

Supporting information

A Novel Method to Construct 2-Aminobenzofurans via [4+1] Cycloaddition Reaction of In Situ Generated *Ortho*-Quinone Methides with Isocyanides

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1. X-ray Crystallographic data of 3ia

The crystal of **3ia** suitable for XRD analysis was prepared by recrystallization from the DMSO. CCDC 1914402 containing the supplementary crystallographic data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. (remarks: The unit cell contains several **3ia** and DMSO, which are weakly clustered together, but this does not affect the structural characterization of compound **3ia**.)

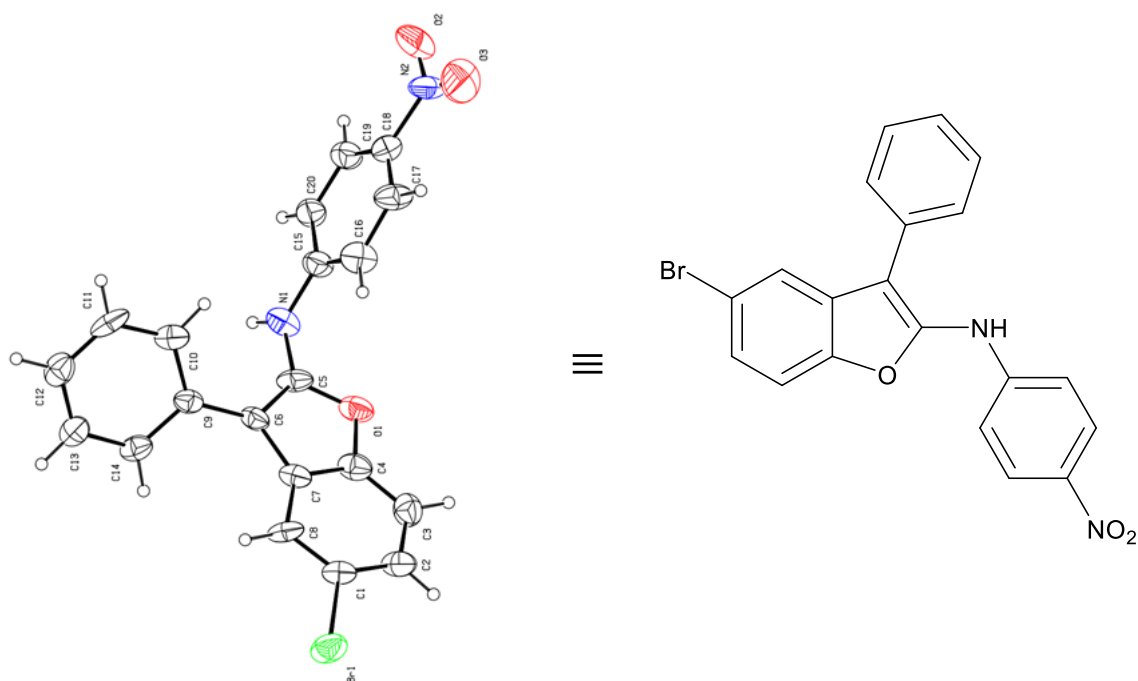


Figure S1. X-ray molecular structure of **3ia**

Table S1 Crystal data and structure refinement for mo_20190105_fence_01_0m_a.

Identification code	mo_20190105_fence_01_0m_a
Empirical formula	C ₂₁ H ₁₆ BrN ₂ O _{3.5} S _{0.5}
Formula weight	448.30
Temperature/K	297.15
Crystal system	triclinic
Space group	P-1

$a/\text{\AA}$	17.968(4)
$b/\text{\AA}$	18.005(4)
$c/\text{\AA}$	18.552(4)
$\alpha/^\circ$	94.914(7)
$\beta/^\circ$	95.055(7)
$\gamma/^\circ$	90.091(8)
Volume/ $\text{\AA}^3$	5956(2)
Z	12
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.500
μ/mm^{-1}	2.150
F(000)	2724.0
Crystal size/ mm^3	$0.21 \times 0.17 \times 0.06$
Radiation	MoK α ($\lambda = 0.71073$)
2Θ range for data collection/ $^\circ$	4.424 to 46.978
Index ranges	$-20 \leq h \leq 20, -20 \leq k \leq 20, -20 \leq l \leq 20$
Reflections collected	71482
Independent reflections	17177 [$R_{\text{int}} = 0.0776, R_{\text{sigma}} = 0.1081$]
Data/restraints/parameters	17177/4/1533
Goodness-of-fit on F^2	1.317
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1164, wR_2 = 0.3325$
Final R indexes [all data]	$R_1 = 0.1660, wR_2 = 0.3867$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.11/-2.40

2. NMR spectra of the products

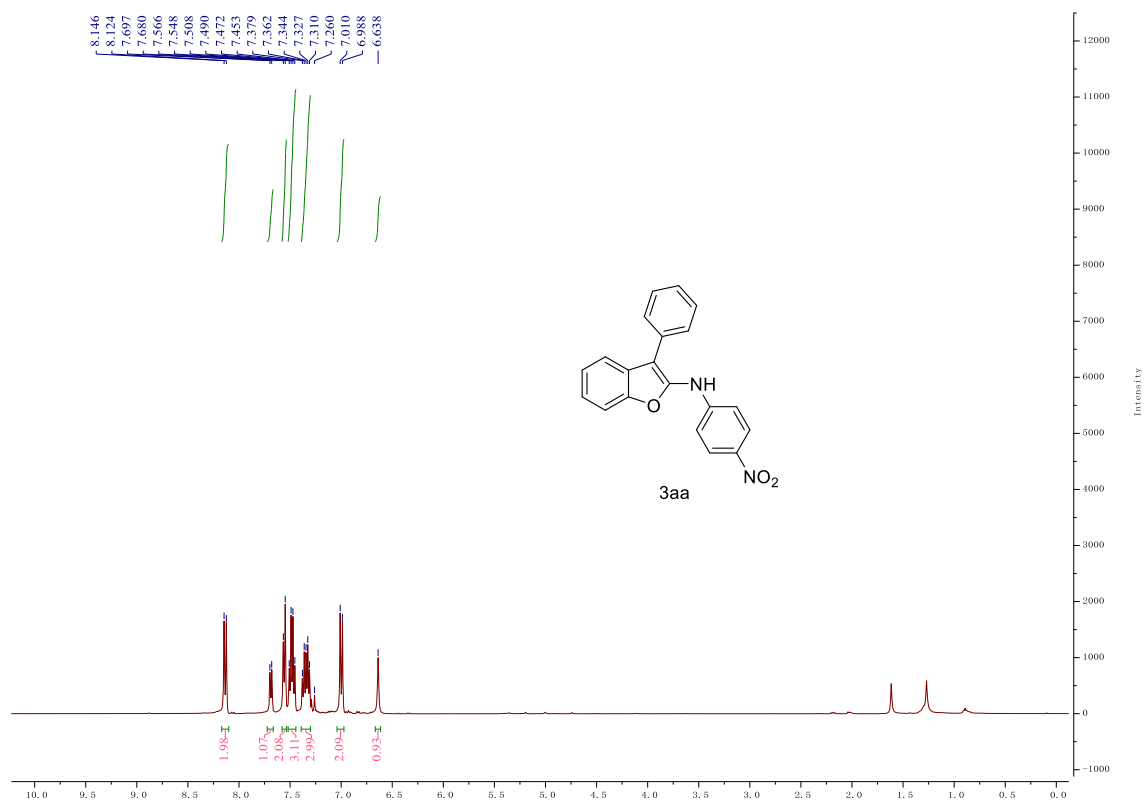


Figure S2. The ¹H NMR of compound 3aa.

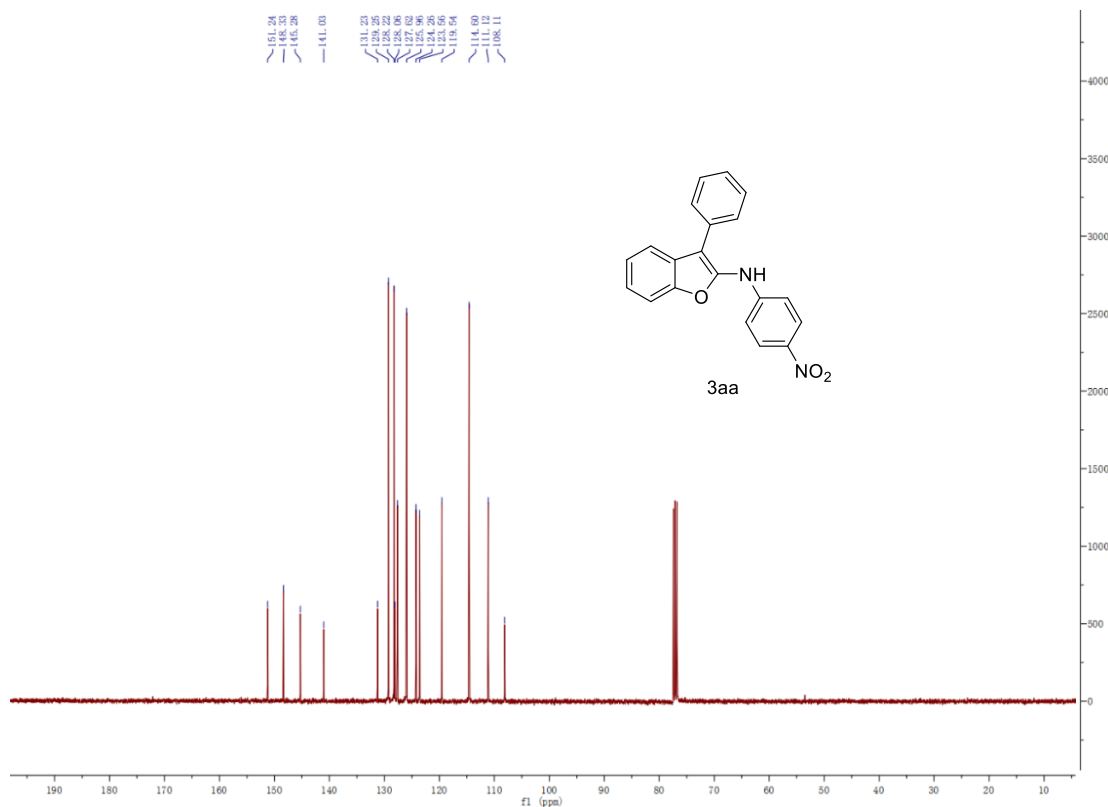


Figure S3. The ¹³C NMR of compound 3aa.

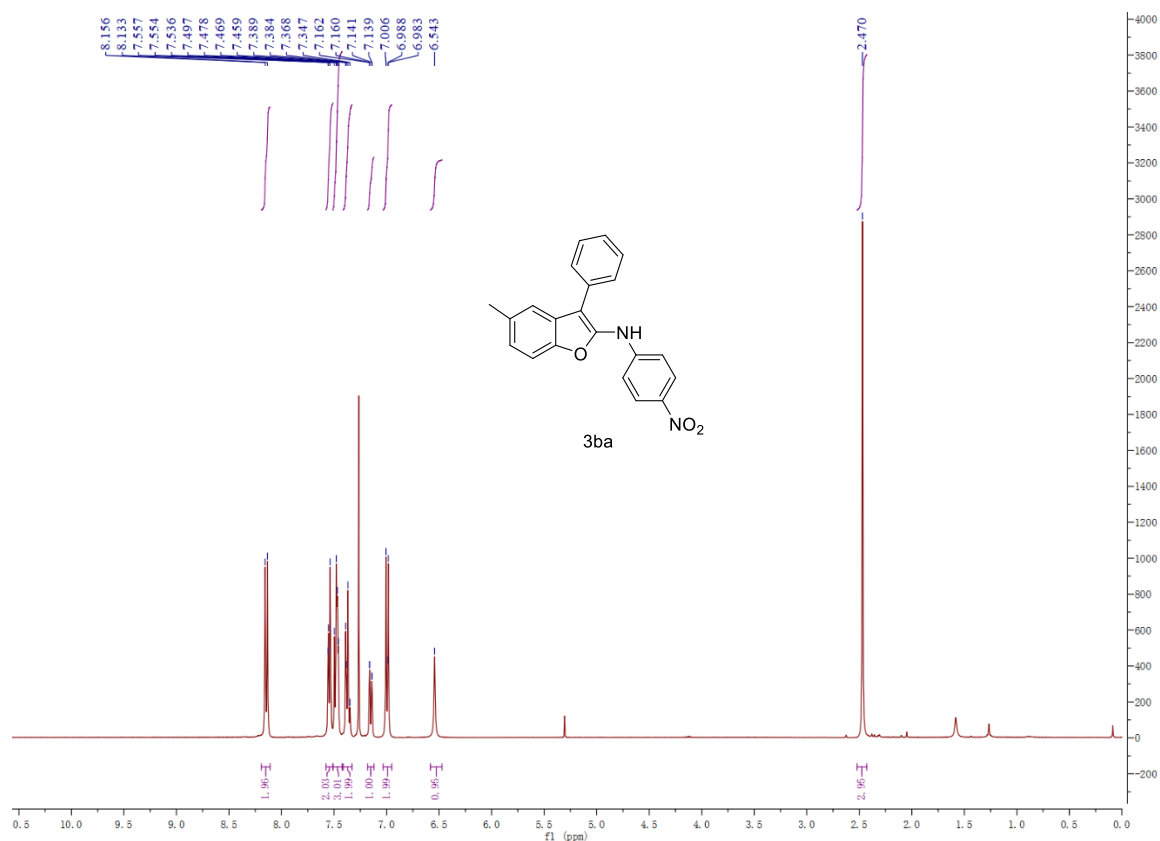


Figure S4. The ¹H NMR of compound 3ba.

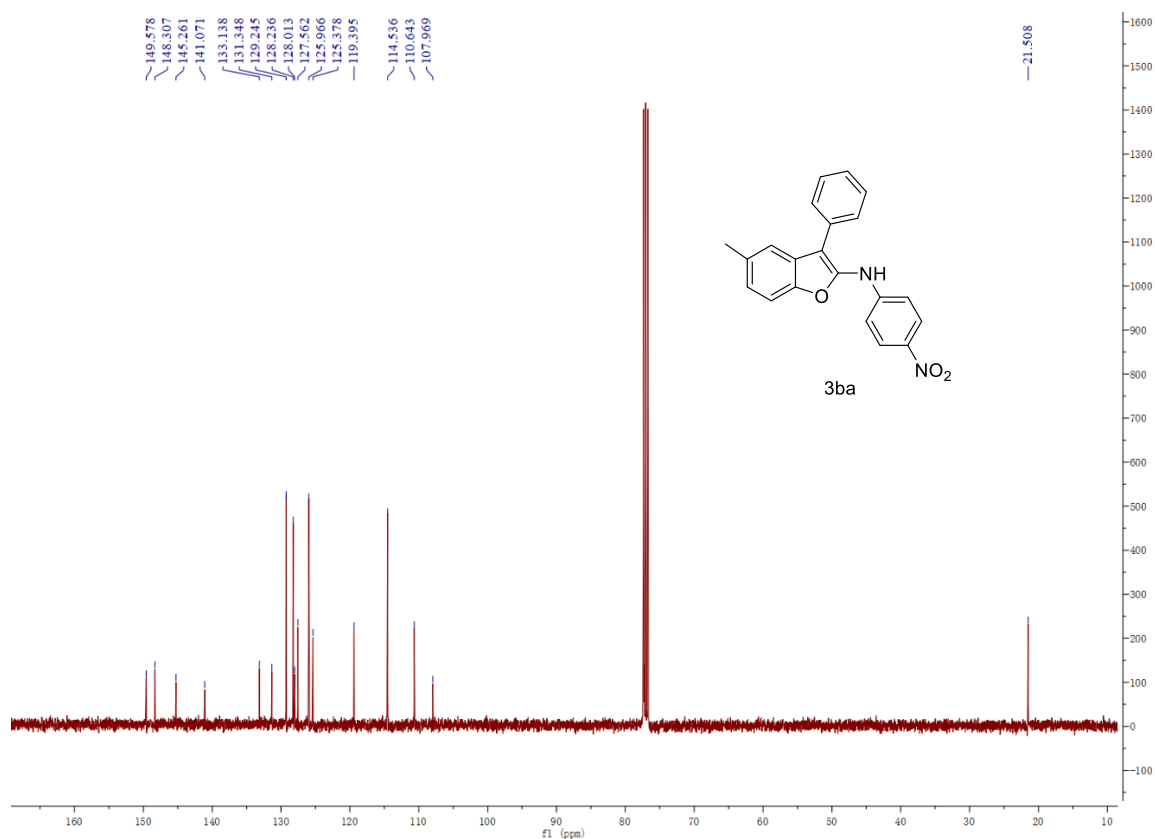


Figure S5. The ¹³C NMR of compound 3ba.

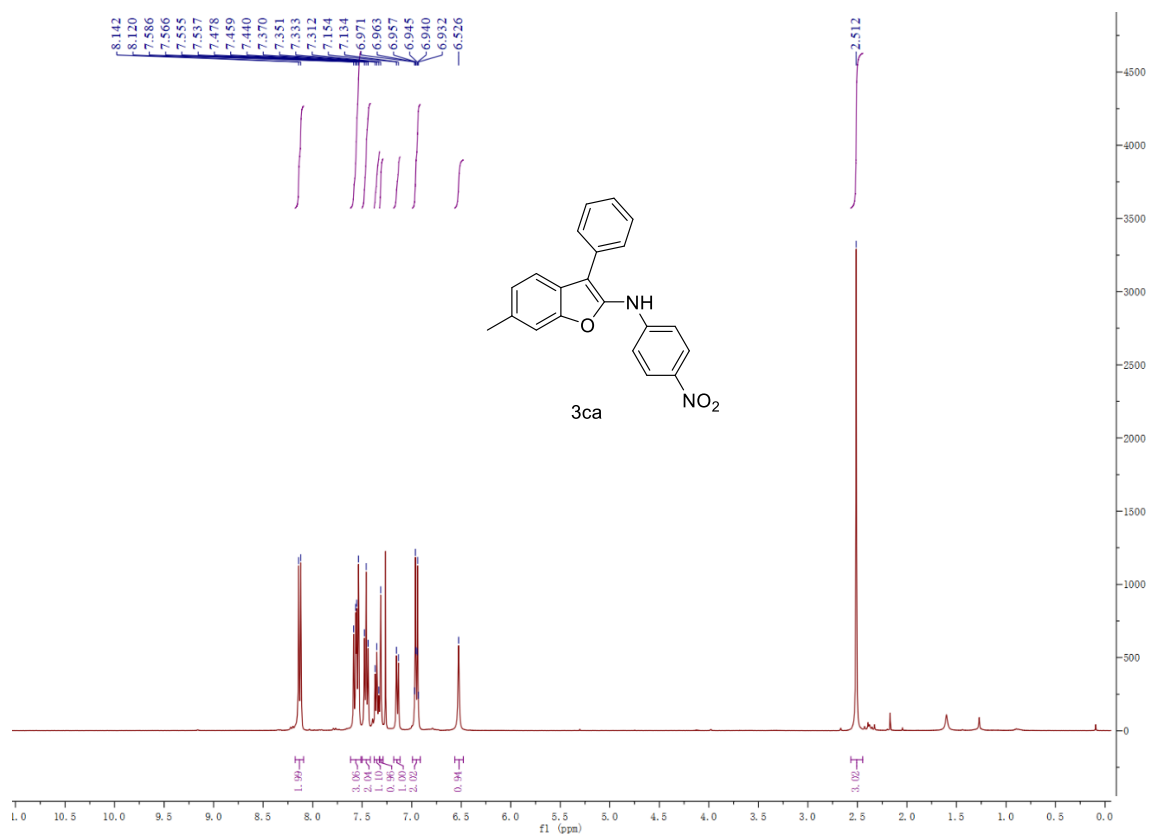


Figure S6. The ¹H NMR of compound 3ca.

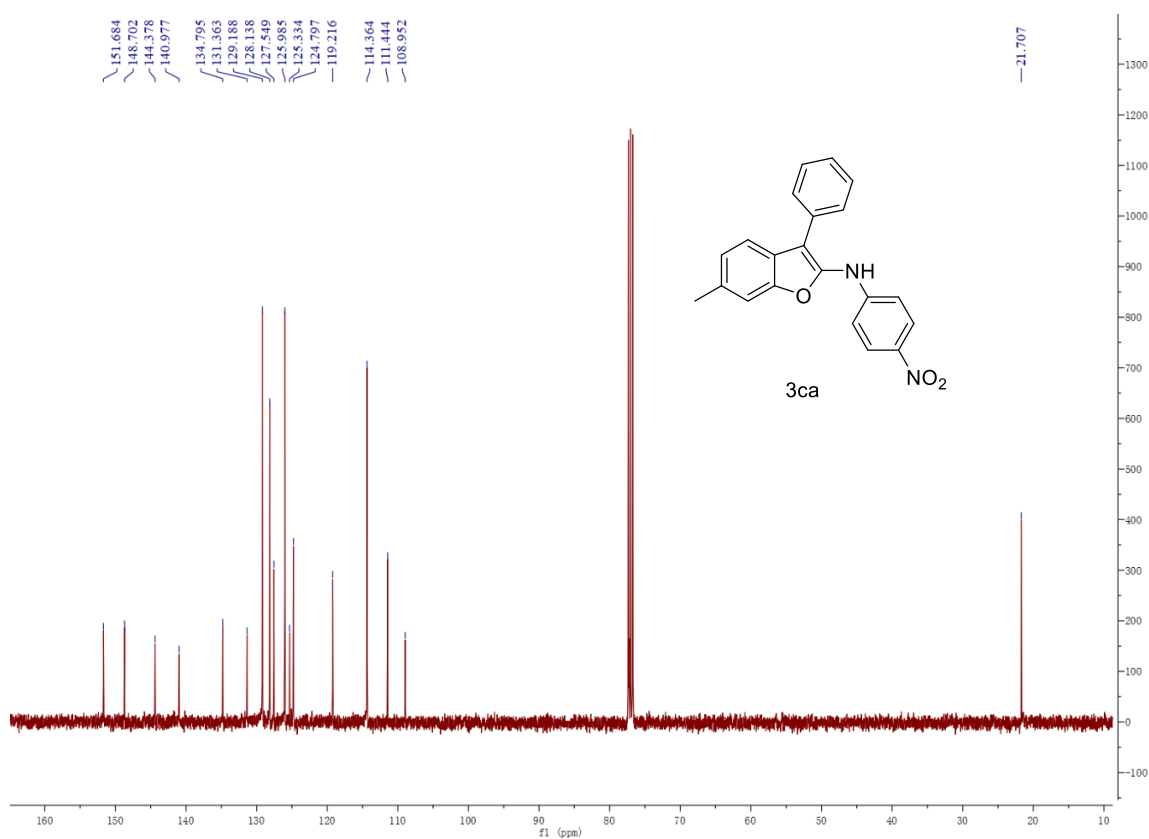


Figure S7. The ¹³C NMR of compound 3ca.

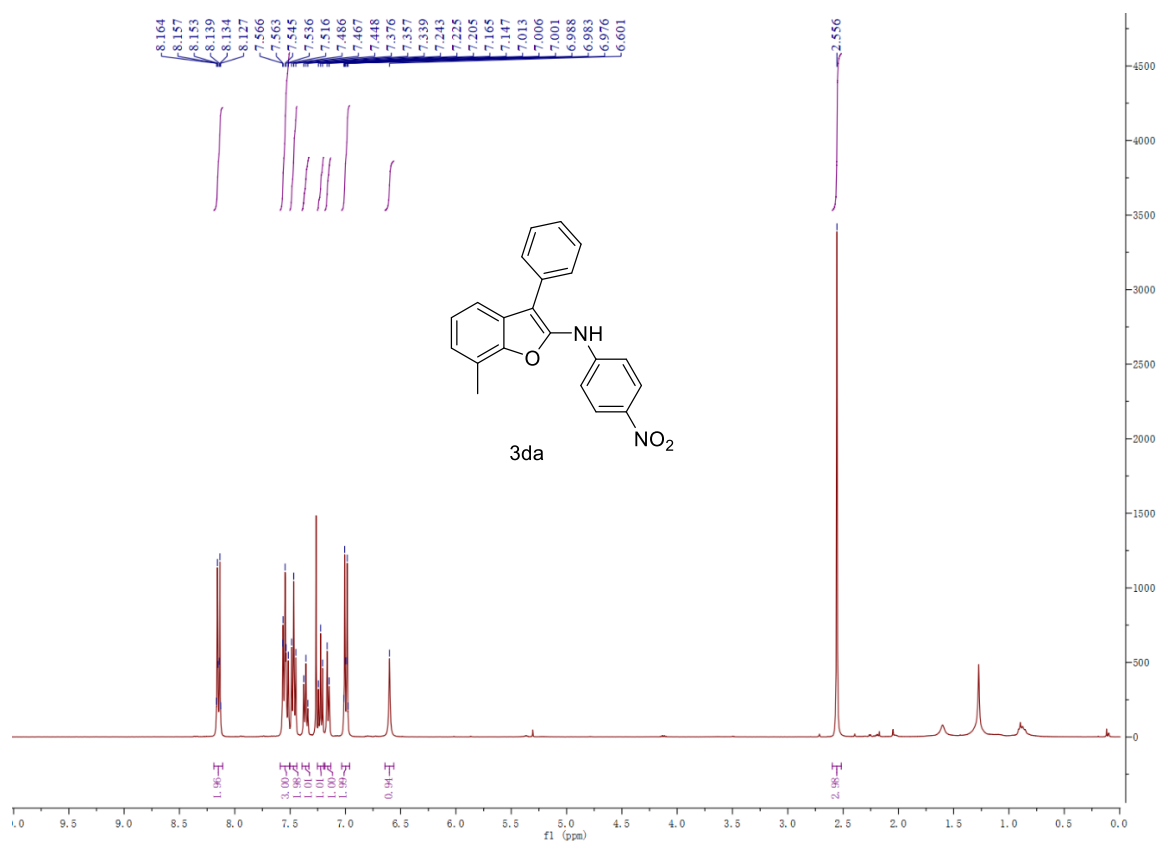


Figure S8. The ¹H NMR of compound 3da.

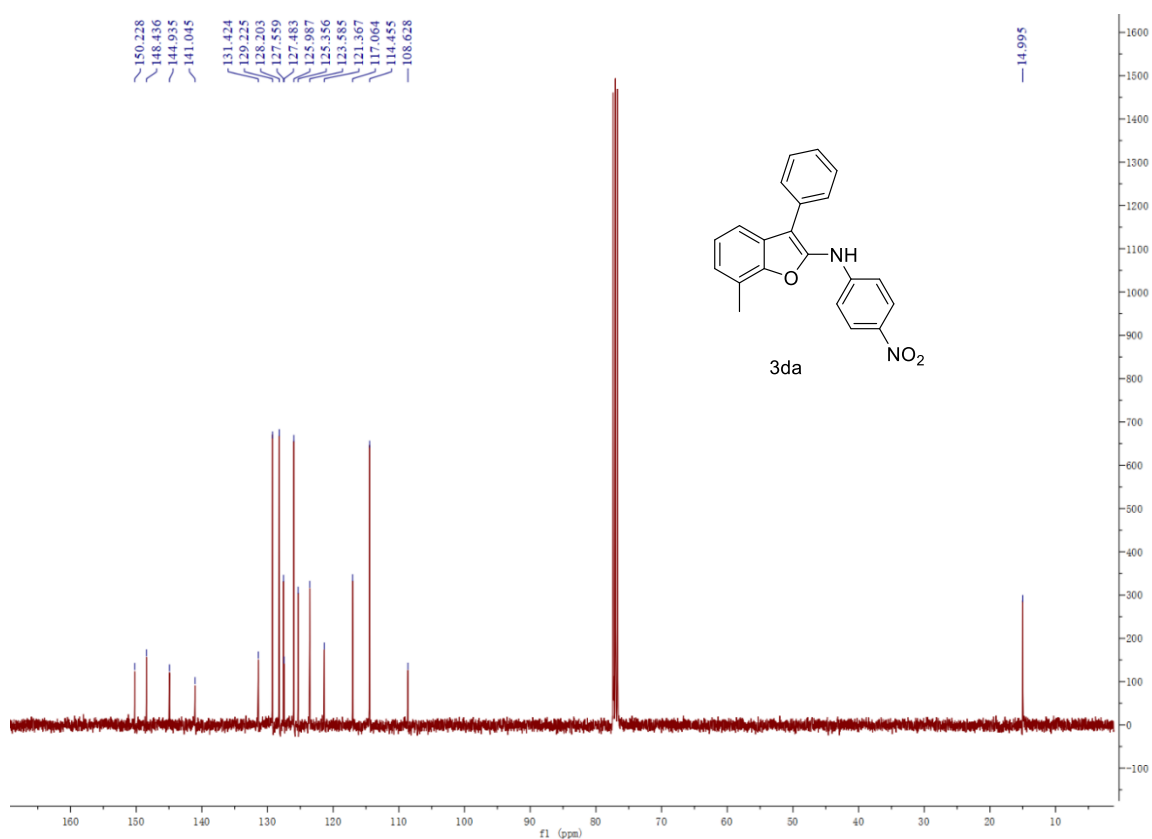


Figure S9. The ¹³C NMR of compound 3da.

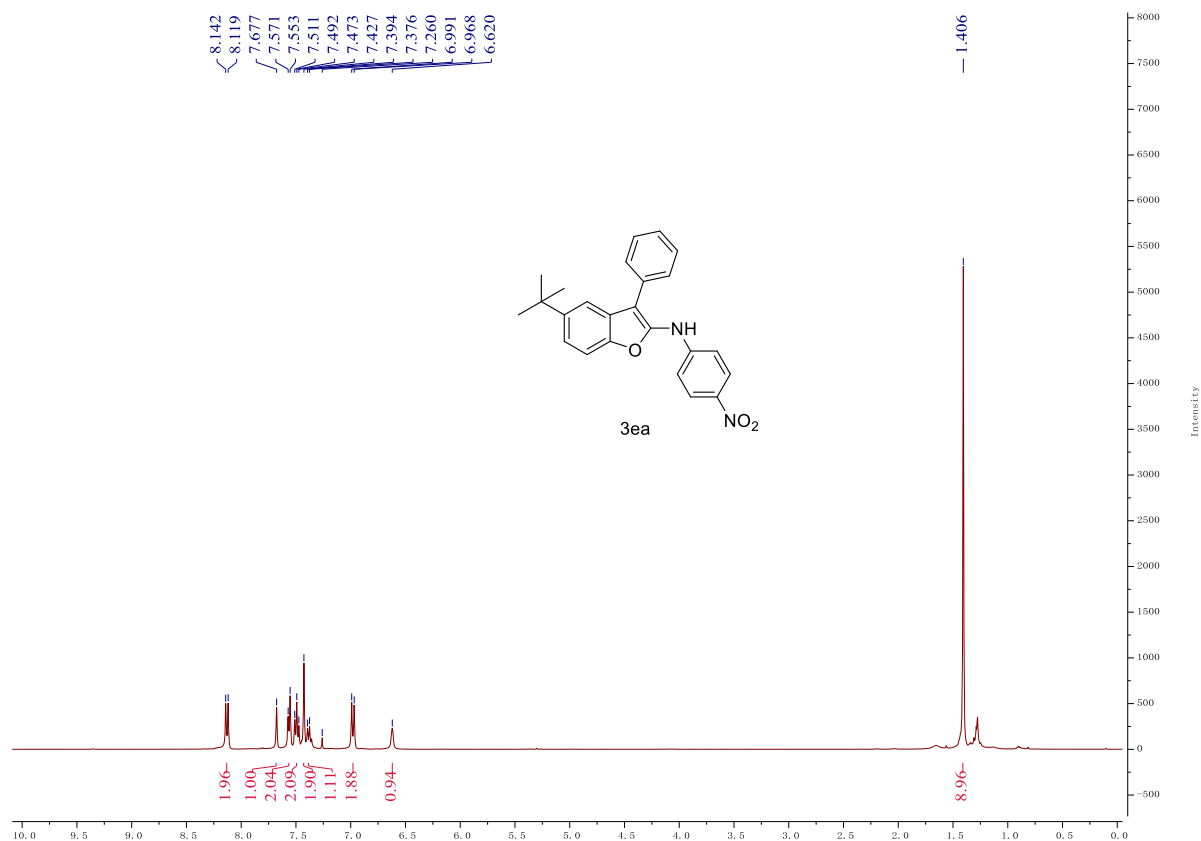


Figure S10. The ¹H NMR of compound 3ea.

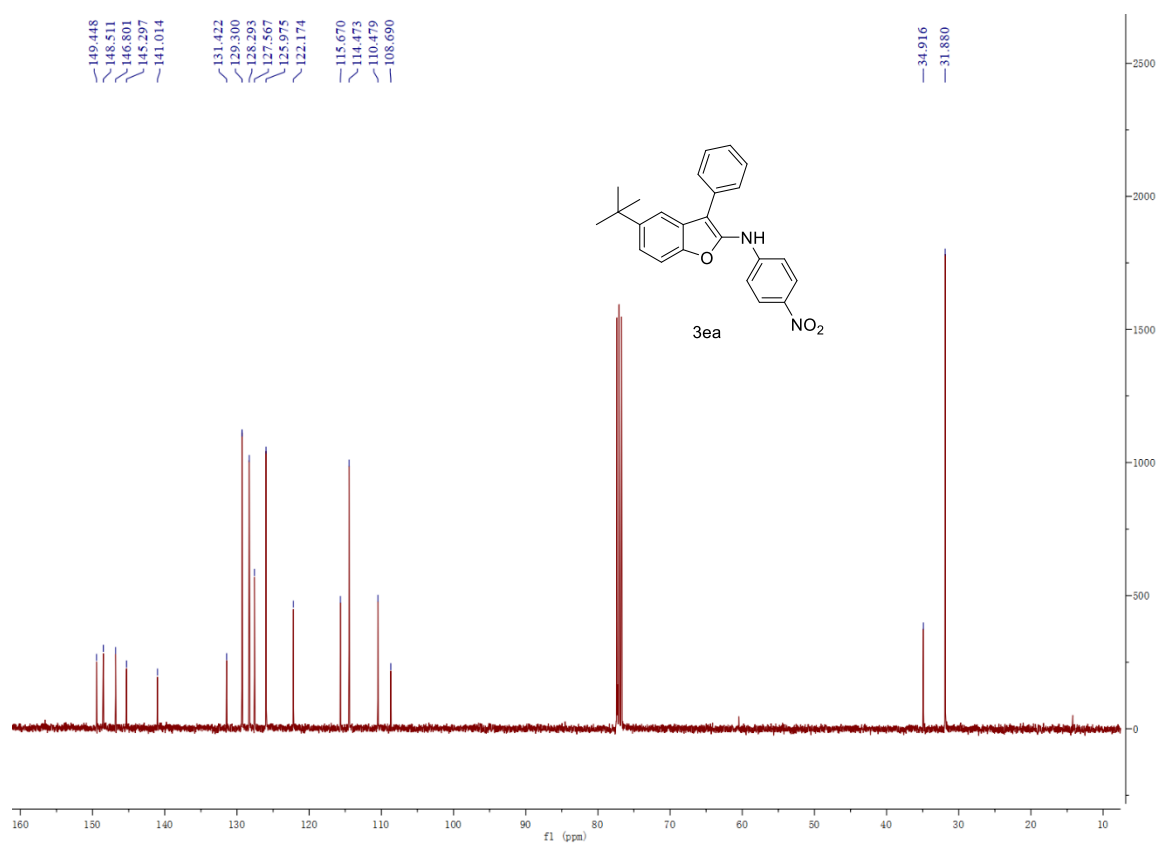


Figure S11. The ¹³C NMR of compound 3ea.

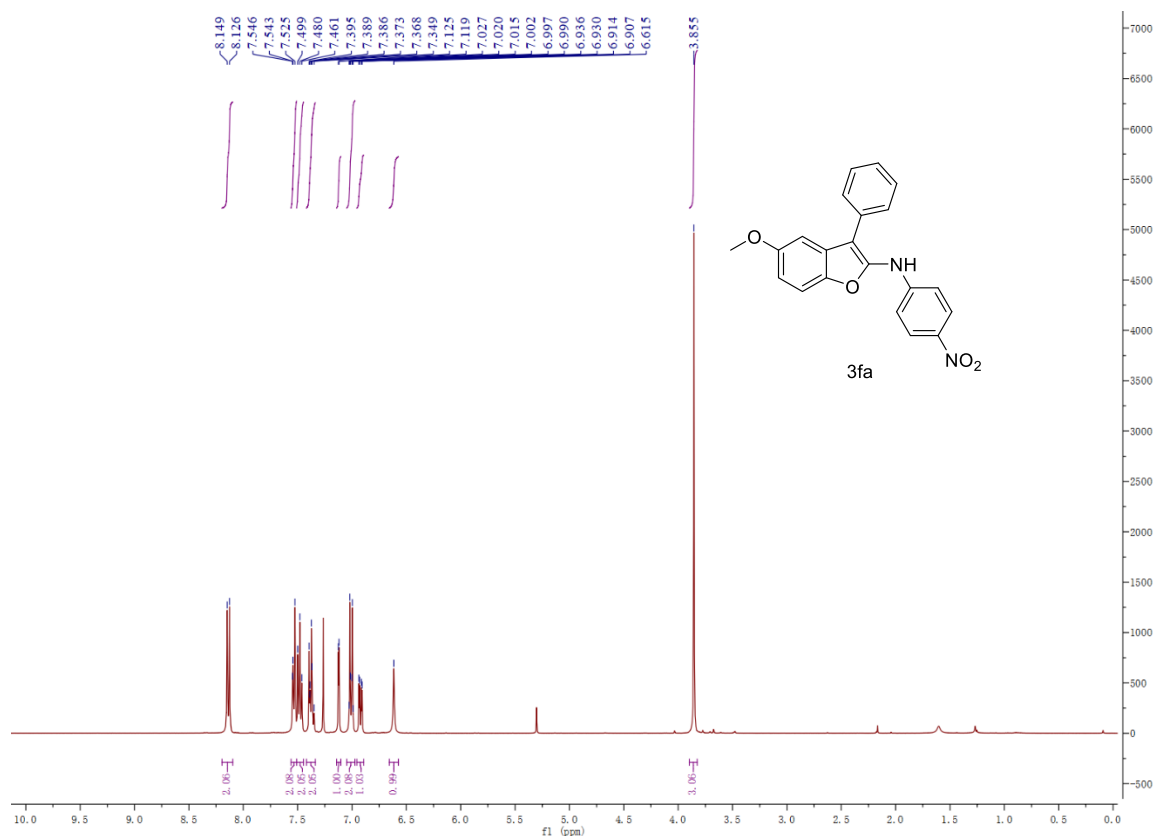


Figure S12. The ¹H NMR of compound 3fa.

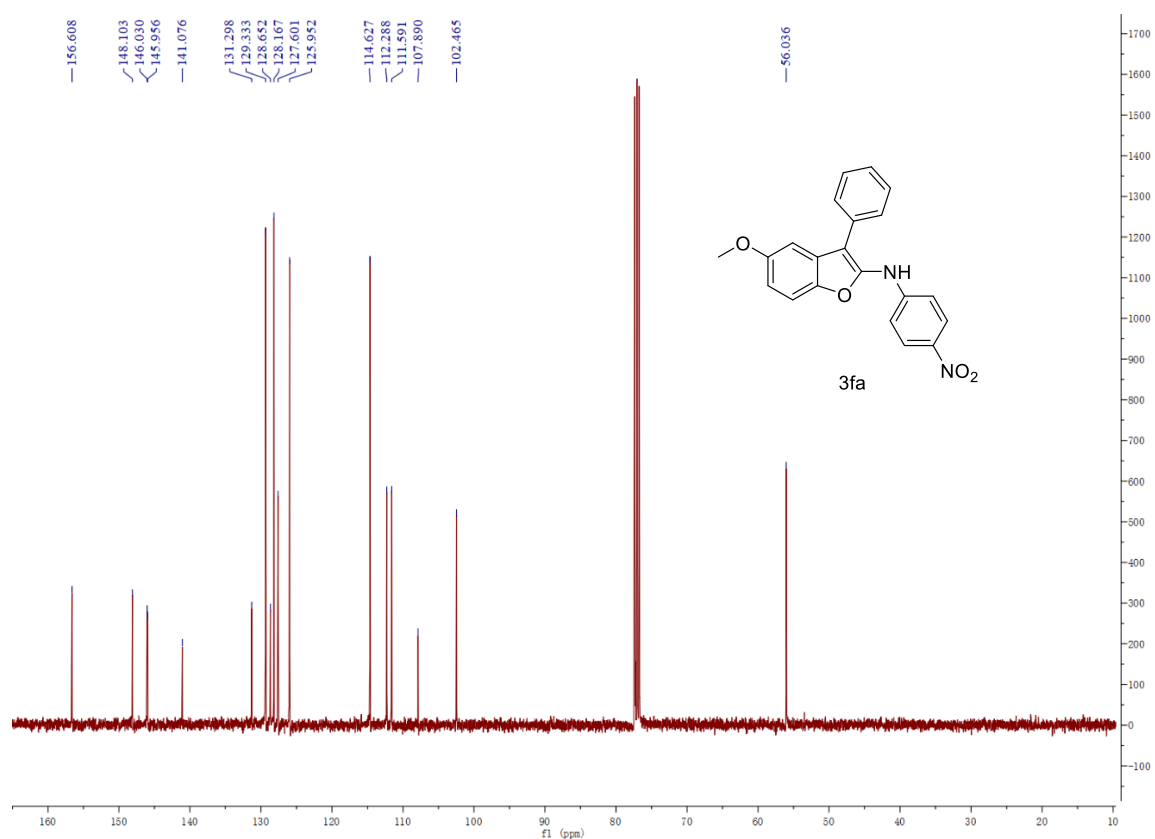


Figure S13. The ¹³C NMR of compound 3fa.

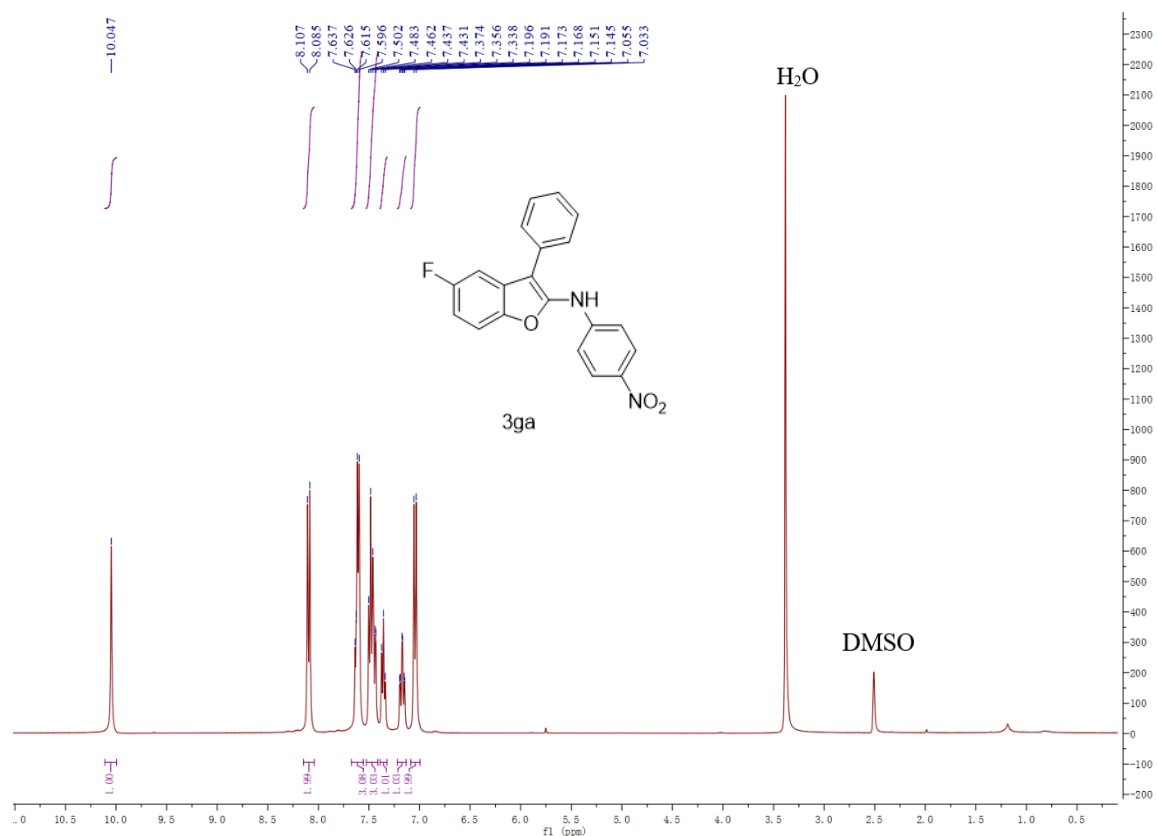


Figure S14. The ¹H NMR of compound 3ga.

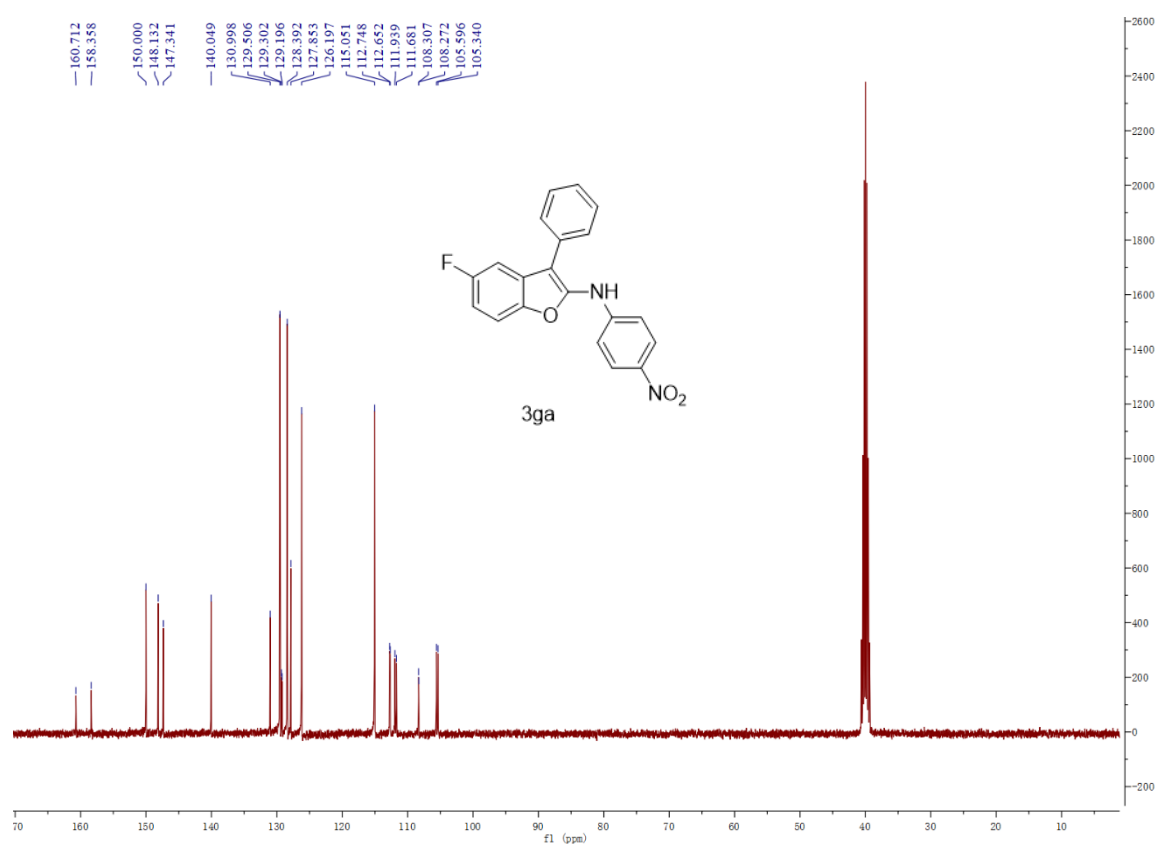


Figure S15. The ¹³C NMR of compound 3ga.

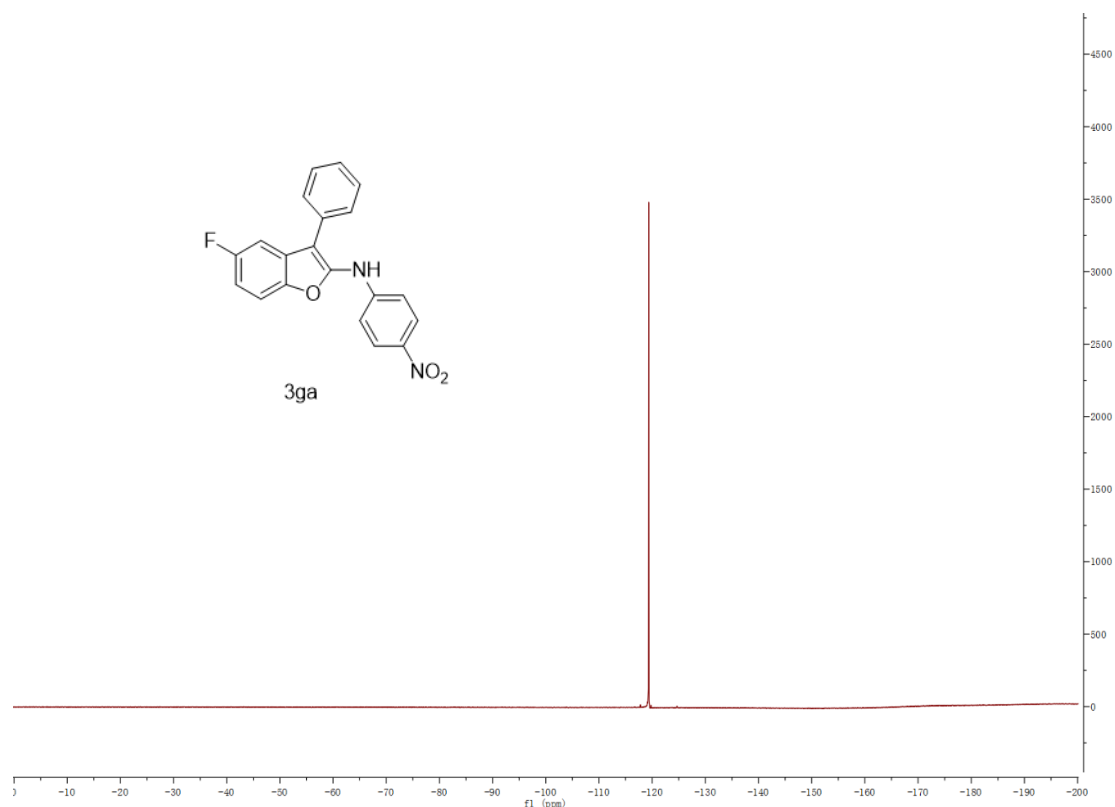


Figure S16. The ¹⁹F NMR of compound 3ga.

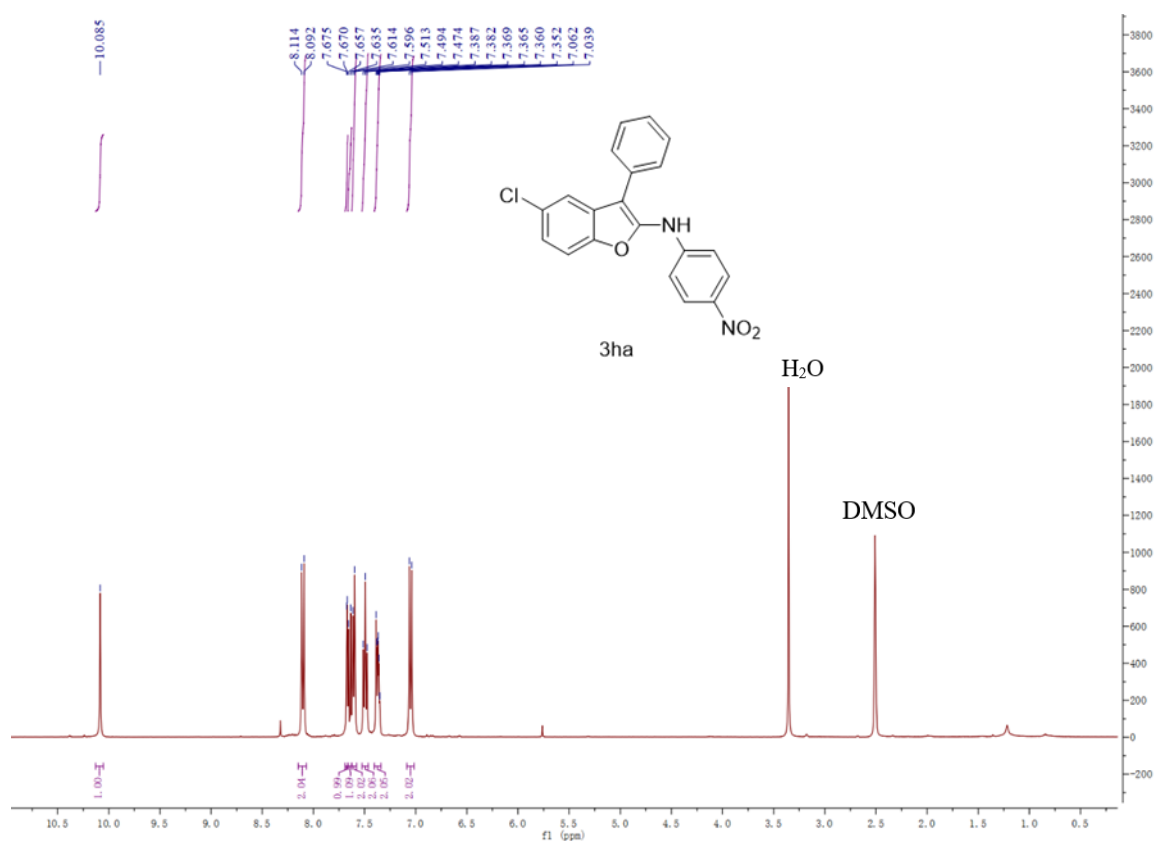


Figure S17. The ¹H NMR of compound 3ha.

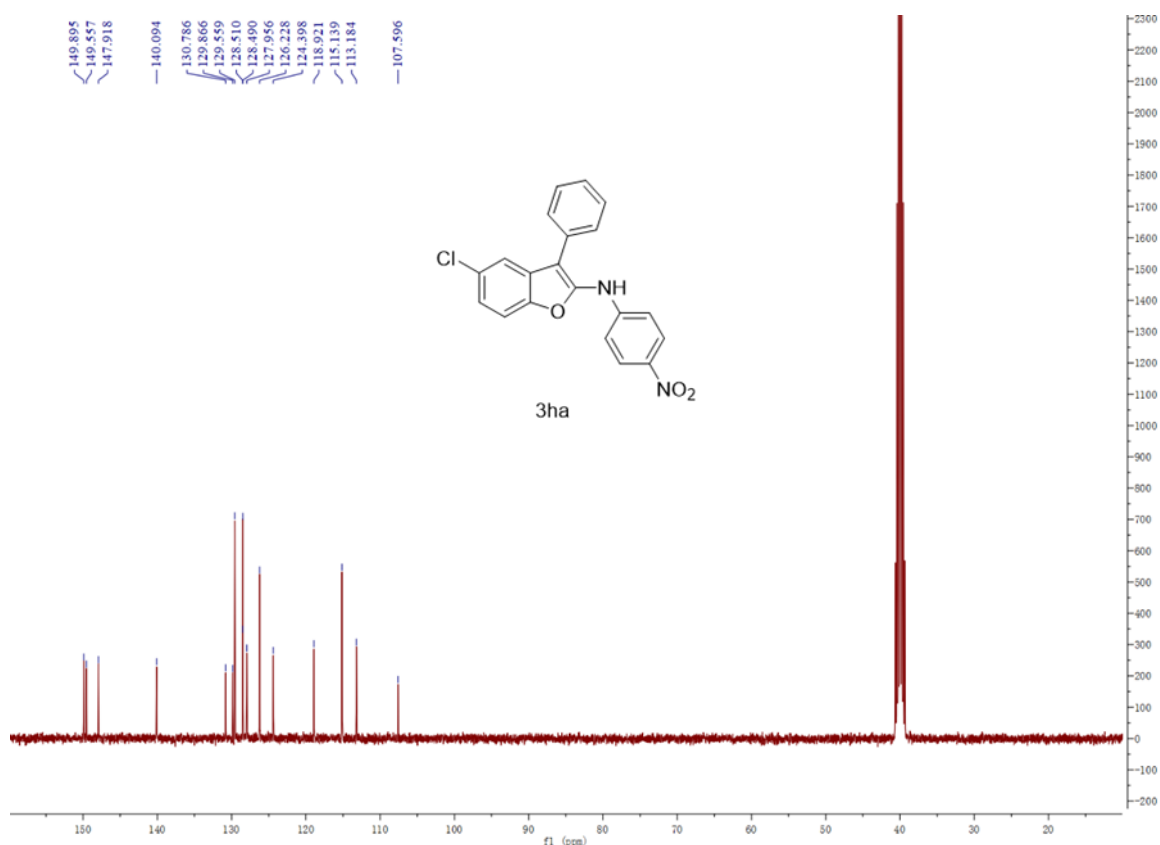


Figure S18. The ¹³C NMR of compound 3ha.

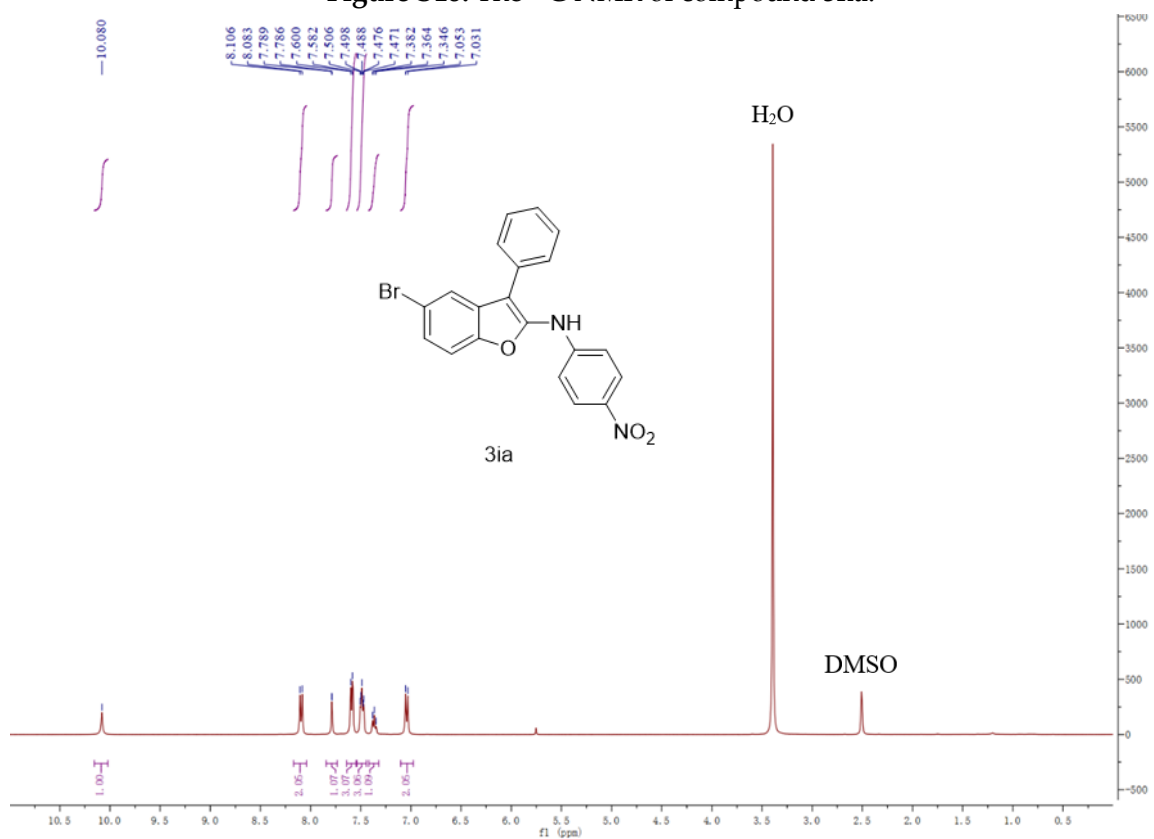


Figure S19. The ¹H NMR of compound 3ia.

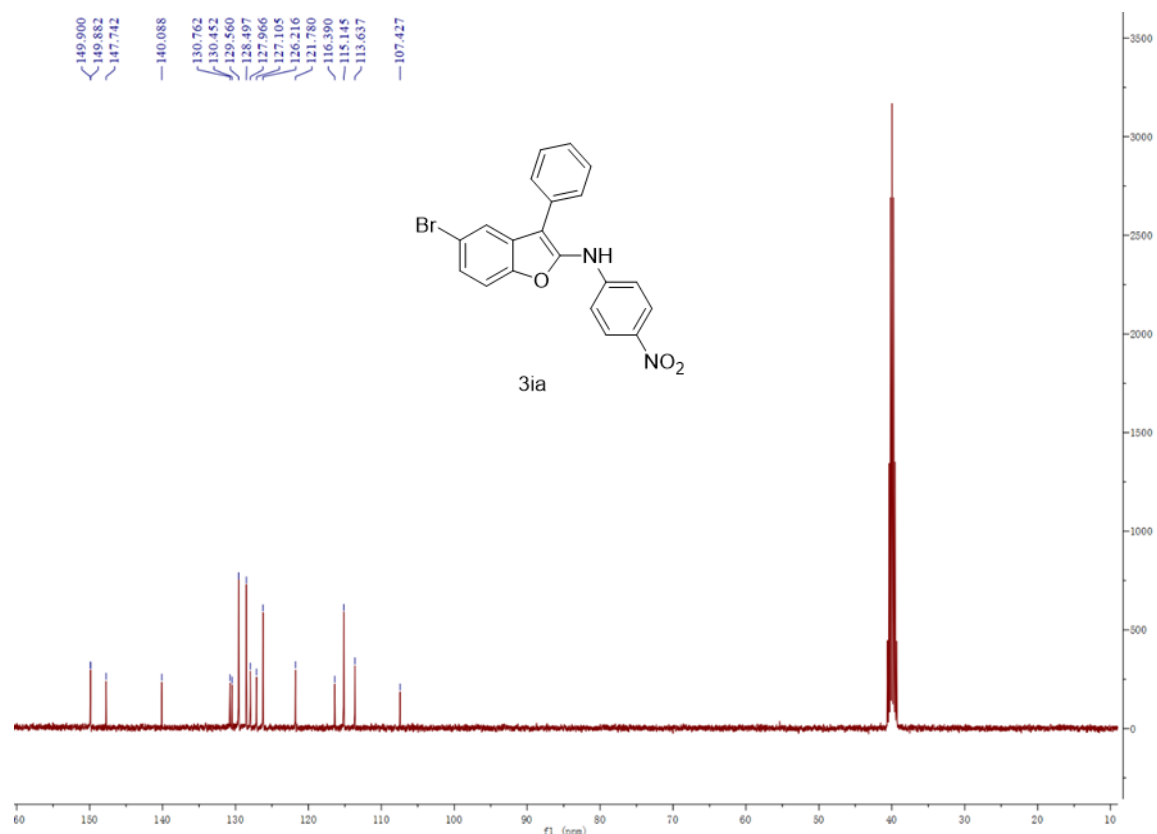


Figure S20. The ¹³C NMR of compound **3ia**.

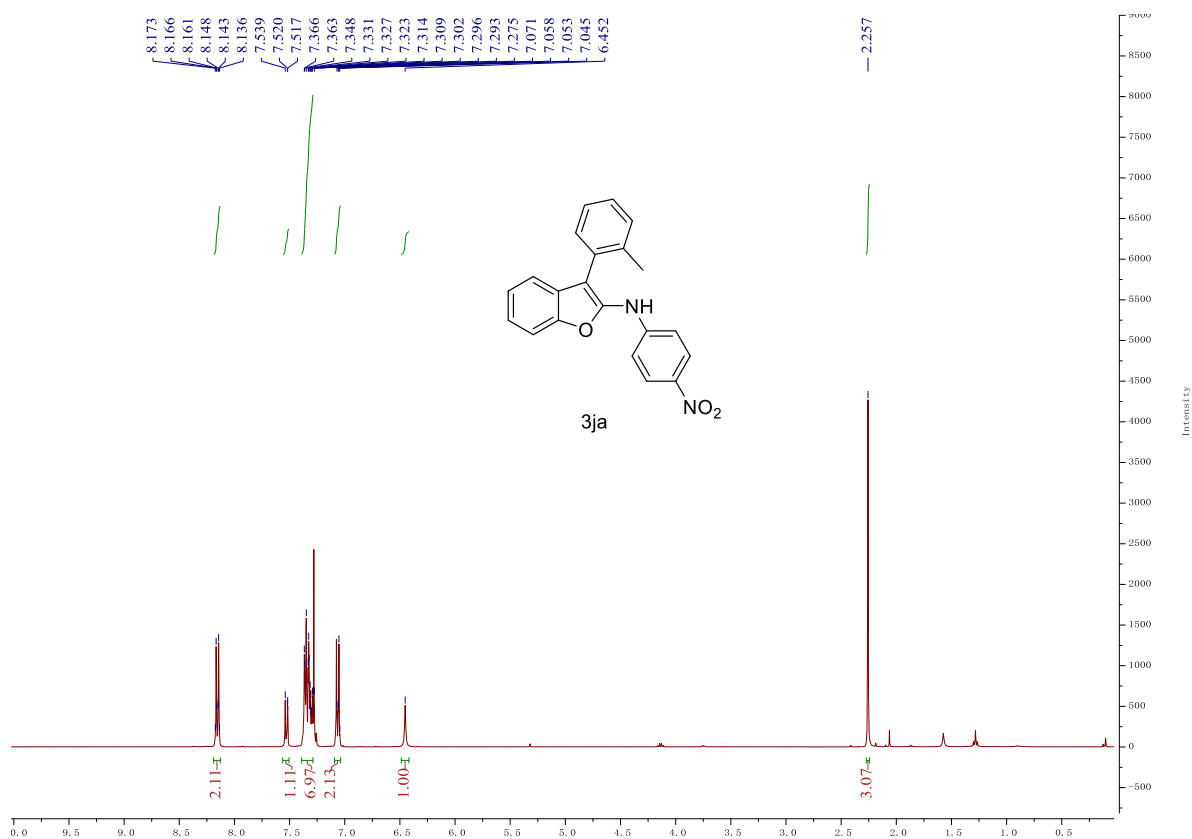


Figure S21. The ¹H NMR of compound **3ja**.

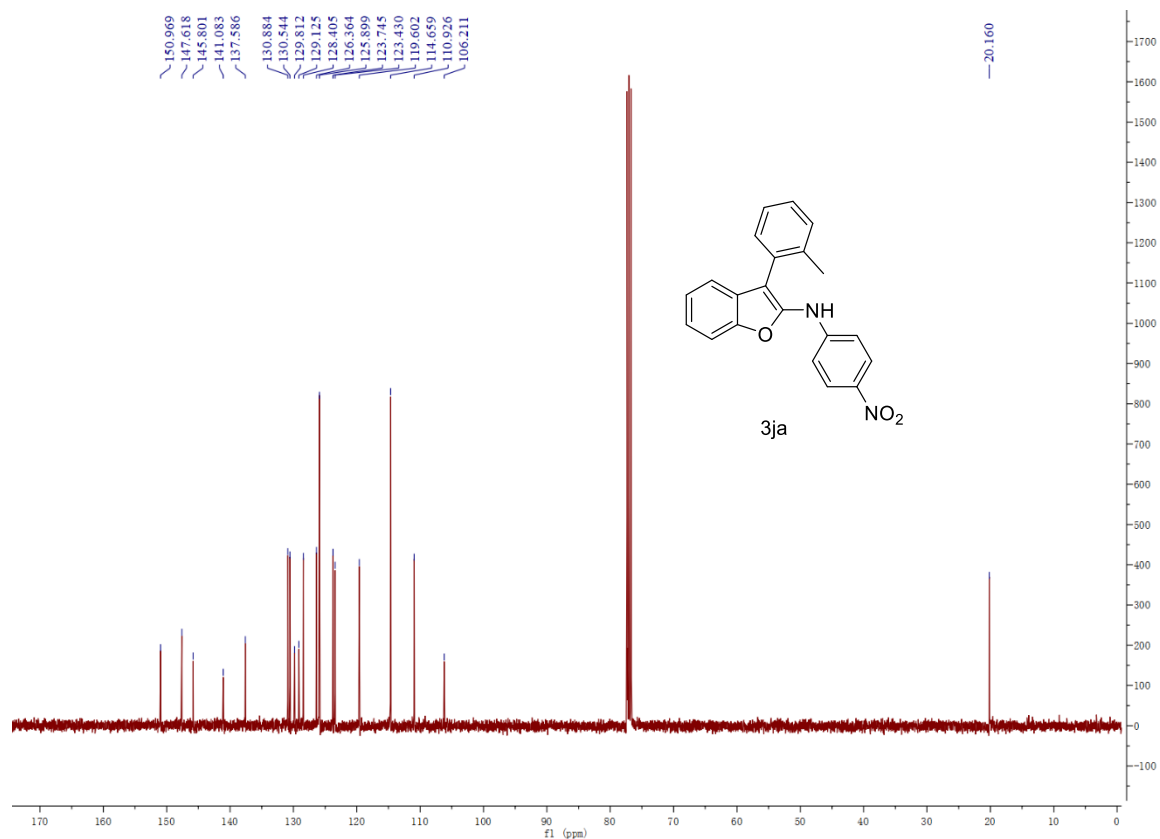


Figure S22. The ¹³C NMR of compound 3ja.

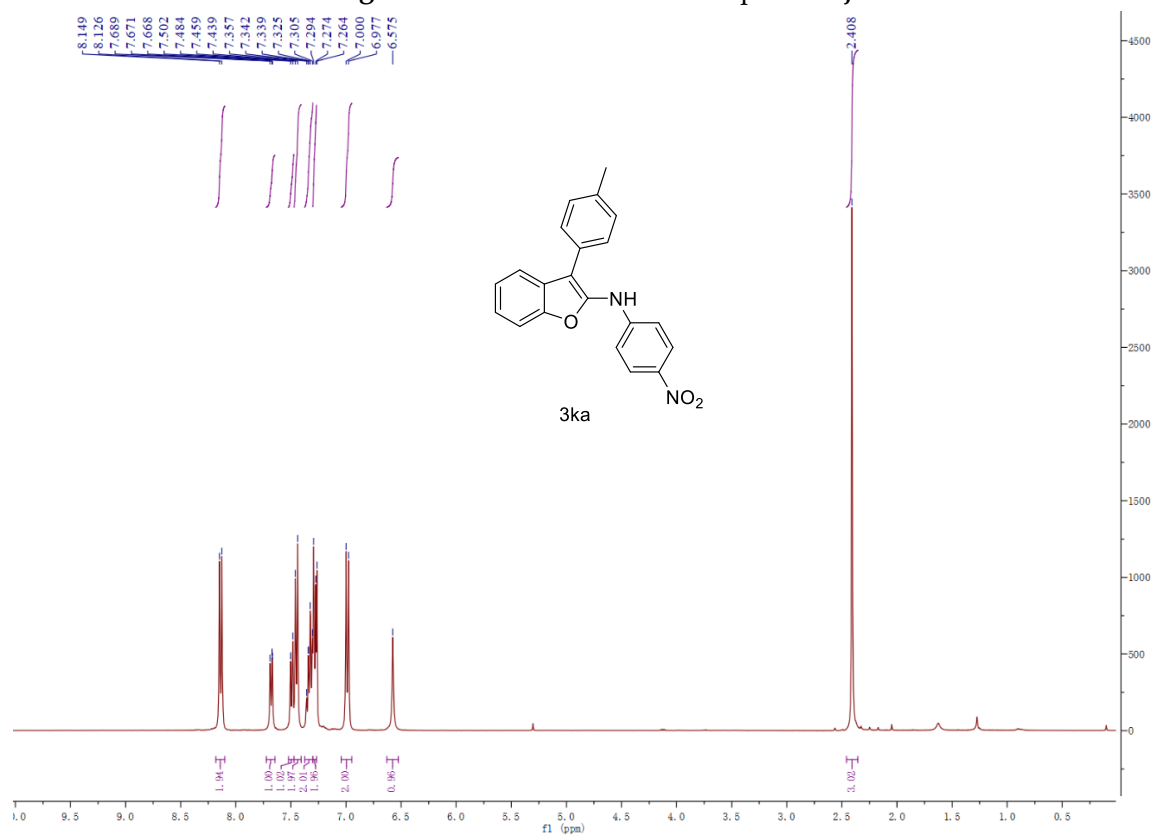


Figure S23. The ¹H NMR of compound 3ka.

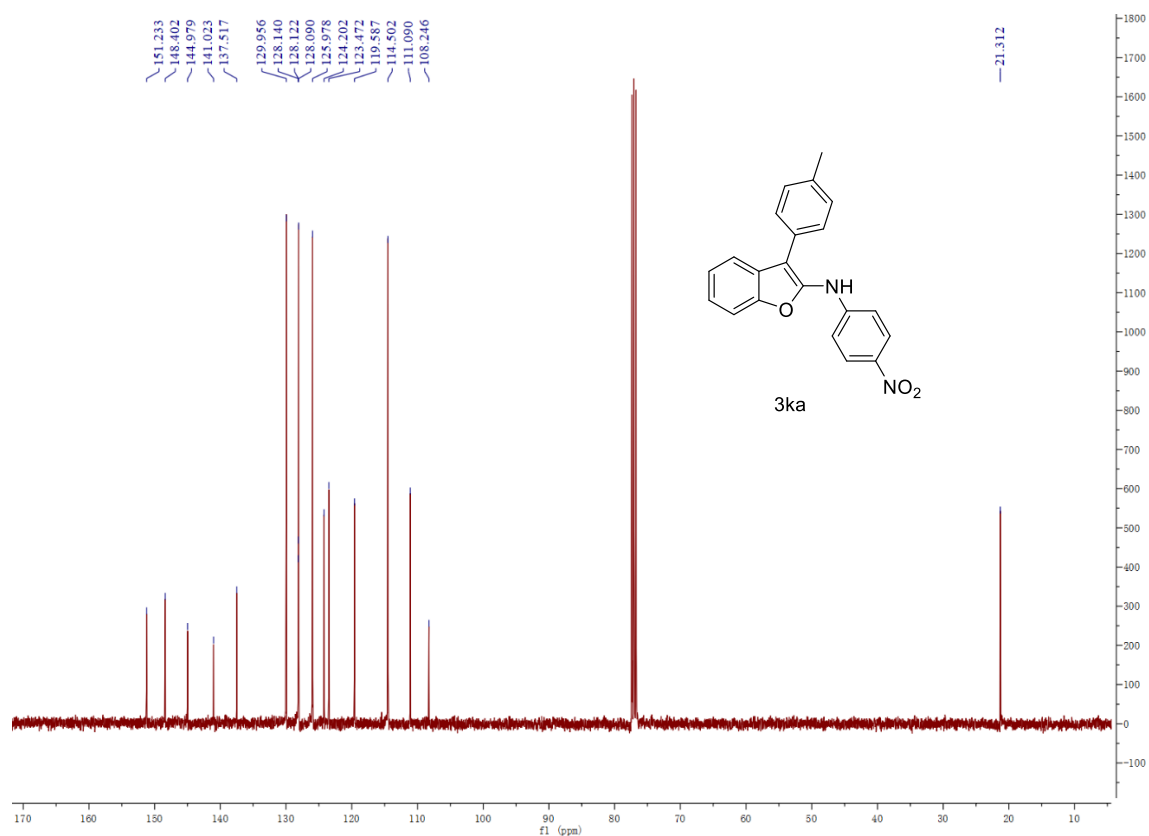


Figure S24. The ¹³C NMR of compound 3ka.

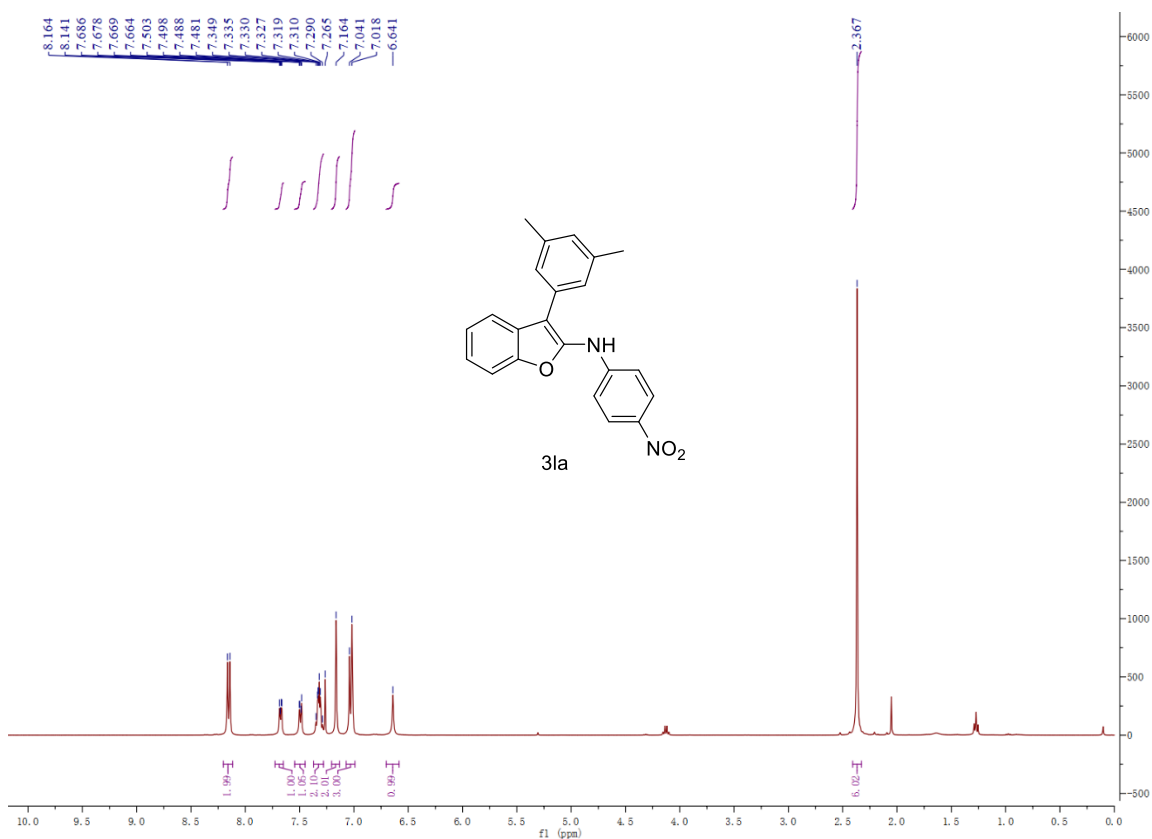


Figure S25. The ¹H NMR of compound 3la.

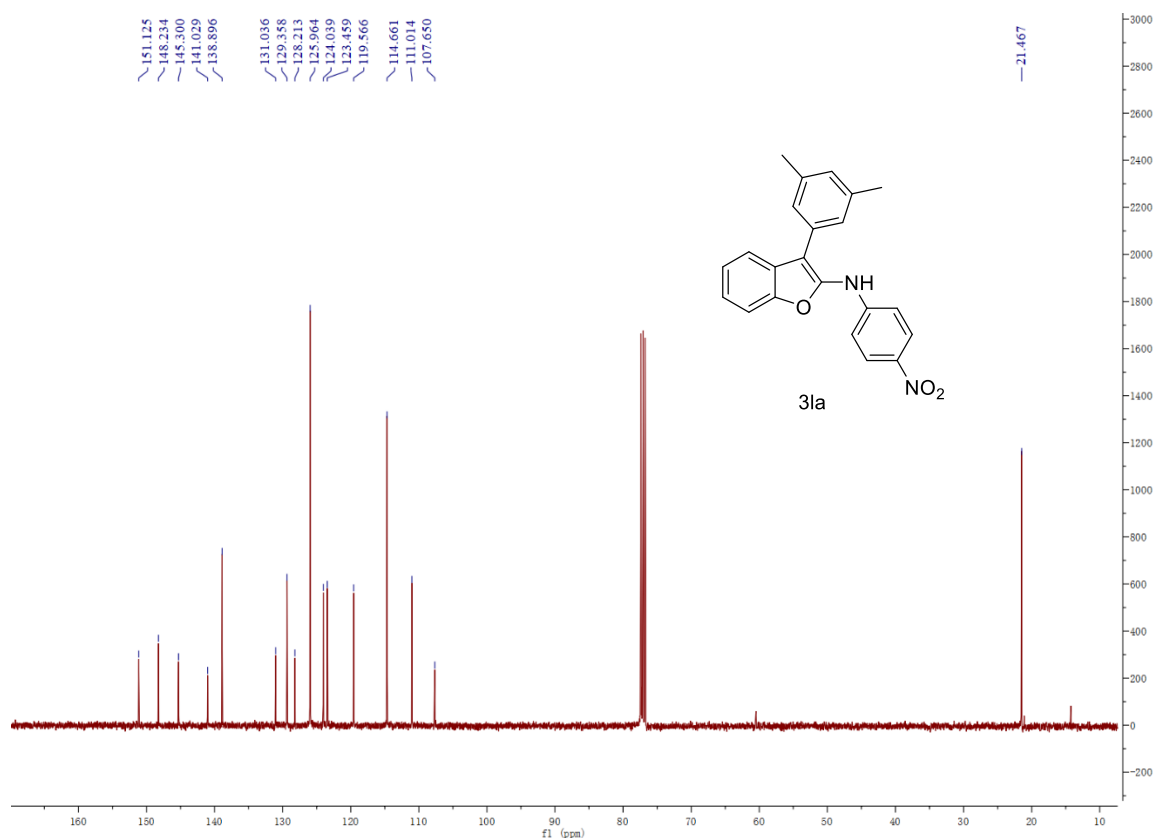


Figure S26. The ¹³C NMR of compound 3la.

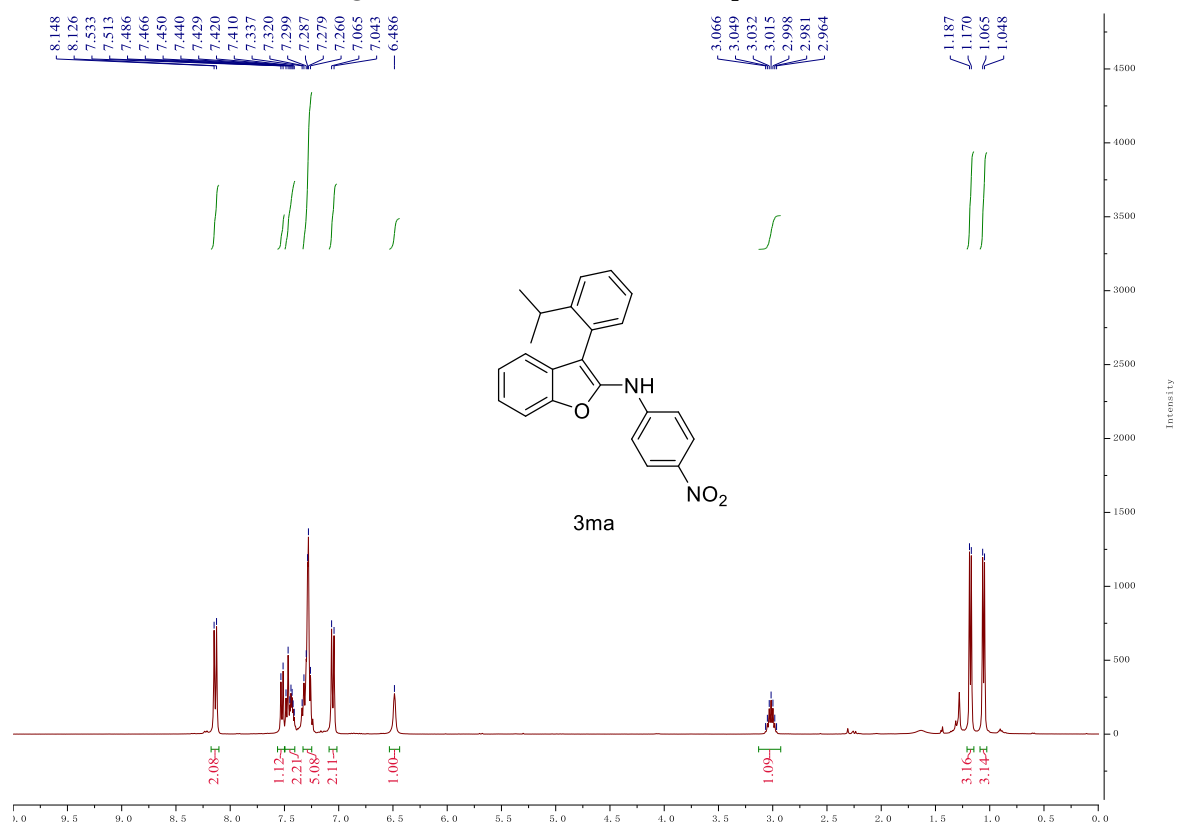


Figure S27. The ¹H NMR of compound 3ma.

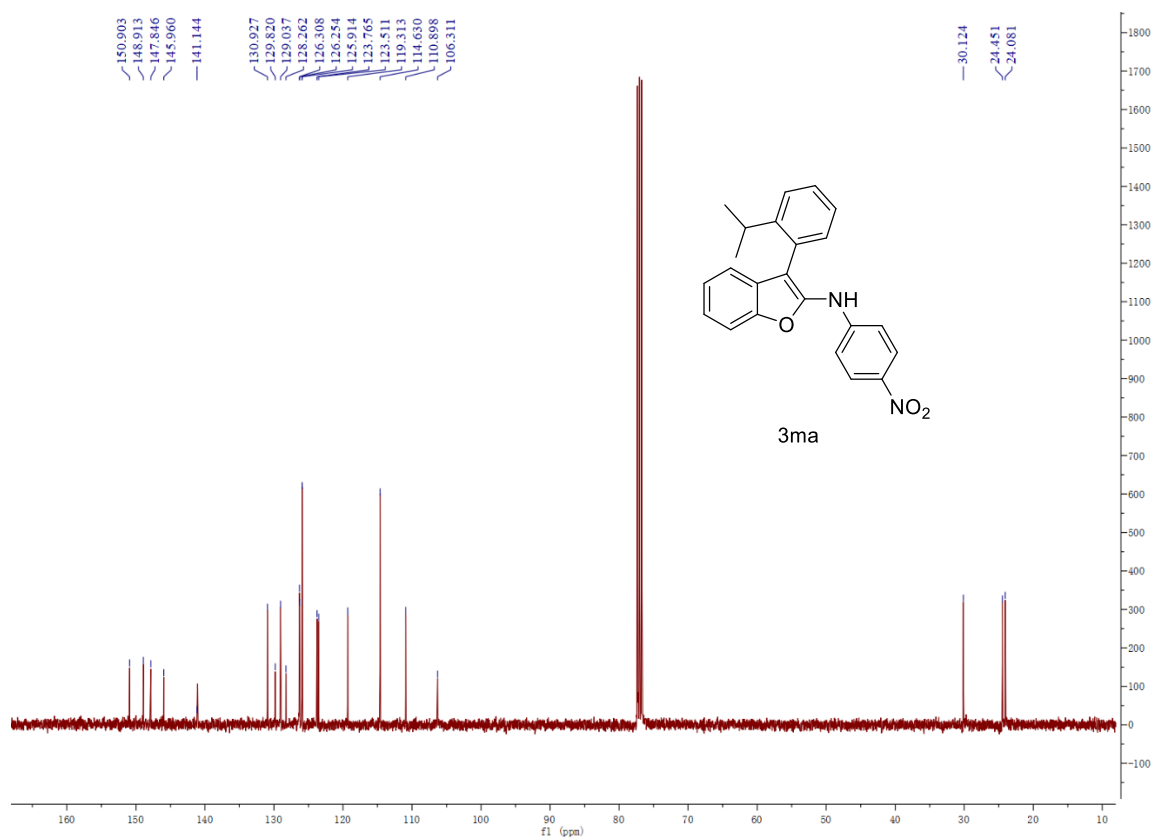


Figure S28. The ¹³C NMR of compound 3ma.

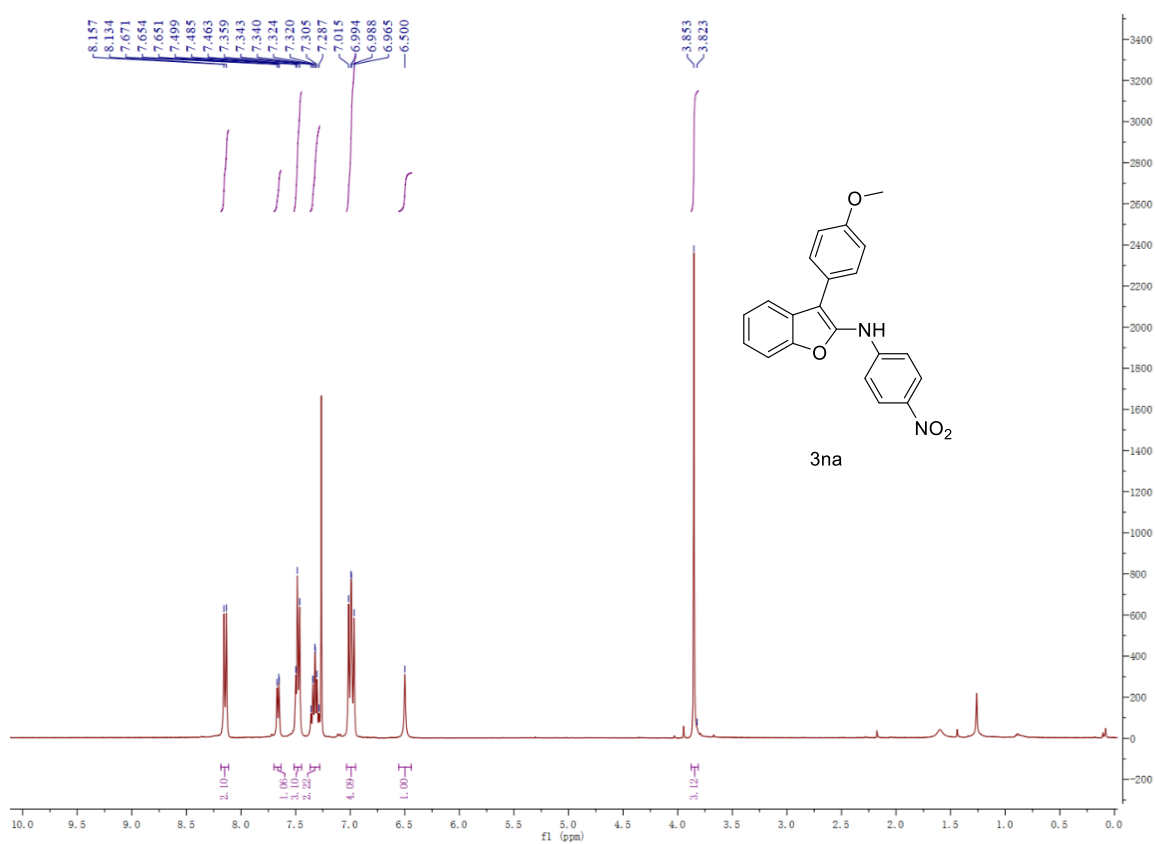


Figure S29. The ¹H NMR of compound 3na.

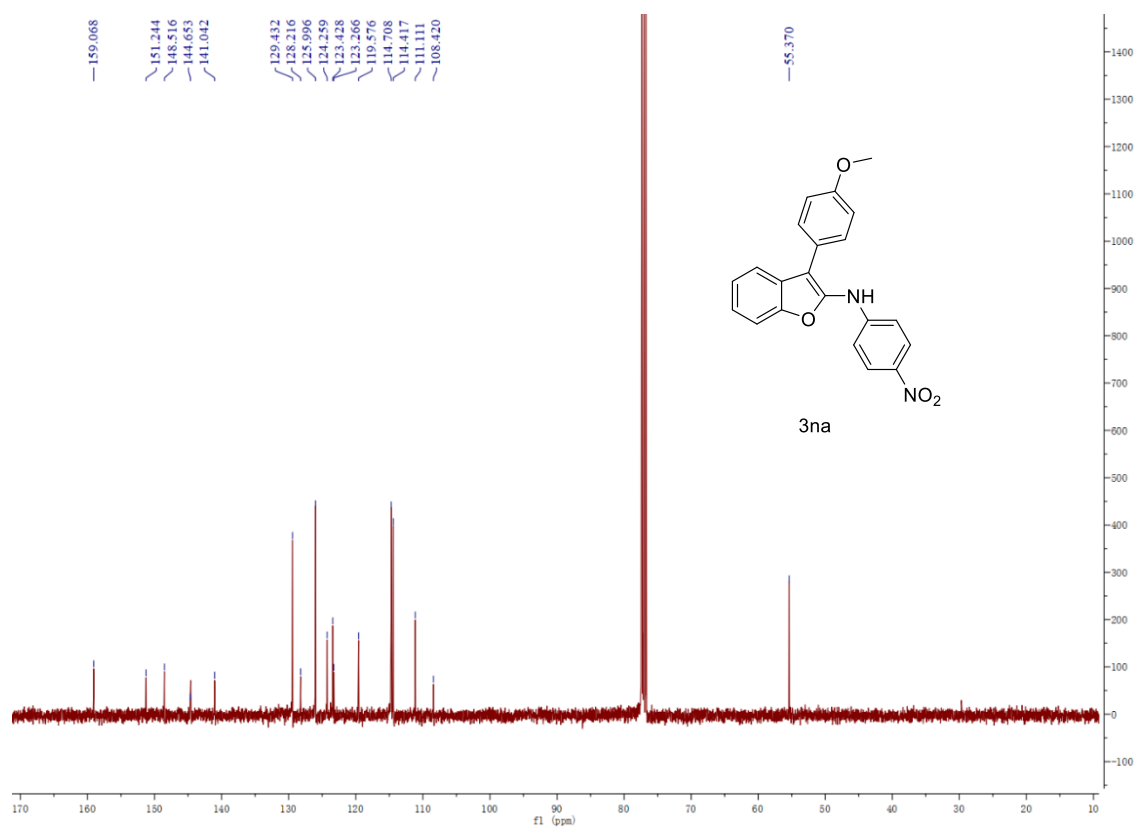


Figure S30. The ¹³C NMR of compound 3na.

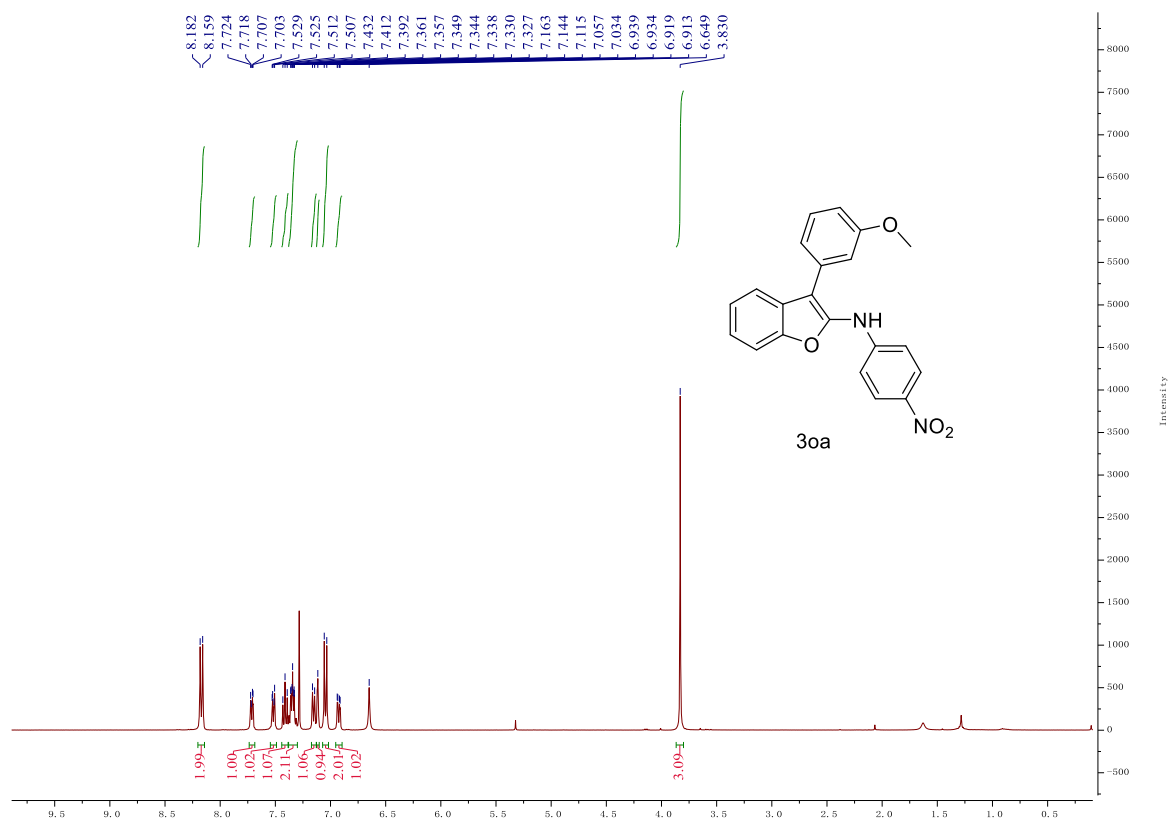


Figure S31. The ¹H NMR of compound 3oa.

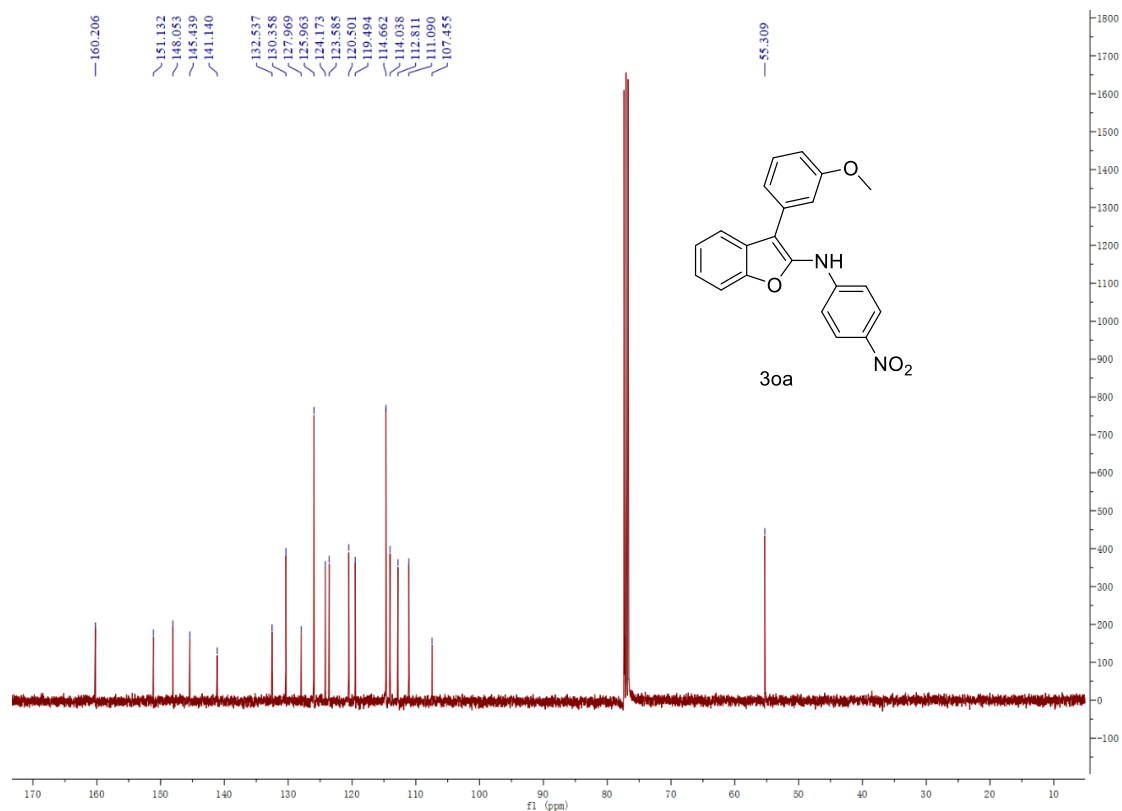


Figure S32. The ¹³C NMR of compound 30a.

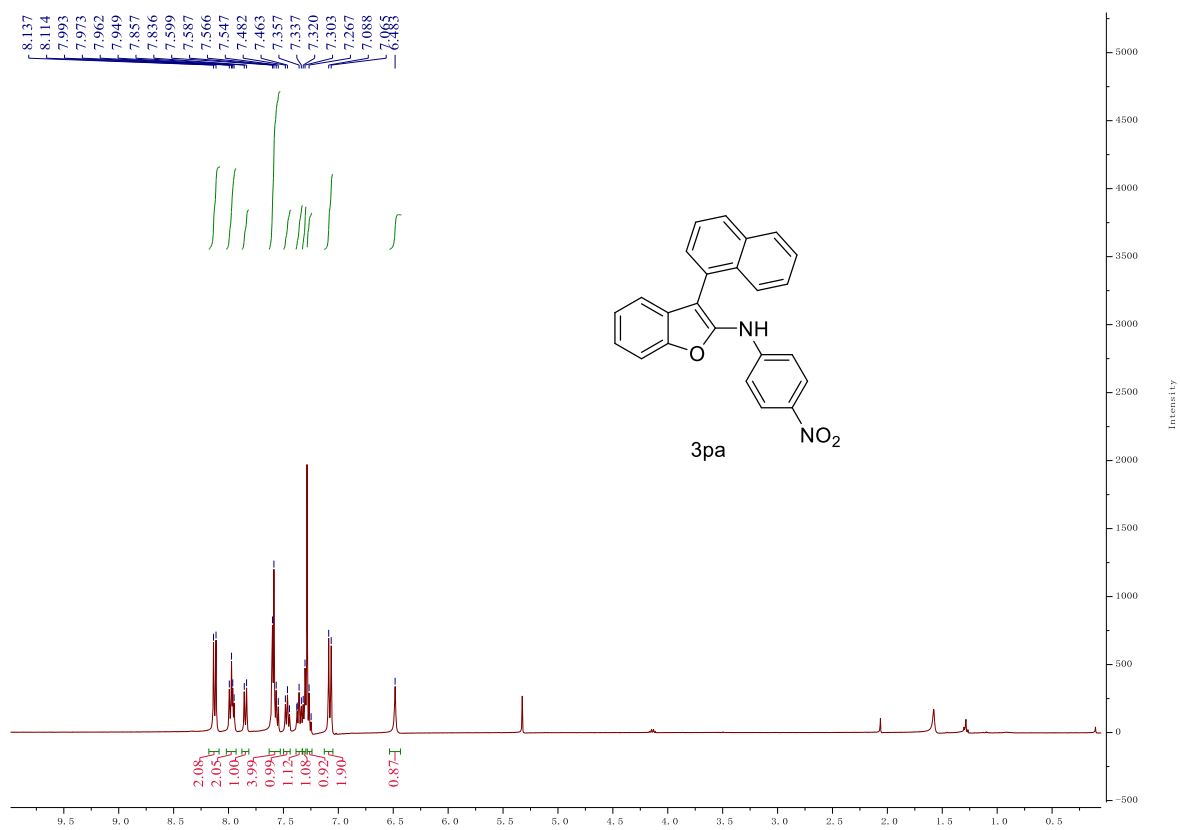


Figure S33. The ¹H NMR of compound 3pa.

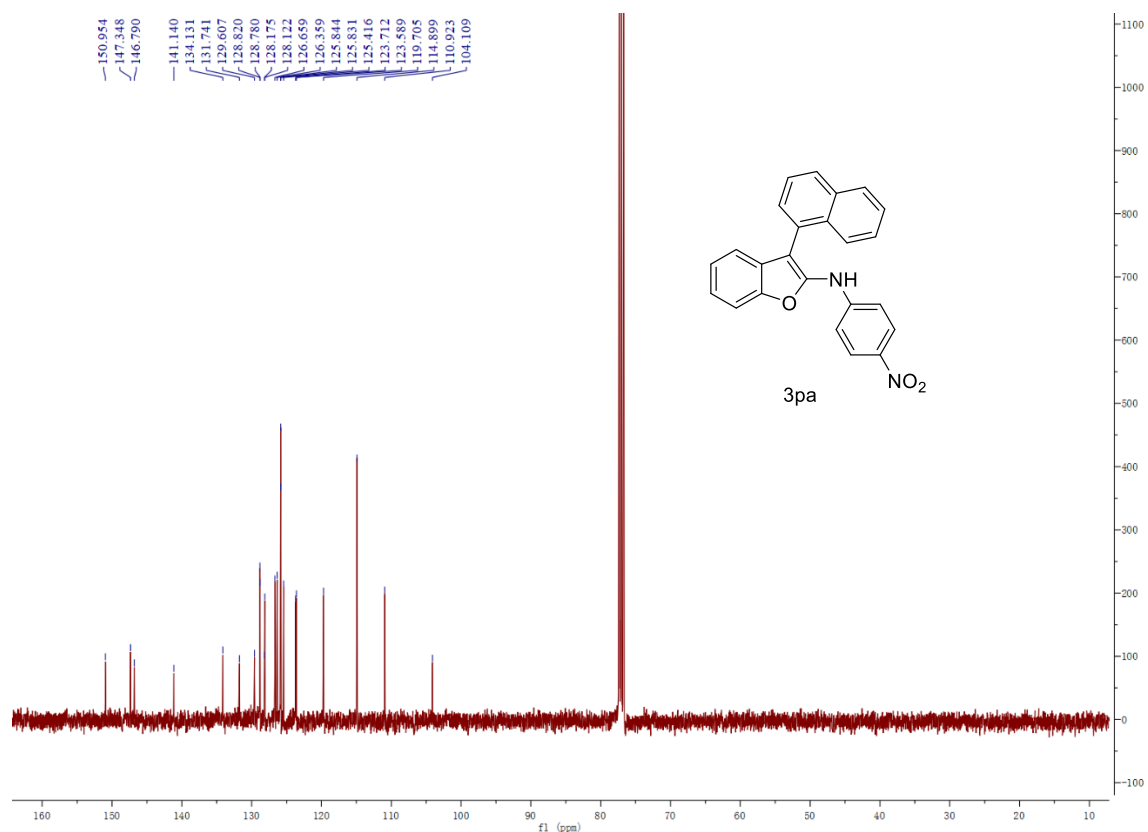


Figure S34. The ¹³C NMR of compound 3pa.

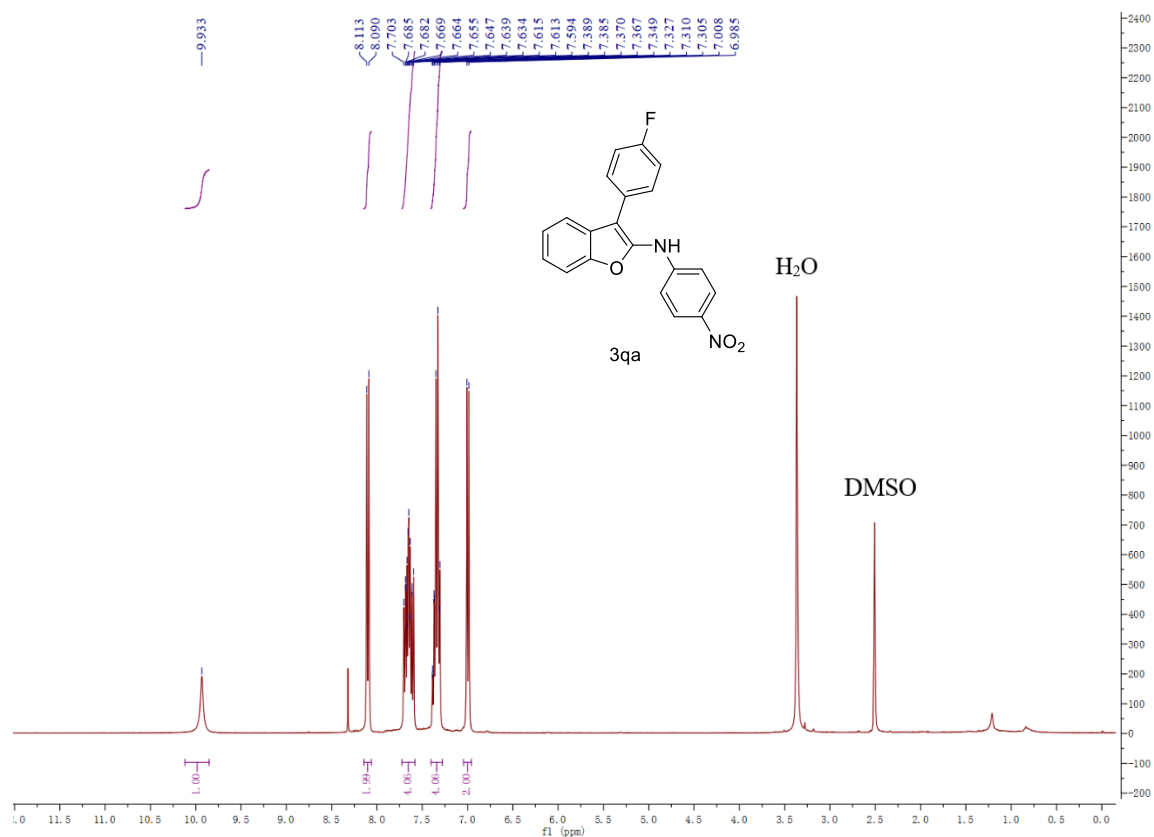


Figure S35. The ¹H NMR of compound 3qa.

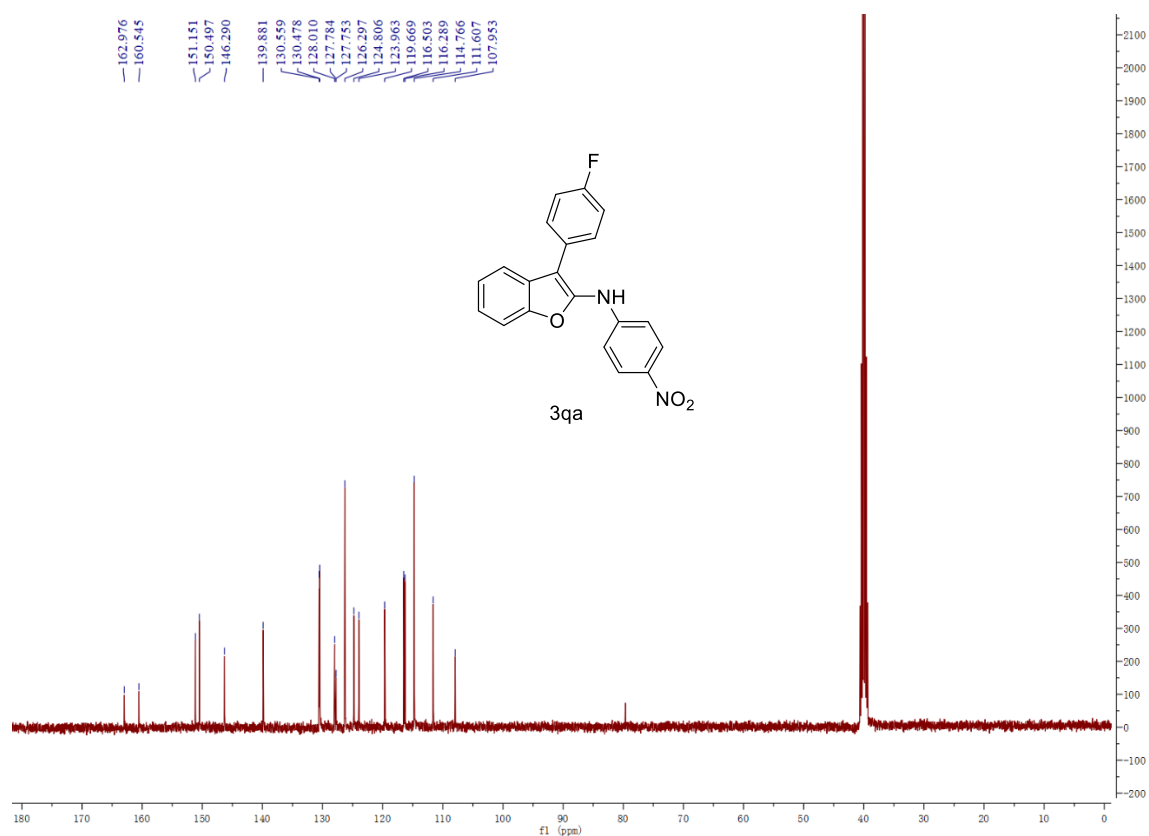


Figure S36. The ¹³C NMR of compound 3qa.

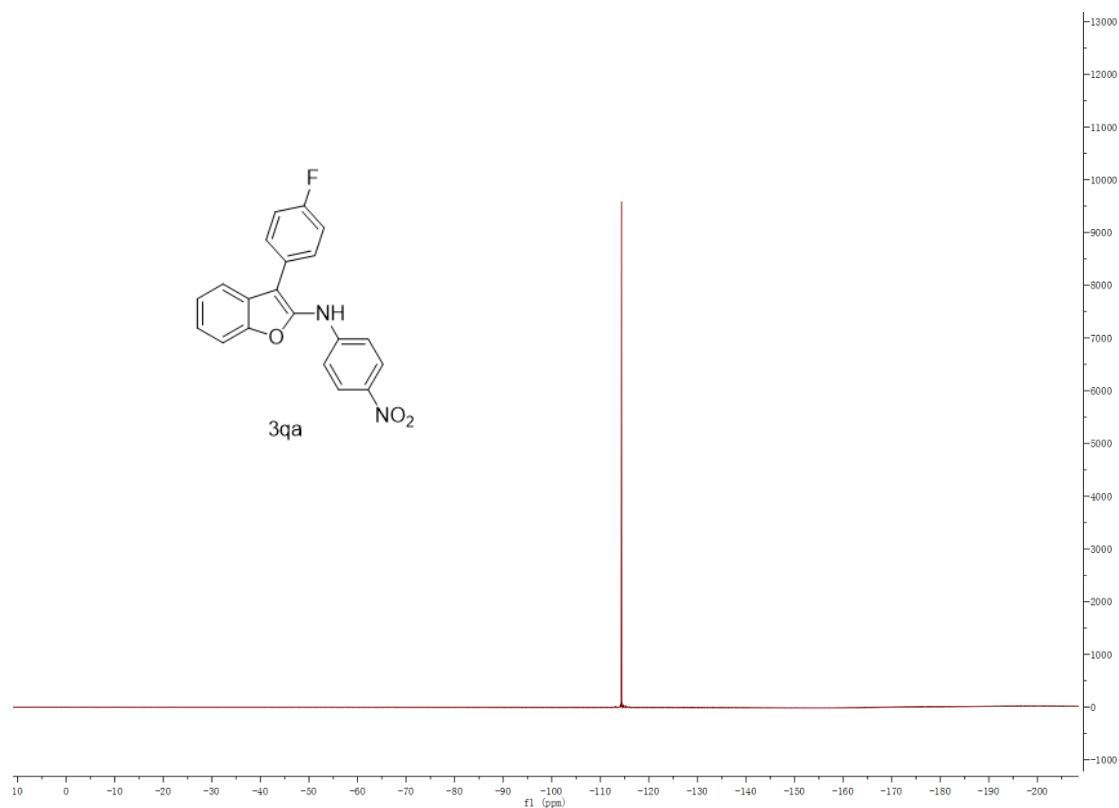


Figure S37. The ¹⁹F NMR of compound 3qa.

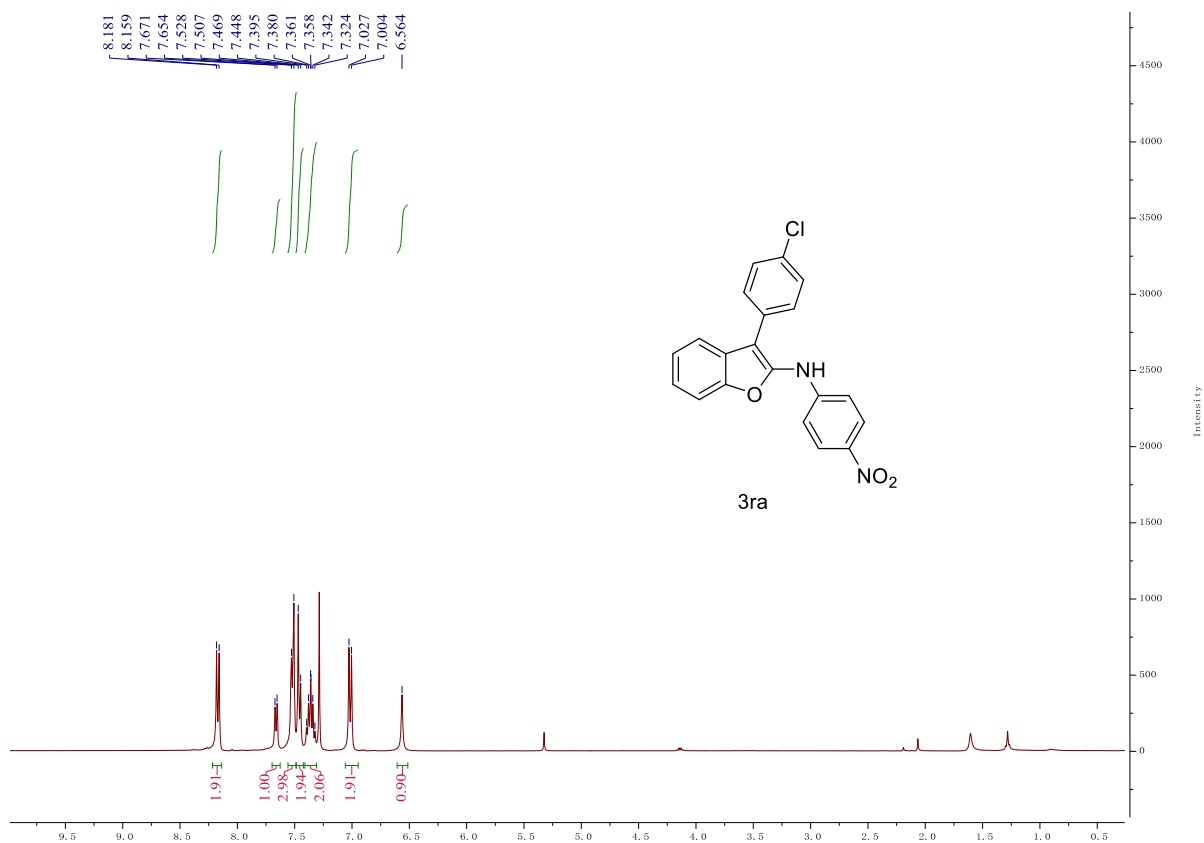


Figure S38. The ¹H NMR of compound 3ra.

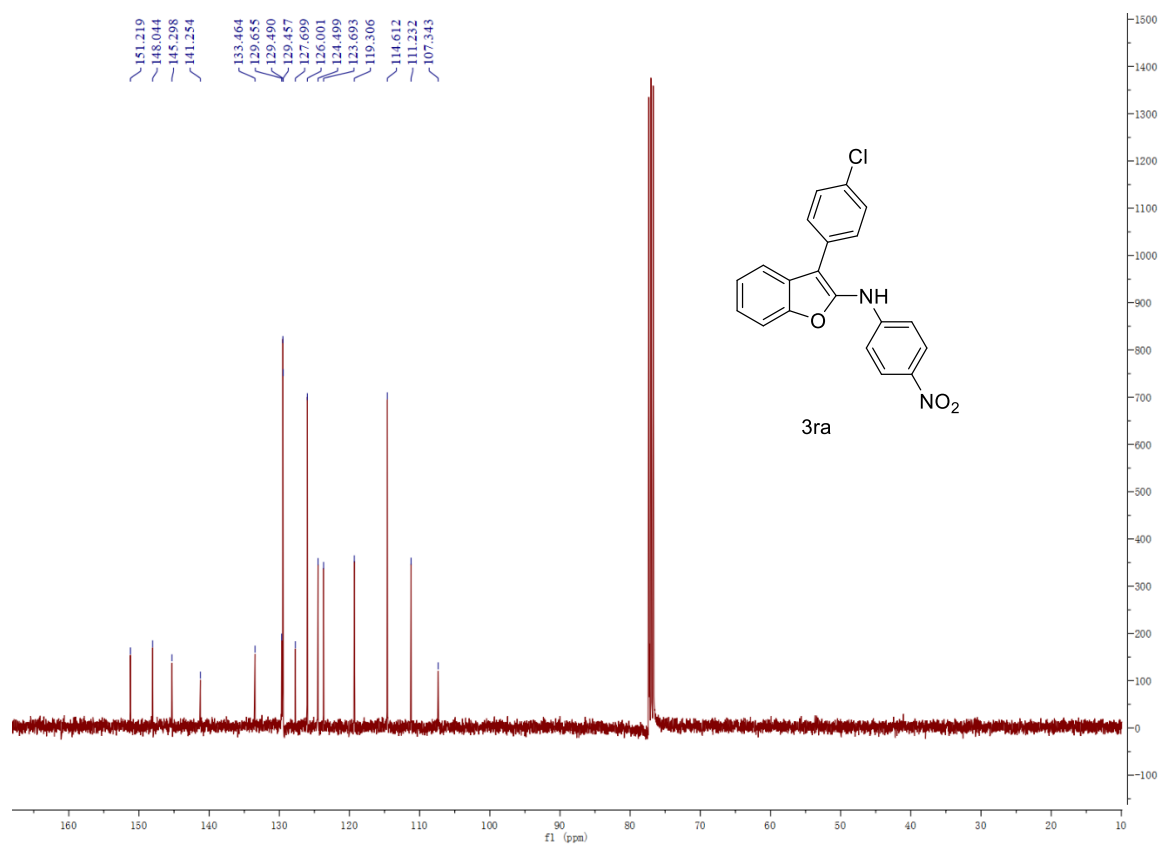


Figure S39. The ¹³C NMR of compound 3ra.

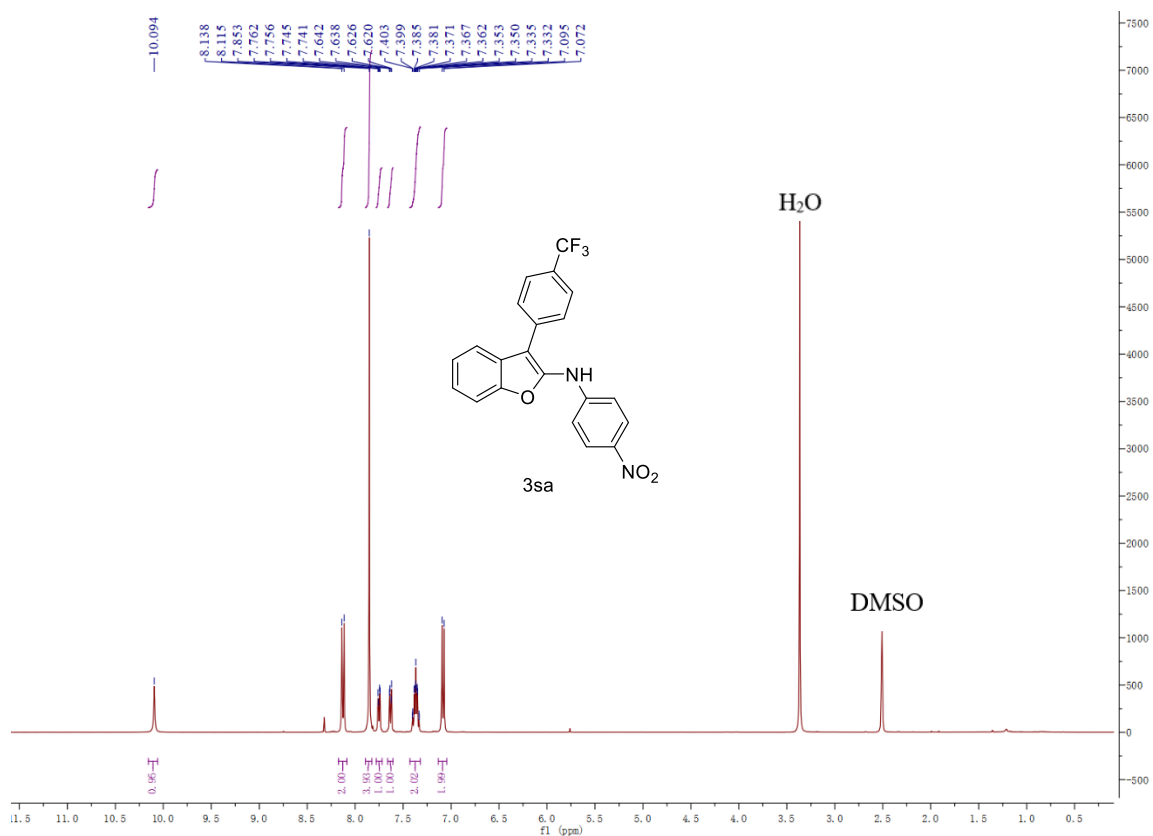


Figure S40. The ¹H NMR of compound 3sa.

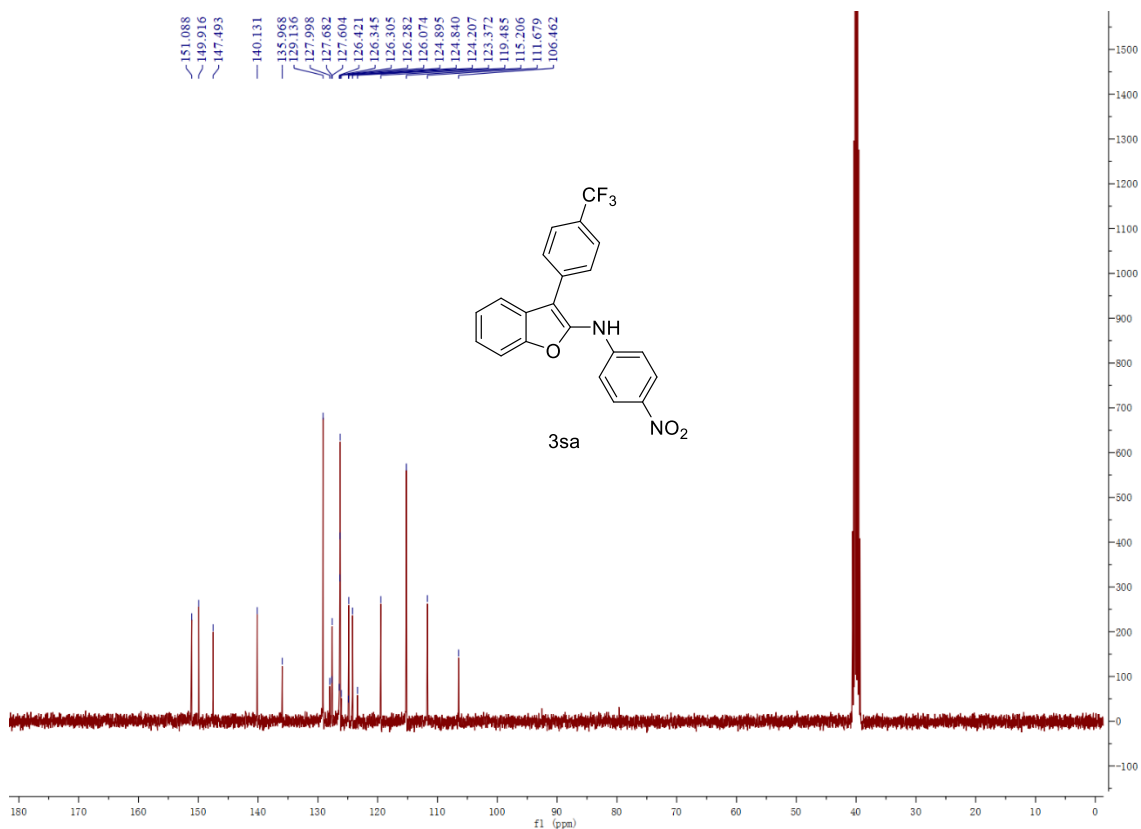


Figure S41. The ¹³C NMR of compound 3sa.

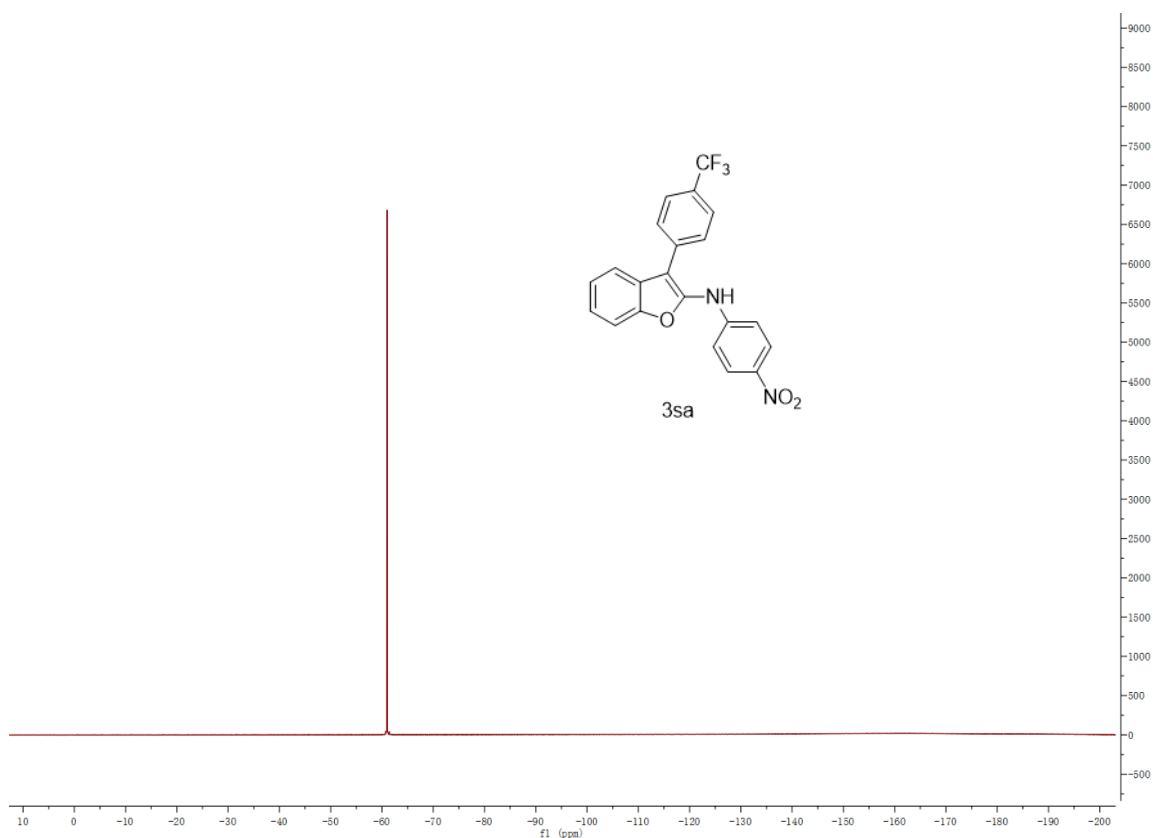


Figure S42. The ¹⁹F NMR of compound 3sa.

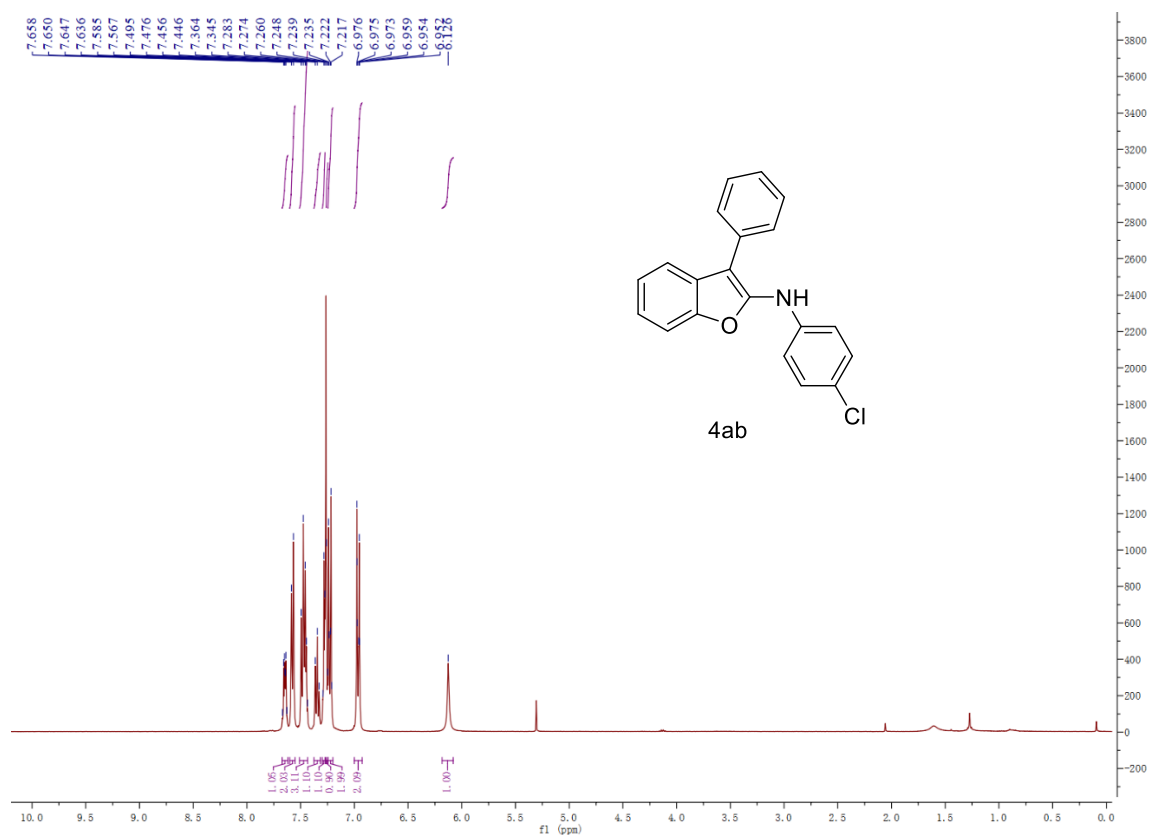


Figure S43. The ¹H NMR of compound 4ab.

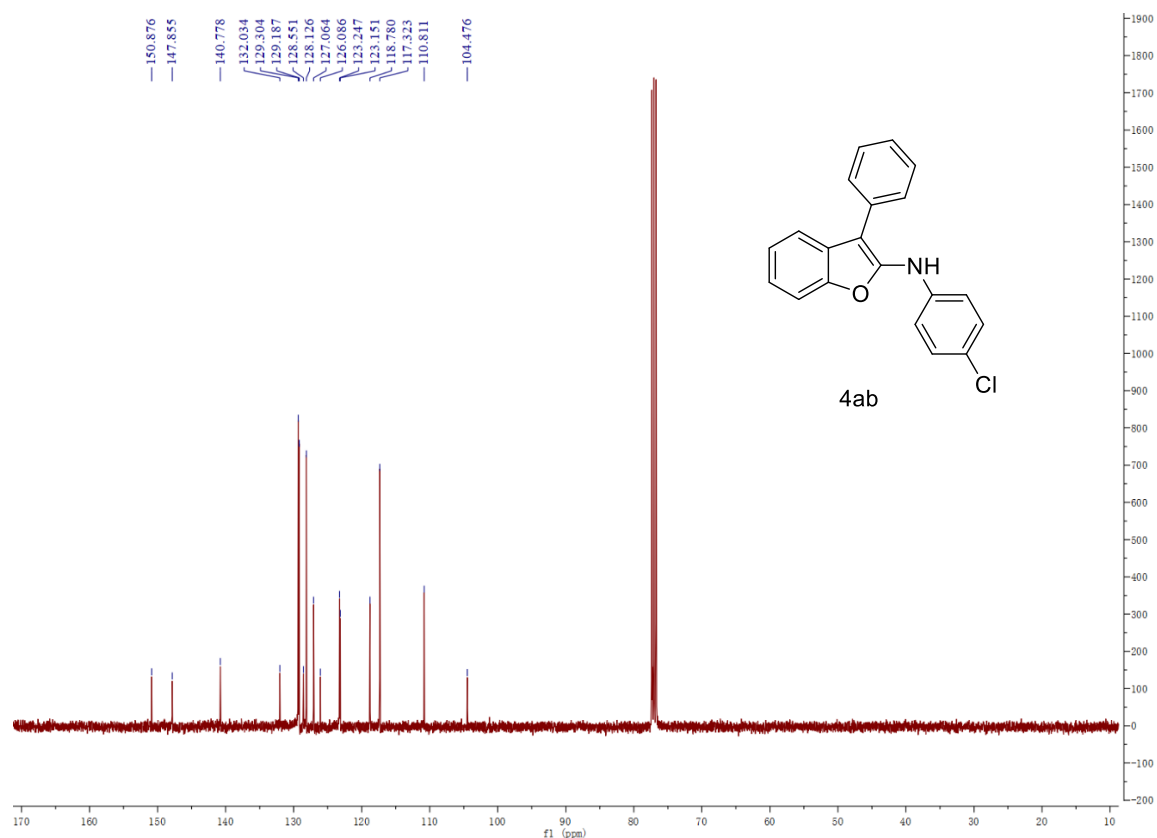


Figure S44. The ¹³C NMR of compound 4ab.

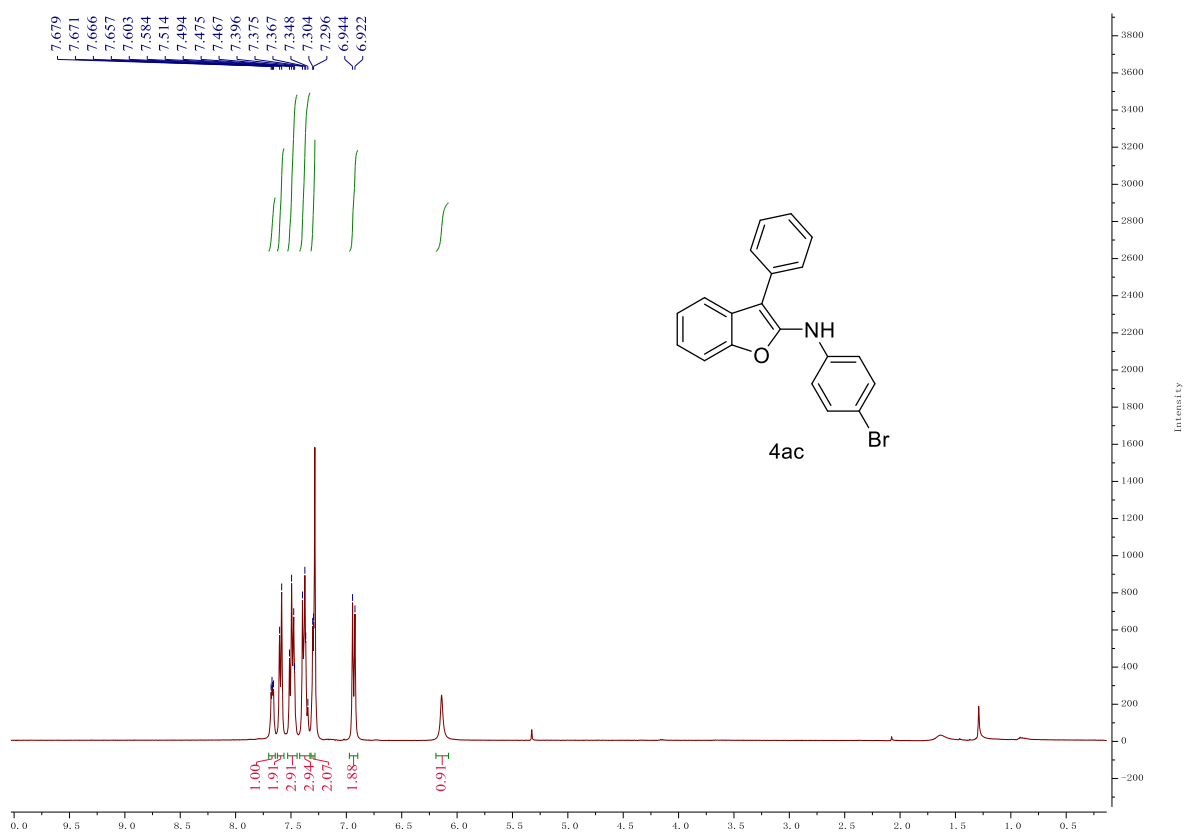


Figure S45. The ¹H NMR of compound 4ac.

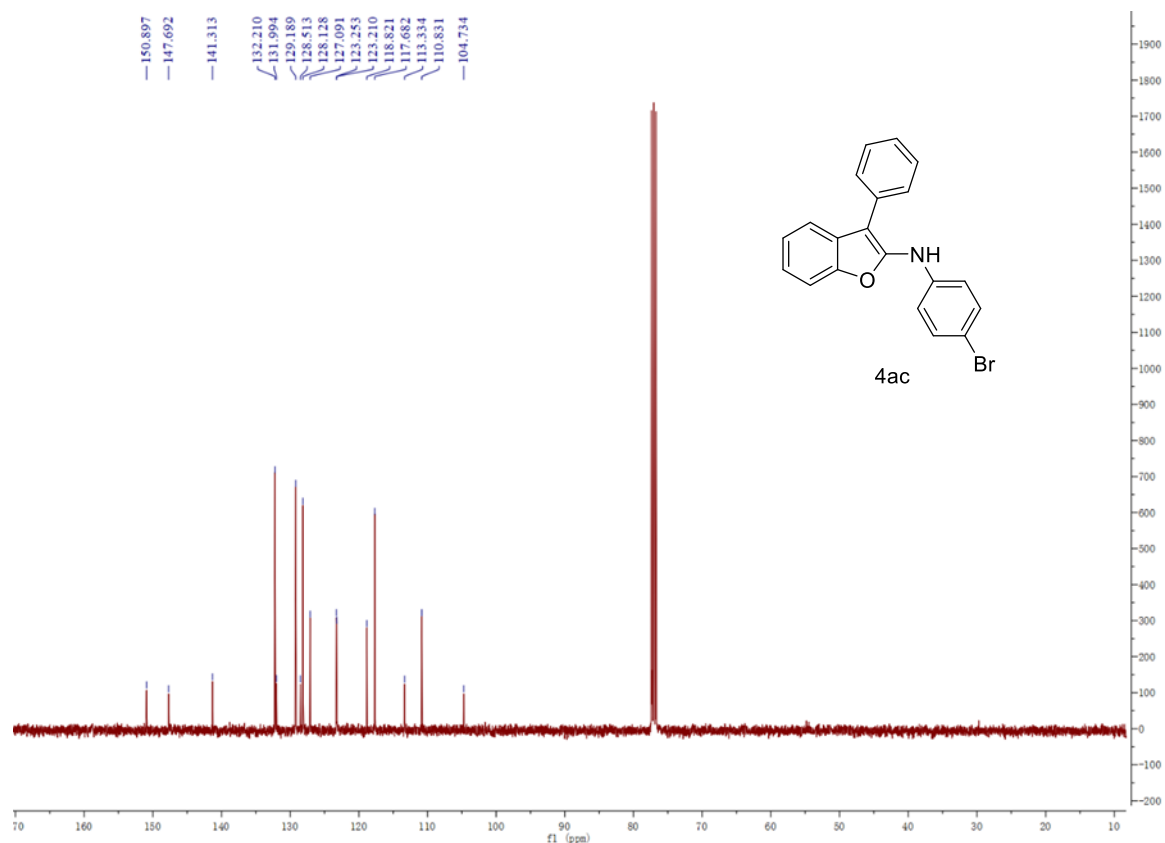


Figure S46. The ¹³C NMR of compound 4ac.

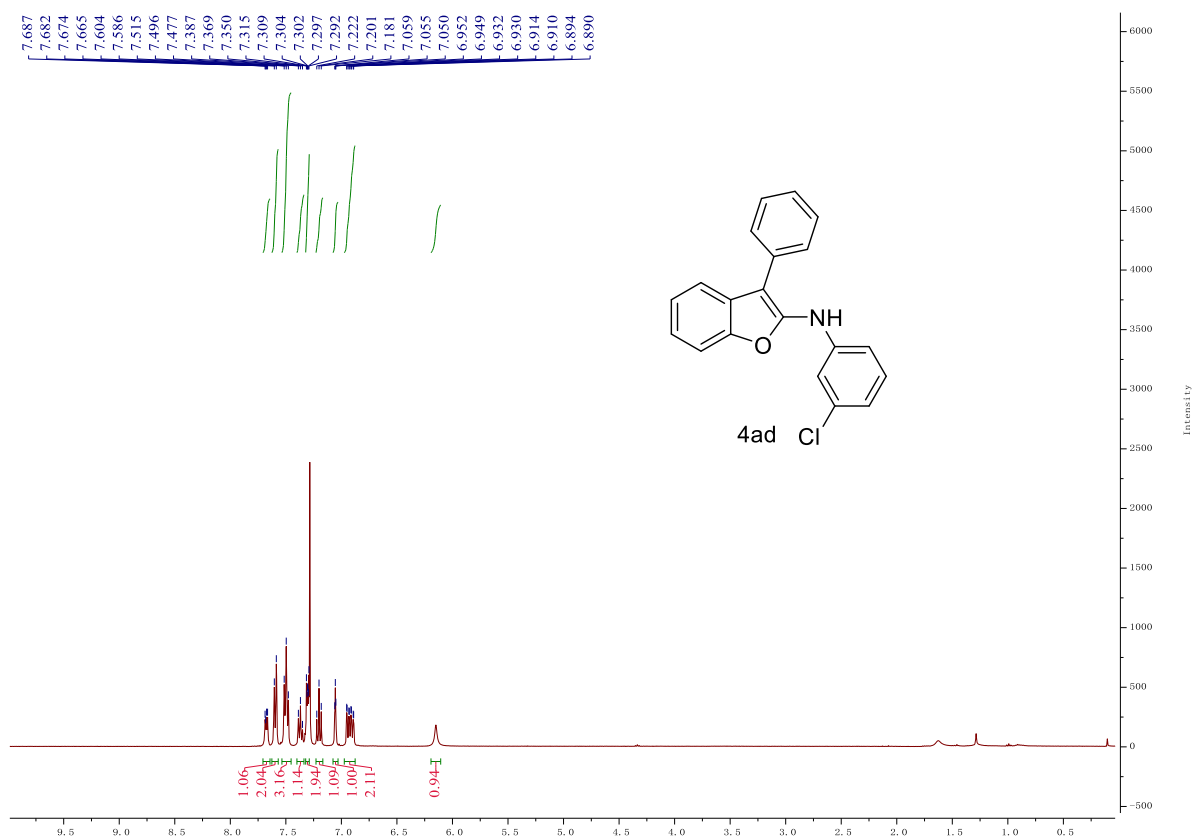


Figure S47. The ¹H NMR of compound 4ad.

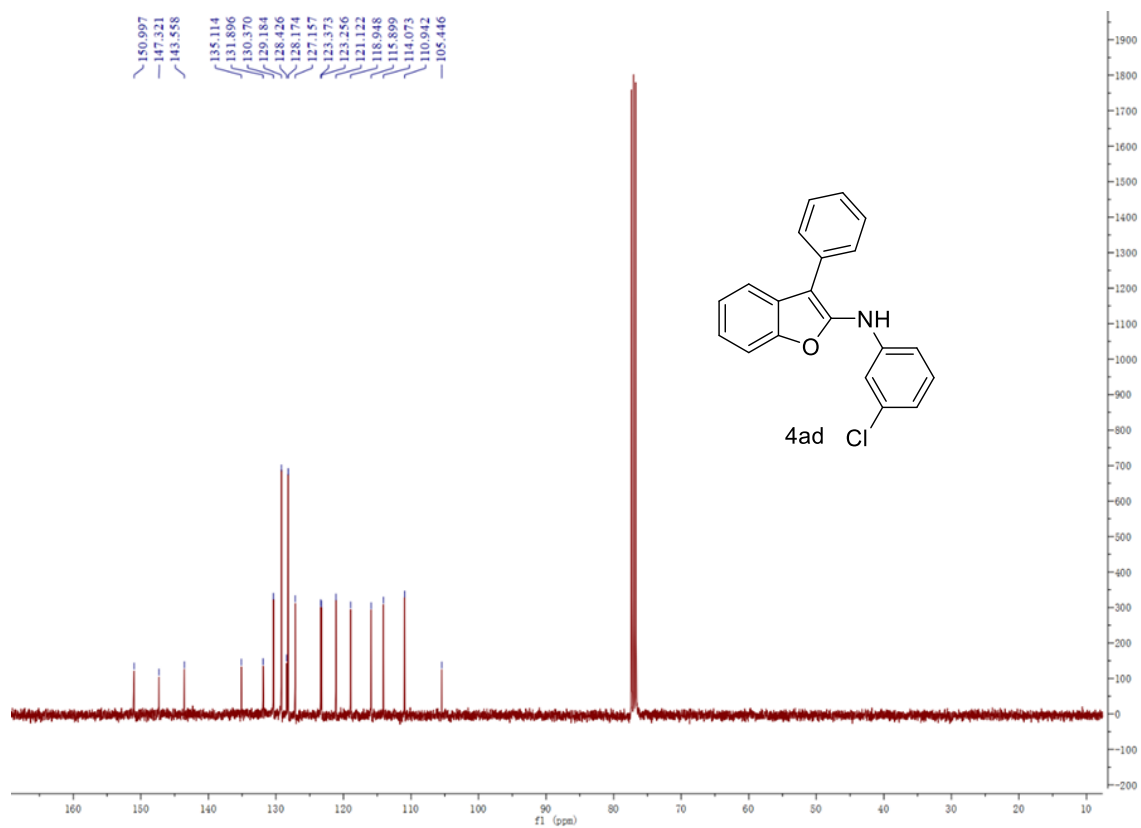


Figure S48. The ¹³C NMR of compound 4ad.

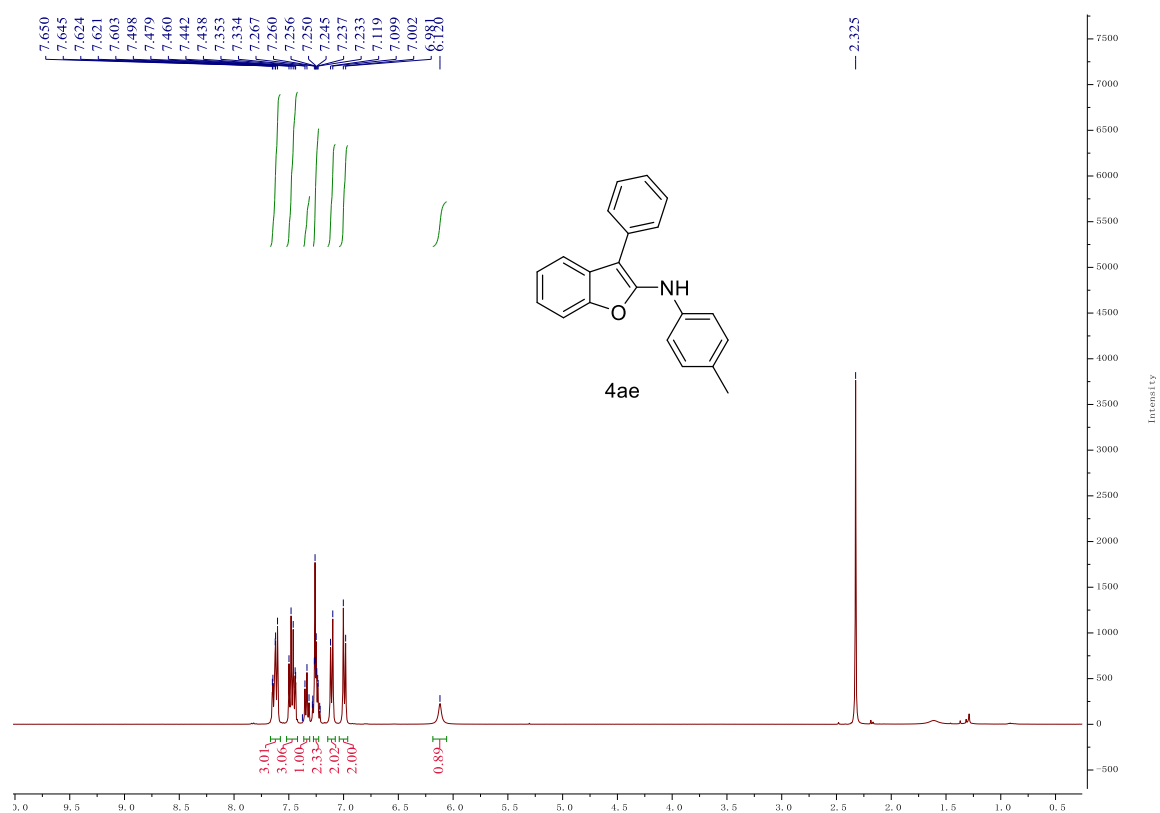


Figure S49. The ¹H NMR of compound 4ae.

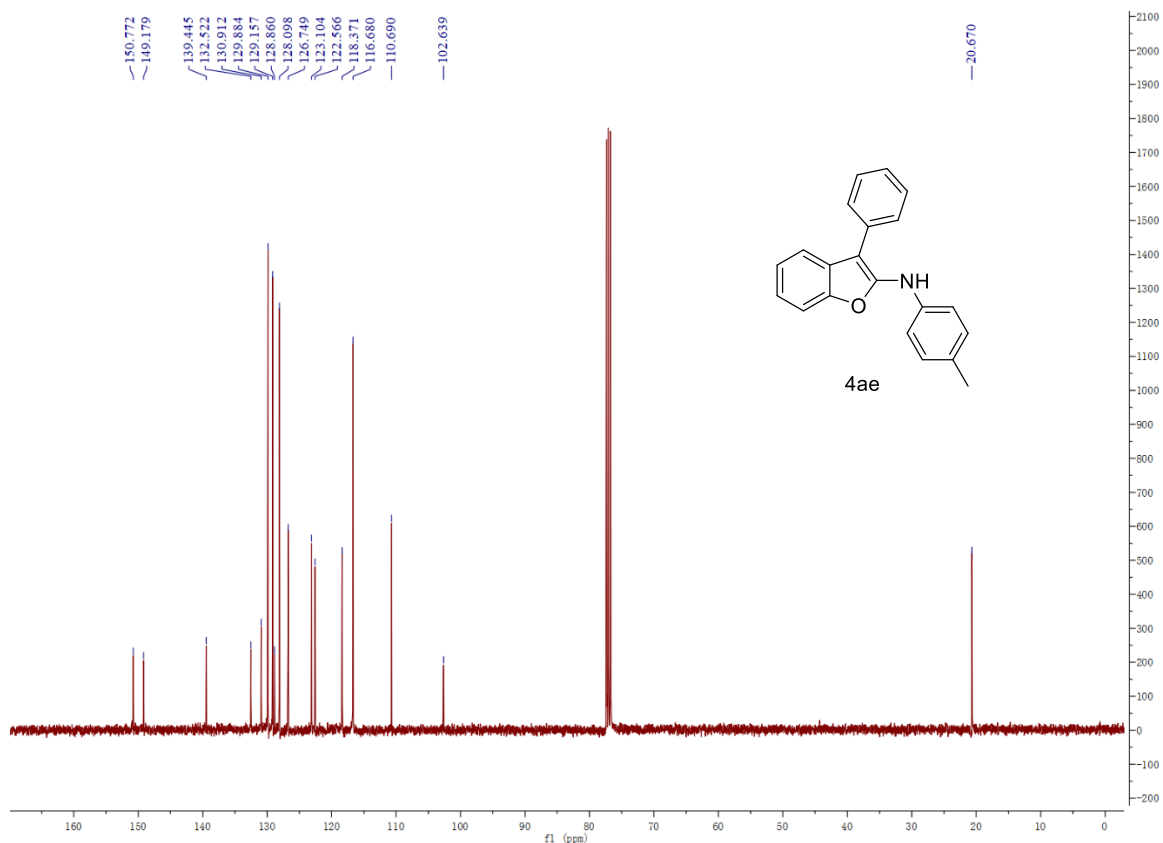


Figure 50. The ¹³C NMR of compound 4ae.

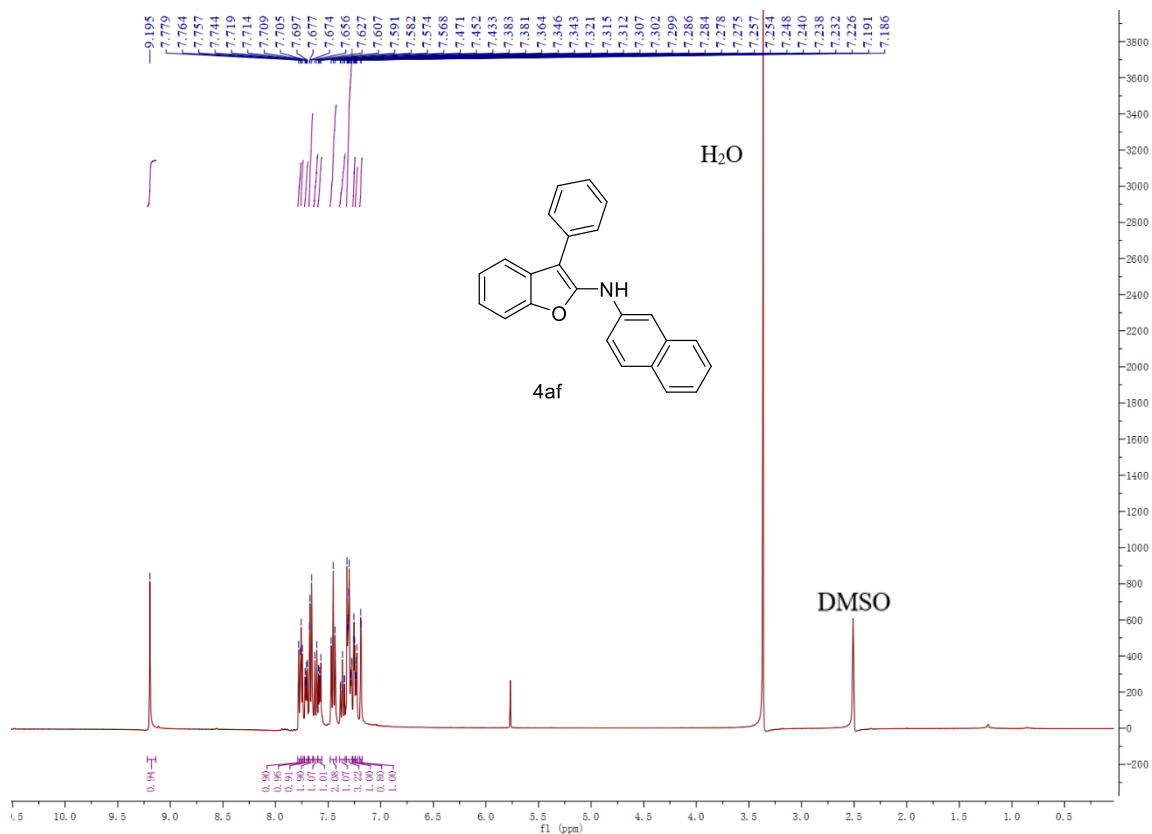


Figure S51. The ¹H NMR of compound 4af.

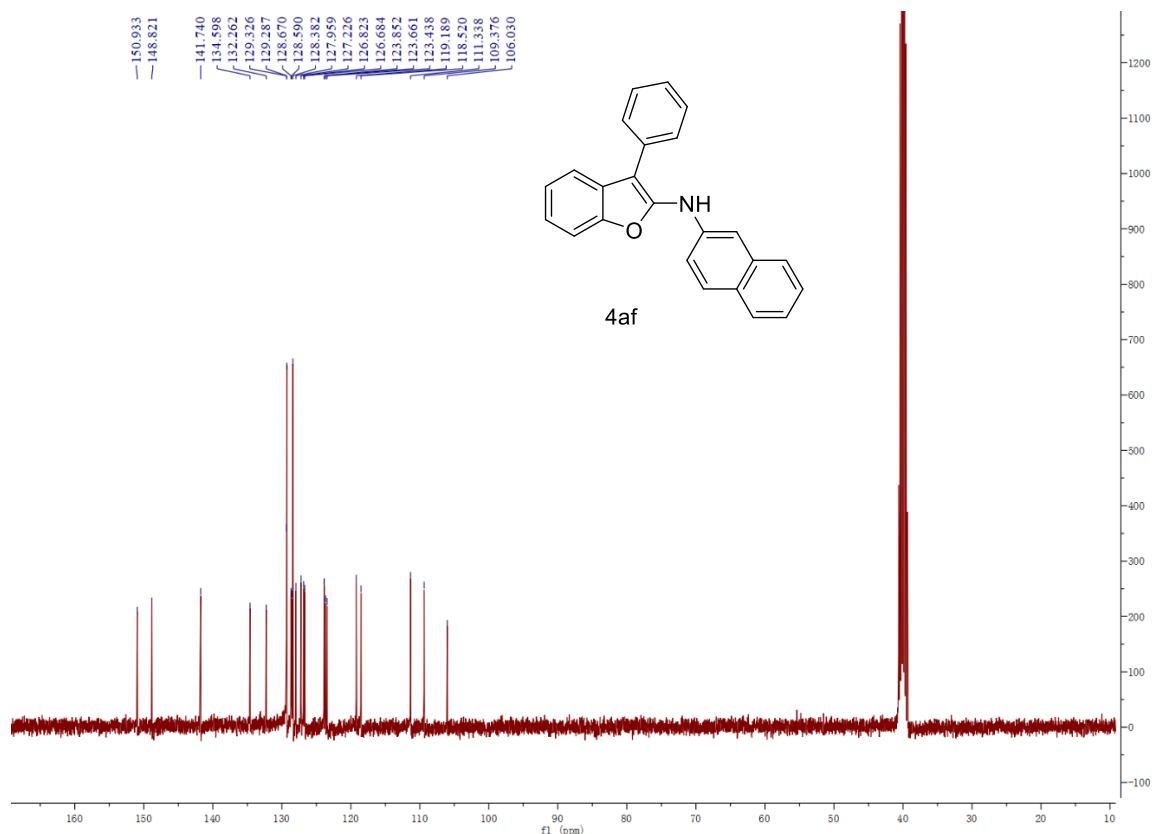


Figure S52. The ¹³C NMR of compound 4af.

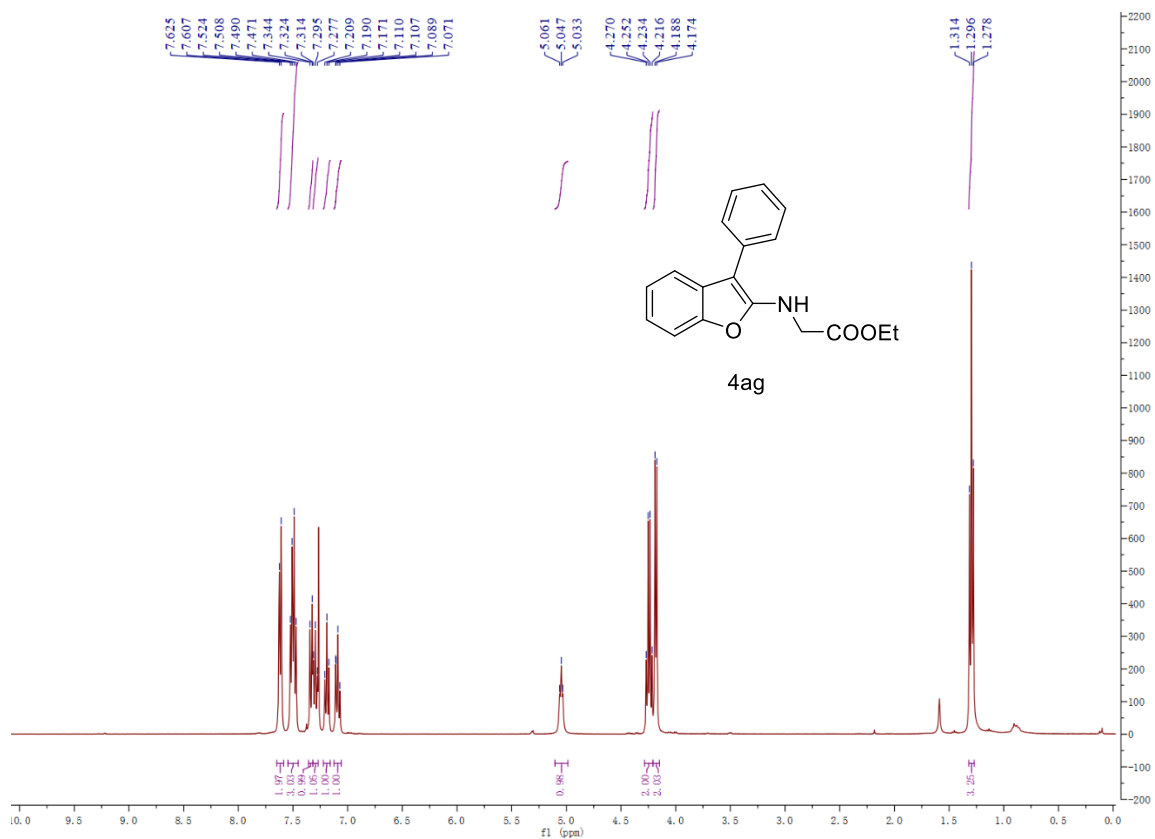


Figure S53. The ¹H NMR of compound 4ag.

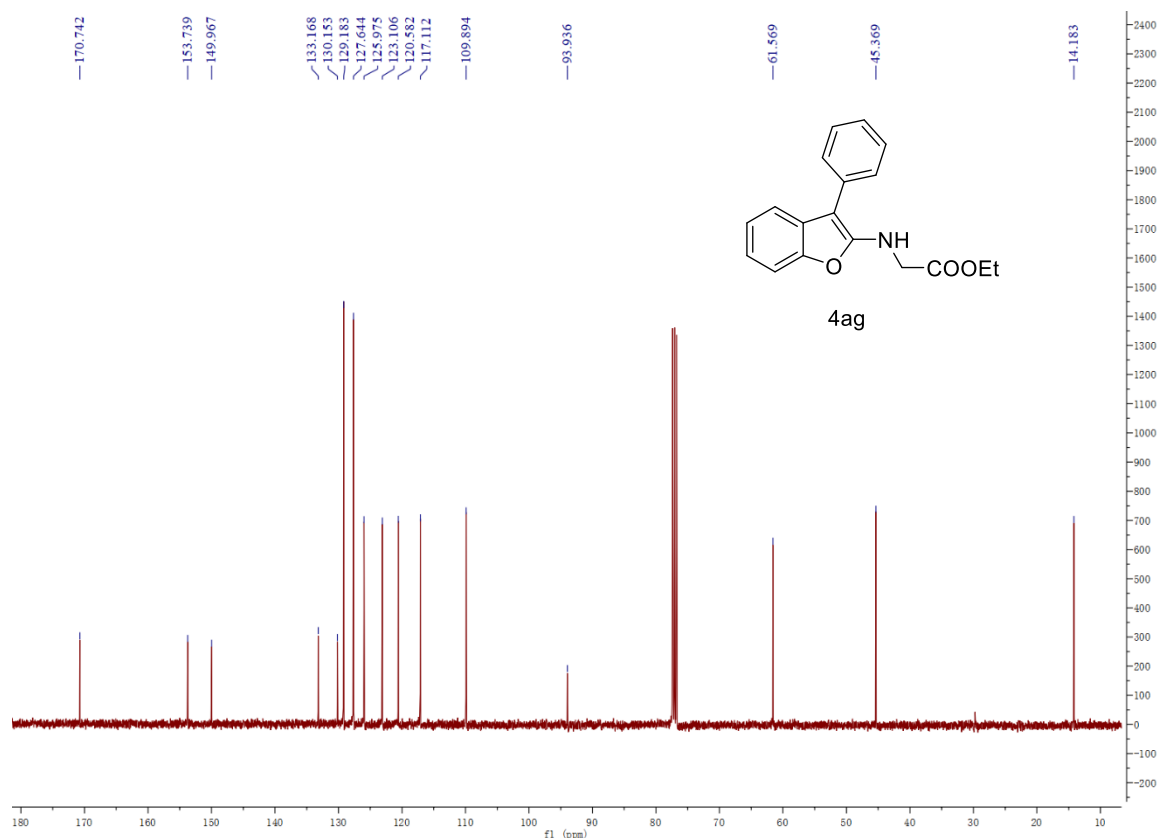


Figure S54. The ¹³C NMR of compound **4ag**.

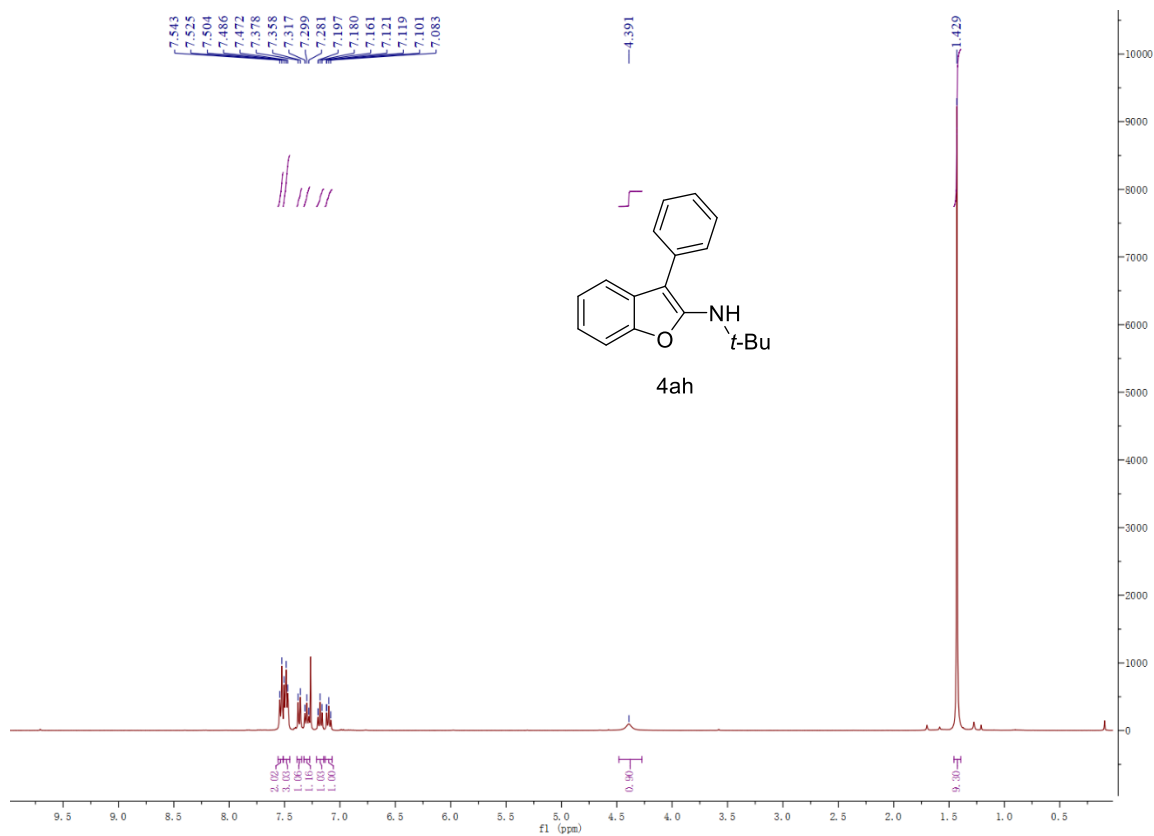


Figure S55. The ¹H NMR of compound **4ah**.

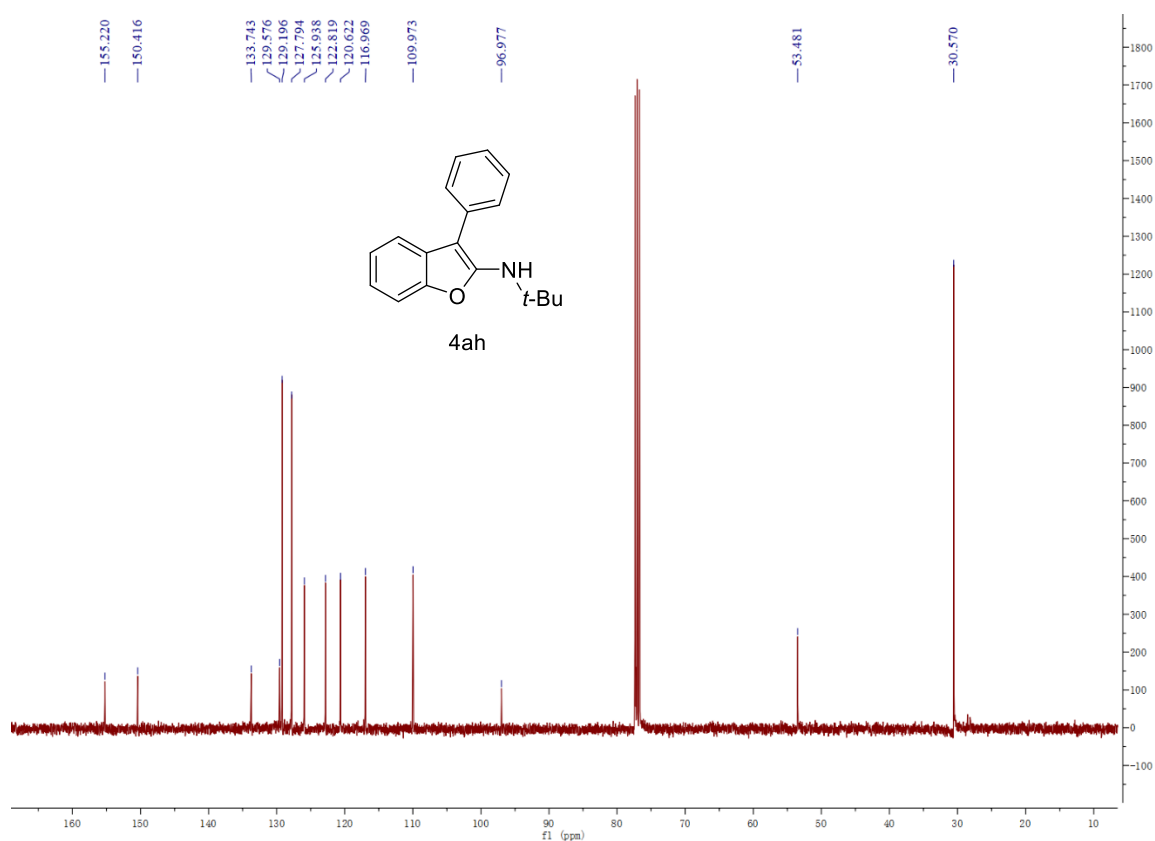


Figure S56. The ¹³C NMR of compound 4ah.