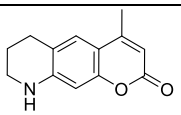
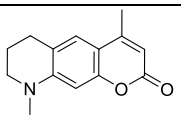
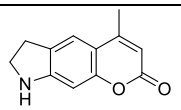
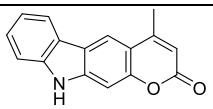
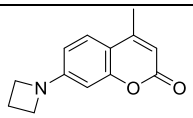
Appendix

Table S1: Photophysical properties of compounds 5, 5a, 6 and 7 in different solvents.

Compound	Compound Structure	λ_{abs} (nm)[a]			λ_{em} (nm)[b]		
		DCM	MeOH	PBS	DCM	MeOH	PBS
5		363	375	378	420	452	459
5a		375	379	383	437	455	465
6		360	371	359	420	451	456
7		362	363	362	448	460	464
2a		360	368	355	430	451	478

λ_{abs} = Absorbance maximum; λ_{em} = emission maximum.

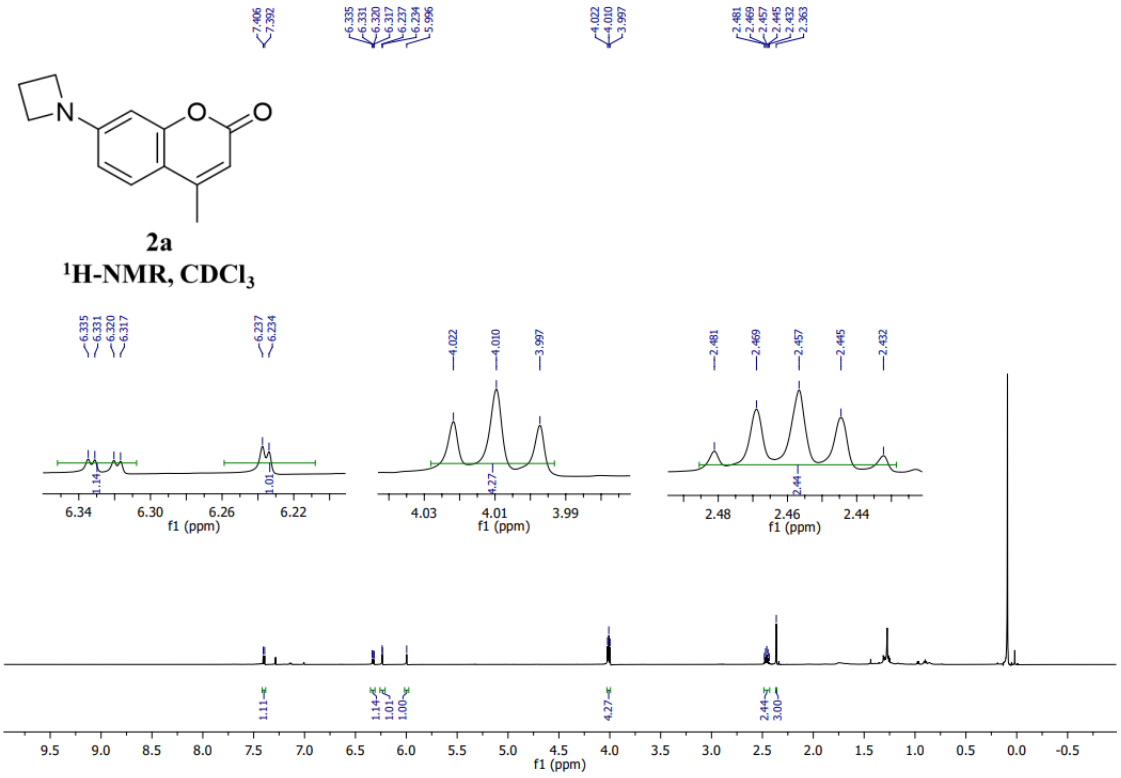


Figure S1. ^{1}H-NMR spectrum of 7-(azetidin-1-yl)-4-methyl-2H-chromen-2-one (2a)

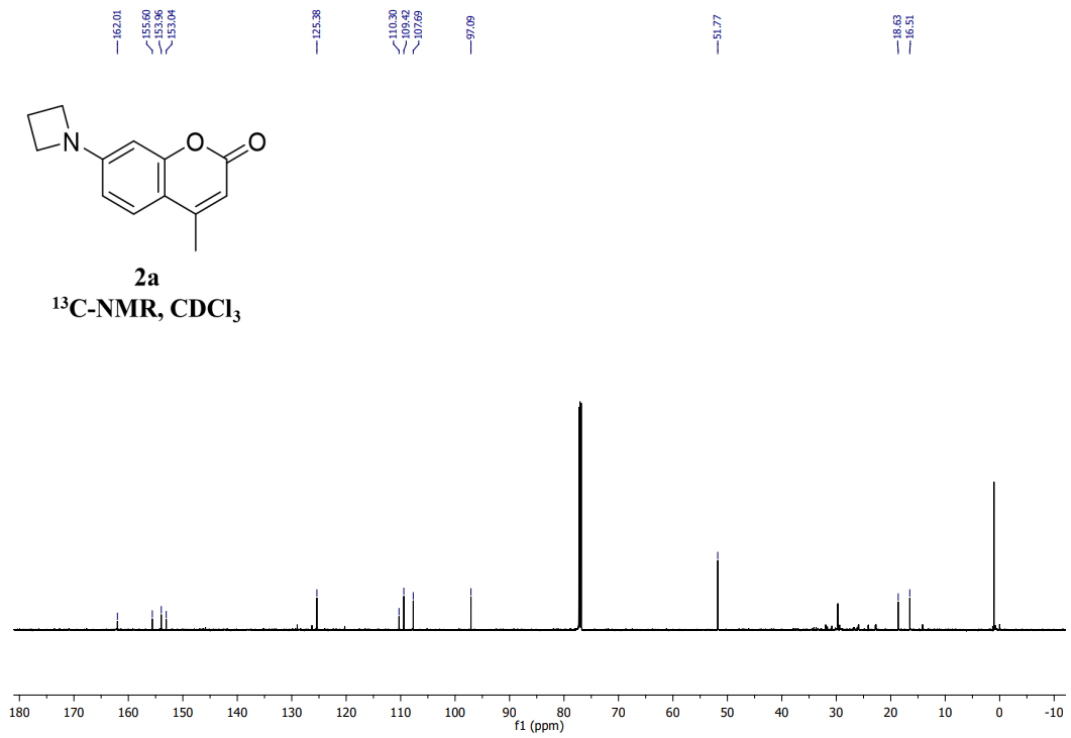


Figure S2. ^{13}C-NMR spectrum of 7-(azetidin-1-yl)-4-methyl-2H-chromen-2-one (2a)

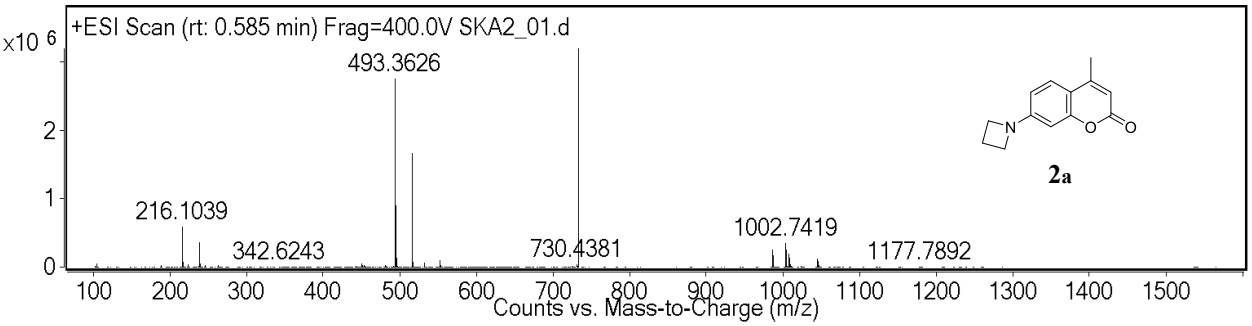


Figure S3. HRMS spectrum of 7-(azetidin-1-yl)-4-methyl-2H-chromen-2-one (2a)

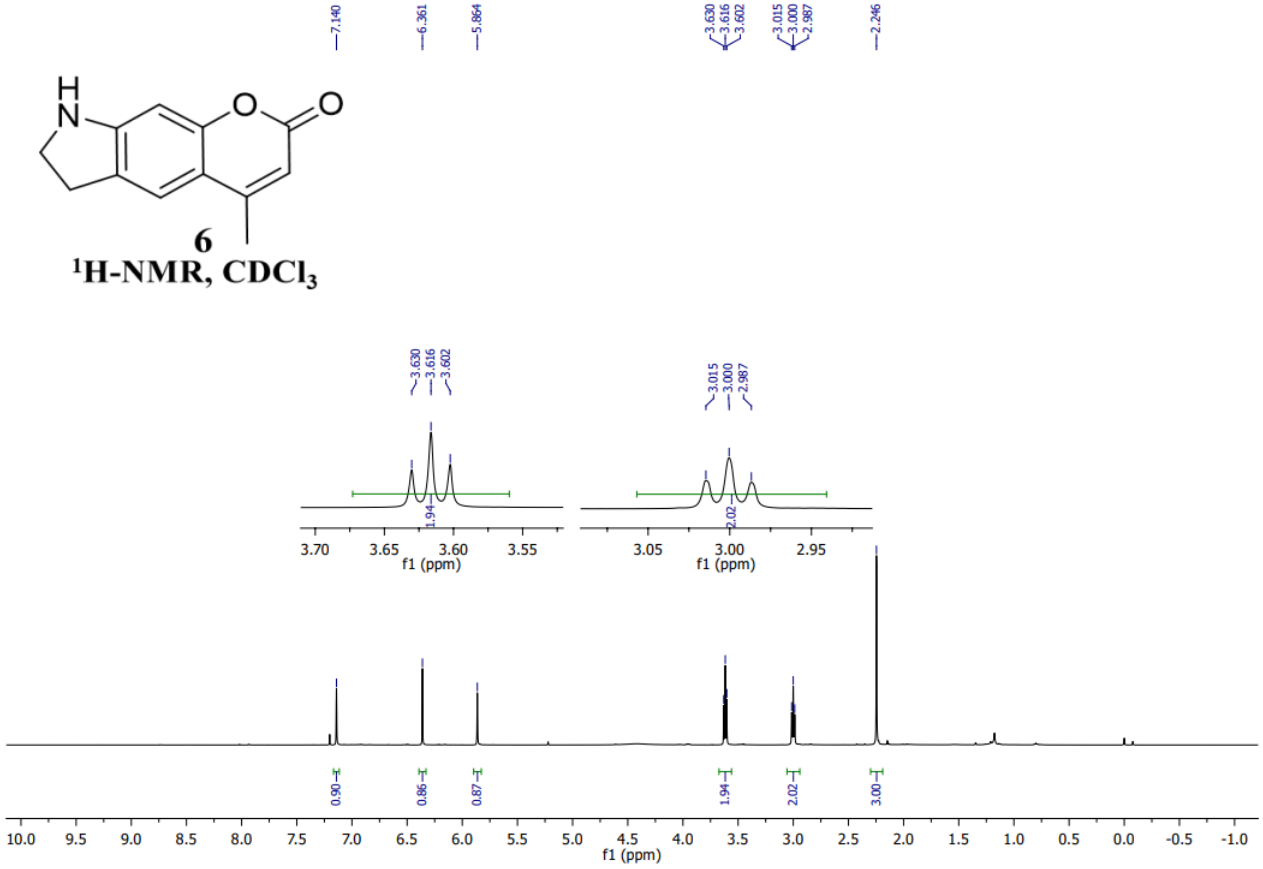


Figure S4. ^{1}H-NMR spectrum of 4-methyl-7,8-dihydropyrano[3,2-f]indol-2(6*H*)-one (6)

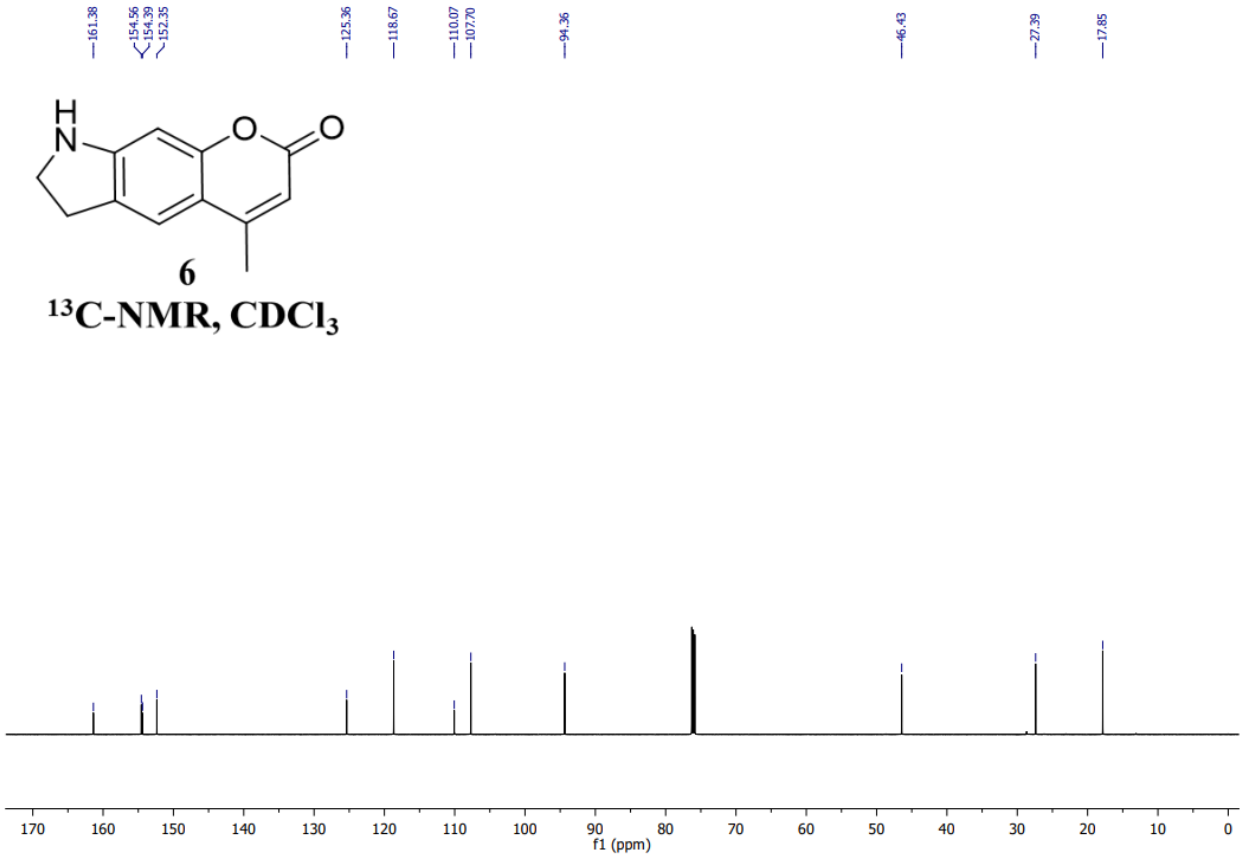


Figure S5. ^{13}C-NMR spectrum of 4-methyl-7,8-dihydropyrano[3,2-f]indol-2(6*H*)-one (6)

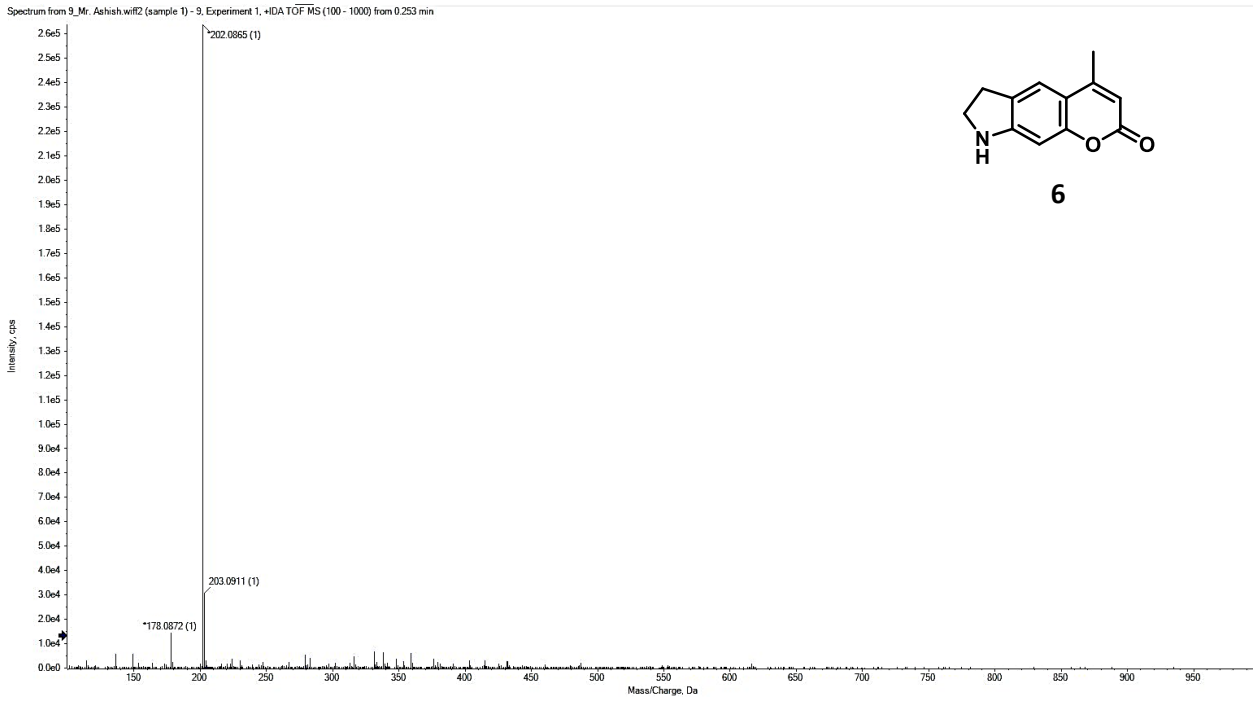


Figure S6. HRMS spectrum of 4-methyl-7,8-dihydropyrano[3,2-f]indol-2(6*H*)-one (6)

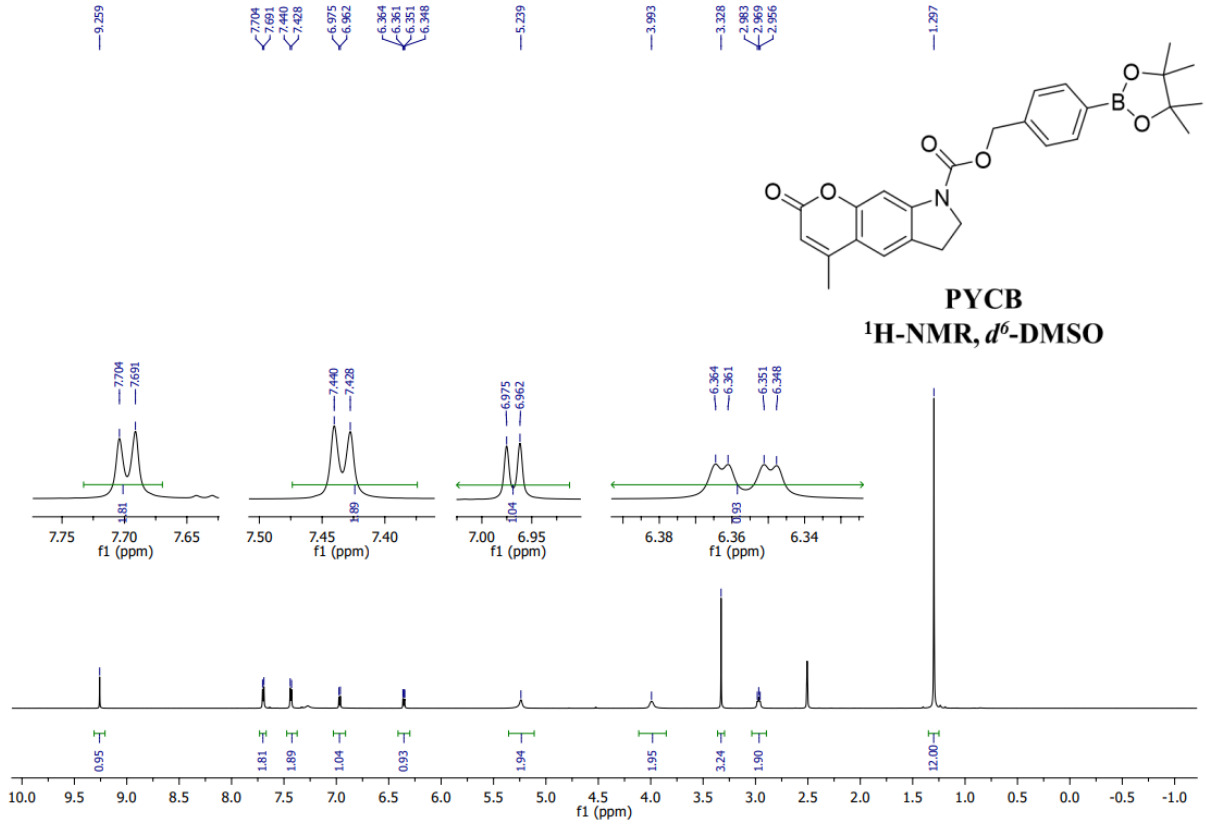


Figure S7. ^{1}H-NMR spectrum of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl-4- methyl-2-oxo-6,7-dihydropyrano [3,2-f]indole-8(2H)-carboxylate (PYCB).

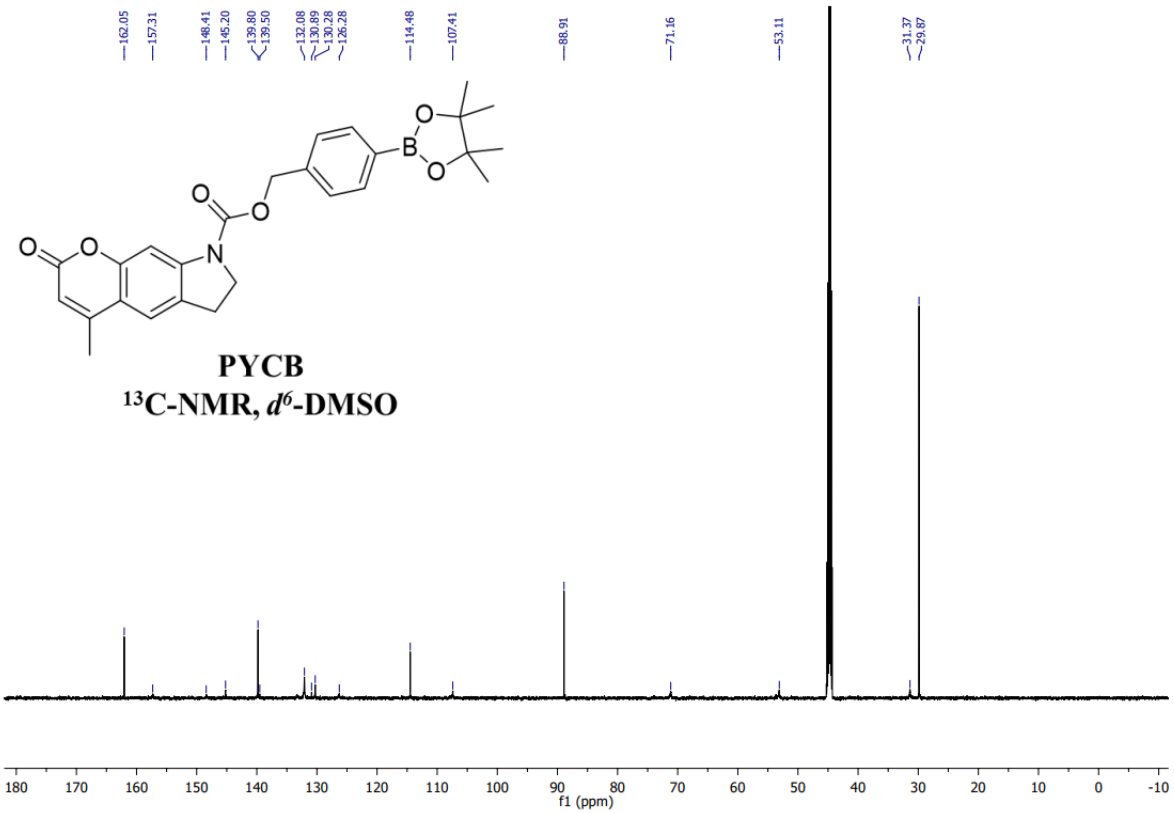


Figure S8. ^{13}C-NMR spectrum of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl-4- methyl-2-oxo-6,7-dihydropyrano [3,2-f]indole-8(2H)-carboxylate (PYCB).

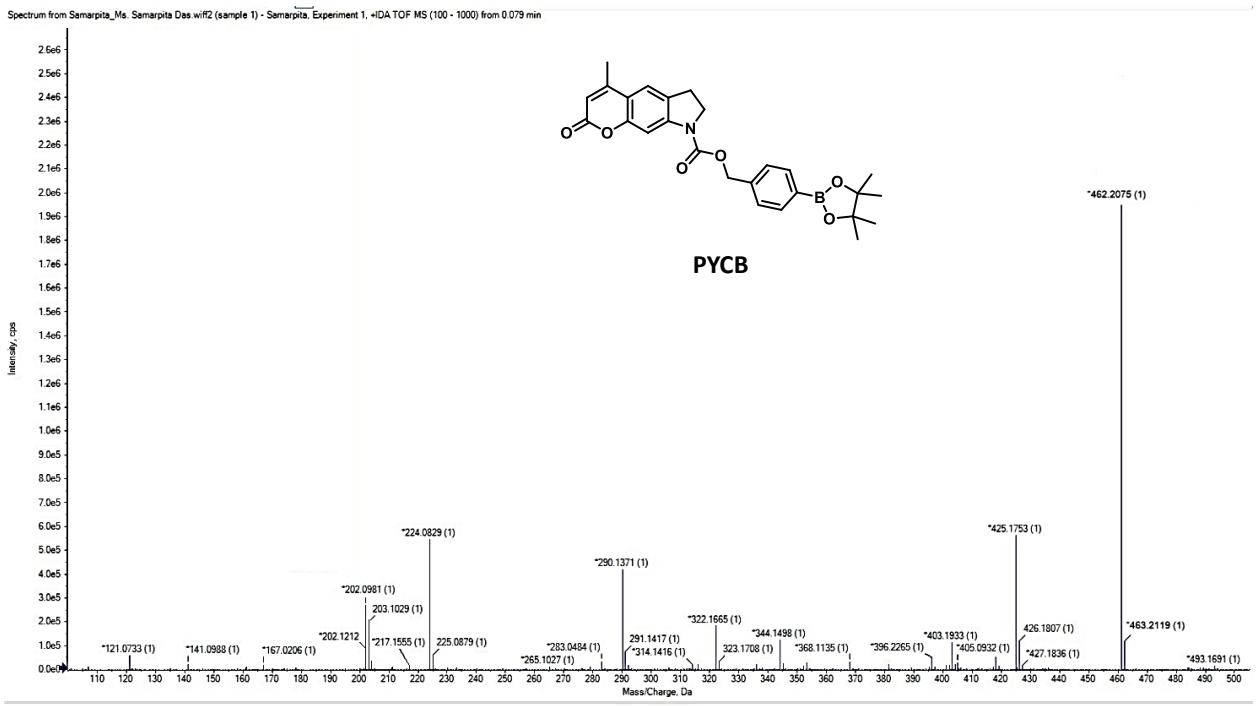


Figure S9. HRMS spectrum of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl-4-methyl-2-oxo-6,7-dihydropyrano [3,2-f]indole-8(2H)-carboxylate (PYCB).

Table S2. Comparison of the practical and theoretical excitation energy (calculated using B3LYP functional and 6-31++g(d,p) basis set).

Sl. No.	Compound	Practical λ_{abs} (nm)	Theoretical λ_{abs} (nm)	HOMO-LUMO energy gap (eV) (after excitation)	Practical λ_{em} (nm)	Theoretical λ_{em} (nm)	HOMO-LUMO energy gap (eV) (after emission)
1.	**4**	355	363.19	3.71	478	414.19	3.26
2.	**6**	363	351.11	3.94	462	418.17	3.38
3.	**7**	360	357.36	3.84	468	404.07	3.31
4.	**8**	355	358.31	3.82	469	404.40	3.311
5.	**9**	370	358.60	3.94	462	402.96	3.31

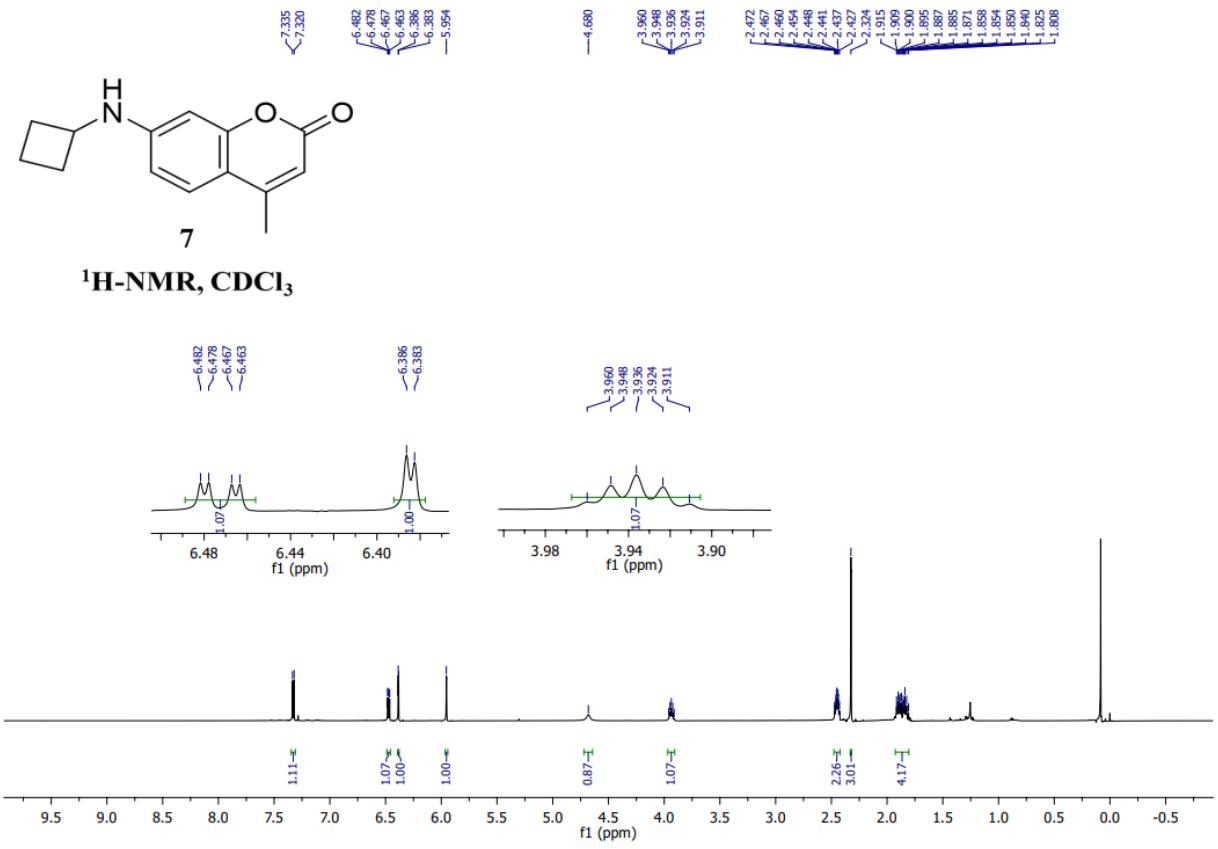


Figure S10. ^{1}H-NMR spectrum of 7-(cyclobutylamino)-4-methyl-2H-chromen-2-one (7)

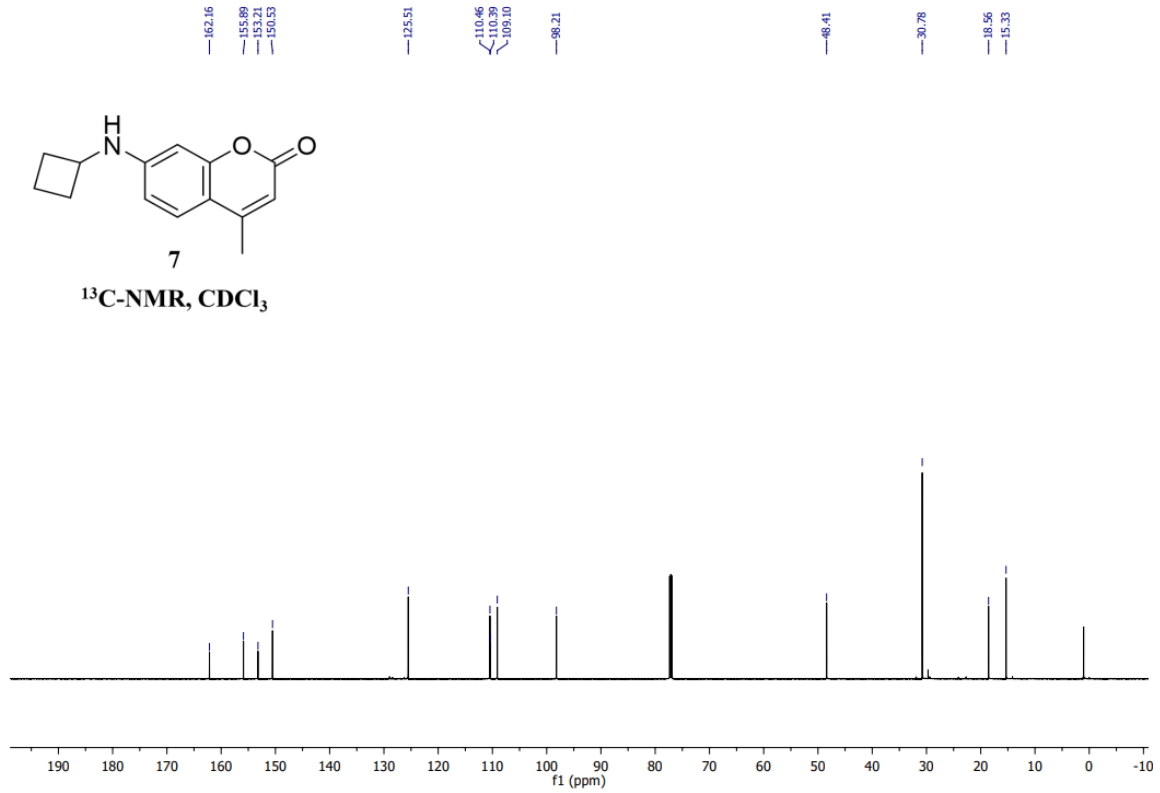


Figure S11. ^{13}C-NMR spectrum of 7-(cyclobutylamino)-4-methyl-2H-chromen-2-one (7)

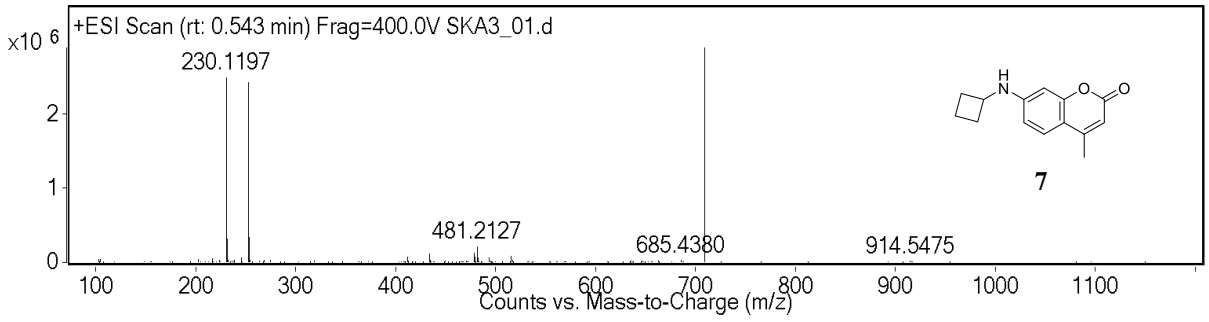


Figure S12. HRMS spectrum of 7-(cyclobutylamino)-4-methyl-2H-chromen-2-one (8)

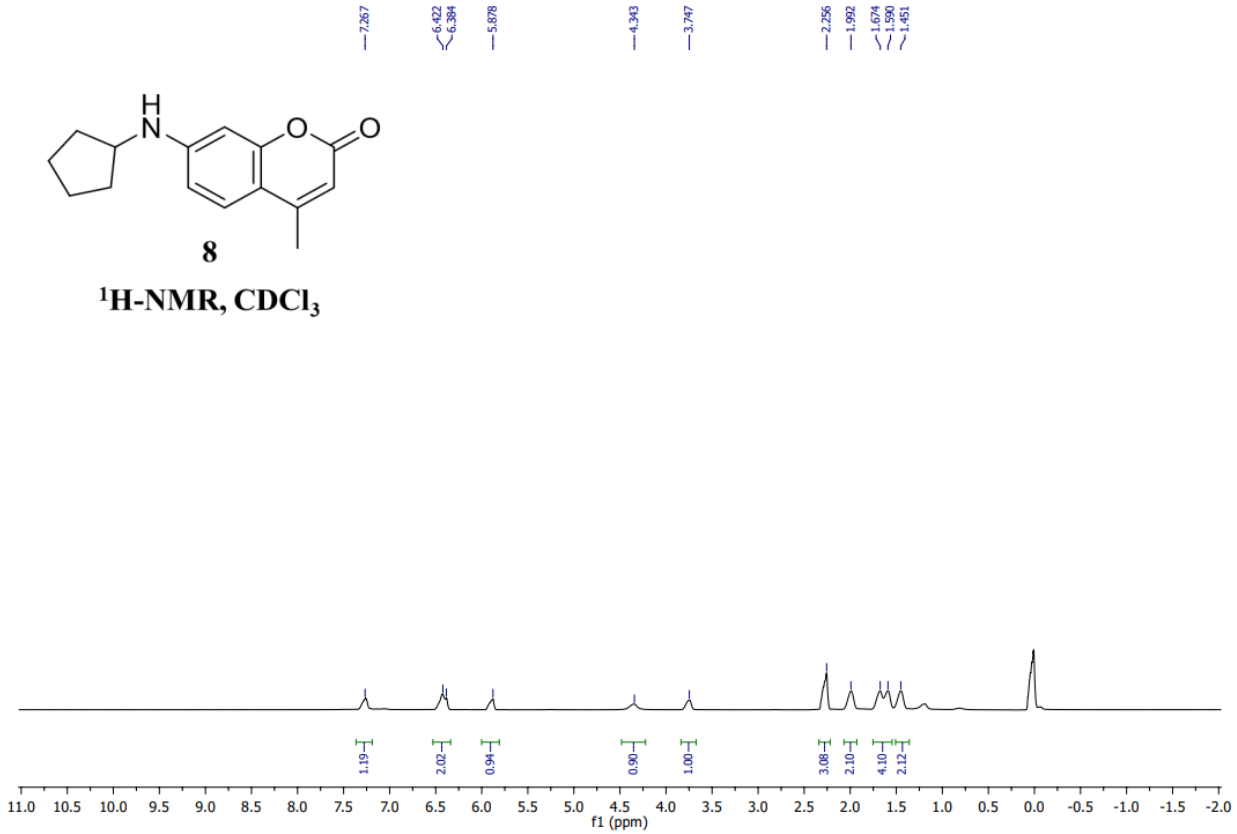


Figure S13. ^{1}H-NMR spectrum of 7-(cyclopentylamino)-4-methyl-2H-chromen-2-one (8)

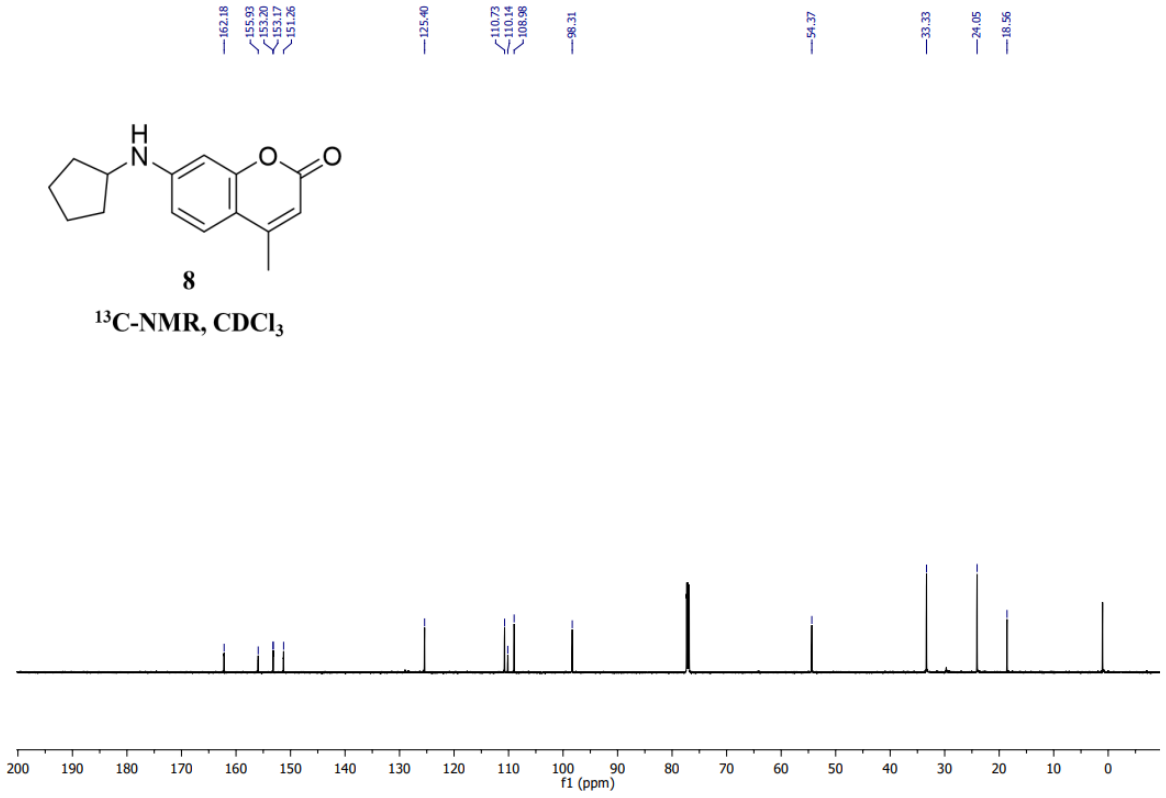


Figure S14. ^{13}C-NMR spectrum of 7-(cyclopentylamino)-4-methyl-2H-chromen-2-one (8)

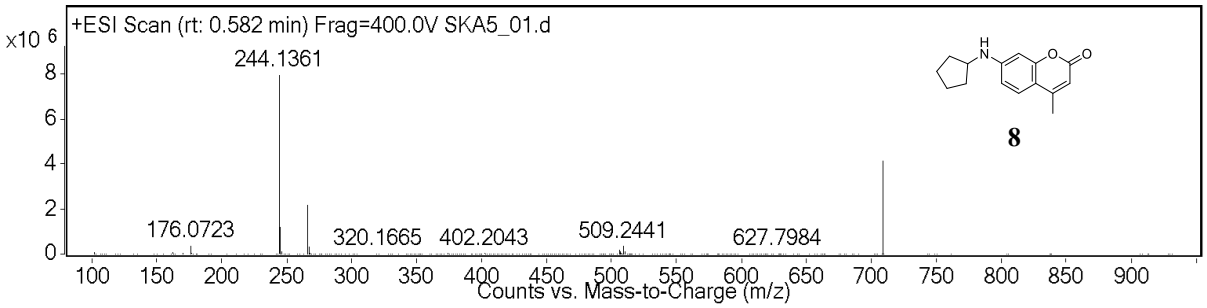
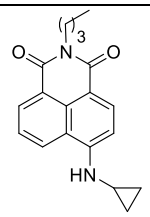
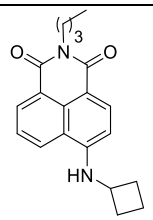
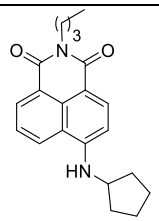
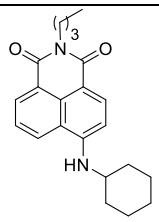
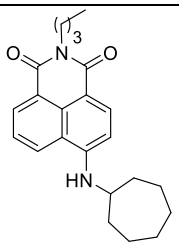
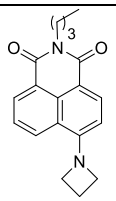
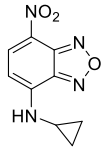
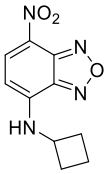
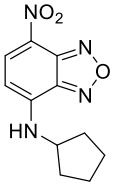
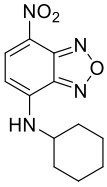
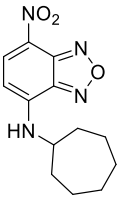
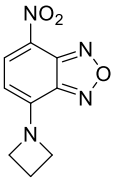


Figure S15. HRMS spectrum of 7-(cyclopentylamino)-4-methyl-2H-chromen-2-one (8)

Table S3. Photophysical properties of compounds 5-5e and 6-6e in different solvents.

Compound	Compound Structure	λ_{abs} (nm)[a]			λ_{em} (nm)[b]		
		DCM	MeOH	PBS	DCM	MeOH	PBS
5a		435	437	448	535	536	553
5b		430	443	454	510	532	549
5c		430	445	447	510	533	549
5d		445	446	448	535	531	549
5e		445	445	444	535	535	541
5		439	448	462	516	540	556

6a		465	463	479	535	537	552
6b		460	467	485	530	533	551
6c		460	469	492	530	536	548
6d		470	470	493	535	537	551
6e		470	471	492	535	536	548
6		480	483	500	530	545	566

[a]λ_{max} (abs) = absorption maxima (nm); [b]λ_{max} (em) = emission maxima (nm).

Table S4. Comparison of the practical and theoretical excitation energy (calculated using B3LYP functional and 6-31++g(d,p) basis set).

Sl. No.	Compound	Practical λ_{abs} (nm)	Theoretical λ_{abs} (nm)	HOMO-LUMO energy gap (eV) (after excitation)	Practical λ_{em} (nm)	Theoretical λ_{em} (nm)	HOMO-LUMO energy gap (eV) (after emission)
1.	**5**	462	438.72	3.209	556	510.08	2.051

2.	**5b**	454	431.12	3.267	549	508.85	2.953
3.	**6**	500	440.15	3.107	566	523.49	2.855
4.	**6b**	485	443.47	3.192	551	537.77	2.900

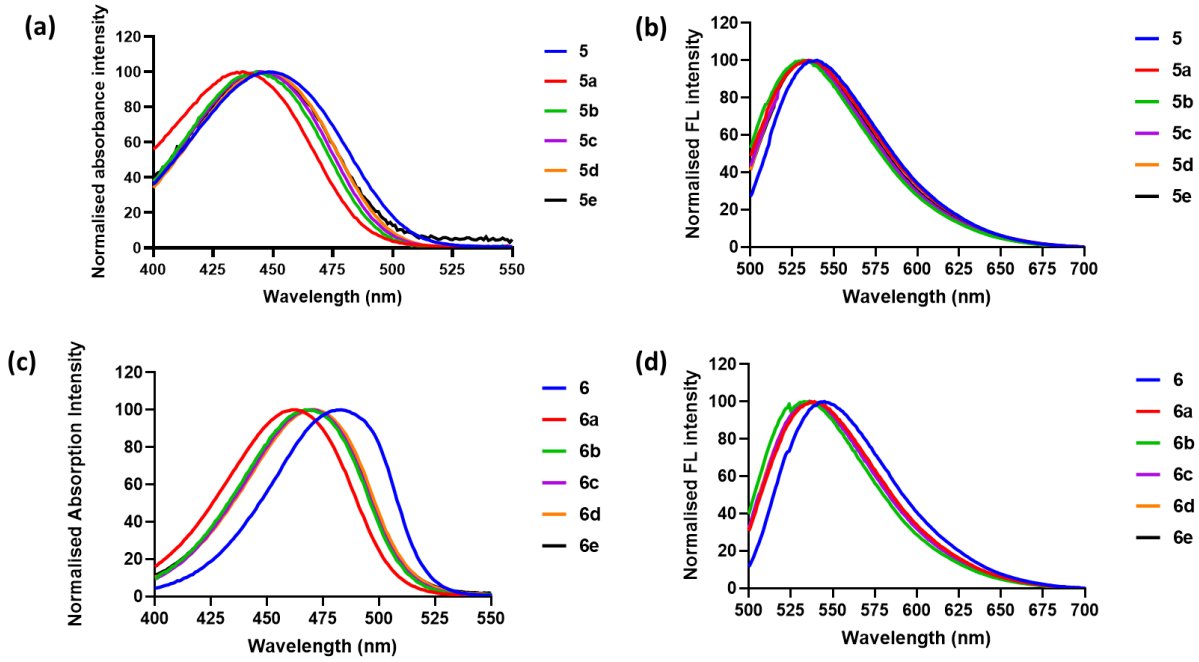


Figure S16. (a,b) Normalised absorption and fluorescence emission peaks of compounds **5a-5e** in methanol in comparison to **5**; (c,d) Normalised absorption and fluorescence emission peaks of compounds **6a-6e** in methanol in comparison to **6**.

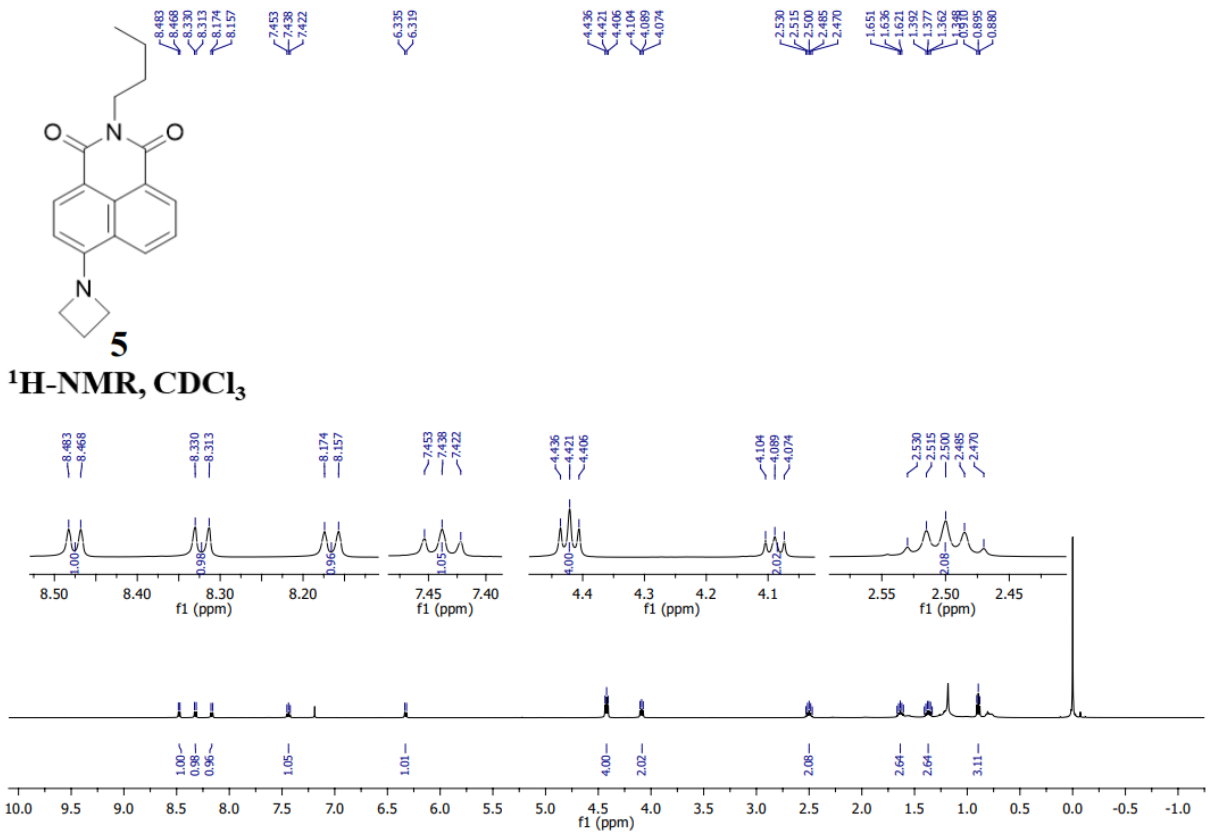


Figure S17. ^{1}H-NMR spectrum of 6-(azetidin-1-yl)-2-butyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (5)

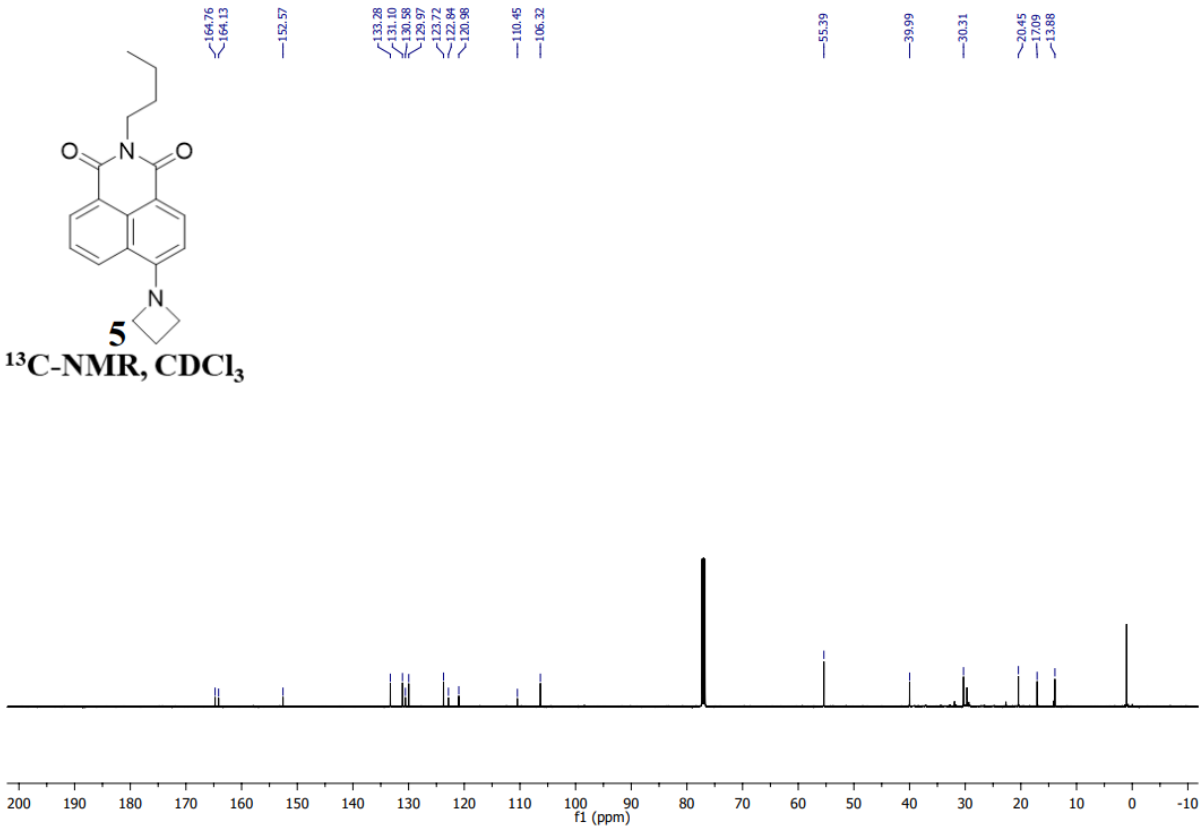


Figure S18. ^{13}C-NMR spectrum of 6-(azetidin-1-yl)-2-butyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (5)

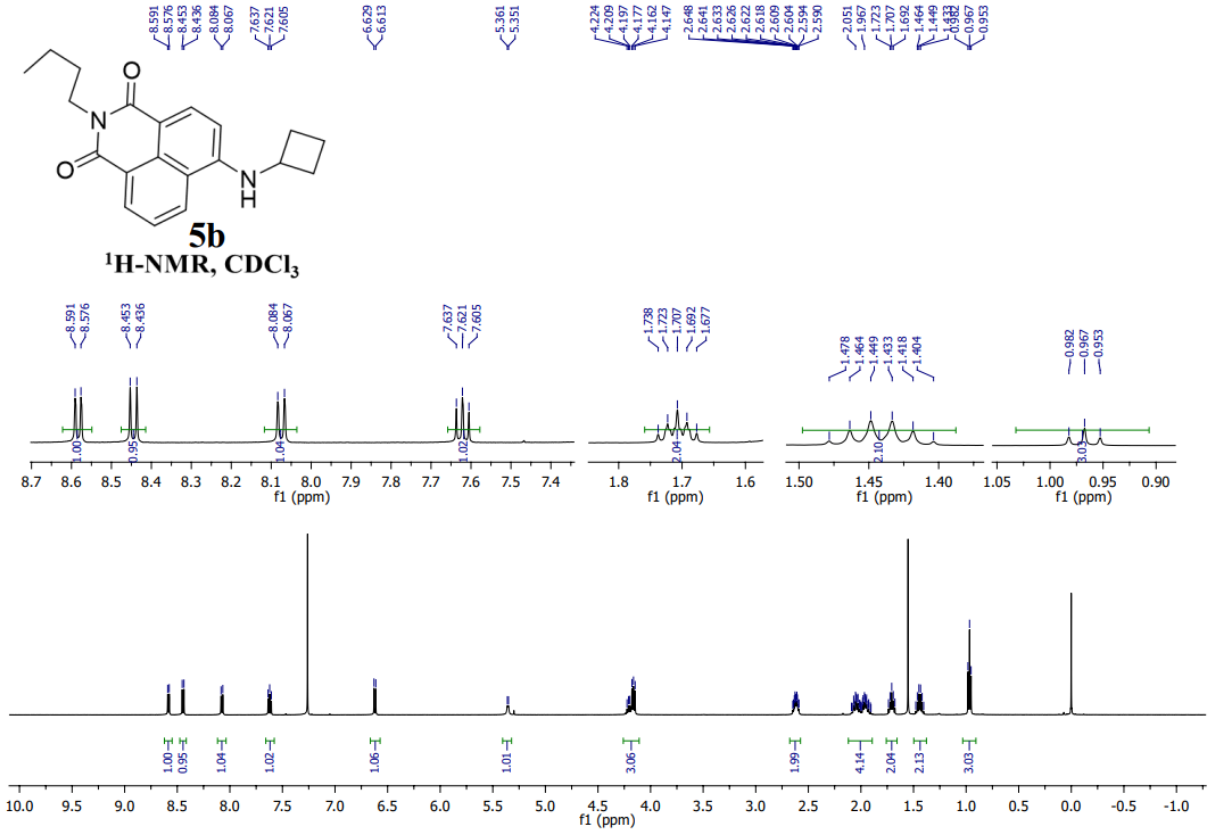


Figure S19. ^{1}H-NMR spectrum of 6-(cyclobutyl)-2-butyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (5b).

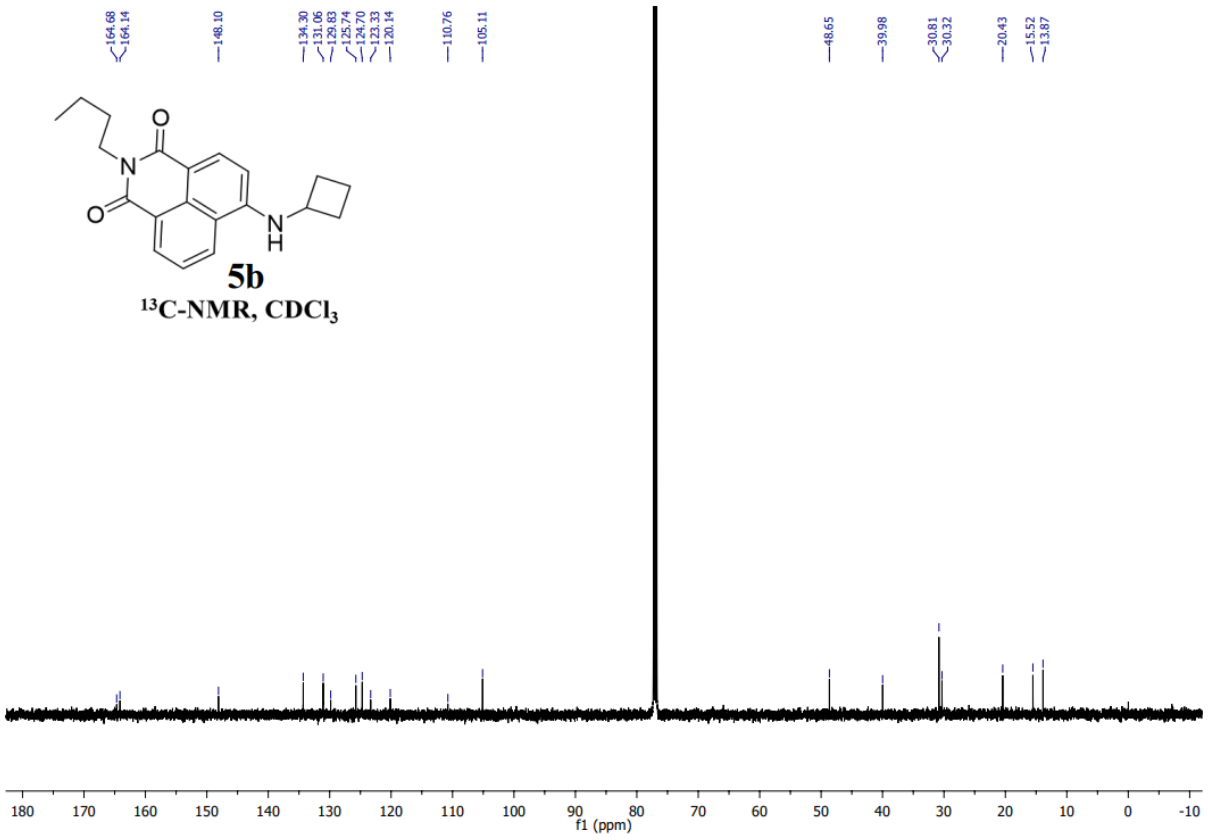


Figure S20. ^{13}C-NMR spectrum of 6-(cyclobutyl)-2-butyl-1H-benzo[de]isoquinoline-1,3(2H)-dione (5b).

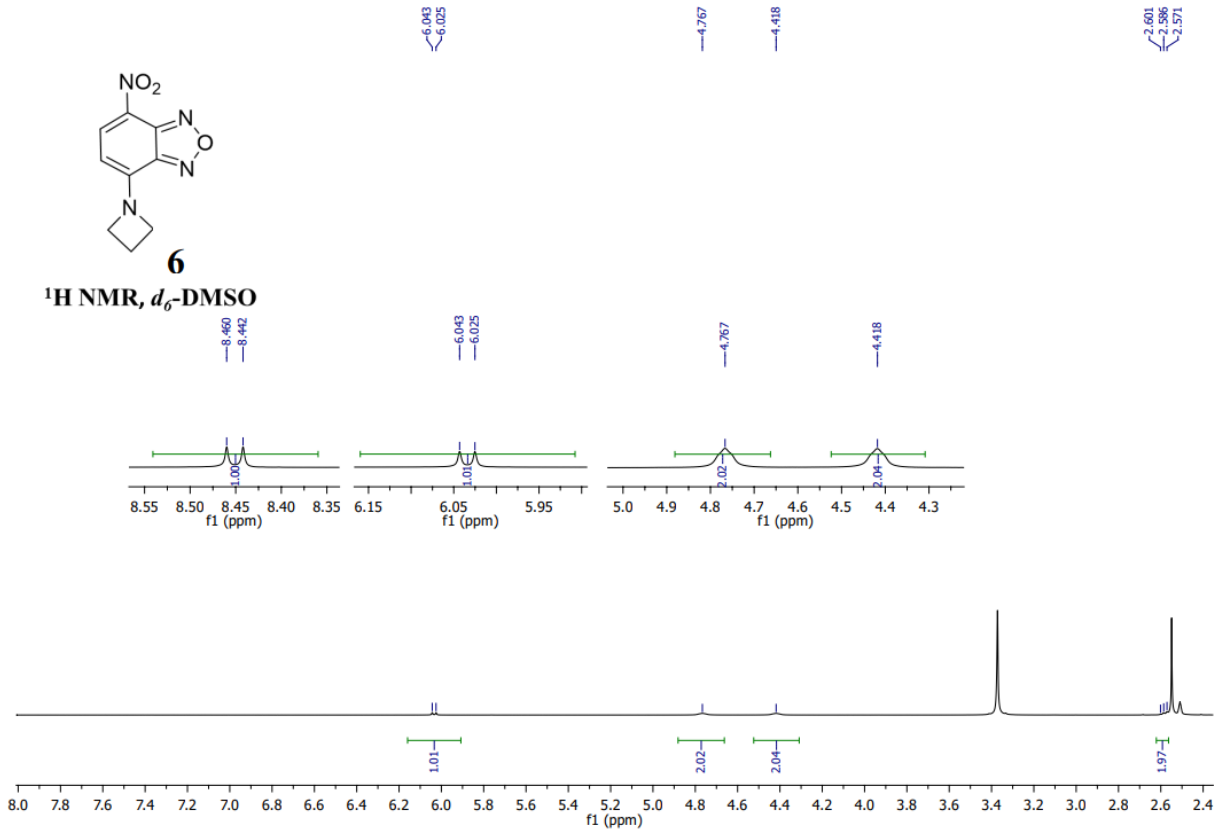


Figure S21. ^{1}H-NMR spectrum of 4-(azetidin-1-yl)-7-nitrobenzo[c][1,2,5]oxadiazole (6).

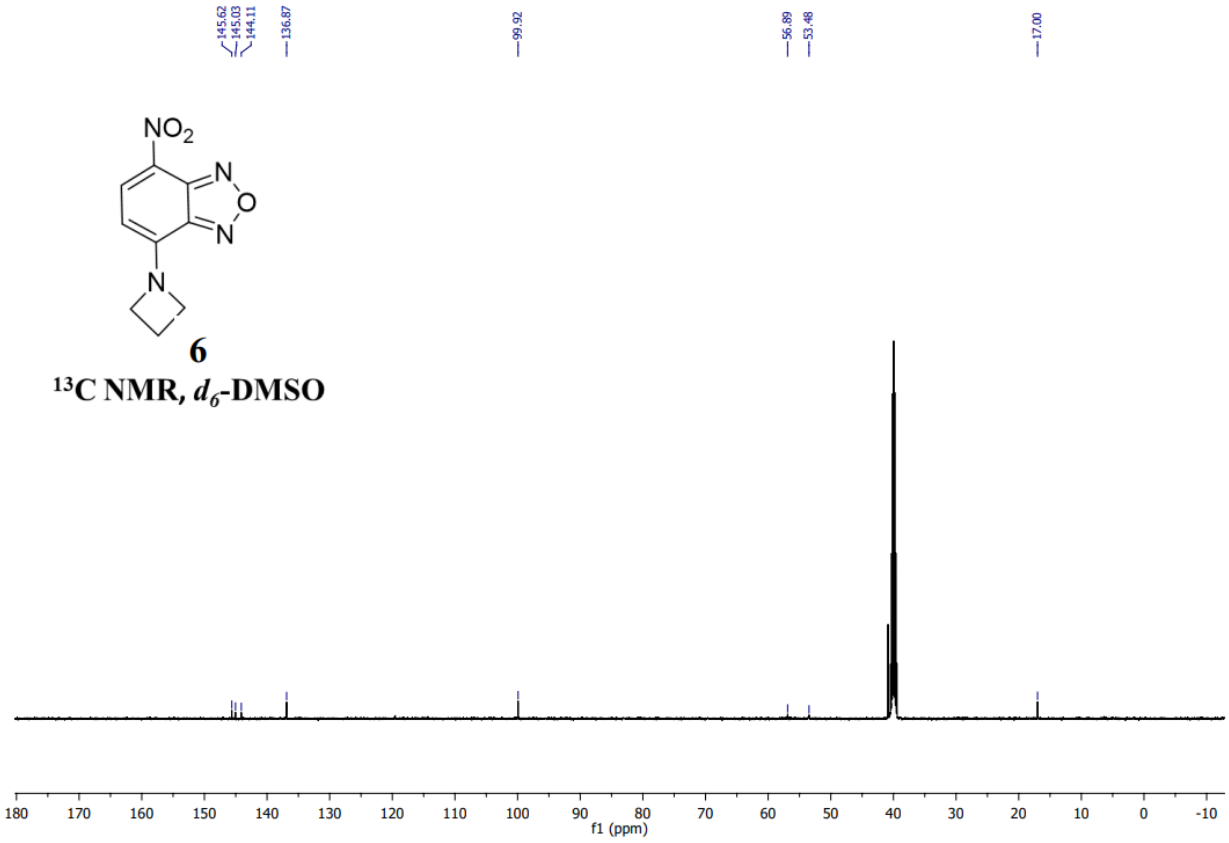


Figure S22. ^{13}C-NMR spectrum of 4-(azetidin-1-yl)-7-nitrobenzo[c][1,2,5]oxadiazole (6).

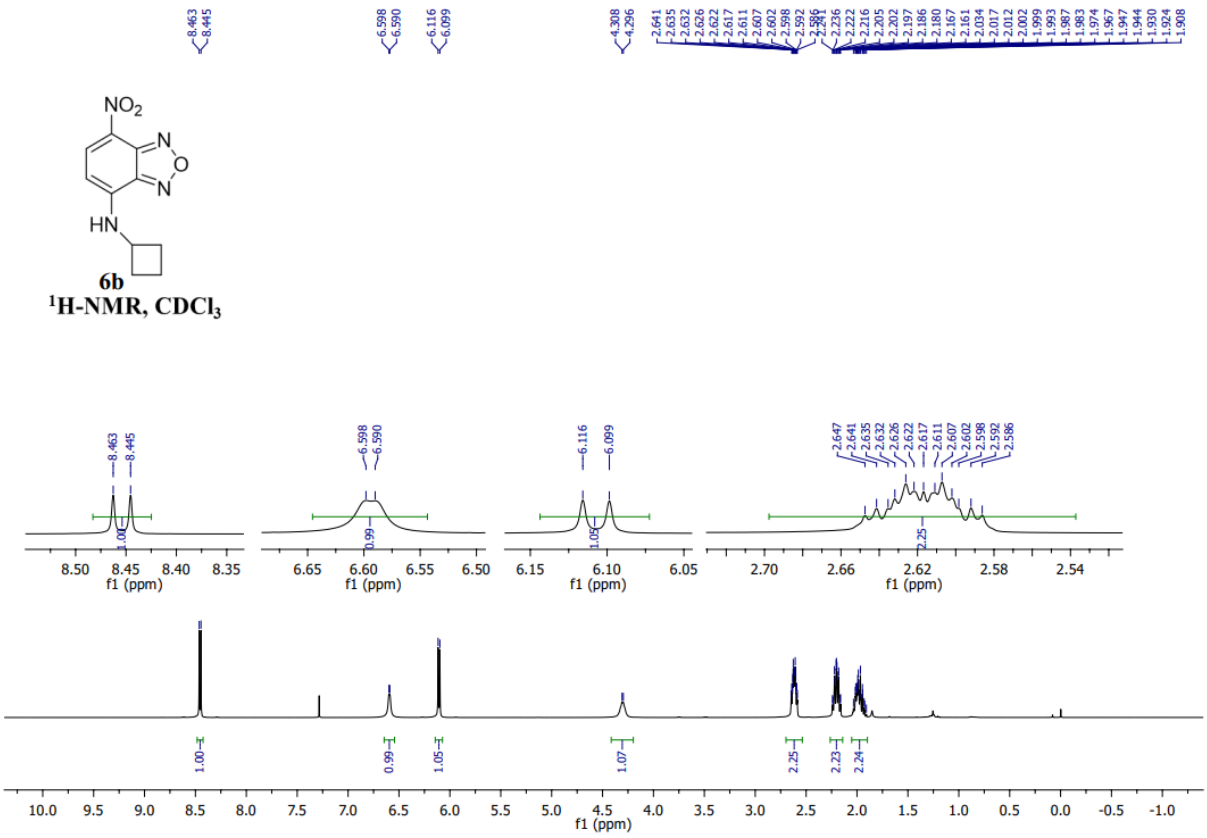


Figure S23. ^{1}H-NMR spectrum of *N*-cyclobutyl-7-nitrobenzo[c][1,2,5]oxadiazol-4-amine (6b).

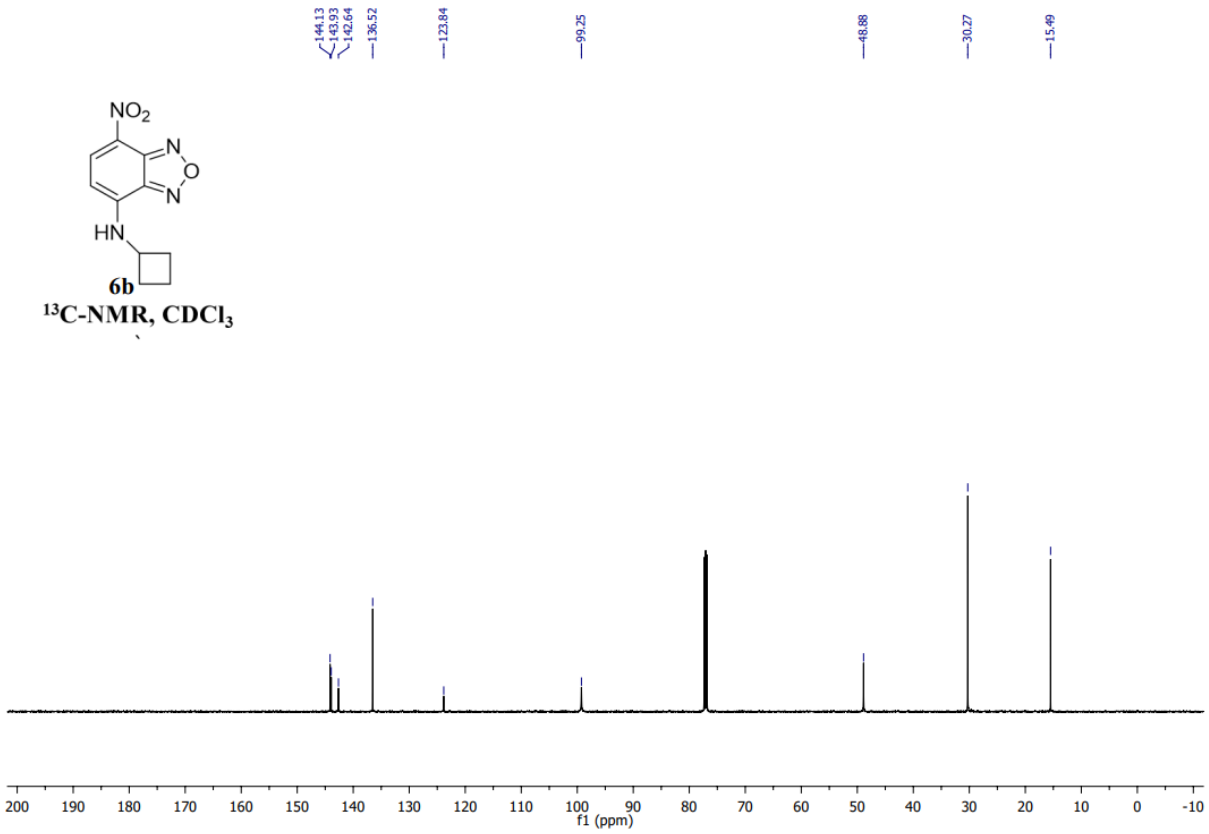


Figure S24. ^{1}H-NMR spectrum of *N*-cyclobutyl-7-nitrobenzo[c][1,2,5]oxadiazol-4-amine (6b).

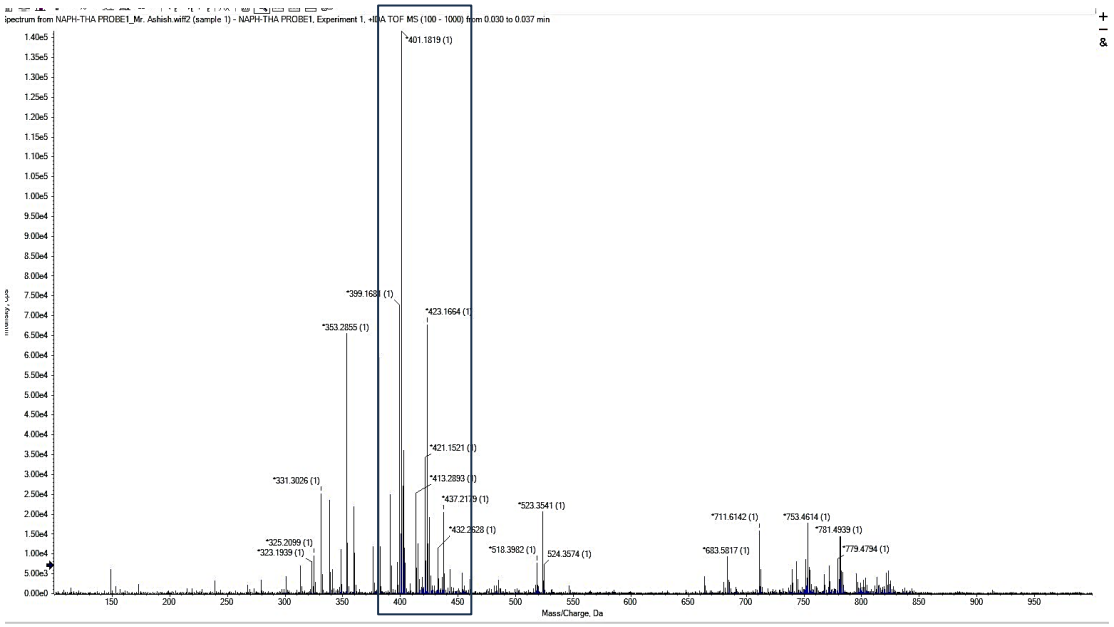


Figure S25. HRMS spectrum of *N*-(2-butyl-1,3-dioxo-2,3-dihydro-1H-benzo[de]isoquinolin-6-yl)-2-chloro-N-cyclobutylacetamide (NAPB)

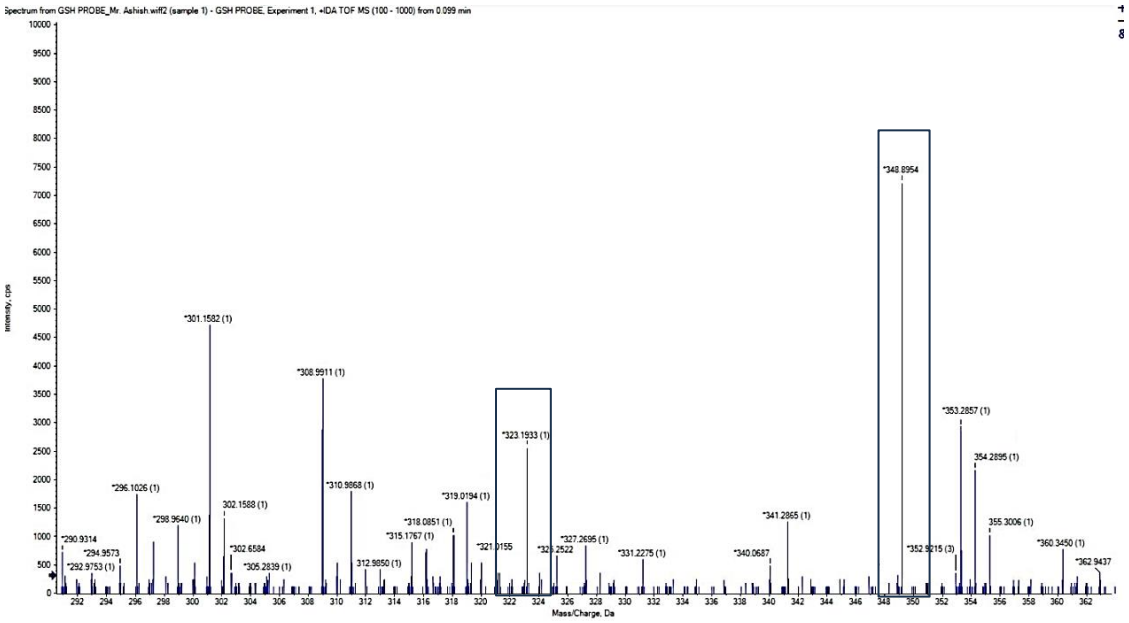


Figure S26. HRMS spectrum of NAPB and GSH reaction mixture

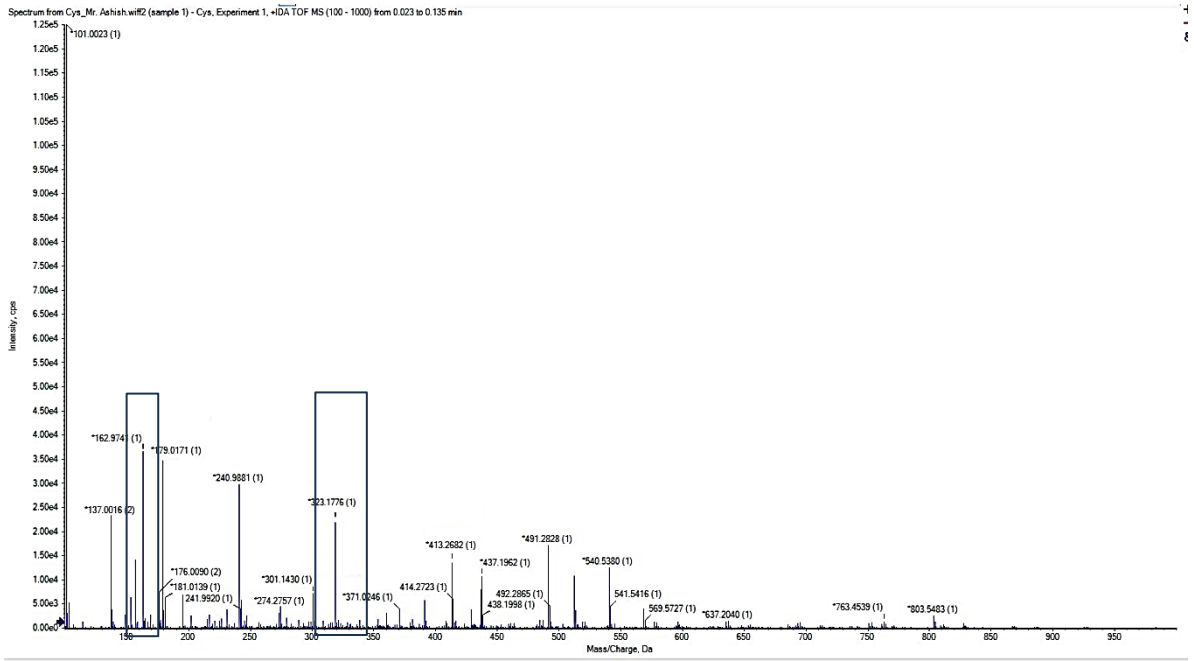


Figure S27. HRMS spectrum of NAPB and Cys reaction mixture

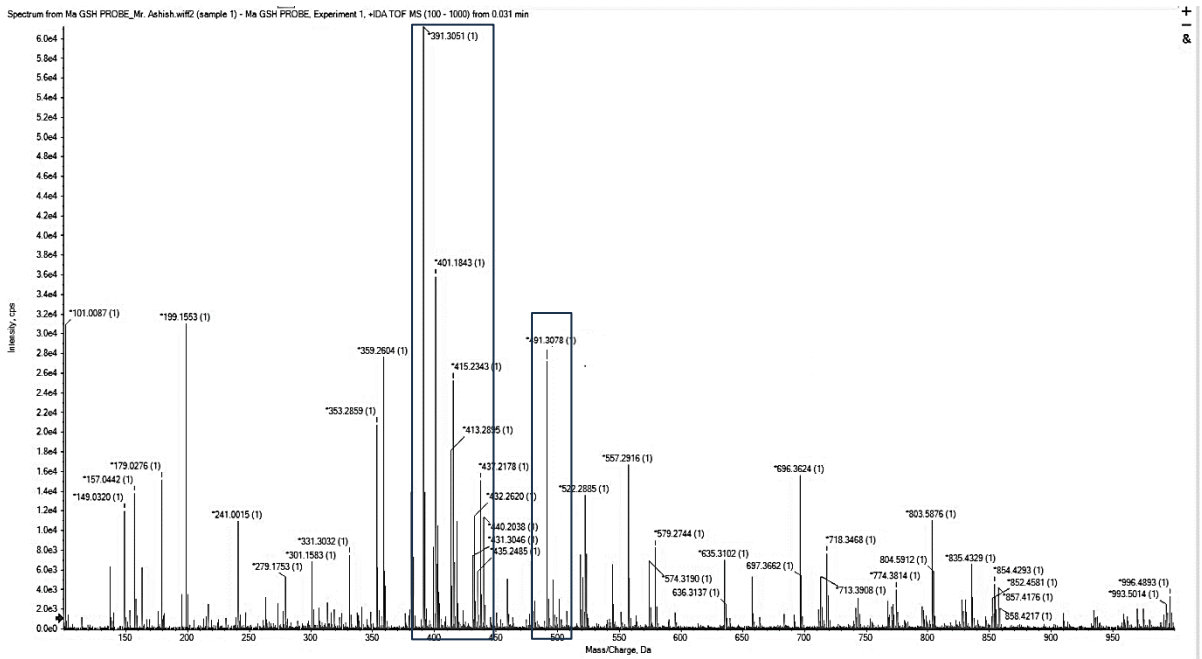


Figure S28. HRMS Spectra of NAPB, GSH and NPM reaction mixture

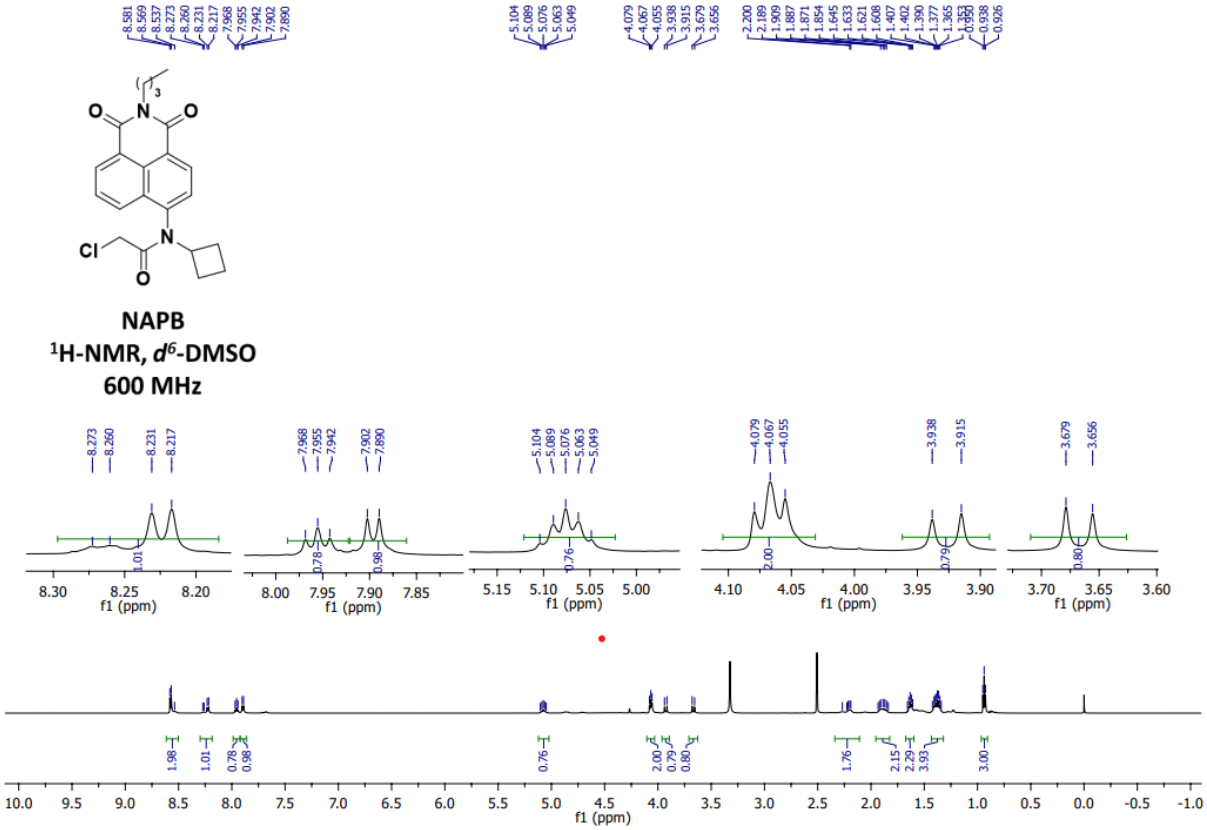


Figure S29. ^{1}H-NMR spectrum of *N*-(2-butyl-1,3-dioxo-2,3-dihydro-1H-benzo[de]isoquinolin-6-yl)-2-chloro-N-cyclobutylacetamide (NAPB).

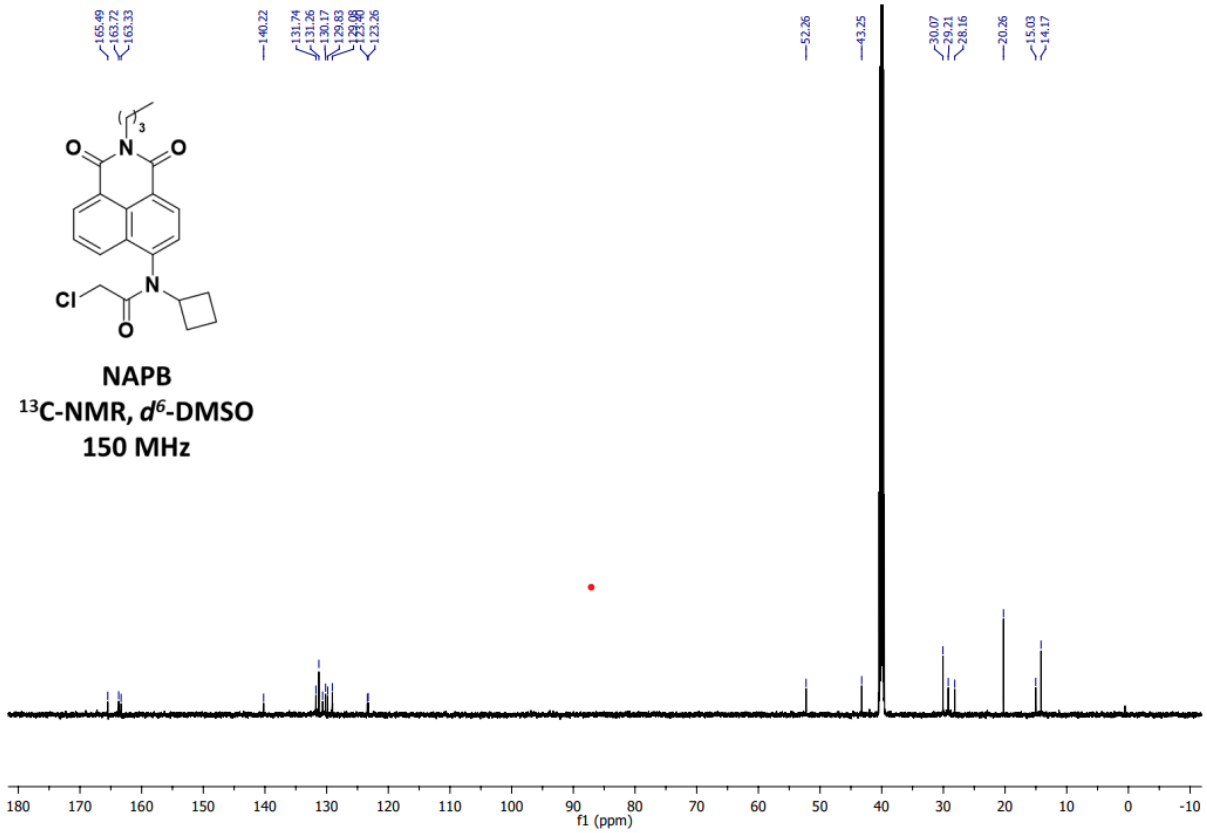


Figure S30. ^{13}C-NMR spectrum of *N*-(2-butyl-1,3-dioxo-2,3-dihydro-1H-benzo[de]isoquinolin-6-yl)-2-chloro-N-cyclobutylacetamide (NAPB).

List of Publications

[1] Das, S.; Goswami, P.; Verma, V. K.; Indurthi, H. K.; Kumar, M.; Koch, B.; Sharma, D. K. Rapid Access to 7-Substituted Cycloalkylamino and Alkylamino Analogues of 4-Methylcoumarin Reveals Surprising Emitters. *Dyes Pigm.* **2023**, *217*, 111407-111415. https://doi.org/10.1016/j.dyepig.2023.111407.

[2] Das, S.; Goswami, P.; Indurthi, H. K.; Koch, B.; Sharma, D. K. Improving the fluorescence brightness of naphthalimide and nitrobenzoxadiazole dyes with cycloalkylamine auxochromes. *Dyes Pigm.* **2024**, *227*, 112206-112213. https://doi.org/10.1016/j.dyepig.2024.112206.

[3] Das, S.; Chaudhuri, A..; Indurthi, H. K.; Agrawal, A. K.; Sharma, D. K. Azacoumarin-based "turn-on" fluorescent probe for the detection and imaging of hydrogen peroxide in living cells. *Org. Biomol. Chem.*, **2024**, *22*, 7332-7336.

[4] Das, S.; Goswami, P.; Indurthi, H. K.; Koch, B.; Sharma, D. K. Cyclobutylamino-naphthalimide-based Ratiometric Fluorescent Probe for Detection of Glutathione in living cells. *(Manuscript under review)*