

Supramolecular Self-associating Amphiphiles: Determination of molecular self-association properties and calculation of critical micelle concentration using a high-throughput, optical density based methodology

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Experimental

General remarks: The NMR spectra were obtained using a Bruker AV2 400 MHz or AVNEO 400 MHz spectrometer. The data was processed using ACD Labs or Topspin software. NMR Chemical shift values are reported in parts per million (ppm) and calibrated to the centre of the residual solvent peak set (s = singlet, br = broad, d = doublet, t = triplet, q = quartet, m = multiplet). The melting point for each compound was measured using Stuart SMP10 melting point apparatus. High resolution mass spectrometry was performed using a Bruker microTOF-Q mass spectrometer and spectra recorded and processed using Bruker's Compass Data Analysis software. Infrared spectra were obtained using a Shimadzu IR-Affinity-1 model Infrared spectrometer. The data are analysed in wavenumbers (cm^{-1}). UV-Vis absorbance and optical density measurements were conducted and analysed using a Clariostar plate reader and MARS data analysis software.

CMC microplate reader studies: Samples of the solutions to be studied were transferred, as 200 μL aliquots, to low UV-transparent 96-well microplates, after an annealing process in which the samples were heated to approximately 313K before being allowed to cool to room temperature. All samples were prepared through serial dilution of the most concentrated sample. After preparation, the low UV-transparent 96-well microplate was then transferred into the plate reader and equilibrated to a temperature of 298 K °C. Optical density (OD) spectral well scan experiments were performed in 10-degree ascending increments, from 298 K to 318 K, using an appropriate absorbance measurement determined from UV-Vis absorbance studies. All experiments were repeated in triplicate to ensure experimental reproducibility. **Data processing:** See also Figure S24. Average OD values obtained for red sections of each well were divided by the average values obtained for the green sections of each well. These values were obtained in triplicate, averaged again, and plotted against molecular concentration. Two linear trend lines were then fitted to these data and the CMC defined as the intersection of these two lines of best fit.

CMC tensiometer studies: All samples underwent an annealing process in which the various solutions were heated to approximately 313 K before being allowed to cool to room temperature, allowing each sample to reach a thermodynamic minimum. All samples were prepared through serial dilution of the most concentrated sample. Three surface tension measurements were obtained for each sample at a given concentration, using a tensiometer through the pendant drop method.^{1,2} The average values were then used to calculate the critical micelle concentration (CMC).

Mass Spectrometry: Approximately 1 mg of each compound was dissolved in 1 mL of methanol. This solution was further diluted 100-fold before undergoing analysis where 10 μL of each sample was injected directly into a flow of 10 mM ammonium acetate in 95 % water (flow rate = 0.02 mL/min).

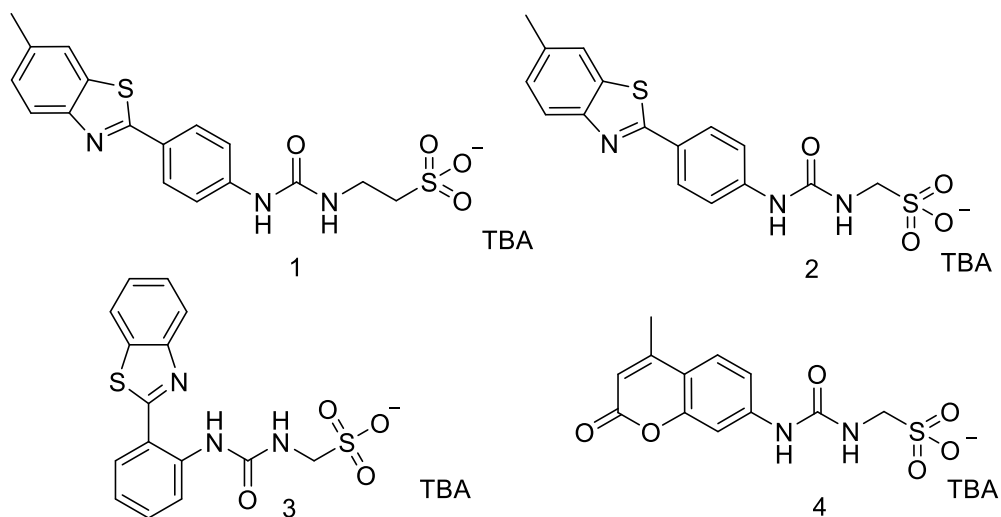
Single Crystal X-ray Studies: A suitable crystal of each amphiphile was selected and mounted on a Rigaku Oxford Diffraction Supernova diffractometer. Data were collected using Cu $K\alpha$ radiation at 100 K. Structures were solved with the ShelXT or ShelXS³ structure solution programs via Direct Methods and refined with ShelXL⁴ by Least Squares minimisation. Olex2 was used as an interface to all ShelX programs (CCDC 1999015).⁵

DLS studies: All vials used for preparing the samples were clean and dry. All solvents used were filtered to remove any particulates that may interfere with the results obtained. Samples of differing concentrations were obtained through serial dilution of a concentrated solution. All samples underwent an annealing process, in which they were heated to 313 K before being allowed to cool to 298 K to allow each sample to reach a thermodynamic minimum. A series of 9 or 10 runs were recorded at 298 K.

Zeta potential studies: All vials used for preparing the samples were clean and dry. All solvents used were filtered to remove any particulates that may interfere with the results obtained. All samples underwent an annealing process, in which they were heated to 313 K before being allowed to cool to

room temperature, allowing each sample to reach a thermodynamic minimum. The final zeta potential value given is an average of the number of experiments conducted at 298 K.

Chemical structures



Chemical synthesis

Compound 1: A mixture of 4-(6-methylbenzothiazole-2-yl)aniline (0.48 g, 2.00 mmol) and CDI (0.39 g, 2.40 mmol) were heated at reflux for 4 hours in chloroform (10 mL), then TBA 1-aminoethane-2-sulfonate (0.73 g, 2.00 mmol) was dissolved in chloroform, added to the original reaction mixture and then heated at reflux overnight. The precipitate was removed and the filtrate re-dissolved in chloroform (10 mL), water washed (15 mL x 3) and the organic layer taken to dryness. Ethyl acetate (10 mL) was added to the resultant oil and sonicated. The resulting pale yellow precipitate was the clean product with a yield of 61% (0.77 g, 1.21 mmol), Melting point: >473 K ^1H NMR (298 K, 400 MHz, $\text{DMSO-}d_6$): δ : 0.93 (t, J = 7.32 Hz, 12H), 1.28-1.32 (m, 8H), 1.56-1.60 (m, 8H), 2.45 (s, 3H), 2.58 (t, J = 6.32 Hz, 2H), 3.14-3.18 (m, 8H), 3.37-3.41 (m, 2H), 6.51 (t, J = 5.40 Hz, 1H), 7.32 (d, J = 8.44 Hz, 1H), 7.59 (d, J = 8.64 Hz, 2H), 7.85-7.92 (m, 4H), 9.30 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, 298K, $\text{DMSO-}d_6$): δ : 13.5 (CH_3), 19.2 (CH_2), 21.0 (CH_3), 23.0 (CH_2), 36.1 (CH_2), 50.9 (CH_2), 57.5 (CH_2), 117.5 (ArCH), 121.7 (ArCH), 121.9 (ArCH), 125.4 (ArC), 127.8 (ArCH), 134.3 (ArC), 134.6 (ArC), 143.9 (ArC), 151.9 (ArC), 154.7 (ArC), 166.3 (C=O); IR (film): ν (cm^{-1}) 2961 (NH stretch), 1686 (C=O stretch), 1179, 1163 (CN stretch), 1038 (S=O); HRMS for the sulfonate-urea ion ($\text{C}_{17}\text{H}_{16}\text{N}_3\text{O}_4\text{S}_2^-$) (ESI $^-$): m/z : act: 390.0575 [M] $^-$ cal: 390.0588 [M] $^-$

Compound 2: This compound was synthesized in line with previously published methods.⁶ Proton NMR was found to match previously published spectra.

Compound 3: This compound was synthesized in line with previously published methods.⁶ Proton NMR was found to match previously published spectra.

Compound 4: A solution of 7-amino-4-methylcoumarin (0.25 g, 1.4 mmol) and triphosgene (0.2 g, 0.7 mmol) in ethyl acetate (20 mL) was heated at reflux for 4 hours in the presence of 4 Å molecular sieves (1.5 g). A solution of tetrabutylammonium aminomethanesulfonate (0.5 g, 1.4 mmol) in ethyl acetate (10 mL) was added dropwise to the reaction mixture, and the solution was heated at reflux overnight. The reaction mixture was then filtrated to remove the molecular sieves and the remaining solid. The filtrate was concentrated, the solid re-dissolved in chloroform and washed with water (10 mL x 3). The organic layer was then dried with Na_2SO_4 , and further dried under reduced pressure. The solid obtained was then recrystallized from methanol, and the product was isolated as a fluffy white solid. (0.35 g, 0.6 mmol) Yield: 45%. Melting point: 449 K; ^1H NMR: (400 MHz, 298 K, $\text{DMSO-}d_6$): δ : 9.63 (s, 1H), 7.47-7.56 (m, 3H), 7.15 (d, J = 8.72 Hz, 1H), 6.05 (s, 1H), 3.99 (d, J = 6.08 Hz, 2H), 3.13-3.17 (m, 8H), 2.31 (s, 3H), 1.55-1.57 (m, 8H), 1.27-1.32 (m, 8H), 0.92 (t, J = 7.44 Hz, 12H); $^{13}\text{C}\{^1\text{H}\}$ NMR: (100 MHz, 298 K, $\text{DMSO-}d_6$): δ : 160.7 (CO), 154.5 (CO), 153.9 (ArC), 153.6 (ArC), 144.5 (ArC), 125.4 (ArCH), 114.4 (ArCH), 113.2 (ArC), 111.0 (ArCH), 103.8 (ArCH), 57.8 (CH_2), 56.1 (CH_2), 23.3 (CH_2), 19.4 (CH_2), 18.1 (CH_3), 13.7 (CH_3); IR (film): ν = 2960 (NH stretch), 1703 (C=O stretch), 1215 (S=O stretch); HRMS for the sulfonate-urea ion ($\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_6\text{S}^-$): m/z : act: 311.0356 [M] $^-$ cal: 311.0343 [M] $^-$.

NMR

Characterisation NMR

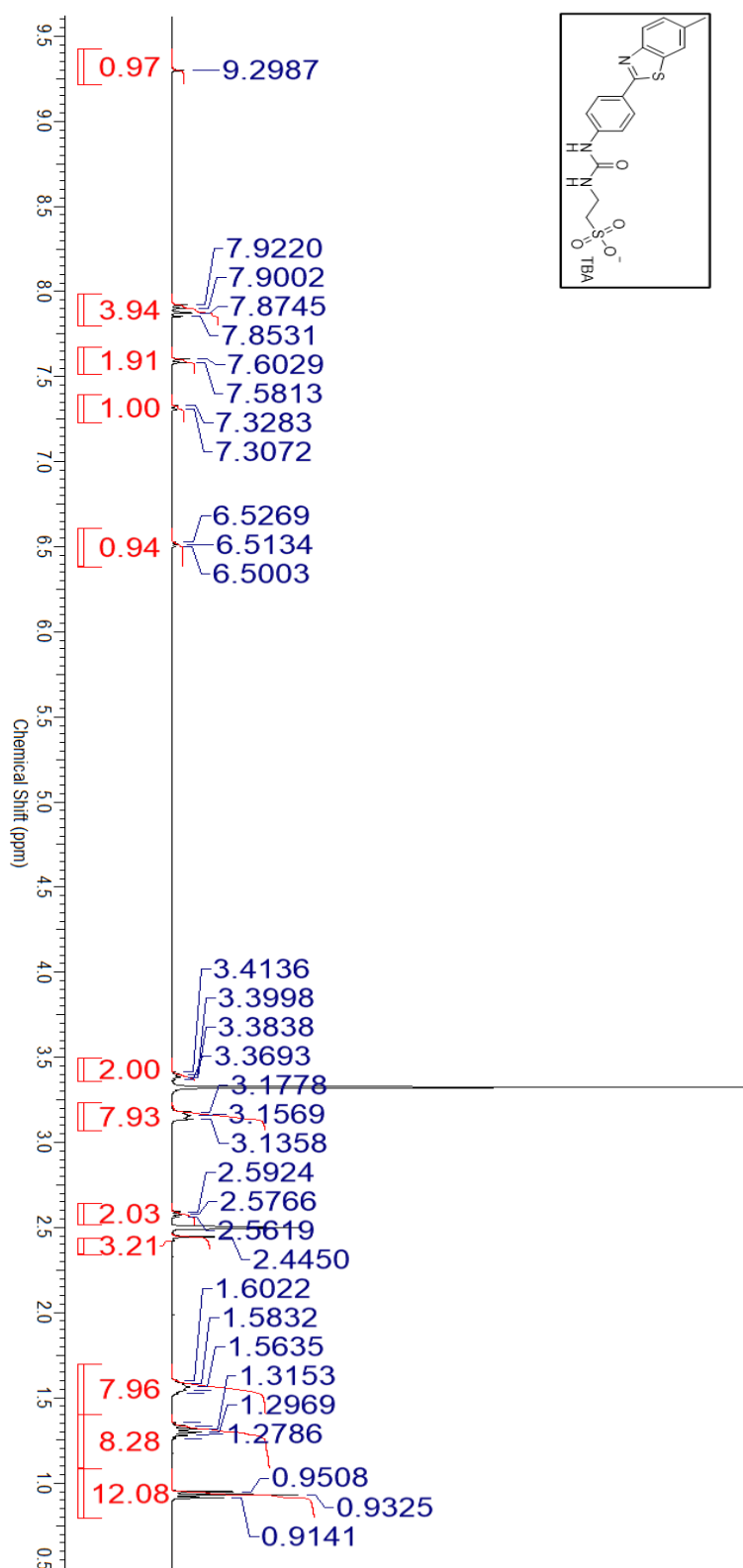


Figure S1: ¹H NMR of compound **1** in DMSO-*d*₆ conducted at 298 K.

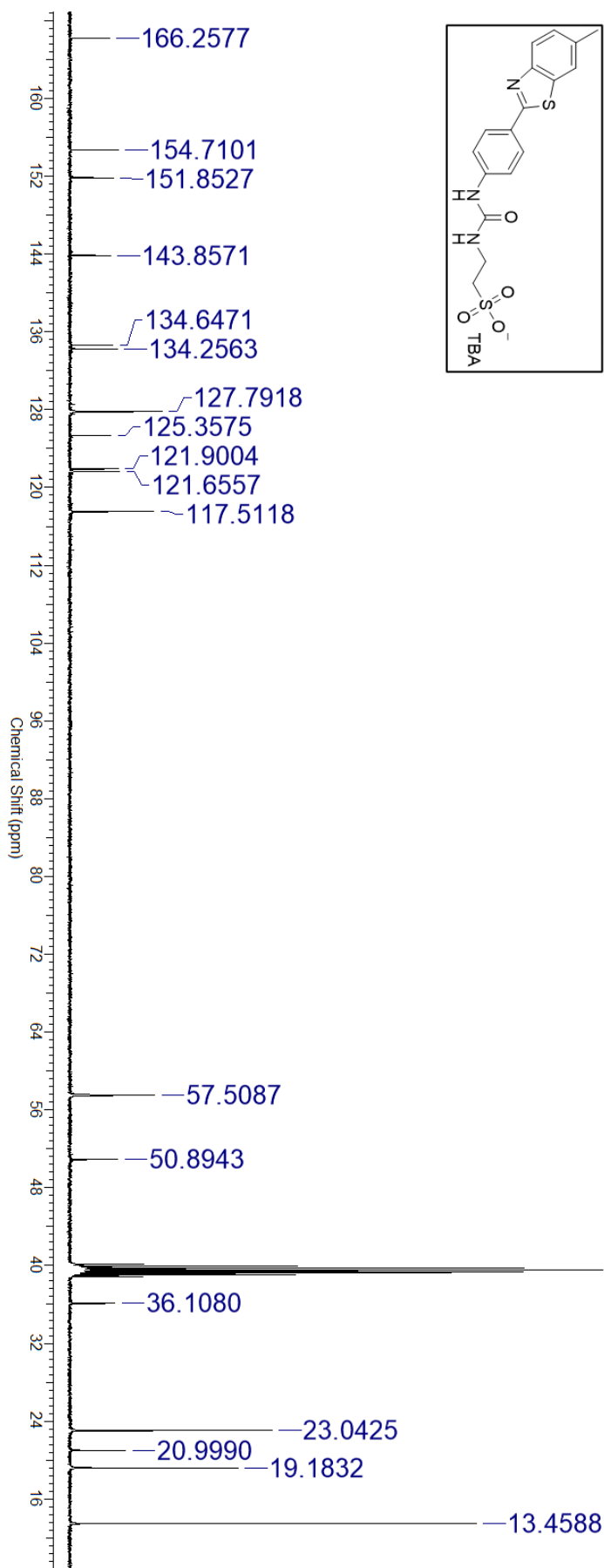


Figure S2: ^{13}C $\{^1\text{H}\}$ NMR of compound **1** in $\text{DMSO-}d_6$ conducted at 298 K.

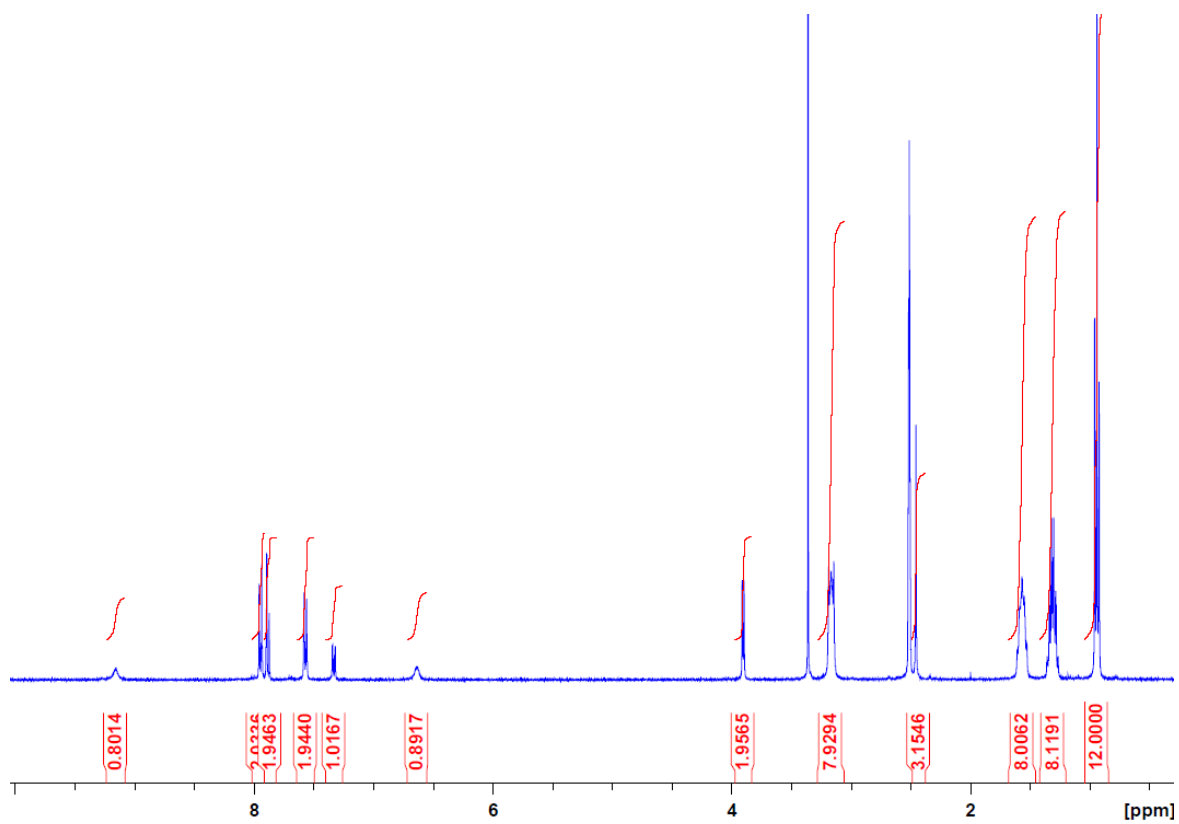


Figure S3: ^1H NMR of compound **2** in $\text{DMSO-}d_6$ conducted at 298 K.

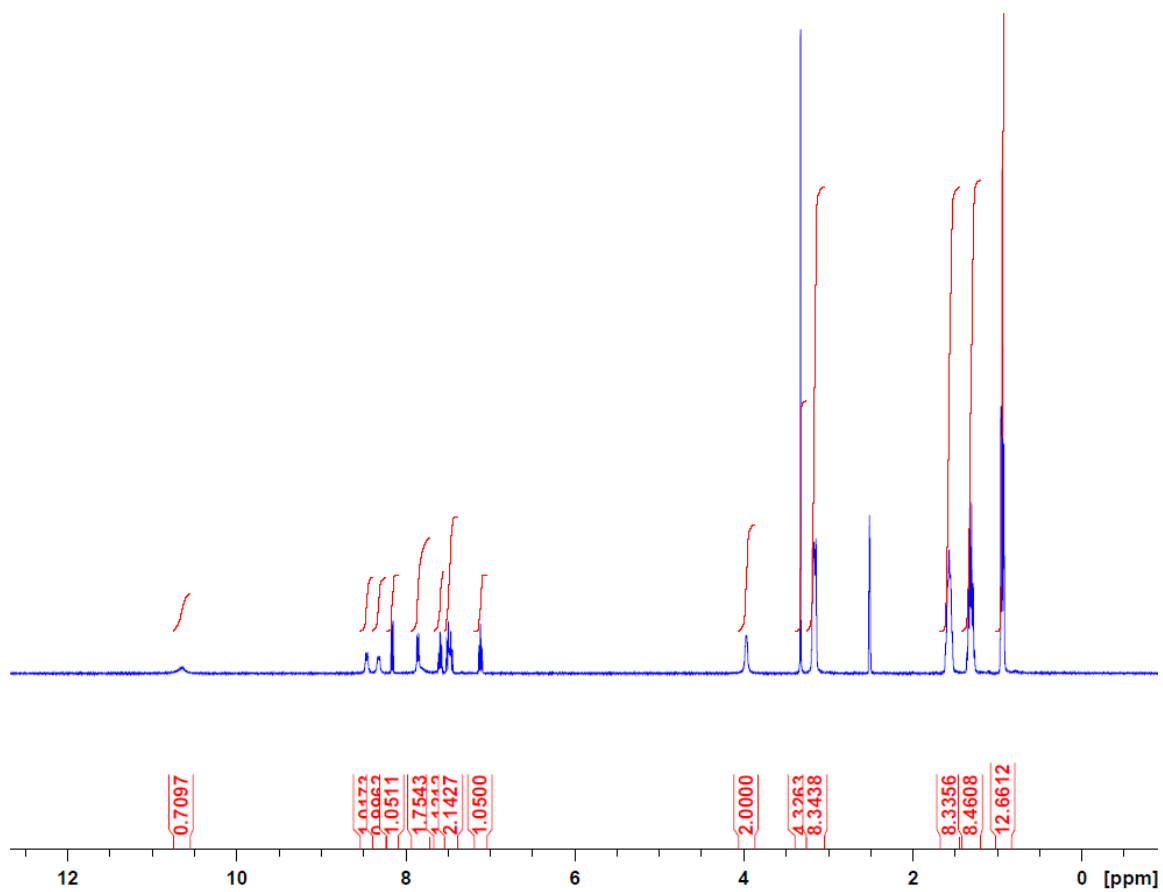


Figure S4: ^1H NMR of compound **3** in $\text{DMSO-}d_6$ conducted at 298 K.

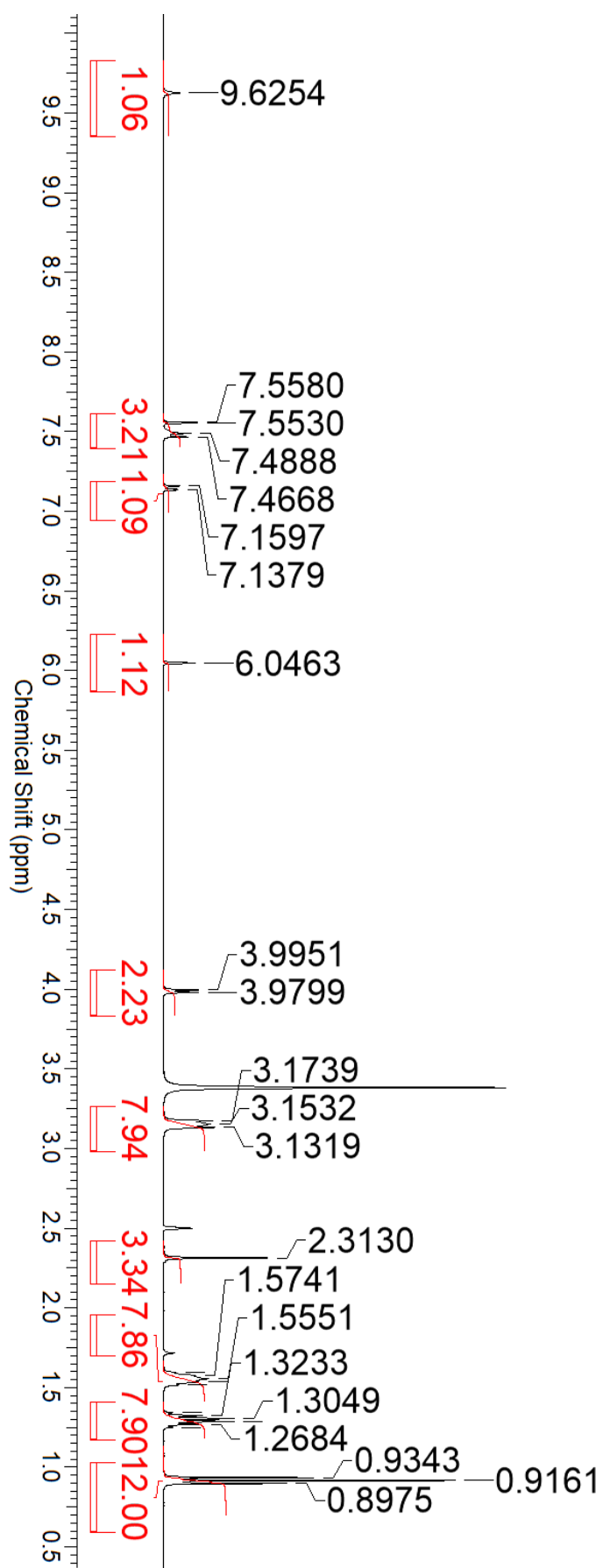


Figure S5: ^1H NMR of compound 4 in $\text{DMSO-}d_6$ conducted at 298 K.

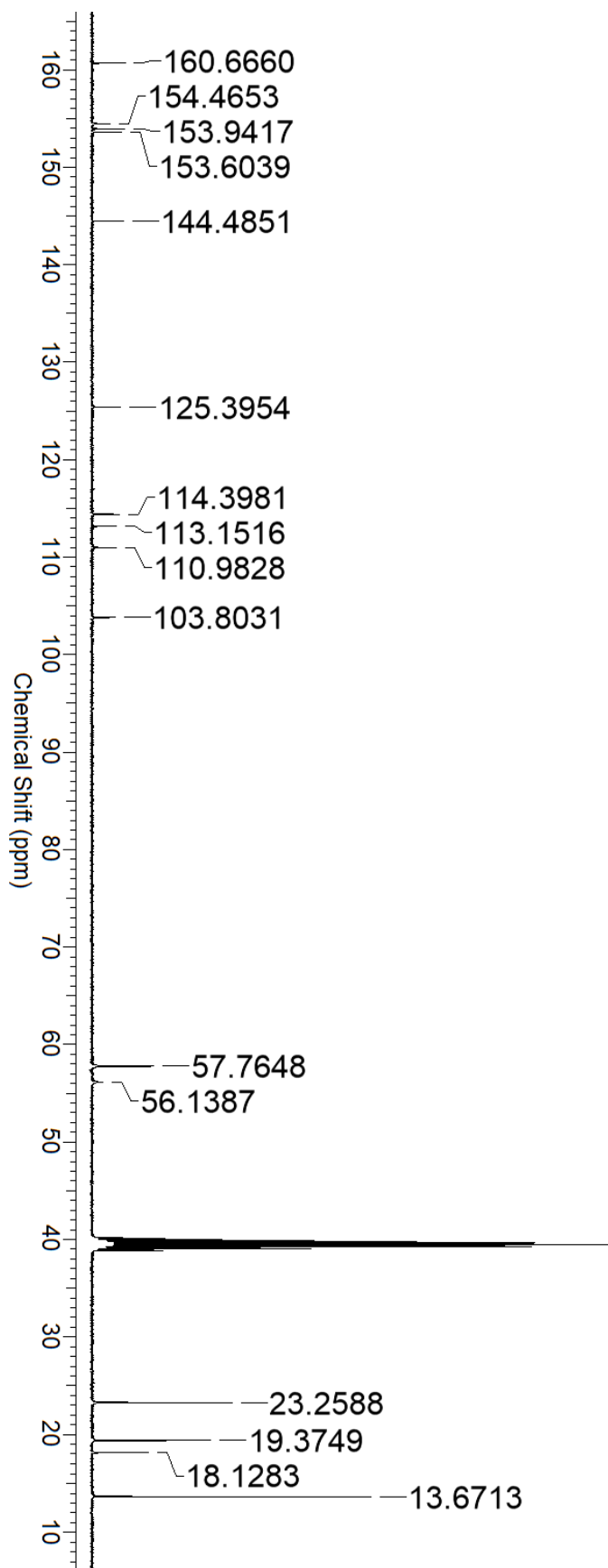


Figure S6: $^{13}\text{C}\{^1\text{H}\}$ NMR of compound **4** in $\text{DMSO-}d_6$ conducted at 298 K.

Quantitative ^1H NMR studies

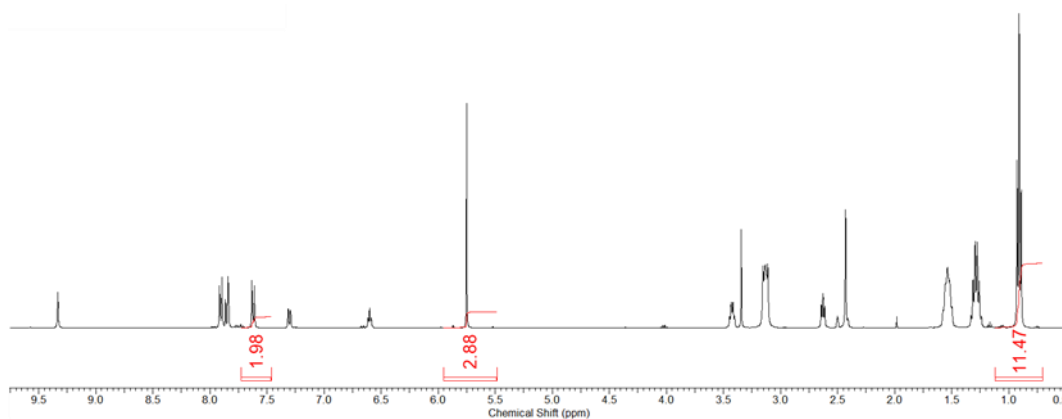


Figure S7: ^1H NMR spectrum ($d_1 = 60$ s) of compound **1** (112 mM) in $\text{DMSO-}d_6/1.0\%$ DCM. Comparative integration indicates 0% of the anionic component of **1** has become NMR silent.

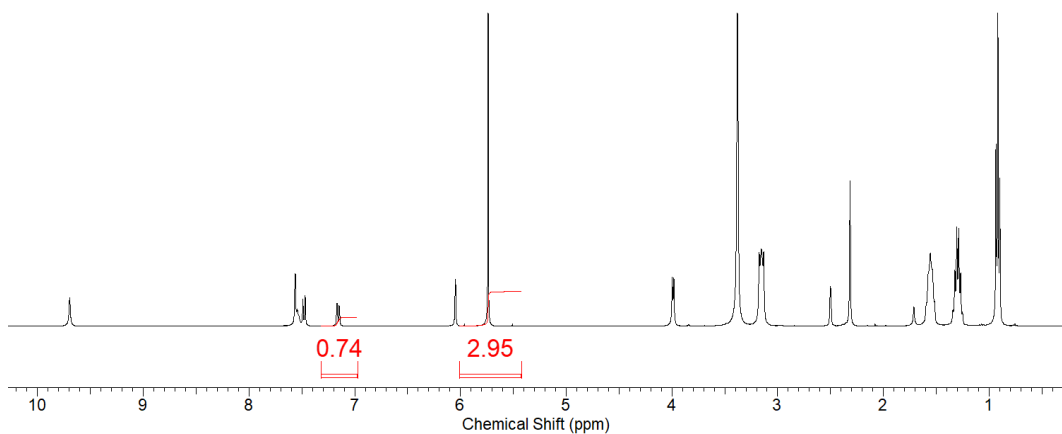


Figure S8: ^1H NMR spectrum ($d_1 = 60$ s) of compound **4** (112 mM) in $\text{DMSO-}d_6/1.0\%$ DCM. Comparative integration indicated 26% of the anionic component of **4** has become NMR silent.

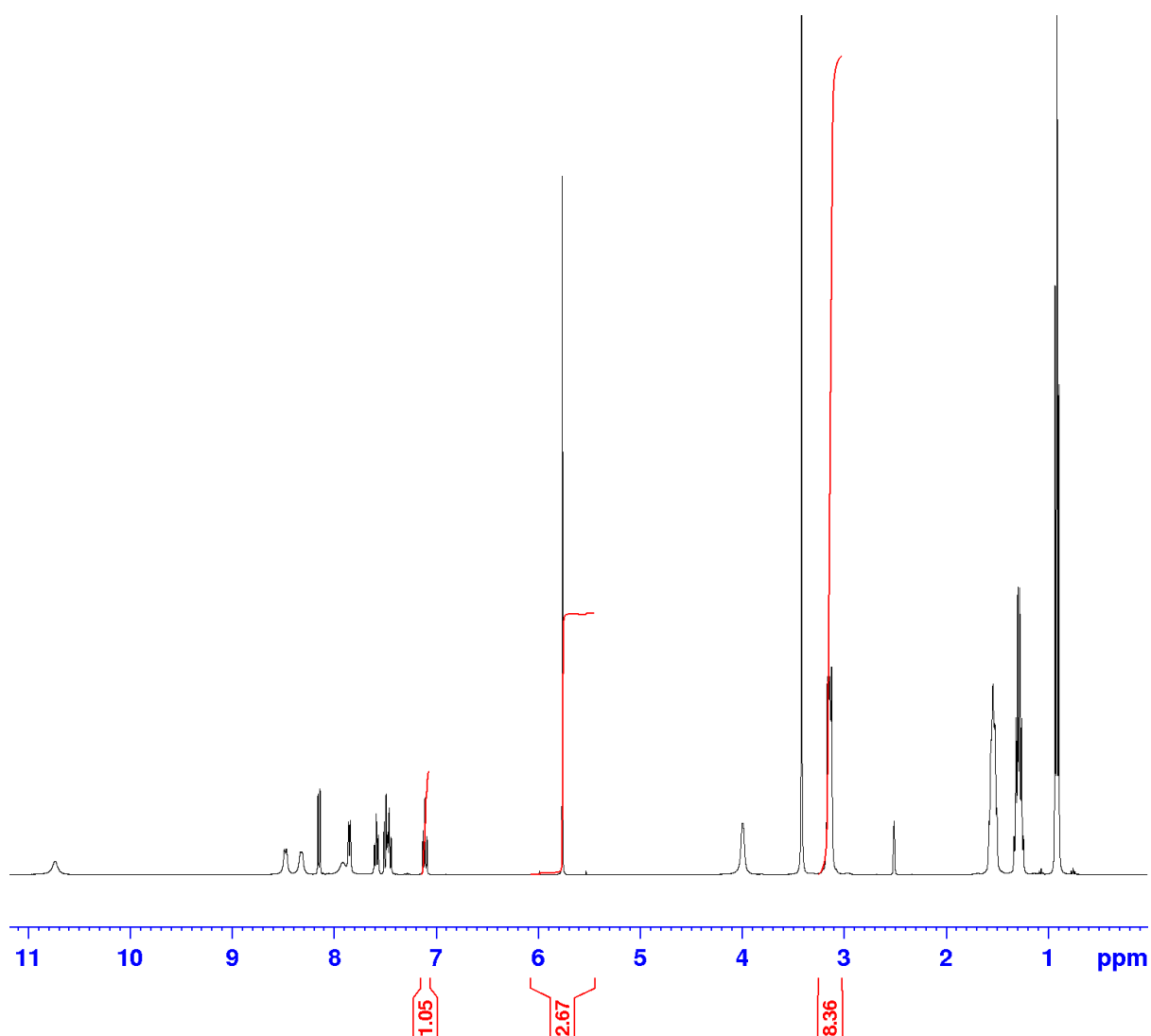


Figure S9: ¹H NMR spectrum ($d_1 = 60$ s) of compound **3** (112 mM) in DMSO- d_6 /1.0% DCM. Comparative integration indicated 0% of the anionic component of **3** has become NMR silent.

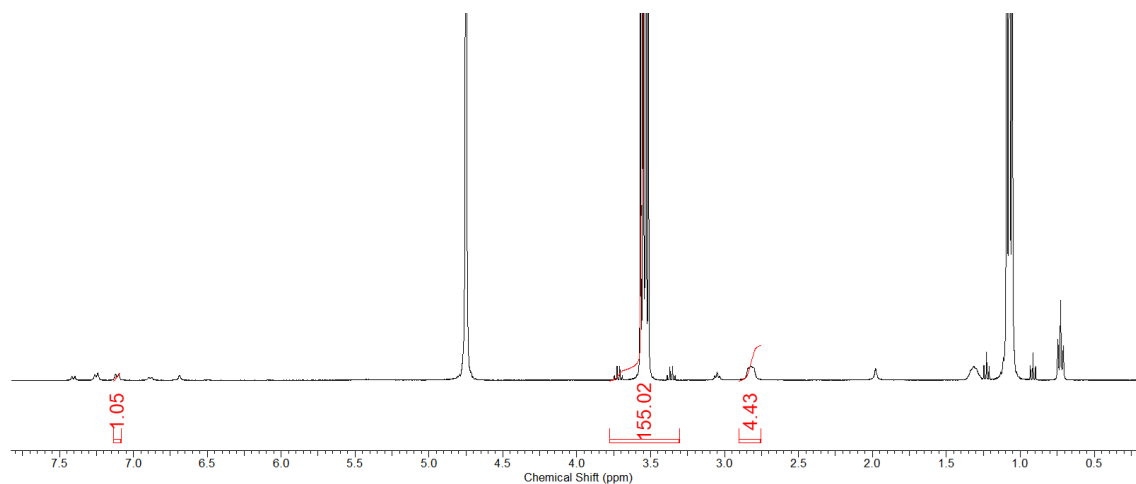


Figure S10: ¹H NMR spectrum ($d_1 = 60$ s) of compound **1** (5.56 mM) in D₂O/5.0% EtOH. Comparative integration indicates 48% of the anionic component of **1** has become NMR silent.

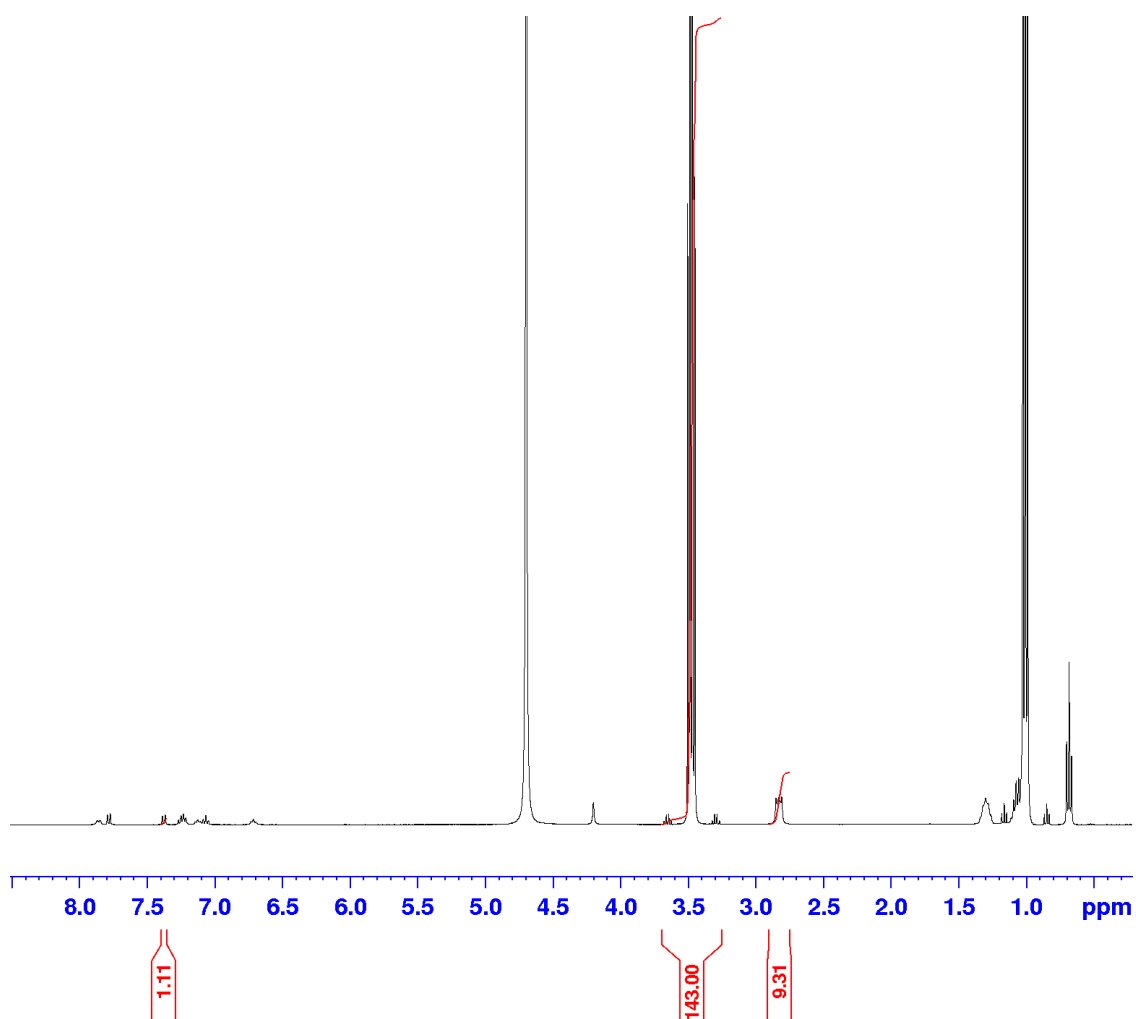


Figure S11: ¹H NMR spectrum with a delay ($d_1 = 60$ s) of compound **3** (5.56 mM) in D₂O/ 5.0% EtOH. Comparative integration indicated 0% of the anionic component of SSA has become NMR silent.

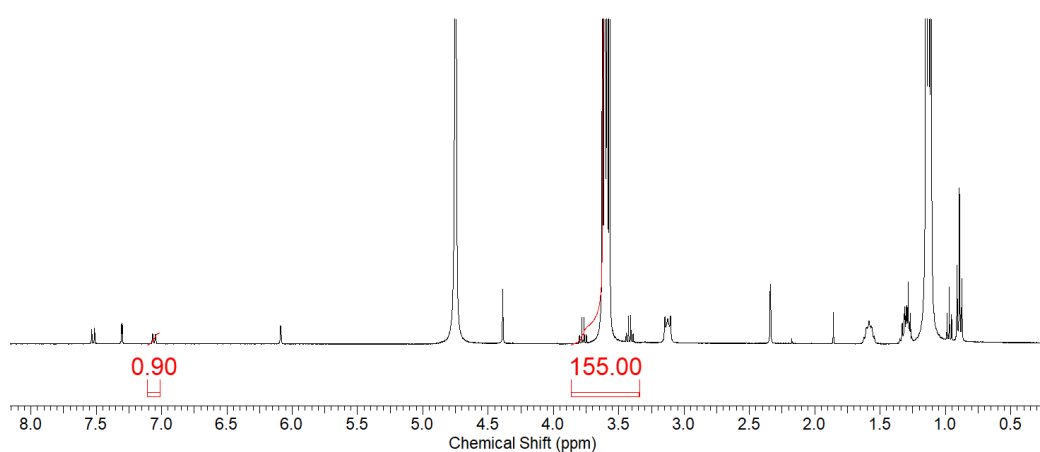


Figure S12: ¹H NMR spectrum with a delay ($d_1 = 60$ s) of compound **4** (5.56 mM) in D₂O/ 5.0% EtOH. Comparative integration indicated 10% of the anionic component of SSA has become NMR silent.

^1H NMR DOSY studies

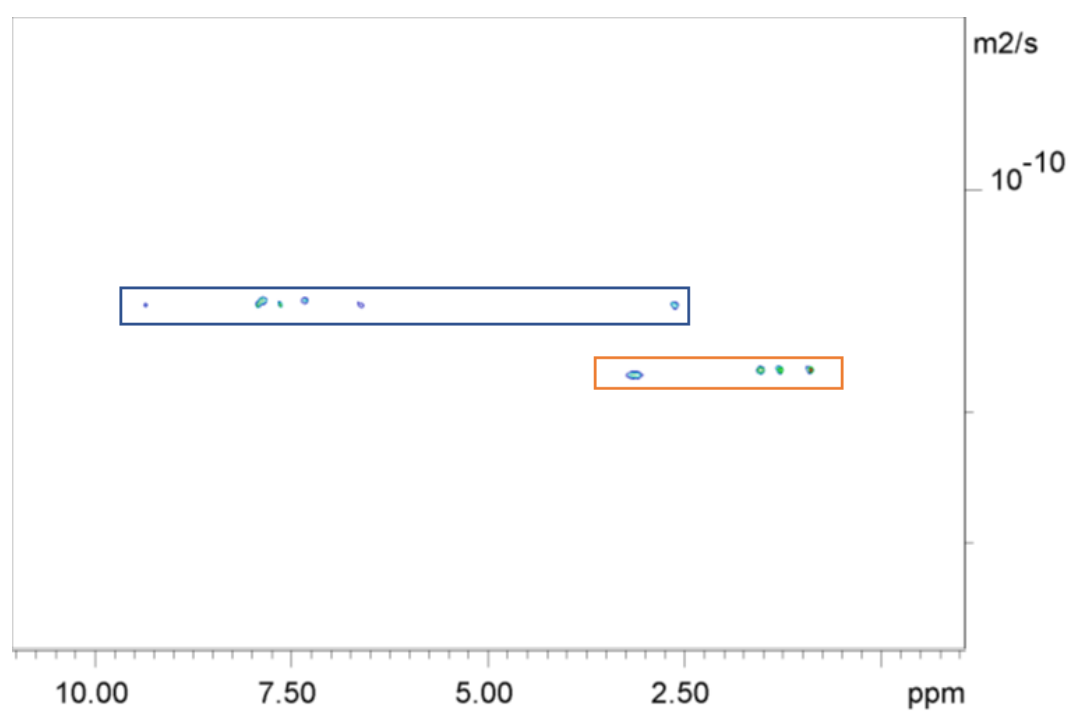
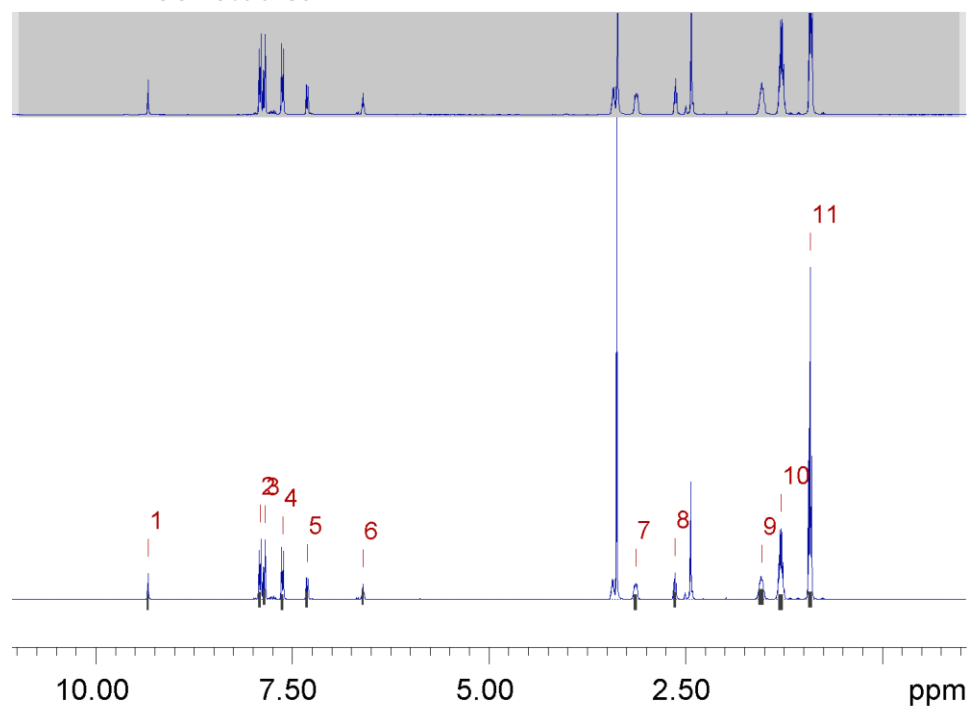


Figure S13: ^1H DOSY NMR spectrum of compound **1** (111.12 mM) in $\text{DMSO-}d_6$ at 298 K. Peaks 1–6 and 8 correspond to the anionic component of **1** while peaks 7, 9–11 correspond to the cationic component of **1**. Data corresponding to this spectrum can be seen in Table S1.

Table S1: ^1H DOSY NMR data table of compound **1** (111.12 mM) in $\text{DMSO-}d_6$ at 298 K, reporting the diffusion constants calculated for each peak used to determine the solvation sphere diameter of the anionic component of **1** ($d_H = 1.54$ nm). Peaks 1–6 and 8 correspond to the anionic component of **1** while peaks 7, 9-11 correspond to the cationic component of **1**. Spectrum corresponding to this data table can be seen in Figure S13.

Peak name	F2 [ppm]	lo	error	D [m ² /s]	error
1	9.335	1.70e+08	1.413e+04	1.42e-10	2.376e-14
2	7.914	5.43e+08	1.631e+04	1.42e-10	8.569e-15
3	7.854	4.99e+08	1.630e+04	1.42e-10	9.285e-15
4	7.626	6.11e+08	1.930e+04	1.42e-10	9.012e-15
5	7.314	2.91e+08	1.747e+04	1.42e-10	1.705e-14
6	6.605	1.42e+08	1.504e+04	1.42e-10	3.021e-14
7	3.138	4.01e+08	2.146e+04	1.77e-10	1.859e-14
8	2.636	3.23e+08	1.711e+04	1.42e-10	1.510e-14
9	1.535	7.55e+08	2.712e+04	1.76e-10	1.246e-14
10	1.288	1.61e+09	2.626e+04	1.76e-10	5.670e-15
11	0.914	3.40e+09	2.349e+04	1.76e-10	2.394e-15

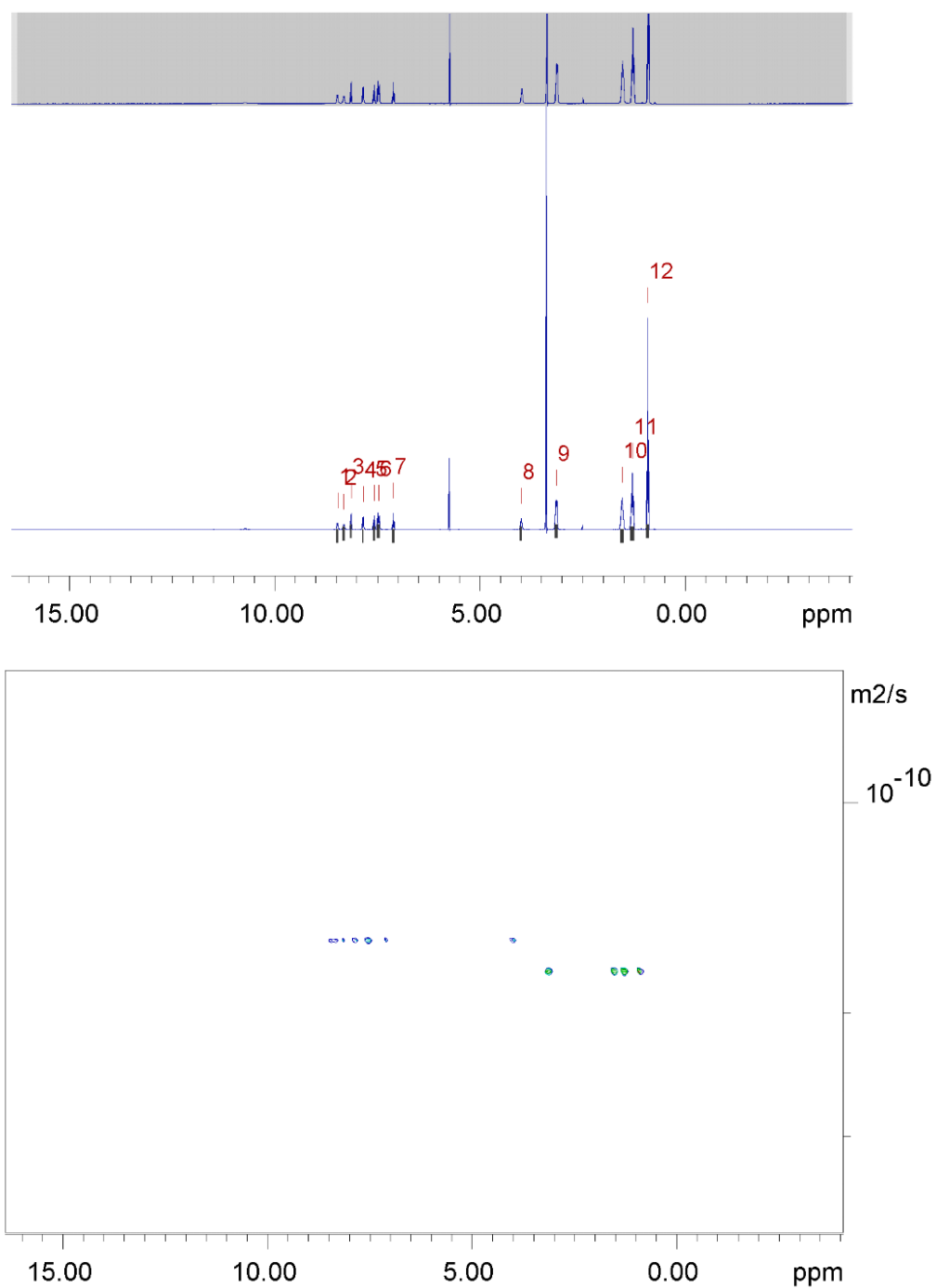


Figure S14: ^1H DOSY NMR spectrum of compound **3** (112.12 mM) in $\text{DMSO}-d_6$ at 298 K. Peaks 1–8 correspond to the anionic component of **3** while peaks 9–12 correspond to the cationic component of **3**. Data corresponding to this spectrum can be seen in Table S2.

Table S2: ¹H DOSY NMR data table of compound **3** (111.12 mM) in DMSO-*d*₆ at 298 K, reporting the diffusion constants calculated for each peak used to determine the solvation sphere diameter of the anionic component of **3** (*d*_H = 1.39 nm). Peaks 1–8 correspond to the anionic component of **3** while peaks 9–12 correspond to the cationic component of **3**. Spectrum corresponding to this data table can be seen in Figure S14.

Peak name	F2 [ppm]	lo	error	D [m ² /s]	error
1	8.475	6.42e+08	3.379e+04	1.58e-10	1.830e-14
2	8.324	5.79e+08	3.333e+04	1.58e-10	2.002e-14
3	8.143	7.52e+08	2.799e+04	1.58e-10	1.294e-14
4	7.848	7.93e+08	2.842e+04	1.58e-10	1.246e-14
5	7.584	8.07e+08	3.288e+04	1.58e-10	1.416e-14
6	7.473	1.63e+09	3.974e+04	1.58e-10	8.485e-15
7	7.110	7.86e+08	3.127e+04	1.58e-10	1.385e-14
8	3.999	1.05e+09	3.234e+04	1.58e-10	1.068e-14
9	3.142	3.88e+09	3.905e+04	1.74e-10	3.822e-15
10	1.540	4.48e+09	4.378e+04	1.74e-10	3.716e-15
11	1.291	5.82e+09	4.730e+04	1.74e-10	3.090e-15
12	0.915	9.57e+09	3.772e+04	1.74e-10	1.499e-15

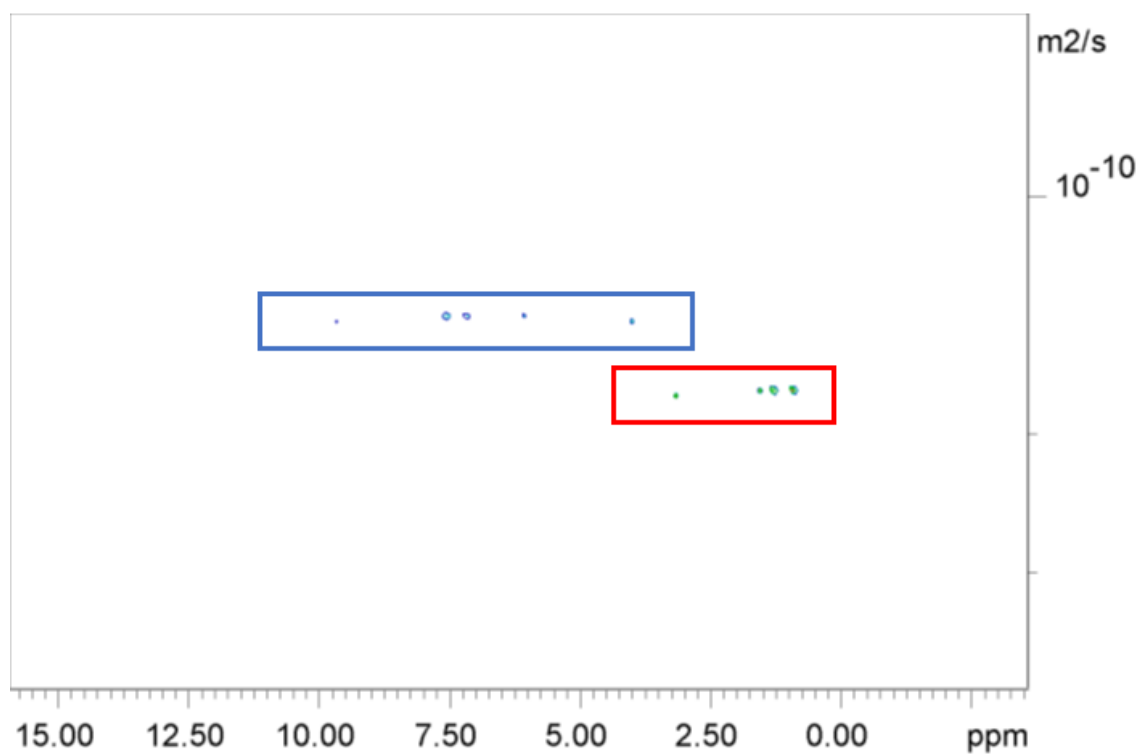
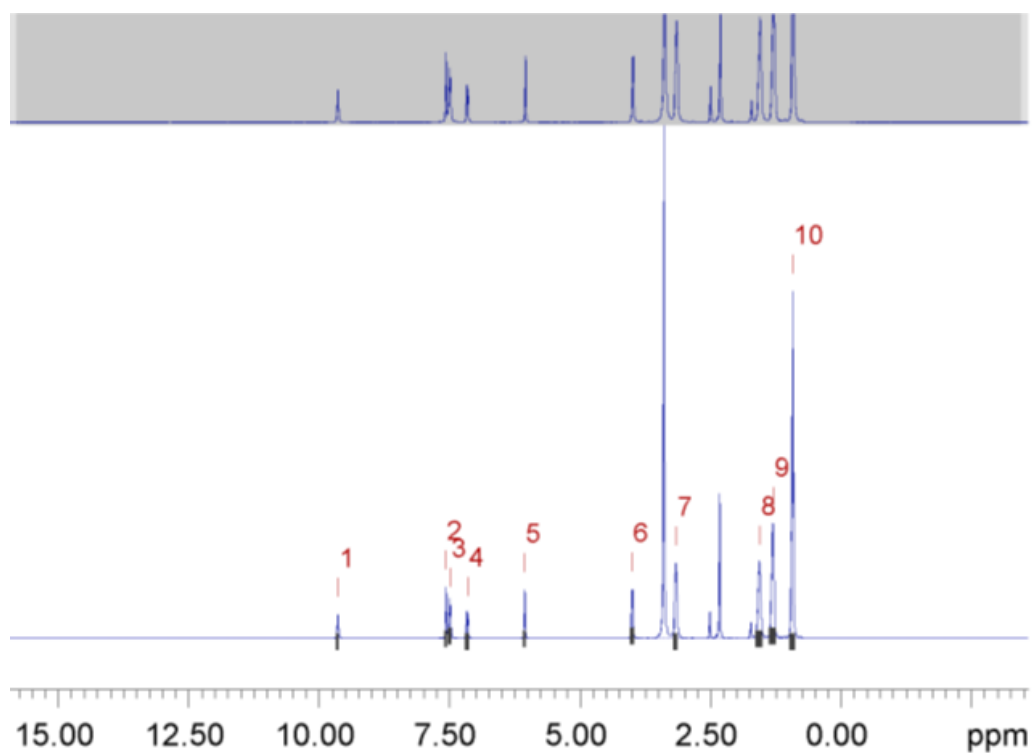


Figure S15: ^1H DOSY NMR spectrum of compound **4** (111.12 mM) in $\text{DMSO-}d_6$ at 298 K. Peaks 1-6 correspond to the anionic component of **4** and peaks 7-10 correspond to the cationic component of **4**. Data corresponding to this spectrum can be seen in Table S3.

Table S3: ^1H DOSY NMR data table of compound **4** (111.12 mM) in $\text{DMSO-}d_6$ at 298 K, reporting the diffusion constants calculated for each peak used to determine the hydrodynamic diameter of the anionic component ($d_H = 1.53$ nm) of **4**. Peaks 1-6 correspond to the anionic component of **4** and peaks 7-10 correspond to the cationic component of **4**. Spectrum corresponding to this data table can be seen in Figure S15.

Peak name	F2 [ppm]	lo	error	D [m ² /s]	error
1	9.638	1.53e+09	1.196e+05	1.44e-10	2.526e-14
2	7.569	2.37e+09	1.192e+05	1.42e-10	1.607e-14
3	7.494	3.68e+09	1.288e+05	1.42e-10	1.121e-14
4	7.158	2.34e+09	1.458e+05	1.42e-10	1.994e-14
5	6.061	2.16e+09	1.288e+05	1.42e-10	1.911e-14
6	4.001	4.04e+09	1.460e+05	1.43e-10	1.160e-14
7	3.165	1.04e+10	1.635e+05	1.78e-10	6.146e-15
8	1.565	1.22e+10	1.929e+05	1.76e-10	6.139e-15
9	1.304	1.56e+10	1.995e+05	1.76e-10	4.974e-15
10	0.928	2.55e+10	1.784e+05	1.76e-10	2.714e-15

¹H NMR self-association studies

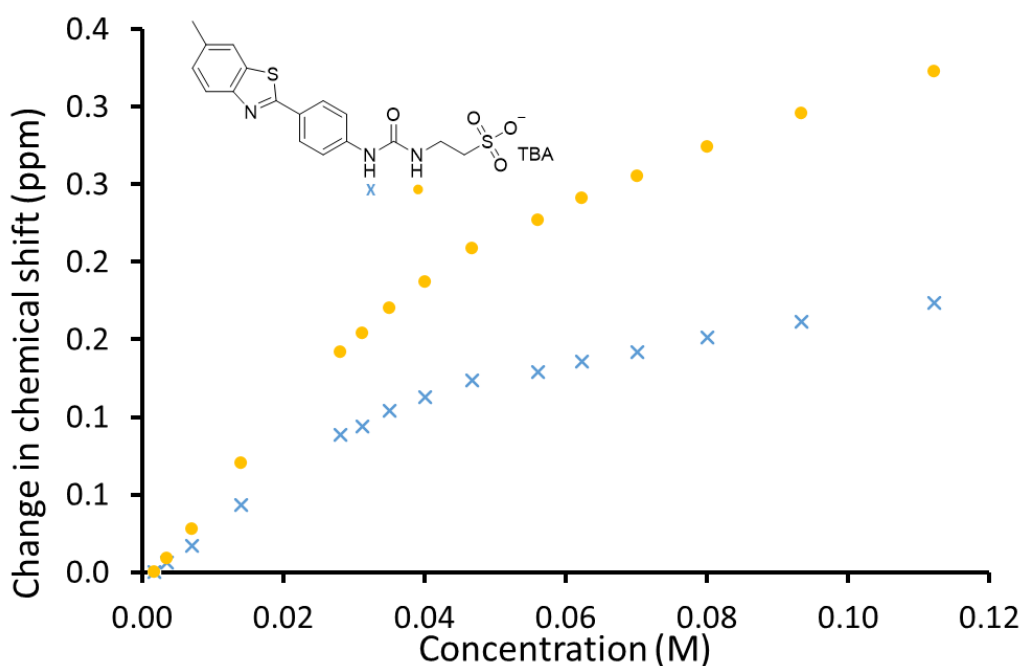


Figure S16: Graph illustrating the ¹H NMR down-field change in chemical shift of urea NH resonances with increasing concentration of compound **1** in DMSO-*d*₆ 0.5% H₂O (298 K).

Self-association constant calculation

Compound **1** – Dilution study in DMSO-*d*₆ 0.5% H₂O. Values calculated from data gathered from both NHs.

Equal K/Dimerisation mode

$$K_e = 8.01 \times 10^{-5} \text{ M}^{-1} \pm 0.0879\%$$

$$K_{dim} = 4.01 \times 10^{-5} \text{ M}^{-1} \pm 4.3951 \times 10^{-2}\%$$

<http://app.supramolecular.org/bindfit/view/fa96db32-f1f4-4cf6-bcc1-97bbcb17d141>

CoEK model

$$K_e = 0.6.09 \text{ M}^{-1} \pm 4.4759\%$$

$$K_{dim} = 3.04 \text{ M}^{-1} \pm 2.2238\%$$

$$\rho = 0.22 \pm 10.1476\%$$

<http://app.supramolecular.org/bindfit/view/4ab2b3d9-dff7-4294-a191-400cf2ad9c74>

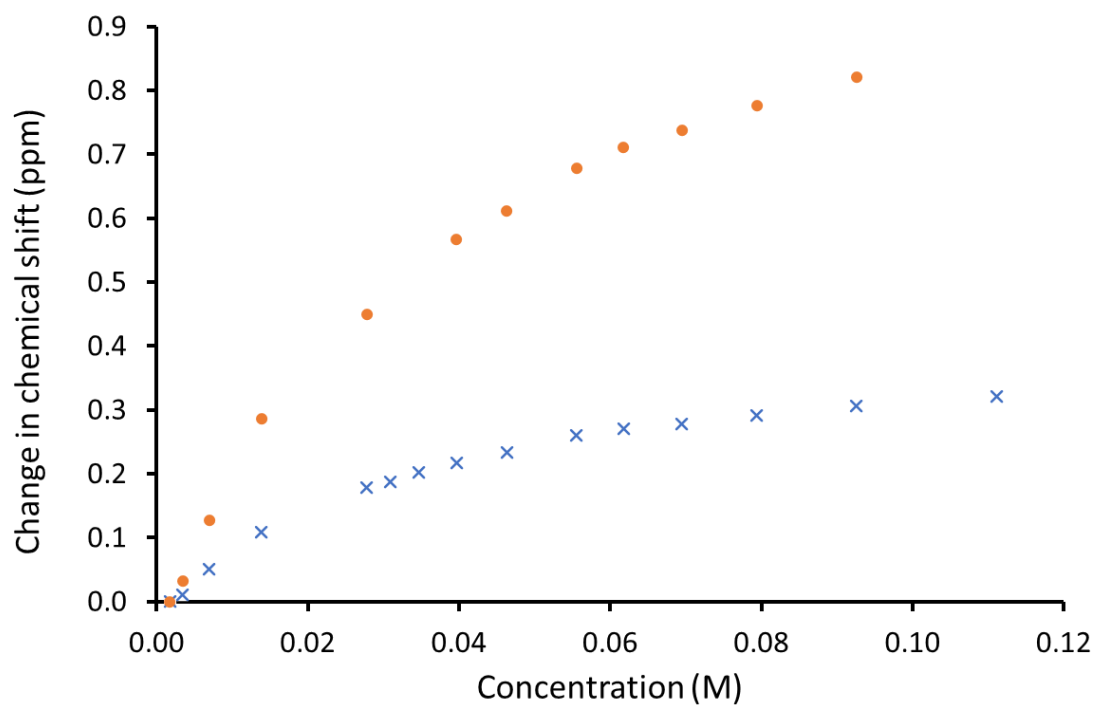


Figure S17: Graph illustrating the ^1H NMR down-field change in chemical shift of urea NH resonances with increasing concentration of compound **4** in $\text{DMSO-}d_6$ 0.5% H_2O (298 K). Orange = NH closest to the sulfonate group and Blue = NH closest to the phenyl ring system.

High-resolution mass spectrometry data

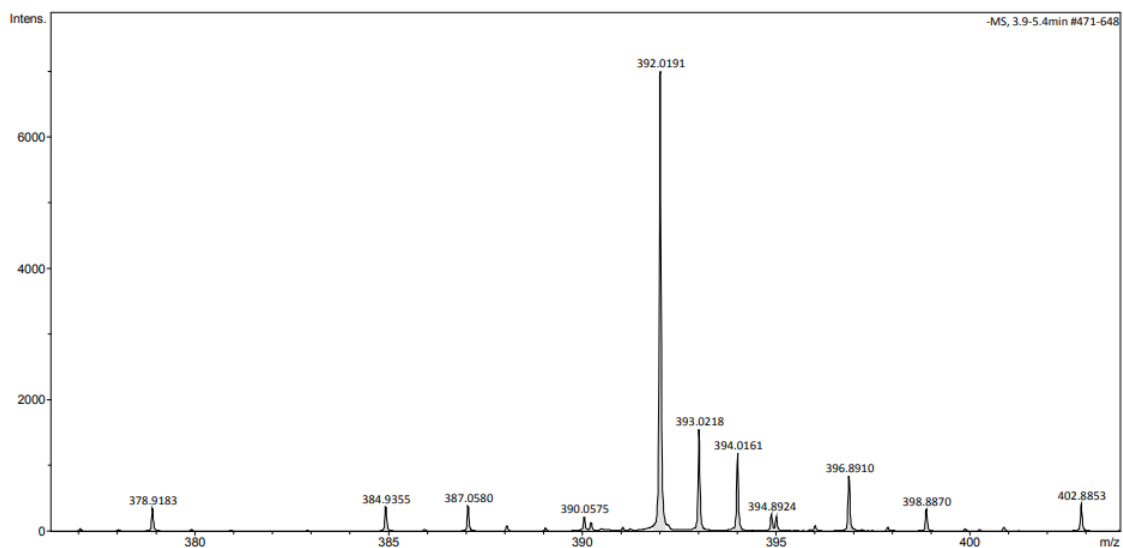


Figure S18: A high-resolution mass spectrum (ESI⁻) obtained for compound **1** in methanol. m/z [M]⁻.

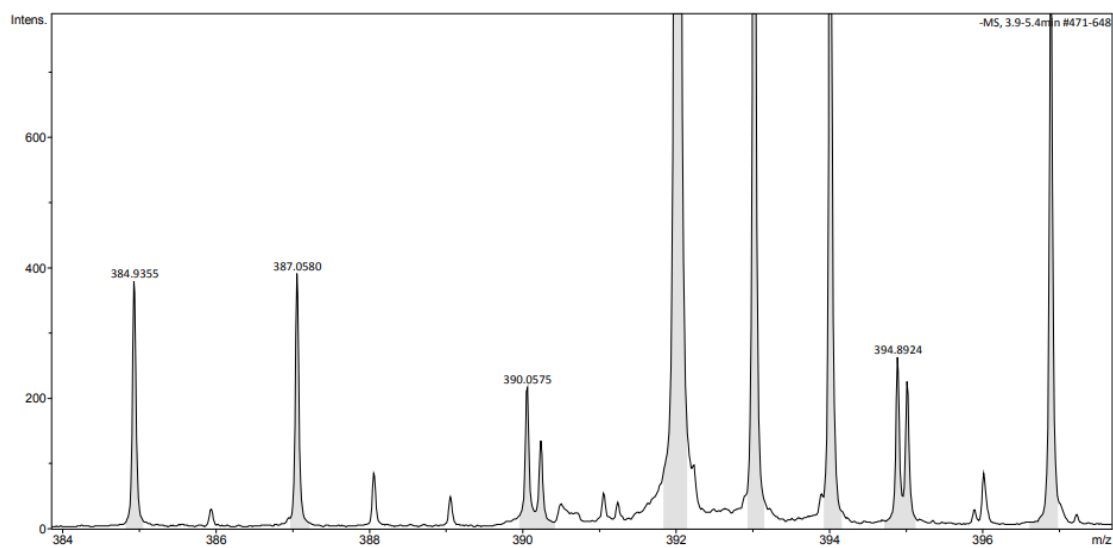


Figure S191: A zoomed in high-resolution mass spectrum (ESI⁻) obtained for compound **1** in methanol. m/z [M]⁻.

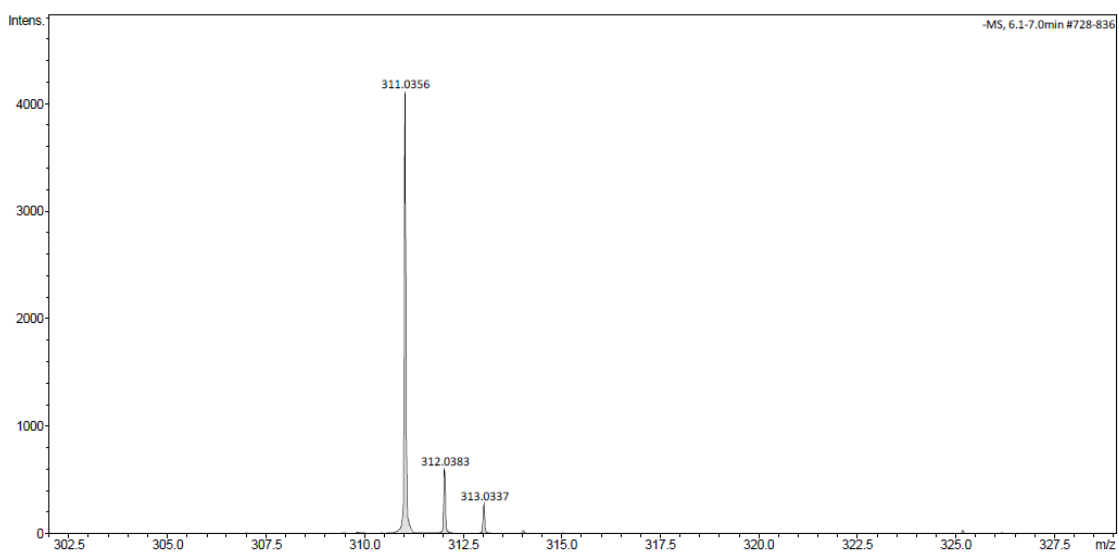


Figure S20: A high-resolution mass spectrum (ESI⁻) obtained for compound **4** in methanol, m/z [M]⁻.

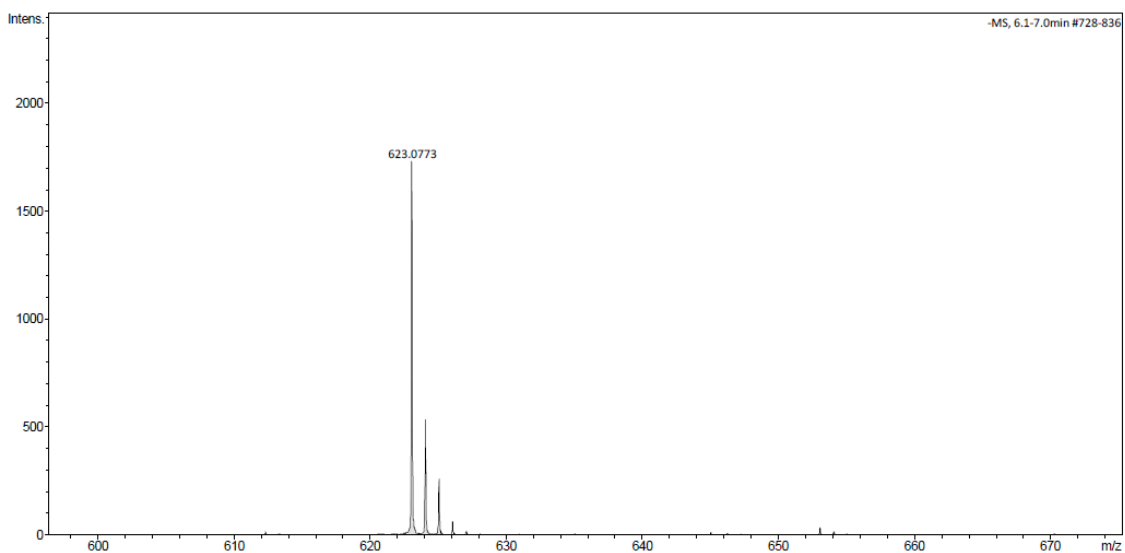


Figure S21: A high-resolution mass spectrum (ESI⁻) obtained for dimeric species of compound **4** in methanol, m/z [M + M + H⁺]⁻.

Overview

Table S4: High resolution ESI⁻ mass spectrometry theoretical and experimentally derived values.

Compound	m/z [M]		m/z [M + M + H ⁺]	
	Theoretical	Actual	Theoretical	Actual
1	390.0588	390.0575	<i>a</i>	<i>a</i>
4	311.0343	311.0356	623.0686	623.0773

a – Dimer not observed.

Single crystal X-ray structures

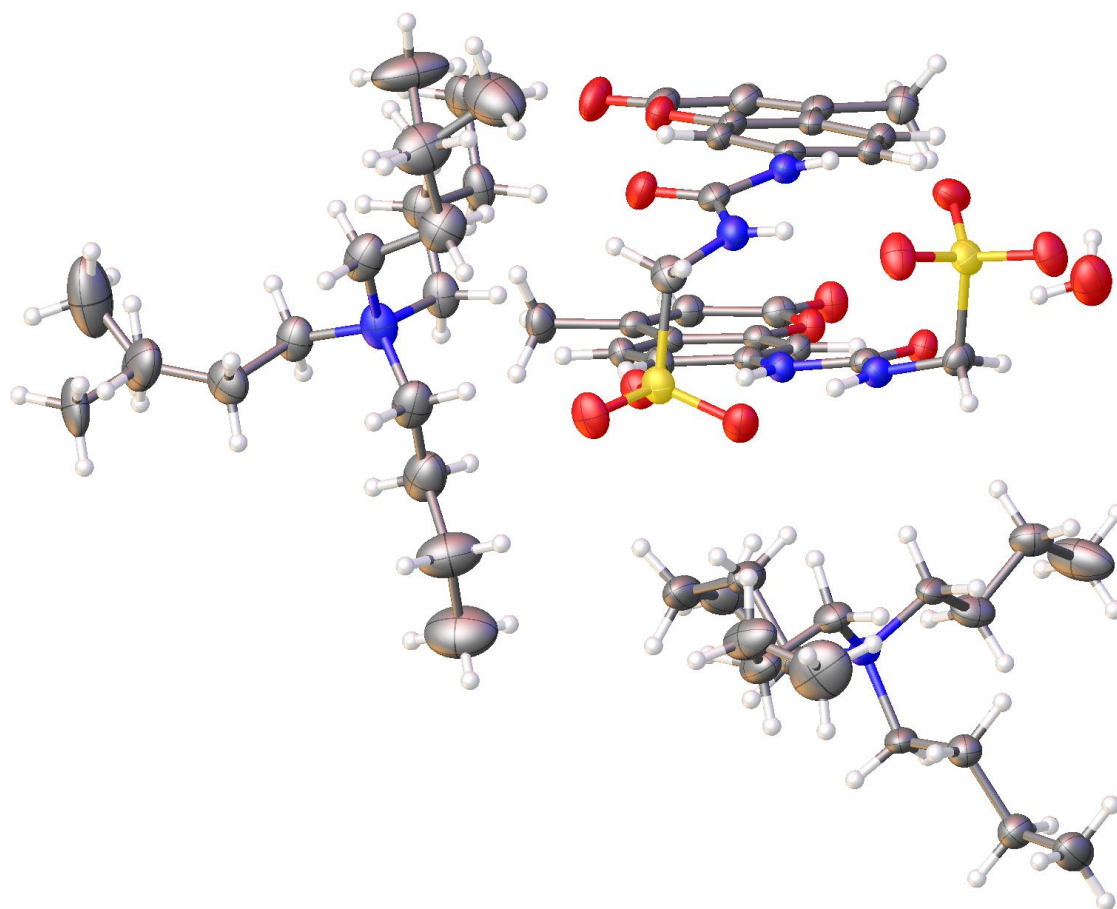


Figure S22: Single crystal X-ray structure of **4**: red = oxygen; yellow = sulfur; blue = nitrogen; white = hydrogen; grey = carbon. CCDC 1999015, $C_{56}H_{96}N_6O_{13}S_2$ ($M = 1125.50$): monoclinic, space group P 21/c, $a = 22.1917(4)$ Å, $b = 11.30152(18)$ Å, $c = 24.5454(4)$ Å, $\alpha = 90^\circ$, $\beta = 96.4591(15)^\circ$, $\gamma = 90^\circ$, $V = 6116.91(17)$ Å³, $Z = 2$, $T = 100(1)$ K, $CuK\alpha = 1.5418$ Å, $D_{calc} = 1.222$ g/cm³, 41676 reflections measured ($7.248 \leq 2\theta \leq 133.186$), 10816 unique ($R_{int} = 0.0408$, $R_{sigma} = 0.0346$) which were used in all calculations. The final R_1 was 0.0601 ($I > 2\sigma(I)$) and wR_2 was 0.1785 (all data). Internal angle of dimerization = $18.01(11)^\circ$.

Table S5: Hydrogen bond distances and angles observed for **4**, calculated from the single crystal X-ray structure shown in Figure S22.

Hydrogen bond donor	Hydrogen bond acceptor	Hydrogen bond length (D•••A) (Å)	Hydrogen bond angle (D-H•••A) (°)
N1	O9	2.921 (3)	164.34 (18)
N2	O8	2.892 (3)	152.44 (16)
N3	O1	2.904 (3)	176.44 (16)
N4	O2	2.893 (3)	165.63 (16)
O13	O10	2.864 (3)	177.40 (6)
O13	O12	2.913 (3)	173.10 (20)

Optical density plate reader data

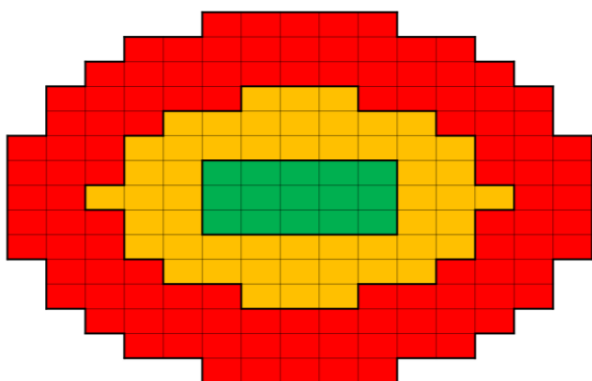


Figure S23: Diagram illustrating the 177 sections monitored during the OD well scan measurement process. Red = 110 sections that are used to monitor the increased OD due to compound aggregation at the well interface. Yellow = 52 'buffer zone' sections. Green = 15 control sections.

Compound 1 CMC calculation at 298 K OD₃₇₀

Table S6: A summary of OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 298 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections									Average of n's			+/- error		
	n = 1			n = 2			n = 3			Red	Yellow	Green	Red	Yellow	Green
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
5	3.37	3.22	3.12	3.42	3.27	3.14	3.43	3.29	3.19	3.40	3.26	3.15	0.03	0.03	0.03
4	3.44	3.25	3.21	3.47	3.31	3.31	3.48	3.36	3.42	3.46	3.31	3.32	0.01	0.05	0.09
3.5	3.38	3.29	3.21	3.35	3.13	3.04	3.37	3.19	3.18	3.36	3.20	3.14	0.01	0.07	0.07
3	3.39	3.08	2.94	3.40	3.15	3.08	3.41	3.18	3.03	3.40	3.14	3.02	0.01	0.04	0.06
2.5	3.36	2.82	2.64	3.39	2.82	2.64	3.40	2.84	2.68	3.39	2.83	2.65	0.02	0.01	0.02
2.25	3.39	2.73	2.53	3.36	2.73	2.56	3.41	2.76	2.54	3.38	2.74	2.54	0.02	0.01	0.01
2	3.34	2.47	2.24	3.29	2.42	2.19	3.34	2.45	2.22	3.32	2.45	2.22	0.02	0.02	0.02
1.9	3.29	2.35	2.11	3.28	2.35	2.11	3.31	2.36	2.10	3.29	2.35	2.11	0.01	0.01	0.00
1.5	3.12	1.89	1.67	3.11	1.91	1.68	3.10	1.86	1.63	3.11	1.89	1.66	0.01	0.02	0.02
1.25	2.94	1.61	1.41	2.96	1.58	1.37	2.98	1.60	1.39	2.96	1.60	1.39	0.02	0.01	0.02
1	2.68	1.17	1.00	2.71	1.19	1.01	2.78	1.18	1.00	2.72	1.18	1.00	0.04	0.01	0.00
0.75	2.58	0.84	0.69	2.48	0.84	0.69	2.56	0.84	0.68	2.54	0.84	0.69	0.04	0.00	0.01
0.5	2.41	0.69	0.55	2.29	0.69	0.55	2.37	0.70	0.56	2.35	0.69	0.55	0.05	0.00	0.00
0.25	2.01	0.39	0.29	1.09	0.35	0.31	1.88	0.39	0.30	1.66	0.38	0.30	0.41	0.02	0.01

Table S7: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Red	Green	Ratio Red: Green
5.00	3.40	3.15	1.08
4.00	3.46	3.32	1.04
3.50	3.36	3.14	1.07
3.00	3.40	3.02	1.13
2.50	3.39	2.65	1.28
2.25	3.38	2.54	1.33
2.00	3.32	2.22	1.50
1.90	3.29	2.11	1.56
1.50	3.11	1.66	1.88
1.25	2.96	1.39	2.13
1.00	2.72	1.00	2.72
0.75	2.54	0.69	3.70
0.50	2.35	0.55	4.27
0.25	1.66	0.30	5.59

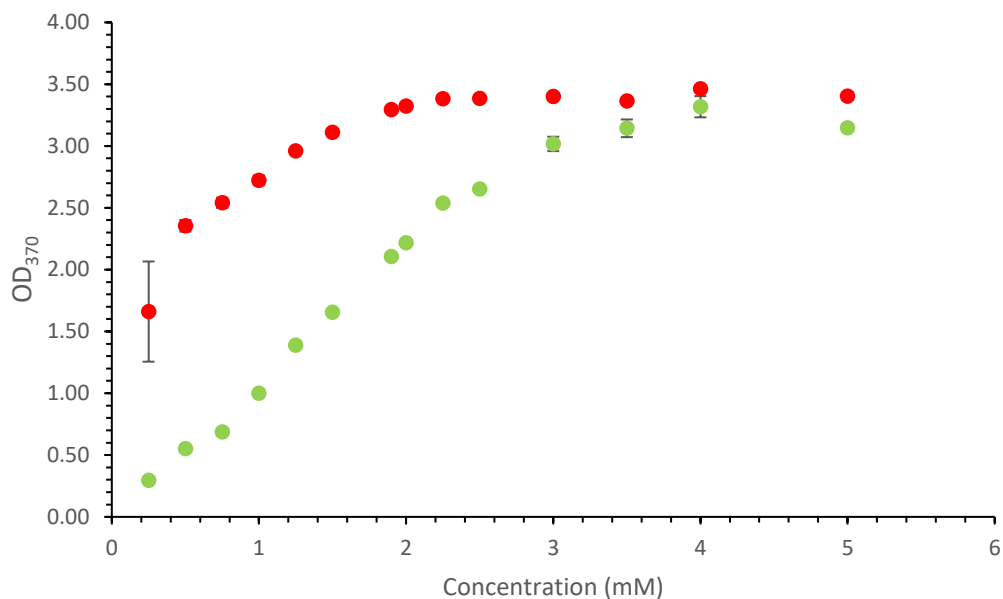


Figure S24: Graph showing average (n=3) red - interface and green - control OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 298 K.

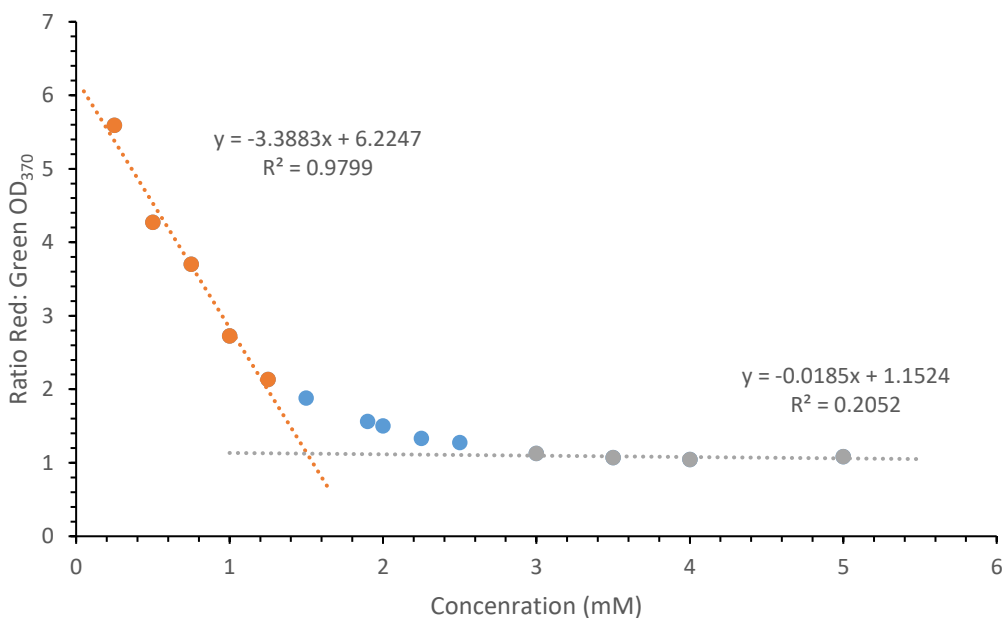


Figure S25: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 at 298 K, plotted against compound concentration. A CMC value of 1.51 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either liner trend.

Raw well data for compound 1 at 298 K OD₃₇₀

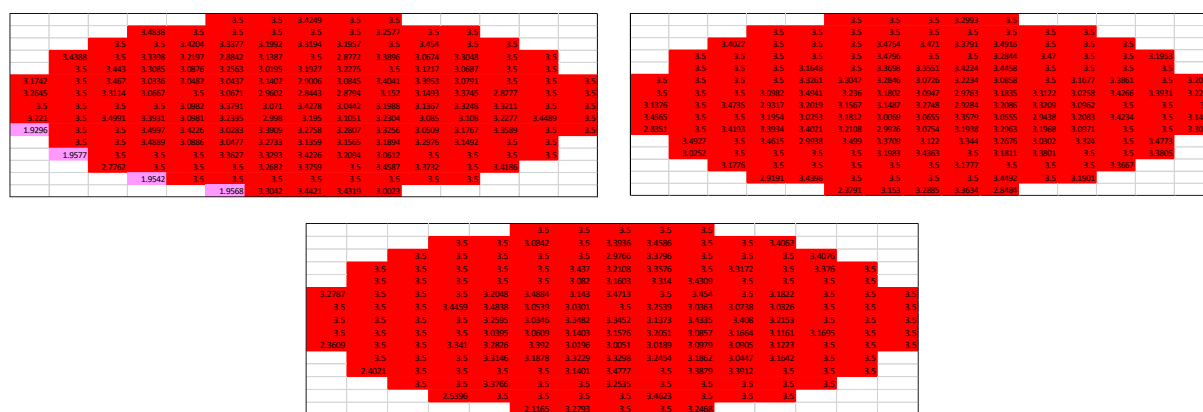


Figure S26: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (5.00 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

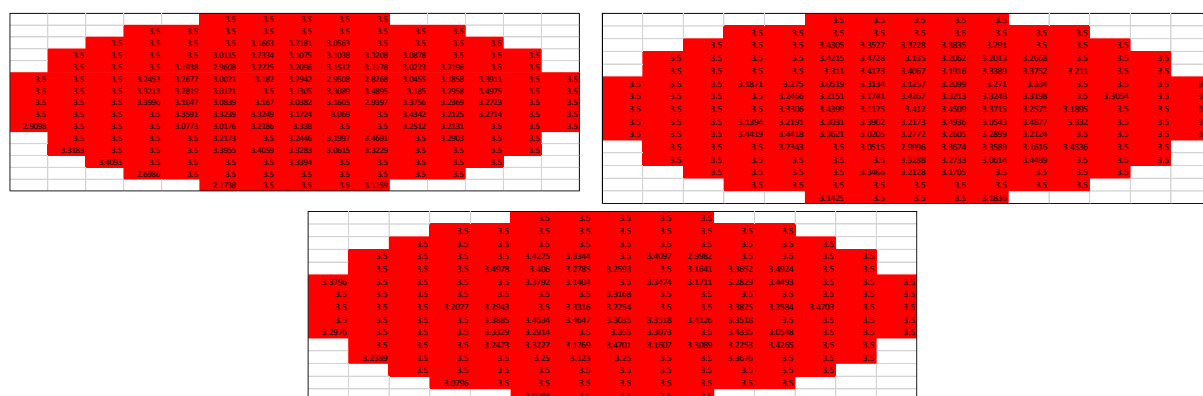


Figure S27: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (4.00 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

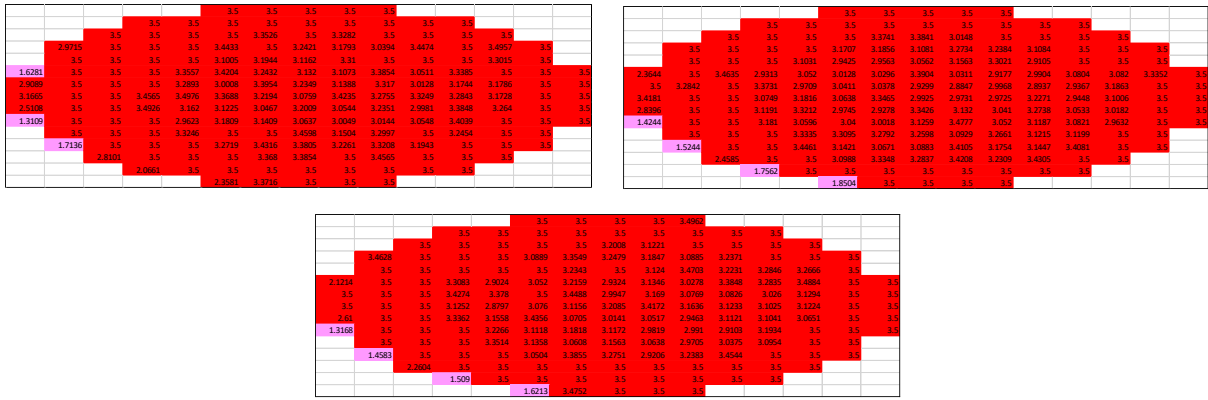


Figure S28: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (3.50 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

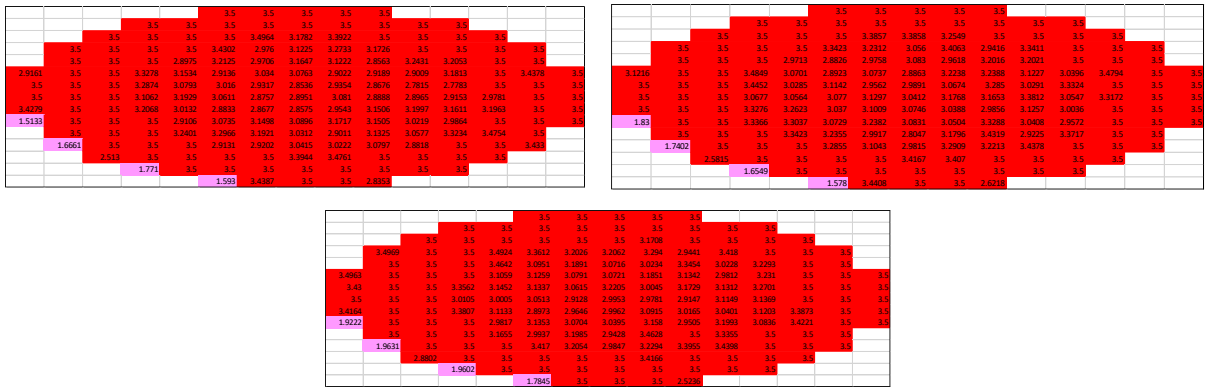


Figure S29: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (3.00 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

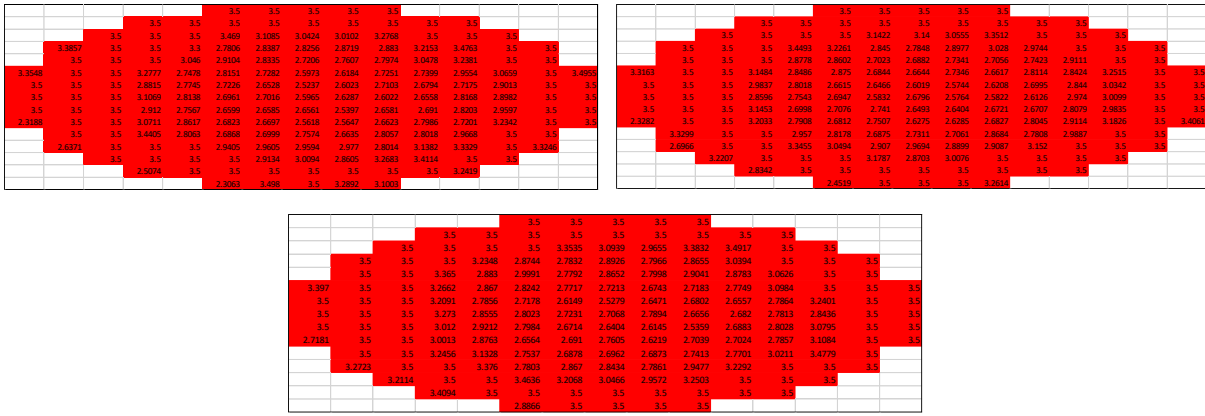


Figure S30: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.50 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

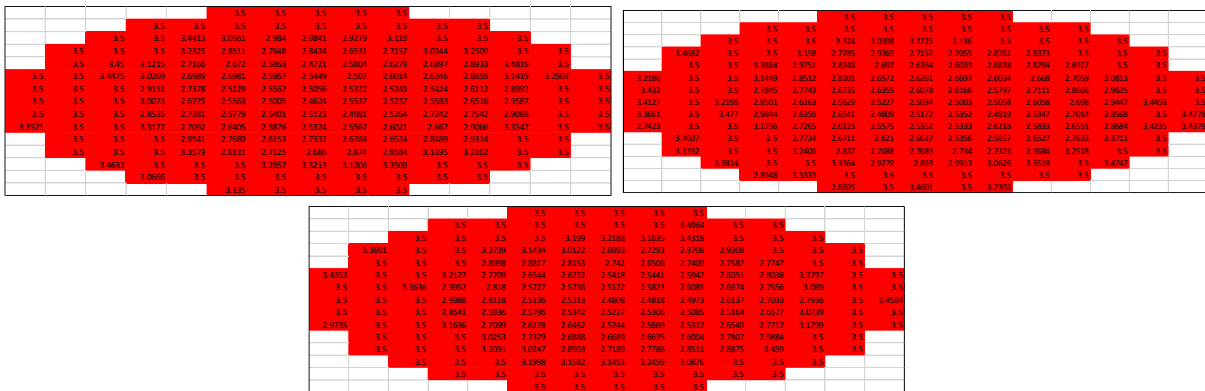


Figure S31: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.25 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

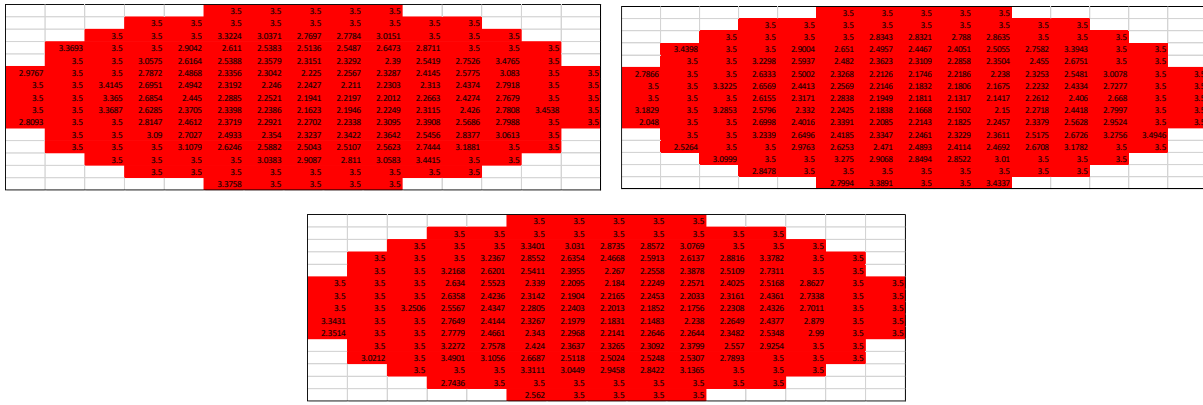


Figure S32: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.00 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

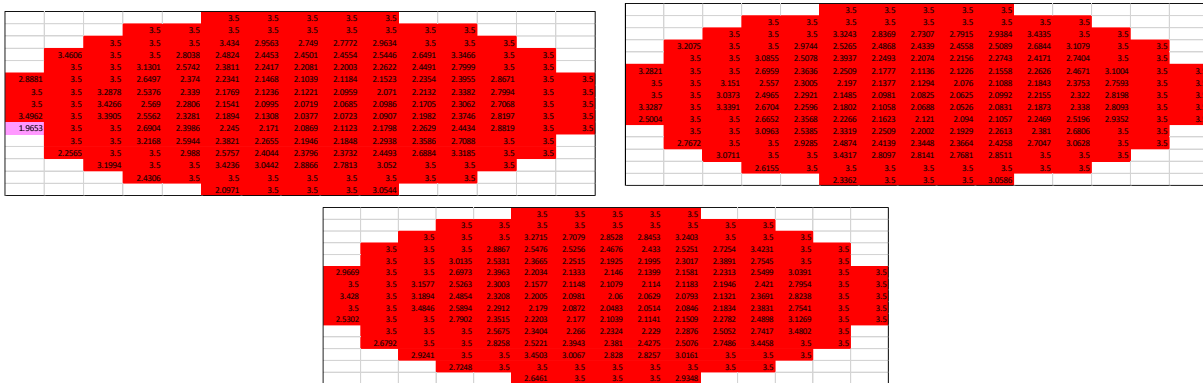


Figure S33: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.90 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



Figure S34: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.50 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

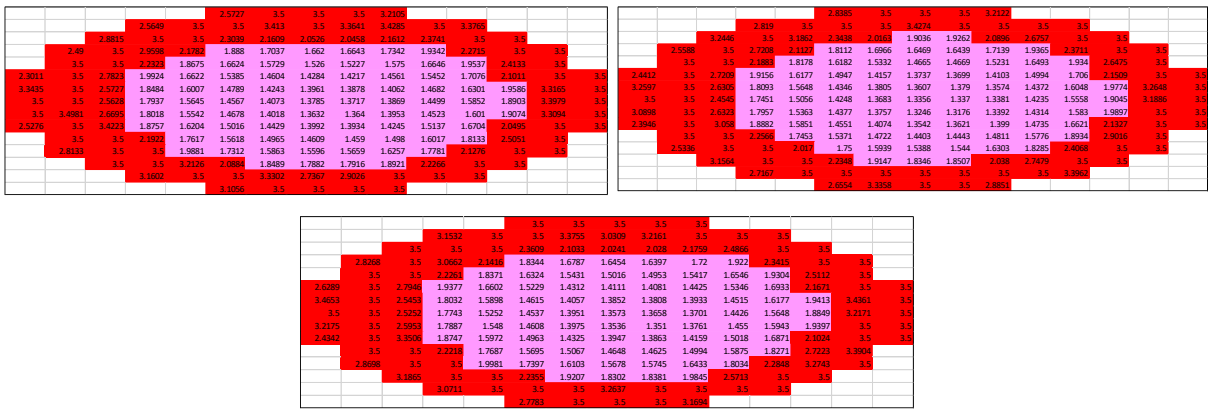


Figure S35: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.25 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



Figure S36: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.00 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

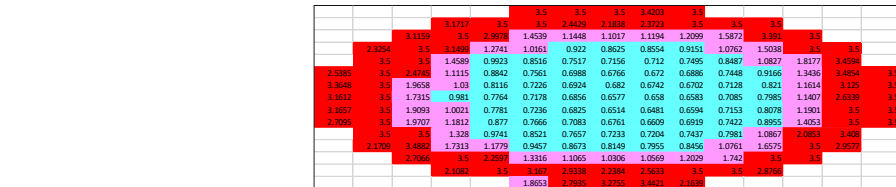
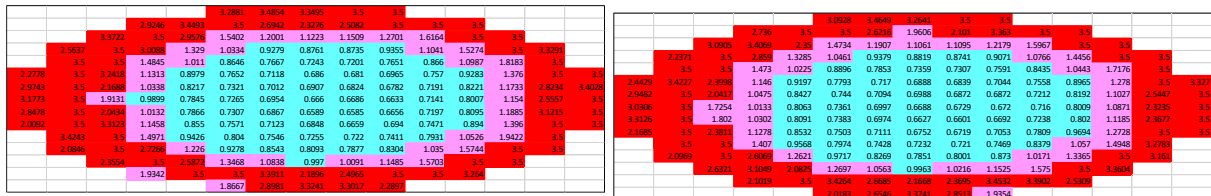


Figure S37: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.75 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

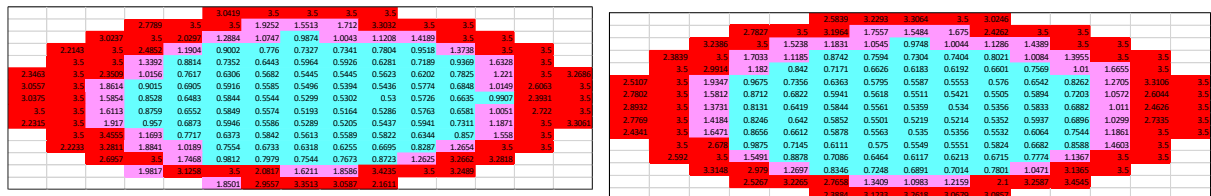


Figure S38: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.50 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

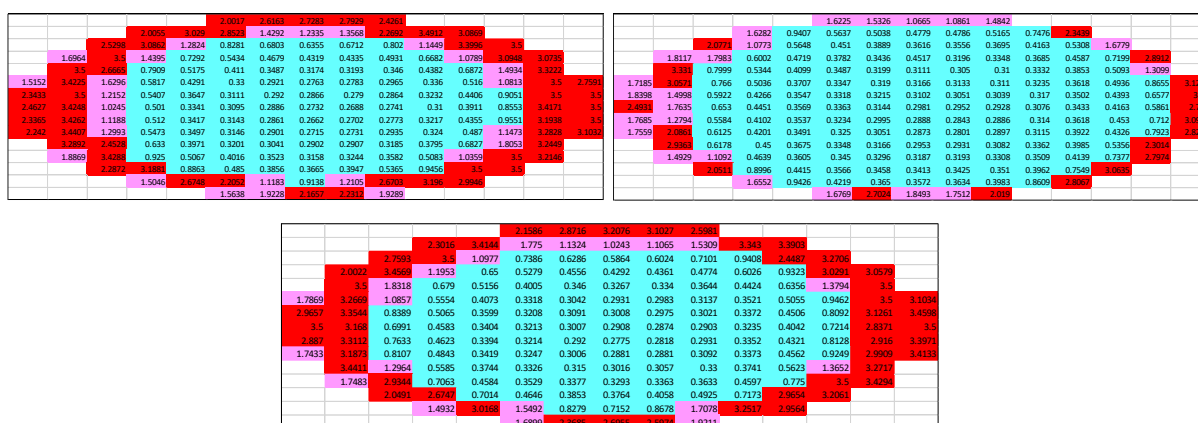


Figure S39: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.25 mM) at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



Figure S40: Raw OD₃₇₀ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 298 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

Compound 1 CMC calculation at 308 K OD₃₇₀

Table S8: A summary of OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 308 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Well sections															
Concentration (mM)	n = 1			n = 2			n = 3			Average of n's			+/- error		
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
5	3.36	3.17	3.09	3.41	3.32	3.22	3.45	3.34	3.24	3.40	3.28	3.18	0.04	0.08	0.07
4	3.43	3.17	3.15	3.47	3.26	3.24	3.46	3.19	3.20	3.45	3.21	3.20	0.02	0.04	0.04
3.5	3.32	2.90	2.79	3.34	3.04	3.01	3.34	3.10	3.02	3.33	3.01	2.94	0.01	0.08	0.11
3	3.35	3.03	2.91	3.37	3.03	2.90	3.40	3.07	2.93	3.37	3.05	2.91	0.02	0.02	0.01
2.5	3.41	2.82	2.62	3.38	2.79	2.58	3.40	2.82	2.61	3.40	2.81	2.60	0.01	0.01	0.01
2.25	3.36	2.65	2.46	3.33	2.67	2.47	3.33	2.62	2.45	3.34	2.65	2.46	0.02	0.02	0.01
2	3.27	2.37	2.15	3.25	2.35	2.12	3.31	2.39	2.15	3.28	2.37	2.14	0.02	0.02	0.01
1.9	3.24	2.29	2.06	3.26	2.30	2.05	3.30	2.32	2.07	3.27	2.31	2.06	0.02	0.01	0.01
1.5	3.10	1.84	1.62	3.10	1.86	1.63	3.11	1.81	1.58	3.10	1.84	1.61	0.01	0.02	0.02
1.25	2.98	1.57	1.36	2.99	1.54	1.32	2.98	1.56	1.35	2.98	1.56	1.34	0.00	0.01	0.01
1	2.75	1.16	0.97	2.73	1.17	0.98	2.83	1.17	0.97	2.77	1.16	0.97	0.04	0.01	0.00
0.75	2.75	0.84	0.67	2.67	0.84	0.67	2.73	0.83	0.66	2.72	0.84	0.67	0.04	0.00	0.01
0.5	2.48	0.69	0.53	2.44	0.68	0.54	2.47	0.69	0.54	2.46	0.69	0.54	0.02	0.00	0.00
0.25	2.05	0.39	0.28	1.26	0.35	0.30	1.93	0.39	0.30	1.75	0.38	0.29	0.35	0.02	0.01

Table S9: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 308 K.

Concentration (mM)	Red	Green	Ratio Red: Green
5.00	3.40	3.18	1.07
4.00	3.45	3.20	1.08
3.50	3.33	2.94	1.13
3.00	3.37	2.91	1.16
2.50	3.40	2.60	1.31
2.25	3.34	2.46	1.36
2.00	3.28	2.14	1.53
1.90	3.27	2.06	1.59
1.50	3.10	1.61	1.93
1.25	2.98	1.34	2.22
1.00	2.77	0.97	2.85
0.75	2.72	0.67	4.08
0.50	2.46	0.54	4.60
0.25	1.75	0.29	5.96

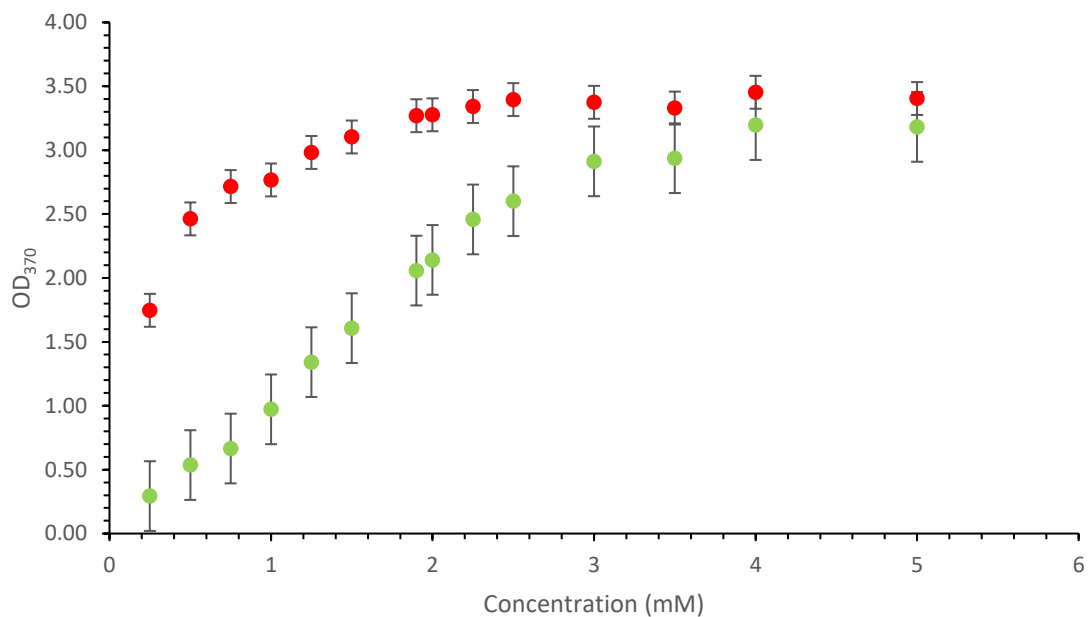


Figure S41: Graph showing average (n=3) red - interface and green - control OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 308 K.

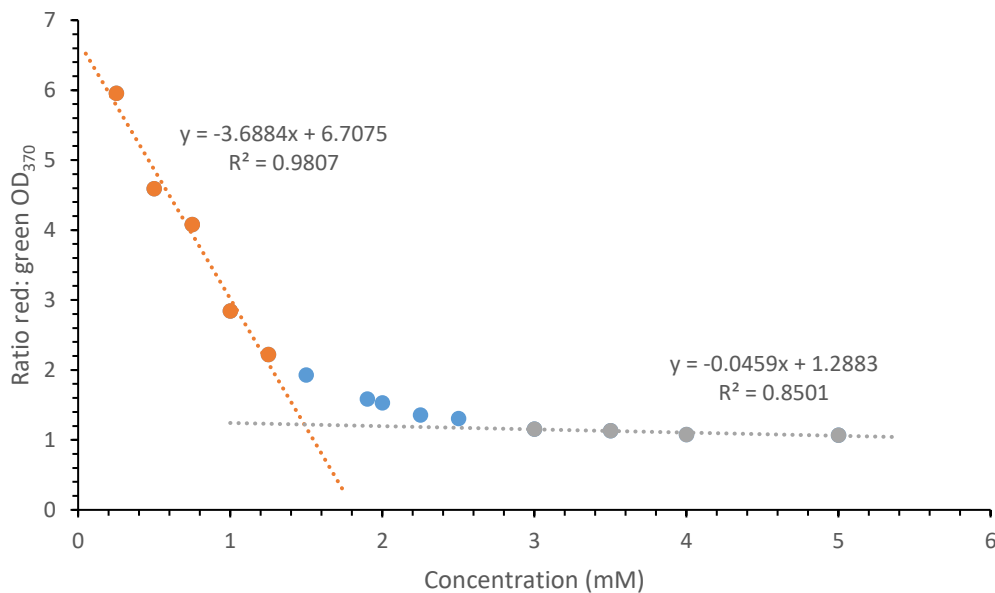


Figure S42: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 308 K, plotted against compound concentration. A CMC value of 1.49 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 1 at 308 K OD₃₇₀

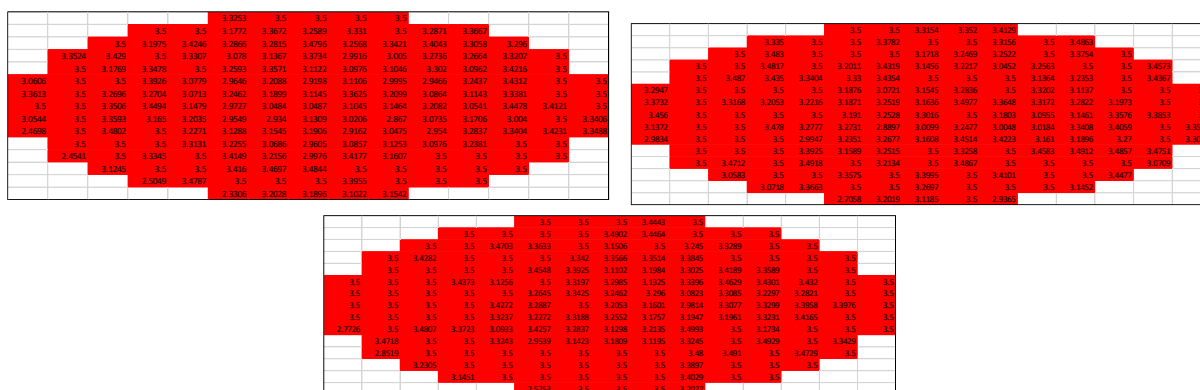


Figure S43: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (5.00 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

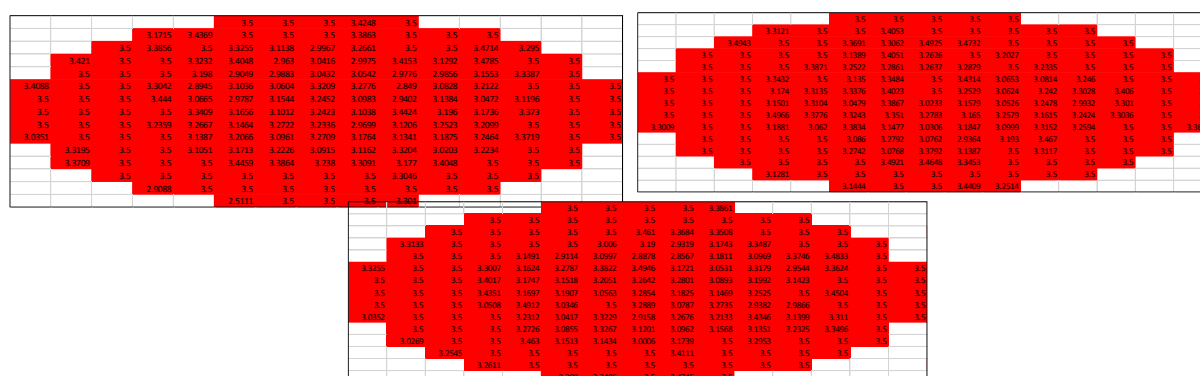


Figure S44: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (4.00 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

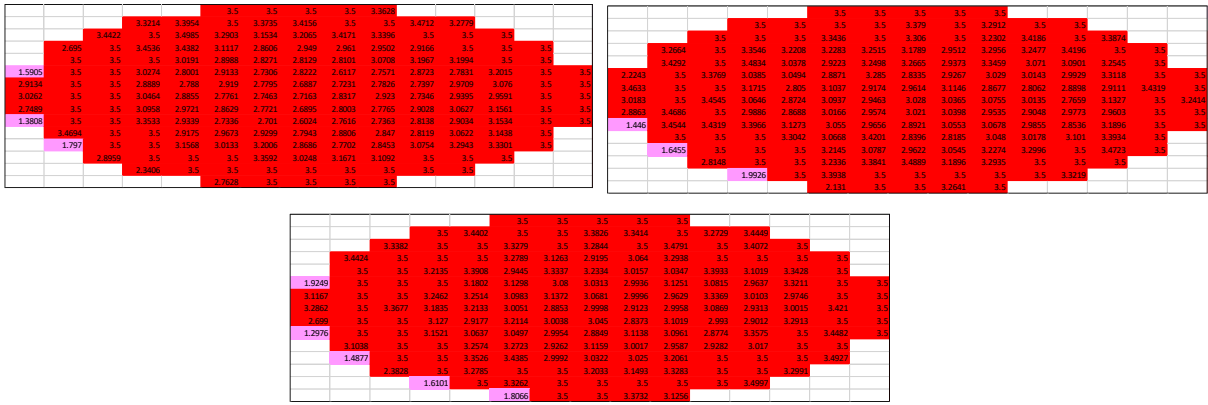


Figure S45: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (3.50 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

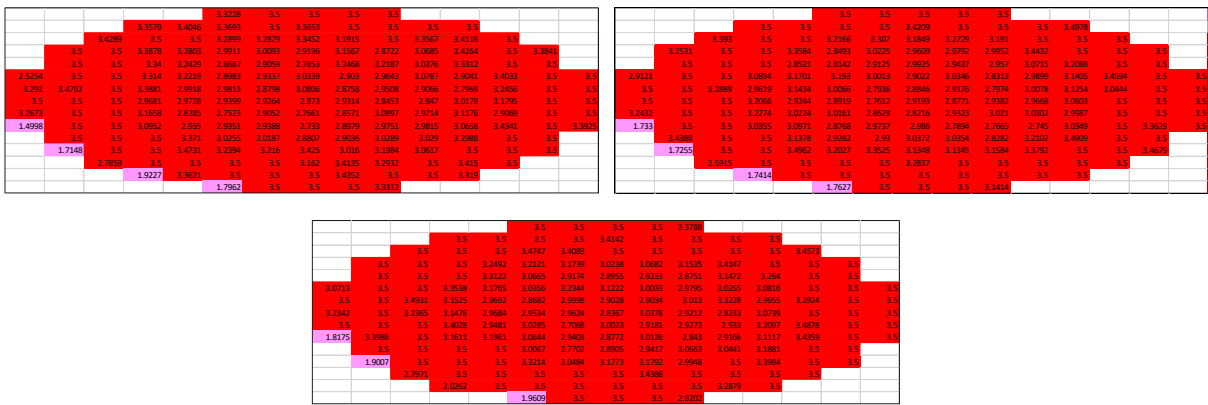


Figure S46: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (3.00 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

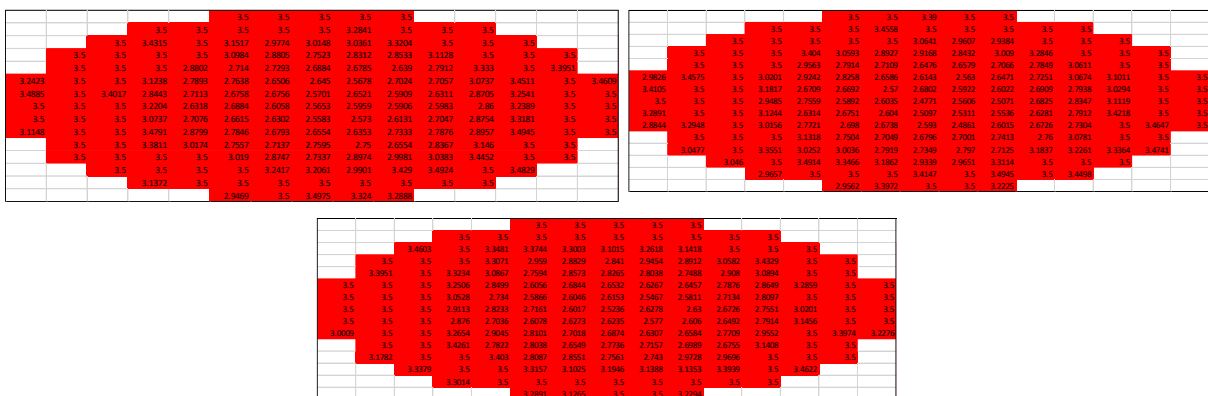


Figure S47: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.50 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

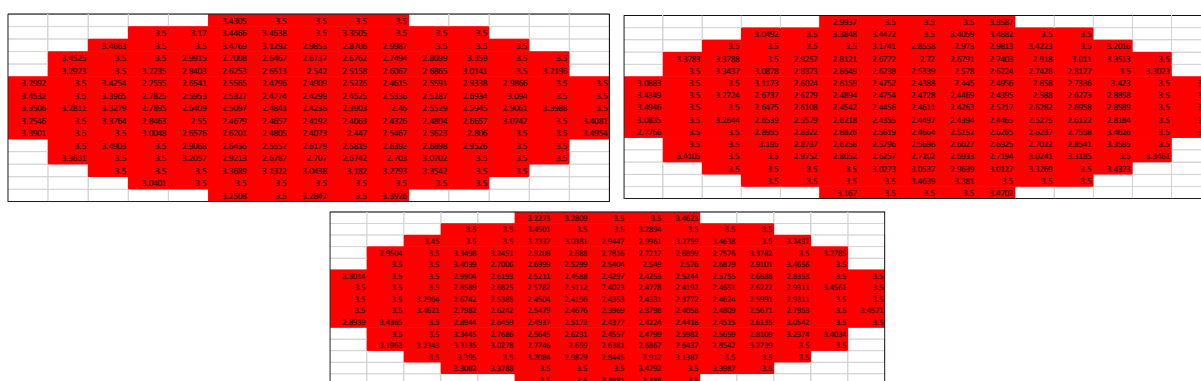


Figure S48: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.25 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

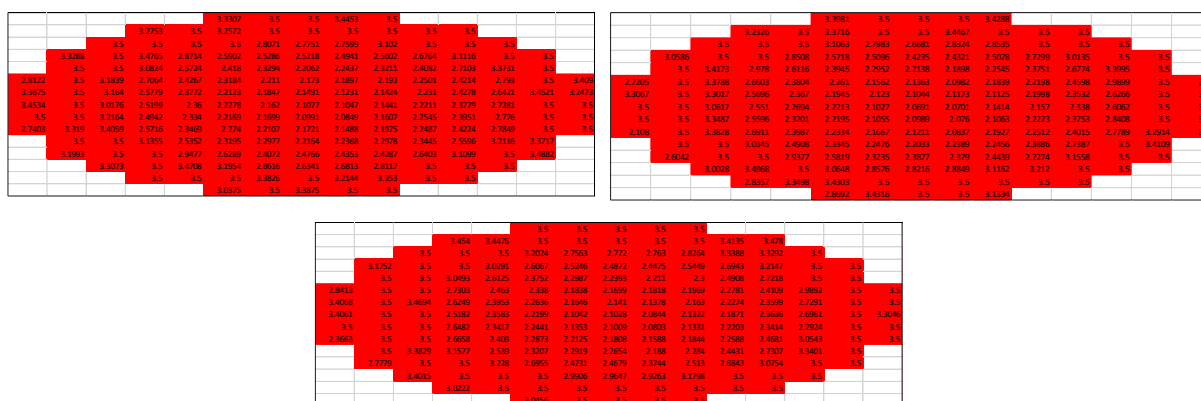


Figure S49: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.00 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

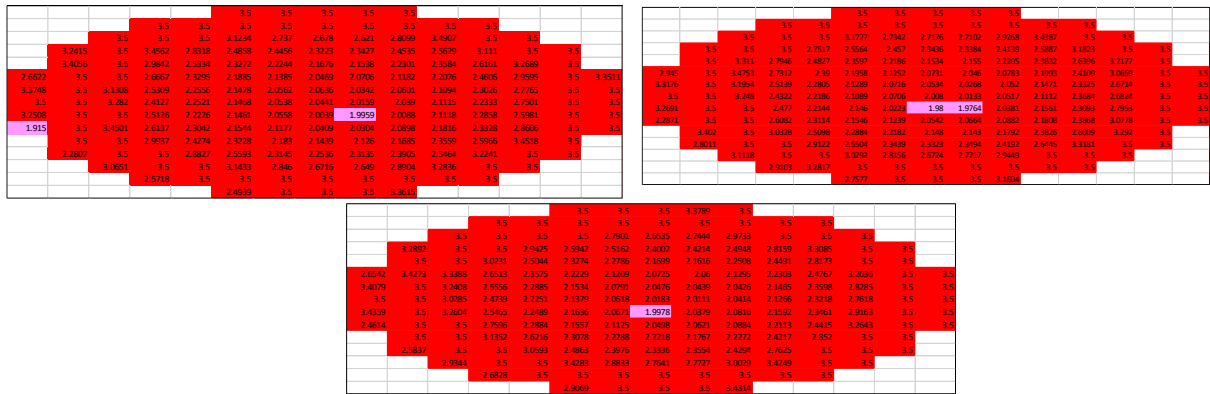


Figure S50: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.90 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

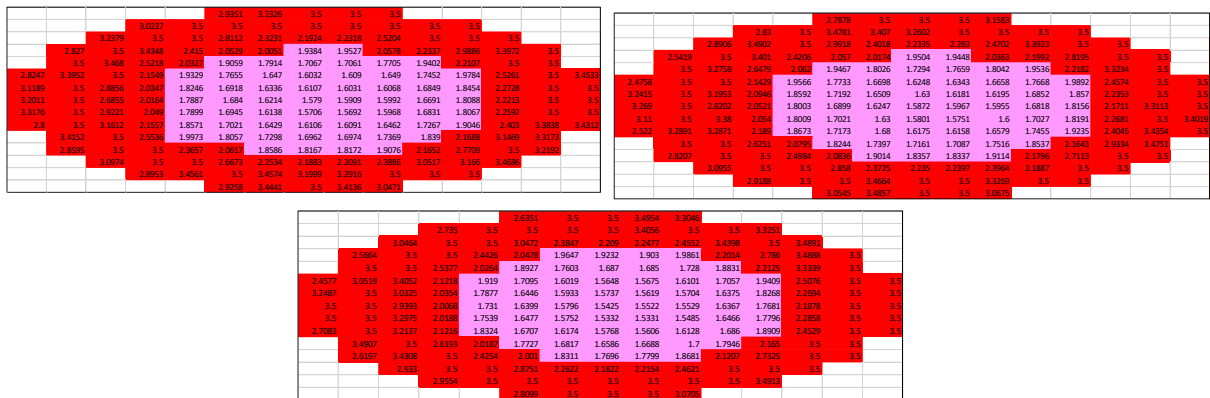


Figure S51: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.50 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

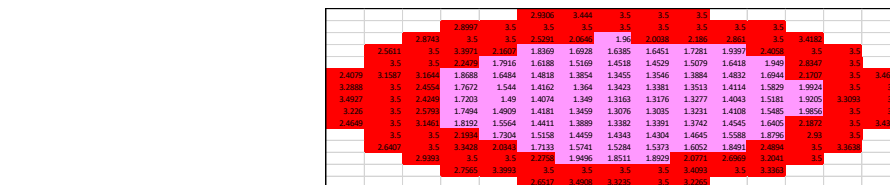
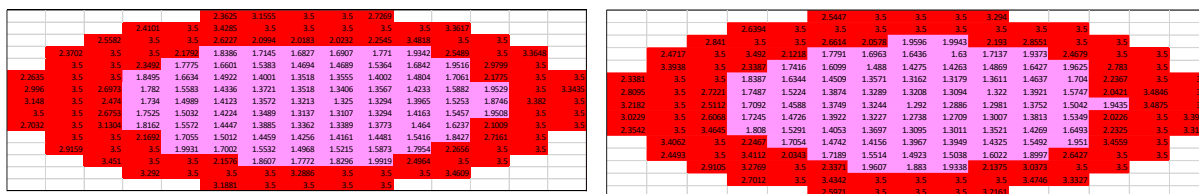


Figure S52: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.25 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

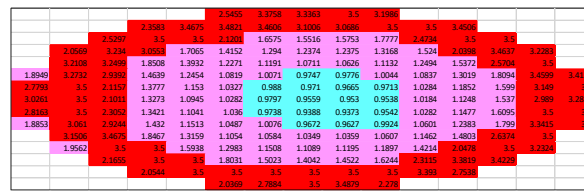


Figure S53: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.00 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

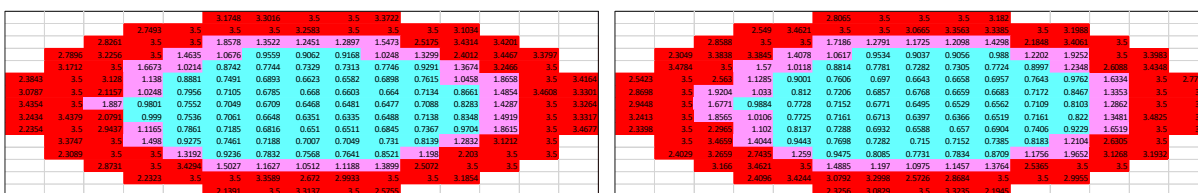


Figure S54: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.75 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



Figure S55: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.50 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

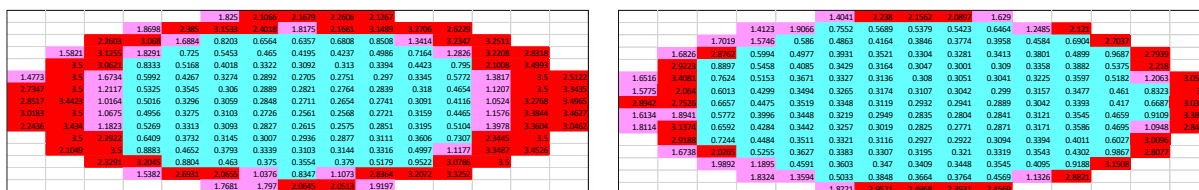


Figure S56: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.25 mM) at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

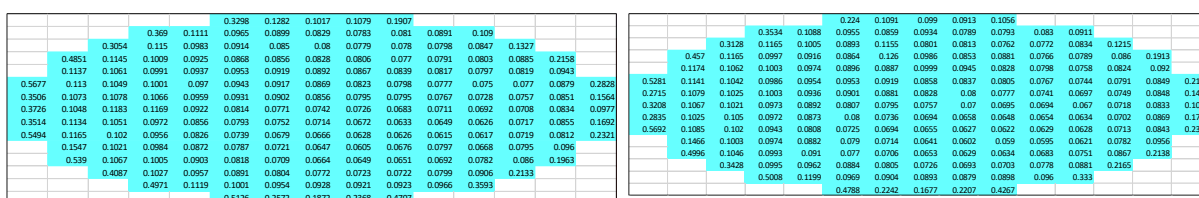
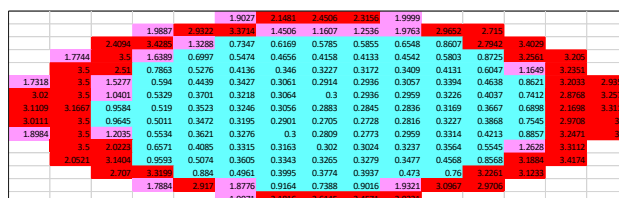
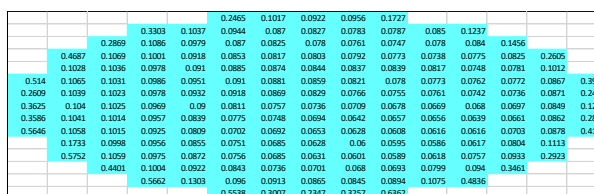


Figure S57: Raw OD₃₇₀ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 308 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



Compound 1 CMC calculation at 318 K OD₃₇₀

Table S11: A summary of OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 318 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections												+/- error		
	n = 1			n = 2			n = 3			Average of n's					
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
5.00	3.44	3.37	3.23	3.47	3.44	3.37	3.47	3.44	3.36	3.46	3.42	3.32	0.01	0.03	0.06
4.00	3.46	3.27	3.01	3.49	3.37	3.18	3.49	3.31	3.02	3.48	3.32	3.07	0.01	0.04	0.08
3.50	3.17	1.87	1.62	3.42	3.20	2.91	3.40	3.19	2.93	3.33	2.75	2.49	0.11	0.62	0.61
3.00	3.40	3.05	2.70	3.39	3.07	2.72	3.41	3.06	2.59	3.40	3.06	2.67	0.01	0.01	0.06
2.50	3.48	2.87	2.44	3.46	2.90	2.49	3.47	2.92	2.54	3.47	2.90	2.49	0.01	0.02	0.04
2.25	3.47	2.77	2.41	3.46	2.81	2.48	3.48	2.75	2.43	3.47	2.78	2.44	0.01	0.03	0.03
2.00	3.44	2.51	2.18	3.38	2.47	2.11	3.39	2.46	2.13	3.40	2.48	2.14	0.03	0.02	0.03
1.90	3.37	2.43	2.08	3.38	2.43	2.06	3.41	2.51	2.08	3.39	2.45	2.08	0.02	0.04	0.01
1.50	3.41	2.05	1.66	3.37	2.05	1.68	3.37	2.00	1.62	3.38	2.03	1.65	0.02	0.02	0.02
1.25	3.27	1.71	1.38	3.30	1.71	1.34	3.30	1.71	1.37	3.29	1.71	1.37	0.01	0.00	0.02
1.00	3.13	1.29	0.97	3.14	1.30	0.99	3.31	1.40	0.98	3.19	1.33	0.98	0.08	0.05	0.00
0.75	3.29	1.09	0.66	3.22	1.05	0.67	3.24	1.09	0.65	3.25	1.08	0.66	0.03	0.02	0.01
0.50	3.04	0.85	0.53	3.01	0.83	0.53	3.04	0.86	0.53	3.03	0.84	0.53	0.01	0.01	0.00
0.25	2.46	0.56	0.28	2.05	0.41	0.30	2.36	0.50	0.29	2.29	0.49	0.29	0.17	0.06	0.01

Table S12: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 318 K.

Concentration (mM)	Red	Green	Ratio Red: Green
5.00	3.46	3.32	1.04
4.00	3.48	3.07	1.13
3.50	3.41	2.92	1.17
3.00	3.40	2.67	1.27
2.50	3.47	2.49	1.39
2.25	3.47	2.44	1.42
2.00	3.40	2.14	1.59
1.90	3.39	2.08	1.63
1.50	3.38	1.65	2.05
1.25	3.29	1.37	2.41
1.00	3.19	0.98	3.26
0.75	3.25	0.66	4.94
0.50	3.03	0.53	5.71
0.25	2.29	0.29	7.89

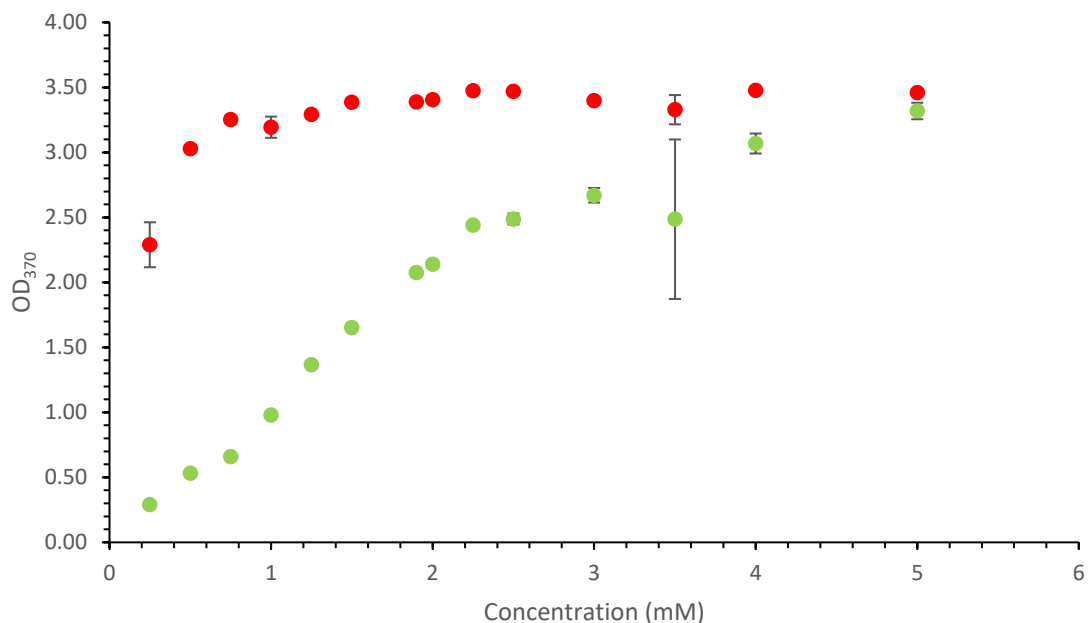


Figure S58: Graph showing average (n=3) red - interface and green - control OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 318 K.

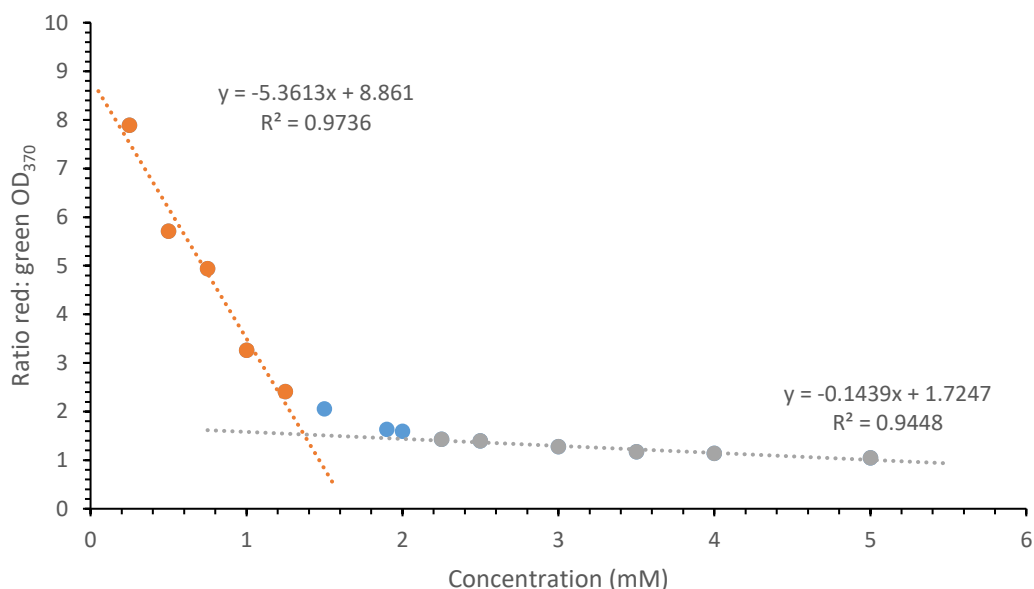


Figure S59: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₇₀ well scan data obtained for **1** in an EtOH/H₂O 1:19 solution at 318 K, plotted against compound concentration. A CMC value of 1.37 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 1 at 318 K OD₃₇₀

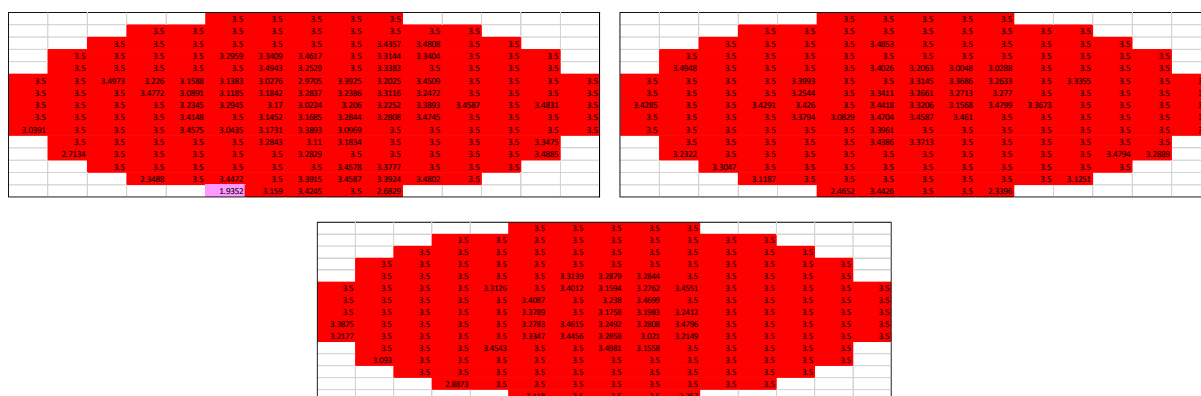


Figure S60: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (5.00 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

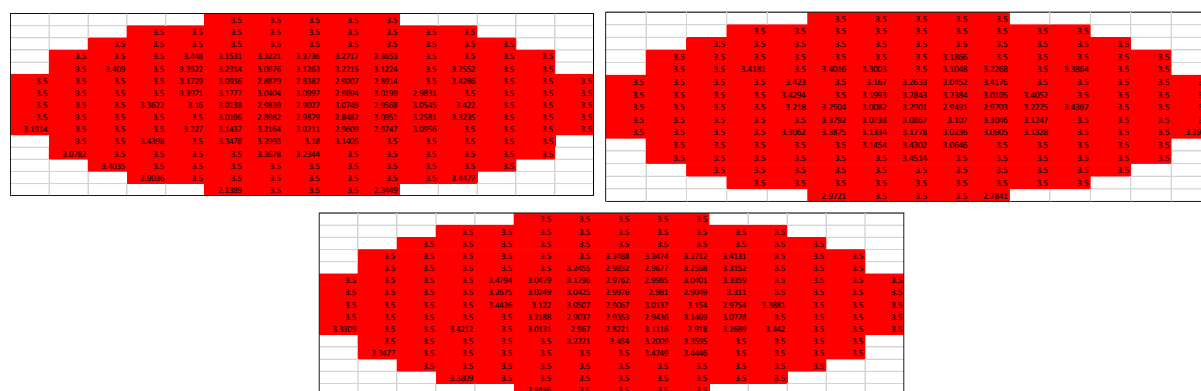


Figure S61: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 1 (4.00 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

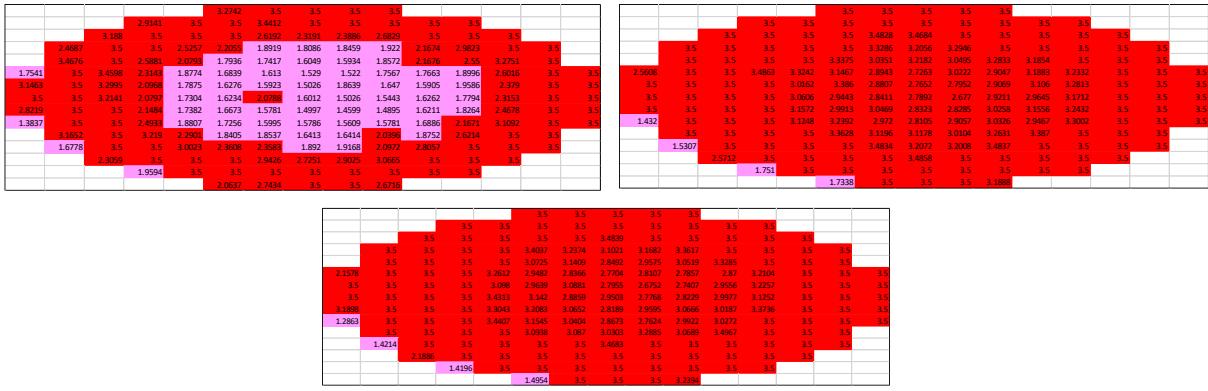


Figure S62: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (3.50 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

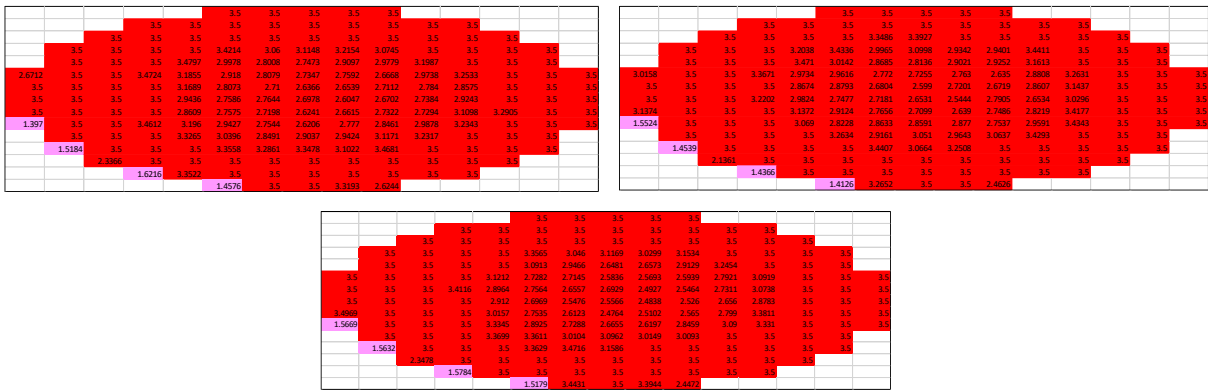


Figure S63: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (3.00 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

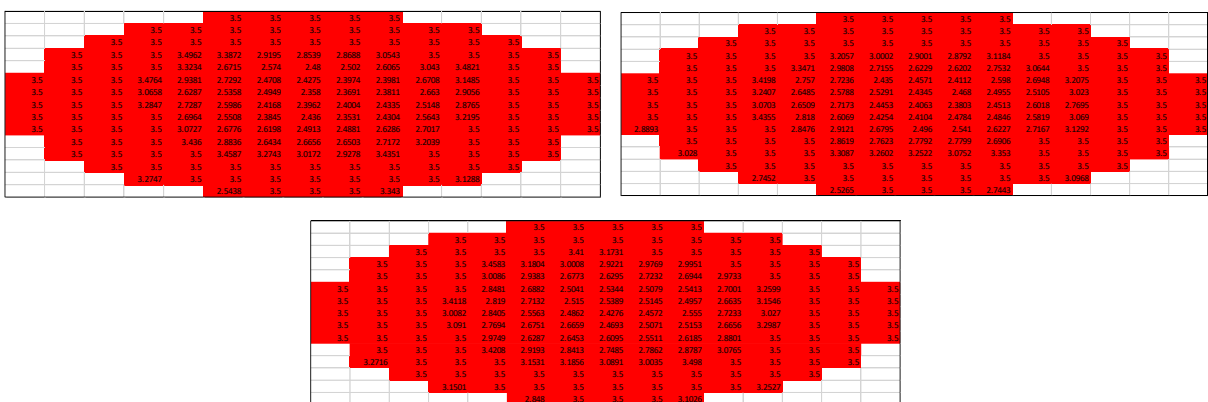


Figure S64: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.50 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

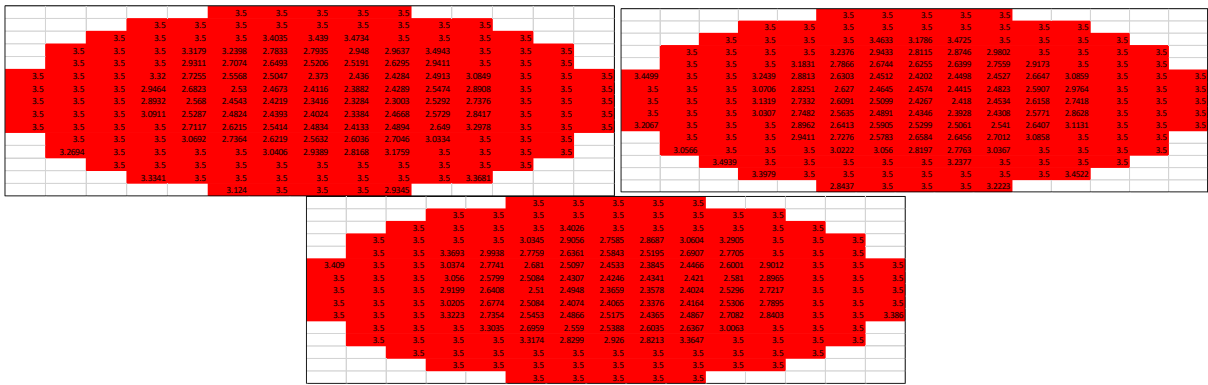


Figure S65: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.25 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

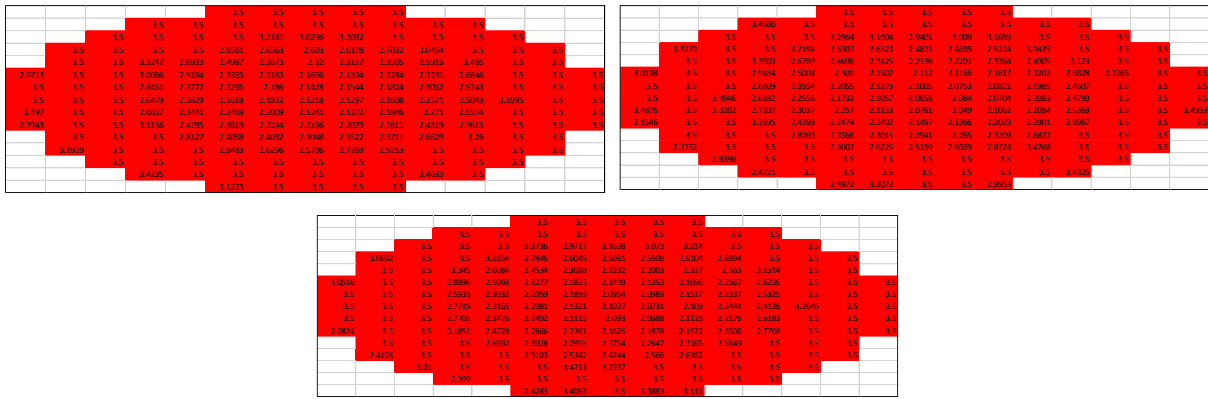


Figure S66: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (2.00 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

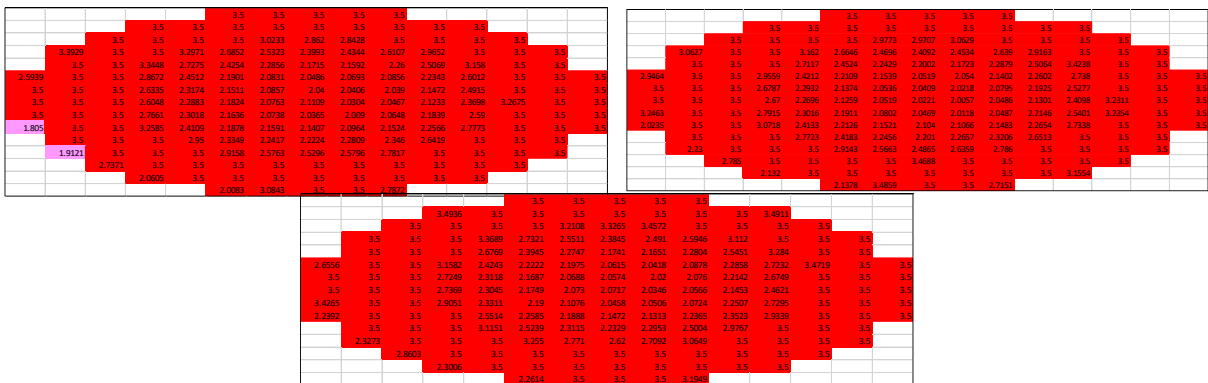


Figure S67: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.90 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

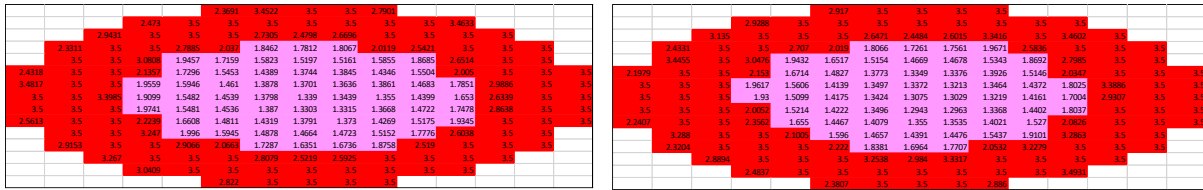


Figure S68: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.50 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

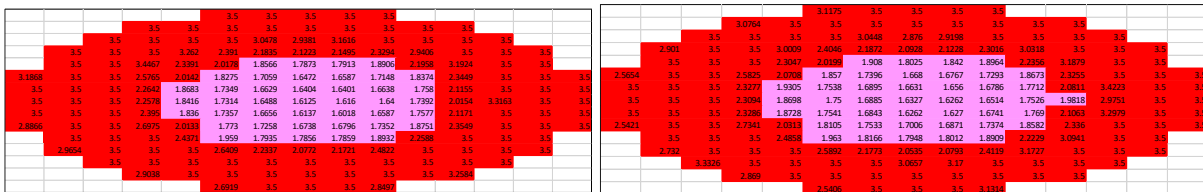
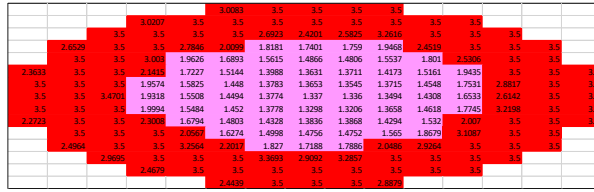


Figure S69: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.25 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

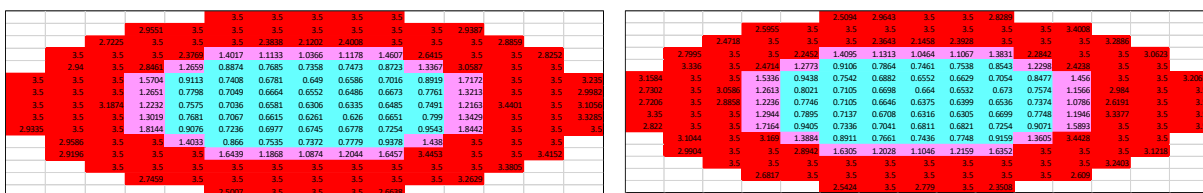
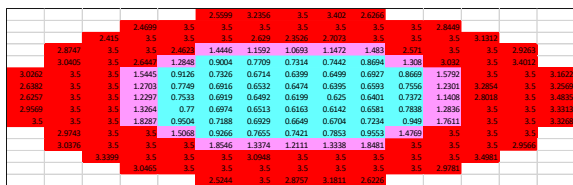


Figure S70: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (1.00 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.



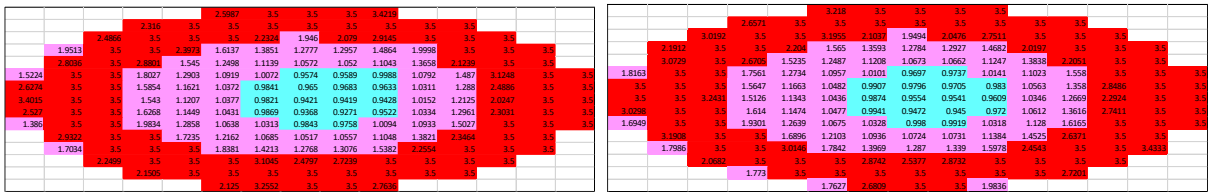


Figure S71: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.75 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

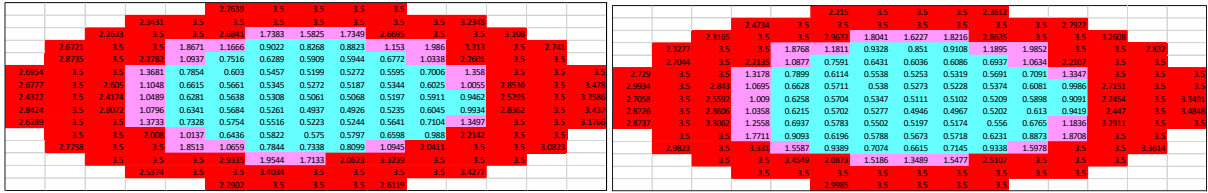


Figure S72: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.50 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

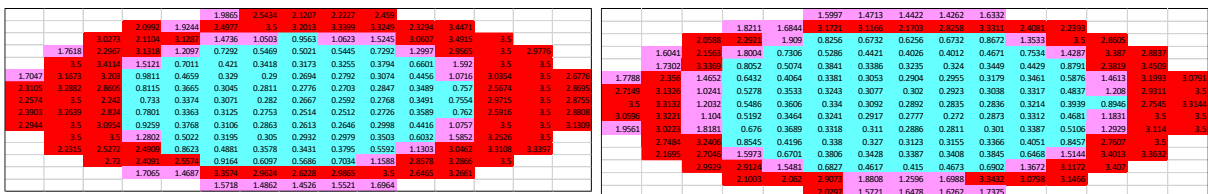


Figure S73: Raw OD₃₇₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **1** (0.25 mM) at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

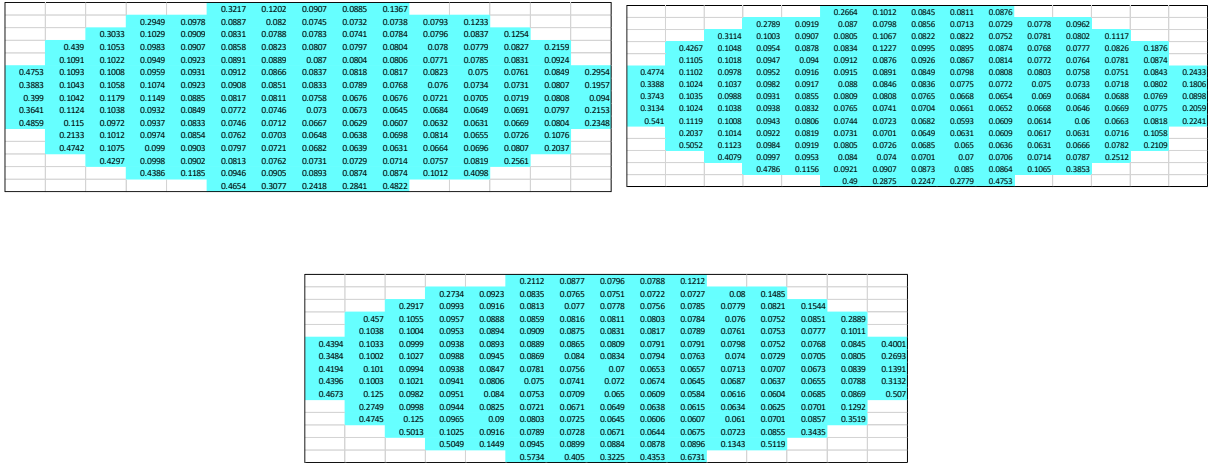


Figure S74: Raw OD₃₇₀ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 318 K. Colour coded regions: Red = OD₃₇₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₇₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₇₀ ≥ 0.0001.

Compound 2 CMC calculation at 298 K OD₃₆₀

Table S12: A summary of OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 298 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections									Average of n's			+/- error		
	n = 1			n = 2			n = 3			Red	Yellow	Green	Red	Yellow	Green
4.50	3.43	3.50	3.49	3.45	3.50	3.50	3.43	3.50	3.50	3.44	3.50	3.50	0.01	0.00	0.00
4.00	3.41	3.50	3.50	3.35	3.50	3.50	3.38	3.50	3.50	3.38	3.50	3.50	0.02	0.00	0.00
3.00	3.38	3.50	3.50	3.34	3.50	3.50	3.41	3.50	3.50	3.38	3.50	3.50	0.03	0.00	0.00
2.00	3.39	3.50	3.50	3.41	3.50	3.50	3.41	3.50	3.50	3.40	3.50	3.50	0.01	0.00	0.00
1.00	3.32	2.27	2.03	3.41	2.68	2.46	3.42	2.70	2.45	3.38	2.55	2.32	0.04	0.20	0.20
0.90	3.35	2.43	2.21	3.30	2.46	2.23	3.23	2.38	2.14	3.29	2.42	2.19	0.05	0.03	0.04
0.70	3.06	1.90	1.70	3.21	1.96	1.74	3.22	1.97	1.74	3.16	1.94	1.73	0.07	0.03	0.02
0.60	3.17	1.71	1.49	3.07	1.72	1.52	3.08	1.71	1.51	3.11	1.71	1.51	0.04	0.01	0.01
0.50	3.01	1.54	1.35	2.92	1.46	1.28	2.93	1.53	1.36	2.95	1.51	1.33	0.04	0.04	0.03
0.40	2.73	1.24	1.08	2.71	1.24	1.08	2.80	1.26	1.08	2.75	1.25	1.08	0.04	0.01	0.00
0.30	2.73	1.11	0.95	2.59	1.11	0.96	2.63	1.05	0.93	2.65	1.09	0.95	0.06	0.03	0.01
0.20	2.45	0.76	0.62	2.35	0.72	0.61	2.44	0.75	0.63	2.41	0.75	0.62	0.04	0.02	0.01
0.10	2.03	0.44	0.35	2.13	0.44	0.35	1.92	0.42	0.34	2.03	0.43	0.35	0.09	0.01	0.01

Table S13: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Red	Green	Ratio Red: Green
4.50	3.44	3.50	0.98
4.00	3.38	3.50	0.97
3.00	3.38	3.50	0.97
2.00	3.40	3.50	0.97
1.00	3.38	2.32	1.46
0.90	3.29	2.19	1.50
0.70	3.16	1.73	1.83
0.60	3.11	1.51	2.06
0.50	2.95	1.33	2.22
0.40	2.75	1.08	2.55
0.30	2.65	0.95	2.80
0.20	2.41	0.62	3.91
0.10	2.03	0.35	5.80

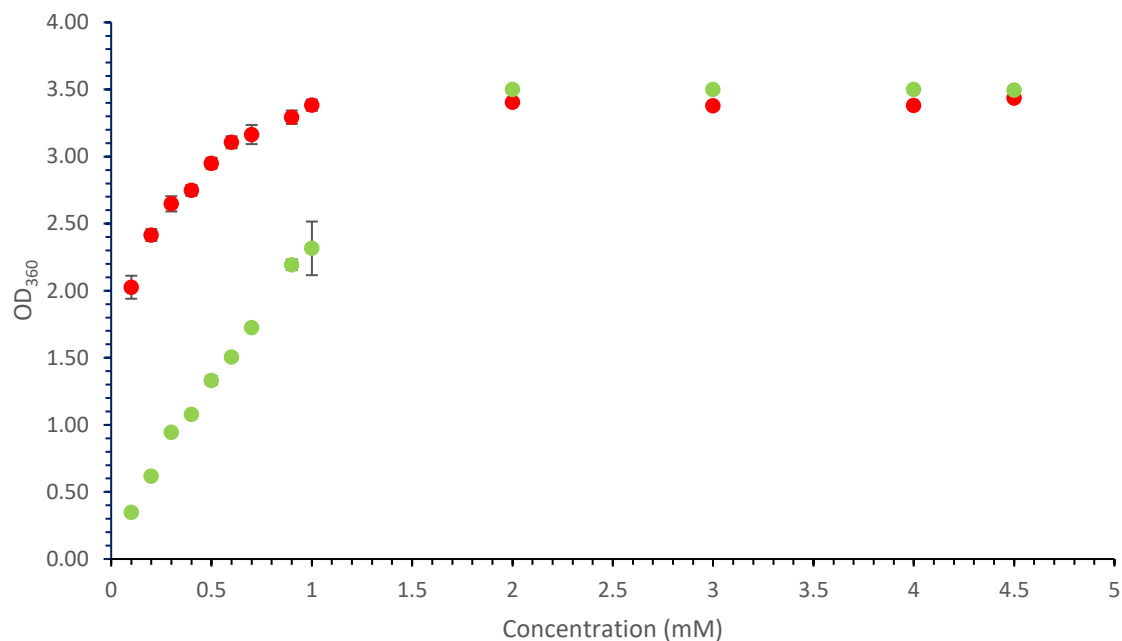


Figure S75: Graph showing average (n=3) red - interface and green - control OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 298 K.

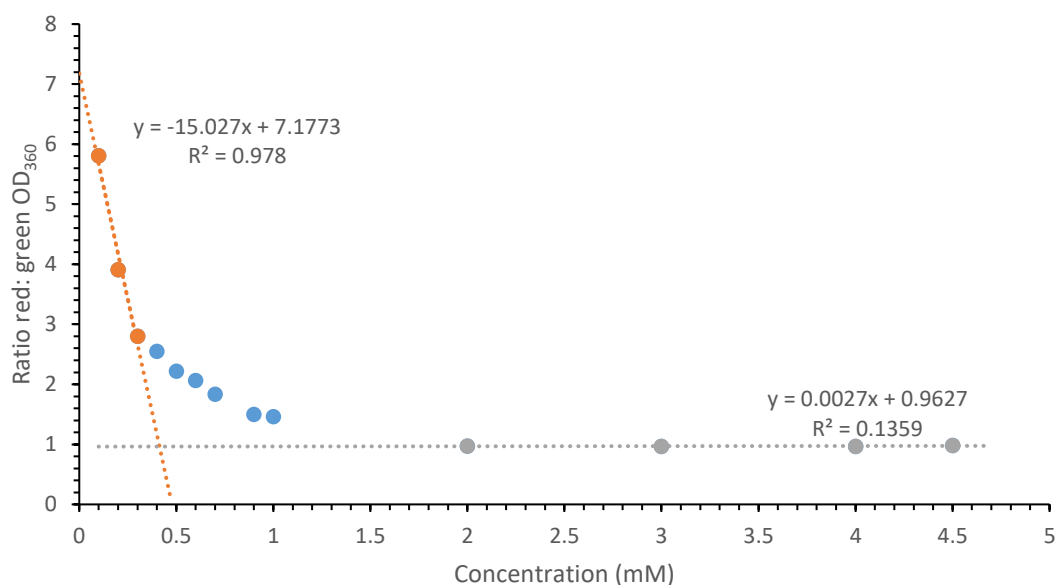


Figure S76: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 298 K, plotted against compound concentration. A CMC value of 0.41 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 2 at 298 K OD₃₆₀

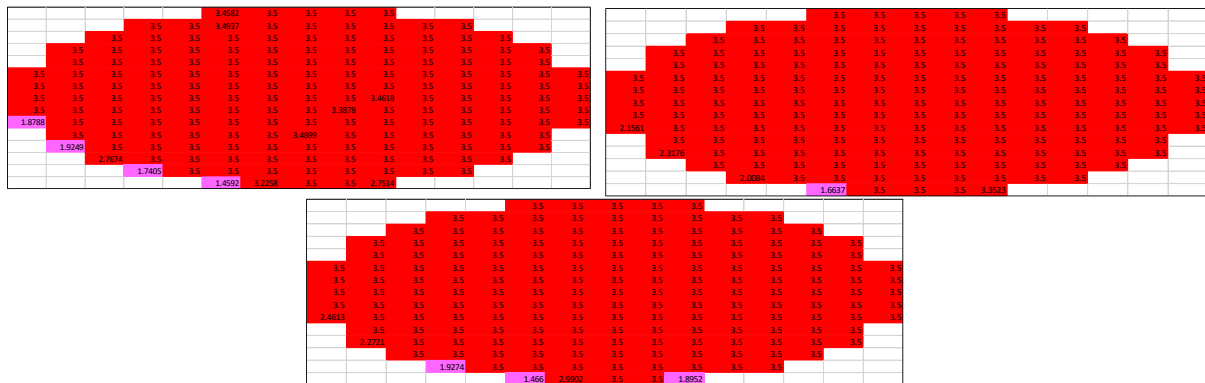


Figure S77: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (4.50 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

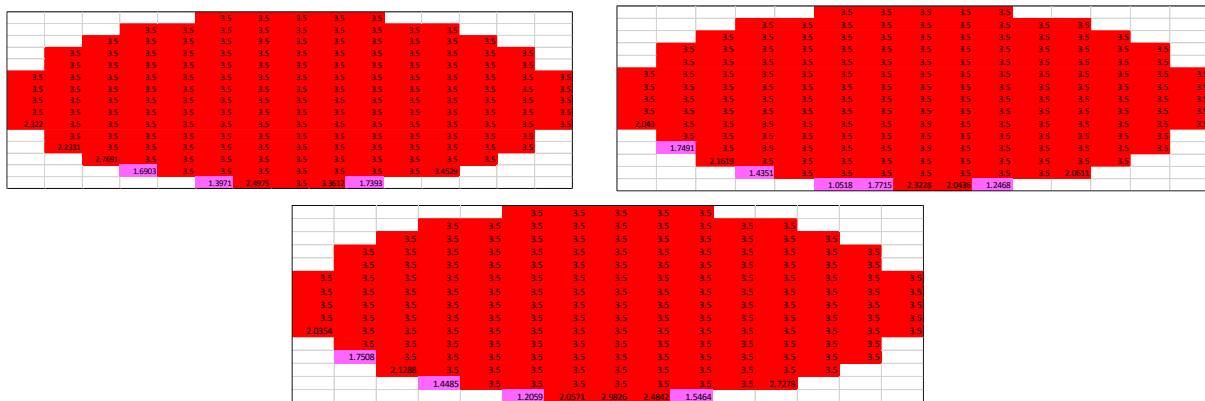


Figure S78: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (4.00 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

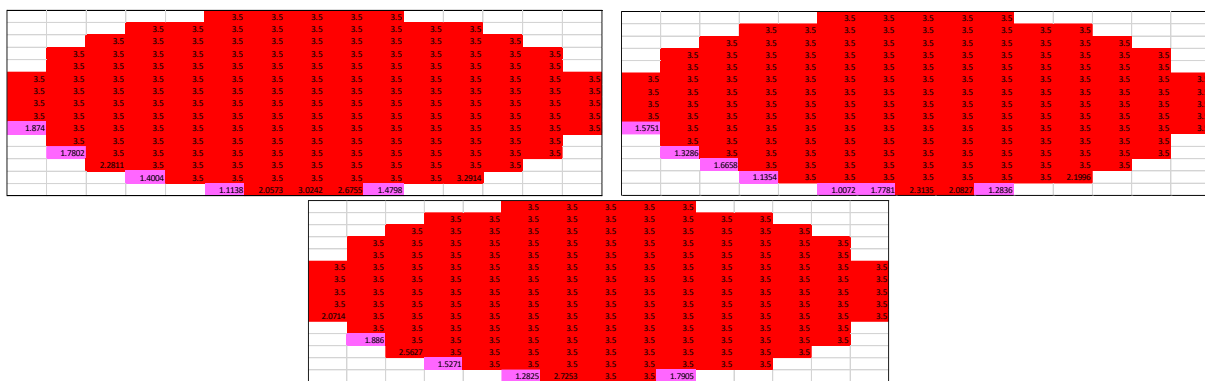


Figure S79: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (3.00 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

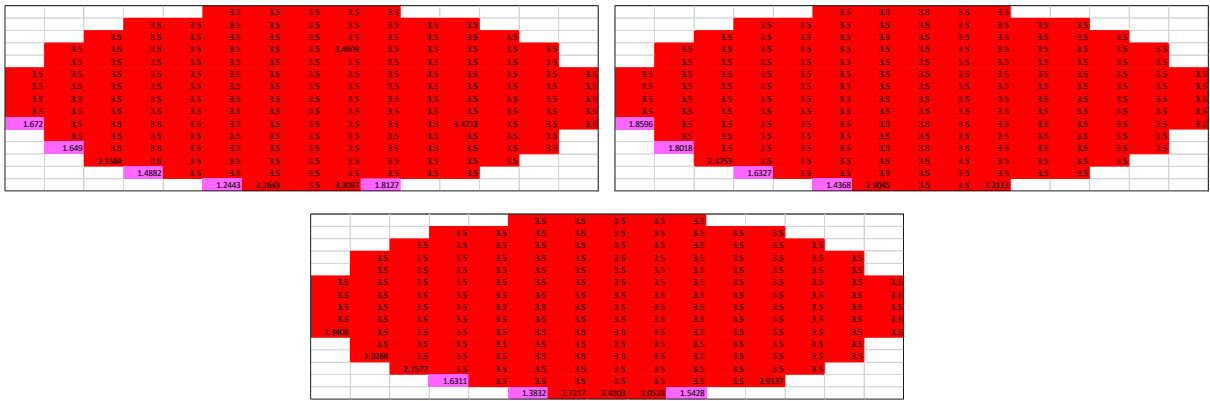


Figure S80: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (2.00 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

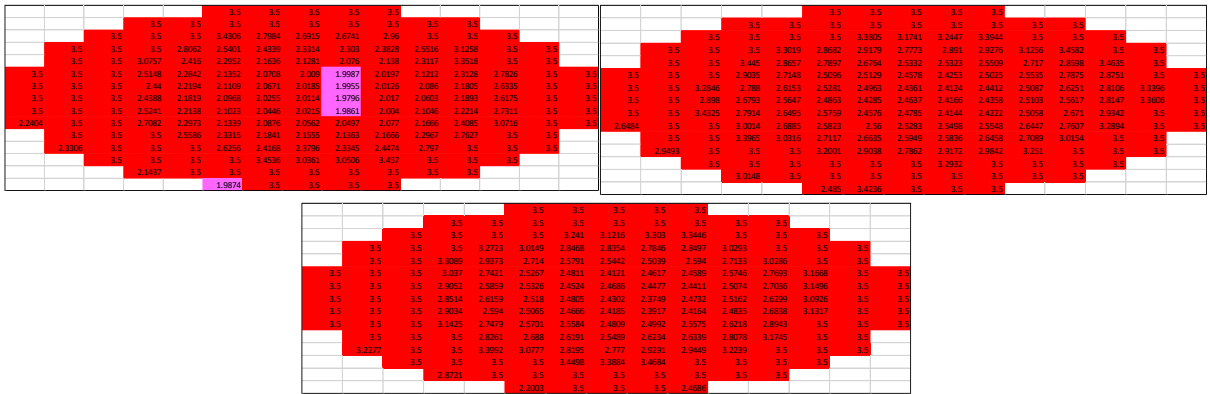


Figure S81: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (1.00 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

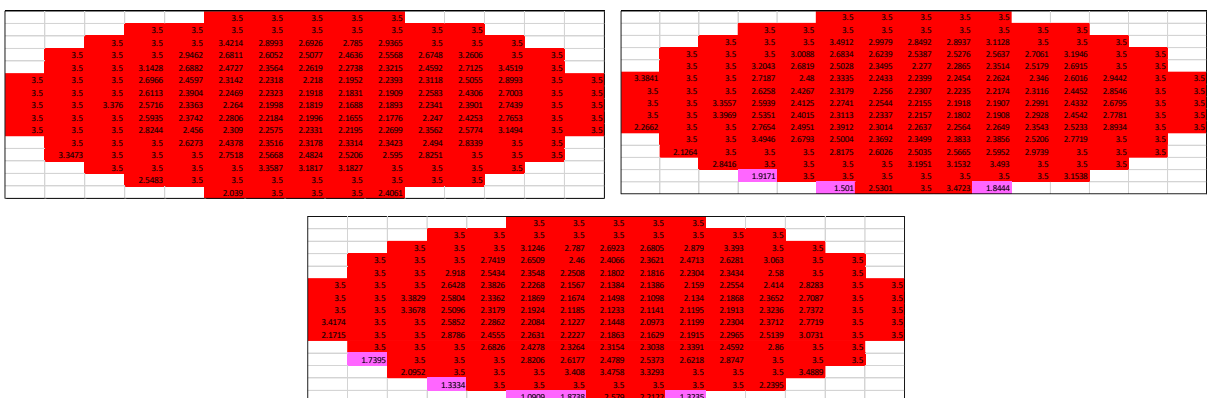


Figure S82: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.90 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

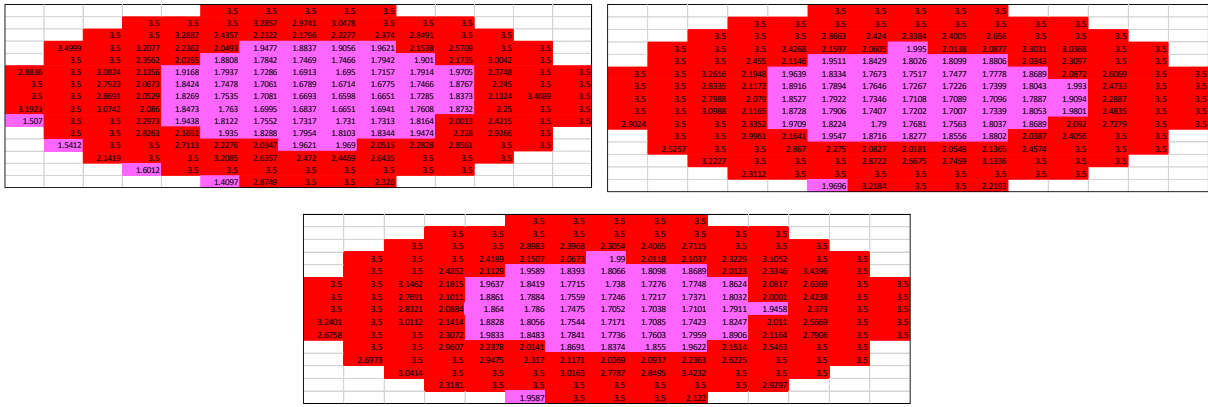


Figure S83: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (0.70 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

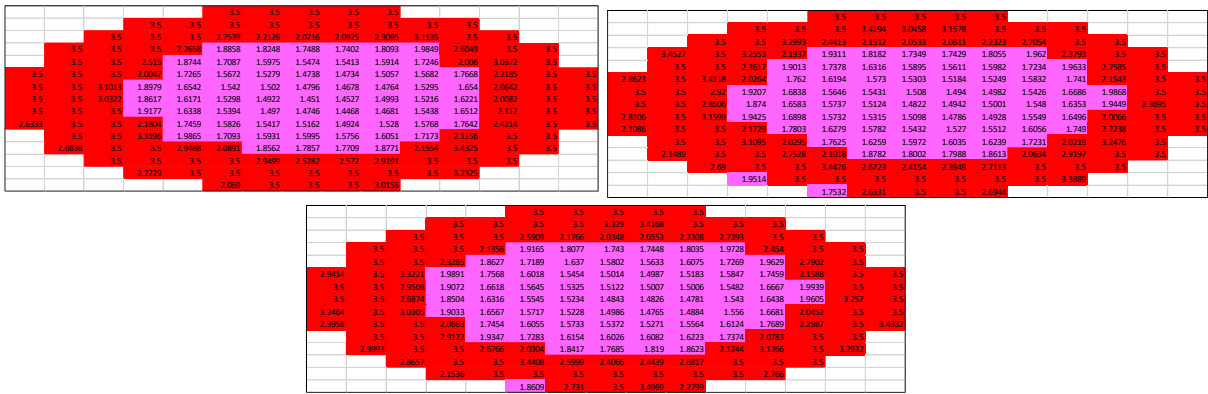


Figure S84: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (0.60 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

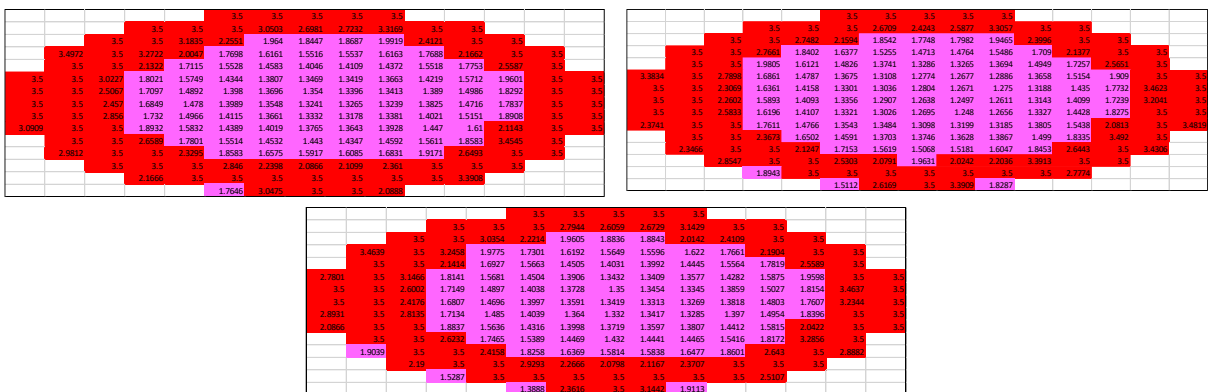


Figure S85: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of 2 (0.50 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S86: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.40 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S87: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.30 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S88: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.20 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

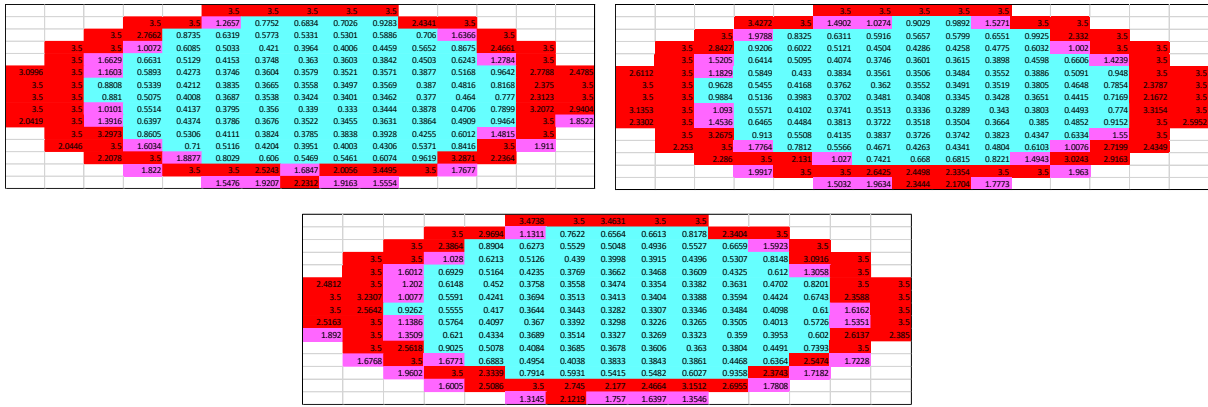


Figure S89: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.10 mM) at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

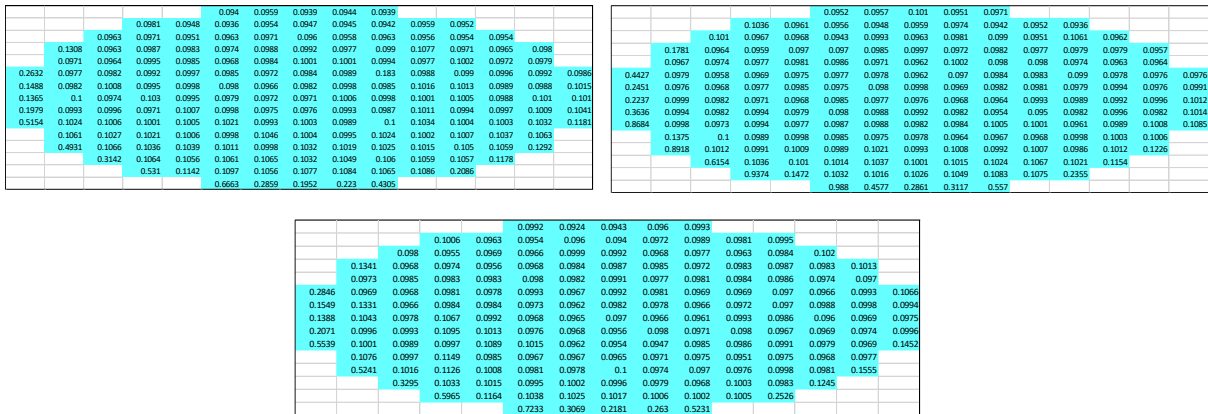


Figure S90: Raw OD₃₆₀ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 298 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

Compound 2 CMC calculation at 308 K OD₃₆₀

Table S14: A summary of OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 308 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections									Average of n's			+/- error		
	n = 1			n = 2			n = 3			Red	Yellow	Green	Red	Yellow	Green
4.50	3.29	3.29	3.33	3.35	3.31	3.30	3.35	3.32	3.35	3.33	3.31	3.33	0.03	0.01	0.02
4.00	3.35	3.31	3.35	3.27	3.33	3.30	3.33	3.36	3.36	3.32	3.34	3.34	0.03	0.02	0.03
3.00	3.35	3.36	3.30	3.31	3.31	3.33	3.36	3.34	3.32	3.34	3.34	3.31	0.02	0.02	0.01
2.00	3.33	3.27	3.24	3.35	3.33	3.29	3.34	3.25	3.25	3.34	3.29	3.26	0.01	0.04	0.02
1.00	3.26	2.19	1.93	3.29	2.50	2.31	3.33	2.54	2.32	3.29	2.41	2.18	0.03	0.16	0.18
0.90	3.24	2.31	2.10	3.21	2.33	2.13	3.14	2.26	2.04	3.20	2.30	2.09	0.04	0.03	0.04
0.70	3.06	1.86	1.63	3.14	1.91	1.67	3.17	1.93	1.68	3.13	1.90	1.66	0.05	0.03	0.02
0.60	3.19	1.70	1.43	3.06	1.71	1.46	3.06	1.69	1.46	3.10	1.70	1.45	0.06	0.01	0.01
0.50	3.04	1.53	1.31	2.97	1.45	1.24	2.96	1.52	1.30	2.99	1.50	1.28	0.03	0.03	0.03
0.40	2.86	1.25	1.04	2.80	1.25	1.04	2.84	1.27	1.04	2.83	1.26	1.04	0.02	0.01	0.00
0.30	2.69	1.11	0.92	2.49	1.08	0.94	2.74	1.11	0.90	2.64	1.10	0.92	0.11	0.02	0.02
0.20	2.56	0.79	0.60	2.35	0.74	0.59	2.42	0.76	0.61	2.45	0.76	0.60	0.09	0.02	0.01
0.10	1.74	0.45	0.35	1.83	0.45	0.35	1.77	0.44	0.34	1.78	0.45	0.35	0.04	0.00	0.00

Table S15: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 308 K.

Concentration (mM)	Well sections		Ratio Red: Green
	Red	Green	
4.50	3.33	3.33	1.00
4.00	3.32	3.34	0.99
3.00	3.34	3.31	1.01
2.00	3.34	3.26	1.02
1.00	3.29	2.18	1.51
0.90	3.20	2.09	1.53
0.70	3.13	1.66	1.88
0.60	3.10	1.45	2.14
0.50	2.99	1.28	2.33
0.40	2.83	1.04	2.72
0.30	2.64	0.92	2.87
0.20	2.45	0.60	4.07
0.10	1.78	0.35	5.13

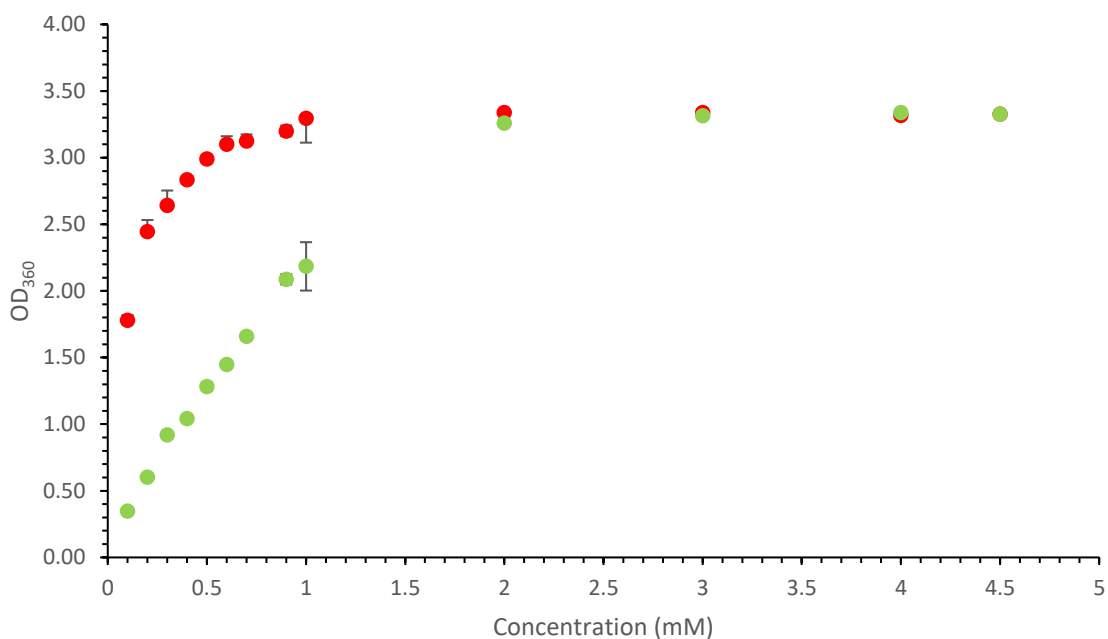


Figure S91: Graph showing average (n=3) red - interface and green - control OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 308 K.

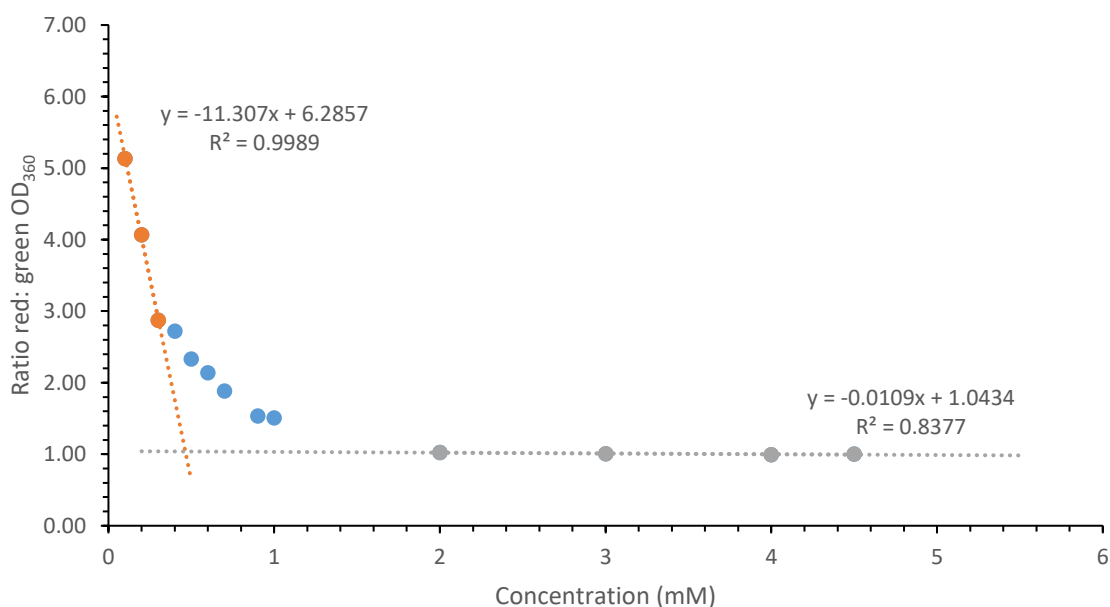


Figure S92: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 308 K, plotted against compound concentration. A CMC value of 0.46 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 2 at 308 K OD₃₆₀

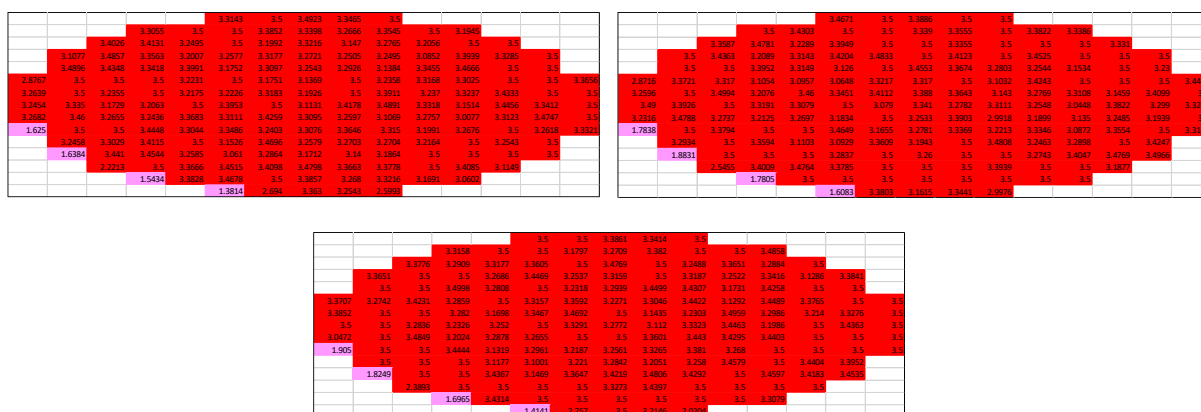


Figure S93: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:199 solutions of **2** (4.50 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S94: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (4.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

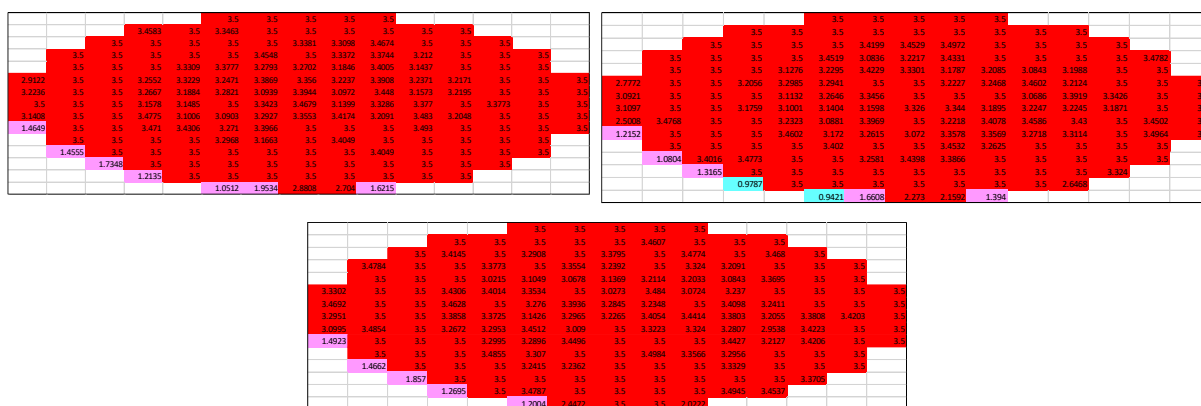


Figure S95: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (3.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

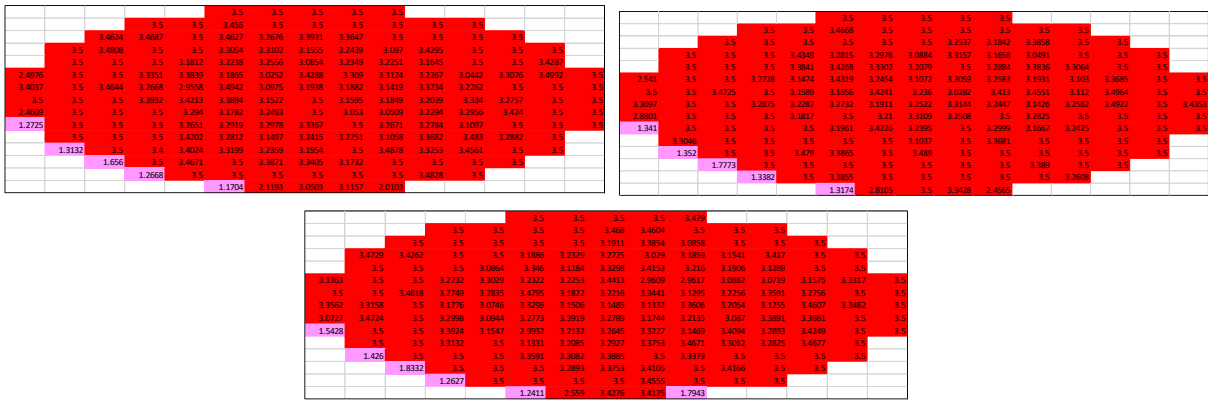


Figure S96: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (2.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

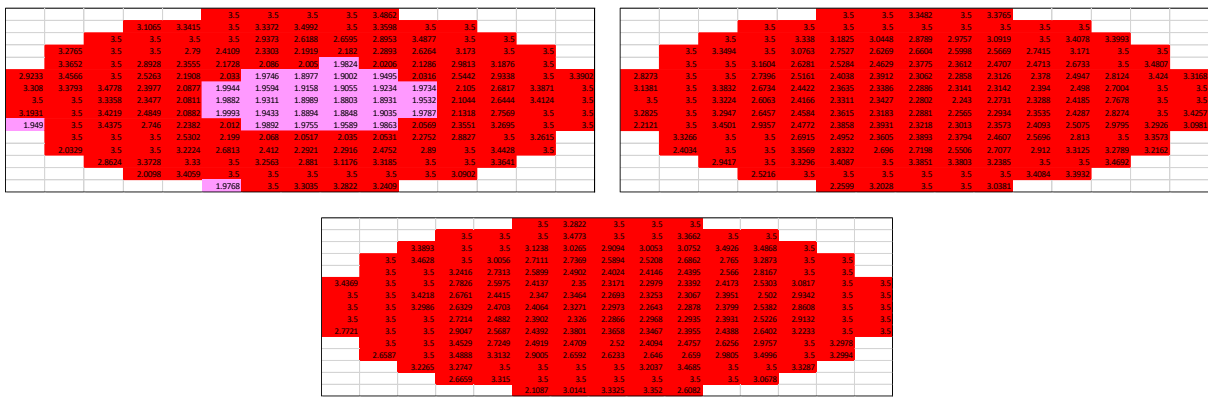


Figure S97: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (1.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

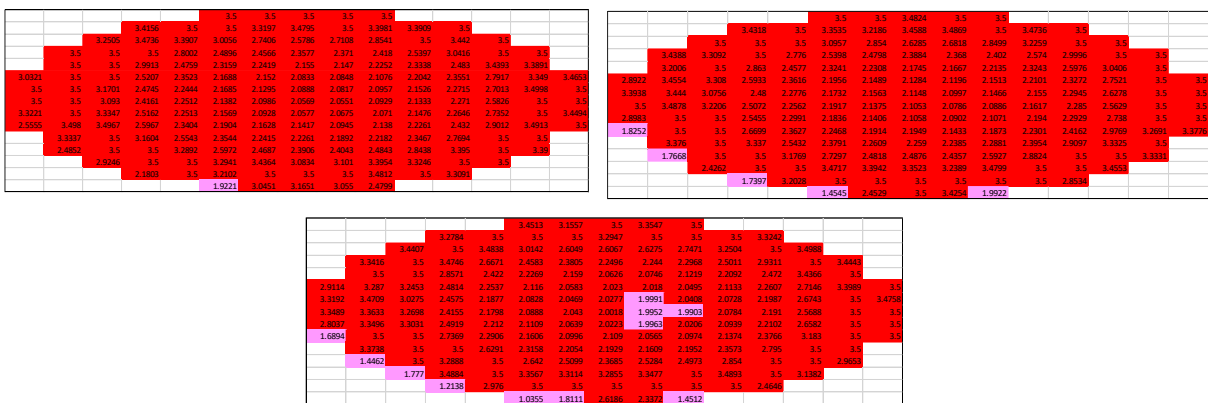


Figure S98: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.90 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

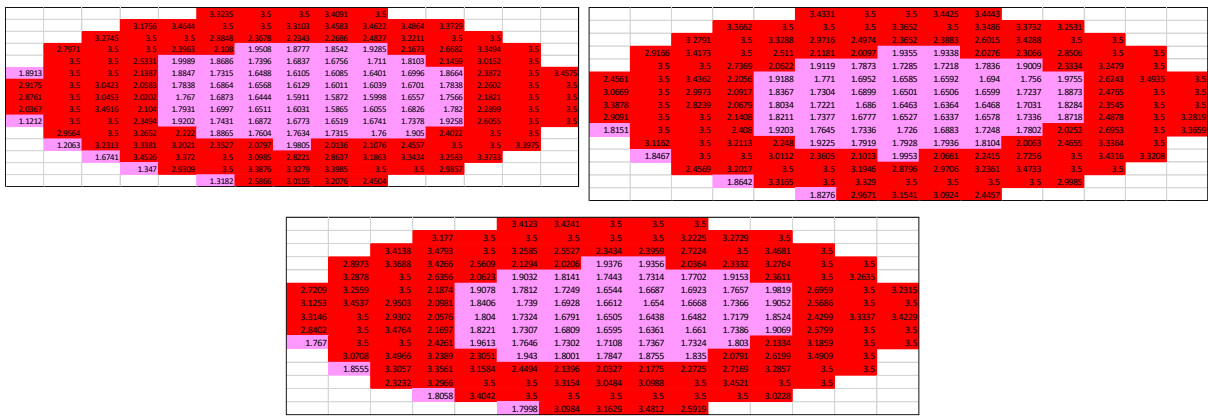


Figure S99: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.70 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

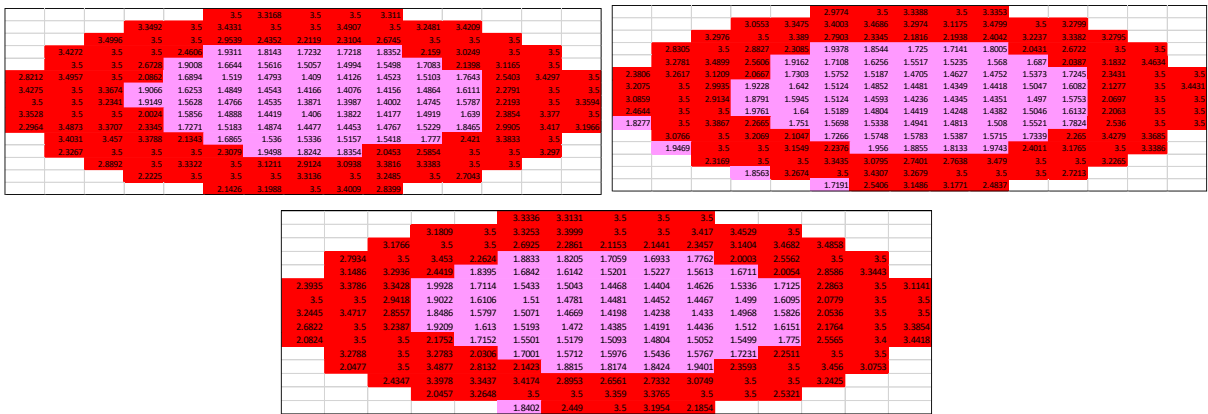


Figure S100: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:199 solutions of **2** (0.60 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S101: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.50 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

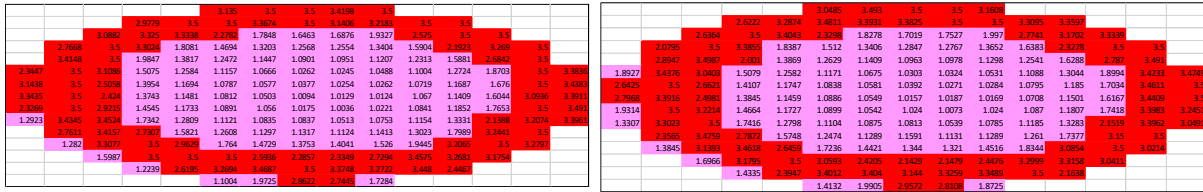


Figure S102: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.40 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

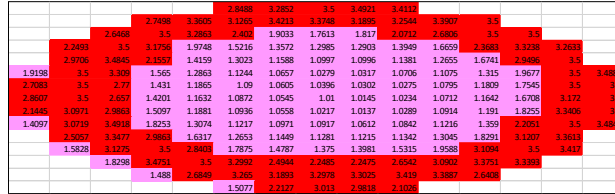


Figure S103: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.30 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

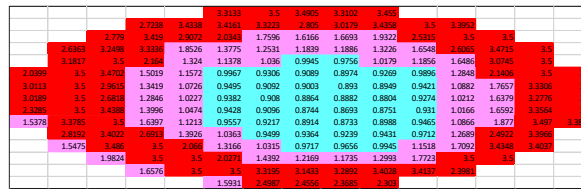


Figure S104: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.20 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

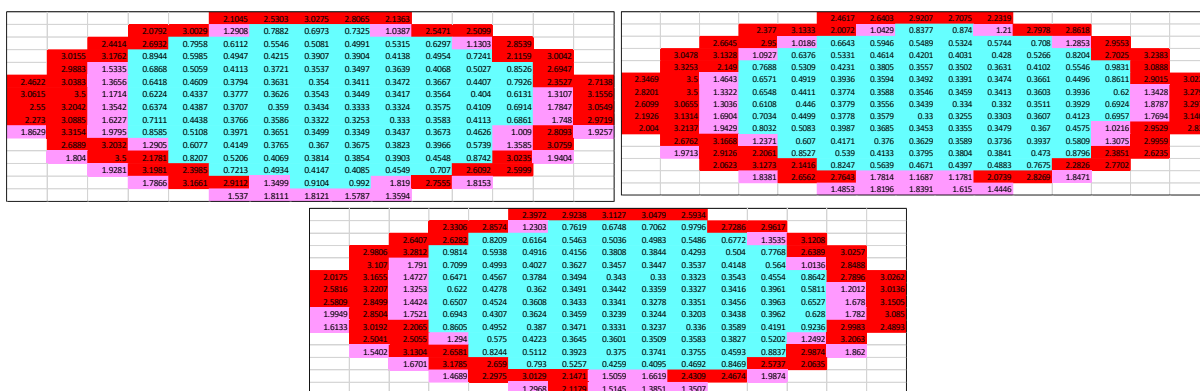


Figure S105: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.10 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

Compound 2 CMC calculation at 318 K OD₃₆₀

Table S16: A summary of OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 318 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Well sections															
Concentration (mM)	n = 1			n = 2			n = 3			Average of n's			+/- error		
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
4.50	3.43	3.50	3.50	3.45	3.50	3.50	3.44	3.50	3.50	3.44	3.50	3.50	0.01	0.00	0.00
4.00	3.42	3.50	3.50	3.36	3.50	3.50	3.39	3.50	3.50	3.39	3.50	3.50	0.02	0.00	0.00
3.00	3.39	3.50	3.50	3.35	3.50	3.50	3.40	3.50	3.50	3.38	3.50	3.50	0.02	0.00	0.00
2.00	3.37	3.50	3.50	3.39	3.50	3.50	3.39	3.50	3.50	3.39	3.50	3.50	0.01	0.00	0.00
1.00	3.42	2.27	1.90	3.45	2.62	2.32	3.46	2.67	2.35	3.44	2.52	2.19	0.02	0.18	0.20
0.90	3.40	2.37	2.09	3.36	2.40	2.12	3.30	2.33	2.02	3.35	2.37	2.08	0.04	0.03	0.04
0.70	3.21	1.89	1.60	3.31	1.95	1.64	3.34	1.99	1.64	3.29	1.94	1.63	0.06	0.04	0.02
0.60	3.39	1.76	1.39	3.28	1.74	1.43	3.25	1.72	1.43	3.31	1.74	1.42	0.06	0.02	0.02
0.50	3.25	1.55	1.27	3.15	1.47	1.21	3.15	1.53	1.27	3.18	1.52	1.25	0.05	0.04	0.03
0.40	3.08	1.28	1.02	3.04	1.29	1.02	3.08	1.32	1.03	3.07	1.30	1.02	0.02	0.01	0.00
0.30	2.90	1.15	0.90	2.81	1.11	0.92	2.95	1.17	0.89	2.89	1.15	0.90	0.06	0.03	0.01
0.20	2.82	0.85	0.59	2.66	0.76	0.59	2.69	0.78	0.61	2.72	0.80	0.59	0.07	0.04	0.01
0.1	1.95	0.44	0.35	1.95	0.45	0.35	1.95	0.43	0.34	1.95	0.44	0.34	0.00	0.01	0.00

Table S17: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 318 K.

Concentration (mM)	Red	Green	Ratio Red: Green
4.50	3.44	3.50	0.98
4.00	3.39	3.50	0.97
3.00	3.38	3.50	0.97
2.00	3.39	3.50	0.97
1.00	3.44	2.19	1.57
0.90	3.35	2.08	1.61
0.70	3.29	1.63	2.02
0.60	3.31	1.42	2.33
0.50	3.18	1.25	2.54
0.40	3.07	1.02	3.00
0.30	2.89	0.90	3.19
0.20	2.72	0.59	4.58
0.10	1.95	0.34	5.68

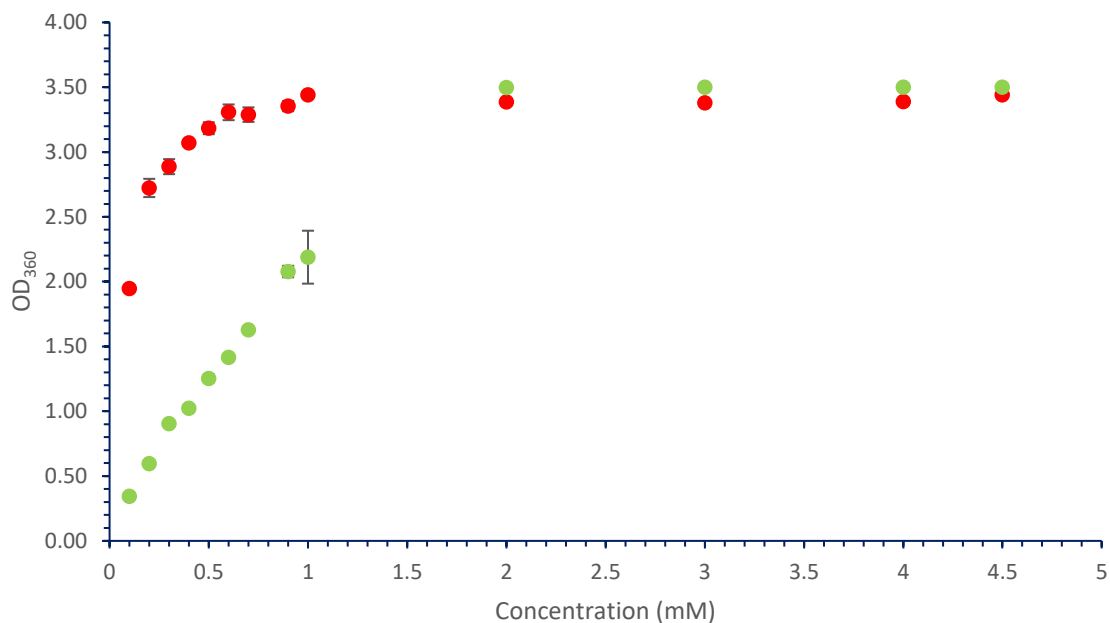


Figure S106: Graph showing average (n=3) red - interface and green - control OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 318 K.

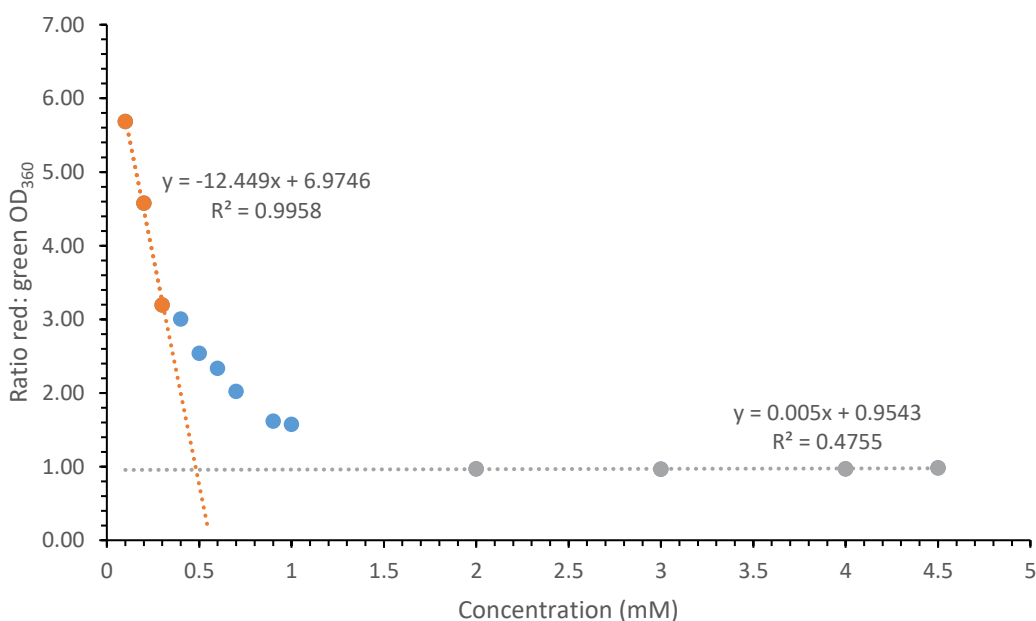


Figure S107: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₆₀ well scan data obtained for **2** in an EtOH/H₂O 1:19 solution at 318 K, plotted against compound concentration. A CMC value of 0.48 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 2 at 318 K OD₃₆₀

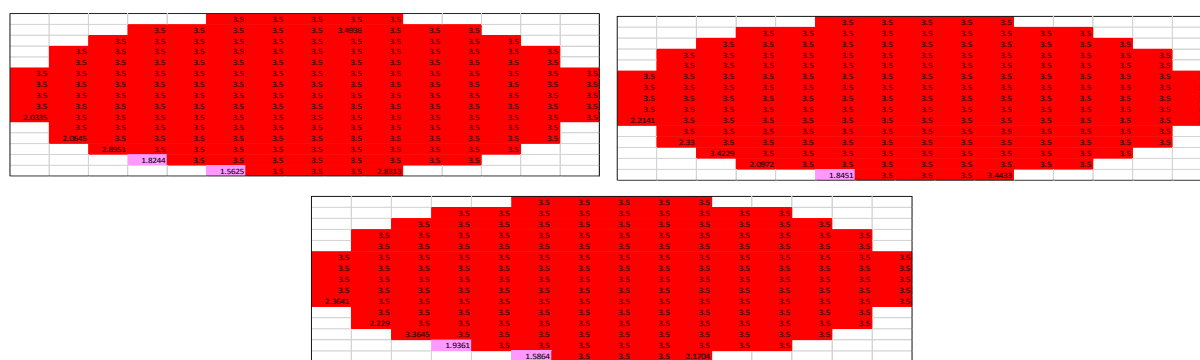


Figure S108: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (4.50 mM) at 318 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

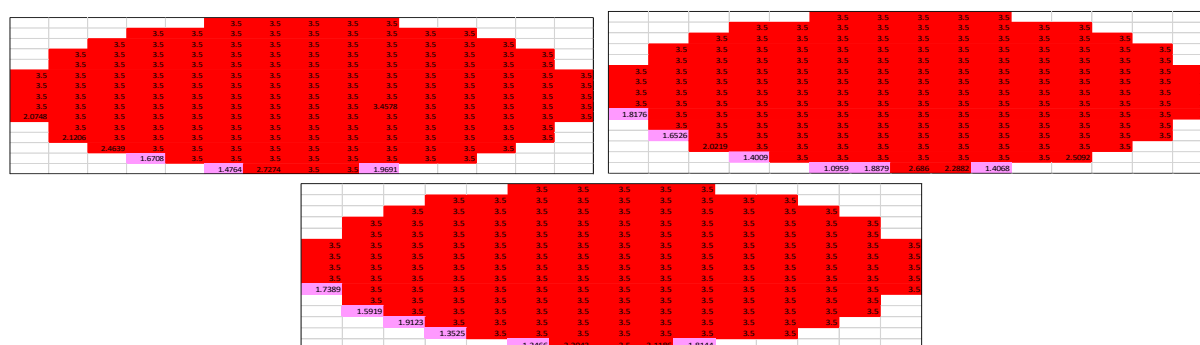


Figure S109: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (4.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

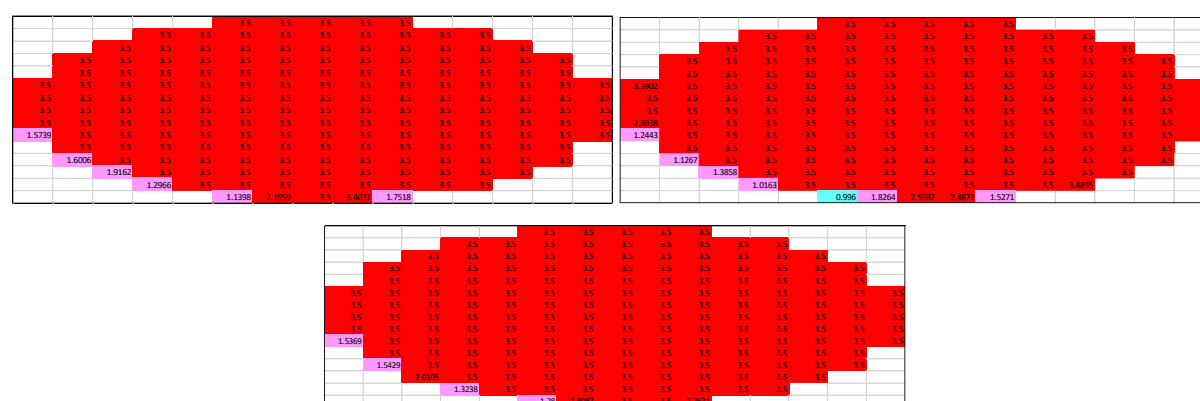


Figure S110: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (3.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

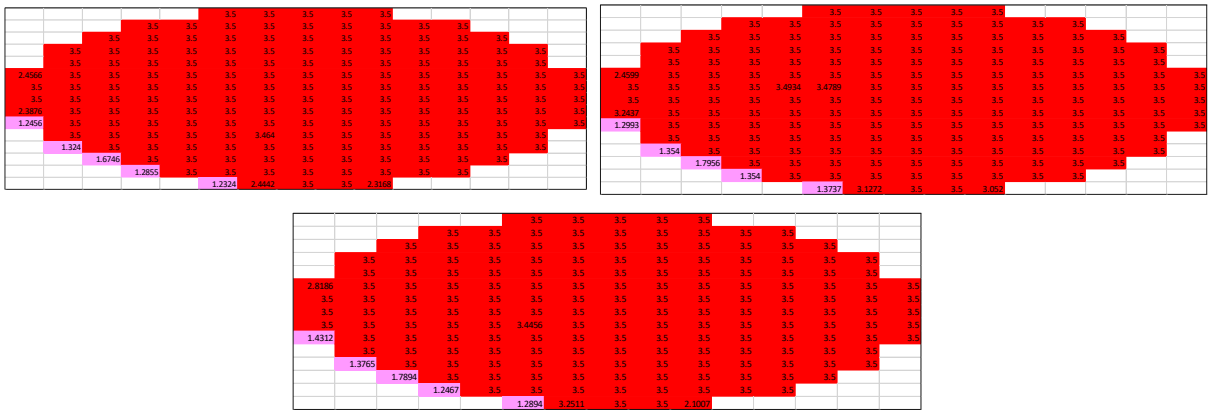


Figure S111: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (2.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

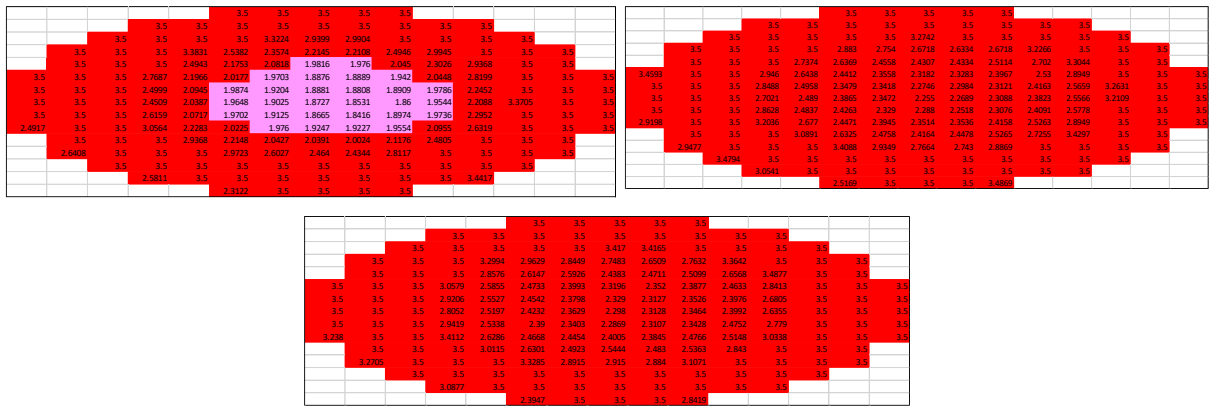


Figure S112: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (1.00 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

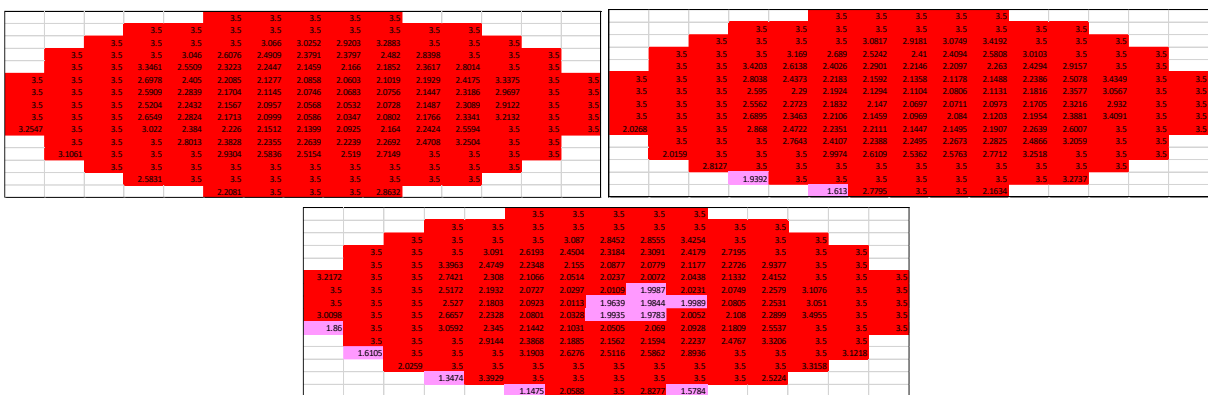


Figure S113: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.90 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

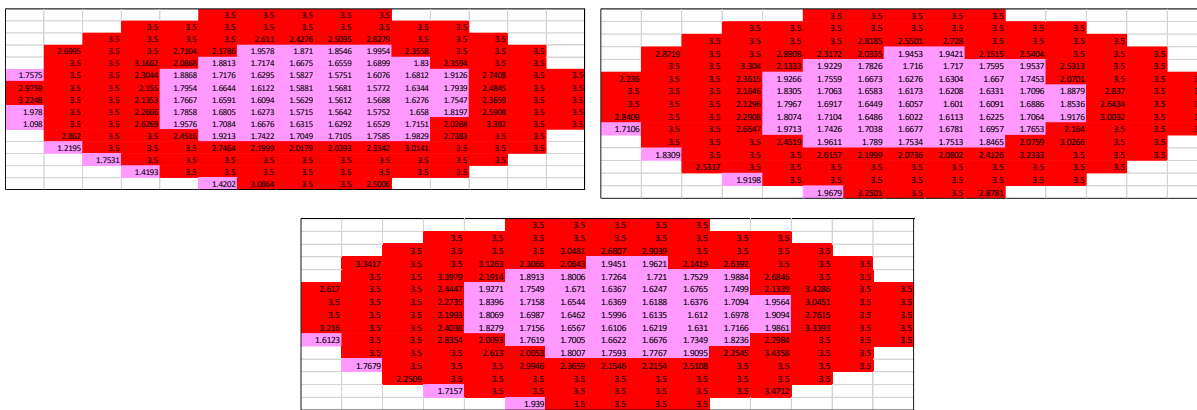


Figure S114: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.70 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

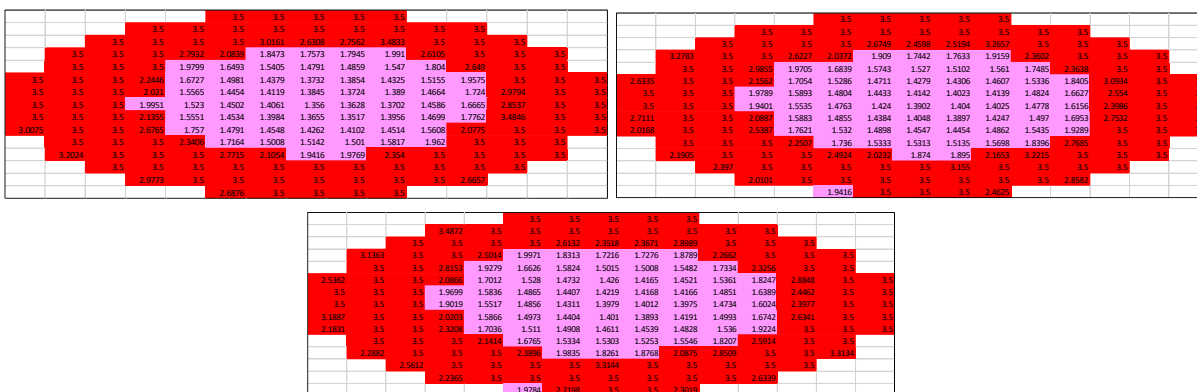


Figure S115: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.60 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

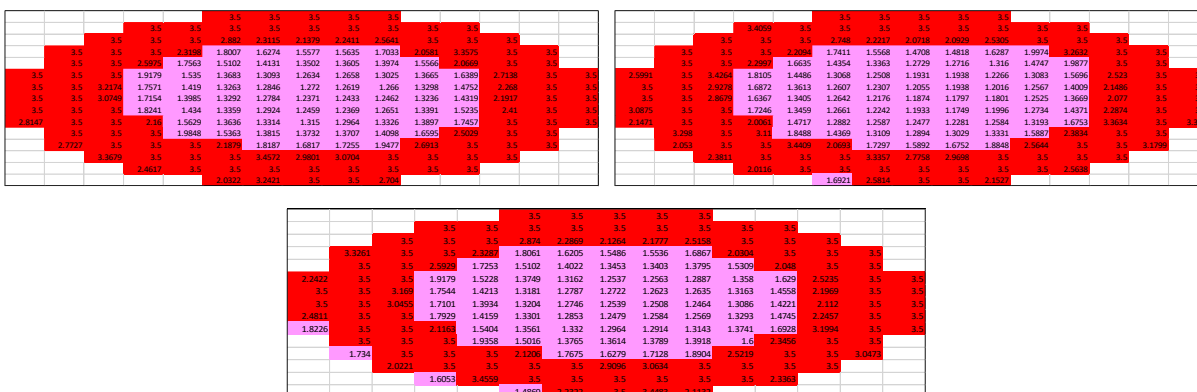


Figure S116: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.50 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S117: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.40 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.



Figure S118: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.30 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

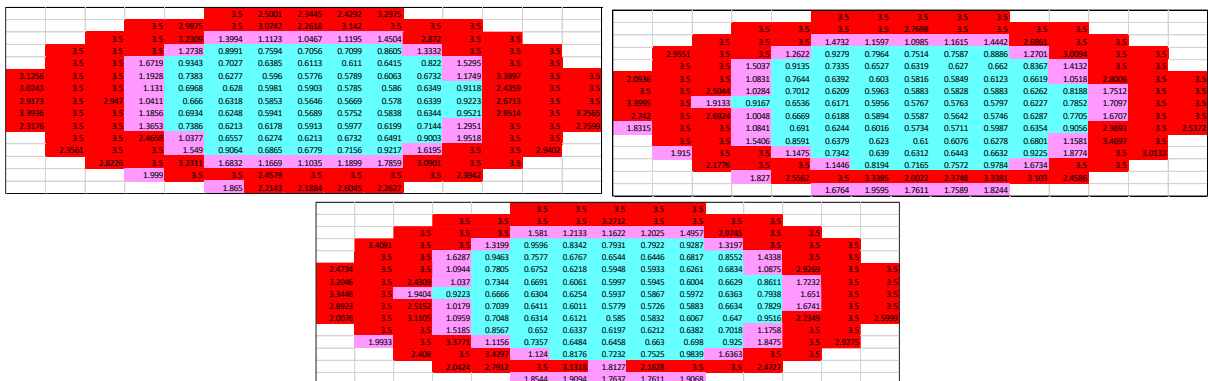


Figure S119: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.20 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

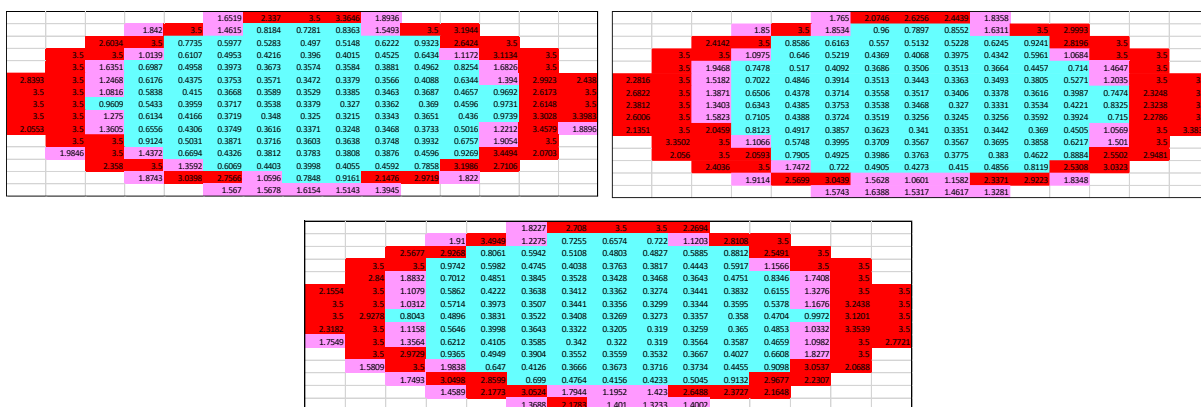


Figure S120: Raw OD₃₆₀ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **2** (0.10 mM) at 308 K. Colour coded regions: Red = OD₃₆₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₆₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₆₀ ≥ 0.0001.

Compound 3 CMC calculation at 298 K OD₃₈₅

Table S18: A summary of OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 298 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Well sections															
Concentration (mM)	n = 1			n = 2			n = 3			Average of n's			+/- error		
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
20	3.05	2.80	2.71	3.08	2.83	2.71	3.07	2.81	2.75	3.07	2.81	2.72	0.01	0.01	0.02
17	2.84	2.42	2.29	2.82	2.53	2.42	/	/	/	2.83	2.47	2.35	0.01	0.05	0.06
15	2.70	2.19	2.05	2.68	2.28	2.14	2.77	2.28	2.13	2.72	2.25	2.11	0.04	0.04	0.04
14	2.60	2.02	1.87	2.66	2.10	1.95	2.65	2.12	1.99	2.63	2.08	1.94	0.03	0.04	0.05
13	2.51	1.85	1.72	2.61	1.95	1.84	2.62	1.97	1.84	2.58	1.92	1.80	0.05	0.05	0.06
12	2.46	1.71	1.59	2.44	1.74	1.62	2.23	1.62	1.51	2.38	1.69	1.57	0.10	0.05	0.04
11	2.21	1.46	1.34	2.24	1.52	1.41	2.26	1.55	1.44	2.23	1.51	1.40	0.02	0.04	0.04
10	2.05	1.24	1.13	2.14	1.29	1.17	2.15	1.33	1.21	2.11	1.28	1.17	0.05	0.03	0.03
9	2.00	1.06	0.95	1.97	1.10	1.00	1.96	1.09	0.99	1.98	1.09	0.98	0.02	0.02	0.02
8	1.87	0.85	0.75	1.83	0.88	0.78	1.79	0.88	0.78	1.83	0.87	0.77	0.03	0.01	0.01
7	1.71	0.69	0.59	1.72	0.71	0.61	1.75	0.72	0.62	1.73	0.71	0.61	0.02	0.02	0.01
6	1.70	0.56	0.46	1.67	0.59	0.49	1.76	0.58	0.47	1.71	0.58	0.47	0.04	0.01	0.01
5	1.68	0.46	0.37	1.67	0.47	0.38	1.68	0.48	0.38	1.68	0.47	0.37	0.00	0.01	0.01
3	1.15	0.26	0.21	0.85	0.25	0.23	1.19	0.26	0.22	1.06	0.26	0.22	0.15	0.00	0.01

Table S19: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Red	Green	Ratio Red: Green
20	3.07	2.72	1.13
17	2.83	2.35	1.20
15	2.72	2.11	1.29
14	2.63	1.94	1.36
13	2.58	1.80	1.44
12	2.38	1.57	1.51
11	2.23	1.40	1.60
10	2.11	1.17	1.80
9	1.98	0.98	2.01
8	1.83	0.77	2.37
7	1.73	0.61	2.84
6	1.71	0.47	3.62
5	1.68	0.37	4.47
3	1.06	0.22	4.88

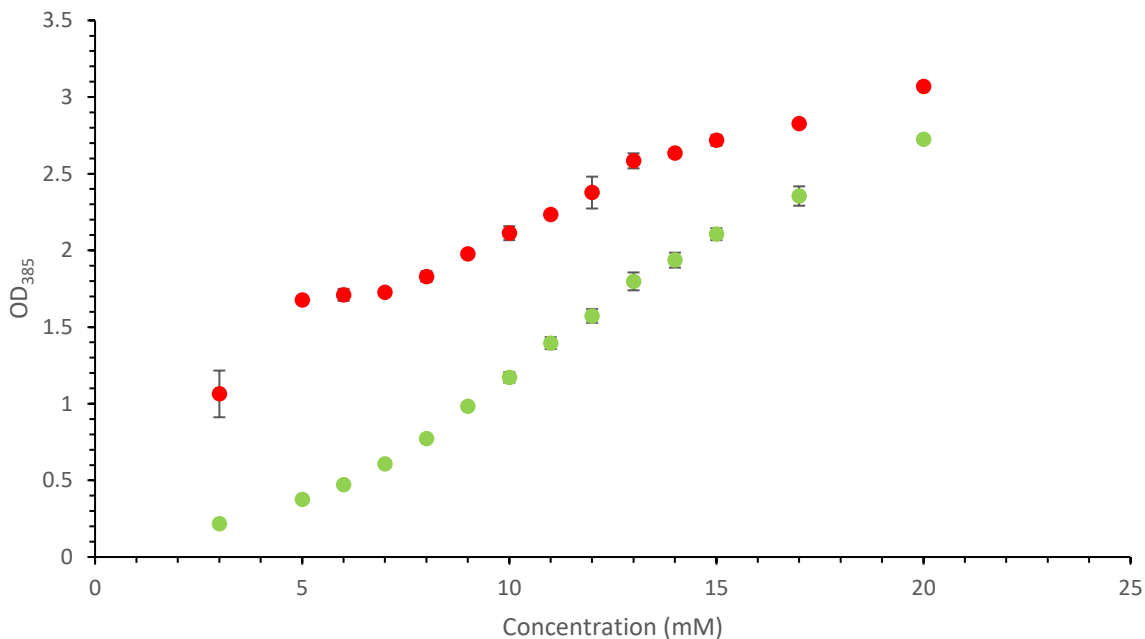


Figure S121: Graph showing average (n=3) red - interface and green - control OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 298 K.

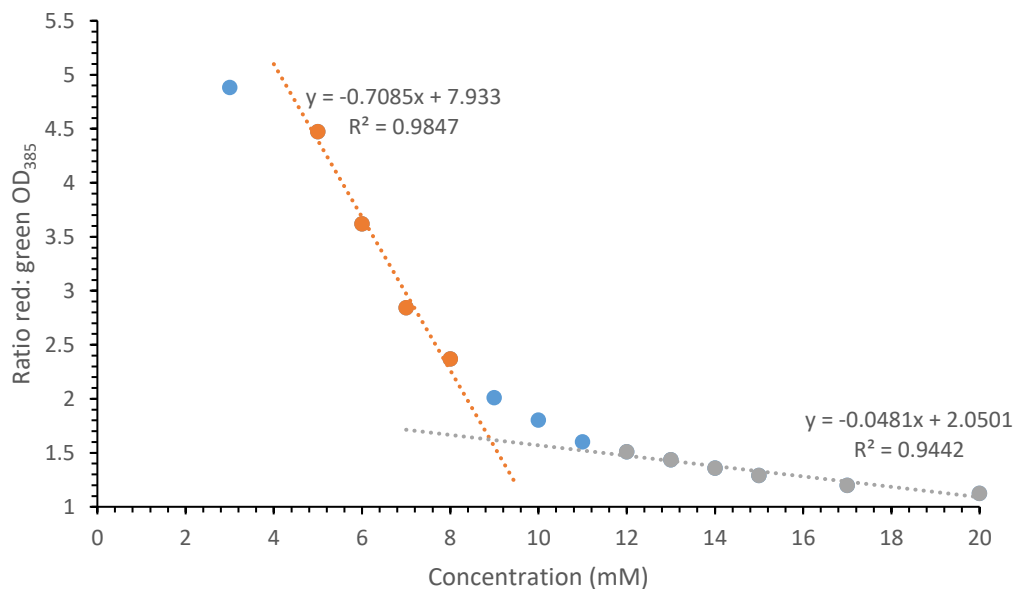


Figure S122: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 298 K, plotted against compound concentration. A CMC value of 8.91 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 3 at 298 K OD₃₈₅



Figure S123: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (20 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

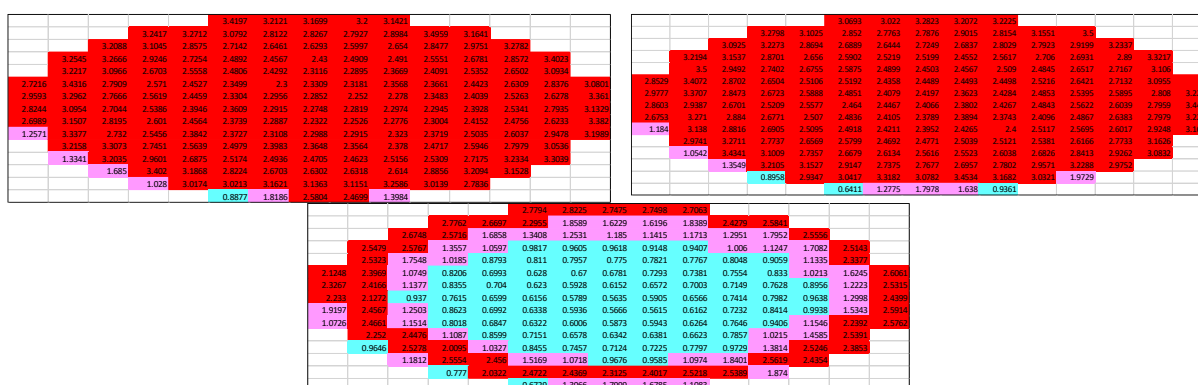


Figure S124: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (17 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S125: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (15 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

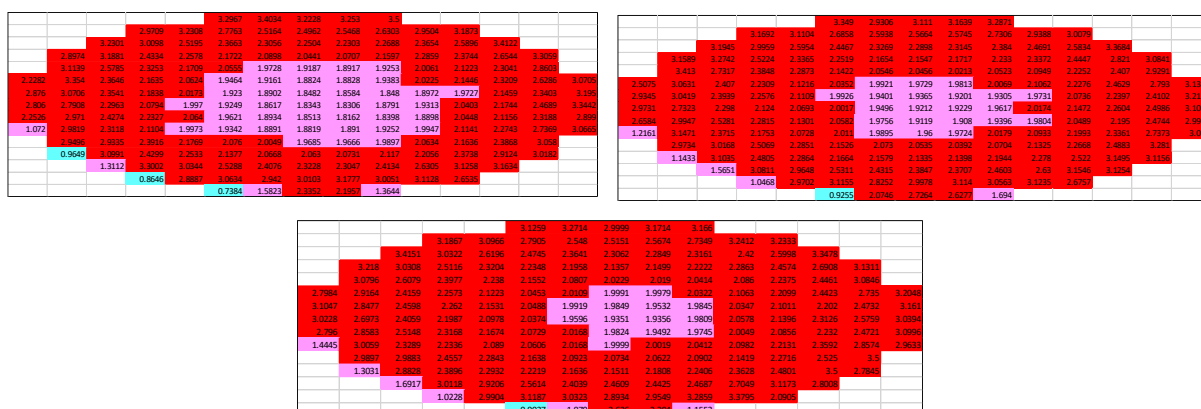


Figure S126: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (14 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

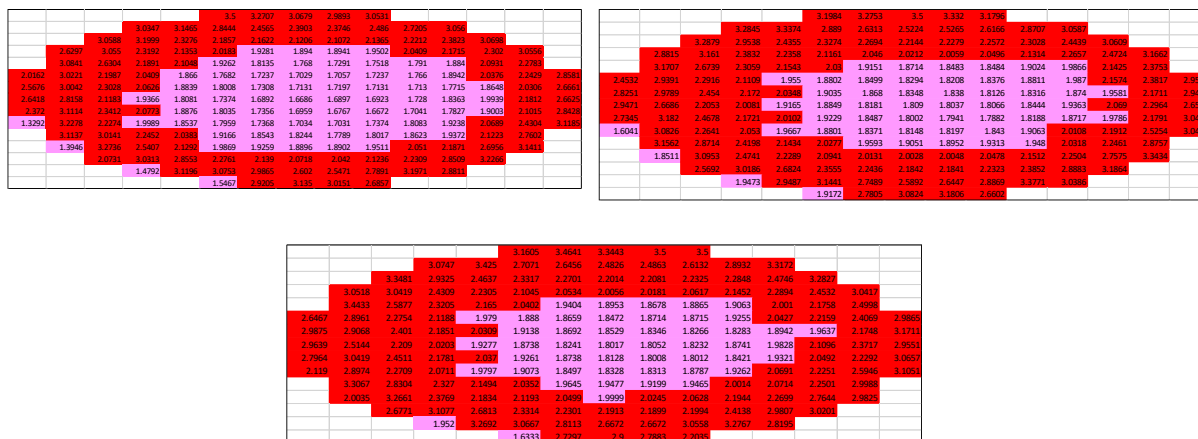


Figure S127: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (13 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S128: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (12 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

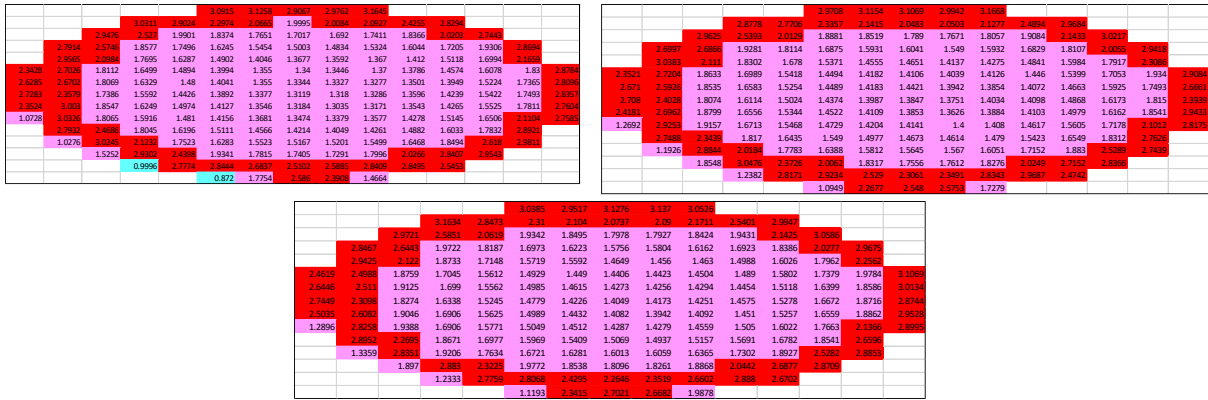


Figure S129: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (11 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

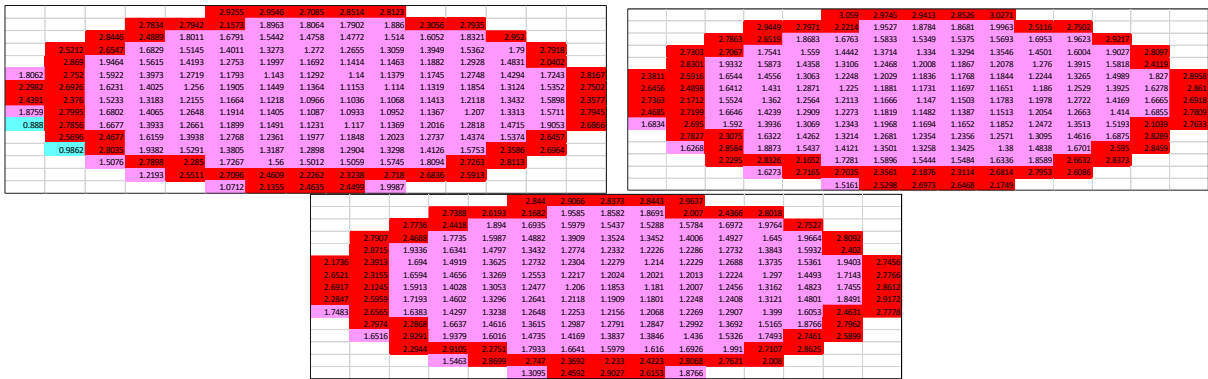


Figure S130: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (10 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S131: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (9 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

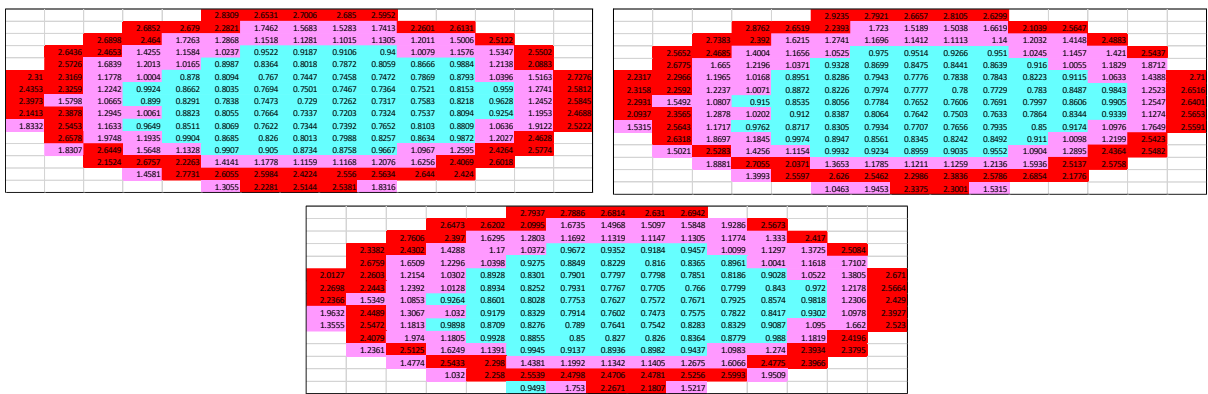


Figure S132: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (8 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

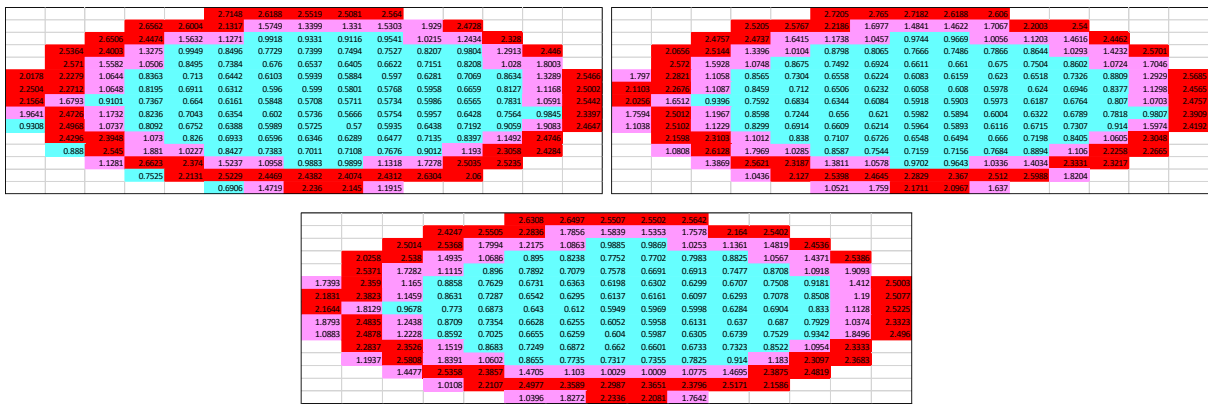


Figure S133: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (7 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

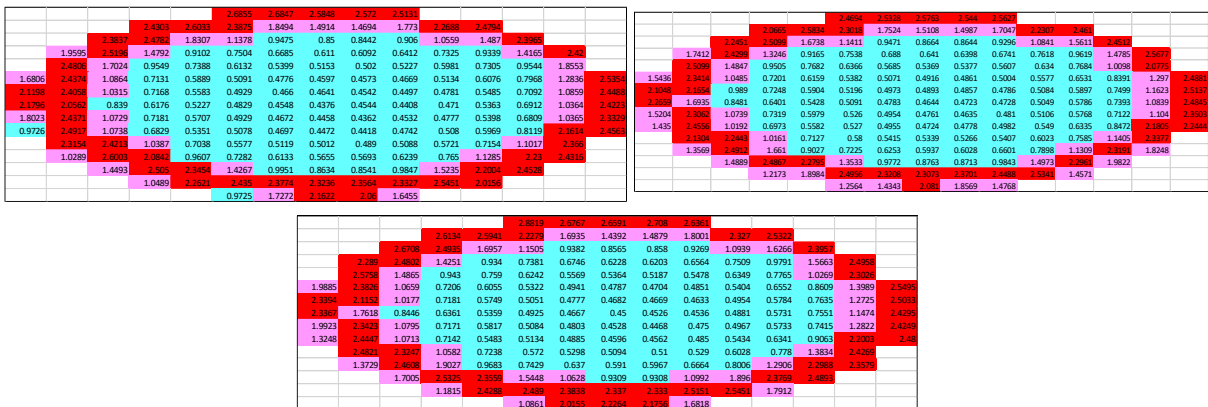


Figure S134: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (6 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

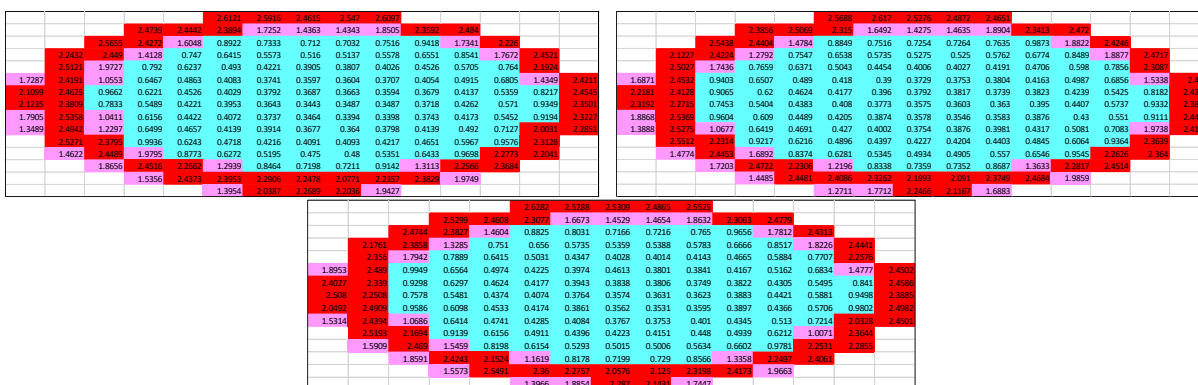


Figure S135: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (5 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

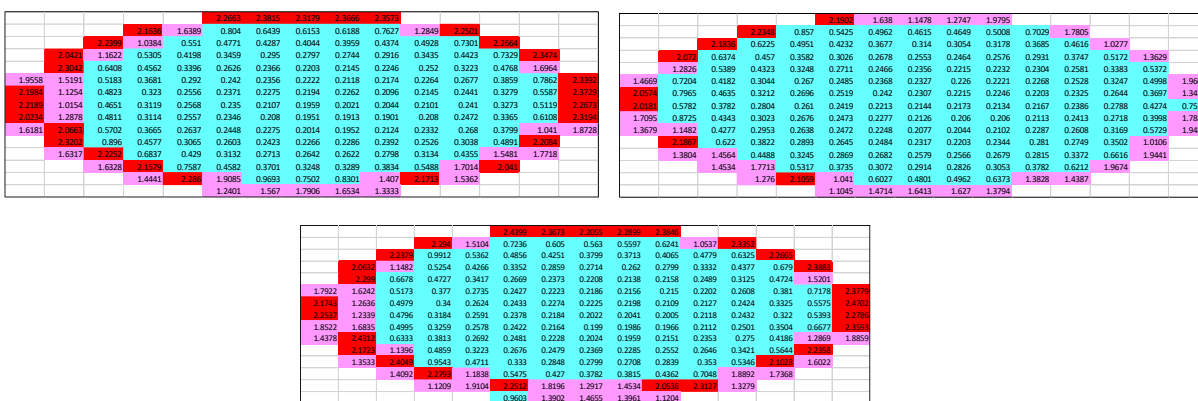


Figure S136: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (3 mM) at 298 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

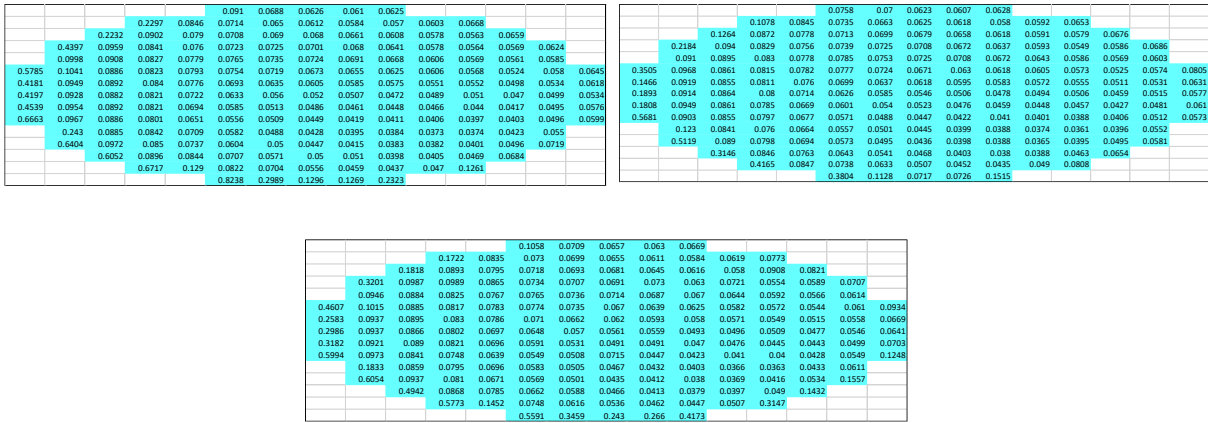


Figure S137: Raw OD₃₈₅ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 298 K. Colour coded regions: Red = OD₃₈₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₀ ≥ 0.0001.

Compound 3 CMC calculation at 308 K OD₃₈₅

Table S20: A summary of OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 308 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections									Average of n's			+/- error		
	n = 1			n = 2			n = 3			Red	Yellow	Green	Red	Yellow	Green
20	3.28	2.97	2.85	3.37	3.11	2.99	3.33	3.07	2.92	3.32	3.05	2.92	0.04	0.06	0.06
17	3.20	2.62	2.44	3.18	2.76	2.59	/	/	/	3.19	2.69	2.52	0.01	0.07	0.08
15	3.01	2.32	2.13	3.00	2.44	2.26	3.05	2.42	2.23	3.02	2.39	2.21	0.02	0.05	0.05
14	2.91	2.15	1.96	2.98	2.24	2.07	2.97	2.27	2.09	2.95	2.22	2.04	0.03	0.05	0.06
13	2.91	1.98	1.81	2.97	2.08	1.92	2.96	2.09	1.93	2.94	2.05	1.89	0.03	0.05	0.05
12	2.77	1.80	1.66	2.71	1.82	1.68	2.48	1.69	1.57	2.65	1.77	1.63	0.12	0.06	0.05
11	2.46	1.53	1.40	2.50	1.59	1.46	2.55	1.63	1.50	2.50	1.58	1.45	0.04	0.04	0.04
10	2.23	1.29	1.18	2.31	1.34	1.22	2.38	1.40	1.27	2.31	1.34	1.22	0.06	0.05	0.04
9	2.29	1.15	1.02	2.22	1.18	1.06	2.18	1.16	1.05	2.23	1.16	1.04	0.05	0.01	0.02
8	2.01	0.90	0.79	1.96	0.93	0.82	1.93	0.93	0.82	1.96	0.92	0.81	0.03	0.01	0.01
7	1.87	0.73	0.61	1.85	0.75	0.64	1.89	0.77	0.65	1.87	0.75	0.63	0.02	0.02	0.01
6	1.82	0.59	0.47	1.79	0.62	0.51	1.89	0.62	0.49	1.84	0.61	0.49	0.04	0.01	0.01
5	1.88	0.49	0.38	1.81	0.49	0.39	1.80	0.50	0.39	1.83	0.49	0.39	0.03	0.00	0.01
3	1.15	0.26	0.22	1.05	0.26	0.23	1.19	0.27	0.22	1.13	0.26	0.23	0.06	0.00	0.00

Table S21: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 308 K.

Concentration (mM)	Red	Green	Ratio Red: Green
20	3.07	2.72	1.13
17	2.83	2.35	1.20
15	2.72	2.11	1.29
14	2.63	1.94	1.36
13	2.58	1.80	1.44
12	2.38	1.57	1.51
11	2.23	1.40	1.60
10	2.11	1.17	1.80
9	1.98	0.98	2.01
8	1.83	0.77	2.37
7	1.73	0.61	2.84
6	1.71	0.47	3.62
5	1.68	0.37	4.47
3	1.06	0.22	4.88

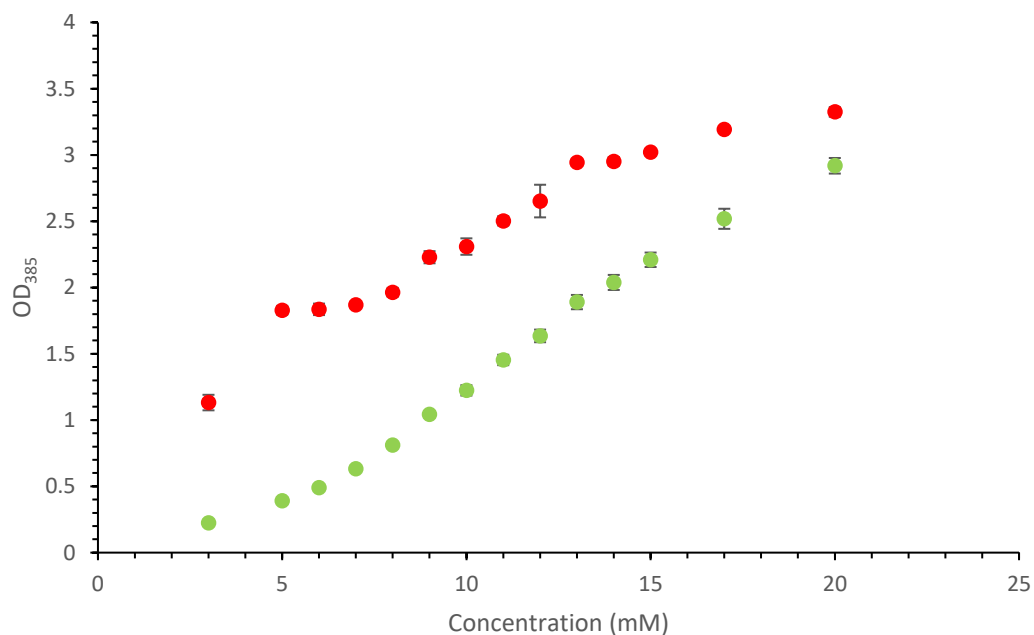


Figure S138: Graph showing average (n=3) red - interface and green - control OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 308 K.

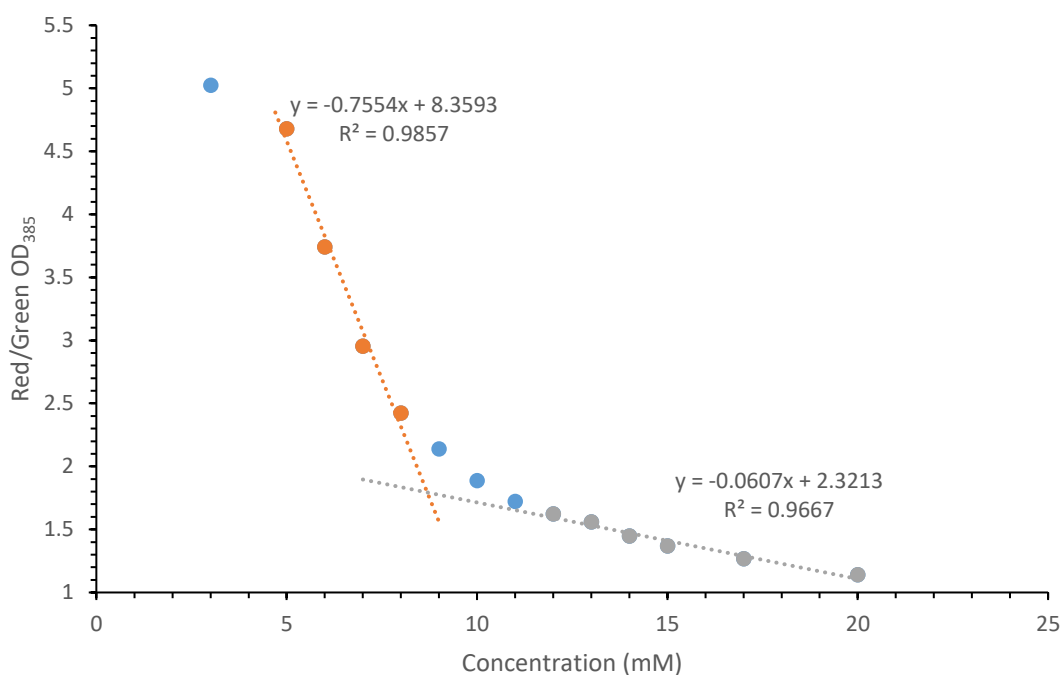


Figure S139: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 308 K, plotted against compound concentration. A CMC value of 8.69 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 3 at 308 K OD₃₈₅s

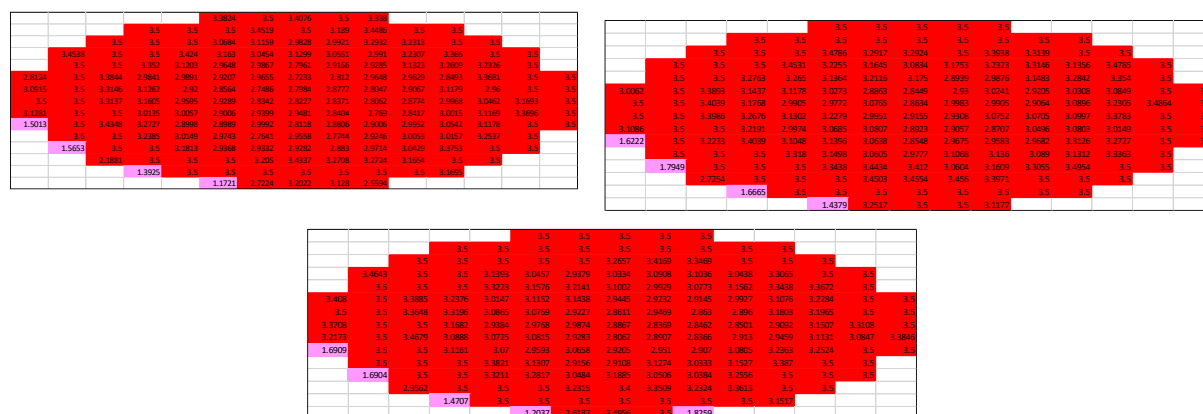


Figure S140: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (20 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

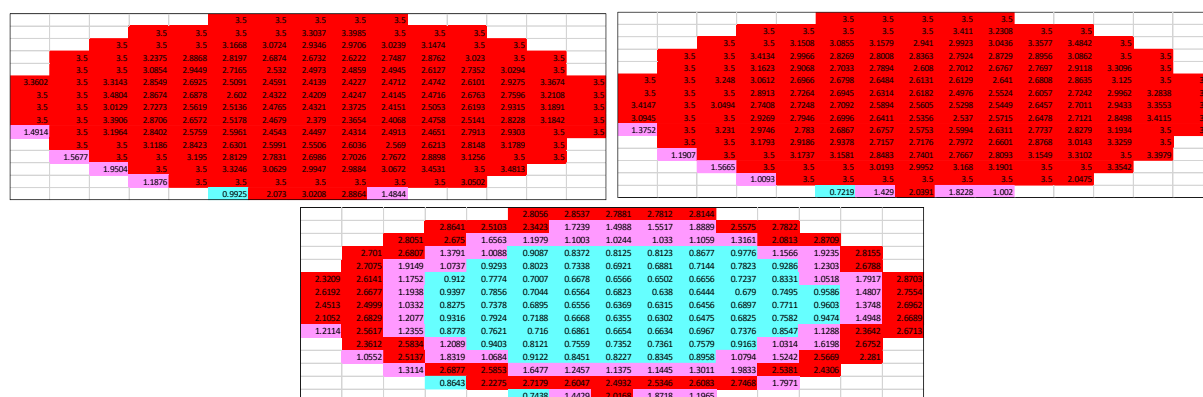


Figure S141: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (17 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

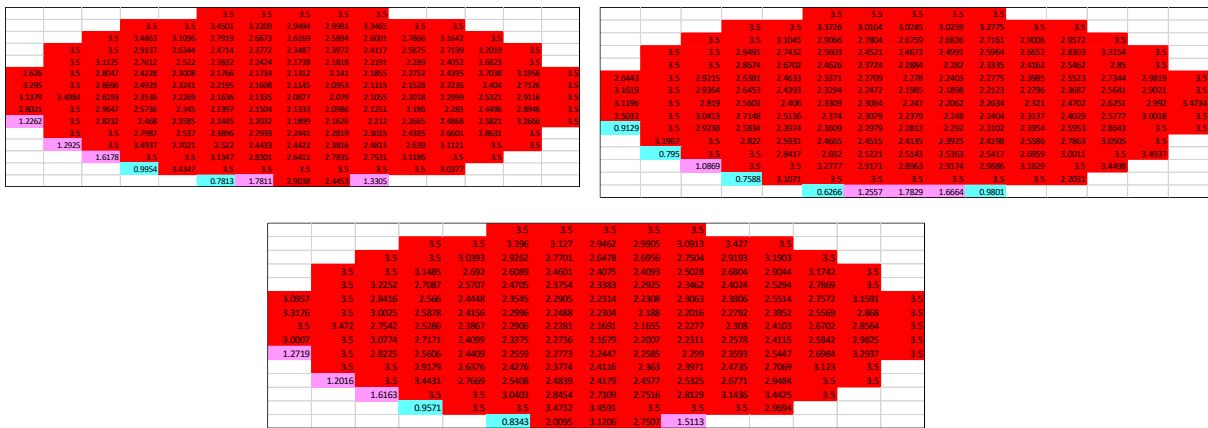


Figure S142: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (15 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

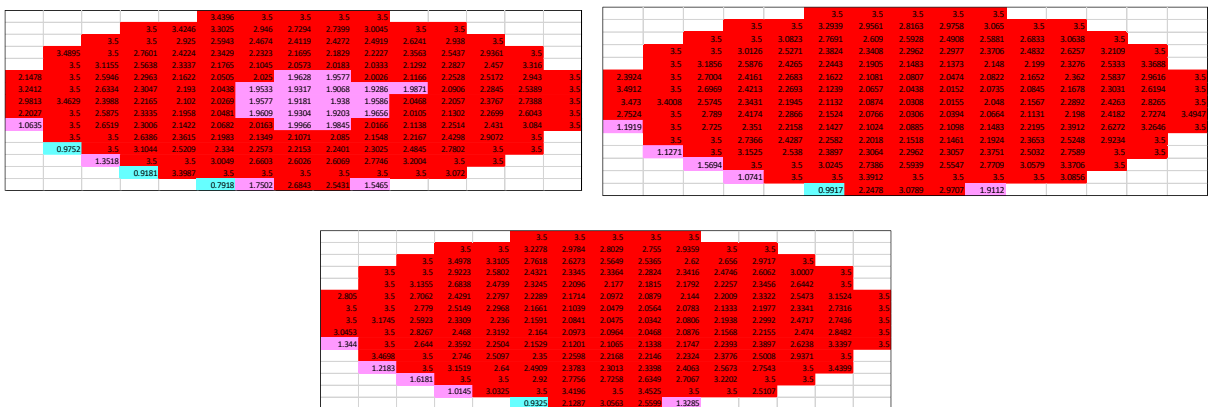


Figure S143: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (14 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

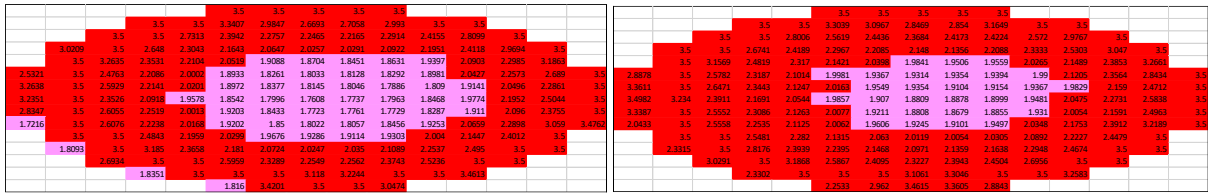


Figure S144: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (13 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

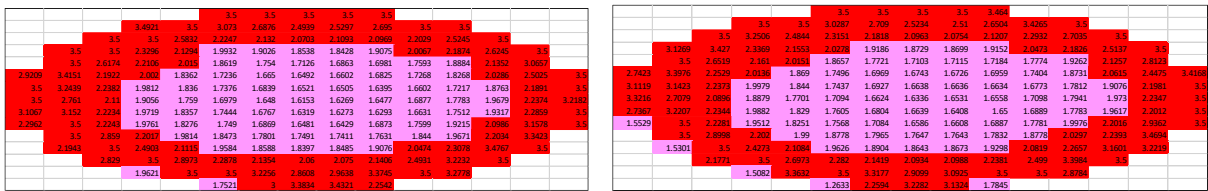


Figure S145: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (12 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

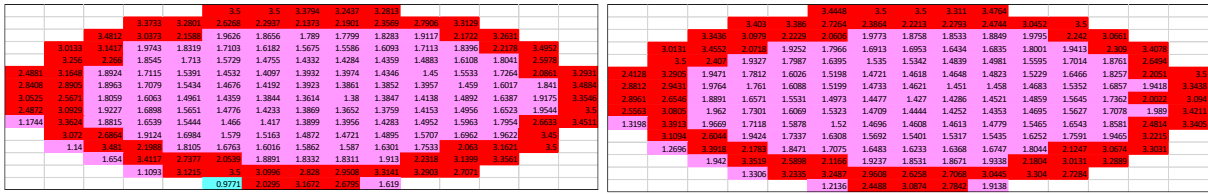


Figure S146: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (11 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S147: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (10 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

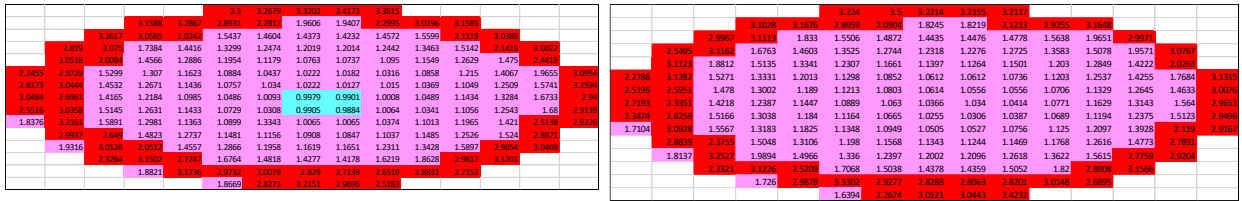


Figure S148: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (9 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

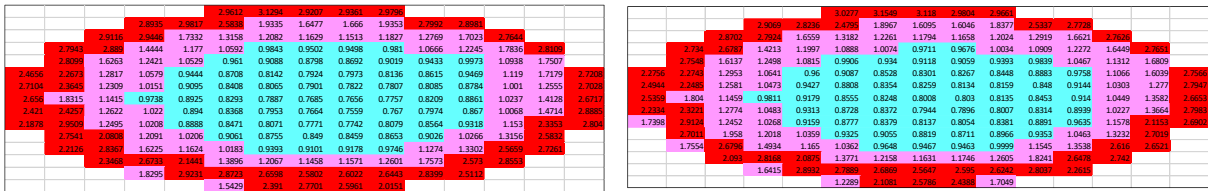


Figure S149: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (8 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



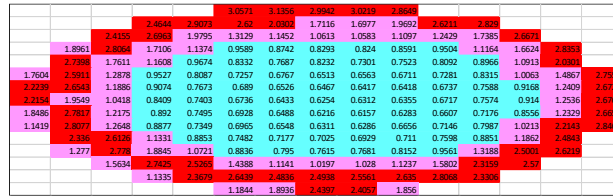
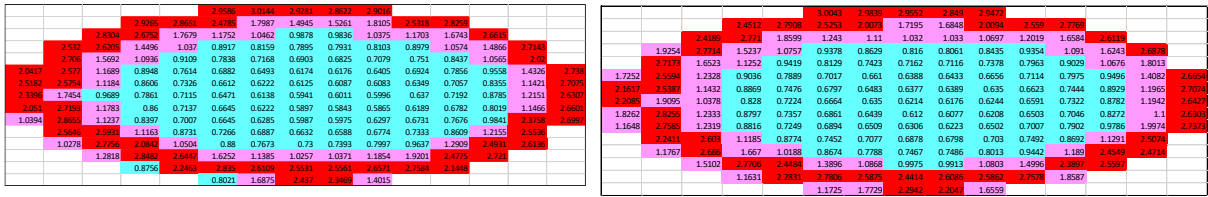


Figure S150: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (7 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

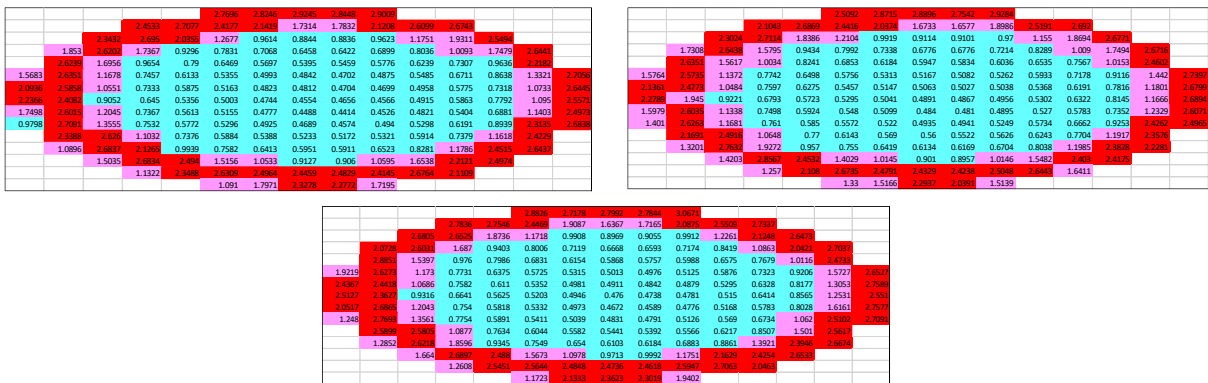


Figure S151: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (6 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

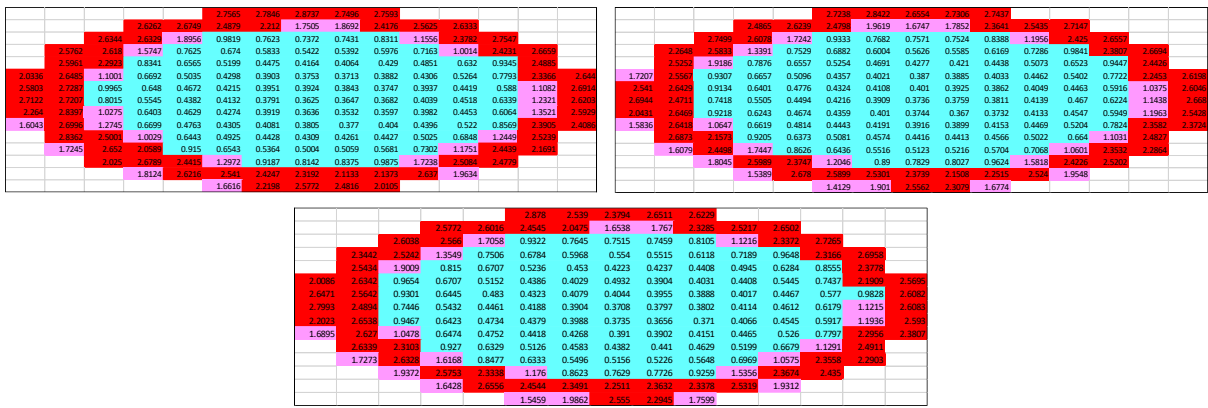


Figure S152: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (5 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

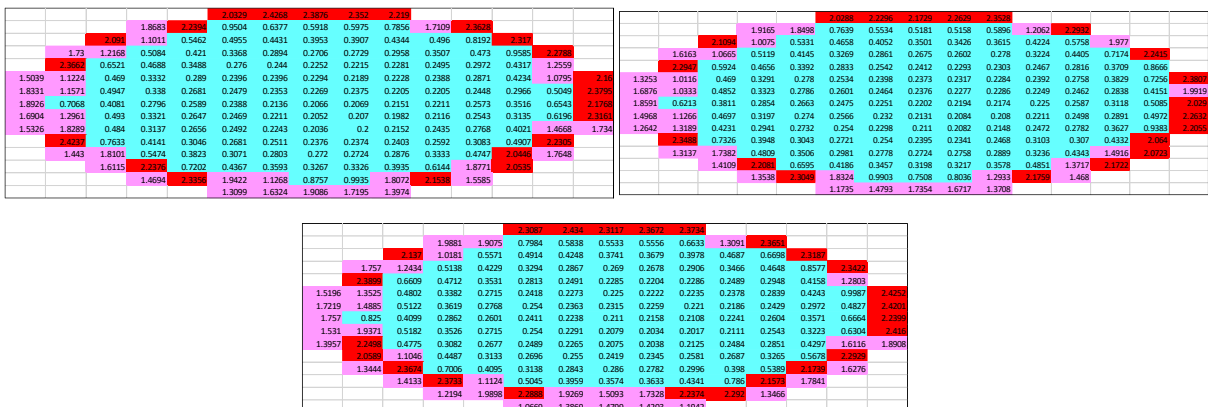


Figure S153: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (3 mM) at 308 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S154: Raw OD₃₈₅ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 308 K. Colour coded regions: Red = $OD_{380} \geq 2.0000$, Pink = $1.9999 \geq OD_{380} \geq 1.0000$, cyan = $0.9999 \geq OD_{380} \geq 0.0001$.

Compound 3 CMC calculation at 318 K OD₃₈₅

Table S22: A summary of OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 318 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections									Average of n's			+/- error		
	n = 1			n = 2			n = 3			Red	Yellow	Green	Red	Yellow	Green
20	3.32	3.03	2.87	3.37	3.08	2.90	3.38	3.11	2.98	3.36	3.07	2.92	0.03	0.03	0.05
17	3.27	2.72	2.52	3.26	2.84	2.66	/	/	/	3.26	2.78	2.59	0.00	0.06	0.07
15	3.13	2.44	2.25	3.07	2.53	2.35	3.14	2.51	2.32	3.11	2.50	2.31	0.03	0.04	0.04
14	3.01	2.27	2.07	3.09	2.37	2.17	3.11	2.41	2.23	3.07	2.35	2.16	0.04	0.06	0.07
13	3.11	2.13	1.94	3.11	2.21	2.02	3.11	2.21	2.03	3.11	2.18	2.00	0.00	0.04	0.04
12	2.94	1.93	1.75	2.91	1.95	1.78	2.70	1.81	1.66	2.85	1.90	1.73	0.11	0.06	0.05
11	2.68	1.65	1.50	2.72	1.72	1.57	2.76	1.76	1.60	2.72	1.71	1.55	0.03	0.05	0.04
10	2.44	1.42	1.27	2.56	1.47	1.32	2.60	1.55	1.39	2.53	1.48	1.33	0.07	0.05	0.05
9	2.56	1.29	1.13	2.47	1.31	1.17	2.42	1.28	1.14	2.49	1.29	1.15	0.06	0.01	0.01
8	2.20	1.00	0.87	2.16	1.03	0.91	2.11	1.02	0.90	2.16	1.01	0.89	0.04	0.01	0.01
7	2.01	0.79	0.67	1.97	0.83	0.70	2.03	0.84	0.71	2.00	0.82	0.69	0.03	0.02	0.02
6	1.95	0.64	0.51	1.93	0.68	0.55	2.05	0.68	0.54	1.98	0.67	0.53	0.05	0.02	0.02
5	2.12	0.57	0.41	2.00	0.55	0.42	1.98	0.54	0.42	2.03	0.55	0.42	0.06	0.01	0.00
3	1.31	0.28	0.23	1.31	0.29	0.24	1.33	0.28	0.23	1.32	0.28	0.23	0.01	0.00	0.00

Table S23: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 318 K.

Concentration (mM)	Well sections		Ratio Red: Green
	Red	Green	
20	3.36	2.92	1.15
17	3.26	2.59	1.26
15	3.11	2.31	1.35
14	3.07	2.16	1.42
13	3.11	2.00	1.56
12	2.85	1.73	1.65
11	2.72	1.55	1.75
10	2.53	1.33	1.91
9	2.49	1.15	2.17
8	2.16	0.89	2.42
7	2.00	0.69	2.88
6	1.98	0.53	3.70
5	2.03	0.42	4.89
3	1.32	0.23	5.66
1	0.42	0.11	3.88

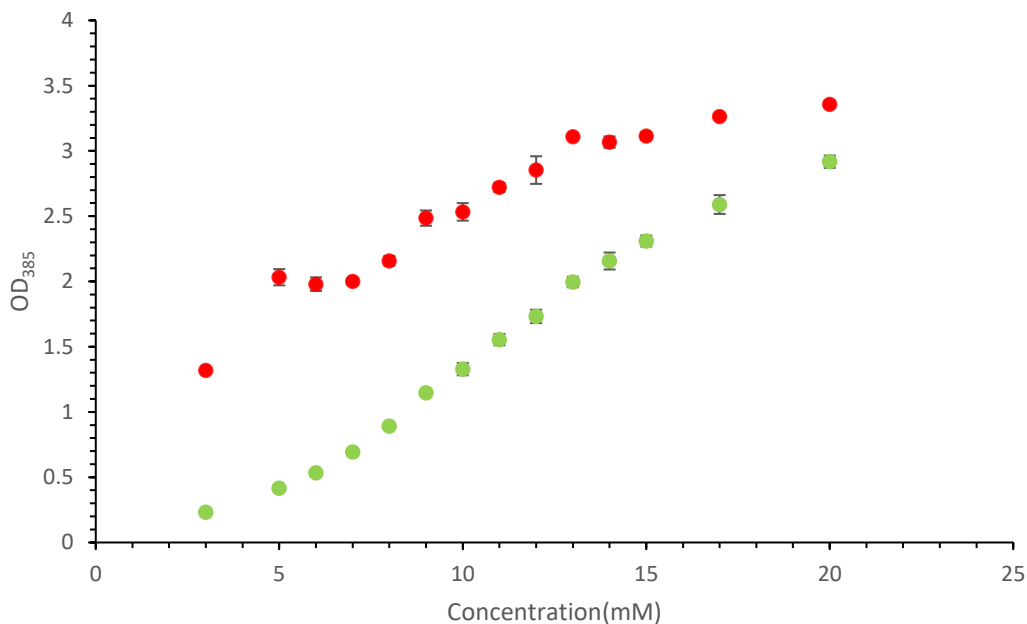


Figure S155: Graph showing average (n=3) red - interface and green - control OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 318 K.

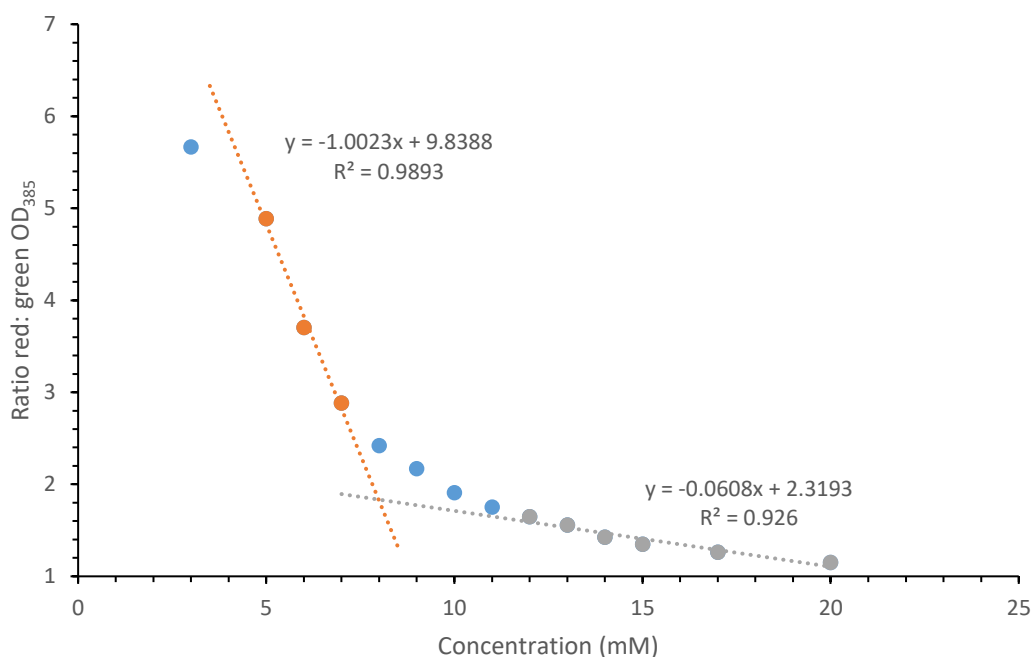


Figure S156: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₅ well scan data obtained for **3** in an EtOH/H₂O 1:19 solution at 318 K, plotted against compound concentration. A CMC value of 7.99 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 3 at 318 K OD₃₈₅

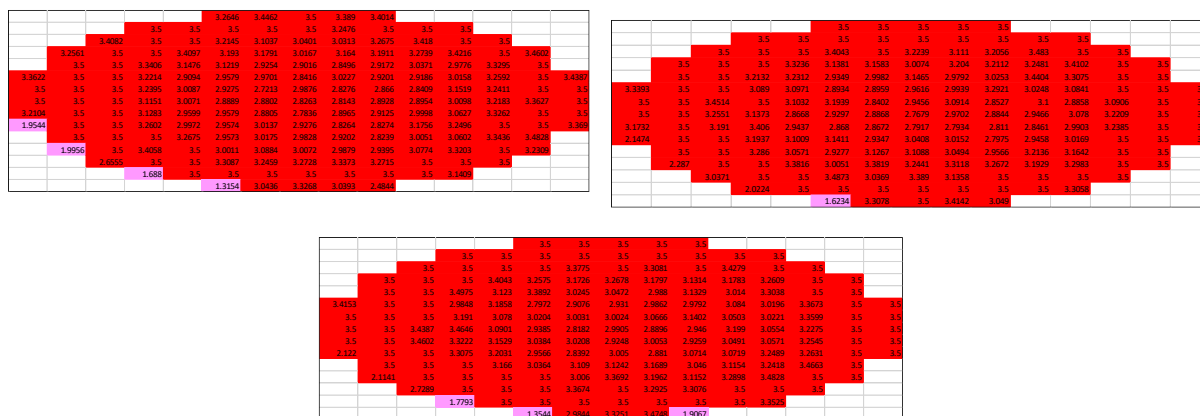


Figure S157: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (20 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

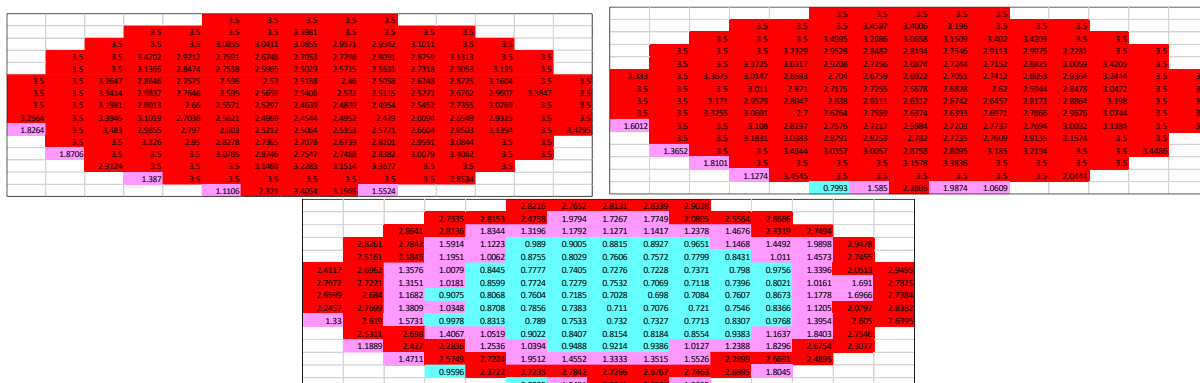


Figure S158: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (17 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S159: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (15 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S160: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (14 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

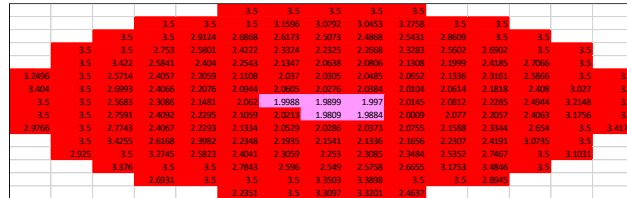
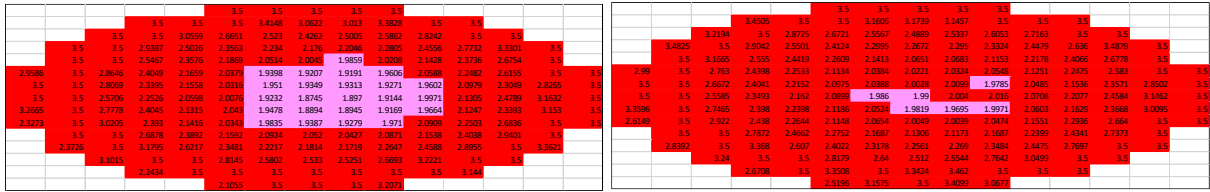


Figure S161: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (13 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

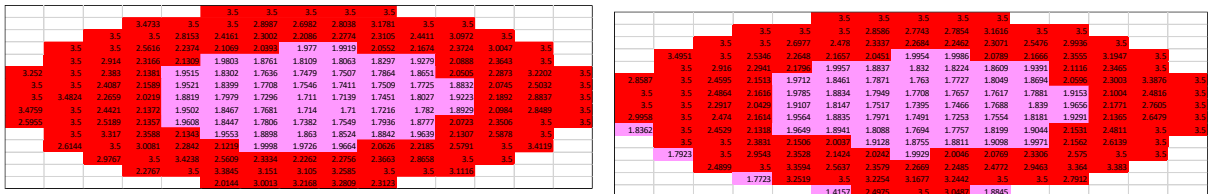


Figure S162: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (12 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

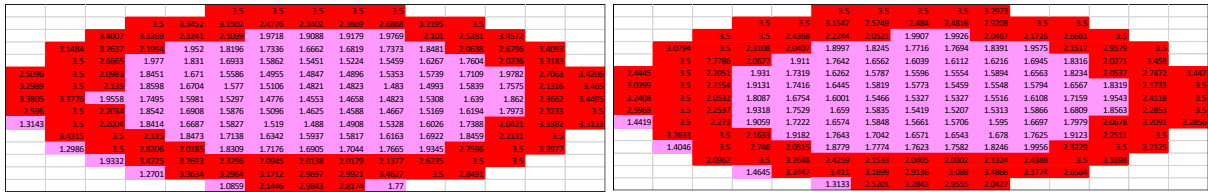


Figure S163: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (11 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

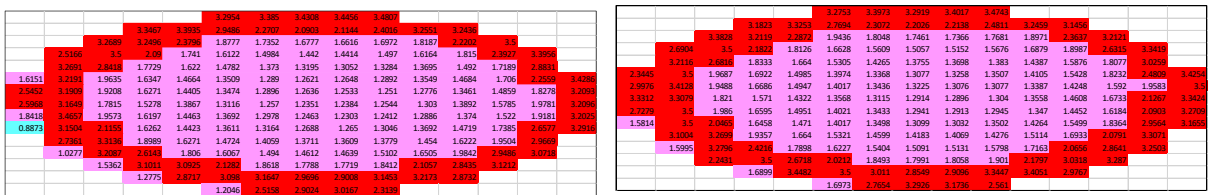


Figure S164: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (10 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

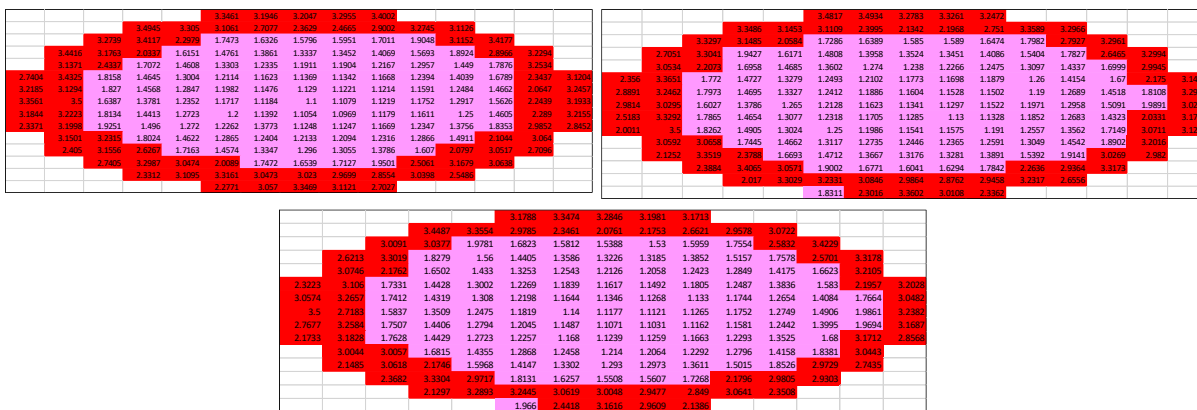


Figure S165: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (9 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S166: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (8 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

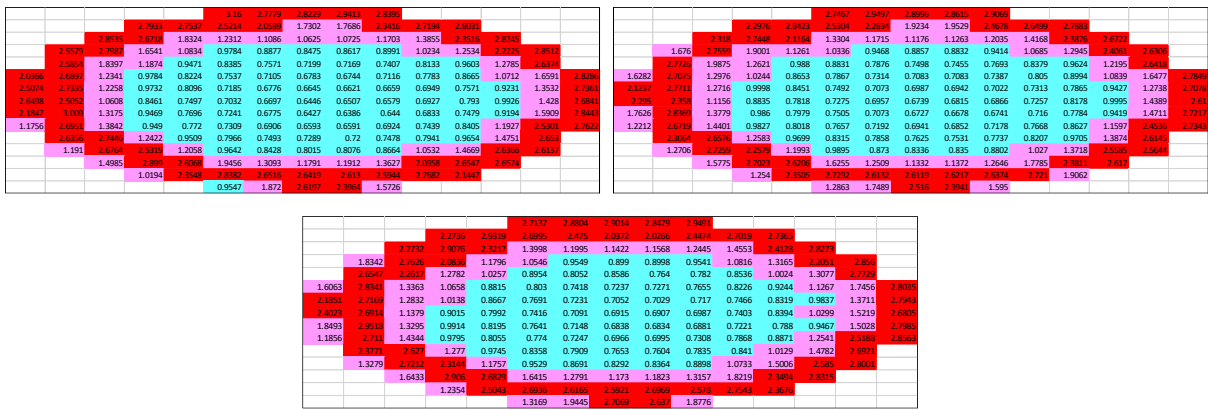


Figure S167: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (7 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



Figure S168: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (6 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

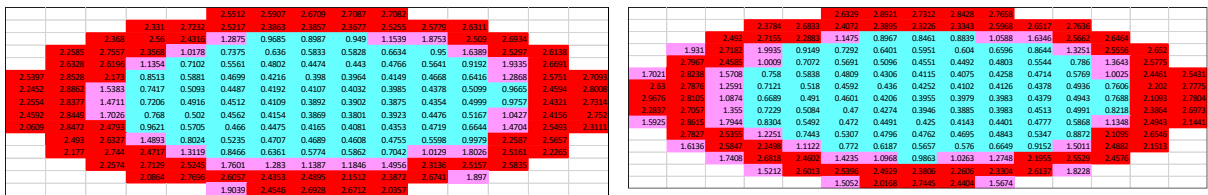


Figure S169: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (5 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.

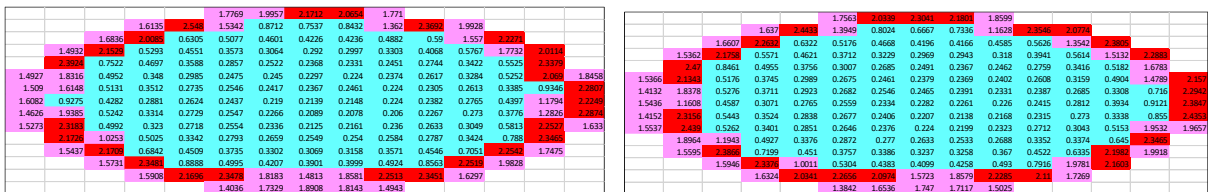
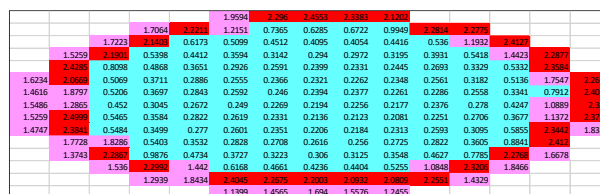


Figure S170: Raw OD₃₈₅ well scan data (n=3) obtained for EtOH/H₂O 1:19 solutions of **3** (3 mM) at 318 K. Colour coded regions: Red = OD₃₈₅ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₅ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₅ ≥ 0.0001.



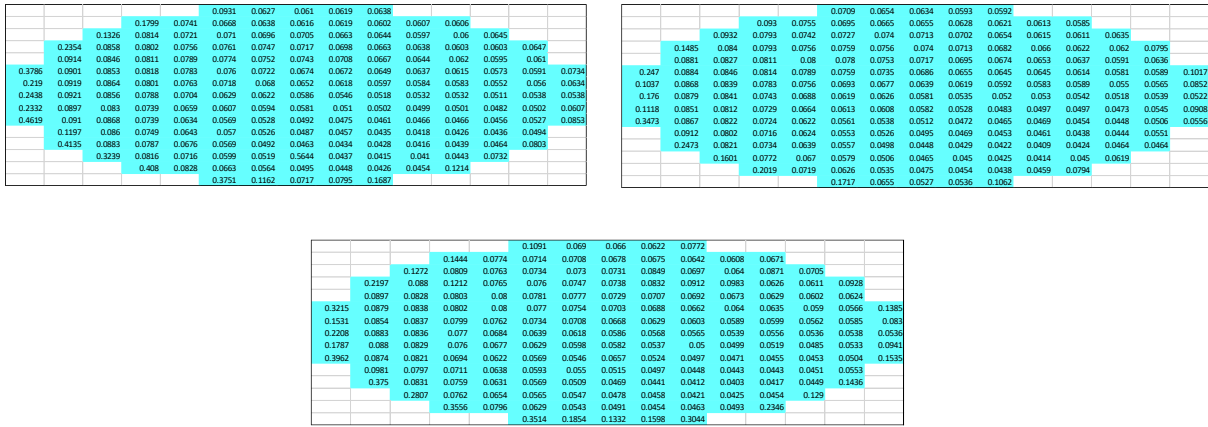


Figure S171: Raw OD₃₈₅ well scan data (n=3) obtained for standard EtOH/H₂O 1:19 solutions at 318 K. Colour coded regions: Red = OD₃₈₀ ≥ 2.0000, Pink = 1.9999 ≥ OD₃₈₀ ≥ 1.0000, cyan = 0.9999 ≥ OD₃₈₀ ≥ 0.0001.

Compound 4 CMC calculation at 298 K OD₃₈₆

Table S24: A summary of OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 298 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Well sections															
Concentration (mM)	n = 1			n = 2			n = 3			Average of n's			+/- error		
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
0.25	0.25	0.09	0.08	0.22	0.09	0.08	0.27	0.09	0.09	0.25	0.09	0.08	0.02	0.00	0.00
1	0.46	0.17	0.16	0.40	0.17	0.16	0.42	0.17	0.16	0.43	0.17	0.16	0.03	0.00	0.00
5	1.44	0.64	0.60	1.47	0.69	0.65	1.55	0.76	0.71	1.49	0.70	0.65	0.05	0.05	0.04
10	2.23	1.39	1.31	2.26	1.48	1.39	2.33	1.50	1.41	2.27	1.45	1.37	0.04	0.05	0.04
12	2.46	1.64	1.55	2.60	1.74	1.65	2.57	1.74	1.63	2.54	1.71	1.61	0.06	0.05	0.04
14	2.71	1.92	1.80	2.83	2.04	1.93	2.80	2.07	1.95	2.78	2.01	1.89	0.05	0.07	0.07
16	3.02	2.18	2.06	3.00	2.23	2.09	3.02	2.26	2.12	3.02	2.22	2.09	0.01	0.03	0.03
18	3.15	2.45	2.32	3.18	2.49	2.37	3.13	2.45	2.32	3.16	2.46	2.34	0.02	0.02	0.02
20	3.21	2.62	2.51	3.30	2.77	2.61	3.31	2.76	2.61	3.27	2.72	2.58	0.04	0.07	0.05
22	3.31	2.86	2.76	3.30	2.83	2.69	3.32	2.83	2.71	3.31	2.84	2.72	0.01	0.01	0.03
24	3.42	3.05	2.93	3.42	3.09	3.02	3.44	3.17	3.05	3.43	3.11	3.00	0.01	0.05	0.05
26	3.44	3.23	3.13	3.40	3.06	2.94	3.40	3.26	3.29	3.41	3.18	3.12	0.02	0.09	0.14
30	3.41	3.42	3.33	3.40	3.42	3.40	3.43	3.43	3.38	3.41	3.42	3.37	0.01	0.01	0.03
45	3.34	3.44	3.40	3.27	3.44	3.45	3.33	3.46	3.39	3.31	3.45	3.41	0.03	0.01	0.03
50	3.34	3.49	3.49	3.40	3.49	3.44	3.39	3.50	3.48	3.37	3.49	3.47	0.02	0.00	0.02

Table S25: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Red	Green	Ratio red: green
0.25	0.25	0.08	2.96
1	0.43	0.16	2.68
5	1.49	0.65	2.27
10	2.27	1.37	1.66
12	2.54	1.61	1.58
14	2.78	1.89	1.47
16	3.02	2.09	1.44
18	3.16	2.34	1.35
20	3.27	2.58	1.27
22	3.31	2.72	1.22
24	3.43	3.00	1.14
26	3.41	3.12	1.09
30	3.41	3.37	1.01
45	3.31	3.41	0.97
50	3.37	3.47	0.97

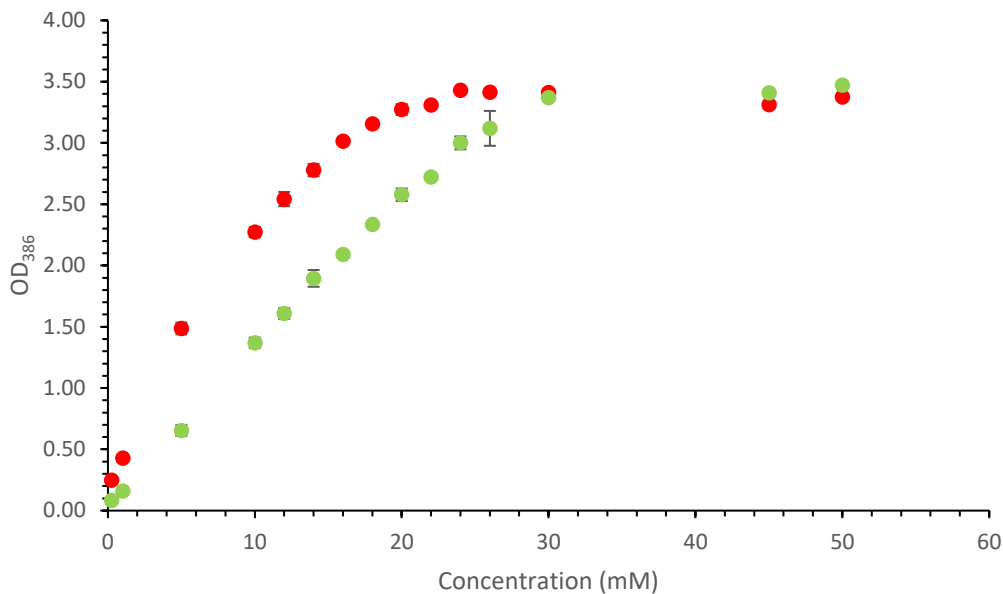


Figure S172: Graph showing average (n=3) red - interface and green - control OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 298 K.

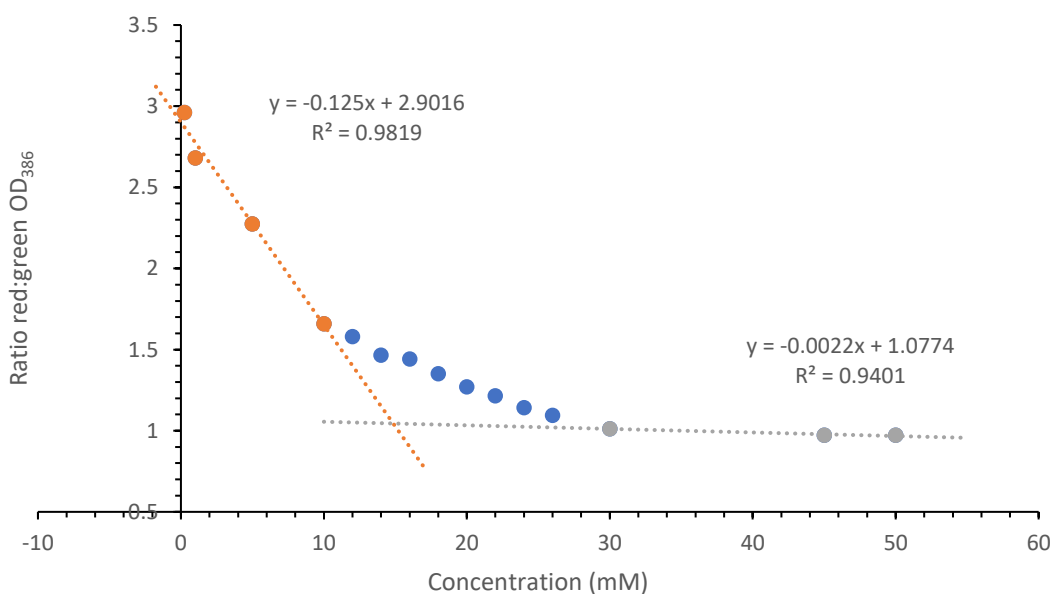


Figure S173: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 298 K, plotted against compound concentration. A CMC value of 14.86 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 4 at 298 K OD₂₈₆.

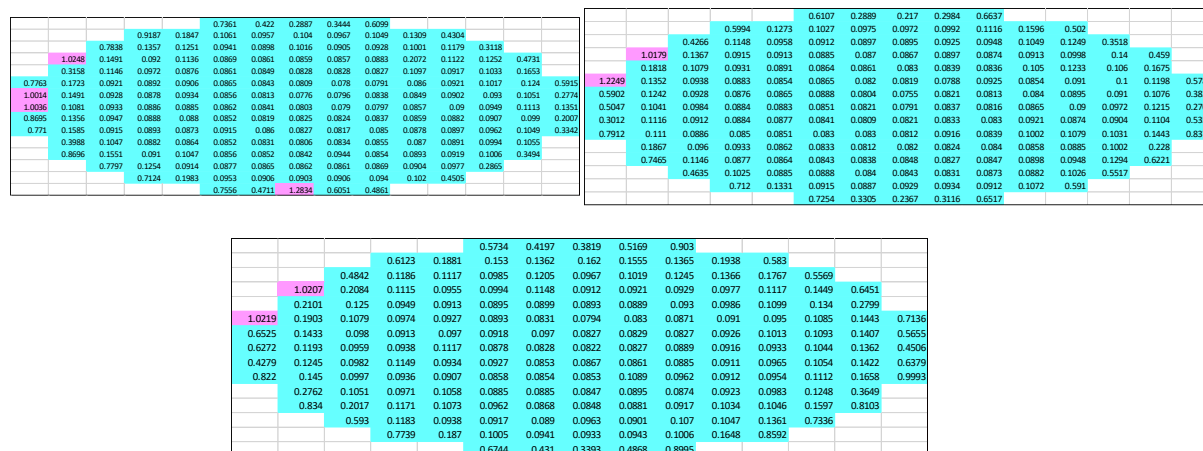


Figure S174: A 0.25 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.



Figure S175: A 1 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

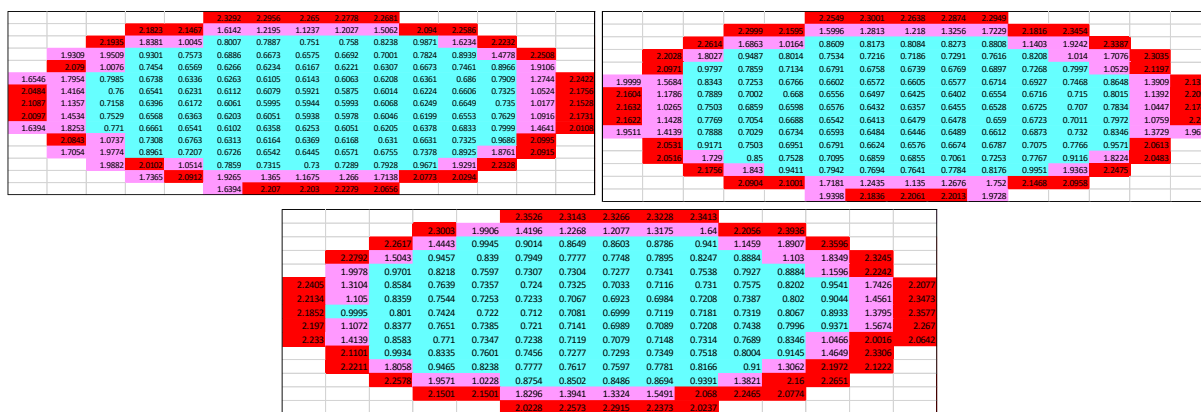


Figure S176: A 5 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

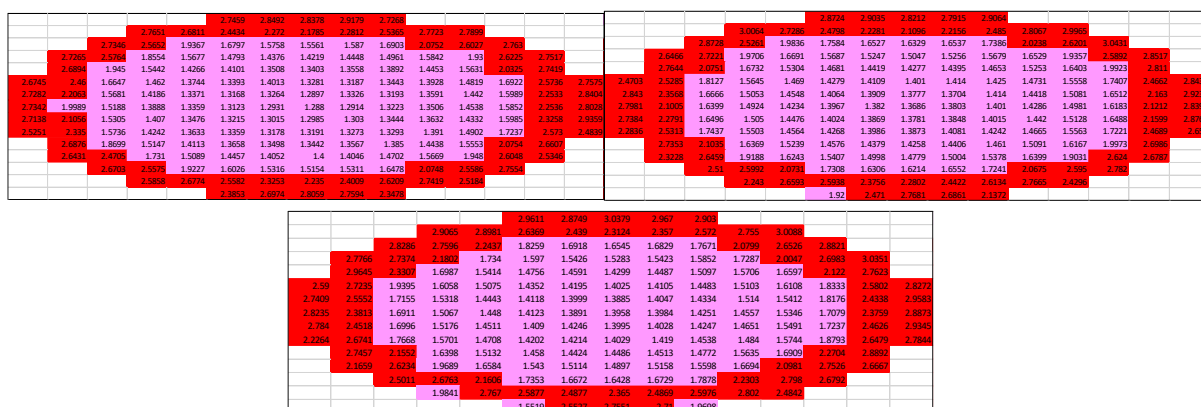


Figure S177: A 10 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.



Figure S178: A 12 mM EtOH/H₂O 1:19 solution of compound **4** at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

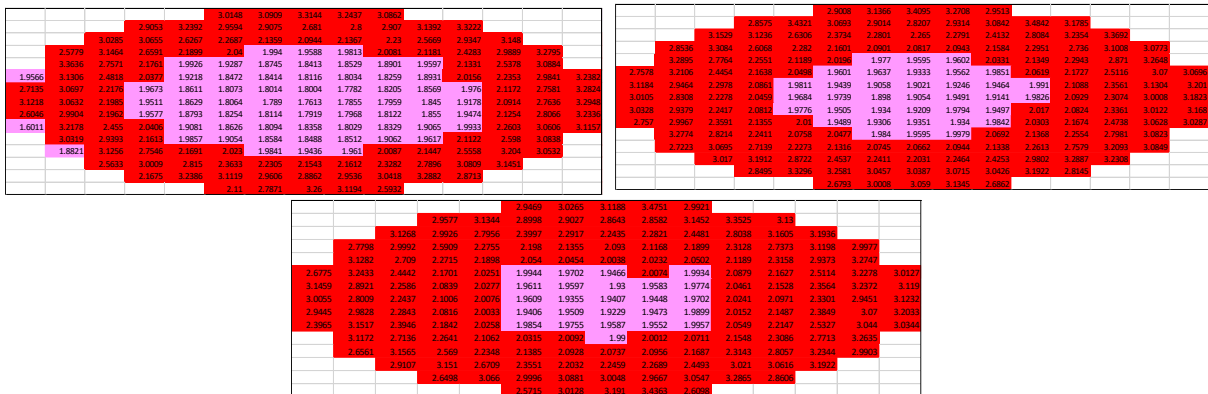


Figure S179: A 14 mM EtOH/H₂O 1:19 solution of compound **4** at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

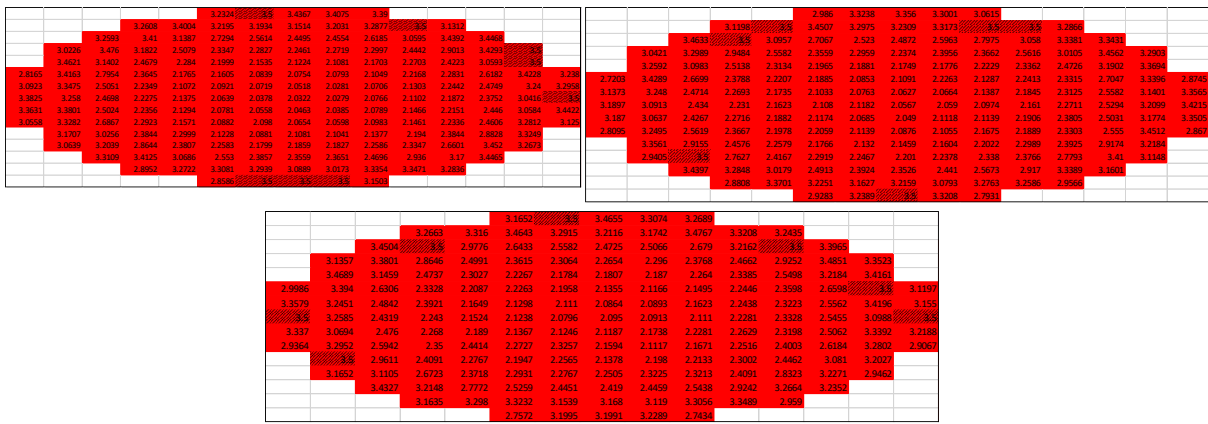


Figure S180: A 16 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

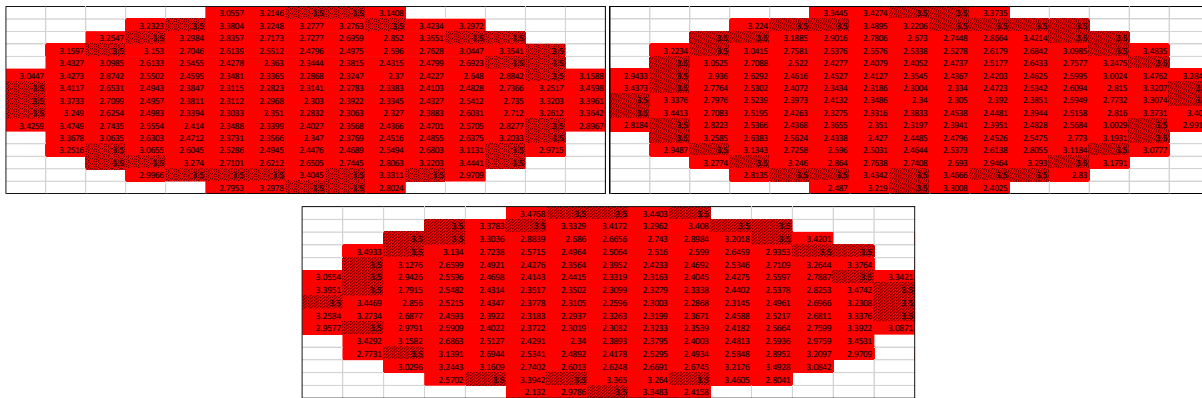


Figure S181: A 18 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

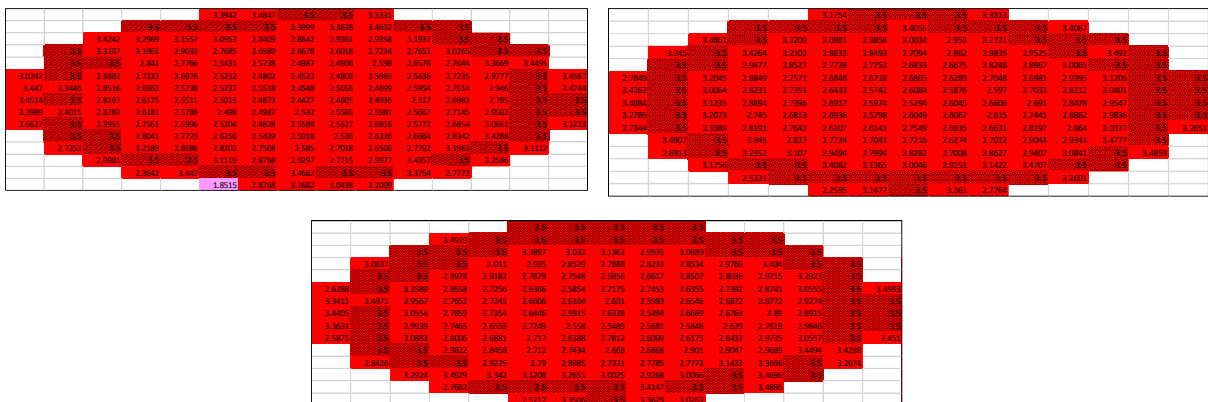


Figure S182: A 20 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

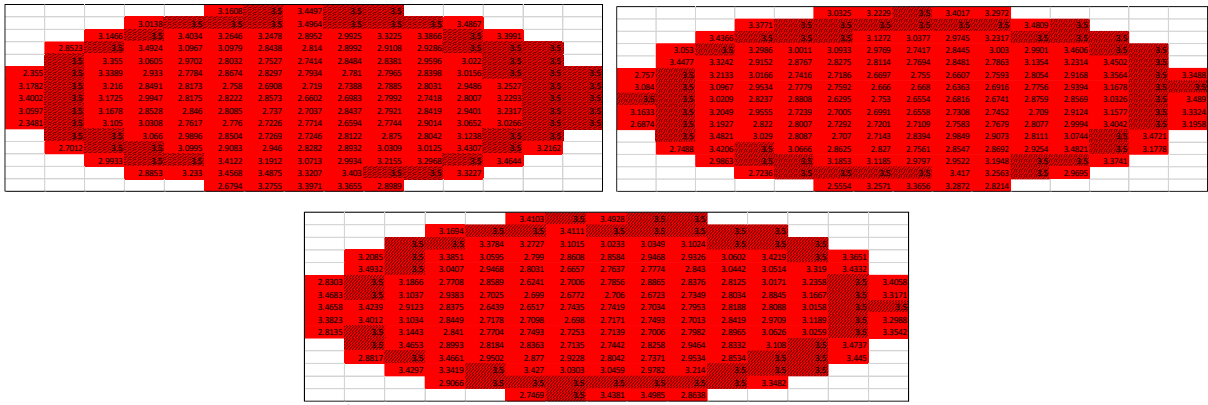


Figure S183: A 22 mM EtOH/H₂O 1:19 solution of compound **4** at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

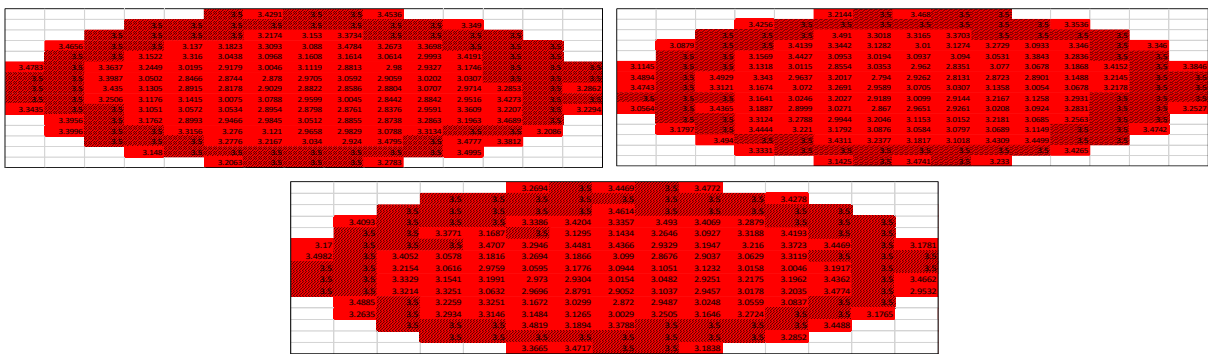


Figure S184: A 24 mM EtOH/H₂O 1:19 solution of compound **4** at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

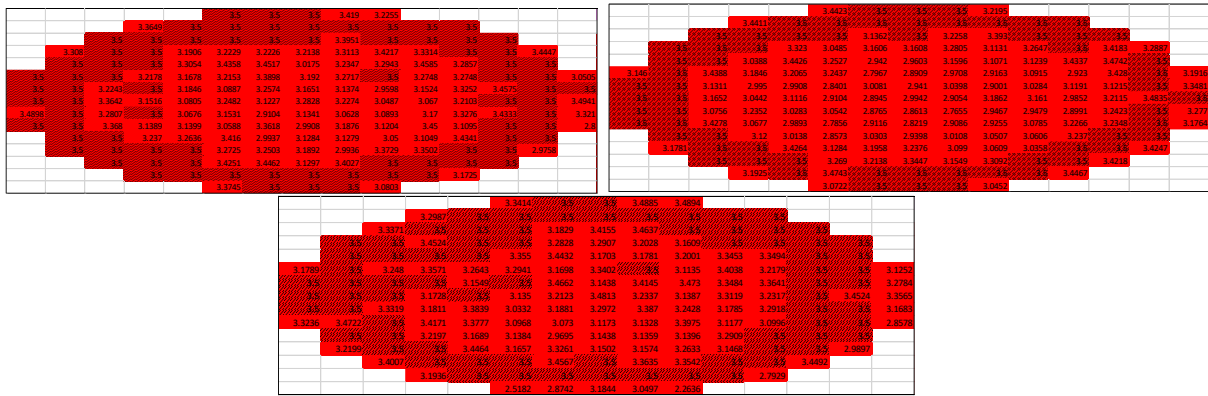


Figure S185: A 26 mM EtOH/H₂O 1:19 solution of compound **4** at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

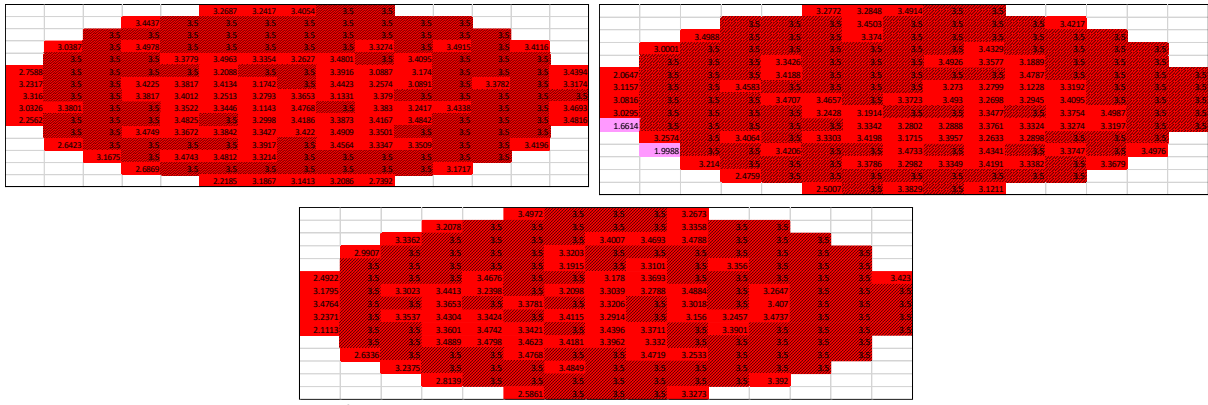


Figure S186: A 30 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.



Figure S187: A 45 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

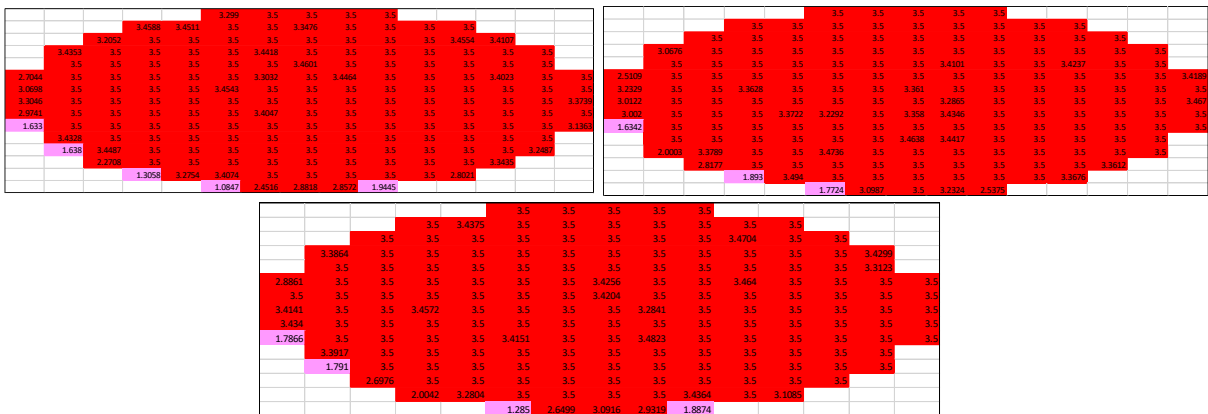


Figure S188: A 50 mM EtOH/H₂O 1:19 solution of compound 4 at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

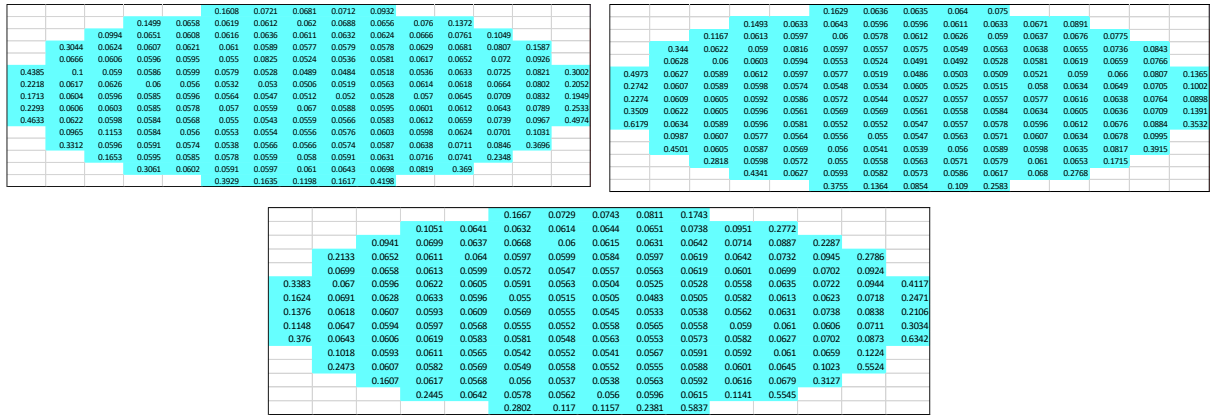


Figure S189: Standard EtOH/H₂O 1:19 solutions at 298 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

Compound 4 CMC calculation at 308 K OD₃₈₆

Table S26: A summary of OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 308 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Well sections															
Concentration (mM)	n = 1			n = 2			n = 3			Average of n's			+/- error		
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
0.25	0.27	0.09	0.08	0.25	0.09	0.08	0.29	0.09	0.09	0.27	0.09	0.08	0.02	0.00	0.00
1	0.41	0.16	0.16	0.38	0.17	0.15	0.42	0.17	0.16	0.40	0.17	0.16	0.02	0.00	0.00
5	1.60	0.63	0.59	1.61	0.67	0.63	1.68	0.74	0.69	1.63	0.68	0.64	0.03	0.04	0.04
10	2.42	1.35	1.25	2.45	1.43	1.33	2.51	1.45	1.35	2.46	1.41	1.31	0.03	0.04	0.04
12	2.64	1.58	1.48	2.77	1.69	1.57	2.76	1.67	1.58	2.72	1.65	1.54	0.06	0.04	0.05
14	2.90	1.85	1.72	3.07	1.96	1.85	3.04	1.99	1.88	3.00	1.93	1.82	0.07	0.06	0.07
16	3.16	2.06	1.92	3.15	2.12	1.98	3.18	2.15	2.05	3.17	2.11	1.98	0.01	0.04	0.05
18	3.25	2.35	2.23	3.25	2.37	2.20	3.25	2.30	2.21	3.25	2.34	2.21	0.00	0.03	0.01
20	3.29	2.53	2.41	3.34	2.69	2.56	3.37	2.64	2.58	3.33	2.62	2.52	0.03	0.07	0.07
22	3.40	2.79	2.71	3.39	2.83	2.76	3.41	2.81	2.64	3.40	2.81	2.70	0.01	0.02	0.05
24	3.47	3.15	3.14	3.47	3.16	3.20	3.47	3.20	3.18	3.47	3.17	3.17	0.00	0.02	0.03
26	3.49	3.32	3.27	3.48	3.06	3.10	3.49	3.42	3.38	3.49	3.27	3.25	0.01	0.15	0.12
30	3.48	3.50	3.50	3.46	3.50	3.50	3.48	3.50	3.50	3.48	3.50	3.50	0.01	0.00	0.00
45	3.41	3.49	3.32	3.33	3.48	3.38	3.37	3.48	3.35	3.37	3.48	3.35	0.03	0.00	0.02
50	3.40	3.50	3.50	3.45	3.50	3.50	3.43	3.50	3.50	3.43	3.50	3.50	0.02	0.00	0.00

Table S27: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 308 K.

Concentration (mM)	Red	Green	Ratio Red: Green
0.25	0.27	0.08	3.26
1	0.40	0.16	2.58
5	1.63	0.64	2.56
10	2.46	1.31	1.88
12	2.72	1.54	1.76
14	3.00	1.82	1.65
16	3.17	1.98	1.60
18	3.25	2.21	1.47
20	3.33	2.52	1.32
22	3.40	2.70	1.26
24	3.47	3.17	1.09
26	3.49	3.25	1.07
30	3.48	3.50	0.99
45	3.37	3.35	1.01
50	3.43	3.50	0.98

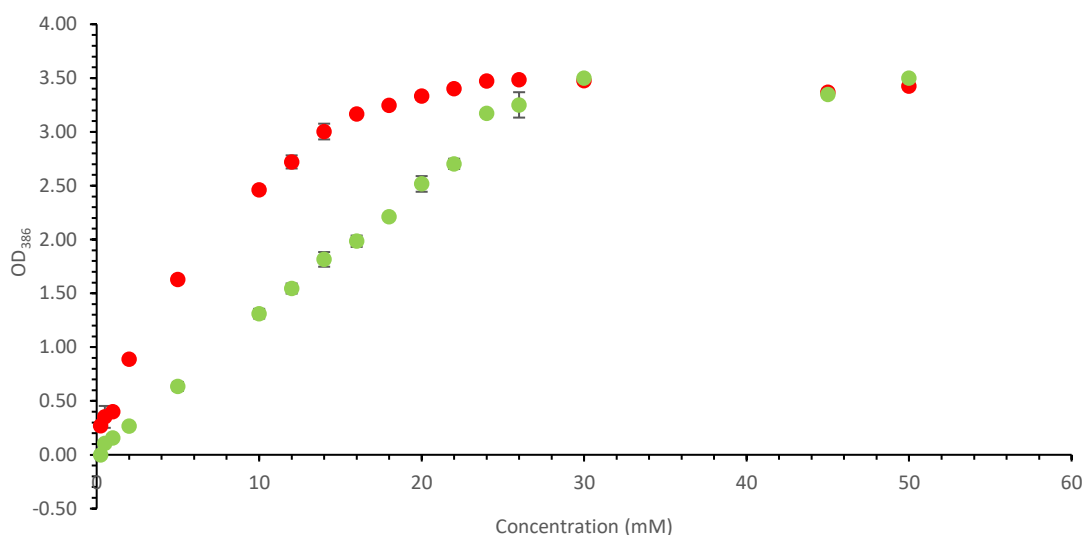


Figure S190: Graph showing average (n=3) red - interface and green - control OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 308 K.

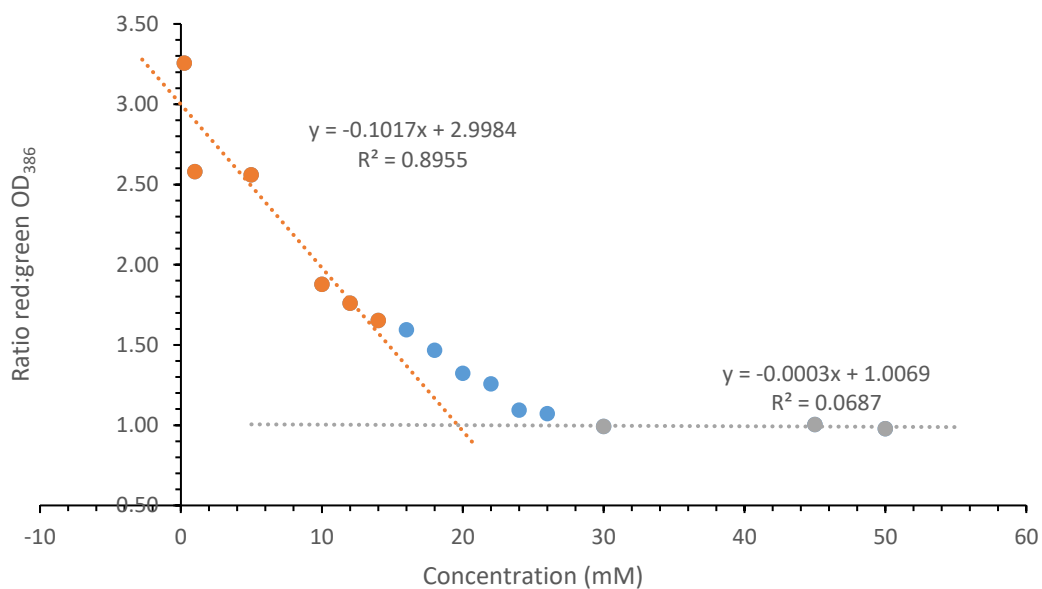


Figure S191: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 308 K, plotted against compound concentration. A CMC value of 19.64 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 4 at 308 K OD₃₈₆



Figure S192: A 0.25 mM EtOH/H₂O 1:19 solution of compound 4 at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

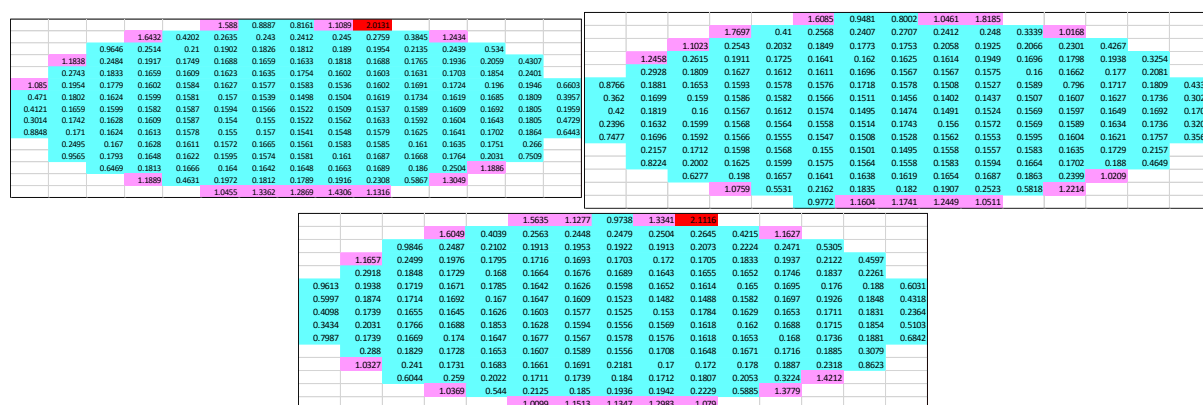


Figure S193: A 1 mM EtOH/H₂O 1:19 solution of compound 4 at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

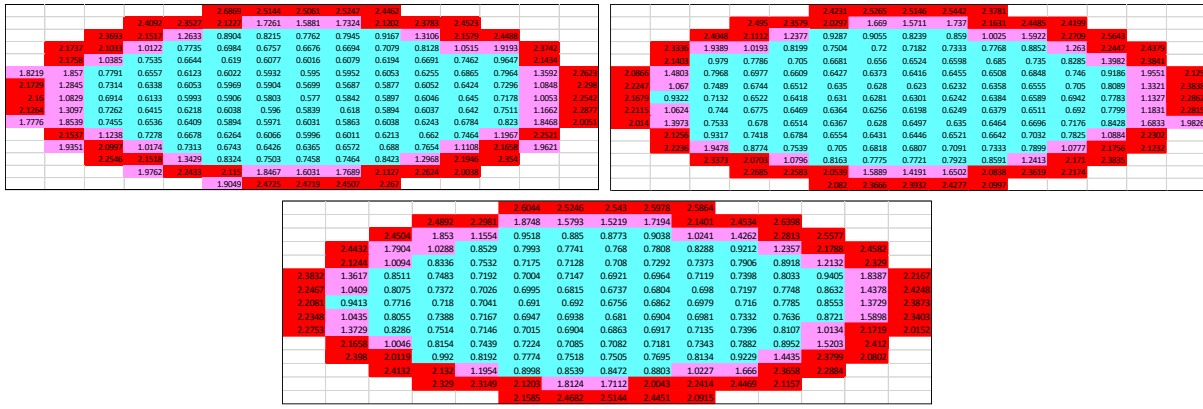


Figure S194: A 5 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

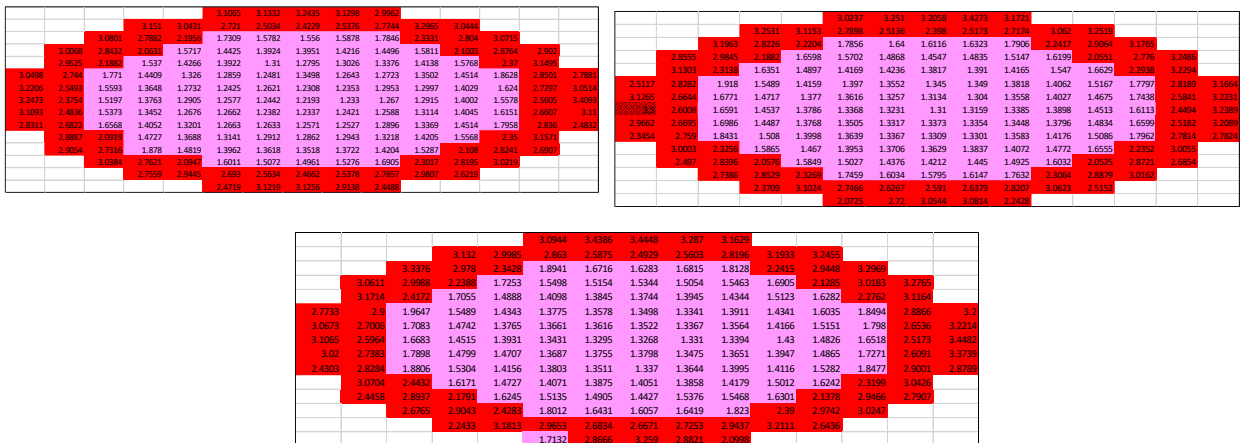


Figure S195: A 10 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

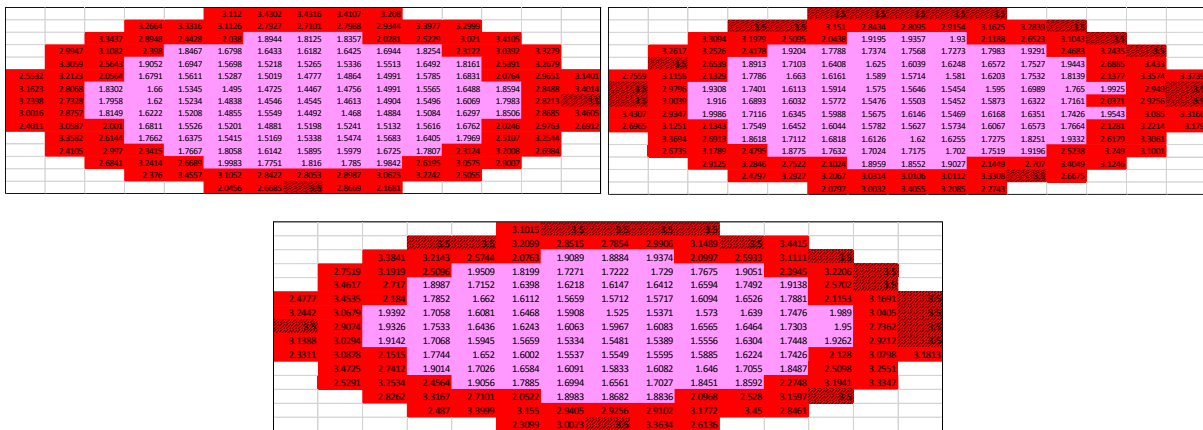


Figure S196: A 12 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

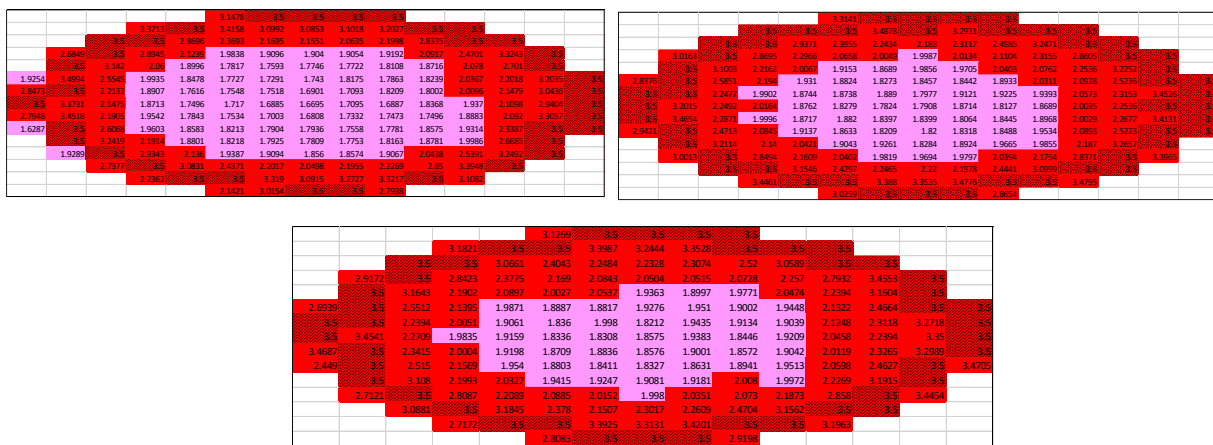


Figure S197: A 14 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

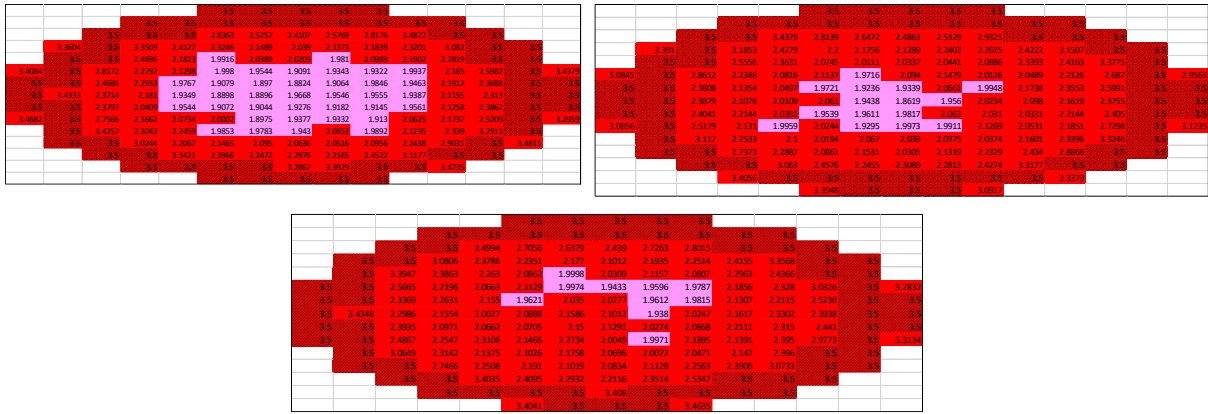


Figure S198: A 16mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

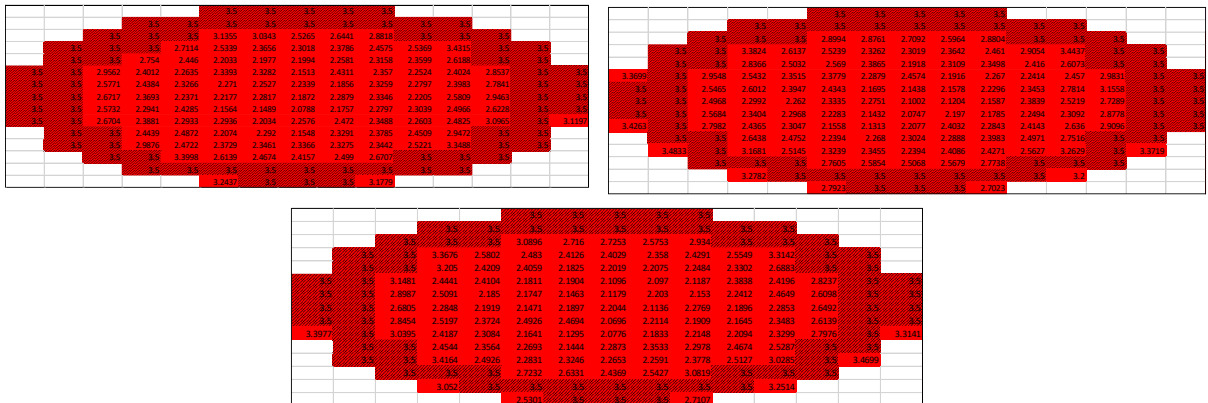


Figure S199: A 18 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

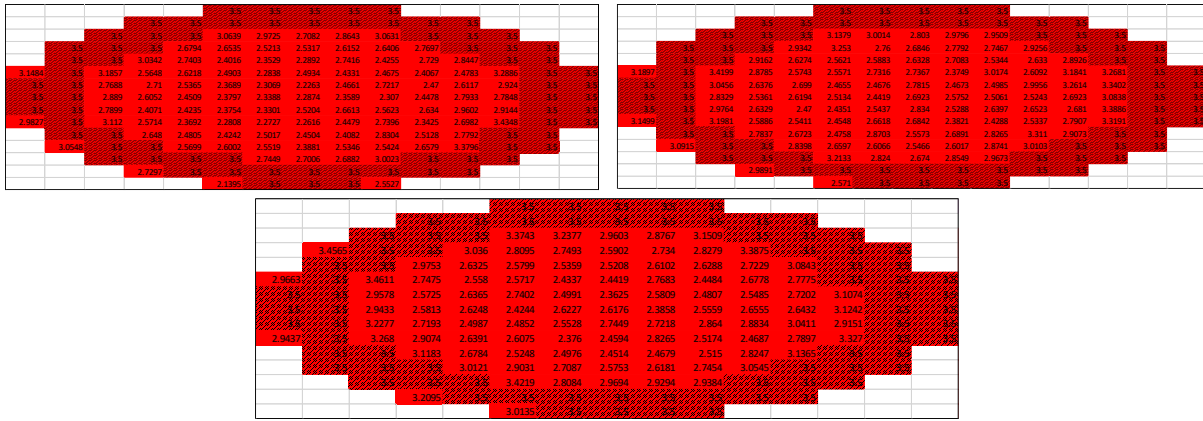


Figure S200: A 20 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

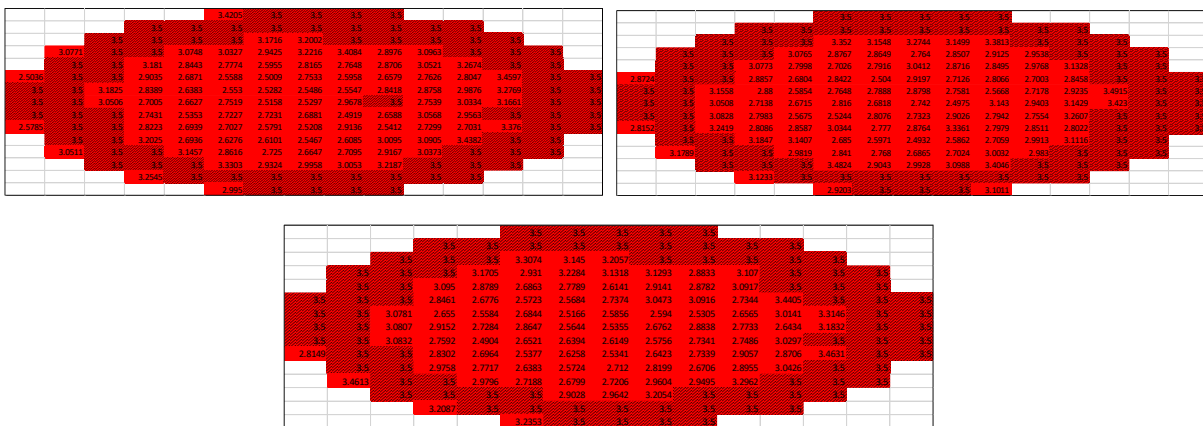


Figure S201: A 22 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

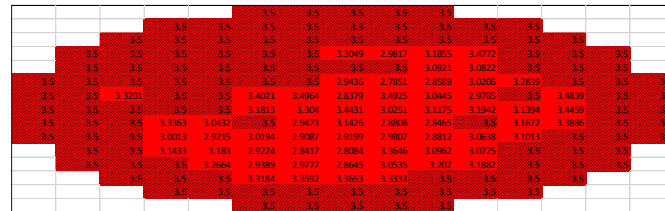
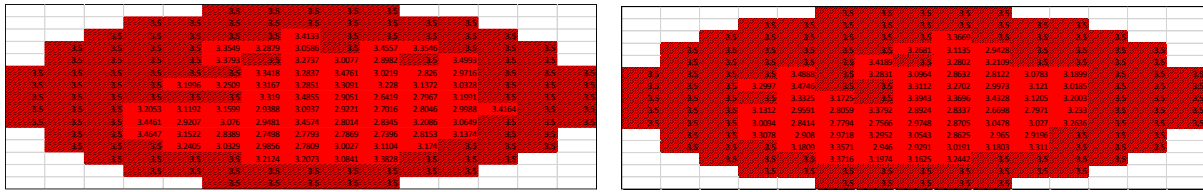


Figure S202: A 24 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

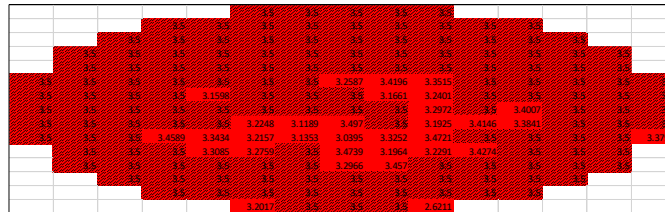
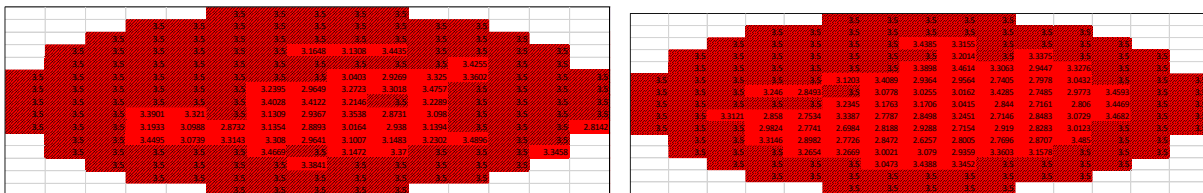


Figure S203: A 26 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

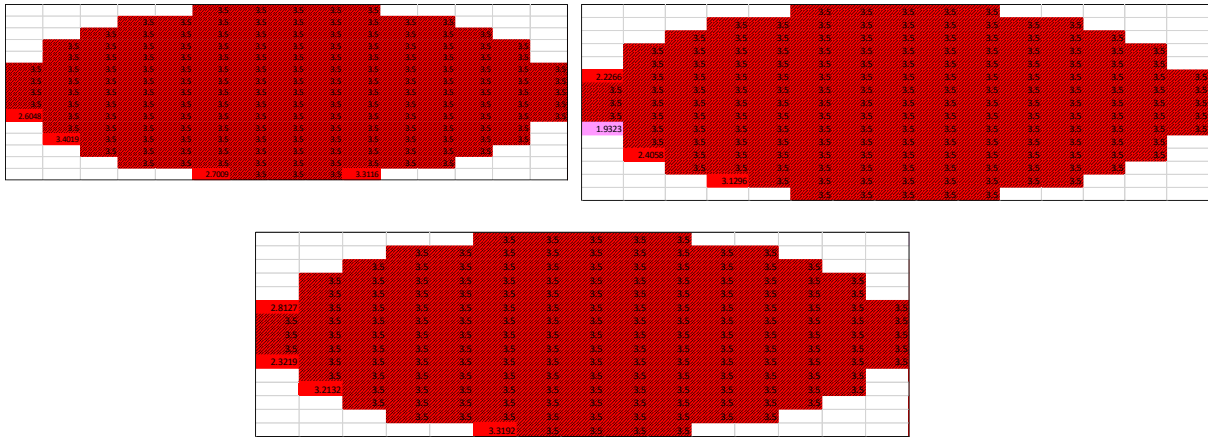


Figure S204: A 30 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

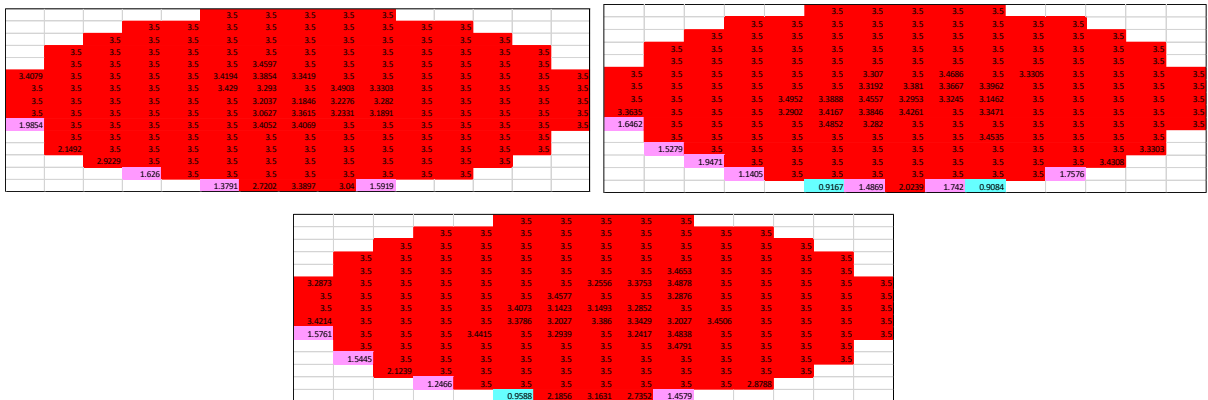


Figure S205: A 45 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

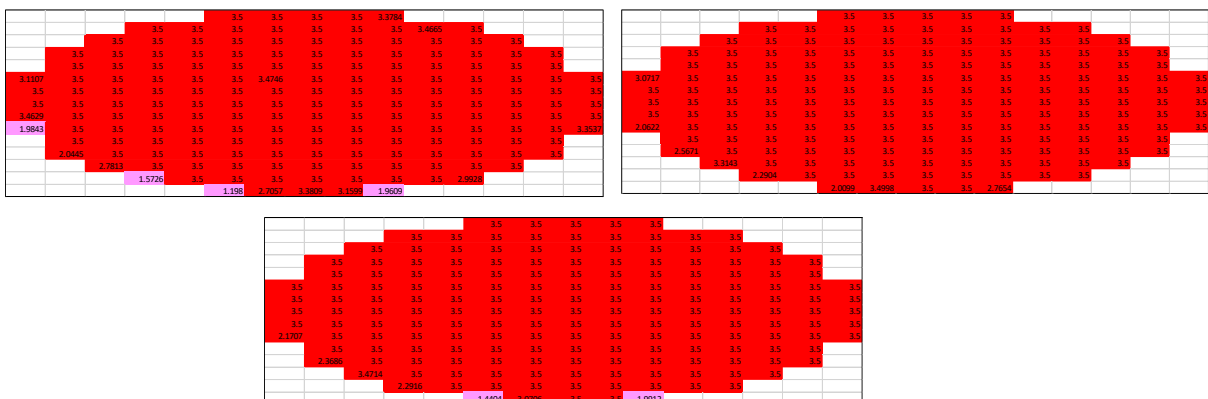


Figure S206: A 50 mM EtOH/H₂O 1:19 solution of compound **4** at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

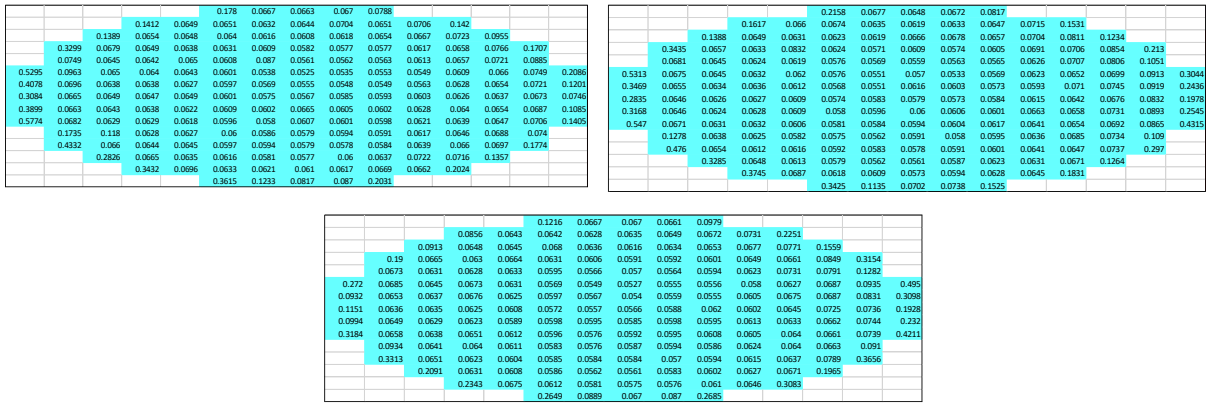


Figure S207: Standard EtOH/H₂O 1:19 solutions at 308 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

Compound 4 CMC calculation at 318 K OD₃₈₆

Table S28: A summary of OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 318 K. These data should be interpreted alongside the appropriate methodology section (CMC microplate reader studies) and diagram given in Figure S27. Error = Standard error of mean.

Concentration (mM)	Well sections												+/- error		
	n = 1			n = 2			n = 3			Average of n's					
	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green	Red	Yellow	Green
0.25	0.26	0.08	0.08	0.23	0.09	0.08	0.23	0.09	0.09	0.24	0.09	0.08	0.01	0.00	0.00
1	0.50	0.16	0.15	0.48	0.17	0.15	0.54	0.16	0.15	0.51	0.16	0.15	0.03	0.00	0.00
5	1.73	0.61	0.57	1.74	0.65	0.60	1.74	0.71	0.66	1.74	0.66	0.61	0.01	0.04	0.04
10	2.33	1.27	1.17	2.36	1.35	1.28	2.39	1.37	1.26	2.36	1.33	1.23	0.02	0.04	0.05
12	2.48	1.48	1.40	2.58	1.57	1.50	2.55	1.57	1.46	2.53	1.54	1.45	0.04	0.04	0.04
14	2.70	1.72	1.70	2.74	1.83	2.01	2.75	1.88	1.96	2.73	1.81	1.89	0.02	0.06	0.13
16	2.99	1.93	2.02	2.95	2.02	2.25	2.97	2.03	2.12	2.97	1.99	2.13	0.02	0.04	0.09
18	3.04	2.19	2.36	3.08	2.20	2.11	3.11	2.19	2.11	3.08	2.19	2.19	0.03	0.01	0.12
20	3.12	2.38	2.62	3.16	2.49	2.87	3.19	2.47	2.43	3.16	2.45	2.64	0.03	0.05	0.18
22	3.24	2.58	2.64	3.25	2.56	2.65	3.29	2.55	2.47	3.26	2.56	2.59	0.02	0.01	0.08
24	3.34	2.74	2.65	3.36	2.81	2.78	3.34	2.88	2.81	3.35	2.81	2.75	0.01	0.06	0.07
26	3.36	3.00	2.89	3.35	2.82	2.79	3.41	3.14	3.17	3.37	2.99	2.95	0.03	0.13	0.16
30	3.48	3.39	3.20	3.46	3.44	3.43	3.47	3.43	3.47	3.47	3.42	3.37	0.01	0.02	0.11
45	3.35	3.01	2.71	3.26	2.93	2.64	3.30	2.97	2.82	3.30	2.97	2.72	0.04	0.03	0.07
50	3.36	3.19	2.91	3.41	3.32	3.12	3.43	3.42	3.40	3.40	3.31	3.14	0.03	0.09	0.20

Table S29: Table summarizing the ratio of Red: Green section values calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 318 K.

Concentration (mM)	Red	Green	Ratio Red: Green
0.25	0.24	0.08	2.86
1	0.51	0.15	3.34
5	1.74	0.61	2.85
10	2.36	1.23	1.91
12	2.53	1.45	1.74
14	2.73	1.89	1.44
16	2.97	2.13	1.39
18	3.08	2.19	1.40
20	3.16	2.64	1.20
22	3.26	2.59	1.26
24	3.35	2.75	1.22
26	3.37	2.95	1.14
30	3.47	3.37	1.03
45	3.30	2.72	1.21
50	3.40	3.14	1.08

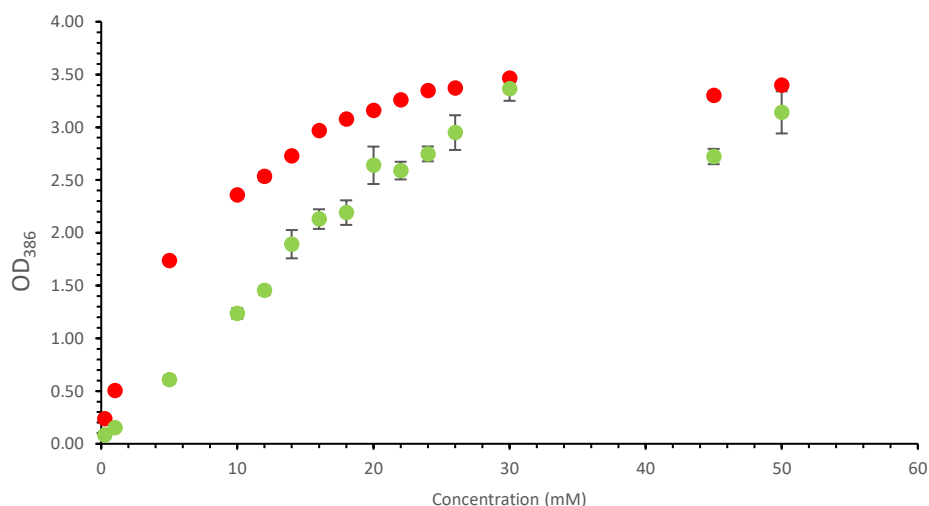


Figure S208: Graph showing average (n=3) red - interface and green - control OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 318 K.

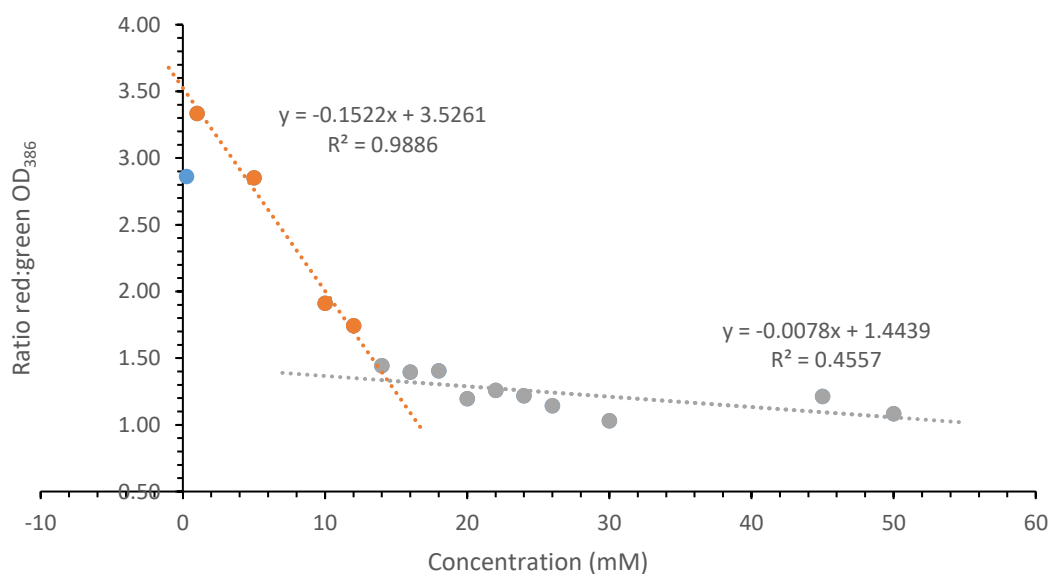


Figure S209: Graph showing the ratio of Red: Green section values, calculated from average (n=3) OD₃₈₆ well scan data obtained for **4** in an EtOH/H₂O 1:19 solution at 318 K, plotted against compound concentration. A CMC value of 14.42 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect. Those data points shown in blue points were not included within the fitting of either linear trend.

Raw well data for compound 4 at 318 K OD₃₈₆



Figure S210: A 0.25 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

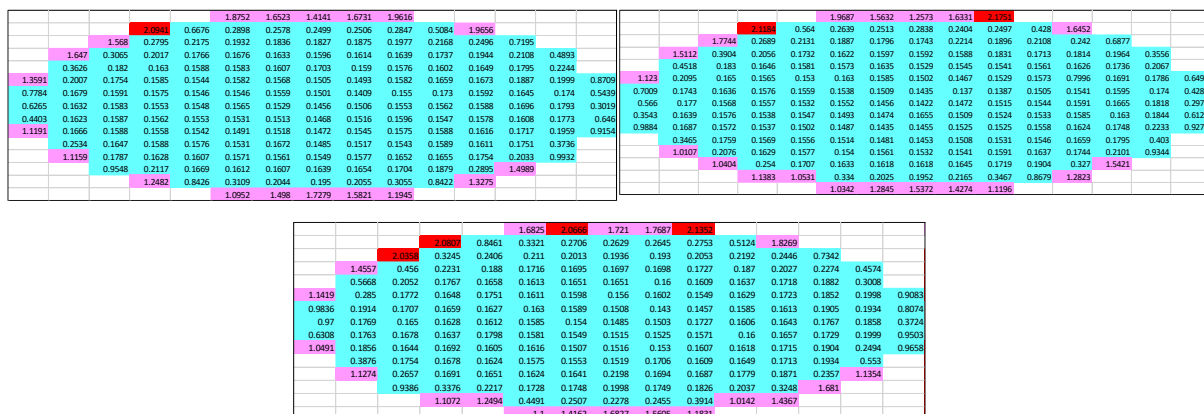


Figure S211: A 1 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

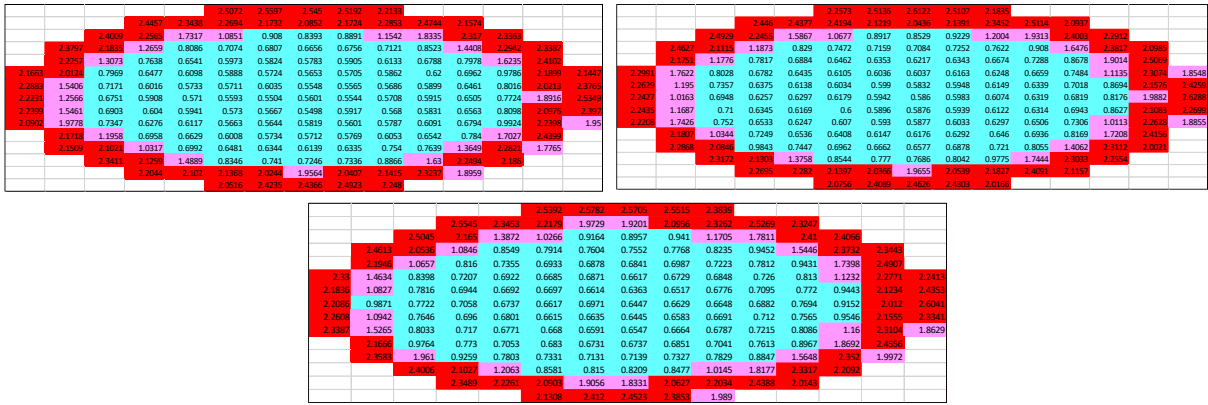


Figure S212: A 5 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

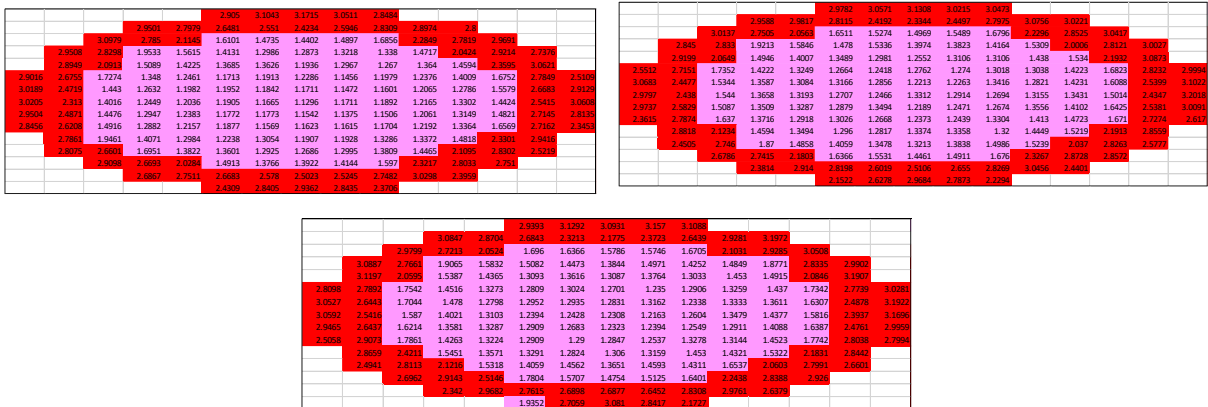


Figure S213: A 10 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

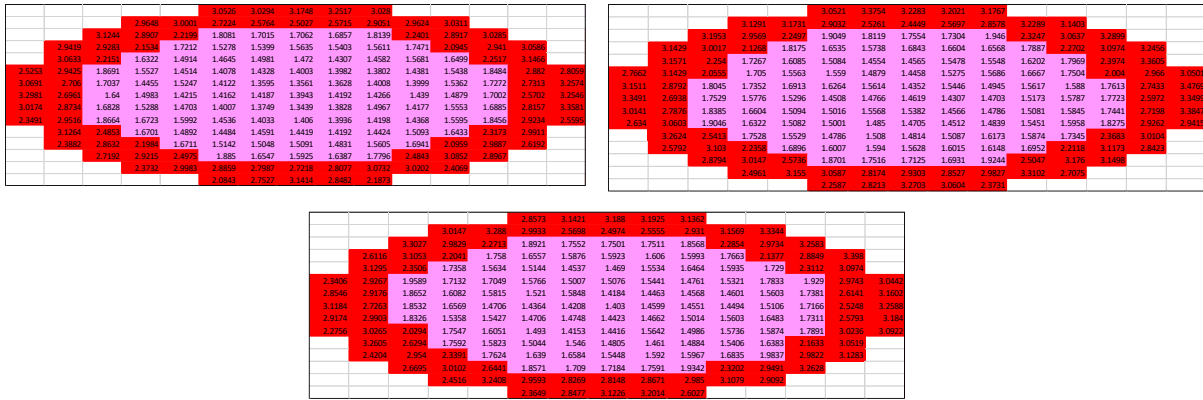


Figure S214: A 12 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.



Figure S215: A 14 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 - 1, cyan = 0.9999 - 0.0001 OD₃₈₆.

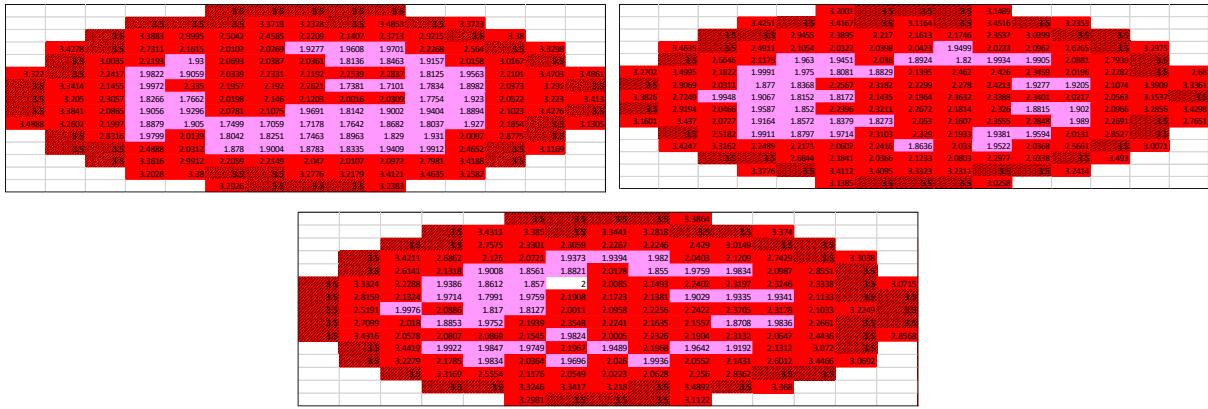


Figure S216: A 16 mM EtOH/H₂O 1:19 solution of compound **4** at 318 KOD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

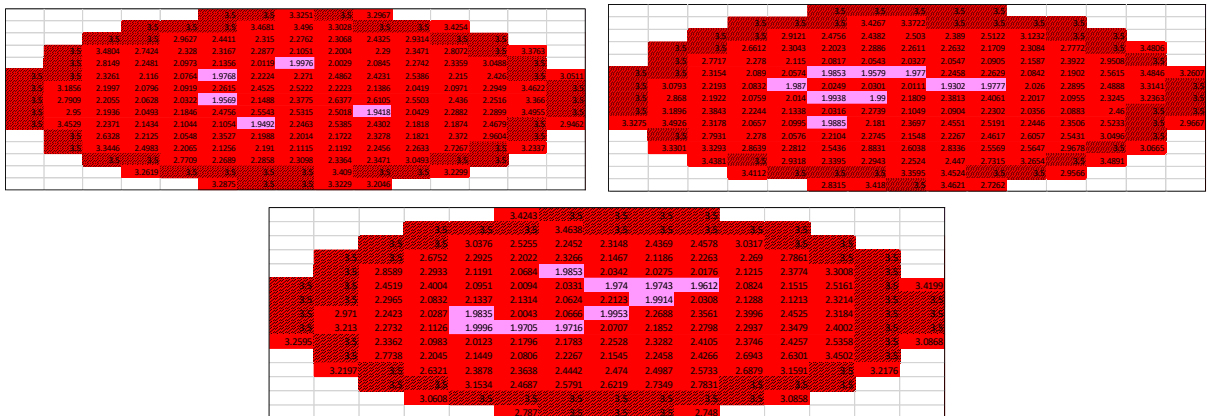


Figure S217: A 18 mM EtOH/H₂O 1:19 solution of compound **4** at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

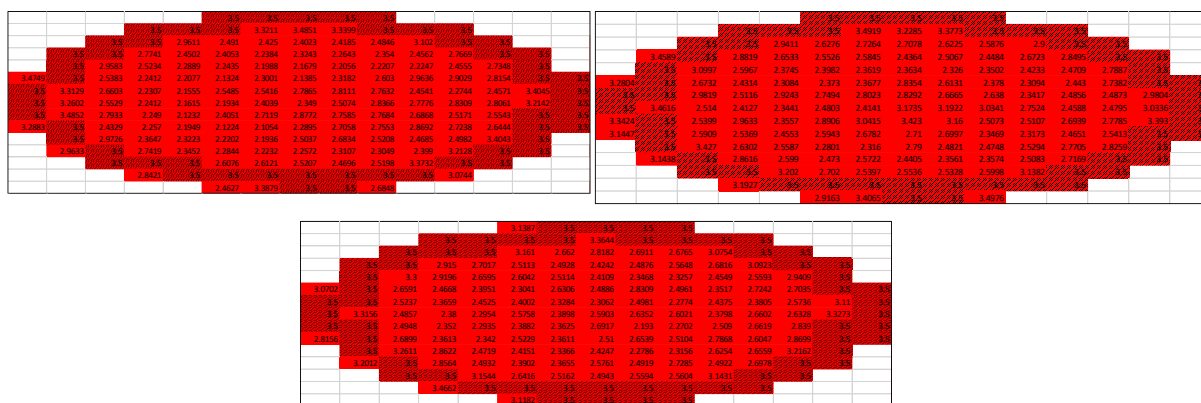


Figure S218: A 20 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

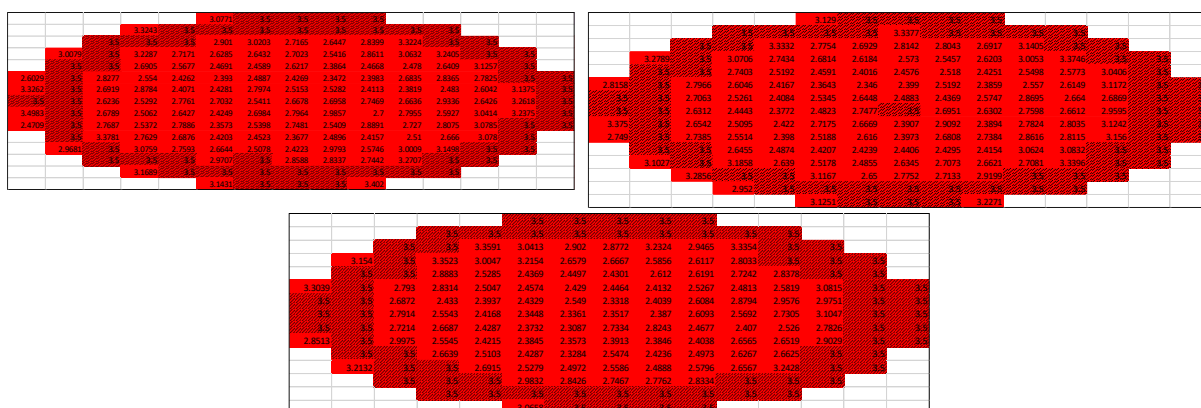


Figure S219: A 22 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2 , Pink = $1.9999 - 1$, cyan = $0.9999 - 0.0001$ OD₃₈₆.

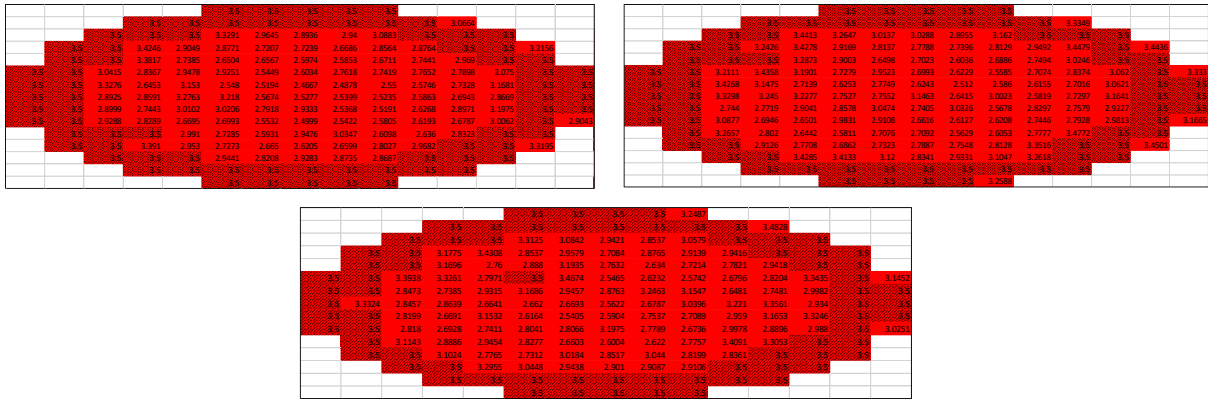


Figure S220: A 24 mM EtOH/H₂O 1:19 solution of compound **4** at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

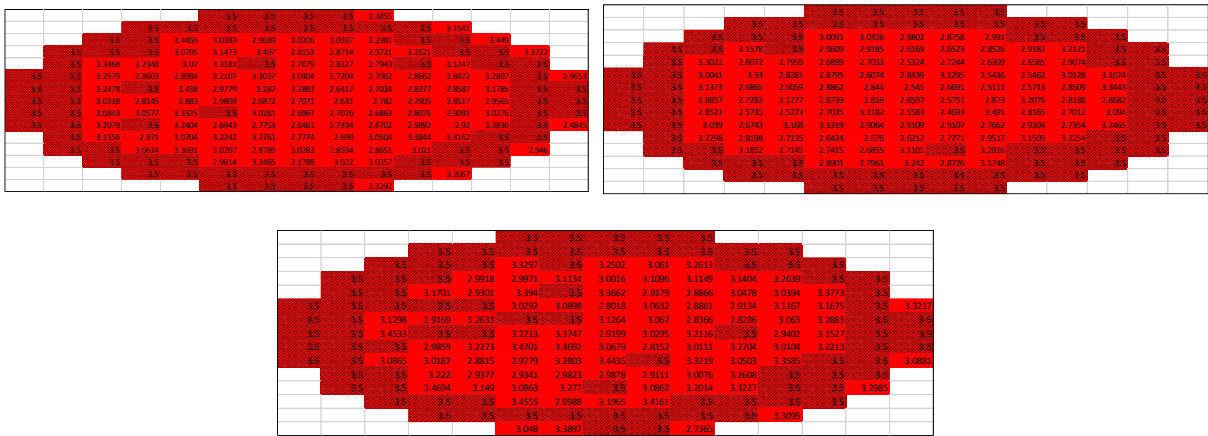


Figure S221: A 26 mM EtOH/H₂O 1:19 solution of compound **4** at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

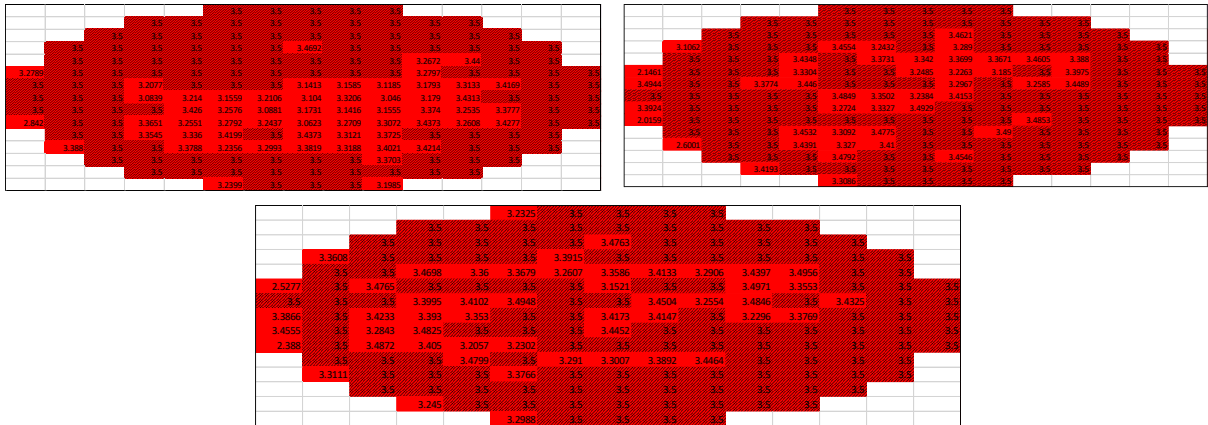


Figure S222: A 30 mM EtOH/H₂O 1:19 solution of compound **4** at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

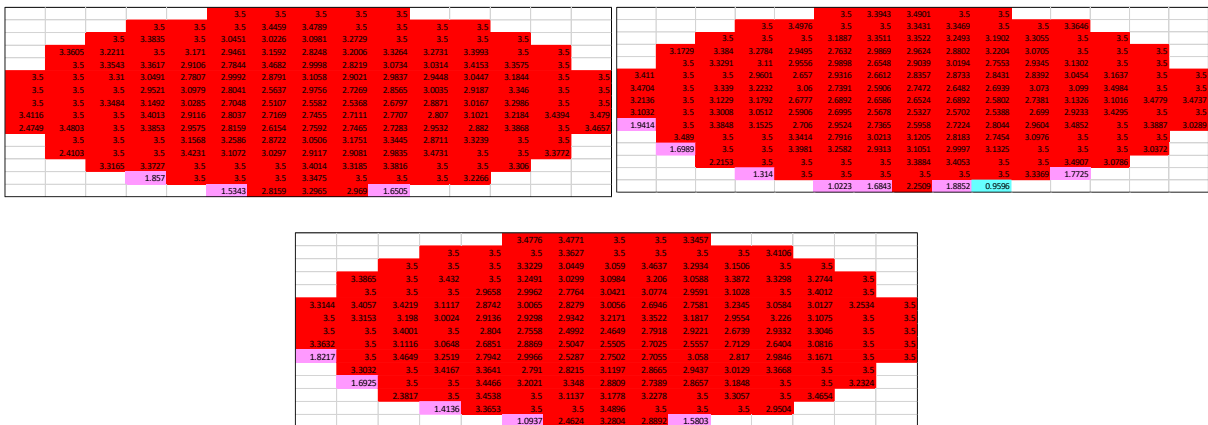


Figure S223: A 45 mM EtOH/H₂O 1:19 solution of compound **4** at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

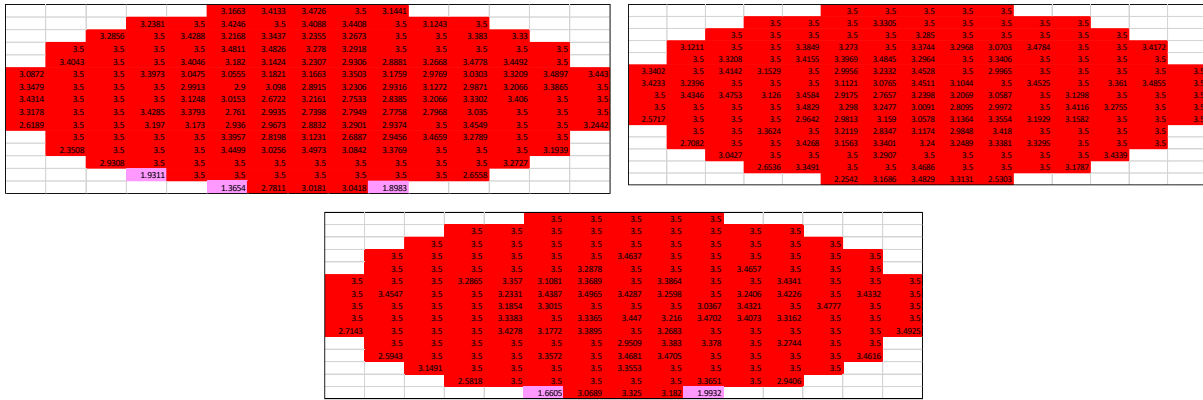


Figure S224: A 50 mM EtOH/H₂O 1:19 solution of compound 4 at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.



Figure S225: Standard EtOH/H₂O 1:19 solutions at 318 K OD₃₈₆. Wells n = 1, n = 2, and n = 3. Colour coded regions: Red = ≥ 2, Pink = 1.9999 – 1, cyan = 0.9999 – 0.0001 OD₃₈₆.

Compound 1 CMC determination via tensiometry

Table S30: Table summarizing surface tension calculated from average (n=3) pendant drop tensiometer data obtained for **1** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Surface tension [mN/m]
6.0	47.72
5.0	47.81
4.0	47.21
3.0	46.94
2.0	46.25
1.0	49.98
0.8	52.42
0.6	54.63

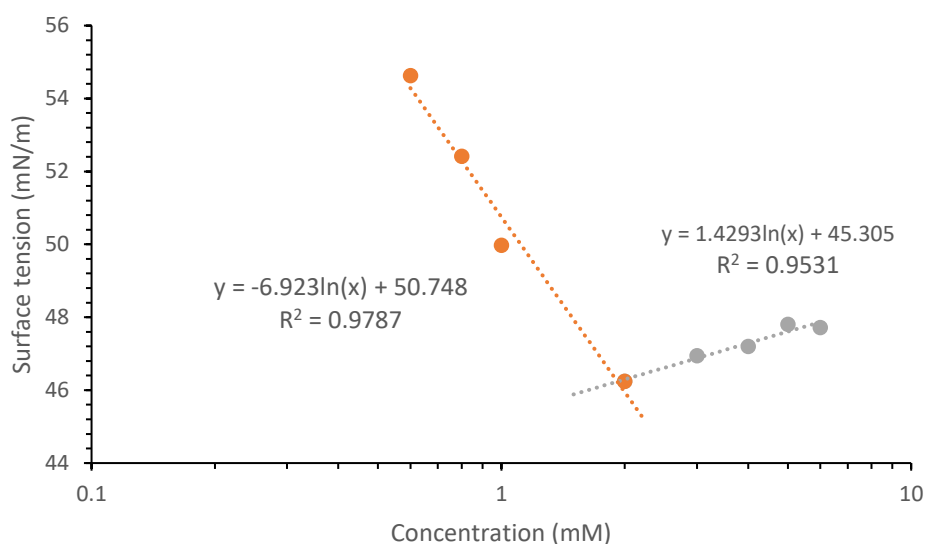


Figure S226: Graph showing surface tension, calculated from average (n=3) tensiometer data obtained for **1** in an EtOH/H₂O 1:19 solution at 298 K, plotted against compound concentration. A CMC value of 1.92 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect.

Compound 4 CMC determination via tensiometry

Table S31: Table summarizing surface tension calculated from average (n=3) pendent drop tensiometer data obtained for **4** in an EtOH/H₂O 1:19 solution at 298 K.

Concentration (mM)	Surface tension [mN/m]
20.0	39.13
17.5	38.26
15.0	38.22
12.5	41.80
11.5	46.11
10.0	48.74
8.0	50.39
7.5	52.58
5.0	53.65
2.5	58.55

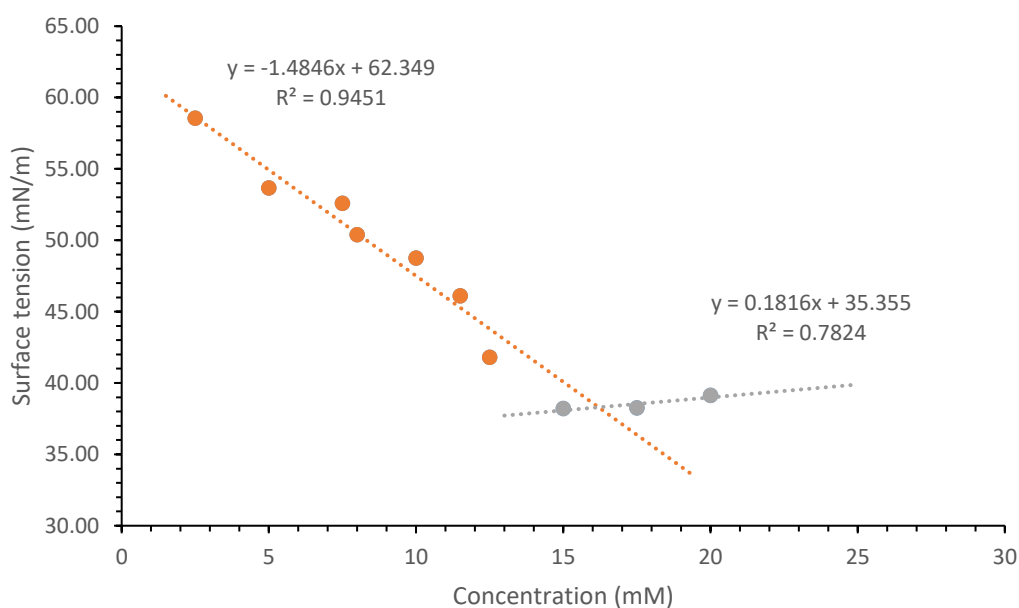


Figure S227: Graph showing surface tension, calculated from average (n=3) tensiometer data obtained for **4** in an EtOH/H₂O 1:19 solution at room temperature, plotted against compound concentration. A CMC value of 16.20 mM was calculated from these data and defined as the point at which the orange and grey linear lines of best fit, fitted to the two linear portions of this data set were found to intersect.

DLS data

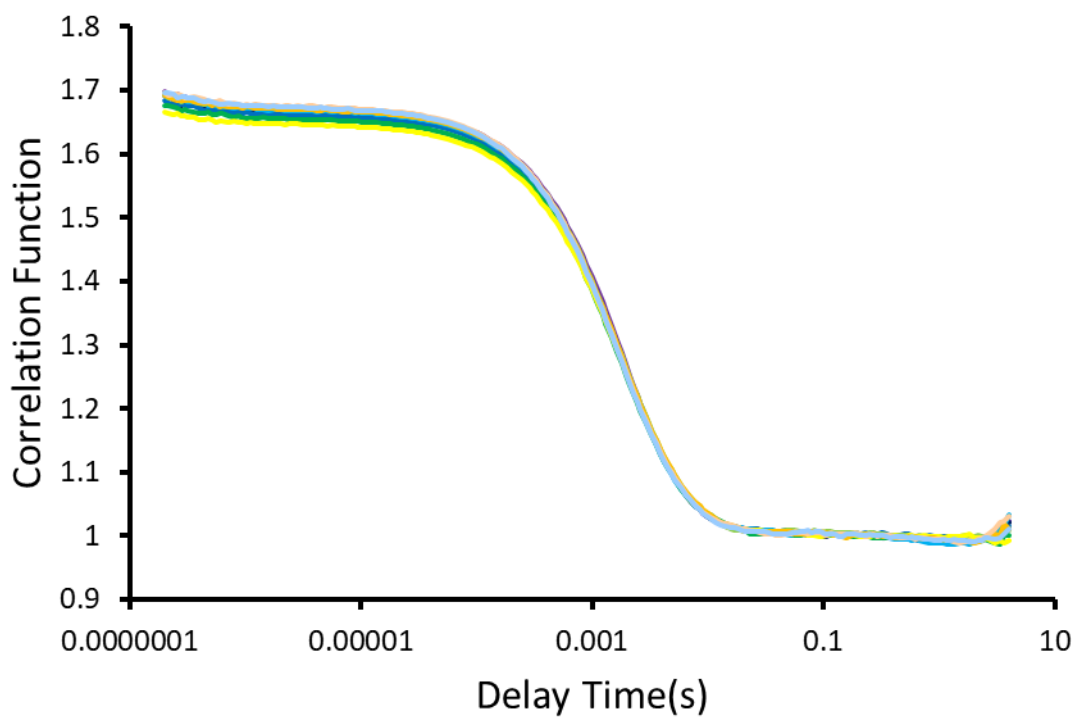


Figure S228: Correlation function data for 10 DLS runs of compound **1** (5.56 mM) in an EtOH/H₂O 1:19 solution at 298 K.

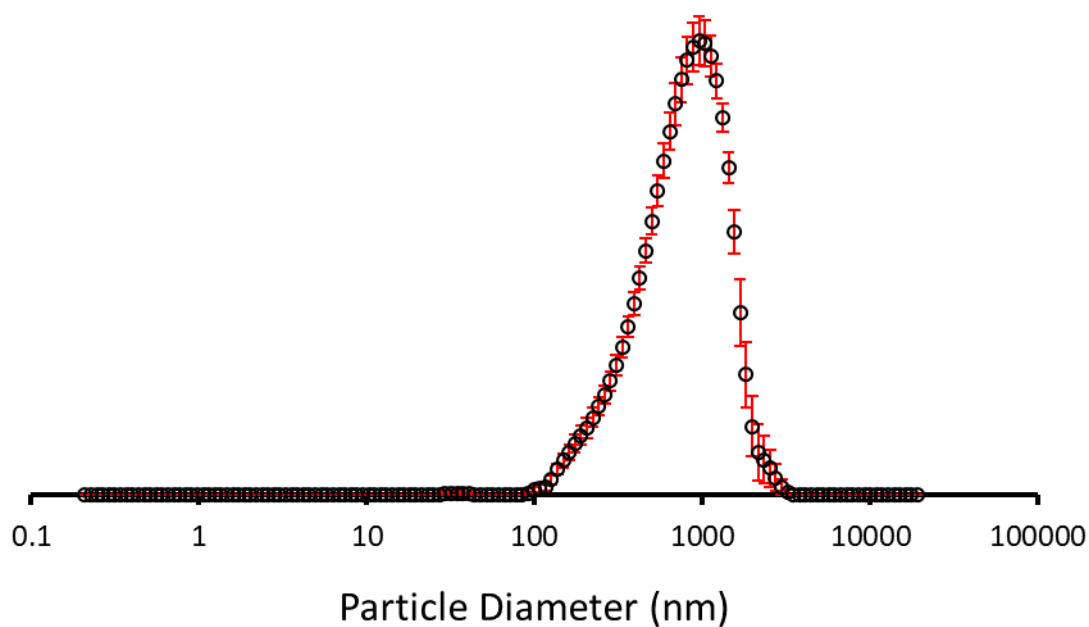


Figure S229: The average intensity particle size distribution calculated (815 nm) using 10 DLS runs for compound **1** (5.56 mM) in an EtOH/H₂O 1:19 solution at 298 K.

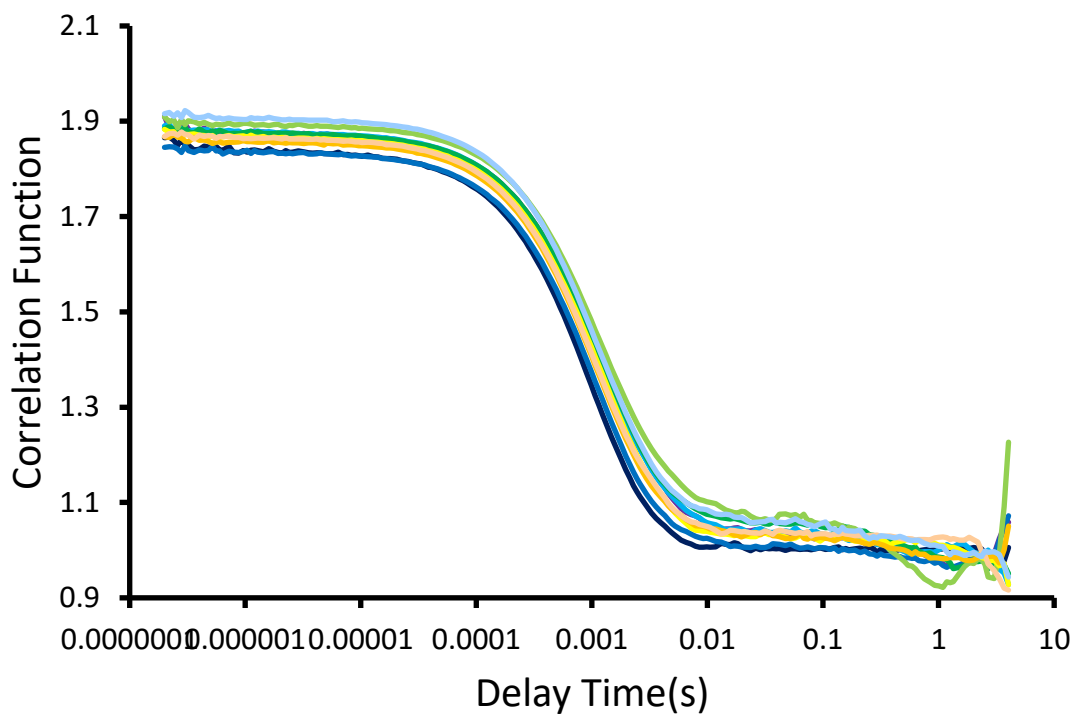


Figure S230: Correlation function data for 10 DLS runs of compound **4** (5.56 mM) in an EtOH/H₂O 1:19 solution at 298 K.

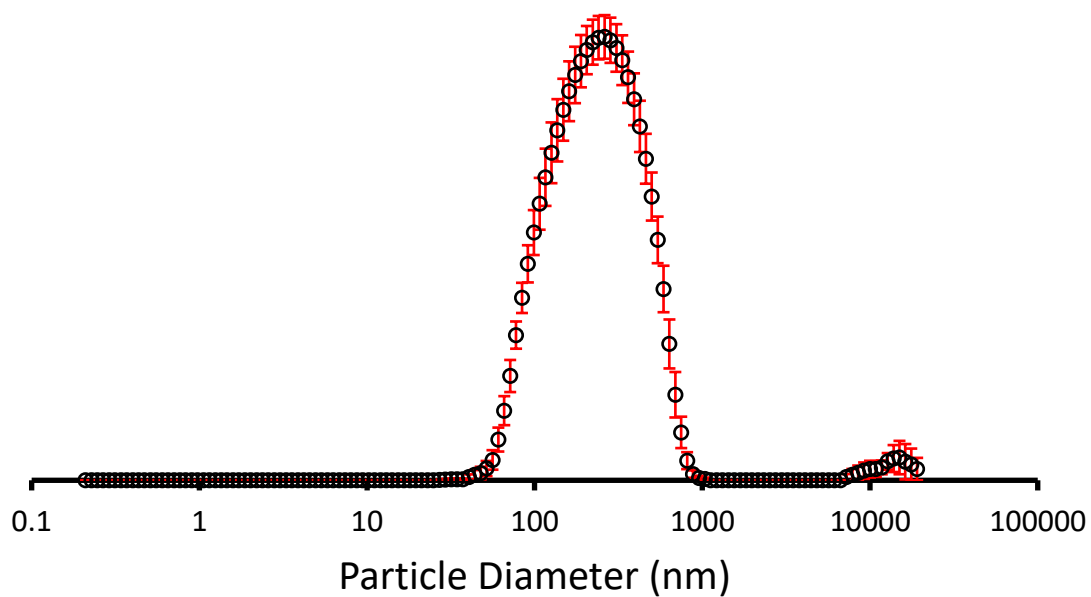


Figure S231: The average intensity particle size distribution calculated (279 nm) using 10 DLS runs for compound **4** (5.56 mM) in an EtOH/H₂O 1:19 solution at 298 K.

Zeta potential data

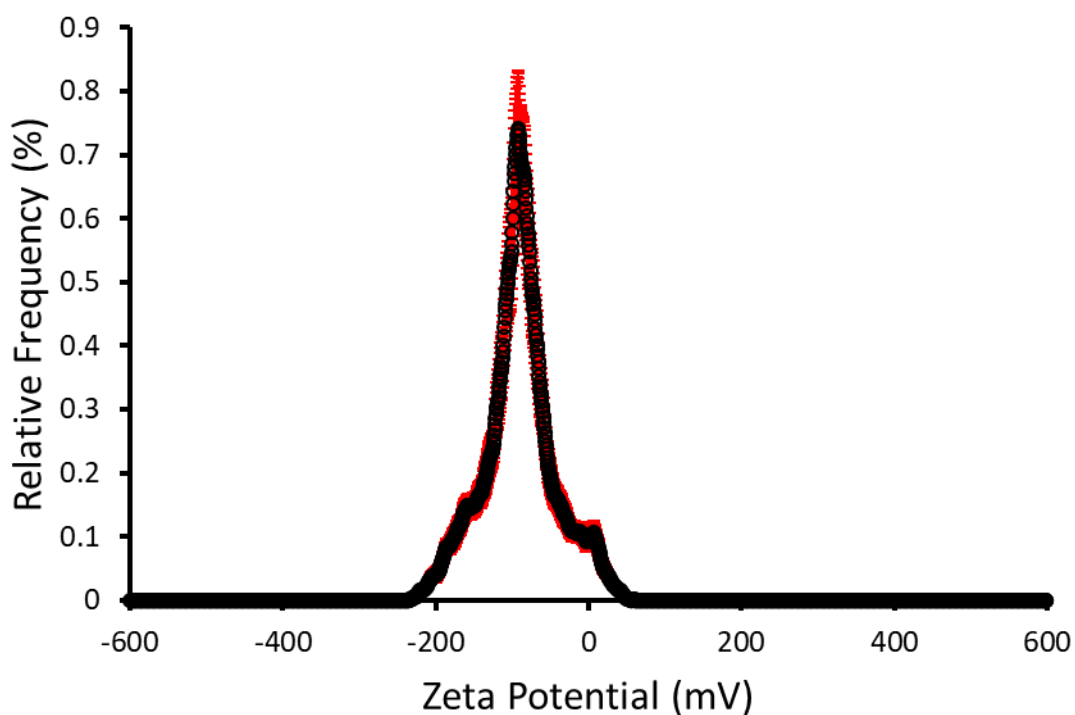


Figure S232: The average zeta potential distribution calculated using 10 runs for compound **1** (5.56 mM) in EtOH/H₂O 1:19 solution at 298 K. Average measurement value -88.29 mV.

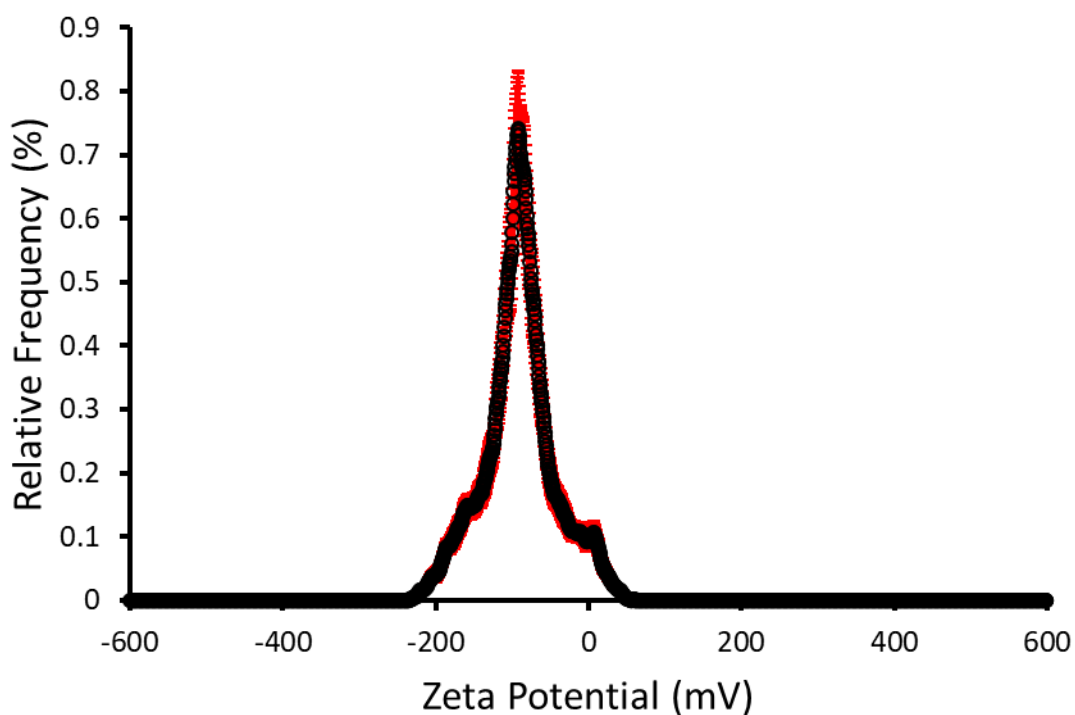


Figure S233: The average zeta potential distribution calculated using 10 runs for compound **4** (5.56 mM) in EtOH/H₂O 1:19 solution at 298 K. Average measurement value -58.55 mV.

References

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