Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Transition Metal-Free Approach Towards Synthesis of β-Carboline Tethered 1,3,4-Oxadiazoles via Oxidative C-O Bond Formation

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Supporting Information

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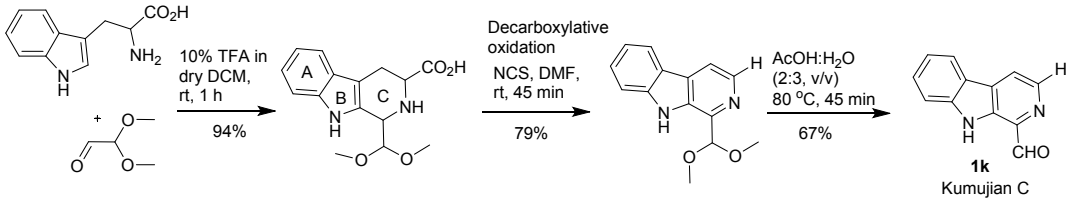
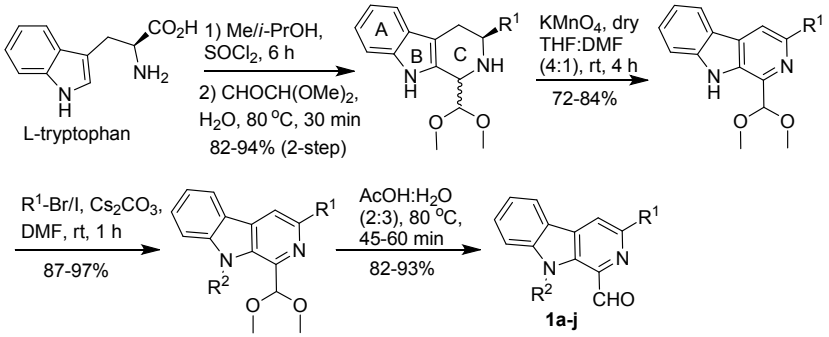
1. Synthesis of Kumujian C and its derivatives



Scheme S1. Synthesis of Kumujian C[24]

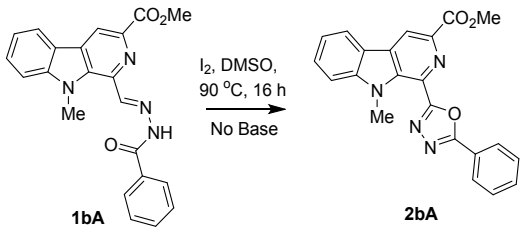


	R^2	R^1
1a	H	CO_2Me
1b	Me	CO_2Me
1c	Et	CO_2Me
1d	*n*-Pr	CO_2Me
1e	allyl	CO_2Me
1f	propargyl	CO_2Me
1g	Bn	CO_2Me
1h	2-NO_2Bn	CO_2Me
1i	H	CO_2*i*Pr
1j	Me	CO_2*i*Pr

Scheme S2. Synthesis of 1-formyl-9*H*-pyrido[3,4-*b*]indole derivatives[24]

pH study during the course of oxidative C-O bond formation : To probe the reaction mechanism and get evidence about the generation of HI acid during the course of reaction, the pH study of reaction medium was conducted in the absence of base. It was observed that at the start of reaction, the pH of medium was 10.03 after addition of benzohydrazone **1bA**. After addition of iodine to reaction medium reduced the pH in acidic range (4.98) giving an inference of generation of HI. The continuous decrease in the pH of medium with the progress of reaction confirmed the generation of HI. It was found that after completion of reaction under base free conditions, the pH of reaction medium was 2.61. The pH for entries 4-7 were measured after cooling the reaction mixture to room temperature.

Table S1. pH study during the course of oxidative C-O bond formation



Entry	Conditions	Time (min.)	pH of reaction medium
1	Anhydrous DMSO, rt	00:00	9.84
2	Addition of **1bA** in DMSO, rt	00:01	10.03
3	Addition of iodine (1.5 equiv.) to **1bA** in DMSO, rt	00:02	4.98
4	After 3 h at 90 ^{o}C (15-20% conversion into **2bA**)	03:00	4.18
5	After 9 h at 90 ^{o}C (40-45% conversion into **2bA**)	09:00	3.14
6	After 16 h at 90 ^{o}C (95-98% conversion into **2bA**)	16:00	2.61
7	After 16 h at 90 ^{o}C (95-98% conversion into **2bA**) then 3 equiv. of Cs_2CO_3 was added to reaction mixture	16.05	8.68

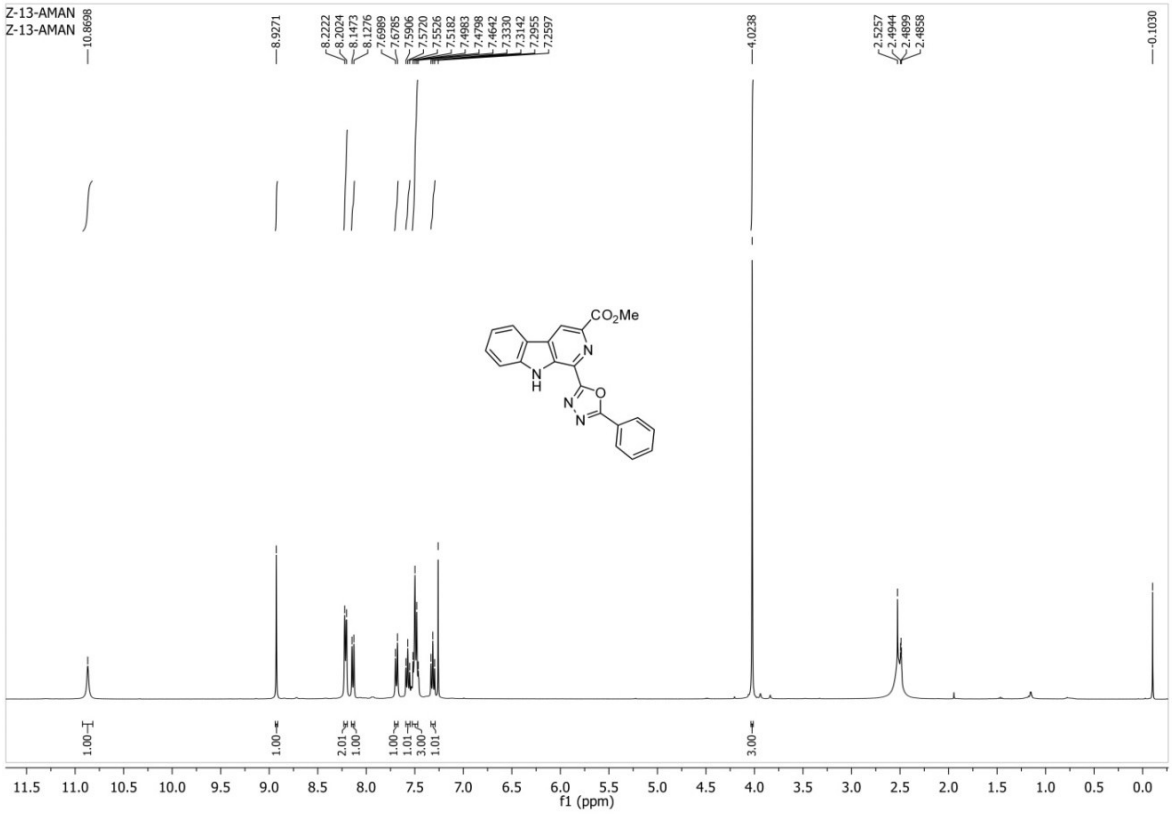


Figure S1. ^{1}H-NMR spectrum of **2aA**.

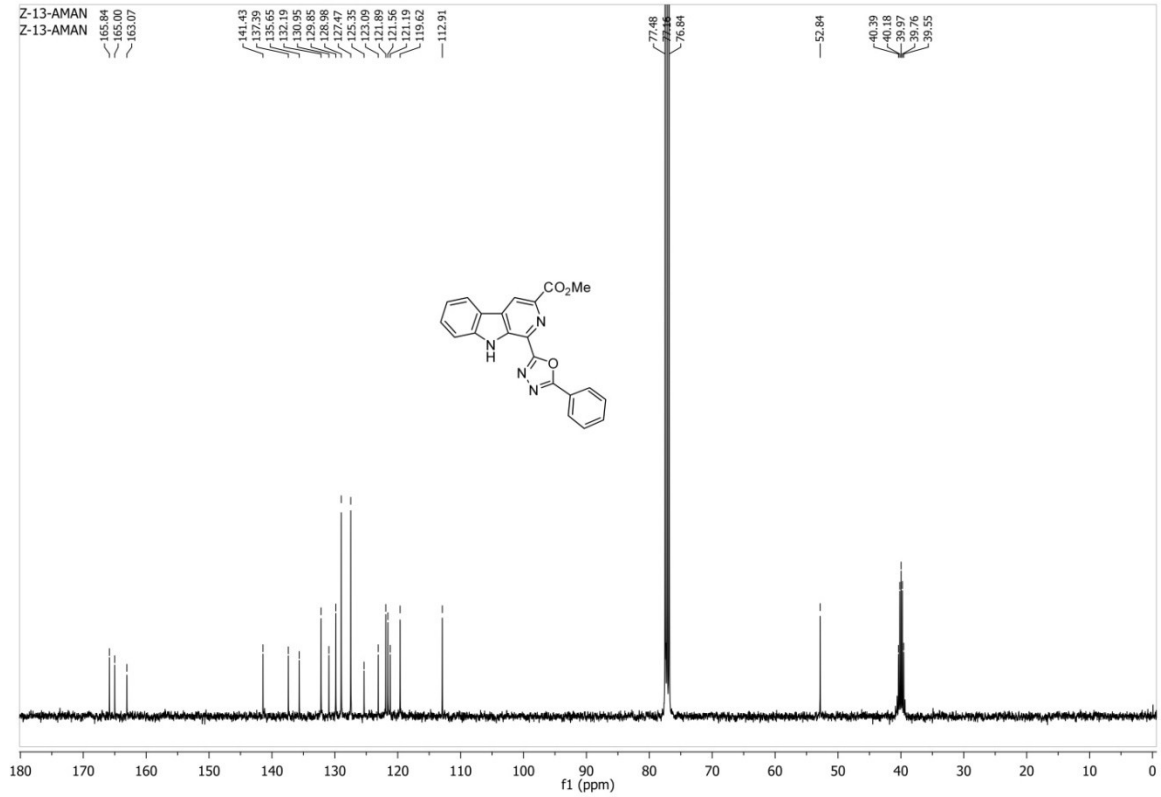


Figure S2. ^{13}C-NMR spectrum of **2aA**.

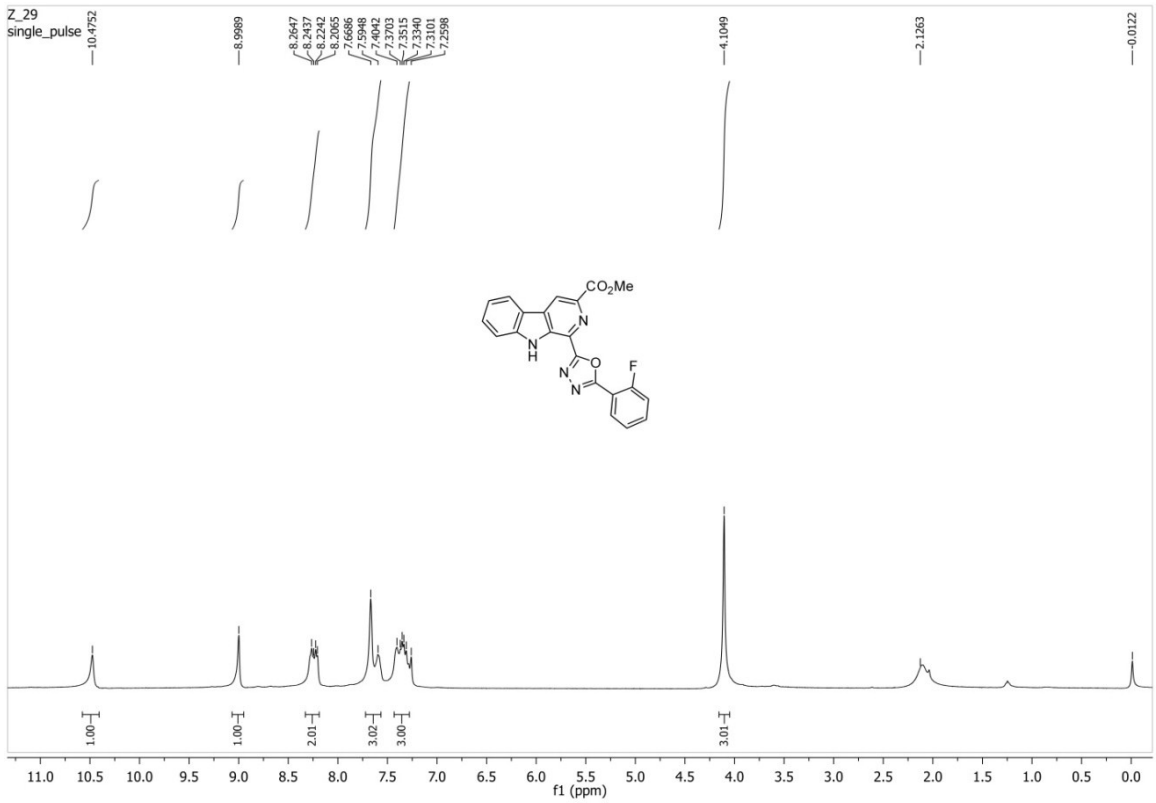


Figure S3. ^{1}H-NMR spectrum of **2aB**.

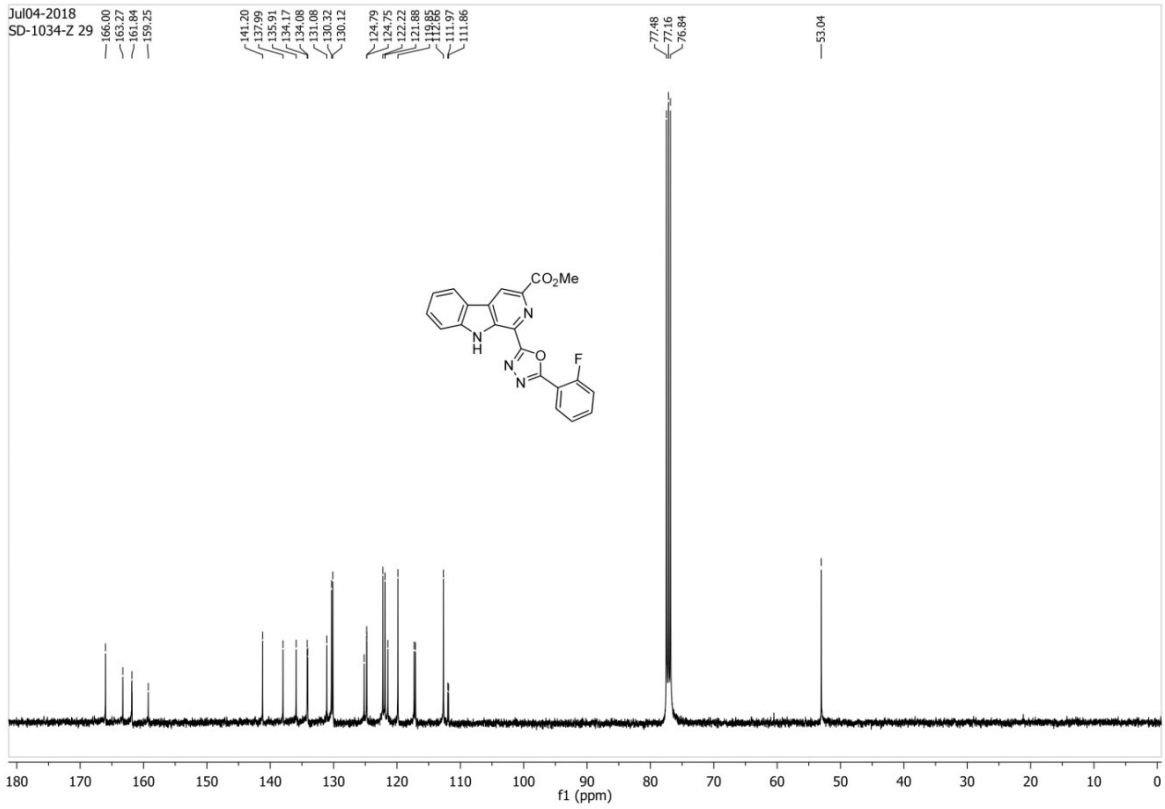


Figure S4. ^{13}C-NMR spectrum of **2aB**.

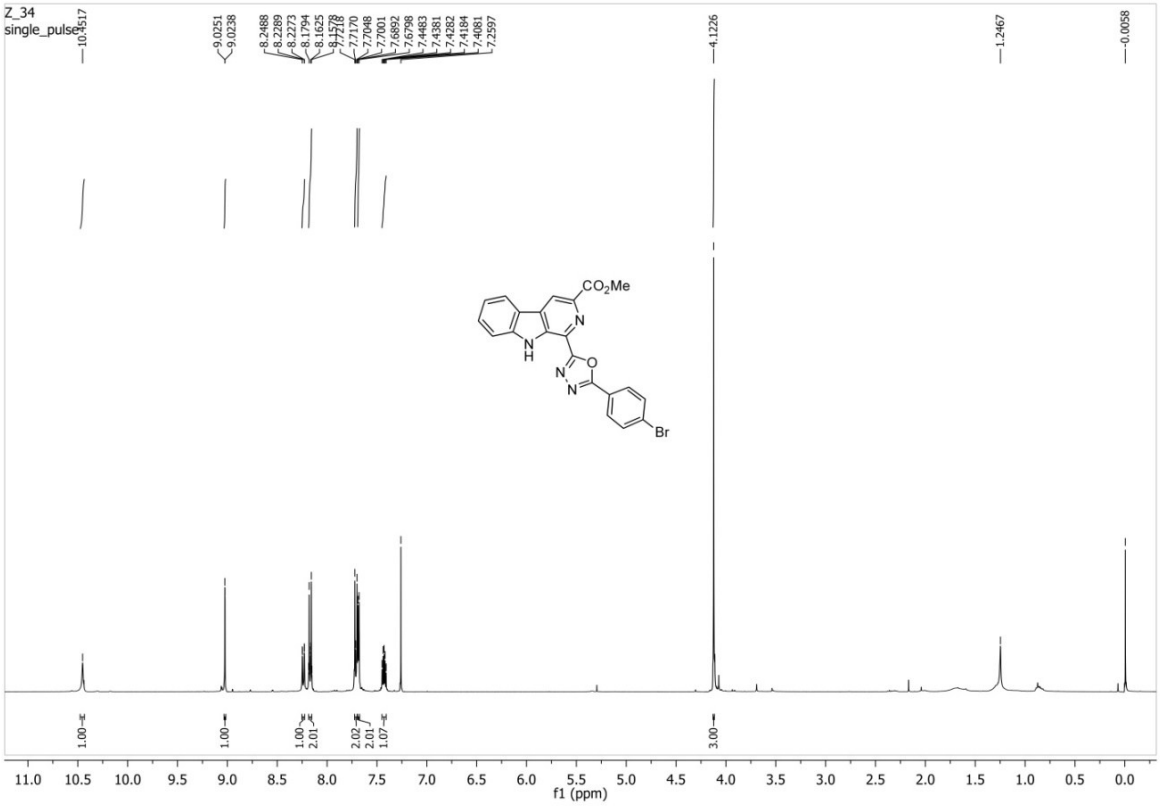


Figure S5.[1]H-NMR spectrum of **2aC**.

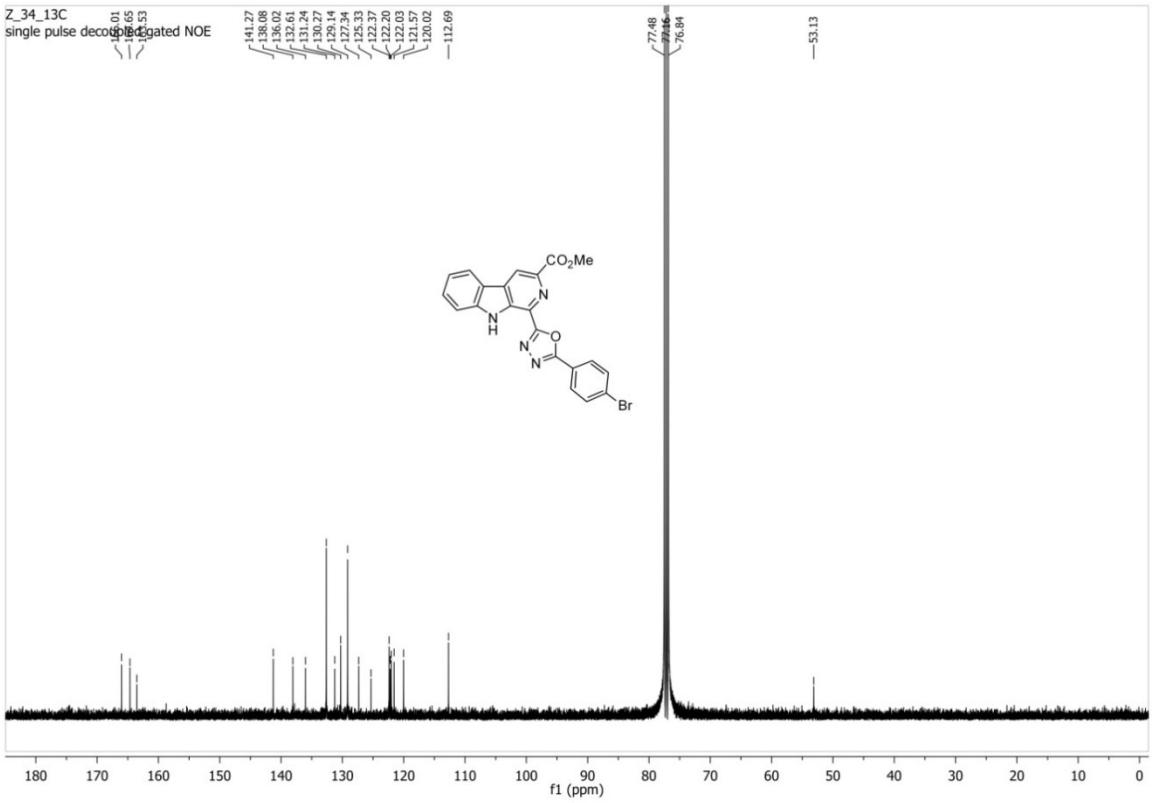


Figure S6. [13]C-NMR spectrum of **2aC**.

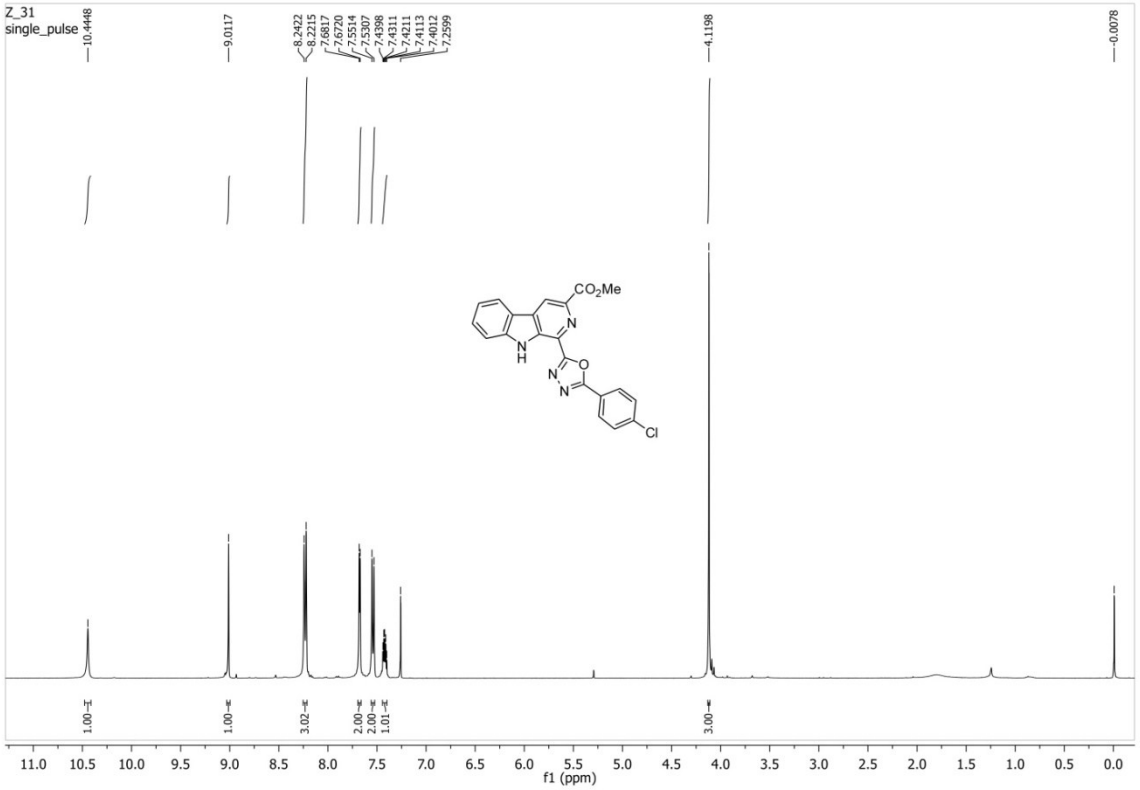


Figure S7. ^{1}H-NMR spectrum of **2aD**.

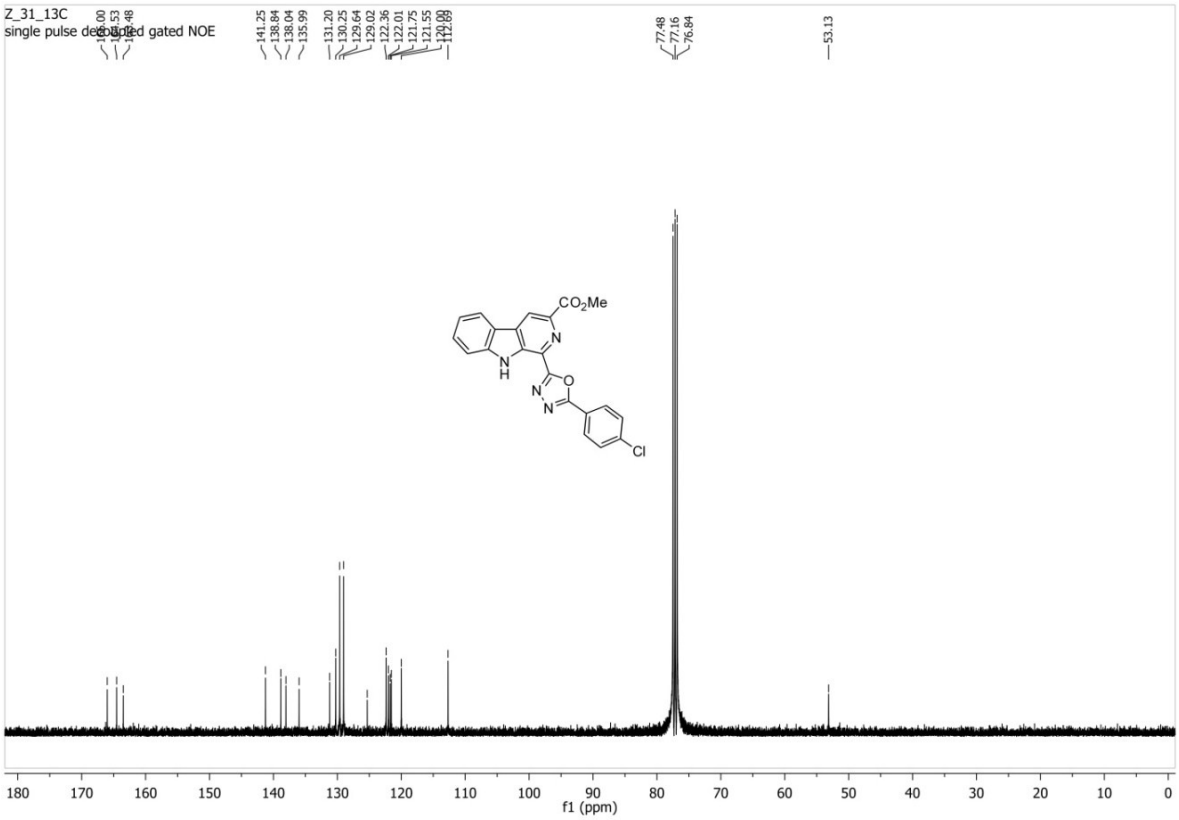


Figure S8. ^{13}C-NMR spectrum of **2aD**.

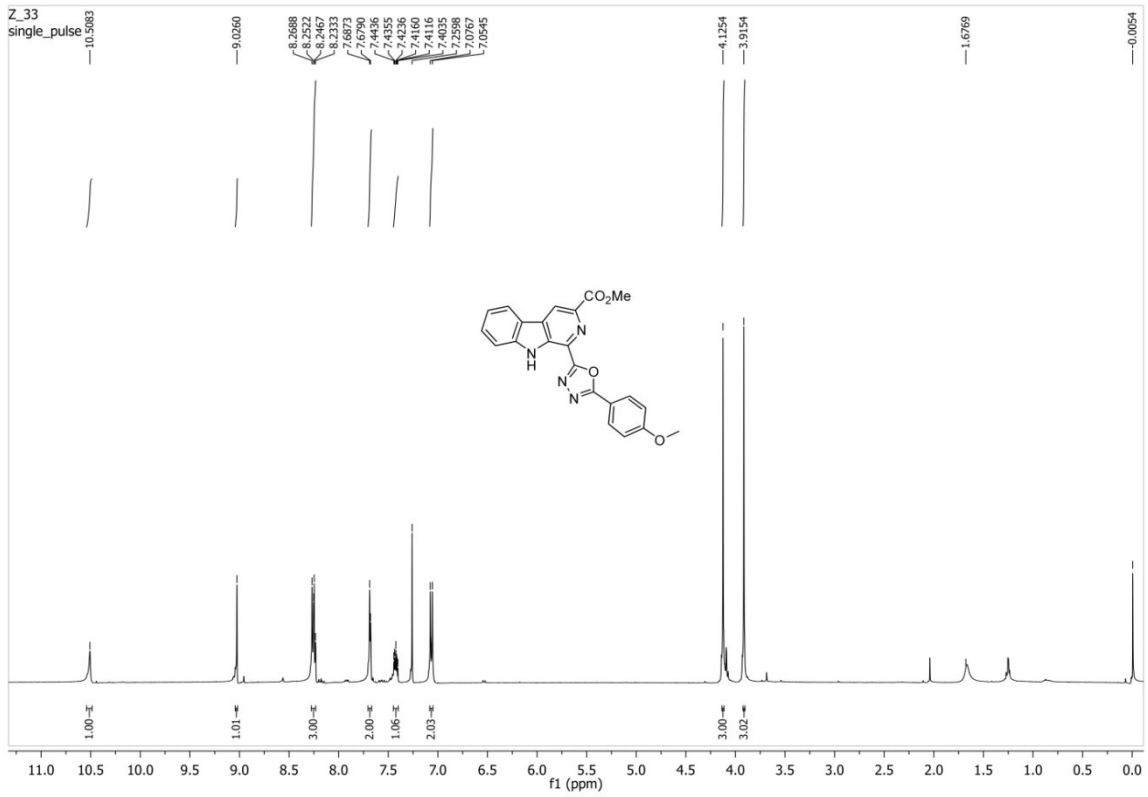


Figure S9. [1]H-NMR spectrum of **2aE**.

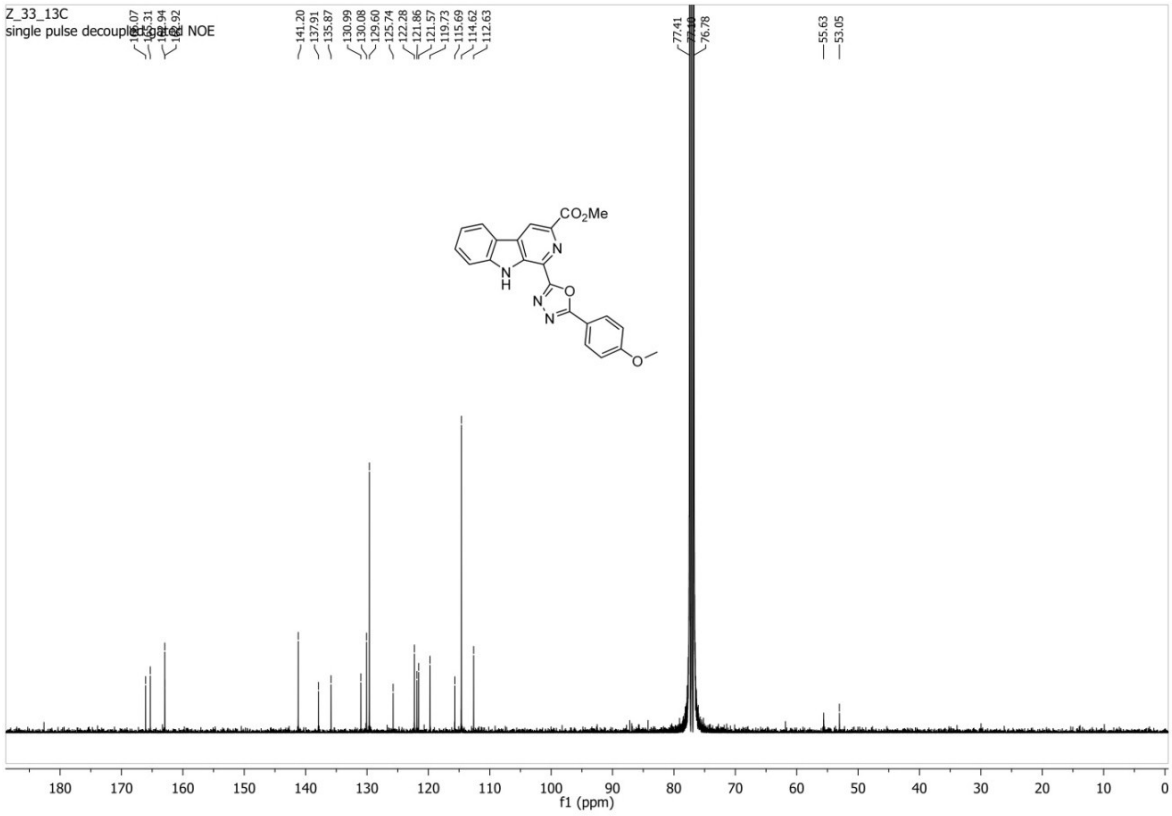


Figure S10. [13]C-NMR spectrum of **2aE**.

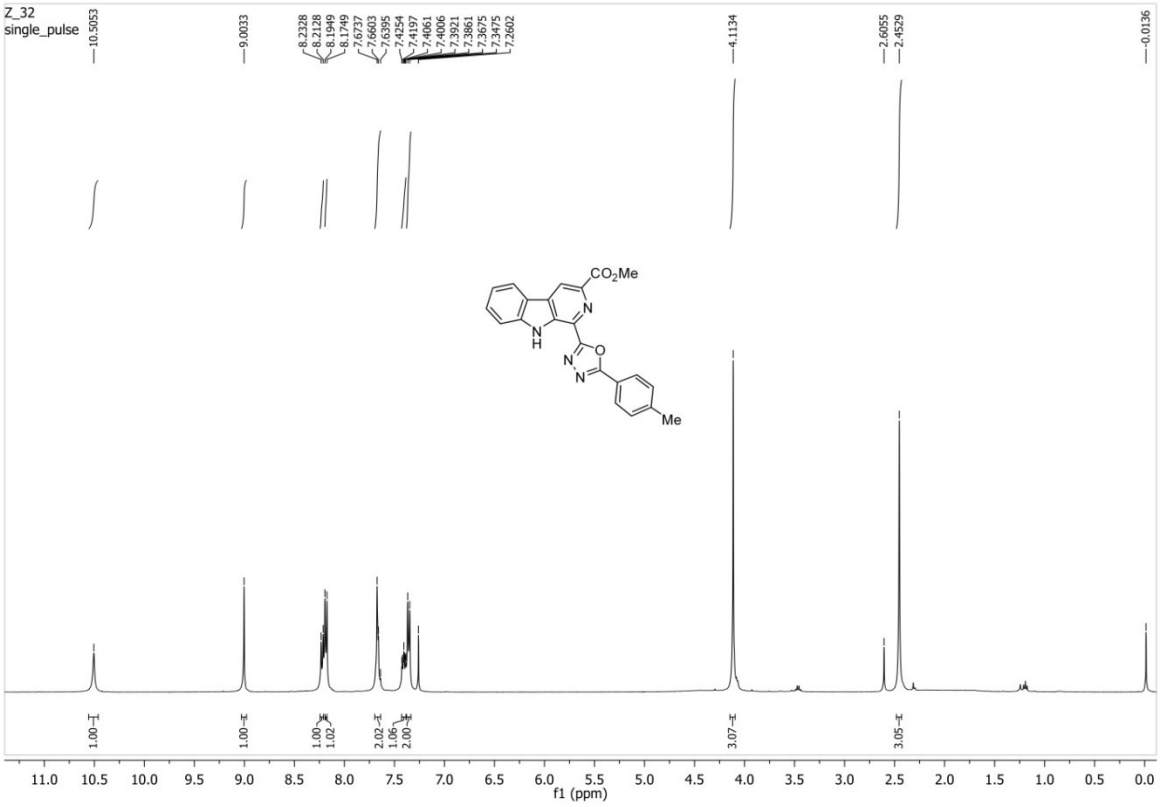


Figure S11. [1]H-NMR spectrum of **2aF**.

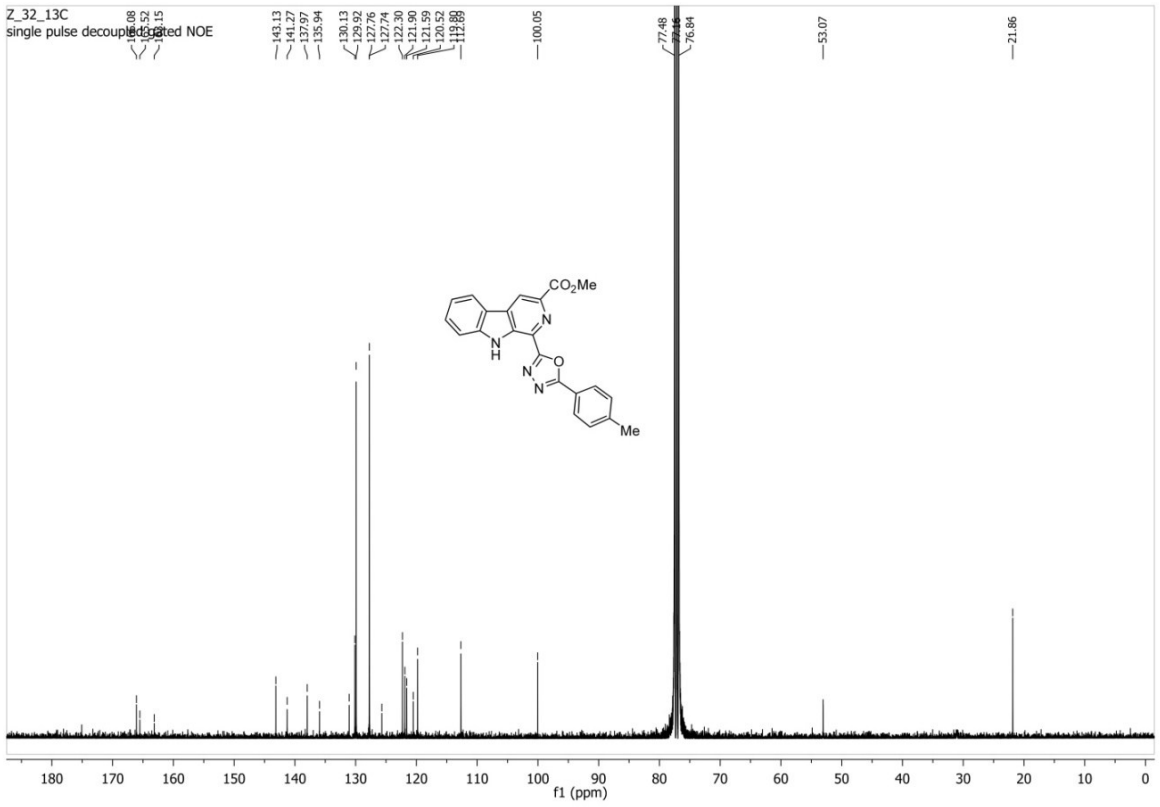


Figure S12. [13]C-NMR spectrum of **2aF**.

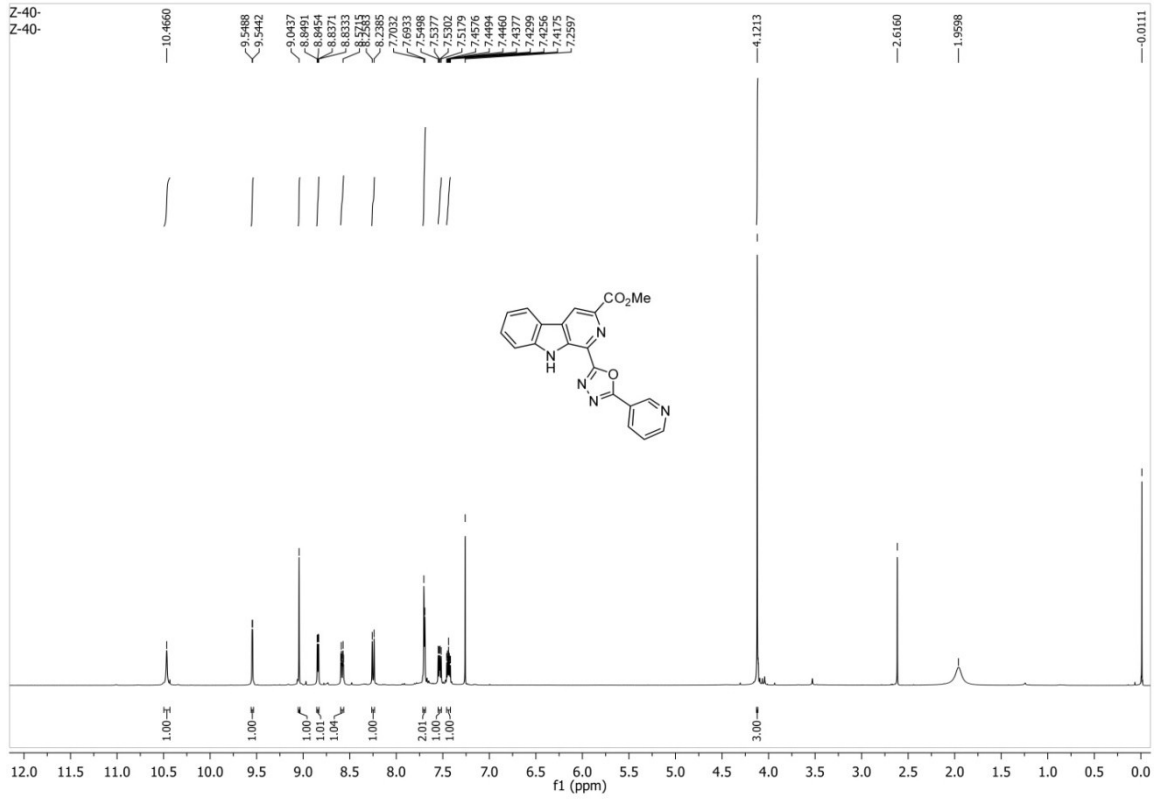


Figure S13. ^{1}H-NMR spectrum of **2aG**.

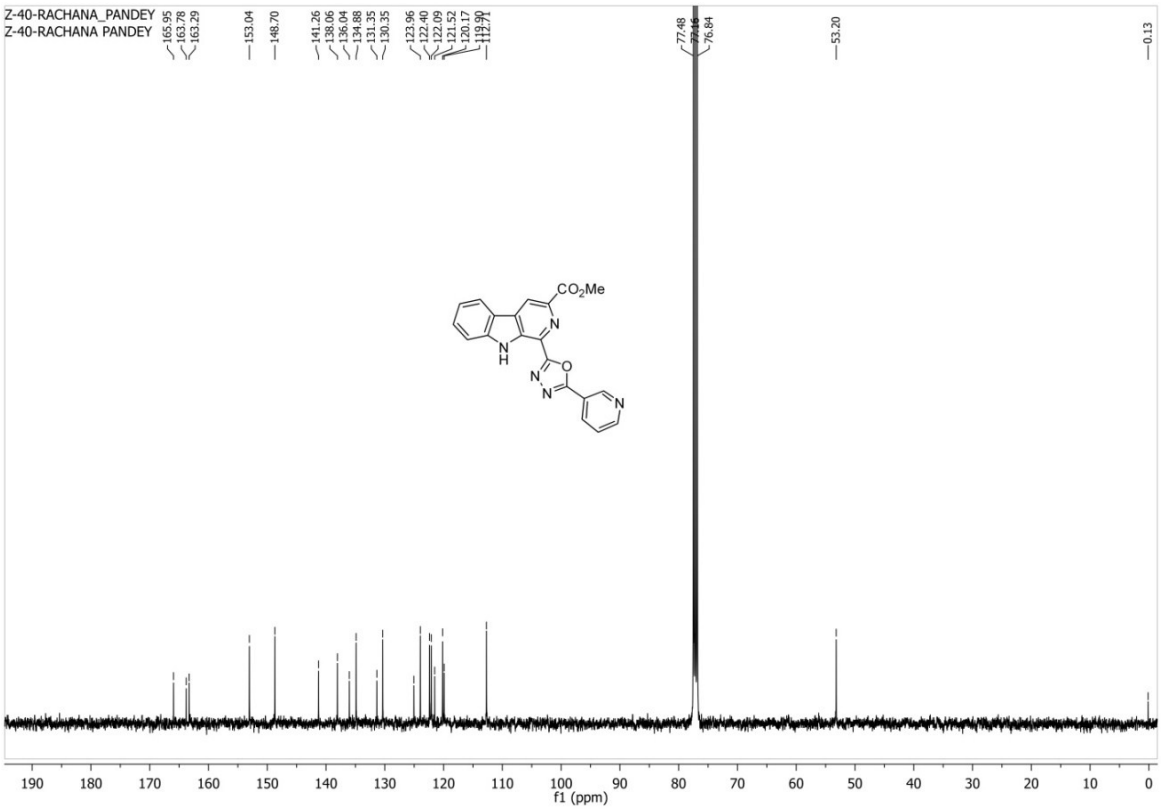


Figure S14. ^{13}C-NMR spectrum of **2aG**.

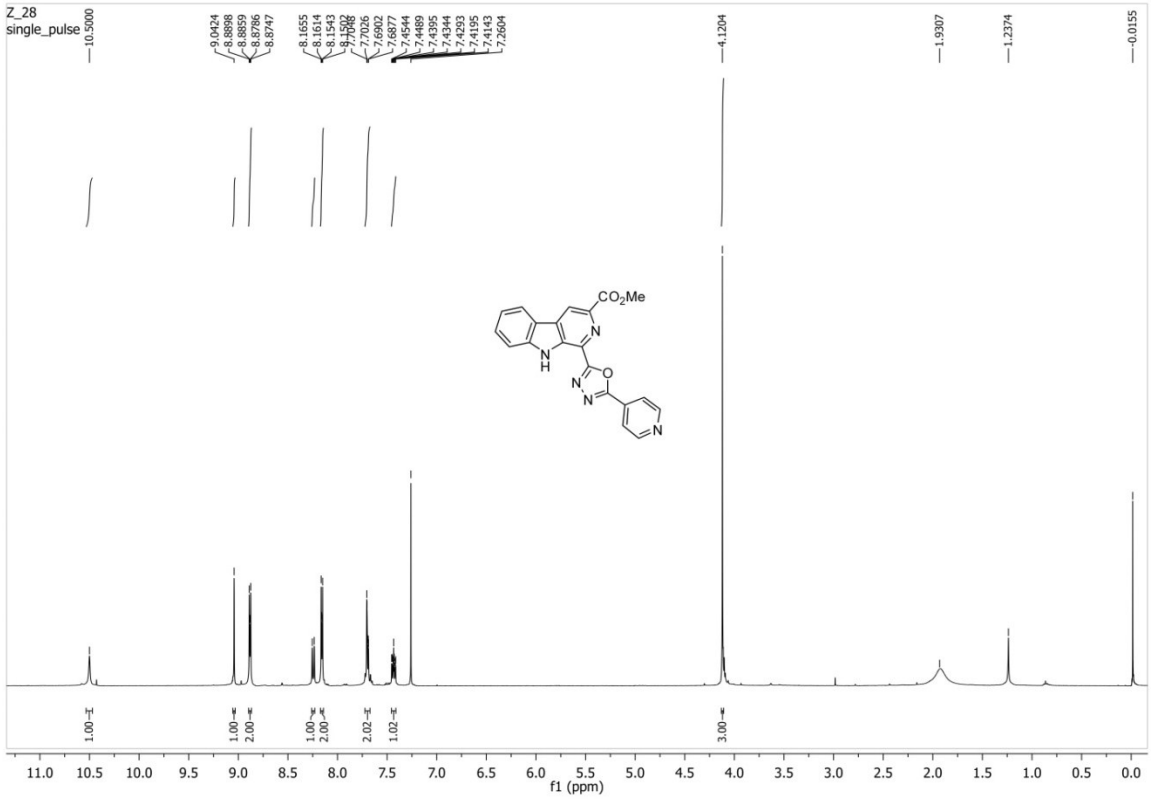


Figure S15. ^{1}H-NMR spectrum of **2aH**.

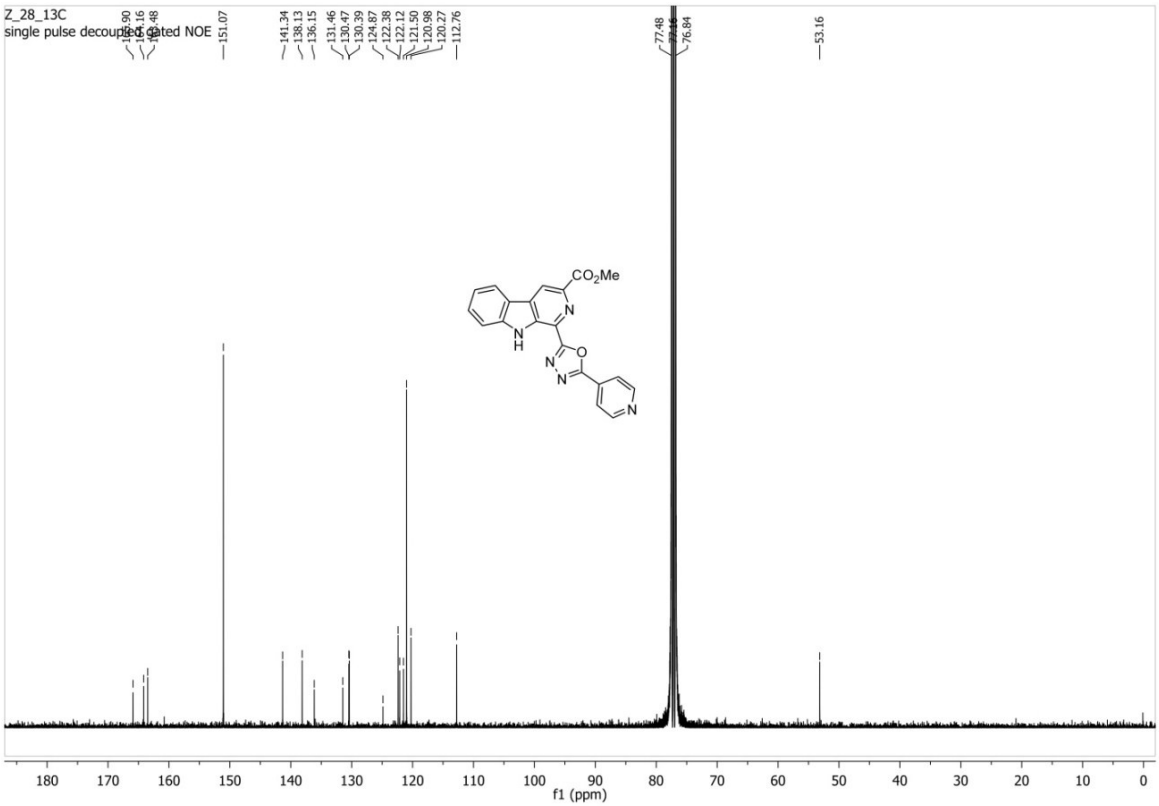


Figure S16. ^{13}C-NMR spectrum of **2aH**.

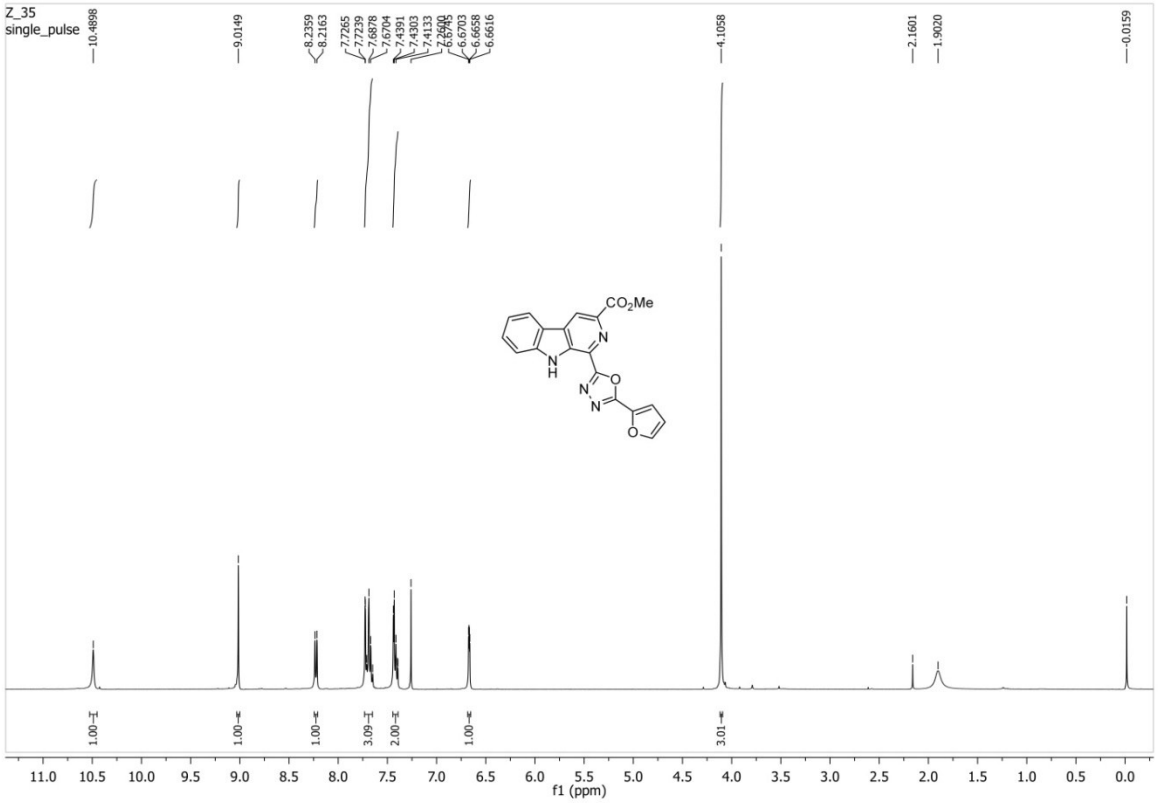


Figure S17. ^{1}H-NMR spectrum of **2aI**.

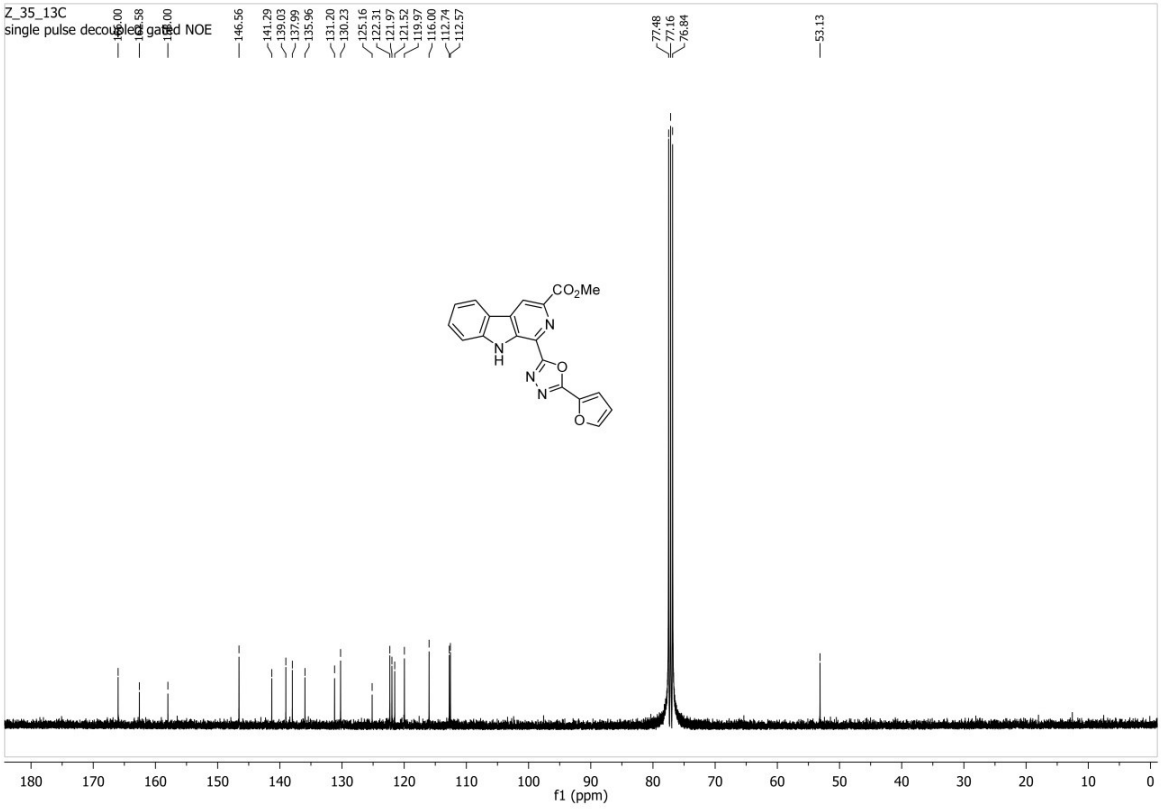


Figure S18. ^{13}C-NMR spectrum of **2aI**.

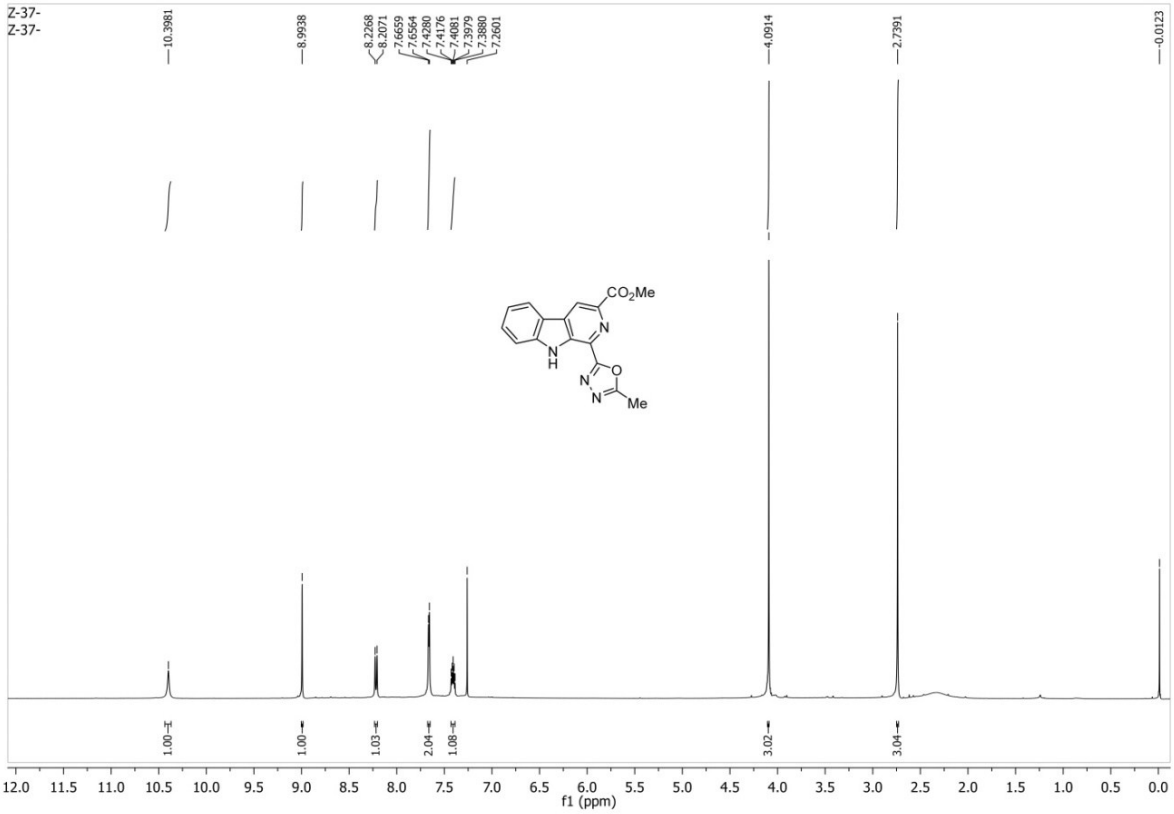


Figure S19. [1]H-NMR spectrum of **2aK**.

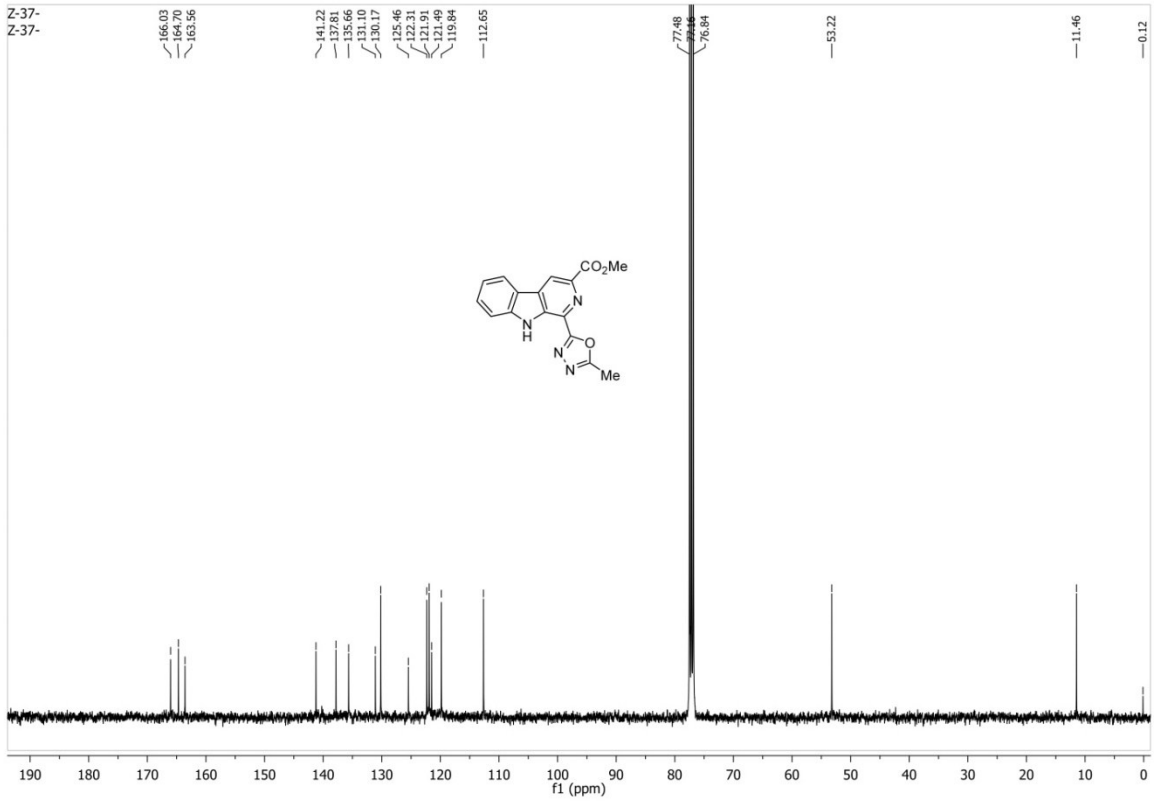


Figure S20. [13]C-NMR spectrum of **2aK**.

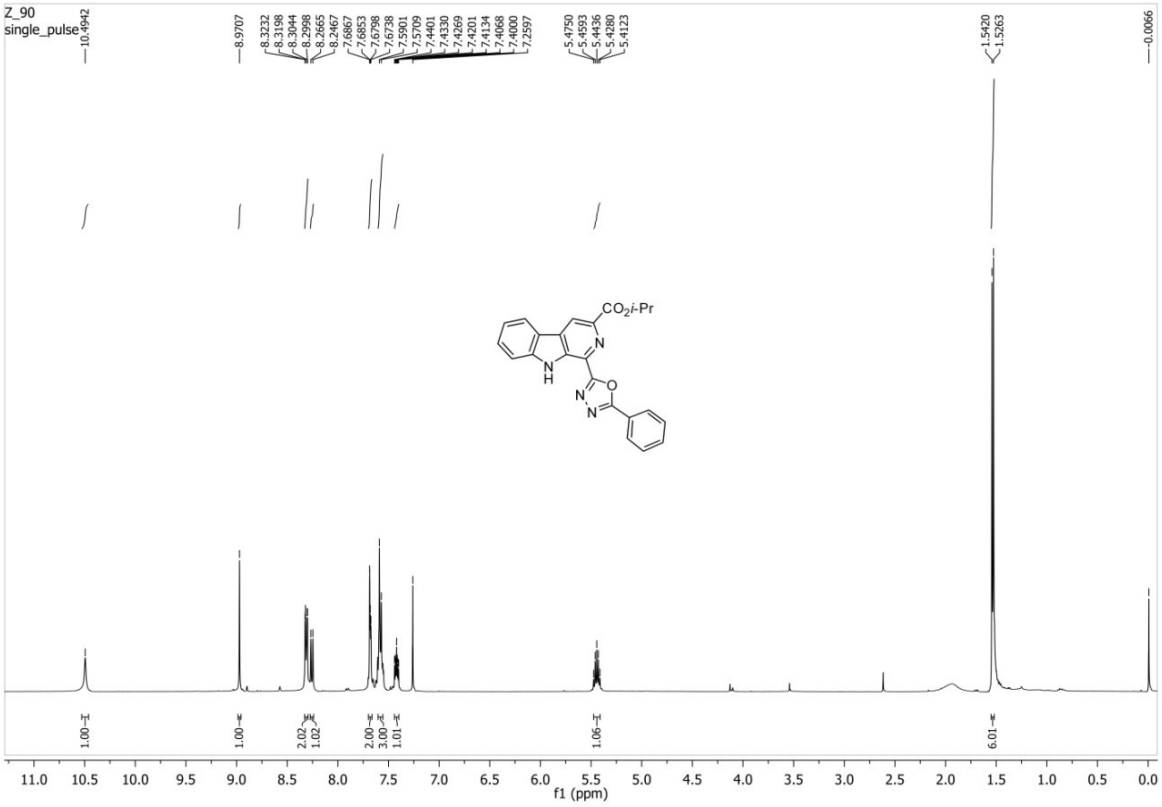


Figure S21. ^{1}H-NMR spectrum of **2iA**.

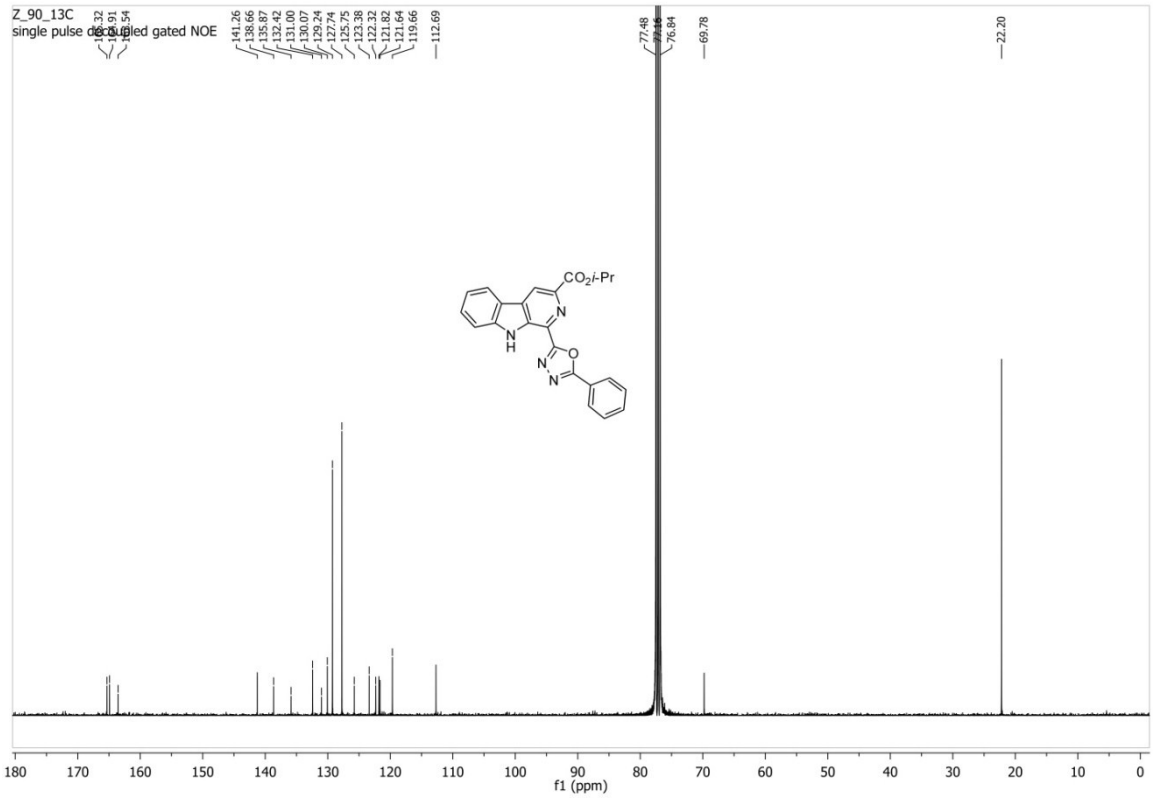


Figure S22. ^{13}C-NMR spectrum of **2iA**.

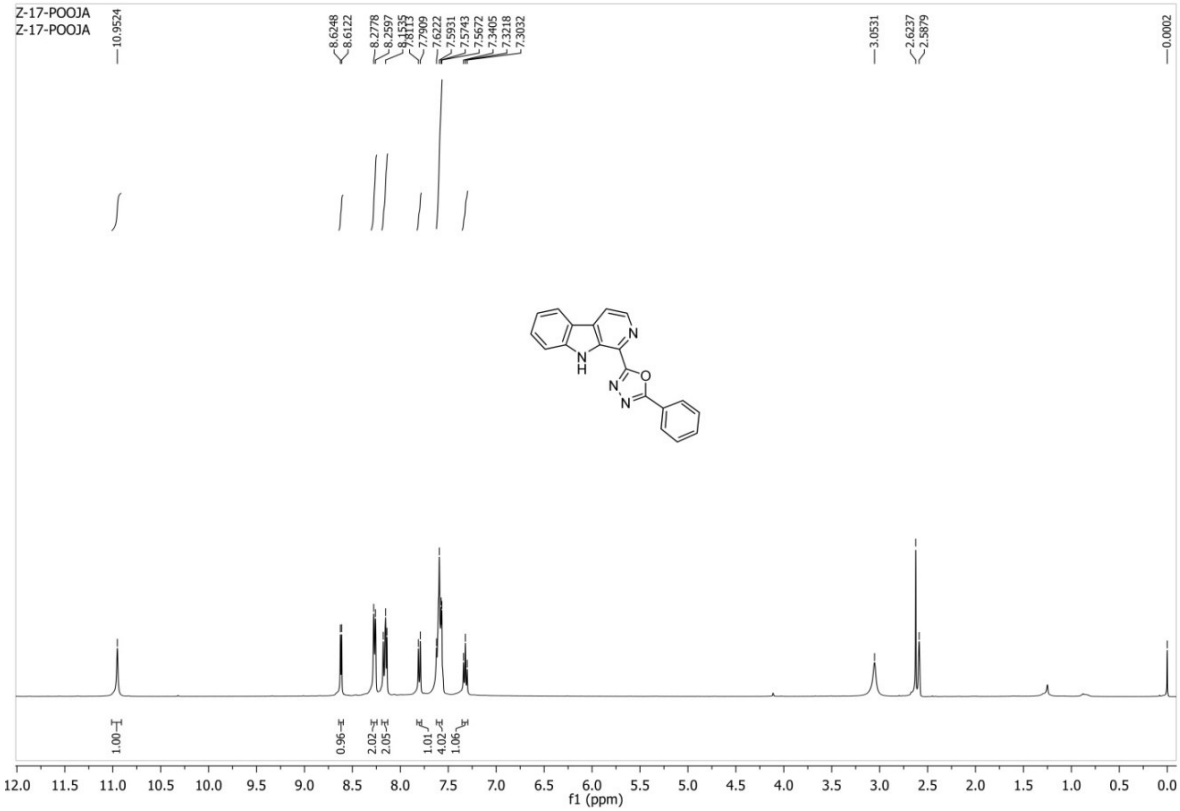


Figure S23. [1]H-NMR spectrum of **2kA**.

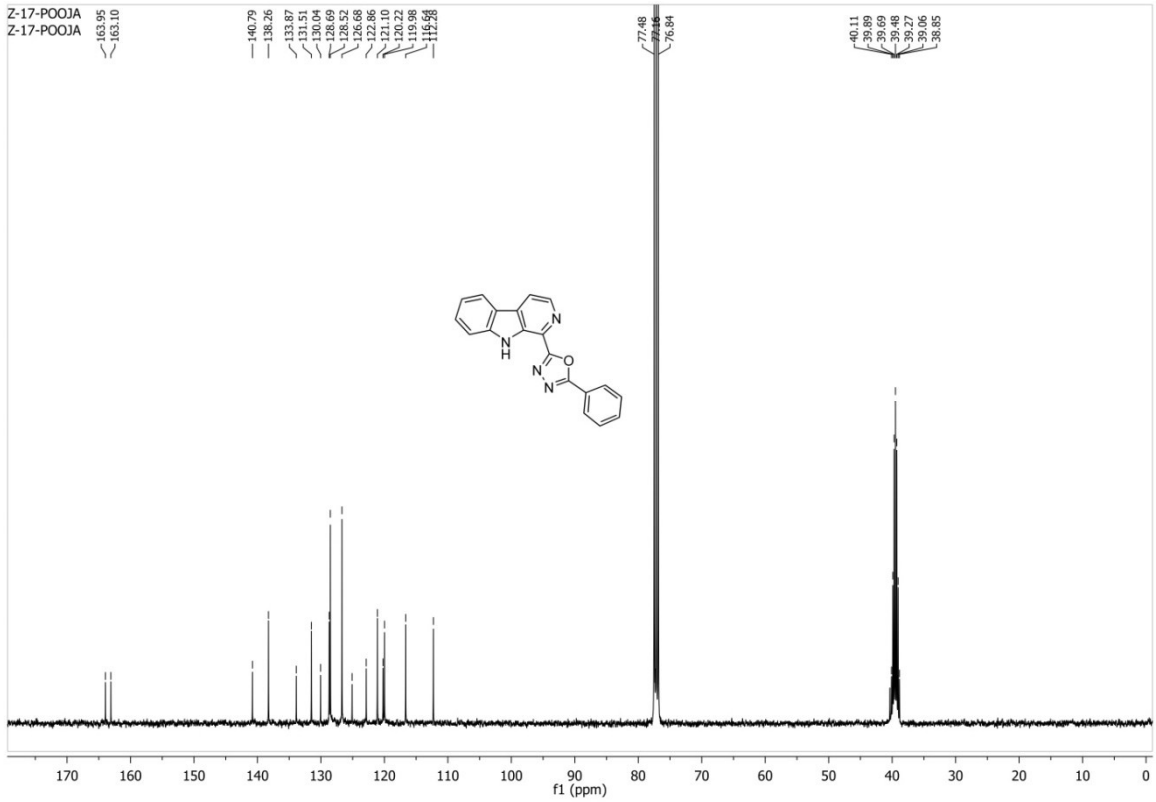


Figure S24. [13]C-NMR spectrum of **2kA**.

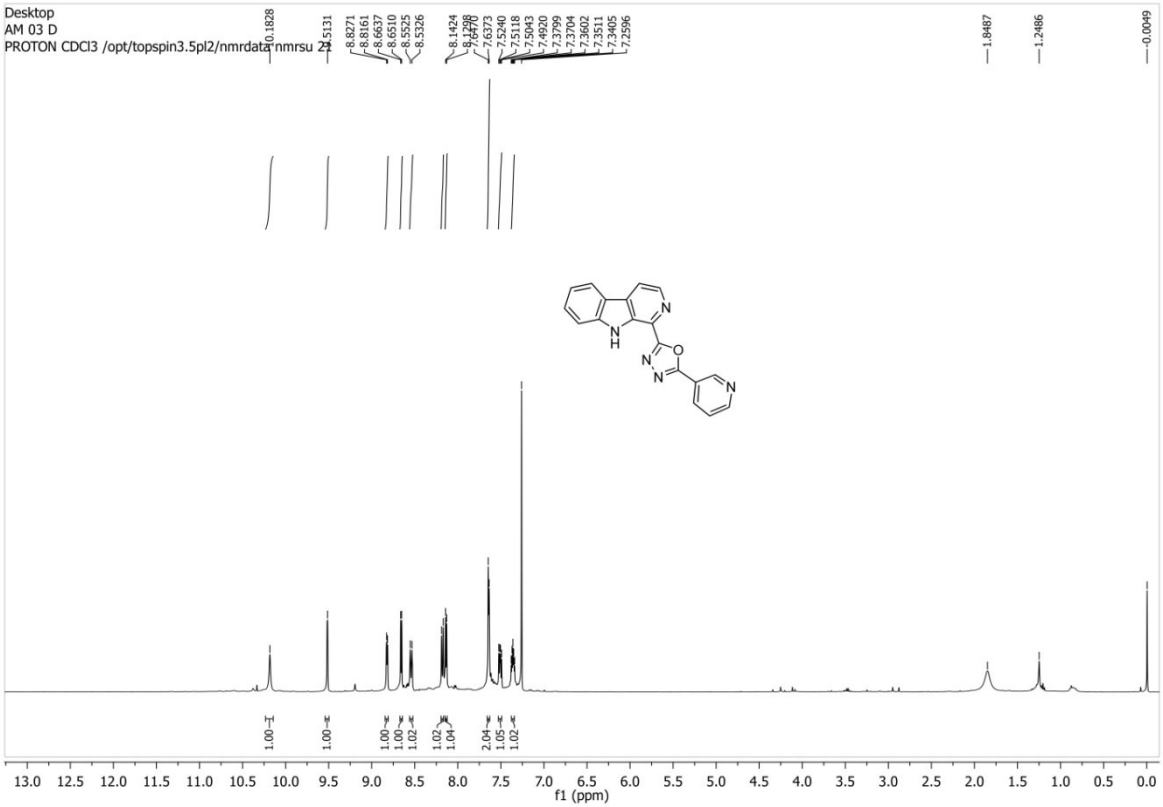


Figure S25. ^{1}H-NMR spectrum of **2kG**.

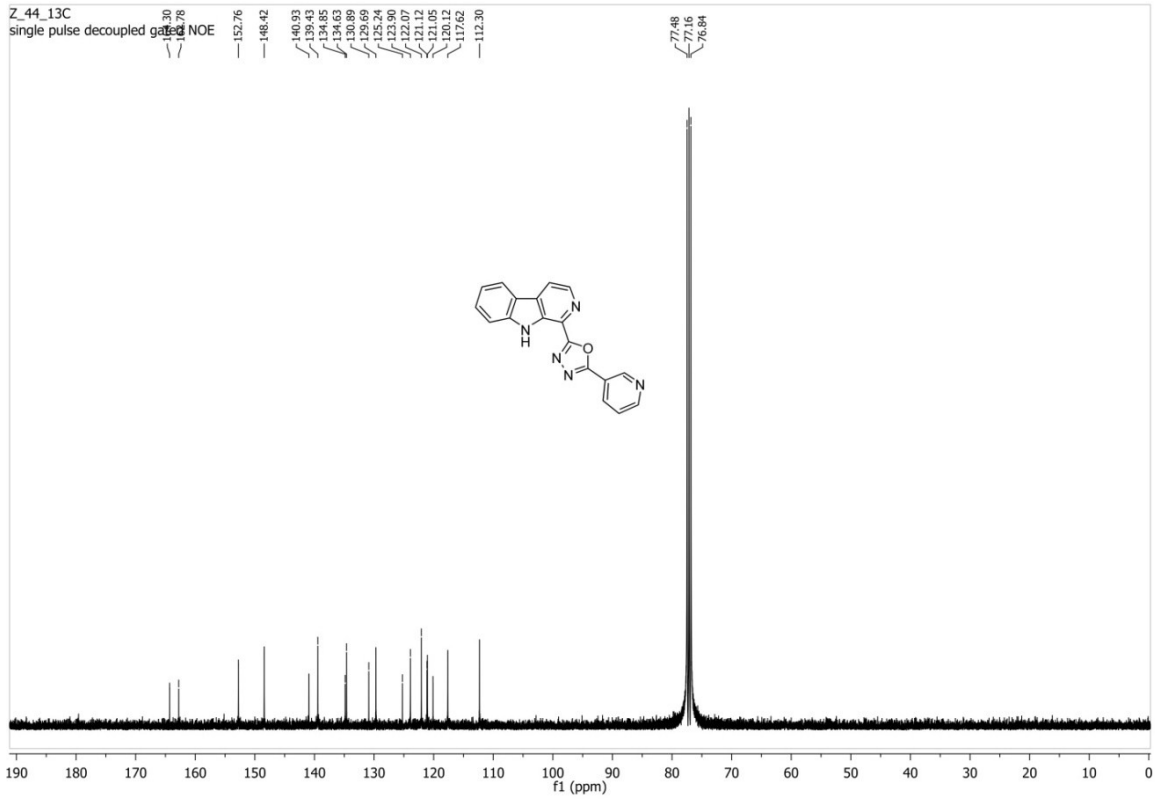


Figure S26. ^{13}C-NMR spectrum of **2kG**.

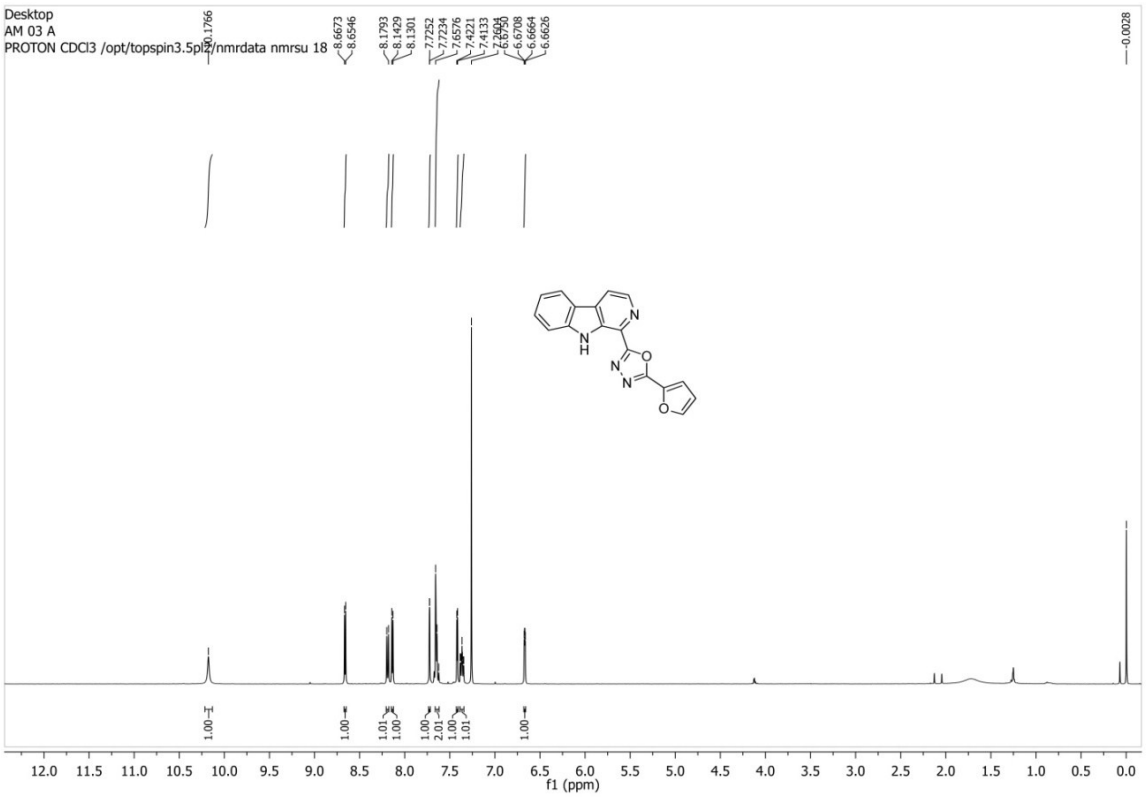


Figure S27. [1]H-NMR spectrum of **2kI**.

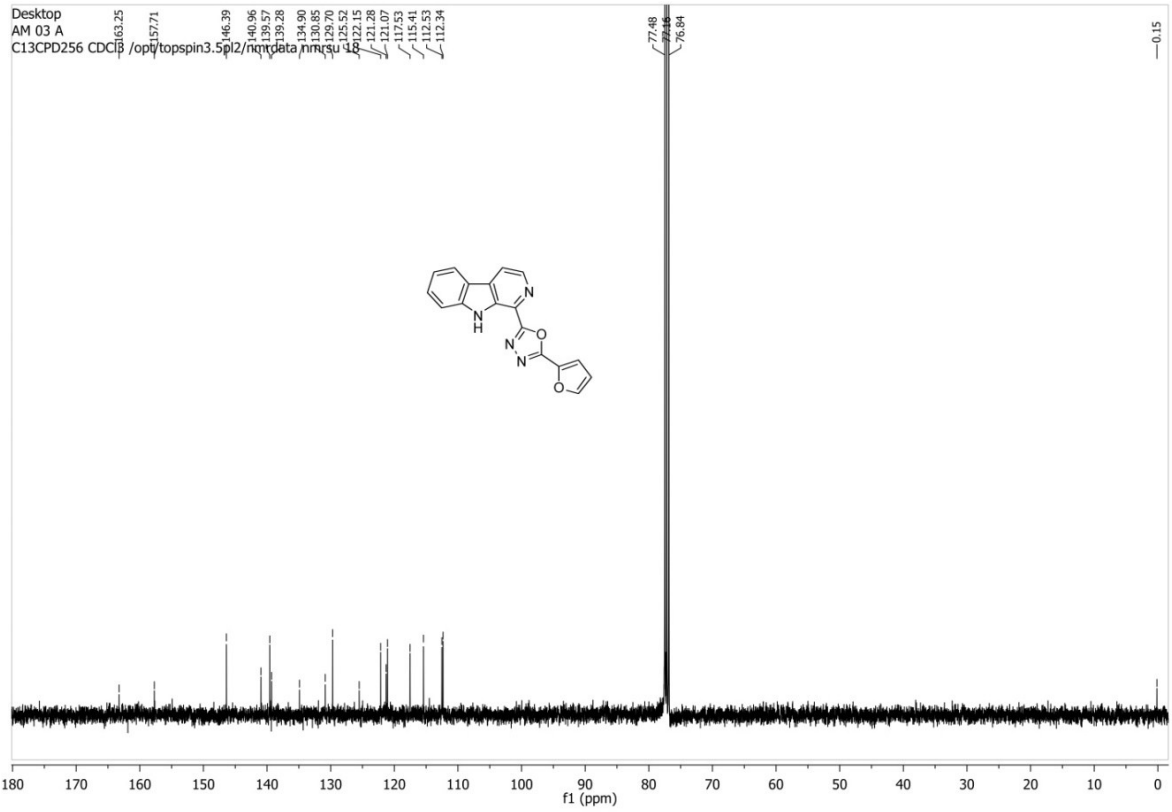


Figure S28. [13]C-NMR spectrum of **2kI**.

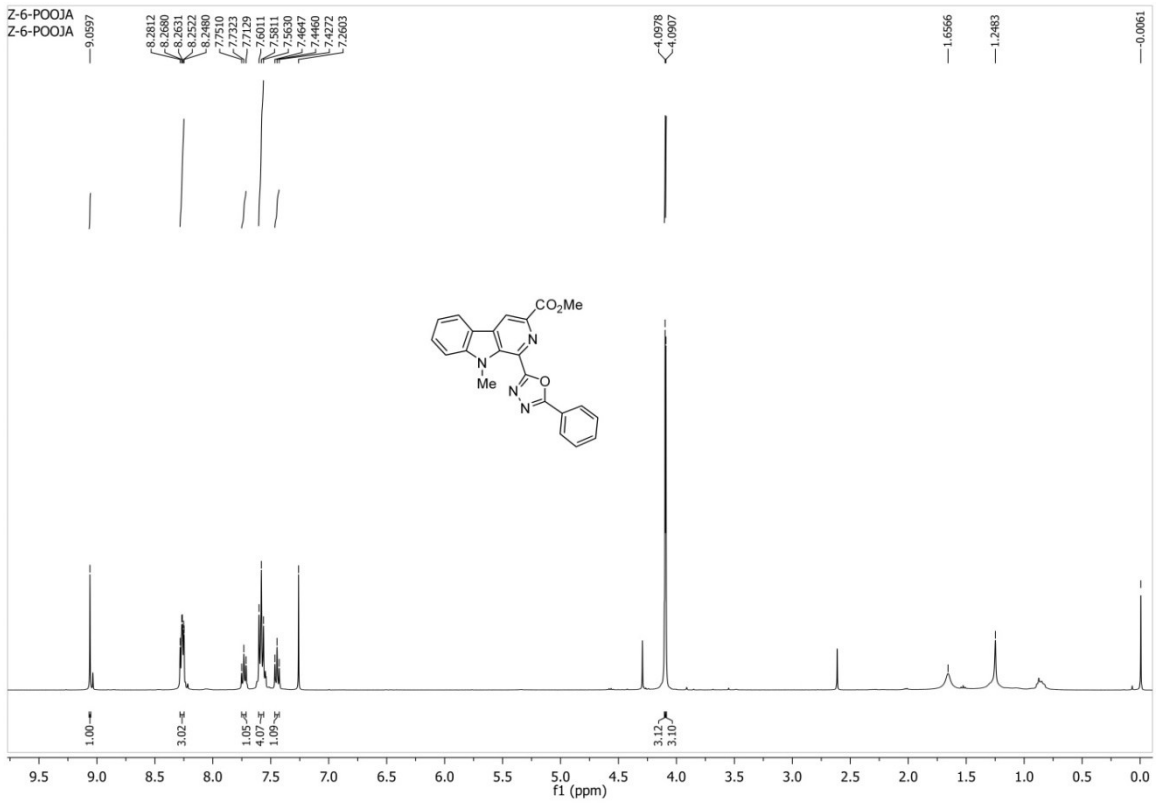


Figure S29. ^{1}H-NMR spectrum of **2bA**.

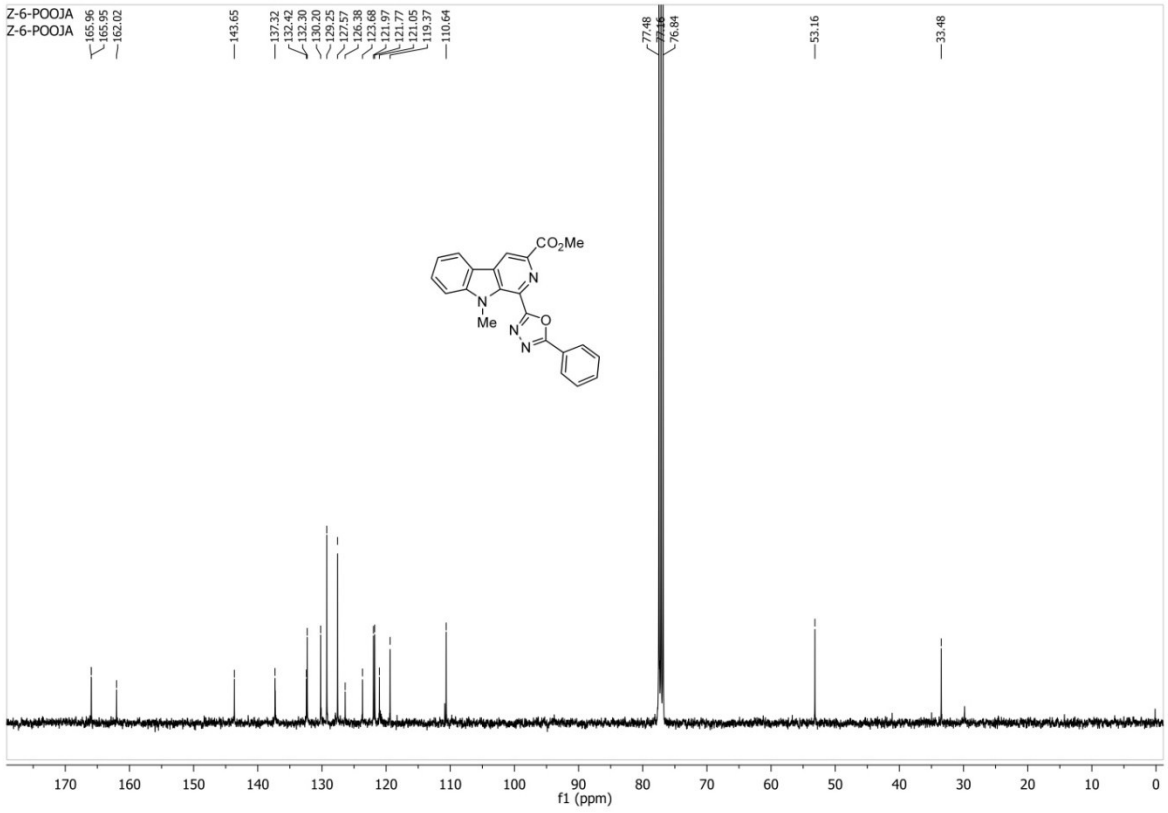


Figure S30. ^{13}C-NMR spectrum of **2bA**.

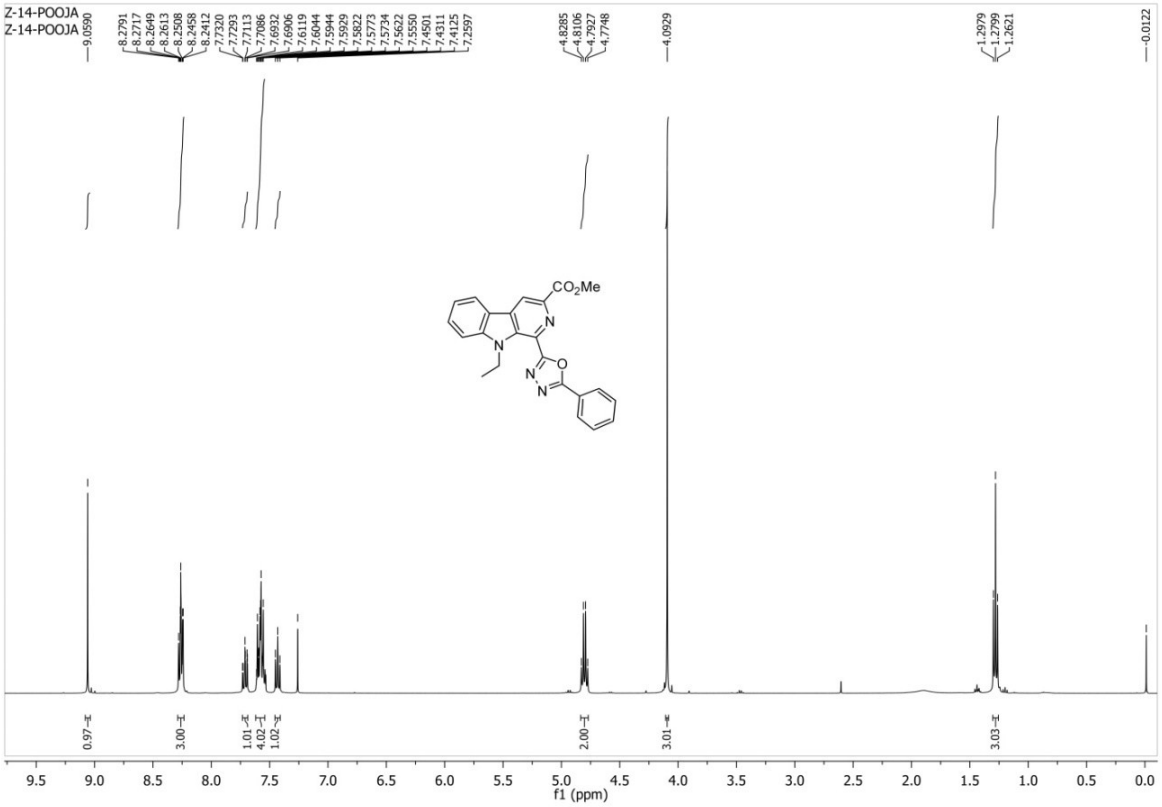


Figure S31. ^{1}H-NMR spectrum of **2cA**.

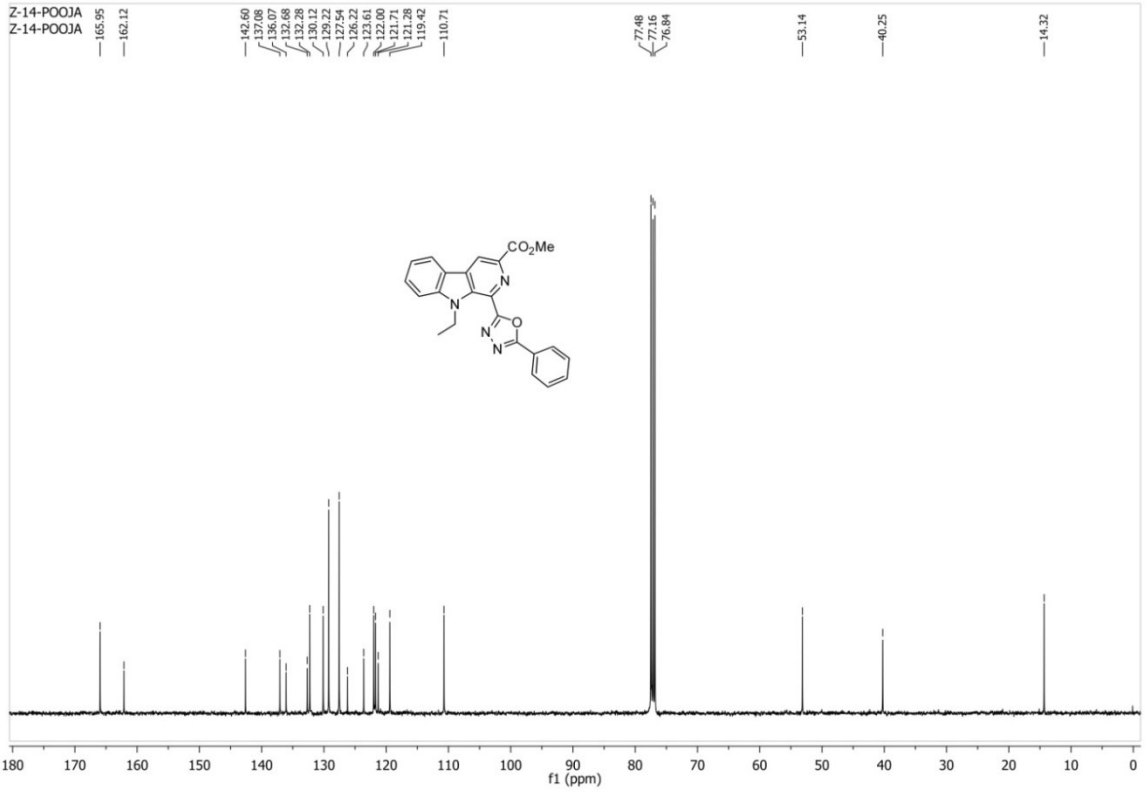


Figure S32. ^{13}C-NMR spectrum of **2cA**.

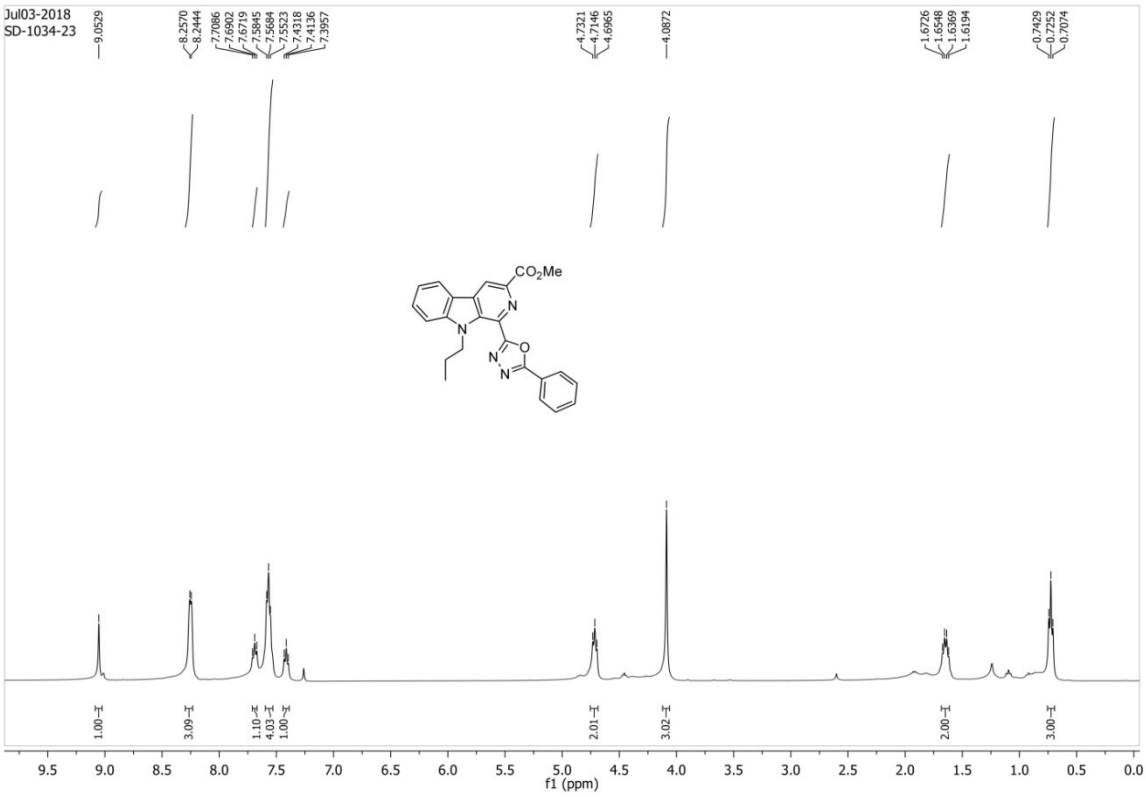


Figure S33. [1]H-NMR spectrum of **2dA**.

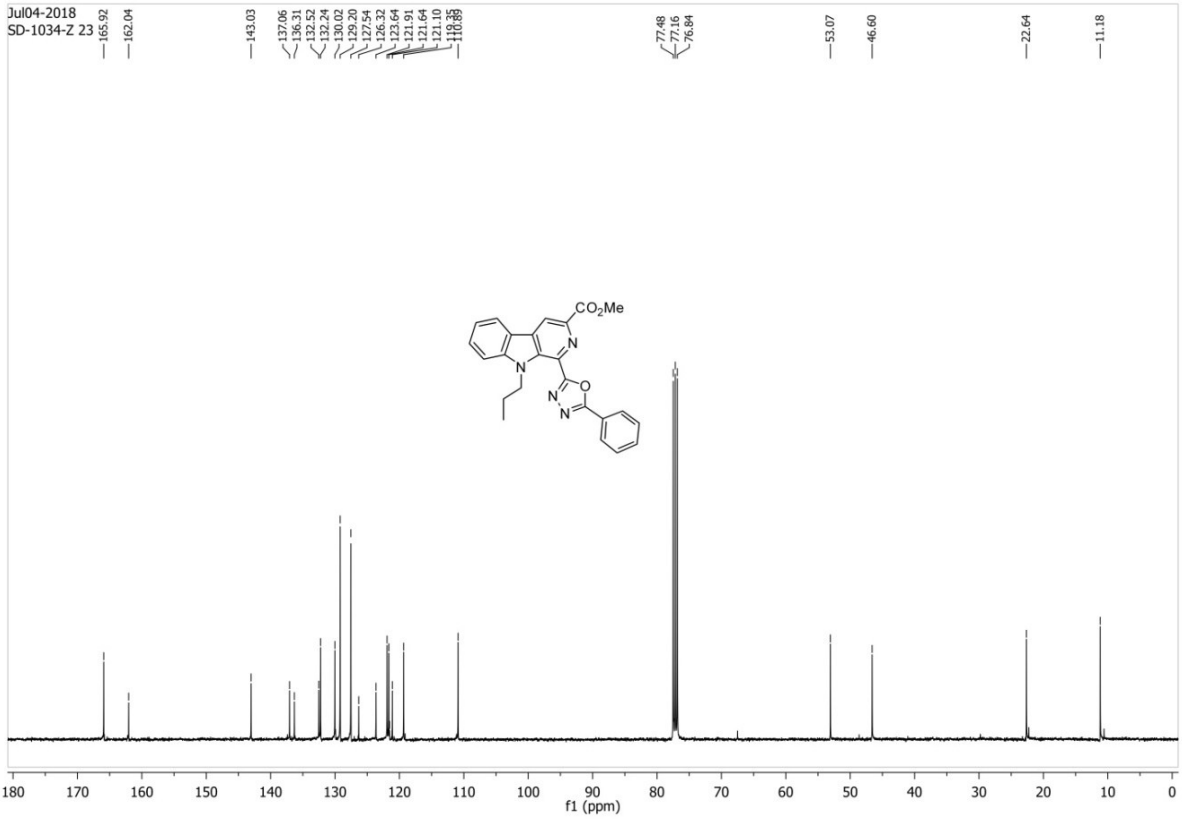
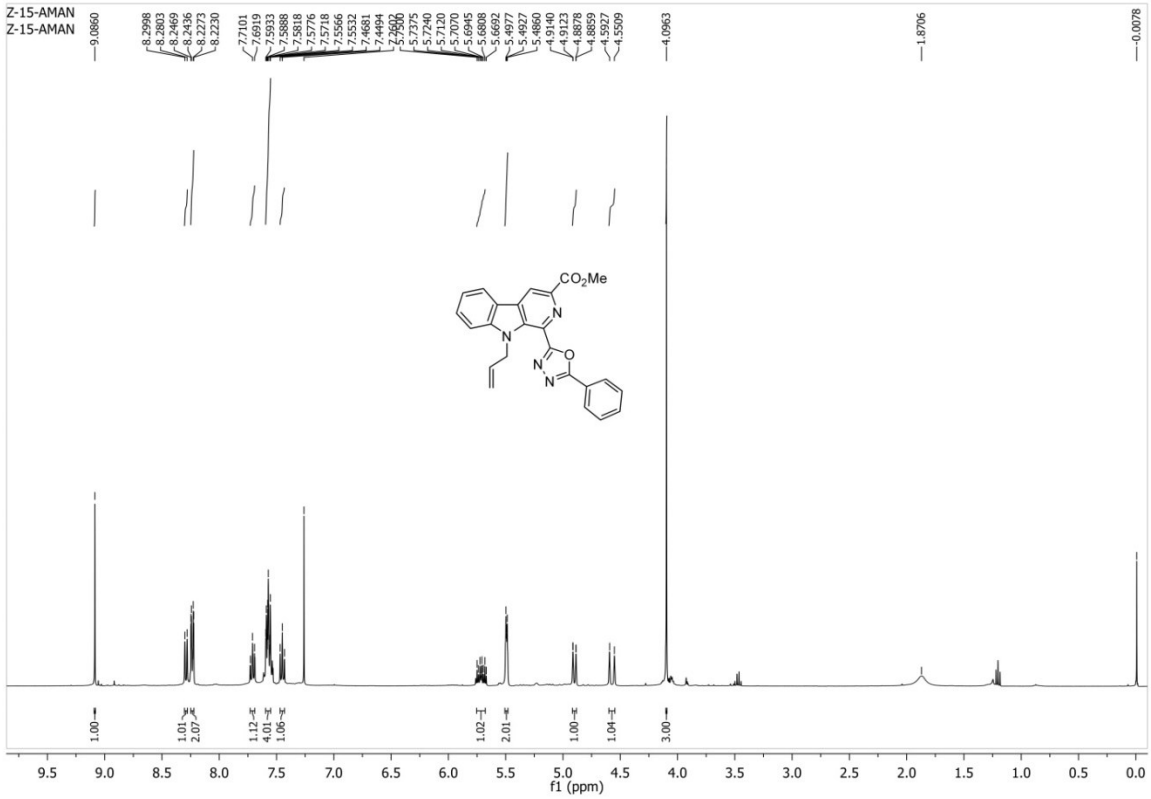


Figure S34. [13]C-NMR spectrum of **2dA**.



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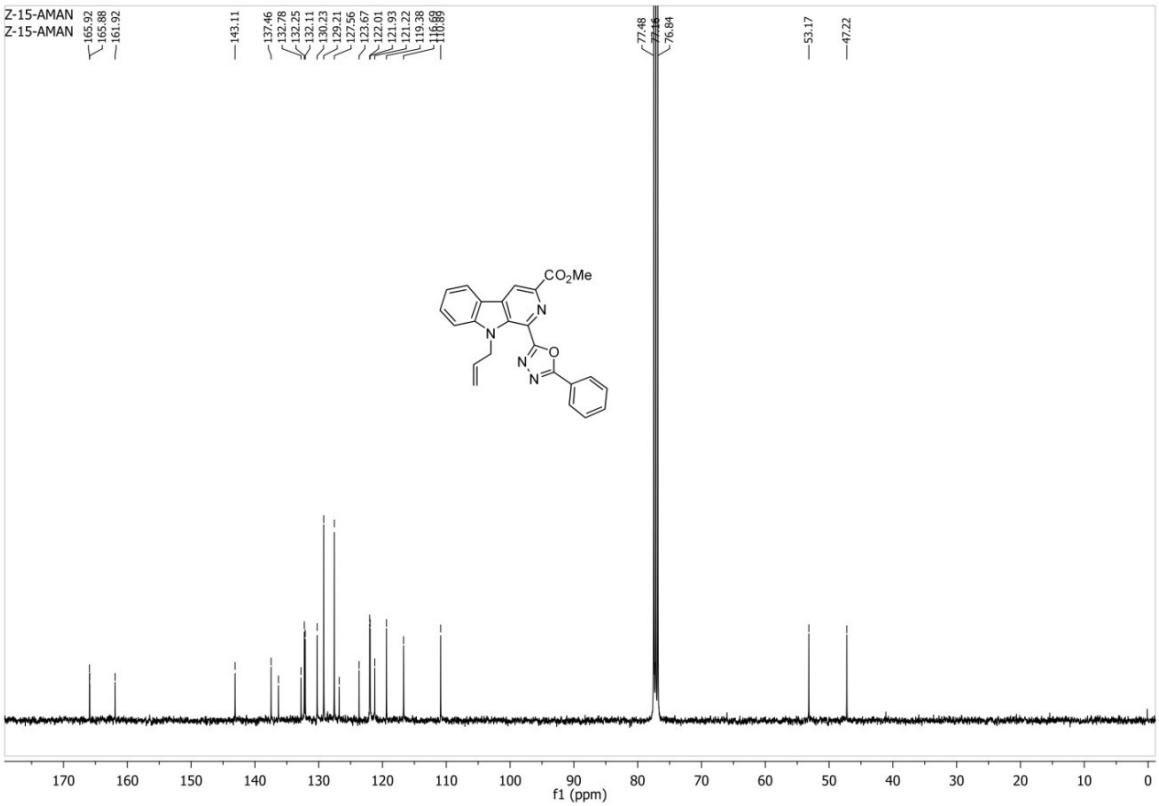

Figure S36. ^{13}C-NMR spectrum of **2eA**.

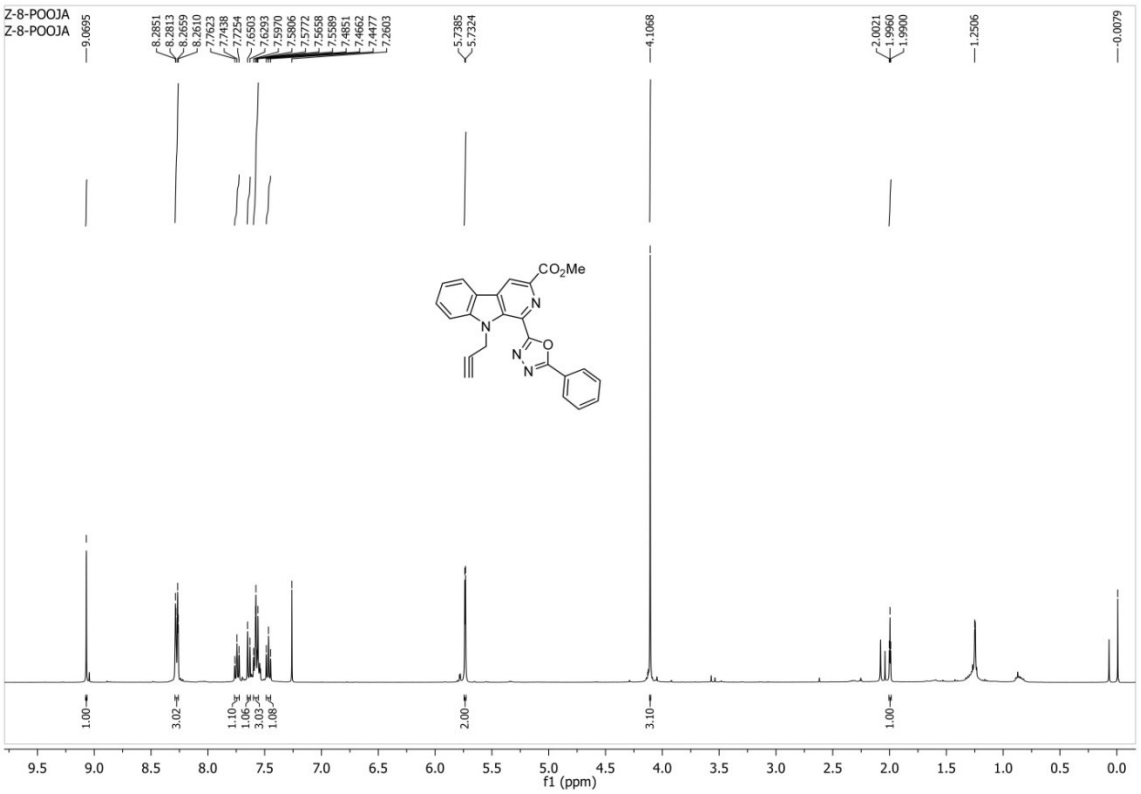

Figure S37. ^{1}H-NMR spectrum of **2fA**.

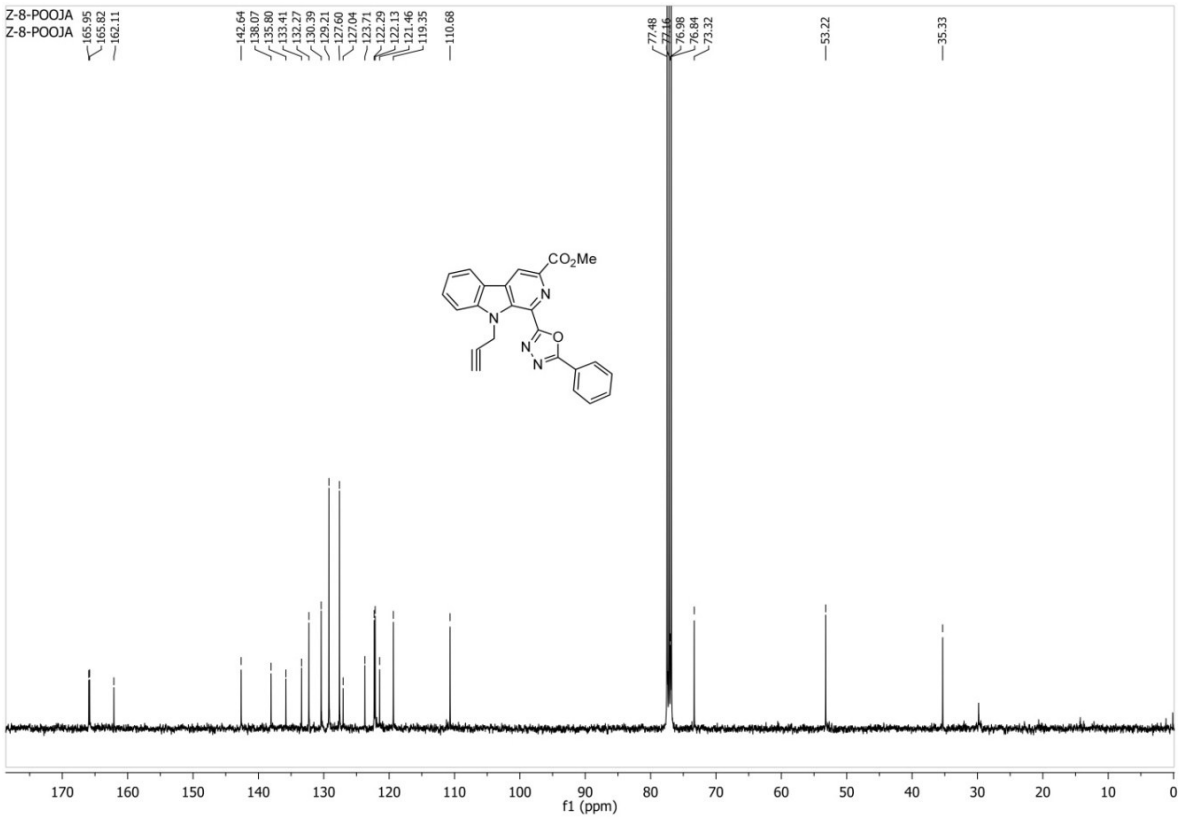

Figure S38. ^{13}C-NMR spectrum of **2fA**.

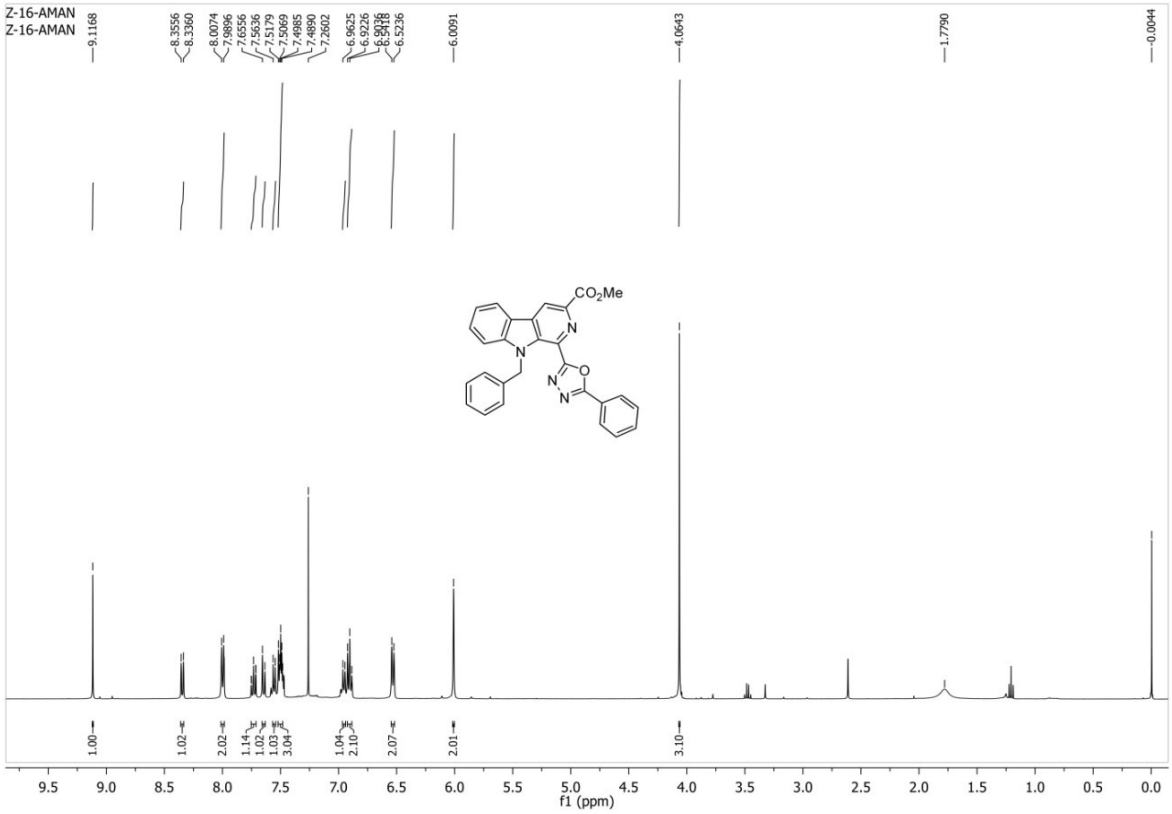

Figure S39. ^{1}H-NMR spectrum of **2gA**.

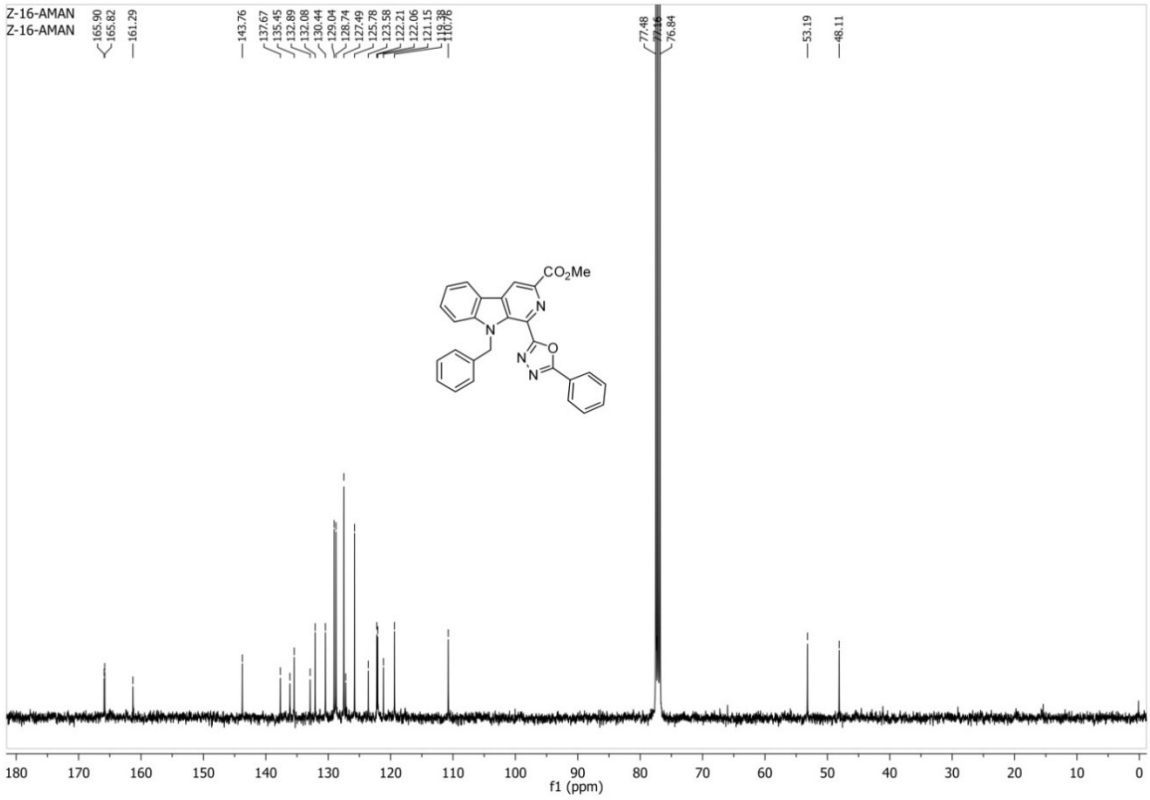

Figure S40. ^{13}C-NMR spectrum of **2gA**.

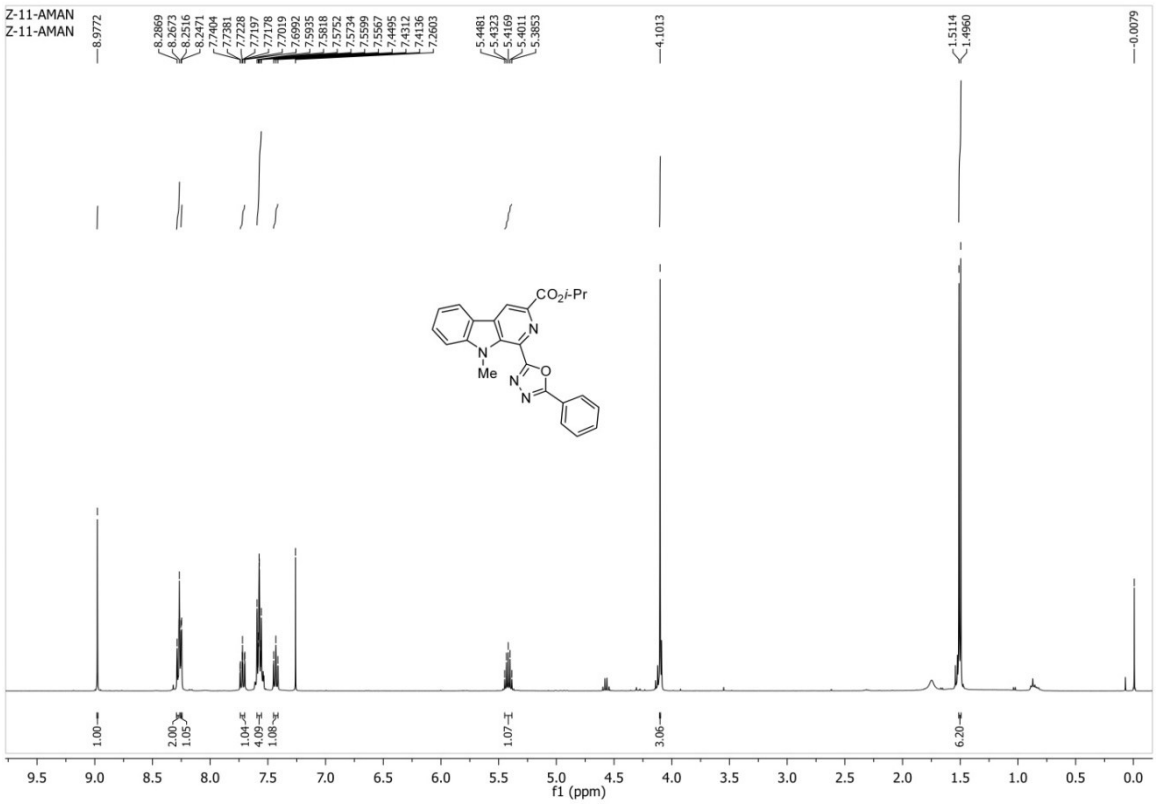

Figure S41. ^{1}H-NMR spectrum of **2jA**.

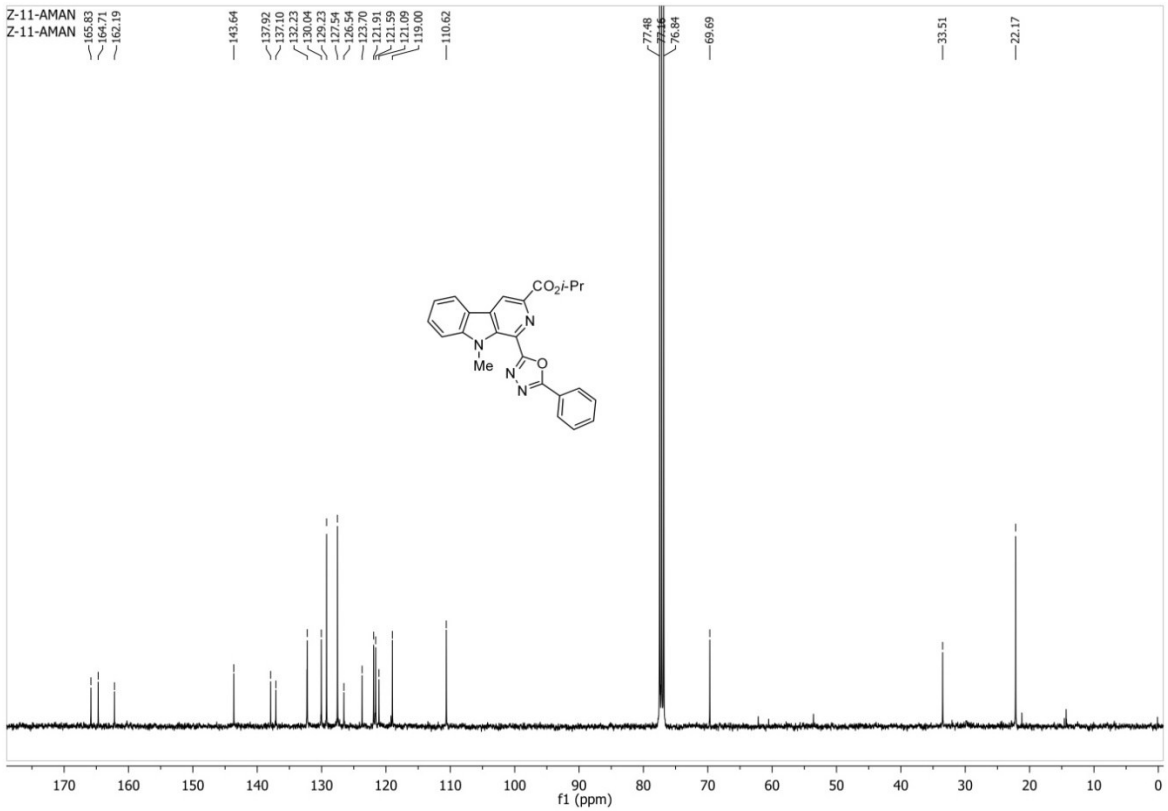

Figure S42. ^{13}C-NMR spectrum of **2jA**.

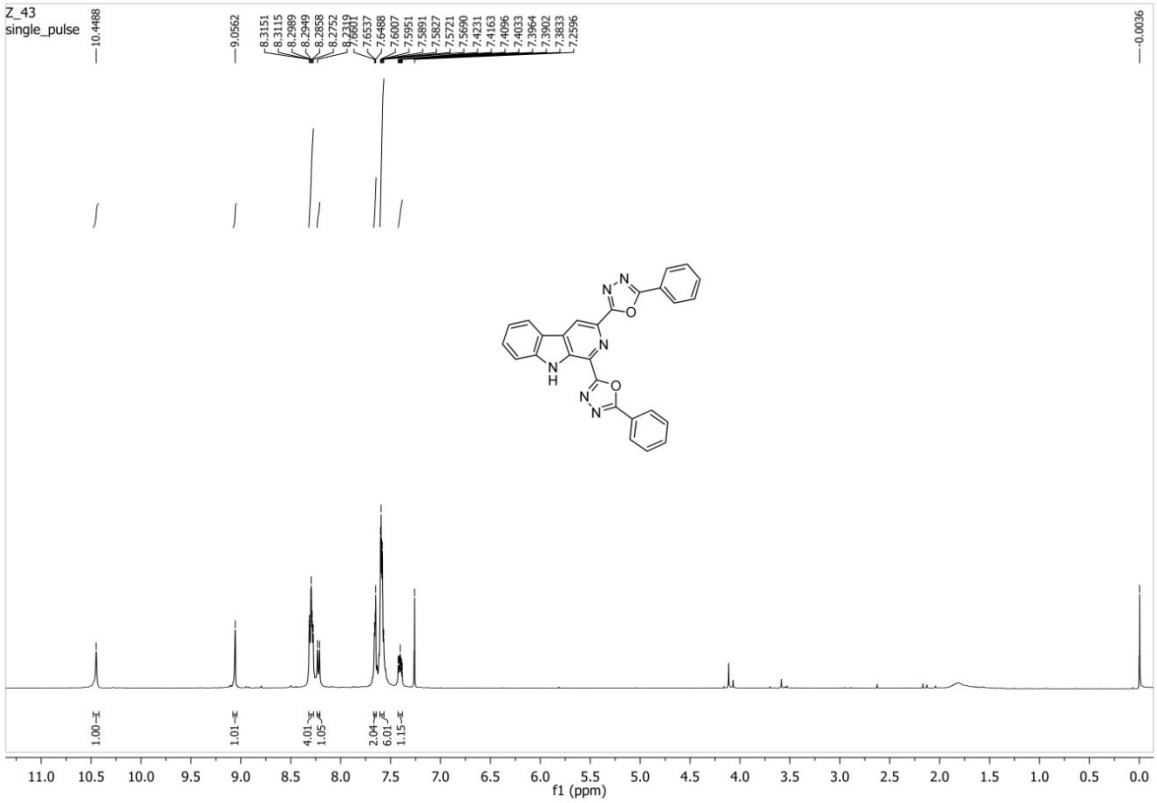

Figure S43. ^{1}H-NMR spectrum of **5A**.

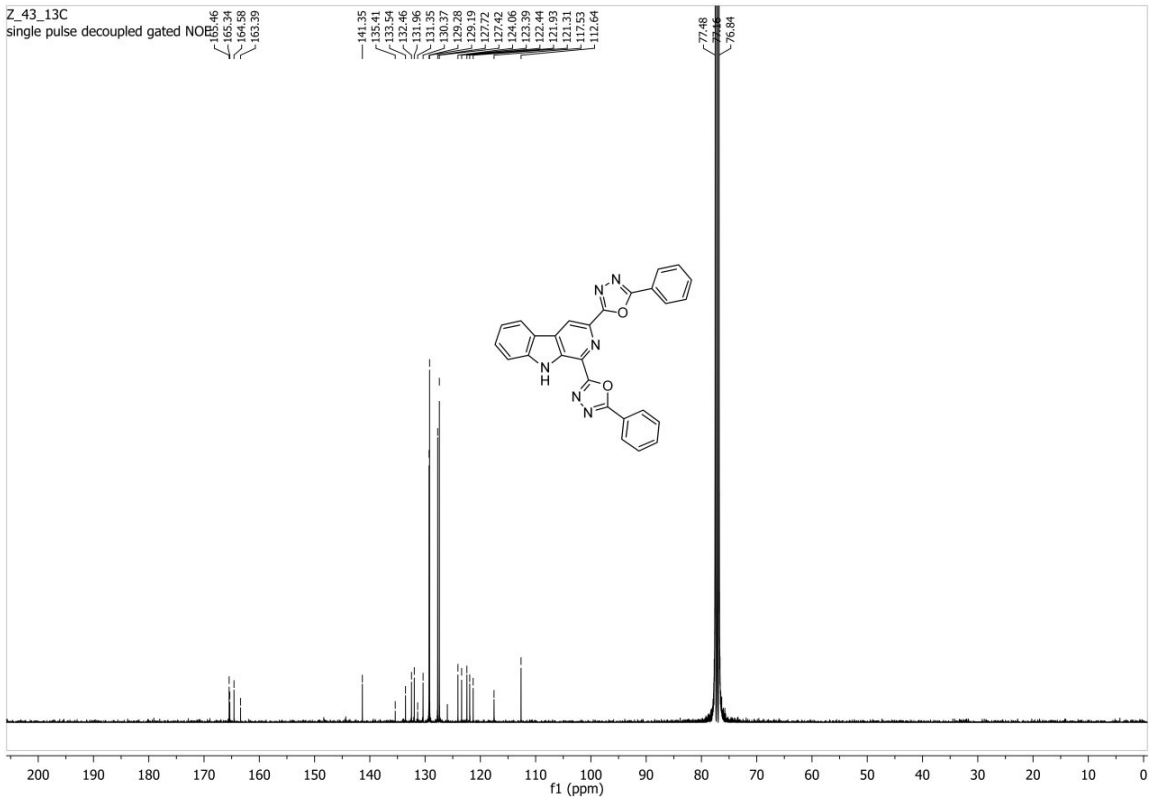

Figure S44. ^{13}C-NMR spectrum of **5A**.

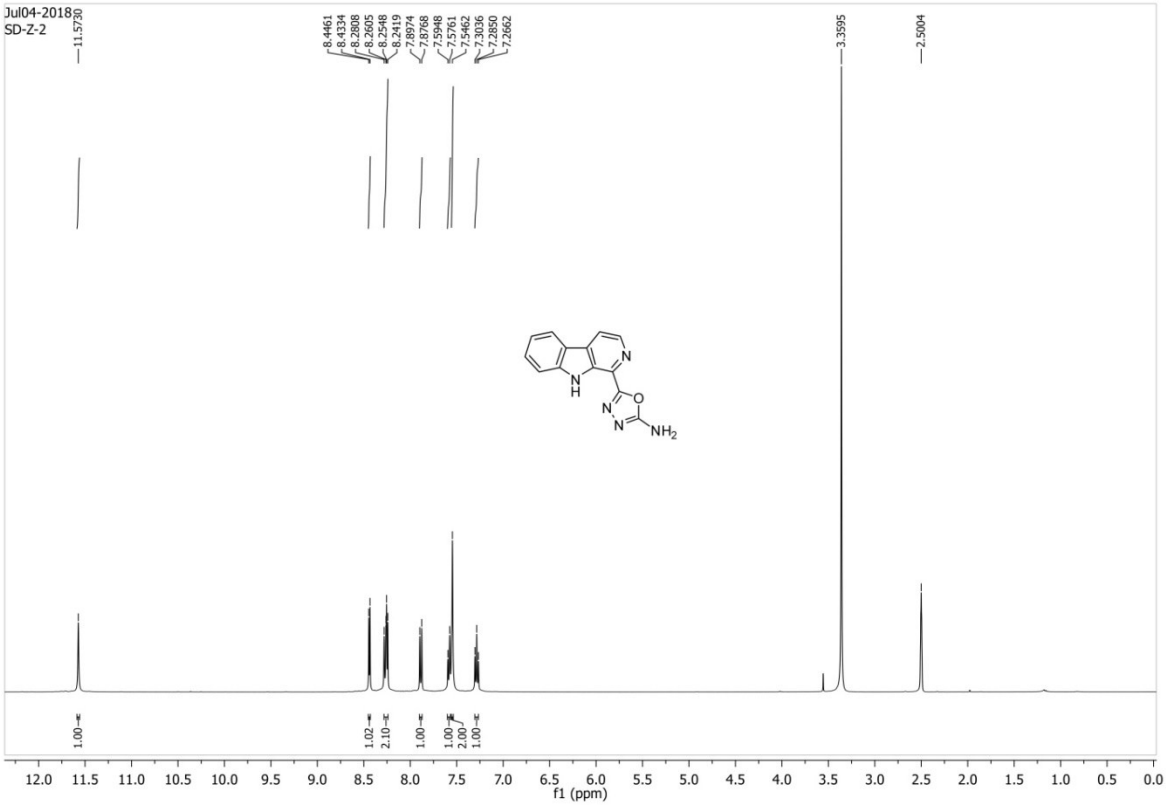

Figure S45. [1]H-NMR spectrum of **2kM**.

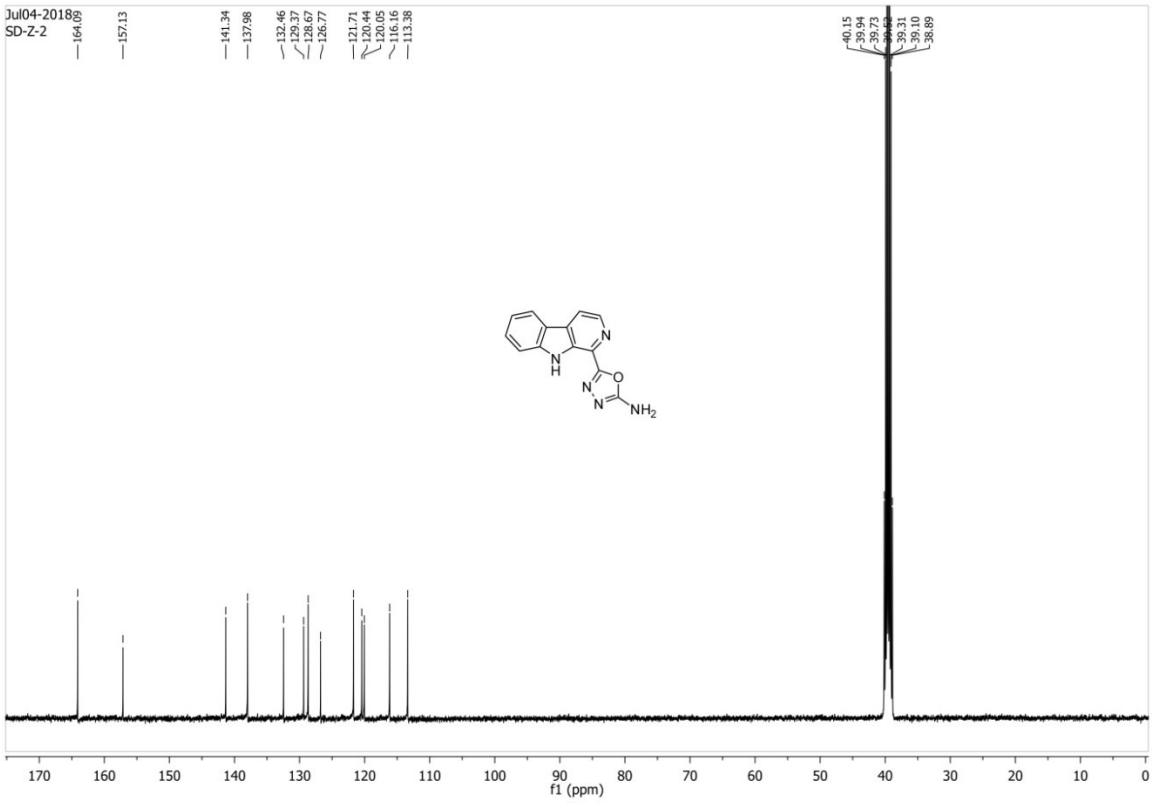

Figure S46. [13]C-NMR spectrum of **2kM**.

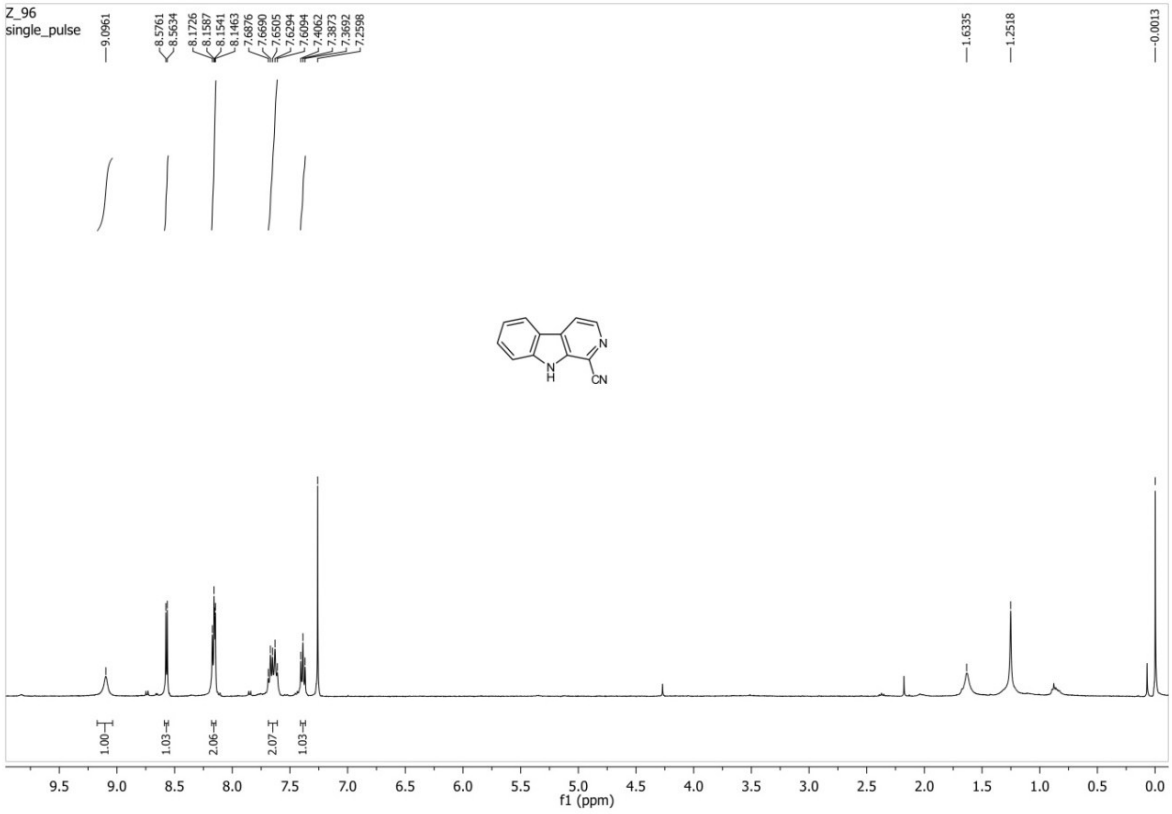

Figure S47. [1]H-NMR spectrum of **6**.

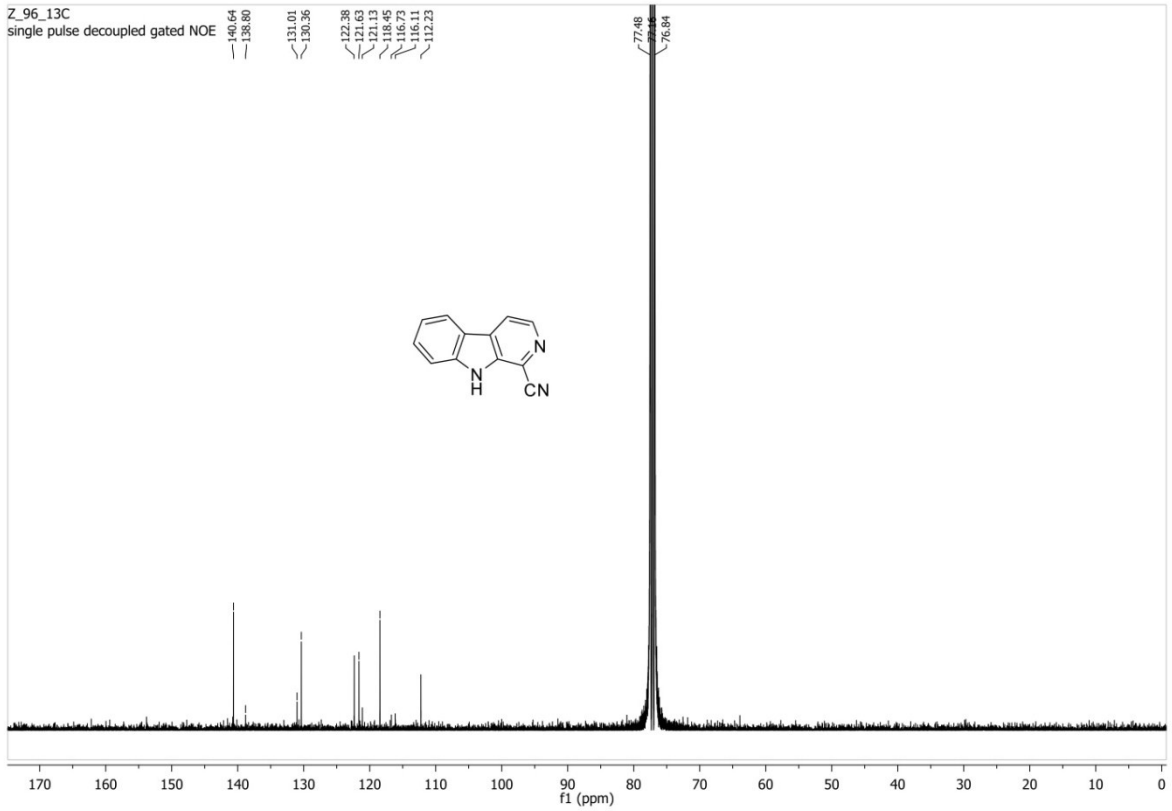

Figure S48. [13]C-NMR spectrum of **6**.