

An Efficient and Step-economical Synthesis of β -Carboline Tethered Imidazopyrido[3,4-*b*]indoles from Acetals

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Supporting Information

Table of Contents

1.	¹H-NMR and ¹³C-NMR spectra of new products	2-31
2.	LCMS data of 15A product	32
3.	Photophysical studies of synthesised compounds	33-38

1.0 ¹H and ¹³C-NMR of the new products

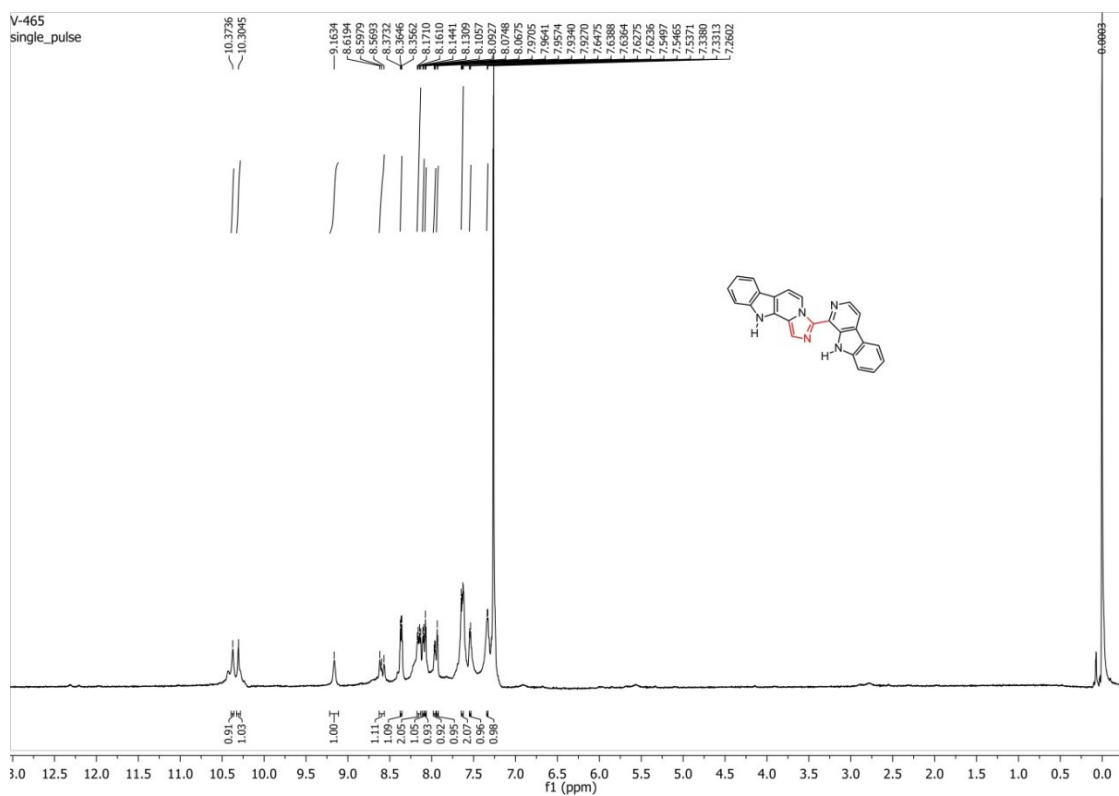


Figure S1. ¹H-NMR spectrum of 14.

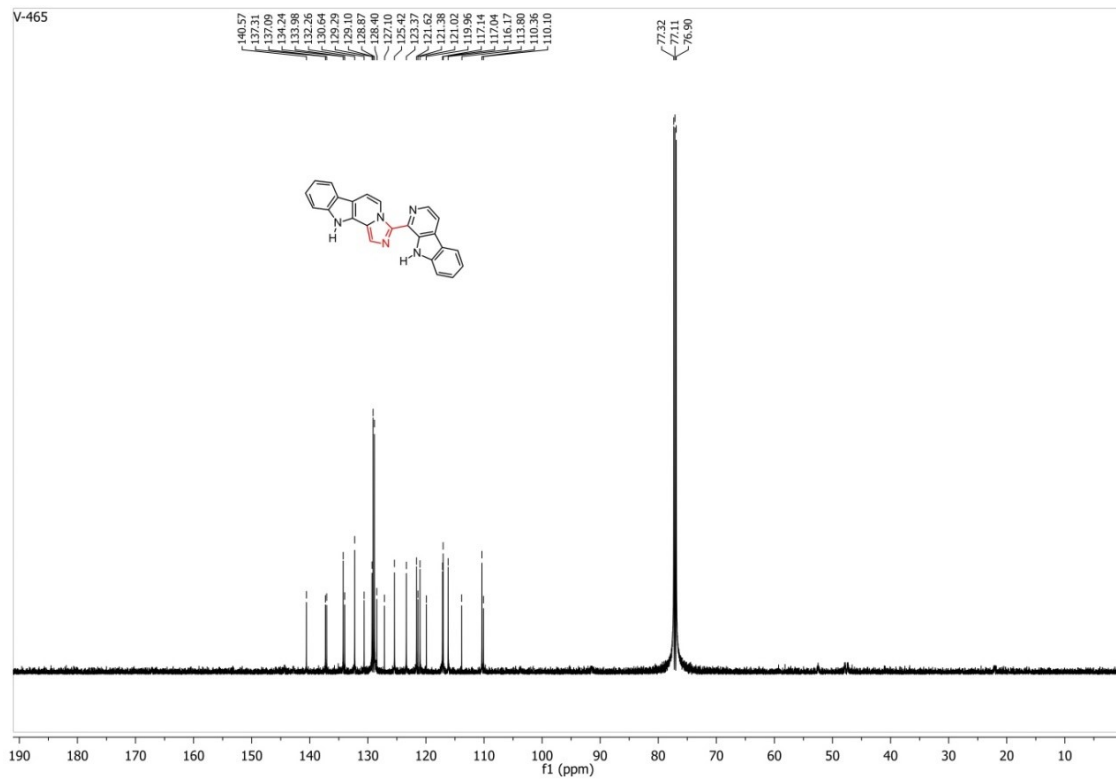


Figure S2. ¹³C-NMR spectrum of 14.

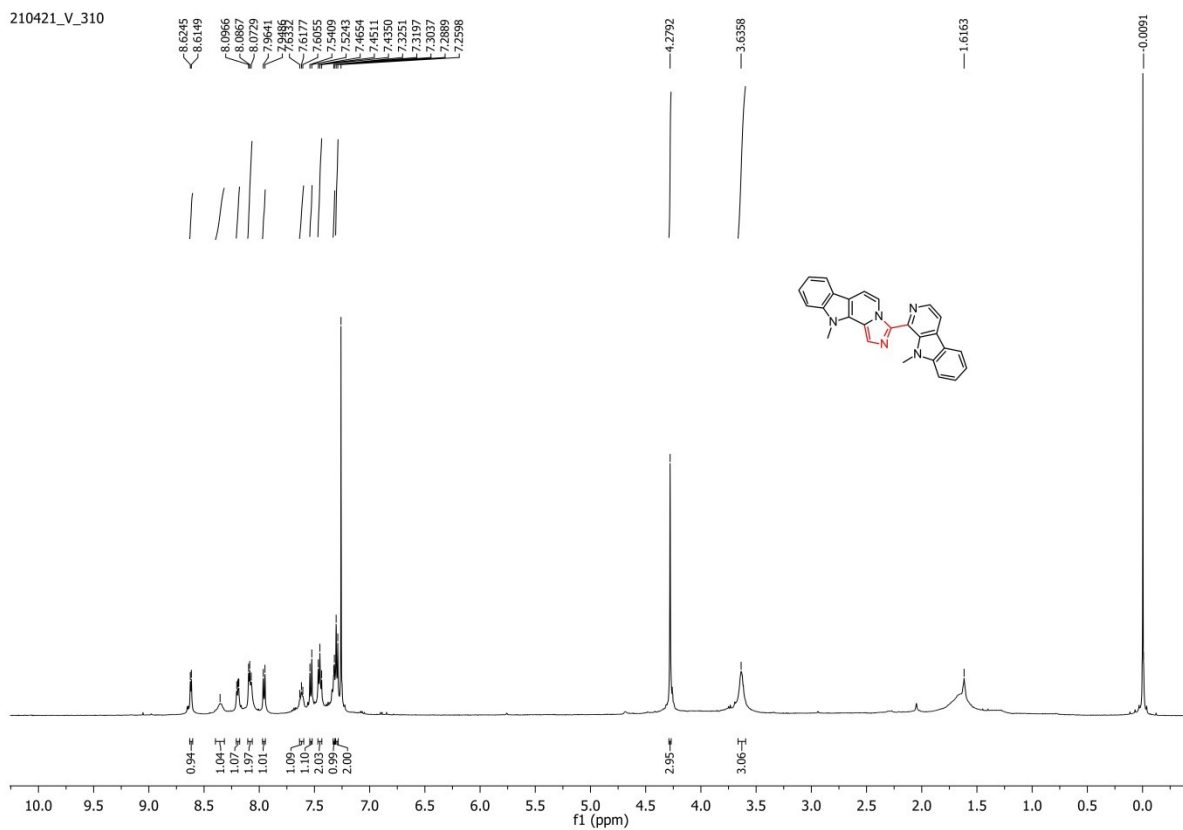


Figure S3. $^1\text{H-NMR}$ spectrum of **15A**.

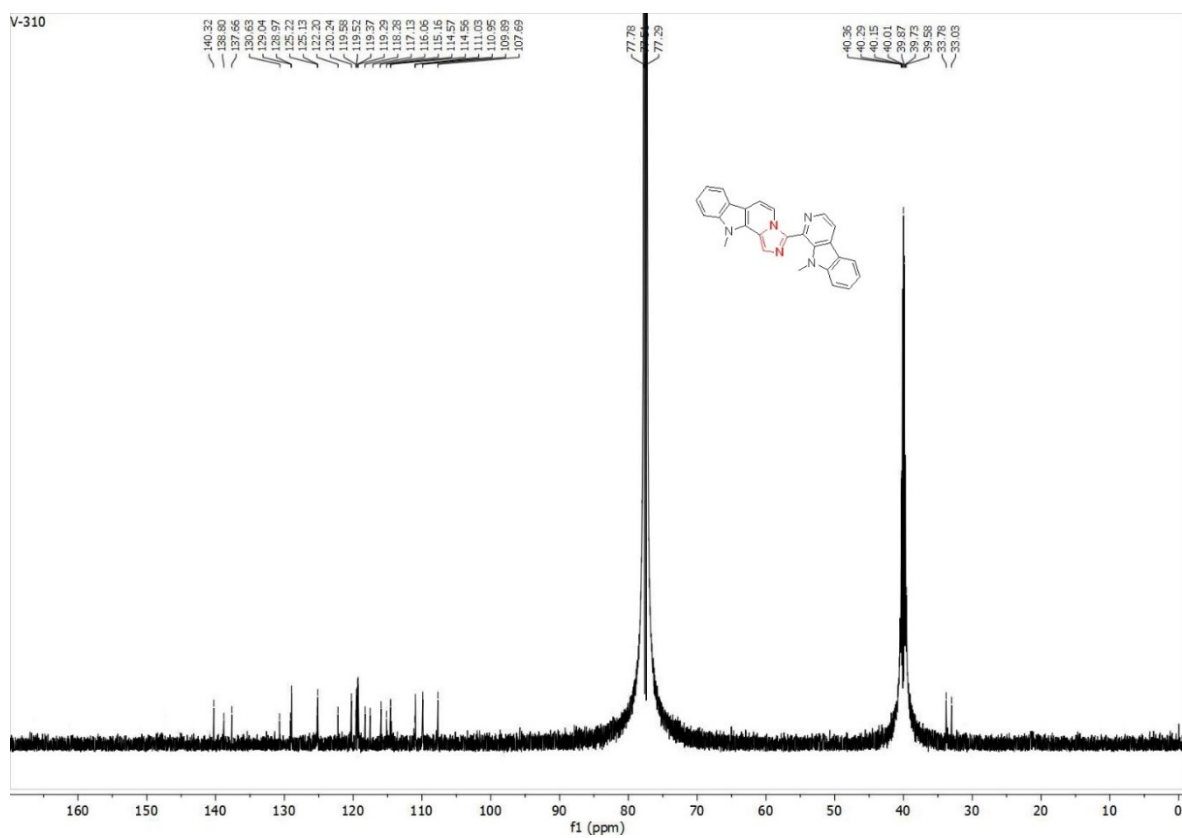


Figure S4. $^{13}\text{C-NMR}$ spectrum of **15A**.

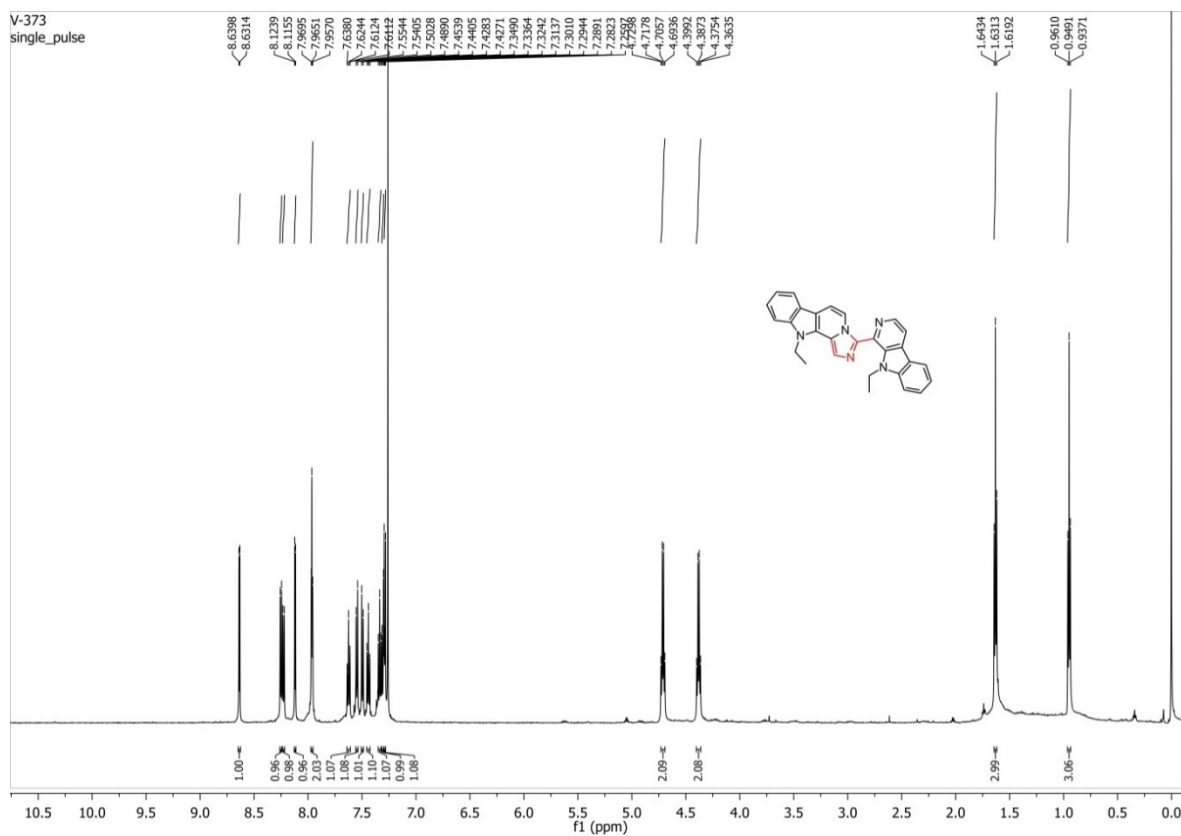


Figure S5. ^1H -NMR spectrum of **15B**.

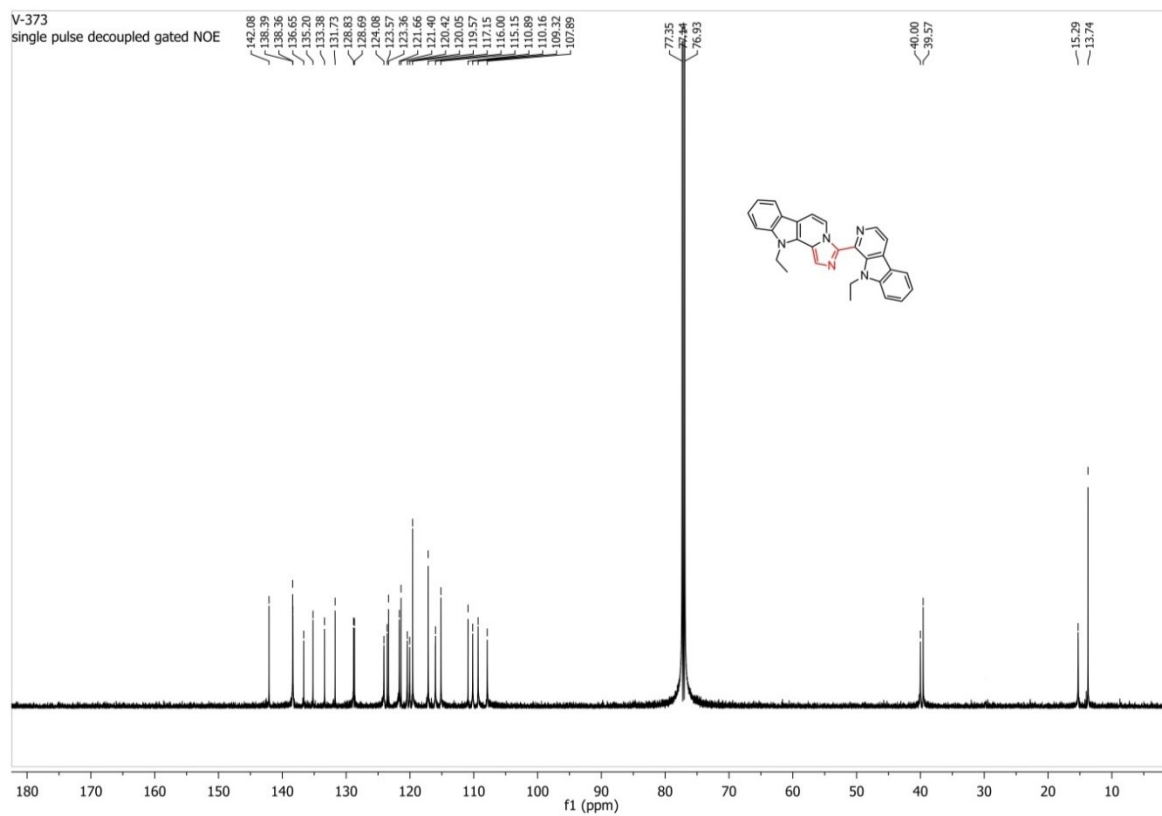


Figure S6. ^{13}C -NMR spectrum of **15B**.

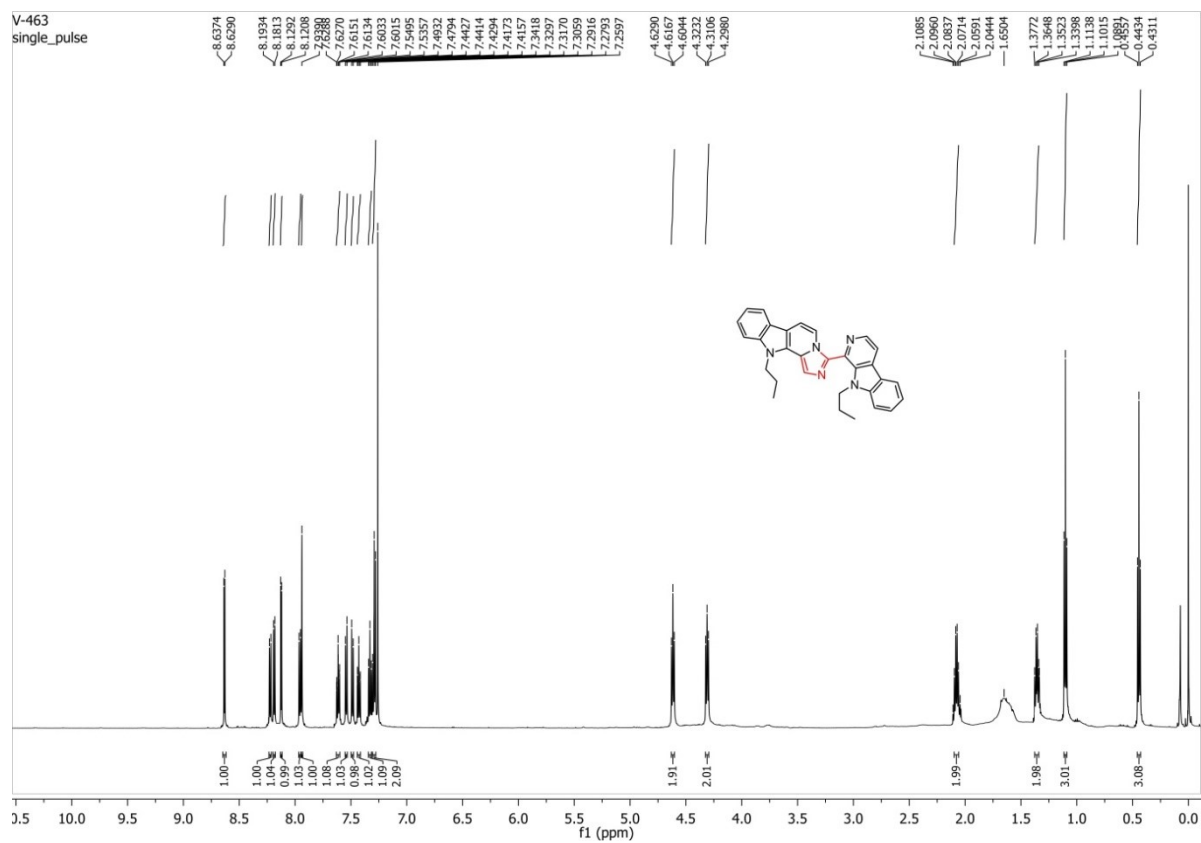


Figure S7. $^1\text{H-NMR}$ spectrum of **15C**.

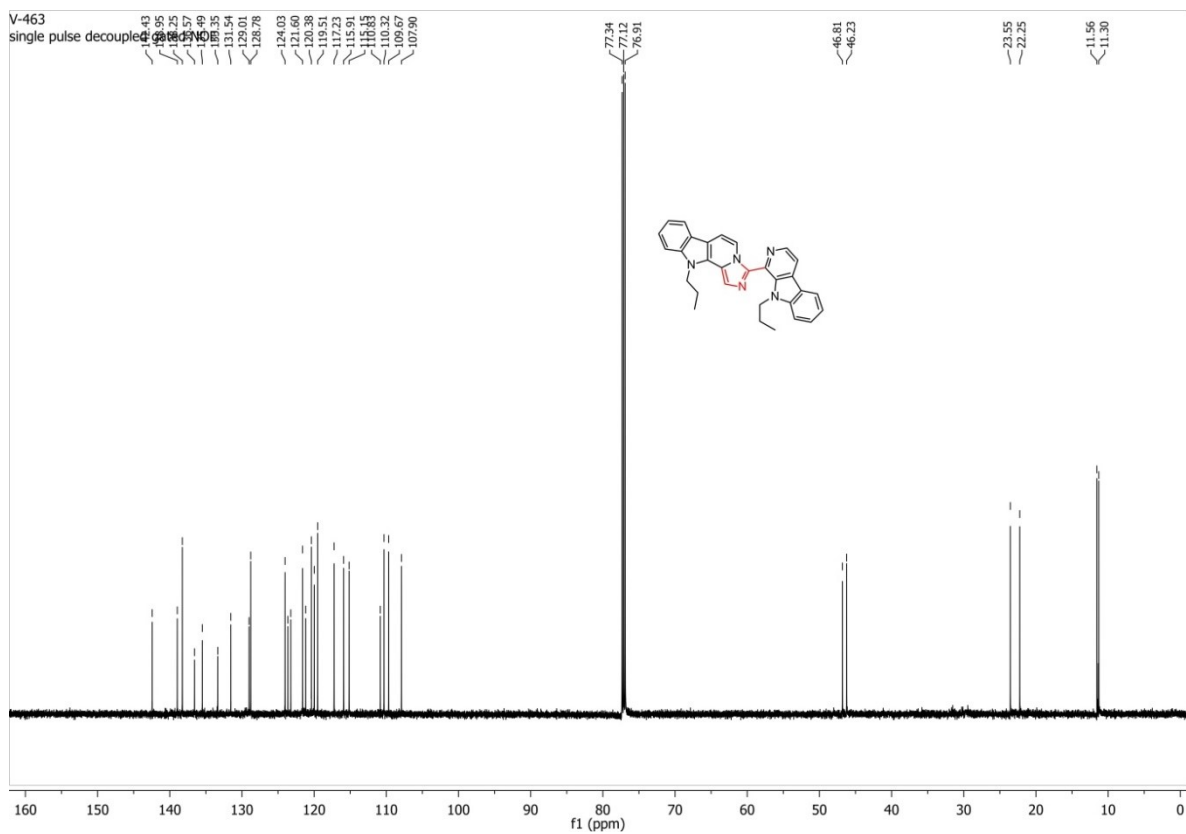


Figure S8. $^{13}\text{C-NMR}$ spectrum of **15C**.

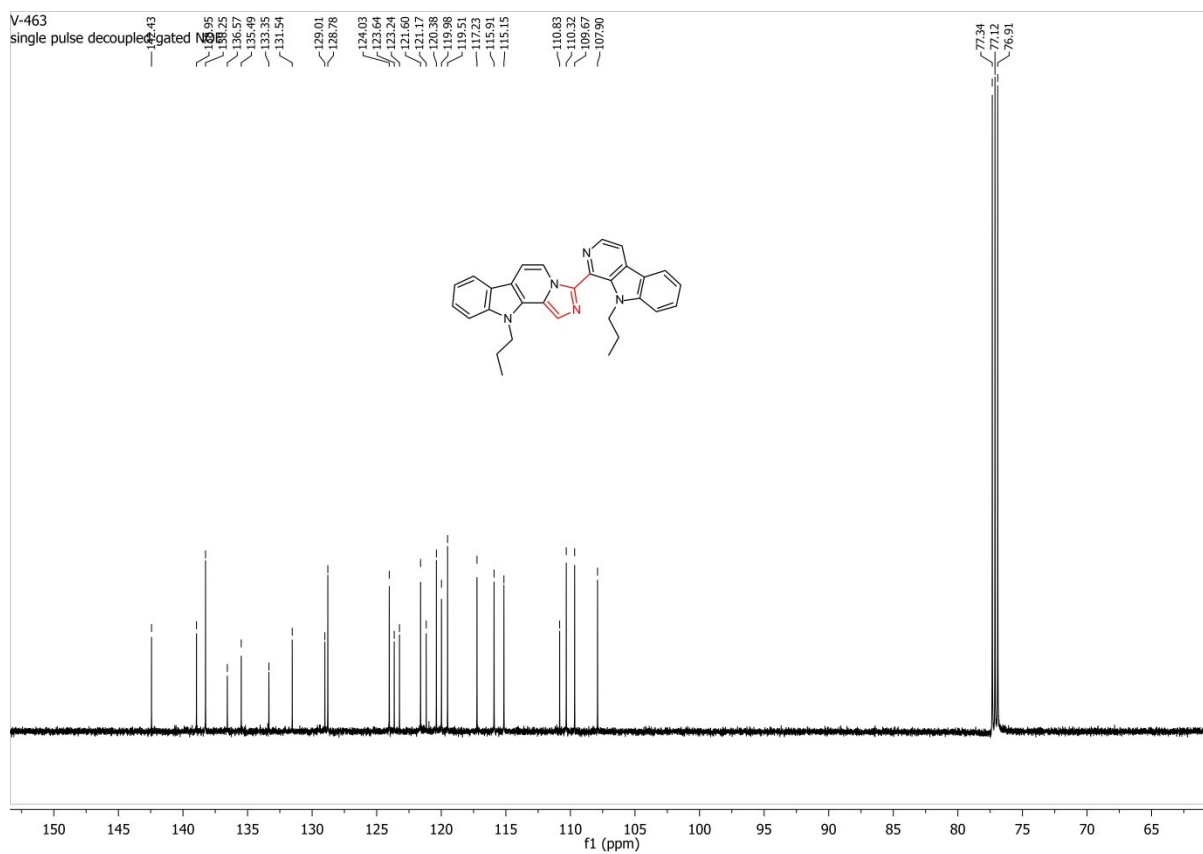


Figure S9. Extended ^{13}C -NMR spectrum of **15C**.

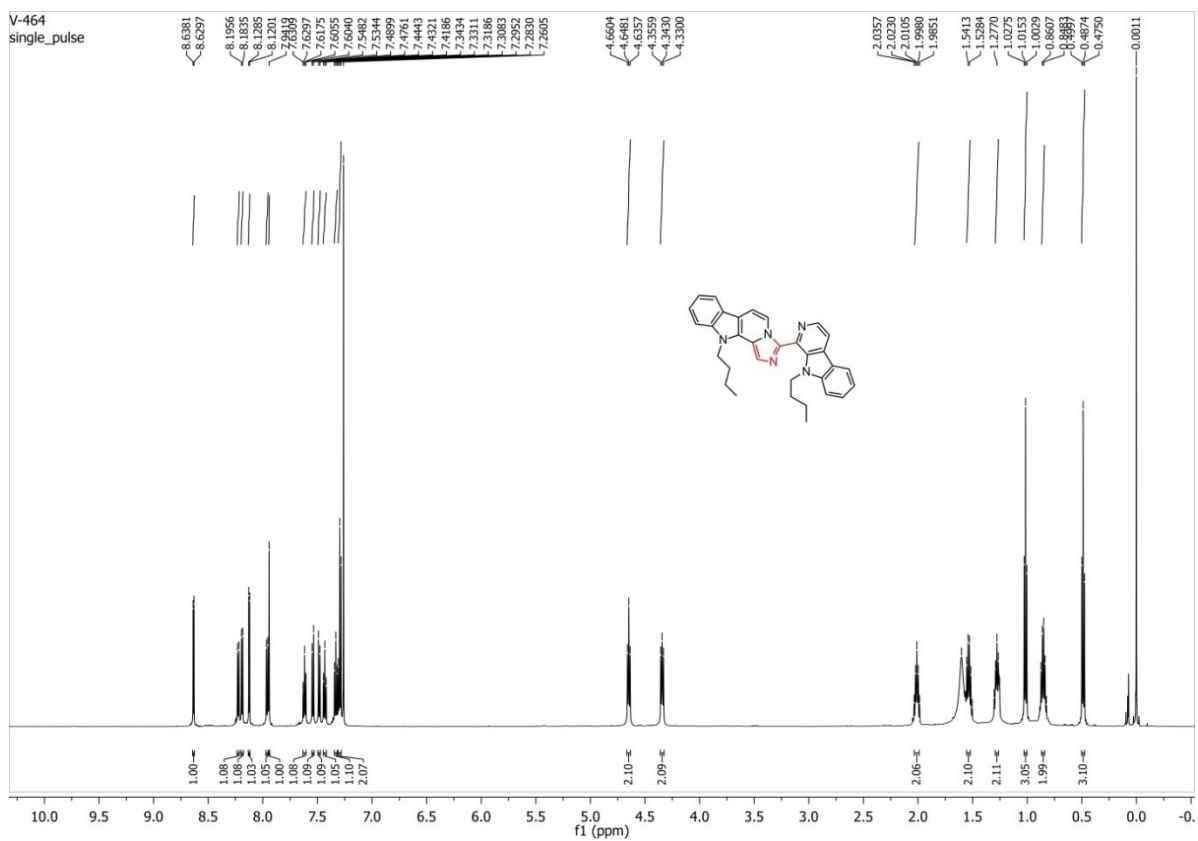


Figure S10. ^1H -NMR spectrum of 15D.

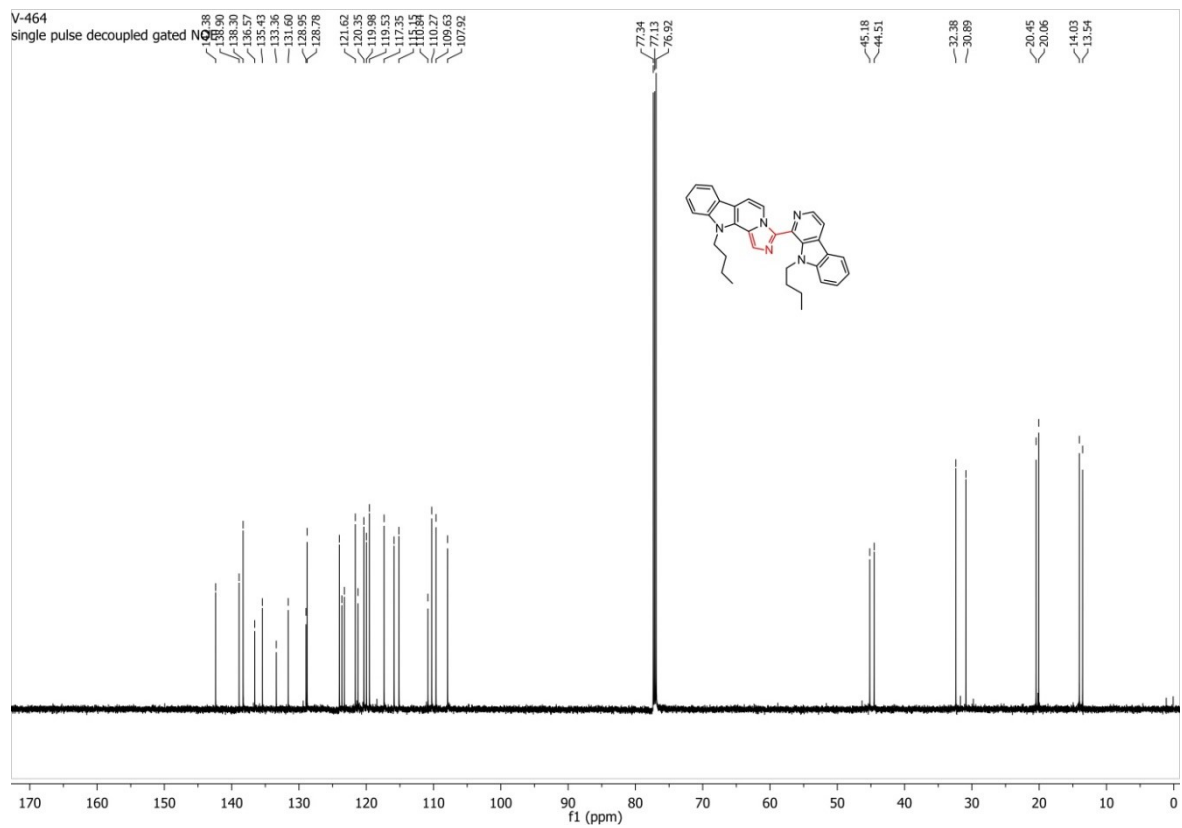


Figure S11. ^{13}C -NMR spectrum of 15D.

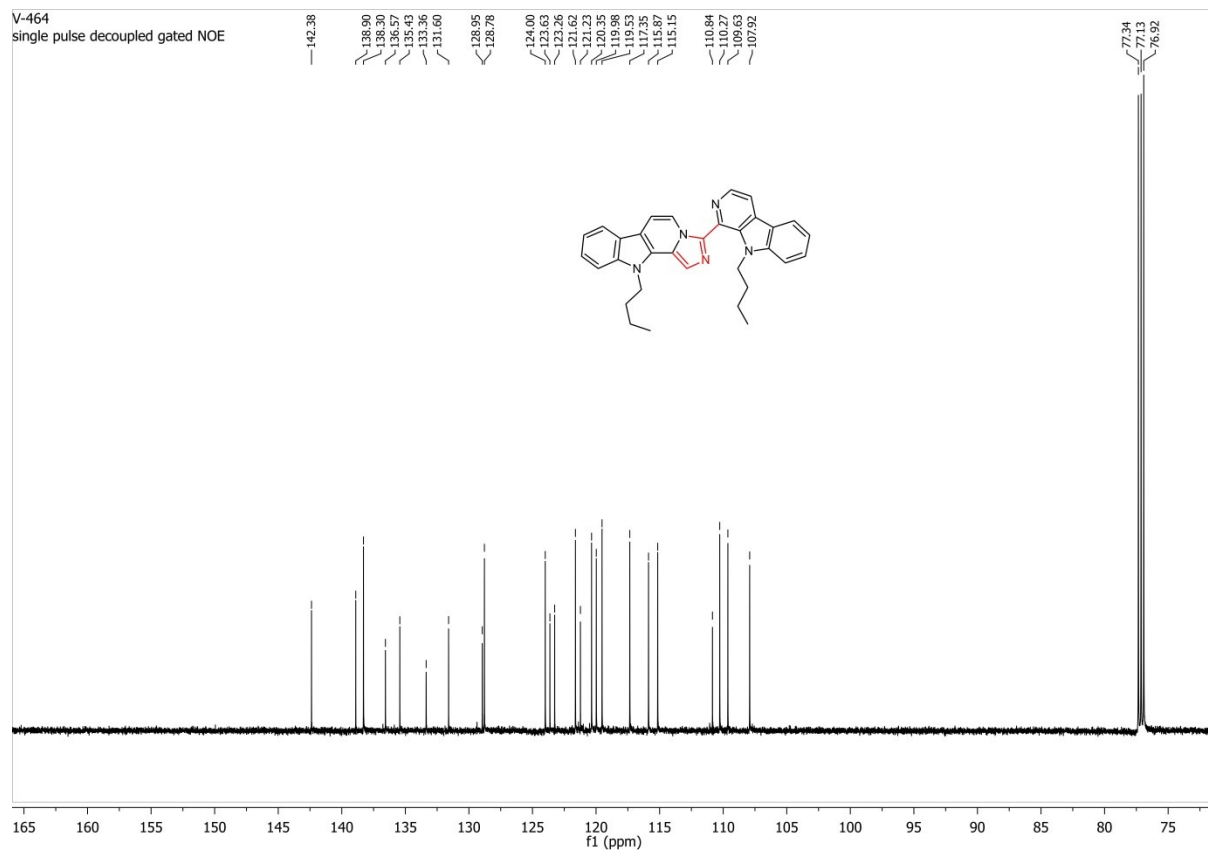


Figure S12. Extended ^{13}C -NMR spectrum of **15D**.

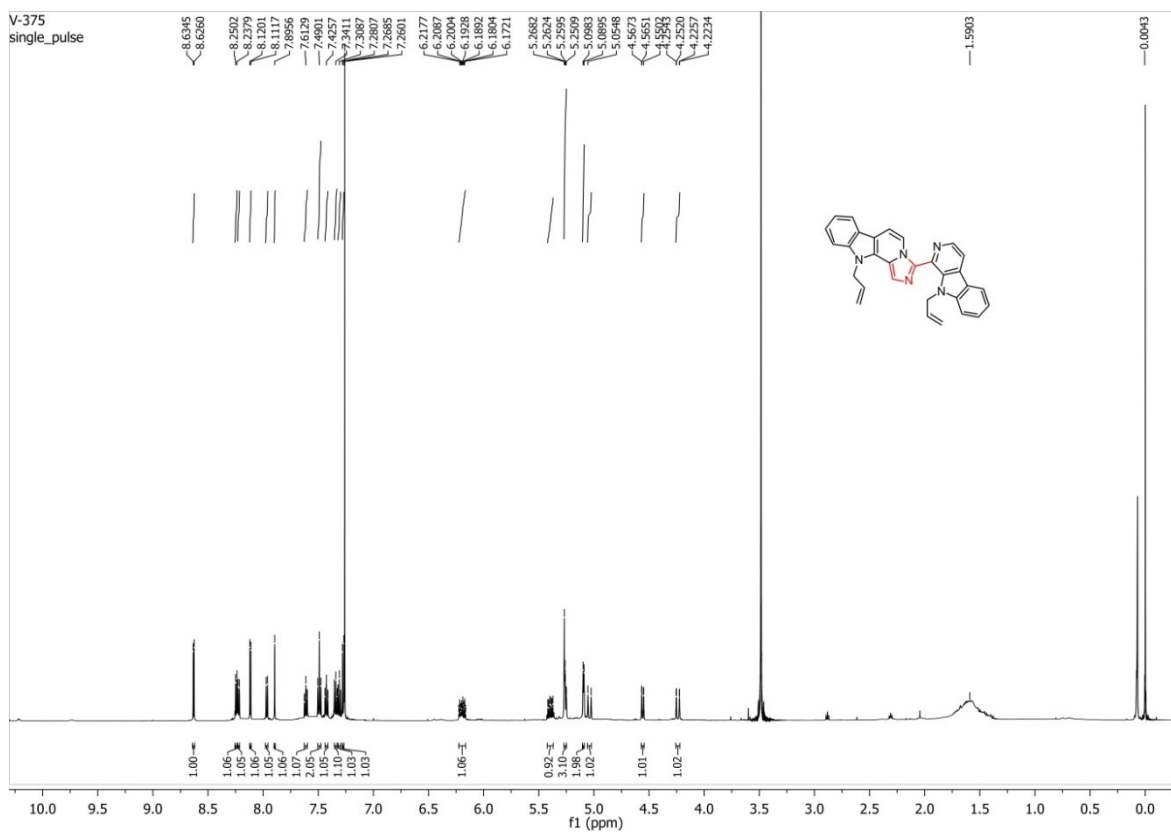


Figure S13. ^1H -NMR spectrum of 15E.

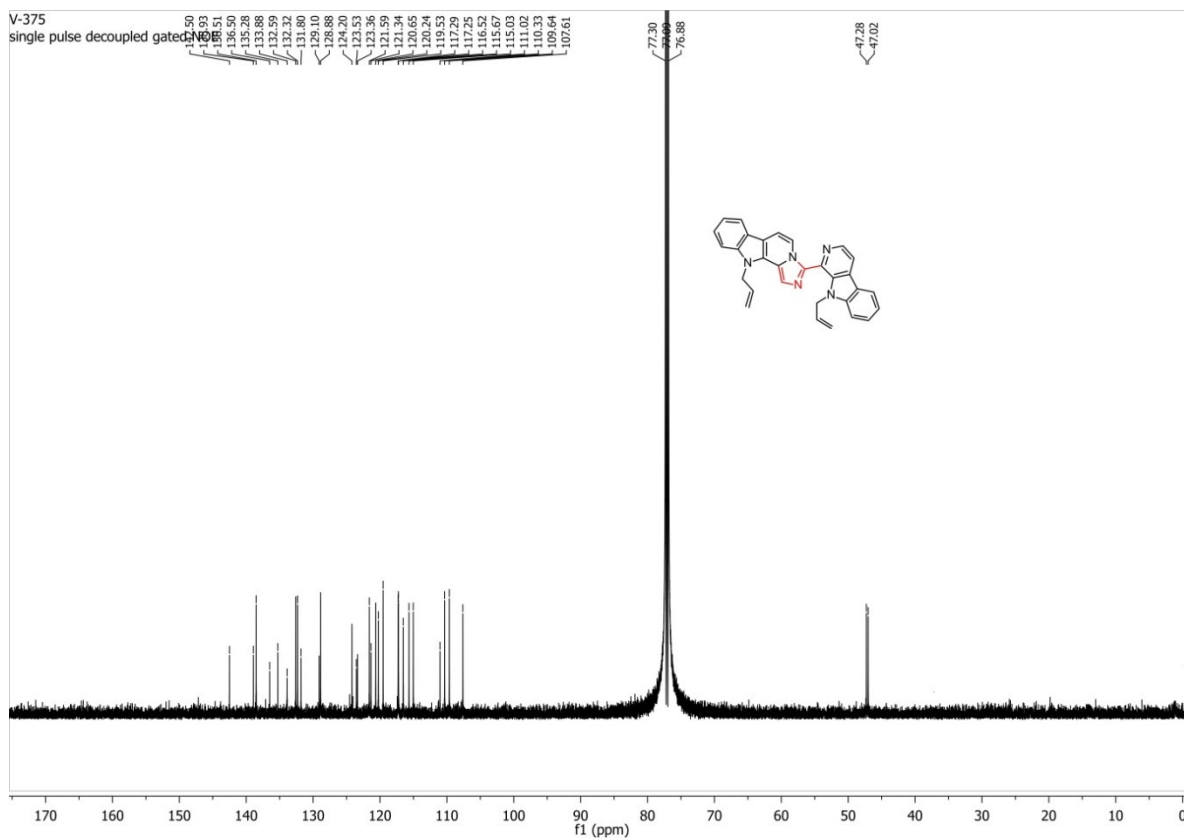


Figure S14. ^{13}C -NMR spectrum of 15E.

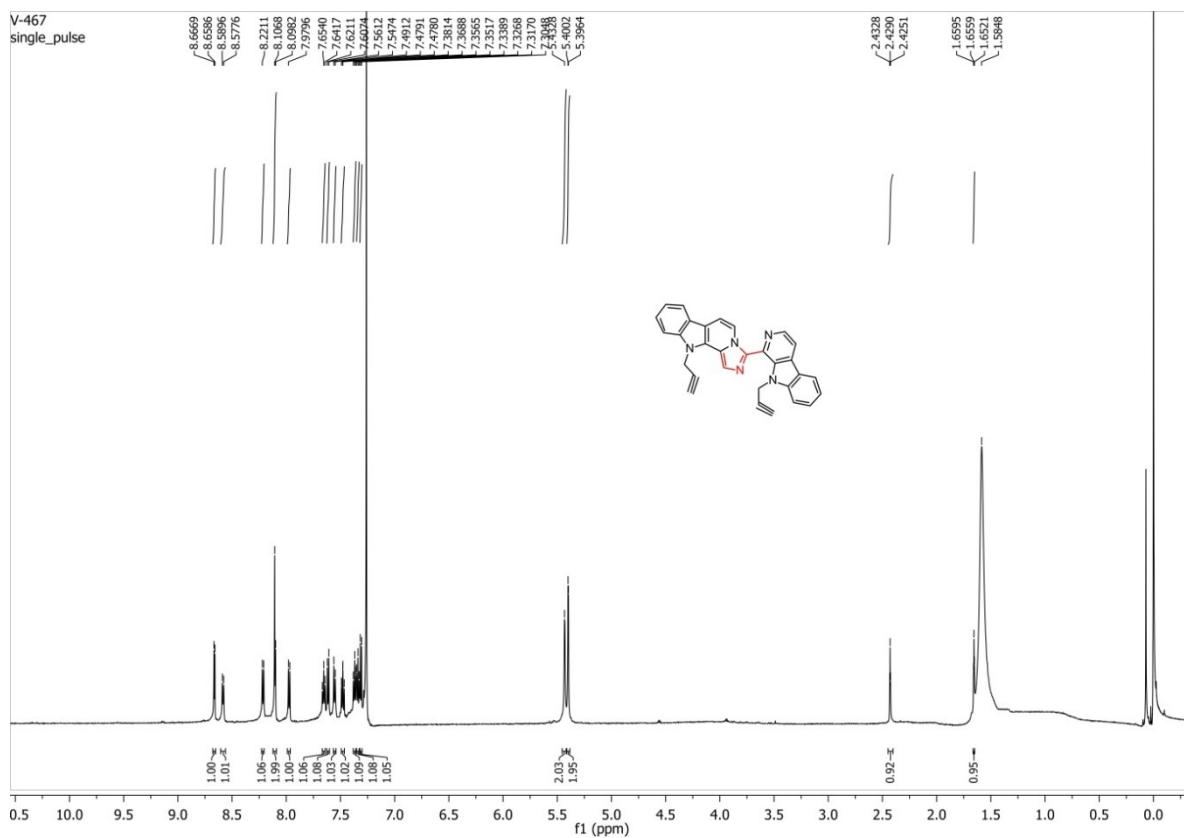


Figure S15. ^1H -NMR spectrum of 15F.

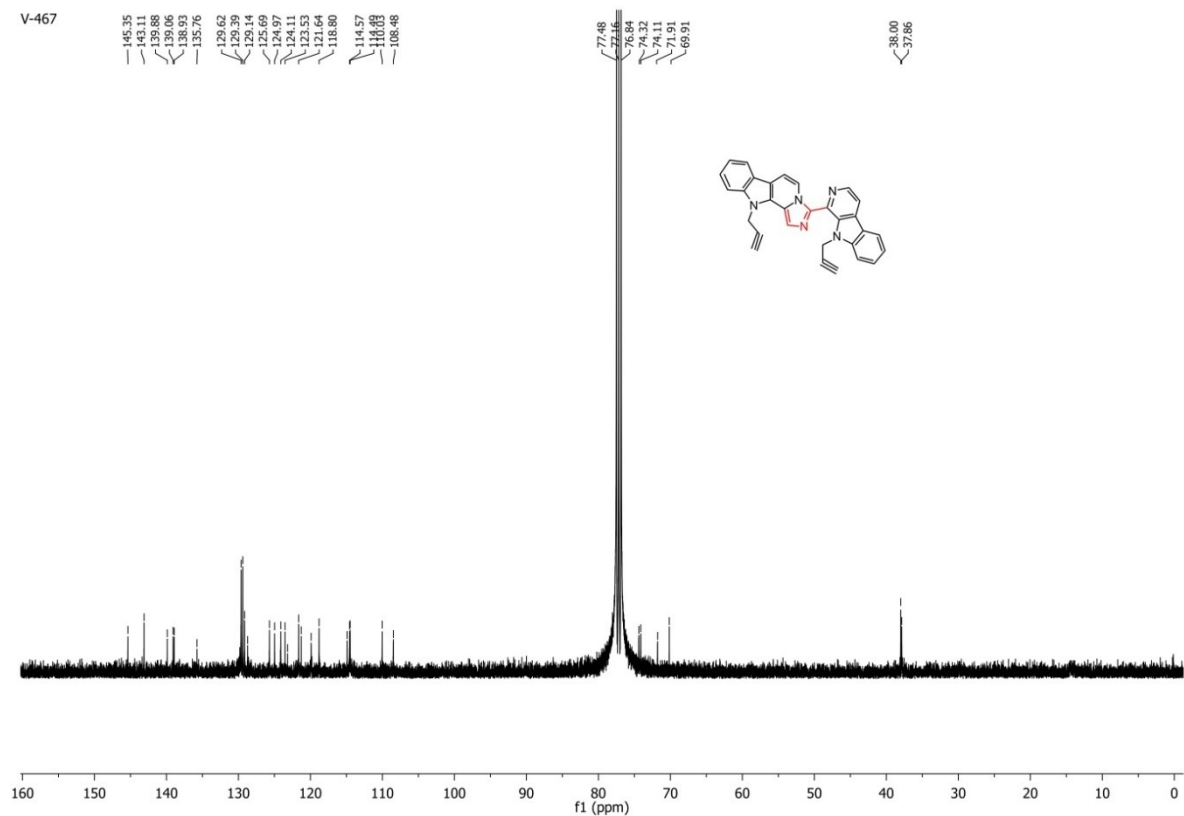
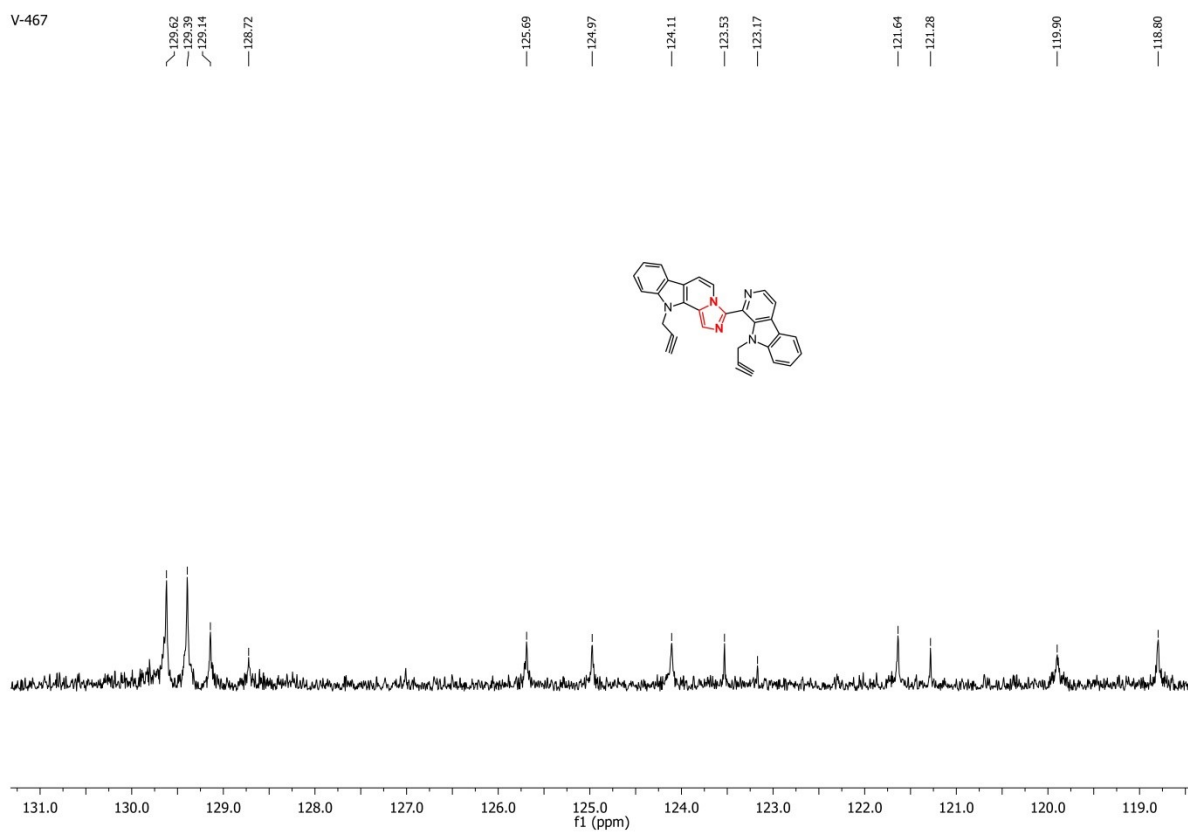


Figure S16. ^{13}C -NMR spectrum of 15F.

V-467



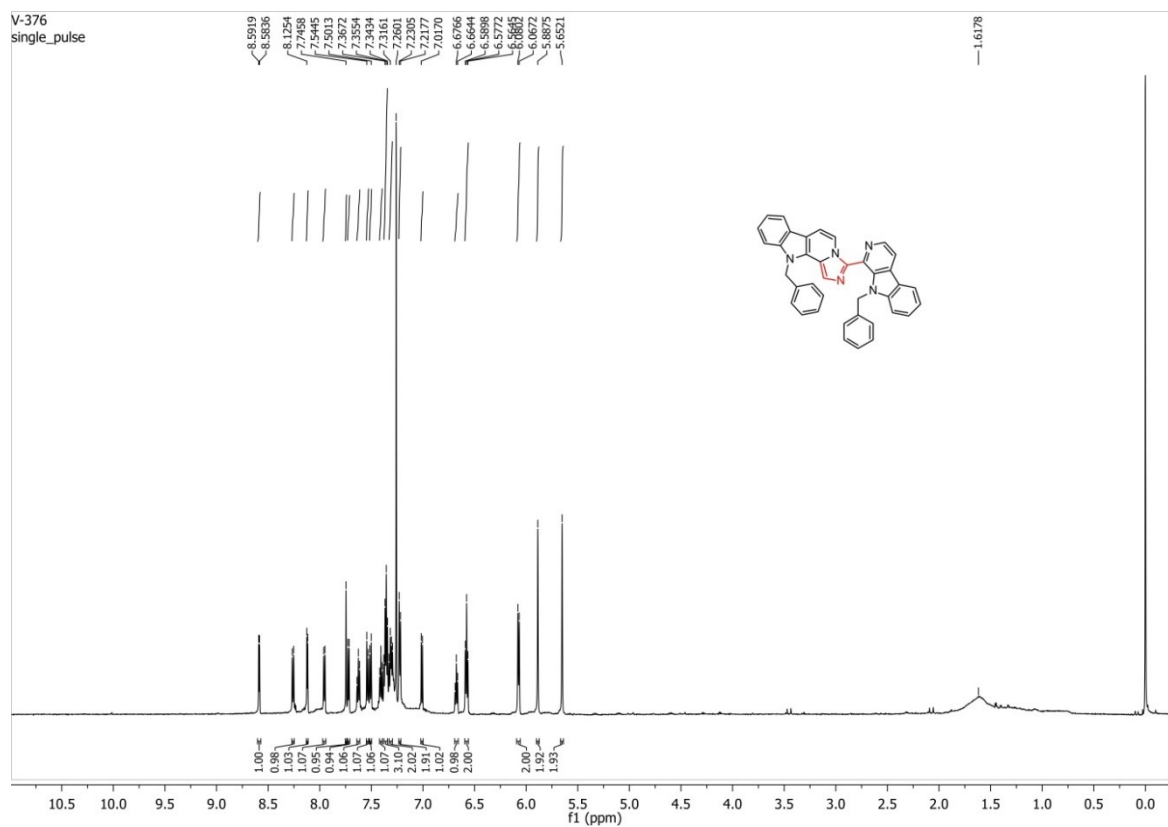


Figure S18. ^1H -NMR spectrum of **15G**.

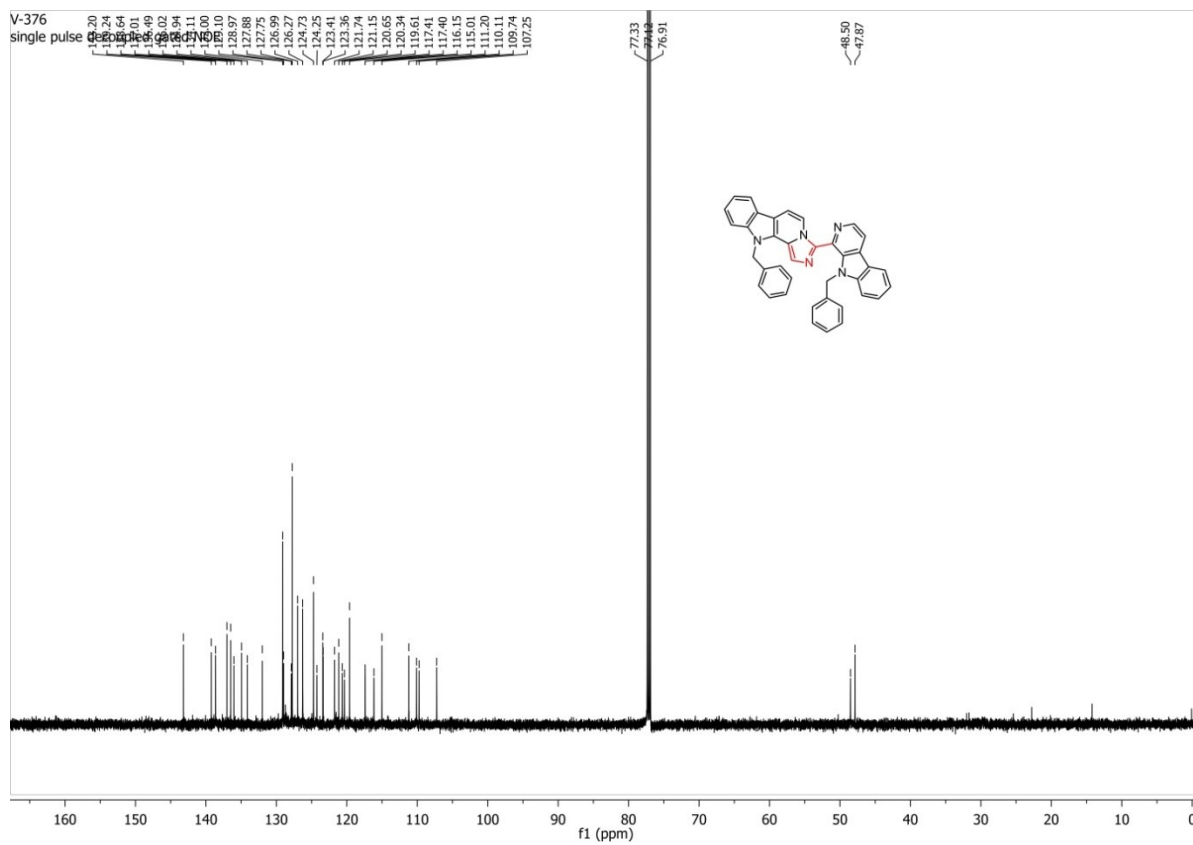


Figure S19. ^{13}C -NMR spectrum of **15G**.

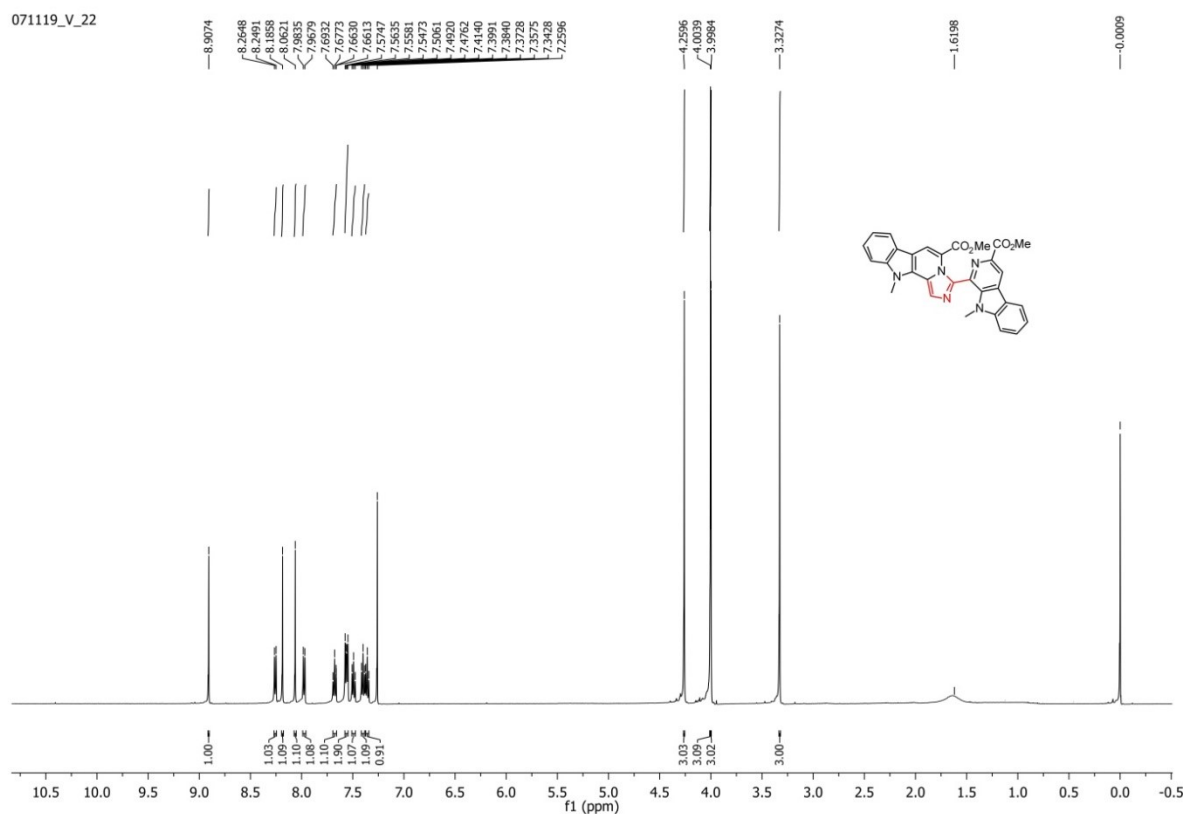


Figure S20. $^1\text{H-NMR}$ spectrum of 16A.

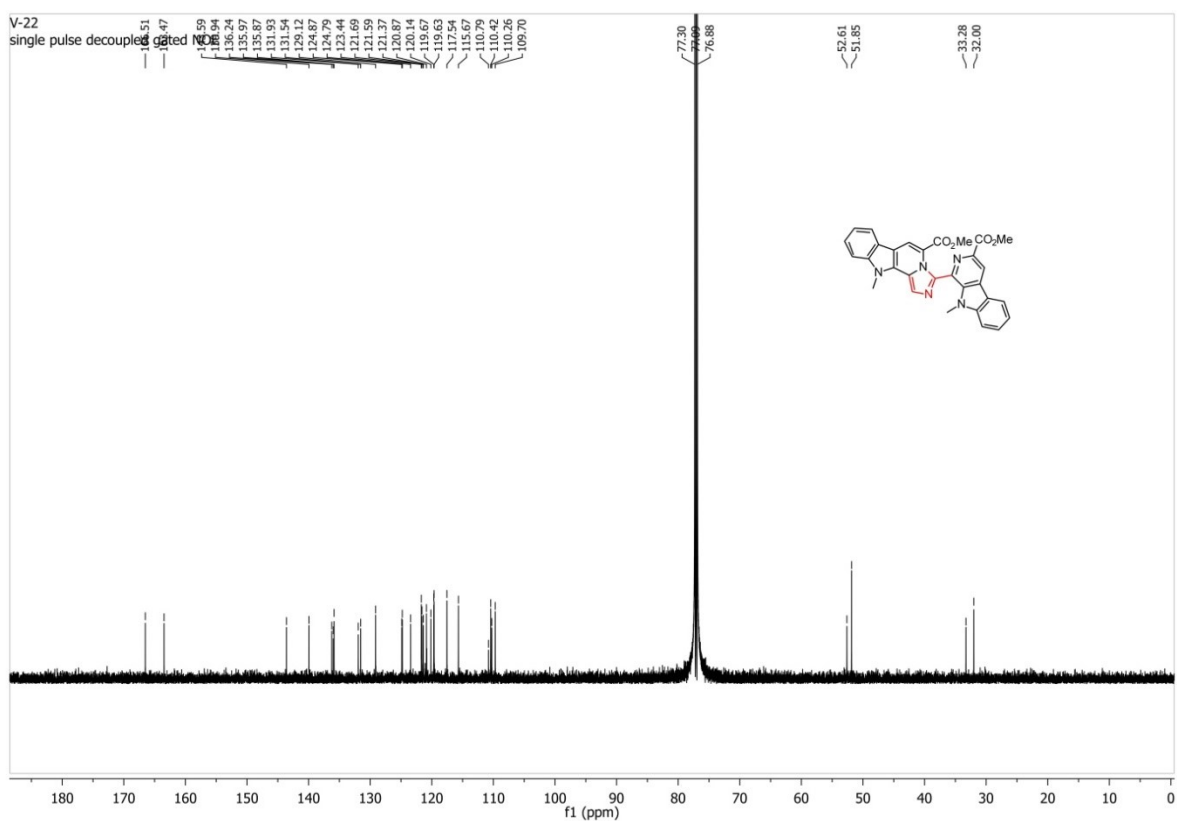


Figure S21. $^{13}\text{C-NMR}$ spectrum of 16A.

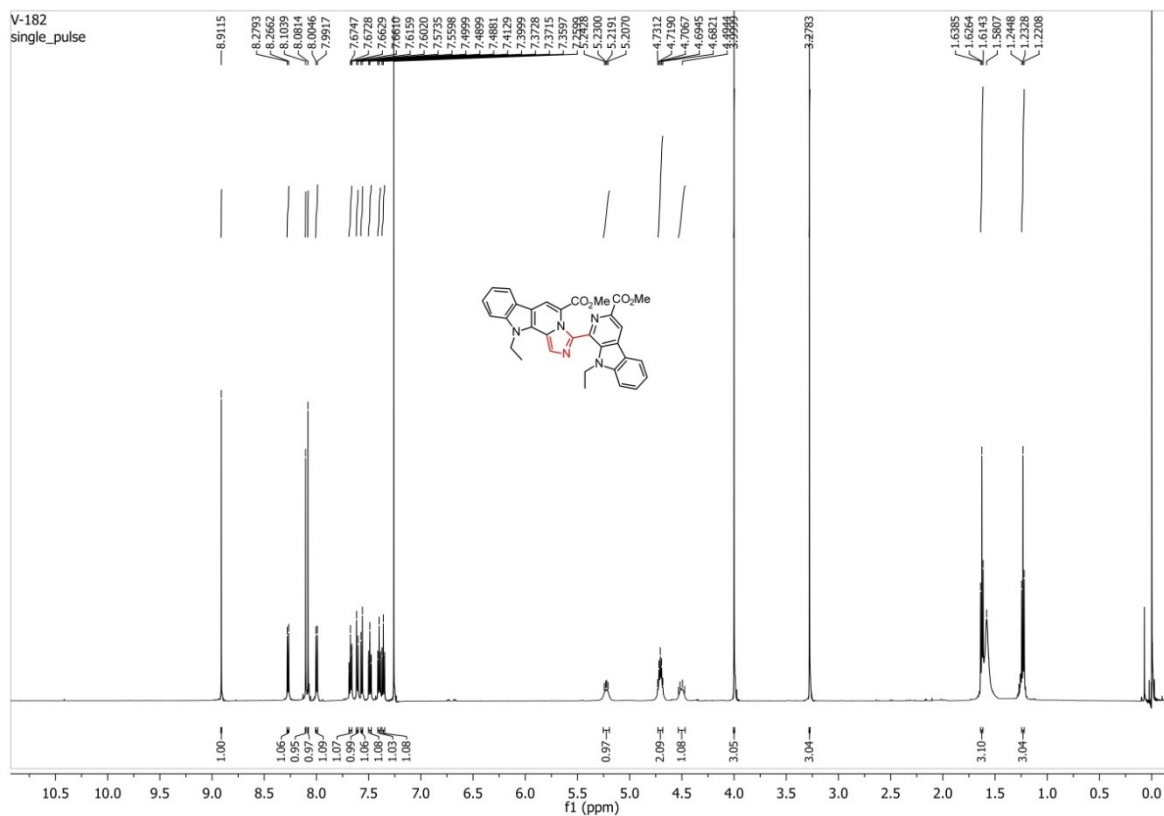


Figure S22. $^1\text{H-NMR}$ spectrum of **16B**.

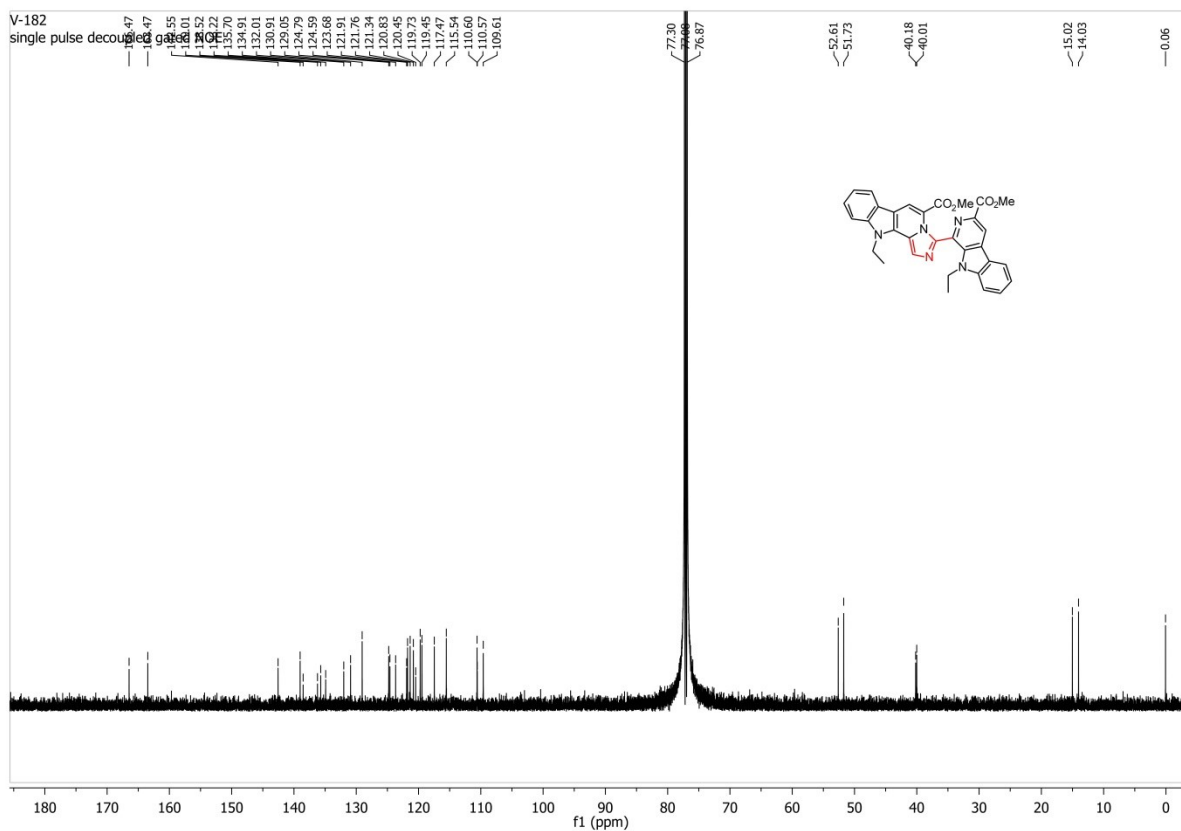
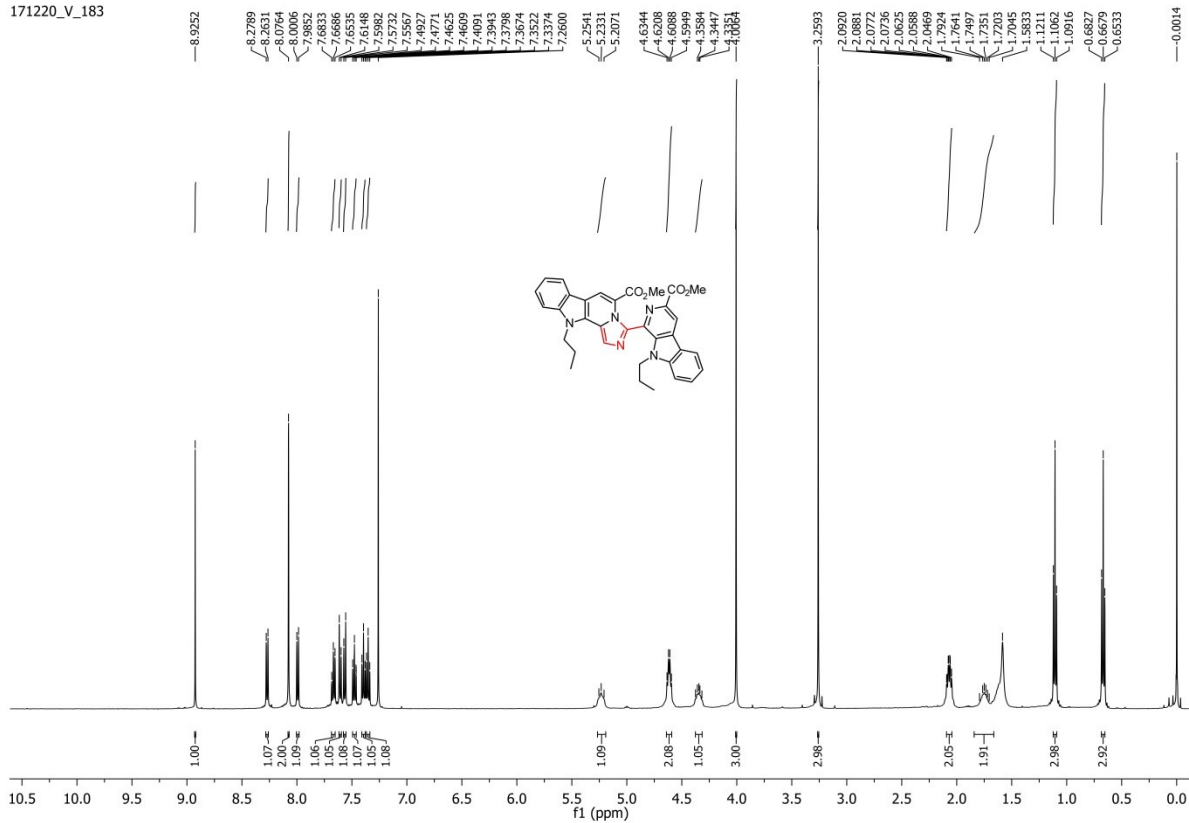
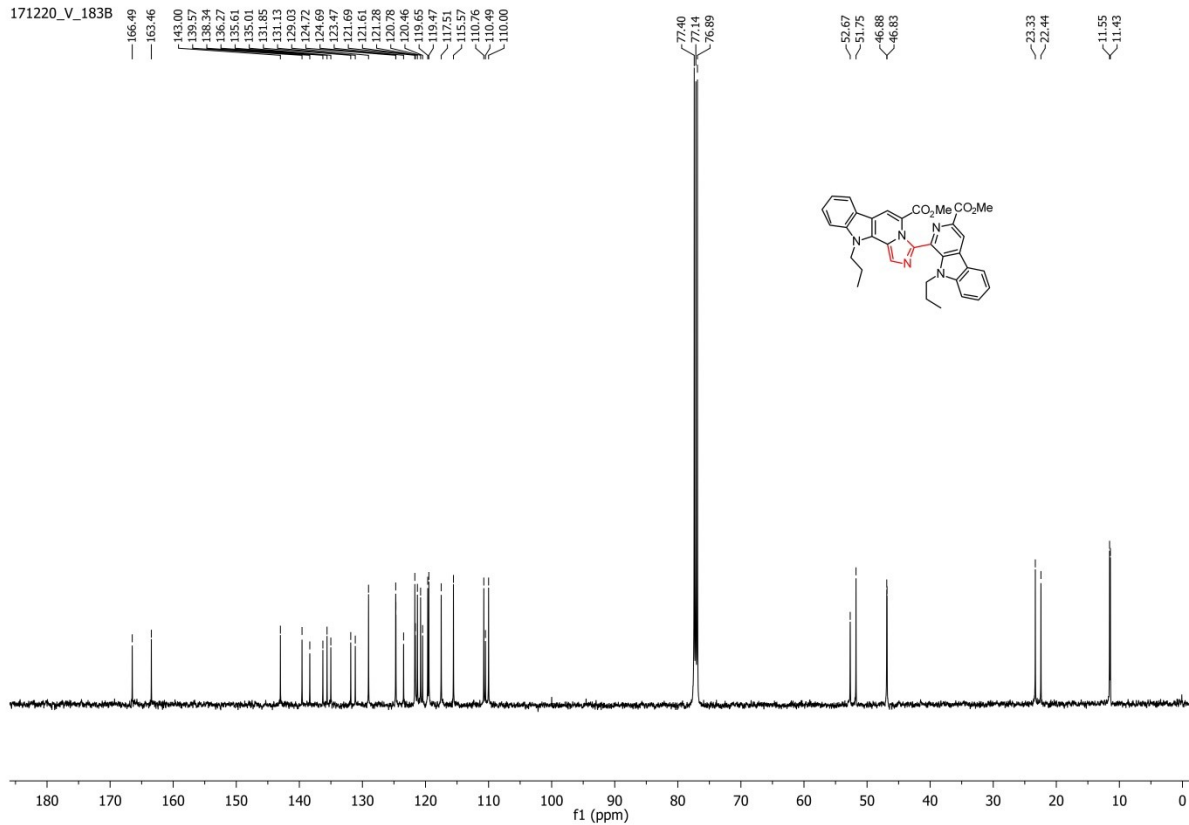


Figure S23. $^{13}\text{C-NMR}$ spectrum of **16B**.

171220_V_183

Figure S24. ¹H-NMR spectrum of 16C.

171220_V_183B

Figure S25. ¹³C-NMR spectrum of 16C.

171220_V_185

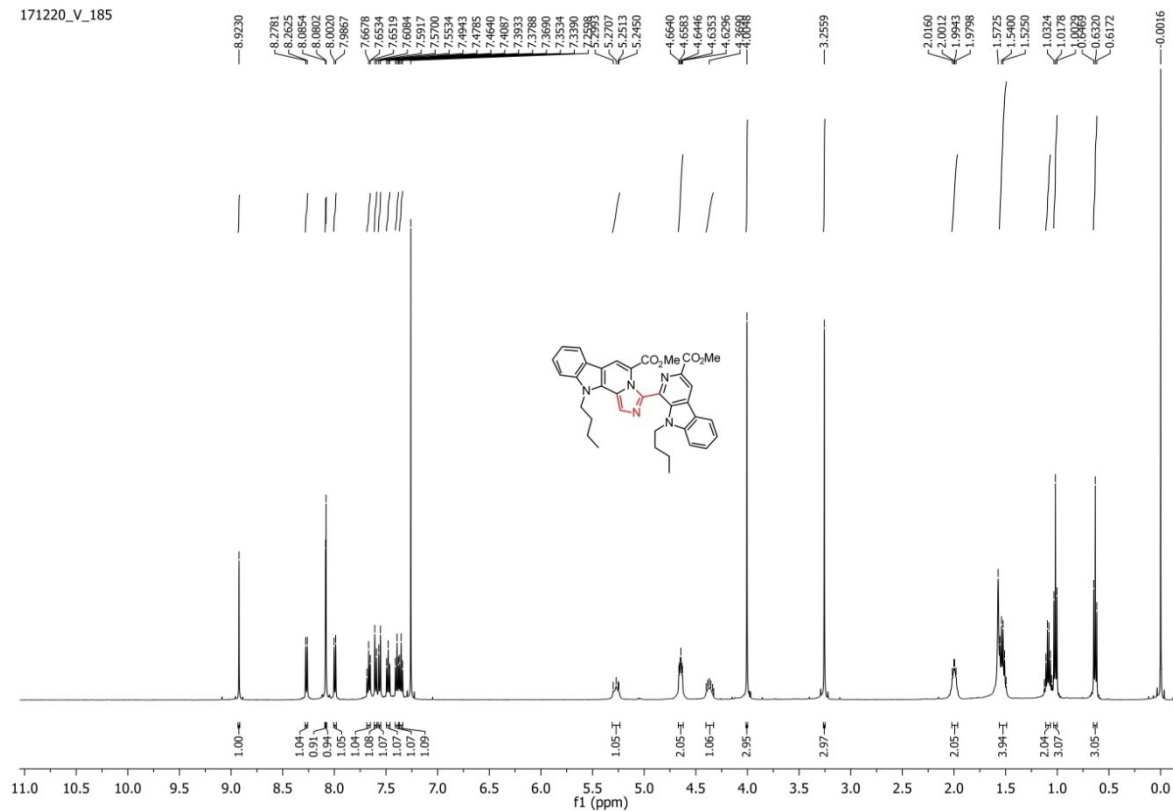


Figure S26. ¹H-NMR spectrum of 16D.

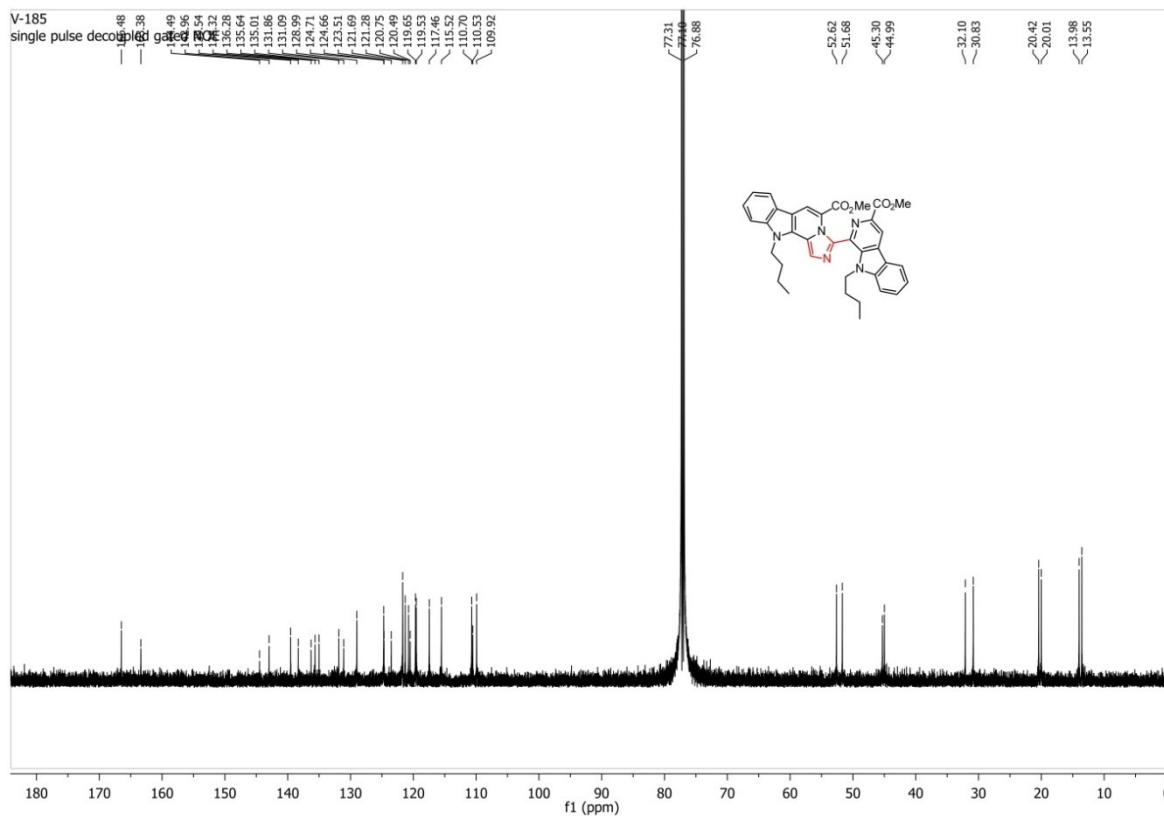
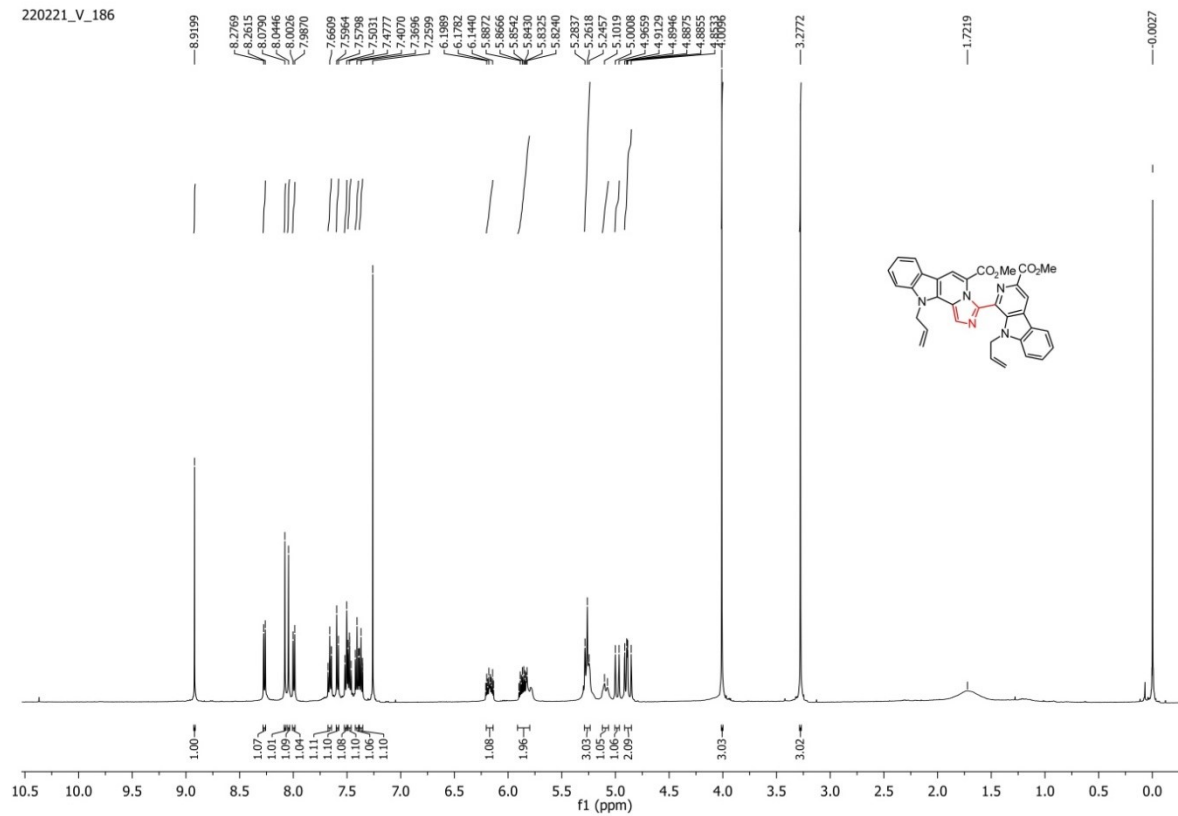
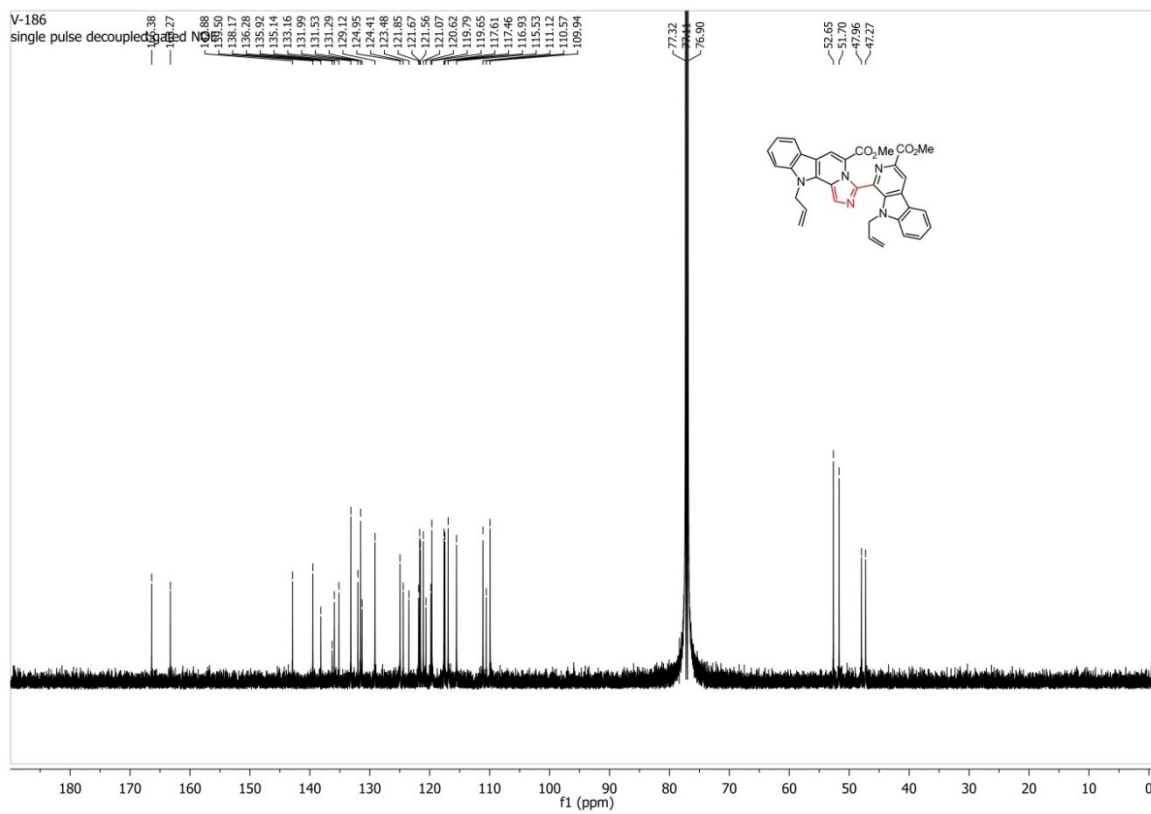


Figure S27. ¹³C-NMR spectrum of 16D.

220221_V_186

Figure S28. ¹H-NMR spectrum of 16E.Figure S29. ¹³C-NMR spectrum of 16E.

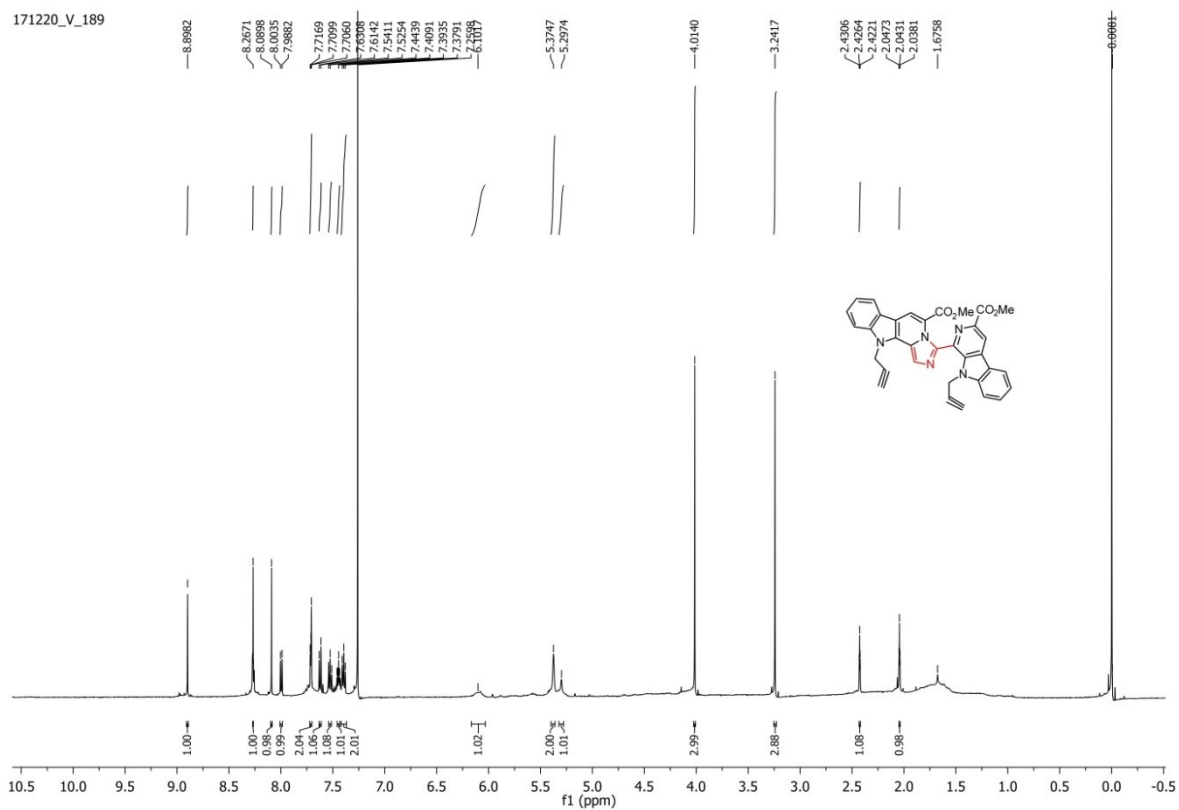


Figure S30. ¹H-NMR spectrum of 16F.

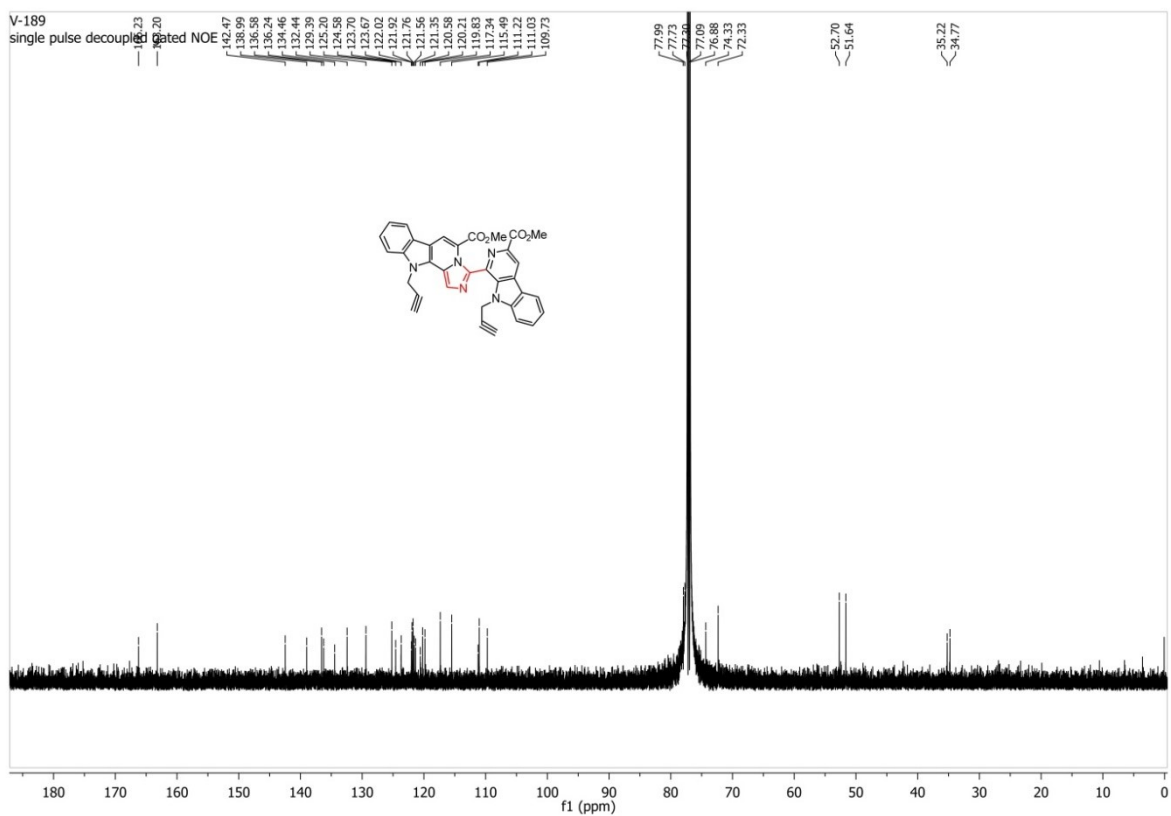


Figure S31. ¹³C-NMR spectrum of 16F.

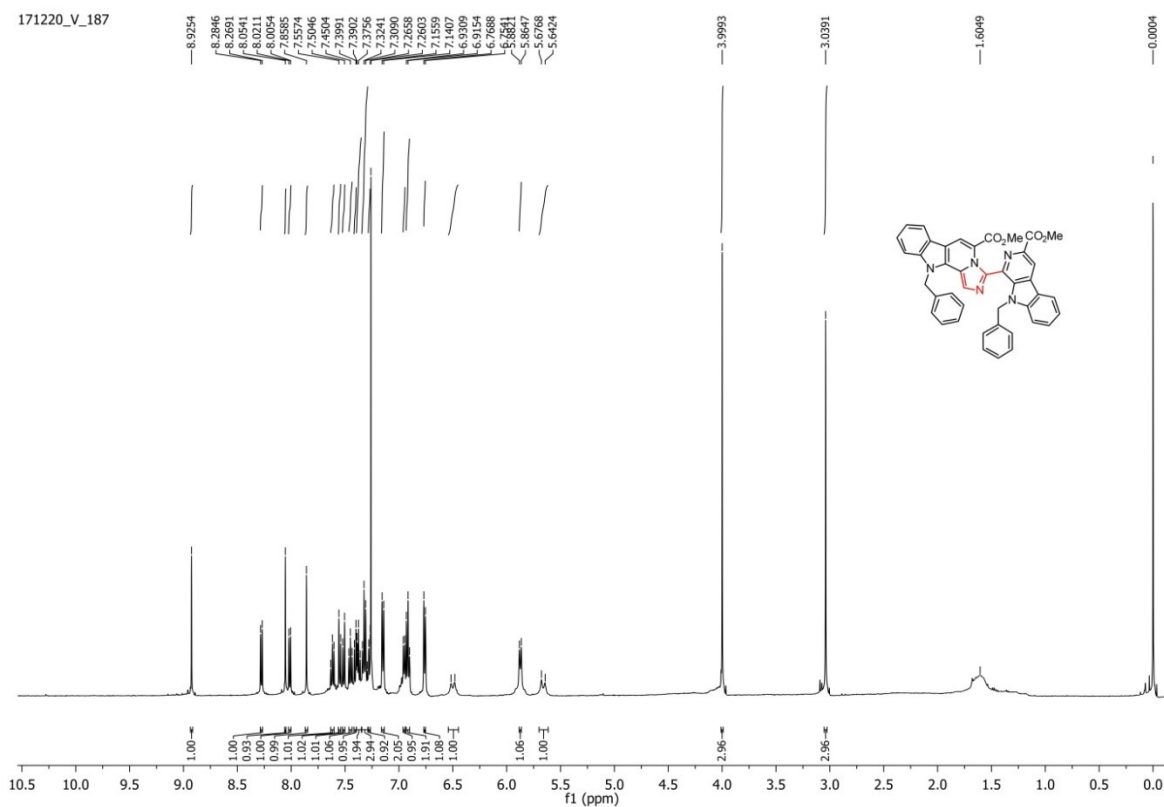


Figure S32. ^1H -NMR spectrum of 16G.

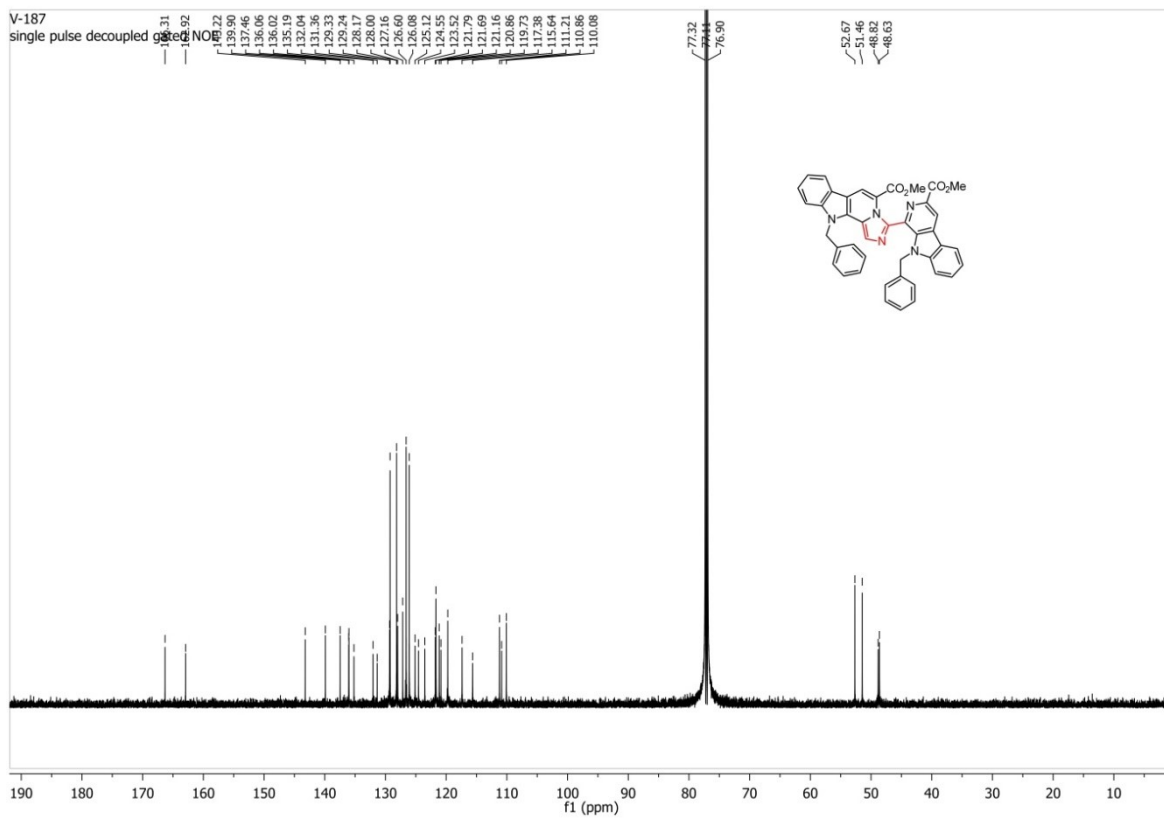
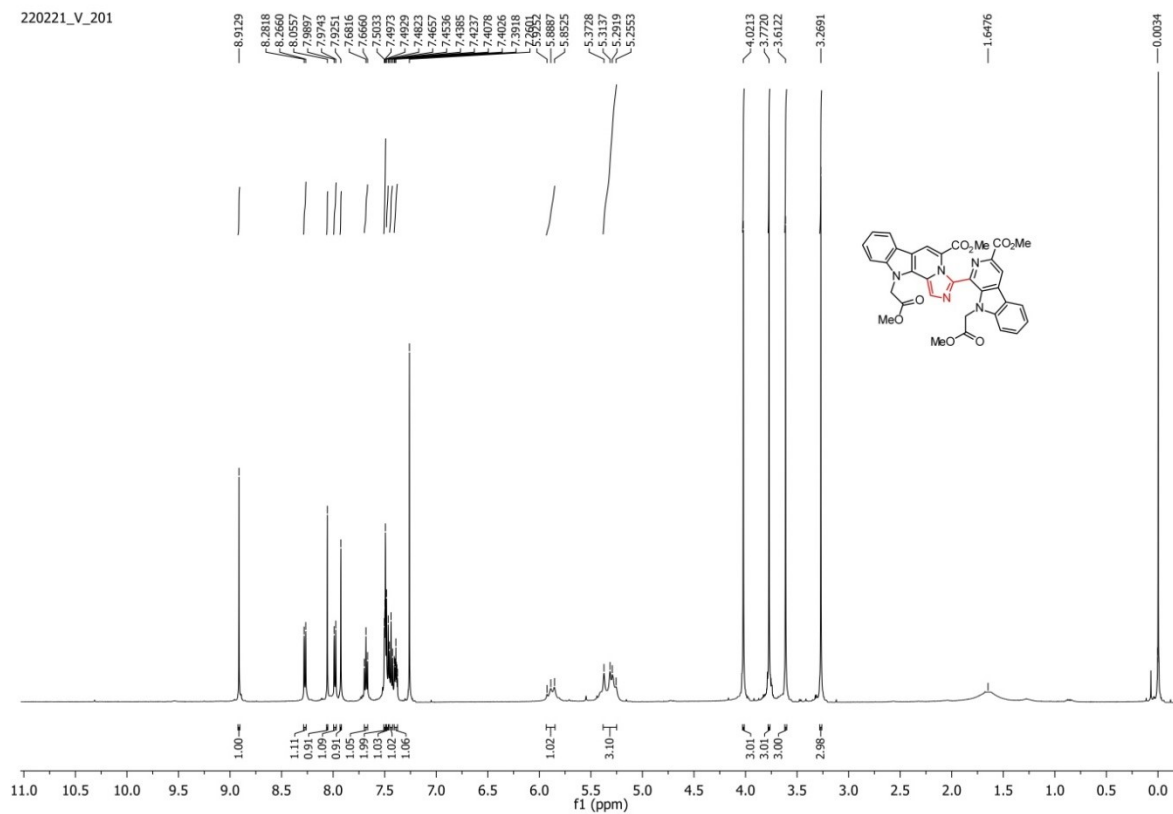
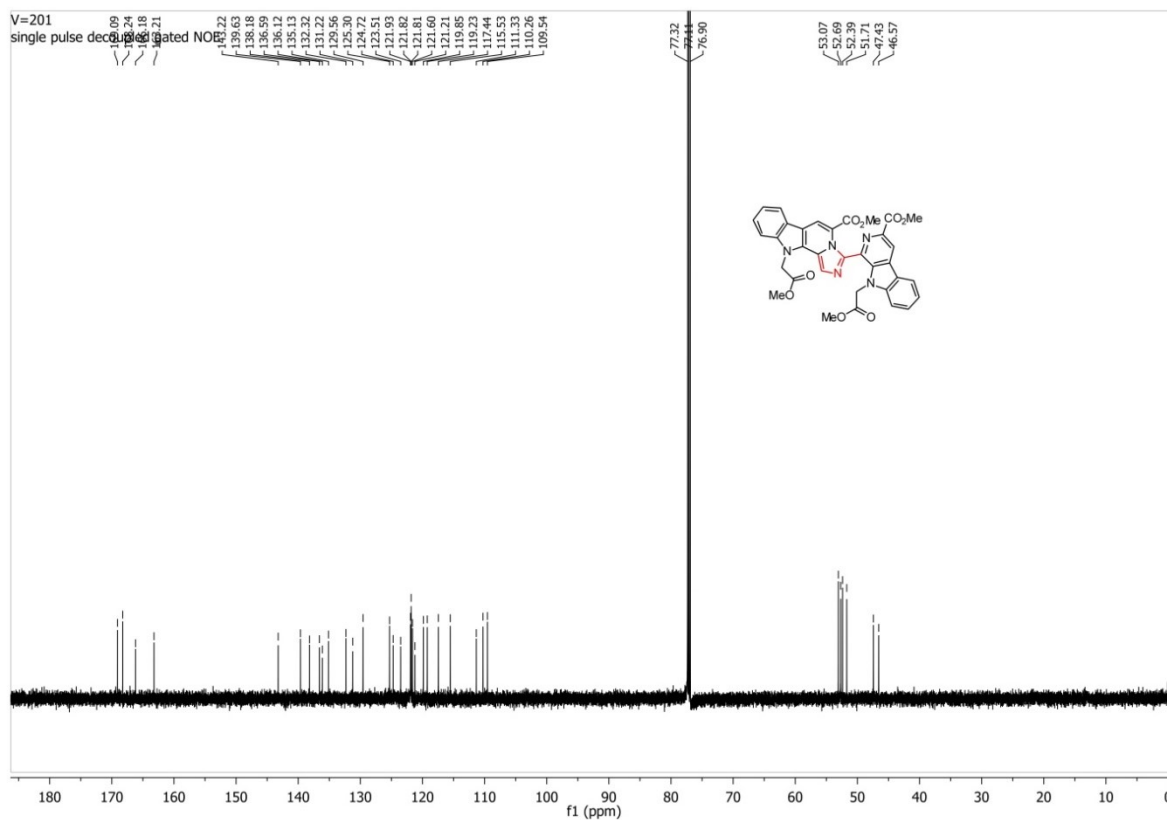


Figure S33. ^{13}C -NMR spectrum of 16G.

220221_V_201

Figure S34. ¹H-NMR spectrum of 16H.Figure S35. ¹³C-NMR spectrum of 16H.

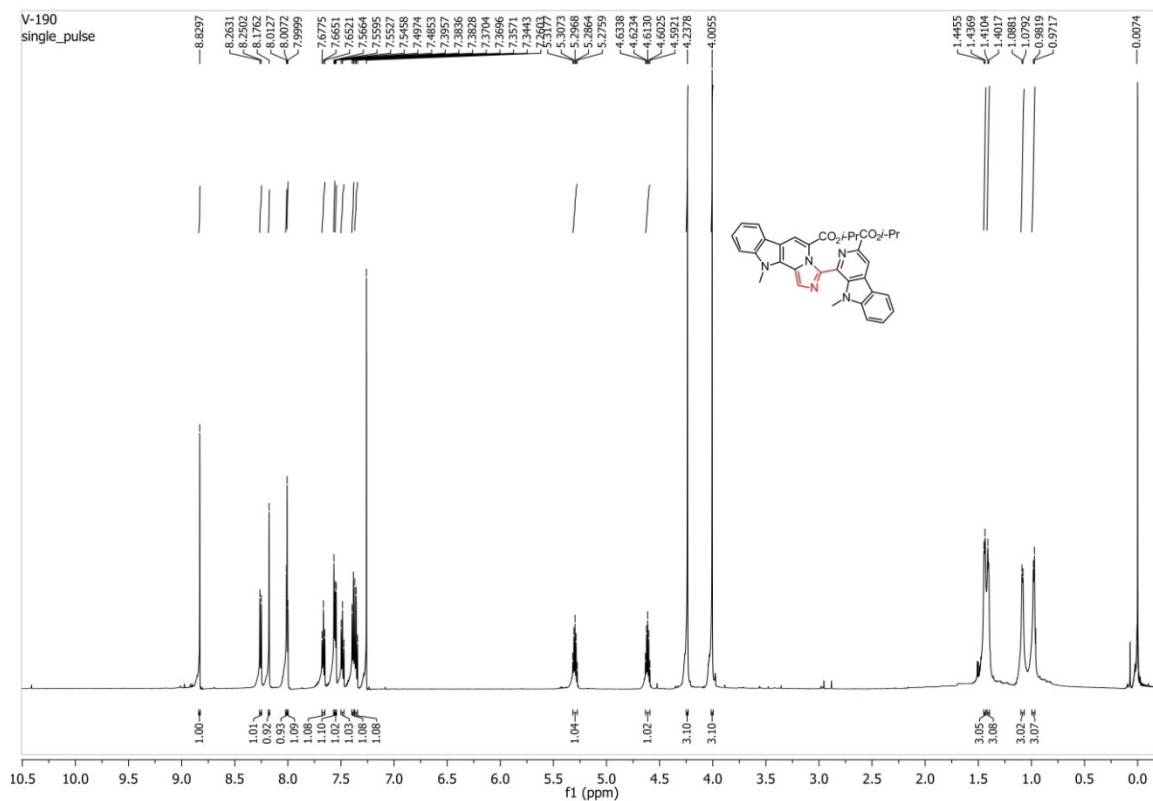


Figure S36. ¹H-NMR spectrum of 17A.

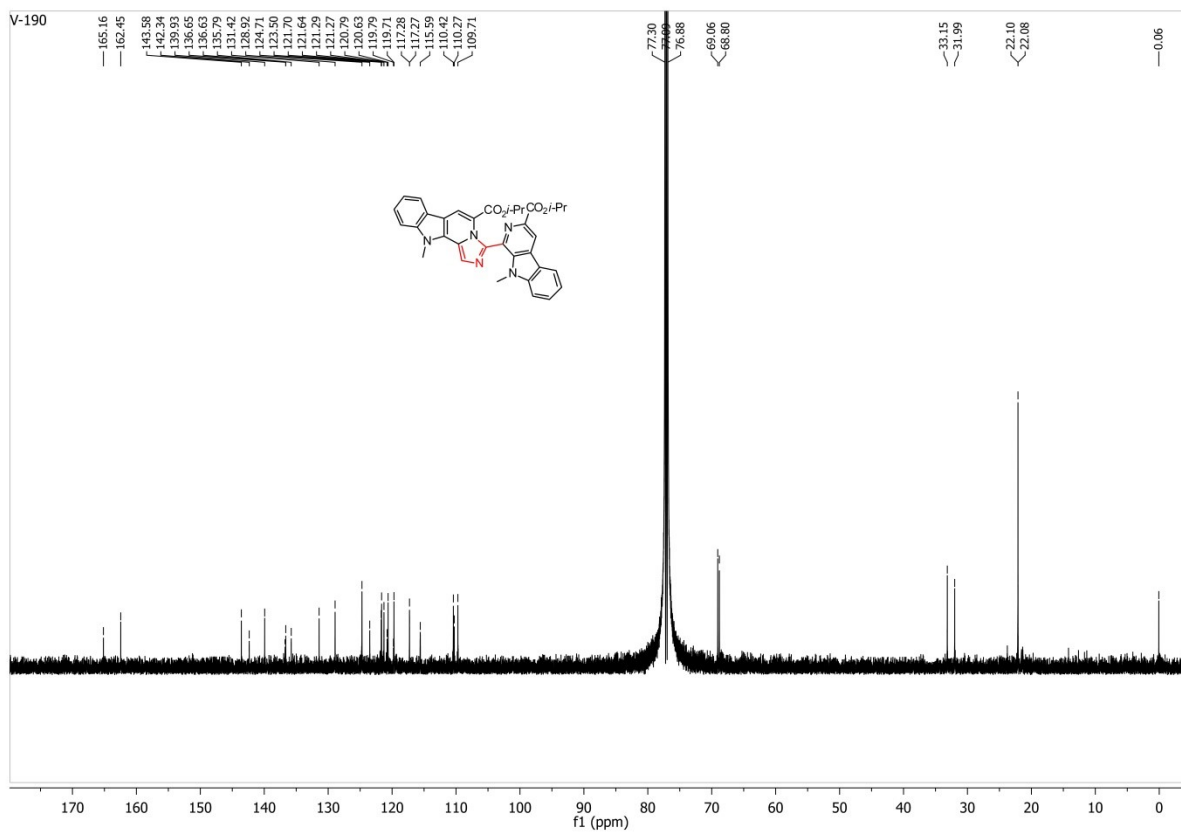


Figure S37. ¹³C-NMR spectrum of 17A.

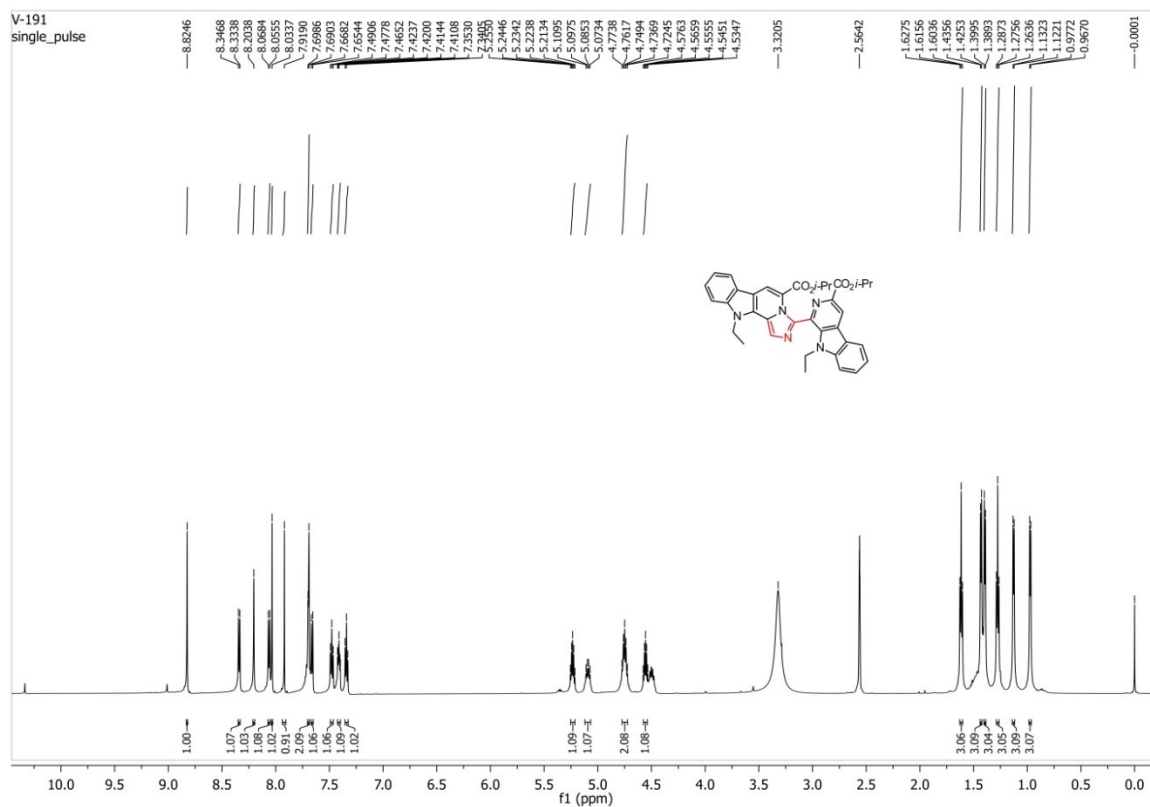


Figure S38. ¹H-NMR spectrum of 17B.

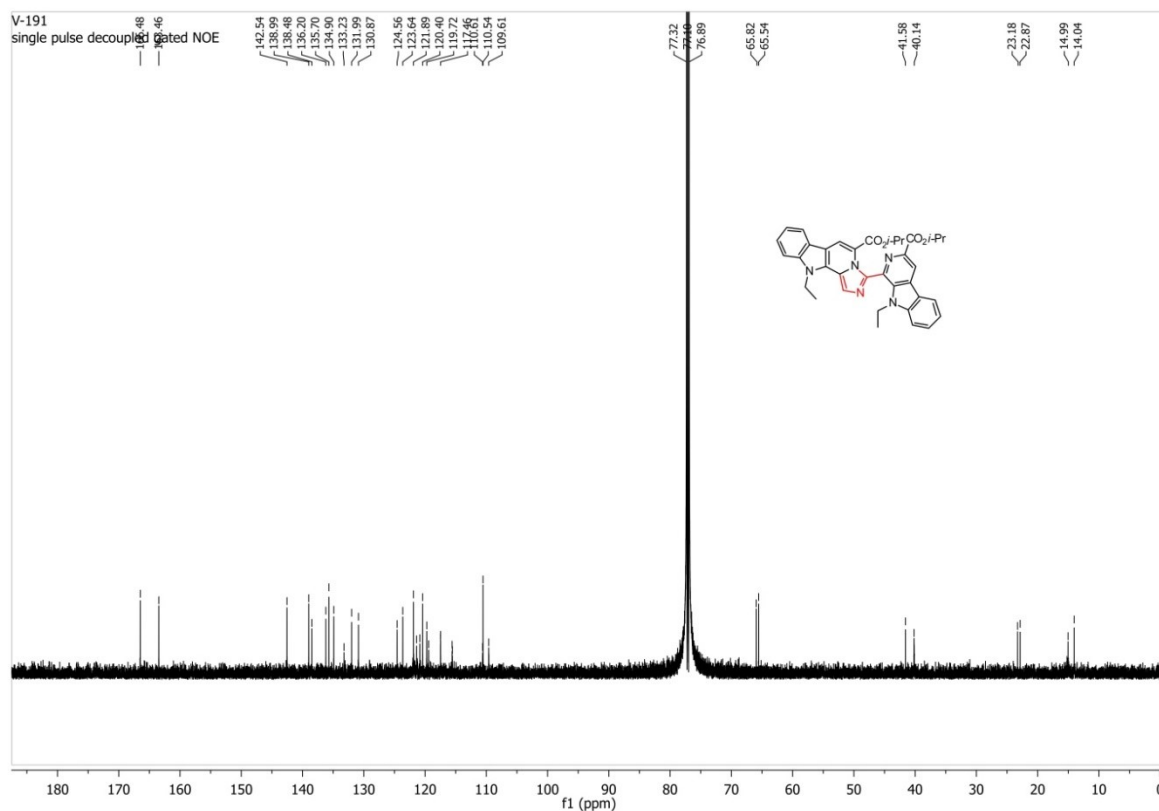


Figure S39. ¹³C-NMR spectrum of 17B.

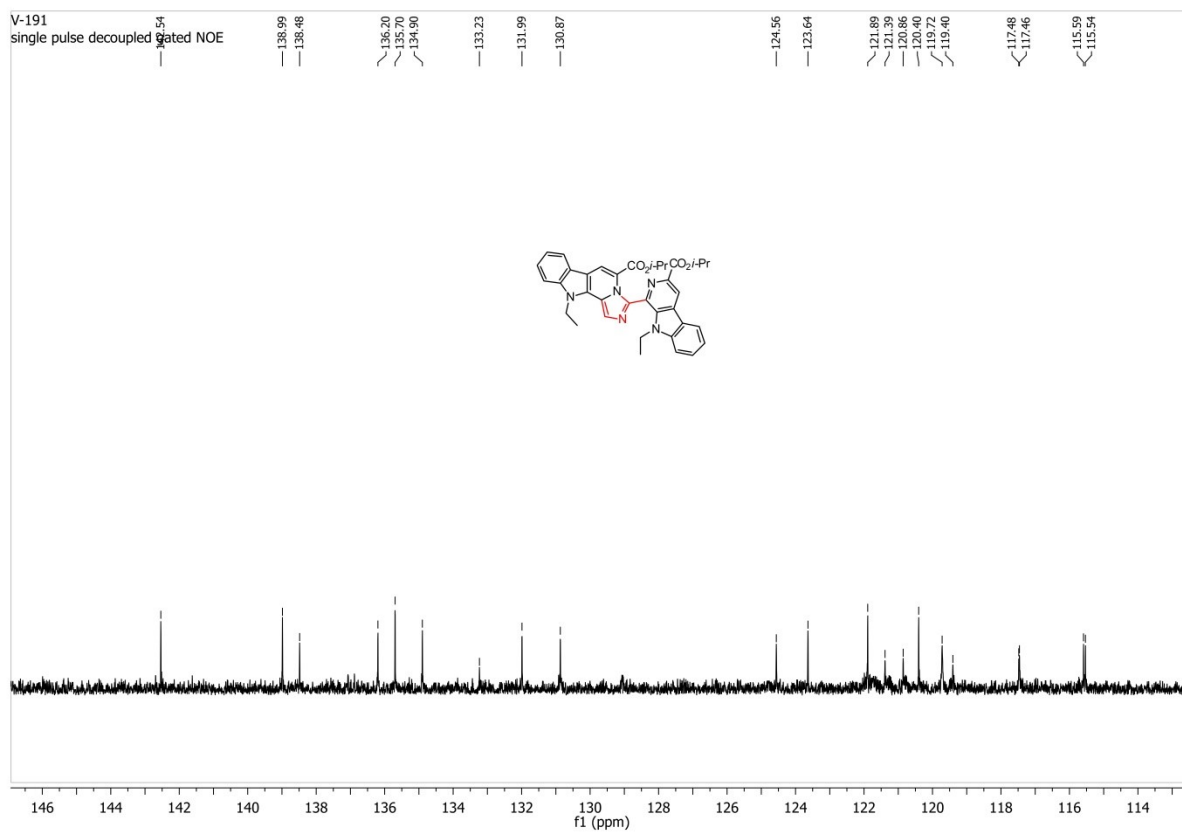


Figure S40. Extended ^{13}C -NMR spectrum of **17B**.

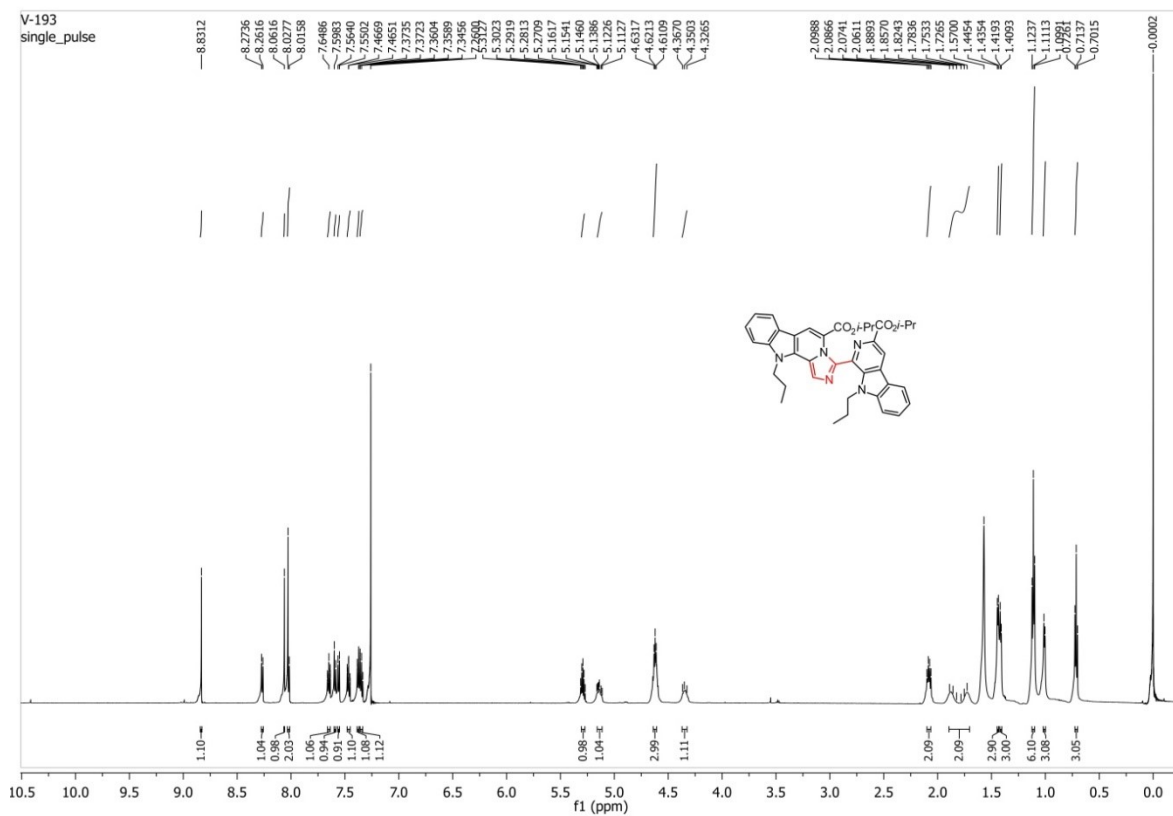


Figure S41. ¹H-NMR spectrum of 17C.

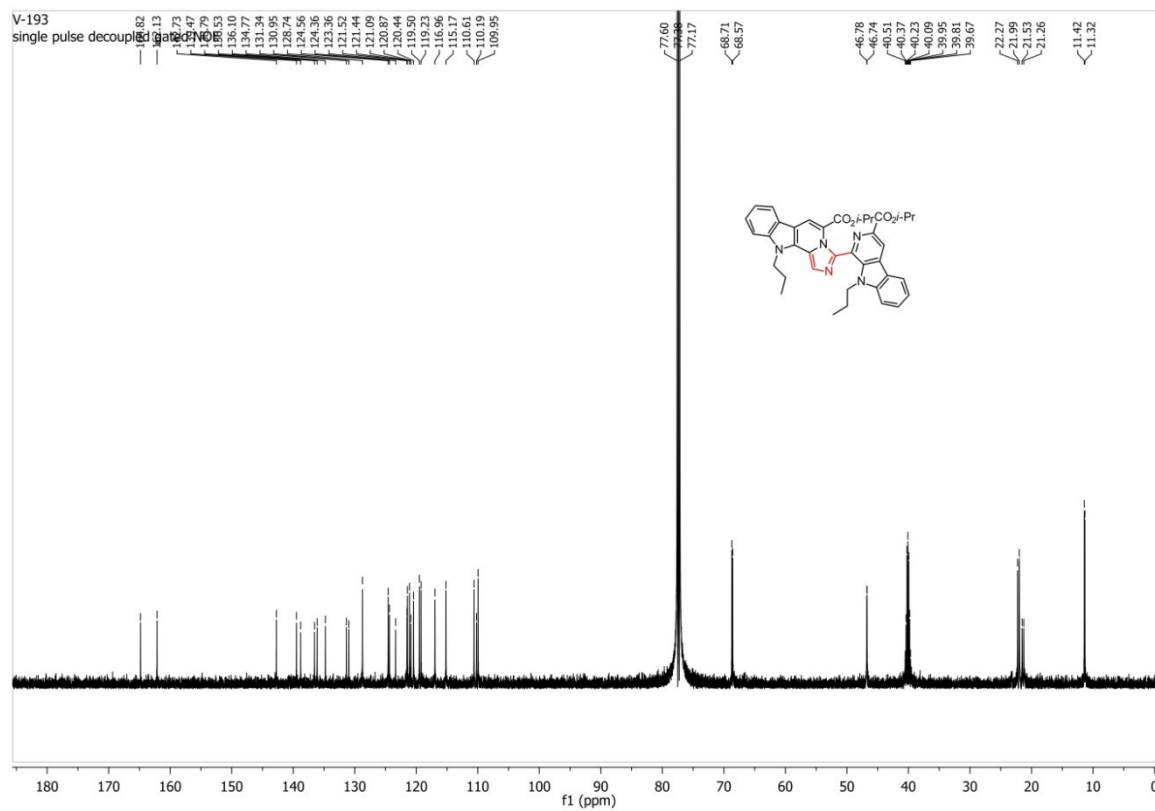


Figure S42. ¹³C-NMR spectrum of 17C.

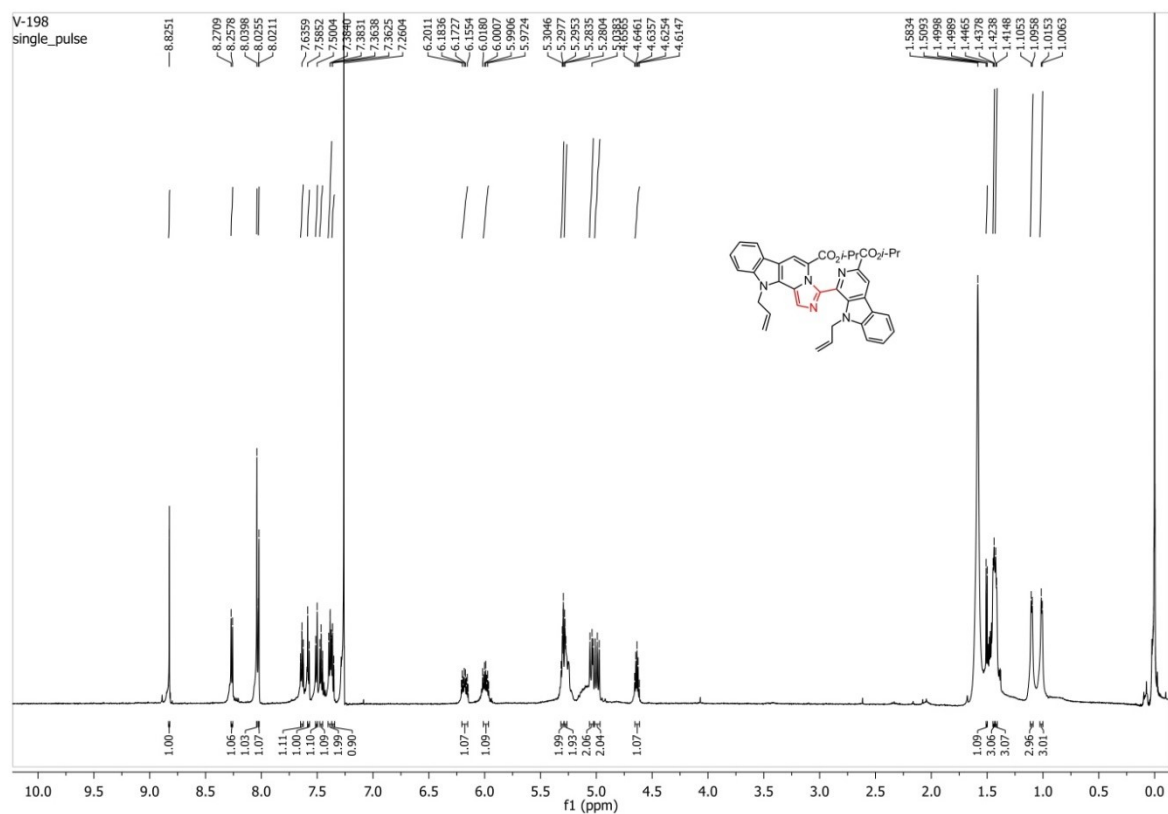


Figure S43. ^1H -NMR spectrum of 17E.

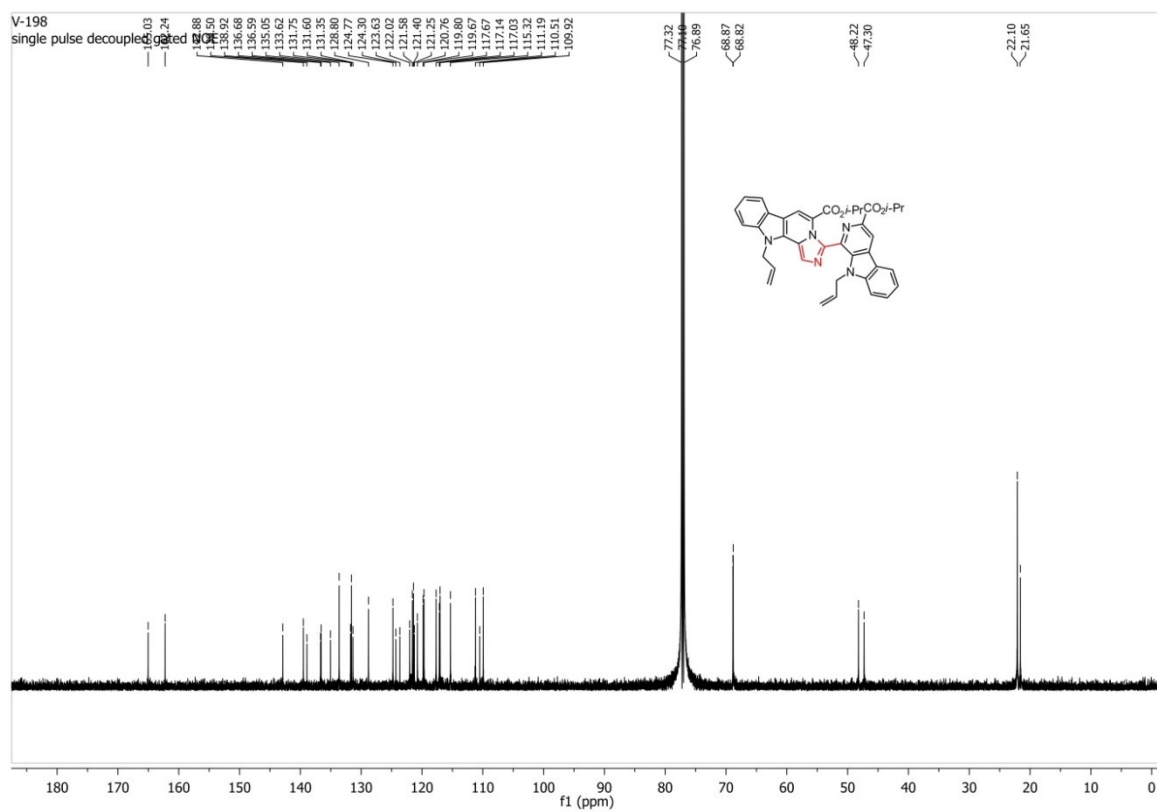


Figure S44. ^{13}C -NMR spectrum of 17E.

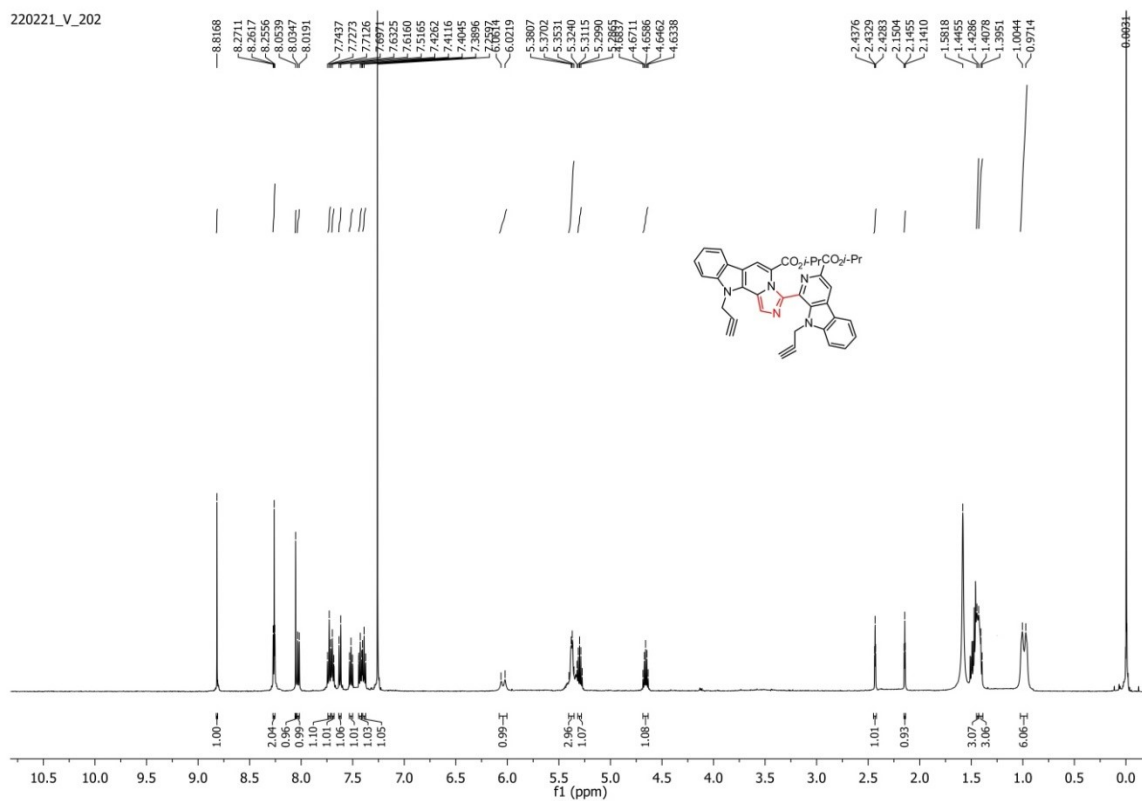


Figure S45. ¹H-NMR spectrum of 17F.

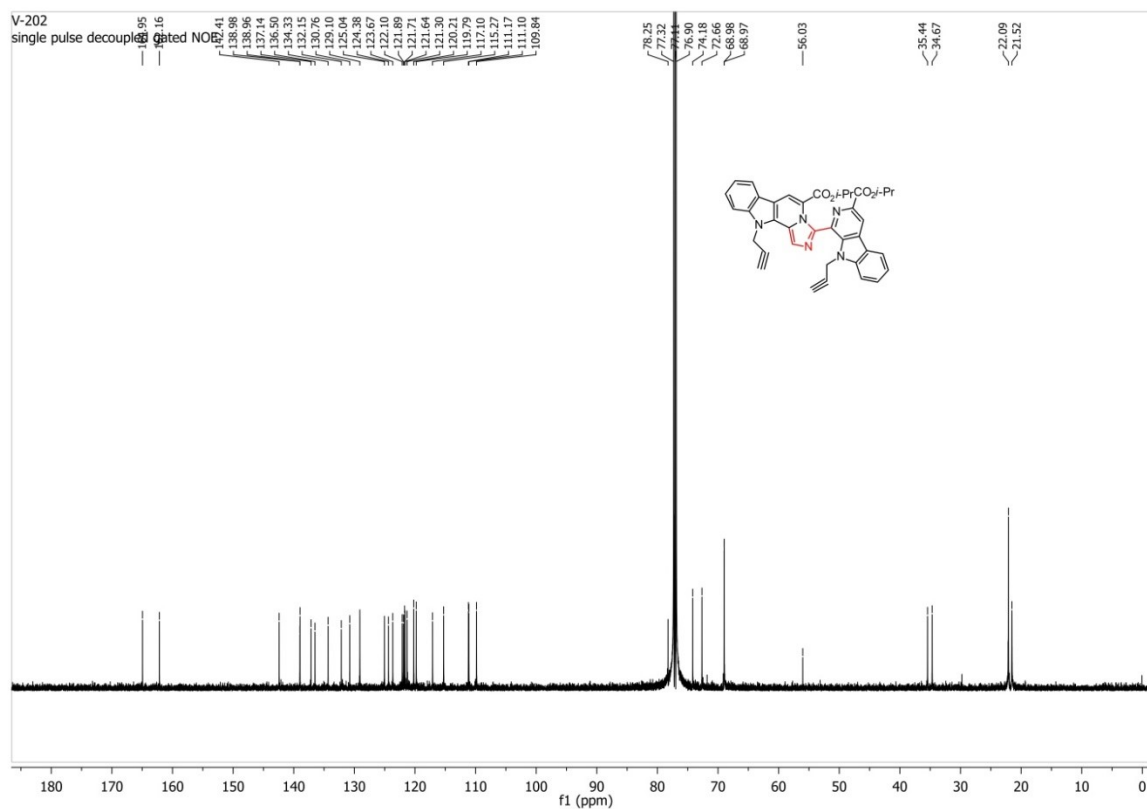
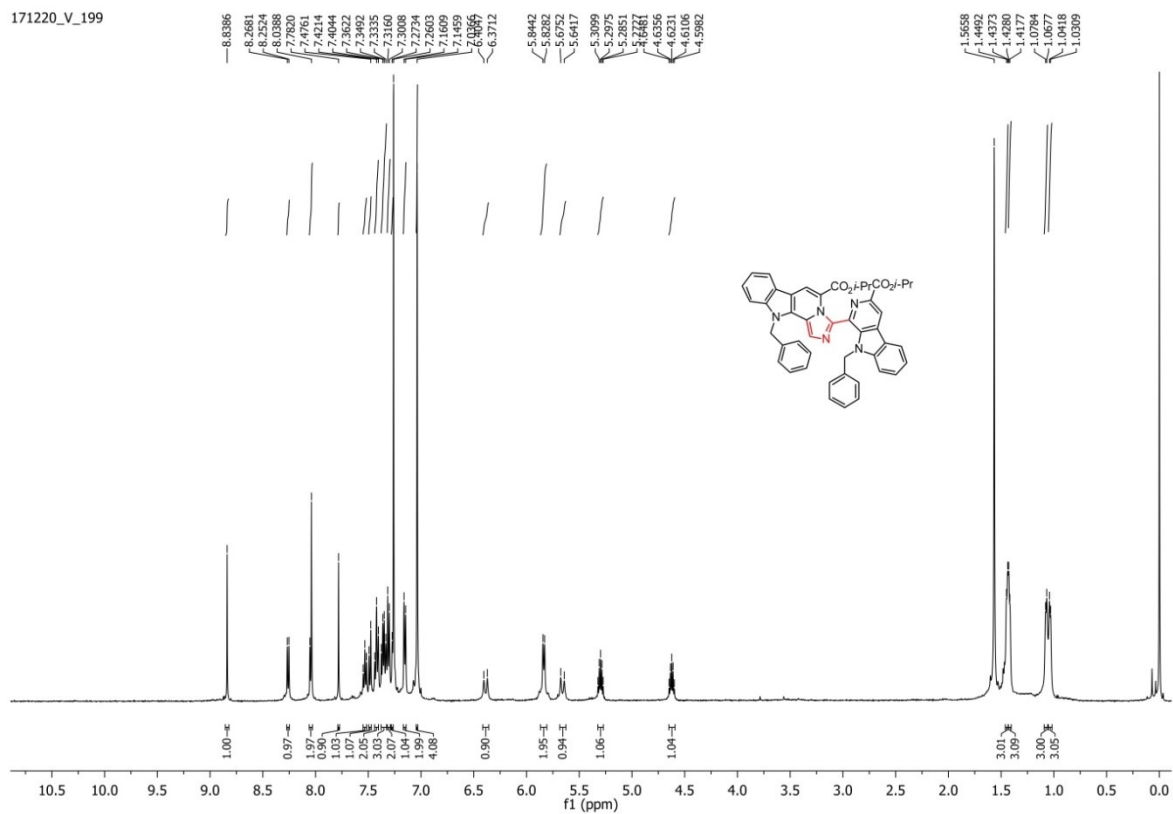
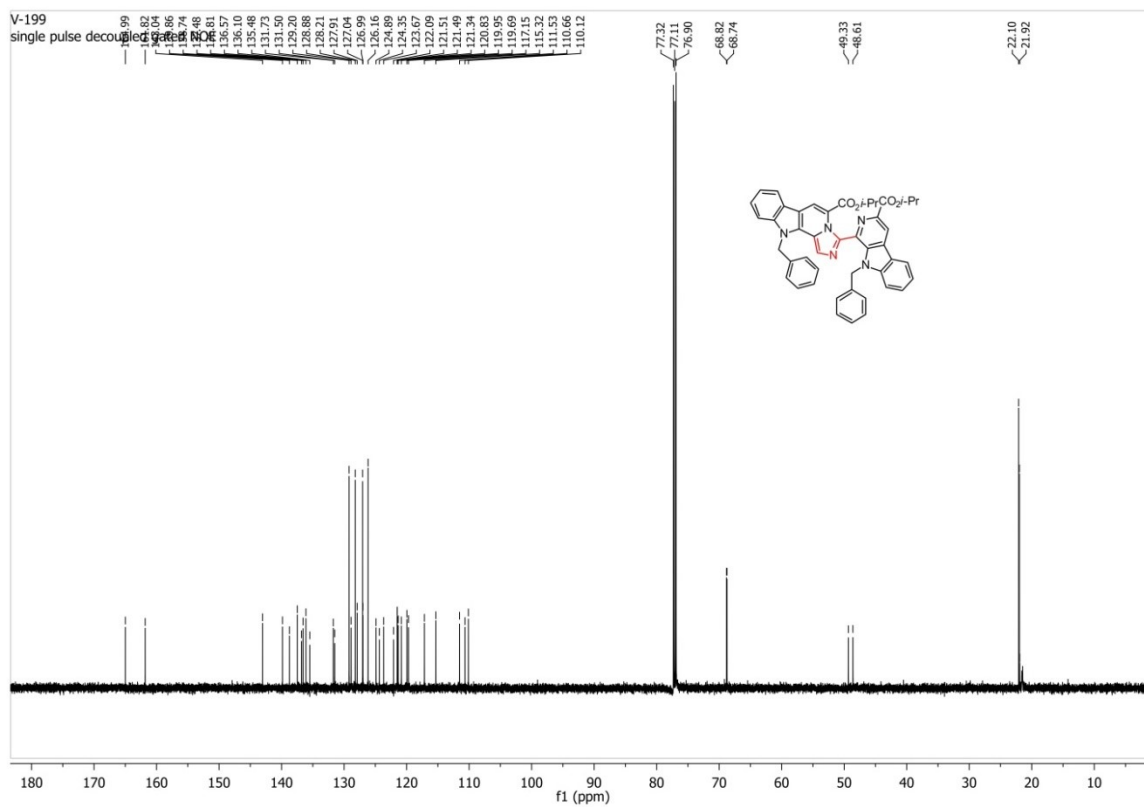


Figure S46. ¹³C-NMR spectrum of 17F.

171220_V_199

Figure S47. ¹H-NMR spectrum of 17G.Figure S48. ¹³C-NMR spectrum of 17G.

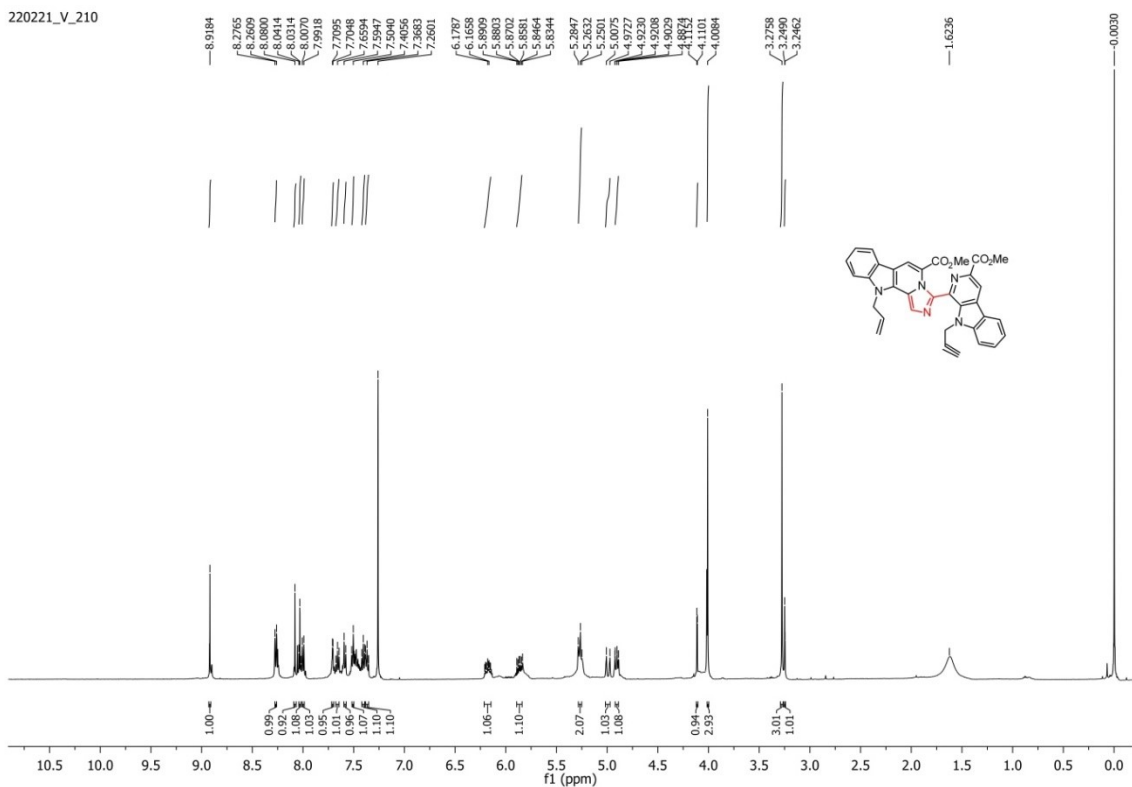


Figure S49. ^1H -NMR spectrum of 18.

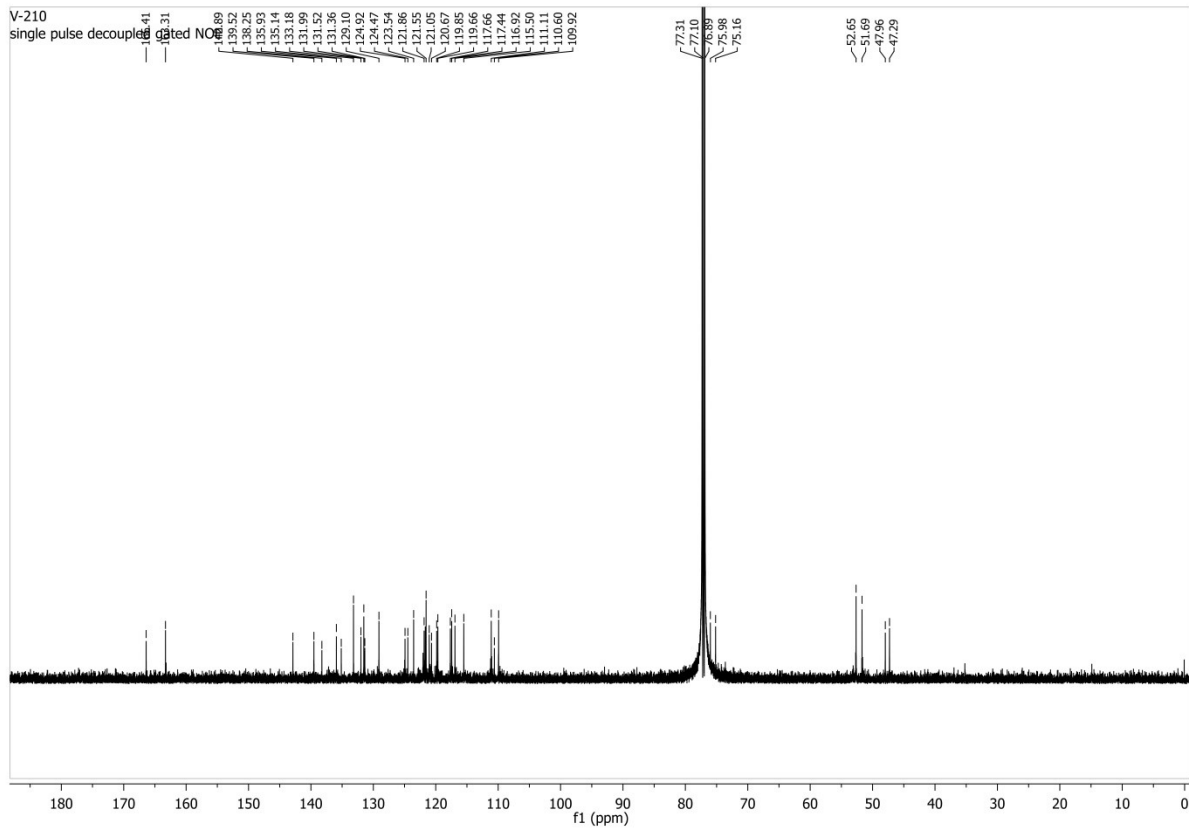


Figure S50. ^{13}C -NMR spectrum of 18.

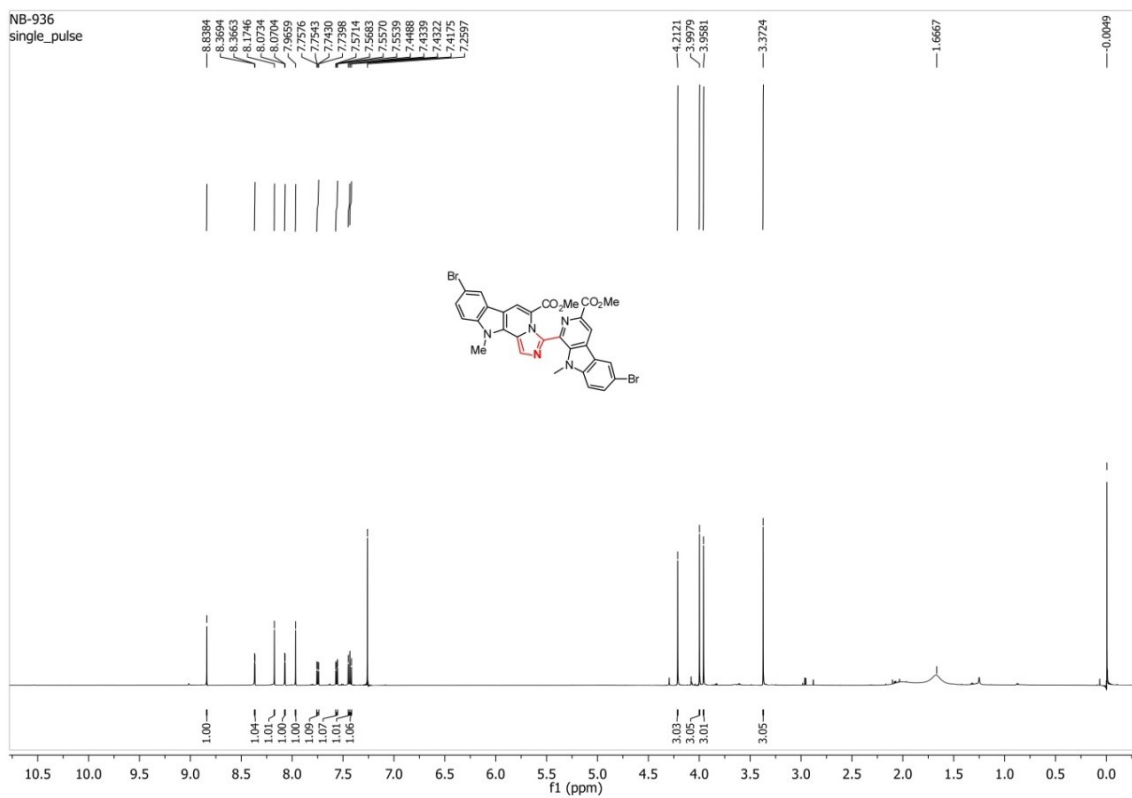


Figure S51. ^1H -NMR spectrum of **19A**.

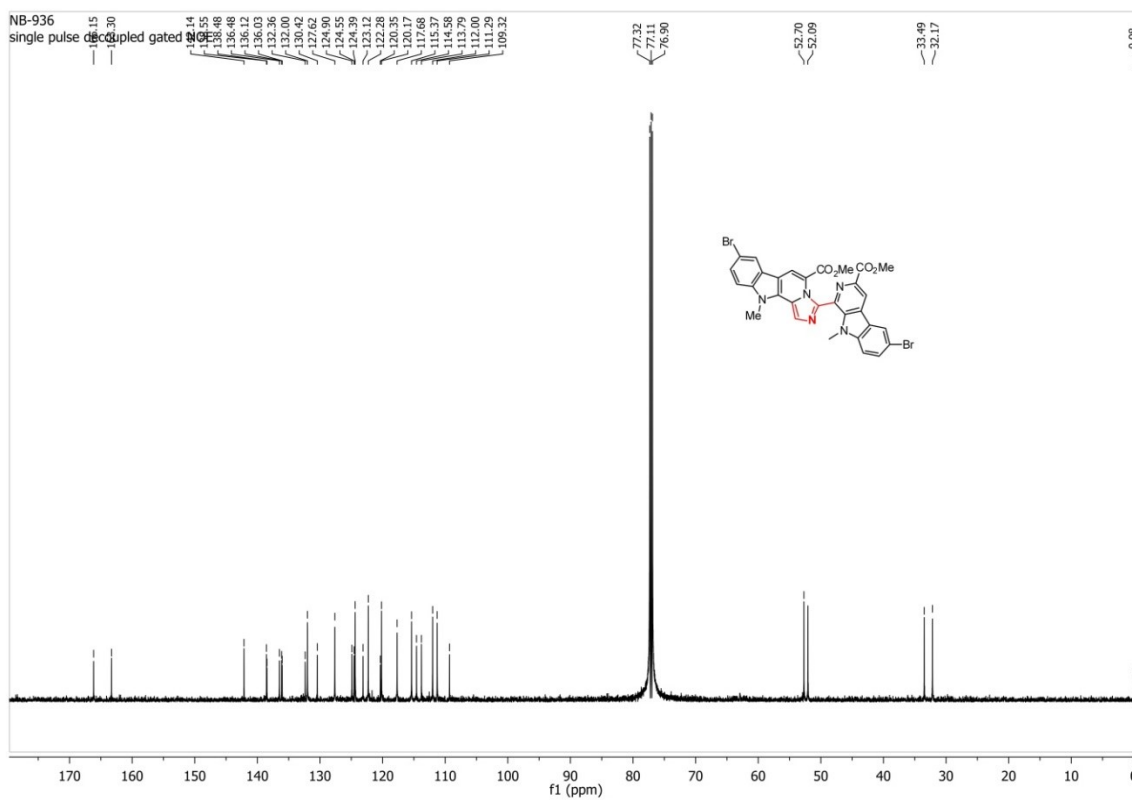


Figure S52. ^{13}C -NMR spectrum of **19A**.

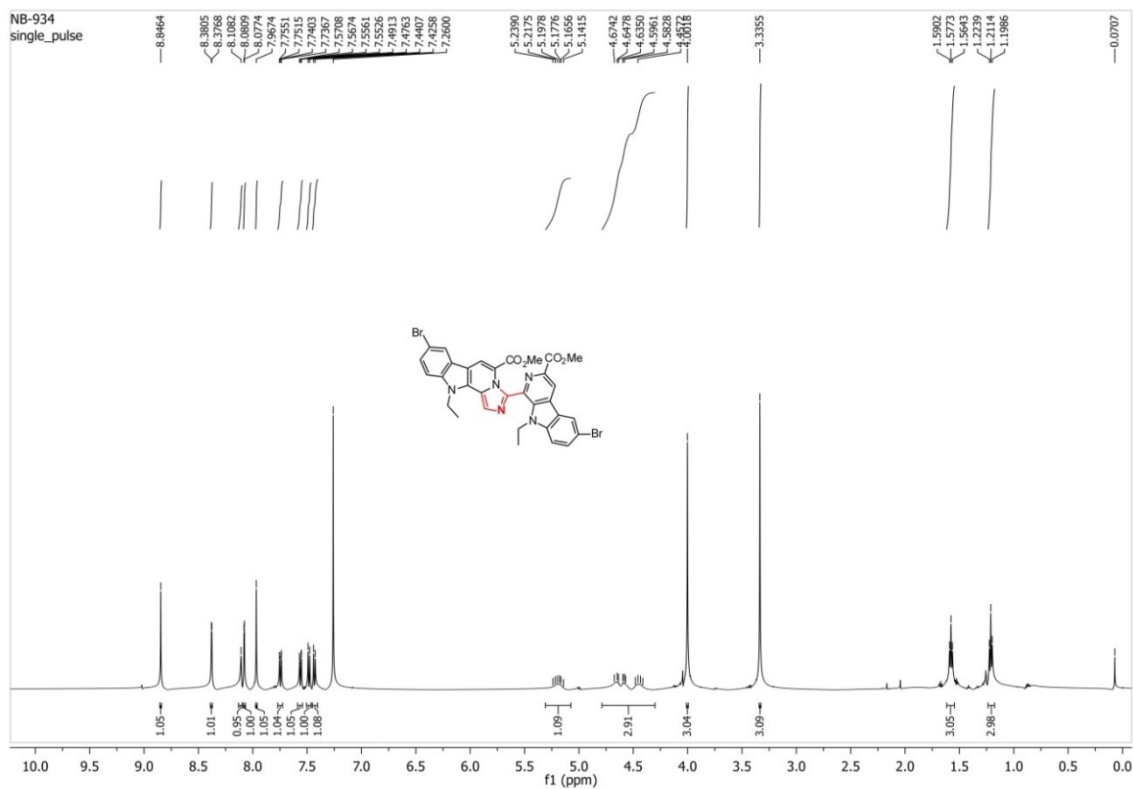


Figure S53. ^1H -NMR spectrum of 19B.

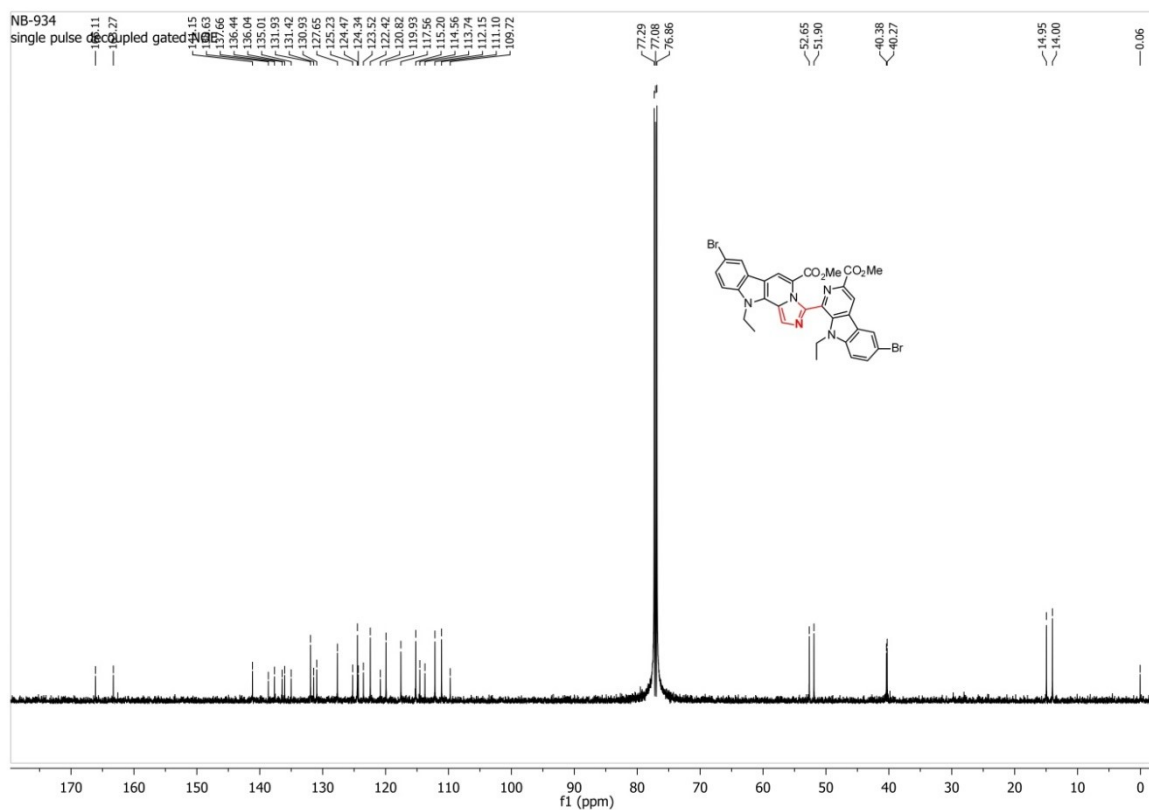


Figure S54. ^{13}C -NMR spectrum of 19B.

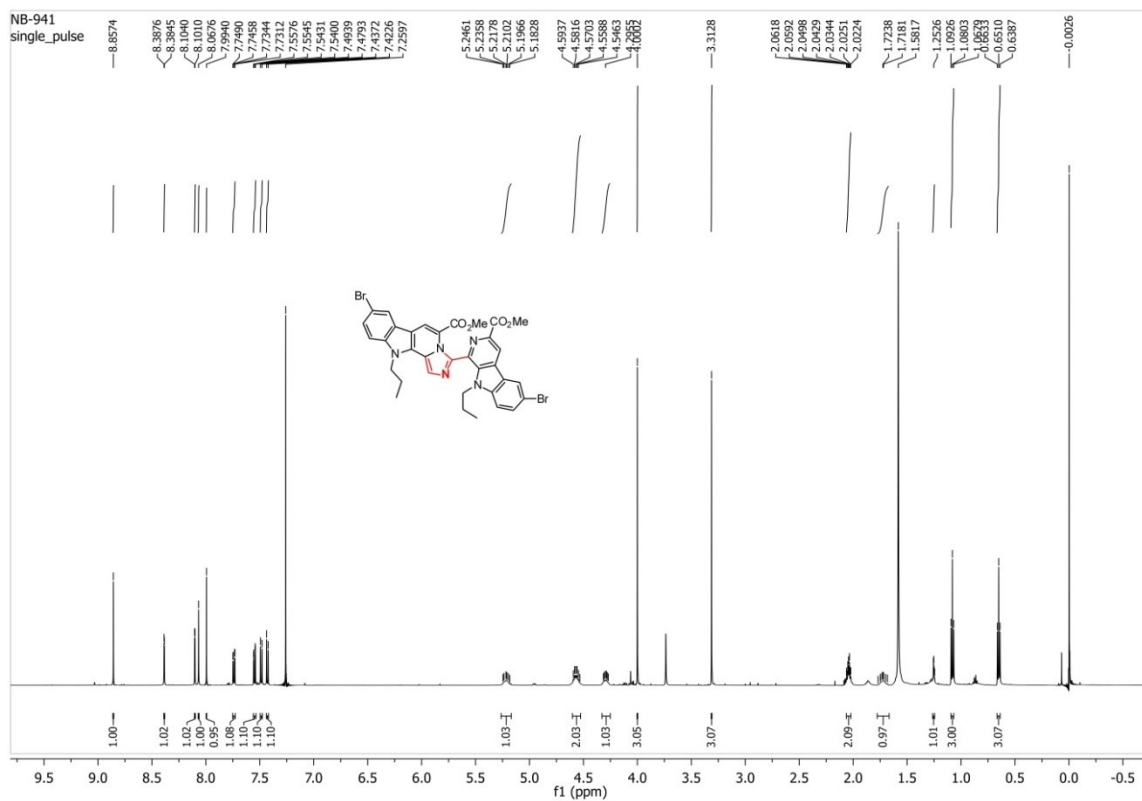


Figure S55. $^1\text{H-NMR}$ spectrum of **19C**.

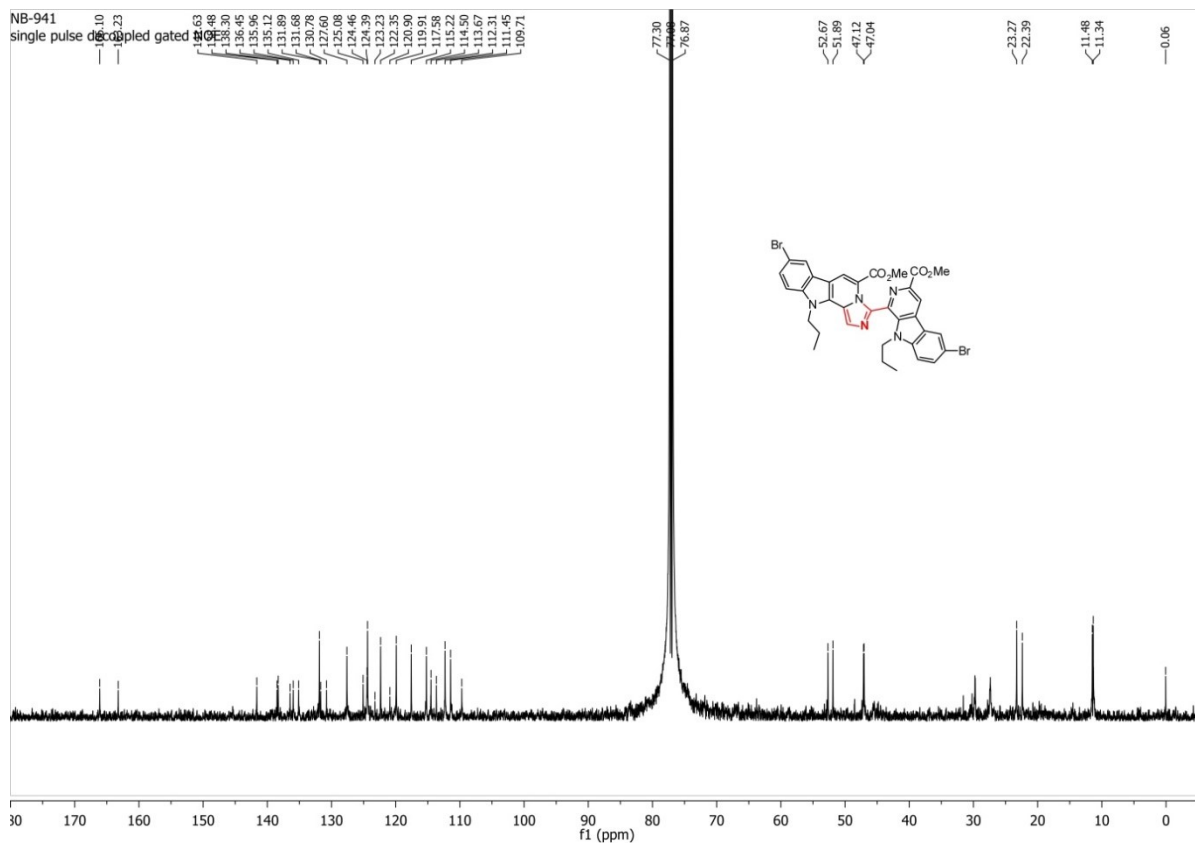


Figure S56. $^{13}\text{C-NMR}$ spectrum of **19C**.

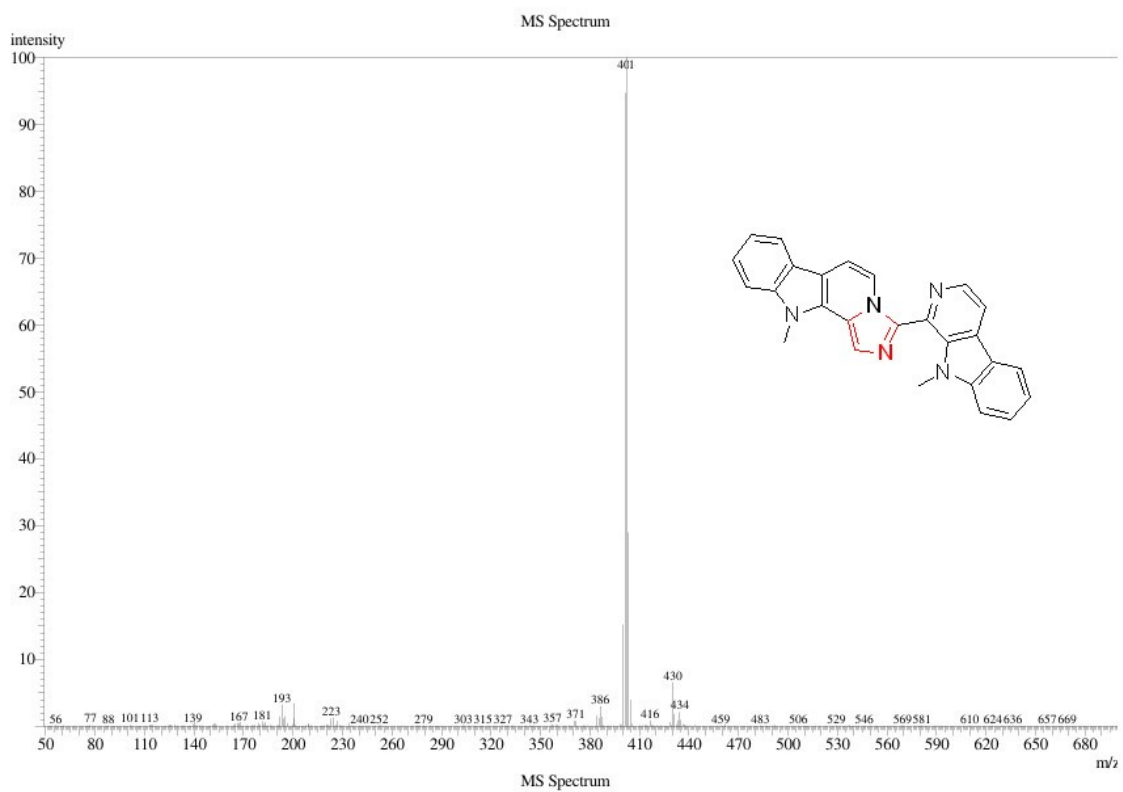


Figure S57. LCMS spectrum of **15A**.

2.0 Photophysical Studies of the Synthesized Compounds:

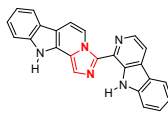
The fluorescent quantum yield (Φ) was measured relative to quinine sulfate ($\Phi = 0.546$) (0.1 M H₂SO₄ at 350 nm excitation) as a reference compound. For the measurement of UV-Vis absorption and fluorescence emission of samples, stock solution (1.0 mM) was prepared in CH₂Cl₂ and diluted to final concentration (5.0 μ M) using CH₂Cl₂. These quantum yields (QY) were calculated by using the equation as follows:

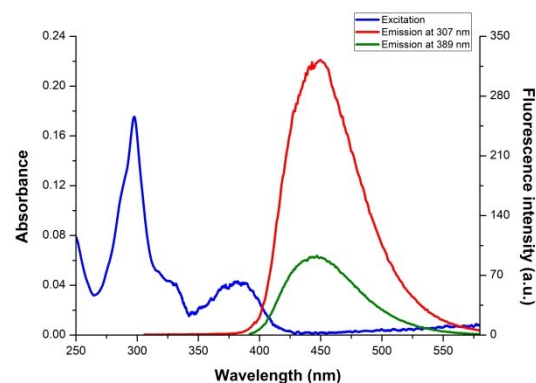
$$\Phi_S = \Phi_R \times \frac{I_S}{I_R} \times \frac{A_R}{A_S} \times \frac{\eta_S^2}{\eta_R^2}$$

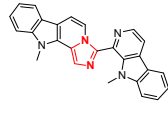
R – Reference; *S* – Sample

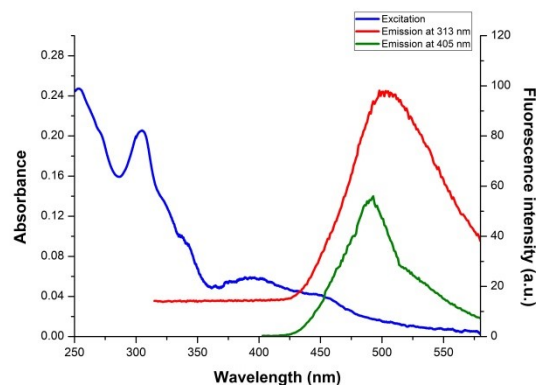
where ϕ is the quantum yields, η is the refractive index of the solvent, I is the integrated fluorescence intensity and A is the absorbance.

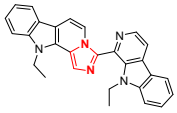
Figure S58. Photophysical properties and graphical data of bis-carboline derivatives:

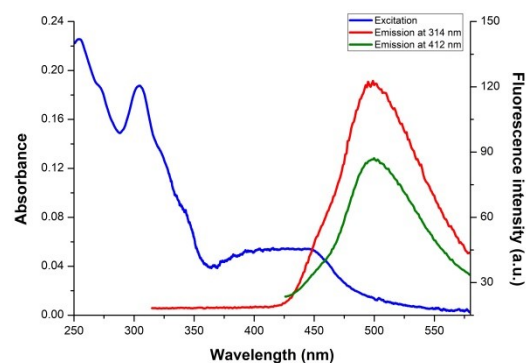
<div style="text-align: center;">14</div> 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	297.26	449.12	323.27		0.34
	379.65	446.72	92.49		0.39

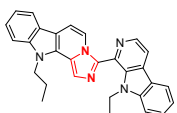


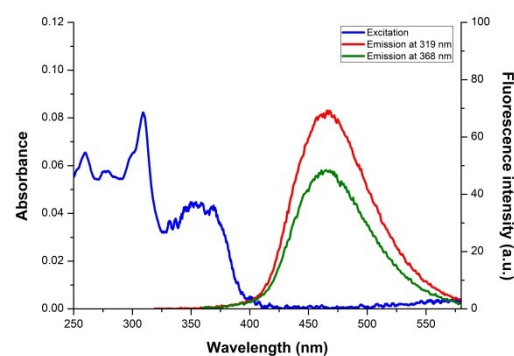
<div style="text-align: center;">15A</div> 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	303.34	497.87	98.09		0.14
	395.16	496.96	50.74		0.15

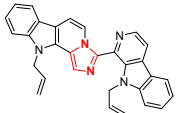


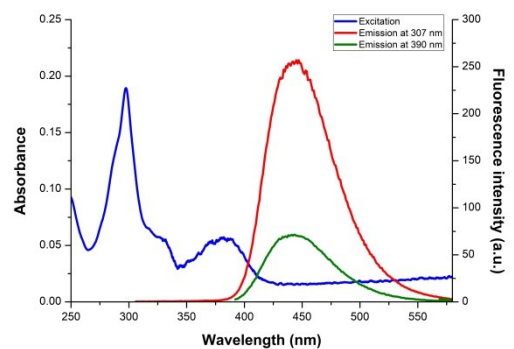
15B 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	304.14	498.93	122.71	0.19	
	402.86	499.84	87.19	0.41	

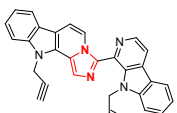


15C 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	309.26	468.10	69.14	0.17	
	358.21	465.35	48.41	0.21	



15E 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	297.89	446.83	257.57	0.24	
	380.60	442.90	71.50	0.23	



15F 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	300.78	451.43	109.31	0.10	

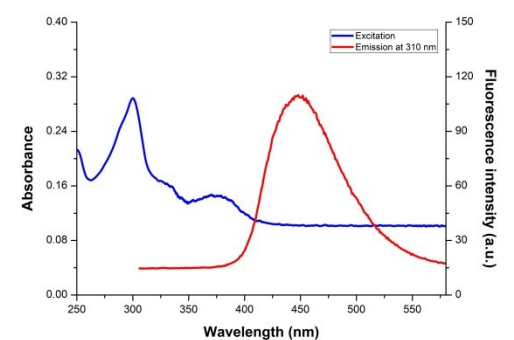
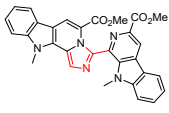
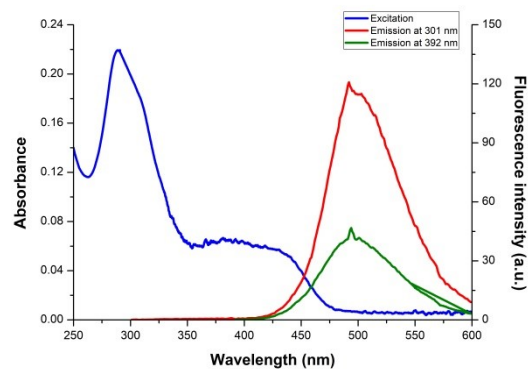
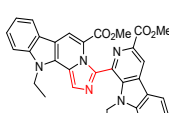


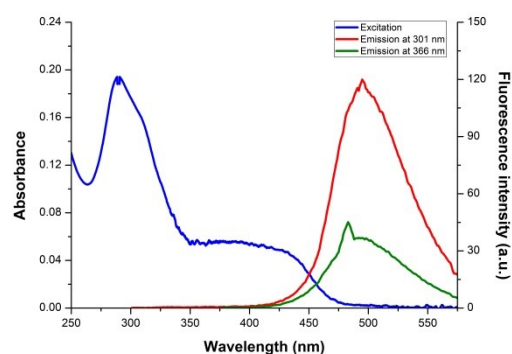
Figure S59. Photophysical properties and graphical data of

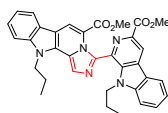
bis-carboline derivatives:

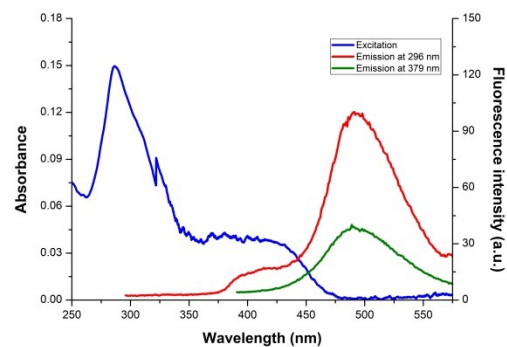
16A 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)	(nm)	(nm)	
	291	492.90	120.75	0.10	
	381	493.93	46.69	0.13	

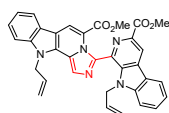


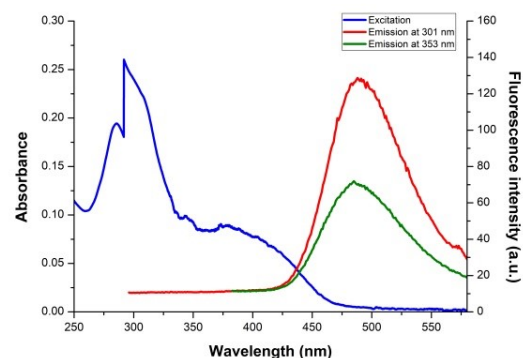
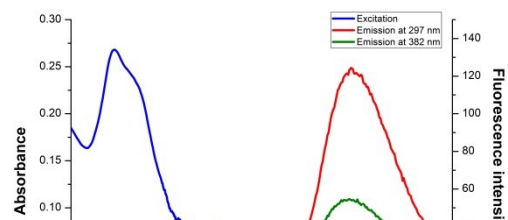
16B 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)	(nm)	(nm)	
	290.70	494.84	119.93	0.11	
	356.30	482.98	45.09	0.13	

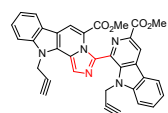


16C 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)	(nm)	(nm)	
	286.22	491.06	100.24	0.15	
	369.41	488.95	40.07	0.20	

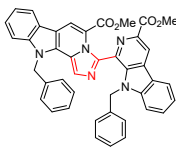


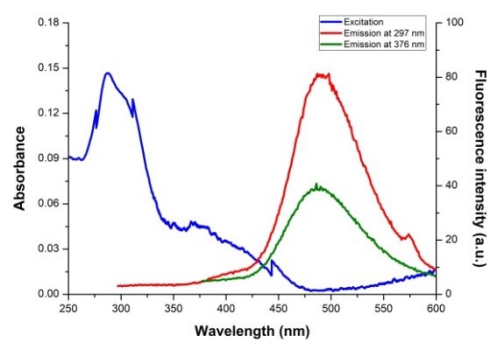
16E 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)	(nm)	(nm)	
	286.97	492.20	124.36	0.10	
	372.43	490.90	54.35	0.18	

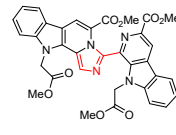


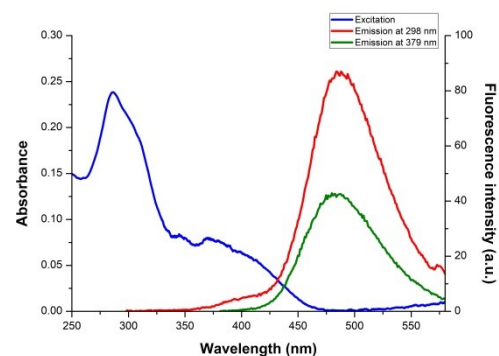
16F 	UV-Vis	Fluorescence	Φ_F
			35

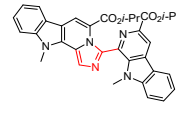
	λ_{Ex} (nm)	λ_{Em} (nm)	Intensity	
	291.52	488	128.72	0.12
	343.32	484.92	71.93	0.18

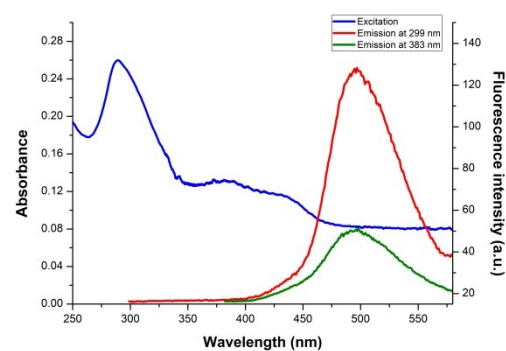
16G 	UV-Vis		Fluorescence		Φ_{F}
	λ_{Ex} (nm)	λ_{Em} (nm)	Intensity		
	287.02	497.87	81.30		
366.80	485.97	40.79		0.21	

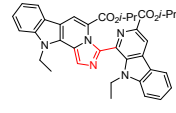


16H 	UV-Vis		Fluorescence		Φ_{F}
	λ_{Ex} (nm)	λ_{Em} (nm)	Intensity		
	287.82	487.47	86.75		
369.41	479.73	42.82		0.11	

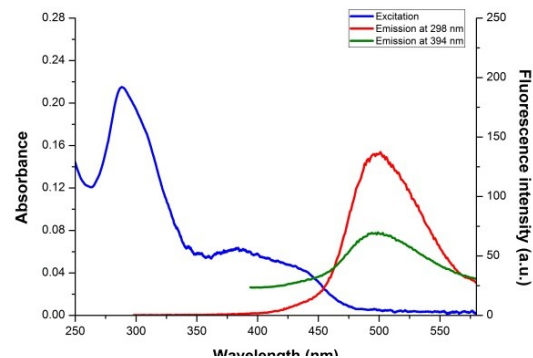


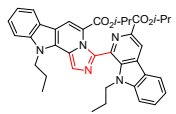
17A 	UV-Vis		Fluorescence		Φ_{F}
	λ_{Ex} (nm)	λ_{Em} (nm)	Intensity		
	289.29	496.96	128.24		
373.14	498.03	51.13		0.12	

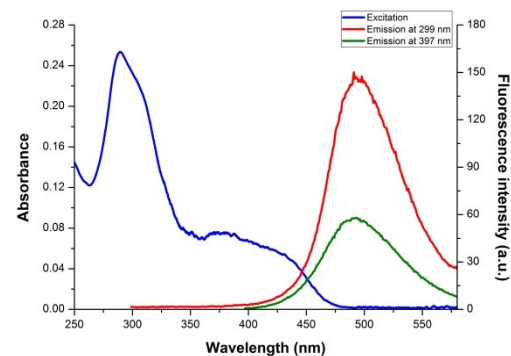


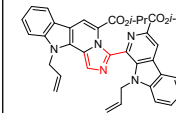
17B 	UV-Vis		Fluorescence		Φ_{F}
	λ_{Ex} (nm)	λ_{Em} (nm)	Intensity		
	288.78	499.04	139.35		

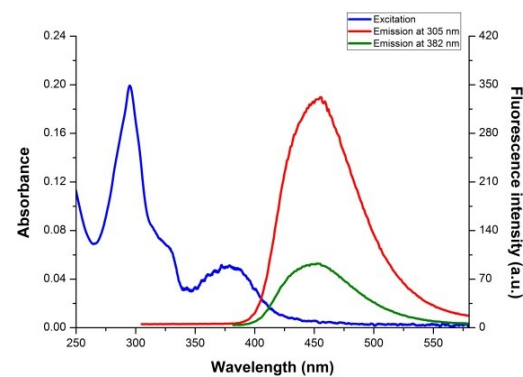
	381.40	493.93	69.50	0.34
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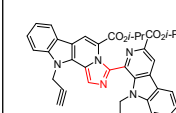


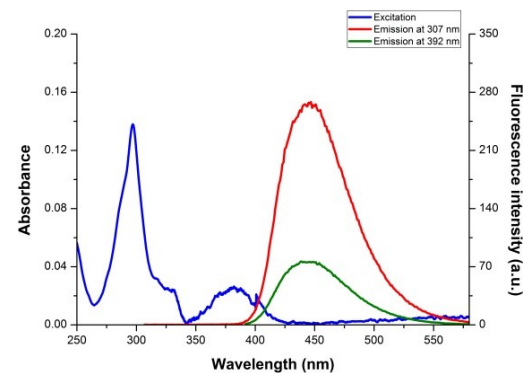
17C 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	289.58	490.90	150.07	0.12	
	388.29	493.03	57.97	0.16	



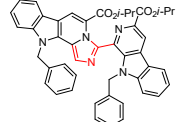
17E 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	295.40	456.16	331.07	0.34	
	379.29	454.02	92.42	0.37	



17F 	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			
	297.27	446.08	267.59	0.35	
	381.41	438.10	76.26	0.55	



17G	UV-Vis		Fluorescence		Φ_F
	λ_{Ex}	λ_{Em}	Intensity		
	(nm)	(nm)			

	295.66	448.19	106.47	0.21
	372.76	453.03	40.01	0.275

