(M+H)+	0.63
478.28266	1	4780.62	C26H33N7O2	(M+H)+	0.43
479.28502	1	601.29	C26H33N7O2	(M+H)+	-0.17
480.28589	1	75.69	C26H33N7O2	(M+H)+	-3.74

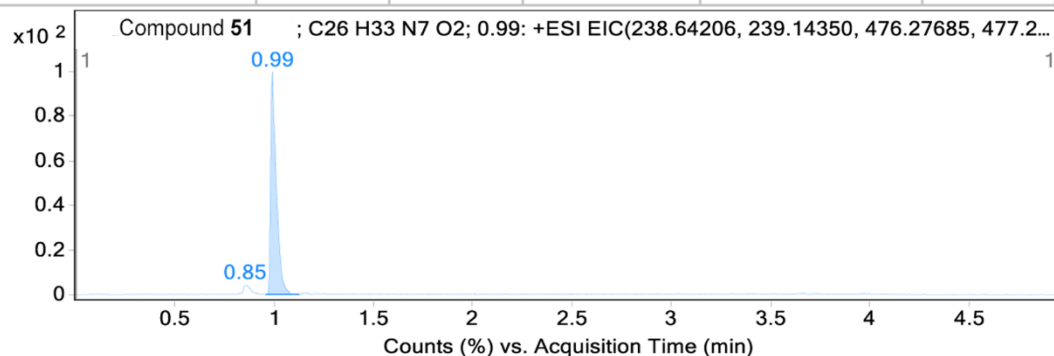
--- End Of Report ---

Compound 53

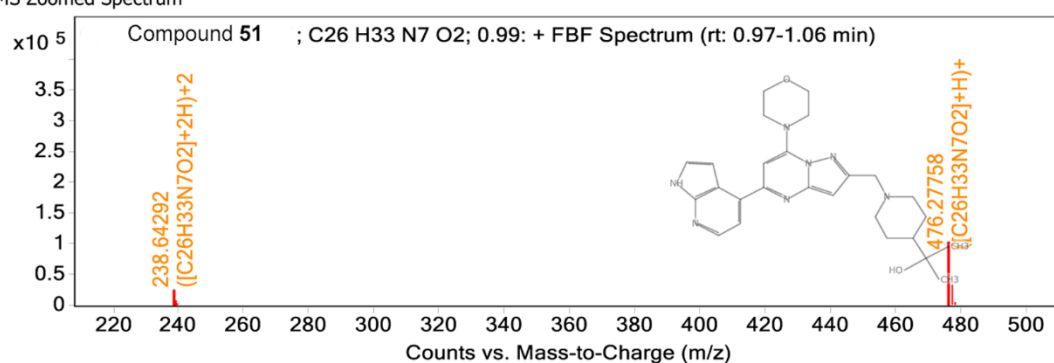


Compound 53

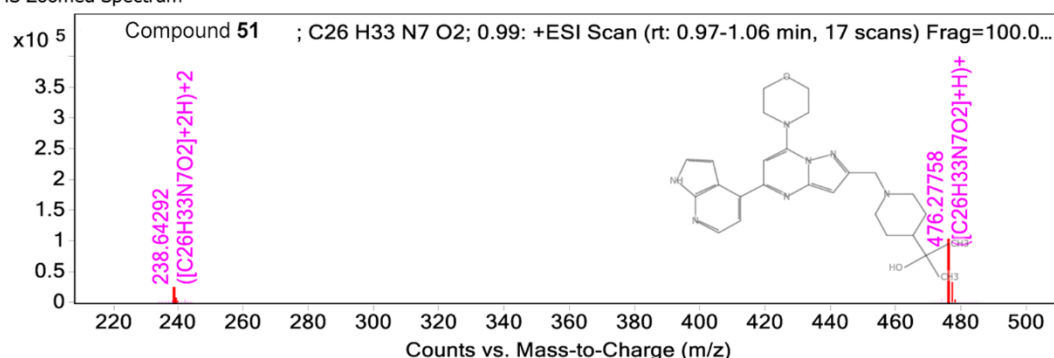
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpd Algorith
Compound 51	476.27758	0.99	475.27041	C26 H33 N7 O2	475.26957	1.76	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum

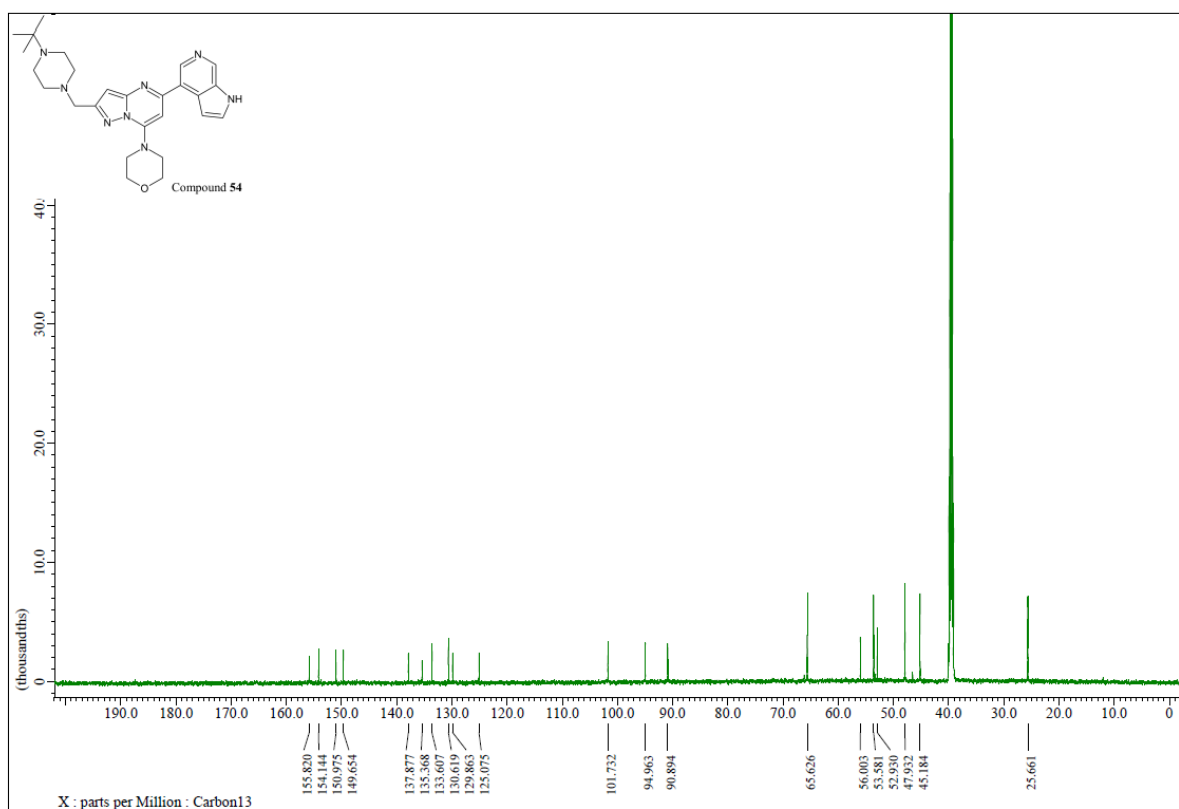
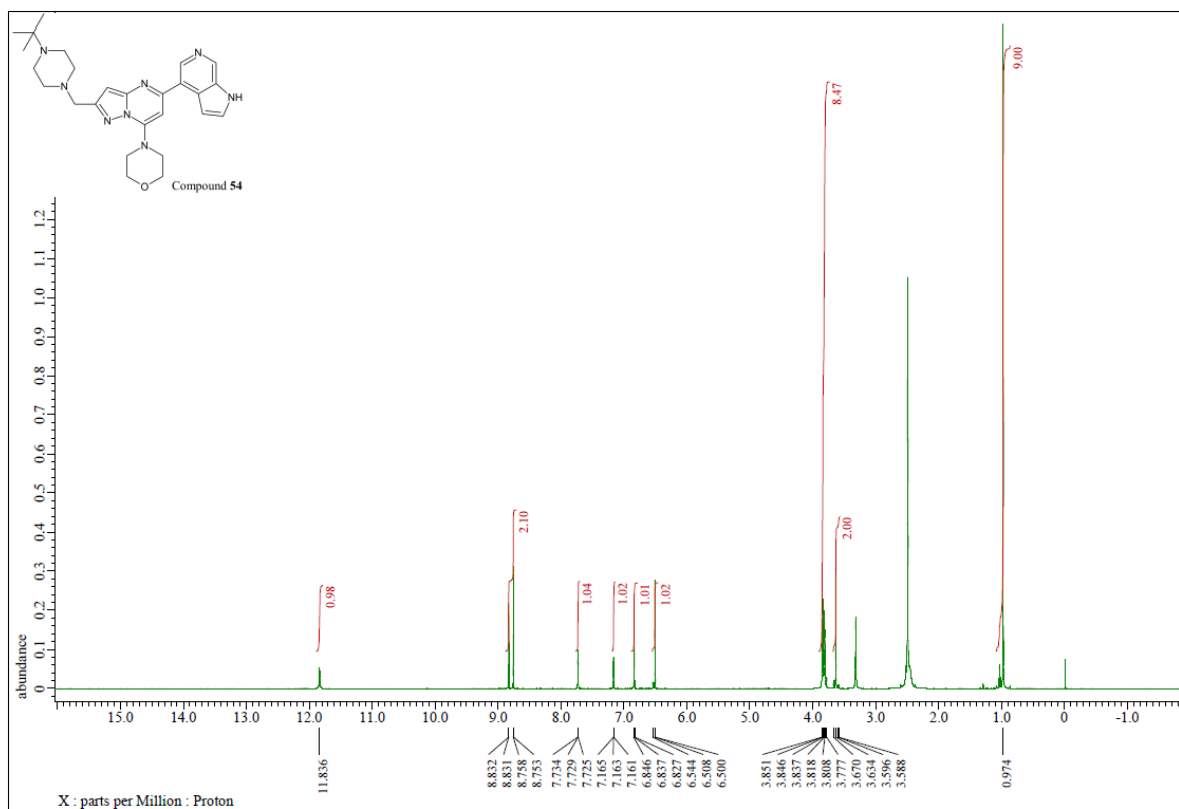


MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.64292	2	23357.19	C26H33N7O2	(M+2H)+2	
239.14466	2	7984.02	C26H33N7O2	(M+2H)+2	
239.64525	2	1242.2	C26H33N7O2	(M+2H)+2	
476.27758	1	101934.38	C26H33N7O2	(M+H)+	
477.28003	1	32395.08	C26H33N7O2	(M+H)+	
478.28266	1	4780.62	C26H33N7O2	(M+H)+	
479.28502	1	601.29	C26H33N7O2	(M+H)+	
480.28589	1	75.69	C26H33N7O2	(M+H)+	
238.64292	2	23357.19	C26H33N7O2	(M+2H)+2	3.58
239.14466	2	7984.02	C26H33N7O2	(M+2H)+2	4.84
239.64525	2	1242.2	C26H33N7O2	(M+2H)+2	1.57
476.27758	1	101934.38	C26H33N7O2	(M+H)+	1.53
477.28003	1	32395.08	C26H33N7O2	(M+H)+	0.63
478.28266	1	4780.62	C26H33N7O2	(M+H)+	0.43
479.28502	1	601.29	C26H33N7O2	(M+H)+	-0.17
480.28589	1	75.69	C26H33N7O2	(M+H)+	-3.74

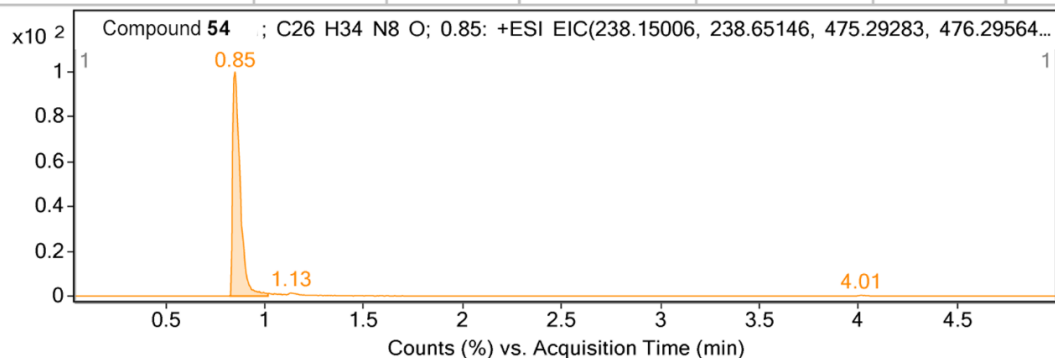
--- End Of Report ---

Compound 54

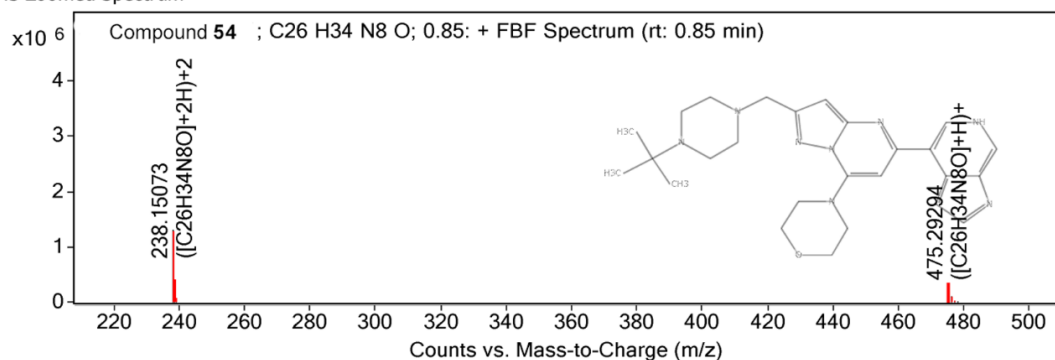


Compound 54

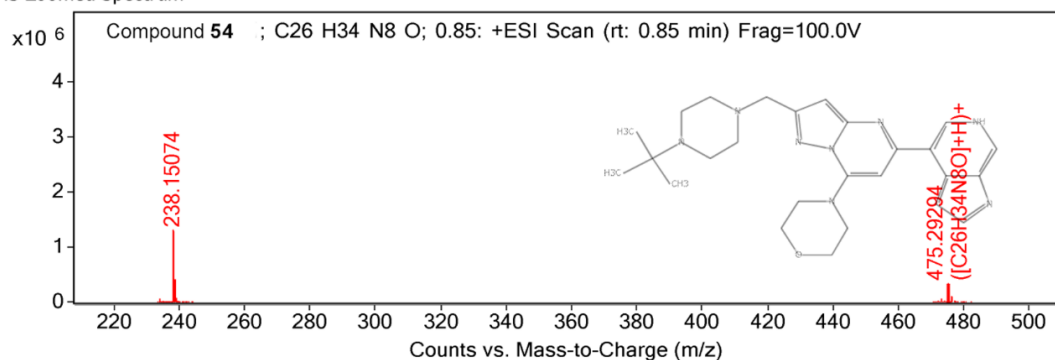
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Alaoirith
Compound 54	475.29294	0.85	474.28648	C26 H34 N8 O	474.28556	1.94	Find by Formula



MS Zoomed Spectrum



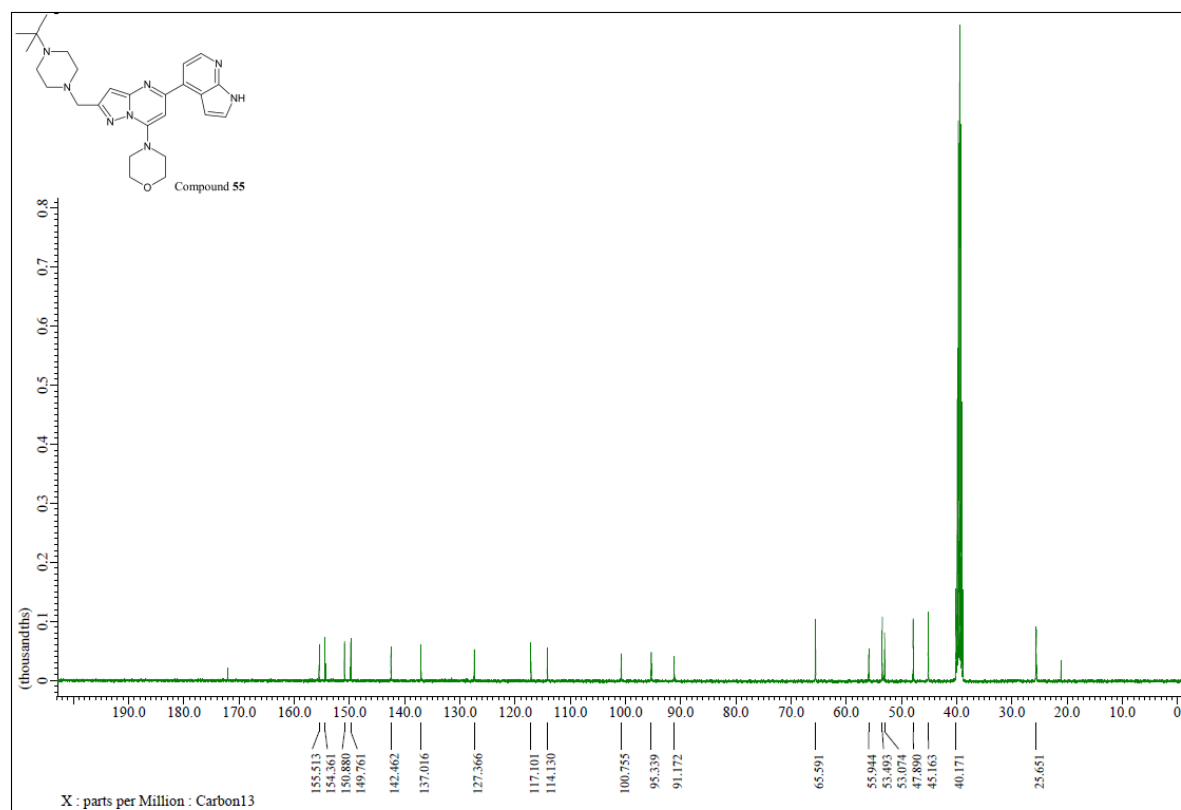
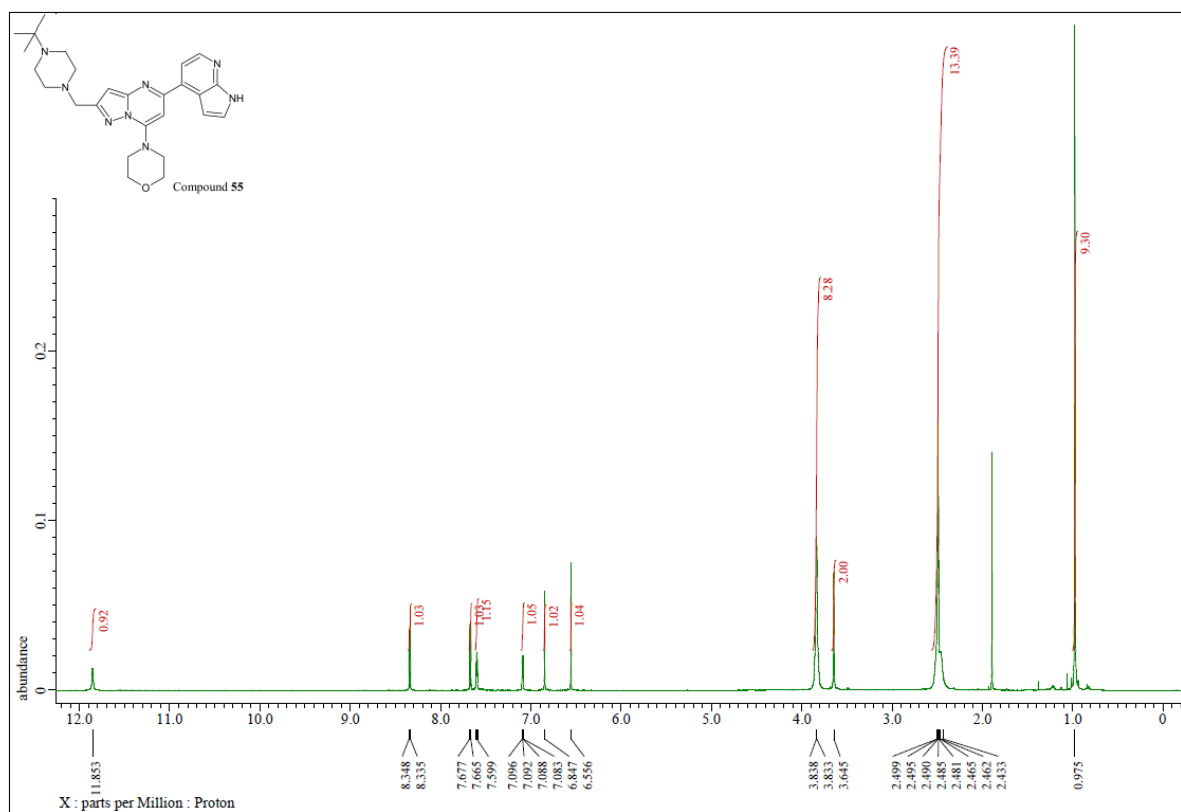
MS Zoomed Spectrum



MS Spectrum Peak List

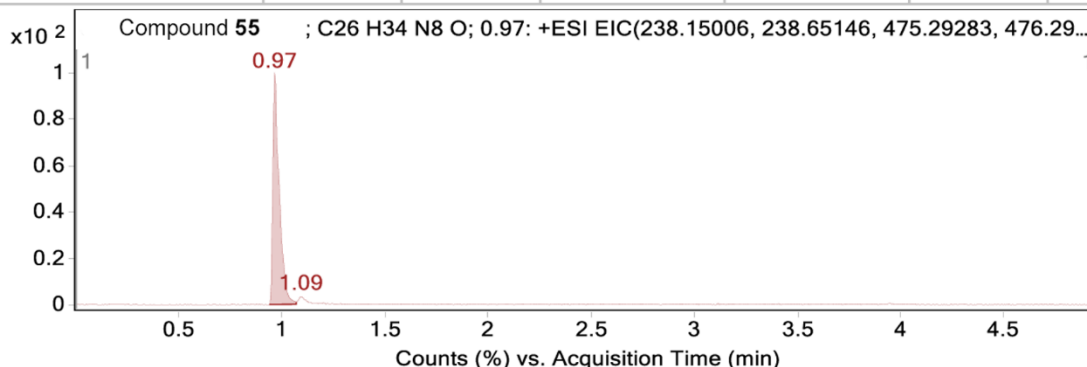
Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.15073	2	1295540.25	C26H34N8O	(M+2H)+2	
238.65175	2	375450.88	C26H34N8O	(M+2H)+2	
239.15293	2	55981.86	C26H34N8O	(M+2H)+2	
475.29294	1	328461.72	C26H34N8O	(M+H)+	
476.29541	1	96053.09	C26H34N8O	(M+H)+	
477.29793	1	13882.22	C26H34N8O	(M+H)+	
478.29997	1	1075.67	C26H34N8O	(M+H)+	
238.15073	2	1295540.25	C26H34N8O	(M+2H)+2	2.85
238.15074		1302772.38			
238.65175	2	375450.88	C26H34N8O	(M+2H)+2	1.22
239.15293	2	55981.86	C26H34N8O	(M+2H)+2	0.43
475.29294	1	328461.72	C26H34N8O	(M+H)+	0.22
476.29541	1	96053.09	C26H34N8O	(M+H)+	-0.48
477.29793	1	13882.22	C26H34N8O	(M+H)+	-0.93
478.29997	1	1075.67	C26H34N8O	(M+H)+	-2.21

Compound 55

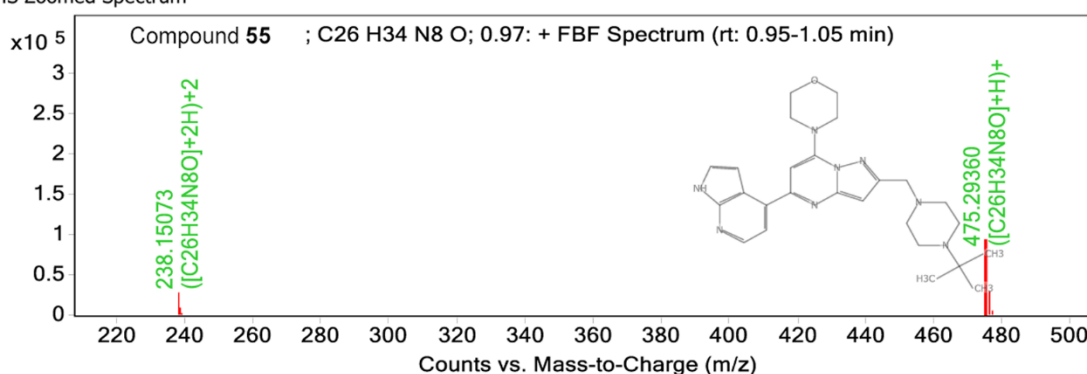


Compound 55

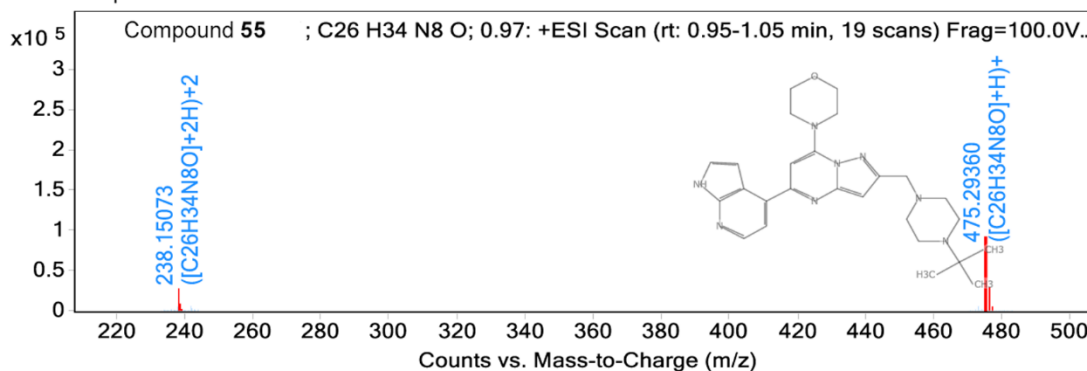
Name	Obs. m/z	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error	Find Cpds Algorith
Compound 55	475.2936	0.97	474.28629	C26 H34 N8 O	474.28556	1.55	Find by Formula



MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope	Tgt Mass Error (ppm)
238.15073	2	27416.88	C26H34N8O	(M+2H)+2	
238.65185	2	8095.95	C26H34N8O	(M+2H)+2	
239.15226	2	1933.05	C26H34N8O	(M+2H)+2	
475.2936	1	92111.73	C26H34N8O	(M+H)+	
476.2959	1	28302.5	C26H34N8O	(M+H)+	
477.29863	1	4277.33	C26H34N8O	(M+H)+	
478.29884	1	406.24	C26H34N8O	(M+H)+	
238.15073	2	27416.88	C26H34N8O	(M+2H)+2	2.83
238.65185	2	8095.95	C26H34N8O	(M+2H)+2	1.65
239.15226	2	1933.05	C26H34N8O	(M+2H)+2	-2.38
475.2936	1	92111.73	C26H34N8O	(M+H)+	1.61
476.2959	1	28302.5	C26H34N8O	(M+H)+	0.54
477.29863	1	4277.33	C26H34N8O	(M+H)+	0.54
478.29884	1	406.24	C26H34N8O	(M+H)+	-4.58

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