Supporting Information

3-(Benzo[*d*]thiazol-2-yl)-4-aminoquinoline derivatives as novel scaffold topoisomerase I inhibitor *via* DNA intercalation: design, synthesis and antitumor activities

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1. X-ray crystallography of compound **6i**

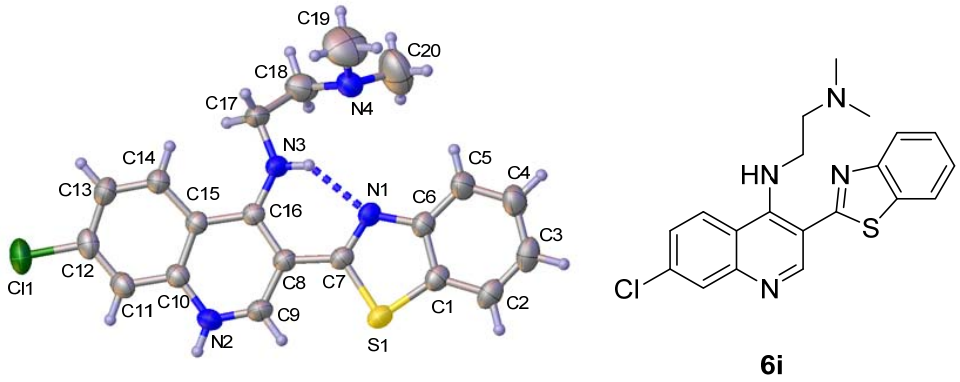


Fig. S1. Crystal structure diagram of compound **6i**.

Table S1

Some crystallographical data for compound **6i**

Empirical formula	$C_{20}H_{19}ClN_4S$
Formula weight	382.91
Temperature/K	296.15
Crystal system	monoclinic
Space group	P21/n
a/Å, b/Å, c/Å	13.793 (5), 8.597 (3), 16.140 (5)
α/°, β/°, γ/°	90.00, 104.275 (5), 90.00
Volume/Å^3	1854.7 (11)
Z	4
ρ_{calc}/mg mm^{-3}	1.375
μ/mm^{-1}	0.33
F (000)	804
Crystal size/mm^3	0.44 × 0.20 × 0.15
2Θ range for data collection	3.48 to 52.74°
Index ranges	$-17 \le h \le 17$, $-10 \le k \le 10$, $-20 \le l \le 20$
Reflections collected	20774
Independent reflections	3791[R(int) = 0.0570]
Data/restraints/parameters	3791/0/237
Goodness-of-fit on F^2	1.026
Final R indexes [I>2σ (I)]	R1 = 0.0592, wR2 = 0.1569
Final R indexes [all data]	R1 = 0.0900, wR2 = 0.1793
Largest diff. peak/hole/e·Å^{-3}	0.923/-0.470

2. Spectrum of UV-vis absorption and fluorescent emission profile for **5a**

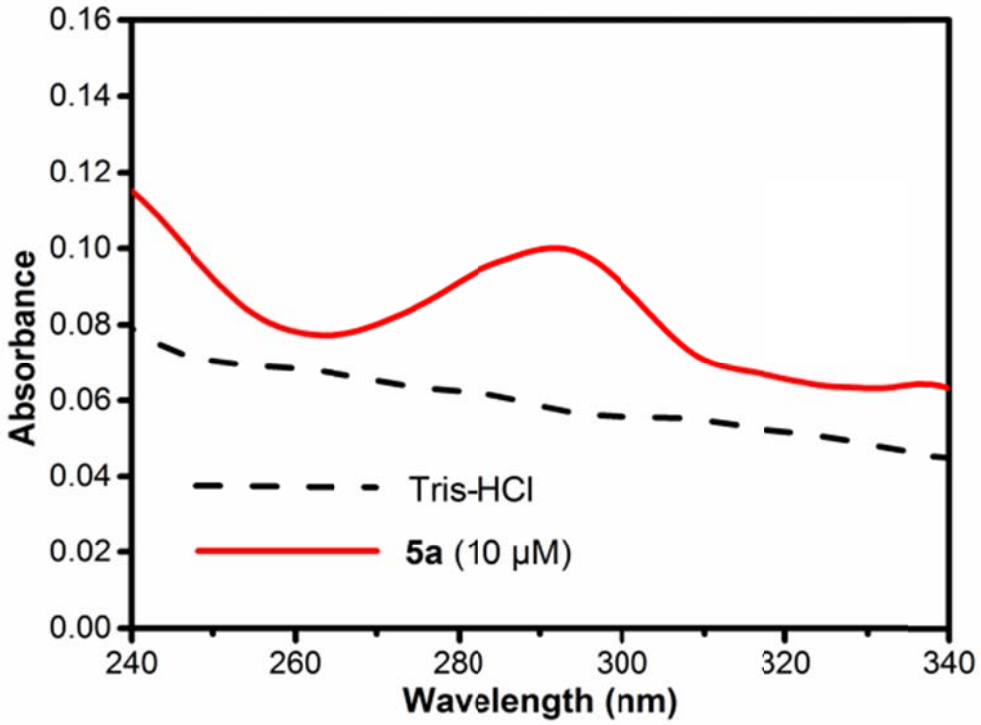


Fig. S2. UV-vis absorption spectrum of **5a**

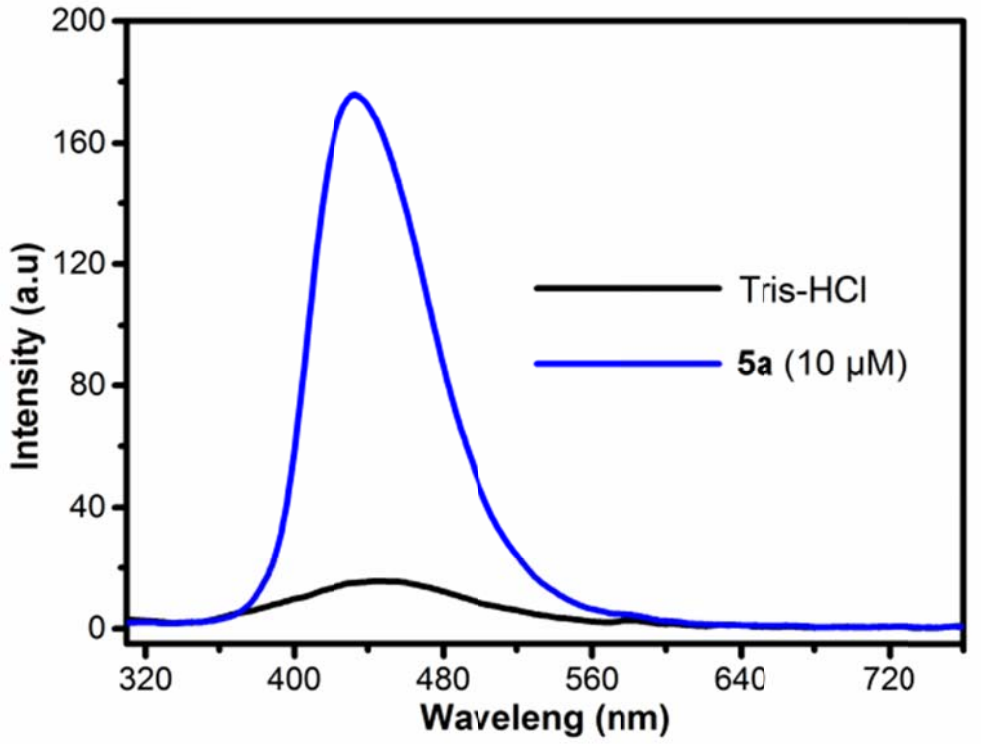
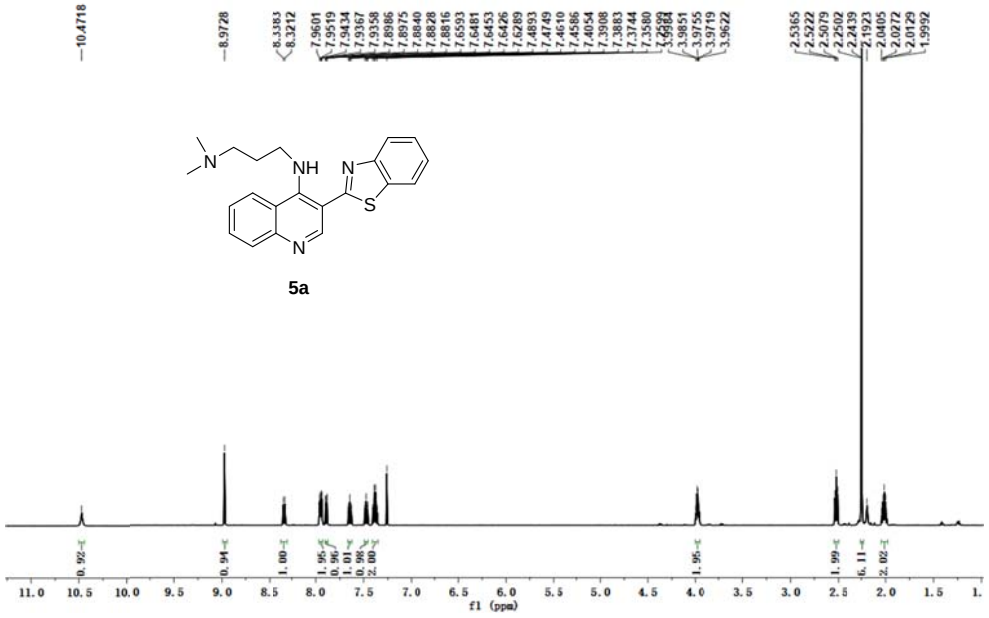
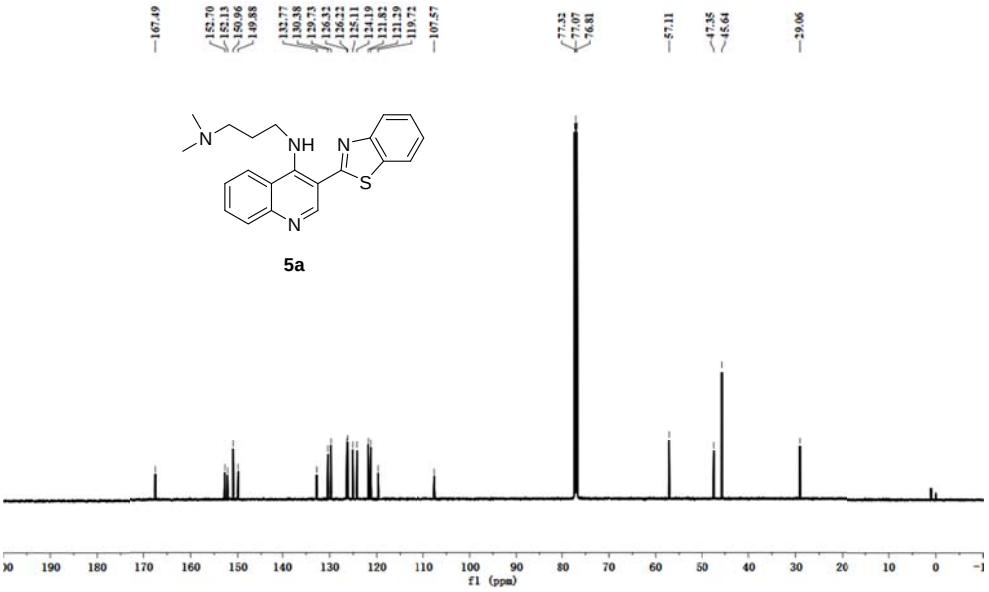


Fig. S3. Fluorescent emission spectrum of **5a**

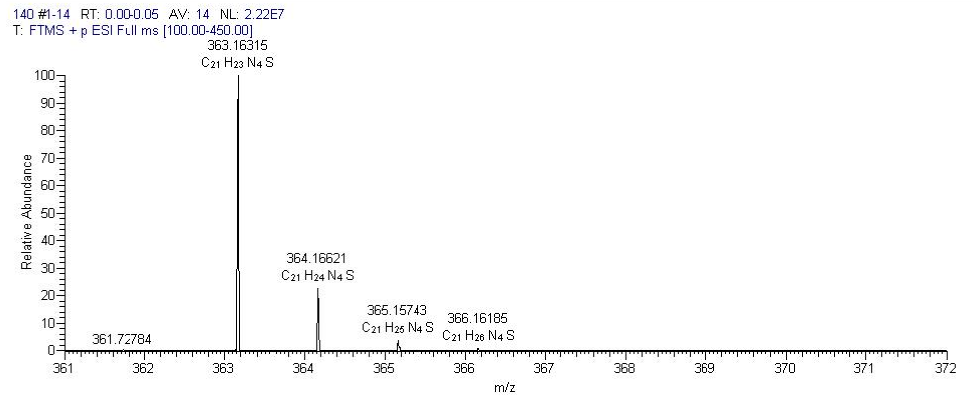
3. NMR and HRMS spectrum for compounds 5a–6n

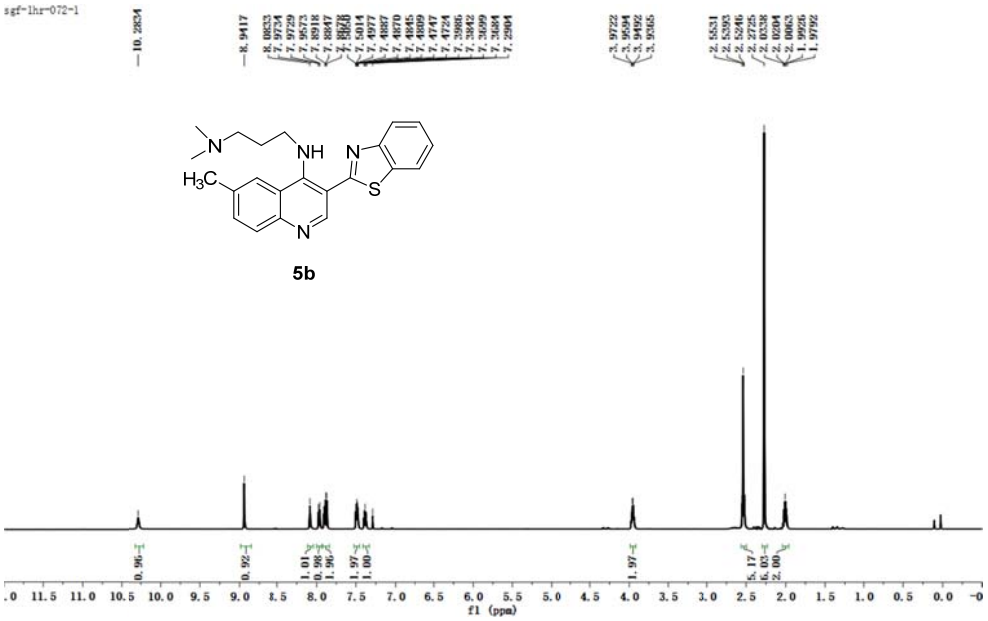


5a



5a

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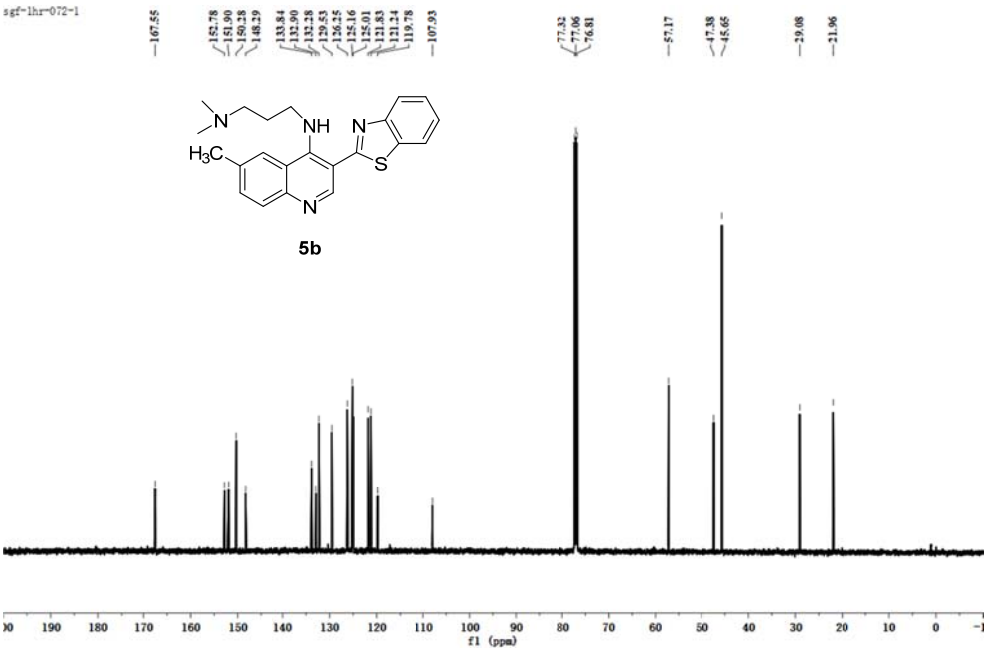
5b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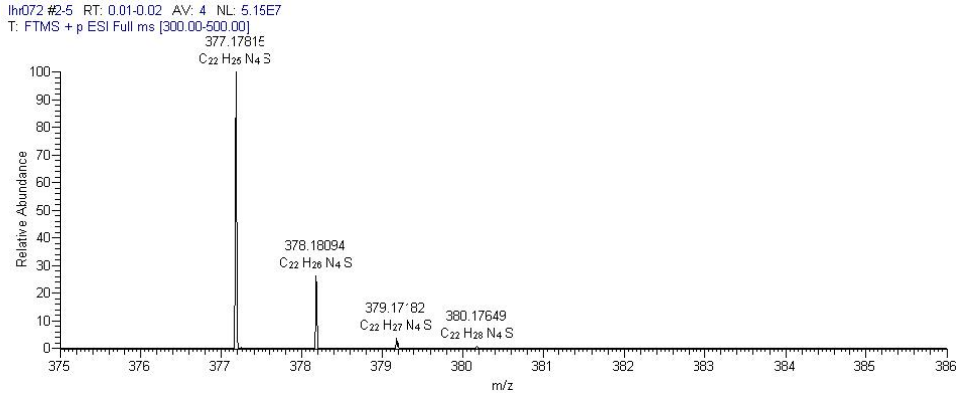
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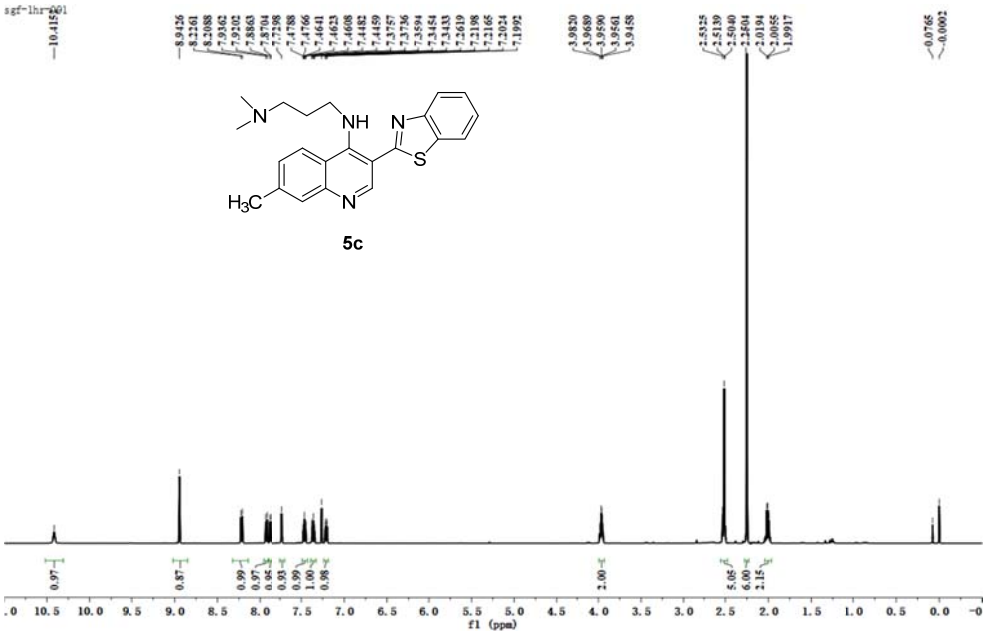
378.18094
C22 H26 N4 S
379.17782
C22 H27 N4 S
380.17649
C22 H28 N4 S
Relative Abundance
m/z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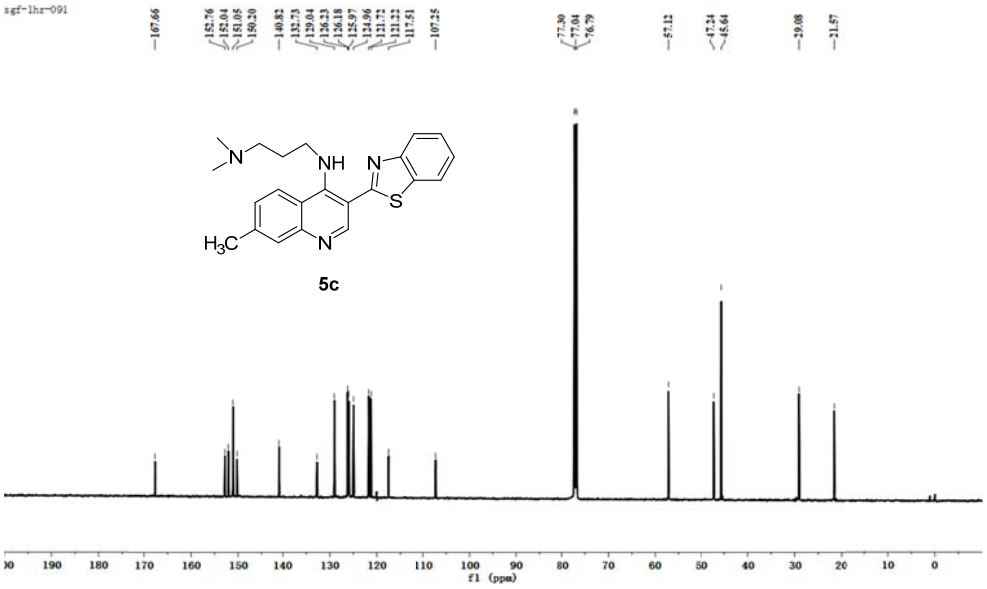
NH
N
S
H_3C
N
f1 (ppm)

5c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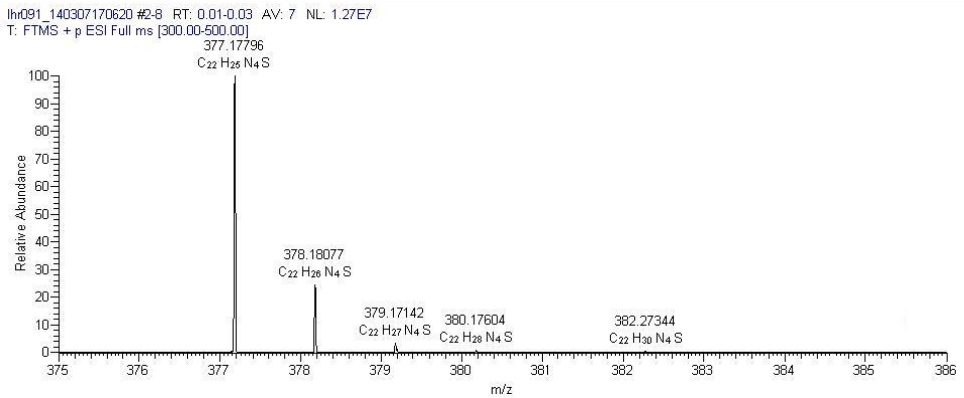
N
S
H_3C
N
f1 (ppm)

5c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$C_{22}H_{26}N_4S$
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$C_{22}H_{27}N_4S$
380.17604
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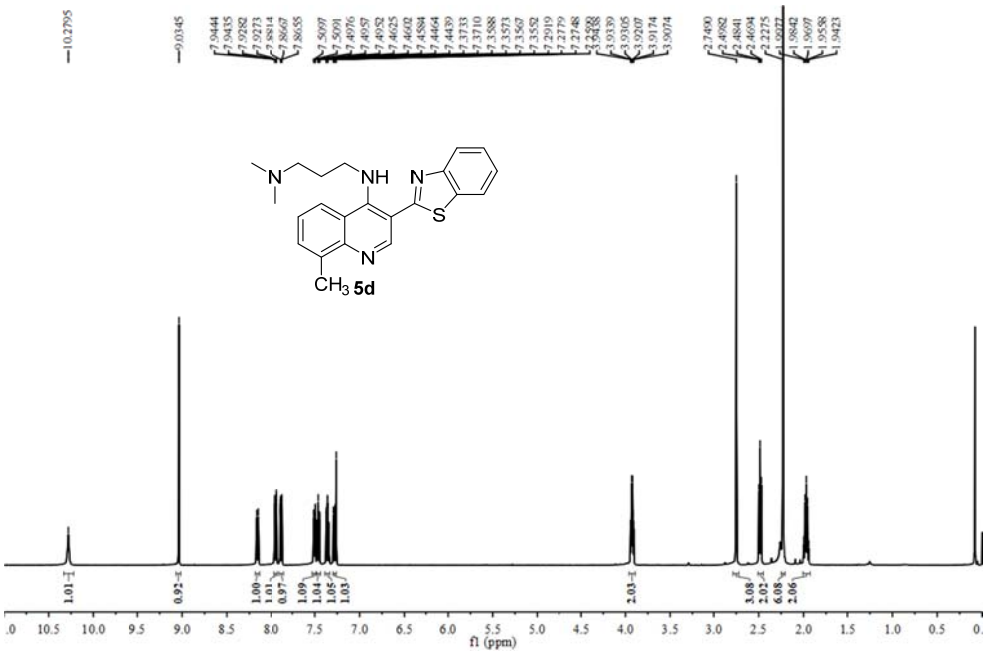
$C_{22}H_{30}N_4S$
Relative Abundance
m/z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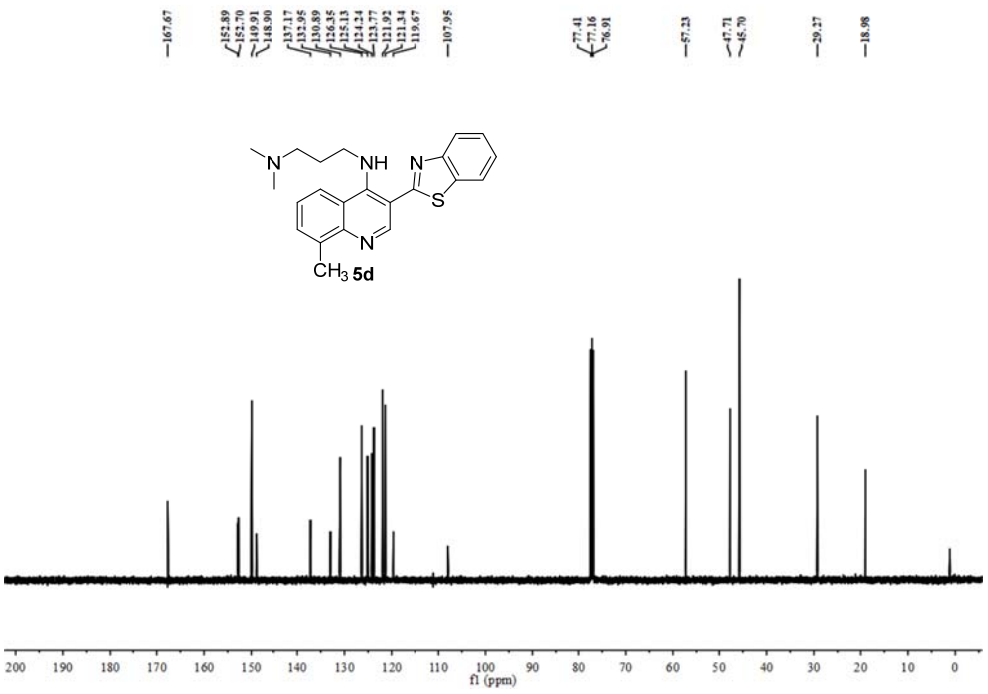
7.4464
7.4439
7.3733
7.3710
7.3588
7.3573
7.3567
7.3552
7.2919
7.2779
7.2748
3.9339
3.9305
3.9207
3.9174
3.9074
2.7490
2.4982
2.4841
2.4694
2.2275
1.9842
1.9697
1.9558
1.9423
1.01
0.92
1.00
1.01
0.97
1.09
1.04
1.05
1.03
2.03
3.08
2.02
6.08
2.06
f1 (ppm)
N
NH
N
S
N
CH3 5d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130.89
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125.13
124.24
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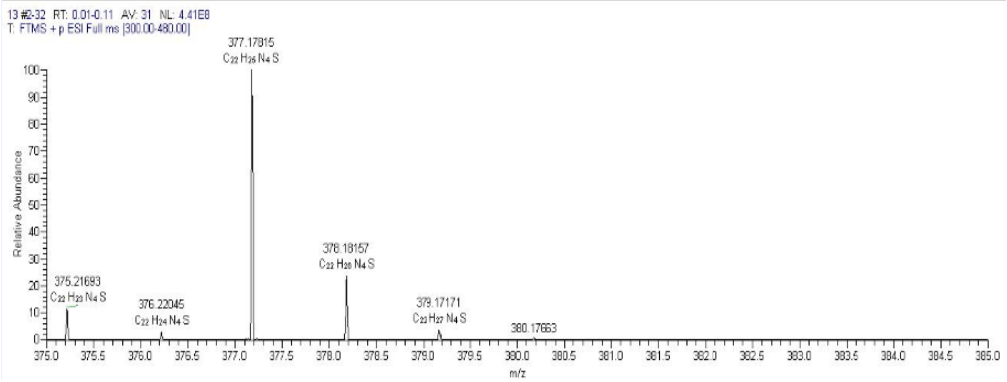
121.92
121.34
119.67
107.95
77.41
77.16
76.91
57.23
47.71
45.70
29.27
18.98
f1 (ppm)
N
NH
N
S
N
CH3 5d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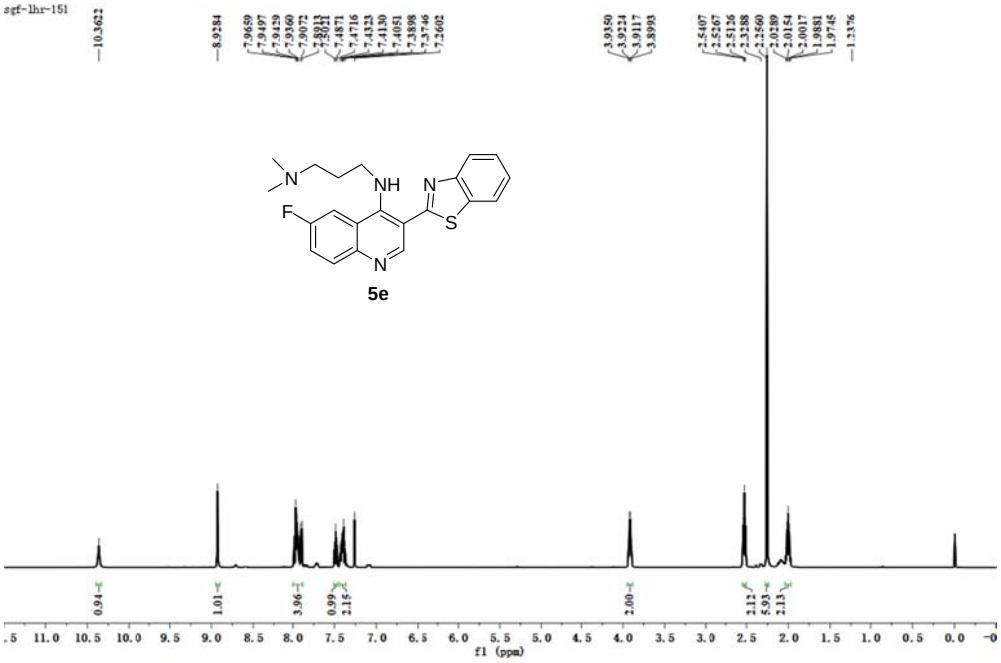
376.18157
C22 H26 N4 S
375.21693
C22 H29 N4 S
376.22045
C22 H24 N4 S
379.17171
C23 H27 N4 S
380.17663
Relative Abundance
m/z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7.9072
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7.8021
7.4871
7.4716
7.4323
7.4130
7.4051
7.3898
7.3746
7.2602
3.9350
3.9224
3.9117
3.8993
2.5407
2.5267
2.5126
2.3388
2.2560
2.0289
2.0154
2.0017
1.9881
1.9745
1.3376
0.94
1.01
3.96
0.99
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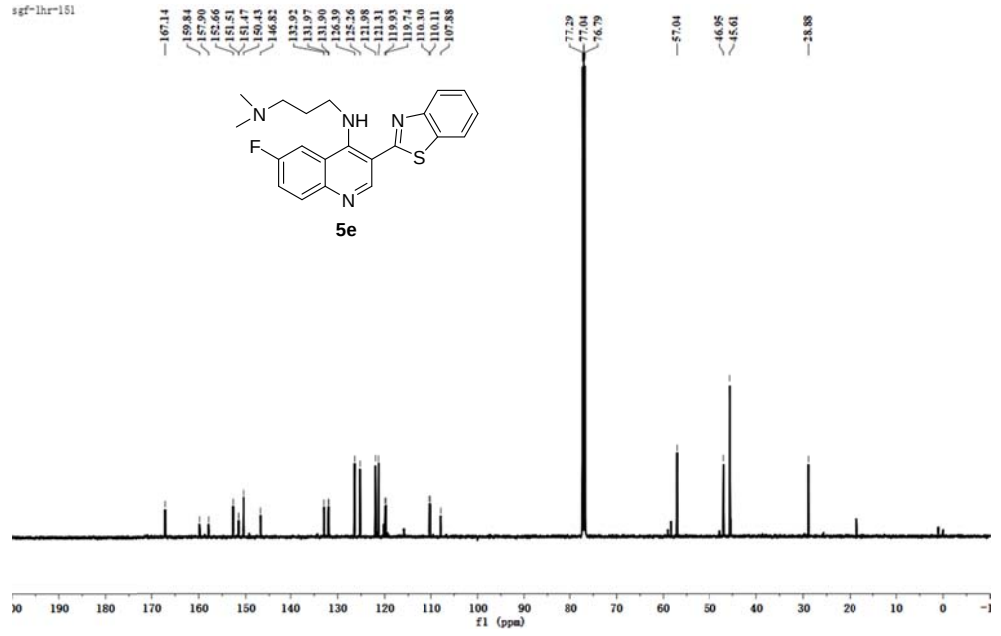
2.00
2.12
5.93
2.13
f1 (ppm)

N
NH
N
F
S
N

5e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131.90
126.39
125.26
121.98
121.31
119.93
119.74
110.16
110.11
107.88
77.29
77.04
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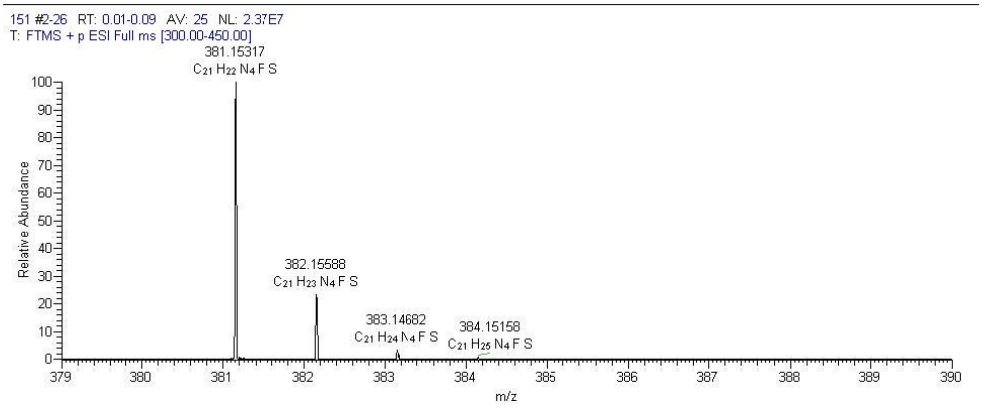
57.04
46.95
45.61
28.88
f1 (ppm)

N
NH
N
F
S
N

5e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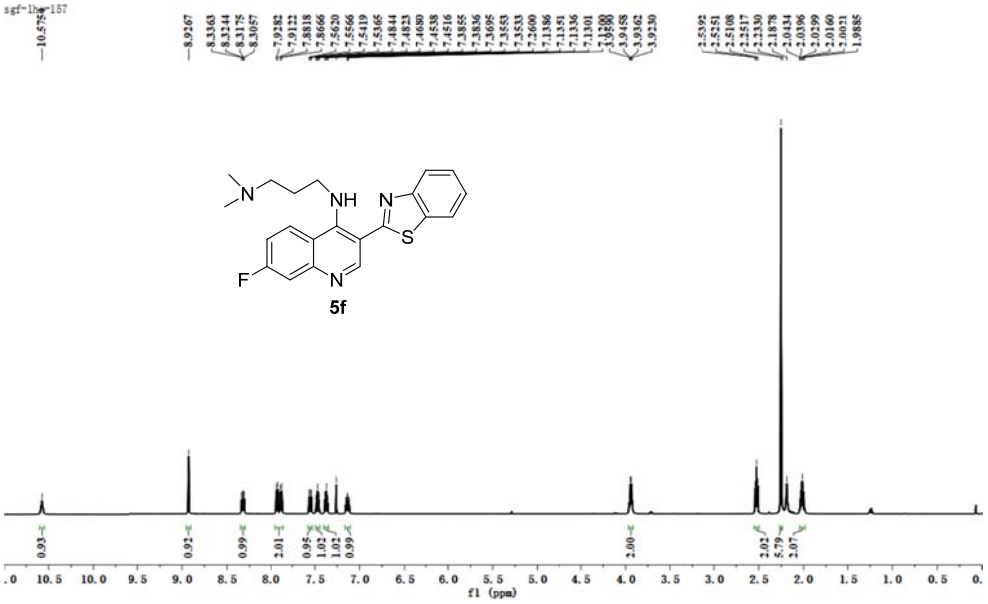
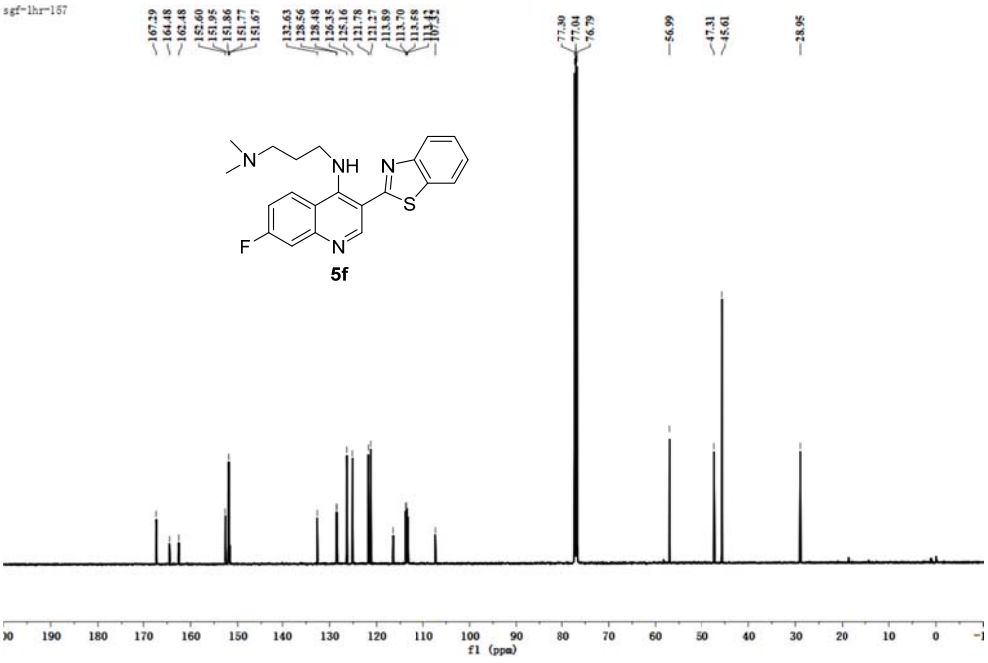
381.15317
C21 H22 N4 F S
382.15588
C21 H23 N4 F S
383.14682
C21 H24 N4 F S
384.15158
C21 H25 N4 F S
Relative Abundance
m/z


5f
f1 (ppm)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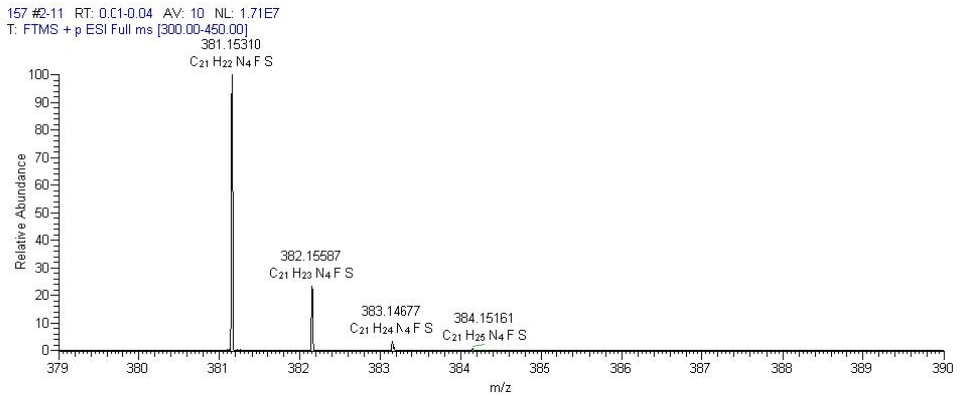
f1 (ppm)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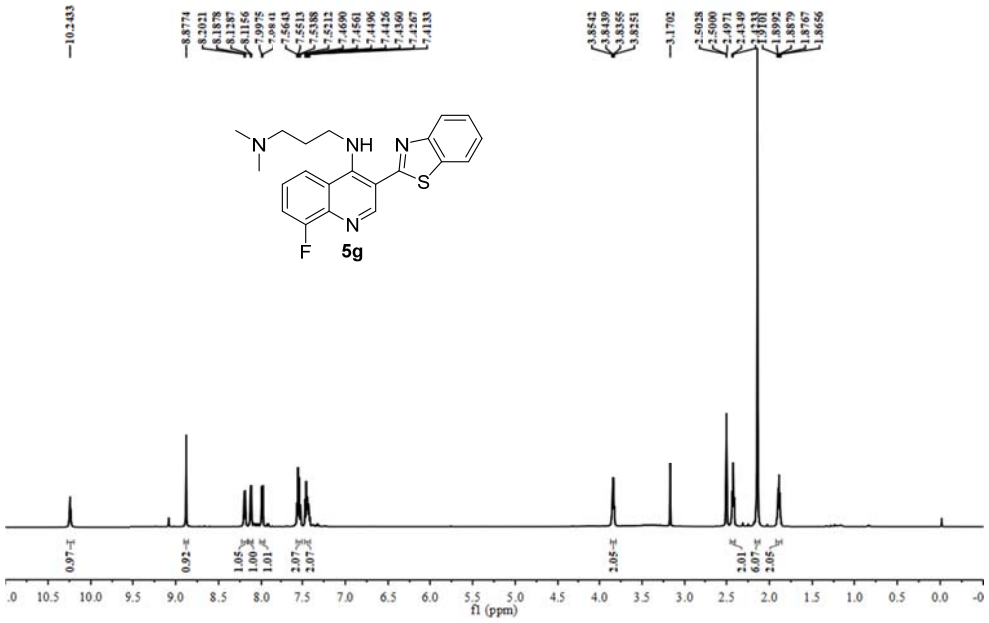
C21 H22 N4 F S
382.15587
C21 H23 N4 F S
383.14677
C21 H24 N4 F S
384.15161
C21 H25 N4 F S
Relative Abundance
m/z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7.5388
7.5212
7.4690
7.4560
7.4496
7.4426
7.4360
7.4267
7.4133
3.8542
3.8439
3.8355
3.8251
3.1702
2.5028
2.5000
2.4971
2.4349
1.8992
1.8879
1.8767
1.8656
NH
N
S
N
F
5g
0.97
0.92
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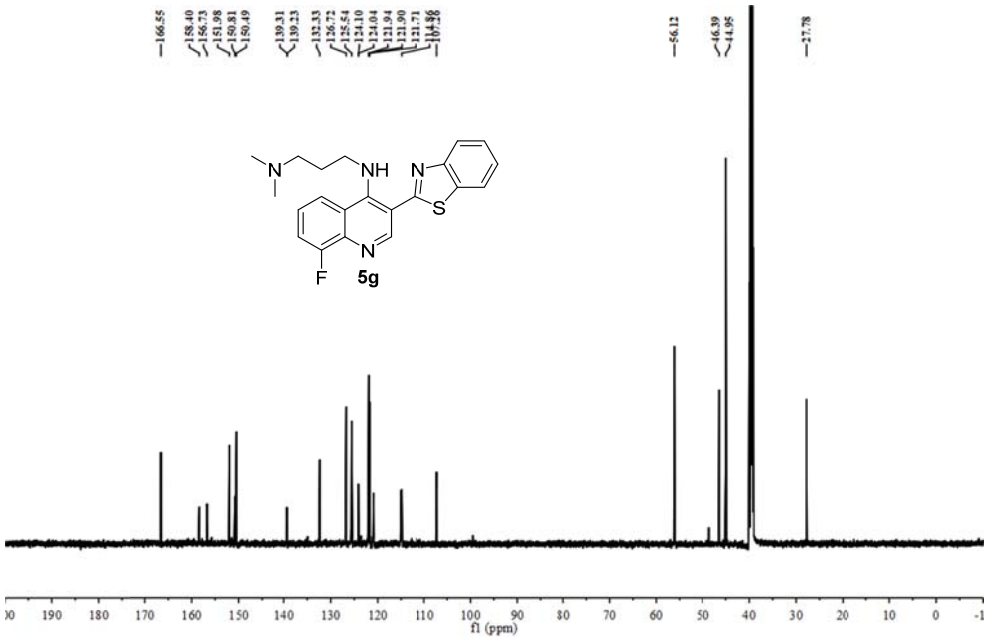
1.00
1.01
2.07
2.07
2.05
2.01
6.07
2.05
f1 (ppm)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124.04
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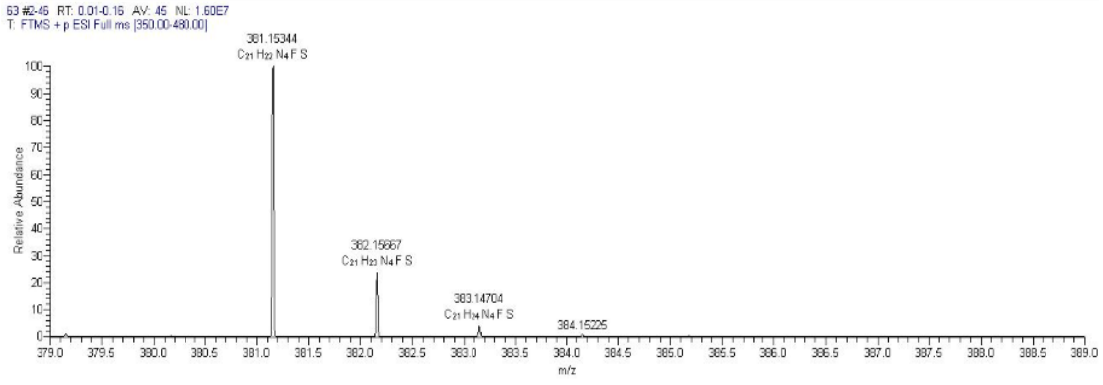
27.78
NH
N
S
N
F
5g
f1 (ppm)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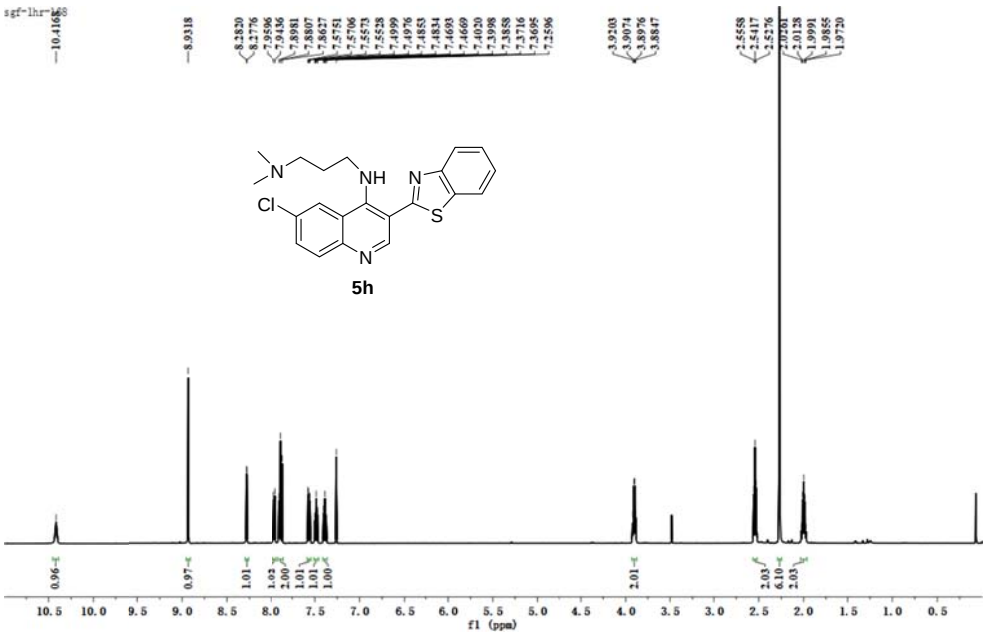
382.15667
C21 H23 N4 F S
383.14704
C21 H14 N4 F S
384.15225
Relative Abundance
m/z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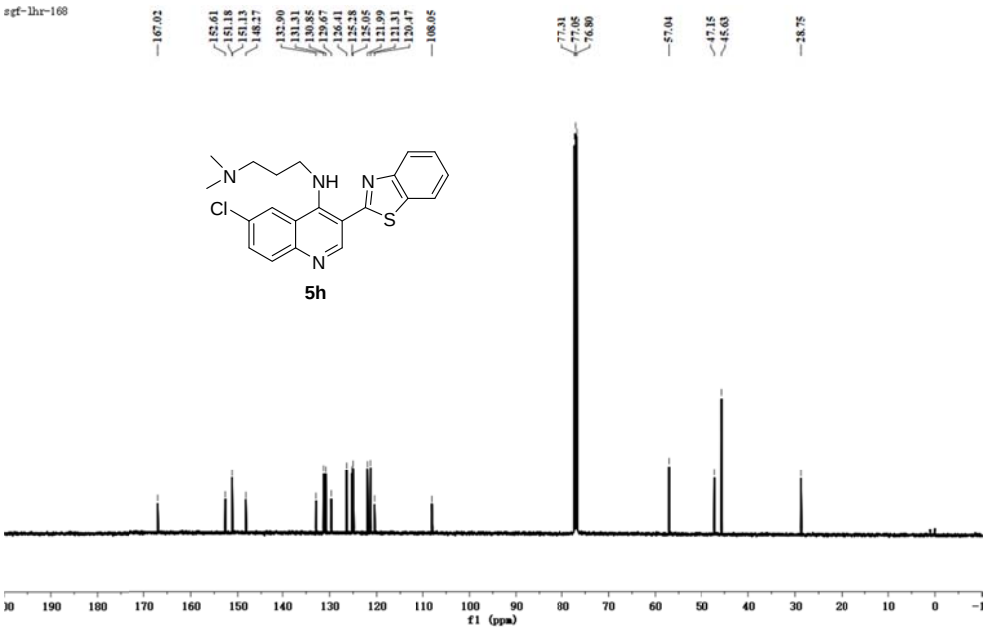
7.5751
7.5706
7.5573
7.5528
7.4999
7.4976
7.4853
7.4834
7.4693
7.4669
7.4020
7.3998
7.3858
7.3716
7.3695
7.2596
3.9203
3.9074
3.8976
3.8847
2.5558
2.5417
2.5276
2.0261
2.0128
1.9991
1.9855
1.9720
0.96
0.97
1.01
1.03
2.00
1.01
1.01
1.00
2.01
2.03
6.10
2.03
f1 (ppm)

5h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151.13
148.27
132.90
131.31
130.85
129.67
126.41
125.28
125.05
121.99
121.31
120.47
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77.31
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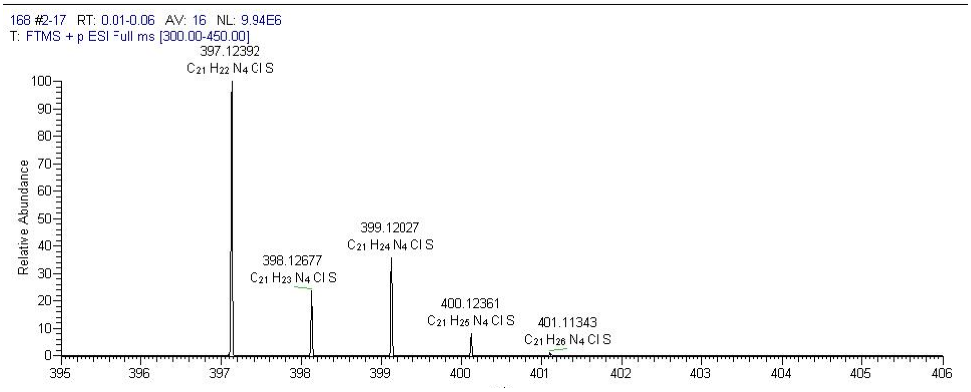
76.80
57.04
47.15
45.63
28.75
f1 (ppm)

5h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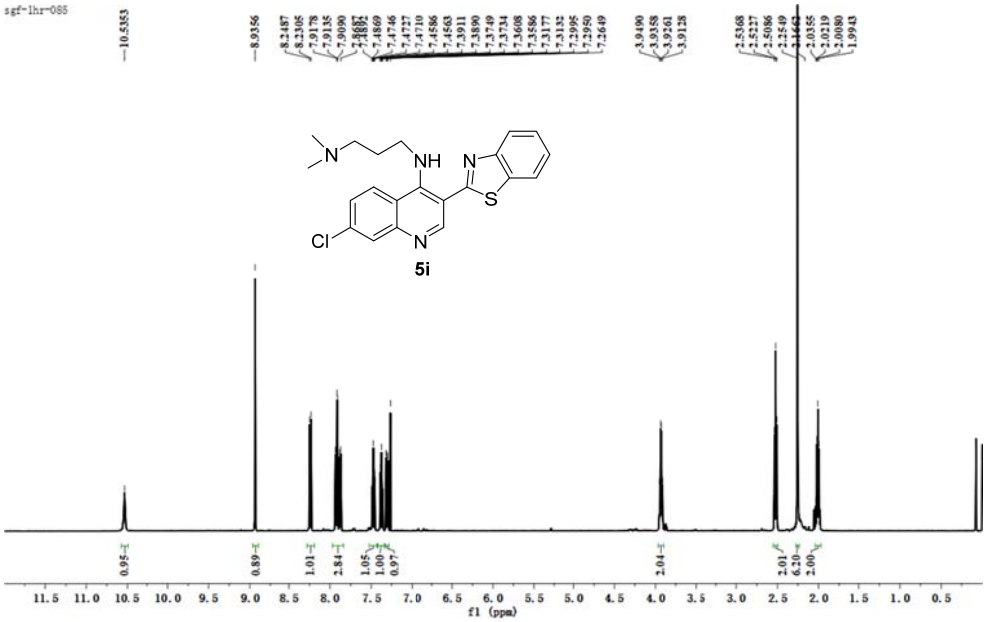
399.12027
C21 H24 N4 Cl S
398.12677
C21 H23 N4 Cl S
400.12361
C21 H25 N4 Cl S
401.11343
C21 H26 N4 Cl S
Relative Abundance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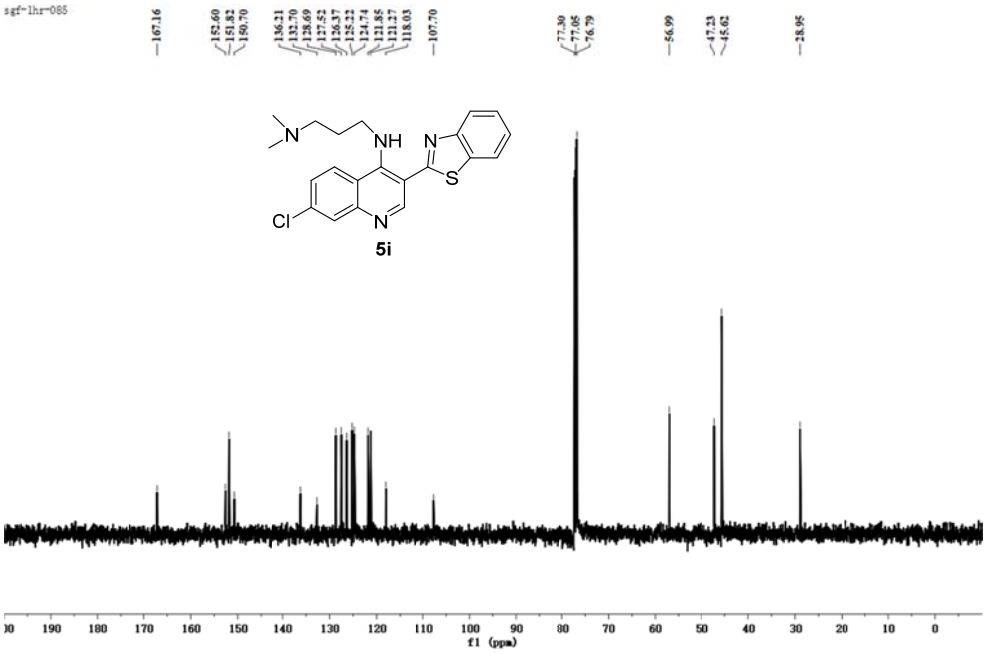
10.5353
8.9356
0.95
0.89
1.01
2.84
1.05
1.00
0.97
2.04
2.01
6.20
2.00
f1 (ppm)
5i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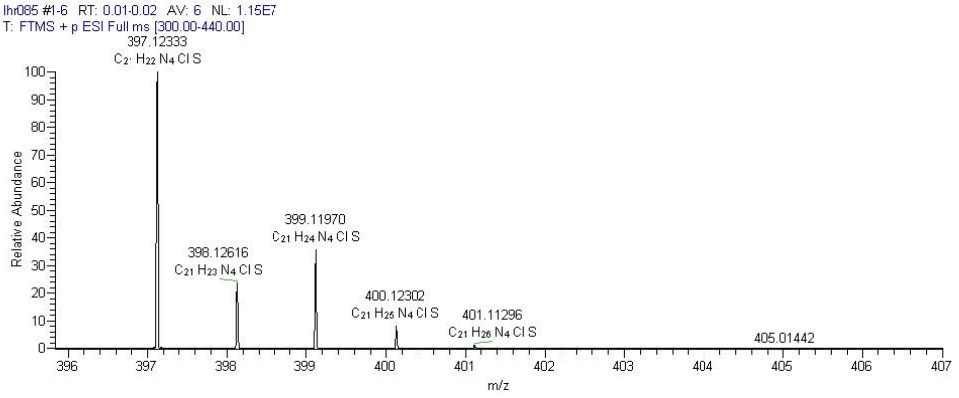
167.16
152.60
151.82
150.70
136.21
132.70
128.69
127.52
126.37
125.22
124.74
121.85
121.27
118.03
107.70
77.30
77.05
76.79
56.99
47.23
45.62
28.95
f1 (ppm)
5i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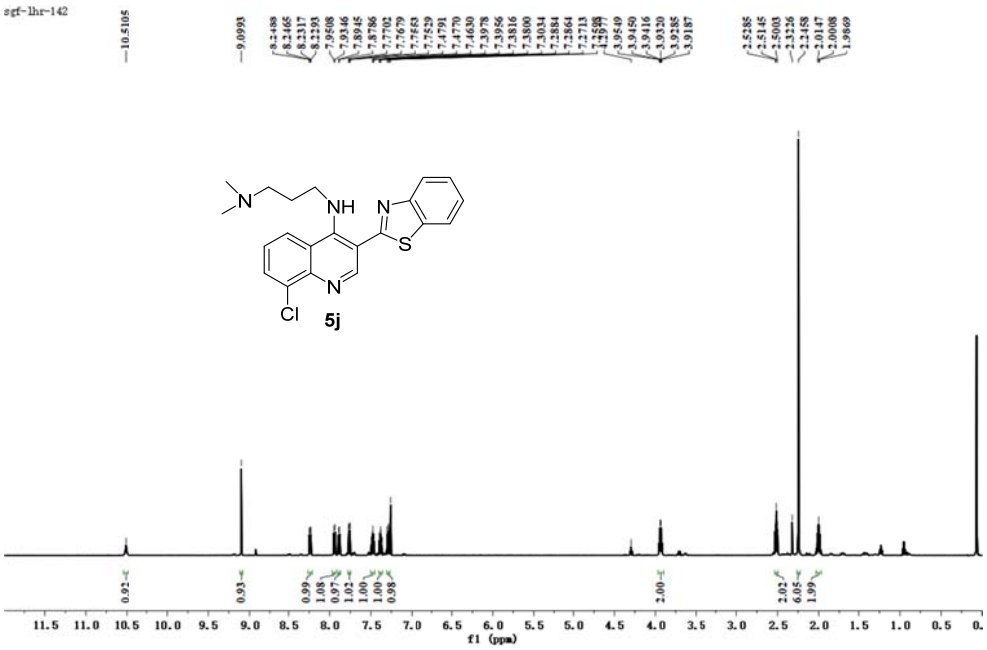
398.12616
C21 H23 N4 Cl S
400.12302
C21 H25 N4 Cl S
401.11296
C21 H26 N4 Cl S
405.01442
Relative Abundance
m/z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7.4770
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7.3800
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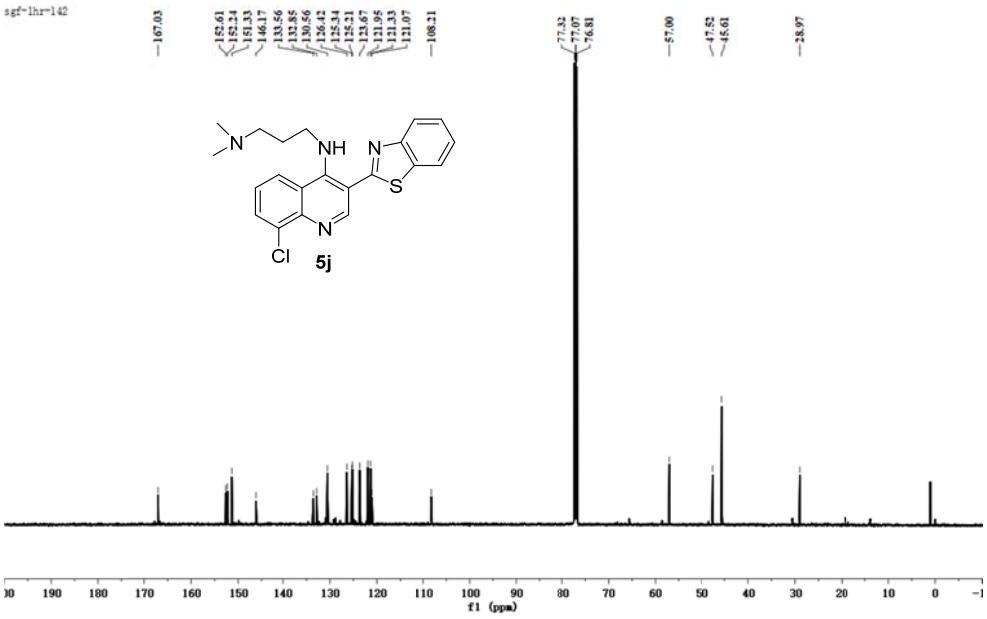
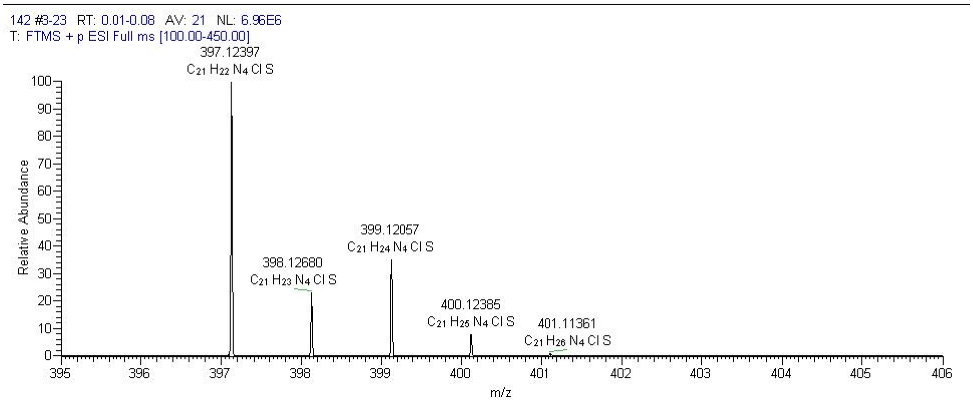
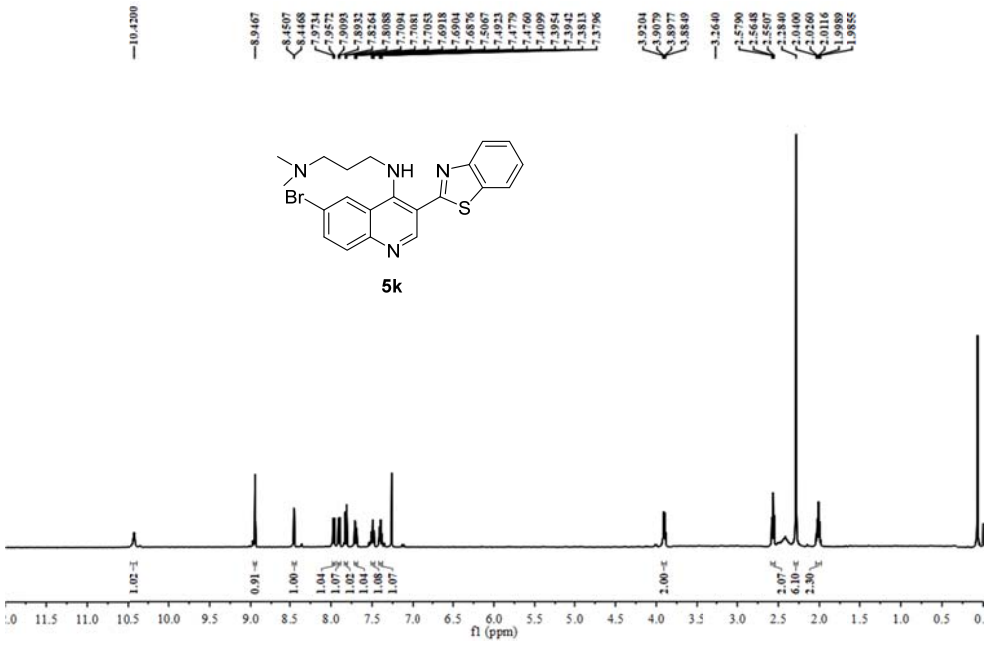
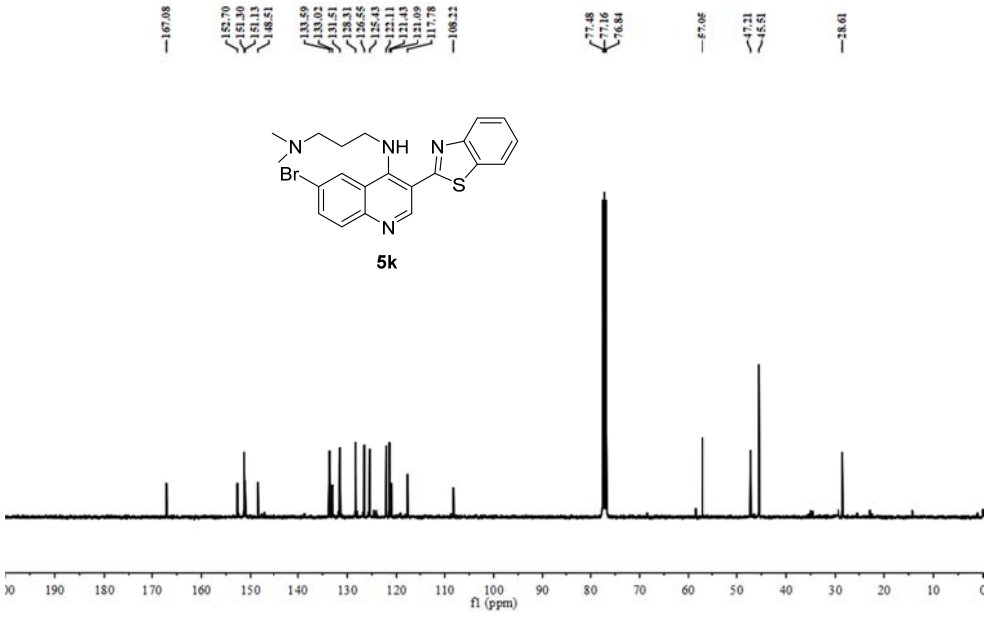
7.2864
7.2713
7.2693
3.9549
3.9450
3.9416
3.9320
3.9285
3.9187
2.5386
2.5145
2.5003
2.3326
2.2458
2.0147
2.0008
1.9869
N
NH
N
S
N
Cl
5j
0.92
0.93
0.99
1.08
0.97
1.02
1.00
1.00
0.98
2.00
2.02
6.05
1.99
f1 (ppm)


sgf-lhr-142
167.03
152.61
152.24
151.33
146.17
133.56
132.85
130.56
126.42
125.34
125.21
123.67
121.95
121.33
121.07
108.21
77.32
77.07
76.81
57.00
47.52
45.61
28.97
N
NH
N
S
N
Cl
5j
f1 (ppm)

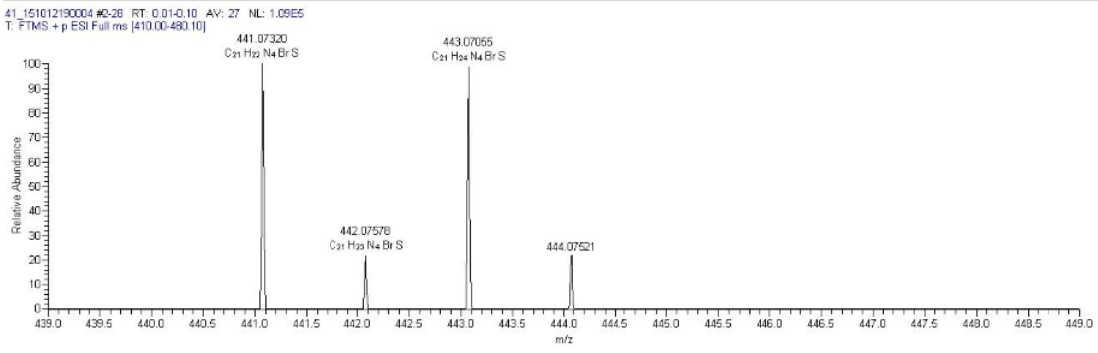

142 #3-23 RT: 0.01-0.08 AV: 21 NL: 6.96E6
T: FTMS + p ESI Full ms [100.00-450.00]
397.12397
C21 H22 N4 Cl S
399.12057
C21 H24 N4 Cl S
398.12680
C21 H23 N4 Cl S
400.12385
C21 H25 N4 Cl S
401.11361
C21 H26 N4 Cl S
Relative Abundance
m/z

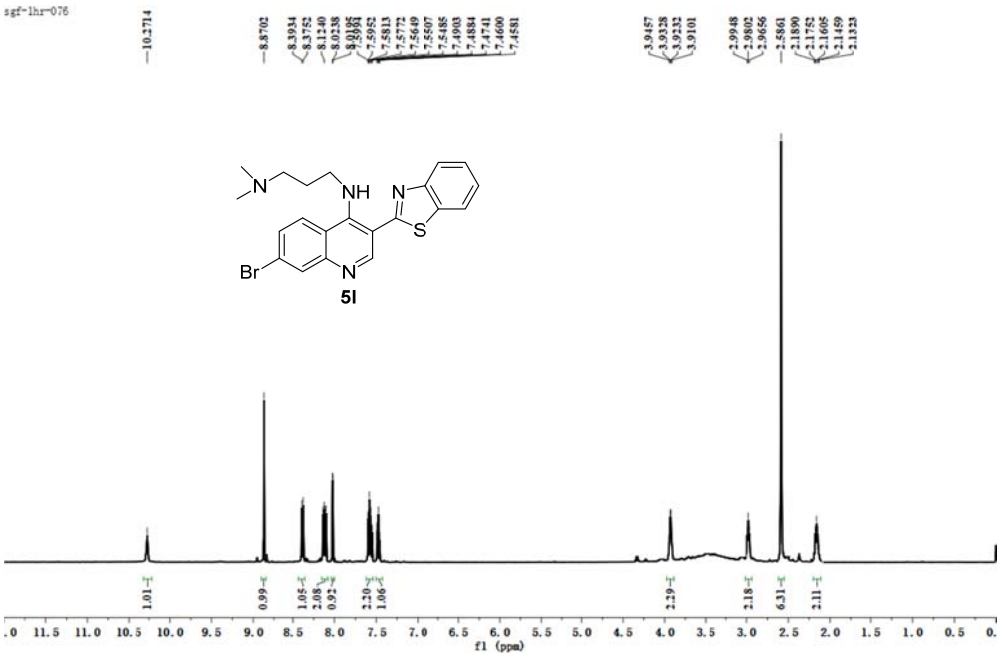

10.4200
8.9467
8.4507
8.4168
7.9724
7.9572
7.9093
7.8932
7.8264
7.8088
7.7094
7.7041
7.7013
7.6918
7.6894
7.6876
7.5067
7.4923
7.4779
7.4760
7.4099
7.3954
7.3912
7.3813
7.3796
3.9204
3.9079
3.8977
3.8849
3.2640
2.5790
2.5648
2.5507
2.2840
2.0400
2.0260
2.0116
1.9989
1.9855
1.02
0.91
1.00
1.04
1.07
1.02
1.04
1.08
1.07
2.00
2.07
6.10
2.30
f1 (ppm)

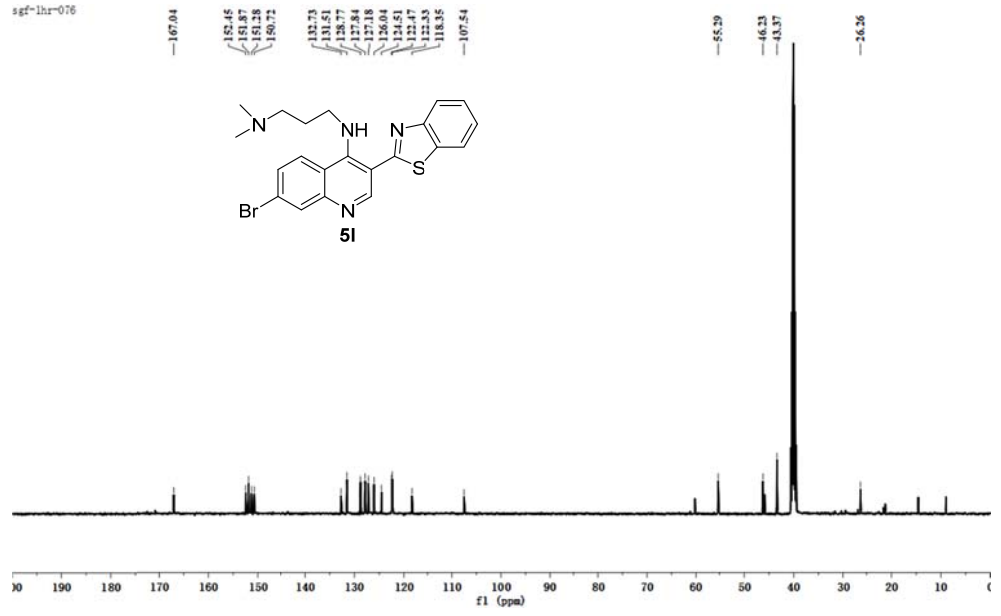
5k

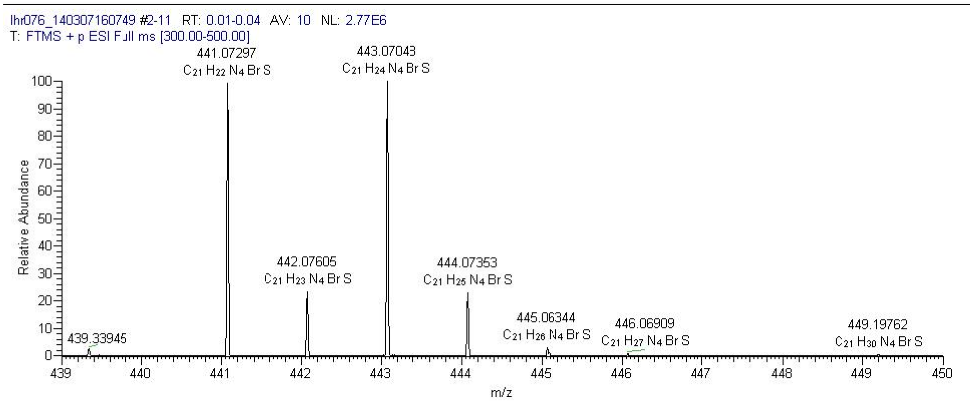

167.08
152.70
151.30
151.13
148.51
133.59
133.02
131.51
128.31
126.55
125.43
122.11
121.43
121.09
117.78
108.22
77.48
77.16
76.84
67.06
47.21
45.51
28.61
f1 (ppm)

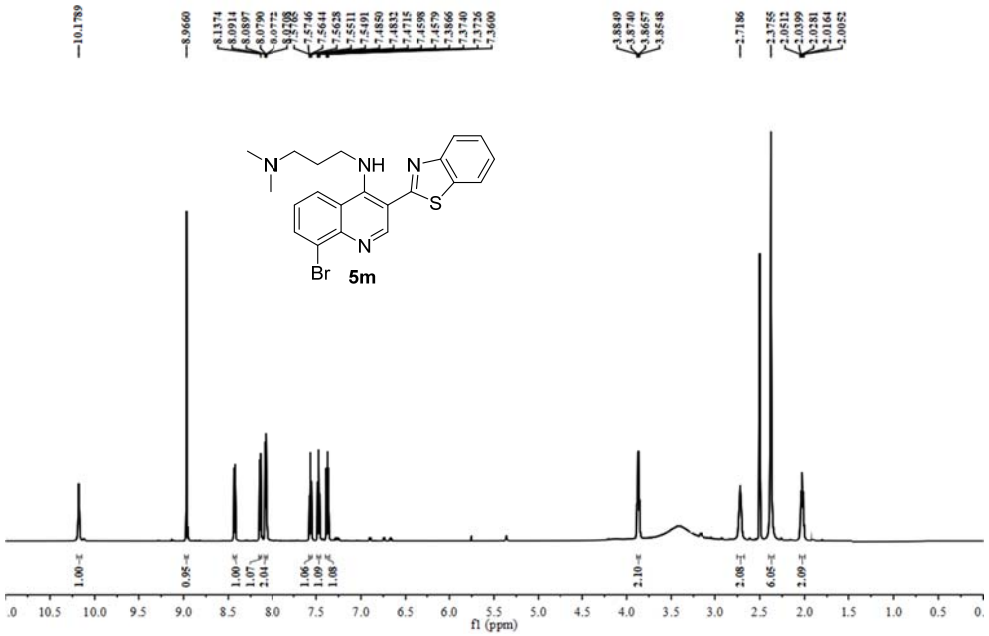
5k

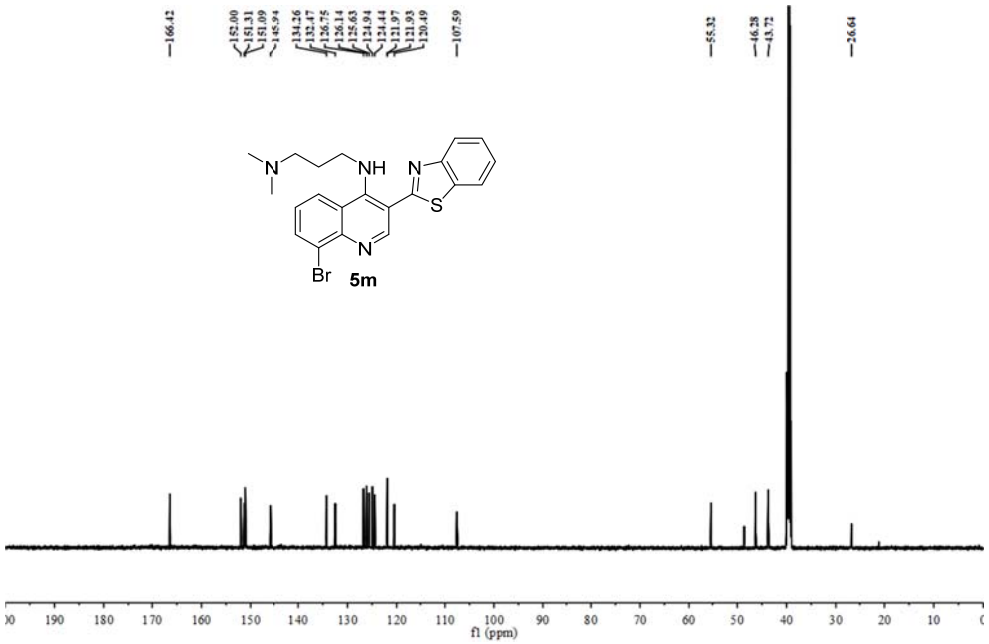

41_151012190004 #2-28 RT: 0.01-0.10 AV: 27 NL: 1.09E5
T: FTMS + p ESI Full ms [410.00-480.10]
441.07320
C21 H22 N4 Br S
443.07055
C21 H24 N4 Br S
442.07578
C21 H23 N4 Br S
444.07521
Relative Abundance
m/z

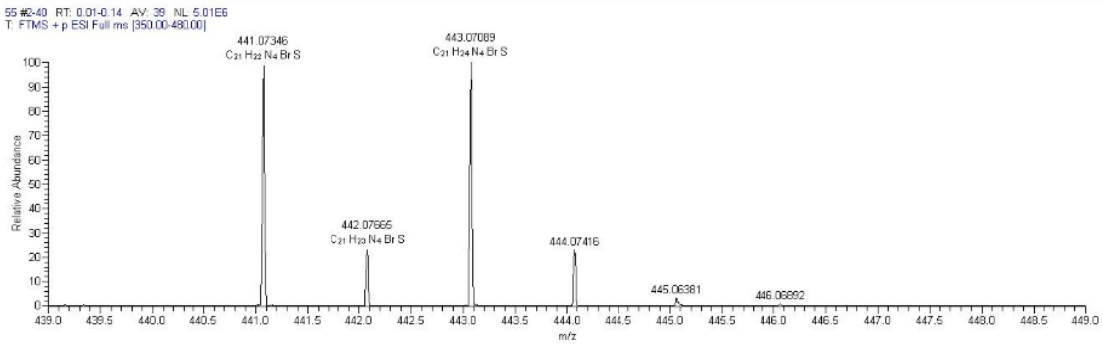

sgf-1hr-076
5l
f1 (ppm)

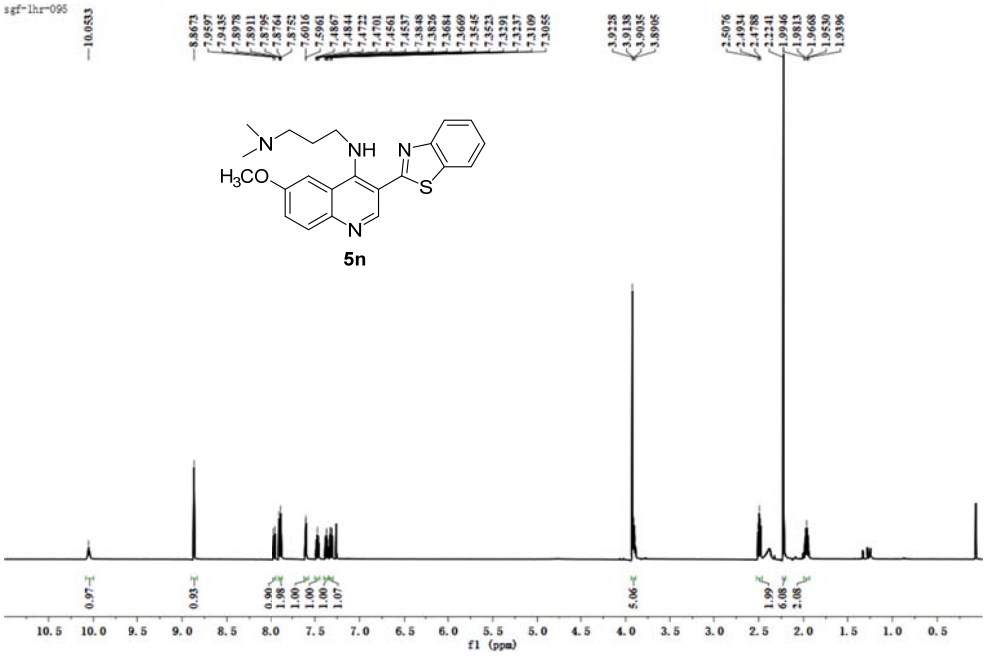

sgf-1hr-076
5l
f1 (ppm)

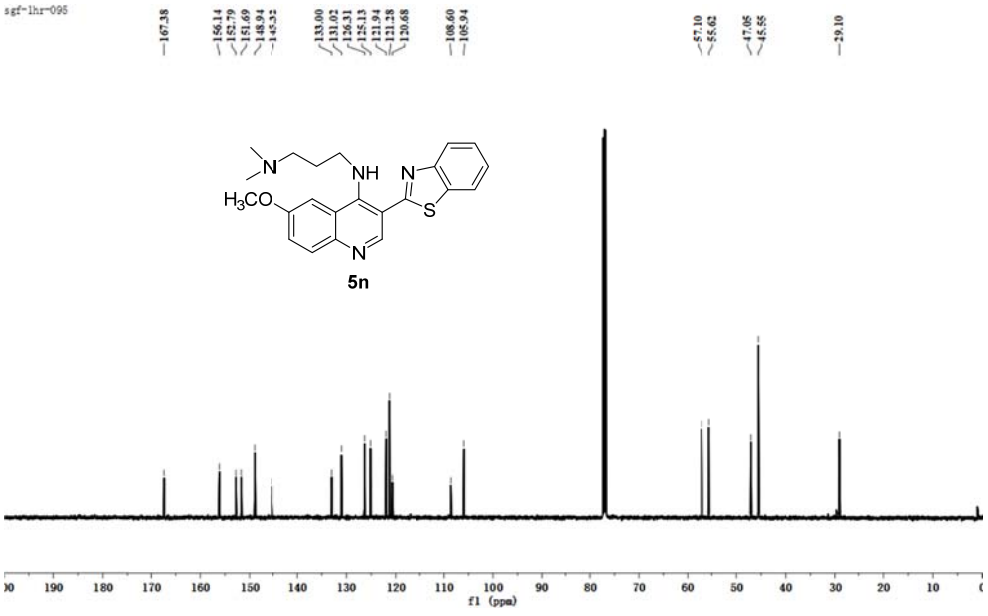

lhr076_140307160749 #2-11 RT: 0.01-0.04 AV: 10 NL: 2.77E6
T: FTMS + p ESI Full ms [300.00-500.00]
441.07297
C21 H22 N4 Br S
443.07043
C21 H24 N4 Br S
442.07605
C21 H23 N4 Br S
444.07353
C21 H25 N4 Br S
445.06344
C21 H26 N4 Br S
446.06909
C21 H27 N4 Br S
449.19762
C21 H30 N4 Br S
439.33945
Relative Abundance
m/z

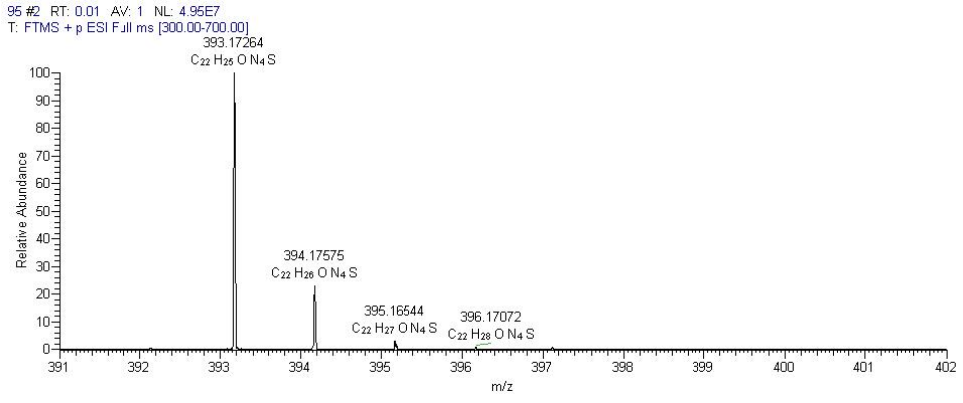

10.1789
8.9660
8.1374
8.0914
8.0597
8.0390
8.0172
7.5746
7.5644
7.5628
7.5511
7.5491
7.4850
7.4832
7.4715
7.4598
7.4579
7.3866
7.3740
7.3726
7.3600
3.8849
3.8740
3.8657
3.8548
2.7186
2.3755
2.0512
2.0399
2.0281
2.0164
2.0052
1.00
0.95
1.00
1.07
2.04
1.06
1.09
1.08
2.10
2.08
6.05
2.09
f1 (ppm)
5m

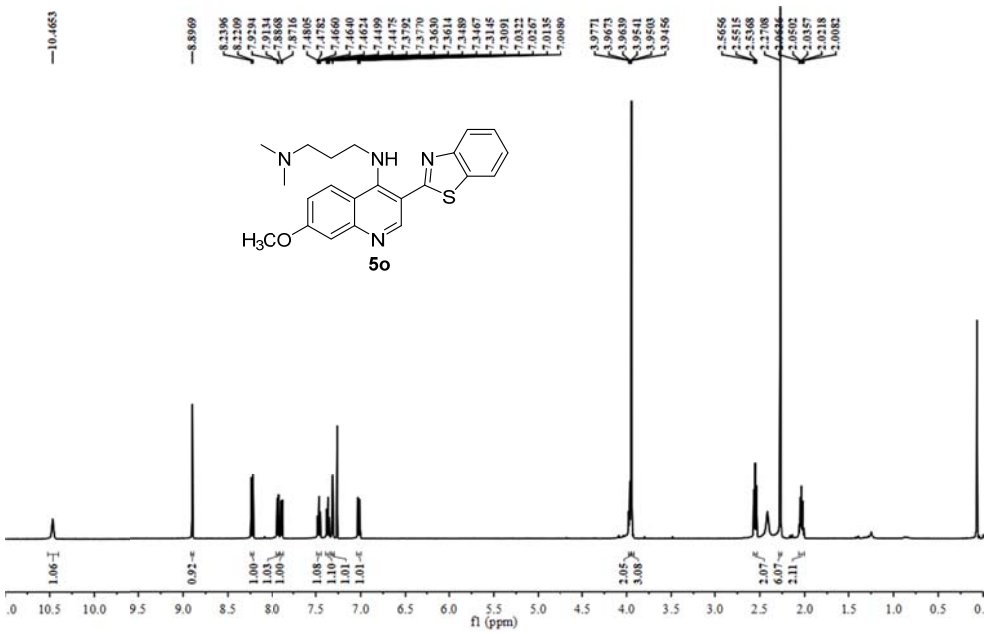

166.42
152.00
151.31
151.09
145.94
134.26
133.47
126.75
126.14
125.63
124.94
124.44
121.97
121.93
120.49
107.59
55.32
46.28
43.72
26.64
f1 (ppm)
5m

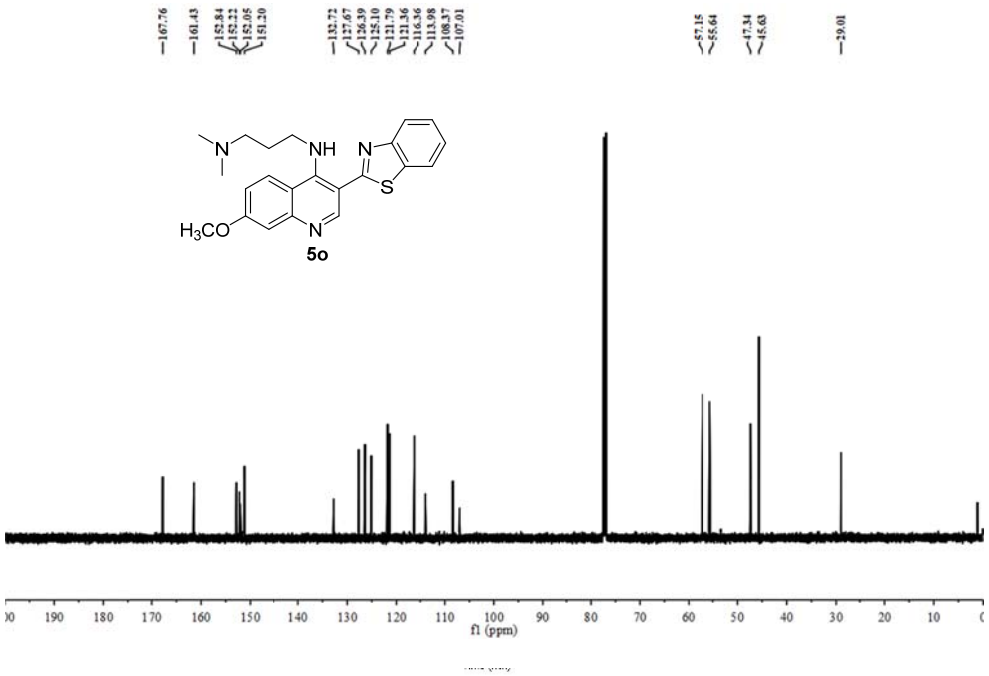

55 #62-80 RT: 0.01-0.14 AV: 39 NL: 5.01E6
T: FTMS + p ESI Full ms [350.00-480.00]
441.07346
C21 H22 N4 Br S
443.07089
C21 H24 N4 Br S
442.07666
C21 H23 N4 Br S
444.07416
445.08381
446.08692
Relative Abundance
m/z

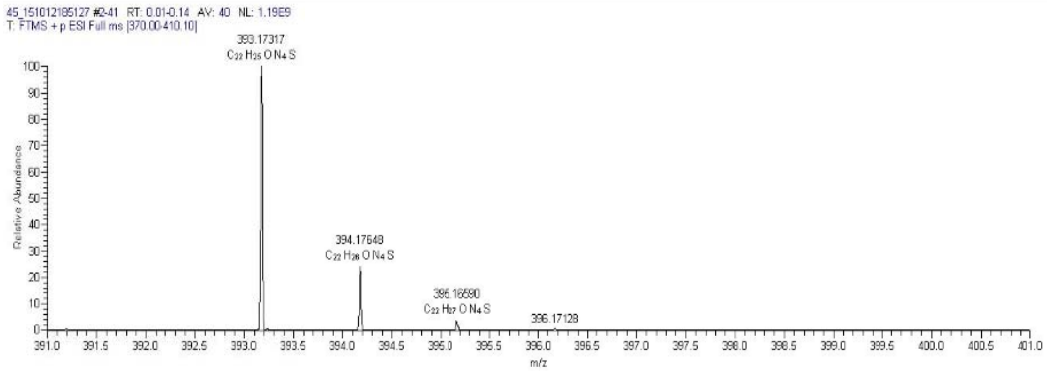

sgf-1hr-095
10.0533
8.8673
7.9597
7.9435
7.8978
7.8911
7.8796
7.8764
7.8752
7.6016
7.5961
7.4867
7.4844
7.4722
7.4701
7.4561
7.4537
7.3848
7.3826
7.3684
7.3669
7.3545
7.3523
7.3291
7.3237
7.3109
7.3055
3.9228
3.9138
3.9035
3.8905
2.5076
2.4934
2.4788
2.2241
1.9946
1.9813
1.9668
1.9530
1.9396
N
NH
N
S
H3CO
N
5n
0.97
0.93
0.90
1.98
1.00
1.00
1.00
1.07
5.06
1.99
6.08
2.08
f1 (ppm)

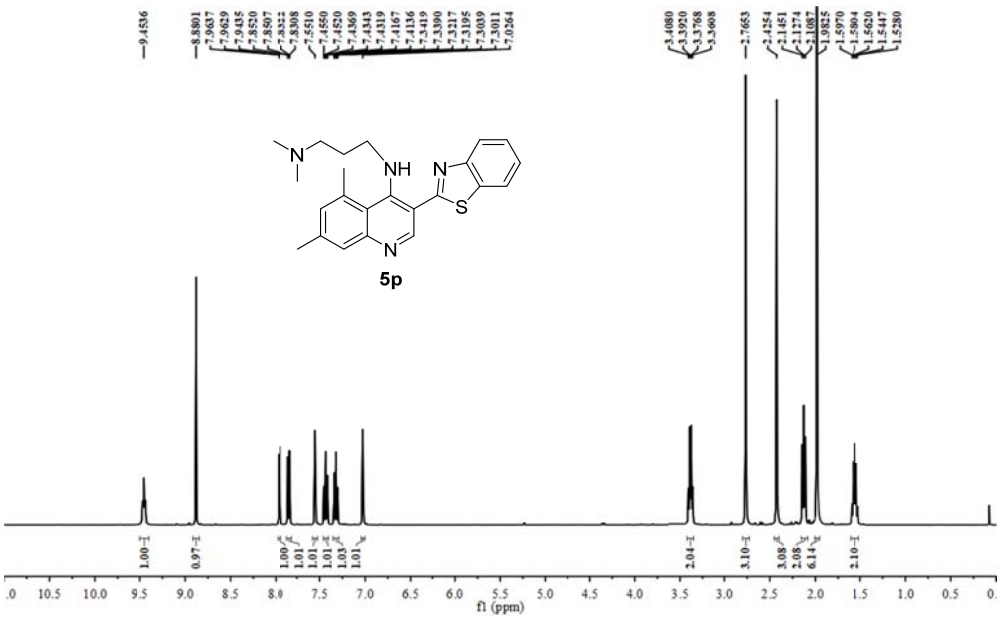

sgf-1hr-095
167.38
156.14
152.79
151.69
148.94
145.52
133.00
131.02
126.31
125.13
121.94
121.28
120.68
108.60
105.94
57.10
55.62
47.05
45.55
29.10
N
NH
N
S
H3CO
N
5n
f1 (ppm)

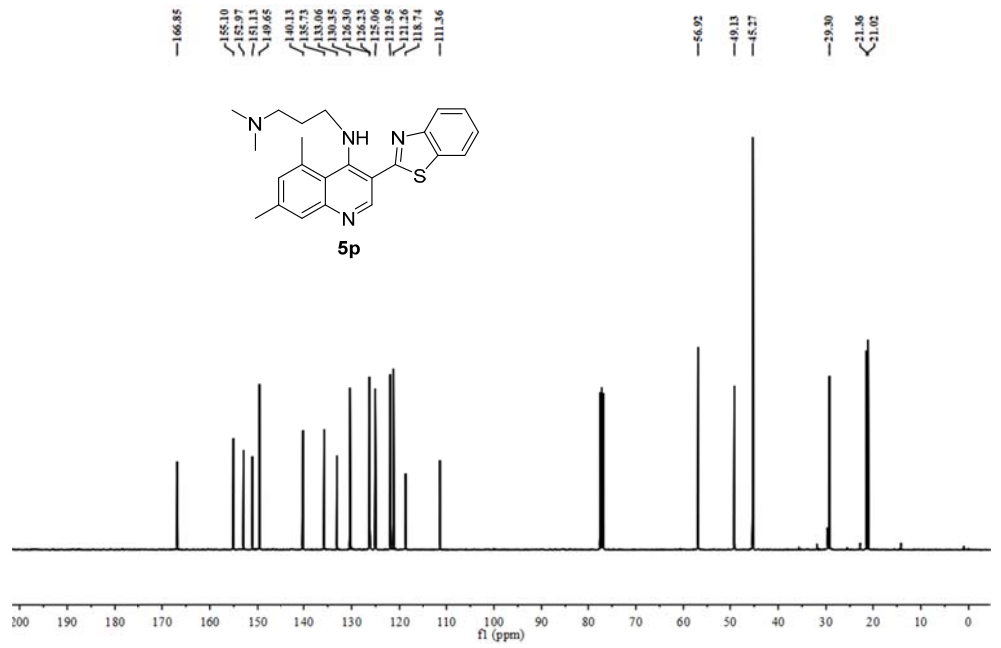

95 #2 RT: 0.01 AV: 1 NL: 4.95E7
T: FTMS + p ESI Full ms [300.00-700.00]
393.17264
C22 H25 O N4 S
394.17575
C22 H26 O N4 S
395.16544
C22 H27 O N4 S
396.17072
C22 H28 O N4 S
Relative Abundance
m/z

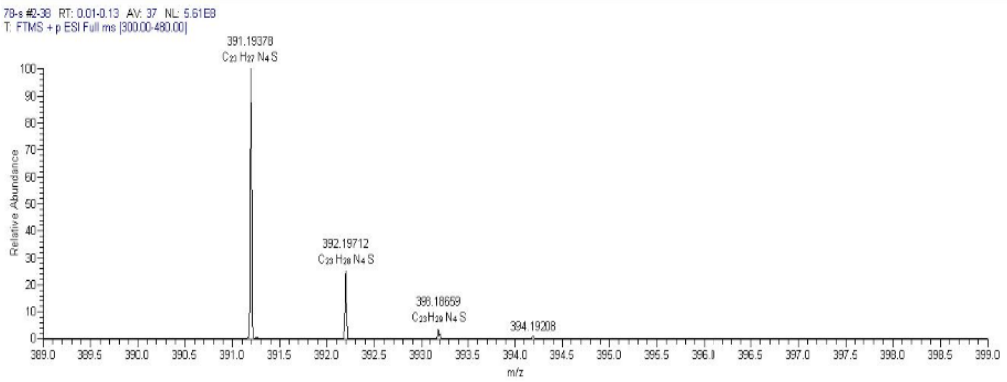

10.4653
8.8969
8.2396
8.2209
7.9294
7.9134
7.8868
7.8716
7.4805
7.4782
7.4660
7.4640
7.4624
7.4499
7.4475
7.3792
7.3770
7.3630
7.3614
7.3489
7.3467
7.3145
7.3091
7.0322
7.0267
7.0135
7.0080
3.9771
3.9673
3.9639
3.9541
3.9503
3.9456
2.5656
2.5515
2.5368
2.2708
2.0644
2.0502
2.0357
2.0218
2.0082
1.06
0.92
1.00
1.03
1.00
1.08
1.10
1.01
1.01
2.05
3.08
2.07
6.07
2.11
f1 (ppm)
5o

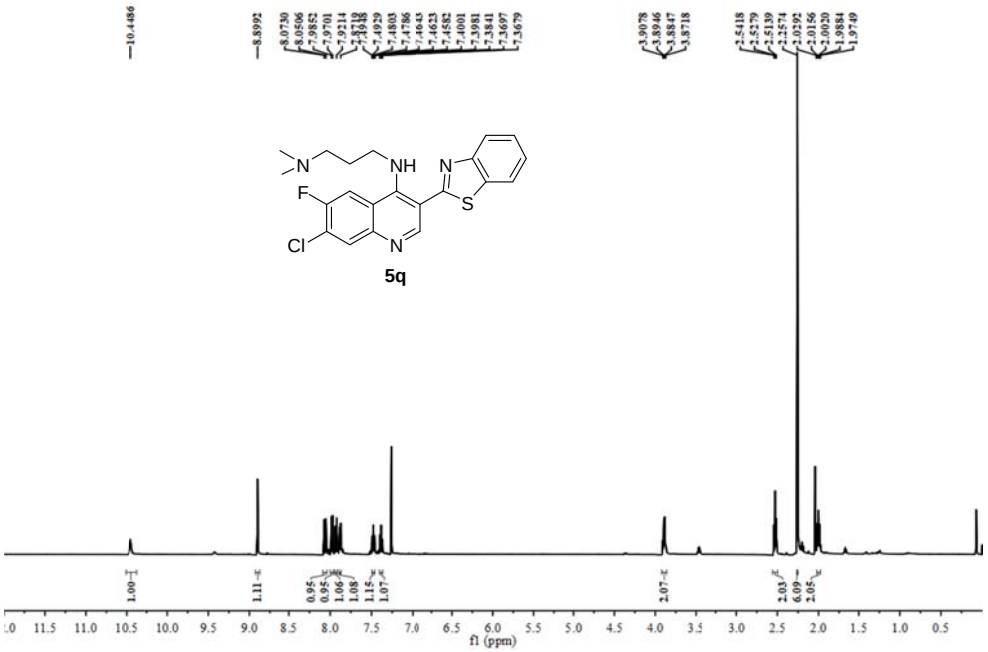

167.76
161.43
152.84
152.22
152.05
151.20
132.72
127.67
126.39
125.10
121.79
121.36
116.36
113.98
108.37
107.01
57.15
55.64
47.34
45.63
29.01
f1 (ppm)
5o

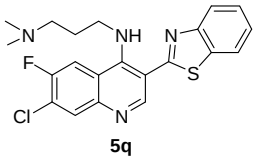

45_151012185127 #2-41 RT: 0.01-0.14 AV: 40 NL: 1.19E9
T: FTMS + p ESI Full ms [370.00-410.10]
393.17317
C22 H25 O N4 S
394.17648
C22 H26 O N4 S
396.16690
C22 H27 O N4 S
396.17128
Relative Abundance
m/z


9.4536
8.8891
7.9637
7.9629
7.9435
7.8520
7.8507
7.8312
7.8308
7.5510
7.4650
7.4520
7.4369
7.4343
7.4319
7.4167
7.4136
7.3419
7.3390
7.3217
7.3195
7.3039
7.3011
7.0264
3.4080
3.3920
3.3768
3.3608
2.7653
2.4254
2.1451
2.1274
2.1087
1.9825
1.5976
1.5804
1.5620
1.5447
1.5280
1.00
0.97
1.00
1.01
1.01
1.03
1.01
2.04
3.10
3.08
2.05
6.14
2.10
f1 (ppm)
5p


166.85
155.10
152.97
151.13
149.65
140.13
135.73
133.06
130.35
126.30
126.23
125.06
121.95
121.26
118.74
111.36
56.92
49.13
45.27
29.30
21.36
21.02
f1 (ppm)
5p


78-s #2-38 RT: 0.01-0.13 AV: 37 NL: 5.61E8
T: FTMS + p ESI Full ms [300.00-480.00]
391.19378
C23 H27 N4 S
392.19712
C23 H28 N4 S
393.18659
C23H28 N4 S
394.19208
Relative Abundance
m/z


10.4486
8.8992
8.0730
8.0506
7.9852
7.9701
7.9211
7.8718
7.8438
7.4929
7.4803
7.4786
7.4643
7.4623
7.4582
7.4001
7.3981
7.3841
7.3697
7.3679
3.9078
3.8946
3.8847
3.8718
2.5418
2.5279
2.5139
2.2574
2.0292
2.0156
2.0020
1.9884
1.9749
1.00
1.11
0.95
0.95
1.06
1.08
1.15
1.07
2.07
2.03
6.09
2.05
f1 (ppm)

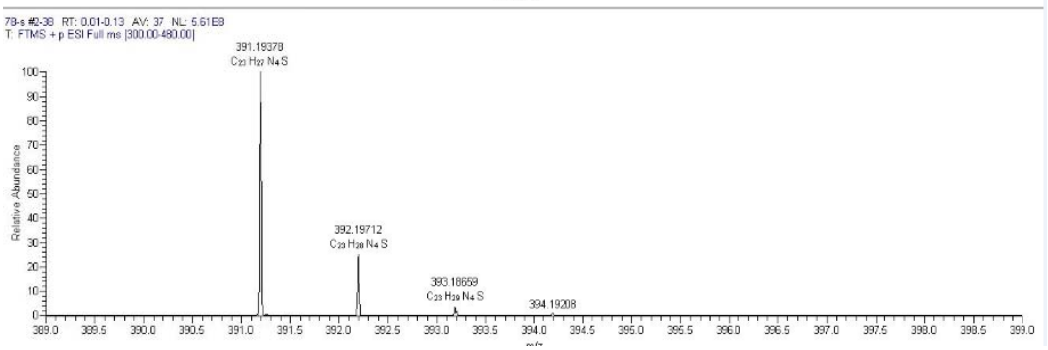

N
NH
N
S
F
Cl
N

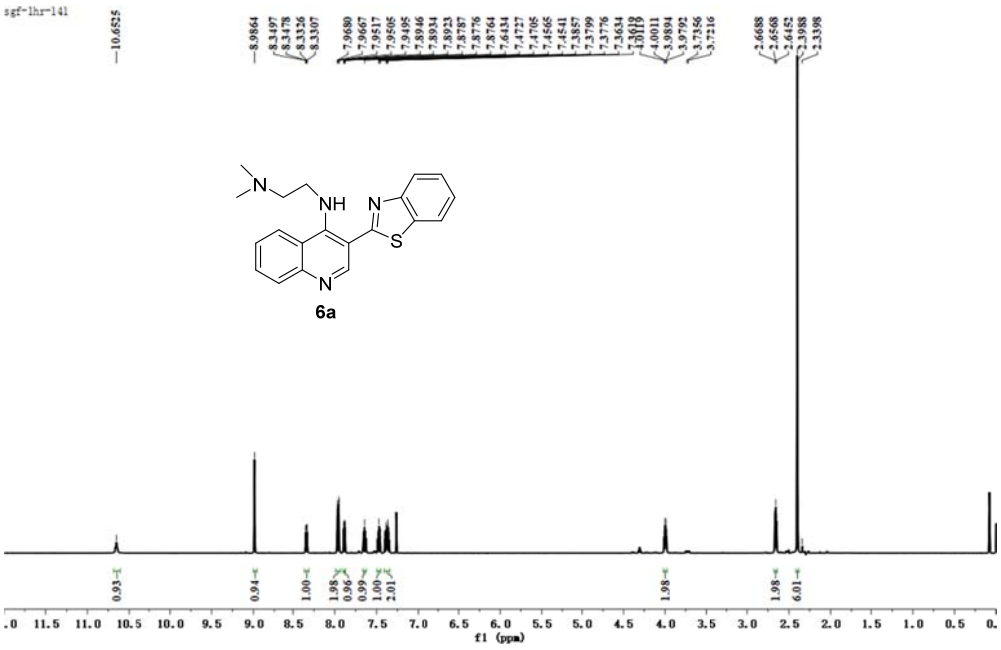
5q

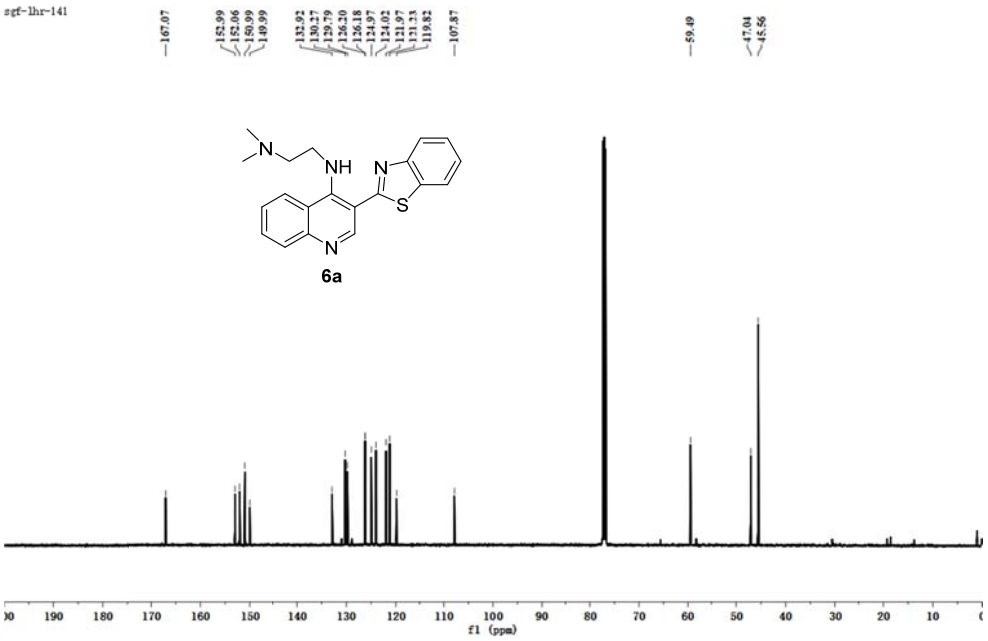
167.00
155.21
153.25
152.68
151.39
151.37
151.26
151.23
147.20
133.94
131.29
126.57
125.48
122.10
121.42
111.68
111.49
108.00
57.02
46.94
45.71
28.93
f1 (ppm)

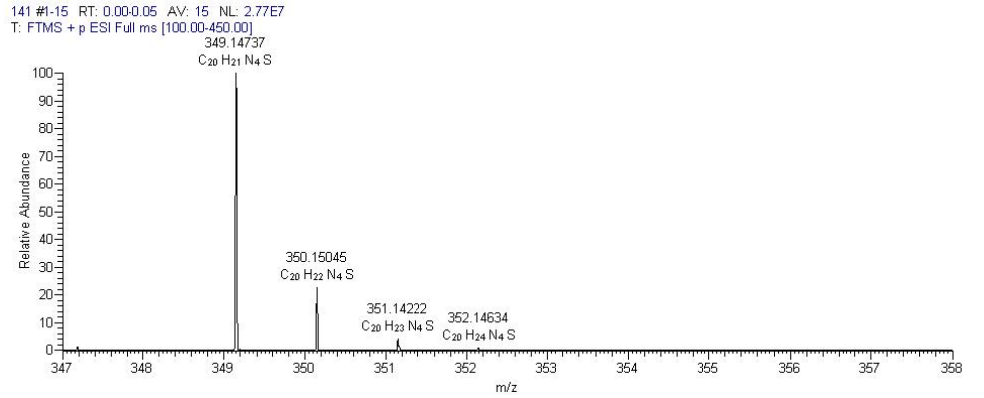
N
NH
N
S
F
Cl
N

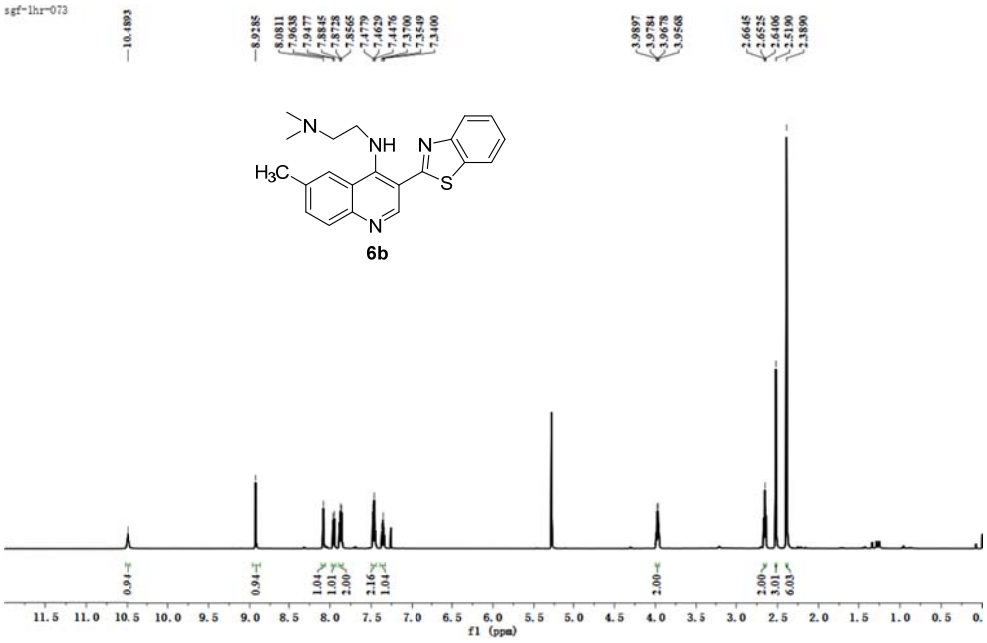
5q

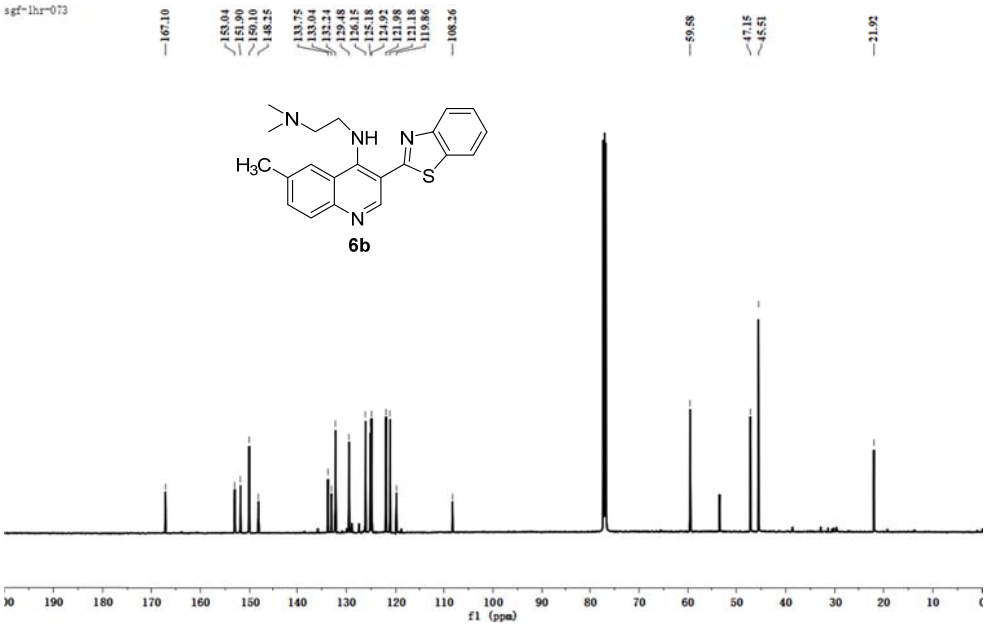

78-s #2-38 RT: 0.01-0.13 AV: 37 NL: 5.61E8
T: FTMS + p ESI Full ms [300.00-480.00]
391.19378
C23 H27 N4 S
392.19712
C23 H28 N4 S
393.18659
C23 H26 N4 S
394.19208
Relative Abundance
m/z

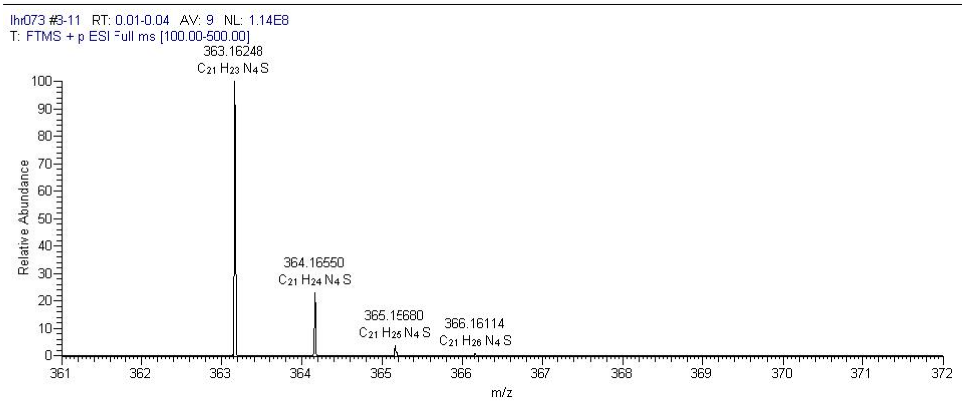

sgf-1hr-141
6a
f1 (ppm)

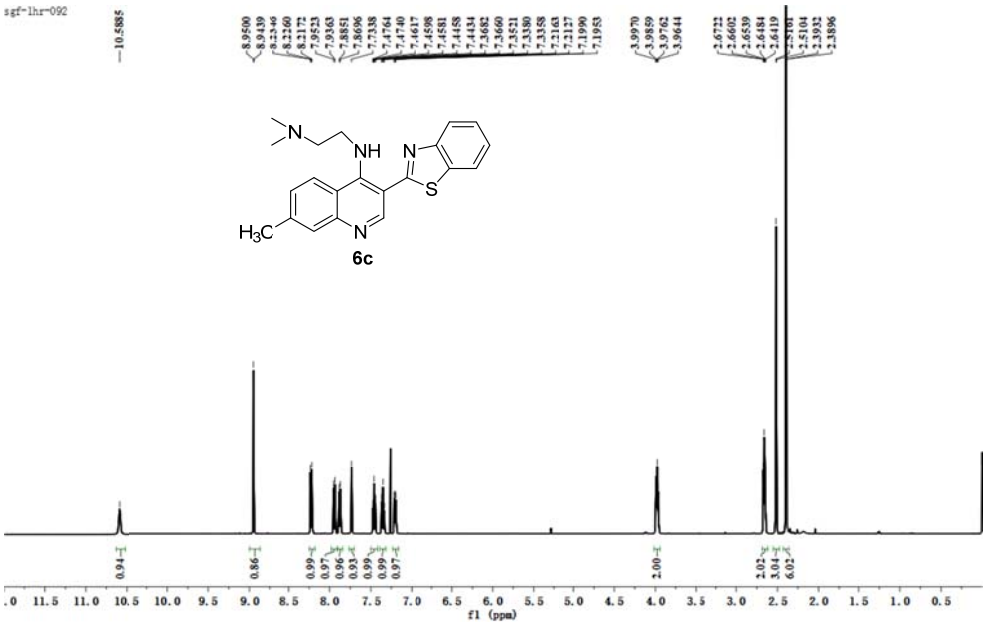

sgf-1hr-141
6a
f1 (ppm)

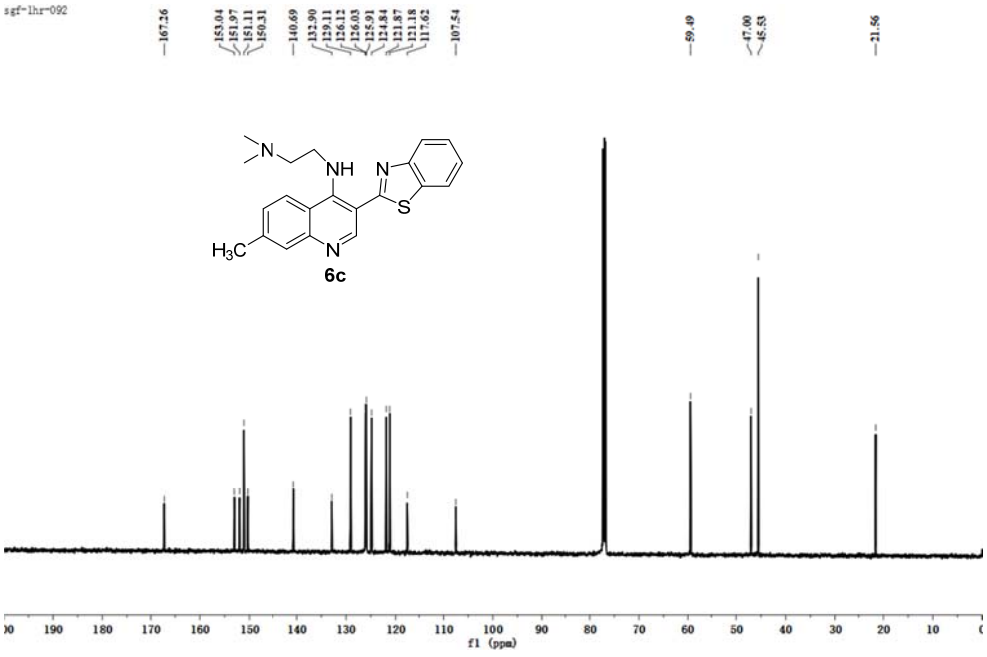

141 #1-15 RT: 0.00-0.05 AV: 15 NL: 2.77E7
T: FTMS + p ESI Full ms [100.00-450.00]
349.14737
C20 H21 N4 S
350.15045
C20 H22 N4 S
351.14222
C20 H23 N4 S
352.14634
C20 H24 N4 S
Relative Abundance
m/z

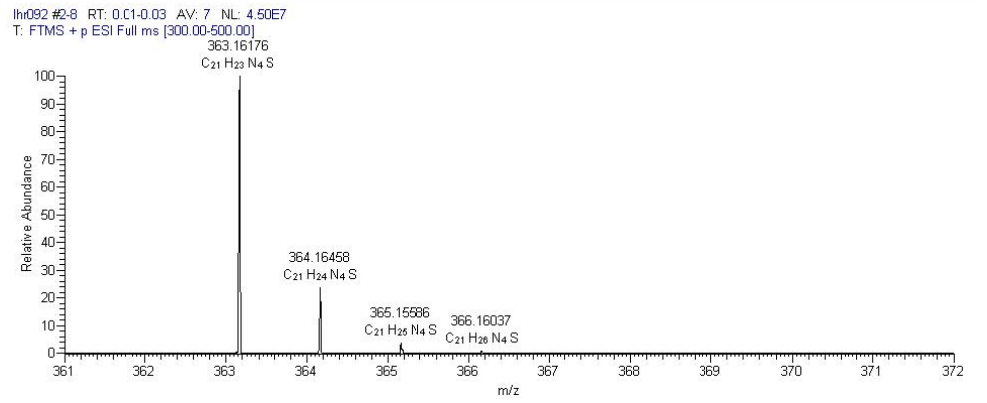

sgf-1hr-073
10.4893
8.9285
8.0811
7.9638
7.9477
7.8845
7.8728
7.8565
7.4779
7.4629
7.4476
7.3700
7.3549
7.3400
3.9897
3.9784
3.9678
3.9568
2.6645
2.6525
2.6406
2.5190
2.3890
N
NH
N
S
H3C
N
6b
0.94
0.94
1.04
1.01
2.00
2.16
1.04
2.00
2.00
3.01
6.03
f1 (ppm)

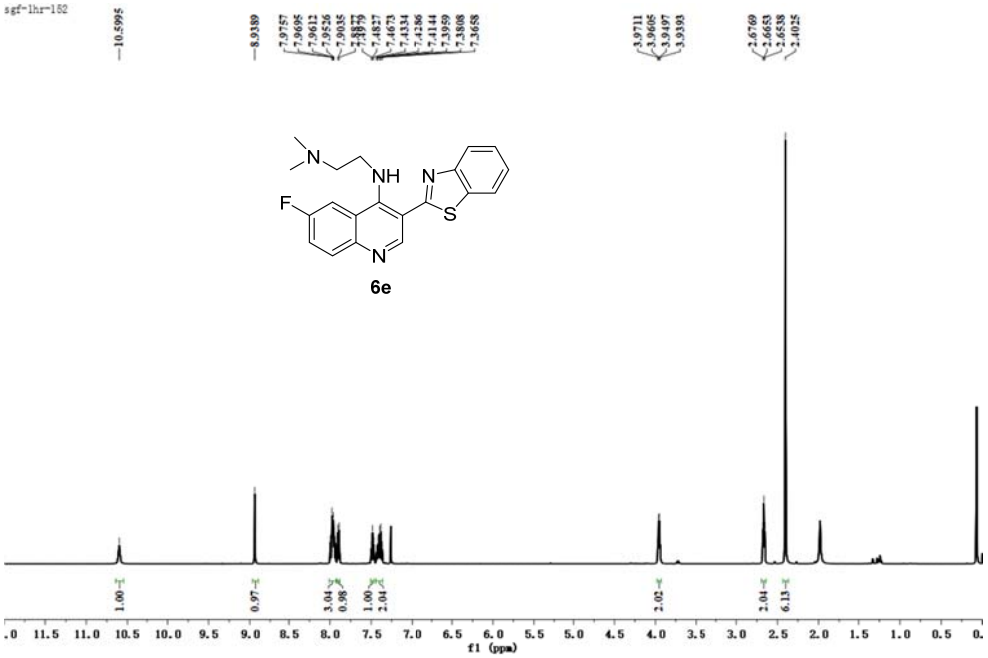

sgf-1hr-073
167.10
153.04
151.90
150.10
148.25
133.75
133.04
132.24
129.48
126.15
125.18
124.92
121.98
121.18
119.86
108.26
59.58
47.15
45.51
21.92
N
NH
N
S
H3C
N
6b
f1 (ppm)


lhr073 #3-11 RT: 0.01-0.04 AV: 9 NL: 1.14E8
T: FTMS + p ESI Full ms [100.00-500.00]
363.16248
C21 H23 N4 S
364.16550
C21 H24 N4 S
365.15680
C21 H26 N4 S
366.16114
C21 H26 N4 S
Relative Abundance
m/z

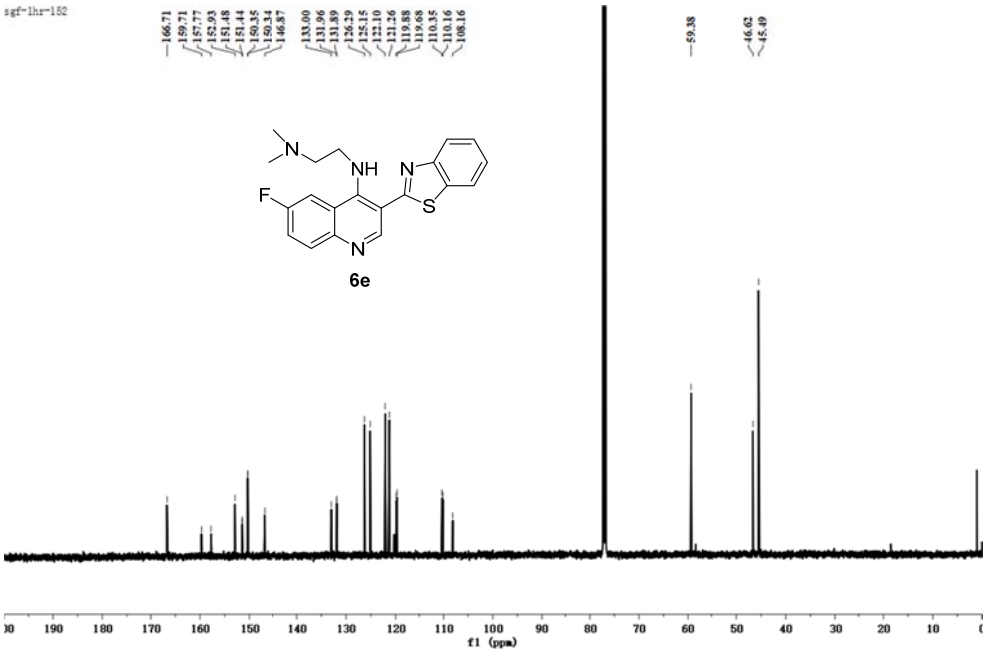

sgf-lhr-092
NH
N
S
H3C
6c
f1 (ppm)


sgf-lhr-092
NH
N
S
H3C
6c
f1 (ppm)

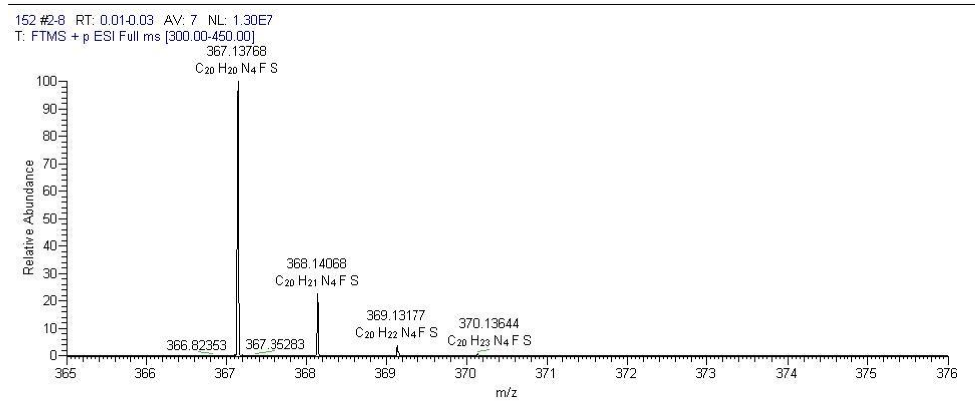

lhr092 #2-8 RT: 0.01-0.03 AV: 7 NL: 4.50E7
T: FTMS + p ESI Full ms [300.00-500.00]
363.16176
C21 H23 N4 S
364.16458
C21 H24 N4 S
365.15586
C21 H25 N4 S
366.16037
C21 H26 N4 S
Relative Abundance
m/z

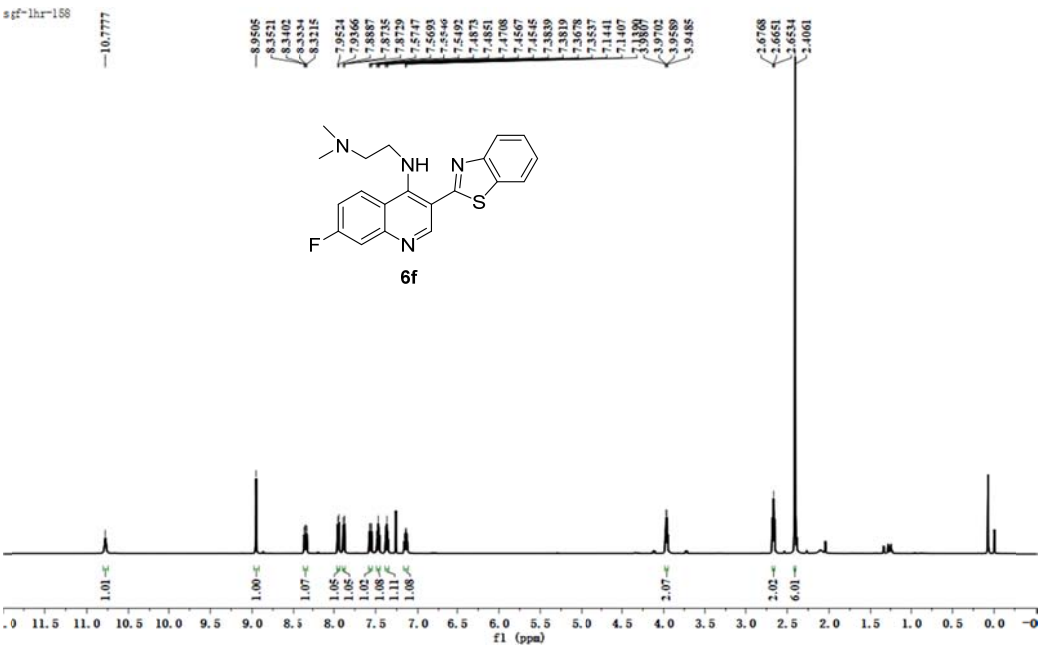

sgf-1hr-152
10.5995
8.9389
7.9757
7.9695
7.9612
7.9526
7.9035
7.4827
7.4673
7.4334
7.4286
7.4144
7.3959
7.3808
7.3658
3.9711
3.9666
3.9497
3.9393
2.6769
2.6653
2.6538
2.4025
1.00
0.97
3.04
0.98
1.00
2.04
2.02
2.04
6.13
f1 (ppm)

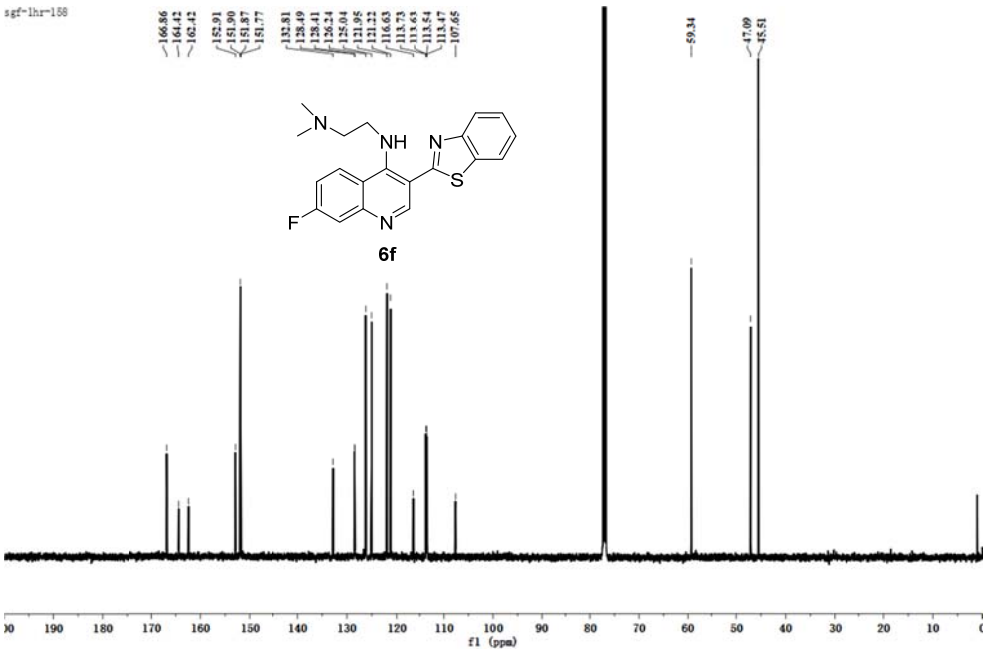
6e

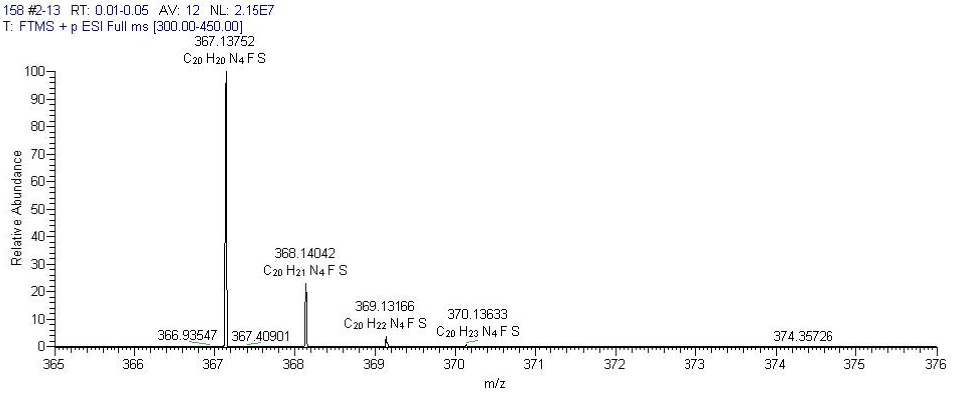

sgf-1hr-152
166.71
159.71
157.77
152.93
151.48
151.44
150.35
150.34
146.87
133.00
131.96
131.89
126.29
125.15
122.10
121.26
119.88
119.68
110.35
110.16
108.16
59.38
46.62
45.49
f1 (ppm)

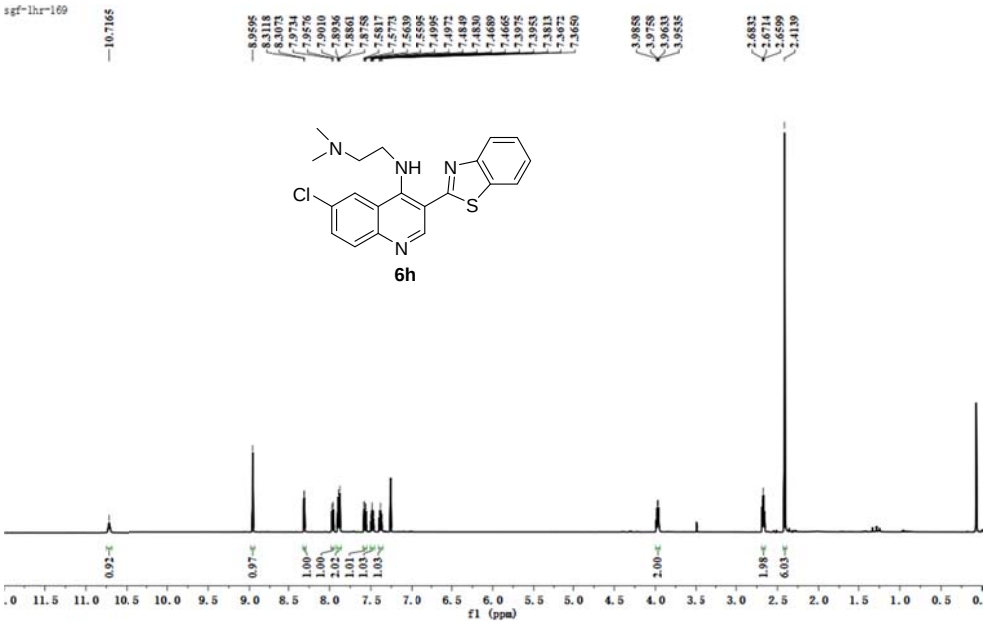
6e

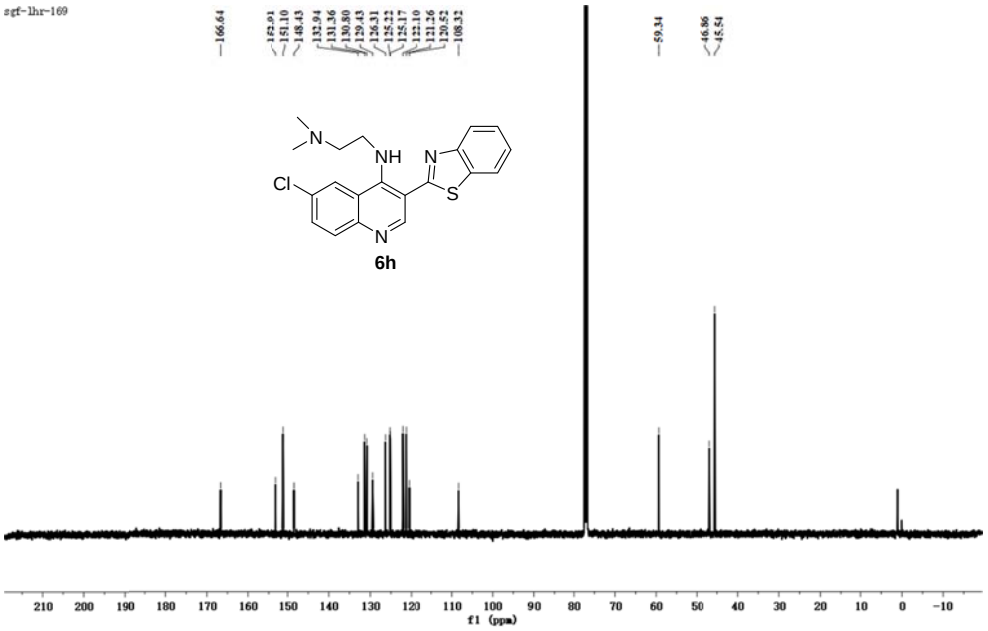

152 #2-8 RT: 0.01-0.03 AV: 7 NL: 1.30E7
T: FTMS + p ESI Full ms [300.00-450.00]
367.13768
C20 H20 N4 F S
368.14068
C20 H21 N4 F S
369.13177
C20 H22 N4 F S
370.13644
C20 H23 N4 F S
366.82353
367.35283
Relative Abundance
m/z

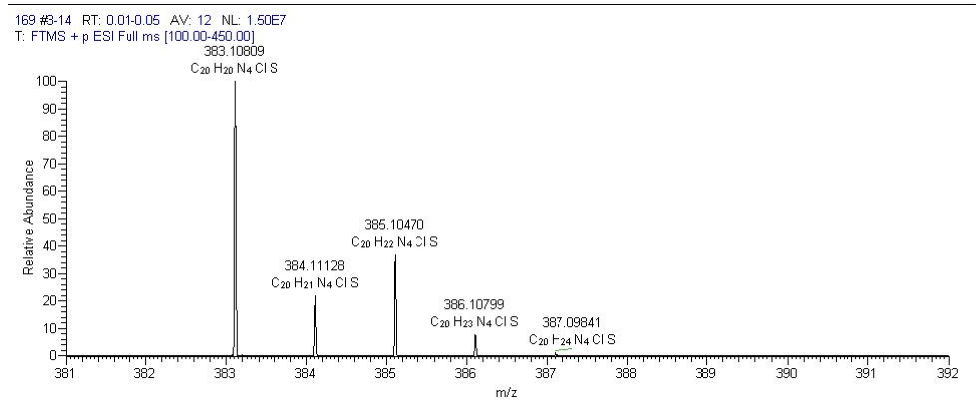

sgf-1hr-158
6f
f1 (ppm)

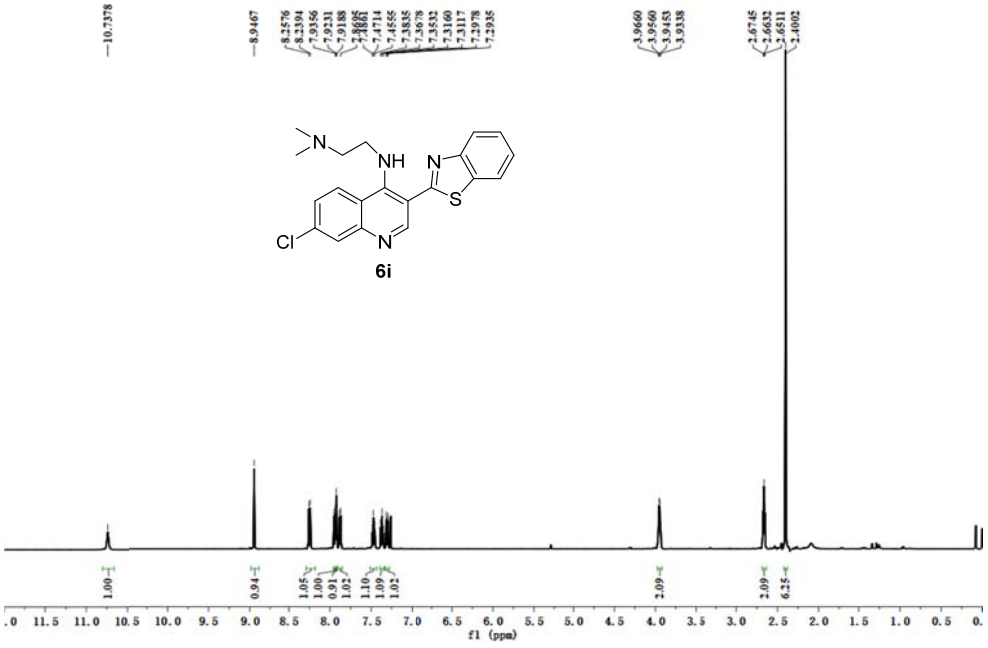

sgf-1hr-158
6f
f1 (ppm)

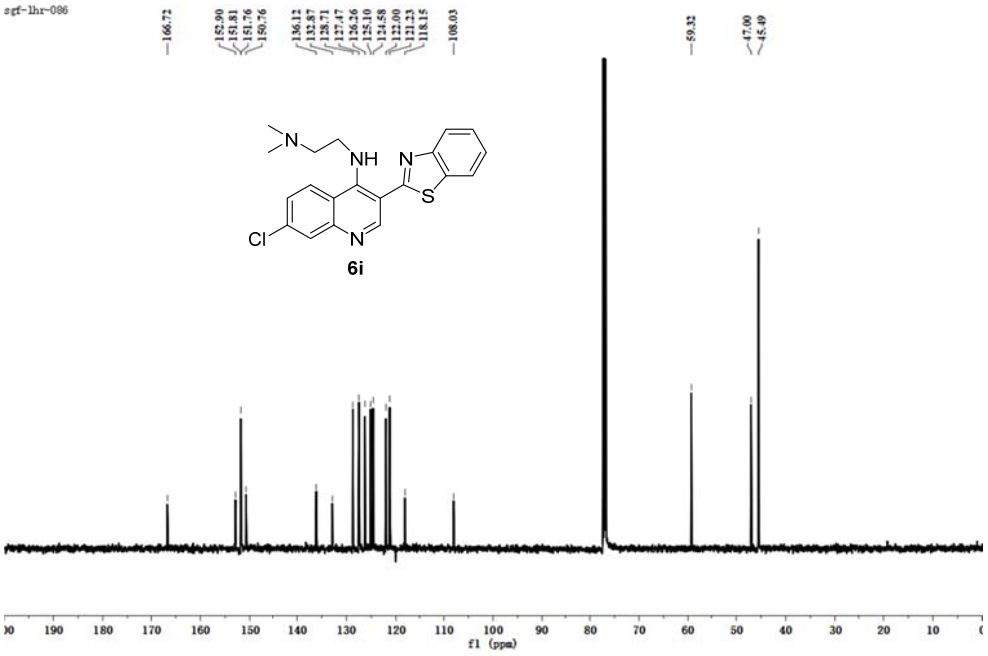

158 #2-13 RT: 0.01-0.05 AV: 12 NL: 2.15E7
T: FTMS + p ESI Full ms [300.00-450.00]
367.13752
C20 H20 N4 F S
368.14042
C20 H21 N4 F S
369.13166
C20 H22 N4 F S
370.13633
C20 H23 N4 F S
366.93547
367.40901
374.35726
Relative Abundance
m/z

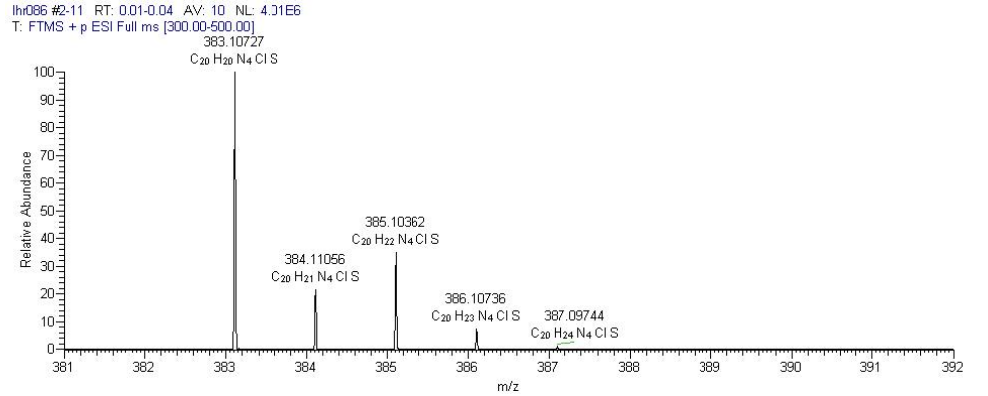

sgf-1hr-169
N
NH
N
Cl
S
N
6h
f1 (ppm)

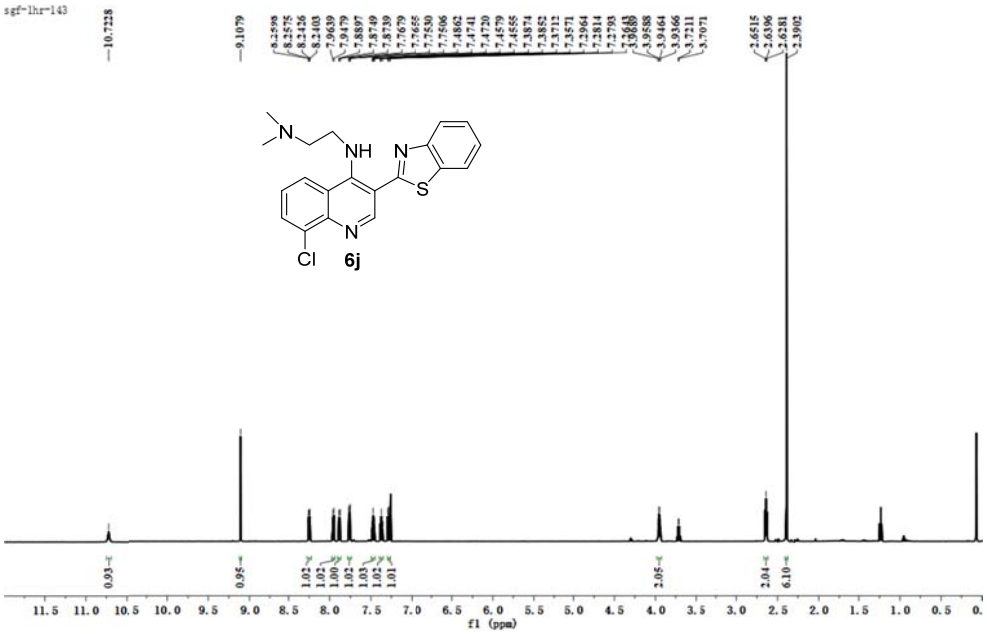

sgf-1hr-169
N
NH
N
Cl
S
N
6h
f1 (ppm)

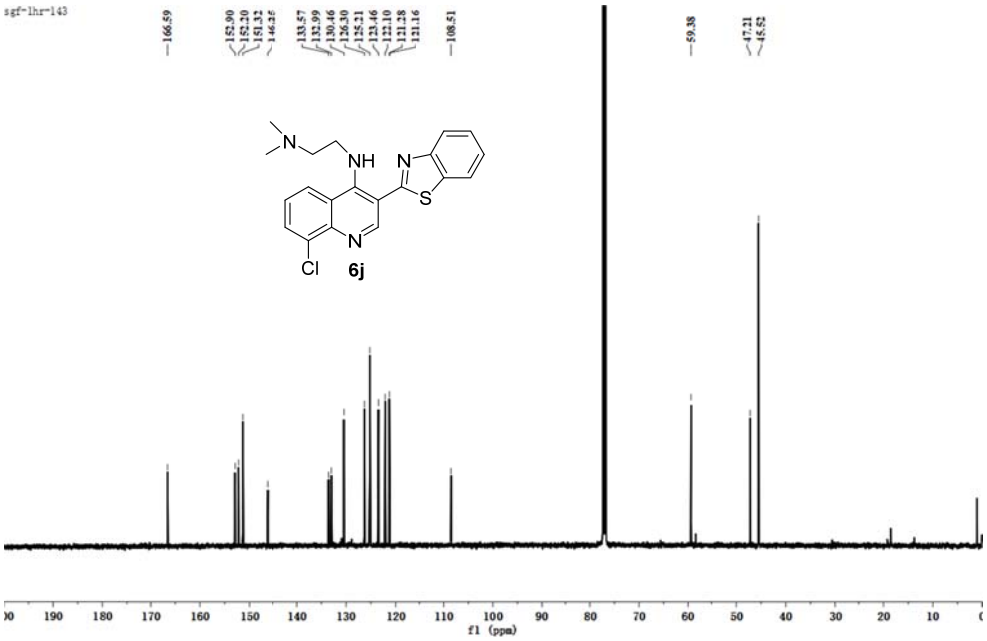

169 #3-14 RT: 0.01-0.05 AV: 12 NL: 1.50E7
T: FTMS + p ESI Full ms [100.00-450.00]
383.10809
C20 H20 N4 Cl S
385.10470
C20 H22 N4 Cl S
384.11128
C20 H21 N4 Cl S
386.10799
C20 H23 N4 Cl S
387.09841
C20 H24 N4 Cl S
Relative Abundance
m/z

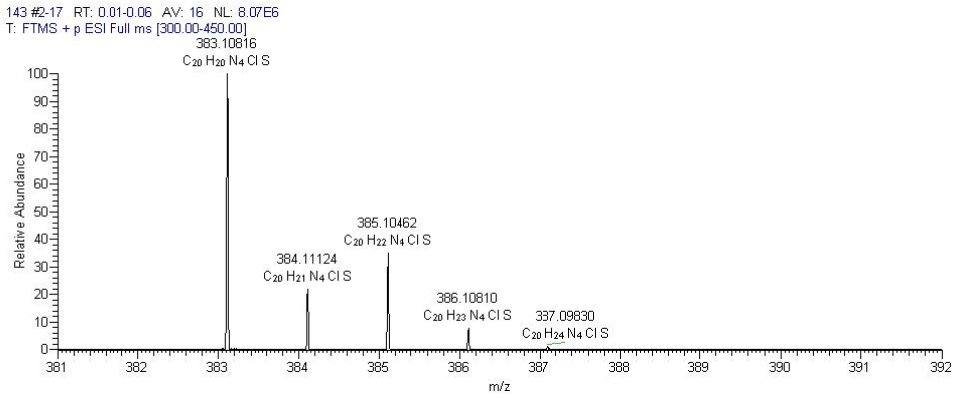

6i
f1 (ppm)

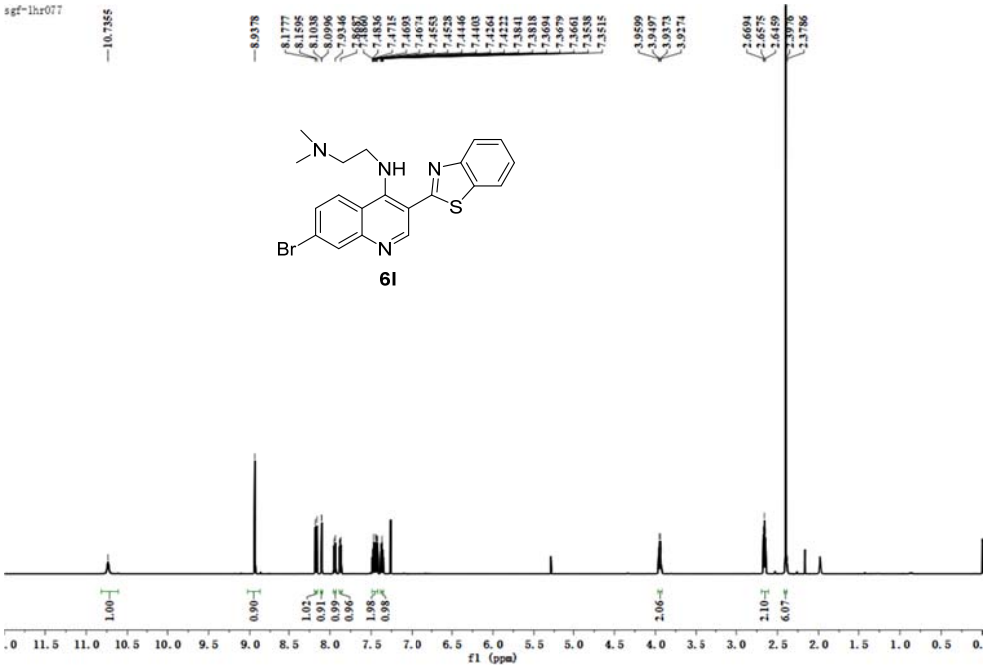

sgf-lhr-086
6i
f1 (ppm)

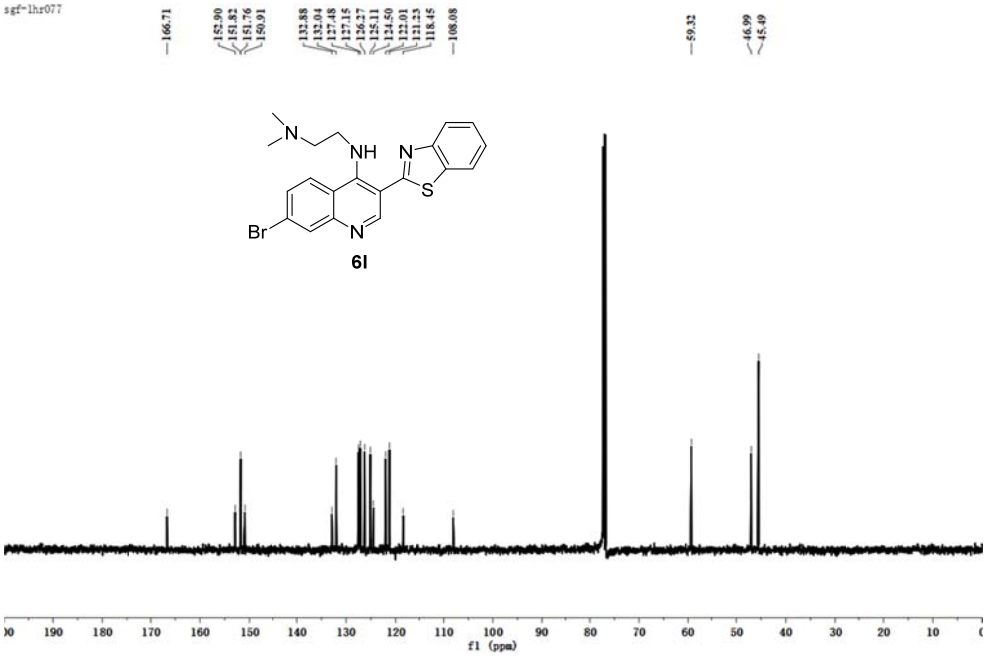

lhr086 #2-11 RT: 0.01-0.04 AV: 10 NL: 4.31E6
T: FTMS + p ESI Full ms [300.00-500.00]
383.10727
C20 H20 N4 Cl S
385.10362
C20 H22 N4 Cl S
384.11056
C20 H21 N4 Cl S
386.10736
C20 H23 N4 Cl S
387.09744
C20 H24 N4 Cl S
Relative Abundance
m/z

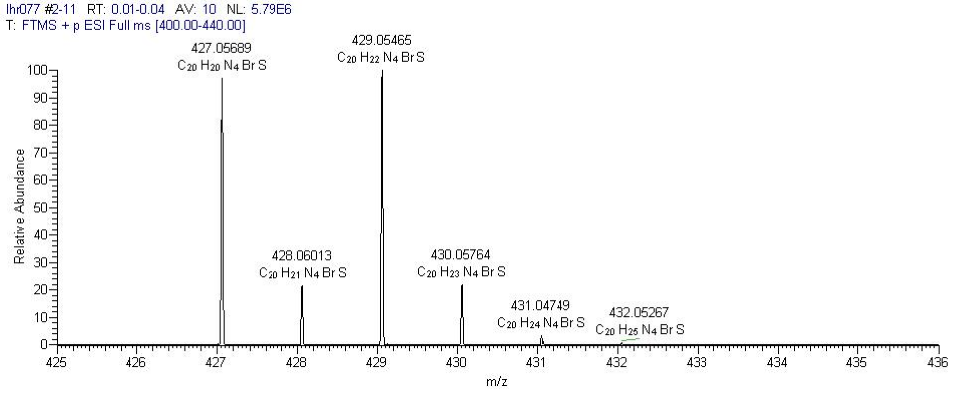

sgf-1hr-143
NH
N
S
N
Cl
6j
f1 (ppm)

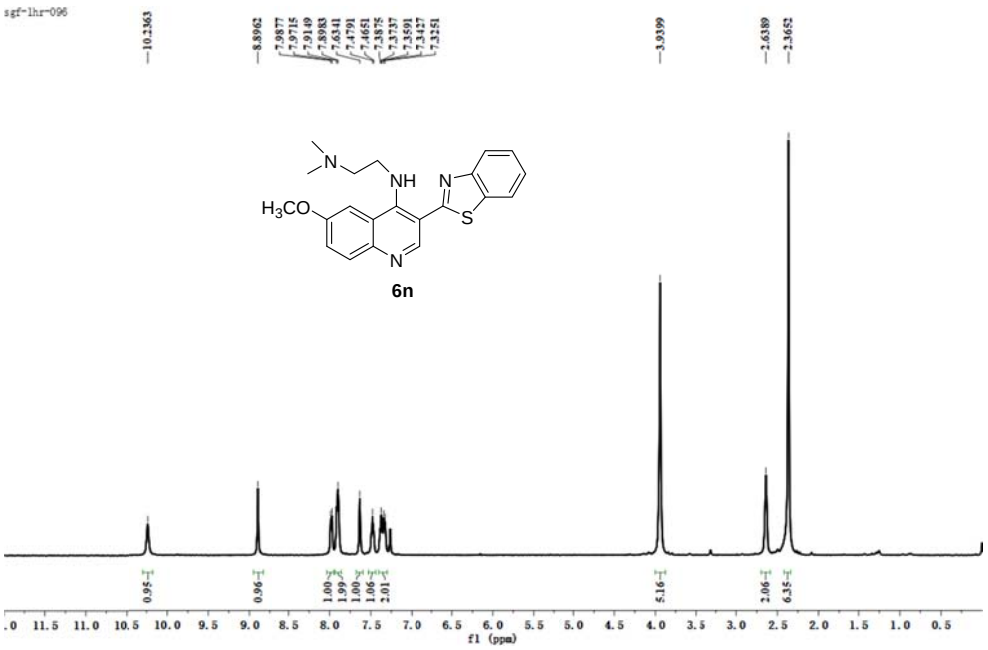

sgf-1hr-143
NH
N
S
N
Cl
6j
f1 (ppm)

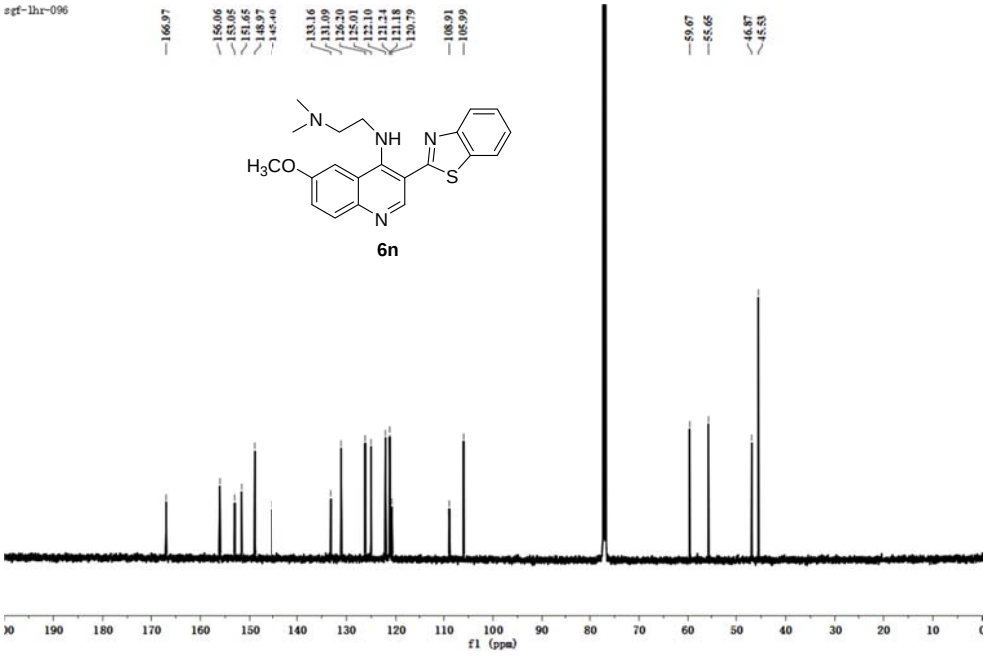

143 #2-17 RT: 0.01-0.06 AV: 16 NL: 8.07E6
T: FTMS + p ESI Full ms [300.00-450.00]
383.10816
C20 H20 N4 Cl S
385.10462
C20 H22 N4 Cl S
384.11124
C20 H21 N4 Cl S
386.10810
C20 H23 N4 Cl S
387.09830
C20 H24 N4 Cl S
Relative Abundance
m/z

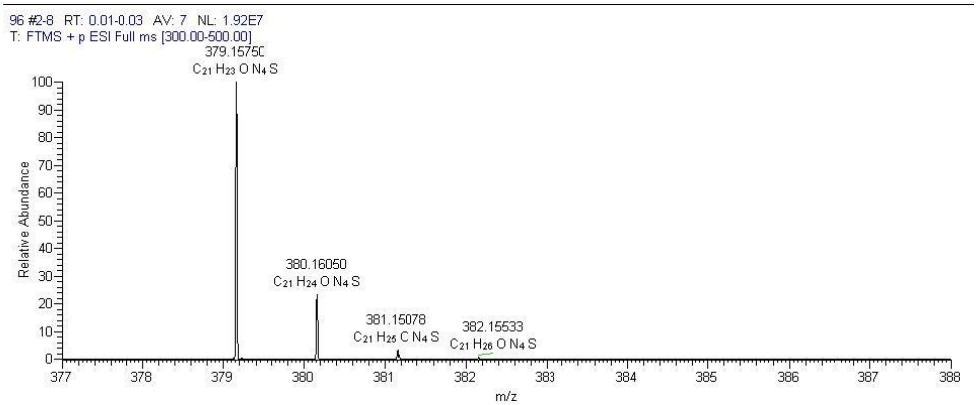

sgf-lhr077
6l
f1 (ppm)


sgf-lhr077
6l
f1 (ppm)

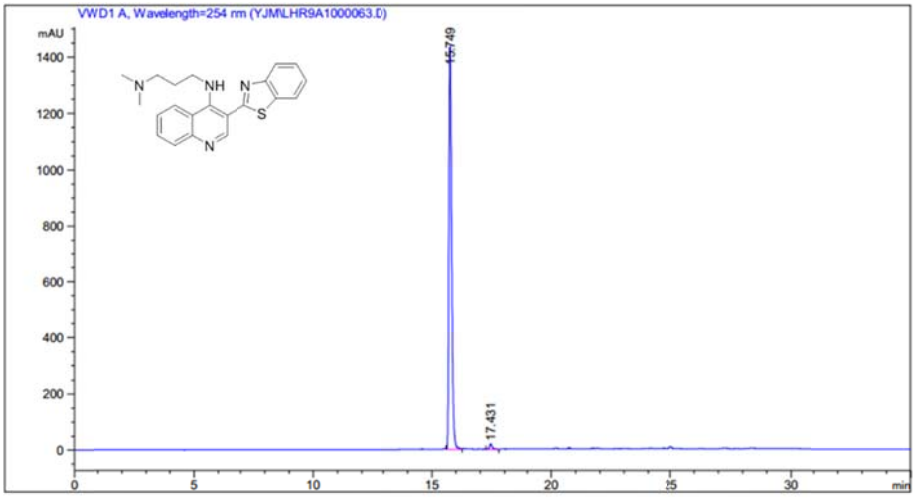

lhr077 #2-11 RT: 0.01-0.04 AV: 10 NL: 5.79E6
T: FTMS + p ESI Full ms [400.00-440.00]
427.05689
C20 H20 N4 Br S
429.05465
C20 H22 N4 Br S
428.06013
C20 H21 N4 Br S
430.05764
C20 H23 N4 Br S
431.04749
C20 H24 N4 Br S
432.05267
C20 H25 N4 Br S
Relative Abundance
m/z


sgf-lhr-096
10.2363
8.8962
7.9877
7.9715
7.9149
7.8983
7.6341
7.4791
7.4651
7.3875
7.3737
7.3591
7.3427
7.3251
3.9399
2.6389
2.3652
NH
N
S
H_3CO
N
6n
0.95
0.96
1.00
1.99
1.00
1.06
2.01
5.16
2.06
6.35
f1 (ppm)

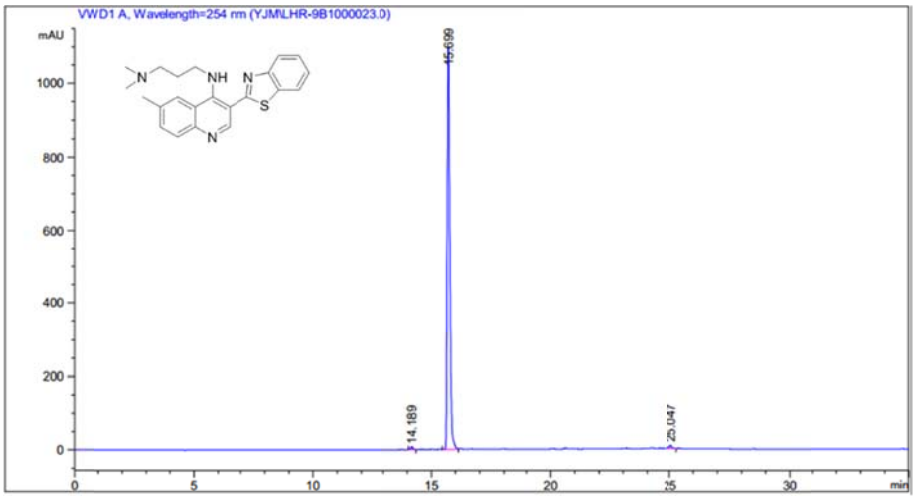

sgf-lhr-096
166.97
156.06
153.05
151.65
148.97
145.40
133.16
131.09
126.20
125.01
122.10
121.24
121.18
120.79
108.91
105.99
59.67
55.65
46.87
45.53
NH
N
S
H_3CO
N
6n
f1 (ppm)


96 #2-8 RT: 0.01-0.03 AV: 7 NL: 1.92E7
T: FTMS + p ESI Full ms [300.00-500.00]
379.15750
$C_{21}H_{23}ON_4S$
380.16050
$C_{21}H_{24}ON_4S$
381.15078
$C_{21}H_{25}CN_4S$
382.15533
$C_{21}H_{26}ON_4S$
Relative Abundance
m/z

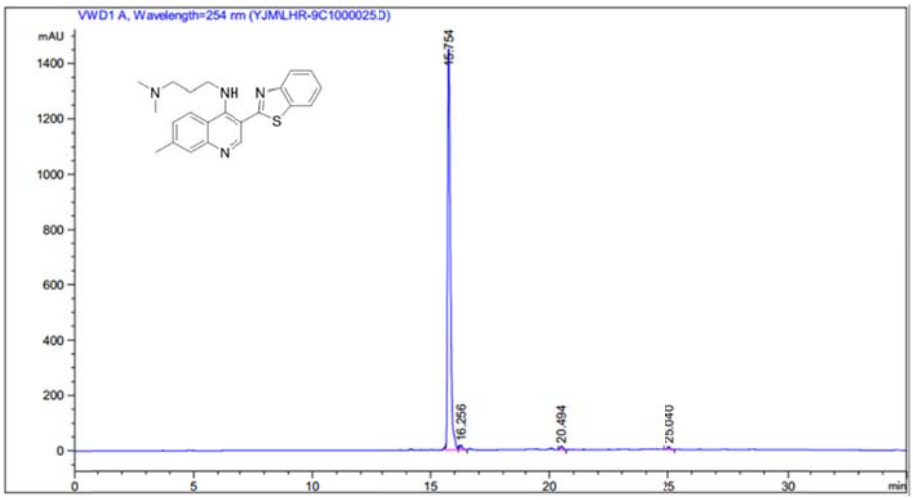
4. The HPLC spectrum of the target compounds.



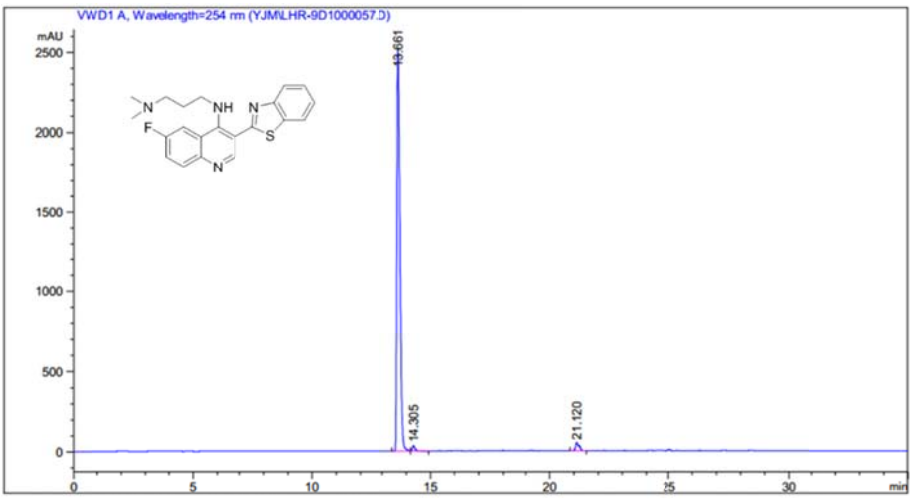
5a



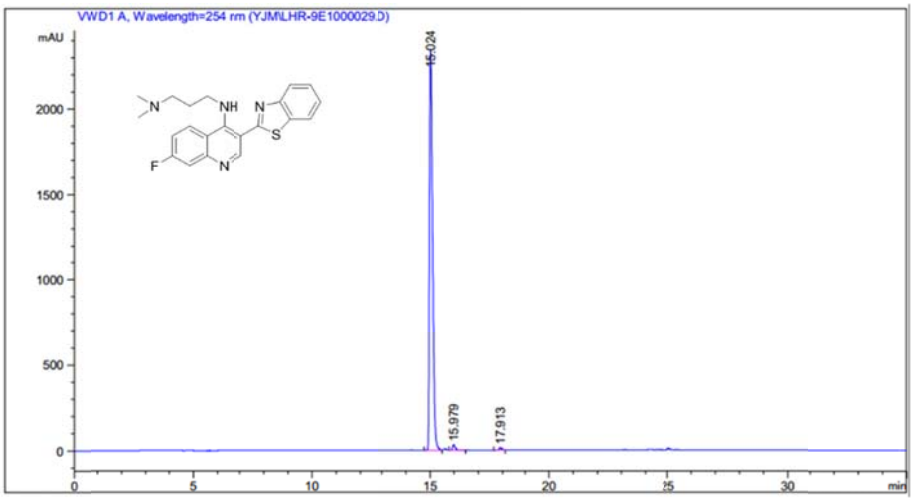
5b



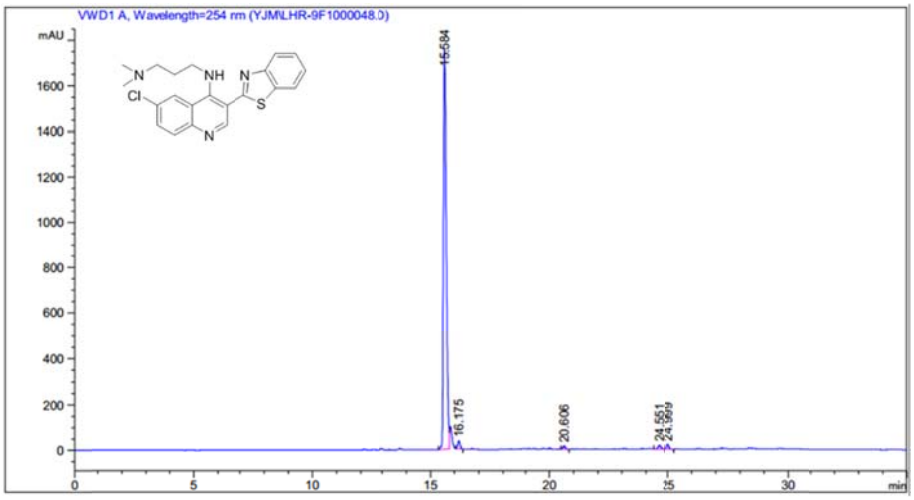
5c


VWD1 A, Wavelength=254 nm (YJM\LHR-9D1000057.D)
mAU
2500
2000
1500
1000
500
0
13.661
14.305
21.120
0
5
10
15
20
30
min

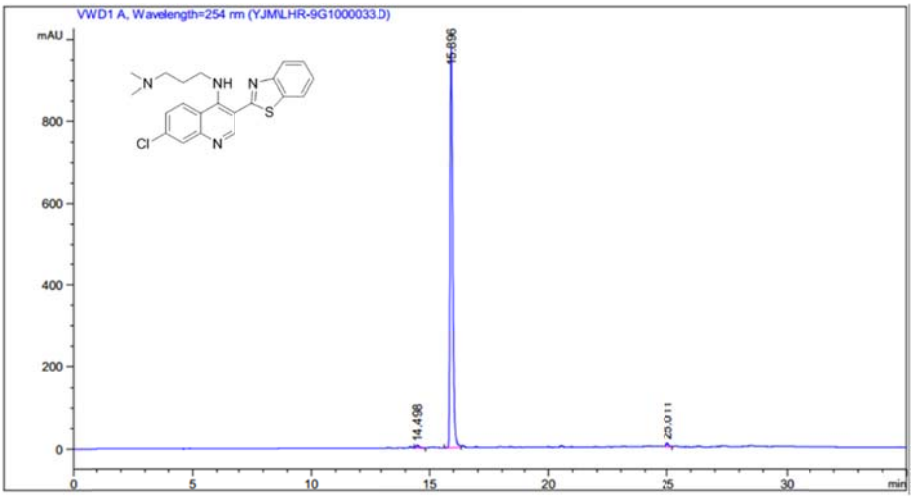
5e


VWD1 A, Wavelength=254 nm (YJM\LHR-9E1000029.D)
mAU
2000
1500
1000
500
0
15.024
15.979
17.913
0
5
10
15
20
30
min

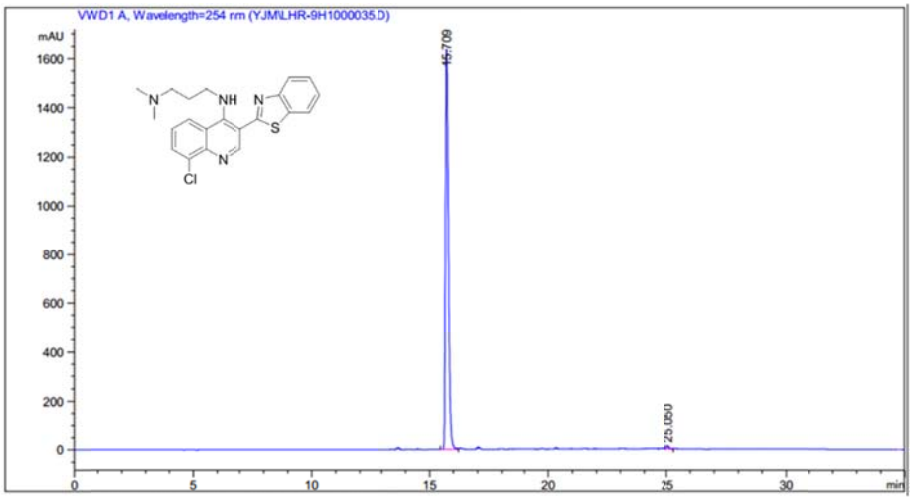
5f


VWD1 A, Wavelength=254 nm (YJM\LHR-9F1000048.D)
mAU
1600
1400
1200
1000
800
600
400
200
0
15.584
16.175
20.606
24.551
24.869
0
5
10
15
20
30
min

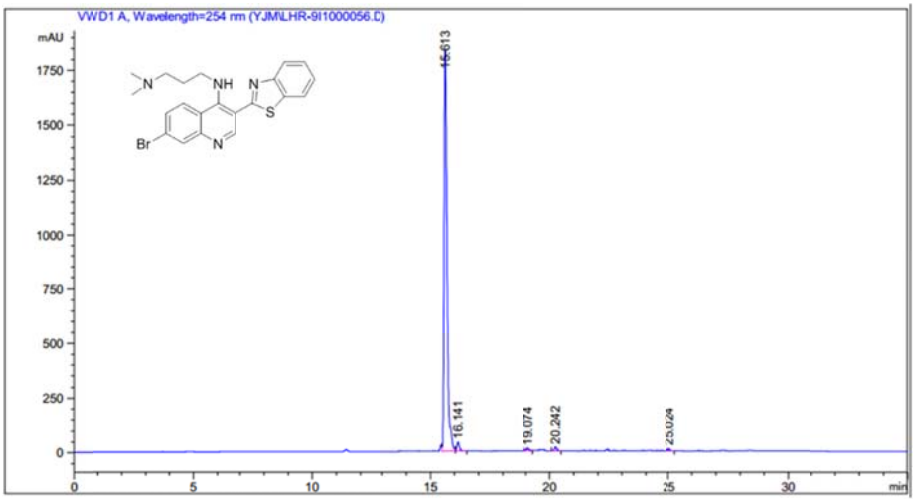
5h


VWD1 A, Wavelength=254 nm (YJM\LHR-9G1000033.D)
mAU
800
600
400
200
0
14.498
15.896
25.011
0
5
10
15
20
30
min

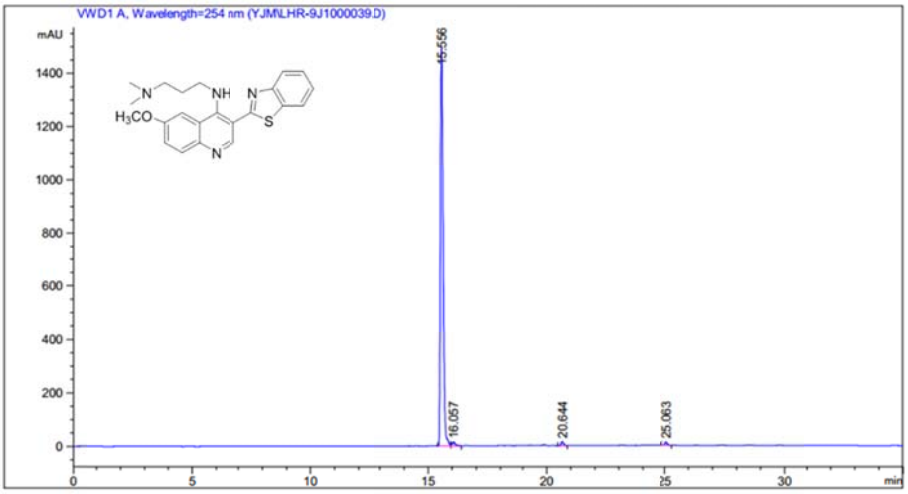
5i


VWD1 A, Wavelength=254 nm (YJM\LHR-9H1000035.D)
mAU
1600
1400
1200
1000
800
600
400
200
0
15.709
25.050
0
5
10
15
20
30
min

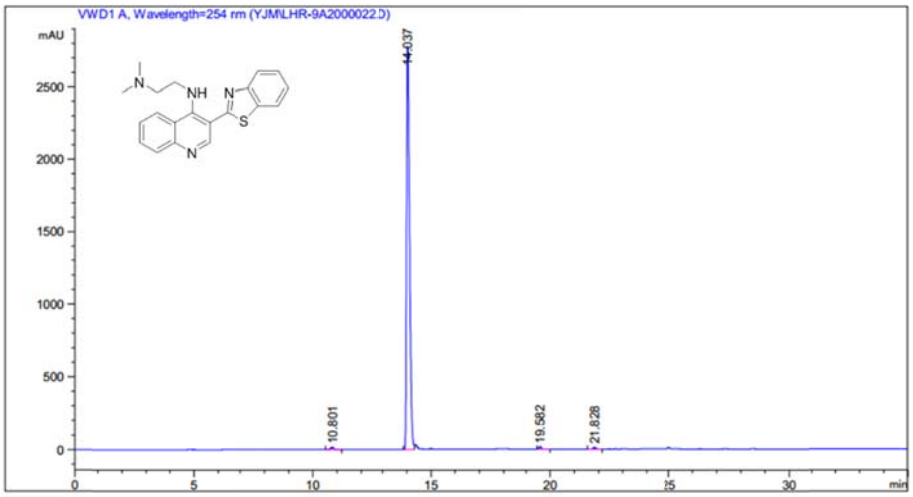
5j


VWD1 A, Wavelength=254 nm (YJM\LHR-9I1000056.D)
mAU
1750
1500
1250
1000
750
500
250
0
15.613
16.141
19.074
20.242
0
5
10
15
20
30
min

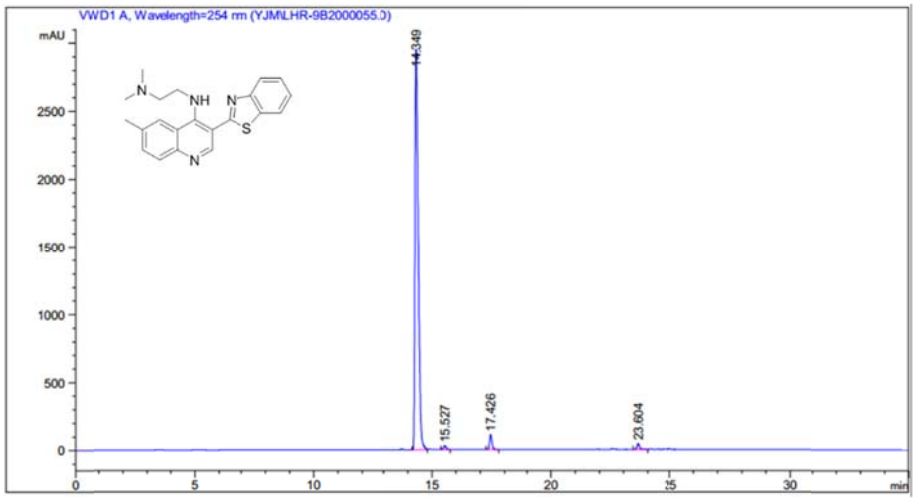
5l


VWD1 A, Wavelength=254 nm (YJM\LHR-9J1000039.D)
mAU
15.556
16.057
20.644
25.063
min

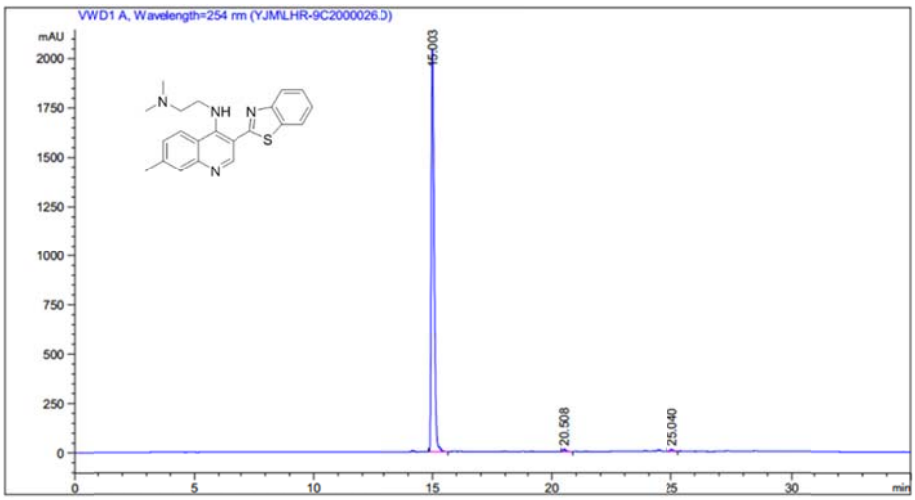
5n


VWD1 A, Wavelength=254 nm (YJM\LHR-9A2000022.D)
mAU
14.037
10.801
19.582
21.828
min

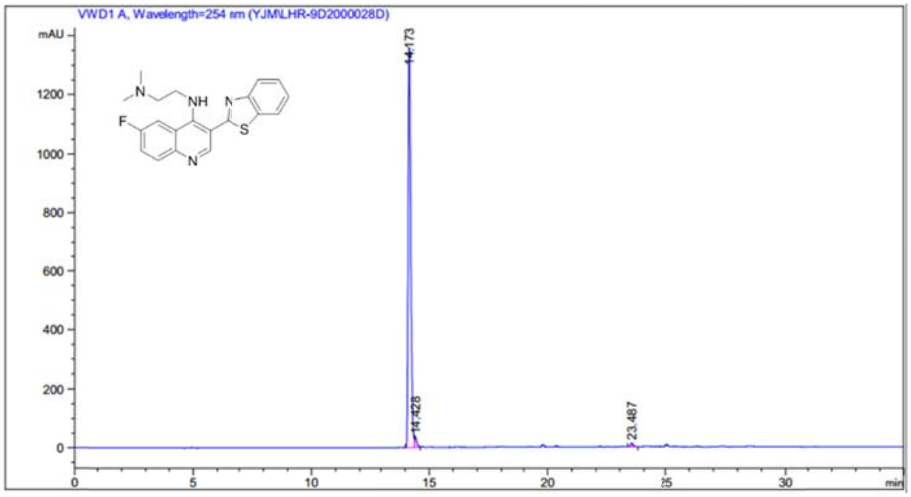
6a


VWD1 A, Wavelength=254 nm (YJM\LHR-9B2000055.D)
mAU
14.349
15.527
17.426
23.604
min

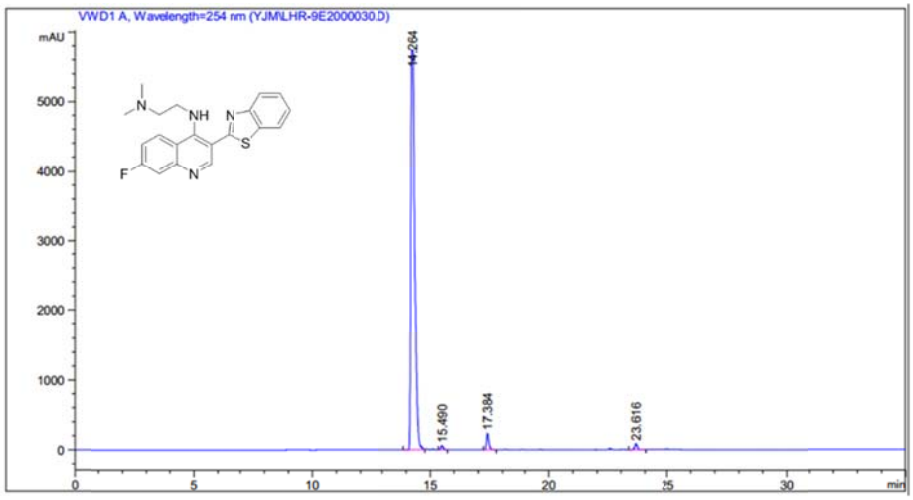
6b


VWD1 A, Wavelength=254 nm (YJM\LHR-9C2000026.D)
mAU
15.003
20.508
25.040
min

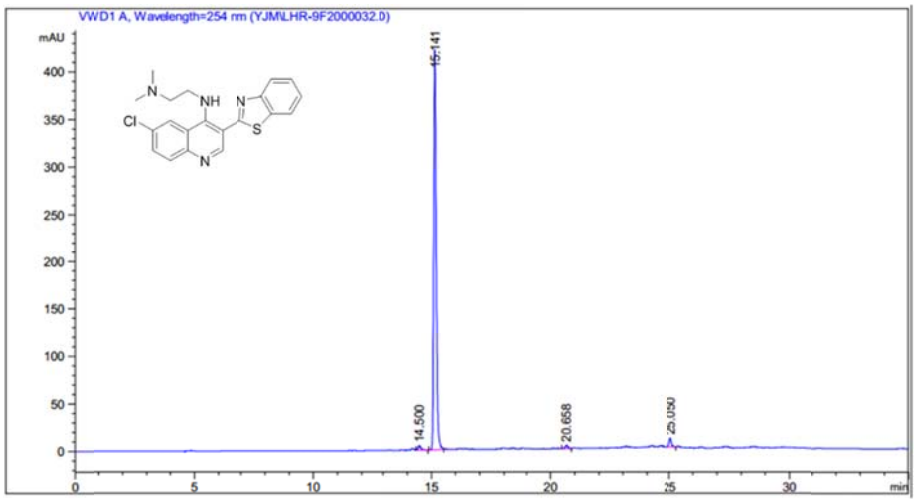
6c


VWD1 A, Wavelength=254 nm (YJM\LHR-9D2000028D)
mAU
14.173
14.428
23.467
min

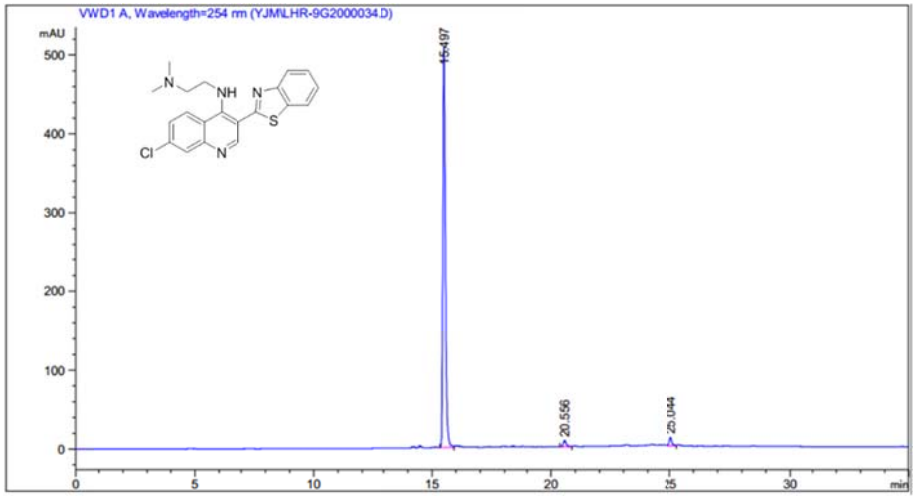
6e


VWD1 A, Wavelength=254 nm (YJM\LHR-9E2000030.D)
mAU
14.264
15.490
17.384
23.616
min

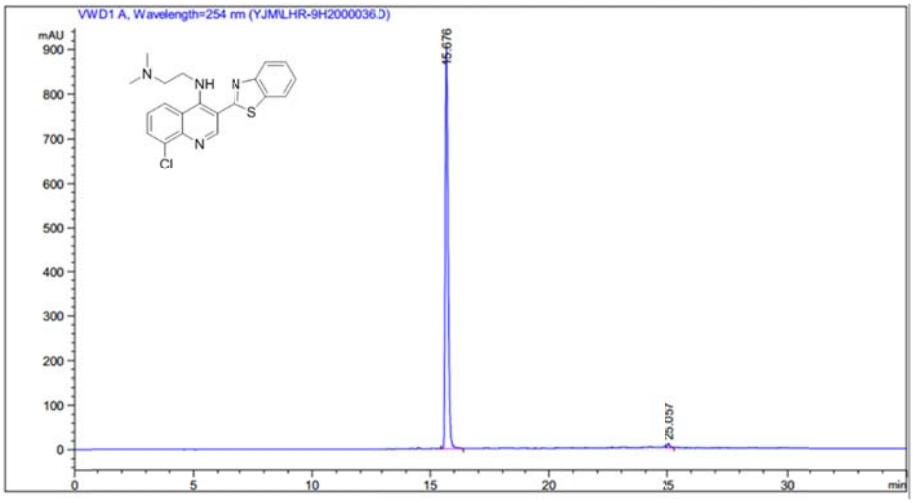
6f


VWD1 A, Wavelength=254 nm (YJM\LHR-9F2000032.D)
mAU
15.141
14.500
20.658
29.050
min

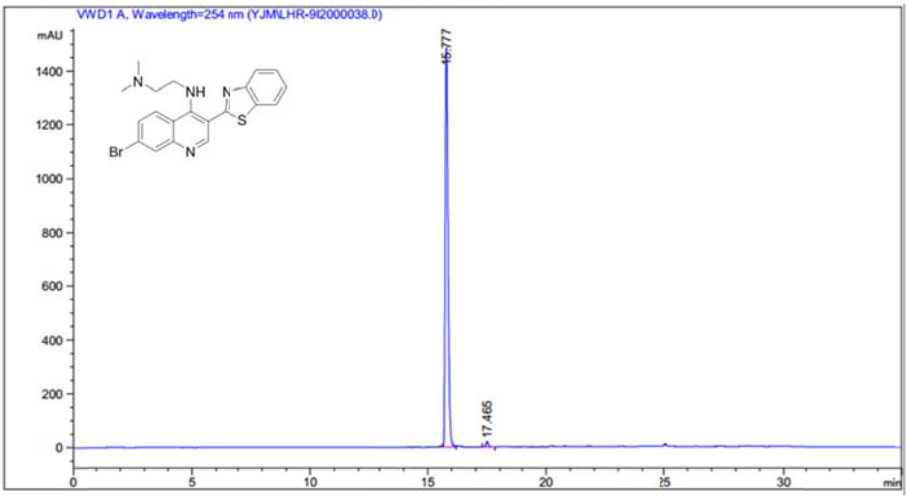
6h


VWD1 A, Wavelength=254 nm (YJM\LHR-9G2000034.D)
mAU
15.497
20.556
29.044
min

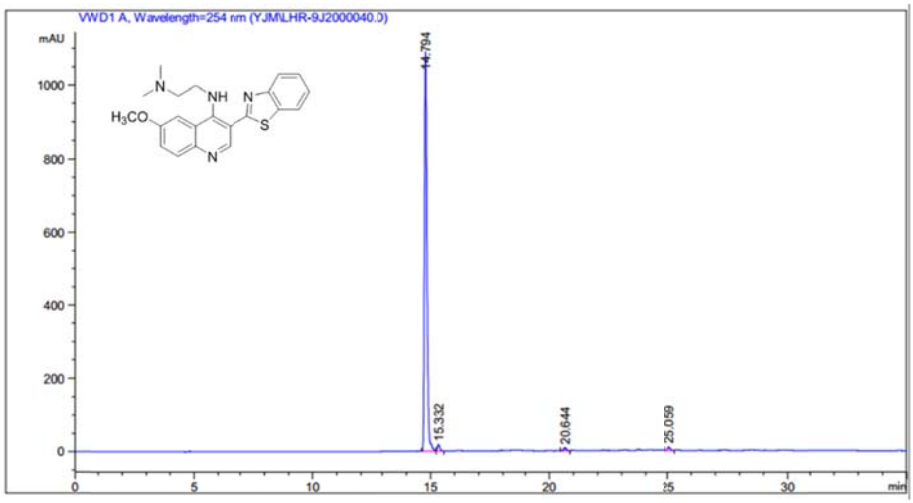
6i


VWD1 A, Wavelength=254 nm (YJM\LHR-9H2000036.D)
mAU
15.676
29.057
min

6j


VWD1 A, Wavelength=254 nm (YJM\LHR-9I2000038.D)
mAU
1400
1200
1000
800
600
400
200
0
16.777
17.465
NH
N
S
Br
N
0
5
10
15
20
30
min

6l


VWD1 A, Wavelength=254 nm (YJM\LHR-9J2000040.D)
mAU
1000
800
600
400
200
0
14.794
15.332
20.644
25.059
NH
N
S
H3CO
N
0
5
10
15
20
30
min

6n