

Design, Synthesis and Biological Evaluation of Phenyl Urea Derivatives as IDO1 Inhibitors

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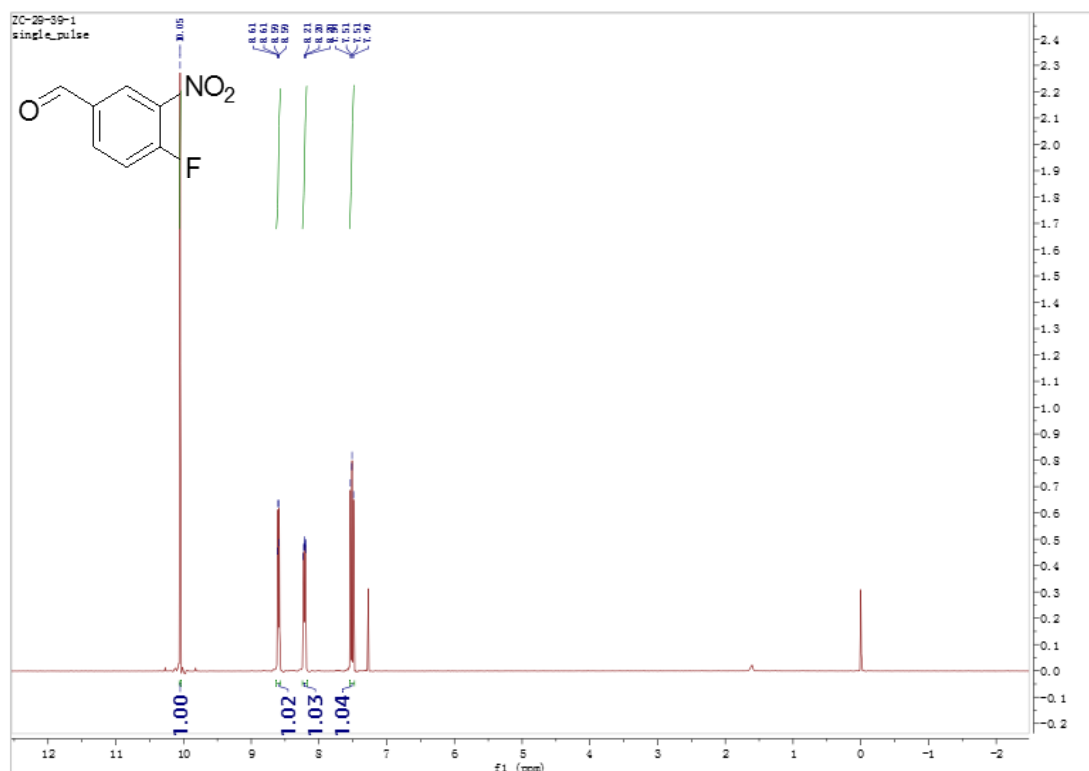
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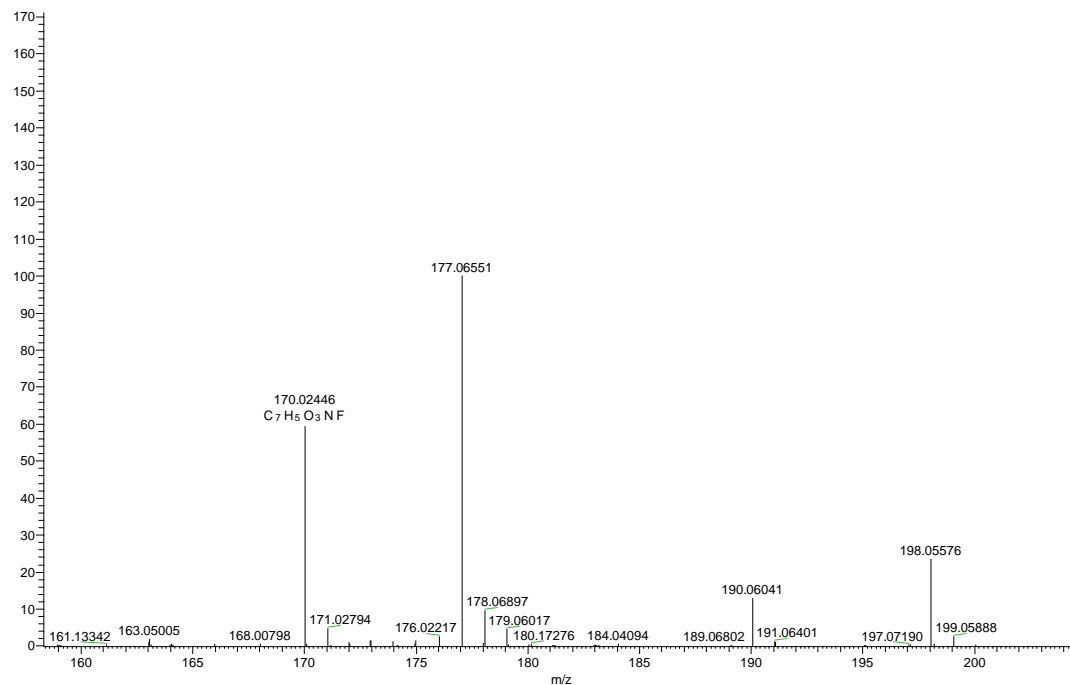
¹H NMR, ¹³C NMR and MS spectra of the synthesized compoundsP2-P53

¹H NMR spectra of compound a



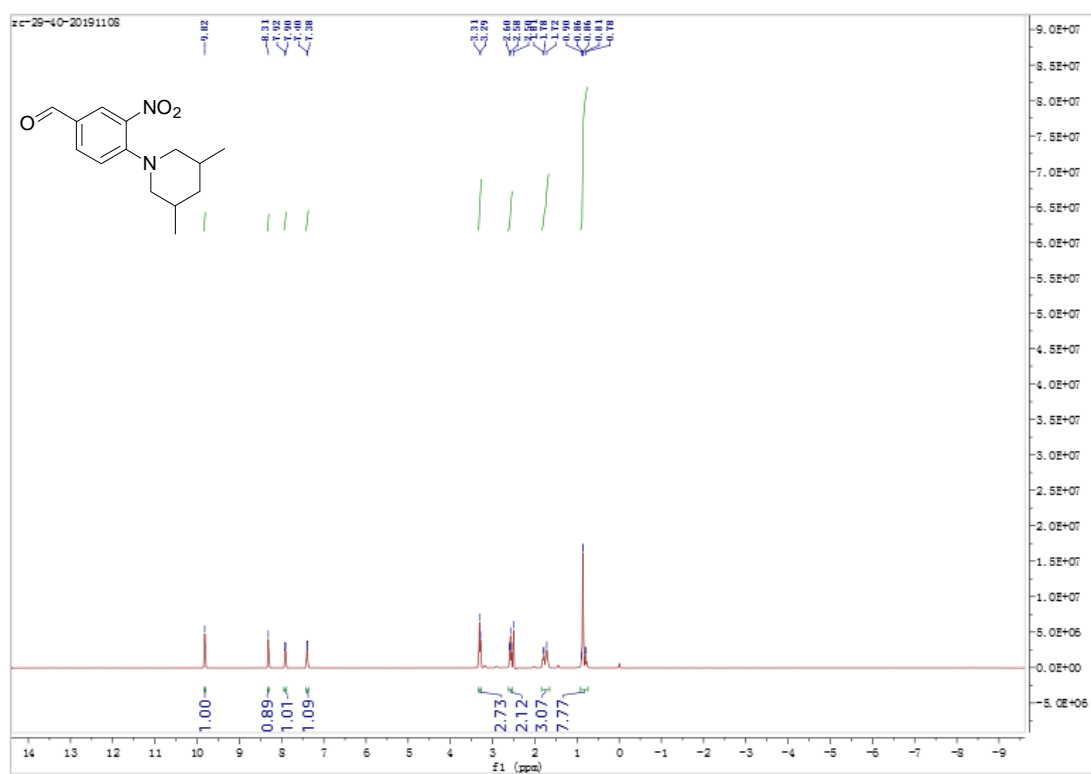
ESI-MS spectra of compound a

ZC-29-39 (2) #1688 RT: 5.03 AV: 1 NL: 5.28E7
T: FTMS + c ESI Full ms [100.0000-1000.0000]



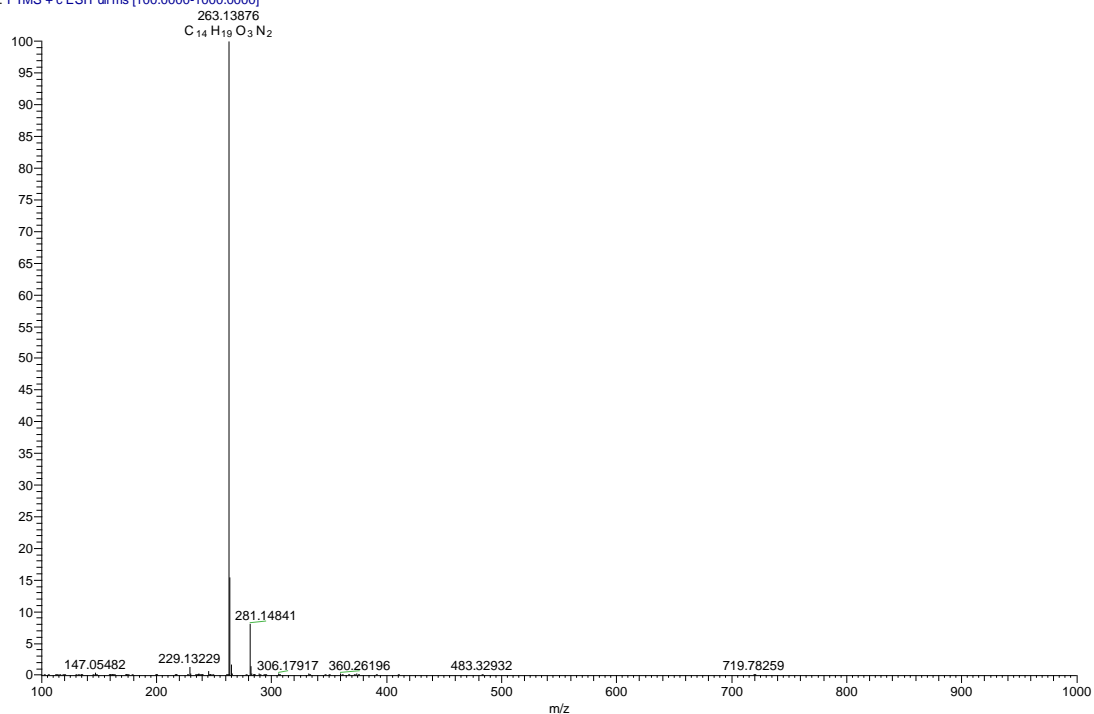
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
170.02446	170.02480	-1.99	5.5	C7 H5 O3 N F

¹H NMR spectra of compound b



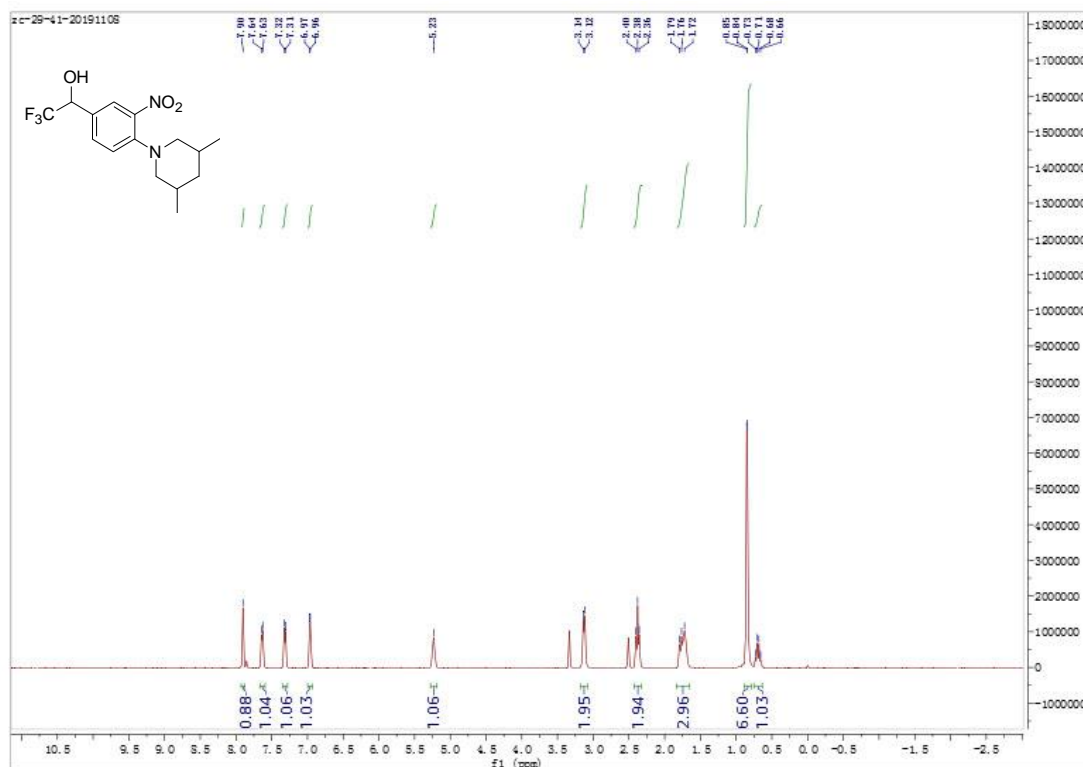
ESI-MS spectra of compound b

ZC-29-40 #2606 RT: 6.30 AV: 1 NL: 9.08E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



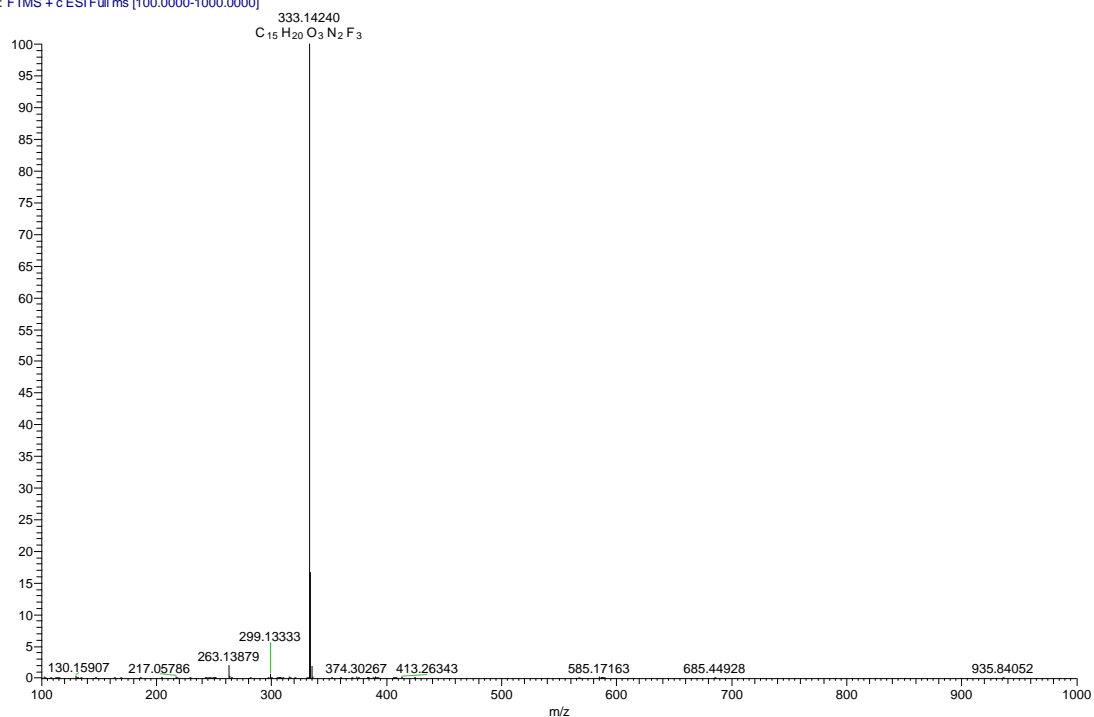
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
263.13876	263.13902	-0.98	6.5	C14 H19 O3 N2

¹H NMR spectra of compound c



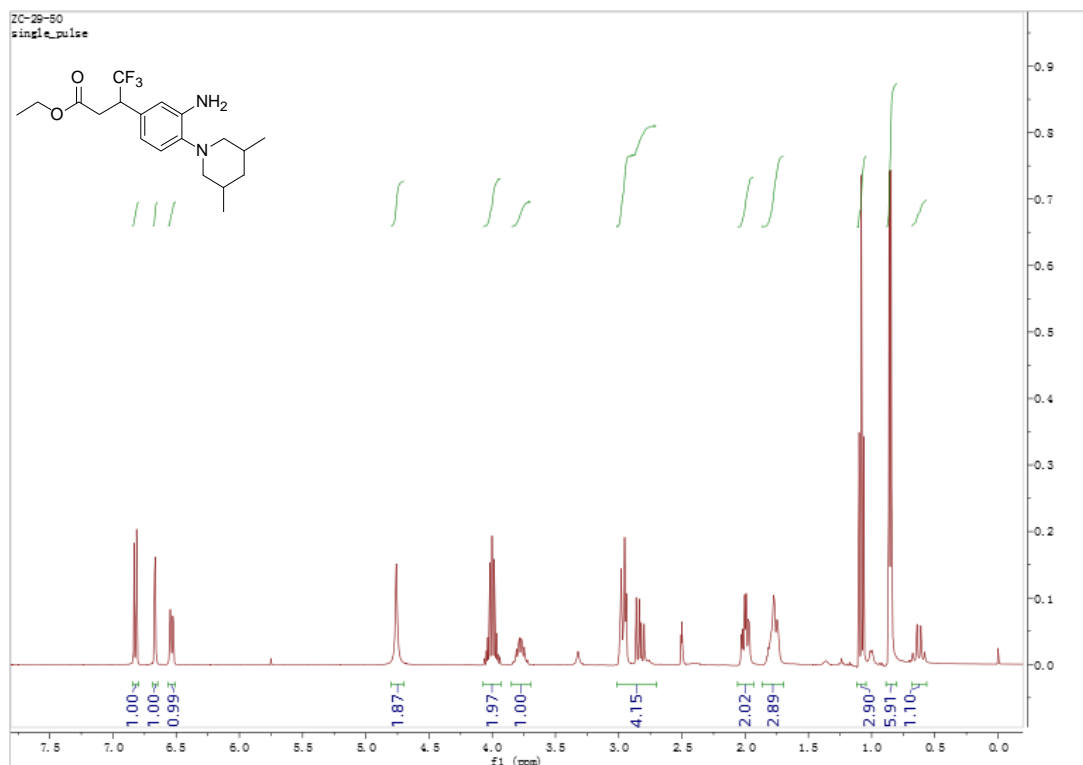
ESI-MS spectra of compound c

ZC-29-41 #3046 RT: 6.75 AV: 1 NL: 3.39E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



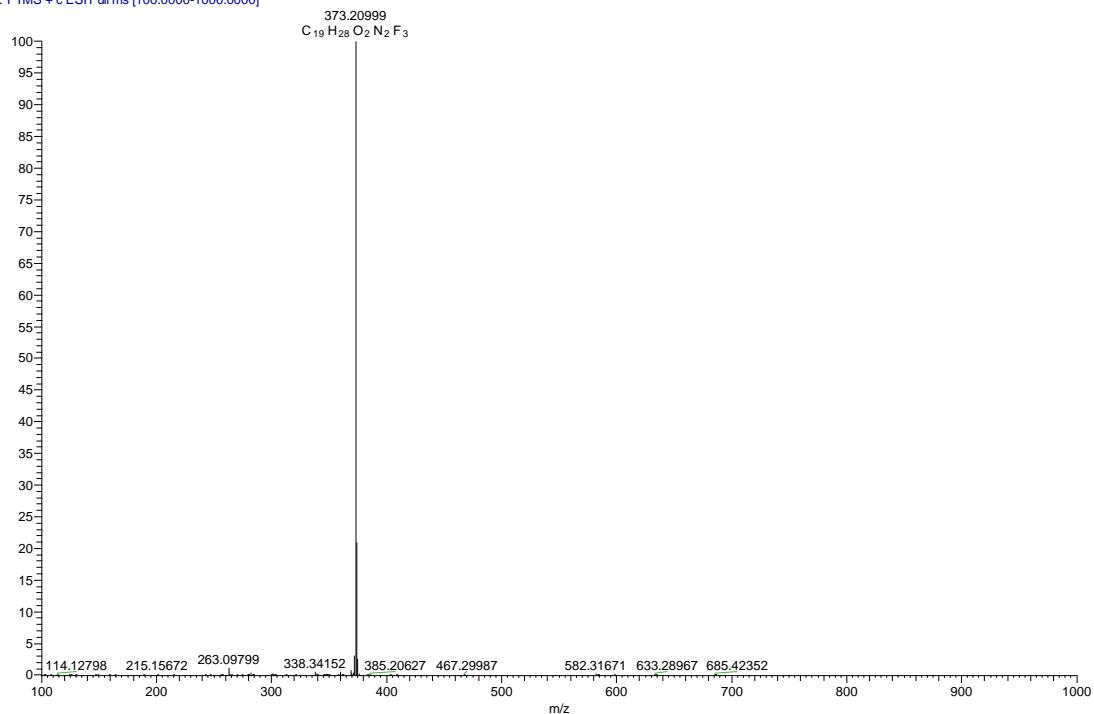
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
333.14246	333.14205	1.22	5.5	C ₁₅ H ₂₀ O ₃ N ₂ F ₃

¹H NMR spectra of compound f



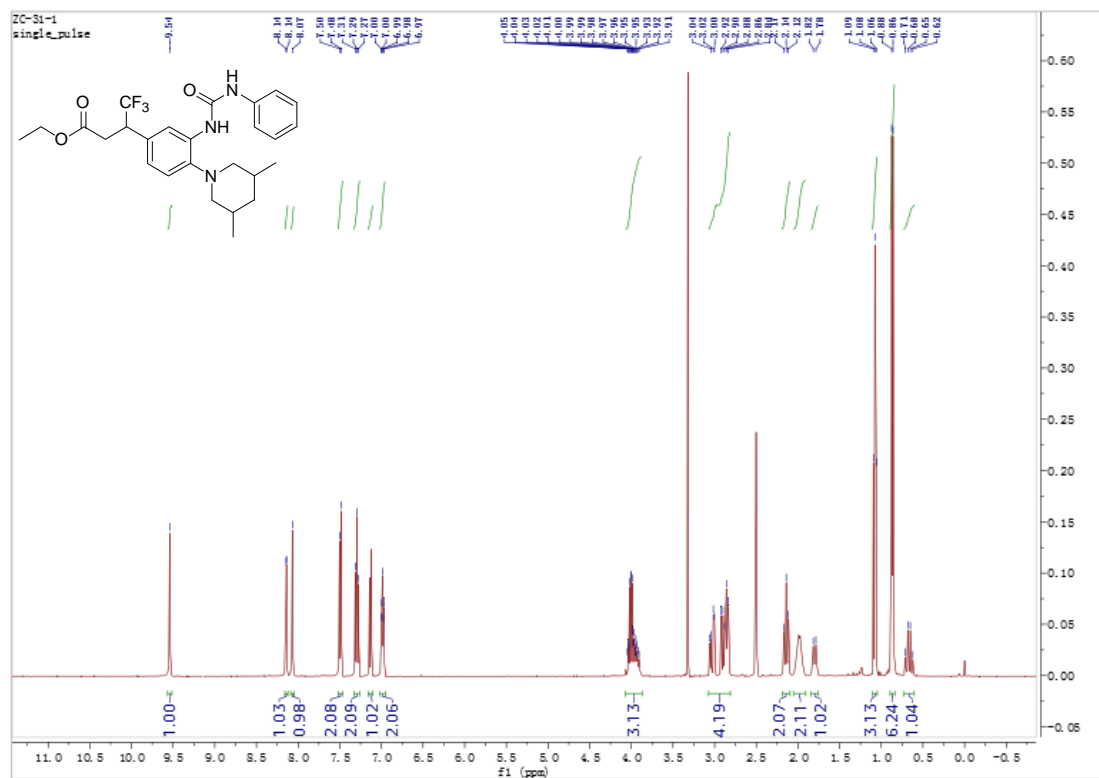
ESI-MS spectra of compound f

ZC-29-50_191112104826 #2497 RT: 7.31 AV: 1 NL: 1.83E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]

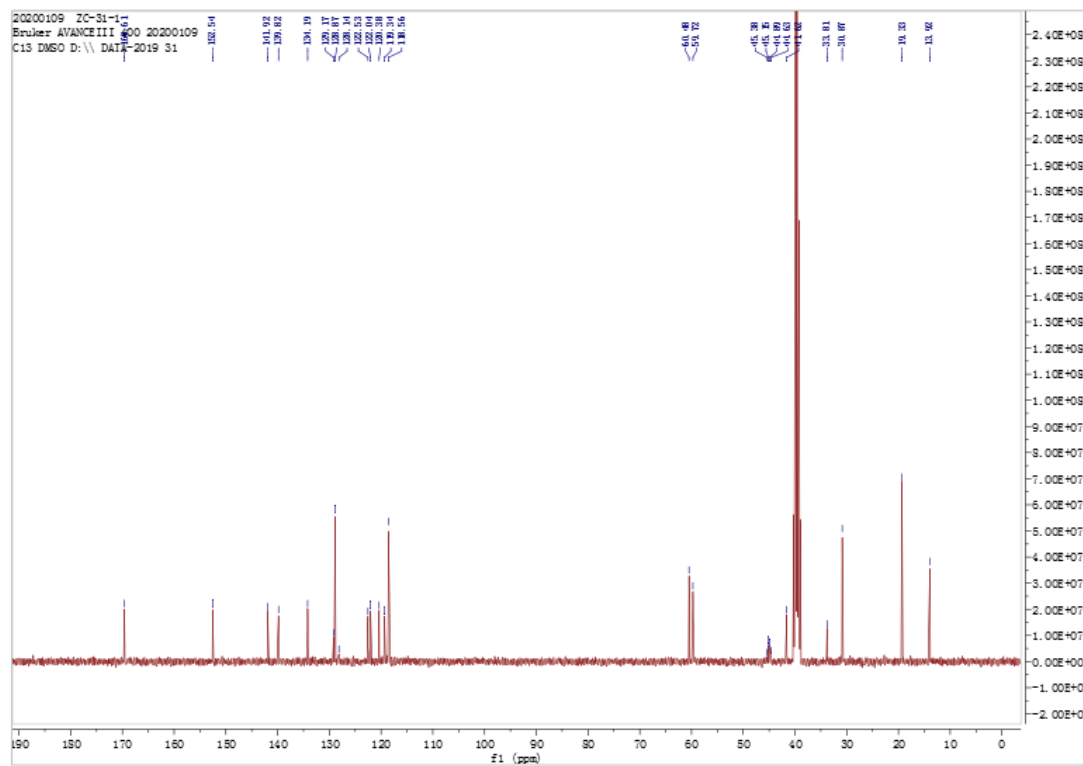


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
373.20999	373.20974	0.67	5.5	C ₁₉ H ₂₈ O ₂ N ₂ F ₃

¹H NMR spectra of compound g1

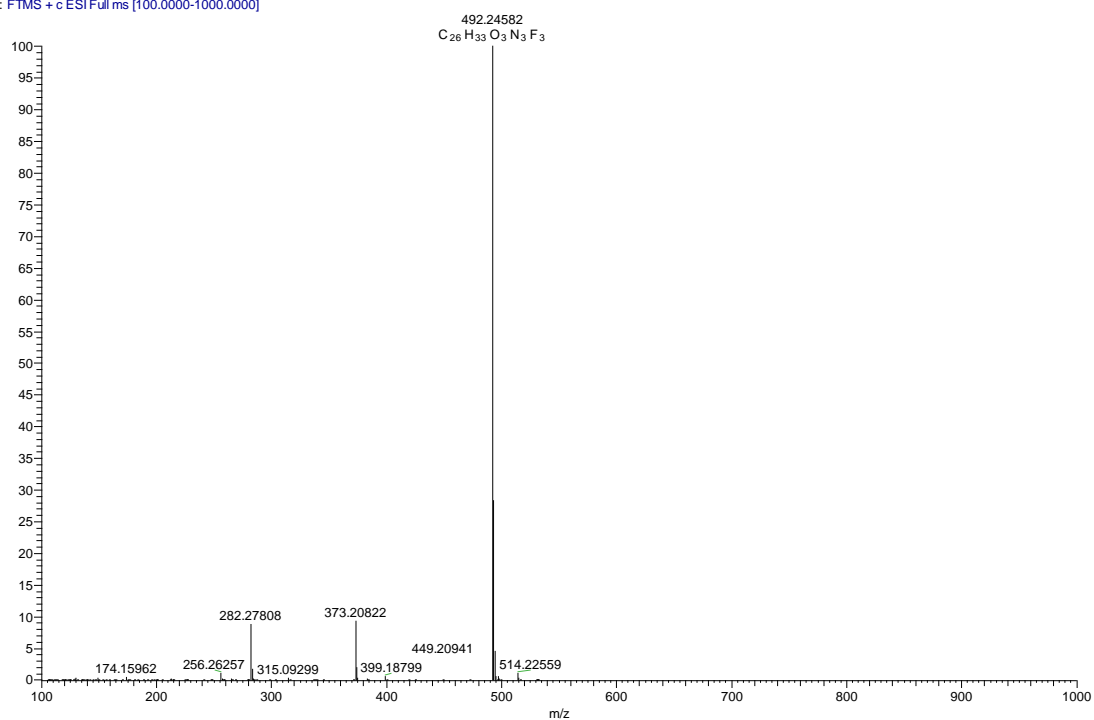


¹³C NMR spectra of compound g1



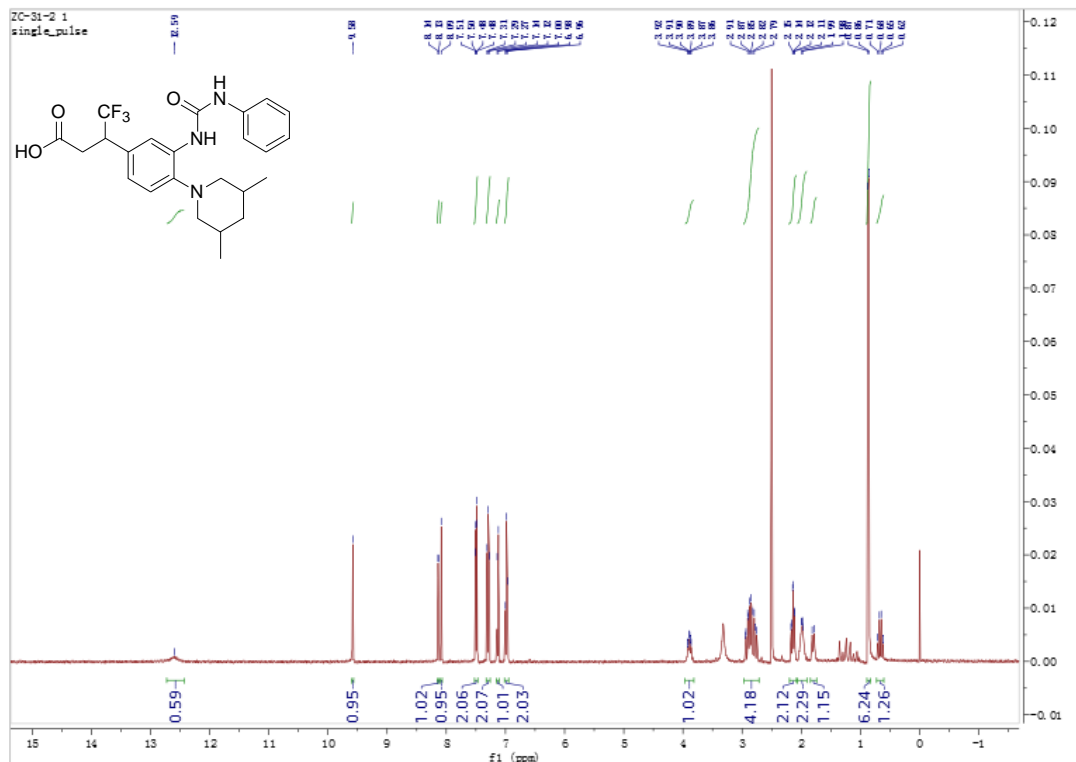
ESI-MS spectra of compound g1

ZC-30-1_191212170659 #1713 RT: 6.14 AV: 1 NL: 1.01E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

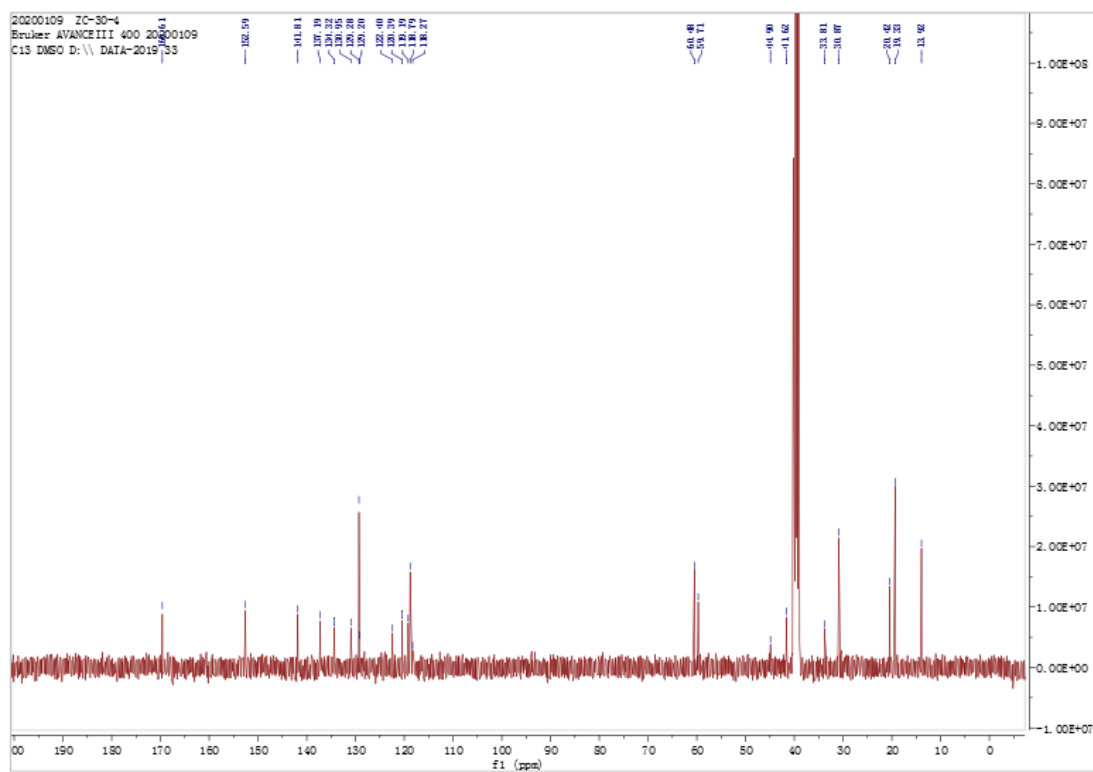


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
492.24582	492.24685	-2.10	10.5	C26 H33 O3 N3 F3

¹H NMR spectra of compound i1

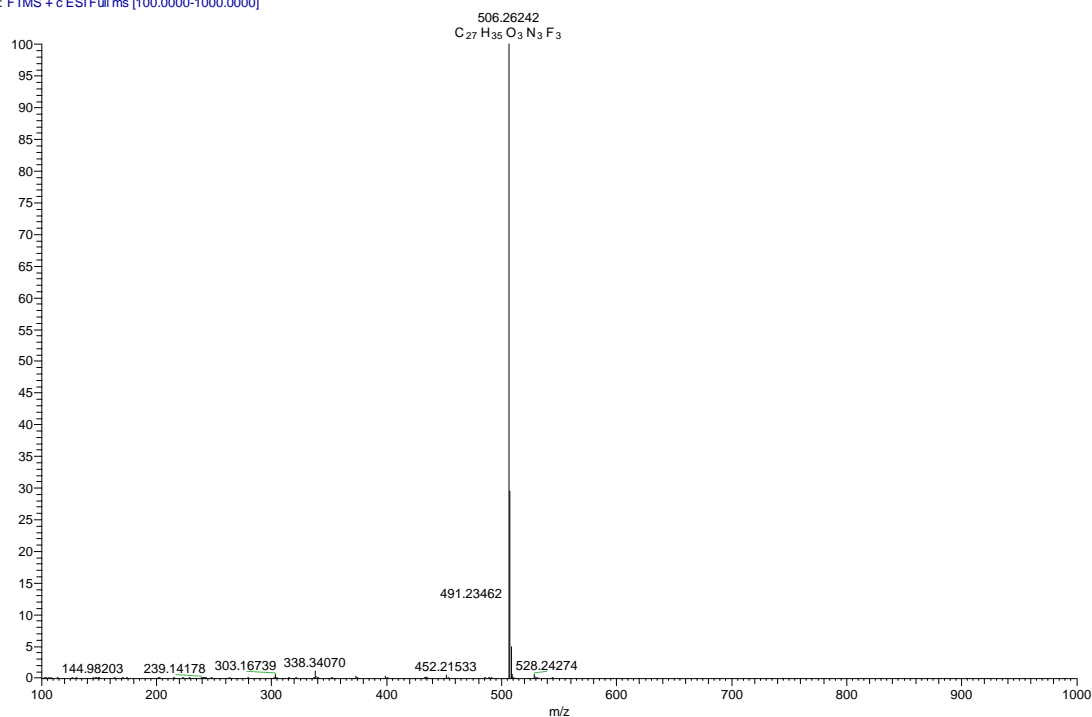


¹³C NMR spectra of compound g2



ESI-MS spectra of compound g2

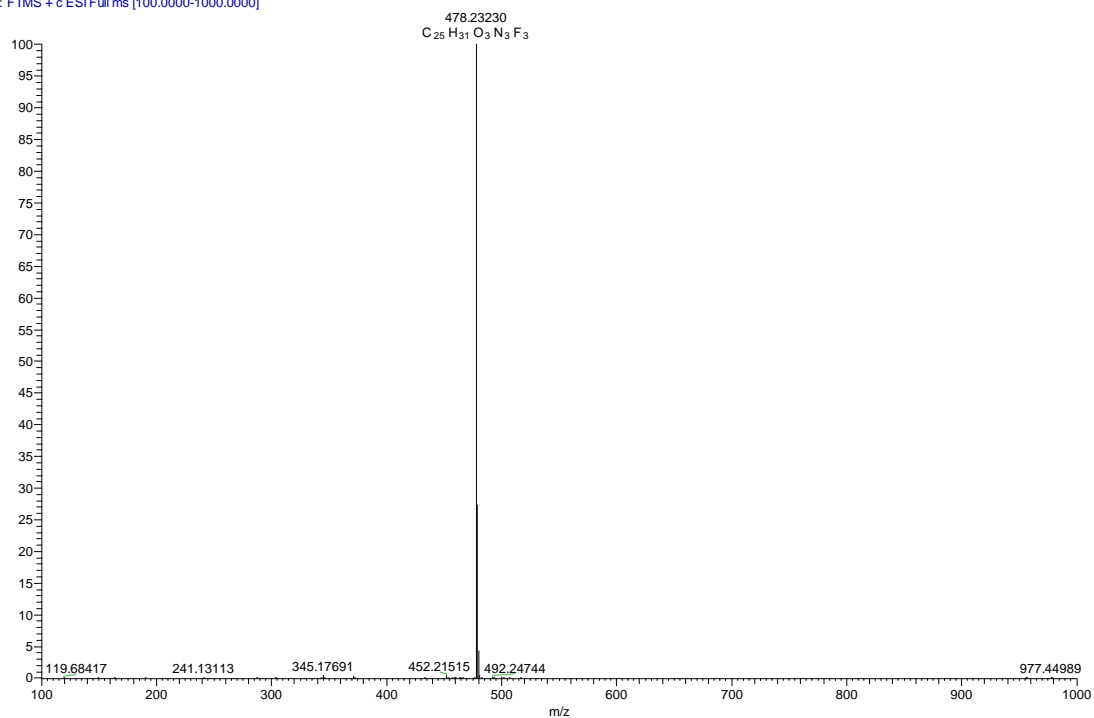
ZC-30-4-2 #1998 RT: 7.13 AV: 1 NL: 1.23E9
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
506.26242	506.26250	-0.16	10.5	C ₂₇ H ₃₅ O ₃ N ₃ F ₃

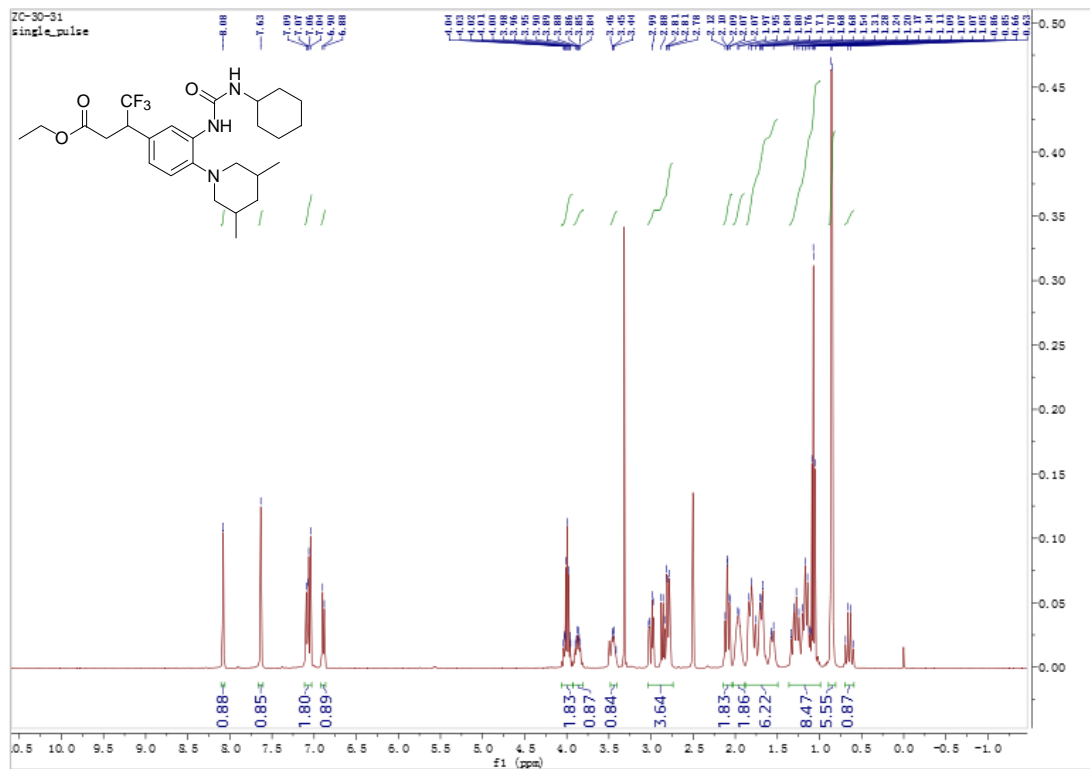
ESI-MS spectra of compound i2

ZC-30-10 #2161 RT: 7.50 AV: 1 NL: 1.16E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



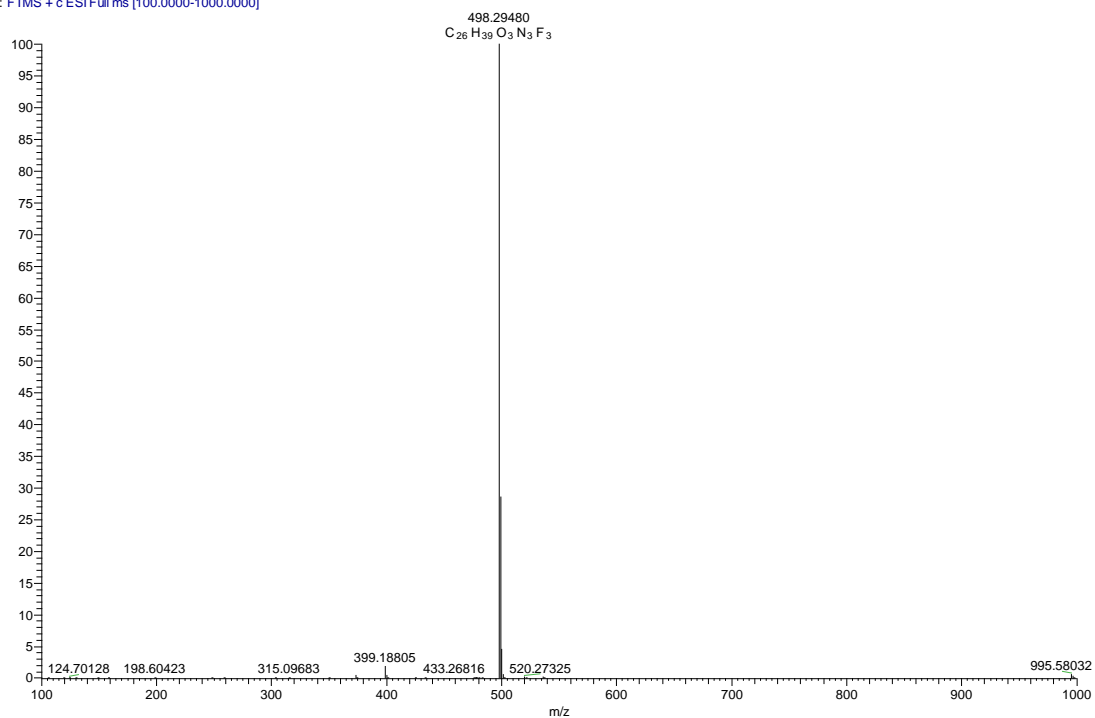
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
478.23230	478.23120	2.29	10.5	C ₂₅ H ₃₁ O ₃ N ₃

¹H NMR spectra of compound g4



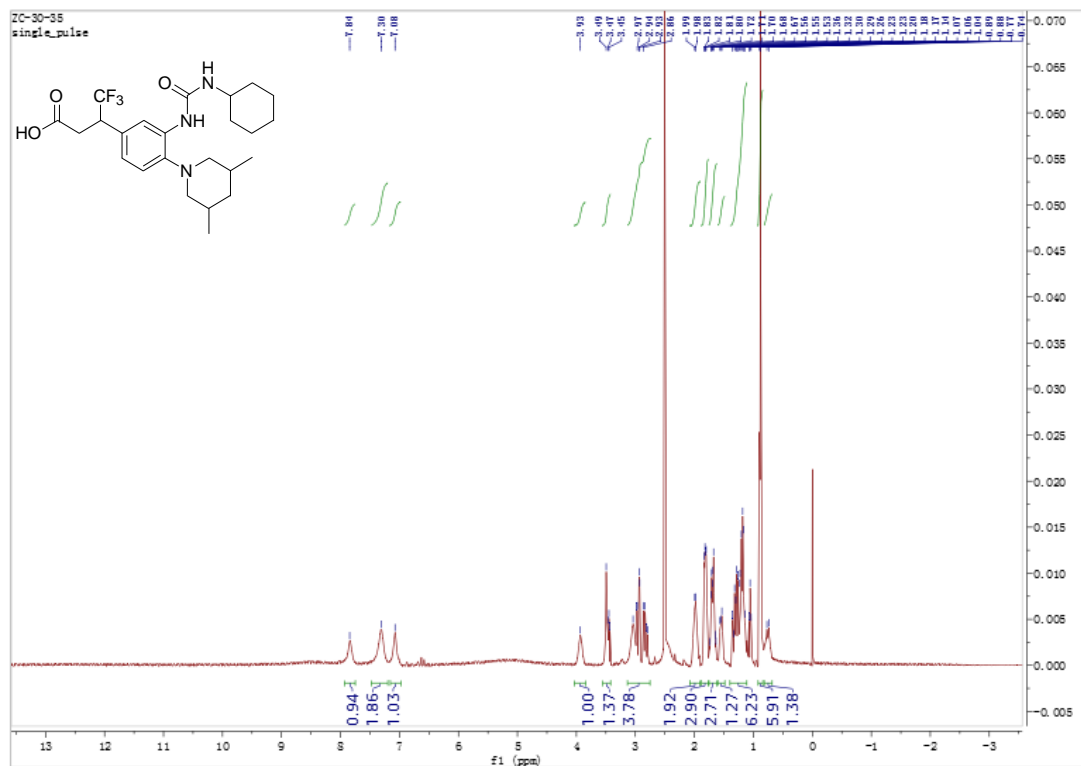
ESI-MS spectra of compound g4

ZC-30-31 #2097 RT: 6.96 AV: 1 NL: 2.19E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



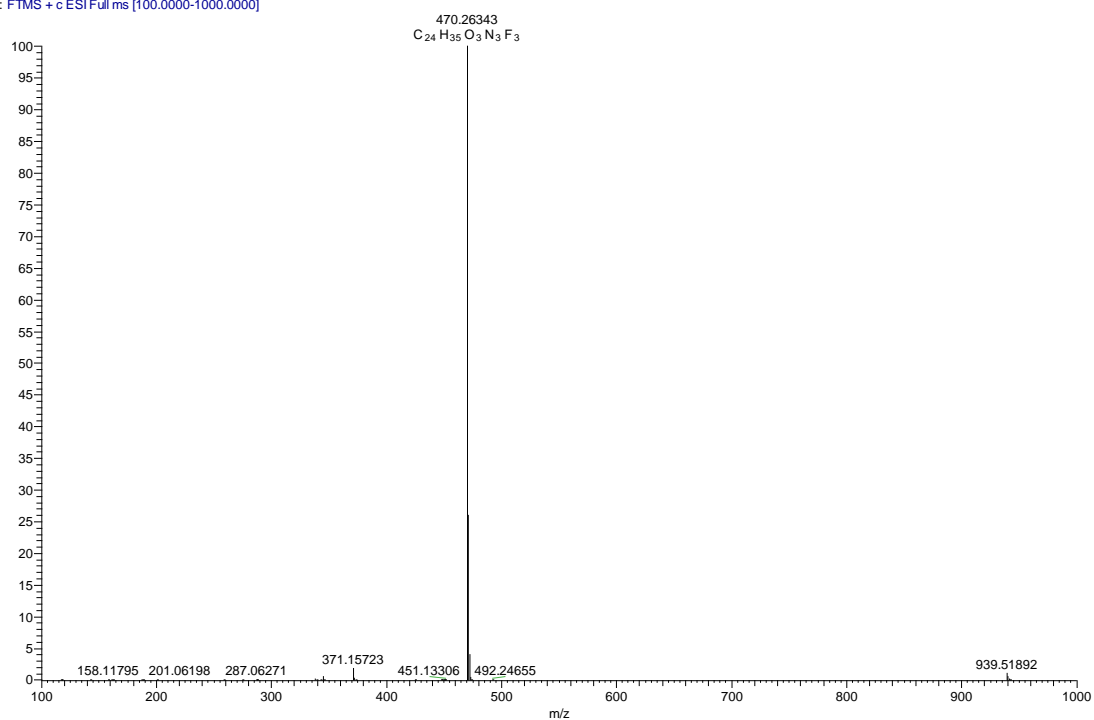
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
498.29480	498.29380	2.00	7.5	C ₂₆ H ₃₉ O ₃ N ₃ F ₃

¹H NMR spectra of compound i4



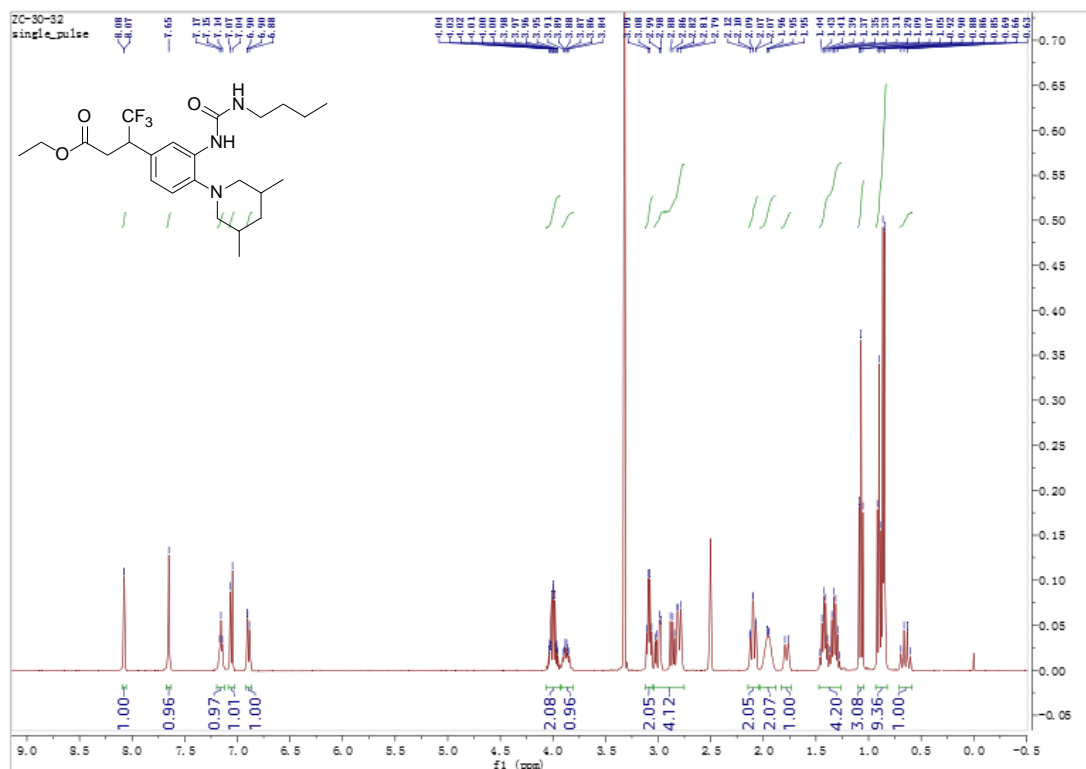
ESI-MS spectra of compound i4

ZC-30-35 #2272 RT: 7.48 AV: 1 NL: 1.13E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



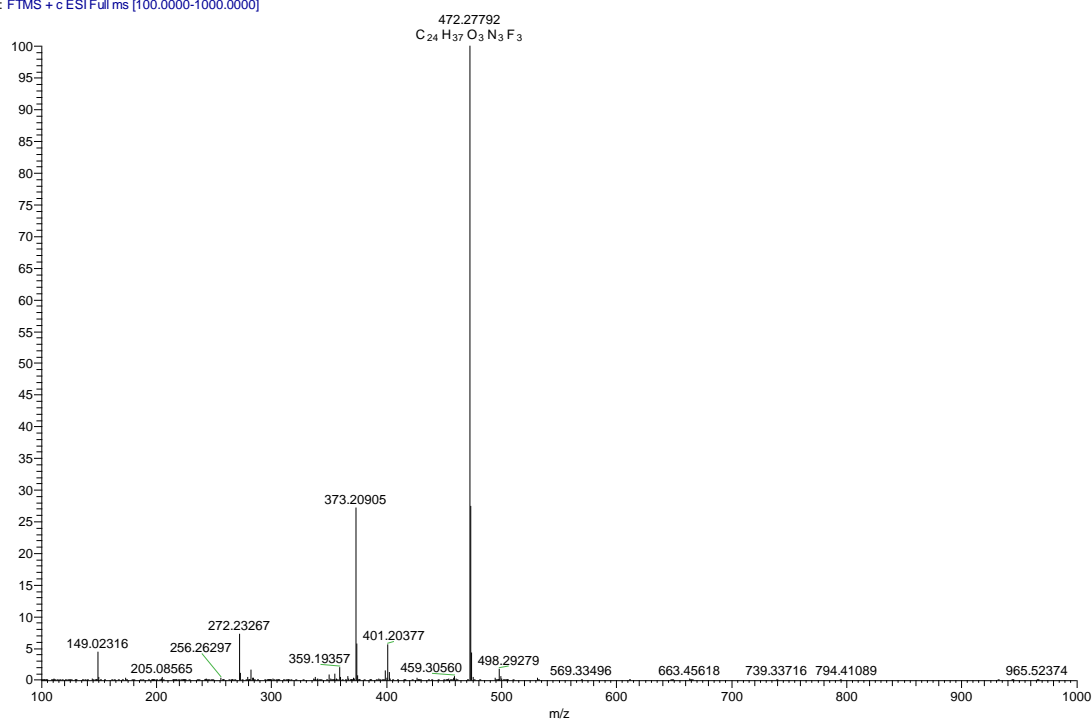
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
470.26343	470.26250	1.97	7.5	C24 H35 O3 N3 F3

¹H NMR spectra of compound g5



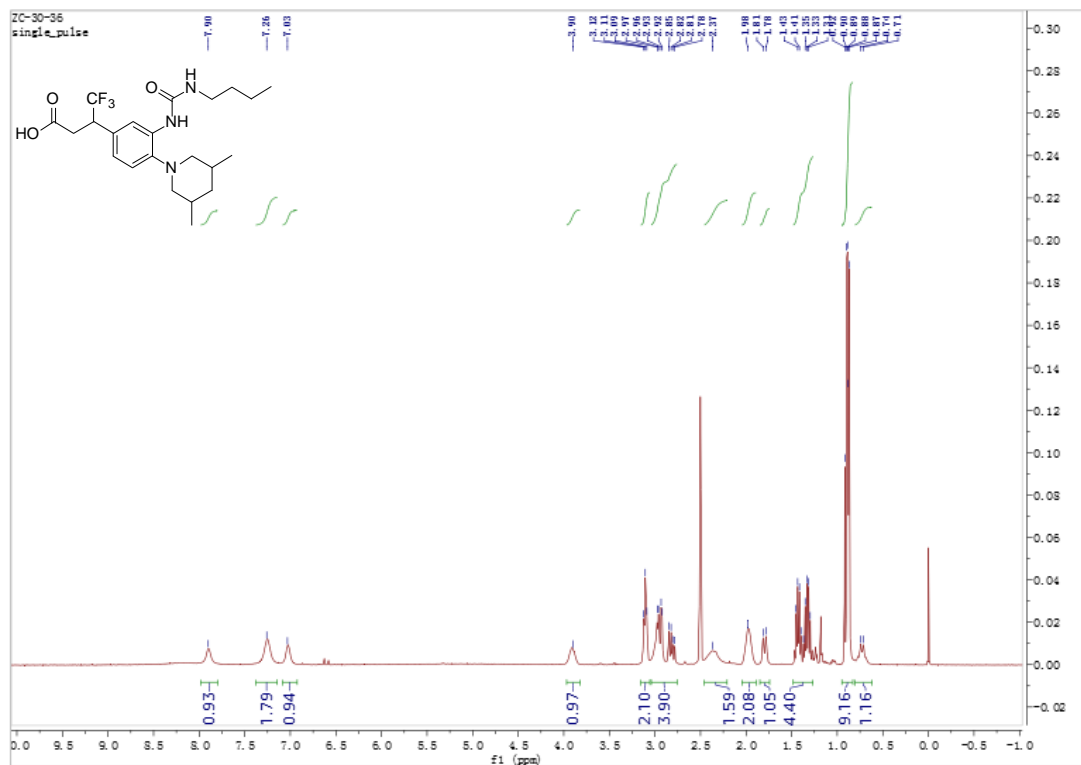
ESI-MS spectra of compound g5

ZC-30-32 #3134 RT: 7.83 AV: 1 NL: 9.04E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]



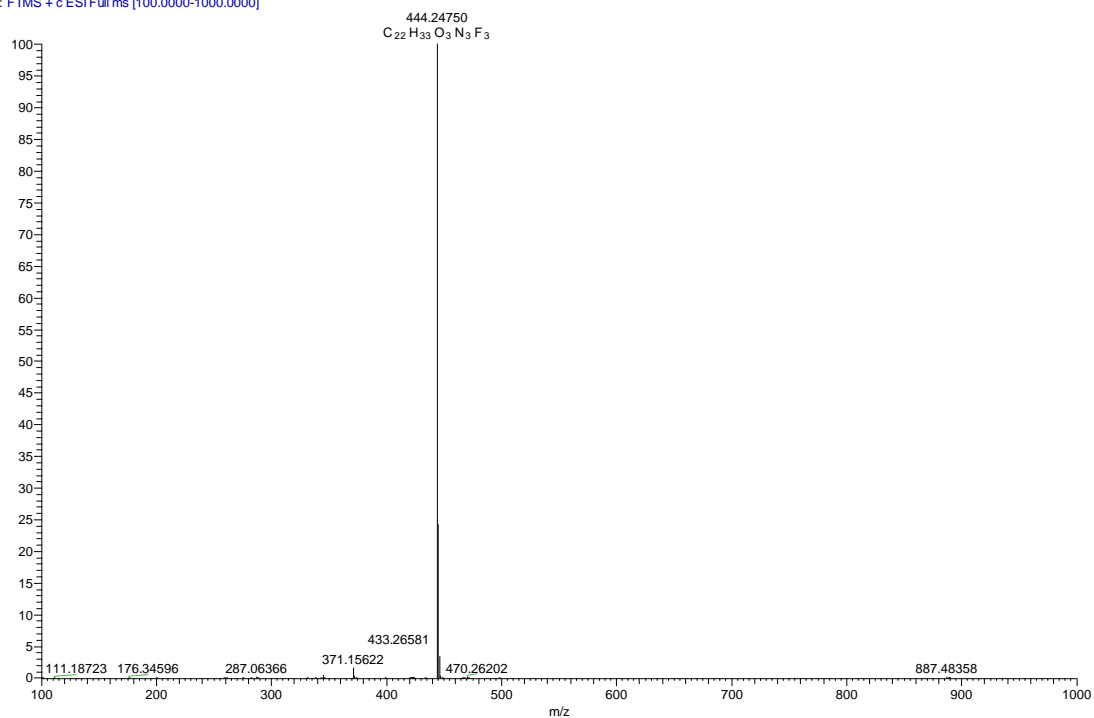
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
472.27792	472.27815	-0.49	6.5	C ₂₄ H ₃₇ O ₃ N ₃ F ₃

¹H NMR spectra of compound i5



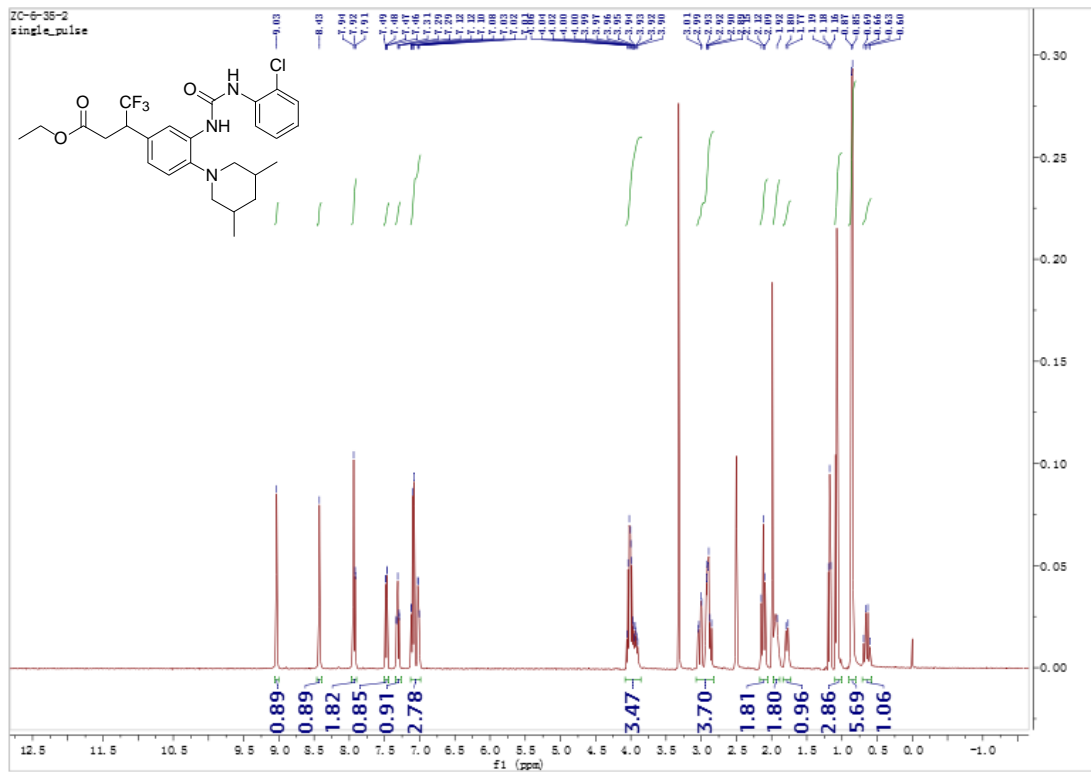
ESI-MS spectra of compound i5

ZC-30-36_191204201711 #2152 RT: 7.25 AV: 1 NL: 1.72E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



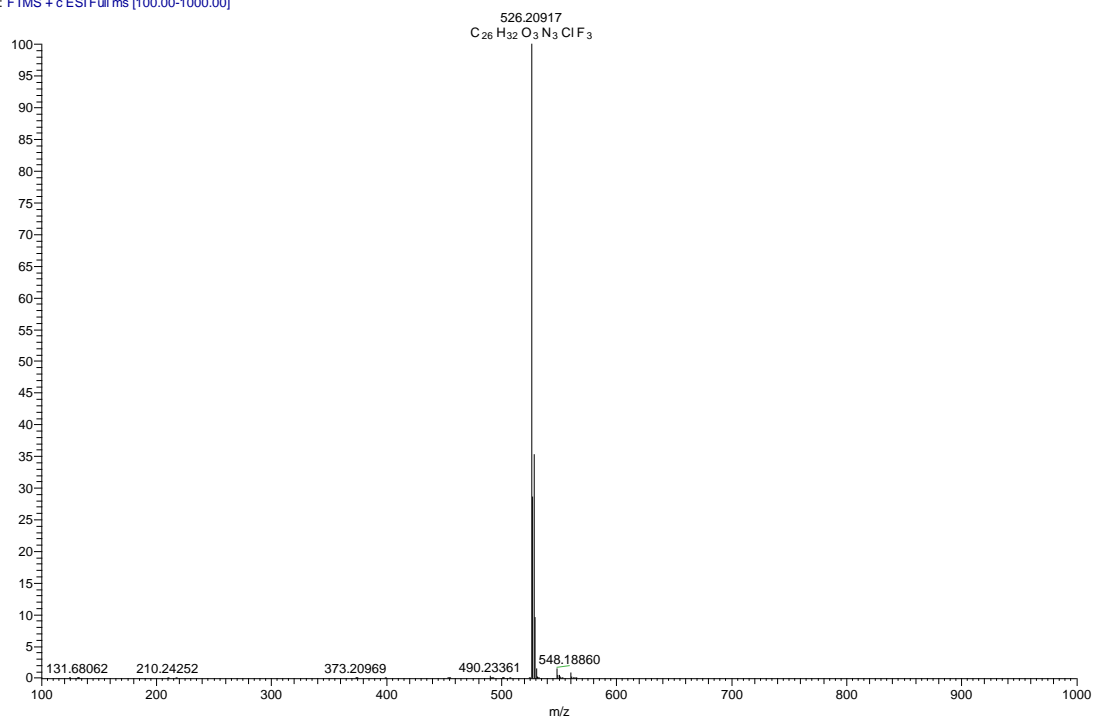
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
444.24750	444.24685	1.46	6.5	C22 H33 O3 N3 F3

¹H NMR spectra of compound g8



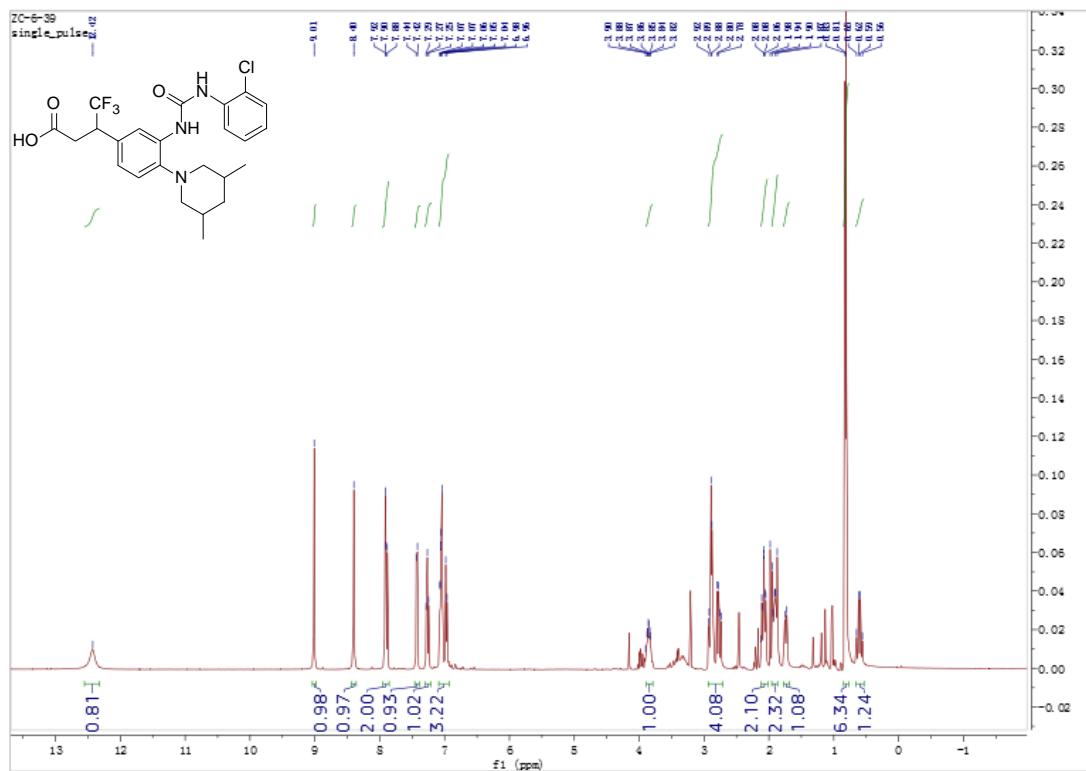
ESI-MS spectra of compound g8

ZC-6-35 #2305 RT: 6.13 AV: 1 NL: 5.30E9
T: FTMS + c ESI Full ms [100.00-1000.00]



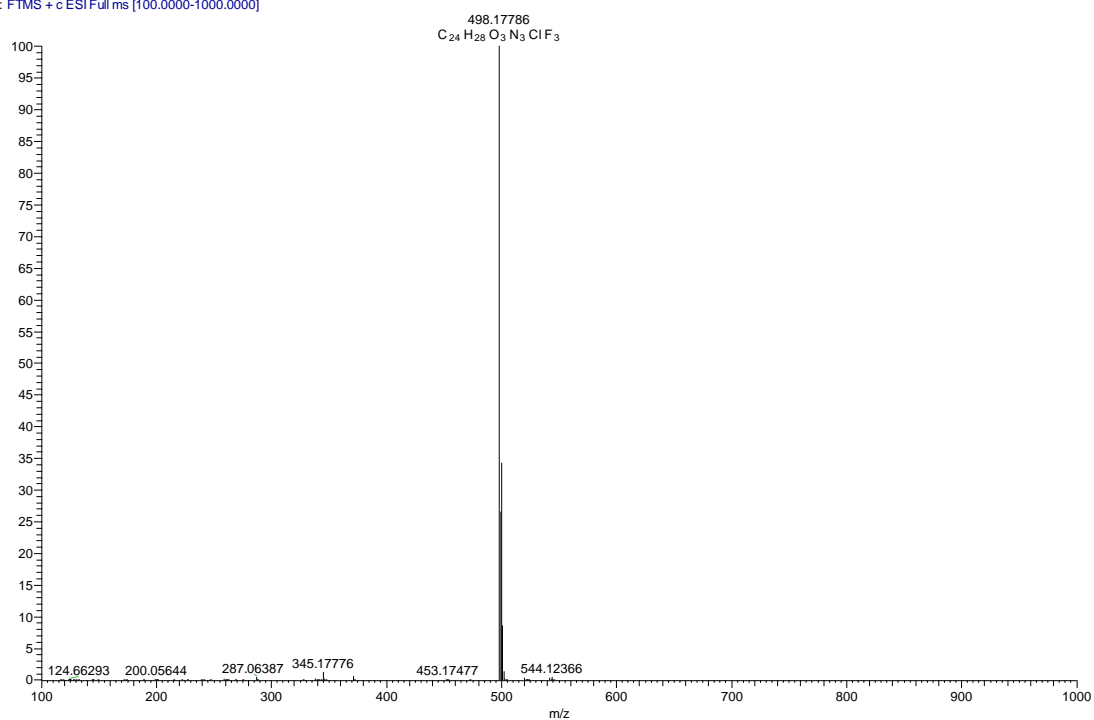
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
526.20917	526.20788	2.45	10.5	C ₂₆ H ₃₂ O ₃ N ₃ ClF ₃

¹H NMR spectra of compound i8



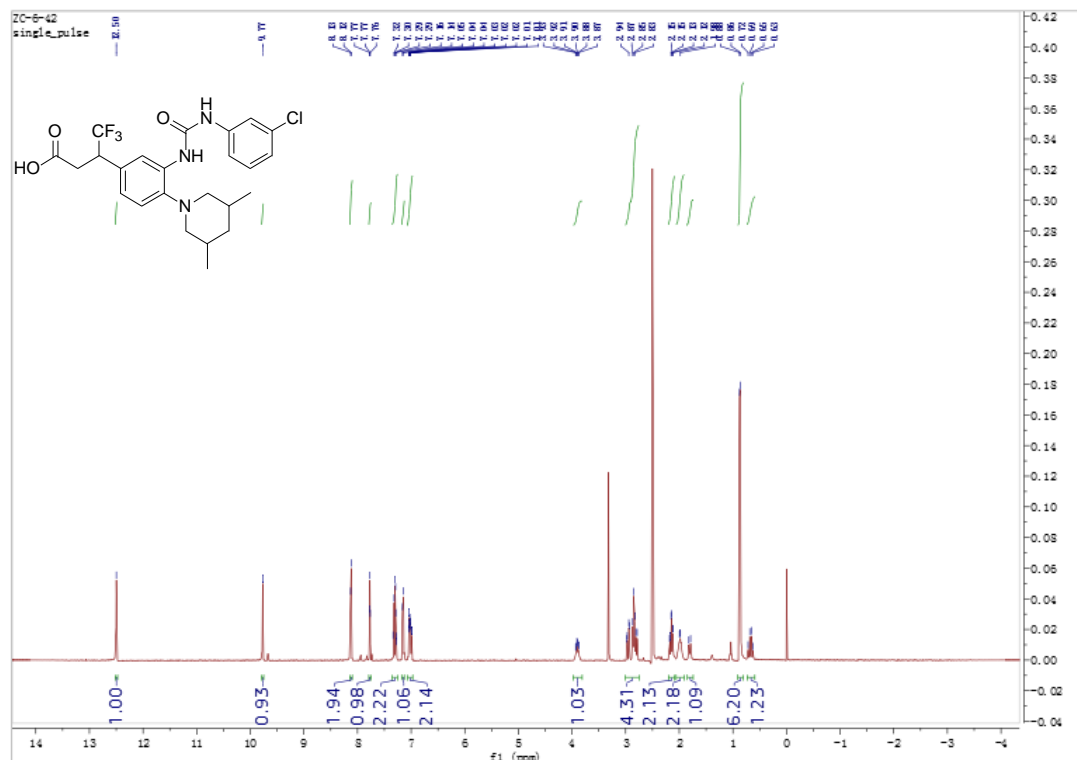
ESI-MS spectra of compound i8

ZC-048 #1697 RT: 5.65 AV: 1 NL: 8.21E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

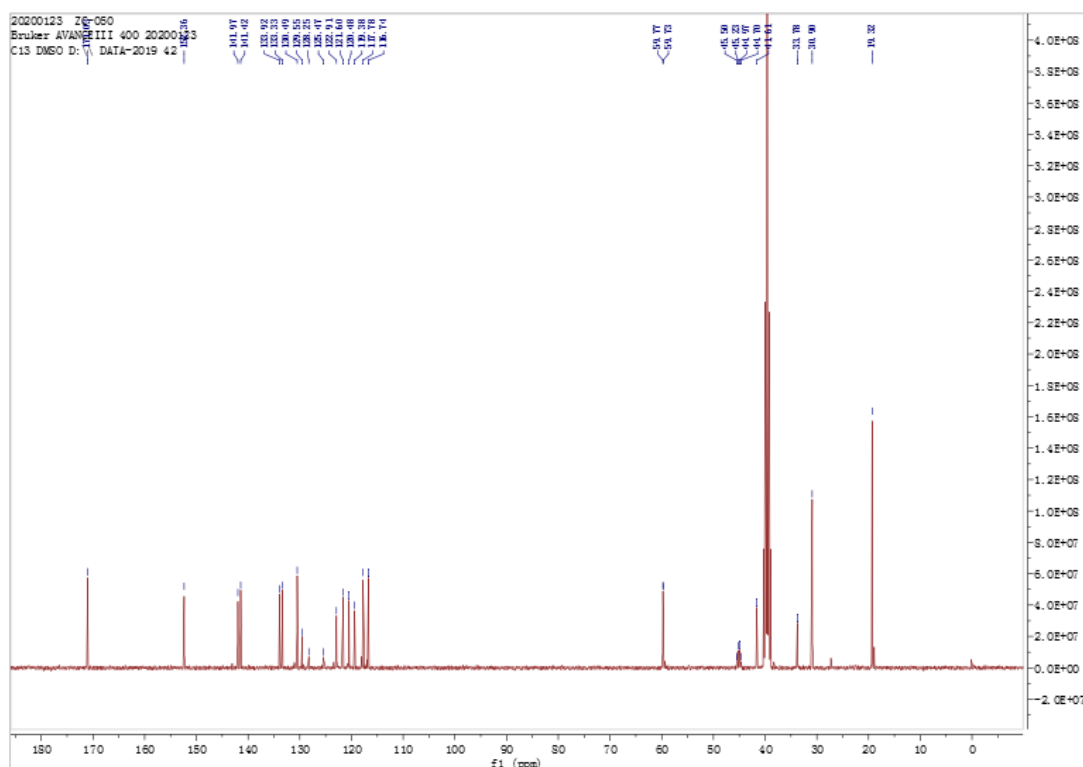


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
498.17786	498.17658	2.57	10.5	C ₂₄ H ₂₈ O ₃ N ₃ ClF ₃

¹H NMR spectra of compound i9

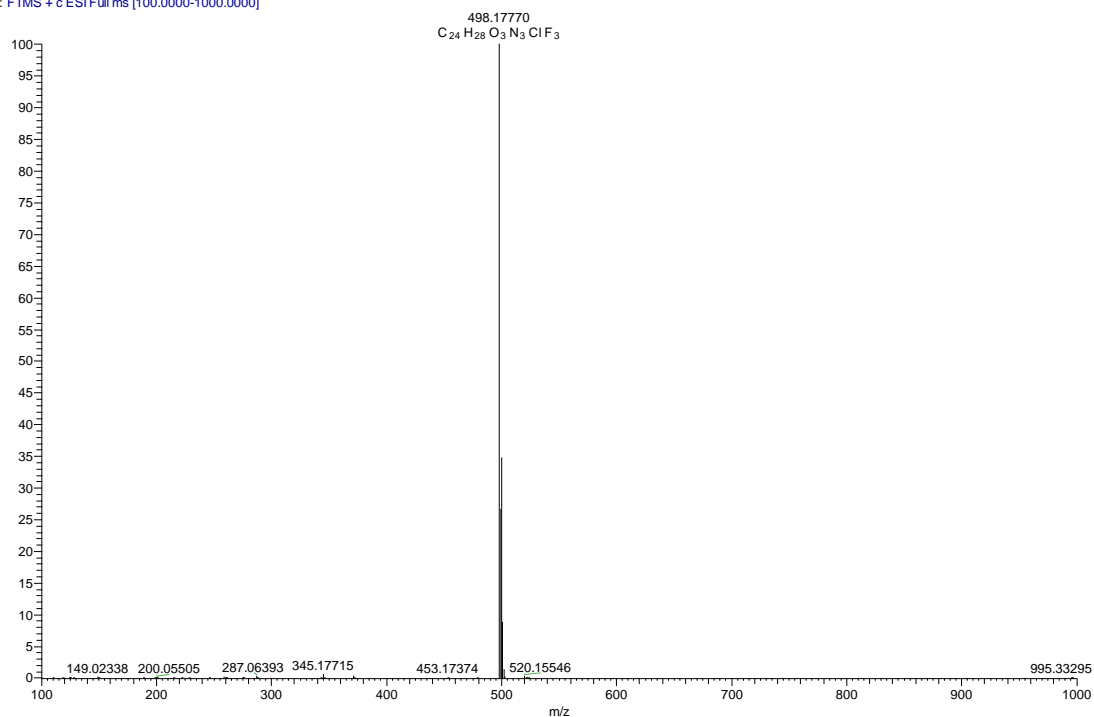


¹³C NMR spectra of compound i9



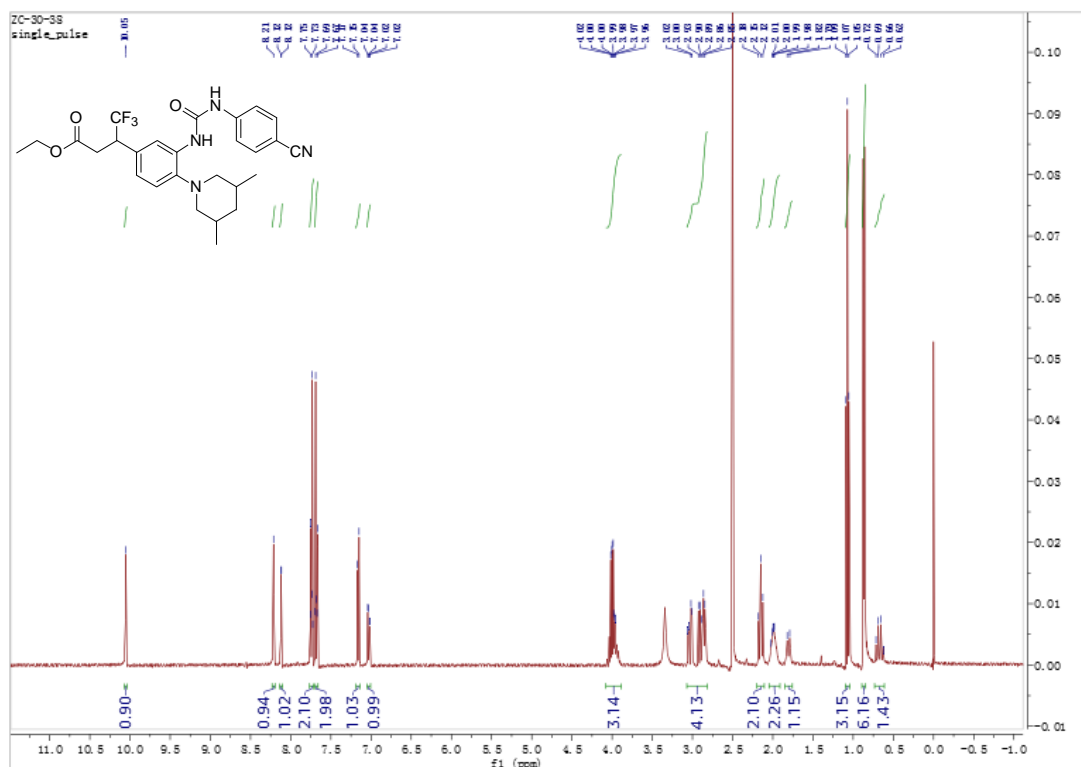
ESI-MS spectra of compound i9

ZC-6-42ZC-050 #1765 RT: 5.78 AV: 1 NL: 1.40E9
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



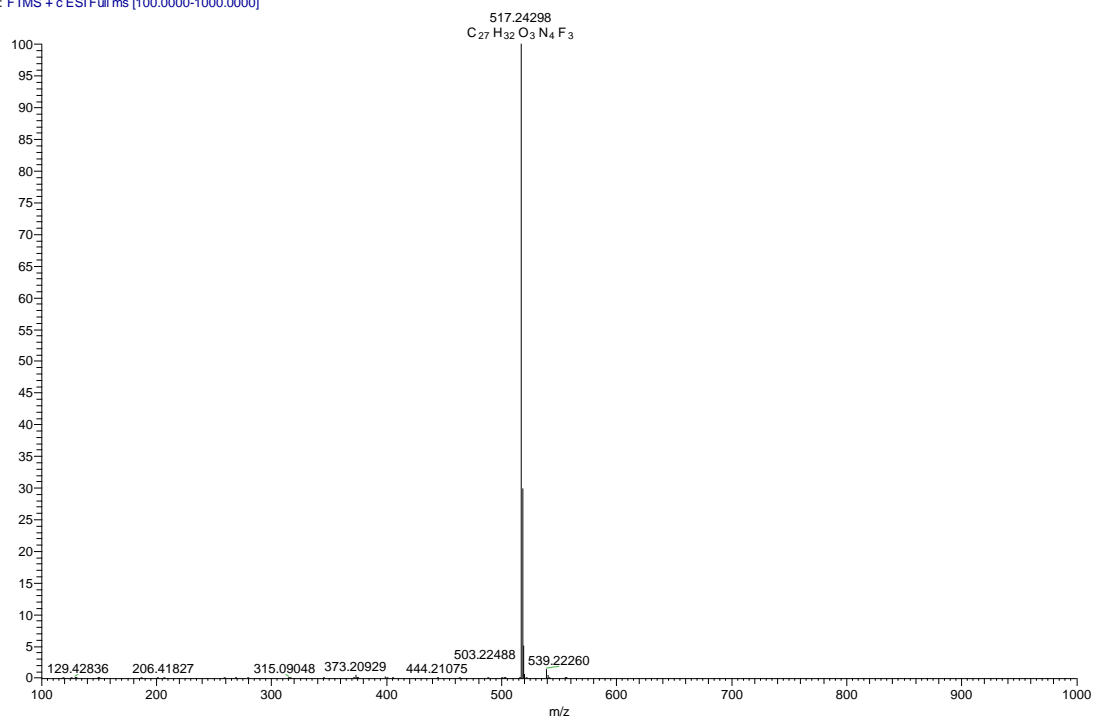
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
498.17770	498.17658	2.25	10.5	C ₂₄ H ₂₈ O ₃ N ₃ ClF ₃

¹H NMR spectra of compound g12



ESI-MS spectra of compound g12

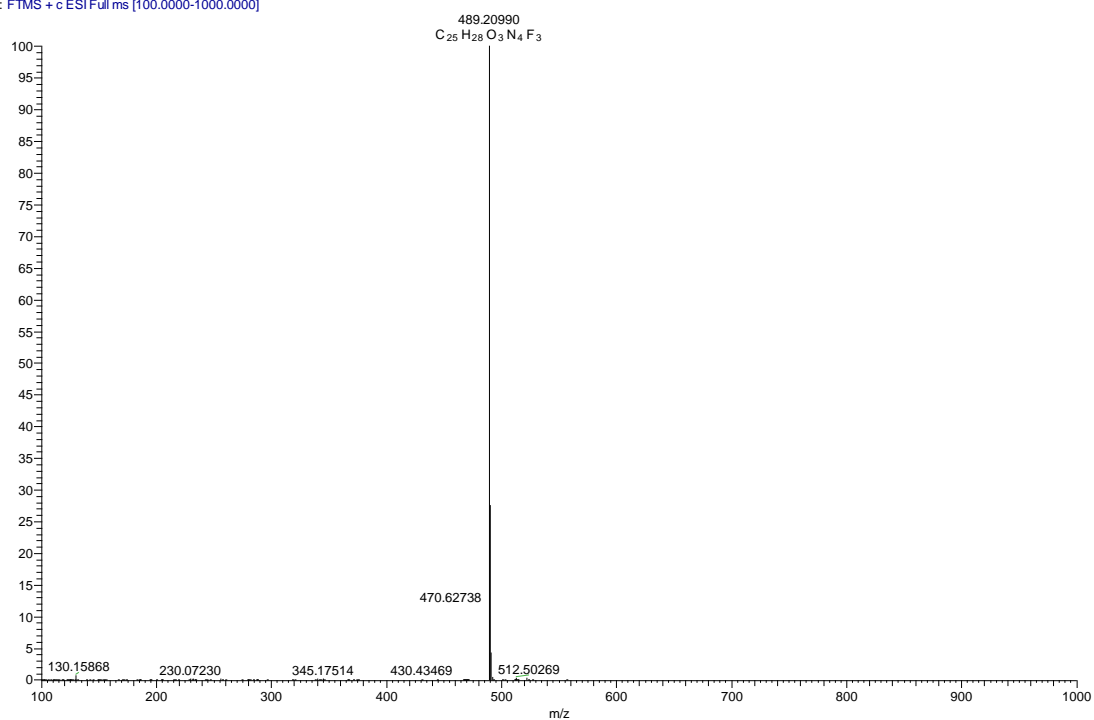
ZC-30-38 #2631 RT: 7.96 AV: 1 NL: 2.66E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
517.24298	517.24210	1.70	12.5	C ₂₇ H ₃₂ O ₃ N ₄ F ₃

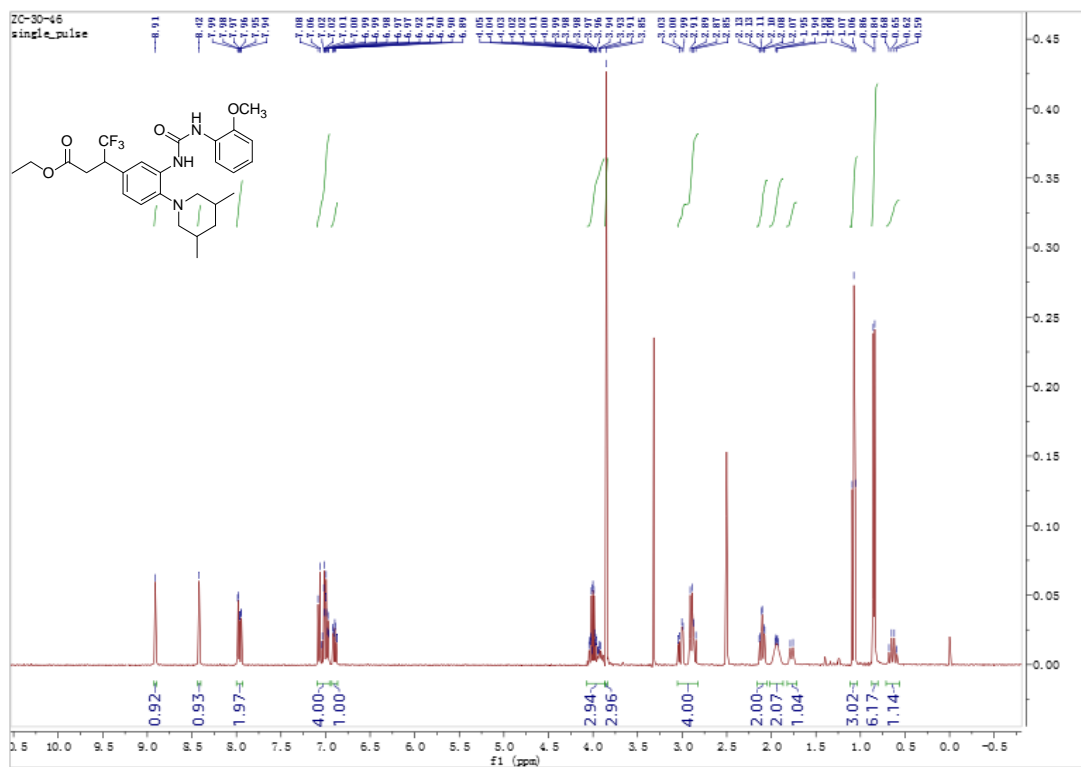
ESI-MS spectra of compound i12

ZC-30-41_191210142927 #1822 RT: 5.45 AV: 1 NL: 2.05E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



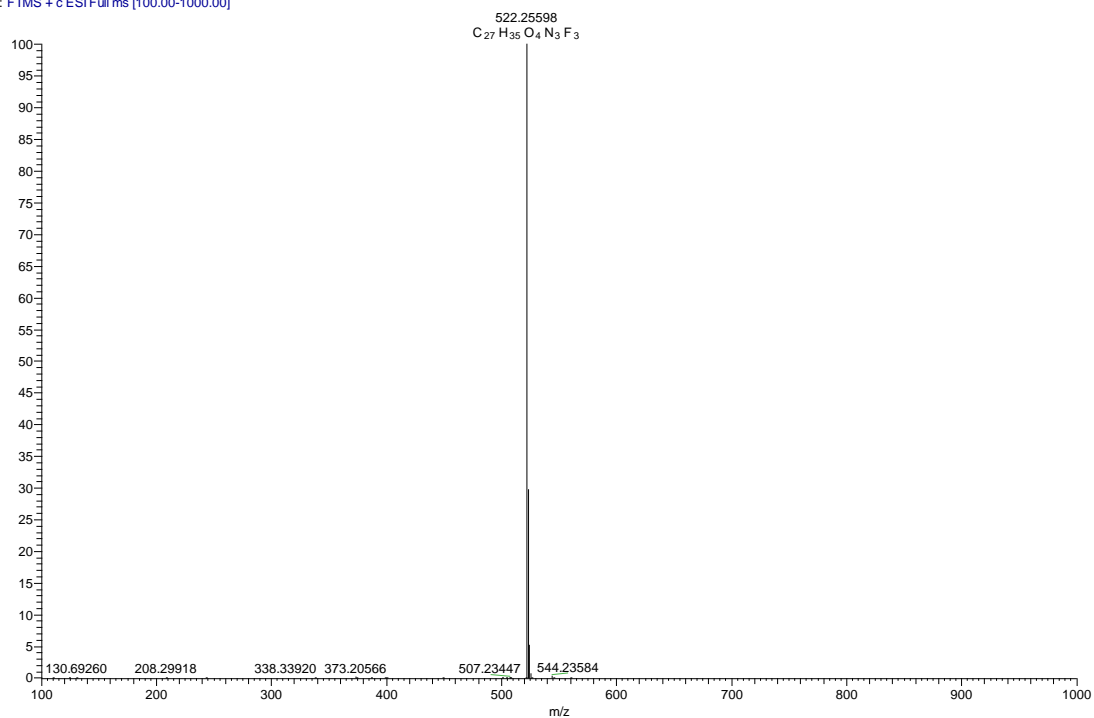
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
489.20990	489.21080	-1.84	12.5	C ₂₅ H ₂₈ O ₃ N ₄ F ₃

¹H NMR spectra of compound g13



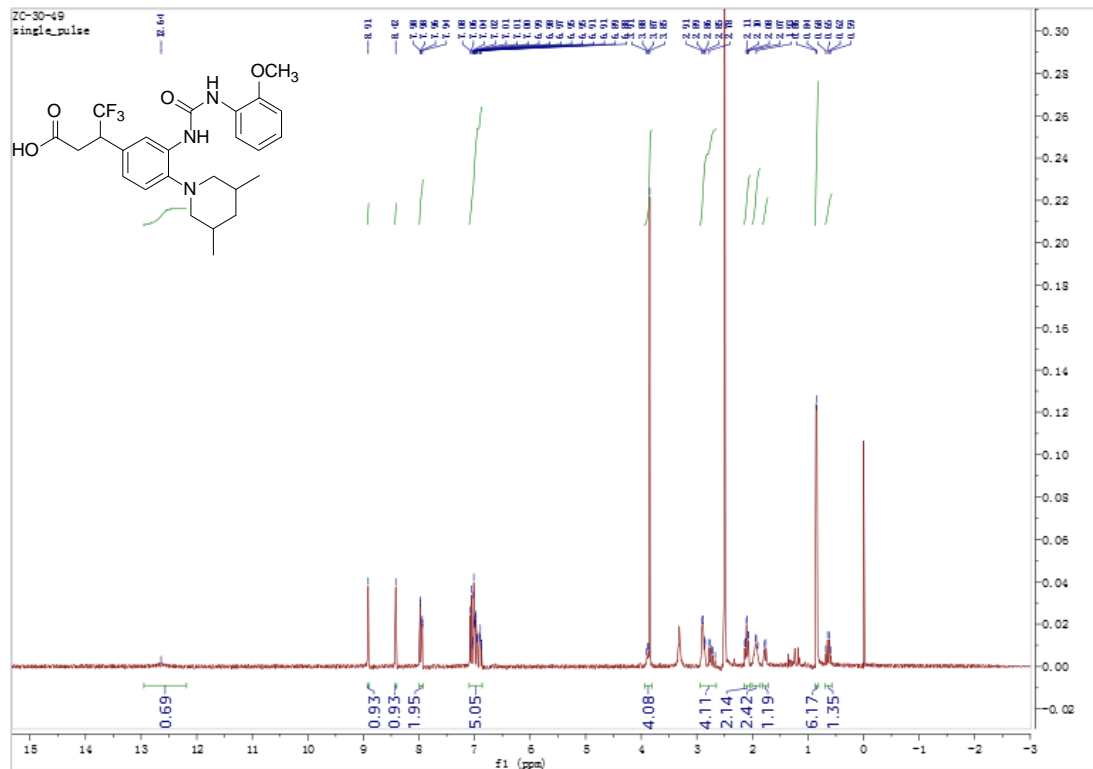
ESI-MS spectra of compound g13

ZC-6-48_170111171942 #2234 RT: 5.80 AV: 1 NL: 9.76E9
T: FTMS + c ESI Full ms [100.00-1000.00]



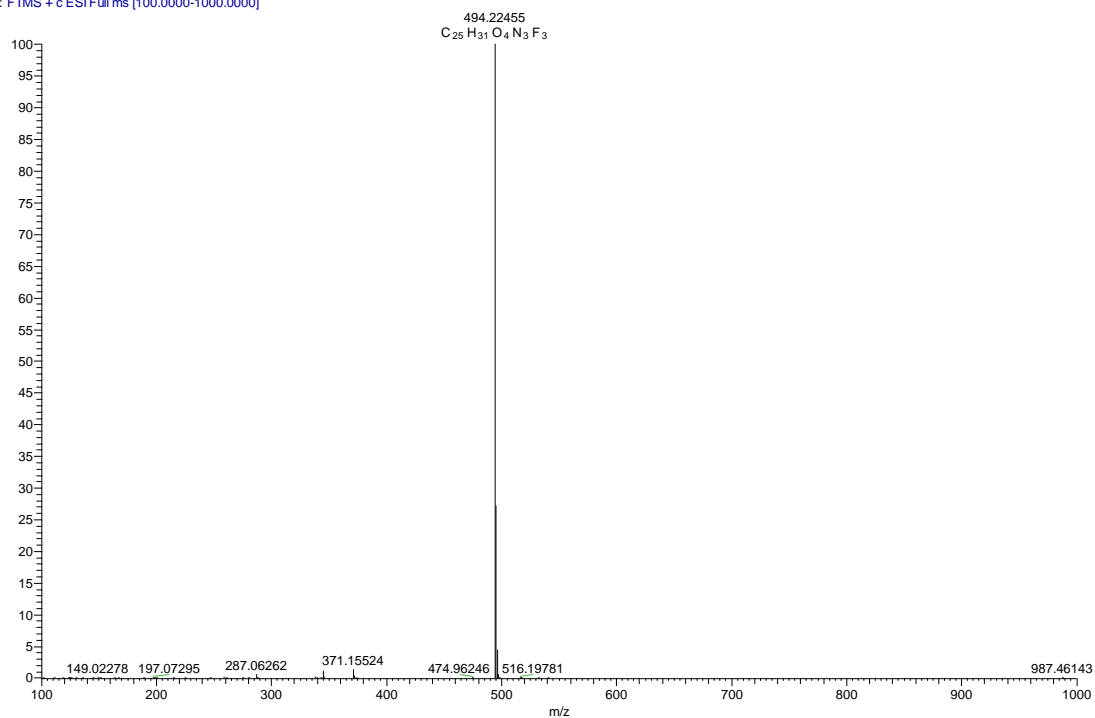
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
522.25598	522.25742	-2.75	10.5	C ₂₇ H ₃₅ O ₄ N ₃ F ₃

¹H NMR spectra of compound i13



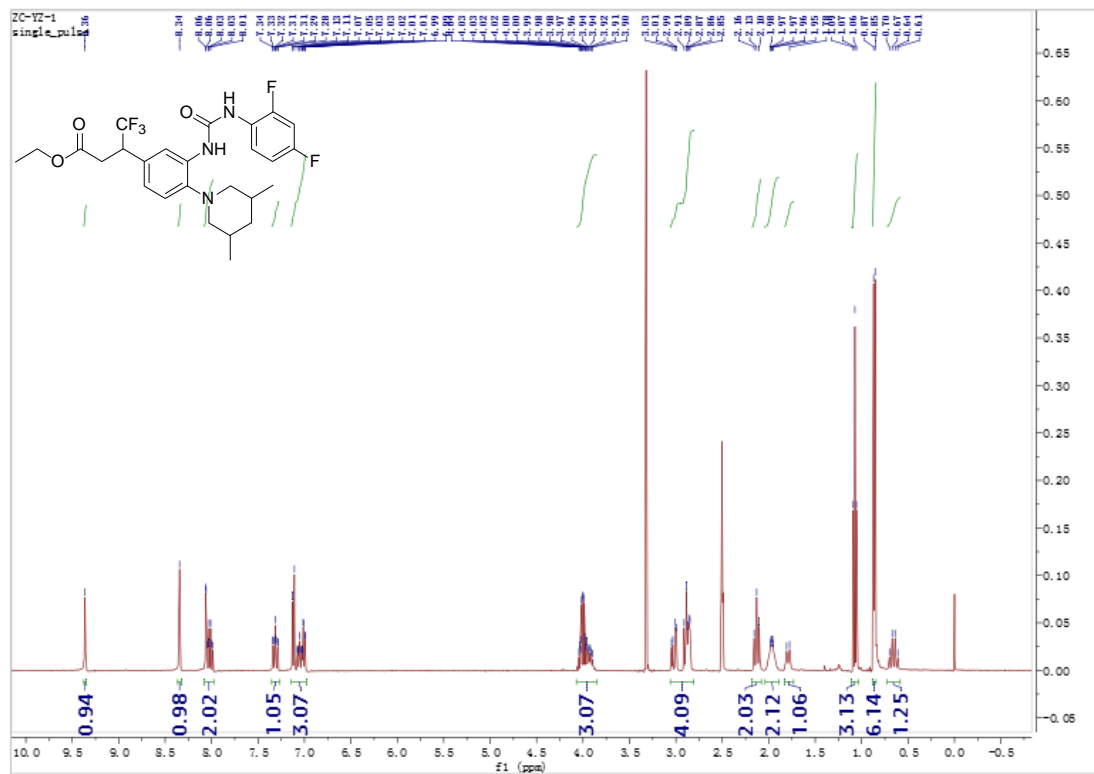
ESI-MS spectra of compound i13

ZC-30-49 #1509 RT: 5.43 AV: 1 NL: 9.48E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

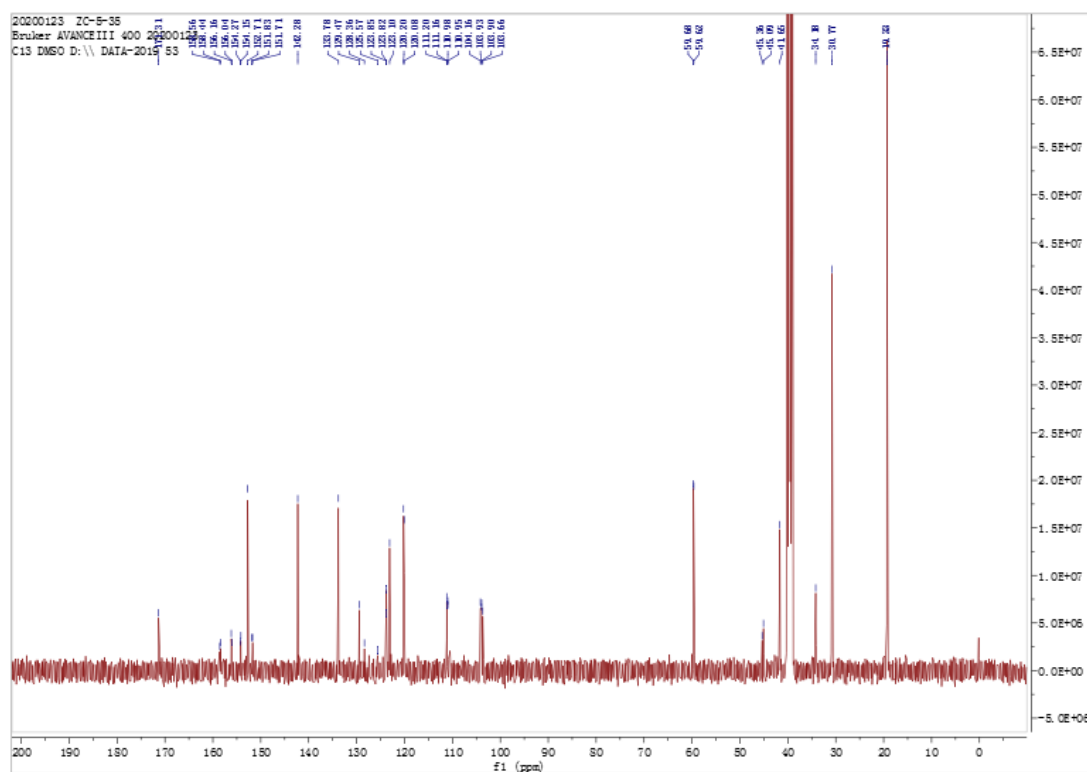


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
494.22455	494.22612	-3.17	10.5	C25 H31 O4 N3 F3

¹H NMR spectra of compound g16

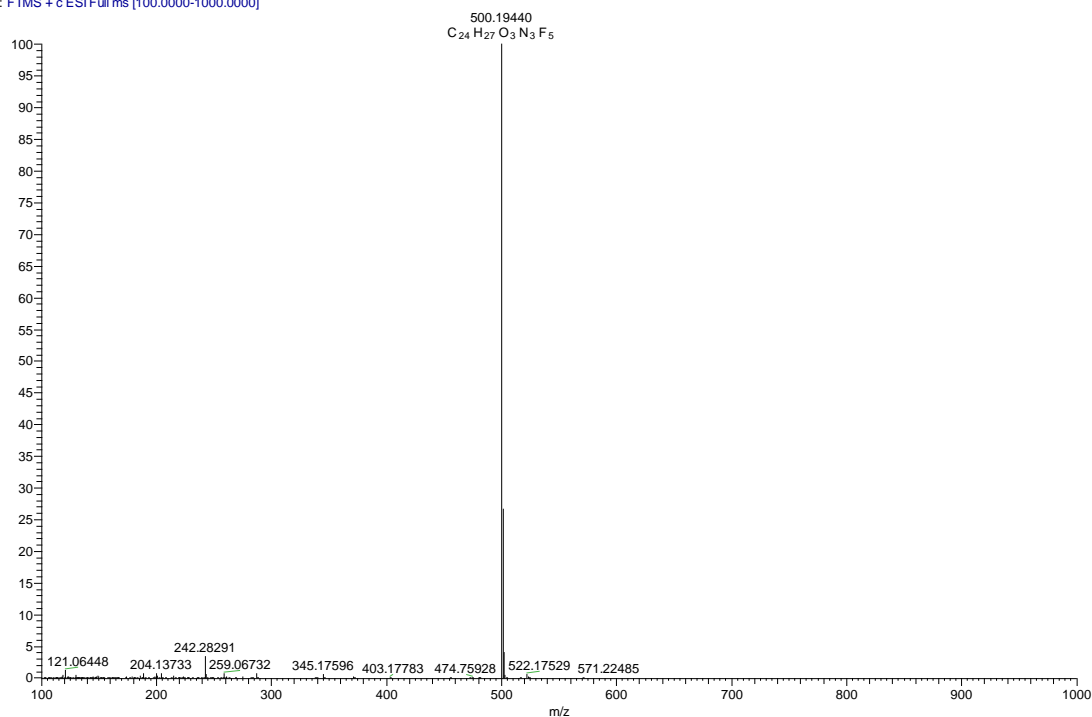


¹³C NMR spectra of compound i16



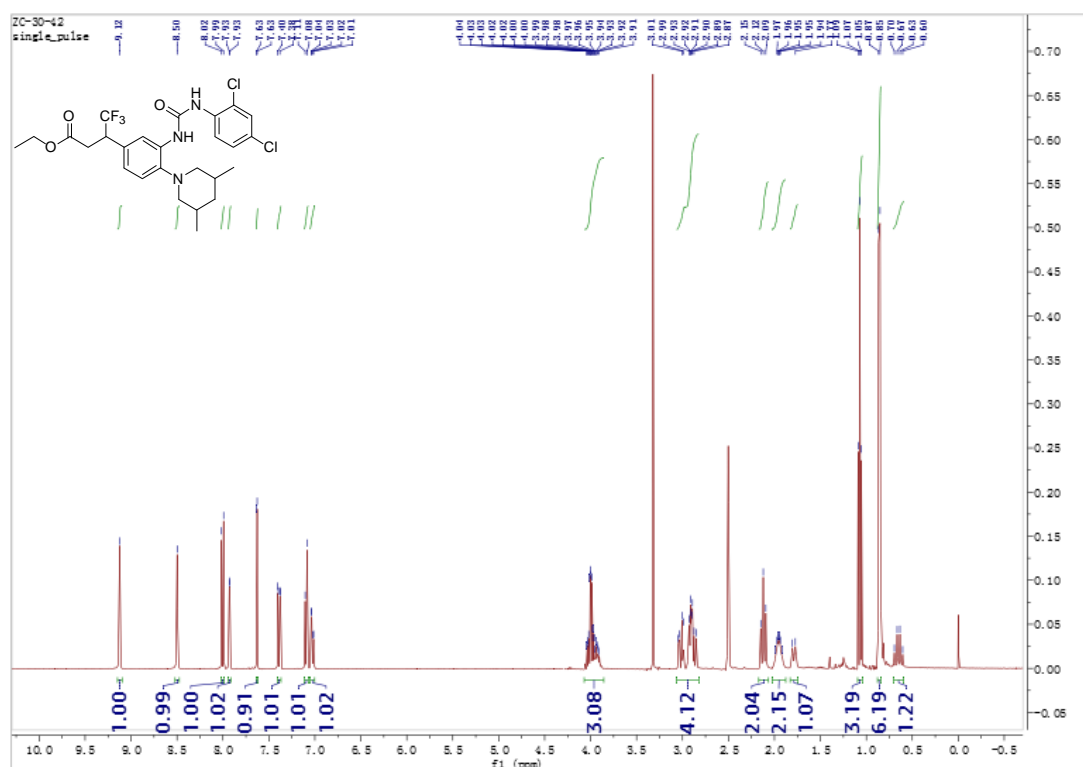
ESI-MS spectra of compound i16

ZC-5-35 #1828 RT: 6.79 AV: 1 NL: 1.81E7
T: FTMS + c ESI Full ms [100.0000-1000.0000]



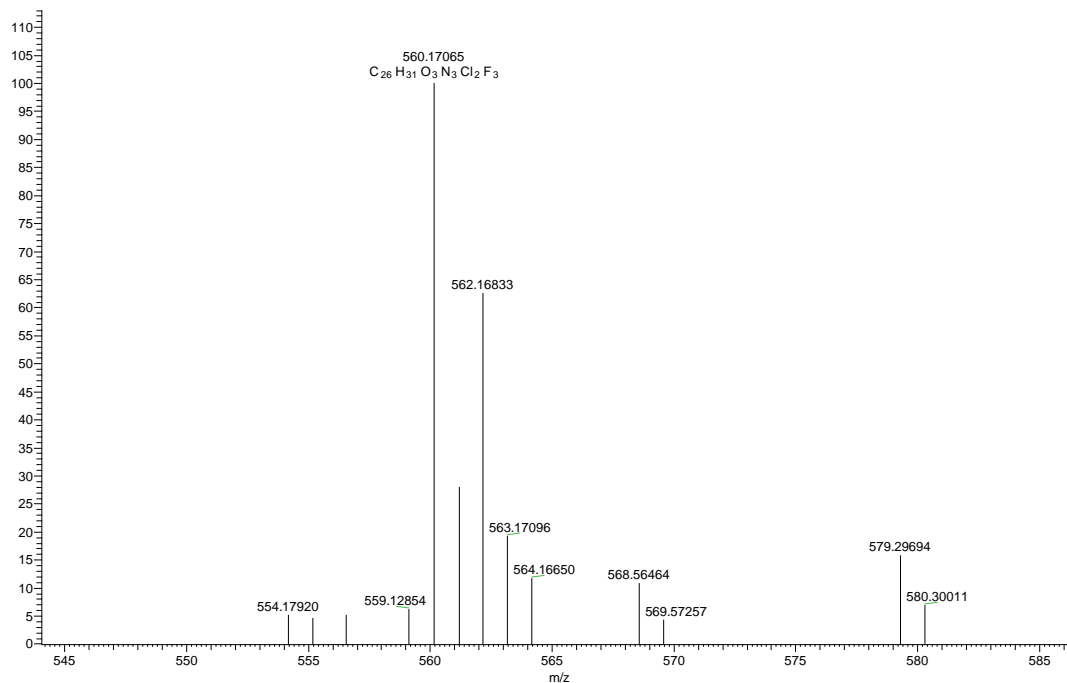
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
500.19440	500.19671	-4.62	10.5	C ₂₄ H ₂₇ O ₃ N ₃ F ₅

¹H NMR spectra of compound g17



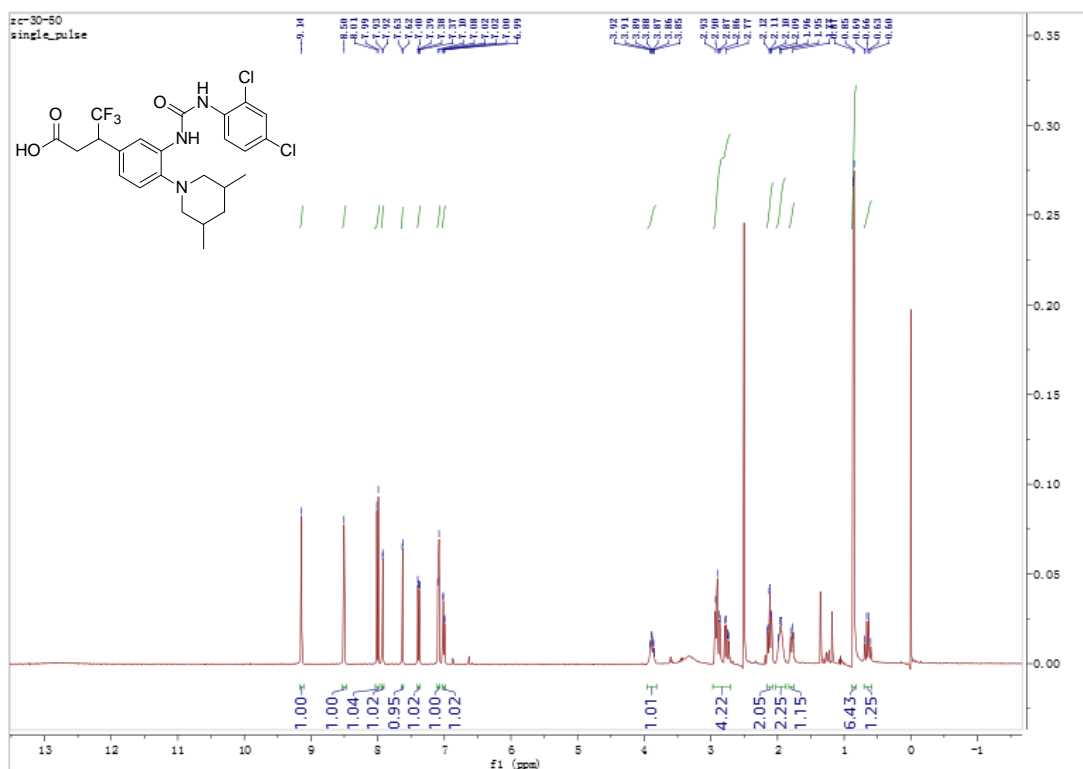
ESI-MS spectra of compound g17

ZC-30-42_191208183414 #2885 RT: 7.95 AV: 1 NL: 5.20E6
T: FTMS + c ESI Full ms [100.0000-1000.0000]

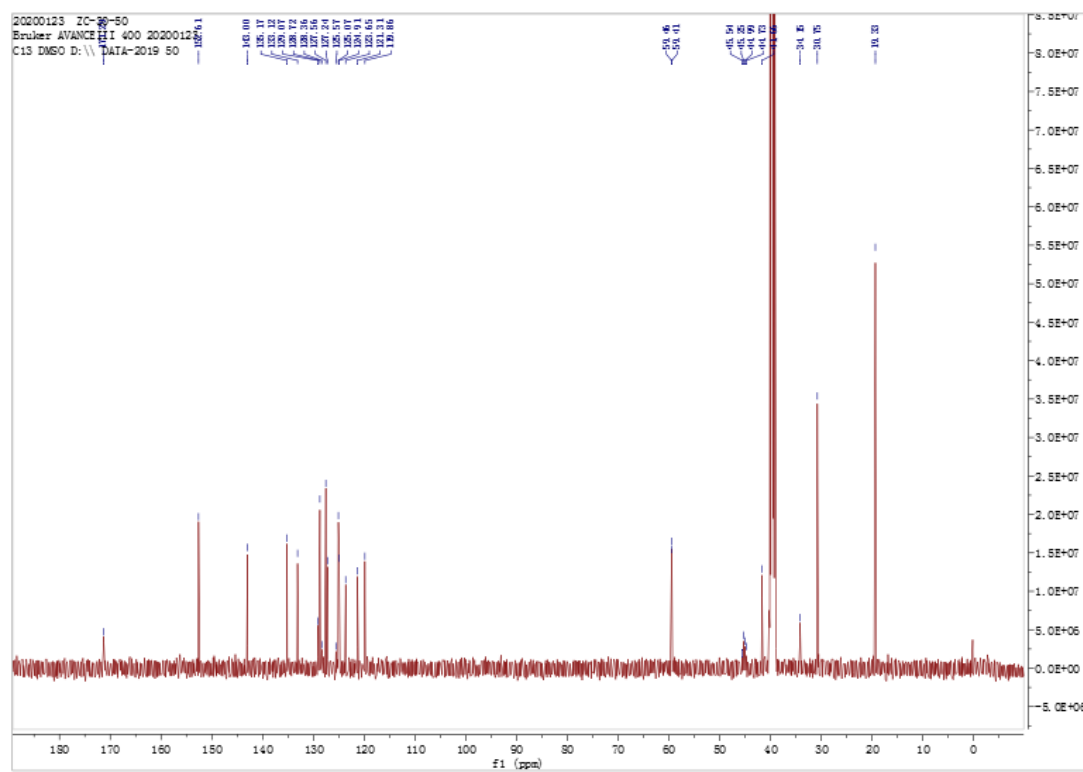


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
560.17065	560.16891	3.11	10.5	C ₂₆ H ₃₁ O ₃ N ₃ Cl ₂ F ₃

¹H NMR spectra of compound i17

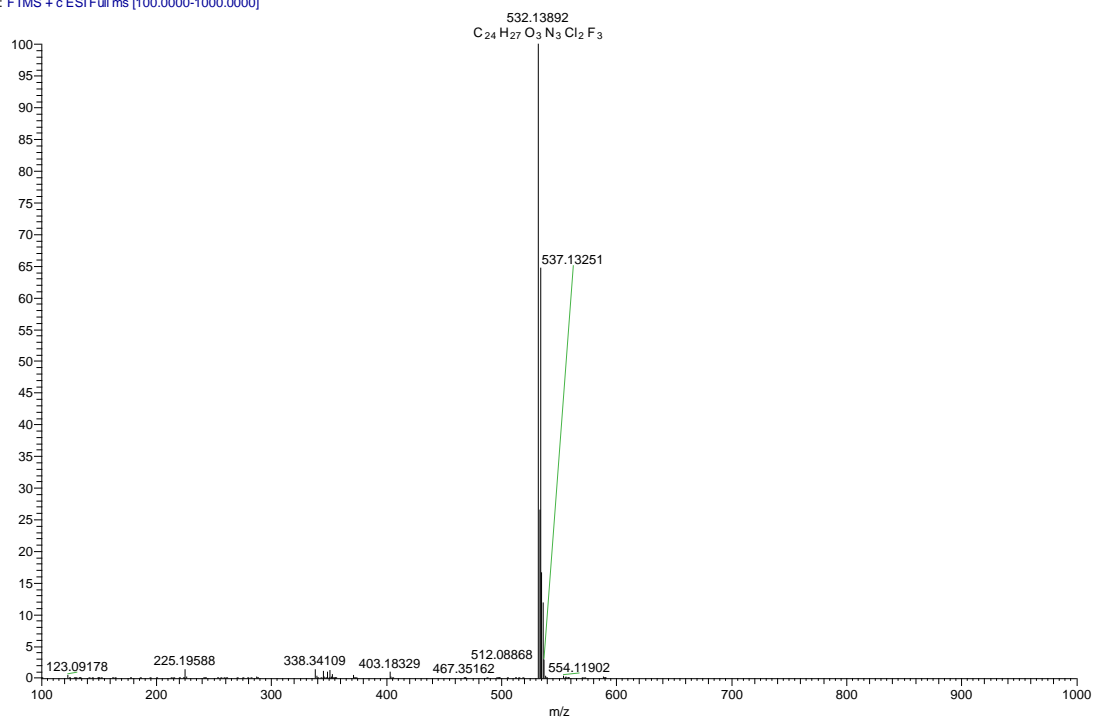


¹³C NMR spectra of compound i17



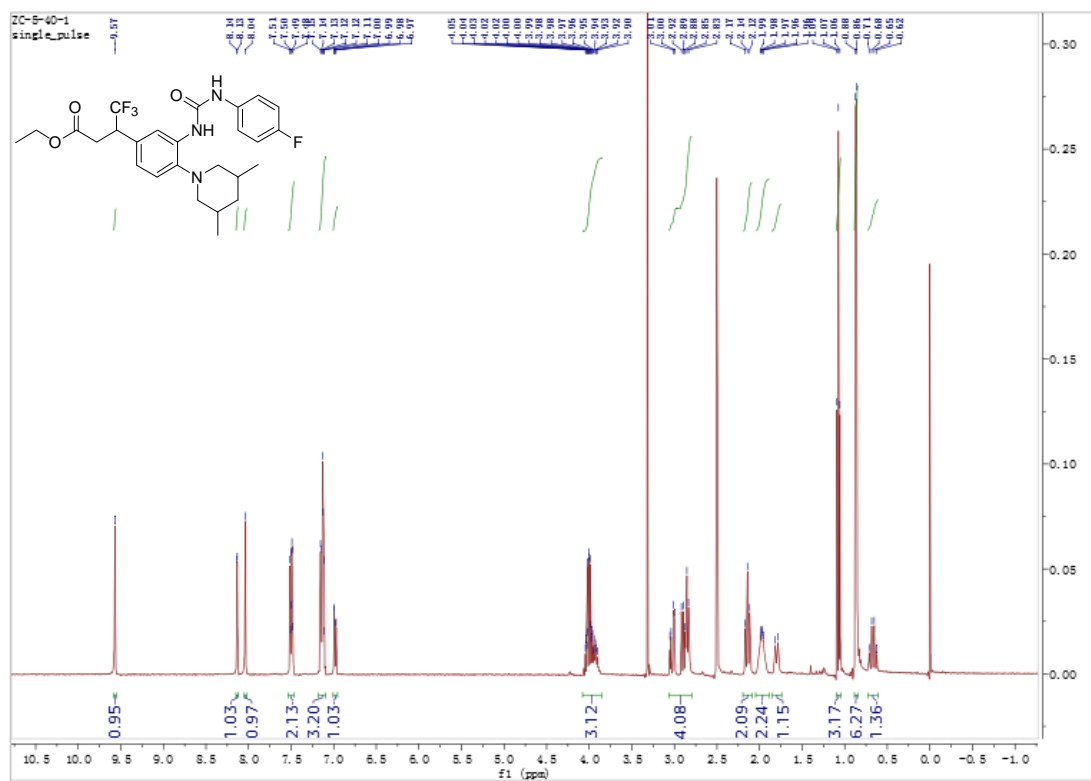
ESI-MS spectra of compound i17

ZC-30-50 #2277 RT: 5.97 AV: 1 NL: 8.92E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

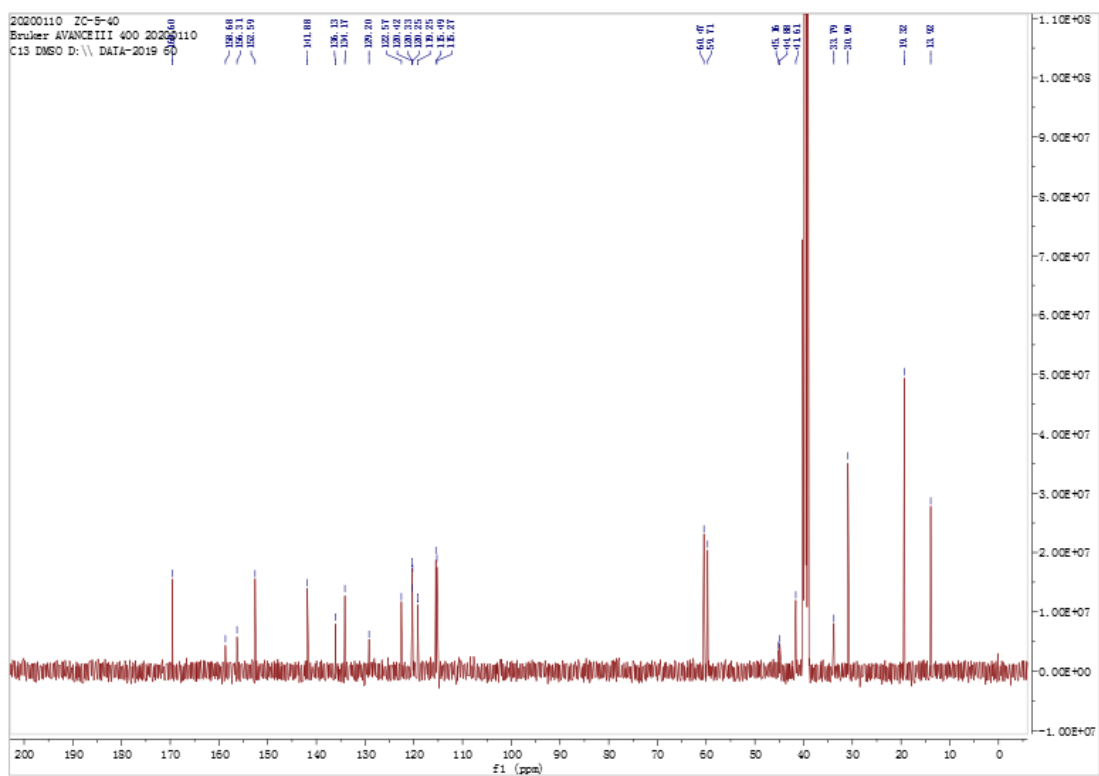


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
532.13892	532.13761	2.47	10.5	C ₂₄ H ₂₇ O ₃ N ₃ Cl ₂ F ₃

¹H NMR spectra of compound g18

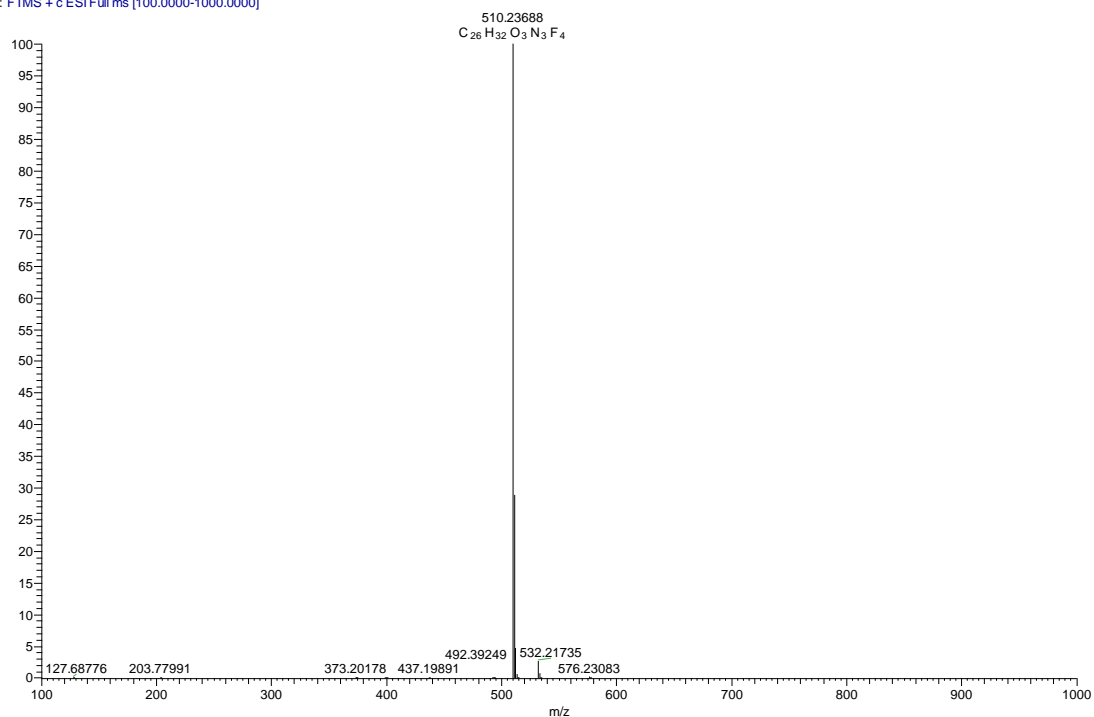


¹³C NMR spectra of compound g18



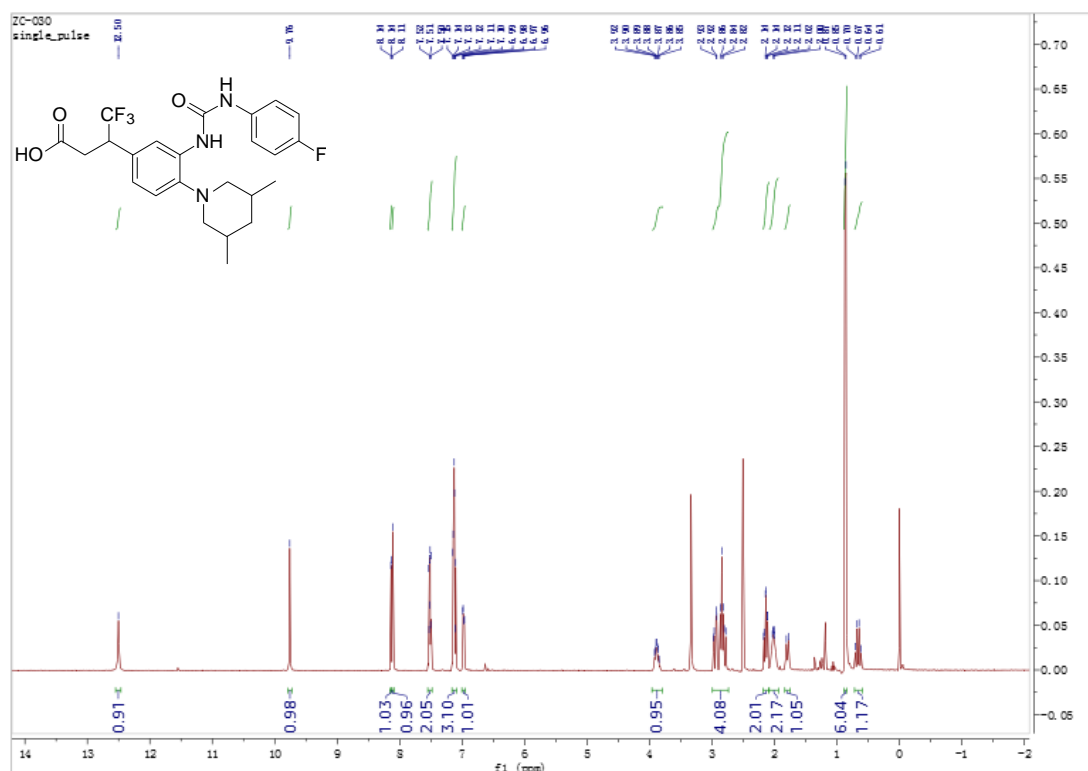
ESI-MS spectra of compound g18

ZC-5-40 #1571 RT: 5.76 AV: 1 NL: 5.31E8
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



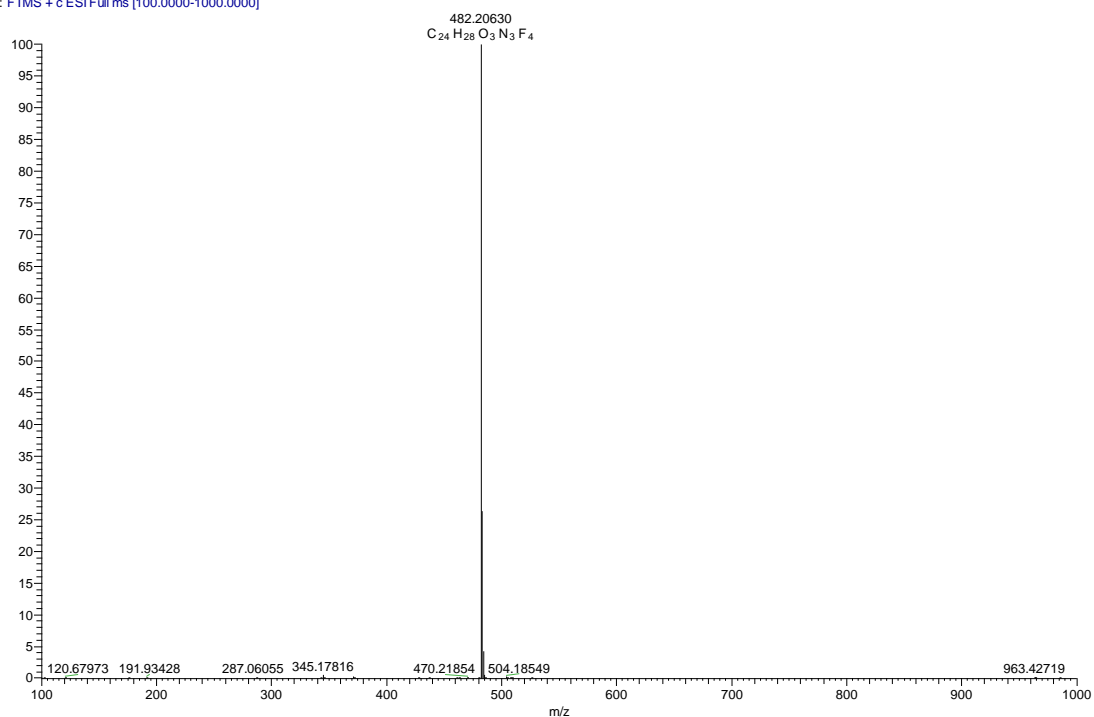
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
510.23688	510.23743	-1.08	10.5	C ₂₆ H ₃₂ O ₃ N ₃ F ₄

¹H NMR spectra of compound i18



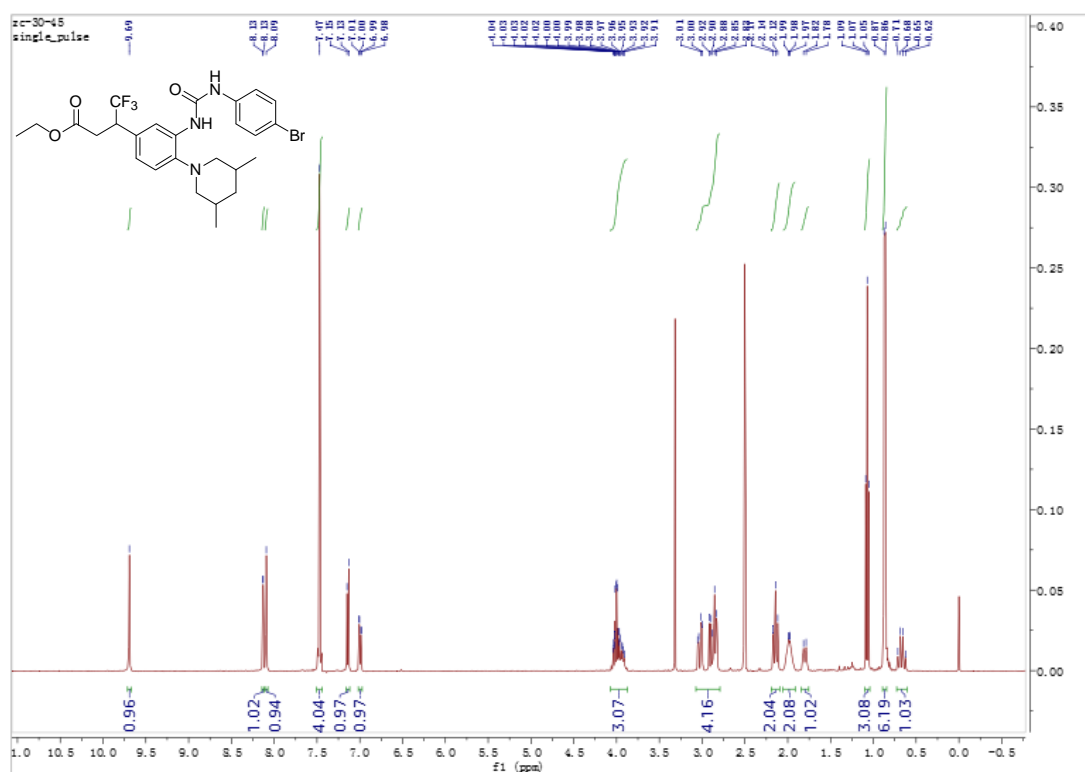
ESI-MS spectra of compound i18

ZC-030 #1954 RT: 6.77 AV: 1 NL: 1.44E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



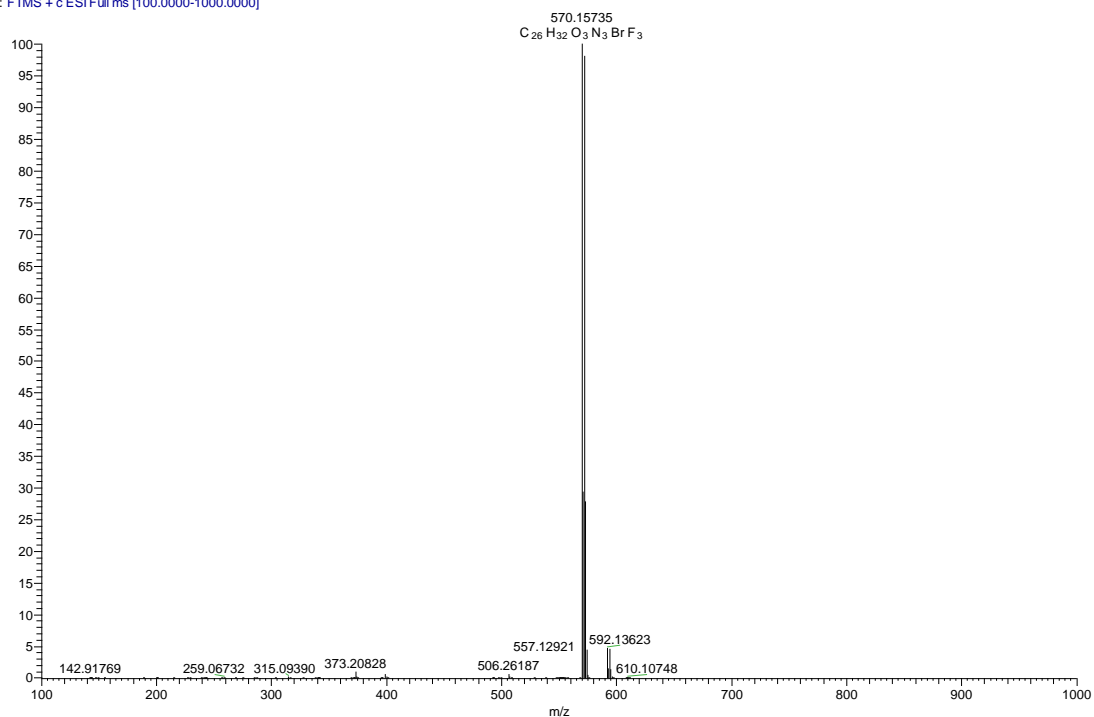
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
482.20630	482.20613	0.35	10.5	C ₂₄ H ₂₈ O ₃ N ₃ F ₄

¹H NMR spectra of compound g19



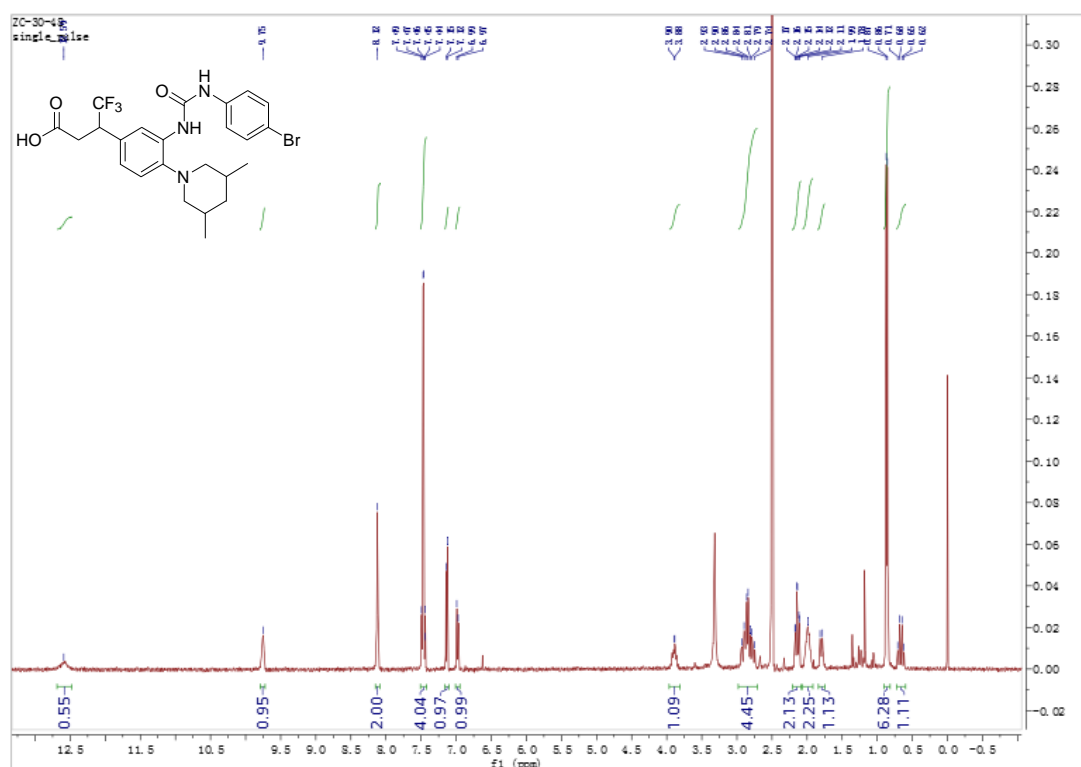
ESI-MS spectra of compound g19

ZC-30-45_191224090752 #1936 RT: 6.50 AV: 1 NL: 4.52E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

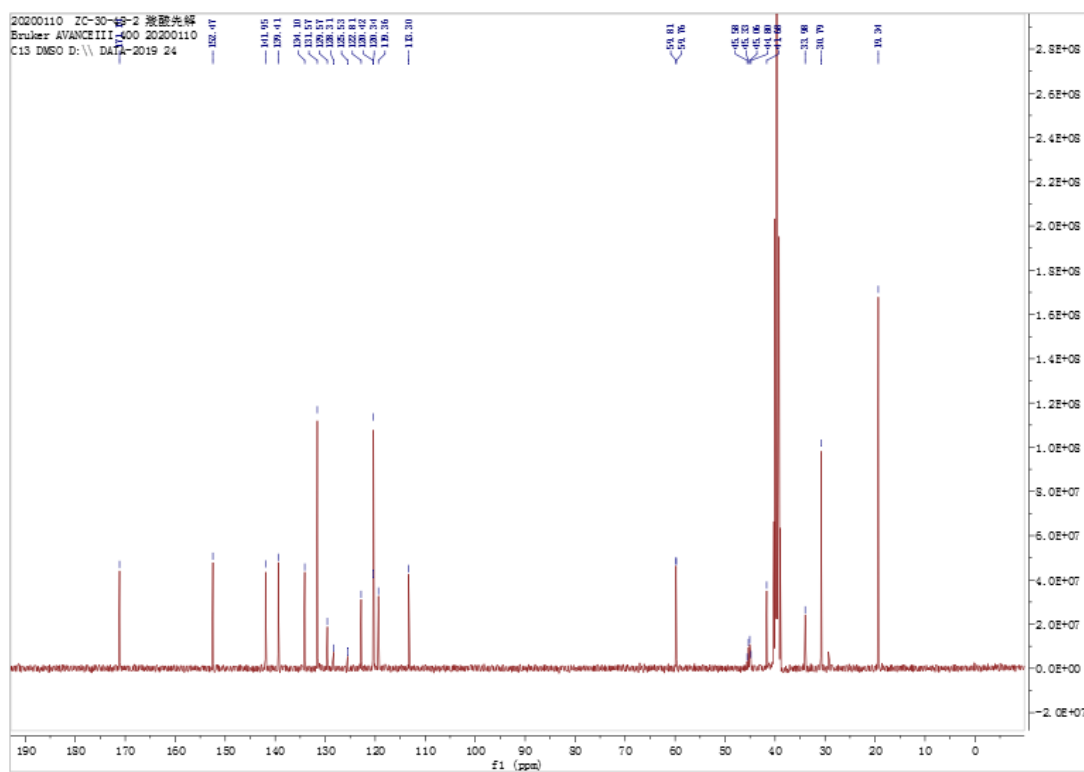


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
570.15735	570.15737	-0.03	10.5	C ₂₆ H ₃₂ O ₃ N ₃ Br F ₃

¹H NMR spectra of compound i19

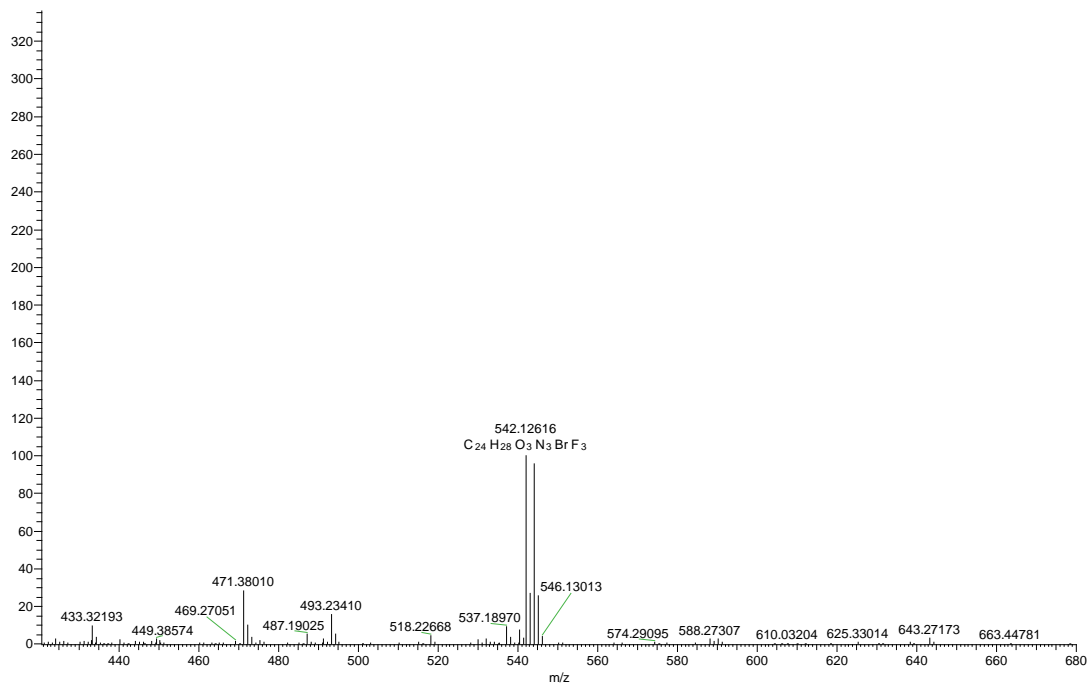


¹³C NMR spectra of compound i19



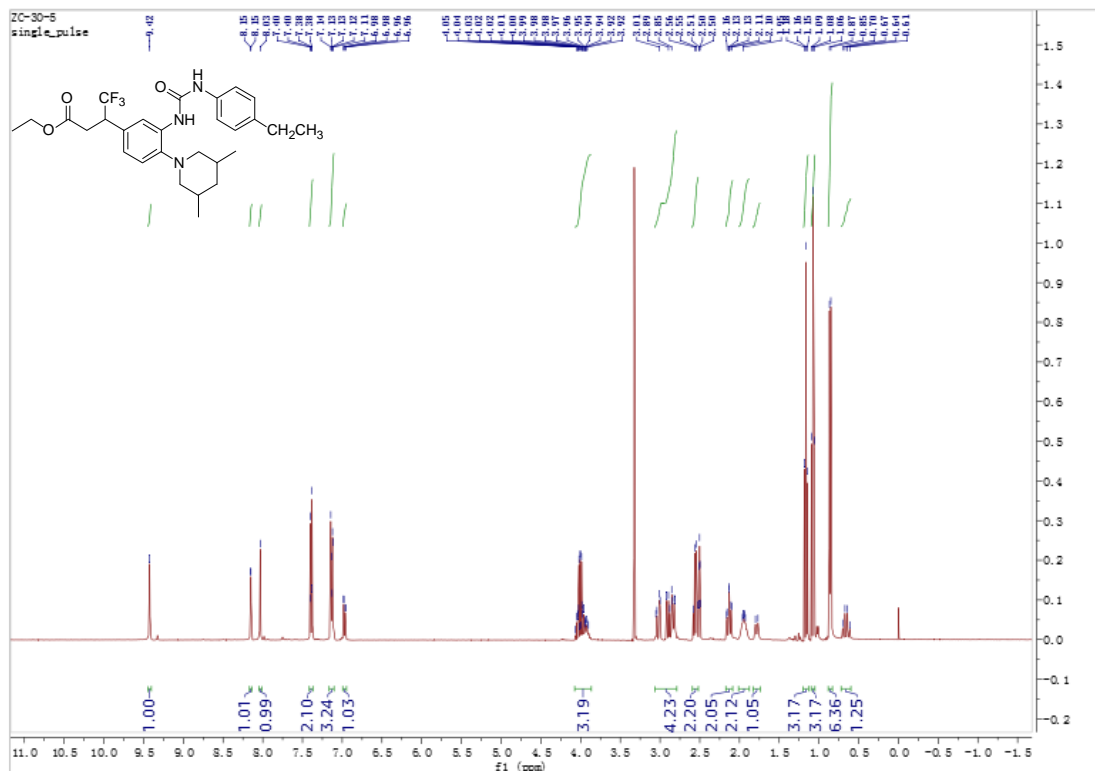
ESI-MS spectra of compound i19

ZC-30-48 #2546 RT: 5.74 AV: 1 NL: 1.97E7
T: FTMS + c ESI Full ms [100.0000-1000.0000]



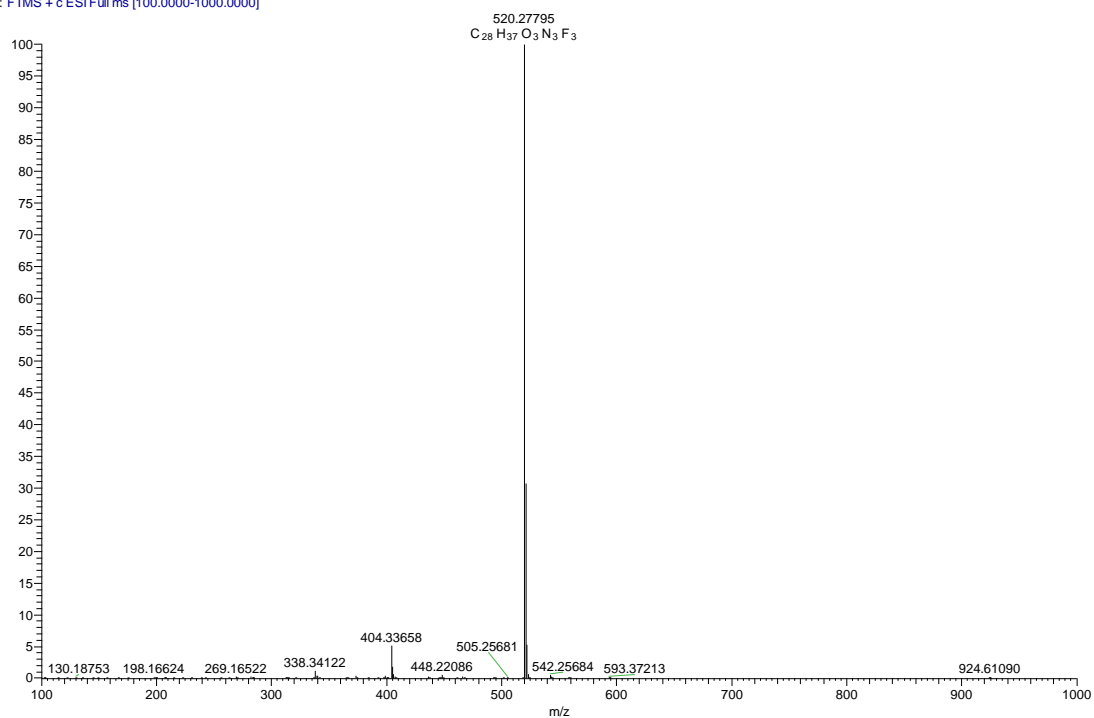
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
542.12616	542.12607	0.17	10.5	C ₂₄ H ₂₈ O ₃ N ₃ Br F ₃

¹H NMR spectra of compound g20



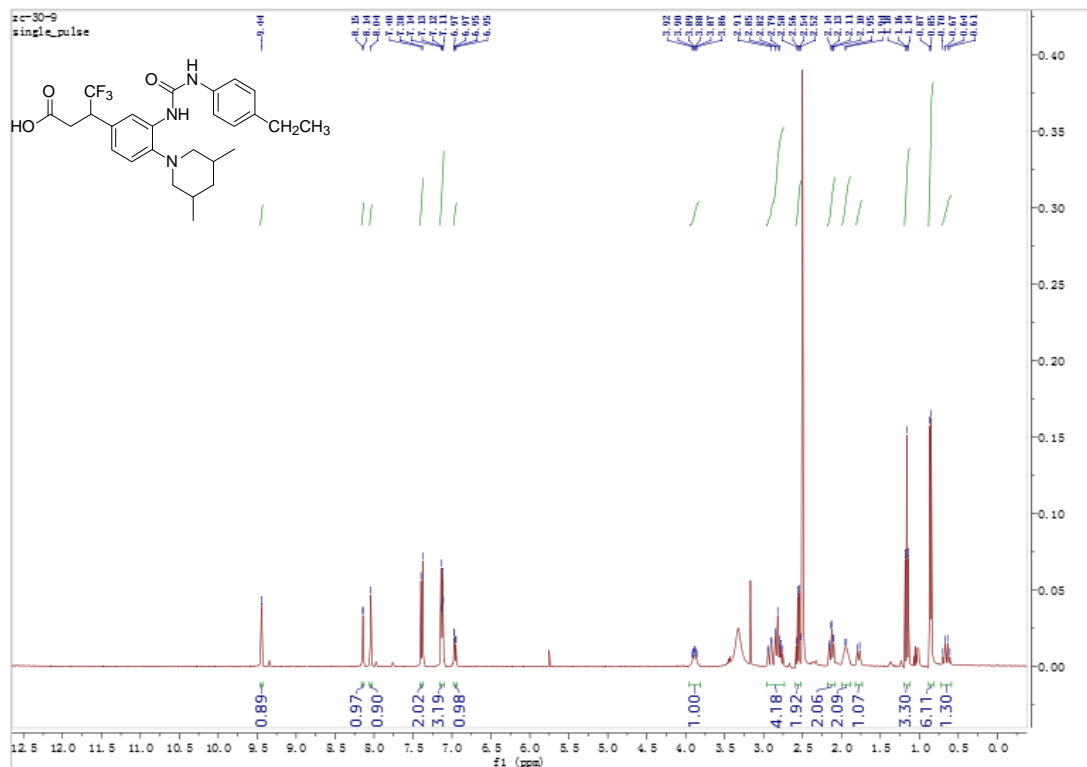
ESI-MS spectra of compound g20

ZC-30-5-2_191115140016 #2172 RT: 7.64 AV: 1 NL: 7.67E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

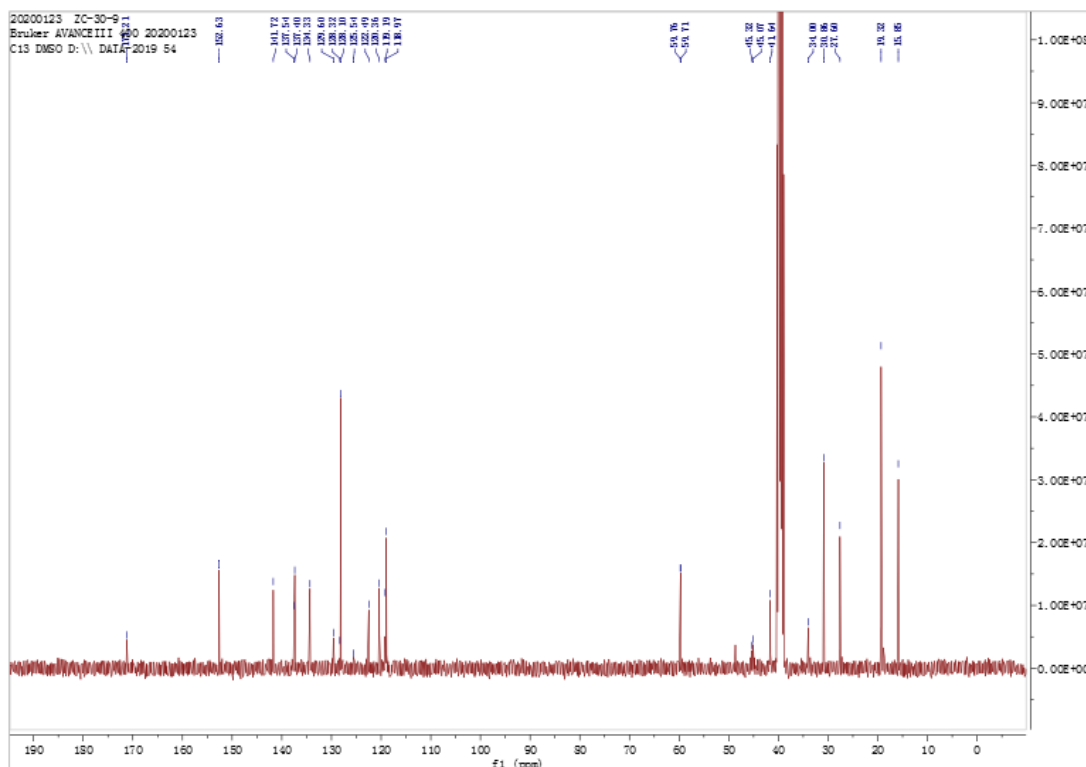


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
520.27795	520.27815	-0.39	10.5	C ₂₈ H ₃₇ O ₃ N ₃ F ₃

¹H NMR spectra of compound i20

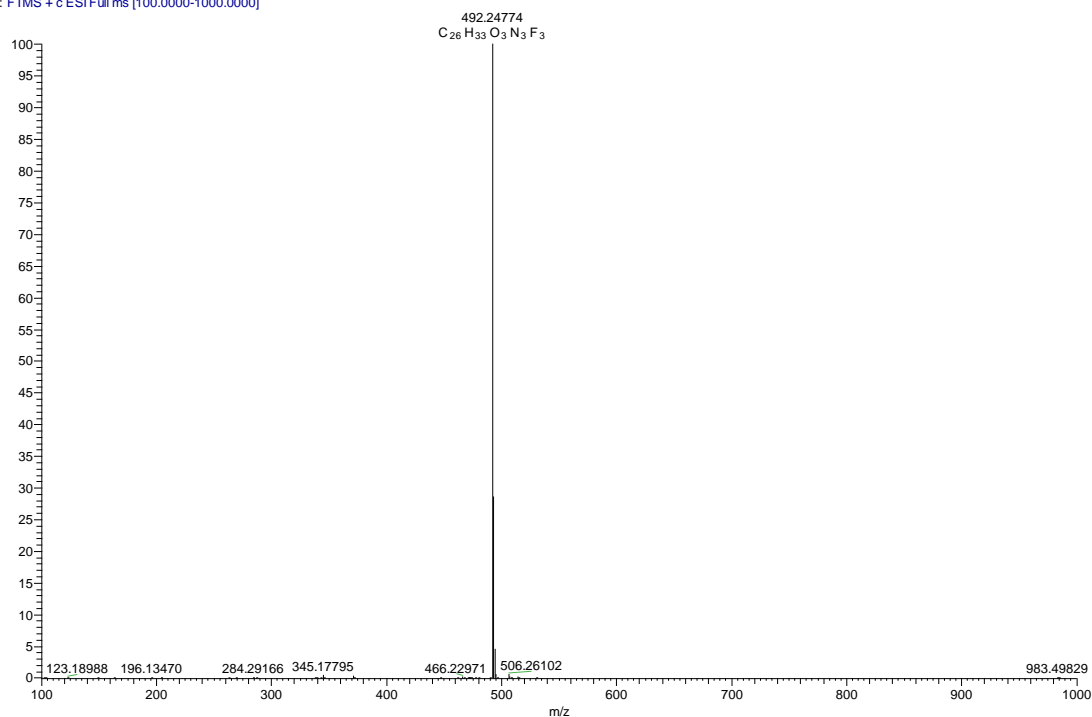


¹³C NMR spectra of compound i20



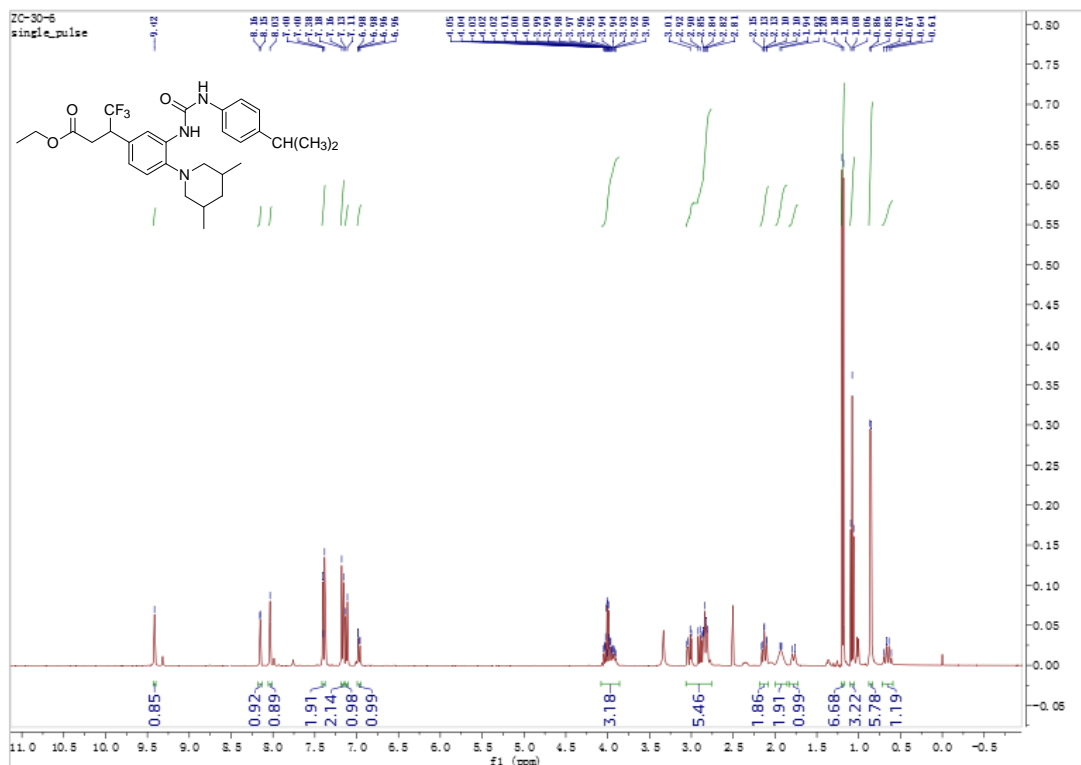
ESI-MS spectra of compound i20

ZC-30-9 #2263 RT: 7.72 AV: 1 NL: 9.33E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]



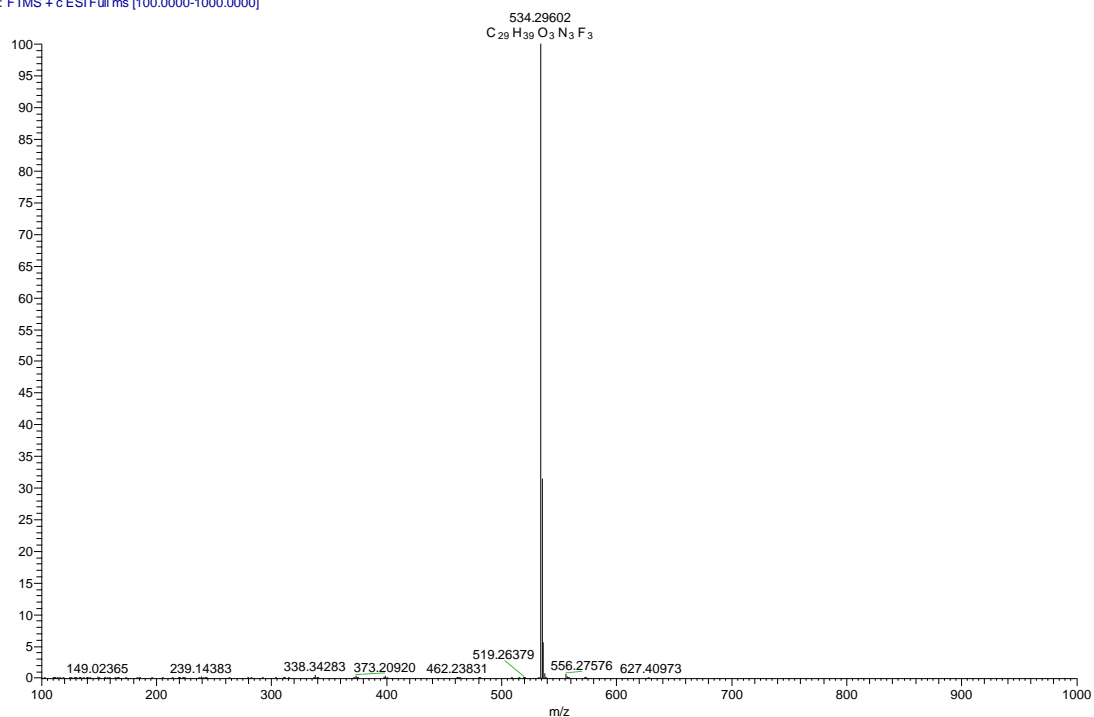
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
492.24774	492.24685	1.80	10.5	C ₂₆ H ₃₃ O ₃ N ₃ F ₃

¹H NMR spectra of compound g21



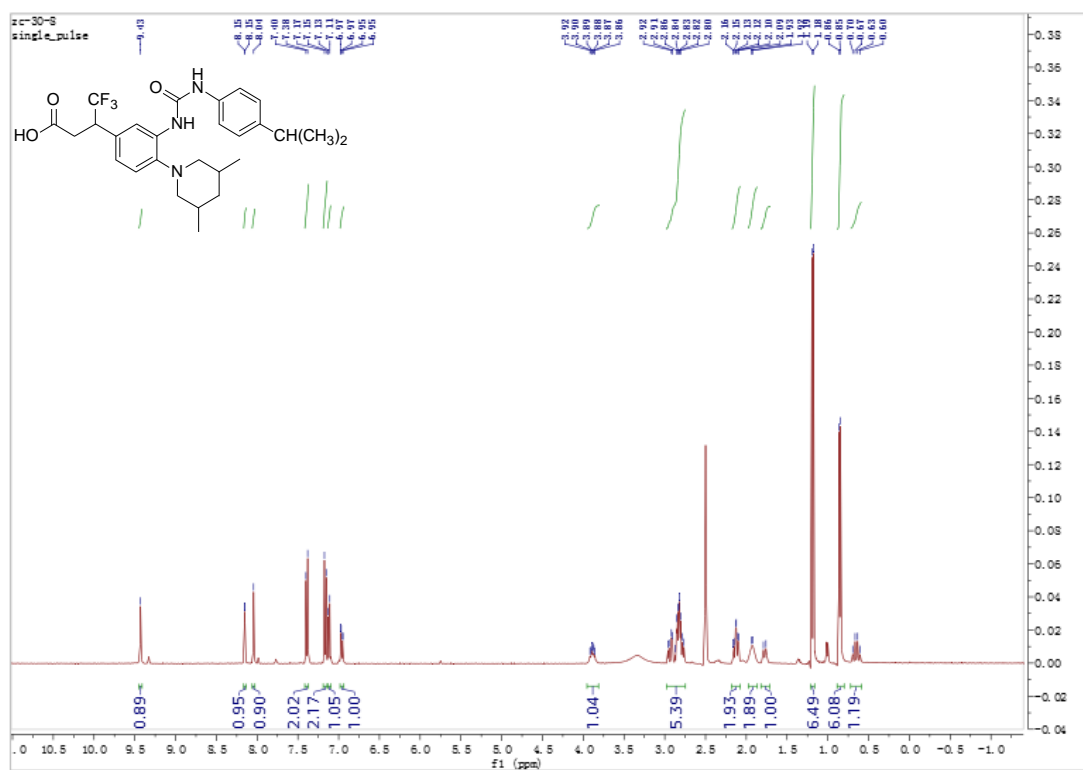
ESI-MS spectra of compound g21

ZC-30-6-4 #2405 RT: 7.94 AV: 1 NL: 9.14E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

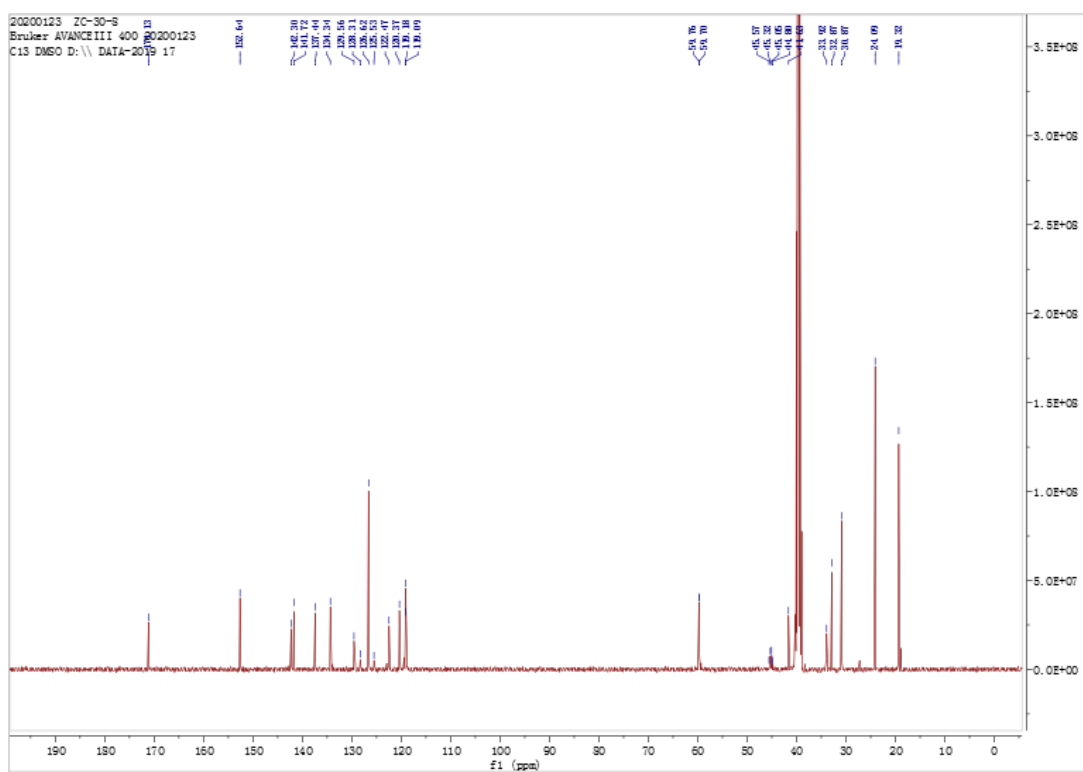


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
534.29602	534.29380	4.15	10.5	C29 H39 O3 N3 F3

¹H NMR spectra of compound i21

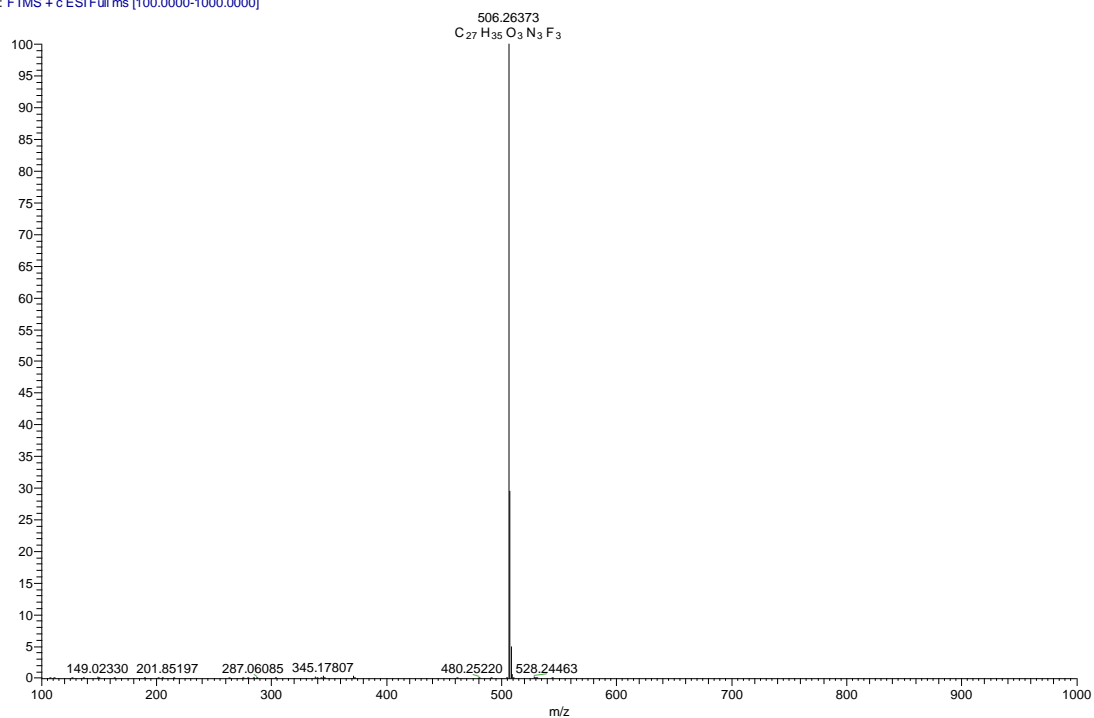


¹³C NMR spectra of compound i21



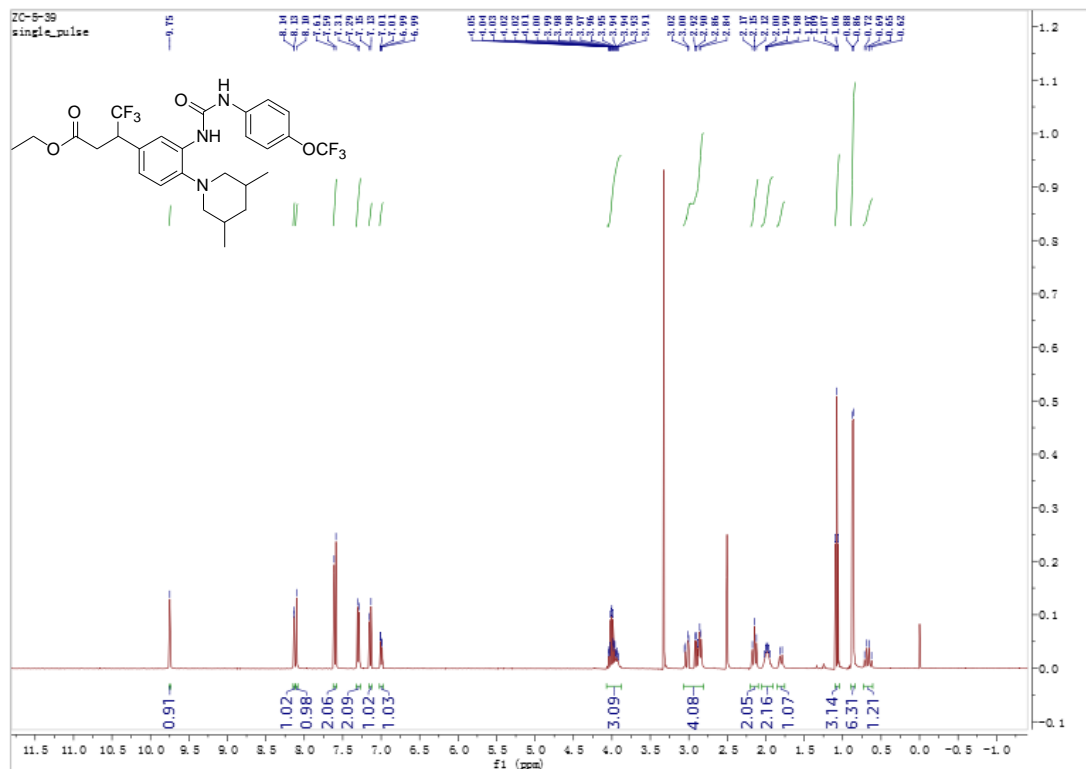
ESI-MS spectra of compound i21

ZC-30-8 #2348 RT: 8.00 AV: 1 NL: 1.56E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



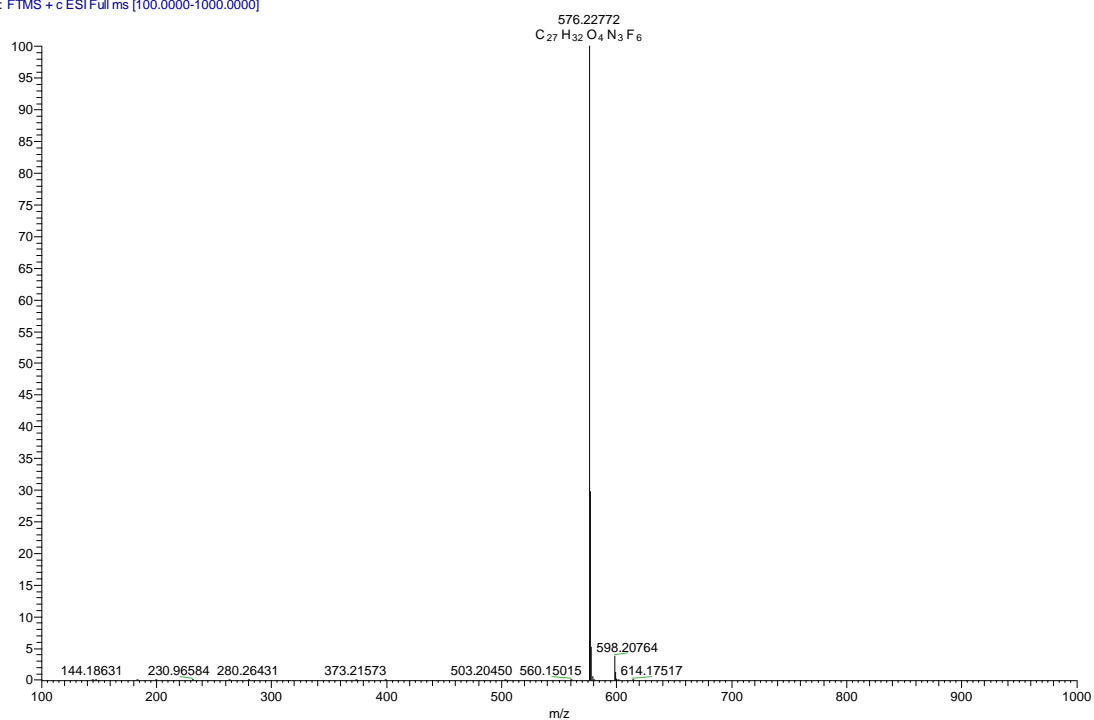
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
506.26373	506.26250	2.42	10.5	C27 H35 O3 N3 F3

¹H NMR spectra of compound g22



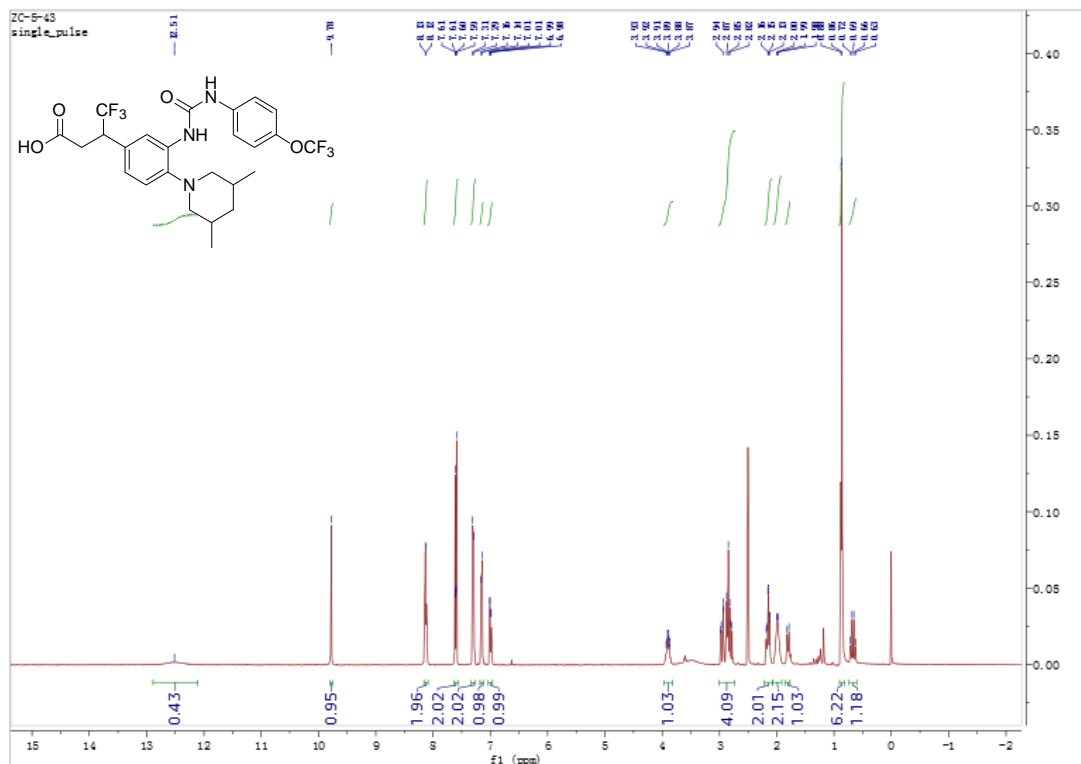
ESI-MS spectra of compound g22

ZC-5-39_200115212721 #1667 RT: 6.12 AV: 1 NL: 3.98E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

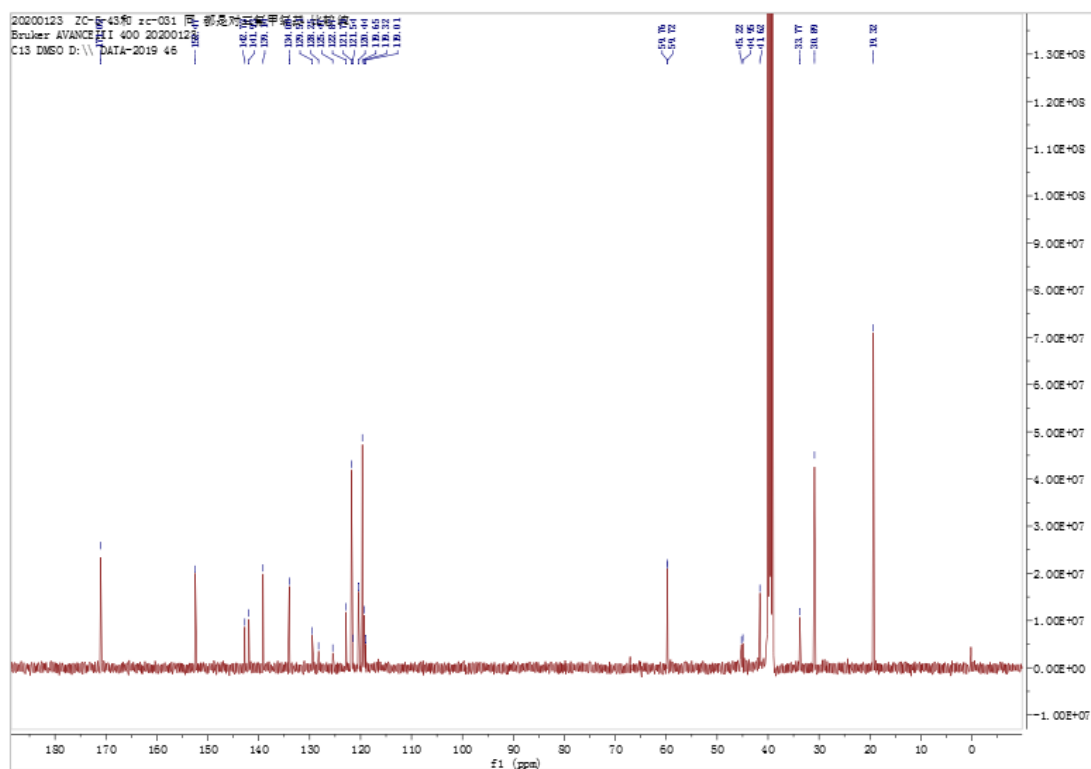


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
576.22772	576.22915	-2.49	10.5	C ₂₇ H ₃₂ O ₄ N ₃ F ₆

¹H NMR spectra of compound i22

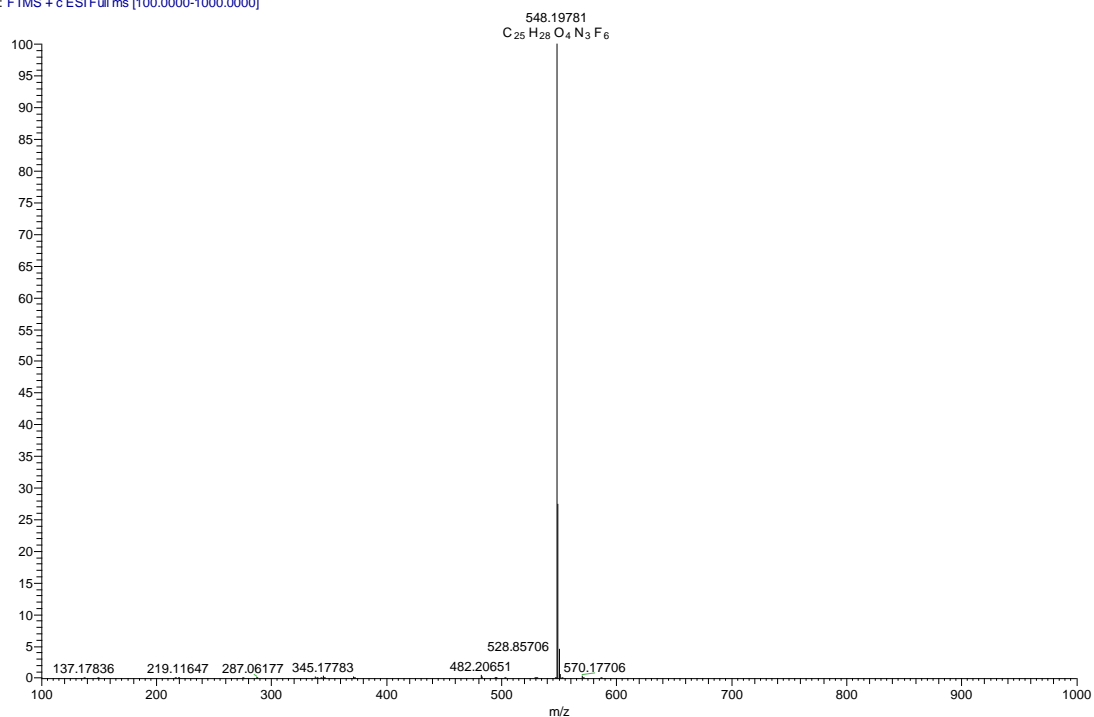


¹³C NMR spectra of compound i22



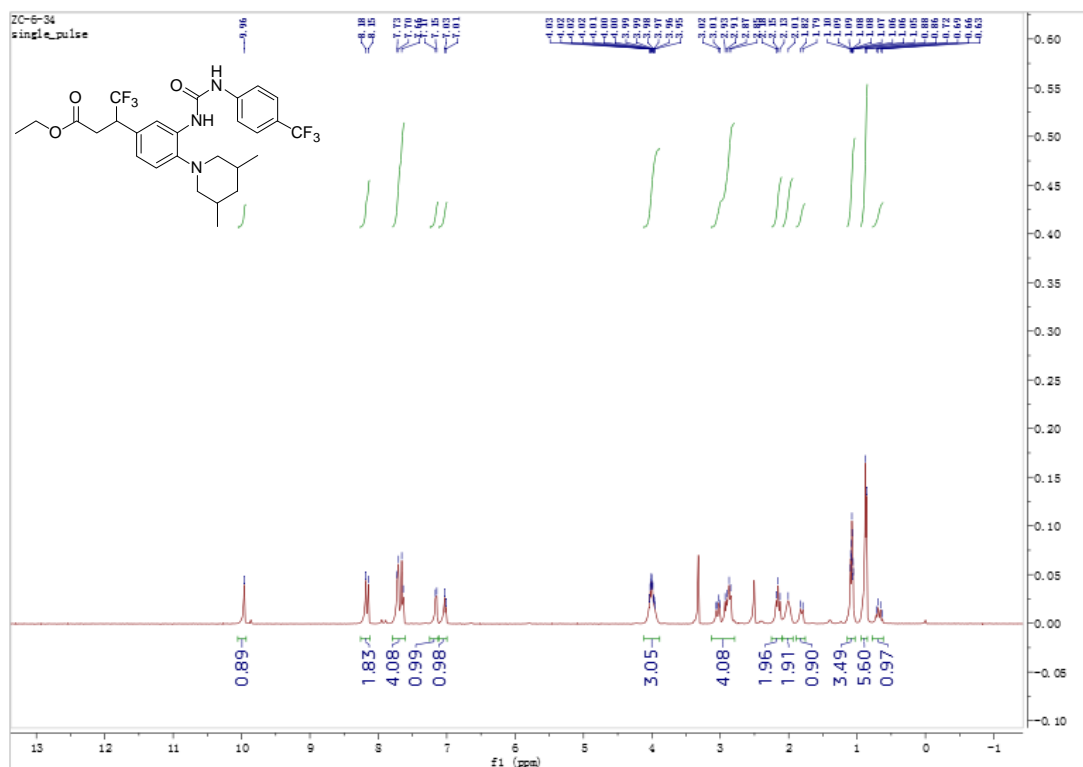
ESI-MS spectra of compound i22

ZC-031 #2127 RT: 6.98 AV: 1 NL: 1.11E9
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



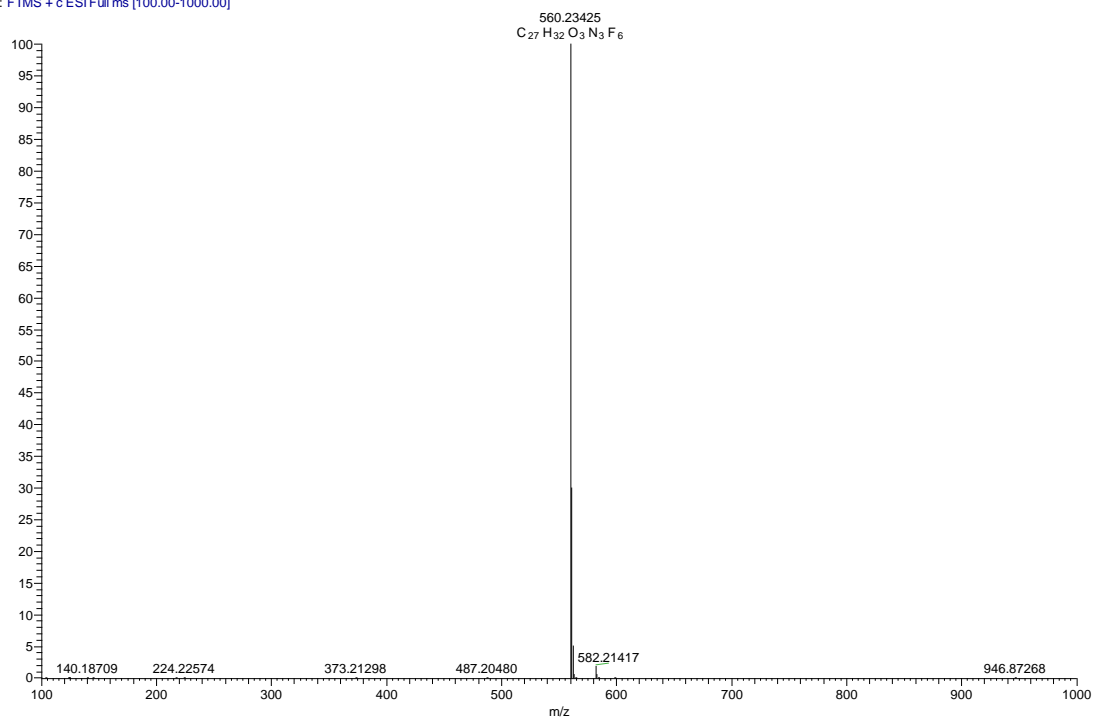
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
548.19781	548.19785	-0.08	10.5	C25 H28 O4 N3 F6

¹H NMR spectra of compound g23



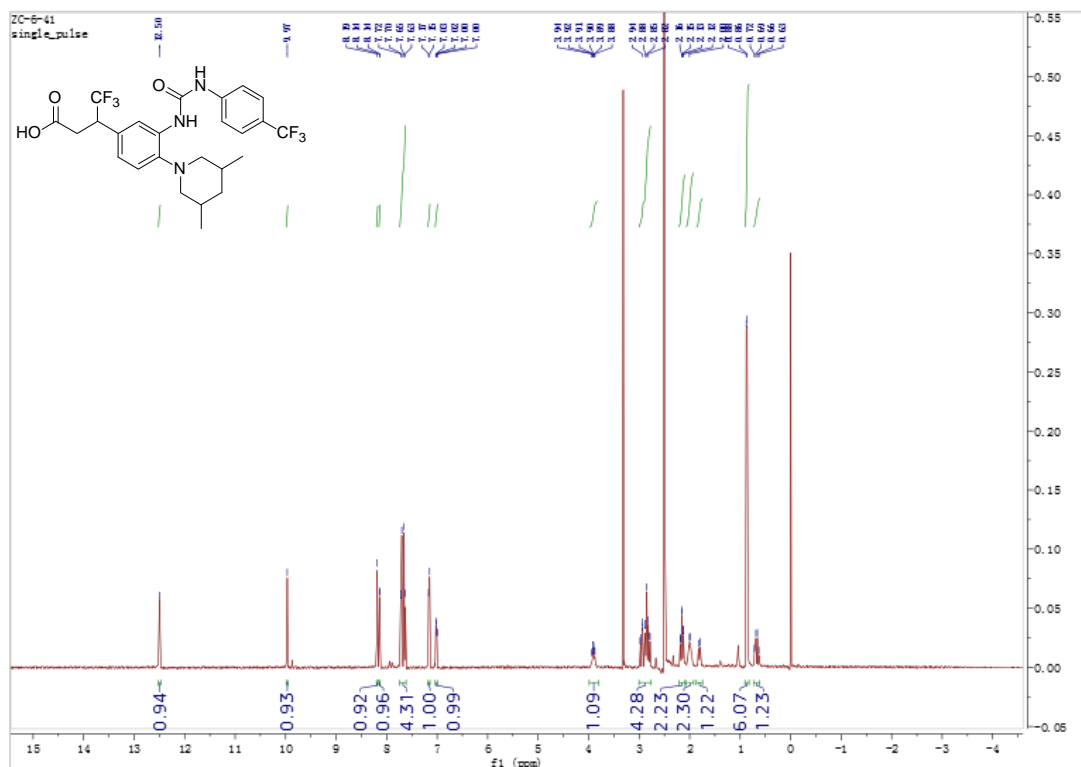
ESI-MS spectra of compound g23

ZC-06-34 #1905 RT: 6.23 AV: 1 NL: 6.61E8
T: FTMS + c ESI Full ms [100.00-1000.00]



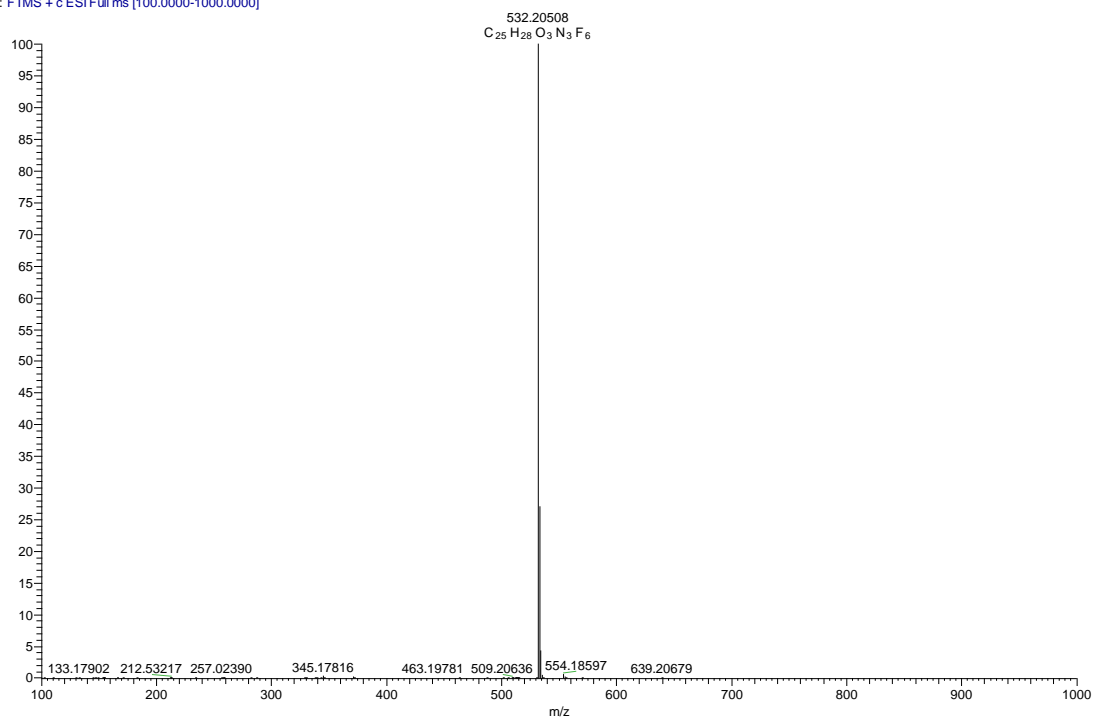
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
560.23425	560.23424	0.02	10.5	C27 H32 O3 N3 F6

¹H NMR spectra of compound i23



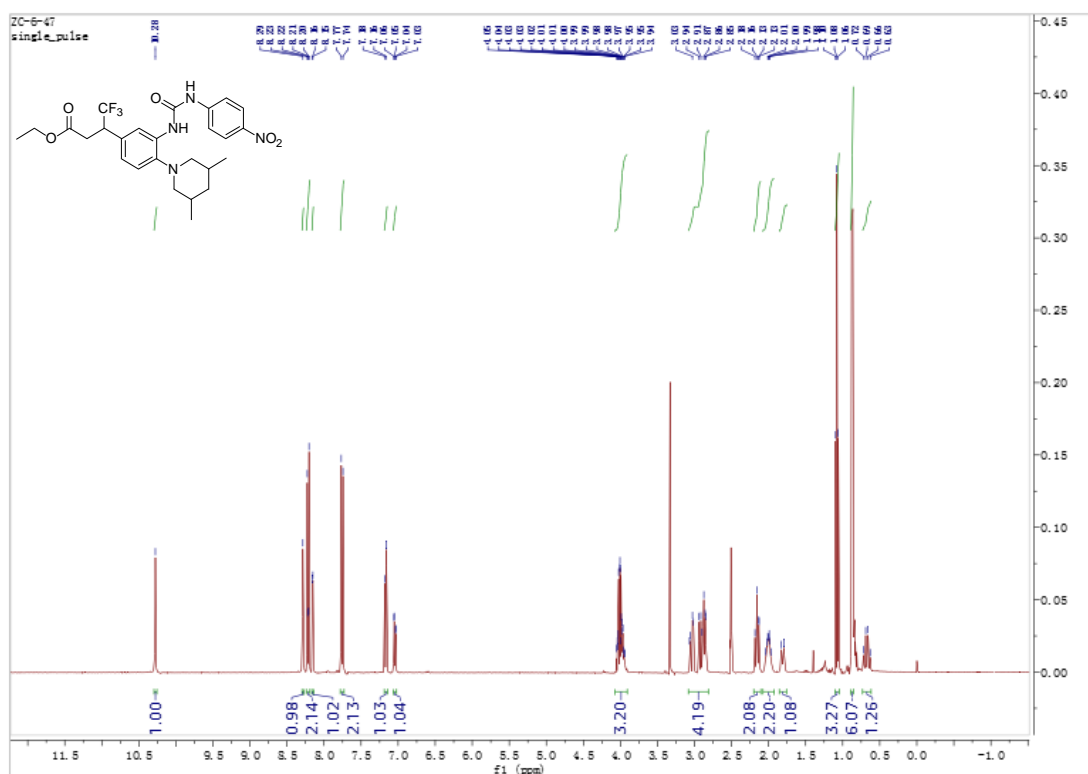
ESI-MS spectra of compound i23

ZC-6-41 #1952 RT: 7.01 AV: 1 NL: 9.58E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]



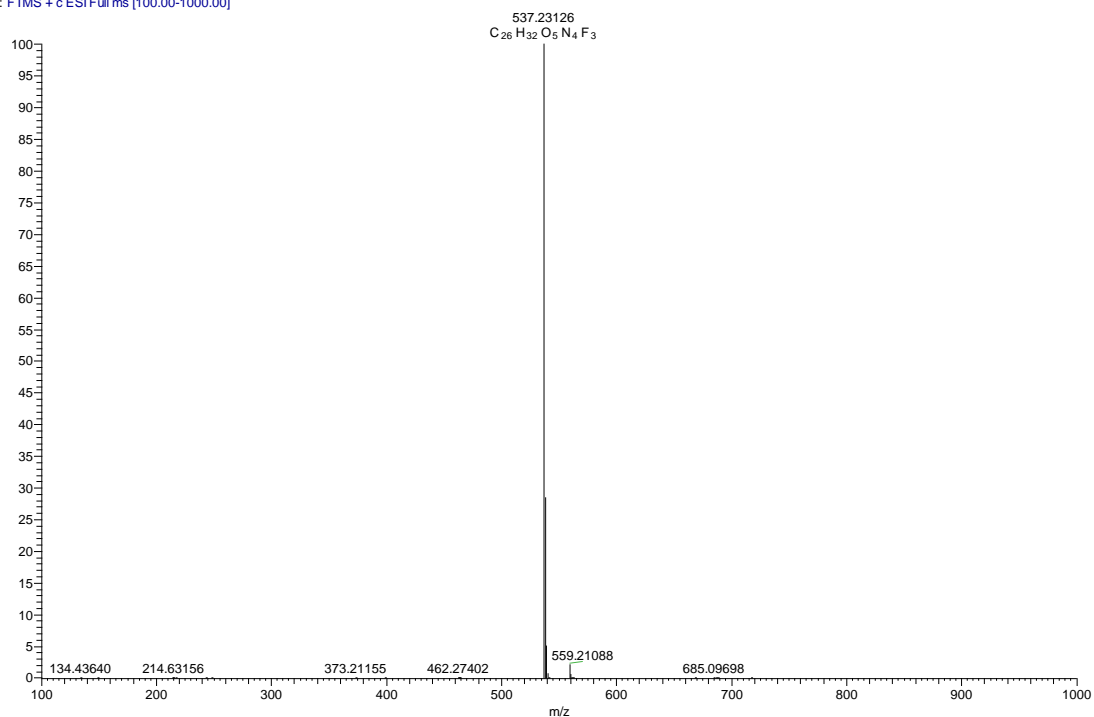
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
532.20508	532.20294	4.03	10.5	C25 H28 O3 N3 F6

¹H NMR spectra of compound g24



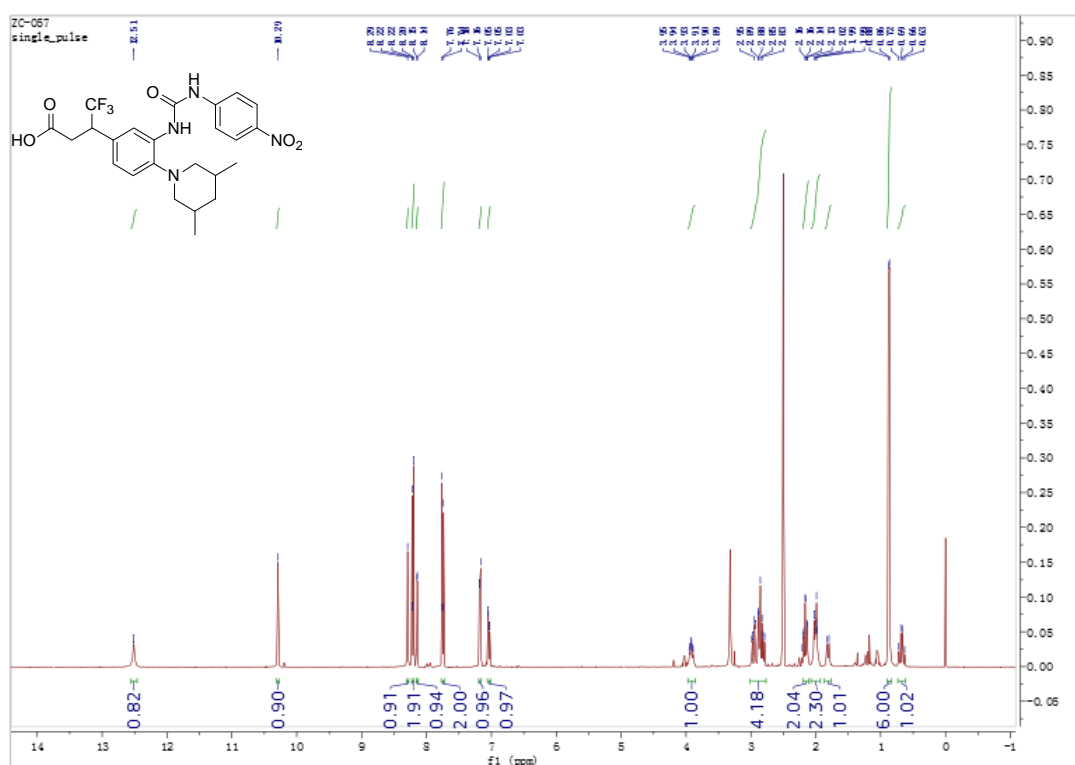
ESI-MS spectra of compound g24

ZC-6-47 #2521 RT: 5.87 AV: 1 NL: 6.15E9
T: FTMS + c ESI Full ms [100.00-1000.00]

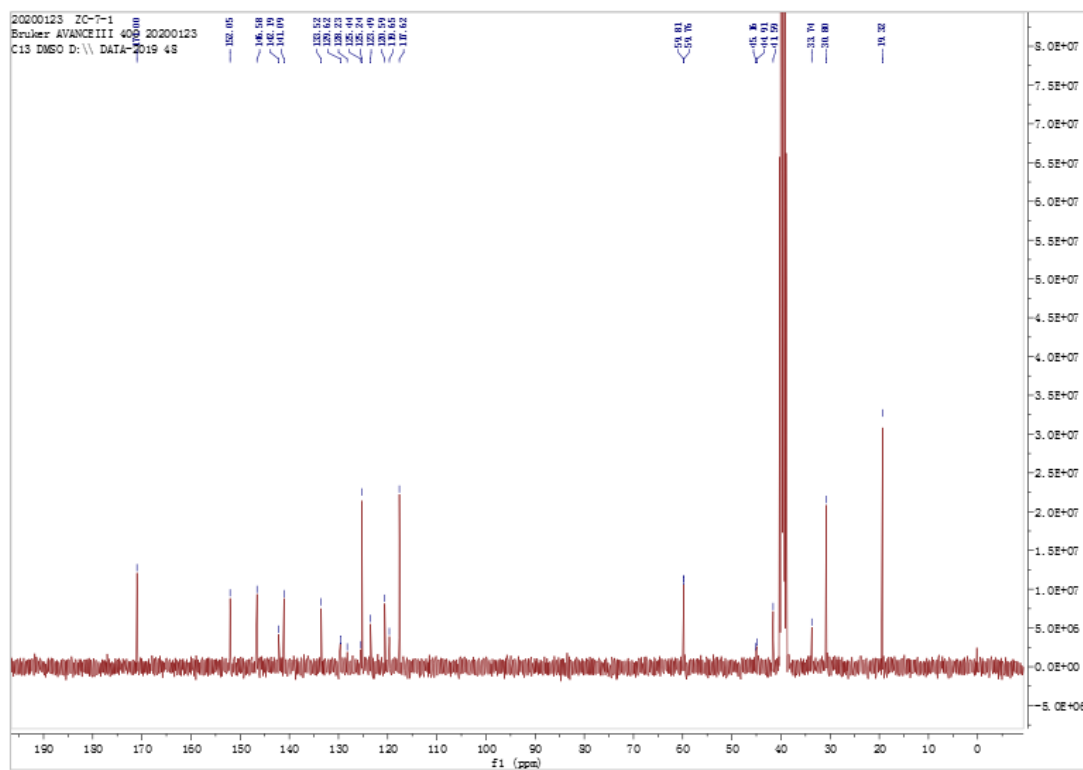


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
537.23126	537.23193	-1.25	11.5	C ₂₆ H ₃₂ O ₅ N ₄ F ₃

¹H NMR spectra of compound i24

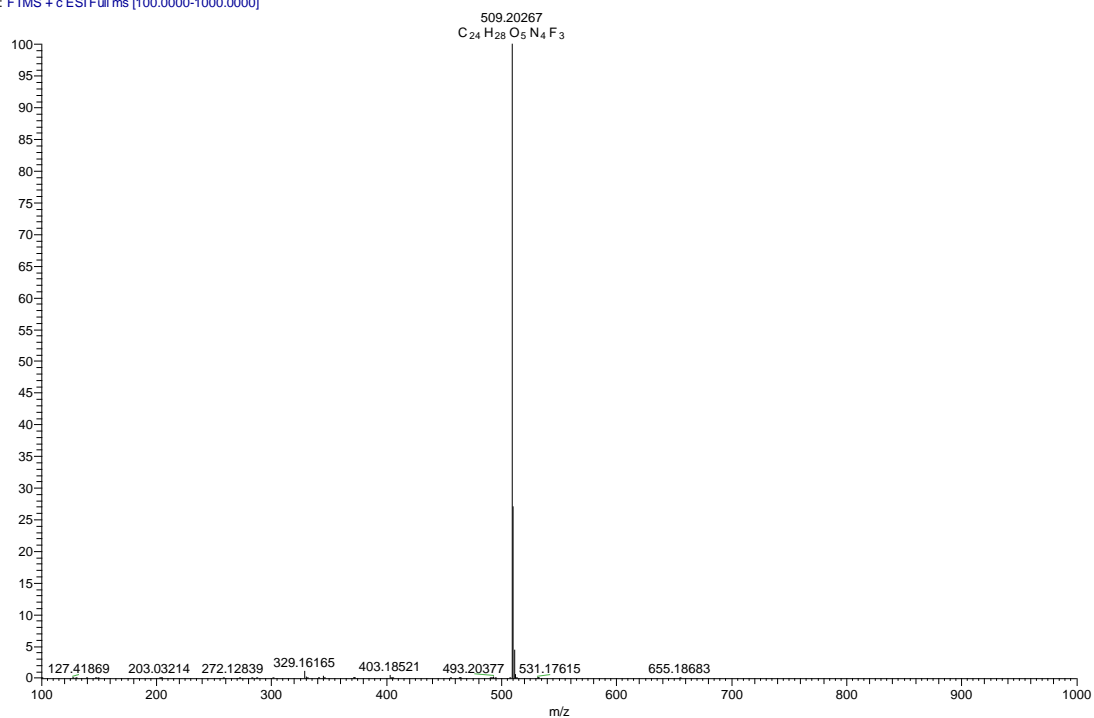


¹³C NMR spectra of compound i24



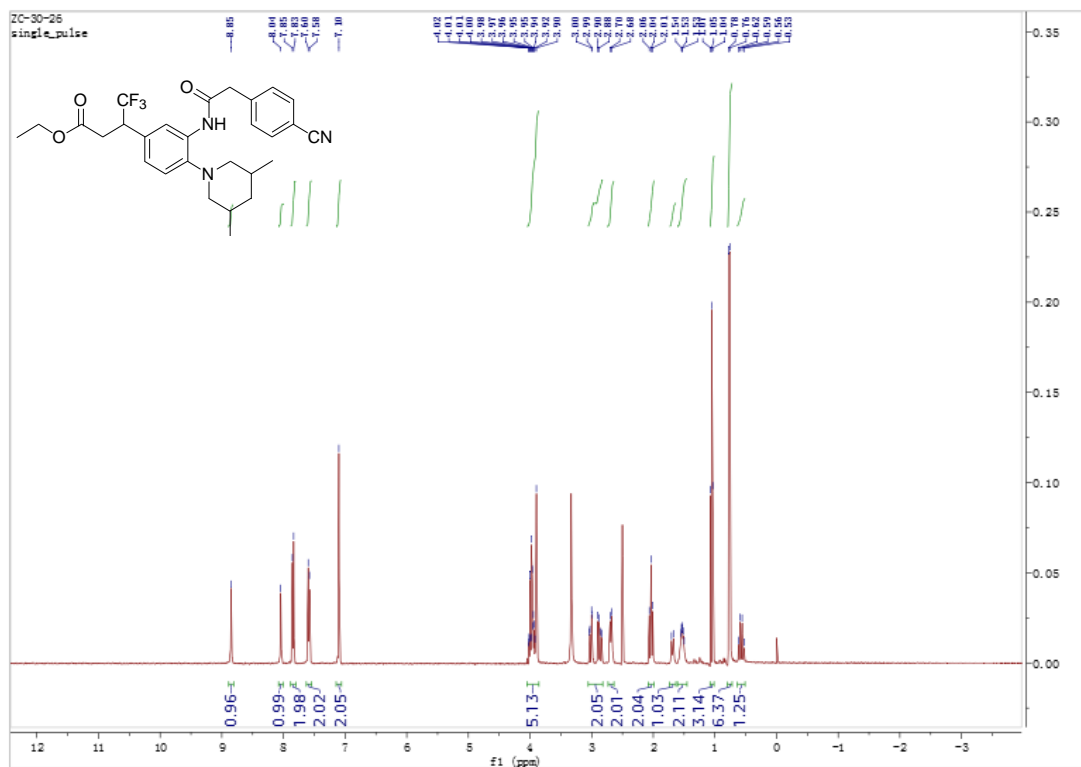
ESI-MS spectra of compound i24

ZC-057 #1866 RT: 6.72 AV: 1 NL: 1.09E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



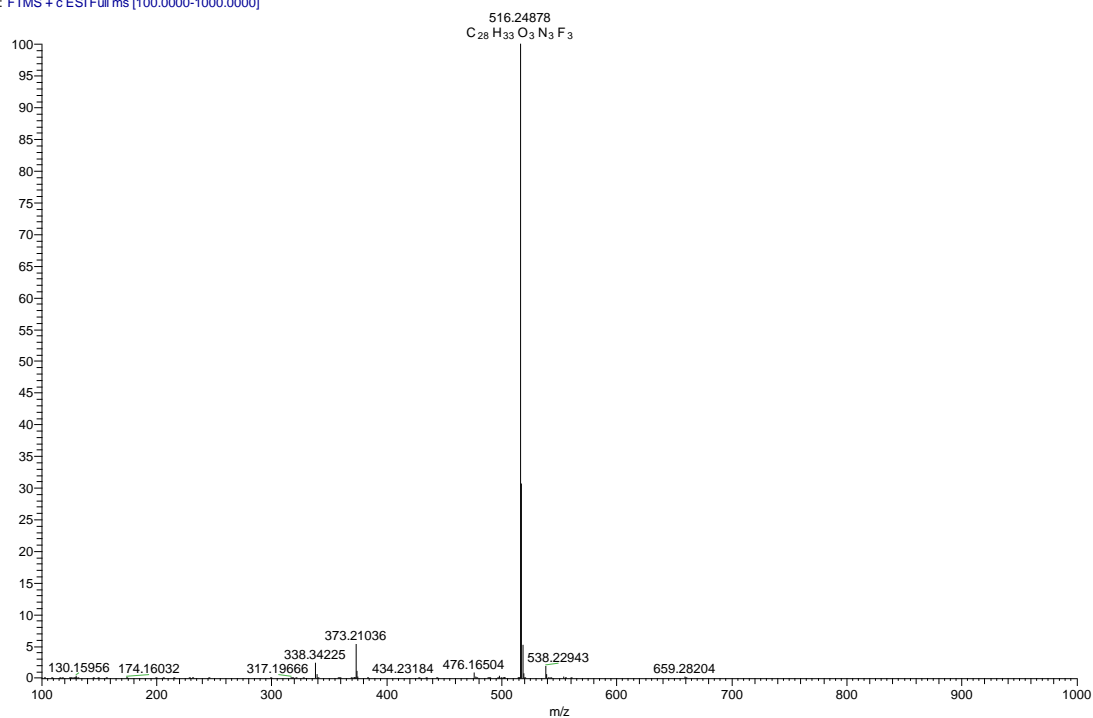
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
509.20267	509.20063	4.00	11.5	C24 H28 O5 N4 F3

¹H NMR spectra of compound h1



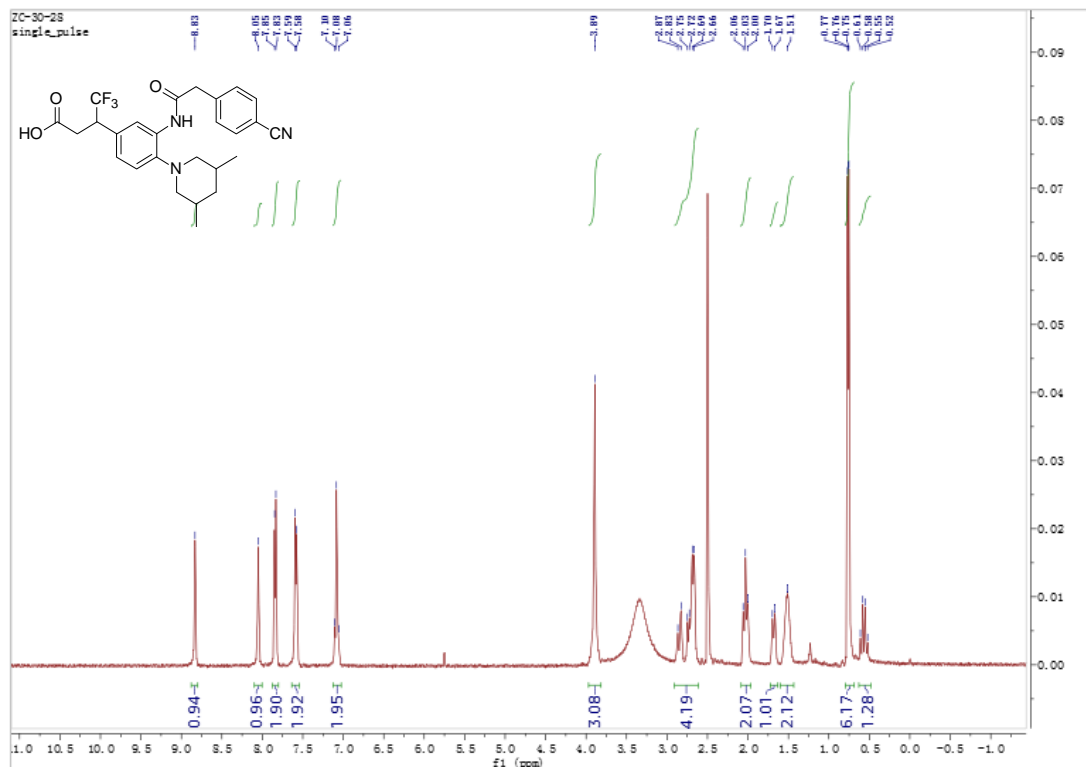
ESI-MS spectra of compound h1

ZC-30-26 #2913 RT: 8.00 AV: 1 NL: 7.09E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]

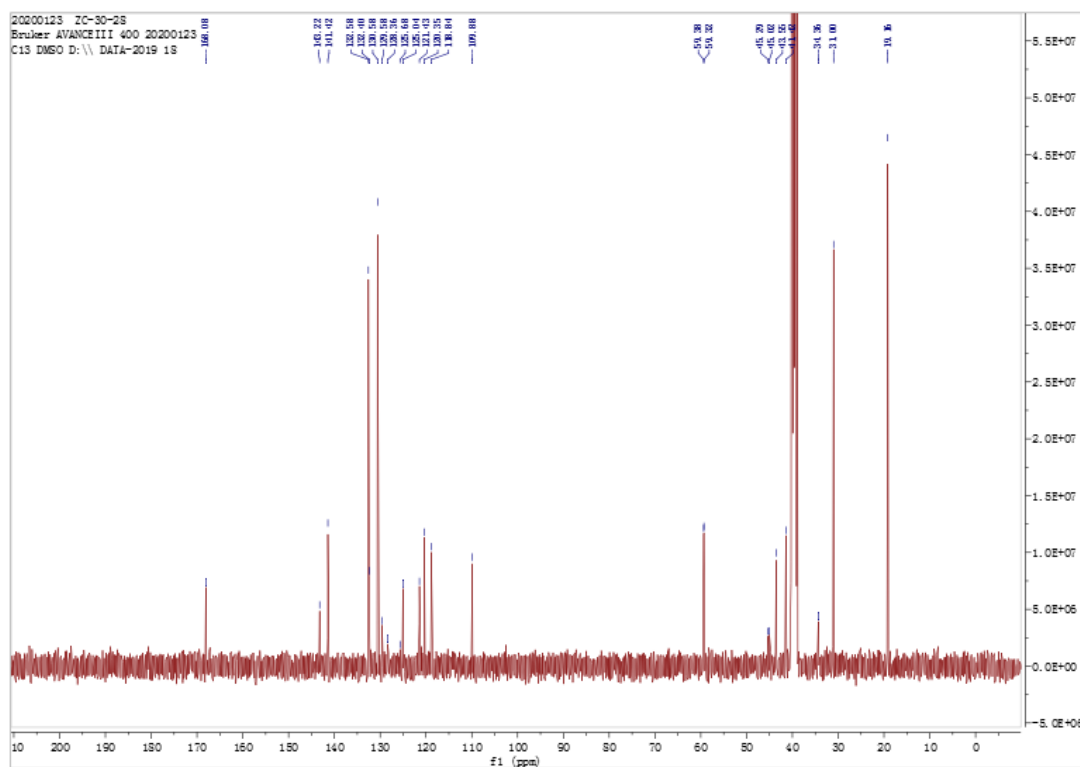


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
516.24878	516.24685	3.73	12.5	C28 H33 O3 N3 F3

¹H NMR spectra of compound j1

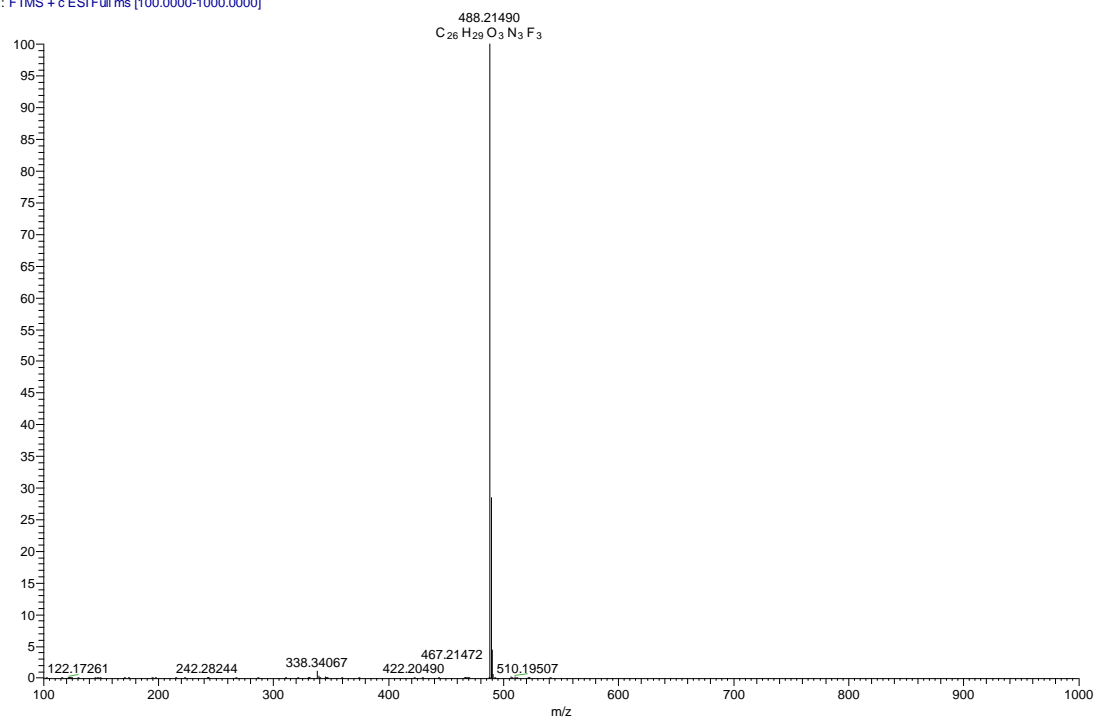


¹³C NMR spectra of compound j1



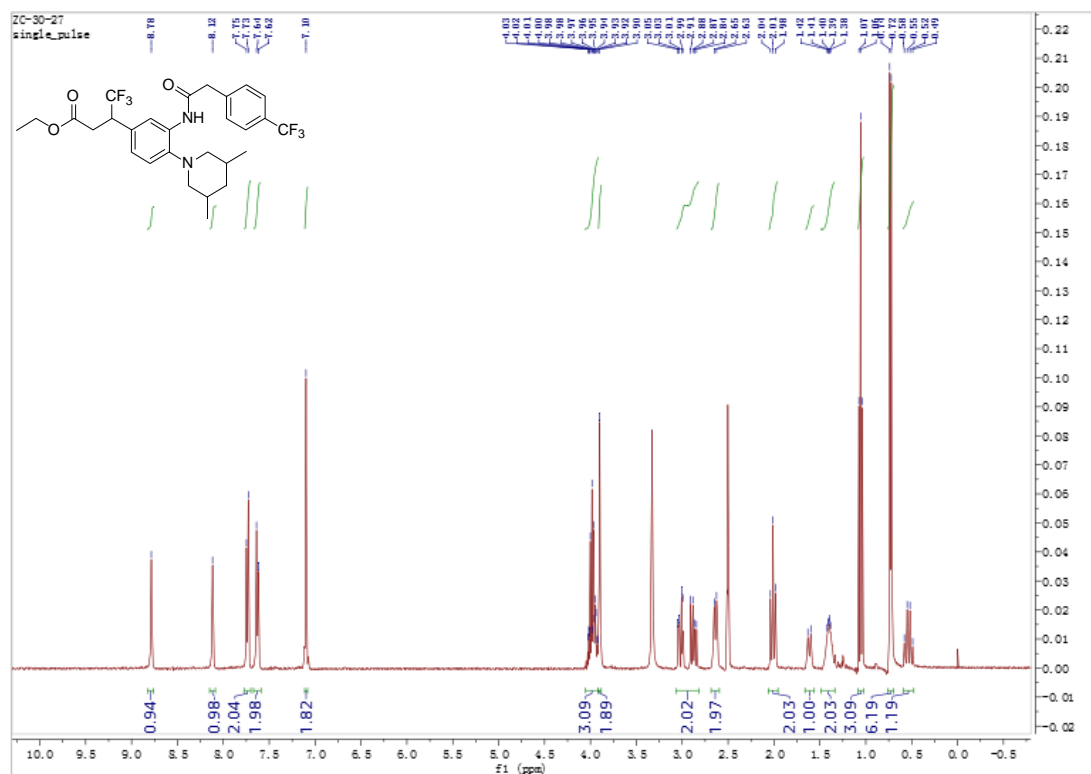
ESI-MS spectra of compound j1

ZC-30-28-2 #2507 RT: 7.35 AV: 1 NL: 2.79E9
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



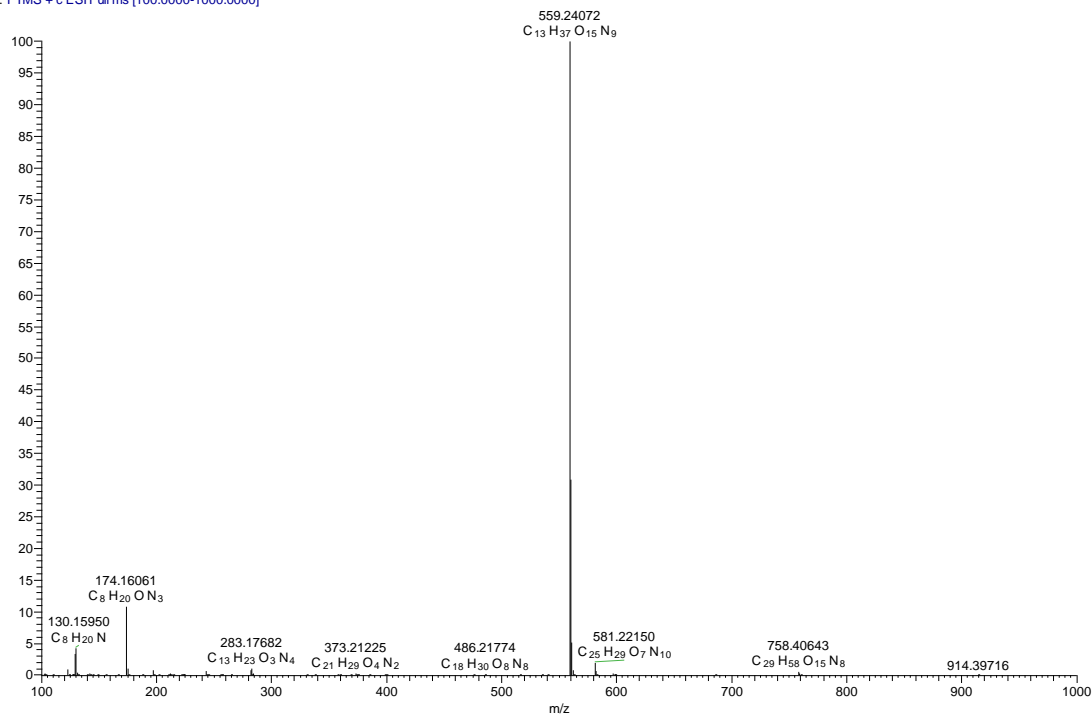
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
488.21490	488.21555	-1.34	12.5	C26 H29 O3 N3 F3

¹H NMR spectra of compound h2



ESI-MS spectra of compound h2

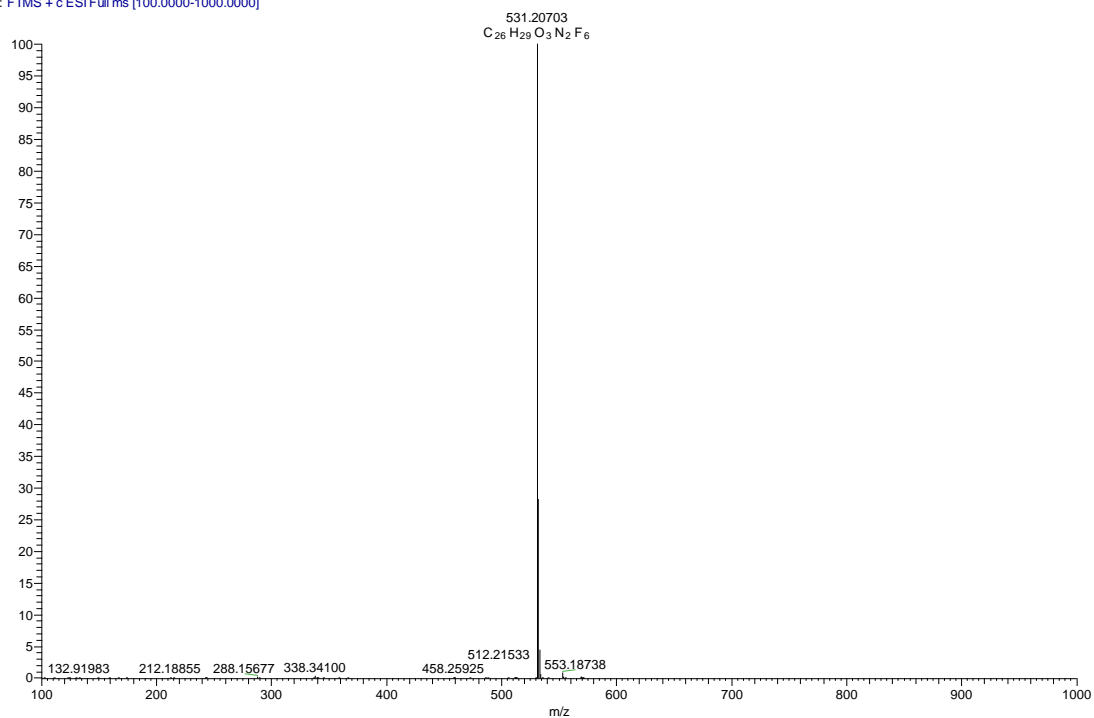
ZC-30-27-2 #3614 RT: 7.96 AV: 1 NL: 8.46E8
T: FTMS + c ESI Full ms [100.0000-1000.0000]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
559.24072	559.23899	3.10	10.5	C28 H33 O3 N2 F6

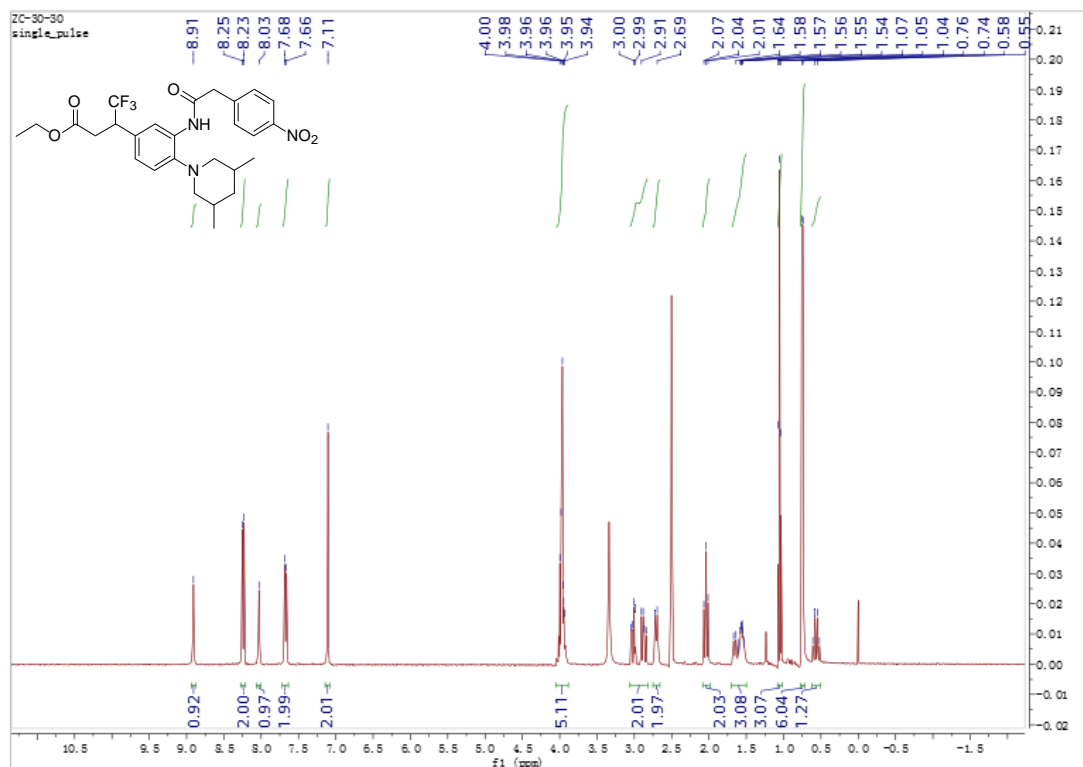
ESI-MS spectra of compound j2

ZC-30-29-2 #2580 RT: 7.89 AV: 1 NL: 1.98E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



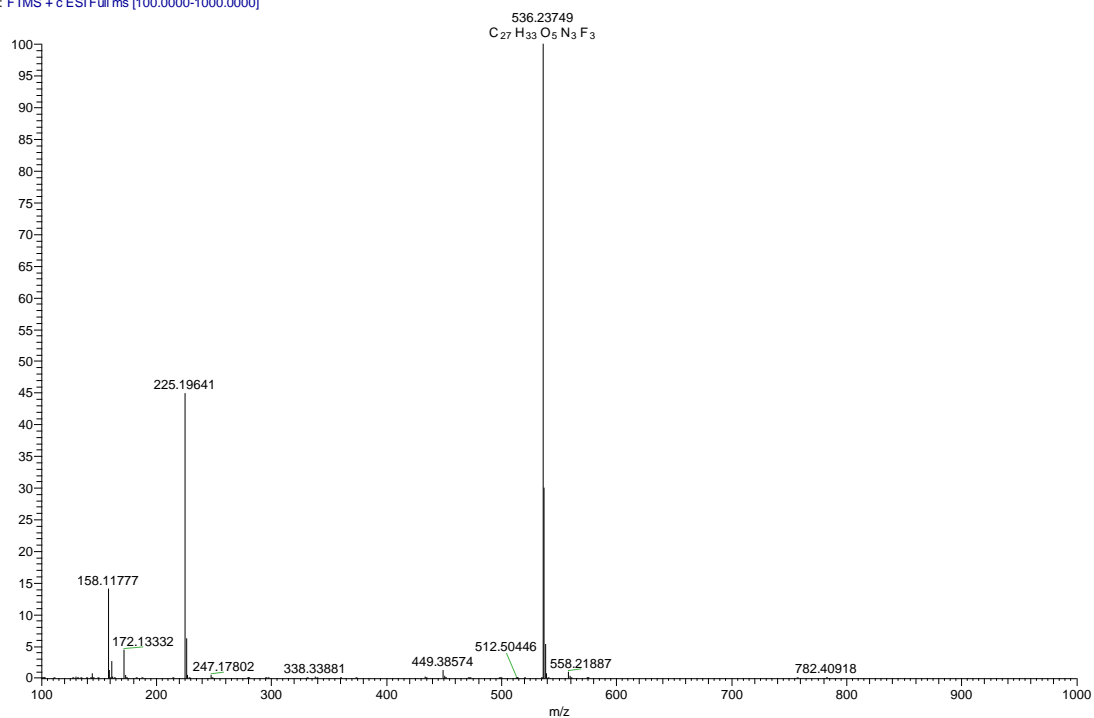
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
531.20703	531.20769	-1.24	10.5	C26 H29 O3 N2 F6

¹H NMR spectra of compound h3



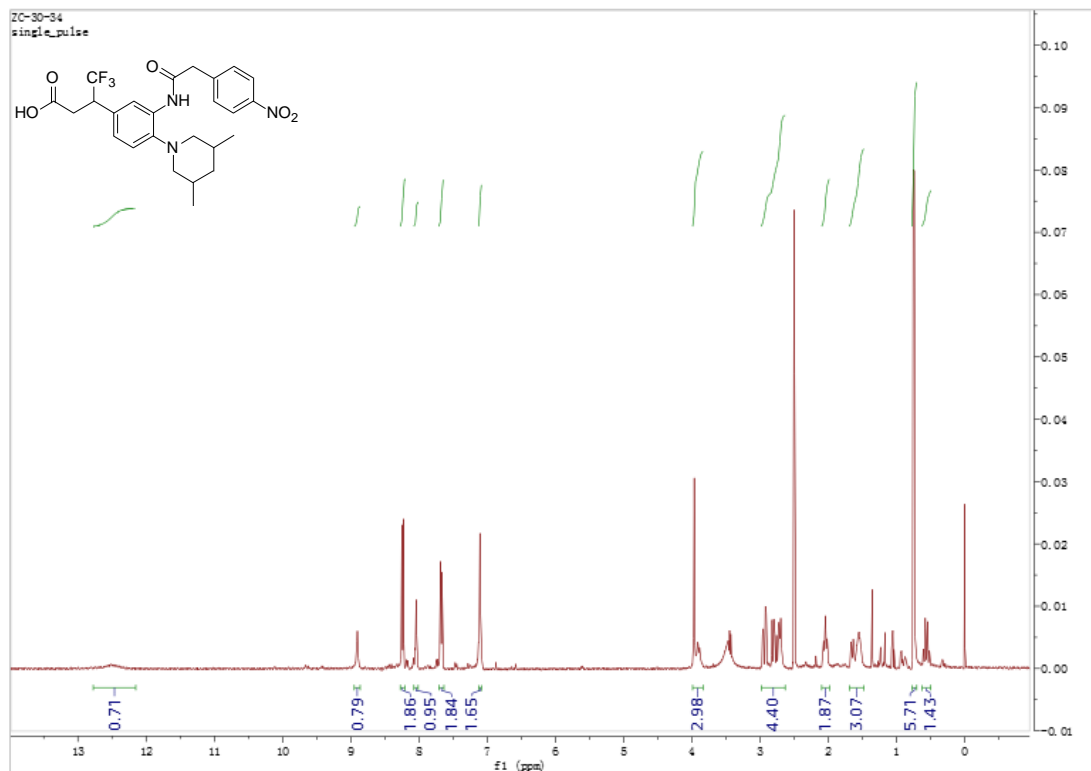
ESI-MS spectra of compound h3

ZC-30-30-3 #2137 RT: 6.96 AV: 1 NL: 1.21E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]

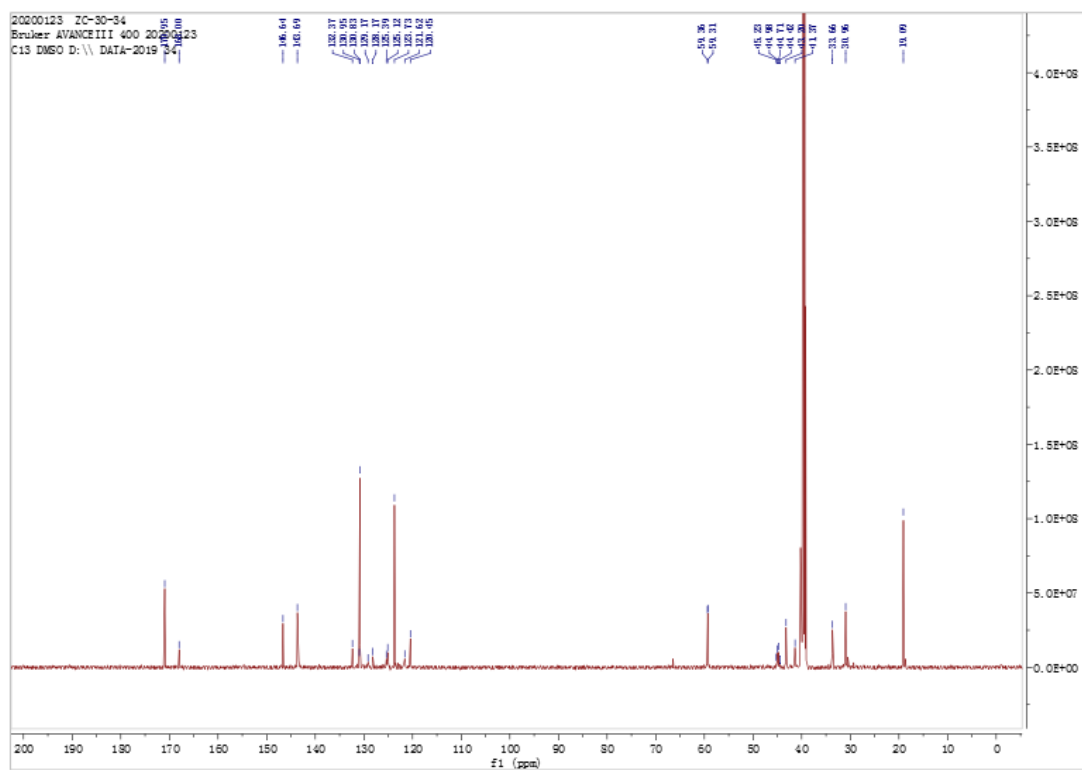


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
536.23749	536.23668	1.51	11.5	C27 H33 O5 N3 F3

¹H NMR spectra of compound j3

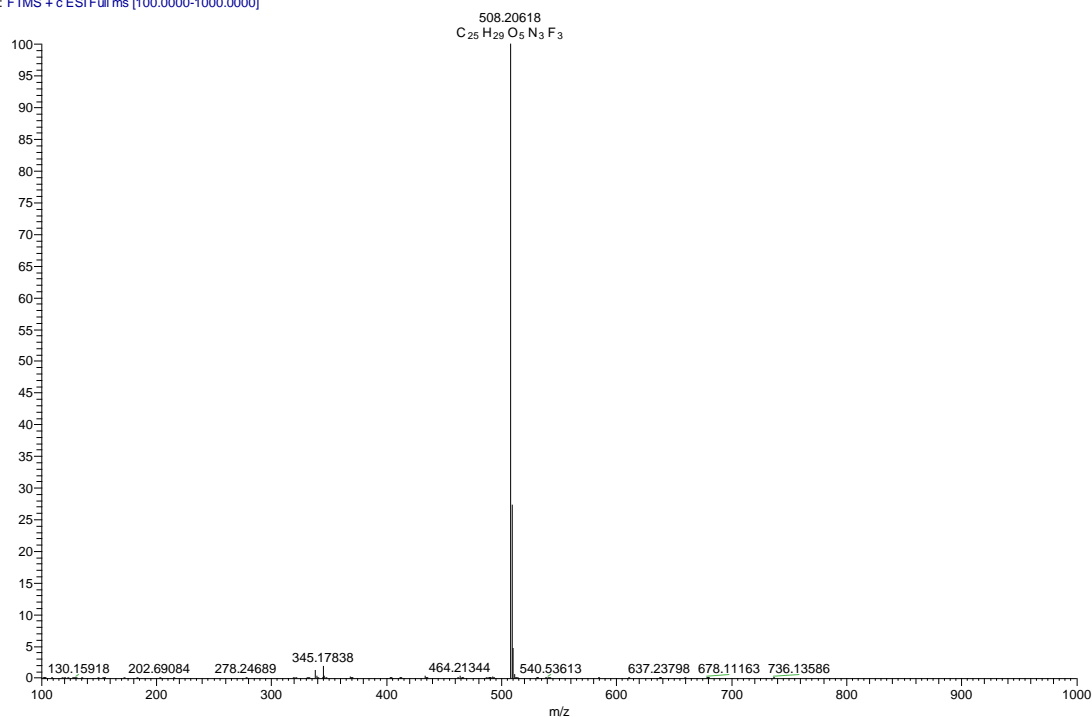


¹³C NMR spectra of compound j3



ESI-MS spectra of compound j3

ZC-30-34_191204200001 #2057 RT: 7.32 AV: 1 NL: 6.56E8
 T: FTMS + c ESI Full ms [100.0000-1000.0000]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
508.20618	508.20538	1.57	11.5	C25 H29 O5 N3 F3