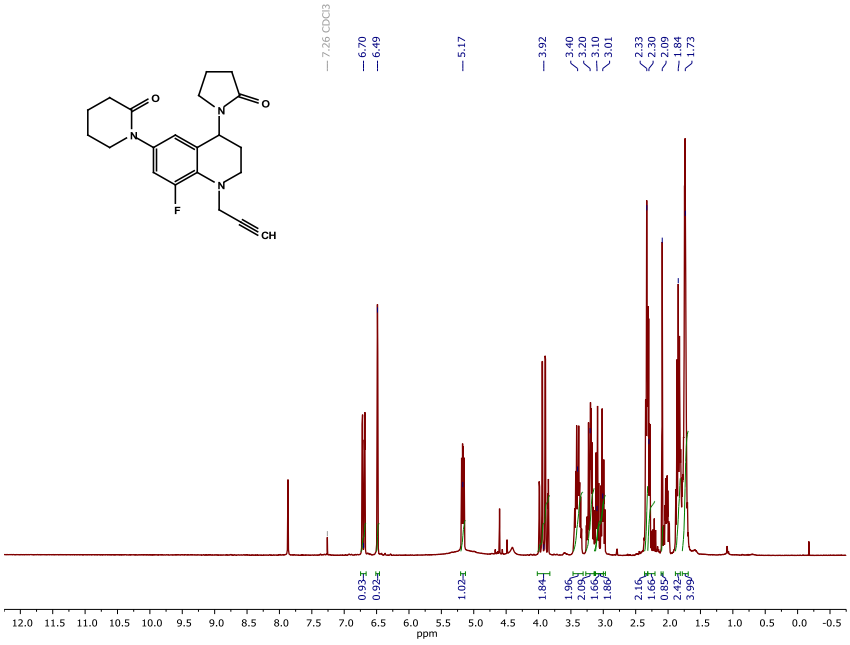
SUPPLEMENTARY MATERIAL

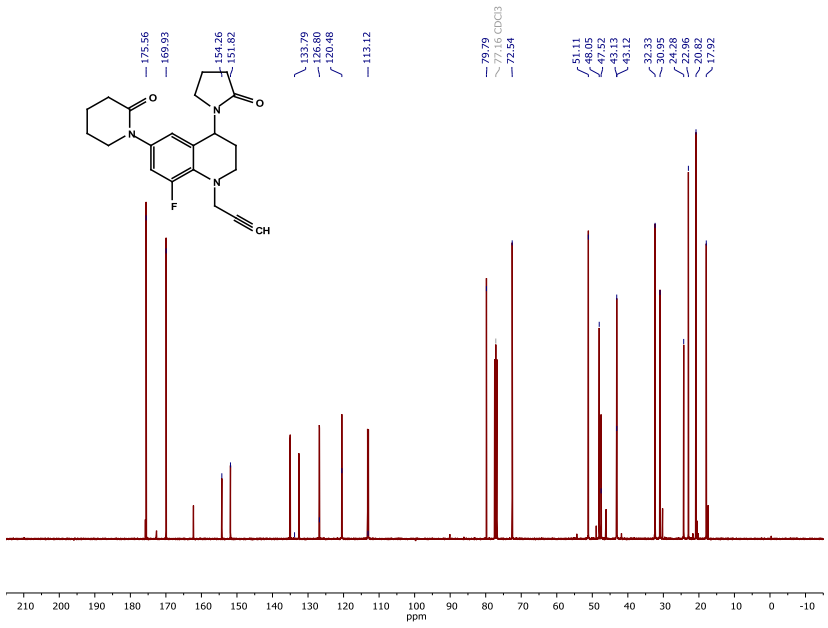
Innovative three-step microwave-promoted synthesis of *N*-propargyltetrahydroquinoline and 1,2,3-triazole derivatives as a potential factor Xa (FXa) inhibitors: drug design, synthesis, and biological evaluation.

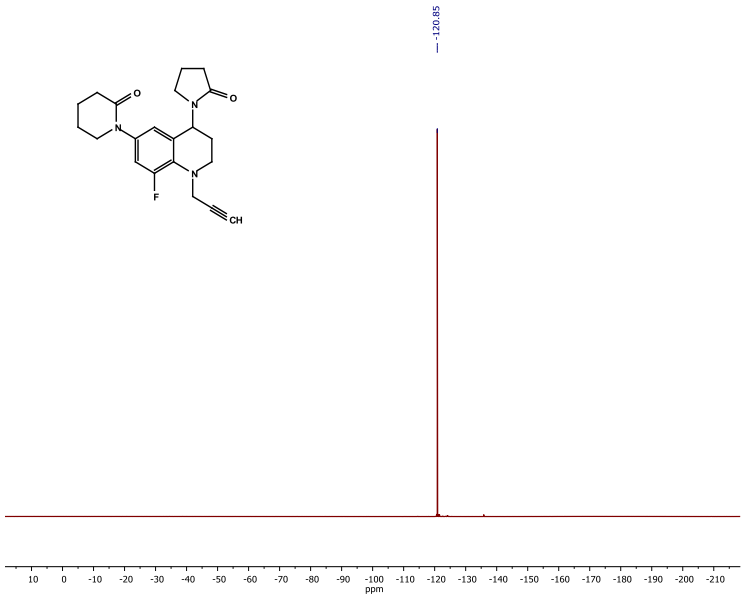
Comentado [FZ1]: The title was changed

TABLE OF CONTENTS

S1. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 17



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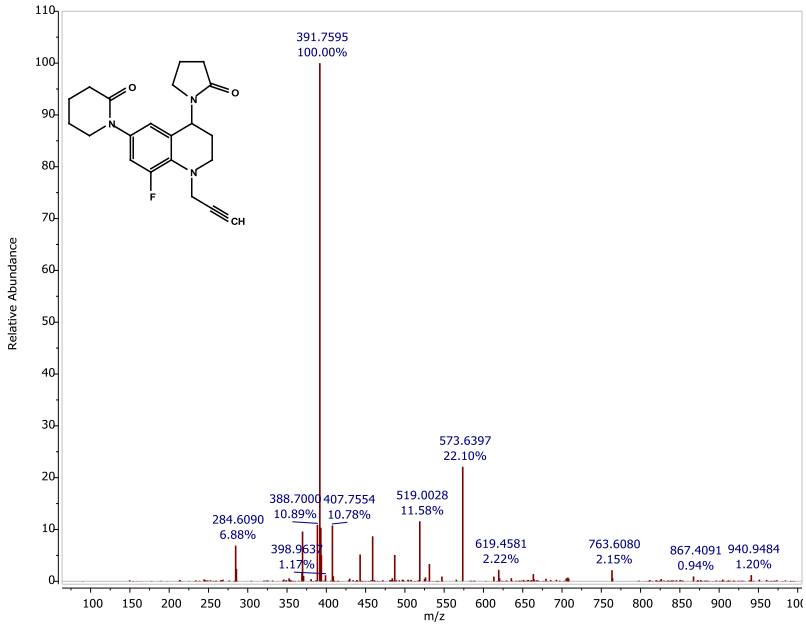
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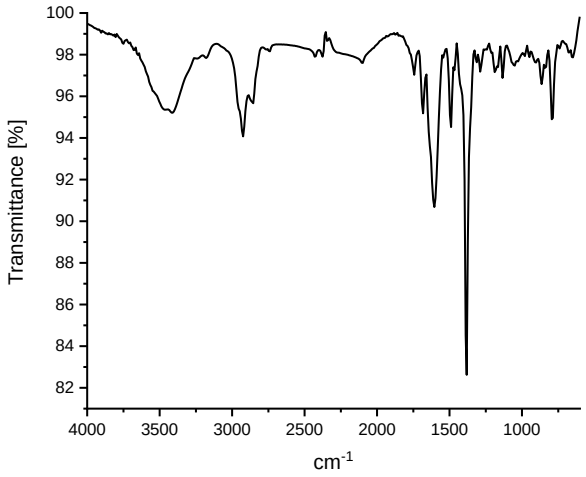
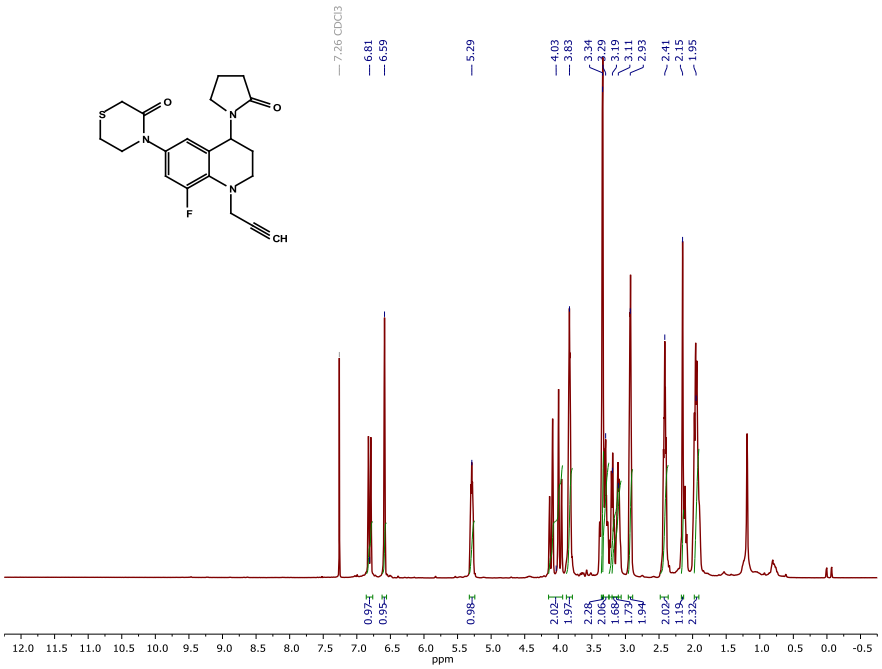
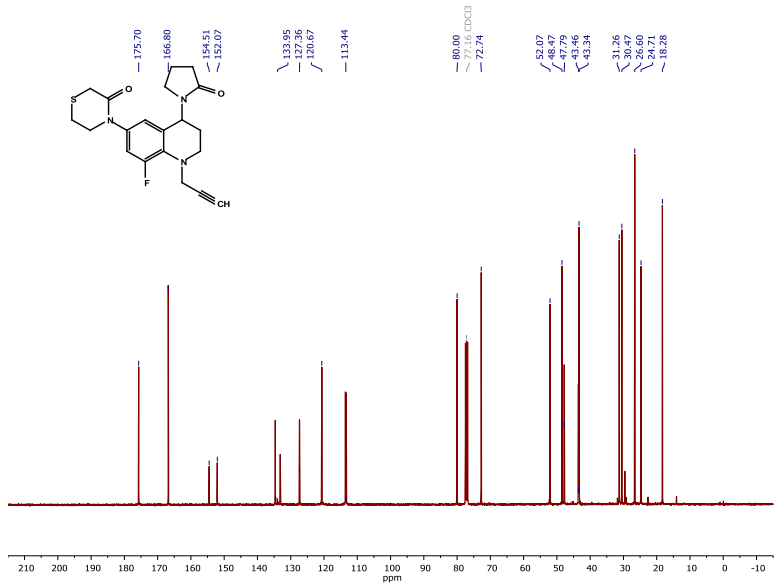
100.00%
573.6397
22.10%
388.7000
10.89%
407.7554
10.78%
519.0028
11.58%
284.6090
6.88%
398.9637
1.17%
619.4581
2.22%
763.6080
2.15%
867.4091
0.94%
940.9484
1.20%
Relative Abundance
m/z



S2. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 19

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166.80
154.51
152.07
133.95
127.36
120.67
113.44
80.00
77.16 CDCl3
72.74
52.07
48.47
47.79
43.46
43.34
31.26
30.47
26.60
24.71
18.28
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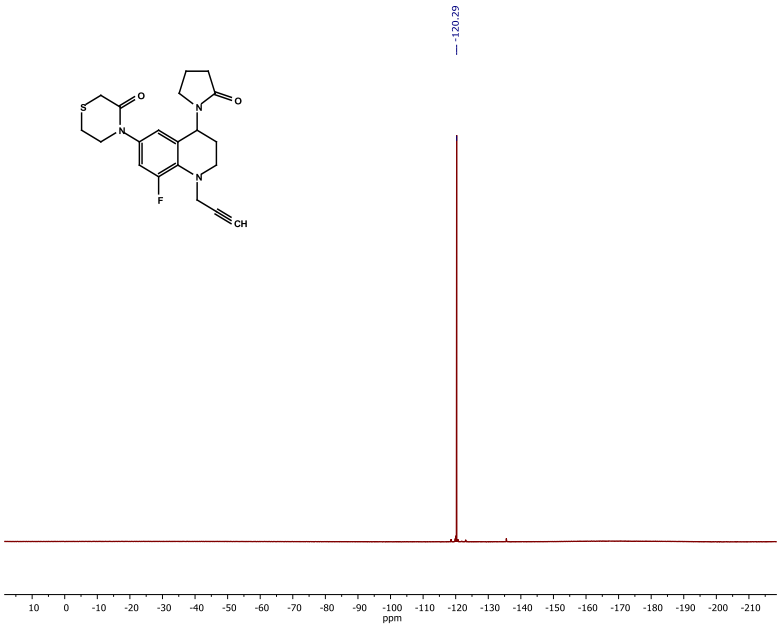
S
N
O
N
F
N
CH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm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S
N
O
N
F
N
CH
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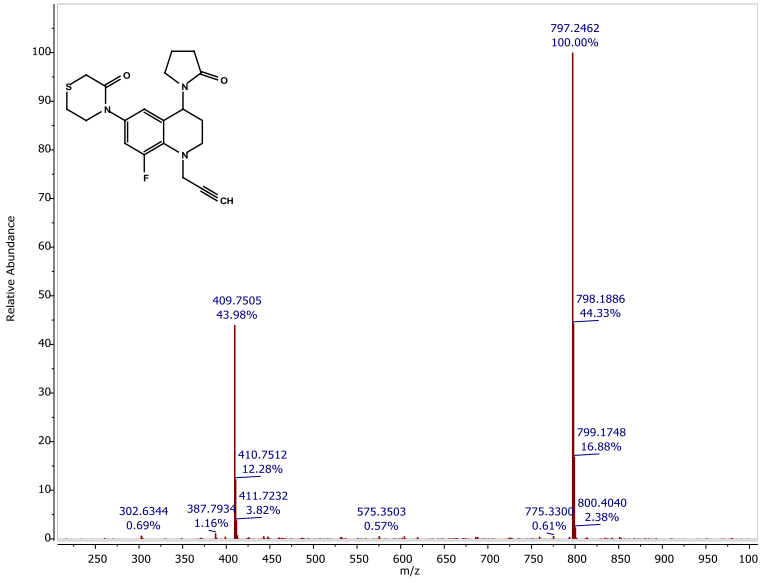
ppm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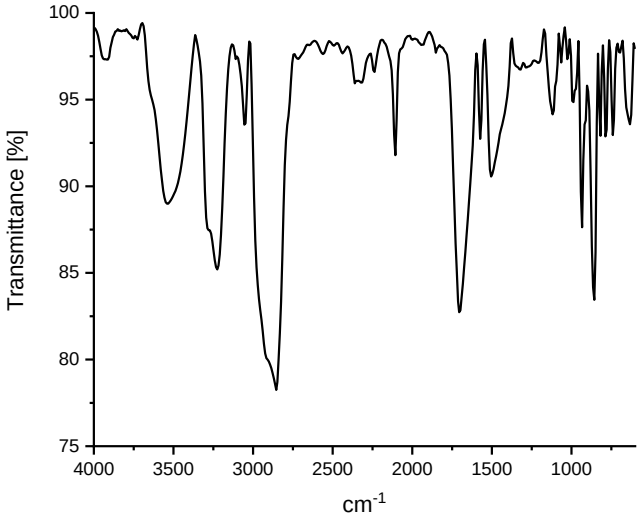
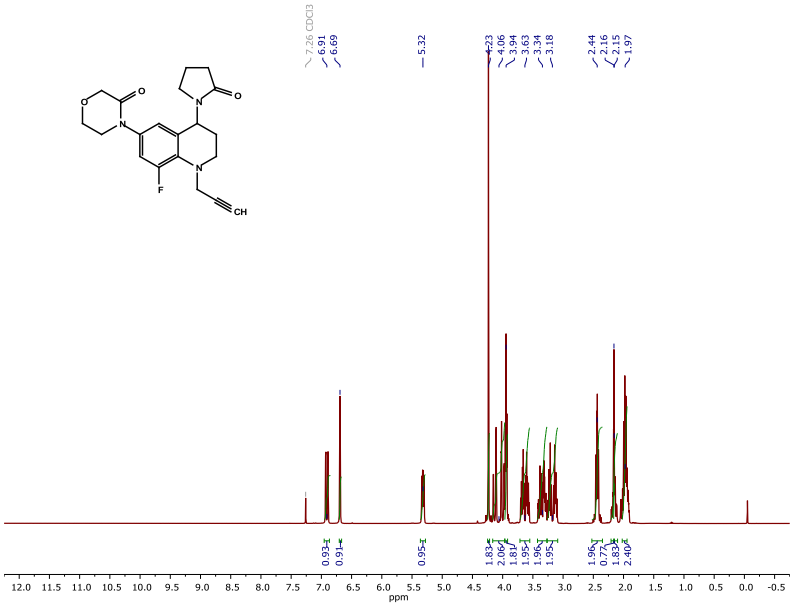
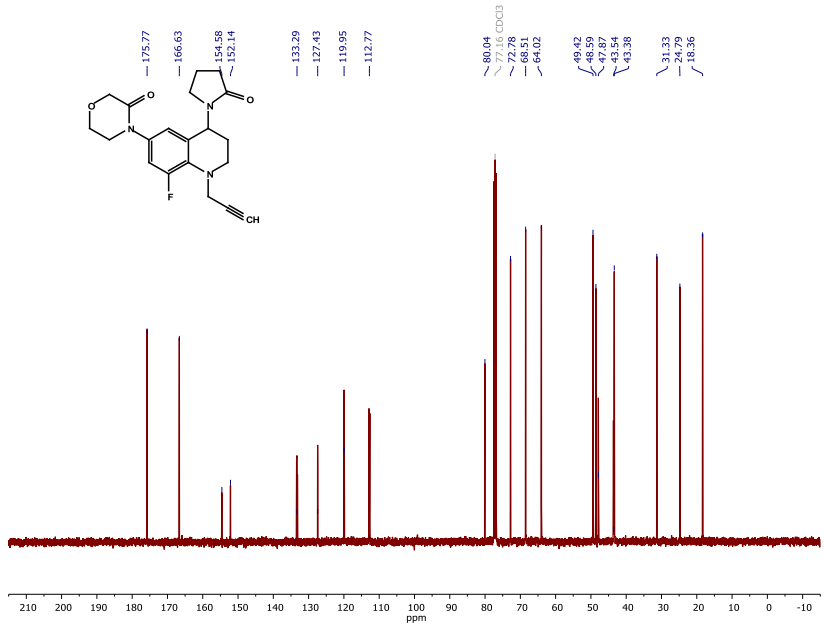
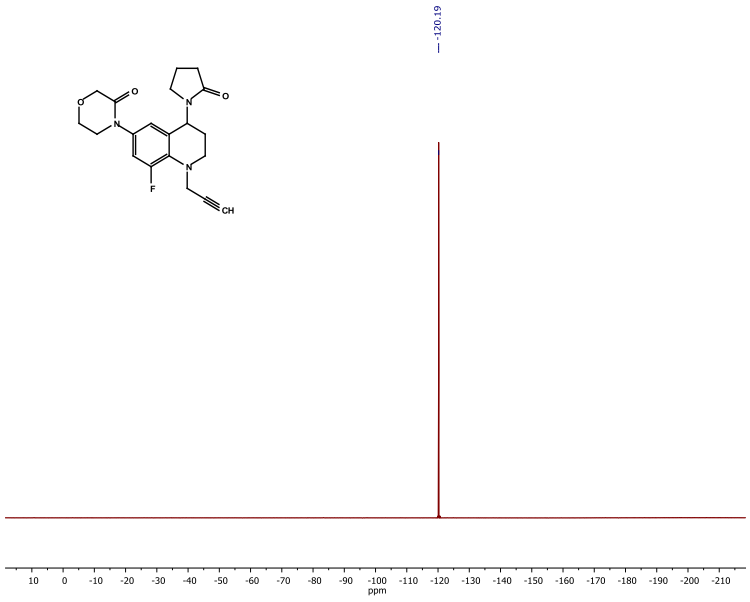
100.00%
409.7505
43.98%
798.1886
44.33%
799.1748
16.88%
410.7512
12.28%
411.7232
3.82%
800.4040
2.38%
302.6344
0.69%
387.7934
1.16%
575.3503
0.57%
775.3300
0.61%
Relative Abundance
m/z


Transmittance [%]
cm-1

S3. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 20



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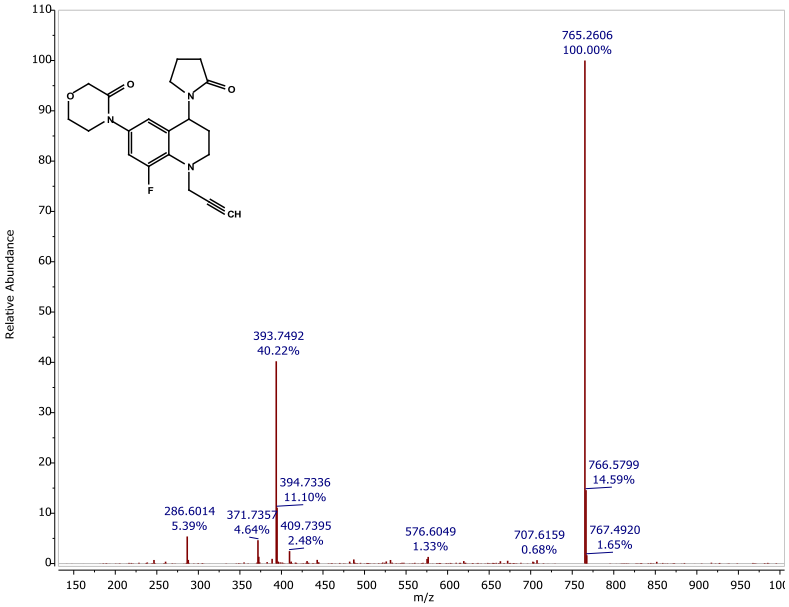
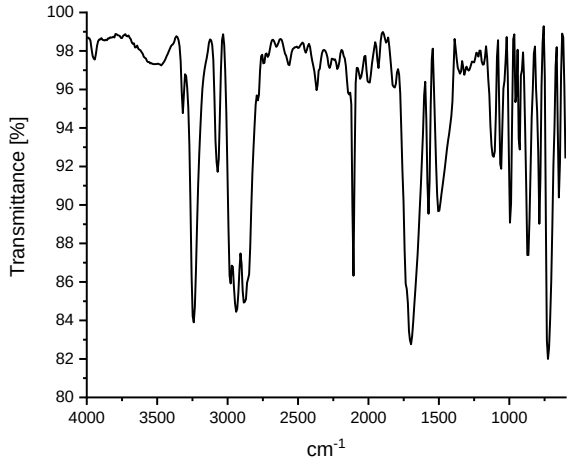
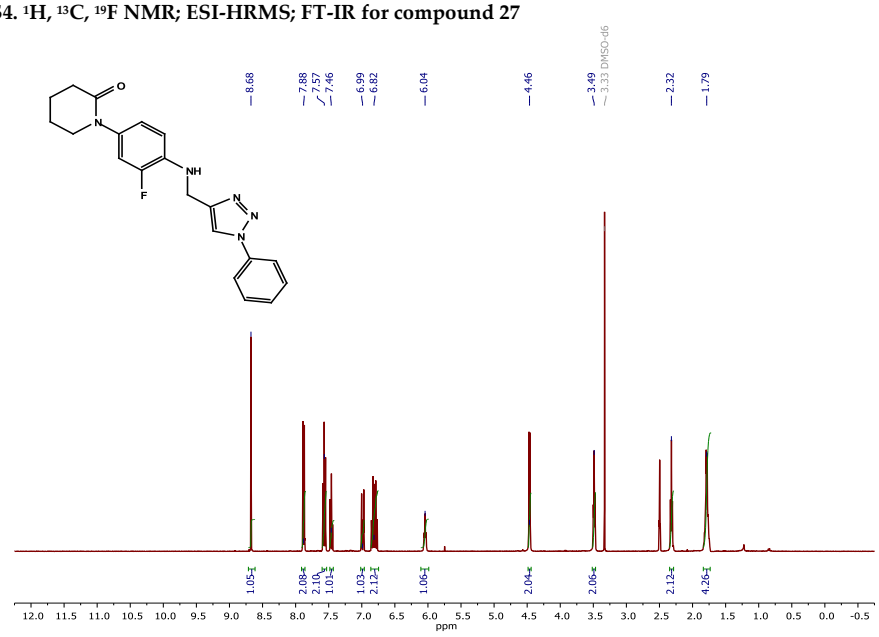
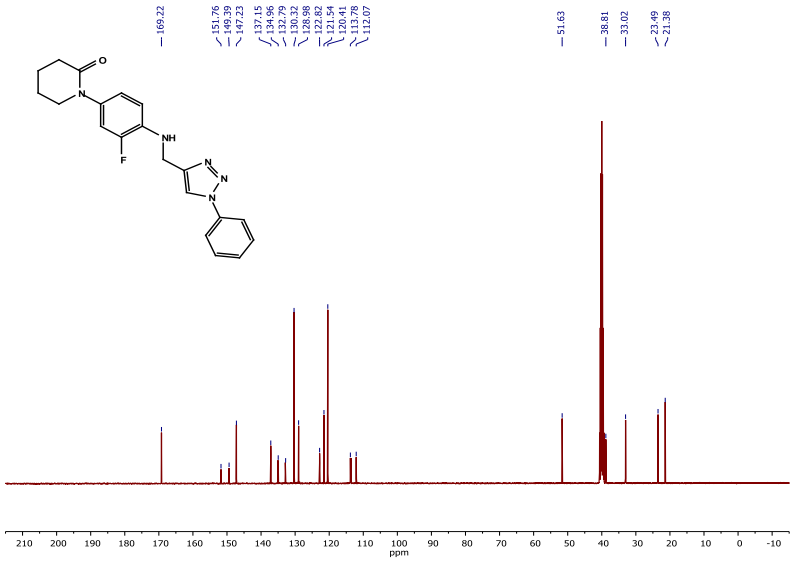
ppm


765.2606
100.00%
393.7492
40.22%
394.7336
11.10%
766.5799
14.59%
286.6014
5.39%
371.7357
4.64%
409.7395
2.48%
576.6049
1.33%
707.6159
0.68%
767.4920
1.65%
Relative Abundance
m/z



S4. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 27

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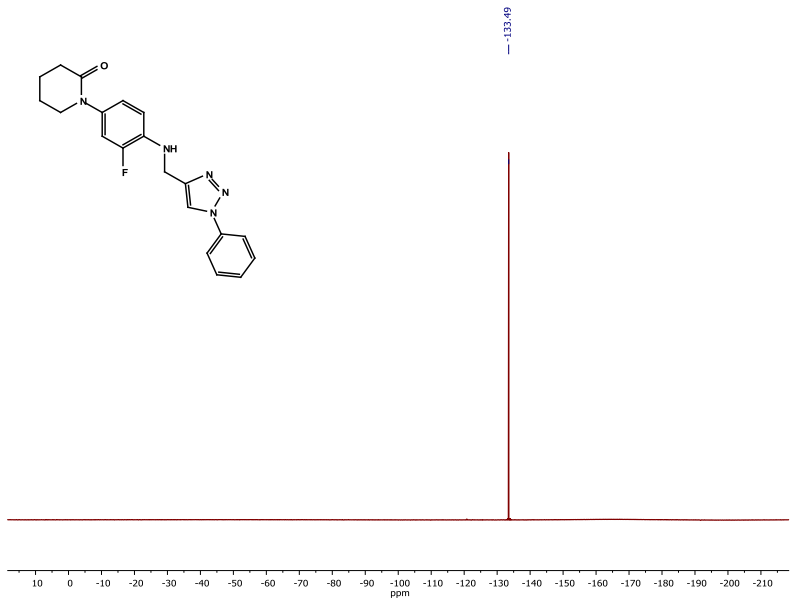
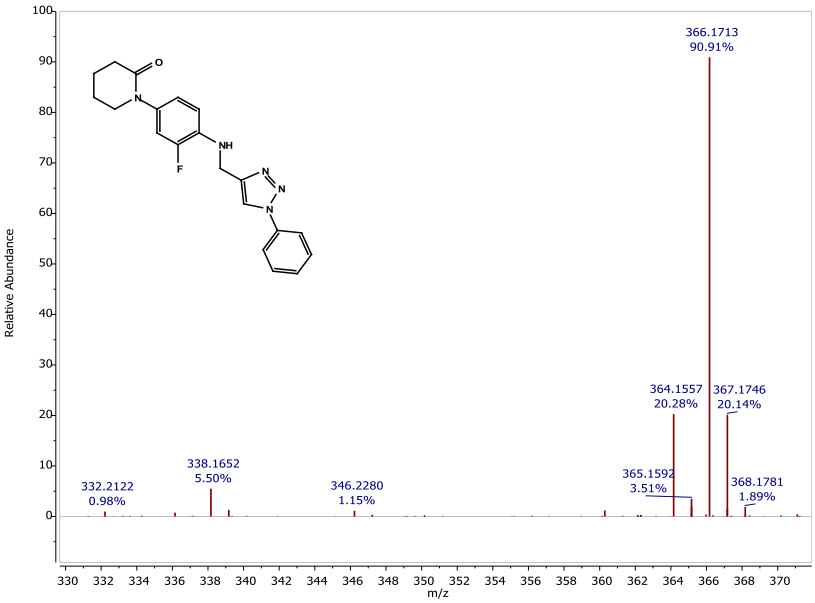
151.76
149.39
147.23
137.15
134.96
132.79
130.32
129.98
122.82
121.54
120.41
113.78
112.07
51.63
38.81
33.02
23.49
21.38
O
N
NH
F
N
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


-133.49
O
N
NH
F
N
N
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
ppm


Relative Abundance
m/z
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364.1557
20.28%
367.1746
20.14%
338.1652
5.50%
332.2122
0.98%
346.2280
1.15%
365.1592
3.51%
368.1781
1.89%
O
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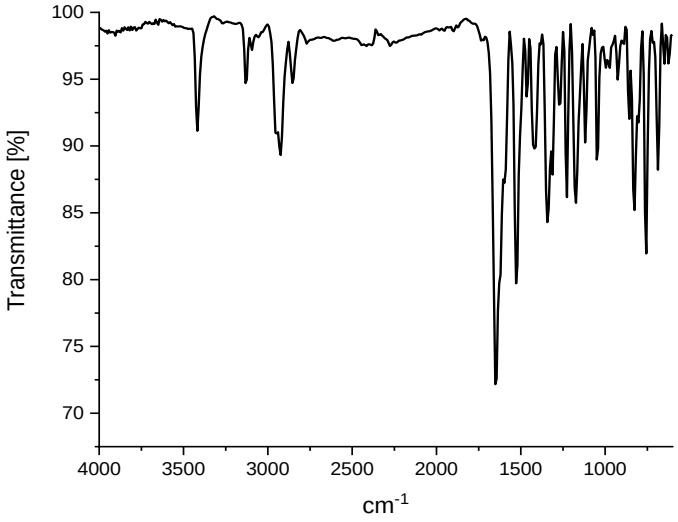
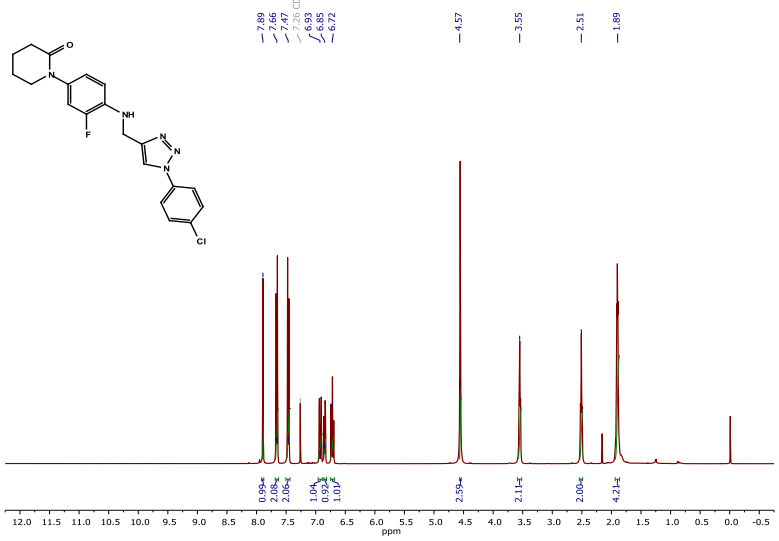
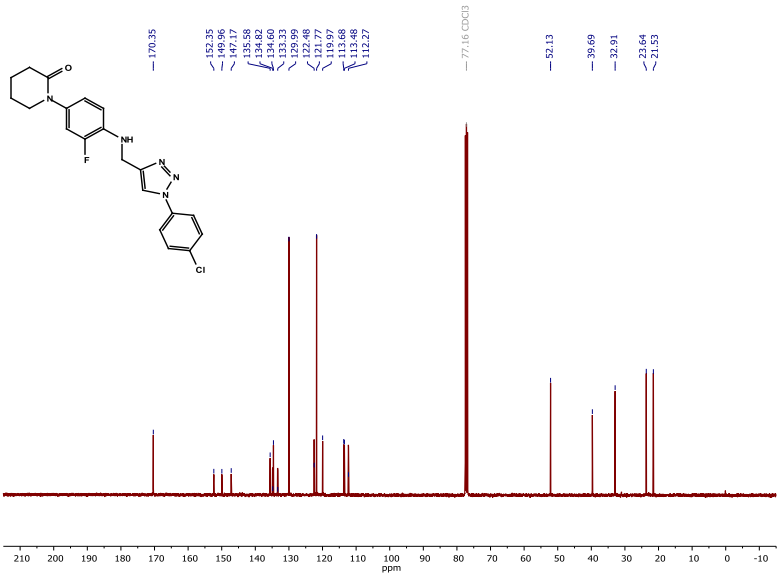
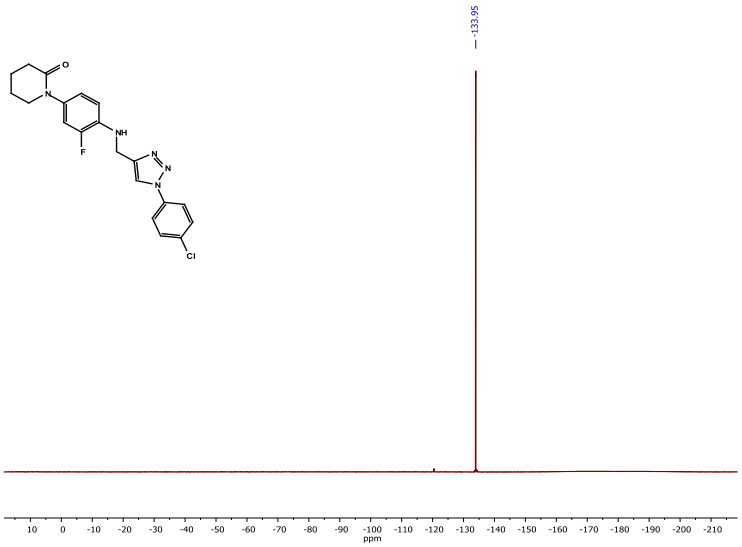
NH
F
N
N
N


Transmittance [%]
cm-1

S5. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 28






-133.95
O
N
NH
F
N
N
N
Cl
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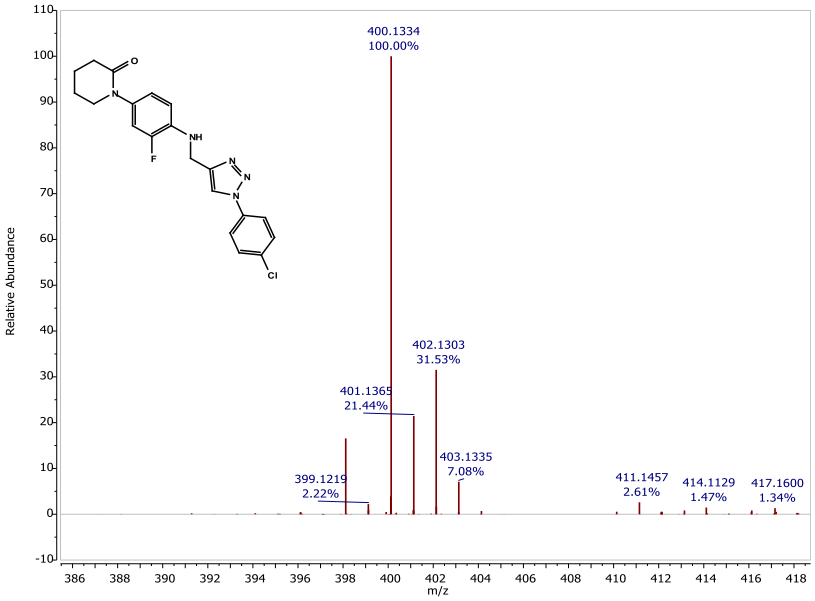
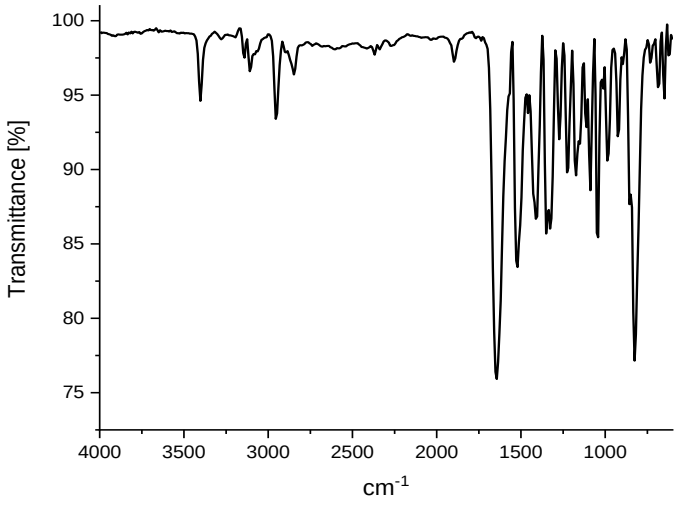
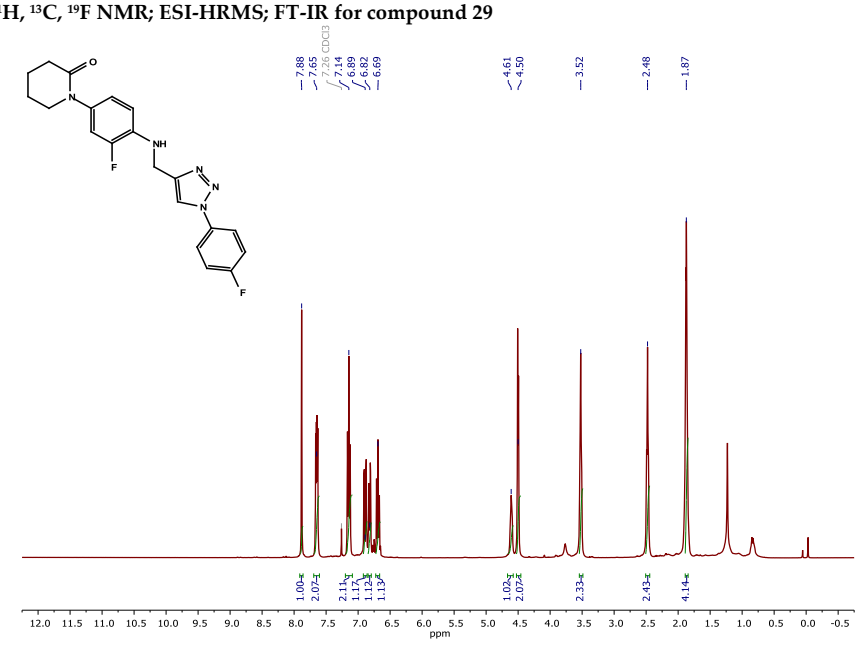
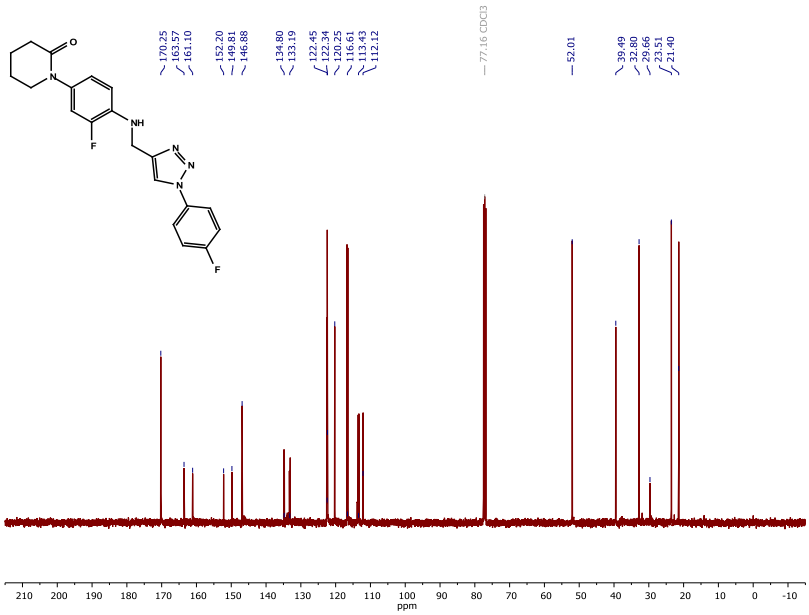
ppm


Relative Abundance
400.1334
100.00%
402.1303
31.53%
401.1365
21.44%
403.1335
7.08%
399.1219
2.22%
411.1457
2.61%
414.1129
1.47%
417.1600
1.34%
O
N
NH
F
N
N
N
Cl
386 388 390 392 394 396 398 400 402 404 406 408 410 412 414 416 418
m/z



S6. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 29

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153.20
149.81
146.88
134.80
133.19
122.45
122.34
120.25
116.61
113.43
112.12
77.16 CDCl3
52.01
39.49
32.80
29.66
23.51
21.40
O
N
NH
F
N
N
N
F
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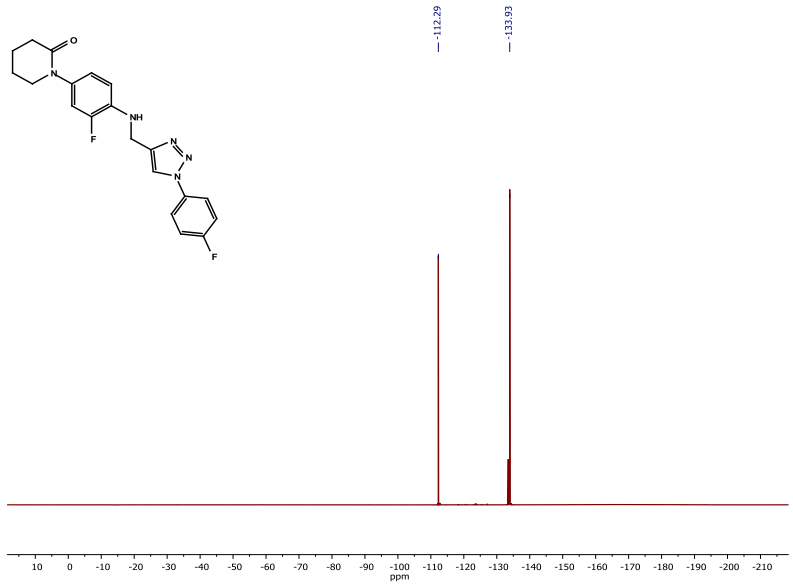
ppm


-112.29
-133.93
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NH
F
N
N
N
F
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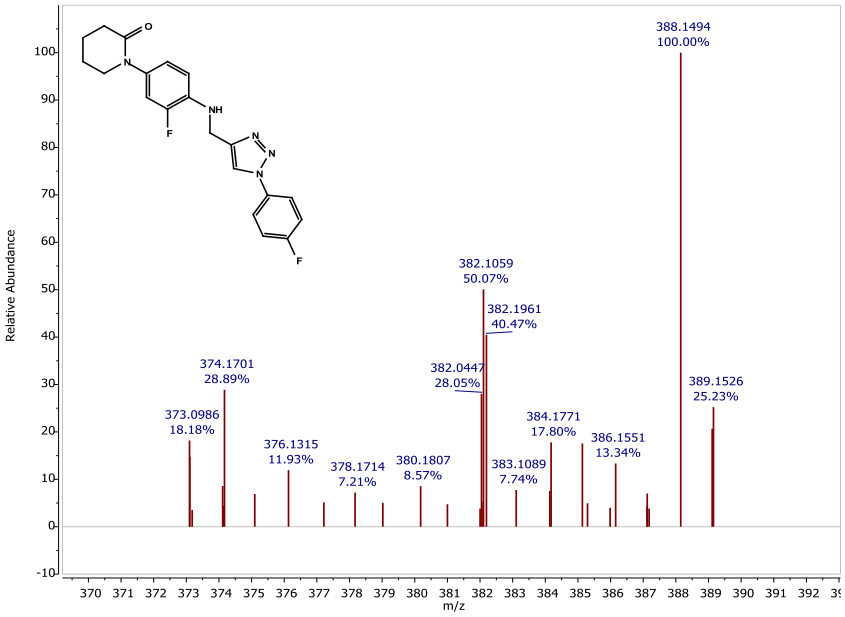
ppm


Relative Abundance
m/z
388.1494
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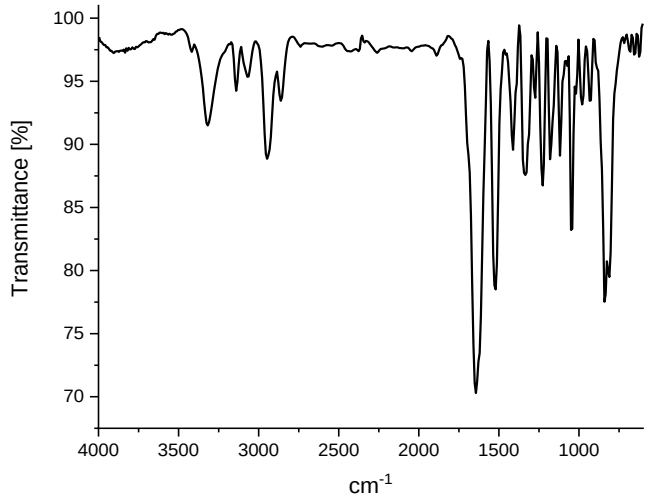
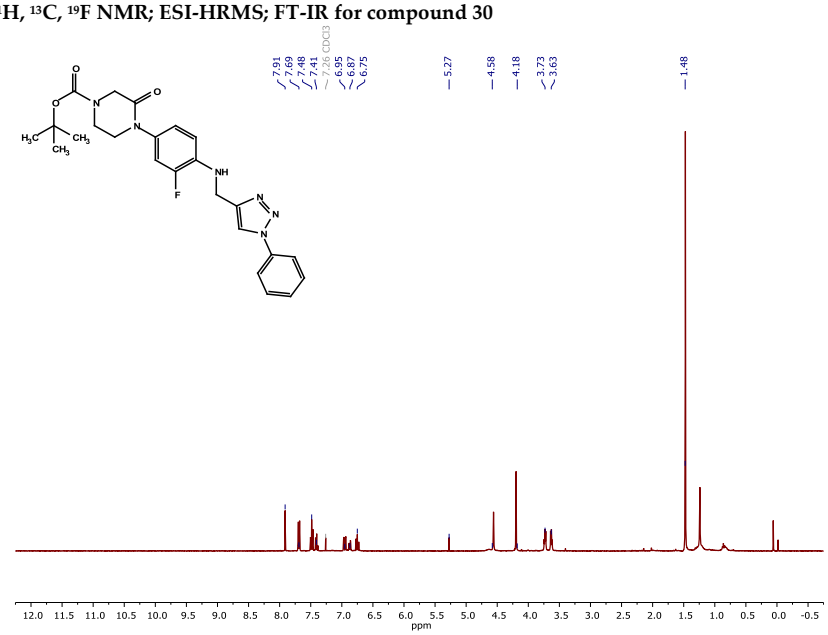
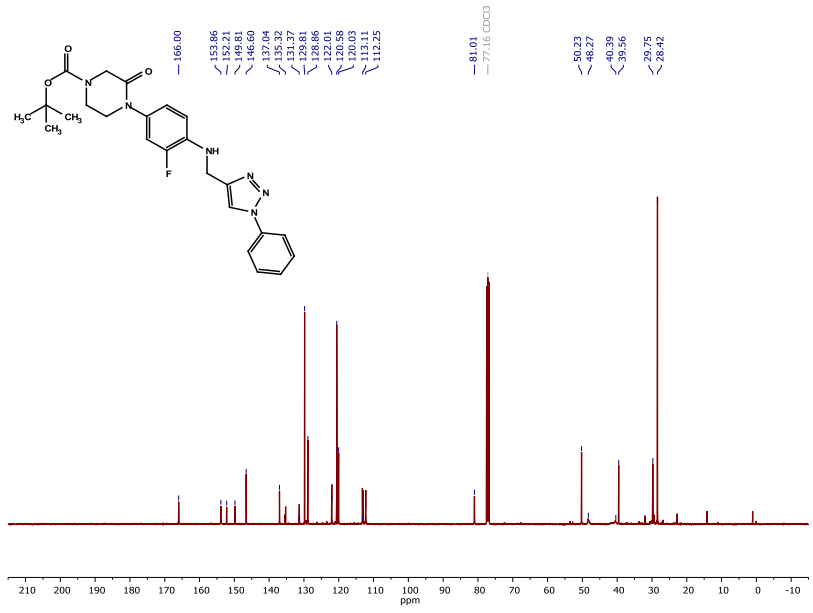
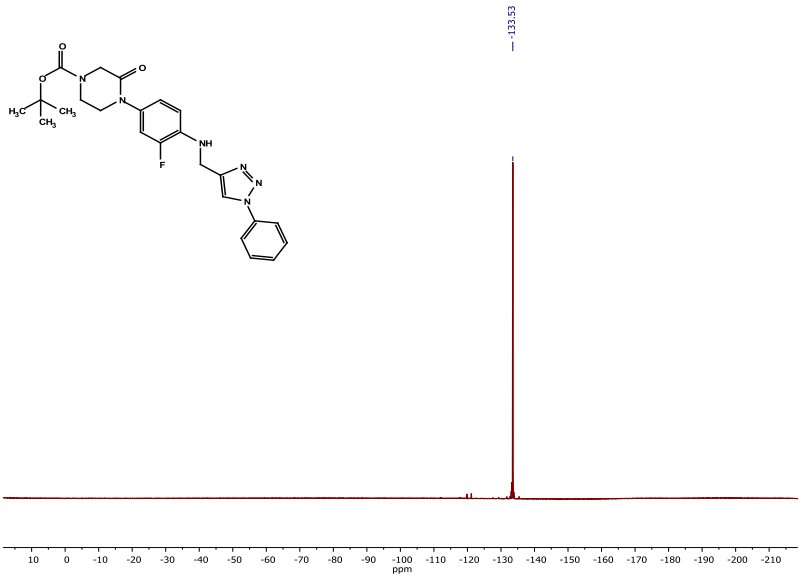
382.1059
50.07%
382.1961
40.47%
374.1701
28.89%
382.0447
28.05%
389.1526
25.23%
373.0986
18.18%
384.1771
17.80%
386.1551
13.34%
376.1315
11.93%
383.1089
7.74%
378.1714
7.21%
380.1807
8.57%


Transmittance [%]
cm-1

S7. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 30



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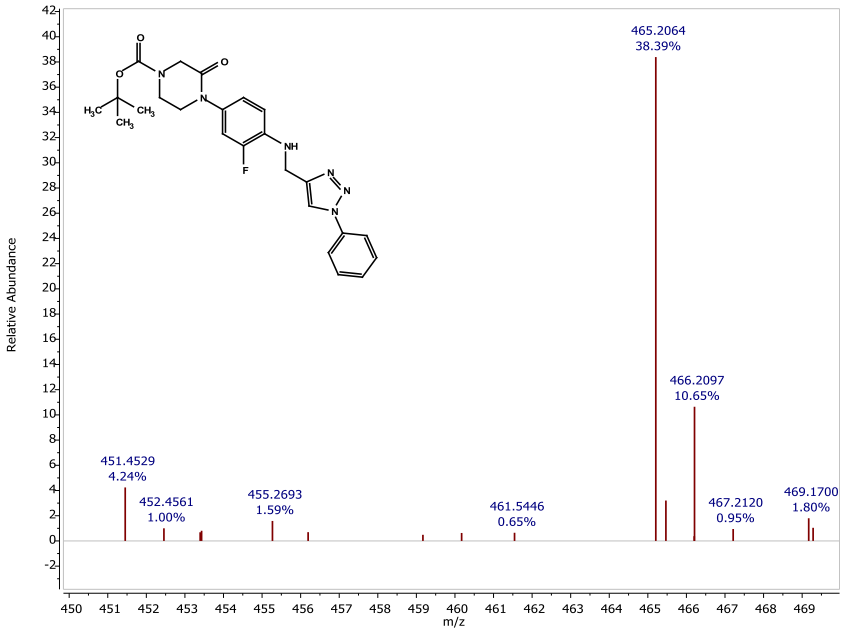
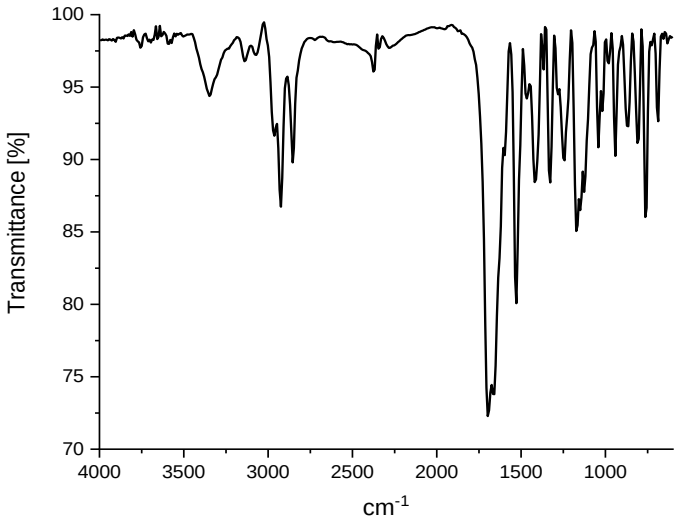
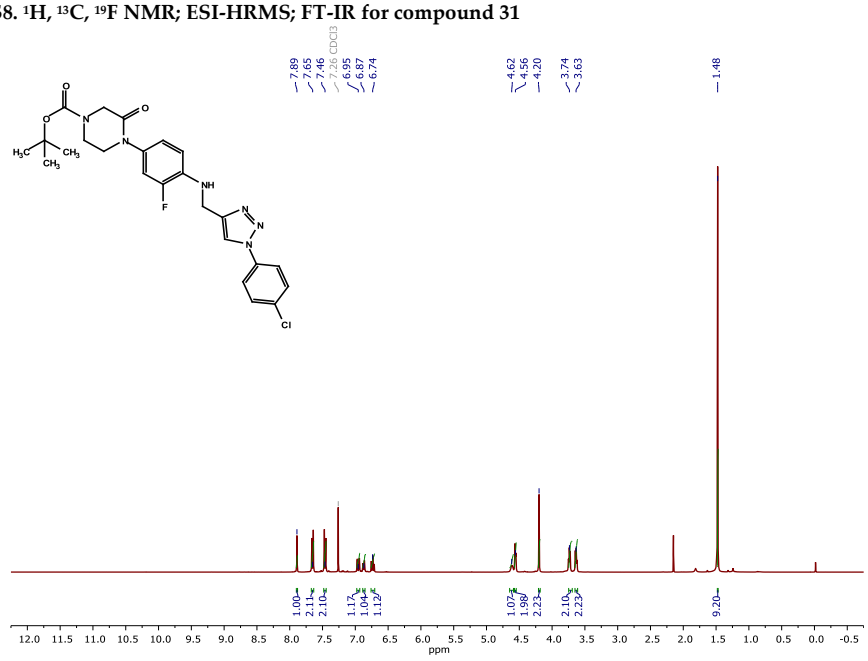
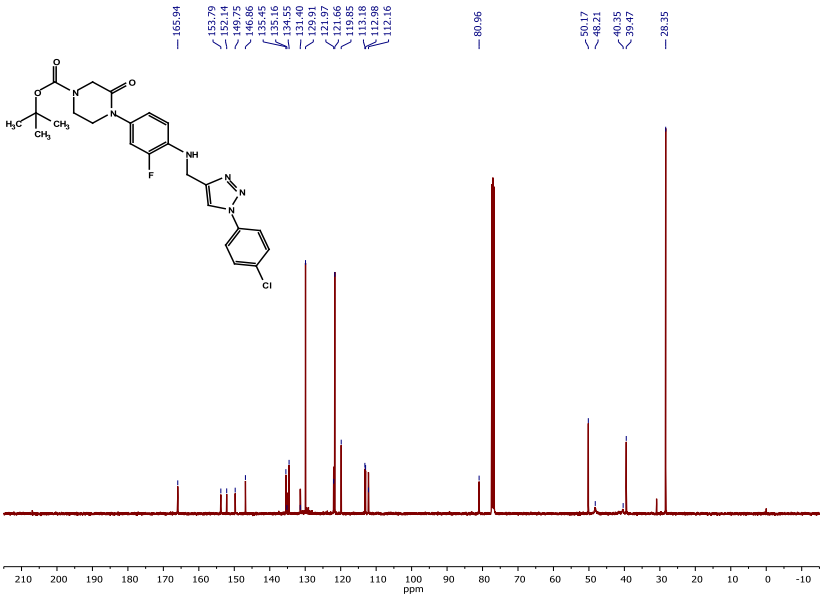
ppm


Relative Abundance
465.2064
38.39%
466.2097
10.65%
451.4529
4.24%
452.4561
1.00%
455.2693
1.59%
461.5446
0.65%
467.2120
0.95%
469.1700
1.80%
450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469
m/z



S8. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 31




165.94
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135.45
135.16
134.55
131.40
129.91
121.97
121.66
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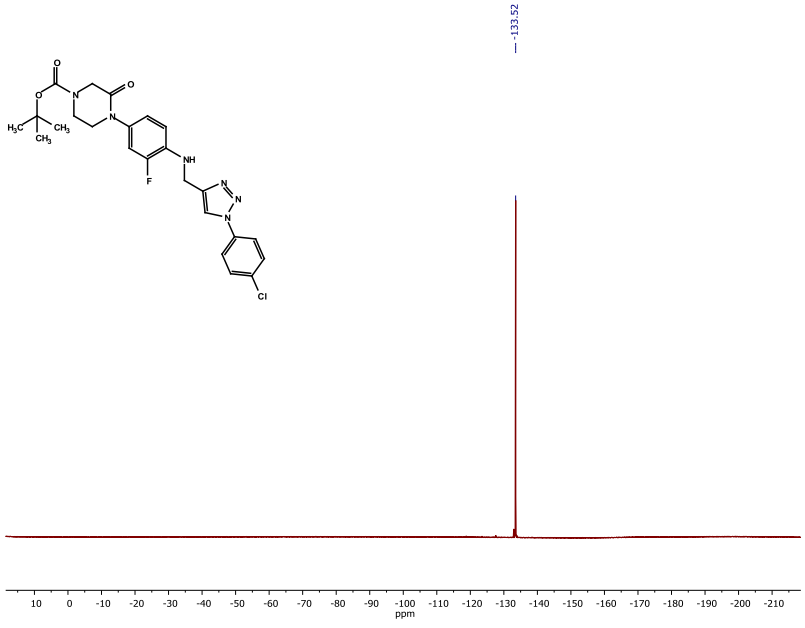
112.16
80.96
50.17
48.21
40.35
39.47
28.35
O
O
O
N
N
O
H3C
CH3
CH3
NH
F
N
N
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm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N
O
H3C
CH3
CH3
NH
F
N
N
N
Cl
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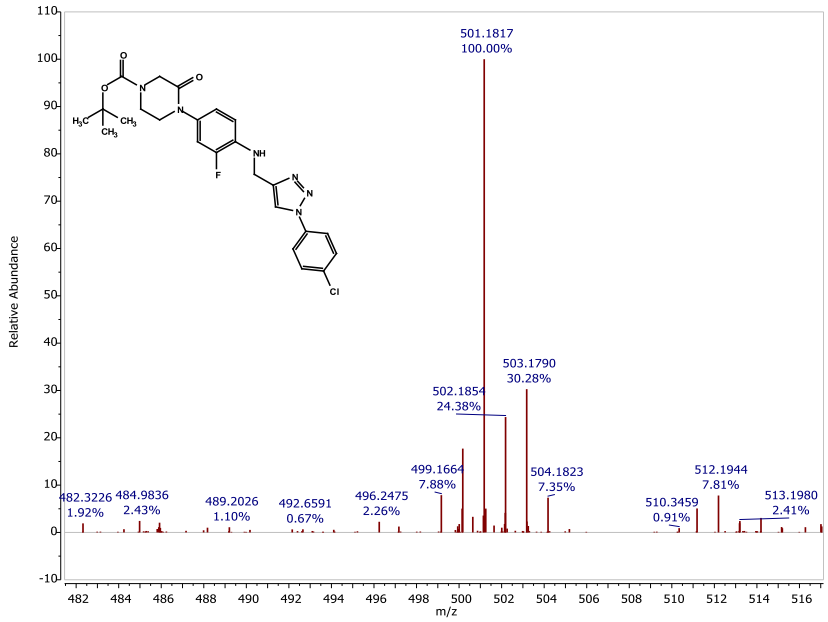
ppm


Relative Abundance
m/z
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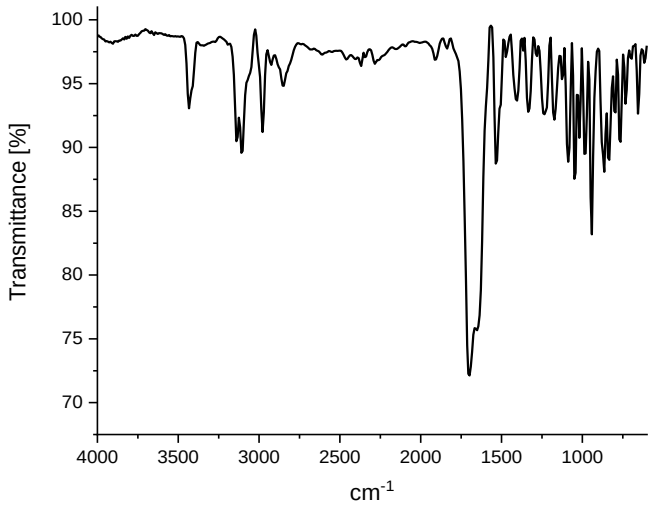
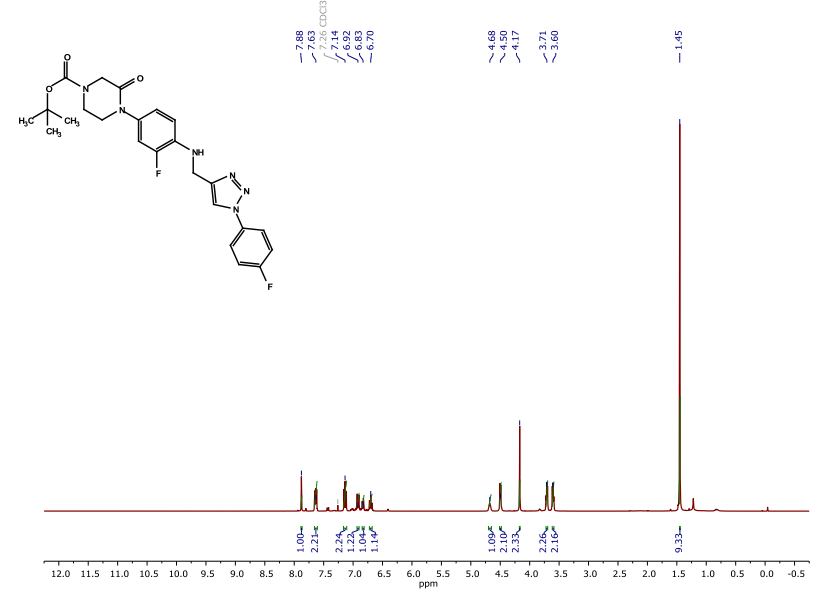
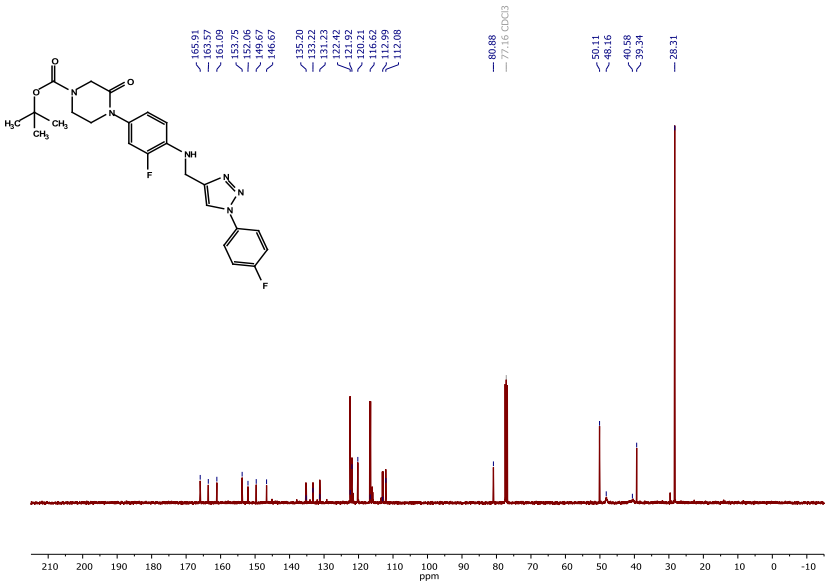
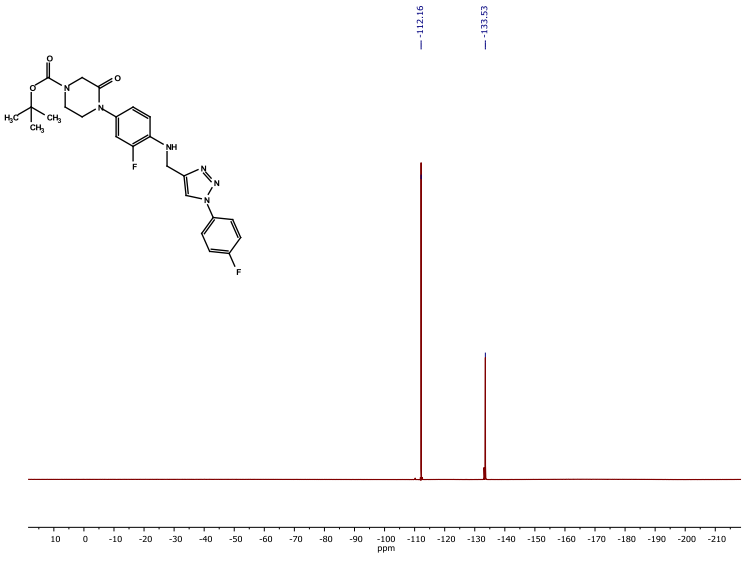
503.1790
30.28%
502.1854
24.38%
499.1664
7.88%
504.1823
7.35%
512.1944
7.81%
513.1980
2.41%
482.3226
1.92%
484.9836
2.43%
489.2026
1.10%
492.6591
0.67%
496.2475
2.26%
510.3459
0.91%
O
O
O
N
N
O
H3C
CH3
CH3
NH
F
N
N
N
Cl

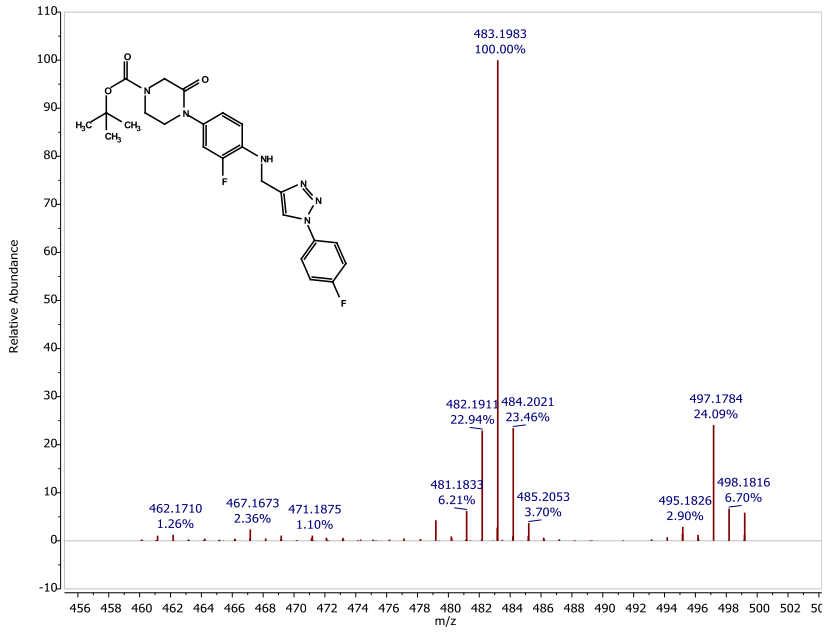

Transmittance [%]
cm-1

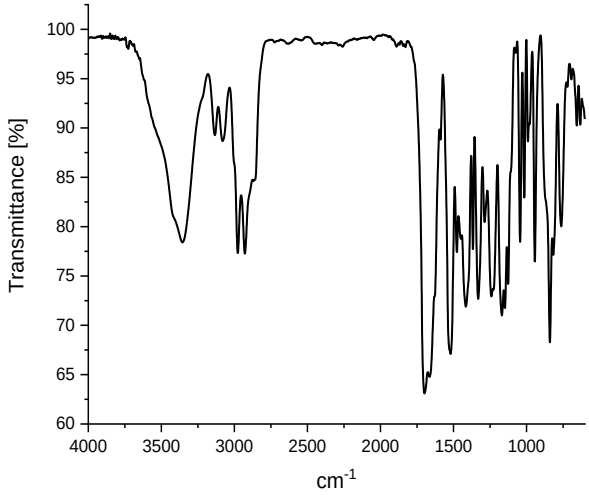
S9. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 32



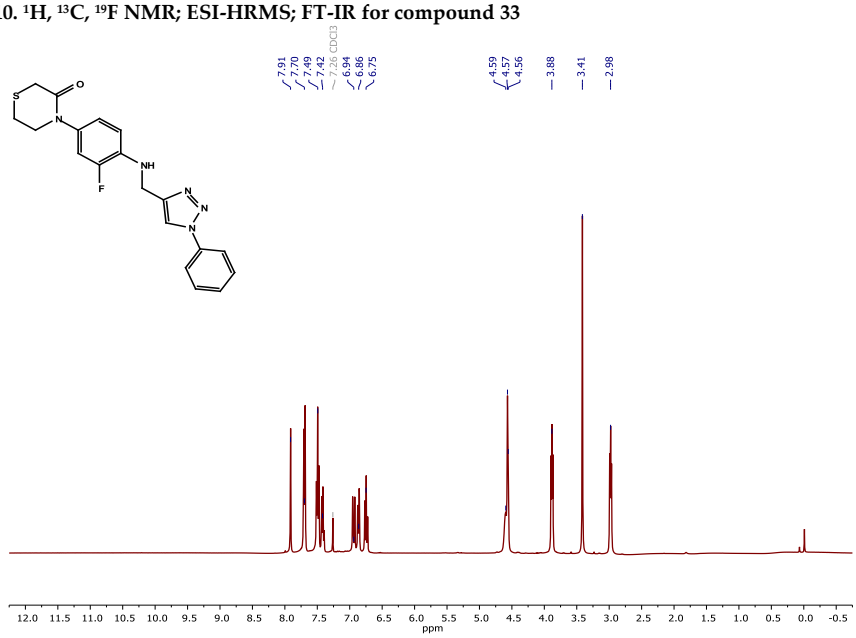


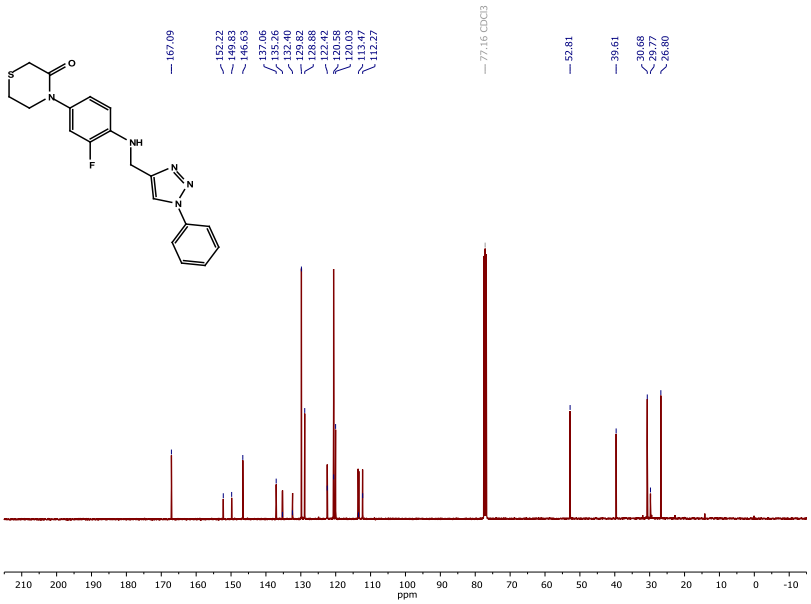

-112.16
-133.53
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
ppm

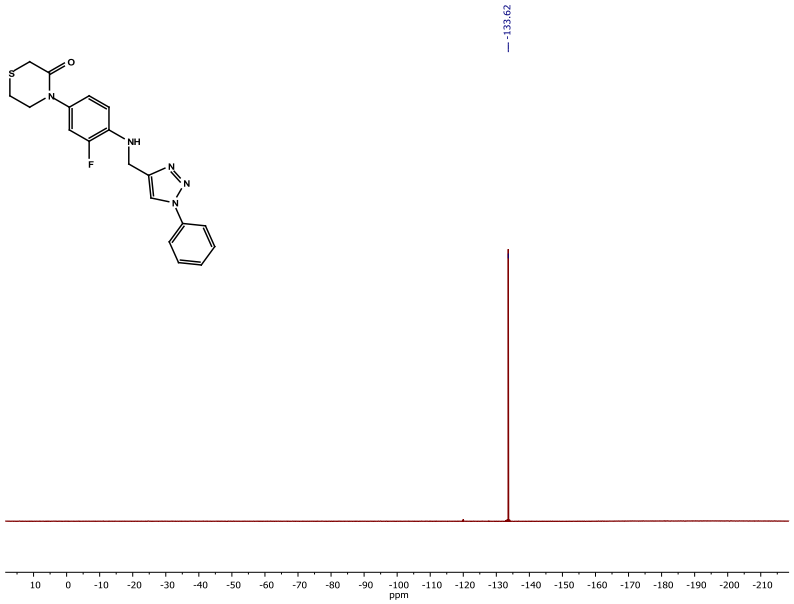

Relative Abundance
m/z
483.1983
100.00%
482.1911
22.94%
484.2021
23.46%
497.1784
24.09%
481.1833
6.21%
485.2053
3.70%
498.1816
6.70%
462.1710
1.26%
467.1673
2.36%
471.1875
1.10%
495.1826
2.90%

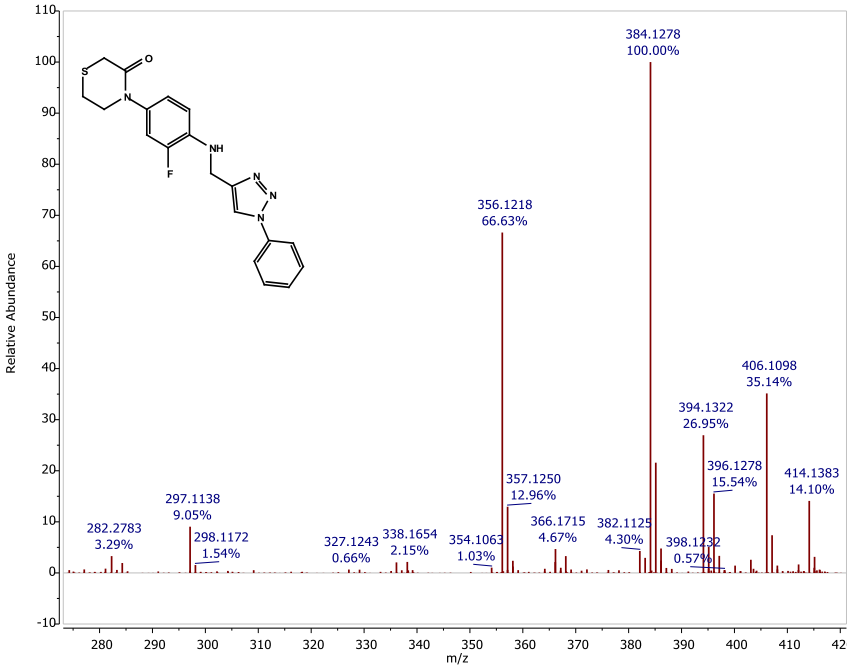


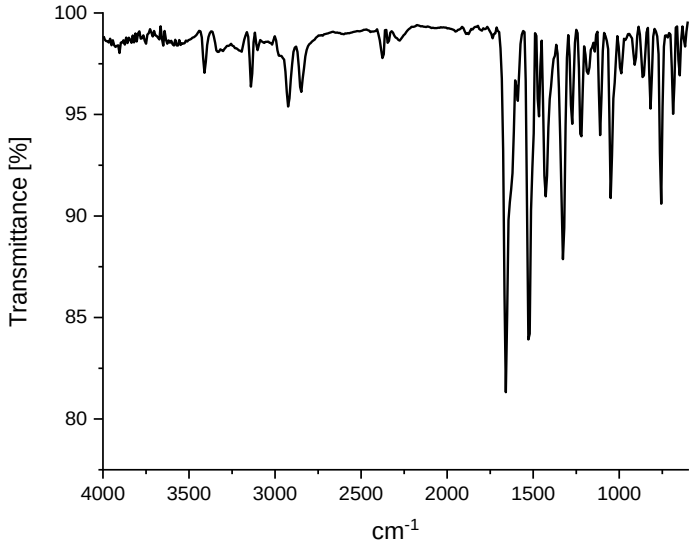
S10. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 33



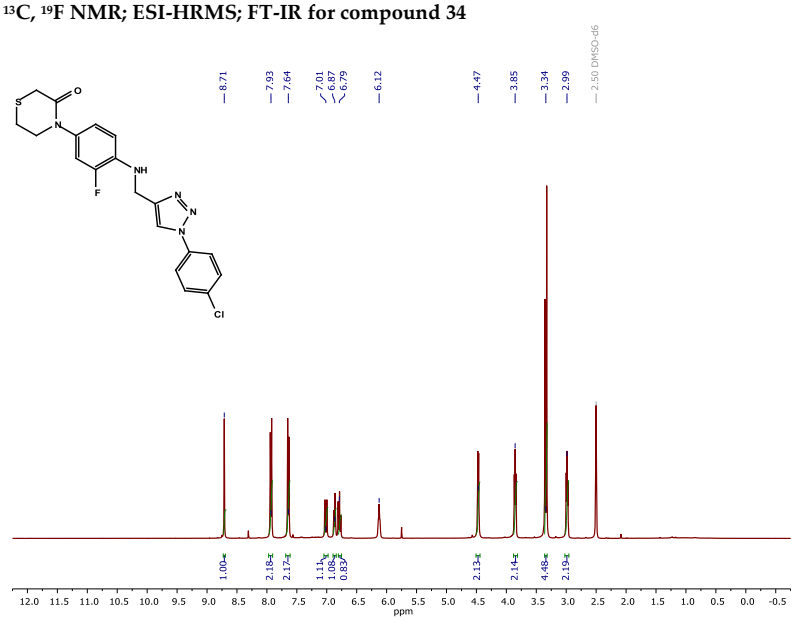

167.09
152.22
149.83
146.63
137.06
135.26
132.40
129.82
128.88
122.42
120.58
120.03
113.47
112.27
77.16 CDCl3
52.81
39.61
30.68
29.77
26.80
ppm

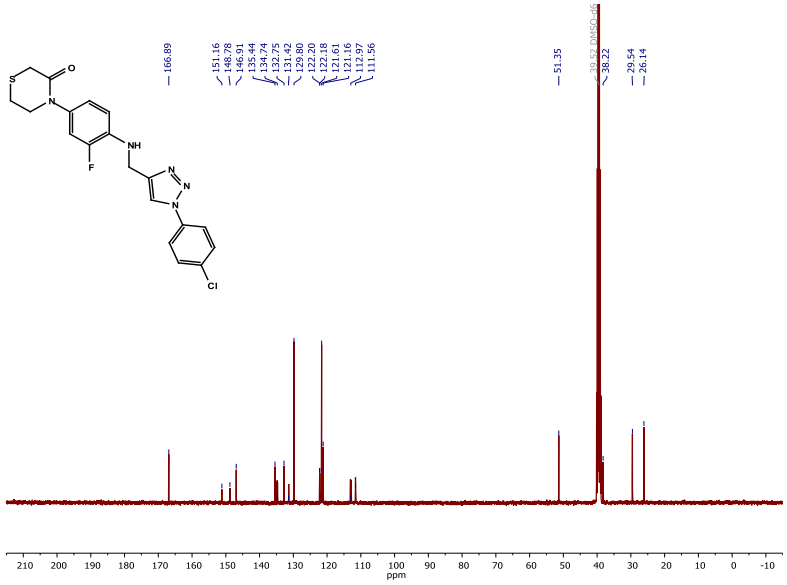

-133.62
ppm

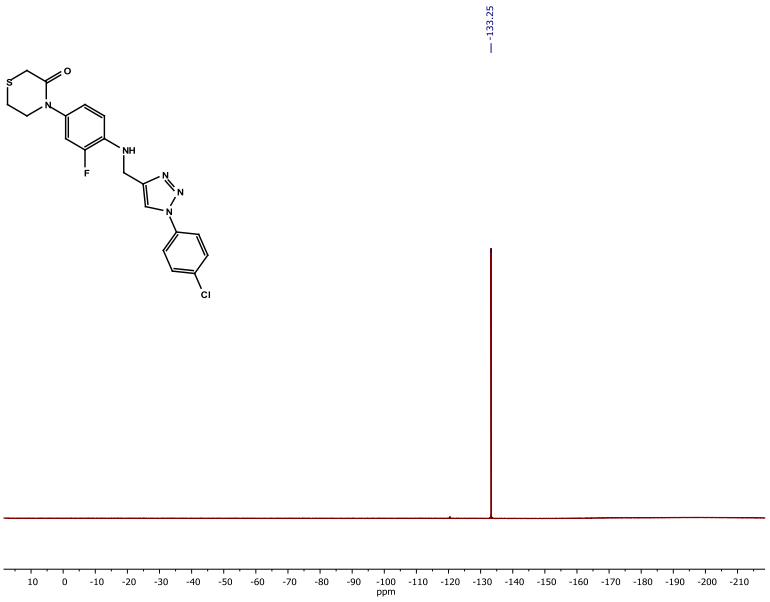

Relative Abundance
m/z
384.1278
100.00%
356.1218
66.63%
406.1098
35.14%
394.1322
26.95%
396.1278
15.54%
414.1383
14.10%
357.1250
12.96%
297.1138
9.05%
366.1715
4.67%
382.1125
4.30%
282.2783
3.29%
298.1172
1.54%
327.1243
0.66%
338.1654
2.15%
354.1063
1.03%
398.1232
0.57%

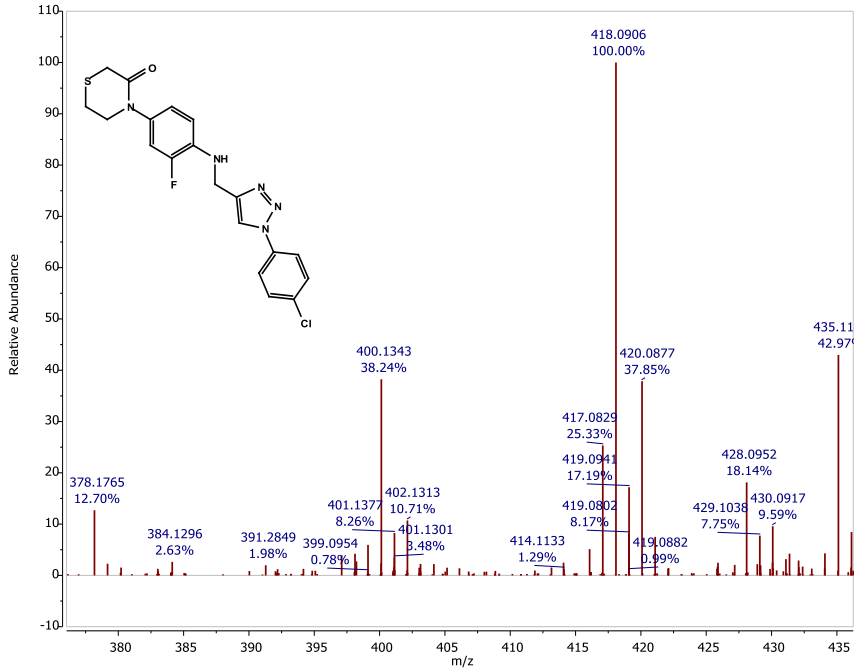

Transmittance [%]
cm-1

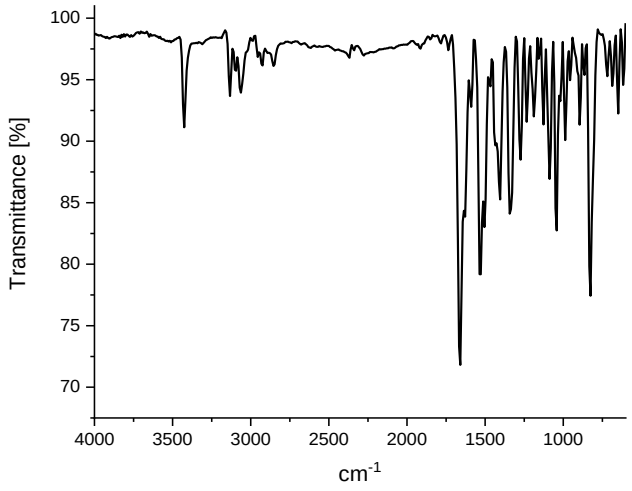
S11. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 34



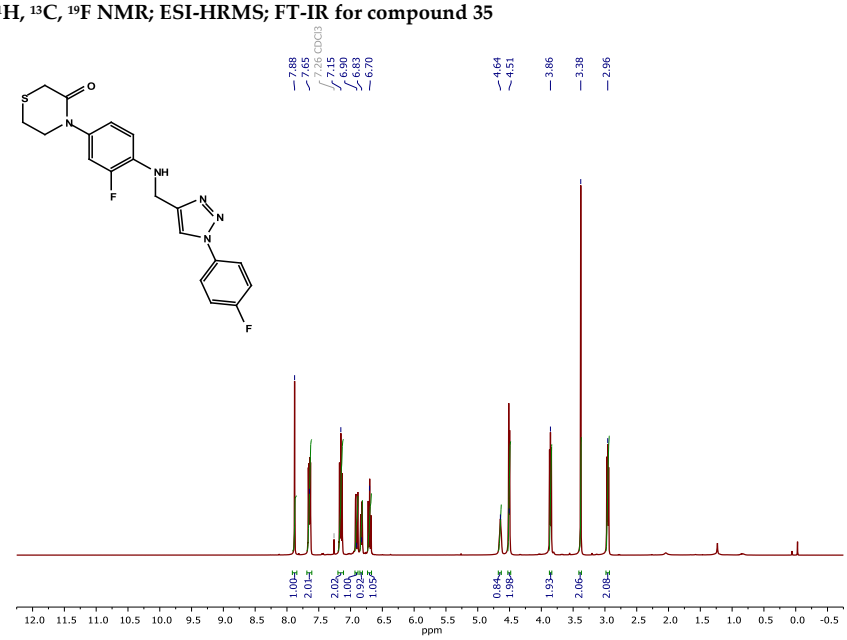


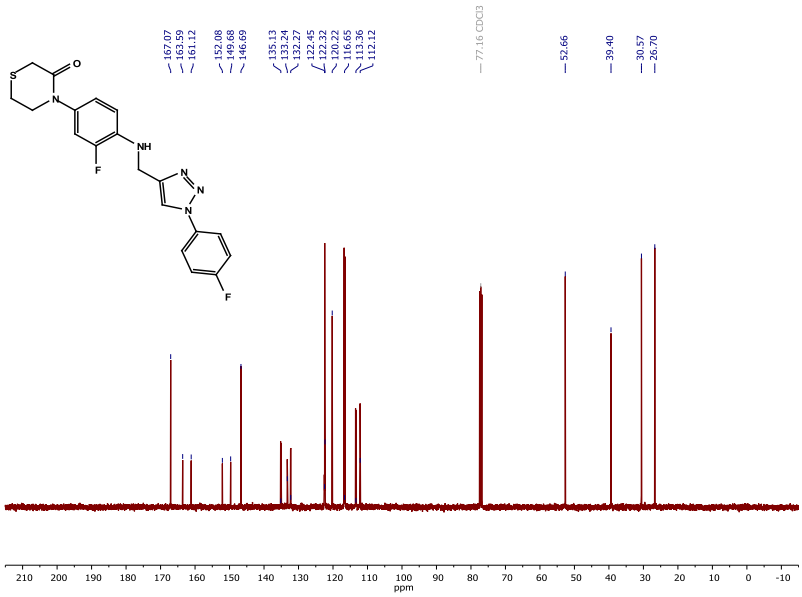

-133.25
ppm

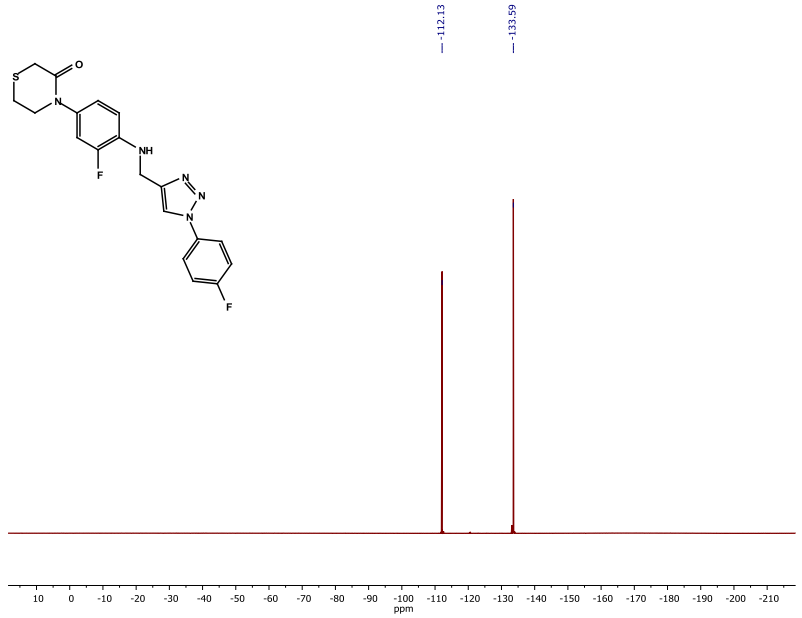

Relative Abundance
m/z
418.0906
100.00%
400.1343
38.24%
420.0877
37.85%
417.0829
25.33%
419.0941
17.19%
428.0952
18.14%
378.1765
12.70%
402.1313
10.71%
401.1377
8.26%
419.0802
8.17%
430.0917
9.59%
429.1038
7.75%
401.1301
3.48%
384.1296
2.63%
391.2849
1.98%
399.0954
0.78%
414.1133
1.29%
419.0882
0.99%

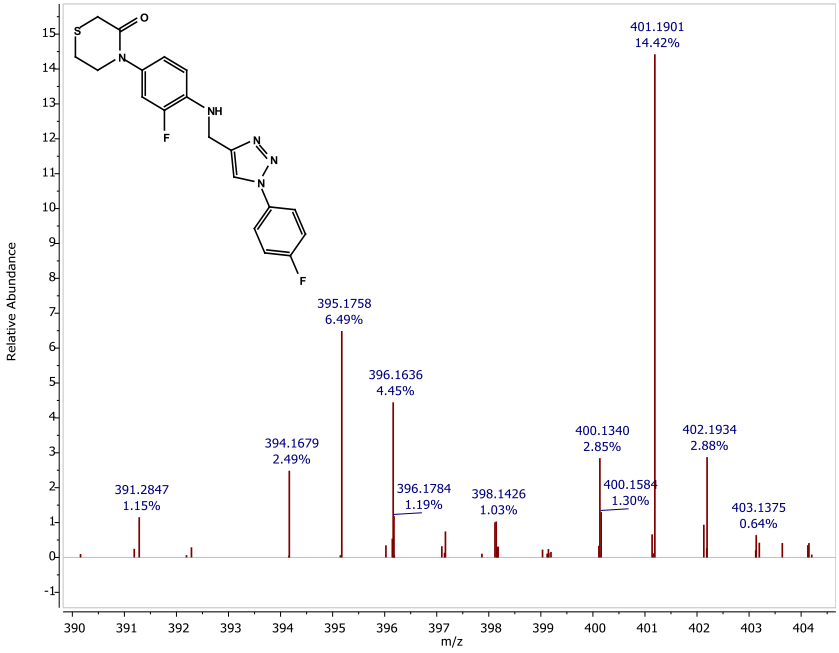


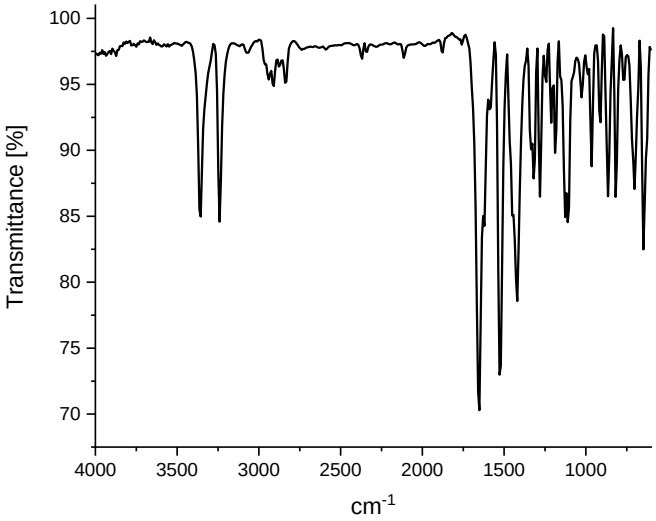
S12. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 35



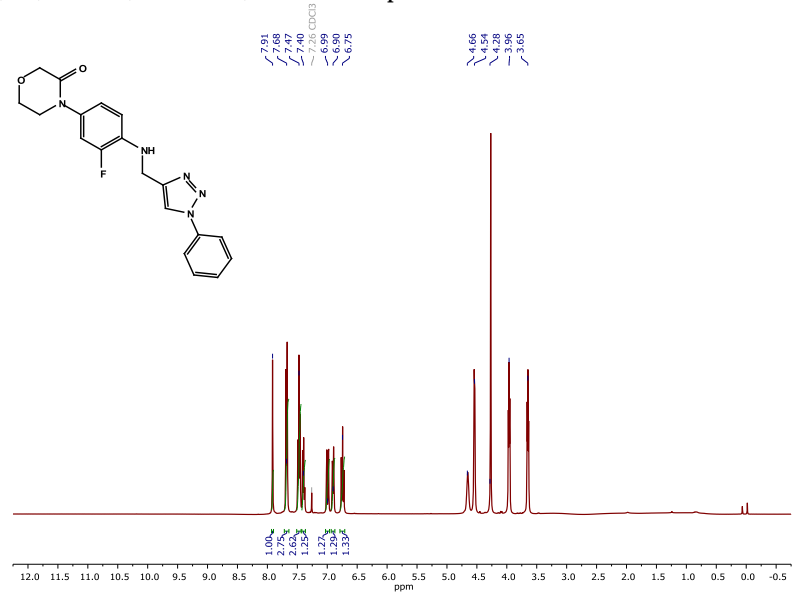

167.07
163.59
161.12
152.08
149.68
146.69
135.13
133.24
132.27
122.45
122.32
120.22
116.65
113.36
112.12
77.16 CDCl3
52.66
39.40
30.57
26.70
ppm

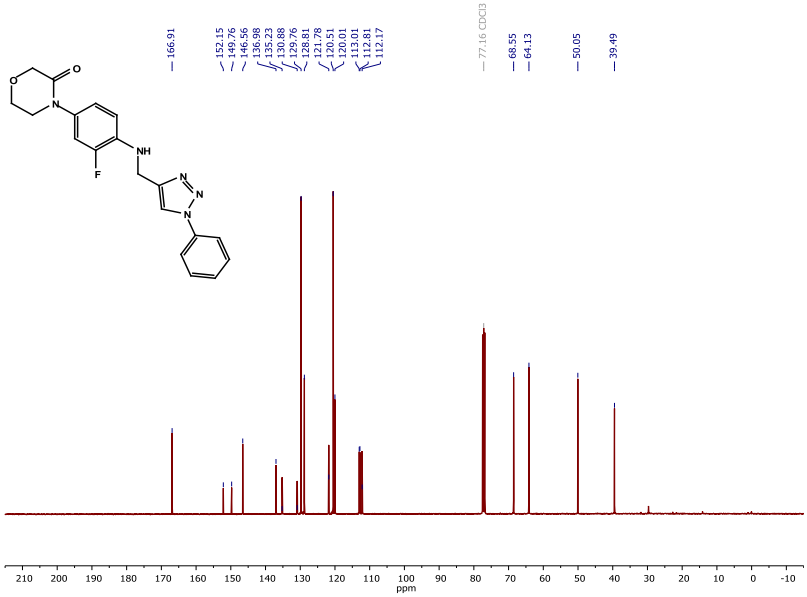

-112.13
-133.59
ppm

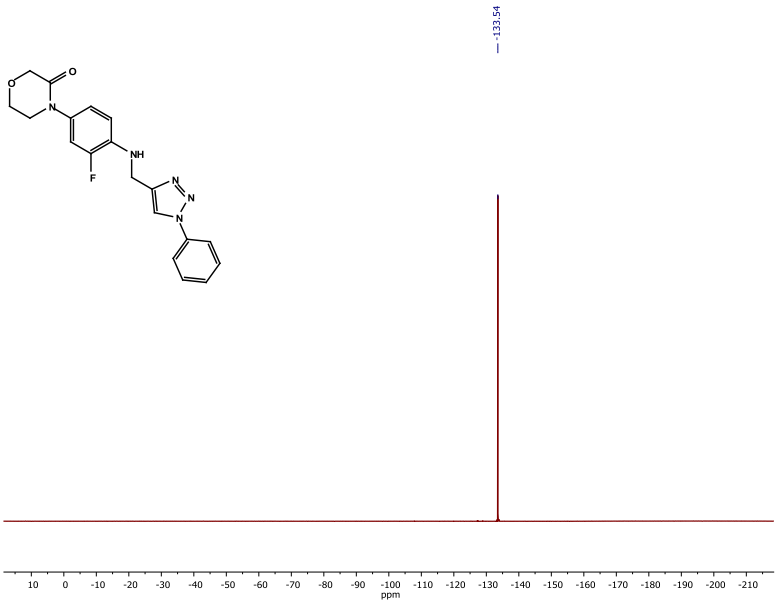

Relative Abundance
m/z
401.1901
14.42%
395.1758
6.49%
396.1636
4.45%
394.1679
2.49%
400.1340
2.85%
402.1934
2.88%
391.2847
1.15%
396.1784
1.19%
398.1426
1.03%
400.1584
1.30%
403.1375
0.64%
O
S
N
NH
F
N
N
N
F

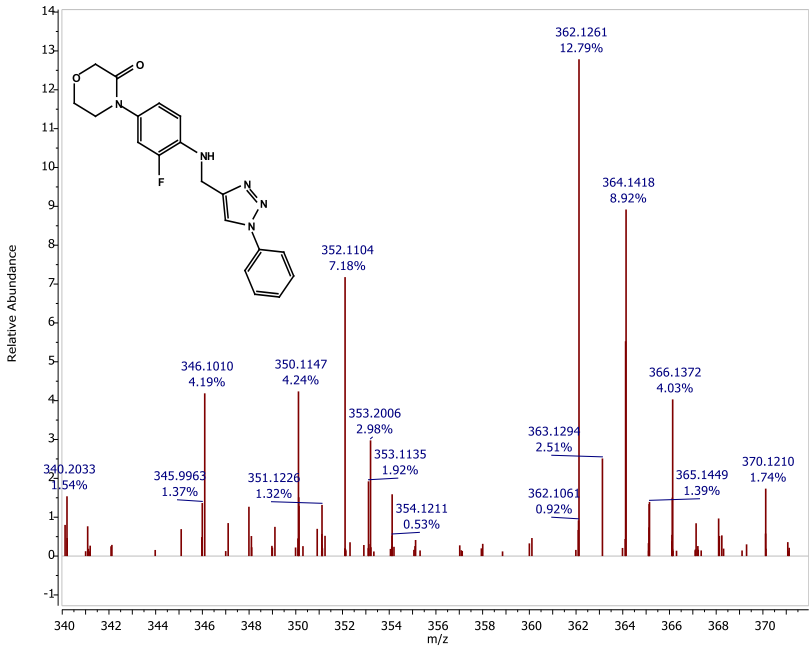

Transmittance [%]
cm-1

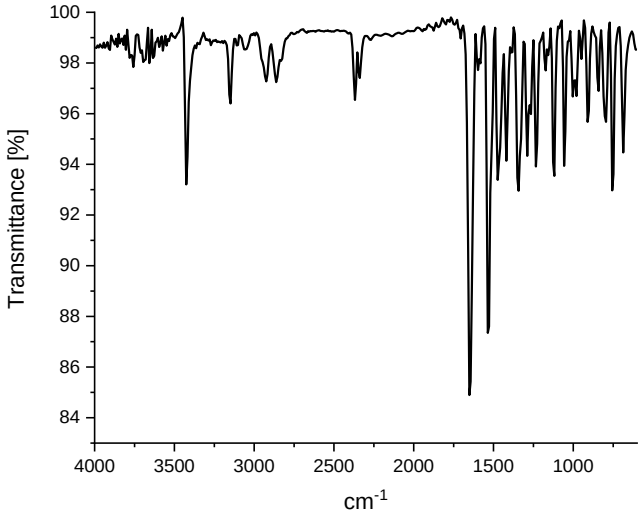
S13. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 36



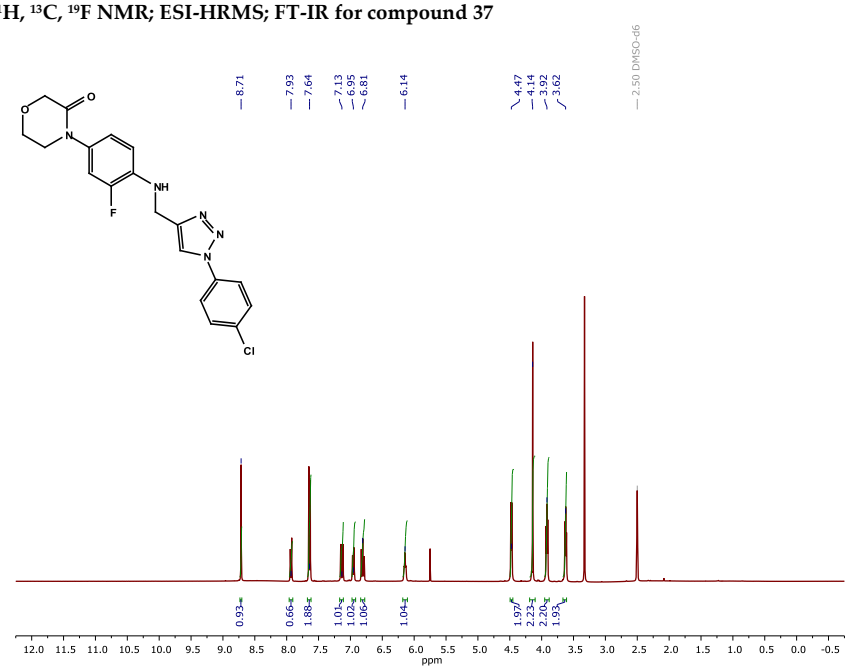


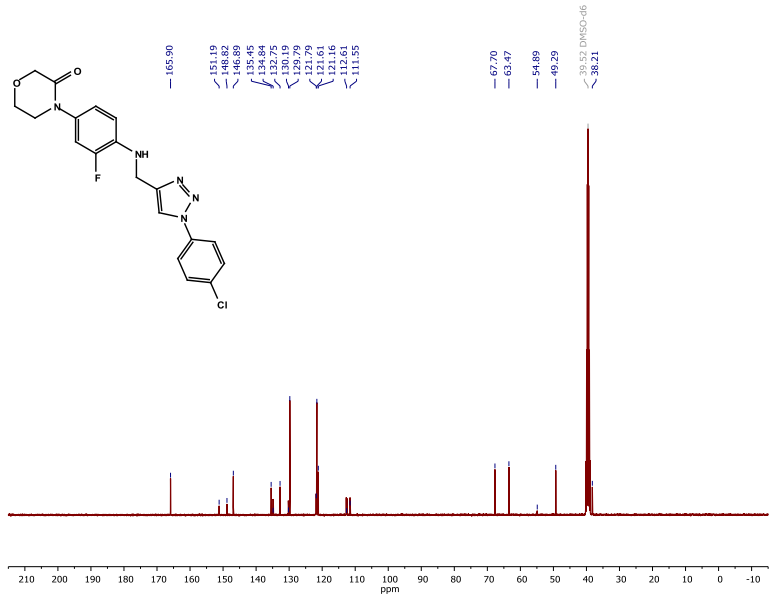

-133.54
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
ppm

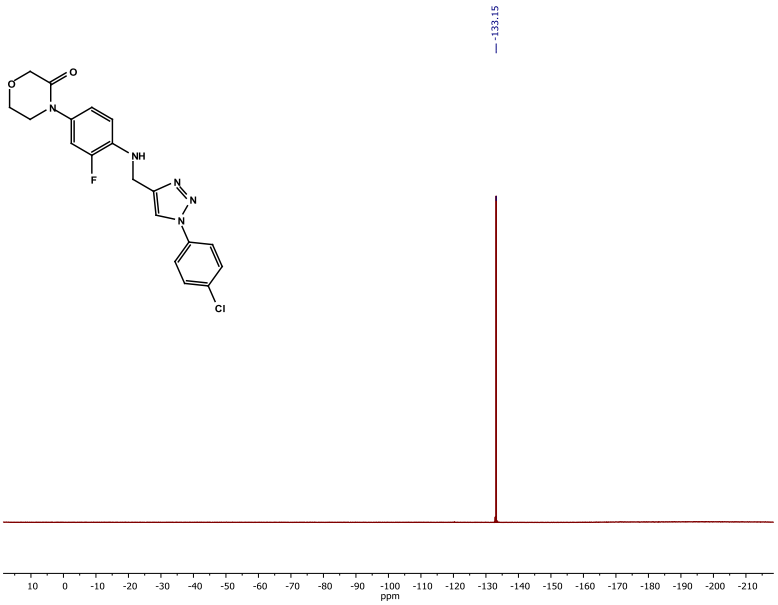

Relative Abundance
362.1261
12.79%
364.1418
8.92%
352.1104
7.18%
346.1010
4.19%
350.1147
4.24%
366.1372
4.03%
353.2006
2.98%
363.1294
2.51%
353.1135
1.92%
340.2033
1.54%
345.9963
1.37%
351.1226
1.32%
365.1449
1.39%
370.1210
1.74%
362.1061
0.92%
354.1211
0.53%
340 342 344 346 348 350 352 354 356 358 360 362 364 366 368 370
m/z

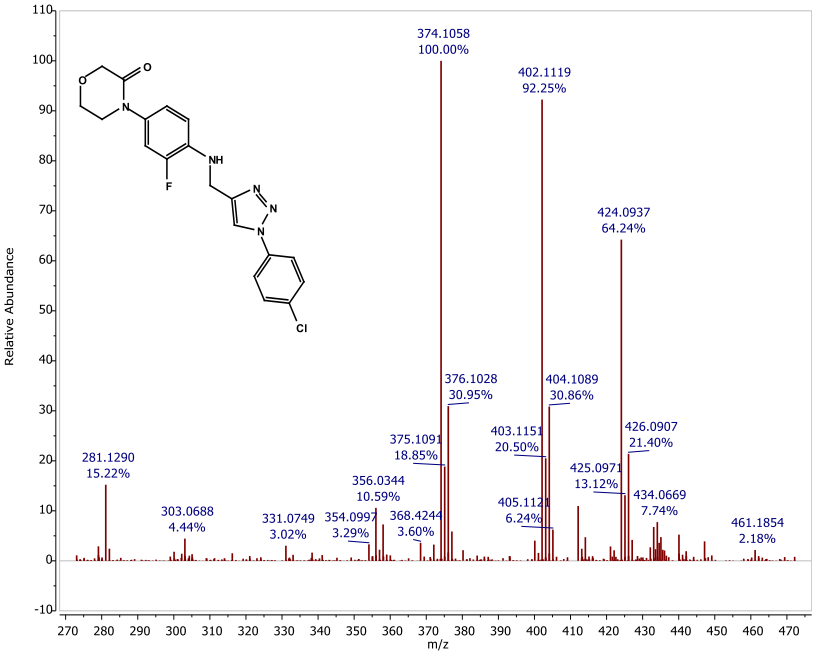


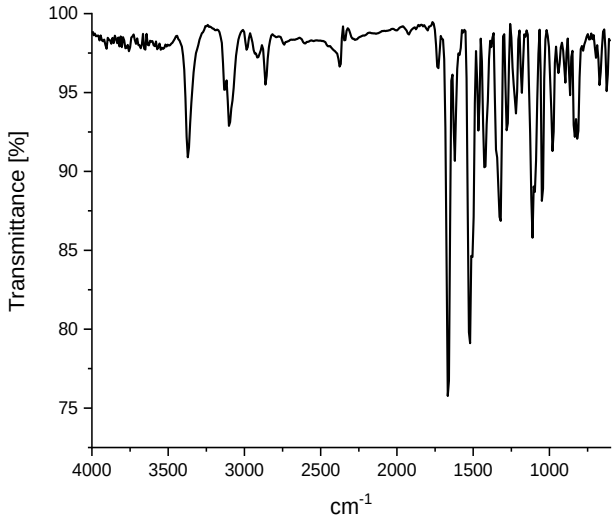
S14. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 37



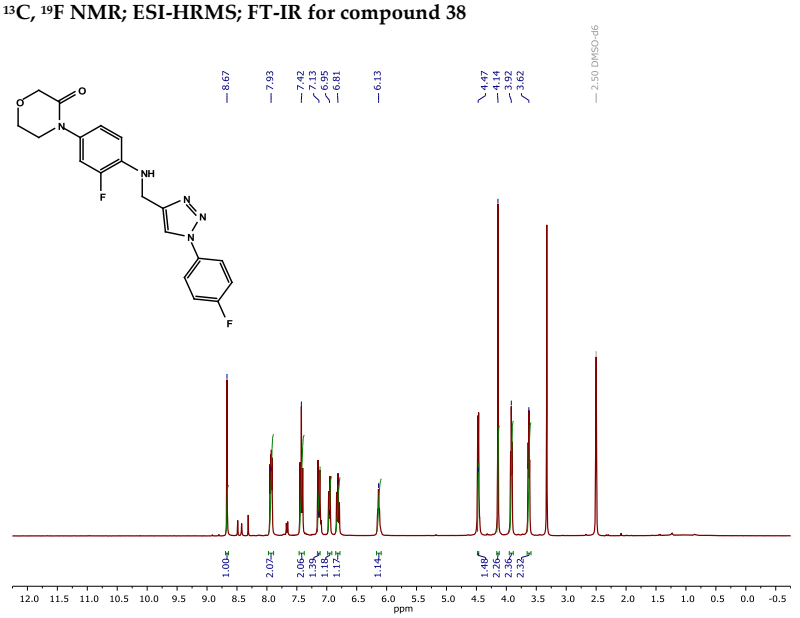

165.90
151.19
148.82
146.89
135.45
134.84
132.75
130.19
129.39
121.79
121.61
121.16
112.61
111.55
67.70
63.47
54.89
49.29
39.52 DMSO-d6
38.21
O
O
N
NH
F
N
N
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

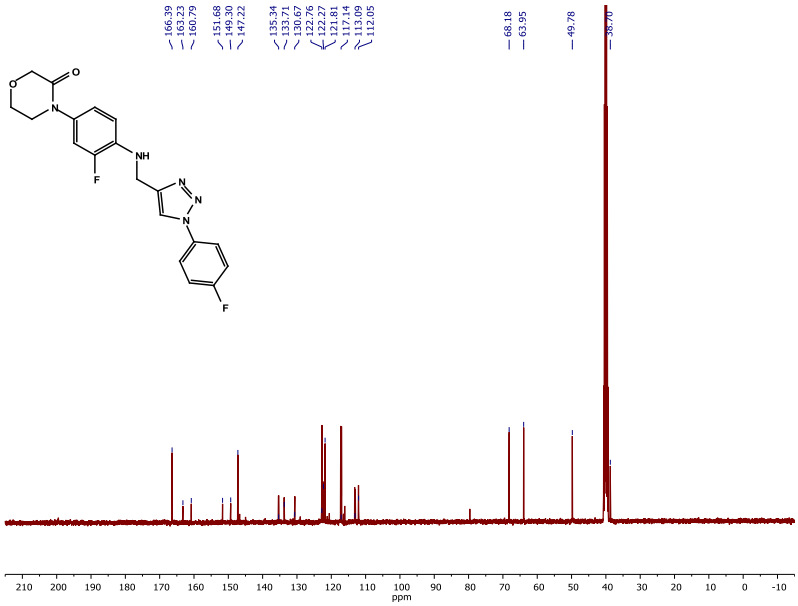

-133.15
O
O
N
NH
F
N
N
N
Cl
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
ppm

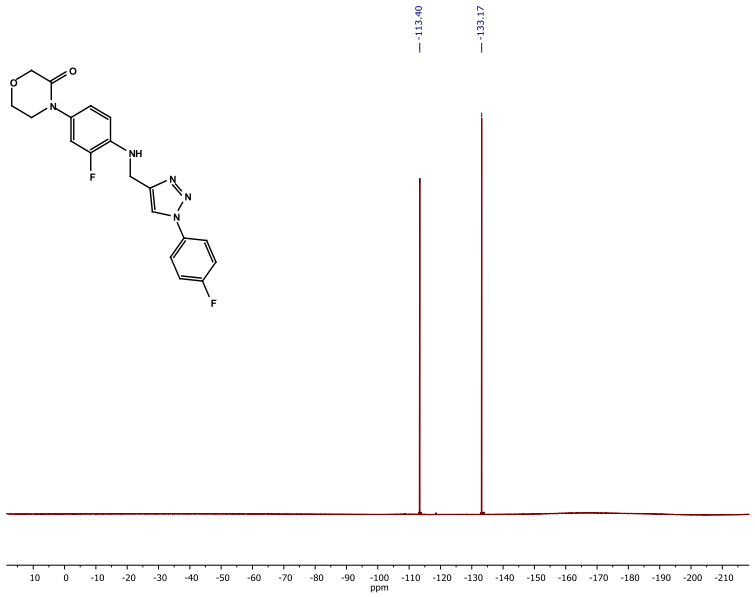

Relative Abundance
m/z
374.1058
100.00%
402.1119
92.25%
424.0937
64.24%
376.1028
30.95%
404.1089
30.86%
426.0907
21.40%
403.1151
20.50%
375.1091
18.85%
425.0971
13.12%
434.0669
7.74%
356.0344
10.59%
405.1121
6.24%
281.1290
15.22%
303.0688
4.44%
331.0749
3.02%
354.0997
3.29%
368.4244
3.60%
461.1854
2.18%
O
O
N
NH
F
N
N
N
Cl

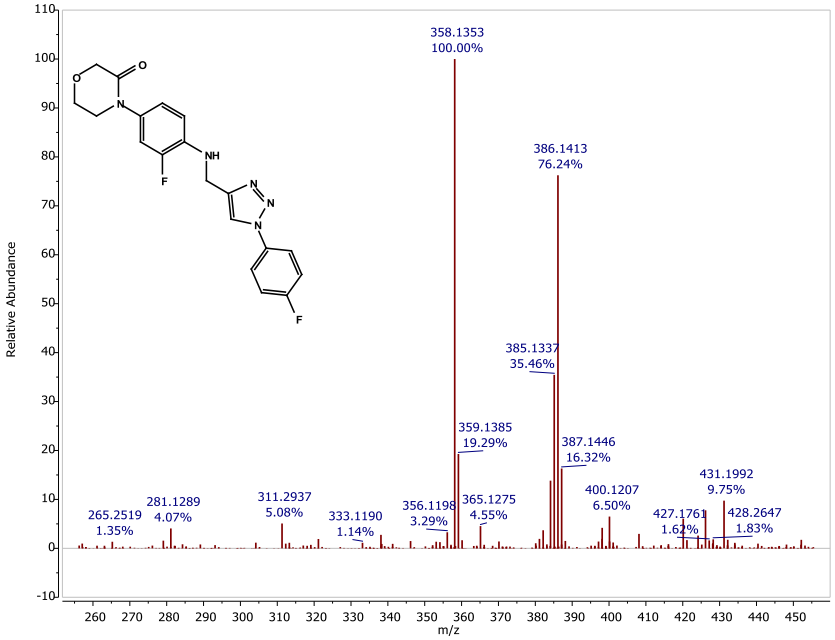

Transmittance [%]
cm-1

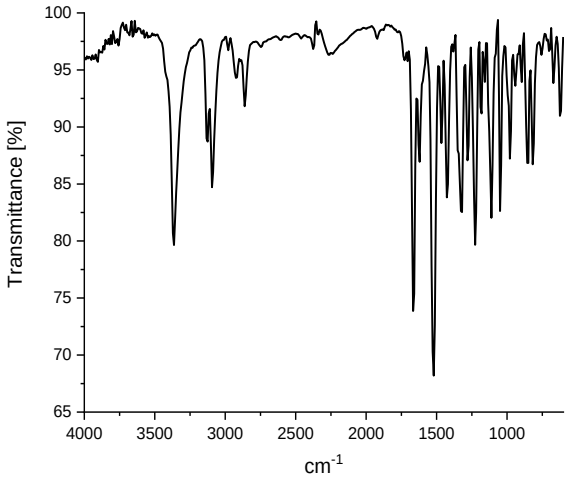
S15. ^{1}H, ^{13}C, ^{19}F NMR; ESI-HRMS; FT-IR for compound 38



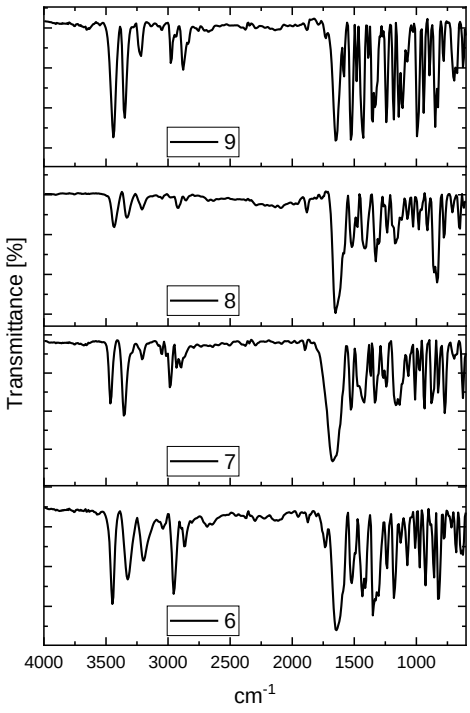


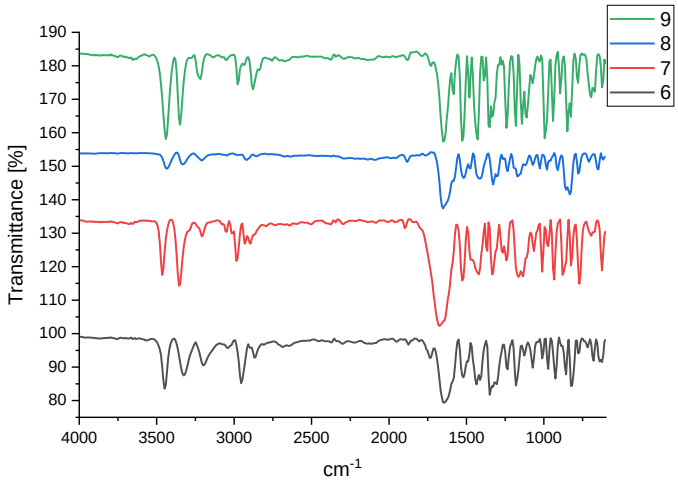

-113.40
-133.17
ppm


358.1353
100.00%
386.1413
76.24%
385.1337
35.46%
359.1385
19.29%
387.1446
16.32%
431.1992
9.75%
400.1207
6.50%
281.1289
4.07%
311.2937
5.08%
265.2519
1.35%
333.1190
1.14%
356.1198
3.29%
365.1275
4.55%
427.1761
1.62%
428.2647
1.83%
Relative Abundance
m/z

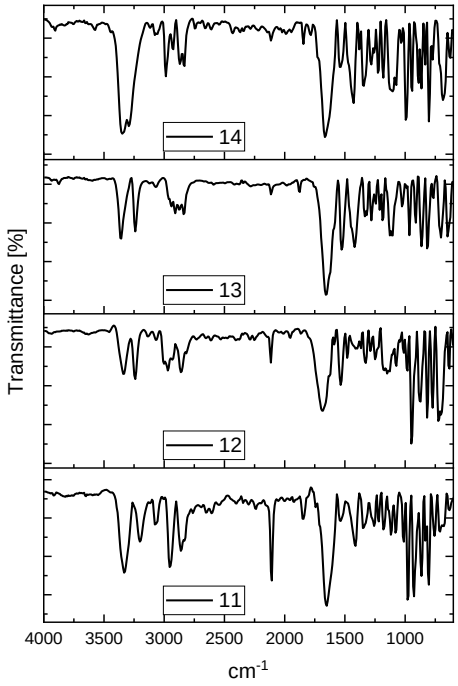

Transmittance [%]
100
95
90
85
80
75
70
65
4000
3500
3000
2500
2000
1500
1000
cm-1

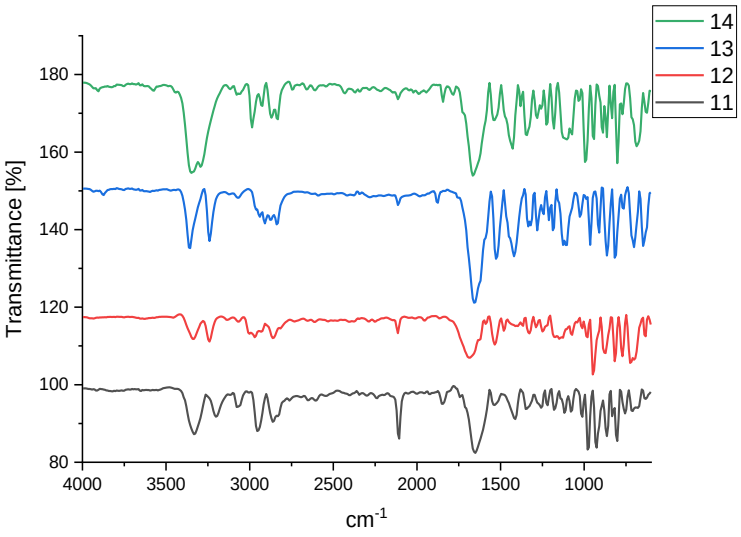
S16. FT-IR stacking for aniline compounds (6-9)



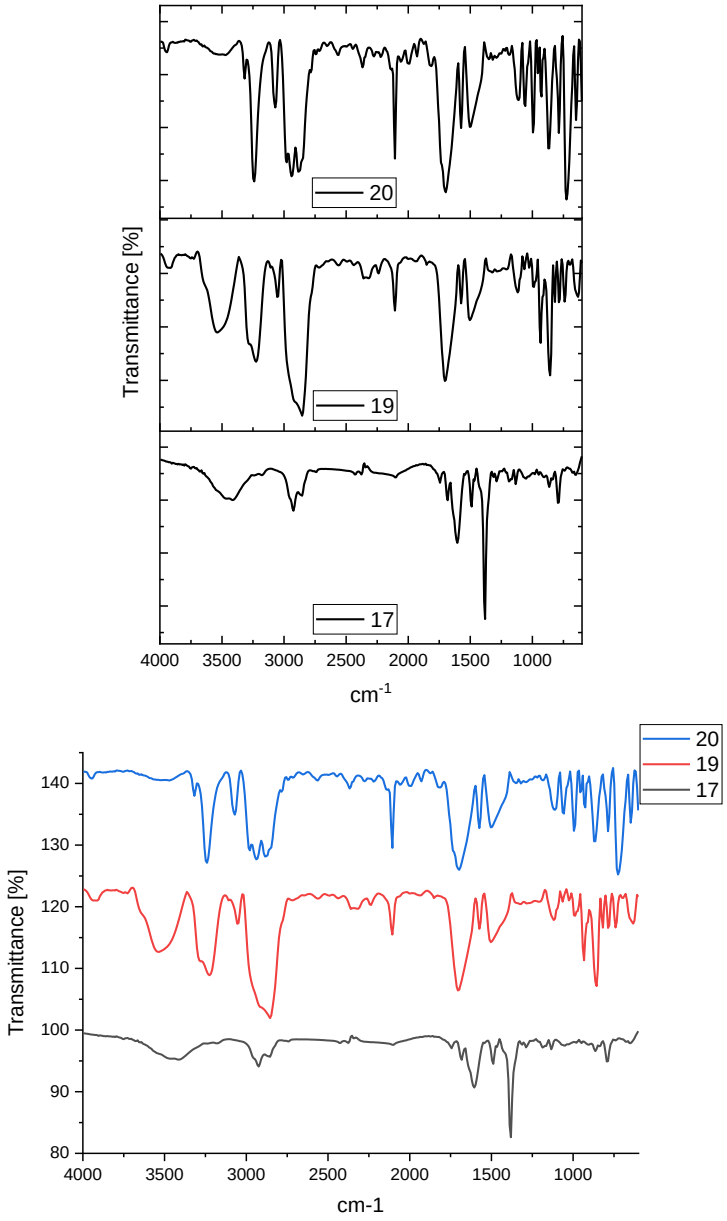


S17. FT-IR stacking for *N*-propargyl aniline compounds (11-14)

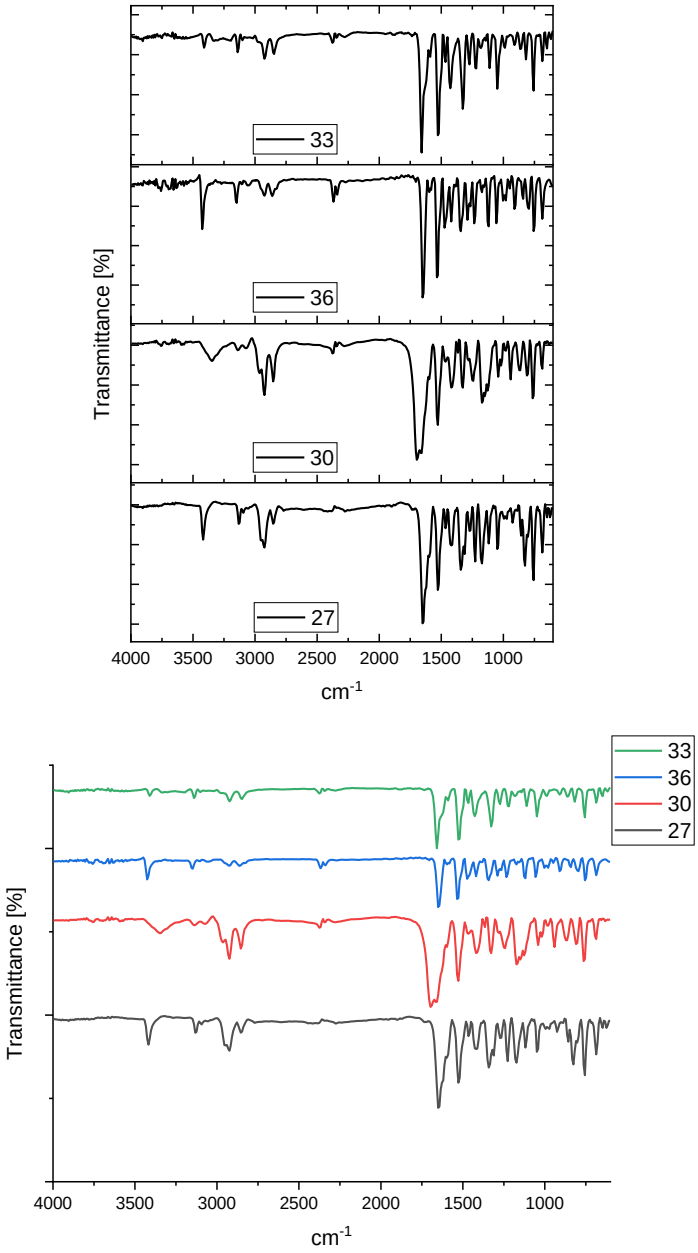




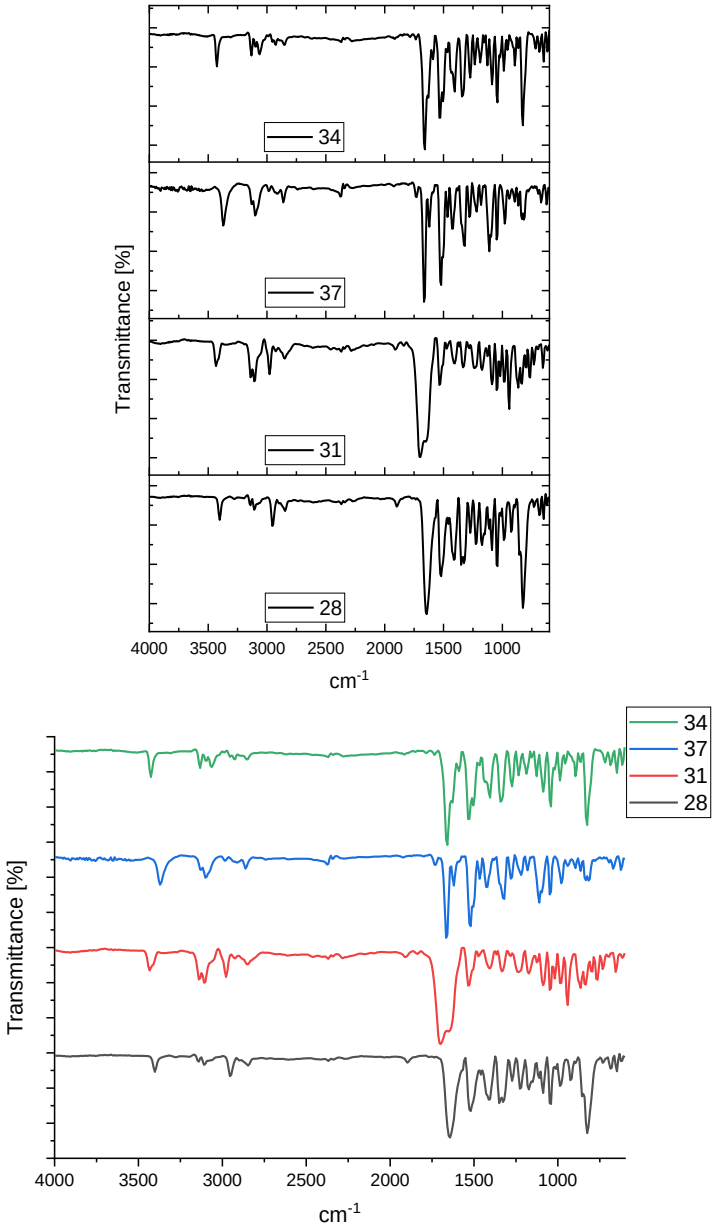
S18. FT-IR stacking for *N*-propargyl tetrahydroquinoline compounds (17-20)



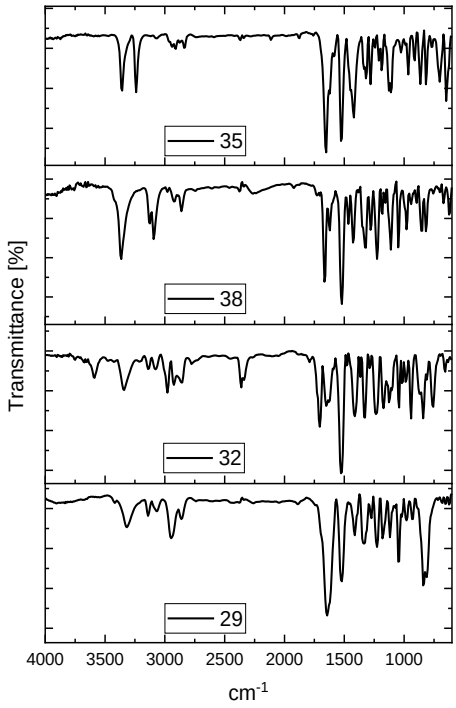
S19. FT-IR stacking for ^{1}H-1,2,3-triazole compounds (27,30,33,36)

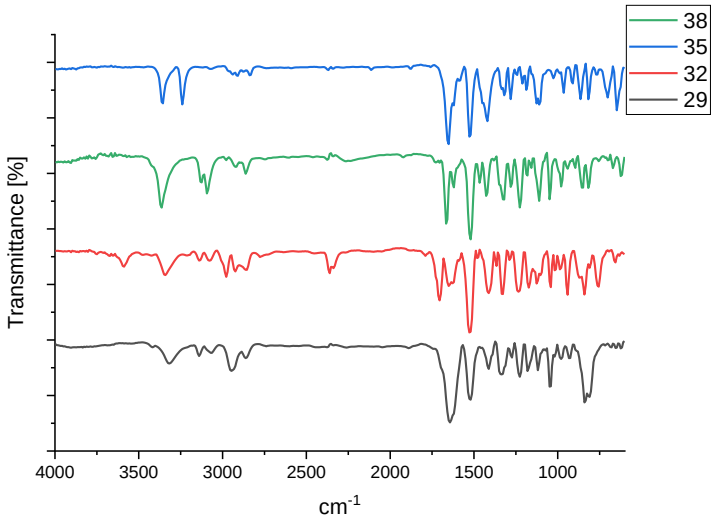


S20. FT-IR stacking for ^{1}H-1,2,3-triazole compounds (28,31,34,37)



S21. FT-IR stacking for ^{1}H-1,2,3-triazole compounds (29,32,35,38)





S22. Table of calculated log P of synthesized compounds (cont.)

Compound	log P[a]	Ilog P[b]	Xlog P3[b]	Wlog P[b]	Mlog P[b]	Silicos-IT[b]	Consensus[b]
6	0.84 ± 0.52	1.91	1.12	1.97	1.84	1.89	1.75
7	0.67 ± 0.65	2.69	1.39	1.66	1.54	1.08	1.67
8	0.35 ± 0.61	1.7	1.15	1.54	1.56	1.85	1.56
9	-0.50 ± 0.57	1.63	0.36	0.82	0.71	1.29	0.96
11	1.60 ± 0.56	2.71	1.90	2.32	2.56	2.84	2.47
12	1.42 ± 0.66	3.45	2.17	2.00	2.18	2.15	2.39
13	1.11 ± 0.63	2.22	1.93	1.88	2.3	2.79	2.22
14	0.25 ± 0.58	2.37	1.14	1.16	1.45	2.23	1.67
17	1.75 ± 0.71	3.39	1.57	1.88	2.86	3.11	2.56
18	1.26 ± 0.76	2.63	1.6	1.45	2.63	3.04	2.27
19	0.40 ± 0.73	3.12	0.8	0.73	1.82	2.48	1.79
20	2.58 ± 0.67	3.27	2.74	3.23	3.04	2.65	2.99
27	3.17 ± 0.68	3.56	3.37	3.89	3.53	3.28	3.52
28	2.63 ± 0.70	3.16	2.84	3.79	3.42	3.06	3.25
29	2.40 ± 0.87	4.19	3.01	2.92	2.68	1.95	2.95
30	3.00 ± 0.88	4.18	3.64	3.57	3.15	2.60	3.43
31	2.45 ± 0.91	4.05	3.11	3.48	3.05	2.38	3.21
32	2.09 ± 0.78	3.06	2.77	2.80	2.81	2.57	2.80
33	2.68 ± 0.80	3.34	3.40	3.45	3.31	3.21	3.34
34	2.14 ± 0.83	2.94	2.88	3.35	3.19	2.99	3.07
35	1.23 ± 0.69	3.19	1.98	2.08	2.01	2.01	2.25
36	1.83 ± 0.70	3.37	2.61	2.73	2.51	2.65	2.77
37	1.28 ± 0.74	3.11	2.08	2.64	2.39	2.43	2.53

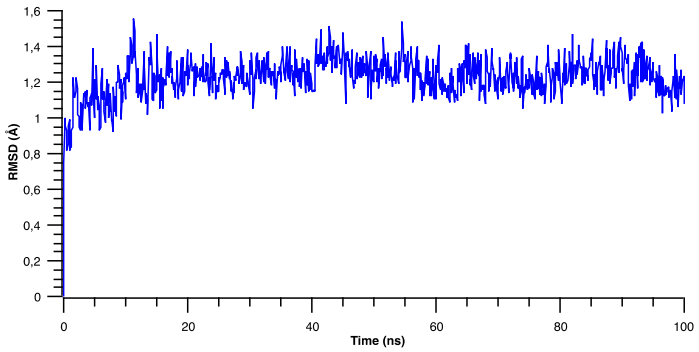
[a]log P of synthesized compounds were calculated using ACD Labs log P predictor. [b] log P of synthesized compounds were calculated using SwissADME log P predictor

S23. Reaction optimization for the synthesis of compounds 7-9

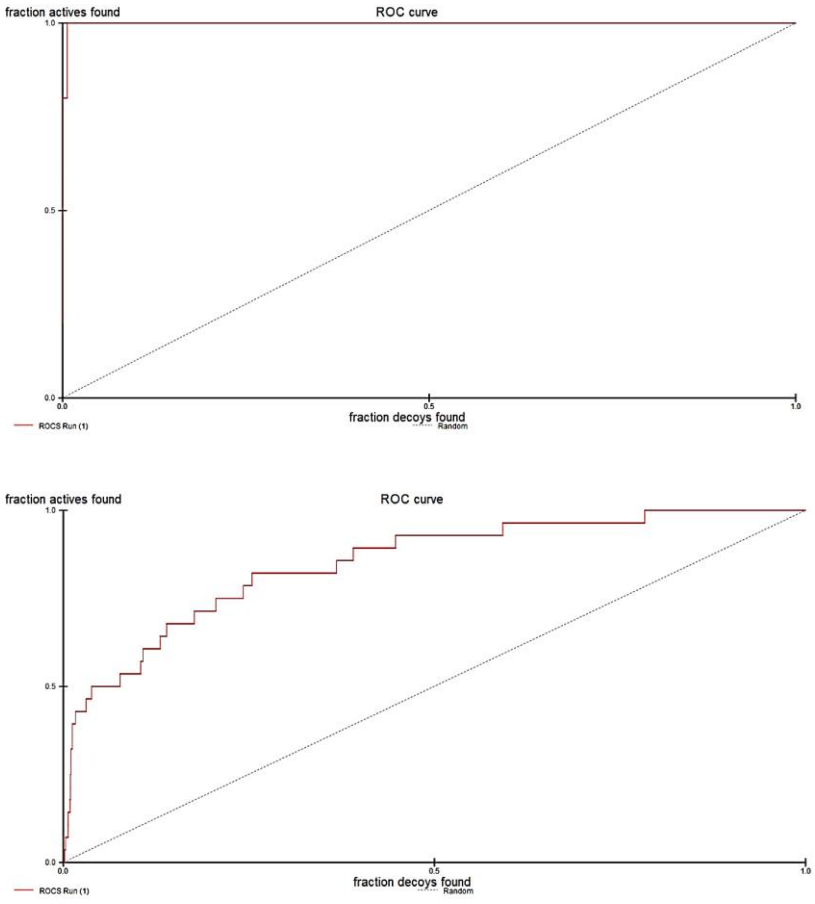
Entry	Lactam (equiv.)	Aniline (equiv.)	CuI (equiv.)	DMEDA (equiv.)	T (°C)	Time (h)	Heating source	Yield (%)[1]	Yield (%)[2]	Yield (%)[3]
1	1.2	1	0.5	0.5	20	96	r.t.	12.74	9.51	15.29
2	1.2	1	0.5	0.5	100	72	conventional	39.5	23.16	40.41
3	1.2	1	0.5	0.5	120	48	conventional	25.48	28.87	45.37
4	1.2	1	0.5	0.5	60	6	sonication	28.55	30.82	62.81
5	1.2	1	0.05	0.1	120	2,0	microwave	6.68	0.91	15,0
6	1.2	1	0.1	0.2	120	2,0	microwave	31.6	3.86	29.67
7	1.2	1	0.15	0.3	120	2,0	microwave	34.87	8.45	52.79
8	1.2	1	0.25	0.5	120	2,0	microwave	39.5	23.16	60.69
9	1.2	1	0.5	0.5	120	2,0	microwave	79.69	62.31	86.91
10	1.2	1	0.5	0.5	160	1.5	microwave	**85.49**[4]	**73.3**	**88.74**
11	**1**	**1.2**	0.5	0.5	160	1.5	microwave	**90.0**[4]	**86.0**	**94.0**

[1]*N*-Boc piperazinone (**7**), [2]Thiomorpholinone (**8**), [3]Morpholinone (**9**), [4]Reaction temperature 90 °C.

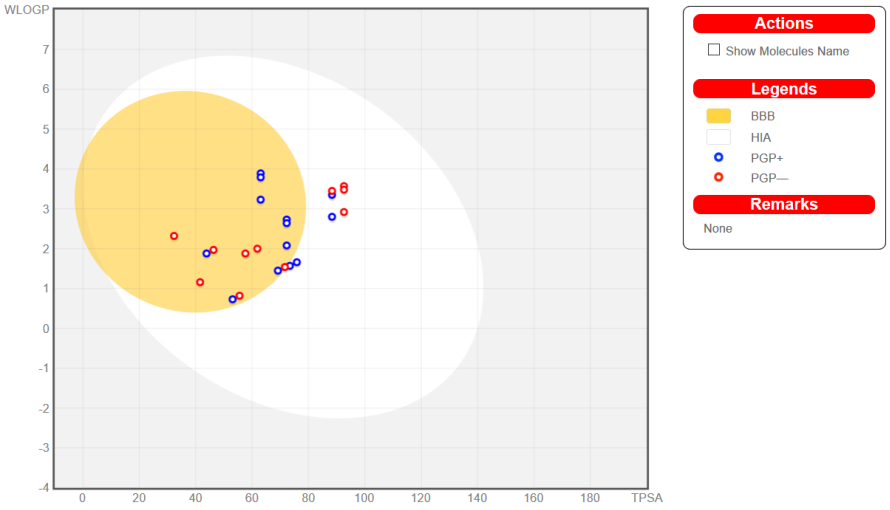
S24. Dynamic RMSD for compound 19

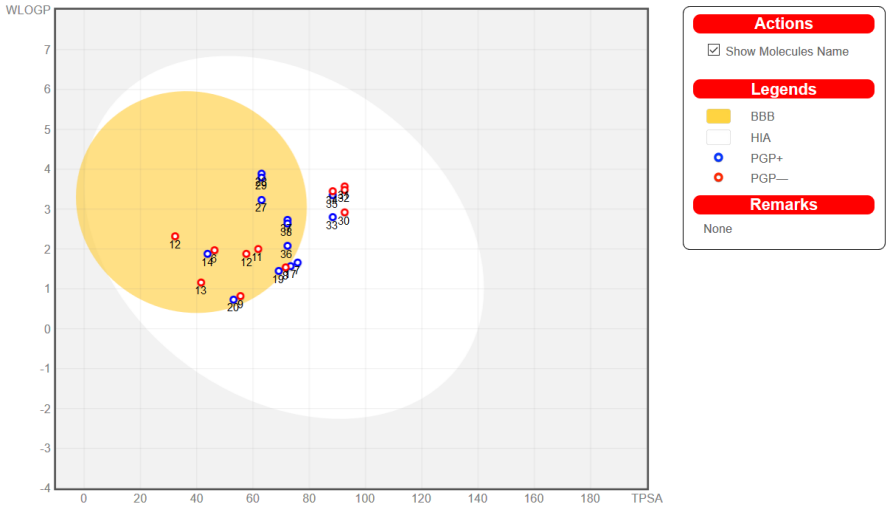


S25. ROCs AUC curve for method enrichment



S26. Boiled egg diagram for blood brain-barrier





S27. Crystal data and structure refinement for compound 6

Identification code	6	
Empirical formula	C11H13FN2O	
Formula weight	208.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1/n)	
Unit cell dimensions	a = 5.6811(8) Å	α= 90°.
	b = 13.3981(19) Å	β= 97.192(5)°.
	c = 13.2740(18) Å	γ = 90°.
Volume	1002.4(2) Å3	
Z	4	
Density (calculated)	1.380 Mg/m3	
Absorption coefficient	0.103 mm-1	
F(000)	440	
Crystal size	0.12 x 0.11 x 0.10 mm3	
Theta range for data collection	2.17 to 26.41°.	
Index ranges	-7<=h<=7, -16<=k<=16, -16<=l<=16	
Reflections collected	28701	
Independent reflections	2050 [$R_{(int)}$ = 0.0472]	
Completeness to theta = 26.41°	99.8 %	
Max. and min. transmission	0.9900 and 0.9874	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2050 / 50 / 199	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2σ(I)]	R_1= 0.0461, wR_2 = 0.1292	
R indices (all data)	R_1= 0.0571, wR_2 = 0.1376	
Largest diff. peak and hole	0.488 and -0.262 e.Å-3	

S28. Crystal data and structure refinement for compound 9

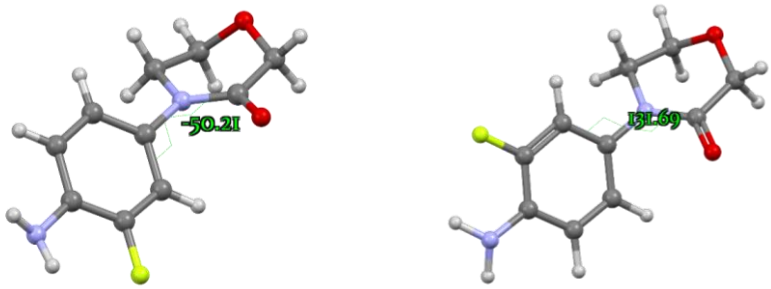
Identification code	9	
Empirical formula	C10H11FN2O2	
Formula weight	210.21	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.2264(16) Å	α= 90°.
	b = 6.3168(5) Å	β= 109.377(2)°.
	c = 16.1031(12) Å	γ = 90°.
Volume	1940.9(3) $Å^3$	
Z	8	
Density (calculated)	1.439 Mg/m^3	
Absorption coefficient	0.114 mm^{-1}	
F(000)	880	
Crystal size	0.27 x 0.21 x 0.13 mm^3	
Theta range for data collection	2.68 to 26.40°.	
Index ranges	-25<=h<=25, -7<=k<=7, -20<=l<=20	
Reflections collected	27057	
Independent reflections	1991 [$R_{(int)}$ = 0.0389]	
Completeness to theta = 26.40°	99.9 %	
Max. and min. transmission	0.9858 and 0.9698	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1991 / 0 / 180	
Goodness-of-fit on F^2	0.789	
Final R indices [I>2σ(I)]	R_1= 0.0343, wR_2 = 0.0944	
R indices (all data)	R_1= 0.0394, wR_2 = 0.0995	
Largest diff. peak and hole	0.231 and -0.186 $e.Å^{-3}$	

S29. Crystal data and structure refinement for compound 20

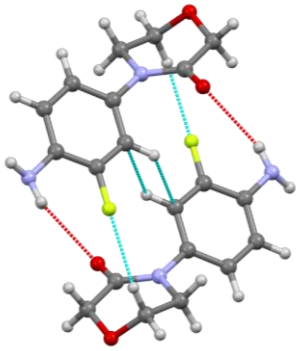
Identification code	20	
Empirical formula	C21H21FN2O3	
Formula weight	368.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7304(9) Å	α= 77.885(3)°.
	b = 9.6126(10) Å	β= 71.698(3)°.
	c = 11.8765(12) Å	γ = 70.361(3)°.
Volume	885.15(16) $Å^3$	
Z	2	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	388	
Crystal size	0.15 x 0.13 x 0.10 mm^3	
Theta range for data collection	1.82 to 26.46°.	
Index ranges	-10<=h<=10, -11<=k<=12, -14<=l<=14	
Reflections collected	32341	
Independent reflections	3639 [$R_{(int)}$ = 0.0429]	
Completeness to theta = 26.46°	99.8 %	
Max. and min. transmission	0.9902 and 0.9851	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3639 / 0 / 244	
Goodness-of-fit on F^2	1.116	
Final R indices [I>2σ(I)]	R1 = 0.0518, wR2 = 0.1552	
R indices (all data)	R1 = 0.0619, wR2 = 0.1666	
Largest diff. peak and hole	0.864 and -0.299 $e.Å^{-3}$	

S30. Dihedral bond angle difference between calculated and experimental compound 9.

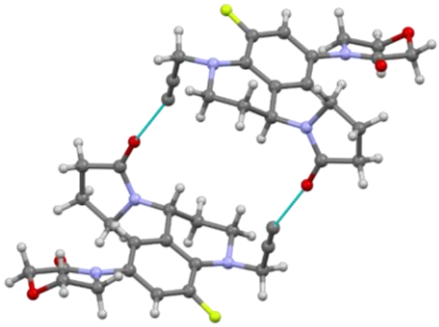
Calculated **Experimental**



S31. Hydrogen bond formed in compound 9 crystal



S32. Interactions between the propargyl and the carbonyl group in the crystal structure of compound 20



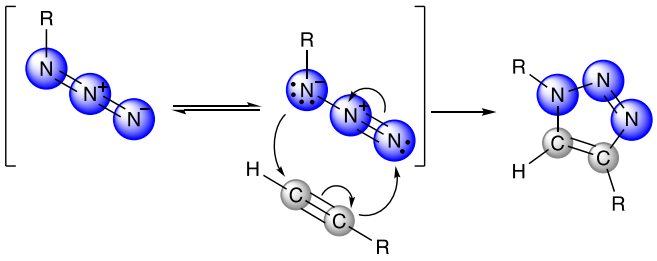
S33. Fukui functions for compound 14

Atom		Neutral	Cation	Anion	f^-	f^+	f°	Δf
Nº	Type							
1	**S**	0.258944	0.353466	0.137422	0.094522	0.121522	0.108022	0.027000
2	**C**	-0.638921	-0.624136	-0.604985	0.014785	0.033936	0.024361	0.019151
3	**C**	-0.143918	-0.133043	-0.117730	0.010875	0.026188	0.018532	0.015313
4	**N**	-0.687981	-0.663278	-0.661368	0.024703	0.026613	0.025658	0.001910
5	**C**	0.576118	0.595208	0.485268	0.019090	0.090850	0.054970	0.071760
6	**C**	-0.748307	-0.714594	-0.732123	0.033713	0.016184	0.024949	-0.017529
7	**C**	0.351941	0.188277	0.322766	0.163664	0.029175	0.096420	-0.134489
8	**C**	-0.244880	-0.033686	-0.295819	0.211194	0.050939	0.131067	-0.160255
9	**C**	0.258751	0.231914	0.240765	0.026837	0.017986	0.022412	-0.008851
10	**C**	0.229809	0.364839	0.182387	0.135030	0.047422	0.091226	-0.087608
11	**C**	-0.121101	-0.123262	-0.151056	0.002161	0.029955	0.016058	0.027794
12	**C**	-0.112750	-0.033566	-0.114877	0.079184	0.002127	0.040656	-0.077057
13	**F**	-0.315098	-0.302832	-0.345970	0.012266	0.030872	0.021569	0.018606
14	**N**	-0.663792	-0.689837	-0.673497	0.026045	0.009705	0.017875	-0.016340
15	**C**	-0.208653	-0.175108	-0.194225	0.033545	0.014428	0.023987	-0.019117
16	**O**	-0.389878	-0.357438	-0.498669	0.032440	0.108791	0.070616	0.076351
17	**C**	0.229584	0.156303	0.257936	0.073281	0.028352	0.050817	-0.044929
18	**C**	-0.526177	-0.432097	-0.591886	0.094080	0.065709	0.079895	-0.028371
19	**H**	0.224413	0.246404	0.175686	0.021991	0.048727	0.035359	0.026736
20	**H**	0.230835	0.256244	0.185958	0.025409	0.044877	0.035143	0.019468
21	**H**	0.202515	0.221628	0.167322	0.019113	0.035193	0.027153	0.016080
22	**H**	0.225757	0.242181	0.168567	0.016424	0.057190	0.036807	0.040766
23	**H**	0.243868	0.280782	0.168761	0.036914	0.075107	0.056011	0.038193
24	**H**	0.256761	0.279102	0.206292	0.022341	0.050469	0.036405	0.028128
25	**H**	0.185274	0.231223	0.140703	0.045949	0.044571	0.045260	-0.001378
26	**H**	0.168206	0.221657	0.121542	0.053451	0.046664	0.050058	-0.006787
27	**H**	0.186011	0.203863	0.152611	0.017852	0.033400	0.025626	0.015548
28	**H**	0.315077	0.404017	0.289489	0.088940	0.025588	0.057264	-0.063352
29	**H**	0.210411	0.271672	0.174992	0.061261	0.035419	0.048340	-0.025842
30	**H**	0.225779	0.276459	0.208341	0.050680	0.017438	0.034059	-0.033242
31	**H**	0.221403	0.257637	0.195397	0.036234	0.026006	0.031120	-0.010228

S34. Fukui functions for compound 25

Atom		Neutral	Cation	Anion	*f*-	*f*+	*f°*	Δ*f*
Nº	Type							
1	C	-0.080679	-0.024180	-0.113052	0.056499	0.032373	0.044436	-0.024126
2	C	-0.149657	-0.117282	-0.162486	0.032375	0.012829	0.022602	-0.019546
3	C	-0.138827	-0.051506	-0.202111	0.087321	0.063284	0.075303	-0.024037
4	C	-0.149657	-0.117282	-0.162486	0.032375	0.012829	0.022602	-0.019546
5	C	-0.080679	-0.024180	-0.113052	0.056499	0.032373	0.044436	-0.024126
6	C	0.025736	0.084568	0.023830	0.058832	0.001906	0.030369	-0.056926
7	N	-0.166497	-0.074790	-0.242773	0.091707	0.076276	0.083992	-0.015431
8	N	0.017948	0.037180	-0.122350	0.019232	0.140298	0.079765	0.121066
9	N	-0.071665	0.080270	-0.295994	0.151935	0.224329	0.188132	0.072394
10	H	0.160865	0.240213	0.076127	0.079348	0.084738	0.082043	0.005390
11	H	0.158119	0.239545	0.081440	0.081426	0.076679	0.079053	-0.004747
12	H	0.156008	0.247687	0.075340	0.091679	0.080668	0.086174	-0.011011
13	H	0.158119	0.239545	0.081440	0.081426	0.076679	0.079053	-0.004747
14	H	0.160865	0.240213	0.076127	0.079348	0.084738	0.082043	0.005390

S35. Reaction species according to Fukui calculations



S36. Calculated thermochemical energies

Compound	E (hartree)	E (eV)	E (kcal/mol)	E (kJ/mol)	ΔH (kcal/mol)	ΔH (kJ/mol)
12	-826.73	-22496.89	-518779.39	-2170571.43	-	-
13	-1188.45	-32340.04	-745762.91	-3120269.84	-	-
14	-1185.62	-32263.15	-743989.80	-3112851.15	-	-
15	-862.63	-23474.02	-541312.09	-2264848.18	-	-
29	-1222.51	-33266.98	-767138.05	-3209703.34	-61.76	-258.39
32	-1584.23	-43110.13	-994121.74	-4159402.43	-61.92	-259.07
35	-1581.41	-43033.25	-992348.76	-4151984.31	-62.06	-259.64
38	-1258.42	-34244.11	-789670.70	-3303979.91	-61.71	-258.22
30	-1682.12	-45773.94	-1055549.11	-4416414.36	-61.58	-257.65
33	-2043.84	-55617.09	-1282532.70	-5366113.04	-61.64	-257.92
36	-2041.02	-55540.20	-1280759.71	-5358694.86	-61.77	-258.43
39	-1718.03	-46751.06	-1078081.71	-4510690.70	-61.48	-257.23
31	-1321.76	-35967.86	-829420.50	-3470292.93	-61.56	-257.57
34	-1683.49	-45811.01	-1056404.14	-4419991.81	-61.67	-258.04
37	-1680.66	-45734.13	-1054631.13	-4412573.55	-61.78	-258.47
40	-1357.67	-36944.99	-851953.11	-3564569.31	-61.47	-257.20
25	-395.69	-10767.41	-248296.90	-1038873.52	-	-
26	-494.94	-13468.30	-310579.55	-1299463.93	-	-
27	-855.30	-23274.37	-536708.14	-2245585.28	-	-