Supporting Information

Unveiling Aggregation-Induced Emission in Benzimidazole–Acrylonitriles for Fluorescent Live-Cell Imaging in HeLa Cells

Munugala Chandrakanth,[a] Ayswarya Mukharjee,[b] Krishnan Rathinasamy,[b] Chinna Ayya Swamy P,[c]* Janardhan Banothu[a]*

[a]Department of Chemistry, National Institute of Technology Calicut, Kozhikode – 673601, Kerala, India

[b]Department of Bioscience and Engineering, National Institute of Technology Calicut, Kozhikode – 673601, Kerala, India

[c]Main group Organometallics Optoelectronic Materials and Catalysis lab, Department of Chemistry, National Institute of Technology Calicut, Kozhikode – 673601, Kerala, India.

Correspondence address:

*Dr. Janardhan Banothu: Room No. 210(C), Department of Chemistry, NIT Calicut, Kozhikode, Kerala-673601, India, Email: janardhan@nitc.ac.in; Tel. 0495-228-5324; ORCID: 0000-0002-2449-1647

*Dr. Chinna Ayya Swamy P: Main Group Organometallics Materials and Catalysis Lab, Department of Chemistry, National Institute of Technology, Calicut 673601, India; Email: swamy@nitc.ac.in; ORCID: 0000- 0001-7875-9517.

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1. ^{1}H & ^{13}C NMR and HRMS Spectra of the Compounds

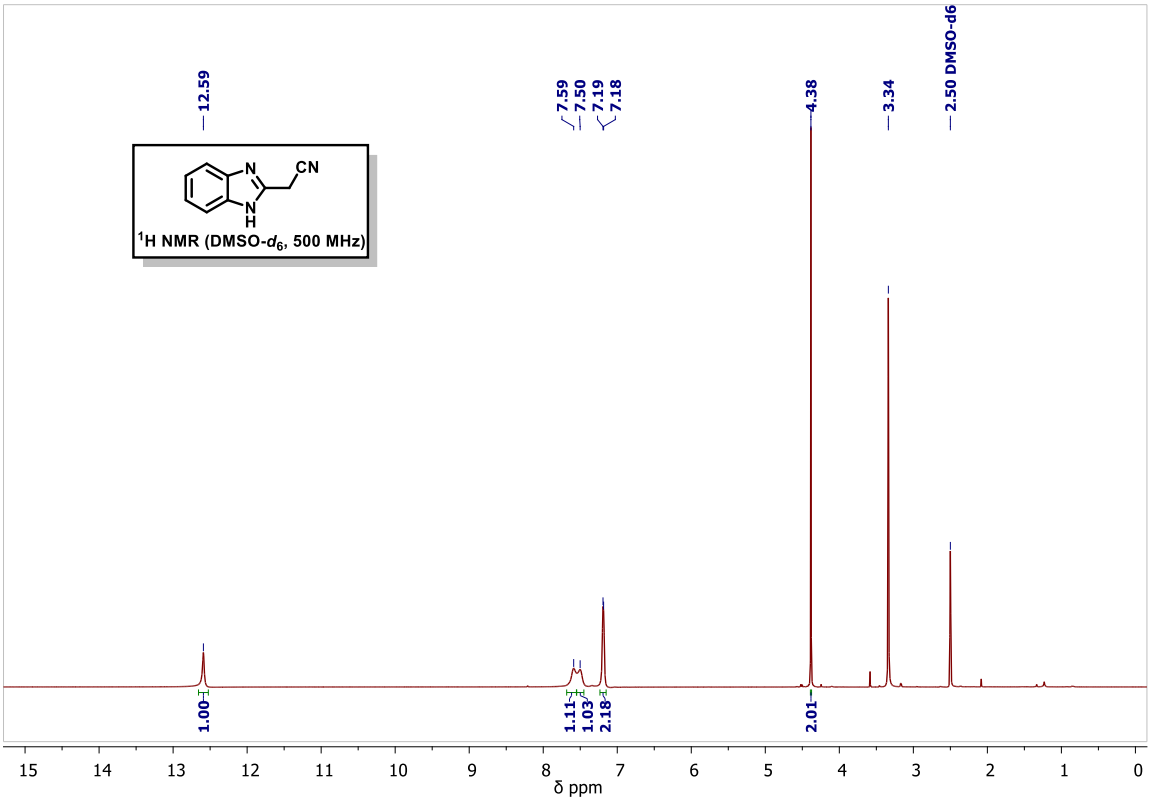


Figure S1. ^{1}H NMR spectra (500 MHz, RT) of compound **A** in DMSO-d_6.

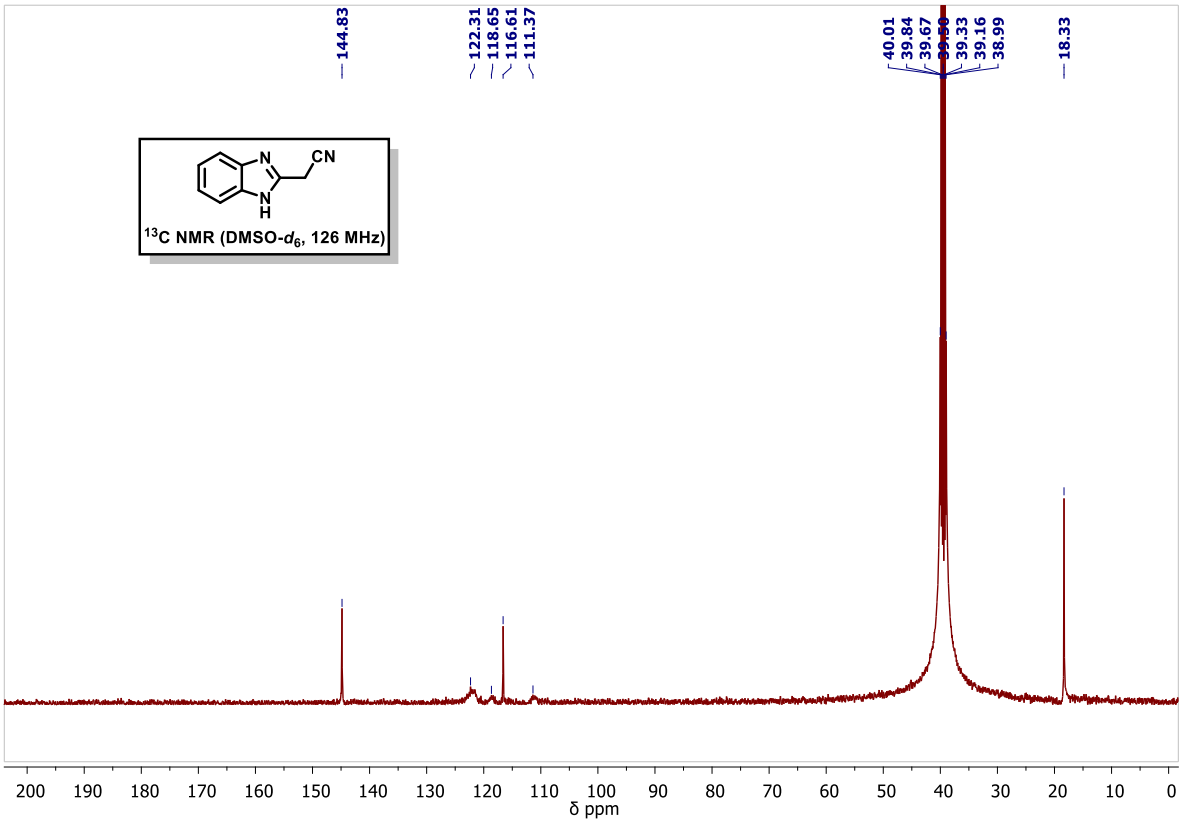


Figure S2. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **A** in DMSO-d_6.

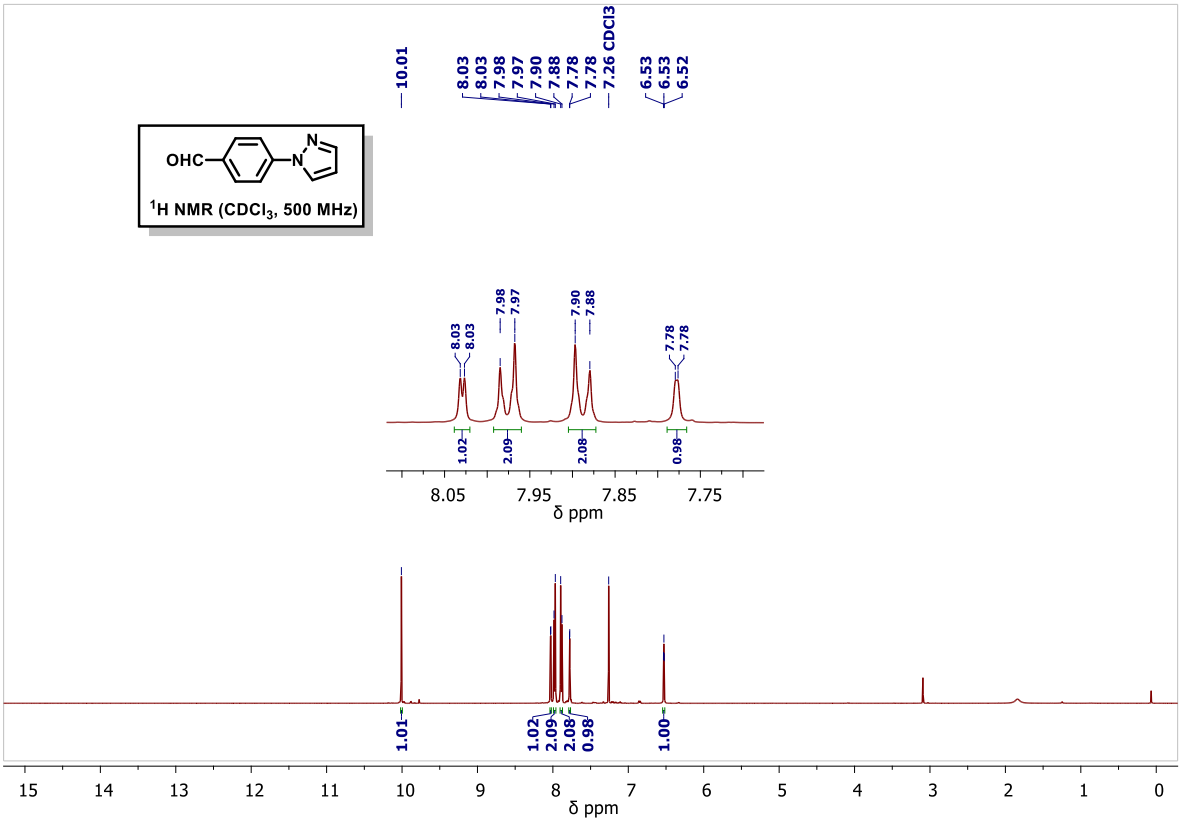


Figure S3. ^{1}H NMR spectra (500 MHz, RT) of compound **B** in $CDCl_3$.

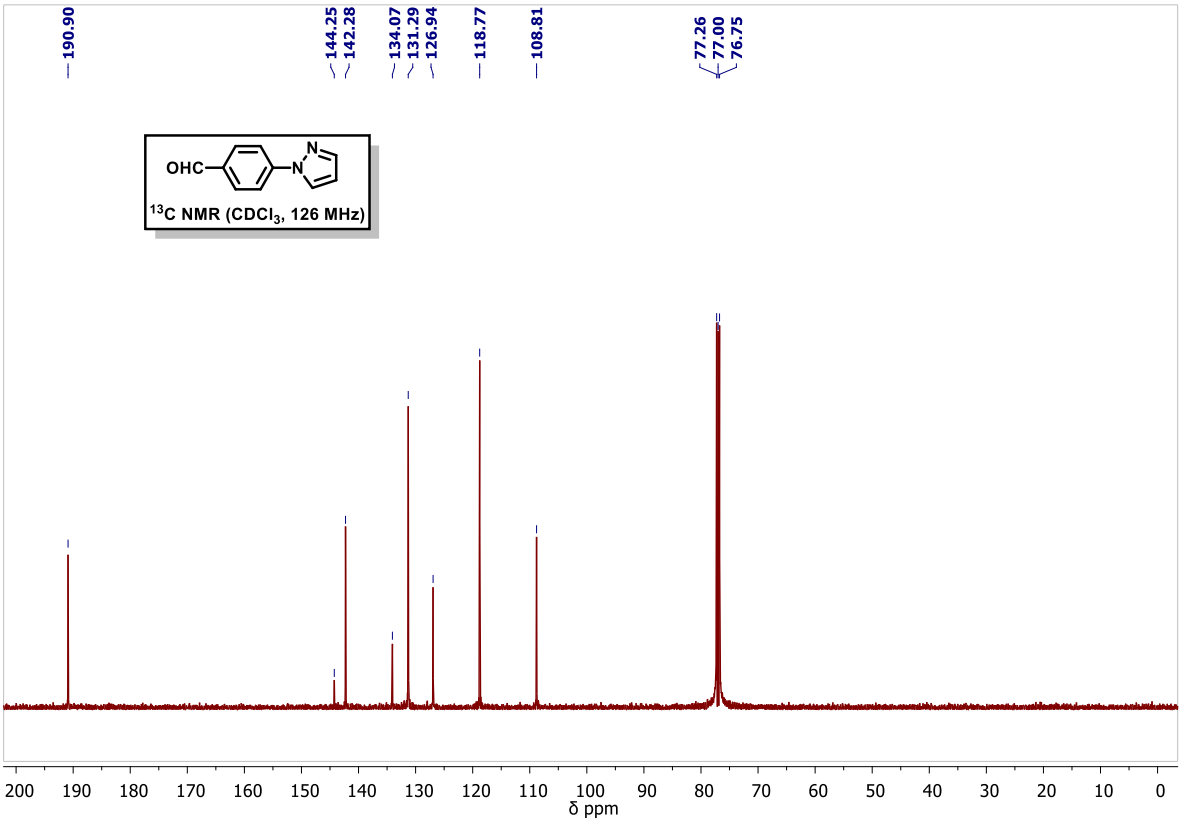


Figure S4. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **B** in $CDCl_3$.

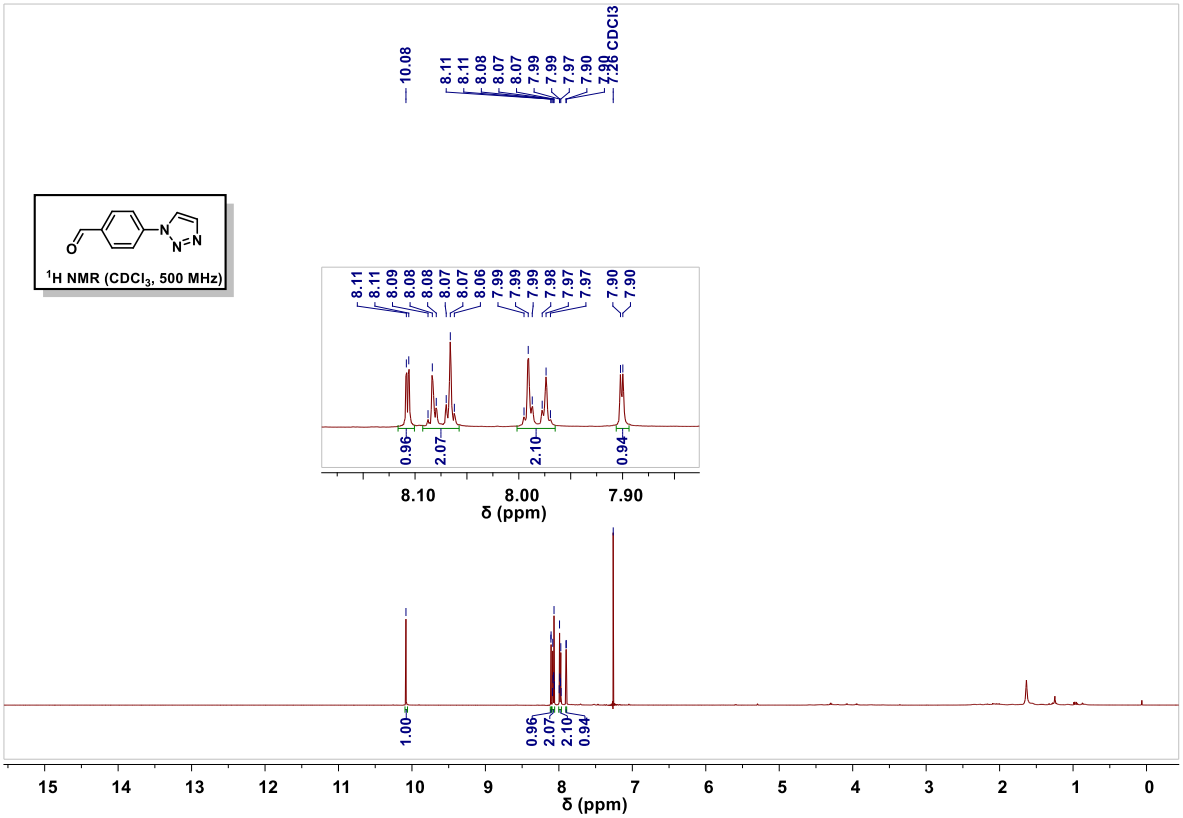


Figure S5. ^{1}H NMR spectra (500 MHz, RT) of compound **C** in $CDCl_3$.

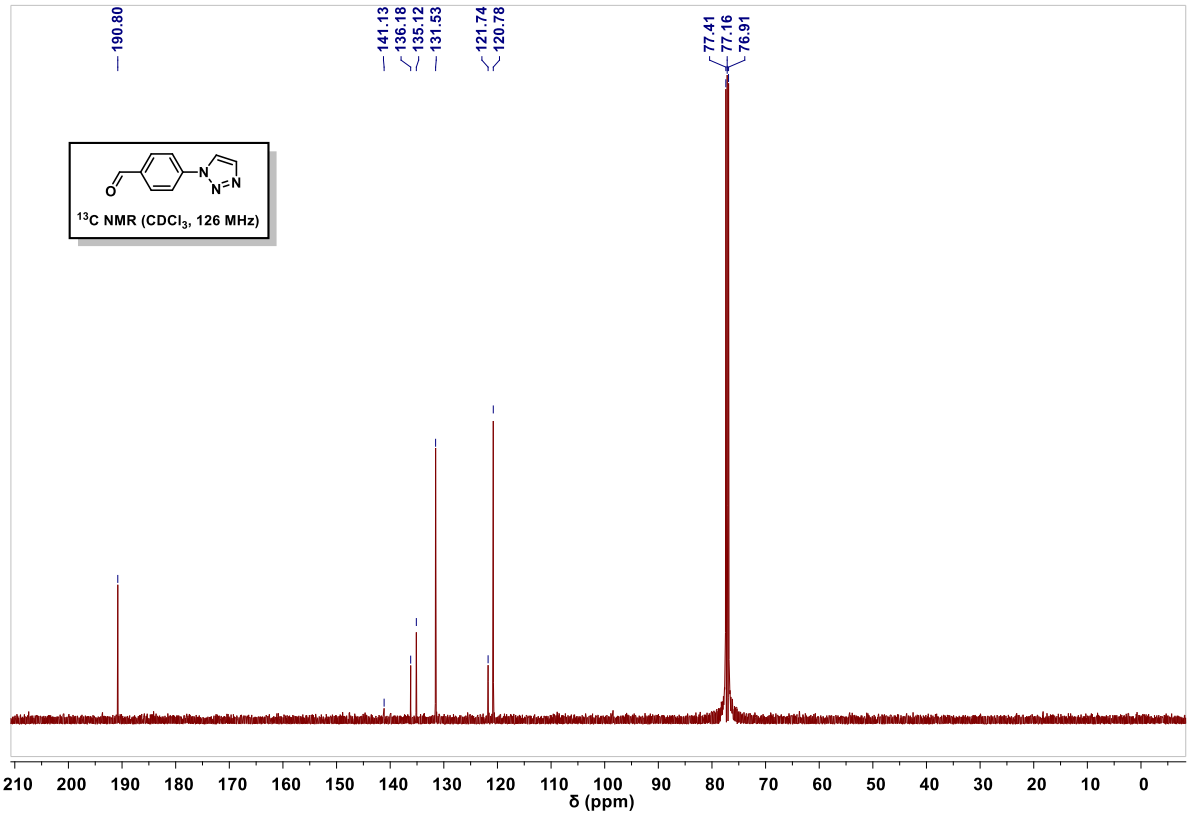


Figure S6. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **C** in $CDCl_3$.

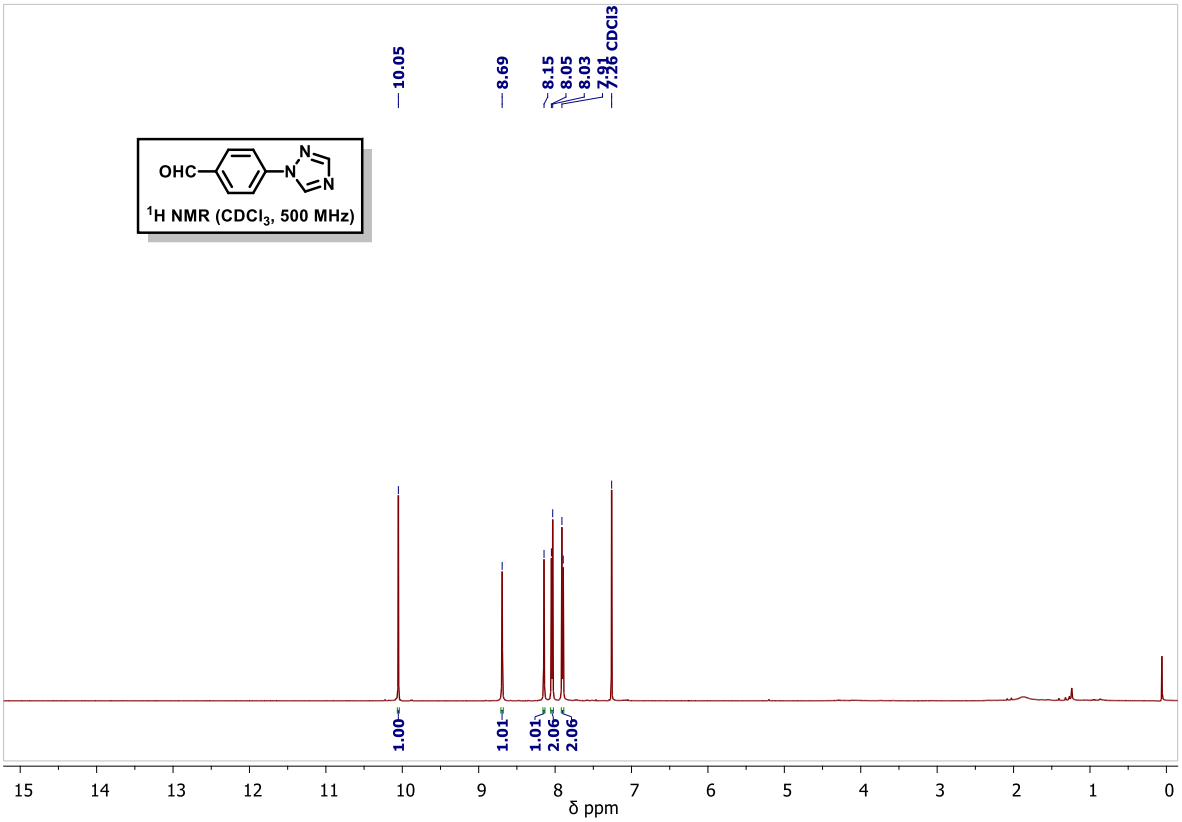


Figure S7. ^{1}H NMR spectra (500 MHz, RT) of compound **D** in $CDCl_3$.

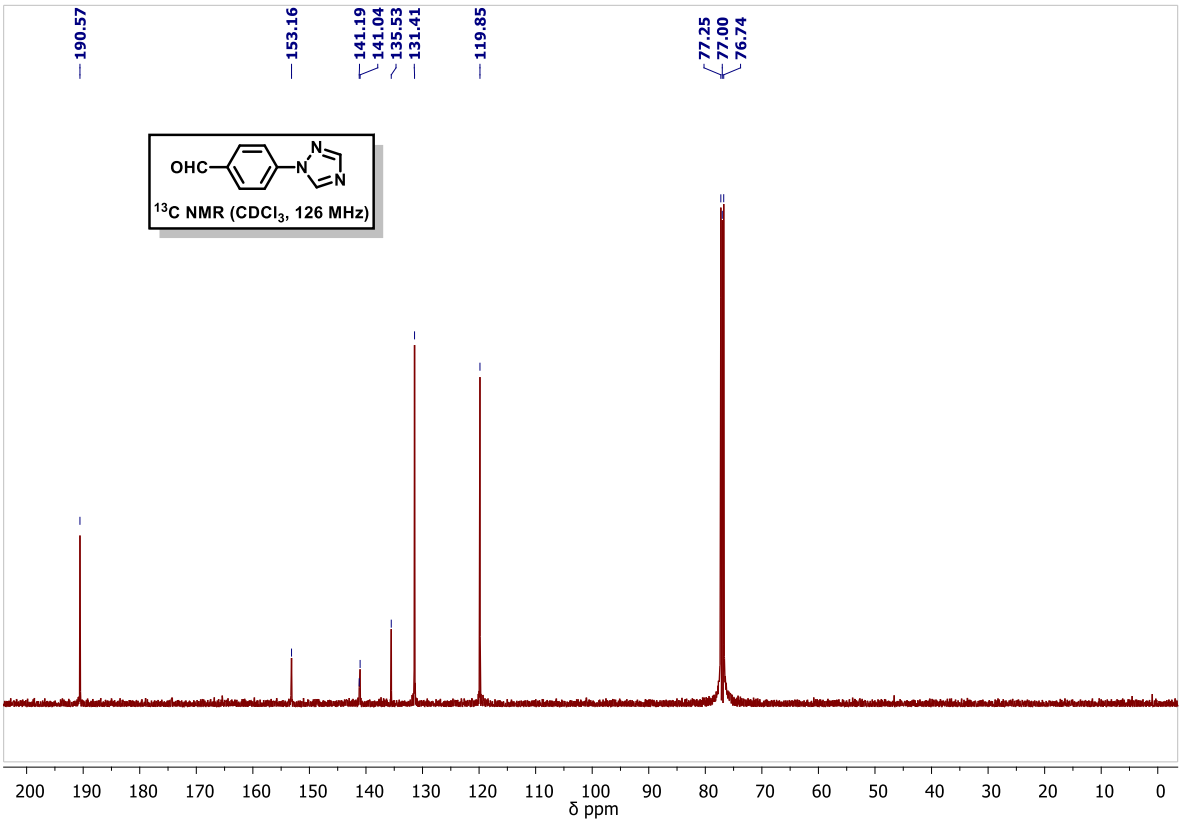


Figure S8. $^{13}C\{^1H\}$ NMR spectra (126 MHz, RT) of compound **D** in $CDCl_3$.

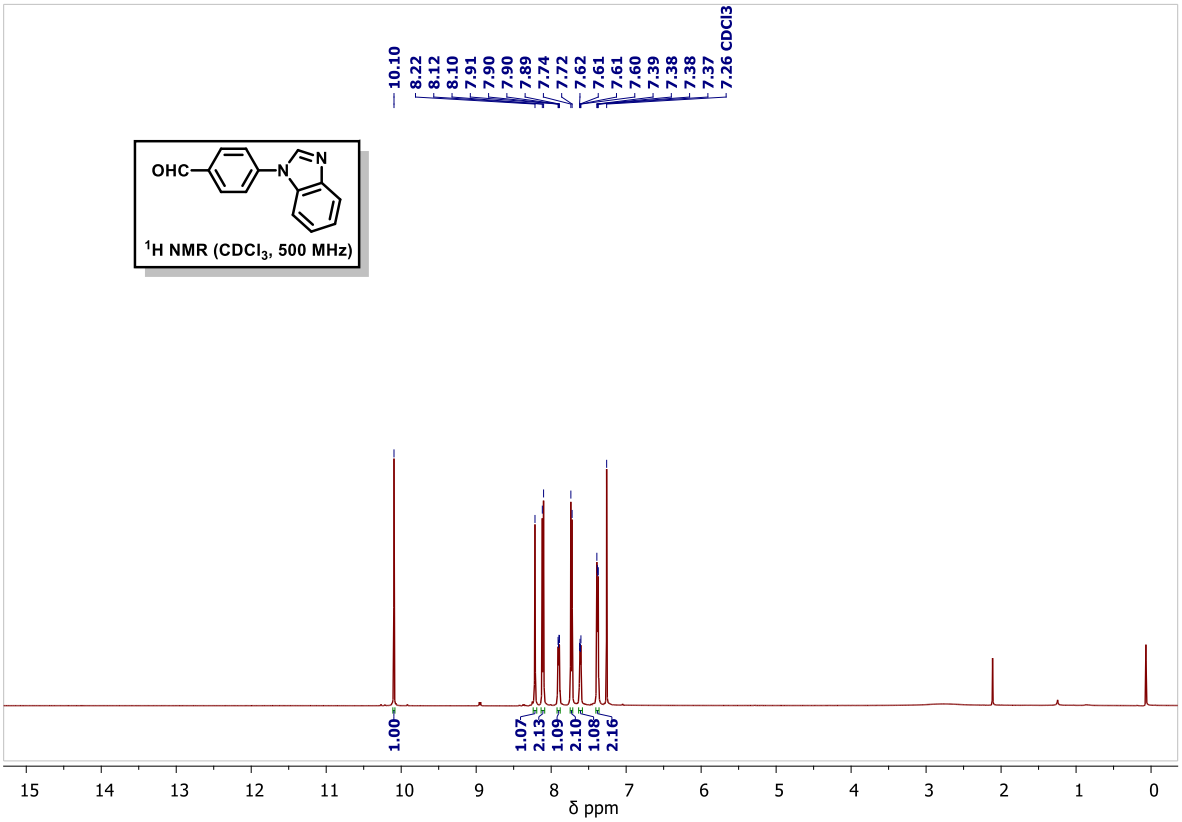


Figure S9. ^{1}H NMR spectra (500 MHz, RT) of compound **E** in $CDCl_3$.

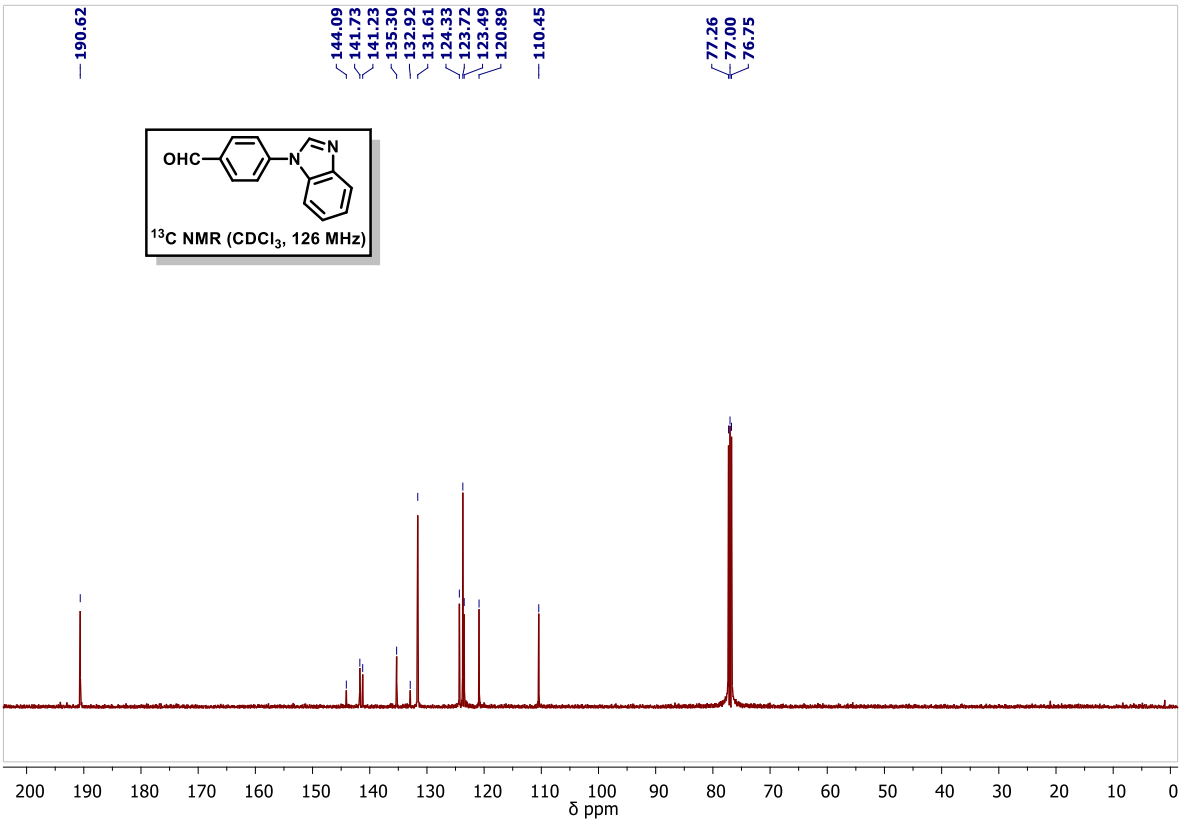


Figure S10. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **E** in $CDCl_3$.

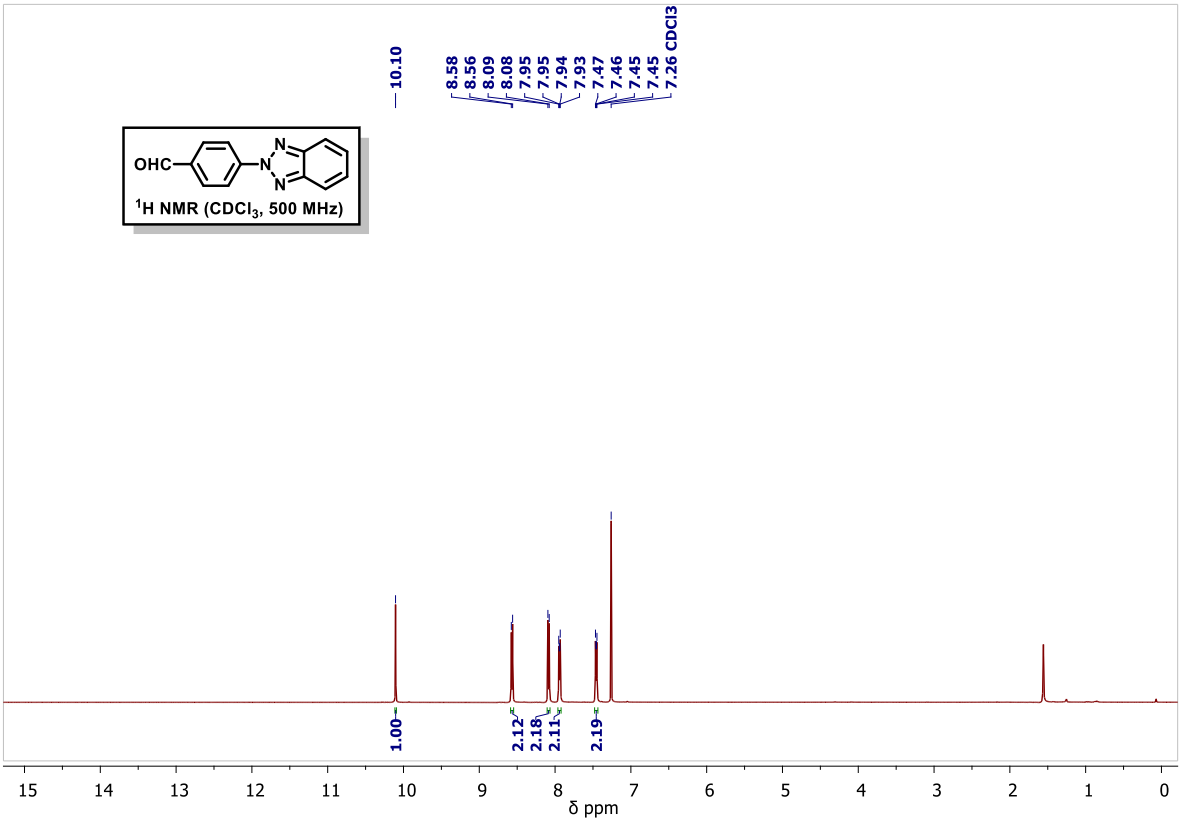


Figure S11. ^{1}H NMR spectra (500 MHz, RT) of compound **F** in $CDCl_3$.

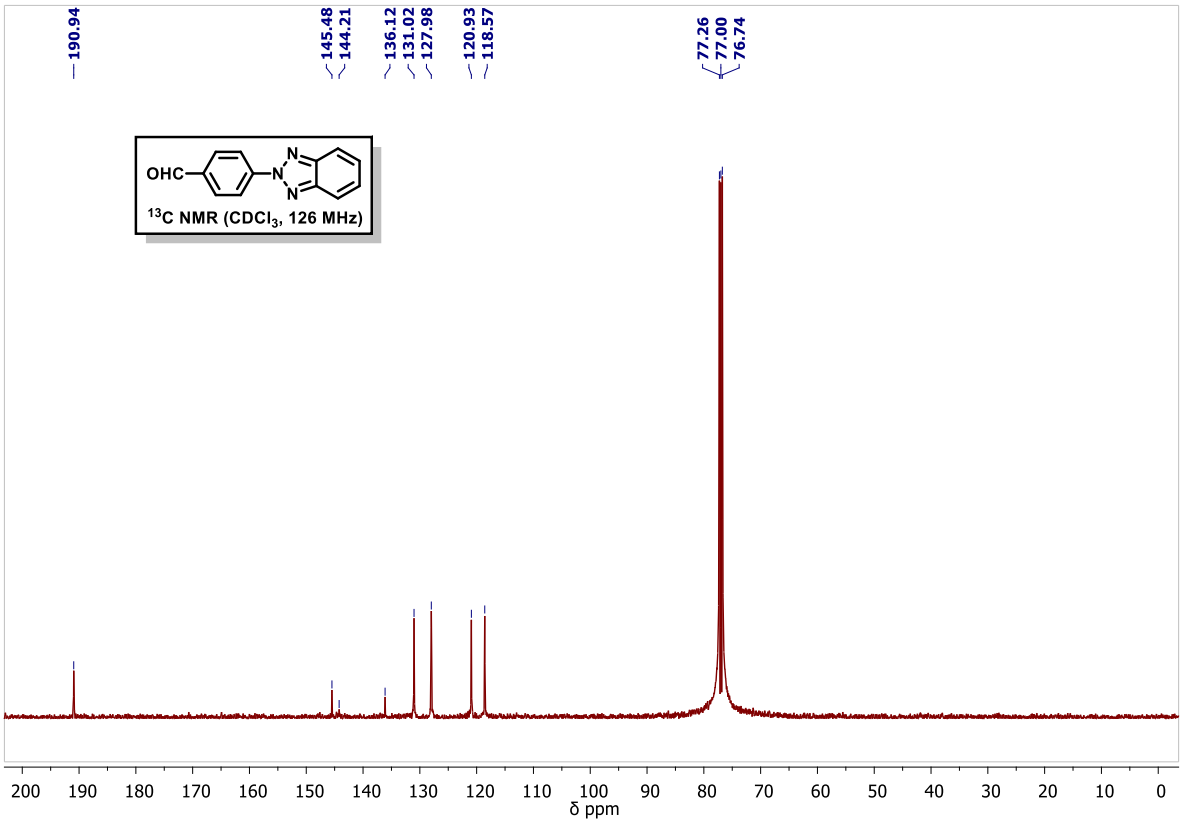


Figure S12. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **F** in DMSO-d_6.

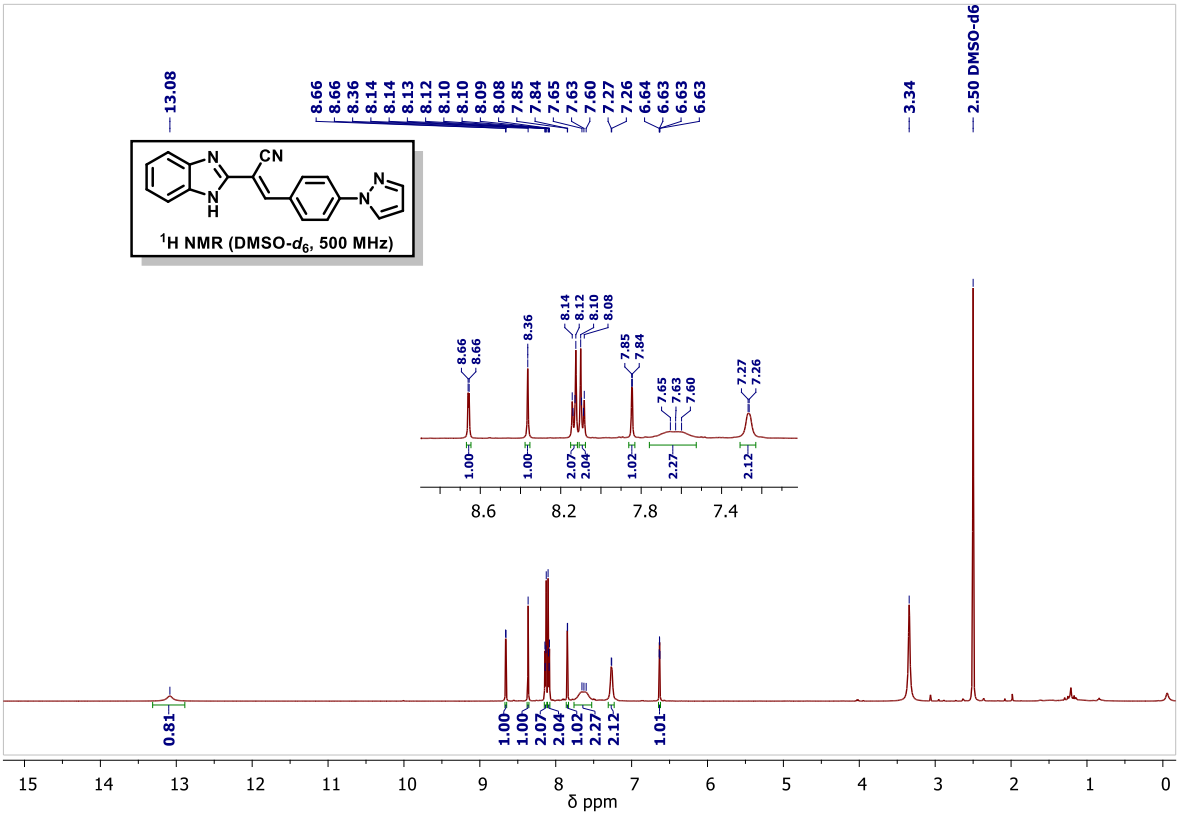


Figure S13. ^{1}H NMR spectra (500 MHz, RT) of compound **1** in DMSO-d_6.

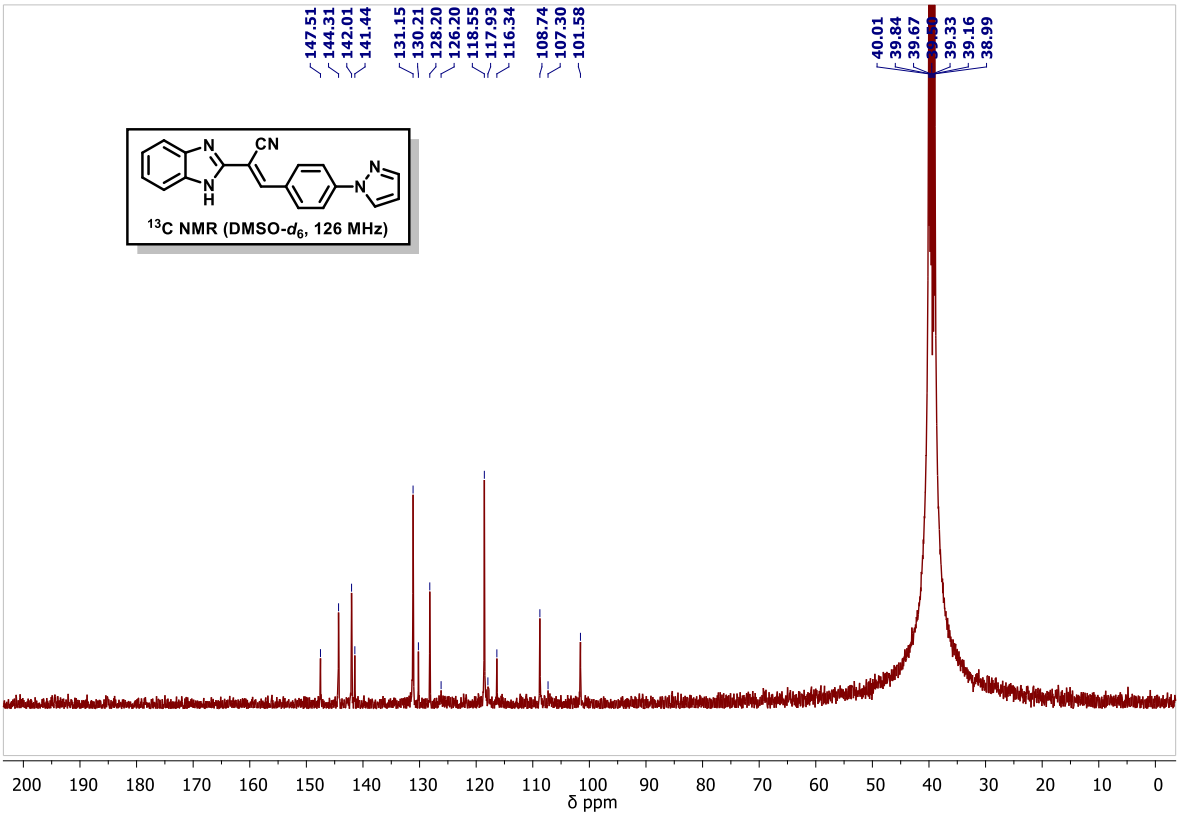


Figure S14. ^{13}C{^{1}H} NMR spectra (126 MHz, RT) of compound **1** in DMSO-d_6.

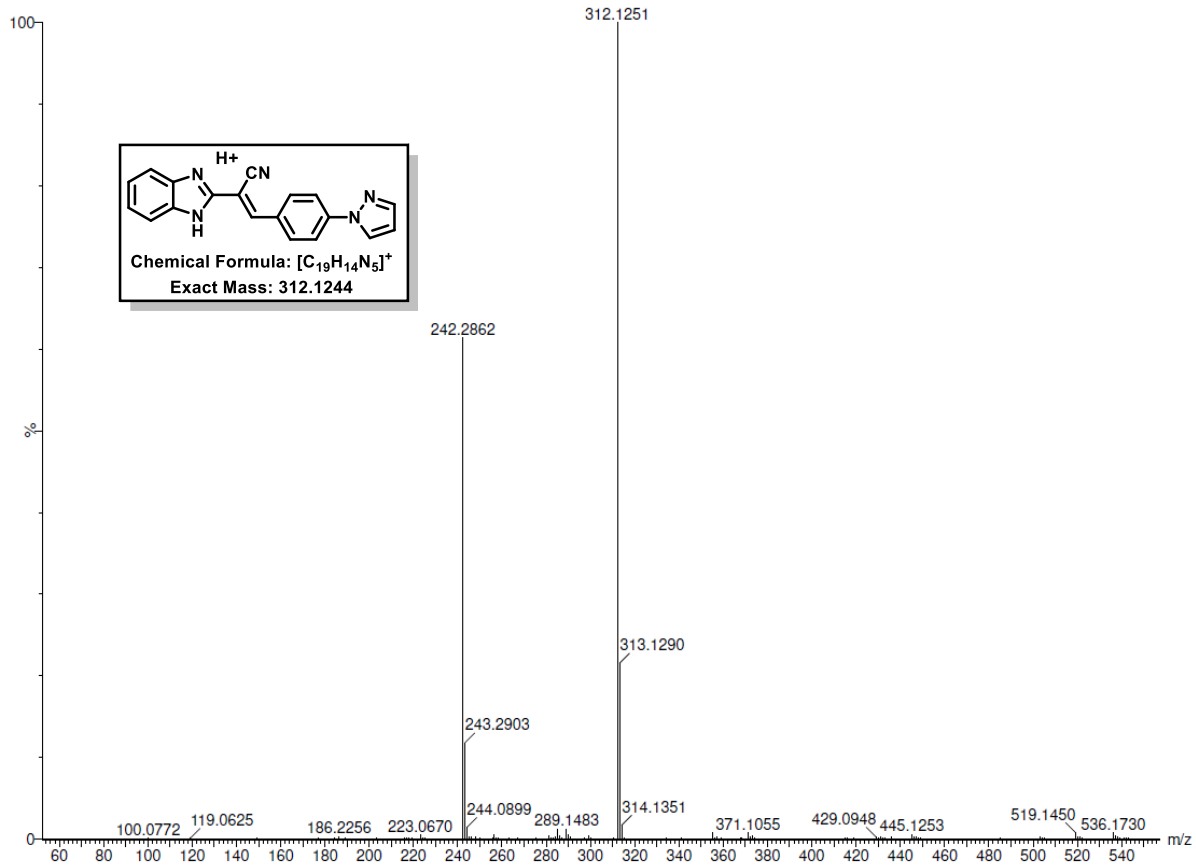


Figure S15. HRMS (ESI-TOF) spectrum of compound **1**.

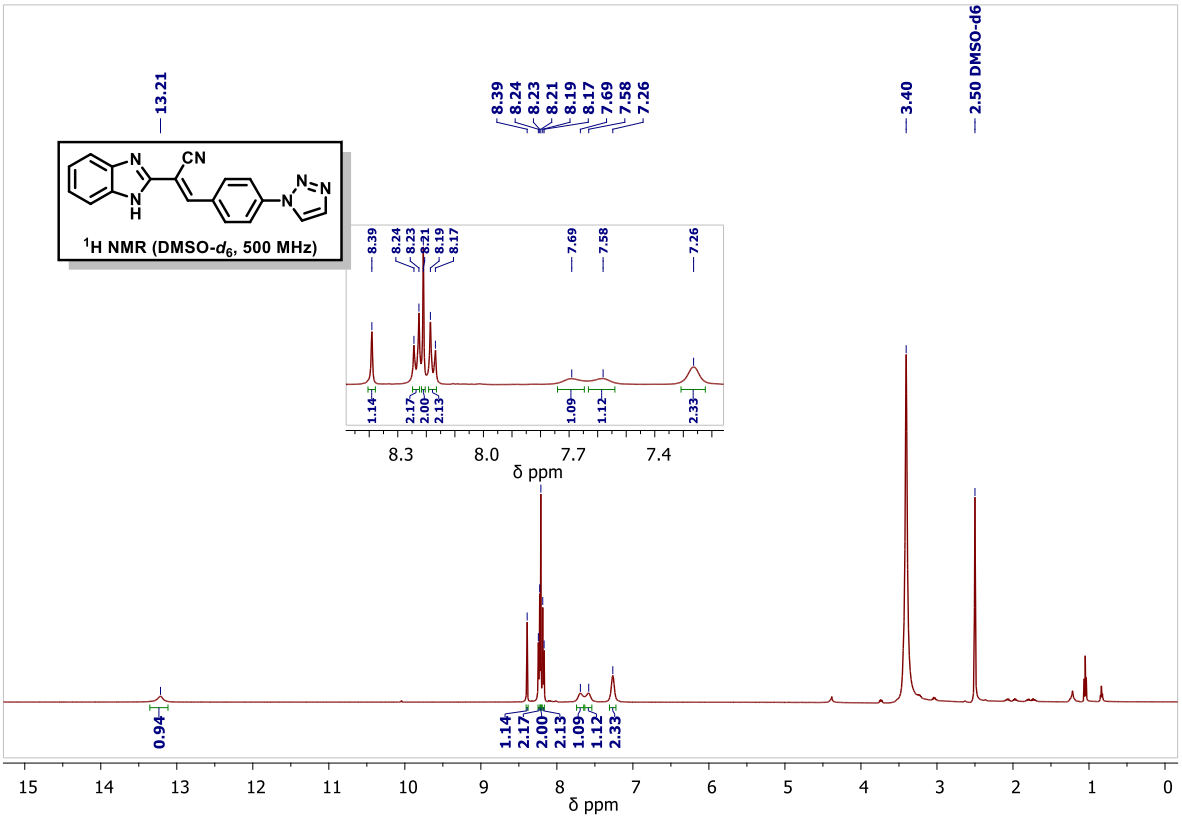


Figure S16. ^{1}H NMR spectra (500 MHz, RT) of compound **2** in DMSO-d_6.

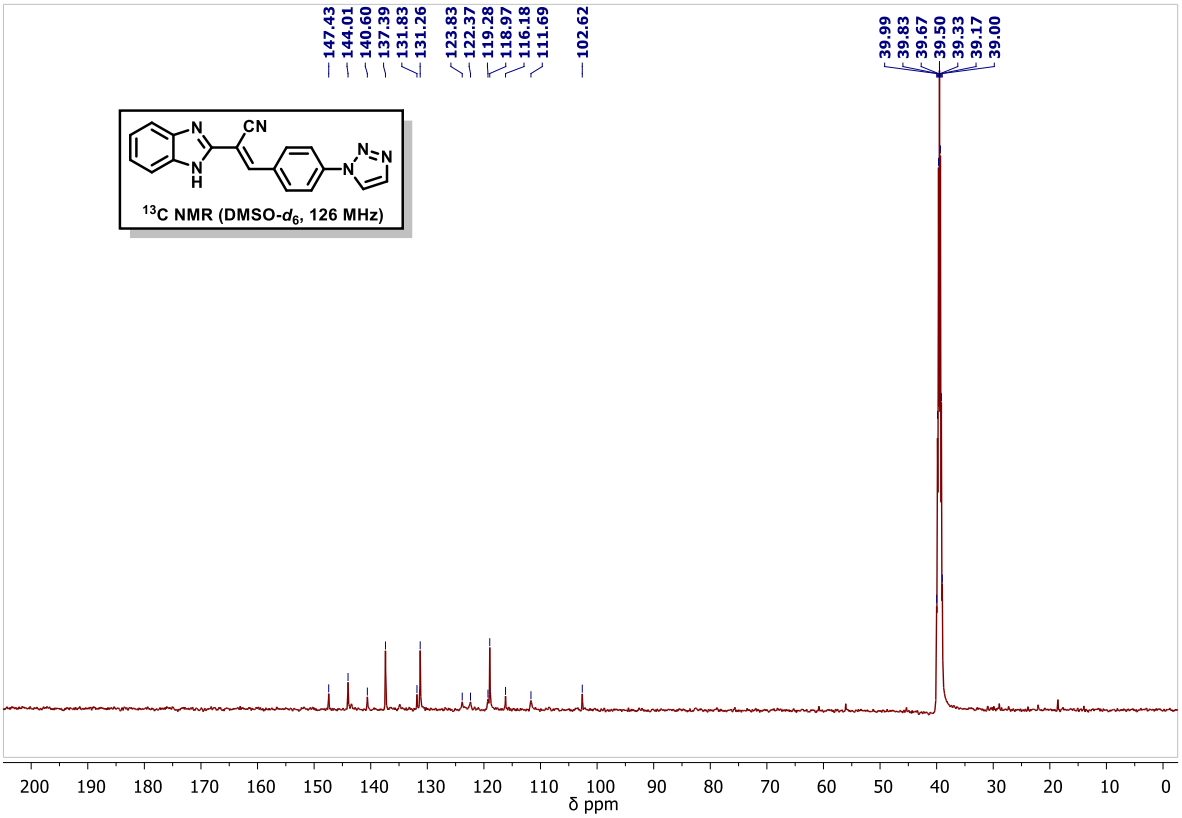


Figure S17. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **2** in DMSO-d_6.

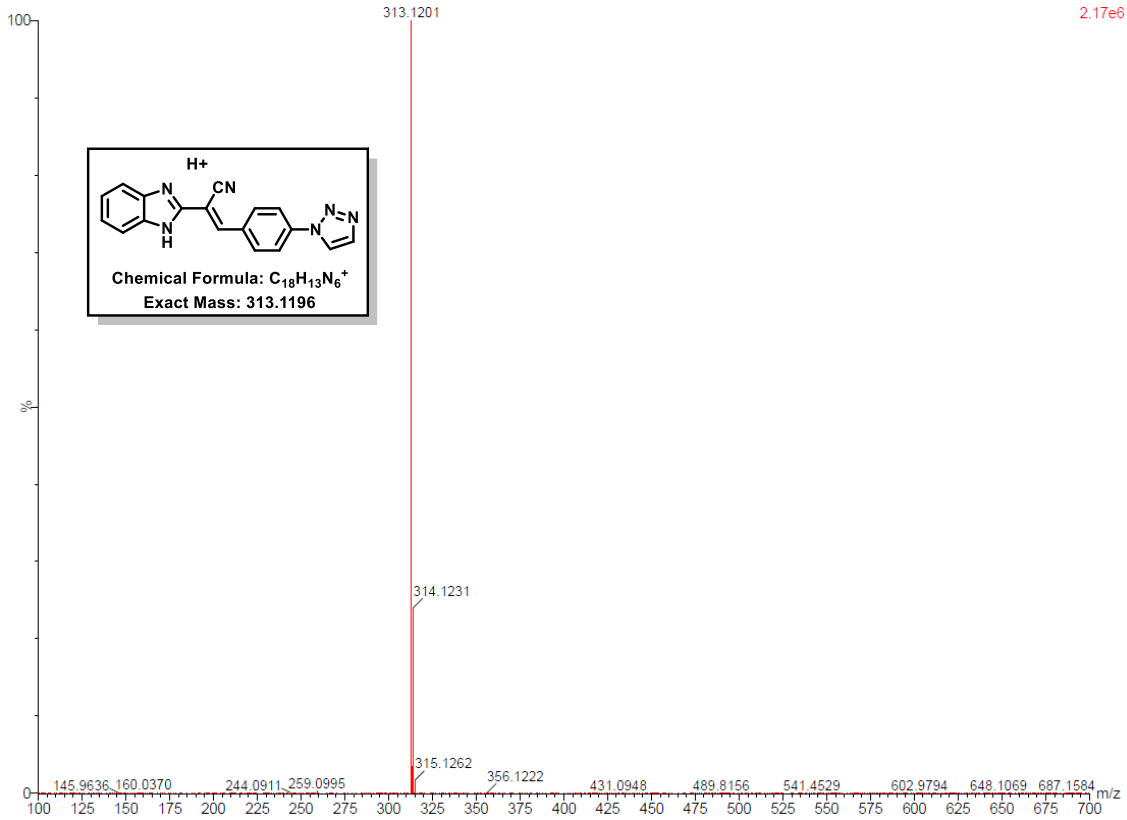


Figure S18. HRMS (ESI-TOF) spectrum of compound **2**.

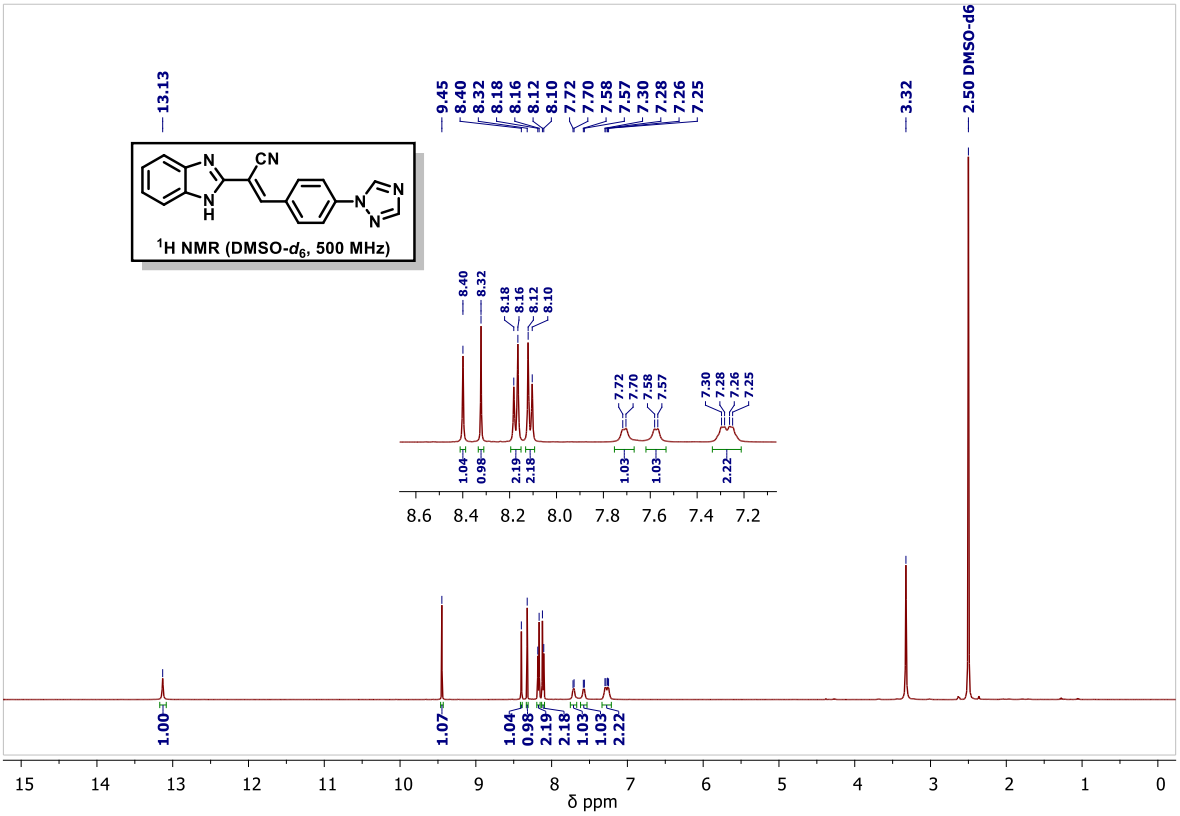


Figure S19. ^{1}H NMR spectra (500 MHz, RT) of compound **3** in DMSO-d_6.

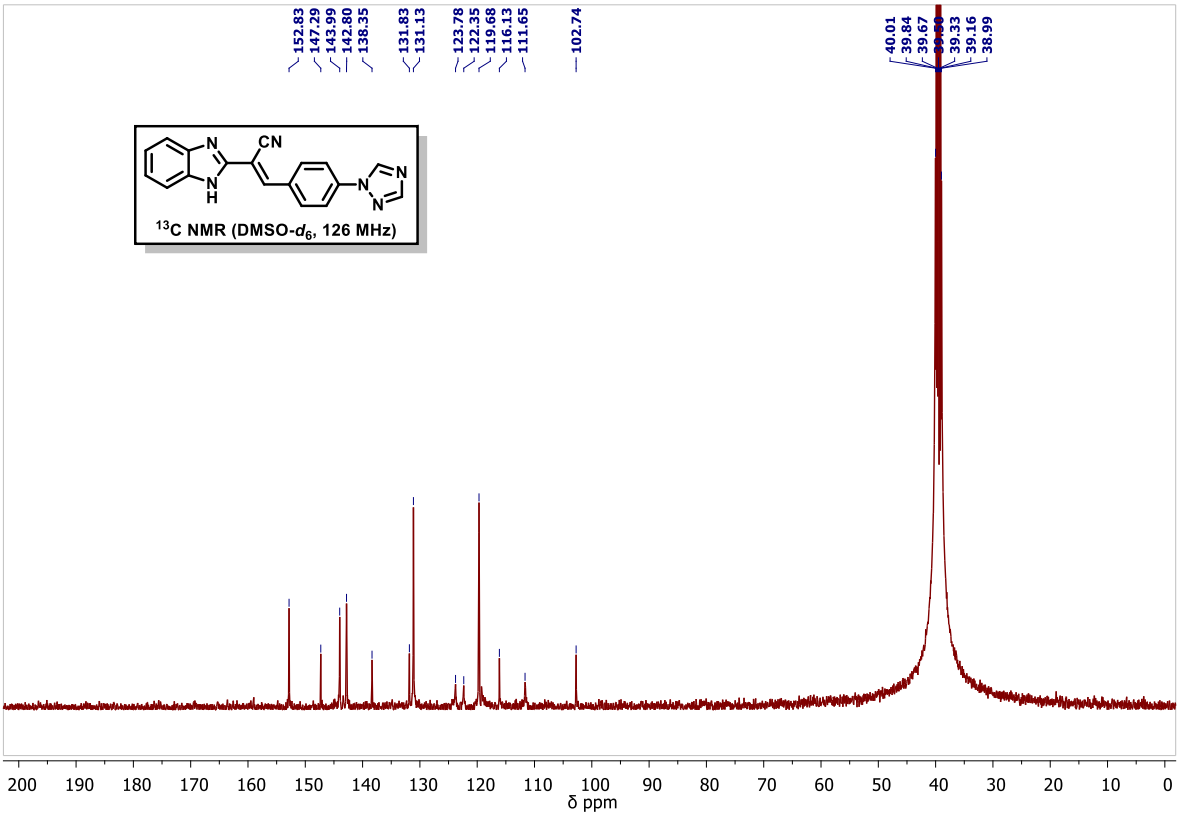


Figure S20. ^{13}C{^{1}H} NMR spectra (126 MHz, RT) of compound **3** in DMSO-d_6.

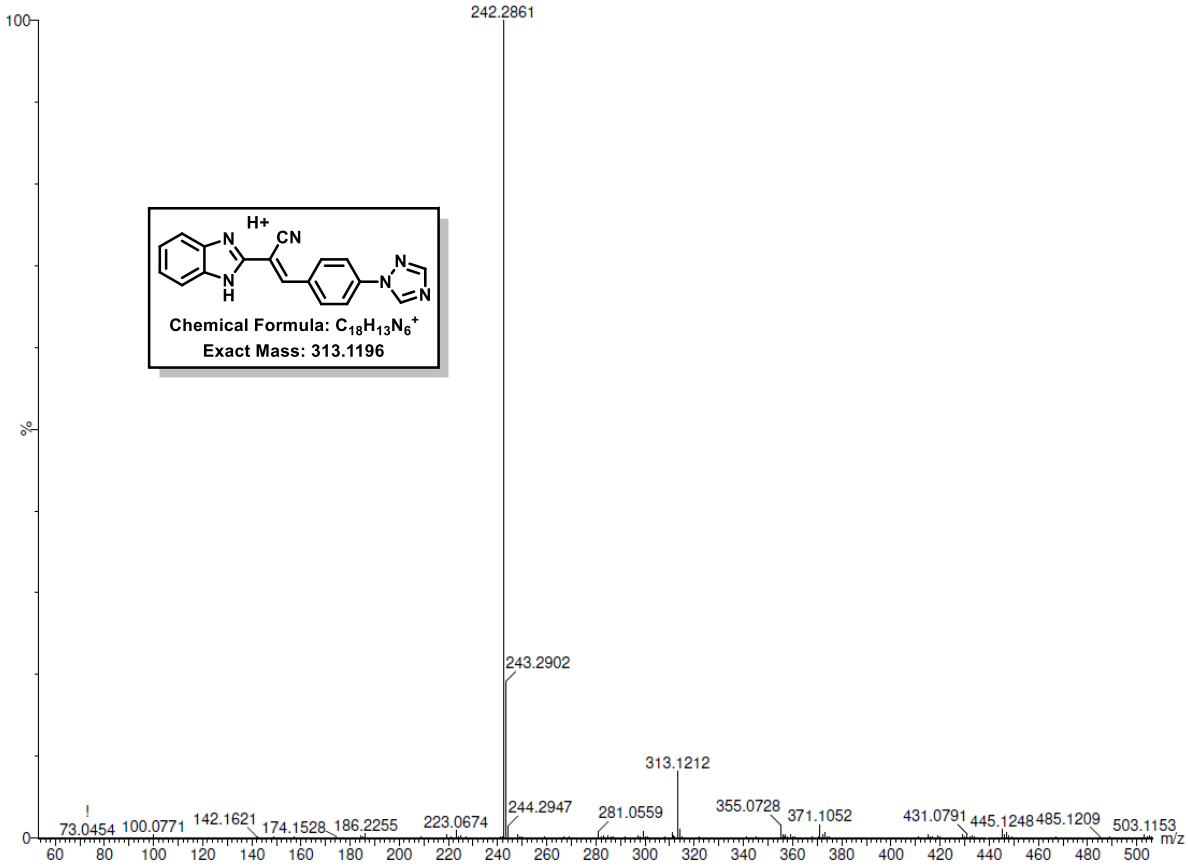


Figure S21. HRMS (ESI-TOF) spectrum of compound **3**.

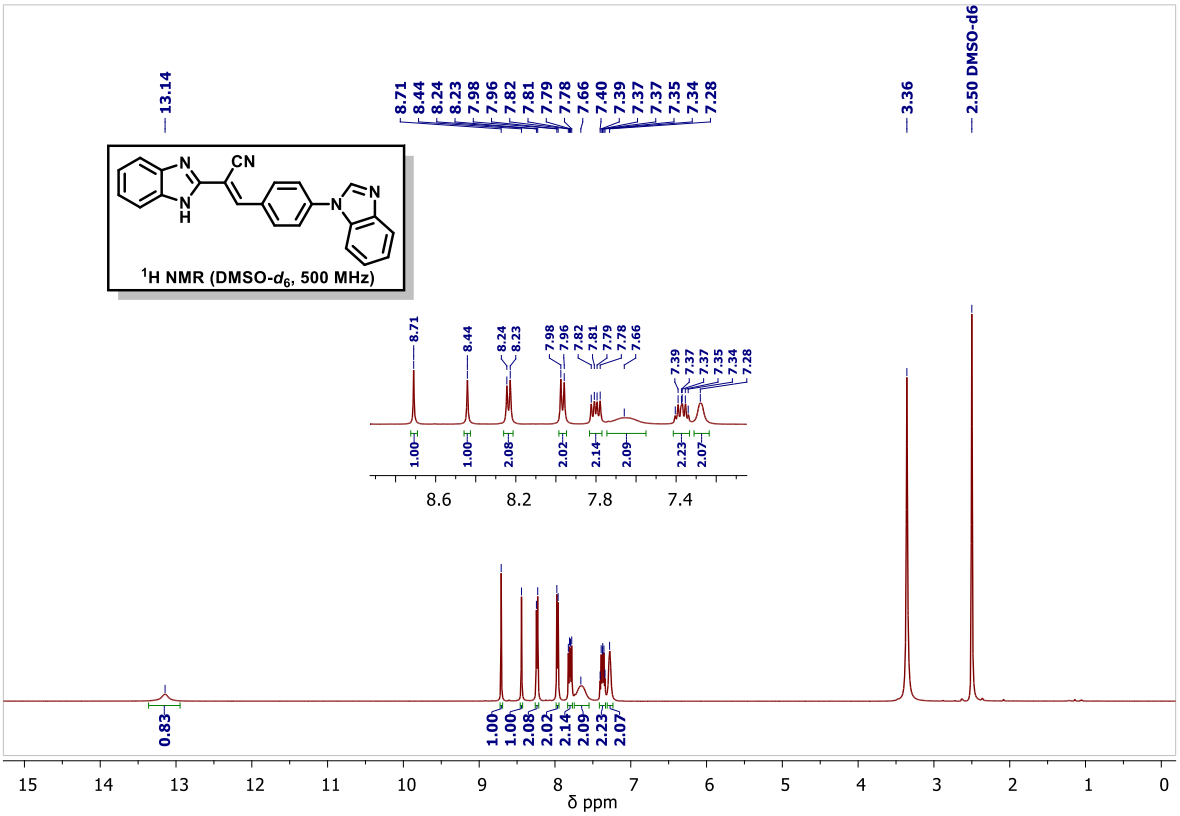


Figure S22. ^{1}H NMR spectra (500 MHz, RT) of compound **4** in DMSO-d_6.

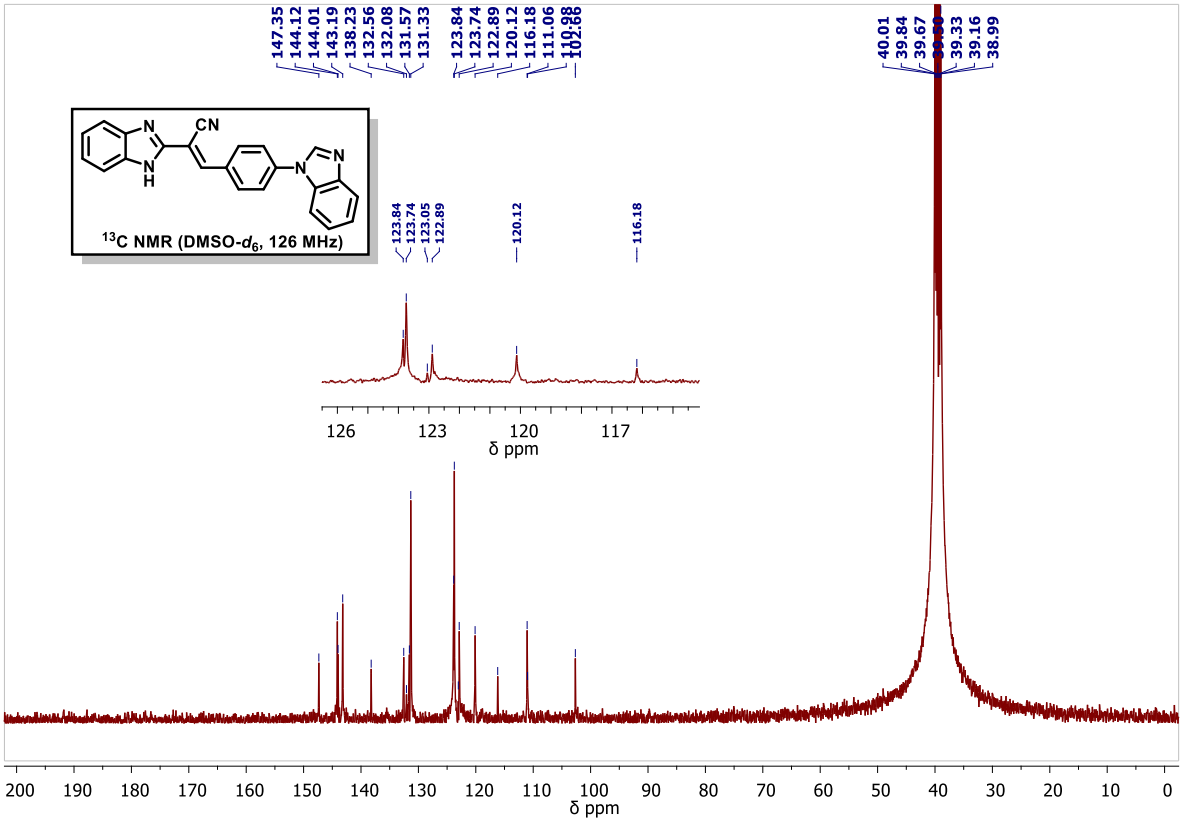


Figure S23. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, RT) of compound **4** in DMSO-d_6.

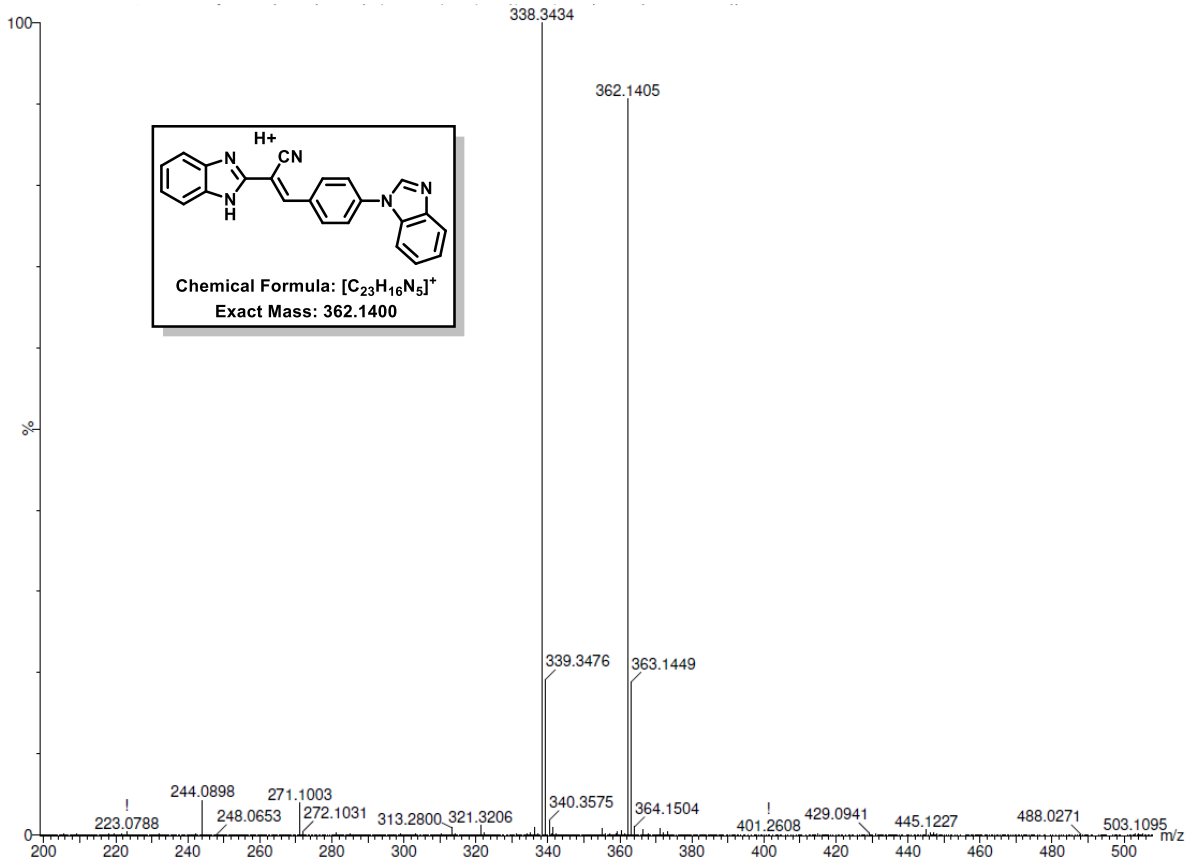


Figure S24. HRMS (ESI-TOF) spectrum of compound **4.**

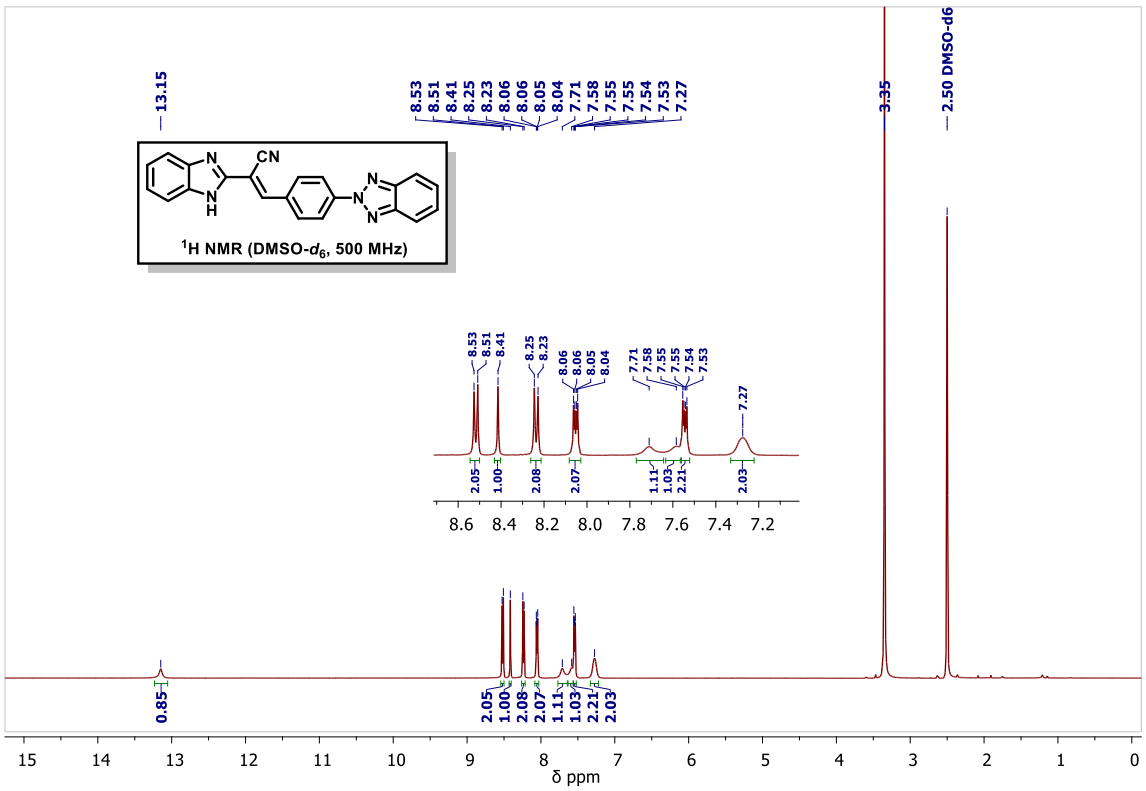


Figure S25. ^{1}H NMR spectra (500 MHz, RT) of compound **5** in DMSO-d_6.

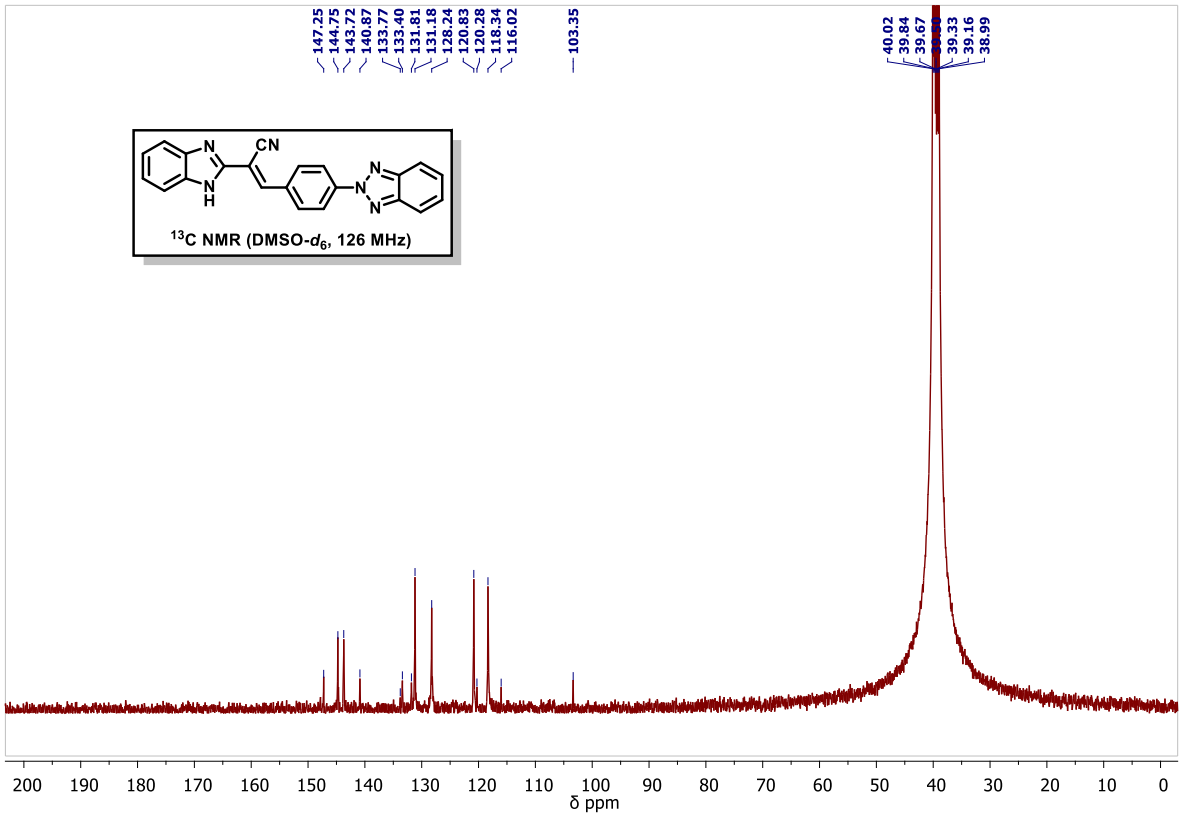


Figure S26. ^{13}C{^{1}H} NMR spectra (126 MHz, RT) of compound **5** in DMSO-d_6.

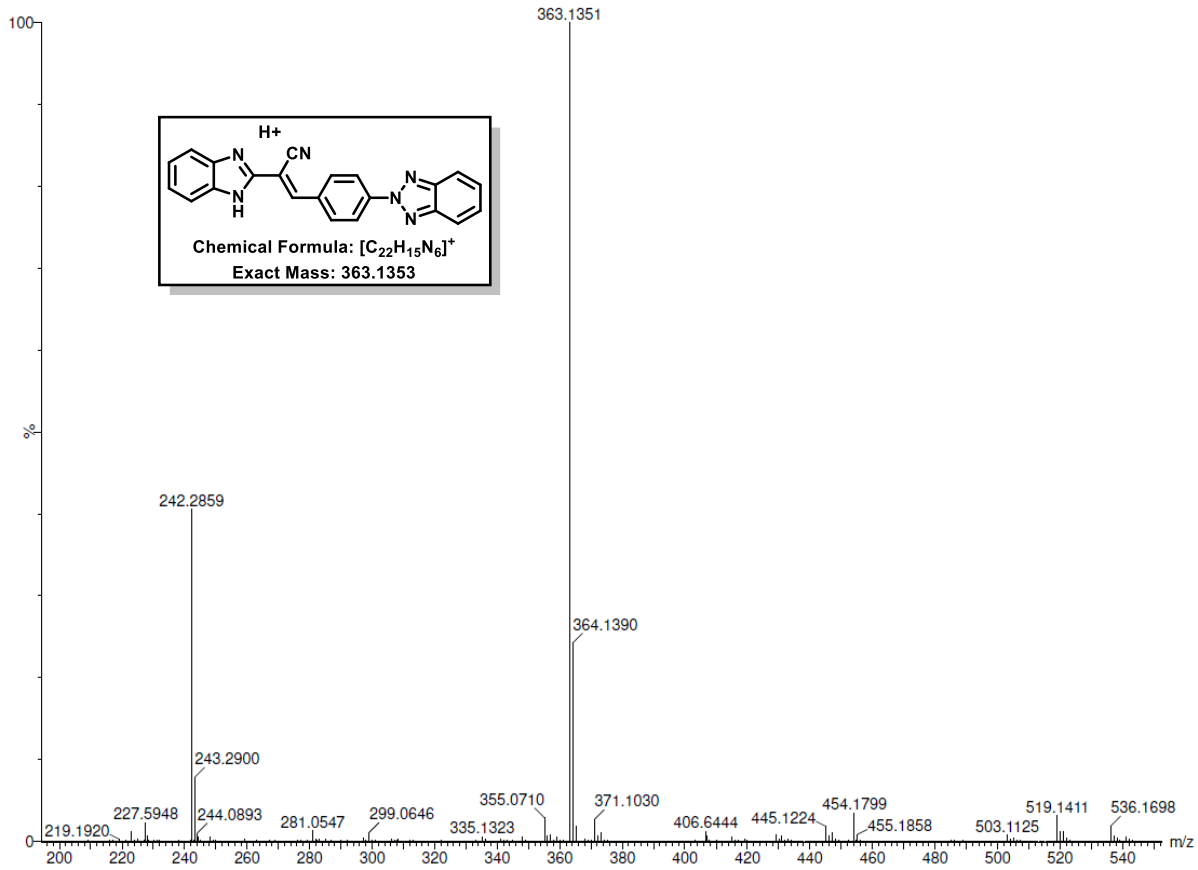


Figure S27. HRMS (ESI-TOF) spectrum of compound **5.**

2. Single Crystal XRD Data

Table S1. Crystal data and structure refinement parameters of compound **5.**

Identification code	**Compound 5**
CCDC Number	2498566
Empirical formula	$C_{22}H_{14}N_6$, C_3H_7NO (DMF)
Formula weight	435.49
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, Space group	Monoclinic, P 21/n
Unit cell dimensions	a = 6.2895(6) Å; α = 90°
	b = 42.092(5) Å; β = 105.185(4)°
	c = 8.6285(10) Å; γ = 90°
Volume	2204.5(4) A^3
Z, Calculated density	4, 1.312 Mg/m^3
Absorption coefficient	0.085 mm^{-1}

F(000)	912
Crystal size	0.365 x 0.258 x 0.175 mm^3
θ range for data collection	2.493 to 25.400 deg.
Index ranges	-7<=h<=6, -50<=k<=50, -10<=l<=10
Reflections collected / unique	23252 / 4048 [R(int) = 0.0767]
Completeness to θ = 25.242°	99.8 %

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **5**. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1067(3)	5172(1)	2035(2)	43(1)
C(2)	-787(4)	5368(1)	1502(3)	57(1)
C(3)	-676(4)	5599(1)	420(3)	56(1)
C(4)	1192(4)	5637(1)	-167(3)	55(1)
C(5)	3001(4)	5450(1)	318(3)	55(1)
C(6)	2929(3)	5210(1)	1443(2)	43(1)
C(7)	4488(3)	4574(1)	4059(2)	40(1)
C(8)	3409(3)	4430(1)	5071(2)	49(1)
C(9)	4360(3)	4172(1)	5987(2)	51(1)
C(10)	6389(3)	4053(1)	5899(2)	42(1)
C(11)	7421(3)	4206(1)	4862(2)	51(1)
C(12)	6504(3)	4467(1)	3953(3)	52(1)
C(13)	7504(3)	3779(1)	6791(2)	44(1)
C(14)	7059(3)	3611(1)	7996(2)	41(1)
C(15)	5324(4)	3691(1)	8715(3)	52(1)
C(16)	8350(3)	3336(1)	8751(2)	41(1)
C(17)	9559(3)	2954(1)	10375(2)	46(1)
C(18)	9961(4)	2729(1)	11605(3)	65(1)
C(19)	11696(4)	2524(1)	11724(3)	72(1)
C(20)	13029(4)	2541(1)	10669(3)	71(1)
C(21)	12673(4)	2762(1)	9452(3)	58(1)
C(22)	10907(3)	2967(1)	9327(2)	44(1)
C(23)	12882(5)	3280(1)	4950(3)	71(1)
C(24)	12032(5)	3640(1)	2723(3)	80(1)

C(25)	15261(5)	3287(1)	3164(4)	98(1)
N(1)	1426(3)	4929(1)	3094(2)	48(1)
N(2)	3447(2)	4835(1)	3097(2)	41(1)
N(3)	4456(3)	4993(1)	2143(2)	48(1)
N(4)	7954(3)	3188(1)	9995(2)	48(1)
N(5)	10078(3)	3212(1)	8279(2)	46(1)
N(6)	3956(4)	3755(1)	9308(3)	82(1)
N(7)	13382(3)	3393(1)	3683(2)	60(1)
O(1)	11342(3)	3367(1)	5476(2)	91(1)

Table S3. Bond lengths [Å] and angles [°] for compound **5**.

C(1)-N(1)	1.352(2)
C(1)-C(2)	1.403(3)
C(1)-C(6)	1.404(3)
C(2)-C(3)	1.363(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.405(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.357(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.409(3)
C(5)-H(5)	0.9300
C(6)-N(3)	1.349(2)
C(7)-C(12)	1.371(3)
C(7)-C(8)	1.378(3)
C(7)-N(2)	1.431(2)
C(8)-C(9)	1.383(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.391(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.393(3)
C(10)-C(13)	1.460(3)
C(11)-C(12)	1.385(3)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.347(3)
C(13)-H(13)	0.9300

C(14)-C(15)	1.430(3)
C(14)-C(16)	1.465(3)
C(15)-N(6)	1.142(3)
C(16)-N(4)	1.319(2)
C(16)-N(5)	1.360(2)
C(17)-N(4)	1.386(3)
C(17)-C(22)	1.392(3)
C(17)-C(18)	1.398(3)
C(18)-C(19)	1.373(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.391(4)
C(19)-H(19)	0.9300
C(20)-C(21)	1.378(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.389(3)
C(21)-H(21)	0.9300
C(22)-N(5)	1.380(2)
C(23)-O(1)	1.227(3)
C(23)-N(7)	1.303(3)
C(23)-H(23)	0.9300
C(24)-N(7)	1.457(3)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-N(7)	1.439(3)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
N(1)-N(2)	1.330(2)
N(2)-N(3)	1.340(2)
N(5)-H(5N)	0.92(2)

N(1)-C(1)-C(2)	130.05(19)
N(1)-C(1)-C(6)	108.91(16)
C(2)-C(1)-C(6)	121.03(18)
C(3)-C(2)-C(1)	117.1(2)
C(3)-C(2)-H(2)	121.4
C(1)-C(2)-H(2)	121.4

C(2)-C(3)-C(4)	121.71(19)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	122.4(2)
C(5)-C(4)-H(4)	118.8
C(3)-C(4)-H(4)	118.8
C(4)-C(5)-C(6)	116.9(2)
C(4)-C(5)-H(5)	121.6
C(6)-C(5)-H(5)	121.6
N(3)-C(6)-C(1)	108.91(16)
N(3)-C(6)-C(5)	130.27(18)
C(1)-C(6)-C(5)	120.81(18)
C(12)-C(7)-C(8)	121.06(18)
C(12)-C(7)-N(2)	120.27(17)
C(8)-C(7)-N(2)	118.67(17)
C(7)-C(8)-C(9)	119.77(18)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(8)-C(9)-C(10)	121.02(18)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	117.30(18)
C(9)-C(10)-C(13)	125.10(17)
C(11)-C(10)-C(13)	117.60(18)
C(12)-C(11)-C(10)	122.34(19)
C(12)-C(11)-H(11)	118.8
C(10)-C(11)-H(11)	118.8
C(7)-C(12)-C(11)	118.50(18)
C(7)-C(12)-H(12)	120.8
C(11)-C(12)-H(12)	120.8
C(14)-C(13)-C(10)	130.92(19)
C(14)-C(13)-H(13)	114.5
C(10)-C(13)-H(13)	114.5
C(13)-C(14)-C(15)	123.06(18)
C(13)-C(14)-C(16)	123.79(18)
C(15)-C(14)-C(16)	113.10(16)
N(6)-C(15)-C(14)	179.1(3)
N(4)-C(16)-N(5)	113.52(17)

N(4)-C(16)-C(14)	122.21(17)
N(5)-C(16)-C(14)	124.26(16)
N(4)-C(17)-C(22)	110.41(17)
N(4)-C(17)-C(18)	129.60(19)
C(22)-C(17)-C(18)	119.98(19)
C(19)-C(18)-C(17)	117.7(2)
C(19)-C(18)-H(18)	121.1
C(17)-C(18)-H(18)	121.1
C(18)-C(19)-C(20)	121.6(2)
C(18)-C(19)-H(19)	119.2
C(20)-C(19)-H(19)	119.2
C(21)-C(20)-C(19)	121.8(2)
C(21)-C(20)-H(20)	119.1
C(19)-C(20)-H(20)	119.1
C(20)-C(21)-C(22)	116.5(2)
C(20)-C(21)-H(21)	121.7
C(22)-C(21)-H(21)	121.7
N(5)-C(22)-C(21)	132.23(19)
N(5)-C(22)-C(17)	105.34(17)
C(21)-C(22)-C(17)	122.43(19)
O(1)-C(23)-N(7)	126.1(3)
O(1)-C(23)-H(23)	116.9
N(7)-C(23)-H(23)	116.9
N(7)-C(24)-H(24A)	109.5
N(7)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
N(7)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(7)-C(25)-H(25A)	109.5
N(7)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(7)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(2)-N(1)-C(1)	102.52(15)
N(1)-N(2)-N(3)	117.25(15)
N(1)-N(2)-C(7)	121.45(15)

N(3)-N(2)-C(7)	121.29(15)
N(2)-N(3)-C(6)	102.40(15)
C(16)-N(4)-C(17)	104.20(16)
C(16)-N(5)-C(22)	106.51(16)
C(16)-N(5)-H(5N)	129.8(15)
C(22)-N(5)-H(5N)	123.7(15)
C(23)-N(7)-C(25)	123.2(3)
C(23)-N(7)-C(24)	120.2(2)
C(25)-N(7)-C(24)	116.6(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **5**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	45(1)	42(1)	42(1)	1(1)	10(1)	4(1)
C(2)	48(1)	61(1)	63(1)	6(1)	19(1)	14(1)
C(3)	51(1)	53(1)	60(1)	5(1)	10(1)	17(1)
C(4)	59(1)	48(1)	55(1)	13(1)	9(1)	8(1)
C(5)	50(1)	55(1)	61(1)	17(1)	18(1)	8(1)
C(6)	41(1)	42(1)	44(1)	4(1)	8(1)	2(1)
C(7)	44(1)	36(1)	40(1)	3(1)	8(1)	1(1)
C(8)	43(1)	53(1)	55(1)	10(1)	18(1)	7(1)
C(9)	51(1)	53(1)	54(1)	14(1)	21(1)	2(1)
C(10)	45(1)	39(1)	41(1)	2(1)	12(1)	1(1)
C(11)	47(1)	52(1)	58(1)	12(1)	21(1)	10(1)
C(12)	52(1)	53(1)	56(1)	16(1)	24(1)	7(1)
C(13)	46(1)	41(1)	46(1)	3(1)	14(1)	1(1)
C(14)	45(1)	37(1)	43(1)	1(1)	13(1)	-2(1)
C(15)	62(1)	45(1)	55(1)	15(1)	26(1)	9(1)
C(16)	46(1)	38(1)	40(1)	1(1)	13(1)	-3(1)
C(17)	52(1)	41(1)	45(1)	4(1)	13(1)	0(1)
C(18)	75(2)	61(1)	63(2)	23(1)	25(1)	10(1)
C(19)	80(2)	61(2)	73(2)	27(1)	18(1)	16(1)
C(20)	68(2)	57(1)	84(2)	13(1)	13(1)	19(1)
C(21)	57(1)	54(1)	66(1)	1(1)	20(1)	7(1)

C(22)	47(1)	37(1)	46(1)	2(1)	11(1)	0(1)
C(23)	78(2)	79(2)	60(2)	2(1)	24(1)	-1(1)
C(24)	98(2)	85(2)	55(2)	5(1)	17(1)	-4(2)
C(25)	85(2)	128(3)	96(2)	-30(2)	49(2)	-6(2)
N(1)	42(1)	51(1)	53(1)	7(1)	16(1)	7(1)
N(2)	40(1)	41(1)	45(1)	4(1)	13(1)	1(1)
N(3)	43(1)	49(1)	53(1)	14(1)	17(1)	7(1)
N(4)	54(1)	44(1)	49(1)	10(1)	20(1)	4(1)
N(5)	52(1)	44(1)	45(1)	6(1)	20(1)	3(1)
N(6)	97(2)	72(1)	99(2)	31(1)	63(2)	29(1)
N(7)	65(1)	72(1)	50(1)	-11(1)	26(1)	-7(1)
O(1)	96(1)	124(2)	68(1)	13(1)	49(1)	12(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **5**.

	x	y	z	U(eq)
H(2)	-2038	5341	1872	68
H(3)	-1868	5735	60	67
H(4)	1189	5796	-915	66
H(5)	4232	5478	-75	66
H(8)	2048	4505	5137	59
H(9)	3631	4076	6674	61
H(11)	8775	4130	4778	61
H(12)	7239	4567	3285	62
H(13)	8728	3709	6474	53
H(18)	9083	2717	12319	78
H(19)	11987	2371	12528	86
H(20)	14193	2398	10790	85
H(21)	13569	2773	8750	70
H(23)	13776	3119	5508	85
H(24A)	10672	3659	3024	120
H(24B)	11726	3586	1606	120
H(24C)	12807	3839	2907	120
H(25A)	16307	3457	3281	148
H(25B)	14796	3224	2058	148
H(25C)	15934	3110	3808	148

H(5N)	10640(40)	3268(6)	7430(30)	69(7)

Table S6. Torsion angles [°] for compound **5**.

N(1)-C(1)-C(2)-C(3)	179.5(2)
C(6)-C(1)-C(2)-C(3)	-1.4(3)
C(1)-C(2)-C(3)-C(4)	1.2(3)
C(2)-C(3)-C(4)-C(5)	-0.8(4)
C(3)-C(4)-C(5)-C(6)	0.5(3)
N(1)-C(1)-C(6)-N(3)	-0.5(2)
C(2)-C(1)-C(6)-N(3)	-179.78(19)
N(1)-C(1)-C(6)-C(5)	-179.61(19)
C(2)-C(1)-C(6)-C(5)	1.2(3)
C(4)-C(5)-C(6)-N(3)	-179.5(2)
C(4)-C(5)-C(6)-C(1)	-0.7(3)
C(12)-C(7)-C(8)-C(9)	-0.5(3)
N(2)-C(7)-C(8)-C(9)	178.58(18)
C(7)-C(8)-C(9)-C(10)	-0.4(3)
C(8)-C(9)-C(10)-C(11)	0.5(3)
C(8)-C(9)-C(10)-C(13)	-178.74(19)
C(9)-C(10)-C(11)-C(12)	0.4(3)
C(13)-C(10)-C(11)-C(12)	179.7(2)
C(8)-C(7)-C(12)-C(11)	1.3(3)
N(2)-C(7)-C(12)-C(11)	-177.75(18)
C(10)-C(11)-C(12)-C(7)	-1.3(3)
C(9)-C(10)-C(13)-C(14)	-9.8(3)
C(11)-C(10)-C(13)-C(14)	171.0(2)
C(10)-C(13)-C(14)-C(15)	-3.7(3)
C(10)-C(13)-C(14)-C(16)	179.14(19)
C(13)-C(14)-C(16)-N(4)	175.65(19)
C(15)-C(14)-C(16)-N(4)	-1.8(3)
C(13)-C(14)-C(16)-N(5)	-2.9(3)
C(15)-C(14)-C(16)-N(5)	179.66(19)
N(4)-C(17)-C(18)-C(19)	-179.4(2)
C(22)-C(17)-C(18)-C(19)	-0.4(4)
C(17)-C(18)-C(19)-C(20)	0.5(4)
C(18)-C(19)-C(20)-C(21)	-0.2(4)
C(19)-C(20)-C(21)-C(22)	-0.3(4)

C(20)-C(21)-C(22)-N(5)	-179.9(2)
C(20)-C(21)-C(22)-C(17)	0.4(3)
N(4)-C(17)-C(22)-N(5)	-0.7(2)
C(18)-C(17)-C(22)-N(5)	-179.9(2)
N(4)-C(17)-C(22)-C(21)	179.07(19)
C(18)-C(17)-C(22)-C(21)	-0.1(3)
C(2)-C(1)-N(1)-N(2)	179.5(2)
C(6)-C(1)-N(1)-N(2)	0.3(2)
C(1)-N(1)-N(2)-N(3)	0.0(2)
C(1)-N(1)-N(2)-C(7)	-179.02(16)
C(12)-C(7)-N(2)-N(1)	175.24(18)
C(8)-C(7)-N(2)-N(1)	-3.9(3)
C(12)-C(7)-N(2)-N(3)	-3.7(3)
C(8)-C(7)-N(2)-N(3)	177.18(18)
N(1)-N(2)-N(3)-C(6)	-0.3(2)
C(7)-N(2)-N(3)-C(6)	178.69(16)
C(1)-C(6)-N(3)-N(2)	0.5(2)
C(5)-C(6)-N(3)-N(2)	179.4(2)
N(5)-C(16)-N(4)-C(17)	0.9(2)
C(14)-C(16)-N(4)-C(17)	-177.79(17)
C(22)-C(17)-N(4)-C(16)	-0.1(2)
C(18)-C(17)-N(4)-C(16)	179.0(2)
N(4)-C(16)-N(5)-C(22)	-1.4(2)
C(14)-C(16)-N(5)-C(22)	177.28(18)
C(21)-C(22)-N(5)-C(16)	-178.5(2)
C(17)-C(22)-N(5)-C(16)	1.2(2)
O(1)-C(23)-N(7)-C(25)	177.8(3)
O(1)-C(23)-N(7)-C(24)	-1.4(4)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for compound **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(5)-H(5N)...O(1)	0.92(2)	1.90(2)	2.814(2)	171(2)

Symmetry transformations used to generate equivalent atoms:

3. Photophysical Properties of the Compounds

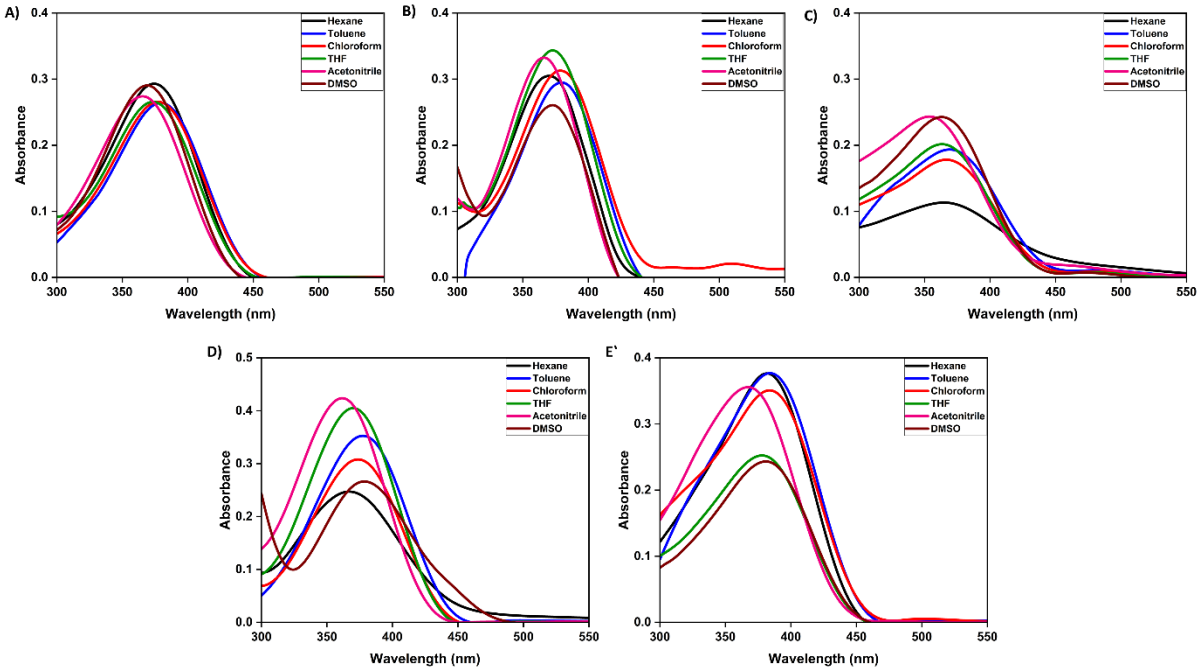


Figure S28. Absorption spectra of compound **1 (A)**, compound **2 (B)**, compound **3 (C)**, compound **4 (D)**, and compound **5 (E)** in different polarity of solvents.

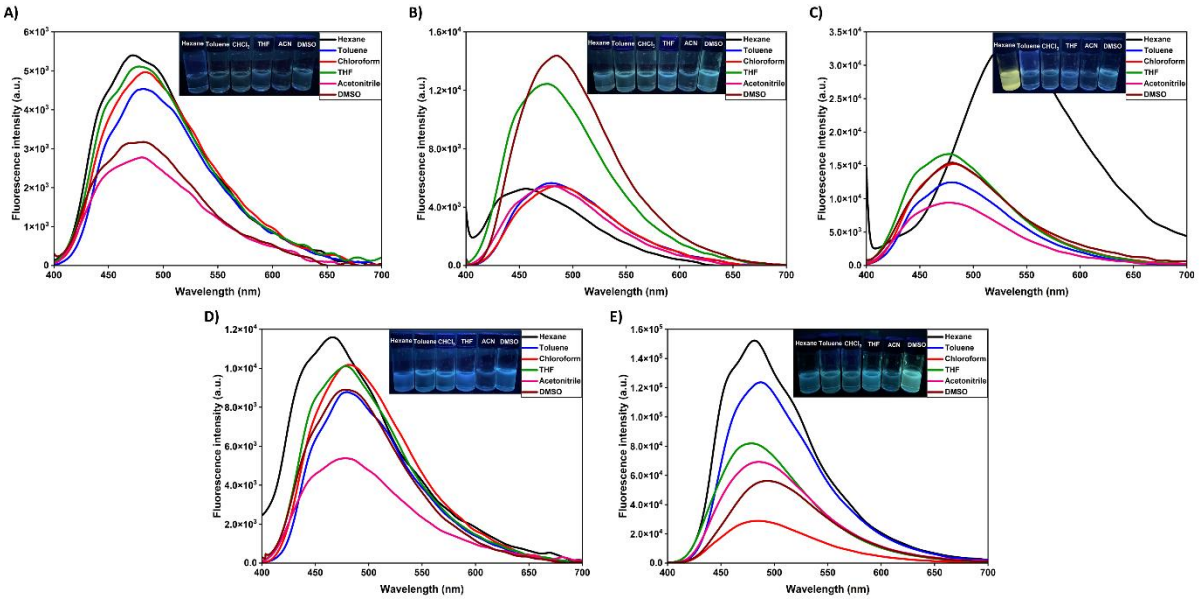


Figure S29. Emission spectra of compound **1 (A)**, compound **2 (B)**, compound **3 (C)**, compound **4 (D)**, and compound **5 (E)** in different polarity of solvents. (Con. 1×10^{-5} M, λ_{ex} = 375 nm). Digital photos taken under UV 365 nm lamp are incorporated alongside the spectral profiles.

Table S8. Photophysical properties of compounds **1-4** in different polarities of solvents (λ_{ex} = 375 nm for compounds).

S. No.	Compound	Solvents	λ_{max}[a] (nm)	λ_{max}[b] (nm)	$\Delta\nu$[c]	ε = A/C. l (mol^{-1}. ltr. cm^{-1})
1	**1**	Hexane	374	473	5596	2.9×10^4
		Toluene	380	482	5569	2.6×10^4
		$CHCl_3$	378	484	5794	2.6×10^4
		THF	374	477	5774	2.6×10^4
		ACN	366	481	6532	2.7×10^4
		DMSO	369	479	6223	2.9×10^4
2	**2**	Hexane	371	456	5024	3.0×10^4
		Toluene	380	480	5482	2.9×10^4
		$CHCl_3$	379	488	5893	3.1×10^4
		THF	373	475	5757	3.4×10^4
		ACN	366	479	6446	3.3×10^4
		DMSO	373	484	6148	2.6×10^4
3	**3**	Hexane	368	534	8447	1.1×10^4
		Toluene	371	480	6121	1.9×10^4
		$CHCl_3$	368	481	6384	1.8×10^4
		THF	365	477	6433	2.0×10^4
		ACN	355	477	7205	2.4×10^4
		DMSO	364	480	6639	2.4×10^4
4	**4**	Hexane	368	465	5669	2.5×10^4
		Toluene	378	479	5578	3.5×10^4
		$CHCl_3$	374	482	5991	3.1×10^4
		THF	371	479	6077	4.1×10^4
		ACN	362	477	6660	4.2×10^4
		DMSO	379	478	5465	2.7×10^4
5	**5**	Hexane	382	481	5388	3.8×10^4
		Toluene	385	487	5440	3.8×10^4

		$CHCl_3$	385	483	5270	3.5×10^4
		THF	379	478	5465	2.5×10^4
		ACN	369	486	6524	3.6×10^4
		DMSO	381	493	5963	2.4×10^4

[a] Peak position of the maximum absorption band in nm. [b] Peak position of emission maxima in nm. [c] Stokes shift in cm^{-1}.

Comparison of Optical Properties: To establish a clear structure–property relationship, the optical properties of compounds **1–5** were systematically compared under solution, solid-state, aggregation-induced emission (AIE), and viscosity-dependent conditions. The relevant absorption and emission maxima are summarized in **Table S9**. In dilute THF solution, all compounds exhibit similar absorption maxima in the range of 365–379 nm, indicating that the ground-state electronic structures are largely comparable across the series. Correspondingly, the emission maxima in THF appear in a narrow window (475–479 nm), suggesting minimal influence of substituent variation on emissive behavior in a freely solvated environment. In contrast, a pronounced red shift in emission is observed in the solid state, with emission maxima extending to 483–580 nm. This significant bathochromic shift reflects the strong influence of molecular packing and restricted molecular motion in the condensed phase. Compounds **1** and **4** display the largest solid-state red shifts, highlighting the role of structural features that favor enhanced intermolecular interactions in the solid state. Under AIE conditions (THF/H_2O = 10:90, v/v), all compounds show red-shifted emission (511–567 nm) relative to solution, confirming aggregation-induced modulation of emissive behavior. Notably, the emission maxima under AIE conditions are generally slightly blue-shifted compared to the solid state, suggesting less compact molecular packing in aggregates than in crystalline or amorphous solids. The extent of the shift varies among the compounds, indicating that aggregation behavior is sensitive to subtle structural differences. To probe the influence of restricted molecular motion independent of aggregation, emission studies were also conducted in viscosity-controlled media (DMSO/glycerol = 10:90, v/v). Under these conditions, all compounds exhibit emission maxima clustered around 481–492 nm, closely resembling their solution-state emission. This observation suggests that viscosity-induced restriction primarily enhances emission intensity rather than significantly altering the emissive energy levels.

Table S9. Comparative optical properties of compounds **1–5** showing absorption and emission maxima in solution (THF), solid state, AIE (THF/H_2O, 10:90, v/v), and viscosity-controlled (DMSO/glycerol, 10:90, v/v) environments.

Code	λ_{abs} (in nm) in THF	λ_{em} (in nm)			
		in THF	in solid-state	in AIE THF/H_2O (10:90, v/v)	in viscosity DMSO/glycerol (10:90, v/v)
1	374	477	576	567	482
2	373	475	492	511	483
3	365	477	483	554	483
4	371	479	580	541	481
5	379	478	543	535	492

4. SEM and DLS Studies

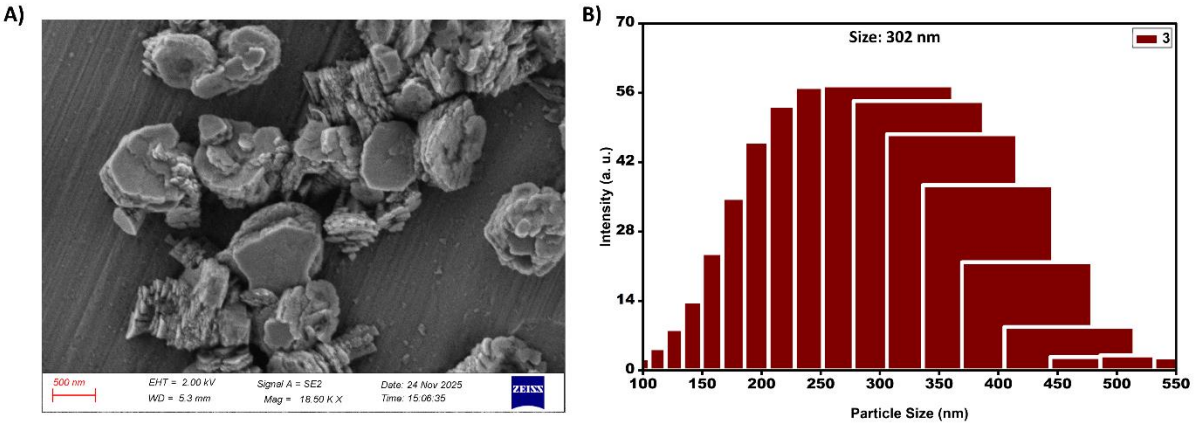


Figure S30. (**A**) FE-SEM image of aggregates of compound **3** (drop-casted from 1×10^{-5} M, hexane solution); (**B**) Size distributions of the aggregates of compound **3** in hexane.

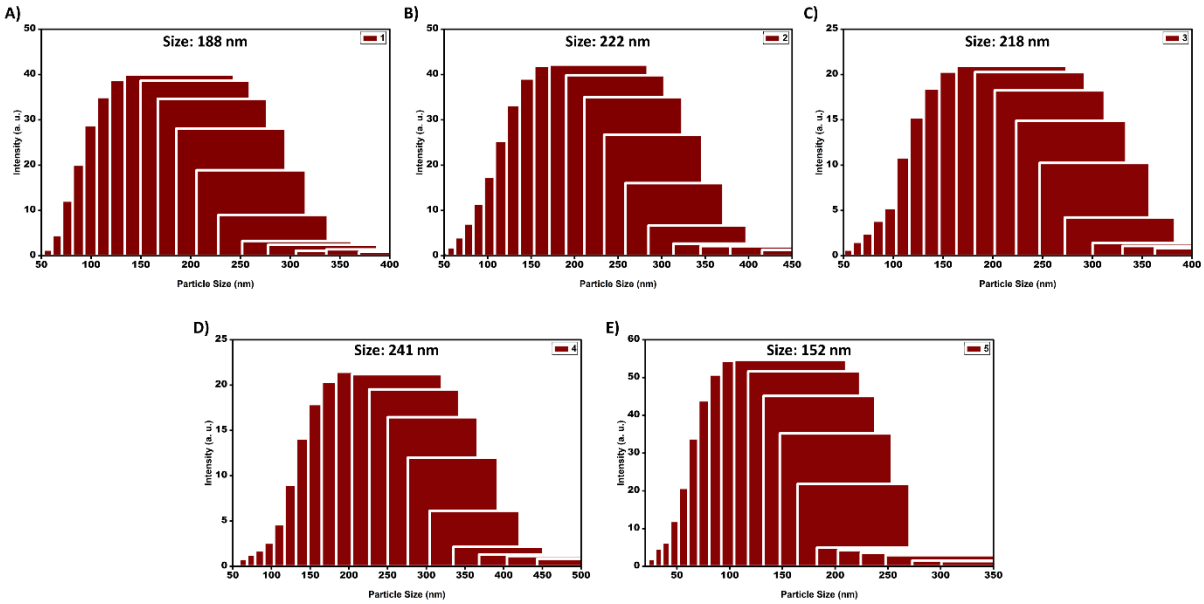


Figure S31. Size distributions of the aggregates of (**A**) **1**, (**B**) **2**, (**C**) **3**, (**D**) **4**, and (**D**) **5**, THF-water mixtures with f_w = 90% (Con. 1×10^{-5} M).

5. Concentration Dependent Fluorescence and Lifetime Data

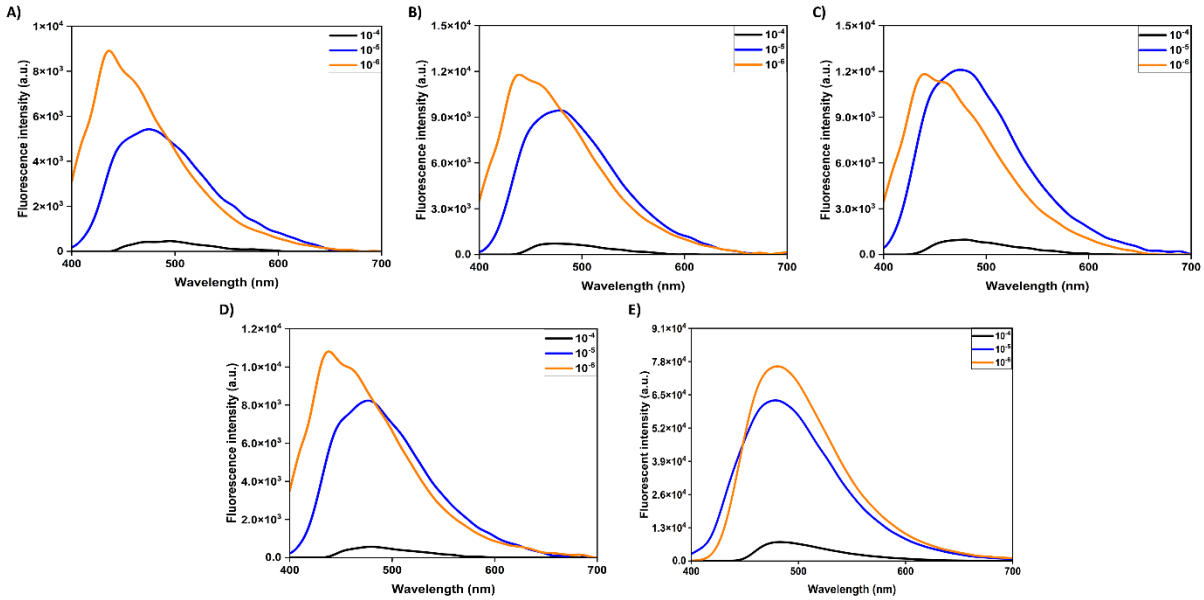


Figure S32. Concentration-dependent fluorescence spectra of compounds **1–5** in THF (λ_{ex} = 375 nm).

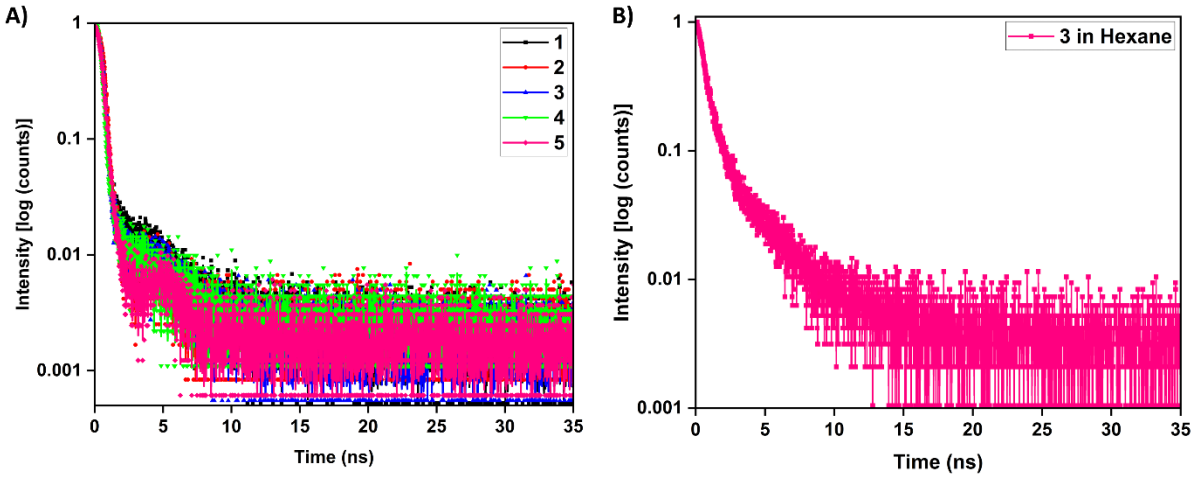


Figure S33. Lifetime profiles of compounds **1-5** in THF solution **(A),** compound **3** in hexane solution **(B)**.

Table S10. Lifetime parameters of compounds **1-5** in solution (THF) and compound **3** in hexane.

Compound	τ_{avr} in THF solution	τ_{avr} in hexane solution
1	0.973	–
2	0.635	–
3	0.741	1.602
4	0.639	–
5	0.592	–

6. Lippert–Mataga Plots

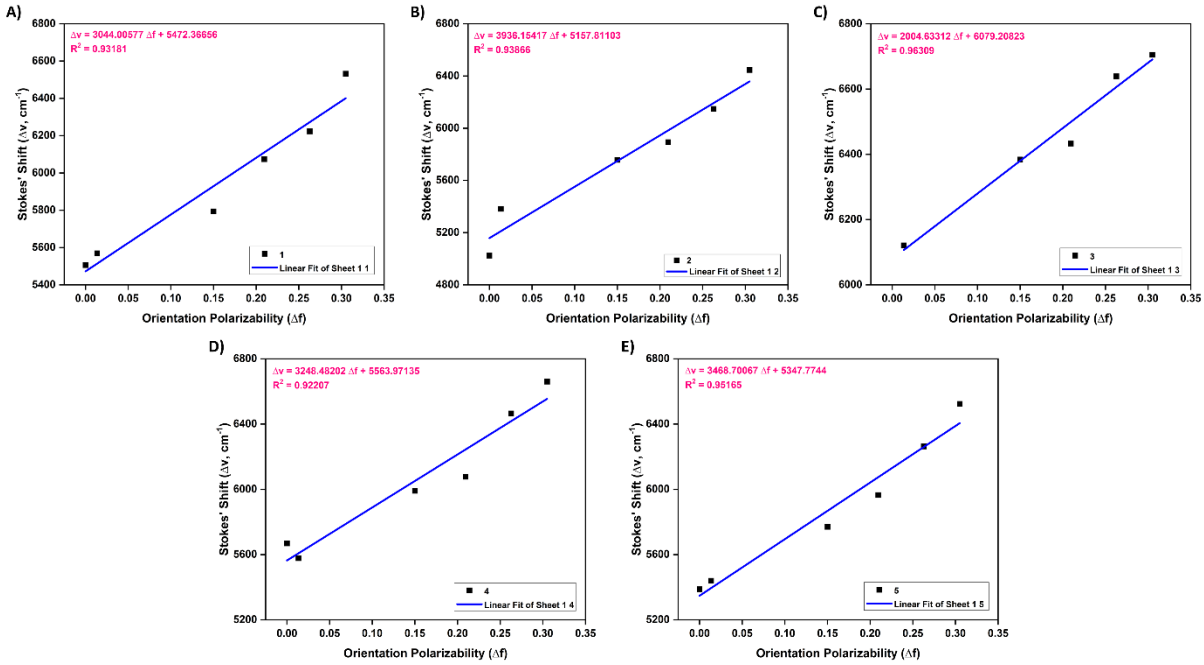


Figure S34. Lippert–Mataga plots for compounds **1** (**A**), **2** (**B**), **3** (**C**), **4** (**D**), and **5** (**E**).

Excited state dipole moment calculations

The excited state dipole moments were calculated from Lippert and Mageta equation (eq-1).

$\Delta\nu = \left[\frac{2(\Delta\mu)^2}{hca_0^3 4\pi\varepsilon_0}\right]\Delta f + A$-------- eq-1

Plot between Δν and Δ*f* gives the slope

$$\left(\frac{2(\Delta\mu)^2}{hca_0^3 4\pi\varepsilon_0}\right)$$

Where Δμ is the change in electric dipole moment upon an electronic transition, h, c, ε_0 and a_0 are Planck's constant, the speed of light, vacuum permittivity constant, and the Onsager radius for compounds **1–5** are ~8.45, 8.47, 8.44, 8.44, and 8.45 Å, respectively.

$\Delta\mu = \mu_g - \mu_e$

Where 'μ_g' and 'μ_e' are the dipole moments in the ground and excited states, respectively

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

Where 'ε' and 'n' are the dielectric constant and refractive index of solvents, respectively.

Table S11. The change in electric dipole moment values (Δμ) of compounds

Compounds	Δμ (Debye)
1	13.50
2	15.42
3	10.94
4	13.94
5	14.42

7. pH-dependent Absorption

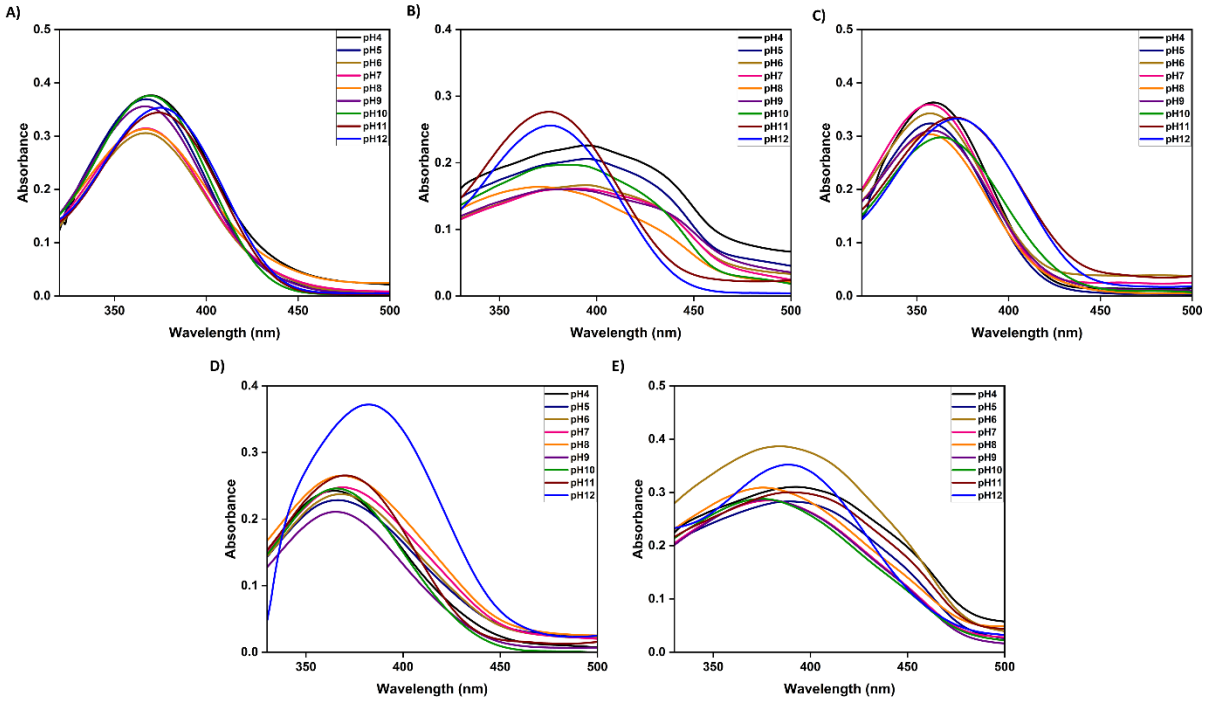


Figure S35. Absorption spectra of compounds **1** (**A**), **2** (**B**), **3** (**C**), **4** (**D**) and **5** (**E**) (Con. 1×10^{-5} M, λ_{ex} = 375 nm) in different pH buffers.

8. Thermal Properties

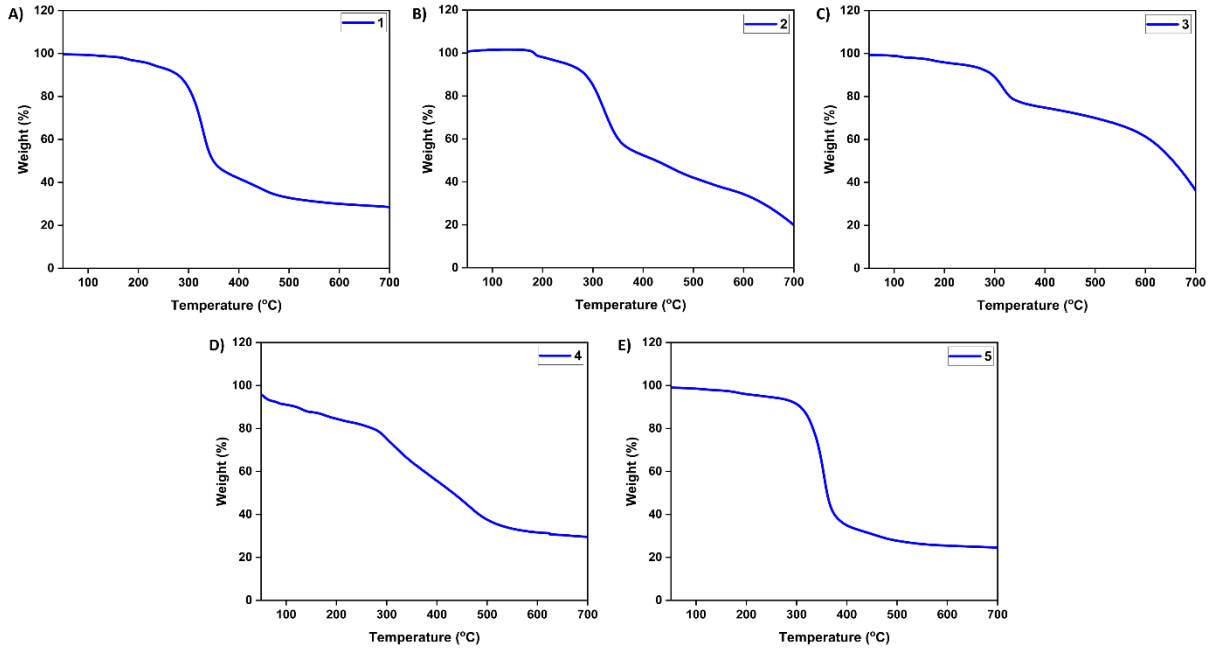


Figure S36. TGA curves of compounds **1** (**A**), **2** (**B**), **3** (**C**), **4** (**D**) and **5** (**E**).

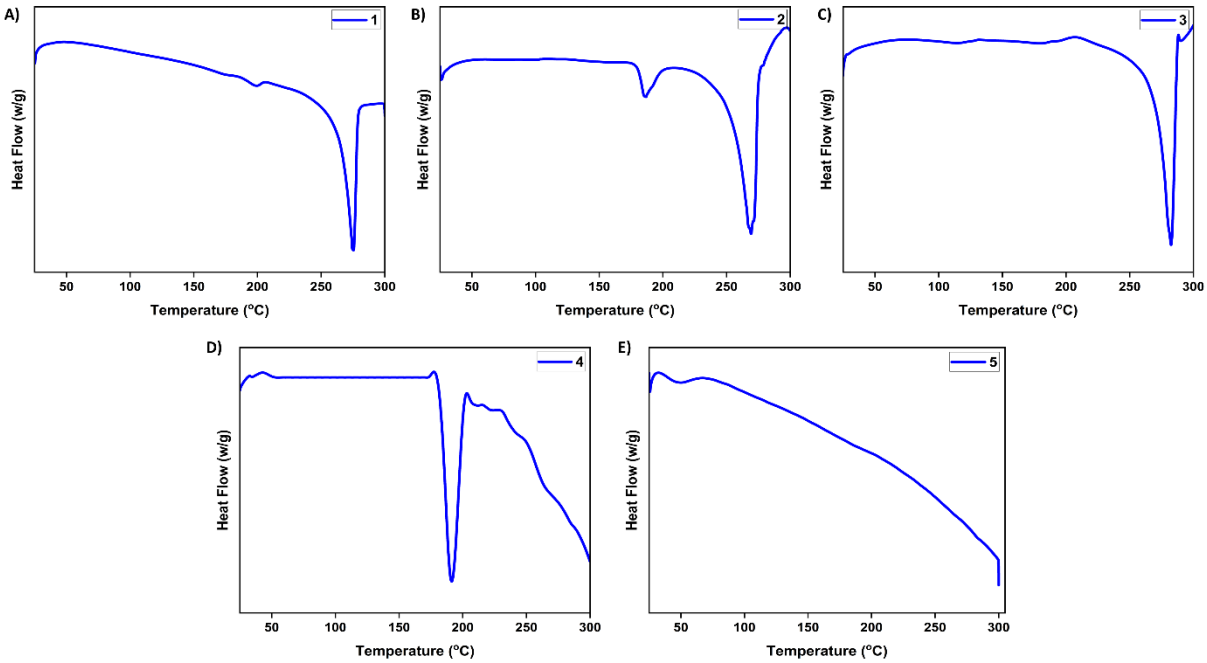


Figure S37. DSC curves of compounds **1** (**A**), **2** (**B**), **3** (**C**), **4** (**D**) and **5** (**E**).

9. DFT Calculations

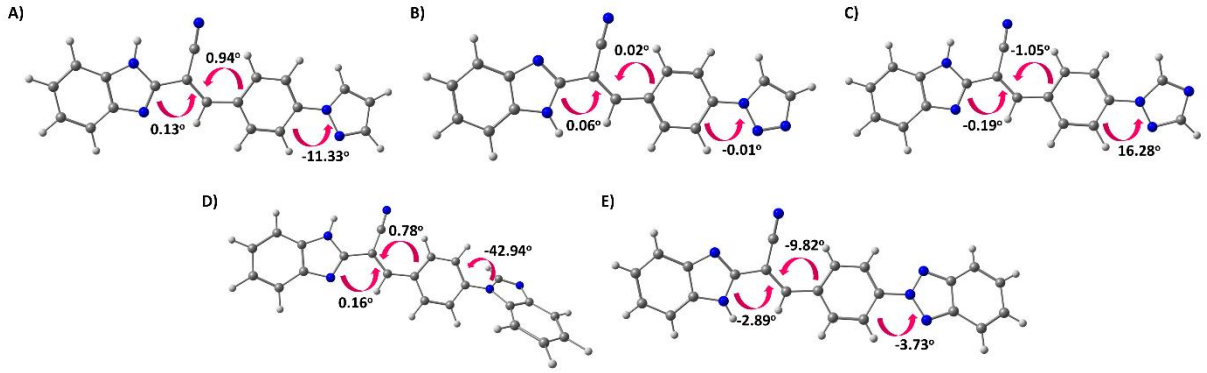


Figure S38. Optimized geometries with selective dihedral angles of compounds (**A**) **1**, (**B**) **2**, (**C**) **3**, (**D**) **4**, and (**E**) **5**.

Table S12. DFT data of molecule **1**.

6	4.527182434	-0.920128892	0.017076631
6	4.929750629	0.440281741	-0.001806910
6	6.272332323	0.827512883	-0.002396918
6	7.218591575	-0.195828191	0.016591514
6	6.836246301	-1.555855599	0.035358448
6	5.496911966	-1.934110634	0.035895022
6	2.714843327	0.231936342	-0.006770566
1	6.570554713	1.872352717	-0.016845573

1	8.274934194	0.058934458	0.016848624
1	7.608495669	-2.320254077	0.049649518
1	5.198461755	-2.978215728	0.050300036
6	1.303358521	0.638596197	-0.017721051
6	0.315163223	-0.304735147	-0.004240075
1	0.695096039	-1.324143693	0.015640930
6	1.076145077	2.050124930	-0.040678242
7	0.976829626	3.211650116	-0.058775610
6	-1.131667947	-0.191104088	-0.009083103
6	-1.861561666	1.017877238	-0.049262543
6	-1.873662870	-1.394218207	0.025183514
6	-3.250051027	1.018164010	-0.051668145
6	-3.261379325	-1.405185893	0.029838123
1	-1.340787630	-2.341427930	0.053699412
6	-3.962338643	-0.191193538	-0.003206944
1	-3.771863716	1.967365672	-0.105807112
7	3.744869549	1.152977555	-0.016979229
7	3.147343586	-1.012930420	0.013461867
1	3.639915851	2.159102211	-0.032188654
1	-1.350120549	1.971849862	-0.089726786
1	-3.813555613	-2.336321862	0.058837787
7	-5.375422184	-0.197988237	0.008071141
6	-6.233573159	0.854024583	0.204782903
6	-7.335684159	-1.035634141	-0.107229354
6	-7.512948907	0.349820456	0.135784309
1	-5.879994014	1.855857120	0.393982950
1	-8.089101167	-1.802546867	-0.232425992
1	-8.437759599	0.897132352	0.250066768
7	-6.052223692	-1.365387371	-0.181594111

Table S13. DFT data of molecule **2**.

6	-7.283709000	1.127155000	-0.035332000
6	-7.227125000	-0.230529000	-0.422383000
6	-6.013211000	-0.903519000	-0.555528000

6	-4.857415000	-0.166402000	-0.286653000
6	-4.895272000	1.195943000	0.102680000
6	-6.127707000	1.854295000	0.230698000
7	-3.510452000	-0.485673000	-0.311615000
6	-2.813841000	0.655453000	0.050592000
7	-3.613834000	1.672000000	0.302881000
6	-1.354019000	0.732965000	0.145123000
6	-0.856276000	2.019292000	0.540497000
6	-0.532404000	-0.325862000	-0.119494000
6	0.916561000	-0.476643000	-0.091196000
6	1.436593000	-1.746383000	-0.431896000
6	2.798825000	-2.011026000	-0.440755000
6	3.697973000	-0.991187000	-0.101831000
6	3.211845000	0.277646000	0.240314000
6	1.845161000	0.531886000	0.245947000
7	5.091991000	-1.256093000	-0.109197000
6	6.141225000	-0.431701000	0.180604000
6	7.253730000	-1.218501000	0.008730000
7	6.851715000	-2.468350000	-0.371742000
7	5.555828000	-2.496389000	-0.444023000
7	-0.417559000	3.048682000	0.858932000
1	-8.253145000	1.609356000	0.055135000
1	-8.152408000	-0.764328000	-0.621472000
1	-5.977189000	-1.947943000	-0.853649000
1	-6.162569000	2.897832000	0.528624000
1	-3.124377000	-1.386482000	-0.550802000
1	-1.036131000	-1.245835000	-0.409825000
1	0.750527000	-2.547516000	-0.697138000
1	3.174457000	-2.991712000	-0.705195000
1	3.889875000	1.081403000	0.505951000
1	1.510440000	1.524767000	0.515962000
1	6.026048000	0.599350000	0.472323000
1	8.297949000	-0.971751000	0.131635000

Table S14. DFT data of molecule **3**.

6	-4.522709754	-0.918932338	0.022787762
6	-4.924634913	0.441647602	-0.002582361
6	-6.267244654	0.829496302	-0.003562770
6	-7.213251541	-0.193490455	0.021778599
6	-6.831440102	-1.553914281	0.046999897
6	-5.492681353	-1.932847774	0.047857387
6	-2.710512207	0.232352301	-0.009181436
1	-6.565245742	1.874259417	-0.023043772
1	-8.269523780	0.061394036	0.021998649
1	-7.604154299	-2.317662326	0.066087782
1	-5.194537504	-2.976917354	0.067207229
6	-1.298239499	0.636308093	-0.023311320
6	-0.312440072	-0.307929810	-0.004175877
1	-0.693088124	-1.326798031	0.022597985
6	-1.068052819	2.047775790	-0.055194549
7	-0.965022131	3.208581295	-0.080293142
6	1.136434839	-0.194906606	-0.010788152
6	1.865662520	1.014089419	-0.061819240
6	1.874873469	-1.399251297	0.031314094
6	3.254661918	1.013073161	-0.067815683
6	3.263632393	-1.411494347	0.035277257
1	1.340407639	-2.345112052	0.066889679
6	3.959857823	-0.197875165	-0.007739754
1	3.782188917	1.958739866	-0.136772780
7	-3.739770122	1.153915072	-0.023068158
7	-3.143200716	-1.012184540	0.018035909
1	-3.635164681	2.160037939	-0.043232050
1	1.354331631	1.967531712	-0.111555703
1	3.815597163	-2.343063183	0.070652719
7	5.376288447	-0.202446255	0.006673670
6	6.251282023	0.803652466	0.291577299
1	5.944219939	1.802208289	0.566703409
6	7.336388600	-0.938114537	-0.136342204

1	8.166187528	-1.612694088	-0.296768692
7	6.083699790	-1.339114176	-0.267220569
7	7.495042078	0.374140704	0.208552554

Table S15. DFT data of molecule **4**.

6	-5.538070367	-1.043254949	-0.197048244
6	-6.037818376	0.227910398	0.187588310
6	-7.403036728	0.484724592	0.340341893
6	-8.270103335	-0.578328370	0.094987772
6	-7.790347113	-1.850966760	-0.288929042
6	-6.429632959	-2.099572316	-0.439187320
6	-3.817855882	0.217077362	0.053808382
1	-7.776090708	1.461709415	0.635304948
1	-9.340488466	-0.424572841	0.201268172
1	-8.503869766	-2.650314543	-0.469805330
1	-6.056506006	-3.075906727	-0.733960224
6	-2.441027180	0.725574649	0.116276015
6	-1.390964180	-0.096013155	-0.176927981
1	-1.696719974	-1.104813858	-0.446363201
6	-2.315317340	2.099358041	0.494966499
7	-2.299817098	3.221953192	0.808315755
6	0.043957036	0.135389858	-0.193579489
6	0.683414430	1.352885056	0.131370211
6	0.864744238	-0.953728562	-0.564591082
6	2.067755052	1.465337973	0.094786704
6	2.248675726	-0.843141021	-0.619070858
1	0.398959150	-1.899491160	-0.829931916
6	2.862852743	0.372043346	-0.284921980
1	2.539581732	2.400022208	0.382689339
7	-4.910034040	1.013070435	0.340391719
7	-4.157620426	-1.014362914	-0.270221718
1	-4.879072482	1.987322370	0.611610899
1	0.104935465	2.217615191	0.432892673
1	2.851687140	-1.685049610	-0.942538268

6	5.254262851	-0.388745034	0.074961536
6	6.481148417	0.241501017	-0.243531527
6	5.201020296	-1.625056955	0.726242804
6	7.695383822	-0.382776356	0.067406493
6	6.420638110	-2.230673825	1.028384862
1	4.261983319	-2.095718990	0.999433686
6	7.650127102	-1.622658914	0.699789079
1	8.636193236	0.101211429	-0.177579662
1	6.420893121	-3.193119953	1.532958703
1	8.576590097	-2.130920210	0.952929531
7	4.268816219	0.510590754	-0.346013836
7	6.252644813	1.475378133	-0.844194735
6	4.954954785	1.595569542	-0.879615304
1	4.415431163	2.430886376	-1.307896057

Table S16. DFT data of molecule **5**.

6	-5.541905050	-1.046798002	-0.171341573
6	-6.039632343	0.234719385	0.180295645
6	-7.404312469	0.496891037	0.328697580
6	-8.272979784	-0.571322872	0.113093870
6	-7.795263911	-1.854146480	-0.238039484
6	-6.435061418	-2.108087143	-0.384067721
6	-3.819935458	0.217936946	0.042992670
1	-7.775796274	1.481750432	0.598359554
1	-9.343011160	-0.413611710	0.217180397
1	-8.509962819	-2.657168383	-0.396716457
1	-6.063493421	-3.092214678	-0.653874460
6	-2.442435241	0.726482325	0.090500641
6	-1.394035350	-0.105566312	-0.177364047
1	-1.701914658	-1.122483711	-0.411617859
6	-2.316123637	2.109684496	0.433356265
7	-2.304564840	3.239402362	0.719917384
6	0.041447800	0.121575969	-0.199552274
6	0.681884891	1.359574629	0.038630049
6	0.859939118	-0.992698334	-0.487944612

6	2.065531201	1.469297674	0.009219781
6	2.245504589	-0.890882181	-0.530491910
1	0.393633817	-1.952409149	-0.695514809
6	2.854726480	0.342590395	-0.268436220
1	2.546506393	2.422324166	0.198630228
7	-4.910785556	1.022348622	0.310132376
7	-4.161607602	-1.021410343	-0.247652813
1	-4.877939625	2.003468033	0.555241811
1	0.101507975	2.247418422	0.258222458
1	2.845508498	-1.755210946	-0.793667489
6	5.254334745	-0.412248864	0.069728751
6	6.443815544	0.292113919	-0.206291782
6	5.274986517	-1.692981913	0.645941368
6	7.701928104	-0.271223105	0.057805674
6	6.527348660	-2.237611477	0.904941986
1	4.367982120	-2.232651890	0.895086817
6	7.726495263	-1.543346510	0.610867230
1	8.610148984	0.281975823	-0.160410403
1	6.587697198	-3.226318978	1.351833591
1	8.678270923	-2.017541455	0.832651876
7	4.262342439	0.468908299	-0.300321029
7	4.834371118	1.637701999	-0.764475056
7	6.115003323	1.534327986	-0.713408943

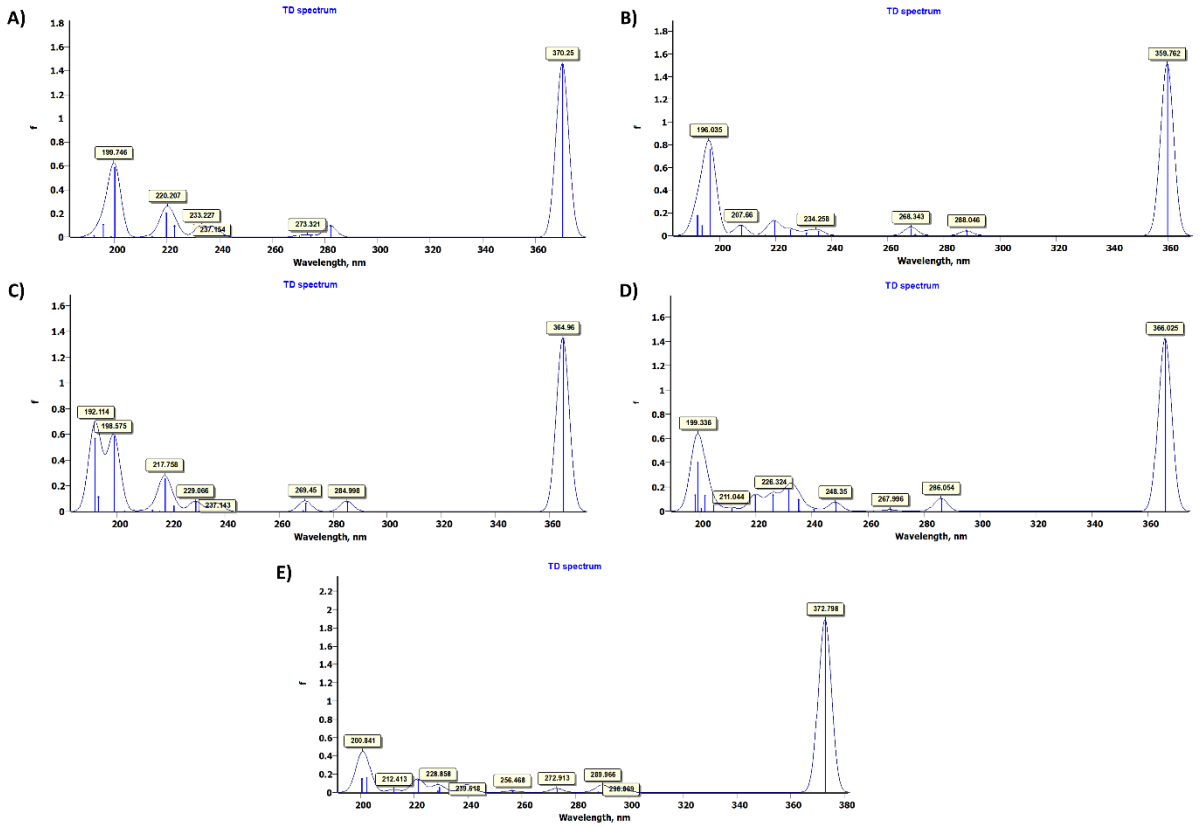


Figure S39. Simulated absorption spectra of compounds **1–5** (**A–E**), respectively, using CAM-B3LYP paired with 6-31+G(d) basis set in tetrahydrofuran solvent.

Table S17. Computed singlet vertical transitions involved in compound **1** from TD-DFT calculation using 6-31+G(d) basis set CAM-B3LYP functional in Gaussian09.

Excited States	**E (eV)**	**λ_{max} (nm)**	***f***	**Major transitions (%)[a]**
S_1	3.3482	370.30	1.4588	HOMO → LUMO (47.0 %)
S_2	4.3960	282.04	0.0997	HOMO-1 → LUMO (42.4 %)
S_3	4.5165	274.51	0.0149	HOMO-2 → LUMO (39.4 %)
S_4	4.5866	270.32	0.0126	HOMO-4 → LUMO (25.3 %)
S_5	5.2092	238.01	0.0806	HOMO → LUMO+2 (16.7 %) HOMO → LUMO+3 (11.1 %)

[a] TD–DFT–predicted electronic transitions highlight only values greater than 10%, as mentioned in the table.

Table S18. Computed singlet vertical transitions involved in compound **2** from TD-DFT calculation using 6-31+G(d) basis set CAM-B3LYP functional in Gaussian09.

Excited States	E (eV)	λ_{max} (nm)	*f*	Major transitions (%)[a]
S_1	3.4461	359.78	1.5123	HOMO → LUMO (46.3 %)
S_2	4.3044	288.04	0.0432	HOMO-1 → LUMO (44.1 %)
S_3	4.5996	269.56	0.0136	HOMO-3 → LUMO (16.3 %) HOMO-2 → LUMO (18.5 %)
S_4	4.6248	268.09	0.0648	HOMO-3 → LUMO (13.8 %) HOMO-2 → LUMO (23.9 %)
S_5	5.2722	235.17	0.0466	HOMO → LUMO+1 (10.7 %) HOMO → LUMO+3 (18.2 %)

[a] TD–DFT–predicted electronic transitions highlight only values greater than 10%, as mentioned in the table.

Table S19. Computed singlet vertical transitions involved in compound **3** from TD-DFT calculation using 6-31+G(d) basis set CAM-B3LYP functional in Gaussian09.

Excited States	E (eV)	λ_{max} (nm)	*f*	Major transitions (%)[a]
S_1	3.3974	364.94	1.3497	HOMO → LUMO (46.6 %)
S_2	4.3491	285.08	0.0830	HOMO-1 → LUMO (45.2 %)
S_3	4.5978	269.66	0.0710	HOMO-2 → LUMO (36.6 %)
S_4	4.6127	268.79	0.0136	HOMO-3 → LUMO (31.0 %)
S_5	5.2285	237.13	0.0671	HOMO → LUMO+2 (12.3 %) HOMO → LUMO+3 (16.7 %)

[a] TD–DFT–predicted electronic transitions highlight only values greater than 10%, as mentioned in the table.

Table S20. Computed singlet vertical transitions involved in compound **4** from TD-DFT calculation using 6-31+G(d) basis set CAM-B3LYP functional in Gaussian09.

Excited States	E (eV)	λ_{max} (nm)	*f*	Major transitions (%)[a]
S_1	3.3868	366.08	1.4235	HOMO → LUMO (46.7 %)
S_2	4.3346	286.03	0.1067	HOMO-2 → LUMO (11.9 %) HOMO-1 → LUMO (33.1 %)
S_3	4.4182	280.62	0.0019	HOMO-3 → LUMO (10.2 %) HOMO-2 → LUMO (25.4 %)
S_4	4.6246	268.10	0.0123	HOMO-5 → LUMO (33.8 %)
S_5	4.7361	261.78	0.0044	HOMO-3 → LUMO (34.0 %)

[a] TD–DFT–predicted electronic transitions highlight only values greater than 10%, as mentioned in the table.

Table S21. Computed singlet vertical transitions involved in compound **5** from TD-DFT calculation using 6-31+G(d) basis set CAM-B3LYP functional in Gaussian09.

Excited States	E (eV)	λ_{max} (nm)	*f*	Major transitions (%)[a]
S_1	3.3265	372.72	1.8924	HOMO → LUMO (44.2 %)
S_2	4.1741	297.03	0.0513	HOMO-2 → LUMO (37.4 %) HOMO-2 → LUMO+1 (11.0 %)
S_3	4.2740	290.09	0.0725	HOMO-3 → LUMO (17.0 %) HOMO-1 → LUMO (20.2 %)
S_4	4.3023	288.18	0.0126	HOMO-3 → LUMO (16.5 %) HOMO-1 → LUMO (21.5 %)
S_5	4.5429	272.92	0.0437	HOMO-4 → LUMO (37.3 %)

[a] TD–DFT–predicted electronic transitions highlight only values greater than 10%, as mentioned in the table.

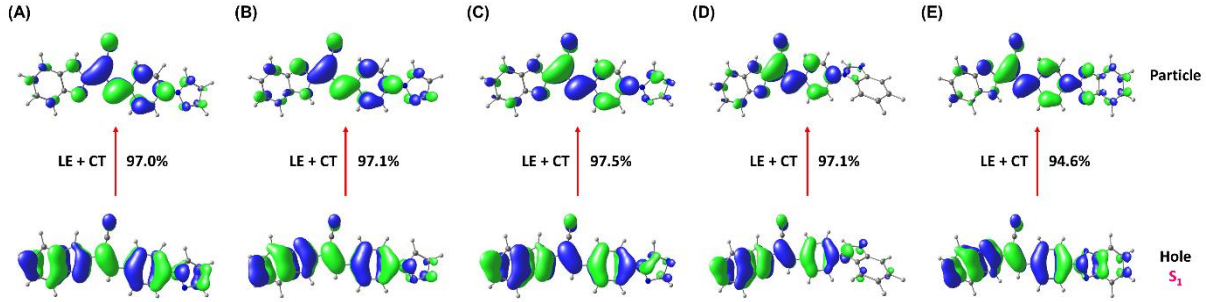


Figure S40. Natural transition orbitals for compound **1** (**A**), **2** (**B**), **3** (**C**), **4** (**D**), and **5** (**E**) through DFT calculation using the CAM-B3LYP functional and 6-31+G(d) as a basis set.

10. Photostability and Cytotoxicity

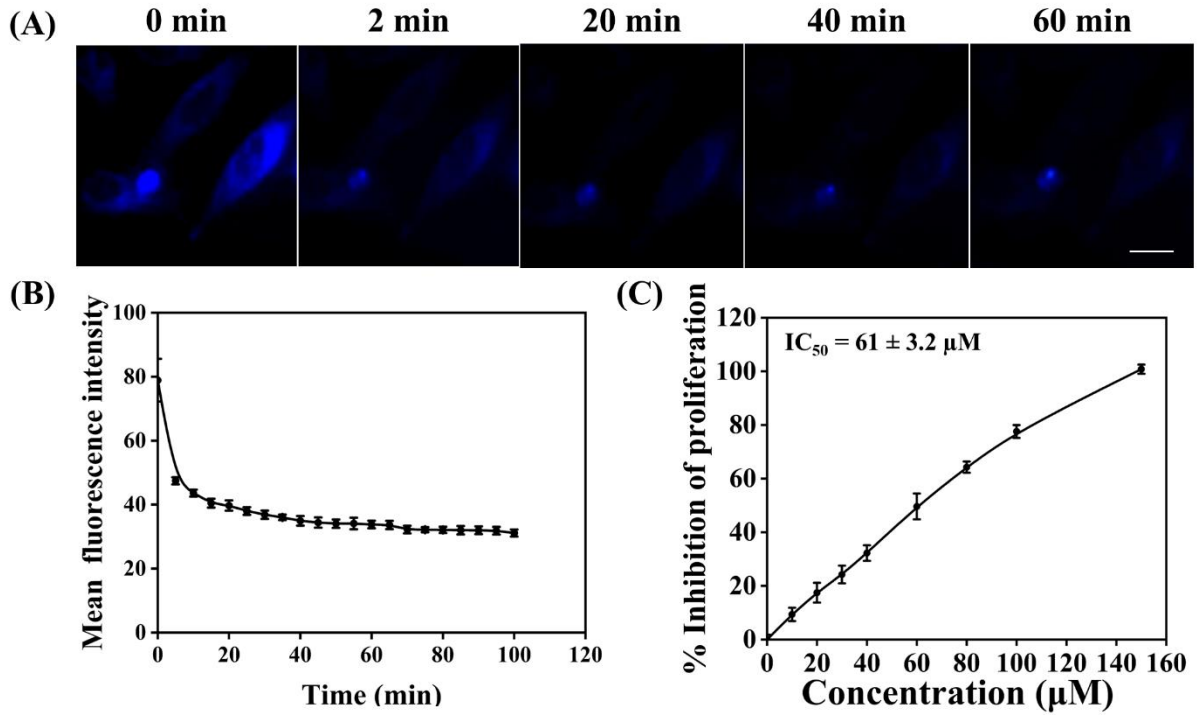
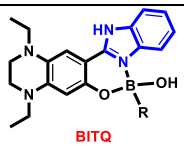
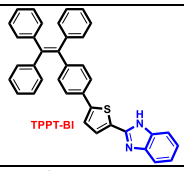
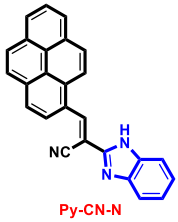
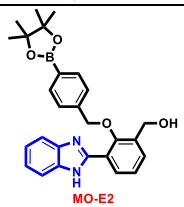
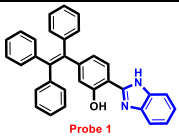
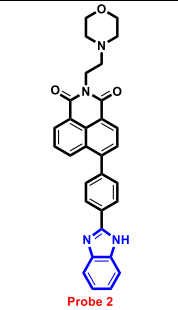
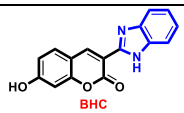
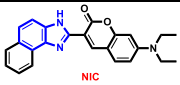
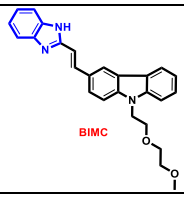
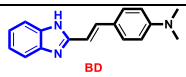
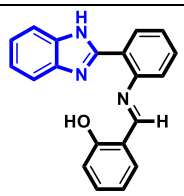


Figure S41. Photostability and Cytotoxicity of compound **1. (A)** HeLa cells were treated with compound **1**, and the images were captured at 0–60 min under continuous UV excitation (362-396 nm). **(B)** Mean fluorescence intensities of compound **1** at different time points. **(C)** HeLa cells were treated with different concentrations of compound **1**, and the cell inhibition was analyzed by SRB assay. Scale bar: 20 µm.

11. Summary of the Literature Survey on Bioimaging Probes

Table S22. Summary of the literature survey on benzimidazole-based blue-emitting bioimaging probes.

S. No.	Structure	λ_{abs}	λ_{em}	Quantum Yield	Cells used for Bioimaging	Cytotoxicity	Ref.
1.	 BITQ	390	480	5.6	T3M-4 cells	–	46
2.	 TPPT-BI	374	475	45.6	HeLa cells	50 µM	47
3.	 Py-CN-N	410	510	6.3	HeLa cells and macrophages RAW 264.7 cells	50 µM	48
4.	 MO-E2	330	450	–	macrophages RAW 264.7 cells	164 µM	49
5.	 Probe 1	347	445	45.6	HeLa cells	40 µM	50
6.	 Probe 2	300, 370	510	–	Human Osteosarcoma MG-63	–	51
7.	 BHC	390	480	0.646	HeLa	200 µM	52
8.	 NIC	440	525	0.703	MCF7	40 µM	53
9.	 BIMC	359	454	0.45	HeLa	100 µM	54

10.	 BD	354	487	–	SNU-423	200 μM	55
11.	 BMSA	288, 301, and 355	425	–	HeLa	50 μM	56