

Supplementary Information

for

Bioinspired Pyrano[2,3-*f*]chromen-8-ones: Ring C-Opened Analogues of Calanolide A. Synthesis and Anti-HIV-1 Evaluation

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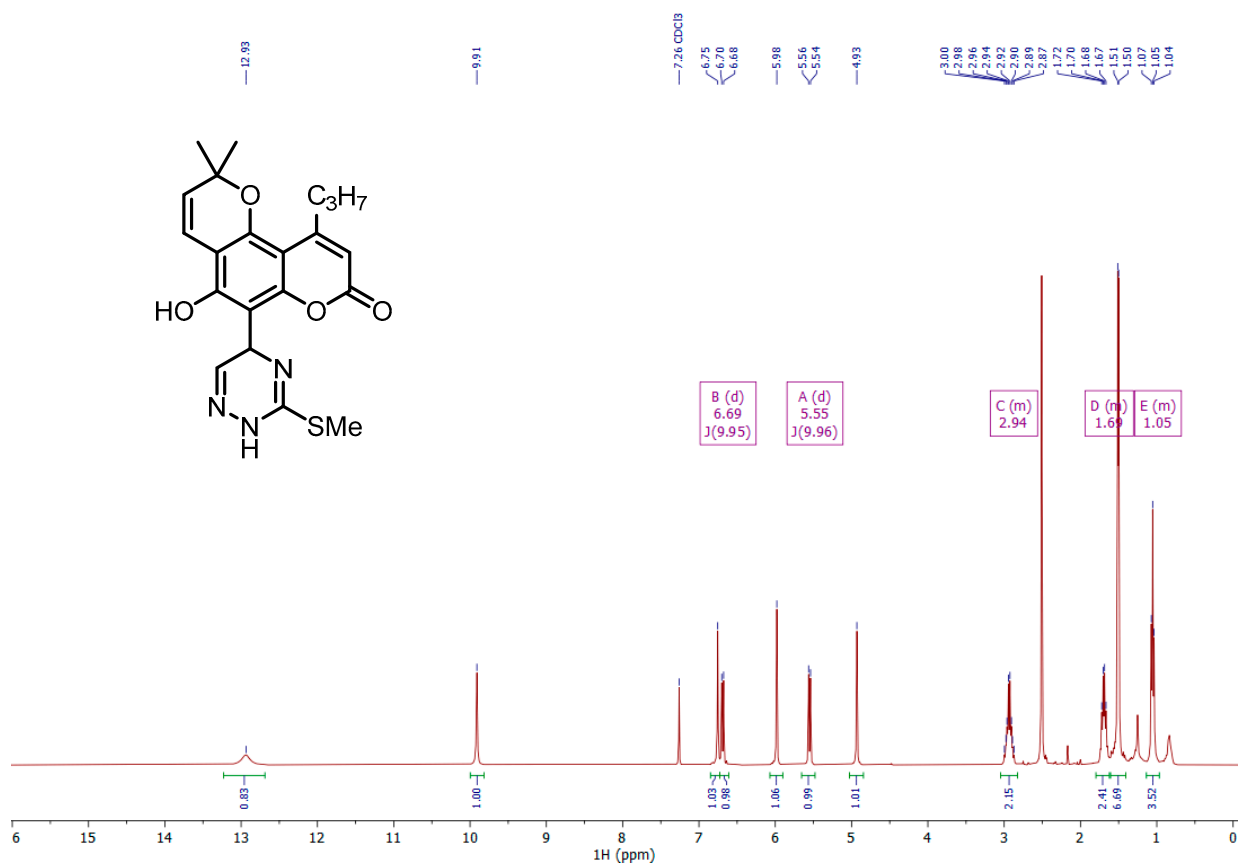
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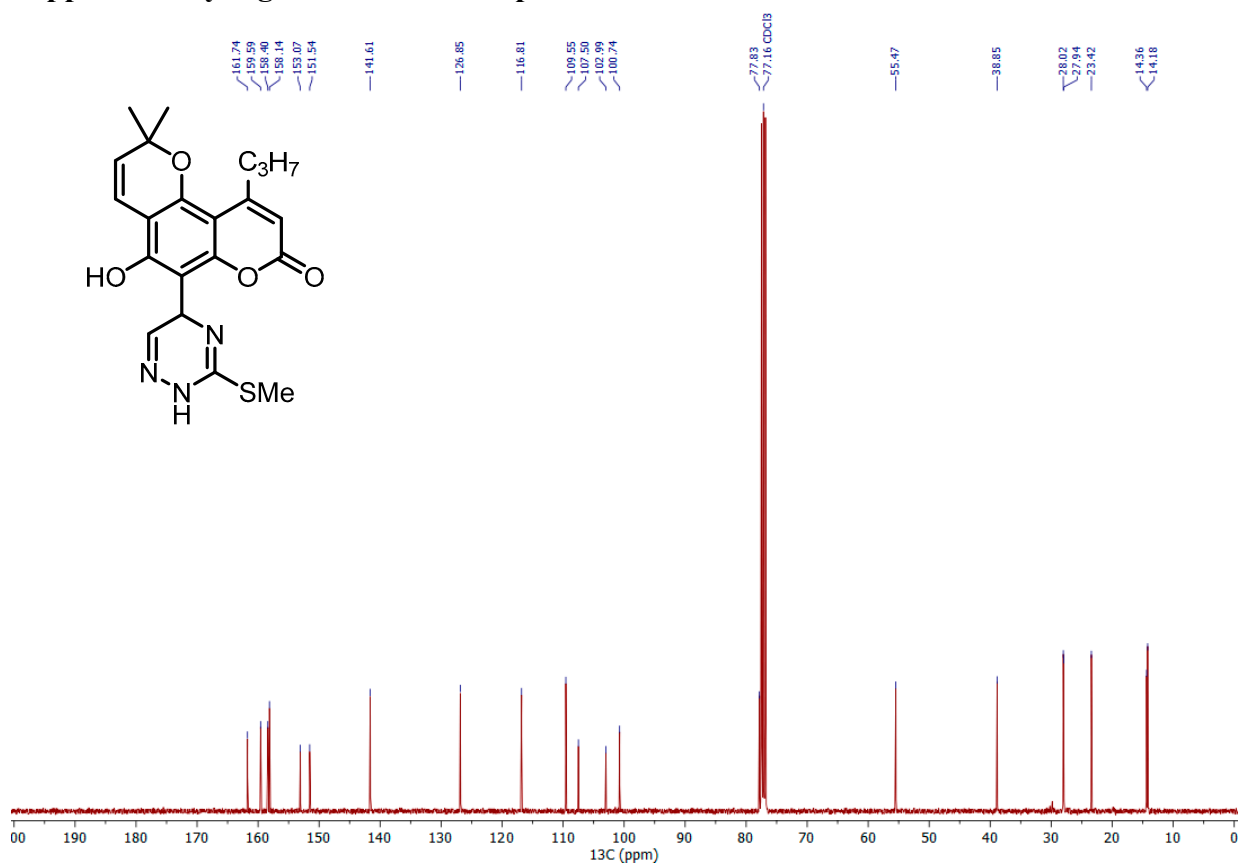
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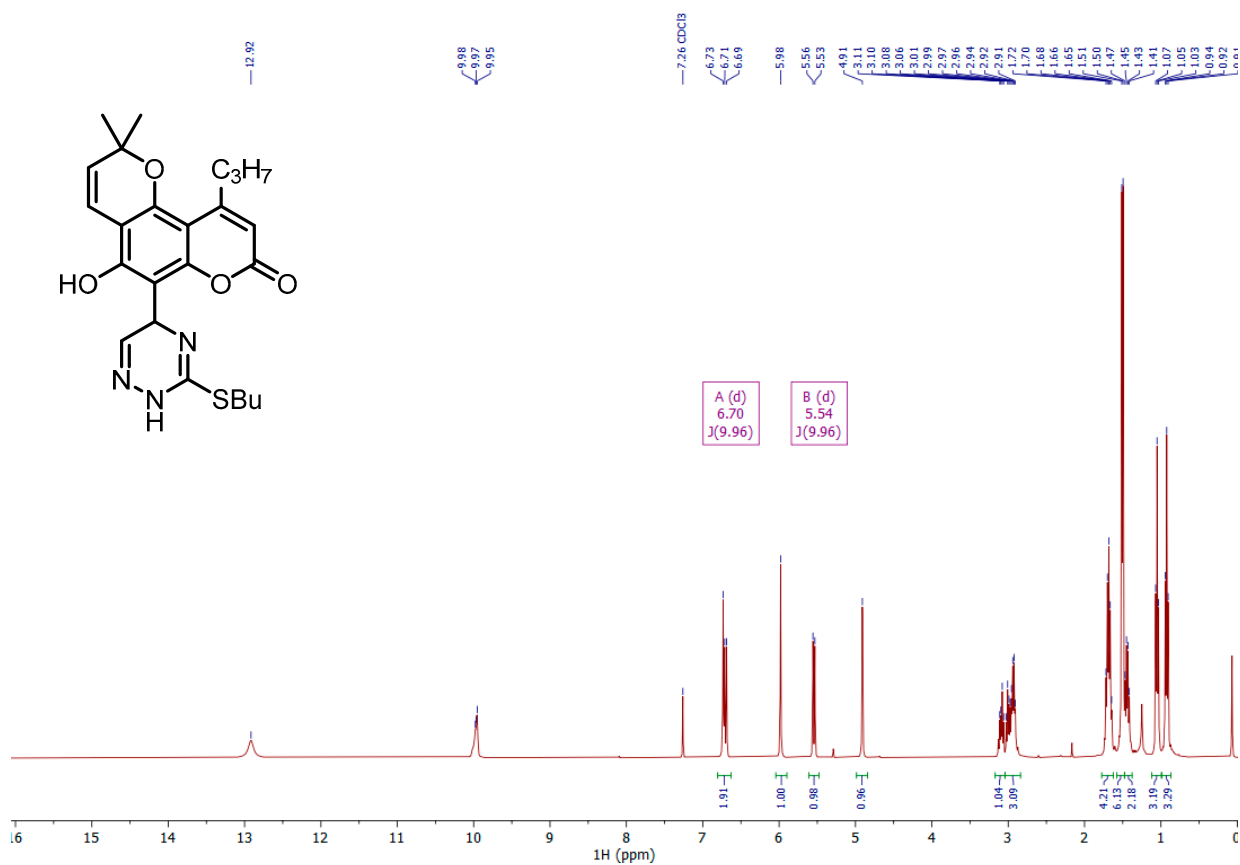
* Correspondence: i.a.khalymbadzha@urfu.ru (I.A.K.); tsurkan@ipfdd.de (M.V.T.)



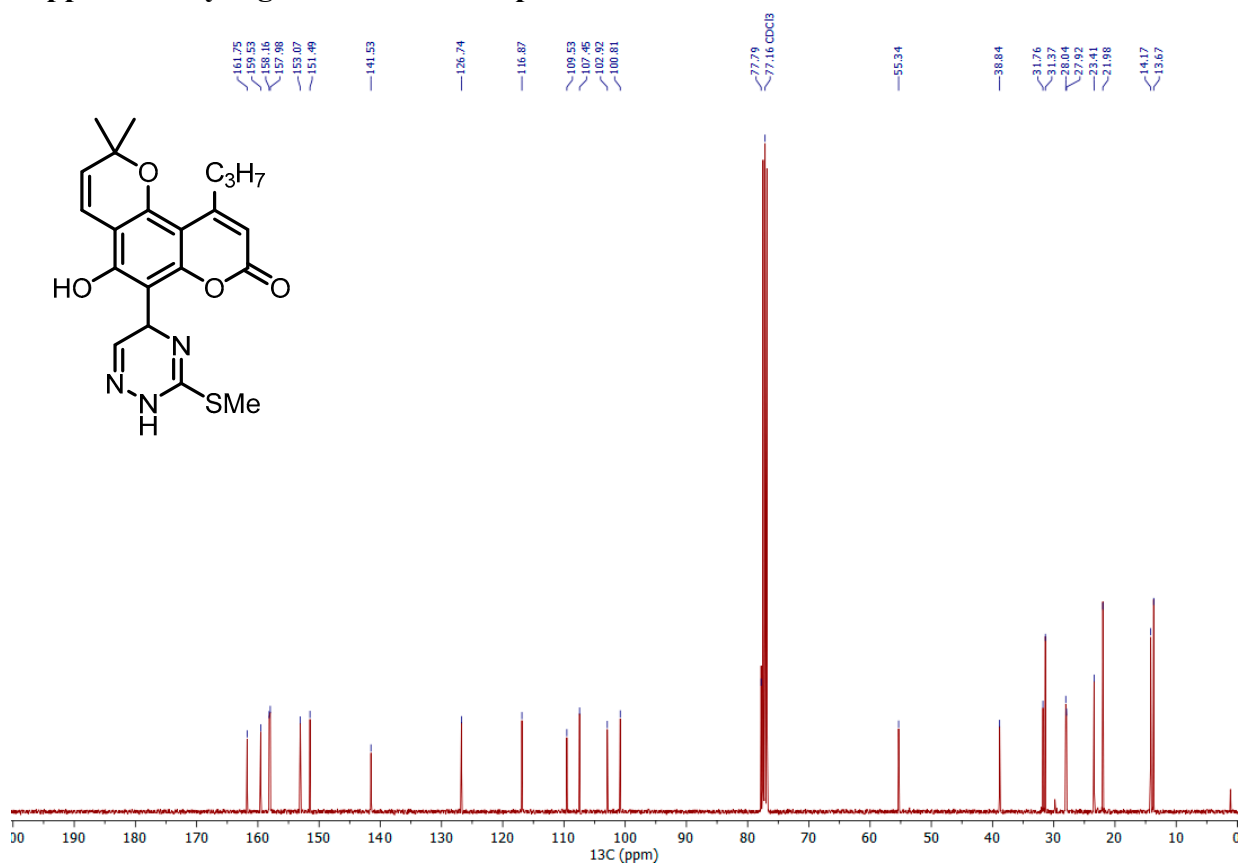
Supplementary Figure S1. ¹H NMR spectrum of 4a



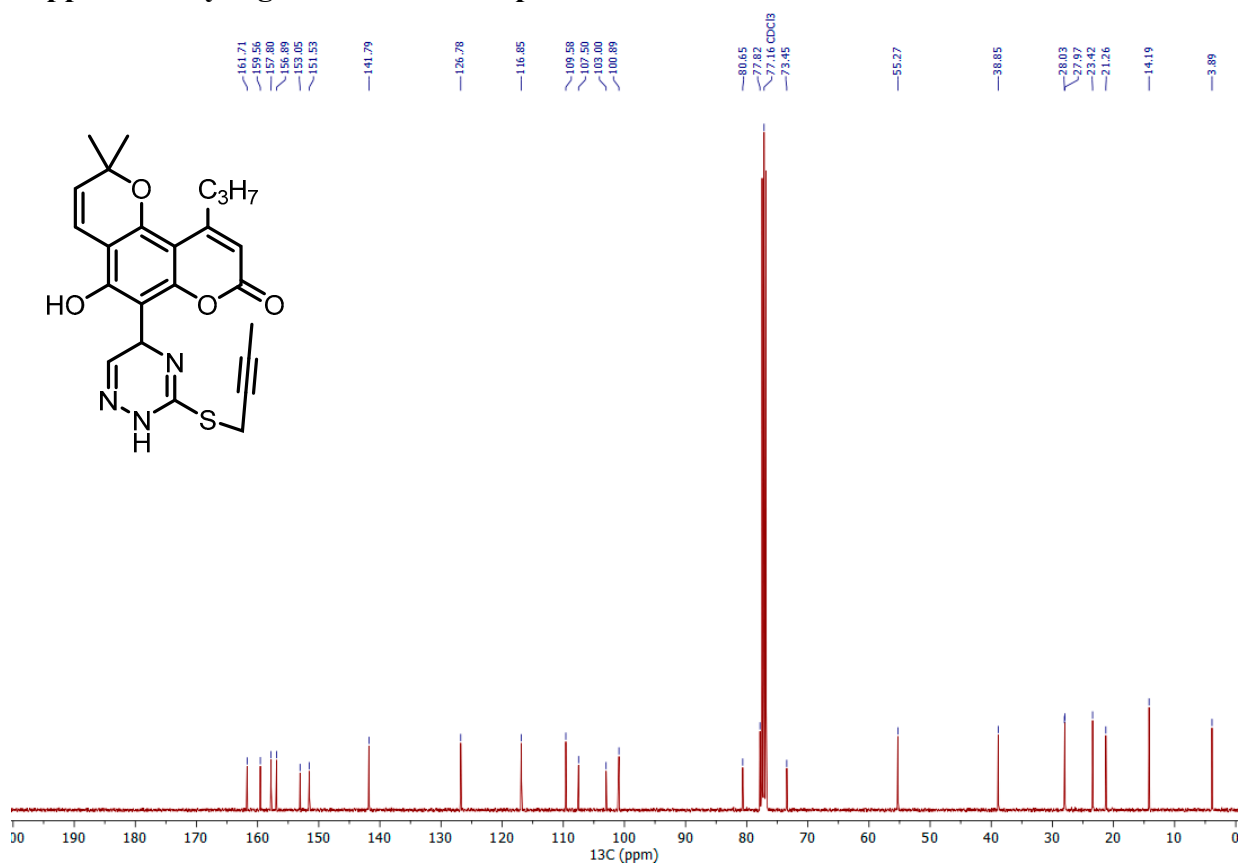
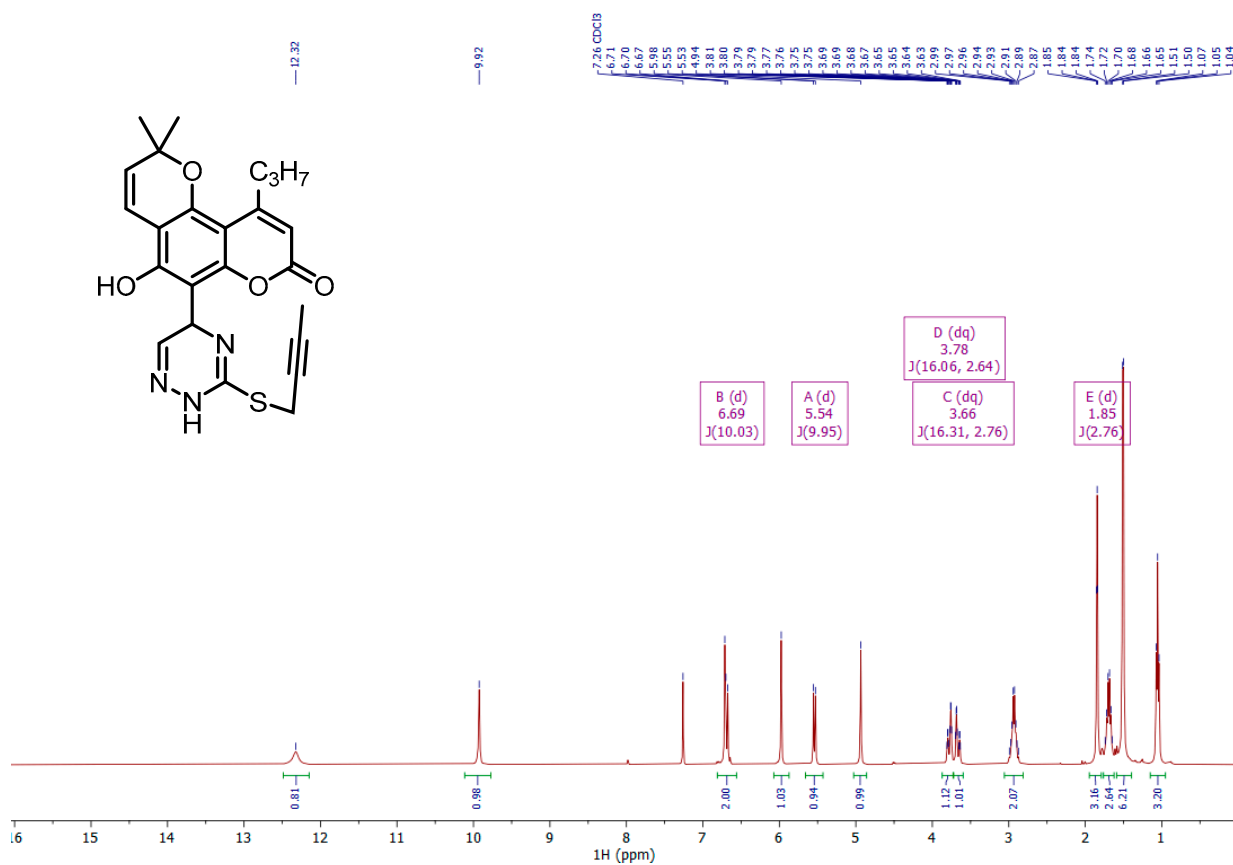
Supplementary Figure S2. ¹³C NMR spectrum of 4a

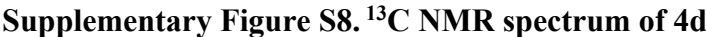
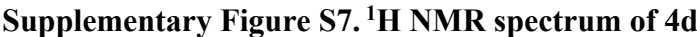


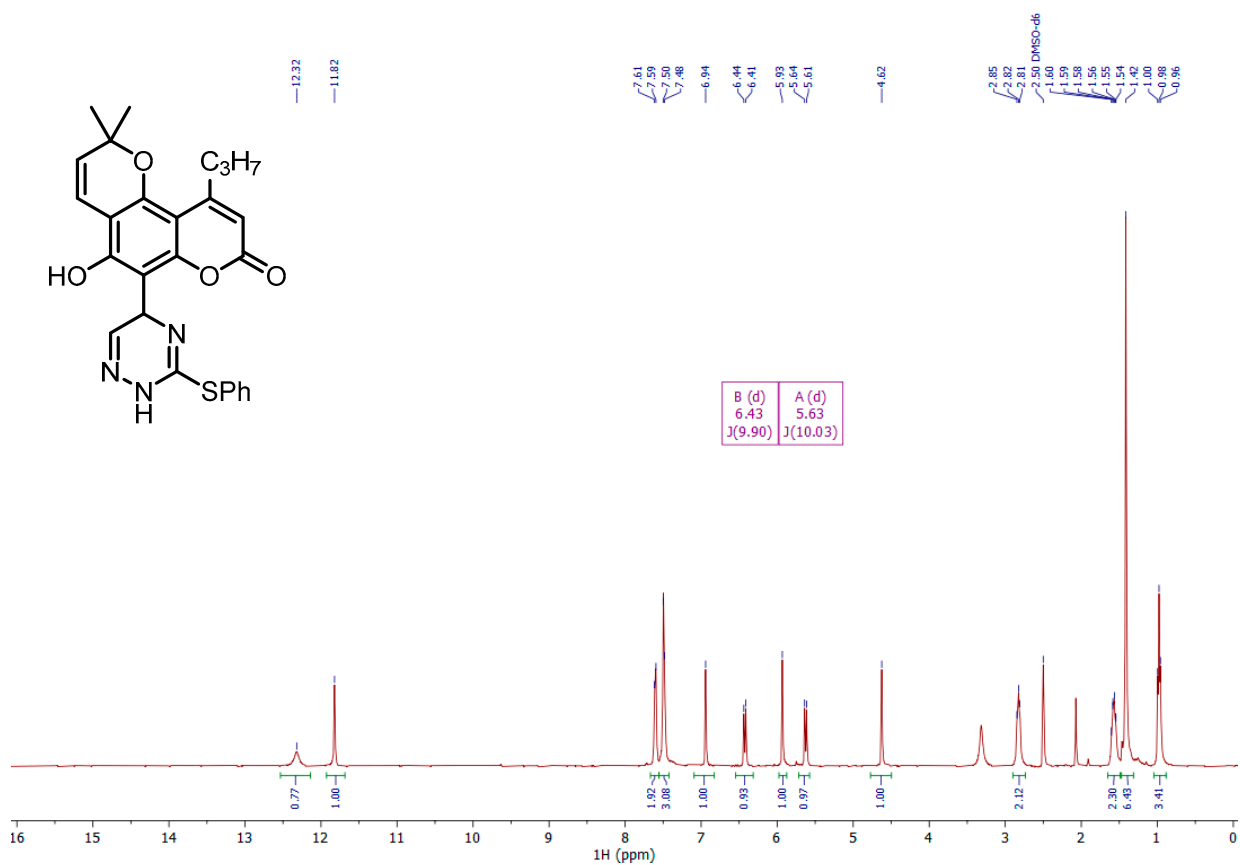
Supplementary Figure S3. ¹H NMR spectrum of 4b



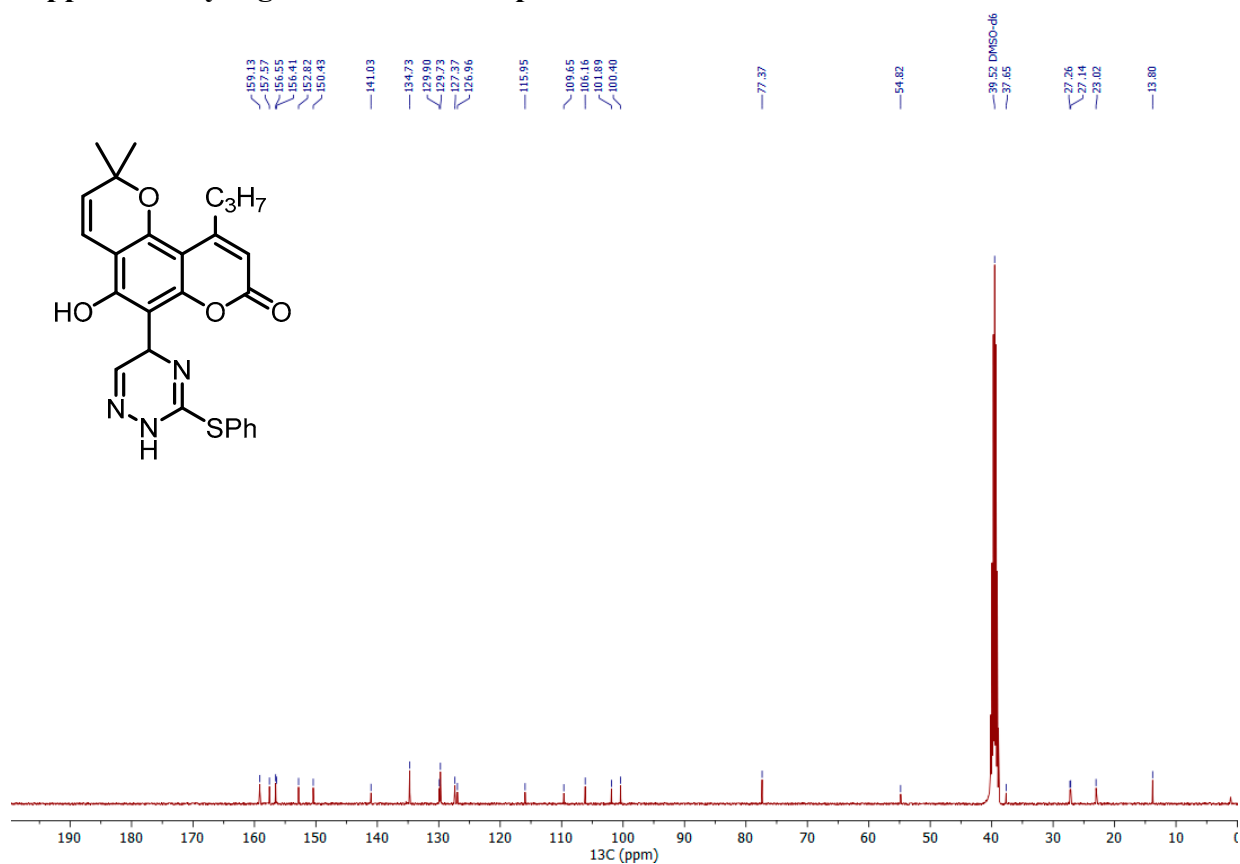
Supplementary Figure S4. ¹³C NMR spectrum of 4b



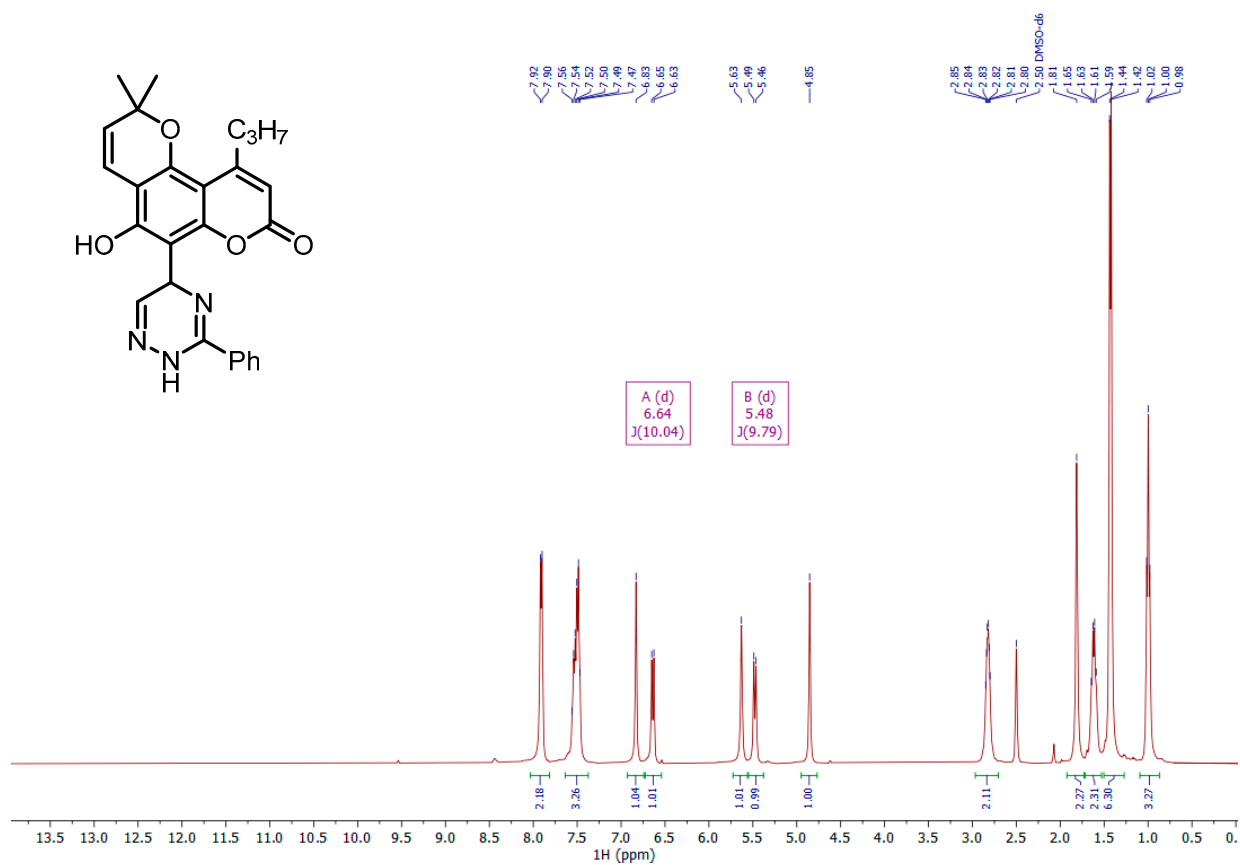




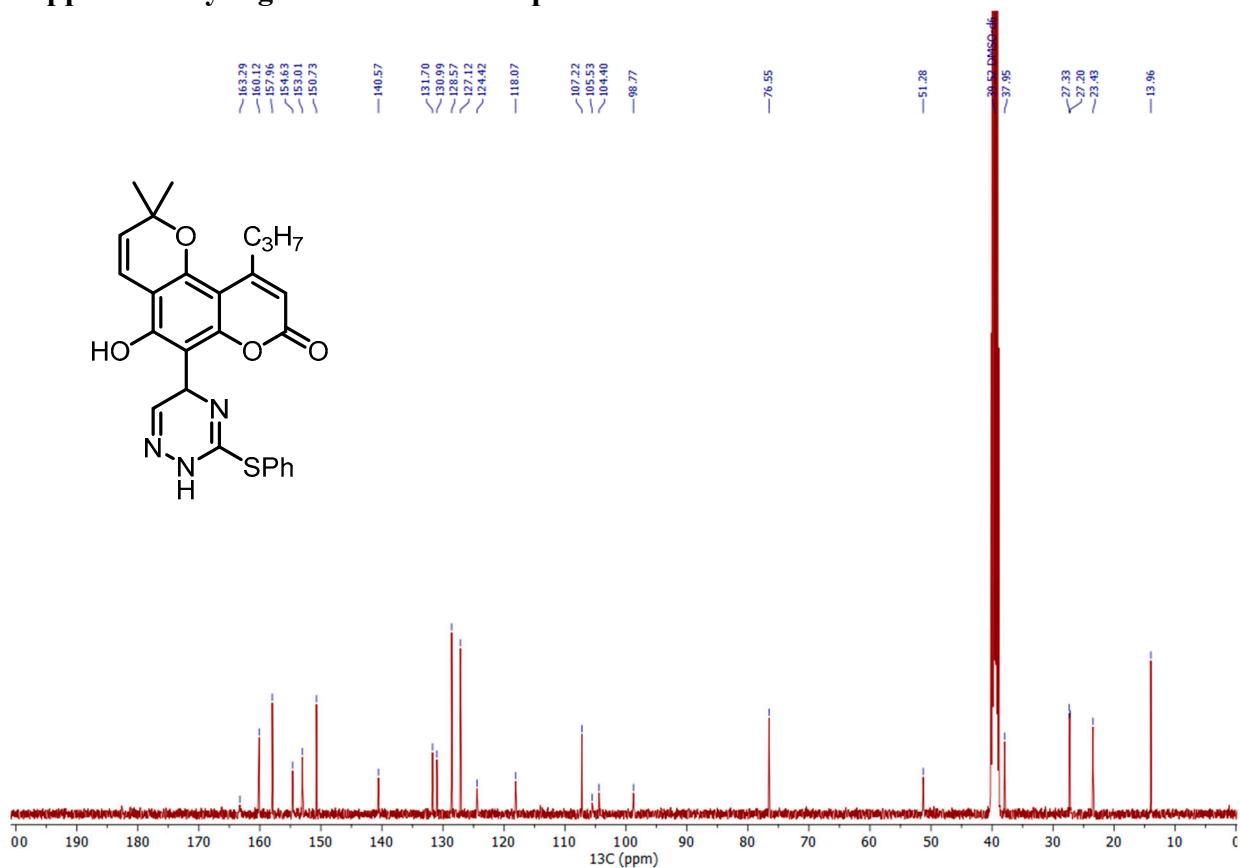
Supplementary Figure S9. ^1H NMR spectrum of 4e



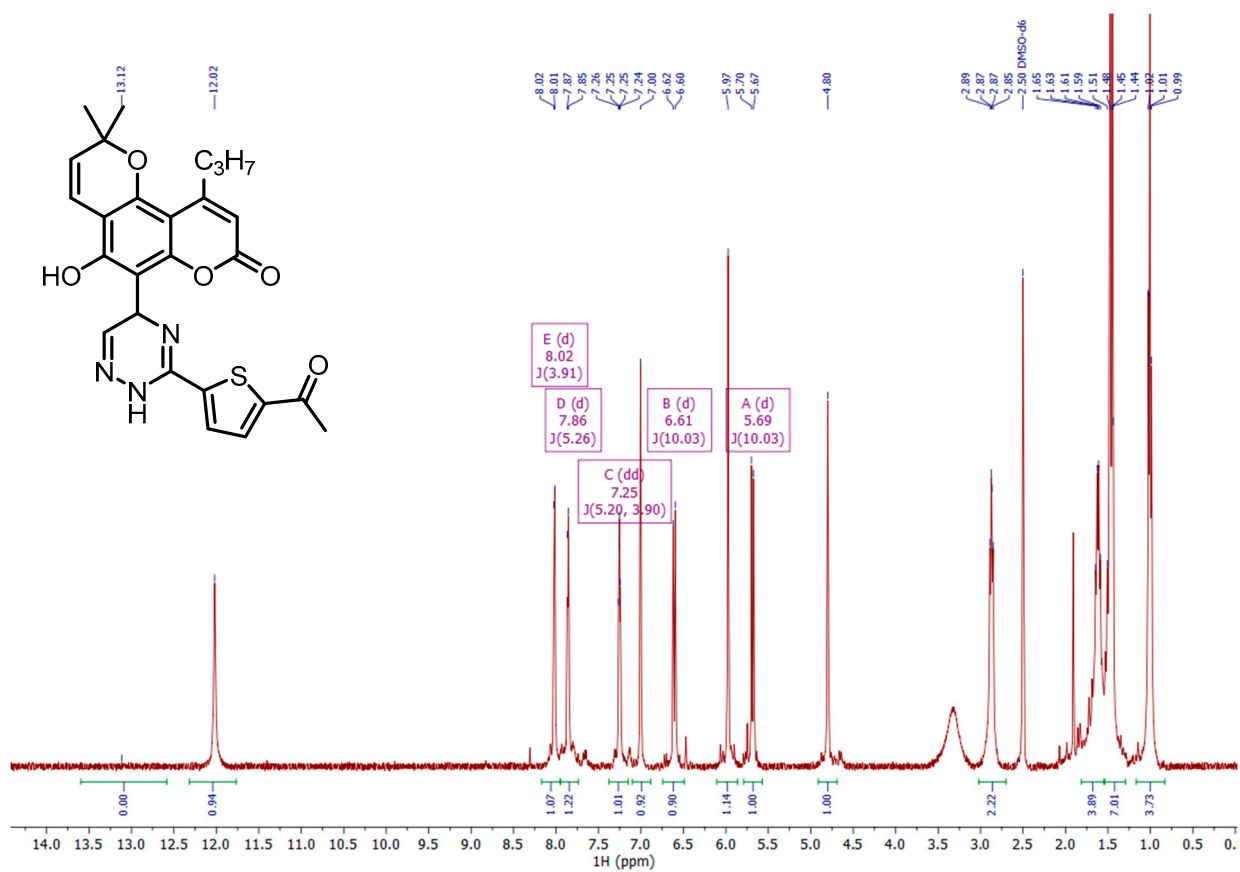
Supplementary Figure S10. ^{13}C NMR spectrum of 4e



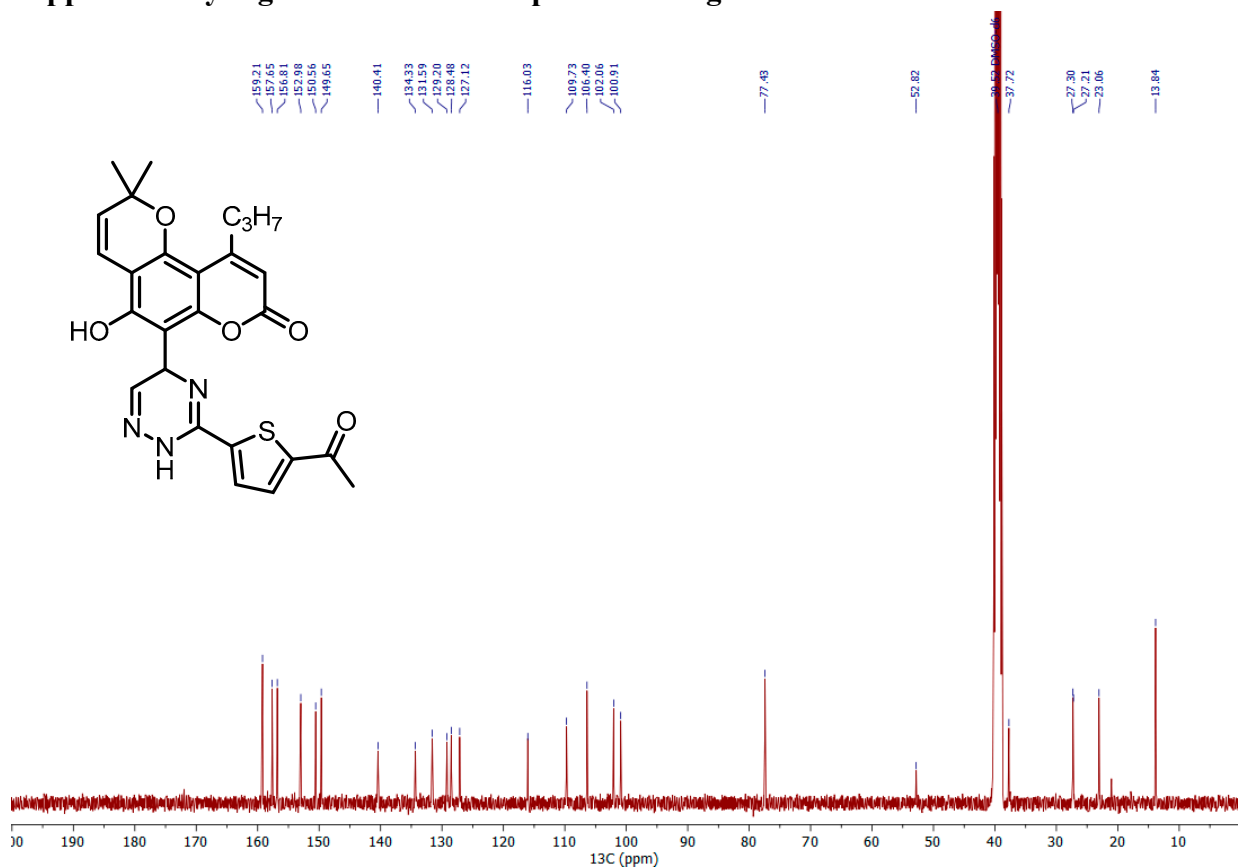
Supplementary Figure S11. ¹H NMR spectrum of 4f



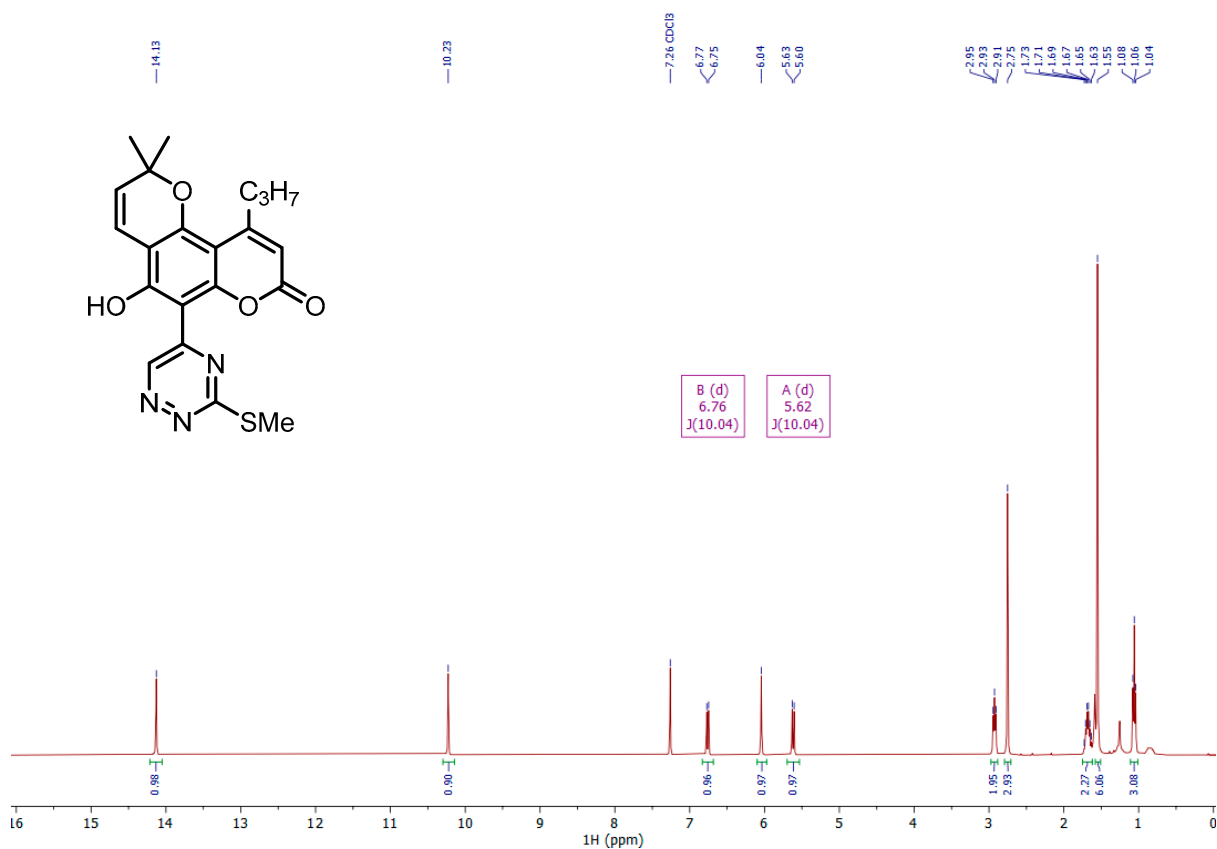
Supplementary Figure S12. ¹³C NMR spectrum of 4f



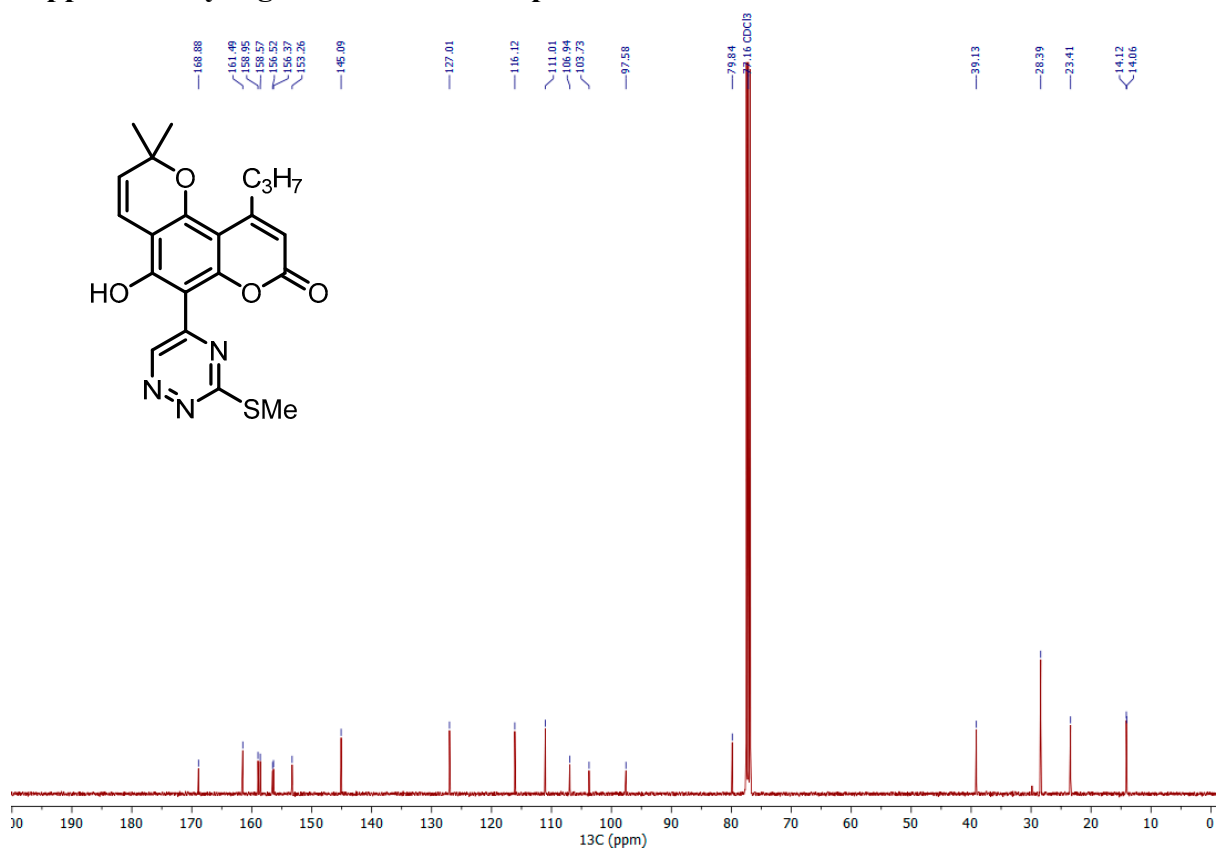
Supplementary Figure S13. ¹H NMR spectrum of 4g



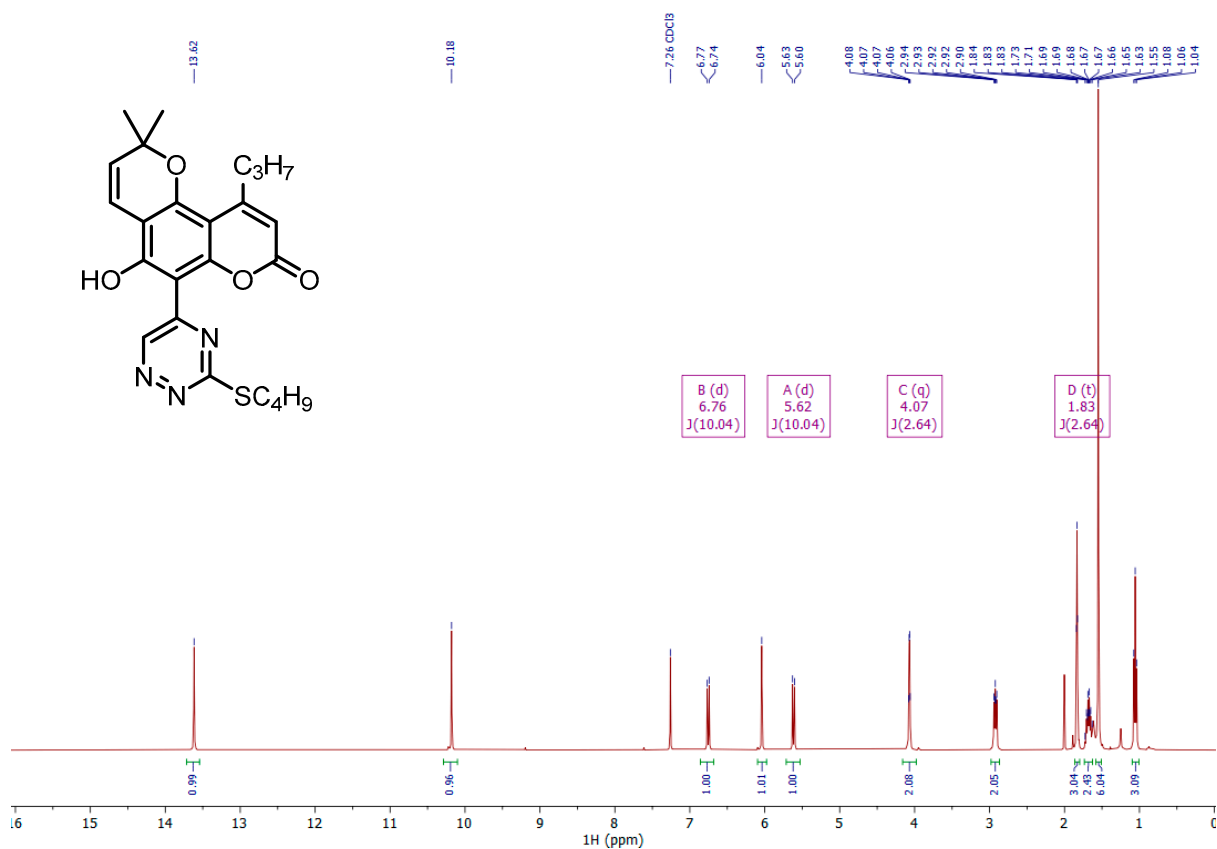
Supplementary Figure S14. ¹³C NMR spectrum of 4g



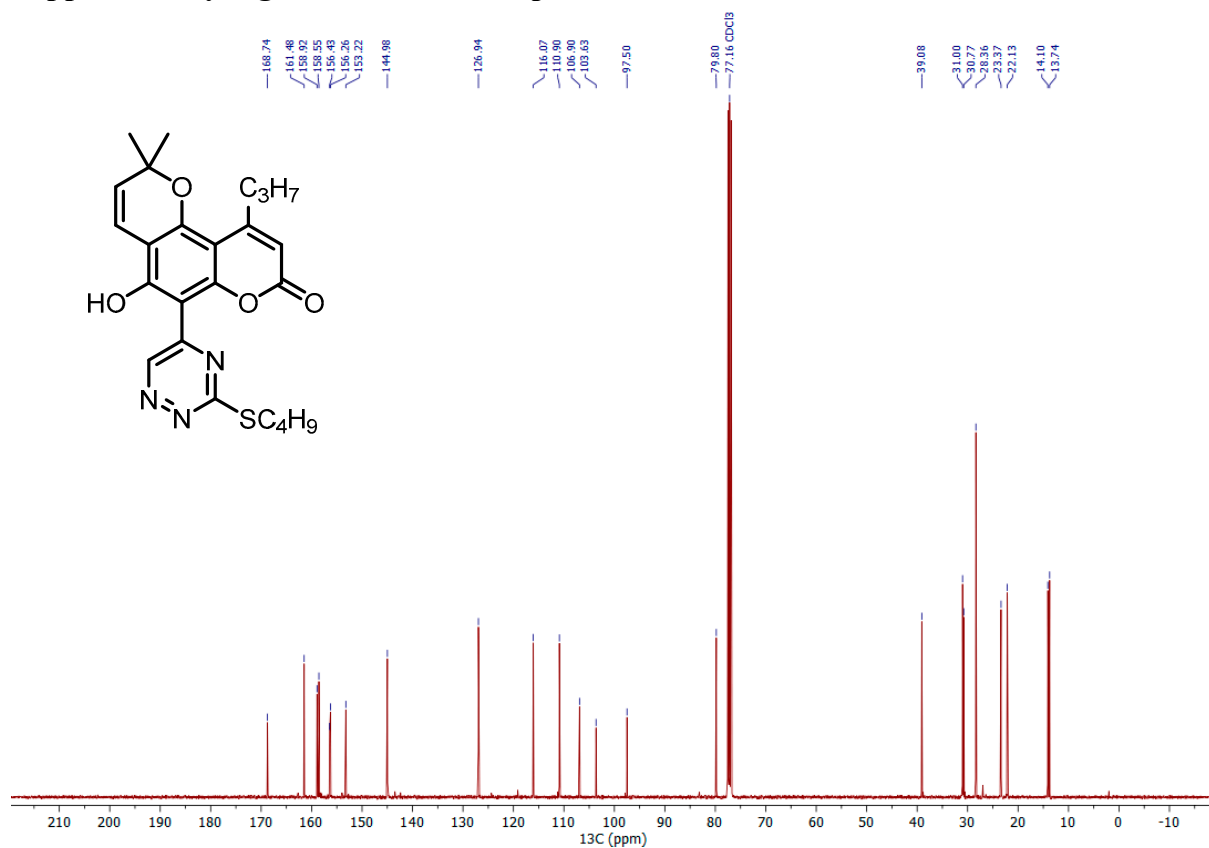
Supplementary Figure S15. ¹H NMR spectrum of 5a



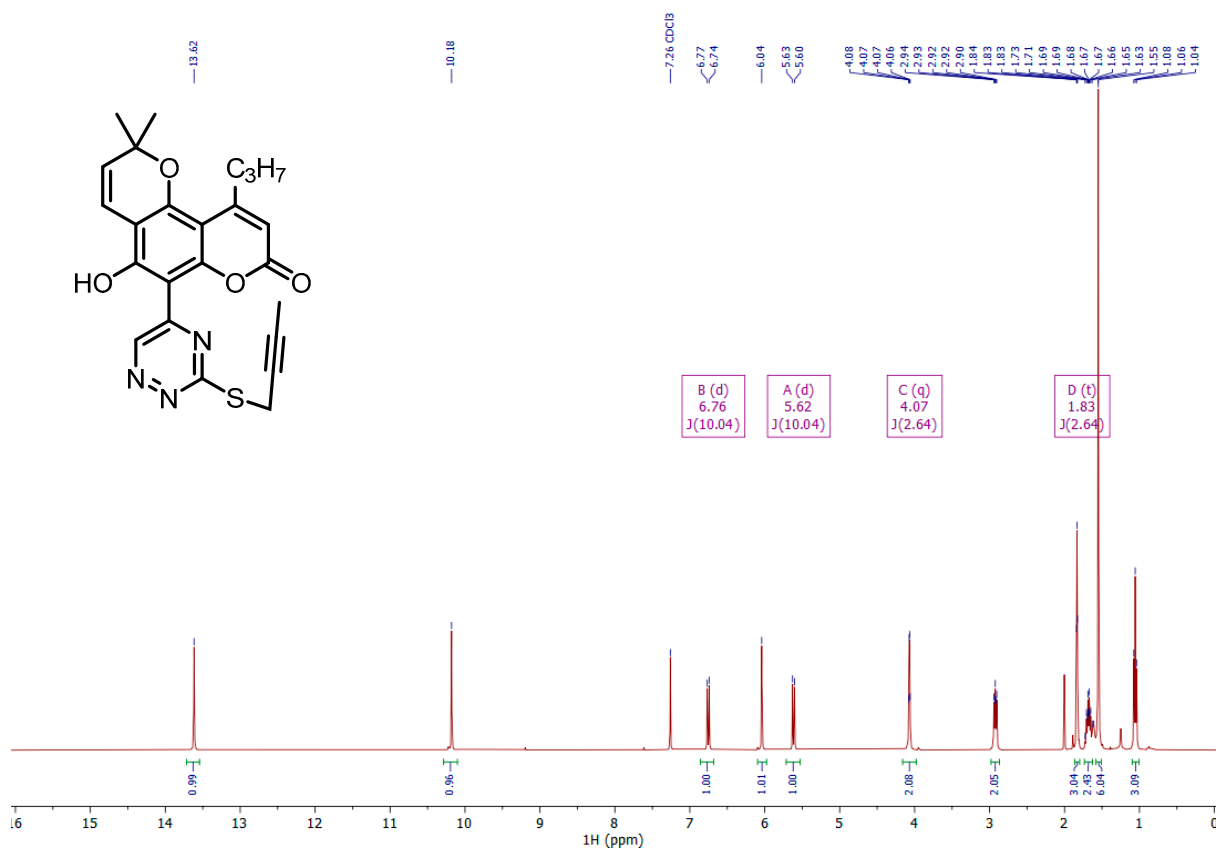
Supplementary Figure S16. ¹³C NMR spectrum of 5a



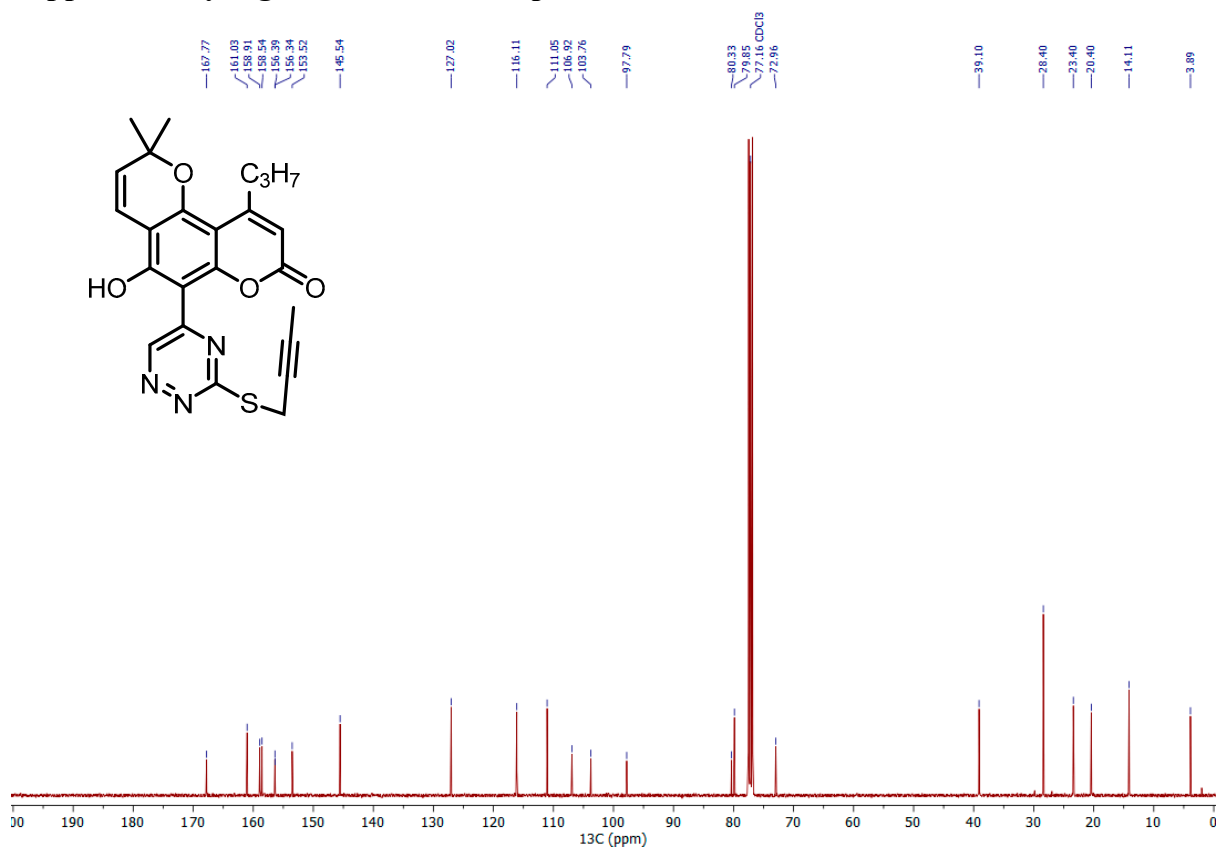
Supplementary Figure S17. ¹H NMR spectrum of 5b



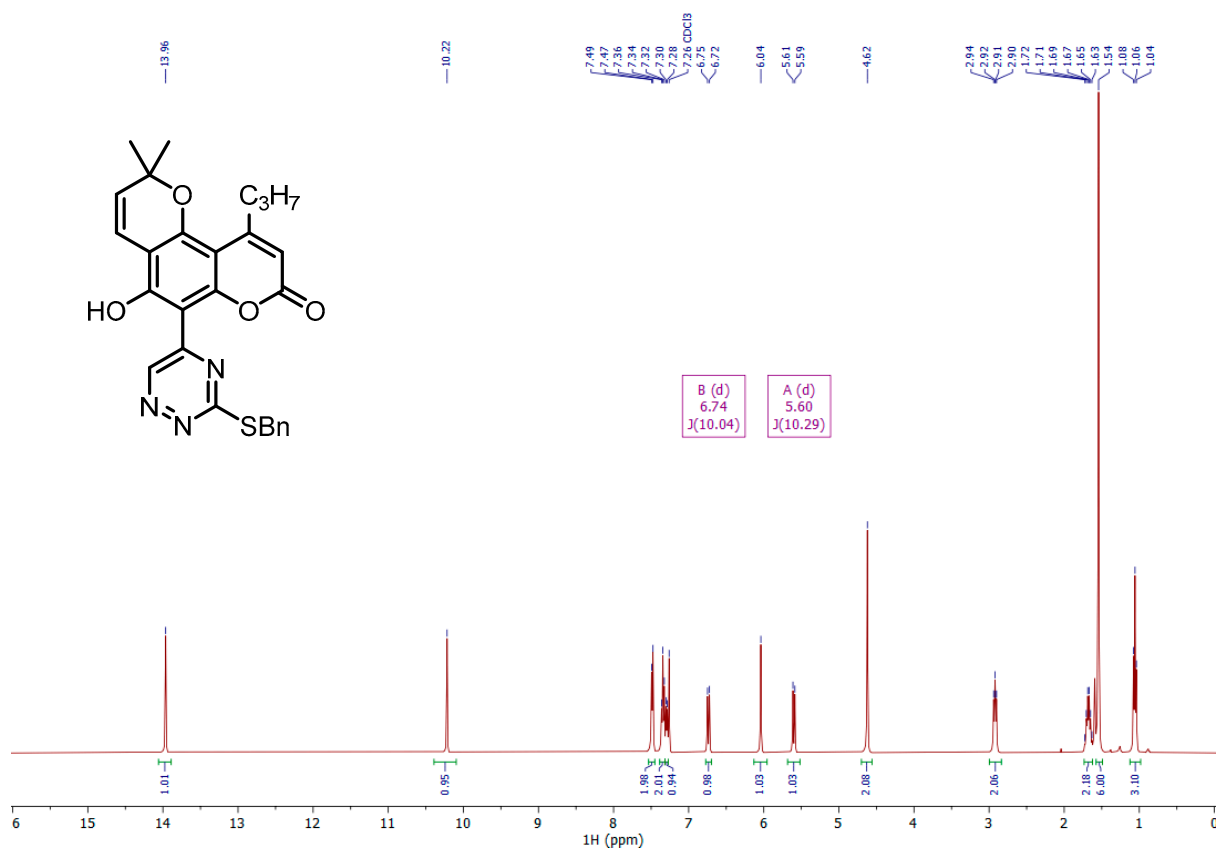
Supplementary Figure S18. ¹³C NMR spectrum of 5b



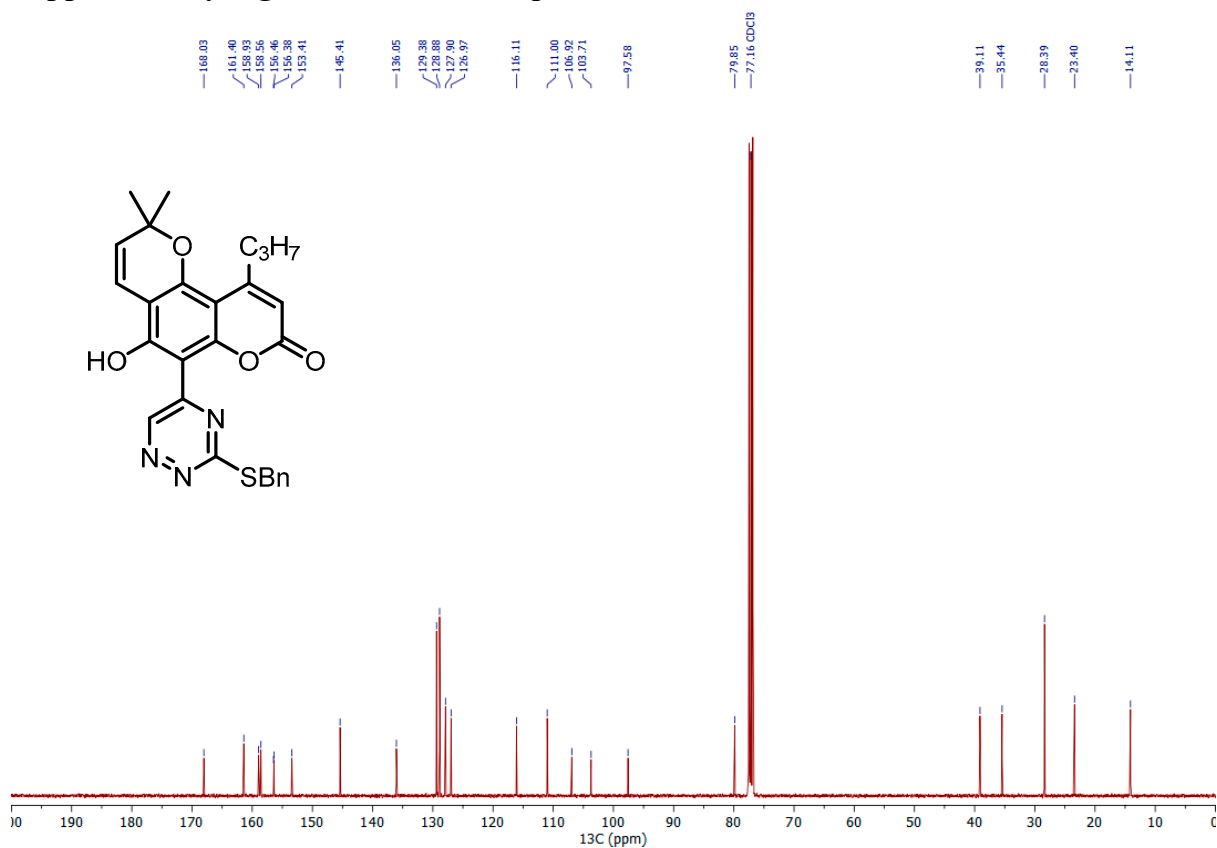
Supplementary Figure S19. ¹H NMR spectrum of 5c



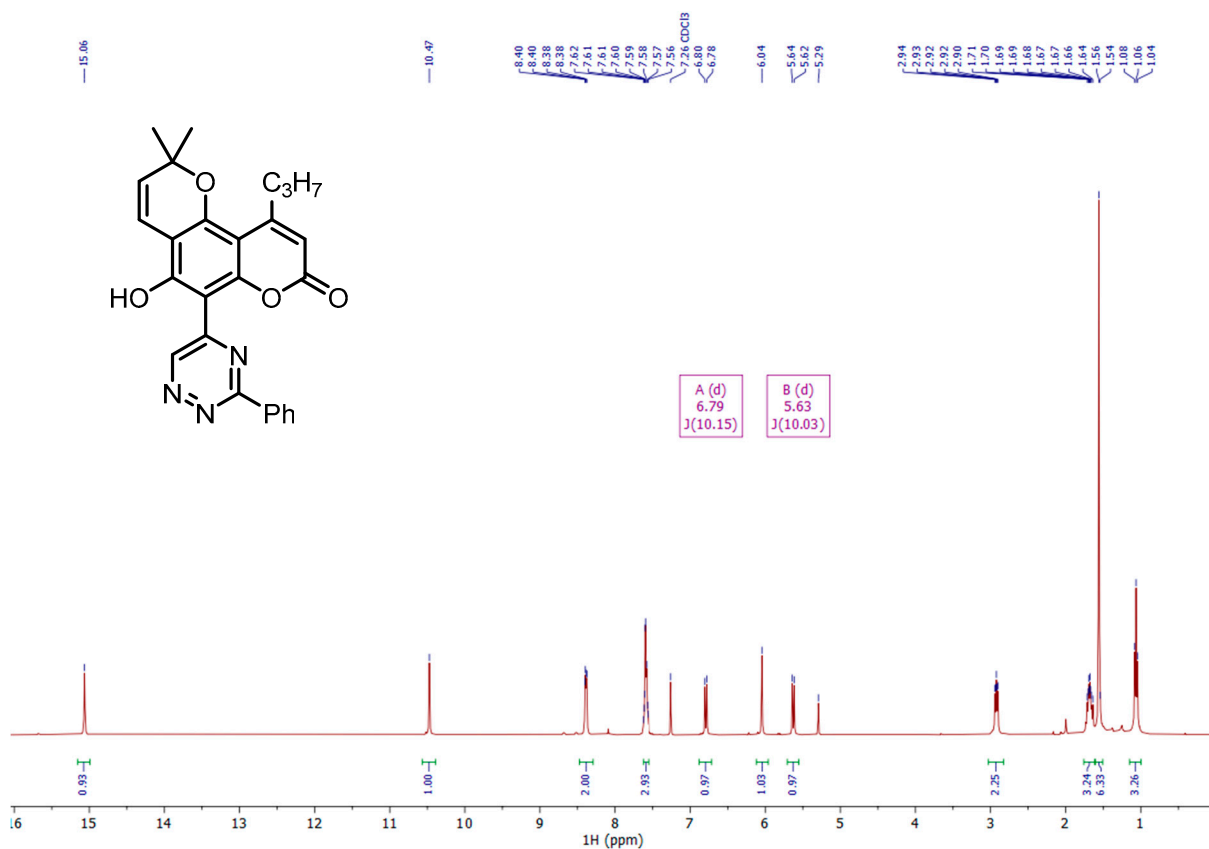
Supplementary Figure S20. ¹³C NMR spectrum of 5c



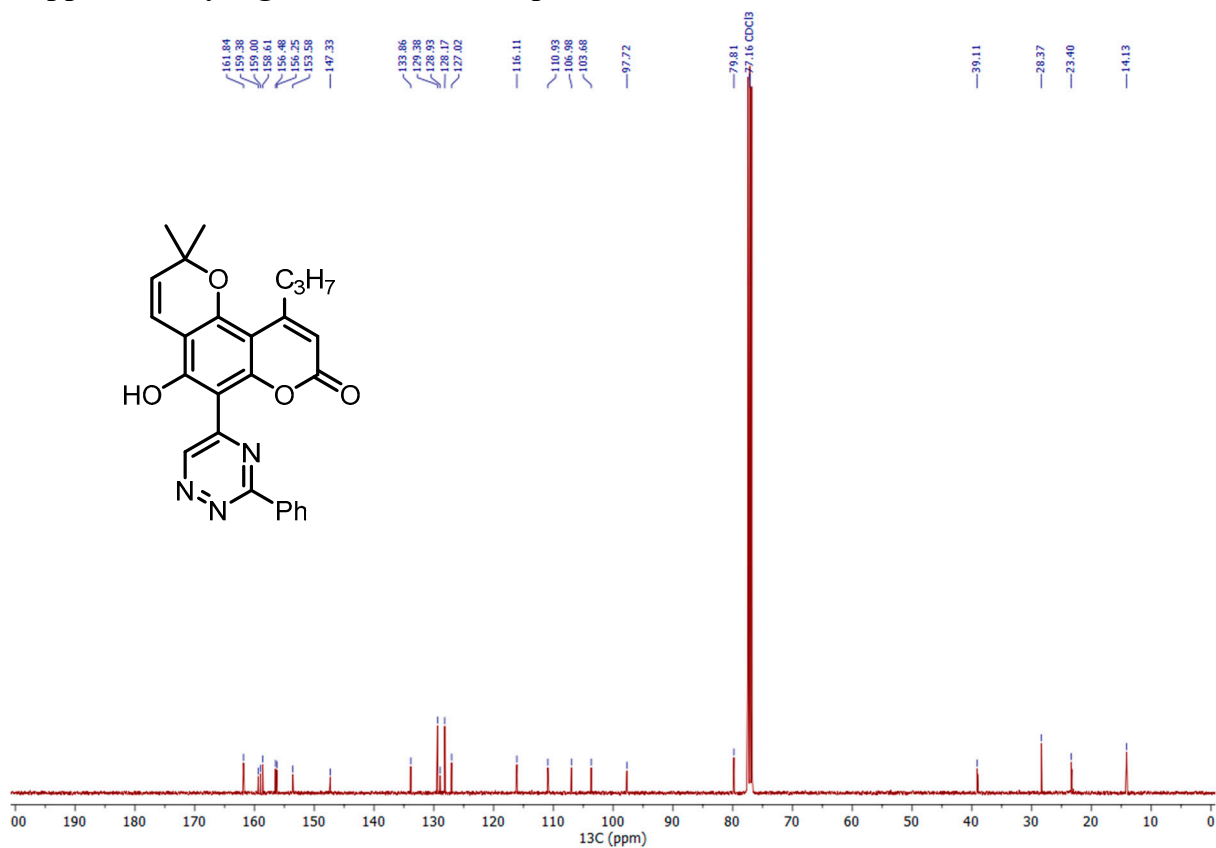
Supplementary Figure S21. ¹H NMR spectrum of 5d



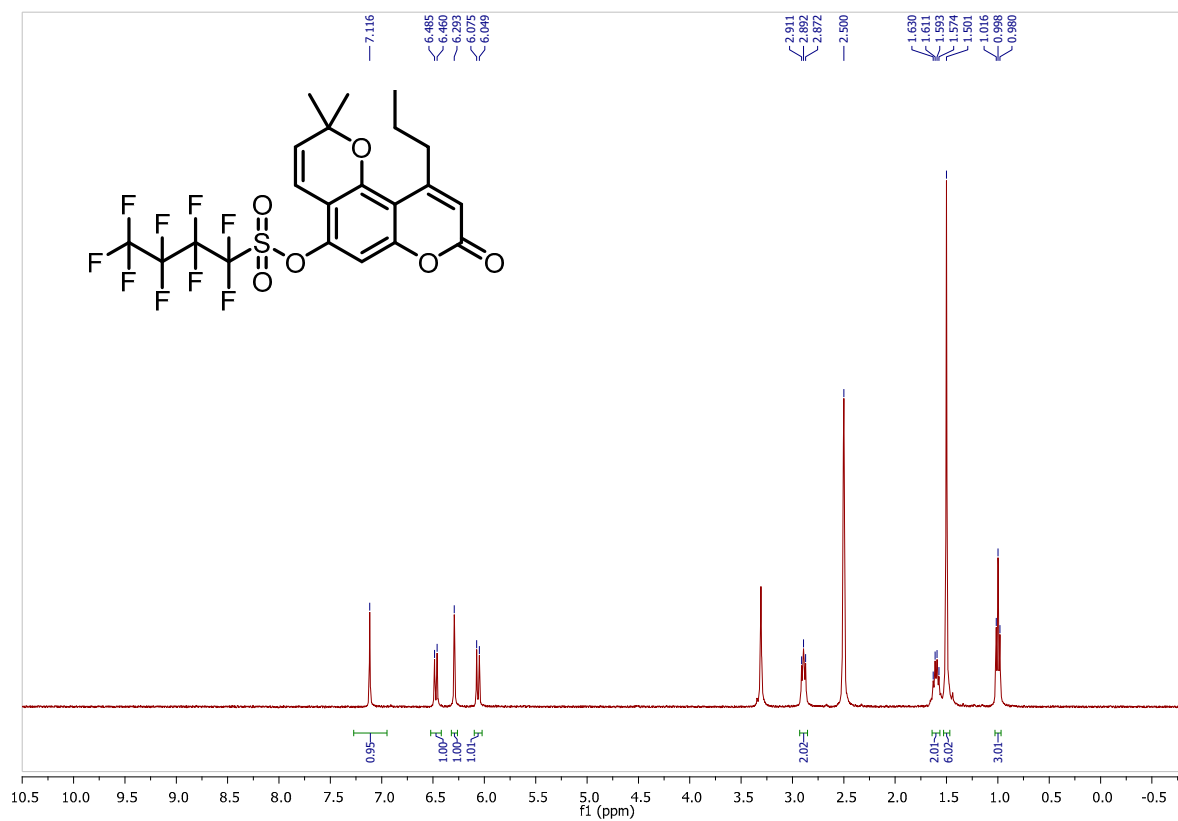
Supplementary Figure S22. ¹³C NMR spectrum of 5d



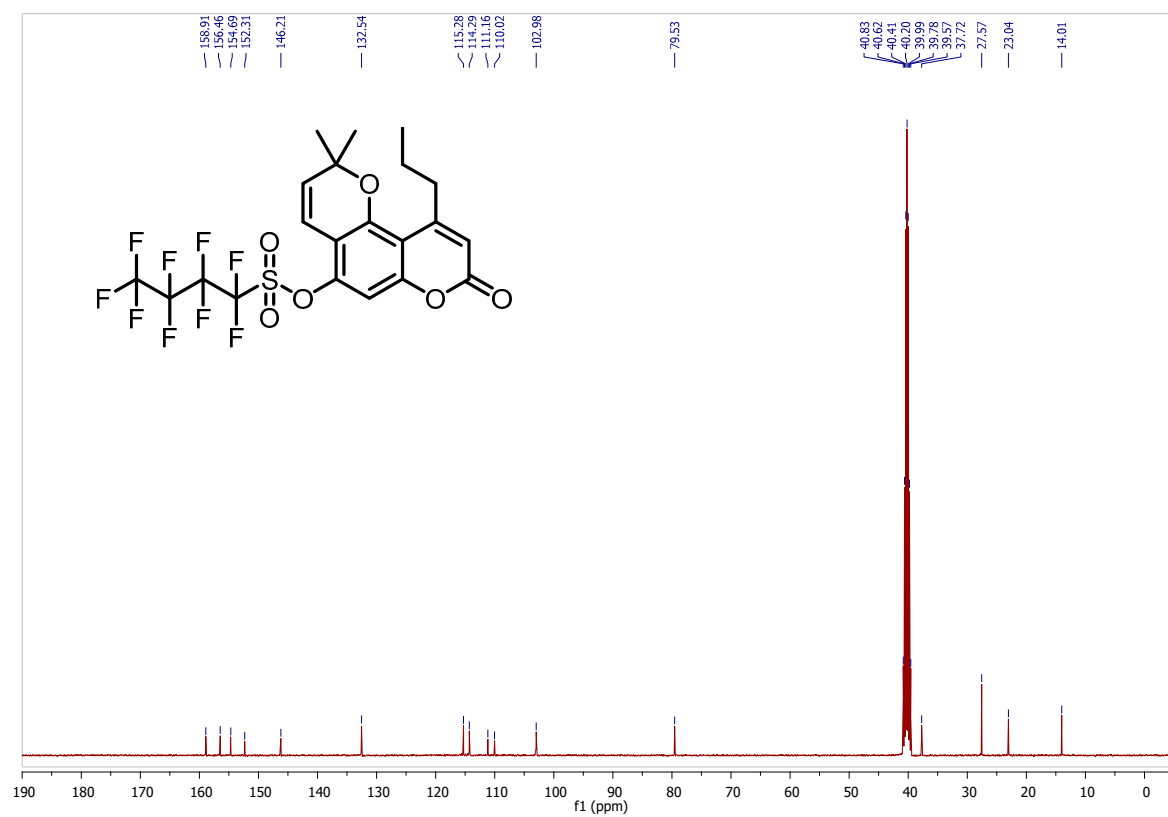
Supplementary Figure S23. ¹H NMR spectrum of 5f



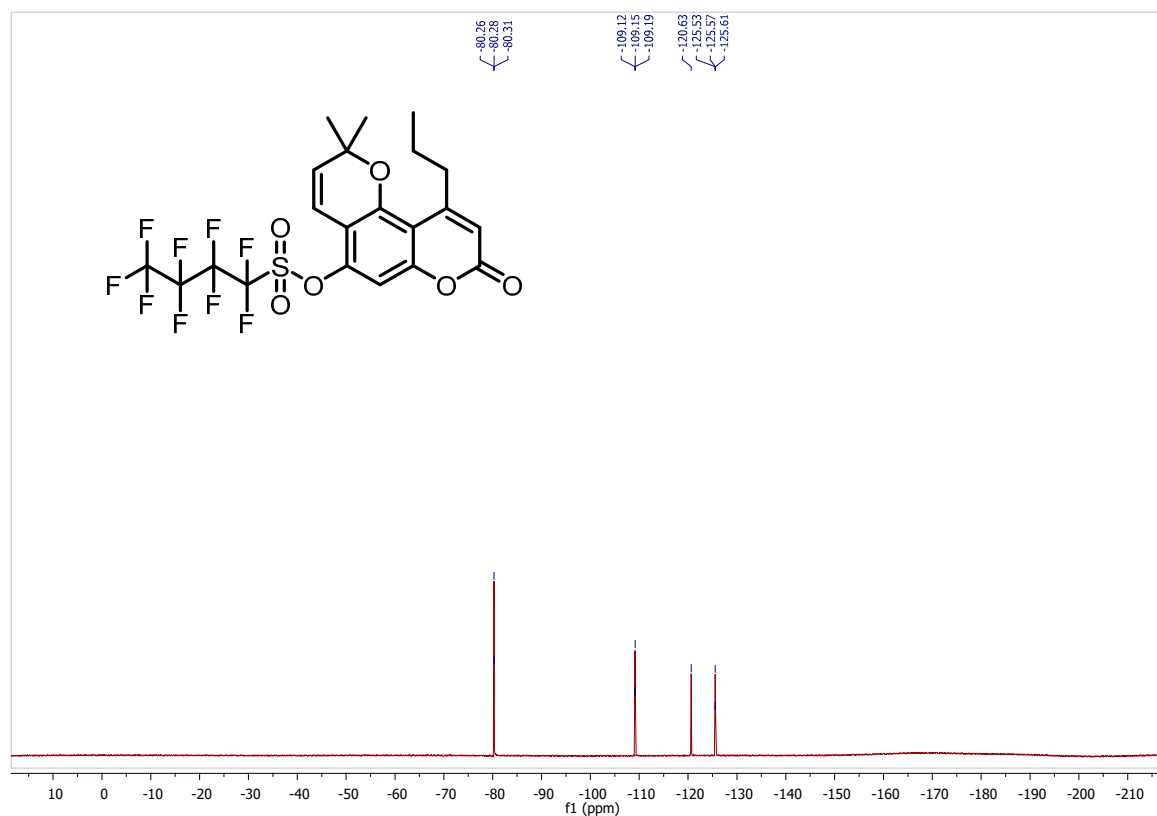
Supplementary Figure S24. ¹³C NMR spectrum of 5f



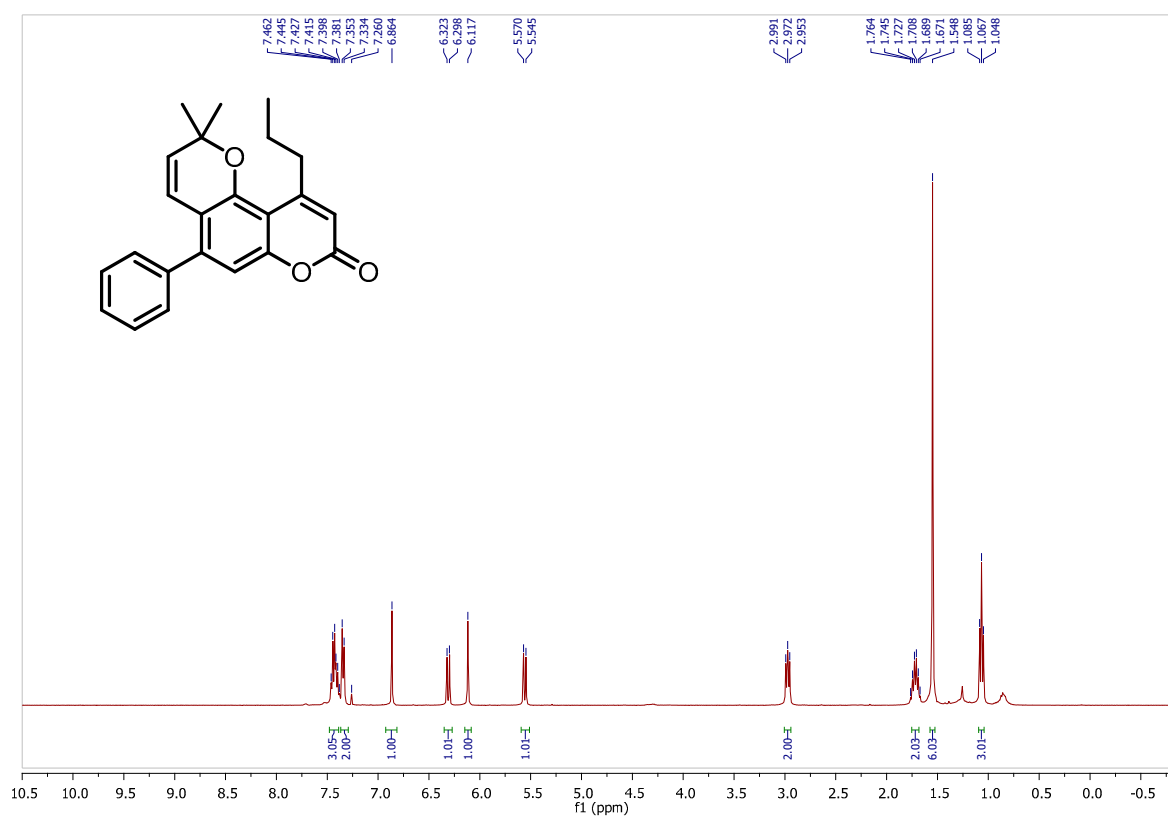
Supplementary Figure S25. ¹H NMR spectrum of 8



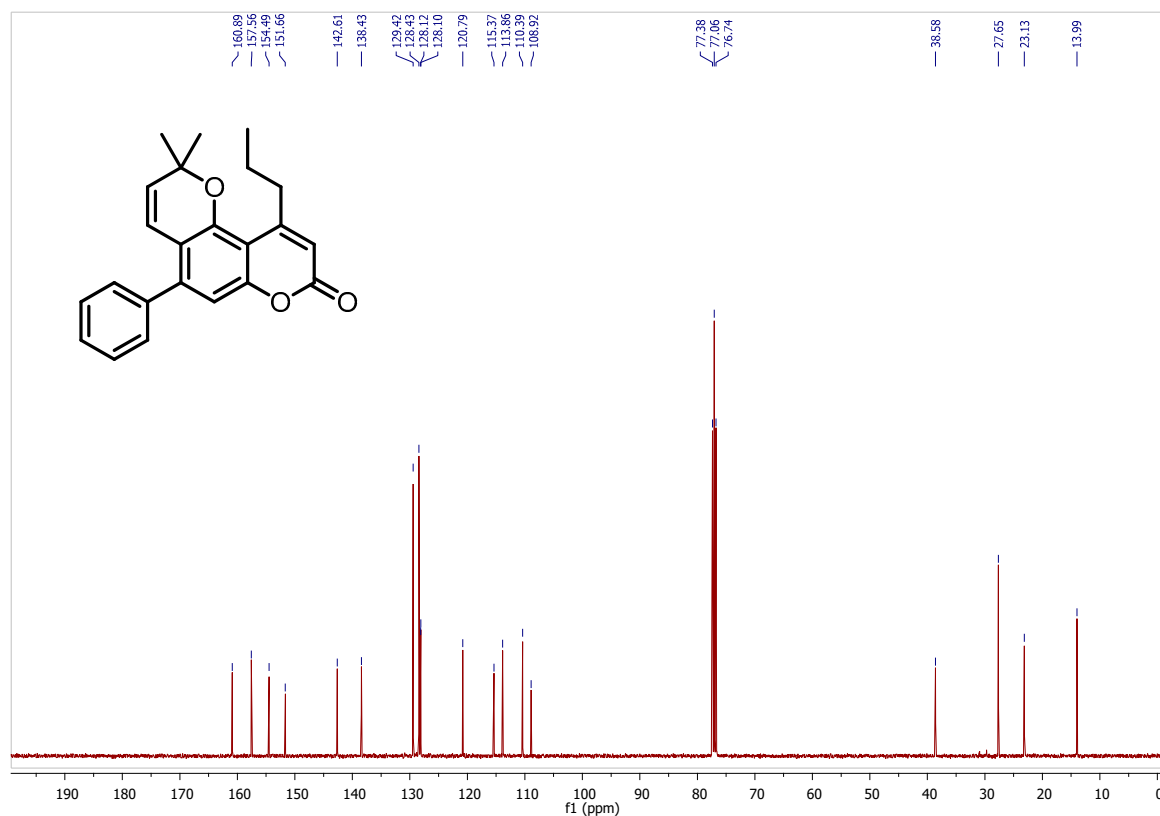
Supplementary Figure S26. ¹³C NMR spectrum of 8



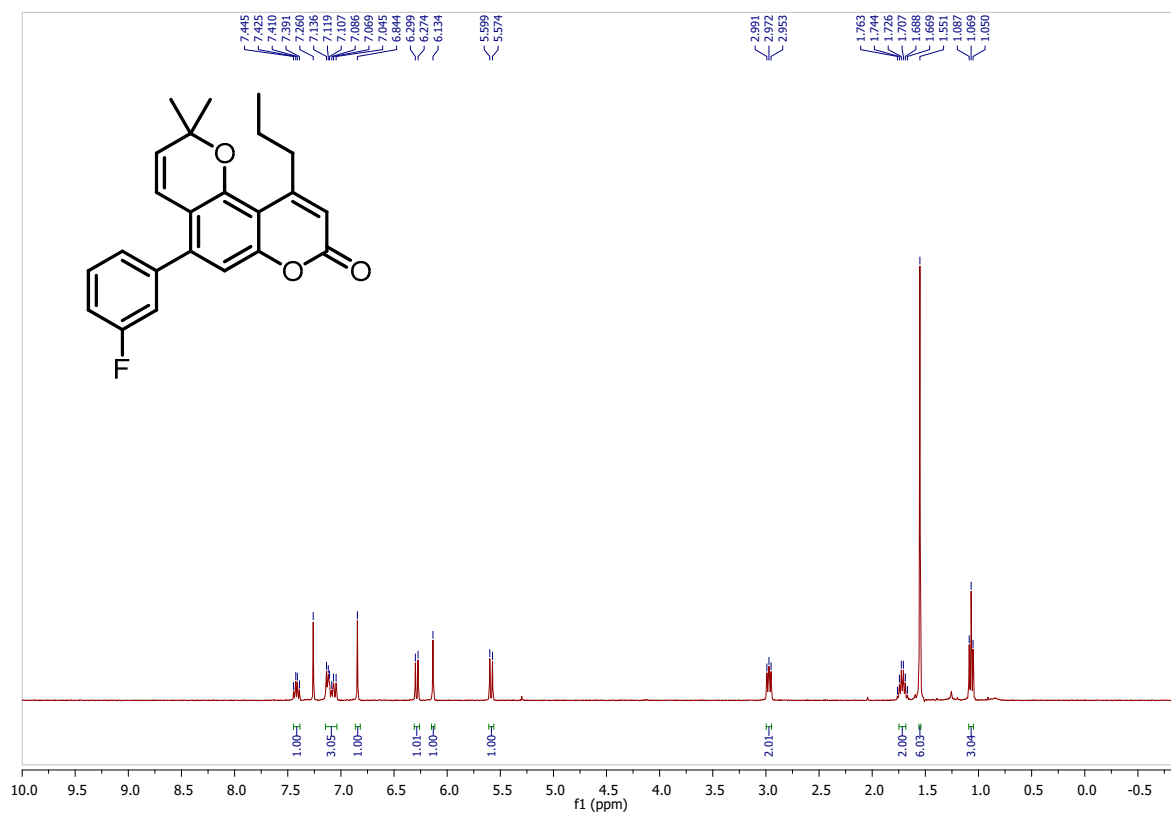
Supplementary Figure S27. ^{19}F NMR spectrum of 8



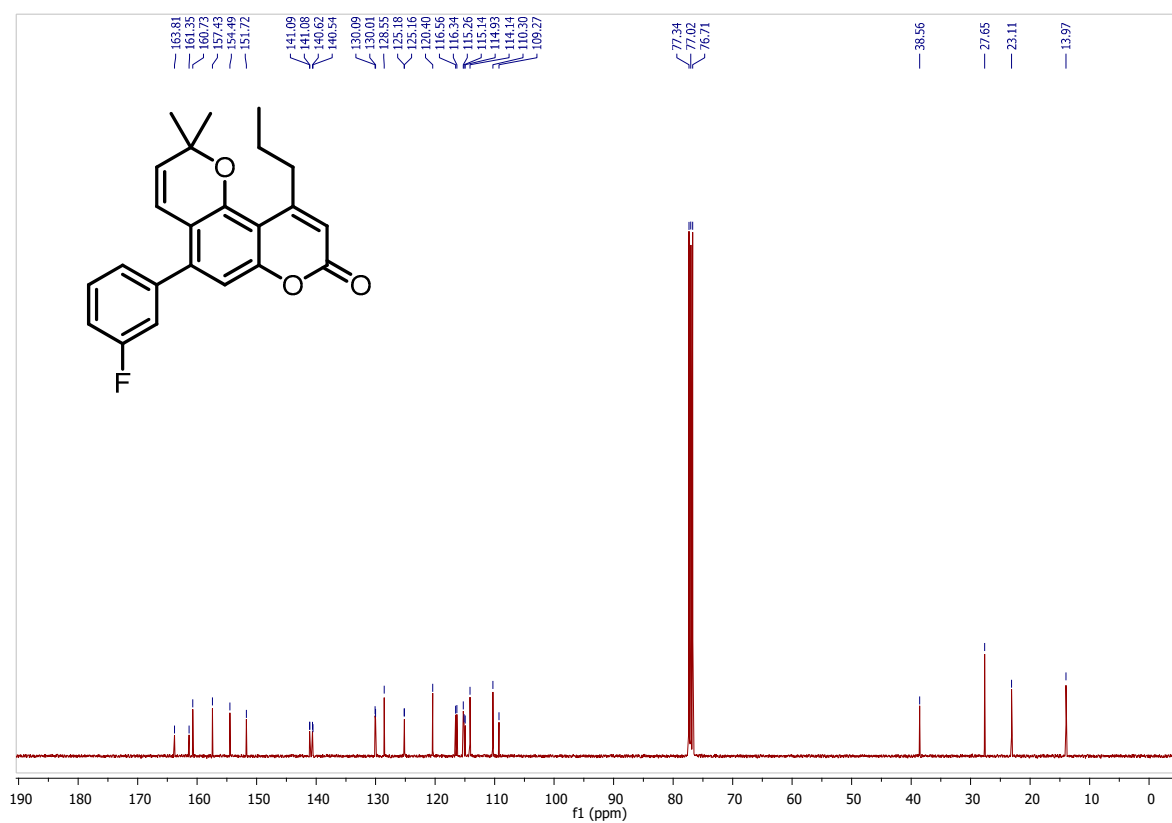
Supplementary Figure S28. ^1H NMR spectrum of 7a



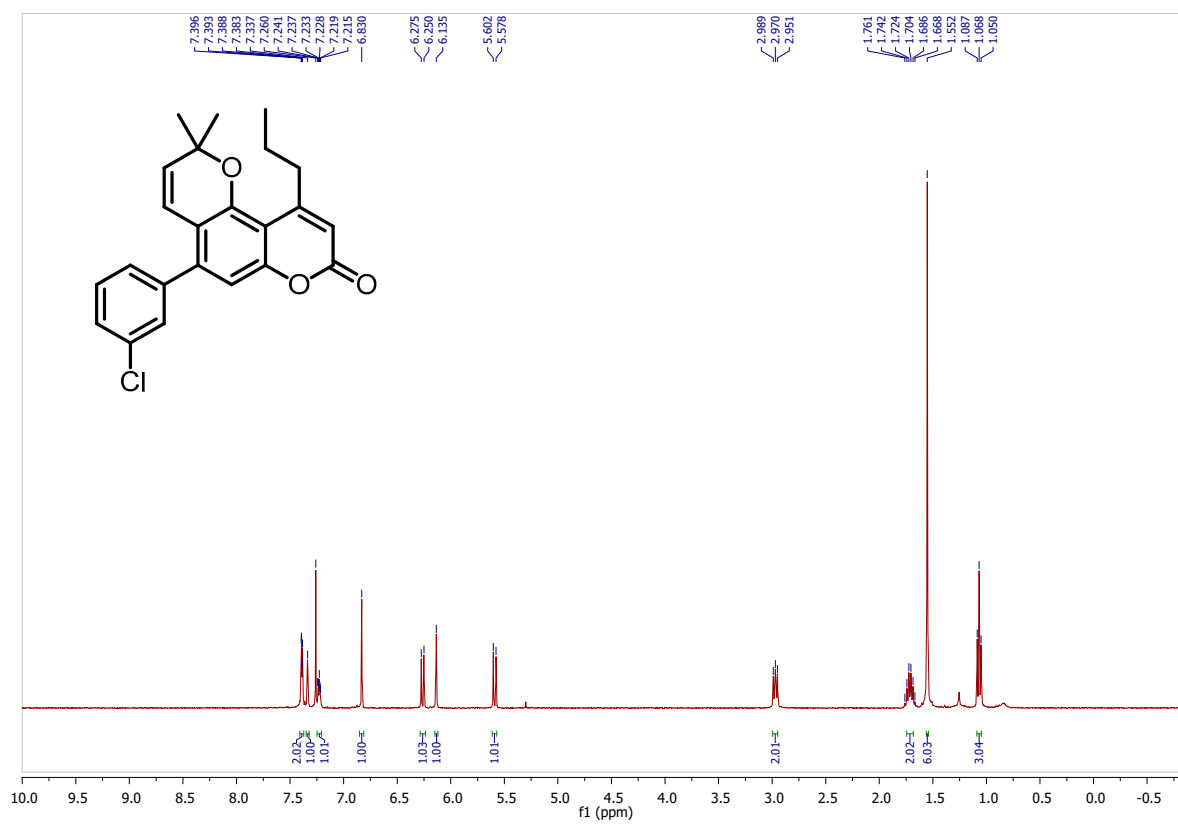
Supplementary Figure S29. ¹³C NMR spectrum of 7a



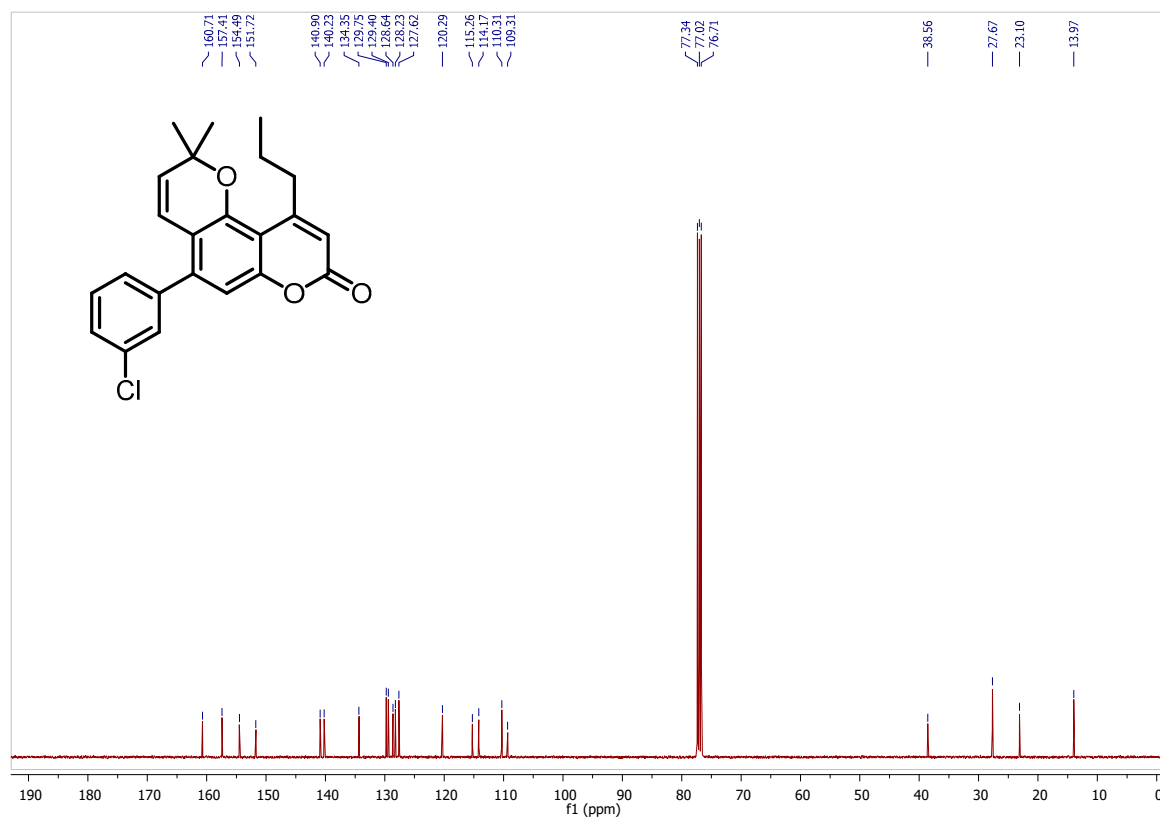
Supplementary Figure S30. ¹H NMR spectrum of 7b



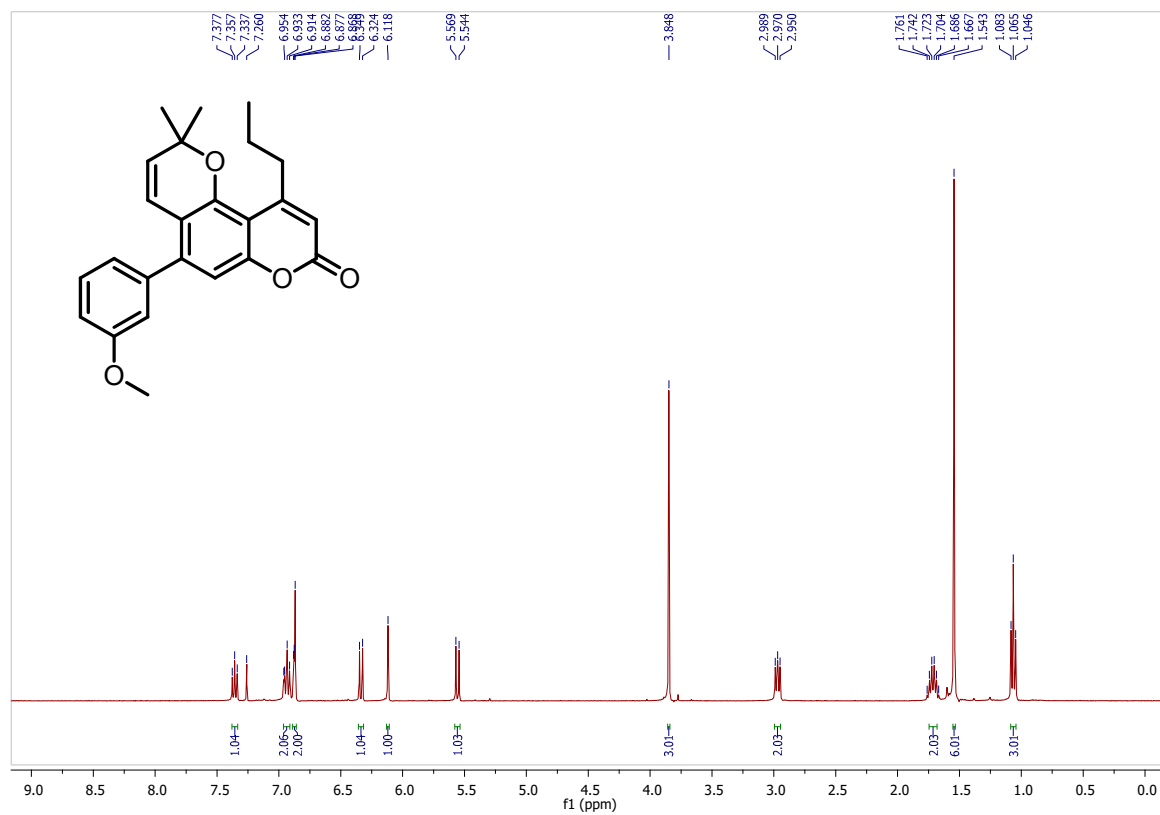
Supplementary Figure S31. ^{13}C NMR spectrum of 7b



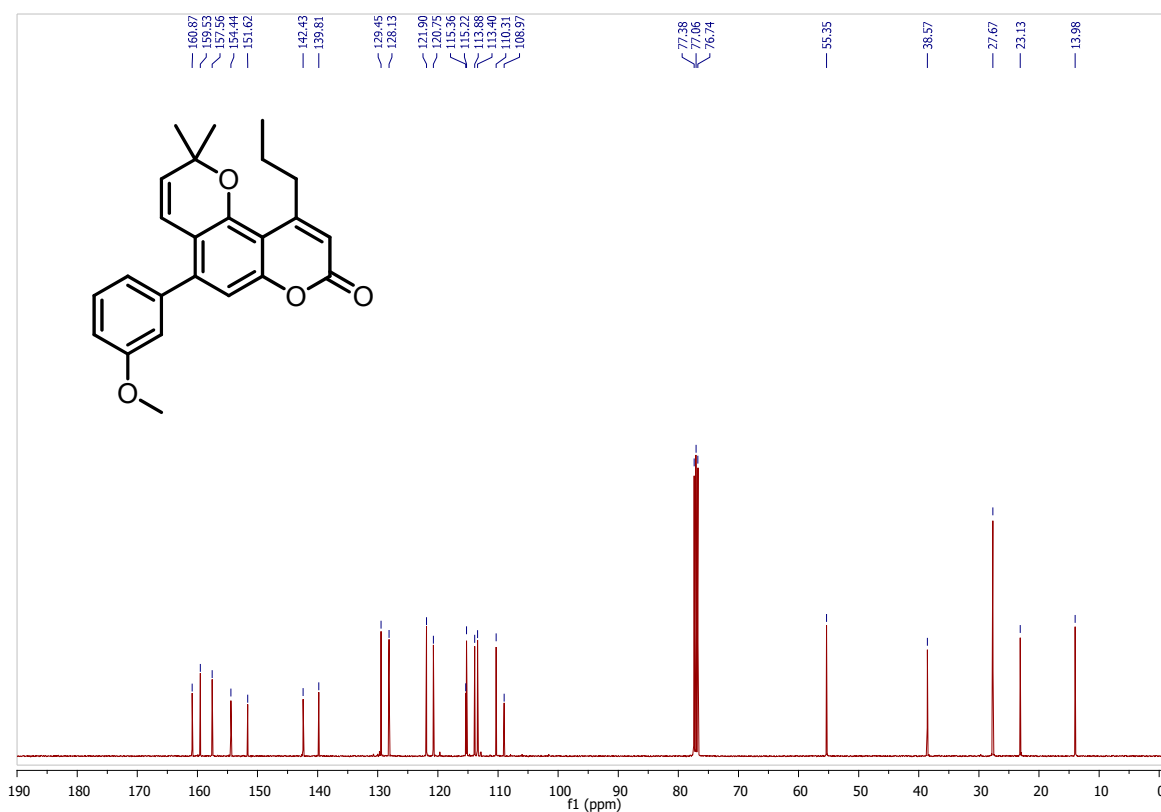
Supplementary Figure S32. ^1H NMR spectrum of 7c



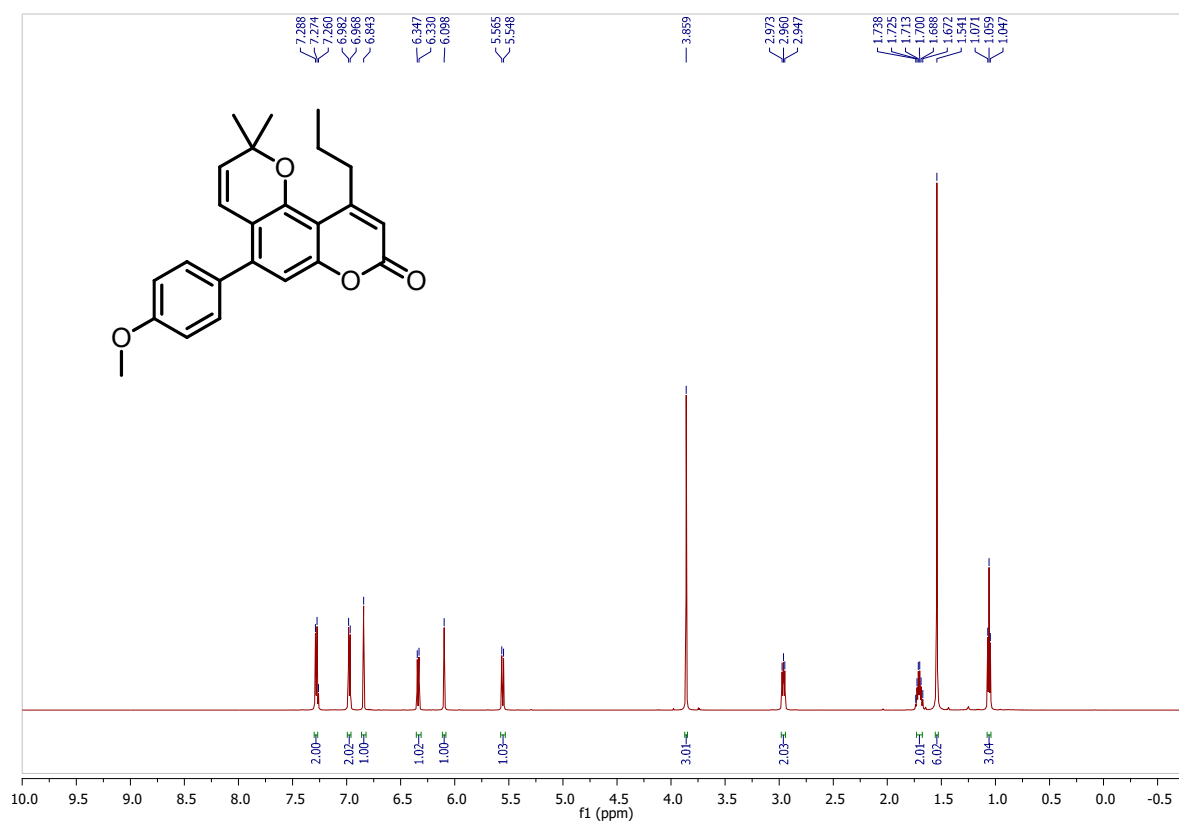
Supplementary Figure S33. ¹³C NMR spectrum of 7c



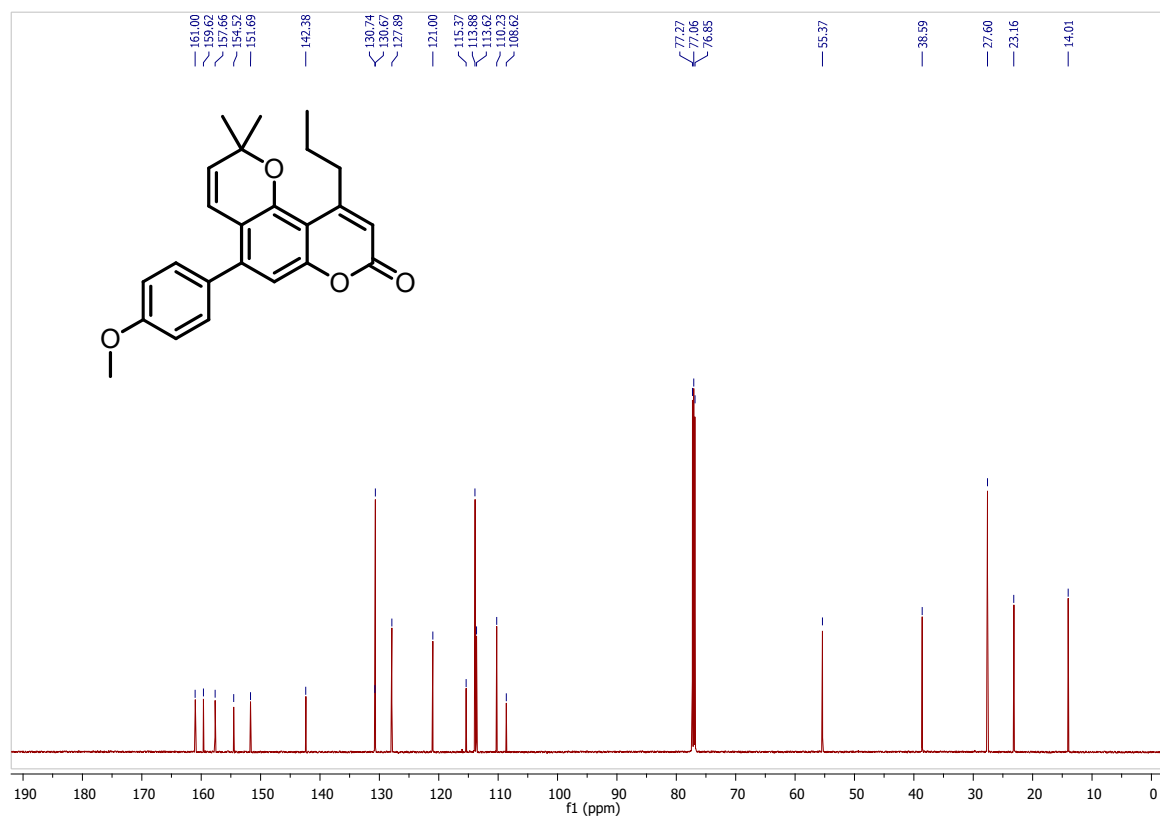
Supplementary Figure S34. ¹H NMR spectrum of 7d



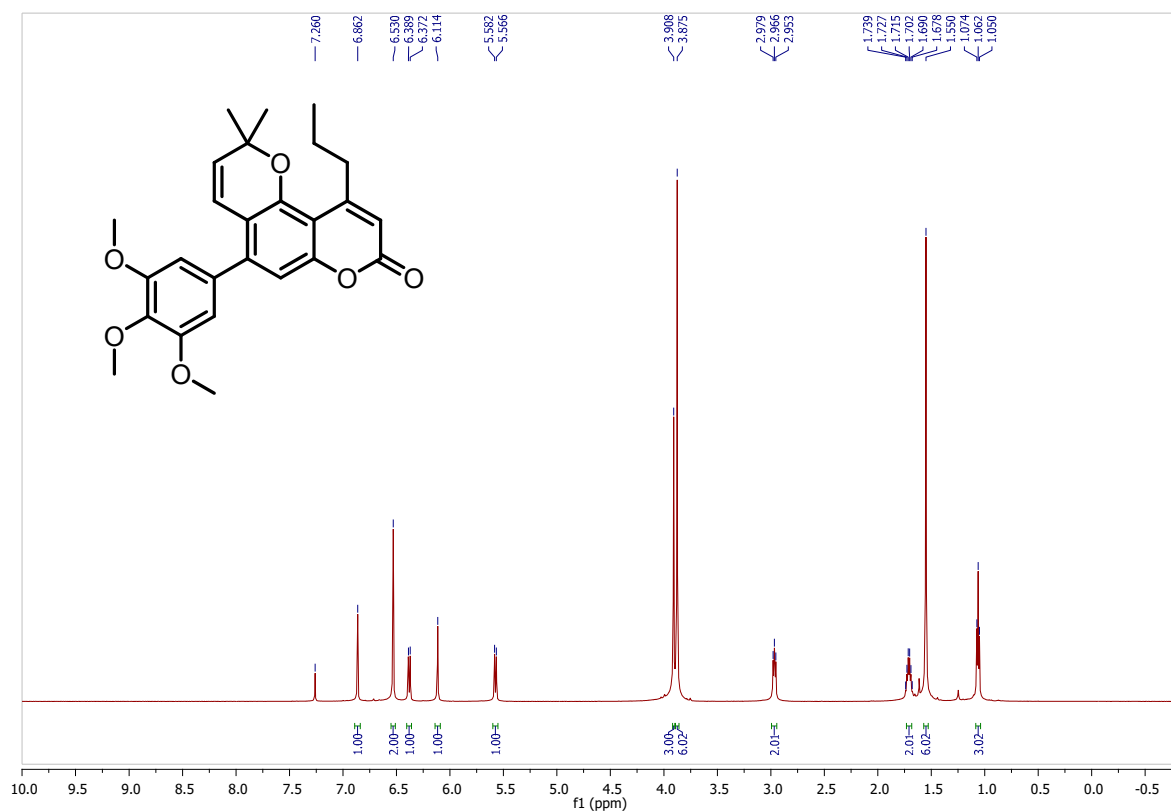
Supplementary Figure S35. ¹³C NMR spectrum of 7d



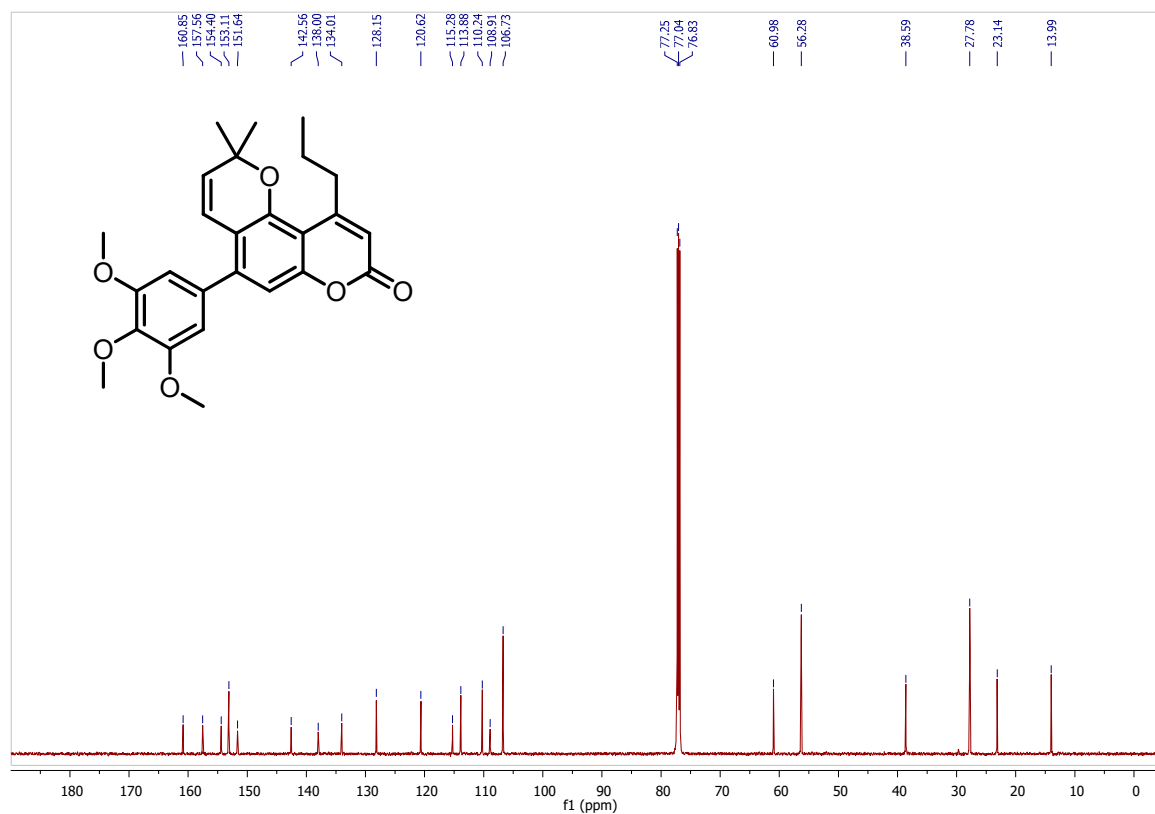
Supplementary Figure S36. ¹H NMR spectrum of 7e



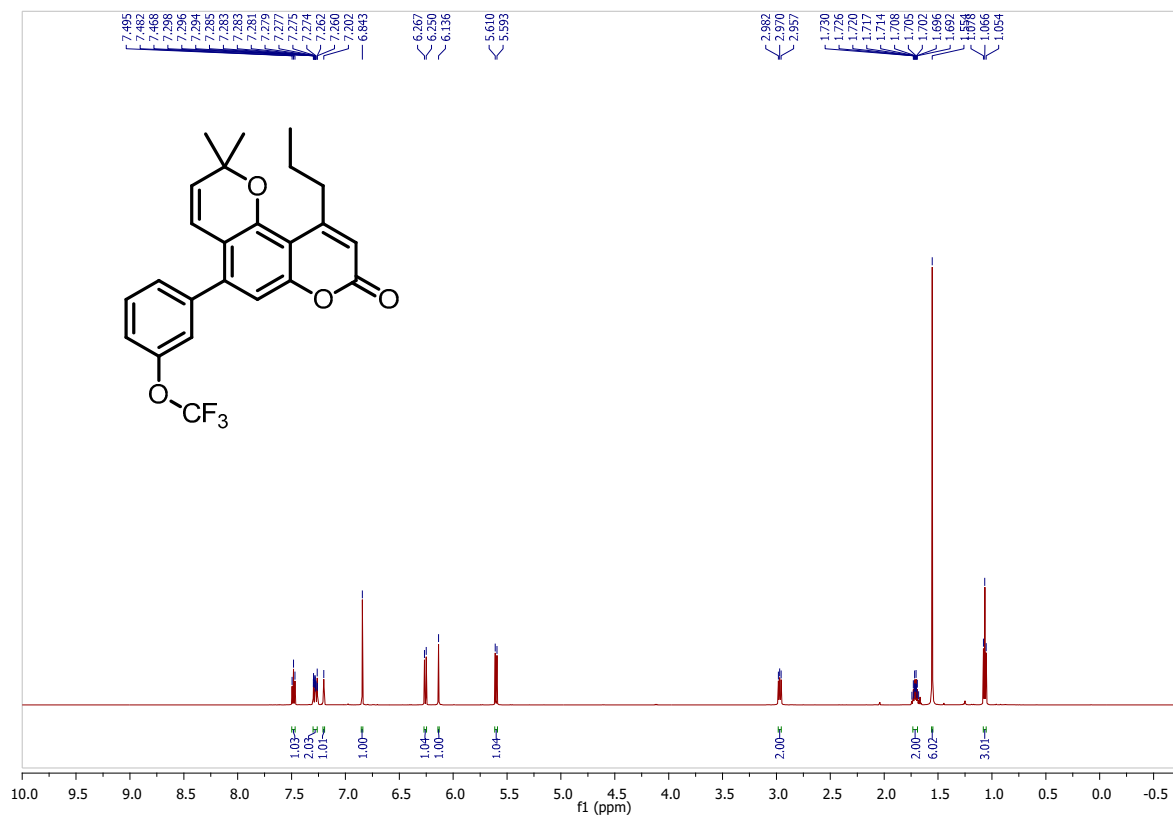
Supplementary Figure S37. ¹³C NMR spectrum of 7e



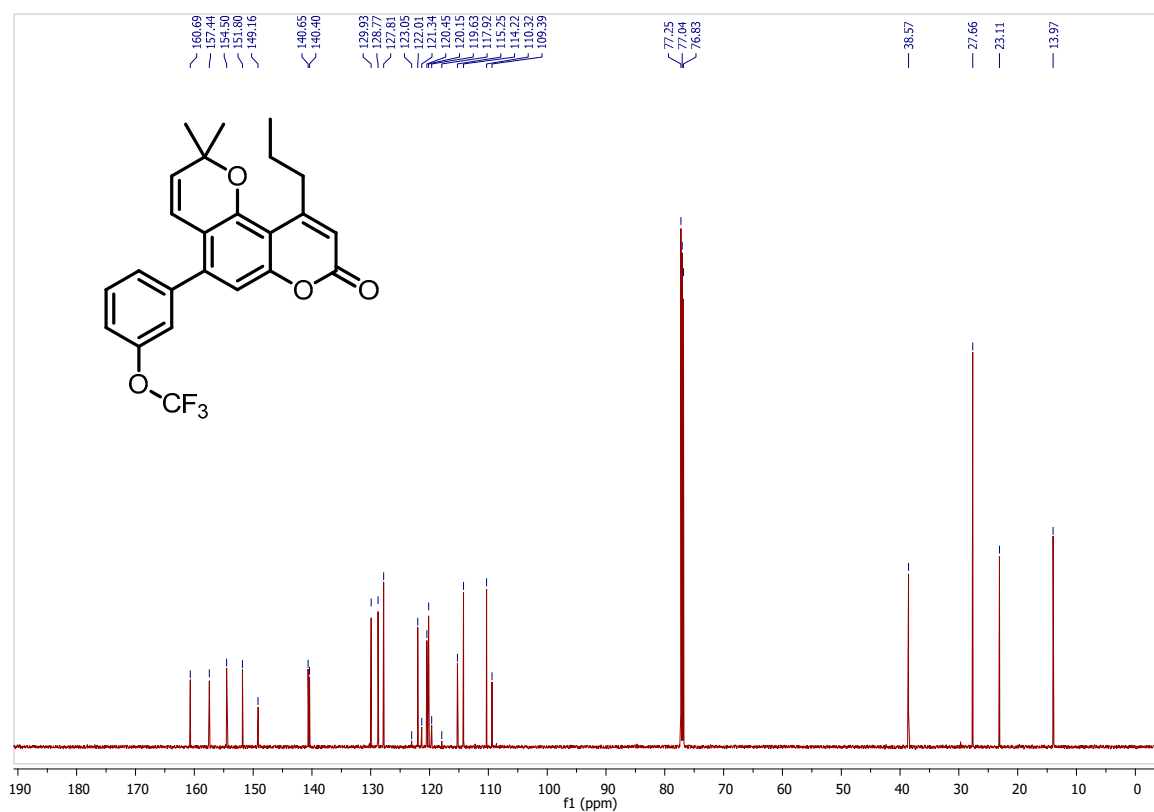
Supplementary Figure S38. ¹H NMR spectrum of 7f



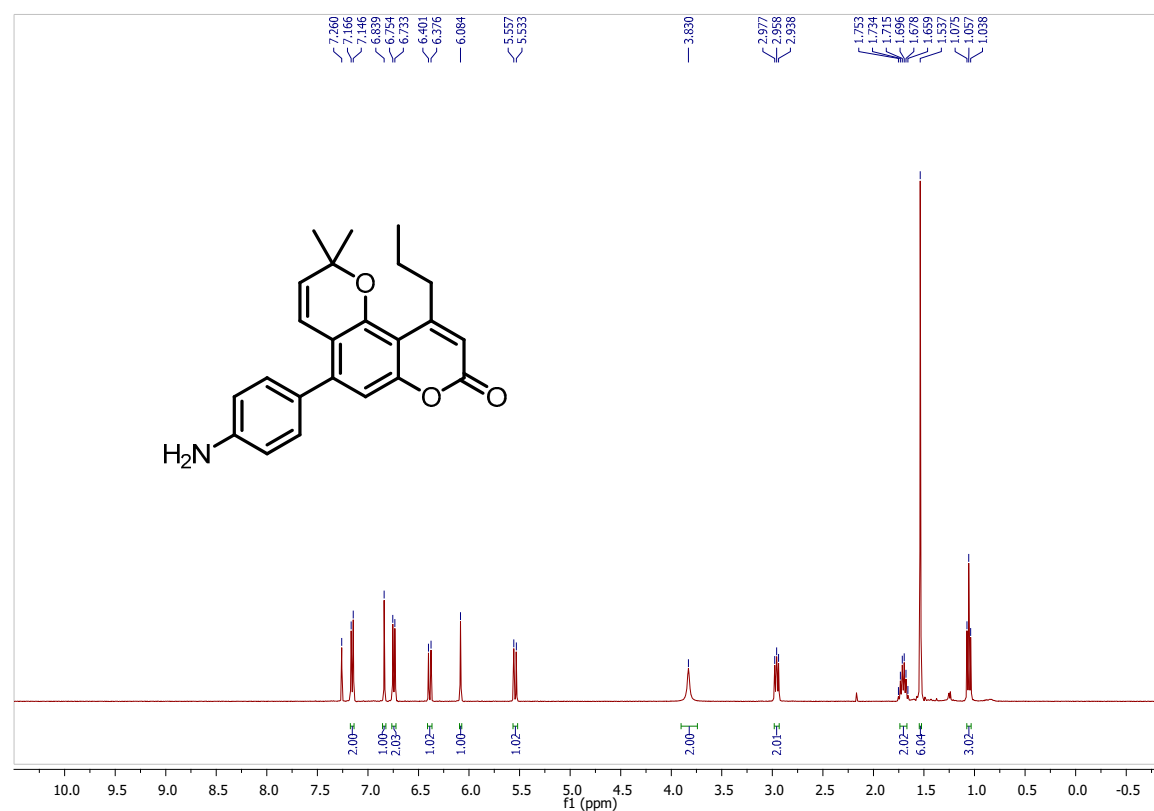
Supplementary Figure S39. ¹³C NMR spectrum of 7f



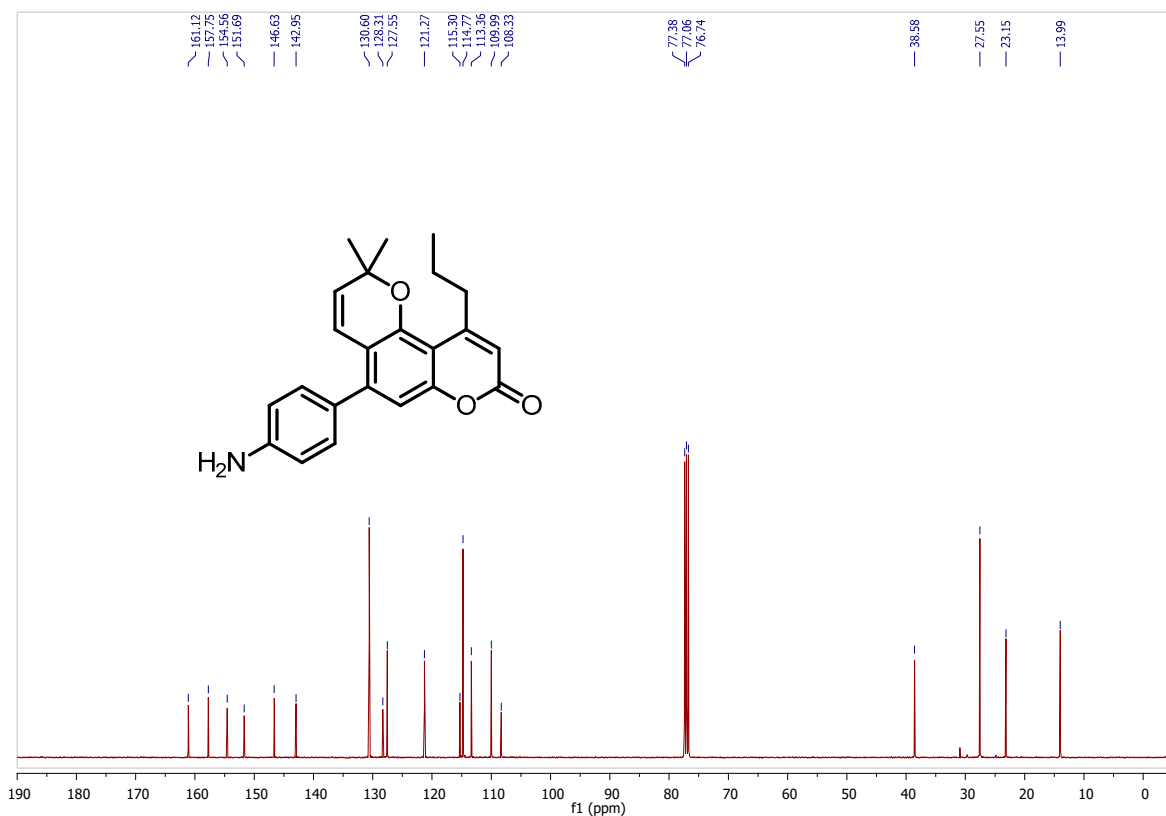
Supplementary Figure S40. ¹H NMR spectrum of 7g



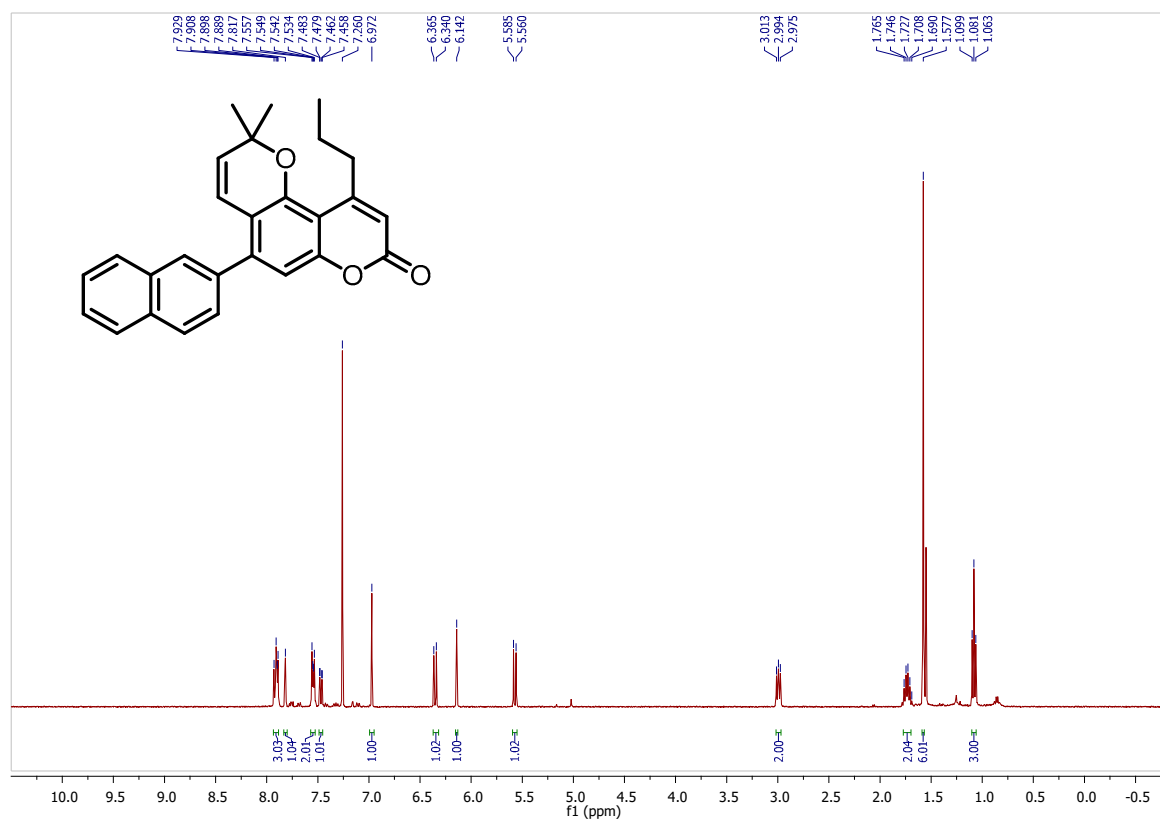
Supplementary Figure S41. ¹³C NMR spectrum of 7g



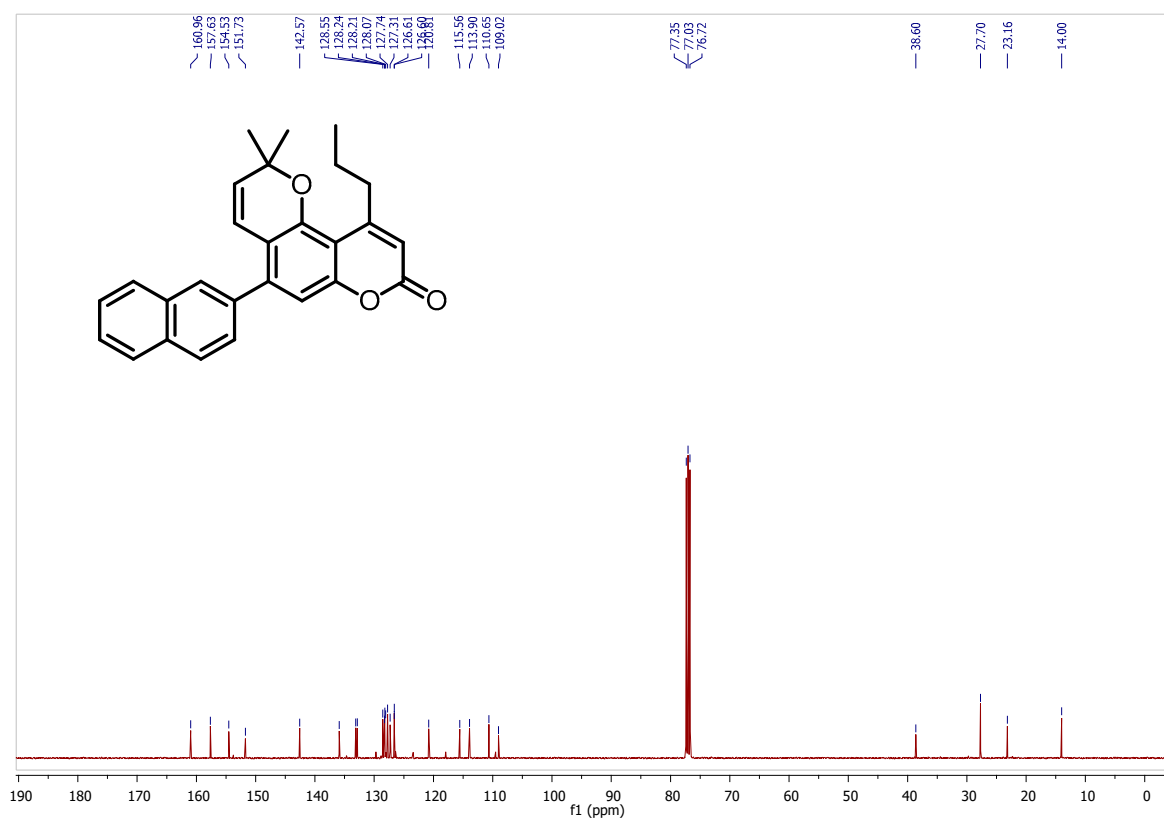
Supplementary Figure S42. ¹H NMR spectrum of 7h



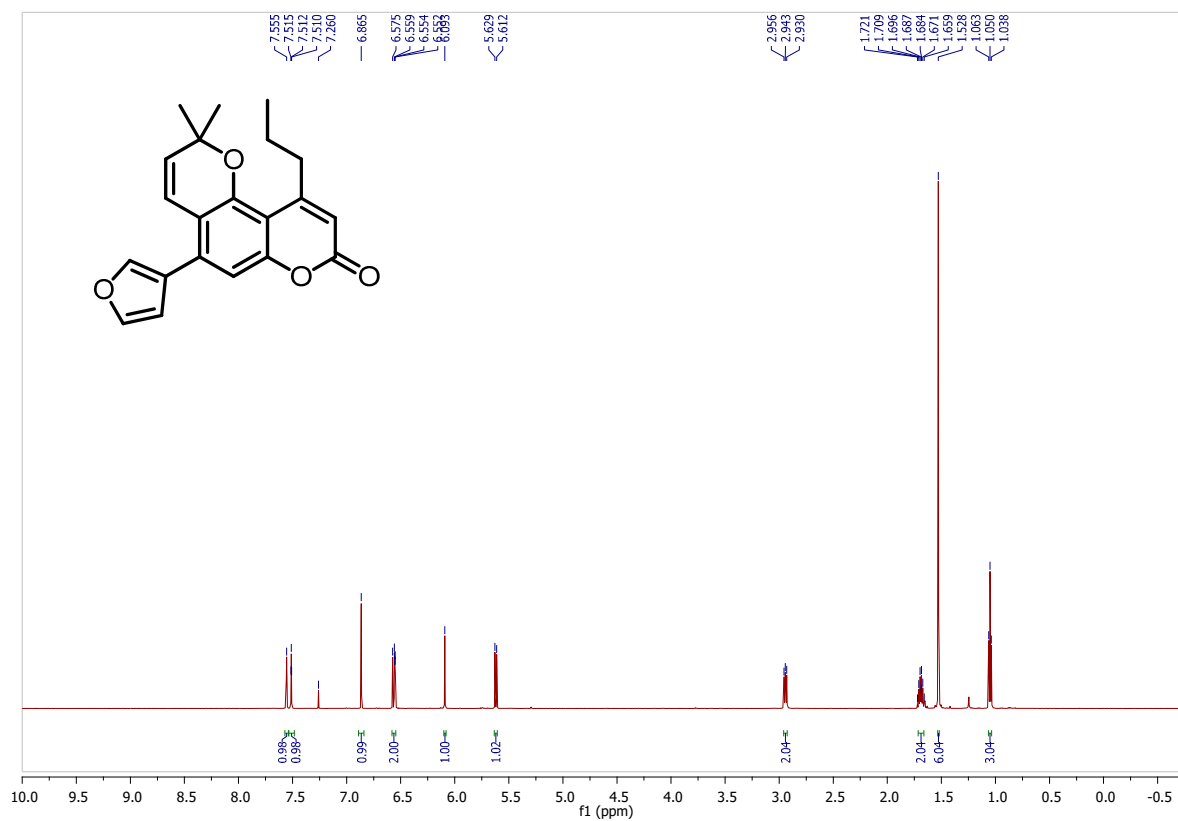
Supplementary Figure S43. ¹³C NMR spectrum of 7h



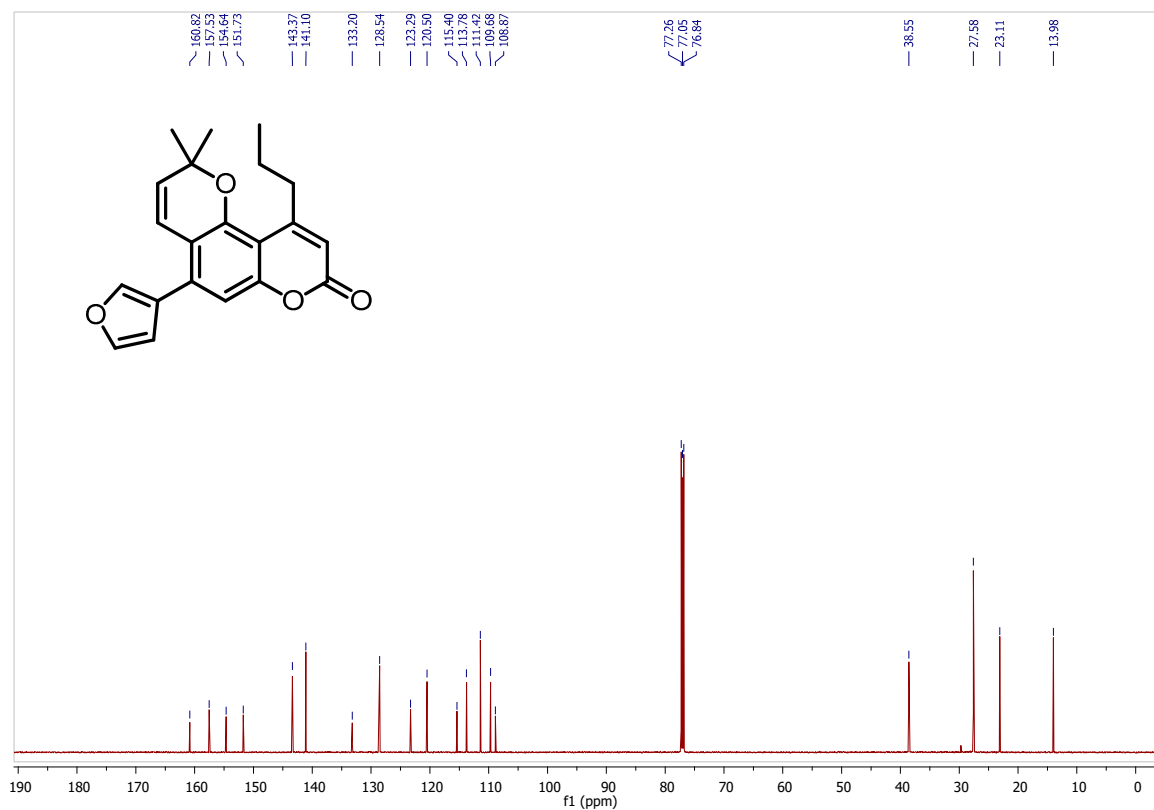
Supplementary Figure S44. ¹H NMR spectrum of 7i



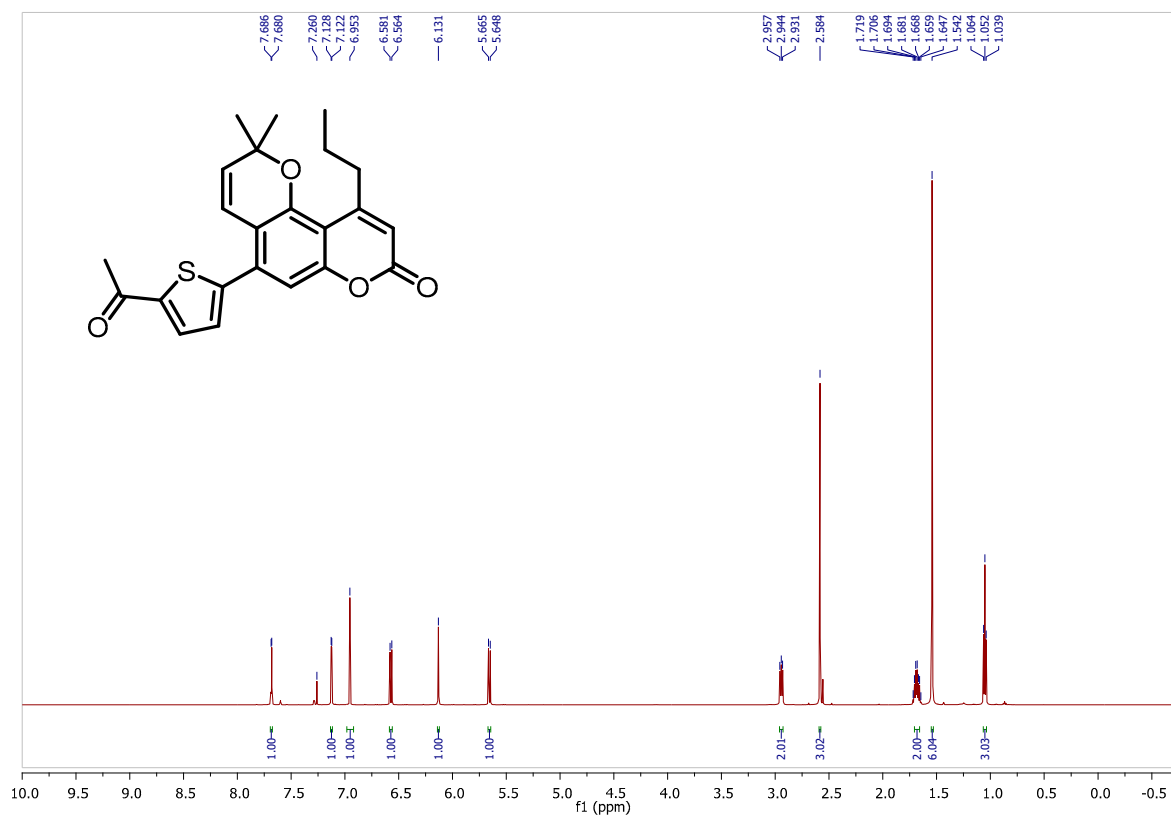
Supplementary Figure S45. ¹³C NMR spectrum of 7i



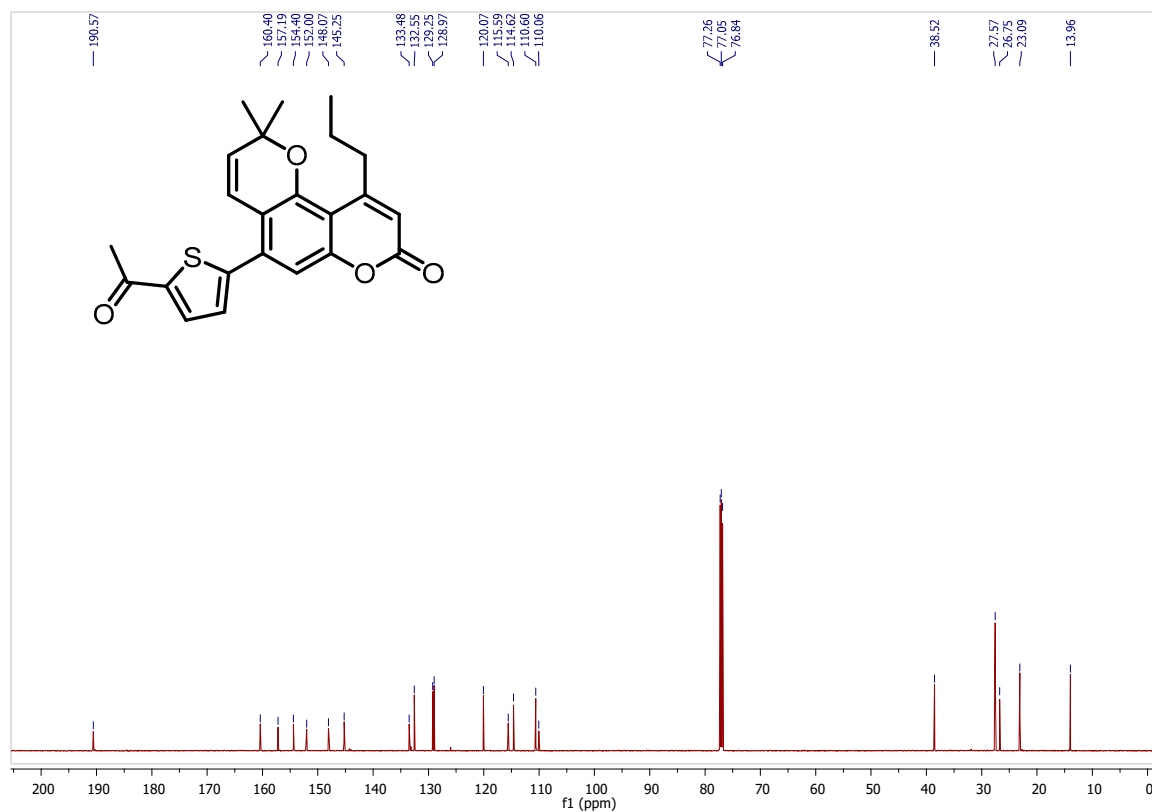
Supplementary Figure S46. ¹H NMR spectrum of 7g



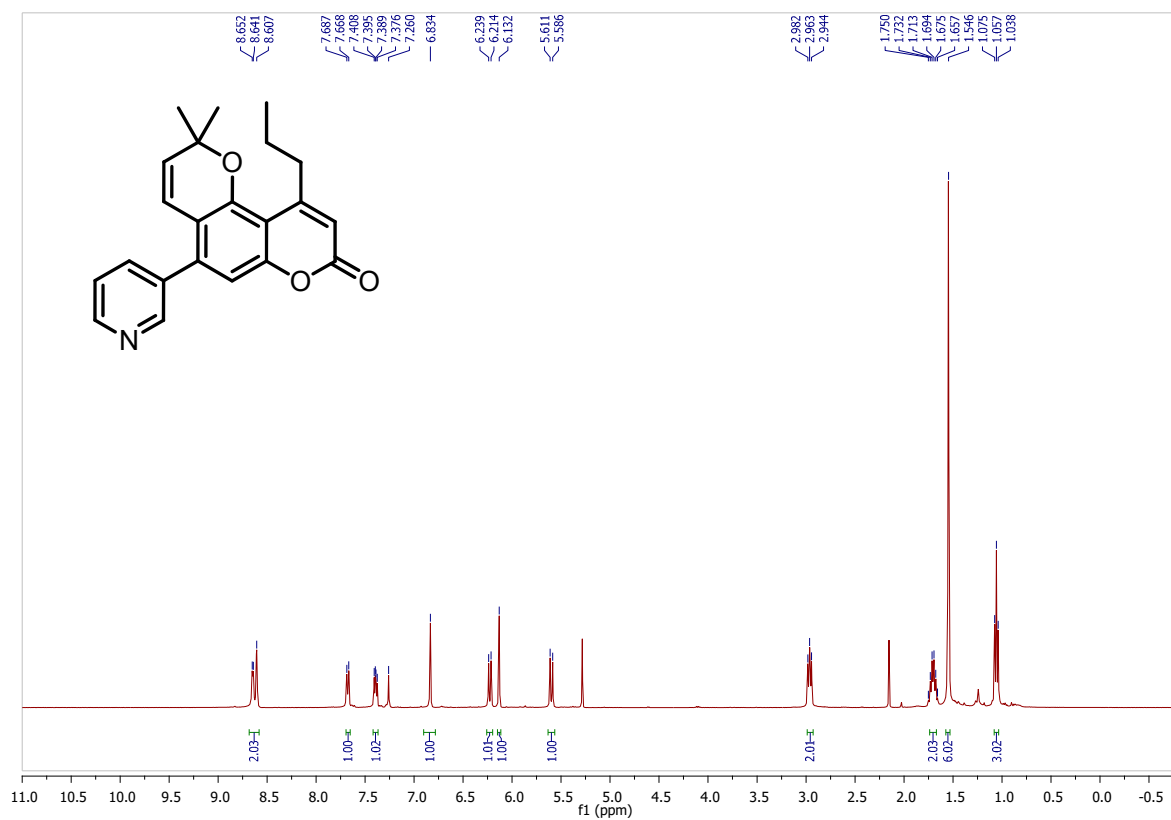
Supplementary Figure S47. ¹³C NMR spectrum of 7g



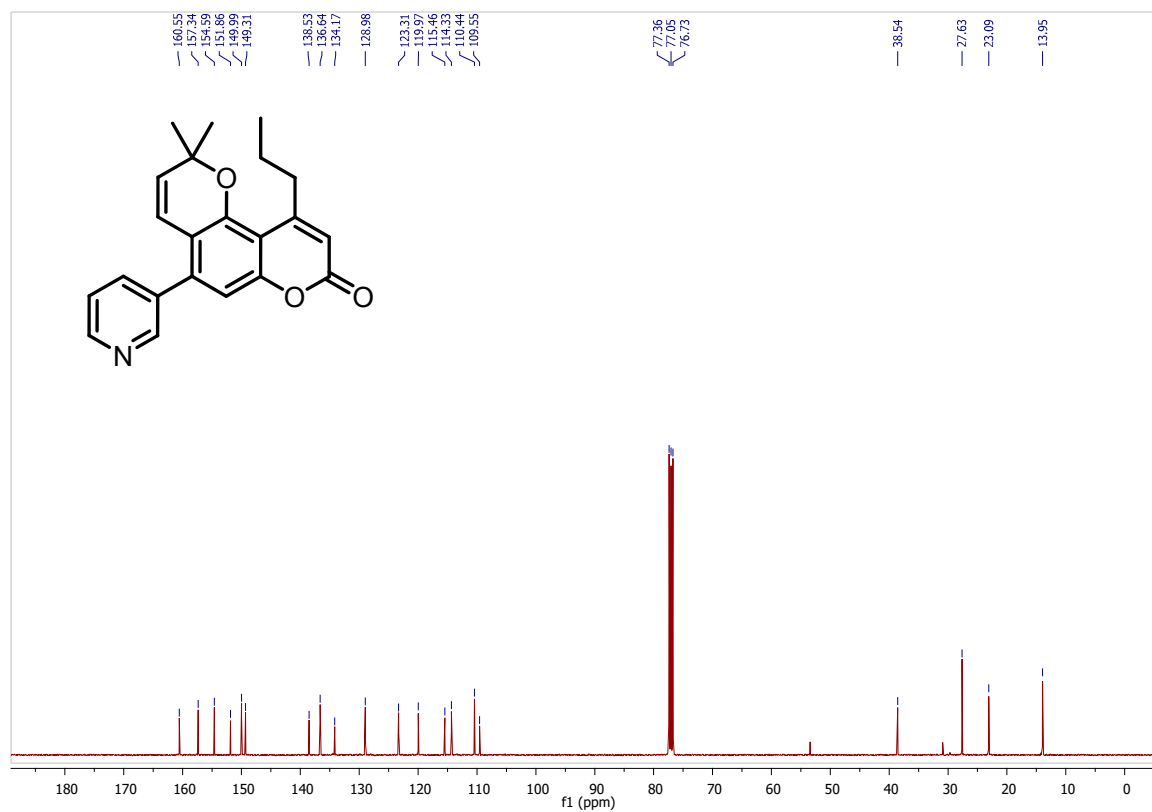
Supplementary Figure S48. ¹H NMR spectrum of 7k



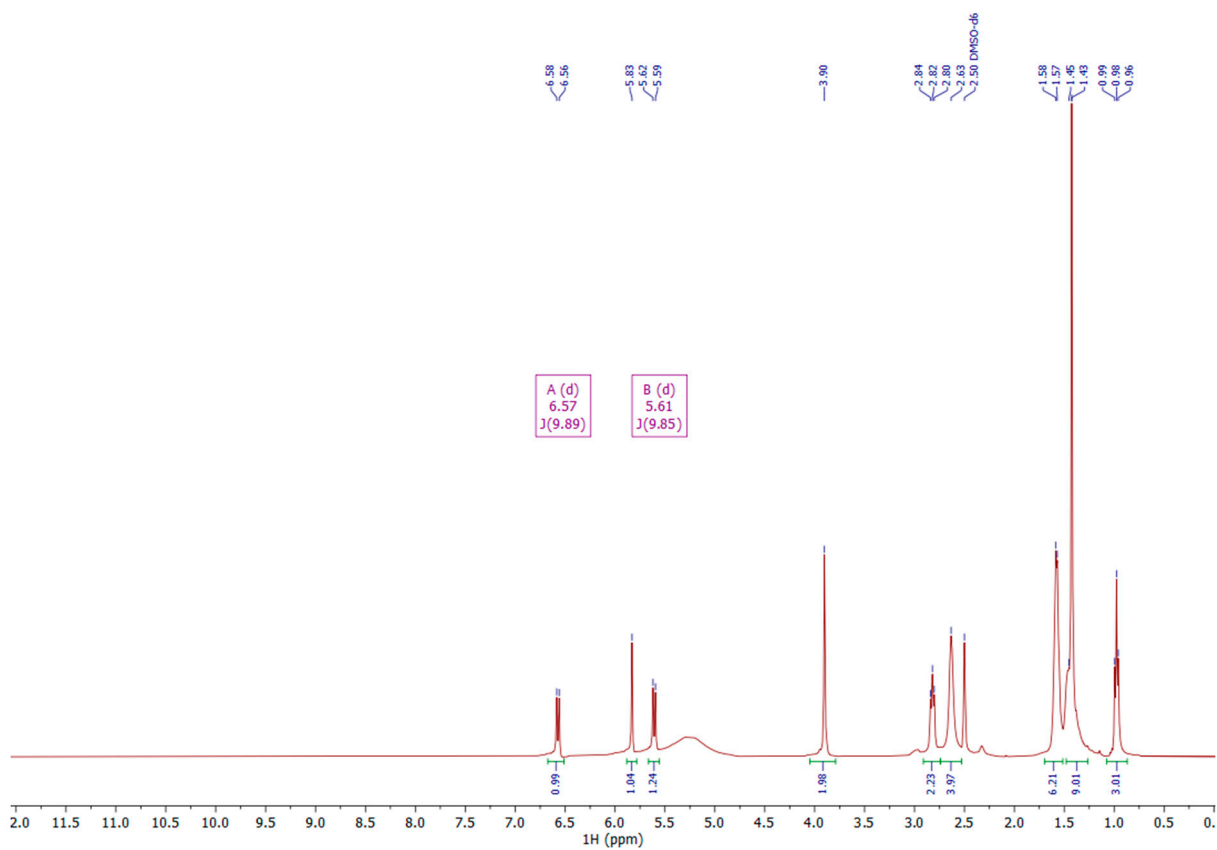
Supplementary Figure S49. ¹³C NMR spectrum of 7k



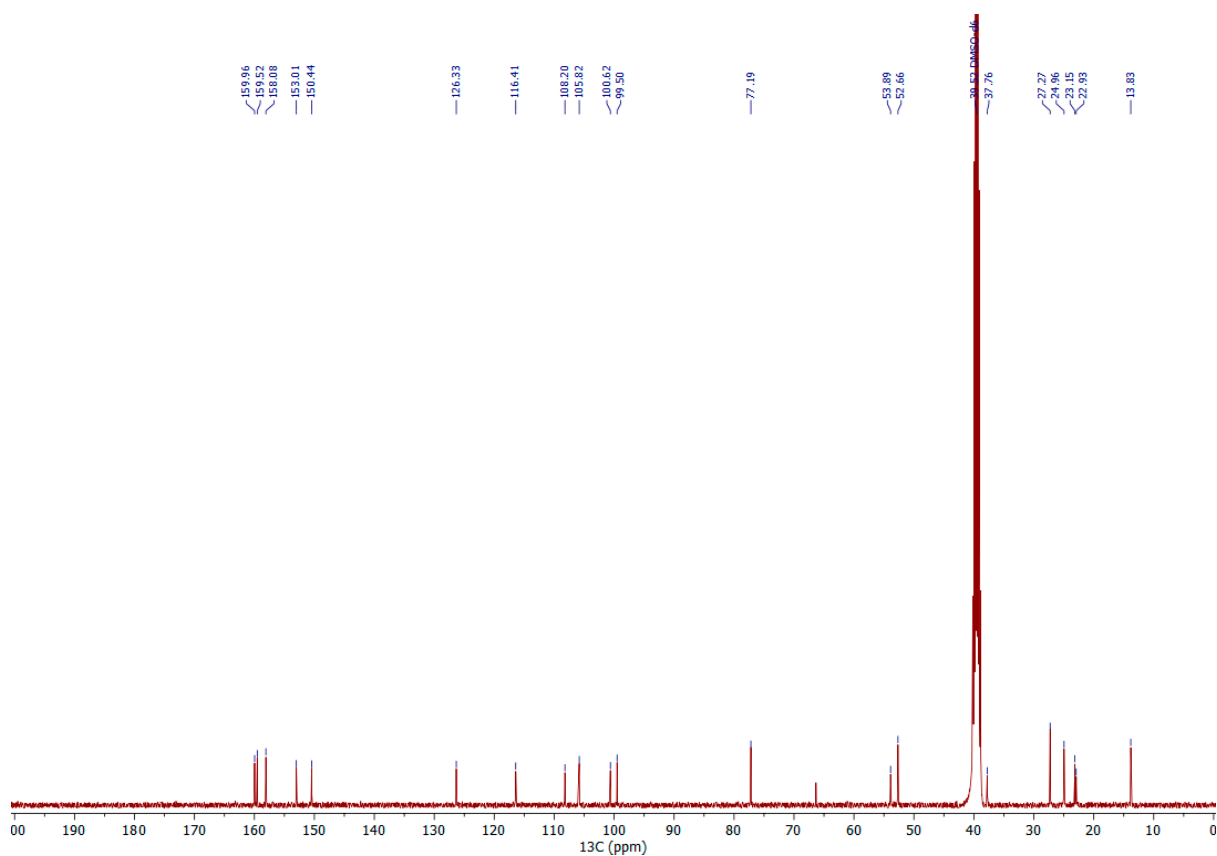
Supplementary Figure S50. ¹H NMR spectrum of 7l



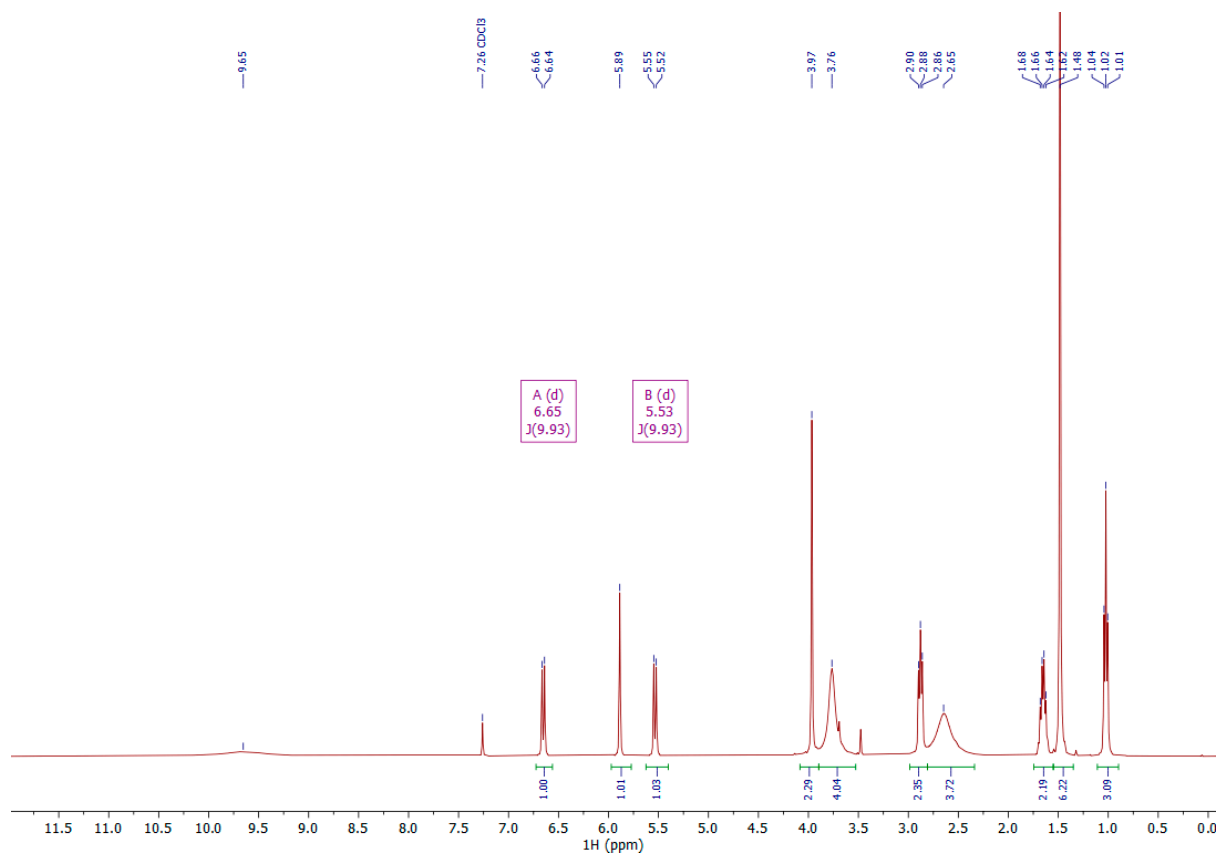
Supplementary Figure S51. ¹³C NMR spectrum of 7l



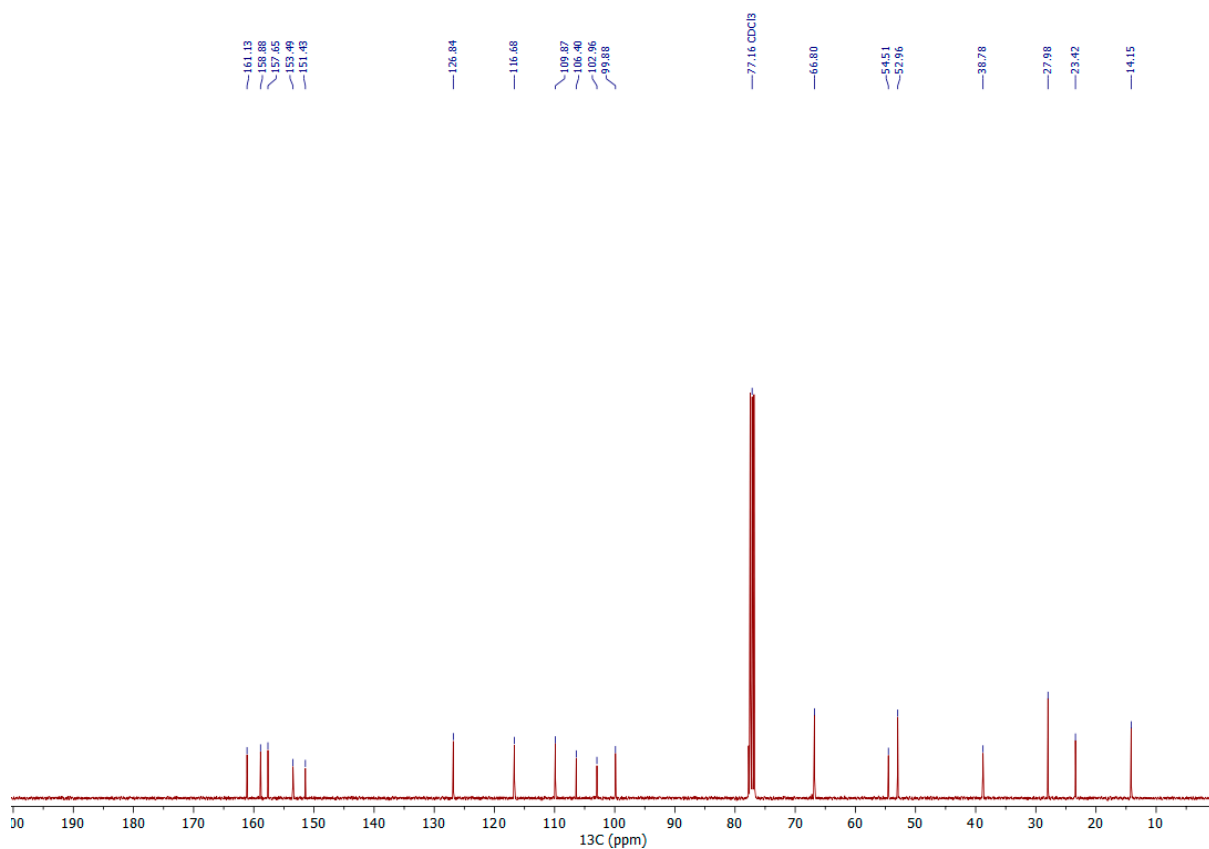
Supplementary Figure S52. ¹H NMR spectrum of 9a



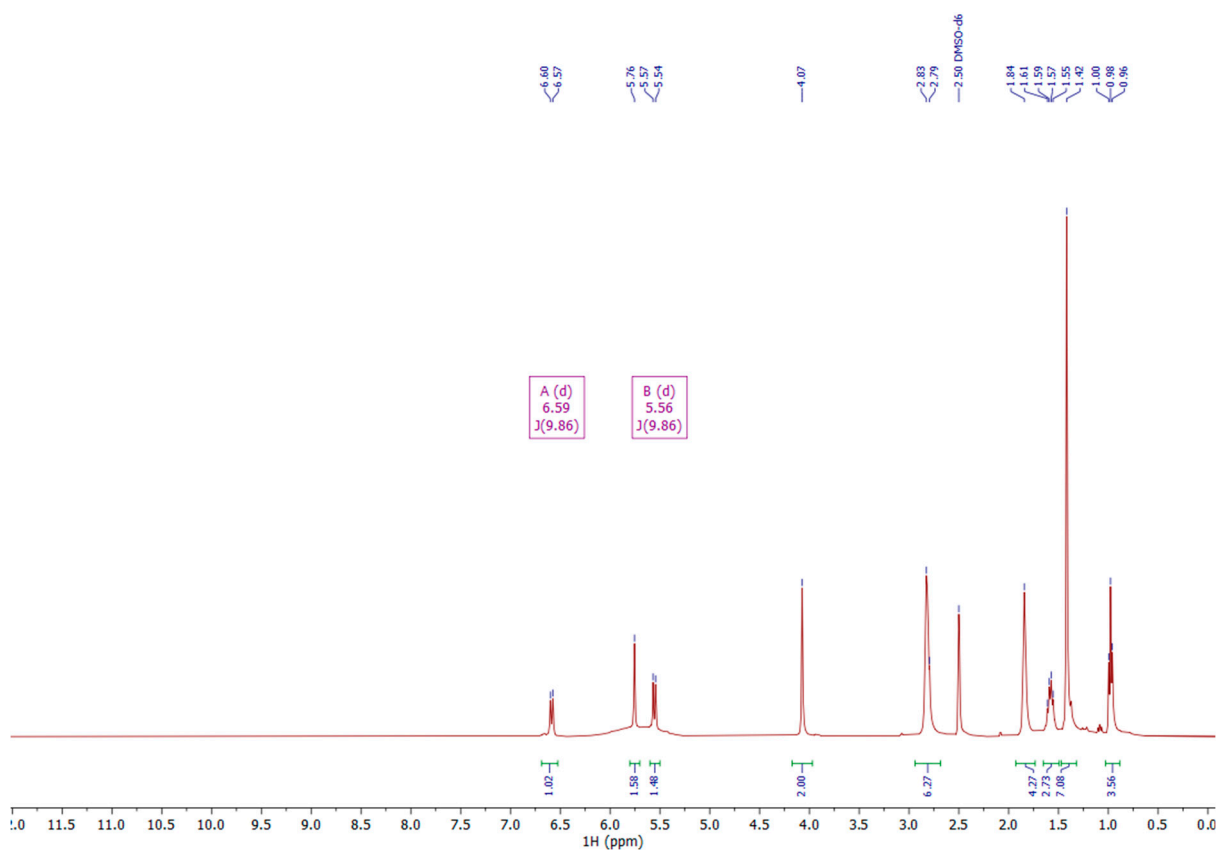
Supplementary Figure S53. ^{13}C NMR spectrum of 9a



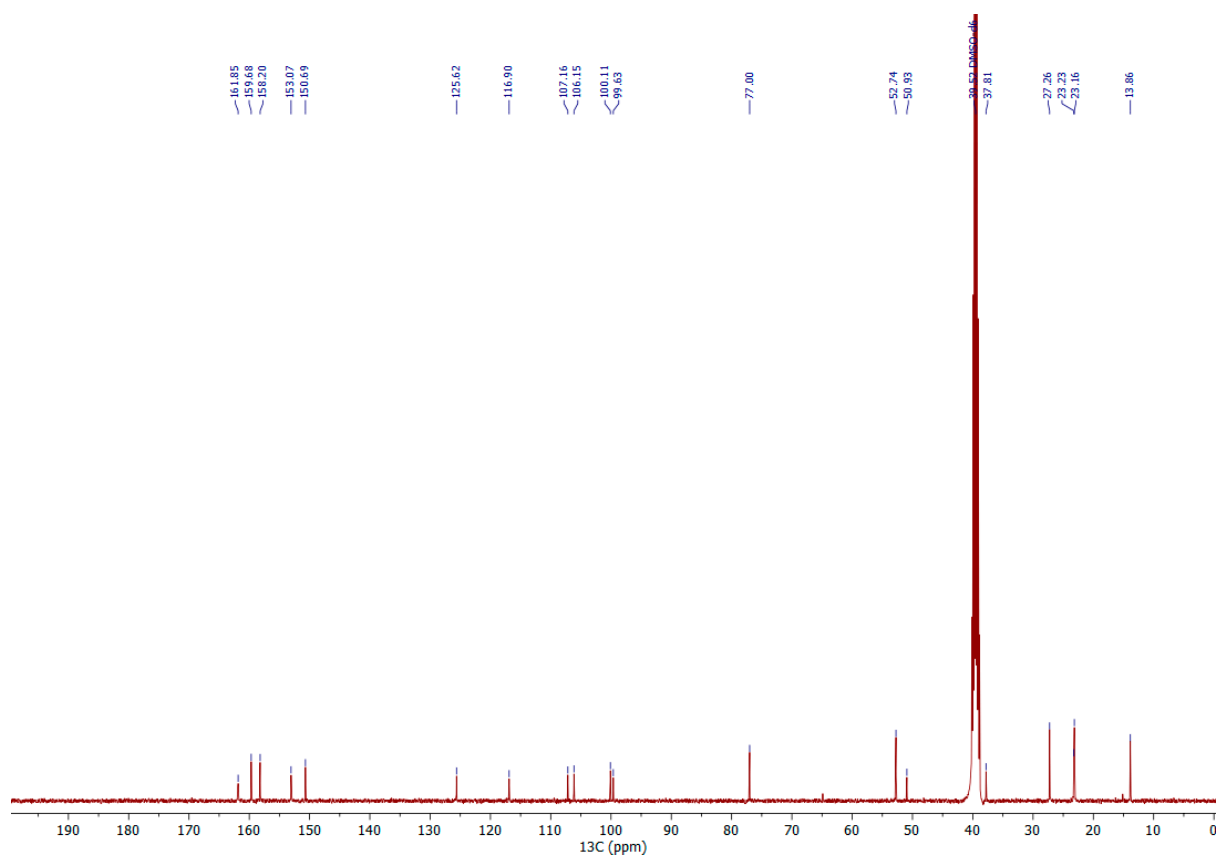
Supplementary Figure S54. ^1H NMR spectrum of 9b



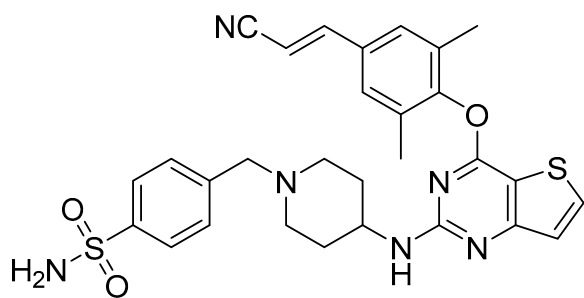
Supplementary Figure S55. ¹³C NMR spectrum of 9b



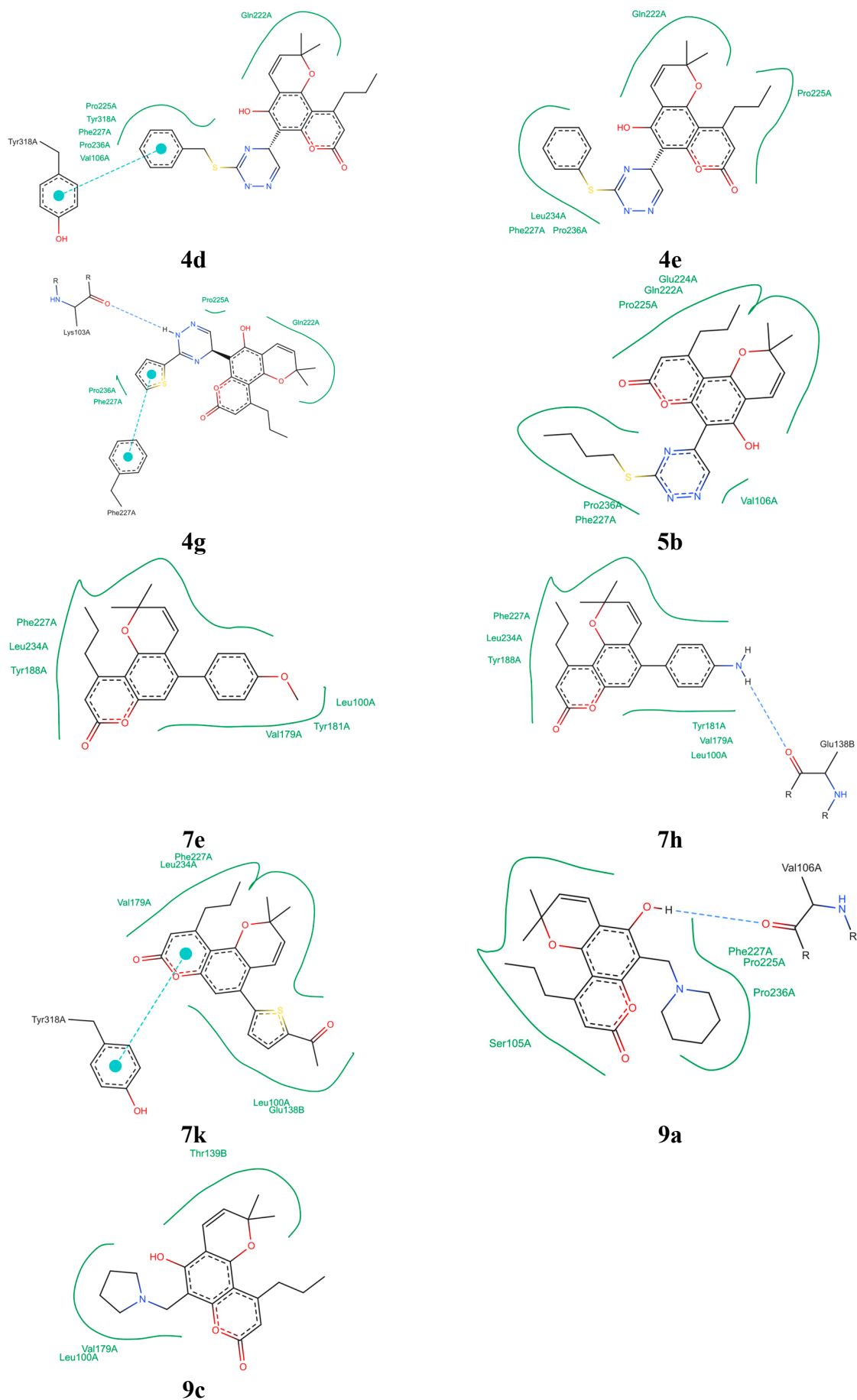
Supplementary Figure S56. ¹H NMR spectrum of 9c



Supplementary Figure S57. ¹³C NMR spectrum of 9c



Supplementary Figure S58. Structure of CHEMBL4094163



Supplementary Figure S59. Two-dimensional maps of non-covalent interactions for the top-1 positions of docked ligands in HIV-RT non-nucleoside binding site

Supplementary Table S1. The results of docking of the known non-nucleoside inhibitors of HIV-1 RT WT

No	Structure	Jamda score	IC ₅₀ , nM	References
1		-2.39	2500	[30]
2		-2.79	6900	
3		-2.37	11200	
4		-2.60	22200	
5		-1.95	32100	
6		-3.36	195	[31]
7		-3.23	1115	[32]
8		-3.13	180	[33]
9		-2.64	6400	[34]
10		-2.51	24	[35]
11		-2.50	3800	[36]
	Pearson coefficient	0.66		
	Spearman coefficient	0.54		