Electronic Supporting Information (ESI) for

Mechanochemically-synthesised AIE-active receptors for selective ceftazidime sensing in high-water-content matrices

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S1. Experimental methods

S1.1 Materials and methods

Materials. Chemical reagents and solvents were of the highest possible purity and were commercially purchased and purified according to the standard methods, if necessary. Thin-layer chromatography (TLC) and preparative thin layer chromatography (PTLC; 2 mm) on SiO_2 were performed using Merck Silica gel 60 F254 plates. PTLC on Al_2O_3 was performed using ALOX-100 UV_{254} plates (Macherey-Nagel).

Mechanochemical syntheses were performed in a Retsch MM400 ball mill using 1.5 mL or 5.0 mL stainless steel jars with 3.0 mm or 5.0 mm stainless steel balls (number of added balls is indicated in the synthesis section), at 30 Hz.

NMR experiments were carried out using a JEOL 600 MHz spectrometer (^{1}H at 600 MHz; {^{1}H}^{13}C NMR at 151 MHz; ^{19}F NMR at 565 MHz) equipped with a multinuclear z-gradient inverse probe head or a Varian VNMRS 500 MHz spectrometer (^{1}H at 500 MHz; {^{1}H}^{13}C NMR at 125 MHz) equipped with a multinuclear z-gradient inverse probe head. The spectra were recorded at 297.15 K, and standard 5 mm NMR tubes were used. ^{1}H NMR (δ_H), {^{1}H}^{13}C NMR (δ_C) and ^{19}F NMR chemical shifts were reported in parts per million (ppm) relative to the solvent signal, i.e., DMSO-*d₆* δ_H (residual DMSO) 2.50 ppm, δ_C (residual DMSO) 39.50 ppm, and δ_F (C_6F_6) −164.9 ppm. For the ^{1}H NMR receptor studies, spectra were recorded in DMSO-d6 with TMS added as an internal standard (reference signal set to TMS, δ_H = 0.00 ppm). NMR spectra were analysed with the MestReNova v12.0 software (Mestrelab Research S.L.).

ESI-HRMS (TOF) measurements were performed with a Q-Exactive ThermoScientific spectrometer.

UV-vis spectra were recorded with a WVR UV-1600PC spectrometer at a spectral resolution of 2 cm^{-1}. For the UV-vis measurements, the wavelengths for the absorption maxima λ_{max} were reported in nm.

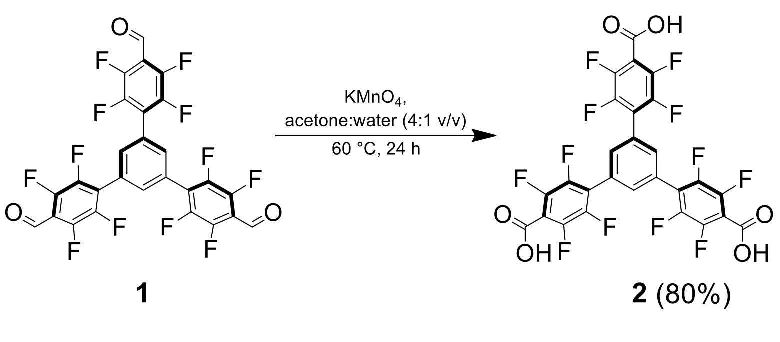
Fluorescence spectra were recorded with a HITACHI F-7100 FL spectrometer. Parameters for the liquid spectra acquisition: scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, EM slit: 5.0 nm, PMT Voltage: 400 V. The wavelengths for the emission maxima (λ_{em}) were reported in nm.

Dynamic light scattering (DLS) measurements were performed with Zetasizer Nano ZS (Malvern).

For sonochemical reactions, Bandelin Sonorex RK 100H (ultrasonic probe; ultrasonic peak output/HF power: 320W/80W; 35kHz) was used.

S1.2 Syntheses

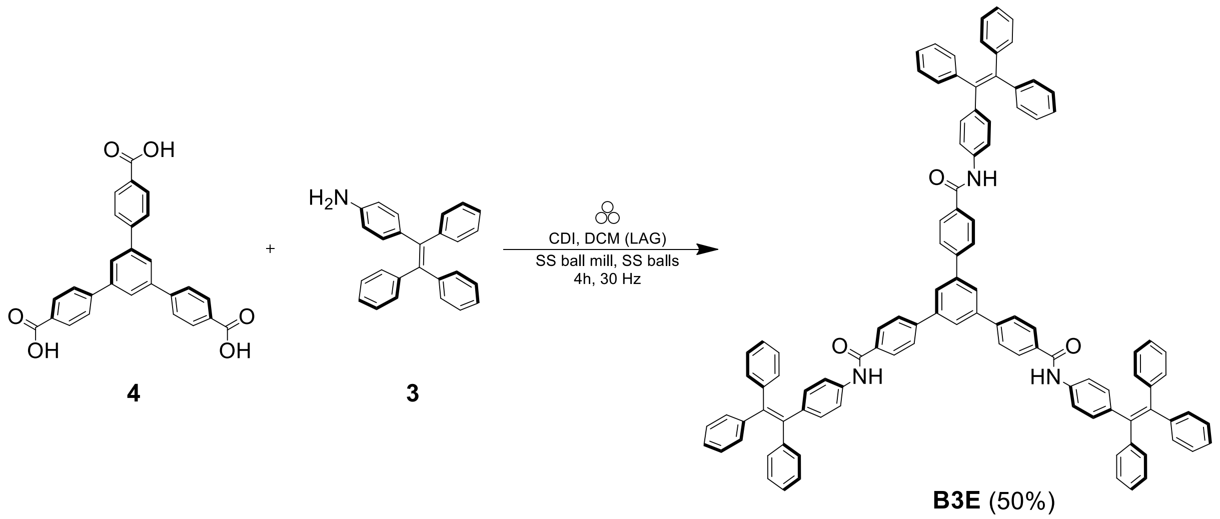
Synthesis of tricarboxylic acid 2



Scheme S1 Synthesis of tricarboxylic acid **2**.

Synthesis via a modified literature procedure[1]. Into a 100 ml round-bottom flask, tricarboxaldehyde **1** (50.0 mg; 0.083 mmol), $KMnO_4$ (160.8 mg; 1.015 mmol), acetone (4 mL) and water (1 mL) were added. The reaction was cautiously heated to 60 °C and mixed for 24 h. The formed brown precipitate (MnO_2) was filtered off under reduced pressure and washed with water (50 mL). To the filtrate, 1 mL of 36% hydrochloric acid was added, and a white, fine precipitate was formed. The precipitate was then filtered and washed with water (20 mL). The precipitate was removed from the filter, which was washed with methanol, then the mixture was distilled off on a rotary evaporator and dried under vacuum. Tricarboxylic acid **2** was an off-white solid, obtained with 80% yield (43.3 mg; 0.66 mmol). NMR spectra were consistent with literature[1].

Synthesis of B3E



Scheme S2 Mechanochemical synthesis of dendritic amide **B3E**

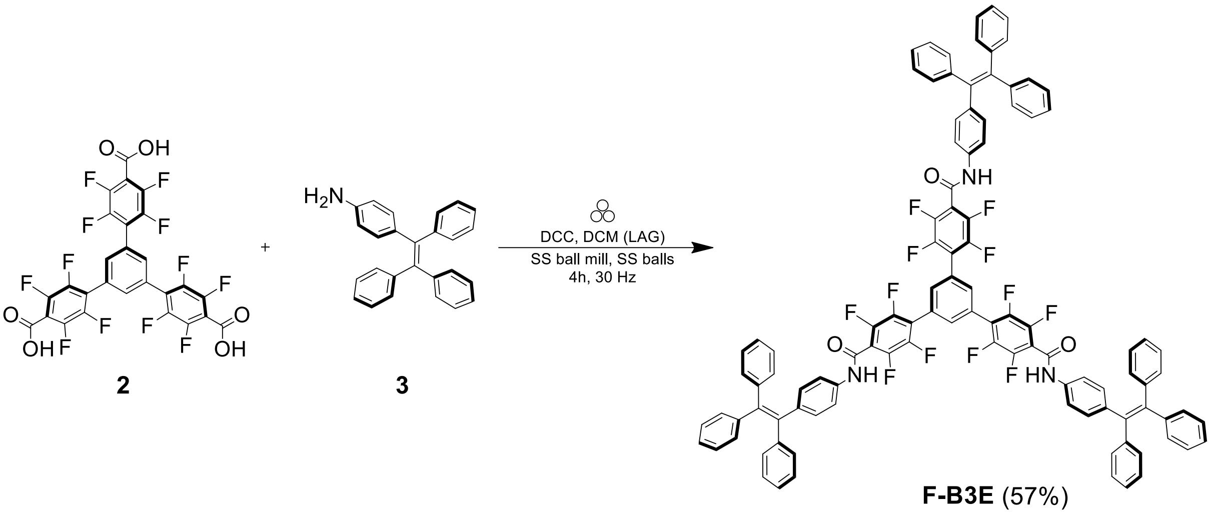
Into a stainless-steel jar (1.5 mL), tricarboxylic acid **4** (6.6 mg, 0.015 mmol, 1.0 equiv.), amine **3** (32.8 mg, 0.090 mmol, 6.0 equiv.), and **CDI** (9.7 mg; 0.060 mmol; 4.0 equiv.) were added. Five stainless steel grinding balls (φ = 3 mm) were added, together with dichloromethane (25 µL). The reaction mixture was ground at 30 Hz for 4 h. Dichloromethane (15 mL) and methanol (2 mL) were added to remove the solid from the jar. 1M HCl (40 mL) was added, and the crude product was extracted with CH_2Cl_2 (3x20 mL). Organic layers were combined and washed with water and brine. After drying with $MgSO_4$ and filtration, the solvents were distilled off on a rotary evaporator. Column chromatography was performed (SiO_2, toluene:cHex:EtOAc = 5:4:1 vol., RF = 0.4), then PTLC was conducted (SiO_2, toluene:cHex:EtOAc =4:4:2 vol., R_F = 0.7). For final purification, another PTLC was performed (Al2O3, toluene:cHex:EtOAc = 3:6:1 vol., RF = 0.25). The collected fraction was then distilled on a rotary evaporator and dried under vacuum. Product (**B3E**) was a colourless solid, obtained with 50% yield (10.4 mg; 0.0075 mmol).

^{1}H NMR (DMSO-d_6; 600 MHz; ppm) δ_H 8.62 (s, 3H), 7.25 (m, 2H); 7.18-7.06 (m, 41H), 6.99-6.94 (m, 23H),6.84 (d, J = 8.7 Hz, 6H)

{^{1}H}^{13}C NMR (DMSO-d_6; 151 MHz; ppm) δ_C 155.3; 143.5; 143.4; 143.3; 140.3; 139.8; 137.3; 136.5; 131.2; 130.7; 130.6; 130.1; 129.3; 128.9; 128.2; 127.9; 127.7; 127.4; 126.5; 126.4; 125.5; 125.3; 117.3

HRMS (ESI) m/z $[M+H_2O-2H]^+$ (associate with H_2O) calcd. for $C_{105}H_{75}N_3O_4$ = 1442.57856, found = 1442.63761

Synthesis of F-B3E



Scheme S3 Mechanochemical synthesis of dendritic amide **F-B3E**

Into a stainless-steel jar (volume 1.5 mL), tricarboxylic acid **2** (4.9 mg, 0.0075 mmol, 1.0 equiv.), amine **3** (15.8 mg, 0.0450 mmol, 6.0 equiv.), and **DCC** (6.2 mg; 0.030 mmol; 4.0 equiv.) were added. Five stainless steel grinding balls (φ = 3 mm) were added, together with dichloromethane (25 µL). The reaction mixture was ground at 30 Hz for 4 h. Dichloromethane (15 mL) and methanol (2 mL) were added to remove the solid from the jar. 1M HCl (40 mL) was added, and the crude product was extracted with CH_2Cl_2 (3 × 20 mL). Organic layers were combined and washed with water and brine. After drying with $MgSO_4$ and filtration, the solvents were distilled off on a rotary evaporator. PTLC purification was performed (SiO_2, hexane:EtOAc 3:1, R_F = 0.5), then column chromatography purification was conducted (Al_2O_3, hexane:EtOAc 7:3). For final purification, another PTLC was conducted (Al_2O_3, cHex:EtOAc =6:4 vol., RF = 0.8). The collected fraction was then distilled on a rotary evaporator and dried under vacuum. Product (**F-B3E**) was a colourless solid, obtained with 57% yield (6.8 mg, 0.0041 mmol).

^{1}H NMR (DMSO-d_6; 600 MHz; ppm) δ_H 11.01 (s, 3H), 7.99 (s, 3H); 7.43 (d, J = 8.7 Hz, 6H), 7.17-7.14 (m, 6H), 7.12-7.06 (m, 22H), 6.99-6.93 (m, 23H)

{^{1}H}^{13}C NMR (DMSO-d_6; 125 MHz; ppm) δ_C 155.3; 143.2; 143.1; 139.9; 139.7; 136.2; 131.4; 130.7; 130.6; 128.0; 127.9; 127.8; 126.6; 118.9

^{19}F NMR (DMSO-d_6; 565 MHz; ppm) δ_F −144.45-144.75 (m, 12F)

HRMS (ESI) m/z [M$^+$] calcd. for $C_{105}H_{63}F_{12}N_3O_3$ = 1642.47059, found = 1642.47245

S1.3 Optimisation of syntheses

Table S1 Optimisation table of **B3E** synthesis

Carboxylic acid (mg; *mmol*; eq)	Amine (mg; *mmol*; eq)	Solvent (µl; *η*)	Coupling agent (mg; *mmol*; eq)	Reaction conditions	Yield
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (2000)	**DCC** (12.4; *0,060*; 4.0)	Sonochemistry, 4 hours T = 60°C	Traces
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (1000)	**CDI** (9.7; *0,060*; 4.0)	Sonochemistry, 4 hours T = 60°C	30%
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (100)	**CDI** (9.7; *0,060*; 4.0)	Sono-Mechanochemistry[a], 4 hours, *WUT Glass Mill*	35%
(4) **TPB-(COOH)$_3$** (13.2; *0.030*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 3.0)	**DCM** (25; *0.40*)	**DCC** (18.6; *0,090*; 3.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (13.2; *0.030*; 1.0)	(3) **TPE-NH$_2$** (62.6; *0,180*; 6.0)	**DCM** (25; *0.25*)	**DCC** (24.8; *0,120*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (25; *0.50*)	**DCC** (12.4; *0,060*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	40%
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (25; *0.51*)	**EDC·HCl** (11.5; *0,060*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (25; *0.53*)	**CDI** (9.7; *0,060*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	**50%**
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**EtOAc** (25; *0.53*)	**CDI** (9.7; *0,060*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	No solvent	**CDI** (9.7; *0,060*; 4.0)	Mechanochemistry, 4 hours, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (6.6; *0.015*; 1.0)	(3) **TPE-NH$_2$** (31.3; *0,090*; 6.0)	**DCM** (50, 1.01)	**CDI** (9.7; *0,060*; 4.0)	Mechanochemistry, 2 hours of CDI-activation, 2 hours of milling with amine, 5×3 mm SS balls	Traces
(4) **TPB-(COOH)$_3$** (33.3; *0.076*; 1.0)	(3) **TPE-NH$_2$** (152.8; *0,450*; 6.0)	**DCM** (125; *0.53*)	**CDI** (48.7; *0,300*; 4.0)	Mechanochemistry, 4 hours, 5×5 mm SS balls	25%

[a]Synthesis in *WUT Glass Mill*[2] with a glass vial placed in the ultrasonic probe

Table S2 Optimisation table of **B3E** synthesis

Carboxylic acid (mg; *mmol*; eq)	Amine (mg; *mmol*; eq)	Solvent (µl; *η*)	Coupling agent (mg; *mmol*; eq)	Reaction conditions	Yield
(4) **F-TPB-(COOH)$_3$** (11.0; *0.015*; 1.0)	(3) **TPE-NH$_2$** (15.7; *0,045*; 3.0)	**DCM** (25; *0.69*)	**DCC** (9.3; *0,045*; 3.0)	Mechanochemistry, 2 hours, 5×3 mm SS balls	25%
(4) **F-TPB-(COOH)$_3$** (5.5; *0.015*; 1.0)	(3) **TPE-NH$_2$** (15.7; *0,045*; 6.0)	**DCM** (25; *0.91*)	**DCC** (6.2; *0,030*; 4.0)	Mechanochemistry, 2 hours, 5×3 mm SS balls	**57%**
(4) **F-TPB-(COOH)$_3$** (16.5; *0.045*; 1.0)	(3) **TPE-NH$_2$** (47.1; *0,135*; 6.0)	**DCM** (75; *0.91*)	**DCC** (18.6; *0,090*; 4.0)	Mechanochemistry, 2 hours, 4×5 mm SS balls	20%

S1.4 Aggregation-Induced Emission (AIE) studies – preparation of the samples

Studies on the AIE effect were conducted by measuring fluorescence spectra. Samples were prepared by subsequently adding 10 µL of receptor stock solution in THF (C = $2\cdot10^{-3}$ M), then different amounts of THF and water (a total of 990 µL). Final samples were a series of receptor solutions (C = $2\cdot10^{-5}$ M) with water content in the range of 0 – 95 % vol.

S1.5 Methodology for fluorescence quantum yield estimation

Measurements of fluorescence quantum yields (Φ_F) for the synthesised monoamides and dendritic-like molecules, as well as their aggregates, were performed at room temperature according to literature procedures. Fluorescence quantum yields (Φ_F) were determined by comparison with quinine sulfate (QS) in 0.5 M H_2SO_4 ($\Phi_{F,ref}$ = 0.551) as the standard. The measurements were performed with highly diluted solutions, for which the absorbance (A) at the highest wavelength was not higher than 0.1. The excitation wavelength (λ_{ex}) for all samples were selected on the basis of the UV-vis spectra as λ_{ex} = 320 nm. Concentrations were as follows: C_{QS} = $2\cdot10^{-6}$ M; $C_{molecule/aggregates}$ = $2\cdot10^{-6}$ M. The following formula was used for the calculation of Φ_F:

$$\Phi_{\mathrm{F}} = \Phi_{\mathrm{F,ref}} \frac{F_{sample}}{F_{reference}} \cdot \frac{1-10^{-A_{ref}}}{1-10^{-A_{sample}}} \cdot \frac{n_{sample}^2}{n_{reference}^2}$$

where $\Phi_{F,\,ref}$ is the quantum yield for QS (0.551), ***F*** is the integrated area under the fluorescence spectra, ***A*** is the absorbance at the excitation wavelength, and ***n*** is the refractive index of the solvent (1.346 for 0.5M H_2SO_4, 1.4072 for THF, and 1.3329 for H_2O, ***n*** for the aggregate solution in the given volume ratio was taken as the weighted arithmetic mean with weights equal to vol% of H_2O and THF in the mixture).

S1.6 Titration experiments methodology - spectrofluorimetry

The binding experiments between **B3E** and **F-B3E** molecules (receptors) and antibiotics (analytes: Ampicillin, Penicillin, Amoxicillin in the form of sodium (Na^+) salts, and Ceftazidime in the form of inner salt) were performed employing the fluorescence spectra titration experiments. The experiments were performed in the H_2O/THF = (80; 95; 99%):(20; 5; 1%) *v/v* systems as follows. A stock solution of amides and dendritic-like molecules ($2\cdot10^{-3}$M) in THF was diluted with an adequate volume of pure THF and H_2O to reach the final sample volume of 3 mL and the desired composition of solvents. The given antibiotic was introduced to the mixture as H_2O/THF solutions of the corresponding solvent content. Stock solution of real antibiotics for additional competitive titration tests were prepared as follows: hard capsules were opened, then content of capsule was introduced into H_2O/THF mixture; tablets were powdered with mortar and pestle, powder was introduced into H_2O/THF mixture. Then, titration experiments were conducted. First, fluorescence of a solution containing only a receptor was measured, then solutions containing the given antibiotic were added in 11 consecutive steps to achieve the following proportions of cation to receptor: 0.00, 0.25, 0.5, 0.75, 1.0, 2.0, 3.0, 4.0, 5.0, 10.0, 30.0 equiv. To ensure proper mixing, the cuvette contents were well mixed with a magnetic stirrer (1400 rpm) before the spectrum was measured.

S1.7 Titration experiments methodology – NMR studies

Into an NMR tube, 400 µL of stock solution of receptor in DMSO-d_6 was placed (C = $7.628\cdot10^{-4}$ M). Then, in the case of the ^{1}H NMR experiment, 100 µL of DMSO-d_6 with 0.03% and 300 µL of DMSO-d_6 were added. In the case of the ^{19}F NMR experiment, 399.8 µL of DMSO-d_6 and 0.2 µL of C_6F_6 were added. NMR spectra at the starting point were measured. Then, appropriate amounts of Cef stock solution in DMSO-d_6 (C = $7.628\cdot10^{-2}$ M) were added in portions (0.25 – 10 equiv.). After each addition the NMR spectrum was measured.

S2. NMR spectra

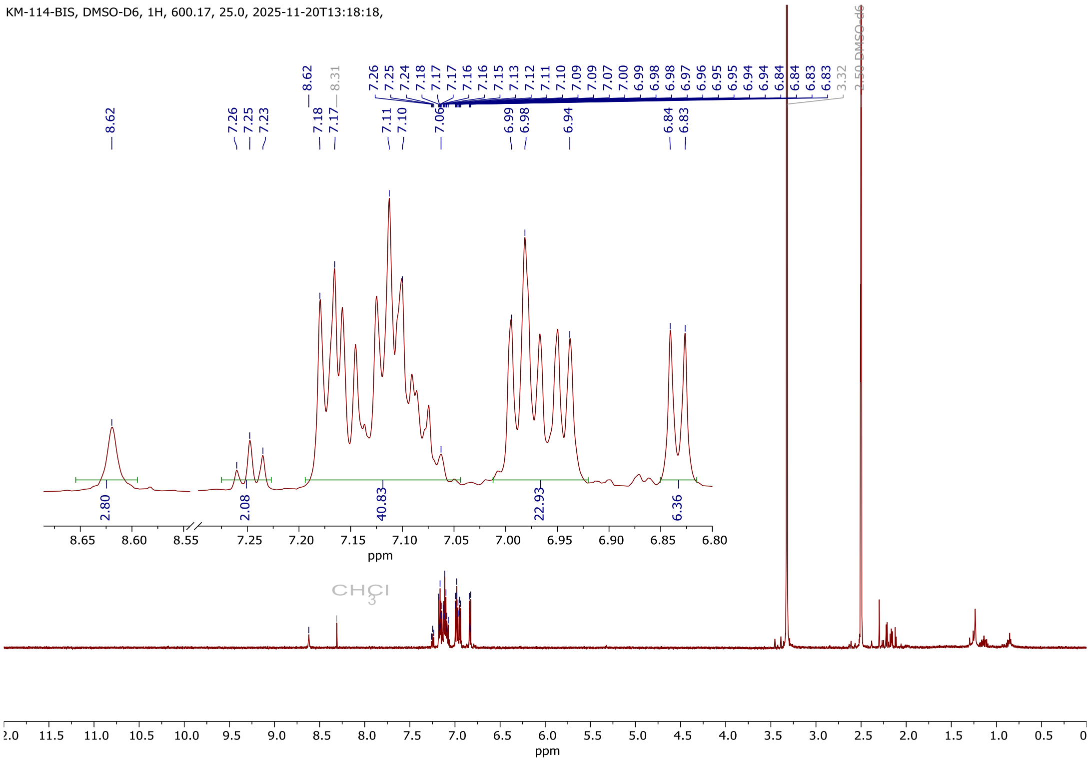


Figure S1 ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **B3E**.

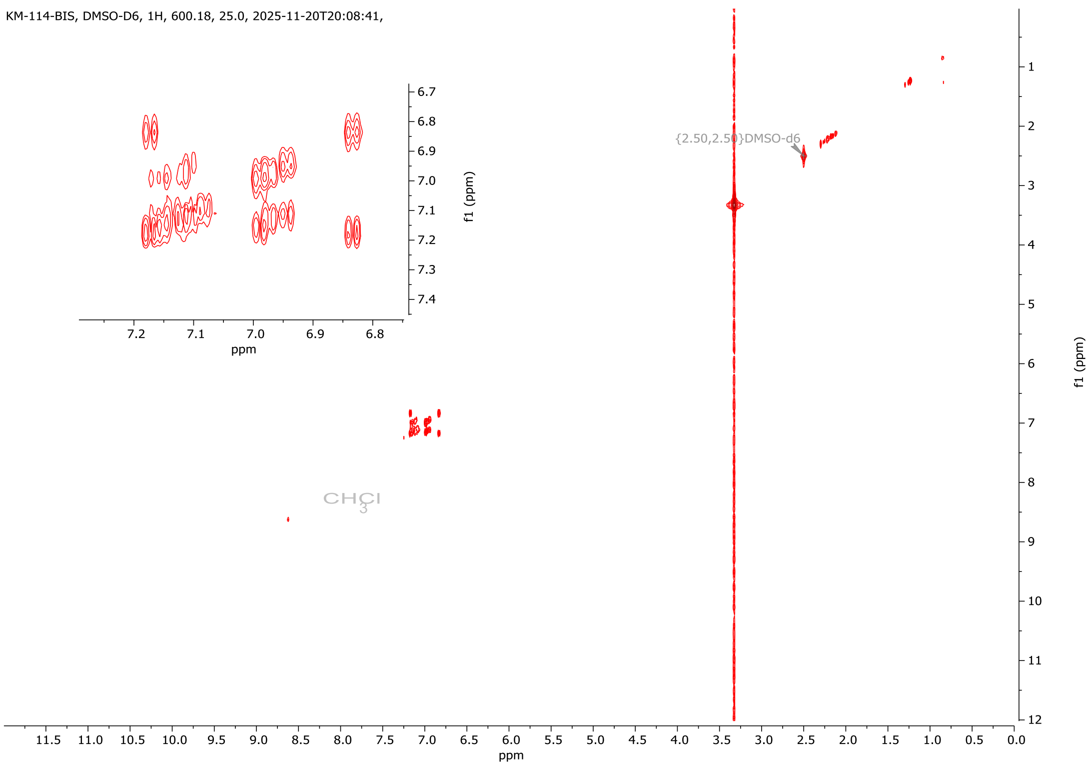


Figure S2 ^{1}H-^{1}H COSY NMR spectrum (600 MHz, DMSO-d6) of **B3E**.

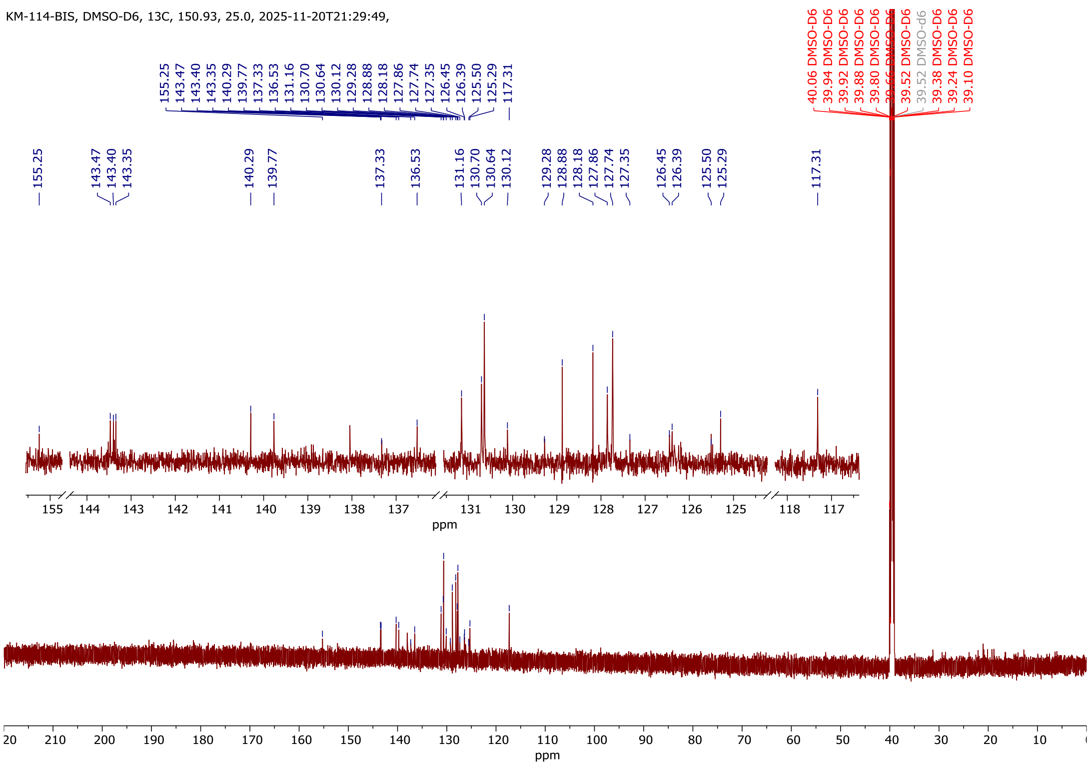


Figure S3 {[1]H}^{13}C NMR spectrum (151 MHz, DMSO-d_6) of **B3E**

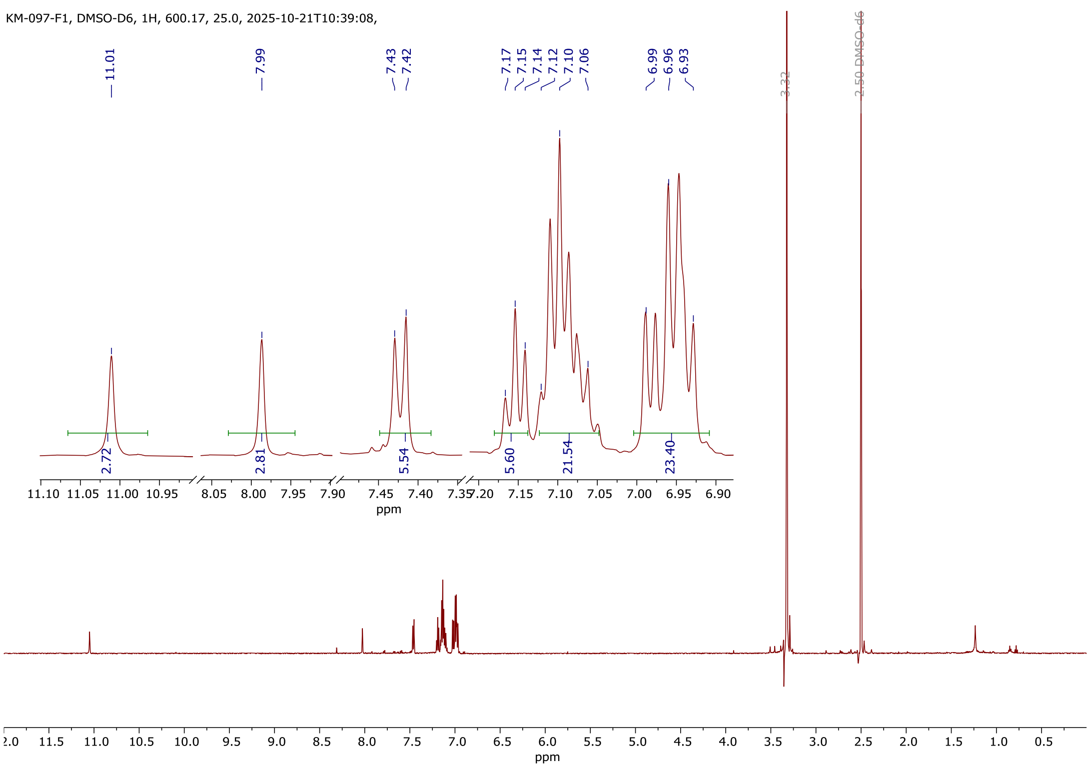


Figure S4 ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of **F-B3E**.

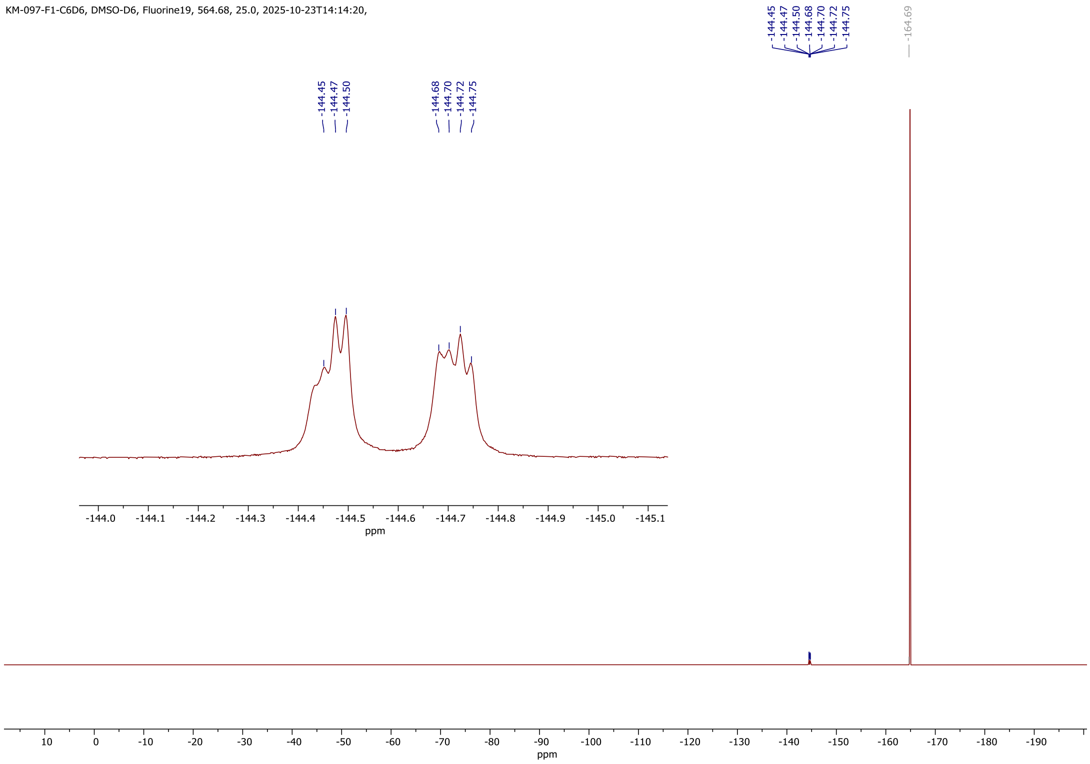


Figure S5 ^{19}F NMR spectrum (565 MHz, DMSO-d_6) of **F-B3E**.

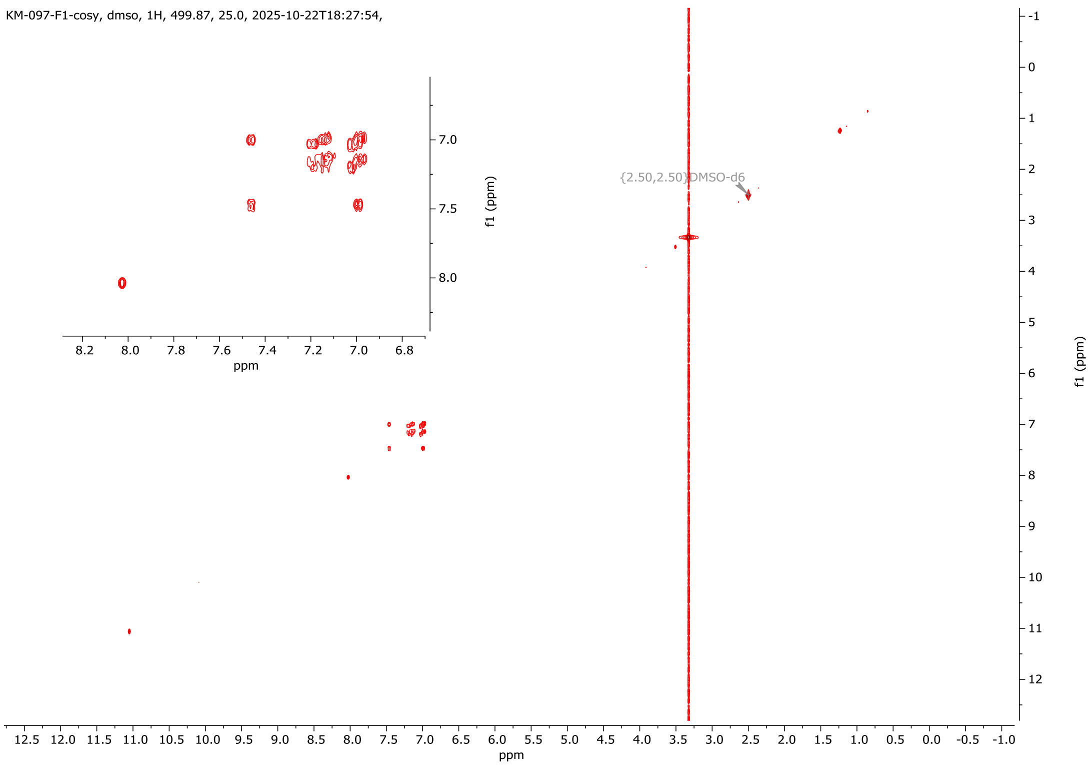


Figure S6 ^{1}H-^{1}H COSY NMR spectrum (500 MHz, DMSO-d6) of **F-B3E**.

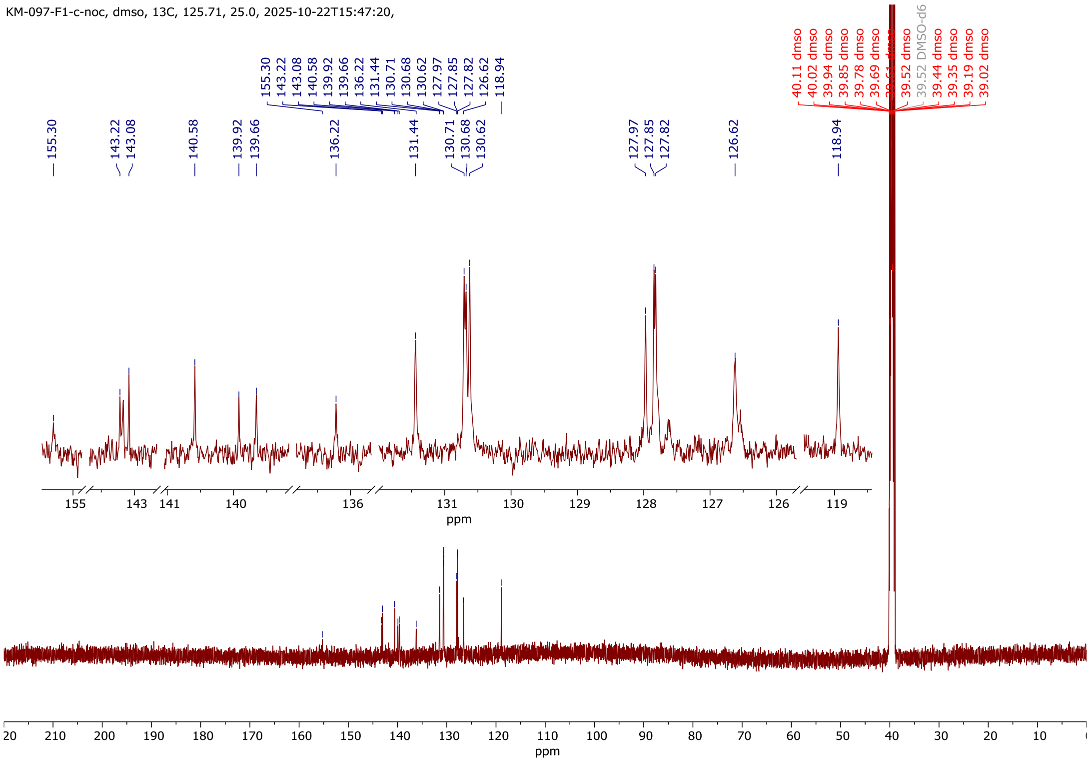


Figure S7 {[1]H}[13]C NMR spectrum (125 MHz, DMSO-d_6) of **F-B3E**.

S.3 HRMS spectra

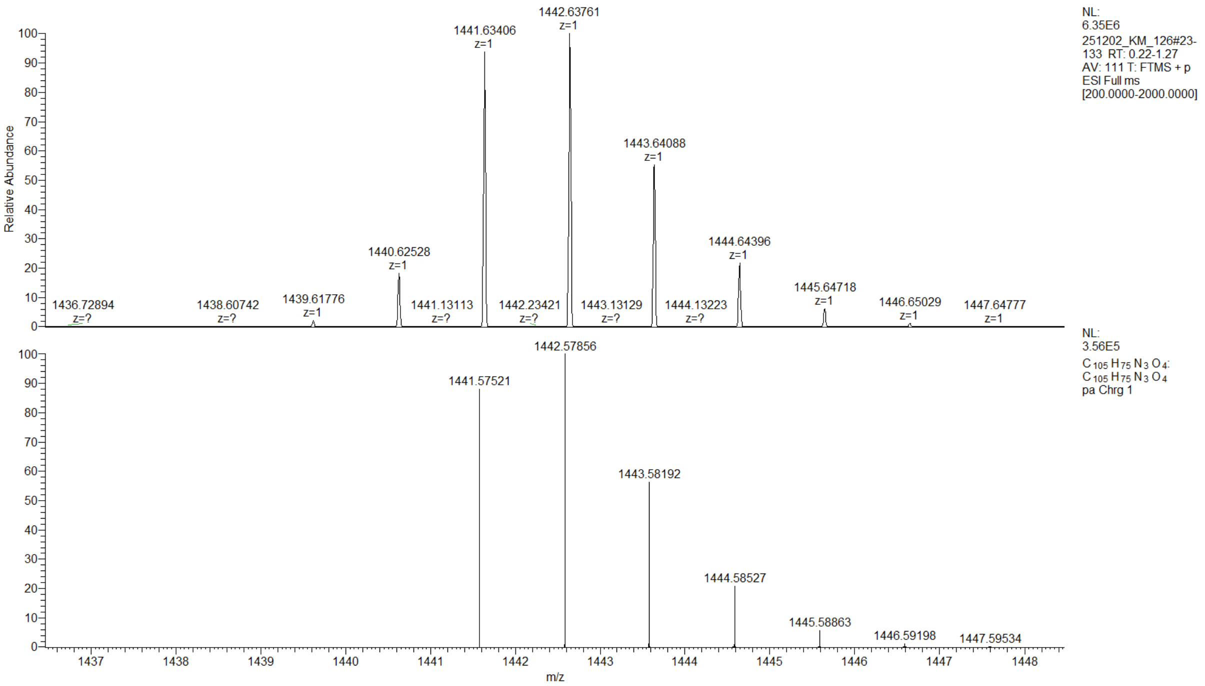


Figure S8 ESI-HRMS (TOF) spectrum of **B3E**.

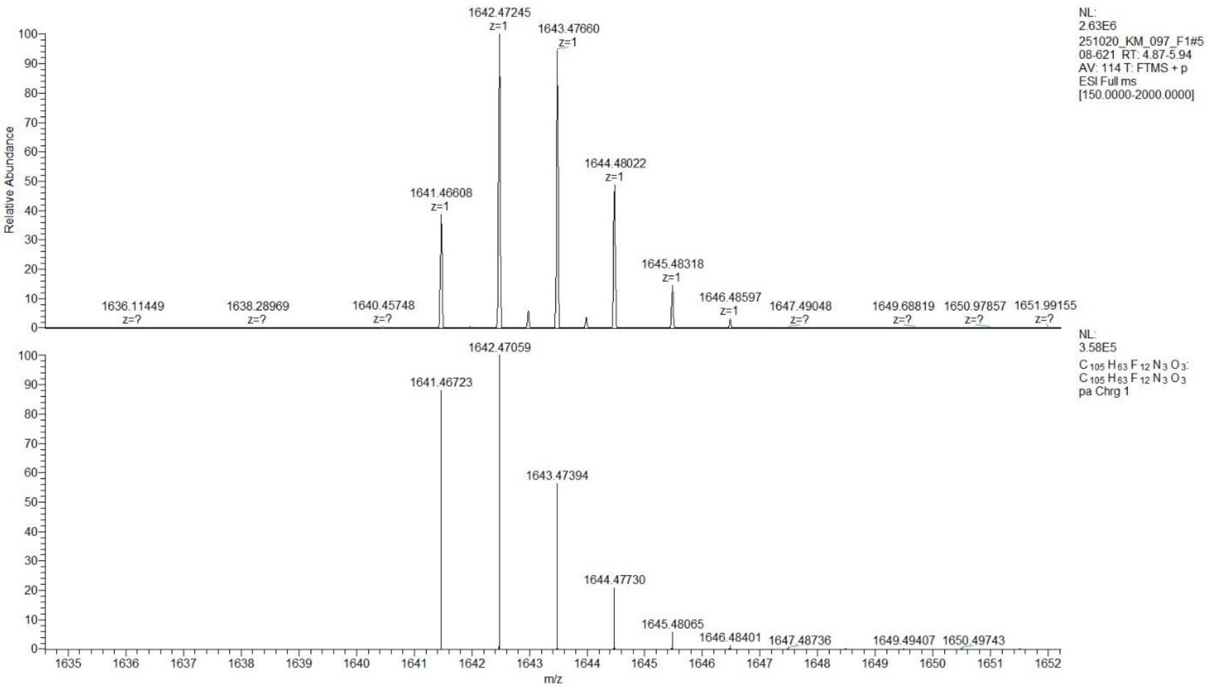


Figure S9 ESI-HRMS (TOF) spectrum of **F-B3E**.

S.4 DFT computations

Density functional theory (DFT) computations (Gaussian software[3]) were performed with the B3LYP functional[4] and the 6-31g(d,p)[5] basis set. After structure optimisation, vibrational frequencies were calculated. All optimised structures represent minima, as no imaginary frequencies were detected. Electrostatic surface potential (ESP) maps were generated and analysed using the GaussView[6] software.

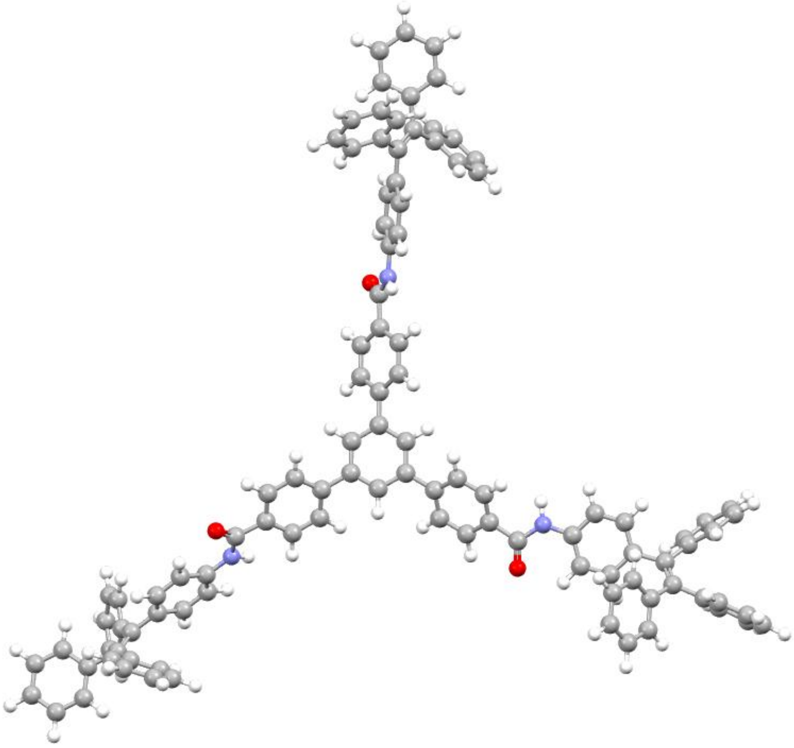


Figure S10 DFT optimised (B3LYP/6-31g(d,p)) structure of **B3E.**

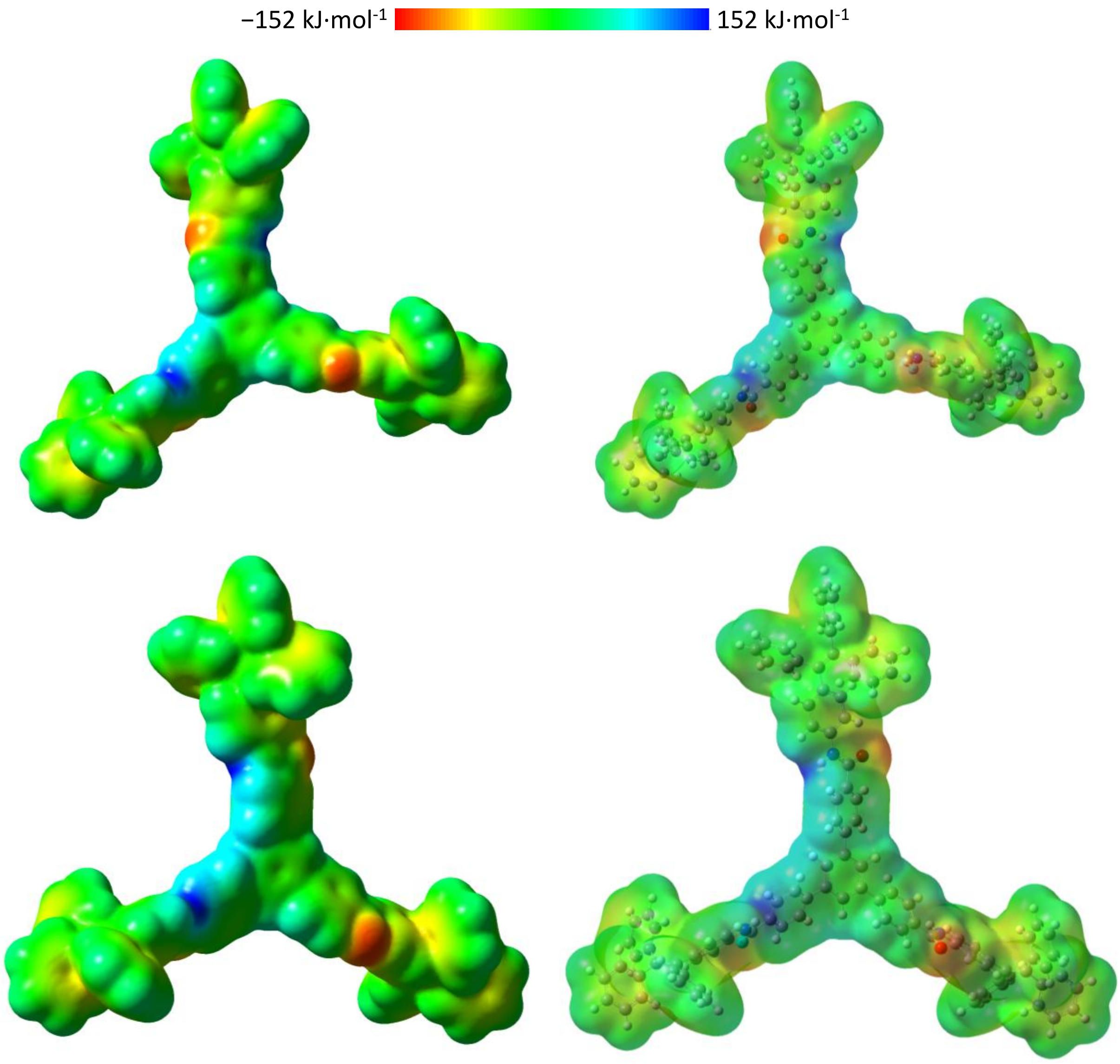


Figure S11 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **B3E**. Views from two perspectives are presented.

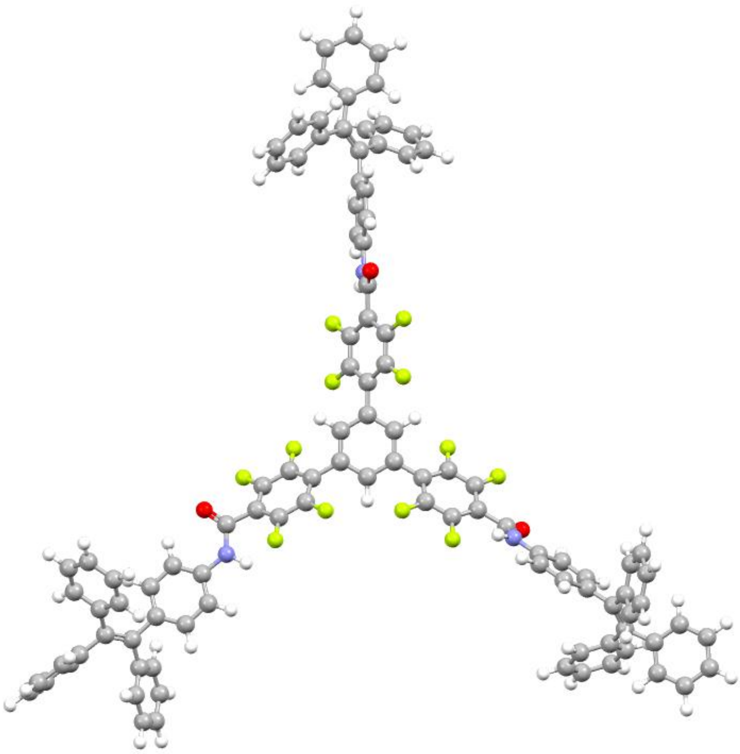


Figure S12 DFT optimised (B3LYP/6-31g(d,p)) structure of **F-B3E**.

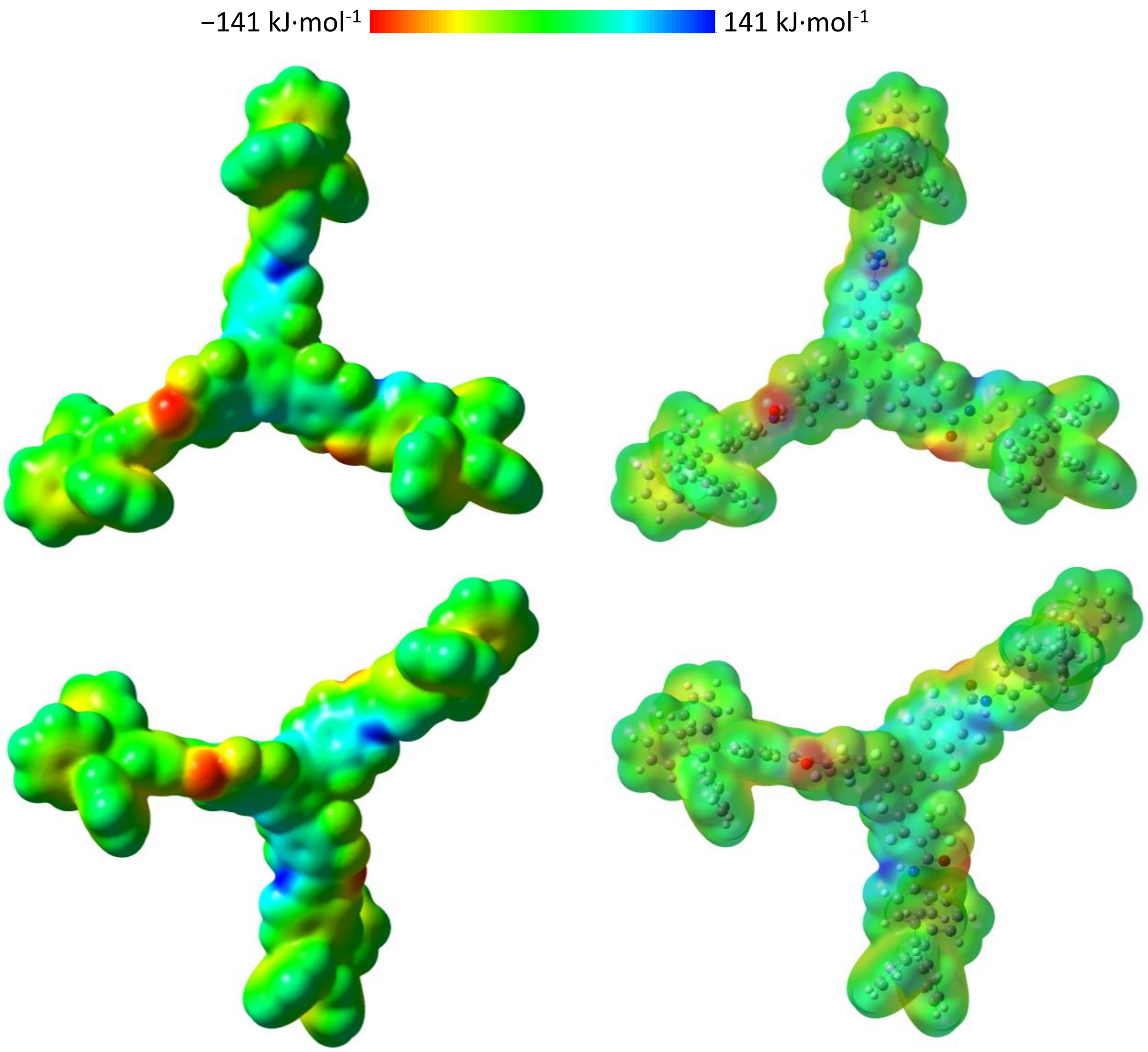


Figure S13 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **F-B3E**. Views from two perspectives are presented**.**

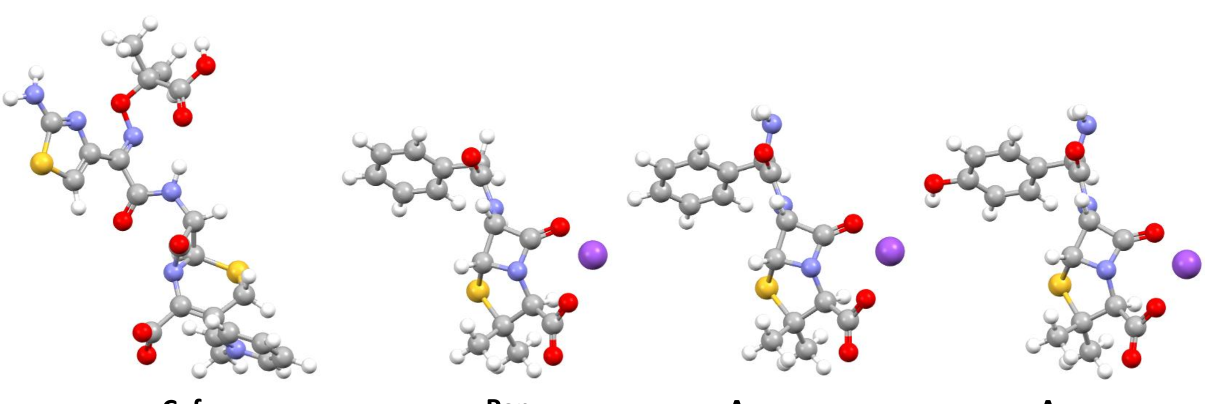


Figure S14 DFT optimised (B3LYP/6-31g(d,p)) structure of (from left to right): **Cef**, **Pen**, **Ampc**, **Amox***,*

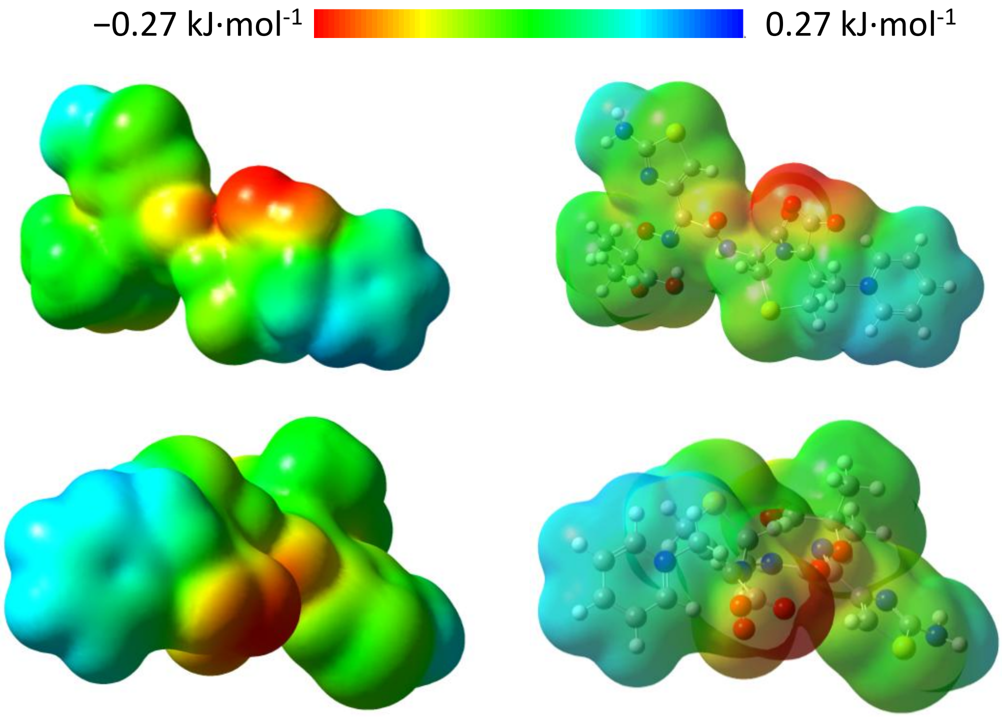


Figure S15 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **Cef**. Views from two perspectives are presented.

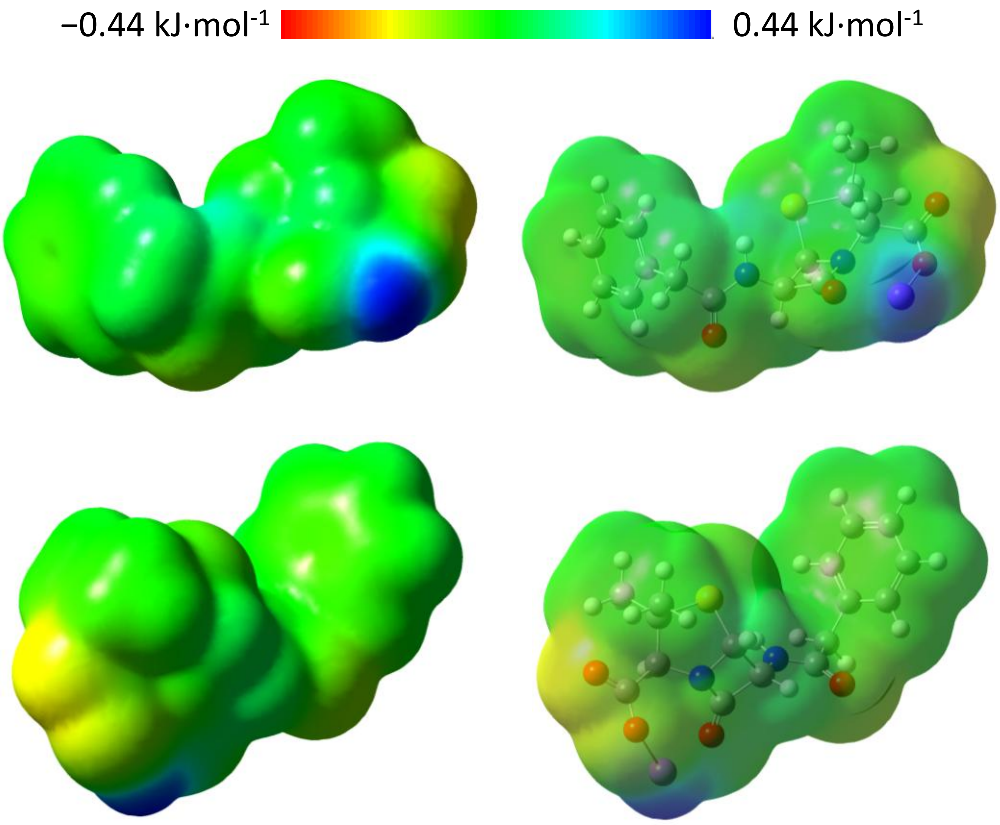


Figure S16 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **Pen**. Views from two perspectives are presented.

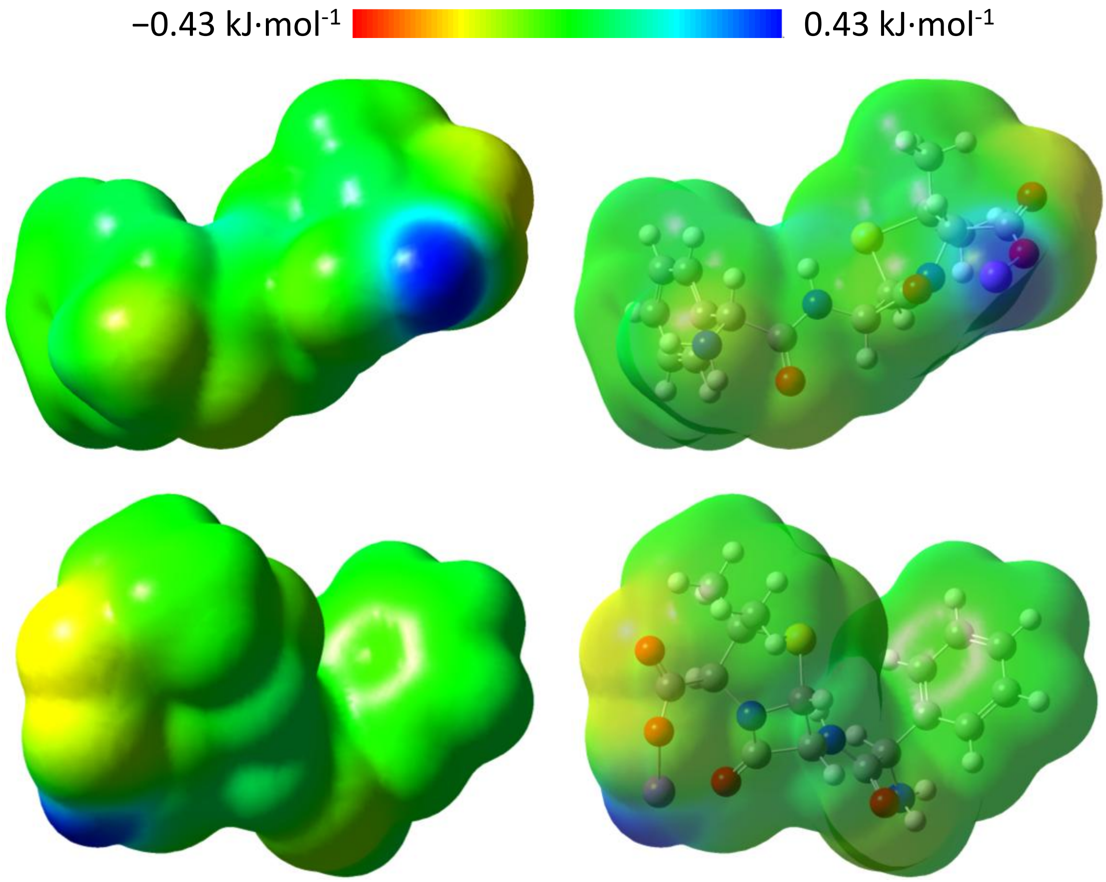


Figure S17 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **Ampc**. Views from two perspectives are presented.

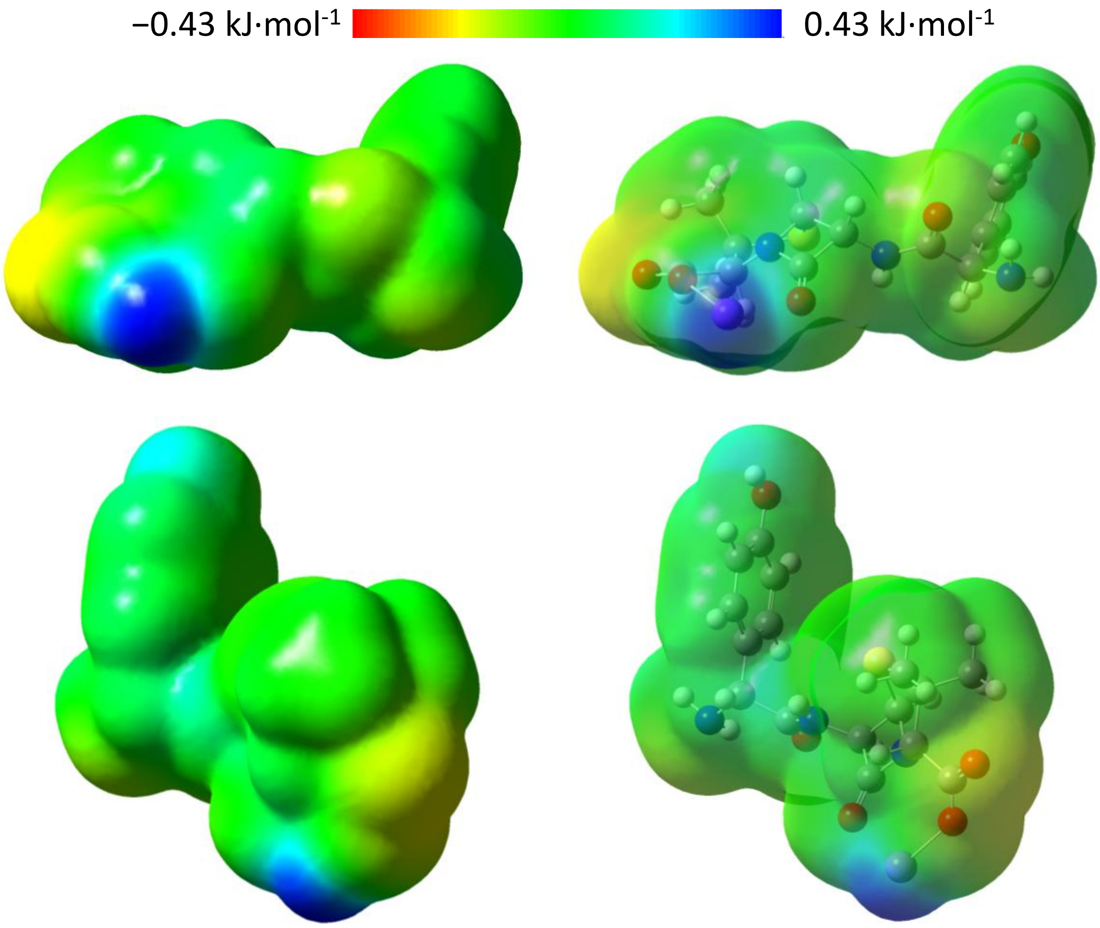


Figure S18 ESP maps for DFT optimised (B3LYP/6-31g(d,p)) **Amox**. Views from two perspectives are presented.

Table S3 Number of hydrogen bonding (HB) donors/acceptors for antibiotics computed with ADMET-predictor™ (ver. 11.0) software.

Compound	HB donors	HB acceptors
Penicillin G sodium salt (Pen)	1	5
Ampicillin sodium salt (Ampc)	2	6
Amoxicillin sodium salt (Amox)	3	7
Ceftazidime (Cef)	3	12

Table S4 Atomic coordinates for the DFT optimised (B3LYP/6-31g(d,p)) **B3E**.

	x	*y*	*z*
C	-0.7189000000	-0.0641000000	-0.2996000000
C	0.1718000000	1.0124000000	-0.1817000000
C	1.5381000000	0.7398000000	-0.0231000000
C	2.0196000000	-0.5764000000	0.0178000000
C	1.1038000000	-1.6307000000	-0.1045000000
C	-0.2683000000	-1.3913000000	-0.2633000000
C	-1.2210000000	-2.5216000000	-0.4080000000
C	3.4674000000	-0.8505000000	0.2050000000
C	-0.3214000000	2.4125000000	-0.2246000000

C	4.4401000000	-0.0451000000	-0.4091000000
C	5.7975000000	-0.3044000000	-0.2404000000
C	6.2262000000	-1.3808000000	0.5488000000
C	5.2606000000	-2.1734000000	1.1833000000
C	3.9062000000	-1.9179000000	1.0082000000
C	-1.5358000000	2.7701000000	0.3836000000
C	-2.0025000000	4.0809000000	0.3387000000
C	-1.2673000000	5.0789000000	-0.3163000000
C	-0.0432000000	4.7333000000	-0.9039000000
C	0.4163000000	3.4227000000	-0.8667000000
C	-0.8834000000	-3.6646000000	-1.1542000000
C	-1.7751000000	-4.7216000000	-1.2887000000
C	-3.0307000000	-4.6819000000	-0.6681000000
C	-3.3815000000	-3.5390000000	0.0640000000
C	-2.4901000000	-2.4772000000	0.1911000000
C	-3.9354000000	-5.8663000000	-0.8690000000
N	-4.8902000000	-6.0403000000	0.1099000000
O	-3.8005000000	-6.6129000000	-1.8324000000
C	7.6691000000	-1.7239000000	0.7979000000
N	8.5450000000	-1.2959000000	-0.1764000000
O	8.0096000000	-2.3523000000	1.7945000000
C	-1.6872000000	6.5205000000	-0.3995000000
O	-0.8642000000	7.4127000000	-0.5748000000
N	-3.0430000000	6.7384000000	-0.2818000000
C	-3.7487000000	7.9581000000	-0.2942000000
C	-5.8892000000	-7.0295000000	0.2067000000
C	9.9462000000	-1.4359000000	-0.2311000000
C	-3.1290000000	9.2163000000	-0.3416000000
C	-3.9120000000	10.3671000000	-0.3340000000
C	-5.3147000000	10.3195000000	-0.2831000000
C	-5.9163000000	9.0489000000	-0.2597000000
C	-5.1507000000	7.8907000000	-0.2526000000
C	-6.6745000000	-7.0393000000	1.3708000000
C	-7.6795000000	-7.9821000000	1.5397000000
C	-7.9581000000	-8.9358000000	0.5449000000
C	-7.1568000000	-8.9164000000	-0.6084000000
C	-6.1360000000	-7.9875000000	-0.7887000000
C	10.7152000000	-1.9861000000	0.8060000000
C	12.0976000000	-2.0673000000	0.6658000000
C	12.7622000000	-1.6182000000	-0.4871000000
C	11.9712000000	-1.0923000000	-1.5237000000
C	10.5925000000	-0.9906000000	-1.3955000000
C	14.2406000000	-1.7475000000	-0.6458000000
C	14.6800000000	-2.3193000000	-1.9561000000
C	15.1252000000	-1.3731000000	0.3267000000

C	16.5729000000	-1.7434000000	0.2866000000
C	14.7220000000	-0.5601000000	1.5147000000
C	-9.0216000000	-9.9630000000	0.7486000000
C	-9.9412000000	-10.2774000000	-0.2127000000
C	-9.0030000000	-10.6231000000	2.0905000000
C	-10.1419000000	-9.4472000000	-1.4397000000
C	-10.8264000000	-11.4785000000	-0.1205000000
C	-6.1476000000	11.5574000000	-0.3179000000
C	-7.2857000000	11.5171000000	-1.2876000000
C	-5.8944000000	12.6430000000	0.4733000000
C	-4.9424000000	12.5979000000	1.6251000000
C	-6.5481000000	13.9697000000	0.2562000000
C	-8.5912000000	11.8560000000	-0.8938000000
C	-9.6530000000	11.7801000000	-1.7936000000
C	-9.4332000000	11.3647000000	-3.1081000000
C	-8.1431000000	11.0150000000	-3.5119000000
C	-7.0838000000	11.0796000000	-2.6085000000
C	-7.1036000000	14.6766000000	1.3375000000
C	-7.6952000000	15.9244000000	1.1500000000
C	-7.7241000000	16.5046000000	-0.1197000000
C	-7.1566000000	15.8249000000	-1.1988000000
C	-6.5757000000	14.5717000000	-1.0132000000
C	-5.0232000000	11.5876000000	2.5984000000
C	-4.1560000000	11.5735000000	3.6893000000
C	-3.1871000000	12.5685000000	3.8311000000
C	-3.1011000000	13.5850000000	2.8779000000
C	-3.9766000000	13.6056000000	1.7937000000
C	15.1237000000	-0.9372000000	2.8082000000
C	14.7723000000	-0.1726000000	3.9192000000
C	14.0310000000	0.9996000000	3.7593000000
C	13.6446000000	1.3992000000	2.4787000000
C	13.9856000000	0.6278000000	1.3692000000
C	15.6625000000	-1.6856000000	-2.7354000000
C	16.0401000000	-2.2048000000	-3.9726000000
C	15.4445000000	-3.3702000000	-4.4582000000
C	14.4594000000	-4.0061000000	-3.7000000000
C	14.0736000000	-3.4798000000	-2.4685000000
C	16.9823000000	-3.0680000000	0.0575000000
C	18.3334000000	-3.4100000000	0.0572000000
C	19.3063000000	-2.4352000000	0.2850000000
C	18.9151000000	-1.1166000000	0.5248000000
C	17.5635000000	-0.7773000000	0.5370000000
C	-10.3037000000	-12.7505000000	0.1686000000
C	-11.1315000000	-13.8707000000	0.2171000000
C	-12.5011000000	-13.7447000000	-0.0215000000

C	-13.0340000000	-12.4893000000	-0.3205000000
C	-12.2041000000	-11.3713000000	-0.3806000000
C	-7.8002000000	-11.1130000000	2.6292000000
C	-7.7689000000	-11.7076000000	3.8893000000
C	-8.9360000000	-11.8048000000	4.6495000000
C	-10.1337000000	-11.3031000000	4.1371000000
C	-10.1669000000	-10.7194000000	2.8718000000
C	-10.2118000000	-10.0510000000	-2.7075000000
C	-10.4231000000	-9.2875000000	-3.8541000000
C	-10.5929000000	-7.9052000000	-3.7563000000
C	-10.5489000000	-7.2943000000	-2.5019000000
C	-10.3252000000	-8.0566000000	-1.3567000000
H	-1.7711000000	0.1347000000	-0.4756000000
H	2.2296000000	1.5630000000	0.1233000000
H	1.4643000000	-2.6537000000	-0.0753000000
H	-4.8101000000	-5.4408000000	0.9177000000
H	8.1265000000	-0.9092000000	-1.0093000000
H	-3.6250000000	5.9139000000	-0.2770000000
H	-2.0518000000	9.2774000000	-0.3953000000
H	-3.4180000000	11.3321000000	-0.3738000000
H	-6.9987000000	8.9699000000	-0.2410000000
H	-5.6438000000	6.9213000000	-0.2200000000
H	-6.4906000000	-6.3047000000	2.1521000000
H	-8.2631000000	-7.9778000000	2.4550000000
H	-7.3329000000	-9.6525000000	-1.3855000000
H	-5.5230000000	-8.0011000000	-1.6781000000
H	10.2245000000	-2.3509000000	1.6965000000
H	12.6777000000	-2.4972000000	1.4753000000
H	12.4457000000	-0.7538000000	-2.4394000000
H	10.0075000000	-0.5660000000	-2.2088000000
H	-8.7687000000	12.1800000000	0.1264000000
H	-10.6547000000	12.0429000000	-1.4655000000
H	-10.2604000000	11.3077000000	-3.8095000000
H	-7.9614000000	10.6875000000	-4.5317000000
H	-6.0851000000	10.7948000000	-2.9257000000
H	-7.0726000000	14.2374000000	2.3300000000
H	-8.1297000000	16.4466000000	1.9978000000
H	-8.1780000000	17.4806000000	-0.2651000000
H	-7.1615000000	16.2731000000	-2.1884000000
H	-6.1350000000	14.0500000000	-1.8562000000
H	-5.7748000000	10.8120000000	2.4944000000
H	-4.2399000000	10.7854000000	4.4323000000
H	-2.5096000000	12.5556000000	4.6798000000
H	-2.3534000000	14.3663000000	2.9805000000
H	-3.9127000000	14.4063000000	1.0631000000

H	15.7113000000	-1.8410000000	2.9385000000
H	15.0815000000	-0.4907000000	4.9108000000
H	13.7626000000	1.5995000000	4.6240000000
H	13.0788000000	2.3164000000	2.3420000000
H	13.6830000000	0.9442000000	0.3764000000
H	16.1295000000	-0.7796000000	-2.3637000000
H	16.7989000000	-1.6954000000	-4.5598000000
H	15.7404000000	-3.7757000000	-5.4214000000
H	13.9870000000	-4.9118000000	-4.0698000000
H	13.2983000000	-3.9724000000	-1.8894000000
H	16.2315000000	-3.8311000000	-0.1186000000
H	18.6259000000	-4.4416000000	-0.1170000000
H	20.3592000000	-2.7020000000	0.2833000000
H	19.6636000000	-0.3508000000	0.7081000000
H	17.2659000000	0.2475000000	0.7377000000
H	-9.2398000000	-12.8562000000	0.3531000000
H	-10.7041000000	-14.8448000000	0.4372000000
H	-13.1461000000	-14.6177000000	0.0177000000
H	-14.0978000000	-12.3805000000	-0.5125000000
H	-12.6232000000	-10.4004000000	-0.6271000000
H	-6.8865000000	-11.0299000000	2.0483000000
H	-6.8307000000	-12.0920000000	4.2797000000
H	-8.9110000000	-12.2615000000	5.6346000000
H	-11.0452000000	-11.3626000000	4.7250000000
H	-11.1011000000	-10.3316000000	2.4793000000
H	-10.0934000000	-11.1272000000	-2.7895000000
H	-10.4593000000	-9.7735000000	-4.8249000000
H	-10.7644000000	-7.3105000000	-4.6488000000
H	-10.6929000000	-6.2212000000	-2.4133000000
H	-10.2929000000	-7.5761000000	-0.3844000000
H	3.1760000000	-2.5349000000	1.5228000000
H	5.5989000000	-2.9819000000	1.8219000000
H	6.5164000000	0.3634000000	-0.7073000000
H	4.1304000000	0.7838000000	-1.0379000000
H	1.3491000000	3.1701000000	-1.3611000000
H	0.5301000000	5.5130000000	-1.3931000000
H	-2.9220000000	4.3241000000	0.8643000000
H	-2.1022000000	2.0212000000	0.9282000000
H	0.0780000000	-3.7100000000	-1.6563000000
H	-1.5236000000	-5.5925000000	-1.8839000000
H	-4.3651000000	-3.4503000000	0.5173000000
H	-2.7758000000	-1.6087000000	0.7765000000

Table S5 Atomic coordinates for the DFT optimised (B3LYP/6-31g(d,p)) **F-B3E**.

	x	*y*	*z*
C	0.8375000000	-0.0127000000	-0.2685000000
C	-0.0041000000	-1.1250000000	-0.1398000000
C	-1.3797000000	-0.9248000000	0.0333000000
C	-1.9150000000	0.3685000000	0.0840000000
C	-1.0588000000	1.4689000000	-0.0493000000
C	0.3185000000	1.2878000000	-0.2287000000
C	1.2182000000	2.4606000000	-0.3776000000
C	-3.3741000000	0.5707000000	0.2768000000
C	0.5542000000	-2.5009000000	-0.1843000000
C	-4.3280000000	-0.2069000000	-0.3927000000
C	-5.6915000000	-0.0127000000	-0.2101000000
C	-6.2029000000	0.9645000000	0.6493000000
C	-5.2538000000	1.7480000000	1.3200000000
C	-3.8875000000	1.5545000000	1.1320000000
C	1.7479000000	-2.8438000000	0.4640000000
C	2.2621000000	-4.1336000000	0.4202000000
C	1.6275000000	-5.1730000000	-0.2669000000
C	0.4351000000	-4.8355000000	-0.9220000000
C	-0.0754000000	-3.5404000000	-0.8822000000
C	0.8743000000	3.5748000000	-1.1546000000
C	1.7144000000	4.6756000000	-1.3039000000
C	2.9639000000	4.7341000000	-0.6714000000
C	3.3046000000	3.6261000000	0.1105000000
C	2.4664000000	2.5277000000	0.2552000000
C	3.8806000000	5.9133000000	-0.9334000000
N	4.6553000000	6.2836000000	0.1357000000
O	3.8762000000	6.4710000000	-2.0202000000
C	-7.6771000000	1.1552000000	0.9491000000
N	-8.5076000000	0.9609000000	-0.1245000000
O	-8.0445000000	1.4802000000	2.0679000000
C	2.0980000000	-6.6145000000	-0.2658000000
O	1.2886000000	-7.5294000000	-0.2762000000
N	3.4602000000	-6.7716000000	-0.2787000000
C	4.2044000000	-7.9708000000	-0.2778000000
C	5.6020000000	7.3274000000	0.2124000000
C	-9.9144000000	1.0628000000	-0.1749000000
C	3.6285000000	-9.2489000000	-0.3327000000
C	4.4521000000	-10.3711000000	-0.3314000000
C	5.8520000000	-10.2732000000	-0.2794000000
C	6.4085000000	-8.9822000000	-0.2492000000
C	5.6027000000	-7.8519000000	-0.2370000000
C	6.3121000000	7.4555000000	1.4167000000

C	7.2499000000	8.4659000000	1.5799000000
C	7.5321000000	9.3725000000	0.5427000000
C	6.8029000000	9.2356000000	-0.6497000000
C	5.8501000000	8.2363000000	-0.8271000000
C	-10.7098000000	1.4544000000	0.9123000000
C	-12.0913000000	1.5288000000	0.7577000000
C	-12.7265000000	1.2266000000	-0.4576000000
C	-11.9082000000	0.8594000000	-1.5405000000
C	-10.5301000000	0.7673000000	-1.4015000000
C	-14.2046000000	1.3497000000	-0.6259000000
C	-14.6330000000	2.0880000000	-1.8540000000
C	-15.0969000000	0.8286000000	0.2688000000
C	-16.5512000000	1.1733000000	0.2514000000
C	-14.6959000000	-0.1321000000	1.3417000000
C	8.5234000000	10.4710000000	0.7386000000
C	9.4774000000	10.7810000000	-0.1900000000
C	8.3927000000	11.2057000000	2.0347000000
C	9.7913000000	9.8937000000	-1.3515000000
C	10.2910000000	12.0333000000	-0.1239000000
C	6.7285000000	-11.4808000000	-0.3193000000
C	7.8634000000	-11.3963000000	-1.2897000000
C	6.5141000000	-12.5767000000	0.4690000000
C	5.5614000000	-12.5682000000	1.6210000000
C	7.2149000000	-13.8785000000	0.2485000000
C	9.1805000000	-11.6894000000	-0.8980000000
C	10.2380000000	-11.5727000000	-1.7984000000
C	10.0022000000	-11.1612000000	-3.1114000000
C	8.7001000000	-10.8568000000	-3.5131000000
C	7.6446000000	-10.9623000000	-2.6091000000
C	7.7948000000	-14.5680000000	1.3281000000
C	8.4300000000	-15.7937000000	1.1374000000
C	8.4792000000	-16.3692000000	-0.1337000000
C	7.8882000000	-15.7073000000	-1.2113000000
C	7.2637000000	-14.4756000000	-1.0226000000
C	5.6074000000	-11.5589000000	2.5975000000
C	4.7394000000	-11.5777000000	3.6878000000
C	3.8048000000	-12.6054000000	3.8254000000
C	3.7541000000	-13.6213000000	2.8690000000
C	4.6306000000	-13.6090000000	1.7856000000
C	-15.1256000000	0.0574000000	2.6669000000
C	-14.7759000000	-0.8455000000	3.6693000000
C	-14.0084000000	-1.9713000000	3.3644000000
C	-13.5940000000	-2.1851000000	2.0486000000
C	-13.9333000000	-1.2753000000	1.0487000000
C	-15.5876000000	1.5488000000	-2.7327000000

C	-15.9545000000	2.2261000000	-3.8944000000
C	-15.3758000000	3.4585000000	-4.2030000000
C	-14.4185000000	4.0028000000	-3.3447000000
C	-14.0432000000	3.3195000000	-2.1894000000
C	-16.9847000000	2.5088000000	0.1968000000
C	-18.3426000000	2.8221000000	0.2176000000
C	-19.2981000000	1.8071000000	0.2922000000
C	-18.8829000000	0.4756000000	0.3575000000
C	-17.5248000000	0.1634000000	0.3490000000
C	9.6867000000	13.2883000000	0.0611000000
C	10.4503000000	14.4540000000	0.0851000000
C	11.8357000000	14.3912000000	-0.0741000000
C	12.4499000000	13.1526000000	-0.2694000000
C	11.6846000000	11.9884000000	-0.3054000000
C	7.1370000000	11.6591000000	2.4758000000
C	7.0021000000	12.3228000000	3.6940000000
C	8.1168000000	12.5278000000	4.5094000000
C	9.3665000000	12.0641000000	4.0947000000
C	9.5030000000	11.4109000000	2.8709000000
C	9.8946000000	10.4255000000	-2.6489000000
C	10.2092000000	9.6100000000	-3.7343000000
C	10.4511000000	8.2483000000	-3.5431000000
C	10.3751000000	7.7104000000	-2.2572000000
C	10.0481000000	8.5238000000	-1.1737000000
F	1.2733000000	5.6843000000	-2.0554000000
F	-0.3044000000	3.6075000000	-1.7991000000
F	4.4785000000	3.5987000000	0.7804000000
F	2.8887000000	1.5187000000	1.0362000000
F	2.4278000000	-1.9240000000	1.1699000000
F	3.4233000000	-4.3577000000	1.0752000000
F	-0.2345000000	-5.7354000000	-1.6424000000
F	-1.2103000000	-3.3031000000	-1.5602000000
F	-3.0511000000	2.3539000000	1.8159000000
F	-5.6257000000	2.7258000000	2.1464000000
F	-3.9424000000	-1.1689000000	-1.2477000000
F	-6.5280000000	-0.8015000000	-0.9205000000
H	1.9001000000	-0.1595000000	-0.4044000000
H	-2.0353000000	-1.7790000000	0.1331000000
H	-1.4660000000	2.4697000000	-0.0139000000
H	4.6068000000	5.6920000000	0.9526000000
H	-8.0742000000	0.6295000000	-0.9741000000
H	4.0110000000	-5.9291000000	-0.1992000000
H	2.5541000000	-9.3506000000	-0.3772000000
H	3.9930000000	-11.3529000000	-0.3752000000
H	7.4874000000	-8.8652000000	-0.2296000000

H	6.0603000000	-6.8657000000	-0.2014000000
H	6.1226000000	6.7609000000	2.2322000000
H	7.7776000000	8.5527000000	2.5244000000
H	6.9829000000	9.9320000000	-1.4615000000
H	5.2998000000	8.1542000000	-1.7530000000
H	-10.2444000000	1.6962000000	1.8566000000
H	-12.6937000000	1.8341000000	1.6065000000
H	-12.3607000000	0.6386000000	-2.5020000000
H	-9.9224000000	0.4695000000	-2.2532000000
H	9.3705000000	-12.0100000000	0.1210000000
H	11.2487000000	-11.8004000000	-1.4720000000
H	10.8262000000	-11.0723000000	-3.8133000000
H	8.5058000000	-10.5328000000	-4.5317000000
H	6.6360000000	-10.7130000000	-2.9250000000
H	7.7482000000	-14.1328000000	2.3218000000
H	8.8826000000	-16.3024000000	1.9839000000
H	8.9670000000	-17.3283000000	-0.2816000000
H	7.9088000000	-16.1525000000	-2.2019000000
H	6.8050000000	-13.9676000000	-1.8643000000
H	6.3326000000	-10.7580000000	2.4970000000
H	4.7960000000	-10.7896000000	4.4333000000
H	3.1265000000	-12.6181000000	4.6735000000
H	3.0332000000	-14.4279000000	2.9687000000
H	4.5946000000	-14.4092000000	1.0525000000
H	-15.7337000000	0.9239000000	2.9086000000
H	-15.1069000000	-0.6717000000	4.6893000000
H	-13.7414000000	-2.6788000000	4.1439000000
H	-13.0078000000	-3.0646000000	1.7983000000
H	-13.6093000000	-1.4479000000	0.0276000000
H	-16.0412000000	0.5914000000	-2.4986000000
H	-16.6914000000	1.7879000000	-4.5614000000
H	-15.6634000000	3.9868000000	-5.1073000000
H	-13.9596000000	4.9597000000	-3.5770000000
H	-13.2896000000	3.7430000000	-1.5323000000
H	-16.2477000000	3.3029000000	0.1404000000
H	-18.6543000000	3.8621000000	0.1800000000
H	-20.3562000000	2.0517000000	0.3069000000
H	-19.6179000000	-0.3219000000	0.4204000000
H	-17.2087000000	-0.8734000000	0.4138000000
H	8.6102000000	13.3449000000	0.1837000000
H	9.9607000000	15.4136000000	0.2240000000
H	12.4305000000	15.2998000000	-0.0540000000
H	13.5268000000	13.0927000000	-0.3991000000
H	12.1673000000	11.0300000000	-0.4713000000
H	6.2639000000	11.4928000000	1.8519000000

H	6.0244000000	12.6768000000	4.0084000000
H	8.0112000000	13.0384000000	5.4621000000
H	10.2381000000	12.2077000000	4.7269000000
H	10.4771000000	11.0532000000	2.5543000000
H	9.7205000000	11.4862000000	-2.8027000000
H	10.2696000000	10.0395000000	-4.7303000000
H	10.7030000000	7.6136000000	-4.3877000000
H	10.5745000000	6.6548000000	-2.0957000000
H	9.9917000000	8.1000000000	-0.1764000000

Table S6 Atomic coordinates for the DFT optimised (B3LYP/6-31g(d,p)) **Cef**.

	x	*y*	*z*
C	1.1887000000	-0.1694000000	0.1544000000
C	2.6675000000	-0.5372000000	-0.0161000000
C	3.1250000000	-0.2440000000	-1.4498000000
C	3.5111000000	0.2951000000	1.0035000000
O	4.2190000000	-0.1585000000	1.8983000000
O	3.4308000000	1.6417000000	0.8273000000
O	2.7109000000	-1.9562000000	0.1753000000
N	4.0239000000	-2.3823000000	0.3753000000
C	4.1448000000	-3.2205000000	1.3705000000
C	3.0608000000	-3.8053000000	2.1740000000
C	3.2553000000	-4.7932000000	3.1280000000
S	1.7766000000	-5.2043000000	3.8876000000
C	0.9700000000	-4.0469000000	2.9195000000
N	1.7256000000	-3.3989000000	2.0721000000
N	-0.3531000000	-3.8450000000	3.0238000000
C	5.5935000000	-3.4646000000	1.7878000000
O	6.0772000000	-4.5819000000	1.7493000000
N	6.2135000000	-2.3114000000	2.2273000000
C	7.5100000000	-2.2731000000	2.9502000000
C	8.6796000000	-3.1884000000	2.4956000000
N	8.4266000000	-4.0223000000	3.6934000000
C	7.5965000000	-3.0801000000	4.2621000000
O	7.2601000000	-2.8674000000	5.4084000000
C	9.4932000000	-4.5407000000	4.3972000000
C	10.5633000000	-3.7874000000	4.7295000000
C	10.7094000000	-2.3914000000	4.2171000000
S	10.2911000000	-2.2889000000	2.4632000000
C	11.6253000000	-4.2876000000	5.6780000000
N	11.5435000000	-3.5452000000	6.9684000000
C	10.4457000000	-3.6837000000	7.7534000000

C	10.3527000000	-3.0083000000	8.9653000000
C	11.3997000000	-2.1963000000	9.3777000000
C	12.5234000000	-2.0772000000	8.5710000000
C	12.5756000000	-2.7685000000	7.3648000000
C	9.4553000000	-5.9835000000	4.9723000000
O	10.2125000000	-6.7885000000	4.3617000000
O	8.9579000000	-6.0597000000	6.1311000000
H	0.9877000000	0.8832000000	-0.0675000000
H	0.8621000000	-0.3636000000	1.1831000000
H	0.5548000000	-0.7829000000	-0.4964000000
H	2.9498000000	0.7972000000	-1.7380000000
H	2.6057000000	-0.8908000000	-2.1662000000
H	4.1971000000	-0.4412000000	-1.5645000000
H	2.8565000000	1.9362000000	0.0971000000
H	4.1708000000	-5.2938000000	3.4158000000
H	-0.9083000000	-4.5922000000	3.4219000000
H	-0.7830000000	-3.3827000000	2.2317000000
H	5.6331000000	-1.4651000000	2.1966000000
H	7.7838000000	-1.2221000000	3.1118000000
H	8.5031000000	-3.7417000000	1.5676000000
H	11.7481000000	-2.0567000000	4.3065000000
H	10.0984000000	-1.6955000000	4.8017000000
H	12.6171000000	-4.1244000000	5.2405000000
H	11.5850000000	-5.3445000000	5.9517000000
H	9.6398000000	-4.3229000000	7.4085000000
H	9.4602000000	-3.1242000000	9.5762000000
H	11.3381000000	-1.6642000000	10.3249000000
H	13.3561000000	-1.4512000000	8.8814000000
H	13.4389000000	-2.7044000000	6.7100000000

Table S7 Atomic coordinates for the DFT optimised (B3LYP/6-31g(d,p)) **Pen**.

	x	*y*	*z*
C	2.8570000000	2.8154000000	1.2054000000
C	2.4520000000	1.9198000000	0.0341000000
C	2.9642000000	0.4635000000	0.2394000000
N	1.9976000000	-0.4001000000	-0.4724000000
C	0.7611000000	0.2206000000	-0.9904000000
S	0.5554000000	1.7334000000	0.0168000000
C	-0.0001000000	-1.0968000000	-0.6199000000
C	1.3671000000	-1.5214000000	-0.0233000000
O	1.7726000000	-2.4683000000	0.6502000000
N	-1.1063000000	-1.0161000000	0.2832000000
C	-2.2865000000	-1.6784000000	0.0408000000
O	-2.4426000000	-2.4110000000	-0.9265000000

C	-3.3996000000	-1.4074000000	1.0516000000
C	-4.3896000000	-0.3734000000	0.5379000000
C	-4.6051000000	0.8181000000	1.2386000000
C	-5.5184000000	1.7647000000	0.7702000000
C	-6.2243000000	1.5302000000	-0.4092000000
C	-6.0116000000	0.3447000000	-1.1170000000
C	-5.1016000000	-0.6013000000	-0.6481000000
C	4.4767000000	0.1683000000	-0.0808000000
O	5.2690000000	1.1100000000	-0.0085000000
C	2.9088000000	2.5282000000	-1.2994000000
O	4.7236000000	-1.0663000000	-0.2849000000
Na	3.9584000000	-2.8545000000	0.4464000000
H	2.4756000000	2.4321000000	2.1570000000
H	2.4847000000	3.8349000000	1.0675000000
H	3.9493000000	2.8391000000	1.2437000000
H	2.8583000000	0.2248000000	1.3080000000
H	0.7930000000	0.4559000000	-2.0563000000
H	-0.3229000000	-1.6919000000	-1.4779000000
H	-1.0352000000	-0.3794000000	1.0648000000
H	-2.9865000000	-1.0851000000	2.0129000000
H	-3.9025000000	-2.3663000000	1.2124000000
H	-4.0600000000	1.0065000000	2.1605000000
H	-5.6753000000	2.6838000000	1.3274000000
H	-6.9353000000	2.2649000000	-0.7753000000
H	-6.5566000000	0.1558000000	-2.0374000000
H	-4.9248000000	-1.5171000000	-1.2035000000
H	3.9978000000	2.6087000000	-1.2874000000
H	2.4667000000	3.5185000000	-1.4350000000
H	2.6251000000	1.9093000000	-2.1560000000

Table S8 Atomic coordinates for the DFT optimized (B3LYP/6-31g(d,p)) **Ampc**.

	x	*y*	*z*
C	2.9758000000	2.7416000000	1.3433000000
C	2.5850000000	1.9098000000	0.1212000000
C	3.0644000000	0.4358000000	0.2706000000
N	2.1021000000	-0.3736000000	-0.5077000000
C	0.8911000000	0.2951000000	-1.0260000000
S	0.6862000000	1.7616000000	0.0475000000
C	0.0974000000	-1.0241000000	-0.7414000000
C	1.4408000000	-1.5036000000	-0.1305000000
O	1.8100000000	-2.4890000000	0.5062000000
N	-1.0303000000	-0.9651000000	0.1374000000
C	-2.2023000000	-1.6134000000	-0.1429000000
O	-2.3507000000	-2.3241000000	-1.1299000000

C	-3.3515000000	-1.3474000000	0.8436000000
C	-4.1075000000	-0.0911000000	0.4013000000
C	-4.2111000000	1.0120000000	1.2551000000
C	-4.9226000000	2.1497000000	0.8673000000
C	-5.5367000000	2.1952000000	-0.3836000000
C	-5.4361000000	1.0987000000	-1.2446000000
C	-4.7281000000	-0.0365000000	-0.8557000000
N	-4.1483000000	-2.5698000000	0.9205000000
C	4.5792000000	0.1248000000	-0.0227000000
O	5.3869000000	1.0468000000	0.1083000000
C	3.0879000000	2.5705000000	-1.1701000000
O	4.8076000000	-1.1052000000	-0.2713000000
Na	3.9937000000	-2.9100000000	0.3624000000
H	2.5625000000	2.3220000000	2.2658000000
H	2.6265000000	3.7736000000	1.2443000000
H	4.0669000000	2.7417000000	1.4103000000
H	2.9240000000	0.1491000000	1.3233000000
H	0.9553000000	0.5807000000	-2.0781000000
H	-0.2105000000	-1.5714000000	-1.6354000000
H	-0.9688000000	-0.3711000000	0.9533000000
H	-2.9196000000	-1.1422000000	1.8333000000
H	-3.7389000000	0.9789000000	2.2344000000
H	-4.9972000000	2.9965000000	1.5433000000
H	-6.0906000000	3.0783000000	-0.6879000000
H	-5.9081000000	1.1306000000	-2.2224000000
H	-4.6404000000	-0.8837000000	-1.5296000000
H	-4.1822000000	-2.9852000000	-0.0084000000
H	-5.0991000000	-2.3462000000	1.1995000000
H	4.1775000000	2.6290000000	-1.1264000000
H	2.6676000000	3.5744000000	-1.2705000000
H	2.8161000000	1.9975000000	-2.0619000000

Table S9 Atomic coordinates for the DFT optimized (B3LYP/6-31g(d,p)) **Amox.**

	x	*y*	*z*
C	2.9900000000	2.8267000000	1.4088000000
C	2.6566000000	1.9974000000	0.1681000000
C	3.2690000000	0.5693000000	0.2682000000
N	2.3714000000	-0.3023000000	-0.5200000000
C	1.0968000000	0.2678000000	-1.0024000000
S	0.7780000000	1.6803000000	0.1151000000
C	0.4295000000	-1.1251000000	-0.7433000000
C	1.8204000000	-1.4971000000	-0.1654000000
O	2.2881000000	-2.4617000000	0.4377000000
N	-0.6840000000	-1.1922000000	0.1523000000

C	-1.8077000000	-1.9172000000	-0.1406000000
O	-1.9127000000	-2.6016000000	-1.1516000000
C	-2.9623000000	-1.7726000000	0.8646000000
C	-3.8118000000	-0.5617000000	0.4744000000
C	-3.9849000000	0.5065000000	1.3579000000
C	-4.7769000000	1.6048000000	1.0189000000
C	-5.4095000000	1.6452000000	-0.2261000000
C	-5.2445000000	0.5831000000	-1.1252000000
C	-4.4549000000	-0.5040000000	-0.7732000000
O	-6.1994000000	2.6858000000	-0.6234000000
N	-3.6631000000	-3.0547000000	0.9065000000
C	4.8008000000	0.4054000000	-0.0540000000
O	5.5241000000	1.3925000000	0.0960000000
C	3.0779000000	2.7366000000	-1.1099000000
O	5.1354000000	-0.7906000000	-0.3443000000
Na	4.4975000000	-2.6791000000	0.2464000000
H	2.6304000000	2.3460000000	2.3239000000
H	2.5480000000	3.8254000000	1.3443000000
H	4.0777000000	2.9232000000	1.4616000000
H	3.1721000000	0.2421000000	1.3140000000
H	1.1176000000	0.5864000000	-2.0467000000
H	0.1570000000	-1.6735000000	-1.6482000000
H	-0.6624000000	-0.6176000000	0.9839000000
H	-2.5341000000	-1.5692000000	1.8565000000
H	-3.5020000000	0.4839000000	2.3322000000
H	-4.9035000000	2.4249000000	1.7225000000
H	-5.7385000000	0.6327000000	-2.0898000000
H	-4.3202000000	-1.3189000000	-1.4785000000
H	-6.2213000000	3.3530000000	0.0751000000
H	-3.6679000000	-3.4435000000	-0.0345000000
H	-4.6277000000	-2.9105000000	1.1904000000
H	4.1584000000	2.8920000000	-1.0786000000
H	2.5676000000	3.7009000000	-1.1754000000
H	2.8447000000	2.1665000000	-2.0143000000

S5. Photophysical and AIE studies

S5.1 Quantum yield measurement

For **B3E** in dissolved state (100% THF), *ΦF* = 0.0118

For **B3E** in aggregated state (H_2O:THF = 95:5 *v:v*), *ΦF* = 0.0586

For **F- B3E** in dissolved state (100% THF), *ΦF* = 0.0208

For **F-B3E** in aggregated state (H_2O:THF = 95:5 *v:v*), *ΦF* = 0.1089

S5.2 UV-vis and fluorescence measurements

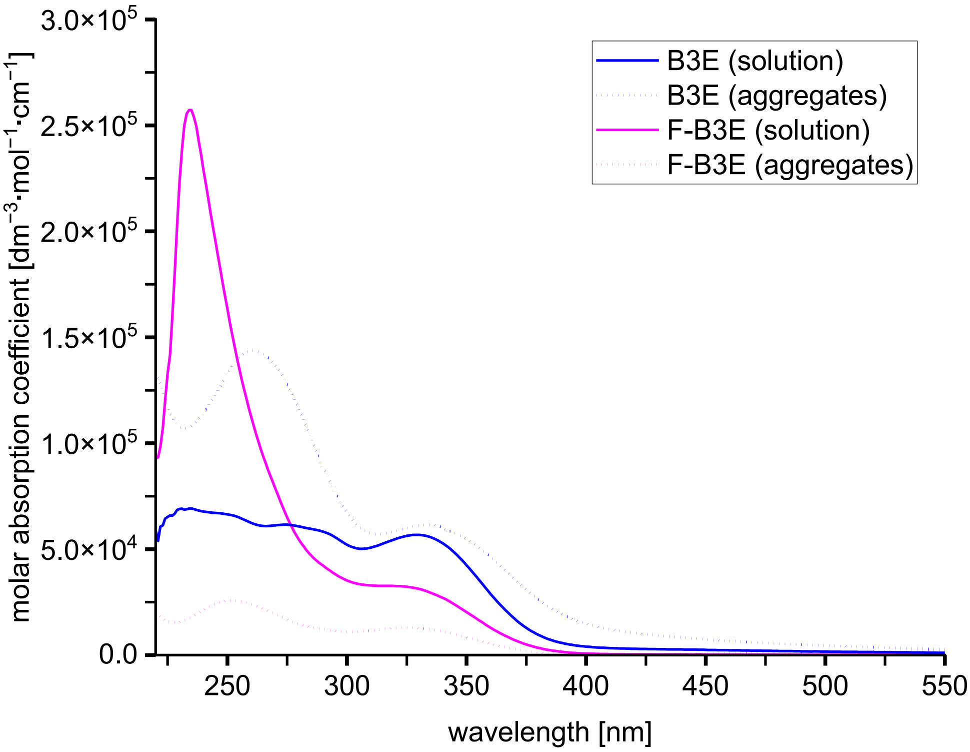


Figure S19 UV-vis stacked spectra of **B3E** and **F-B3E** ($C = 2·10^{-6}$) in solution (100% THF) and in aggregated state (95:5 H_2O:THF *v/v*). ($C = 2·10^{-6}$).

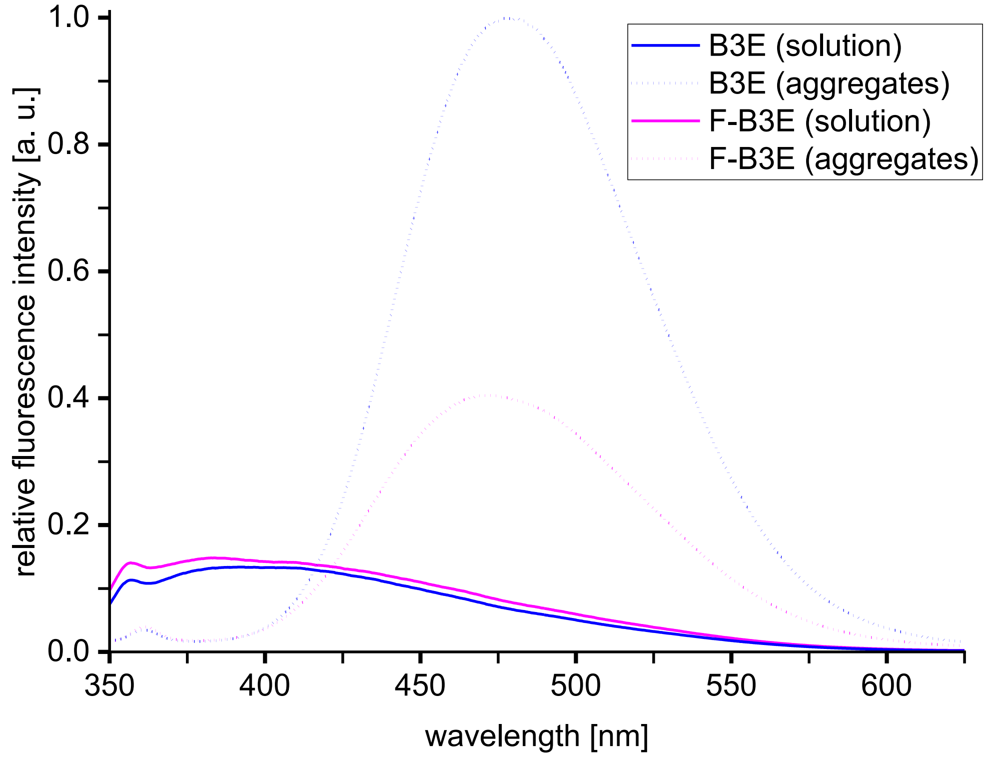


Figure S 20 Stacked fluorescence spectra of **B3E** and **F-B3E** ($C = 2{\cdot}10^{-6}$) in solution (100% THF) and in aggregated state (95:5 H_2O:THF *v/v*). ($C = 2{\cdot}10^{-6}$).

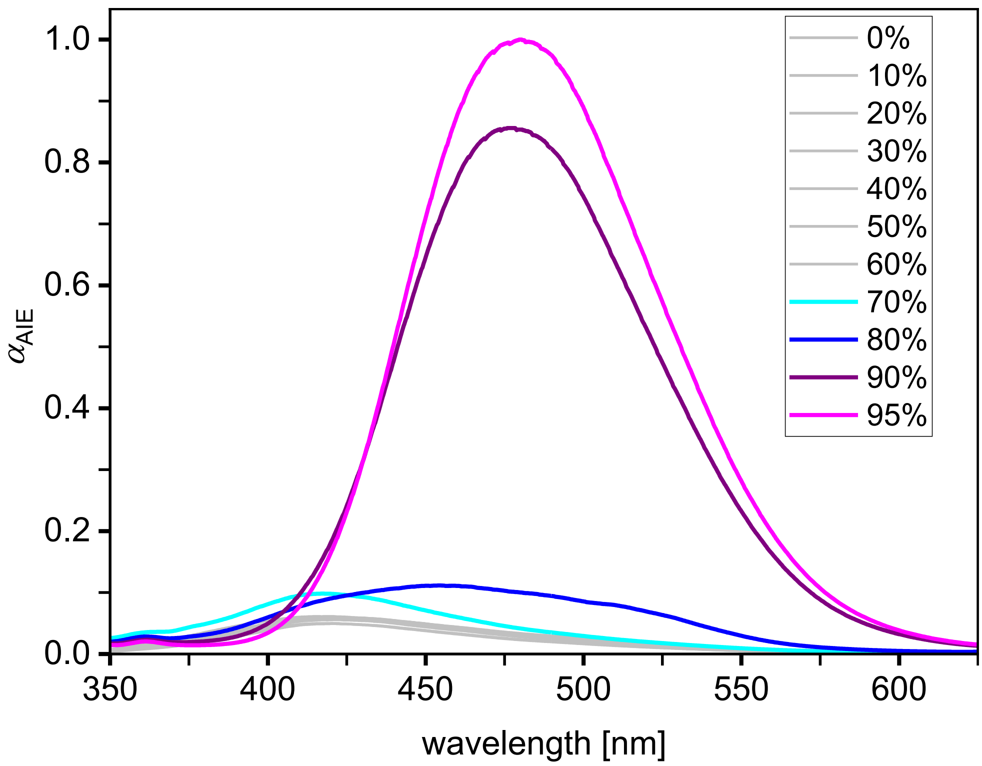


Figure S21 Relative fluorescence intensity of **B3E** a in water:THF systems with increasing water content ($C = 2{\cdot}10^{-5}$ M, λ_{ex} = 320 nm).

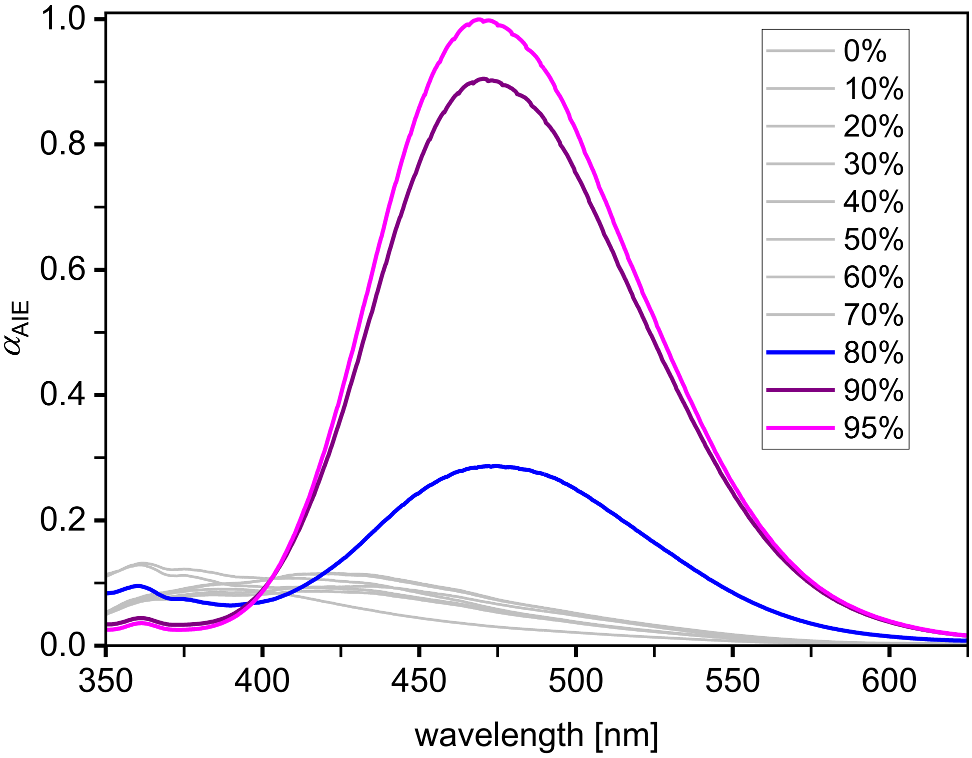


Figure S22 Relative fluorescence intensity of **B3E** a in water:THF systems with increasing water content ($C = 2\cdot10^{-5}$ M, $\lambda_{ex} = 320$ nm).

S5.3 Dynamic Light Scattering measurements

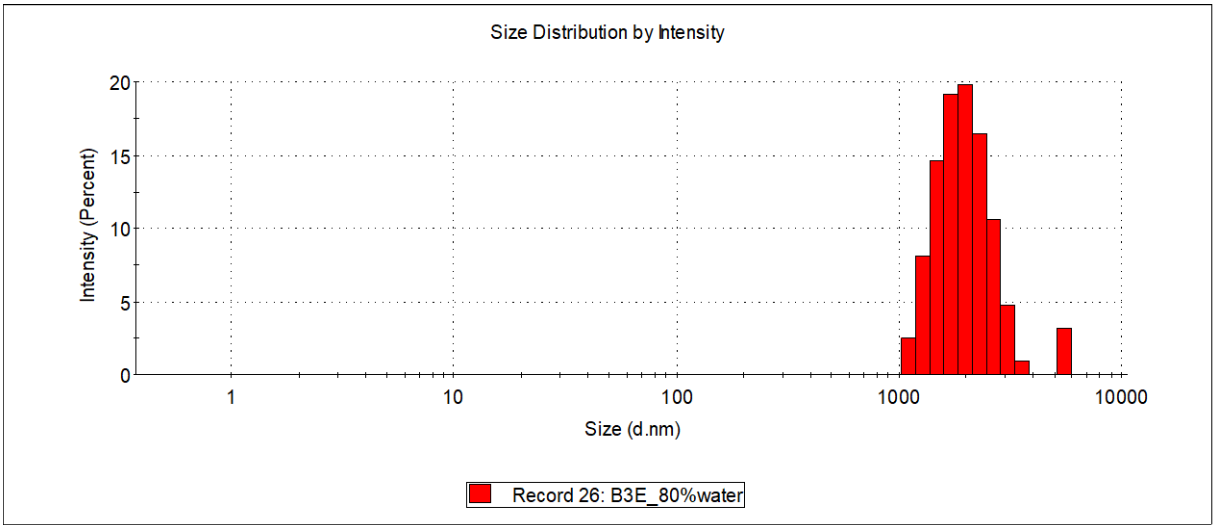


Figure S23 DLS experiment results: size distribution by intensity for **B3E** in H_2O:THF 80:20 *v/v*. Average aggregate size in dominant peak: d = 1974 nm.

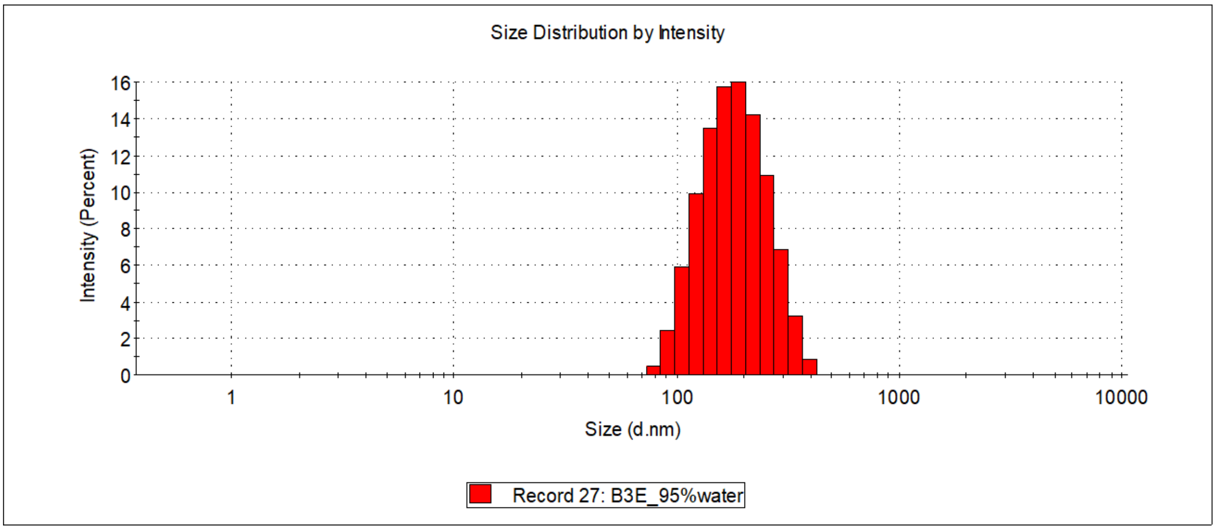


Figure S24 DLS experiment results: size distribution by intensity for **B3E** in H_2O:THF 95:5 *v/v*. Average aggregate size in dominant peak: d = 190.1 nm.

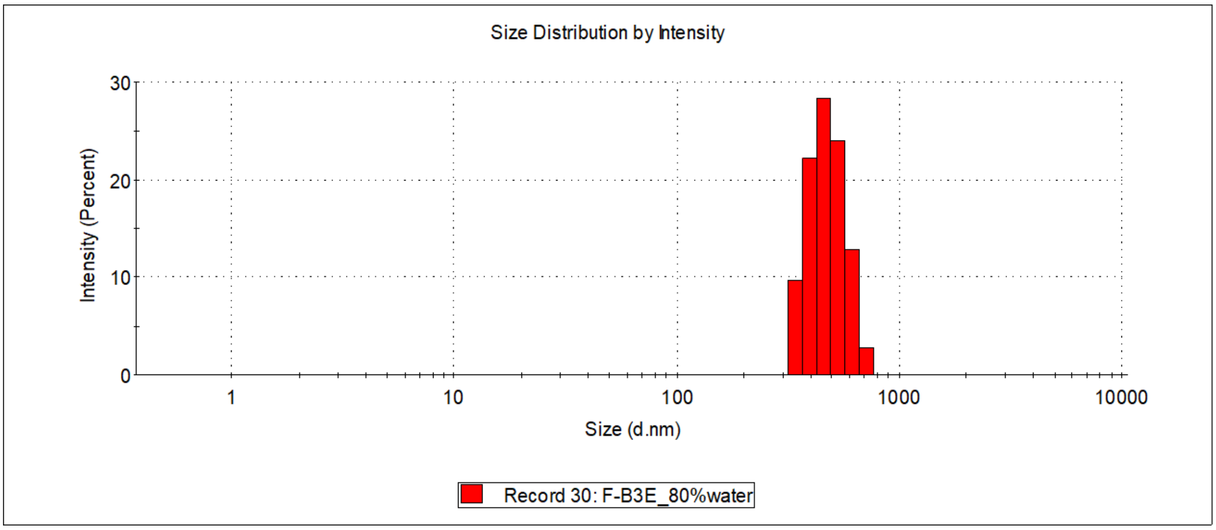


Figure S25 DLS experiment results: size distribution by intensity for **F-B3E** in H_2O:THF 80:20 *v/v*. Average aggregate size in dominant peak: d = 478.1 nm.

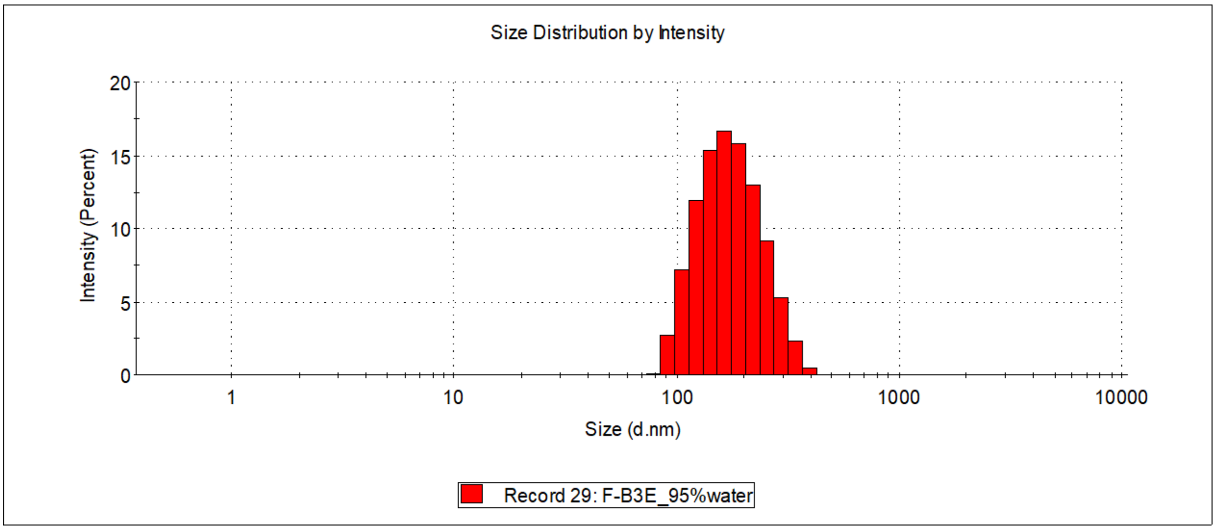


Figure S26 DLS experiment results: size distribution by intensity for **F-B3E** in H_2O:THF 95:5 *v/v*. Average aggregate size in dominant peak: d = 181.4 nm.

S6. Receptor studies

S6.1 Spectrofluorimetry

For the calculation of Stern-Volmer constant values equation:

$$\frac{I_0}{\mathrm{I}} - 1 = K_{S-V} \cdot C_{analyte}$$

where:

I_0 – fluorescence intensity at starting point [a. u.]

I - fluorescence intensity at measured point [a. u.]

$K_{S\text{-}V}$ – Stern-Volmer constant value [M^{-1}]

$C_{analyte}$ – concentration of analyte at measured point [M]

was used. $K_{S\text{-}V}$ were calculated as the slope of linear regression from experimental points. LOD values were calculated as $\frac{3 \cdot \sigma}{K_{S-V}}$.

Table S10. Comparison of $K_{S\text{-}V}$, K_a and LOD values for **B3E** and **F-B3E** in different solvent systems (water:THF).

Water content	Solvent – receptor system		$K_{s\text{-}v} \cdot 10^3$ [M^{-1}]	LOD [μM]
95% vol.	Ultrapure water 95%	**B3E**	3.049 ± 0.111	5.7
		F-B3E	2.972 ± 0.124	6.5
99% vol.	Ultrapure water	**B3E**	3.459 ± 0.025	1.1
		F-B3E	3.103 ± 0.216	10.8
	Buffer, pH 5.14	**B3E**	3.203 ± 0.155	7.5
		F-B3E	2.452 ± 0.148	9.4
	Buffer, pH 7.4	**B3E**	4.581 ± 0.068	2.3
		F-B3E	4.337 ± 0.176	6.3
	Buffer, pH 8.29	**B3E**	4.107 ± 0.079	3.0
		F-B3E	2.700 ± 0.154	8.9
	Tap water	**B3E**	3.369 ± 0.153	7.1
		F-B3E	3.159 ± 0.133	6.5
	Seawater (filtered)	**B3E**	4.070 ± 0.077	2.9
		F-B3E	5.411 ± 0.228	6.5
	Seawater (non-filtered)	**B3E**	4.101 ± 0.178	6.7
		F-B3E	4.346 ± 0.152	5.4
	Artesian groundwater	**B3E**	4.115 ± 0.179	6.4
		F-B3E	2.423 ± 0.198	12.7

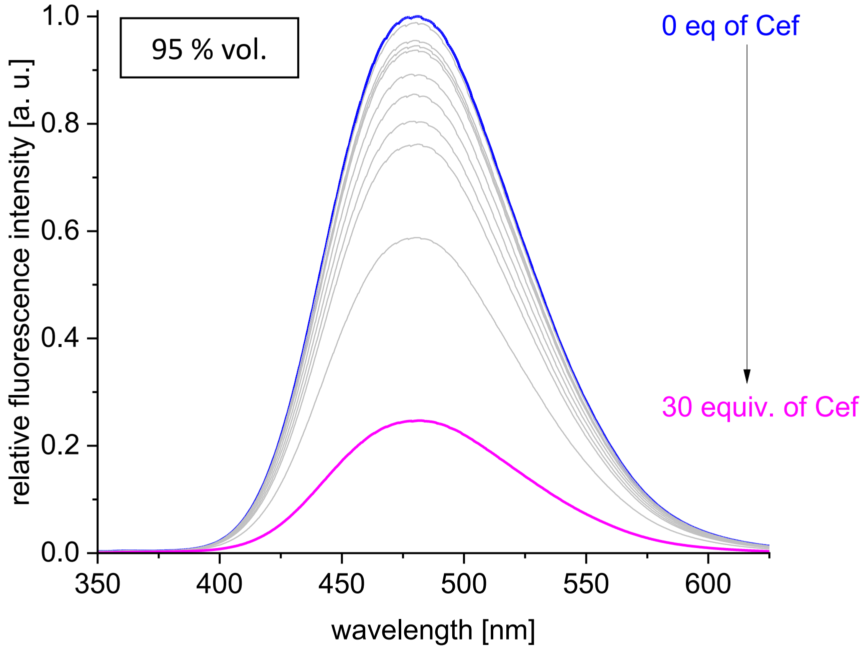


Figure S27 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

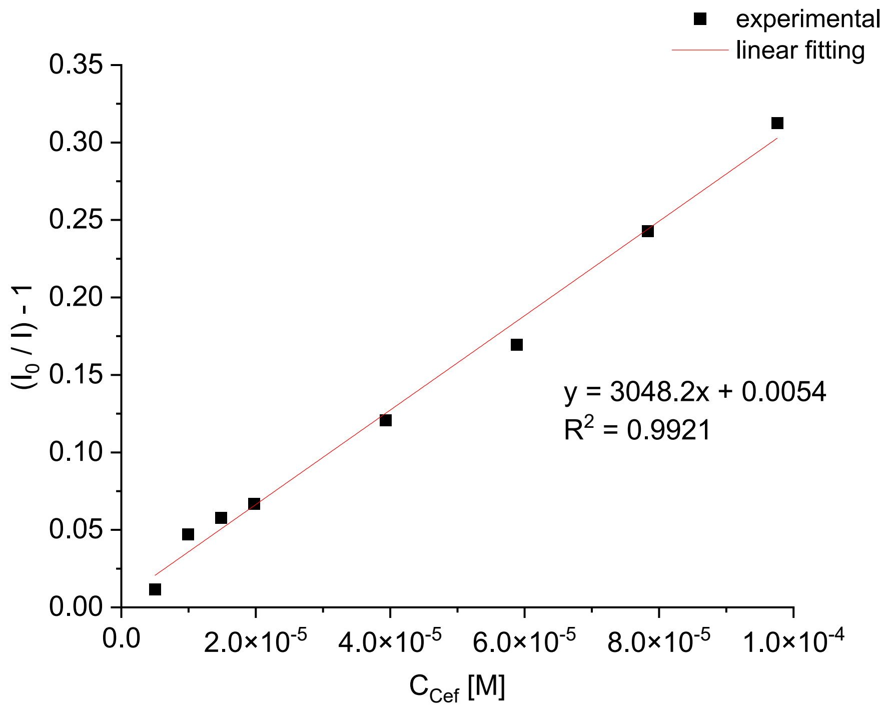


Figure S28 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

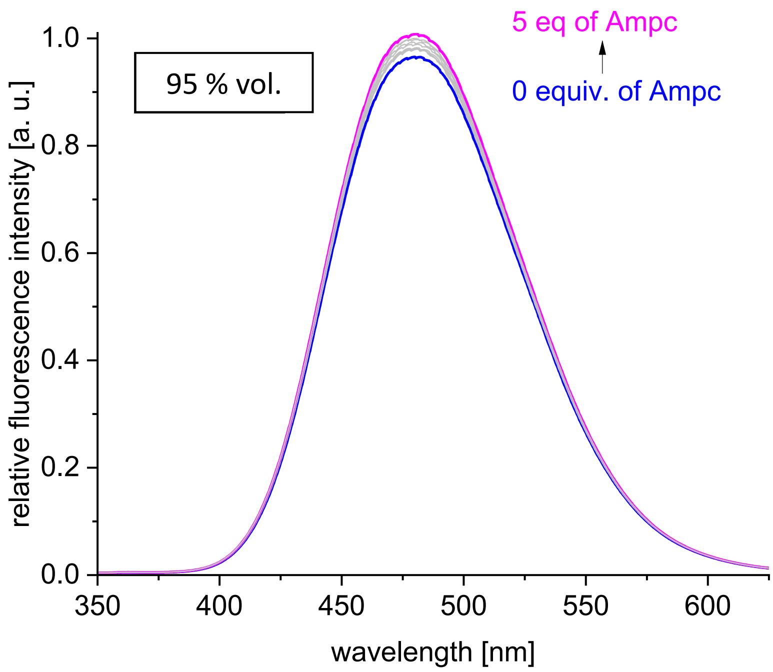


Figure S29 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ampicillin (Ampc). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

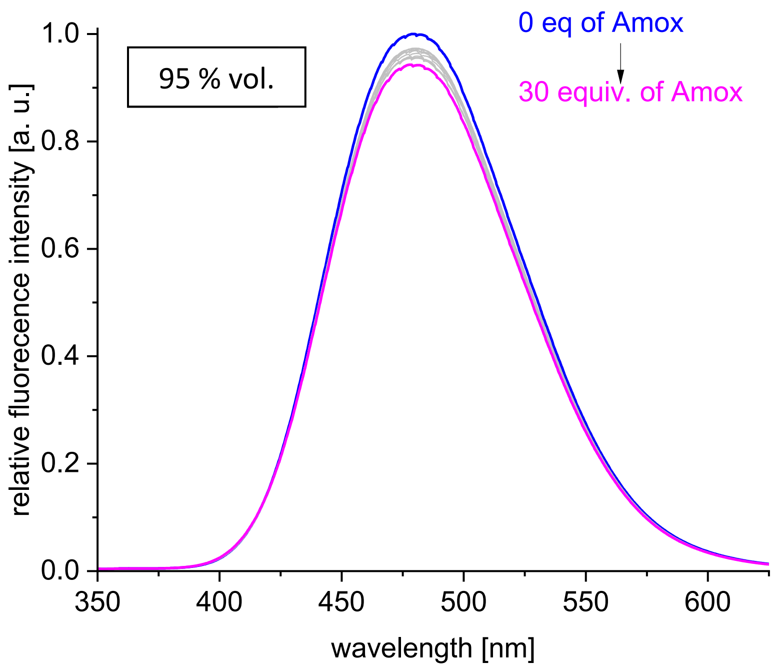


Figure S30 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Amoxicillin (Amox). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

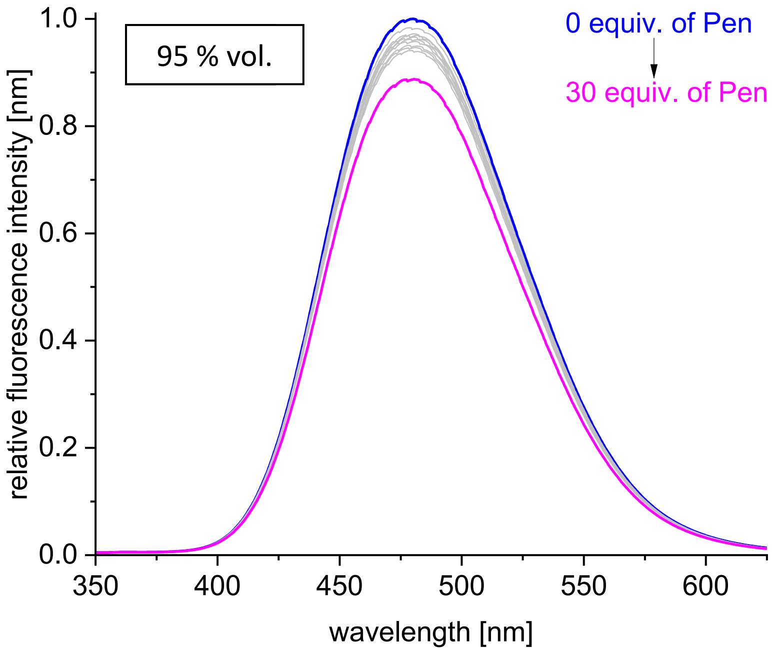


Figure S31 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Penicillin (Pen). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

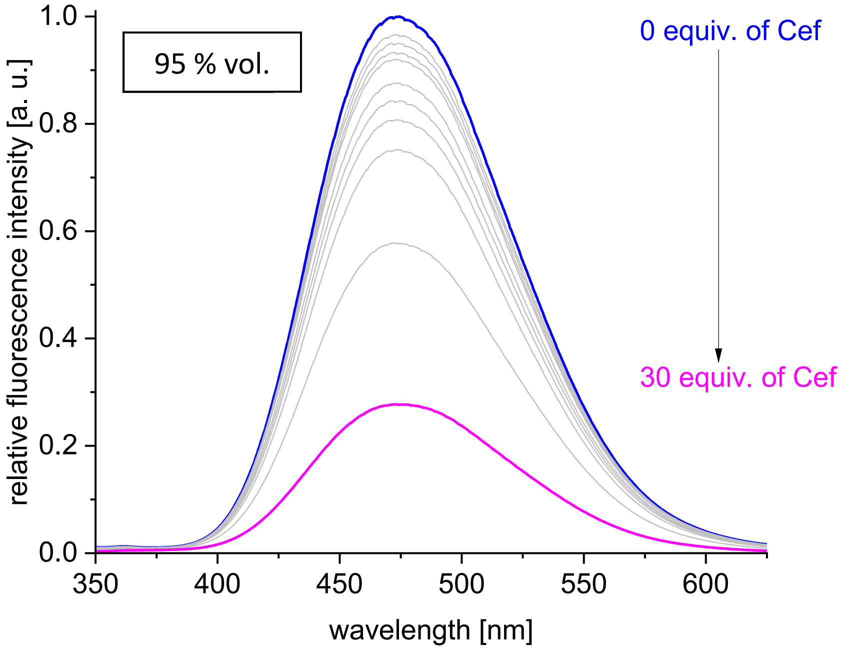


Figure S32 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.For convenience, the value in the frame shows the water content.

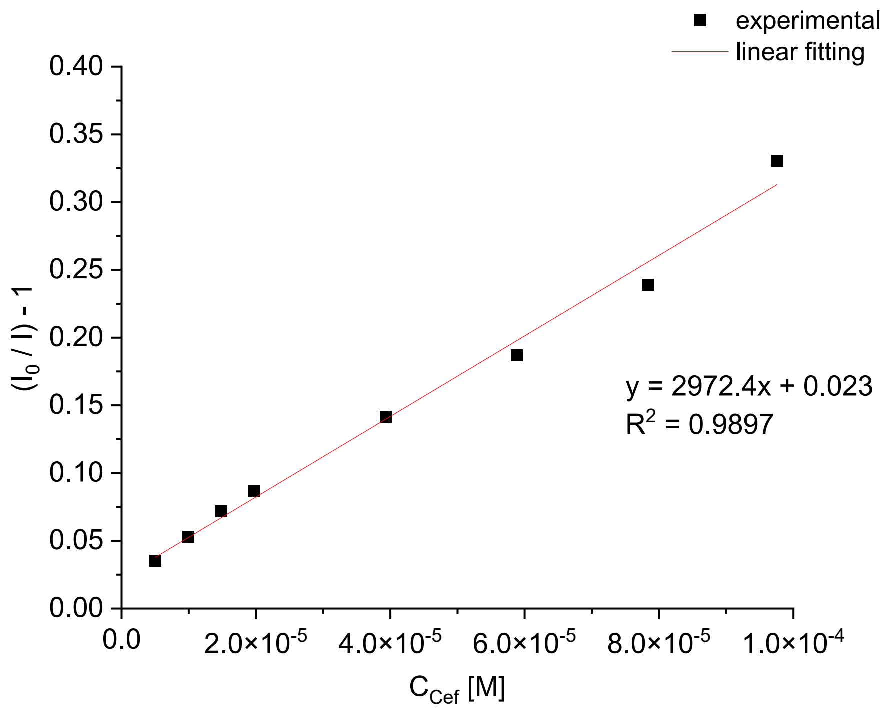


Figure S33 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

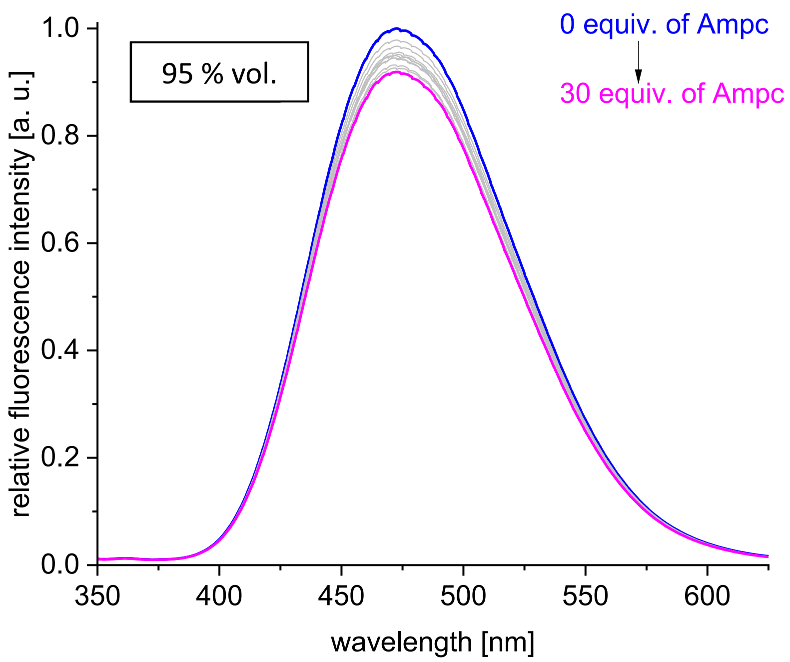


Figure S34 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ampicillin (Ampc). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

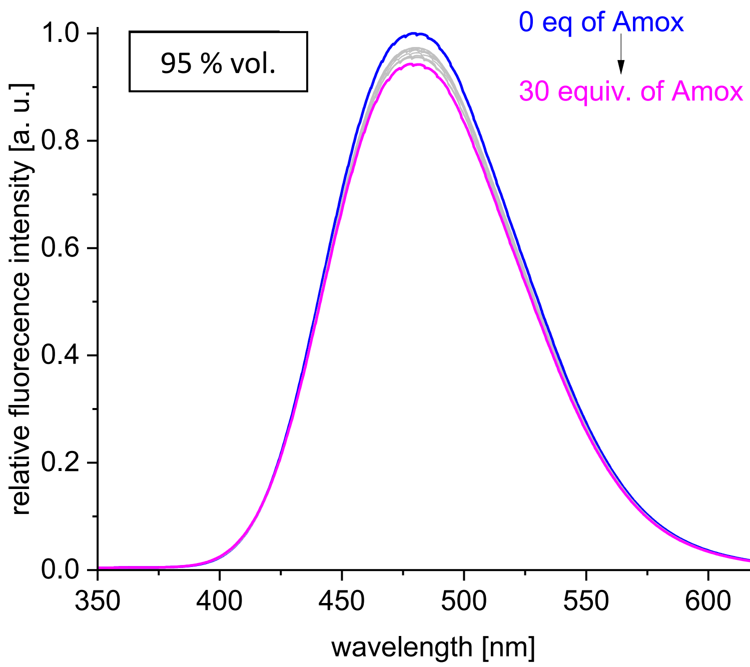


Figure S35 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Amoxicillin (Amox). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

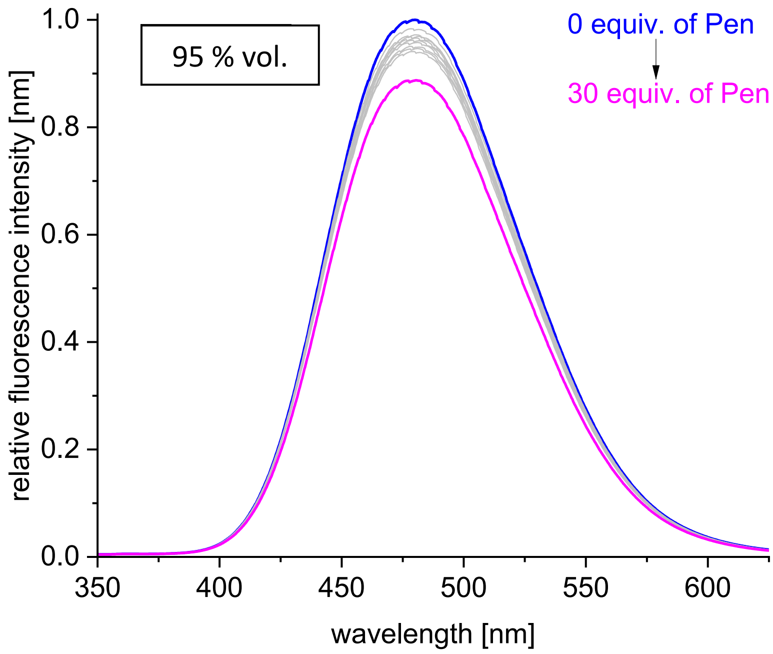


Figure S36 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Penicillin (Pen). Conditions: H_2O:THF = 95:5 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

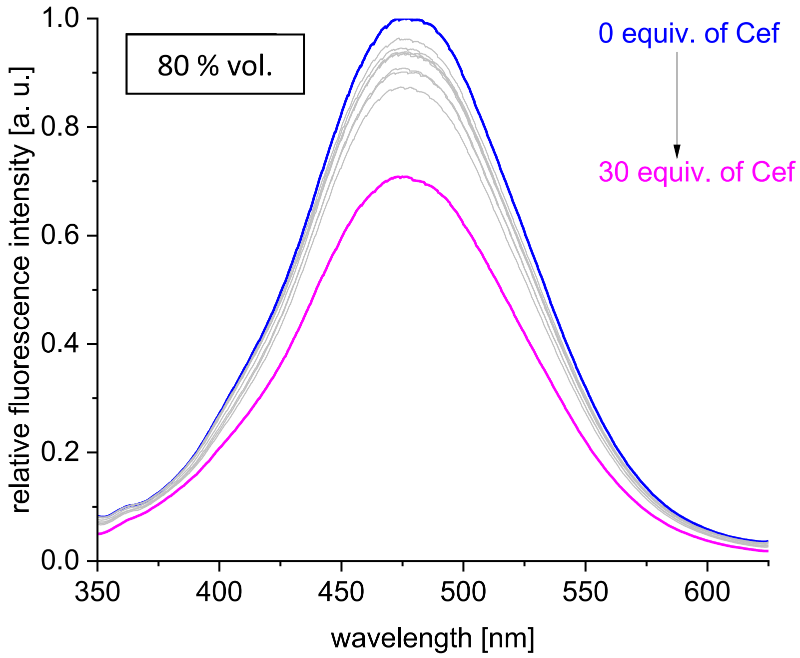


Figure S37 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 80:20 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

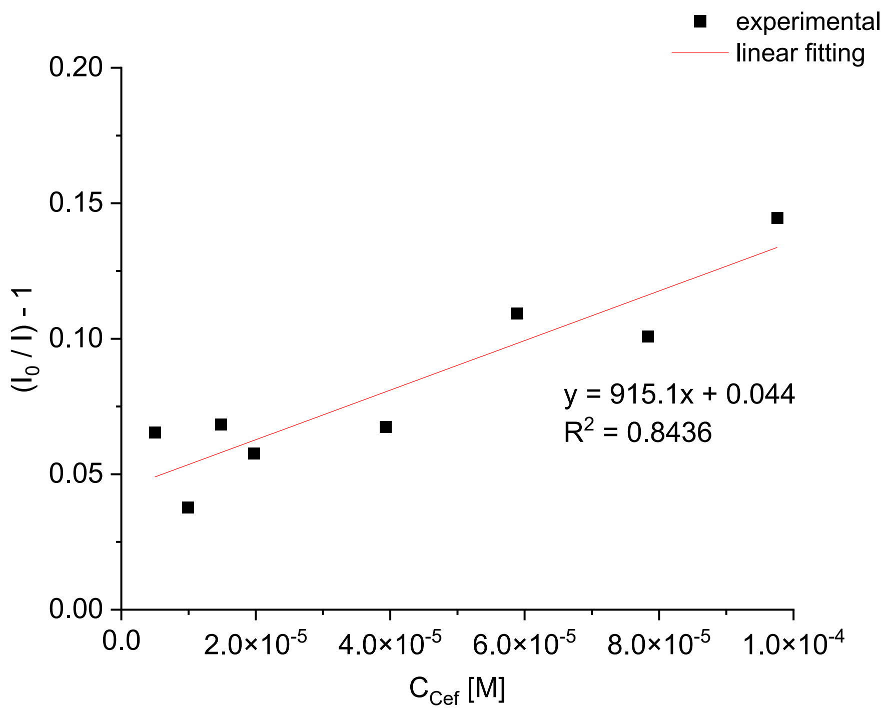


Figure S38 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 80:20 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

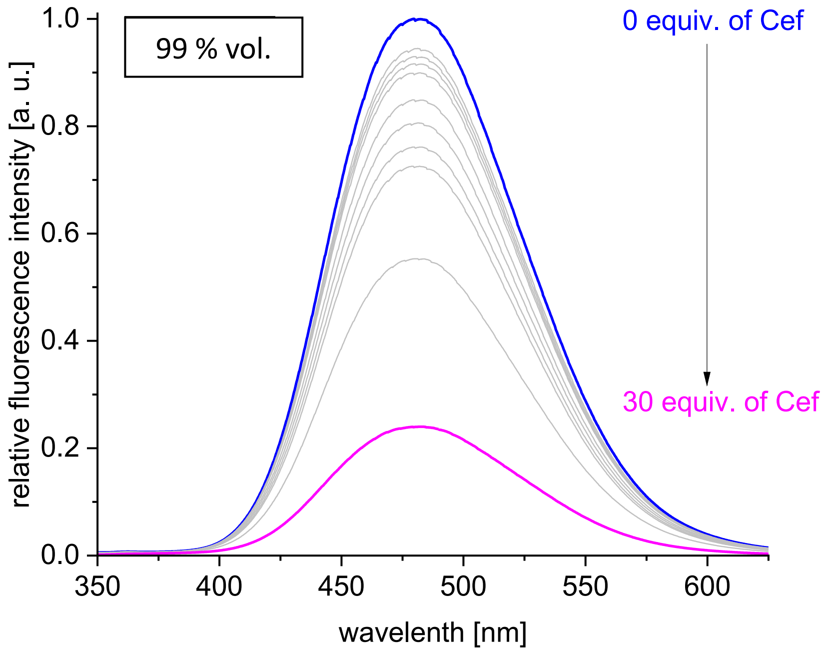


Figure S39 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

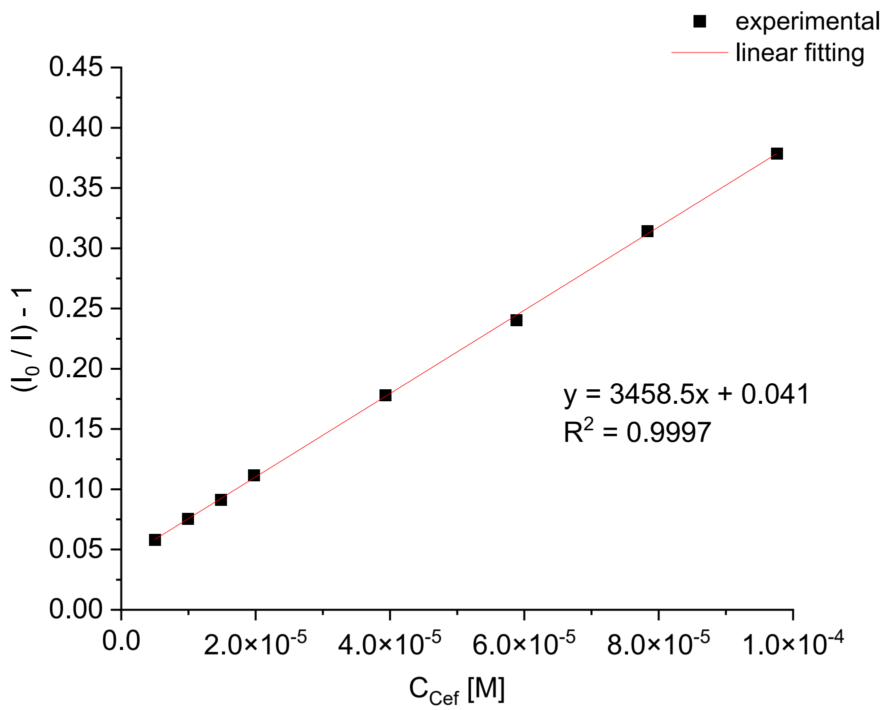


Figure S40 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v/v*, C = $2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

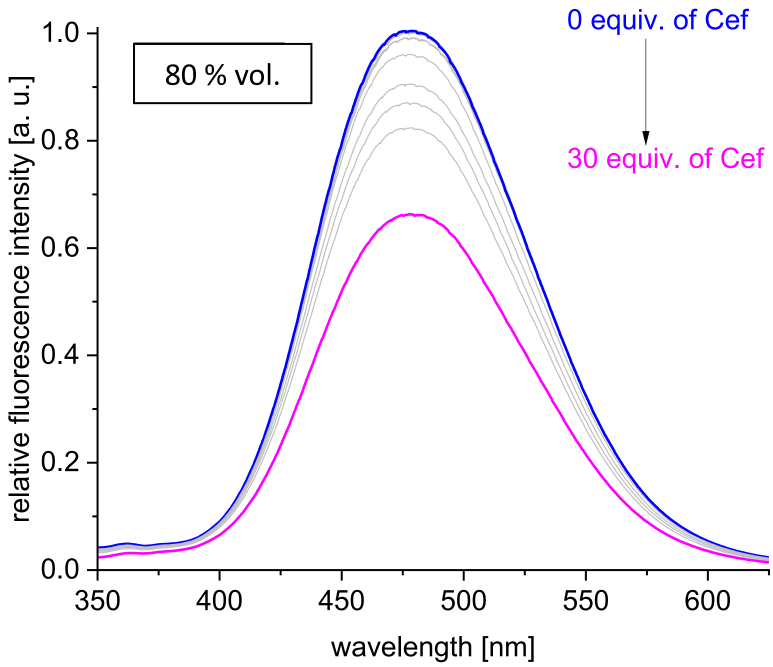


Figure S41 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 80:20 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

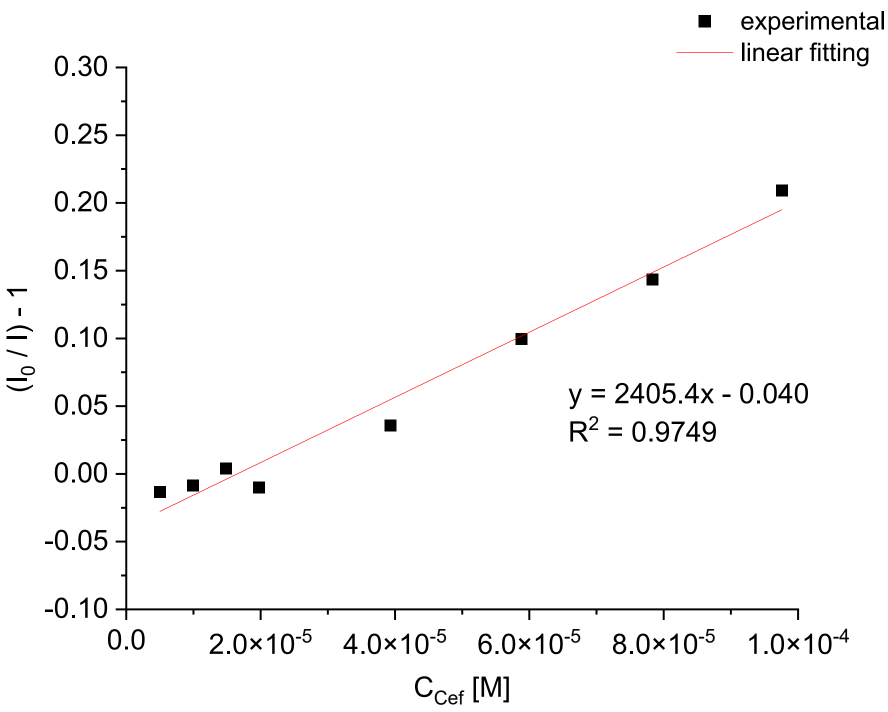


Figure S42 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 80:20 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

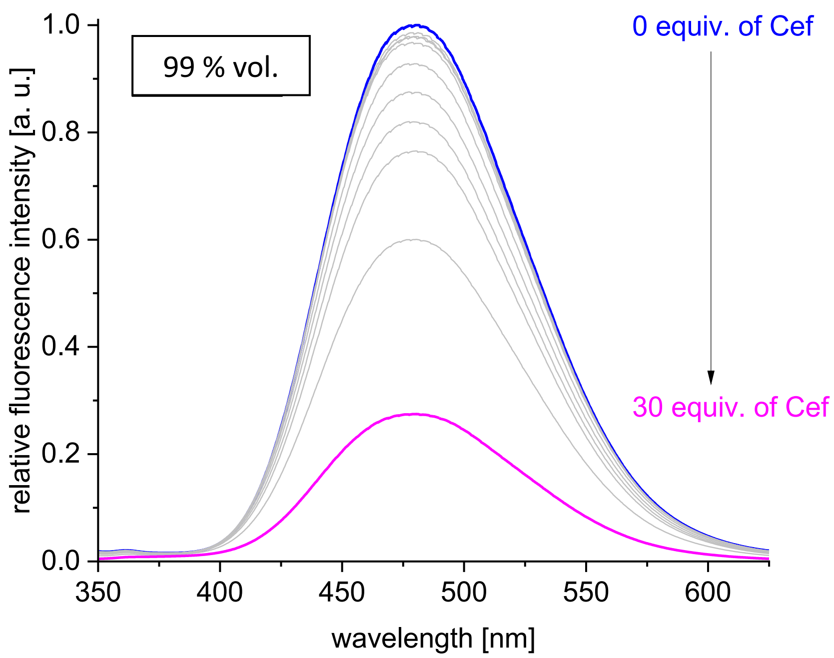


Figure S43 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v*/*v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

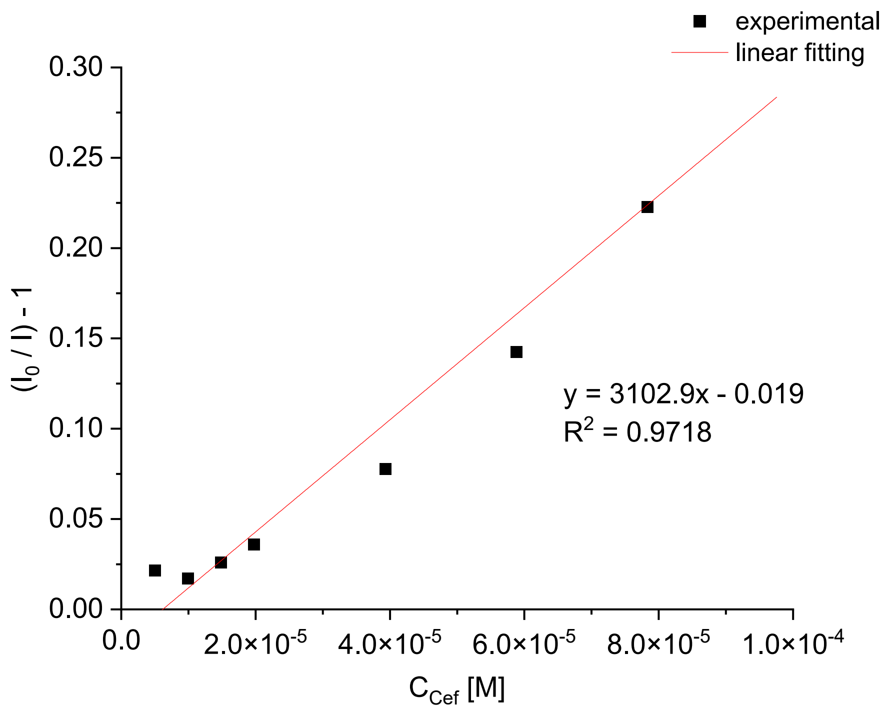


Figure S44 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v*/*v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

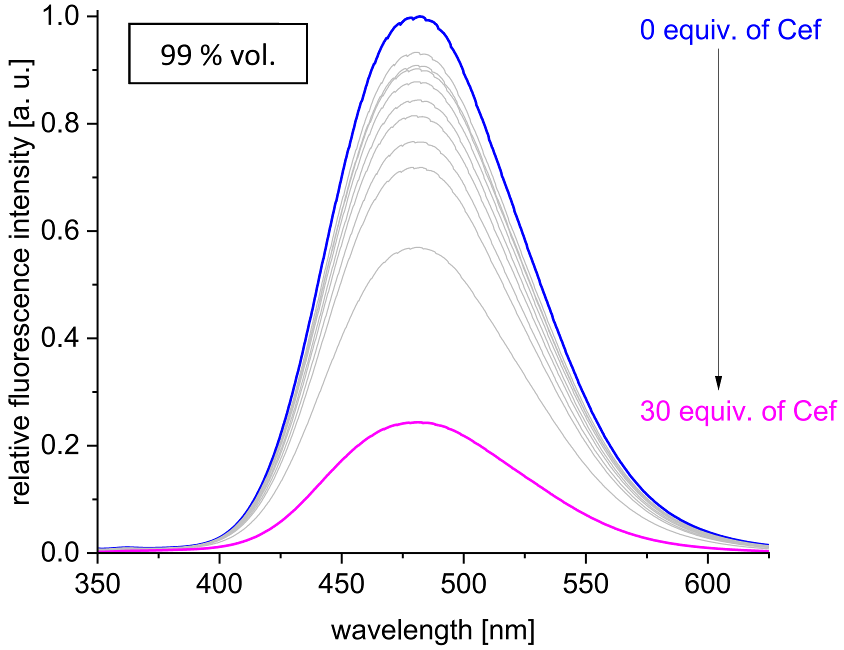


Figure S45 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (MES, pH = 5.14, C = 0.01M):THF = 99:1 v/v, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

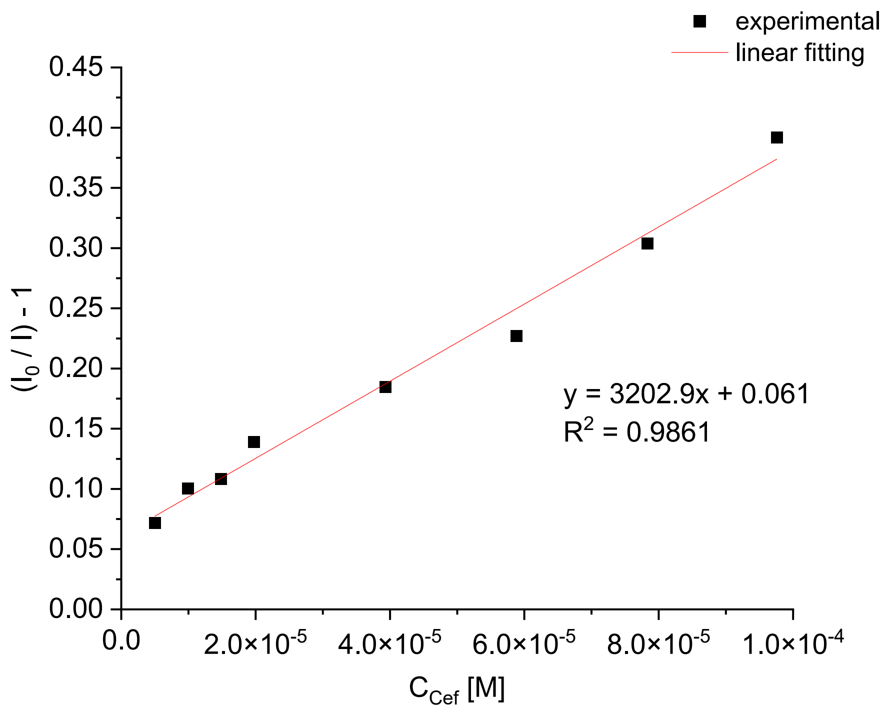


Figure S 46 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: buffer (MES, pH = 5.14, C = 0.01M):THF = 99:1, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

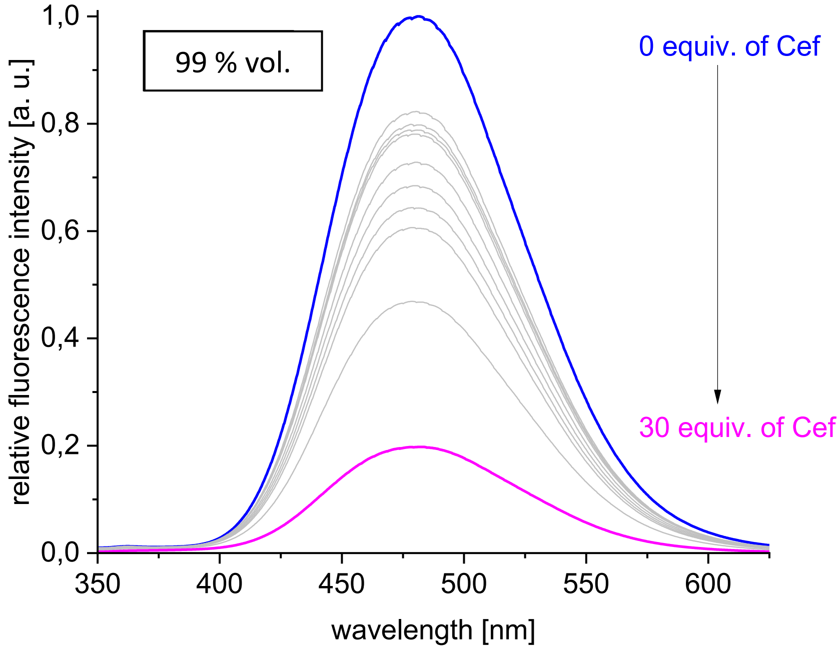


Figure S47 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (PBS, pH = 7.40, C = 0.01M):THF = 99:1 v/v, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

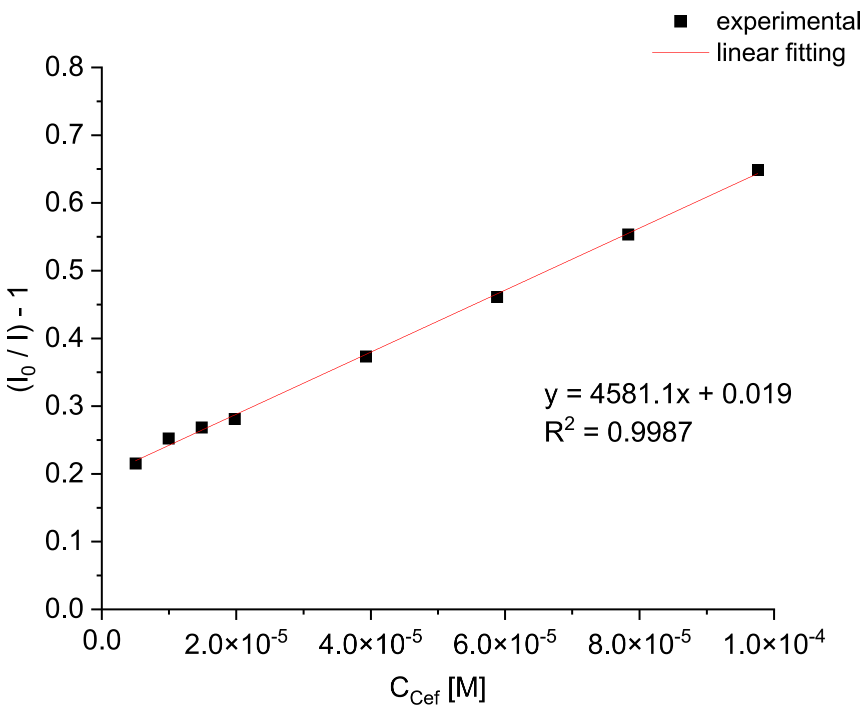


Figure S48 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: buffer (PBS, pH = 7.40, C = 0.01M):THF = 99:1, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

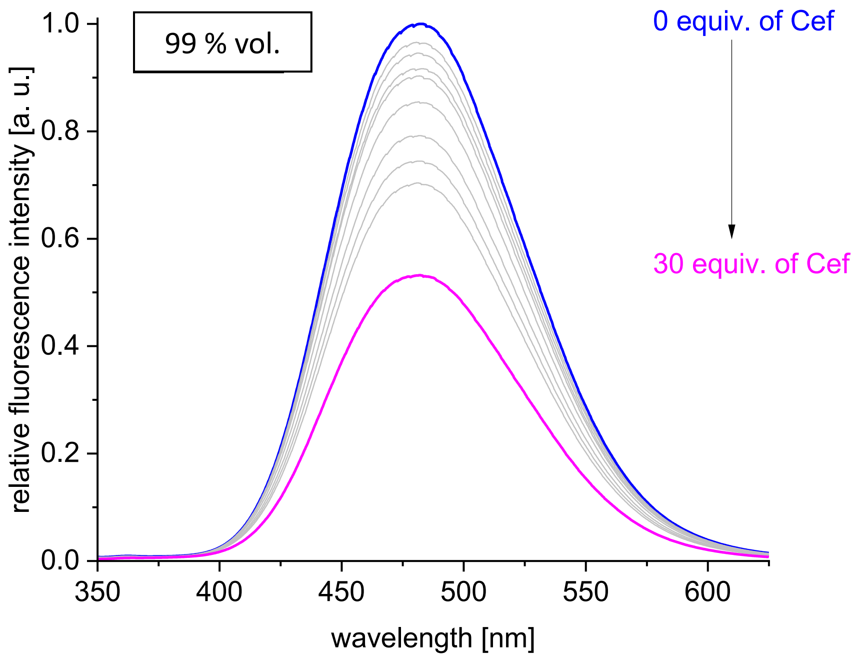


Figure S49 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (Tris, pH = 8.29, C = 0.01M):THF = 99:1 v/v, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

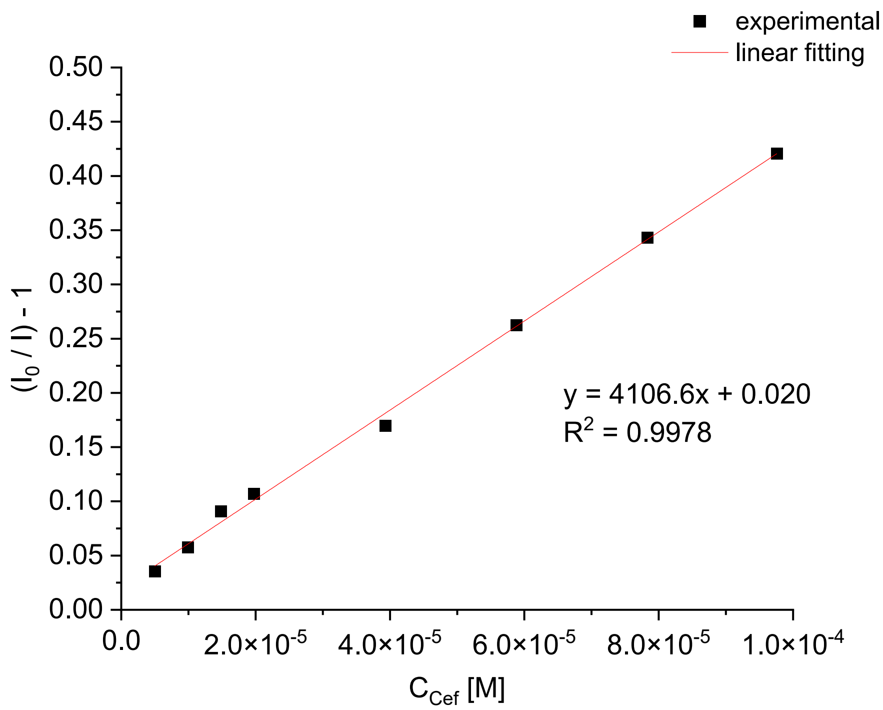


Figure S 50 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: buffer (Tris, pH = 7.40, C = 0.01M):THF = 99:1, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

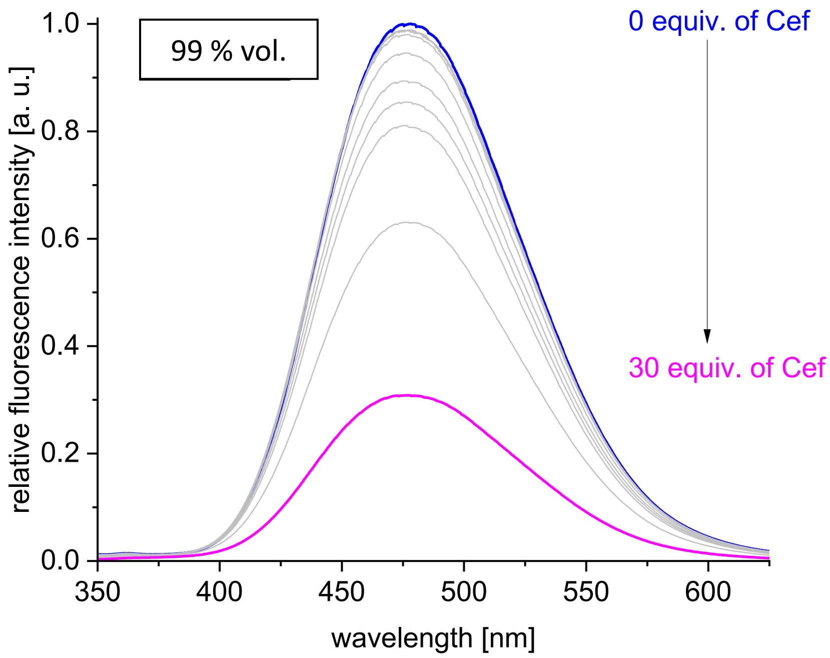


Figure S51 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (MES, pH = 5.14, C = 0.01M):THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

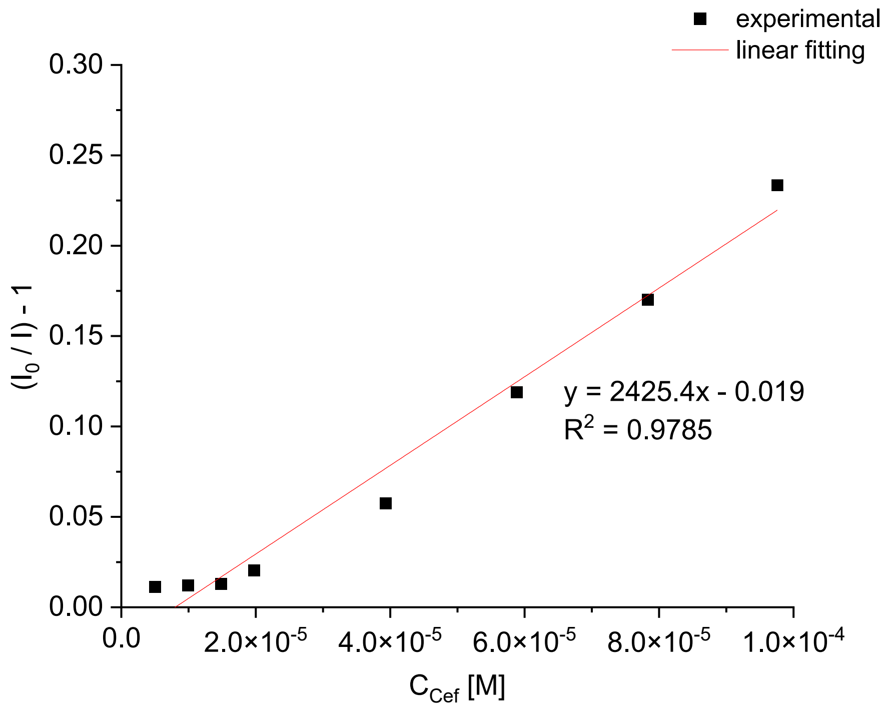


Figure S52 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: buffer (MES, pH = 5.14, C = 0.01M):THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

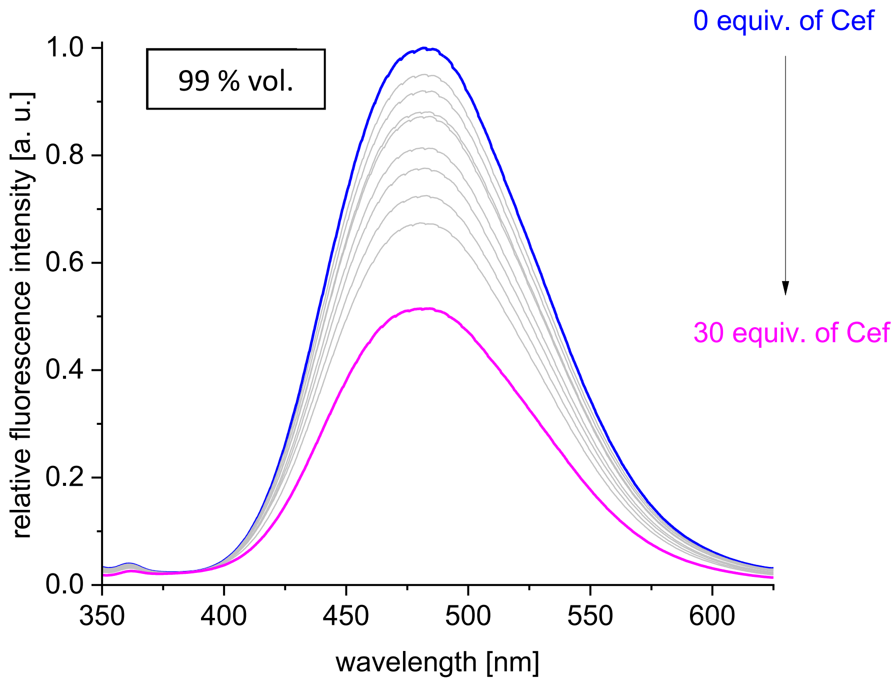


Figure S 53 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (PBS, pH = 7.40, C = 0.01M):THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

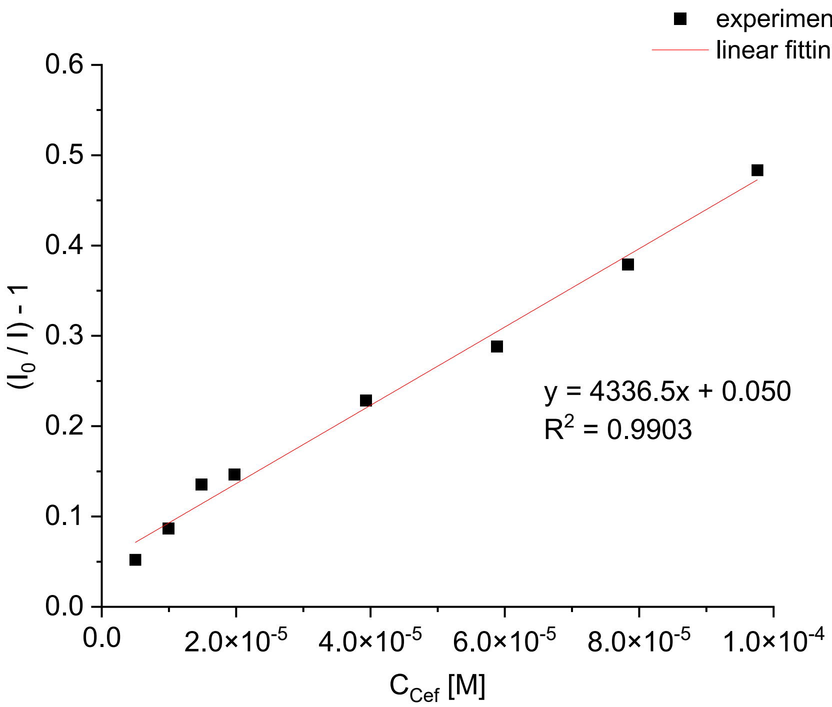


Figure S54 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: buffer (PBS, pH = 7.40, C = 0.01M):THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

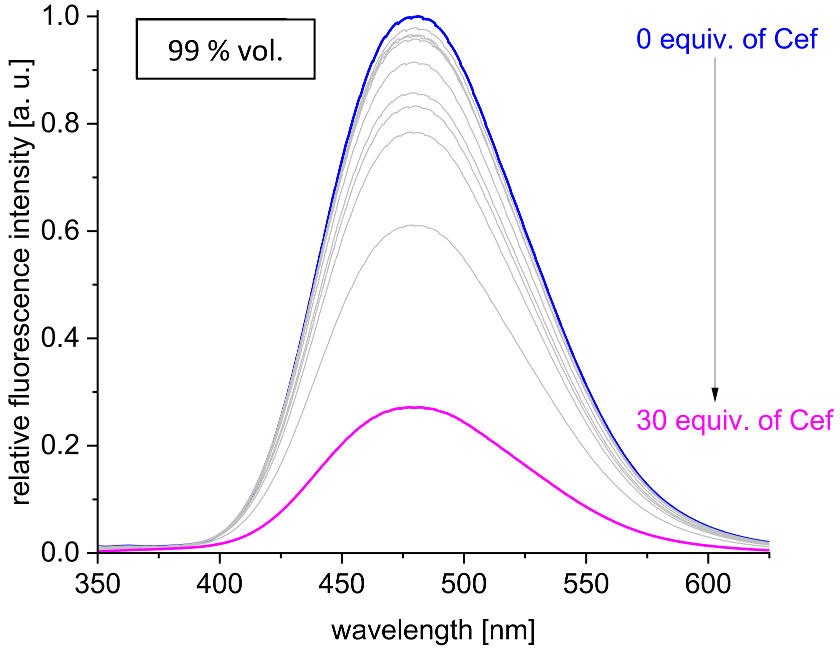


Figure S55 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: buffer (Tris, pH = 8.29, C = 0.01M):THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

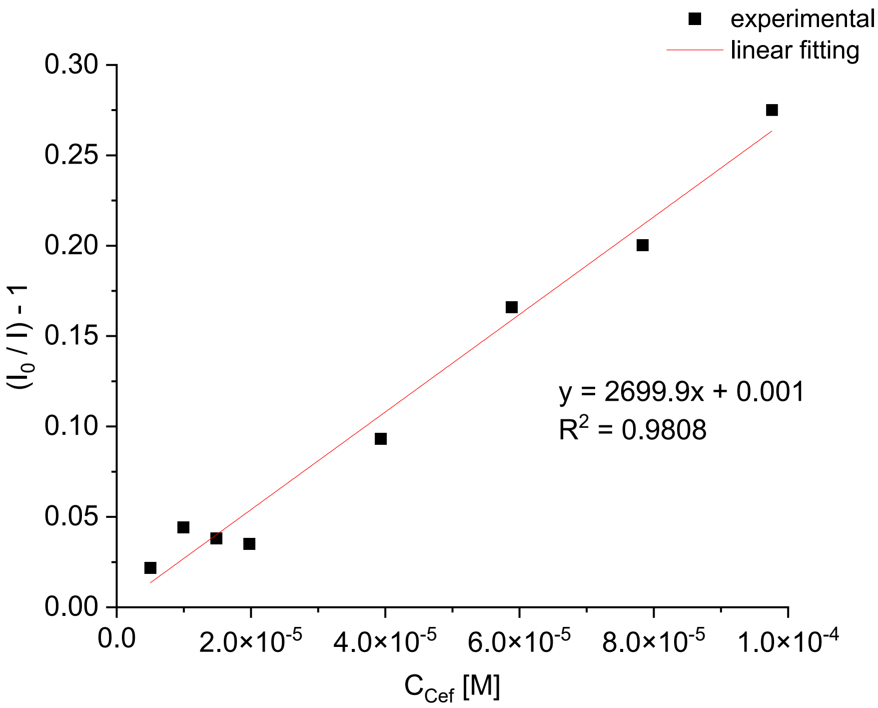


Figure S56 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: buffer (Tris, pH = 8.29, C = 0.01M):THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

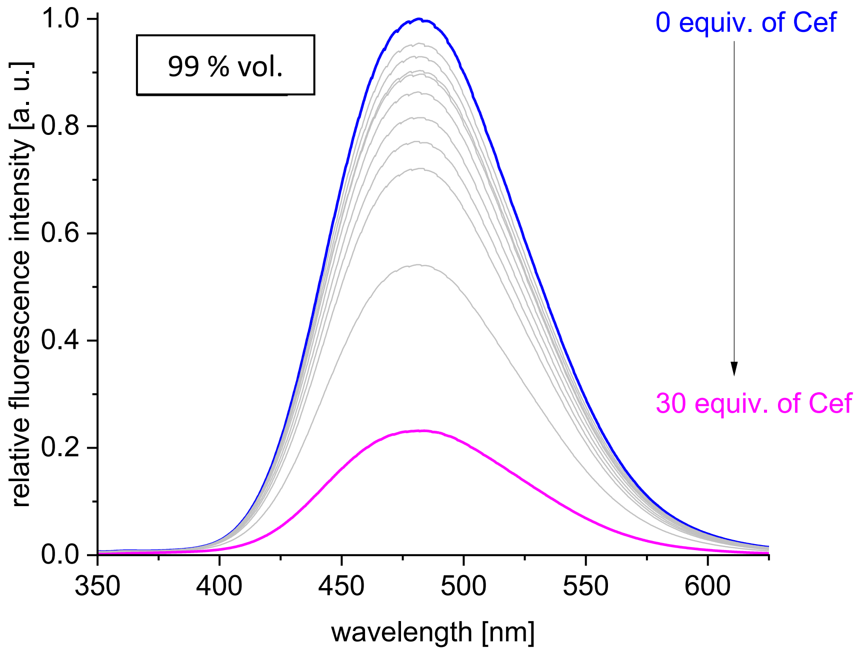


Figure S57 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: tap water:THF = 99:1 v/v, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

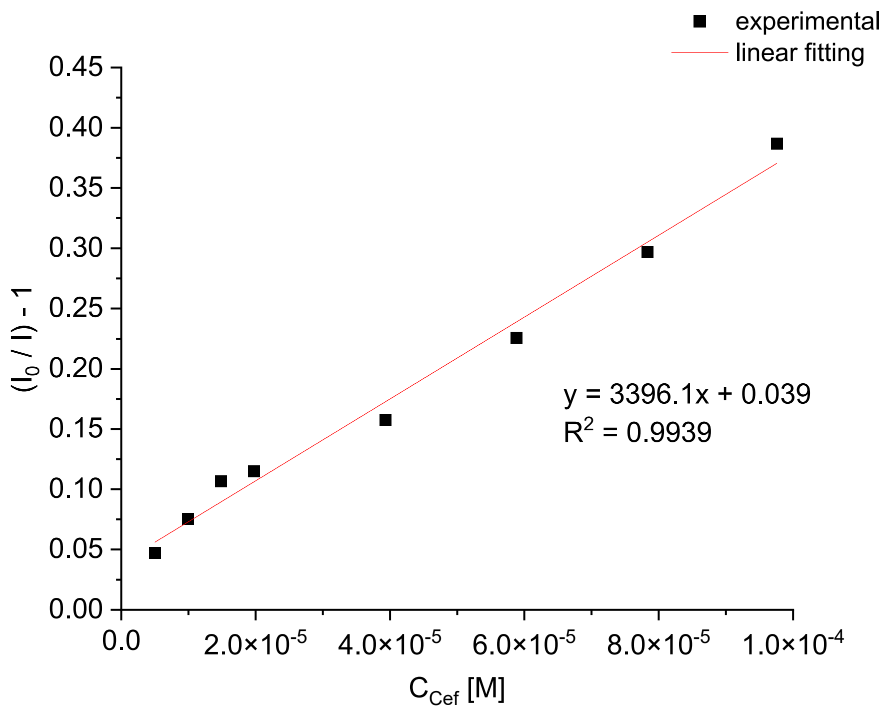


Figure S58 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: tap water:THF = 99:1, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

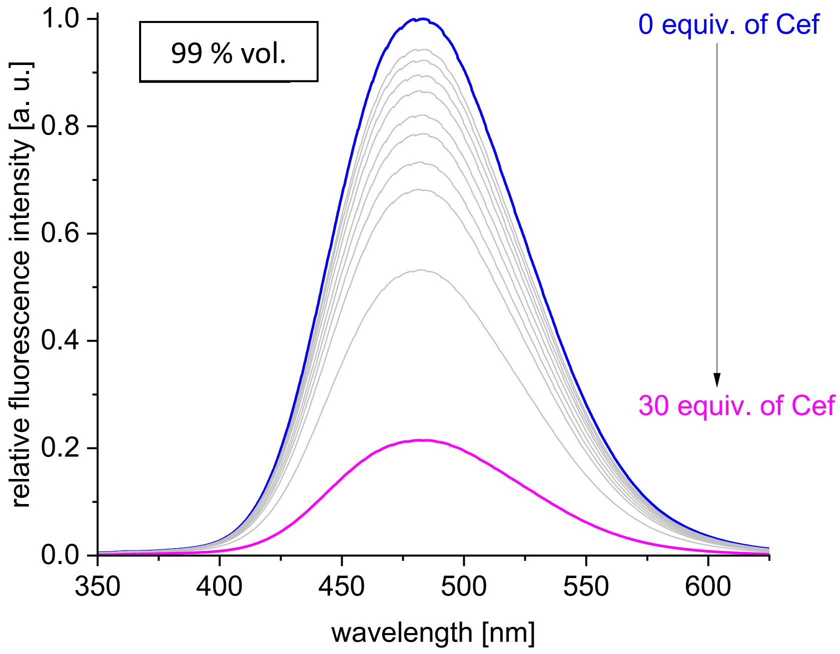


Figure S59 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: artesian groundwater:THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

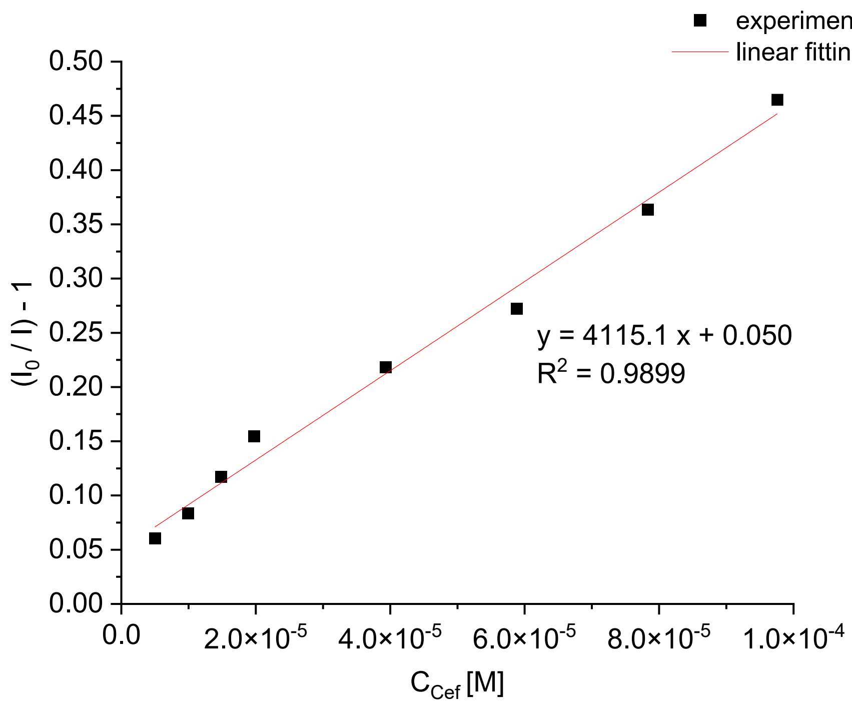


Figure S60 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: artesian water:THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

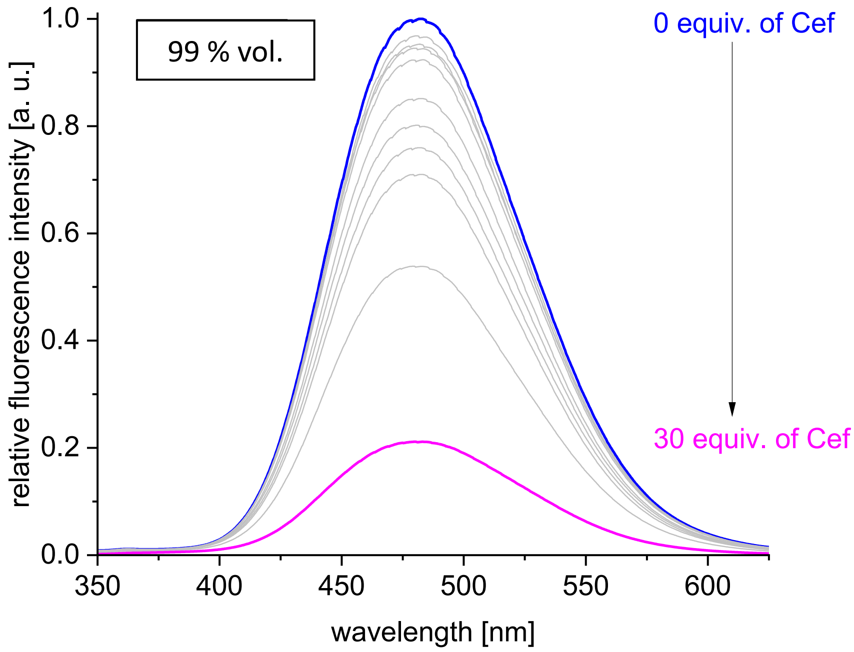


Figure S61 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: filtered seawater:THF = 99:1 v/v, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

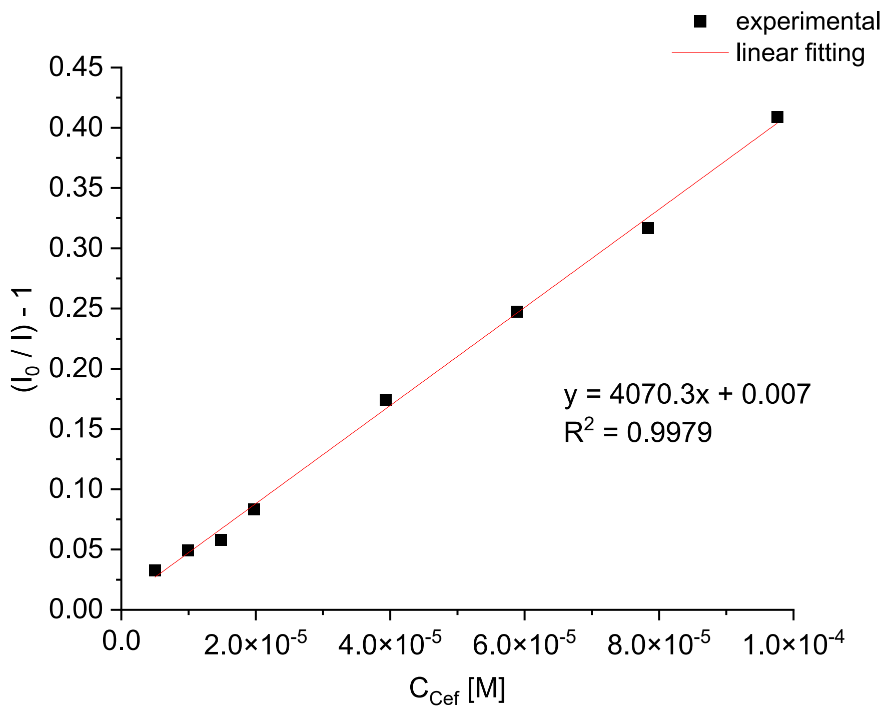


Figure S62 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: filtered seawater:THF = 99:1, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

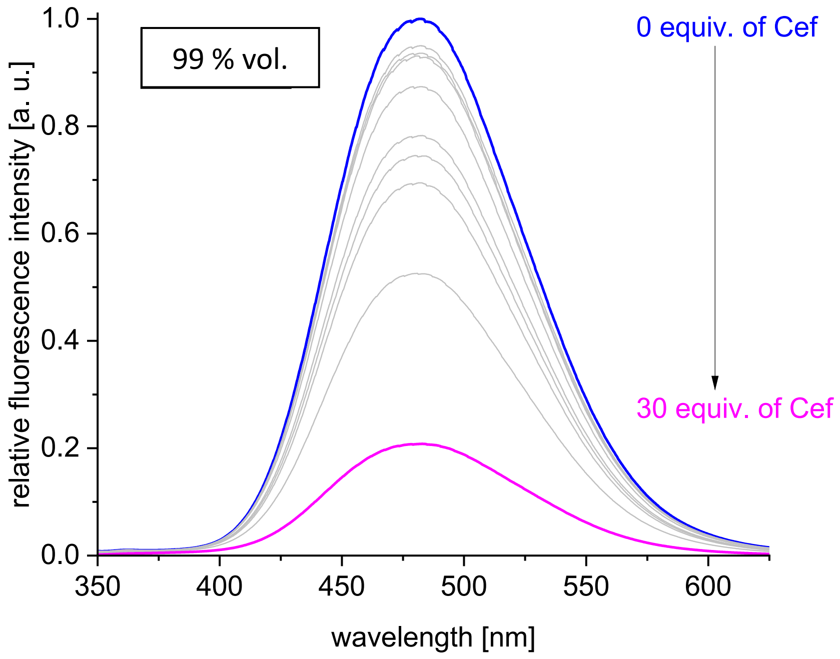


Figure S63 Emission spectra of aggregated **B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: non-filtered seawater:THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

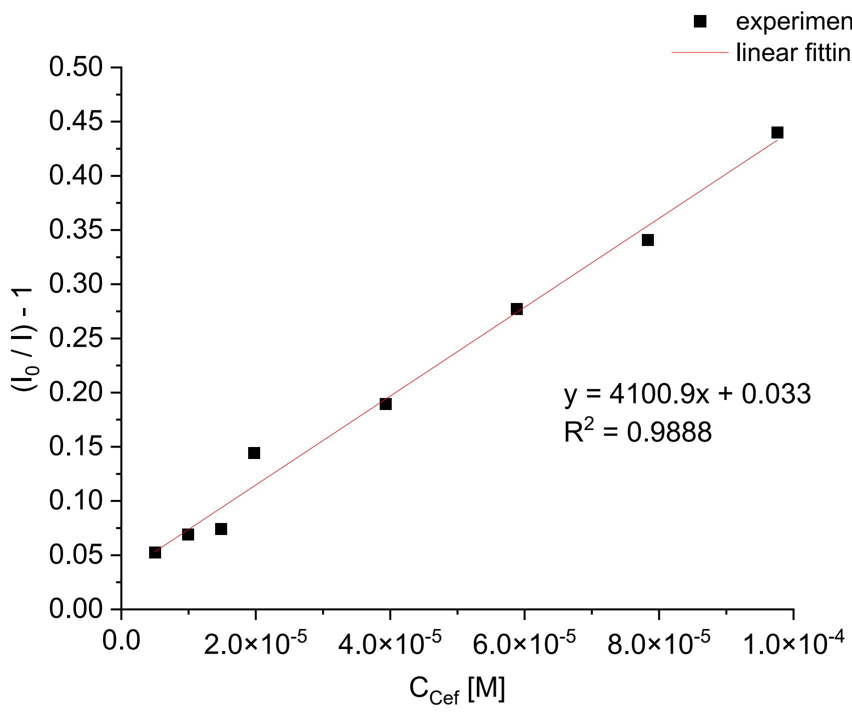


Figure S64 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **B3E** with Ceftazidime (Cef). Conditions: non-filtered seawater:THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

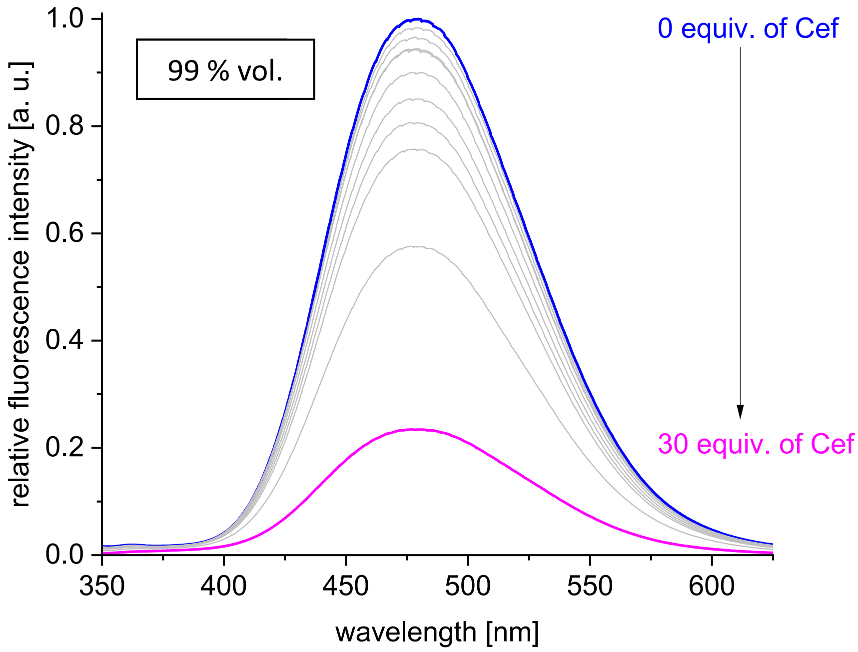


Figure S65 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: tap water:THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

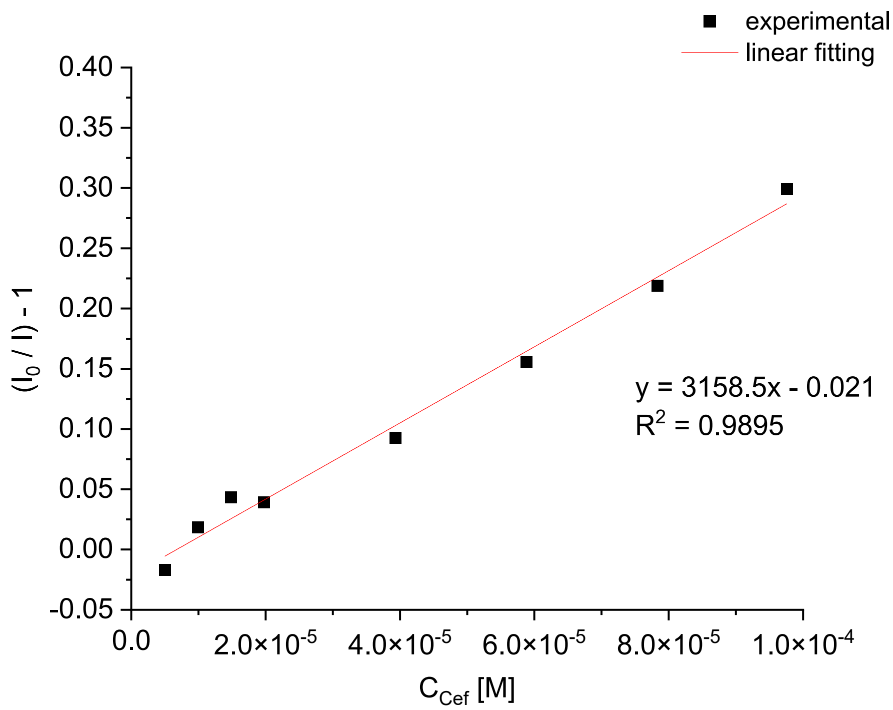


Figure S66 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: tap water:THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

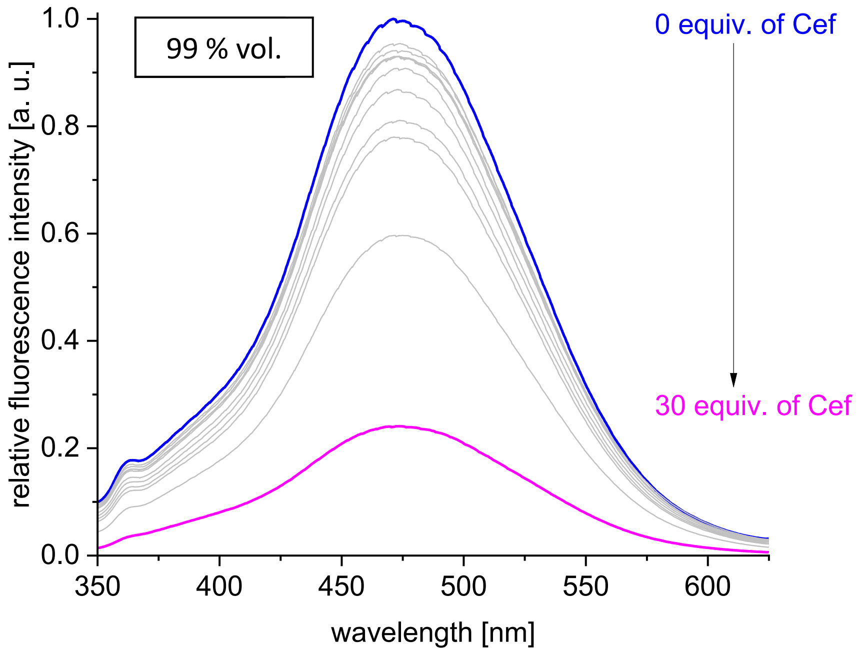


Figure S67 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: artesian groundwater:THF = 99:1 v/v, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

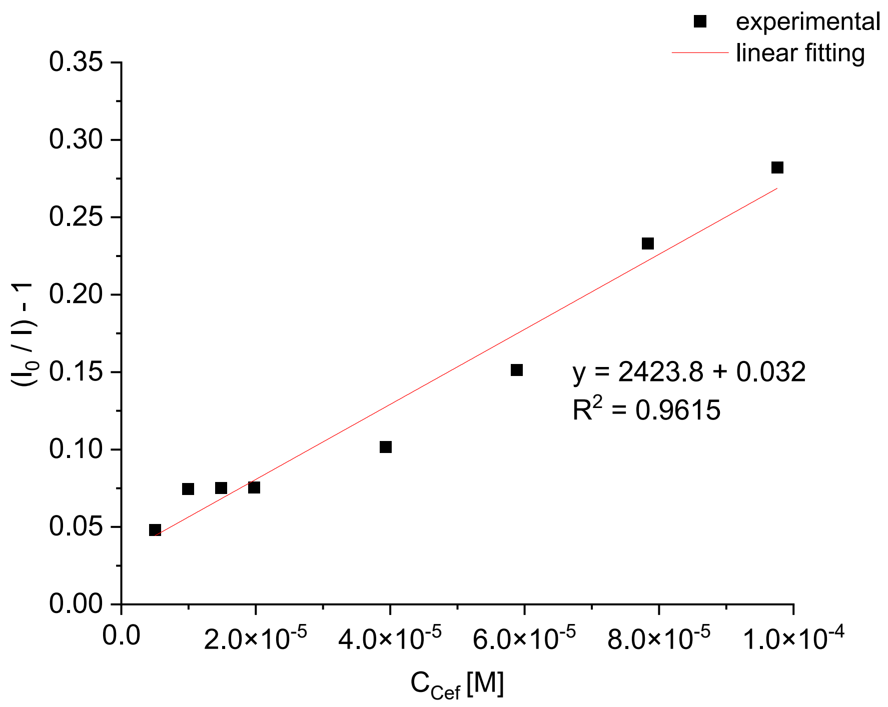


Figure S68 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: artesian water:THF = 99:1, $C = 2 \cdot 10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

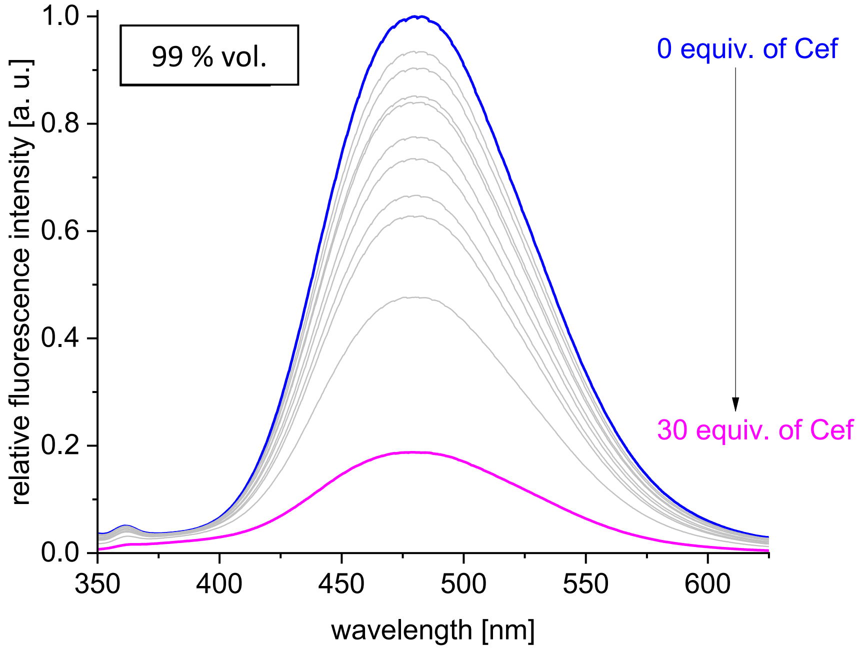


Figure S69 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: filtered water:THF = 99:1 v/v, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

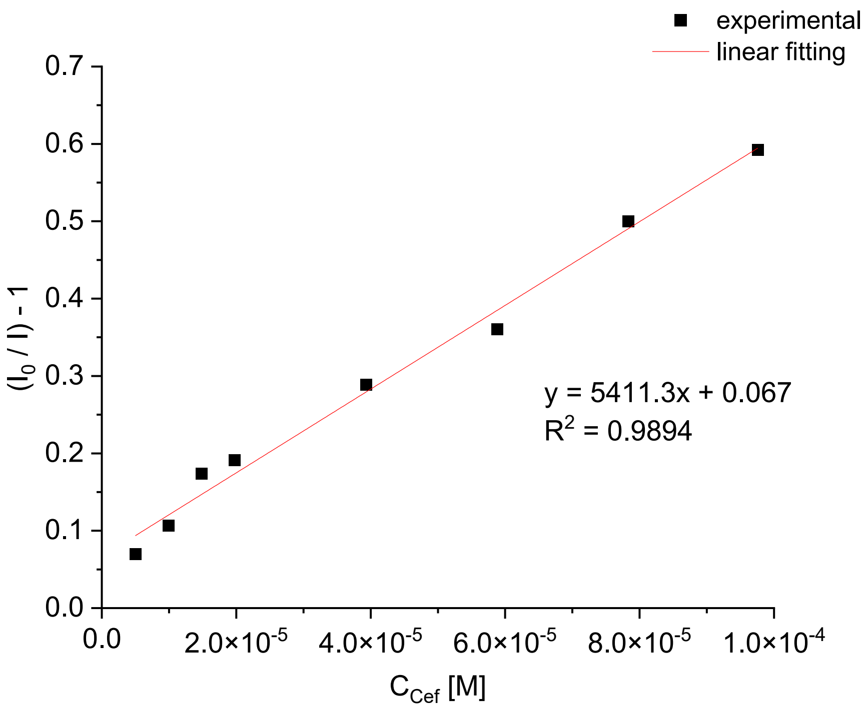


Figure S70 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: filtered water:THF = 99:1, $C = 2\cdot10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

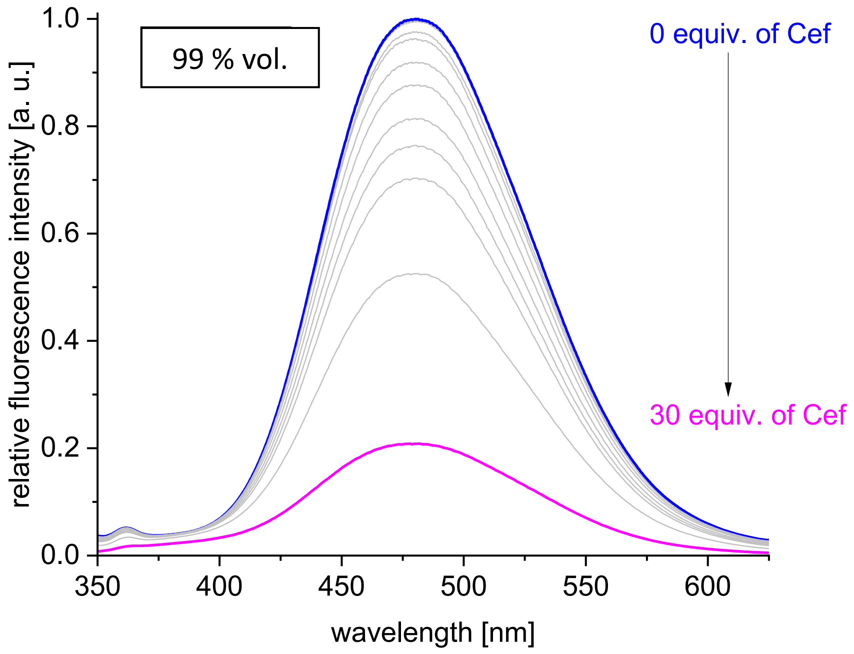


Figure S71 Emission spectra of aggregated **F-B3E** in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: non-filtered water:THF = 99:1 v/v, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content.

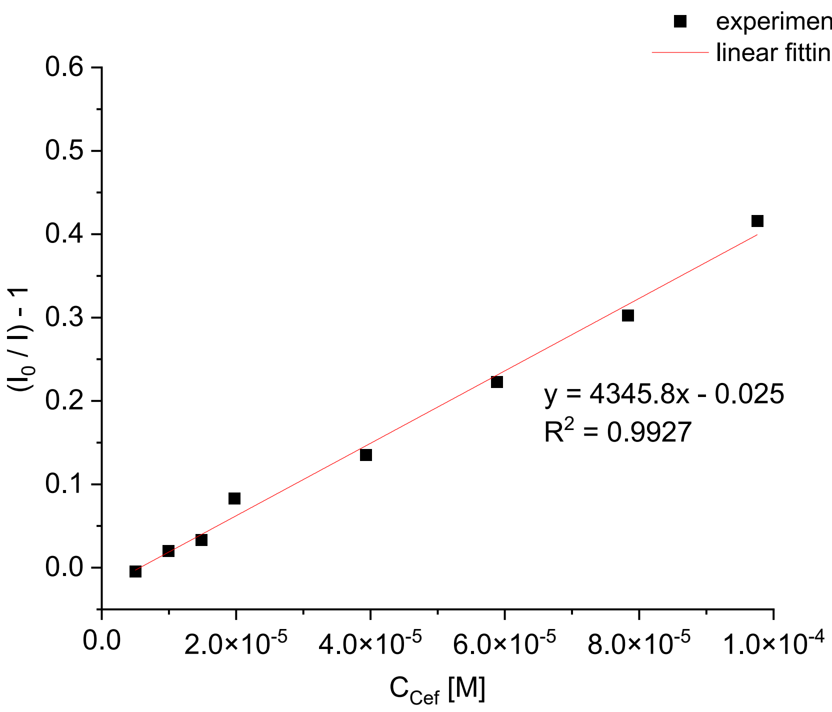
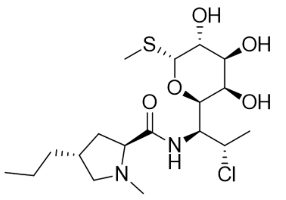


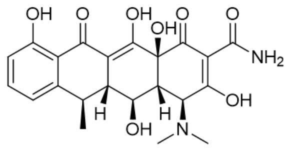
Figure S72 Experimental points and linear fitting of Stern-Volmer correlation for spectrofluorimetric titration of **F-B3E** with Ceftazidime (Cef). Conditions: non-filtered water:THF = 99:1, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm.

Clindamycin
(Dalacin C)



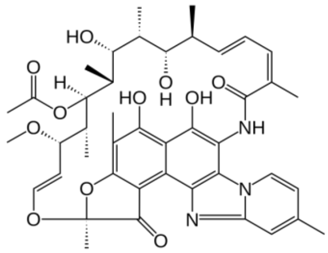
- Lincosamide antibiotic
- Hard capsules (300 mg)
- Contained also:
  talc, magnesium stearate, lactose, TiO_2, gelatine, corn starch

Doxycycline
(Doxycyclinum FP)



- Tetracycline antibiotic
- Hard capsules (100 mg)
- Contained also:
  talc, magnesium stearate, TiO2, gelatine, corn starch, cellulose, E132, E104

Rifaximin
(Xifaxan)



- Tetracycline antibiotic
- Tablets (200 mg)
- Contained also:
  sodium glycolate, glycerol distearate, SiO_2, talc, cellulose, hydroxypropylcellulose, TiO_2, Fe_2O_3, sodium edetate

Figure S73 Chemical structures, description and containment of real medical products used as antibiotic source for additional competitive titrations.

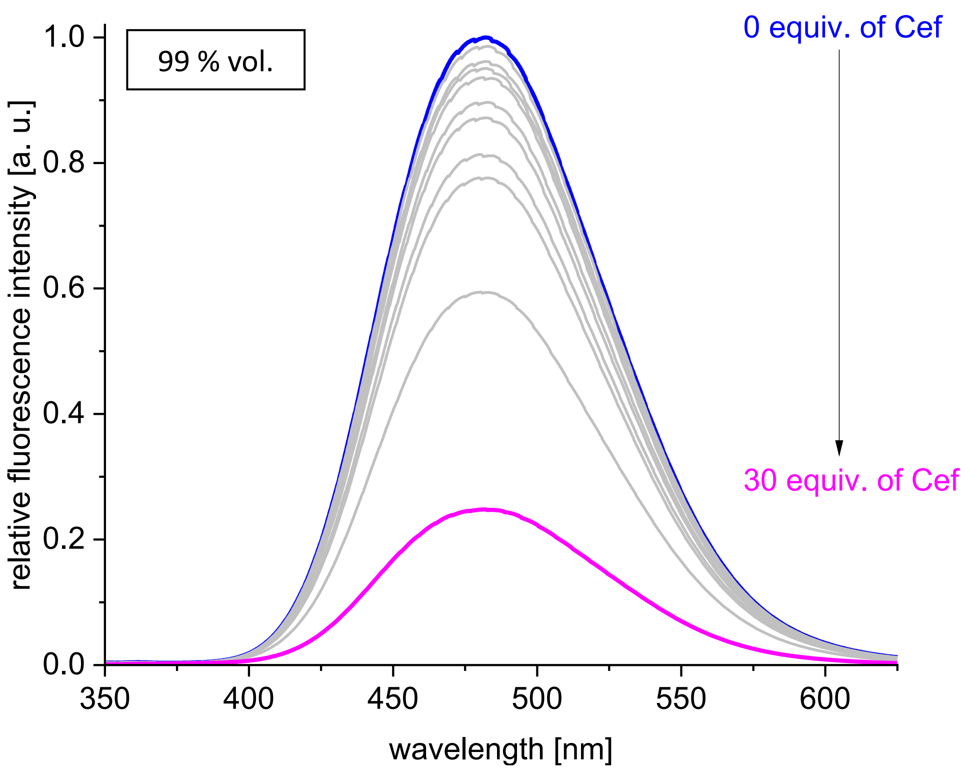


Figure S74 Emission spectra of aggregated **B3E** with addition of Ampicillin (1 molar equiv.) in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content. Calculated Stern-Volmer constant: $K_{S\text{-}V}$ = 2795 ± 126 M^{-1}.

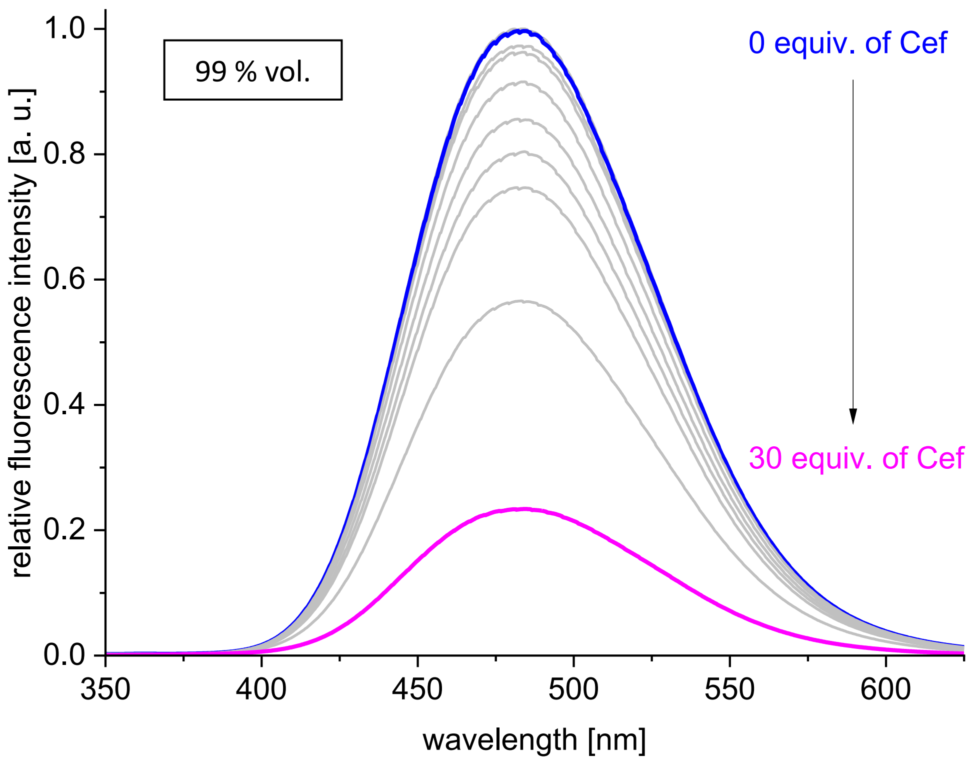


Figure S75 Emission spectra of aggregated **B3E** with addition of Clindamycin (1 molar equiv.) in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v*/*v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content. Calculated Stern-Volmer constant: $K_{S\text{-}V}$ = 2597 ± 155 M^{-1}.

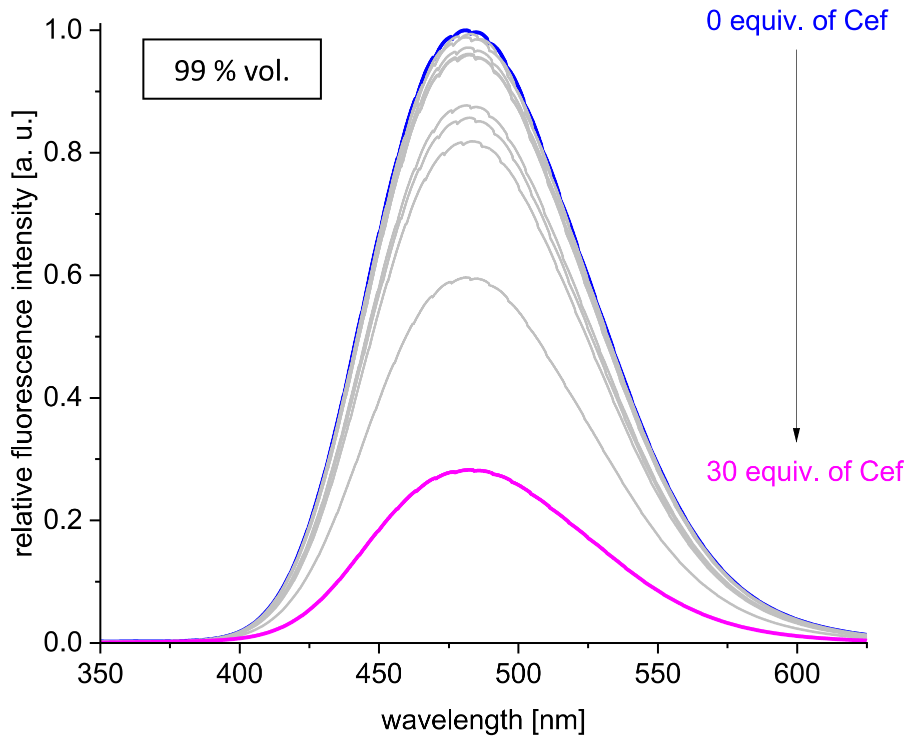


Figure S76 Emission spectra of aggregated **B3E** with addition of Doxycyclin (1 molar equiv.) in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v*/*v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content. Calculated Stern-Volmer constant: $K_{S\text{-}V}$ = 2161 ± 160 M^{-1}.

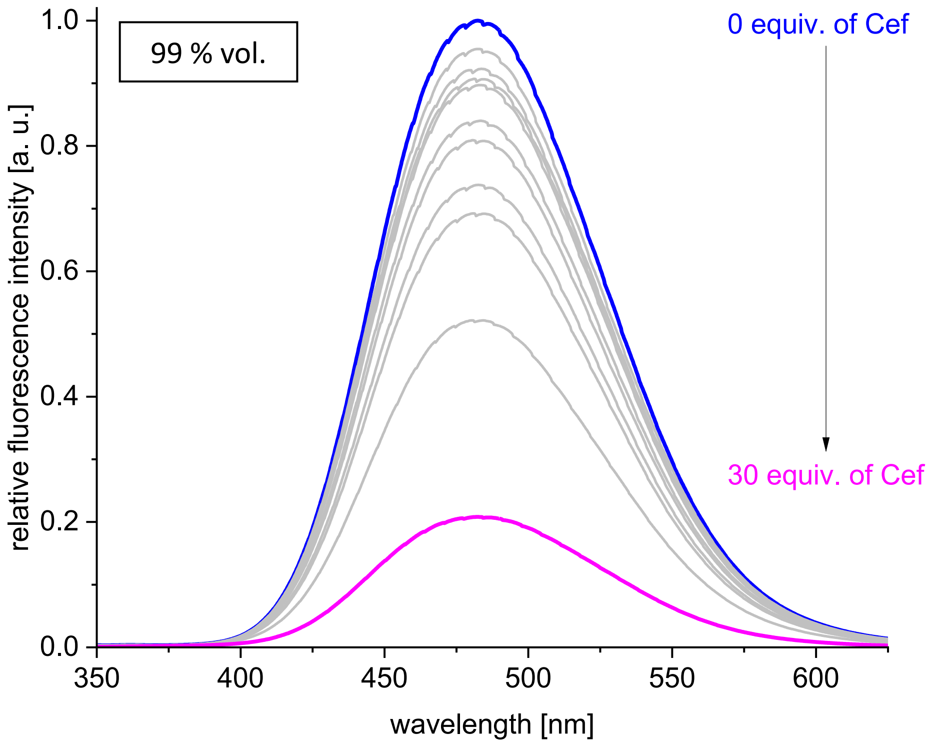


Figure S77 Emission spectra of aggregated **B3E** with addition of Rifaximin (1 molar equiv.) in the presence of increasing molar equivalents of Ceftazidime (Cef). Conditions: H_2O:THF = 99:1 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. For convenience, the value in the frame shows the water content. Calculated Stern-Volmer constant: $K_{S\text{-}V}$ = 4060 ± 188 M^{-1}.

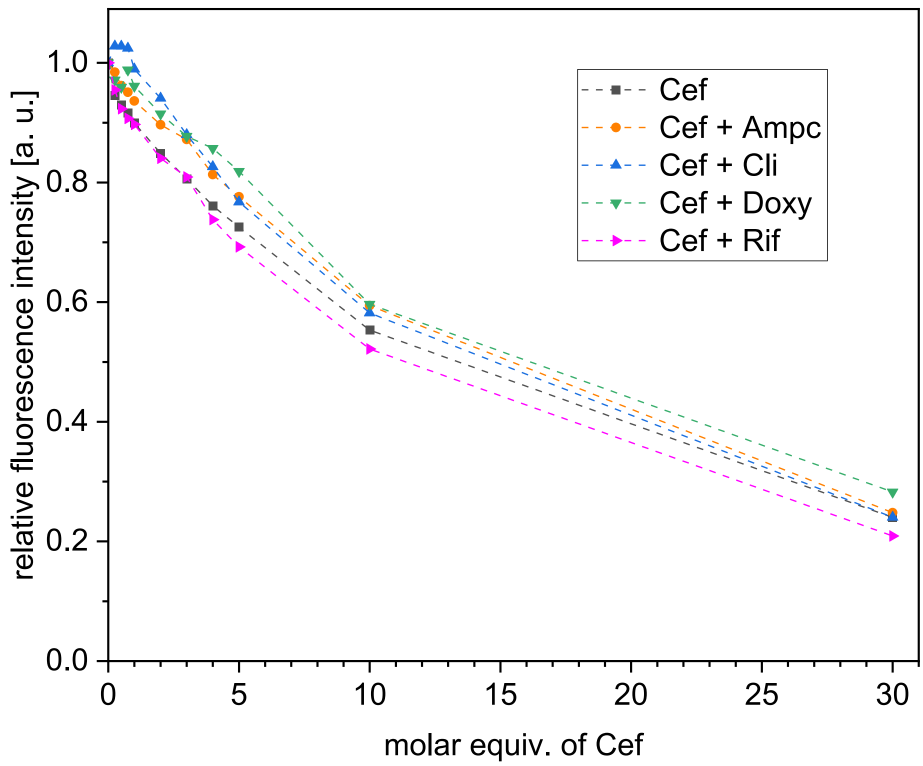


Figure S78 Titration curves for interactions between aggregated **B3E** and Cef in the absence or presence of antibiotic interferents (1 molar equiv.). Conditions: H_2O:THF = 99:1 *v/v*, $C = 2{\cdot}10^{-5}$ mol·dm^{-3}, λ_{ex} = 320 nm. Ampc = Ampicillin. Cli = Clindamycin. Doxy = Doxycyclin. Rif = Rifaximin.

S6.2 NMR studies

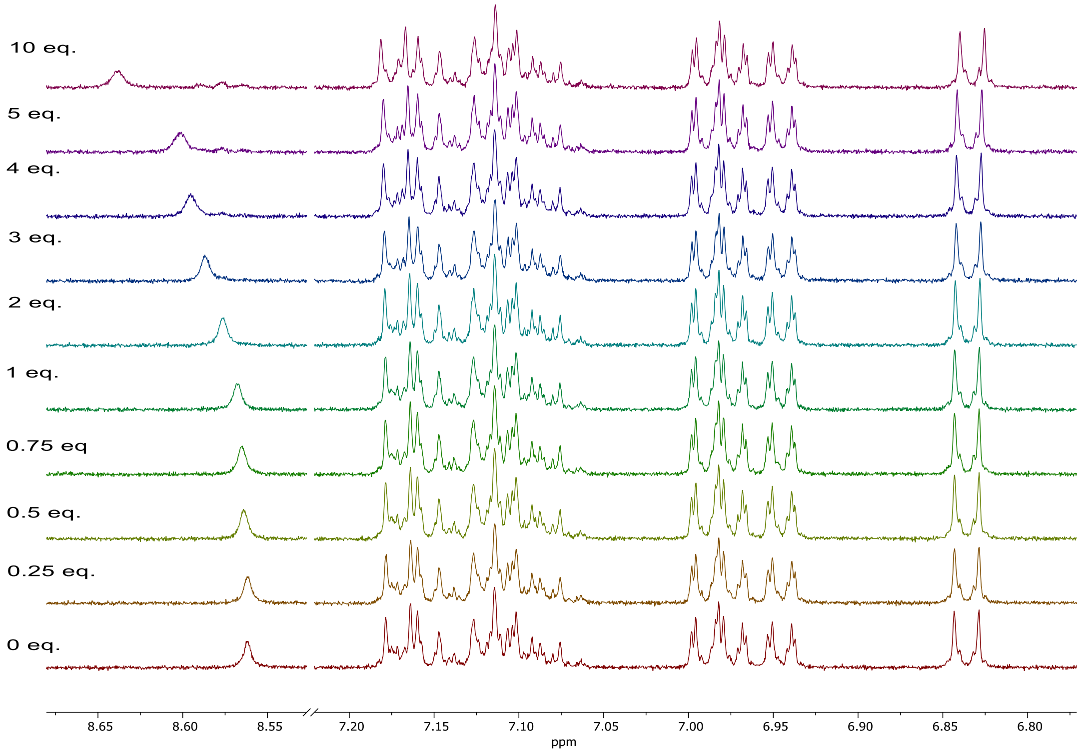


Figure S79 Evolution of ^{1}H NMR spectra (600 MHz, DMSO-d_6 + TMS, $C_{\mathbf{B3E}}$ = 3.8·10^{-4} M) for titration of **B3E** with 0-10 equiv. of Cef. Insets presenting signals from **B3E** protons.

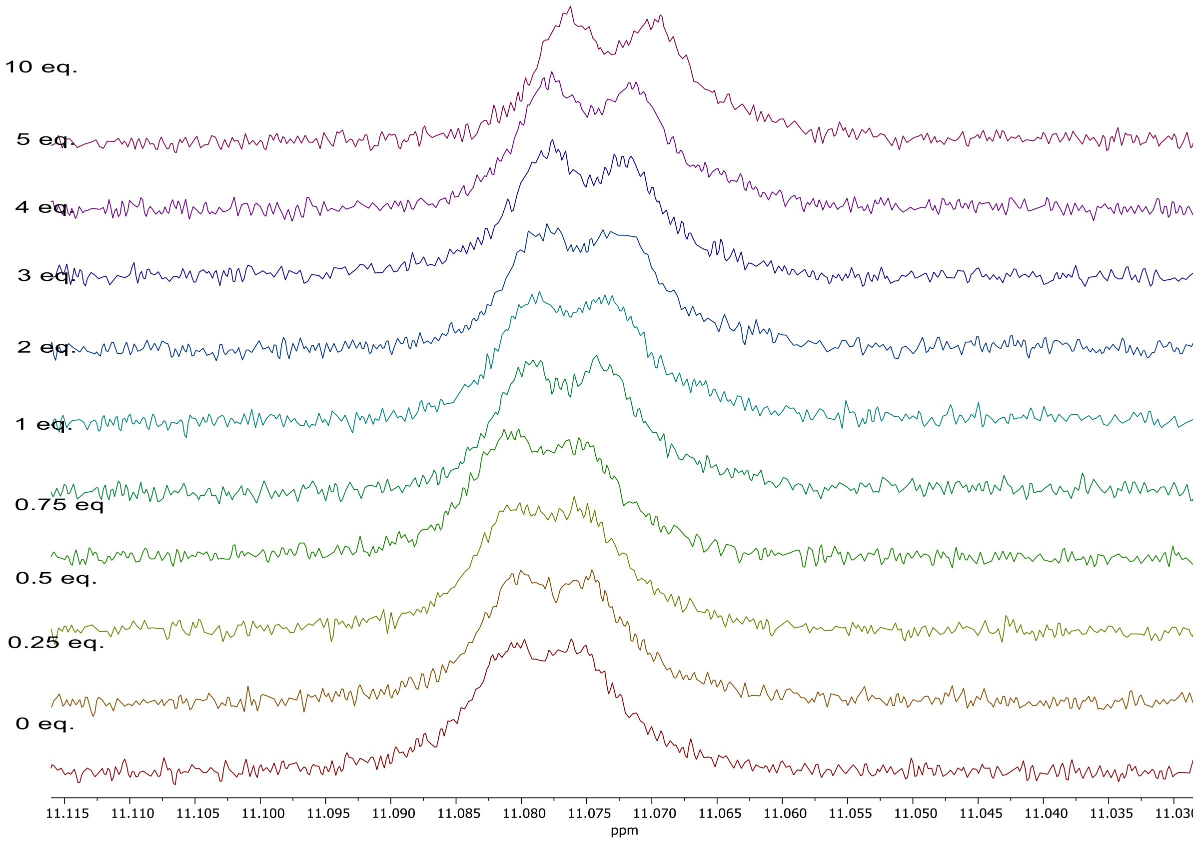


Figure S80 Evolution of ^{1}H NMR spectra (600 MHz, DMSO-d_6 + TMS, $C_{\mathbf{F\text{-}B3E}}$ = 3.8·10^{-4} M) for titration of **F-B3E** with 0-10 equiv. of Cef. Inset presenting N-**H** signal from **F-B3E** protons.

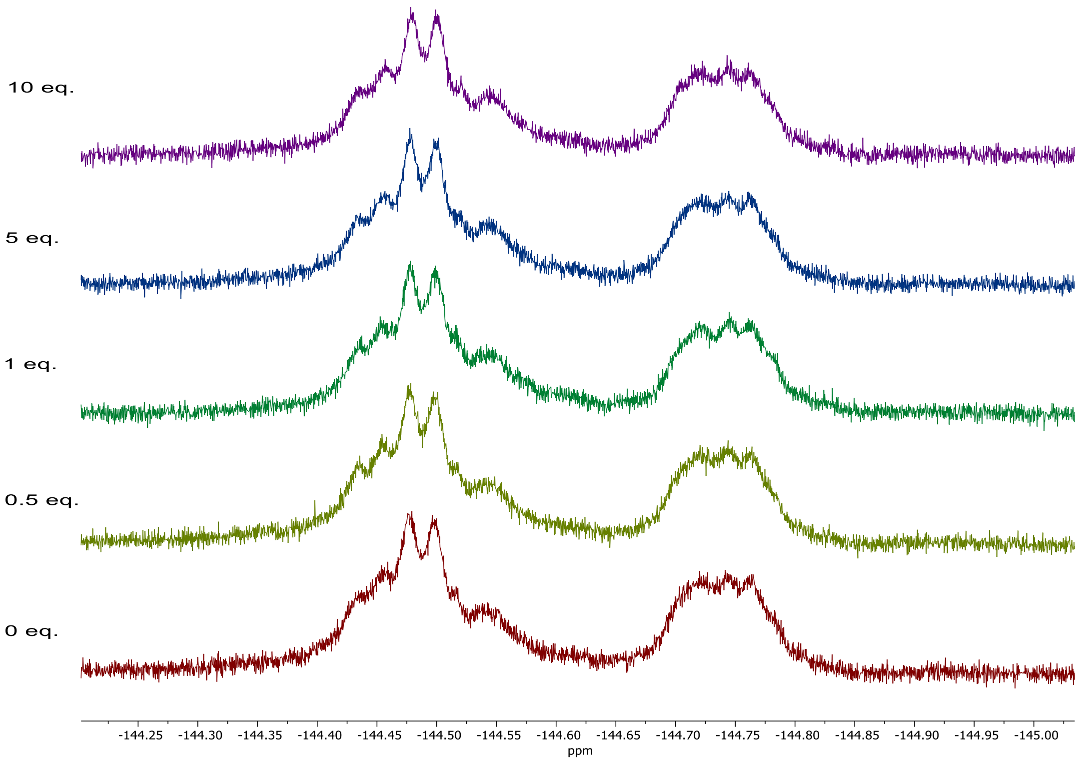
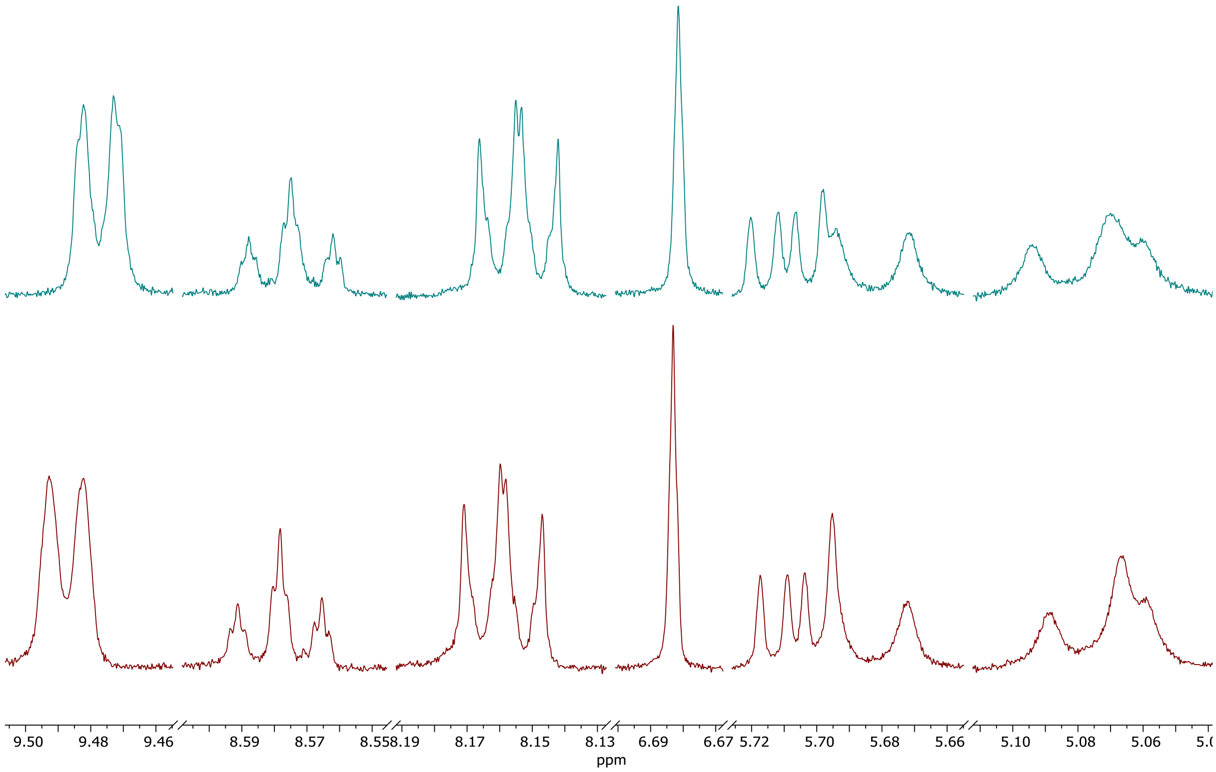


Figure S 81 Evolution of ^{19}F NMR spectra (565 MHz, DMSO-d_6 + C_6F_6, $C_{\mathbf{F\text{-}B3E}}$ = $3.8 \cdot 10^{-4}$ M) for titration of **F-B3E** with 0-10 equiv. of Cef. Insets presenting signals from **F-B3E** ^{19}F nuclei.



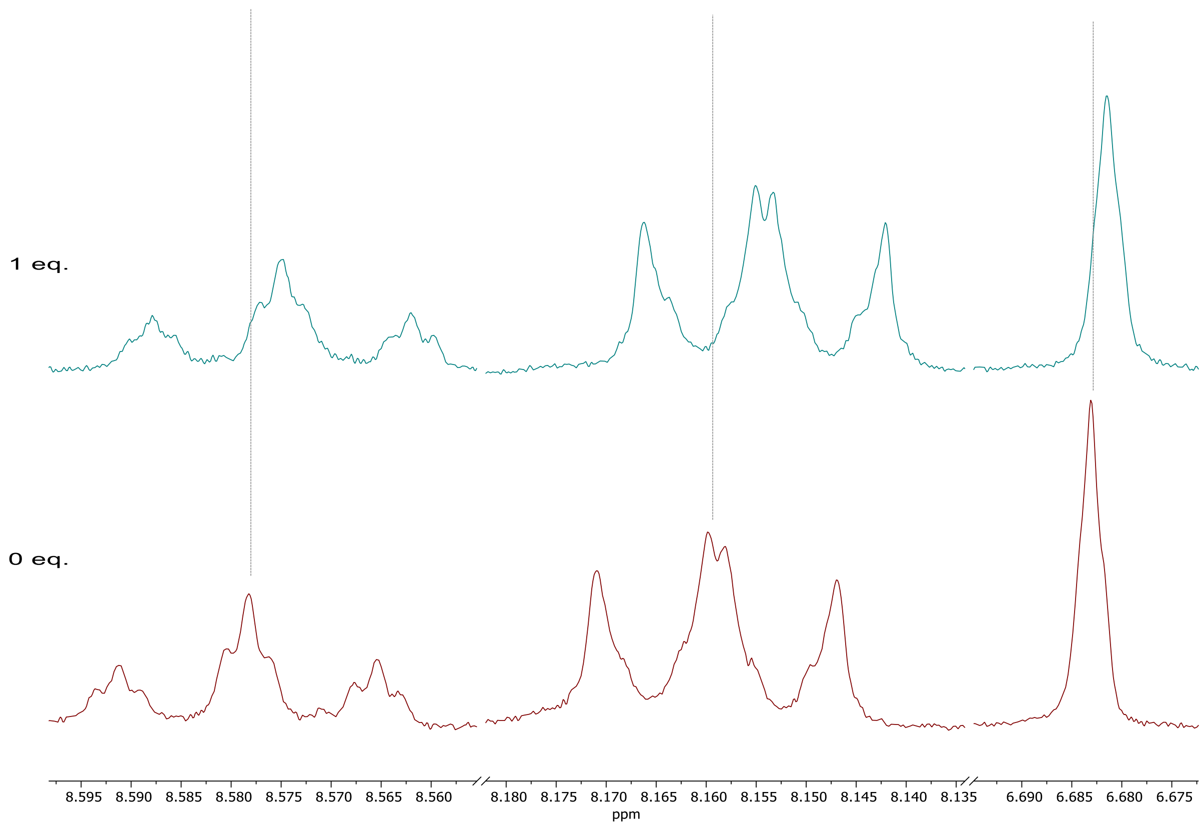


Figure S82 Stacked ^{1}H NMR spectra (600 MHz, DMSO-d_6) of Ceftazidime with and without presence of 1 molar equiv. of **B3E**: (**top**) all Cef signals, (**bottom**) inset – pyridinium moiety protons.

S6.3 DLS studies

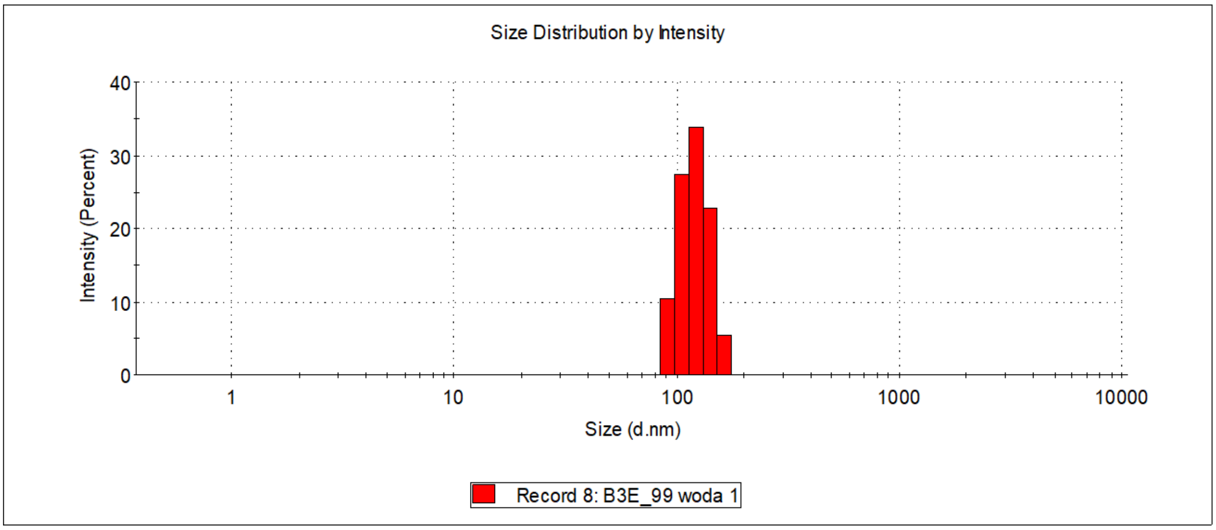


Figure S83 DLS experiment results: size distribution by intensity for **B3E** in H_2O:THF 99:1 *v/v*. $C = 2{\cdot}10^{-5}$ M. Average aggregate size in dominant peak: d = 121.3 nm.

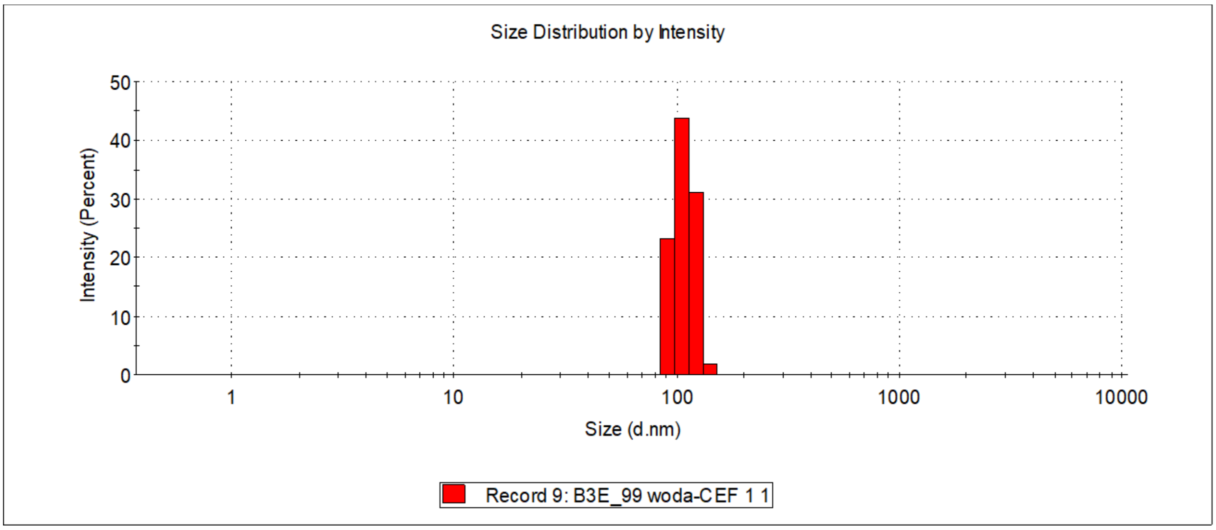


Figure S84 DLS experiment results: size distribution by intensity for **B3E** in H_2O:THF 99:1 *v/v* in presence of 1 equiv. of Cef. $C = 2{\cdot}10^{-5}$ M. Average aggregate size in dominant peak: d = 108.2 nm.

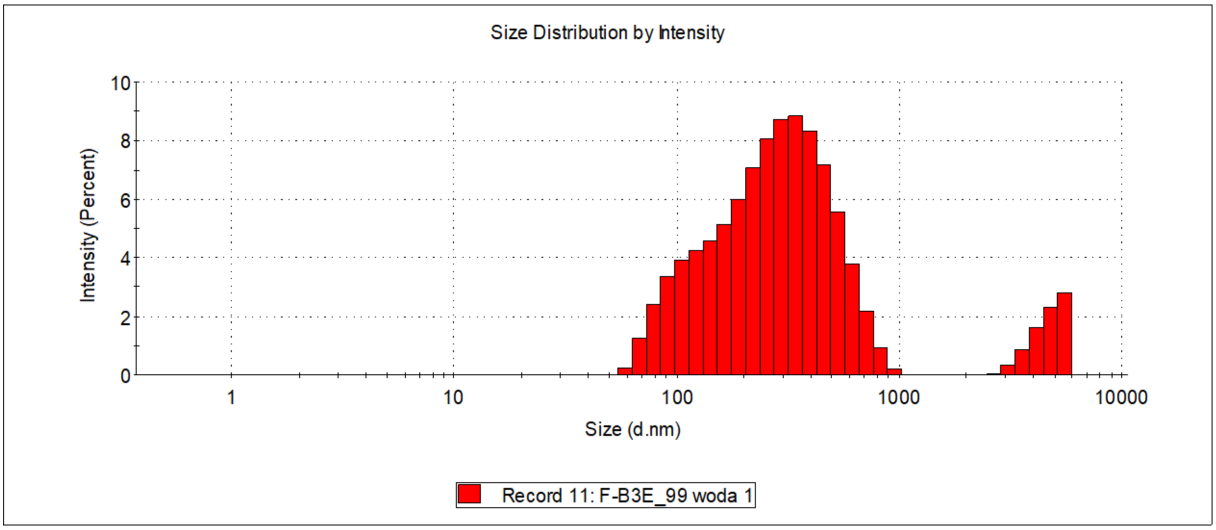


Figure S85 DLS experiment results: size distribution by intensity for **F-B3E** in H_2O:THF 99:1 *v/v*. $C = 2 \cdot 10^{-5}$ M. Average aggregate size in dominant peak: d = 302.1 nm.

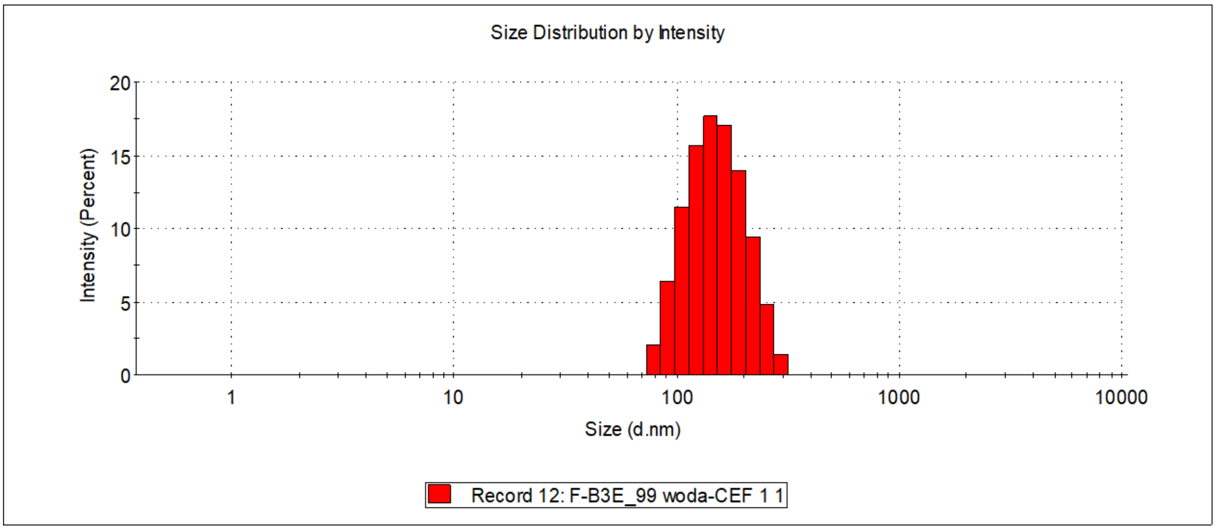


Figure S86 DLS experiment results: size distribution by intensity for **F-B3E** in H_2O:THF 99:1 *v/v* in presence of 1 equiv. of Cef. $C = 2 \cdot 10^{-5}$ M. Average aggregate size in dominant peak: d = 218.6 nm.

S7. Water and analytes characteristics

As ultrapure water LiChrosolv® Water for chromatography (LC-MS Grade) from Supelco® (Merck) was used.

A tap water sample was collected from the house faucet (Warsaw, Poland, produced by Warsaw Waterworks) on 15.01.2026.

A seawater sample was collected from the Baltic Sea in Karwia, Poland 54°49'59.7"N, 18°11'44.5"E) on 18.01.2026.

An artesian well water sample was collected from a public well (Warsaw, Zajączka Str. 7) on 04.02.2026.

Water samples were characterised by ICP-MS for presence of 23 elements (**Table 10**)

Table S11 Characteristics of water samples (ICP-MS)

Sample		Ultrapure water	Tap water	Artesian water	Seawater
Li	*C* [µg/L]	3.8354	11.6115	46.5121	41.3274
	Variance [µg/L]	2.3644	1.8605	3.3297	2.8881
Na	*C* [µg/L]	< LOQ	67.2061	122.4429	1936.1519
	Variance [µg/L]		1.2561	1.2033	20.3419
Mg	*C* [µg/L]	< LOQ	14.9759	12.5920	248.9977
	Variance [µg/L]		0.2236	0.1876	3.1814
Al	*C* [µg/L]	11.3194	41.2143	32.5819	50.5783
	Variance [µg/L]	3.5000	3.7262	3.8467	35.6992
K	*C* [µg/L]	<LOQ	12.3571	10.3715	74.9475
	Variance [µg/L]		0.2140	0.1209	0.9866
Ca	*C* [µg/L]	0.6019	92.9393	42.9102	107.4244
	Variance [µg/L]	0.0861	1.6868	0.9243	1.4342
Fe	*C* [µg/L]	8.2163	36.6901	74.4229	36.1414
	Variance [µg/L]	1.1941	3.6710	2.1667	2.1358
Y	*C* [µg/L]	0.4339	1.2111	1.6644	1.6765
	Variance [µg/L]	0.0057	0.1035	0.0850	0.0922
La	*C* [µg/L]	0.0008	0.1058	0.0507	0.0058
	Variance [µg/L]	0.0159	0.0561	0.0612	0.0457
V	*C* [µg/L]	< LOQ	< LOQ	< LOQ	3.3850
	Variance [µg/L]				2.9615
Cr	*C* [µg/L]	0.0060	0.3004	0.0120	0.9349
	Variance [µg/L]	0.0749	0.0782	0.0400	0.1018
Mn	*C* [µg/L]	0.1013	1.3240	104.2899	2.0512
	Variance [µg/L]	0.0303	0.0549	1.6105	0.0583
Co	*C* [µg/L]	0.0506	0.1607	0.0979	0.1338
	Variance [µg/L]	0.0363	0.0250	0.0195	0.0210
Ni	*C* [µg/L]	0.0583	3.0054	1.0628	1.7981
	Variance [µg/L]	0.1195	0.3949	0.2527	0.3176
Cu	*C* [µg/L]	2.2112	59.2647	86.6914	61.0410
	Variance [µg/L]	0.4173	2.6043	2.3228	11.7759
Zn	*C* [µg/L]	< LOQ	83.5593	29.1310	7.5022
	Variance [µg/L]		1.7795	1.4118	0.8702

As	*C* [µg/L]	0.09188	0.6547	0.1959	1.6387
	Variance [µg/L]	0.0157	0.1295	0.0771	0.2448
Se	*C* [µg/L]	1.1988	4.7785	4.6083	93.0353
	Variance [µg/L]	0.3538	0.7757	0.6983	2.8926
Mo	*C* [µg/L]	0.5745	3.2183	1.5171	5.9255
	Variance [µg/L]	0.2890	0.4574	0.2570	1.1584
Ag	*C* [µg/L]	0.0432	0.9825	0.1993	3.0847
	Variance [µg/L]	0.0336	0.0962	0.0277	0.1113
Cd	*C* [µg/L]	0.1109	1.1308	0.3956	1.0442
	Variance [µg/L]	0.0492	0.1267	0.0584	0.1070
Ba	*C* [µg/L]	0.0873	47.7408	12.5286	22.7566
	Variance [µg/L]	0.1928	0.7848	0.3606	0.4581
Pb	*C* [µg/L]	0.4447	60.02542	19.3513	57.4245
	Variance [µg/L]	0.1802	0.8241	0.4189	0.8679

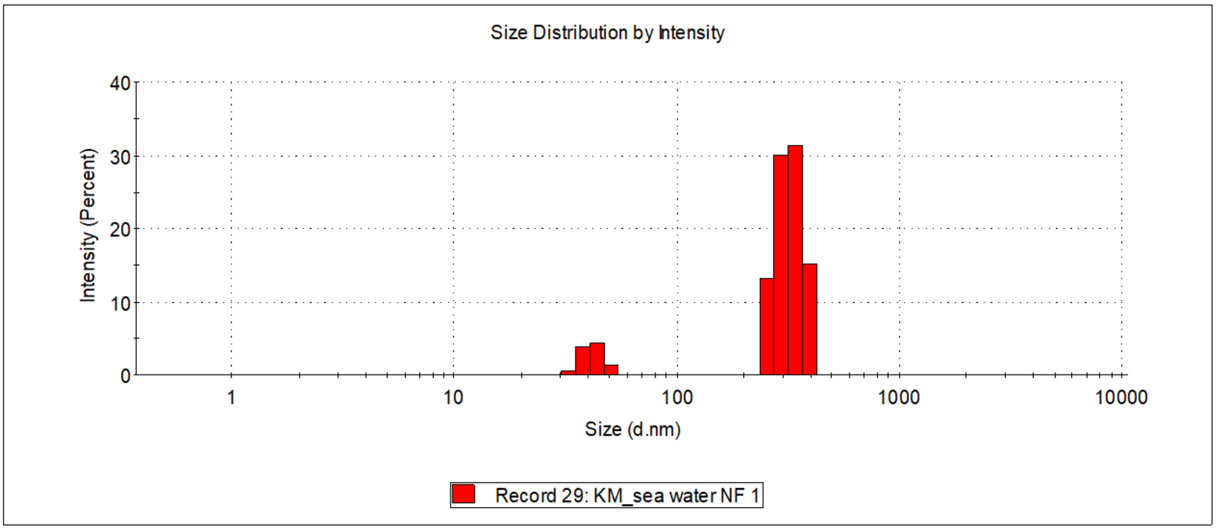


Figure S87 DLS experiment results: size distribution by intensity for non-filtered (crude) seawater. Average aggregate size: d = 840.5 nm

S8. References

1 S. S. Sebastian, H. Lee, S. Badarukhiya, R. K. Christoffels, J. M. Gebauer and U. Ruschewitz, *Chem. Eur. J.*, 2024, **30**, e202402334.
2 J. S. Cyniak and A. Kasprzak, *RSC Adv.*, 2024, **14**, 13227–13236.
3 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT*, 2016.
4 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
5 J. S. Binkley, J. A. Pople and W. J. Hehre, *J. Am. Chem. Soc.*, 1980, **102**, 939–947.
6 R. Dennington, T. A. Keith and J. M. Millam, *GaussView, Version 6.1, Semichem Inc., Shawnee Mission, KS*, 2016.