

**FeCl₃·6H₂O/TMSBr Catalyzed Rapid Synthesis of Dihydropyrimidinones and
Dihydropyrimidinethiones under Microwave Irradiation**

Supporting Information

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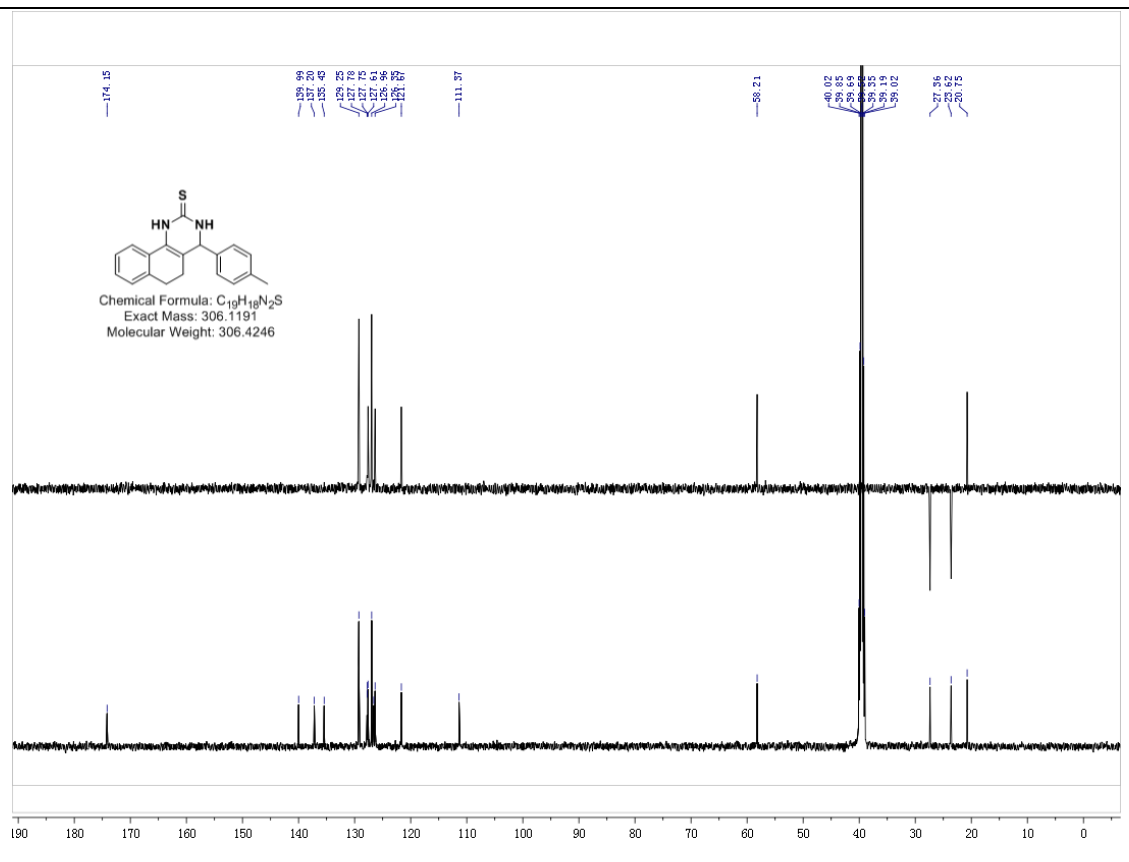
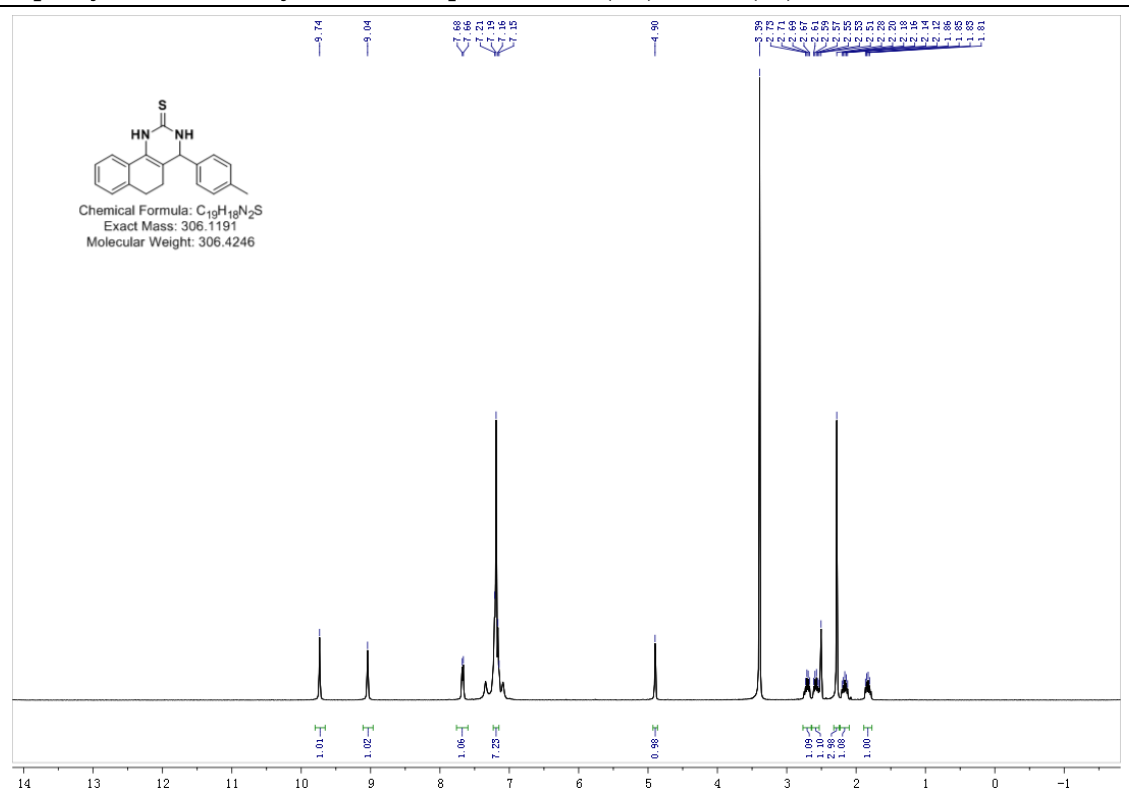
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4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazoline-2(1*H*)-thione (4a)

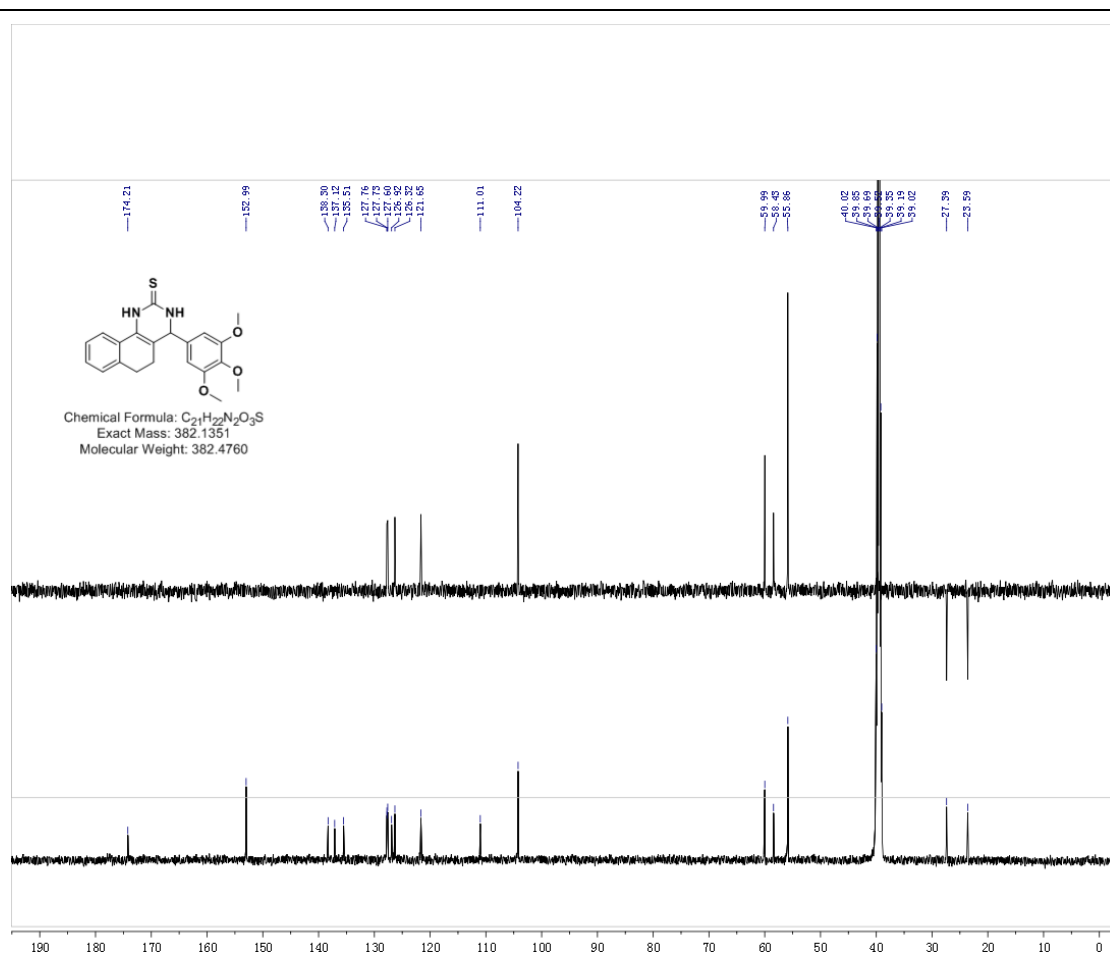
4-*p*-tolyl-3,4,5,6-tetrahydrobenzo[*h*]quinazoline-2(1*H*)-thione (4b)



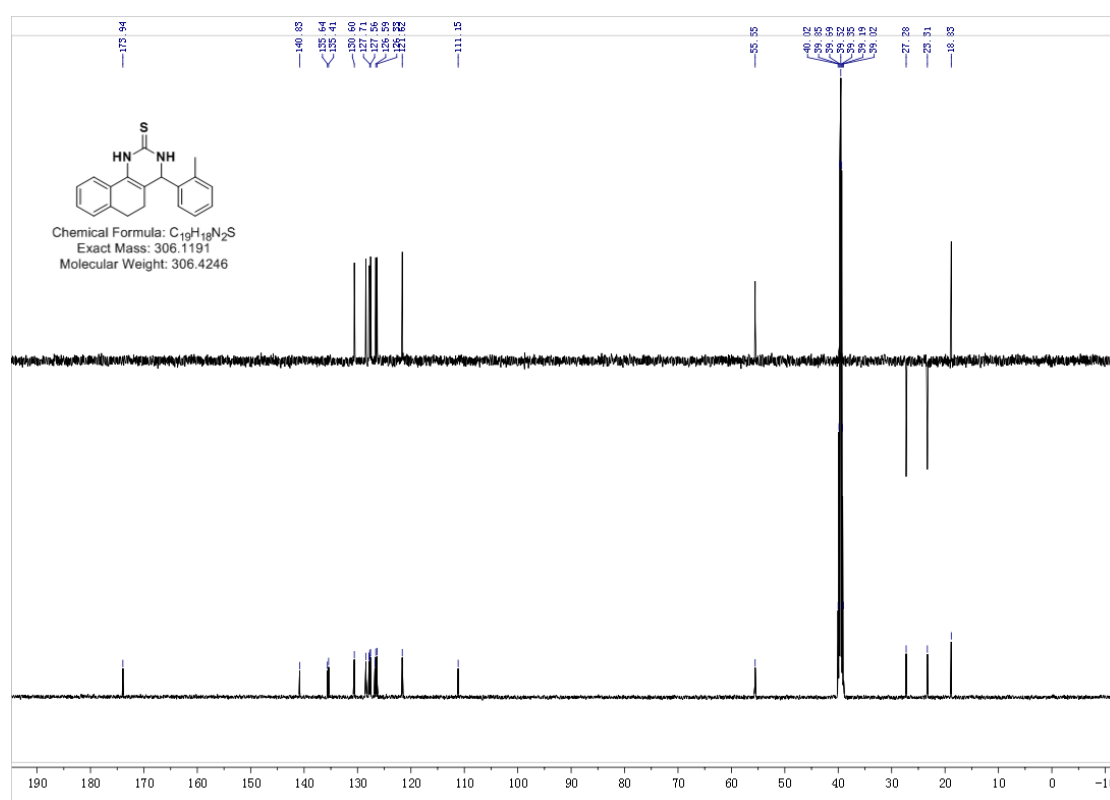
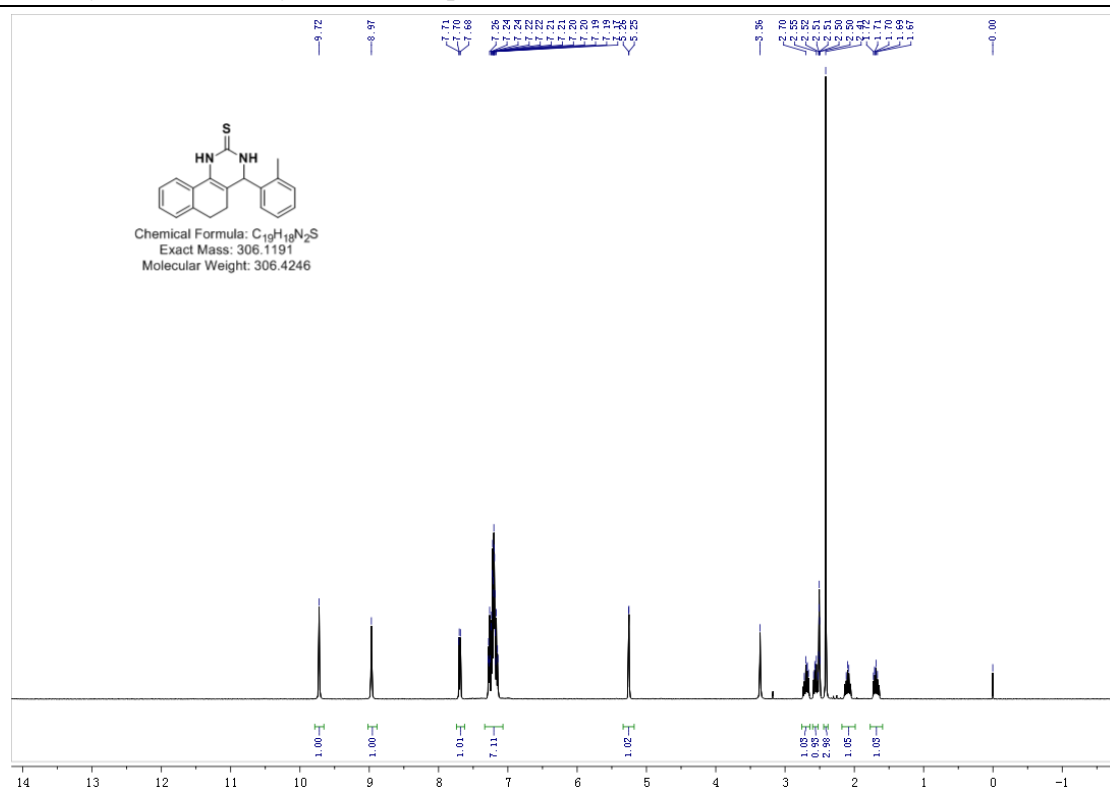
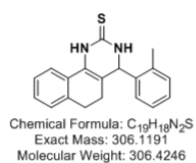
Chemical Formula: $C_{21}H_{22}N_2O_3S$
Exact Mass: 382.1351
Molecular Weight: 382.4760

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7.18
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2.67
2.11

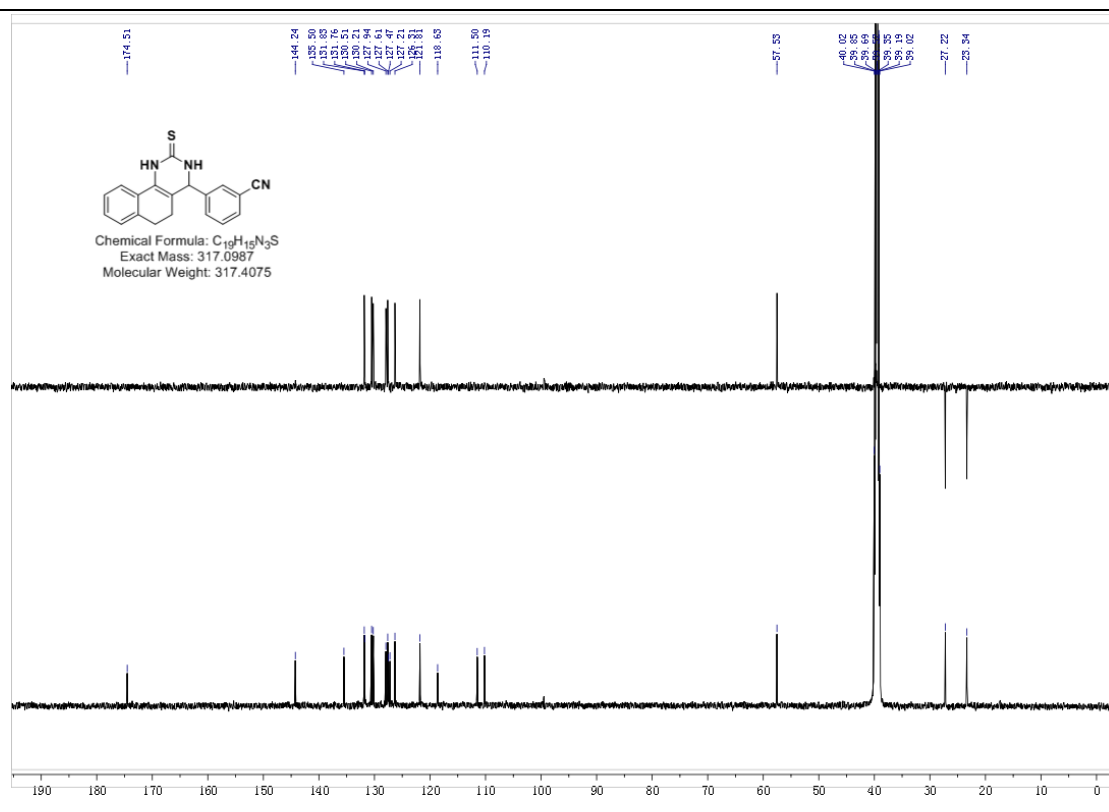
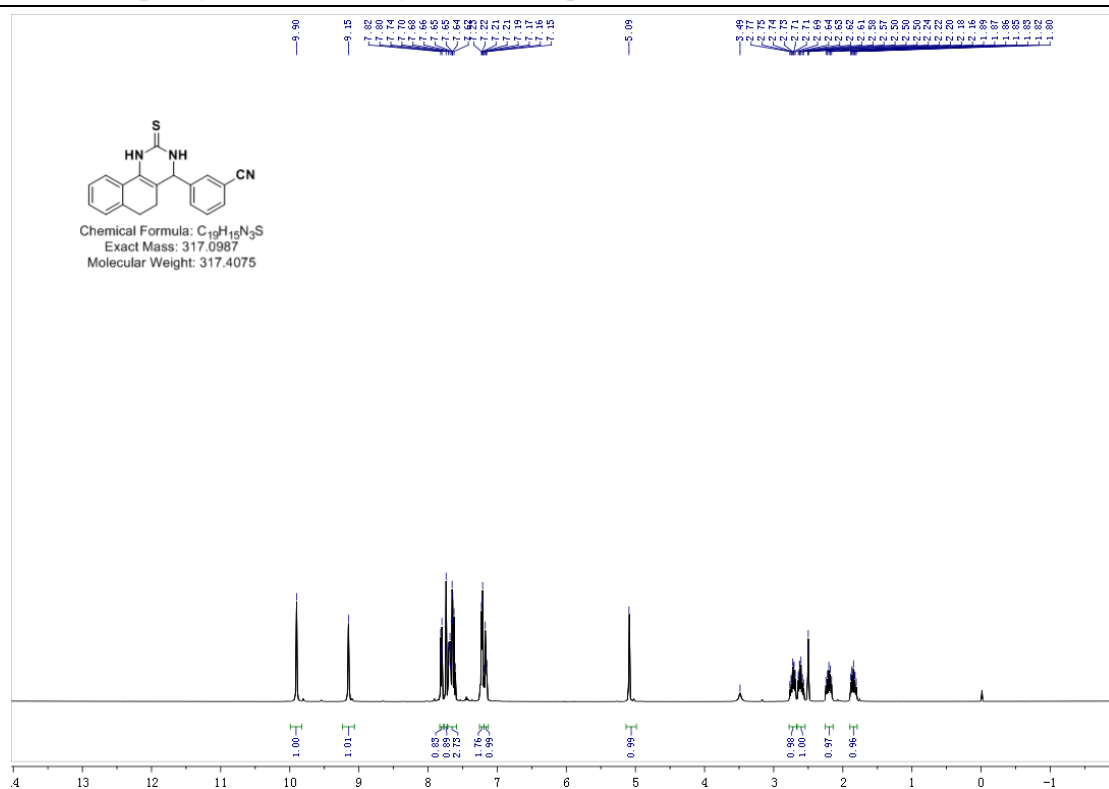
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6.72
1.05
1.06
1.00
1.11



4-*o*-tolyl-3,4,5,6-tetrahydrobenzo[*h*]quinazoline-2(1*H*)-thione (4d)



4-(3-nitrilephenyl)-3,4,5,6-tetrahydrobenzo[h]quinazoline-2(1H)-thione (4e)

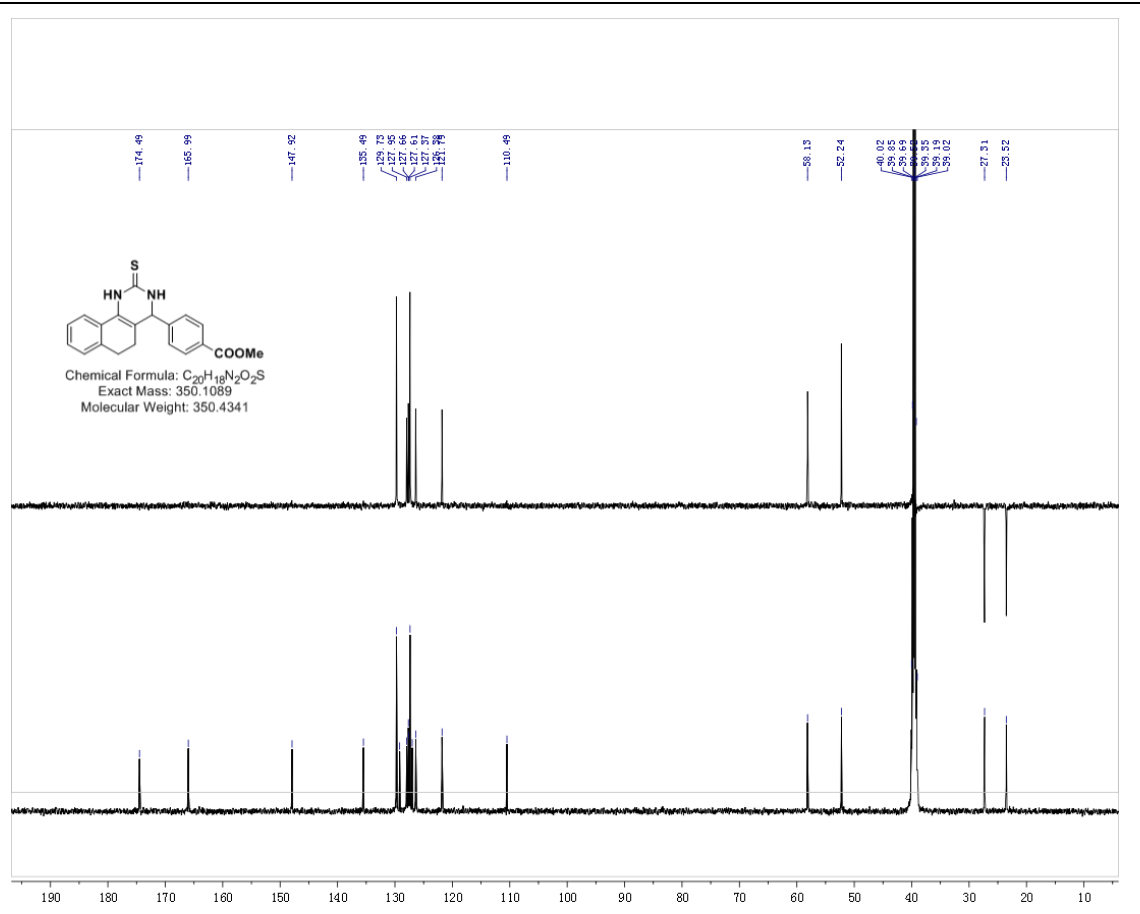


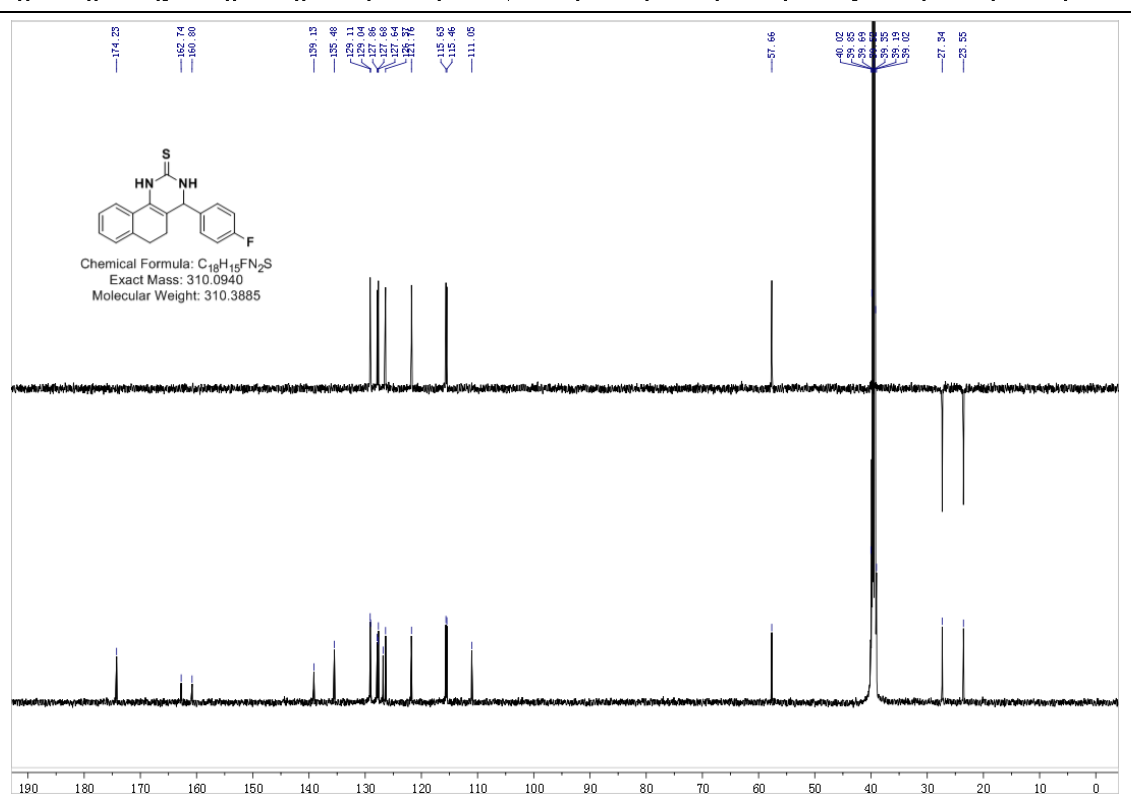
Chemical structure of the compound is shown above the spectrum. The compound is a benzimidazole derivative with a phenyl ring substituted with a methoxycarbonyl group (COOMe).

Chemical Formula: $C_{20}H_{18}N_2O_2S$
Exact Mass: 350.1089
Molecular Weight: 350.4341

The spectrum displays chemical shifts from 14 to -1 ppm. Key peaks are labeled with their chemical shifts and integrations:

- Peak at ~10.0 ppm (Integration: 1.00)
- Peak at ~9.5 ppm (Integration: 1.00)
- Peak at ~7.8 ppm (Integration: 2.00)
- Peak at ~7.5 ppm (Integration: 0.05)
- Peak at ~7.2 ppm (Integration: 1.00)
- Peak at ~7.0 ppm (Integration: 1.00)
- Peak at ~6.8 ppm (Integration: 1.00)
- Peak at ~5.0 ppm (Integration: 1.00)
- Peak at ~3.8 ppm (Integration: 3.00)
- Peak at ~3.6 ppm (Integration: 3.00)
- Peak at ~3.4 ppm (Integration: 1.00)
- Peak at ~3.2 ppm (Integration: 1.00)
- Peak at ~2.8 ppm (Integration: 1.00)
- Peak at ~2.6 ppm (Integration: 1.00)
- Peak at ~2.4 ppm (Integration: 1.00)
- Peak at ~2.2 ppm (Integration: 1.00)
- Peak at ~2.0 ppm (Integration: 1.00)
- Peak at ~1.8 ppm (Integration: 1.00)
- Peak at ~1.6 ppm (Integration: 1.00)
- Peak at ~1.4 ppm (Integration: 1.00)
- Peak at ~1.2 ppm (Integration: 1.00)
- Peak at ~1.0 ppm (Integration: 1.00)
- Peak at ~0.8 ppm (Integration: 1.00)
- Peak at ~0.6 ppm (Integration: 1.00)
- Peak at ~0.4 ppm (Integration: 1.00)
- Peak at ~0.2 ppm (Integration: 1.00)
- Peak at ~0.0 ppm (Integration: 1.00)

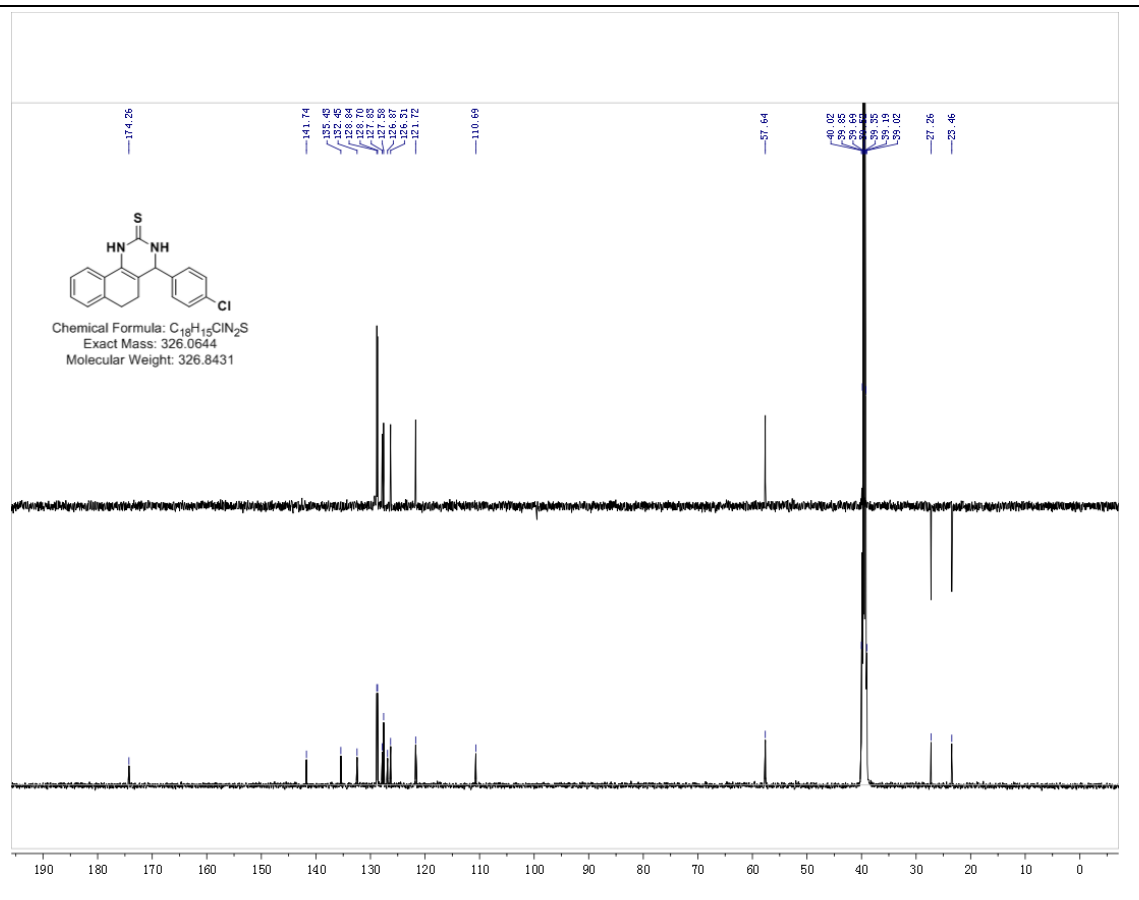


[illegible]

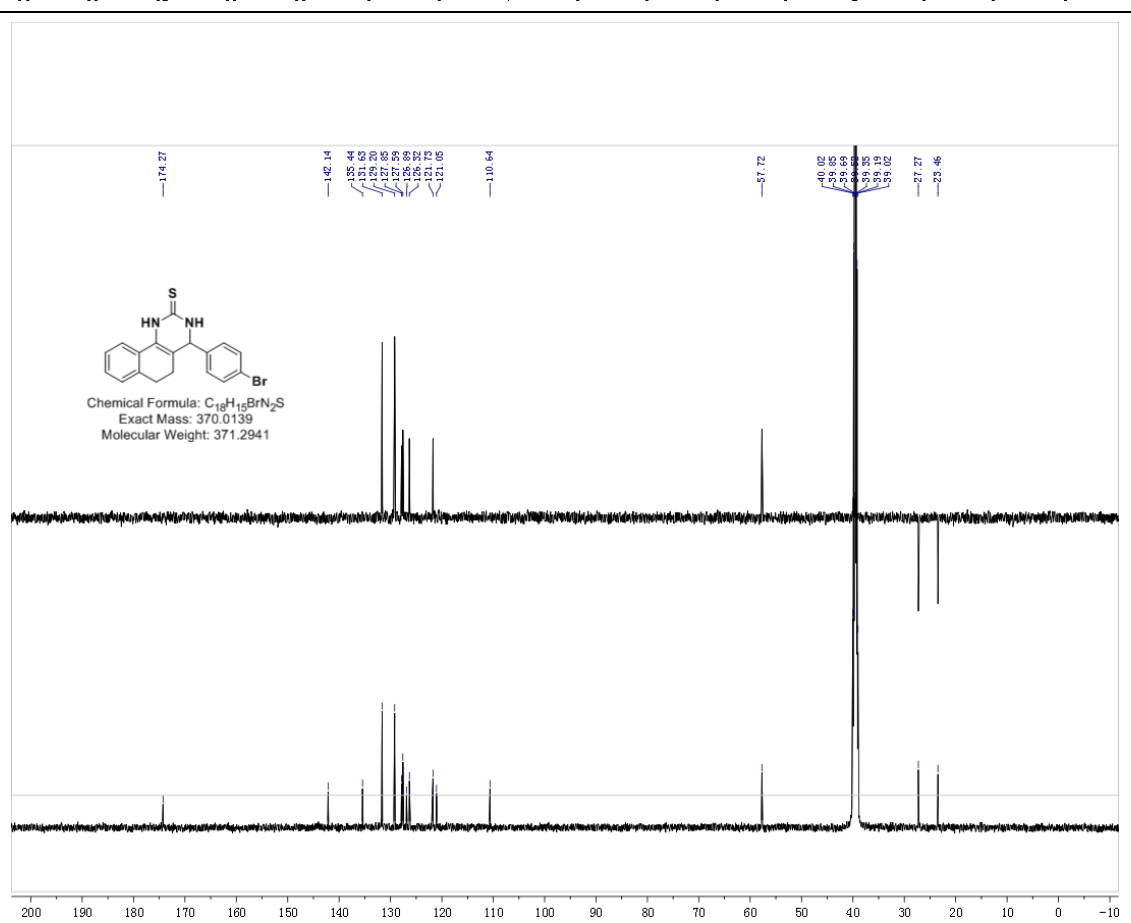
Chemical structure: Clc1ccc(cc1)C2=NC(=S)Nc3ccccc23

Chemical Formula: $C_{18}H_{15}ClN_2S$
Exact Mass: 326.0644
Molecular Weight: 326.8431

1H NMR spectrum (CDCl₃) showing peaks in the aromatic region (7.0-7.8 ppm), a thione NH peak (9.8 ppm), a solvent peak (3.3 ppm), and aliphatic peaks (2.2-2.5 ppm). Integration values are provided below the baseline.

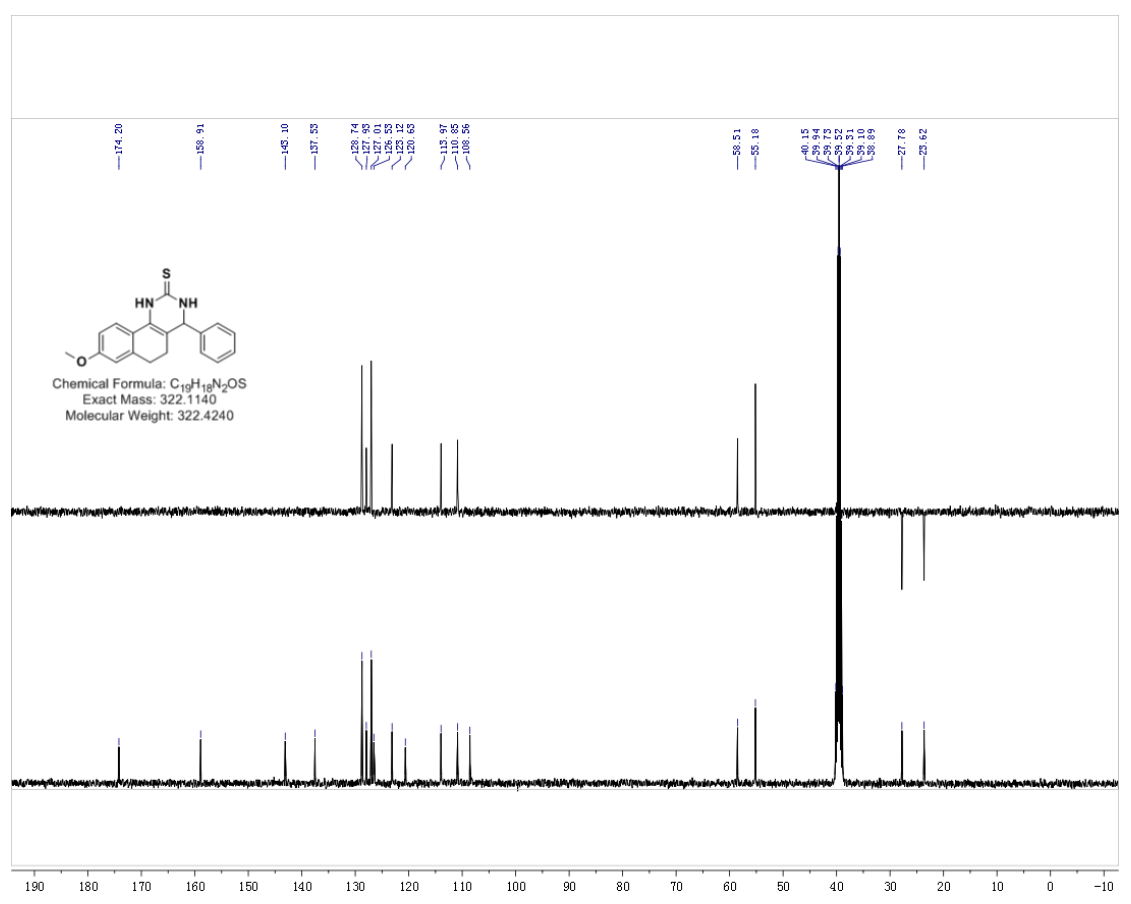


Chemical Formula: C₁₈H₁₆BrN₂S
Exact Mass: 370.0139
Molecular Weight: 371.2941

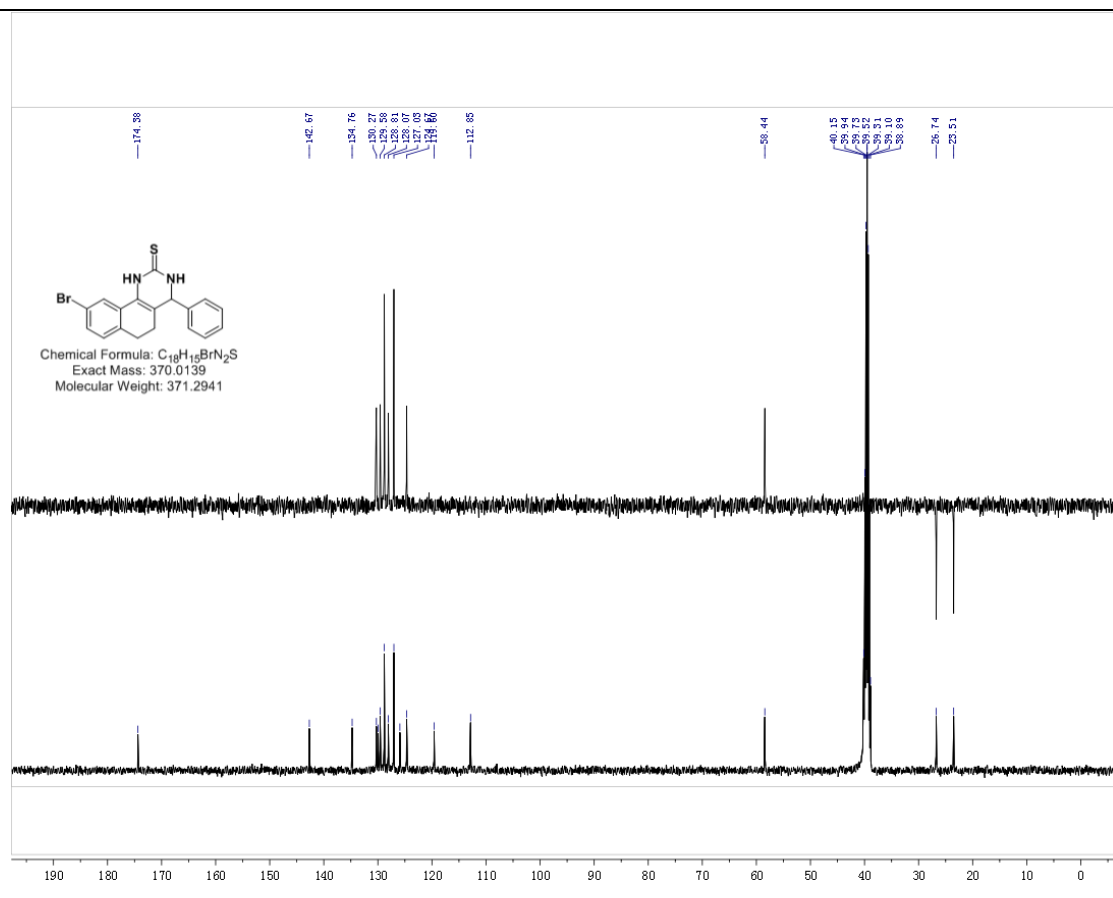
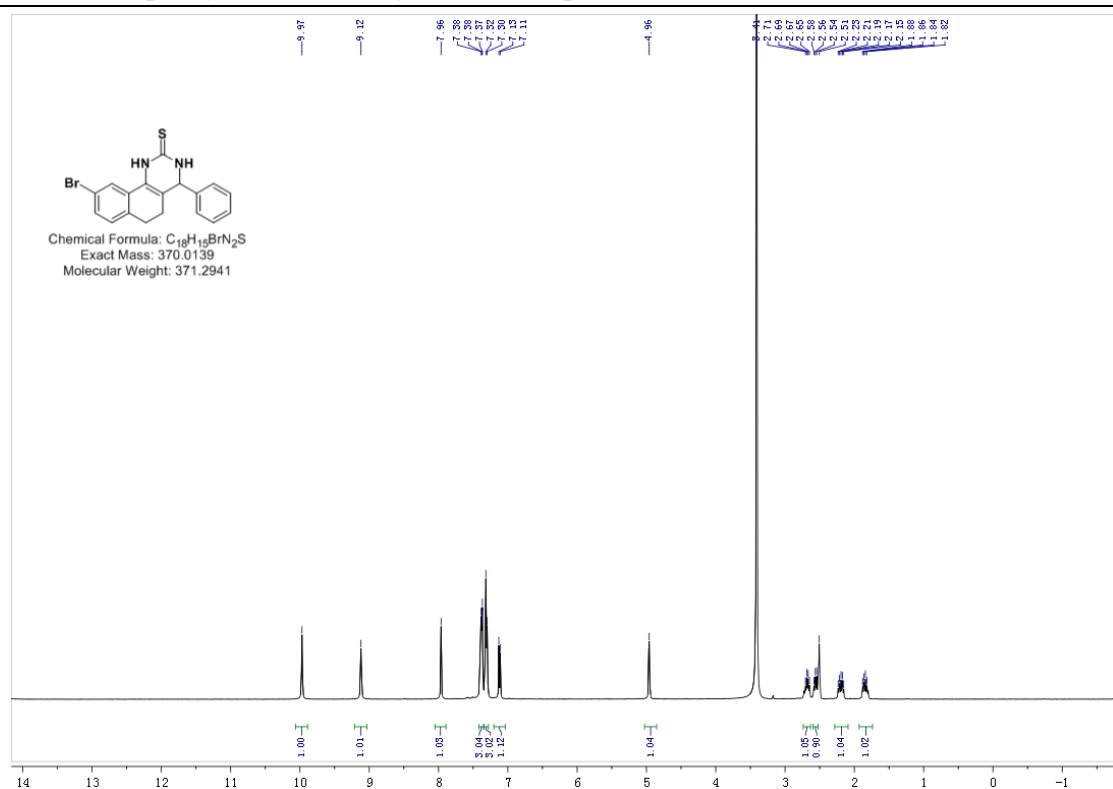


Chemical Formula: C₁₉H₁₈N₂OS
Exact Mass: 322.1140
Molecular Weight: 322.4240

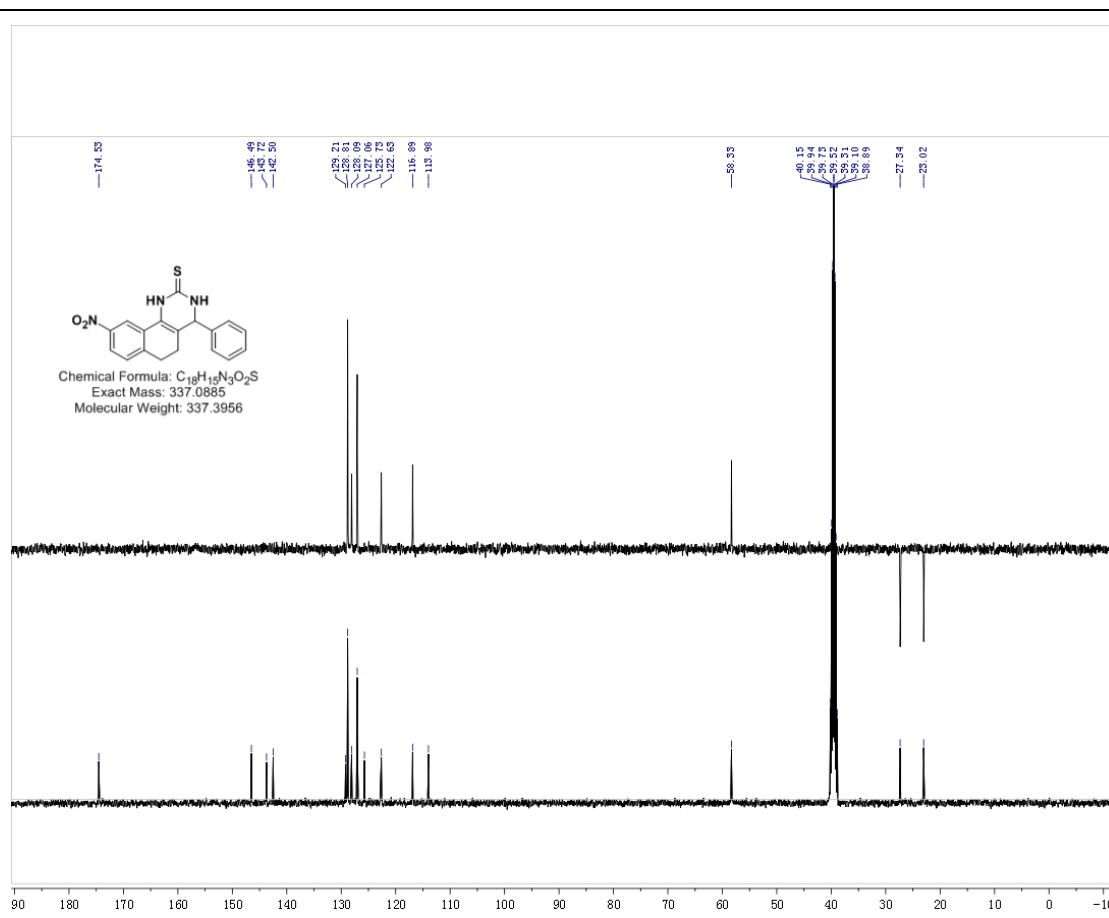
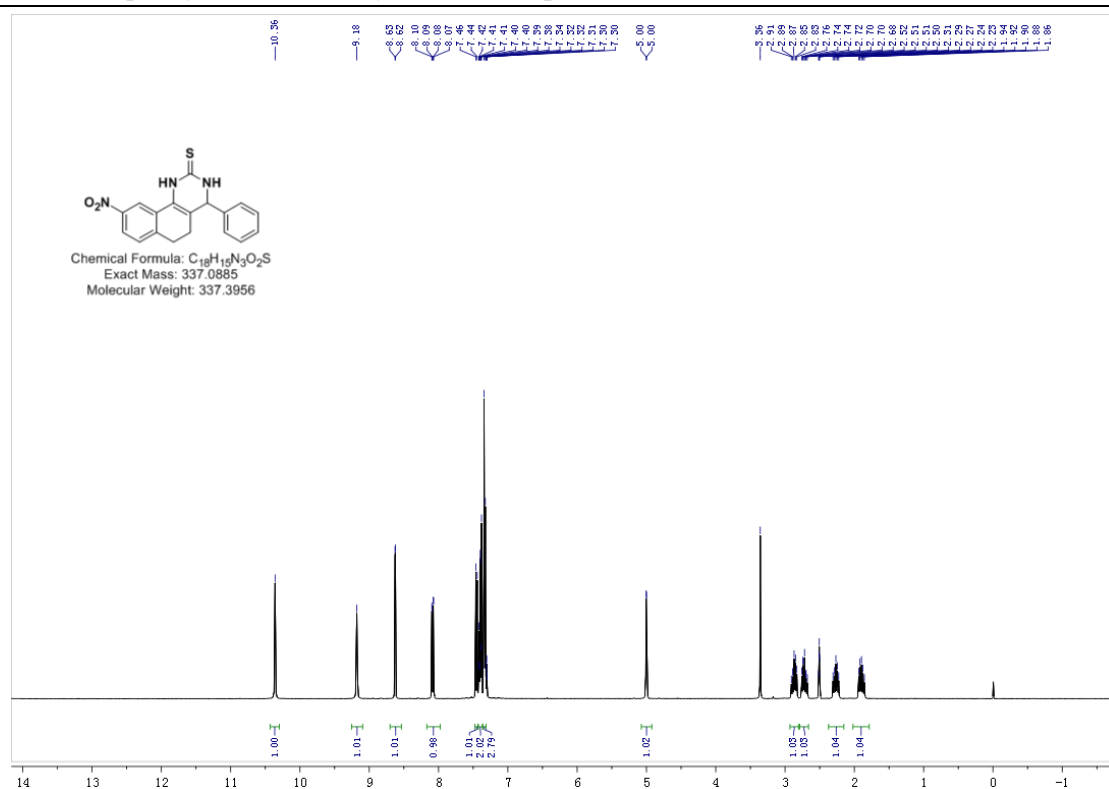
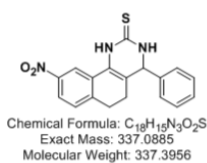
1H NMR spectrum (400 MHz, CDCl₃) of 2-(4-methoxyphenyl)-2-phenyl-1,2,3,4-tetrahydroquinoline-5-carbonylthiohydrazide. The spectrum shows peaks from 0 to 10 ppm. Key features include a methoxy singlet at 3.8 ppm, aromatic signals between 6.5-7.5 ppm, and a thiohydrazide NH singlet at 9.7 ppm. Integration values are provided below the baseline.



9-bromo-4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazoline-2(1H)-thione (4k)

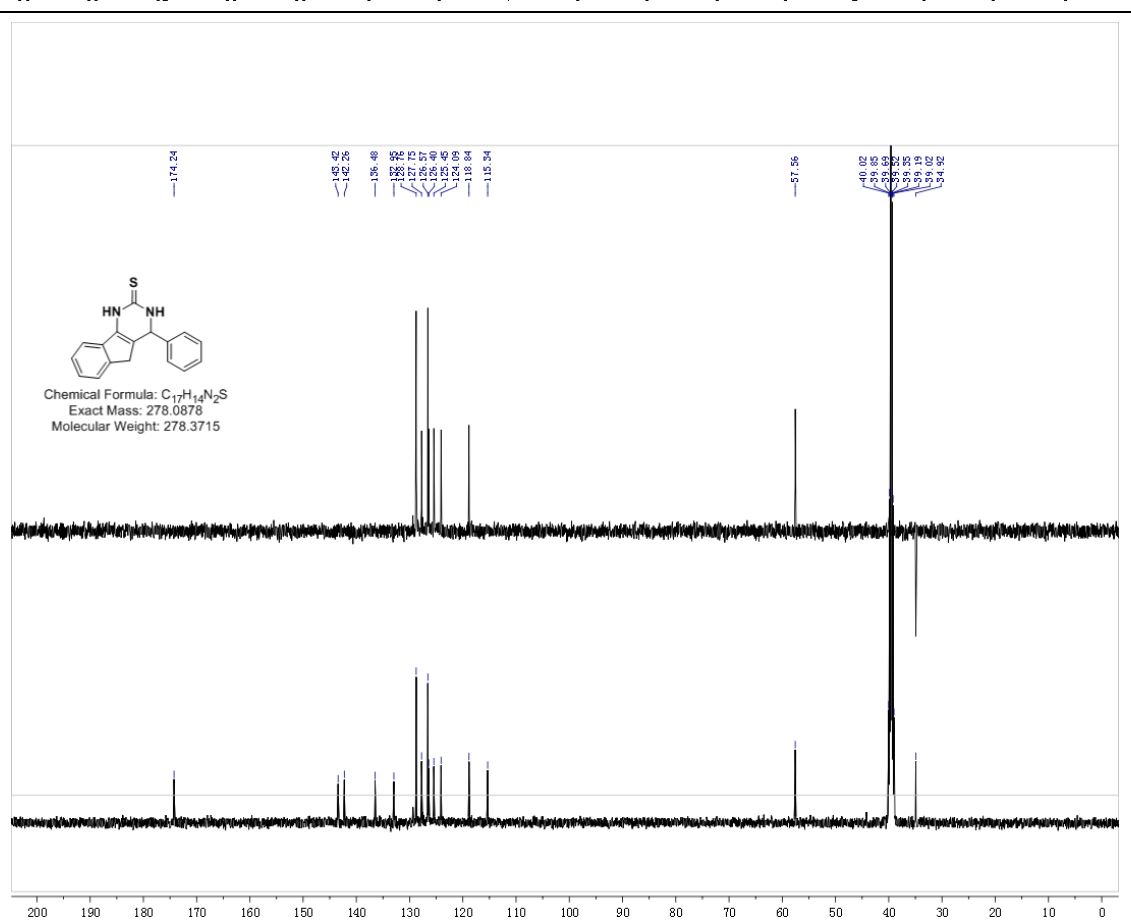


9-nitro-4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazoline-2(1H)-thione (4l)

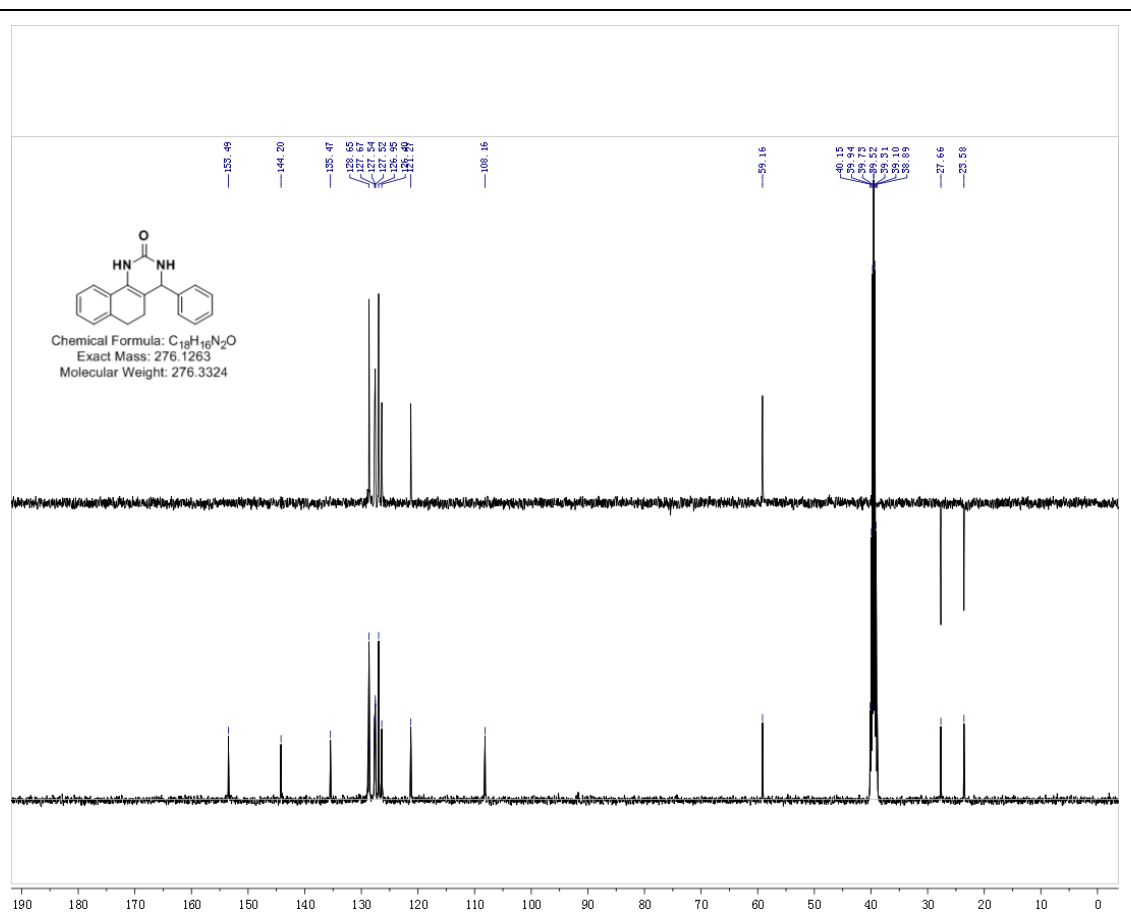
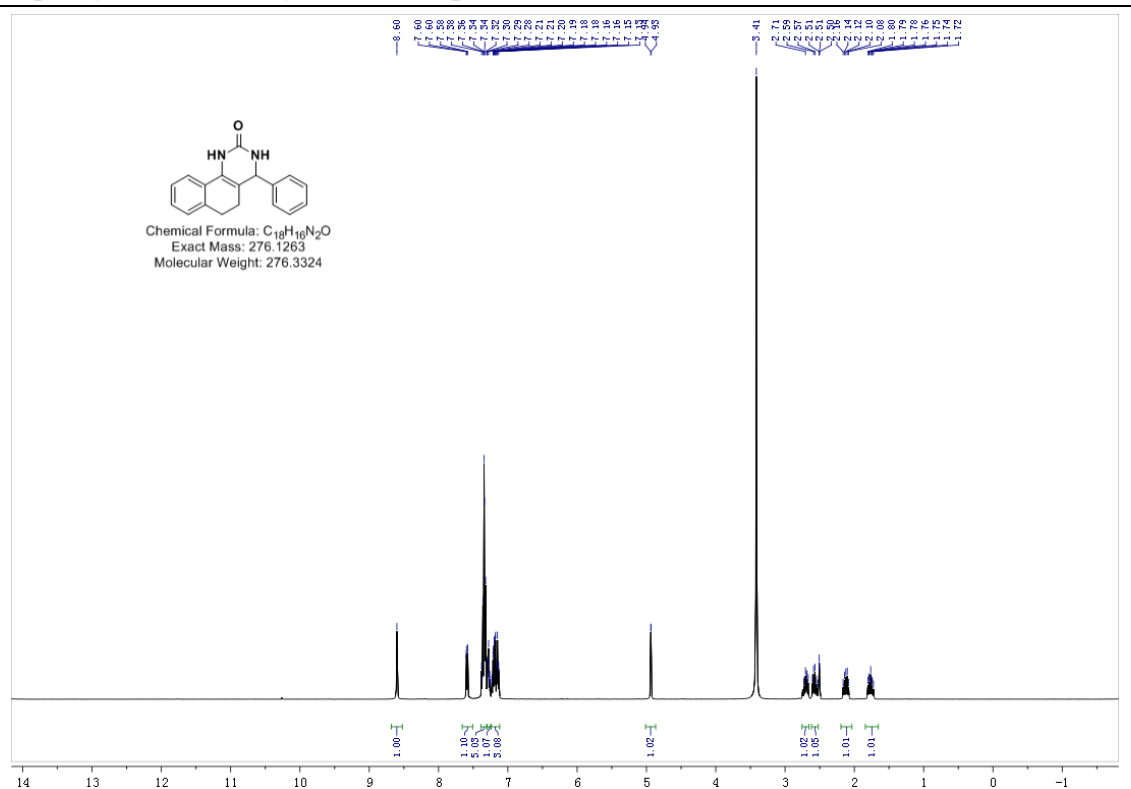


Chemical Formula: C₁₇H₁₄N₂S
Exact Mass: 278.0878
Molecular Weight: 278.3715

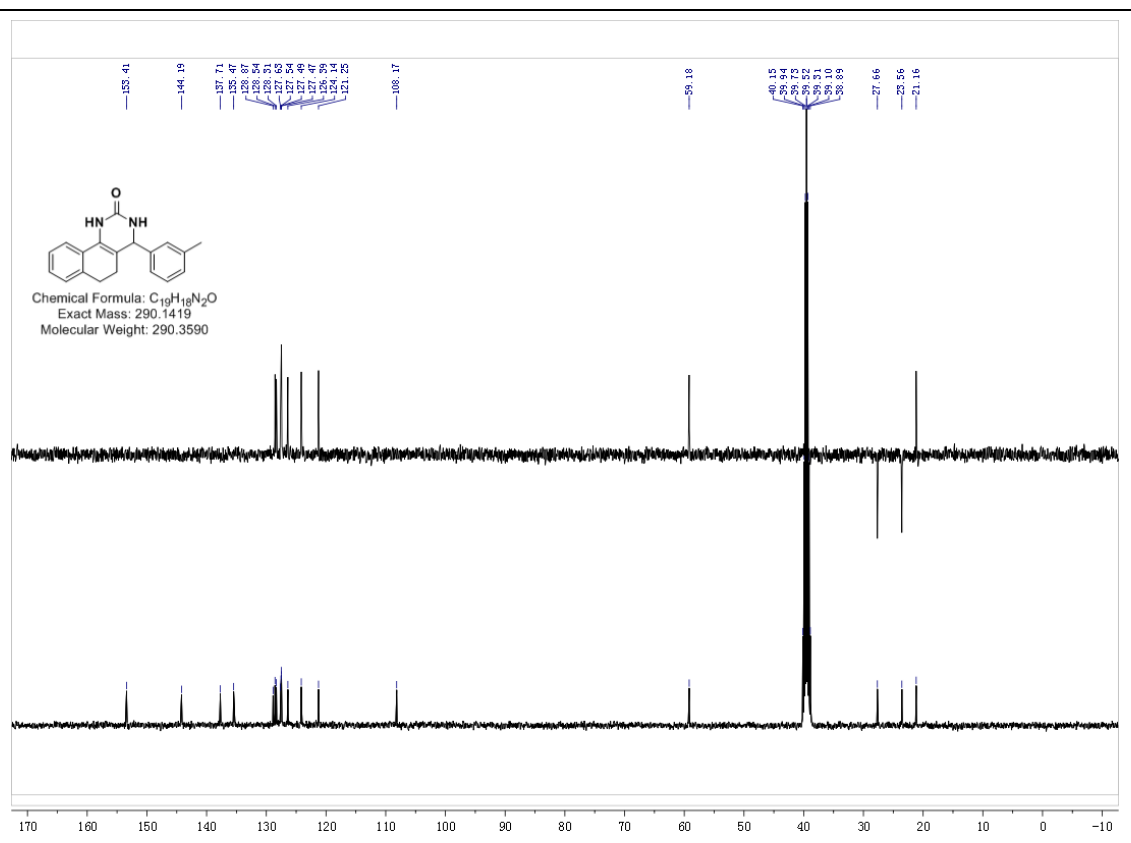
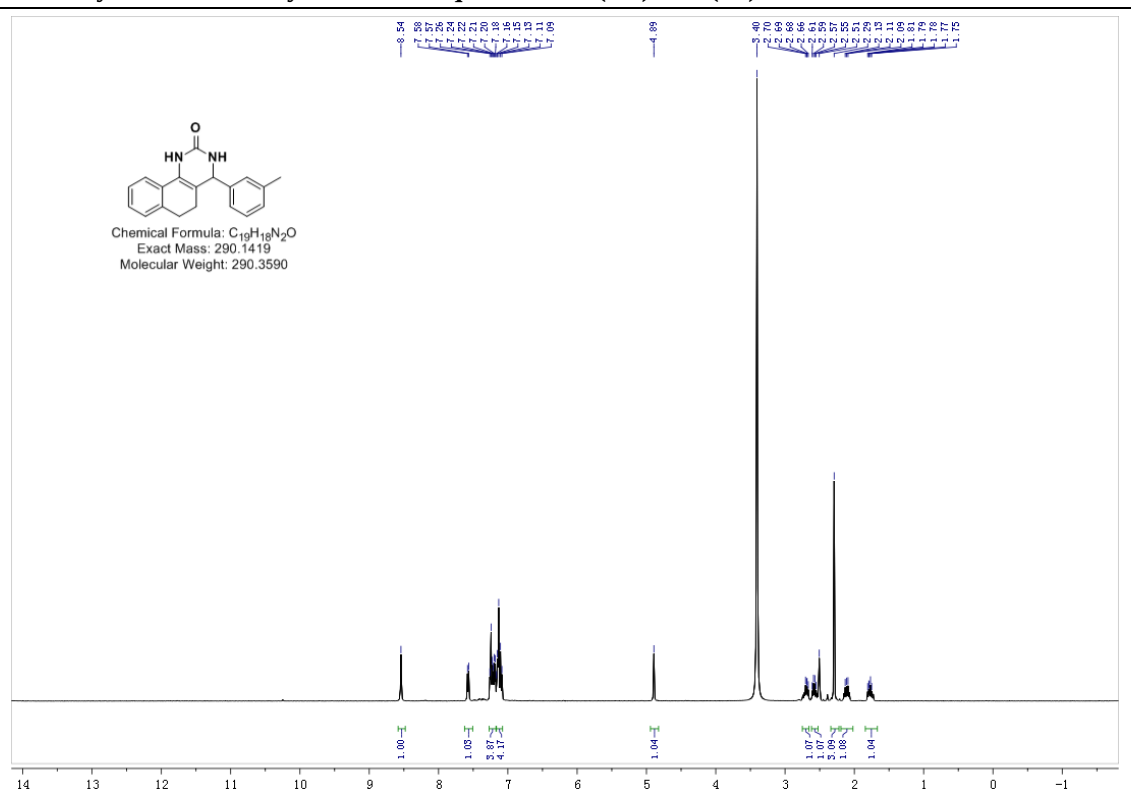
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1.01
1.40
1.10



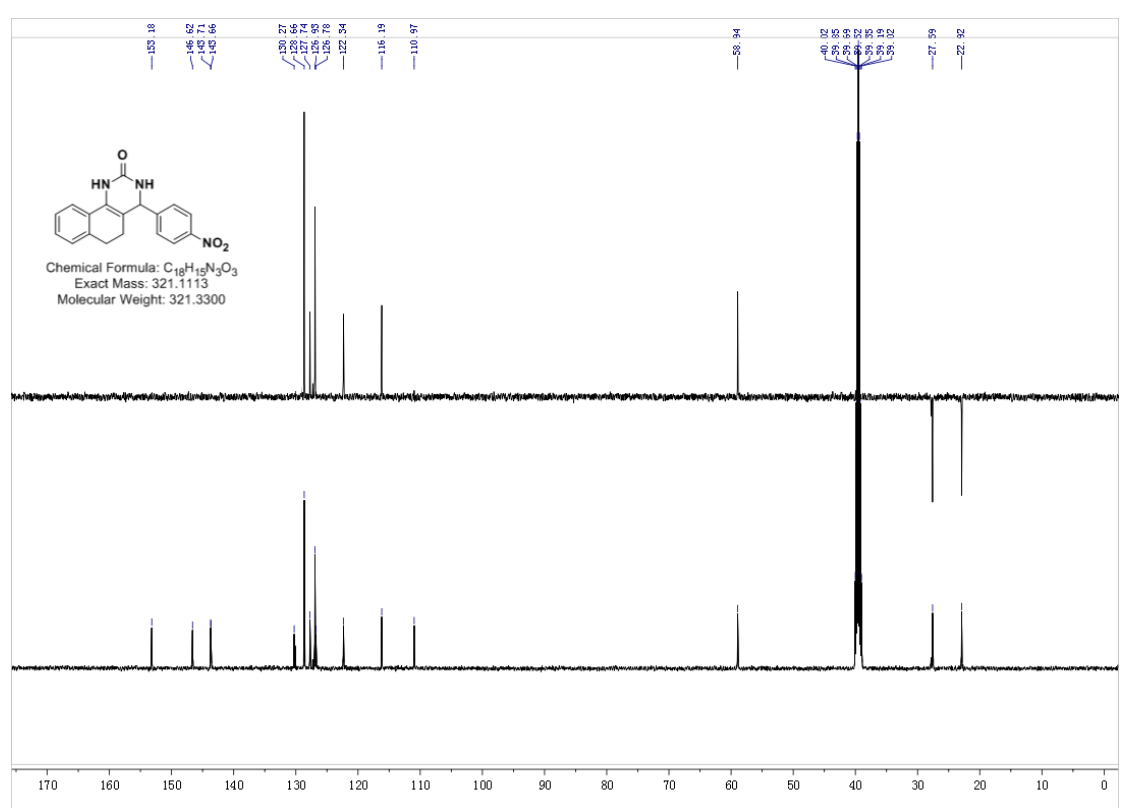
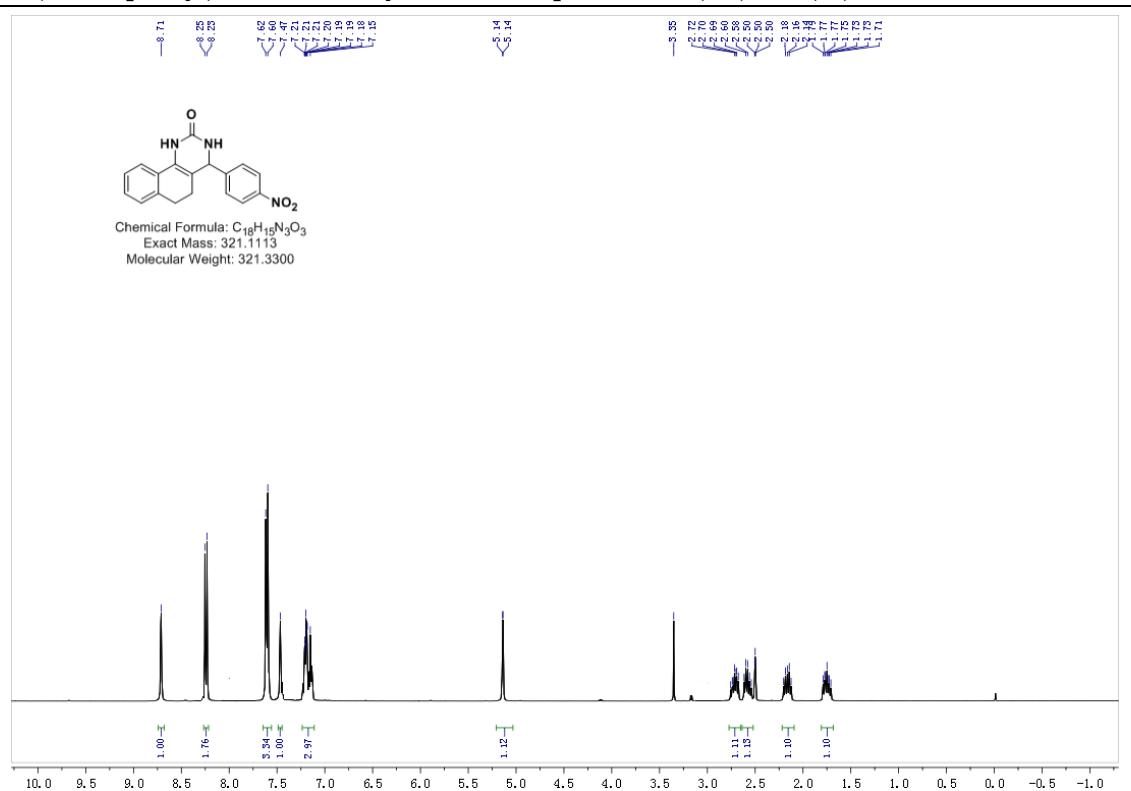
4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6a)



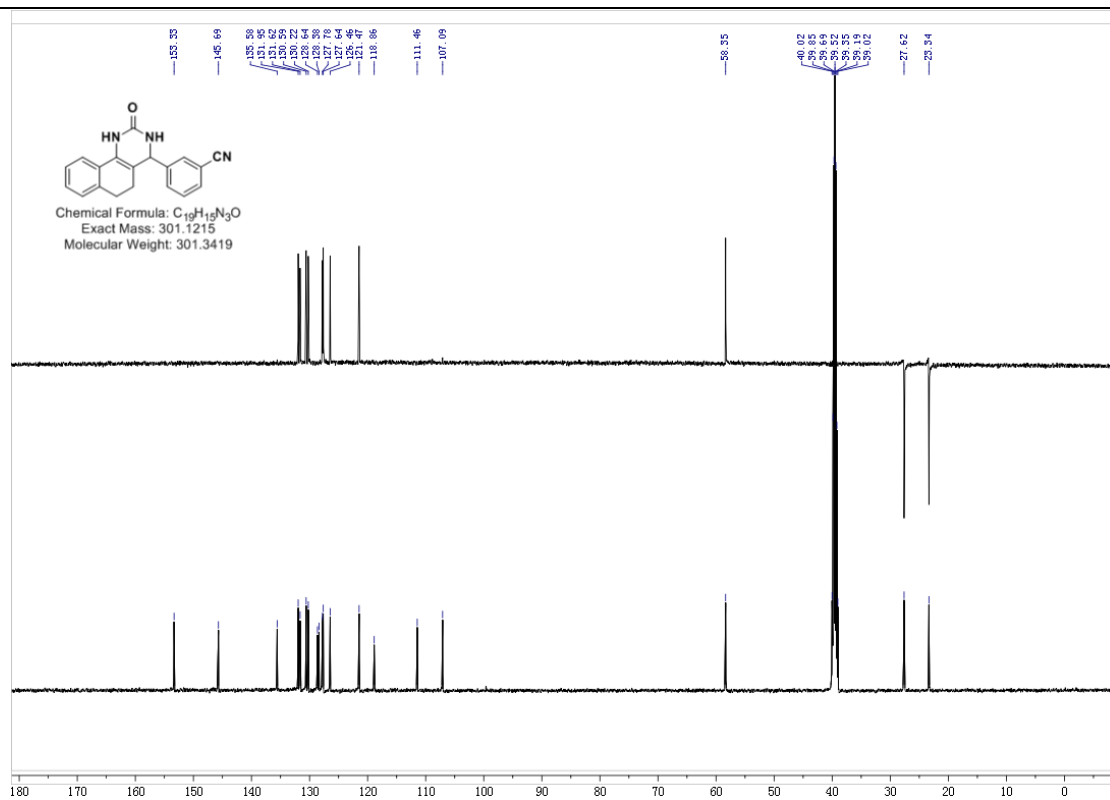
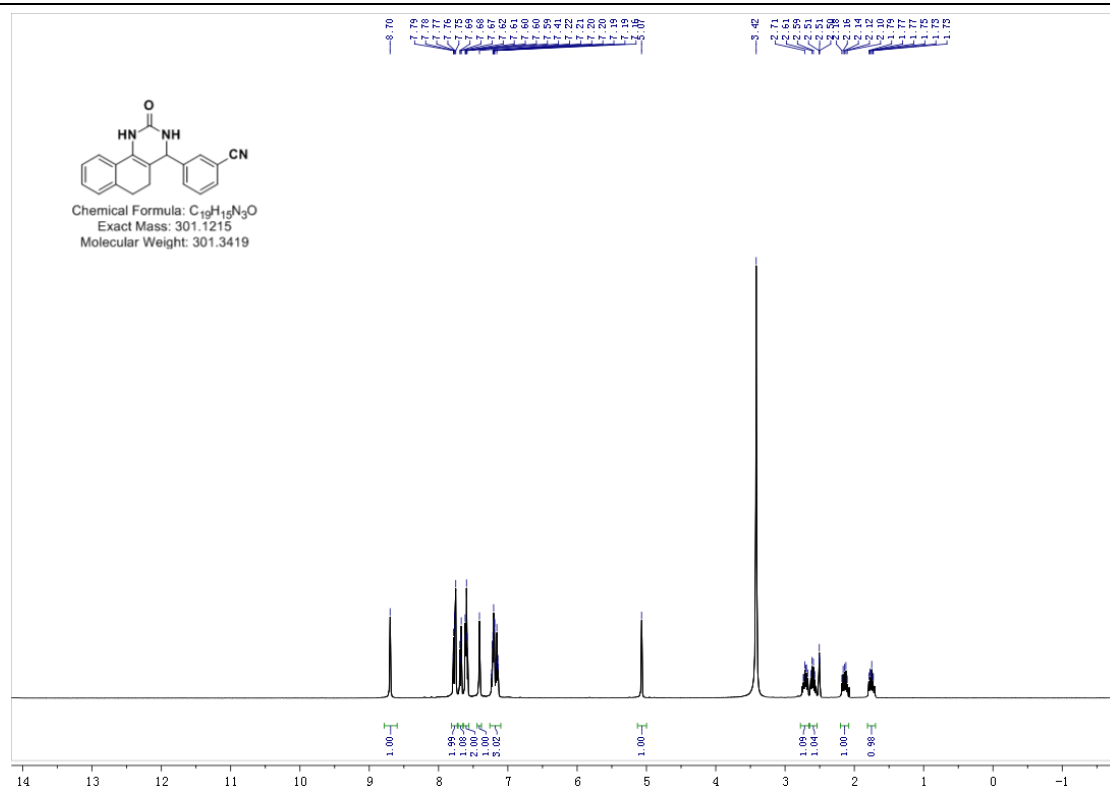
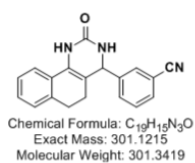
4-*m*-tolyl-3,4,5,6-tetrahydrobenzo[*h*]quinazolin-2(1*H*)-one (6b)



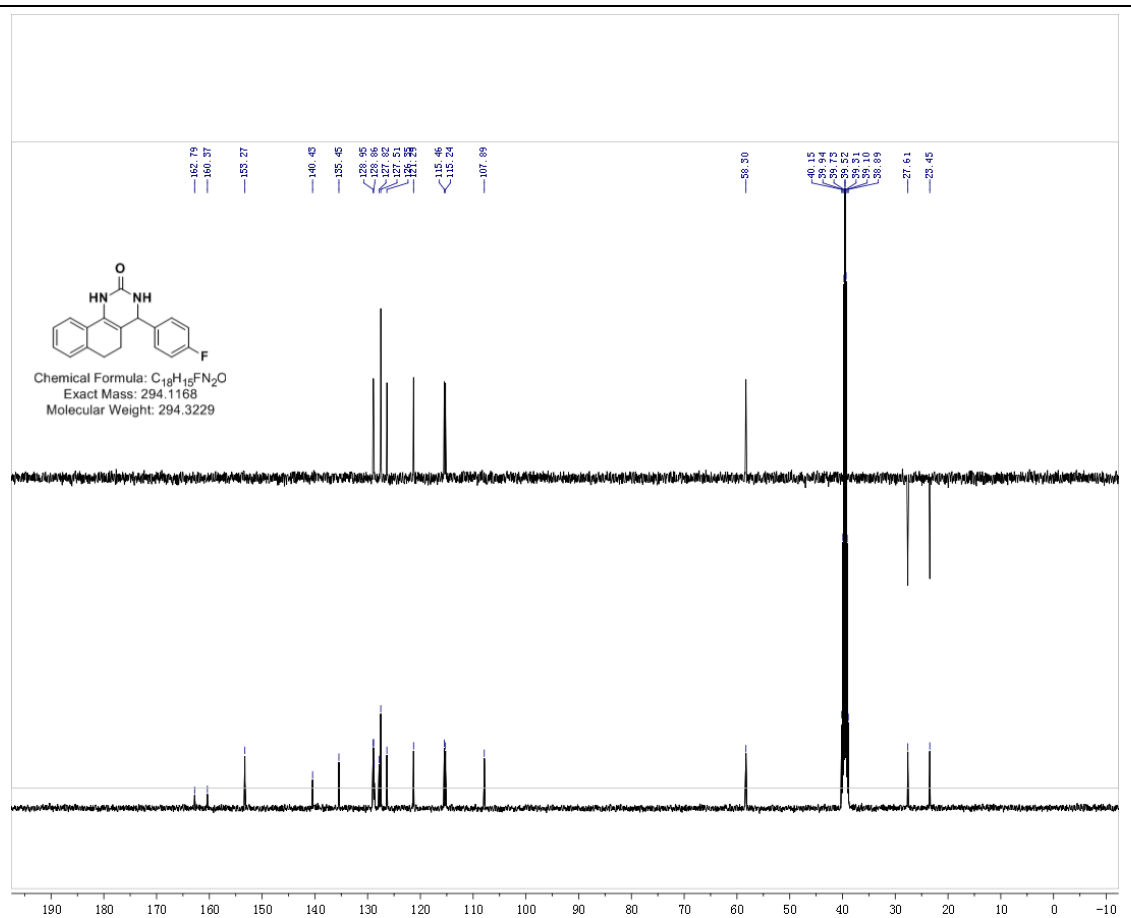
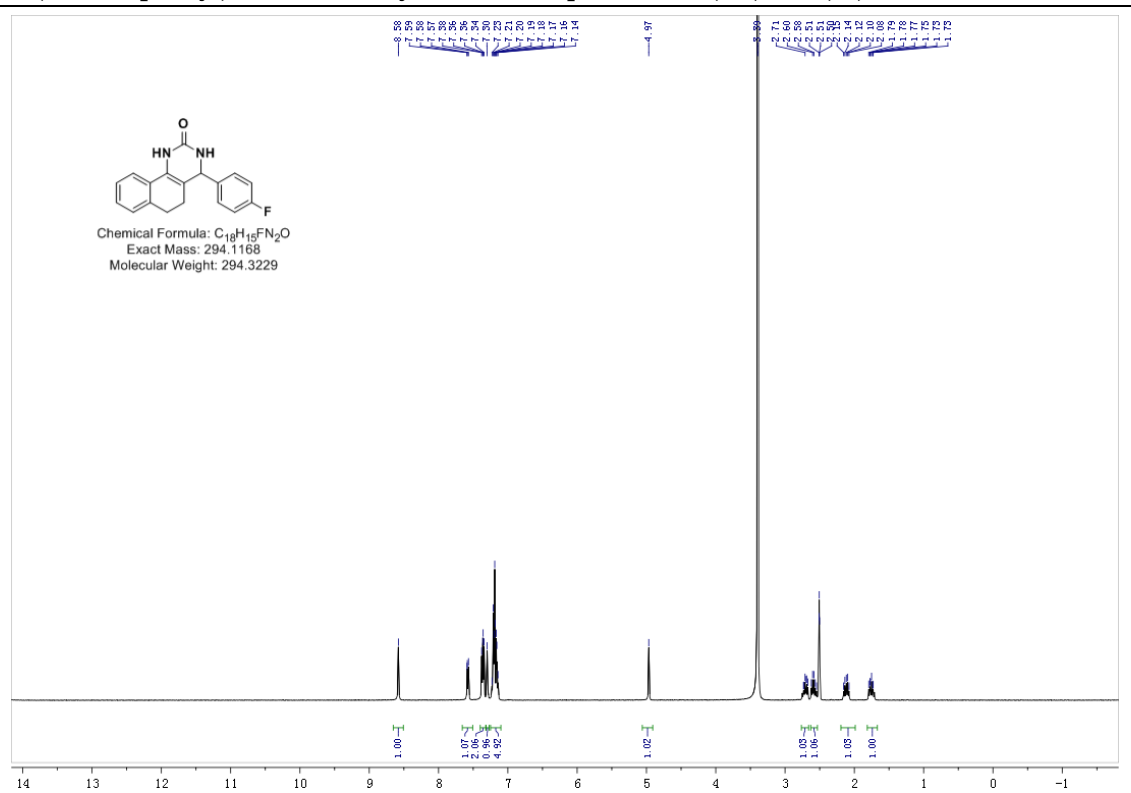
4-(4-nitrophenyl)-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6c)



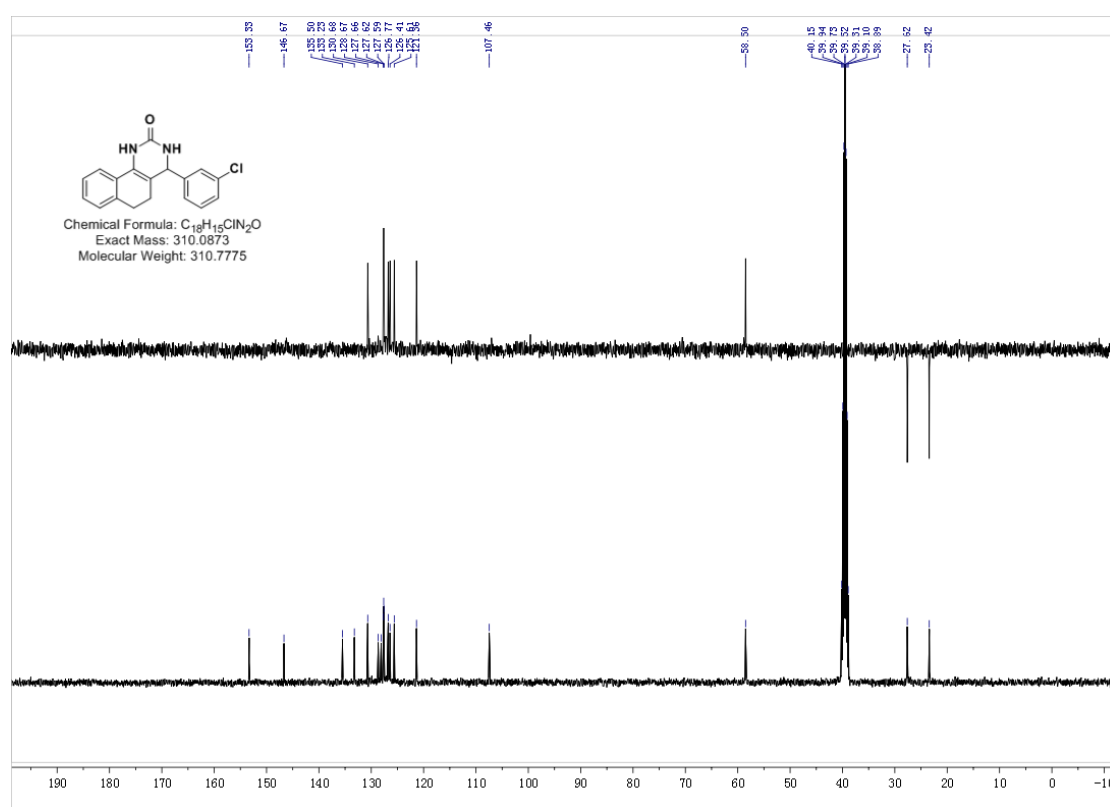
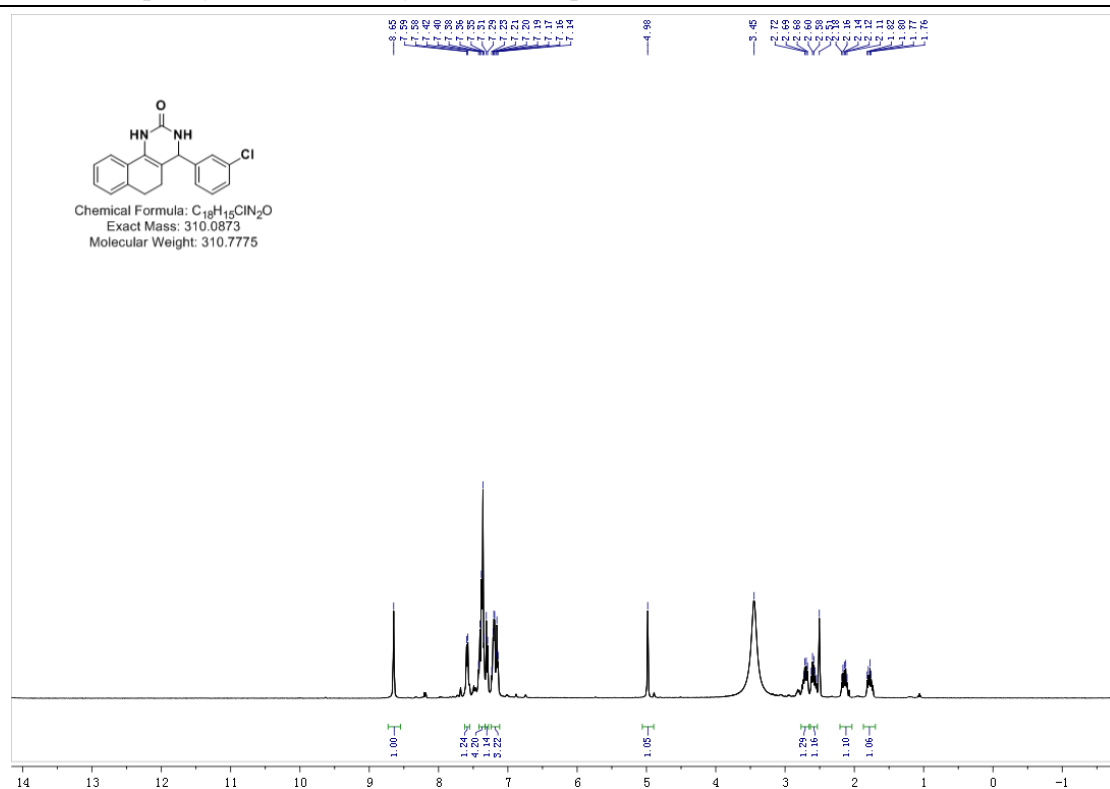
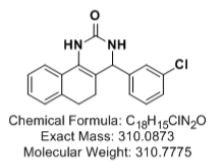
3-(2-oxo-1,2,3,4,5,6-hexahydrobenzo[h]quinazolin-4-yl)benzonitrile (6d)



4-(4-fluorophenyl)-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6e)



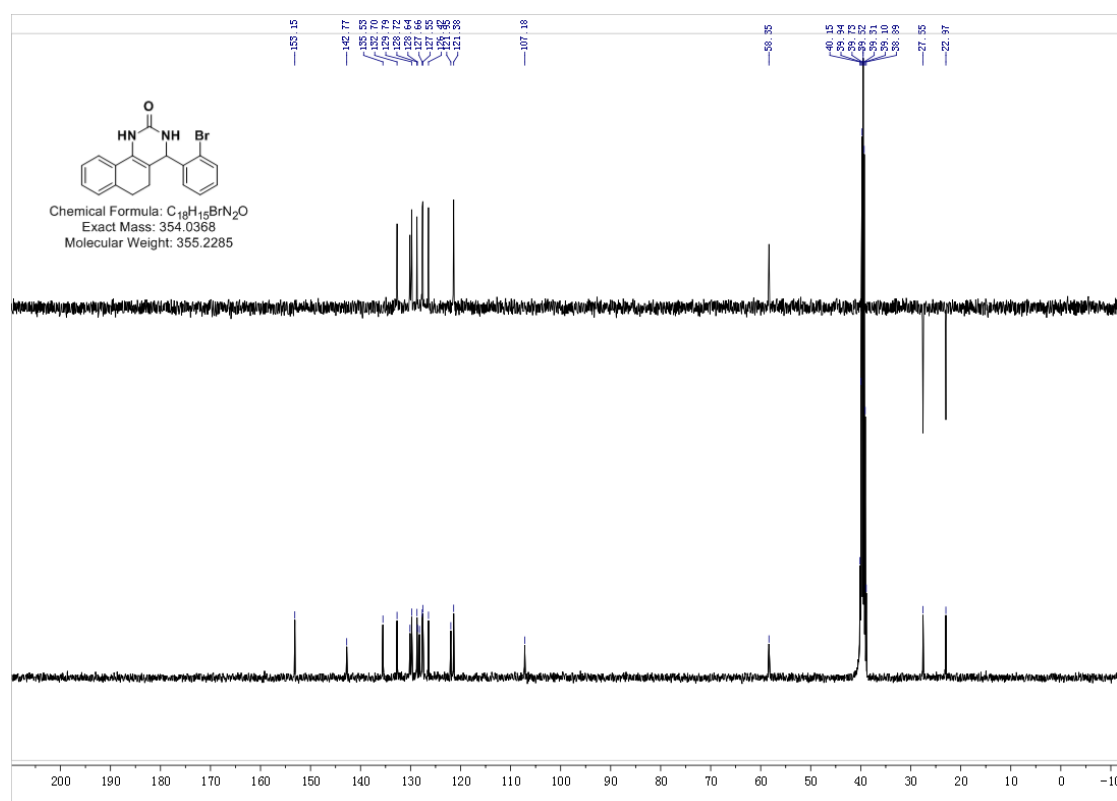
4-(3-chlorophenyl)-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6f)



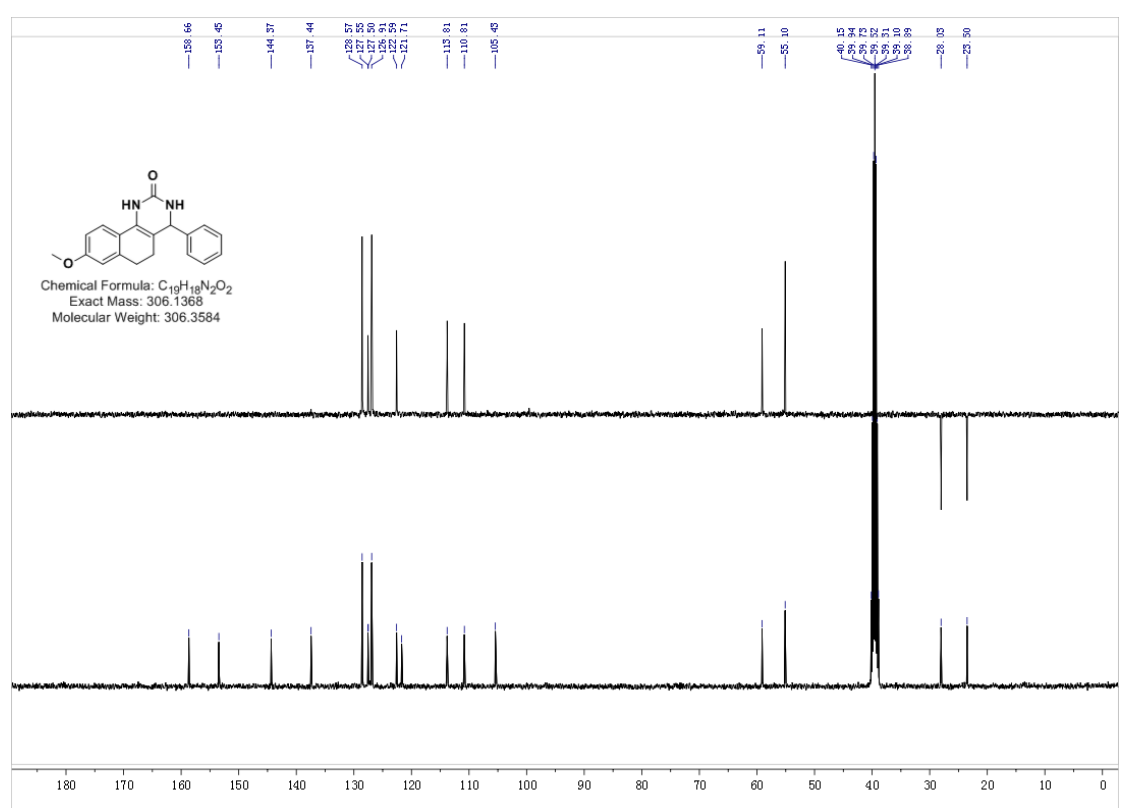
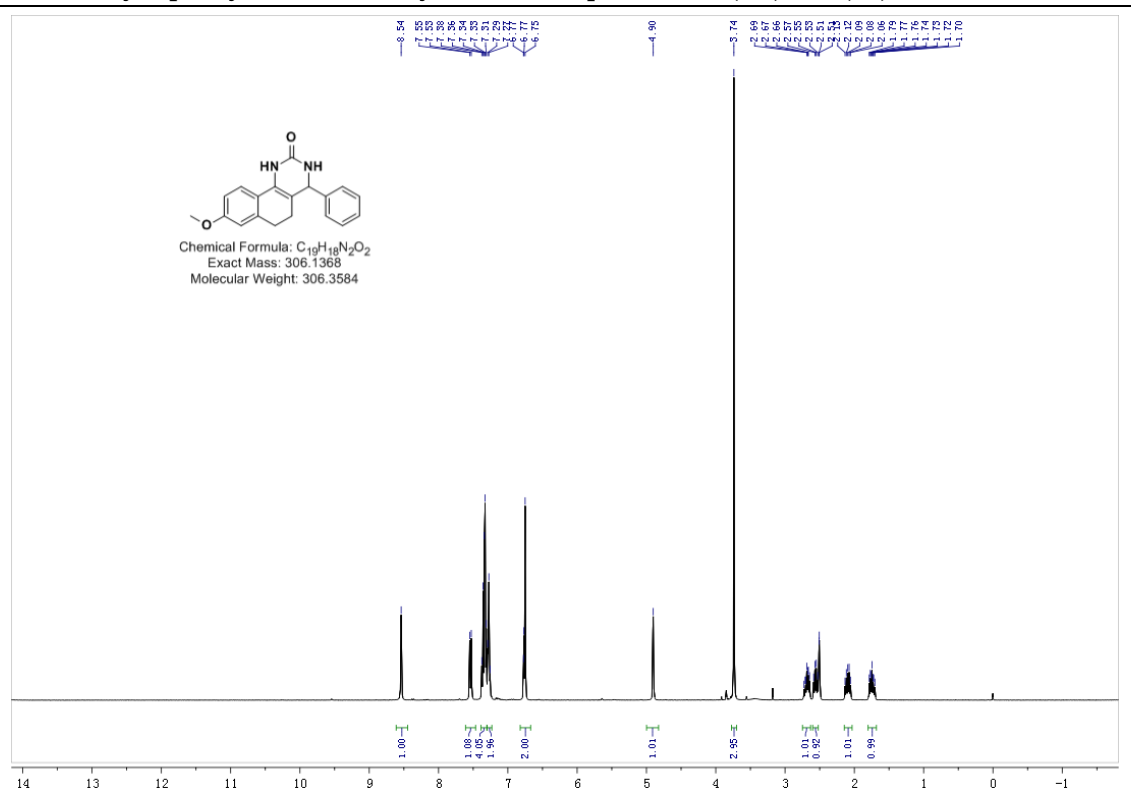
O=C1NC2=CC=CC=C2C3=CC=CC=C3C1C4=CC=C(C=C4)Br

4-(2-bromophenyl)-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one

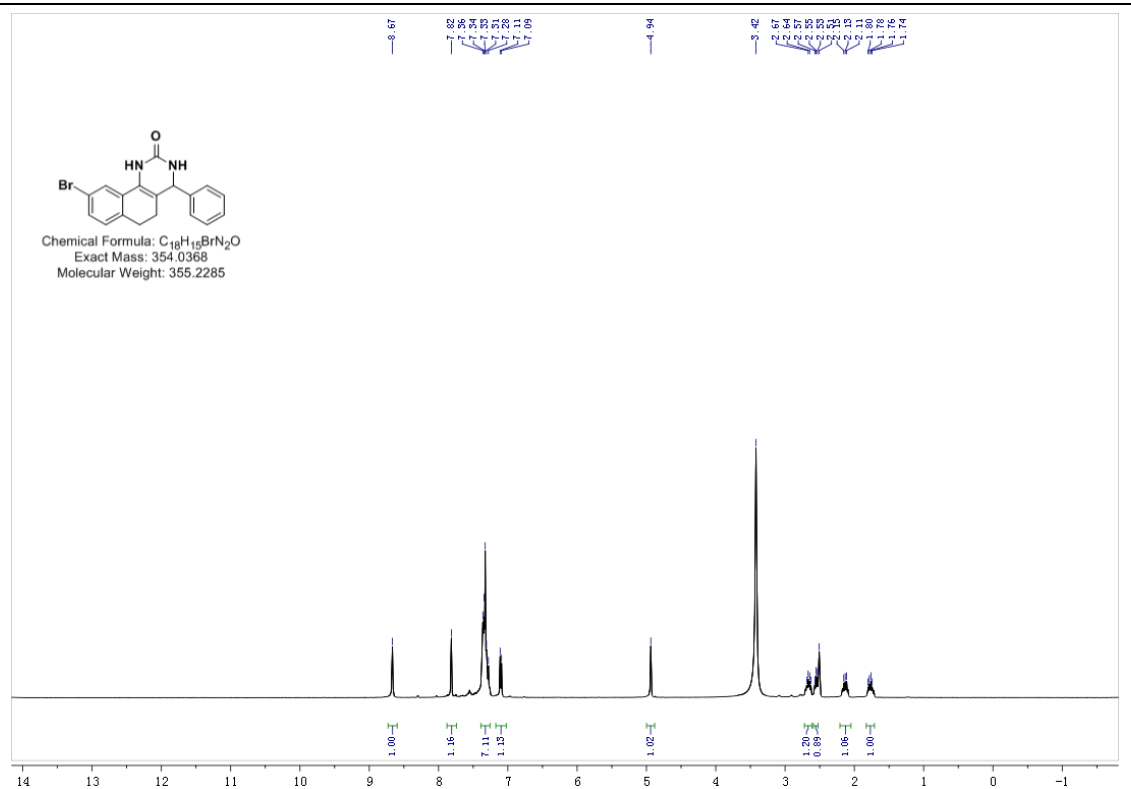
¹H NMR spectrum (CDCl₃) of 4-(2-bromophenyl)-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one. The spectrum shows peaks at 8.25 (s, 1H), 7.5-7.8 (m, 5H), 5.5 (s, 1H), 3.3 (s, 3H), 2.5 (m, 2H), and 1.8 (m, 2H). Integration values are 1.00, 3.97, 1.00, 3.00, 1.00, and 2.01 respectively.



8-methoxy-4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6h)



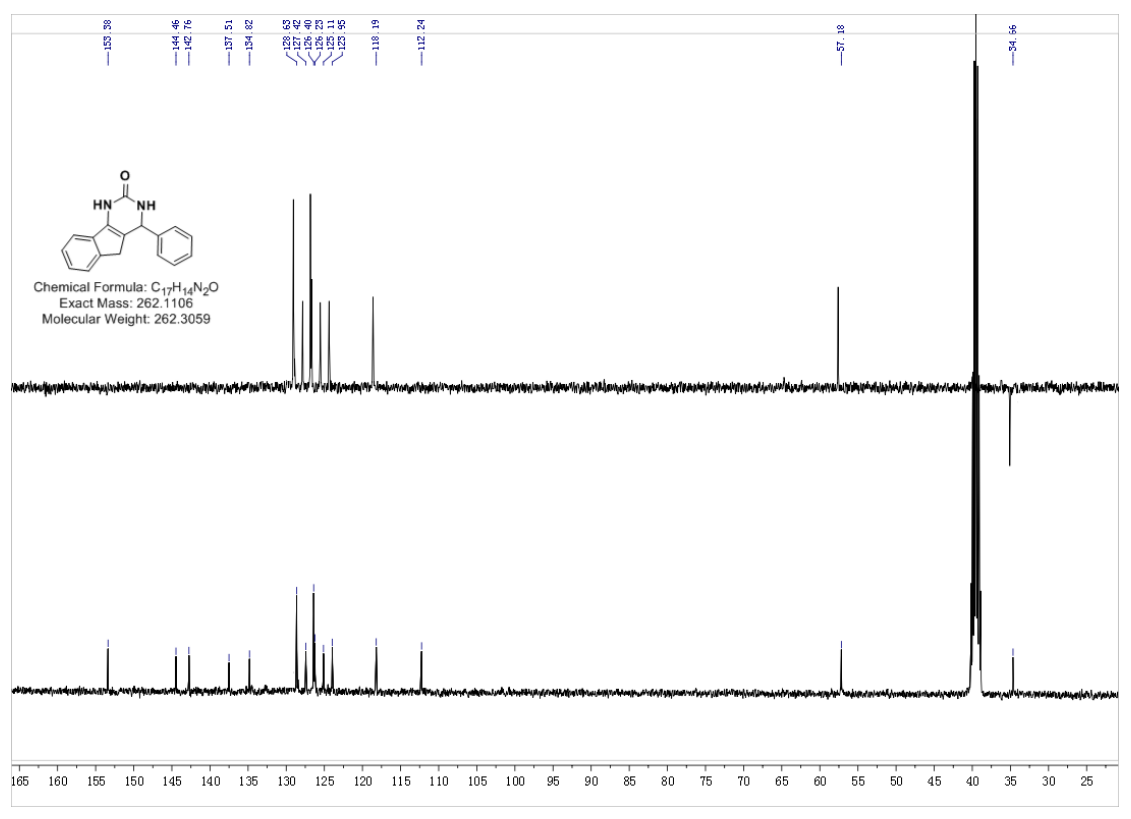
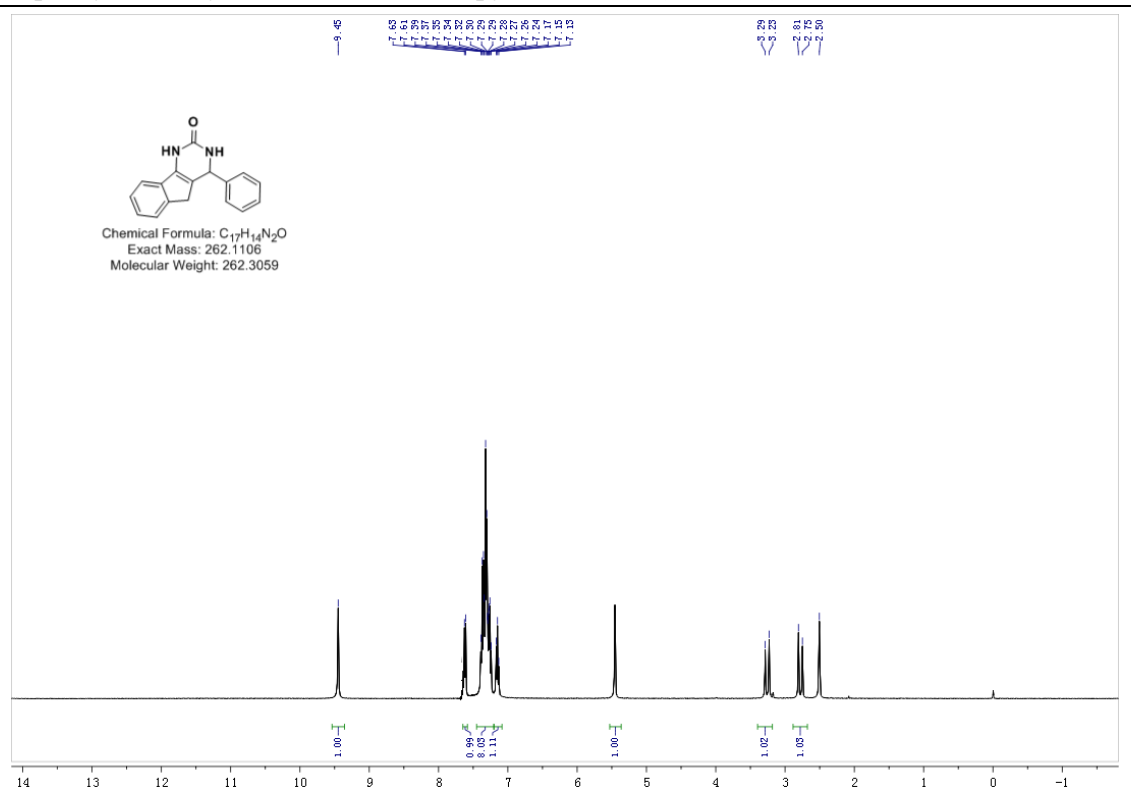
9-bromo-4-phenyl-3,4,5,6-tetrahydrobenzo[h]quinazolin-2(1H)-one (6i)



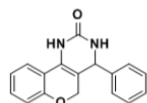
Chemical Formula: C₁₈H₁₅N₃O₃
Exact Mass: 321.1113
Molecular Weight: 321.3300

Chemical Formula: C₁₈H₁₅N₃O₃
Exact Mass: 321.1113
Molecular Weight: 321.3300

4-phenyl-3,4-dihydro-1H-indeno[1,2-d]pyrimidin-2(5H)-one (6k)



4-phenyl-3,4-dihydro-1H-chromeno[4,3-d]pyrimidin-2(5H)-one (6l)



Chemical Formula: $C_{17}H_{14}N_2O_2$
Exact Mass: 278.1055
Molecular Weight: 278.3053

