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Article

Red-Shifted Environmental Fluorophores and Their Use for the Detection of Gram-Negative Bacteria

Alicia Megia-Fernandez [1,*], Maxime Klausen [1], Bethany Mills [2], Gillian E. Brown [3], Heather McEwan [1], Neil Finlayson [3], Kevin Dhaliwal [2] and Mark Bradley [1]

[1] EaStCHEM School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK; mklausen@ed.ac.uk (M.K.); H.McEwan-1@sms.ed.ac.uk (H.M.); Mark.Bradley@ed.ac.uk (M.B.)

[2] EPSRC Proteus IRC Hub, Centre for Inflammation Research, Queen's Medical Research Institute, University of Edinburgh, 47 Little France Crescent, Edinburgh EH16 4TJ, UK; Beth.Mills@ed.ac.uk (B.M.); Kev.Dhaliwal@ed.ac.uk (K.D.)

[3] Institute for Integrated Micro and Nano Systems, School of Engineering, University of Edinburgh, Edinburgh EH9 3FF, UK; g.e.brown@ed.ac.uk (G.E.B.); N.Finlayson@ed.ac.uk (N.F.)

* Correspondence: A.Megia@ed.ac.uk

Supplementary Information

CONTENT

1. Chemical characterization of compounds **1** and **2**

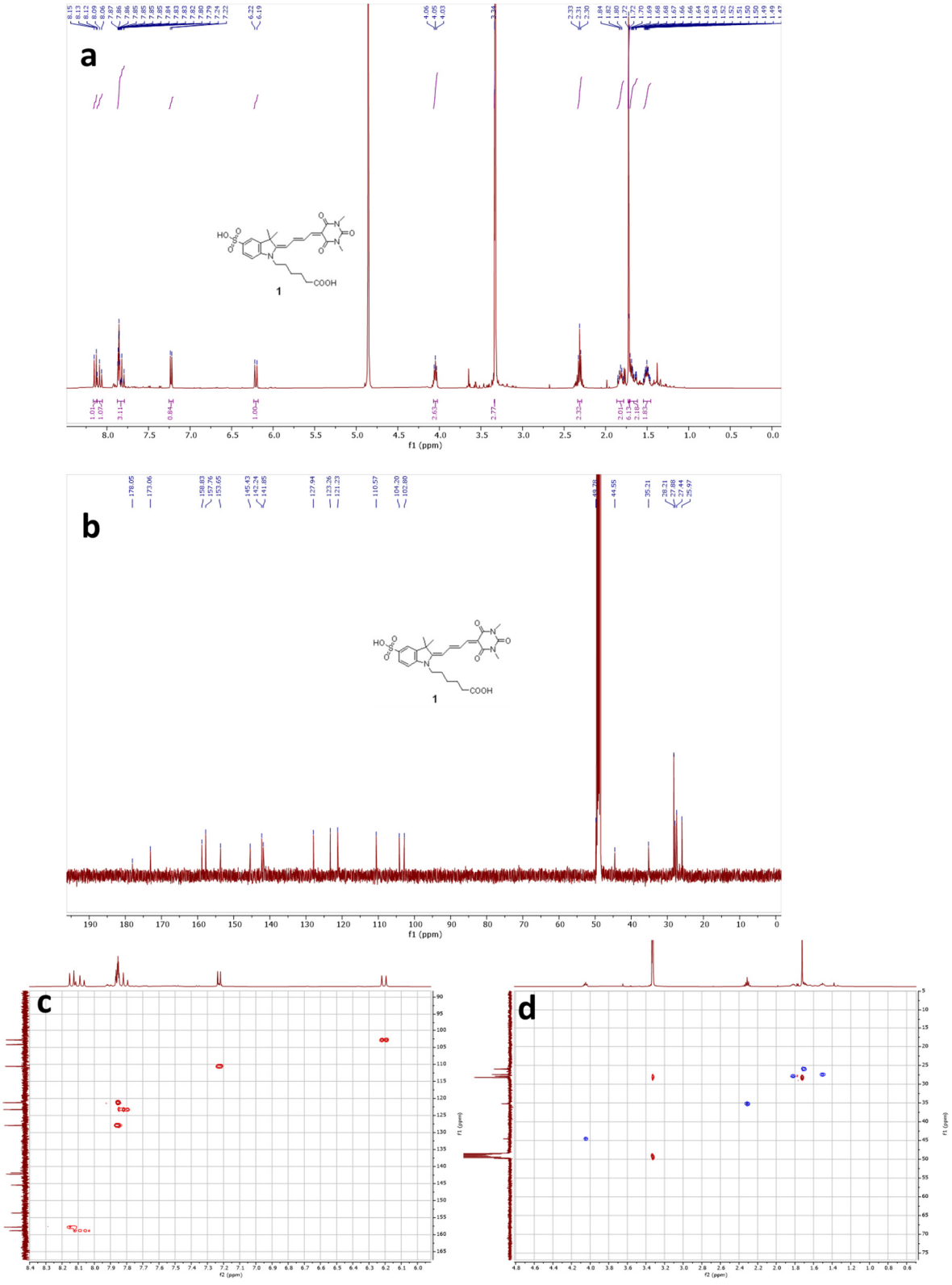


Figure S1. a) ^{1}H-NMR spectrum of **1**; **b**) 13C-NMR spectrum of **1**; **c**) Multiplicity-edited HSQC 2D-NMR spectrum of **1**, zoom 8-6 ppm; **d**) Multiplicity-edited HSQC 2D-NMR spectrum of **1**, zoom 4-1 ppm.

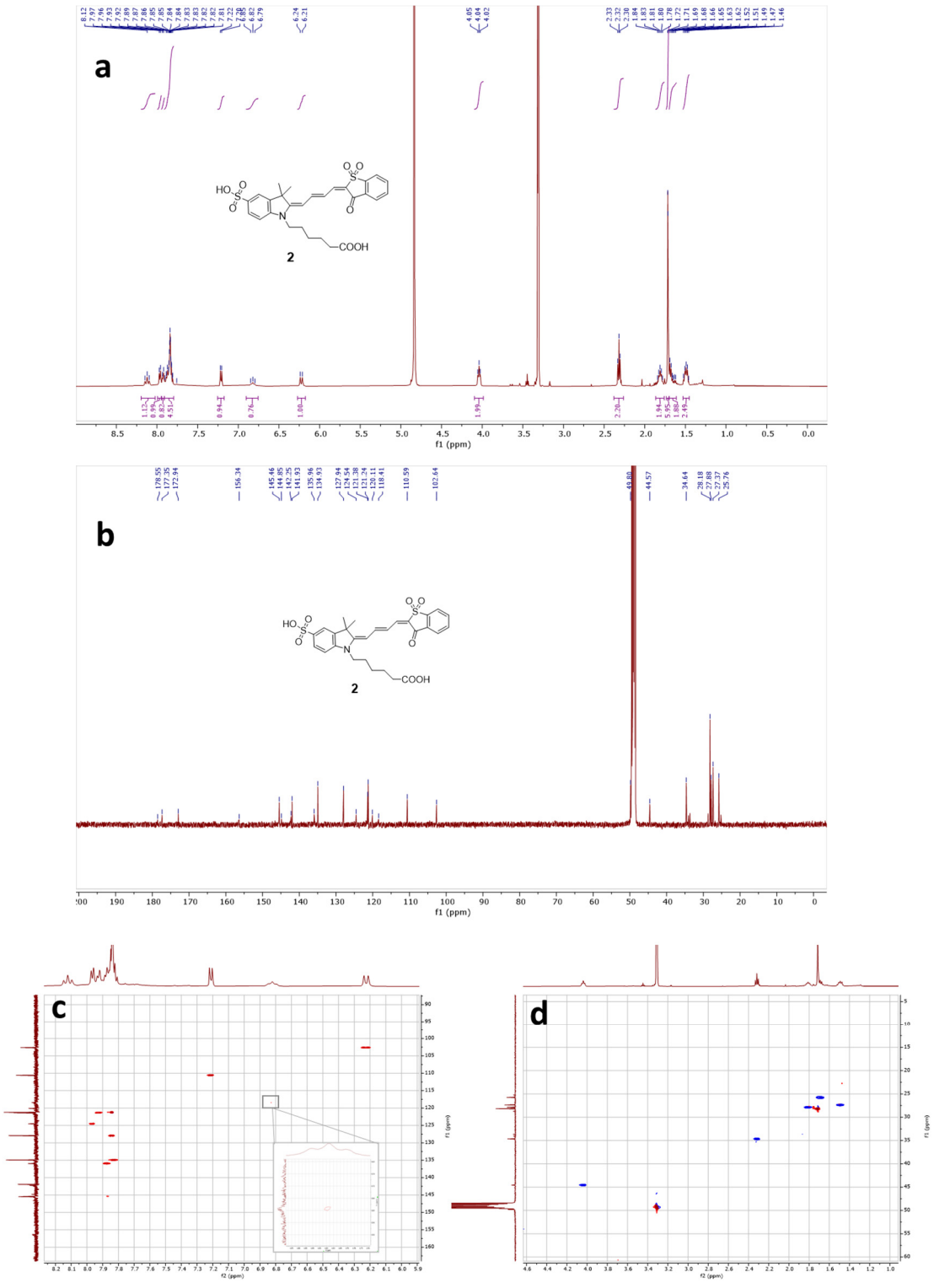


Figure S2. a) ^{1}H-NMR spectrum of **2**; **b**) 13C-NMR spectrum of **2**; **c**) Multiplicity-edited HSQC 2D-NMR spectrum of **2**, zoom 8-6 ppm; **d**) Multiplicity-edited HSQC 2D-NMR spectrum of **2**, zoom 4-1 ppm.

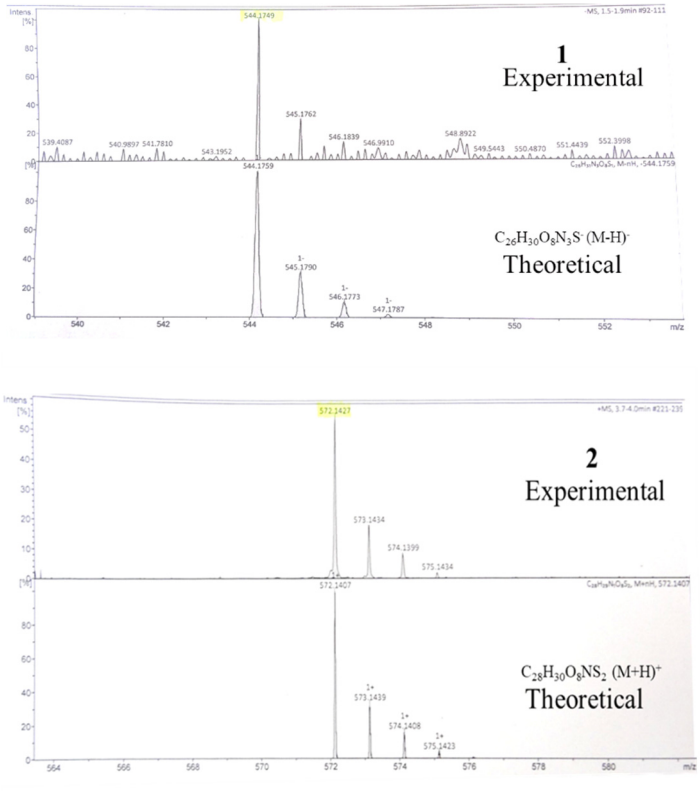


Figure S3. HR-MS spectrum of **1** (up) and **2** (down).

2. Photophysical characterization of compounds **1** and **2**

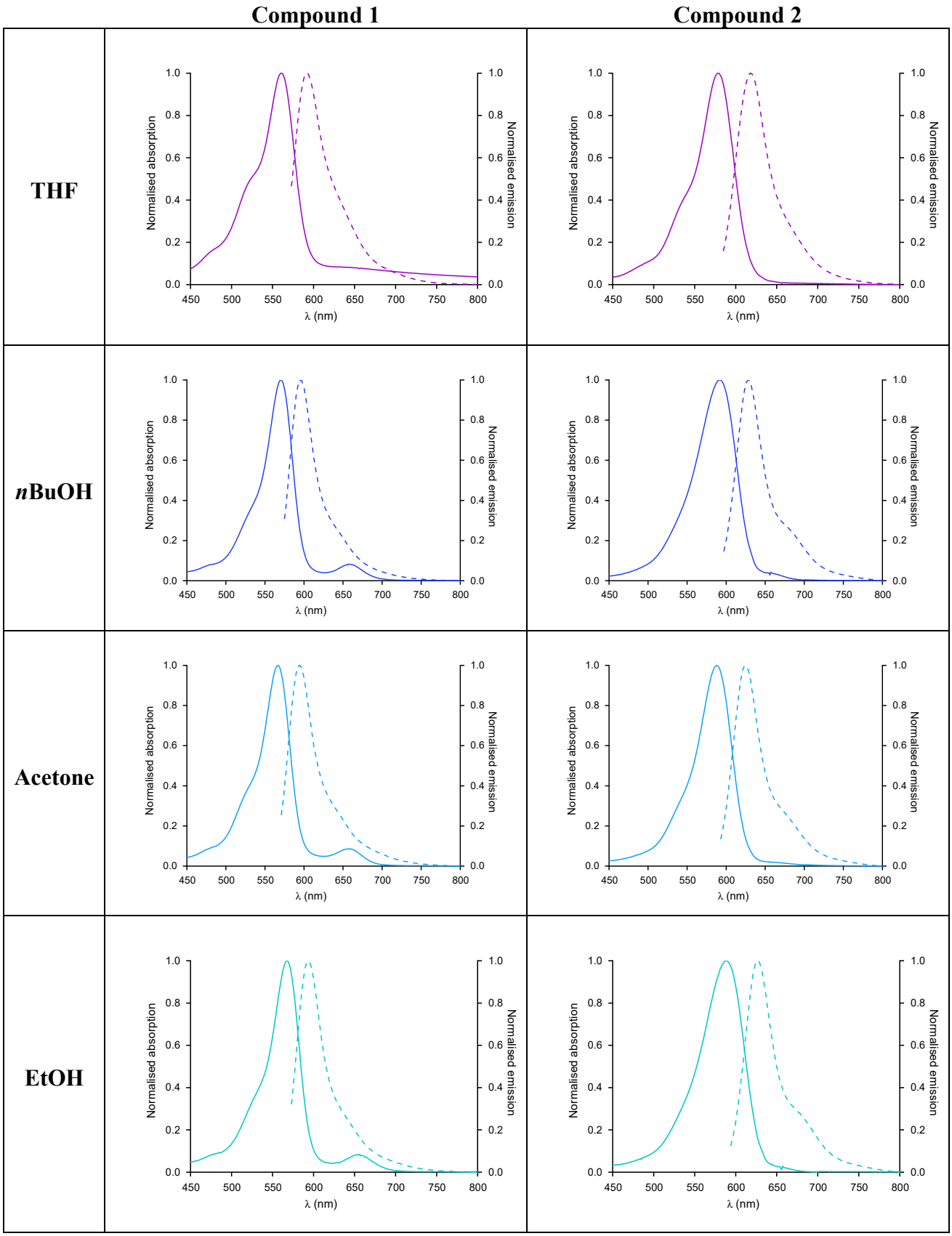


Figure S4. Normalised absorption and emission spectra of **1** and **2** in different solvents.

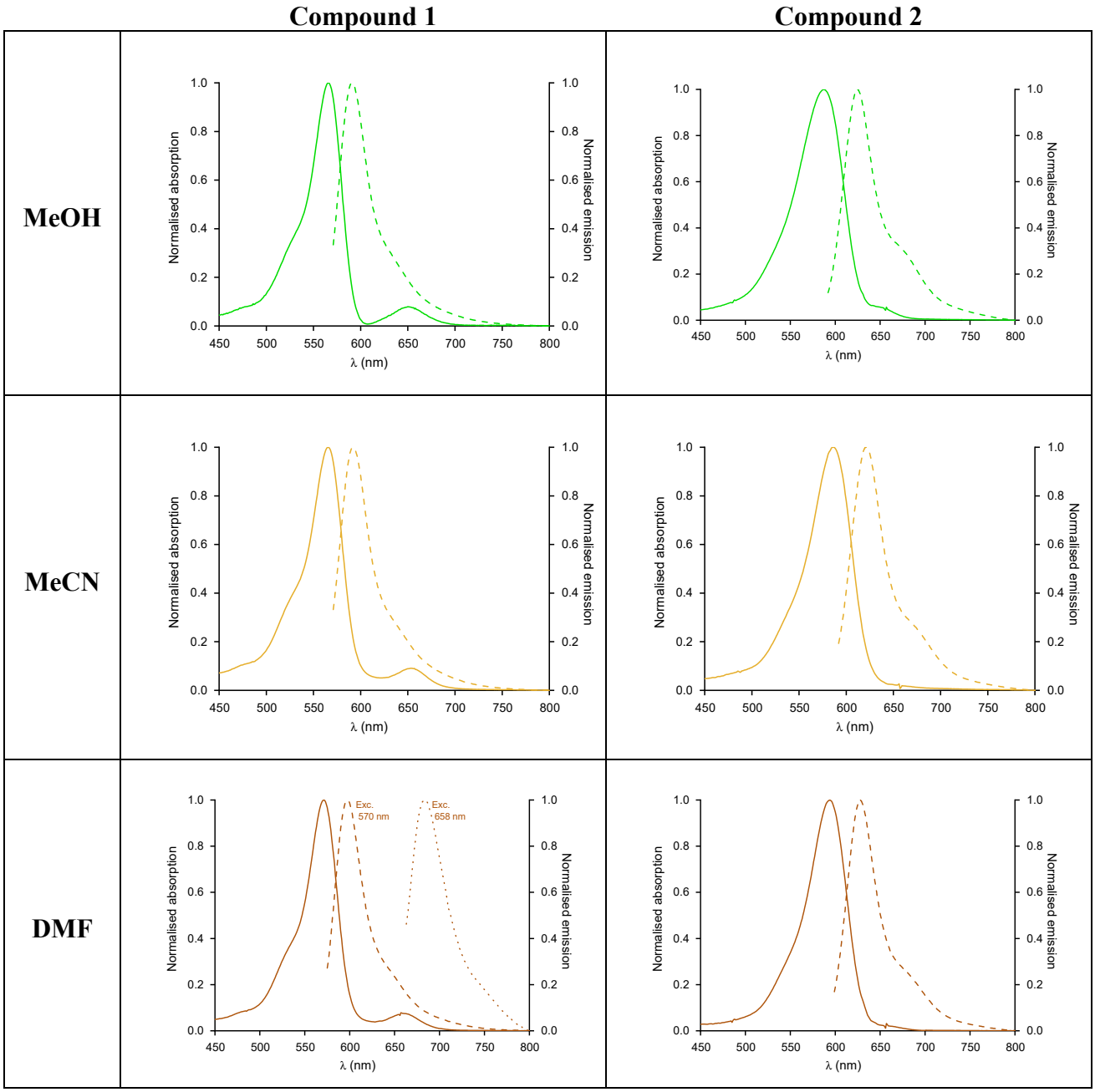


Figure S4. Normalised absorption and emission spectra of **1** and **2** in different solvents (continued).

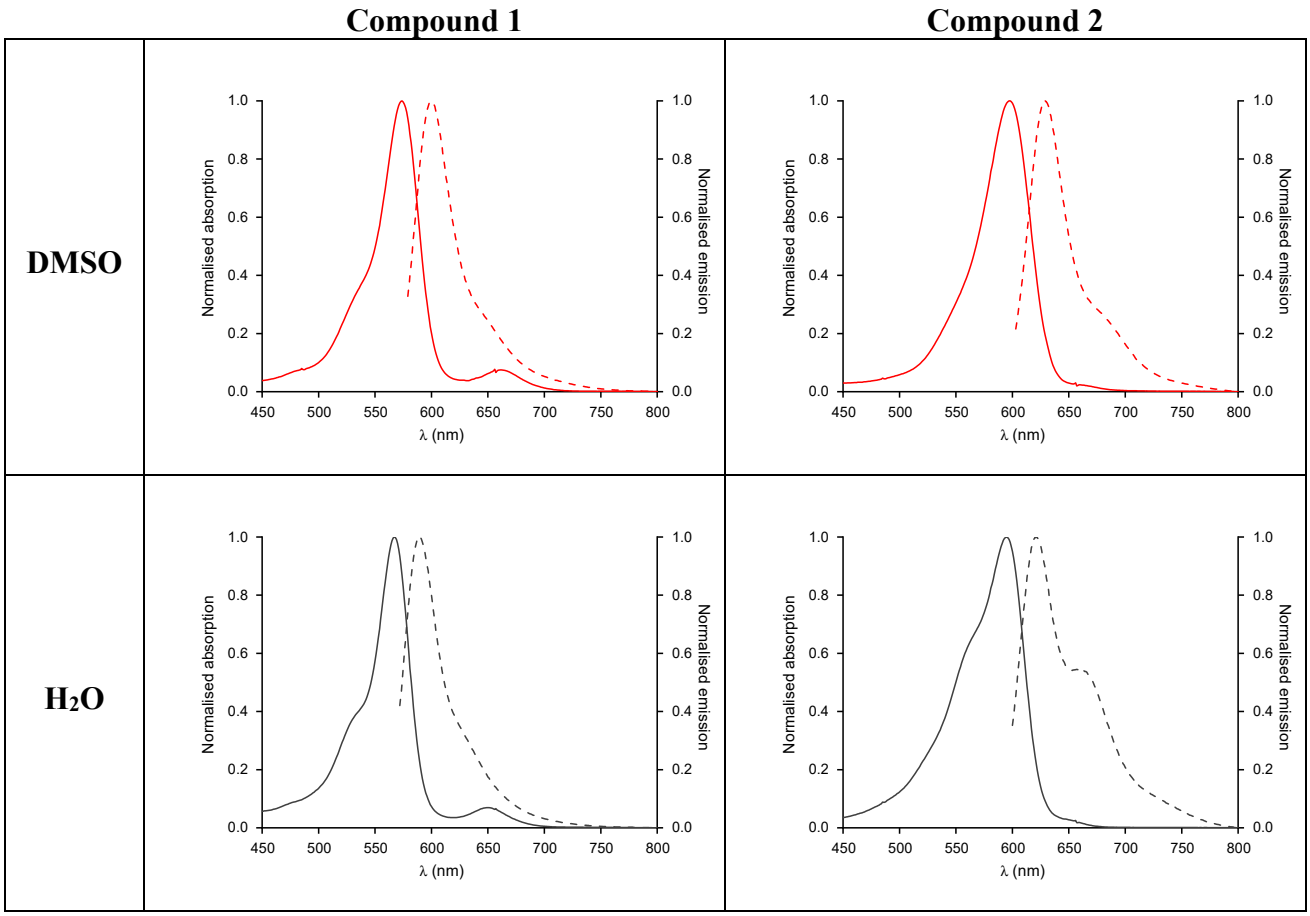


Figure S4. Normalised absorption and emission spectra of **1** and **2** in different solvents (continued).

Solvent and environmental effect

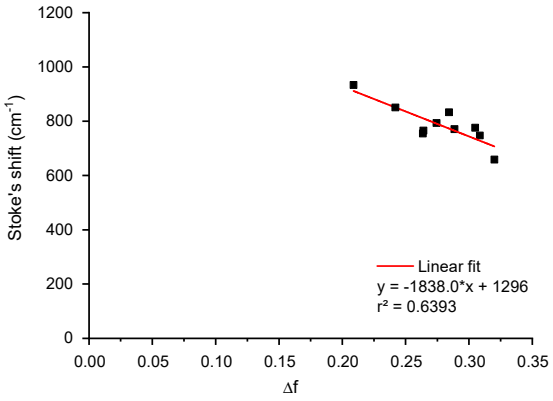
The behaviour of the merocyanine sub-units was investigated in solvents of various polarities. Both fluorophores exhibited a complex behaviour in solution, and did not show a linear dependence of their Stoke's shift to the orientation-polarisability parameter as stated by the Lippert-Mataga equation [1,2]:

$$\nu_{abs} - \nu_{em} = 2\Delta\mu^2\Delta f / (hca^3) + \text{const}$$

where ν_{abs} (ν_{em}) is the wavenumber of the absorption (fluorescence) maximum, $\Delta\mu$ is the change of dipole moment between the relaxed emissive excited state and corresponding Frank Condon ground state, h is the Planck constant, c is the light velocity, a is the radius of the Onsager spherical cavity, and the orientation polarizability is $\Delta f = (\varepsilon - 1)/(2\varepsilon + 1) - (n^2 - 1)/(2n^2 + 1)$, where ε is the dielectric constant and n the refractive index of the solvent.

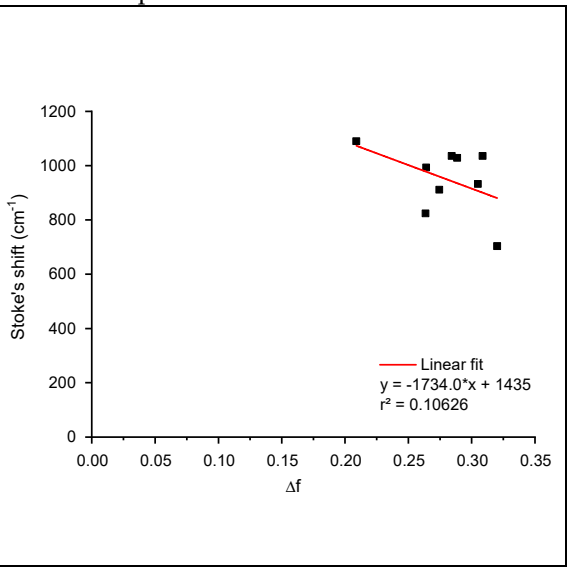
Lippert-Mataga model applied to compound **1**.

Solvent	λ_{Abs} [nm]	λ_{em} [nm]	Stoke's Shift	Δf
THF	561	592	933	0.20888
*n*BuOH	570	596	765	0.26402
Acetone	566	594	833	0.28427
EtOH	568	594	771	0.28856
MeOH	566	591	774	0.30862
MeCN	566	592	776	0.30492
DMF	570	597	793	0.27445
DMSO	574	600	755	0.26358
H_2O	567	589	659	0.32009



Lippert-Mataga model applied to compound **2**.

Solvent	λ_{Abs} [nm]	λ_{em} [nm]	Stoke's Shift [cm-1]	Δf
THF	579	618	1090	0.20888
*n*BuOH	592	629	994	0.26402
Acetone	587	625	1036	0.28427
EtOH	589	627	1029	0.28856
MeOH	587	625	1036	0.30862
MeCN	587	621	933	0.30492
DMF	594	628	911	0.27445
DMSO	598	629	824	0.26358
H_2O	595	621	704	0.32009



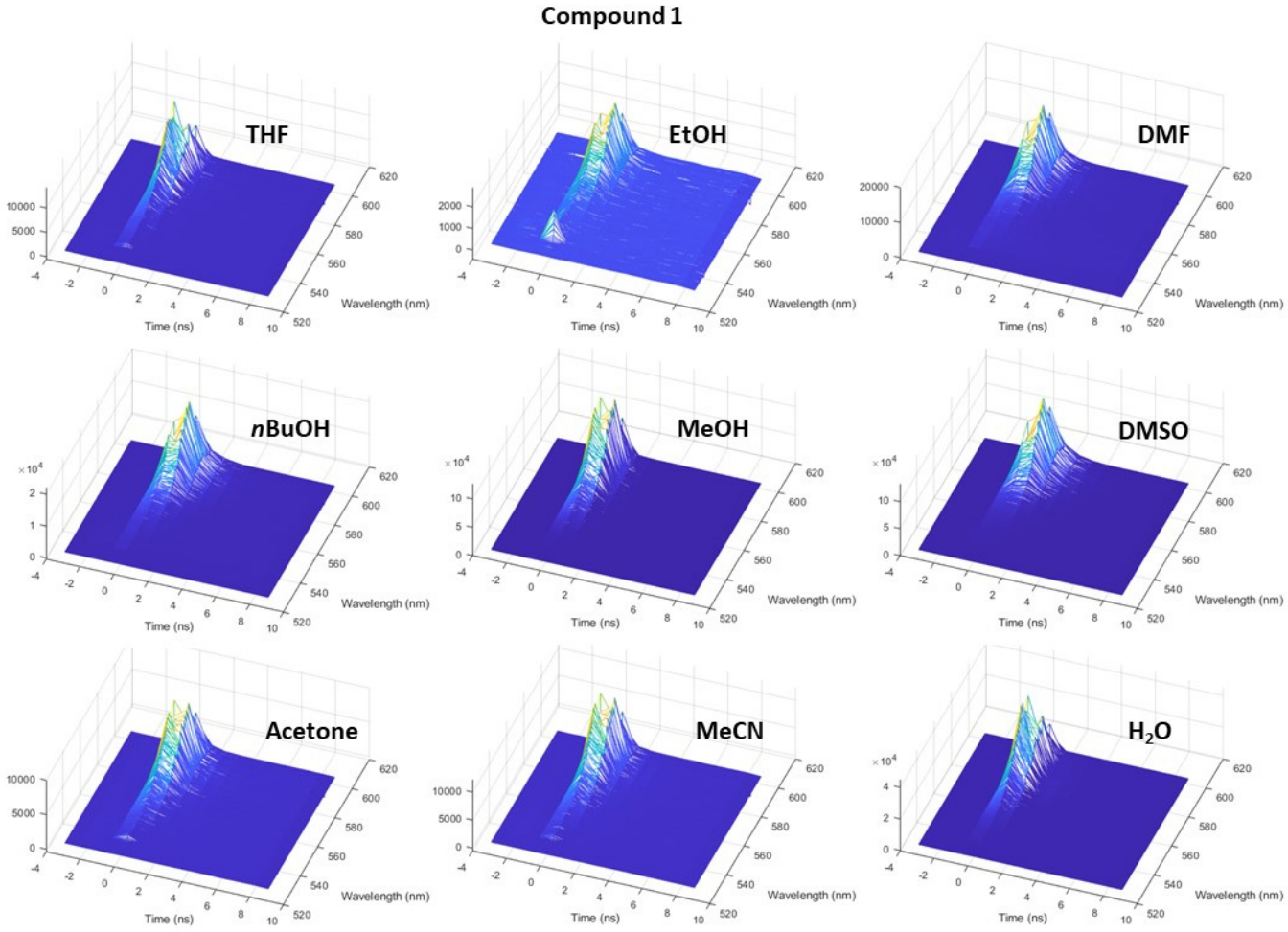


Figure S5. Time-resolved fluorescence spectra of compound **1** in different solvents.

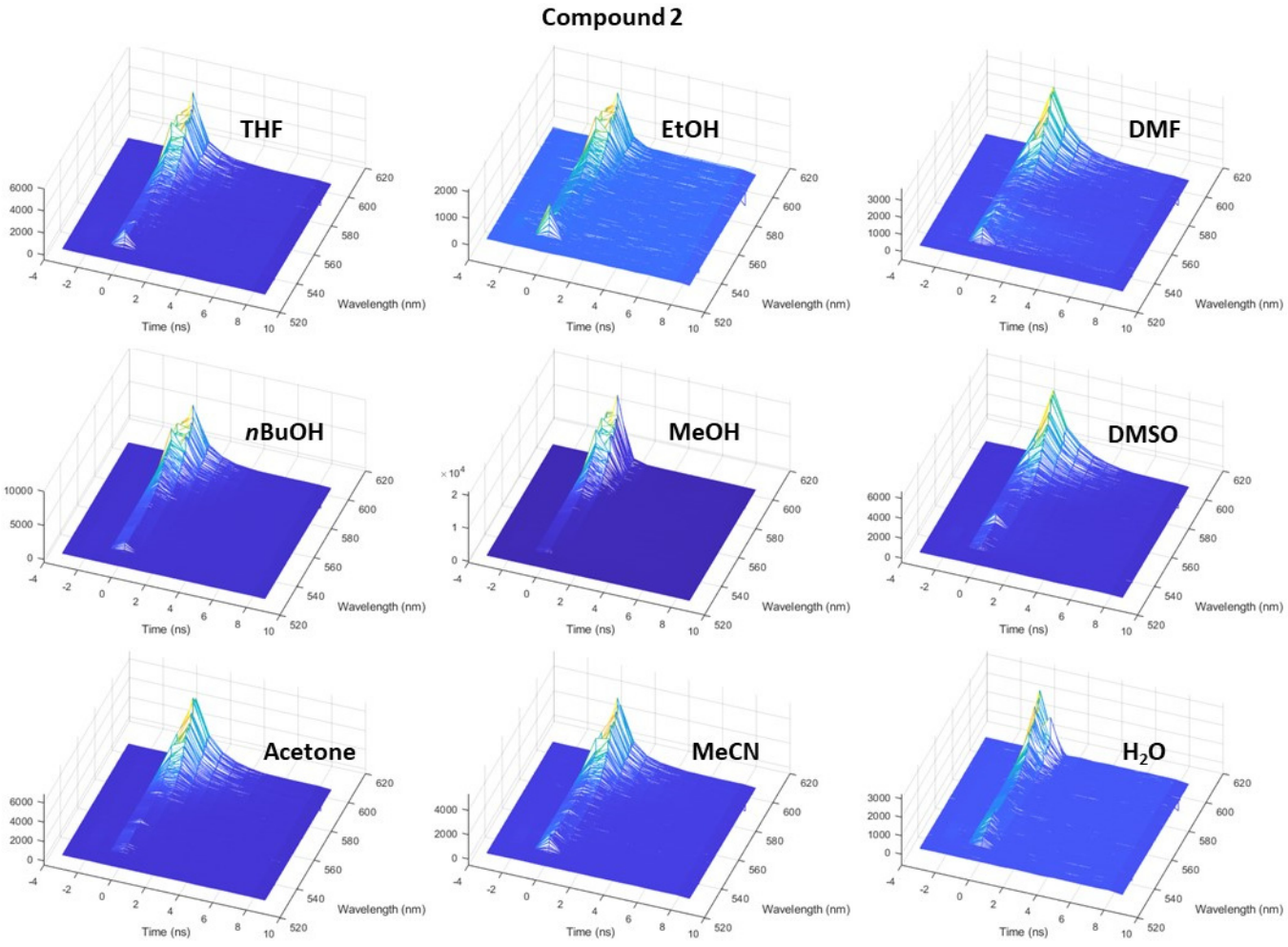


Figure S6. Time-resolved fluorescence spectra of compound **2** in different solvents.

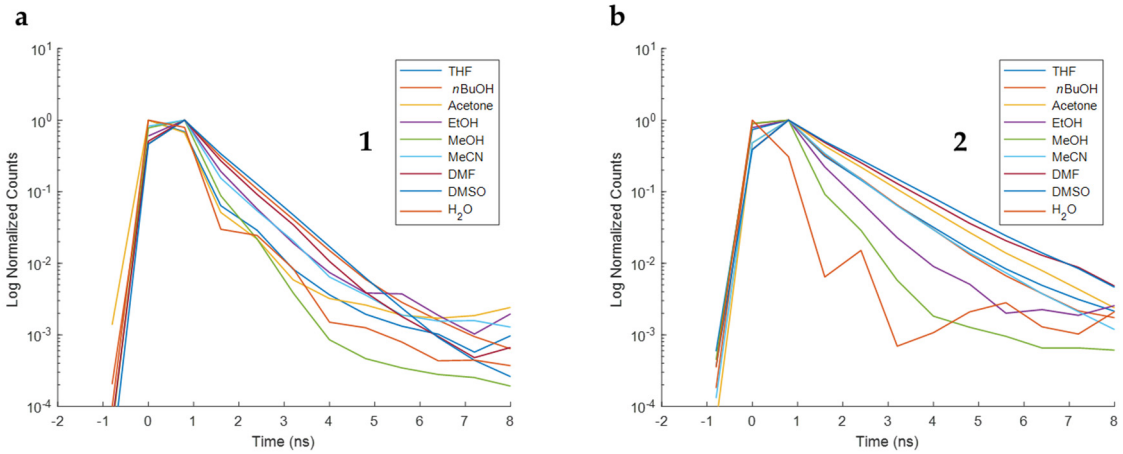


Figure S7. Time-resolved fluorescence decay curves for compounds (a) **1** and (b) **2** in all solvents. The logarithm of normalized counts vs time over a nine nanosecond time range with 800 ps time resolution. Fluorescence counts were summed and normalised over a 586-603 nm wavelength range.

References

1. Lippert, E. Dipolmoment und Elektronenstruktur von angeregten Molekülen. *Zeitschrift für Naturforschung A* **1955**, *10*, 541–545, doi:https://doi.org/10.1515/zna-1955-0707.

2. Mataga, N.; Kaifu, Y.; Koizumi, M. The Solvent Effect on Fluorescence Spectrum, Change of Solute-Solvent Interaction during the Lifetime of Excited Solute Molecule. *Bulletin of the Chemical Society of Japan* **1955**, *28*, 690–691.