

Supporting Information

I₂-Catalyzed Carbonylation of α -Methylene Ketones to Synthesize 1,2-Diaryl Diketones and Antiviral Quinoxalines in One Pot

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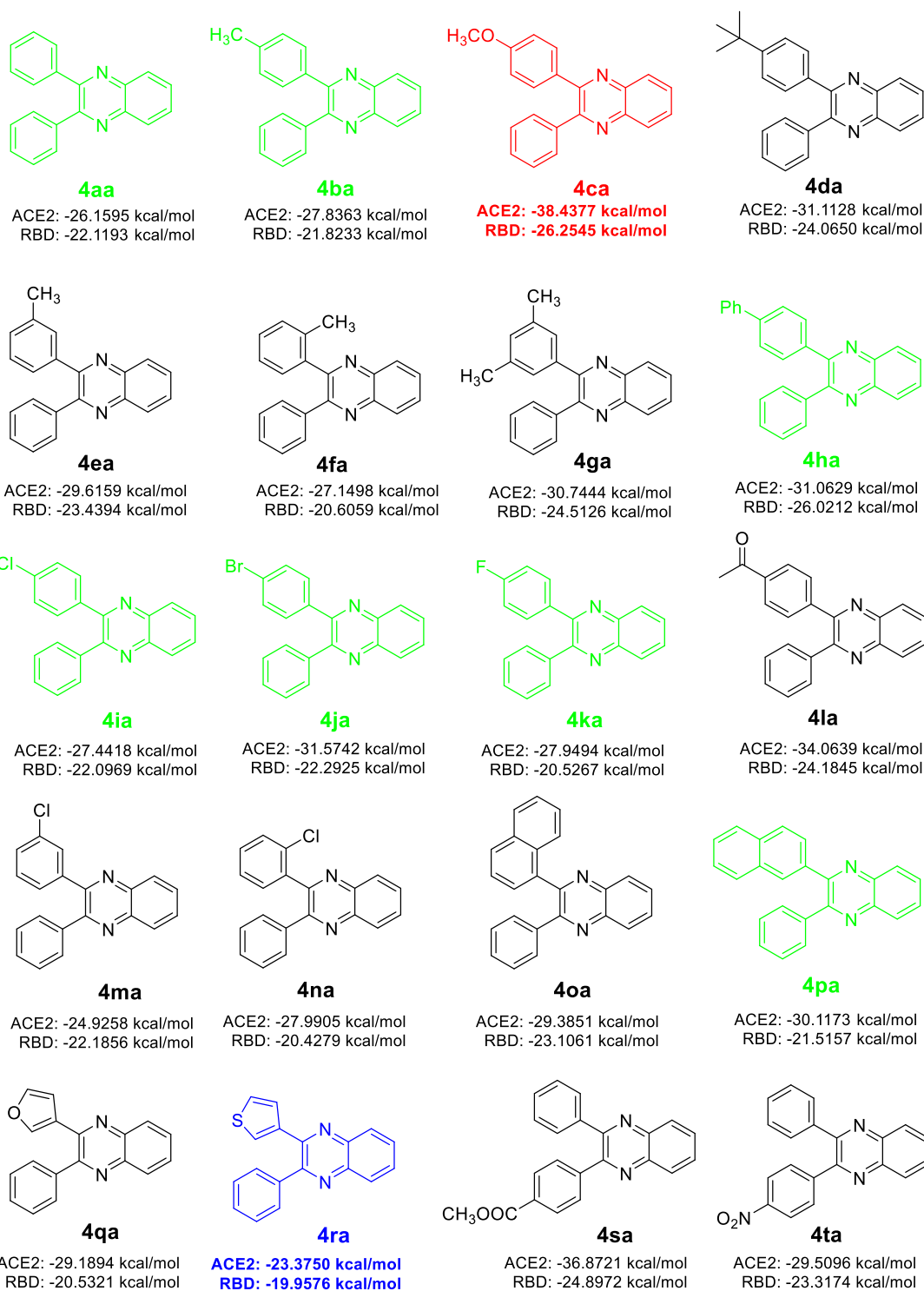
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Scheme S1 Twenty quinoxalines from diketones **2a** - **2t**

Table S1 Calculated binding energy (kcal/ mol) of twenty quinoxalines with human ACE2 and SARS-CoV-2 spike RBD proteins by molecular docking study

Supplementary Figure 1- Supplementary Figure 74 The ¹H- and ¹³C-NMR spectra of the products **2** and **4**.

Supplementary Figure 75- Supplementary Figure 111 HRMS spectra of the products **2** and **4**.

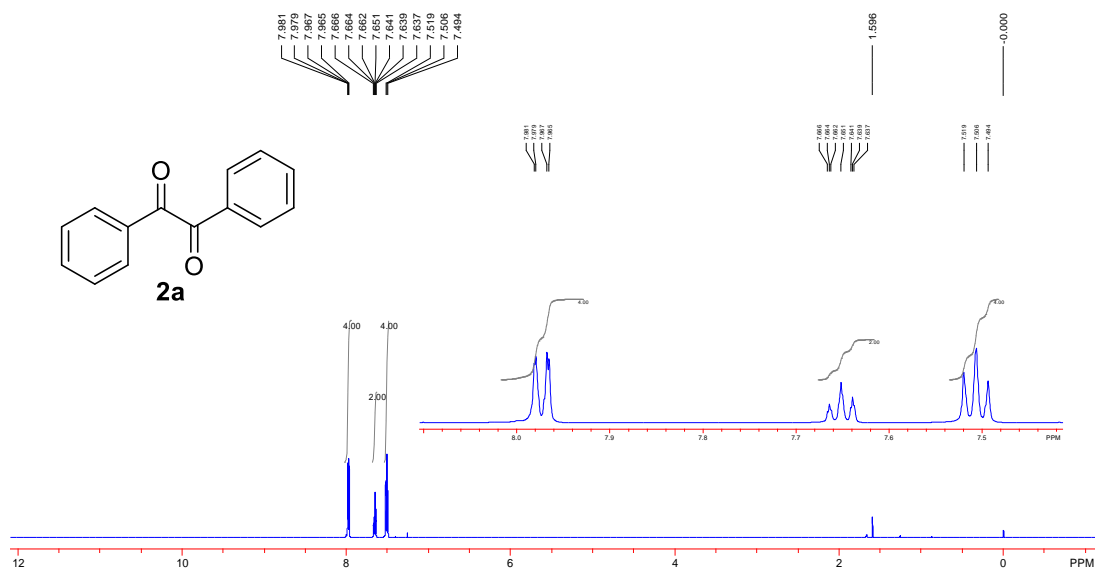


Scheme S1 Twenty quinoxalines from diketones **2a** - **2t** with calculated binding energy with both human ACE2 and SARS-CoV-2 spike RBD proteins by molecular docking study. Quinoxalines **4ca** (in red) has the lowest binding energy with both ACE2 and Spike RBD proteins, while **4ra** (in blue) has the highest binding energy with both proteins among all 20 quinoxalines. Nine quinoxalines **4aa**-

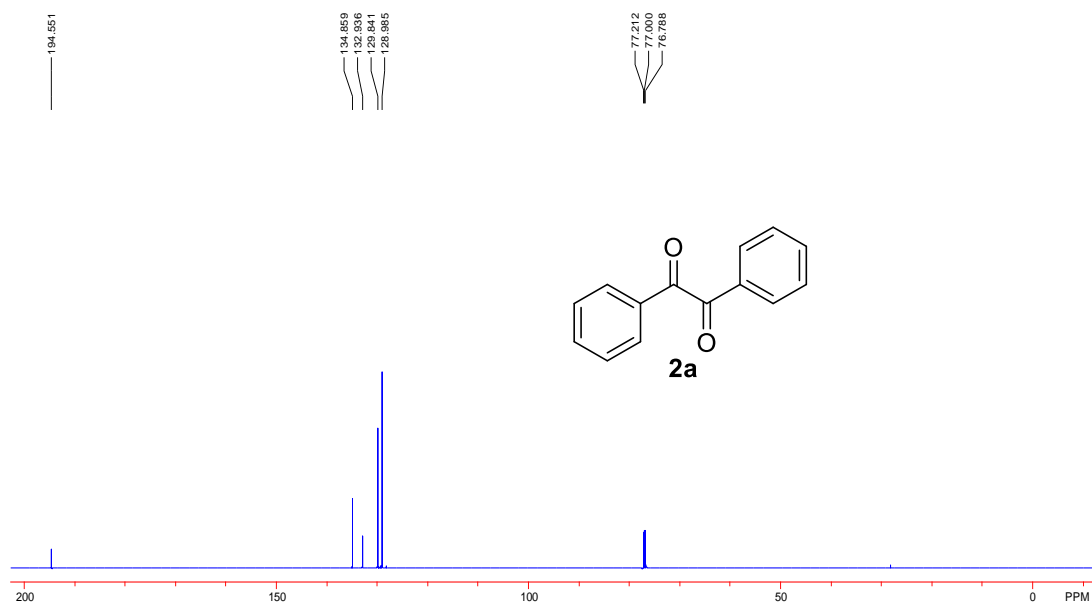
4ca, **4ha**, **4ia-4ka**, **4pa** and **4ra** were selected as representatives to be synthesized for subsequent antiviral entry evaluation against SARS-CoV-2 pseudovirus.

Table S1 Calculated binding energy (kcal/ mol) of twenty quinoxalines with human ACE2 and SARS-CoV-2 spike RBD proteins by molecular docking study

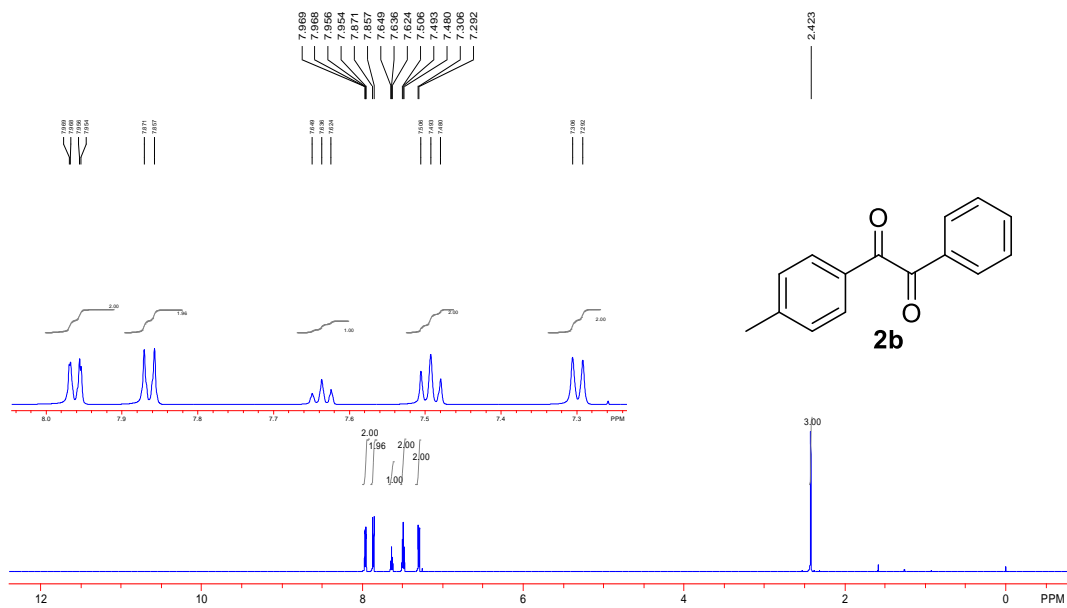
Quinoxalines	ACE2	Spike RBD
4aa	-26.1595	-22.1193
4ba	-27.8363	-21.8233
4ca	-38.4377	-26.2545
4da	-31.1128	-24.065
4ea	-29.6159	-23.4394
4fa	-27.1498	-20.6059
4ga	-30.7444	-24.5126
4ha	-31.0629	-26.0212
4ia	-27.4418	-22.0969
4ja	-31.5742	-22.2925
4ka	-27.9494	-20.5267
4la	-34.0639	-24.1845
4ma	-24.9258	-22.1856
4na	-27.9905	-20.4279
4oa	-29.3851	-23.1061
4pa	-30.1173	-21.5157
4qa	-29.1894	-20.5321
4ra	-23.375	-19.9576
4sa	-36.8721	-24.8972
4ta	-29.5096	-23.3174



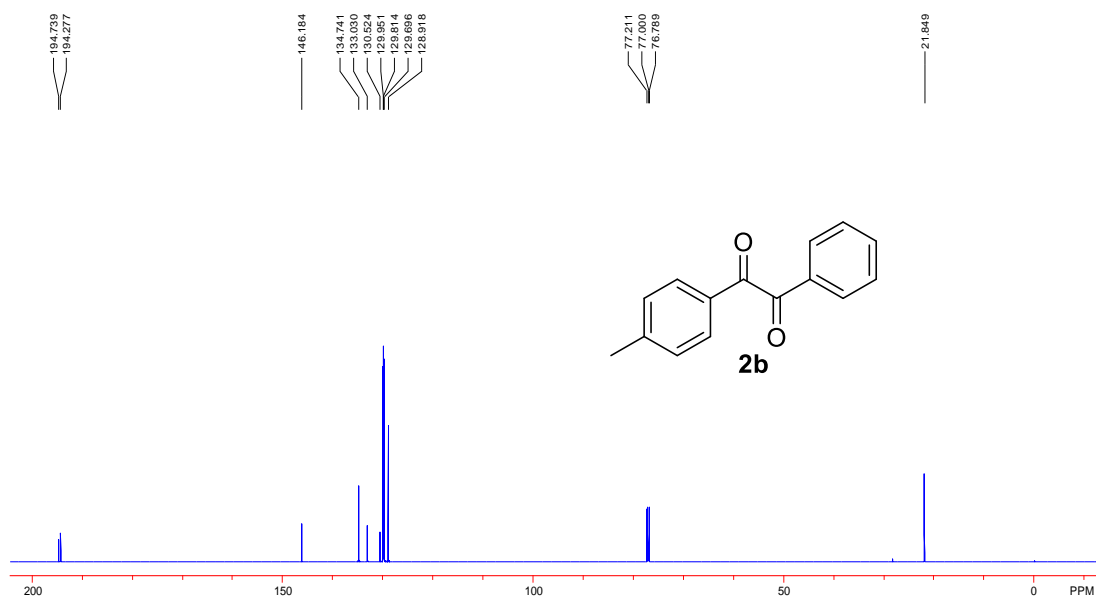
Supplementary Figure 1. ¹H-NMR spectrum of Compound **2a** in CDCl₃



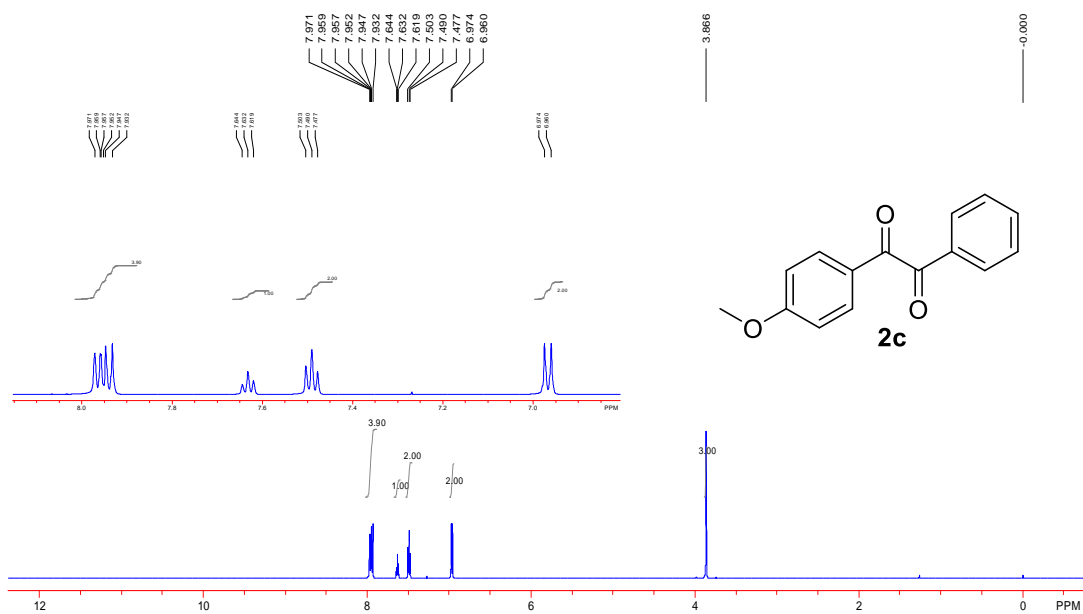
Supplementary Figure 2. ¹³C-NMR spectrum of Compound **2a** in CDCl₃



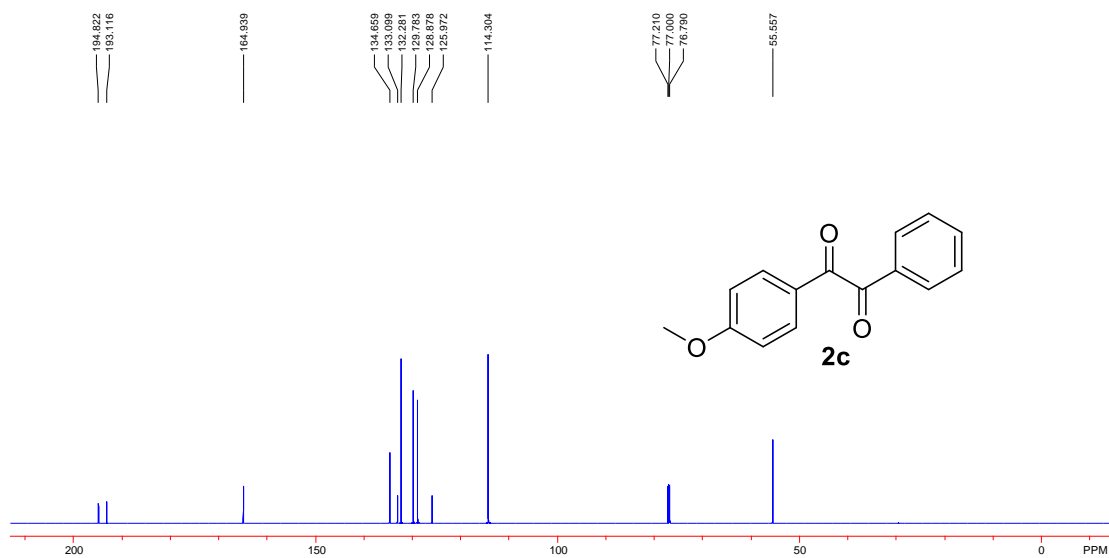
Supplementary Figure 3. ¹H-NMR spectrum of Compound **2b** in CDCl₃



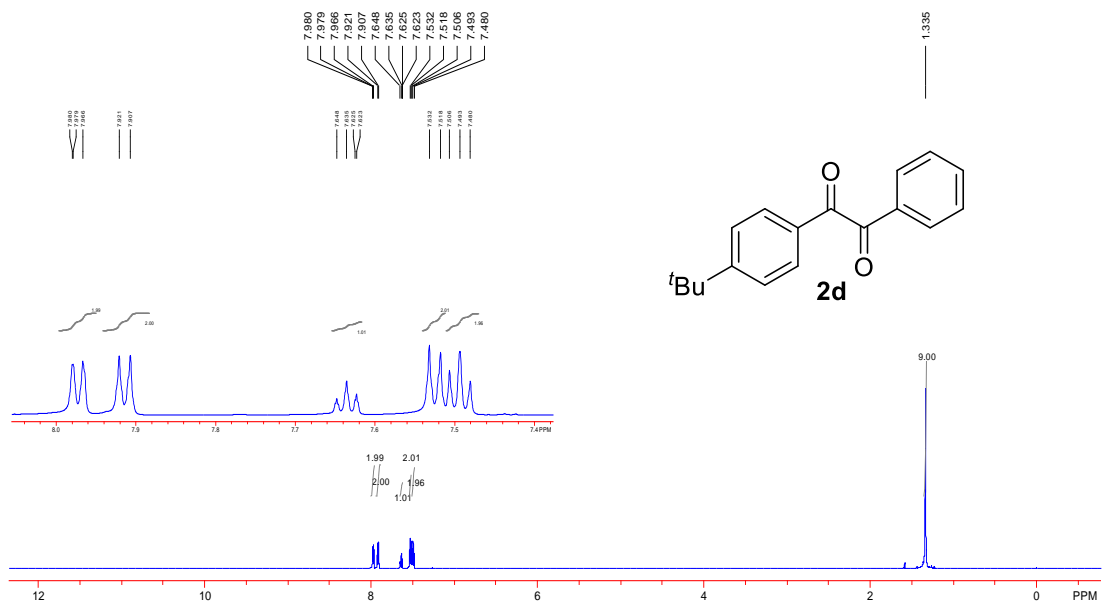
Supplementary Figure 4. ¹³C-NMR spectrum of Compound **2b** in CDCl₃



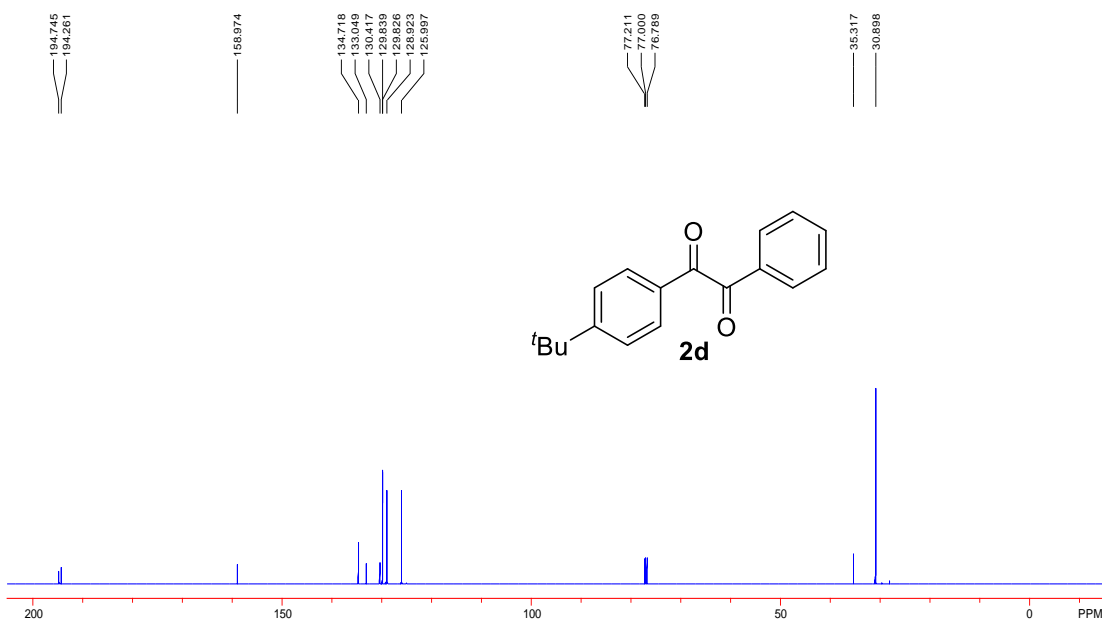
Supplementary Figure 5. ¹H-NMR spectrum of Compound 2c in CDCl₃



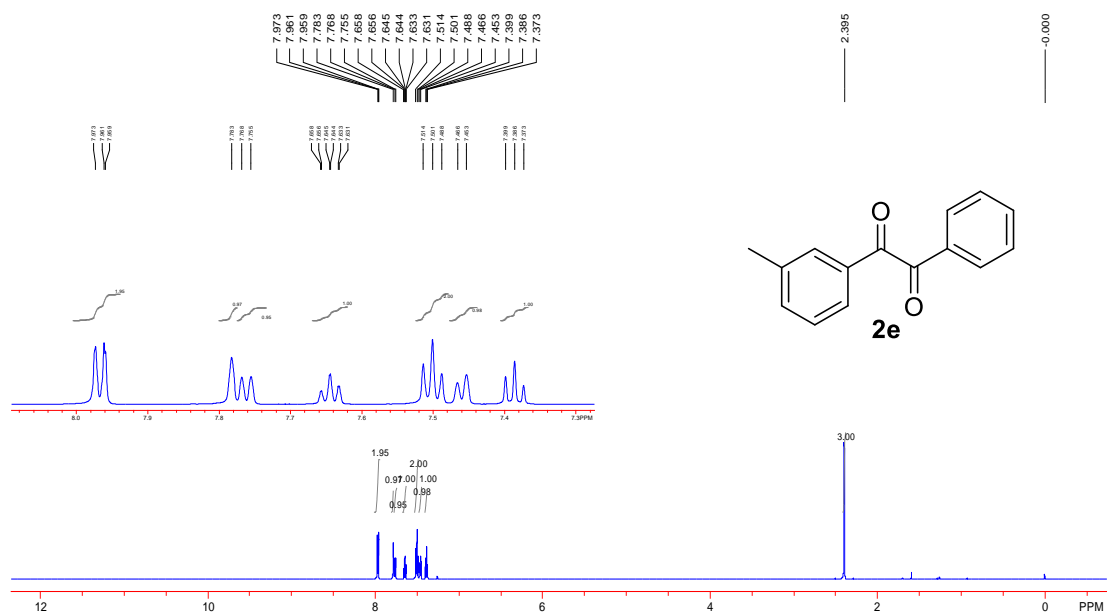
Supplementary Figure 6. ¹³C-NMR spectrum of Compound 2c in CDCl₃



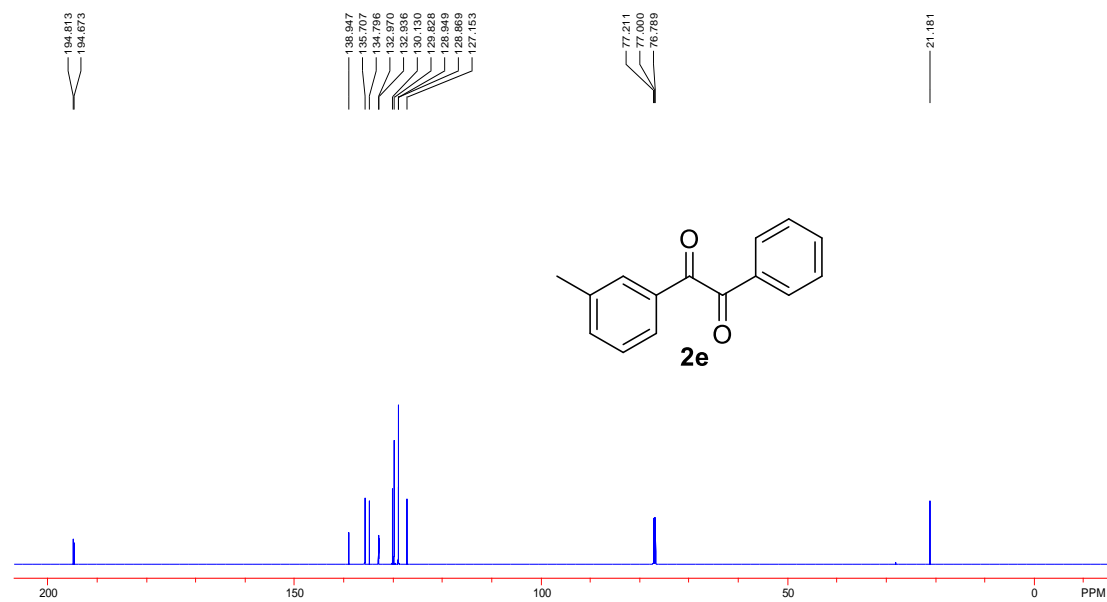
Supplementary Figure 7. ¹H-NMR spectrum of Compound **2d** in CDCl₃



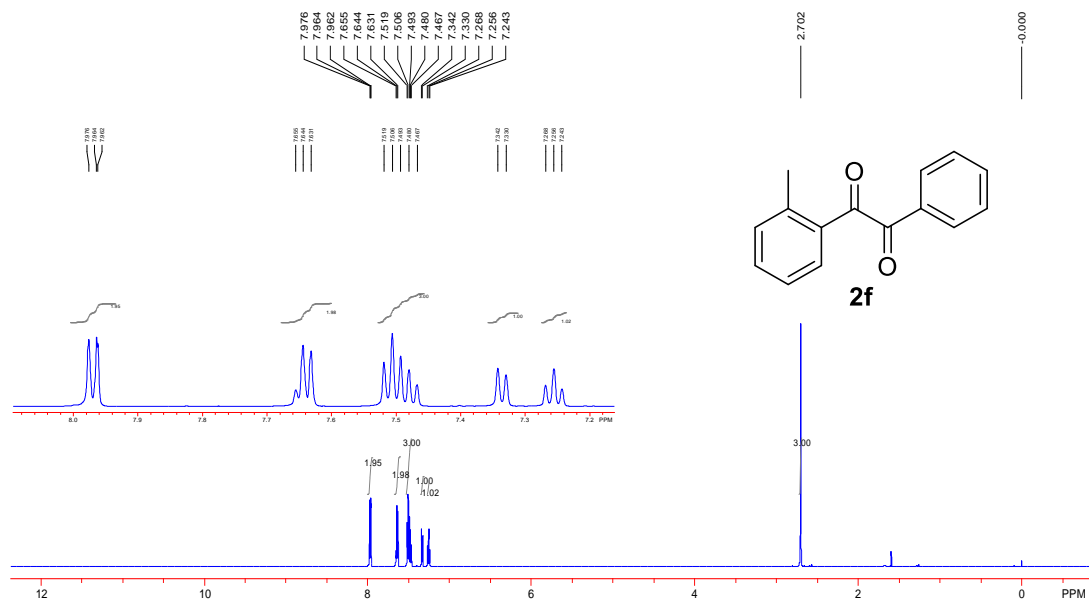
Supplementary Figure 8. ¹³C-NMR spectrum of Compound **2d** in CDCl₃



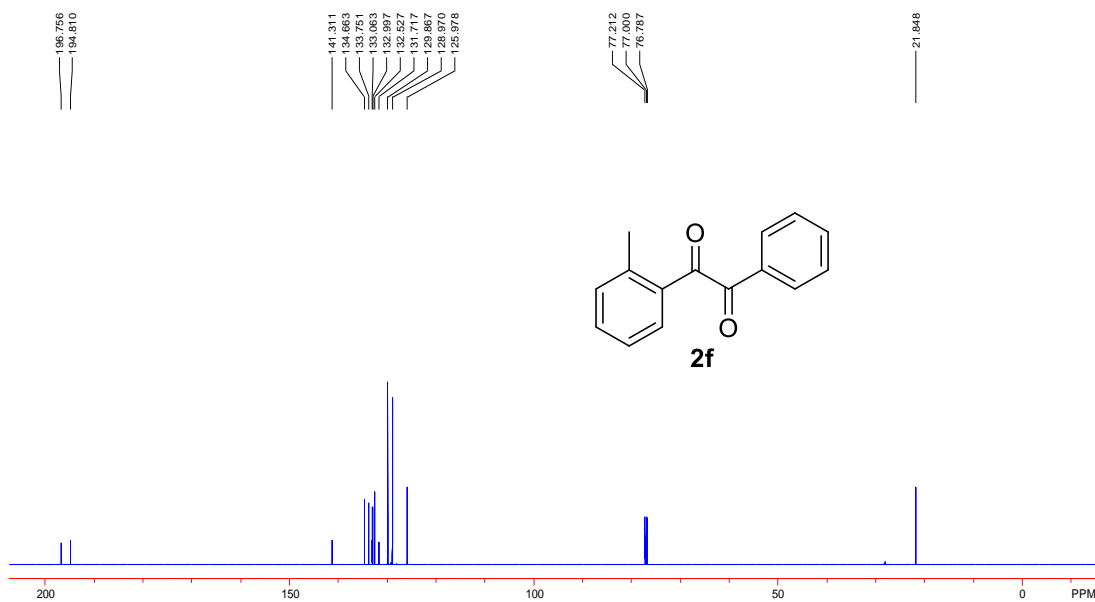
Supplementary Figure 9. ¹H-NMR spectrum of Compound 2e in CDCl₃



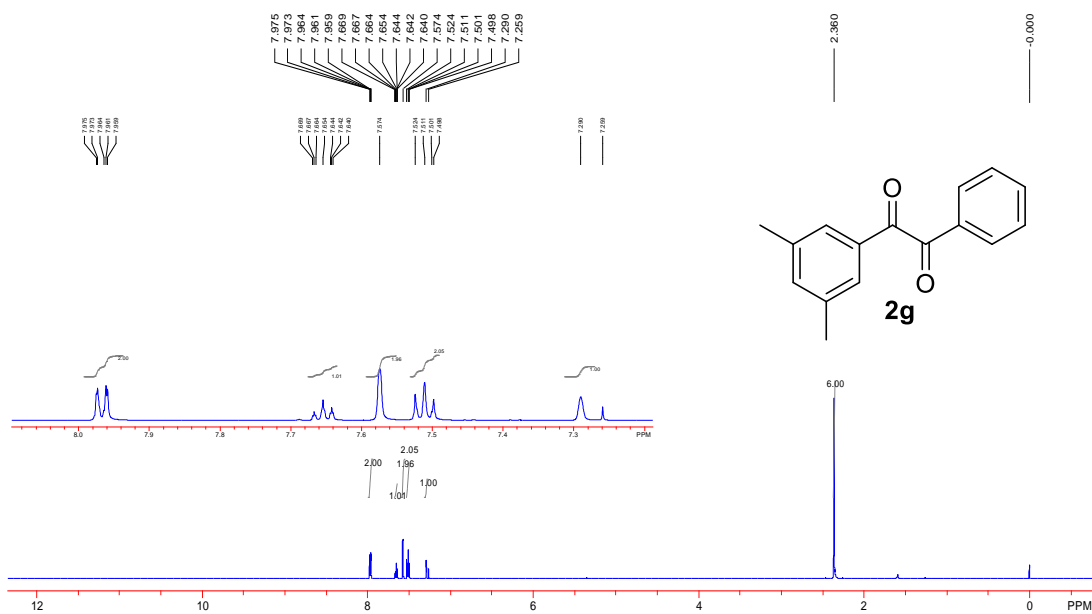
Supplementary Figure 20. ¹³C-NMR spectrum of Compound 2e in CDCl₃



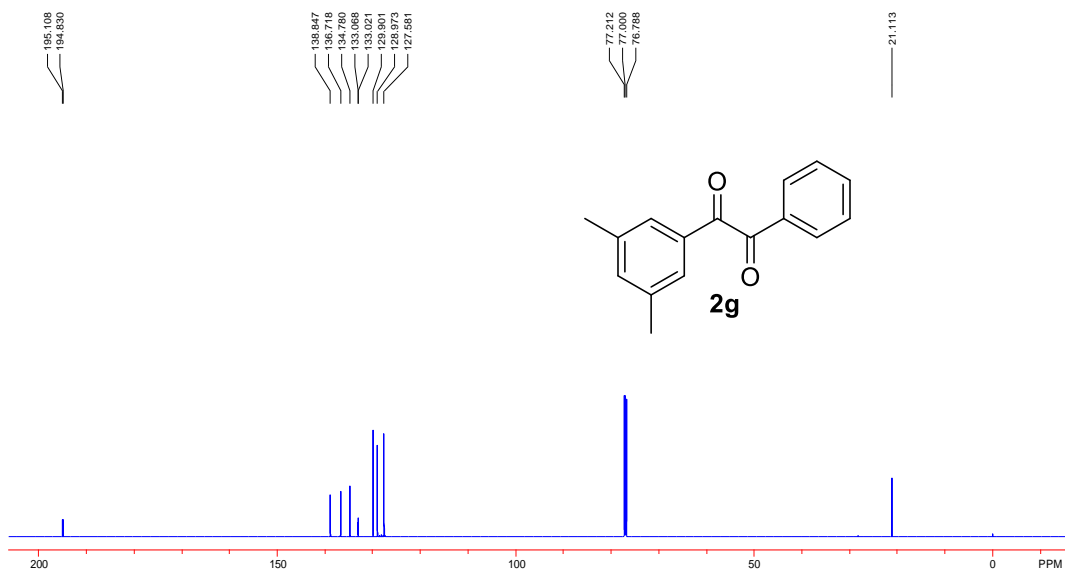
Supplementary Figure 31. ¹H-NMR spectrum of Compound **2f** in CDCl₃



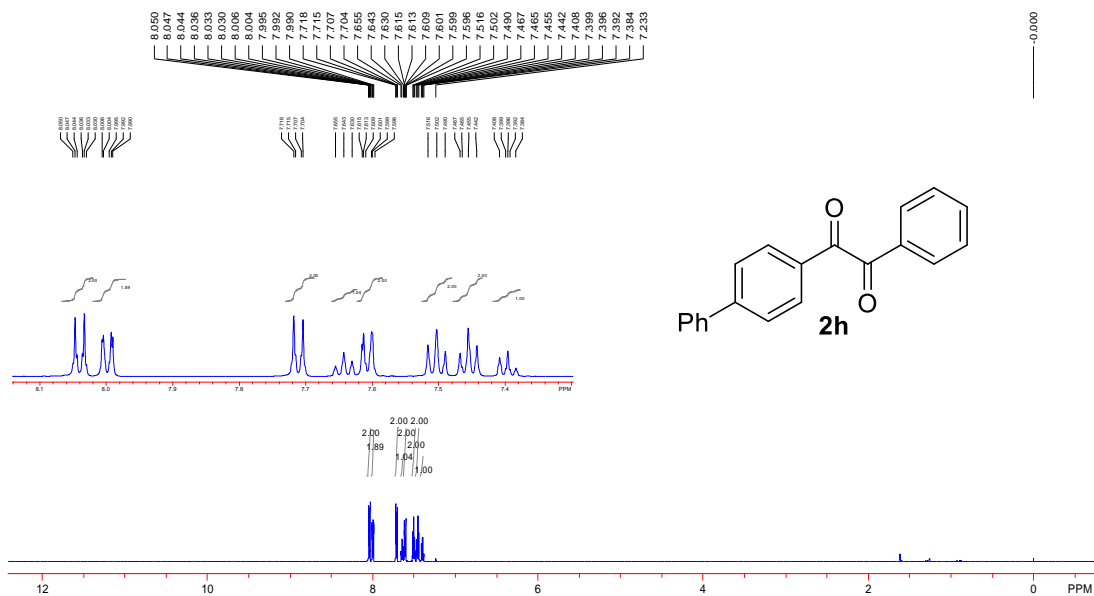
Supplementary Figure 42. ¹³C-NMR spectrum of Compound **2f** in CDCl₃



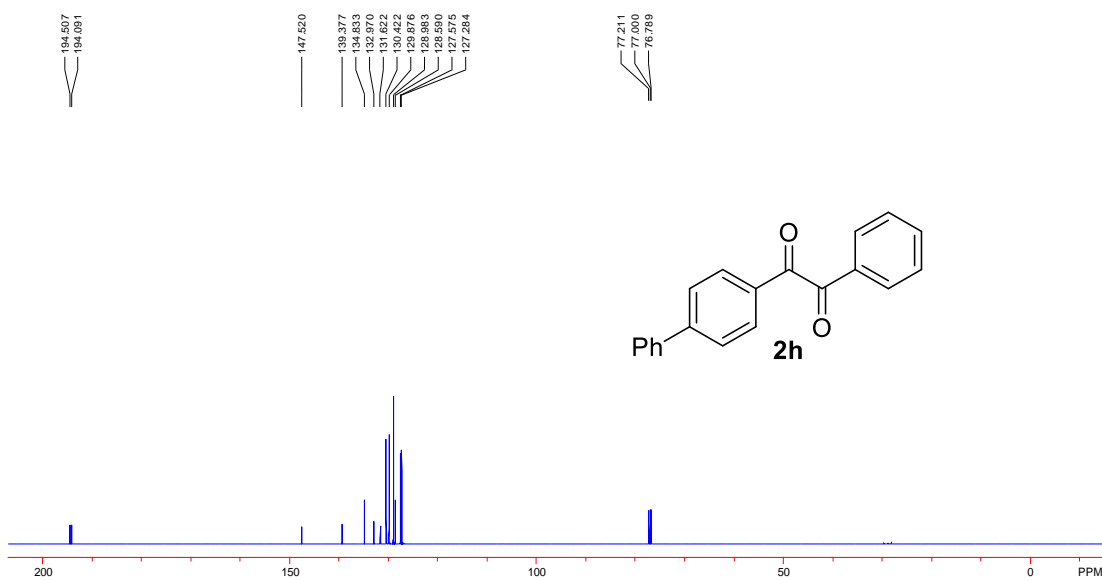
Supplementary Figure 53. ¹H-NMR spectrum of Compound **2g** in CDCl₃



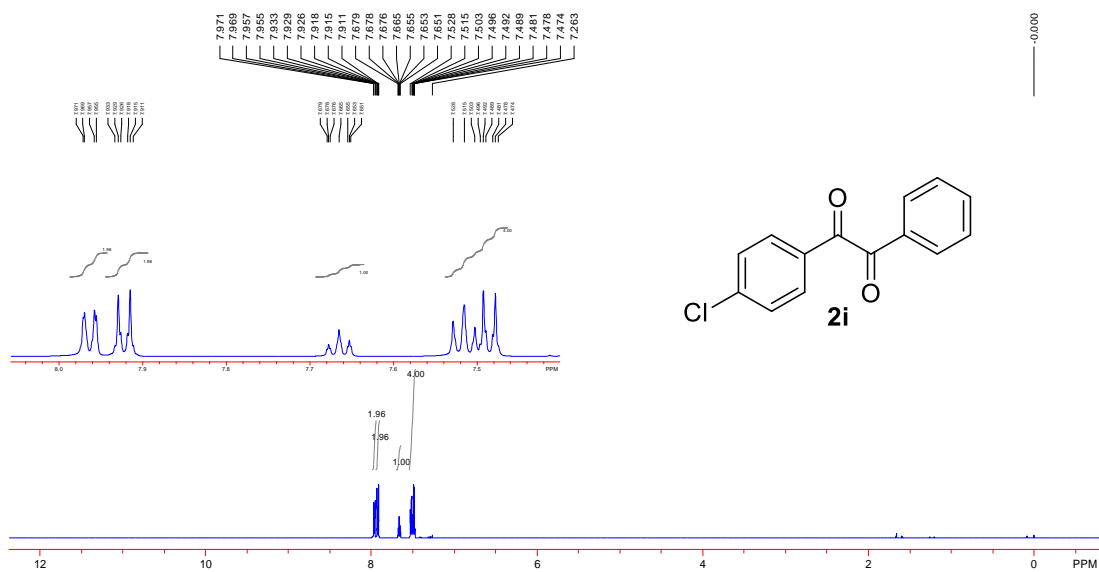
Supplementary Figure 64. ¹³C-NMR spectrum of Compound **2g** in CDCl₃



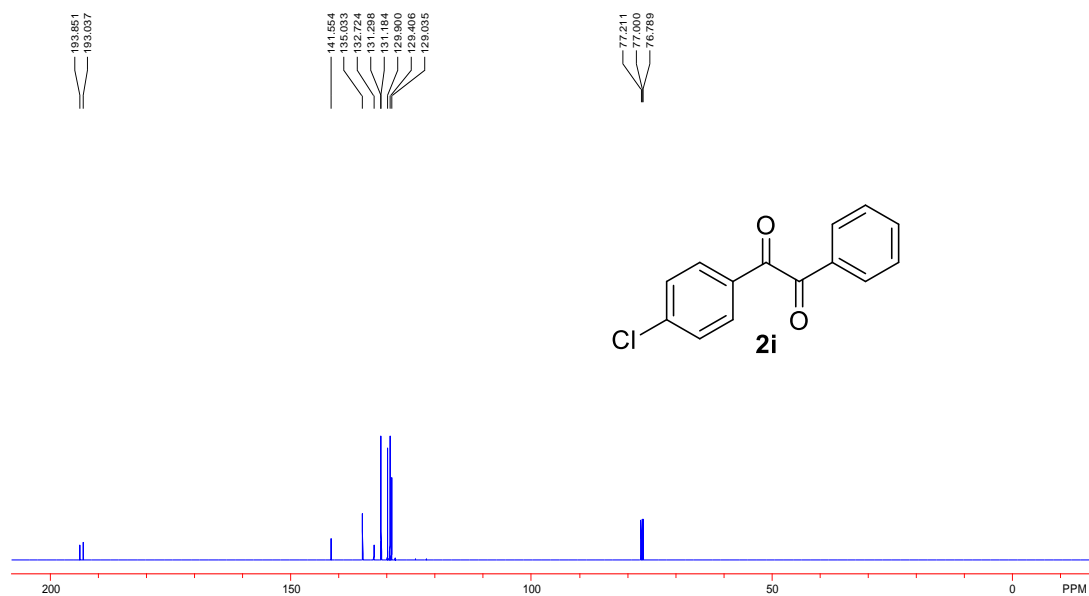
Supplementary Figure 75. ¹H-NMR spectrum of Compound 2h in CDCl₃



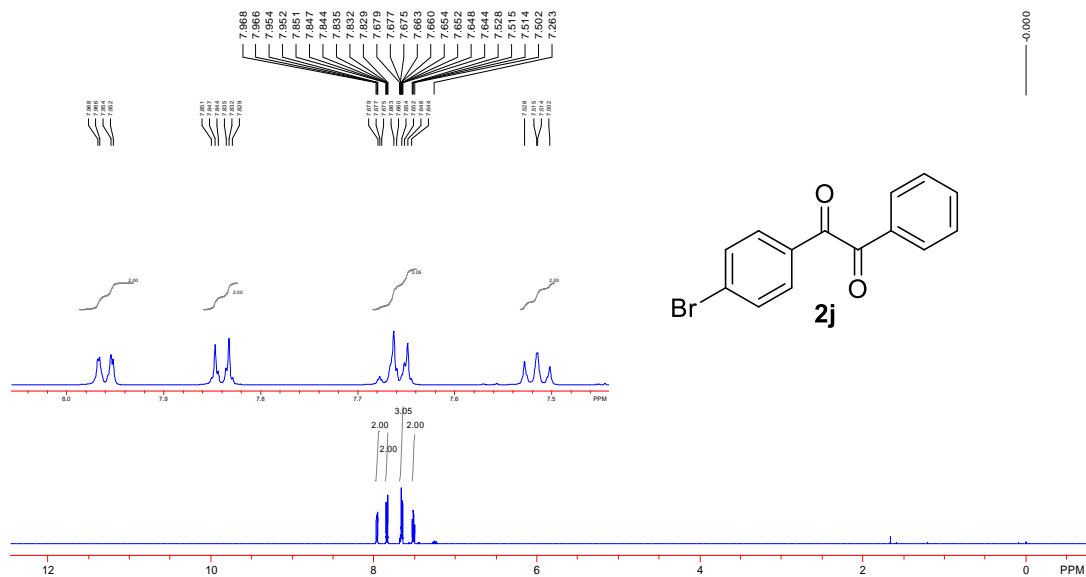
Supplementary Figure 86. ¹³C-NMR spectrum of Compound 2h in CDCl₃



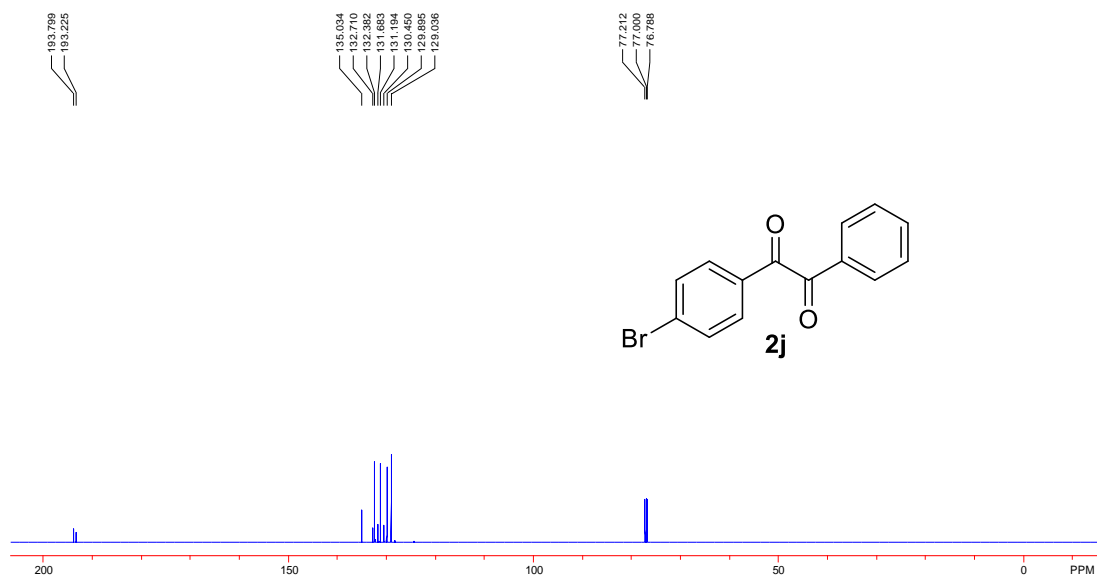
Supplementary Figure 97. ¹H-NMR spectrum of Compound **2i** in CDCl₃



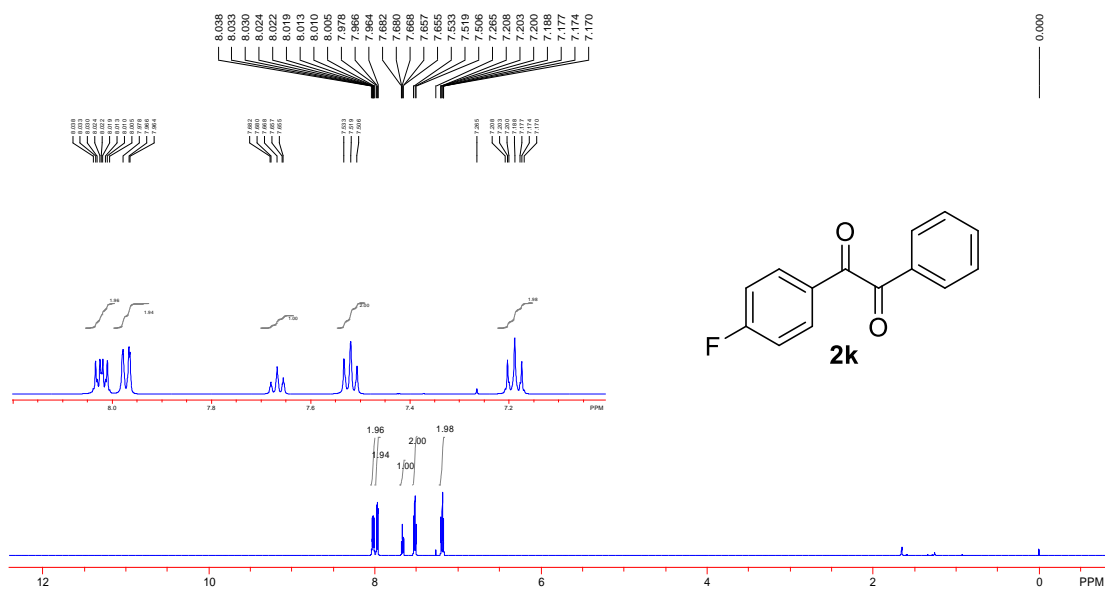
Supplementary Figure 108. ¹³C-NMR spectrum of Compound **2i** in CDCl₃



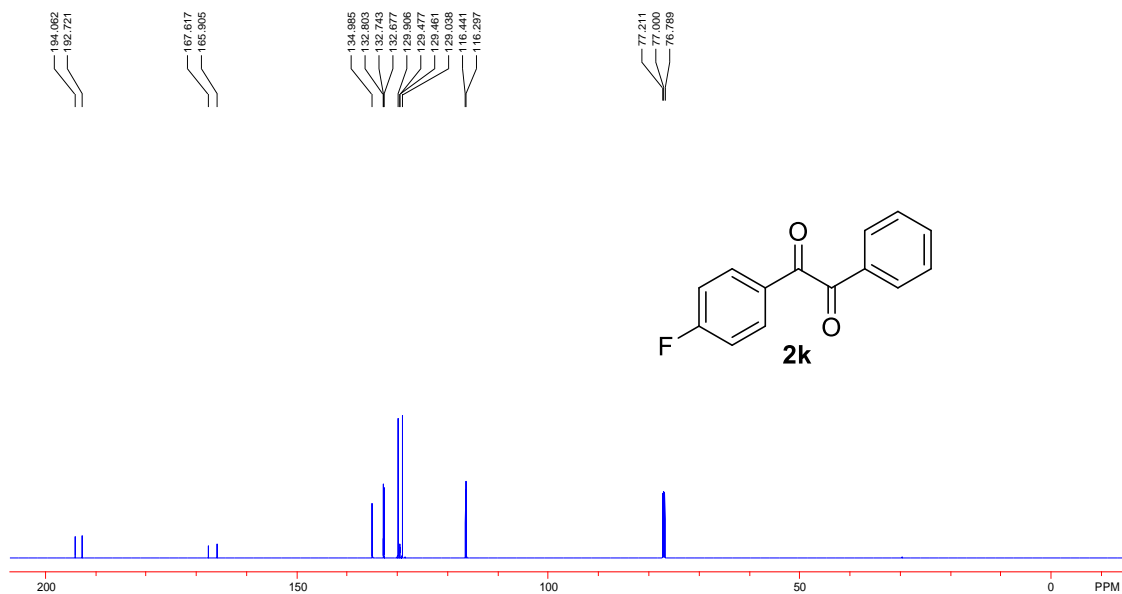
Supplementary Figure 119. ¹H-NMR spectrum of Compound **2j** in CDCl₃



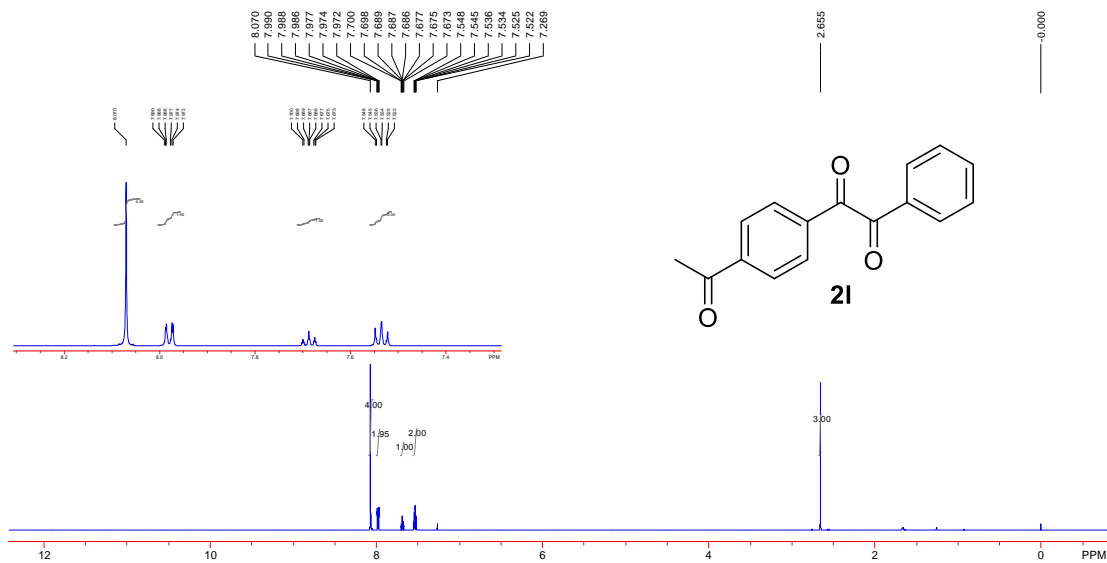
Supplementary Figure 20. ¹³C-NMR spectrum of Compound **2j** in CDCl₃



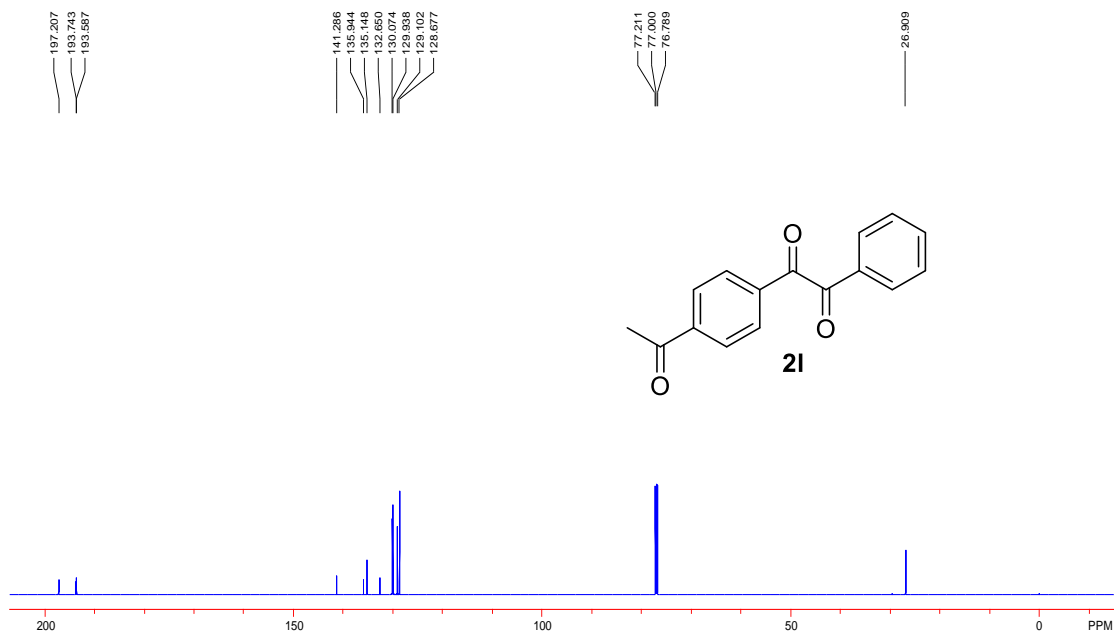
Supplementary Figure 21. ¹H-NMR spectrum of Compound **2k** in CDCl₃



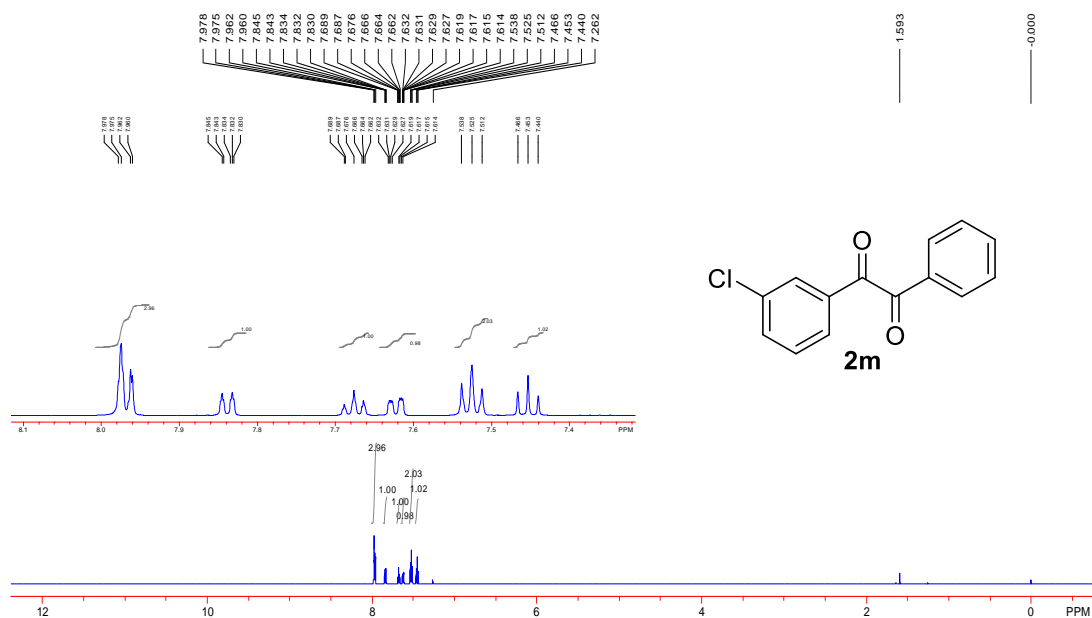
Supplementary Figure 22. ¹³C-NMR spectrum of Compound **2k** in CDCl₃



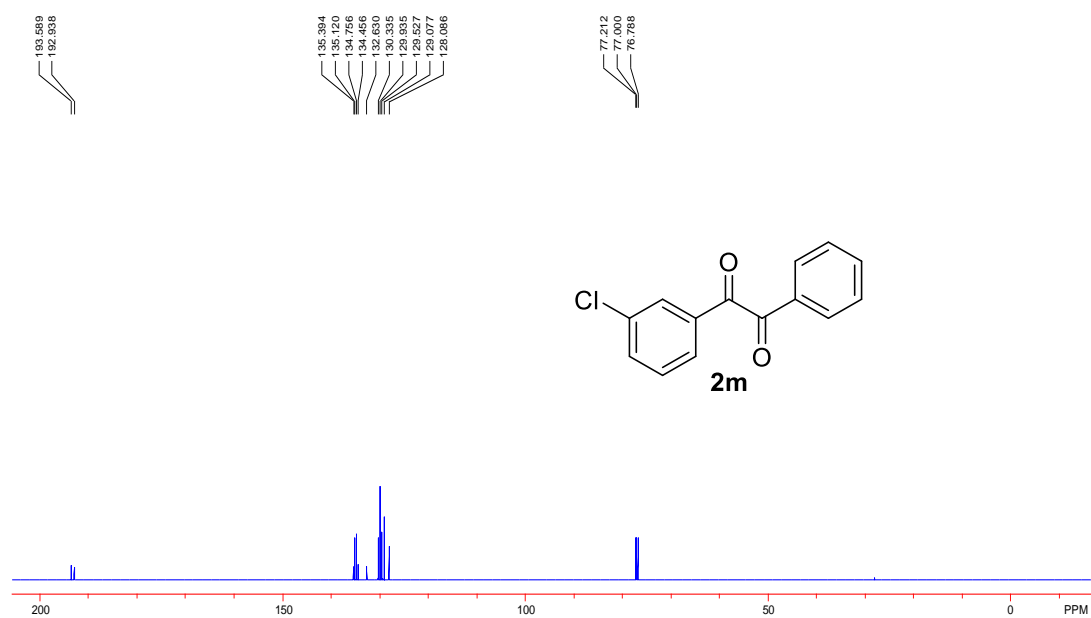
Supplementary Figure 23. ¹H-NMR spectrum of Compound **2I** in CDCl₃



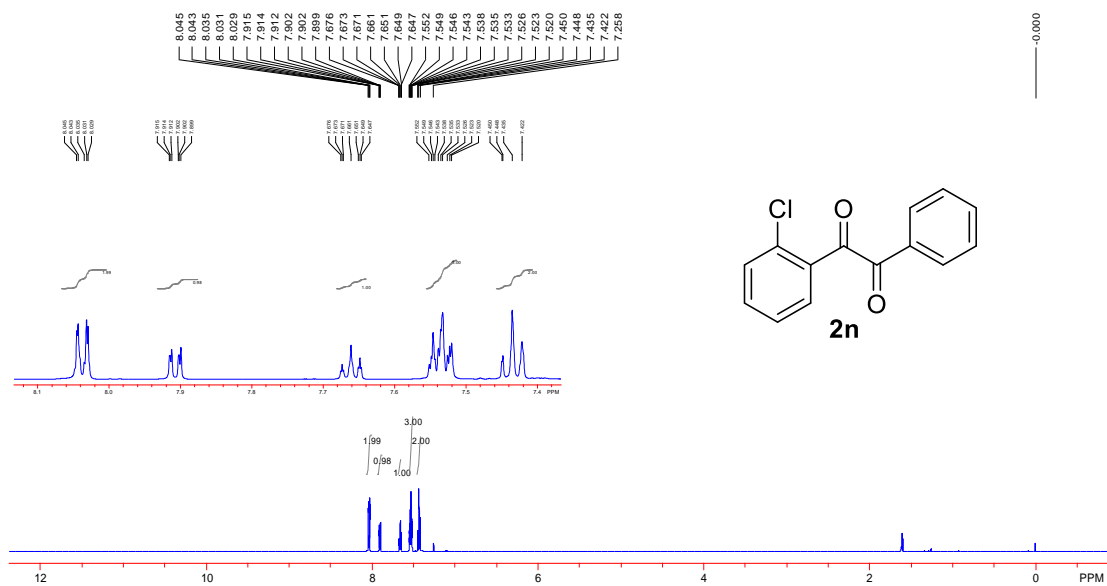
Supplementary Figure 24. ¹³C-NMR spectrum of Compound **2I** in CDCl₃



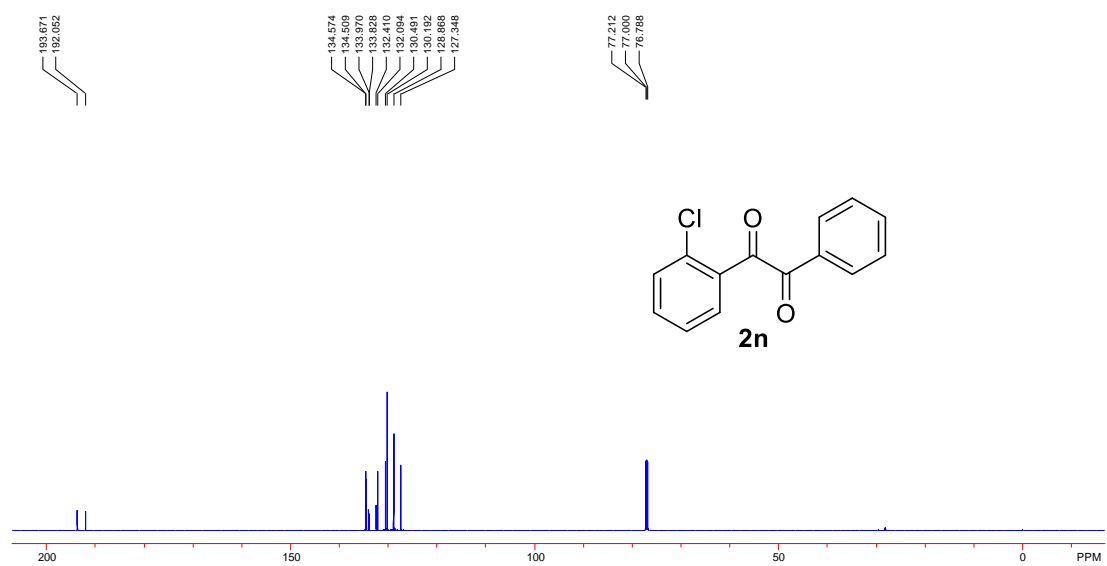
Supplementary Figure 25. ¹H-NMR spectrum of Compound **2m** in CDCl₃



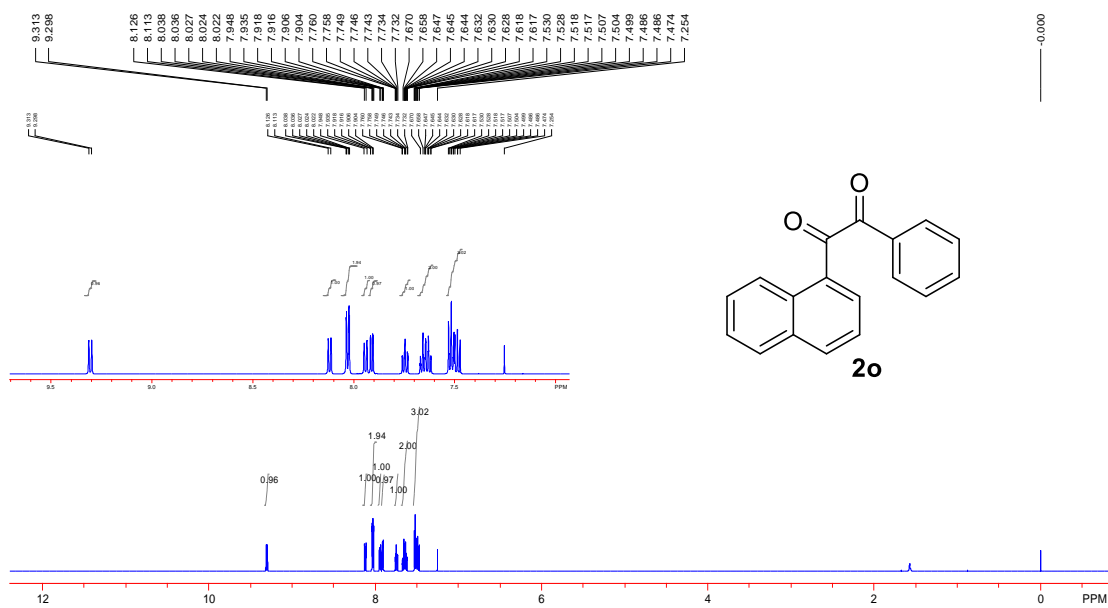
Supplementary Figure 26. ¹³C-NMR spectrum of Compound **2m** in CDCl₃



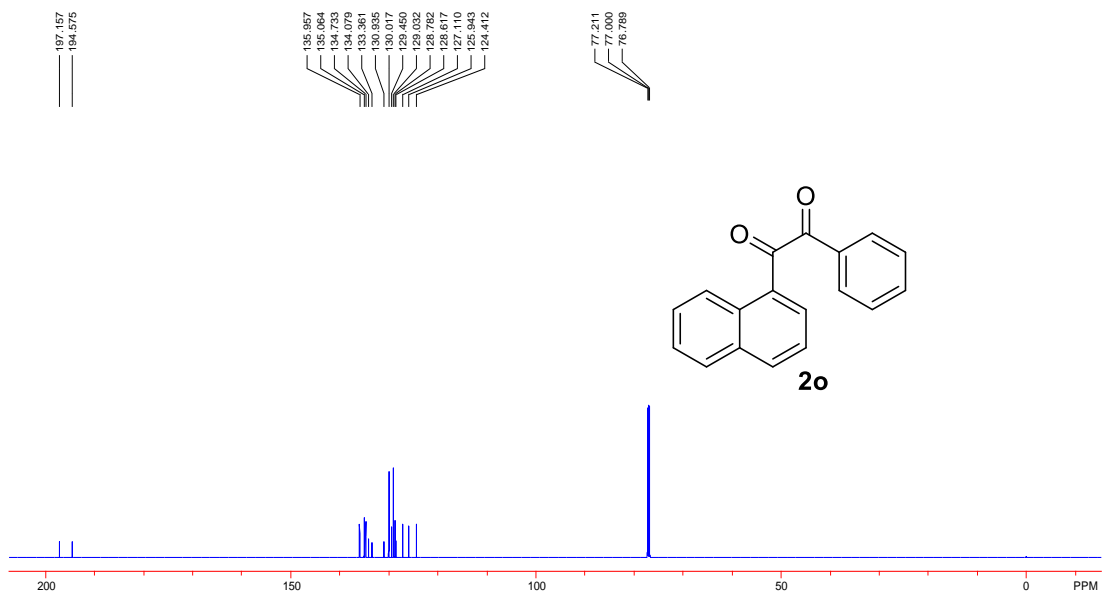
Supplementary Figure 27. ¹H-NMR spectrum of Compound **2n** in CDCl₃



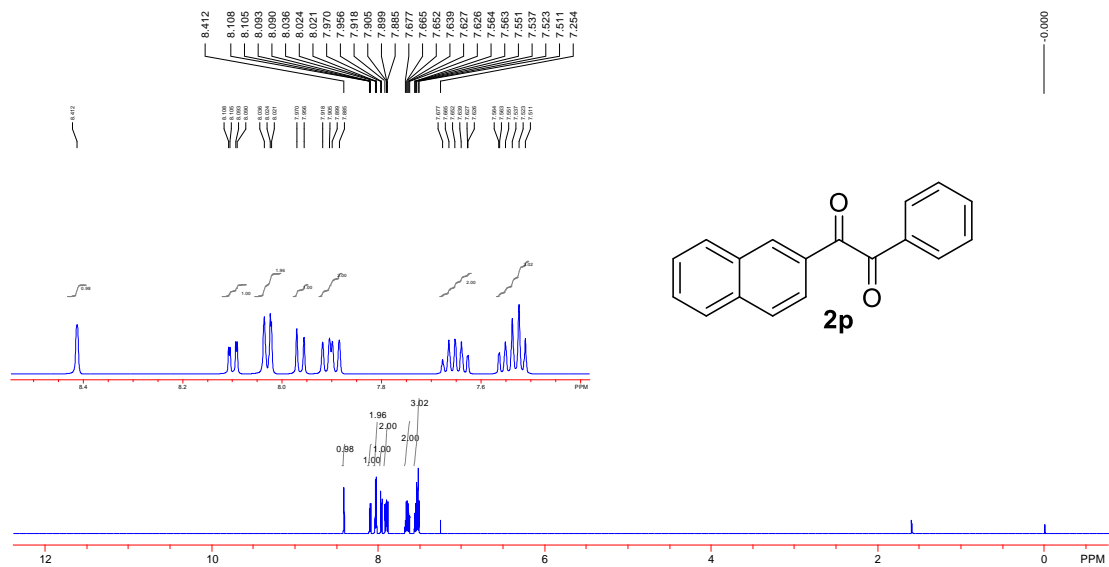
Supplementary Figure 28. ¹³C-NMR spectrum of Compound **2n** in CDCl₃



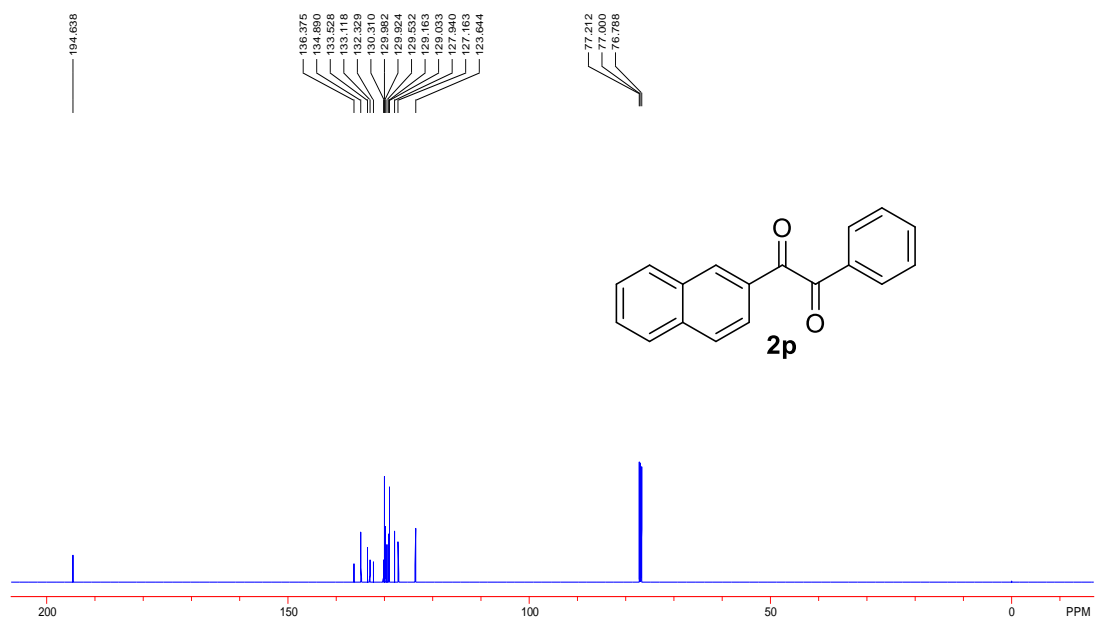
Supplementary Figure 29. ¹H-NMR spectrum of Compound 2o in CDCl₃



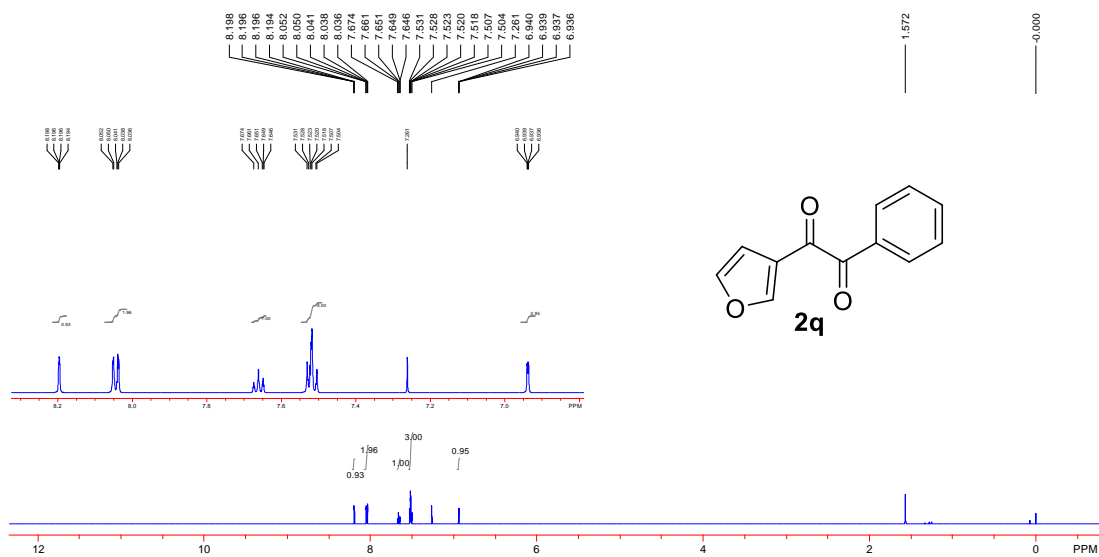
Supplementary Figure 30. ¹³C-NMR spectrum of Compound 2o in CDCl₃



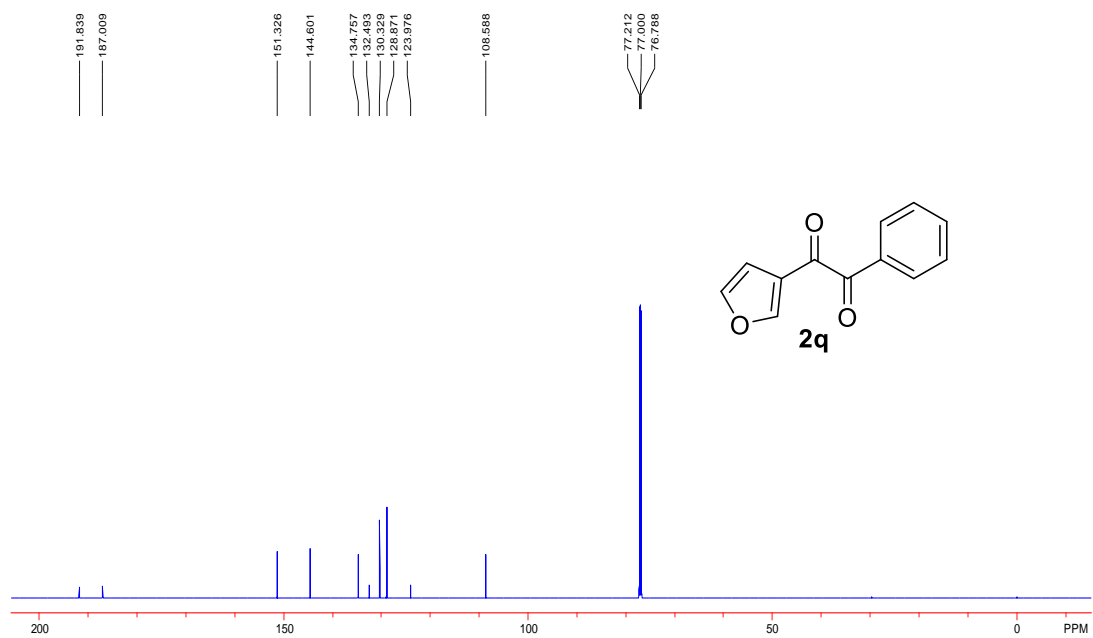
Supplementary Figure 31. ¹H-NMR spectrum of Compound **2p** in CDCl₃



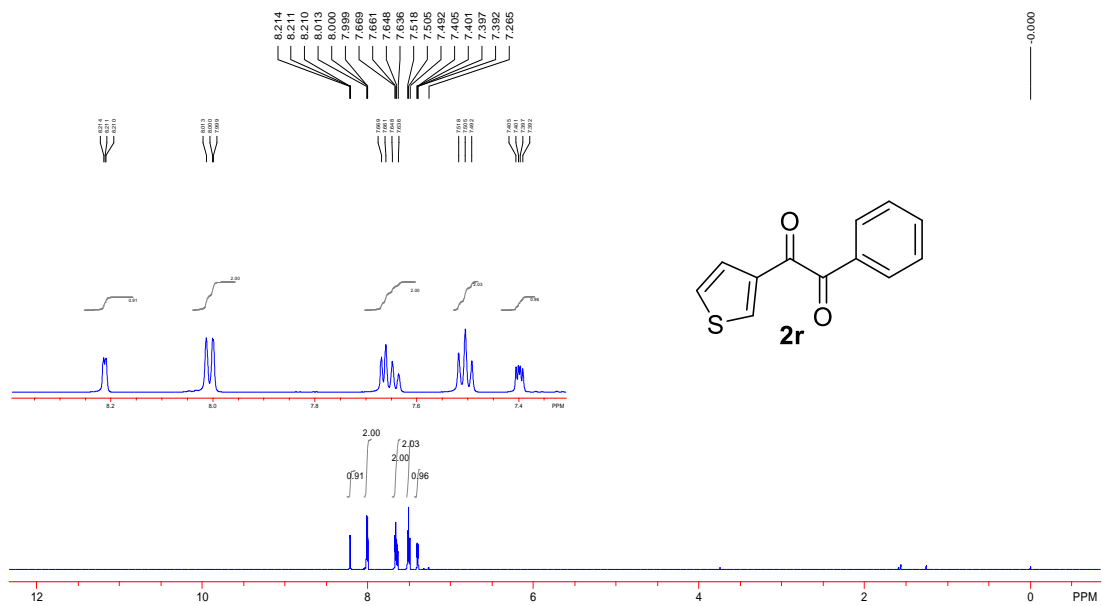
Supplementary Figure 32. ¹³C-NMR spectrum of Compound **2p** in CDCl₃



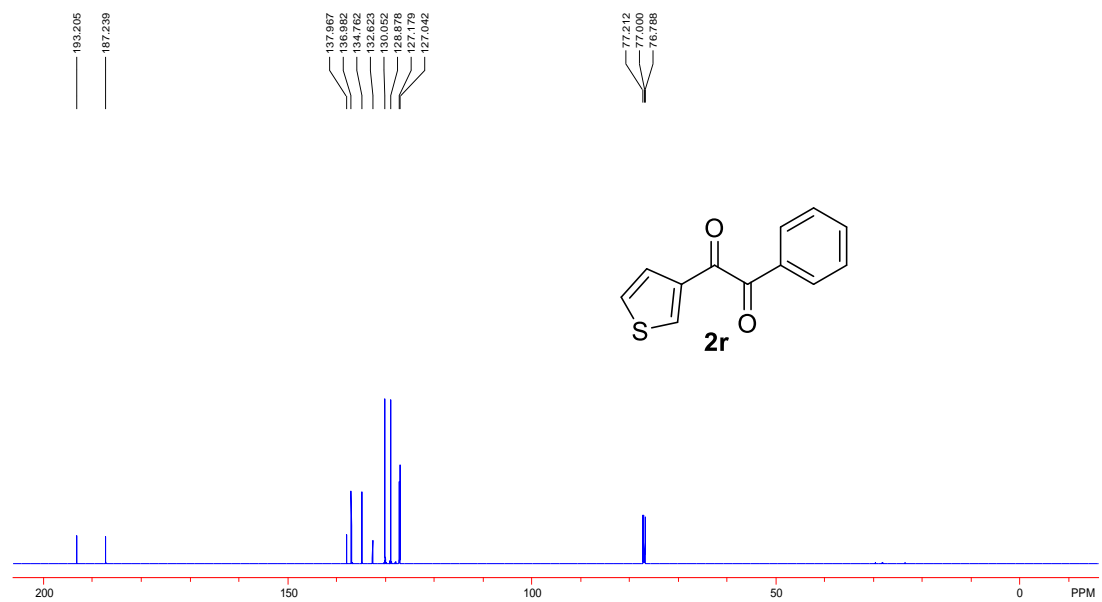
Supplementary Figure 33. ¹H-NMR spectrum of Compound **2q** in CDCl₃



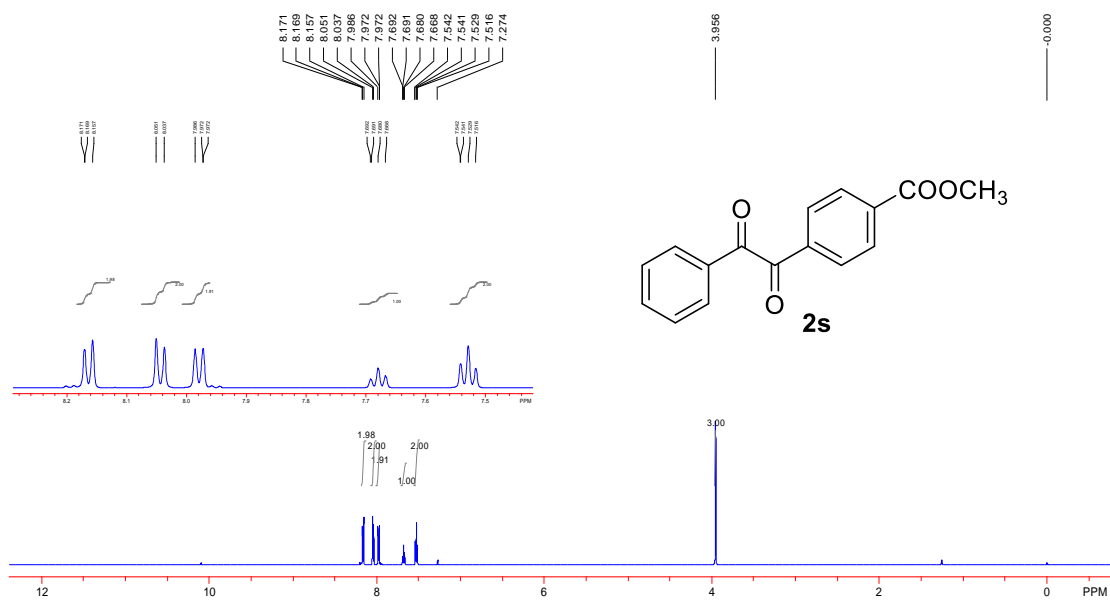
Supplementary Figure 34. ¹³C-NMR spectrum of Compound **2q** in CDCl₃



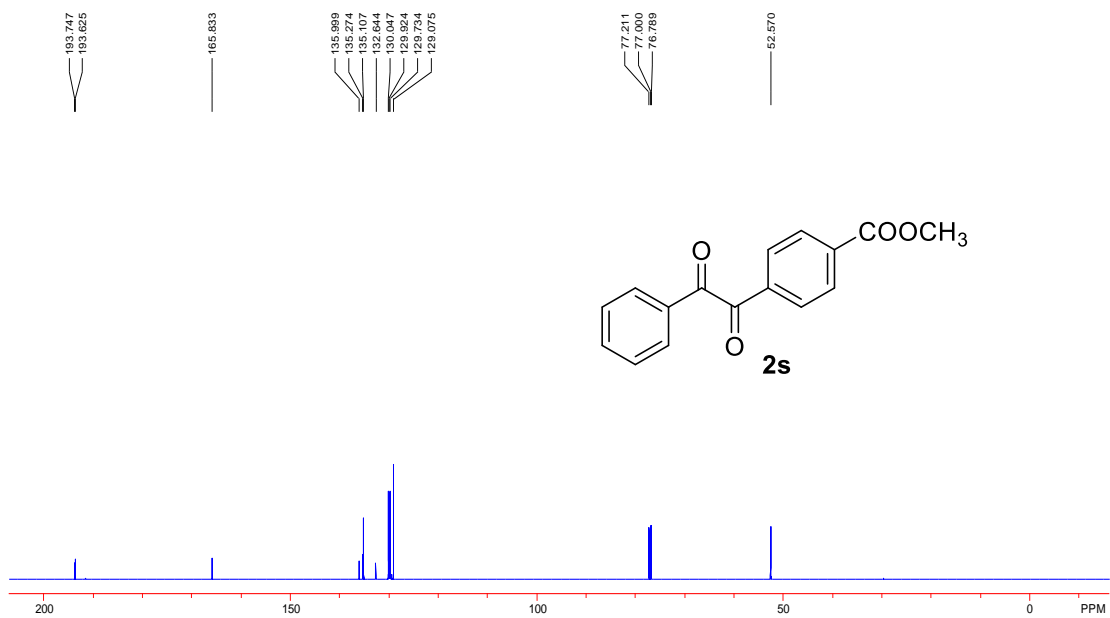
Supplementary Figure 35. ¹H-NMR spectrum of Compound **2r** in CDCl₃



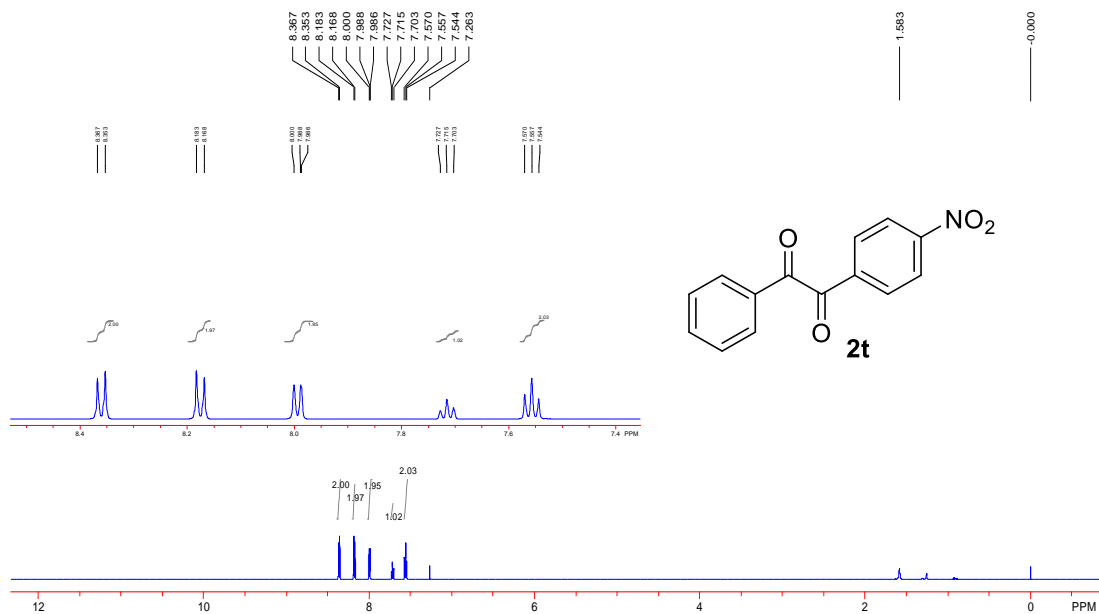
Supplementary Figure 36. ¹³C-NMR spectrum of Compound **2r** in CDCl₃



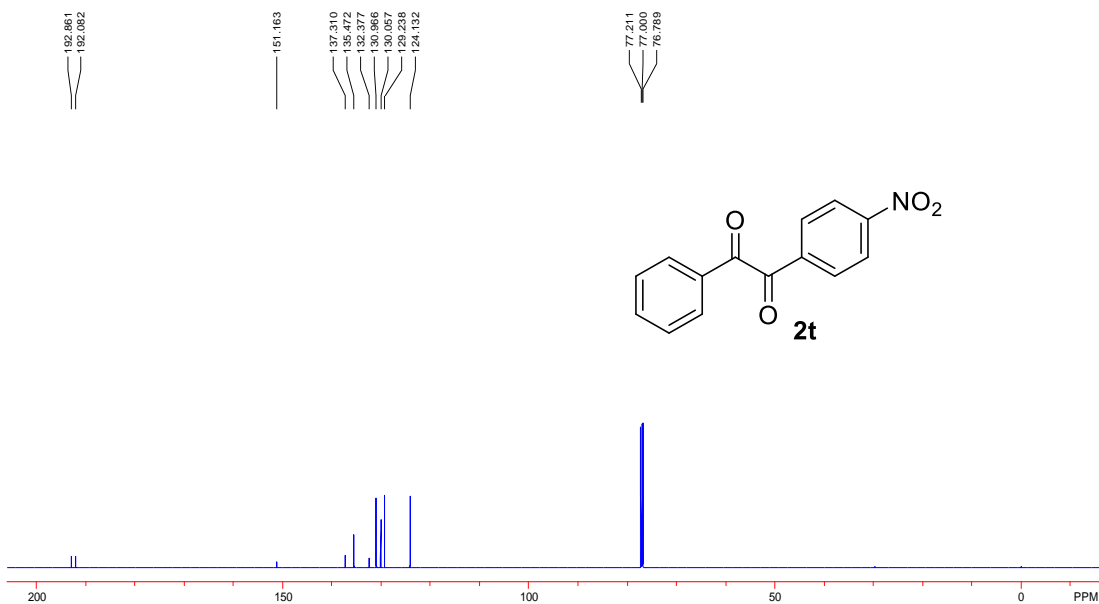
Supplementary Figure 37. ¹H-NMR spectrum of Compound **2s** in CDCl₃



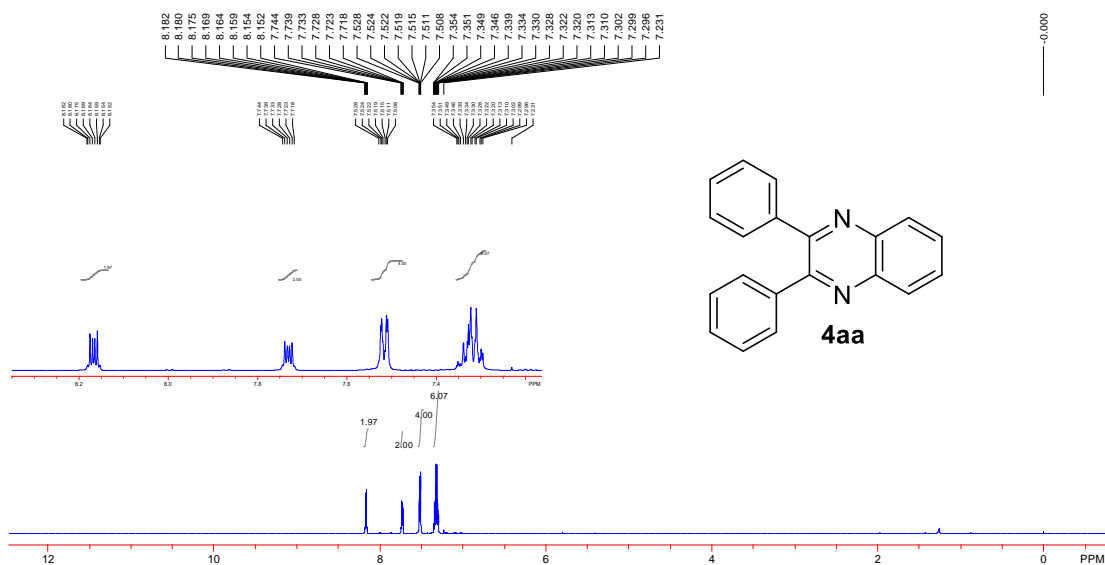
Supplementary Figure 38. ¹³C-NMR spectrum of Compound **2s** in CDCl₃



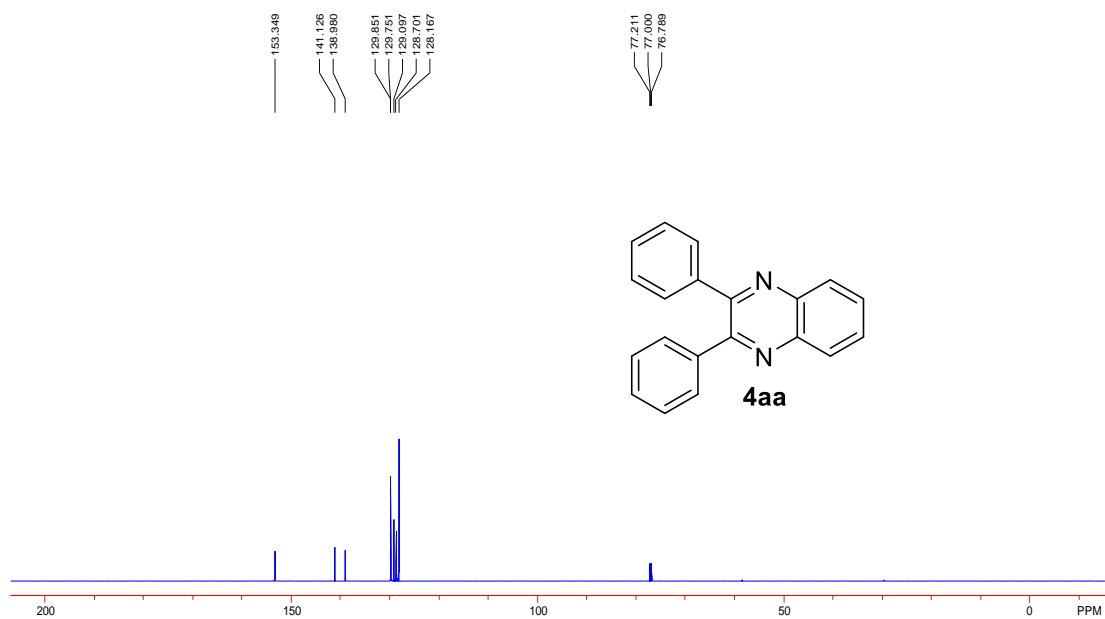
Supplementary Figure 39. ¹H-NMR spectrum of Compound **2t** in CDCl₃



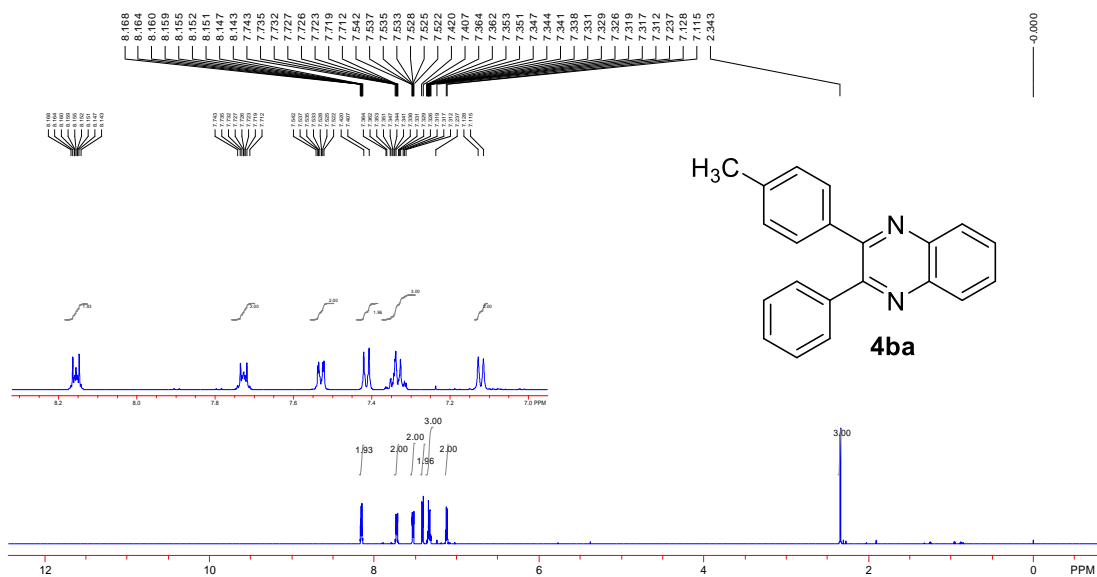
Supplementary Figure 40. ¹³C-NMR spectrum of Compound **2t** in CDCl₃



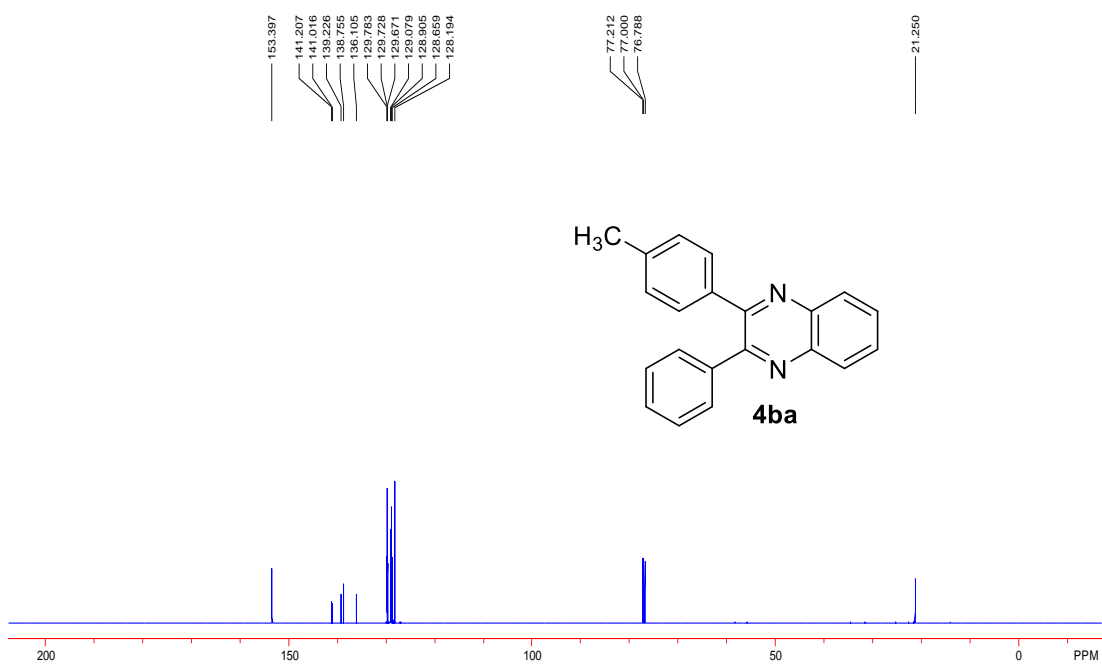
Supplementary Figure 41. ¹H-NMR spectrum of Compound **4aa** in CDCl₃



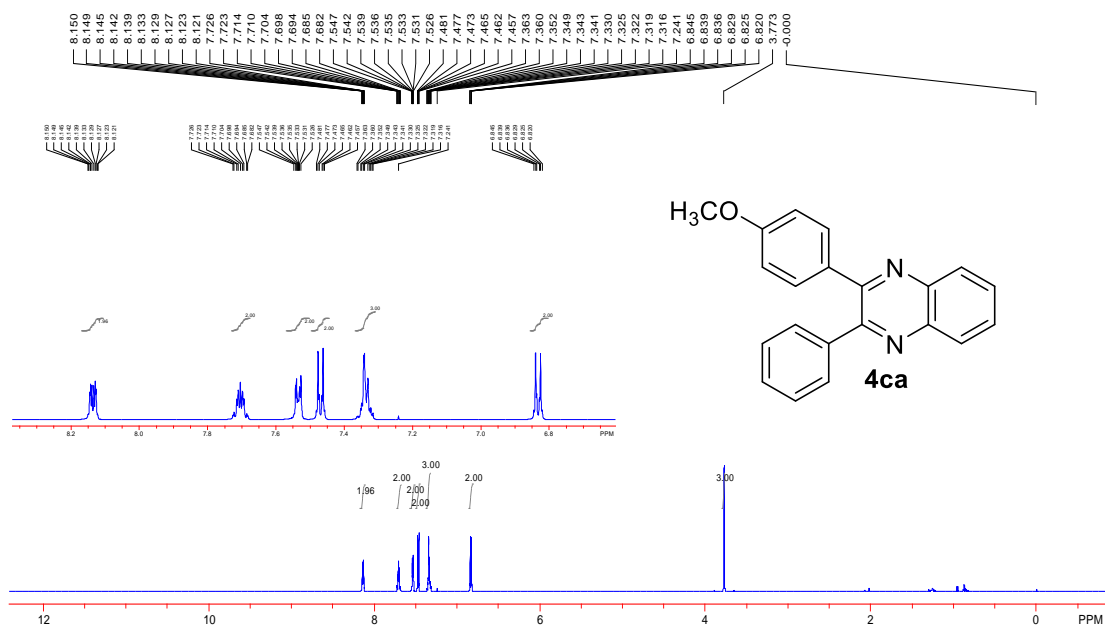
Supplementary Figure 42. ¹³C-NMR spectrum of Compound **4aa** in CDCl₃



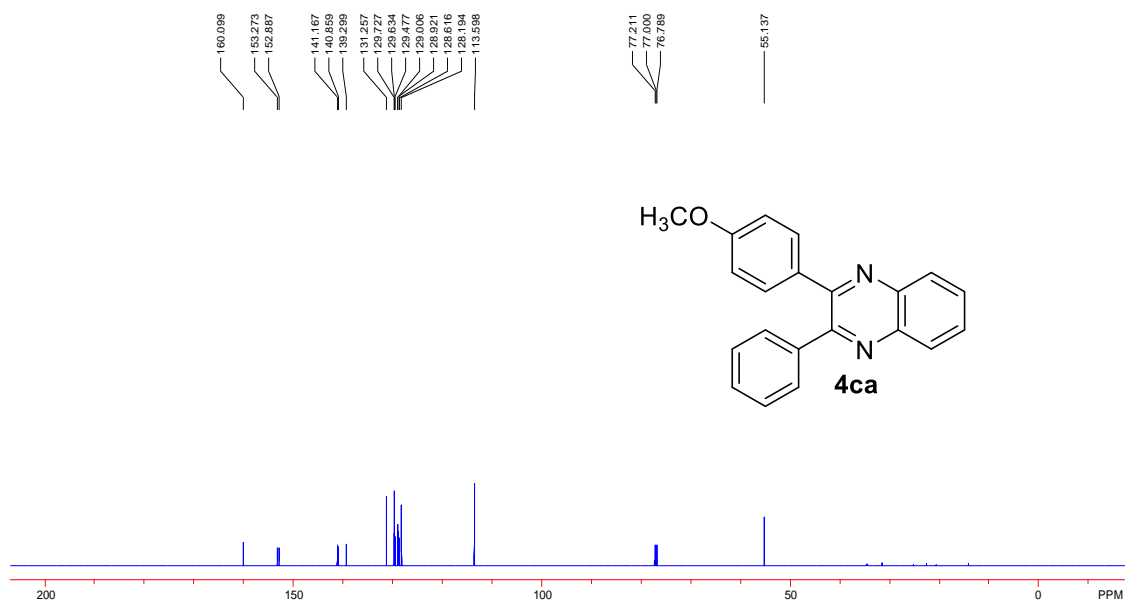
Supplementary Figure 43. ¹H-NMR spectrum of Compound **4ba** in CDCl₃



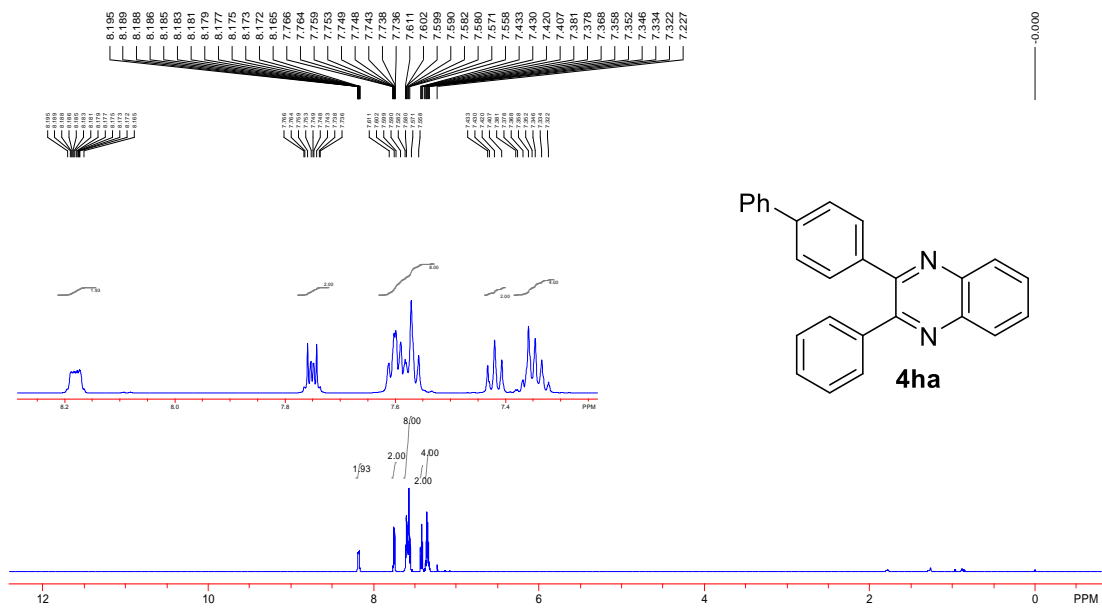
Supplementary Figure 44. ¹³C-NMR spectrum of Compound **4ba** in CDCl₃



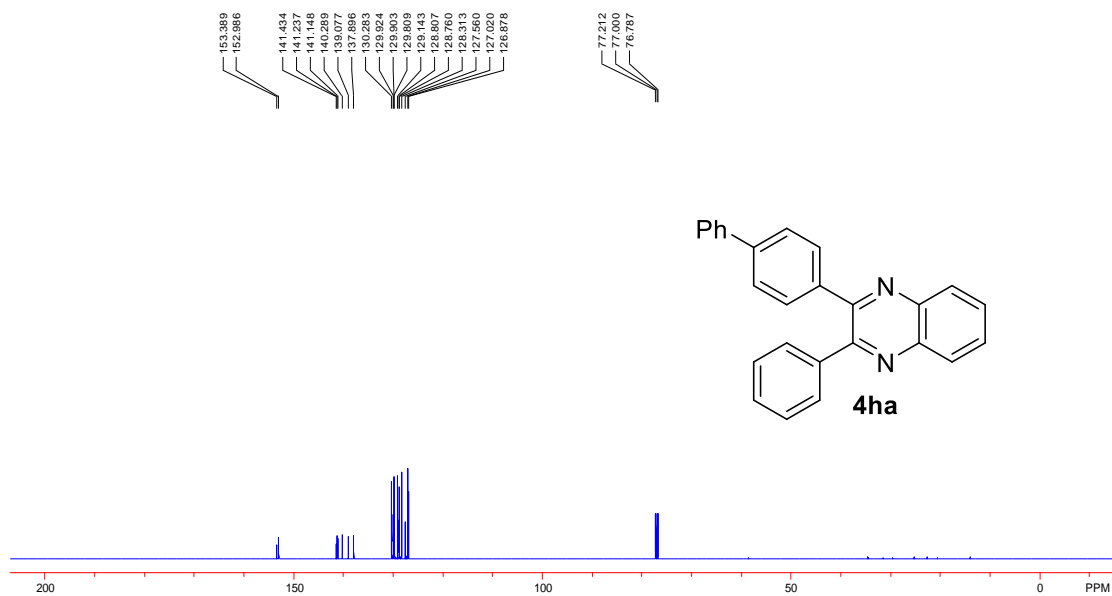
Supplementary Figure 45. ¹H-NMR spectrum of Compound **4ca** in CDCl₃



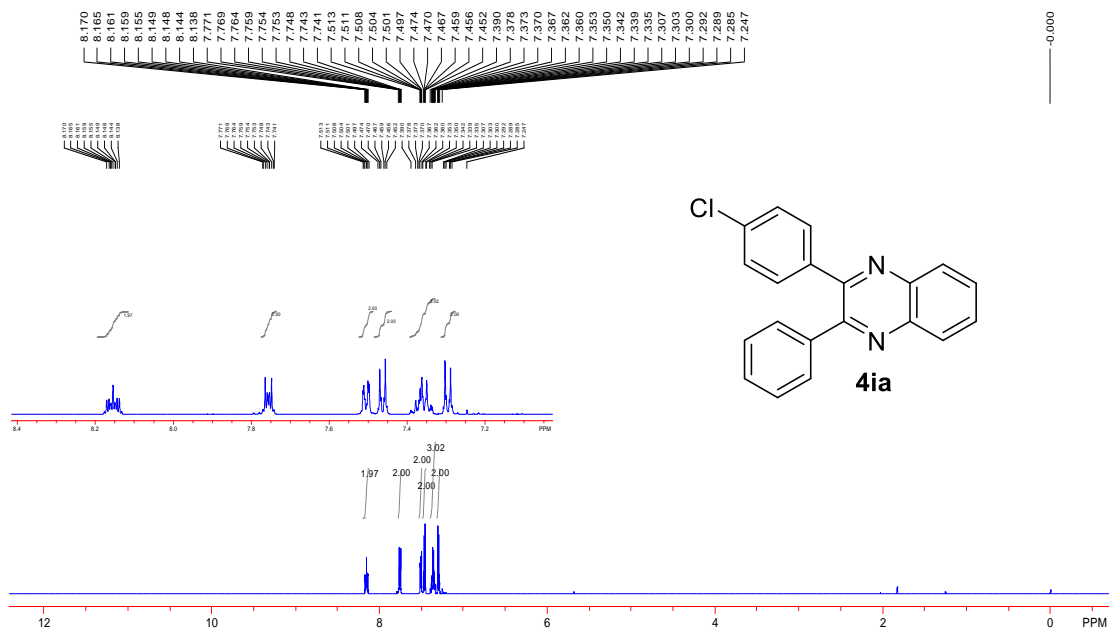
Supplementary Figure 46. ¹³C-NMR spectrum of Compound **4ca** in CDCl₃



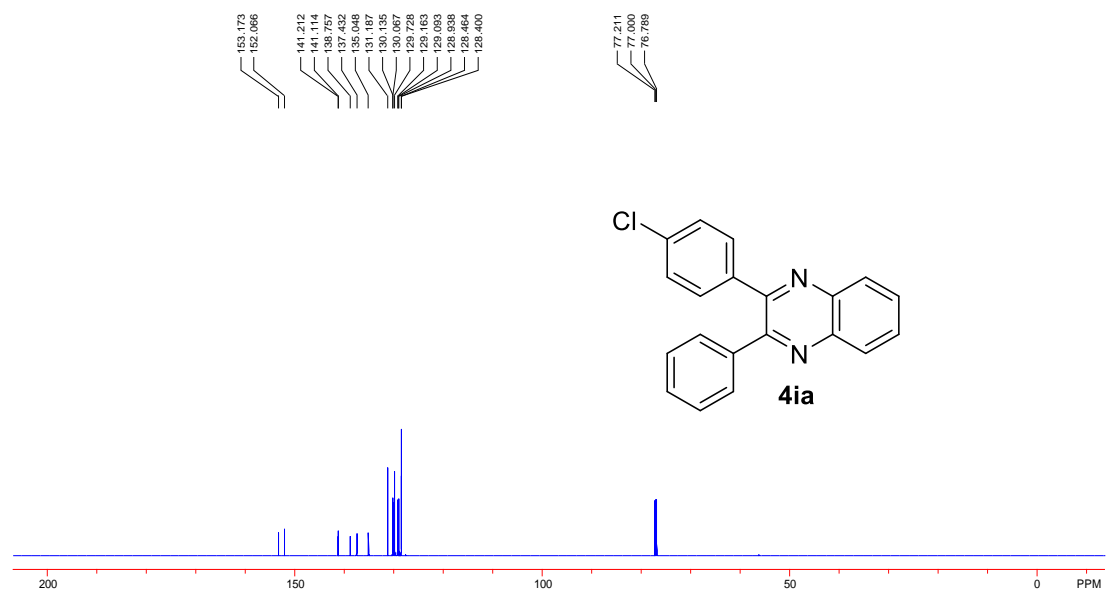
Supplementary Figure 47. ¹H-NMR spectrum of Compound **4ha** in CDCl₃



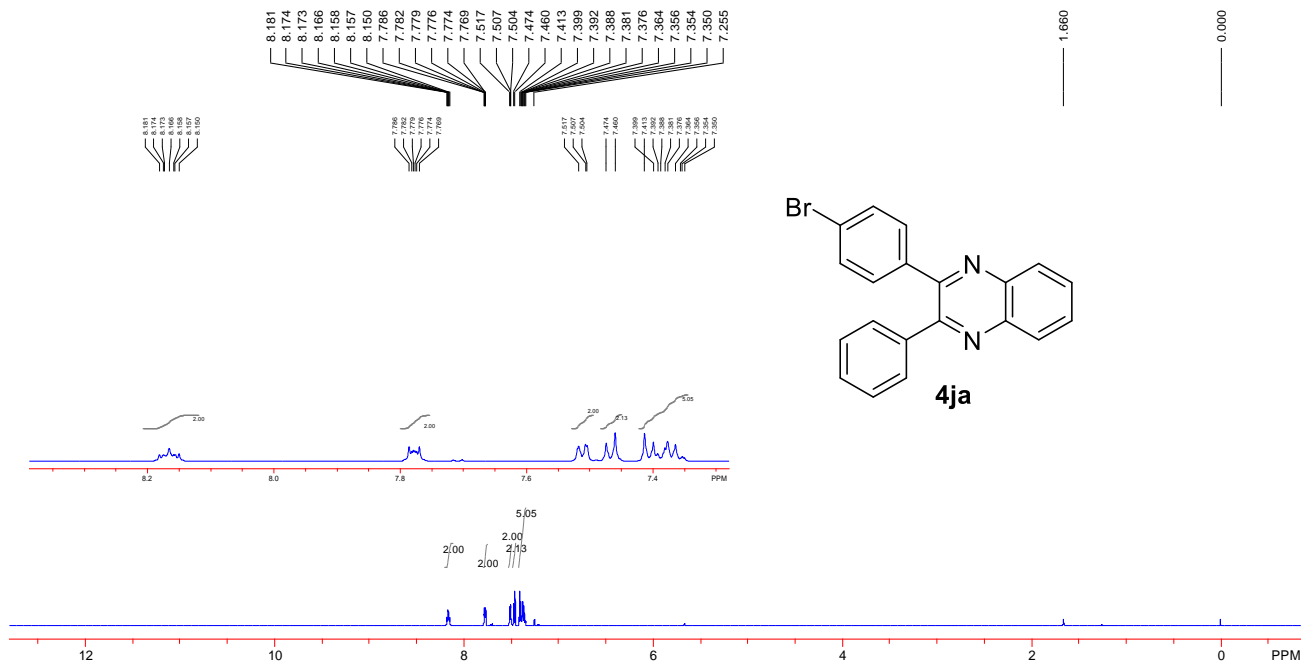
Supplementary Figure 48. ¹³C-NMR spectrum of Compound **4ha** in CDCl₃



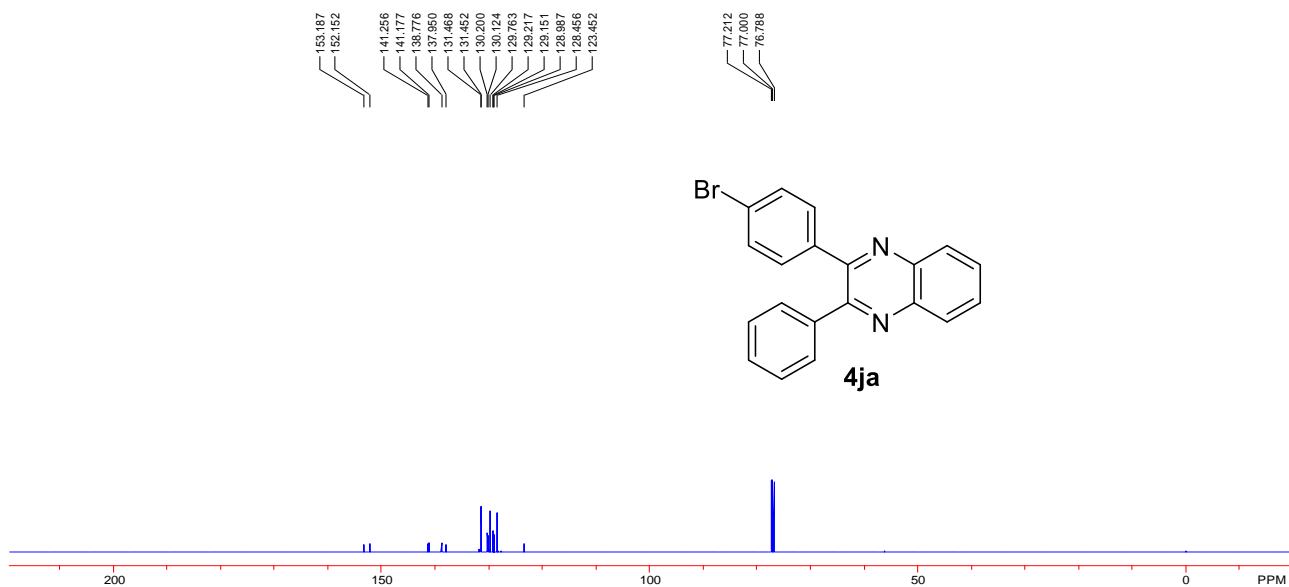
Supplementary Figure 49. ¹H-NMR spectrum of Compound **4ia** in CDCl₃



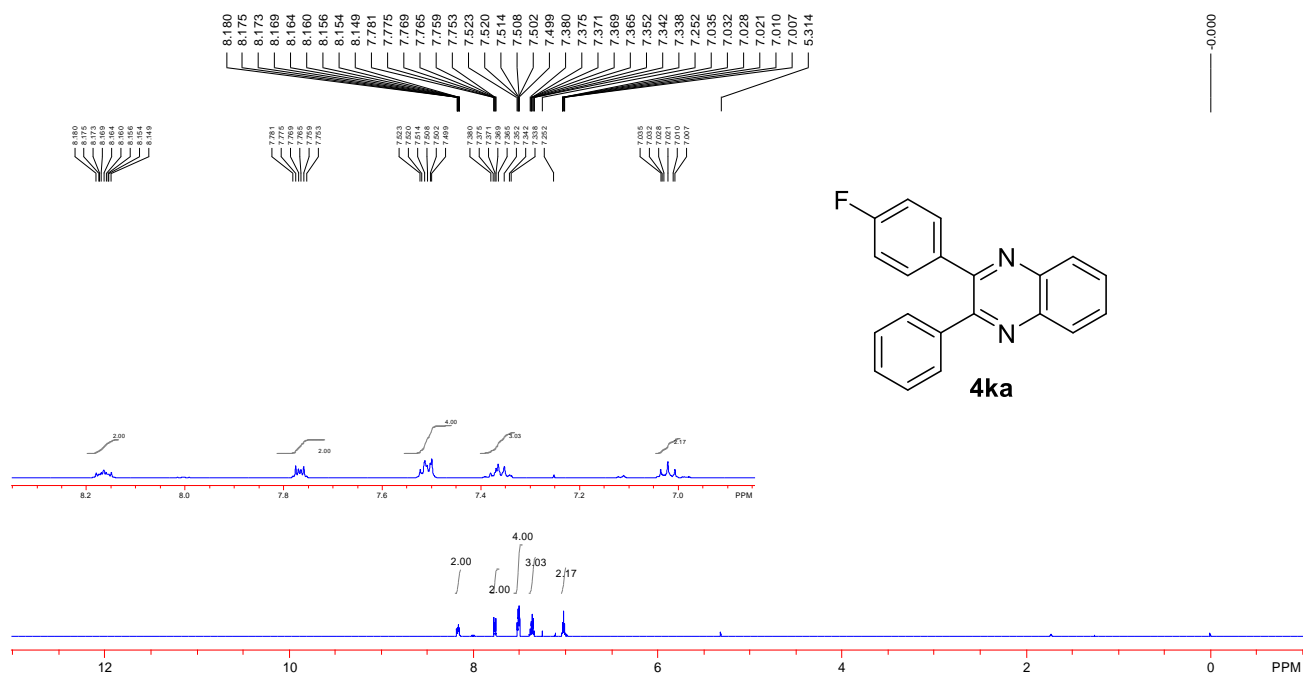
Supplementary Figure 50. ¹³C-NMR spectrum of Compound **4ia** in CDCl₃



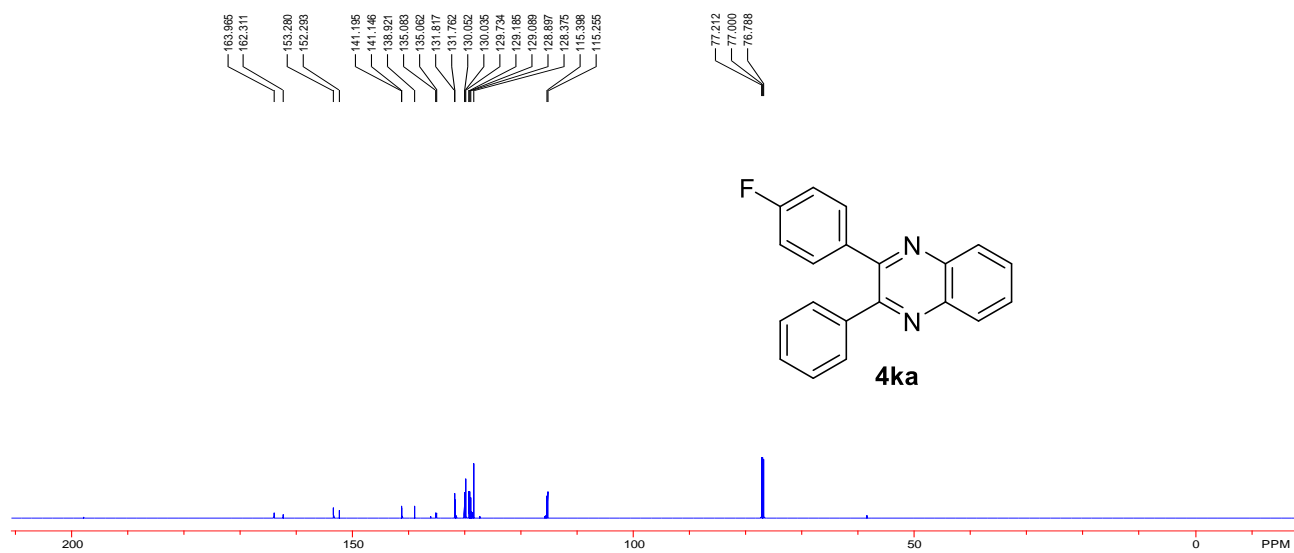
Supplementary Figure 51. ¹H-NMR spectrum of Compound 4ja in CDCl₃



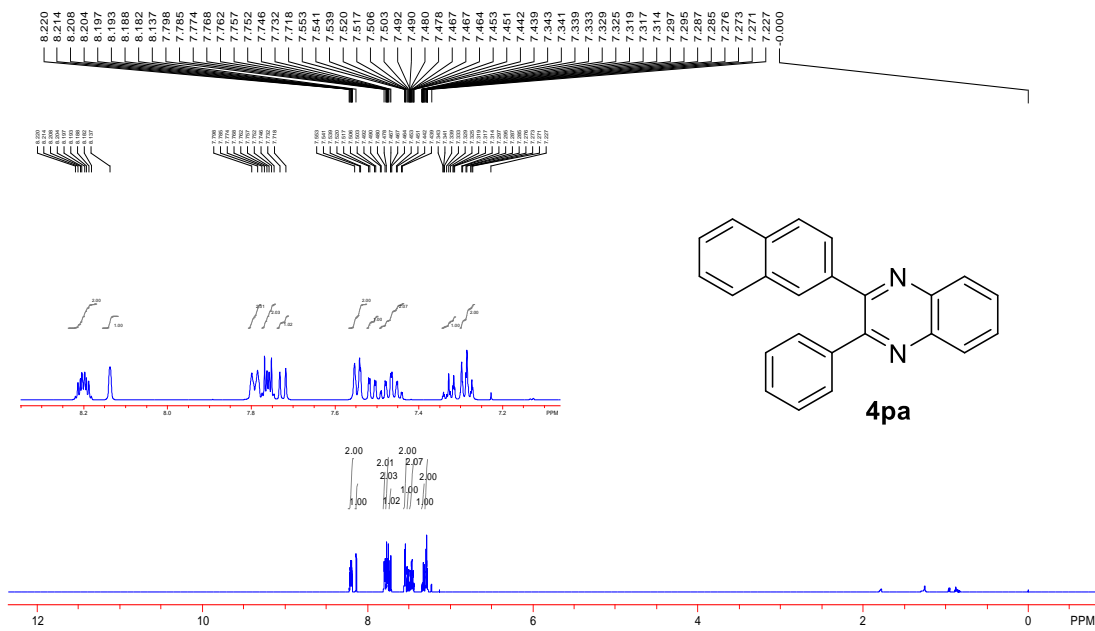
Supplementary Figure 52. ¹³C-NMR spectrum of Compound 4ja in CDCl₃



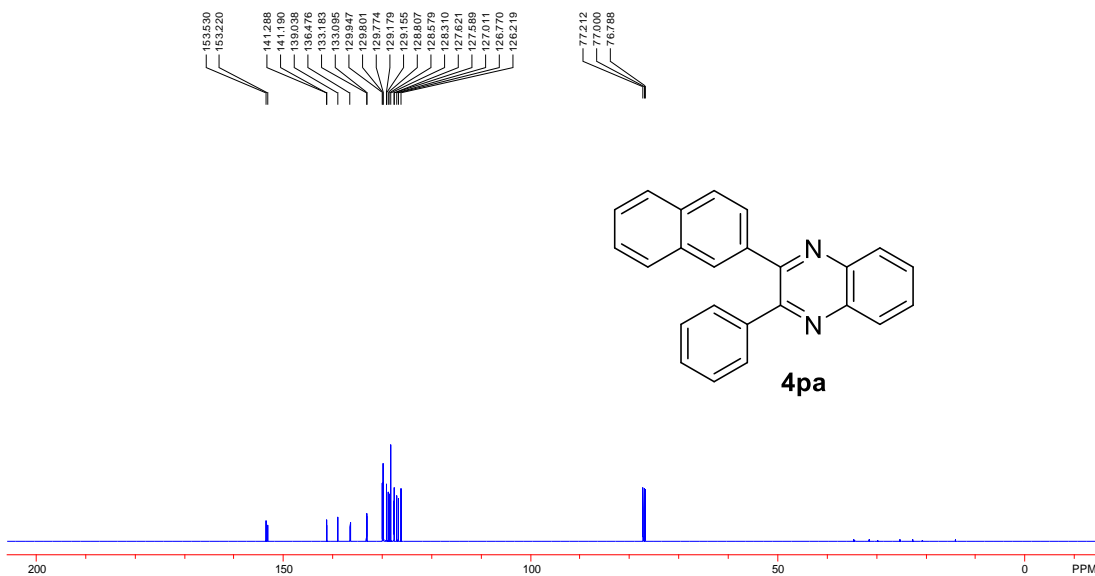
Supplementary Figure 53. ¹H-NMR spectrum of Compound **4ka** in CDCl₃



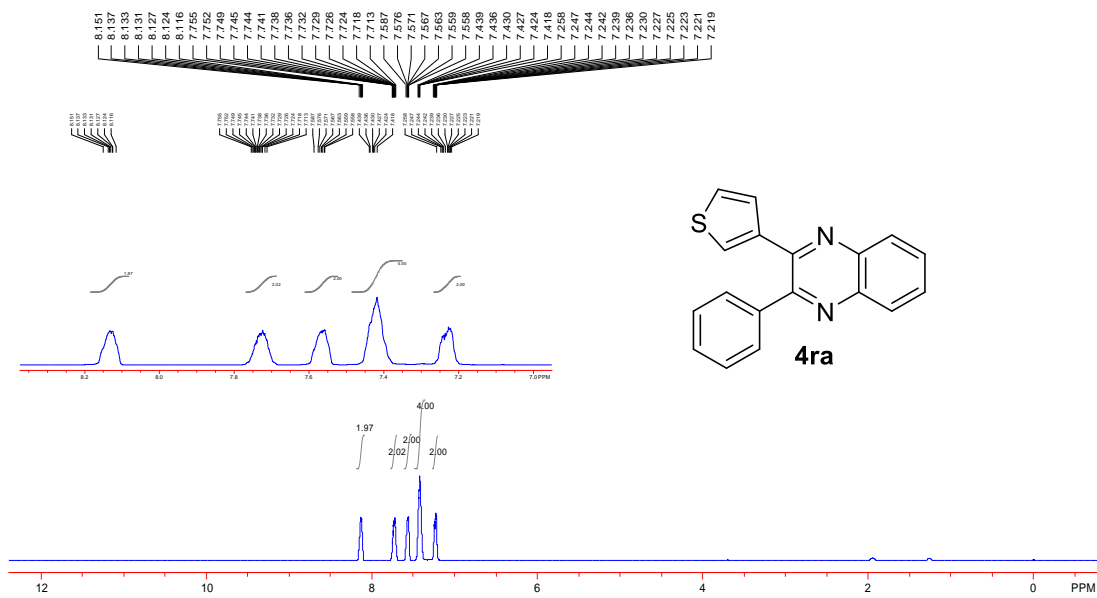
Supplementary Figure 54. ¹³C-NMR spectrum of Compound **4ka** in CDCl₃



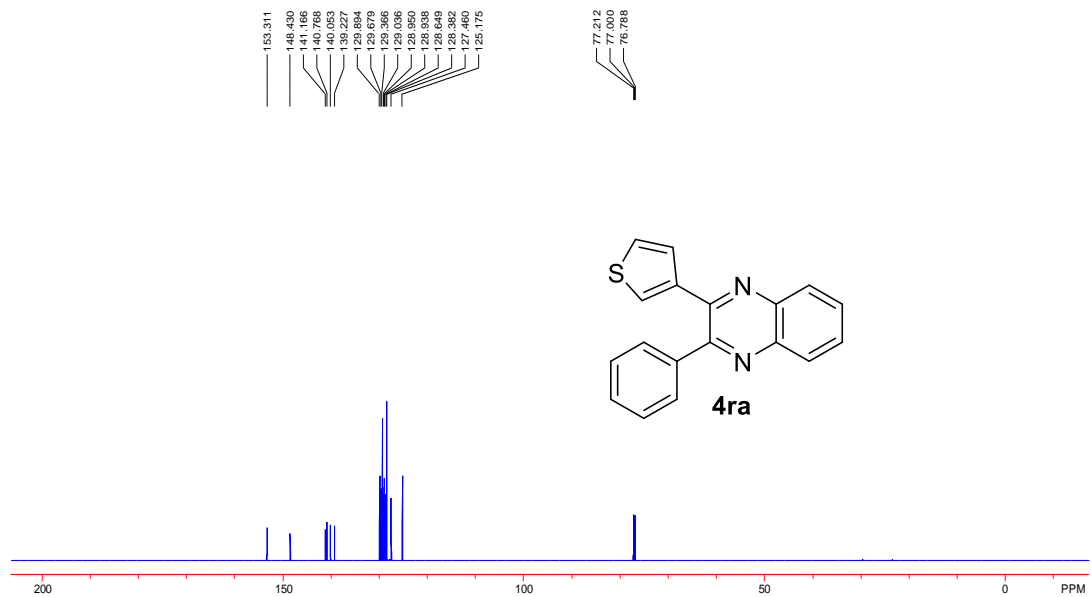
Supplementary Figure 55. ¹H-NMR spectrum of Compound **4pa** in CDCl₃



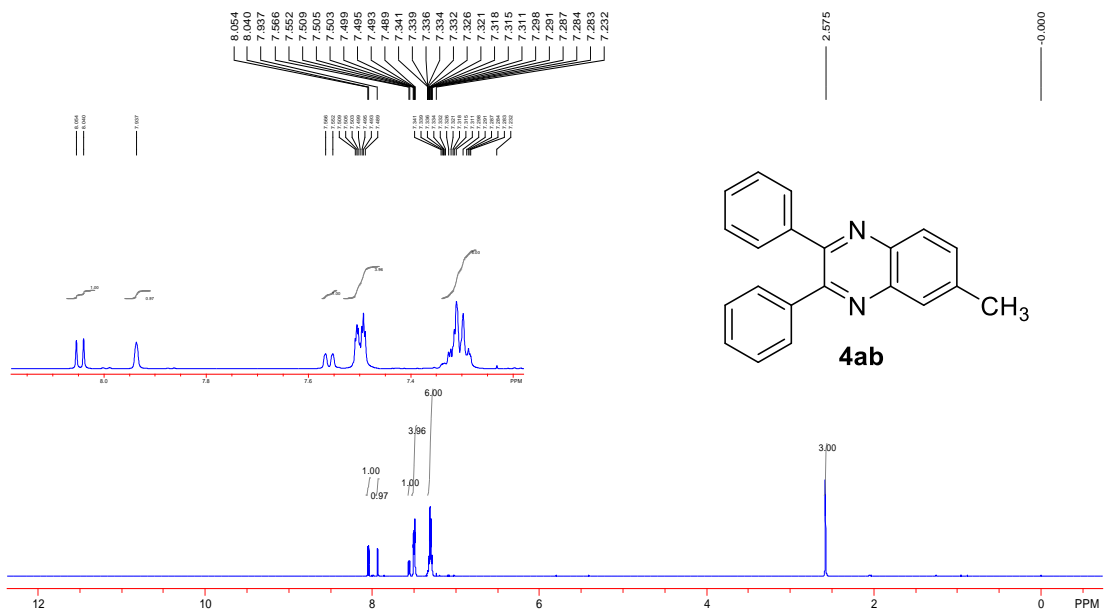
Supplementary Figure 56. ¹³C-NMR spectrum of Compound **4pa** in CDCl₃



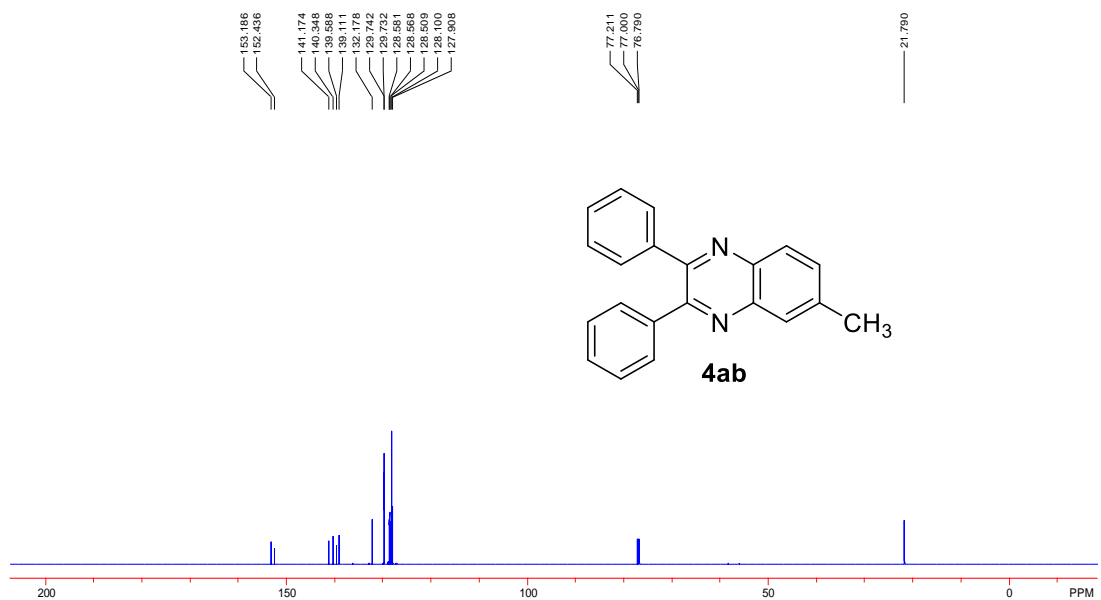
Supplementary Figure 57. ¹H-NMR spectrum of Compound **4ra** in CDCl₃



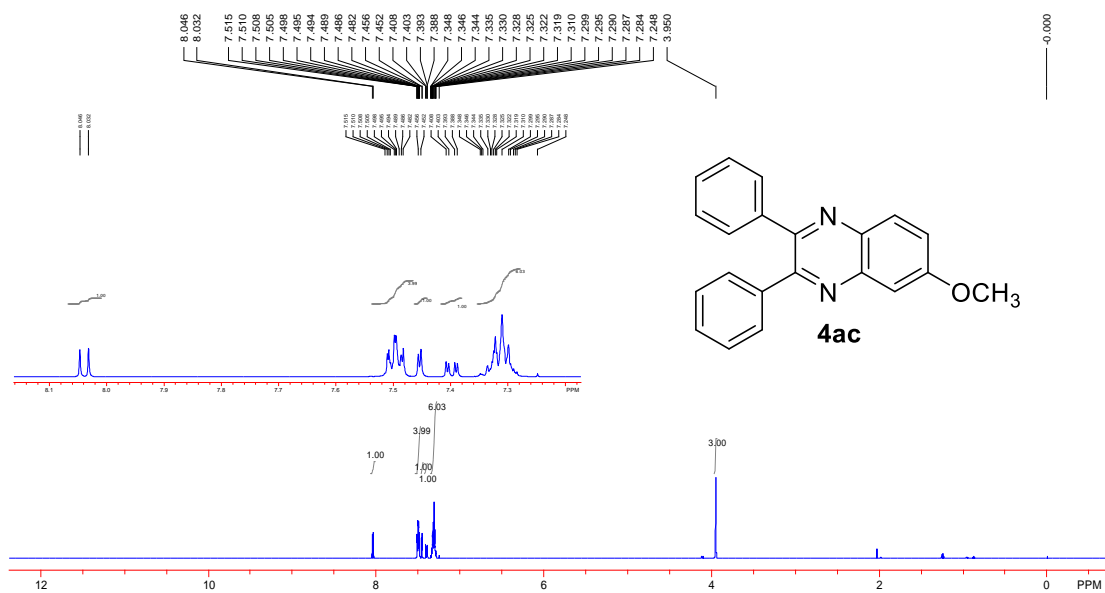
Supplementary Figure 58. ¹³C-NMR spectrum of Compound **4ra** in CDCl₃



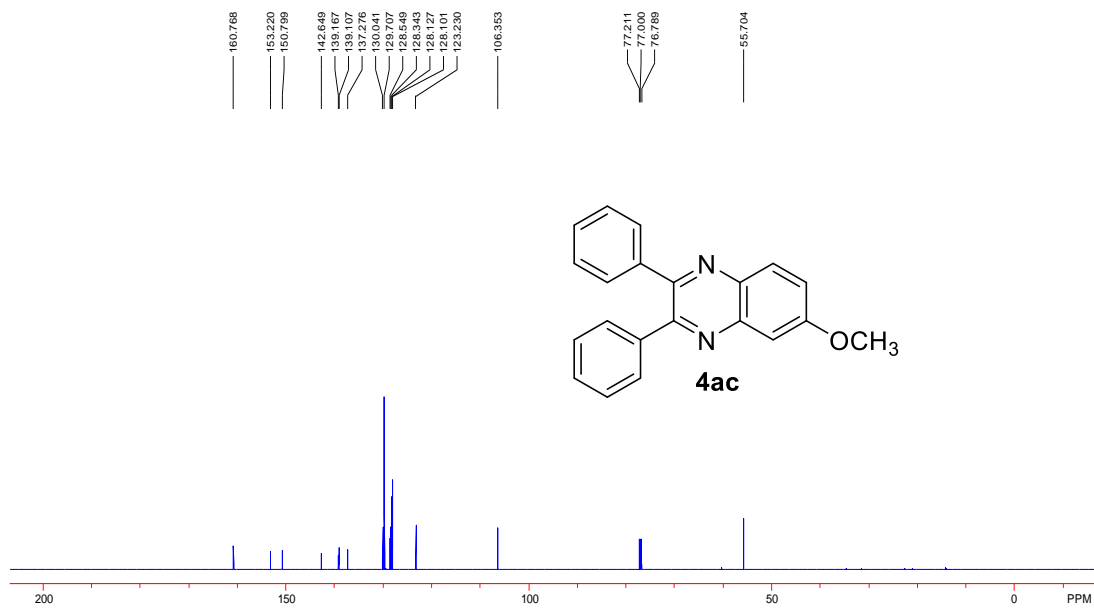
Supplementary Figure 59. ¹H-NMR spectrum of Compound **4ab** in CDCl₃



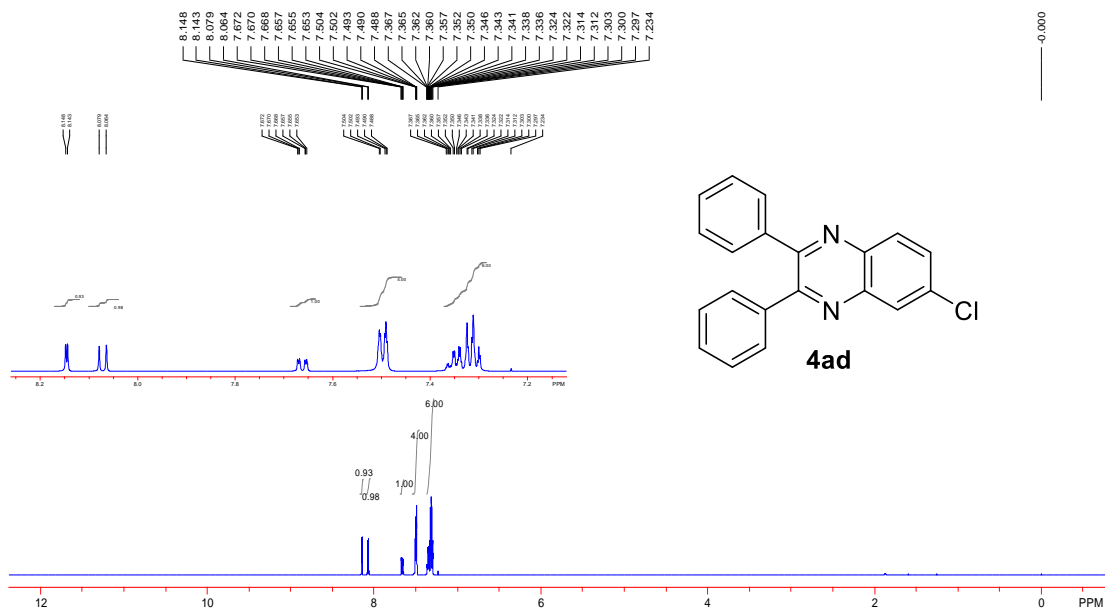
Supplementary Figure 60. ¹³C-NMR spectrum of Compound **4ab** in CDCl₃



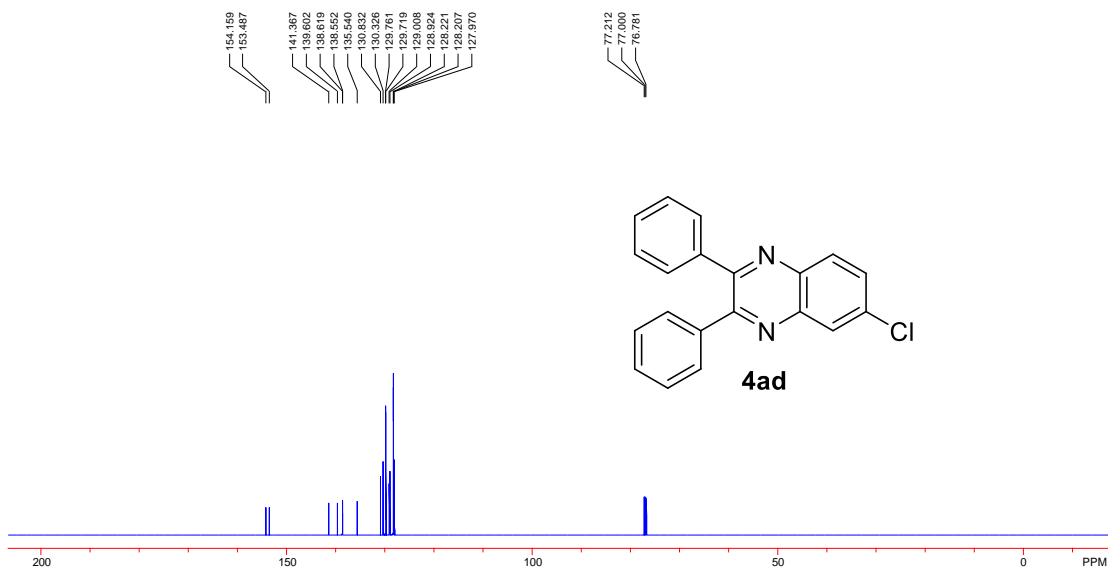
Supplementary Figure 61. ¹H-NMR spectrum of Compound **4ac** in CDCl₃



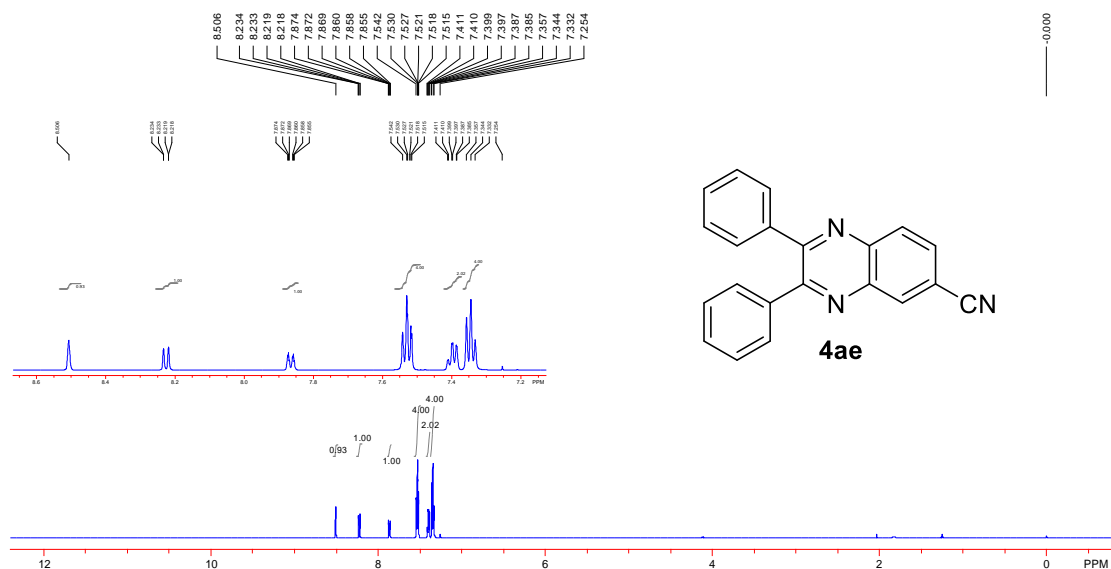
Supplementary Figure 62. ¹³C-NMR spectrum of Compound **4ac** in CDCl₃



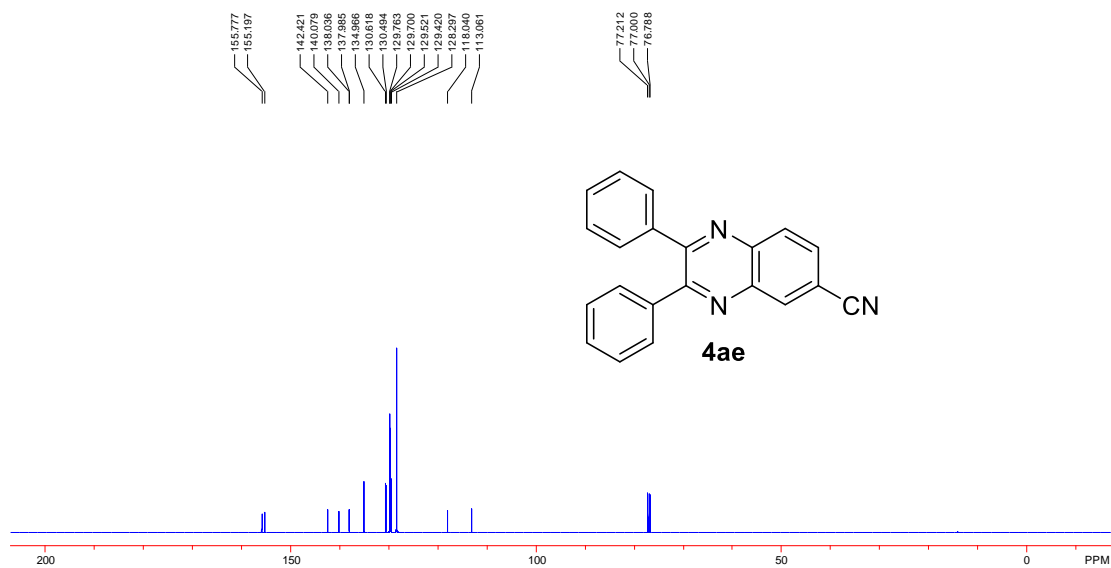
Supplementary Figure 63. ¹H-NMR spectrum of Compound **4ad** in CDCl₃



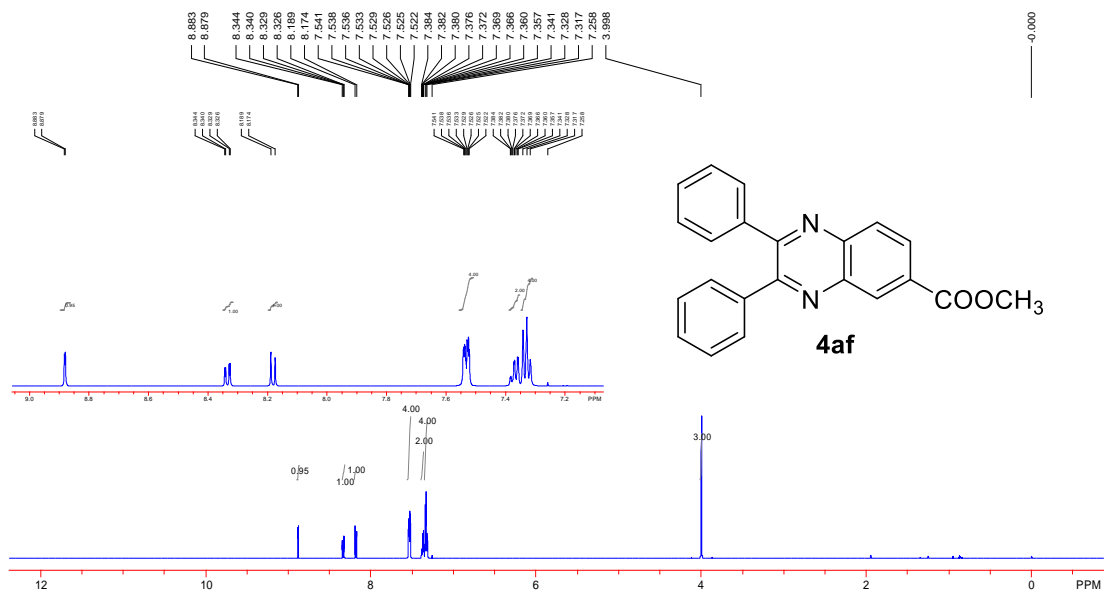
Supplementary Figure 64. ¹³C-NMR spectrum of Compound **4ad** in CDCl₃



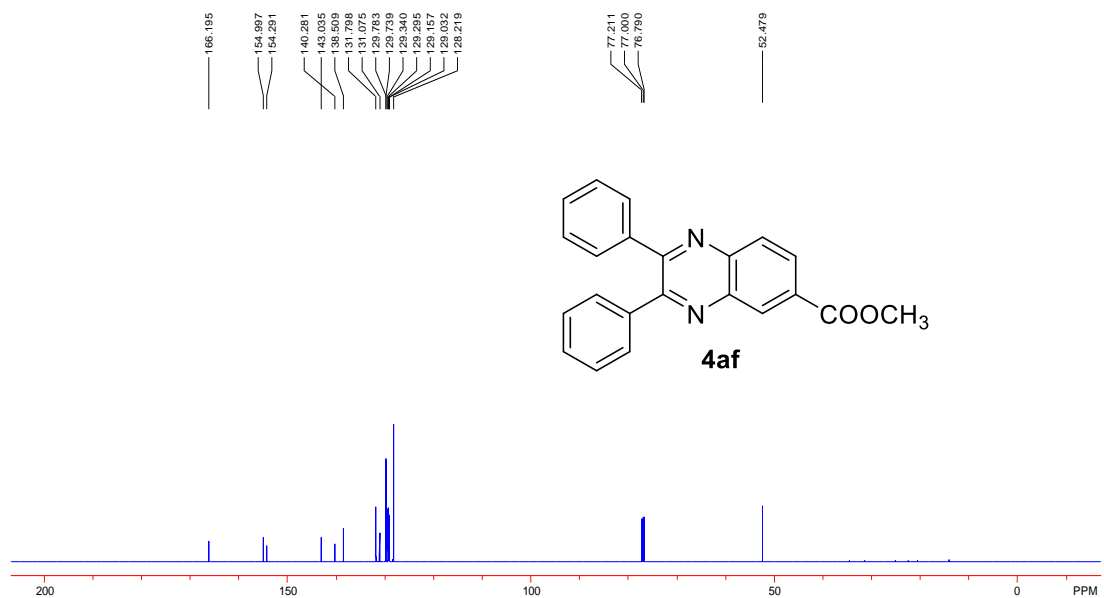
Supplementary Figure 65. ¹H-NMR spectrum of Compound **4ae** in CDCl₃



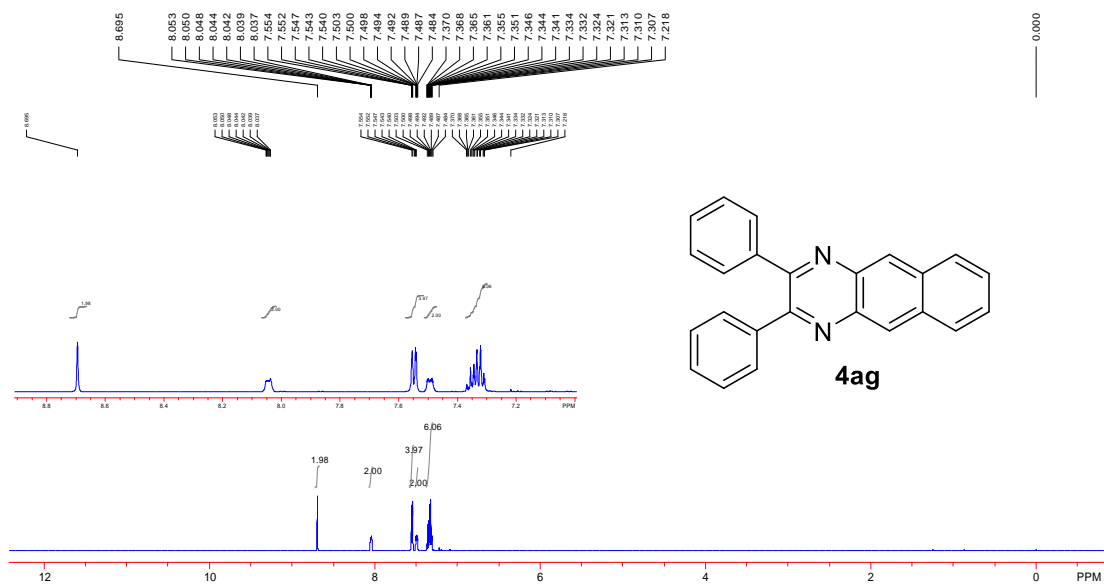
Supplementary Figure 66. ¹³C-NMR spectrum of Compound **4ae** in CDCl₃



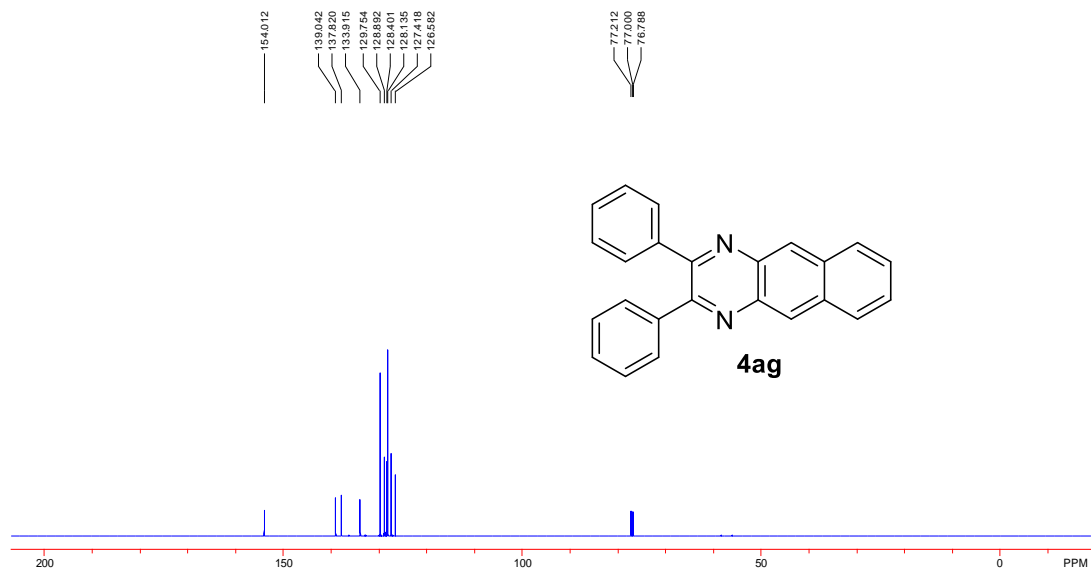
Supplementary Figure 67. ¹H-NMR spectrum of Compound **4af** in CDCl₃



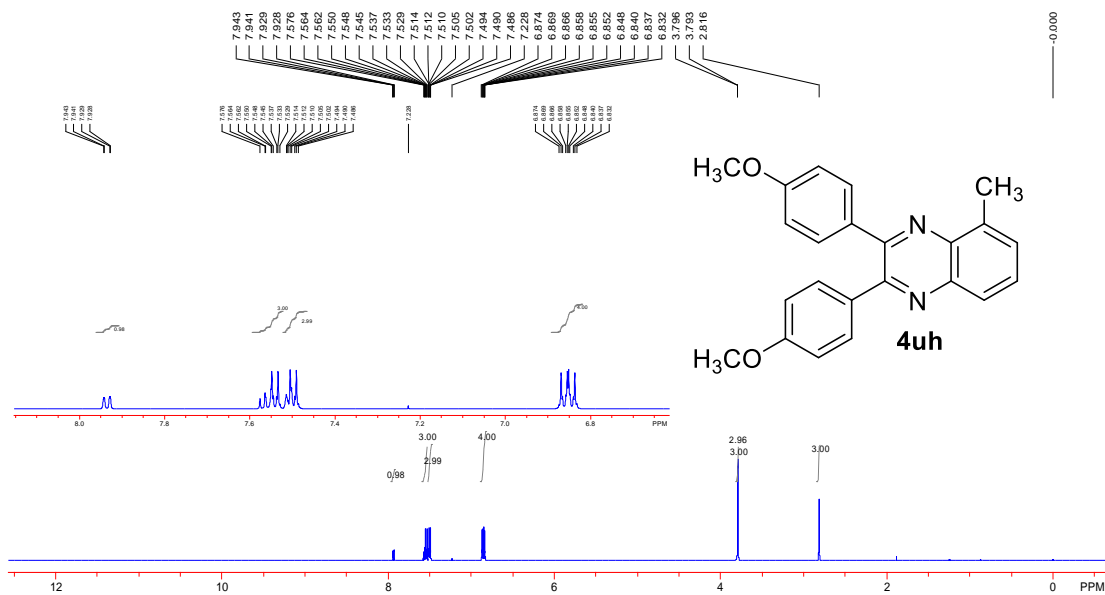
Supplementary Figure 68. ¹³C-NMR spectrum of Compound **4af** in CDCl₃



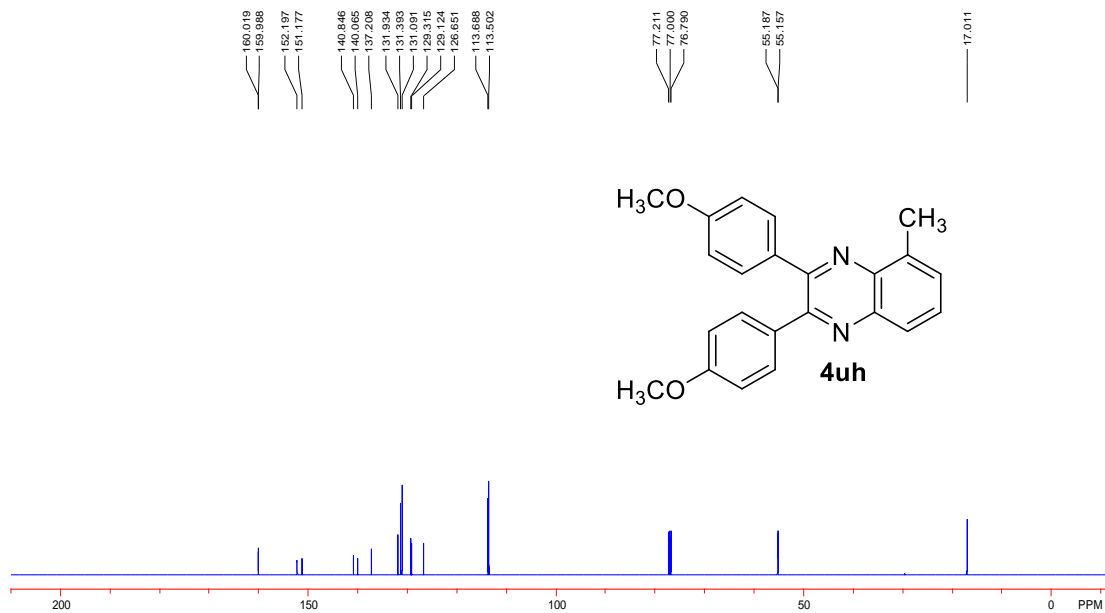
Supplementary Figure 69. ¹H-NMR spectrum of Compound **4ag** in CDCl₃



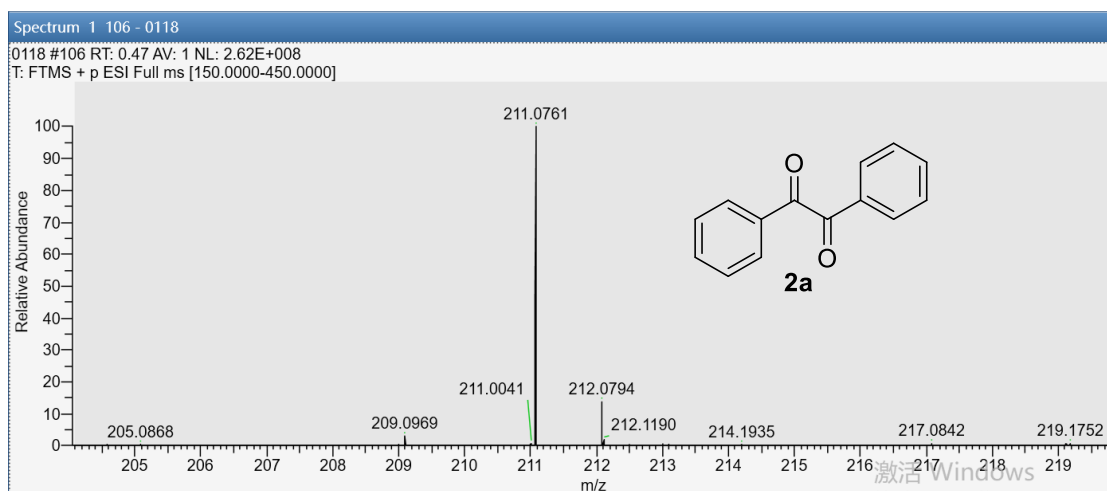
Supplementary Figure 70. ¹³C-NMR spectrum of Compound **4ag** in CDCl₃



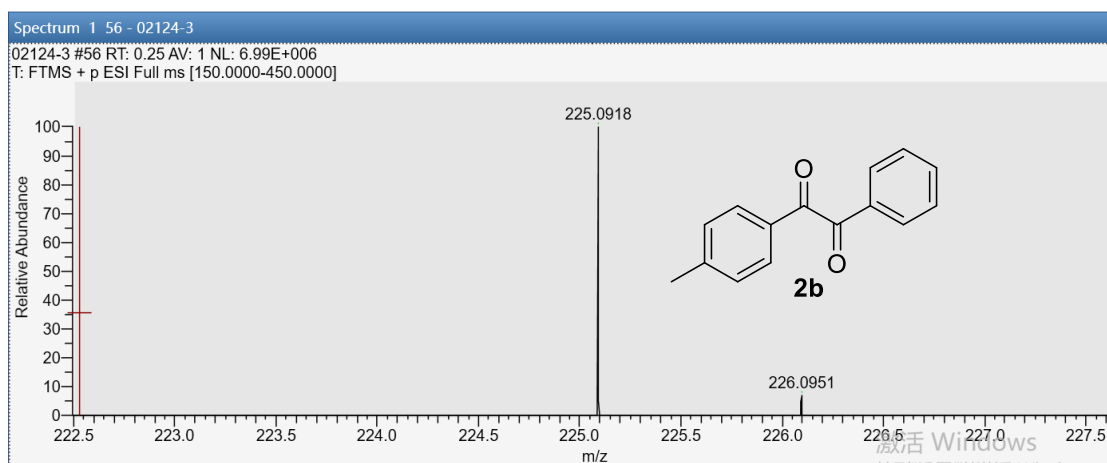
Supplementary Figure 73. ¹H-NMR spectrum of Compound **4uh** in CDCl₃



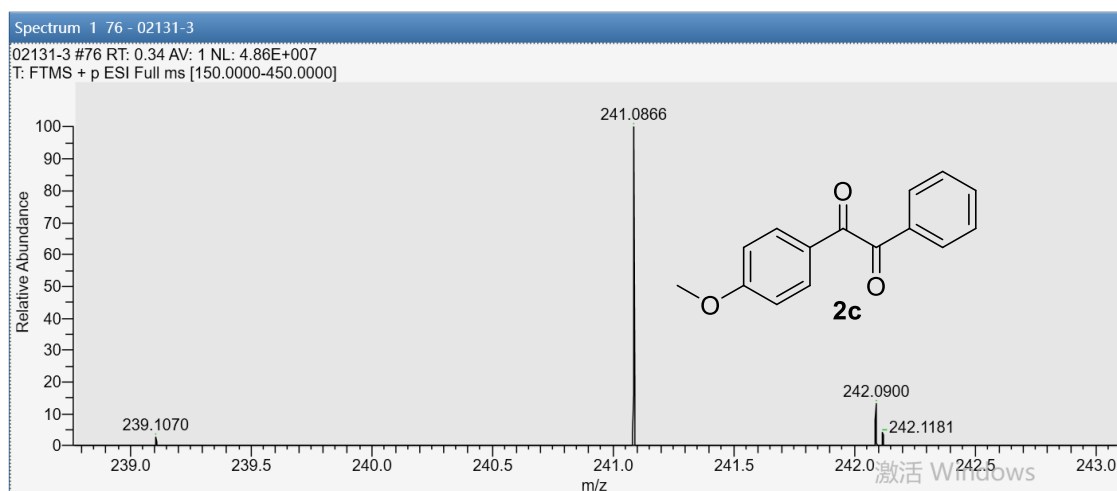
Supplementary Figure 74. ¹³C-NMR spectrum of Compound **4uh** in CDCl₃



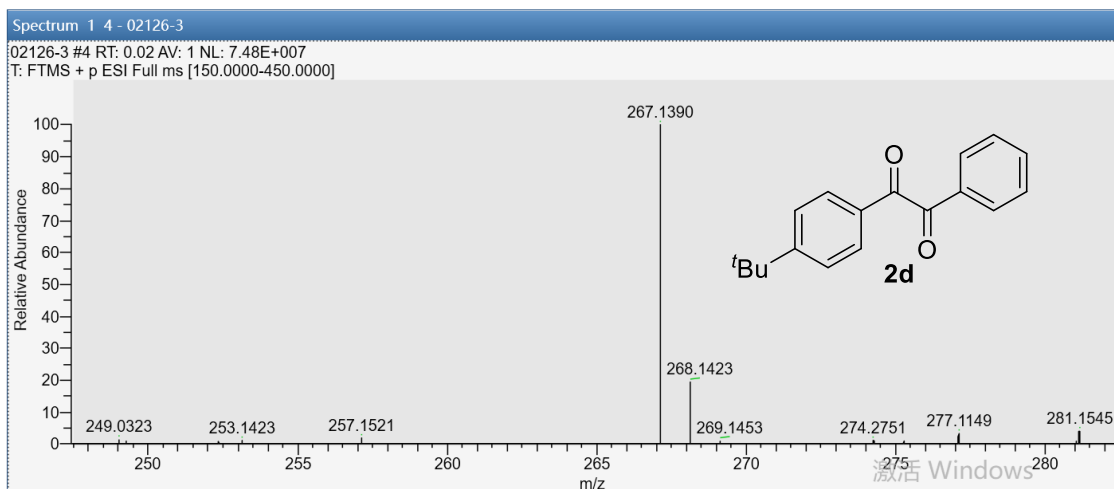
Supplementary Figure 75. HRMS spectrum of Compound **2a**.



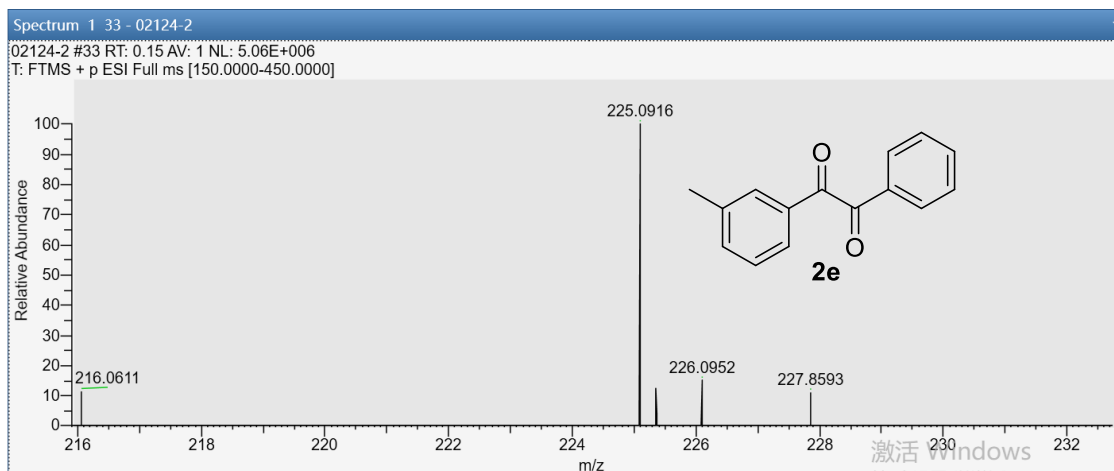
Supplementary Figure 76. HRMS spectrum of Compound **2b**.



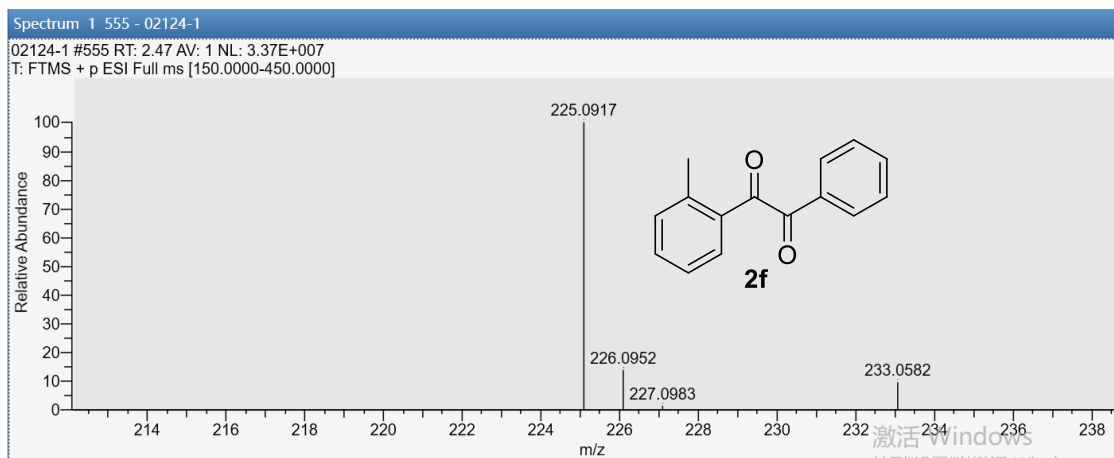
Supplementary Figure 77. HRMS spectrum of Compound **2c**.



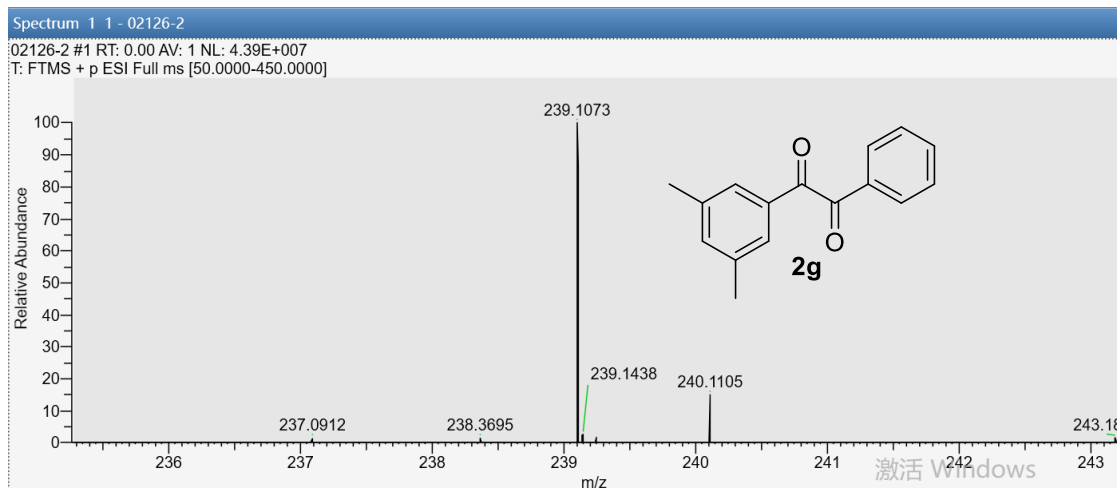
Supplementary Figure 78. HRMS spectrum of Compound 2d.



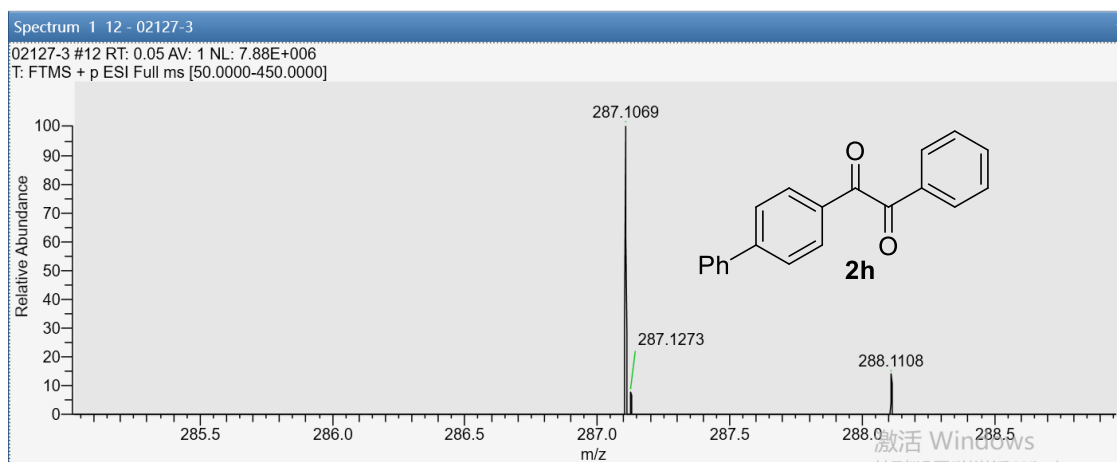
Supplementary Figure 79. HRMS spectrum of Compound 2e.



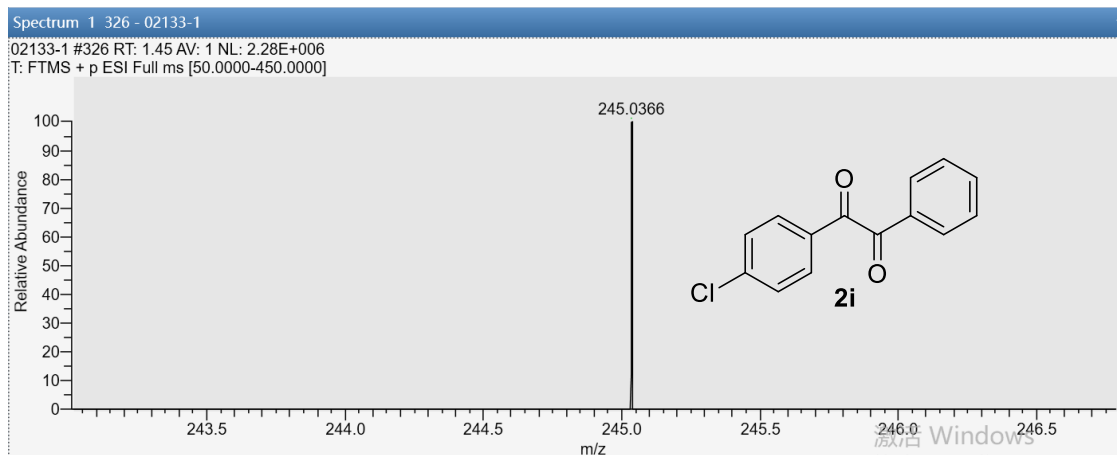
Supplementary Figure 80. HRMS spectrum of Compound 2f.



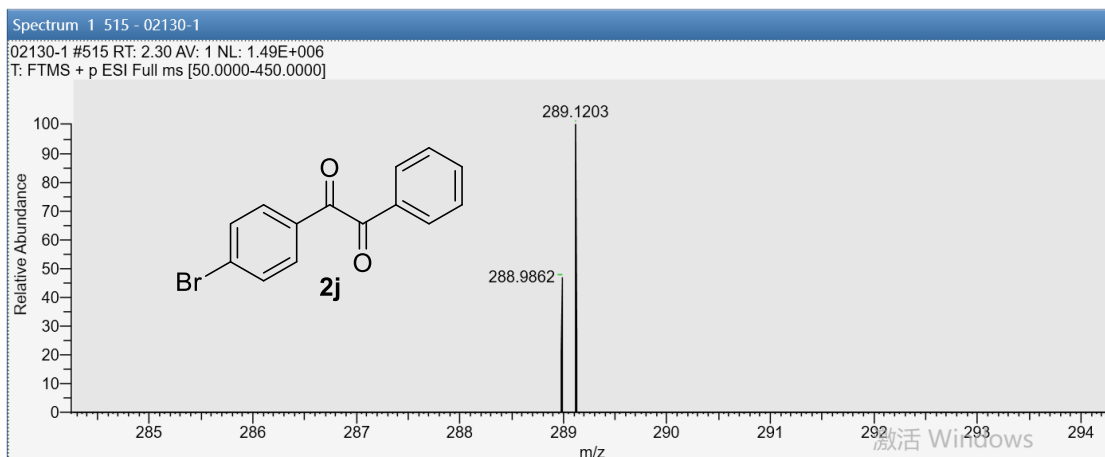
Supplementary Figure 81. HRMS spectrum of Compound **2g**.



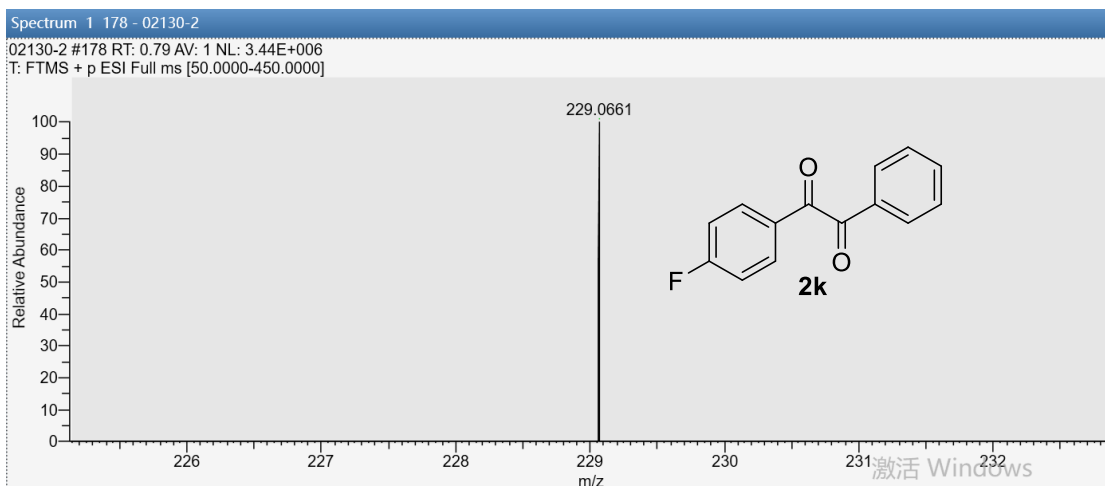
Supplementary Figure 82. HRMS spectrum of Compound **2h**.



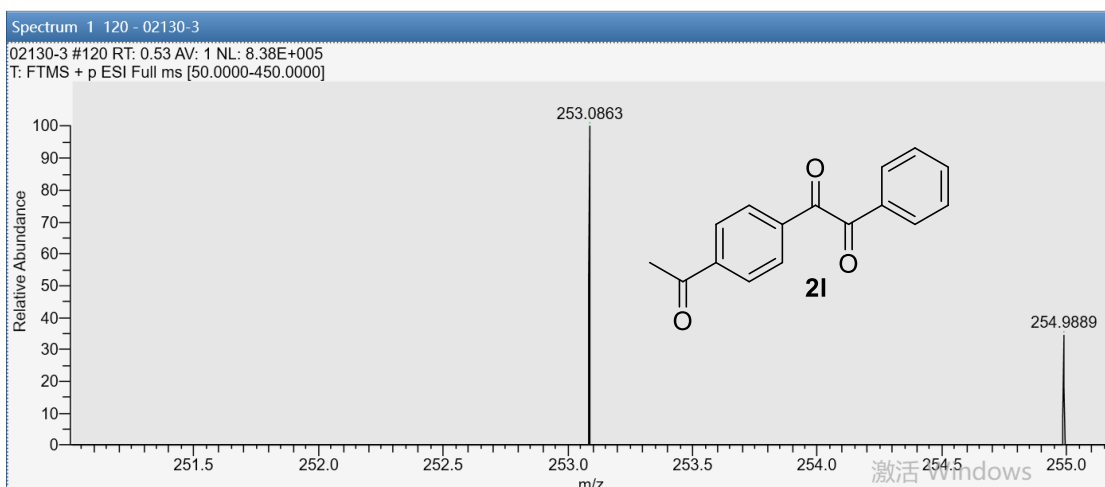
Supplementary Figure 83. HRMS spectrum of Compound **2i**.



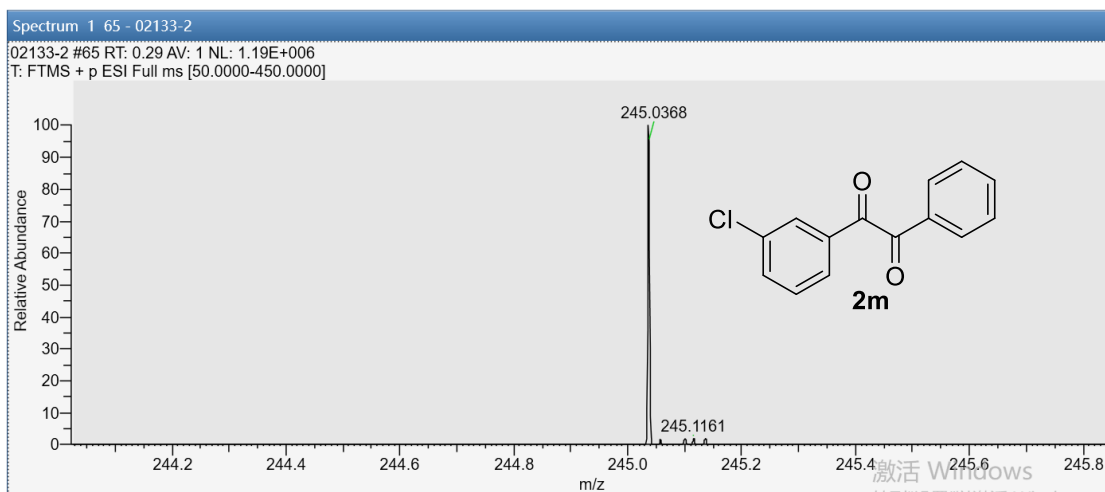
Supplementary Figure 84. HRMS spectrum of Compound **2j**.



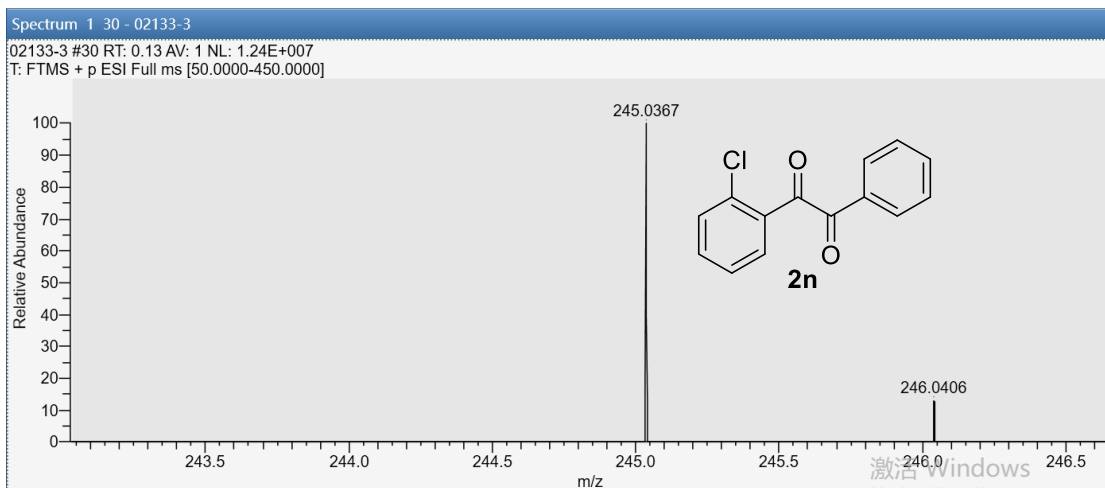
Supplementary Figure 85. HRMS spectrum of Compound **2k**.



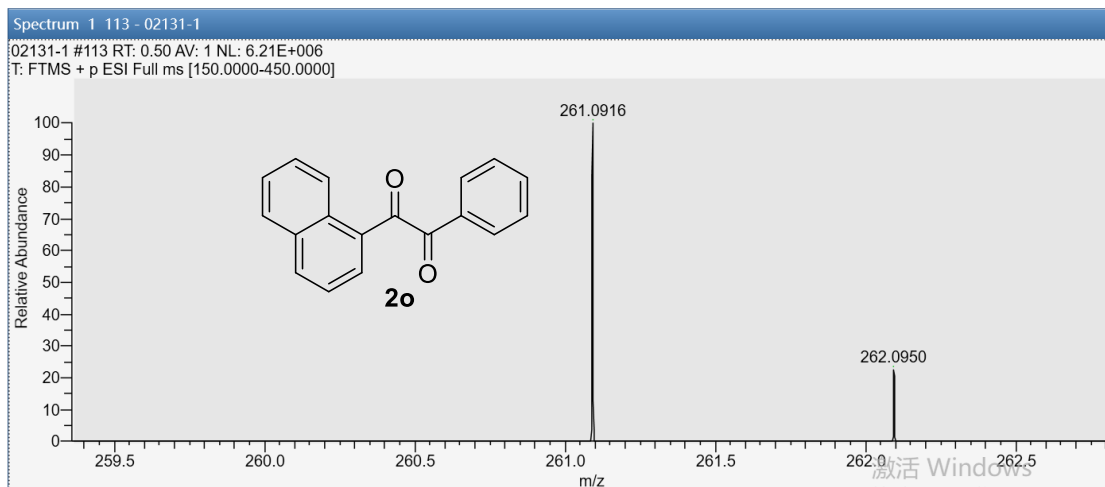
Supplementary Figure 86. HRMS spectrum of Compound **2l**.



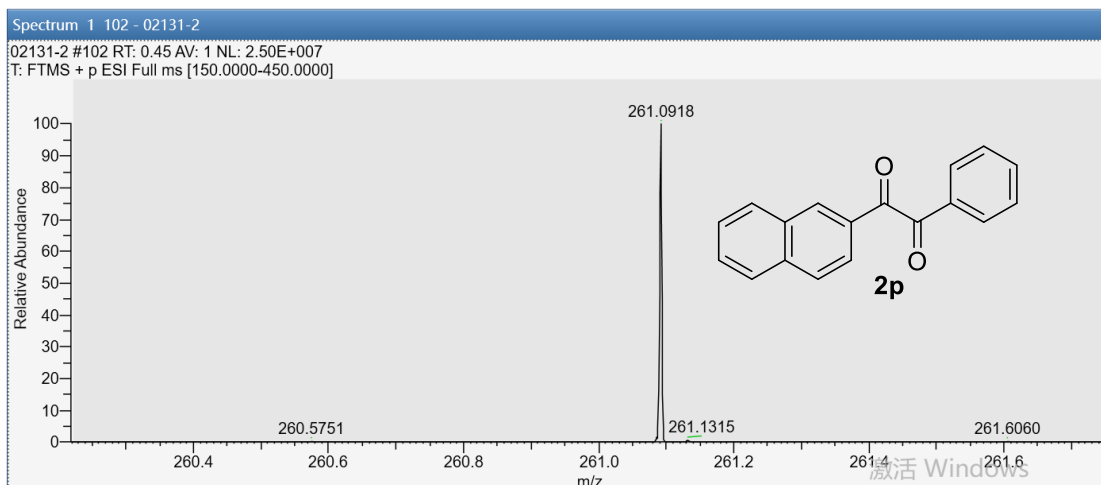
Supplementary Figure 87. HRMS spectrum of Compound **2m**.



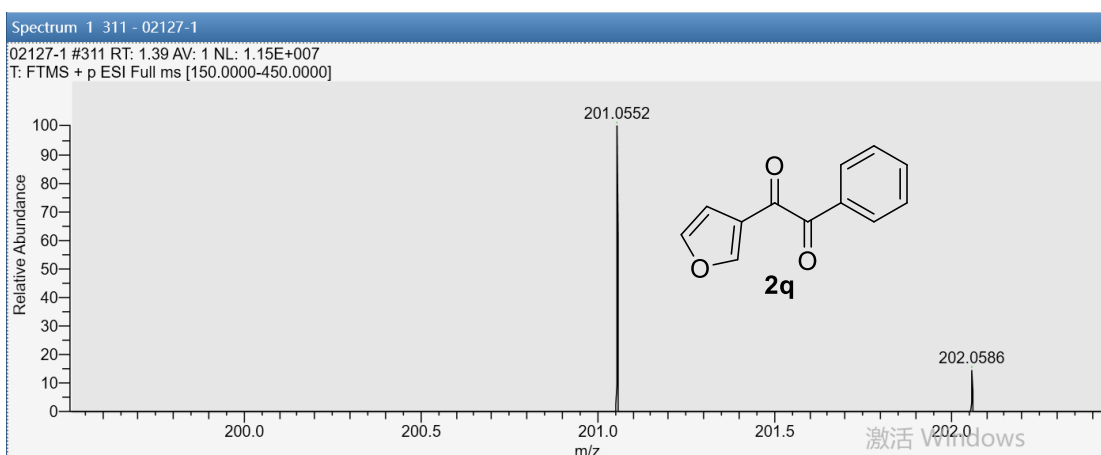
Supplementary Figure 88. HRMS spectrum of Compound **2n**.



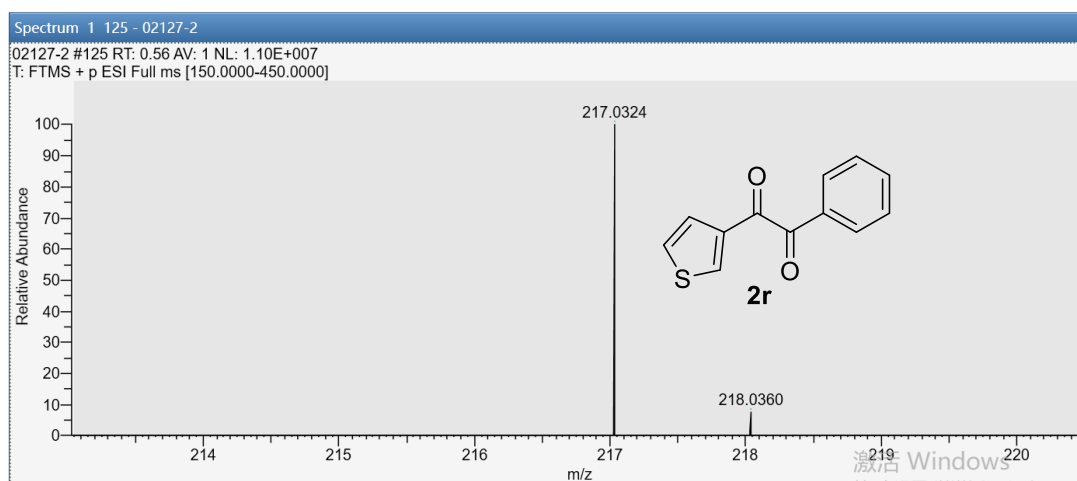
Supplementary Figure 89. HRMS spectrum of Compound **2o**.



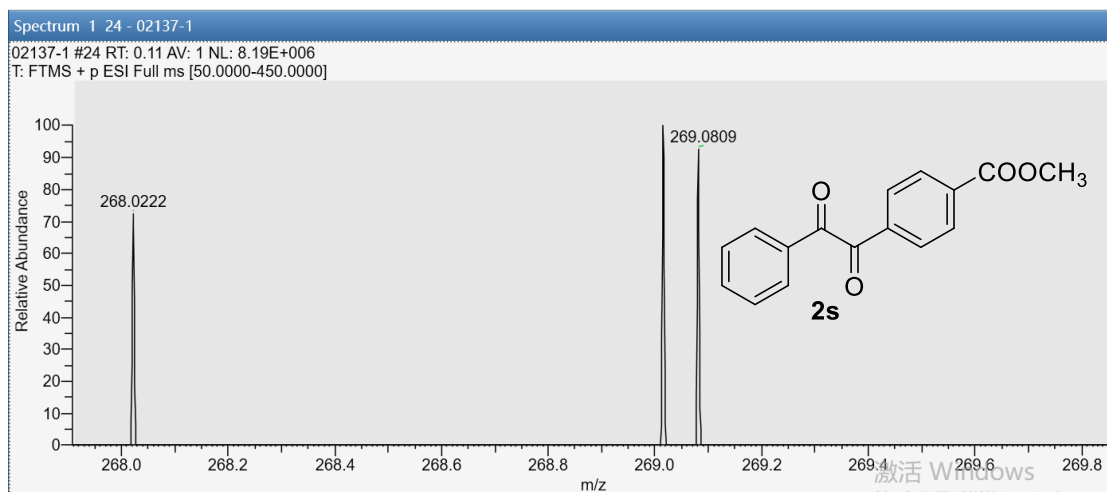
Supplementary Figure 90. HRMS spectrum of Compound **2p**.



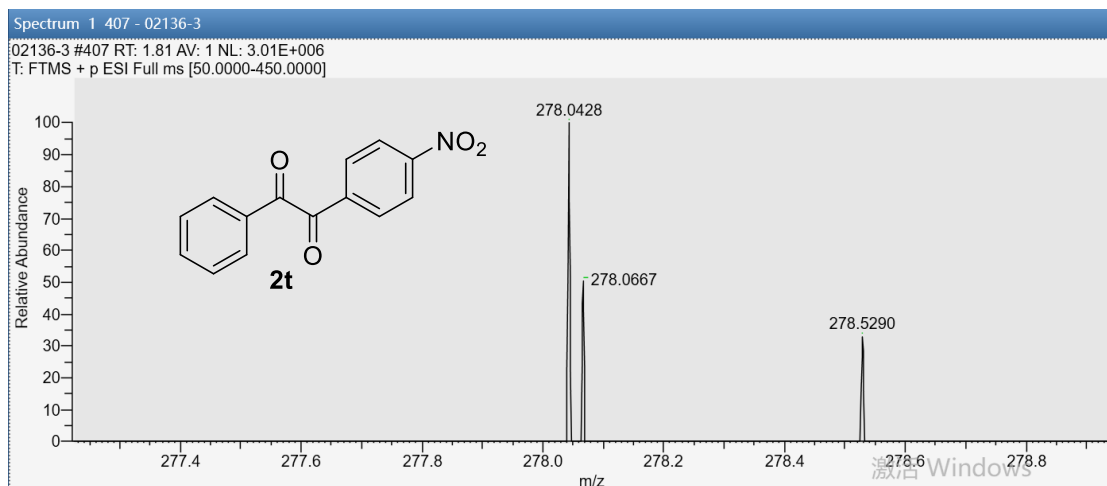
Supplementary Figure 91. HRMS spectrum of Compound **2q**.



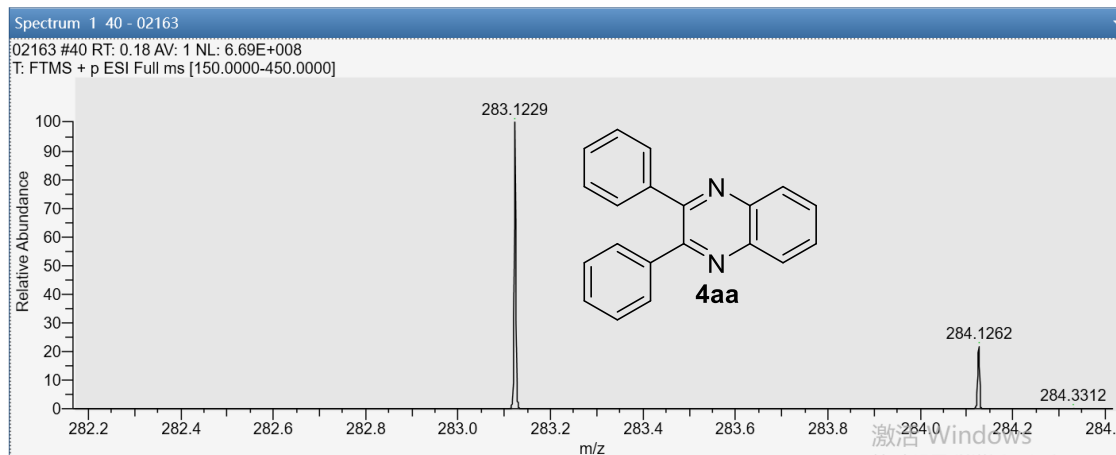
Supplementary Figure 92. HRMS spectrum of Compound **2r**.



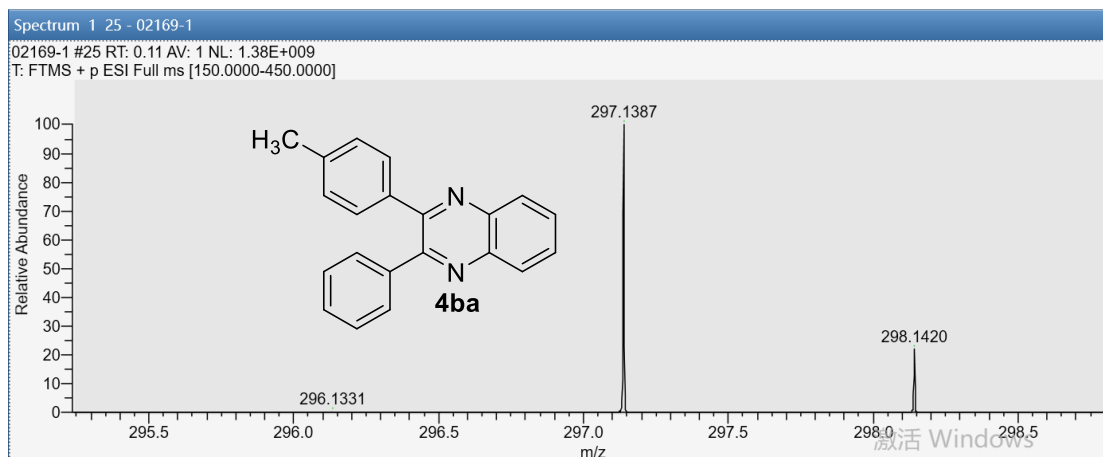
Supplementary Figure 93. HRMS spectrum of Compound **2s**.



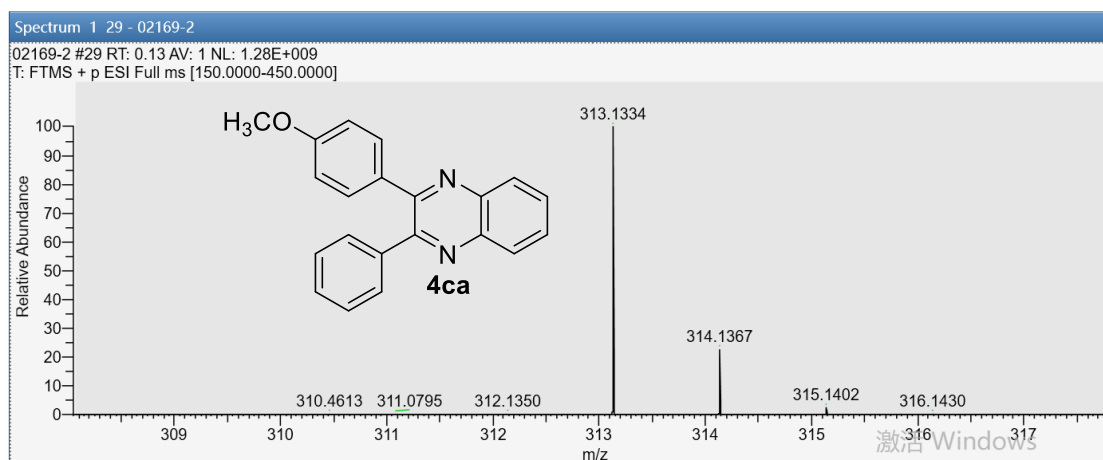
Supplementary Figure 94. HRMS spectrum of Compound **2t**.



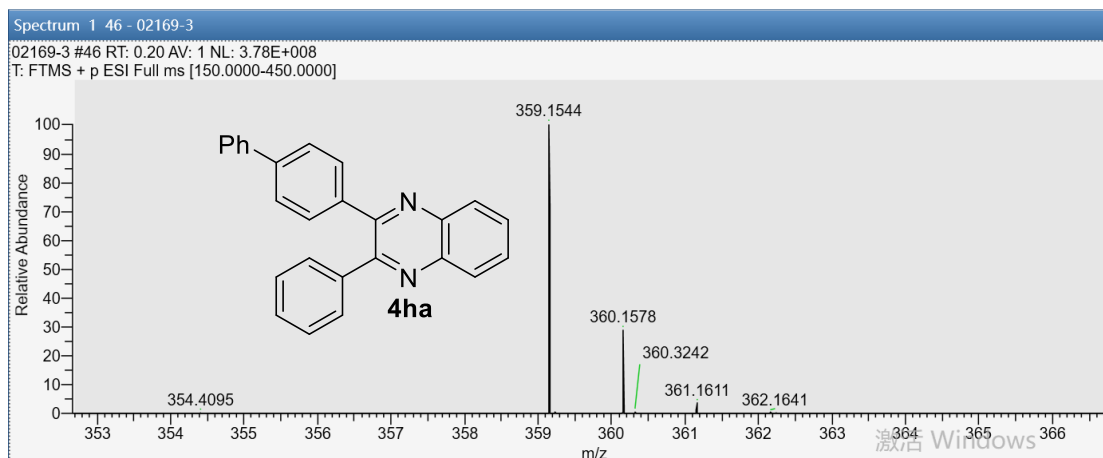
Supplementary Figure 95. HRMS spectrum of Compound **4aa**.



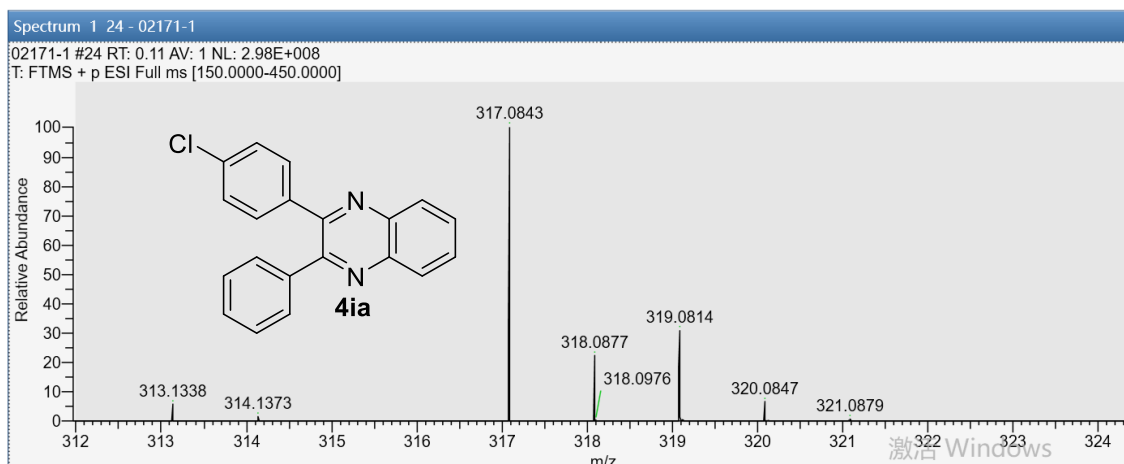
Supplementary Figure 96. HRMS spectrum of Compound **4ba**.



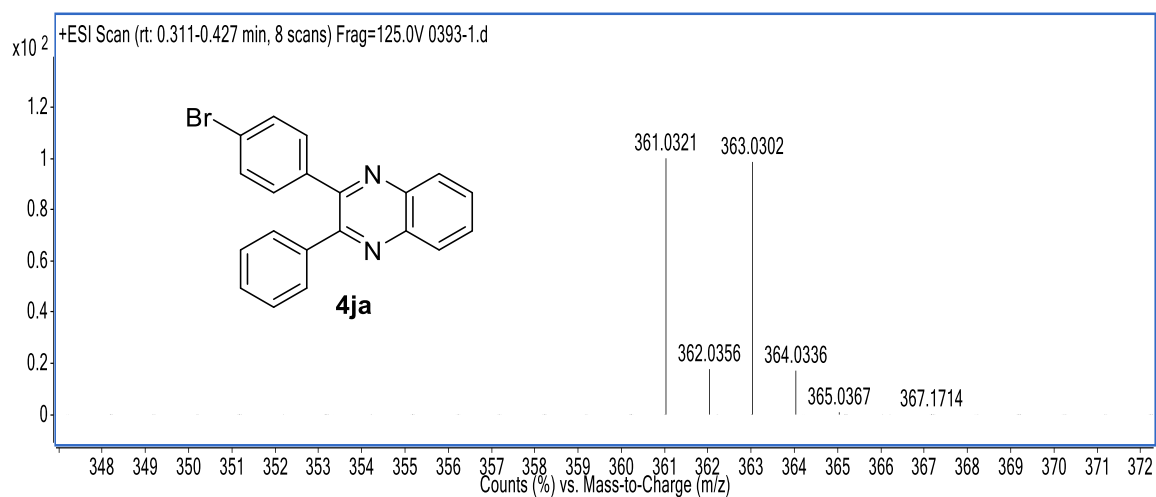
Supplementary Figure 97. HRMS spectrum of Compound **4ca**.



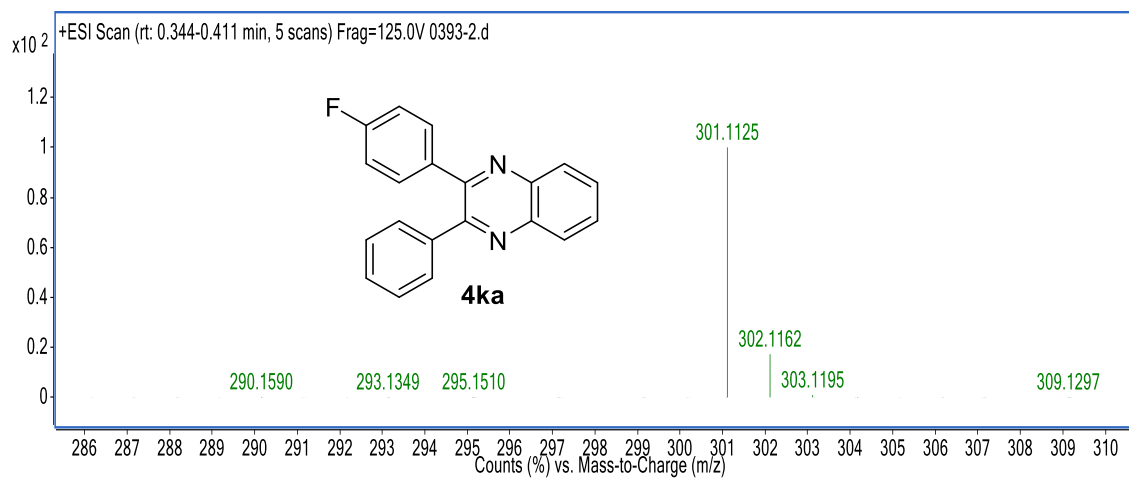
Supplementary Figure 98. HRMS spectrum of Compound **4ha**.



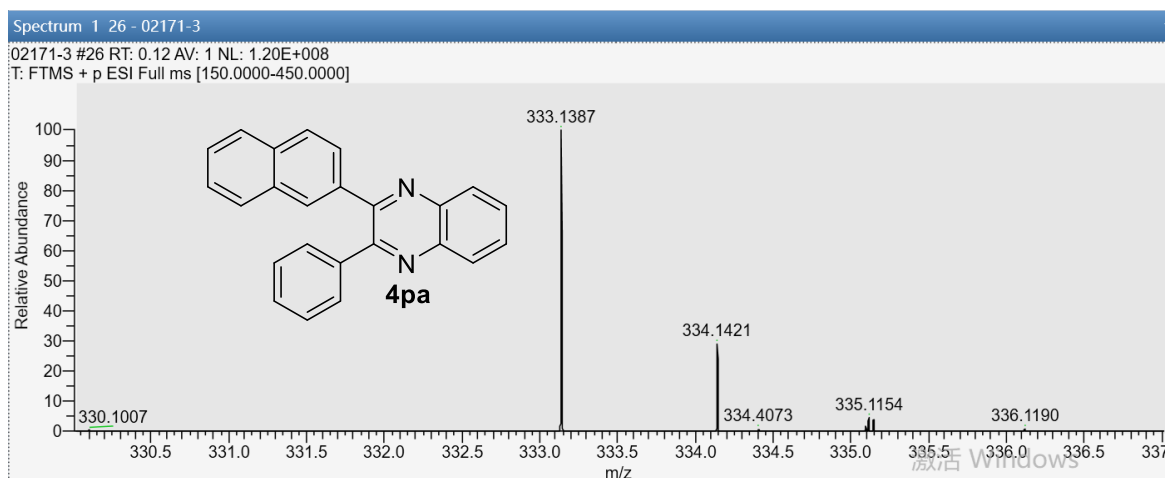
Supplementary Figure 99. HRMS spectrum of Compound **4ia**.



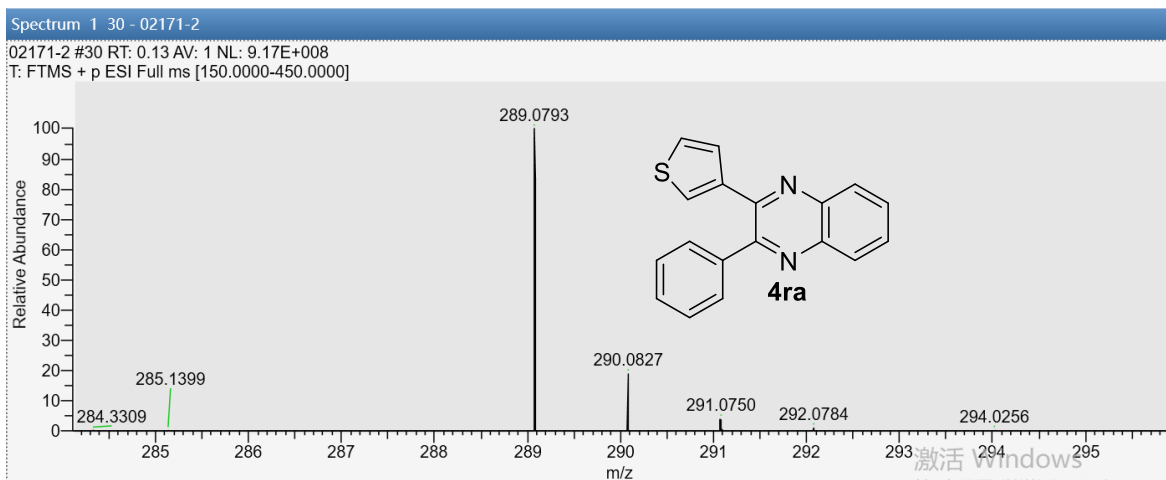
Supplementary Figure 100. HRMS spectrum of Compound **4ja**.



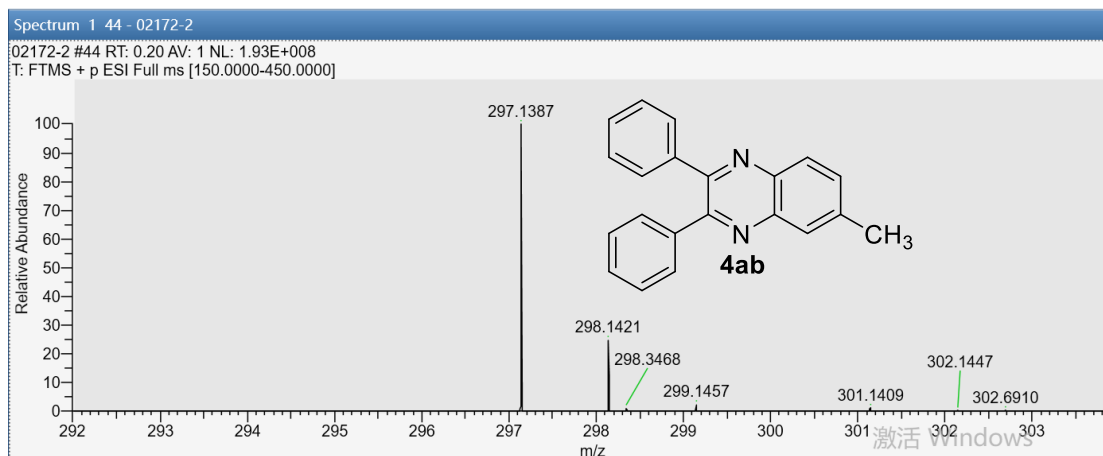
Supplementary Figure 101. HRMS spectrum of Compound **4ka**.



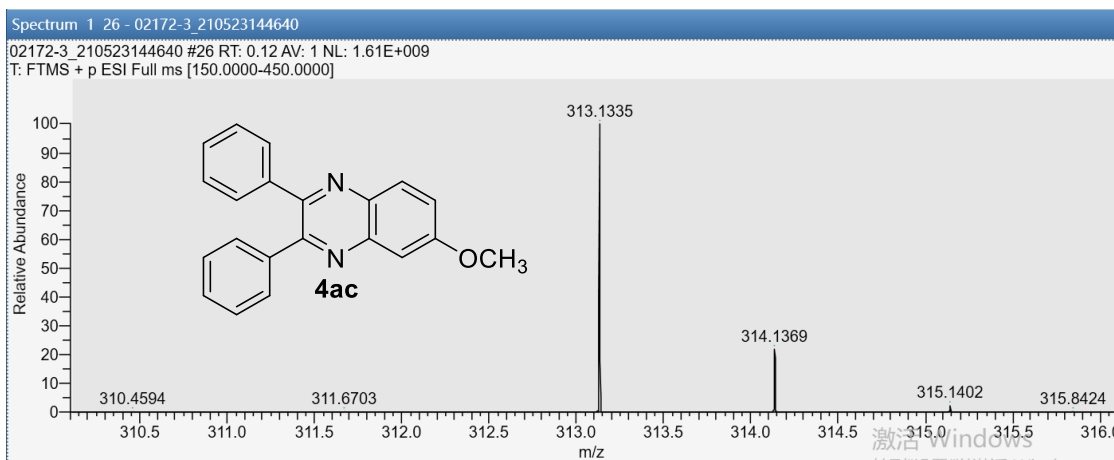
Supplementary Figure 102. HRMS spectrum of Compound **4pa**.



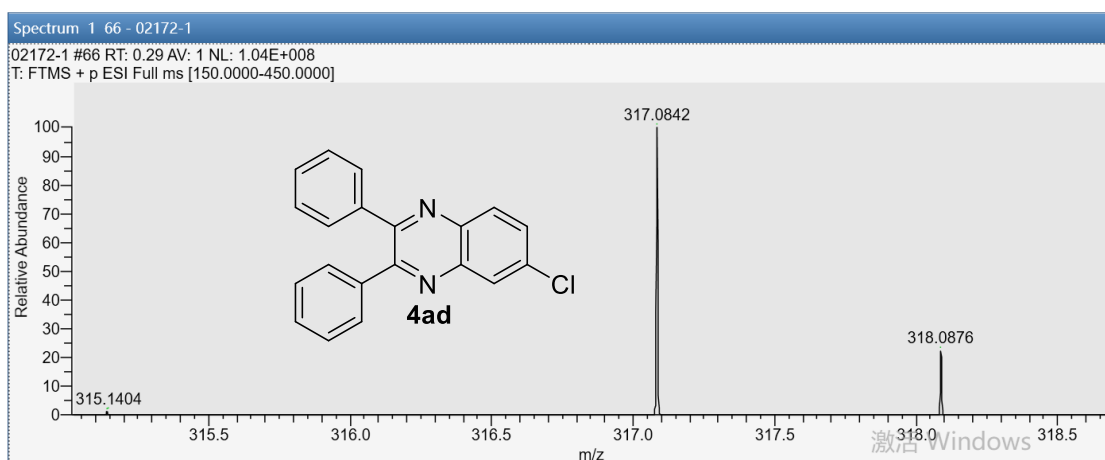
Supplementary Figure 103. HRMS spectrum of Compound **4ra**.



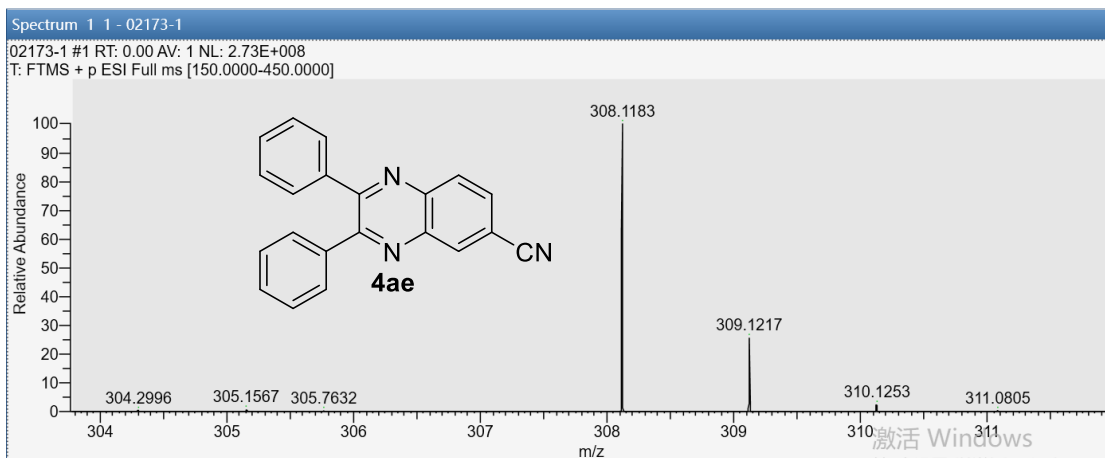
Supplementary Figure 104. HRMS spectrum of Compound **4ab**.



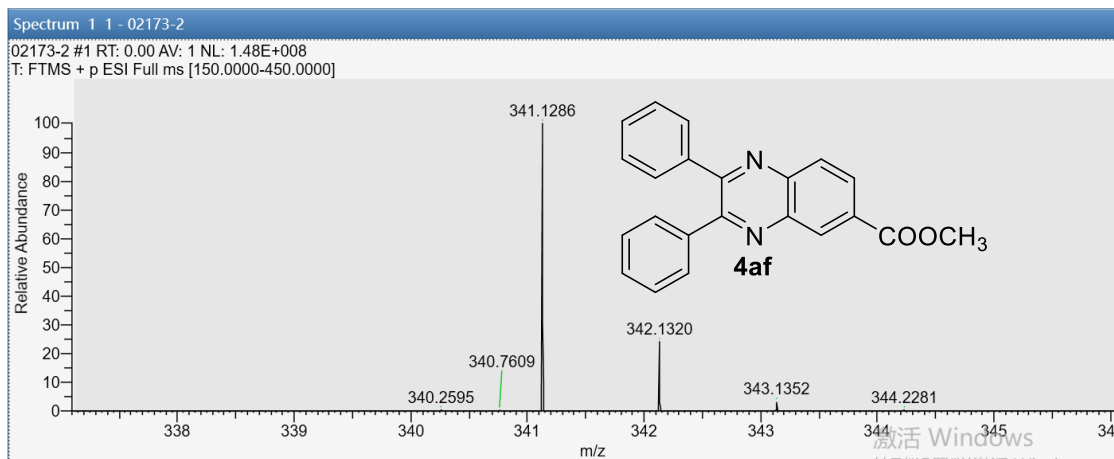
Supplementary Figure 105. HRMS spectrum of Compound **4ac**.



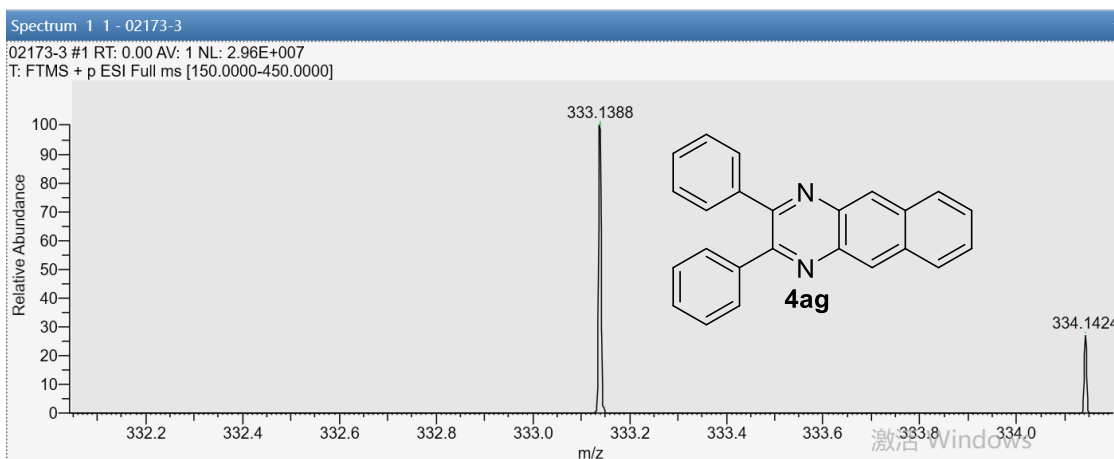
Supplementary Figure 106. HRMS spectrum of Compound **4ad**.



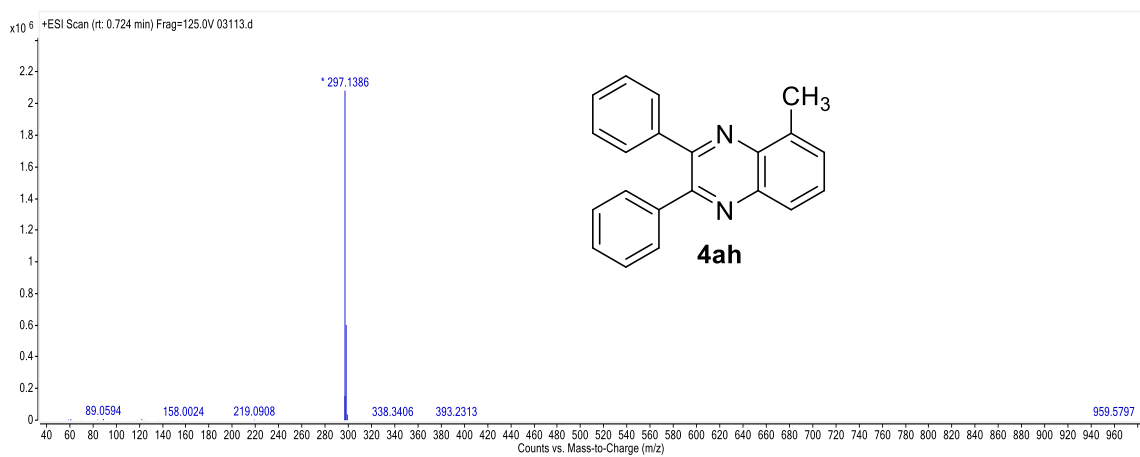
Supplementary Figure 107. HRMS spectrum of Compound **4ae**.



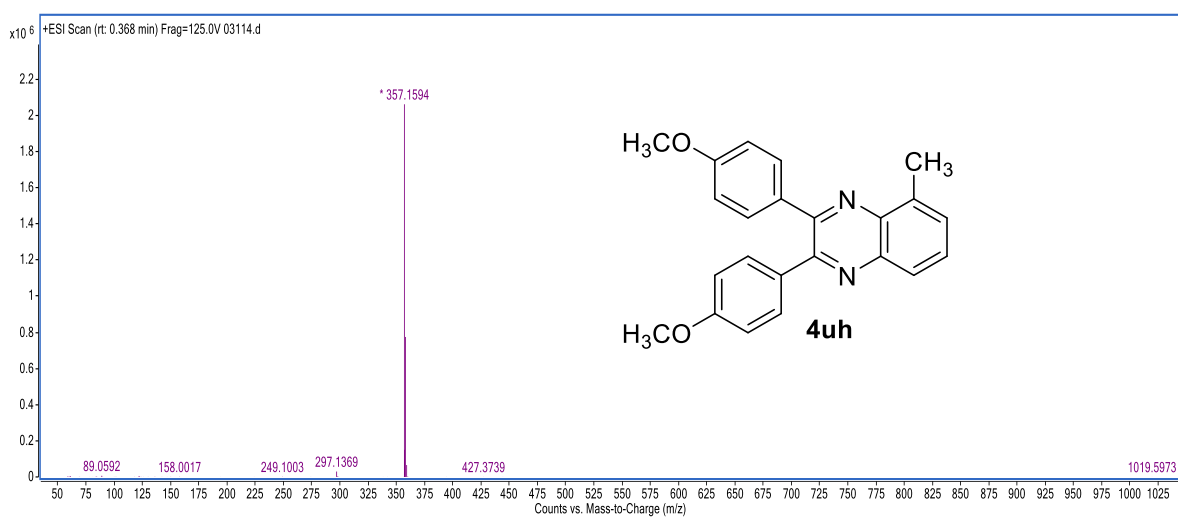
Supplementary Figure 108. HRMS spectrum of Compound **4af**.



Supplementary Figure 109. HRMS spectrum of Compound **4ag**.



Supplementary Figure 110. HRMS spectrum of Compound **4ah**.



Supplementary Figure 111. HRMS spectrum of Compound **4uh**.