Supplementary Information

Synthesis, Antioxidant Activity, Acetylcholinesterase Inhibition and Quantum Studies of Thiosemicarbazones

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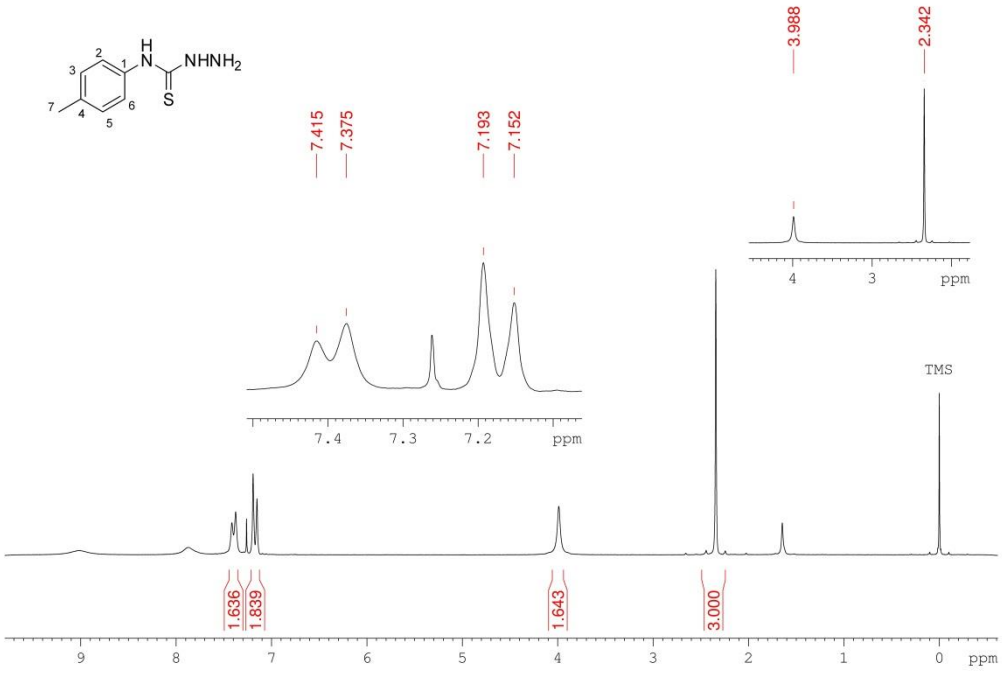

Figure S1. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **1**.

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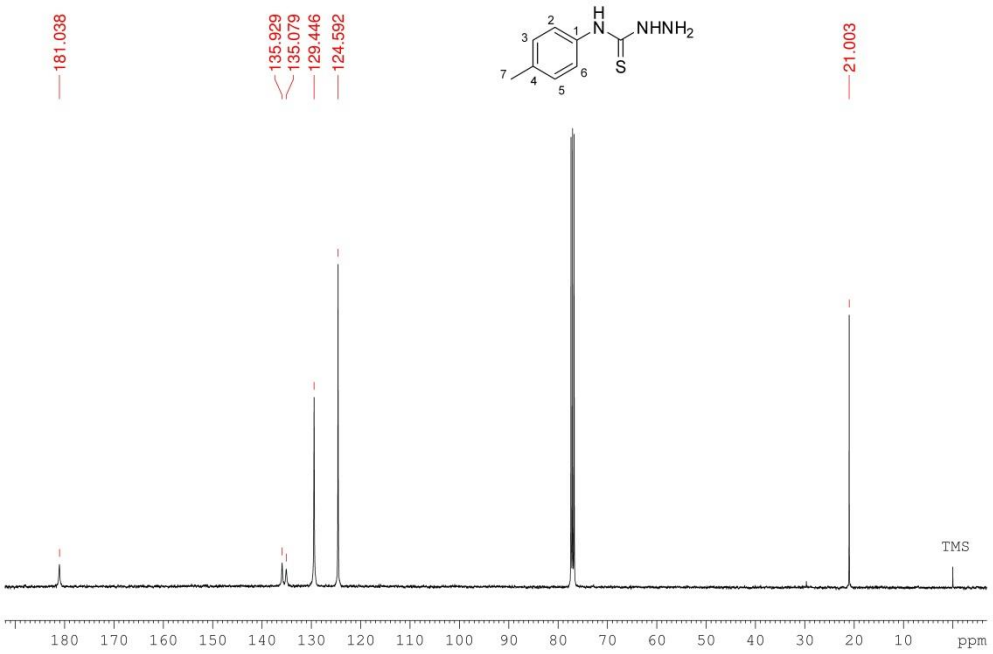

Figure S2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **1**.

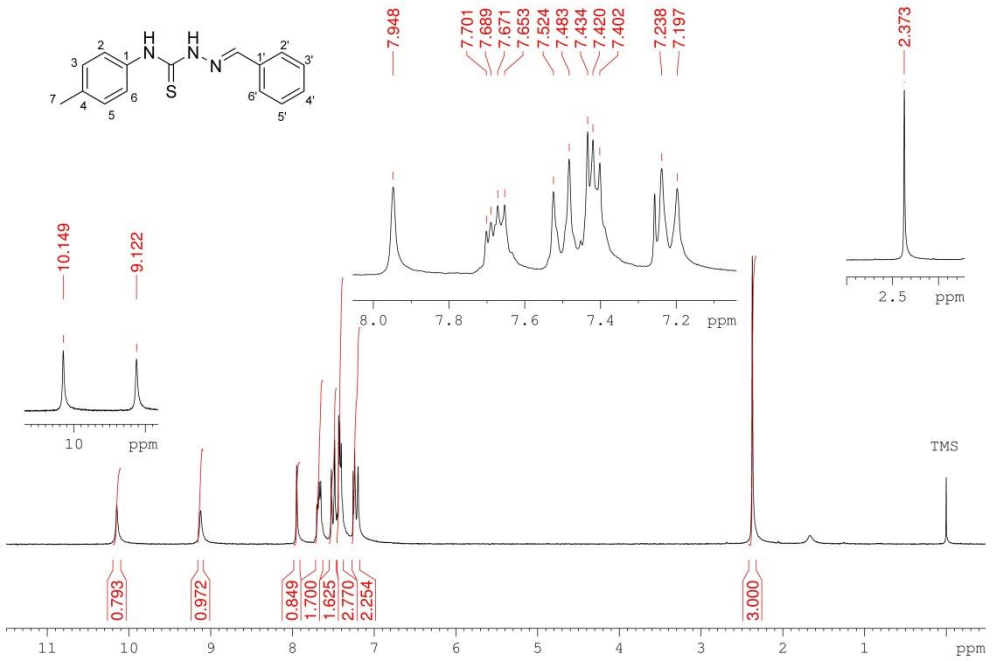

Figure S3. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2a**.

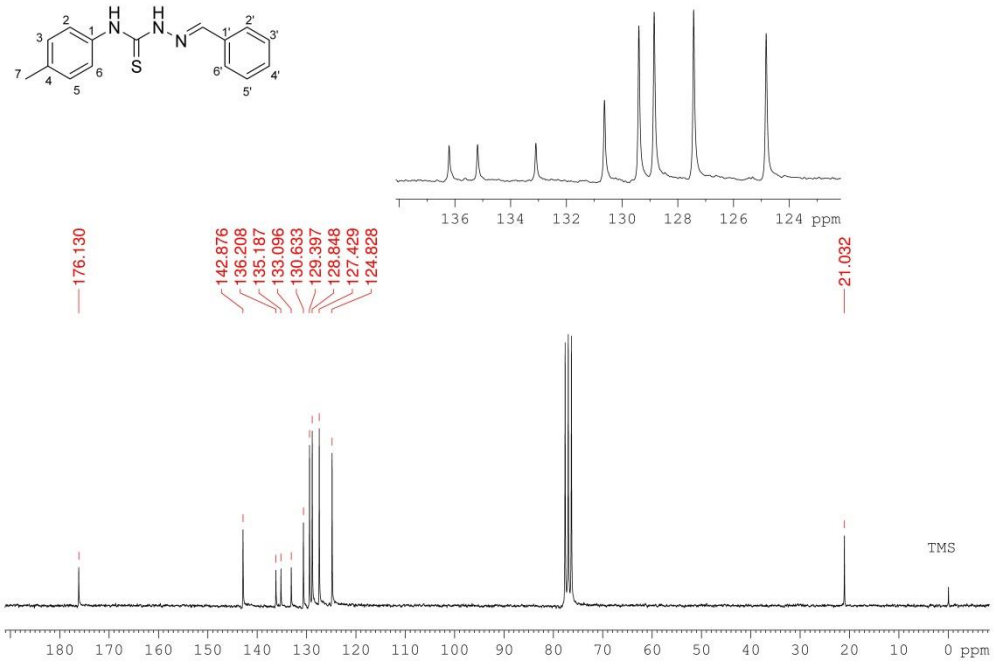

Figure S4. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2a**.

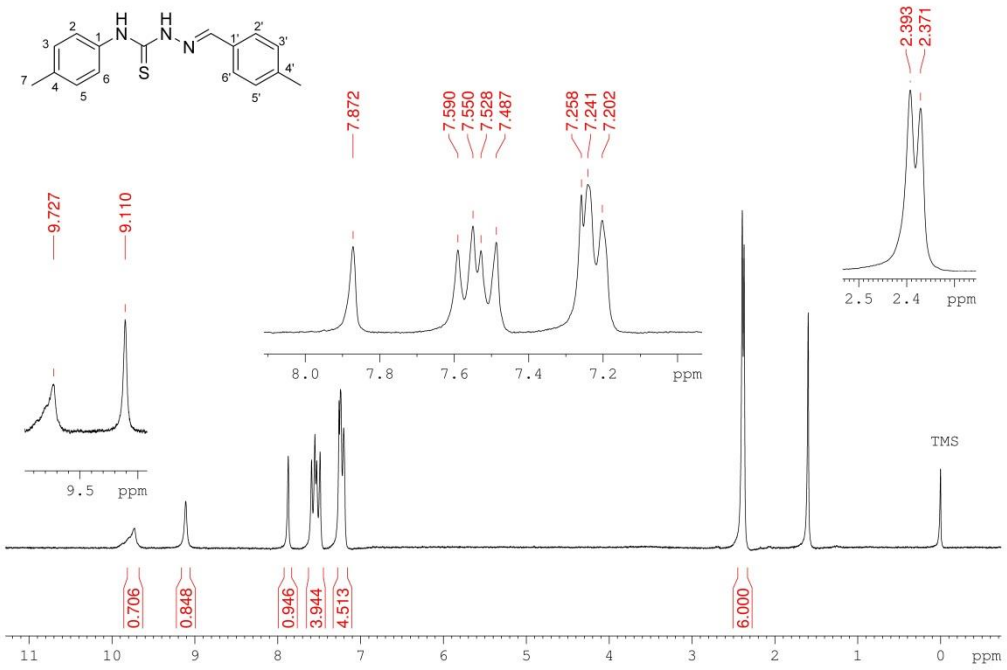

Figure S5. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2b**.

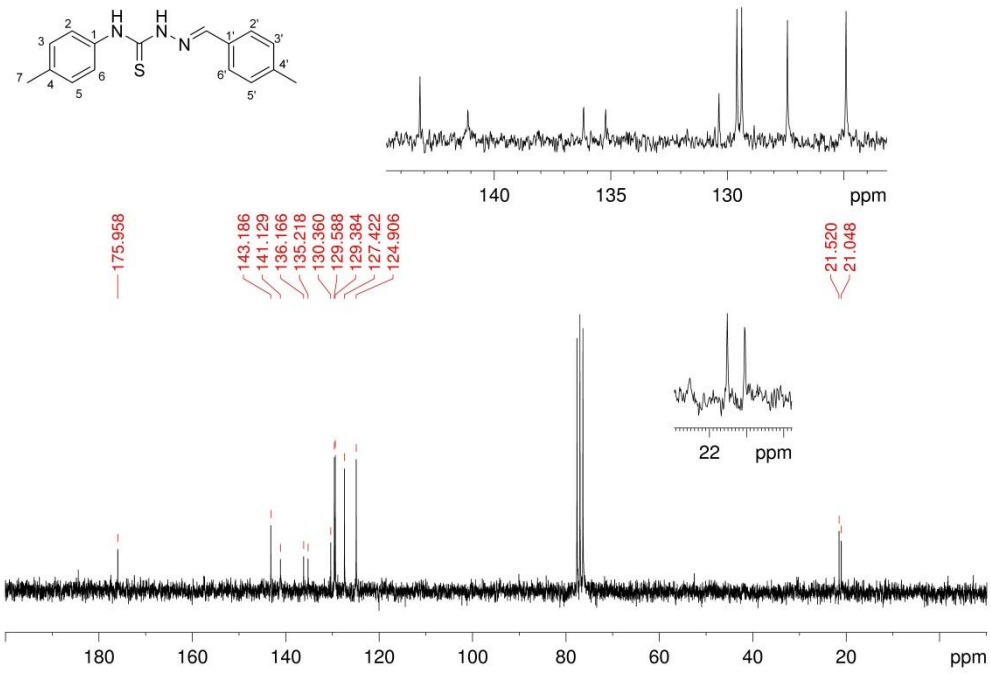

Figure S6. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2b**.

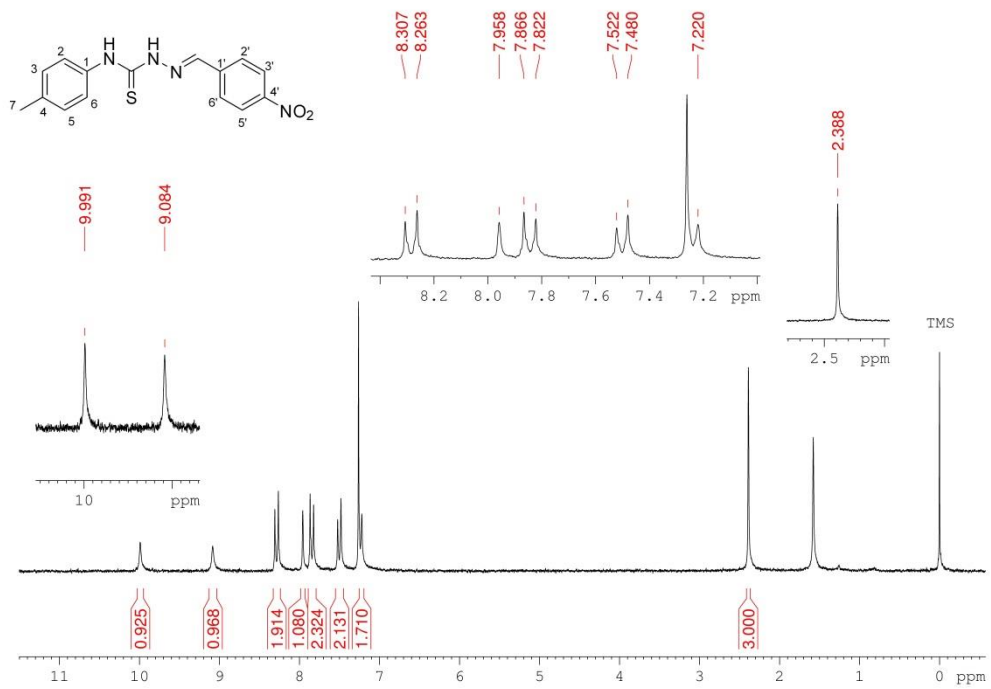

Figure S7. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2c**.

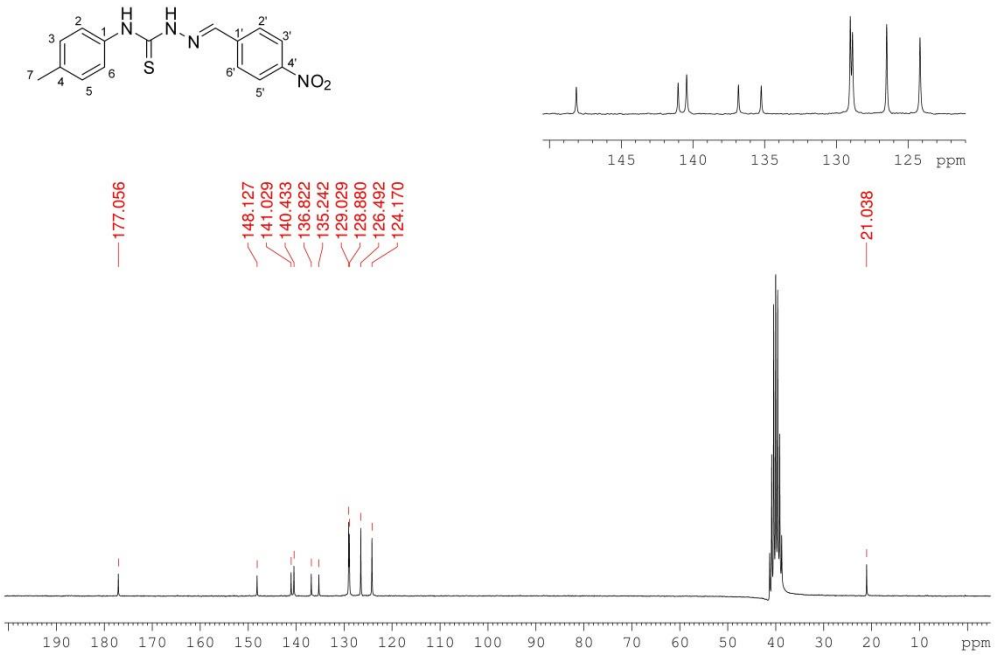

Figure S8. ^{13}C NMR spectrum (50 MHz, DMSO) of compound **2c**.

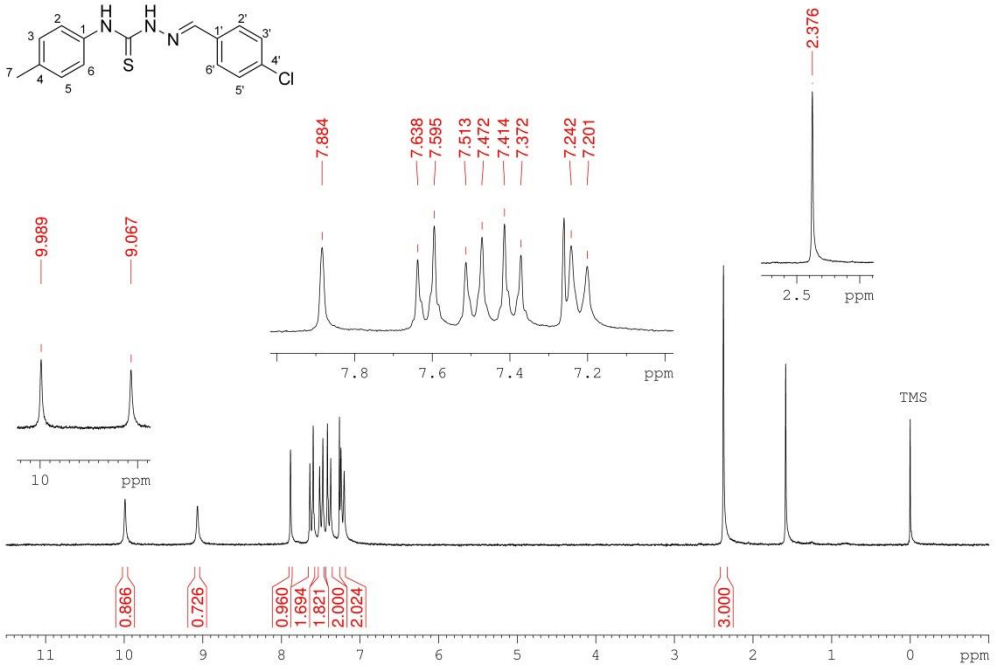

Figure S9. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2d**.

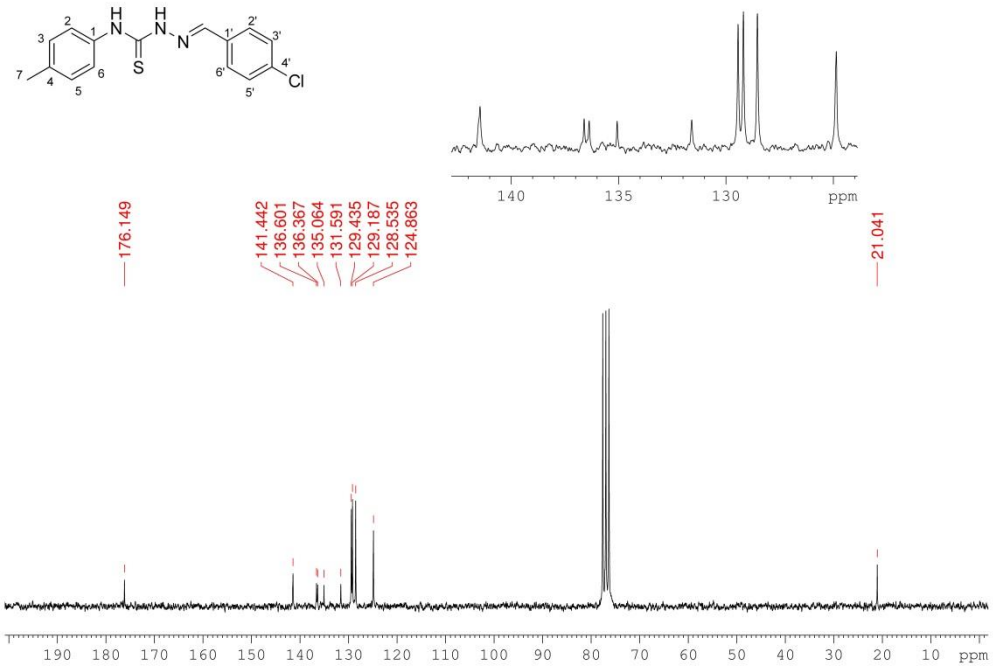

Figure S10. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2d**.

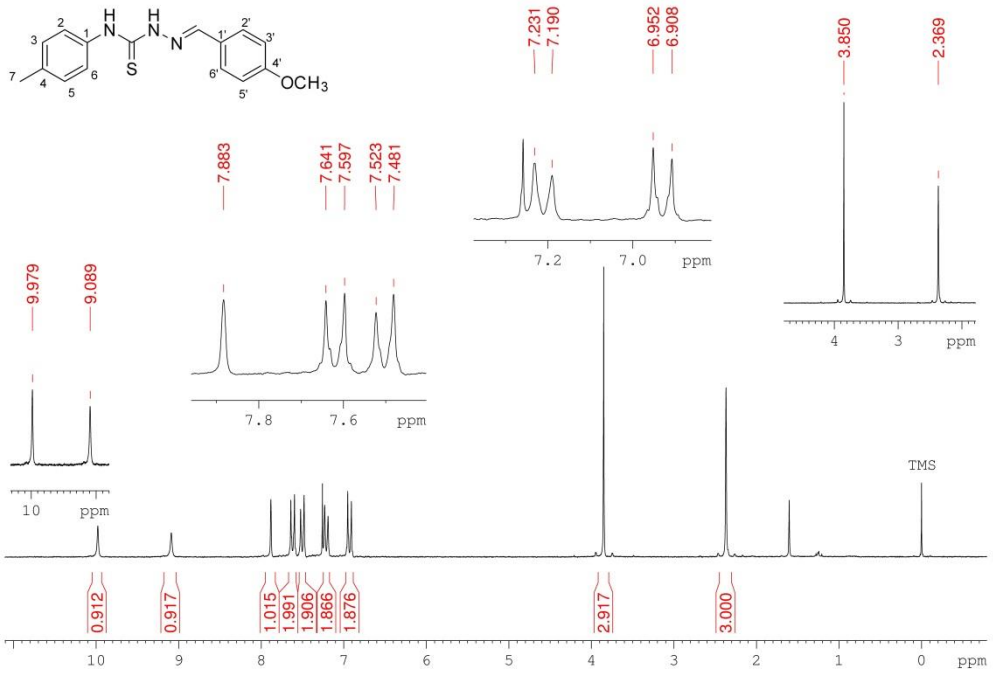

Figure S11. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2e**.

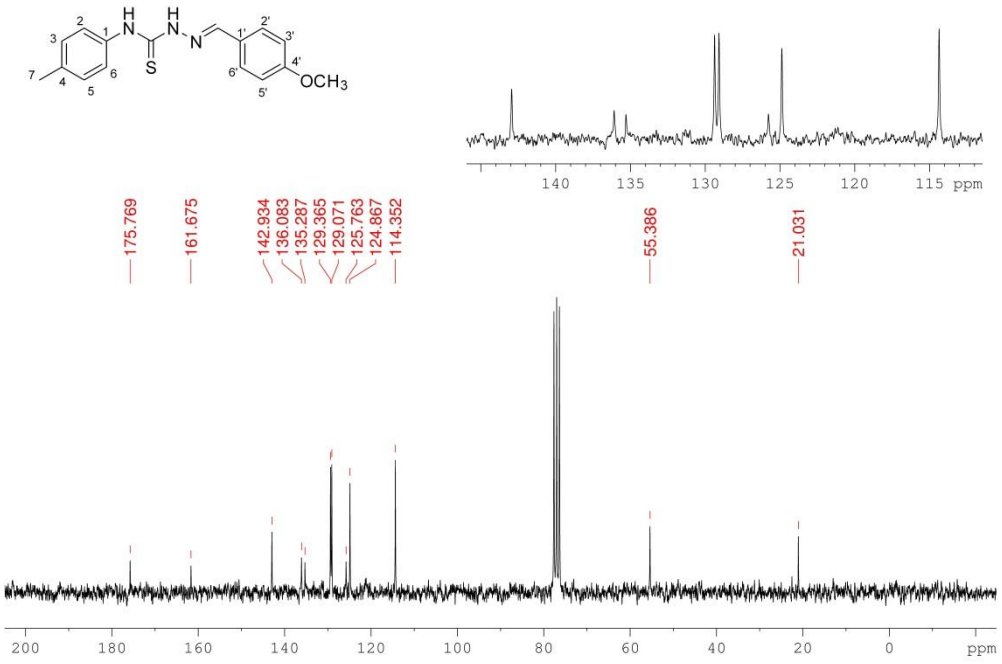

Figure S12. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2e**.

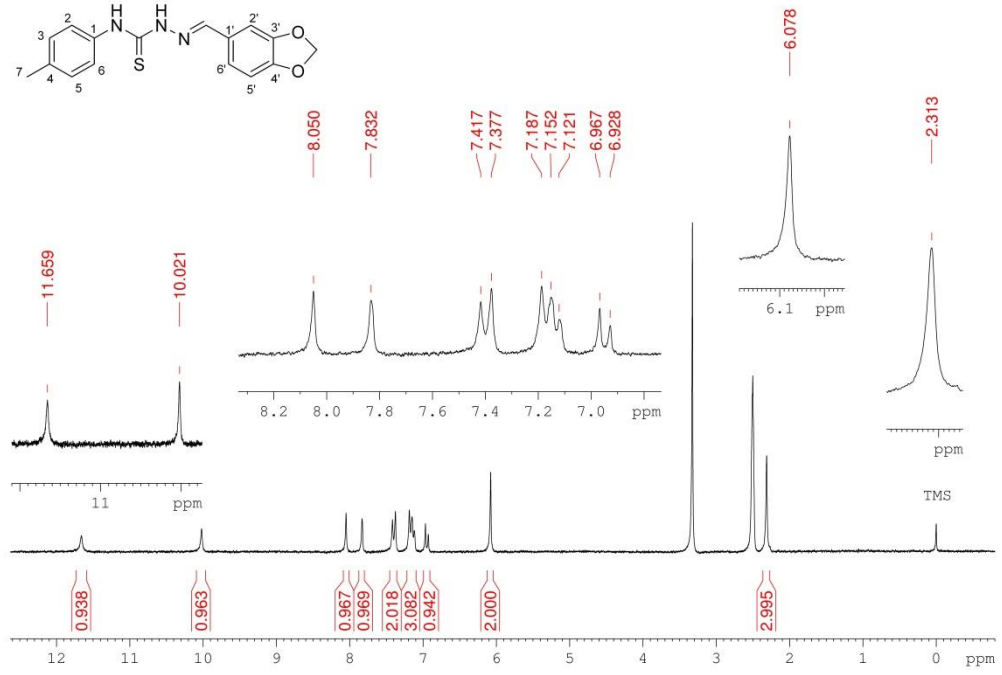

Figure S13. ^{1}H NMR spectrum (200 MHz, DMSO) of compound **2f**.

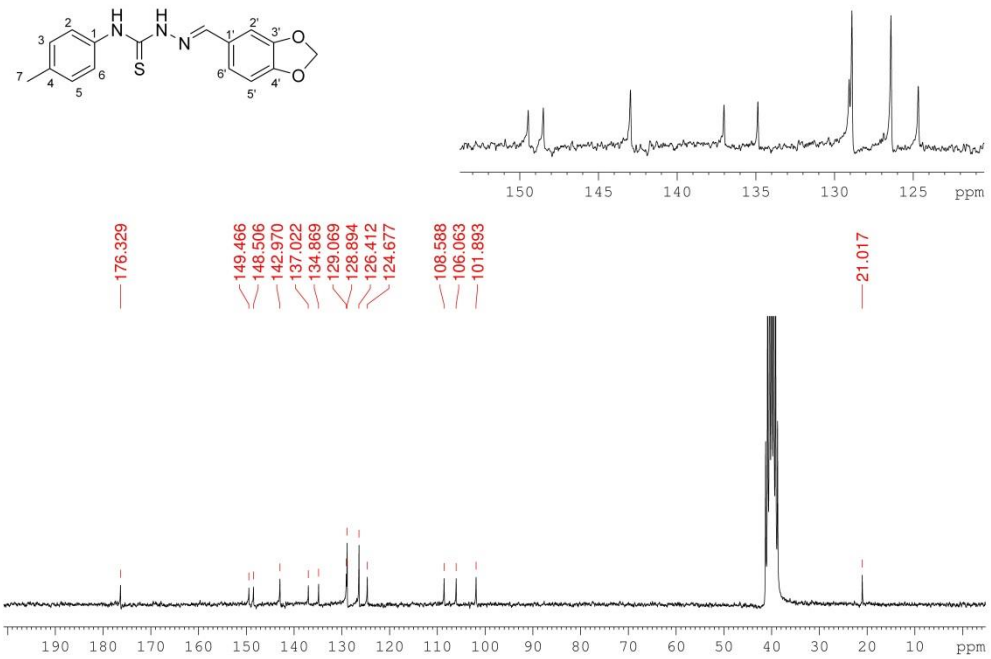

Figure S14. ^{13}C NMR spectrum (50 MHz, DMSO) of compound **2f**.

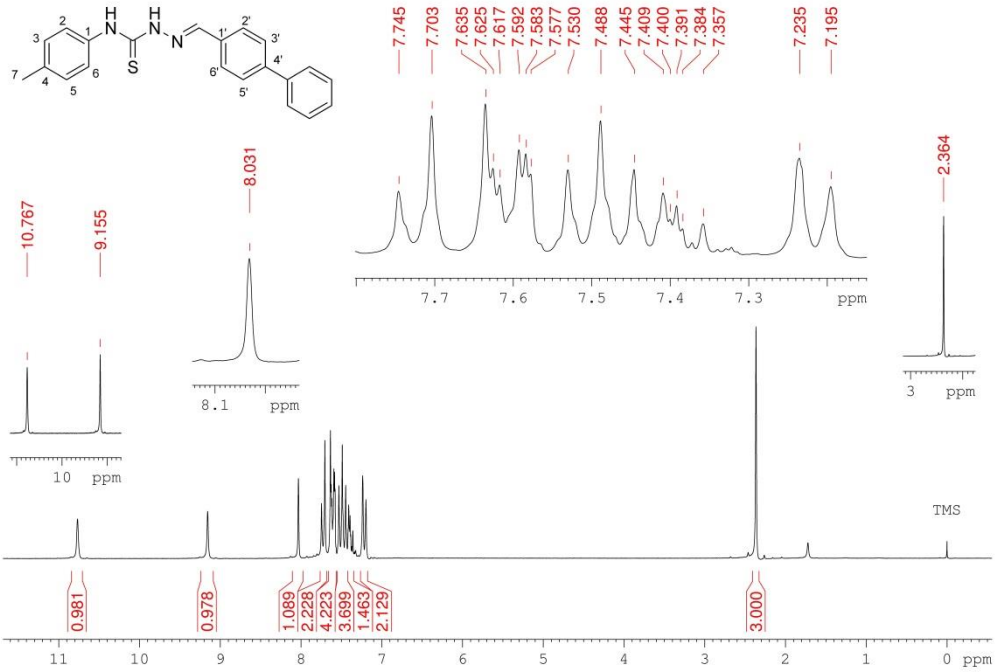

Figure S15. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2g**.

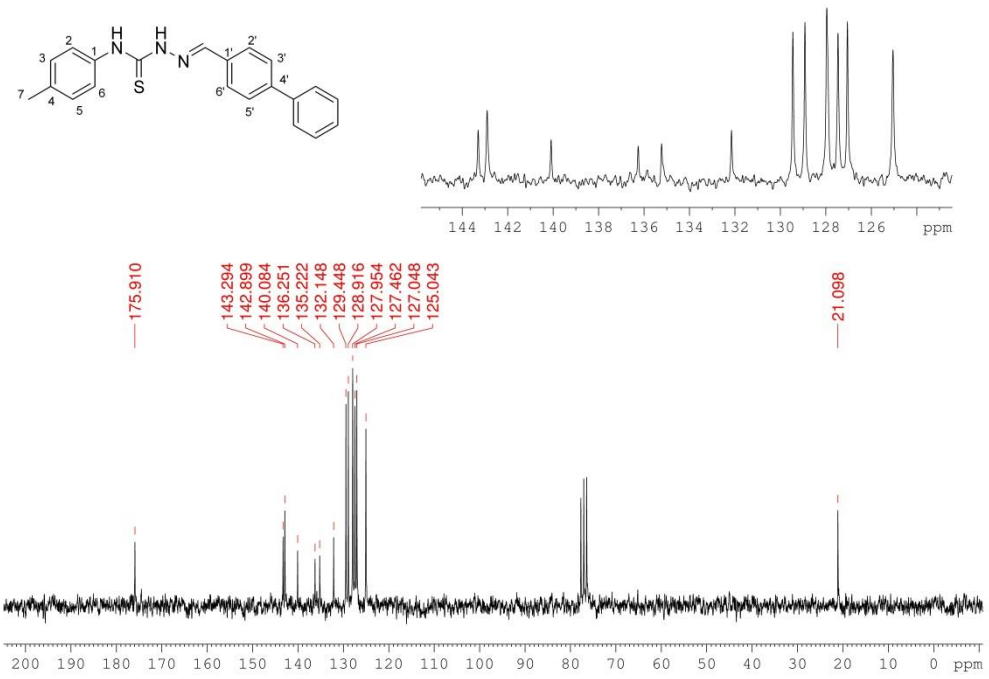

Figure S16. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2g**.

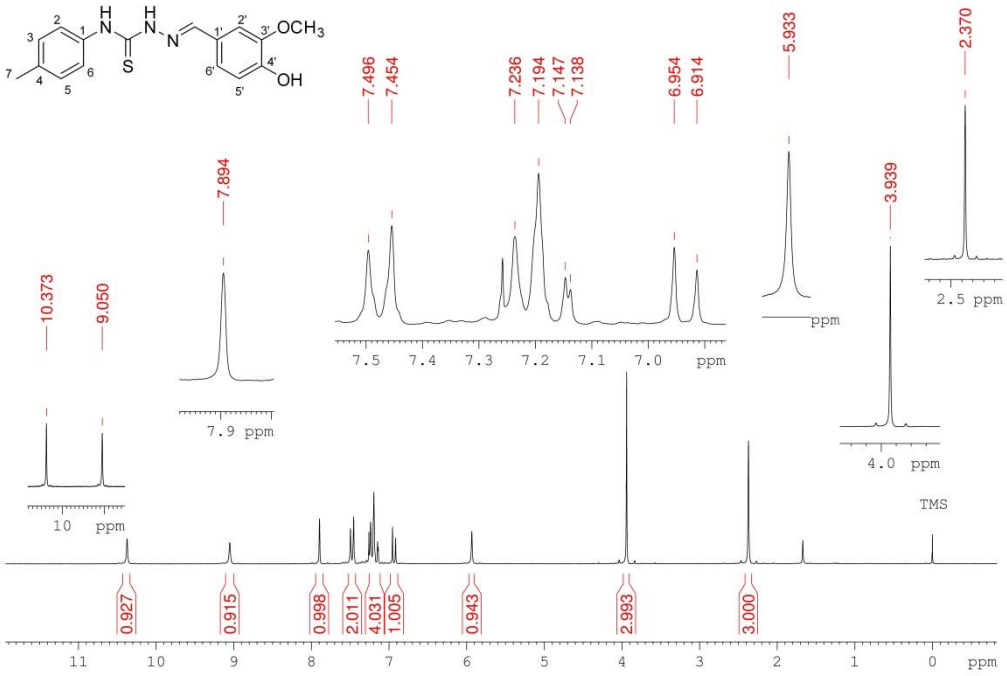

Figure S17. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2h**.

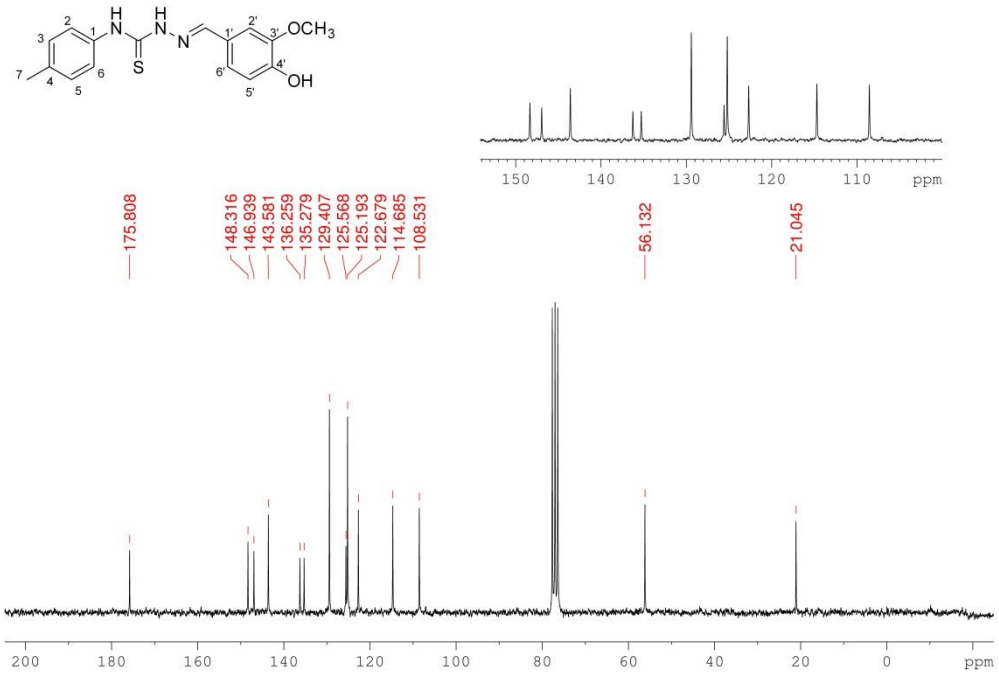

Figure S18. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2h**.

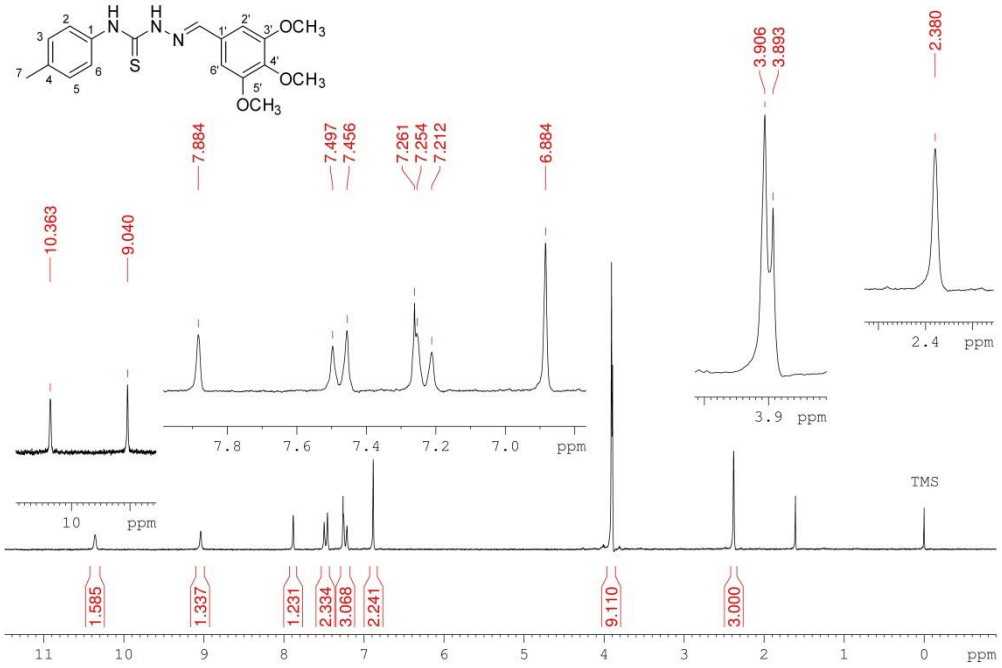

Figure S19. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2i**.

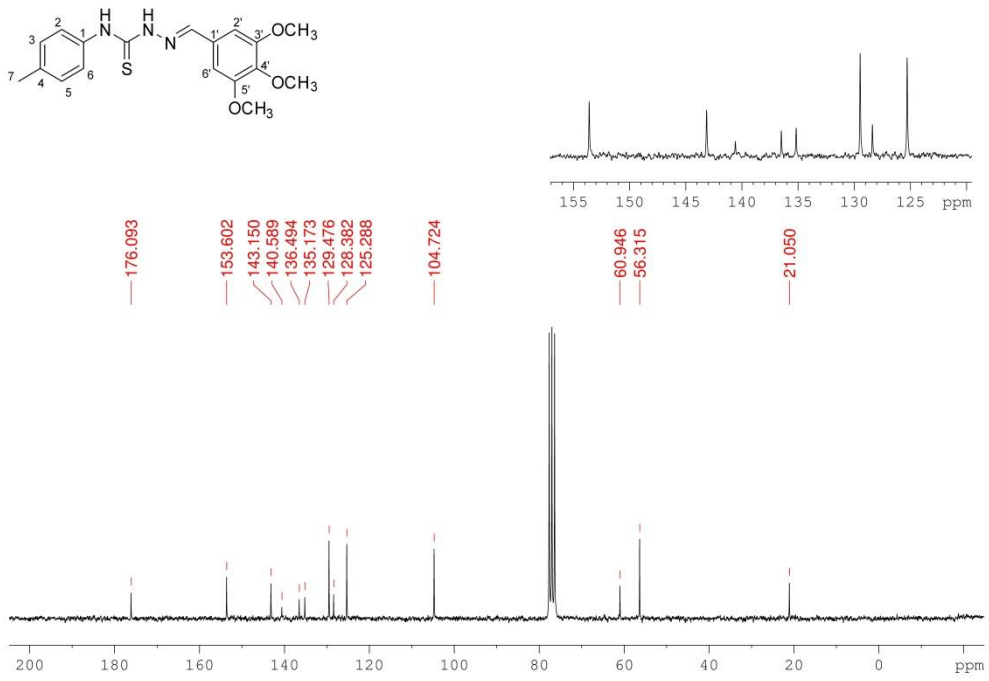

Figure S20. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2i**.

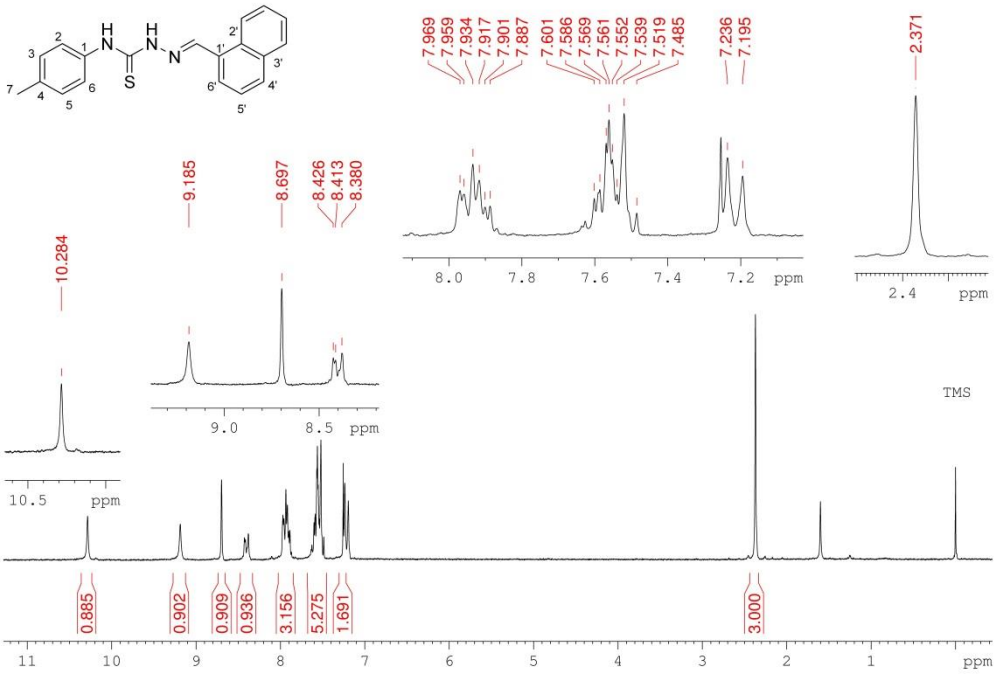

Figure S21. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2j**.

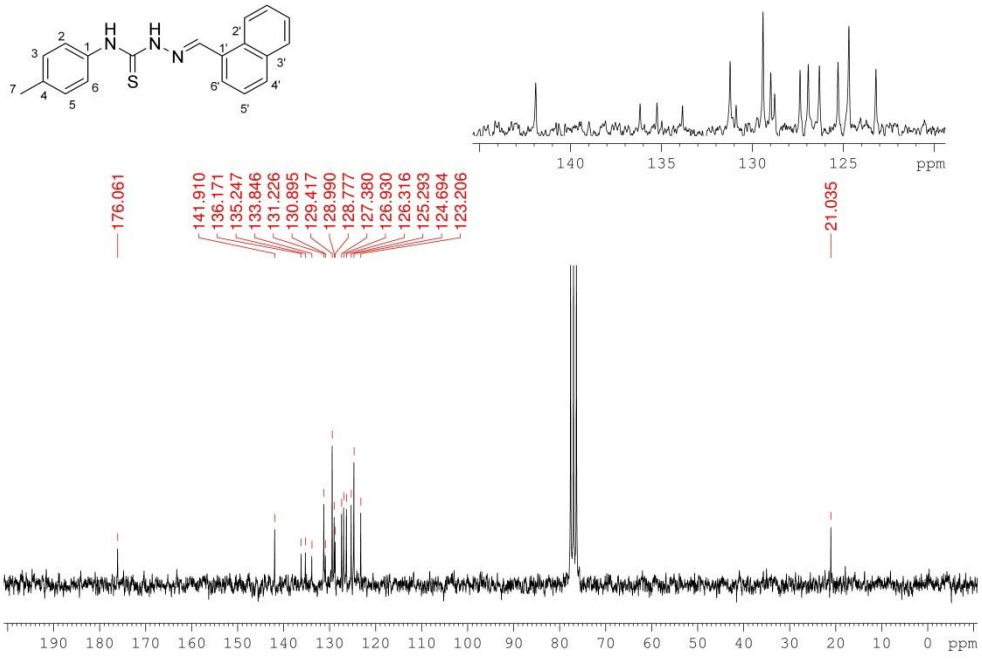

Figure S22. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2j**.

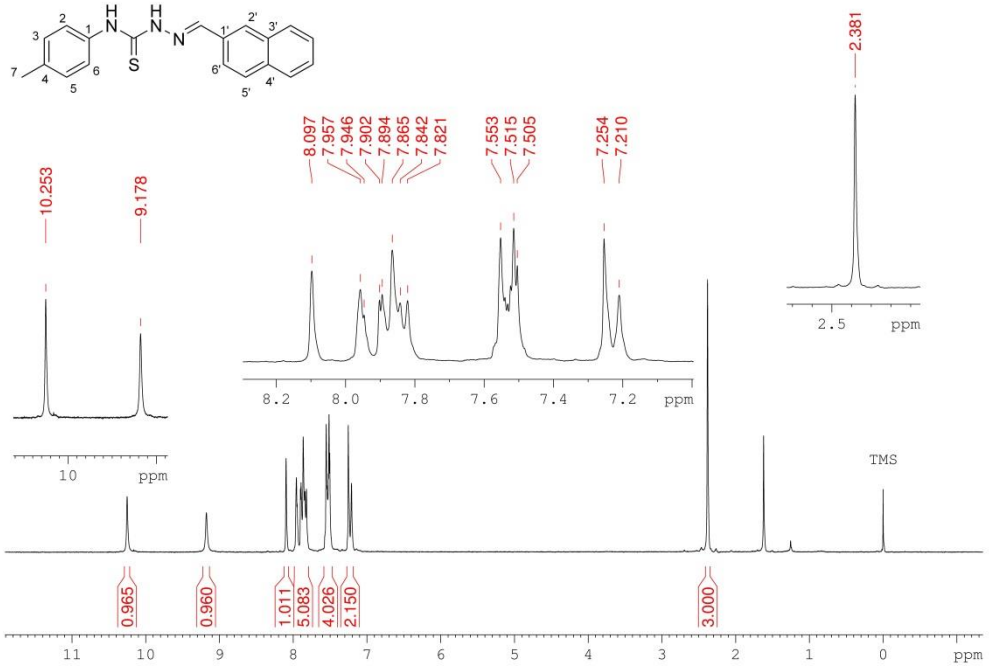

Figure S23. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2k**.

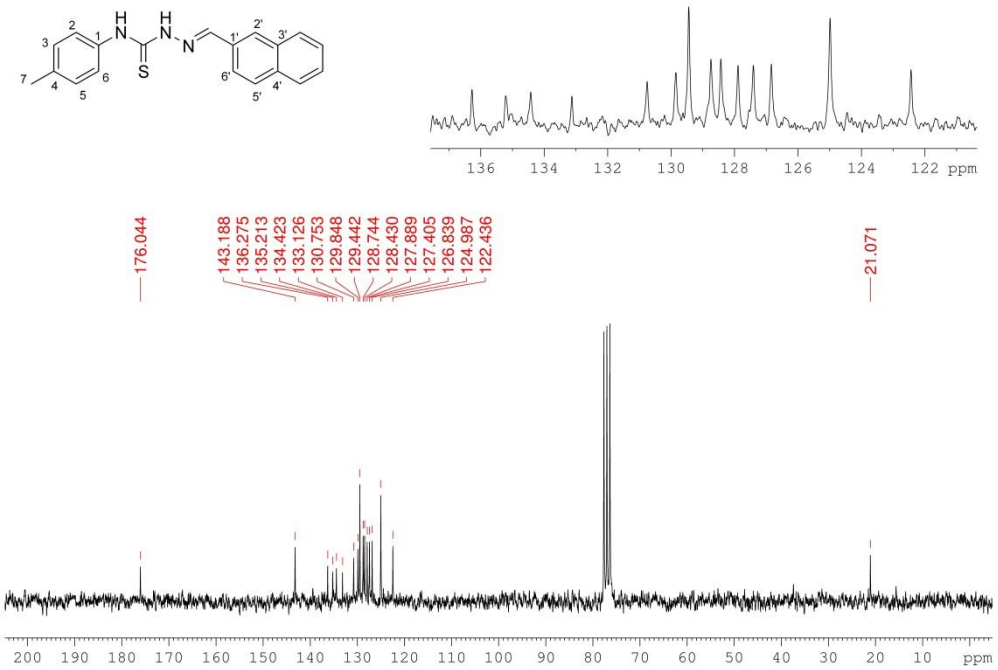

Figure S24. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2k**.

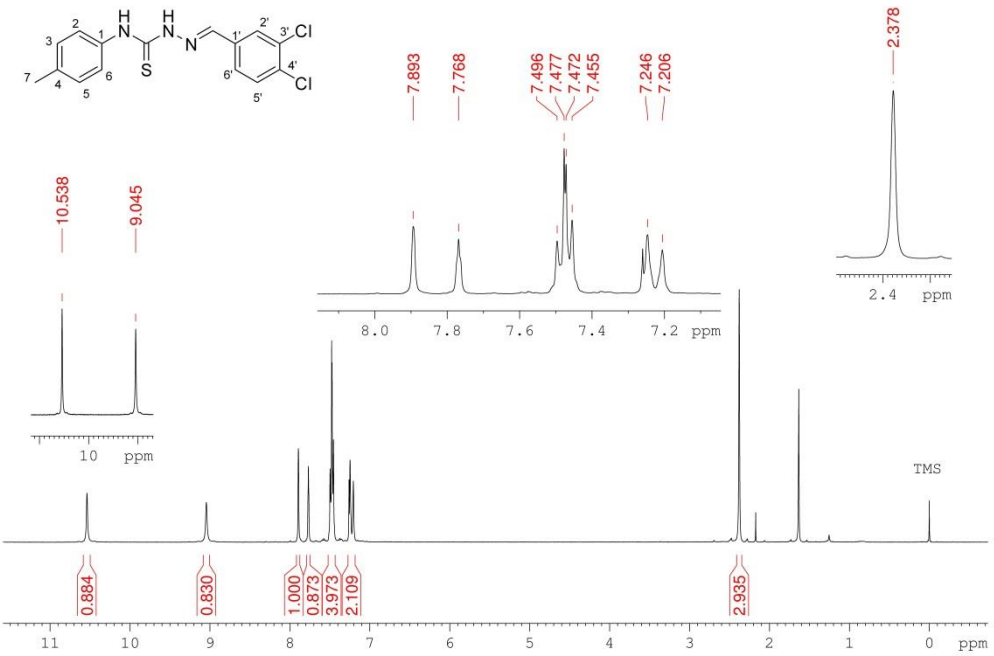

Figure S25. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2l**.

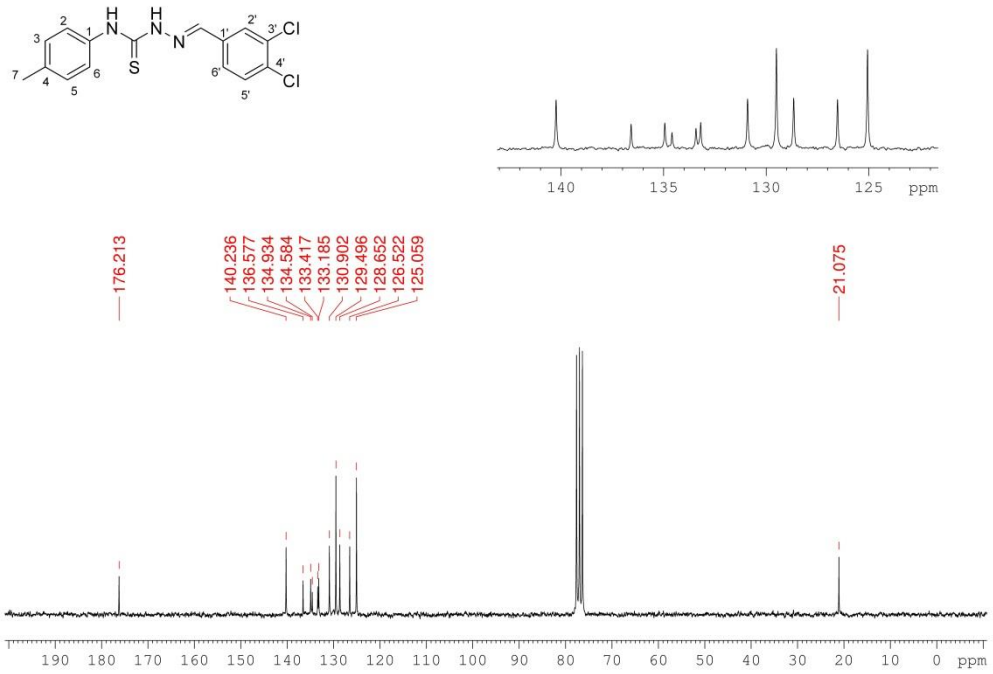

Figure S26. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2l**.

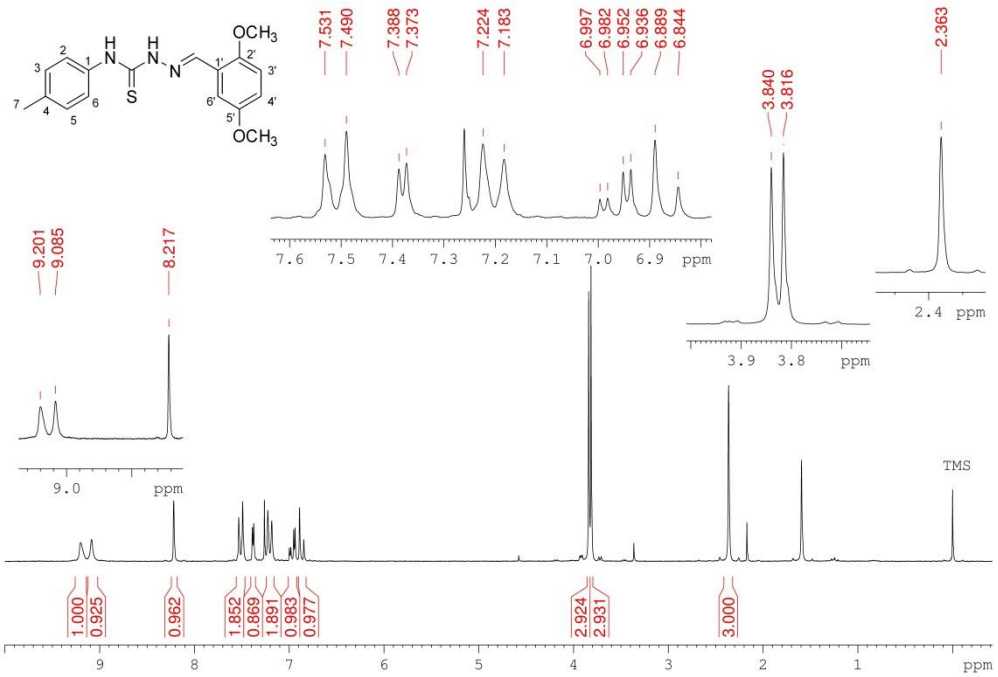

Figure S27. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2m**.

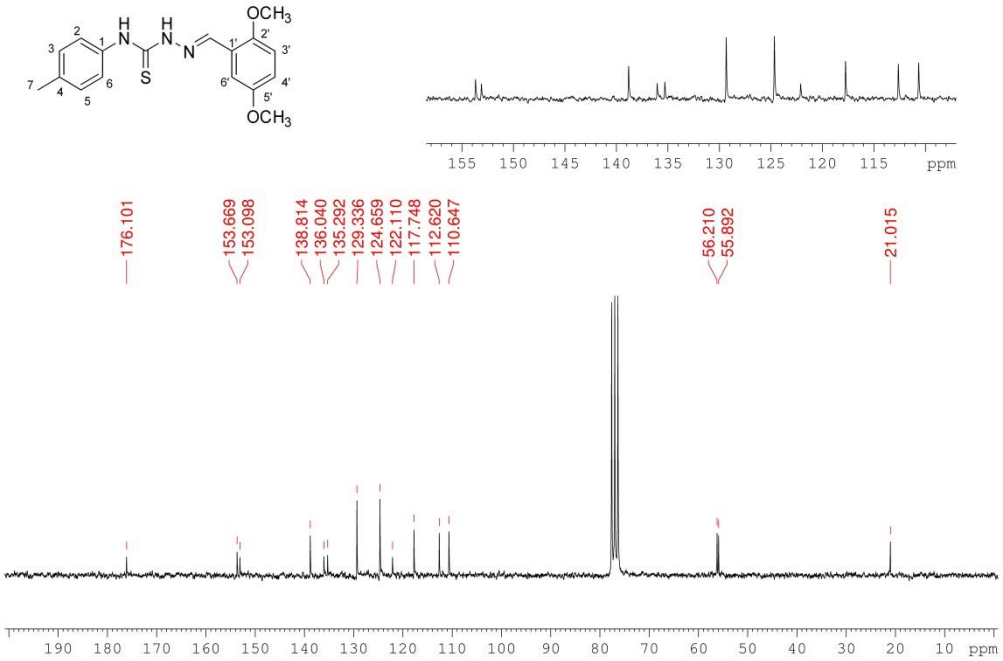

Figure S28. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2m**.

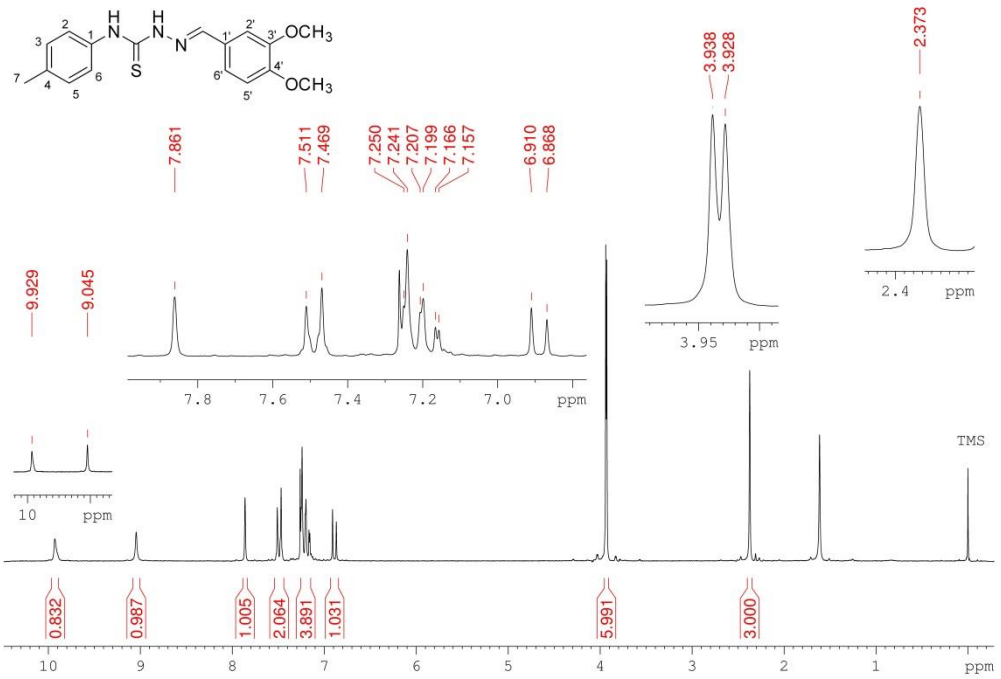

Figure S29. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2n**.

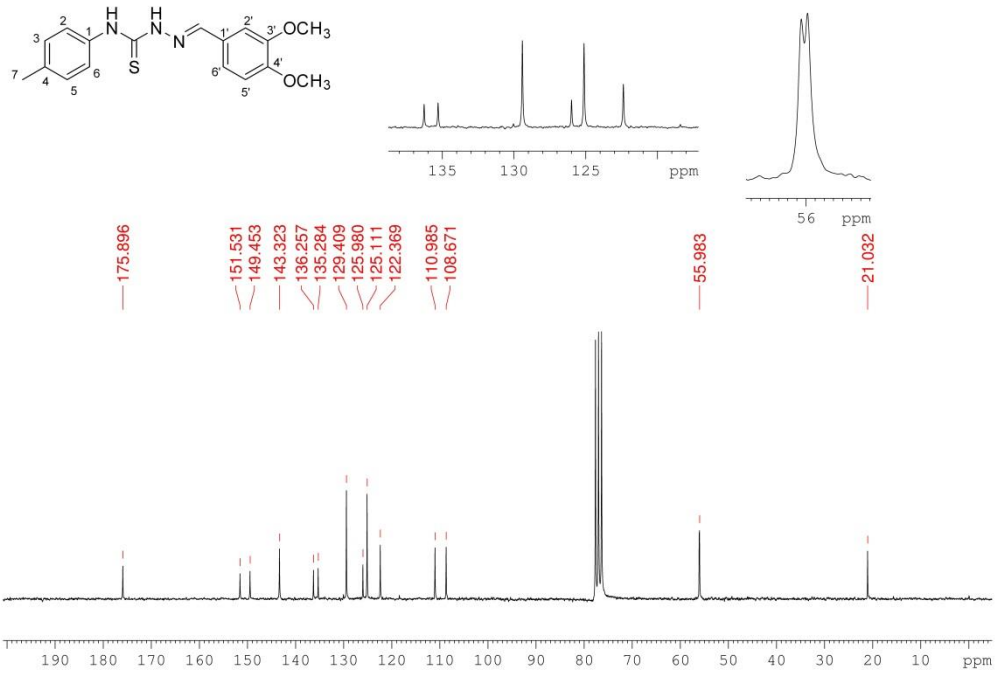

Figure S30. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2n**.

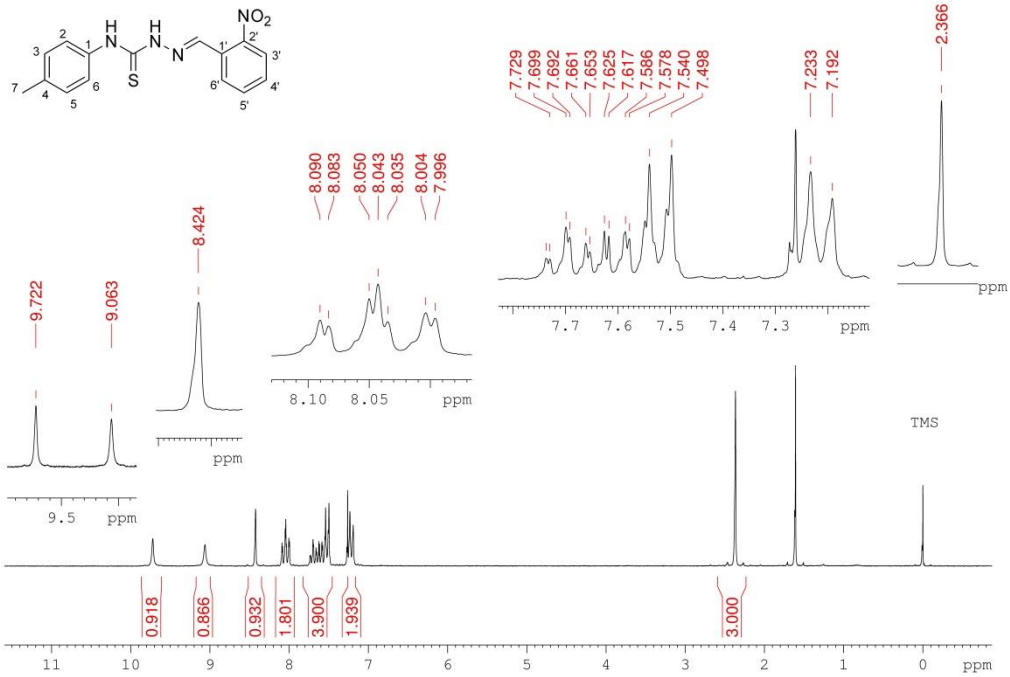

Figure S31. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2o**.

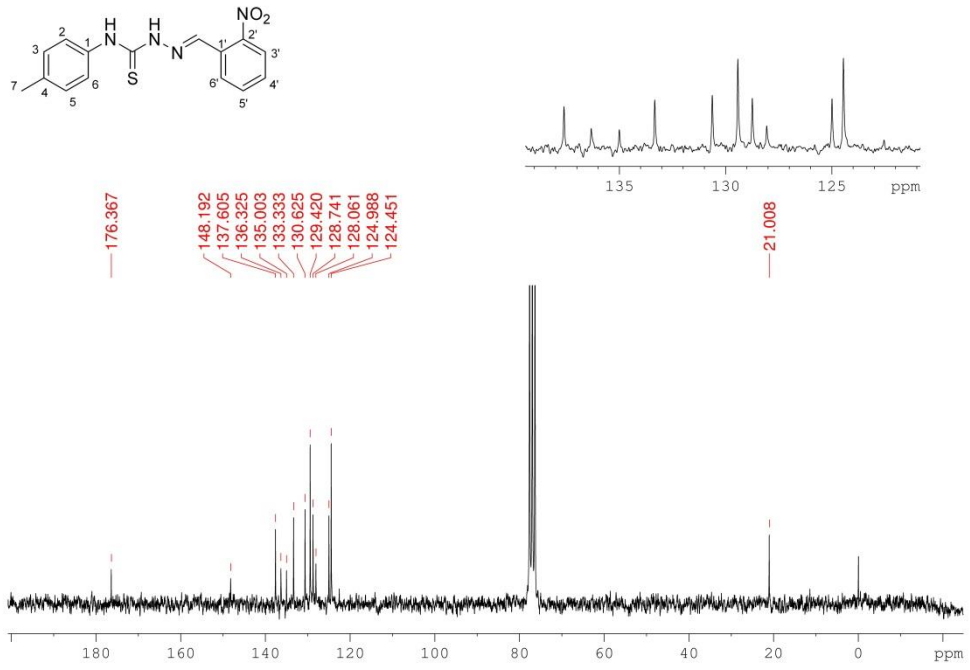

Figure S32. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2o**.

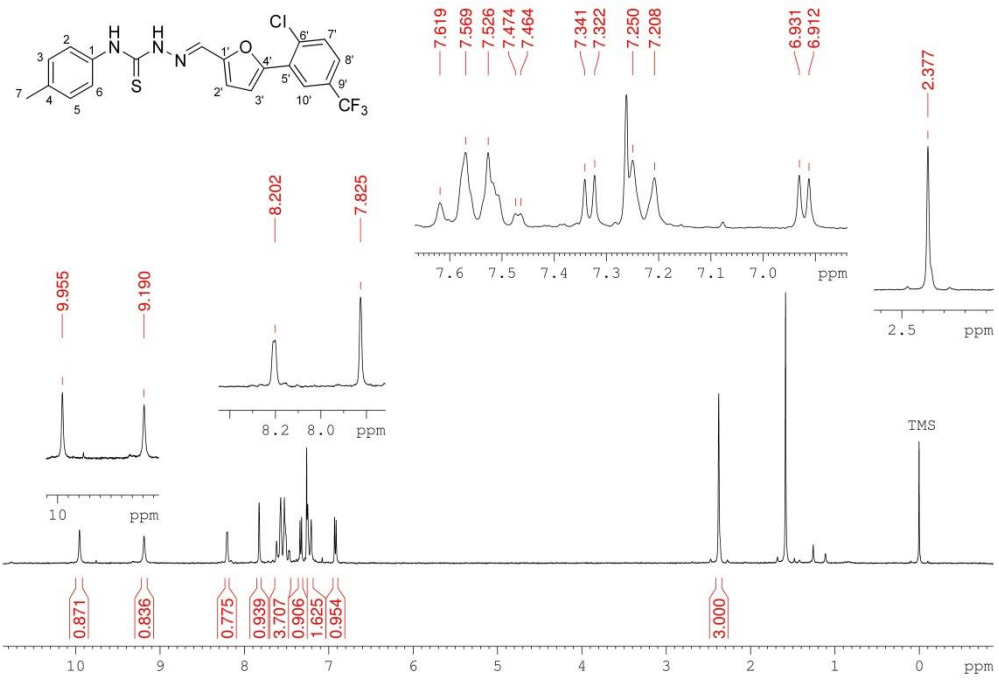

Figure S33. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2p**.

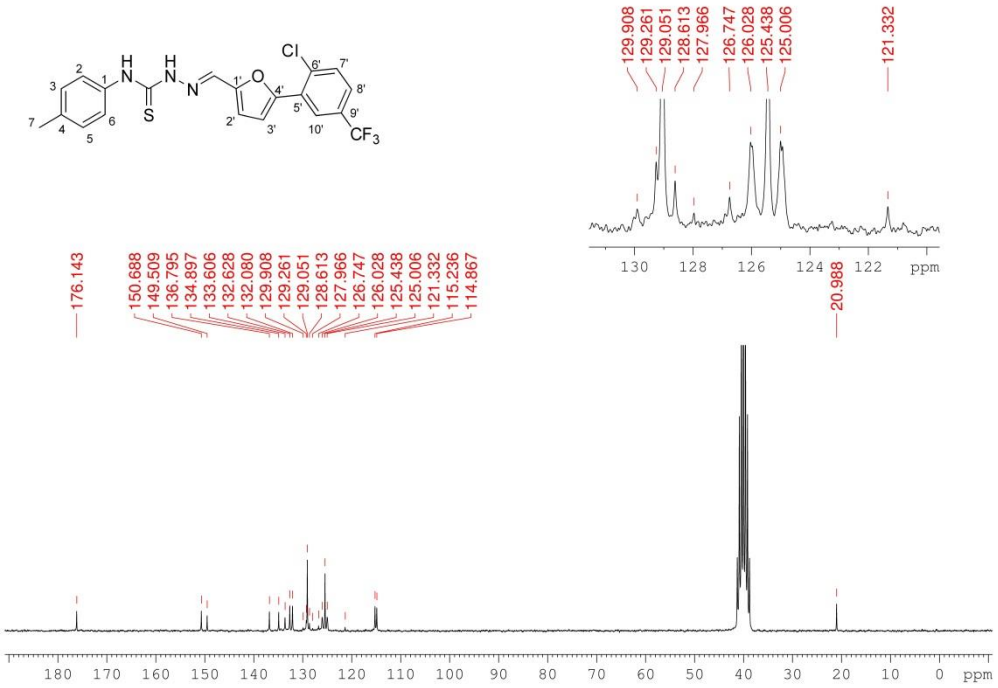

Figure S34. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2p**.

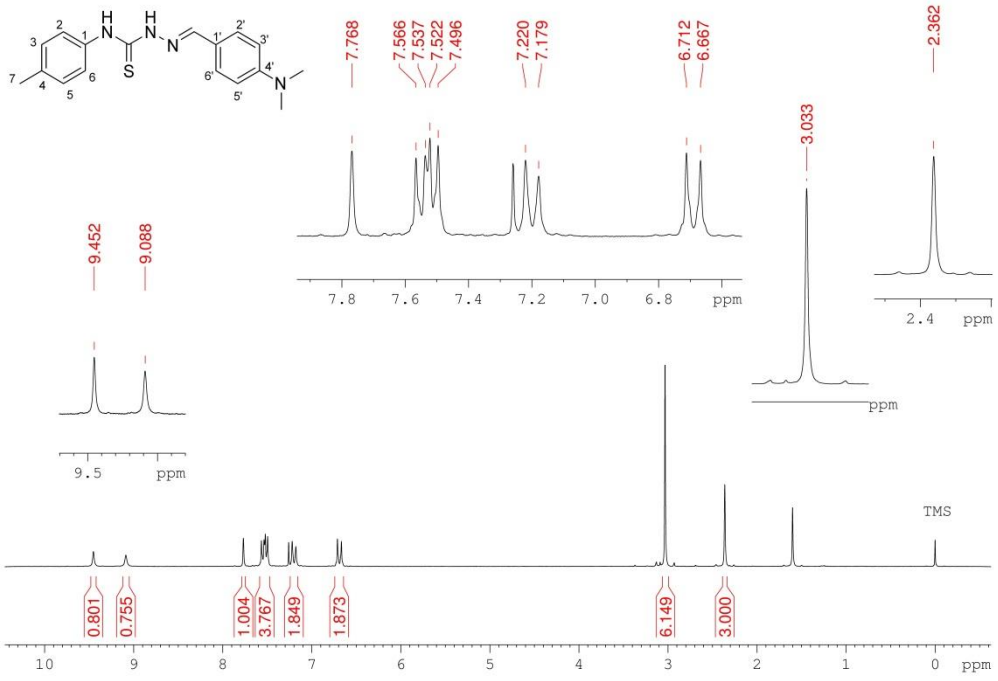

Figure S35. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of compound **2q**.

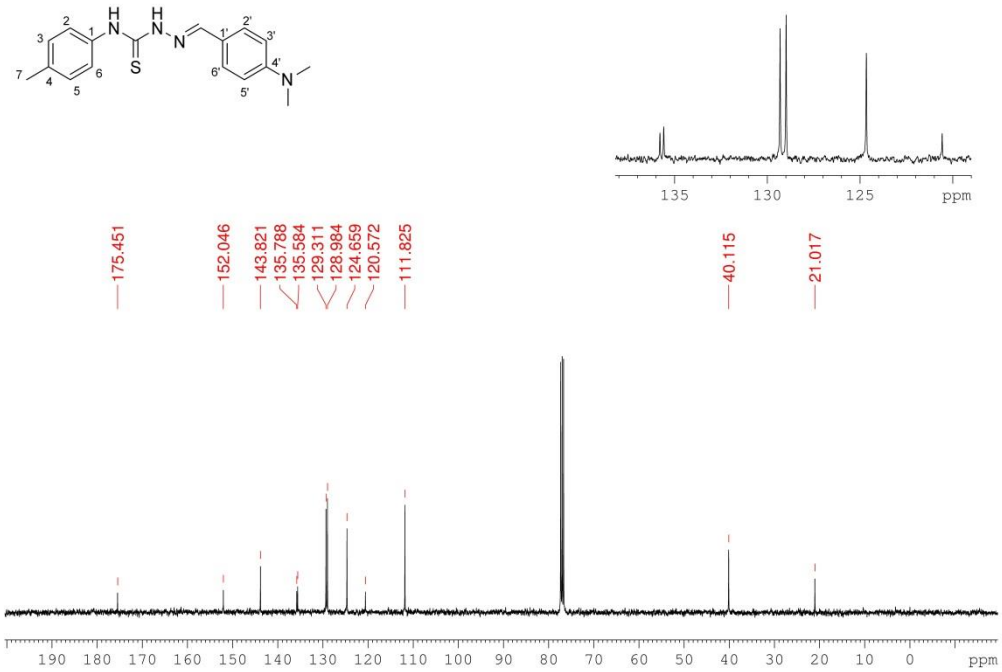

Figure S36. ^{13}C NMR spectrum (50 MHz, $CDCl_3$) of compound **2q**.

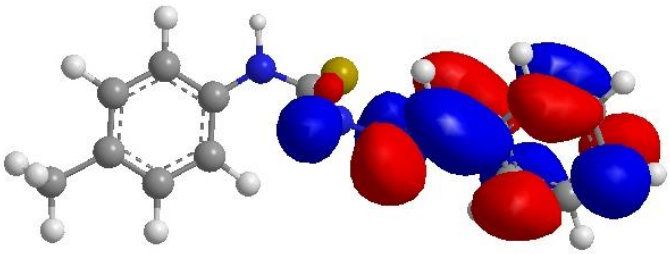

Figure S37. Lowest unoccupied molecular orbital (LUMO) of compound **2a**.

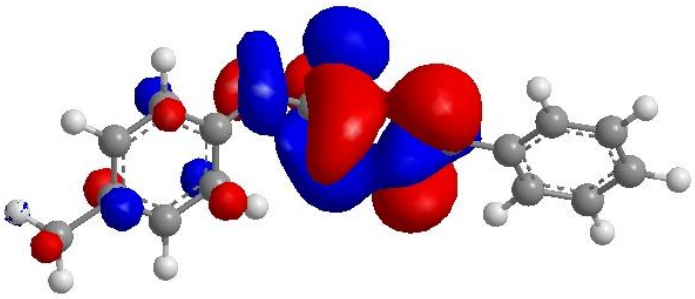

Figure S38. Highest occupied molecular orbital (HOMO) of compound **2a**.

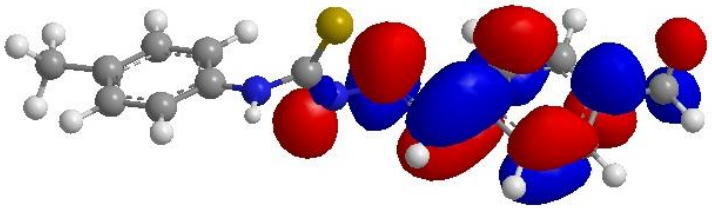

Figure S39. Lowest unoccupied molecular orbital (LUMO) of compound **2b**.

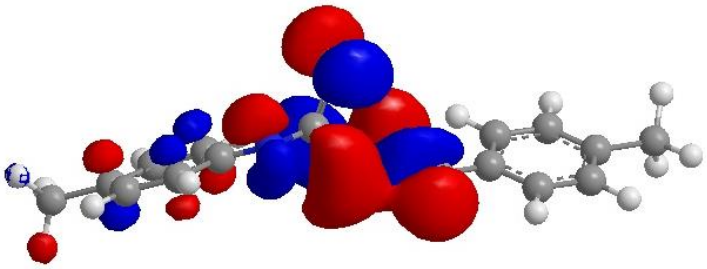

Figure S40. Highest occupied molecular orbital (HOMO) of compound **2b**.

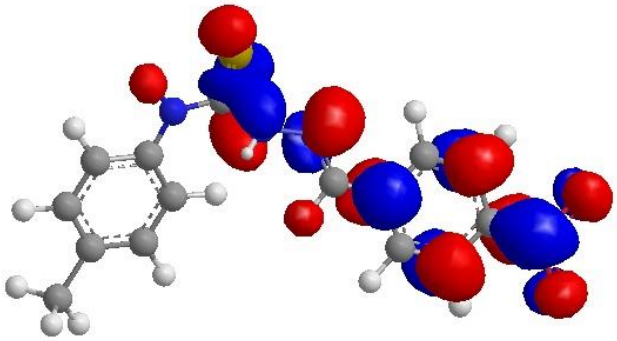

Figure S41. Lowest unoccupied molecular orbital (LUMO) of compound **2c**.

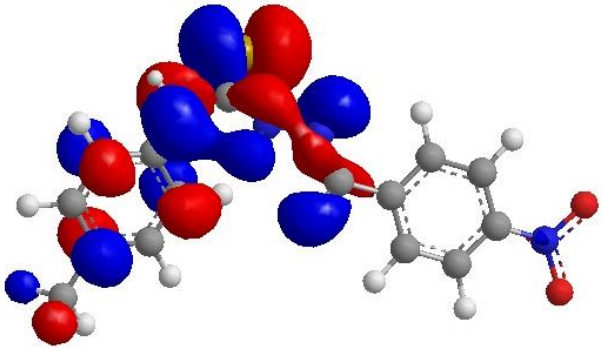

Figure S42. Highest occupied molecular orbital (HOMO) of compound **2c**.

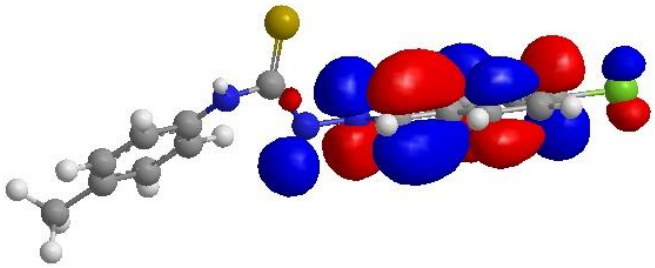

Figure S43. Lowest unoccupied molecular orbital (LUMO) of compound **2d**.

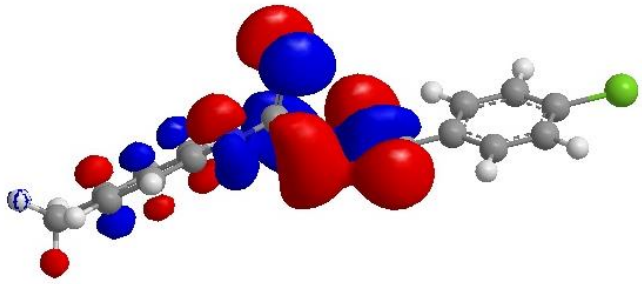

Figure S44. Highest occupied molecular orbital (HOMO) of compound **2d**.

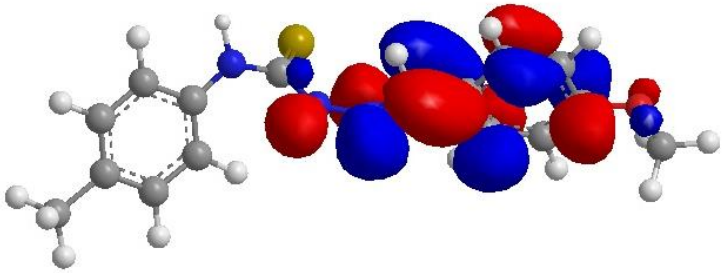

Figure S45. Lowest unoccupied molecular orbital (LUMO) of compound **2e**.

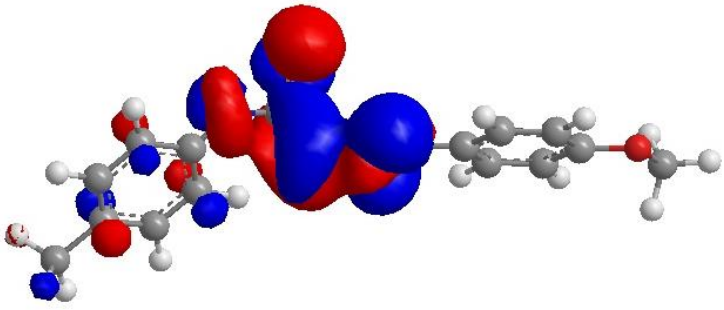

Figure S46. Highest occupied molecular orbital (HOMO) of compound **2e**.

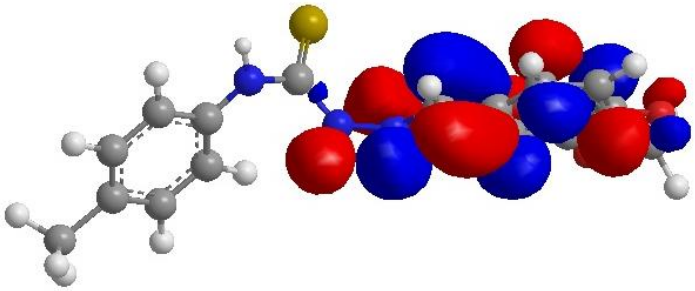

Figure S47. Lowest unoccupied molecular orbital (LUMO) of compound **2f**.

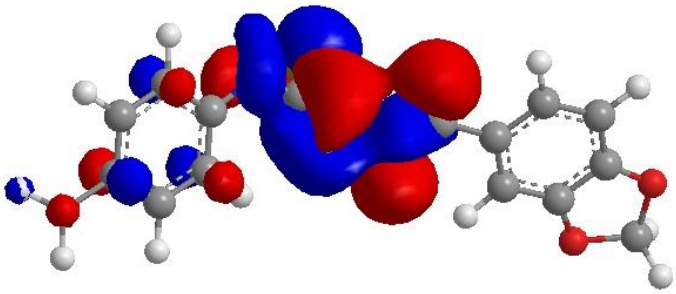

Figure S48. Highest occupied molecular orbital (HOMO) of compound **2f**.

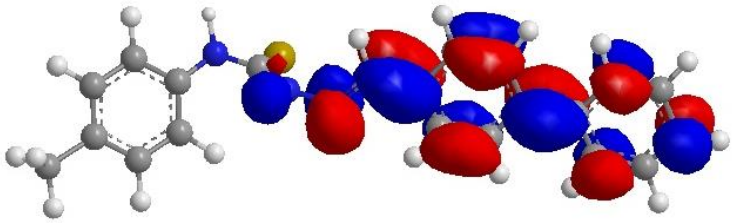

Figure S49. Lowest unoccupied molecular orbital (LUMO) of compound **2g**.

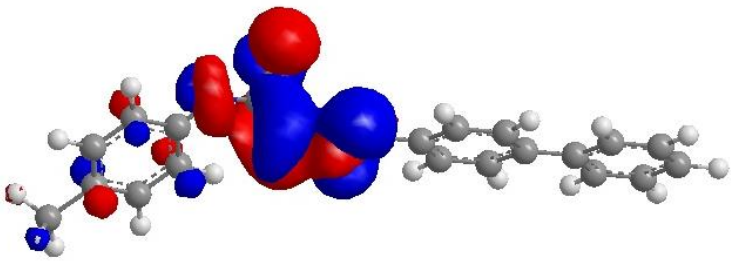

Figure S50. Highest occupied molecular orbital (HOMO) of compound **2g**.

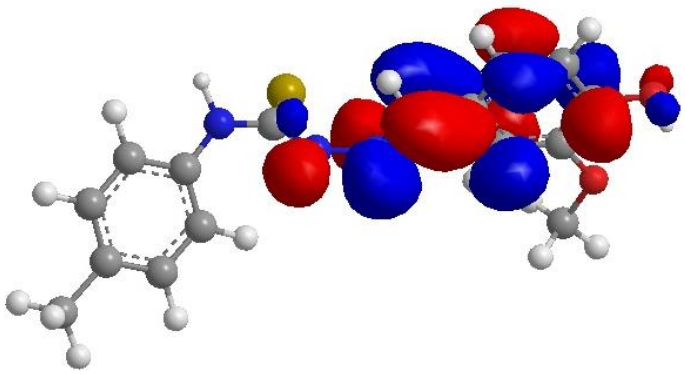

Figure S51. Lowest unoccupied molecular orbital (LUMO) of compound **2h**.

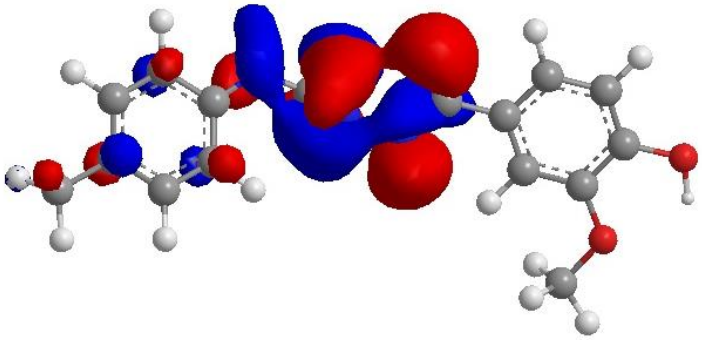

Figure S52. Highest occupied molecular orbital (HOMO) of compound **2h**.

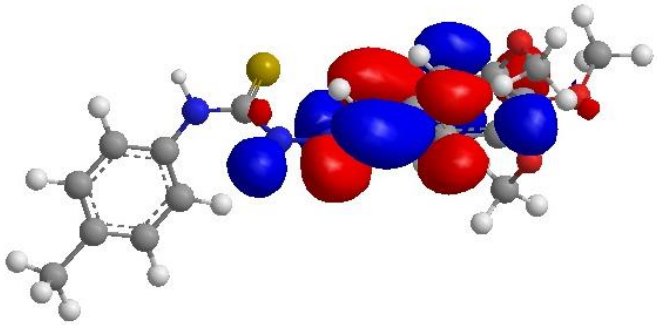

Figure S53. Lowest unoccupied molecular orbital (LUMO) of compound **2i**.

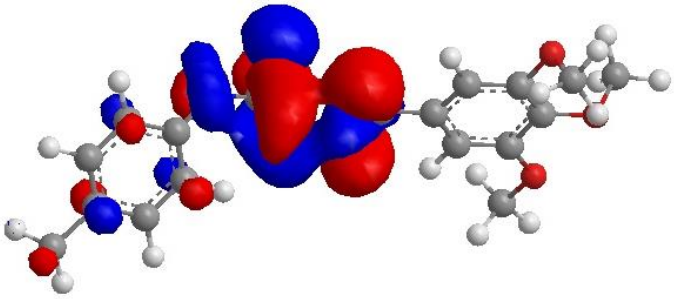

Figure S54. Highest occupied molecular orbital (HOMO) of compound **2i**.

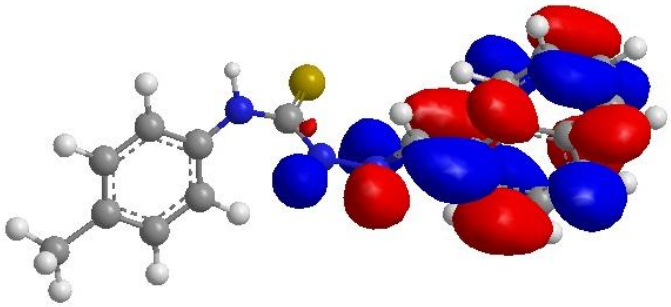

Figure S55. Lowest unoccupied molecular orbital (LUMO) of compound **2j**.

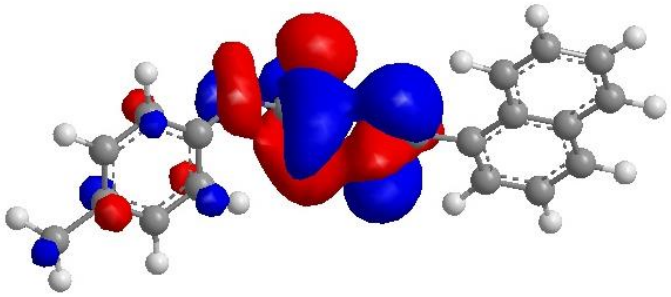

Figure S56. Highest occupied molecular orbital (HOMO) of compound **2j**.

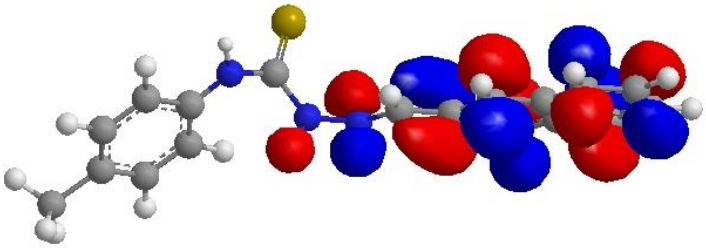

Figure S57. Lowest unoccupied molecular orbital (LUMO) of compound **2k**.

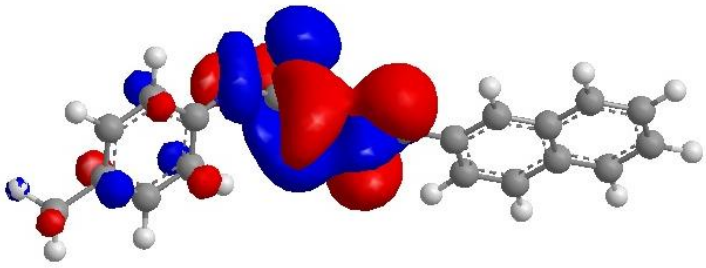

Figure S58. Highest occupied molecular orbital (HOMO) of compound **2k**.

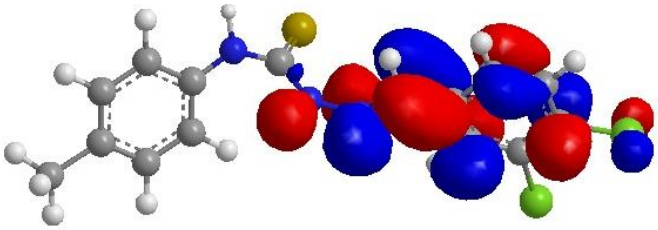

Figure S59. Lowest unoccupied molecular orbital (LUMO) of compound **2l**.

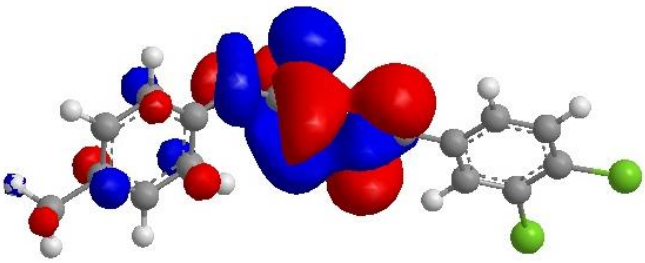

Figure S60. Highest occupied molecular orbital (HOMO) of compound **2l**.

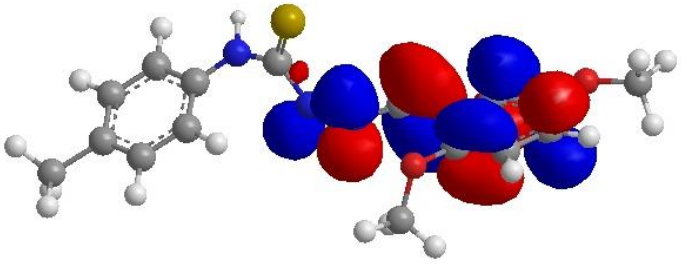

Figure S61. Lowest unoccupied molecular orbital (LUMO) of compound **2m**.

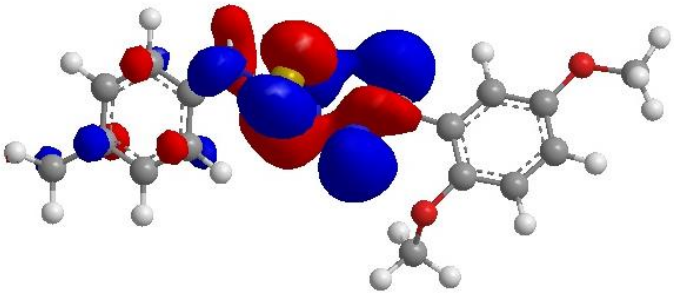

Figure S62. Highest occupied molecular orbital (HOMO) of compound **2m**.

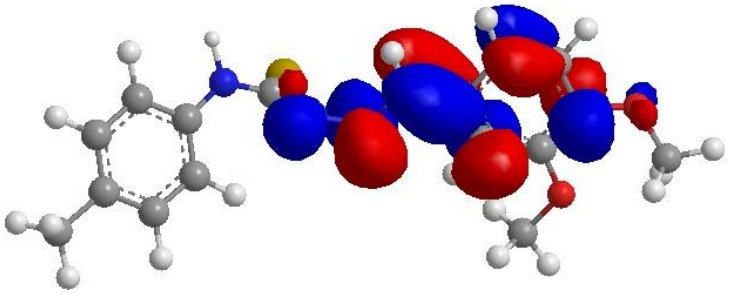

Figure S63. Lowest unoccupied molecular orbital (LUMO) of compound **2n**.

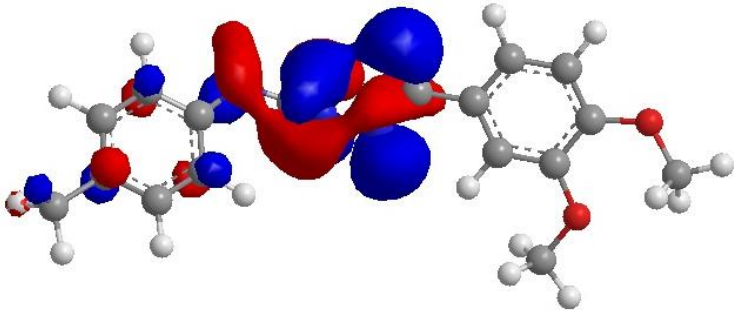

Figure S64. Highest occupied molecular orbital (HOMO) of compound **2n**.

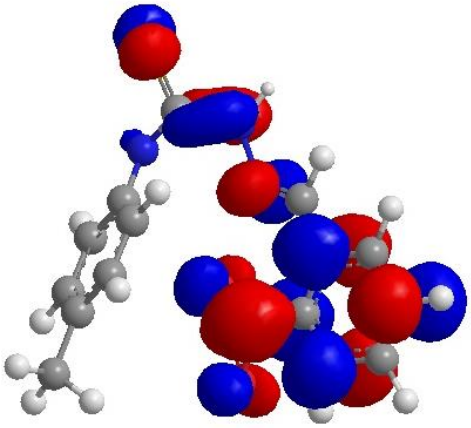

Figure S65. Lowest unoccupied molecular orbital (LUMO) of compound **2o**.

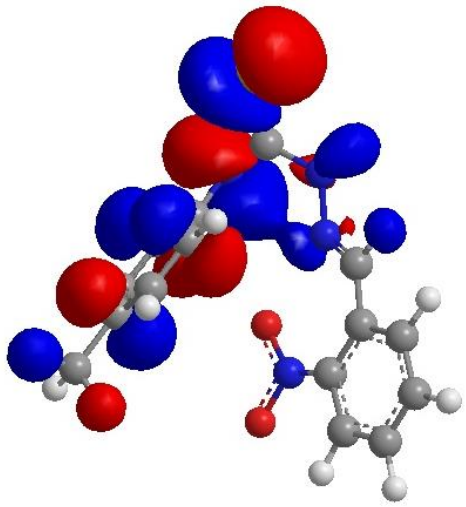

Figure S66. Highest occupied molecular orbital (HOMO) of compound **2o**.

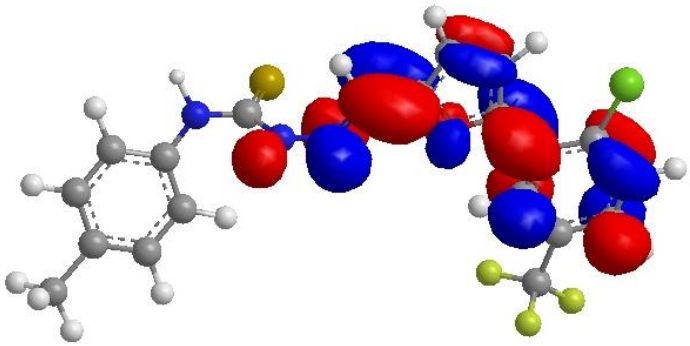

Figure S67. Lowest unoccupied molecular orbital (LUMO) of compound **2p**.

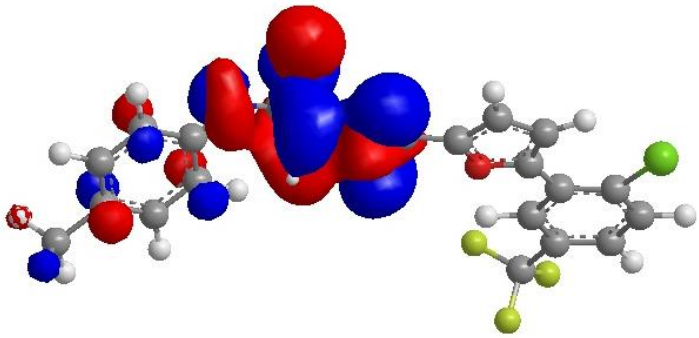

Figure S68. Highest occupied molecular orbital (HOMO) of compound **2p**.

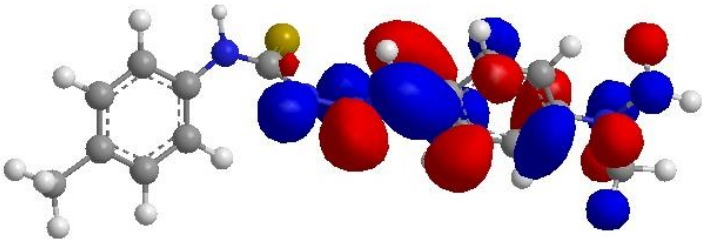

Figure S69. Lowest unoccupied molecular orbital (LUMO) of compound **2q**.

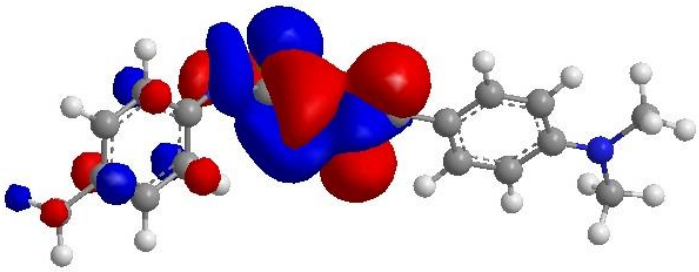

Figure S70. Highest occupied molecular orbital (HOMO) of compound **2q**.