Manganese(I)-Catalyzed Transfer Hydrogenation and Acceptorless Dehydrogenative Condensation: Promotional Influence of the Uncoordinated N-Heterocycle

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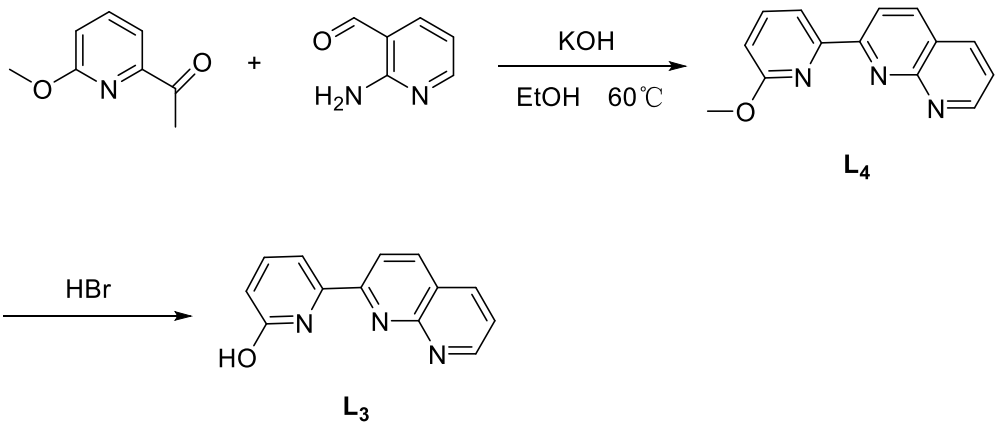
Crystallographic Details

3: A total of 11725 reflections ($-10 \leq h \leq 10$, $-11 \leq k \leq 11$, $-12 \leq l \leq 12$) were collected at T = 173(2) K in the range of 2.308 to 24.997° of which 3104 were unique (R_{int} = 0.0340); Mo_K radiation (λ = 0.71073 Å). The structure was solved by the direct methods. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were placed in calculated idealized positions. The residual peak and hole electron densities were 0.301 and -0.268 eA^{-3}, respectively. The least squares refinement converged normally with residuals of $R(F)$ = 0.0232, $wR(F^2)$ = 0.0512 and a GOF = 1.031 ($I>2\sigma(I)$). $C_{17}H_{13}BrMnN_3O_5$, Mw = 474.15, space group P-1, triclinic, a = 8.9986(4), b = 10.0301(4), c = 10.1404(4) Å, V = 894.28(6) $Å^3$, Z = 2, ρ_{calcd} = 1.761 Mg/m^3. CCDC-1939902 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Scheme S1. Synthesis of **L_3**



^{1}H NMR Spectra

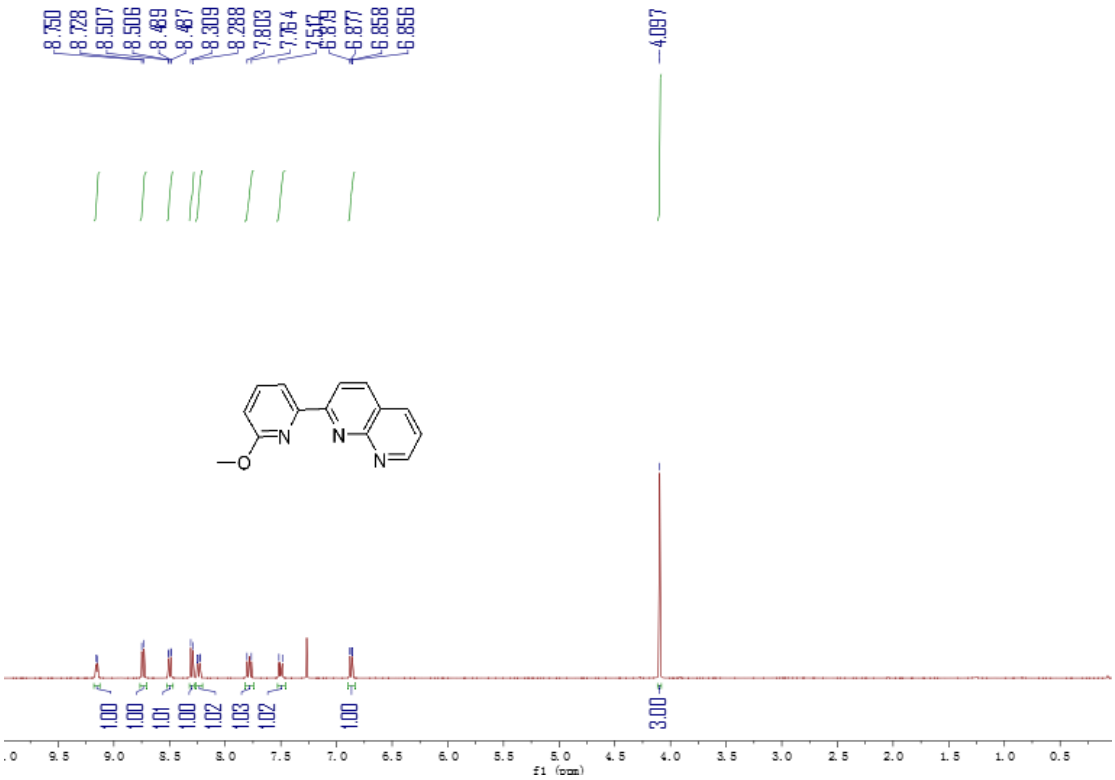


Figure S1. ^{1}H NMR spectrum of 2-(6-methoxypyridin-2-yl)-1,8-naphthyridine in $CDCl_3$.

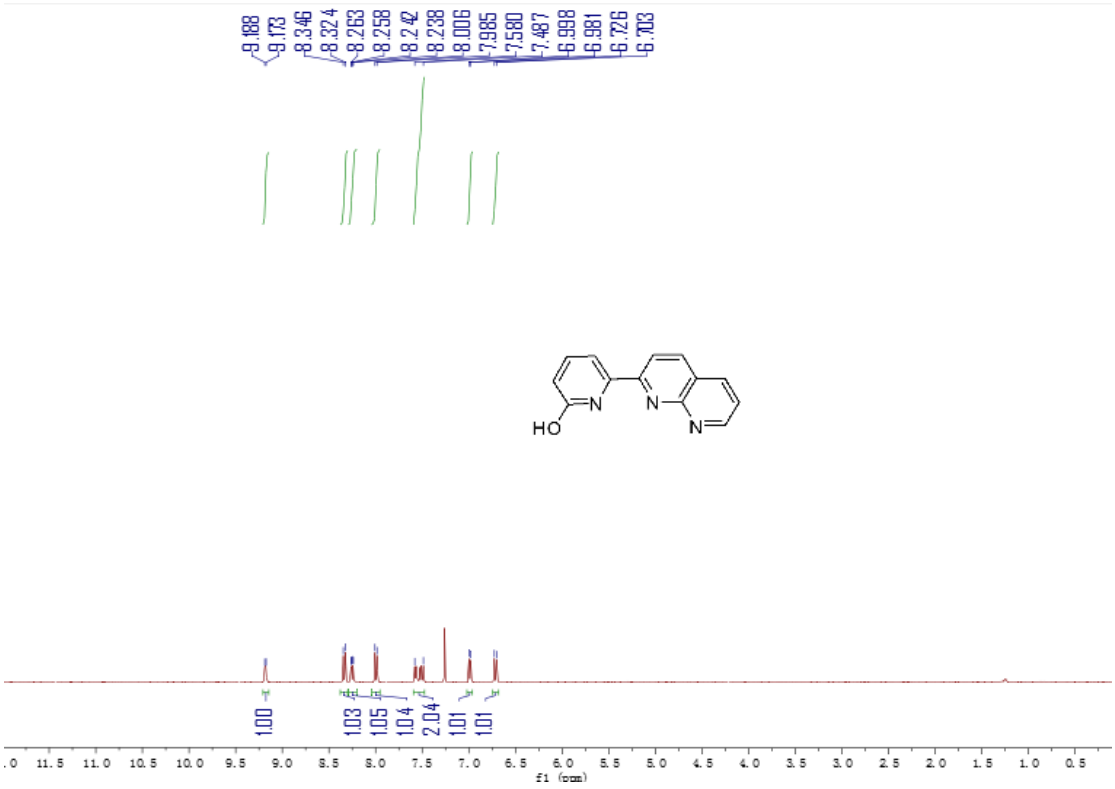


Figure S2. ^{1}H NMR spectrum of 6-(1,8-naphthyridin-2-yl)pyridin-2-ol in $CDCl_3$.

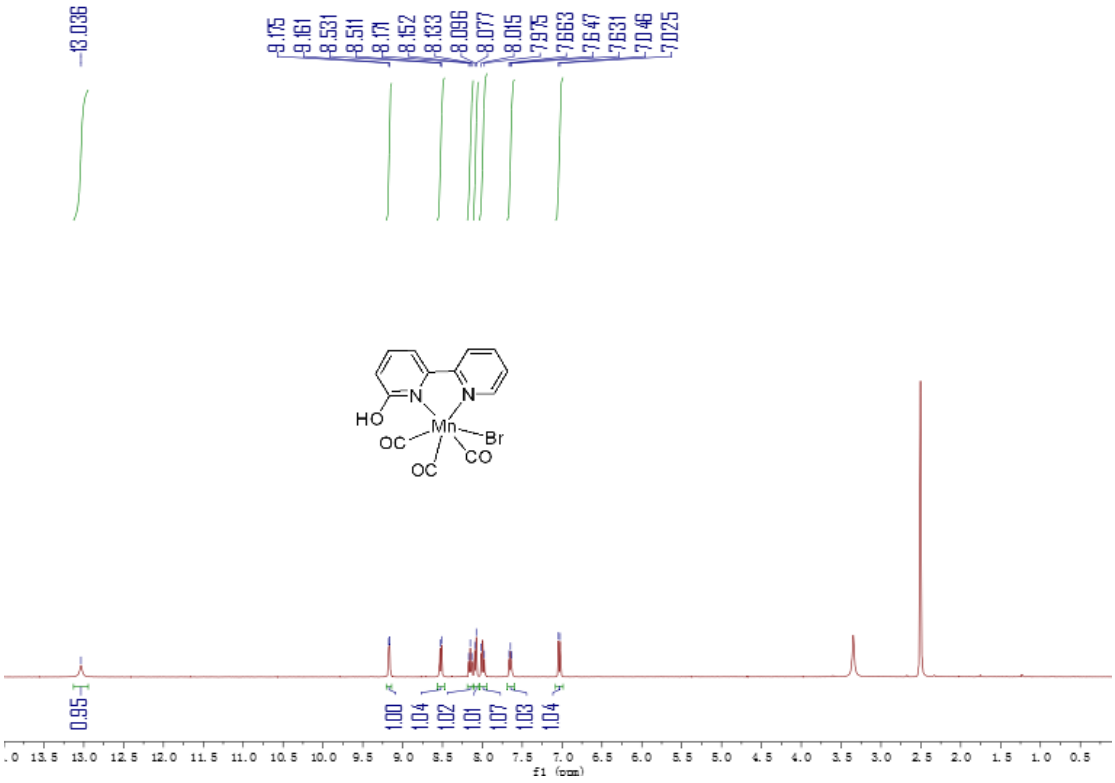


Figure S3. ^{1}H NMR spectrum of **1** in d_6-DMSO.

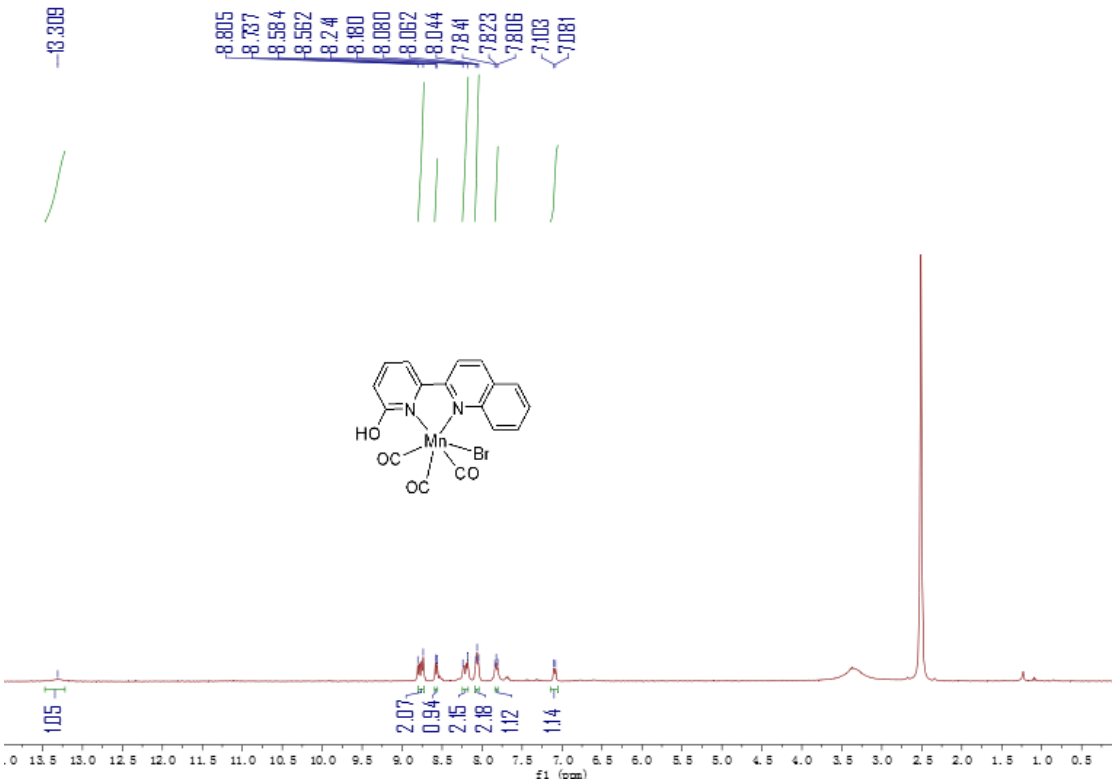


Figure S4. ^{1}H NMR spectrum of **2** in d_6-DMSO.

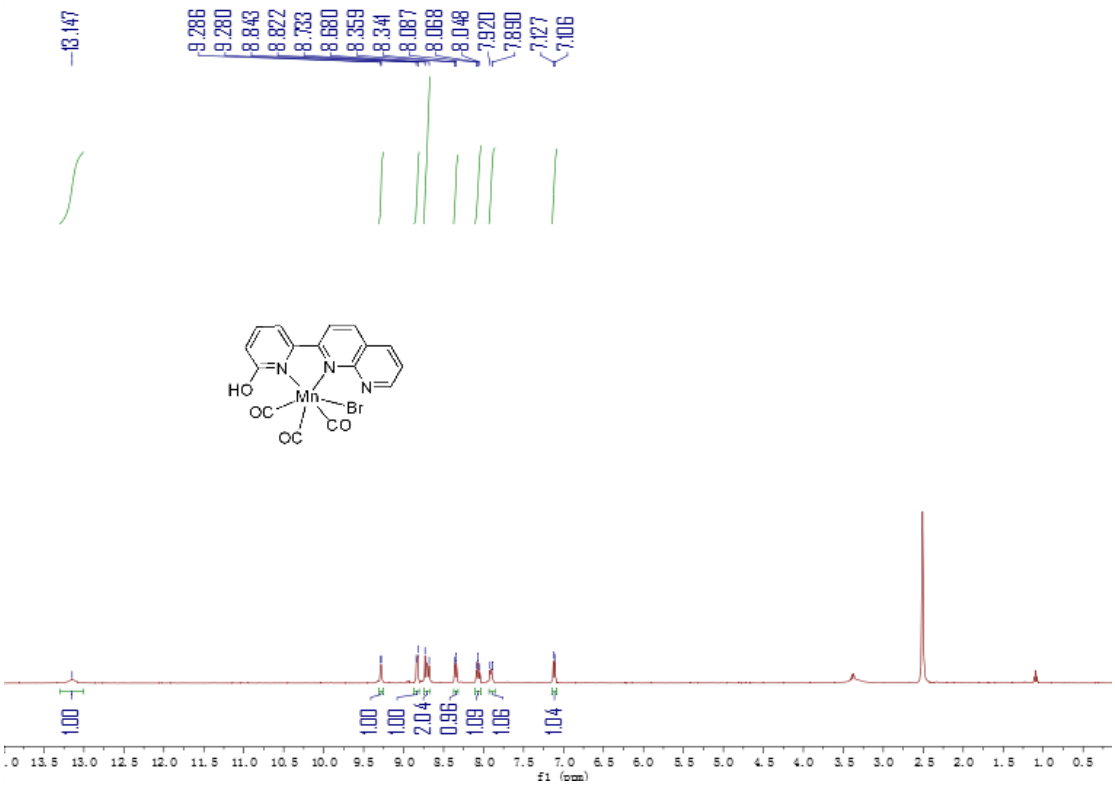


Figure S5. ^{1}H NMR spectrum of **3** in d_6-DMSO.

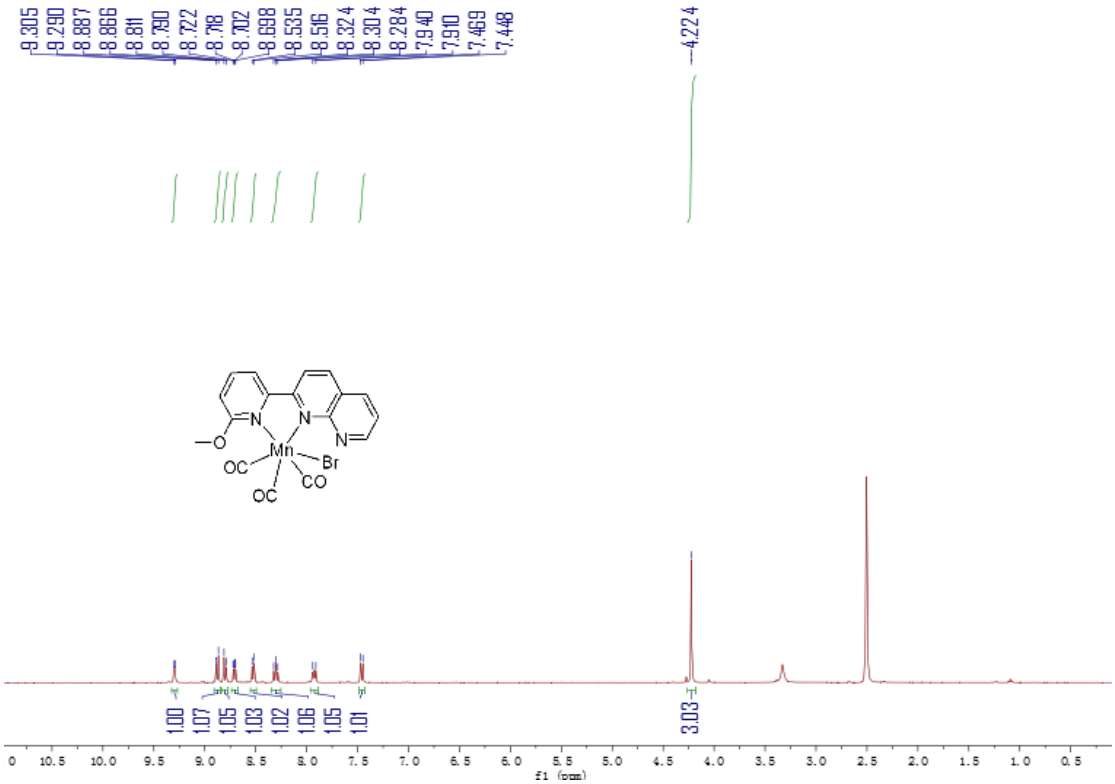


Figure S6. ^{1}H NMR spectrum of **4** in d_6-DMSO.

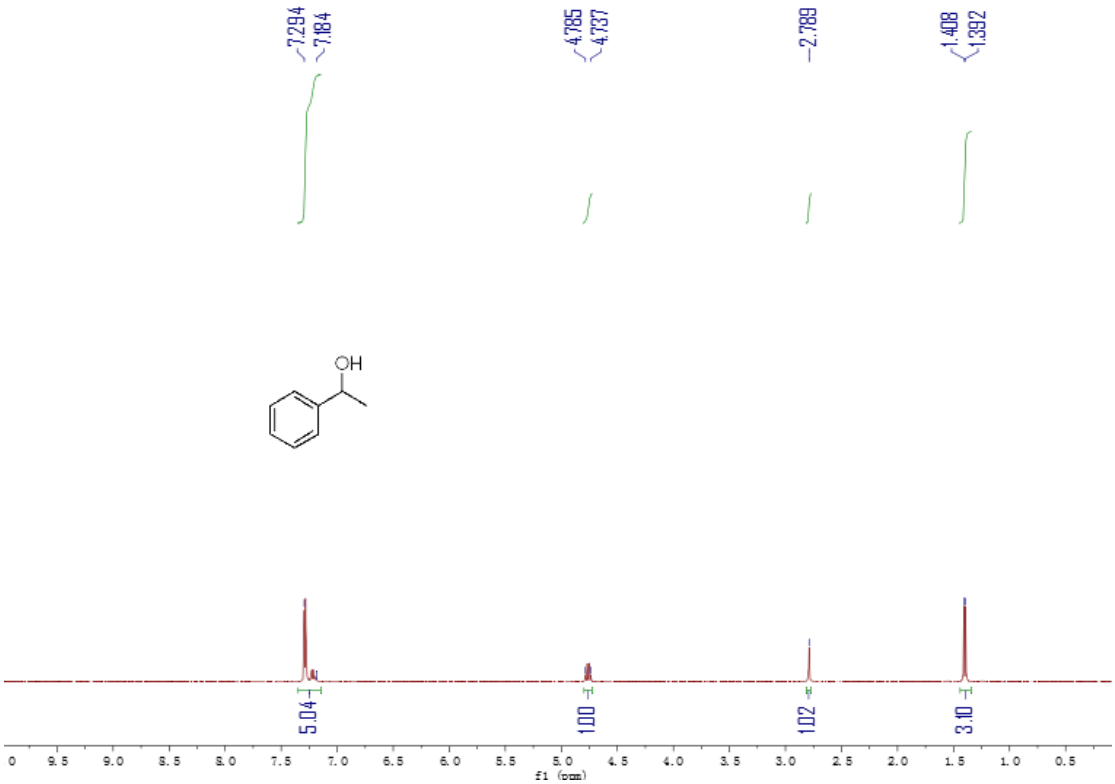


Figure S7. ^{1}H NMR spectrum of 1-phenylethan-1-ol in $CDCl_3$.

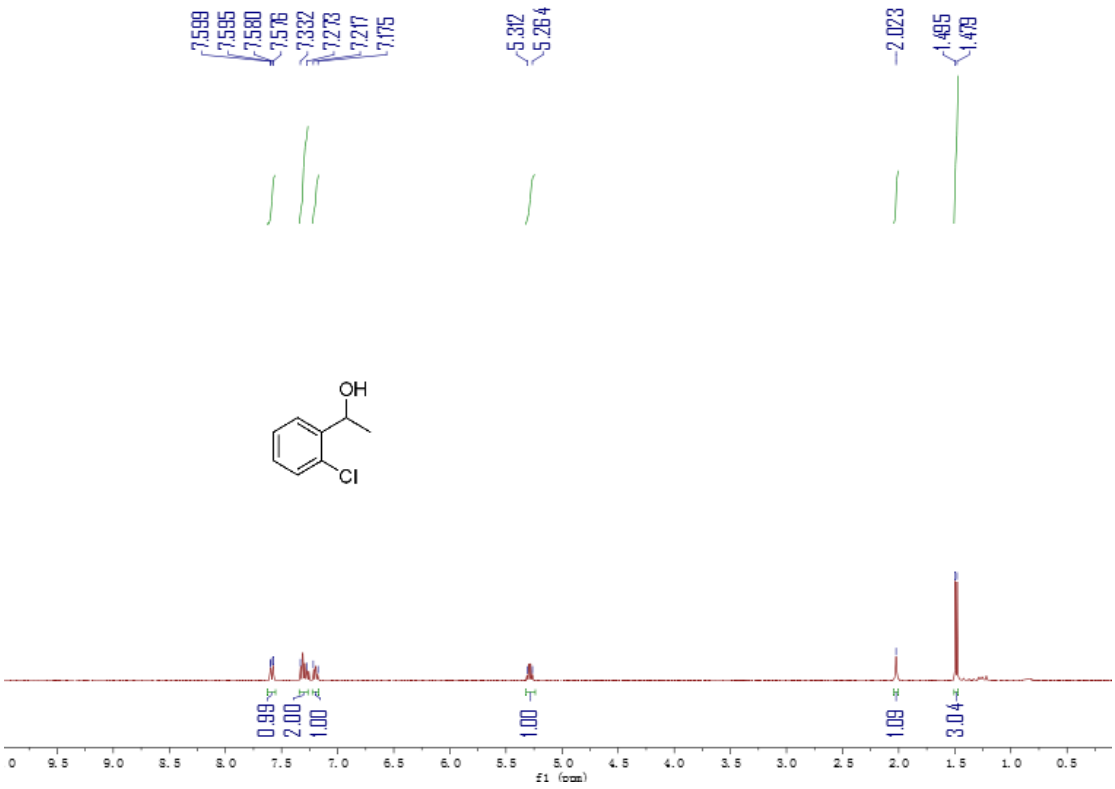


Figure S8. ^{1}H NMR spectrum of 1-(2-chlorophenyl)ethan-1-ol in $CDCl_3$.

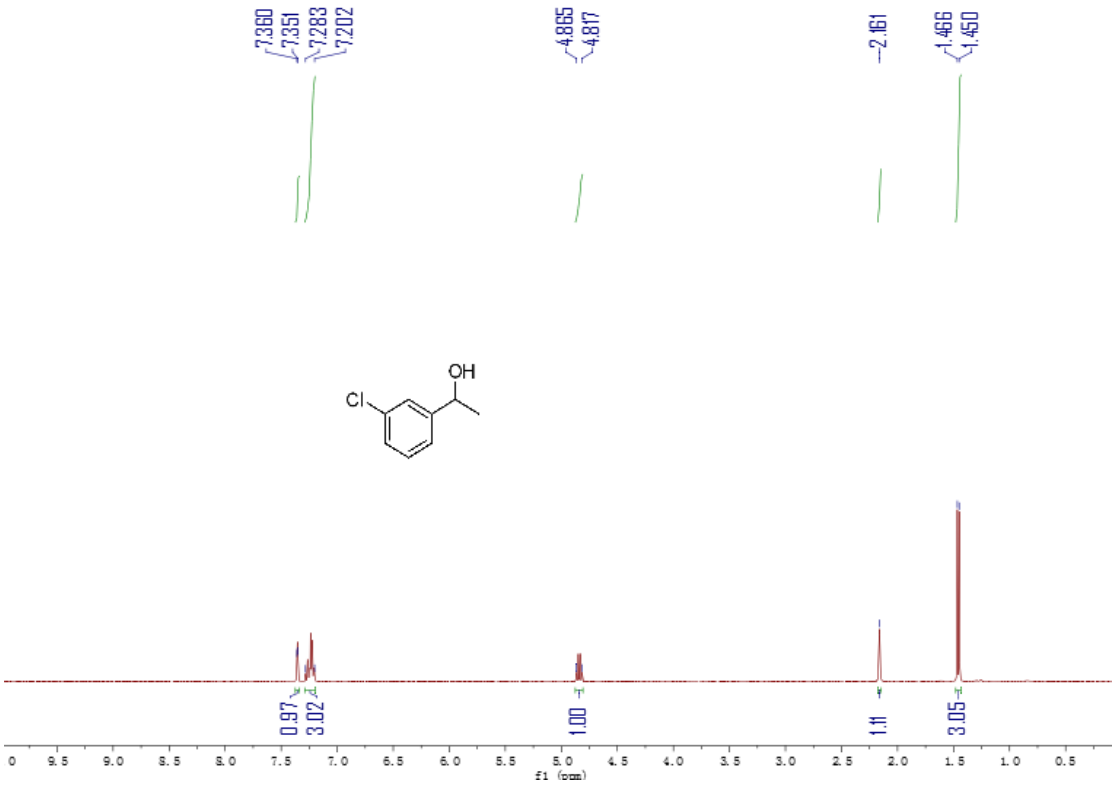


Figure S9. ^{1}H NMR spectrum of 1-(3-chlorophenyl)ethan-1-ol in $CDCl_3$.

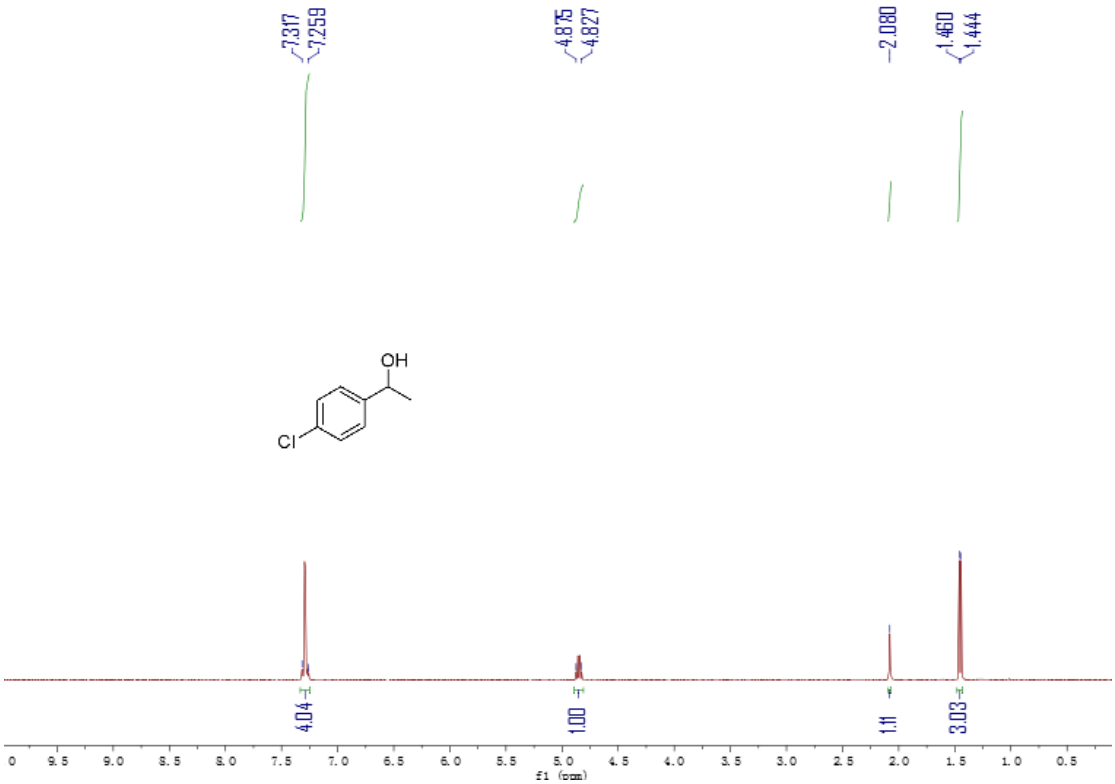


Figure S10. ^{1}H NMR spectrum of 1-(4-chlorophenyl)ethan-1-ol in $CDCl_3$.

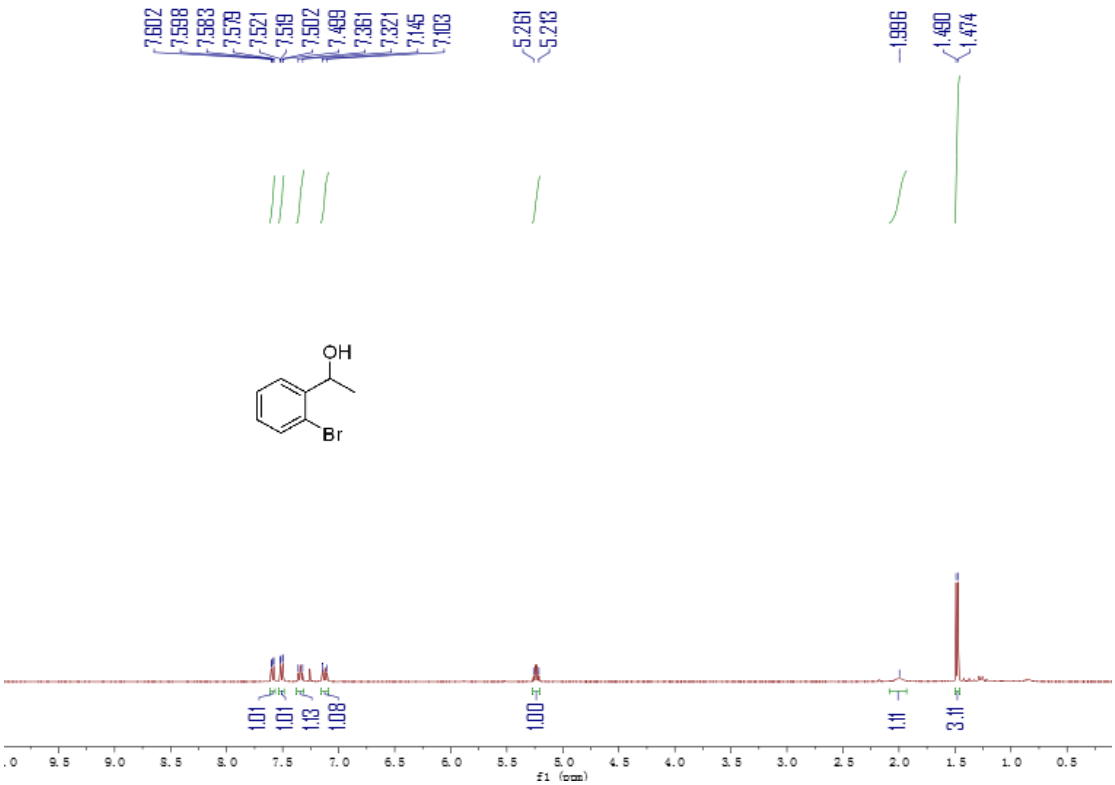


Figure S11. ^{1}H NMR spectrum of 1-(2-bromophenyl)ethan-1-ol in $CDCl_3$.

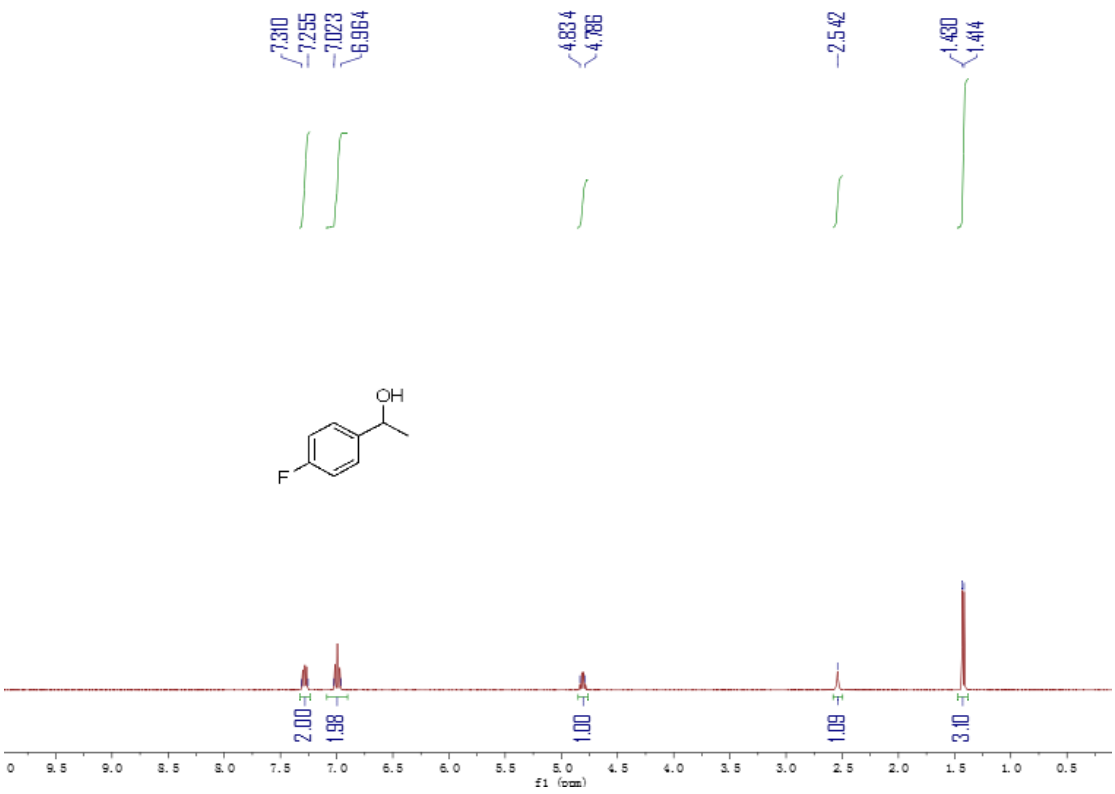


Figure S12. ^{1}H NMR spectrum of 1-(4-fluorophenyl)ethan-1-ol in $CDCl_3$.

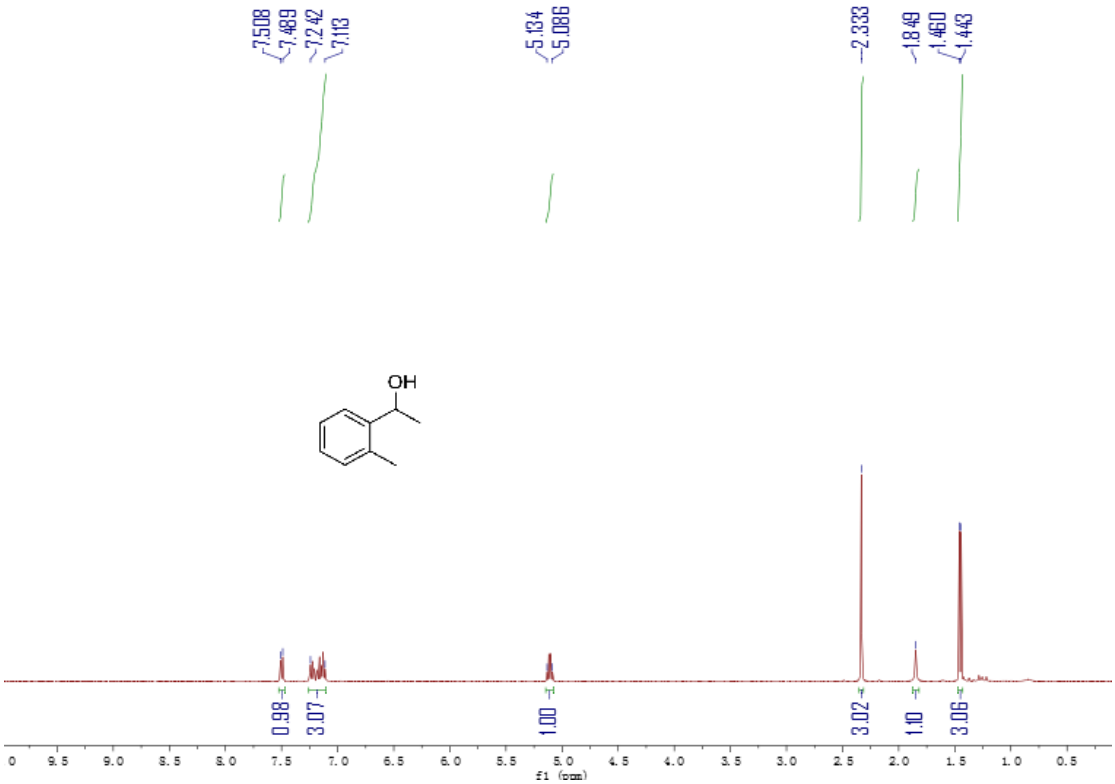


Figure S13. ^{1}H NMR spectrum of 1-(o-tolyl)ethan-1-ol in $CDCl_3$.

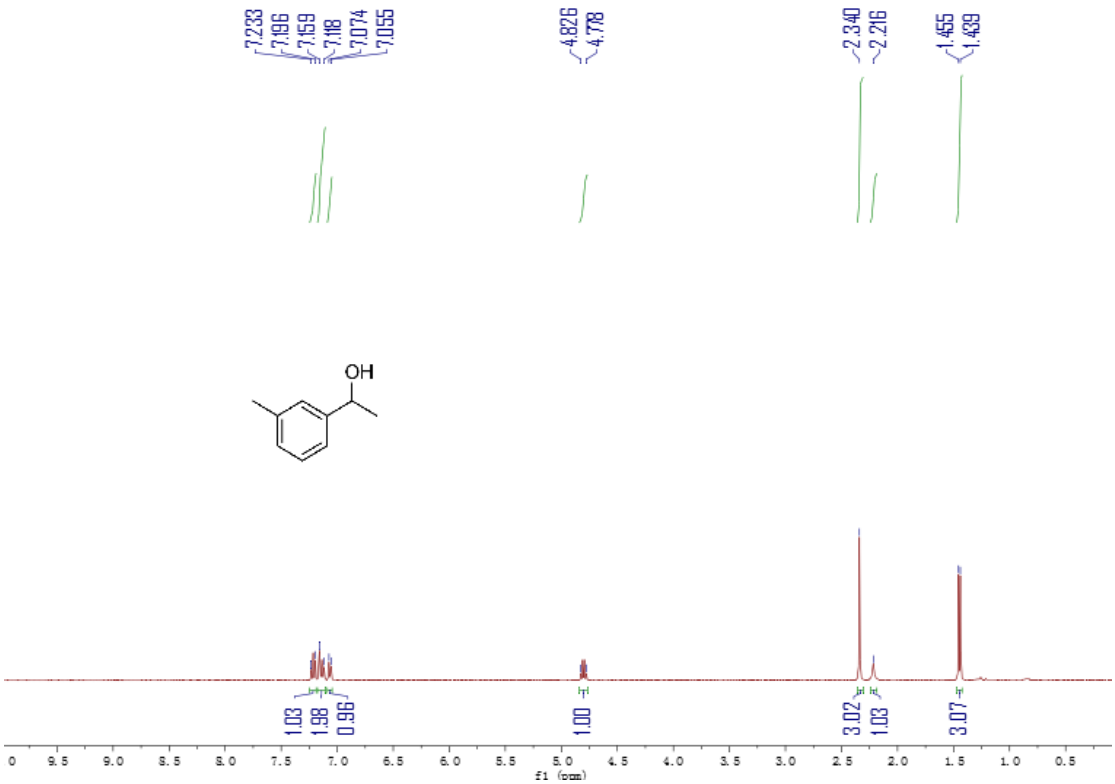


Figure S14. ^{1}H NMR spectrum of 1-(m-tolyl)ethan-1-ol in $CDCl_3$.

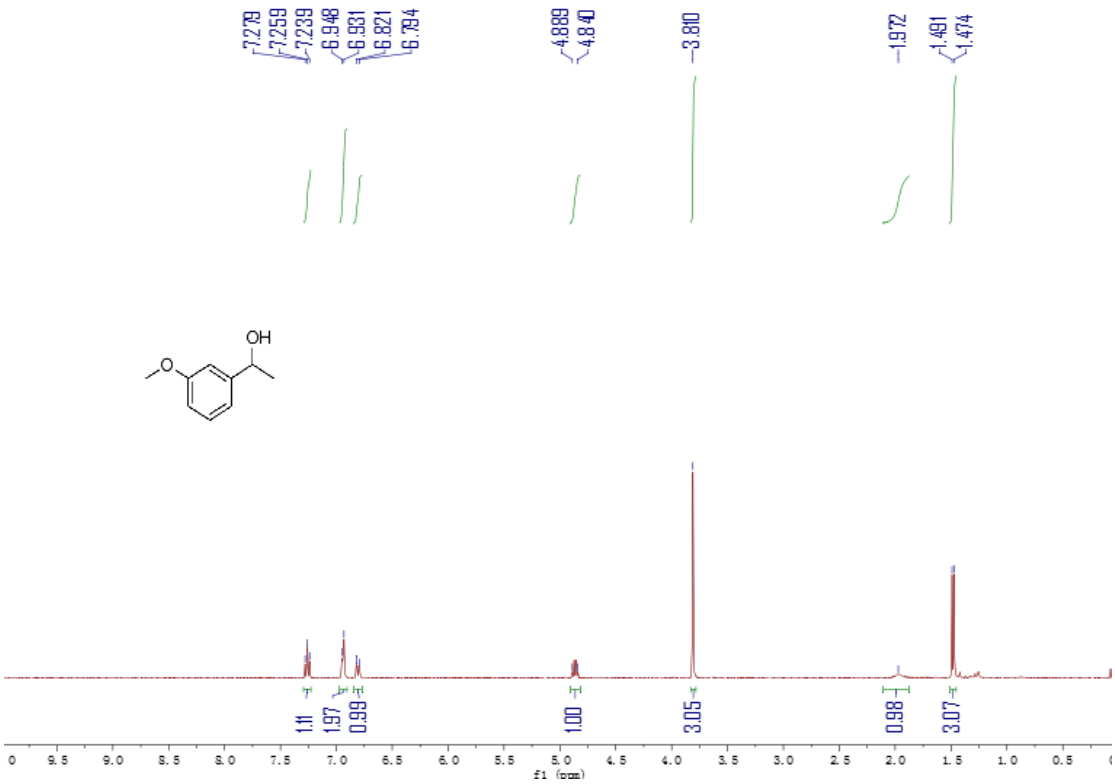


Figure S15. ^{1}H NMR spectrum of 1-(3-methoxyphenyl)ethan-1-ol in $CDCl_3$.

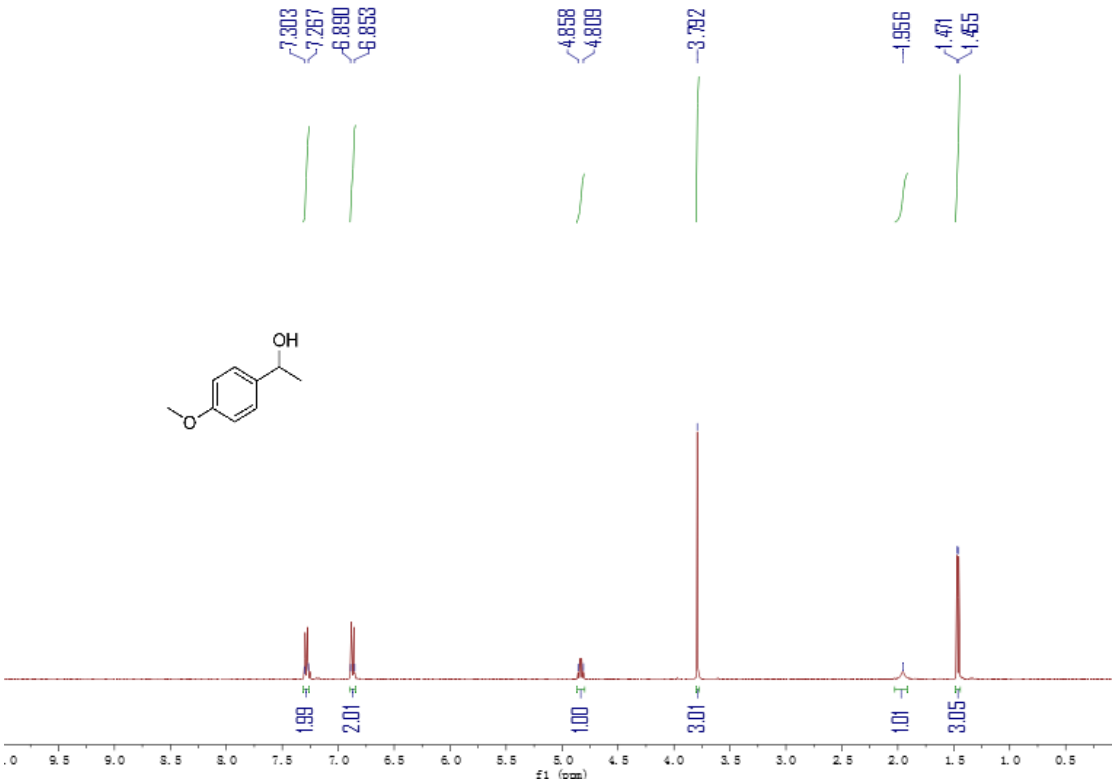


Figure S16. ^{1}H NMR spectrum of 1-(4-methoxyphenyl)ethan-1-ol in $CDCl_3$.

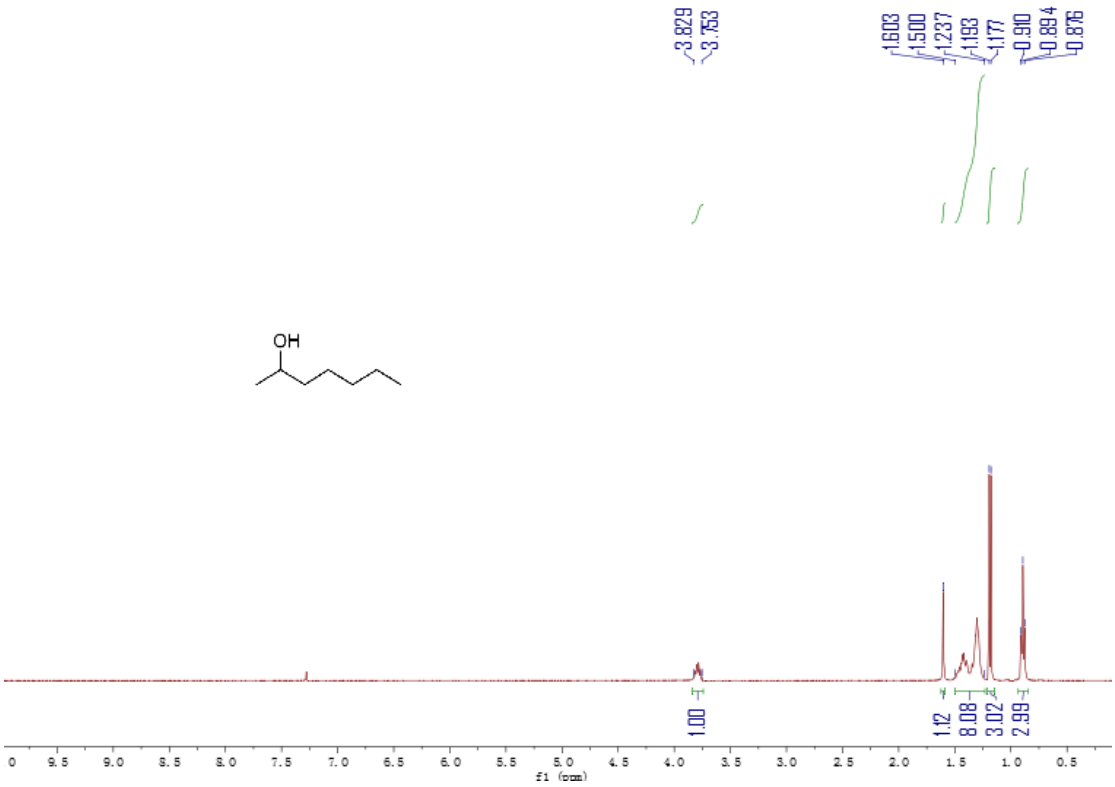


Figure S17. ^{1}H NMR spectrum of heptan-2-ol in $CDCl_3$.

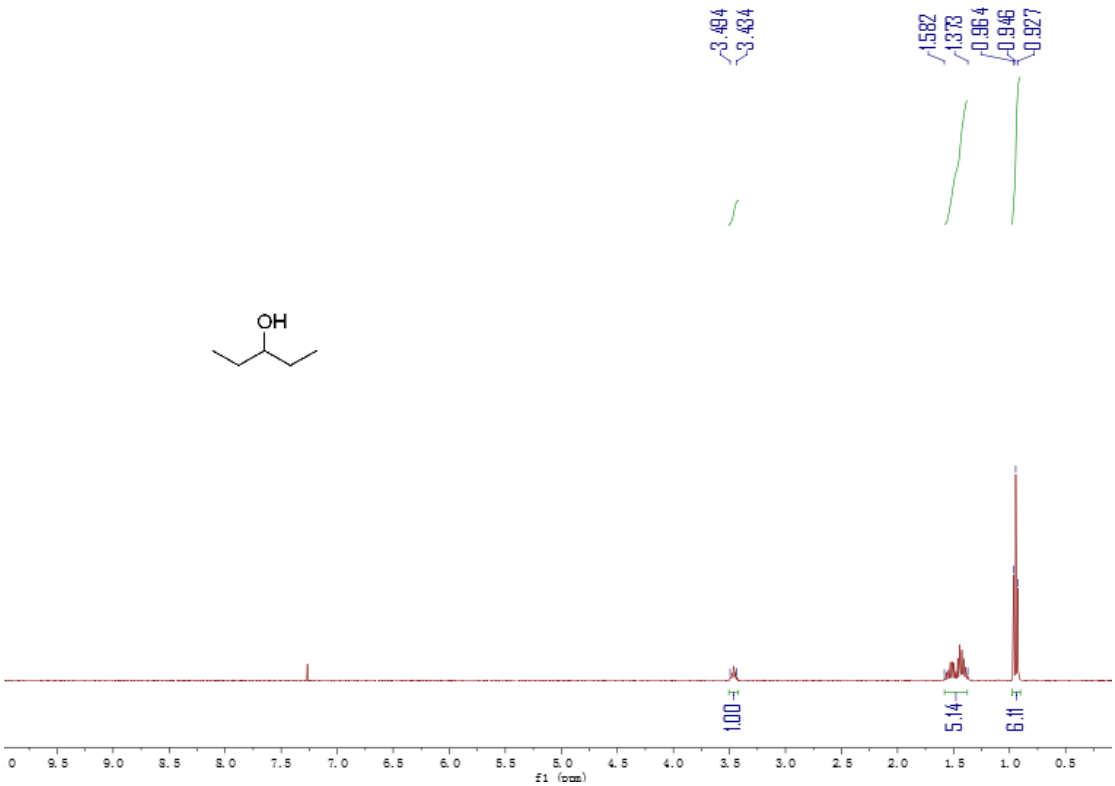


Figure S18. ^{1}H NMR spectrum of pentan-3-ol in $CDCl_3$.

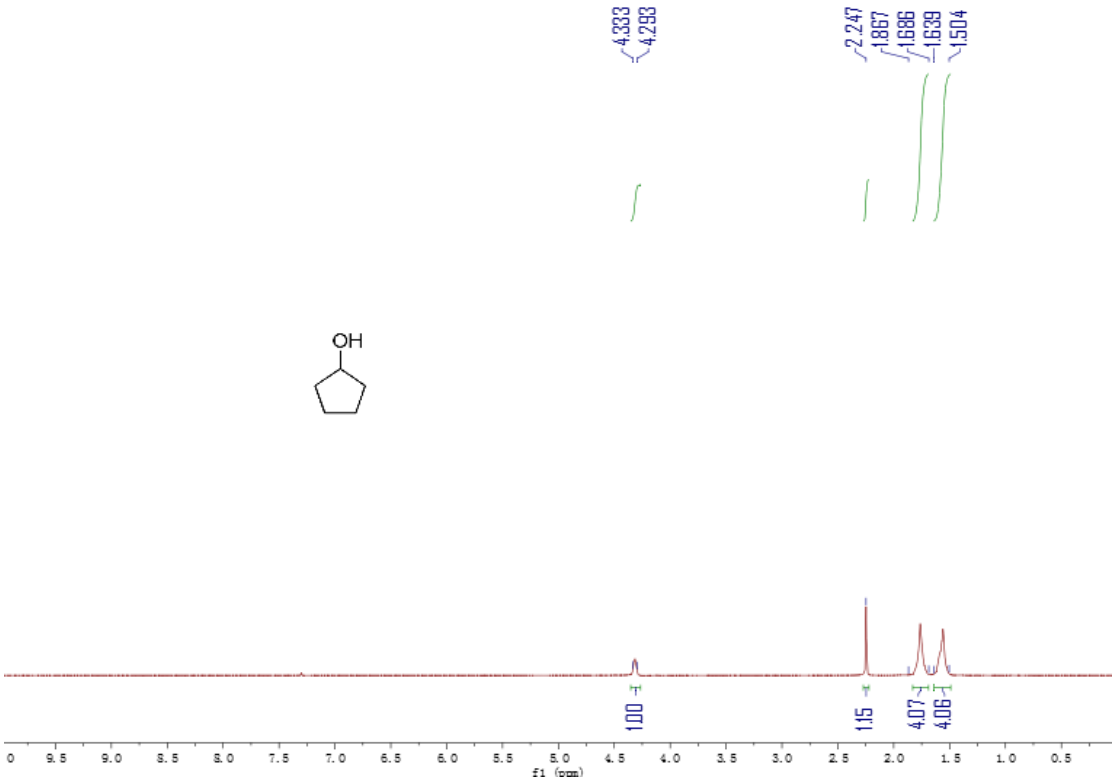


Figure S19. ^{1}H NMR spectrum of cyclopentanol in $CDCl_3$.

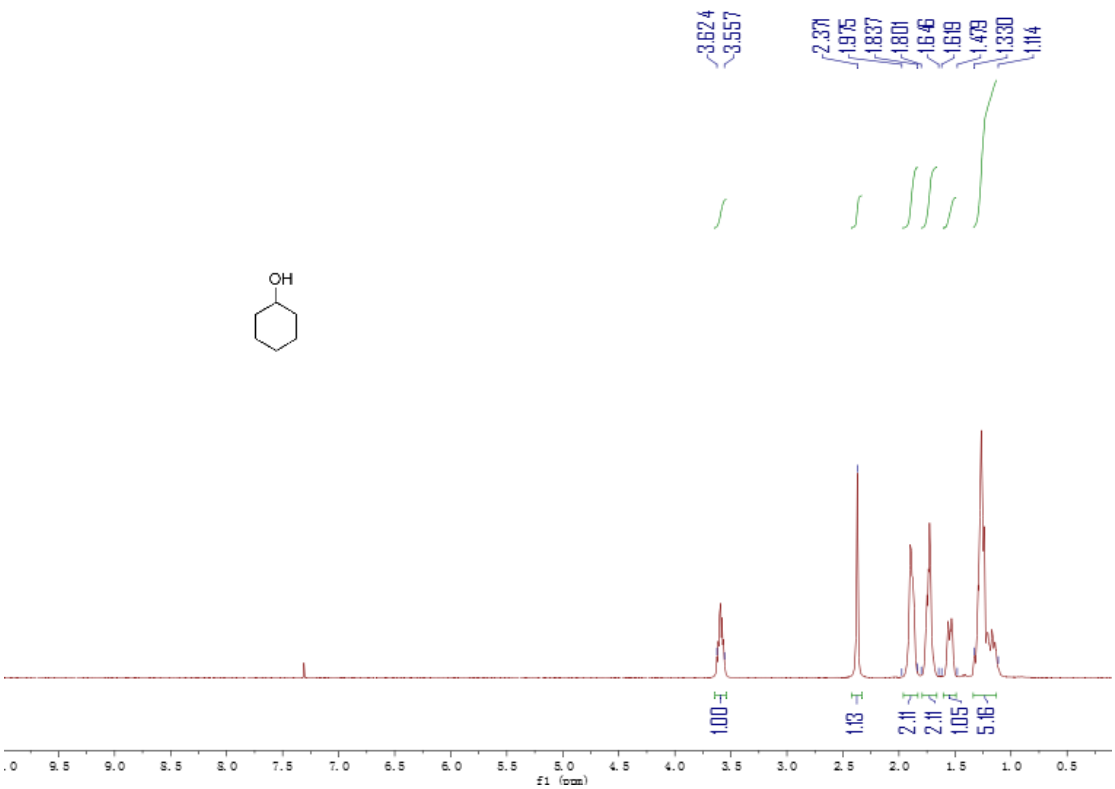


Figure S20. ^{1}H NMR spectrum of cyclohexanol in $CDCl_3$.

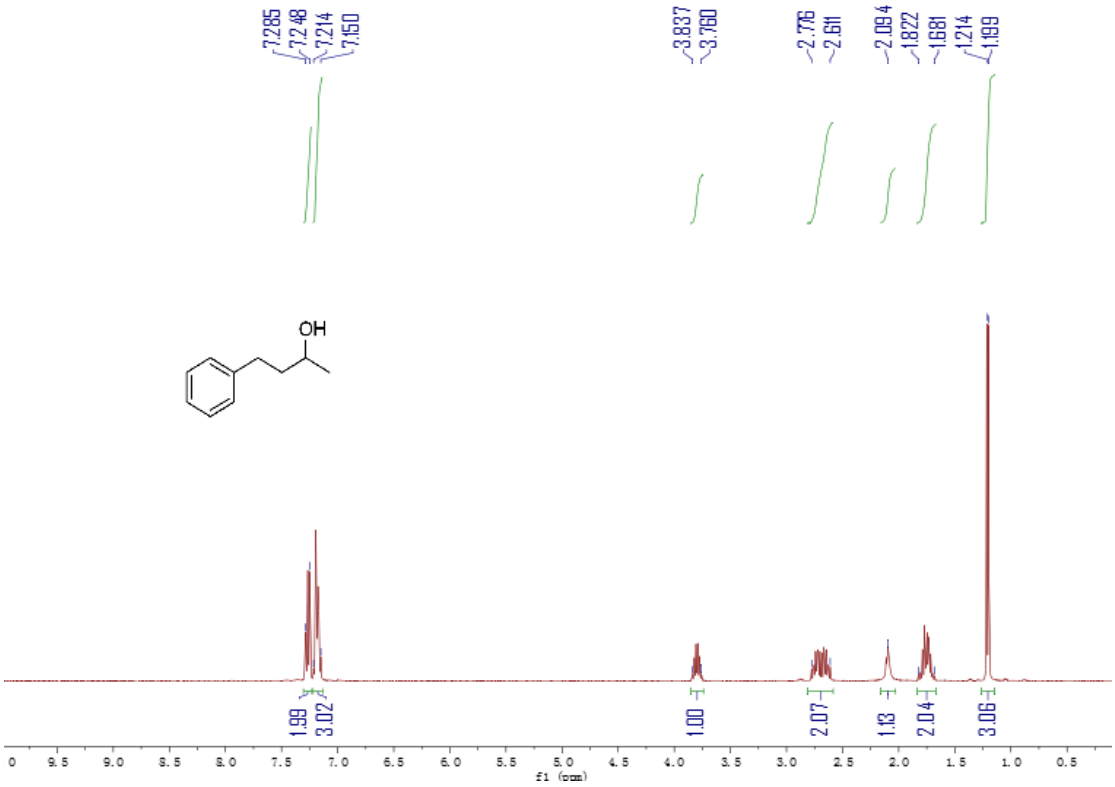


Figure S21. ^{1}H NMR spectrum of 4-phenylbutan-2-ol in $CDCl_3$.

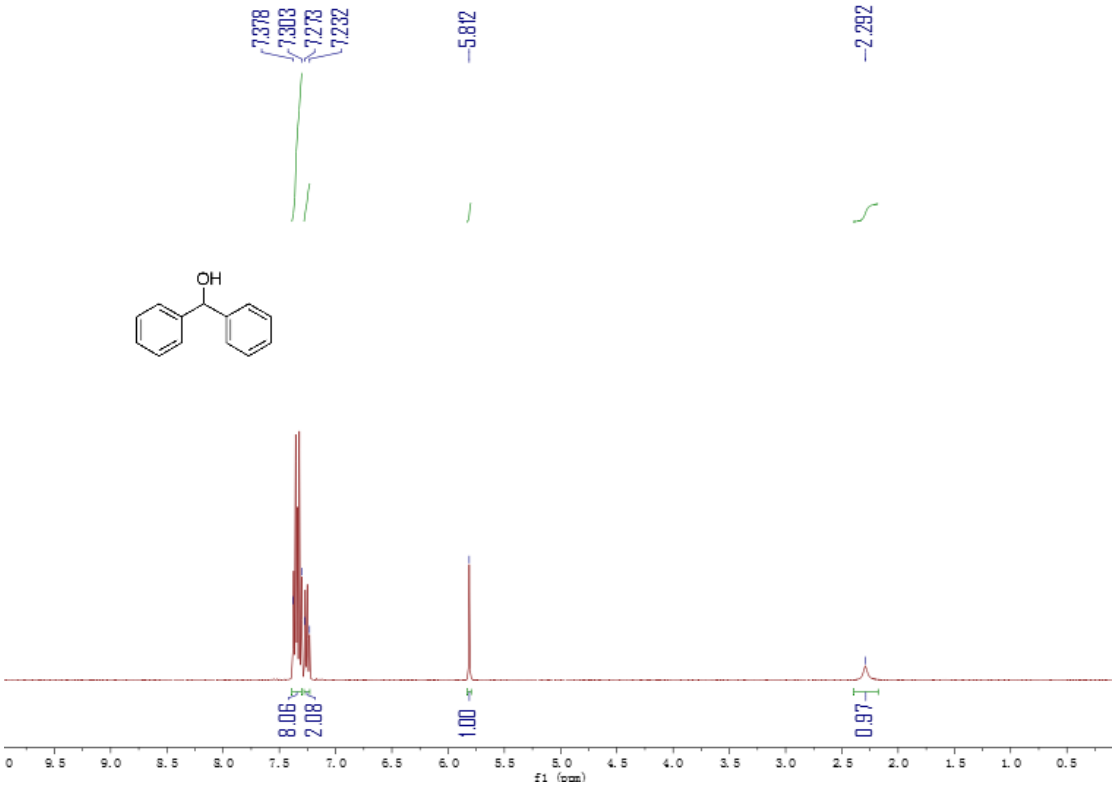


Figure S22. ^{1}H NMR spectrum of diphenylmethanol in $CDCl_3$.

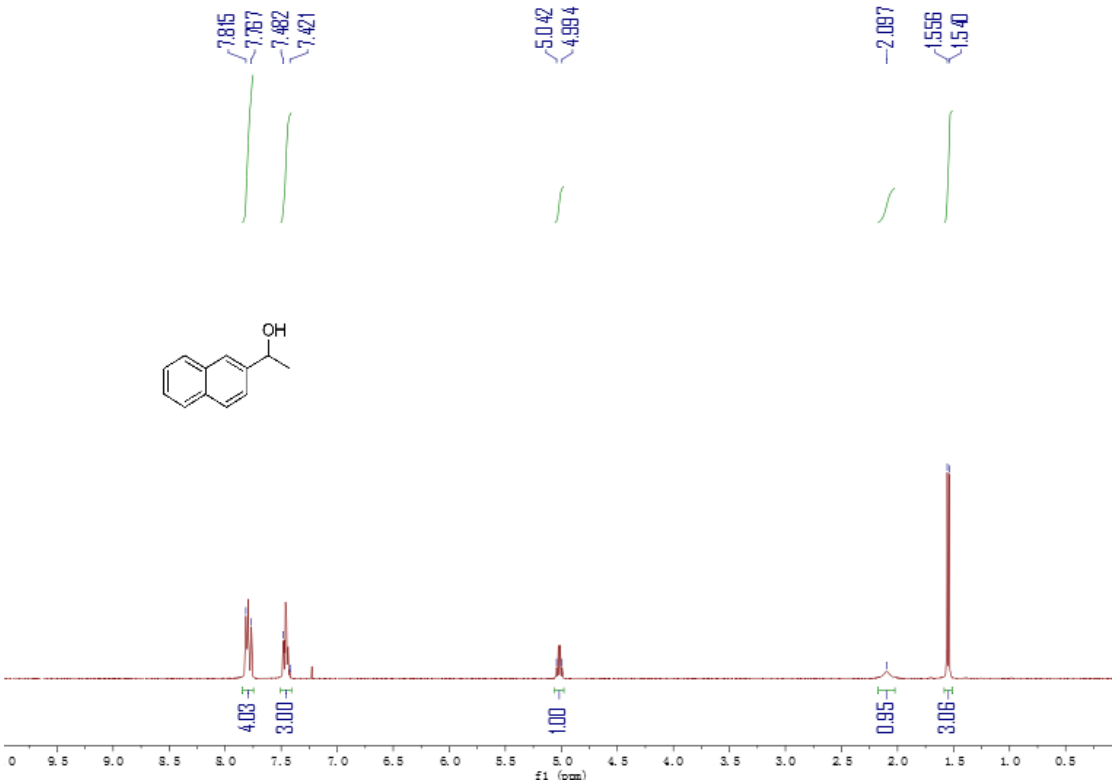


Figure S23. ^{1}H NMR spectrum of 1-(naphthalen-2-yl)ethan-1-ol in $CDCl_3$.

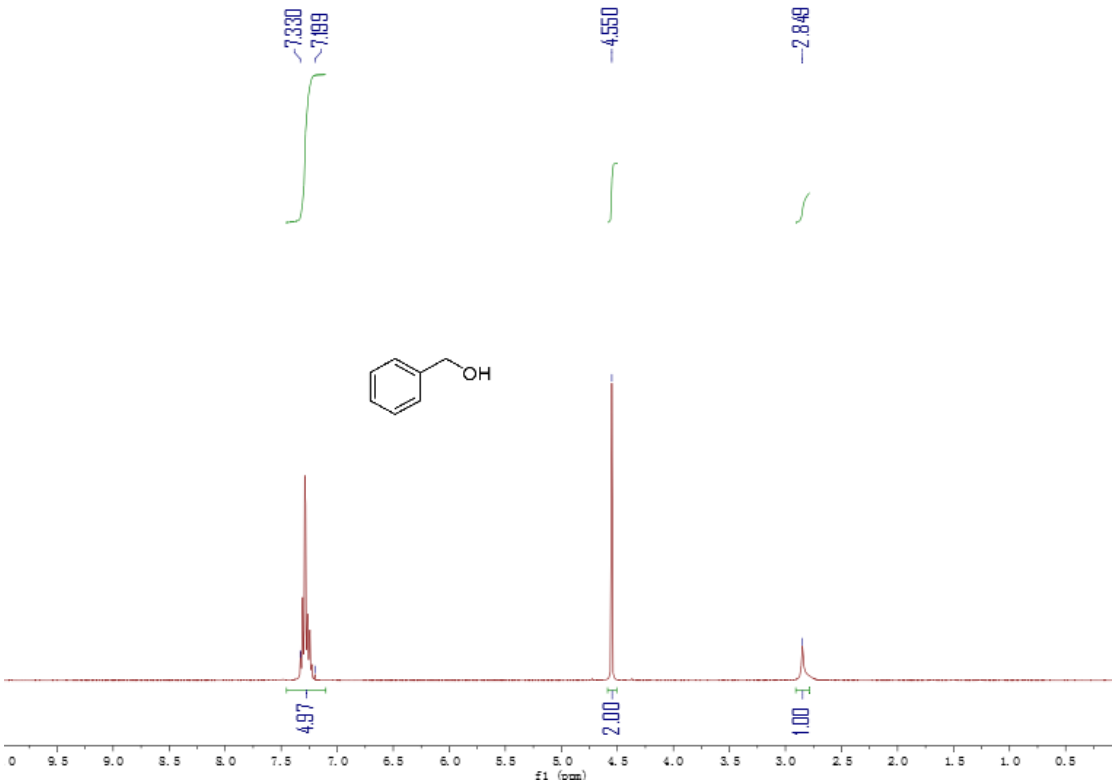


Figure S24. ^{1}H NMR spectrum of phenylmethanol in $CDCl_3$.

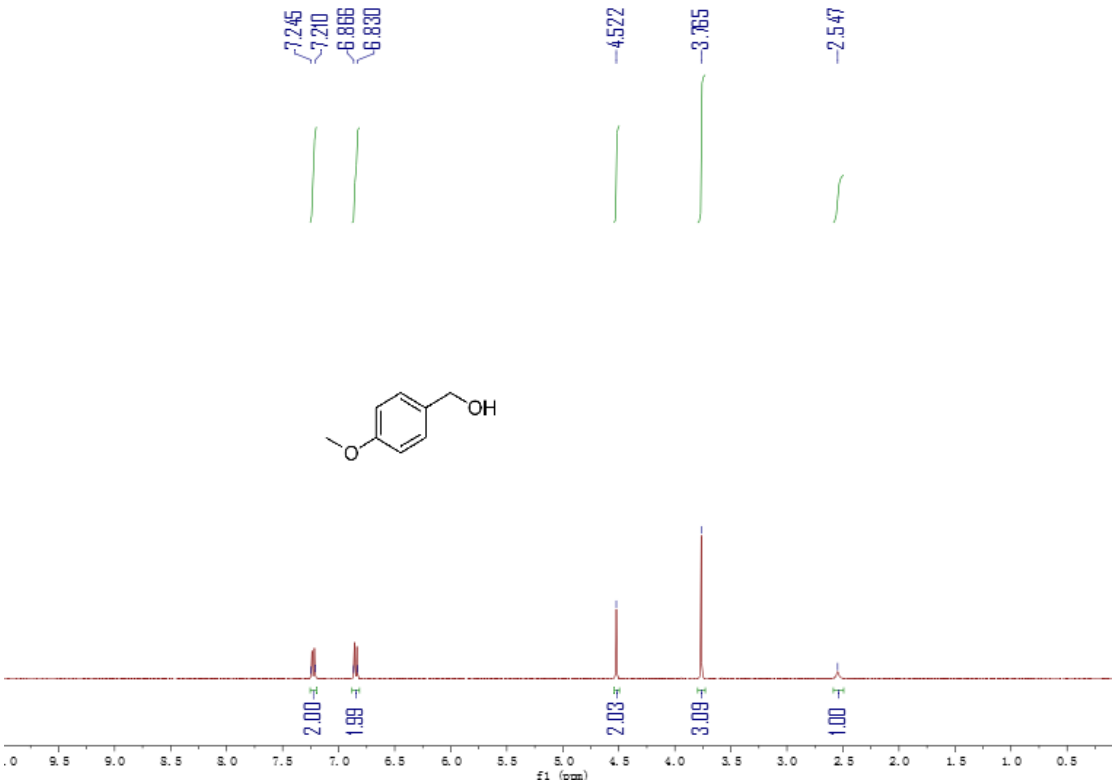


Figure S25. ^{1}H NMR spectrum of (4-methoxyphenyl)methanol in $CDCl_3$.

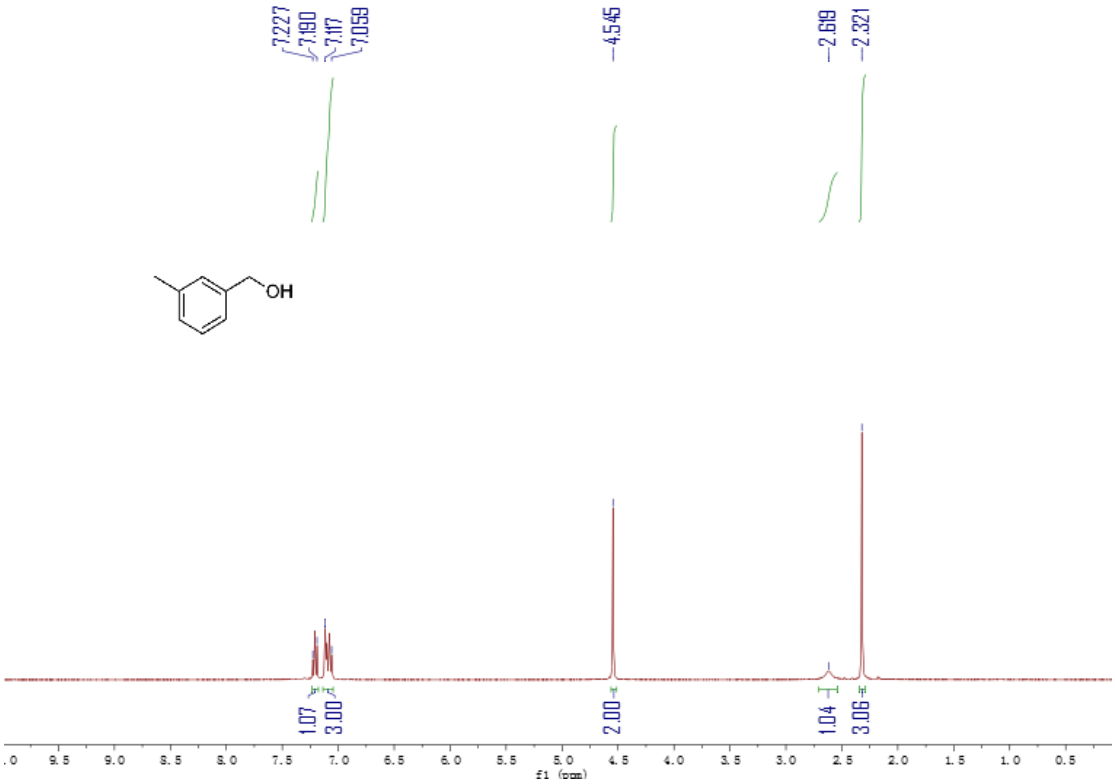


Figure S26. ^{1}H NMR spectrum of m-tolylmethanol in $CDCl_3$.

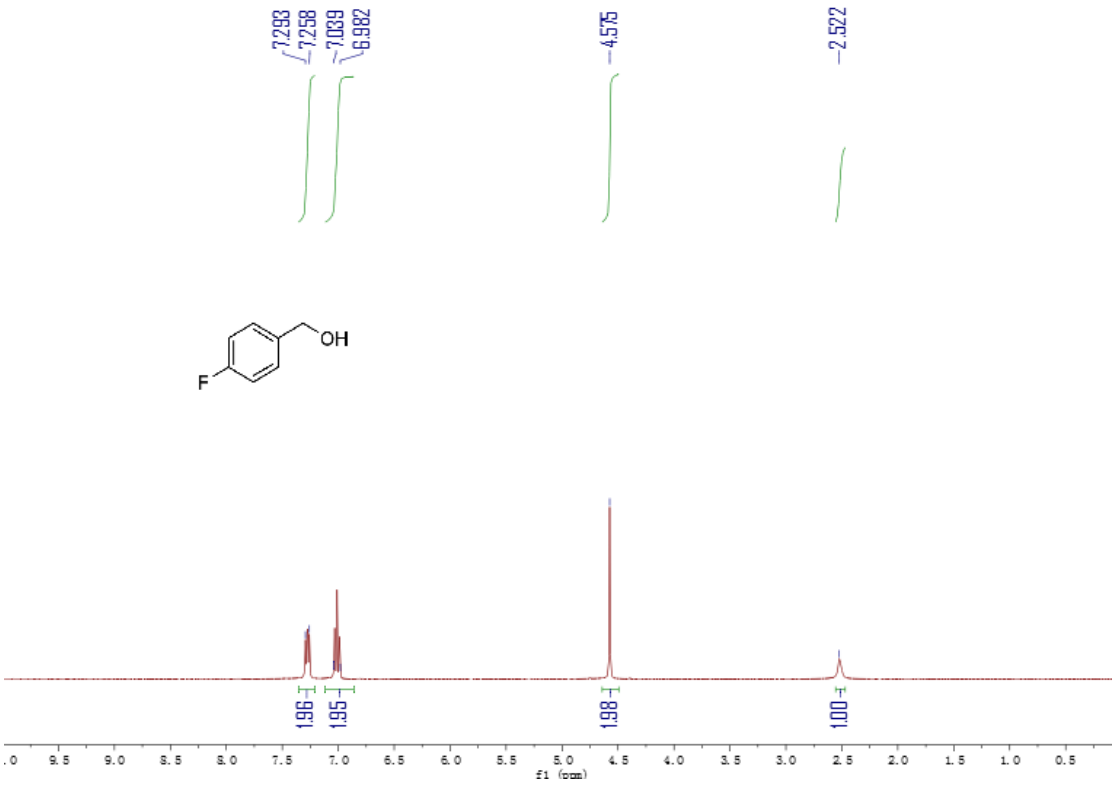


Figure S27. ^{1}H NMR spectrum of (4-fluorophenyl)methanol in $CDCl_3$.

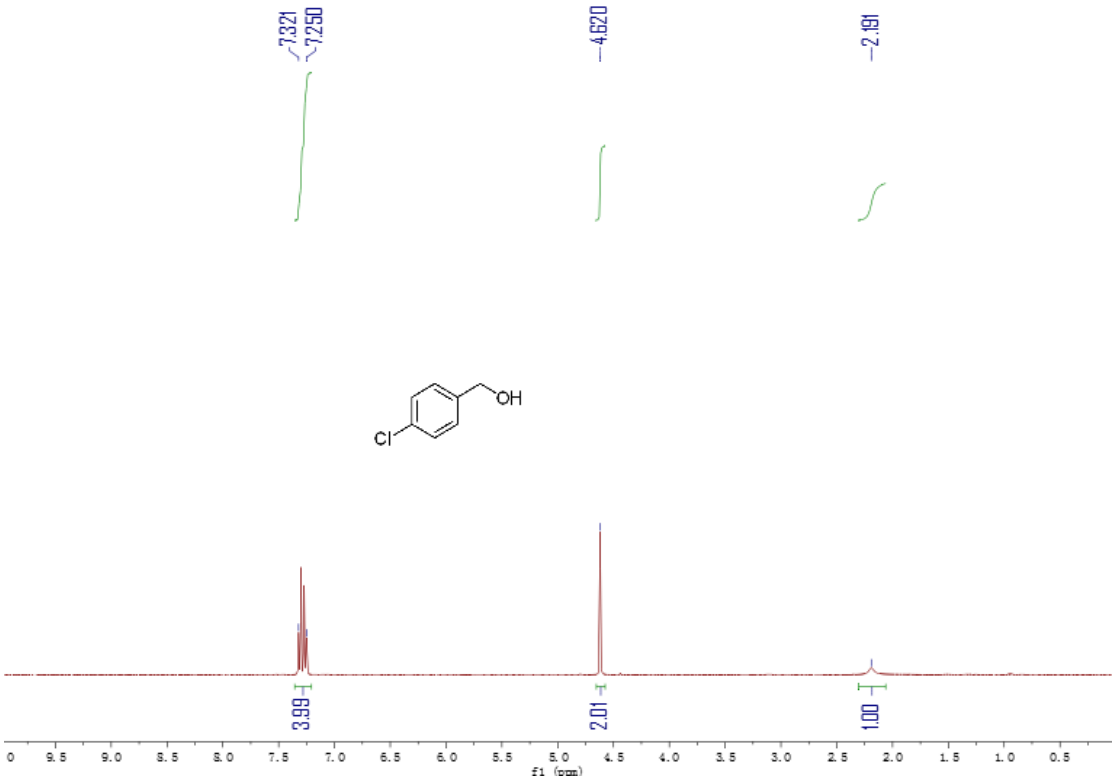


Figure S28. ^{1}H NMR spectrum of (4-chlorophenyl)methanol in $CDCl_3$.

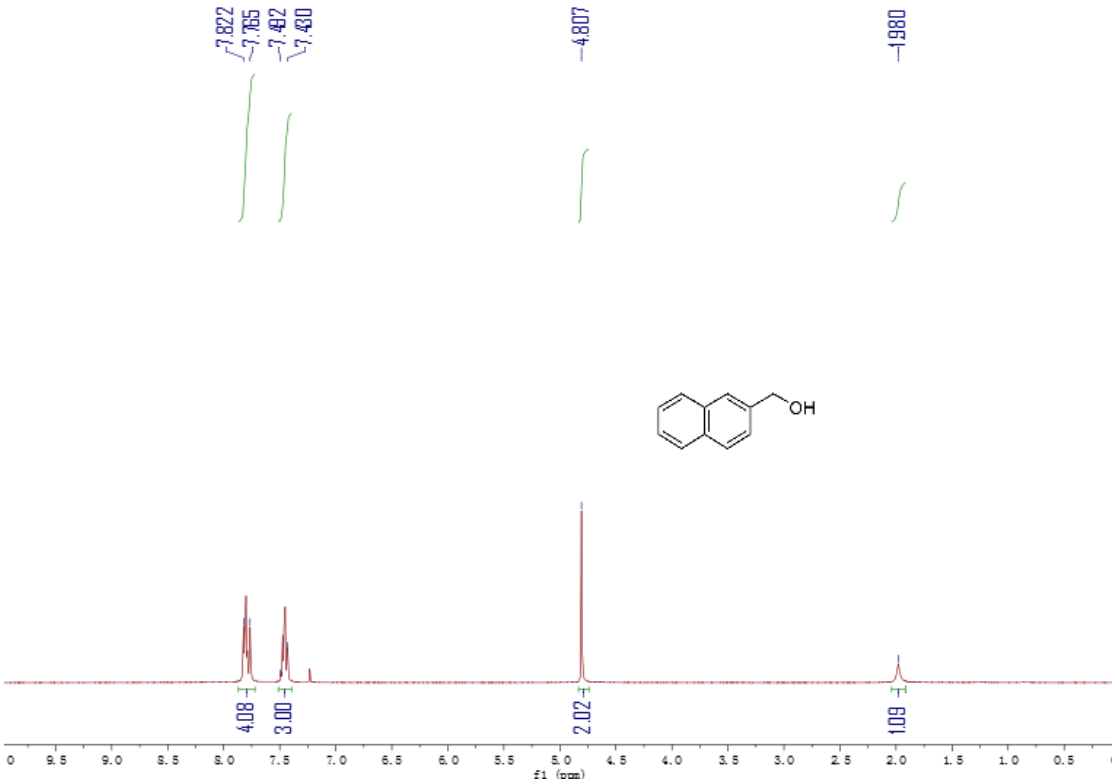


Figure S29. ^{1}H NMR spectrum of naphthalen-2-ylmethanol in $CDCl_3$.

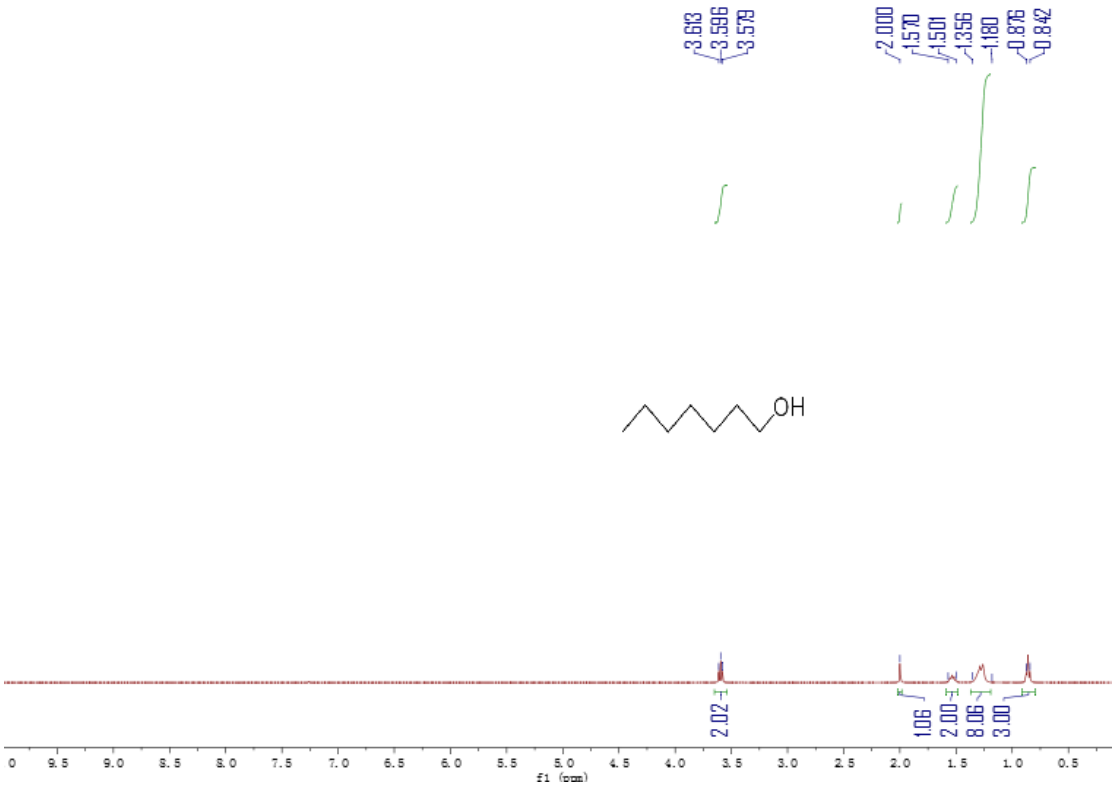


Figure S30. ^{1}H NMR spectrum of heptan-1-ol in $CDCl_3$.

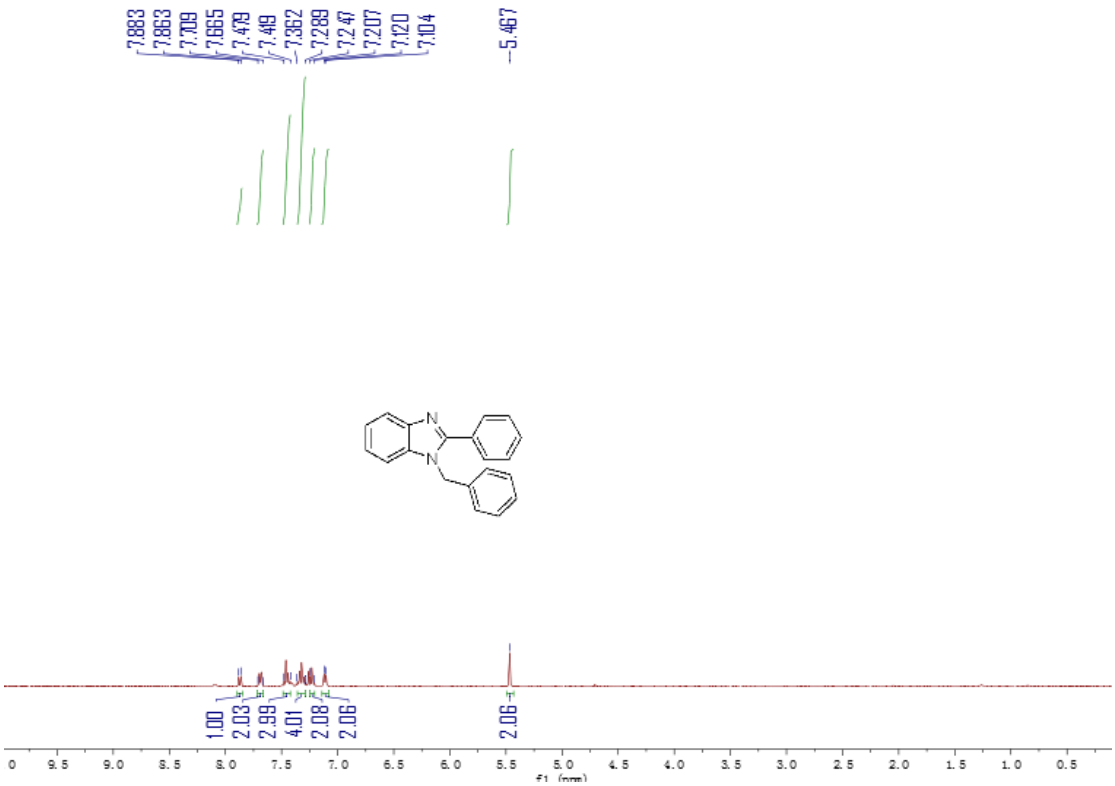


Figure S31. ^{1}H NMR spectrum of 1-benzyl-2-phenyl-1H-benzo[d]imidazole in $CDCl_3$.

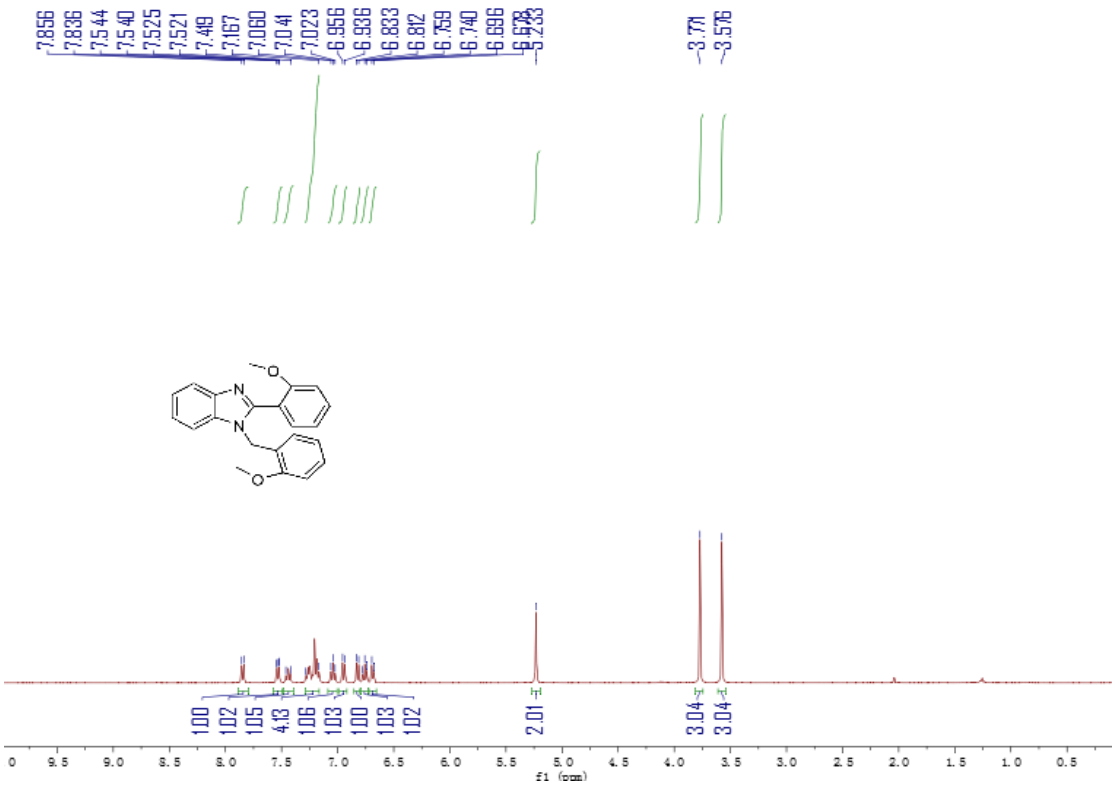


Figure S32. ^{1}H NMR spectrum of 1-(2-methoxybenzyl)-2-(2-methoxyphenyl)-1H-benzo[d]imidazole in $CDCl_3$.

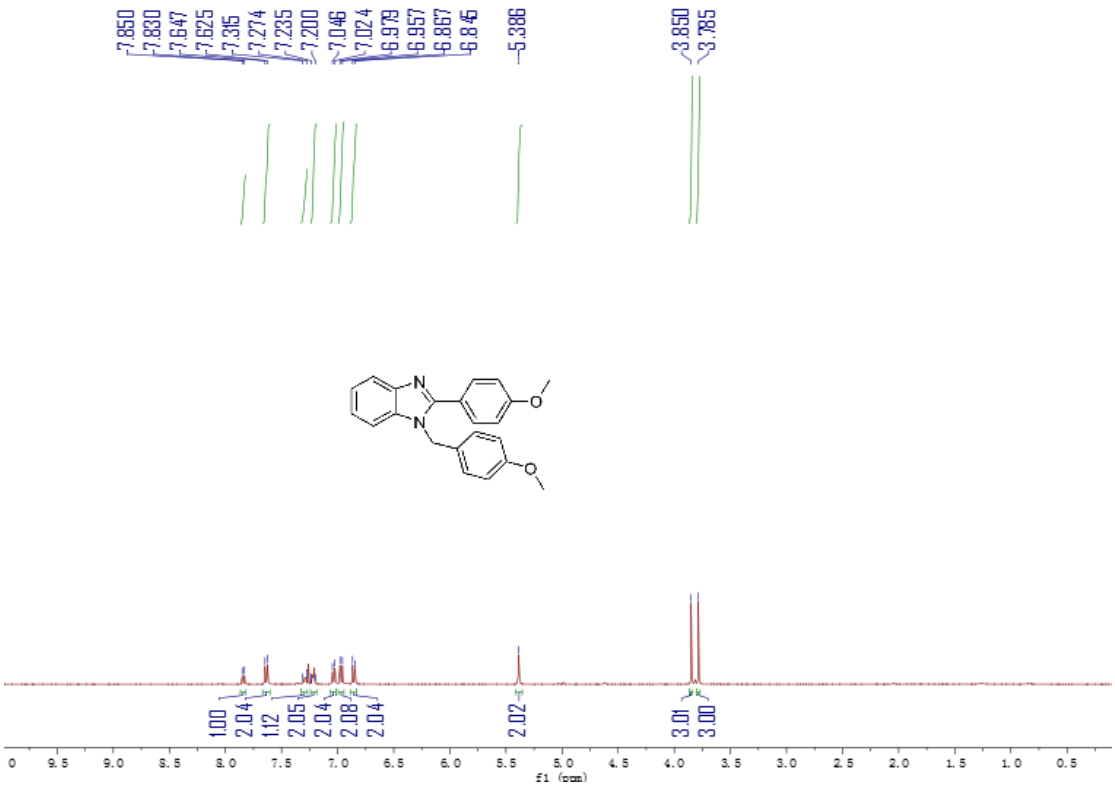


Figure S33. ^{1}H NMR spectrum of 1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1H-benzo[d]imidazole in $CDCl_3$.

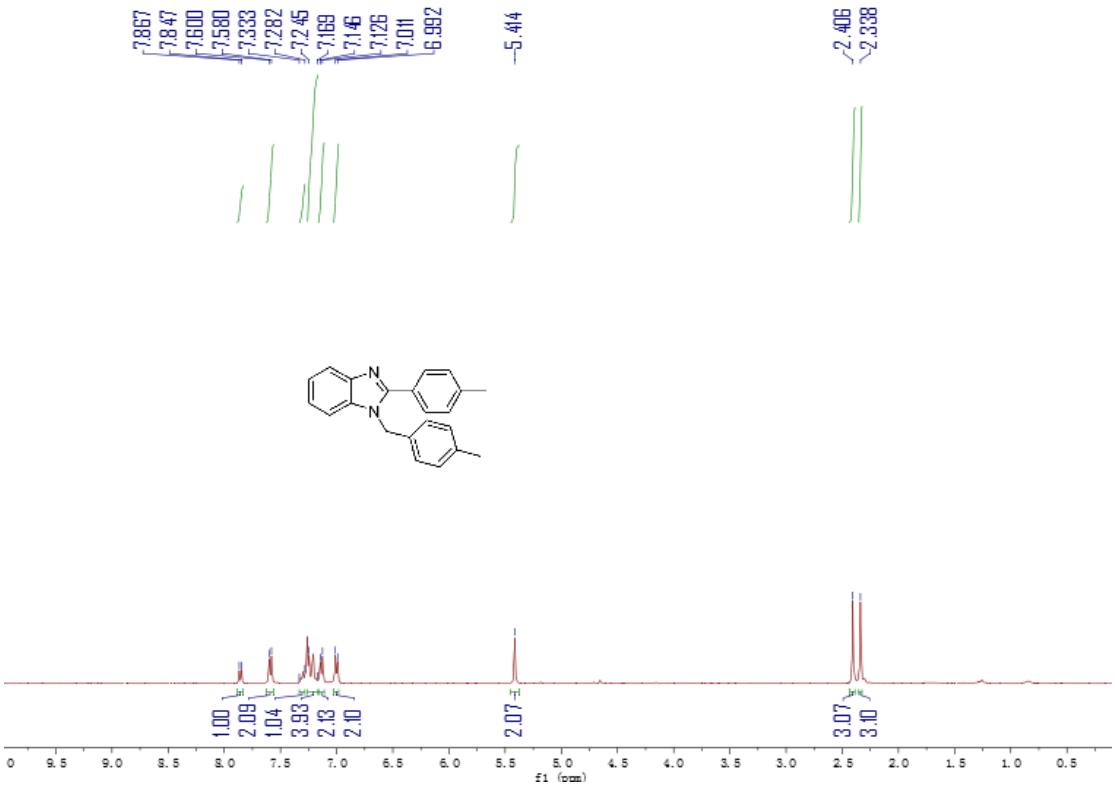


Figure S34. ^{1}H NMR spectrum of 1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole in $CDCl_3$.

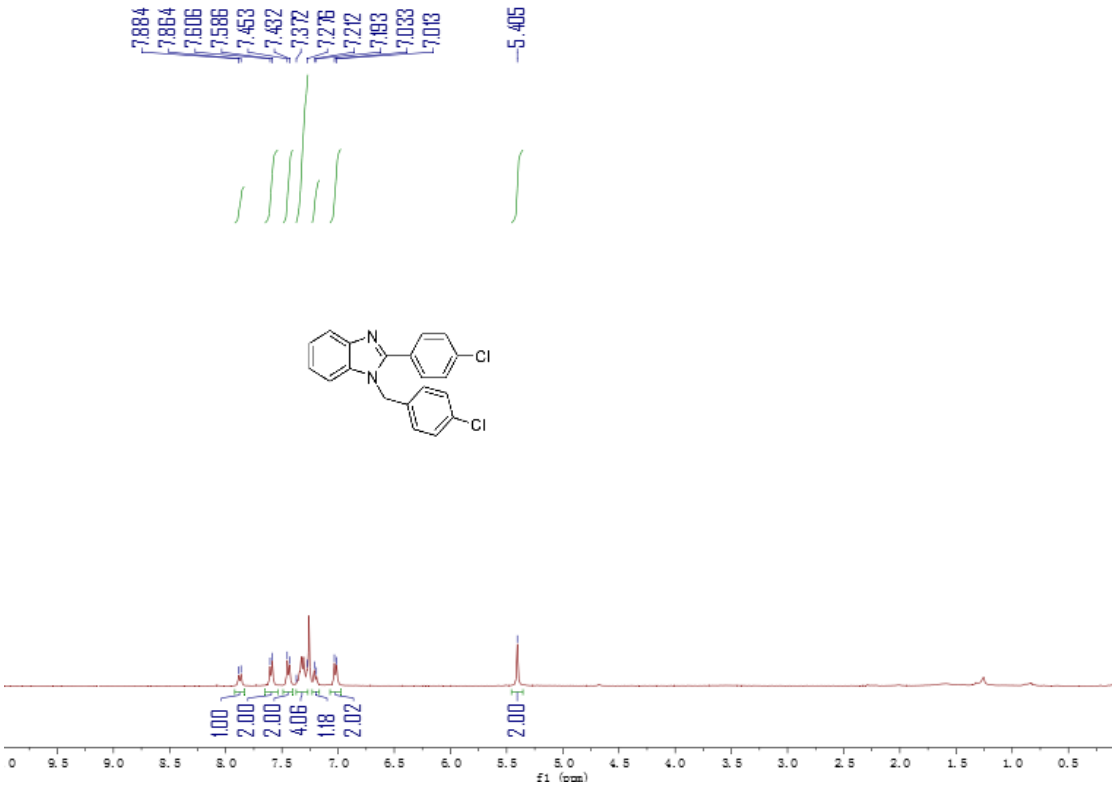


Figure S35. ^{1}H NMR spectrum of 1-(4-chlorobenzyl)-2-(4-chlorophenyl)-1H-benzo[d]imidazole in $CDCl_3$.

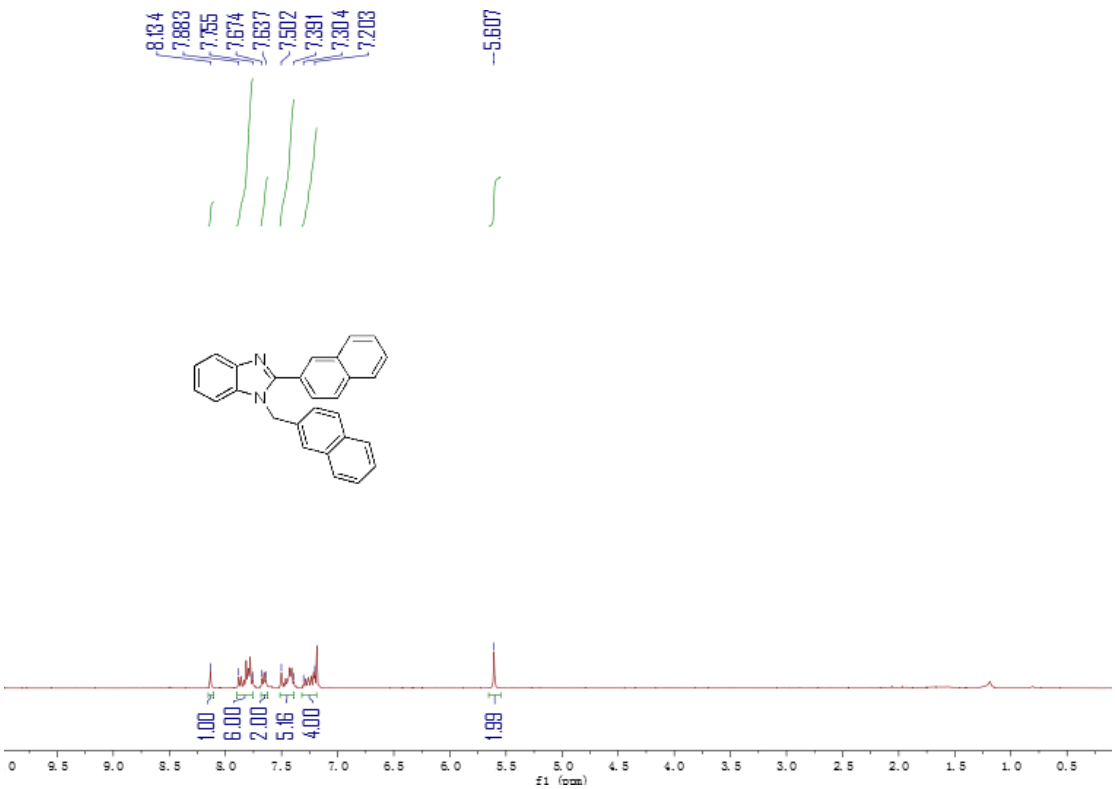


Figure S36. ^{1}H NMR spectrum of 2-(naphthalen-2-yl)-1-(naphthalen-2-ylmethyl)-1H-benzo[d]imidazole in $CDCl_3$.

Figure S37. ^{1}H NMR spectrum of 2-phenylquinoline in $CDCl_3$.

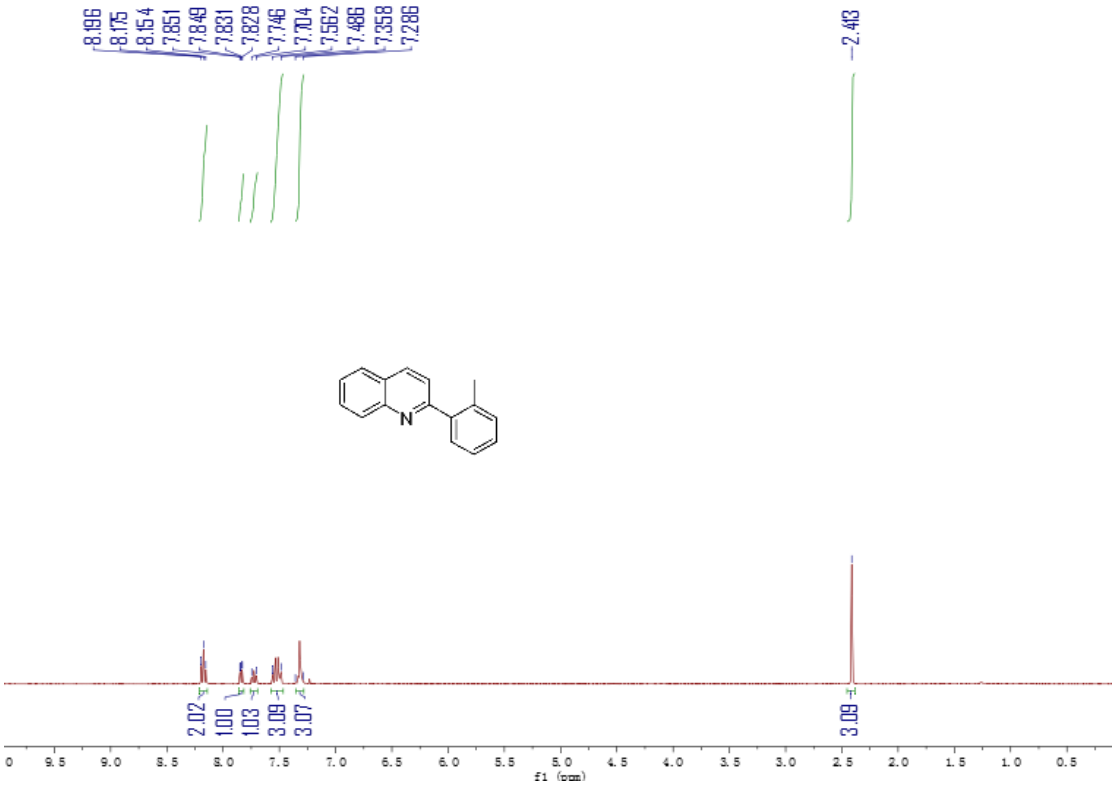


Figure S38. ^{1}H NMR spectrum of 2-(o-tolyl)quinoline in $CDCl_3$.

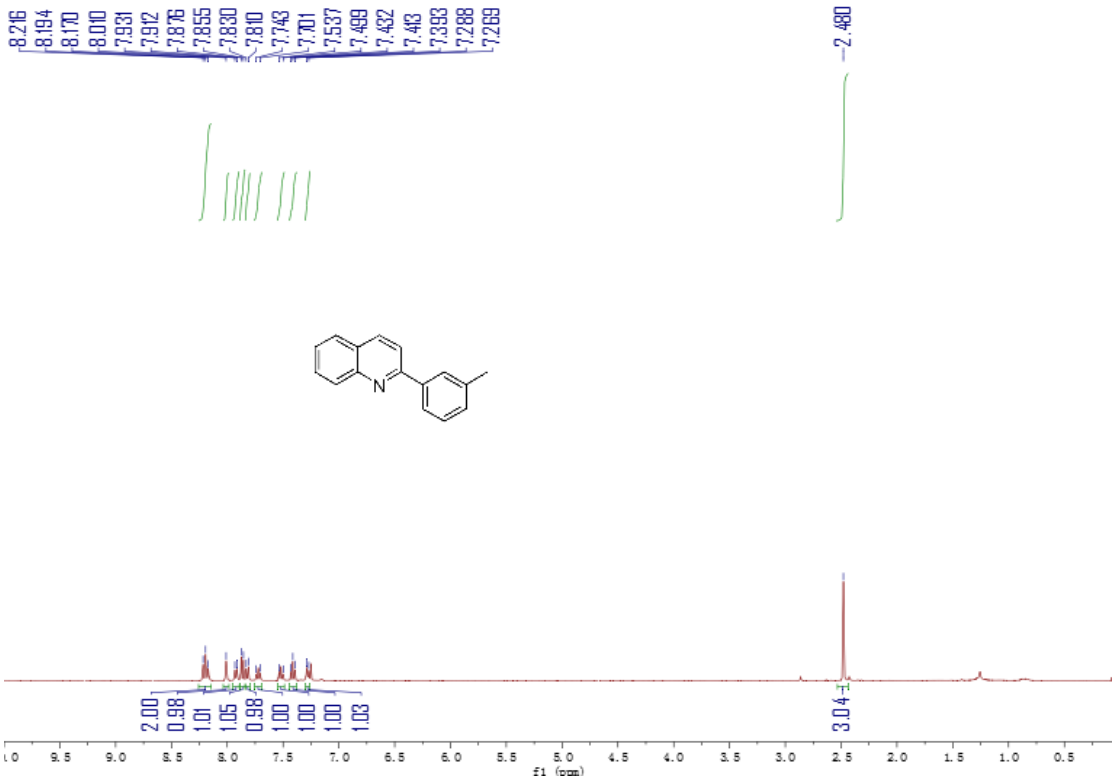


Figure S39. ^{1}H NMR spectrum of 2-(m-tolyl)quinoline in $CDCl_3$.

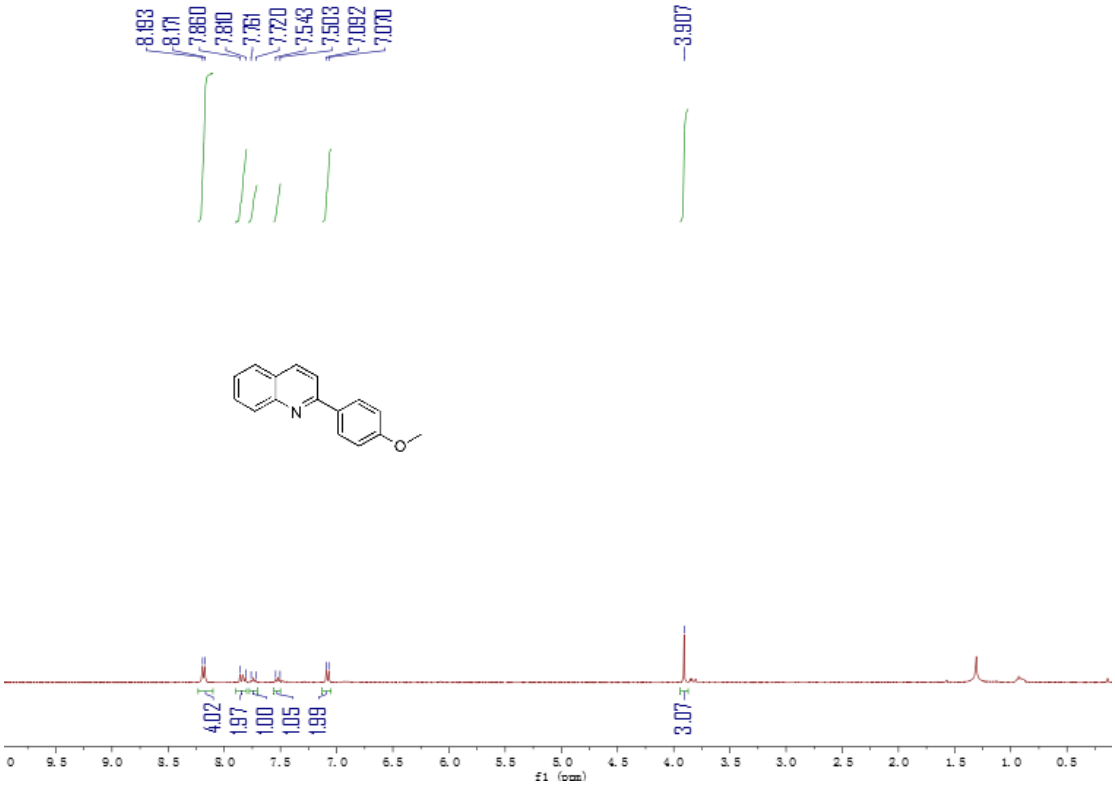


Figure S40. ^{1}H NMR spectrum of 2-(4-methoxyphenyl)quinolone in $CDCl_3$.

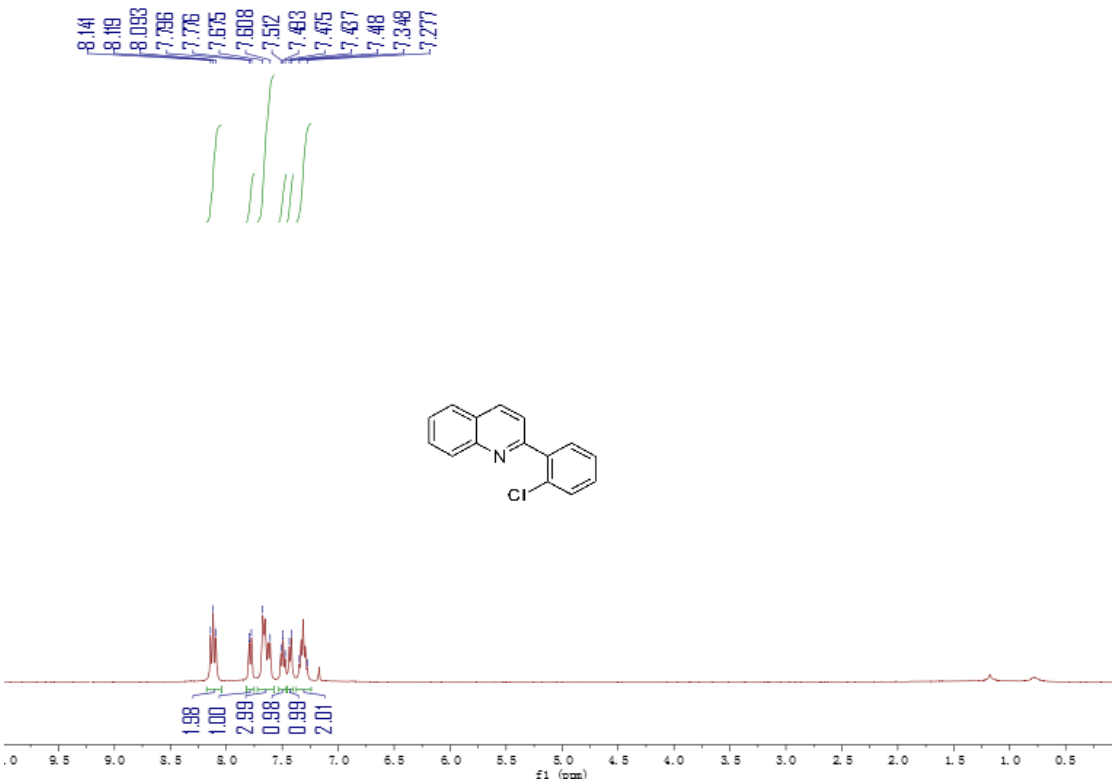


Figure S41. ^{1}H NMR spectrum of 2-(2-chlorophenyl)quinolone in $CDCl_3$.

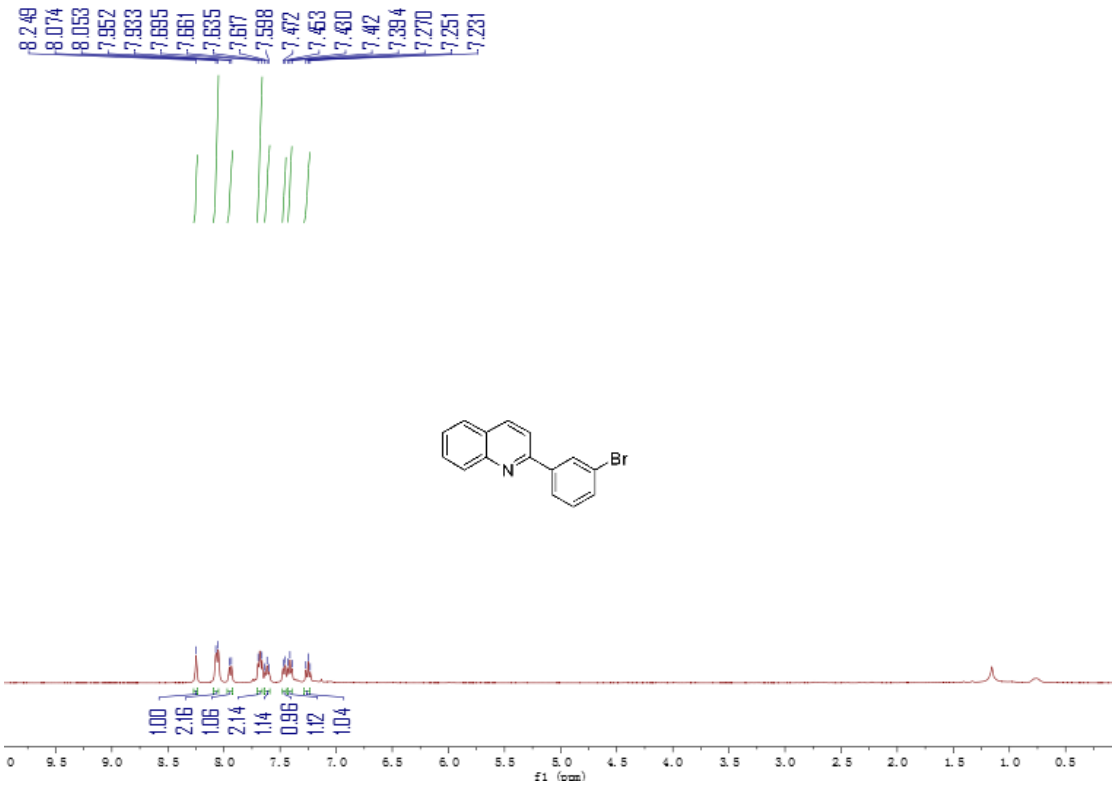


Figure S42. ^{1}H NMR spectrum of 2-(3-bromophenyl)quinolone in $CDCl_3$.

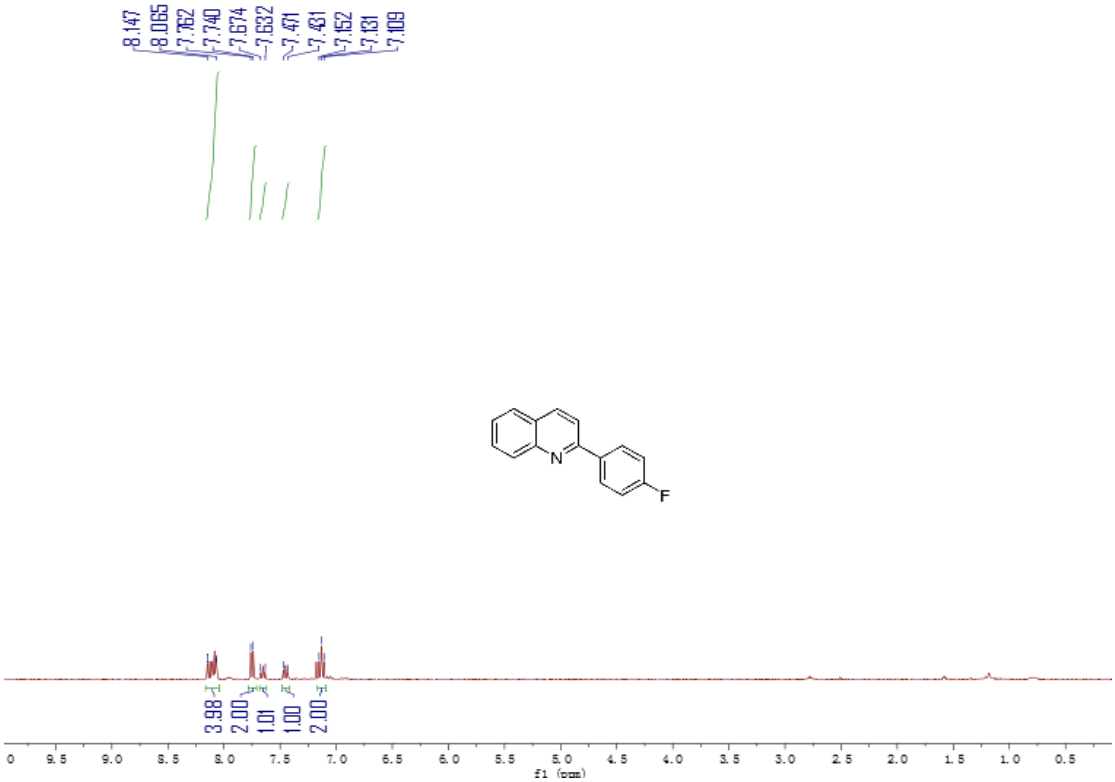


Figure S43. ^{1}H NMR spectrum of 2-(4-fluorophenyl)quinolone in $CDCl_3$.

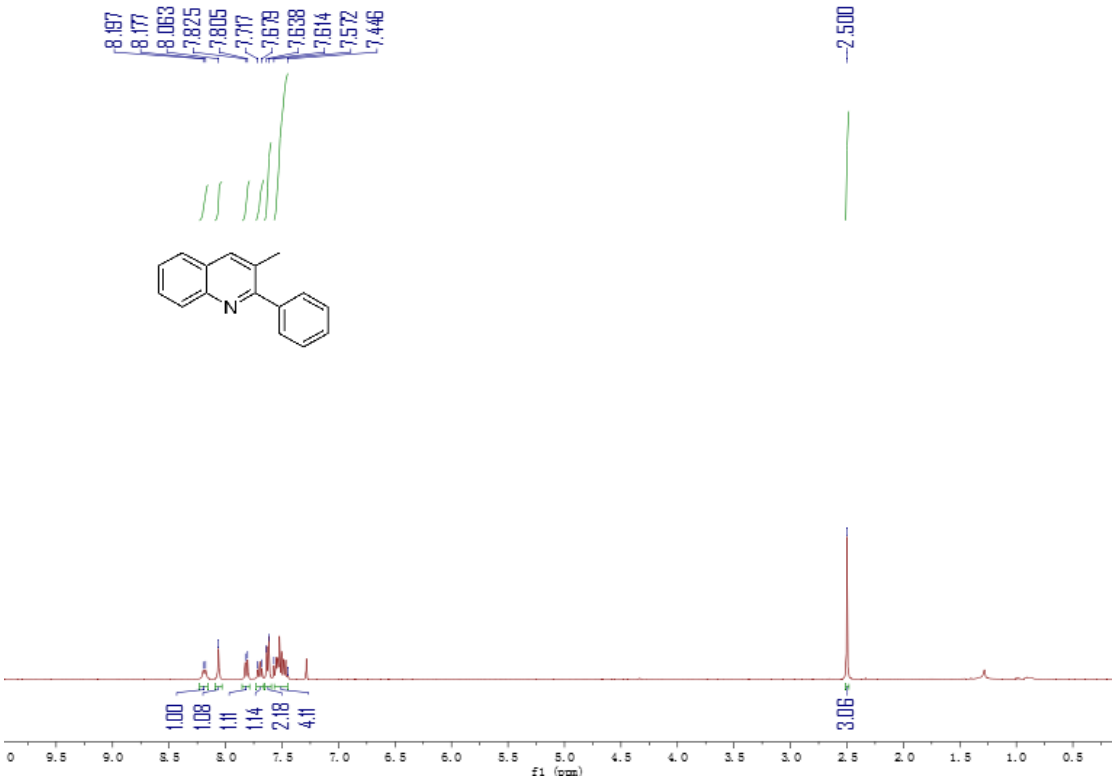


Figure S44. ^{1}H NMR spectrum of 3-methyl-2-phenylquinoline in $CDCl_3$.

^{13}C NMR Spectra

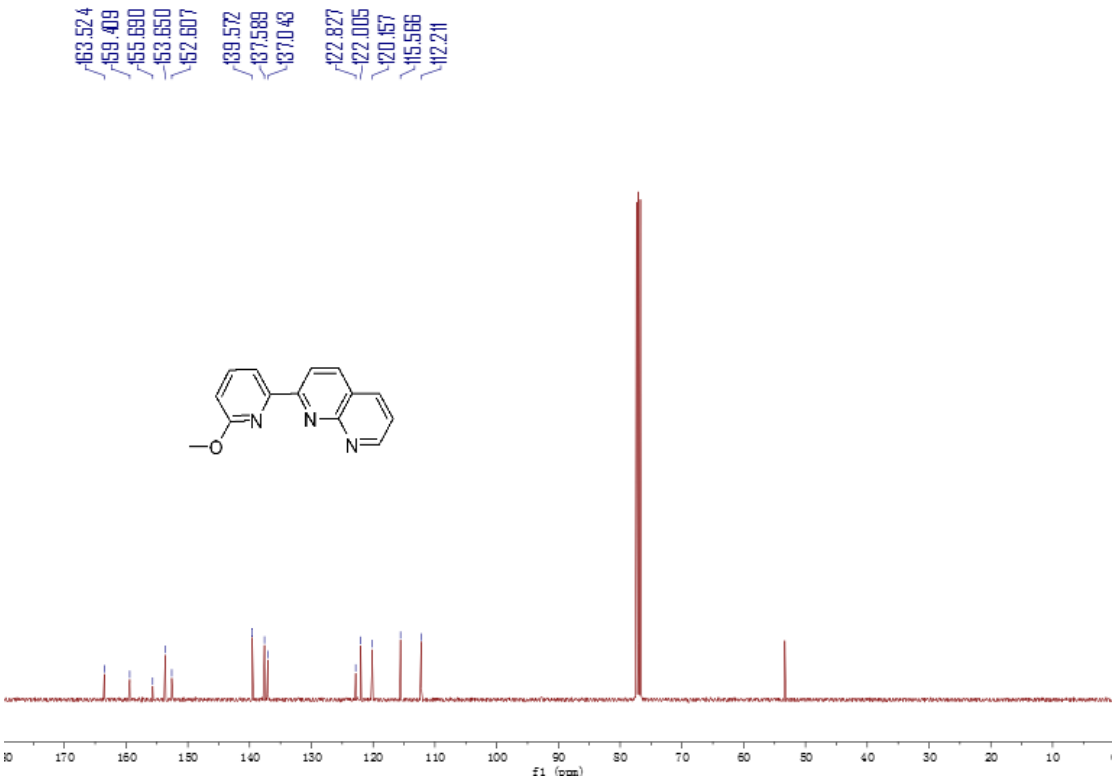


Figure S45. ^{13}C NMR spectrum of 2-(6-methoxypyridin-2-yl)-1,8-naphthyridine in $CDCl_3$.

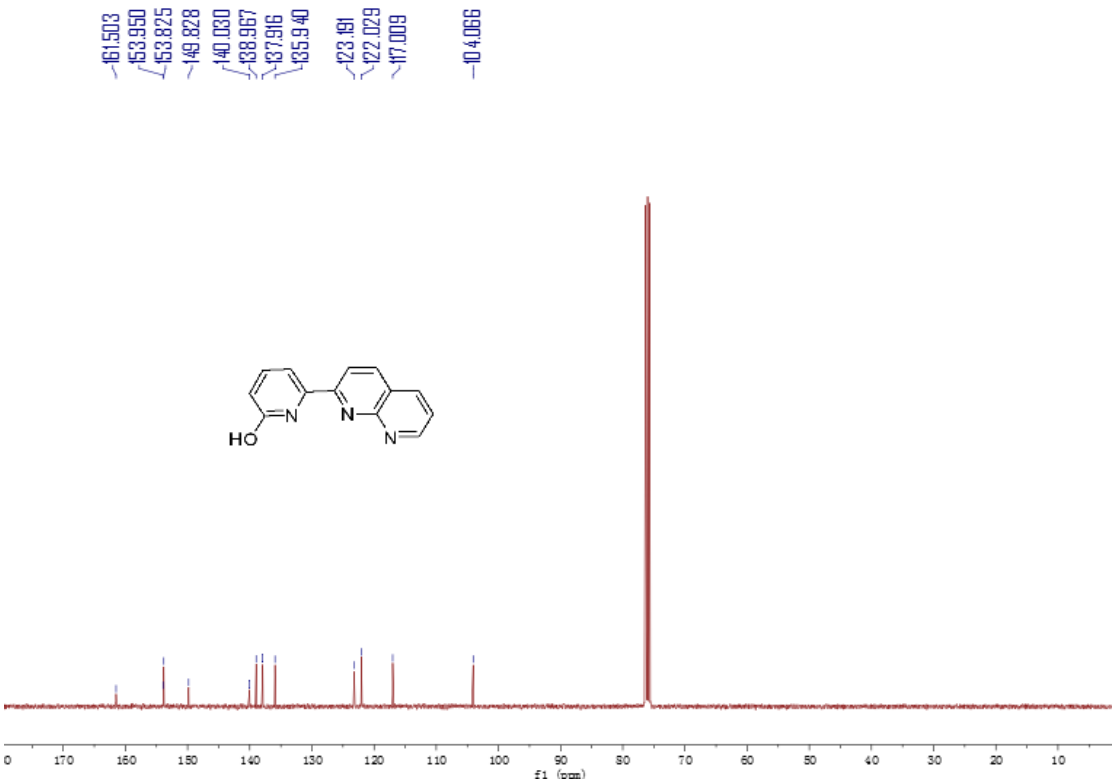


Figure S46. ^{13}C NMR spectrum of 6-(1,8-naphthyridin-2-yl)pyridin-2-ol in $CDCl_3$.

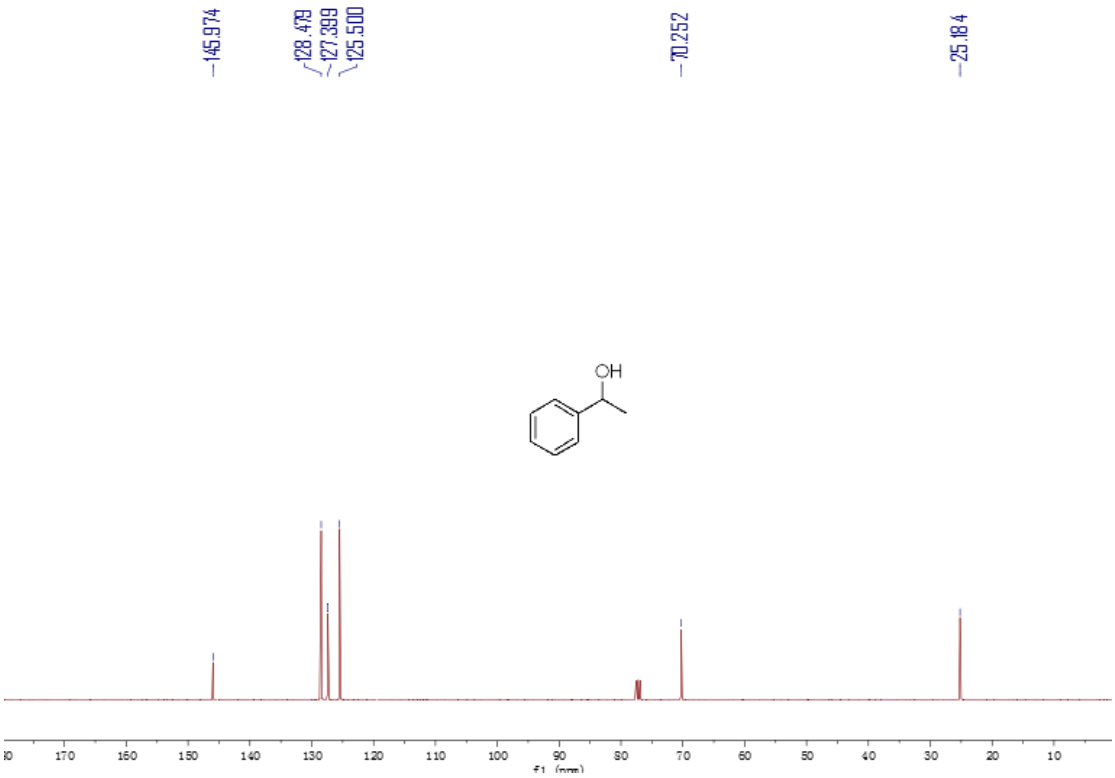


Figure S47. ^{13}C NMR spectrum of 1-phenylethan-1-ol in $CDCl_3$.

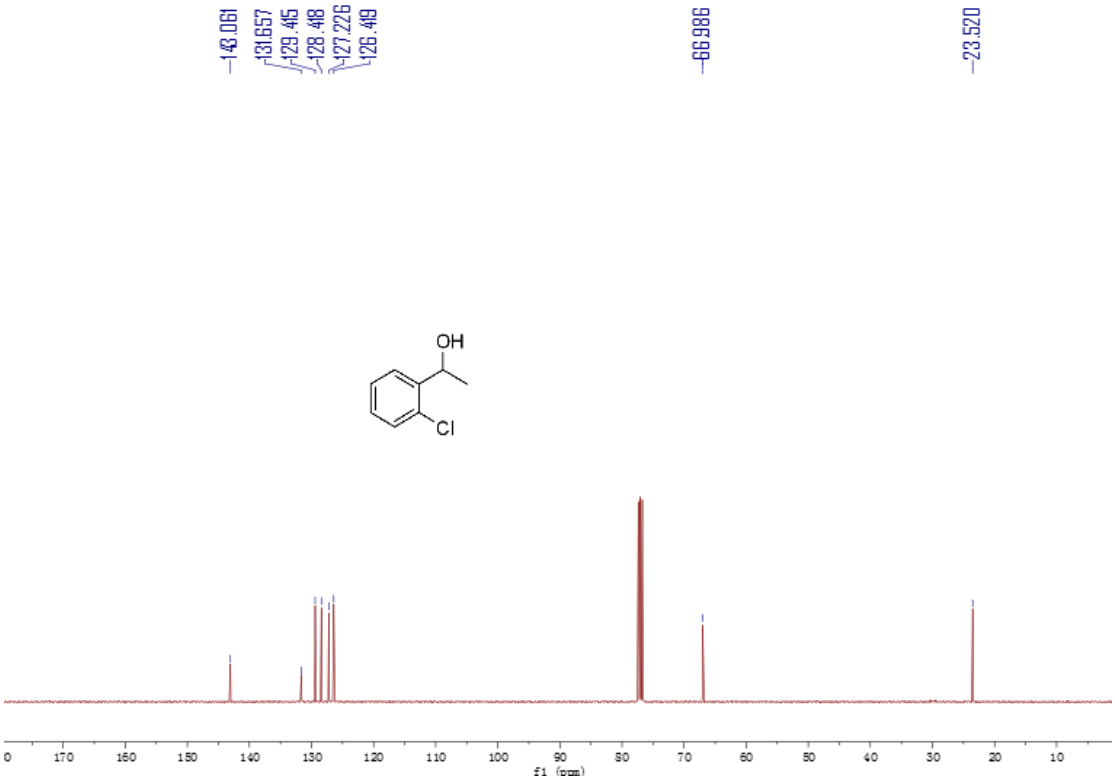


Figure S48. ^{13}C NMR spectrum of 1-(2-chlorophenyl)ethan-1-ol in $CDCl_3$.

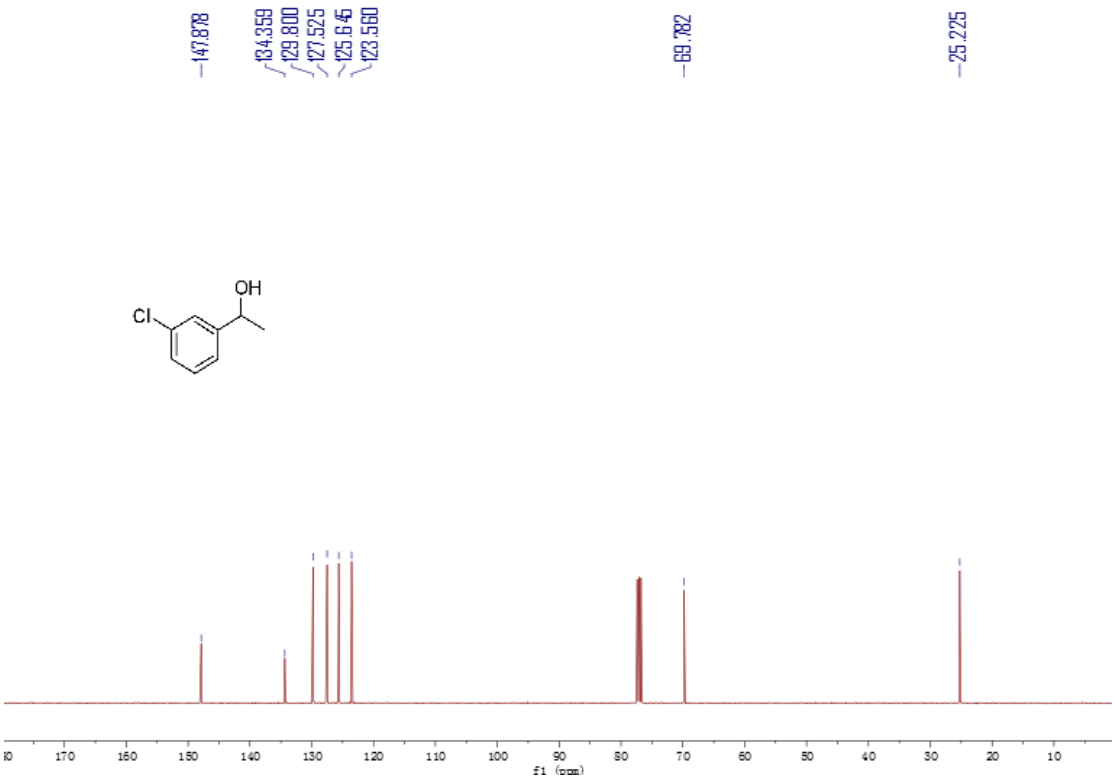


Figure S49. ^{13}C NMR spectrum of 1-(3-chlorophenyl)ethan-1-ol in $CDCl_3$.

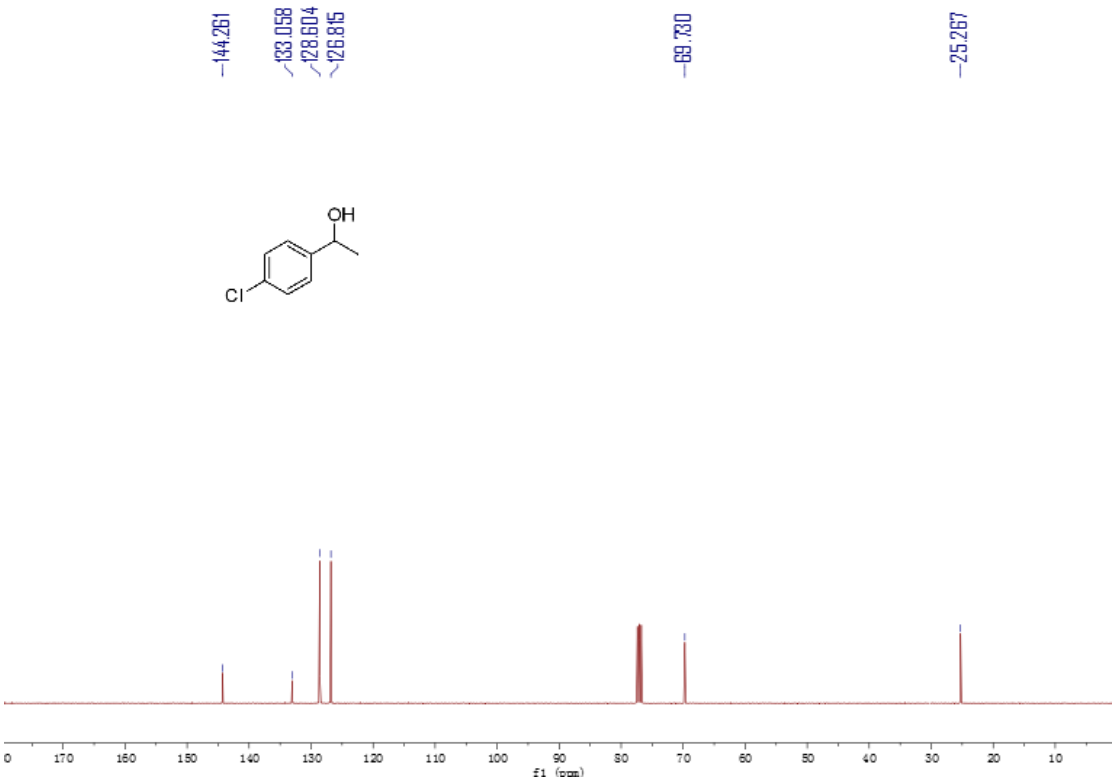


Figure S50. ^{13}C NMR spectrum of 1-(4-chlorophenyl)ethan-1-ol in $CDCl_3$.

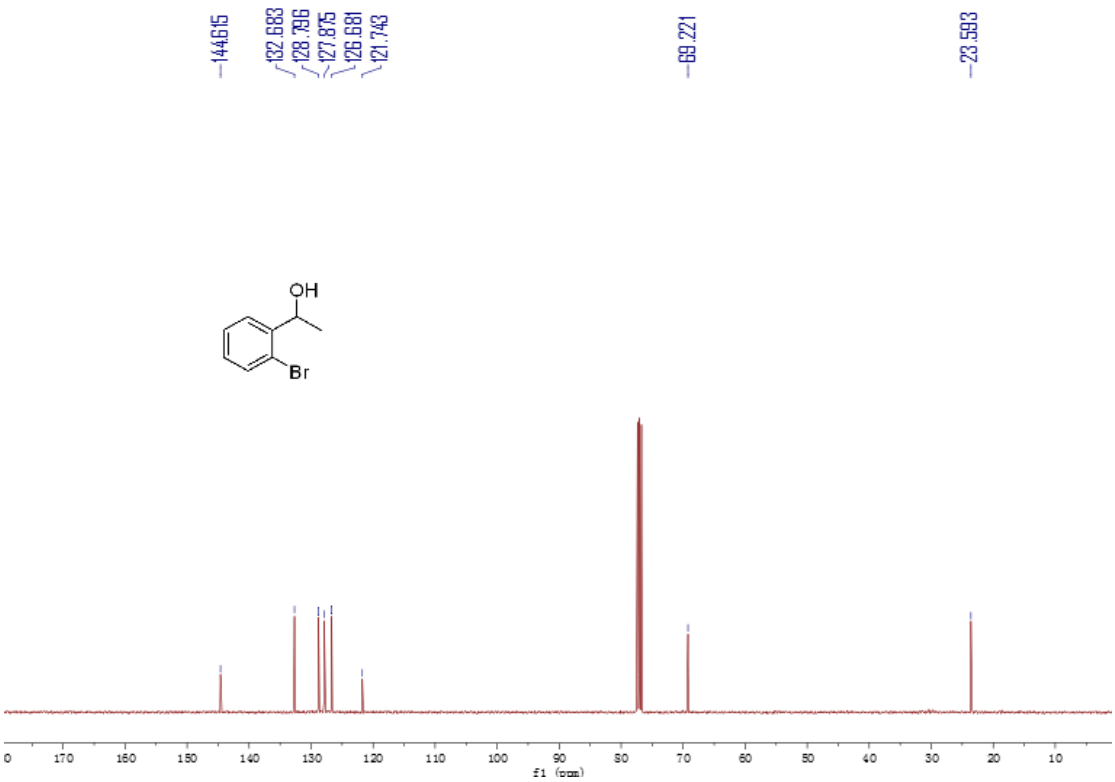


Figure S51. ^{13}C NMR spectrum of 1-(2-bromophenyl)ethan-1-ol in $CDCl_3$.

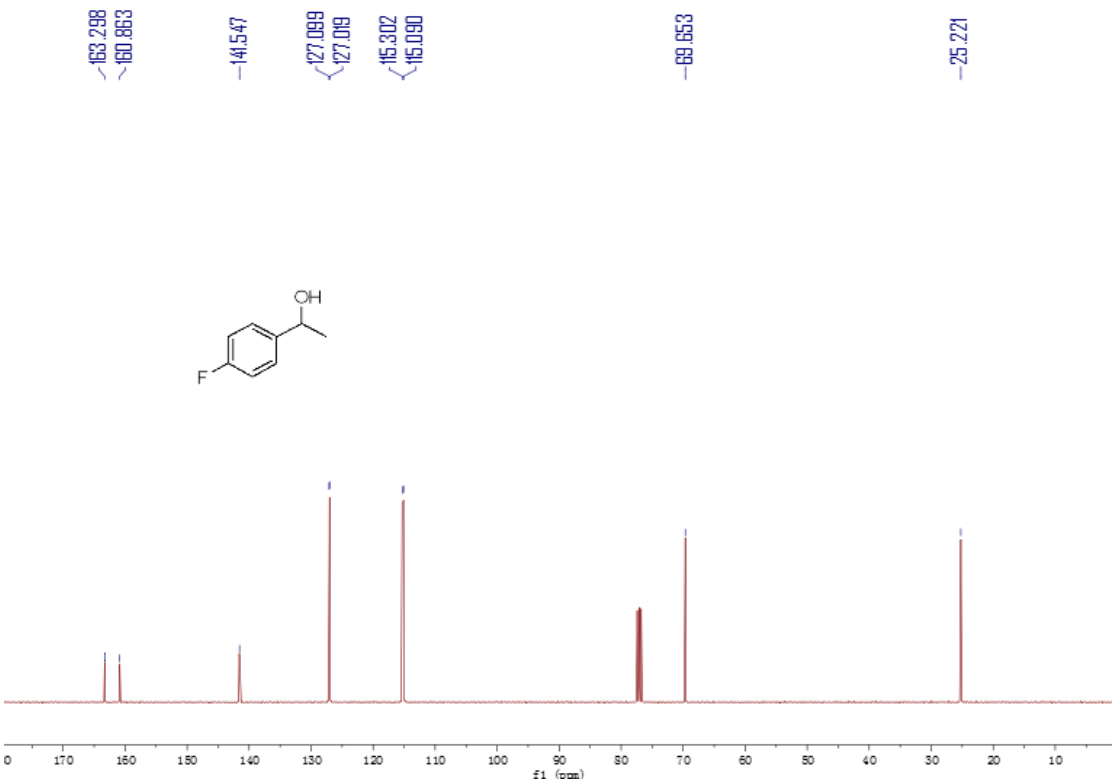


Figure S52. ^{13}C NMR spectrum of 1-(4-fluorophenyl)ethan-1-ol in $CDCl_3$.

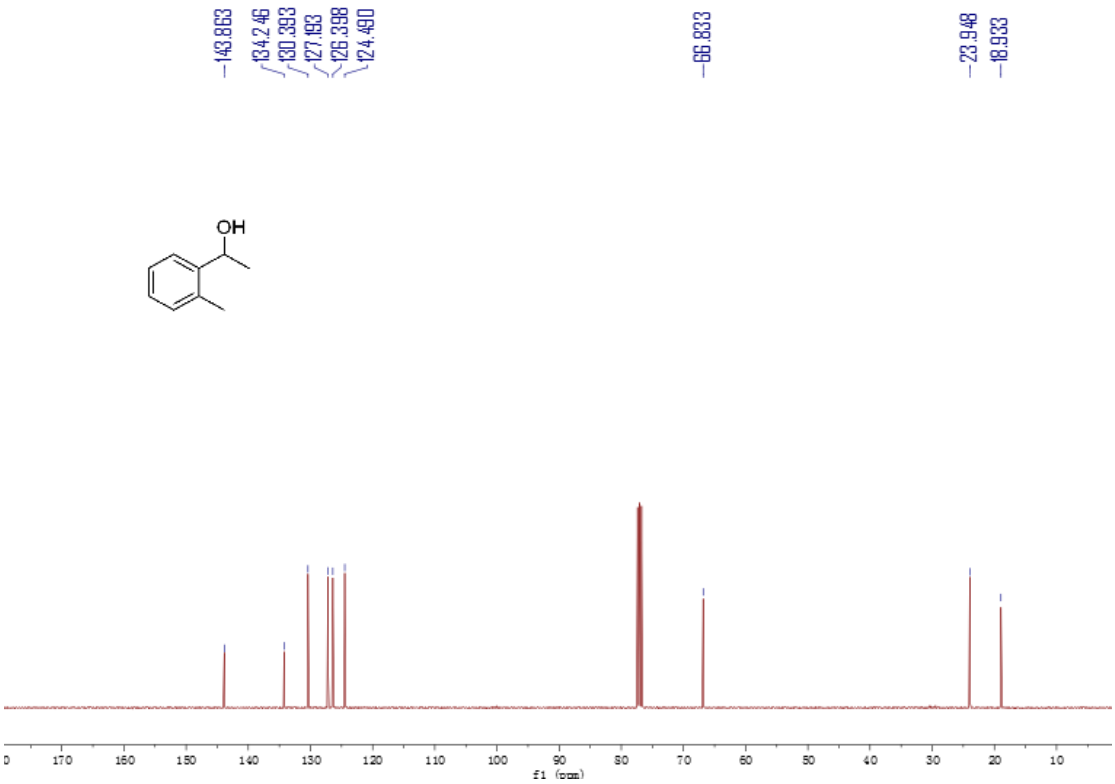


Figure S53. ^{13}C NMR spectrum of 1-(o-tolyl)ethan-1-ol in $CDCl_3$.

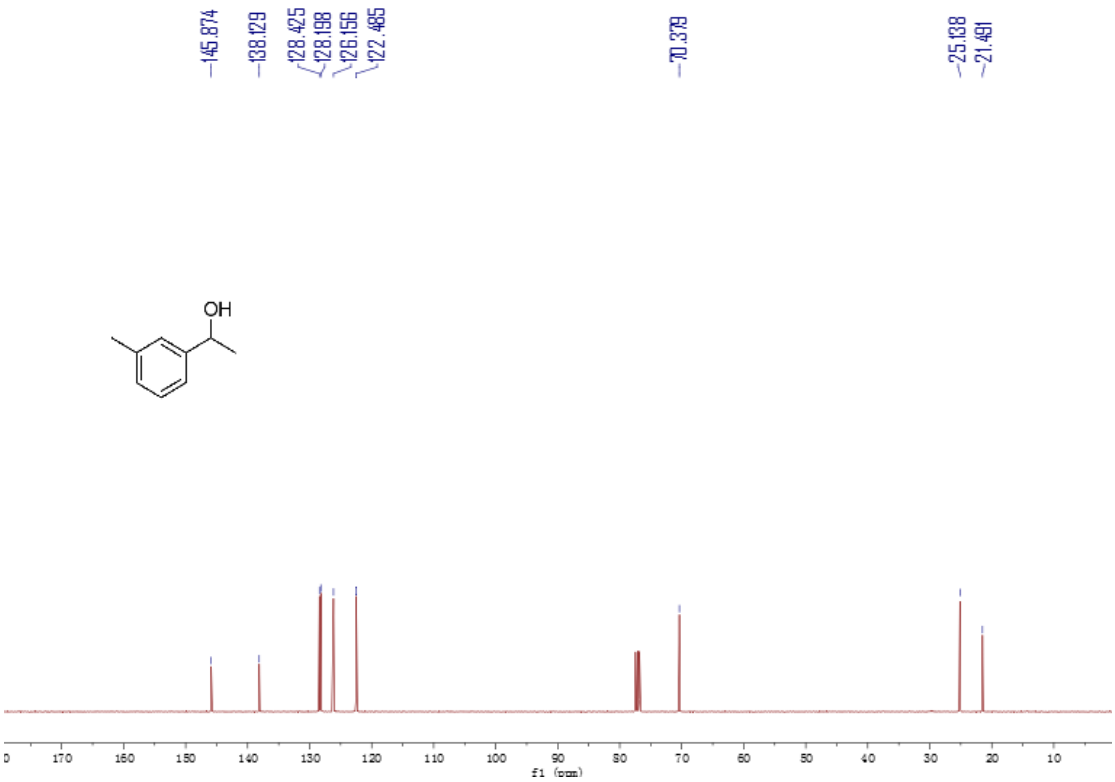


Figure S54. ^{13}C NMR spectrum of 1-(m-tolyl)ethan-1-ol in $CDCl_3$.

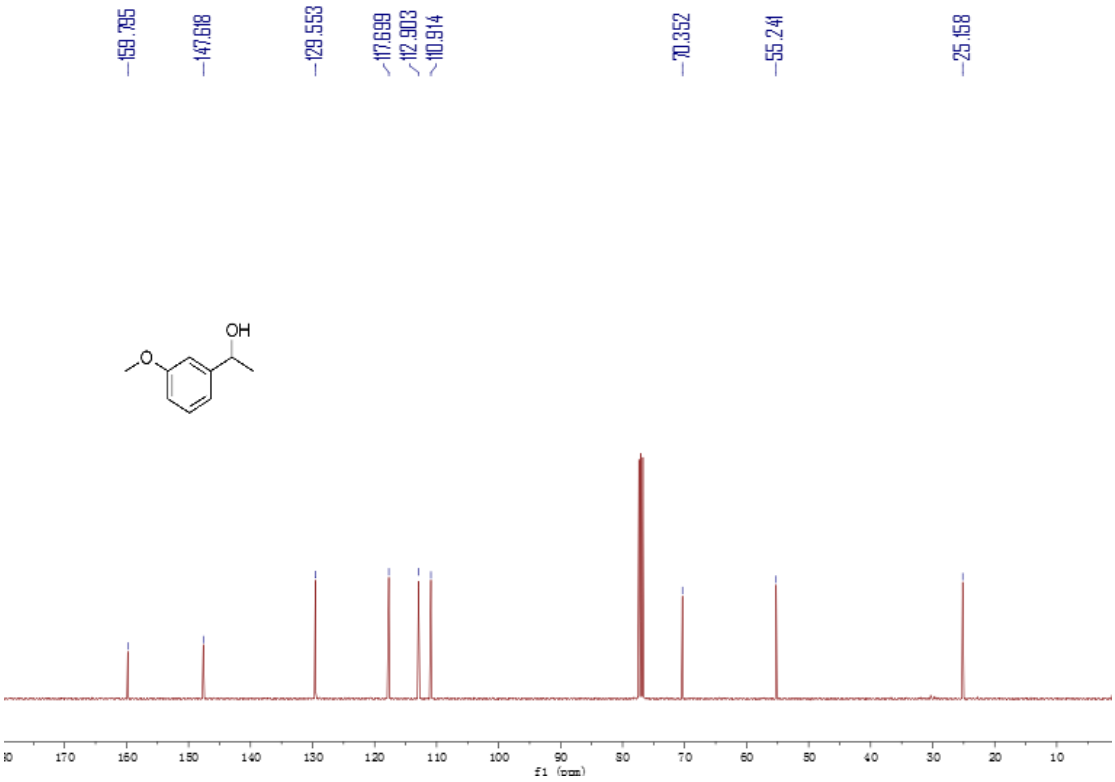


Figure S55. ^{13}C NMR spectrum of 1-(3-methoxyphenyl)ethan-1-ol in $CDCl_3$.

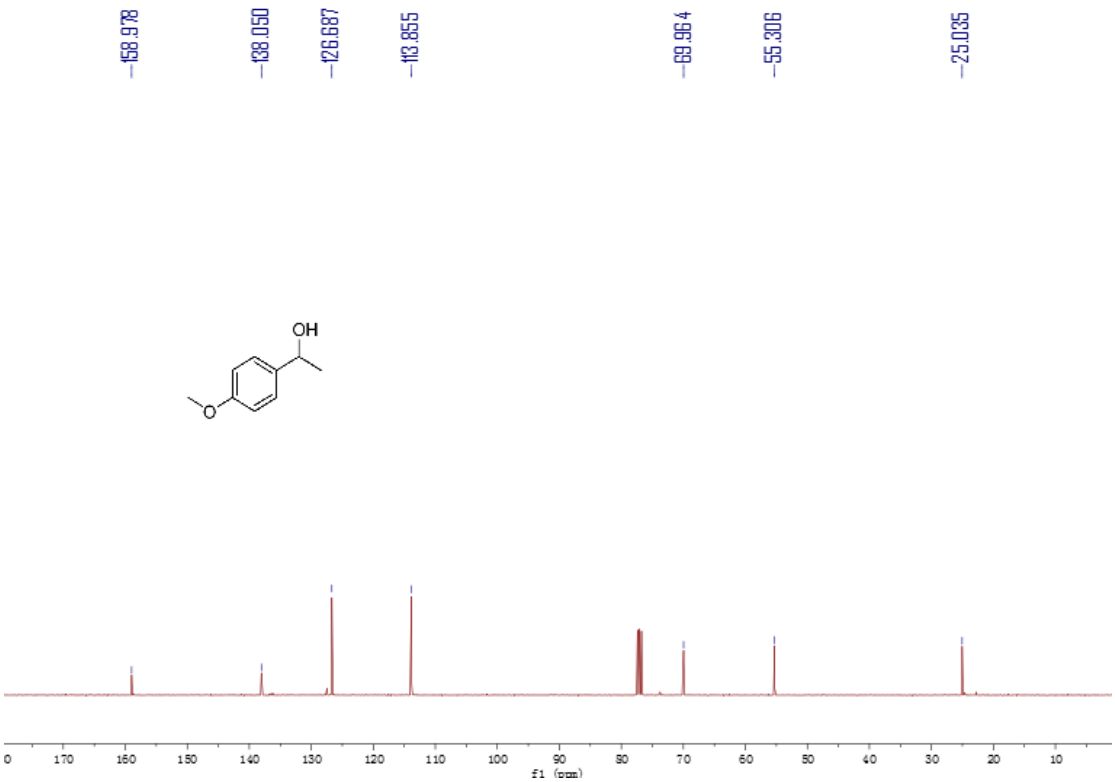


Figure S56. ^{13}C NMR spectrum of 1-(4-methoxyphenyl)ethan-1-ol in $CDCl_3$.

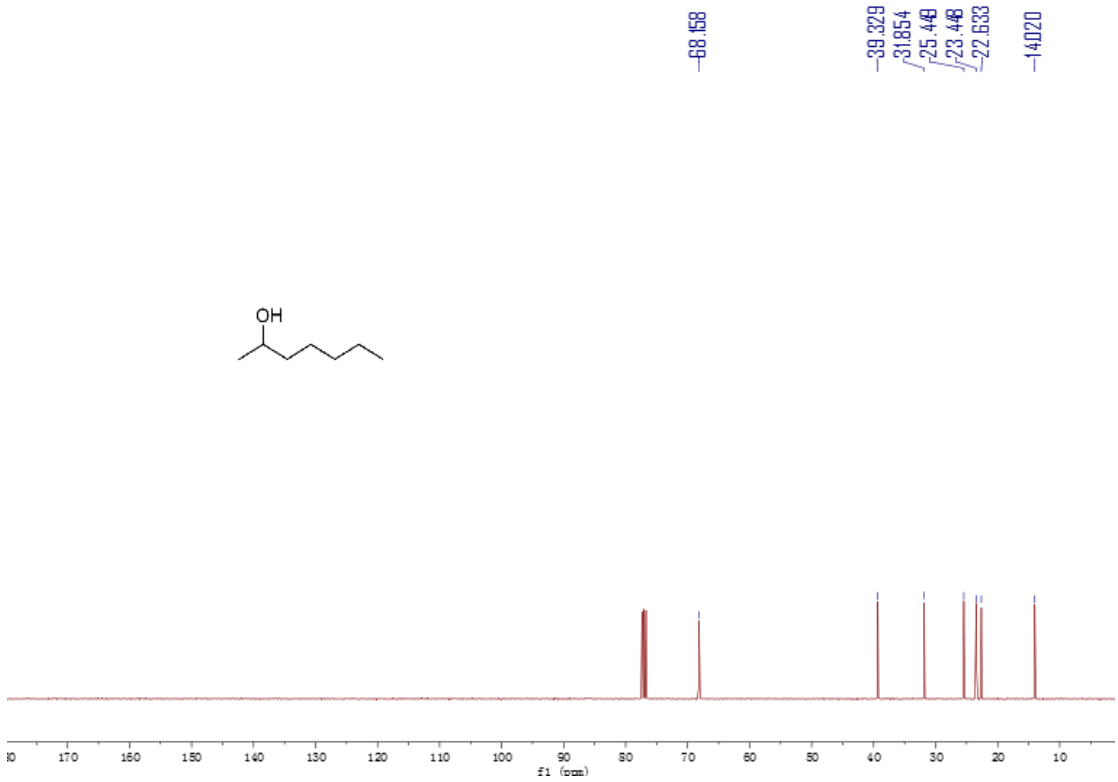


Figure S57. ^{13}C NMR spectrum of heptan-2-ol in $CDCl_3$.

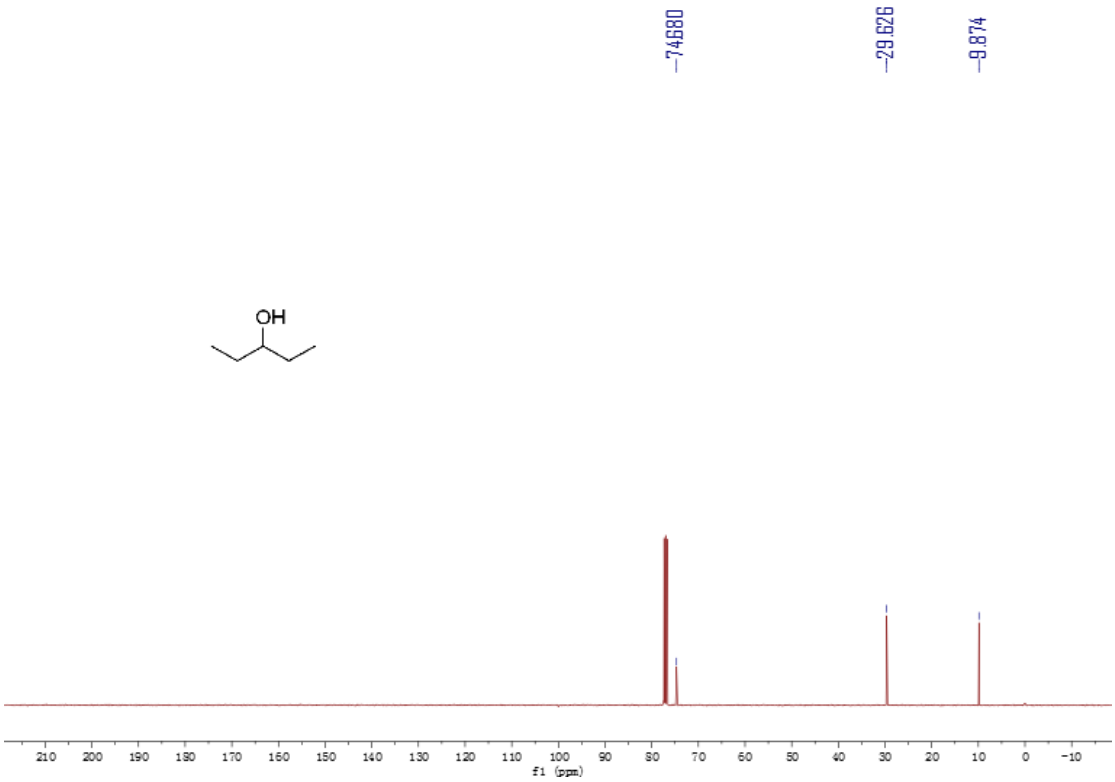


Figure S58. ^{13}C NMR spectrum of pentan-3-ol in $CDCl_3$.

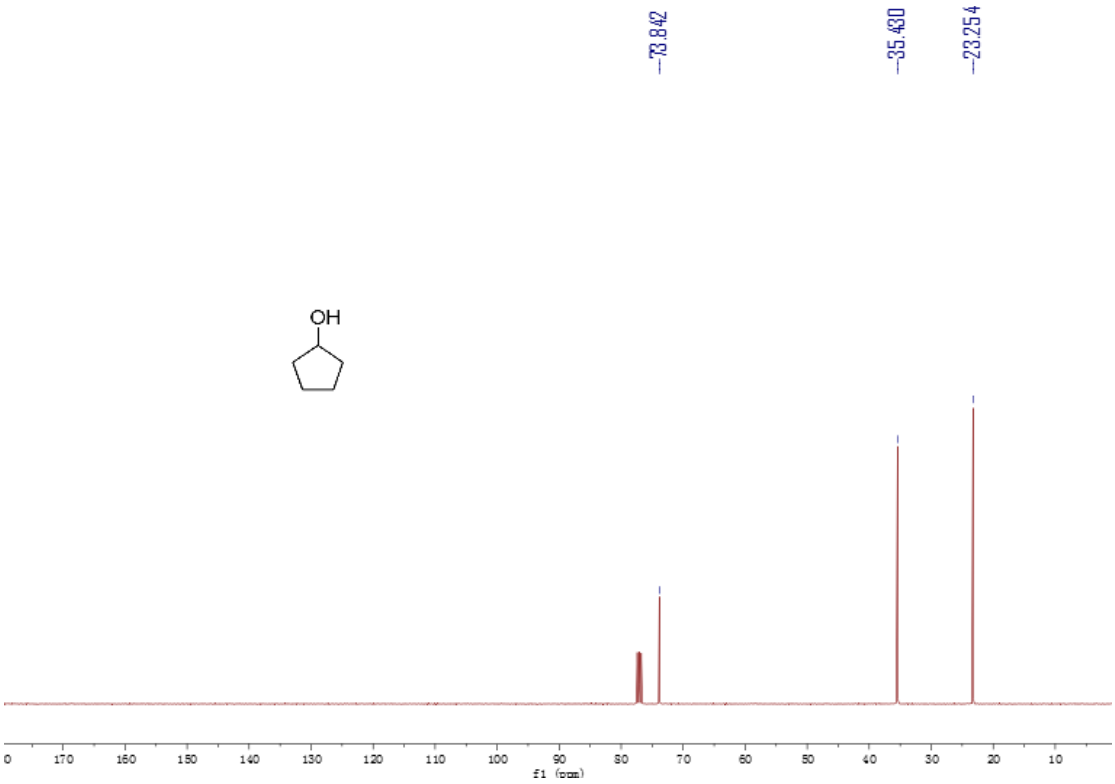


Figure S59. ^{13}C NMR spectrum of cyclopentanol in $CDCl_3$.

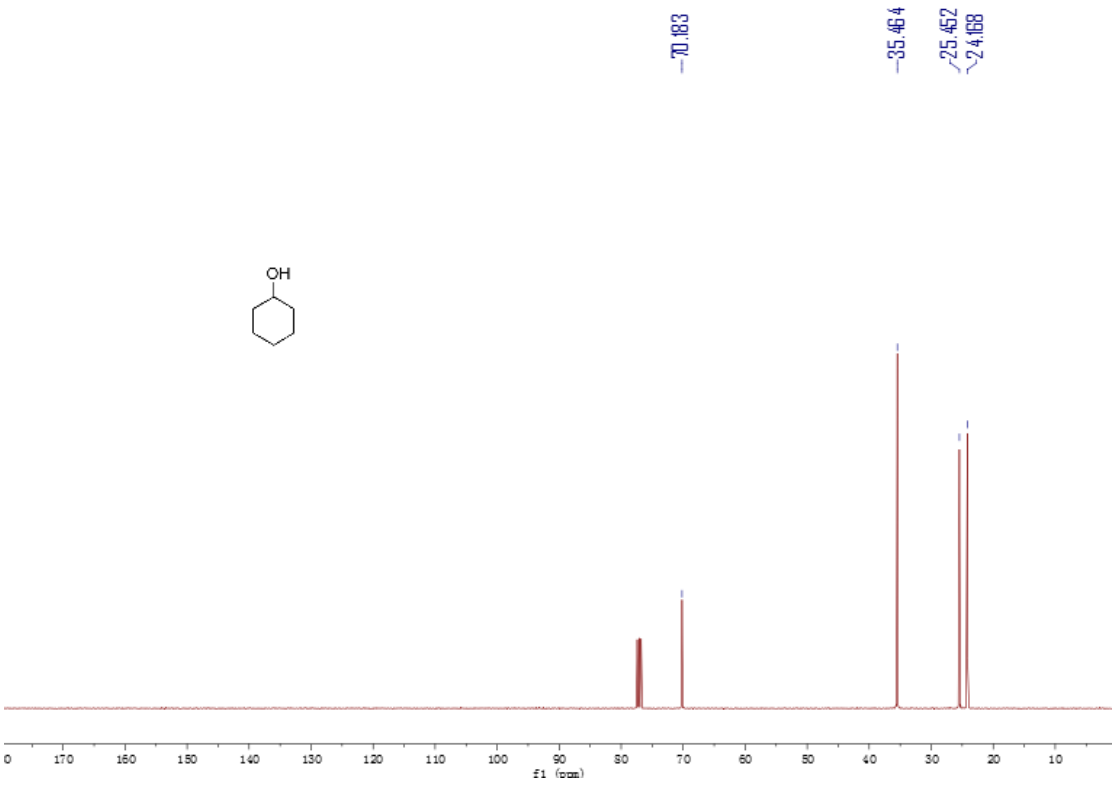


Figure S60. ^{13}C NMR spectrum of cyclohexanol in $CDCl_3$.

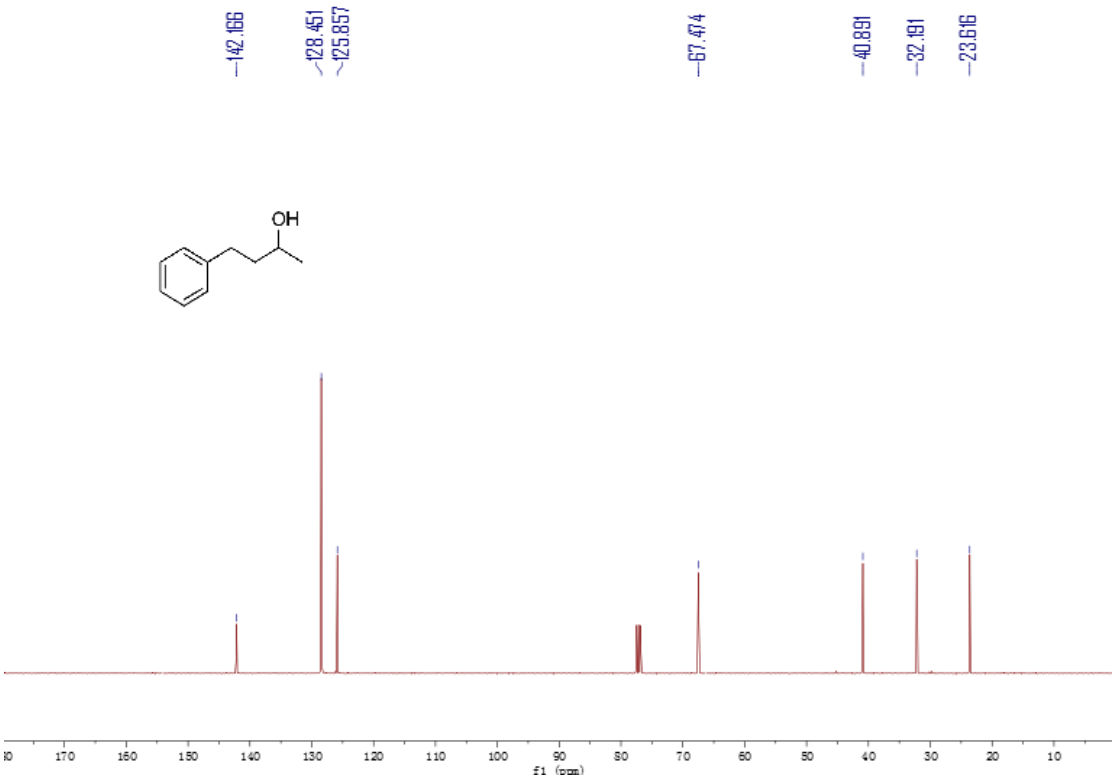


Figure S61. ^{13}C NMR spectrum of 4-phenylbutan-2-ol in $CDCl_3$.

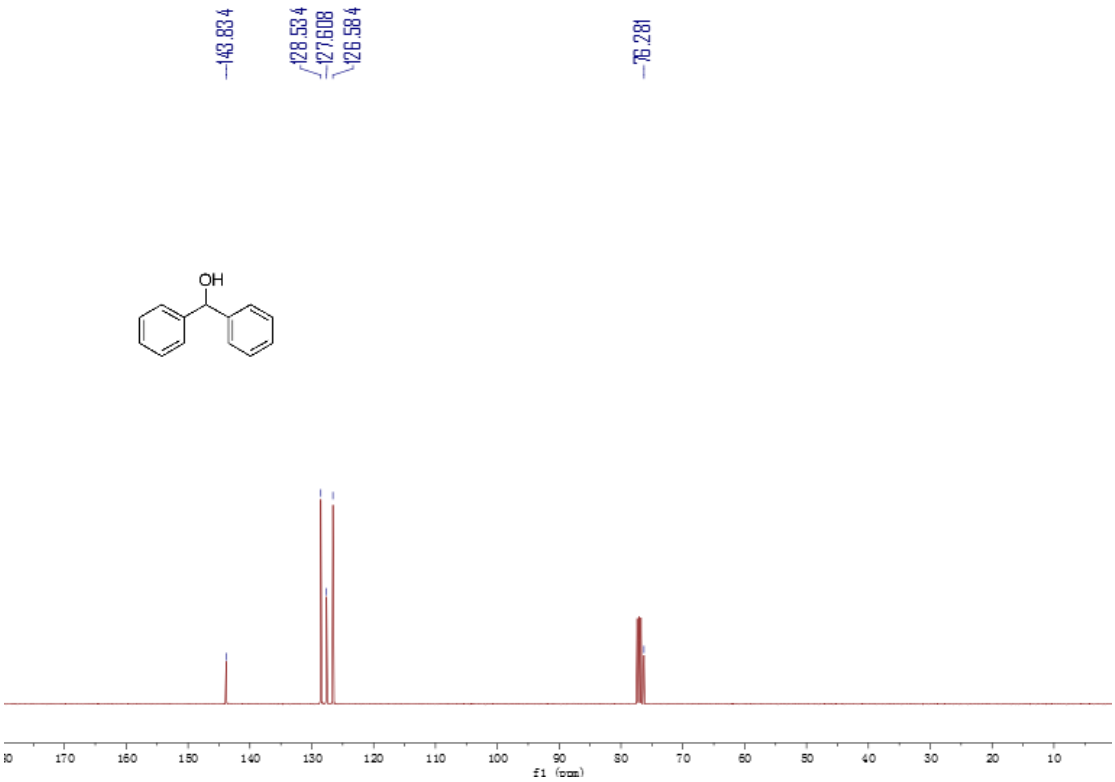


Figure S62. ^{13}C NMR spectrum of diphenylmethanol in $CDCl_3$.

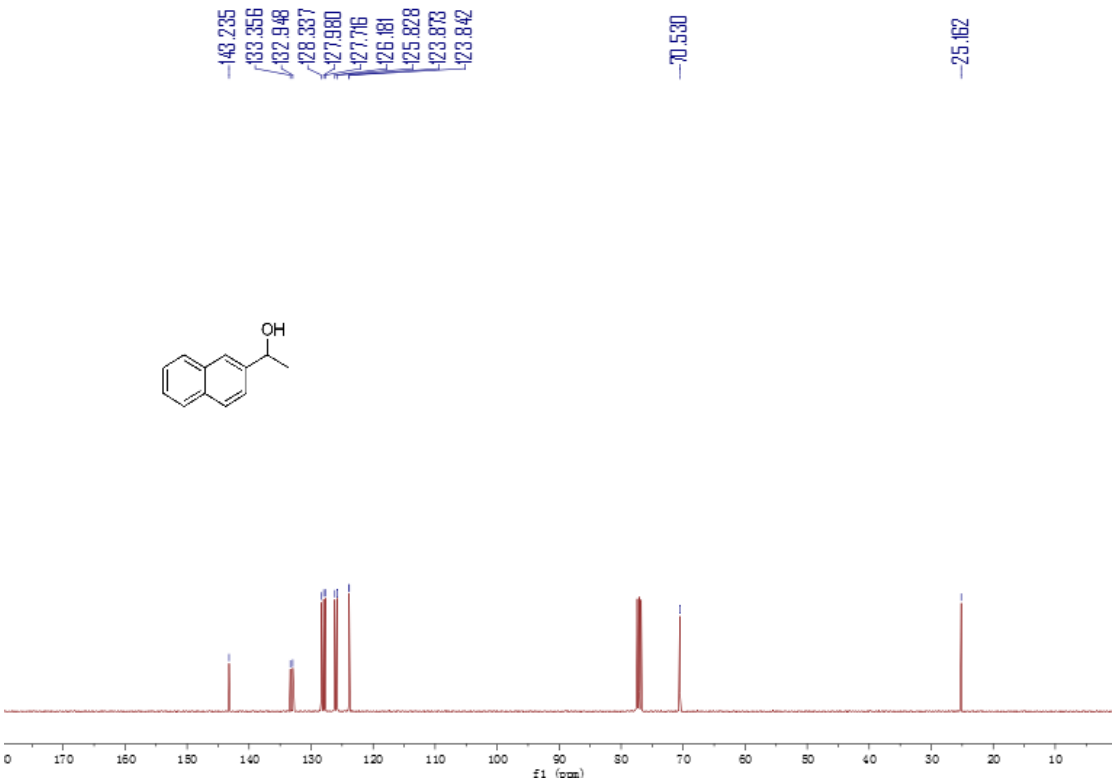


Figure S63. ^{13}C NMR spectrum of 1-(naphthalen-2-yl)ethan-1-ol in $CDCl_3$.

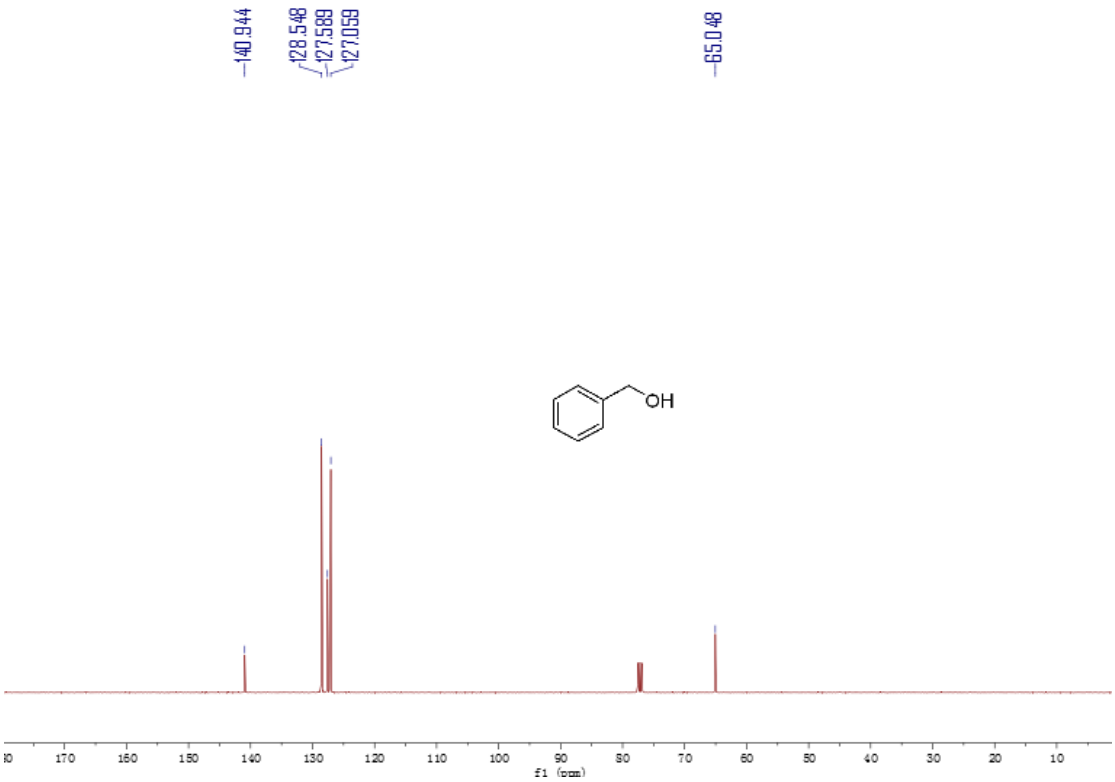


Figure S64. ^{13}C NMR spectrum of phenylmethanol in $CDCl_3$.

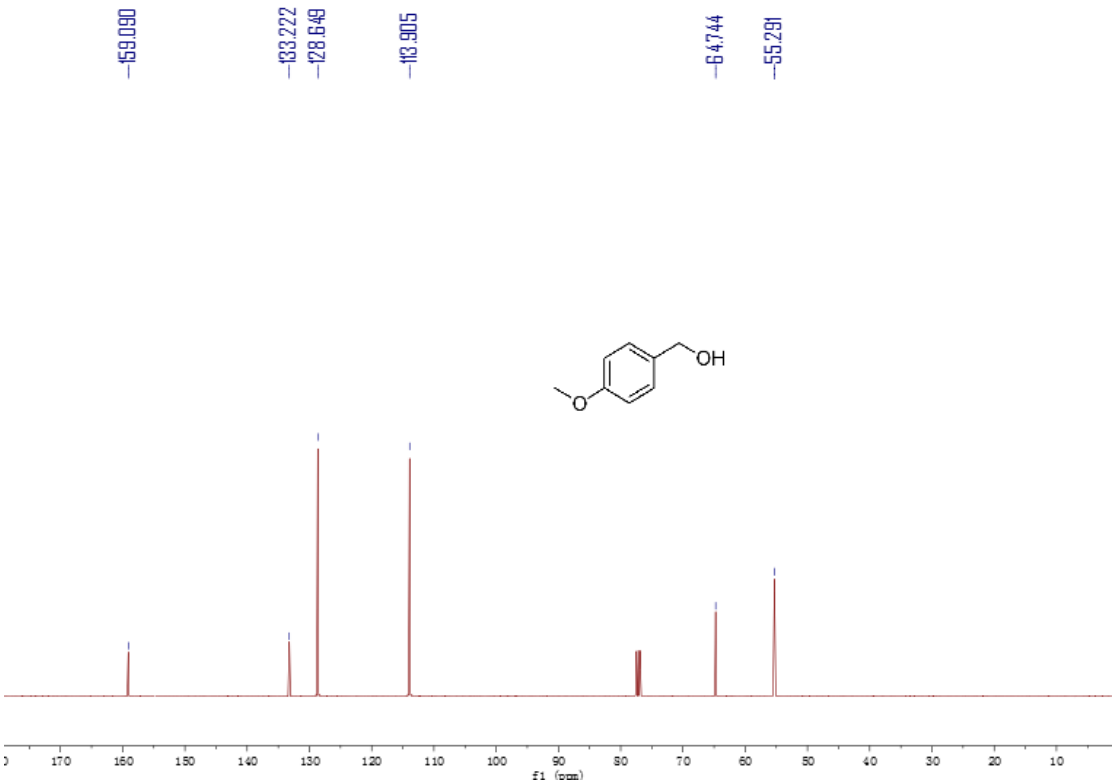


Figure S65. ^{13}C NMR spectrum of (4-methoxyphenyl)methanol in $CDCl_3$.

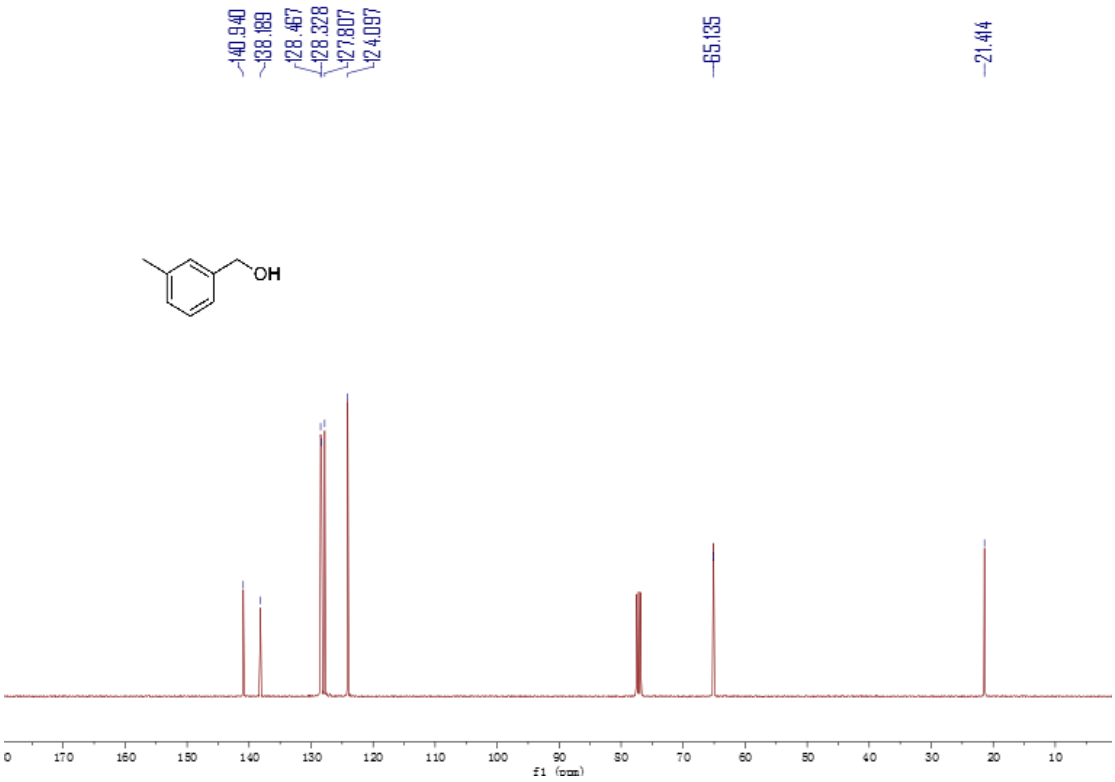


Figure S66. ^{13}C NMR spectrum of m-tolylmethanol in $CDCl_3$.

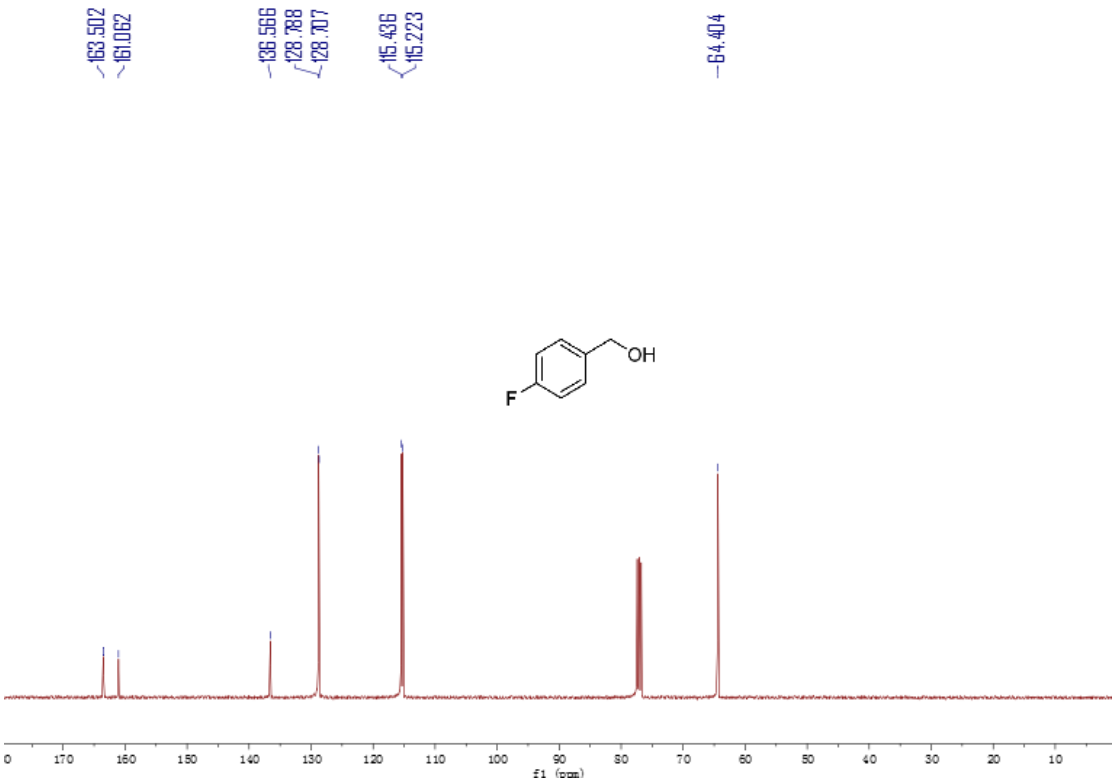


Figure S67. ^{13}C NMR spectrum of (4-fluorophenyl)methanol in $CDCl_3$.

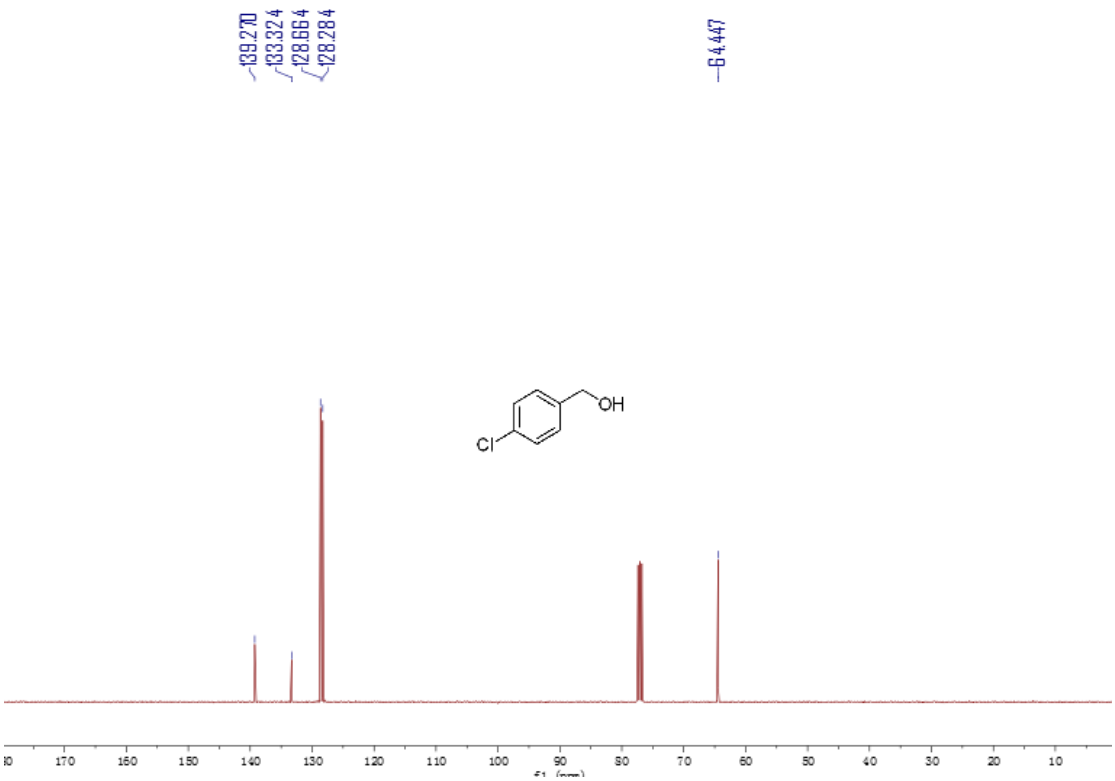


Figure S68. ^{13}C NMR spectrum of (4-chlorophenyl)methanol in $CDCl_3$.

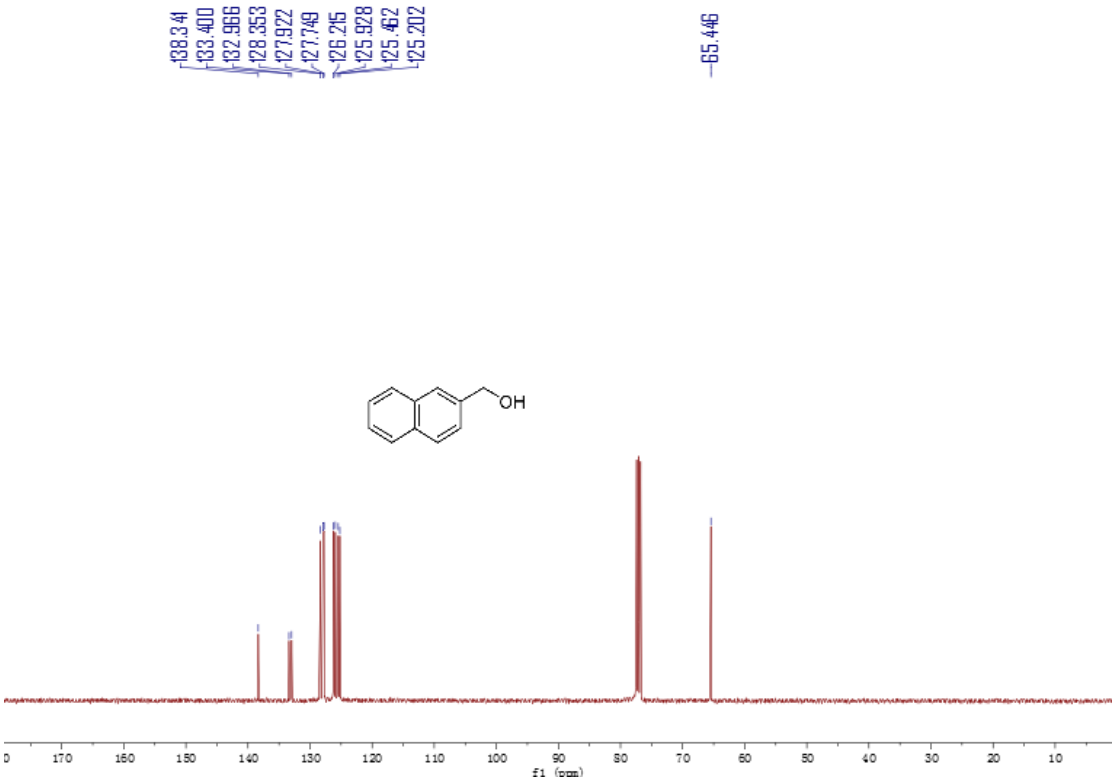


Figure S69. ^{13}C NMR spectrum of naphthalen-2-ylmethanol in $CDCl_3$.

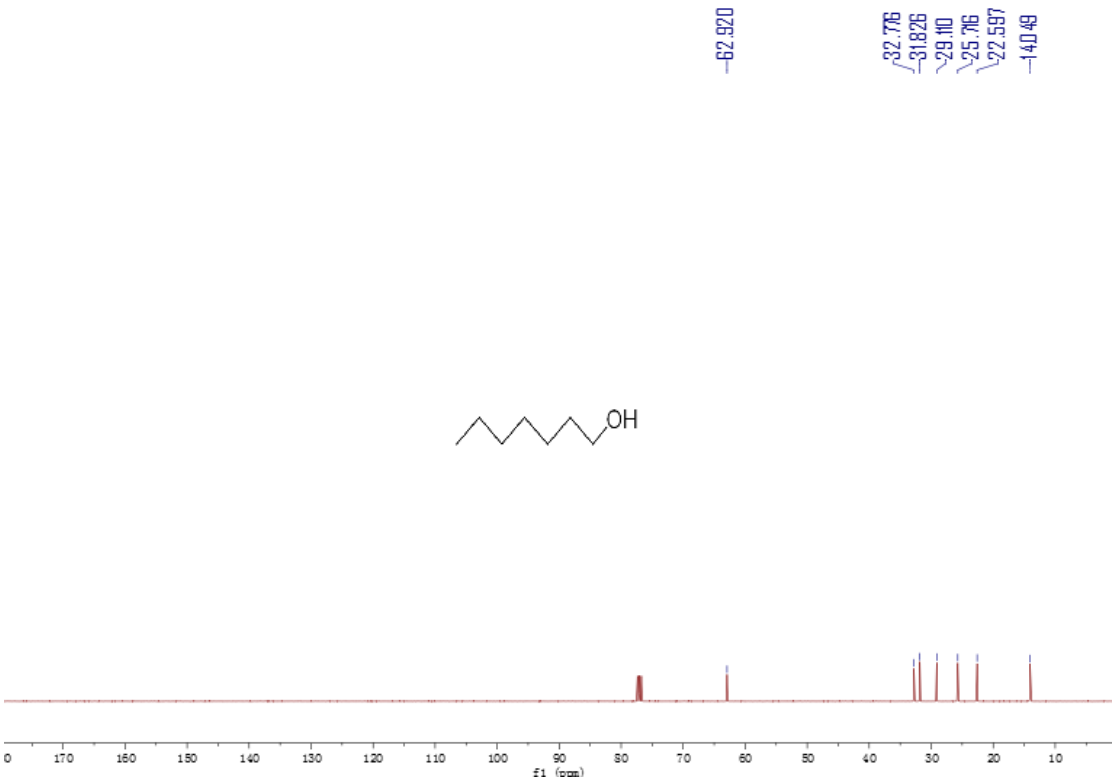


Figure S70. ^{13}C NMR spectrum of heptan-1-ol in $CDCl_3$.

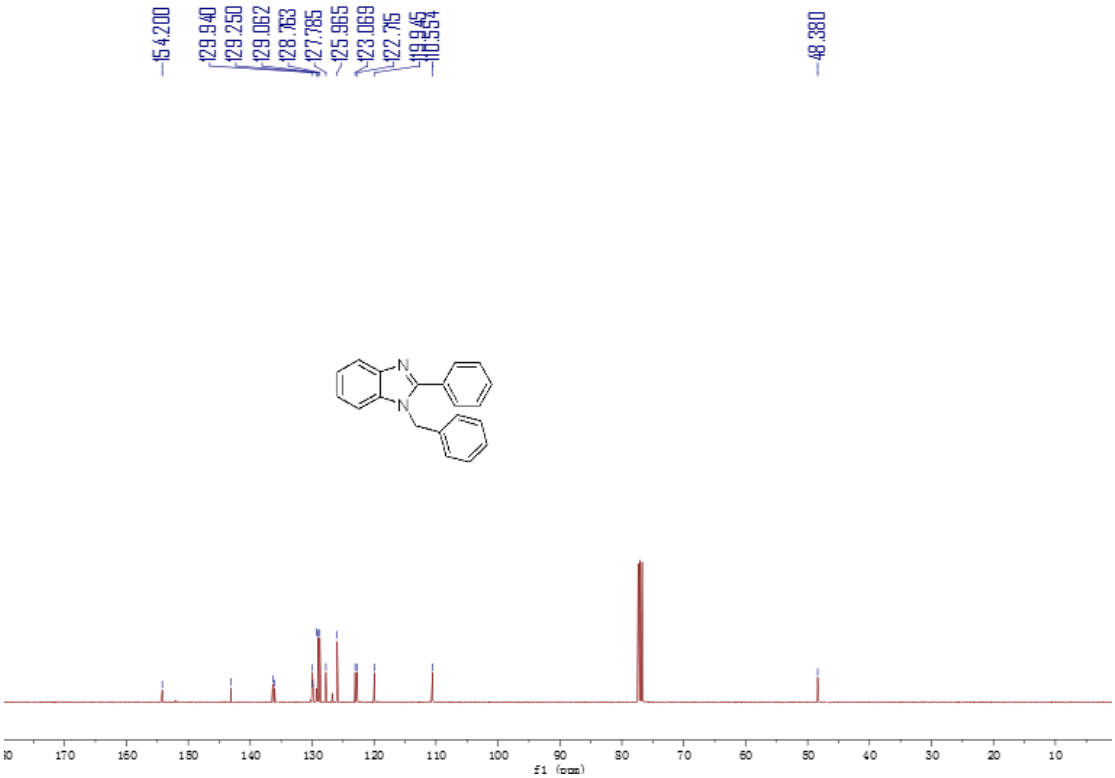


Figure S71. ^{13}C NMR spectrum of 1-benzyl-2-phenyl-1H-benzo[d]imidazole in $CDCl_3$.

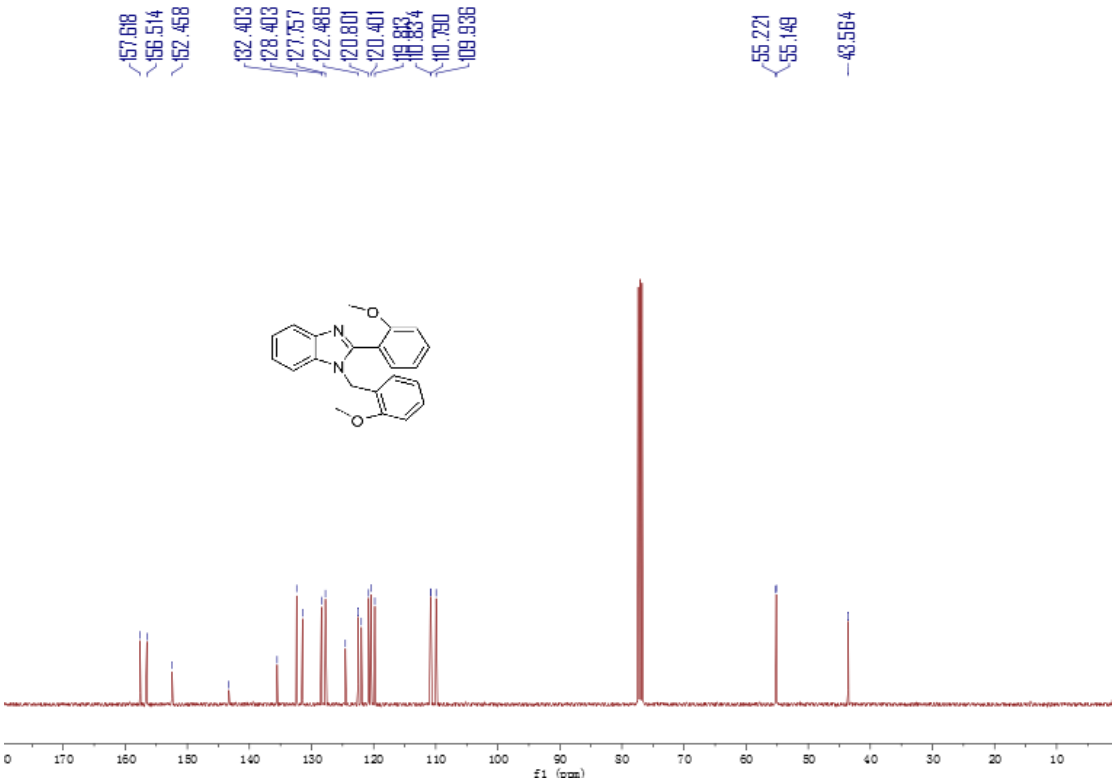


Figure S72. ^{13}C NMR spectrum of 1-(2-methoxybenzyl)-2-(2-methoxyphenyl)-1H-benzo[d]imidazole in $CDCl_3$.

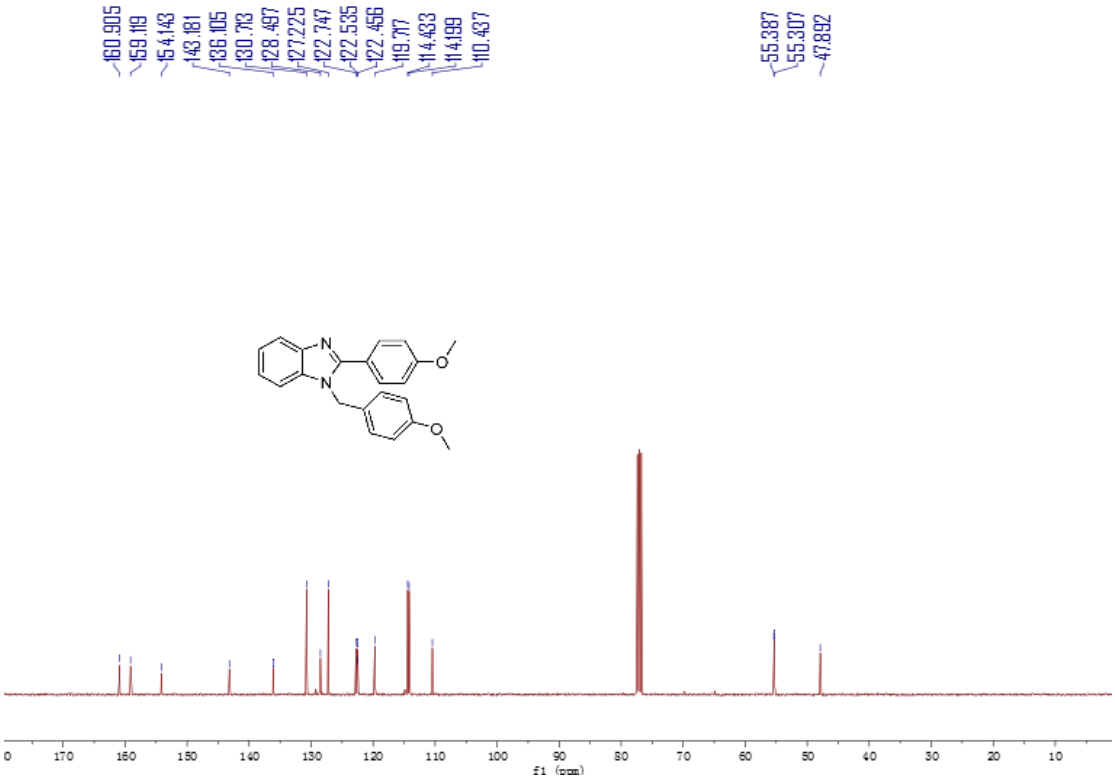


Figure S73. ^{13}C NMR spectrum of 1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1H-benzo[d]imidazole in $CDCl_3$.

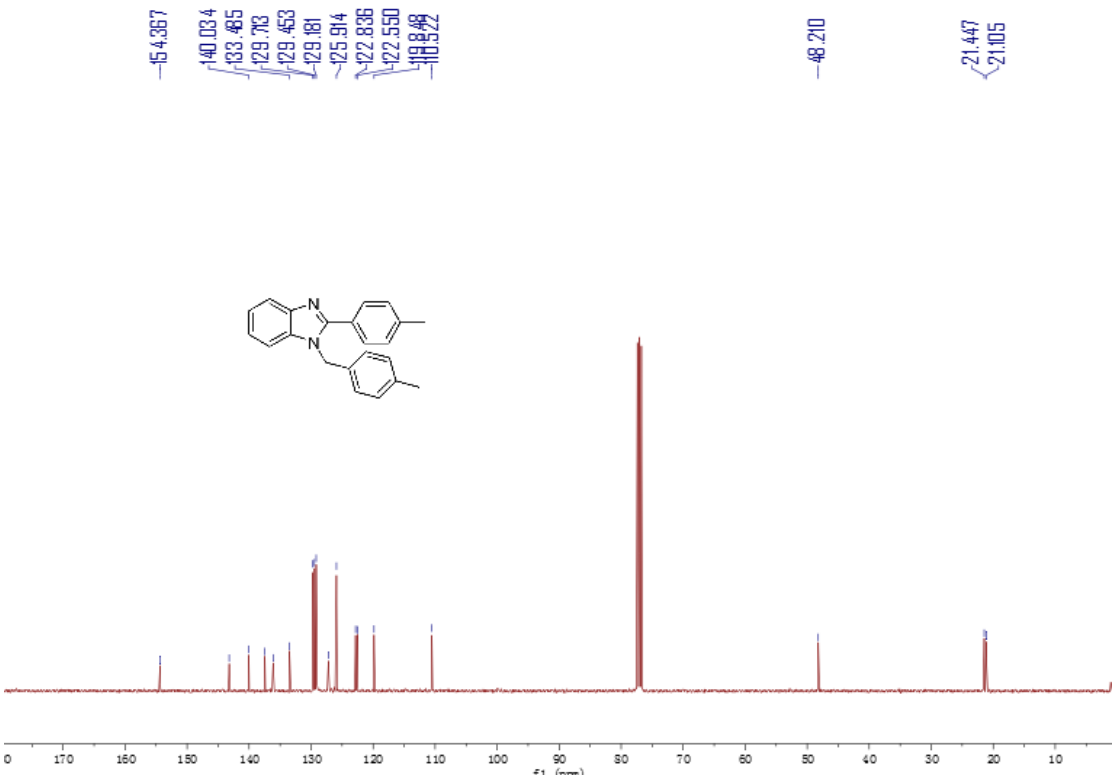


Figure S74. ^{13}C NMR spectrum of 1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole in $CDCl_3$.

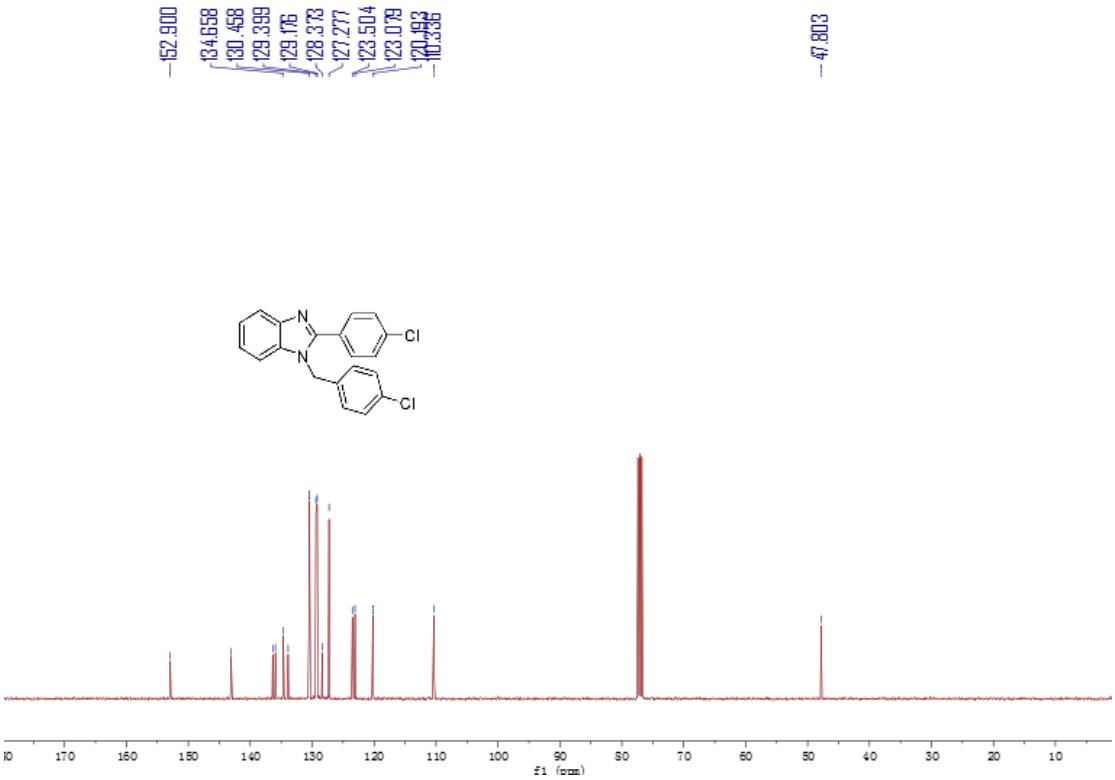


Figure S75. ^{13}C NMR spectrum of 1-(4-chlorobenzyl)-2-(4-chlorophenyl)-1H-benzo[d]imidazole in $CDCl_3$.

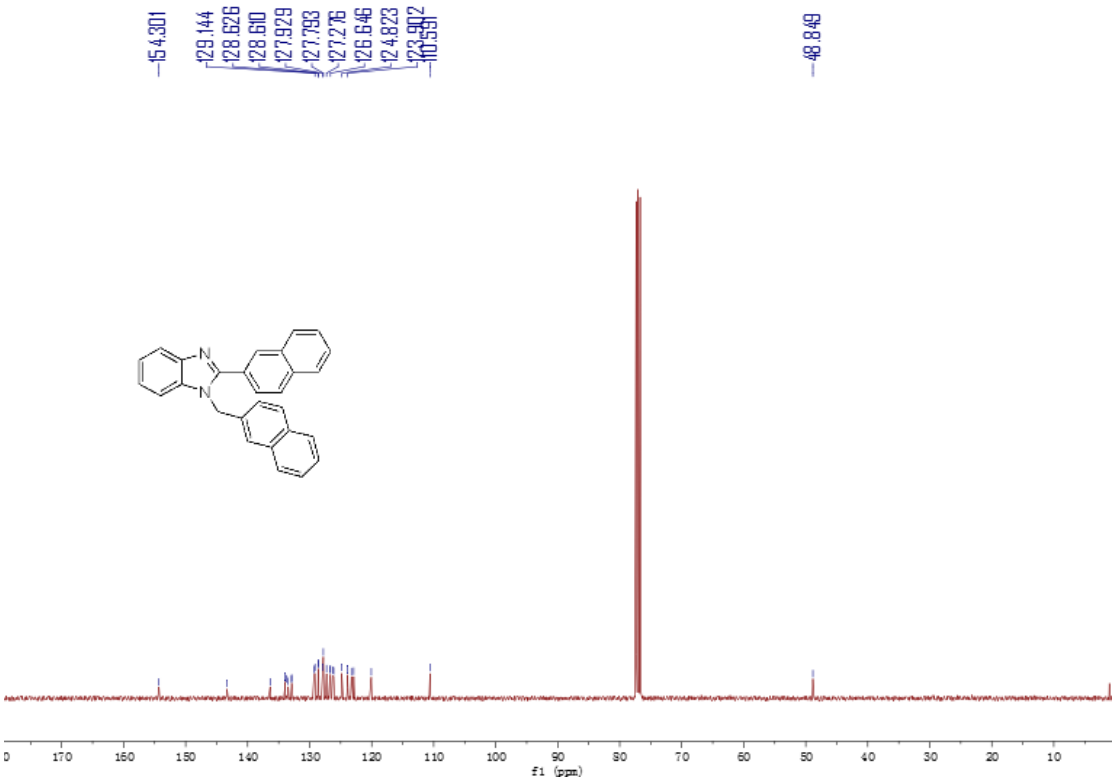


Figure S76. ^{13}C NMR spectrum of 2-(naphthalen-2-yl)-1-(naphthalen-2-ylmethyl)-1H-benzo[d]imidazole in $CDCl_3$.

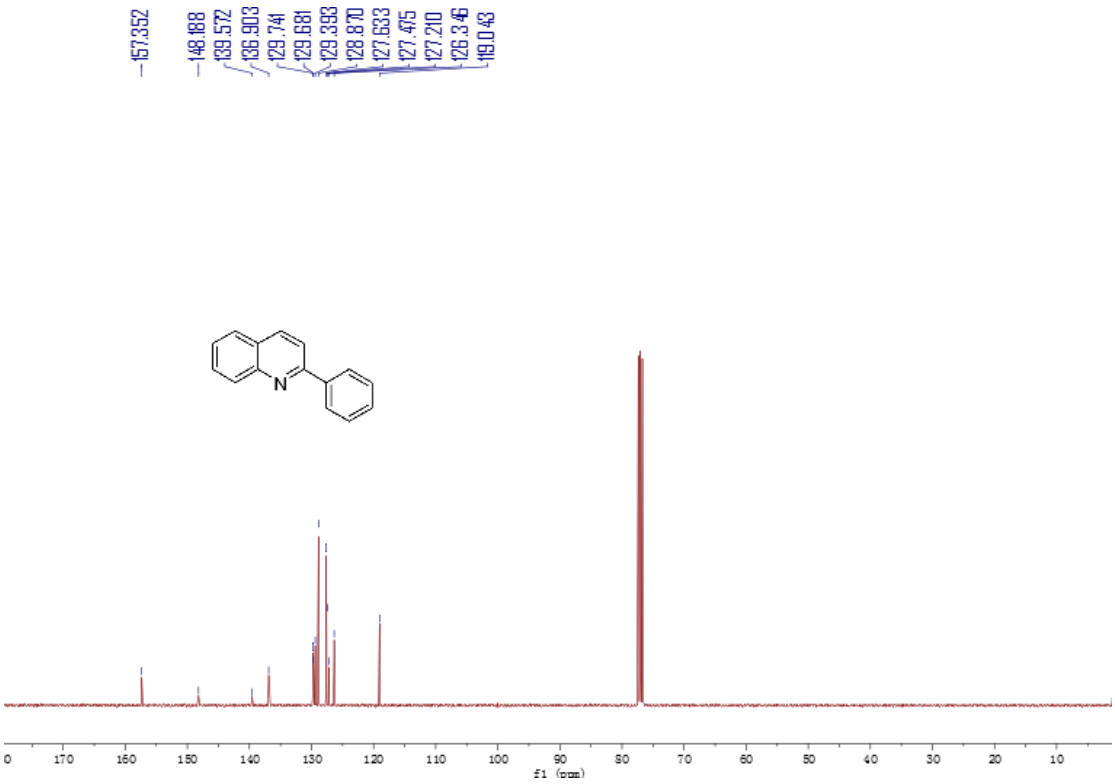


Figure S77. ^{13}C NMR spectrum of 2-phenylquinoline in $CDCl_3$.

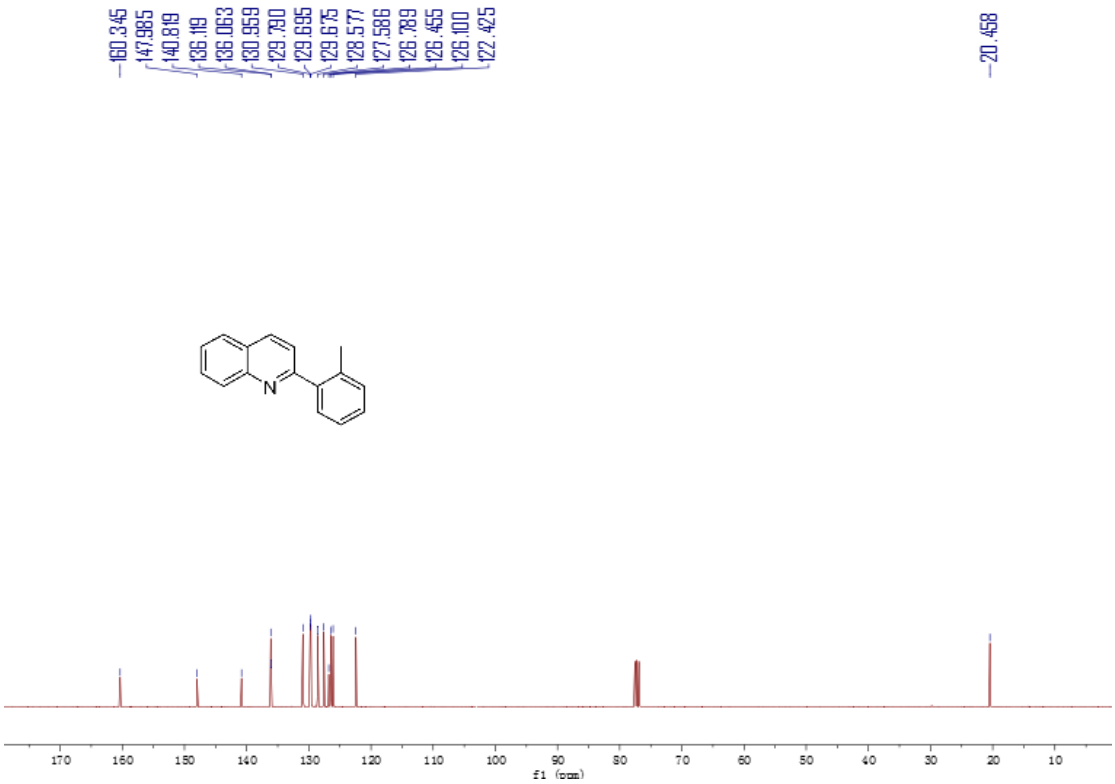


Figure S78. ^{13}C NMR spectrum of 2-(o-tolyl)quinoline in $CDCl_3$.

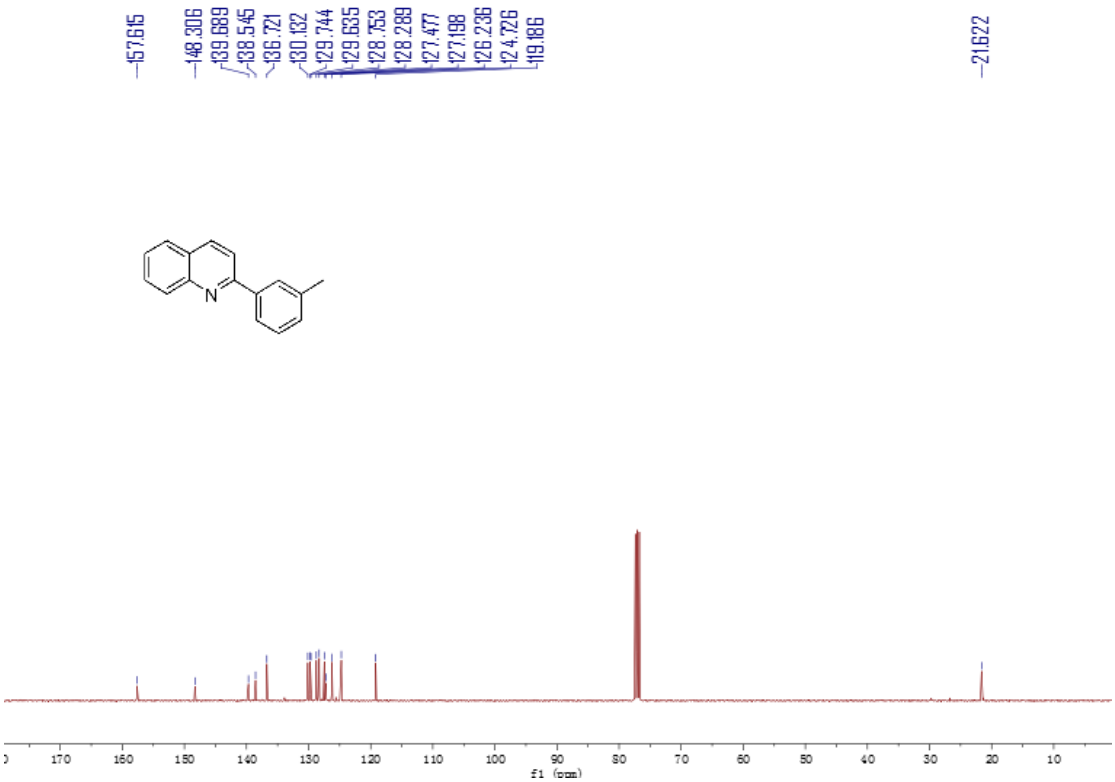


Figure S79. ^{13}C NMR spectrum of 2-(m-tolyl)quinoline in $CDCl_3$.

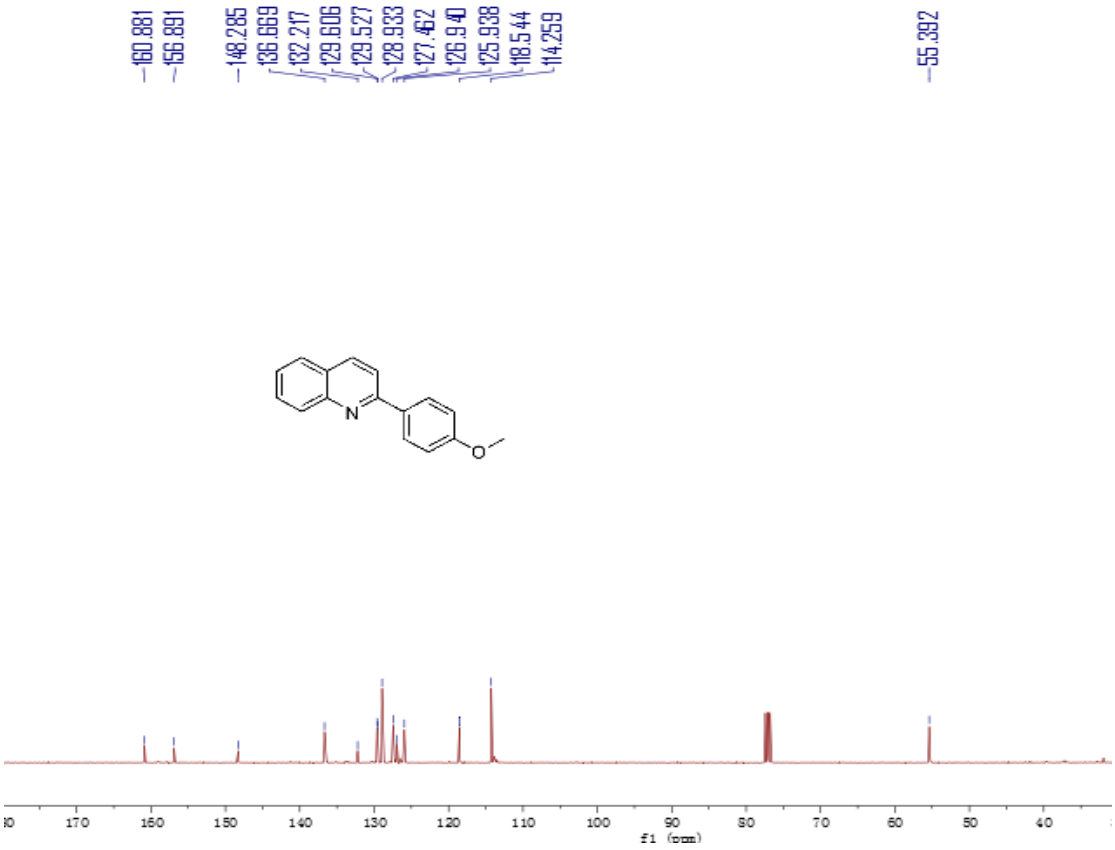


Figure S80. ^{13}C NMR spectrum of 2-(4-methoxyphenyl)quinolone in $CDCl_3$.

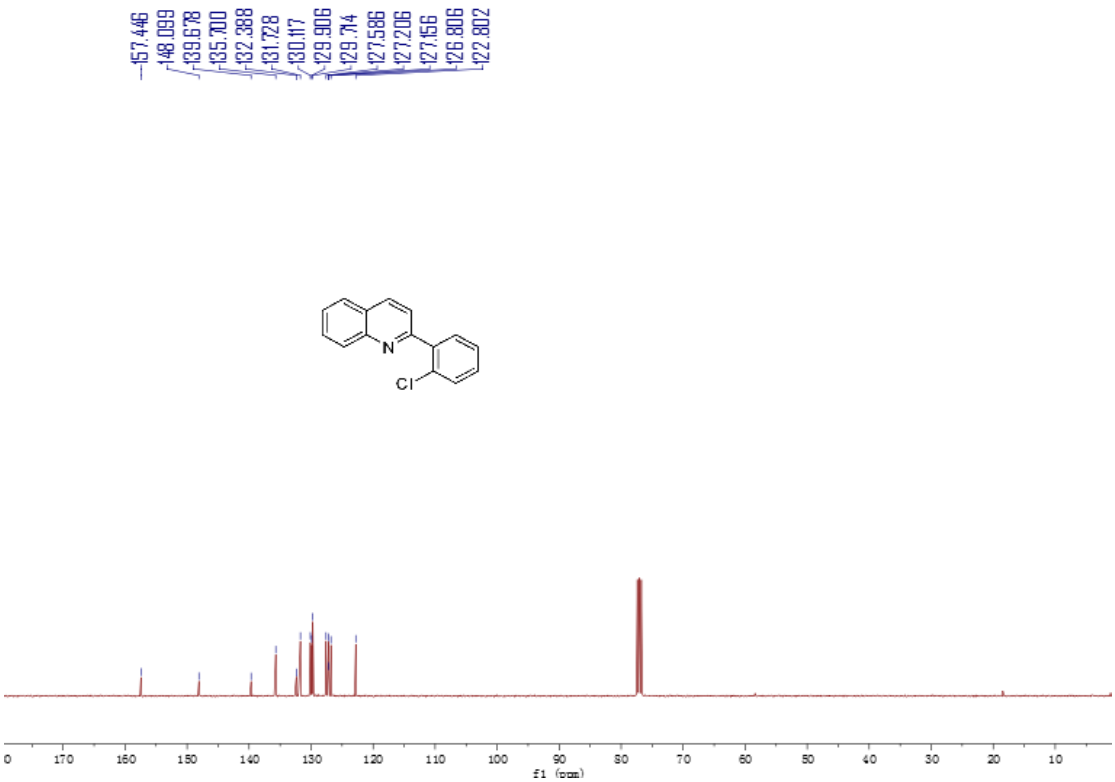


Figure S81. ^{13}C NMR spectrum of 2-(2-chlorophenyl)quinolone in $CDCl_3$.

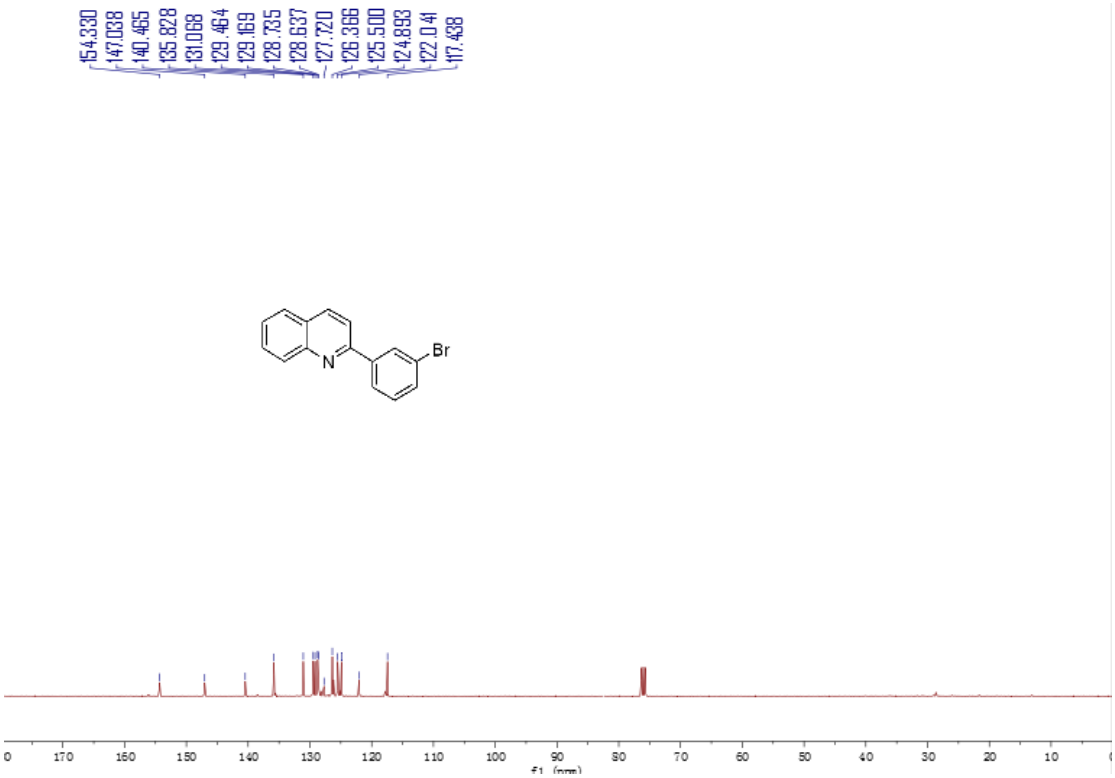


Figure S82. ^{13}C NMR spectrum of 2-(3-bromophenyl)quinolone in $CDCl_3$.

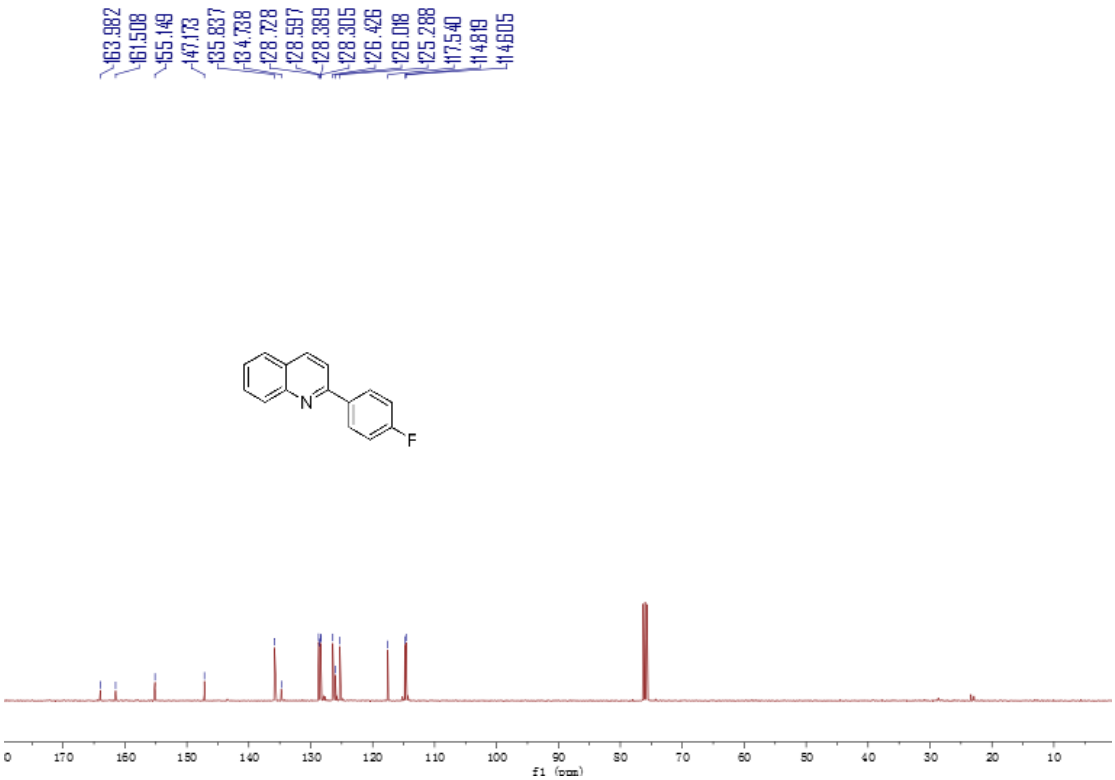


Figure S83. ^{13}C NMR spectrum of 2-(4-fluorophenyl)quinolone in $CDCl_3$.

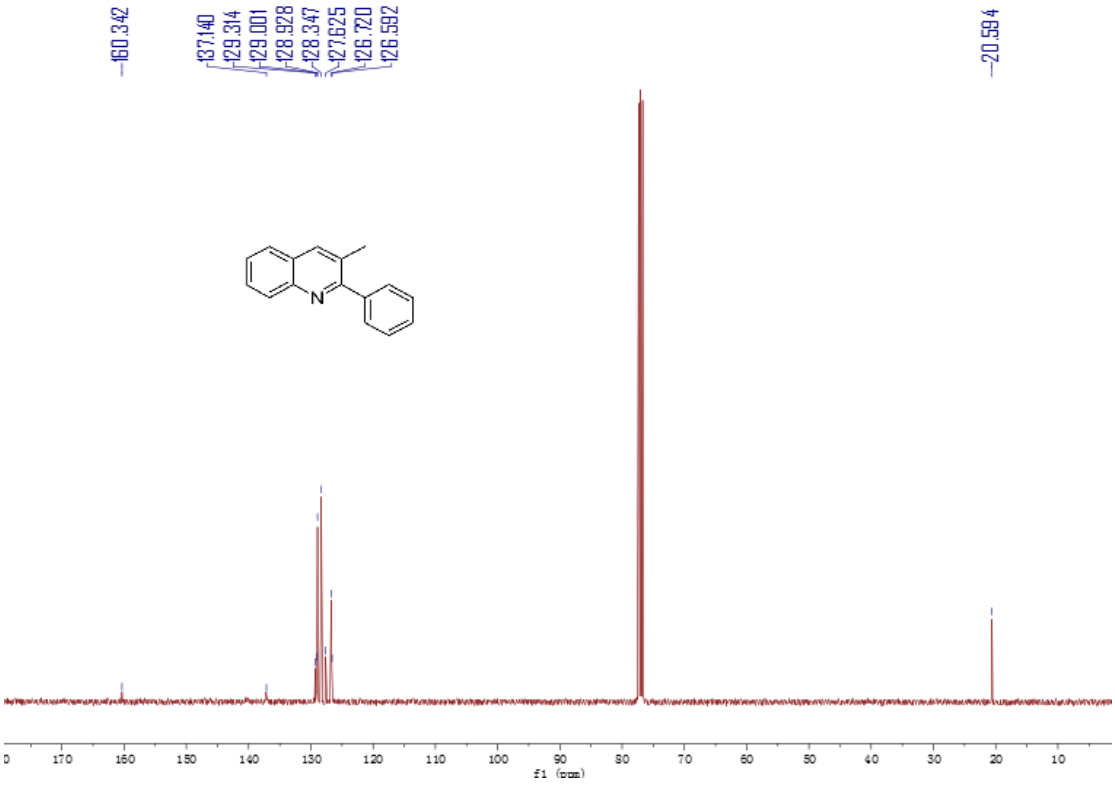


Figure S84. ^{13}C NMR spectrum of 3-methyl-2-phenylquinoline in $CDCl_3$.

IR Spectra

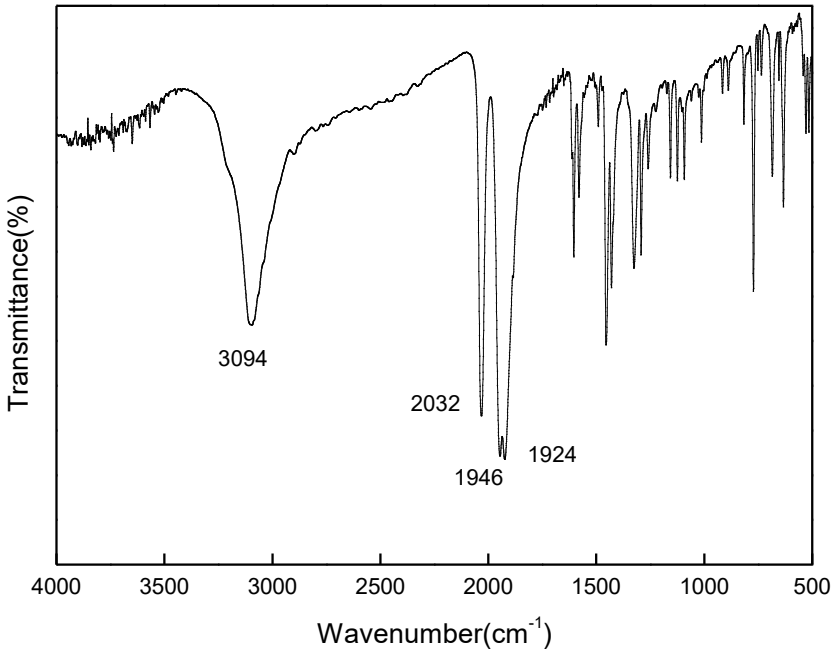


Figure S85. IR spectrum of **1** in KBr.

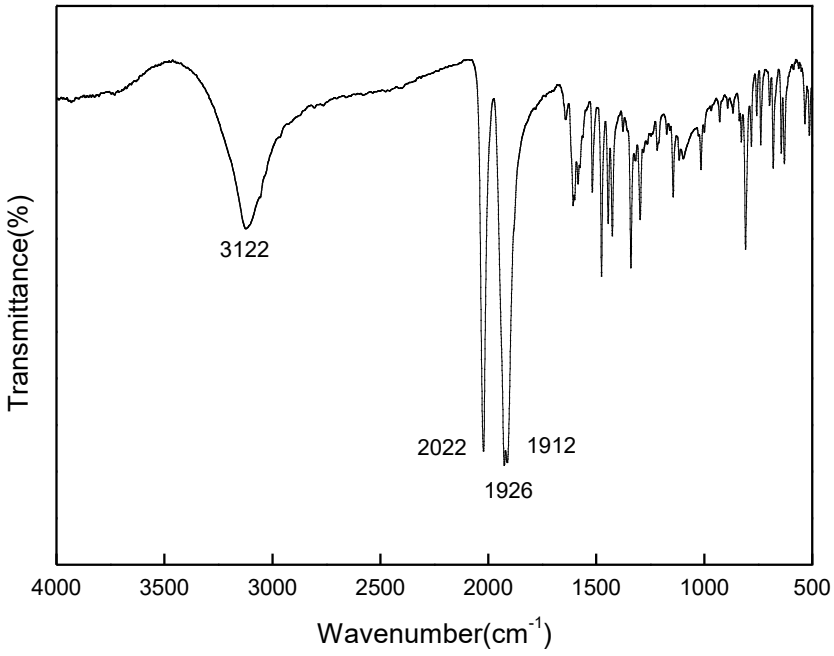


Figure S86. IR spectrum of **2** in KBr.

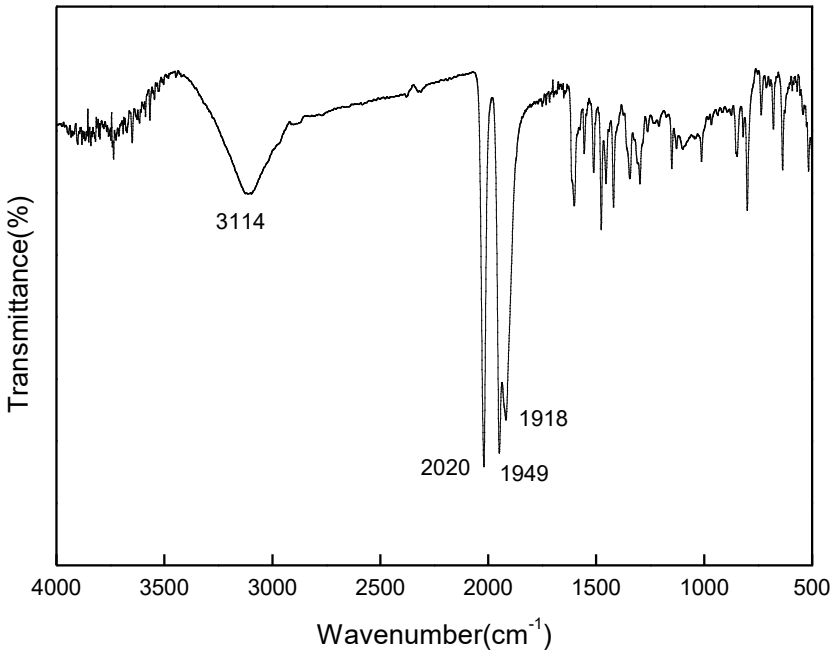


Figure S87. IR spectrum of **3** in KBr.

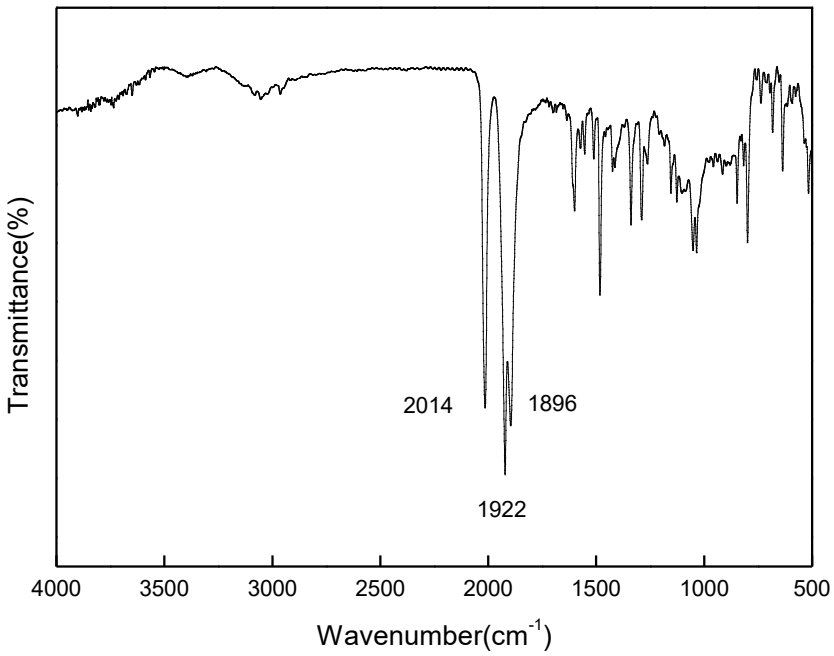


Figure S88. IR spectrum of **4** in KBr.