

Supporting information

Copper-mediated thiolation of carbazole derivatives and related N-heterocycle compounds

Longzhi Zhu,^a Xin Cao,^a Renhua Qiu,^{a,b*} Takanori Iwasaki,^b Vutukuri Prakash Reddy,^b Xinhua Xu,^a

Shuang-Feng Yin^{a*} and Nobuaki Kambe^{a,b*}

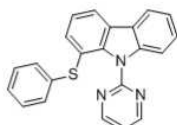
^a*College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, P.R. China;*

^b*Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan ;*

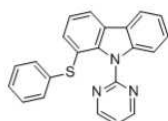
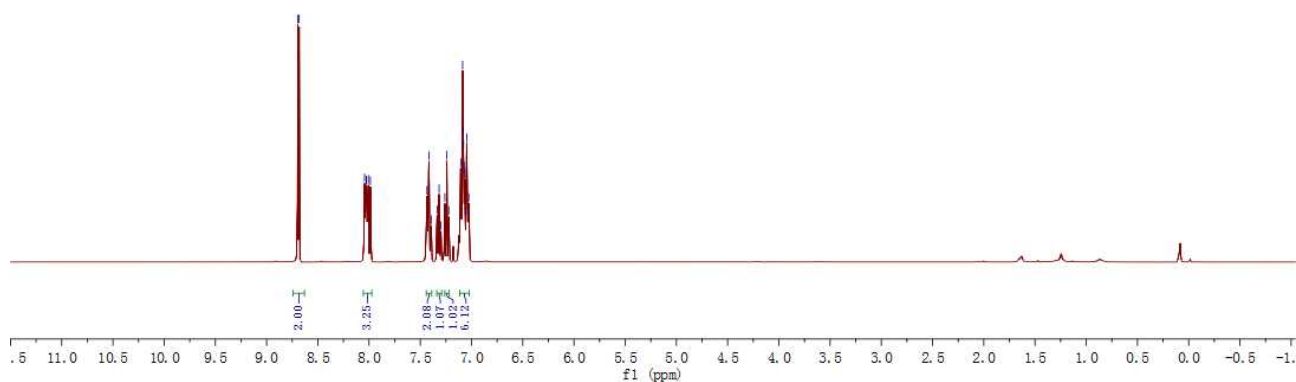
renhuaqiu@hnu.edu.cn; sf_yin@hnu.edu.cn; kambe@chem.eng.osaka-u.ac.jp

1. Data of ^1H NMR and ^{13}C NMR of Compounds of 3a-3l, 5a-5e, 7a-7g, 9 and 1b.

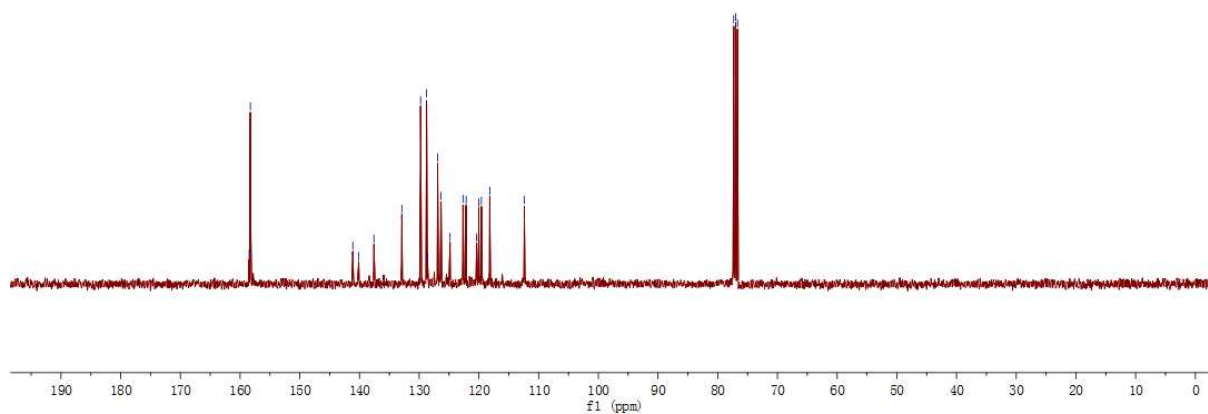
1-(Phenylthio)-9-(pyrimidin-2-yl)-9H-carbazole (3a)



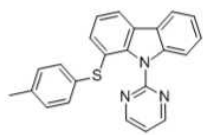
Chemical Formula: $\text{C}_{22}\text{H}_{15}\text{N}_3\text{S}$
Molecular Weight: 353.44



Chemical Formula: $\text{C}_{22}\text{H}_{15}\text{N}_3\text{S}$
Molecular Weight: 353.44



1-((4-Methylphenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole(3b)

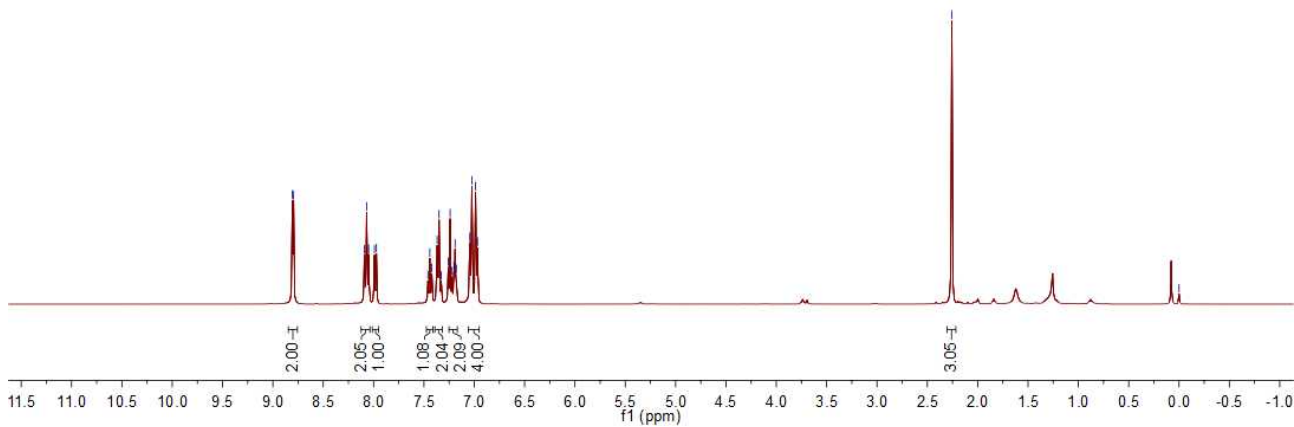


Chemical Formula: C₂₃H₁₇N₃S
Molecular Weight: 367.47

8.8061
8.7944
8.0691
8.0488
7.9909
7.9719
7.4604
7.4419
7.4219
7.3685
7.3495
7.3282
7.2584
7.2398
7.2205
7.2024
7.1905
7.1786
7.0439
7.0240
6.9876
6.9678

2.2569

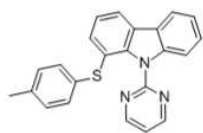
0.0001



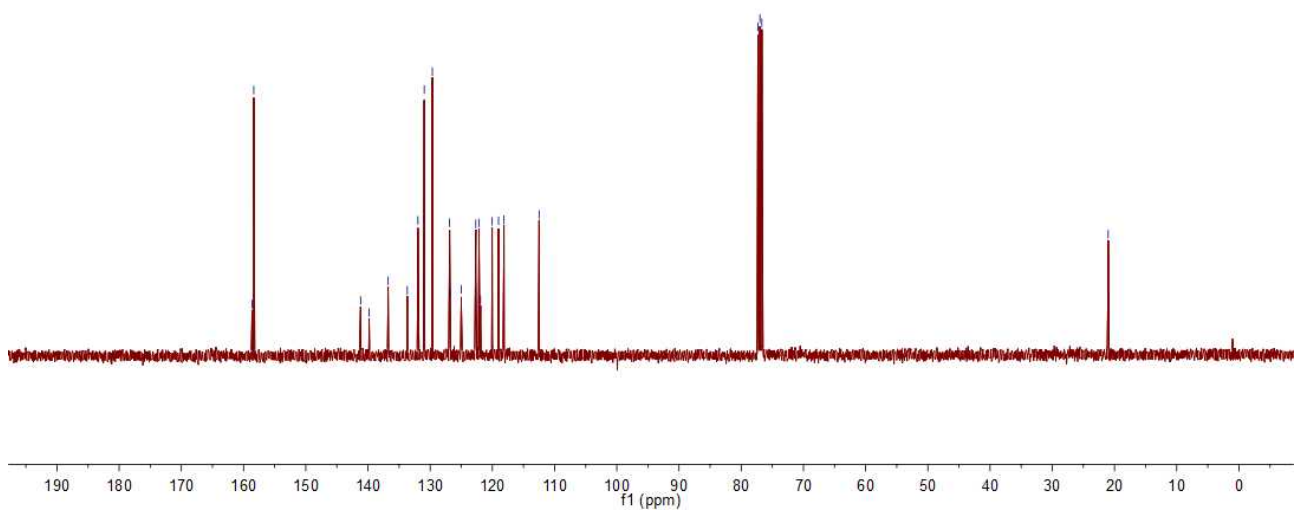
158.6340
158.3606
141.1823
139.8062
136.7666
133.6812
131.9693
130.9550
129.6523
126.8728
126.7983
125.0058
122.6875
122.1533
121.9059
120.0357
119.0082
118.1358
112.4920

77.3174
76.9997
76.6820

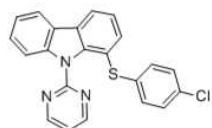
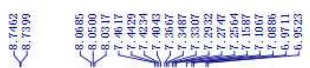
21.0078



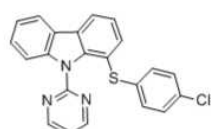
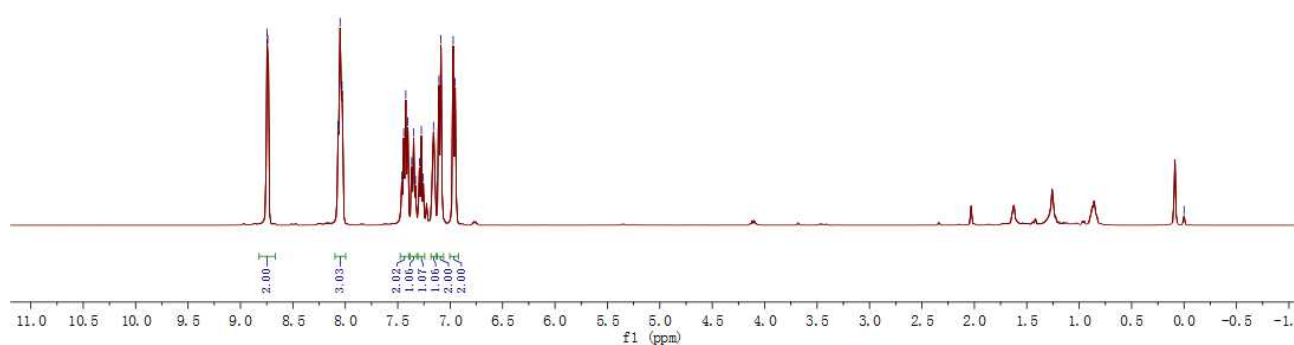
Chemical Formula: C₂₃H₁₇N₃S
Molecular Weight: 367.47



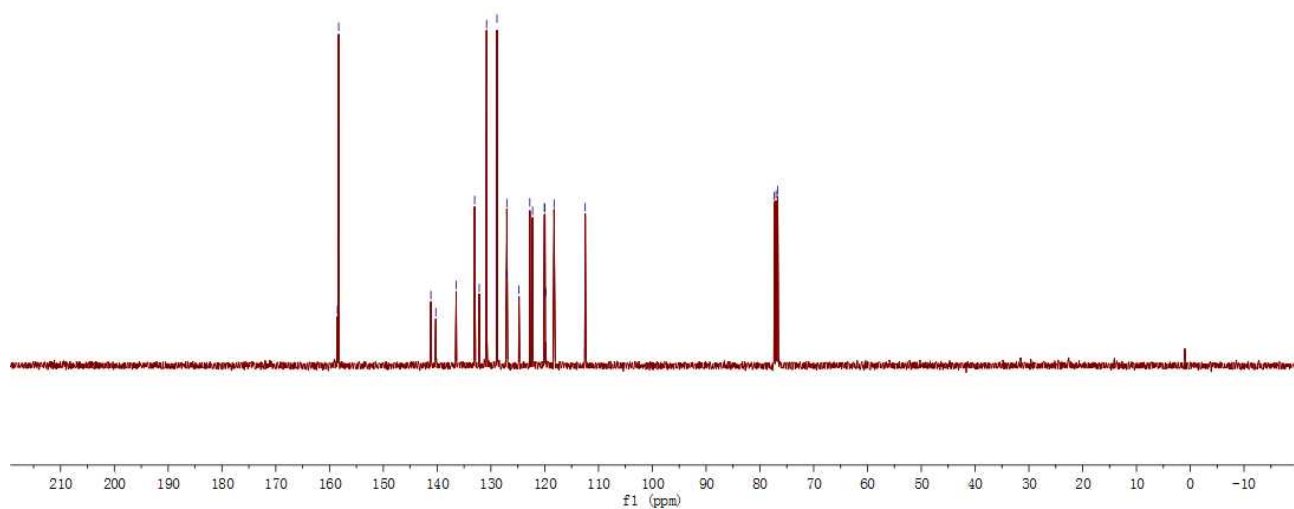
1-(4-Chlorophenyl)thio-9-(pyrimidin-2-yl)-9H-carbazole (3c)



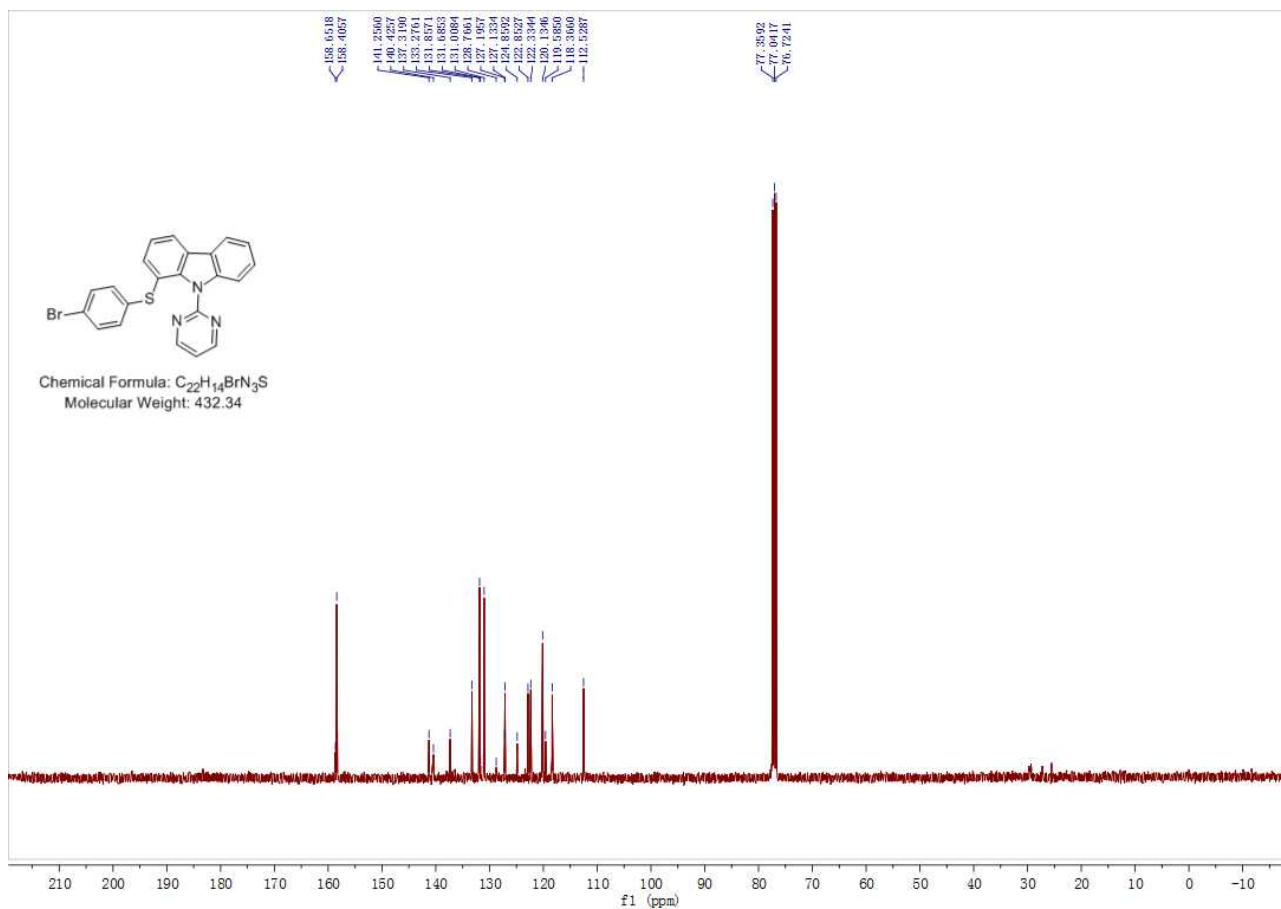
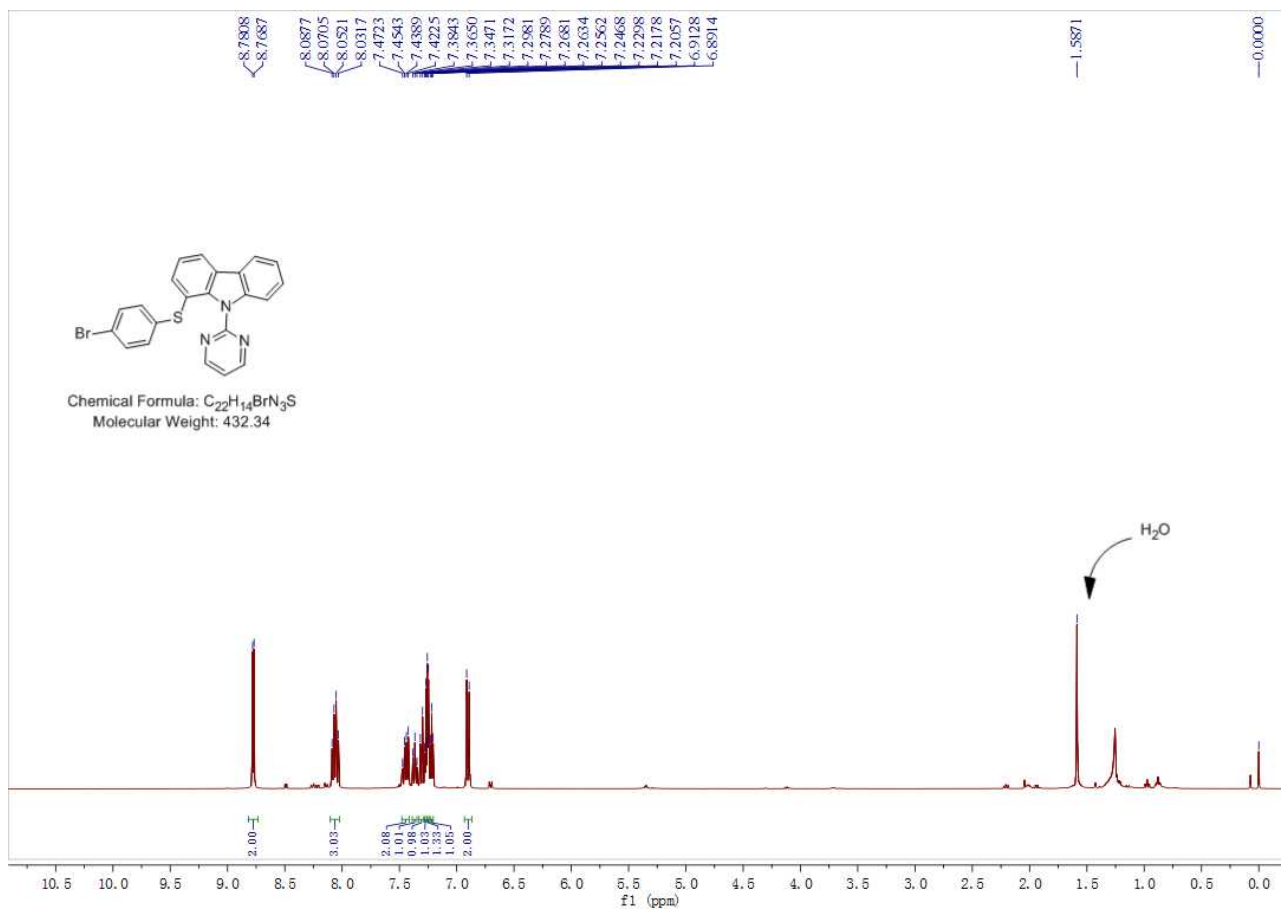
Chemical Formula: C₂₂H₁₄ClN₃S
Molecular Weight: 387.88



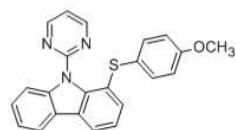
Chemical Formula: C₂₂H₁₄ClN₃S
Molecular Weight: 387.88



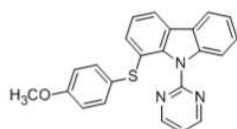
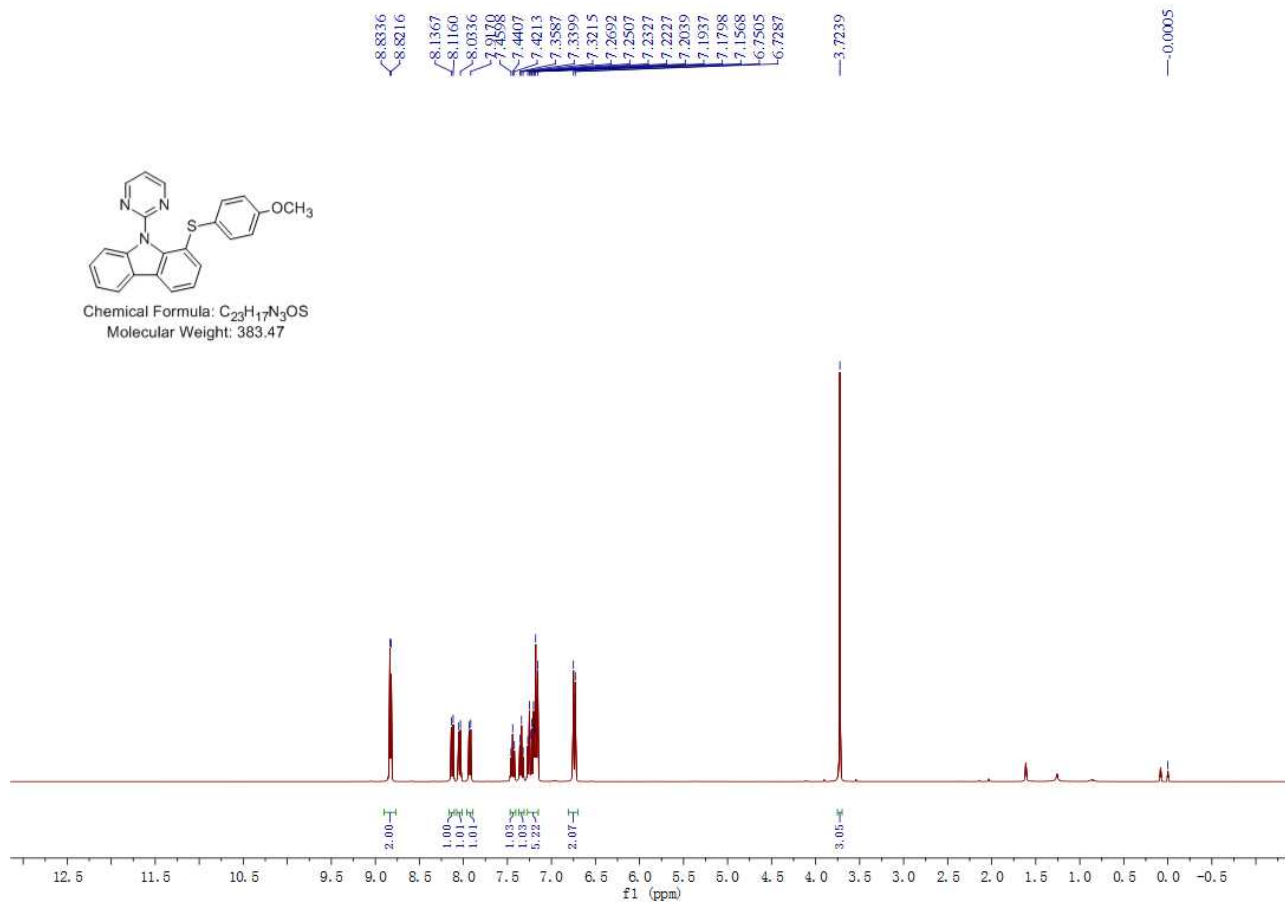
1-((4-Bromophenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole (3d)



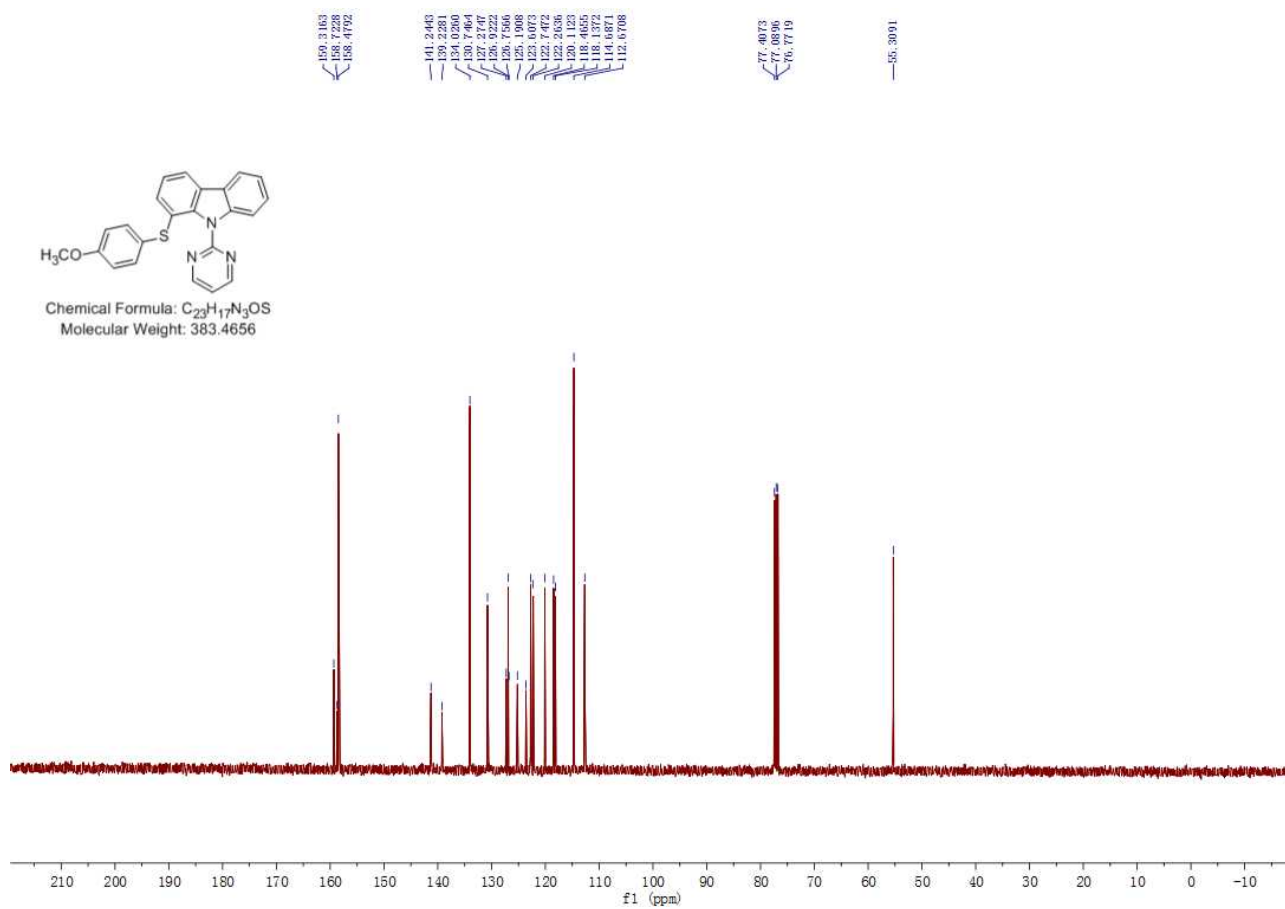
1-((4-Methoxyphenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole (3e)



Chemical Formula: C₂₃H₁₇N₃OS
Molecular Weight: 383.47



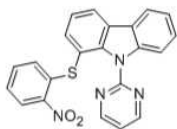
Chemical Formula: C₂₃H₁₇N₃OS
Molecular Weight: 383.4656



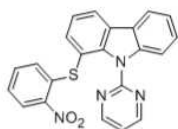
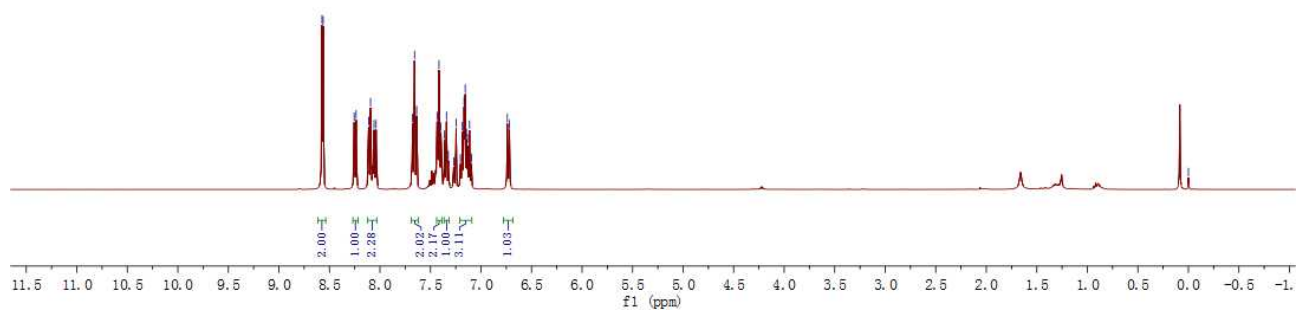
1-((2-Nitrophenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole (3f)



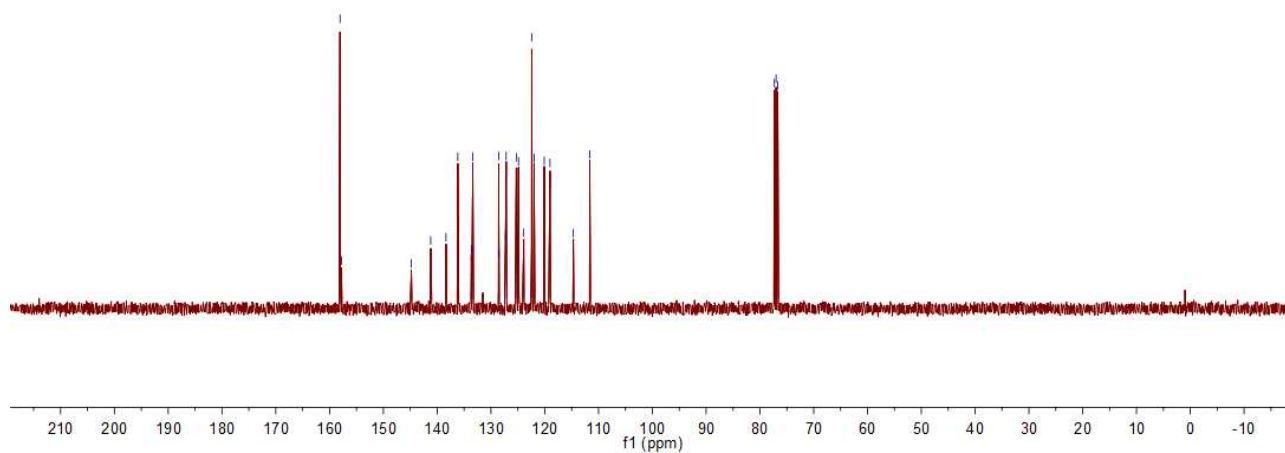
-0.0002



Chemical Formula: C₂₂H₁₄N₄O₂S
Molecular Weight: 398.4372

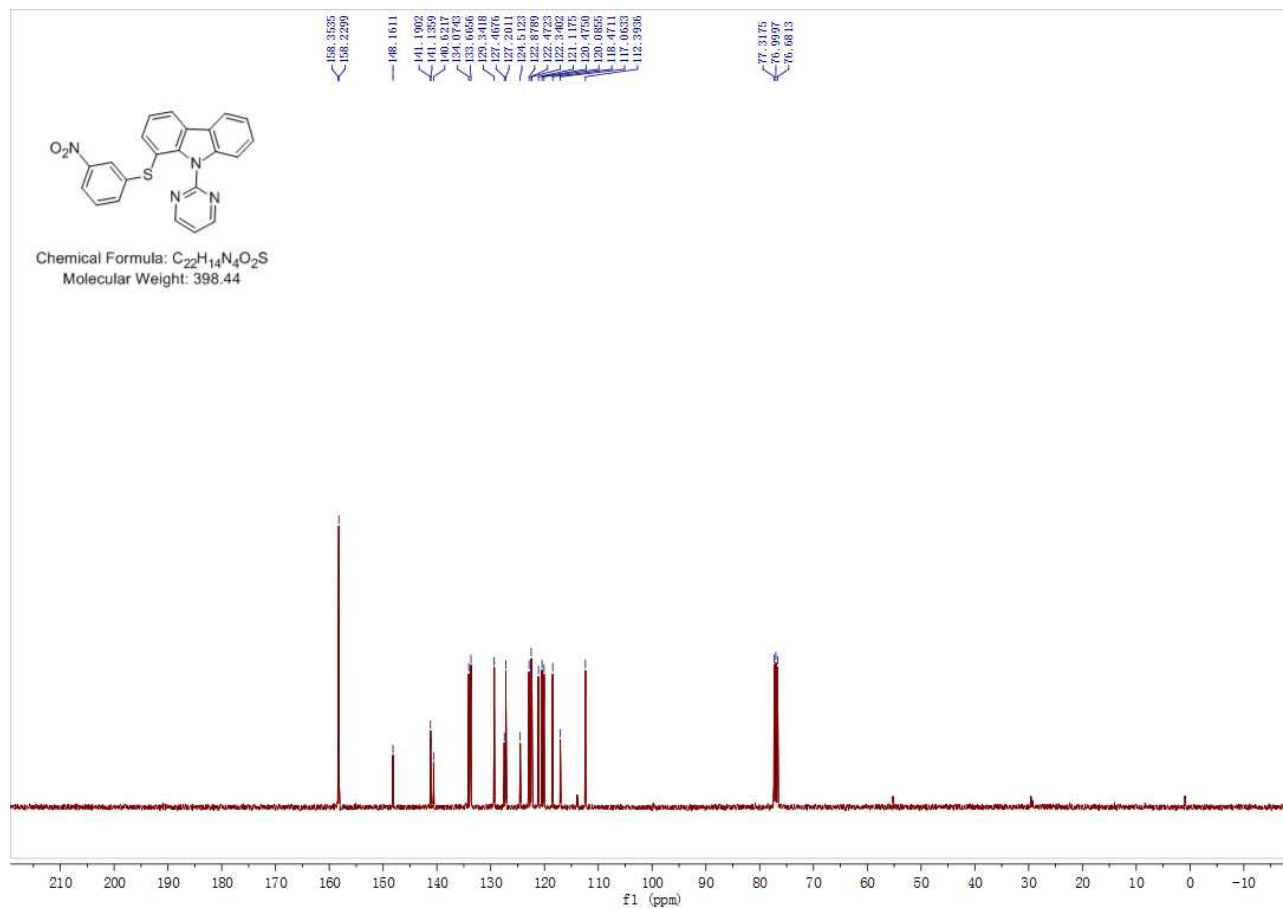
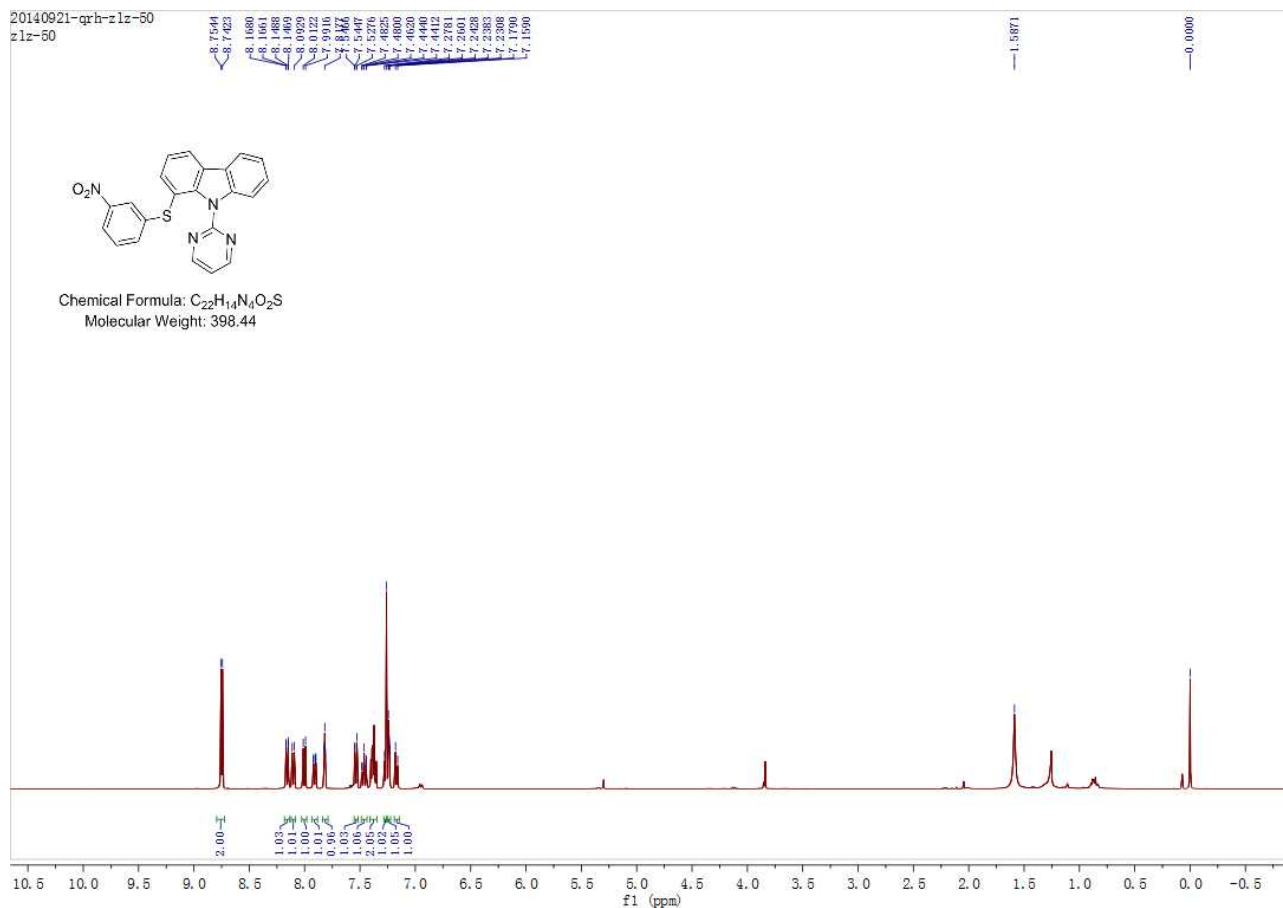


Chemical Formula: C₂₂H₁₄N₄O₂S
Molecular Weight: 398.4372

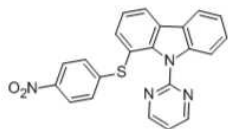


1-((3-Nitrophenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole (3g)

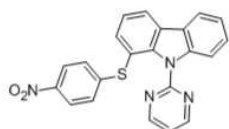
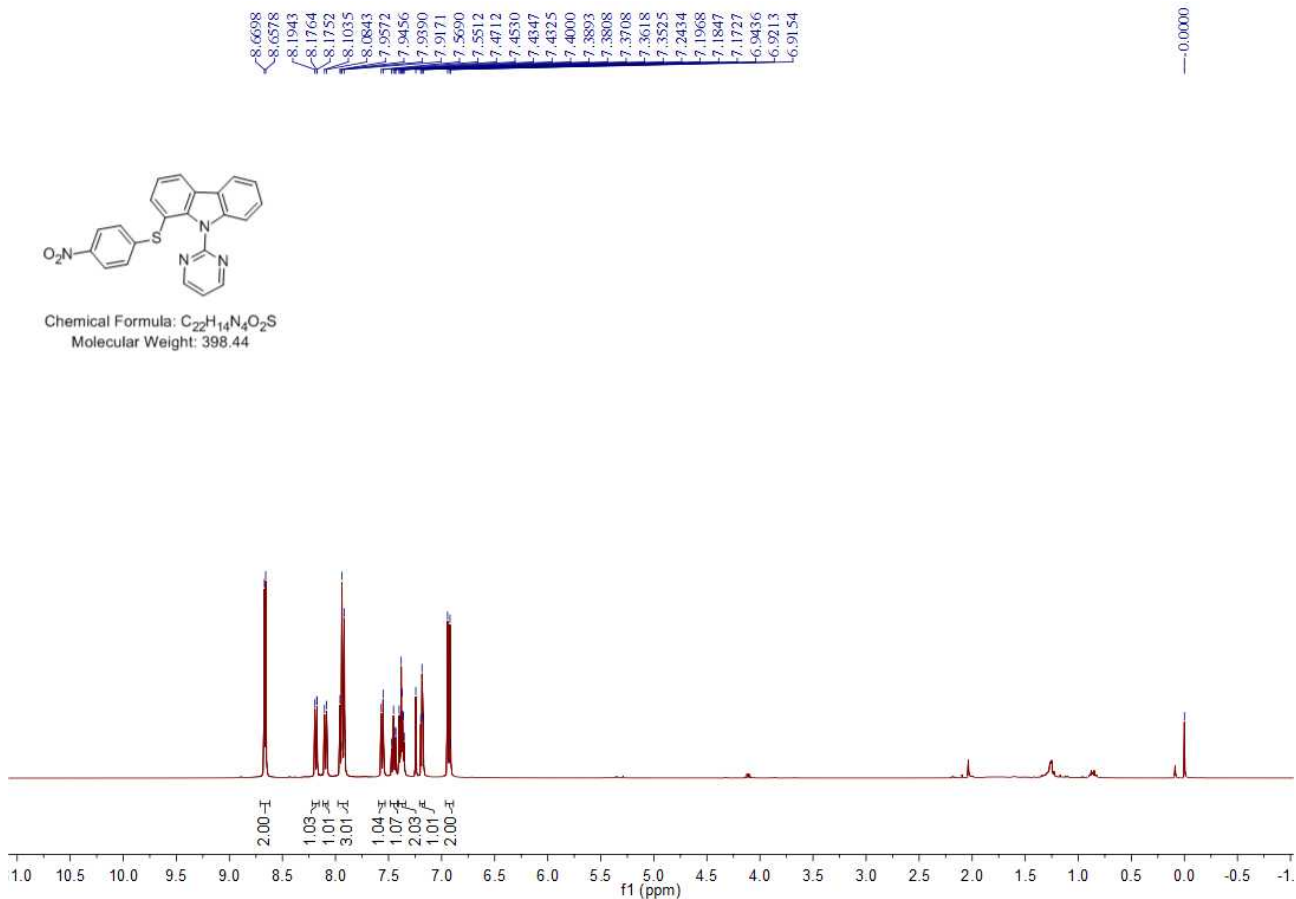
20140921-qrh-zlz-50
z1z-50



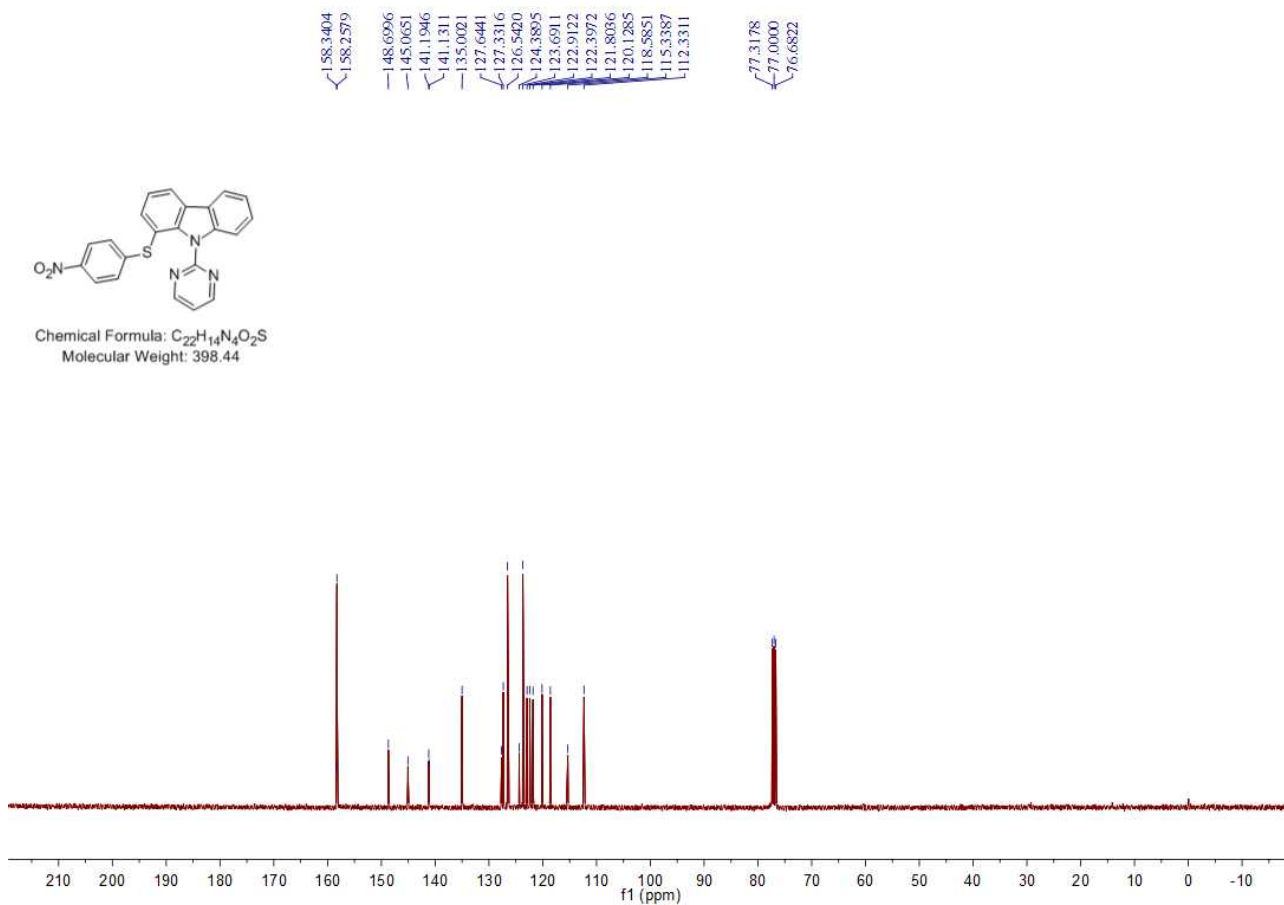
1-((4-Nitrophenyl)thio)-9-(pyrimidin-2-yl)-9H-carbazole (3h)



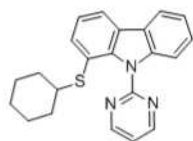
Chemical Formula: C₂₂H₁₄N₄O₂S
Molecular Weight: 398.44



Chemical Formula: C₂₂H₁₄N₄O₂S
Molecular Weight: 398.44

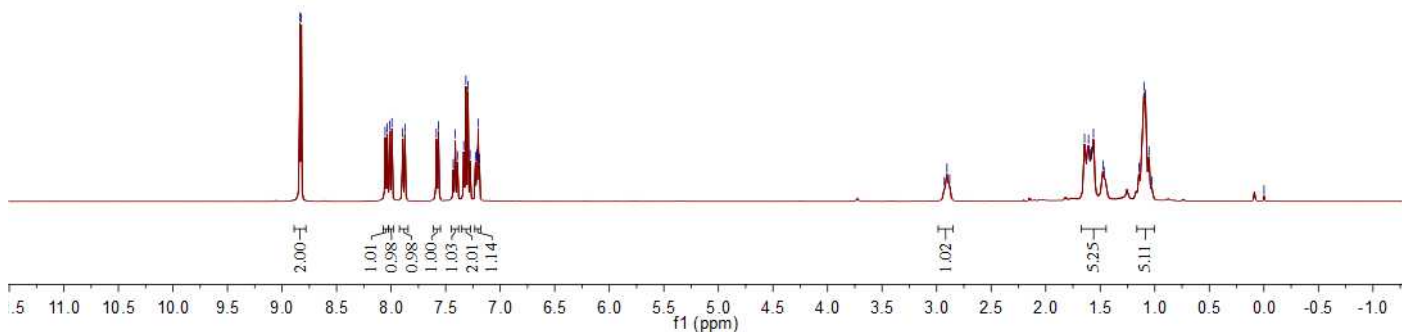


1-(Cyclohexylthio)-9-(pyrimidin-2-yl)-9H-carbazole (3i)

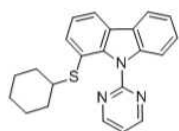


Chemical Formula: C₂₂H₂₁N₃S
Molecular Weight: 359.49

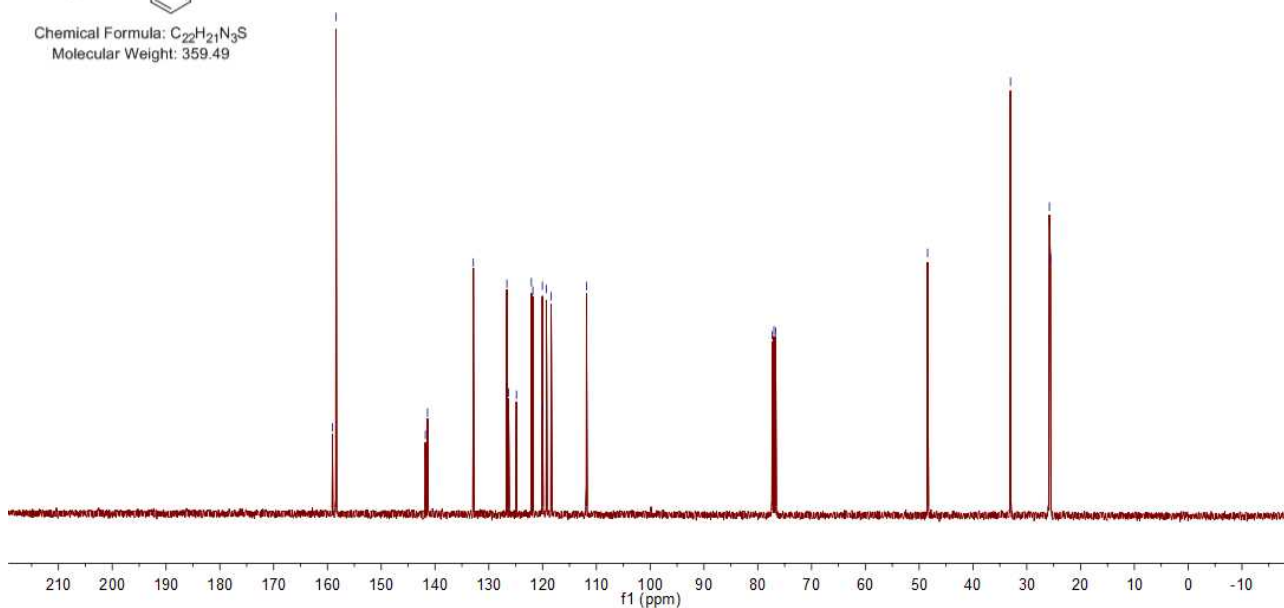
8.8351, 8.8230, 8.0544, 8.0352, 8.0120, 7.9928, 7.8938, 7.8732, 7.8653, 7.5664, 7.4308, 7.4123, 7.3923, 7.3344, 7.3150, 7.2956, 7.2762, 7.2266, 7.2143, 7.2076, 7.2023, 7.1903, 2.9290, 2.9049, 2.8805, 1.6440, 1.6070, 1.5896, 1.5800, 1.5622, 1.4749, 1.4640, 1.1433, 1.0973, 1.0847, 1.0530, 1.0270, -0.0015



159.0675, 158.4021, 141.7994, 141.3853, 132.8729, 126.6312, 126.3257, 124.8605, 122.0800, 121.8049, 120.0385, 119.9669, 119.2910, 118.4046, 111.8458, 77.3184, 76.9996, 76.6824, 48.4314, 33.0271, 25.7909, 25.5919



Chemical Formula: C₂₂H₂₁N₃S
Molecular Weight: 359.49



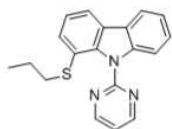
1-(Propylthio)-9-(pyrimidin-2-yl)-9H-carbazole (3j)

8.8778
8.8660
8.0677
8.0485
8.0345
8.0138
7.9850
7.9659
7.5647
7.5456
7.4565
7.4382
7.4180
7.3615
7.3494
7.3429
7.3318
7.3244
7.3128
7.2925
7.2468
7.2351

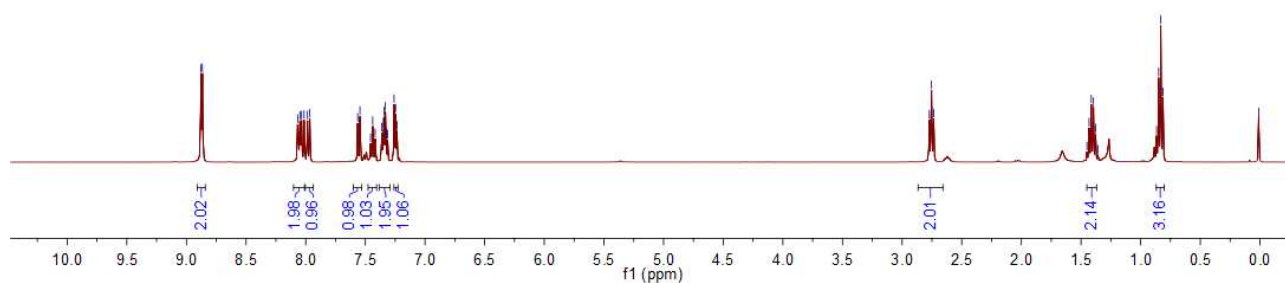
2.7717
2.7534
2.7353

1.4504
1.4324
1.4142
1.3959
1.3777
1.3595
0.8664
0.8491
0.8313
0.8129

0.0094



Chemical Formula: C₁₉H₁₇N₃S
Molecular Weight: 319.42



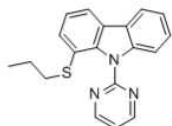
158.9653
158.4351
141.4050
140.5895
130.1887
126.7907
126.5415
125.1708
122.5383
122.3095
122.0743
120.1304
118.5046
118.2541
112.2912

77.3803
77.0629
76.7448

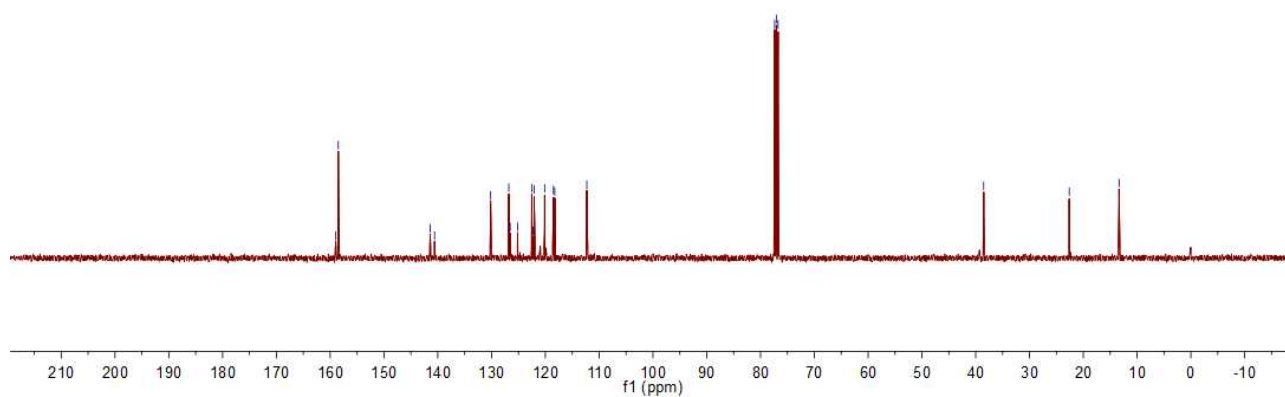
38.5188

22.8062

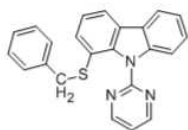
13.3481



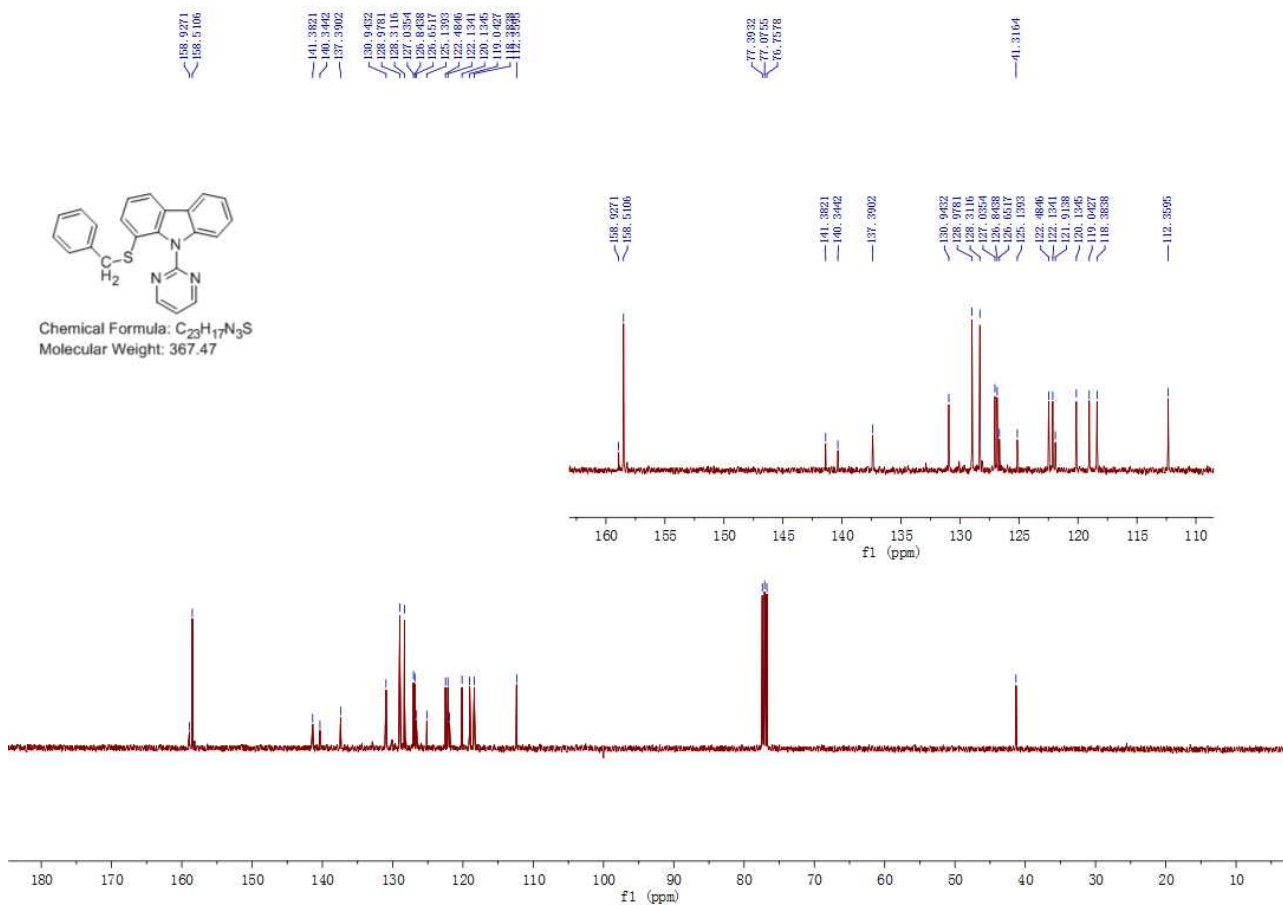
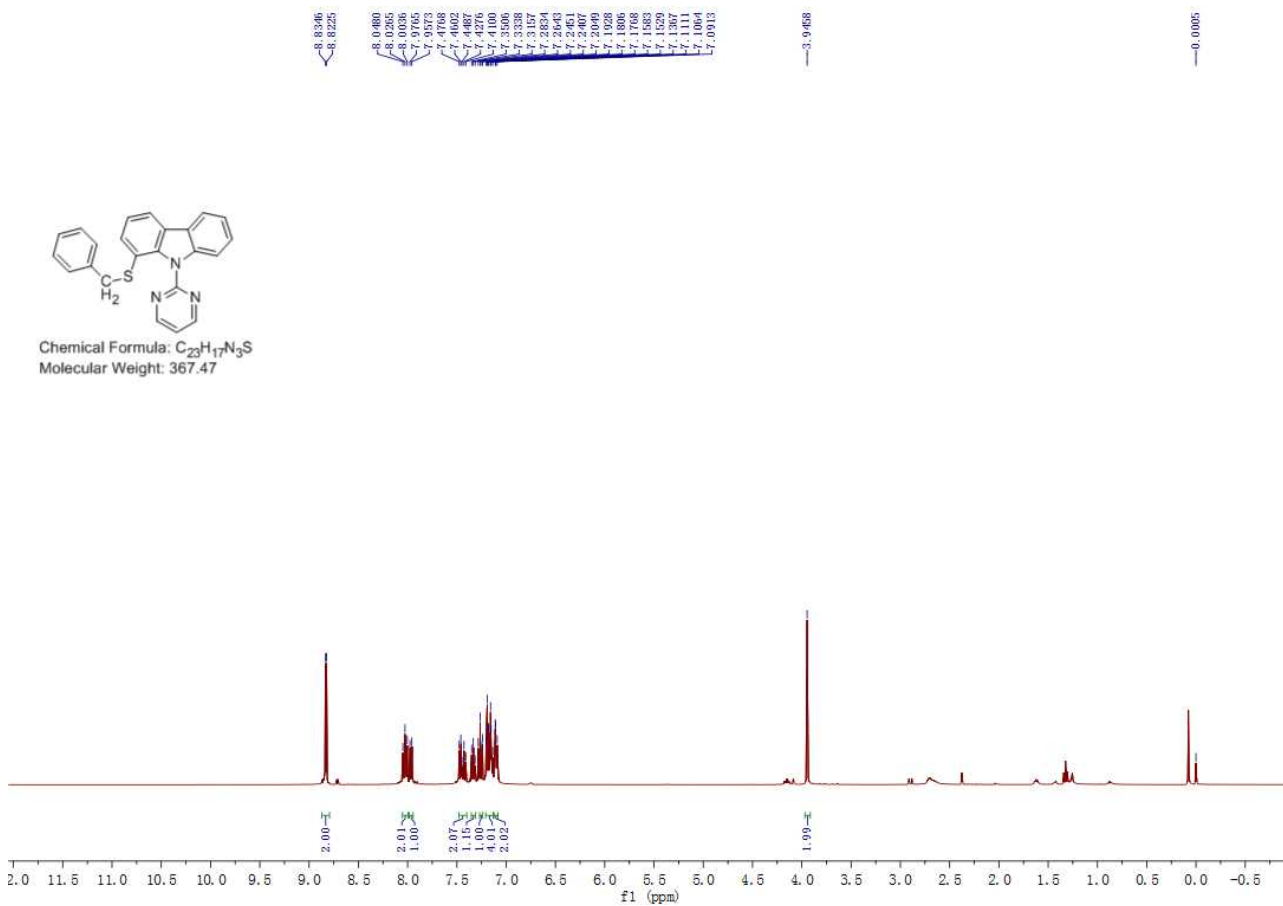
Chemical Formula: C₁₉H₁₇N₃S
Molecular Weight: 319.42



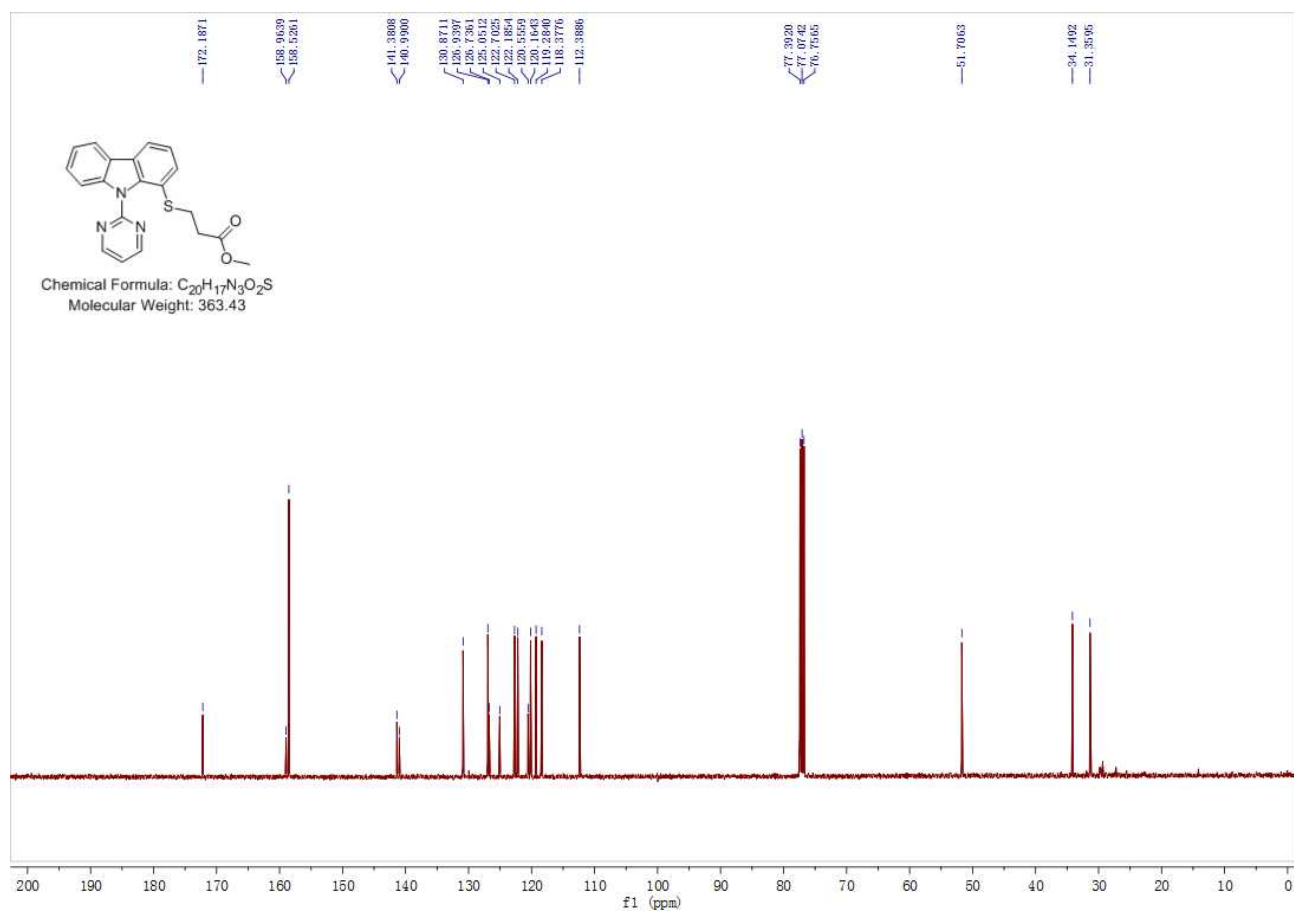
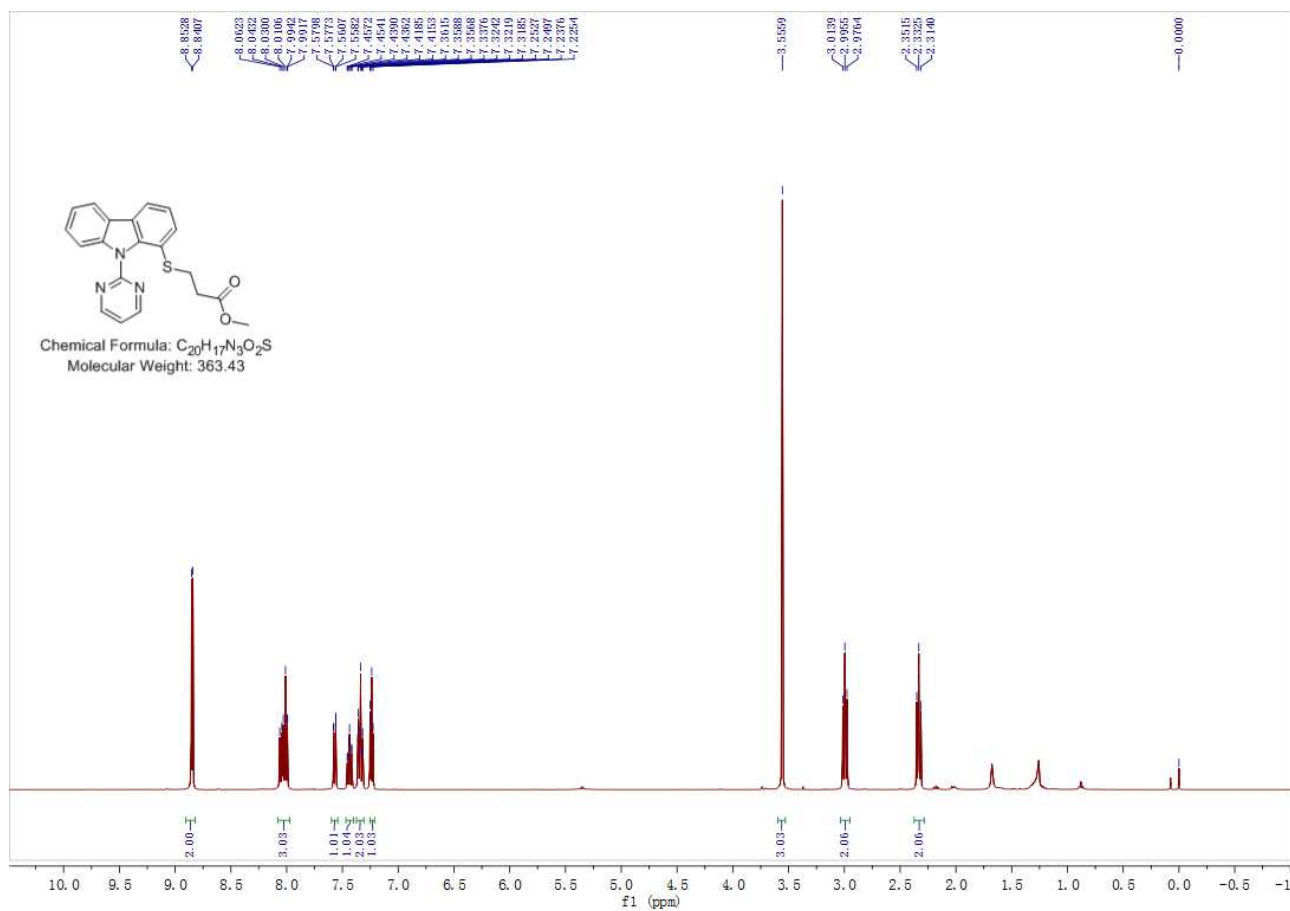
1-(Benzylthio)-9-(pyrimidin-2-yl)-9H-carbazole (3k)



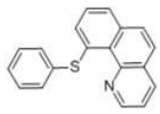
Chemical Formula: $C_{23}H_{17}N_3S$
Molecular Weight: 367.47



Methyl 3-((9-(pyrimidin-2-yl)-9H-carbazol-1-yl)thio)propano-ate(3I)



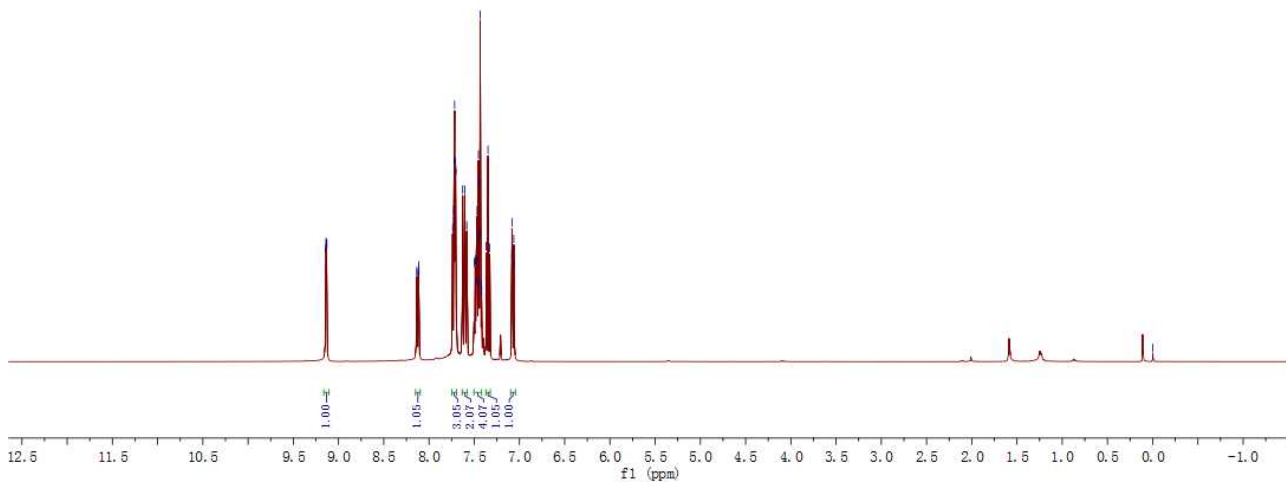
10-(Phenylthio)benzo[h]quinoline (5a)



Chemical Formula: C₁₉H₁₃NS
Molecular Weight: 287.38

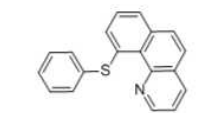
9.1440
9.1396
9.1351
9.1286
8.1859
8.1311
8.1151
8.1111
7.7384
7.7291
7.7251
7.7197
7.7165
7.7063
7.7026
7.6956
7.6920
7.5819
7.4883
7.4771
7.4751
7.4683
7.4632
7.4501
7.4457
7.4374
7.4347
7.4303
7.4200
7.4171
7.4156
7.3476
7.3460
7.3285
7.0847
7.0822
7.0807
7.0625

-0.0002

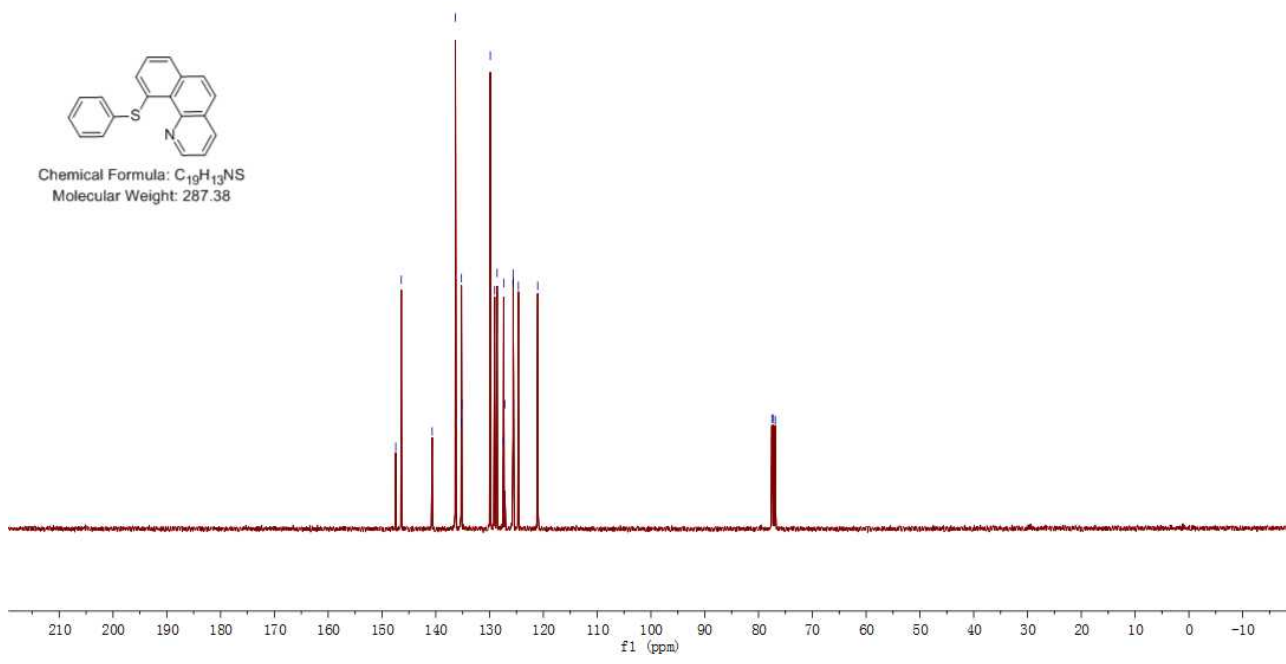


147.4832
146.4728
140.6728
136.3459
135.2678
135.2213
134.8416
129.8816
129.0506
128.5964
127.4386
127.3790
125.6107
125.5615
124.6300
121.0397

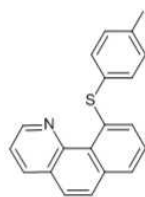
77.5173
77.0911
76.6811



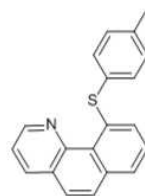
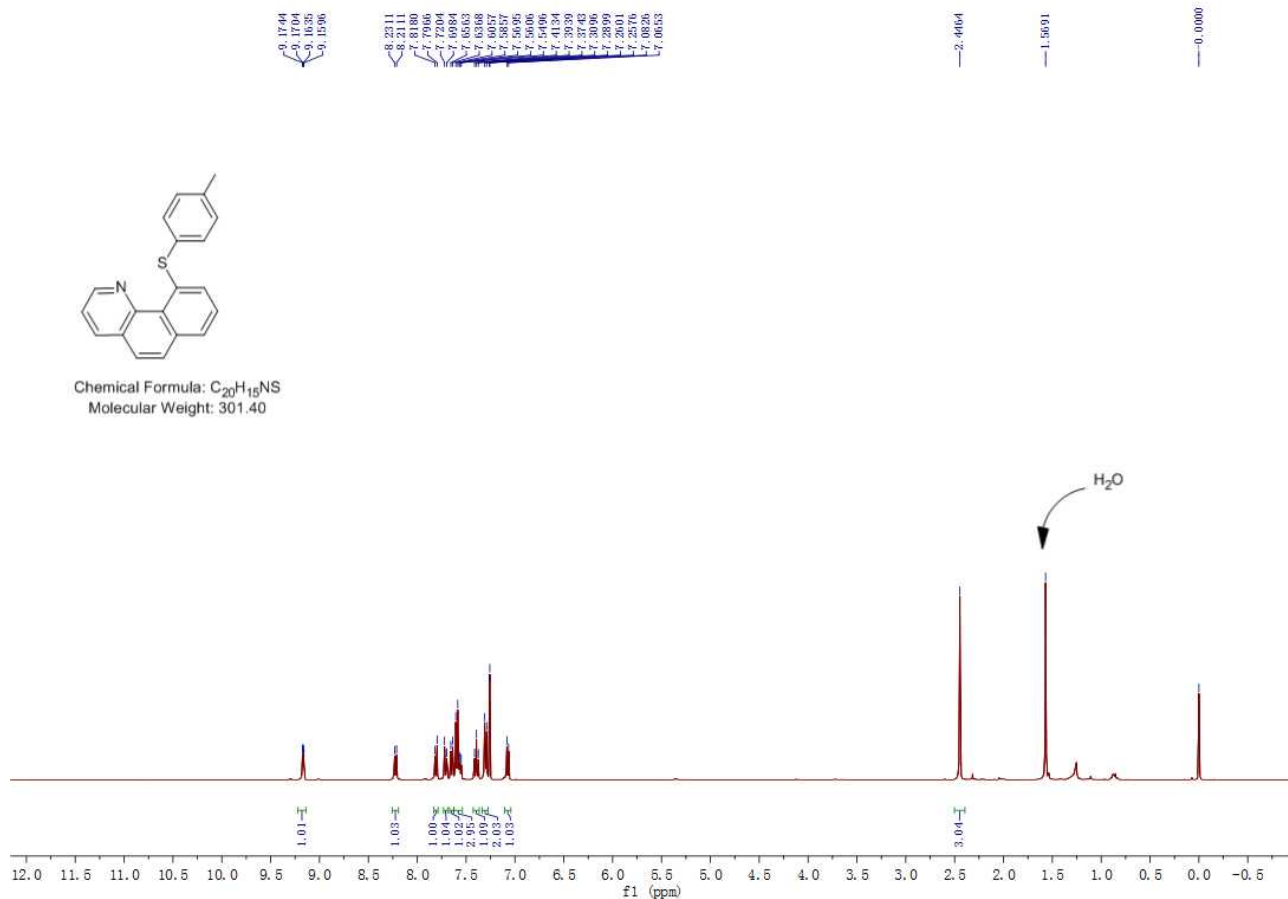
Chemical Formula: C₁₉H₁₃NS
Molecular Weight: 287.38



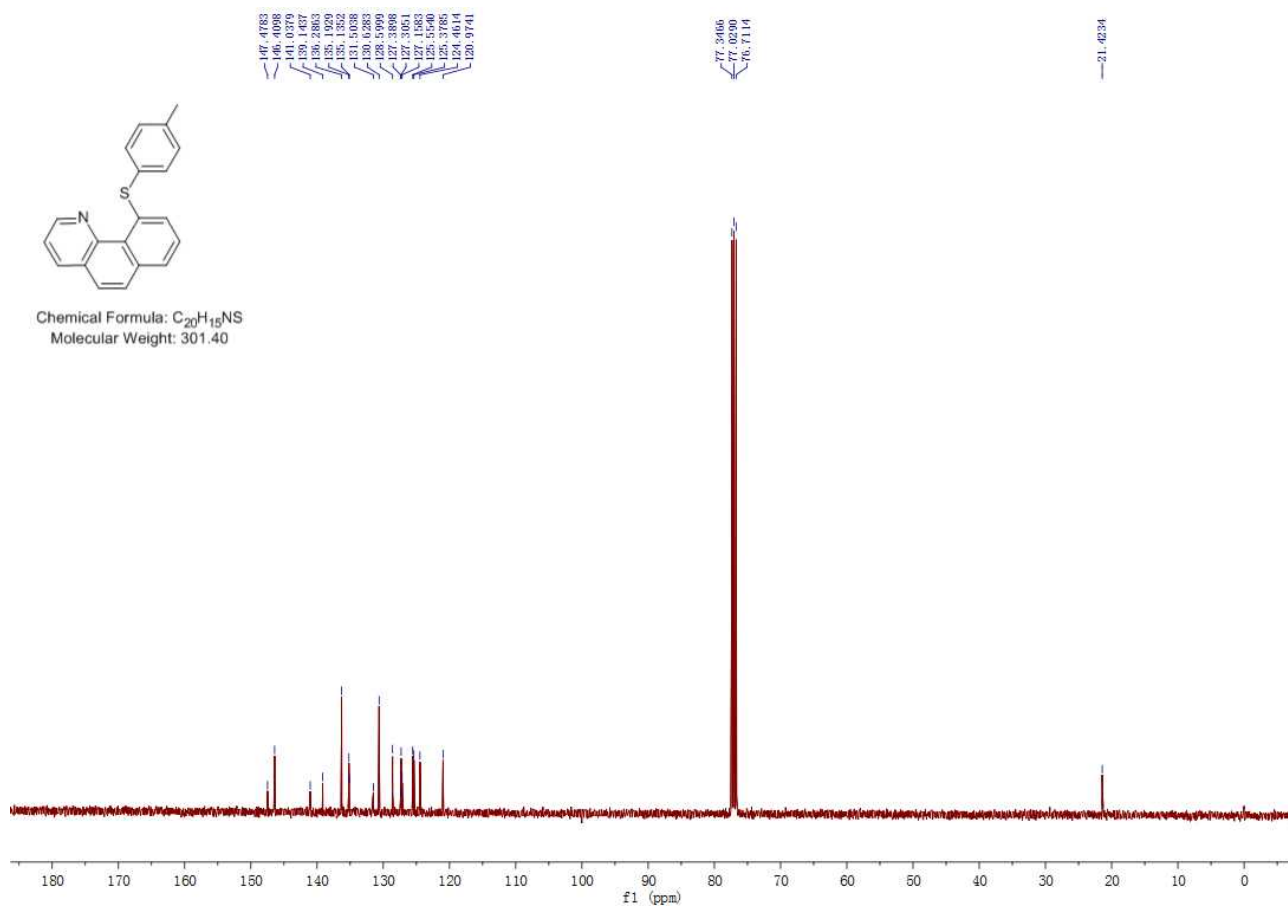
10-(4-Methylphenyl)thio)benzo[*h*]quinoline (5b)



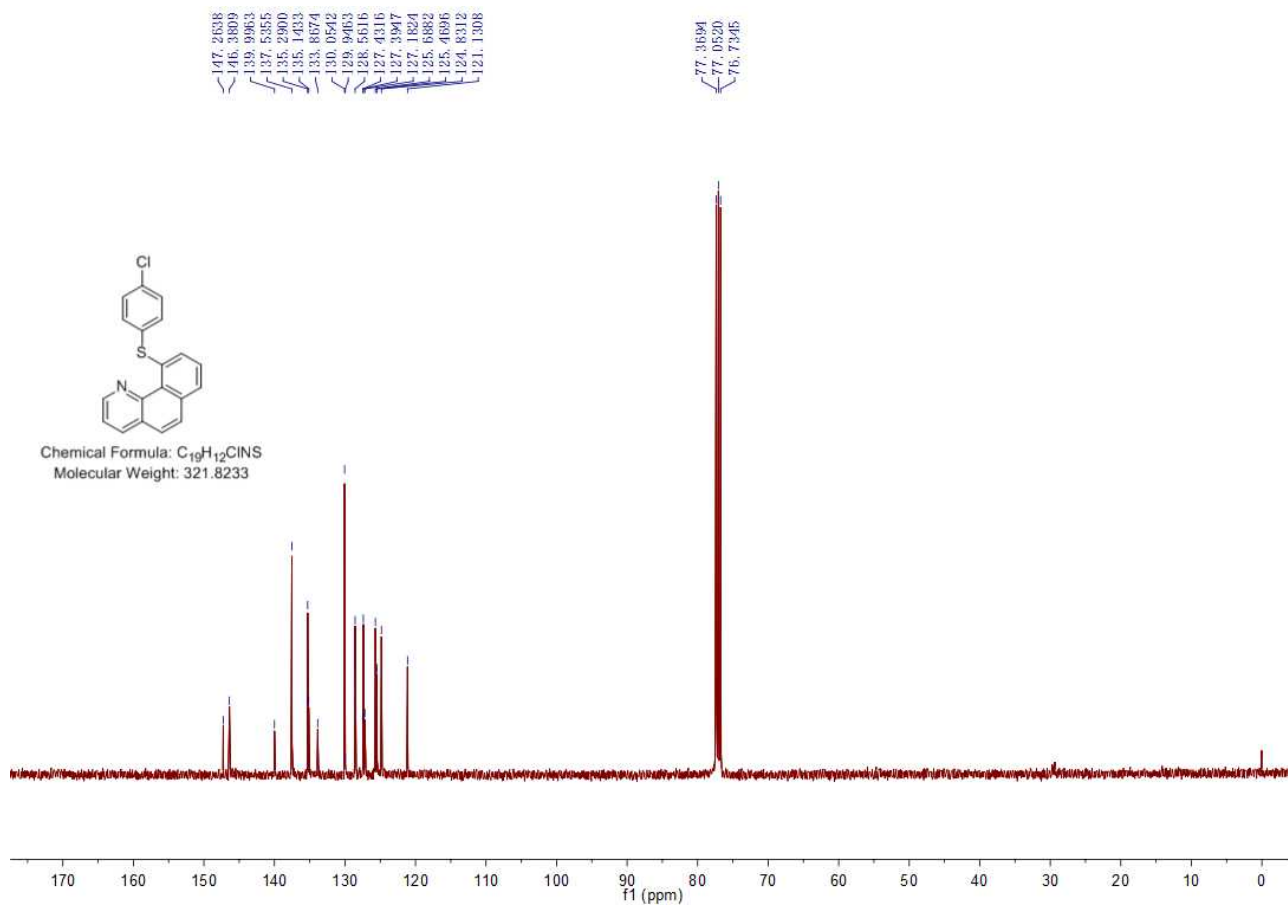
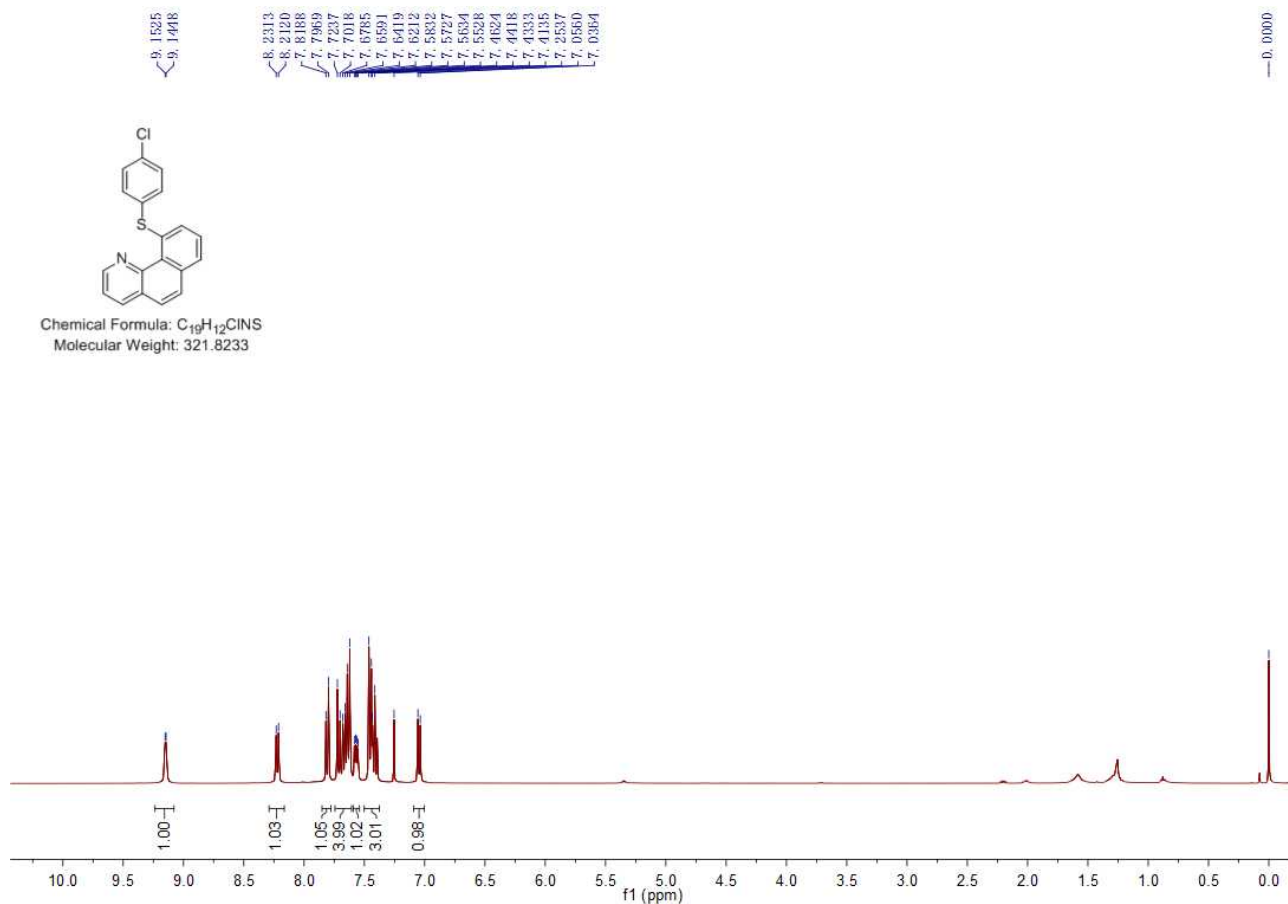
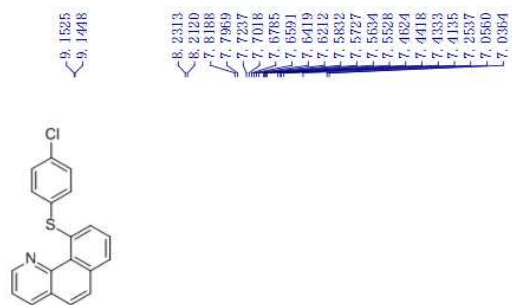
Chemical Formula: C₂₀H₁₅NS
Molecular Weight: 301.40



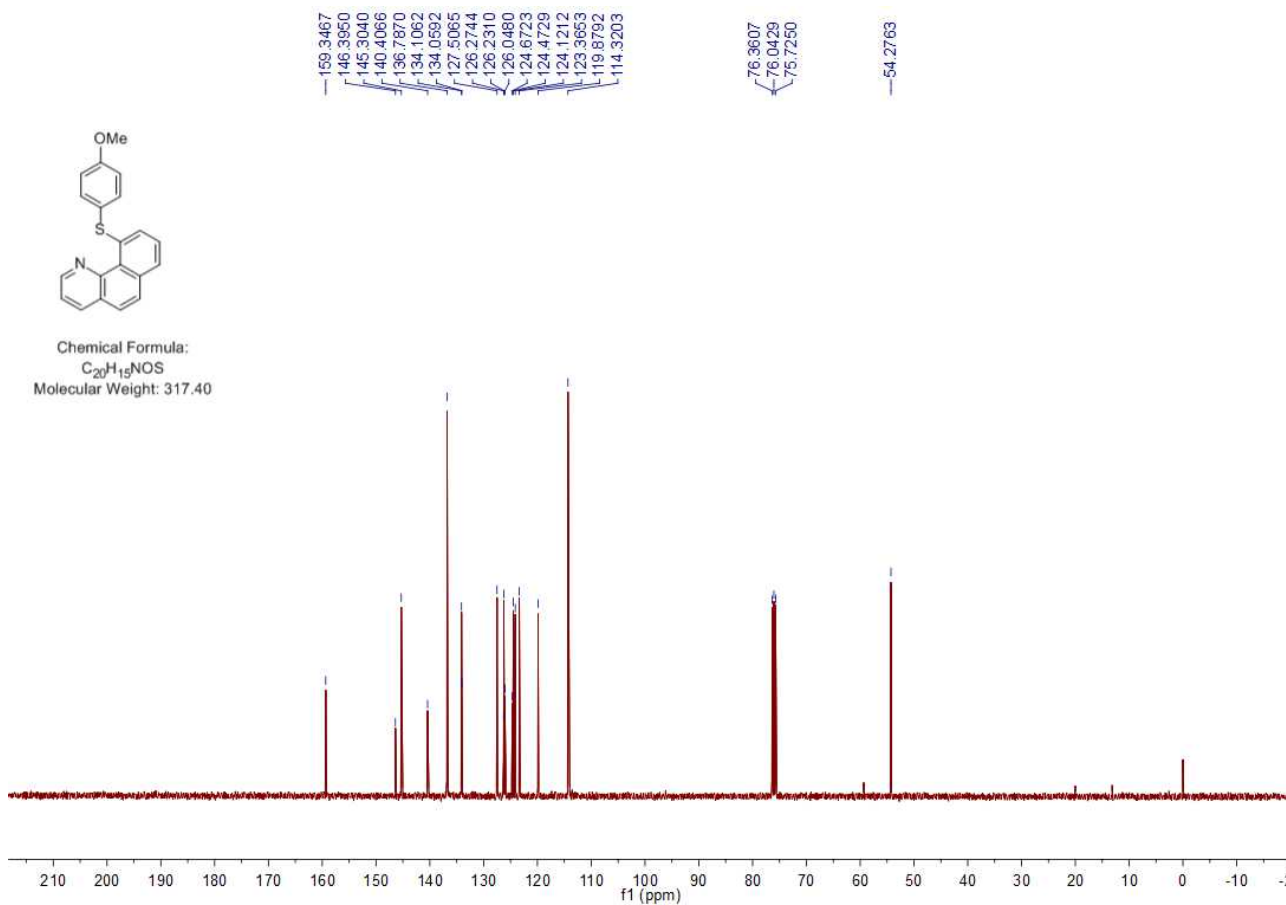
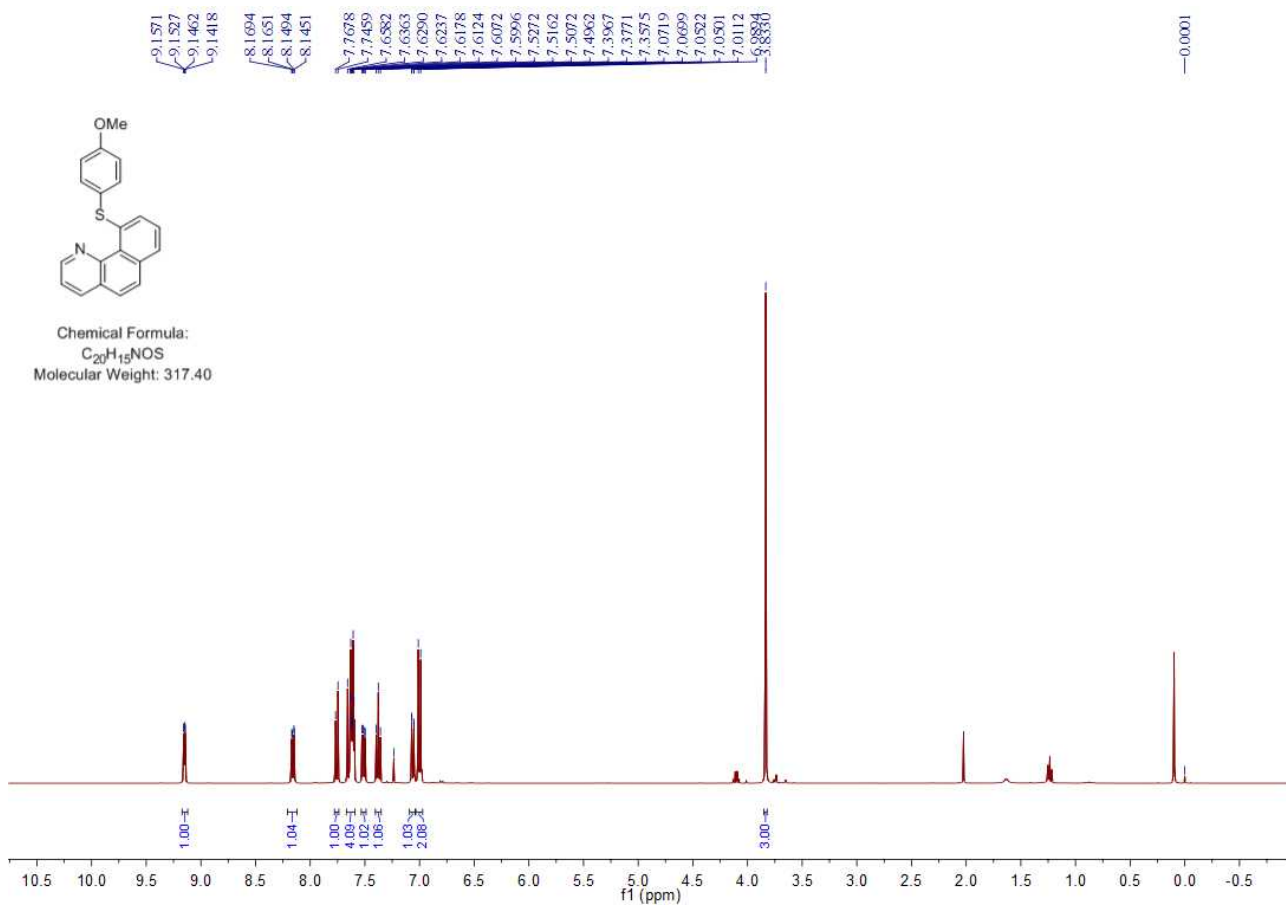
Chemical Formula: C₂₀H₁₅NS
Molecular Weight: 301.40



10-(4-chlorophenyl)thio)benzo[h]quinoline (5c)



10-((4-methoxyphenyl)thio)benzo[*h*]quinoline (5d)



10-(Propylthio)benzo[h]quinoline (5e)

9.1389
8.1324
8.1259
8.1214

8.1696
8.1498
7.7914
7.7696
7.6905
7.6780
7.6579
7.6549
7.6199
7.6079
7.5213
7.5194
7.3014
7.2894
7.2581

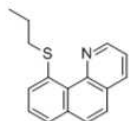
3.6985

3.0517
3.0332
3.0140

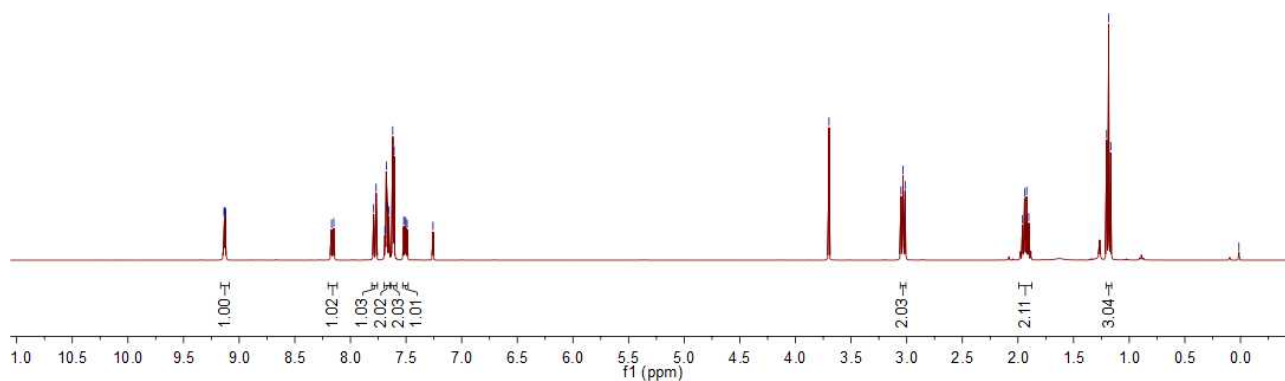
1.9591
1.9404
1.9216
1.9031

1.2030
1.1896
1.1851

0.0140



Chemical Formula: C₁₆H₁₅NS
Molecular Weight: 253.36



147.4442
146.2465

139.6032
135.2211
134.9808
128.5603
127.9924
127.2544
127.0108
125.5513
123.9566
123.0203
120.6853

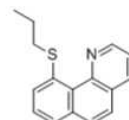
77.3182
77.0003
76.6826

66.9533

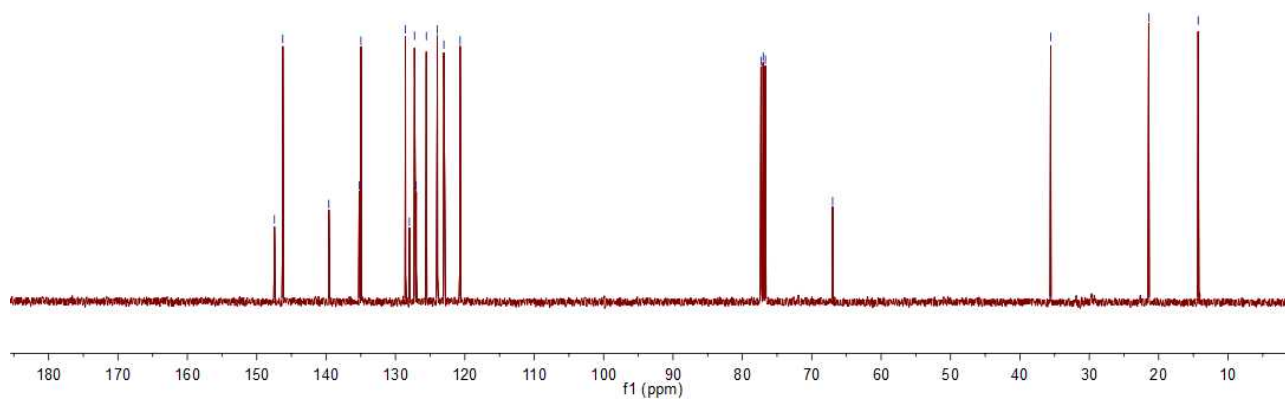
35.5670

21.4337

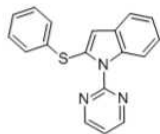
14.3054



Chemical Formula: C₁₆H₁₅NS
Molecular Weight: 253.36



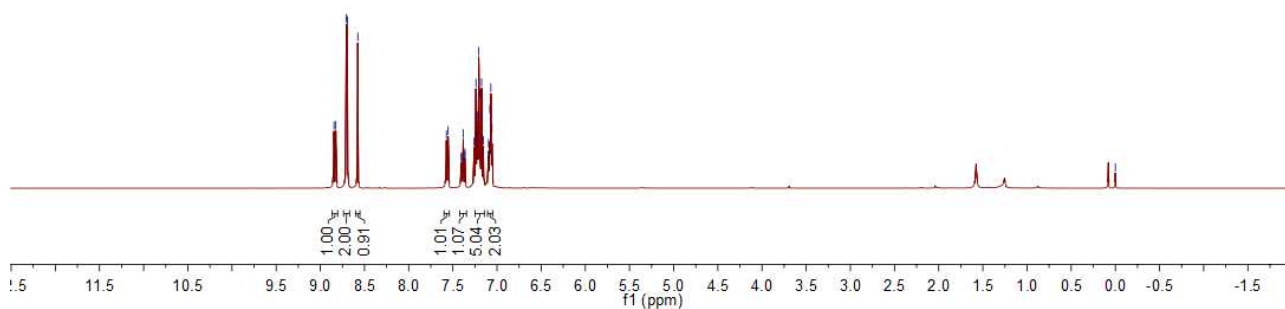
2-((Phenylthio)thio)-1-(pyrimidin-2-yl)-1H-indole (7a)



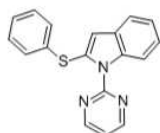
Chemical Formula: C₁₈H₁₃N₃S
Molecular Weight: 303.38

8.8453
8.8242
8.7057
8.6937
8.5760
7.5728
7.5533
7.4033
7.4009
7.3827
7.3644
7.3620
7.2895
7.2884
7.2280
7.2239
7.2063
7.1927
7.1747
7.1547
7.0987
7.0955
7.0815
7.0812
7.0695
7.0575

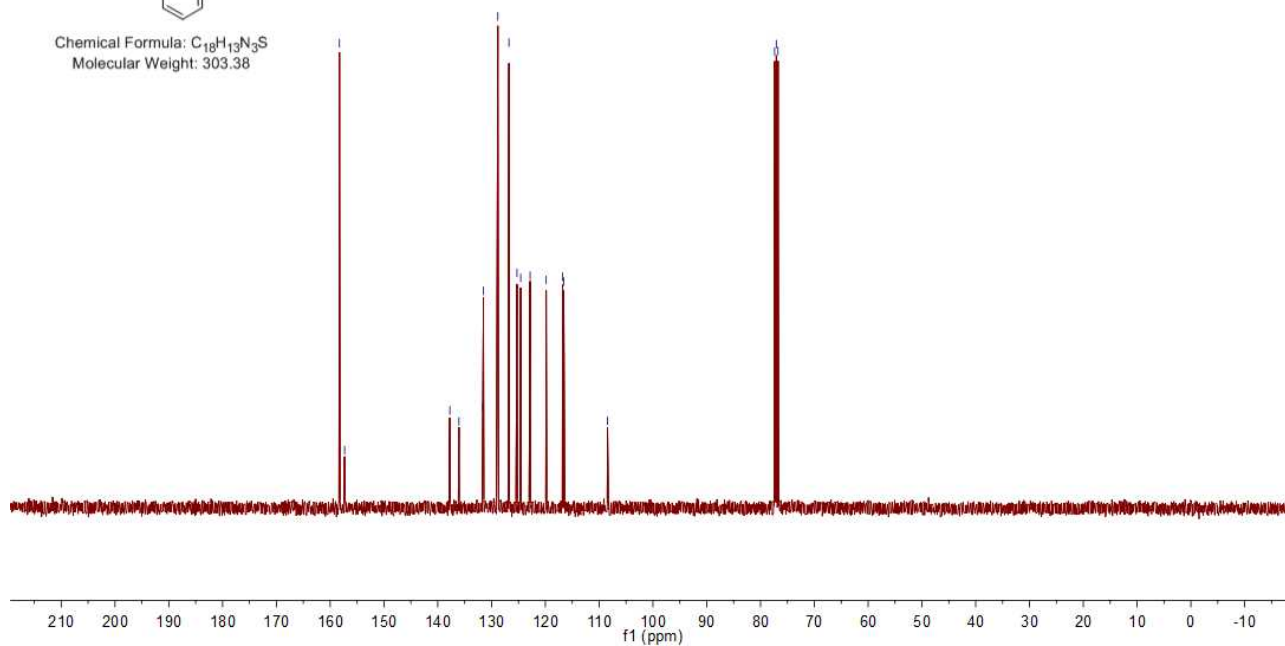
-0.0001



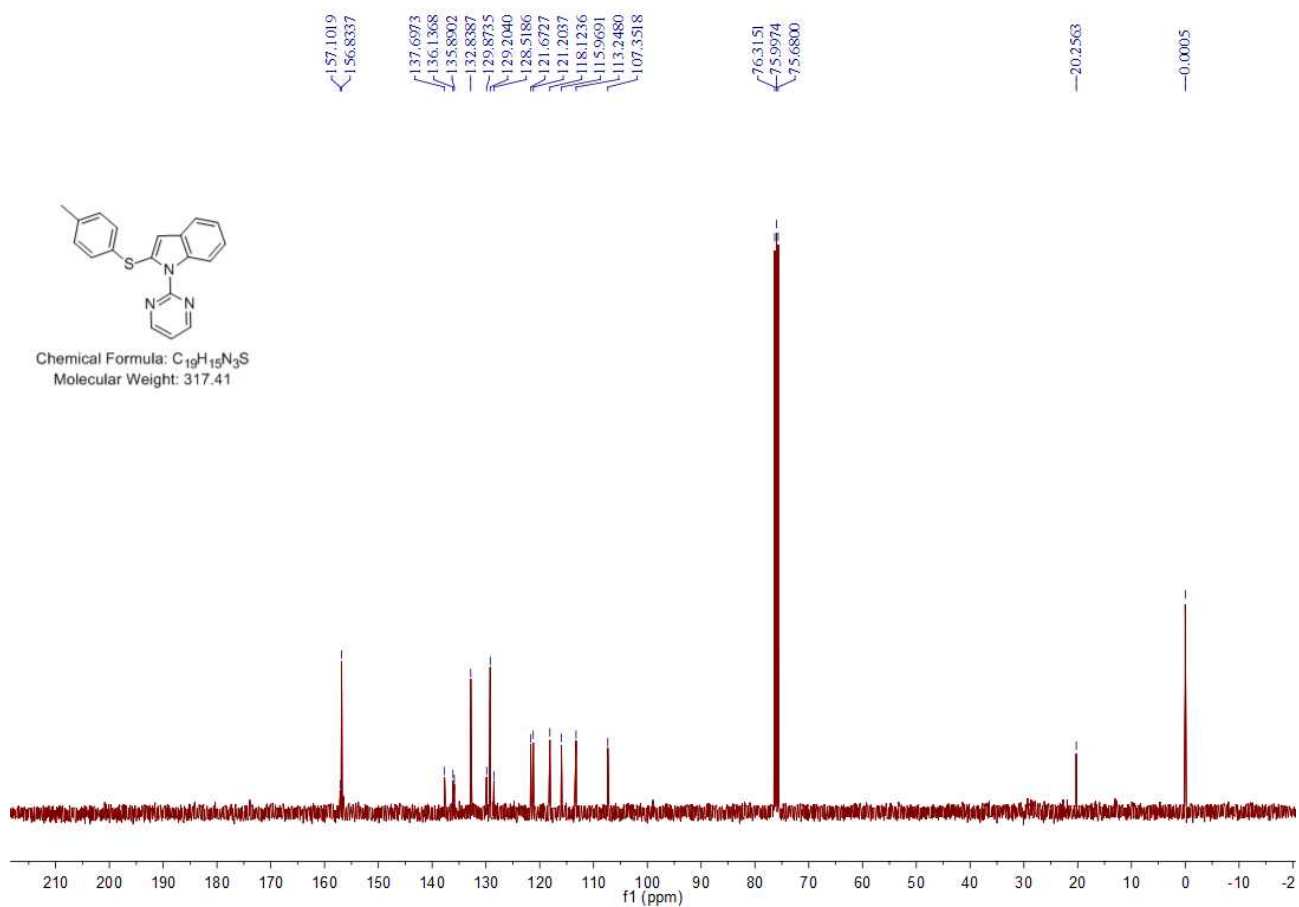
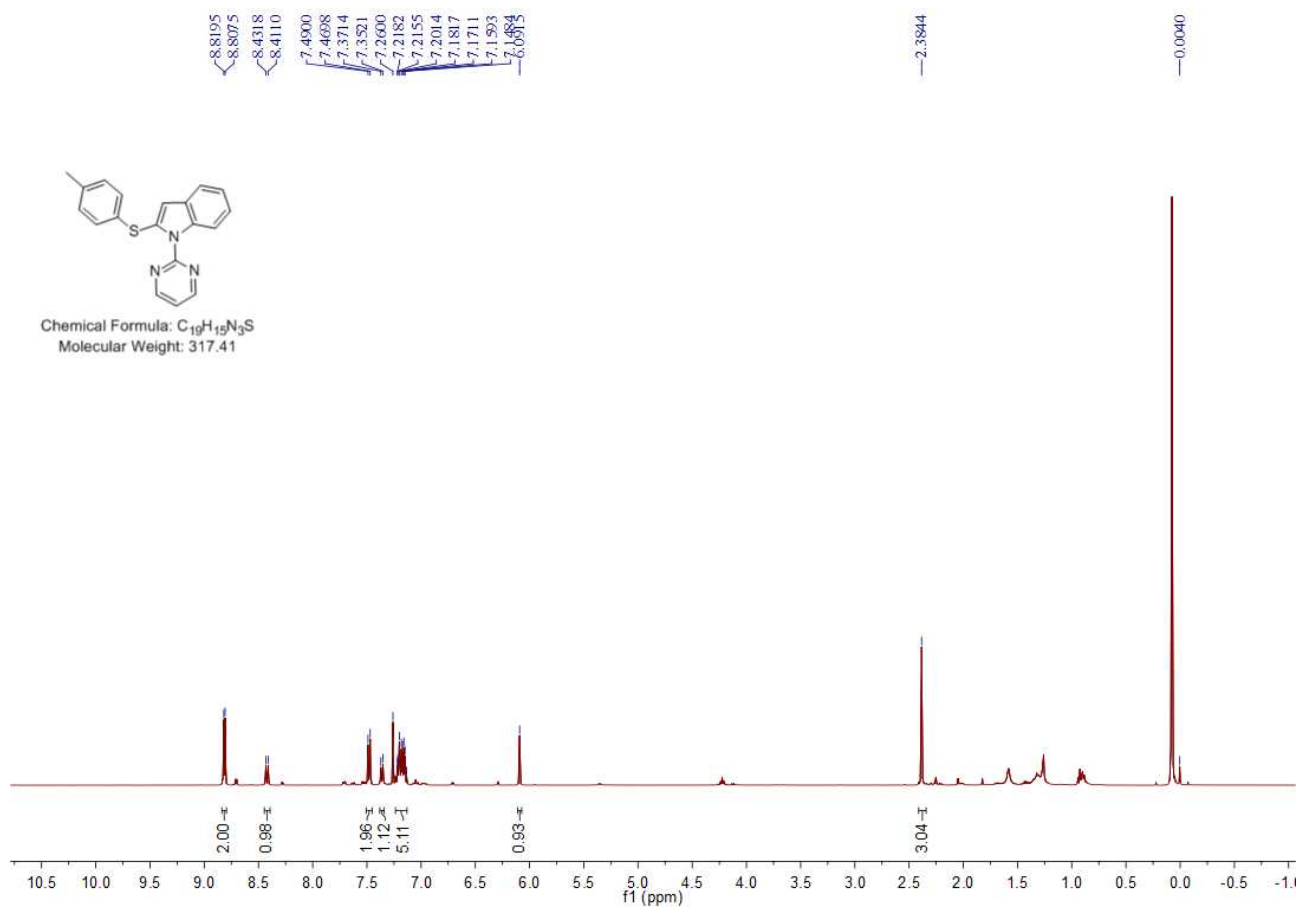
158.2778
157.3086
137.7532
136.0694
135.6665
131.5191
128.8342
126.7688
125.2753
124.5780
122.8342
119.8434
116.7943
116.5735
108.4329
77.3883
77.0885
76.7511



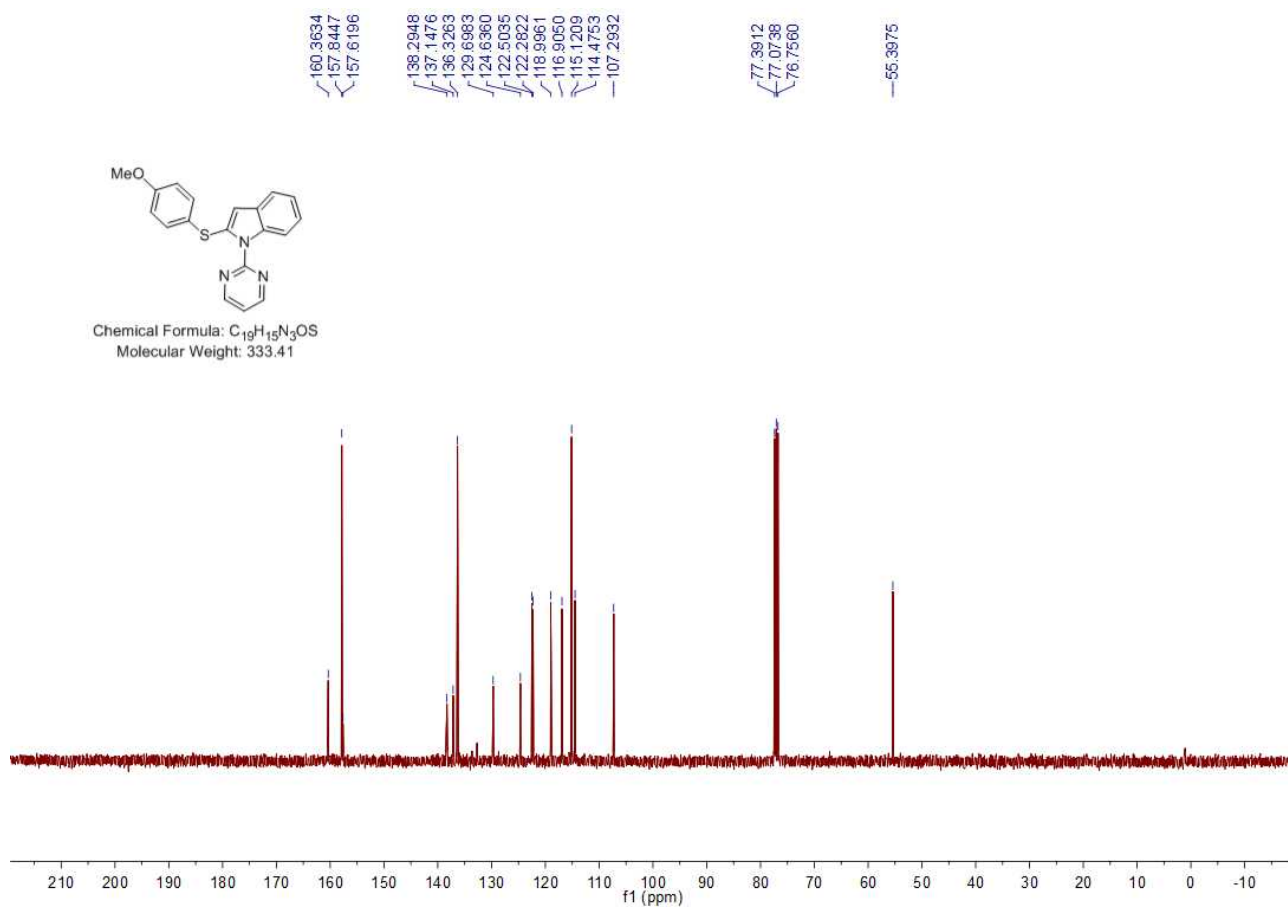
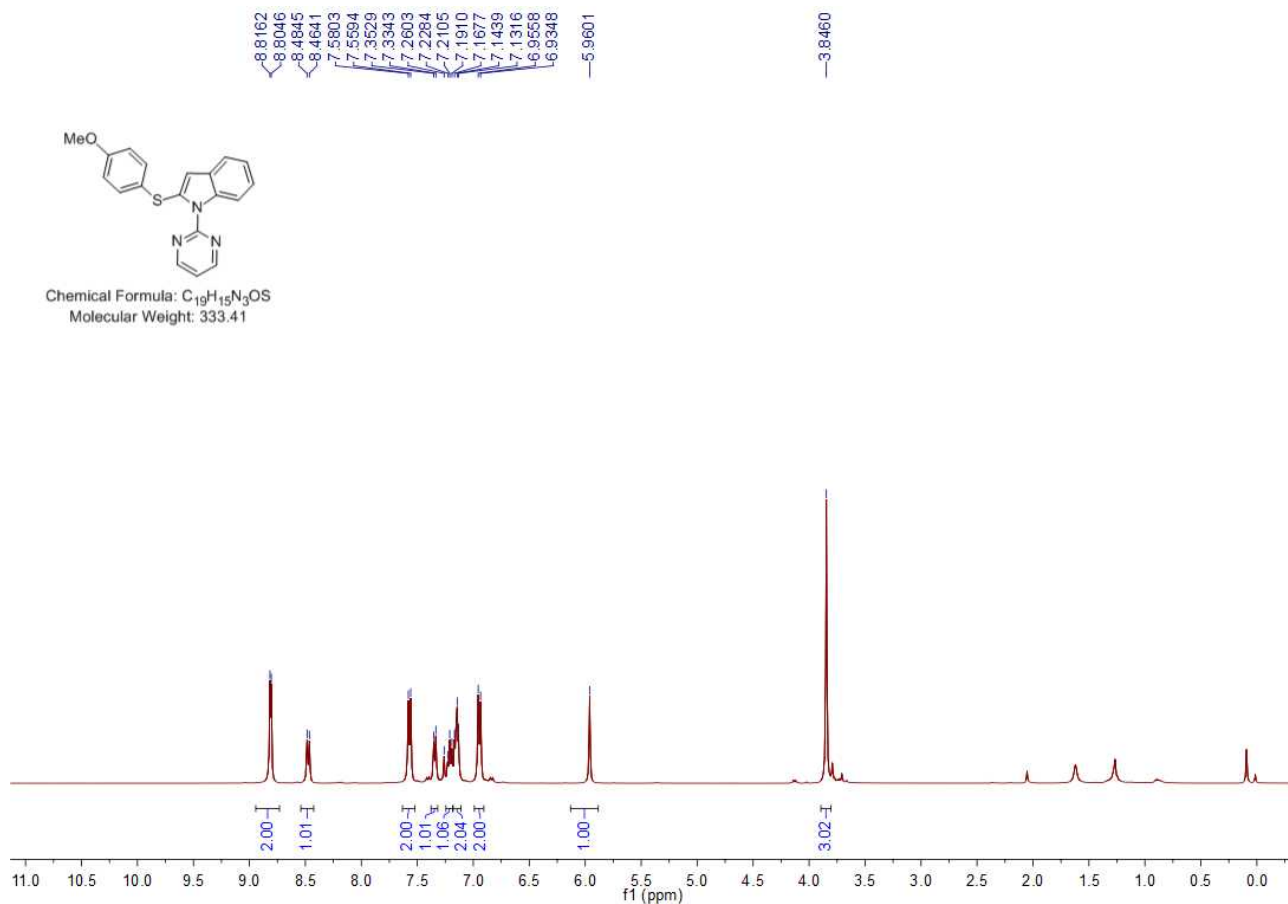
Chemical Formula: C₁₈H₁₃N₃S
Molecular Weight: 303.38



2-((4-methylphenyl)thio)-1-(pyrimidin-2-yl)-1H-indole (7b)



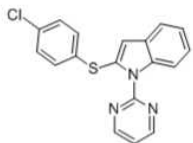
2-((4-Methoxyphenyl)thio)-1-(pyrimidin-2-yl)-1H-indole (7c)



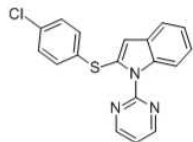
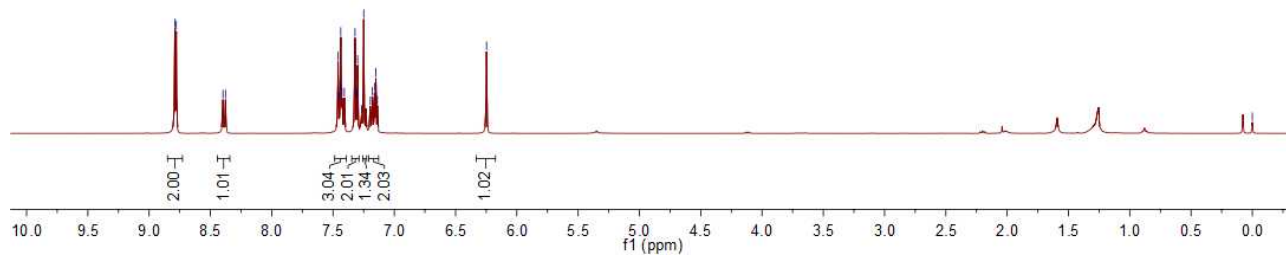
2-((4-Chlorophenyl)thio)-1-(pyrimidin-2-yl)-1H-indole (7d)



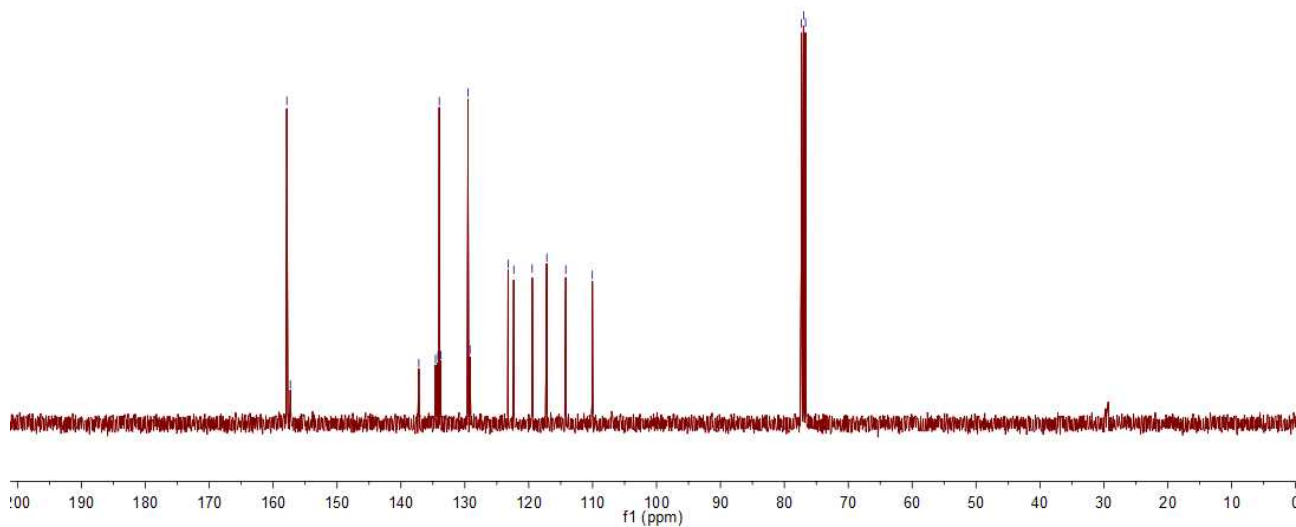
0.0001



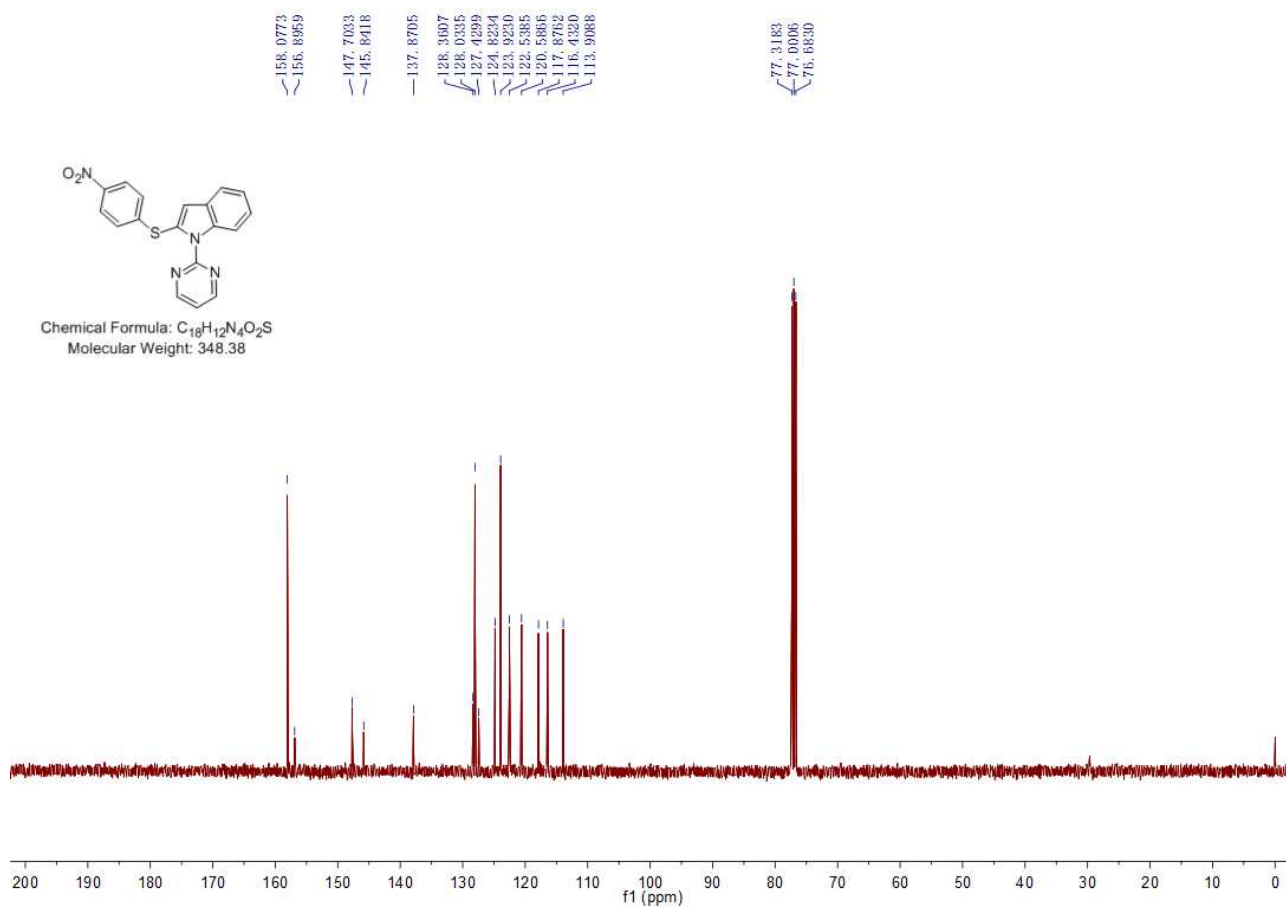
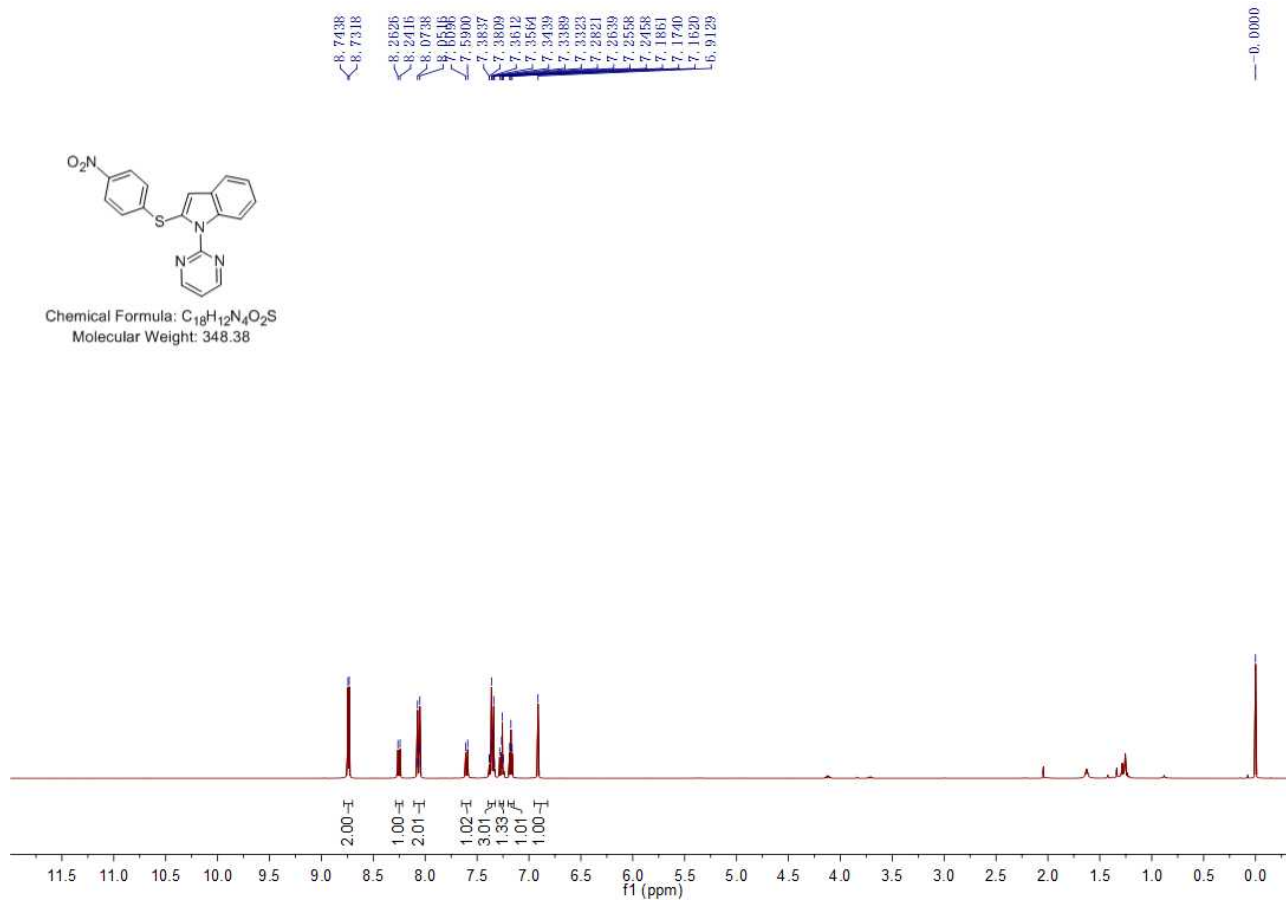
Chemical Formula: C₁₈H₁₂ClN₃S
Molecular Weight: 337.83



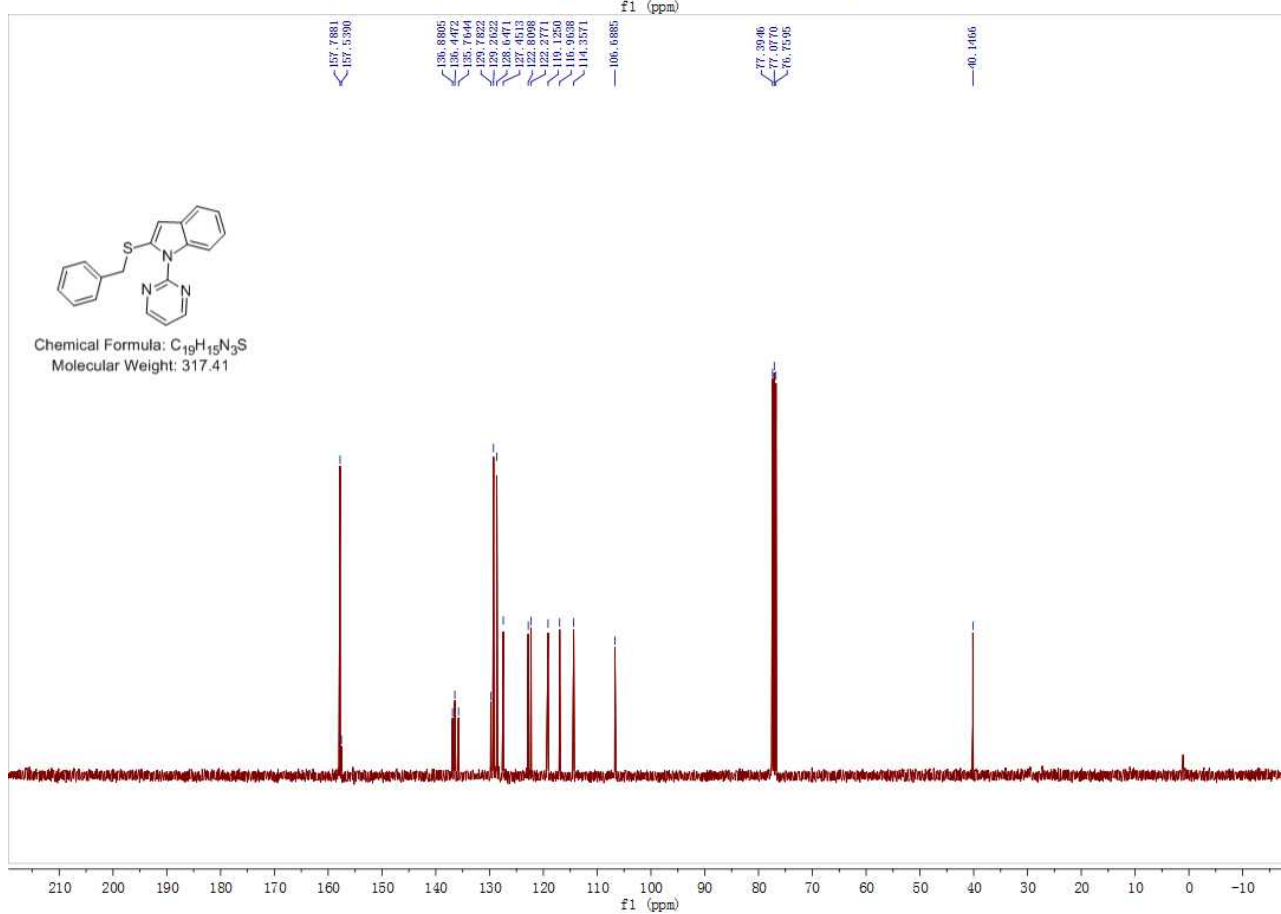
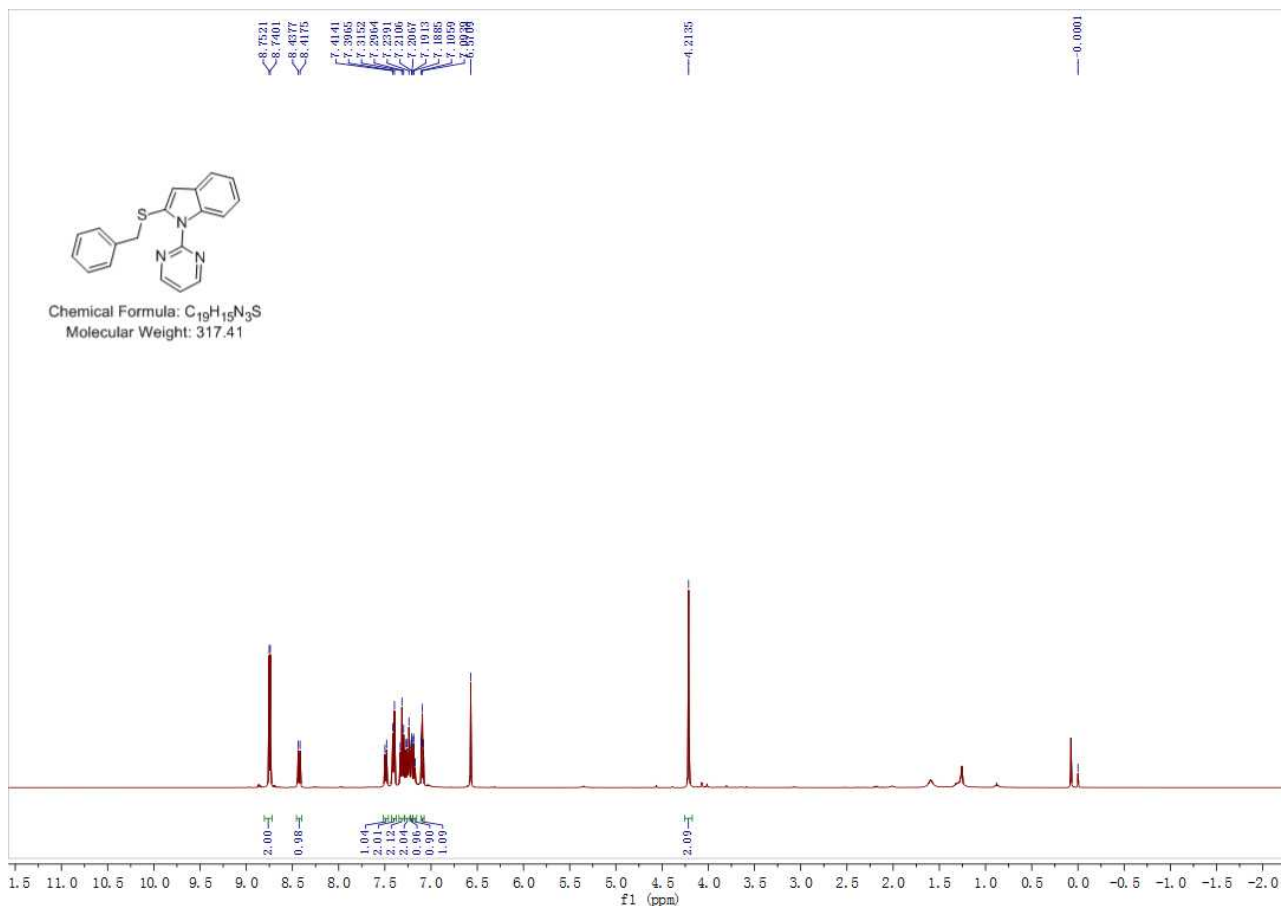
Chemical Formula: C₁₈H₁₂ClN₃S
Molecular Weight: 337.83



2-((4-Nitroxyphenyl)thio)-1-(pyrimidin-2-yl)-1H-indole (7e)



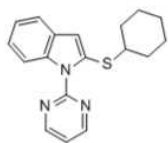
2-((Benzyl)thio)-1-(pyrimidin-2-yl)-1H-indole (7f)



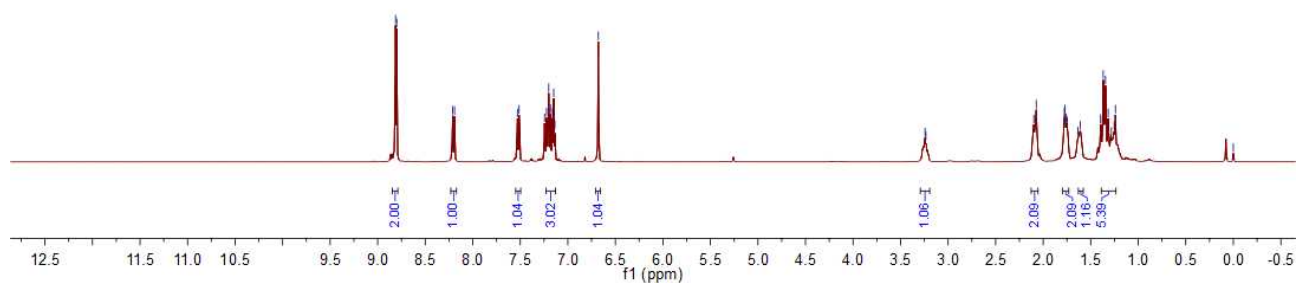
2-(Cyclohexylthio)-1-(pyrimidin-2-yl)-1H-indole (7g)

8.8120
8.8000
8.2116
8.1917
7.5126
7.2337
7.2008
7.1834
7.1609
6.6751

3.2424
3.2337
2.0987
2.0728
1.7776
1.7704
1.7567
1.7475
1.6348
1.6089
1.3960
1.3685
1.3446
1.3169
1.2830
1.2529
1.2401
0.0001



Chemical Formula: C₁₈H₁₉N₃S
Molecular Weight: 309.43



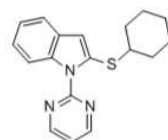
157.9713
157.4700

137.2349
133.3688
129.4223
122.8962
122.0527
119.3103
117.3967
113.4671
109.1487

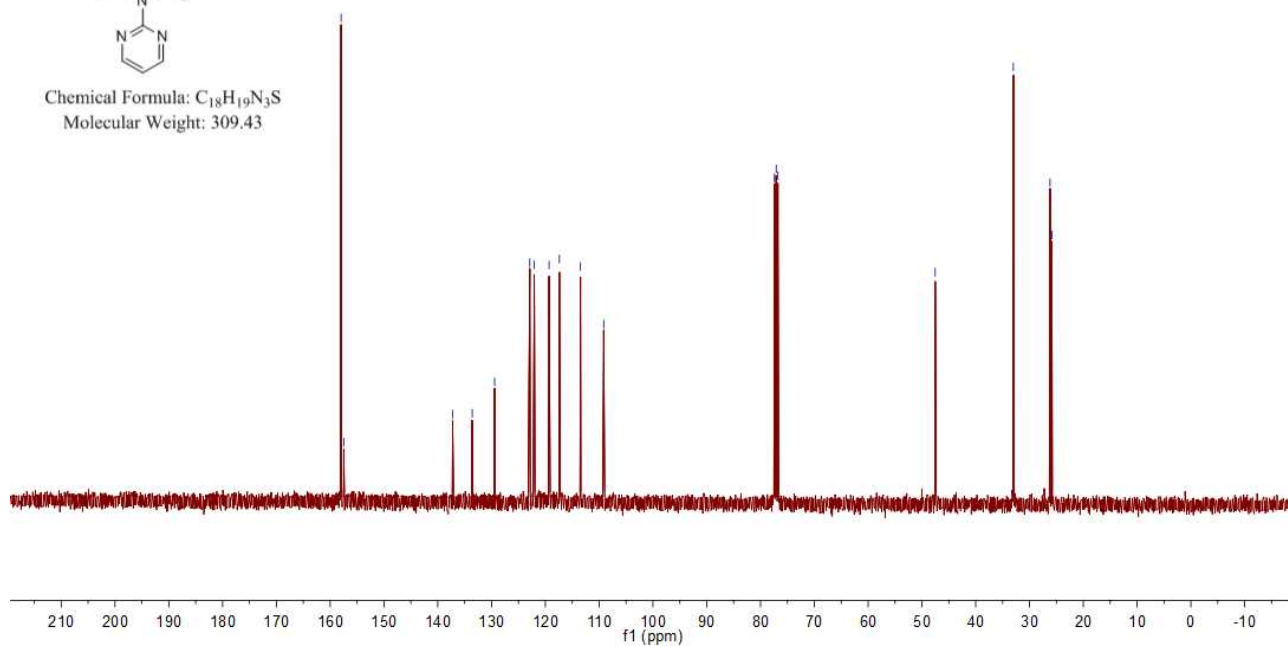
77.4033
77.0878
76.7702

47.5275

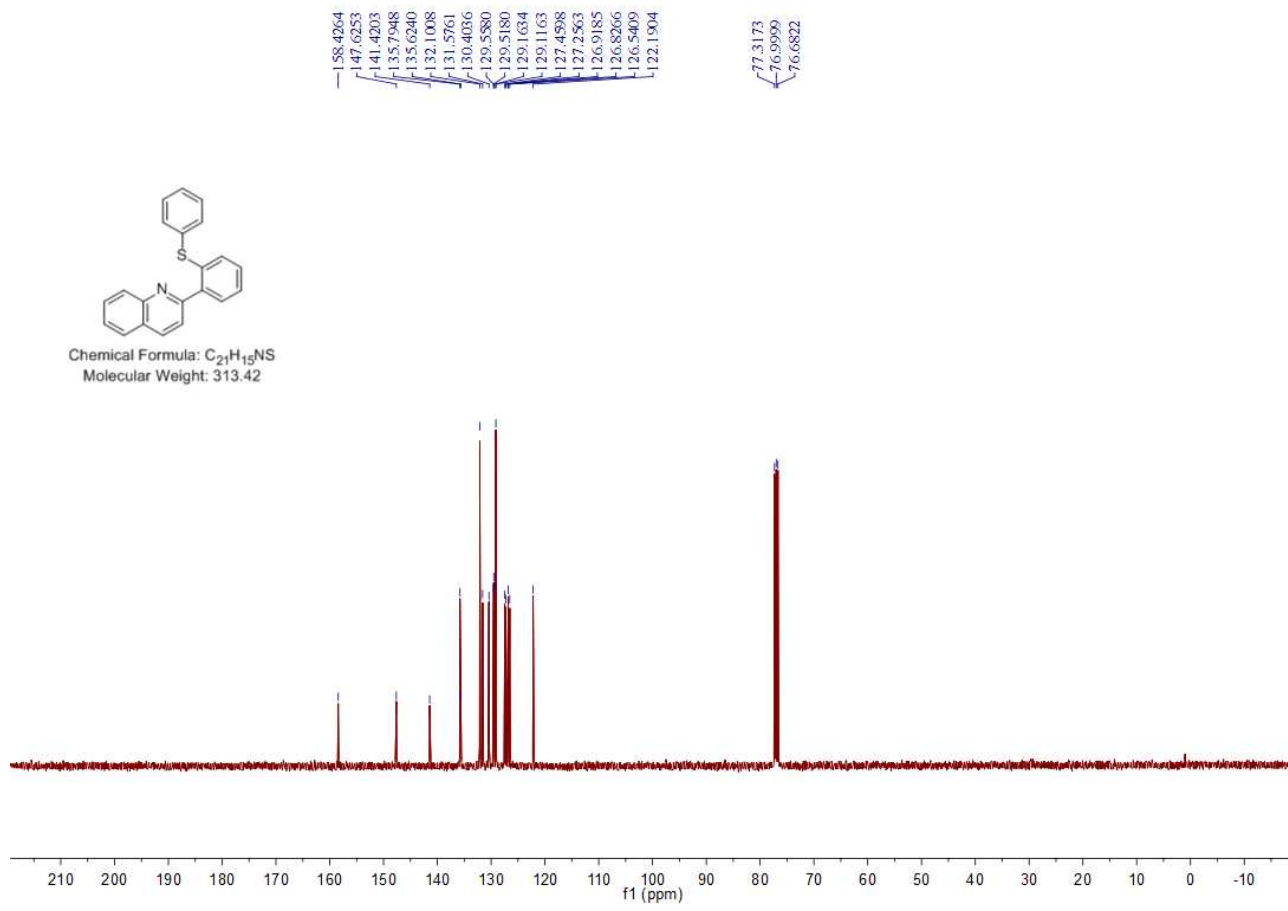
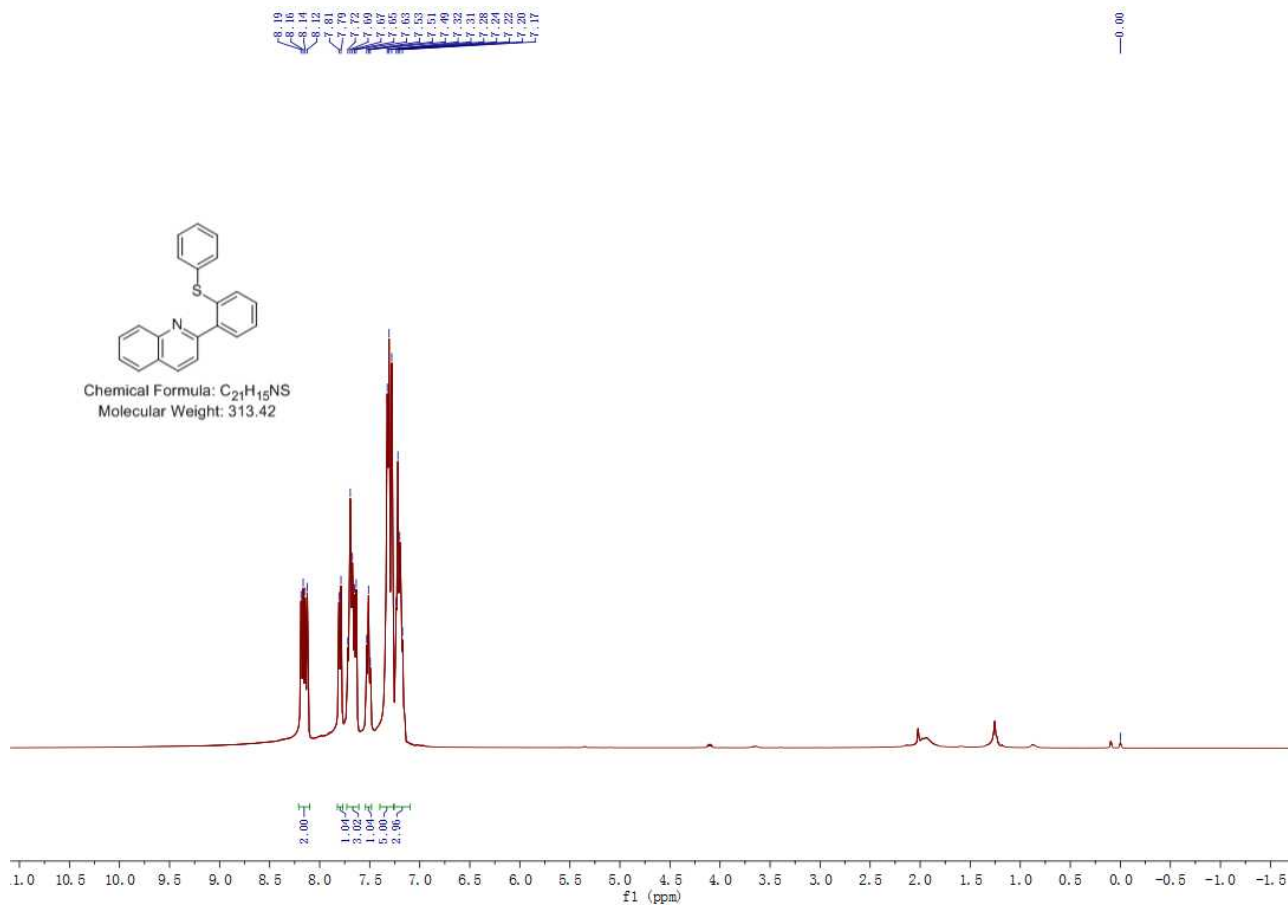
33.0011
26.1848
25.8461



Chemical Formula: C₁₈H₁₉N₃S
Molecular Weight: 309.43

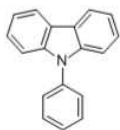


2-(2-(phenylthio)phenyl)quinoline(9)

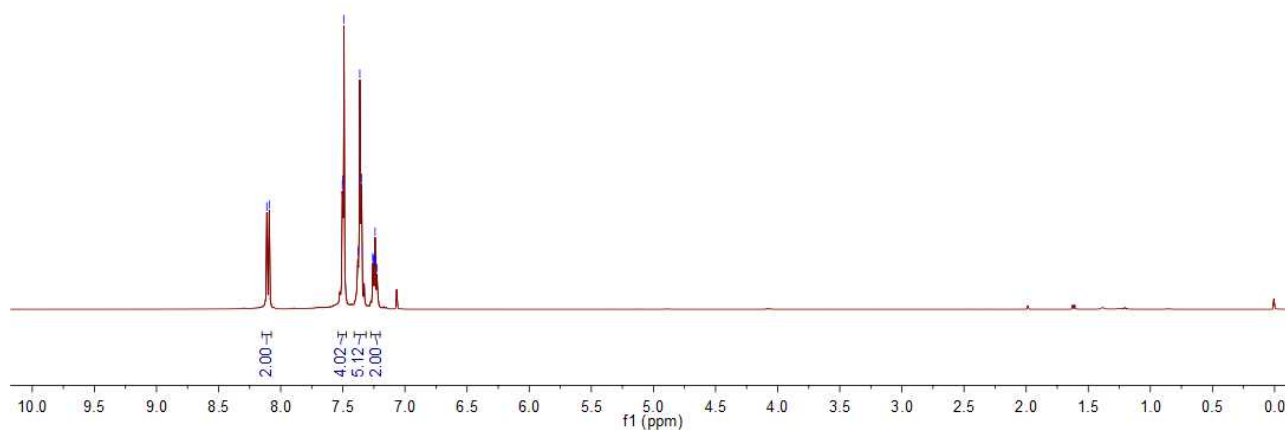


N-Phenyl carbazole (1b)

8.1119
8.0925
7.5040
7.4994
7.4909
7.3782
7.3637
7.3497
7.2802
7.2543
7.2451
7.2405
7.2357
7.2264

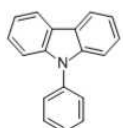


Chemical Formula: C₁₈H₁₃N
Molecular Weight: 243.3025



140.823
137.633
129.770
127.330
127.035
125.866
123.303
120.242
119.854
109.697

77.318
77.000
76.682



Chemical Formula: C₁₈H₁₃N
Molecular Weight: 243.3025

