Electronic Supplementary Material (ESI) for RSC Advances.

BODIPY dyes functionalized with 2-(2-dimethylaminophenyl)ethanol moieties as sensitive and selective fluorescent chemodosimeters for the nervous agents mimics DCNP and DFP

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Supplementary Information

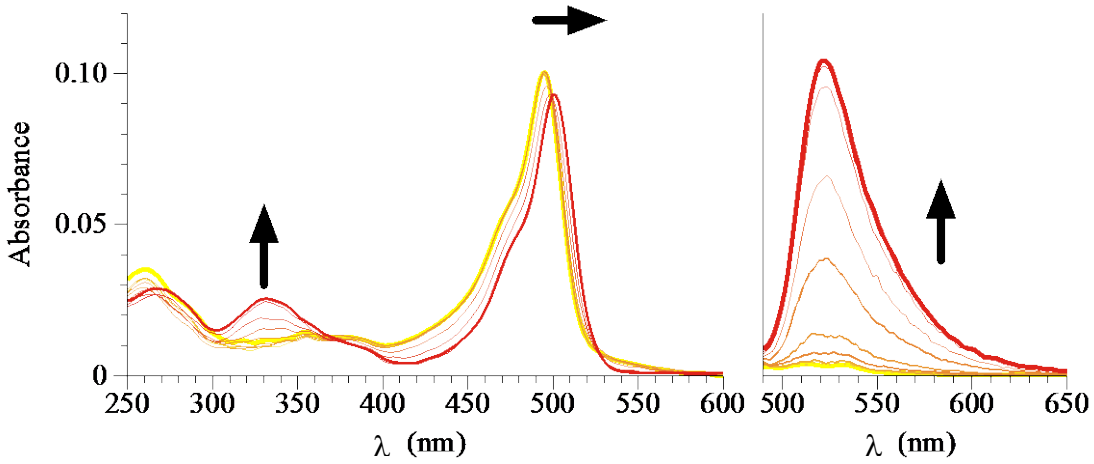

Figure S-1. UV-vis (left) and emission (right, λ_{exc}=480 nm) spectrum of compound **1** ($1x10^{-6}$M in MeCN) titrated with DCNP (from 100 μM to 20 mM) Yellow: free ligand, red: ligand+DCNP 20 mM

Crystallographic Data Compound 1:

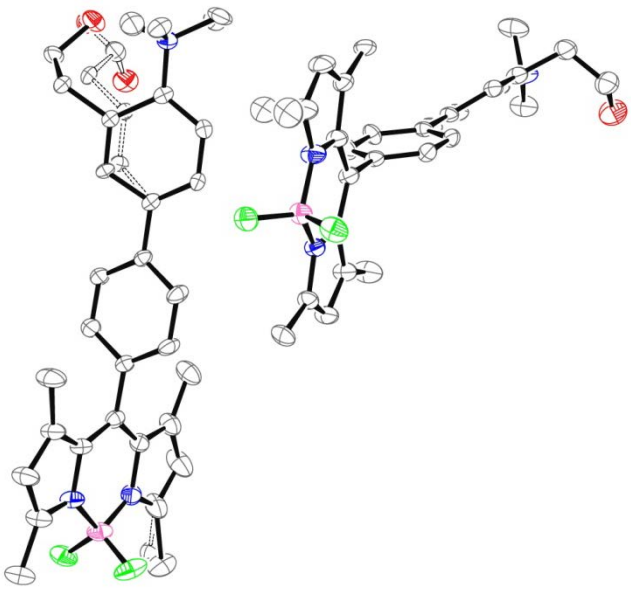

Figure S-2. Asymmetric unit of structure of compound **2**, including disorders atoms. Hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for compound **2**.

Empirical formula	$C_{58}\,H_{47}\,B_2\,F_4\,N_6\,O_2$
Formula weight	957.64
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 15.7361(3) Å
	b = 16.6946(4) Å β = 103.168(3)º
	c = 20.2283(7) Å
Volume	5174.4(2) $Å^3$
Z, Calculated density	4, 1.229 mg/m^3
Absorption coefficient	0.085 mm^{-1}
F(000)	1996
Crystal size	0.17 x 0.11 x 0.09 mm
θ range for data collection	2.86 to 25.00º
Limiting indices	-18<=h<=12, -19<=k<=19, -24<=l<=24
Reflections collected / unique	29796 / 9092 [R(int) = 0.0522]
Completeness to θ = 25.00	99.8 %
Max. and min. transmission	0.9924 and 0.9857
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9092 / 884 / 777
Goodness-of-fit on F^2	1.256
Final R indices [I>2σ(I)]	R1 = 0.1007, wR_2 = 0.3103
R indices (all data)	R1 = 0.1330, wR_2 = 0.3511
Extinction coefficient	0.0014(10)
Largest diff. peak and hole	1.161 and -0.842 $e.A^{-3}$

Figure S-3. ^{1}H NMR spectrum of compound **1** in CD_2Cl_2.

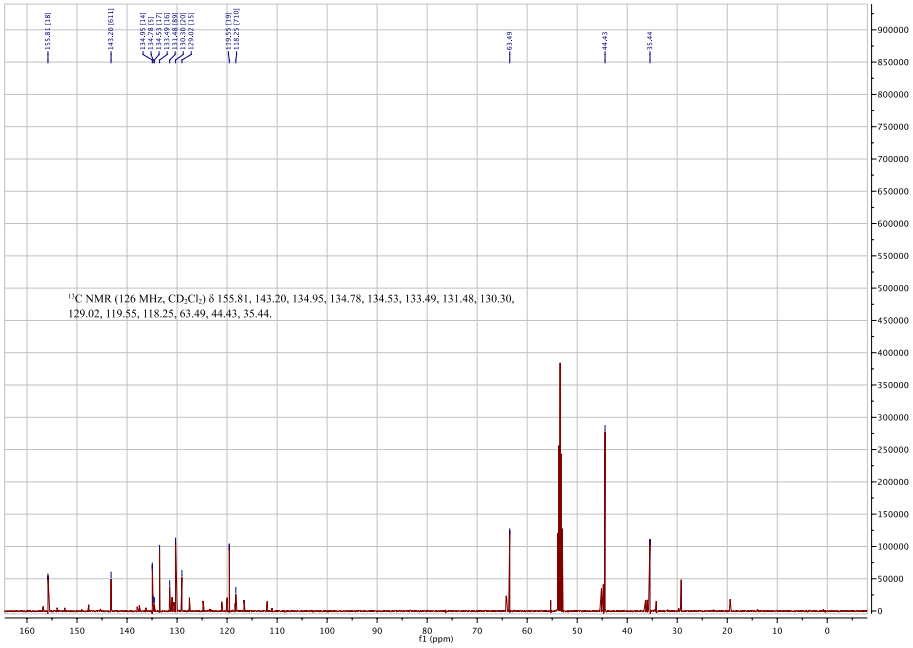

Figure S-4. ^{13}C NMR spectrum of compound **1** in CD_2Cl_2.

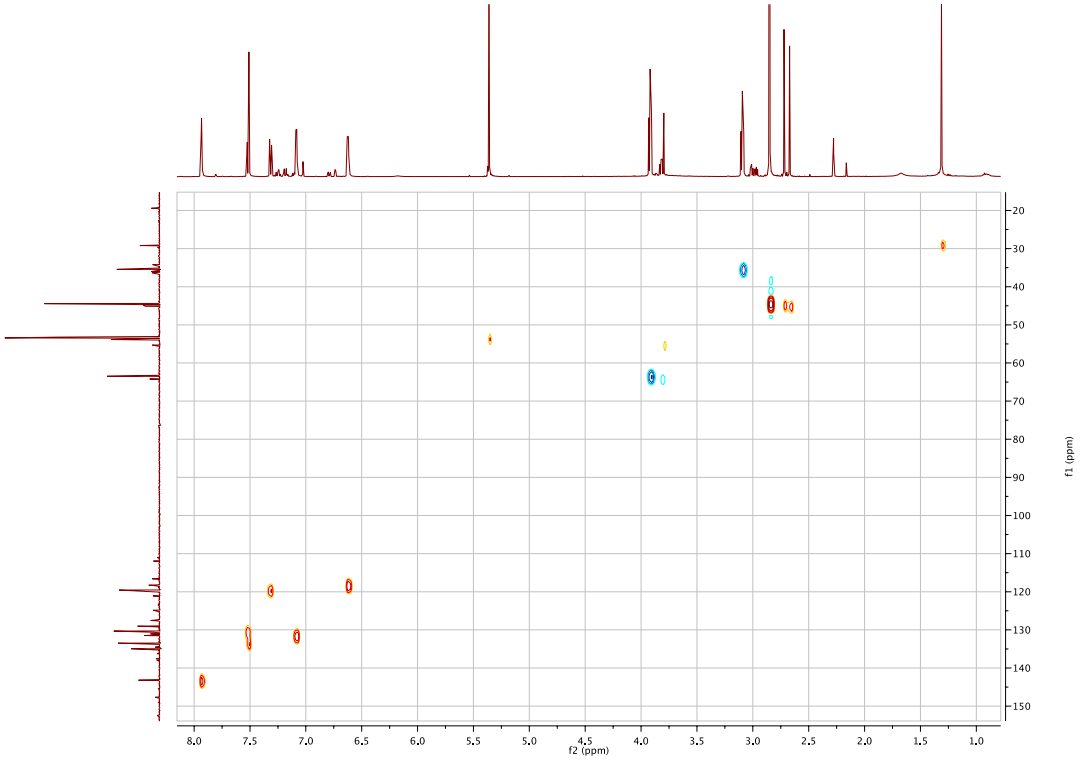

Figure S-5. HSQC spectrum of compound **1** in CD_2Cl_2.

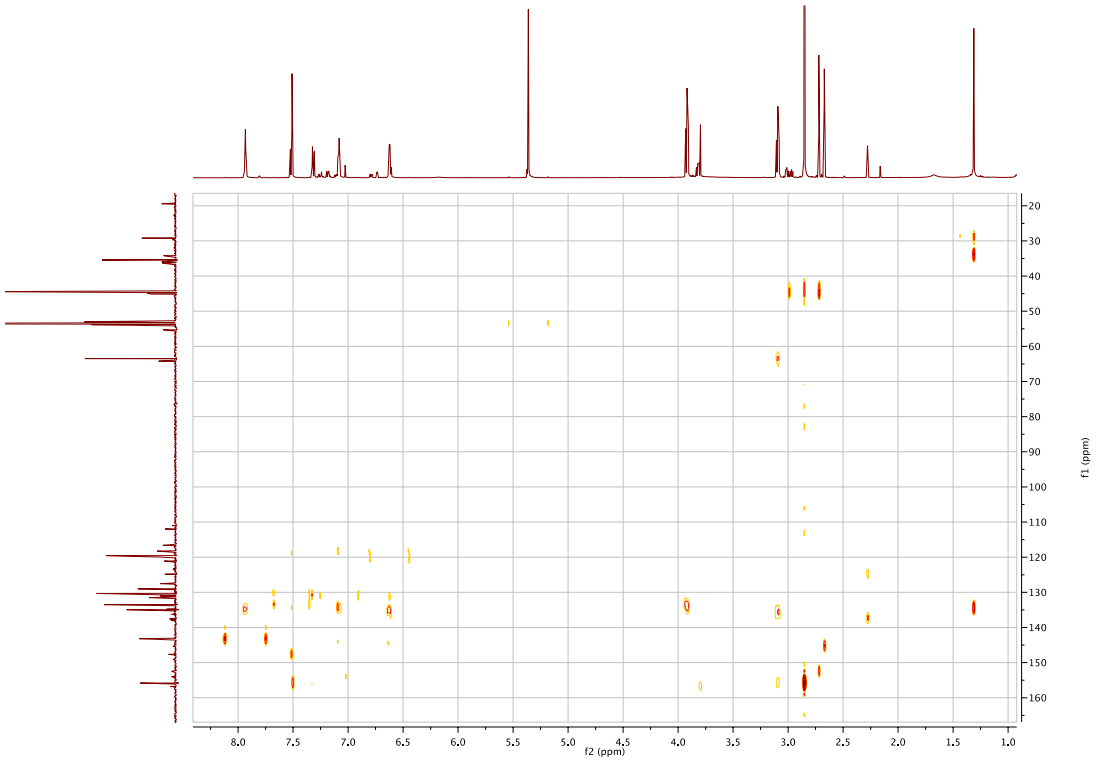

Figure S-6. HMBC spectrum of compound **1** in CD_2Cl_2.

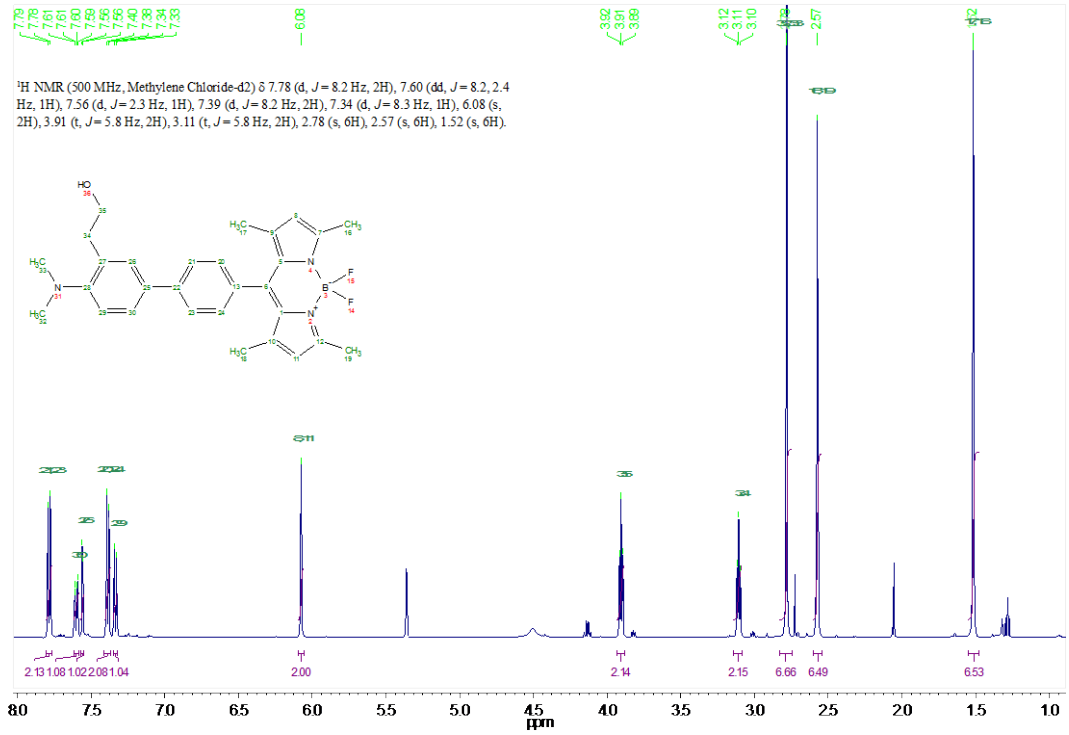

Figure S-7. ^{1}H NMR spectrum of compound **2** in CD_2Cl_2.

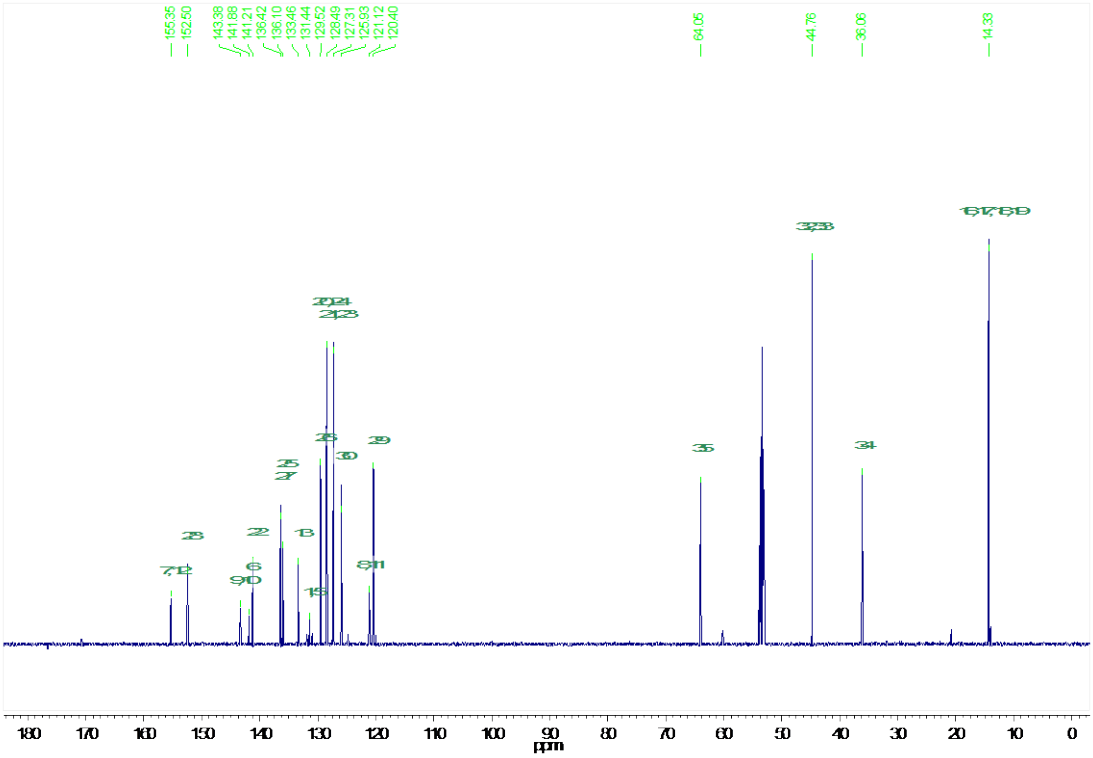

Figure S-8. ^{13}C NMR spectrum of compound **2** in CD_2Cl_2.

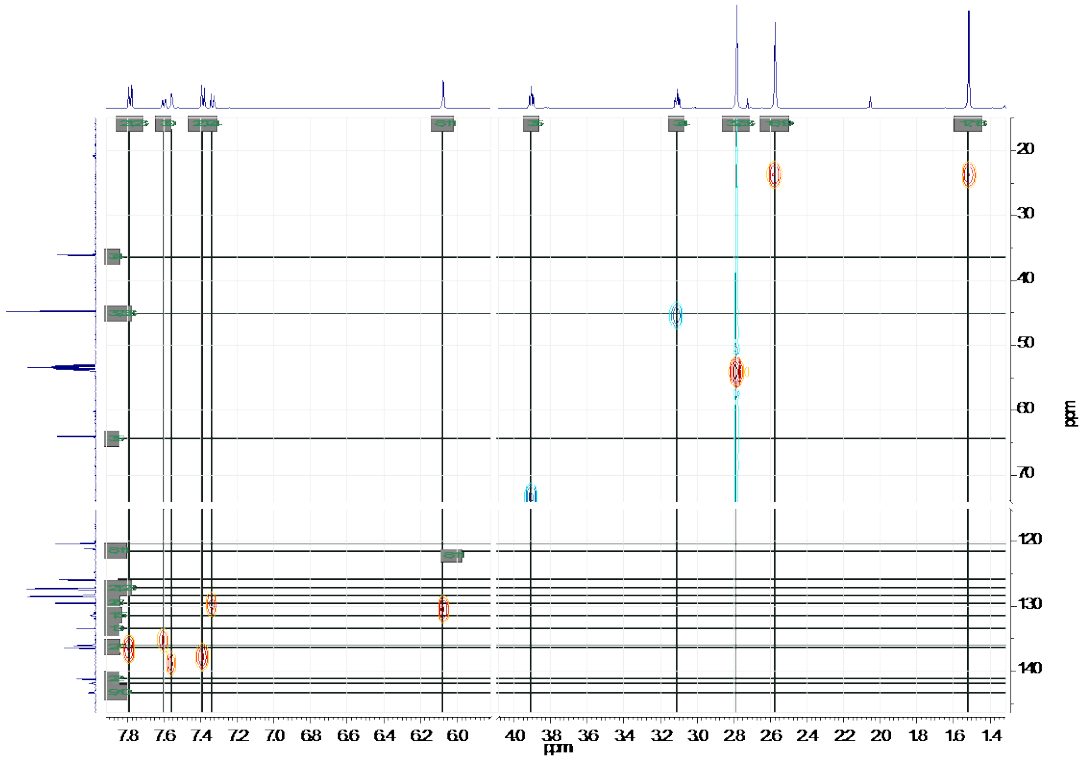

Figure S-9. HSQC spectrum of compound **2** in CD_2Cl_2.

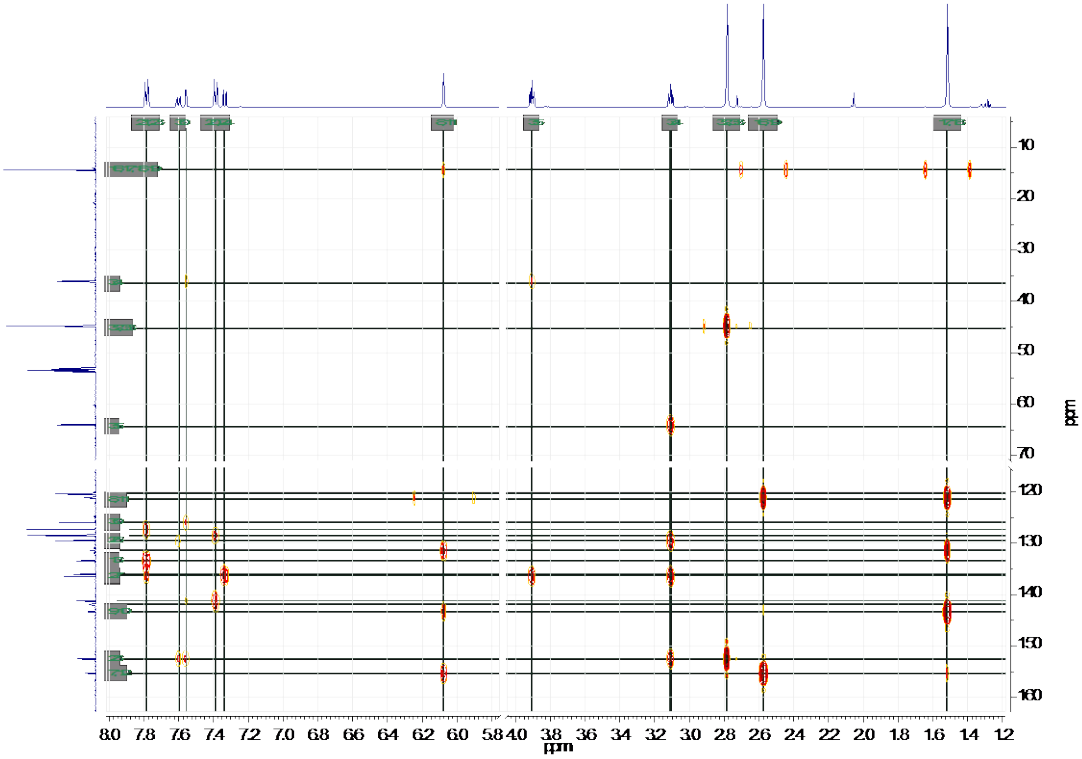

Figure S-10. HMBC spectrum of compound **2** in CD_2Cl_2.

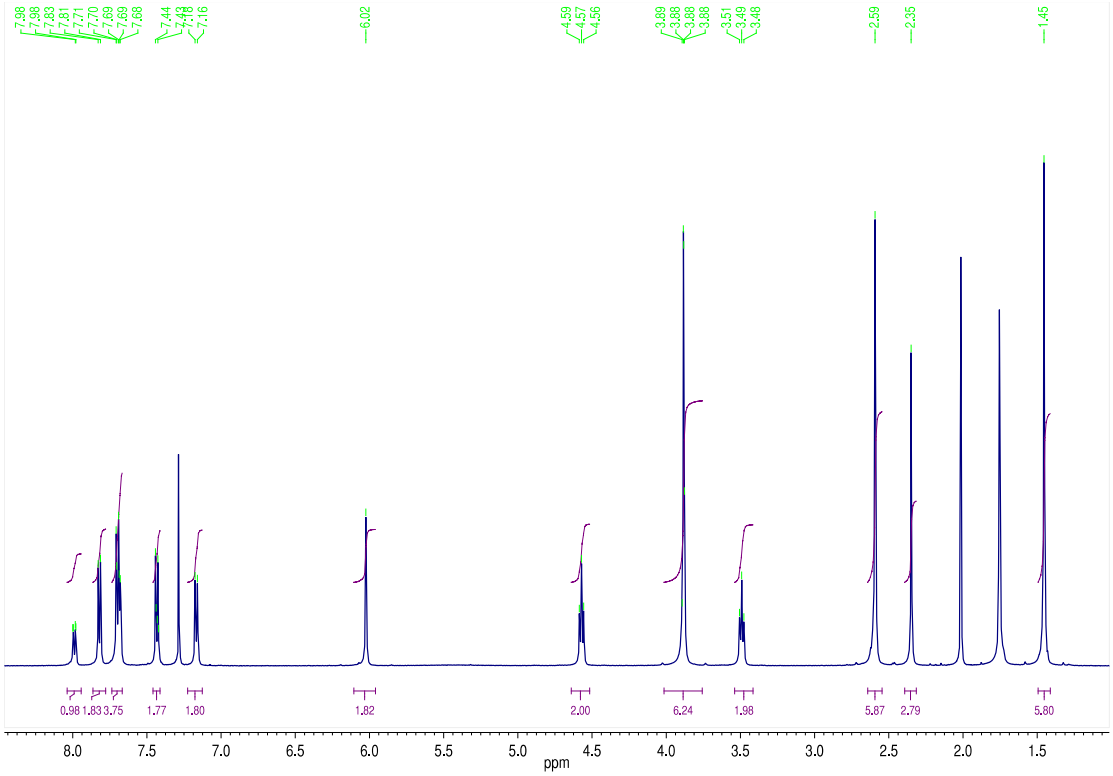

Figure S-11. ^{1}H NMR spectrum of compound **8** in $CDCl_3$.

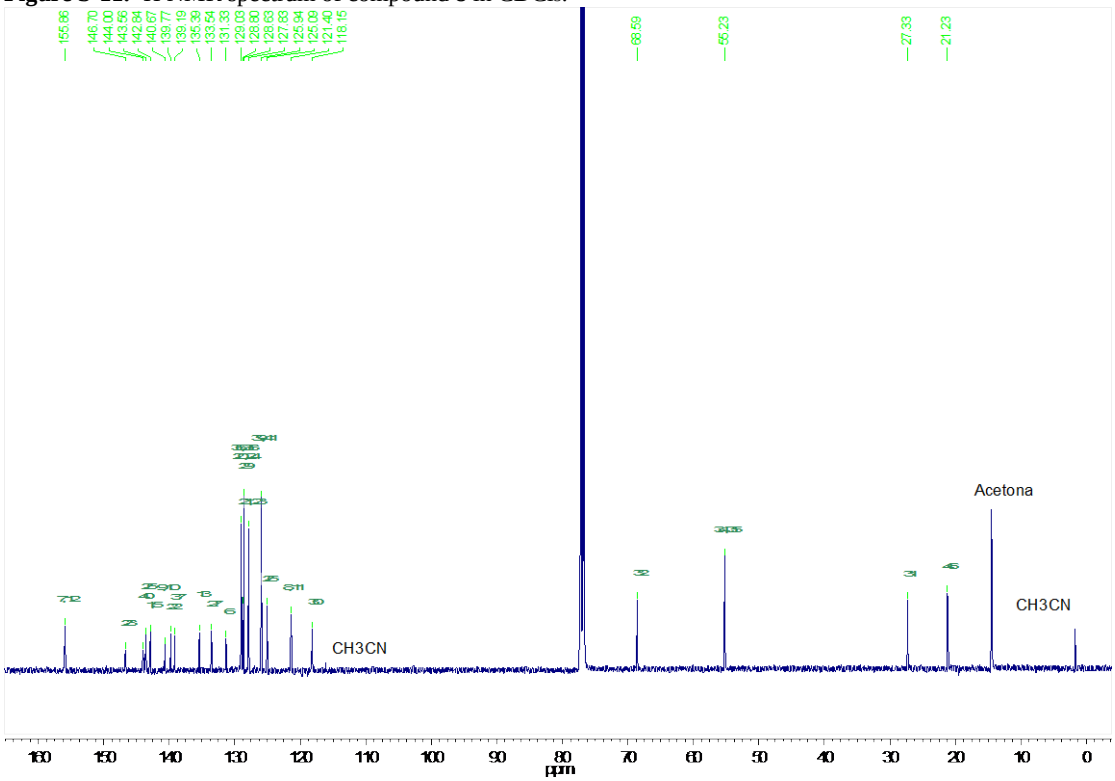

Figure S-12. ^{13}C NMR spectrum of compound **8** in $CDCl_3$.

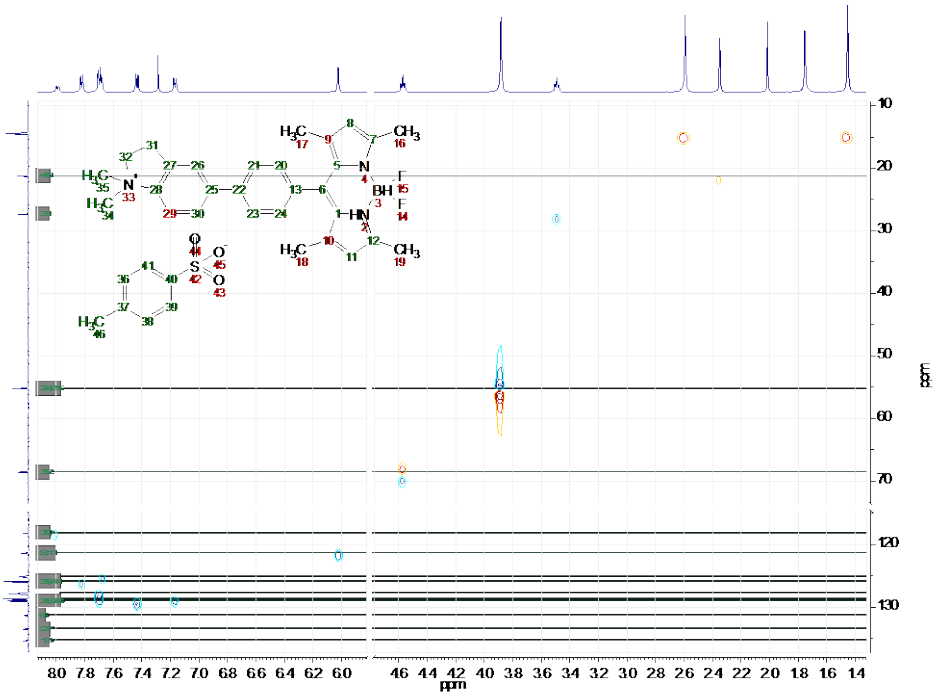

Figure S-13. HSQC NMR spectrum of compound **8** in $CDCl_3$.

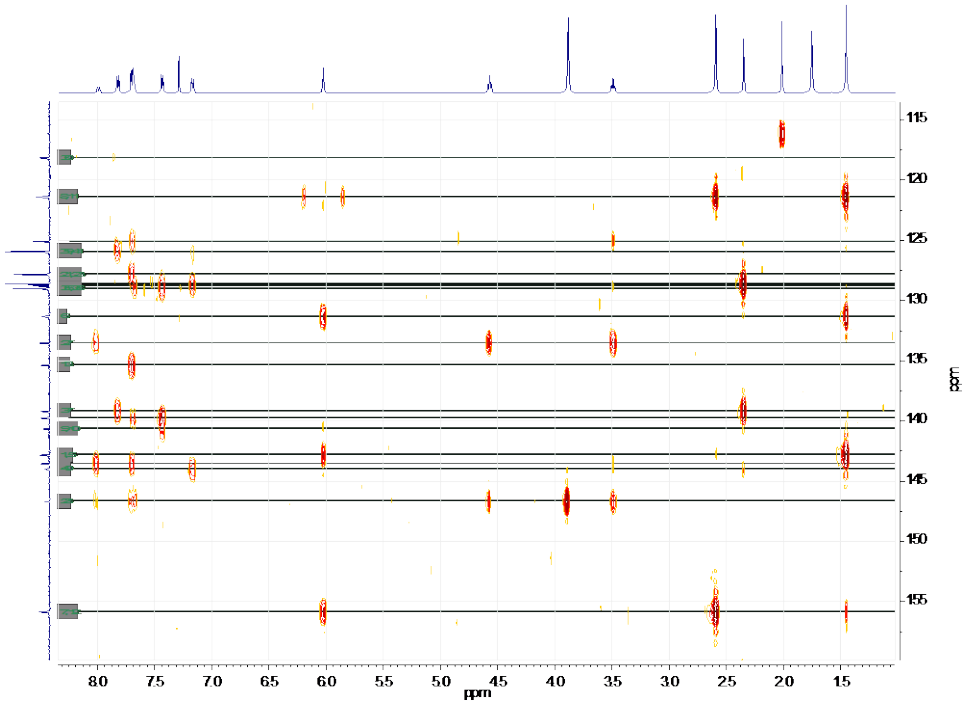

Figure S-14. HMBC NMR spectrum of compound **8** in $CDCl_3$.

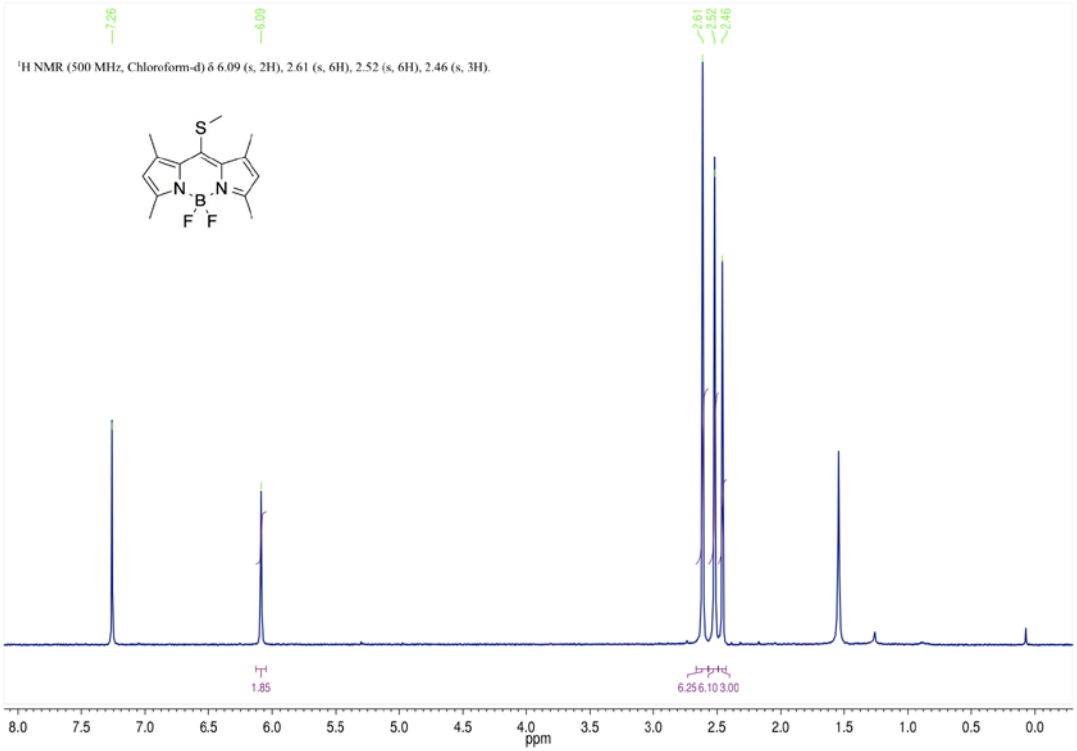

Figure S-15. ^{1}H NMR spectrum of tetramethylated derivative of **4** in $CDCl_3$.

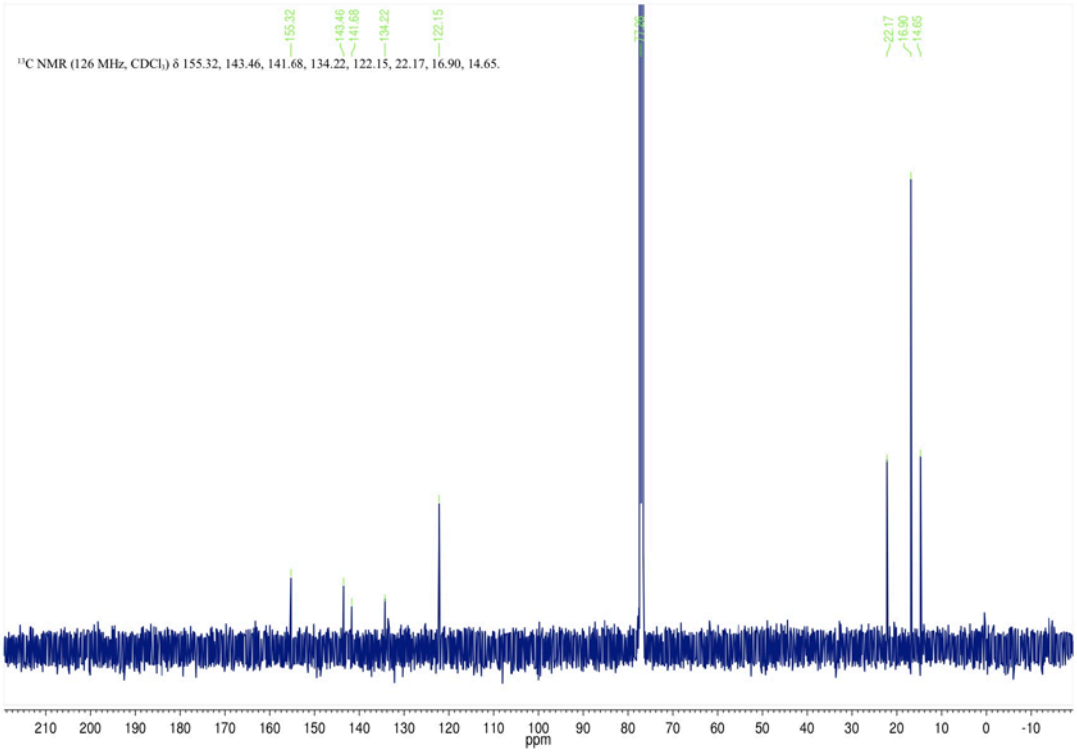

Figure S-16. ^{13}C NMR spectrum of tetramethylated derivative of **4** in $CDCl_3$.

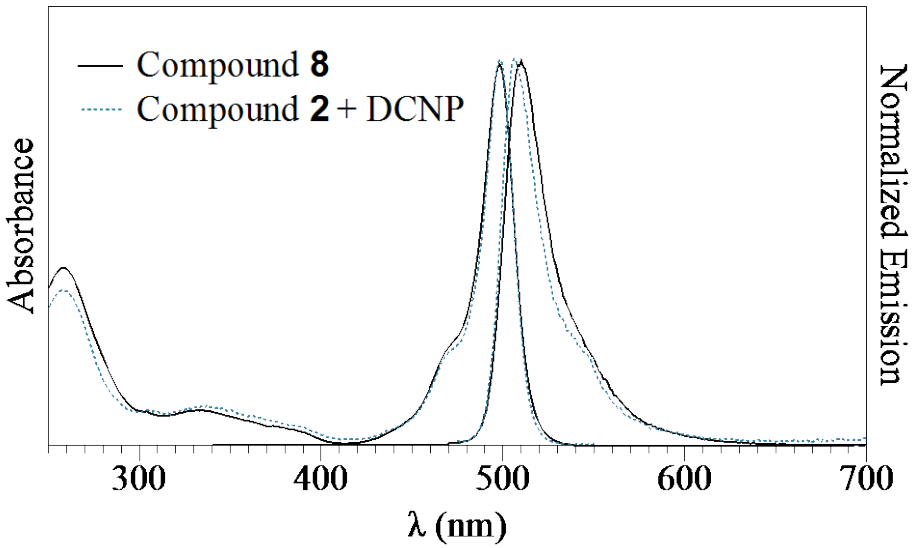

Figure S-17. Absorption and emission spectra of compound **8** 10^{-6} M in MeCN (Black line). Absorption and emission spectra of compound **2** + DCNP 20 mM (Blue dotted lines) are included for comparison purposes.

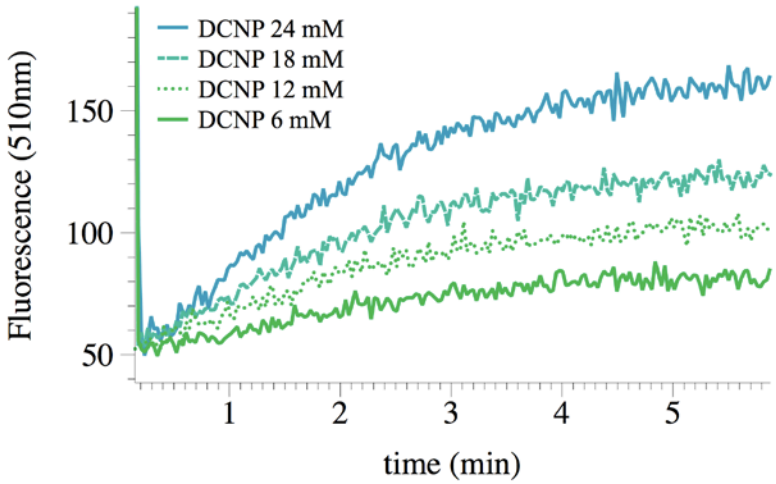

Figure S-18. Kinetic profile of the emission intensity at 510 nm of probe **1** after the addition of 6, 12, 18 and 24 mM DCNP. Probe **1** is 10^{-6} M in pH=5.5 buffered water/acetonitrile 3:1 v/v mixture.

Notes

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