

Electronic supplementary information for the article

Facile chemical access to biologically active norcantharidin derivatives from biomass

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NMR and MS spectra of synthesized compounds

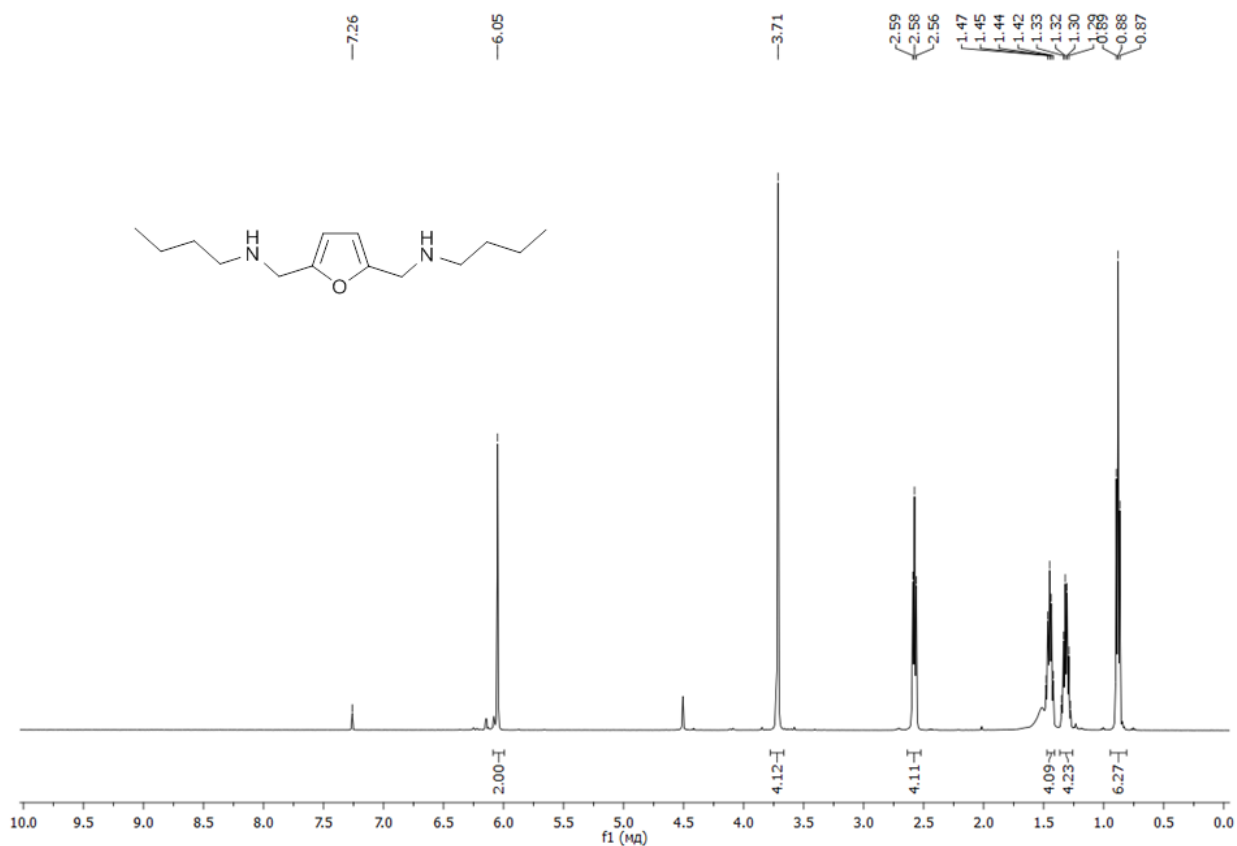


Fig. S1. ¹H NMR spectrum of compound 3 (CDCl₃, 298 K, 500 MHz).

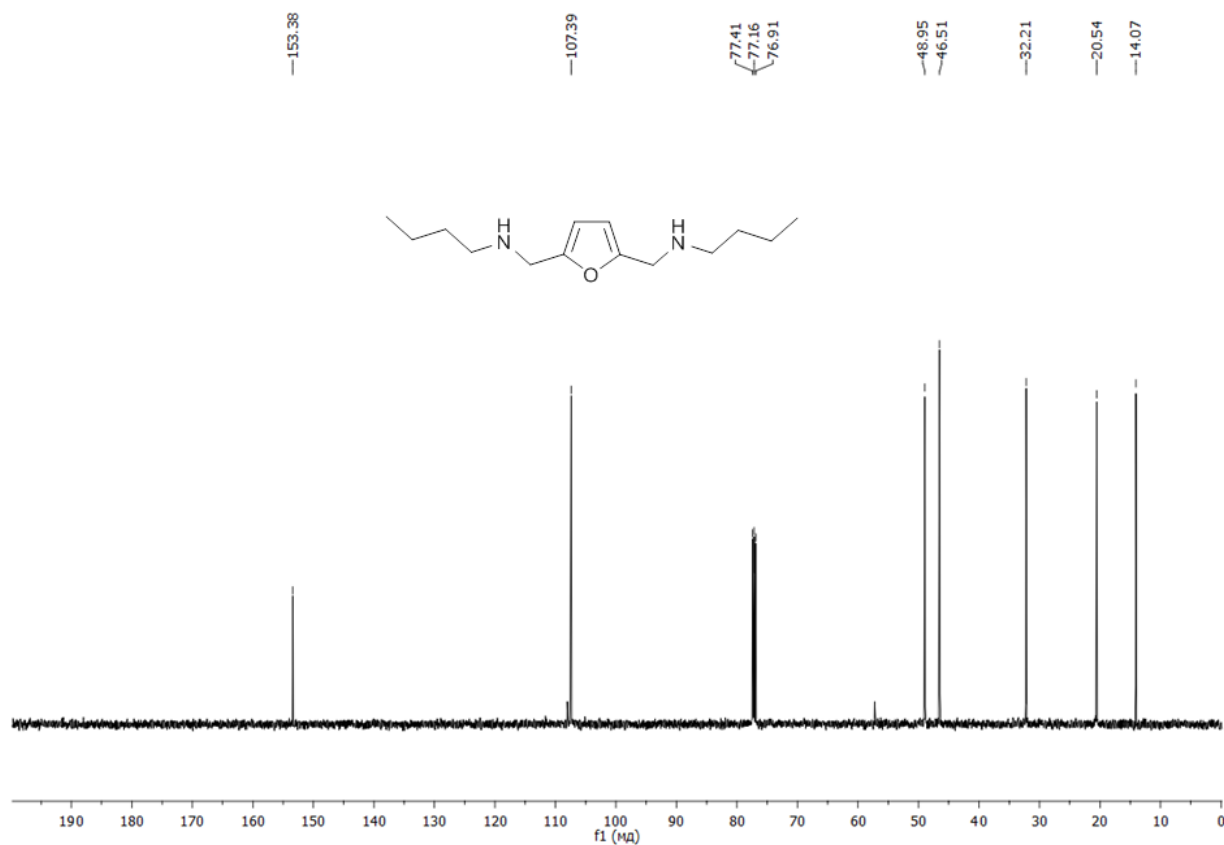


Fig. S2. ¹³C NMR spectrum of compound 3 (CDCl₃, 298 K, 126 MHz).

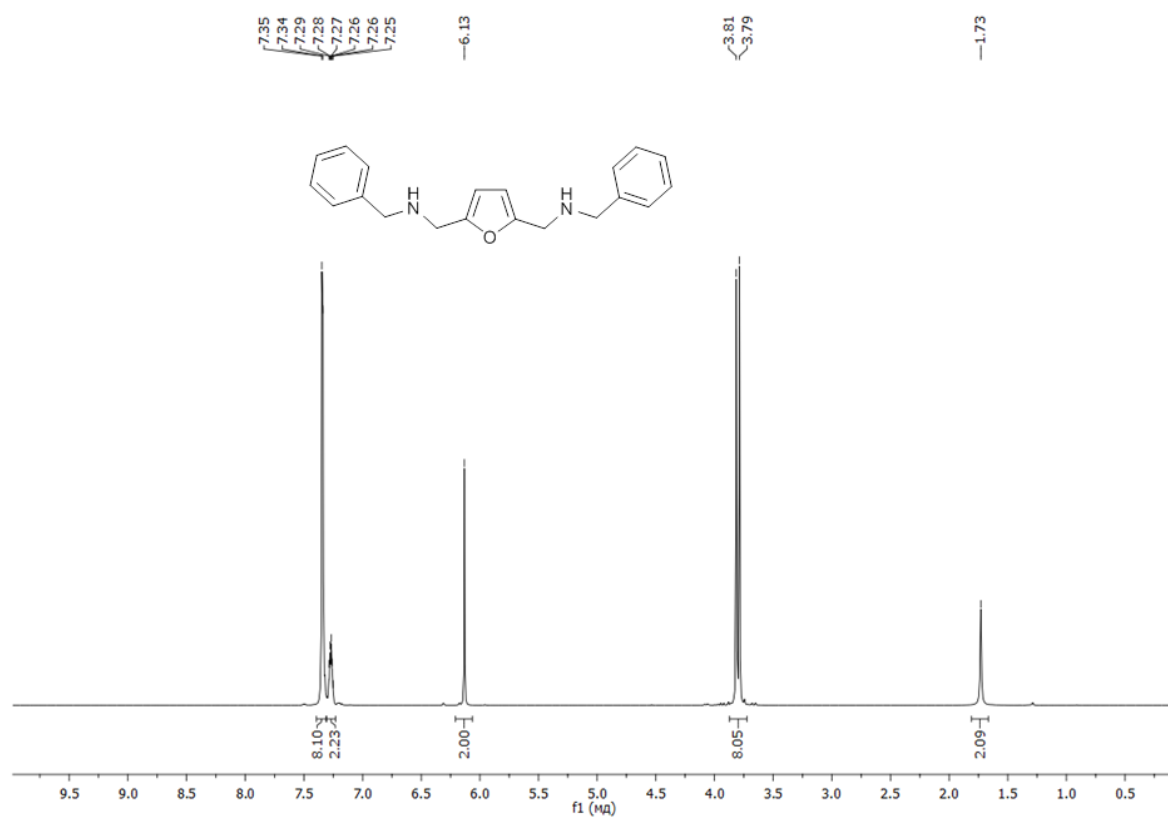


Fig. S3. ¹H NMR spectrum of compound 4 (CDCl₃, 298 K, 500 MHz).

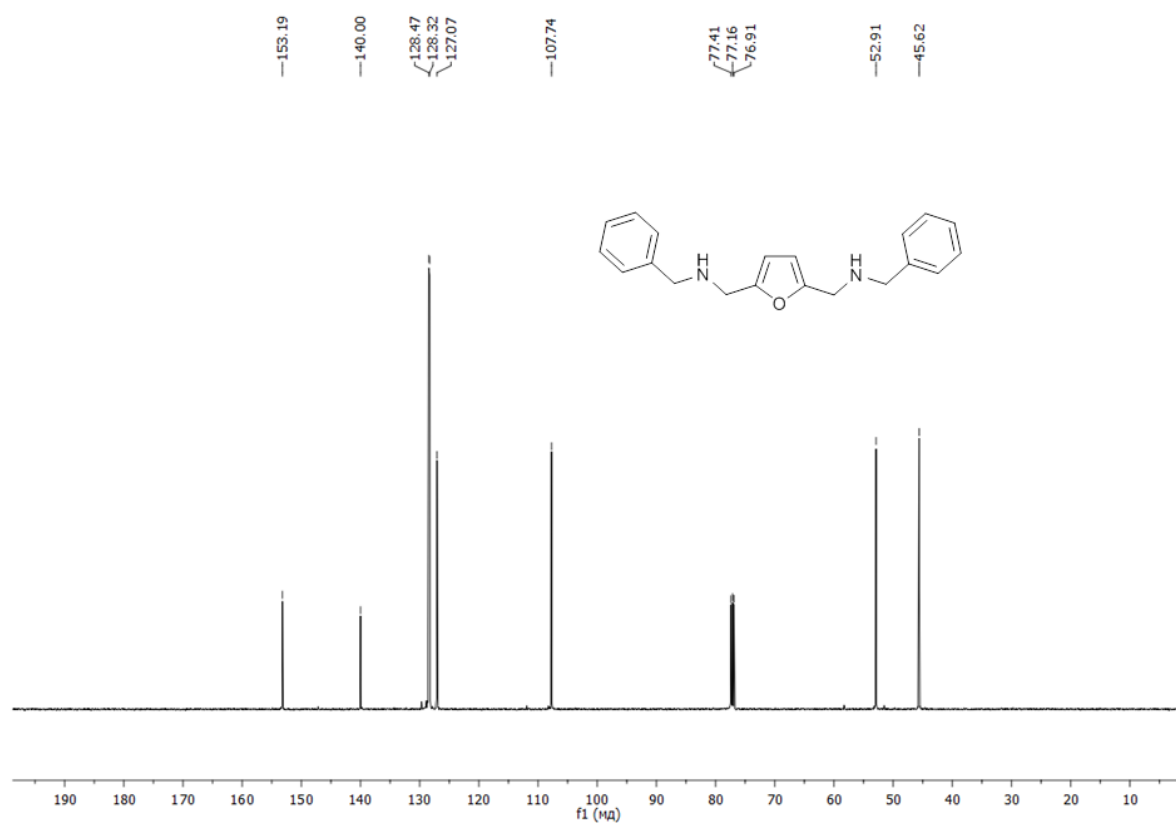


Fig. S4. ¹³C NMR spectrum of compound 4 (CDCl₃, 298 K, 126 MHz).

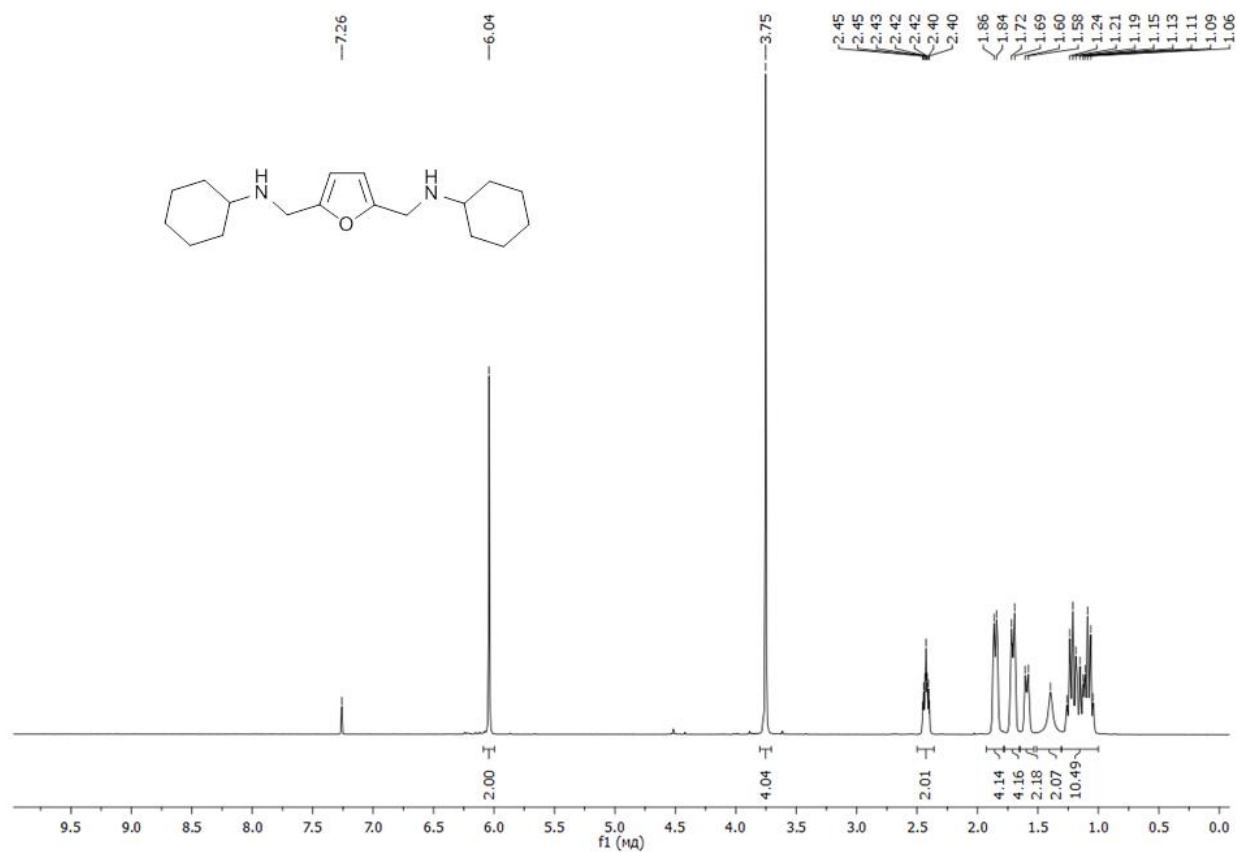


Fig. S5. ¹H NMR spectrum of compound 5 (CDCl₃, 298 K, 500 MHz).

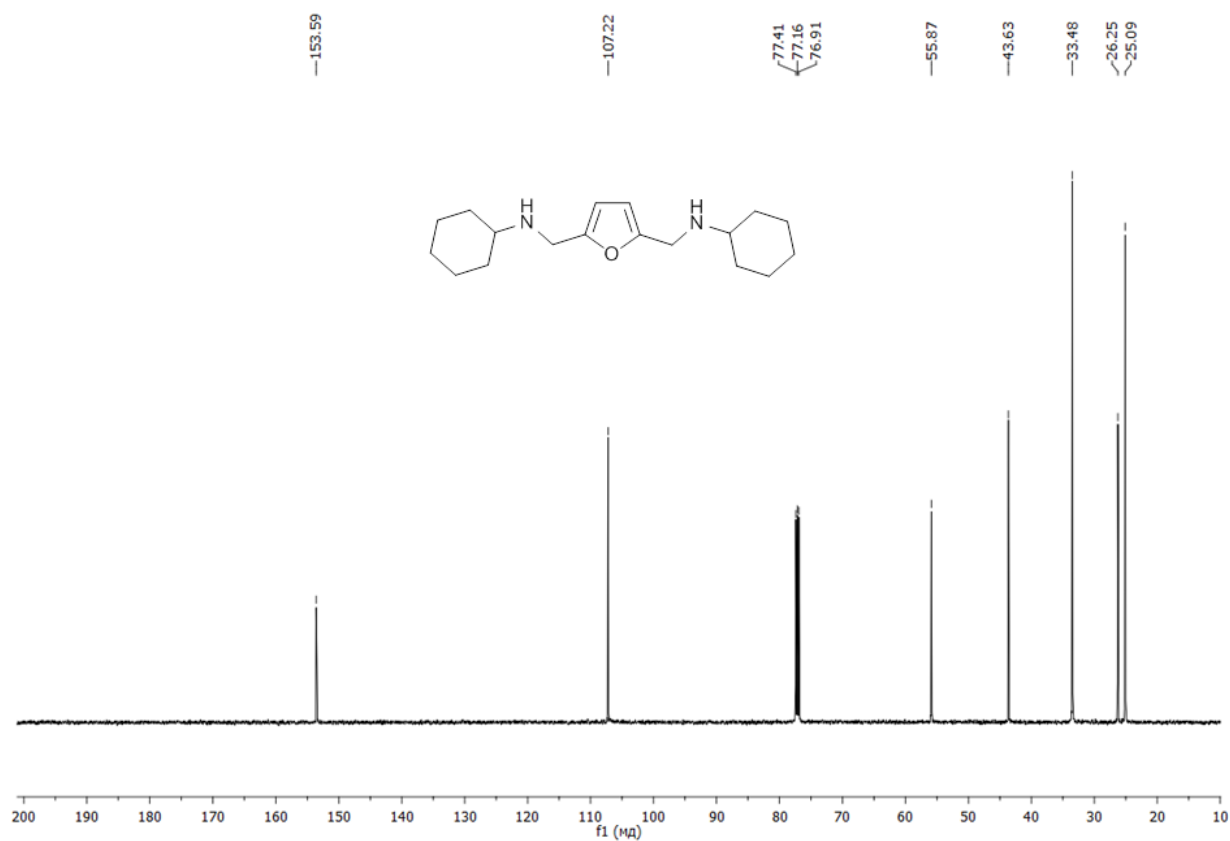


Fig. S6. ¹³C NMR spectrum of compound 5 (CDCl₃, 298 K, 126 MHz).

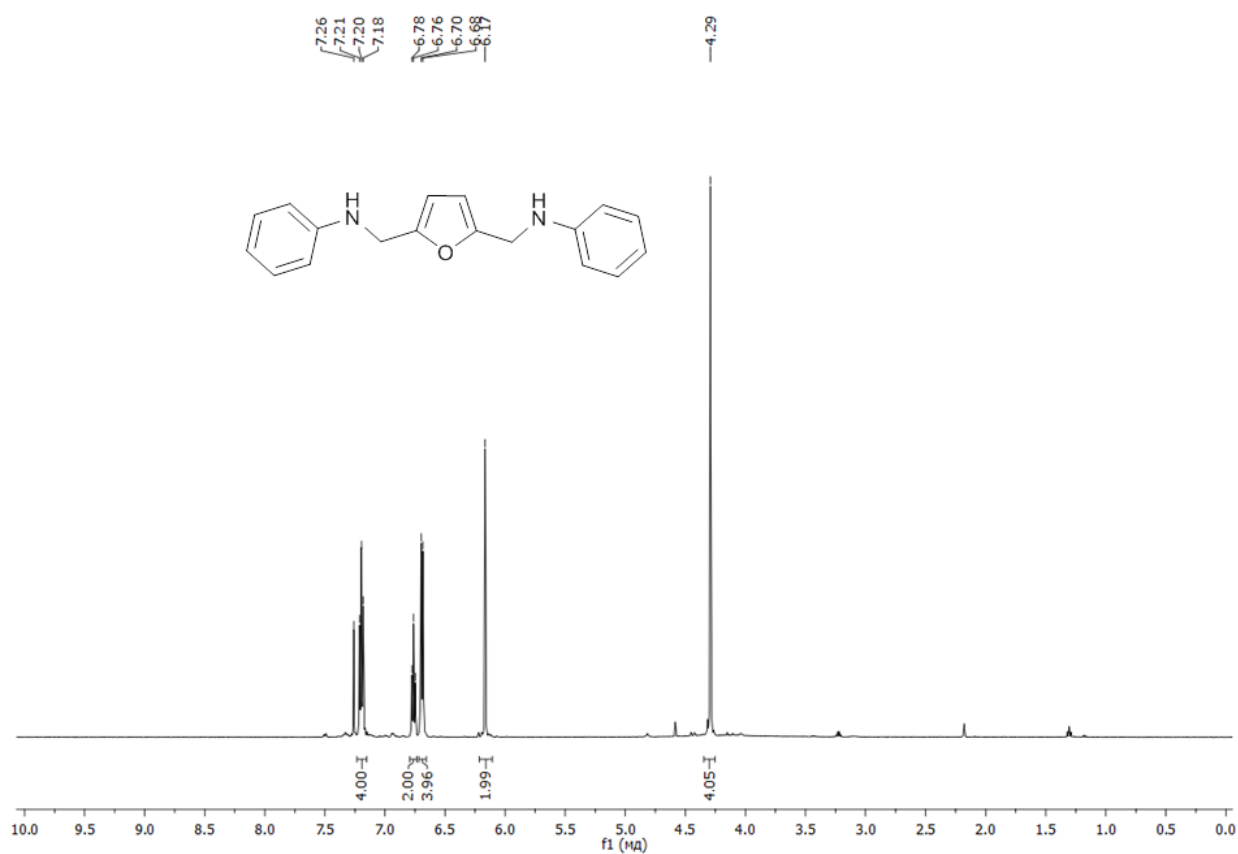


Fig. S7. ¹H NMR spectrum of compound 6 (CDCl₃, 298 K, 500 MHz).

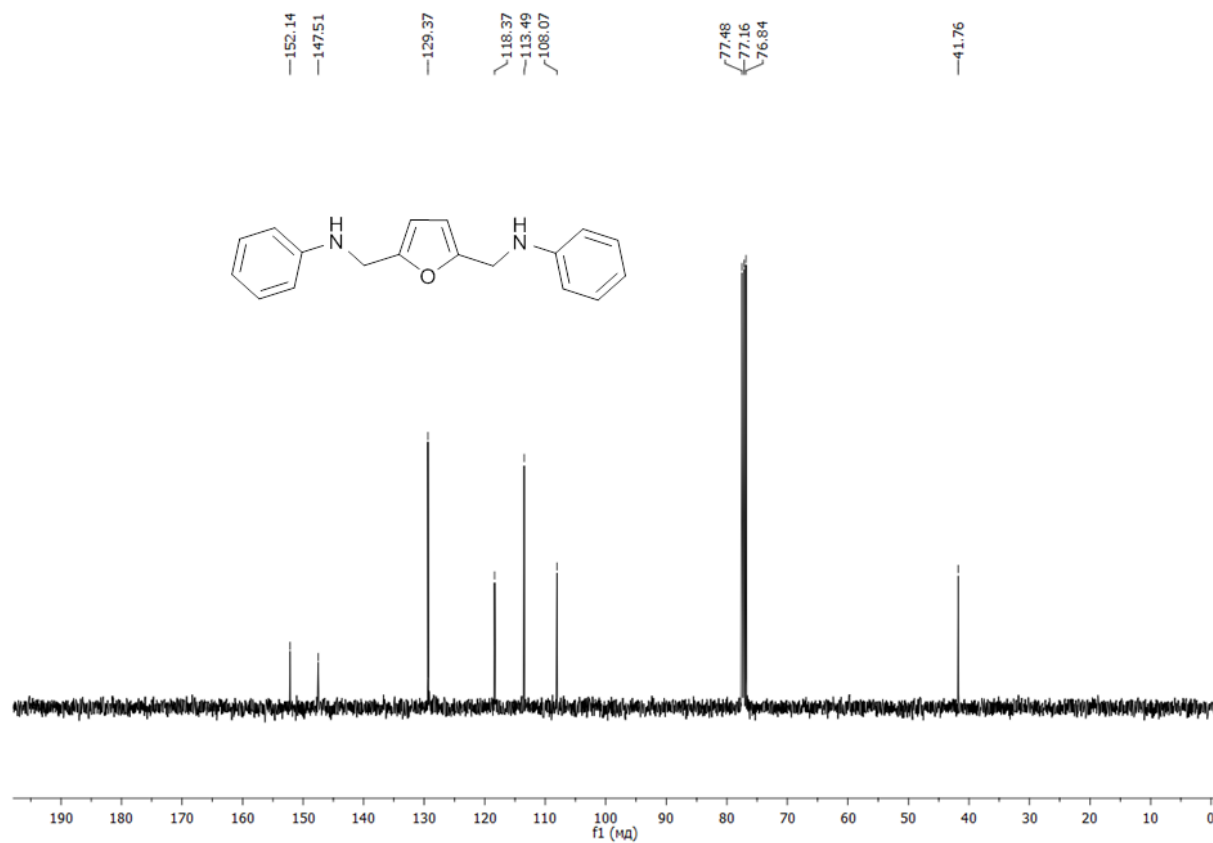


Fig. S8. ¹³C NMR spectrum of compound 6 (CDCl₃, 298 K, 126 MHz).

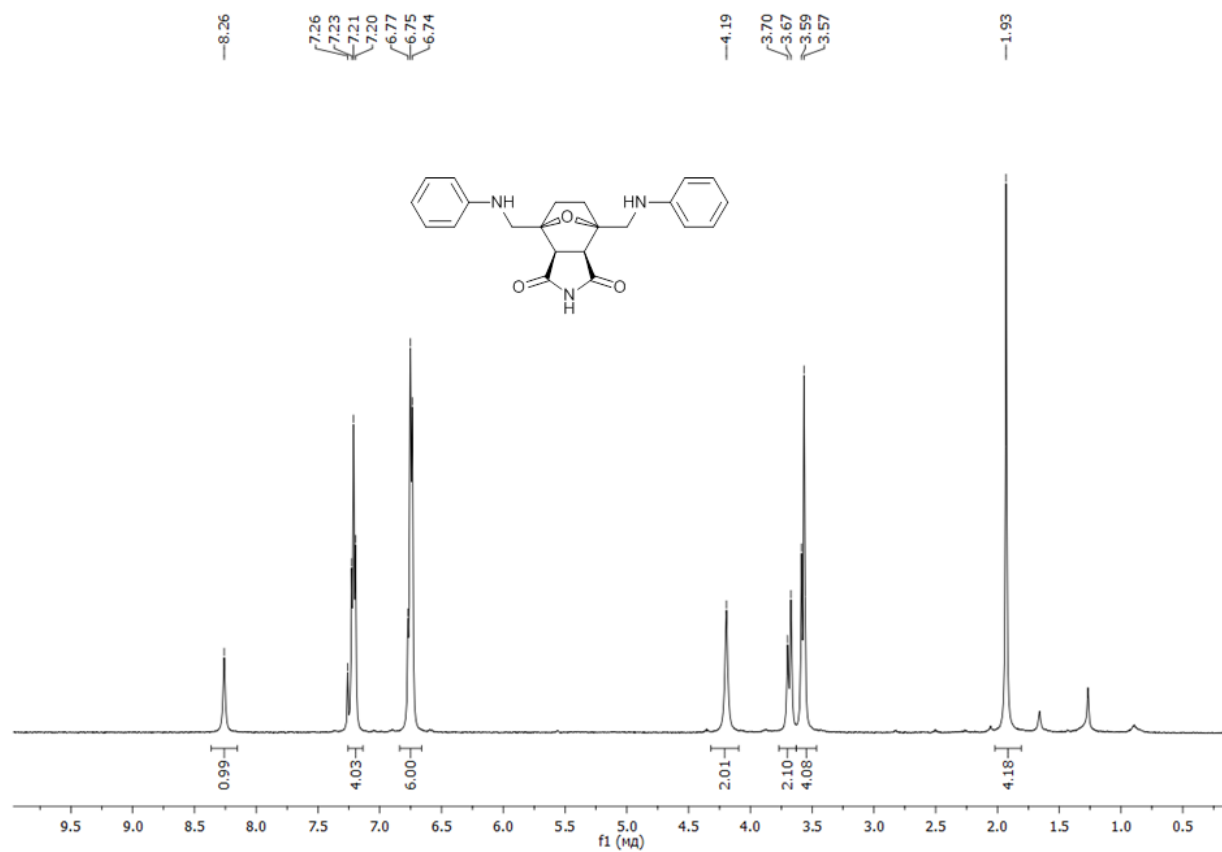


Fig. S9. ¹H NMR spectrum of compound 9 (CDCl₃, 298 K, 500 MHz).

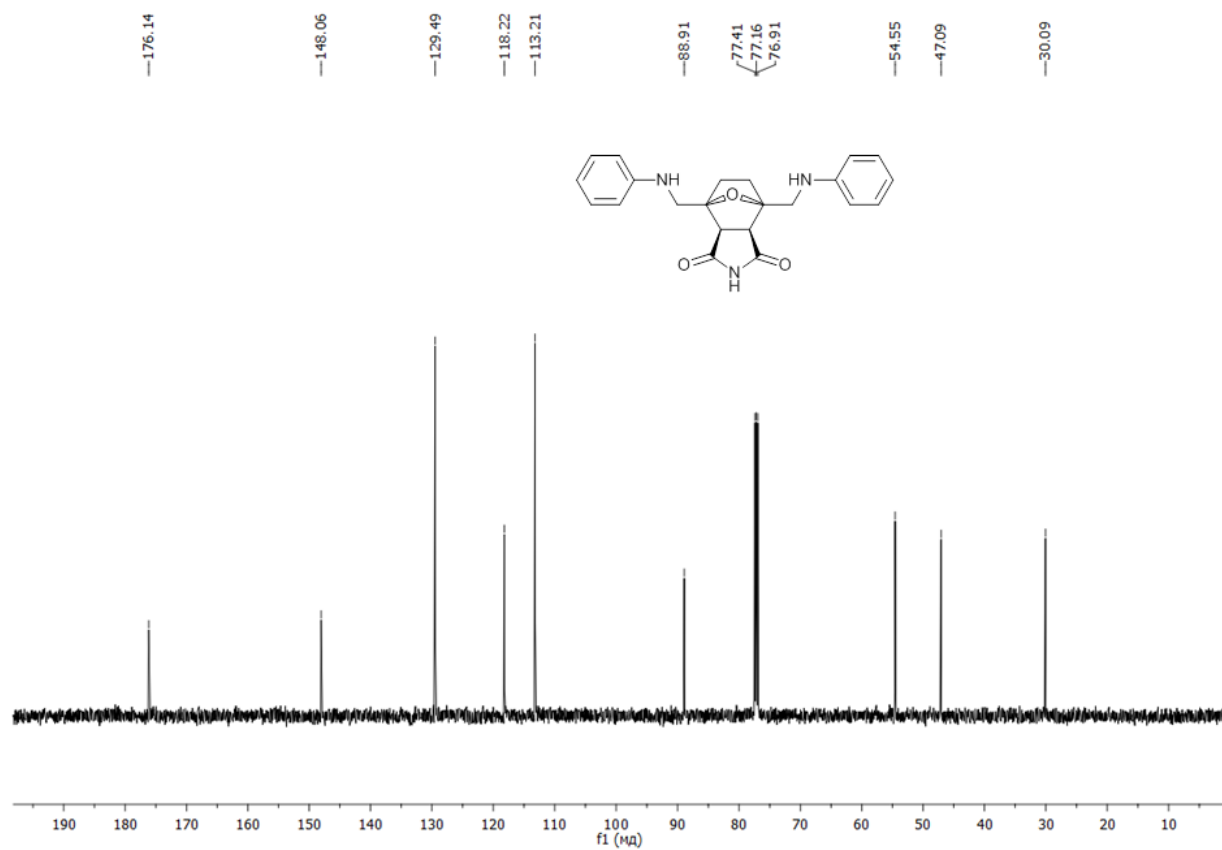


Fig. S10. ¹³C NMR spectrum of compound 9 (CDCl₃, 298 K, 126 MHz).

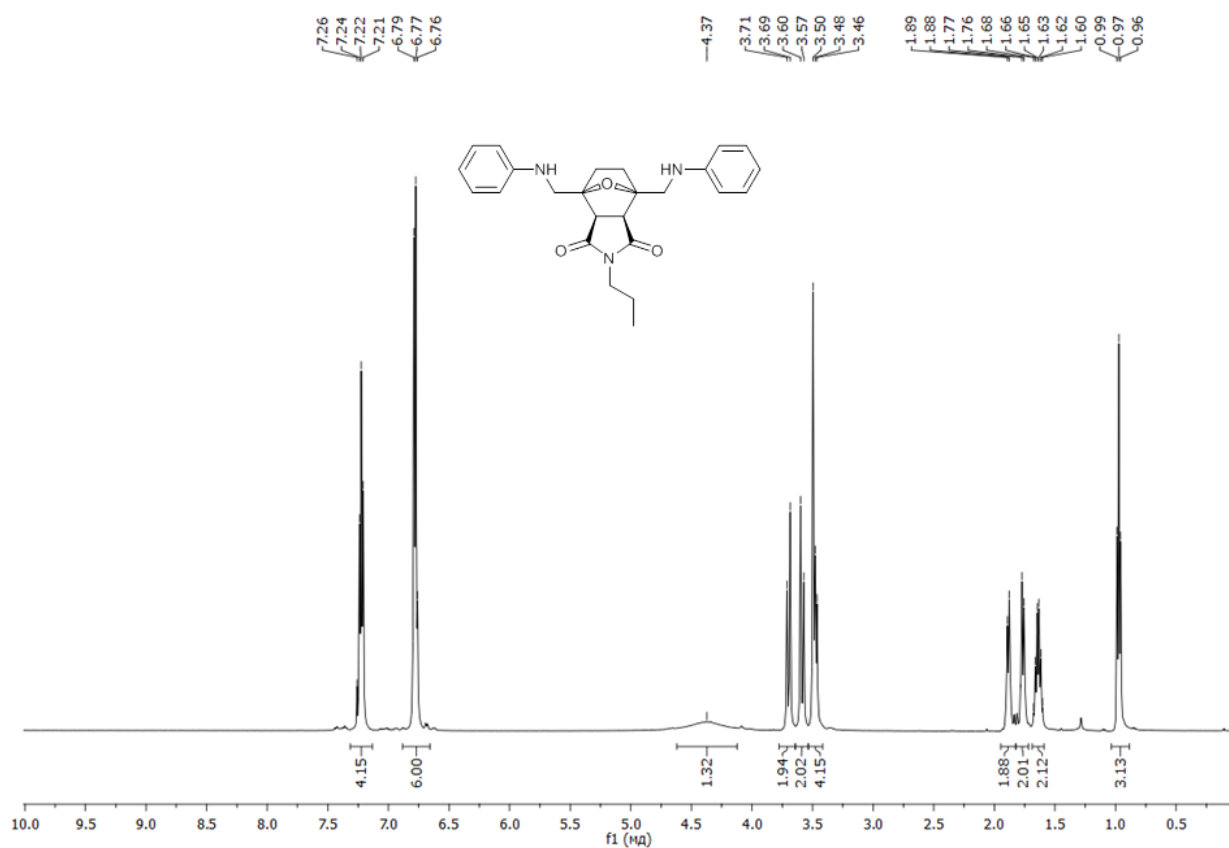


Fig. S11. ¹H NMR spectrum of compound 10-endo (CDCl₃, 298 K, 500 MHz).

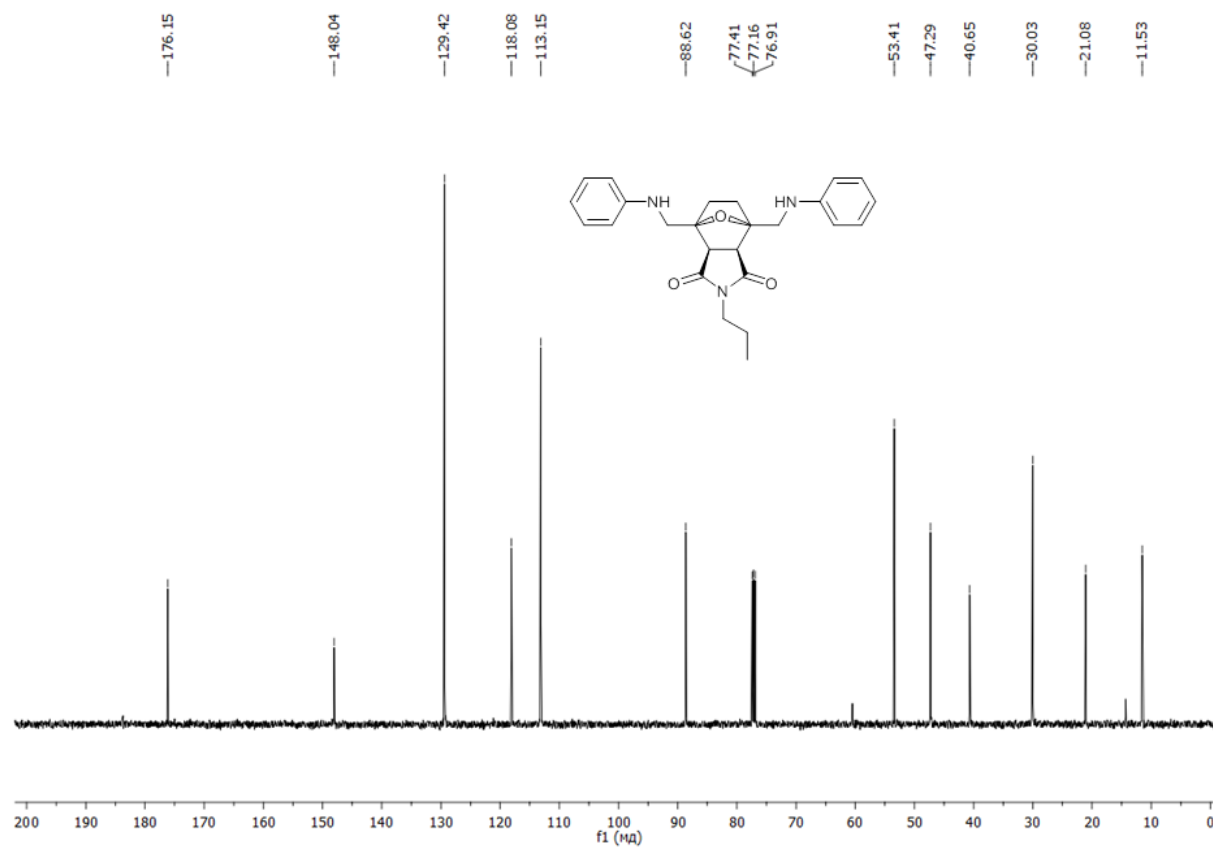


Fig. S12. ¹³C NMR spectrum of compound 10-endo (CDCl₃, 298 K, 126 MHz).

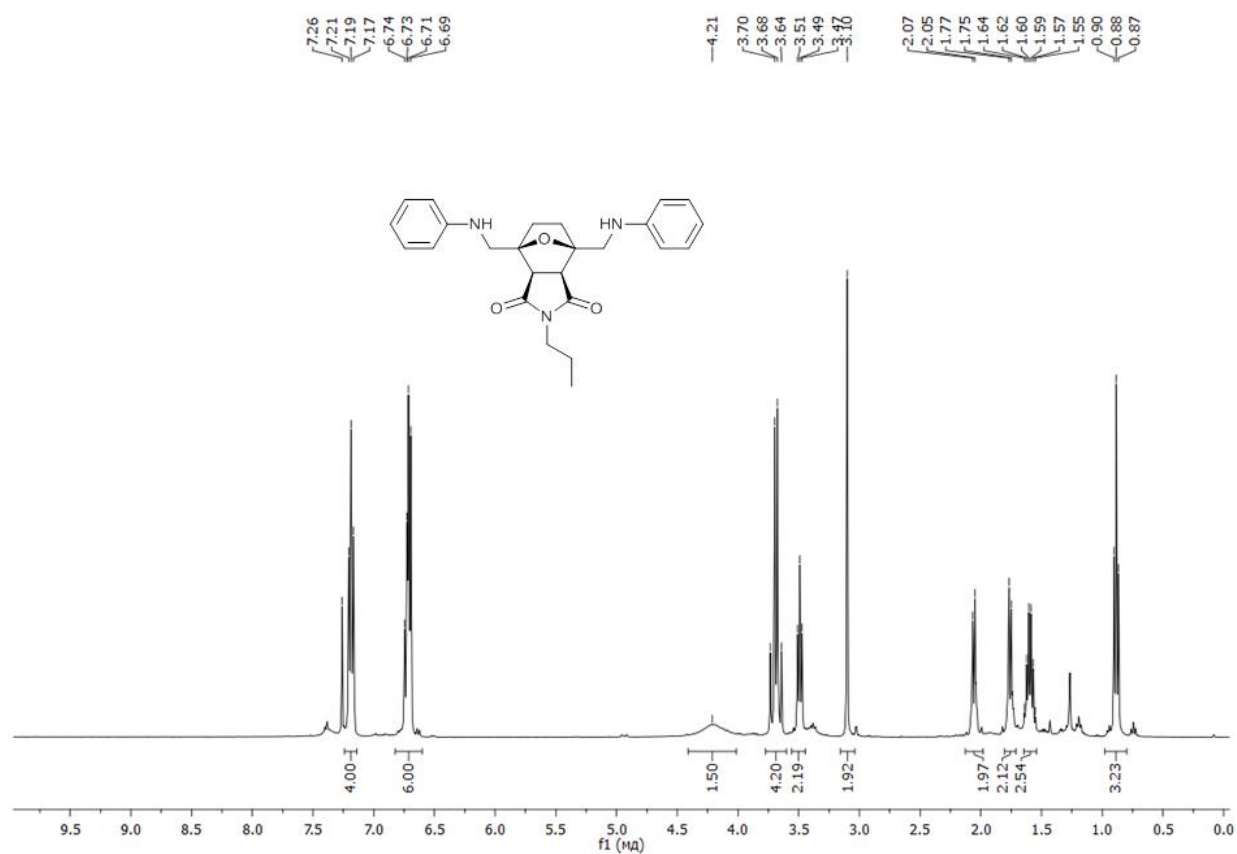


Fig. S13. ¹H NMR spectrum of compound 10-exo (CDCl₃, 298 K, 400 MHz).

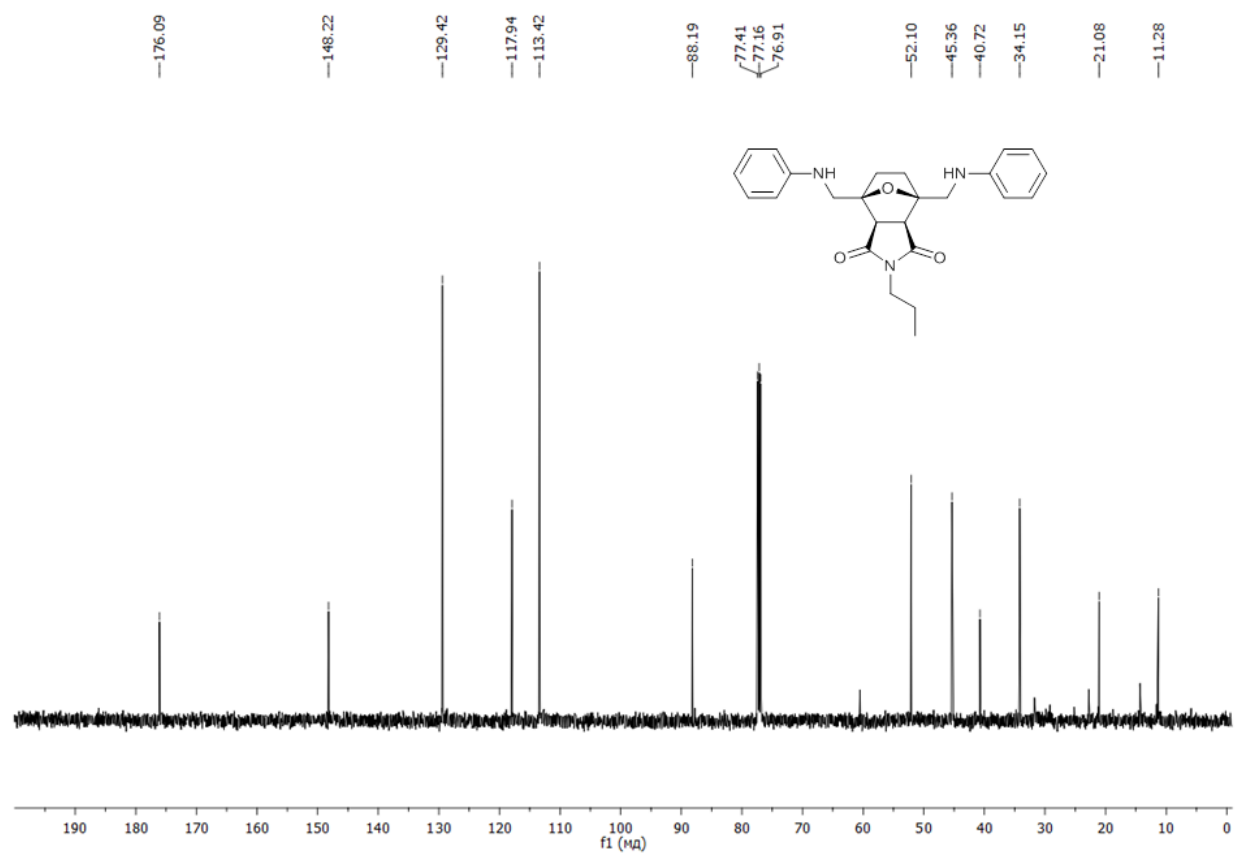


Fig. S14. ¹³C NMR spectrum of compound 10-exo (CDCl₃, 298 K, 126 MHz).

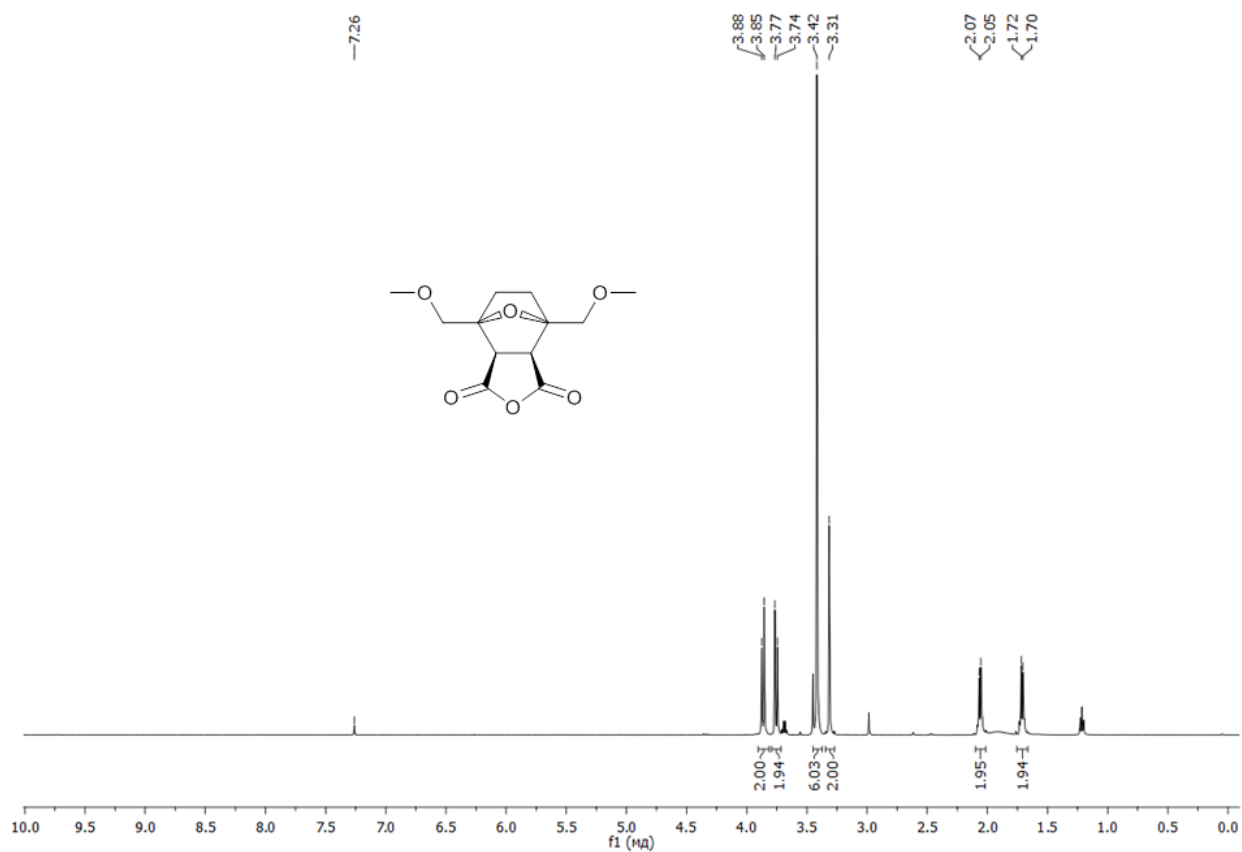


Fig. S15. ¹H NMR spectrum of compound 17 (CDCl₃, 298 K, 500 MHz).

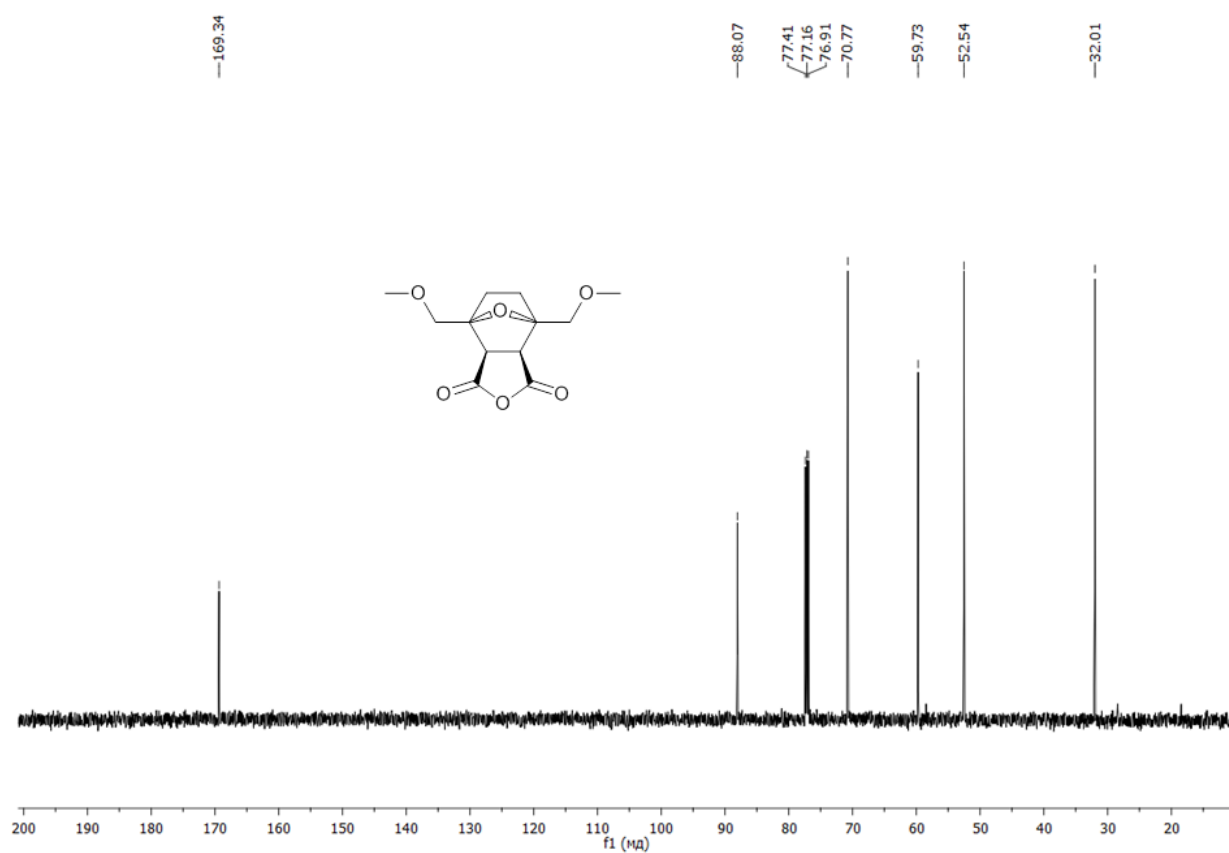


Fig. S16. ¹³C NMR spectrum of compound 17 (CDCl₃, 298 K, 126 MHz).

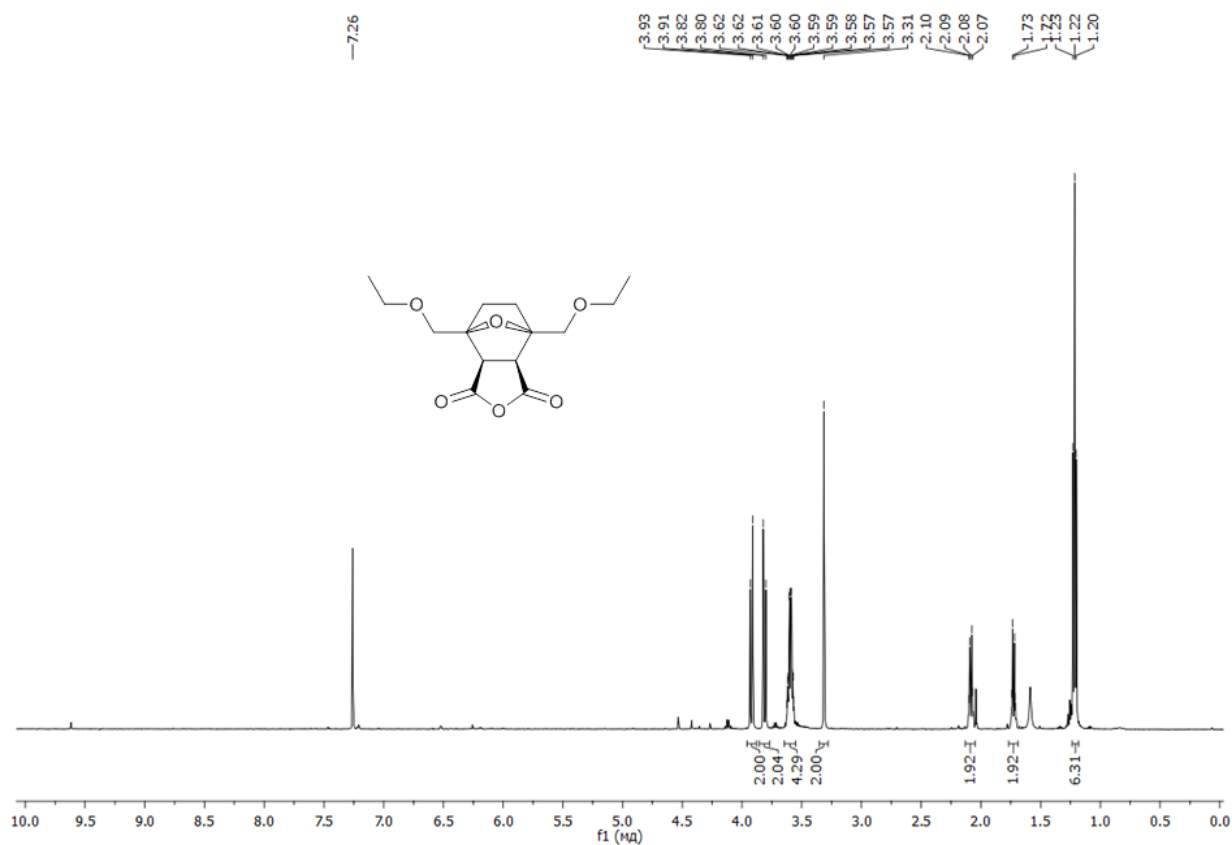


Fig. S17. ¹H NMR spectrum of compound 18 (CDCl₃, 298 K, 500 MHz).

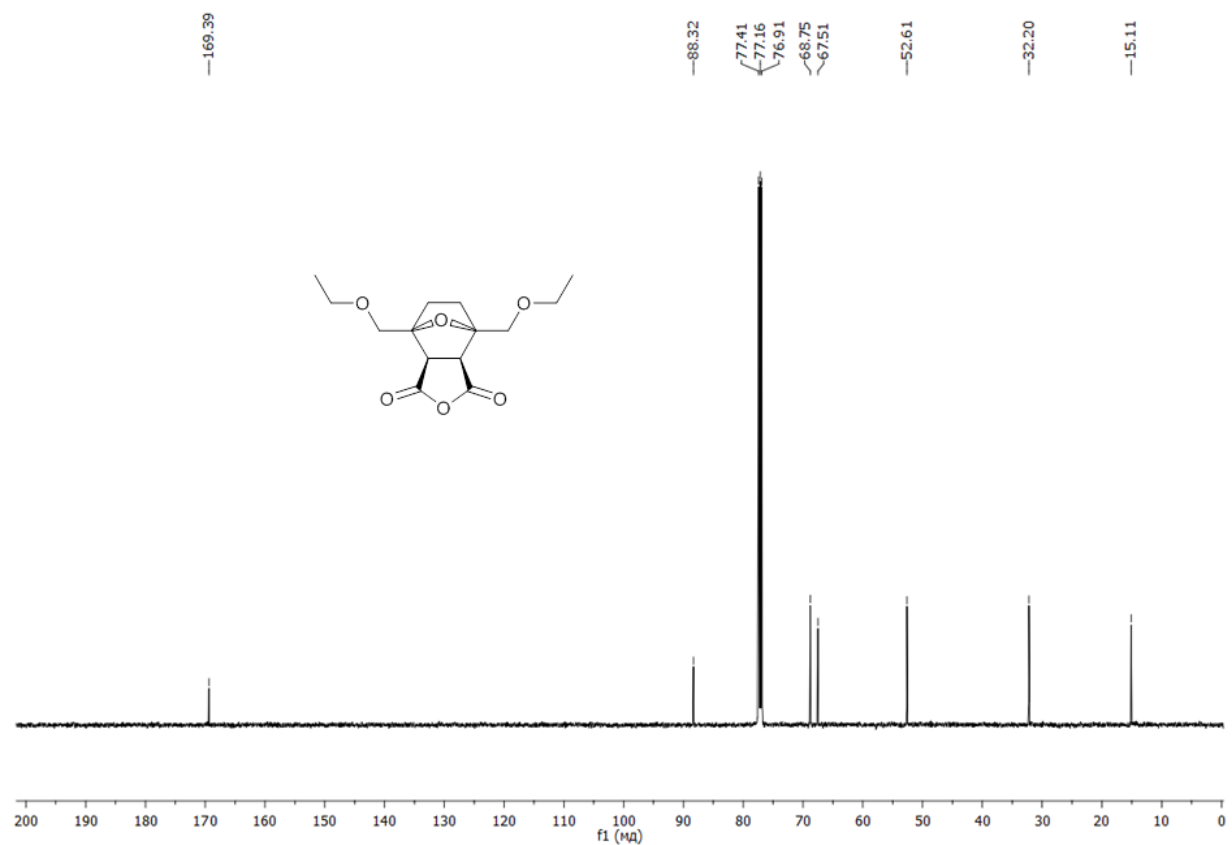


Fig. S18. ¹³C NMR spectrum of compound 18 (CDCl₃, 298 K, 126 MHz).

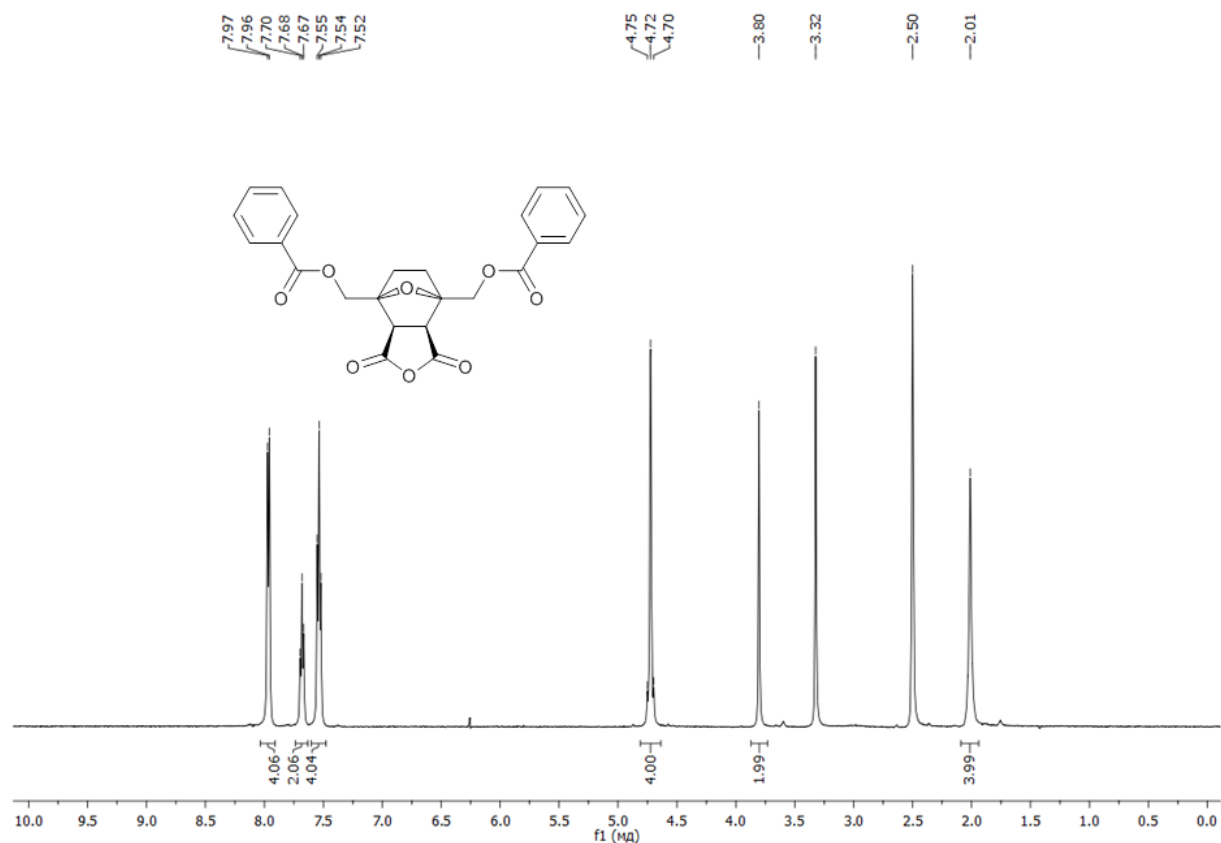


Fig. S19. ¹H NMR spectrum of compound 19 (DMSO-*d*₆, 298 K, 500 MHz).

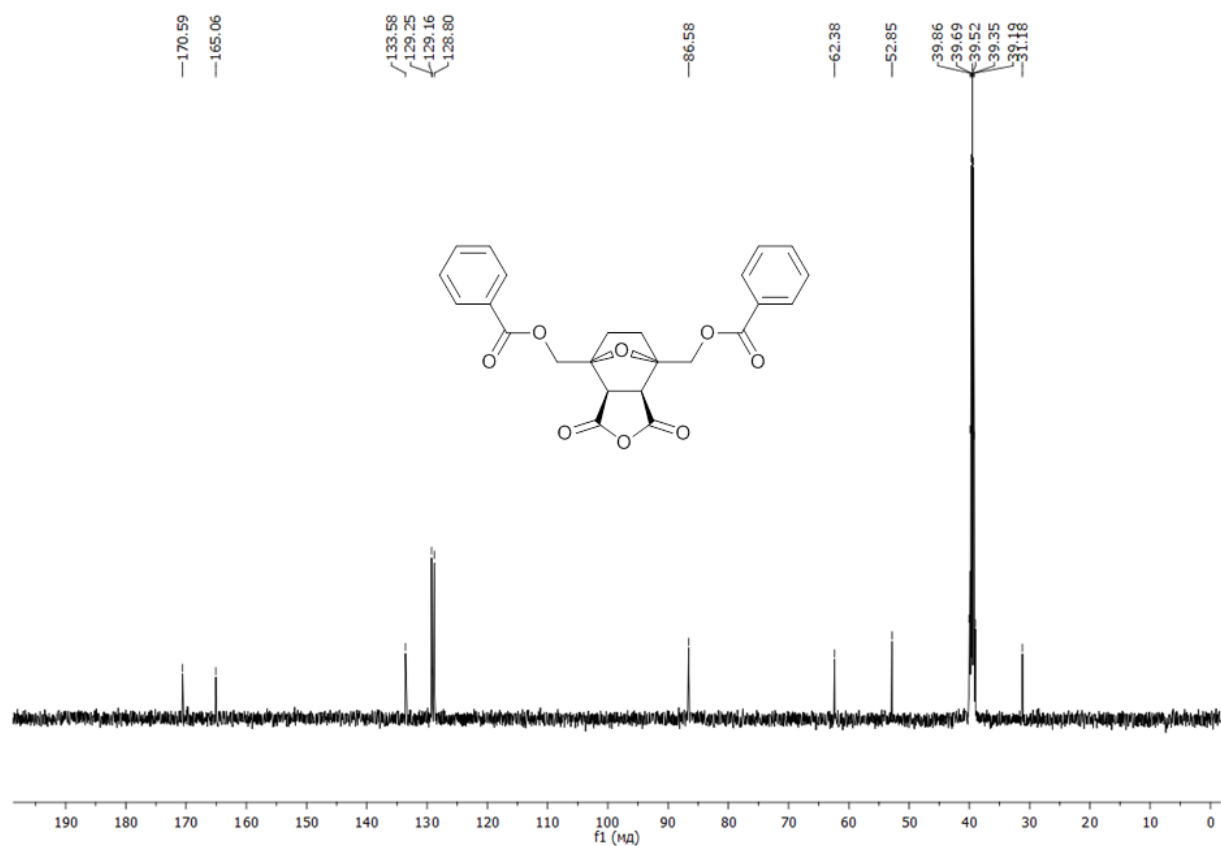


Fig. S20. ¹³C NMR spectrum of compound 19 (DMSO-*d*₆, 298 K, 126 MHz).

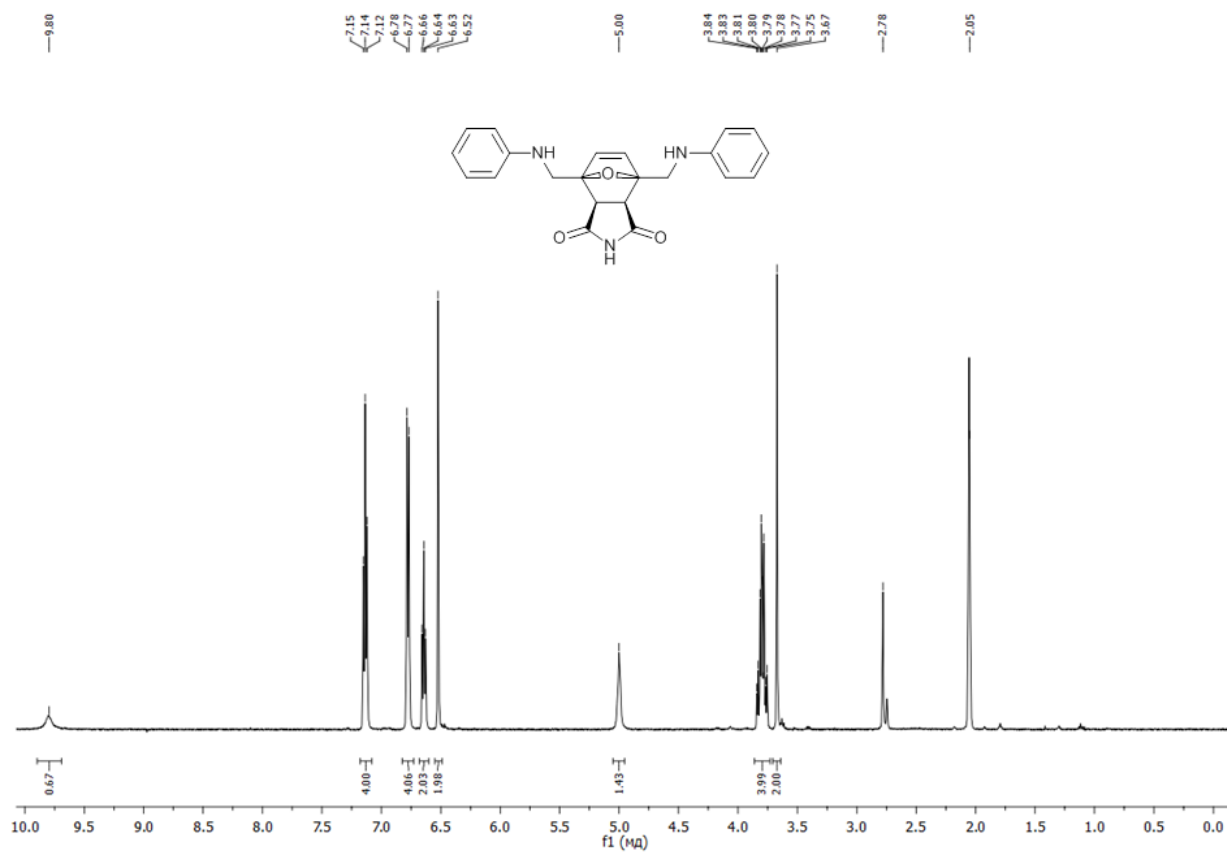


Fig. S21. ¹H NMR spectrum of compound 9a (acetone-*d*₆, 298 K, 500 MHz).

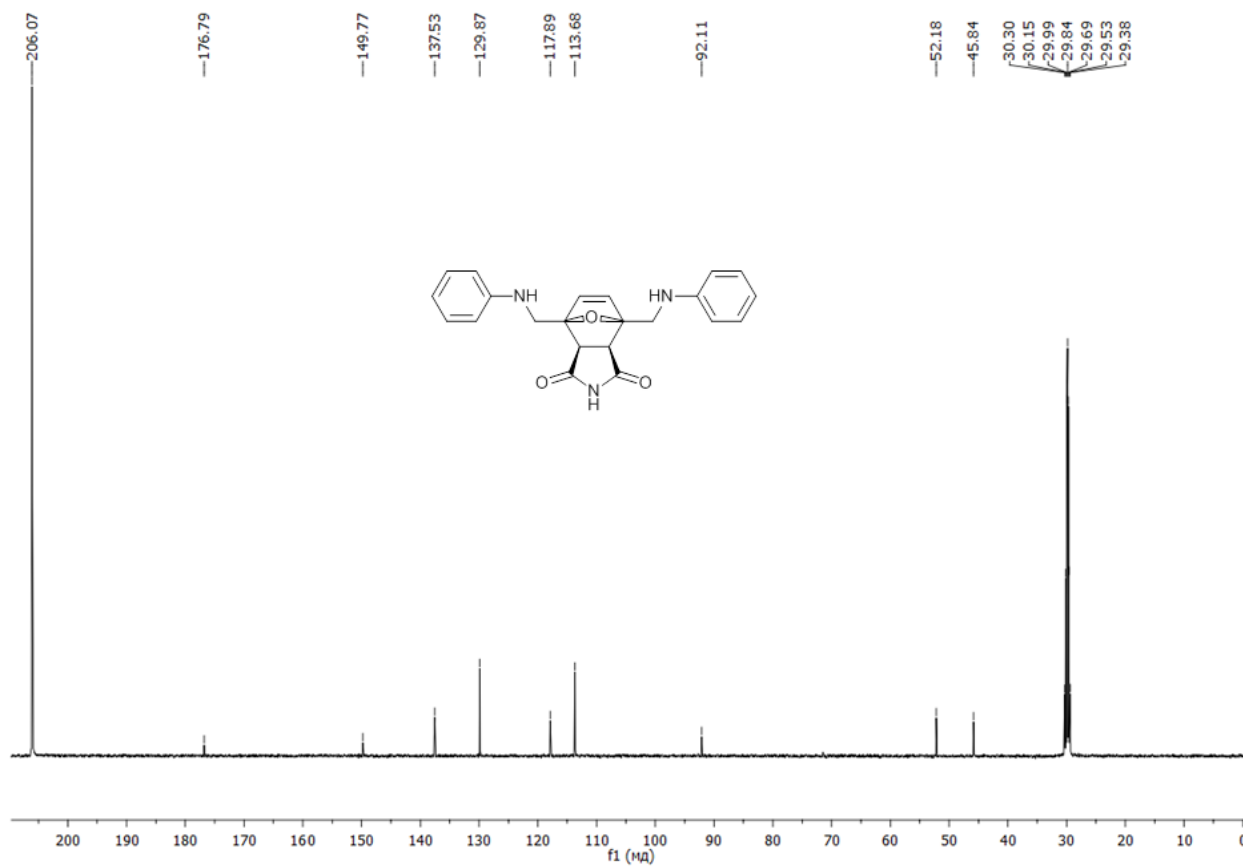


Fig. S22. ¹³C NMR spectrum of compound 9a (acetone-*d*₆, 298 K, 126 MHz).

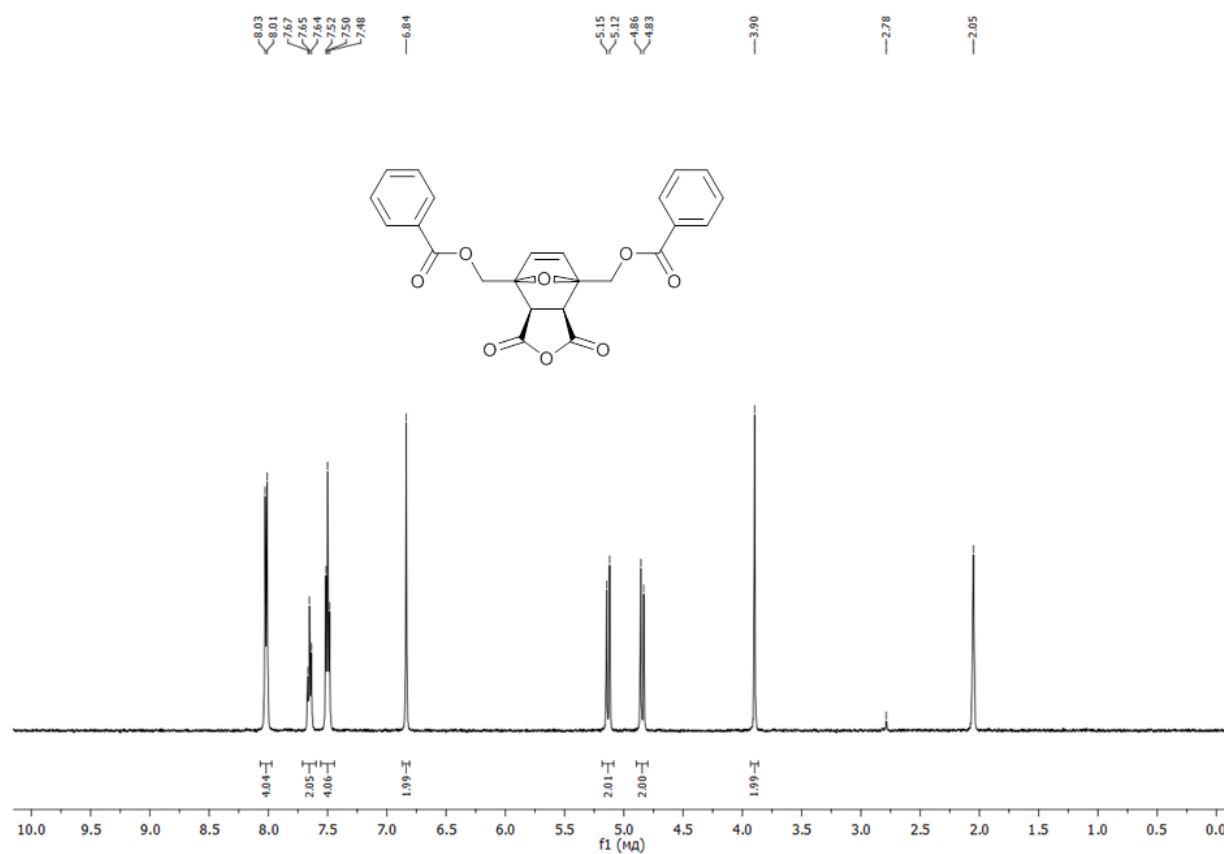


Fig. S23. ¹H NMR spectrum of compound 19a (acetone-*d*₆, 298 K, 500 MHz).

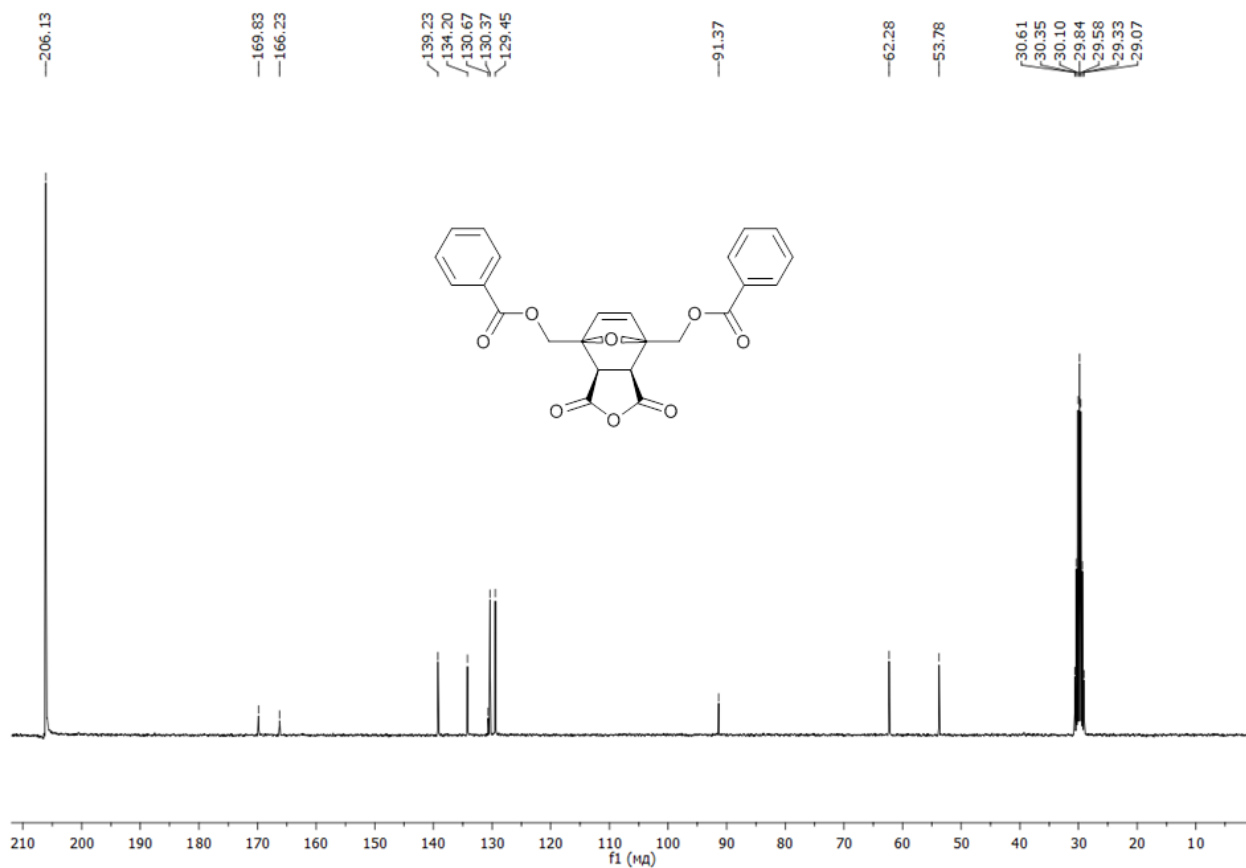


Fig. S24. ¹³C NMR spectrum of compound 19a (acetone-*d*₆, 298 K, 75 MHz).

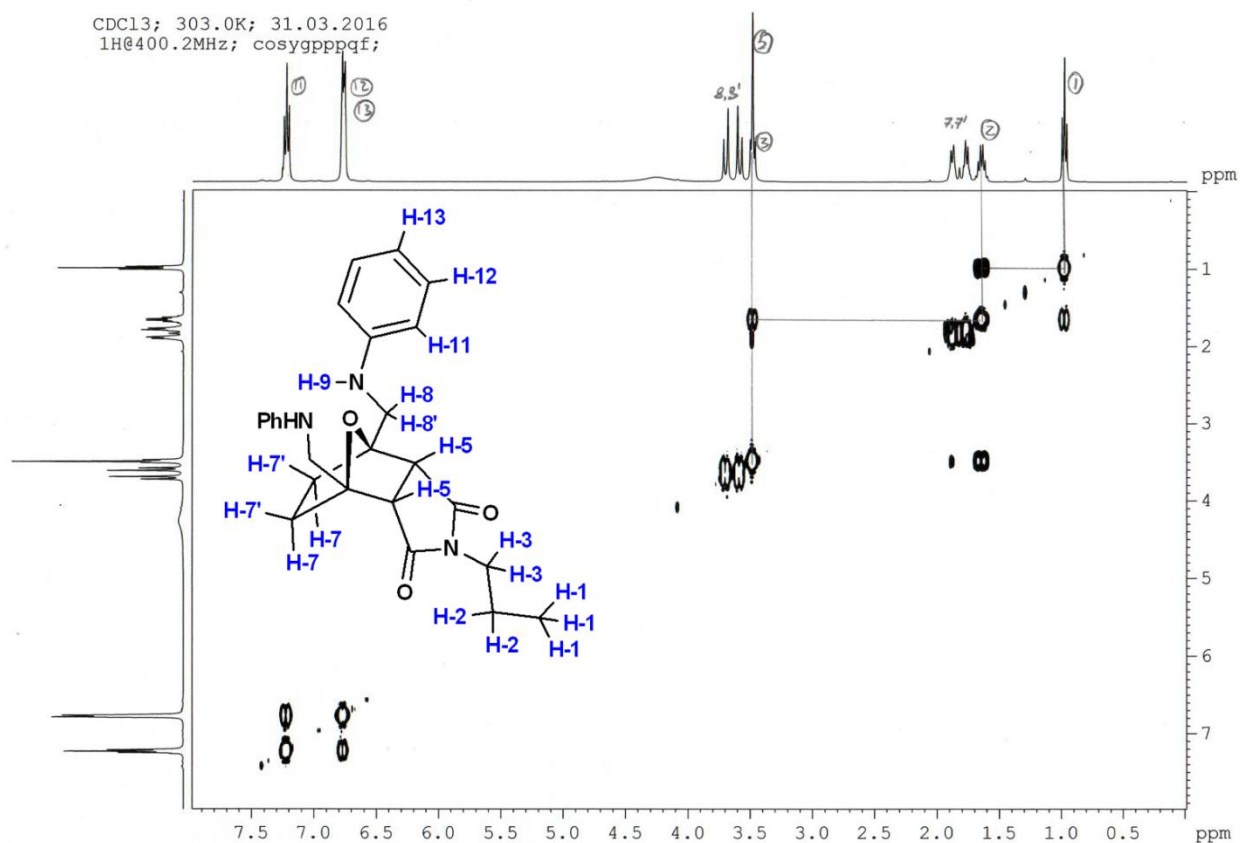


Fig. S25. COSY spectrum of compound 10-endo (CDCl₃, 298 K, 400 MHz).

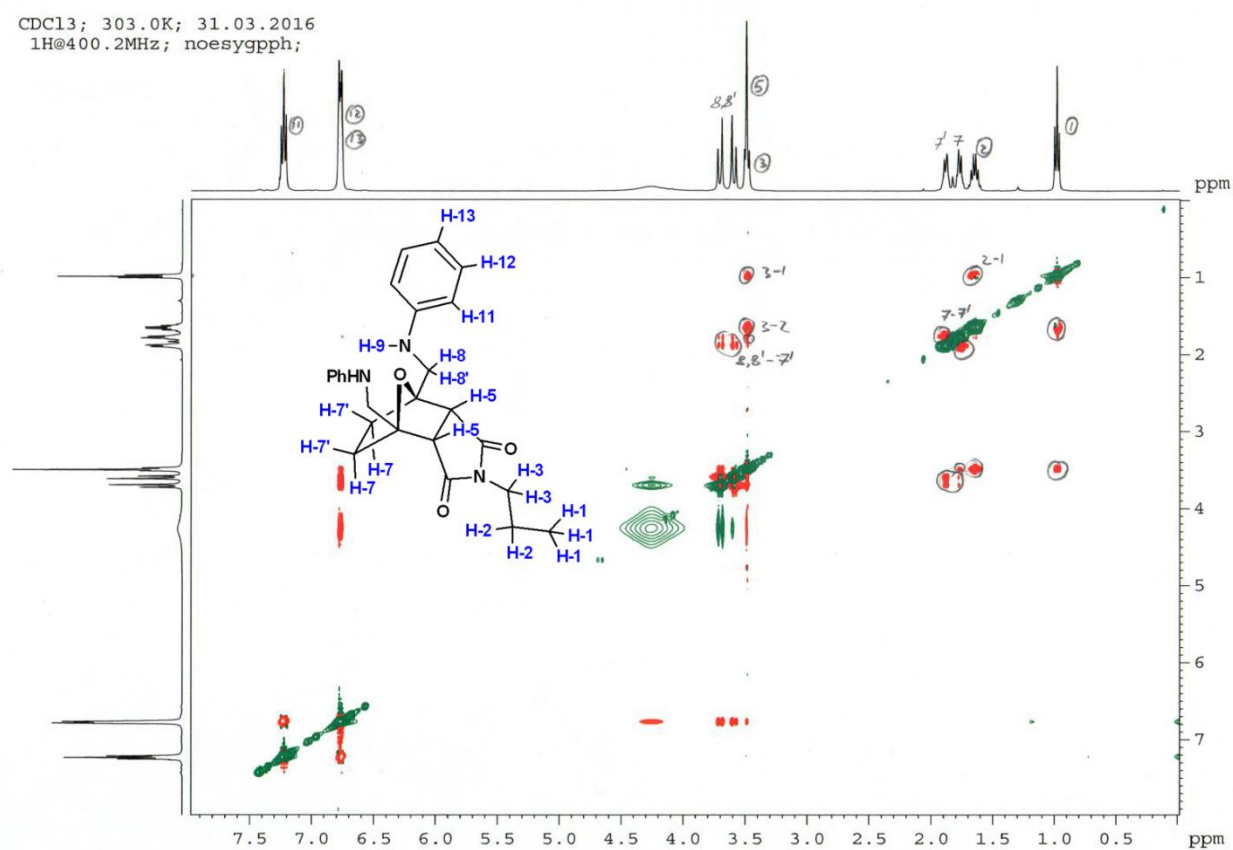


Fig. S26. NOESY spectrum of compound 10-endo (CDCl₃, 303 K, 400 MHz).

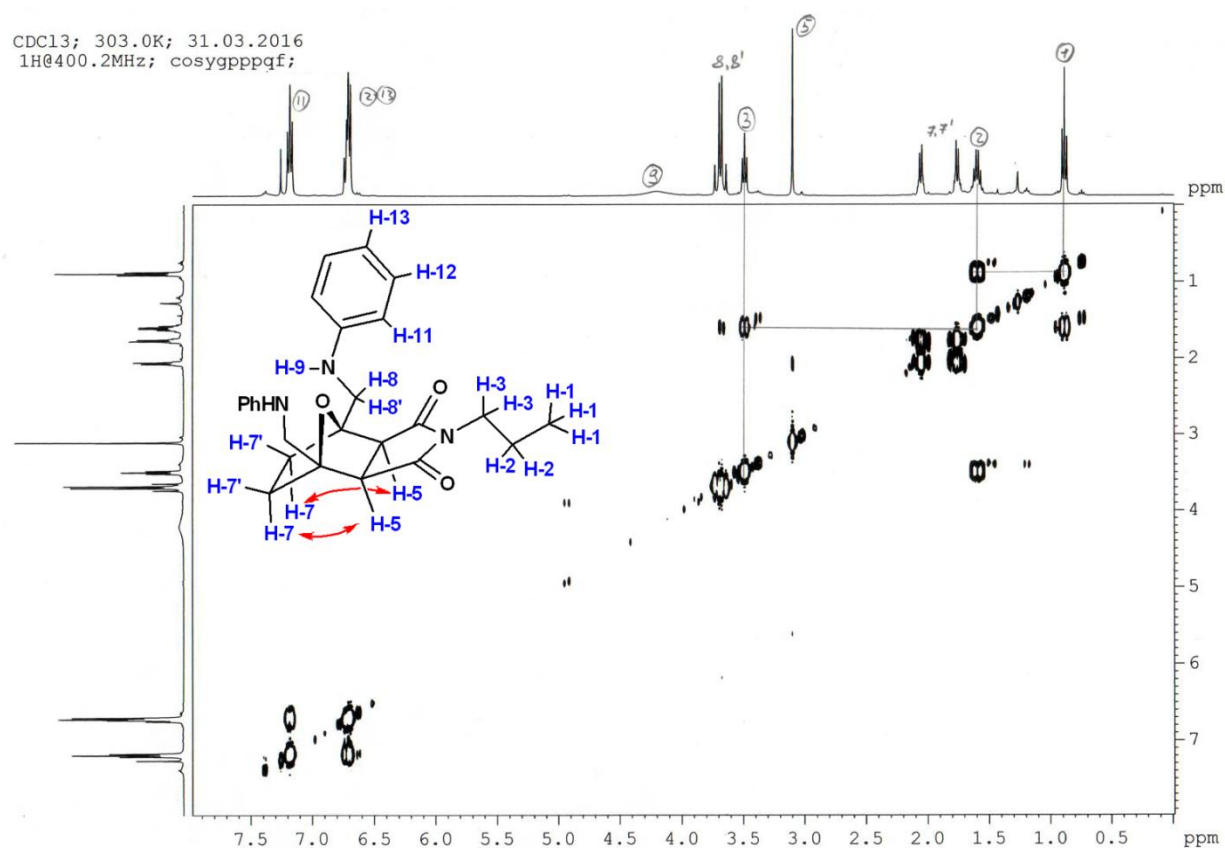


Fig. S27. COSY spectrum of compound 10-exo (CDCl₃, 303 K, 400 MHz).

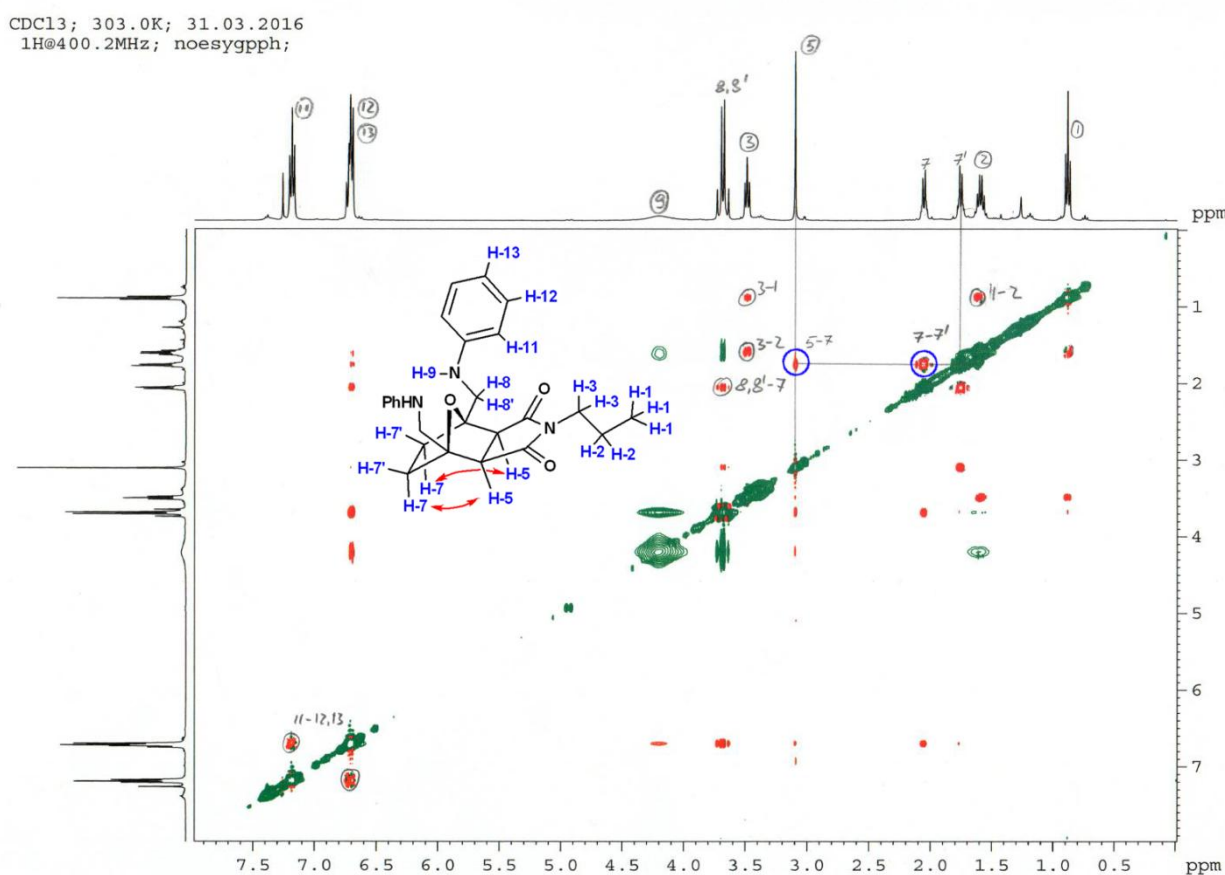


Fig. S28. NOESY spectrum of compound 10-exo (CDCl₃, 298 K, 400 MHz).

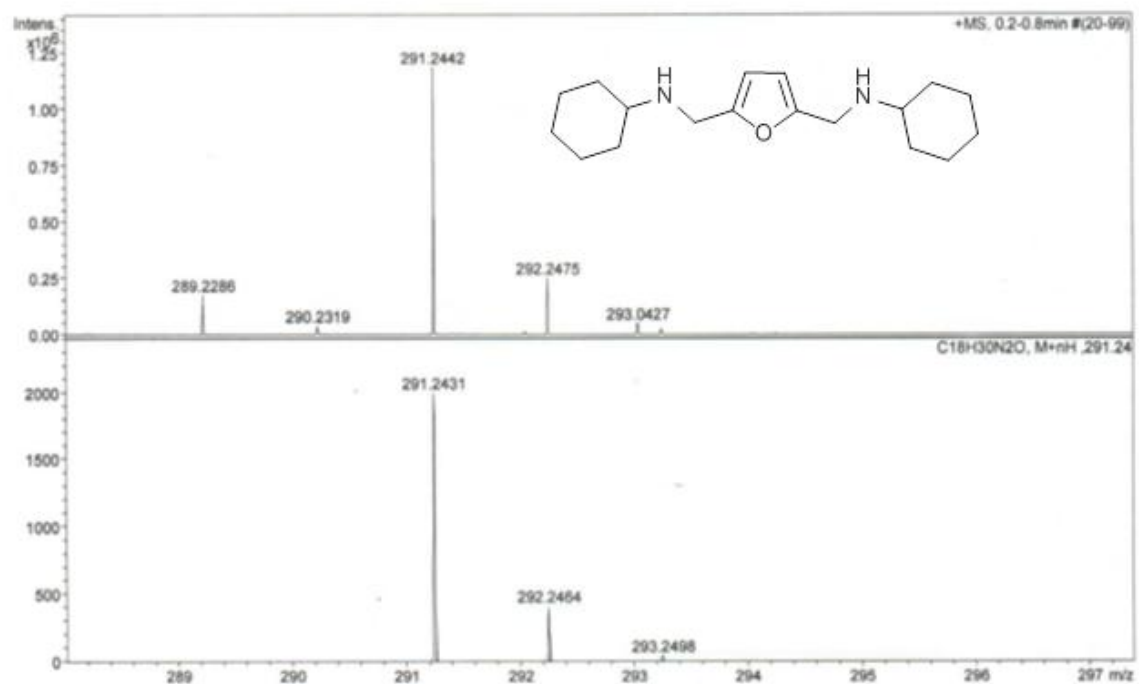


Fig. S29. HRMS (ESI) spectrum of compound 5.

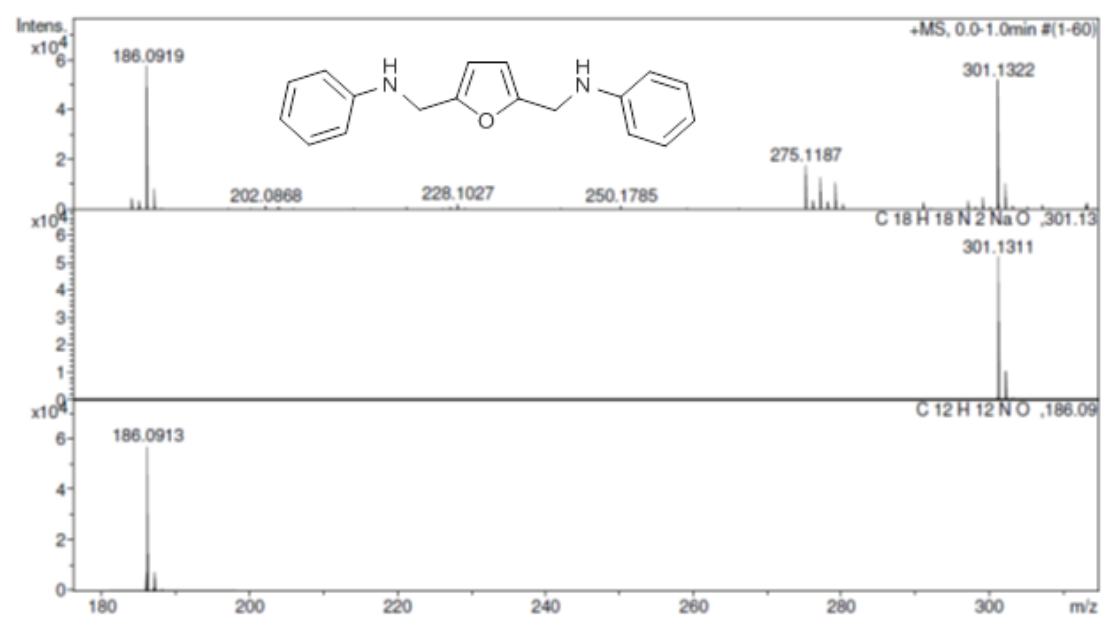


Fig. S30. HRMS (ESI) spectrum of compound 6.

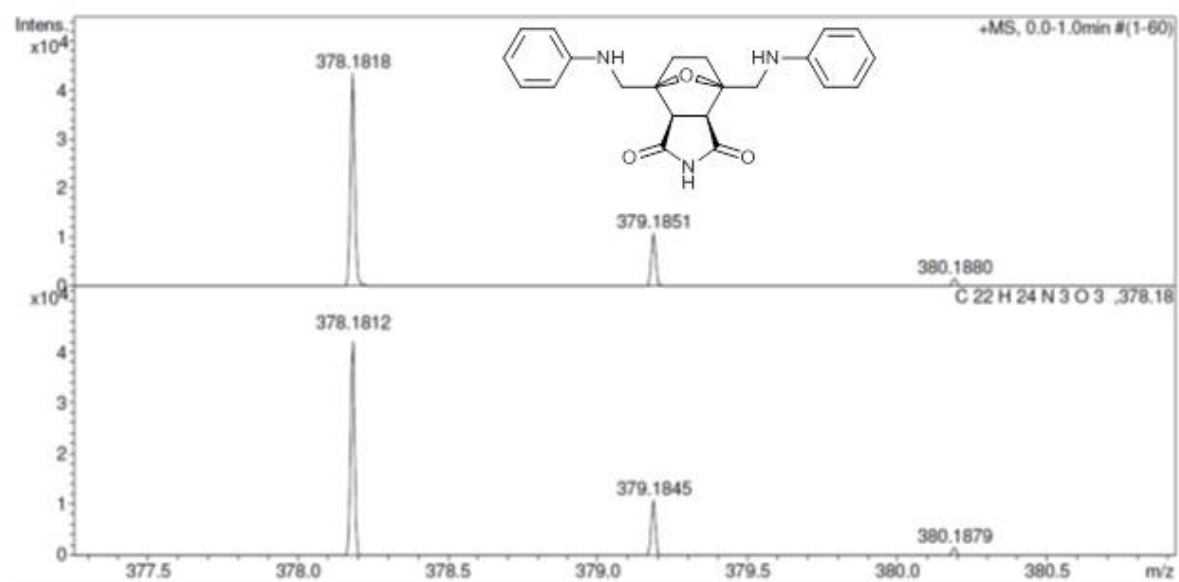


Fig. S31. HRMS (ESI) spectrum of compound 9.

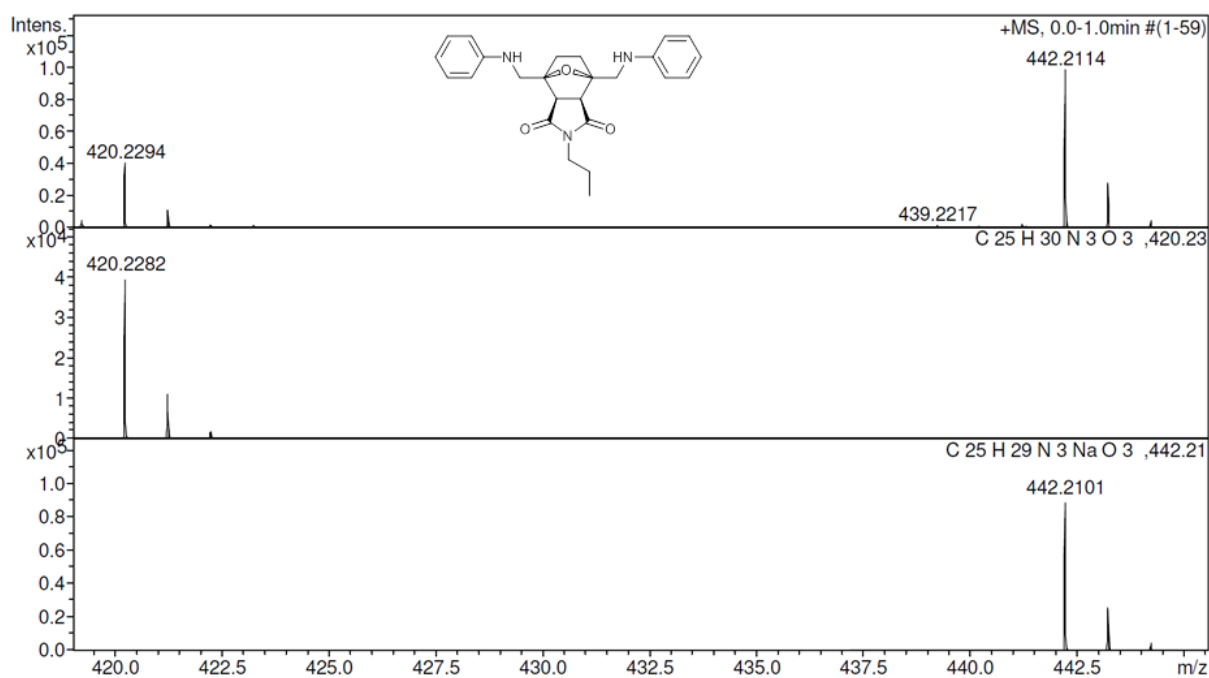


Fig. S32. HRMS (ESI) spectrum of compound 10-endo.

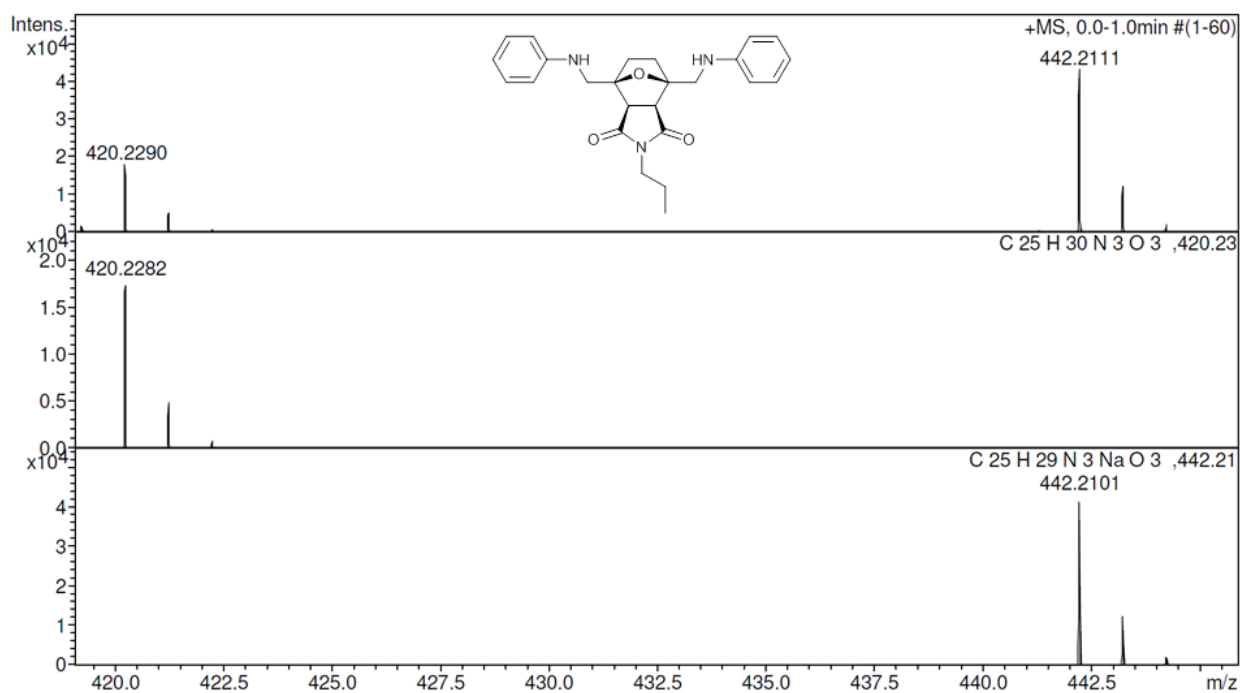


Fig. S33. HRMS (ESI) spectrum of compound 10-exo.

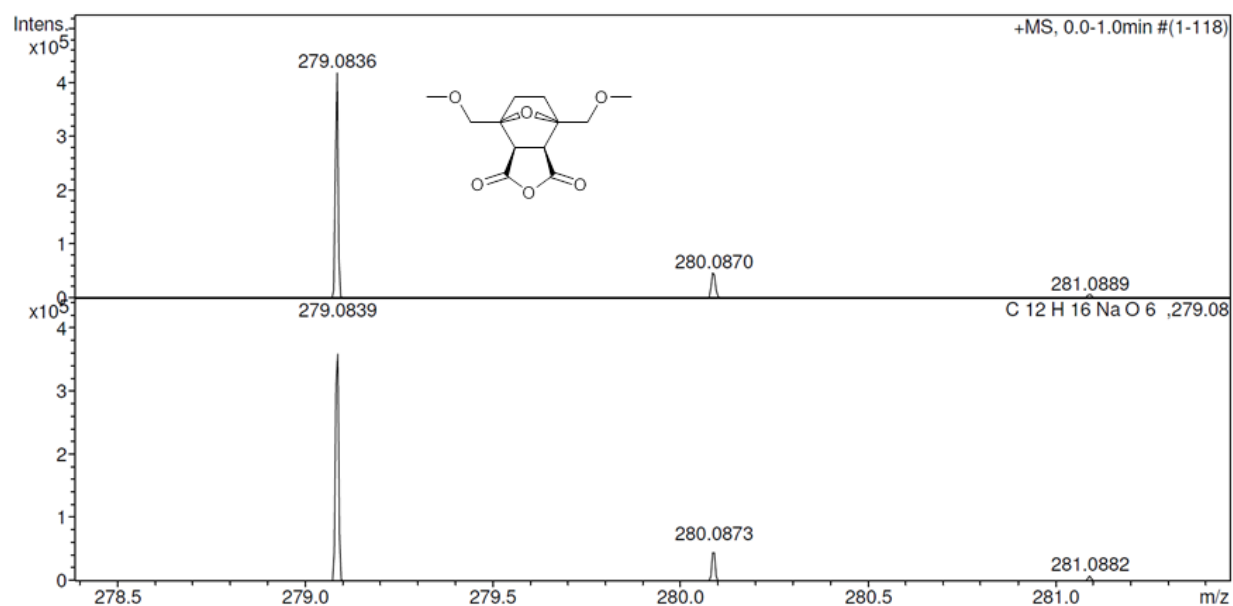


Fig. S34. HRMS (ESI) spectrum of compound 17.

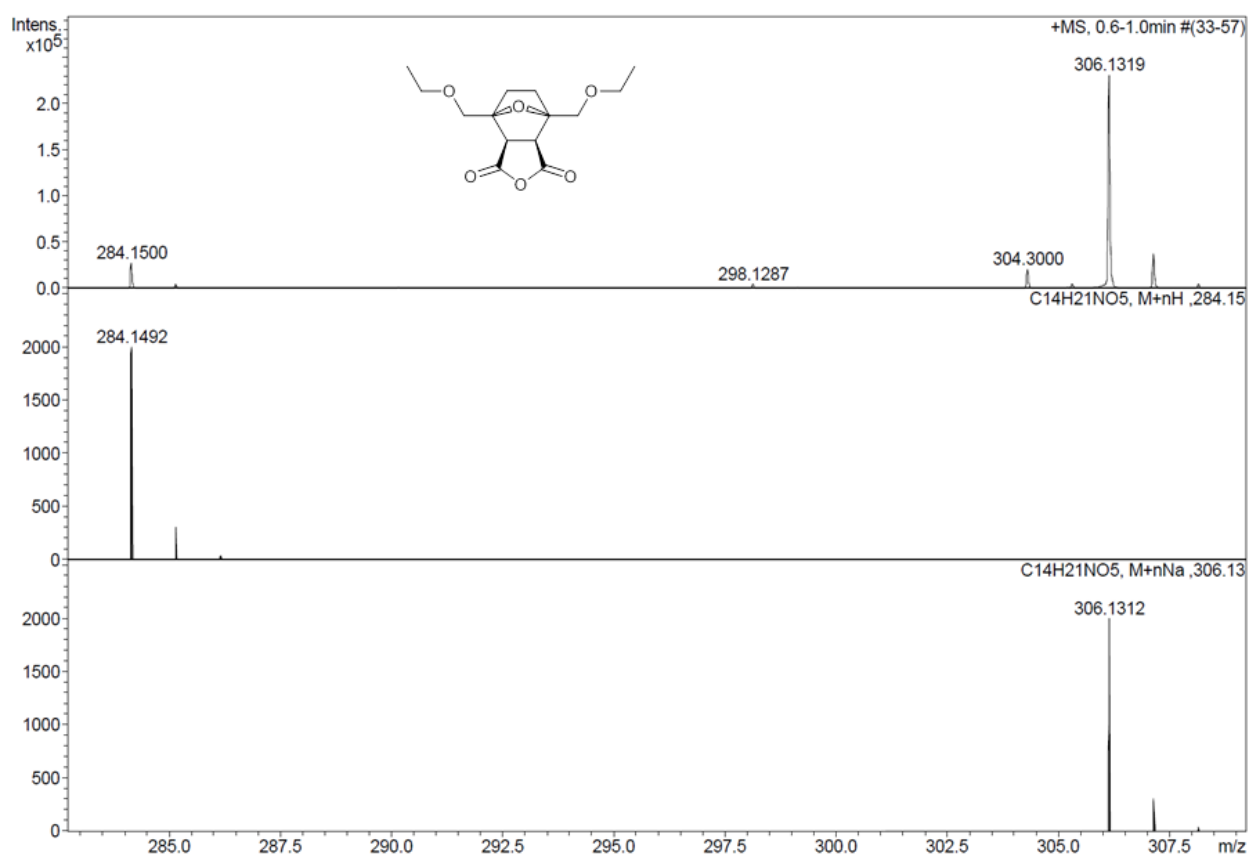


Fig. S35. HRMS (ESI) spectrum of compound 18.

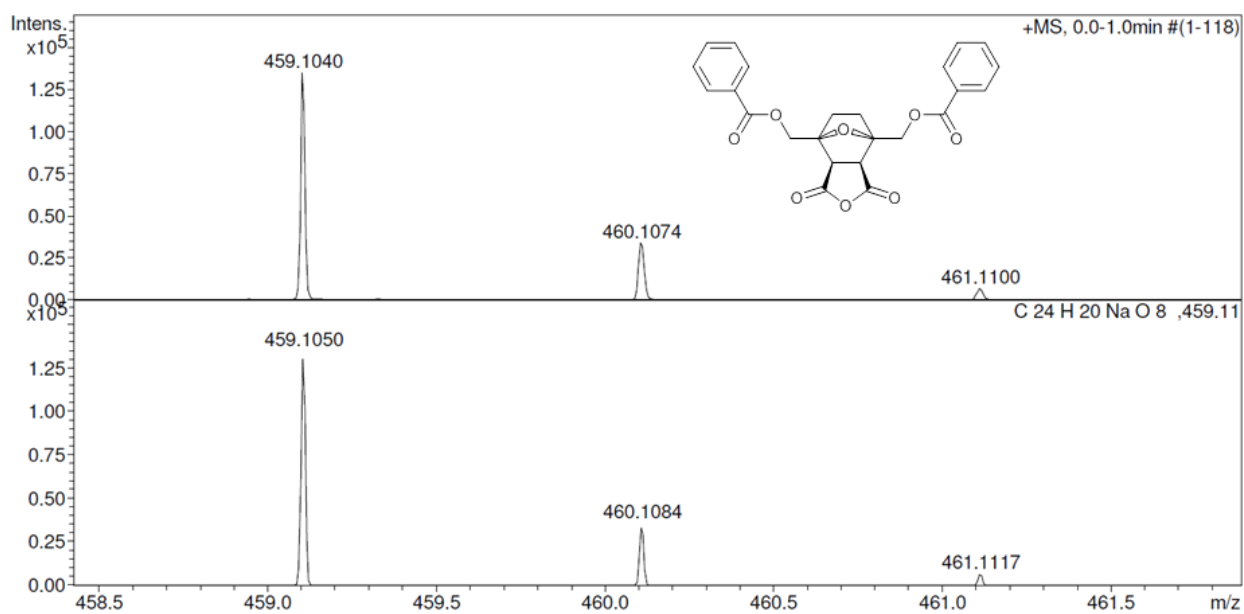


Fig. S36. HRMS (ESI) spectrum of compound 19.

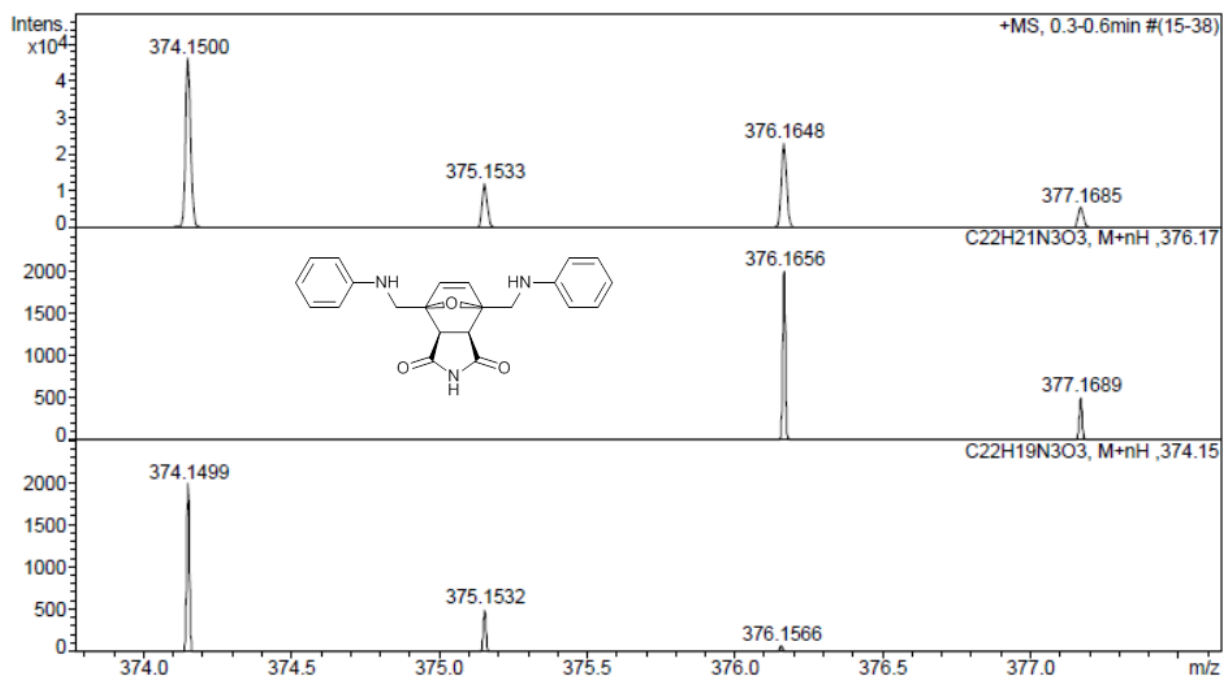


Fig. S37. HRMS (ESI) spectrum of compound 9a.

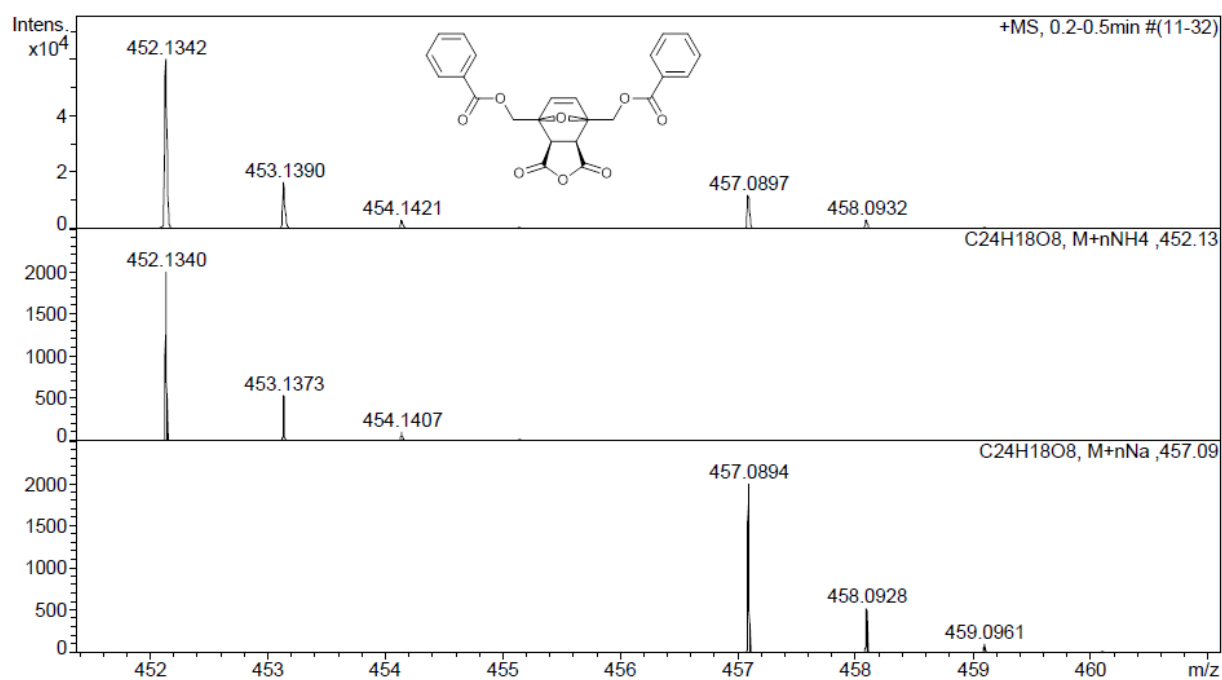
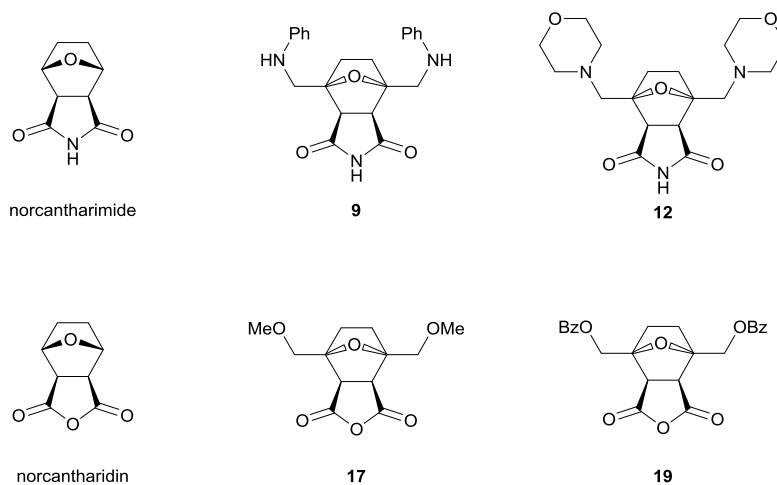


Fig. S38. HRMS (ESI) spectrum of compound 19a.

Preliminary studies of cytotoxicity of selected substances

Table S1. Cytotoxicity of selected substances towards HT-29 cells.



Entry	Substance	48-h IC ₅₀ , μM	72-h IC ₅₀ , μM
1	Norcantharidin	180	26
2	Norcantharimide	>5000	- ^b
3	9	350 ^a	250
4	12	>5000	- ^b
5	17	>1000	- ^b
6	19	- ^c	- ^c

^a - Did not kill all cells at the maximum concentration tested. ^b – Not tested due to low effect shown in 48h experiment. ^c - Hydrolysis of the product.