

Supporting Information

DMAP-catalyzed one-pot synthesis of quinazoline-2,4-diones from 2-aminobenzamides and di-*tert*-butyl dicarbonate

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General Information

The reagents and solvents were obtained from commercial suppliers and used without further purification. TLC was performed on silica gel plates (GF254) with visualization of components by UV light (254 nm). ^1H and ^{13}C NMR spectra were recorded on Varian 400 or 500 MHz NMR spectrometer with $\text{DMSO-}d_6$ as a solvent. Chemical shifts are referenced to the residual solvent peak and reported in ppm (δ scale) and all coupling constant (J) values are given in Hz. The following multiplicity abbreviations are used: (s) singlet, (d) doublet, (t) triplet, (q) quartet, (m) multiplet, and (br) broad. ESI-HRMS data were measured on Thermo Exactive Orbitrap plus spectrometer. Melting points were determined on Yanaco MP-J3 microscope melting point apparatus. All microwave reactions were carried out in single-mode CEM Explorer SP 48.

^1H NMR and ^{13}C NMR Spectra

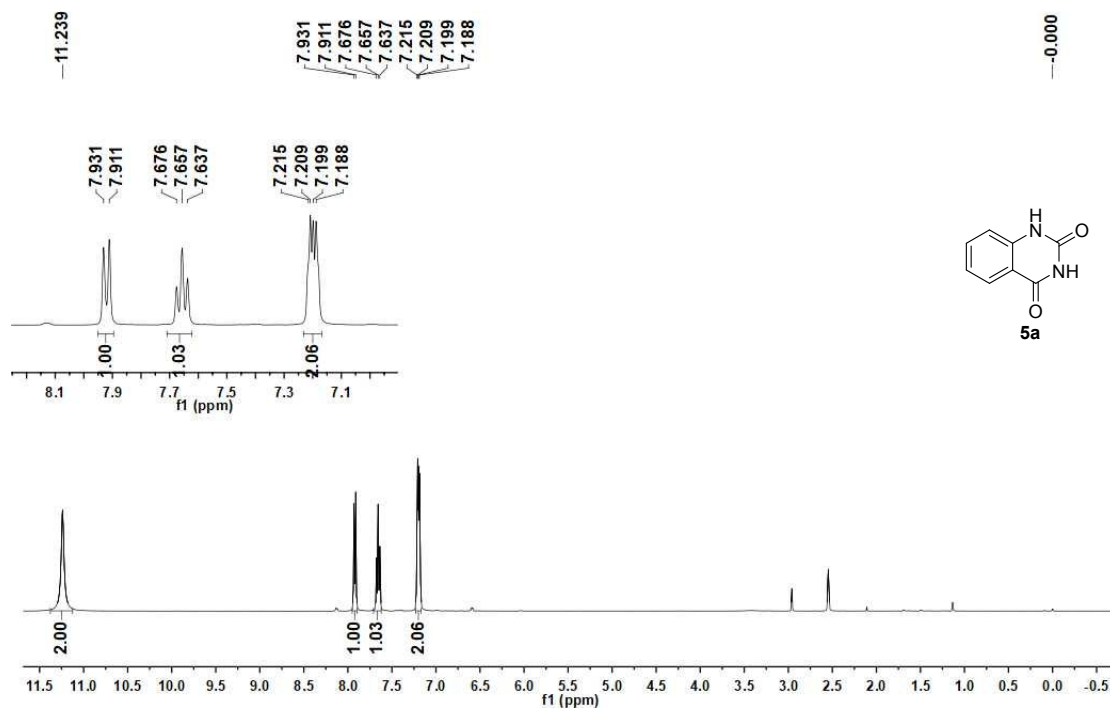


Figure S1. ^1H NMR spectra of quinazoline-2,4(1*H*,3*H*)-dione (**5a**)

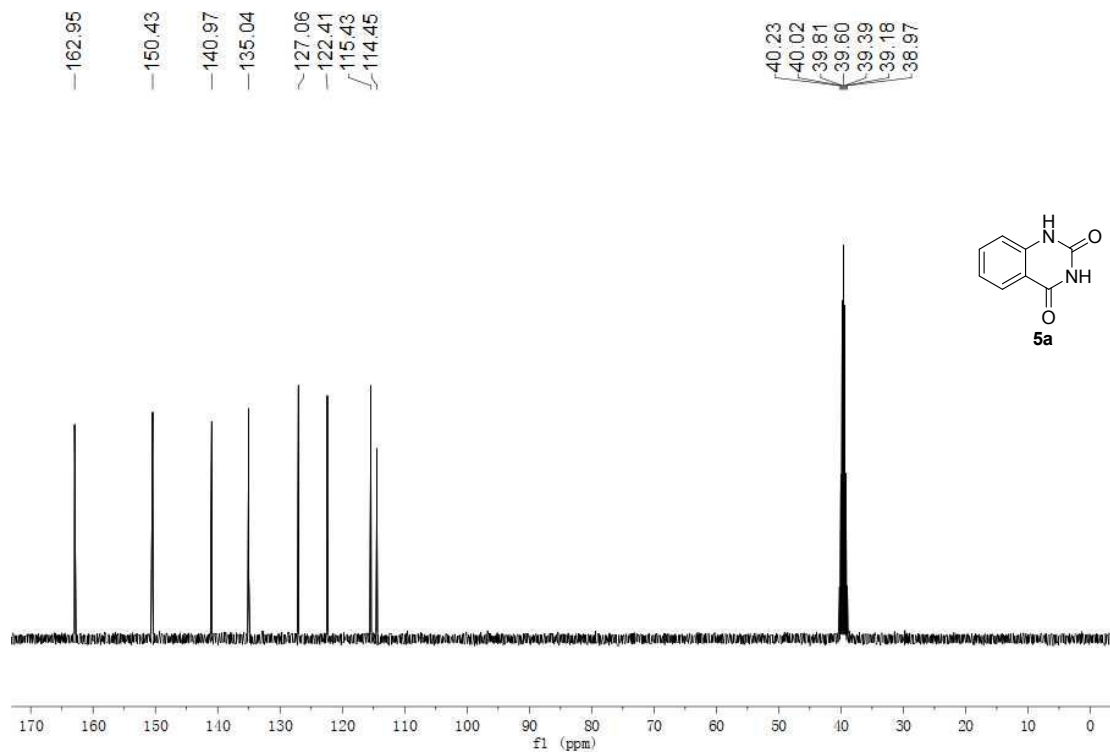


Figure S2. ^{13}C NMR spectra of quinazoline-2,4(1*H*,3*H*)-dione (**5a**)

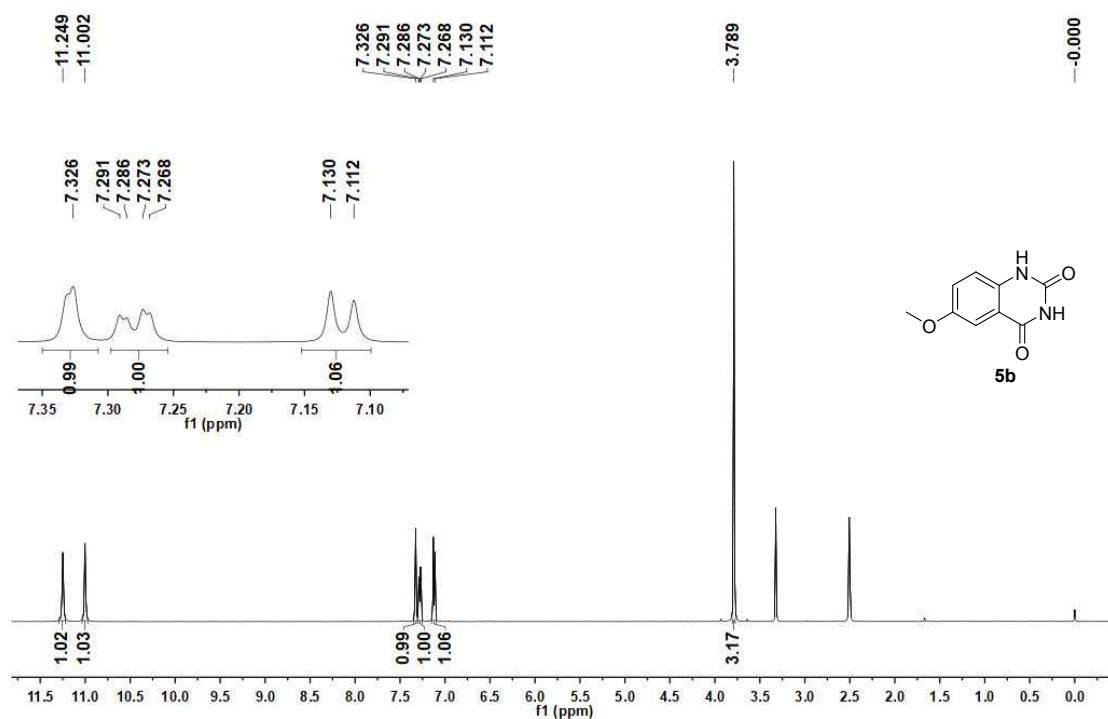


Figure S3. ¹H NMR spectra of 6-methoxyquinazoline-2,4(1*H*,3*H*)-dione (5b)

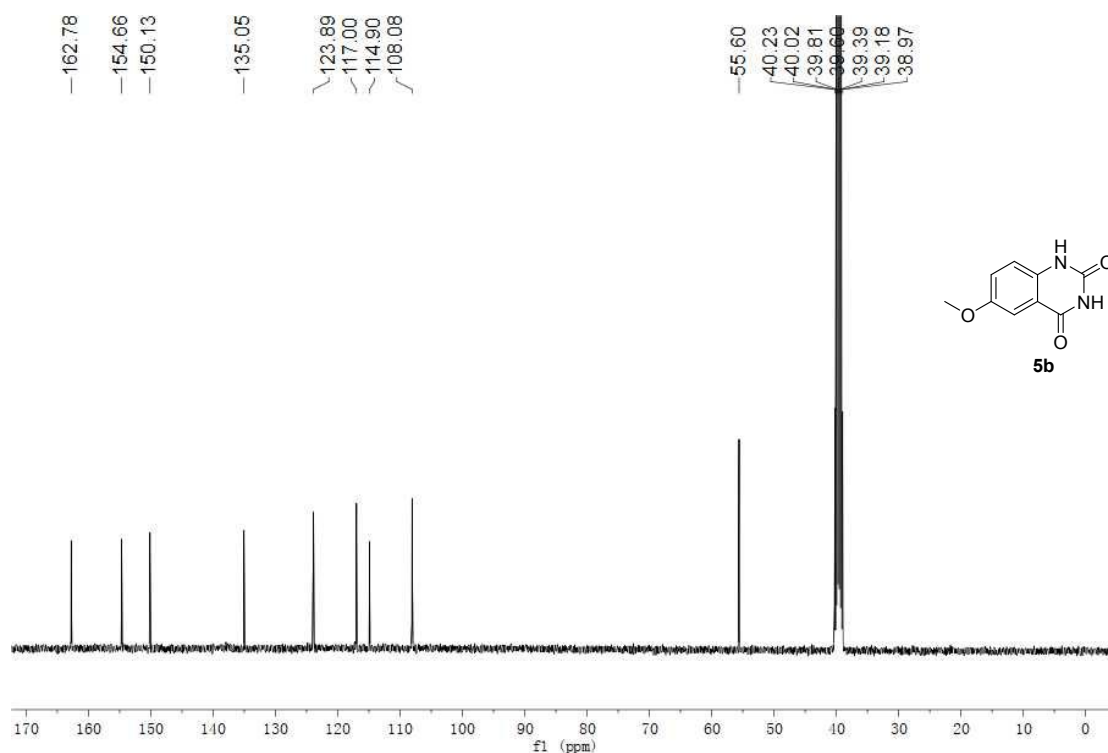


Figure S4. ¹³C NMR spectra of 6-methoxyquinazoline-2,4(1*H*,3*H*)-dione (5b)

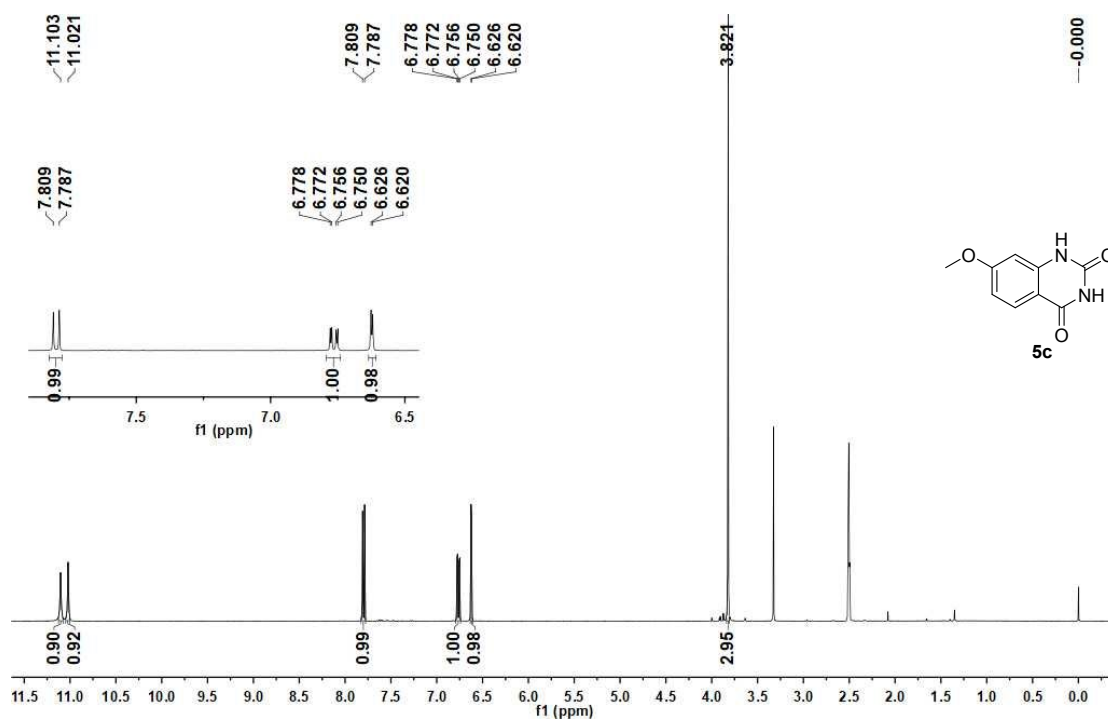


Figure S5. ¹H NMR spectra of 7-methoxyquinazoline-2,4(1*H*,3*H*)-dione (5c)

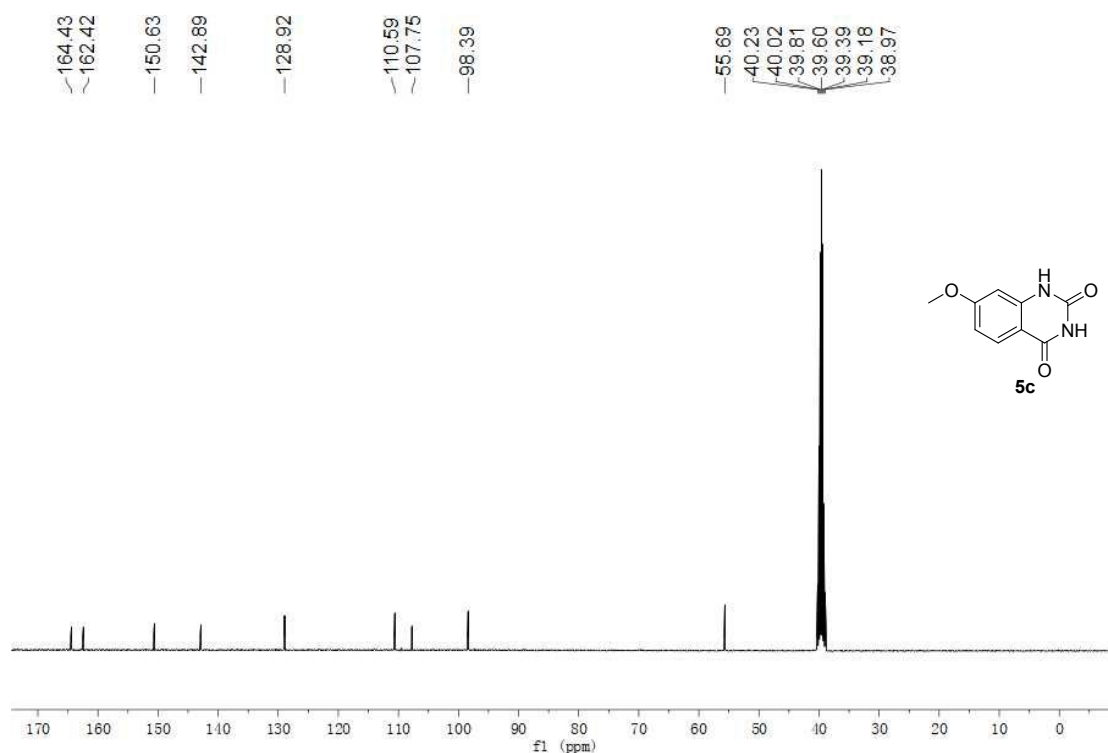


Figure S6. ¹³C NMR spectra of 7-methoxyquinazoline-2,4(1*H*,3*H*)-dione (5c)

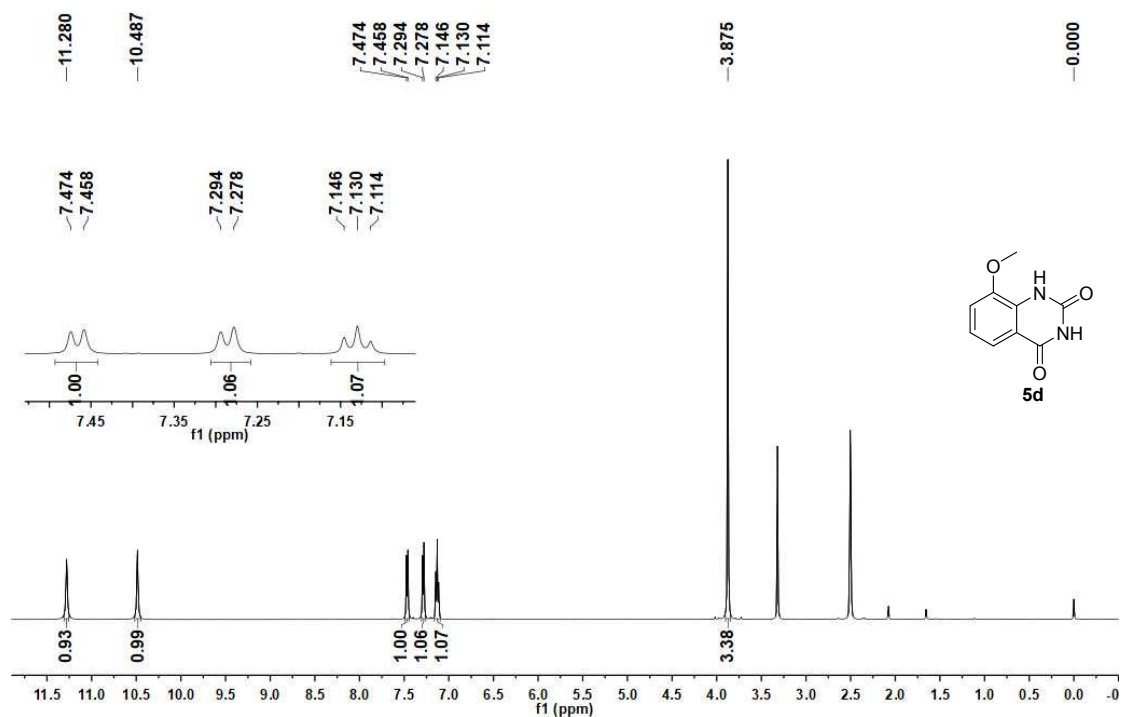


Figure S7. ^1H NMR spectra of 8-methoxyquinazoline-2,4(1H,3H)-dione (5d)

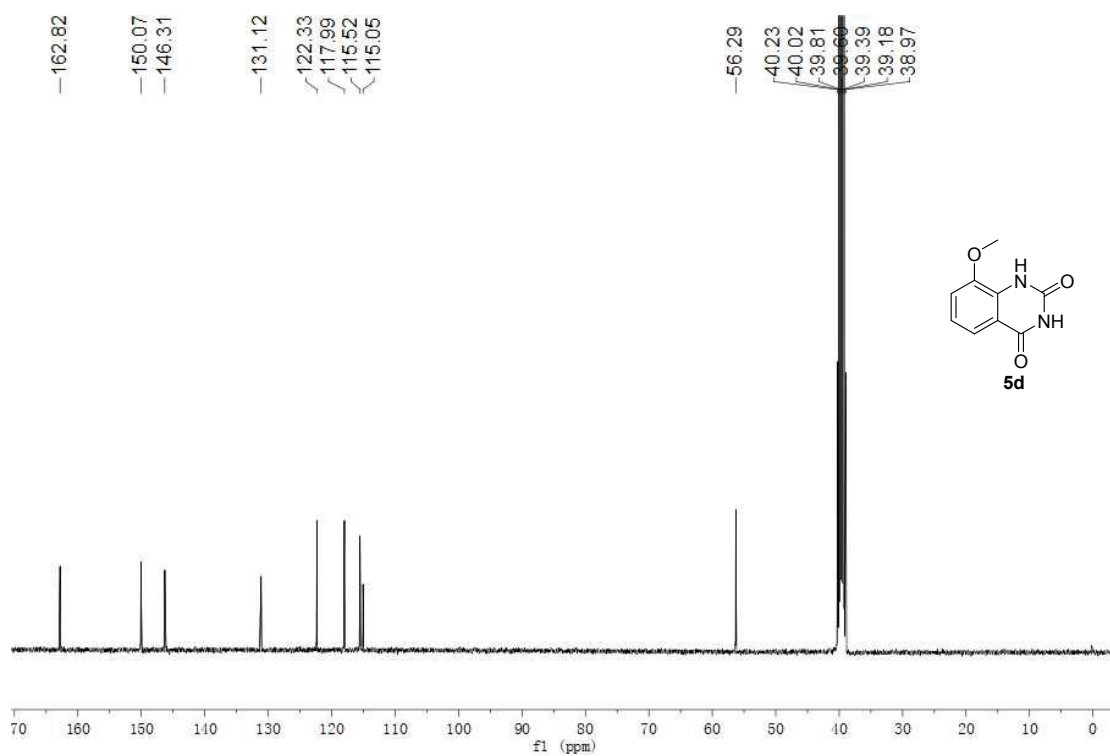


Figure S8. ^{13}C NMR spectra of 8-methoxyquinazoline-2,4(1H,3H)-dione (5d)

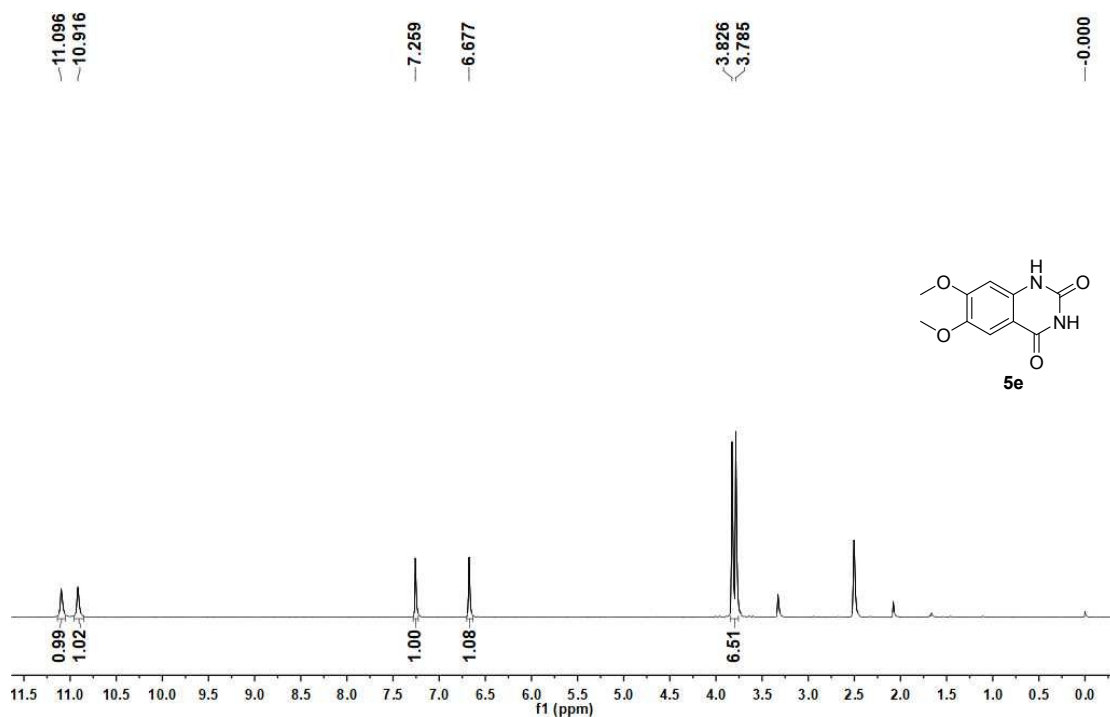


Figure S9. ^1H NMR spectra of 6,7-dimethoxyquinazoline-2,4(1H,3H)-dione (5e)

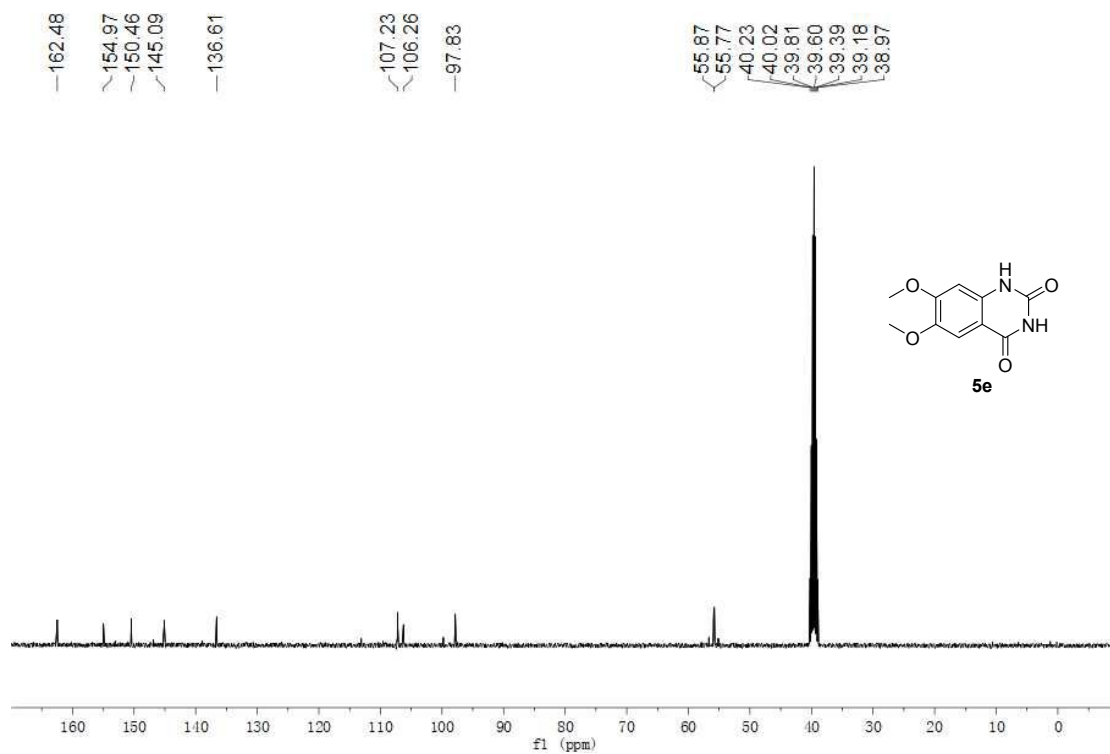


Figure S10. ^{13}C NMR spectra of 6,7-dimethoxyquinazoline-2,4(1H,3H)-dione (5e)

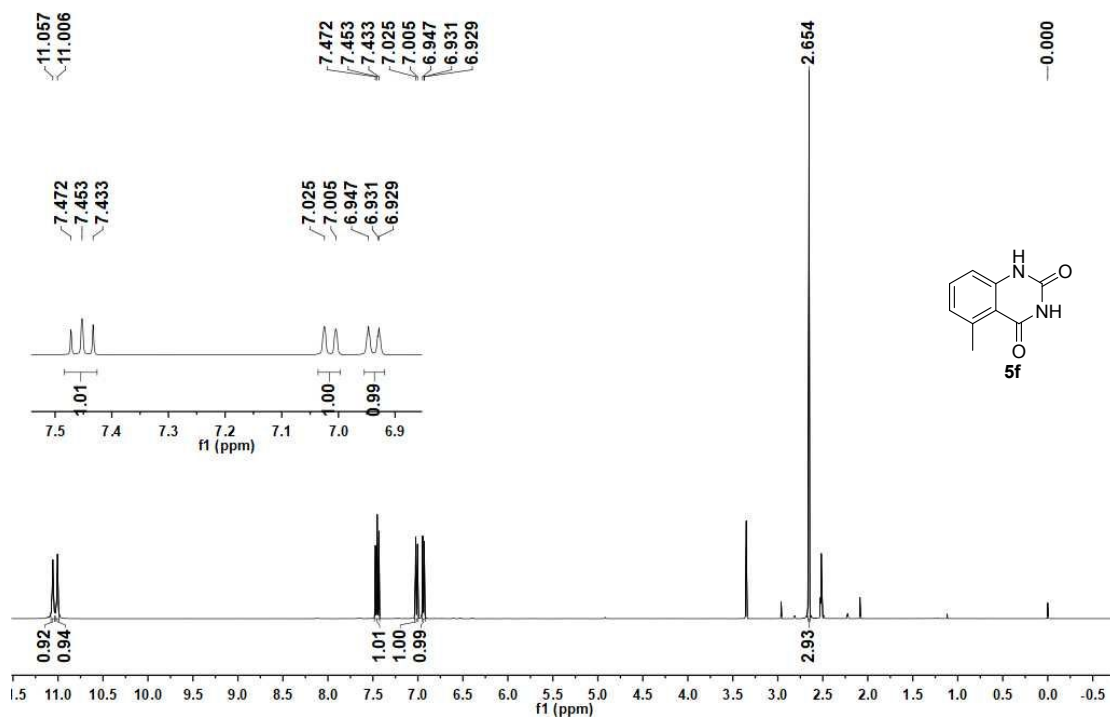


Figure S11. ¹H NMR spectra of 5-methylquinazoline-2,4(1*H*,3*H*)-dione (5f)

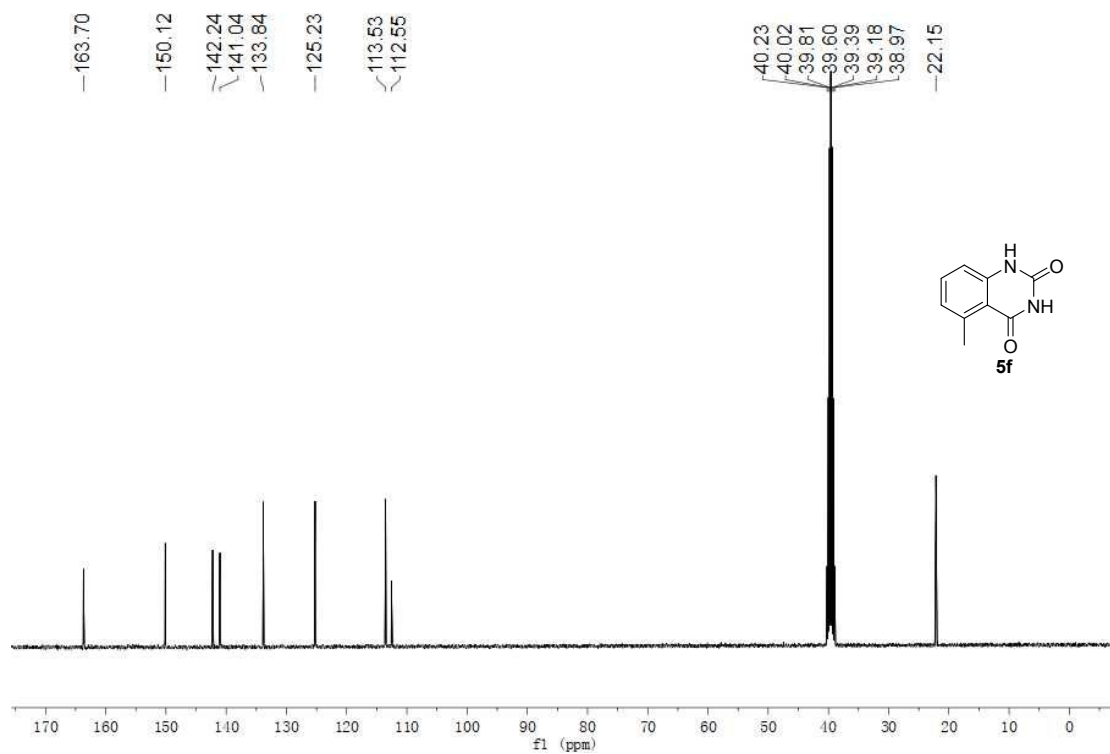


Figure S12. ¹³C NMR spectra of 5-methylquinazoline-2,4(1*H*,3*H*)-dione (5f)

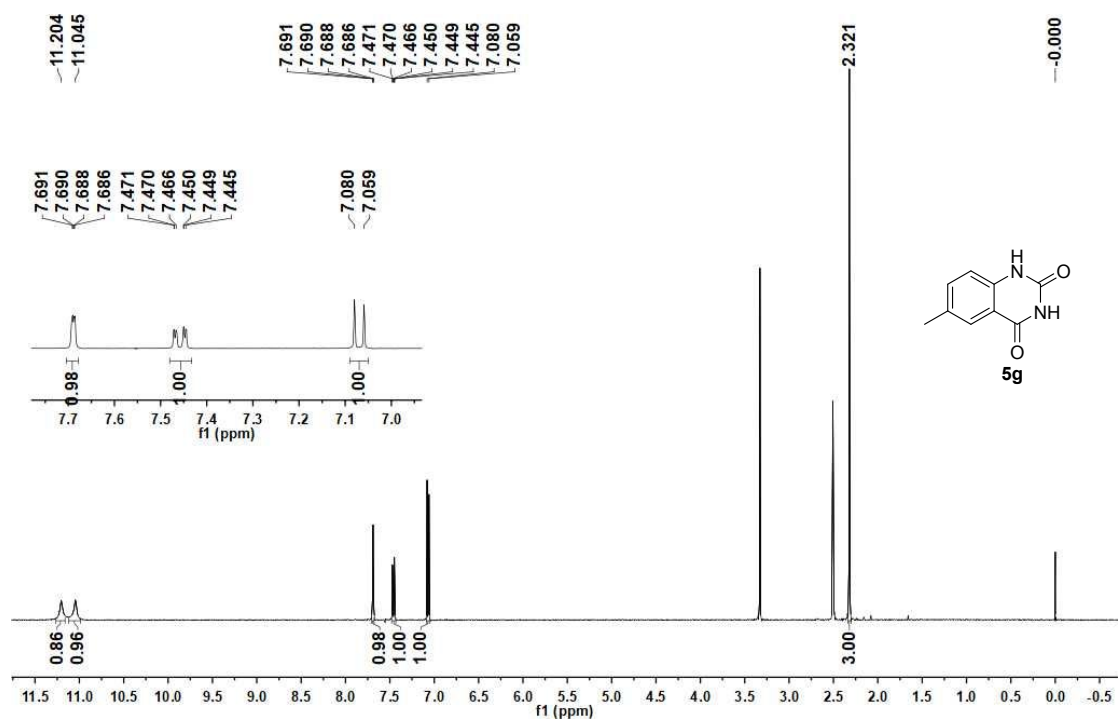


Figure S13. ^1H NMR spectra of 6-methylquinazoline-2,4(1H,3H)-dione (5g)

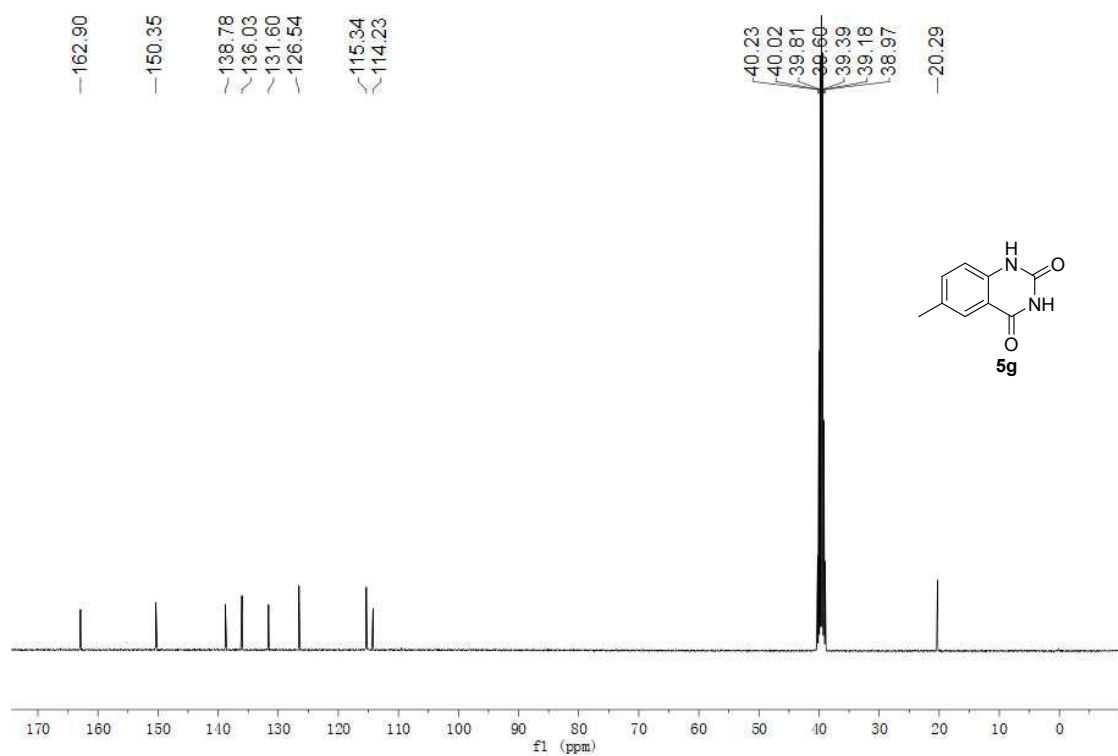


Figure S14. ^{13}C NMR spectra of 6-methylquinazoline-2,4(1H,3H)-dione (5g)

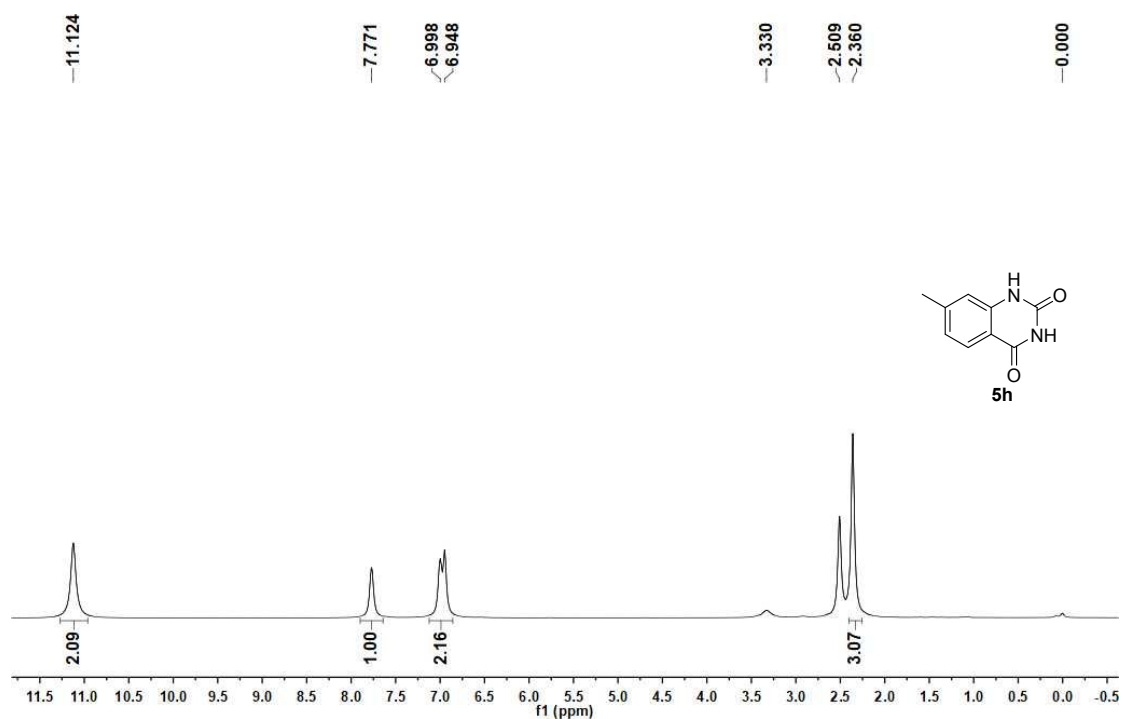


Figure S15. ^1H NMR spectra of 7-methylquinazoline-2,4(1H,3H)-dione (5h)

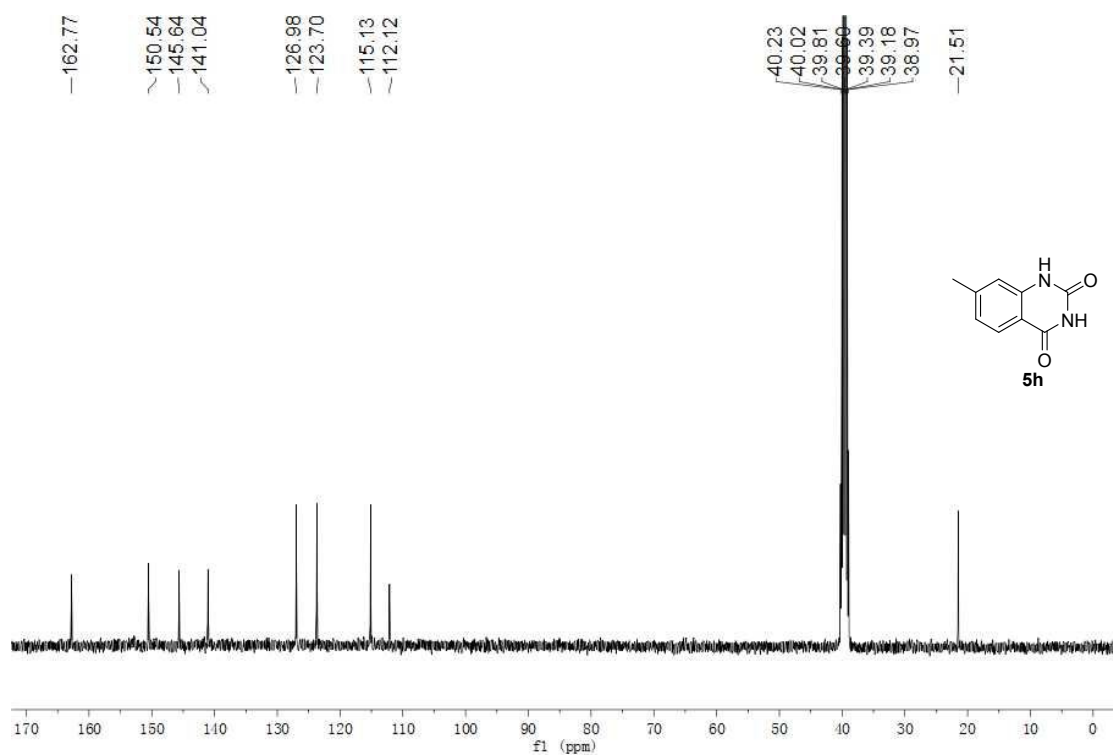


Figure S16. ^{13}C NMR spectra of 7-methylquinazoline-2,4(1H,3H)-dione (5h)

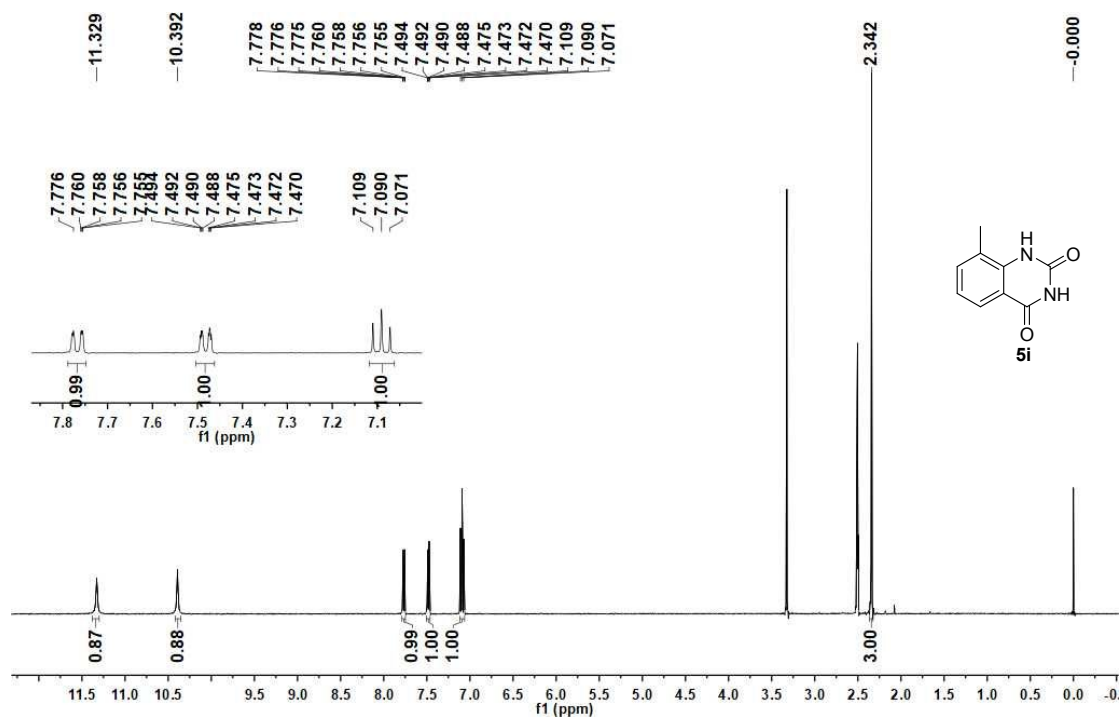


Figure S17. ¹H NMR spectra of 8-methylquinazoline-2,4(1H,3H)-dione (5i)

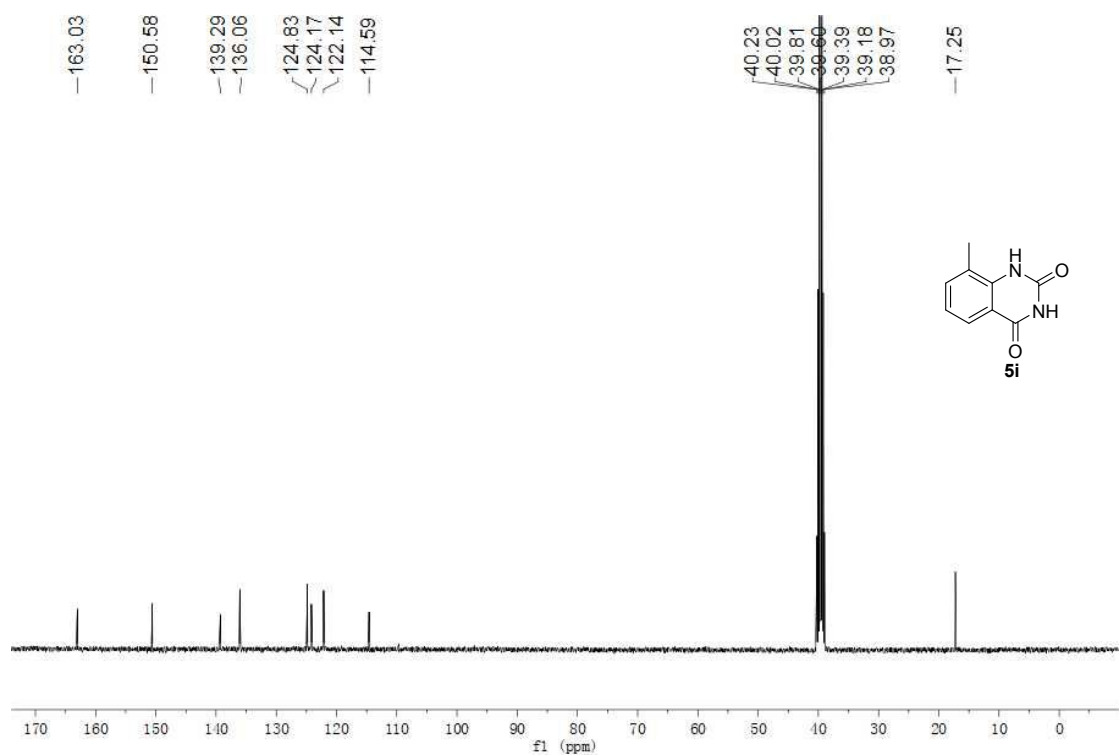


Figure S18. ¹³C NMR spectra of 8-methylquinazoline-2,4(1H,3H)-dione (5i)

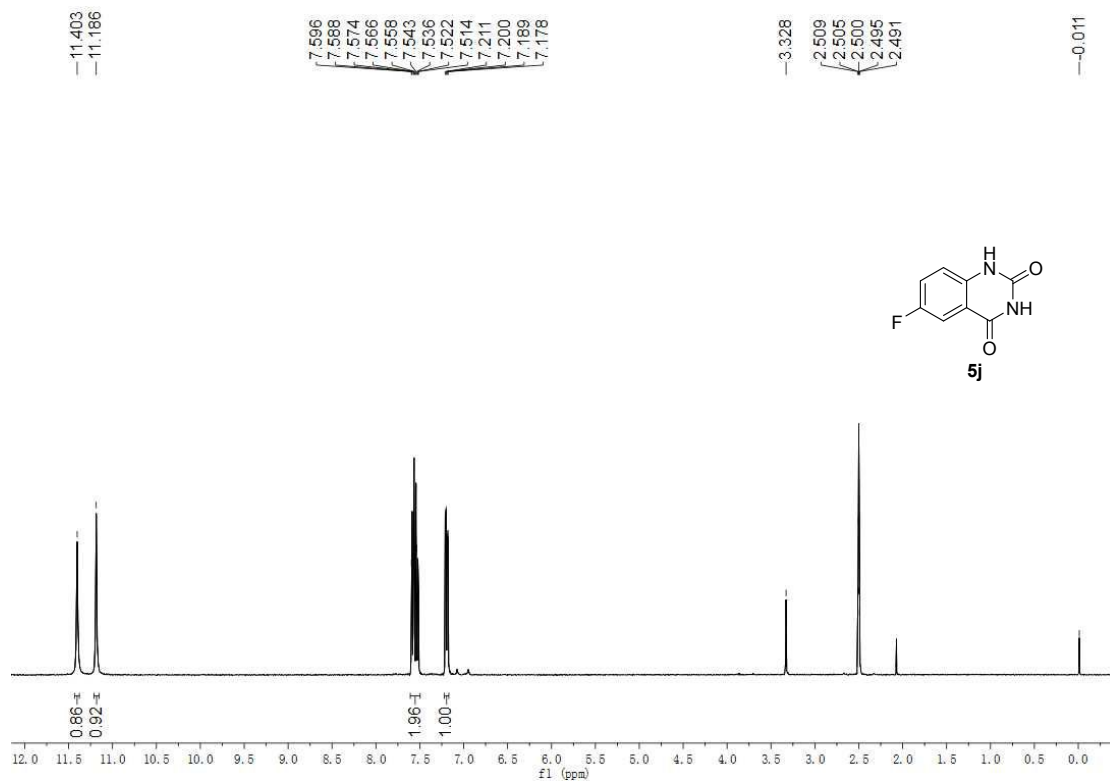


Figure S19. ^1H NMR spectra of 6-fluoroquinazoline-2,4(1H,3H)-dione (5j)

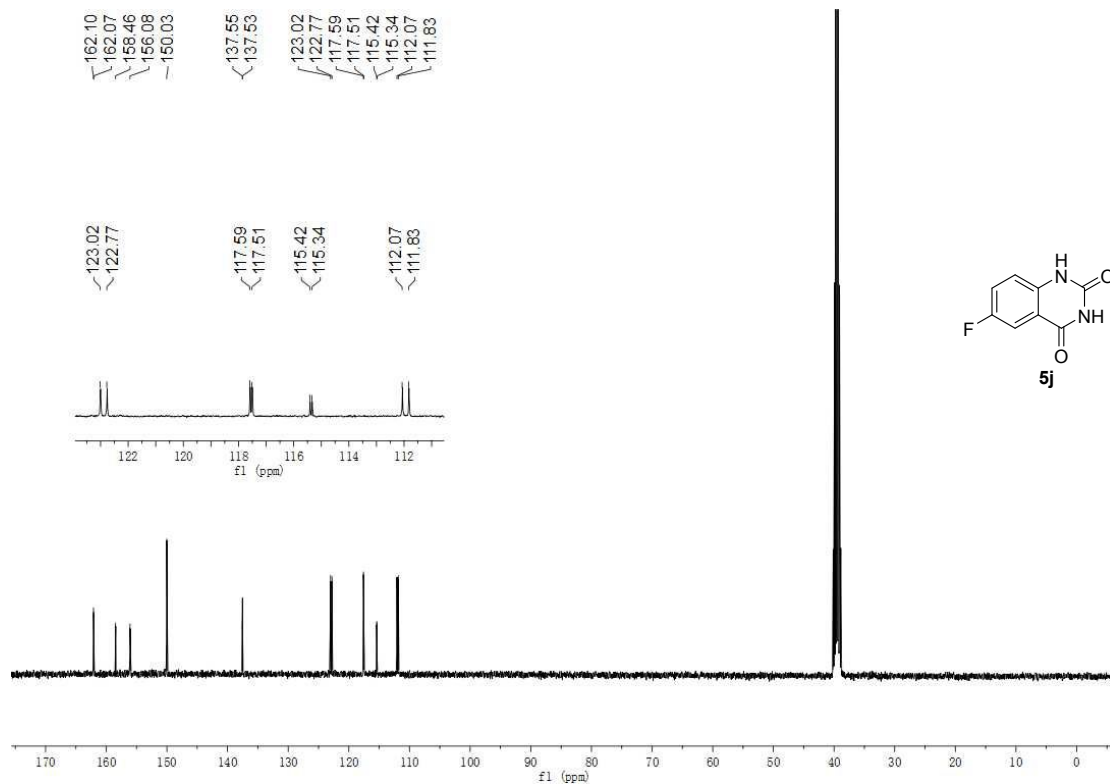


Figure S20. ^{13}C NMR spectra of 6-fluoroquinazoline-2,4(1H,3H)-dione (5j)

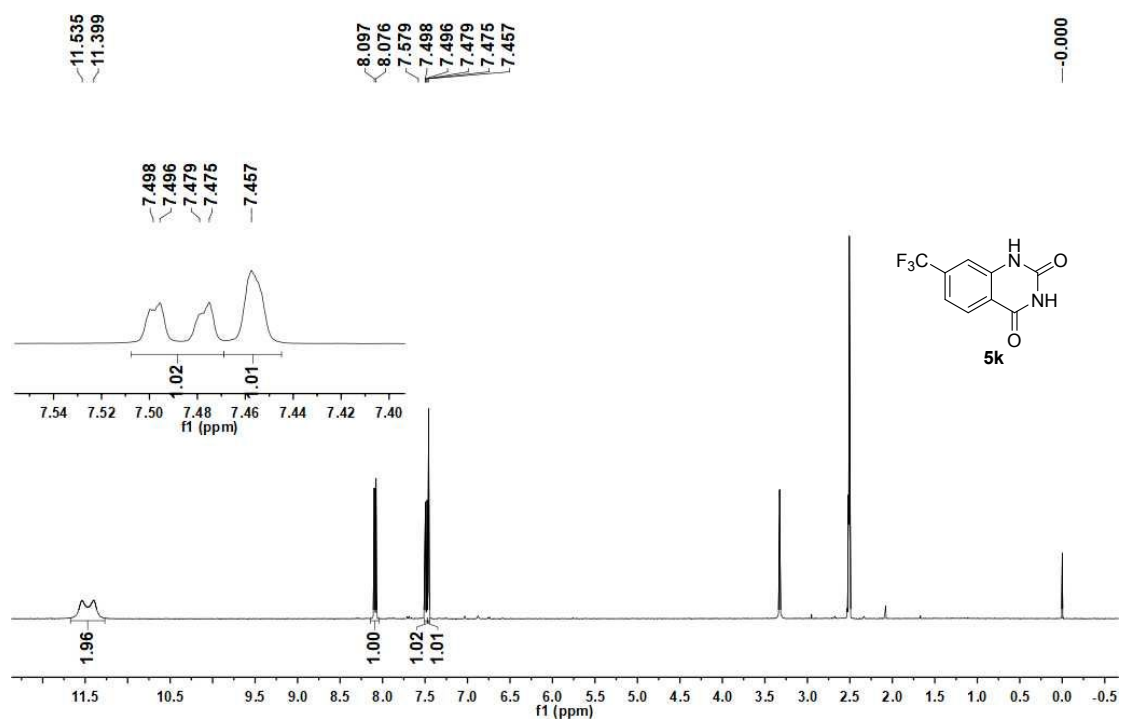


Figure S21. ^1H NMR spectra of 7-(trifluoromethyl)quinazoline-2,4(1H,3H)-dione (5k)

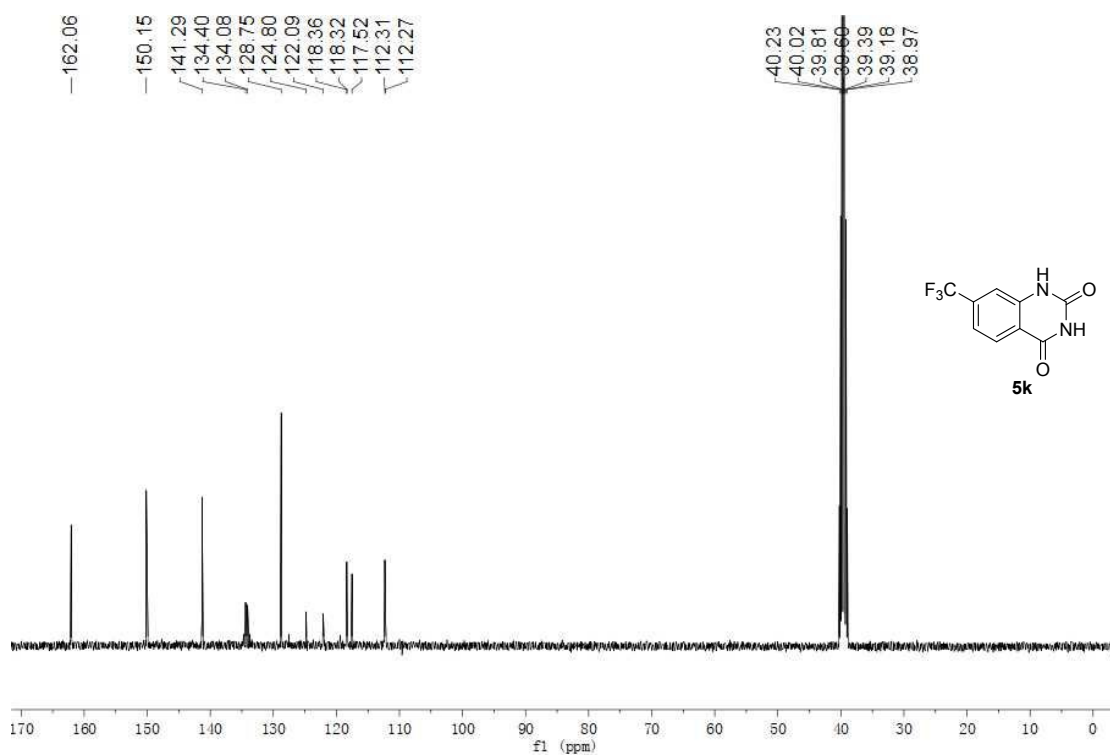


Figure S22. ^{13}C NMR spectra of 7-(trifluoromethyl)quinazoline-2,4(1H,3H)-dione (5k)

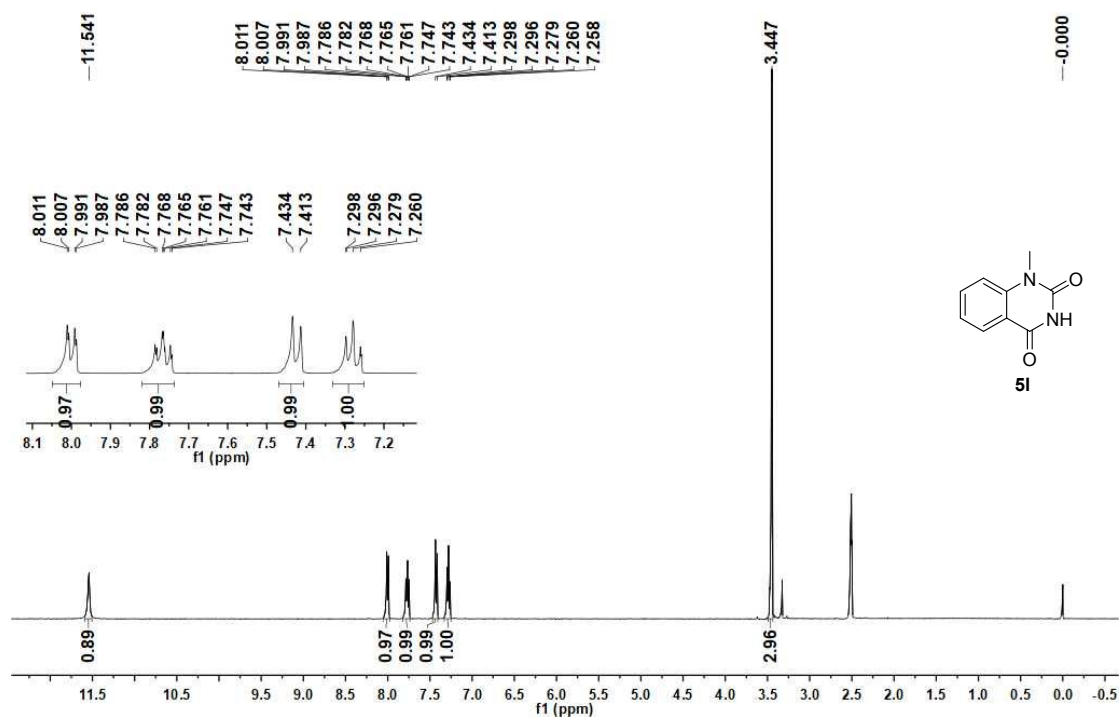


Figure S23. ¹H NMR spectra of 1-methylquinazoline-2,4(1H,3H)-dione (5I)

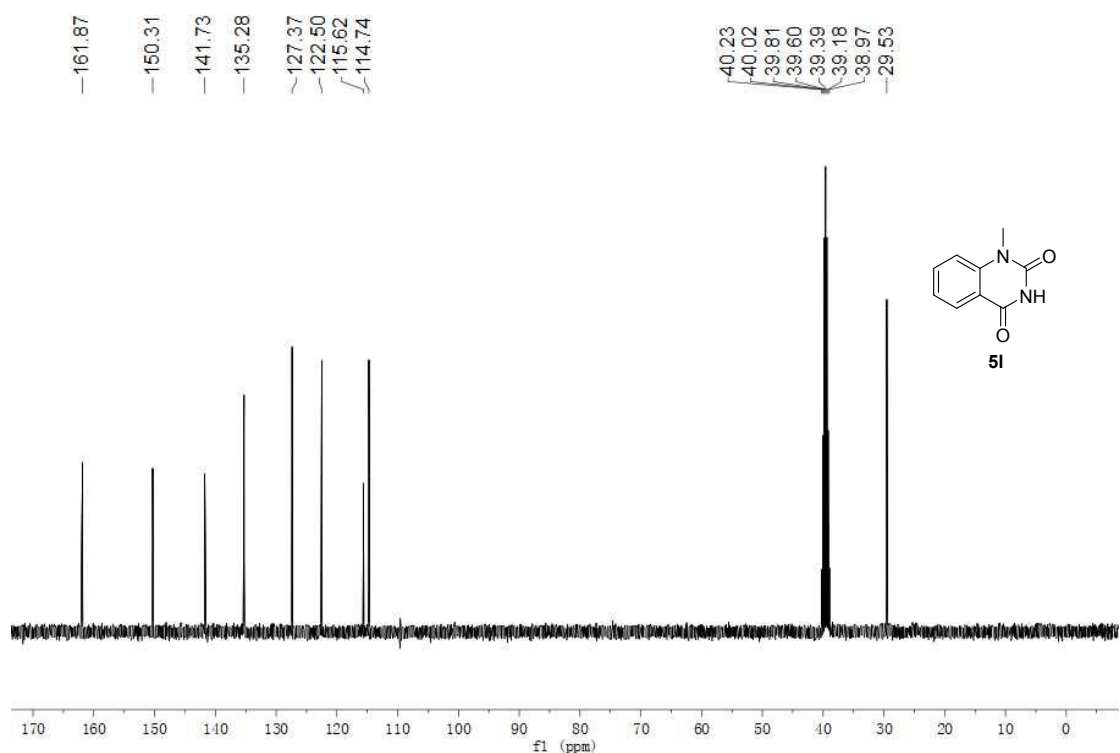


Figure S24 ¹³C NMR spectra of 1-methylquinazoline-2,4(1H,3H)-dione (5I)

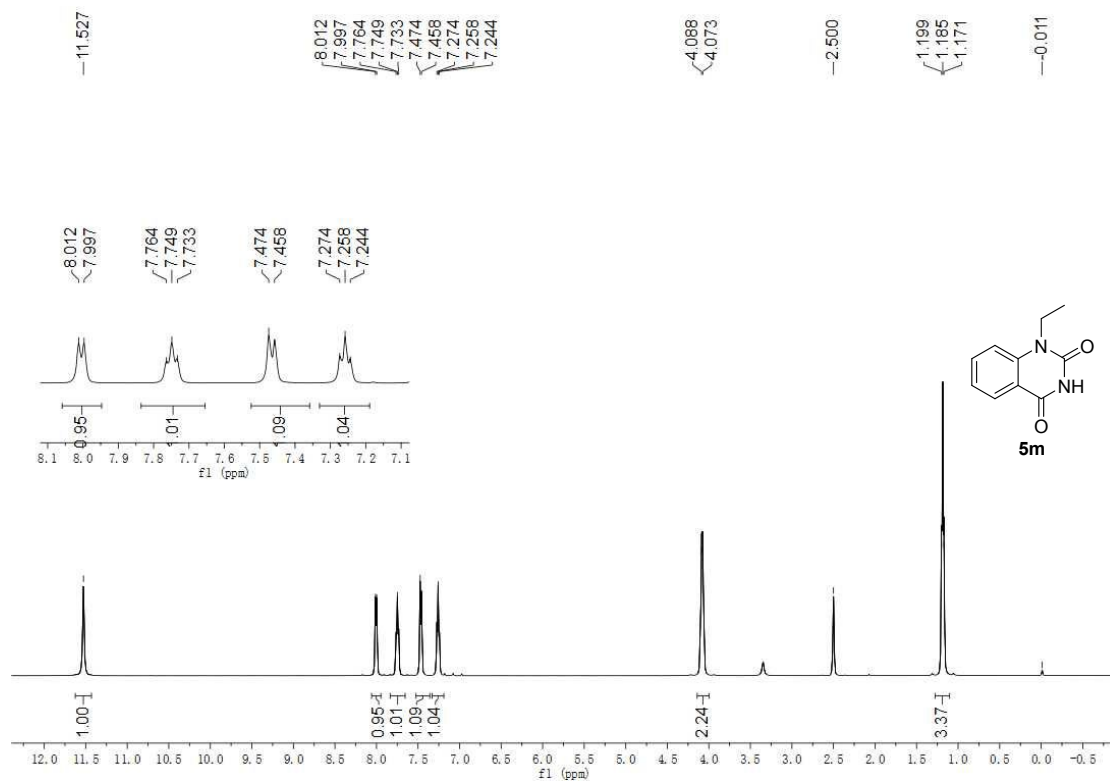


Figure S25. ^1H NMR spectra of 1-ethylquinazoline-2,4(1H,3H)-dione (5m)

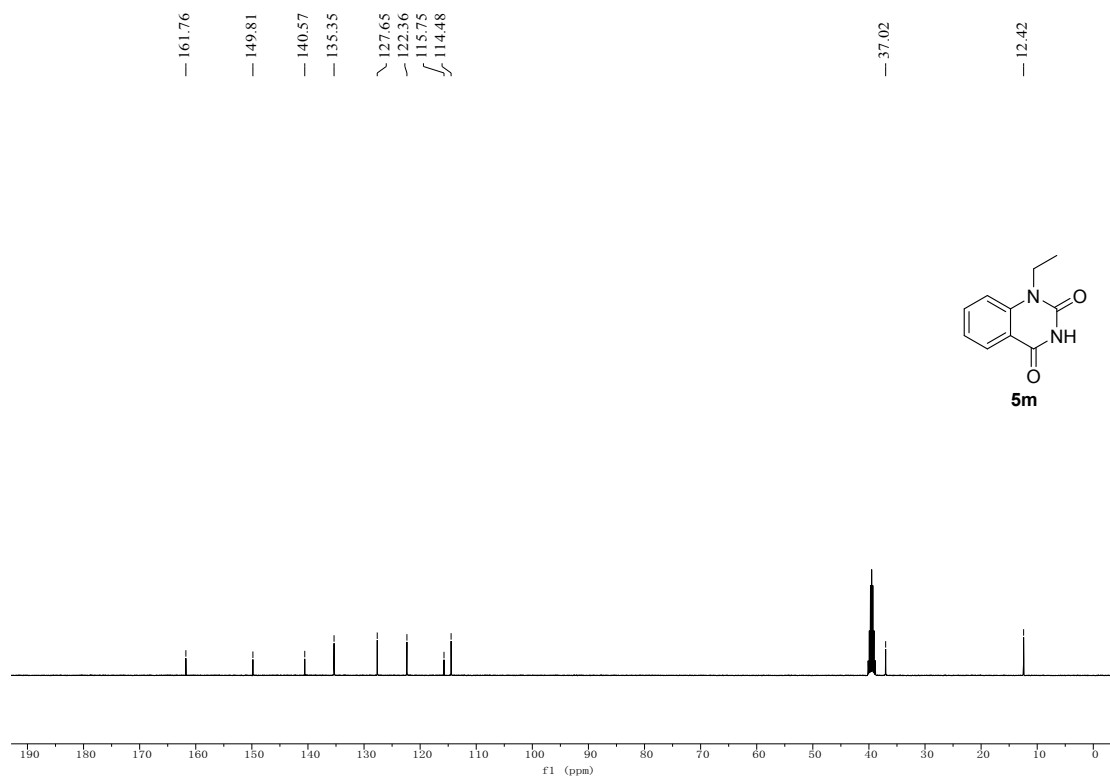


Figure S26. ^{13}C NMR spectra of 1-ethylquinazoline-2,4(1H,3H)-dione (5m)

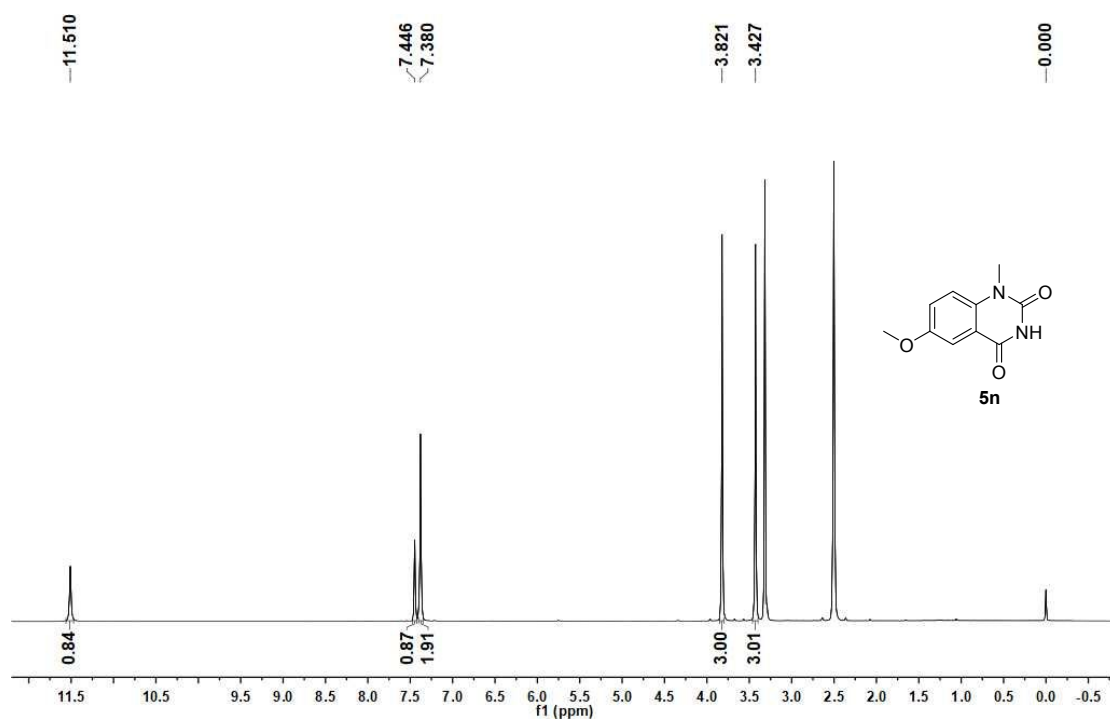


Figure S27. ^1H NMR spectra of 6-methoxy-1-methylquinazoline-2,4(1H,3H)-dione (5n)

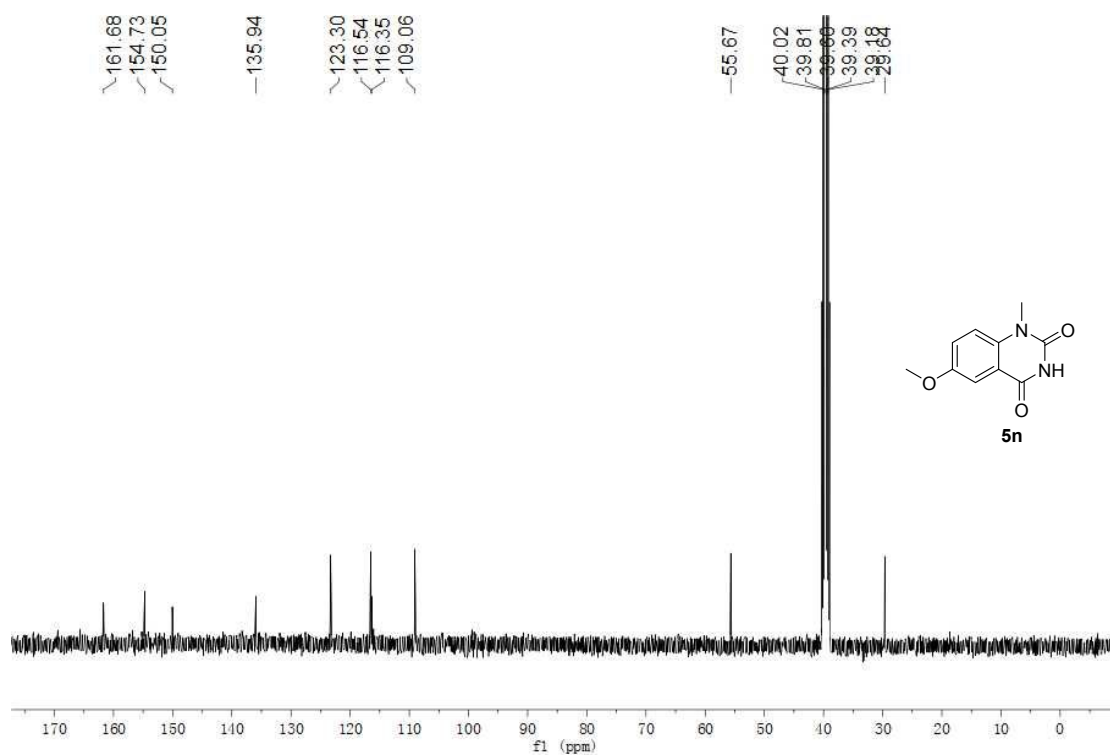


Figure S28. ^{13}C NMR spectra of 6-methoxy-1-methylquinazoline-2,4(1H,3H)-dione (5n)

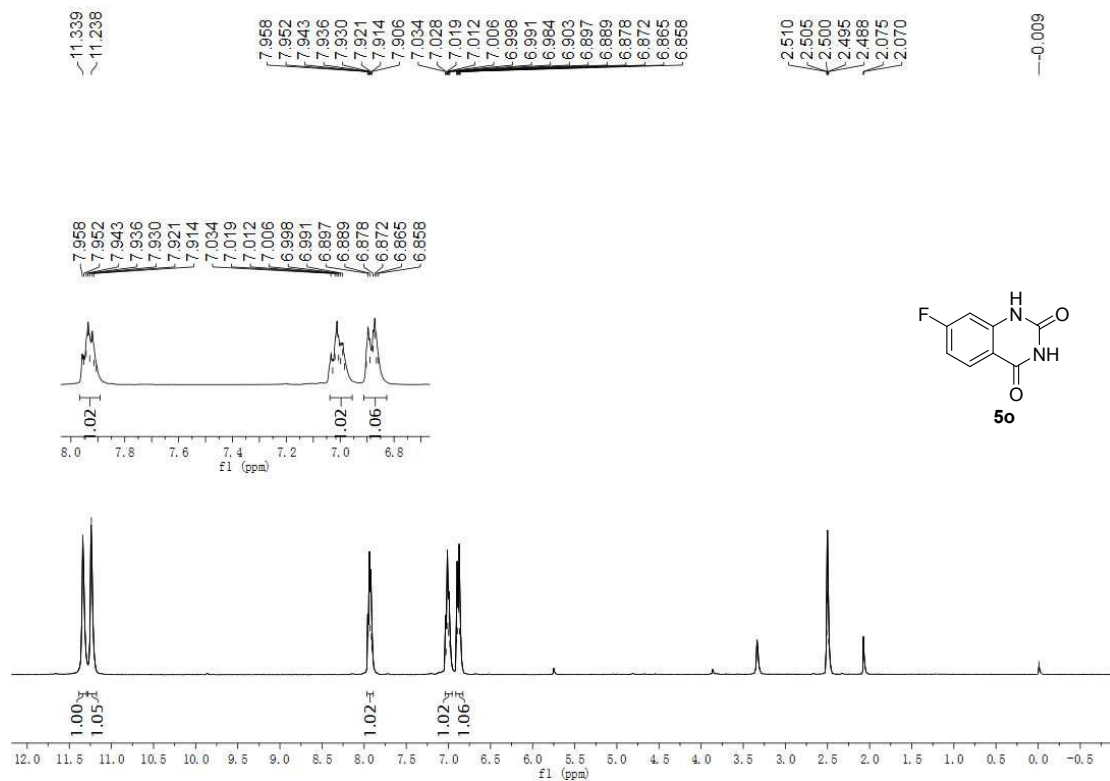


Figure S29. ¹H NMR spectra of 7-fluoroquinazoline-2,4(1H,3H)-dione (5o)

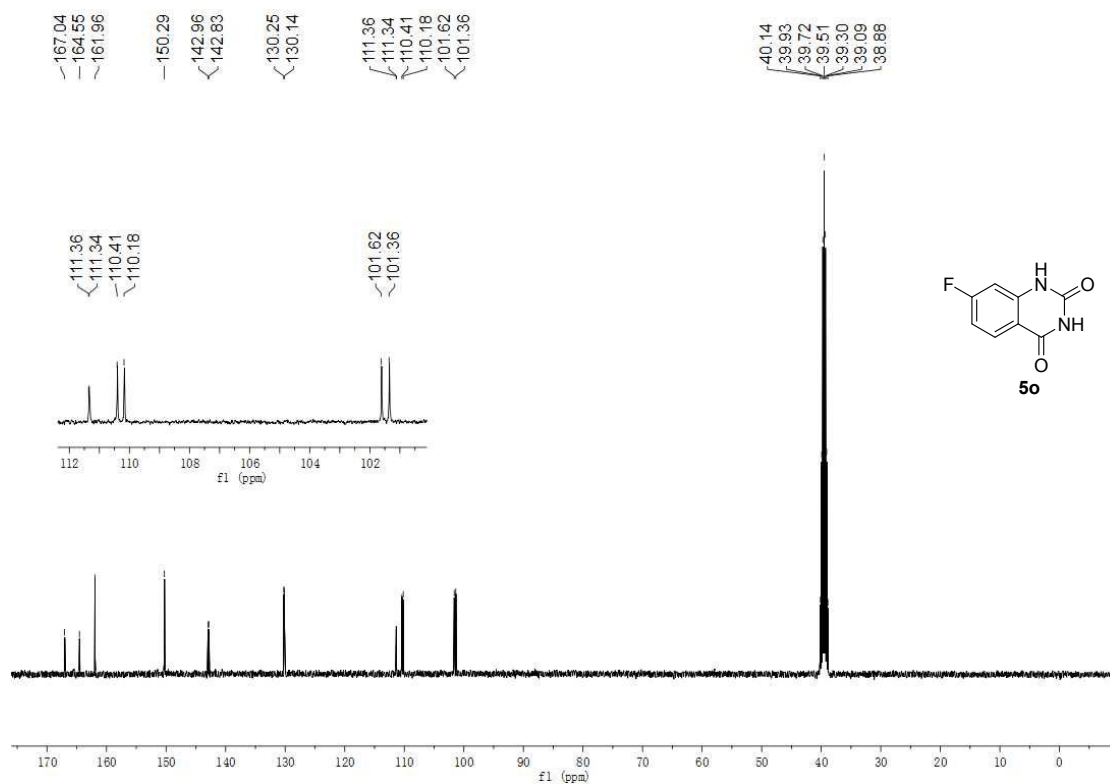


Figure S30. ¹³C NMR spectra of 7-fluoroquinazoline-2,4(1H,3H)-dione (5o)

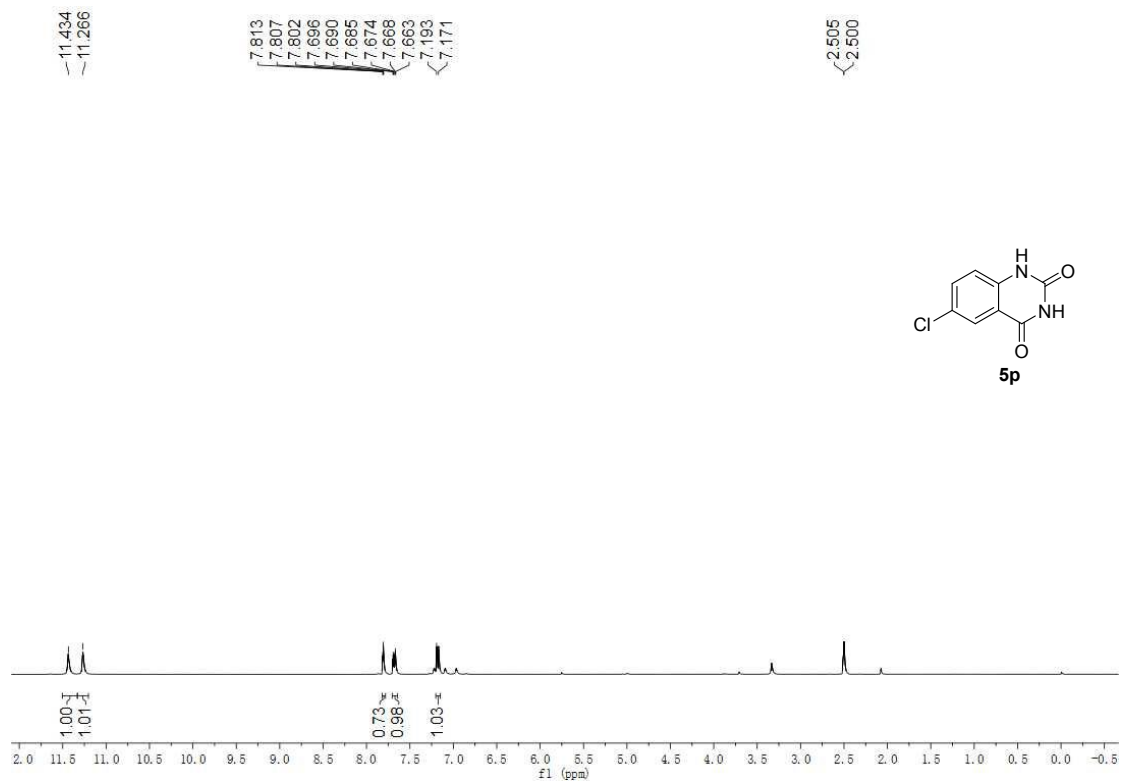


Figure S31. ¹H NMR spectra of 6-chloroquinazoline-2,4(1H,3H)-dione (5p)

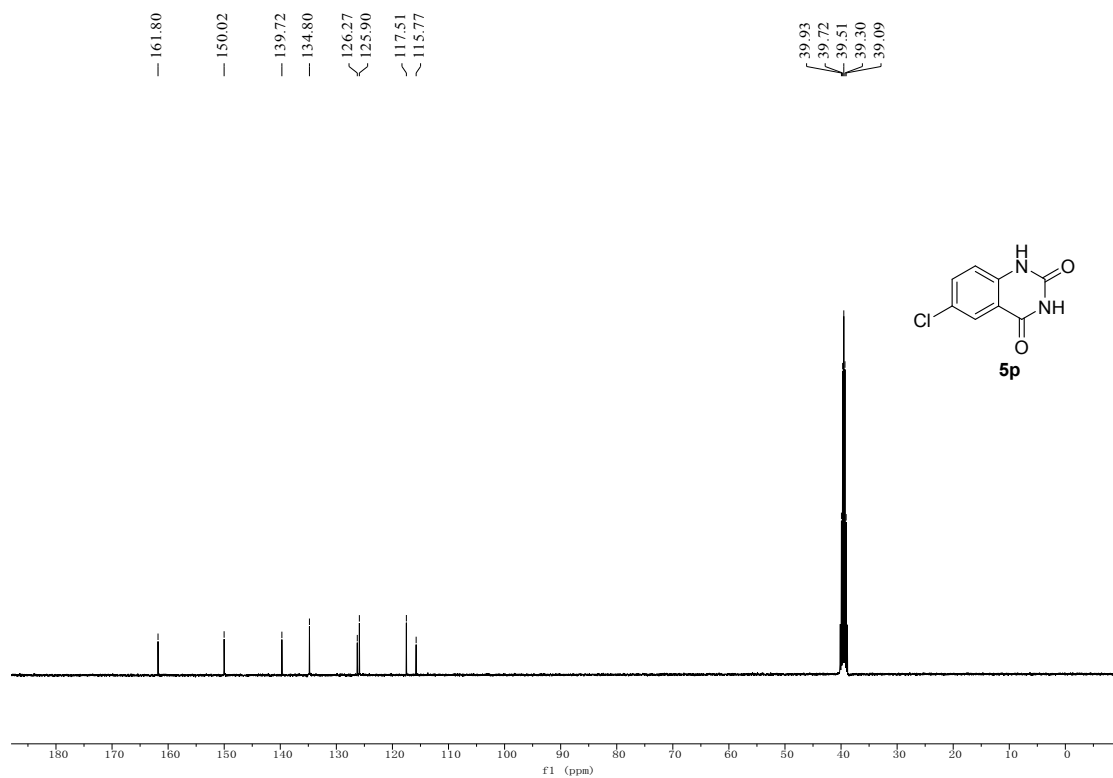


Figure S32. ¹³C NMR spectra of 6-chloroquinazoline-2,4(1H,3H)-dione (5p)

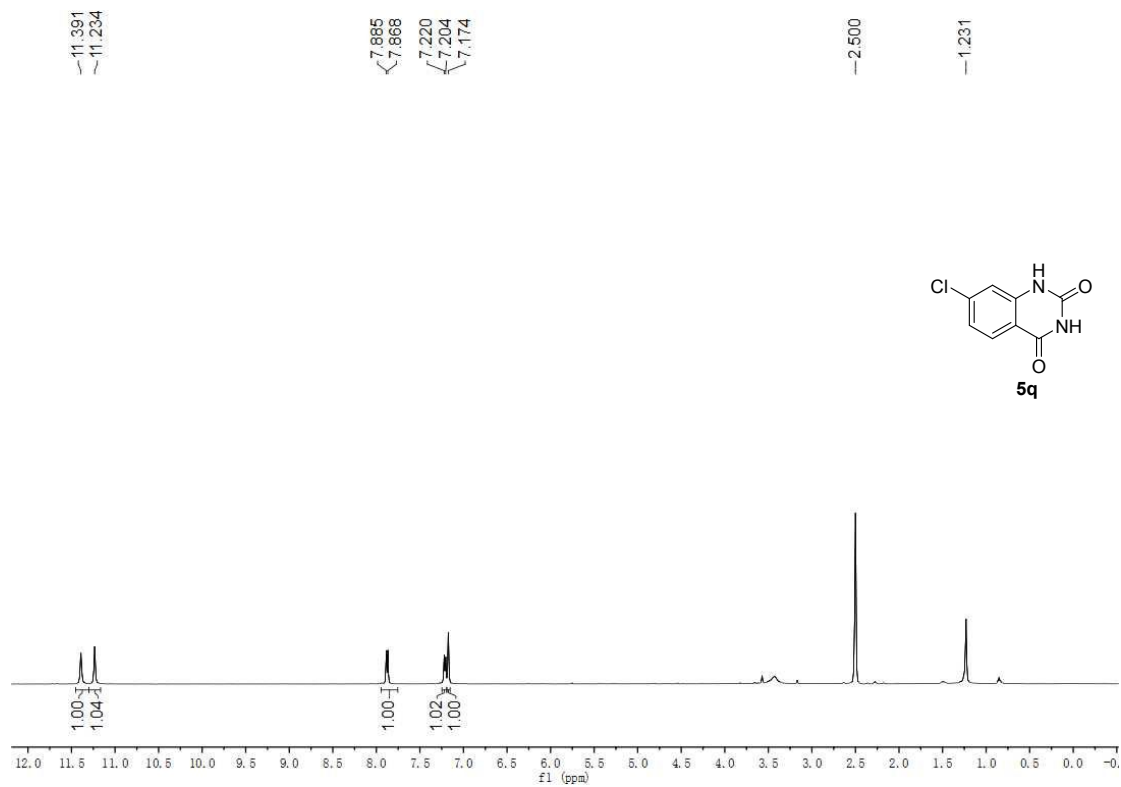


Figure S33. ¹H NMR spectra of 7-chloroquinazoline-2,4(1H,3H)-dione (5q)

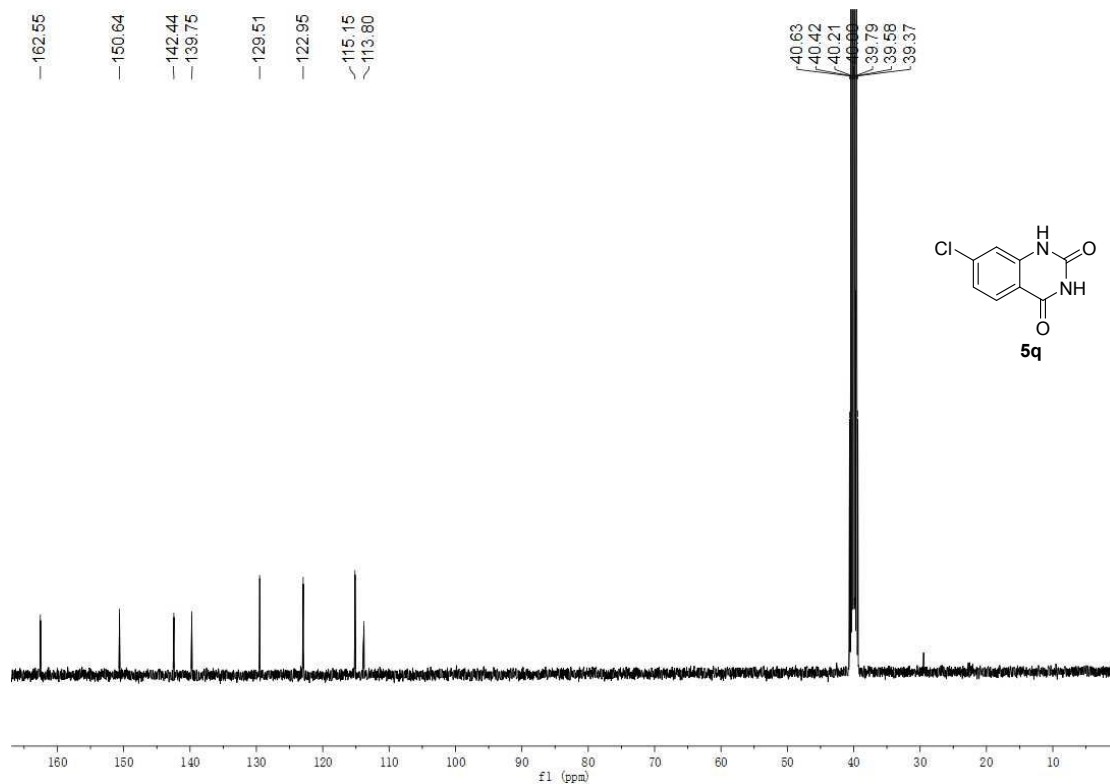


Figure S34. ¹³C NMR spectra of 7-chloroquinazoline-2,4(1H,3H)-dione (5q)

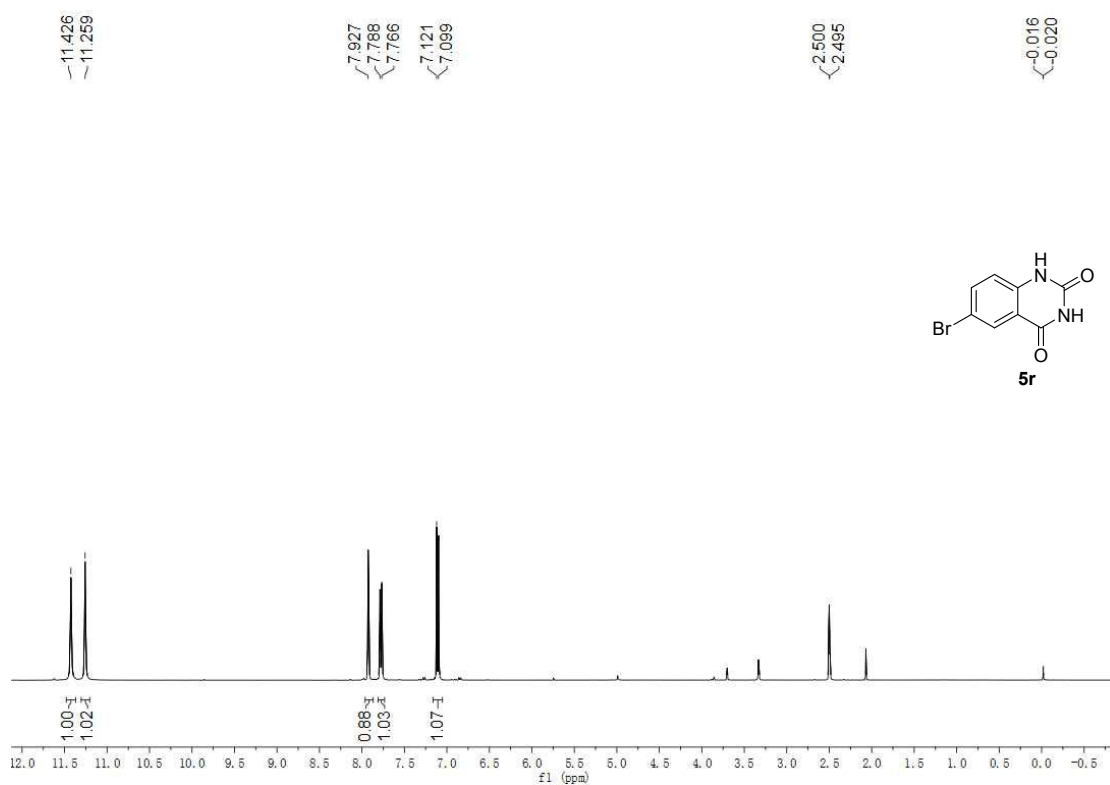


Figure S35. ^1H NMR spectra of 6-bromoquinazoline-2,4(1*H*,3*H*)-dione (5r)

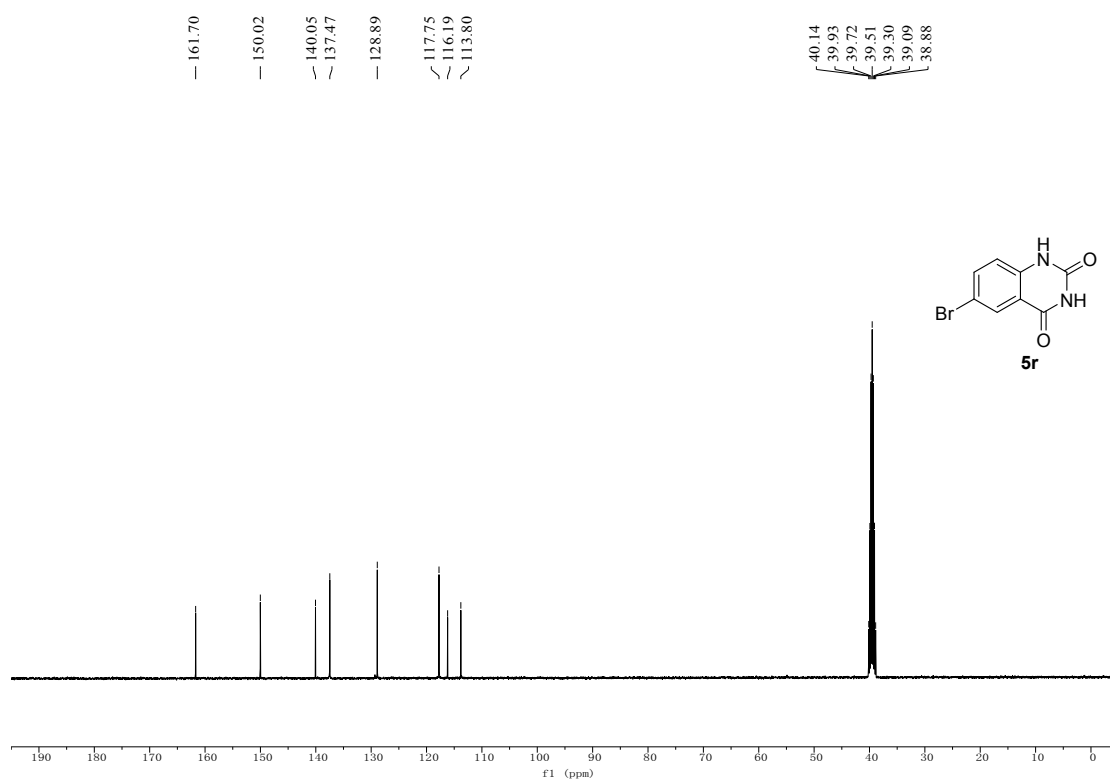


Figure S36. ^{13}C NMR spectra of 6-bromoquinazoline-2,4(1*H*,3*H*)-dione (5r)

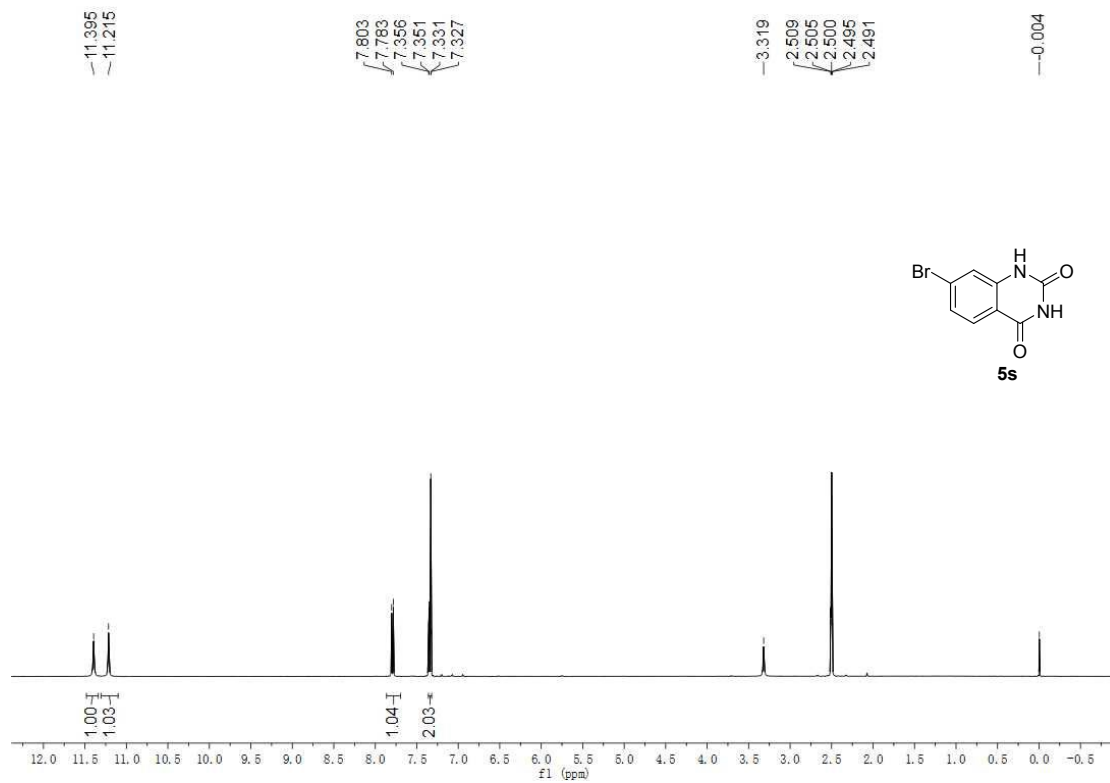


Figure S37. ¹H NMR spectra of 7-bromoquinazoline-2,4(1H,3H)-dione (5s)

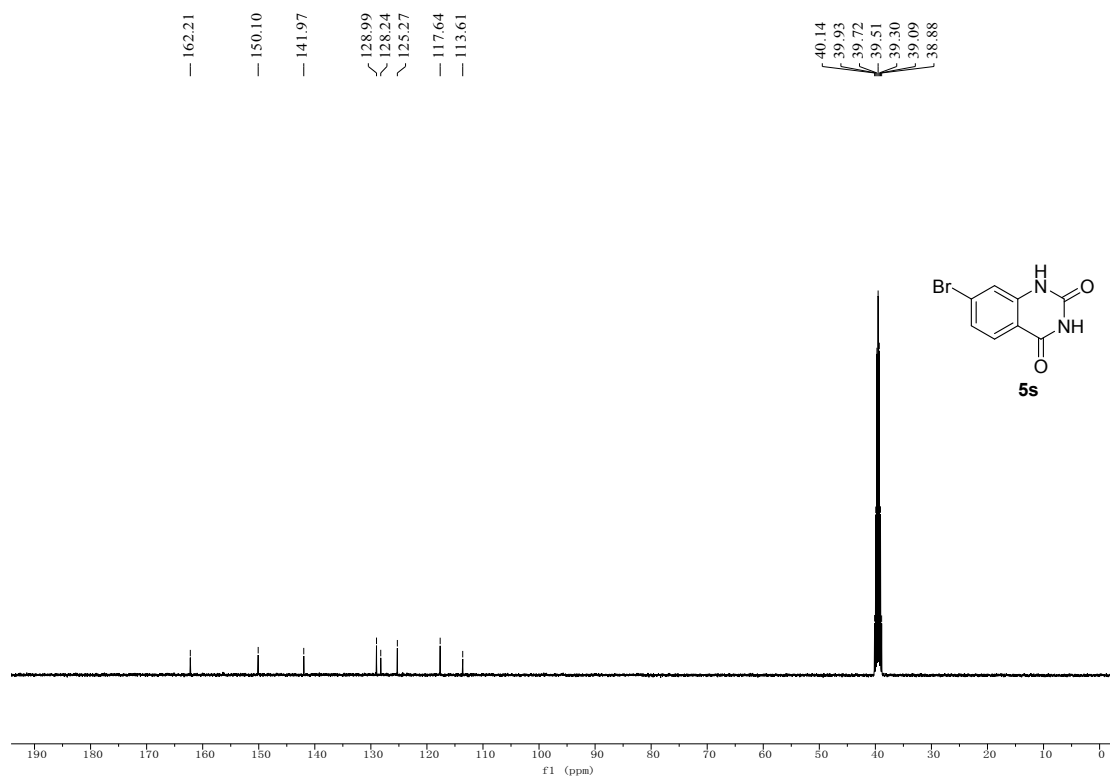


Figure S38. ¹³C NMR spectra of 7-bromoquinazoline-2,4(1H,3H)-dione (5s)

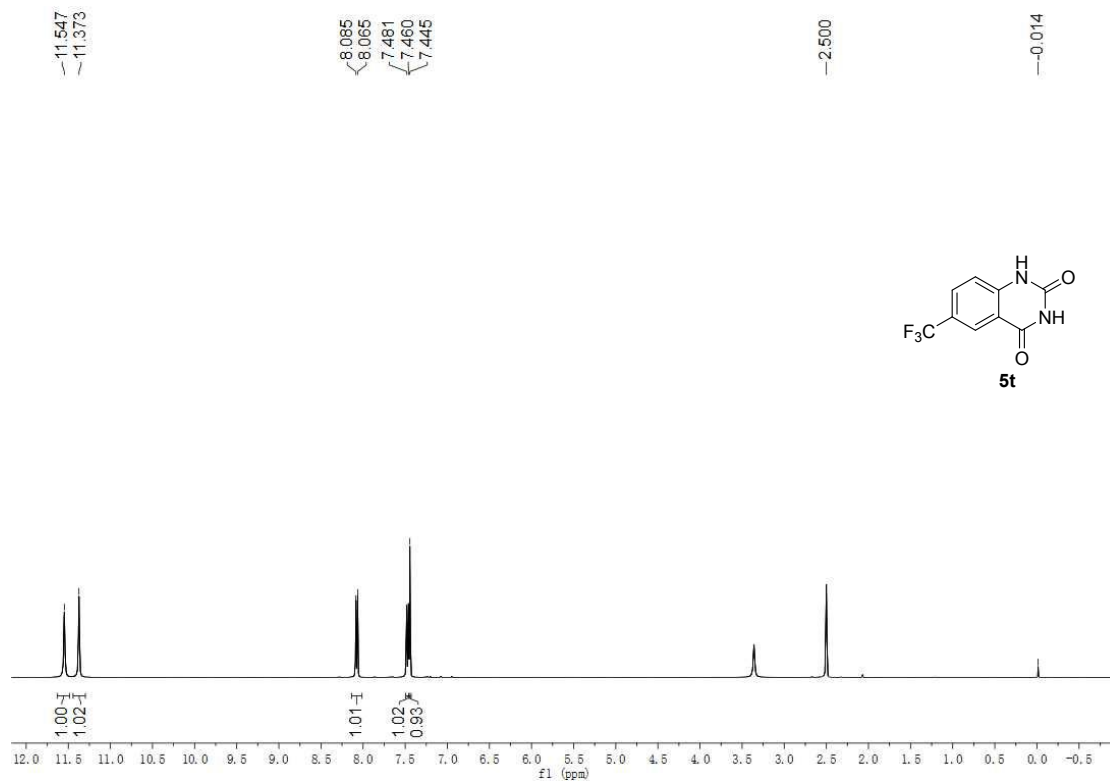


Figure S39. ^1H NMR spectra of 6-(trifluoromethyl)quinazoline-2,4(1H,3H)-dione (5t)

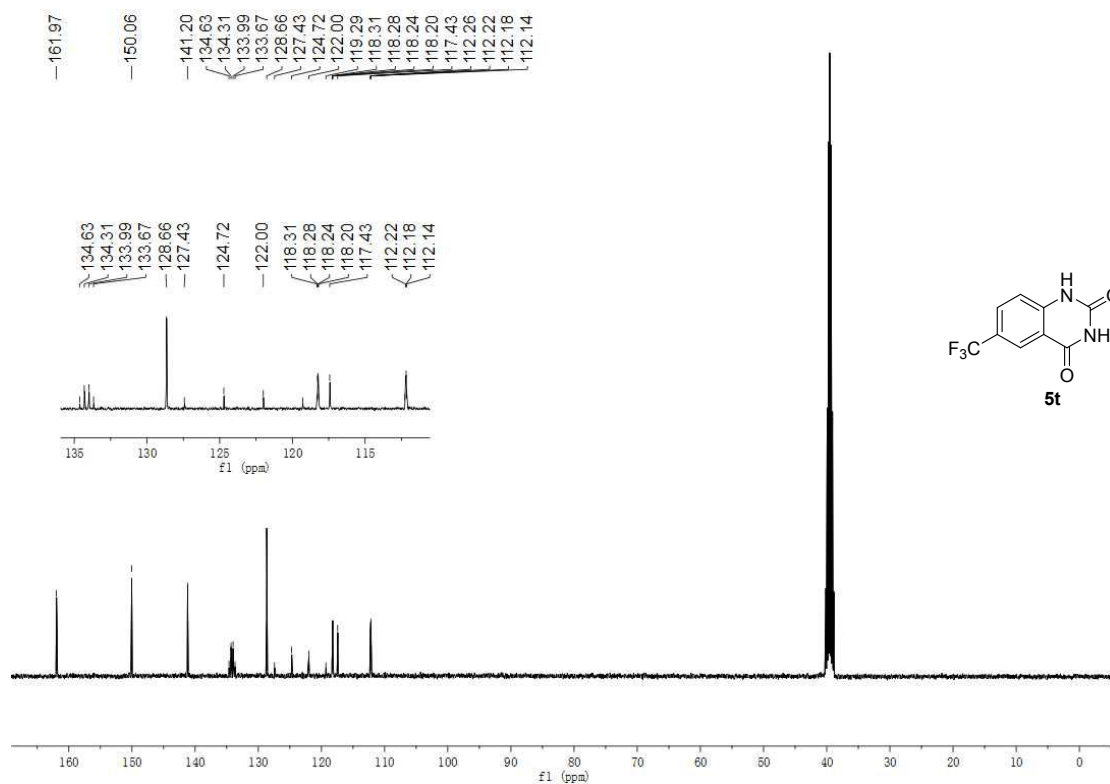


Figure S40. ^{13}C NMR spectra of 6-(trifluoromethyl)quinazoline-2,4(1H,3H)-dione (5t)

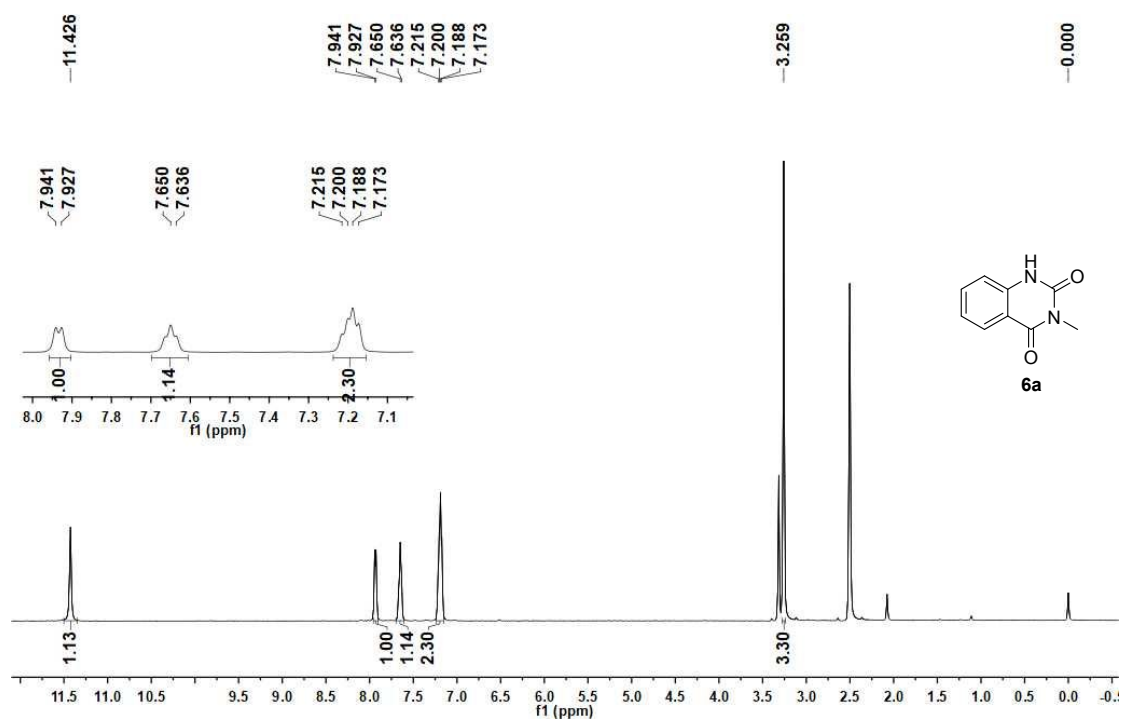


Figure S41. ^1H NMR spectra of 3-methylquinazoline-2,4(1H,3H)-dione (6a)

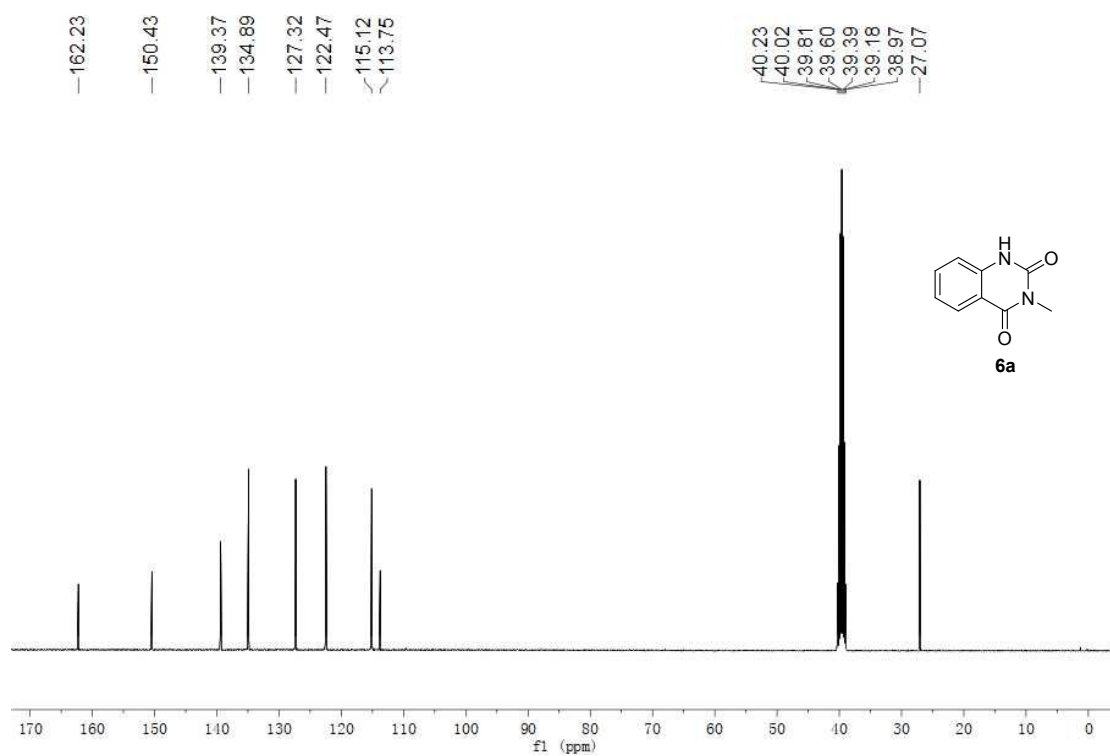


Figure S42. ^{13}C NMR spectra of 3-methylquinazoline-2,4(1H,3H)-dione (6a)

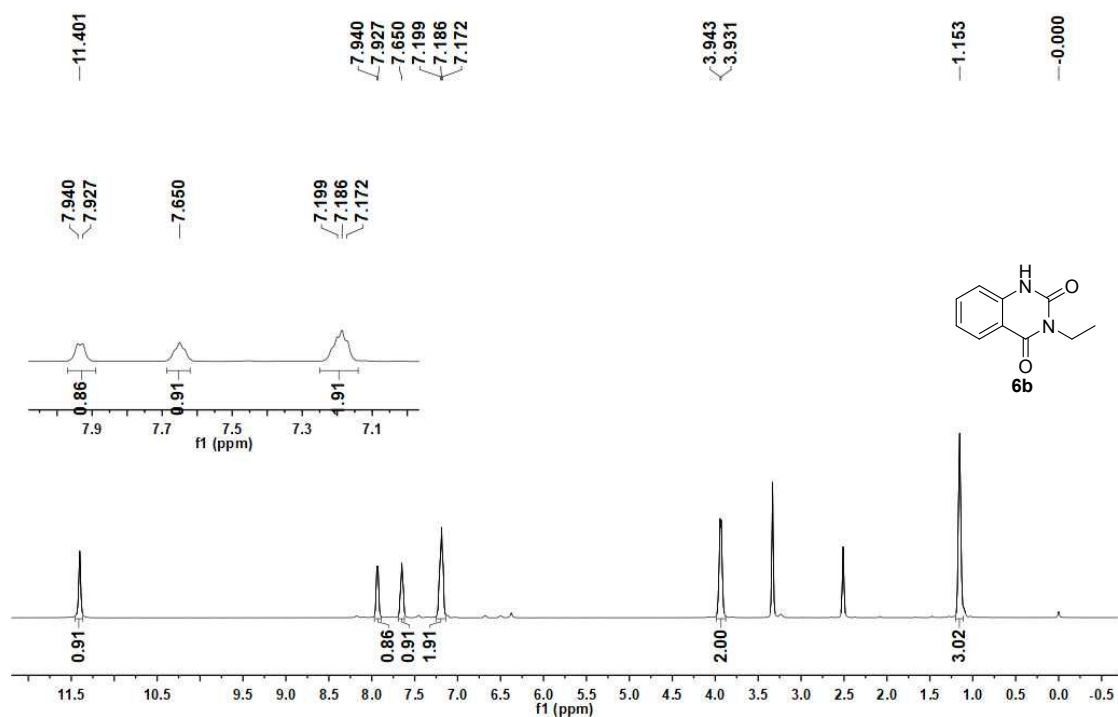


Figure S43. ¹H NMR spectra of 3-ethylquinazoline-2,4(1*H*,3*H*)-dione (6b)

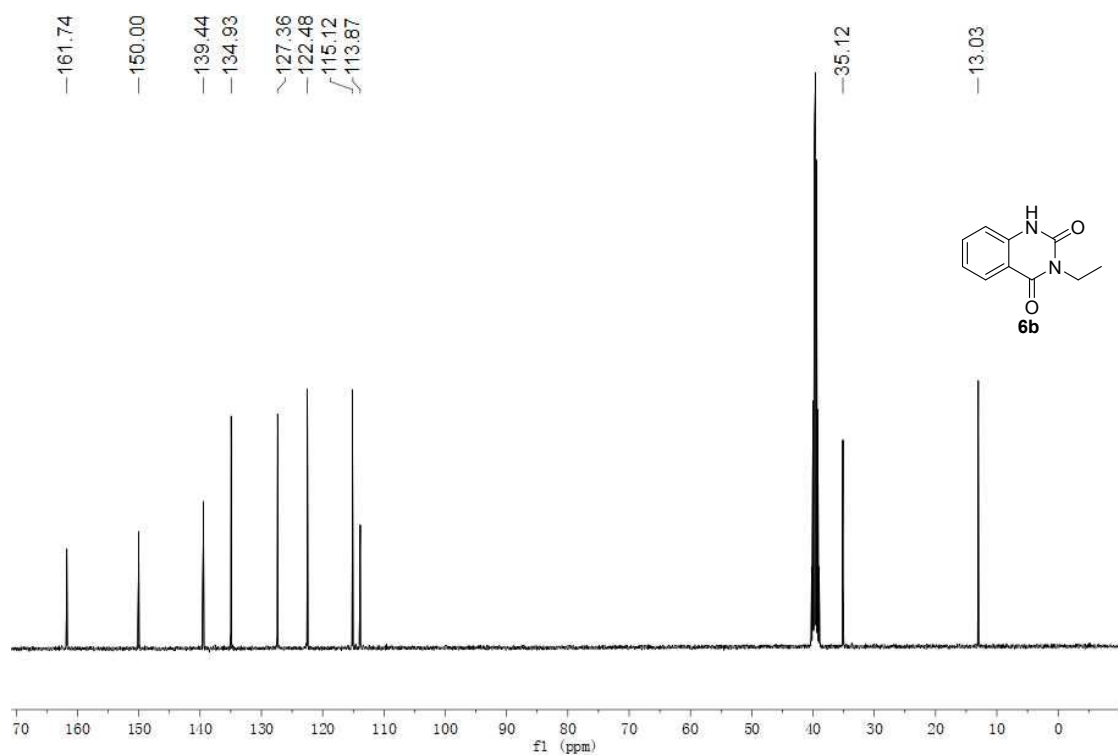


Figure S44. ¹³C NMR spectra of 3-ethylquinazoline-2,4(1*H*,3*H*)-dione (6b)

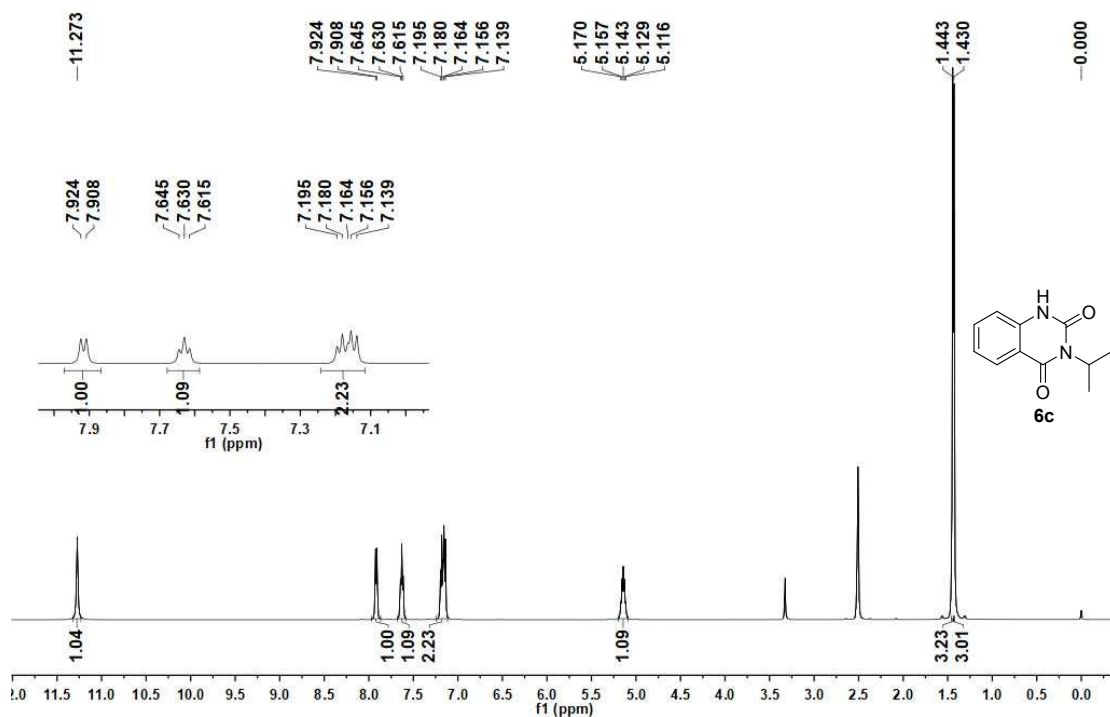


Figure S45. ^1H NMR spectra of 3-isopropylquinazoline-2,4(1H,3H)-dione (6c)

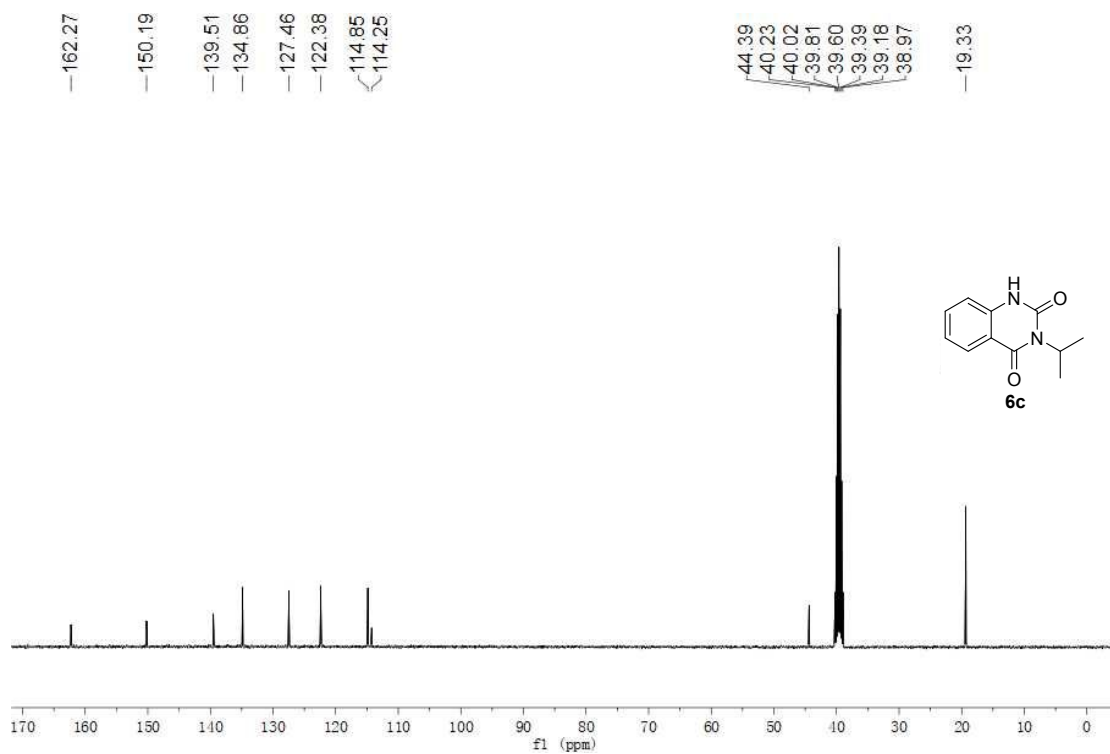


Figure S46. ^{13}C NMR spectra of 3-isopropylquinazoline-2,4(1H,3H)-dione (6c)

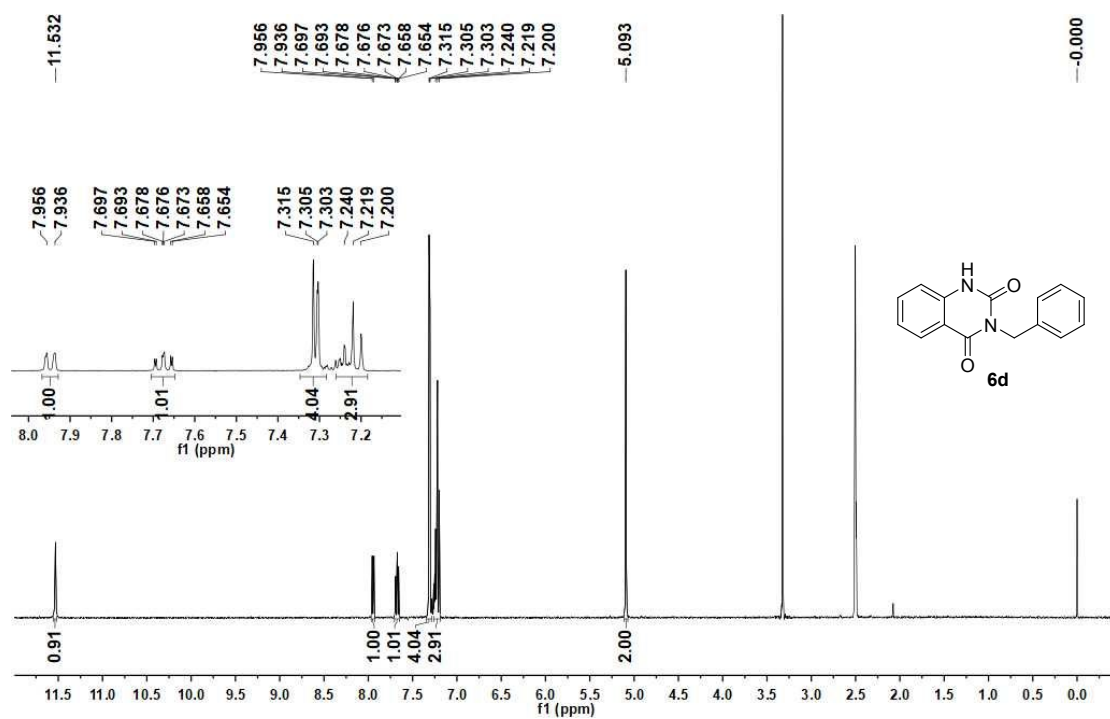


Figure S47. ^1H NMR spectra of 3-benzylquinazoline-2,4(1H,3H)-dione (6d)

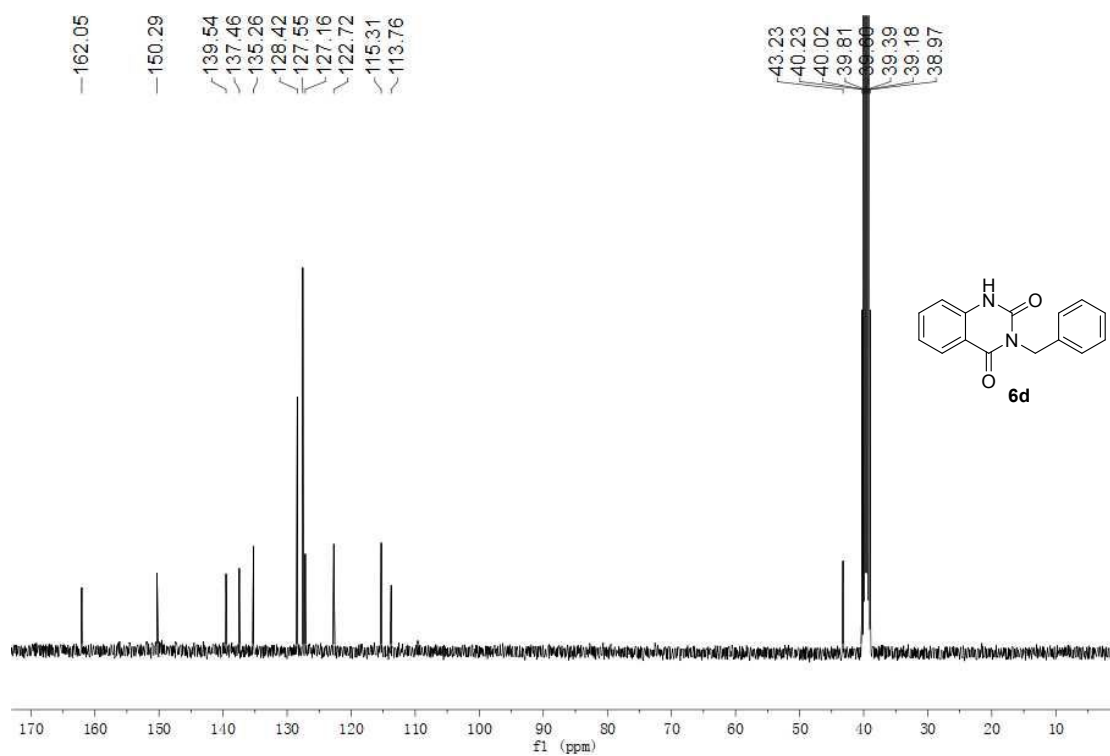


Figure S48. ^{13}C NMR spectra of 3-benzylquinazoline-2,4(1H,3H)-dione (6d)

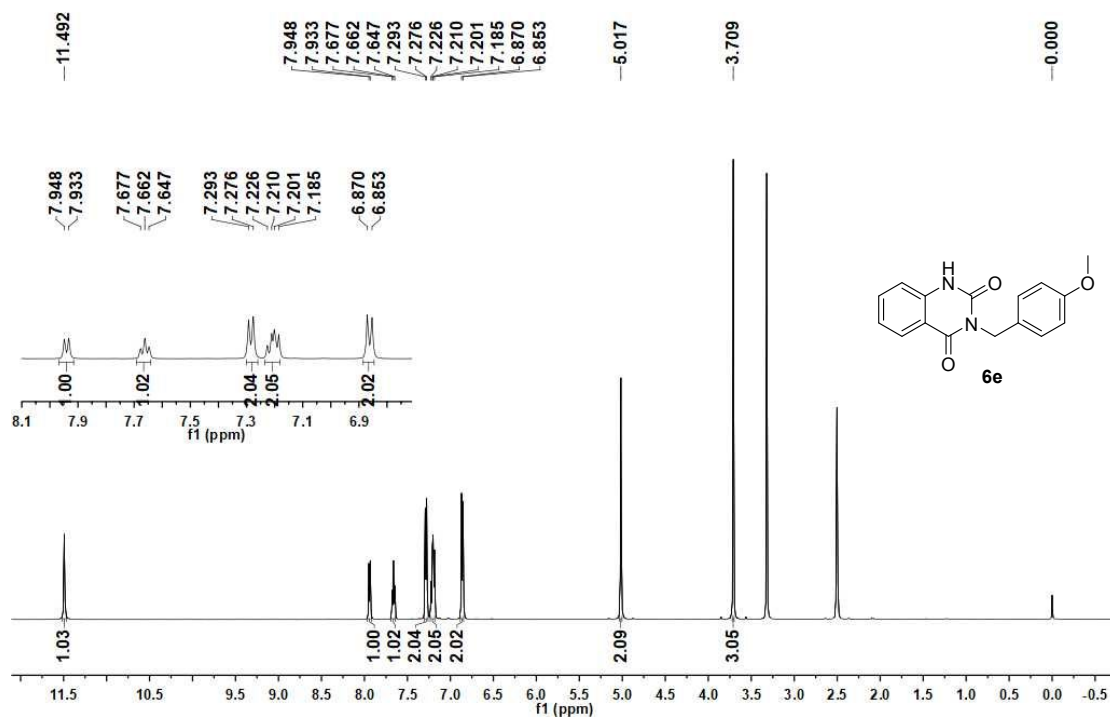


Figure S49. ¹H and spectra of 3-(4-methoxybenzyl)quinazoline-2,4(1*H*,3*H*)-dione (6e)

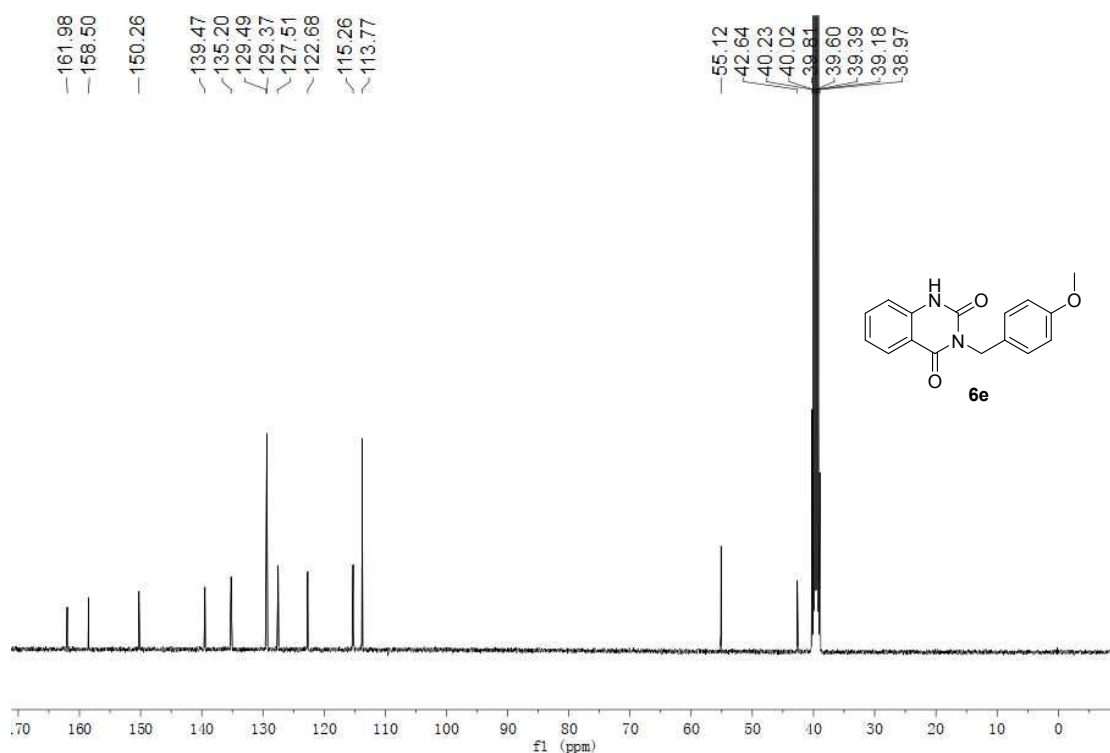


Figure S50. ¹³C NMR spectra of 3-(4-methoxybenzyl)quinazoline-2,4(1*H*,3*H*)-dione (6e)

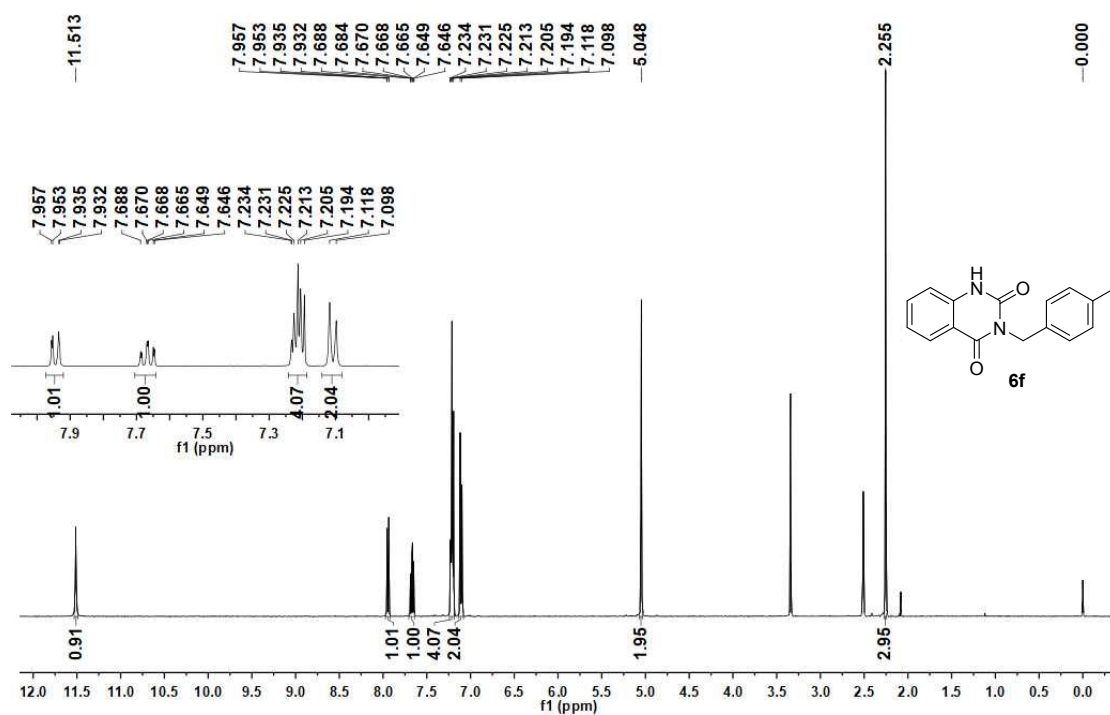


Figure S51. ¹H NMR spectra of 3-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (6f)

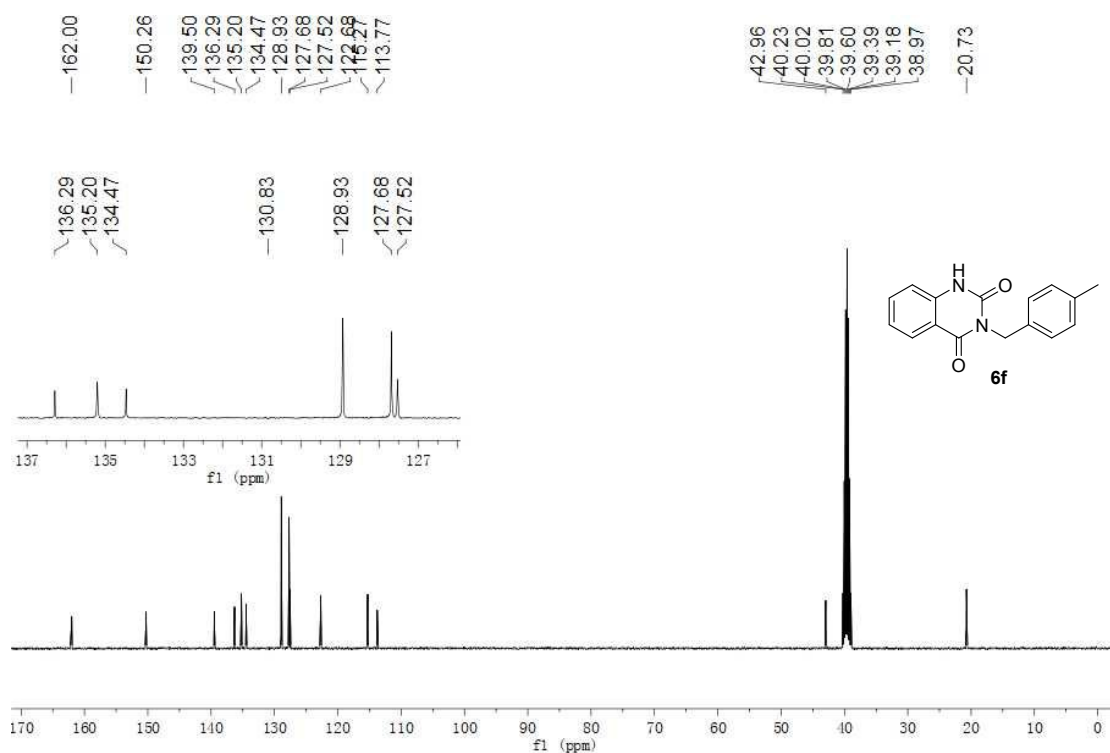


Figure S52. ¹³C NMR spectra of 3-(4-methylbenzyl)quinazoline-2,4(1H,3H)-dione (6f)

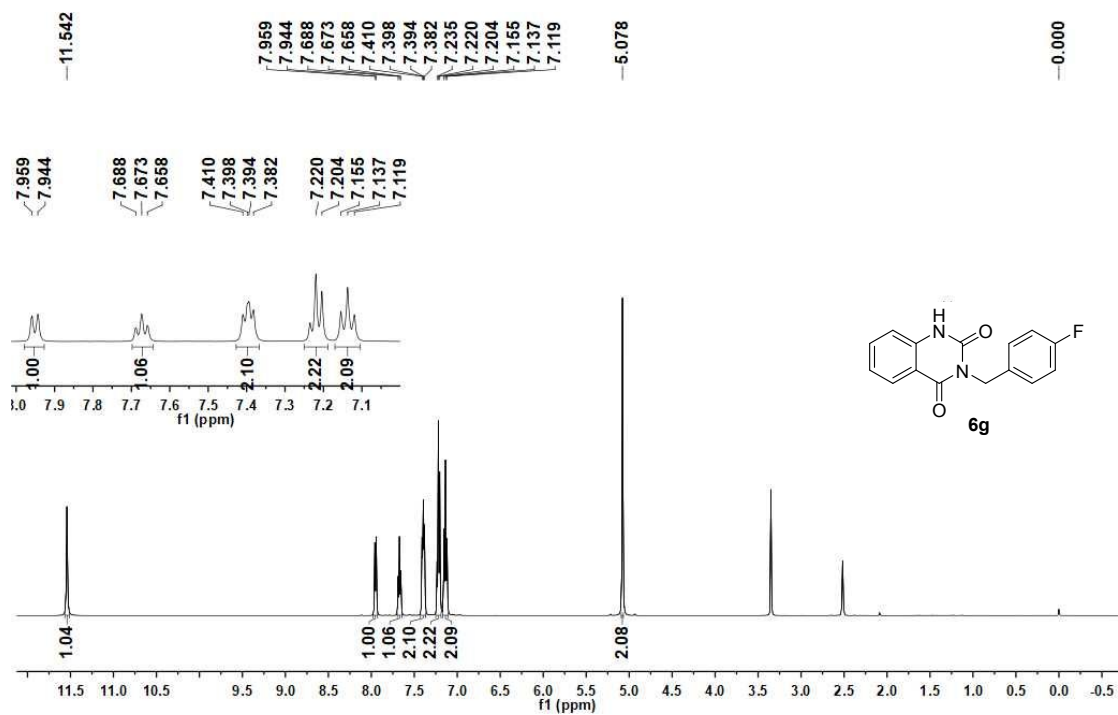


Figure S53. ¹H NMR spectra of 3-(4-fluorobenzyl)quinazoline-2,4(1*H*,3*H*)-dione (6g)

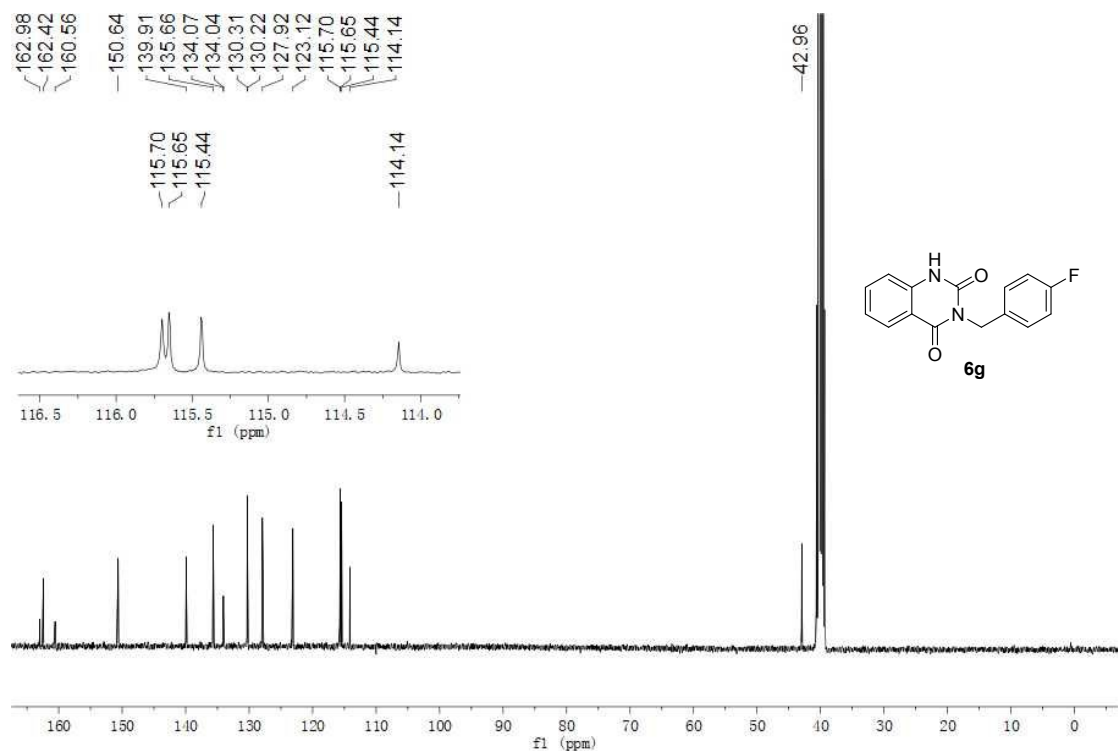


Figure S54. ¹³C NMR spectra of 3-(4-fluorobenzyl)quinazoline-2,4(1*H*,3*H*)-dione (6g)

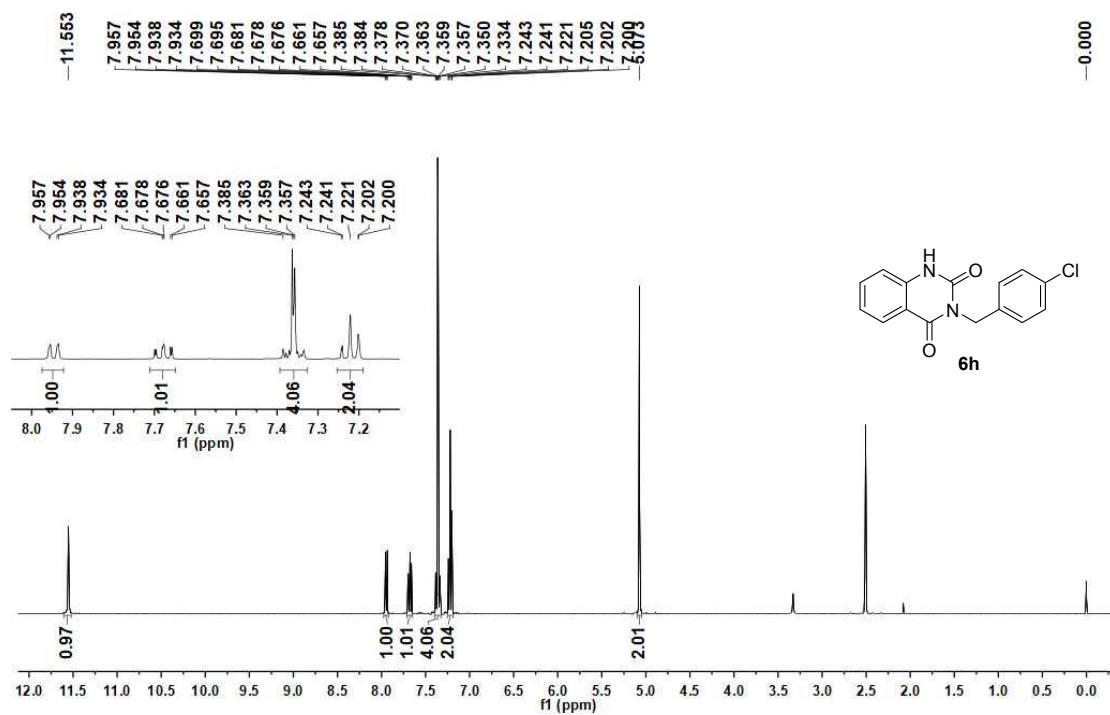


Figure S55. ¹H NMR spectra of 3-(4-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (6h)

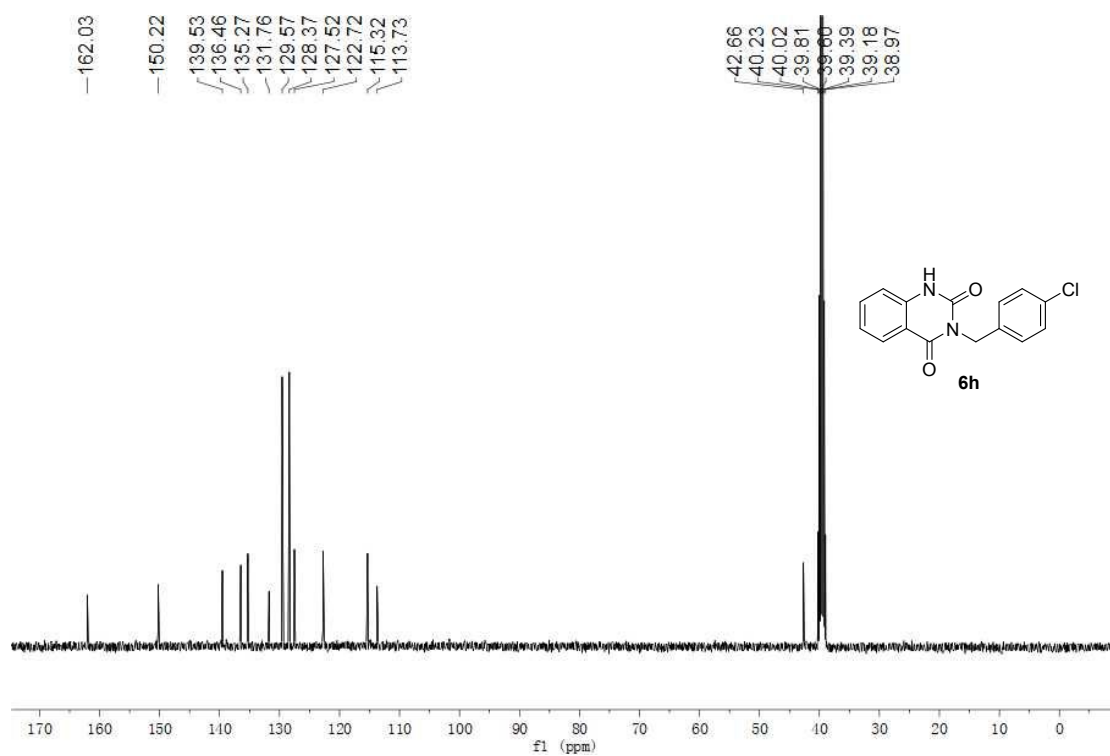


Figure S56. ¹³C NMR spectra of 3-(4-chlorobenzyl)quinazoline-2,4(1H,3H)-dione (6h)

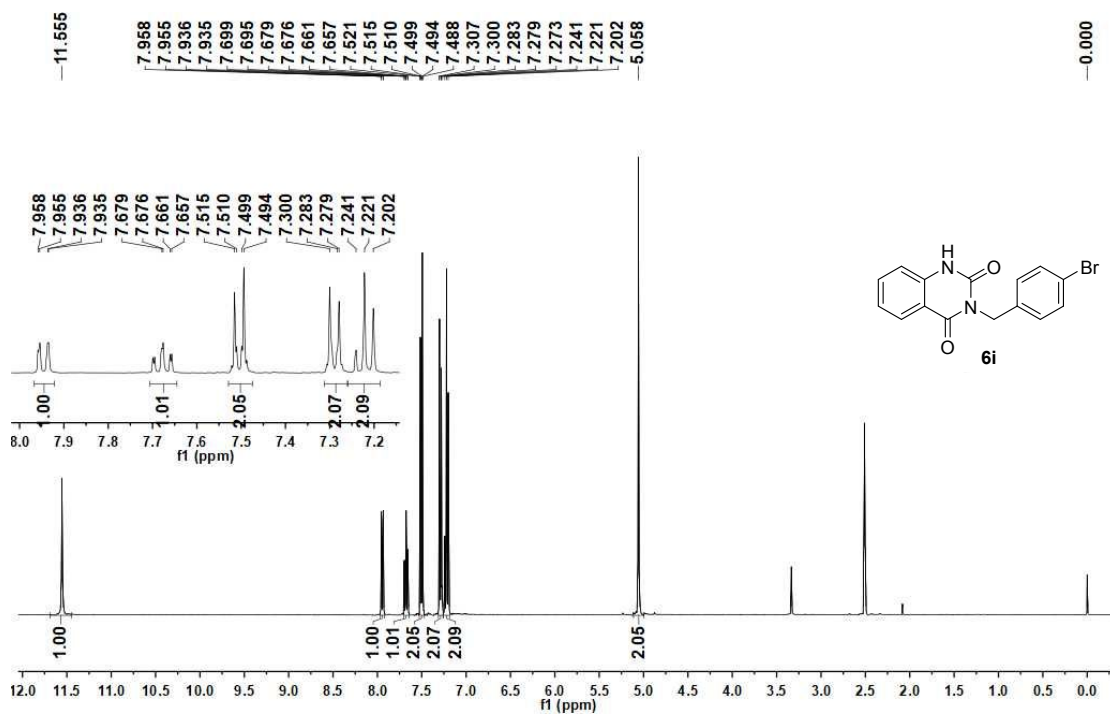


Figure S57. ¹H NMR spectra of 3-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (6i)

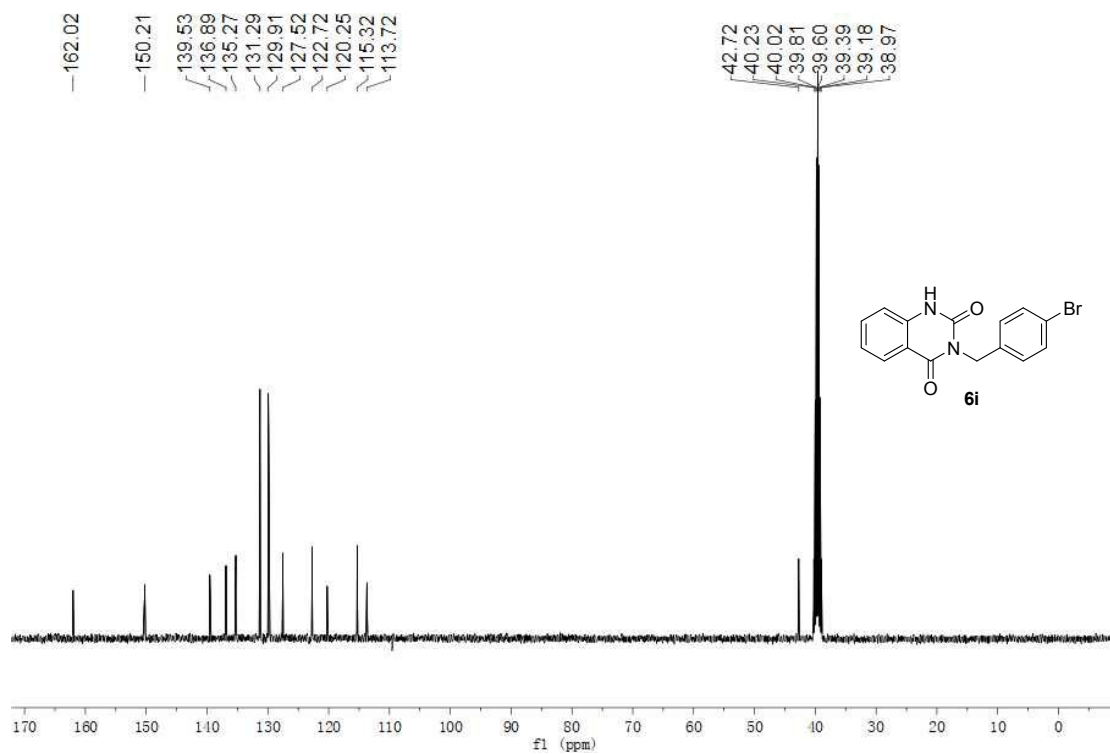


Figure S58. ¹³C NMR spectra of 3-(4-bromobenzyl)quinazoline-2,4(1H,3H)-dione (6i)

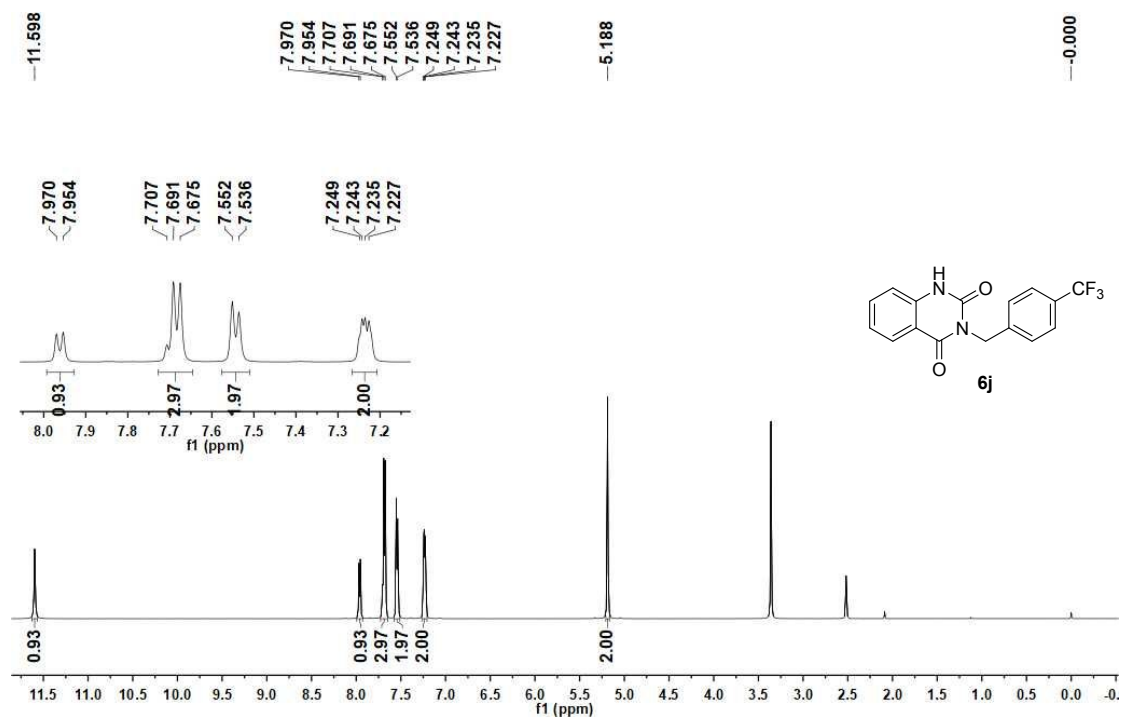


Figure S59. ¹H NMR spectra of 3-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (6j)

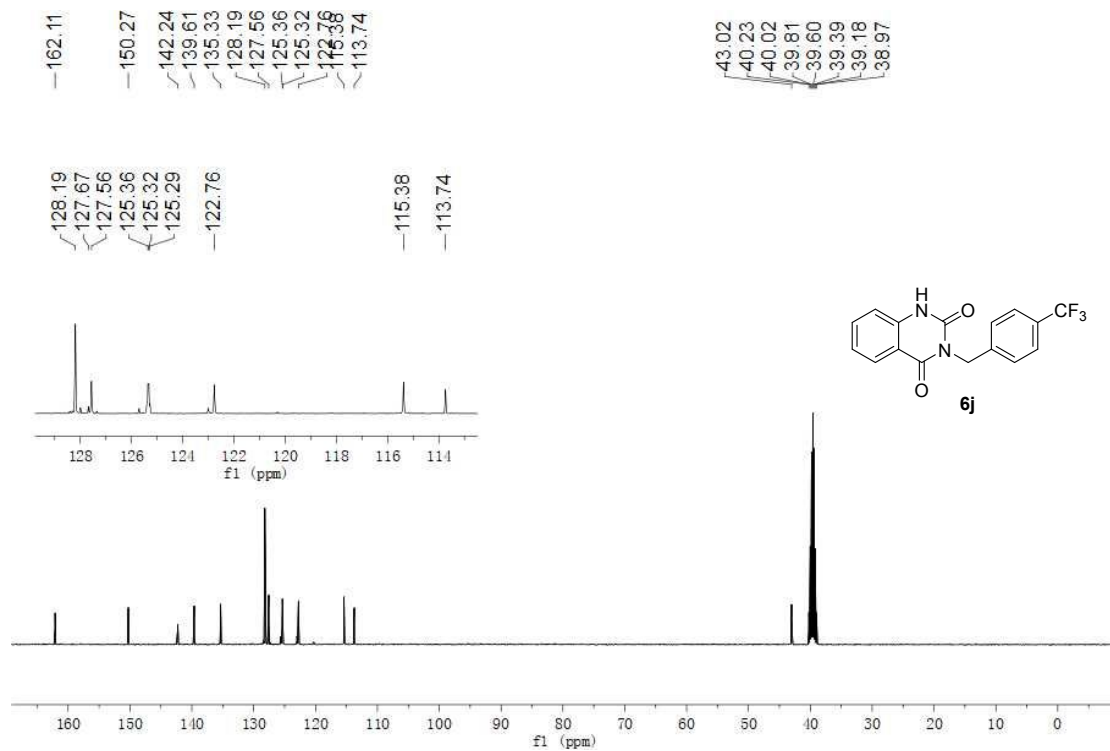


Figure S60. ¹³C NMR spectra of 3-(4-(trifluoromethyl)benzyl)quinazoline-2,4(1H,3H)-dione (6j)

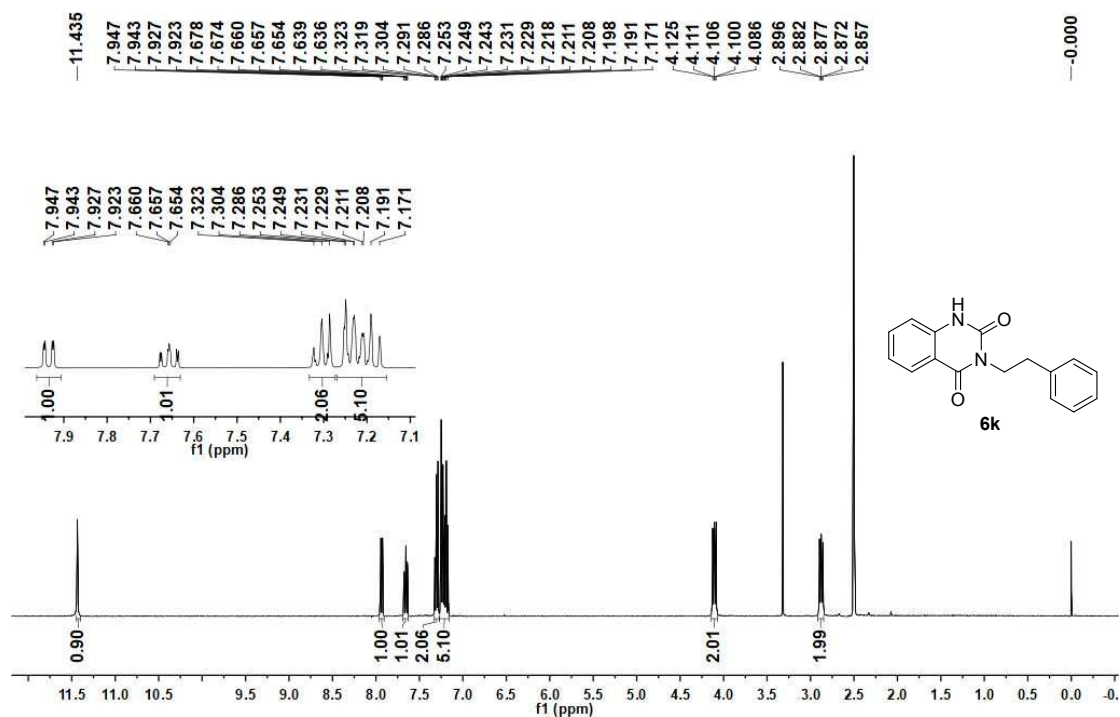


Figure S61. ¹H NMR spectra of 3-phenethylquinazoline-2,4(1H,3H)-dione (6k)

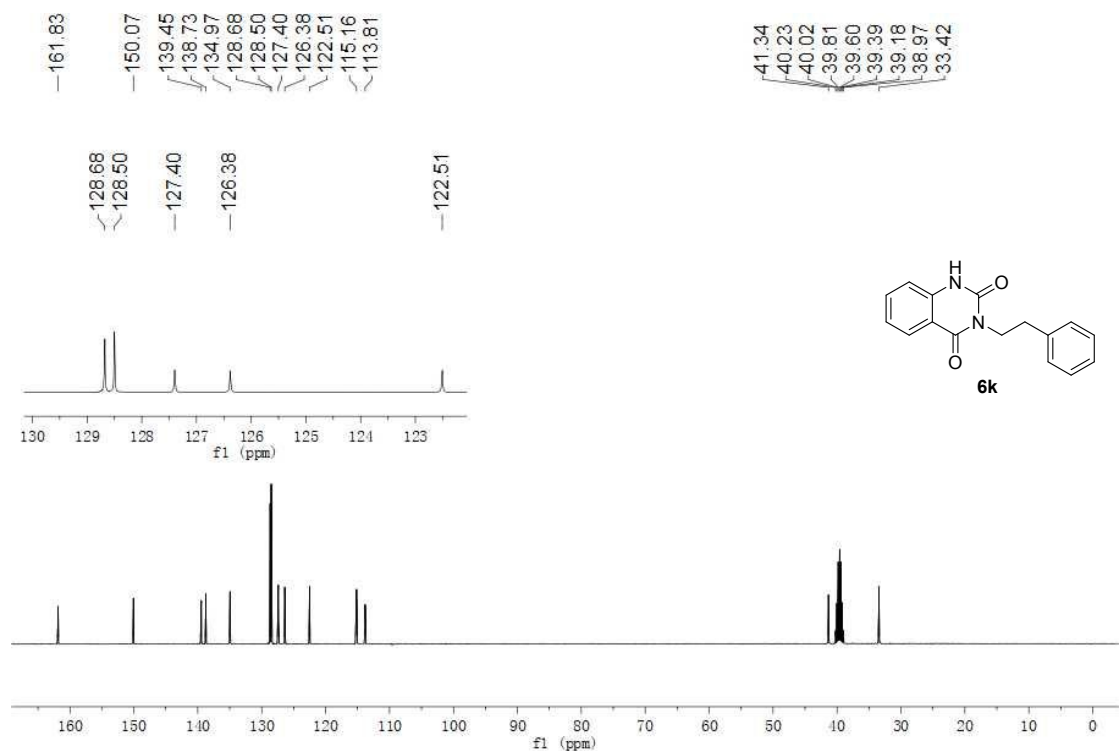


Figure S62. ¹³C NMR spectra of 3-phenethylquinazoline-2,4(1H,3H)-dione (6k)

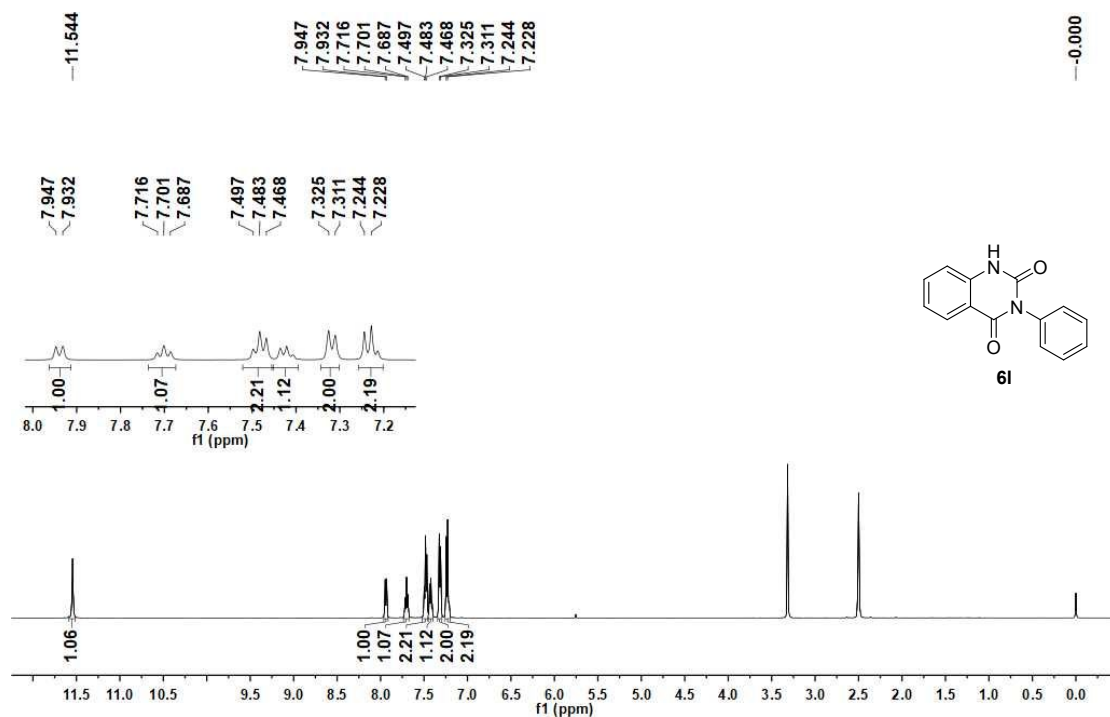


Figure S63. ¹H NMR spectra of 3-phenylquinazoline-2,4(1H,3H)-dione (6l)

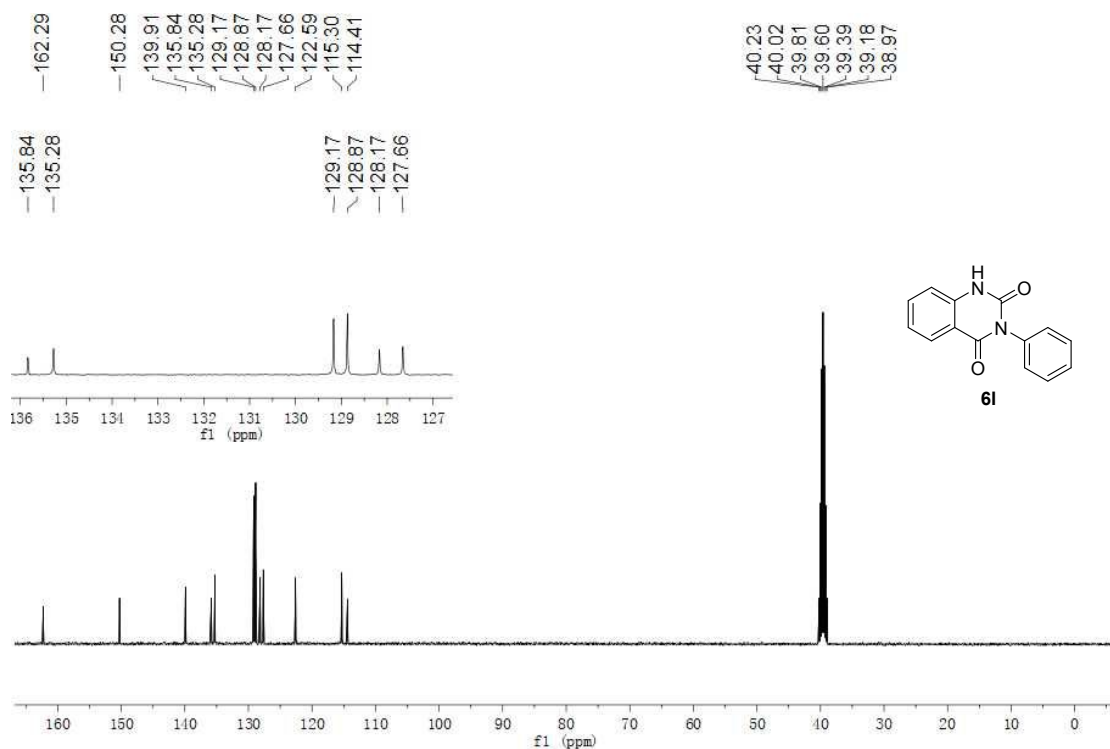


Figure S64. ¹³C NMR spectra of 3-phenylquinazoline-2,4(1H,3H)-dione (6l)

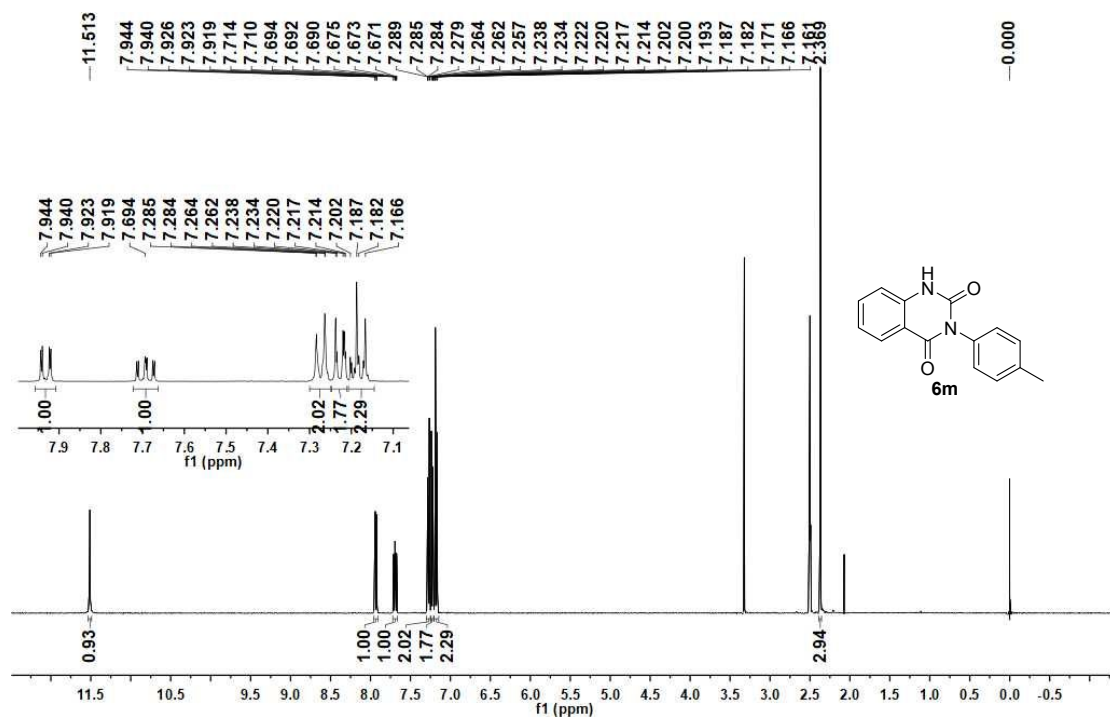


Figure S65. ¹H NMR spectra of 3-(4-methylphenyl)quinazoline-2,4(1H,3H)-dione (6m)

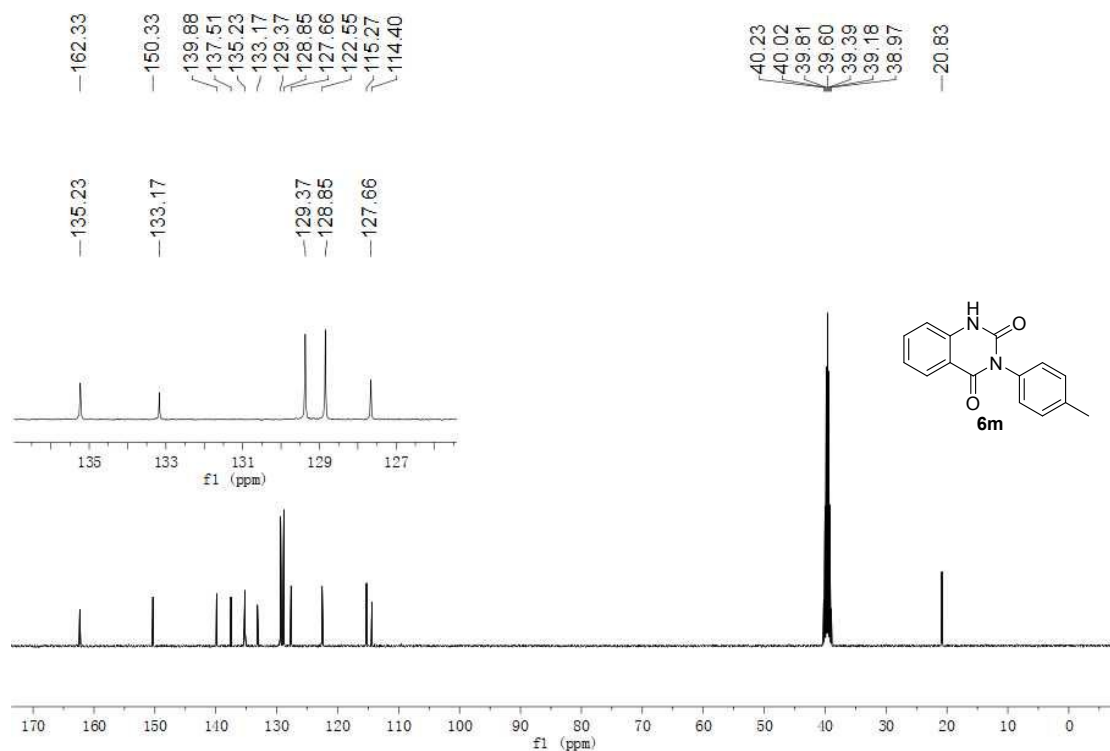


Figure S66. ¹³C NMR spectra of 3-(4-methylphenyl)quinazoline-2,4(1H,3H)-dione (6m)

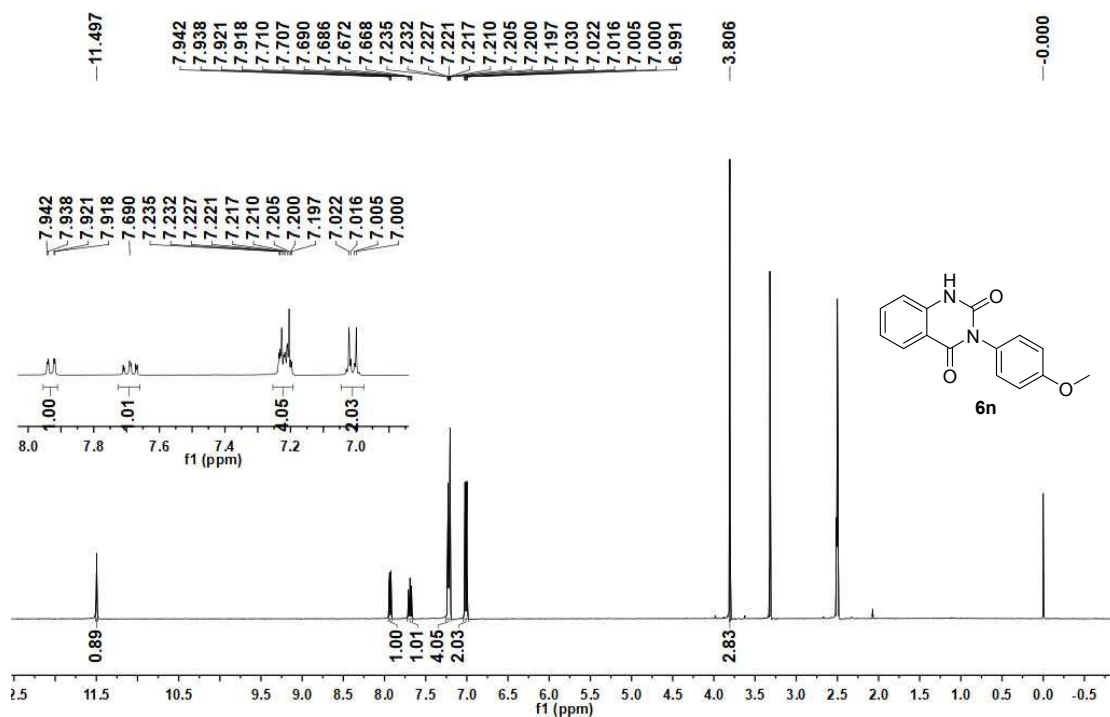


Figure S67. ¹H NMR spectra of 3-(4-methoxyphenyl)quinazoline-2,4(1H,3H)-dione (6n)

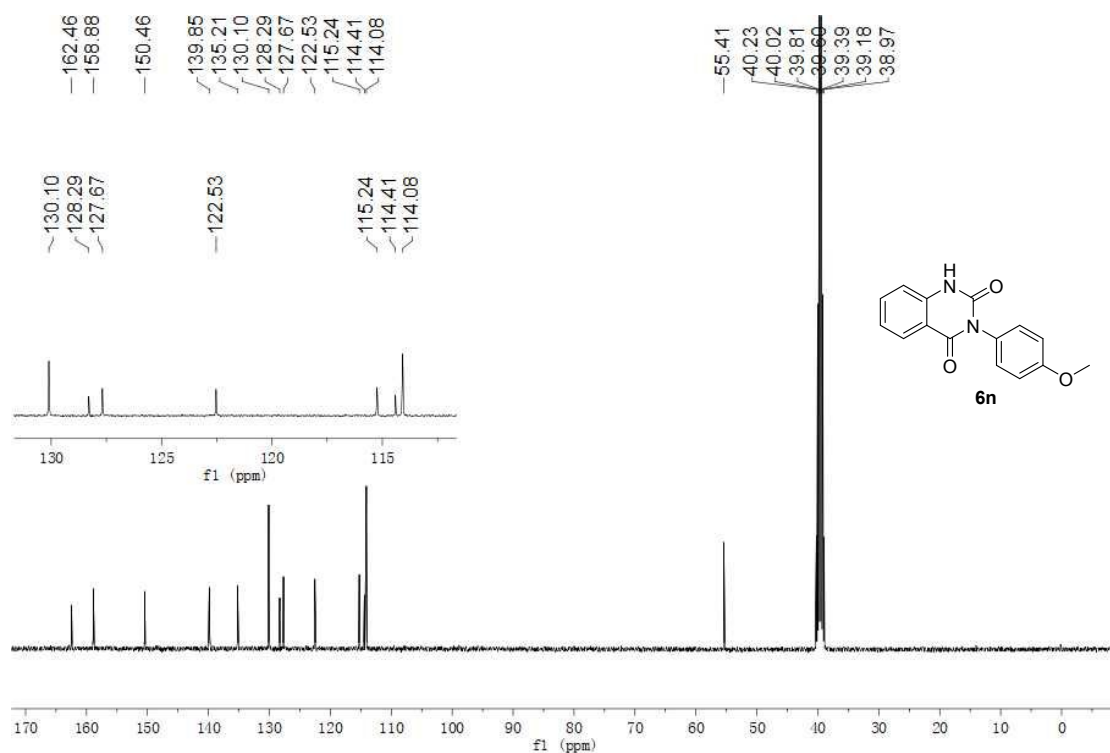


Figure S68. ¹³C NMR spectra of 3-(4-methoxyphenyl)quinazoline-2,4(1H,3H)-dione (6n)

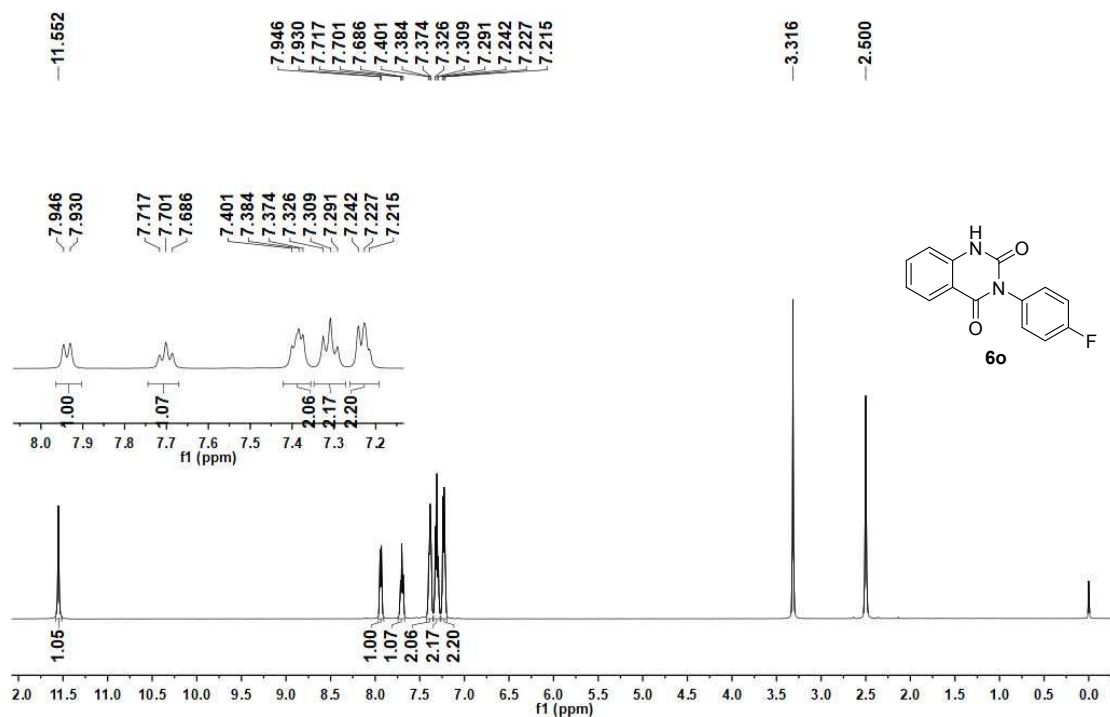


Figure S69. ¹H NMR spectra of 3-(4-fluorophenyl)quinazoline-2,4(1H,3H)-dione (6o)

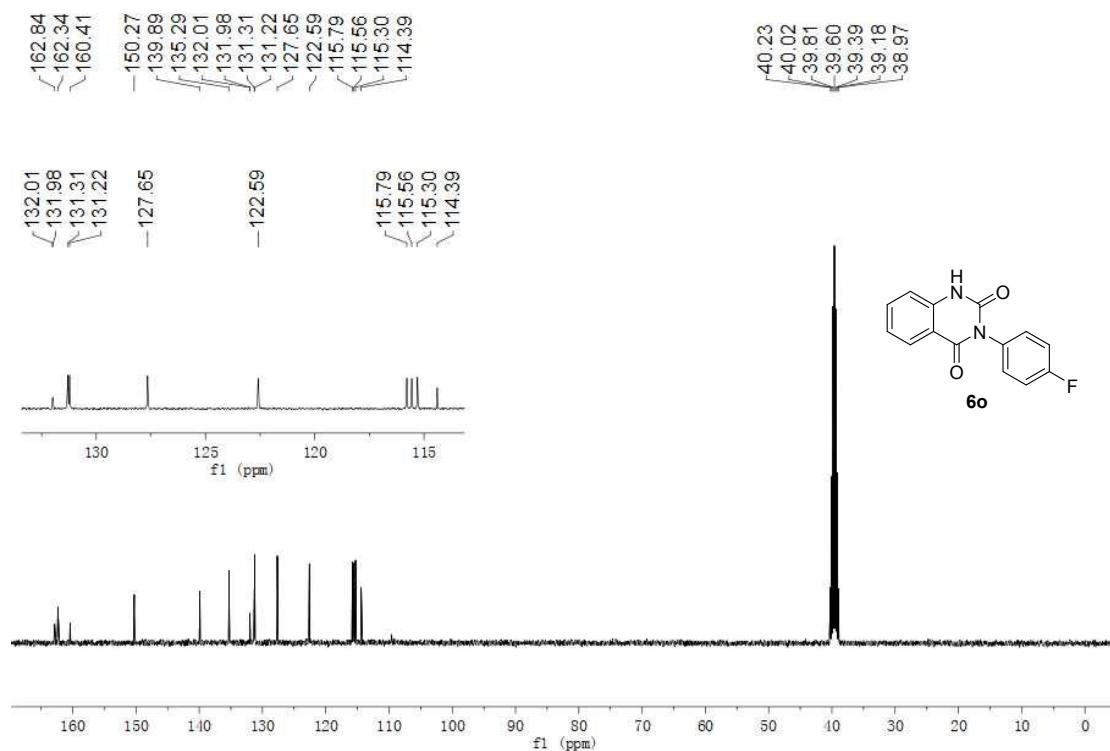


Figure S70. ¹³C NMR spectra of 3-(4-fluorophenyl)quinazoline-2,4(1H,3H)-dione (6o)

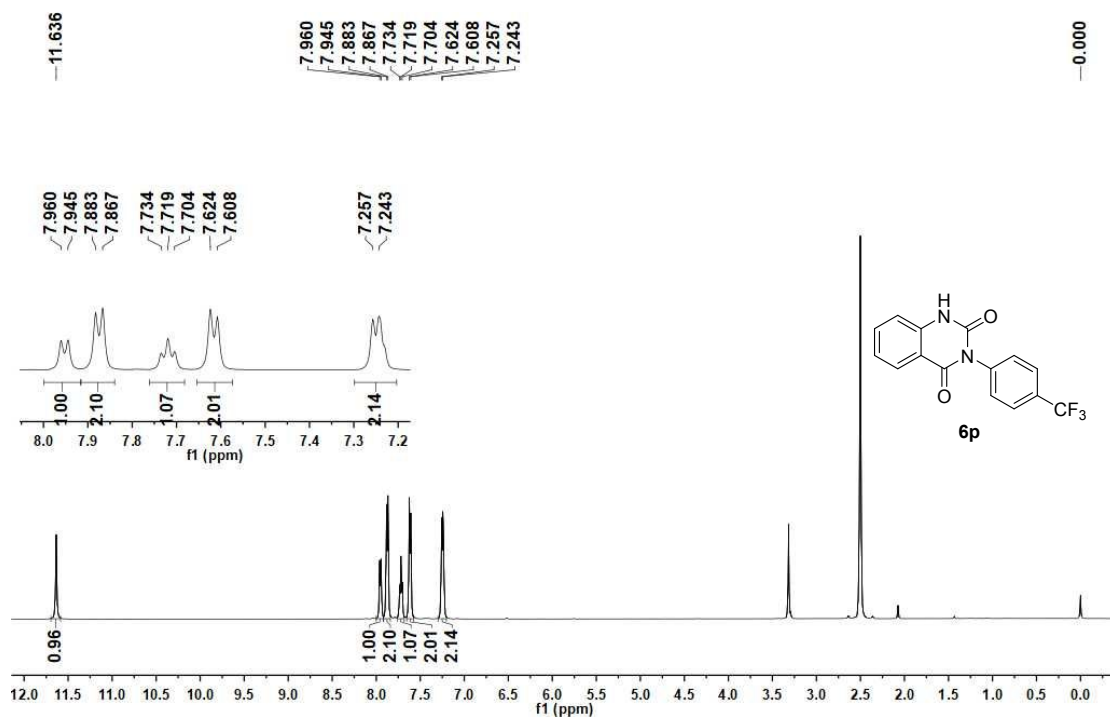


Figure S71. ¹H NMR spectra of 3-(4-(trifluoromethyl)phenyl)quinazoline-2,4(1H,3H)-dione (6p)

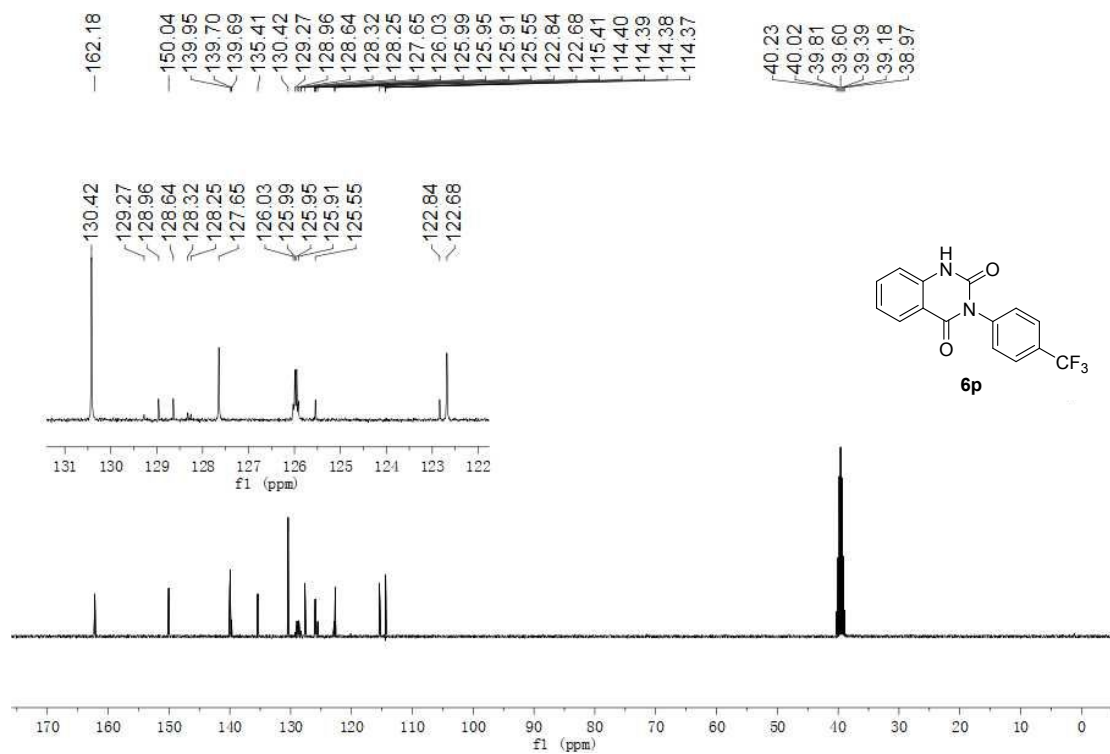


Figure S72. ¹³C NMR spectra of 3-(4-(trifluoromethyl)phenyl)quinazoline-2,4(1H,3H)-dione (6p)

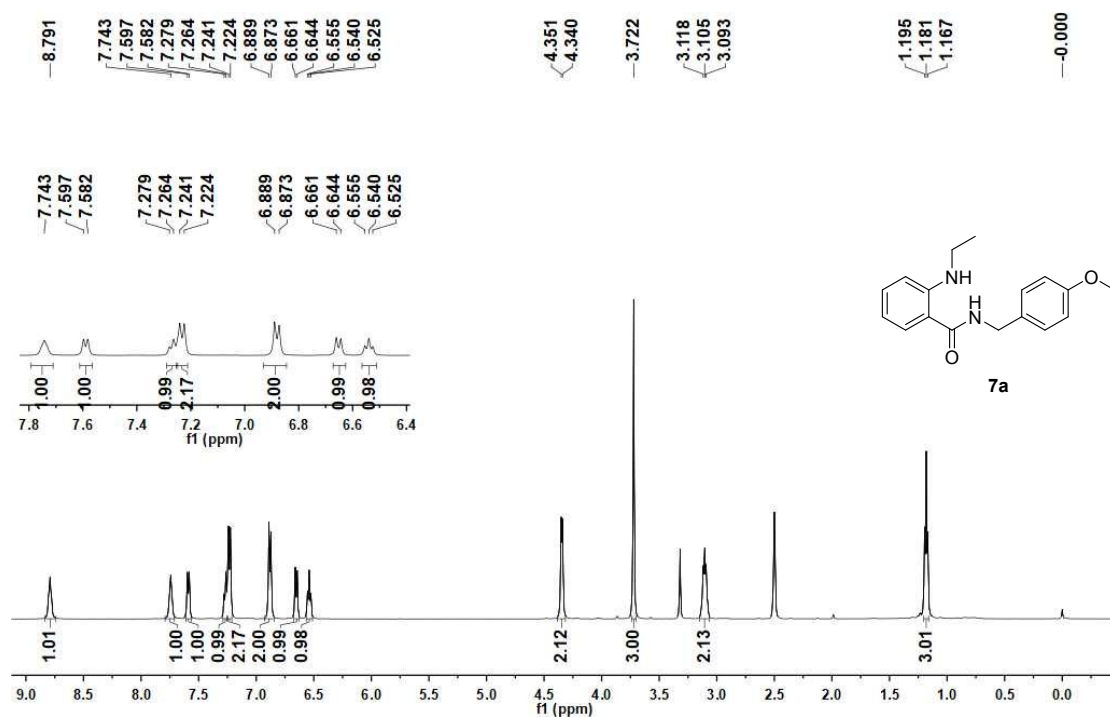


Figure S73. ¹H NMR spectra of 2-(ethylamino)-N-(4-methoxybenzyl)benzamide (7a)

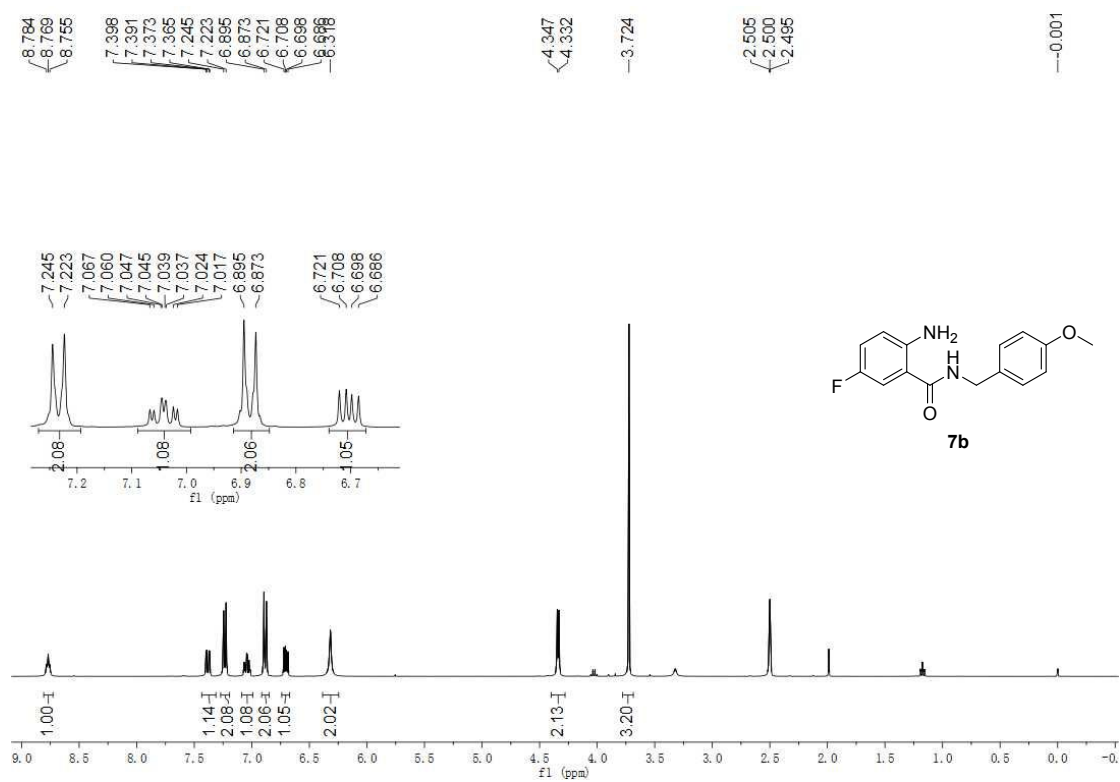


Figure S74. ¹H NMR spectra of 2-amino-5-fluoro-N-(4-methoxybenzyl)benzamide (7b)

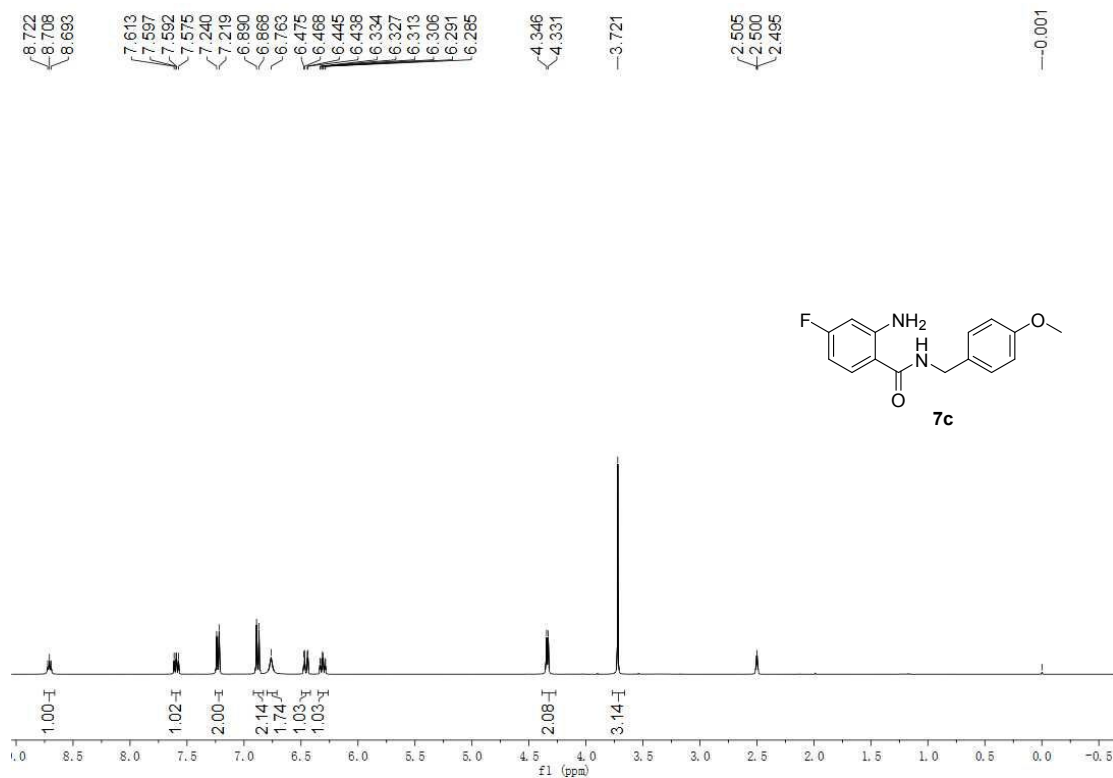


Figure S75. ¹H NMR spectra of 2-amino-4-fluoro-N-(4-methoxybenzyl)benzamide (7c)

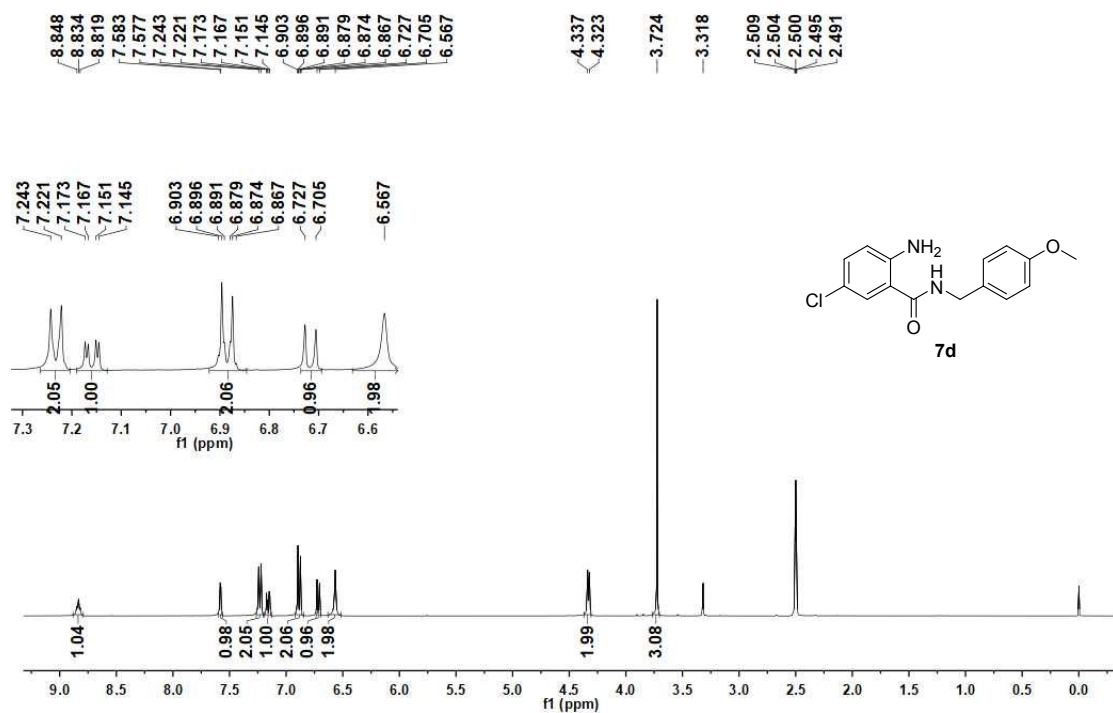


Figure S76. ¹H NMR spectra of 2-amino-5-chloro-N-(4-methoxybenzyl)benzamide (7d)

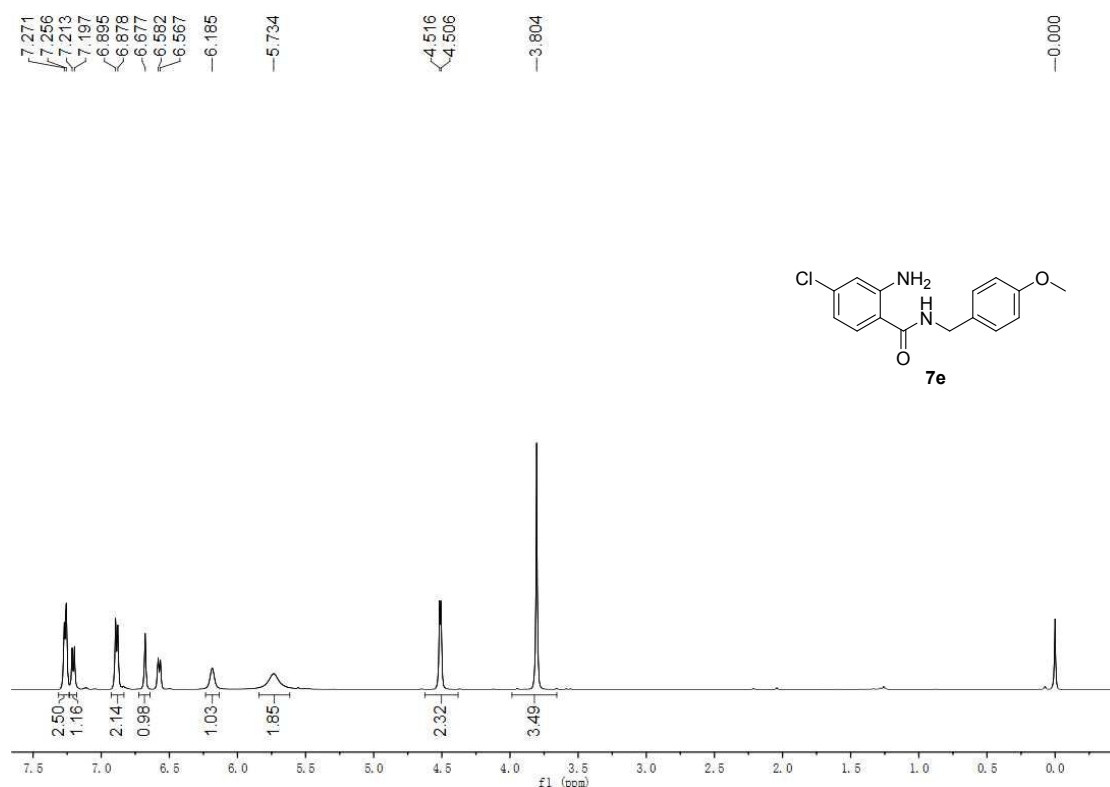


Figure S77. ¹H NMR spectra of 2-amino-4-chloro-N-(4-methoxybenzyl)benzamide (7e)



Figure S78. ¹H NMR spectra of 2-amino-5-bromo-N-(4-methoxybenzyl)benzamide (7f)

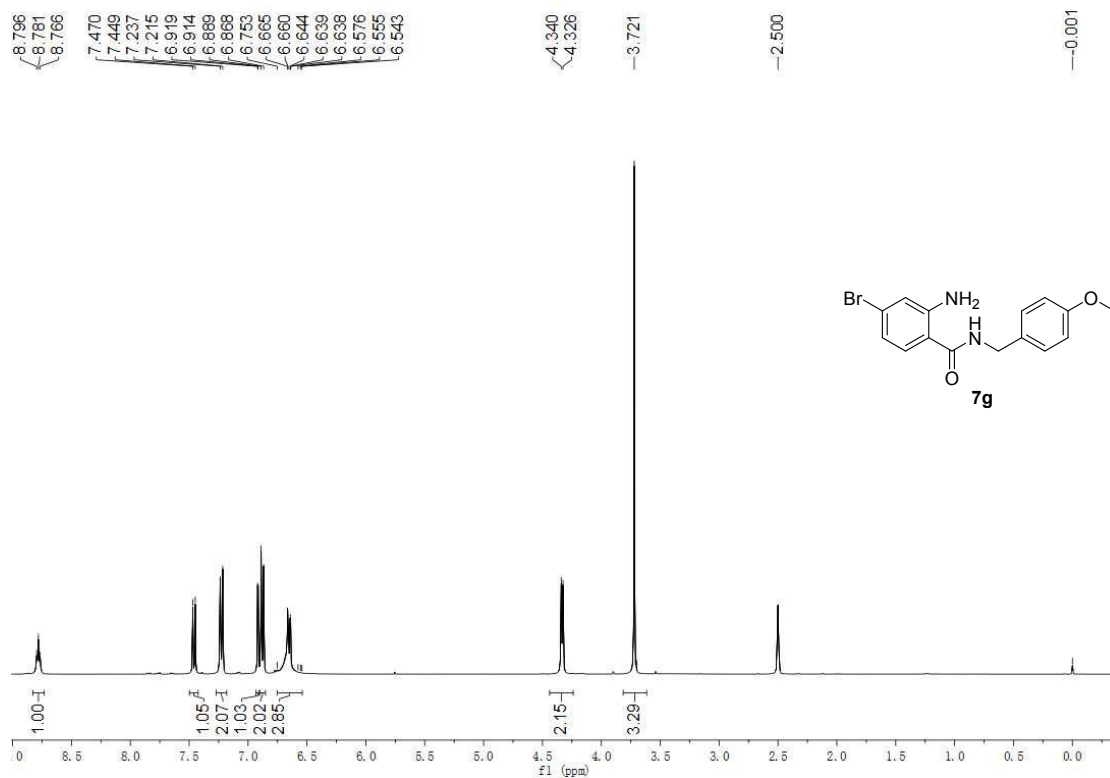


Figure S79. ¹H NMR spectra of 2-amino-4-bromo-*N*-(4-methoxybenzyl)benzamide (7g)

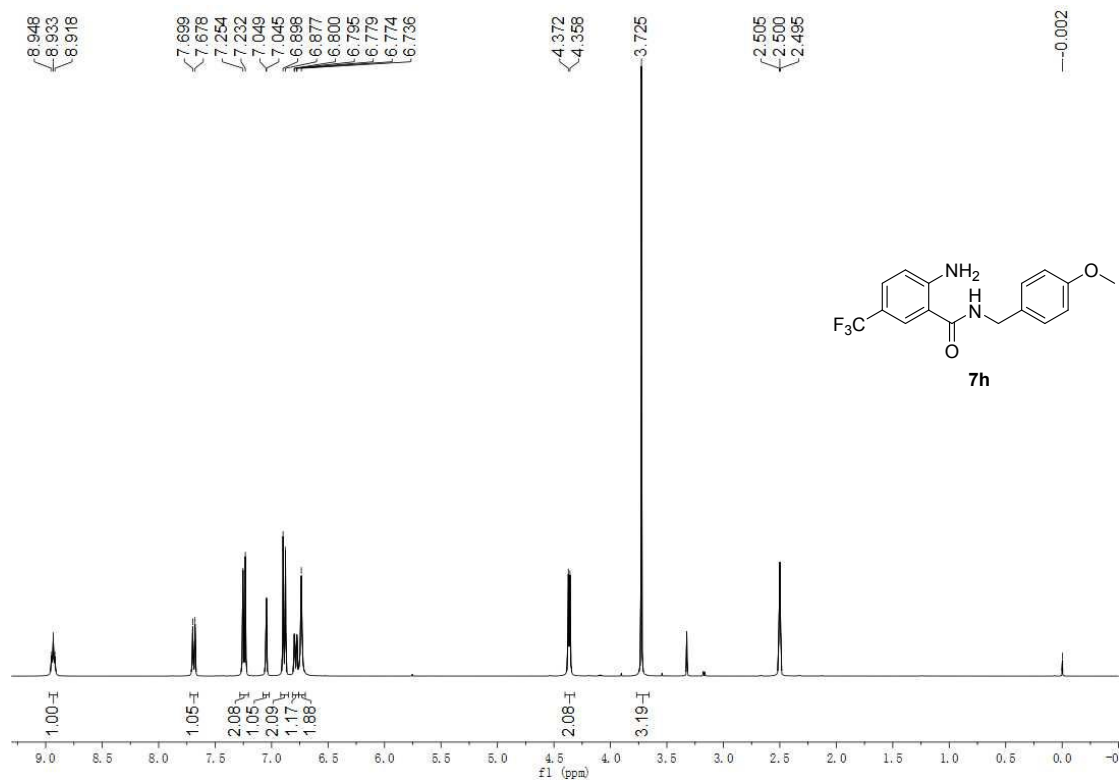


Figure S80. ¹H NMR spectra of 2-amino-*N*-(4-methoxybenzyl)-5-(trifluoromethyl)benzamide (7h)

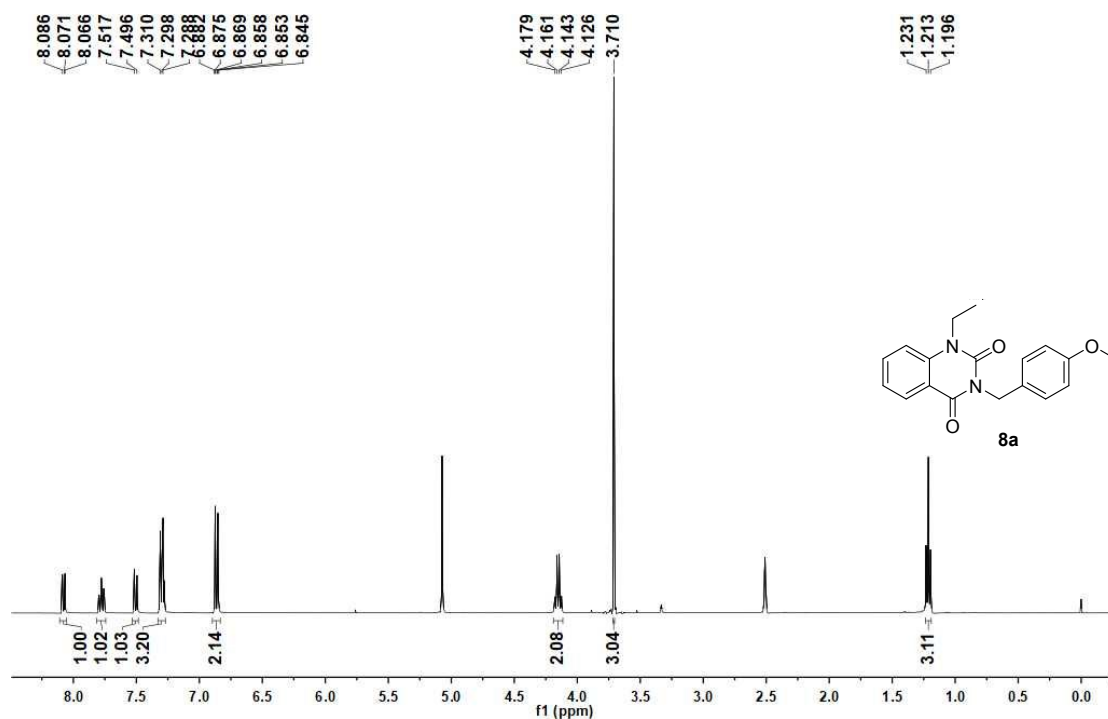


Figure S81. ^1H NMR spectra of 1-ethyl-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8a)

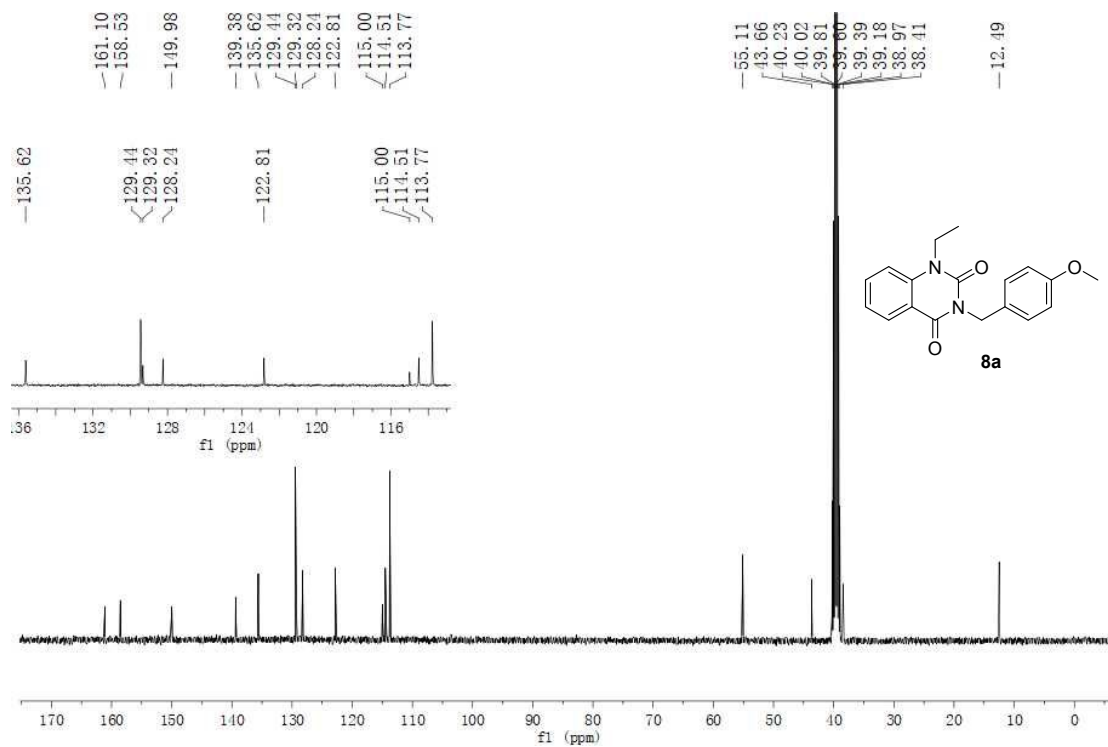


Figure S82. ^{13}C NMR spectra of 1-ethyl-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8a)

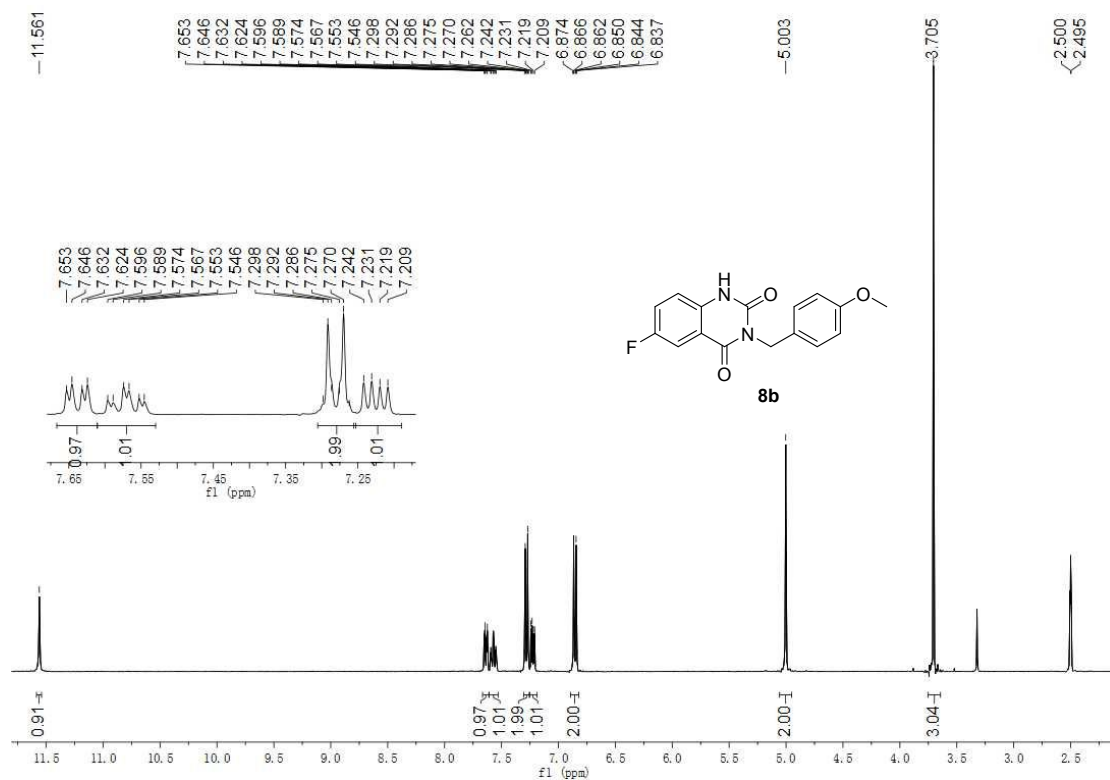


Figure S83. ¹H NMR spectra of 6-fluoro-3-(4-methoxybenzyl)quinazoline-2,4(1*H*,3*H*)-dione (8b)

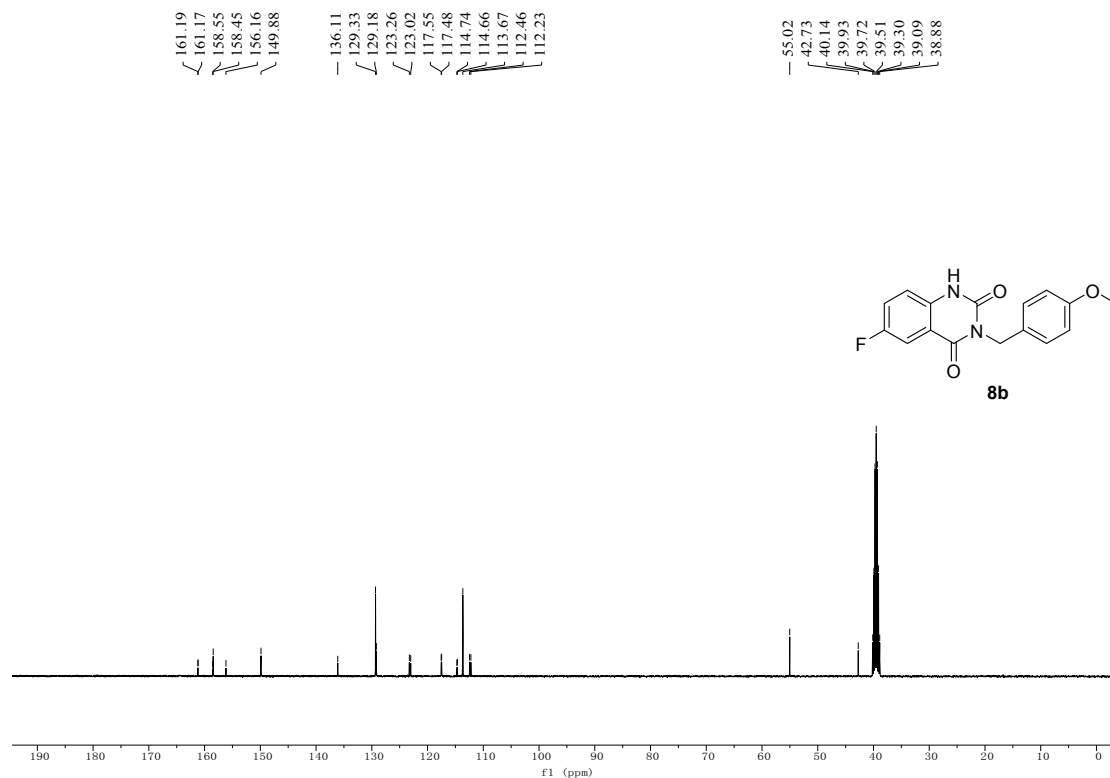


Figure S84. ¹³C NMR spectra of 6-fluoro-3-(4-methoxybenzyl)quinazoline-2,4(1*H*,3*H*)-dione (8b)

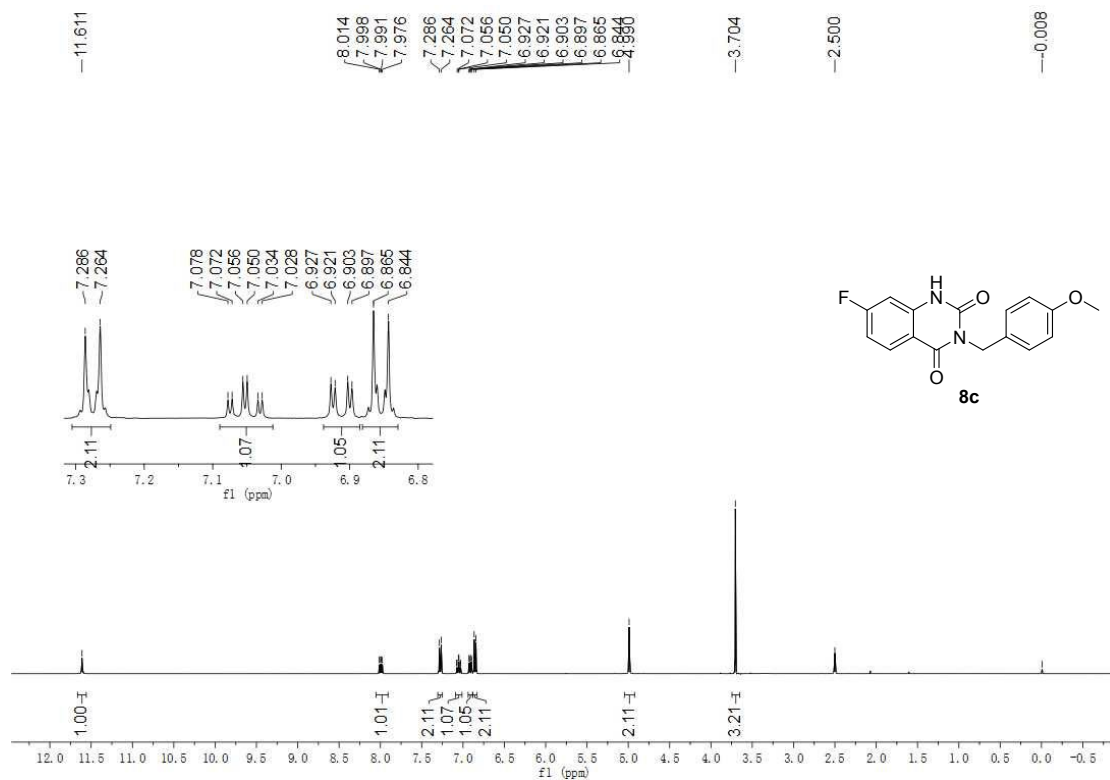


Figure S85. ¹H NMR spectra of 7-fluoro-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8c)

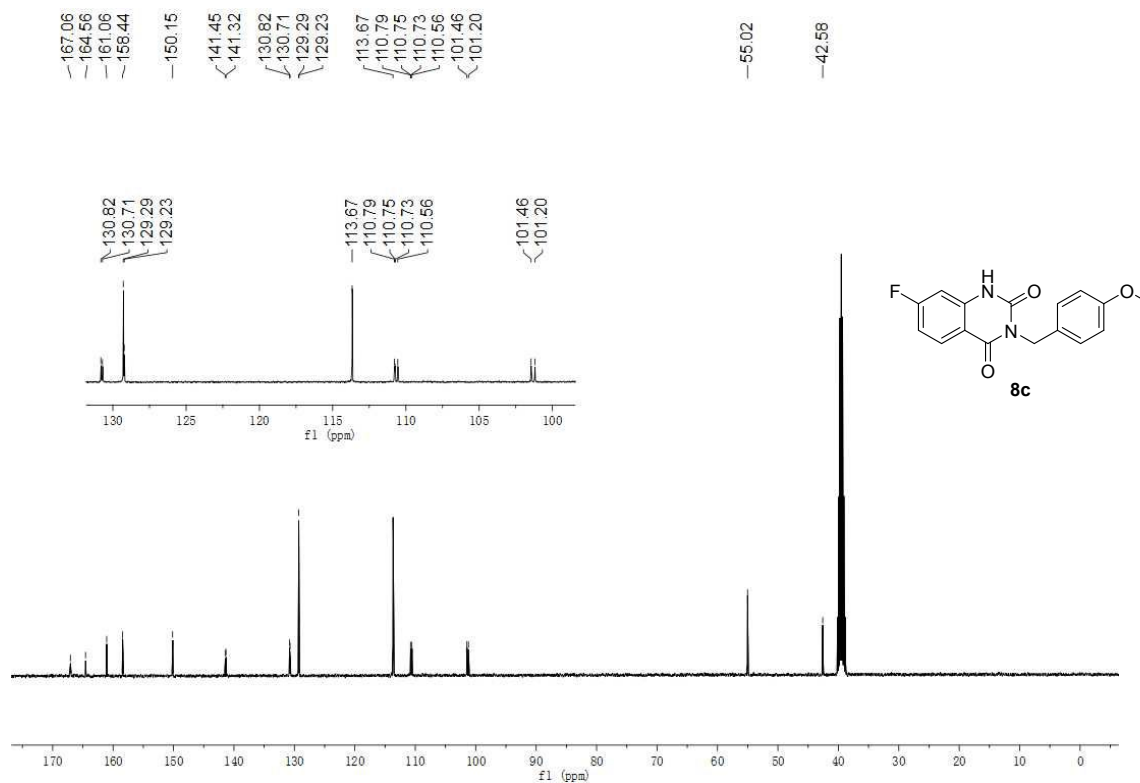
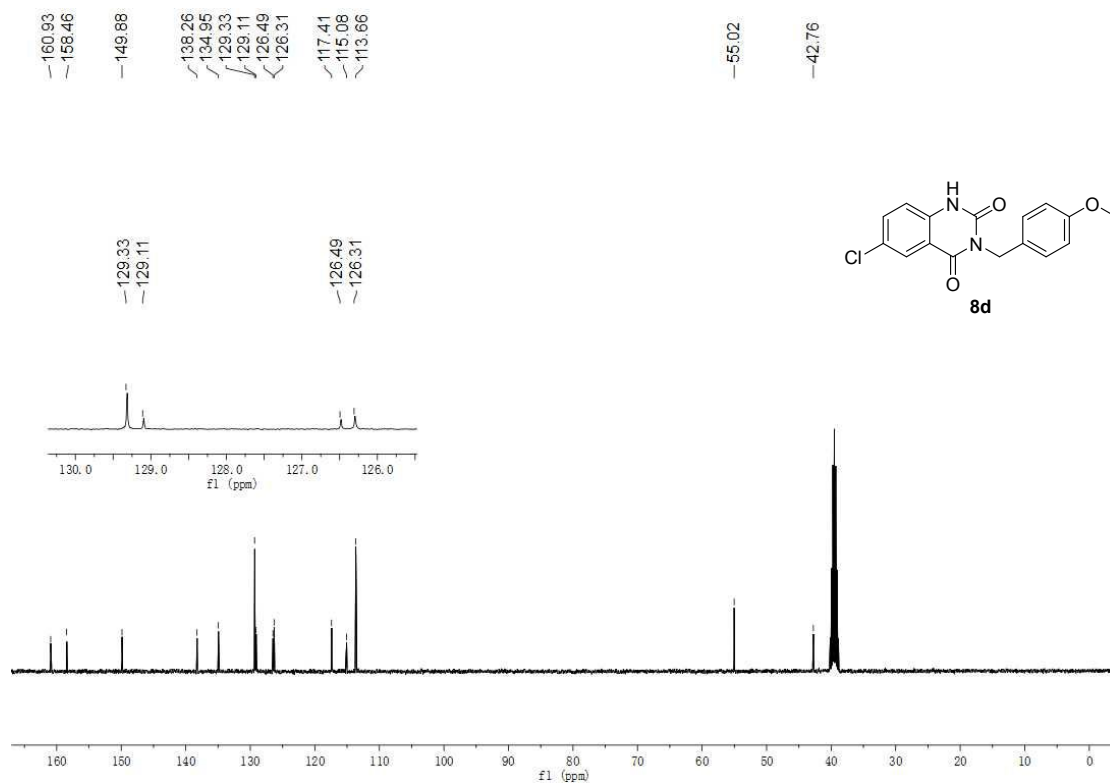
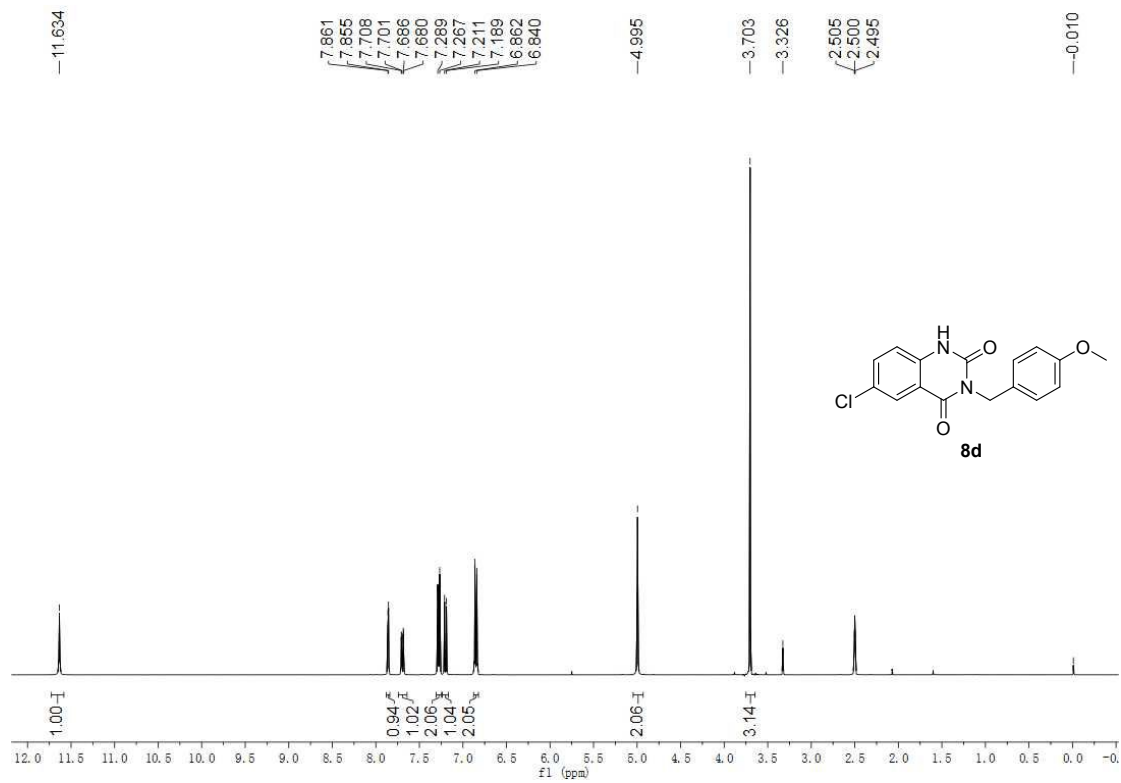


Figure S86. ¹³C NMR spectra of 7-fluoro-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8c)



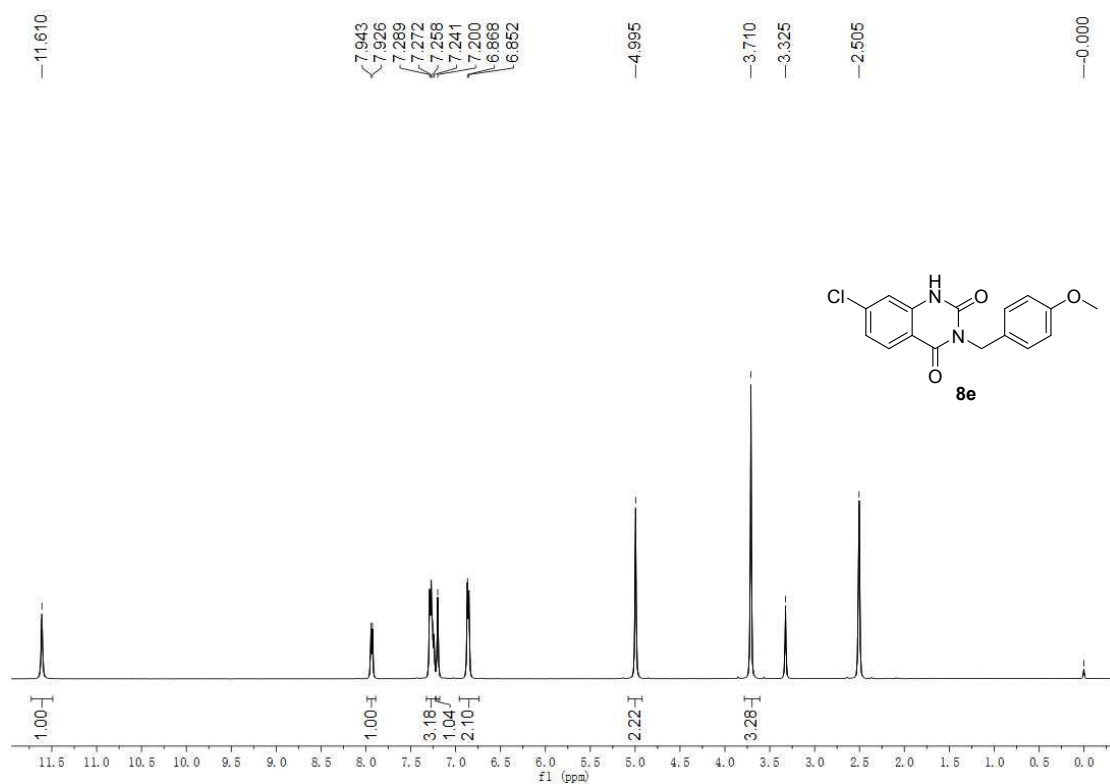


Figure S89. ¹H NMR spectra of 7-chloro-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8e)

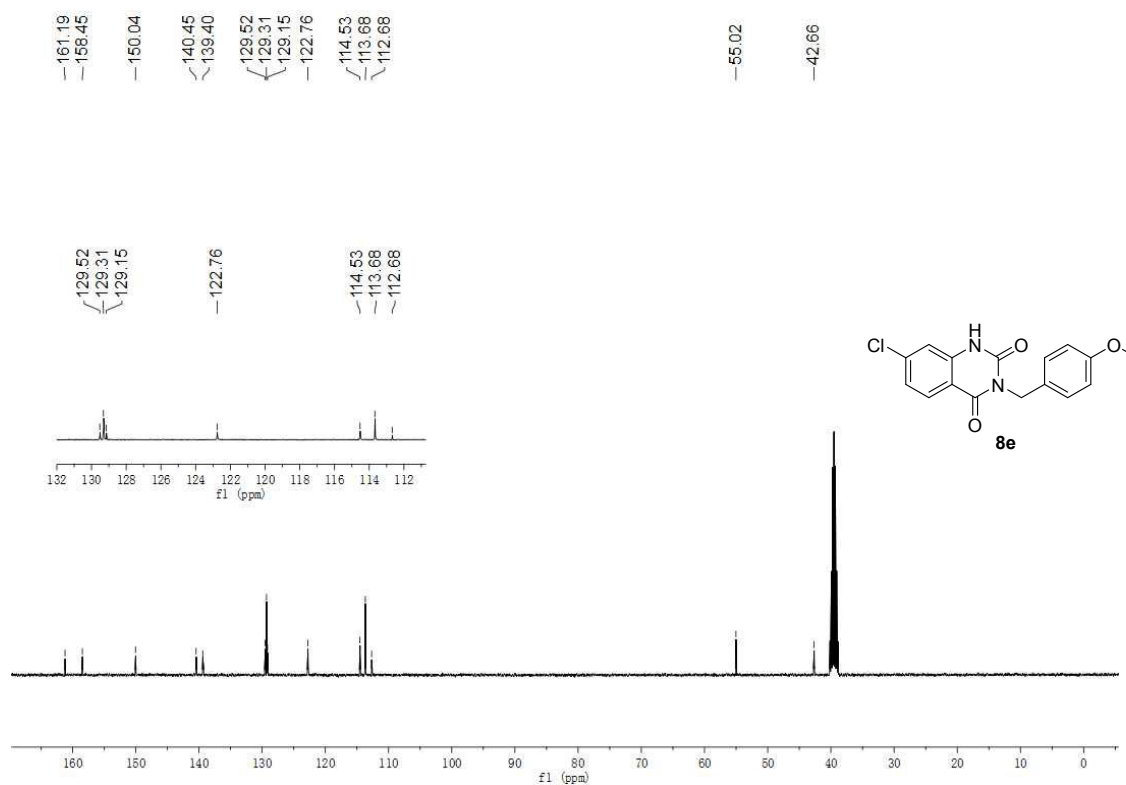


Figure S90. ¹³C NMR spectra of 7-chloro-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8e)

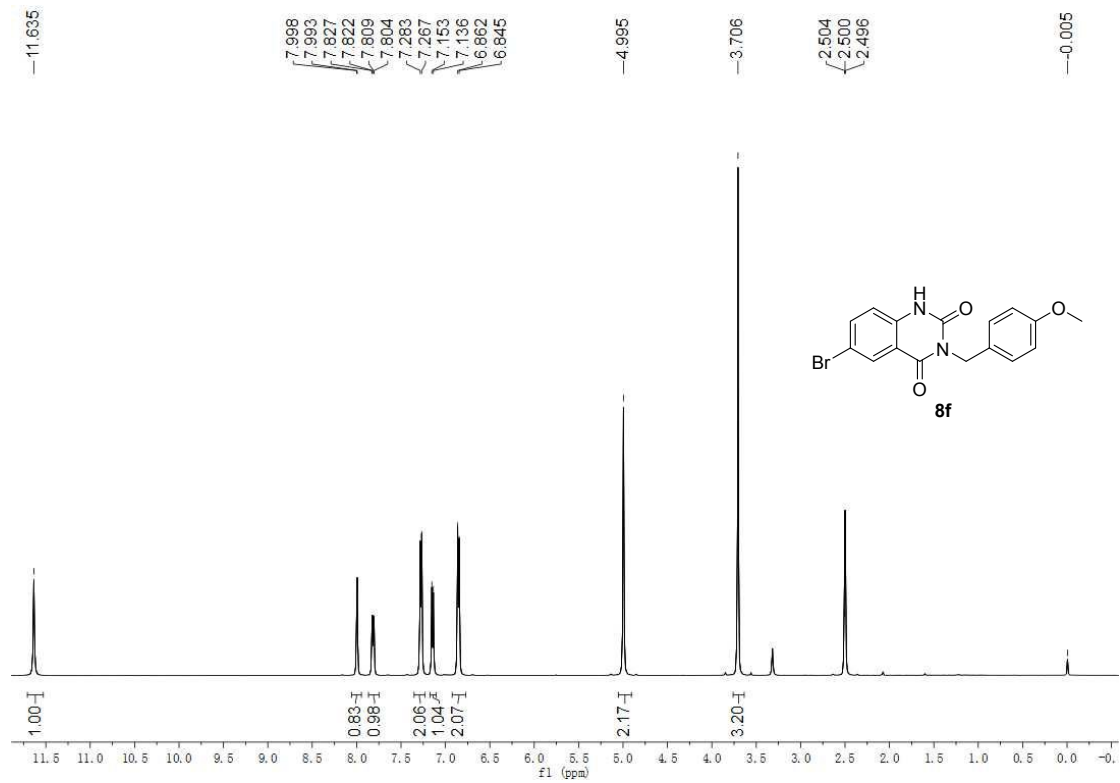


Figure S91. ¹H NMR spectra of 6-bromo-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8f)

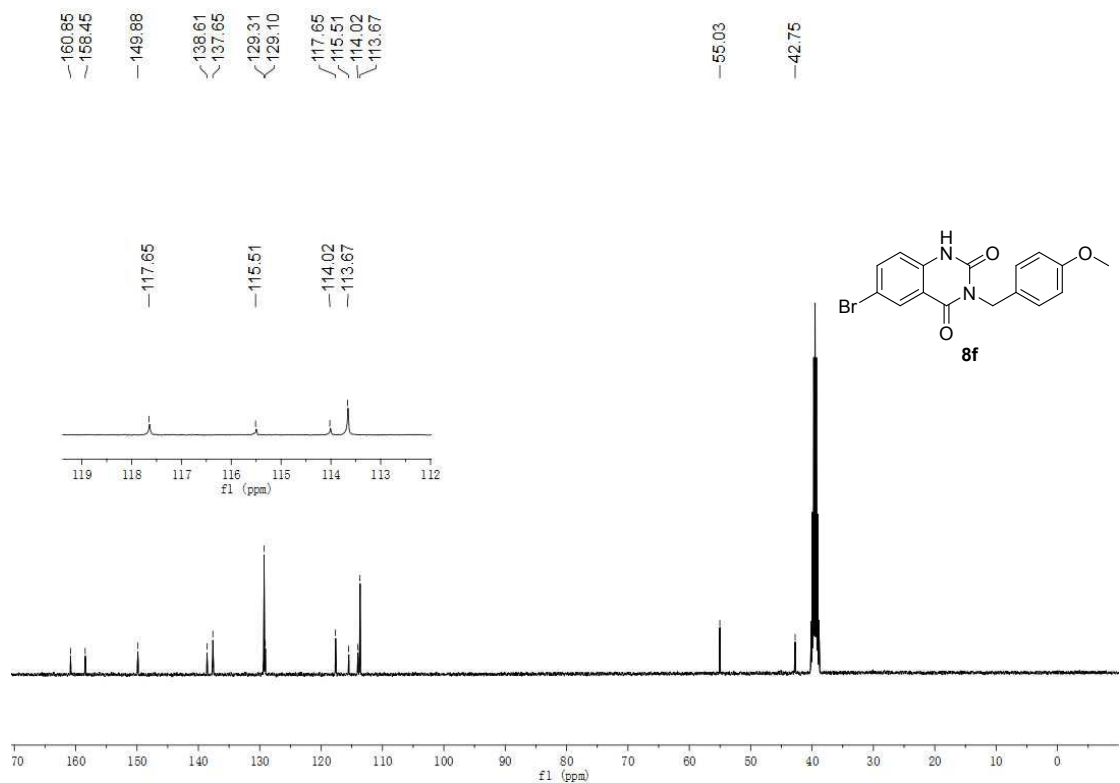


Figure S92. ¹³C NMR spectra of 6-bromo-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8f)

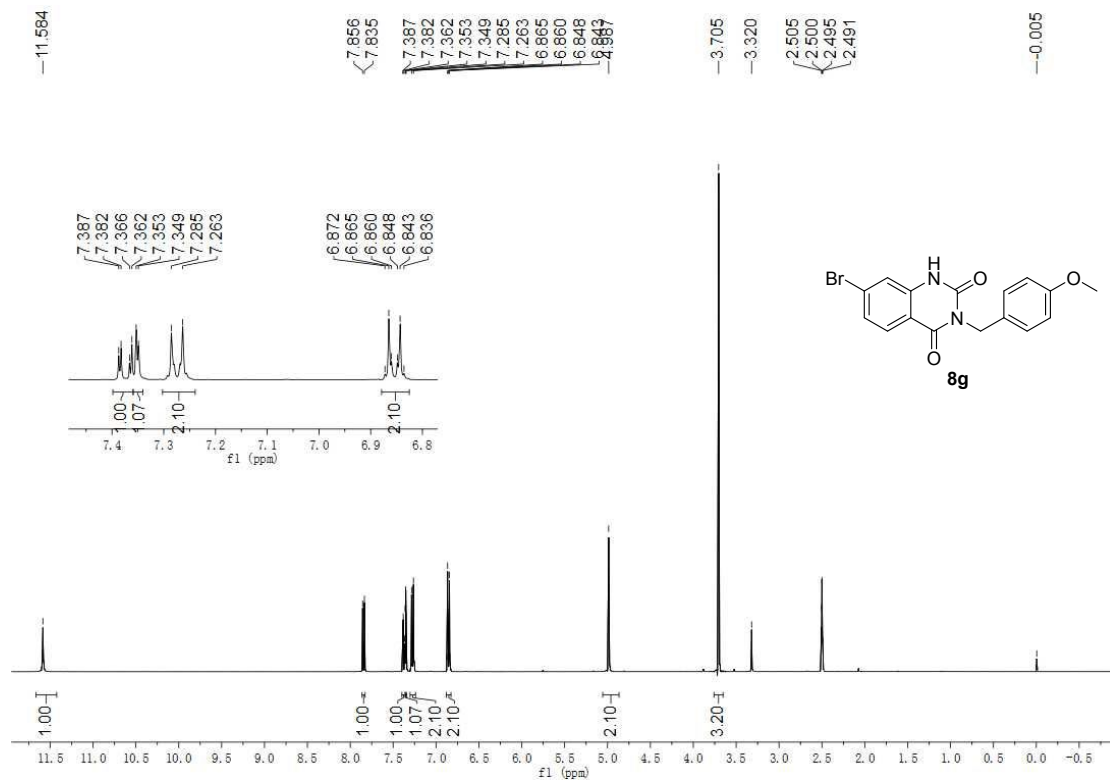


Figure S93. ¹H NMR spectra of 7-bromo-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8g)

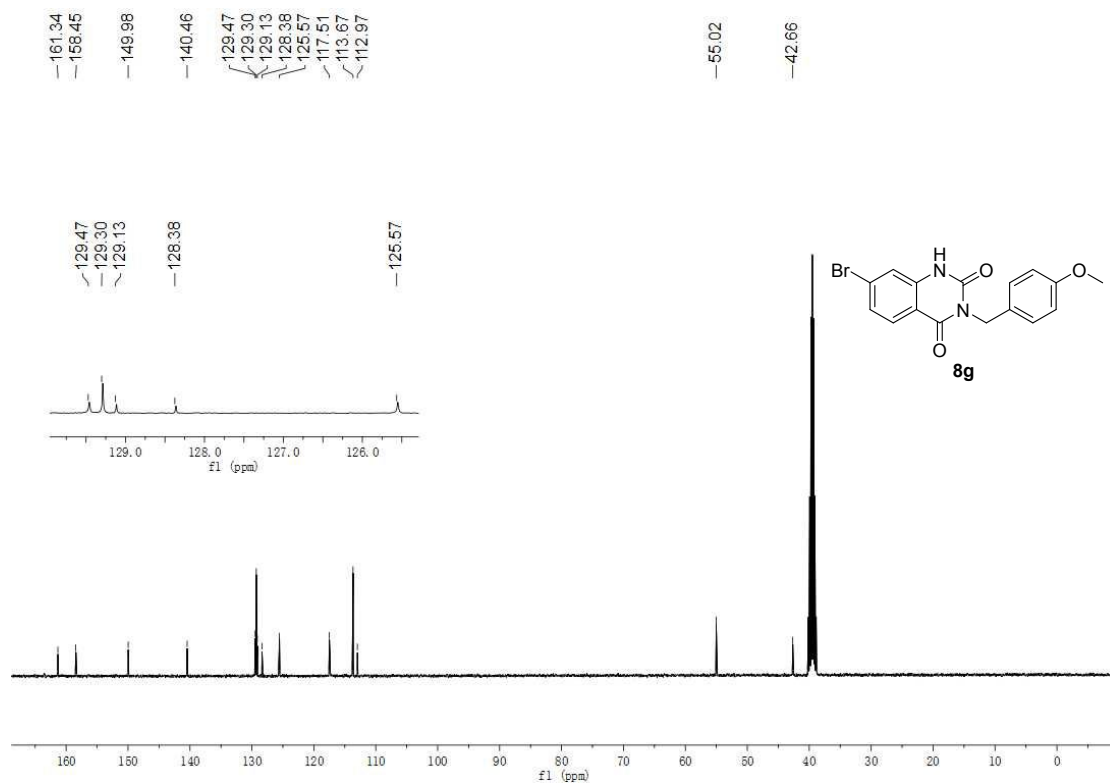
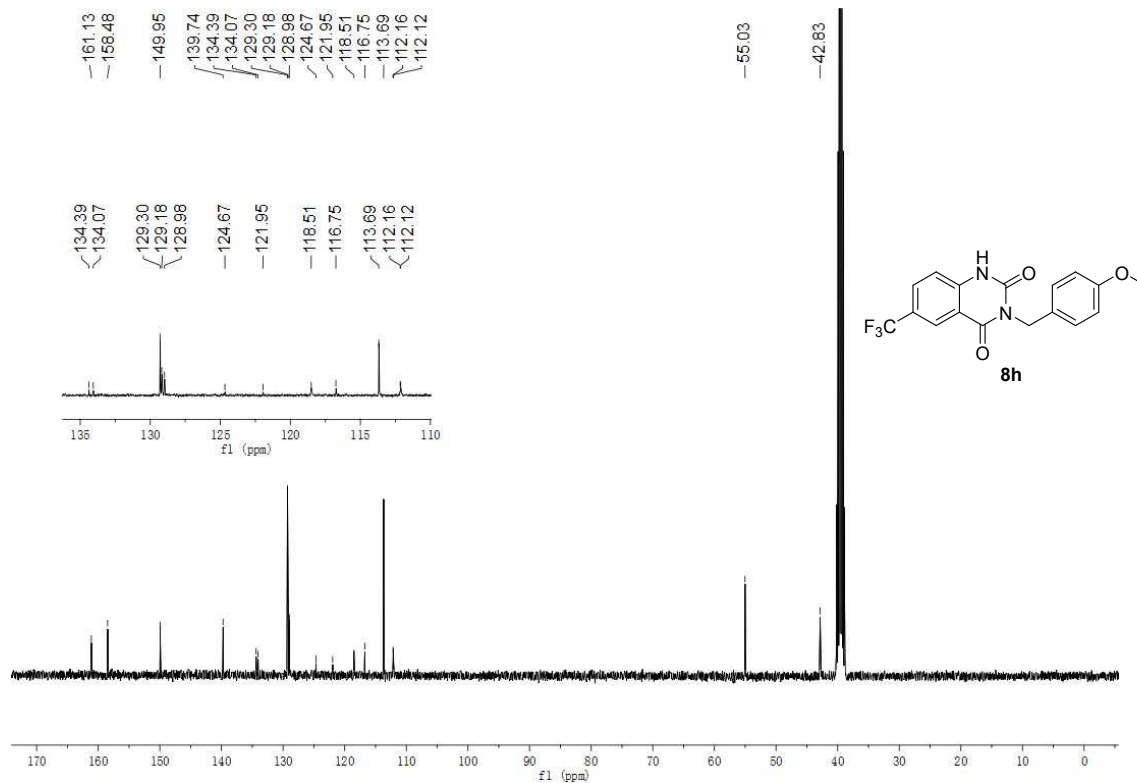
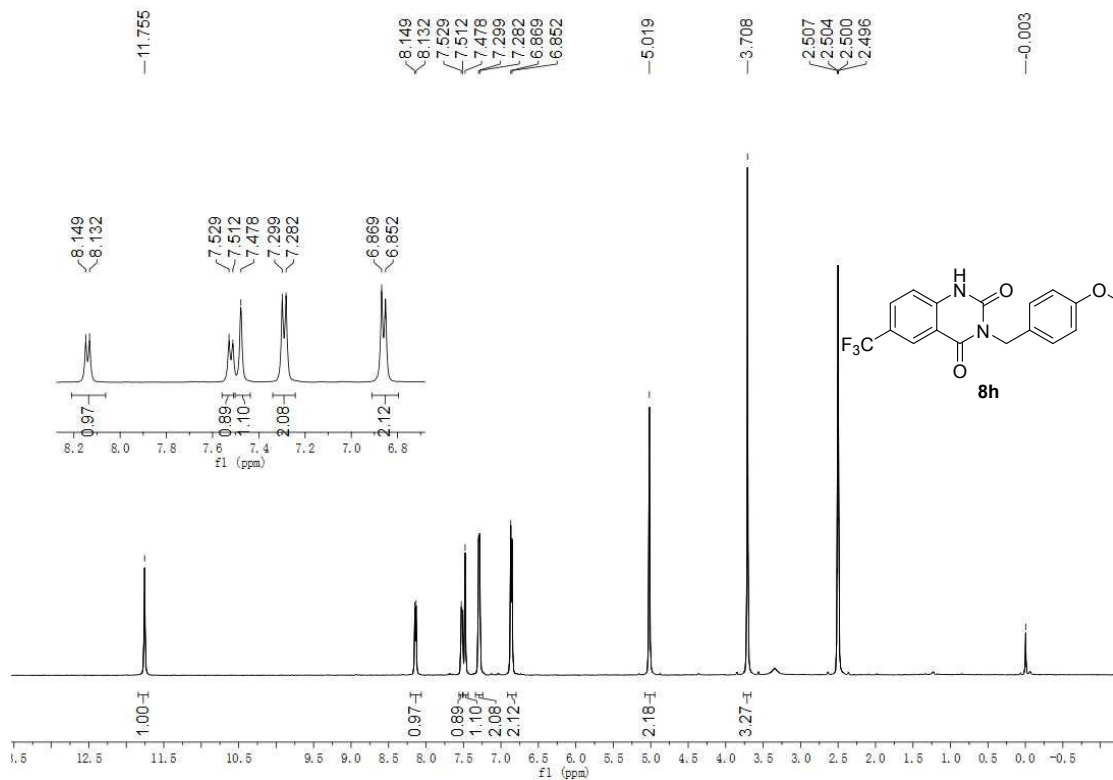


Figure S94. ¹³C NMR spectra of 7-bromo-3-(4-methoxybenzyl)quinazoline-2,4(1H,3H)-dione (8g)



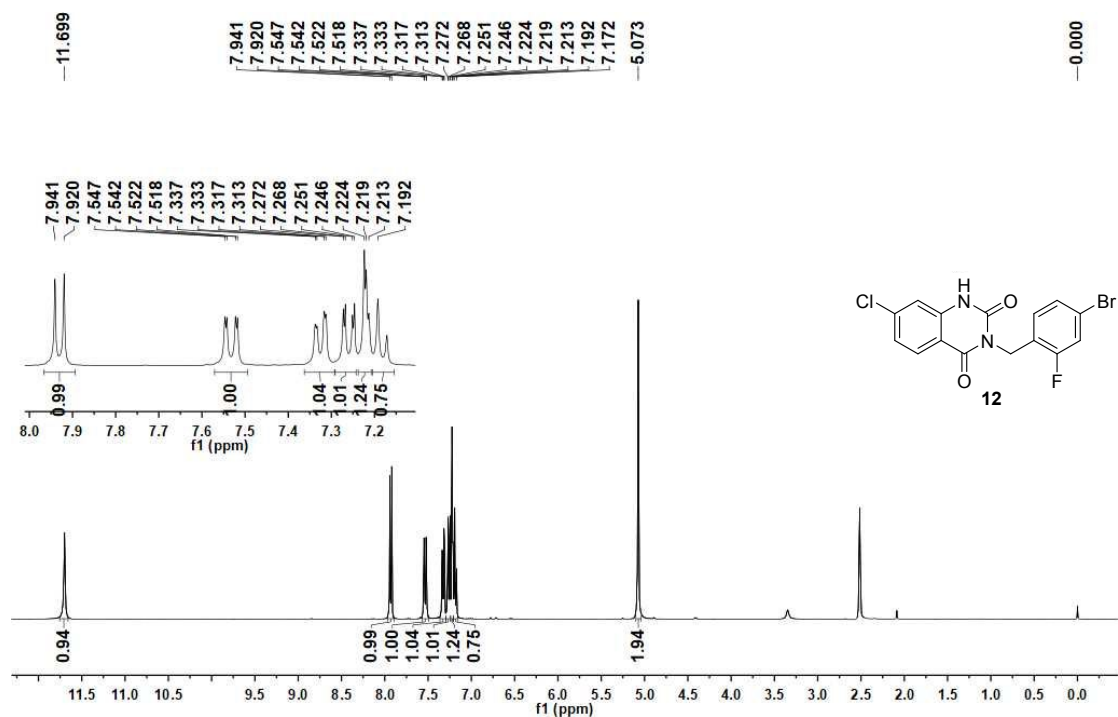


Figure S97. ¹H NMR spectra of 3-(4-bromo-2-fluorobenzyl)-7-chloroquinazoline-2,4(1H,3H)-dione (12)

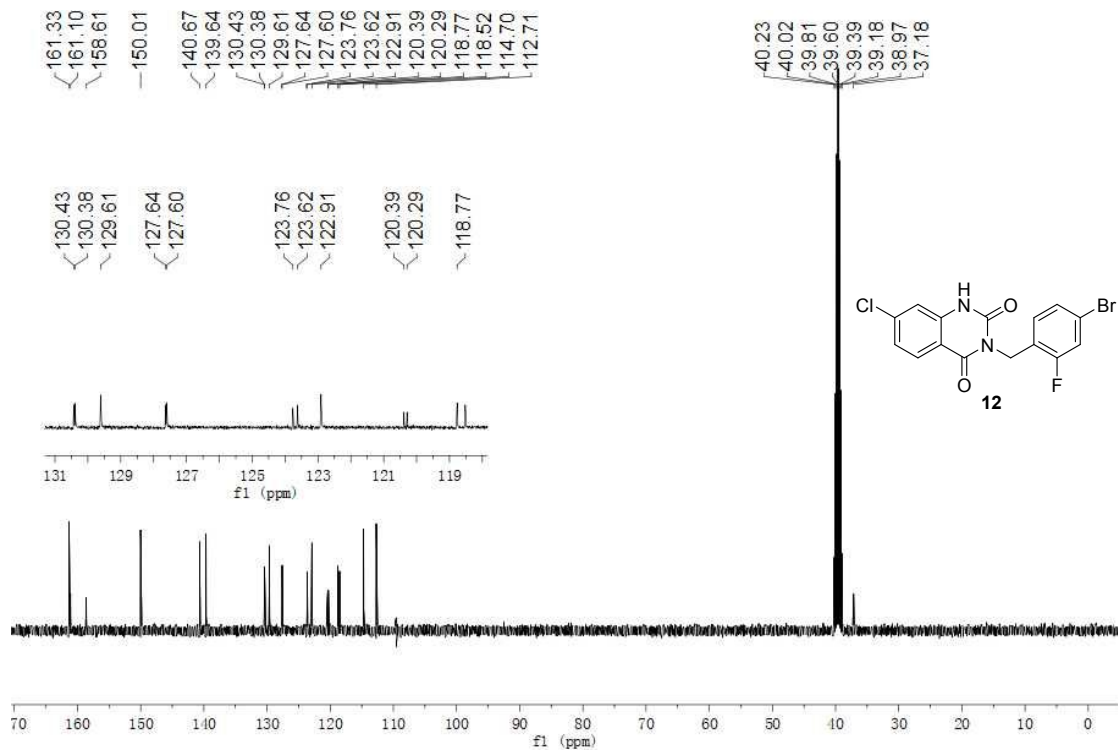


Figure S98. ¹³C NMR spectra of 3-(4-bromo-2-fluorobenzyl)-7-chloroquinazoline-2,4(1H,3H)-dione (12)

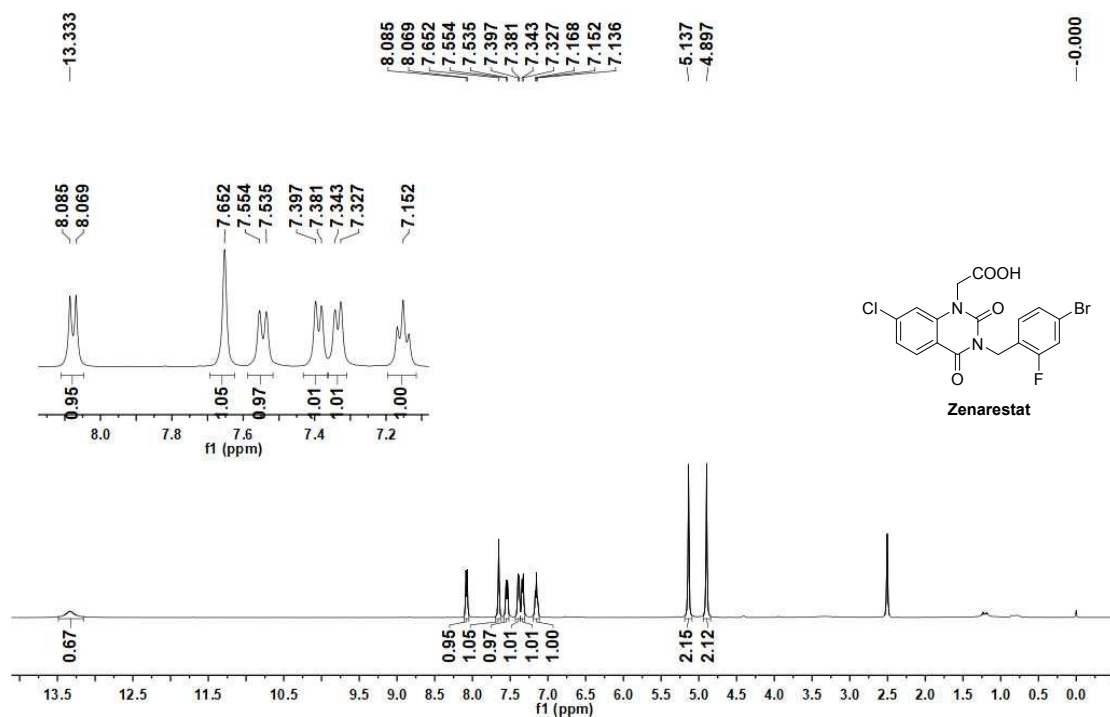


Figure S99. ¹H NMR spectra of Zenarestat

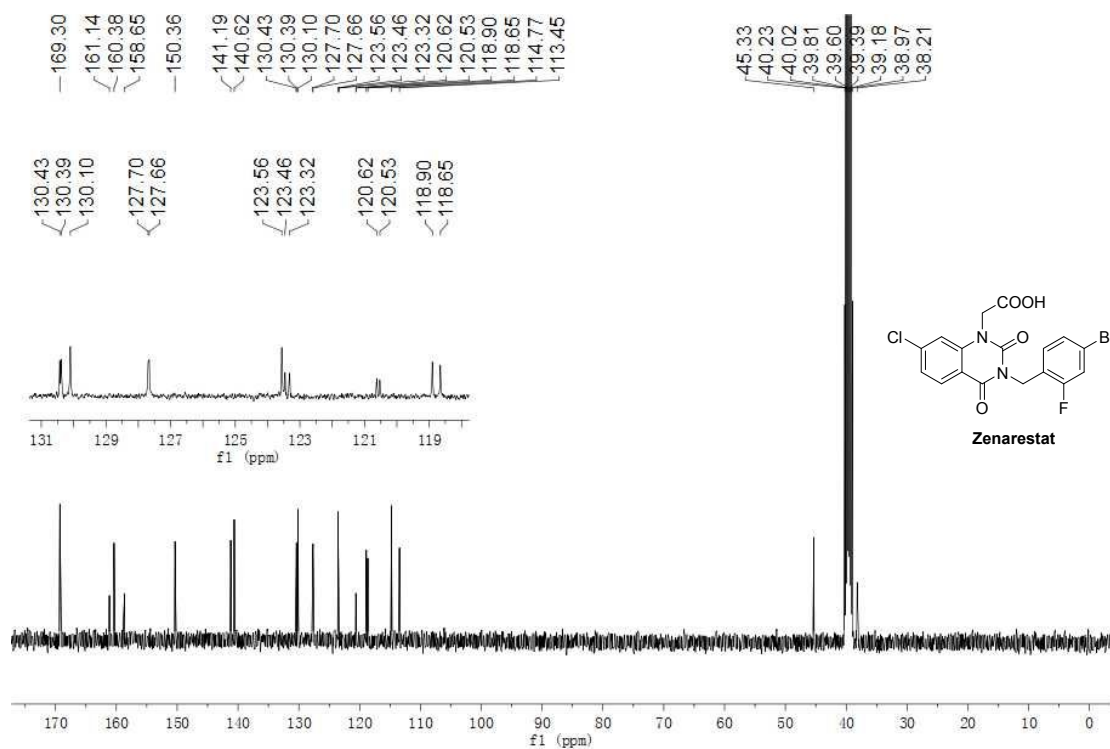


Figure S100. ¹³C NMR spectra of Zenarestat