# **Electronic Supplementary Information (ESI) for**

# Grind, shine and detect: Mechanochemical synthesis of AIE-active polyaromatic amide and its application as molecular receptor of monovalent anions or nucleotides

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## List of abbreviations:

- EDCI: 1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride
- **DMAP:** *N*,*N*-Dimethylpyridin-4-amine
- **k-Oxyma:** (Z)-ethyl 2-cyano-3-hydroxyacrylate potassium salt
- NHS: *N*-hydroxysuccinimide
- **sulfo-NHS:** *N*-hydroxy- sulfosuccinimide
- **CDI:** 1,1'-Carbonyldiimidazole
- **HBTU:** 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate
- EDC: 1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide
- **DIC:** *N*,*N'*-Diisopropylcarbodiimide
- DCC: N,N'-Dicyclohexylcarbodiimide
- **AMP:** adenosine monophosphate
- **ADP:** adenosine diphosphate
- ATP: adenosine triphosphate
- NADP: nicotinamide adenine dinucleotide phosphate
- FAD: flavin adenine dinucleotide
- RT: room temperature
- h: hours

## S1. Experimental section

#### S1.1 Materials and methods

Chemical reagents and solvents for the synthesis were commercially purchased and purified according to the standard methods, if necessary. Thin layer chromatography (TLC) was performed using Merck Silica gel 60 F254 plates.

**The NMR experiments** were conducted using a Varian VNMRS 500 MHz spectrometer (<sup>1</sup>H at 500 MHz, <sup>13</sup>C{<sup>1</sup>H} NMR at 125 MHz) equipped with a multinuclear z-gradient inverse probe head. The spectra were recorded at 25 °C and standard 5 mm NMR tubes were used. <sup>1</sup>H and <sup>13</sup>C chemical shifts ( $\delta$ ) were reported in parts per million (ppm) relative to the solvent signal, *i.e.*, DMSO-*d*<sub>6</sub>:  $\delta_{H}$  (residual DMSO) 2.50 ppm,  $\delta_{C}$  (residual DMSO) 39.5 ppm. In the case of NMR spectra were analyzed with the MestReNova v12.0 software (Mestrelab Research S.L).

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

**Elemental analyzes** were performed using CHNS Elementar Vario EL III apparatus. Each elemental composition was reported as an average of two analyses.

**UV-vis** measurements were performed with a WVR UV-1600PC spectrometer, with the spectral resolution of 2 cm<sup>-1</sup>. For the UV-Vis measurements, the wavelengths for the absorption maxima  $\lambda_{max}$  were reported in nm.

**Emission spectra** were recorded with a HITACHI F-7100 FL spectrometer; parameters for the spectra of liquid samples (DMSO solution): scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, EM slit: 5.0 nm, PMT voltage: 700 V; parameters for the spectra of samples of aggregates (DMSO/H<sub>2</sub>O solution in various proportions): scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, EM slit: 5.0 nm, PMT voltage: 400 V parameters for the spectra of solid samples: scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, EM slit: 5.0 nm, PMT voltage: 400 V parameters for the spectra of solid samples: scan speed: 1200 nm/min, delay: 0.0 s, EX slit: 5.0 nm, PMT voltage: 400 V. The wavelengths for the emission maxima ( $\lambda_{em}$ ) were reported in nm.

**SEM** Field emission scanning electron microscope Helios 5 PFIB (Thermo Scientific) with the use of SE (secondary electron) detector.

**Dynamic light scattering (DLS) measurements** were performed with Brookhaven Instruments Particle Size Analyser 90Plus **For grinding in hand-held morta**r agate mortar with pestle was used (mortar diameter: 62 mm, pestle diameter: 24 mm)

**For grinding in glass vial** a vial (diameter: 18 mm) and rod (diameter: 8 mm) made of borosilicate glass were used.

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

### S1.2 Synthesis of compound 3 – synthesis in solvent

### General method for the synthesis of compound 3 in solvent

In a round-bottom flask, 4-(1,2,2-triphenylvinyl) benzoic acid (1) was placed. Then 5'-phenyl-[1,1':3',1"-terphenyl]-4-amine (2) was added, followed by an addition of coupling agent and an organic solvent (see Table S1). The reaction mixture was stirred at room temperature under an argon atmosphere. Then, a 1 mol·dm<sup>-3</sup> hydrochloric acid solution was added to the reaction mixture, and the crude product was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3x20 mL). Organic layers were combined, washed with water and brine. After drying with MgSO<sub>4</sub> followed by filtration, volatiles were distilled off on a rotary evaporator. Finally, the product was purified using a column chromatography (SiO<sub>2</sub>, 2% hex/CH<sub>2</sub>Cl<sub>2</sub>) to provide the target compound **3** as a yellow solid (*Note: Compound 3 can also be purified by column chromatography with 50% c-hex/AcOEt, Rf = 0.9*).

<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 500 MHz, ppm),  $\delta_{H}$  10.29 (s, 1H) 7.91-7.85 (m, 11H), 7.78-7.76 (m,2H), 7.53-7,50 (m, 4H), 7.43-7,40 (m, 2H), 7.20-7.12 (m, 11H), 7.04-7.00 (m, 6H); {<sup>1</sup>H}<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz, ppm), 165.0, 146.7, 142.9, 142.8, 142.7, 141.6, 141.1, 140.2, 139.7, 138.9, 135.1, 132.6x2, 130.6, 128.9, 128.0, 127.9x2, 127.8, 127.7, 127.3x2, 127.2, 126.9, 126.7, 124.0x2, 120.6; HRMS (ESI) *m/z* [M]<sup>+</sup> calcd. for C<sub>51</sub>H<sub>37</sub>NO = 680.2948, found = 680.2942 m/z; Elemental analysis: Anal. Calcd for C<sub>51</sub>H<sub>37</sub>NO: C, 90.1; H, 5.49; N. 2.06. Found: C, 89.86; H, 5.49; N, 2.08. R<sub>f</sub> (2% hex/CH<sub>2</sub>Cl<sub>2</sub>) = 0.91

no.	carboxylic acid (1) (mg; <i>mol</i> ; <u>eq</u> )	amine (2) (mg; <i>mol</i> ; <u>eq</u> )	solvent (ml)	coupling agent (mg; <i>mol</i> ; <u>eq</u> )	time/ temp.	yield (mg; %)
1	20; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	DCM (4)	SOCl₂ 7.58; 6.37 <i>·10⁻</i> 5; <u>1.2</u>	24h/ RT	3.3 mg 9%
2	20; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DMF (4)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> DMAP 1.30; 1.06·10 <sup>-5</sup> ; <u>0.2</u>	24h/ RT	7.8 mg 28%
3	20; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	EtOAc (4)	EDCI 10.0; 5.31 · 10 <sup>-5</sup> ; <u>1.0</u> DMAP 1.30; <i>1.06 · 10<sup>-5</sup>; <u>0.2</u></i>	24h/ RT	16.7 mg 46%
4	20; <i>5.31·10<sup>.5</sup>; <u>1.0</u></i>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	THF (4)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> DMAP 1.30; 1.06·10 <sup>-5</sup> ; <u>0.2</u>	170h/ RT	16.7 mg 46%
5	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (4)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> DMAP 1.30; 1.06·10 <sup>-5</sup> ; <u>0.2</u>	170h/ RT	17.3 mg 48%

Table S1 Conditions for the reaction in solvent

### S1.3 Synthesis of compound 3 – mechanochemistry

### General method for the mechanochemical synthesis of compound 3

4-(1,2,2-Triphenylvinyl) benzoic acid (1), 5'-phenyl-[1,1':3',1"-terphenyl]-4amine (2) and a coupling agent were grinded in presence of small amount of organic solvent (LAG – Liquid Assisted Grinding) at room temperature (see Table S2). Then a 1 mol·dm<sup>-3</sup> hydrochloric acid solution was added to the reaction mixture, and the crude product was extracted with  $CH_2Cl_2$  (3x20 mL). Organic layers were combined, washed with water and brine. After drying with MgSO<sub>4</sub> followed by filtration, volatiles were distilled off on a rotary evaporator. Finally, the product was purified using a column chromatography (SiO<sub>2</sub>, 2% hex/CH<sub>2</sub>Cl<sub>2</sub>) to provide the target compound **3** as a yellow solid.

# Table S2 Conditions for the mechanochemical synthesis

no.	carboxylic acid (1) (mg; <i>mol</i> ; <u>eq</u> )	amine (2) (mg; <i>mol</i> ; <u>eq</u> )	solvent (µl)	coupling agent (mg; <i>mol</i> ; <u>eq</u> )	time/ temp.	yield (mg; %)
6	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	k-Oxyma 9.56; <i>5.31·10⁻</i> 5; <u>1</u>	15min/ RT	grinding in hand-held mortar 0.0 mg / 0%
7	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> NHS 6.11; 5.31·10 <sup>-5</sup> ; <u>1</u>	15min/ RT	grinding in hand-held mortar 1.0 mg / 3%
8	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	CDI 8.61; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 2.7 mg / 5%
9	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	HBTU 20.1; <i>5.31·10⁻⁵</i> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 2.8 mg / 8%
10	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> FeCl <sub>3</sub> 43.1; 1.59·10 <sup>-4</sup> ; <u>3</u>	15 min/ RT	grinding in hand-held mortar 4.2 mg / 12%
11	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; 6.44·10 <sup>-5</sup> ; <u>1.2</u> K <sub>3</sub> PO <sub>4</sub> 33.8; 1.59·10 <sup>-4</sup> ; <u>3</u>	15 min/ RT	grinding in hand-held mortar 7.9 mg / 22%
12	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	-	EDC 10.0; <i>6.44·10<sup>-5</sup></i> ; <u>1.2</u>	15 min/ RT	grinding in hand-held mortar 7.9 mg / 22%
13	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> DIPEA 20.6; 1.59·10 <sup>-4</sup> ; <u>3.0</u>	15 min/ RT	grinding in hand-held mortar 8.4 mg / 23%
14	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> K <sub>2</sub> CO <sub>3</sub> 22.0; 1.59·10 <sup>-4</sup> ; <u>3.0</u>	15 min/ RT	grinding in hand-held mortar 8.8 mg / 24%
15	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5. <i>31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> DMAP 1.50; 1.06·10 <sup>-5</sup> ; 0.2	15 min/ RT	grinding in hand-held mortar 9.3 mg / 26%
16	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5. <i>31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; 5.31 · 10 <sup>-5</sup> ; <u>1.0</u> sulfo-NHS 11.5; 5.31 · 10 <sup>-5</sup> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 12.7 mg / 35%
17	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	DIC 6.70; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 13.4 mg / 37%
18	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	-	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 14.8 mg / 41%
19	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	DCC 10.9; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 16.5 mg / 45%

20	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	DCM (50)	DCC 10.9; <i>5.31·10⁻⁵</i> ; <u>1.0</u>	15 min/ RT	grinding in glass tube 16.2 mg / 45%
21	20; 5 <i>.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 18.9 mg / 52%
22	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5.31 <sup>.</sup> 10 <sup>-5</sup> ; <u>1.0</u>	EtOAc (50)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	15 min/ RT	grinding in hand-held mortar 18.9 mg / 52%
23	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	5 min/ RT	grinding in hand-held mortar 19.3 mg / 53%
24	20; 5 <i>.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> NaCI 18.7; 3.2·10 <sup>-4</sup> ; <u>6.0</u>	15 min/ RT	grinding in hand-held mortar 19.9 mg / 55%
25	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u> SiO <sub>2</sub> 20 mg	15 min/ RT	grinding in hand-held mortar 19.9 mg / 55%
26	20; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	DCM (50)	EDCI 10.0; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	30 min/ RT	grinding in hand-held mortar 19.9 mg / 55%
27	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	EtOAc (50)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	30 min/ RT	grinding in glass tube 28.4 mg / 80%
28	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	DCM (50)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	15 min/ RT	grinding in glass tube 30.5 mg / 84%
29	20; 5.31·10⁻⁵; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>;</i> <u>1.0</u>	DCM (50)	EDCI 10.0; <i>5.31·10⁻</i> 5; <u>1.0</u>	30 min/ RT	grinding in glass tube 34.8 mg / 96%

To check the repeatability of the designed grinding-induced protocol, we performed the mechanochemical synthesis of the target compound **3** under optimized mechanochemical conditions (grinding in glass vial with glass rod, reaction time: 30 minutes, 1.0 equiv. of EDCI) three times (independent runs), at the similar scales and on different days. The obtained isolated yields were consistent and equalled 93±3%. <sup>1</sup>H NMR analyses supported the isolation of pure **3** in each synthesis. The data for these experiments are presented below:

#### Run#1:

Synthesis date: 6.12.2022, reaction scale (mmol of amine **2**): 0.0531, mmol of the product **3** obtained: 0.0510, isolated yield of **3**: 96%

#### Run#2:

Synthesis date: 15.03.2024, reaction scale (mmol of amine **2**): 0.0531, mmol of the product **3** obtained: 0.0478, isolated yield of **3**: 90%

#### Run#3:

Synthesis date: 18.03.2024, reaction scale (mmol of amine **2**): 0.0531, mmol of the product **3** obtained: 0.0489, isolated yield of **3**: 92%

<sup>1</sup>H NMR spectra (DMSO- $d_6$ ) of the samples of compound **3** from the above-listed mechanochemical reaction runs:



## S1.4 Synthesis of compound 3 – sonochemistry

### General method for the sonochemical synthesis of compound 3

In a round-bottom flask 4-(1,2,2-triphenylvinyl) benzoic acid (**1**) was placed. Then 5'-phenyl-[1,1':3',1"-terphenyl]-4-amine (**2**) was added, followed by coupling agent and organic solvent. The flask was then placed in an ultrasonic bath Then a 1 mol·dm<sup>-3</sup> hydrochloric acid solution was added to the reaction mixture, and the crude product was extracted with  $CH_2Cl_2$  (3x20 mL). Organic layers were combined, washed with water and brine. After drying with MgSO<sub>4</sub> followed by filtration, volatiles were distilled off on a rotary evaporator. Finally, the product was purified using a column chromatography (SiO<sub>2</sub>, 2% hex/CH<sub>2</sub>Cl<sub>2</sub>) to provide the target compound **3** as yellow solid.

no.	carboxylic acid (1) (mg; <i>mol</i> ; <u>eq</u> )	amine (2) (mg; <i>mol</i> ; <u>eq</u> )	solvent (ml)	coupling agent (mg; <i>mol</i> ; <u>eq</u> )	time/ temp.	yield (mg; %)
33	20; <i>5.31·10<sup>-5</sup>; <u>1.0</u></i>	17.1; <i>5.31·10<sup>-5</sup>;</i> <u>1.0</u>	EtOAc (4)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	60 min/ RT	11.6 mg / 32%
34	20; 5.31·10 <sup>-5</sup> ; <u>1.0</u>	17.1; <i>5.31·10<sup>-5</sup>;</i> <u>1.0</u>	DCM (0.2)	EDCI 10.0; <i>5.31·10<sup>-5</sup></i> ; <u>1.0</u>	60 min/ RT	28.1 mg / 78%

### **Table S3** Conditions for the sonochemical synthesis

# S1.5 Green chemistry metrics

## Safety considerations

compound	hazard statements	meaning	thermal stability	
TPE-COOH	H302	Harmful if swallowed		
	H315	Causes skin irritation		
	H319	Causes serious eye irritation		
	H335	May cause respiratory	n/a	
		irritation	n/a	
TPB-NH <sub>2</sub>	H302	Harmful if swallowed		
	H315	Causes skin irritation		
	H319	Causes serious eye irritation		
	H332	Acute toxicity, innaiation	(	
	H335	Specific target organ toxicity,	n/a	
		single exposure; Respiratory		
		system		
NH <sub>2</sub>				
EDCI	H302	Harmful if swallowed		
	H315	Causes skin irritation		
	H319	Causes serious eye irritation	n/a	
$\sim \sim \sim c_{N}$	H335	May cause respiratory	n/a	
HCI		irritation		
	H301, H331	Toxic if swallowed or if		
DMAP		inhaled		
	H310	Fatal in contact with skin		
`N <sup>∕</sup>	H315	Causes skin irritation		
	H318	Causes serious eye damage	n/a	
	H370	Causes damage to organs		
N		(Nervous system)		
	H411	Toxic to aquatic life with long		
		lasting effects		
	H315	Causes skin irritation		
	H319	Causes serious eye irritation		
dichloromethane	H336	May cause drowsiness or	n/a	
		dizziness		
	H351	Suspected of causing cancer		

# Table S4 Hazards of the coupling reagents and solvents

# First pass green metrics calculations

EDC	I/ DMA	AP, syn	thesis i	n solutio	on				Su	mmary of Fi	irst Pa	ss Metr	ics To	olkit			
Reactant (Limiting Reactant First)	Mass (g)	MW (g/mol)	Mol	Catalyst	Mass (g)	Reagent	Mass (g)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g⋅mΓ <sup>1</sup> )	Mass (g)	Density (g·cm⁻¹)	Mass (g)				
TPE-COOH	0.02	376.45	5.31E-05			DMAP	0.0013	DCM	4	1.33	5.32			n-hexane	3	0.661	1.983
TPB-NH <sub>2</sub>	0.017	321.41	5.31E-05											DCM	147	1.33	195.51
EDCI	0.01	191.17	5.31E-05														
Total	0.047	889.03					0.0013				5.32						197.49
								1									
Yield		48.0			Mass (g)	MW	Mol					Solve	nts (first p	oass)			Tick
Selectiv	ity	100.0		Product	0.03477	679.846	0.0000511			Preferred solvents	water, Et	:OH, <i>n-</i> BuOl	H, <i>i</i> -PrOH s	l, EtOAc, <i>i</i> -Pr sulfolane	OAc, <i>n-</i> Bu	OAc, anisole,	
AE		67.2		Unreacted Limited Reactant	0.0008					Problematic solvents	DMSO,	AcOH, Acet cycloł	onitrile, Ac nexane, ch	cOMe, THF, h Ilotrobenzene,	eptane, tol Me-THF	uene, MTBE,	
RME		71.9			mass	of isolated	product 10	0		Hazardous solvents		dioxane	, TEA, DI	ME, <b>DCM</b> , DM	IF, hexane		+
OE		96.3		AE =	me = total	mass of re	eactants x It	x 100		Highly hazardous solvents	hly dous $Et_2O$ , benzene, $CCl_4$ , chloroform, nitromethane, $CS_2$ ents						
PMI tot	al	5834.4			total moleci	ular weigh	t of reactants										
PMI react	tion	154.4										Catalyst/e	nzyme (Fi	irst pass)			Tick
Reagents, catalyst         0.047         PMI = mass intensity =					ensity = $\frac{to}{-}$	tal mass in	a process or	process step	0	catalyst or enzy	/me used	or reaction t	akes place	e without any o	catalyst/	Green Flag	
PMI reaction solvents 153.0					n	hass of produ	ct		Us	e of stoic	hometric qua	antities of	reagents		Amber Flag	+	
PMI reage	ents	0.037	1		OE	$= \frac{\text{RME}}{\text{m}} \mathbf{x}$	100				use	of reagents	in excess			Red Flag	
PMI workup c	hemical	0.0			01	AE											
PMI workup solvent 5680.0																	

EC	DCI/ DMAP, s	ynthesis	in soluti	on																							
Critic	al Elements									Tick	1			Re	maining	years										2	
Suppl	ly Remaining	Flag Colour	Note element			React	tion run a	t reflux	Red Flag		1.00	4		kı (bas	nown res ed on curre	erves nt rate of					0	5	6	7 8	9	4.00250 10	
5-	50 years	Red Flag				Reaction r solve	Reaction run 5°C or below the solvent boiling point		Green Flag	+	654 11	i Be 1 9.012180	2		5-50 yea	ars ears						B 10.811	C 12.0107 14	N 14.00674 1 15 1	0 F 5.9994 18.99 6 17	Ne 20.1797 18	
50-	500 years	Amber Flag									N 22.9	Na         Mg         100-500 γr           22.58977         24.3050         21         22         23         3				ears						AI 26.98153	Si 28.0855	P 39.97376 3	S C	Ar 27 39.948	
+5	500 years	Green Flag	+				Workup			Tick	K Ca Sc Ti V				Cr I	Vin Fi	e Co	28 Ni	20 Cu	30 Zn	" Ga	Ge	As	Se B	r Kr		
							quenchin filtration	lg			39.0	983 40.078 38	44.95591 39	47.867 40	50.9415 S	1.9961 54 2 43	55.84	5 58,9332	0 58.6934 45	63.546	65.39 48		72.61	14 52 540 - 2 51 - 5	8.96 79.90 2 53	s 83.80 54	
						Ce	entrifugat	ion			85.4	b Sr 578 87.42	¥ 88.9085	Zr 91.224	Nb 92.90638 9	Mo 6.94 (98	TC Ri	r soz.905	Pd 106.42	Ag	Cd	In 114815	Sn 138.760	Sb 121.740 1	Te	Xe 131.29	
	Energy		Tick			cr	rystalisati	ion	Green Flag		55	s Ba	57 La *	77 Hf	73 Ta	9 25 W	Re O	s Ir	" Pt	Au	80 Hg	an TI	<sup>82</sup> Pb	er e Bi	Po A	85 Rn	
Reaction	run between 0 to 70°C	Green Flag	+			low temperature distillation evaporation/ sublimation		distillation/ plimation			132: 87	117.327 88 r Ra	138.9055 89 Ac‡	178.49 394 Rf	180.9479 1 105 1 Db	82.24 18 06 30 Sg 1	6.207 19602 7 108 Bh H	1 192,217 109 s Mt	110 DS	111 Rq	200.59 112 Uub	204 2422 113 Uut	270.2 114 Uuq	715 SHOP ( 115 1 Uup	209  (210) 16 117 Lv Ut	(222) 118 IS Uuo	8
Reaction ru or 7	n between -20 to 0 0 to 140°C	Amber Flag				solvent ex into a	xchange, iqueous s	quenching solvent	Amber Flag		[223] 226.025 [227] (252		(257)	(257) (260) (263) 58 59		2] (265)	(266) 62 Sm	63 Fu	Gd (277)	(285) 65 Tb	(284) (289) (288) 66 67 68		(288) ( 8 67 Fr	69 20 21			
Reaction run between below - 20 or above 140°C		Red Flag				chro	omatogra	aphy	Red Flag	+			Actinides #			140,0077         164,24         (145)         13           90         91         00         91         91         91         91         91         91         91         91         92			36         151,964         157,25         1           94         95         9         9         9         9         9         1           Vp         Pu         Am         2         2         244)         243)         2			162.50 98 Cf (251)	150         164,9303         167           99         100           Cf         Es         1           53)         (252)         (2		88.9342 173.0 11 342 Md No 589 (259)	174.967 103 0 Lr (262)	
Ba	Batch/Flow					high multip	h tempera	ature lisation																			
Flow	Gren Flag										_																
Batch	Amber Flag	+																									
Healt	h and Safety																										
	,	Red Flag	Amber Flag	Green Flag	_ist subs	tances nad	H-codes	List subs	tances nad H	l-codes	List subs	stance	es na	d H-	code	s											
Highl	ly Explosive	H200, H201, H202, H203	H205, H220, H224	Н flag								TPE-	coo	н													
Explosive	thermal runaway	H230, H240, H250	H241	agged Ireen								трв	B-NH <sub>2</sub>	2													
	Тохіс	H300, H310, H330	H301, H311, H331	nber fla then g		DMAP			DMAP																		
Long Term Toxicity		H340, H350, H360, H370, H372	H341, H351, H361, H371, H373	no red or ar des present								D	см														
Environme	ental Implications	H400, H410, H411, H420	H401, H412	lf r coc																							
Use of che	micals of environm	ental concern		List of sul	ostances																						
Chemical High Conce	Chemical identified as Substances of igh Concern by ChemSec which are		Red Flag																								

EDO	CI, mec	hanocl	hemistr	у				Sı	ummar	y of First Pa	ass Met	rics Too	olkit				
Reactant (Limiting Reactant First)	Mass (g)	MW (g/mol)	Mol	Catalyst	Mass (g)	Reagent	Mass (g)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g·ml <sup>⁻1</sup> )	Mass (g)	Workup chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g·cm⁻¹)	Mass (g)
TPE-COOH	0.02	376.45	5.30E-05					DCM	0.05	1.33	0.0665			n-hexane	3	0.661	1.983
TPB-NH <sub>2</sub>	0.017	321.41	5.30E-05											DCM	147	1.33	195.51
EDCI	0.01	191.17	5.30E-05														
Total	0.047	889.03									0.07						197.49
Yiel	d	96.0				Mass (g)	MW	Mol				Solve	nts (first pass	s)			Tick
Selecti	ivity	100.0		Proc	duct	0.03477	679.846	0.0000511		Preferred solvents	water, EtOH, <i>n</i> -BuOH, <i>i</i> -PrOH, EtOAc, <i>i</i> -PrOAc, <i>n</i> -BuOAc, anisole, sulfolane						
AE		76.4		Unreacted Limited Reactant 0.0008 0.0008 Problematic DMSO, AcOH, Acetonitrile, AcOMe, THF, heptane, to solvents DMSO, AcOH, Acetonitrile, AcOMe, THF, heptane, to								cOMe, THF, heptane, toluene, MTBE, hlotrobenzene, Me-THF					
RM	E	73.4				··]]]	J			Hazardous solvents		dioxane	», TEA, DME,	DCM, DMF,	hexane		+
OE	1	96.1		RME =	= mass of total m	ass of reacta	$\frac{\text{duct}}{\text{ants}} \ge 100$			Highly hazardous solvents	I	Et <sub>2</sub> O, benzei	ne, CCl <sub>4</sub> , chloi	roform, nitron	nethane, CS	S <sub>2</sub>	
PMI to	otal	5683.2		$AE = \frac{1}{2}$	total mole	cular weight	of reactants	x 100									
PMI rea	ction	3.3				culai weight	orreactante					Catalyst/e	nzyme (First	pass)			Tick
Reagents,	catalyst	0.000				total mass	s in a proces	s or process	step	catalyst or enzyr	me used or r	eaction take	s place withou	ut any catalys	t/ reagent	Green Flag	
PMI reaction	solvents	nts 1.9 PMI = mass intensity =					mass of pr	oduct			Use of stoid	chometric qu	antities of rea	igents		Amber Flag	+
PMI reag	gents	0.0				RME					Us	e of reagent	s in excess			Red Flag	
PMI workup	workup chemical 0.0				OE = -	AE x 100											
PMI workup	solvent	5680.0	5680.0														

Critical Elements										Tick	1	H 0794	Rei unt kn	naining years il depletion o own reserves	f					4.002602	
Supply Remaining		Flag Colour	Note element			F	Reaction run a	at reflux	Red Flag		3	Li Be	(base	d on current rate extraction) S-S0 years	of			B C	7 8 N 0	9 10 F Ne	
5-50 years		Red Flag				Reac	Reaction run 5°C or below the solvent boiling point			+	31 22-5 19	Na         J2           98977         24.3050           20         20           K         Ca           0983         40.078	21 22 Sc Ti 64.99995 47.567	50-100 years 00-500 years 13 24 V Cr 60415 51.9961	25 25 Mn Fe 34 51001 55345	27 28 Co M 58/93320 58/0	20 50 Cu Zr M 6556 6539	30         34           30         34           Al         34           36.98153         28.0855           31         39           34         34           35         28.0855           36         Ga           69.723         72.61	15         36           P         S           39.93736         32.066           30         34           As         Se           34.937360         78.96	Inc. 1997         18           Cl         Ar           35.4527         39.948           35         36           Br         Kr           29304         81.80	
50-500 years		Amber Flag									20 F	Rb Sr	39 40 1 Y Zr 88,9085 95,224 1	Nb Mo	Tc Ru	Rh P	d Ag Co	I In Sn	51 52 50 Te 101,500 127,60	1 Xe	
+500 years		Green Flag	+				Workup			Tick	55	Cs Ba	57 77 La * Hf	Ta W	Re Os	ir a Ir P	t Au Hg	TI Pb	Bi Po	as 86 At Rn	
						filtration		ng n	_		112	Fr Ra	138.9055 178.89 89 504 Ac ‡ Rf	05 106 Db Sg	107 108 Bh Hs	199,213 PM	111 200.59 5 Rq Uu	2002 2702 113 114 b Uut Uuq	115 116 Uup Lv	(210) (222) 117 118 Uus Uuo	
							centrifugation		Green Flag		[22]	3) 226.025	(227) (257)	260) (263)	(262) (265)	(266) (271)	[272] [285]	(284) (285)	(288) (292)		
Energy			Tick			low	crystalisa	tion distillation/				La	nthanides *	e Pr	Nd Pm	Sm Eu	Gd Tb	65 67 Dy Ho	en ov Er Tm	70 71 Yb Lu	
Reaction run between 0 to 70°C		Green Flag	+			ev	aporation/ su	blimation					Actinides ‡ T	141,24 (1 91 (1 h Pa	U Np	51364 15735 54 95 Pu Am	158.9253 158.925 96 97 Cm Bk	1 562.50 1661.9303 98 99 Cf Es	167.26 168.9342 100 101 Fm Md	102 103 No Lr	
Reaction run between -20 to 0 or 70 to 140°C		Amber Flag				solven	t exchange, q aqueous sc	quenching into	Amber Flag				232	2381 231.0289 2	28.0299 (237)	(244) (243)	(243) (243)	(253)	(257) (258)	(255) (242)	
Reaction run between below -20 or above 140°C		Red Flag				chromatogra		raphy													
						high tempera		rature	Red Flag	+											
Batch/Flow		Tick				multiple crystal		alisation													
Flow	Gren Flag																				
Batch	Amber Flag	+																			
Health and Safety																					
		Red Flag	Amber Flag	Green Flag	List sub	ist substances nad H-codes		List substances nad H-codes			List substances nad H-codes										
Highly Explosive		H200, H201, H202, H203	H205, H220, H224	d H flag						ТРЕ-СООН											
Explosive thermal runaway		H230, H240, H250	H241	flagge i green							TPB-NH <sub>2</sub>										
Toxic		H300, H310, H330	H301, H311, H331	mber it ther							EDCI										
Long Term Toxicity		H340, H350, H360, H370, H372	H341, H351, H361, H371, H373	no red or a des presen								DCM									
Environmental Implications		H400, H410, H411, H420	H401, H412	, T 00			ň														
						_															
Use of chemicals of environmental concern				List of sub	stances																
Chemical identified as Substances of Very High Concern by ChemSec which are utilised																					

#### S1.6 Characterisation of aggregation induced emission effect

The characterisation of aggregation induced emission behavior of compound **3** was performed employing measurements of the emission spectra. The experiments were performed in the DMSO/H<sub>2</sub>O solvent mixture. Stock solution of **3** ( $2 \cdot 10^{-3}$  M) in DMSO was diluted with proper volume of pure DMSO followed by addition of H<sub>2</sub>O to reach given vol% of H<sub>2</sub>O in the sample.

### S1.7 Anion binding experiments

### S1.7.1 <sup>1</sup>H NMR spectroscopy

The binding experiments between compound **3** (receptor) and anions (Br<sup>-</sup>, AMP and ADP) were performed employing the <sup>1</sup>H NMR titration experiments. Tetrabutylammonium bromide ([N(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>]<sup>+</sup>) was used in these experiments. The experiments were performed in DMSO-d<sub>6</sub> containing TMS (tetramethylsilane, 0.03% *vol*) as follows. To a stock solution of **3** ( $7.5 \cdot 10^{-3}$  M) in DMSO-d<sub>6</sub> a stock solution of analyte ( $7.5 \cdot 10^{-3}$  M) in DMSO-d<sub>6</sub> was added, followed by addition of DMSO-d<sub>6</sub> to reach given concentration of analyte in the sample (in case of AMP and ADP stock solution of **3** and stock solution of analyte were mixed in such a way that the sum of receptor (**3**) and analyte concentrations in the sample were on the constant level with varying molar fractions). Final volume of the samples was 1 mL.

### S1.7.2 Spectrofluorimetry

The anion binding experiments between compound **3** (receptor) and anions (analytes; Br<sup>-</sup>, I<sup>-</sup>, HSO<sub>4</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, ClO<sub>4</sub><sup>-</sup>, CN<sup>-</sup>, AMP, ADP, ATP, NADP and FAD) were performed employing the emission spectra titration experiments. In all cases, tetrabutylammonium ([N(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>]<sup>+</sup>) salts of anions were used. The experiments were performed in the DMSO/H<sub>2</sub>O = 1:1 *v*/*v* system as follows. Stock solution of **3** (2·10<sup>-3</sup> M) in DMSO was diluted with adequate volume of pure DMSO (to reach volume of 1 mL), followed by addition of H<sub>2</sub>O solution containing given anion (final concentration of anion was between 5·10<sup>-6</sup> M and 2·10<sup>-4</sup> M)

### S1.9 Estimation of fluorescence quantum yield

The measurements were performed at room temperature according to the published procedures.<sup>1,2</sup> Fluorescence quantum yields ( $\Phi_F$ ) were determined by comparison with quinine sulfate (QS) in 0.5M H<sub>2</sub>SO<sub>4</sub> ( $\Phi_{F,ref}$  = 0.55 <sup>3</sup>) as the standard. The measurements were performed with diluted solutions (absorbance for the highest wavelength A < 0.1 a.u.). The selected excitation

wavelengths ( $\lambda_{ex}$ ) were as follows:  $C_{QS} = 2 \cdot 10^{-6}$  M;  $C_3 = 2 \cdot 10^{-6}$  M,  $\lambda_{ex} = 351$  nm;  $C_{3agg.} = 2 \cdot 10^{-6}$  M,  $\lambda_{ex} = 343$  nm.

The following formula was used for the calculation of  $\Phi_F$ :

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

where  $\Phi_{F,ref}$  is the quantum yield for QS (0.55<sup>1</sup>), *F* is the integrated area under the fluorescence spectra, *A* is the absorbance at the excitation wavelength, *n* is the refractive index of the solvent (1.346 for 0.5M H<sub>2</sub>SO<sub>4</sub>, 1.4772 for DMSO, *n* for the aggregates solution (DMSO/H<sub>2</sub>O = 1:1 v/v) was taken as weighted arithmetic mean with weights equal to vol% of H<sub>2</sub>O (*n* = 1.3329) and DMSO in the mixture). The calculated  $\Phi_F$  for **3** and aggregates of **3**, were 0.0042 and 0.2437, respectively.

## S2. NMR spectra



Figure S 1 <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) spectrum of 3



Figure S 2  ${^{1}H}^{13}C$  NMR (125 MHz, DMSO- $d_{6}$ ) spectrum of 3



Figure S 3 <sup>1</sup>H-<sup>1</sup>H COSY NMR (500 MHz, DMSO-d<sub>6</sub>) spectrum of 3



Figure S 4 <sup>1</sup>H-<sup>13</sup>C HSQC NMR (DMSO-d<sub>6</sub>) spectrum of 3

# S3 HRMS spectrum



Figure S 5 ESI-HRMS (TOF) spectrum of 3

# S4. Absorption and emission spectra



Figure S 6 UV-vis spectrum of compound 3 (DMSO,  $C_3 = 2 \cdot 10^{-5}$  M)



**Figure S 7** Emission spectra of **3** (DMSO,  $C_3 = 2 \cdot 10^{-5}$  M,  $\lambda_{ex} = 270$  nm (top),  $\lambda_{ex} = 340$  nm (bottom))



**Figure S 8** 3D emission spectrum of **3** (DMSO,  $C_3 = 2 \cdot 10^{-5}$  M)



**Figure S 9** Emission spectra ( $\lambda_{ex}$  = 270 nm) of compound **3** in DMSO/H<sub>2</sub>O system containing different vol% of water in the sample (C<sub>3</sub> = 2·10<sup>-5</sup> M,)



**Figure S 10** Emission spectra ( $\lambda_{ex}$  = 340 nm) of compound **3** in DMSO/H<sub>2</sub>O system containing different vol% of water in the sample (C<sub>3</sub> = 2·10<sup>-5</sup> M)



**Figure S 11** 3D emission spectra of **3** (DMSO/H<sub>2</sub>O = 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M)

### S5. Anions binding experiments

For anions for which a decrease in emission intensity was observed (I, HSO<sub>4</sub>, BF<sub>4</sub>, H<sub>2</sub>PO<sub>4</sub>, CN, AMP, ADP, ATP, NADP, FAD) the Stern-Volmer constant values (K<sub>sv</sub>) were estimated using the Stern-Volmer method, given by the equation:

$$\frac{I_0}{I} = 1 + K_{SV}$$

where  $I_0$  and I are the fluorescence intensities of **3** in the absence and presence of given anion, respectively.  $K_{SV}$  were taken as slope of  $1/C(A_-)$  vs.  $1/\Delta I$  linear plots.

The limit of detection (LOD) values were estimated from the plot: of  $(I-I_{min})/(I_{max}-I_{min})$  vs Log ([A-]).

For CIO<sub>4</sub> where an increase in emission intensity was observed the apparent binding constant ( $K_{app}$ ) values were estimated using the Benesi-Hildebrand <sup>4,5</sup> method, given by the equation:

$$\frac{1}{I-I_0} = \frac{1}{a} + \frac{1}{a \cdot K_{app} \cdot C(A^-)}$$

where  $I_0$  and I are the fluorescence intensities of **3** in the absence and presence of given anion, respectively, **a** is a constant, and  $C(A^-)$  is the concentration of given anion in solution.  $K_{app}$  were determined as a ratio of intercept-to-slope of  $1/(I - I_0)$  vs.  $1/C(A^-)$  linear plots.

The data (for the estimation of  $K_{app}$  for the studied systems were collected from emission maxima ( $\lambda_{em}$ ) = 496 nm ( $\lambda_{ex}$  = 270 nm).

The limit of detection (LOD) values were estimated by the equation: LOD = 3S/b

Where S is standard error of intercept, and b is slope of regression line

The stoichiometry of the complexes formed was estimated using Job's plot method, from the plot:  $(1 - x) \cdot (\delta - \delta_0)$  vs x. The x stands from the mole fraction of nucleotide. The expected stoichiometry is indicated by the maximum on the plot.

All the spectra and plots are presented below.

### S5.1 <sup>1</sup>H NMR spectroscopy



**Figure S 12** <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of Br<sup>-</sup>



.311 10.309 10.307 10.305 10.303 10.301 10.299 10.297 10.295 10.293 10.291 10.289 10.287 10.285 10.285

**Figure S 13** Inset of the <sup>1</sup>H NMR (500 MHz, DMSO-d6) spectrum of **3** in presence of various molar equivalents of Br<sup>-</sup>

Signals on the <sup>1</sup>H NMR spectra were assigned according to the literature data<sup>6</sup>.



**Figure S 14** Chemical formula of adenosine monophosphate (**AMP**) with the marked protons (a, b) for which the shifts of signals were observed in the <sup>1</sup>H NMR spectrum



**Figure S 15** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **AMP** (grey colour indicates signals that are shifted)



**Figure S 16** Insets of the <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **AMP** 



**Figure S 17** Insets of the <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **AMP** (amplification of the shifted proton signals of the nucleobase of the nucleotide)



Figure S 18 Job's plot regarding the interactions between 3 and AMP (the red arrow indicates the estimated stoichiometry of the complex formed)



**Figure S 19** Chemical formula of adenosine diphosphate (**ADP**) with the marked protons (a, b), whose signals are shifted in the <sup>1</sup>H NMR spectrum



**Figure S 20** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **ADP** (grey colour indicates signals that are shifted)



**Figure S 21** Insets of the <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **ADP** (amplification of the shifted proton signals of the amide group)



**Figure S 22** Insets of the <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of **3** in presence of various molar equivalents of **ADP** (amplification of the shifted proton signals of the nucleobase of the nucleotide)



Figure S 23 Job's plot regarding the interactions between 3 and ADP (the red arrow indicates the estimated stoichiometry of the complex formed)

## S5.2 Emission spectra



**Figure S 24** Emission spectra of **3** in the presence of various molar equivalents of Br (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 25 Stern-Volmer plot regarding the interactions between 3 and Br. The data for the linear plot are also presented.



**Figure S 26** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{Br}-)$  of the interactions between **3** and **Br**. The data for the linear plot are also presented.



**Figure S 27** Emission spectra of **3** in the presence of various molar equivalents of  $I^{-1}$  (DMSO/H<sub>2</sub>O 1:1 *v*/*v*, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



**Figure S 28** Stern-Volmer plot regarding the interactions between **3** and **I**. The data for the linear plot are also presented.



**Figure S 29** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{I})$  regarding the interactions between **3** and **I**. The data for the linear plot are also presented.



**Figure S 30** Emission spectra of **3** in the presence of various molar equivalents of **HSO**<sub>4</sub> (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 31 Stern-Volmer plot regarding the interactions between 3 and HSO<sub>4</sub>. The data for the linear plot are also presented.



**Figure S 32** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{HSO_{4}^{-}})$  regarding the interactions between **3** and **HSO**<sub>4</sub>. The data for the linear plot are also presented.



**Figure S 33** Emission spectra of **3** in the presence of various molar equivalents of **BF**<sub>4</sub> (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



**Figure S 34** Stern-Volmer plot regarding the interactions between **3** and **BF**<sub>4</sub>. The data for the linear plot are also presented.



**Figure S 35** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{BF_{4}^{-}})$  regarding the interactions between **3** and **BF**<sub>4</sub>. The data for the linear plot are also presented.



**Figure S 36** Emission spectra of **3** in the presence of various molar equivalents of  $H_2PO_4^-$  (DMSO/H<sub>2</sub>O 1:1 *v*/*v*, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 37 Stern-Volmer plot regarding the interactions between 3 and  $H_2PO_4$ . The data for the linear plot are also presented.



**Figure S 38** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{H_2PO_4^-})$  regarding the interactions between **3** and  $H_2PO_4^-$ . The data for the linear plot are also presented.



**Figure S 39** Emission spectra of **3** in the presence of various molar equivalents of CIO<sub>4</sub><sup>-</sup> (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



**Figure S 40** Benesi-Hildebrand plots regarding the interactions between **3** and **CIO**<sub>4</sub><sup>-</sup>. The data for the linear plot are also presented.



**Figure S 41** Emission spectra of **3** in the presence of various molar equivalents of **CN**<sup>-</sup> (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 42 Stern-Volmer plot regarding the interactions between 3 and CN<sup>-</sup>. The data for the linear plot are also presented.



**Figure S 43** Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{CN}^{-})$  regarding the interactions between **3** and **CN**<sup>-</sup>. The data for the linear plot are also presented.



**Figure S 44** Emission spectra of **3** in the presence of various molar equivalents of **AMP** (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 45 Stern-Volmer plot regarding the interactions between 3 and AMP. The data for the linear plot are also presented.



Figure S 46 Plot for  $(I-I_{min})/(I_{max}-I_{min})$  versus  $log(C_{AMP})$  of the interactions between 3 and AMP. The data for the linear plot are also presented.



**Figure S 47** Emission spectra of **3** in the presence of various molar equivalents of **ADP** (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 48 Stern-Volmer plot regarding the interactions between 3 and ADP. The data for the linear plot are also presented.



**Figure S 49** Plot for (I-I<sub>min</sub>)/(I<sub>max</sub>-I<sub>min</sub>) versus log(C<sub>AMP</sub>) of the interactions between **3** and **ADP**. The data for the linear plot are also presented.



**Figure S 50** Emission spectra of **3** in the presence of various molar equivalents of **ATP** (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 51 Stern-Volmer plot of the interactions between 3 and ATP. The data for the linear plot are also presented.



**Figure S 52** Plot for (I-I<sub>min</sub>)/(I<sub>max</sub>-I<sub>min</sub>) versus log(C<sub>AMP</sub>) of the interactions between **3** and **ATP**. The data for the linear plot are also presented.



**Figure S 53** Emission spectra of **3** in the presence of various molar equivalents of **NADP** (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



**Figure S 54** Stern-Volmer plot of the interactions between **3** and **NADP**. The data for the linear plot are also presented.



**Figure S 55** Plot for (I-I<sub>min</sub>)/(I<sub>max</sub>-I<sub>min</sub>) versus log(C<sub>AMP</sub>) regarding the interactions between **3** and **NADP**. The data for the linear plot are also presented.



**Figure S 56** Emission spectra of **3** in the presence of various molar equivalents of **FAD** (DMSO/H<sub>2</sub>O 1:1 v/v, C<sub>3</sub> = 2·10<sup>-5</sup> M,  $\lambda_{ex}$  = 270 nm).



Figure S 57 Stern-Volmer plot of the interactions between 3 and FAD. The data for the linear plot are also presented.



**Figure S 58** Plot for (I-I<sub>min</sub>)/(I<sub>max</sub>-I<sub>min</sub>) versus log(C<sub>AMP</sub>) of the interactions between **3** and **NADP**. The data for the linear plot are also presented.

### S6. DLS measurements



Figure S 59 Size distribution pattern of 3 in DMSO



Figure S 60 Size distribution pattern of 3 in DMSO/H<sub>2</sub>O = 1/1 v/v system



Figure S 61 Size distribution pattern of 3 in DMSO/H<sub>2</sub>O = 9/1 v/v system

# S7 SEM images



Figure S 62 SEM image of solid 3 obtained after column chromatography



Figure S 63 SEM image of dried aggregates of 3

### **S8** Supporting references

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