

Liposomal formulations of novel BODIPY dimers as promising photosensitizers for antibacterial and anticancer treatment

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NMR data of

2

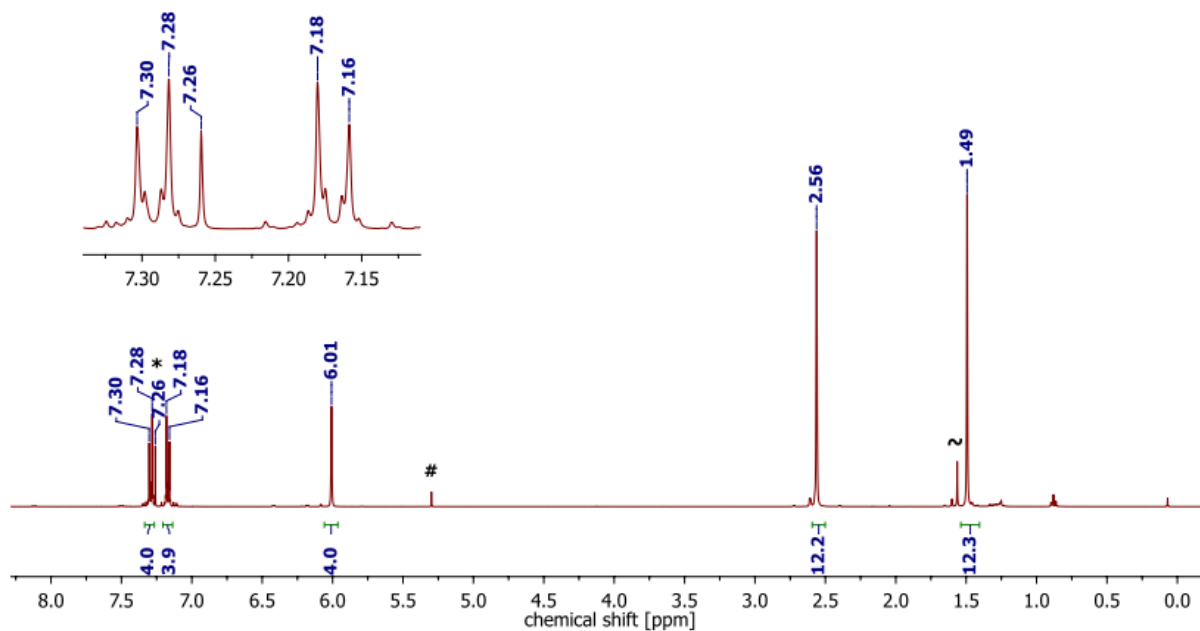


Fig. S1. ^1H NMR of **2**. Closely spaced signals are expanded in box above. The symbols *, # and ~ indicate chloroform, dichloromethane and water residual peaks, respectively.

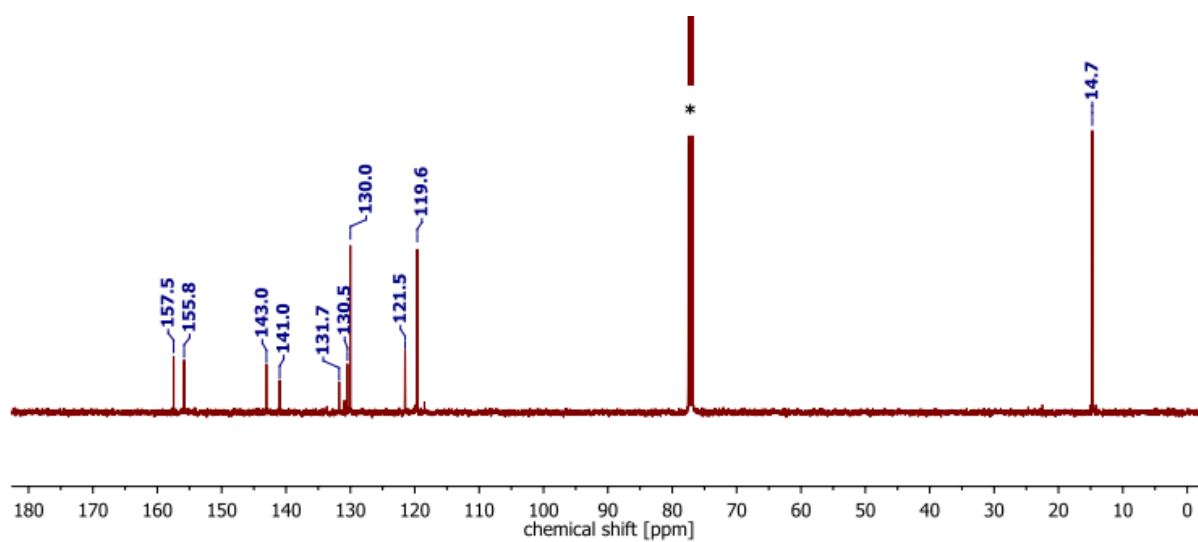


Fig. S2. ^{13}C NMR of **2**. The symbol * indicates chloroform residual peak.

Table S1. NMR data for **2** including key correlations from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

^1H δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ [Hz])	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.49	s	2.56, 6.01	14.7	121.5, 131.7, 143.0, 155.8
2.56	s	1.49	14.7	121.5, 143.0, 155.8
6.01	s	1.49	121.5	14.7, 131.7, 143.0, 155.8
7.17	d (9)	7.29	119.6	130.5, 157.5
7.29	d (9)	7.17	130.0	130.5, 141.0, 157.5
δ_{C} [ppm] from ^{13}C NMR: 157.5, 155.8, 143.0, 141.0, 131.7, 130.5, 130.0, 121.5, 119.6, 14.7				

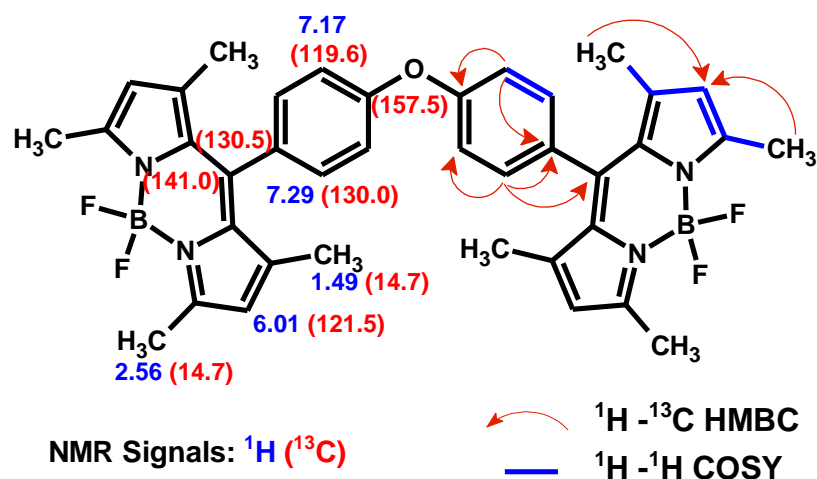


Fig. S3. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in 2D NMR spectra of **2**.

3

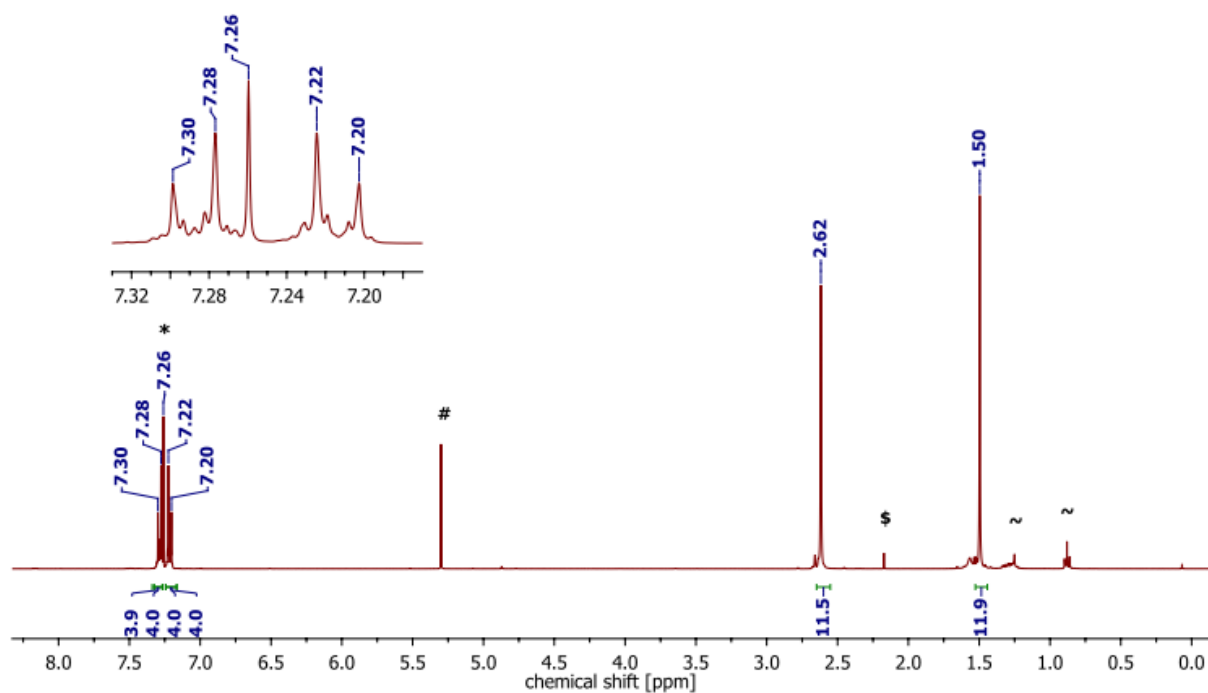


Fig. S4. ^1H NMR of **3**. Closely spaced signals are expanded in box above. The symbols *, #, ~ and \$ indicate chloroform, dichloromethane, acetone and hexane residual peaks, respectively.

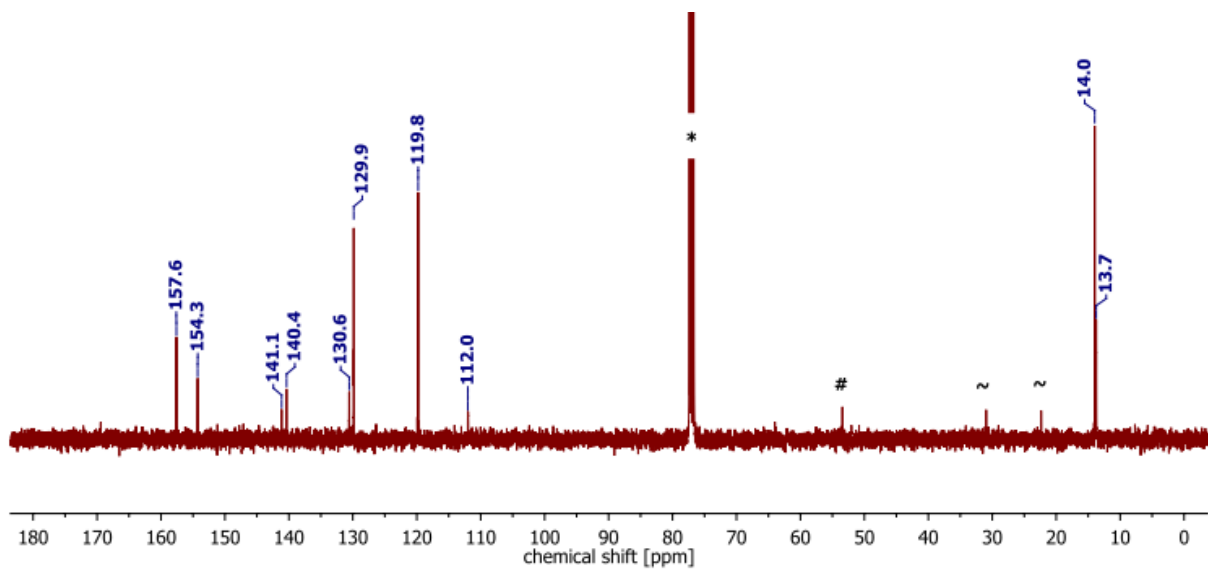


Fig. S5. ^{13}C NMR of **3**. The symbols *, # and ~ indicate chloroform, dichloromethane and hexane residual peaks, respectively.

Table S2. NMR data for **3** including key correlations from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

^1H δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ [Hz])	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.50	s	2.62	14.0	112.0, 130.6, 154.3, 140.4
2.62	s	1.50	13.7	112.0, 154.3, 140.4
7.21	d (9)	7.29	119.8	130.6, 157.6
7.29	d (9)	7.21	129.9	119.8, 141.1, 157.6
δ_{C} [ppm] from ^{13}C NMR: 157.6, 154.3, 141.1, 140.4, 130.6, 129.9, 119.8, 112.0, 14.0, 13.7				

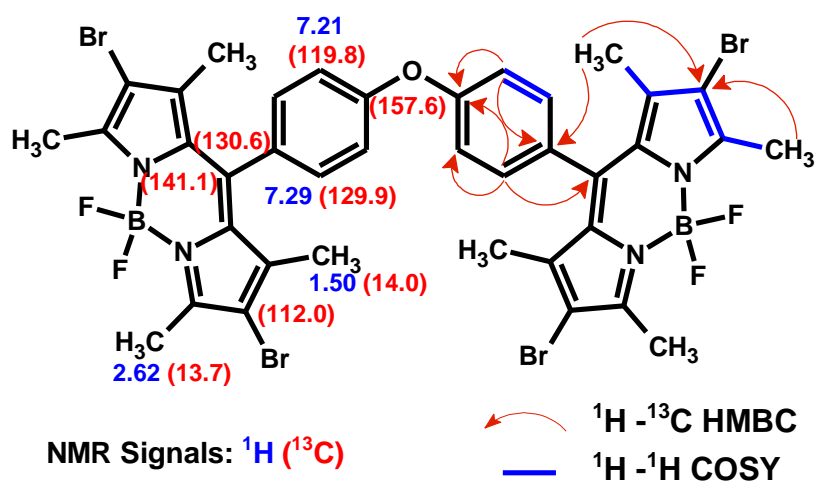


Fig. S6. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in 2D NMR spectra of **3**.

13C NMR spectrum of compound 1. The x-axis represents chemical shift in ppm, ranging from 180 to 0. The spectrum shows several sharp peaks. Key peaks are labeled with their chemical shifts: 157.6, 157.1, 145.1, 140.4, 131.5, 130.2, 129.9, 119.8, 85.9, 16.1, and 17.3. A reference peak for TMS is marked with an asterisk (*) at approximately 77 ppm.

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Table S3. NMR data for **4** including key correlations from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

^1H δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ [Hz])	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.51	s	2.66	17.3	85.9, 131.5, 145.1, 157.1
2.66	s	1.51	16.1	85.9, 140.4, 145.1, 157.1
7.21	d (9)	7.28	119.8	130.2, 157.6
7.28	d (9)	7.21	129.9	140.4, 157.6

δ_{C} [ppm] from ^{13}C NMR: 157.6, 157.1, 145.1, 140.4, 131.5, 130.2, 129.9, 119.8, 85.9, 17.3, 16.1

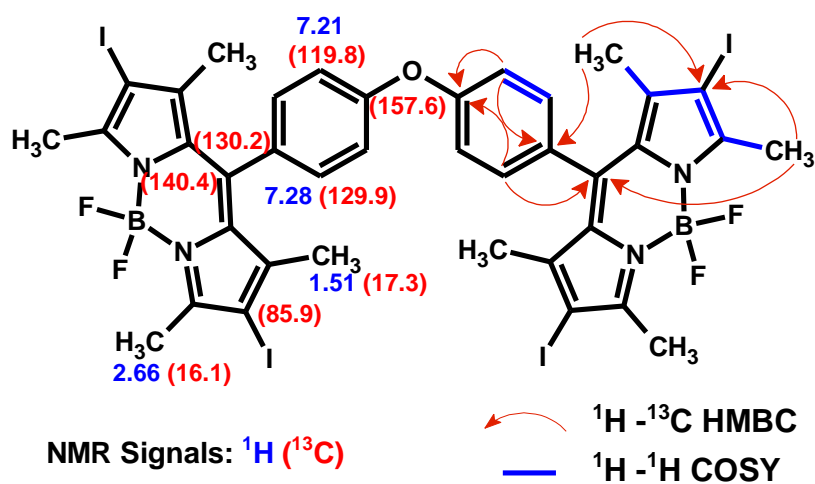


Fig. S9. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in 2D NMR spectra of **4**.

Mass Spectrometry data of

2

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3900 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

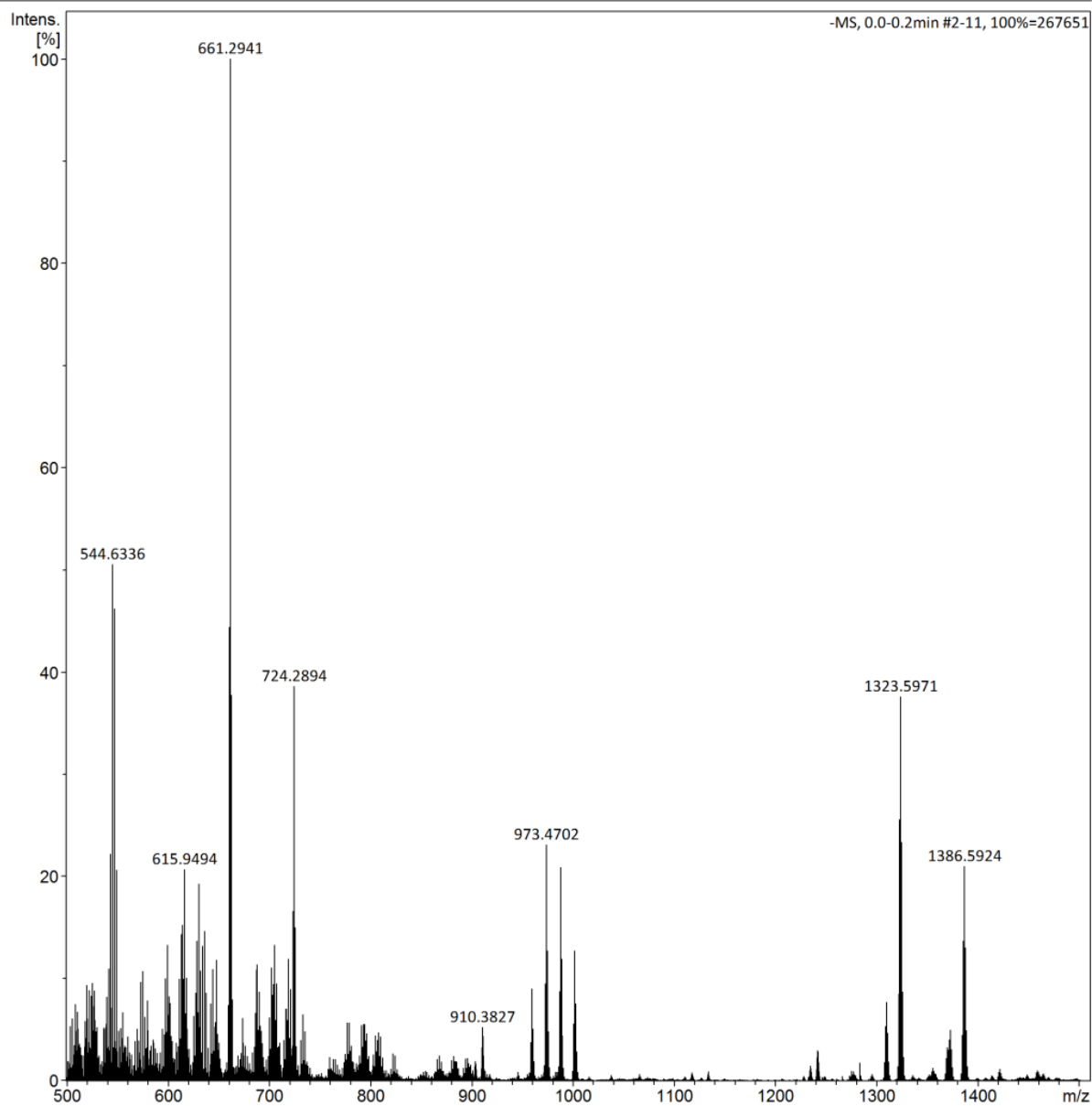
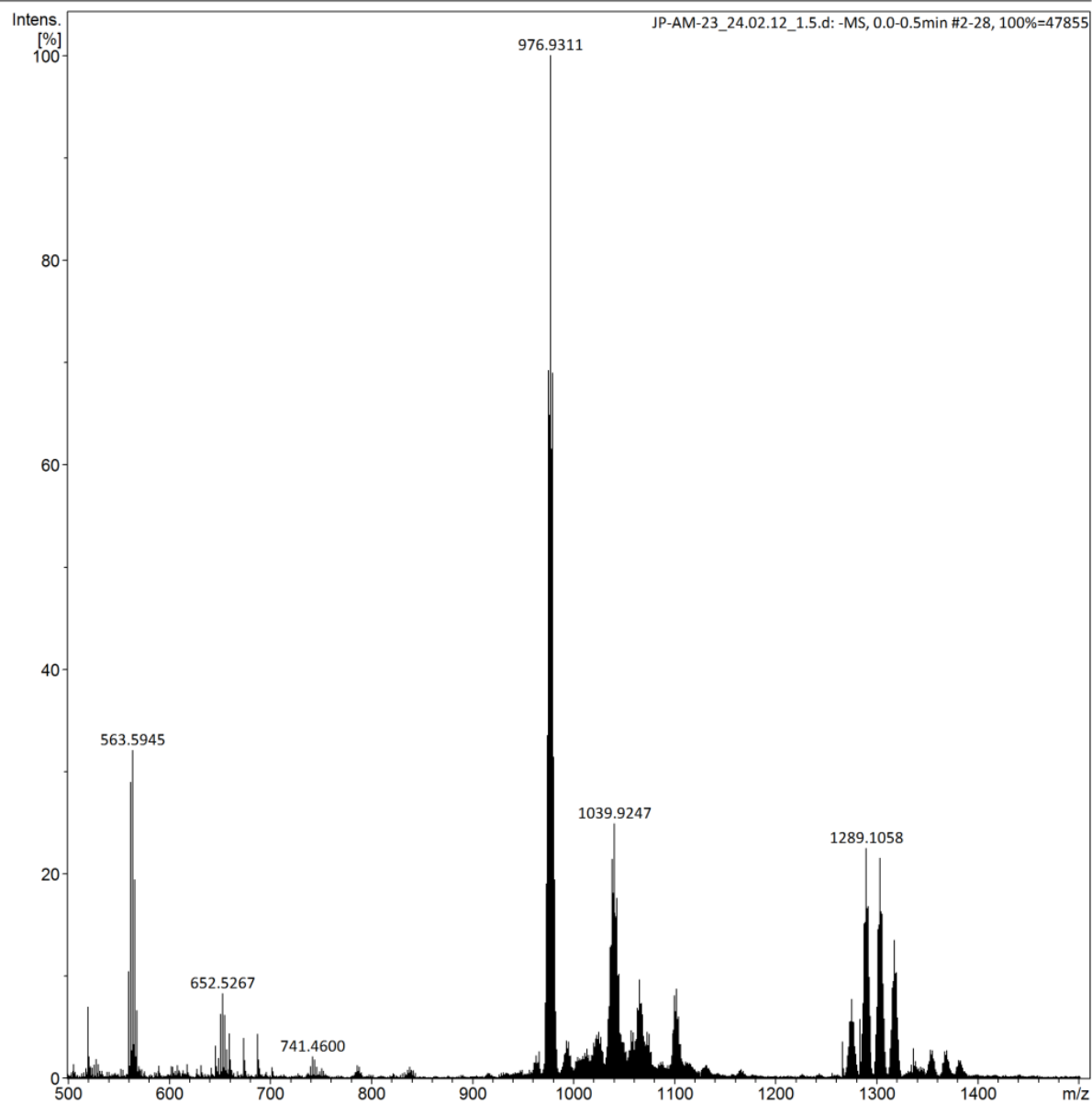


Fig. S10. HRMS spectrum of 2.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3900 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3900 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

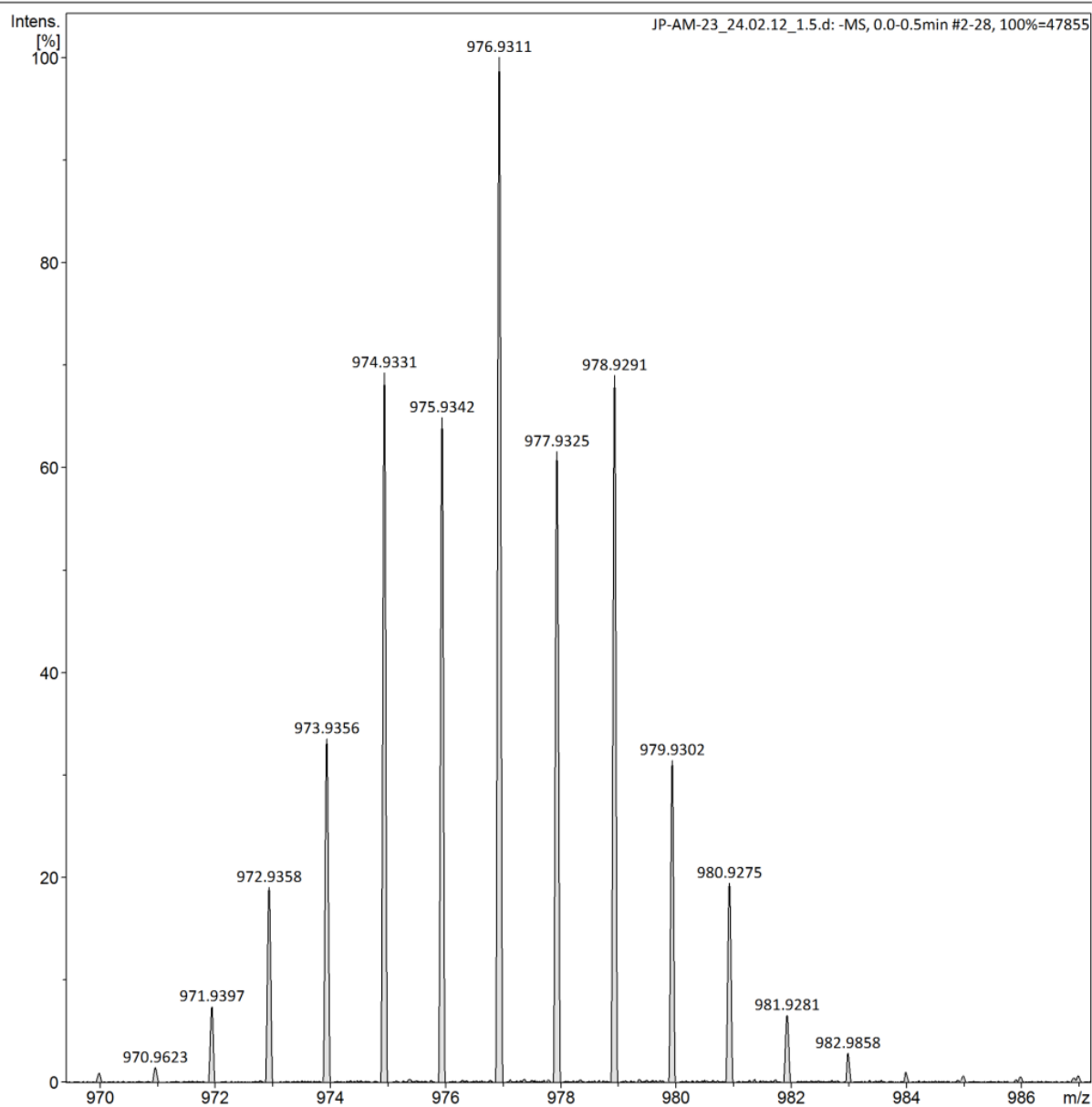


Fig. S11. HRMS spectra of **3**.

4

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	350 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

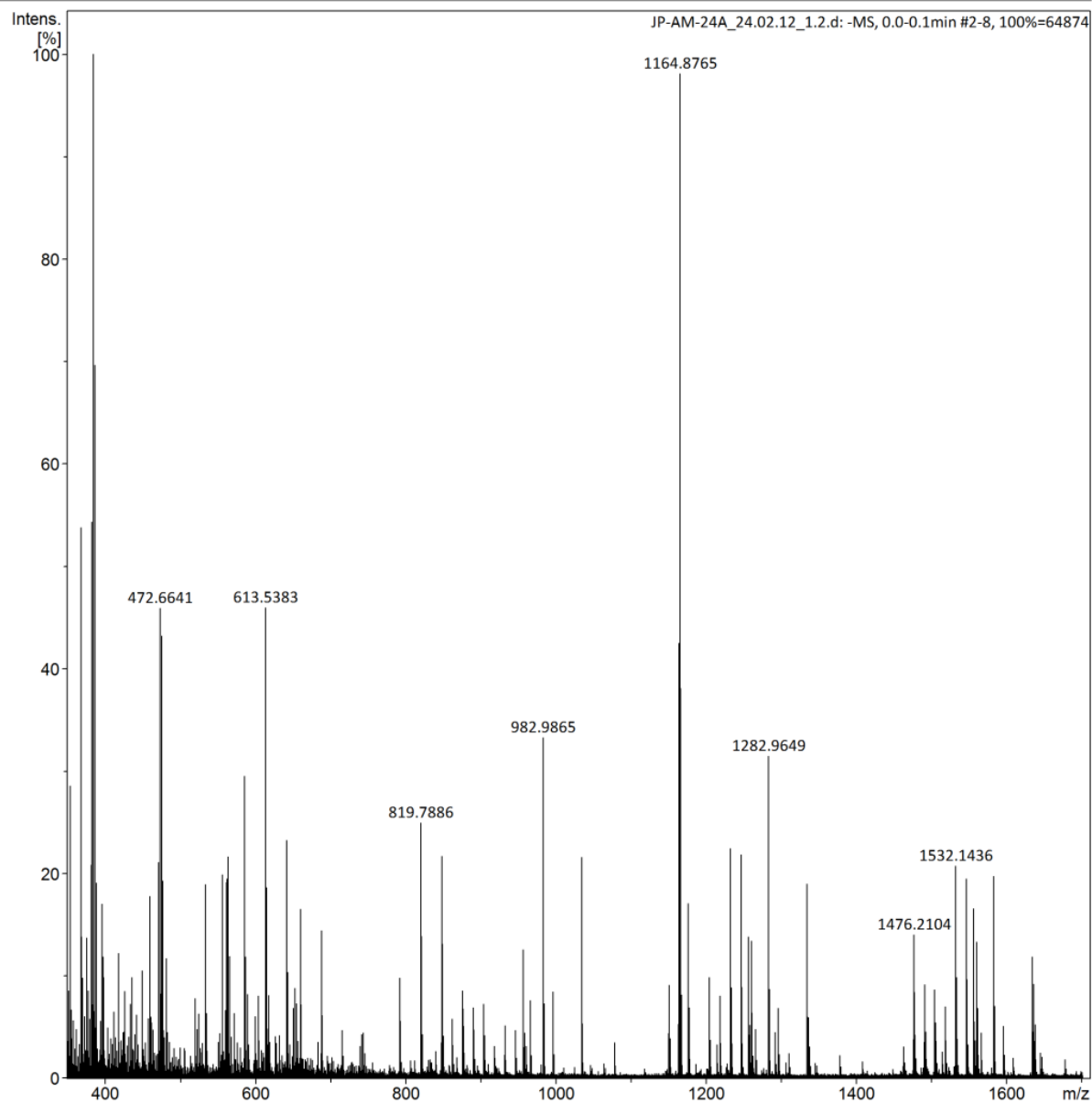


Fig. S12. HRMS spectrum of **4**.

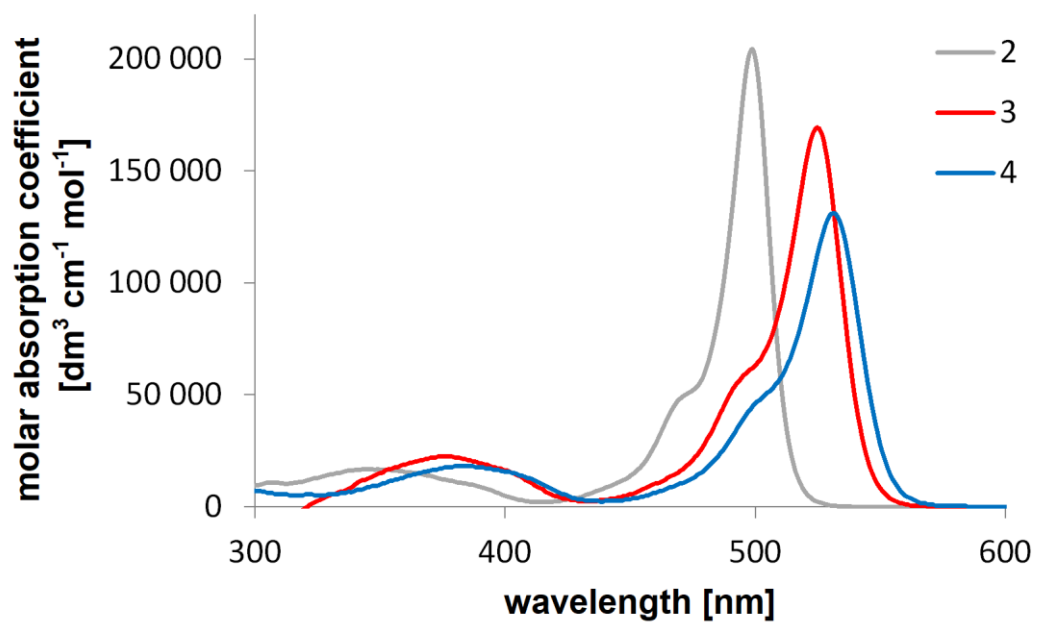


Fig S13. Absorption spectra of compounds **2-4** in methanol.

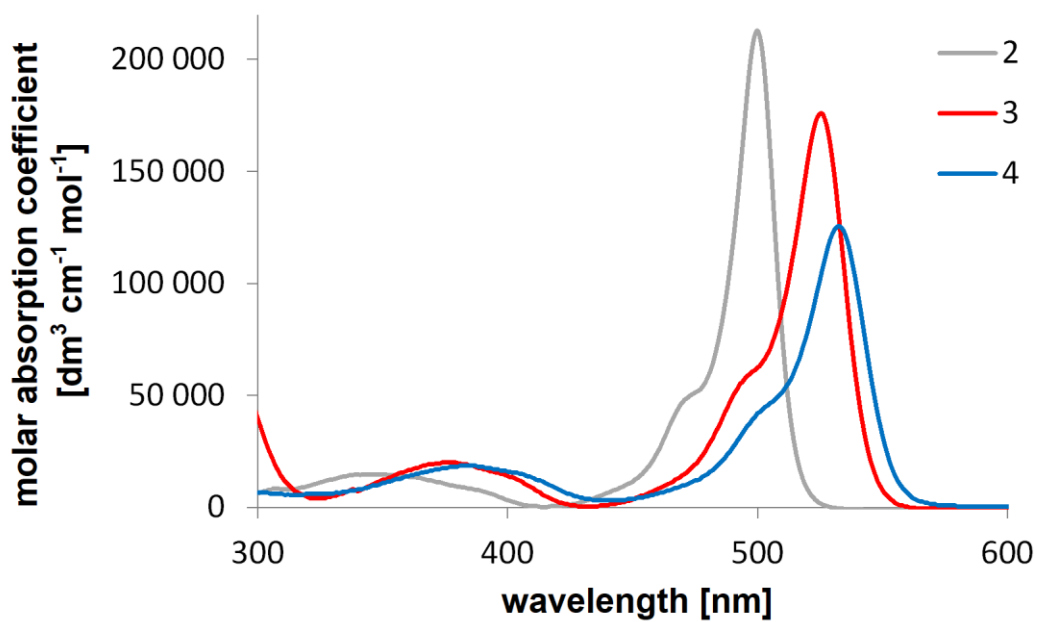


Fig S14. Absorption spectra of compounds **2-4** in ethanol.

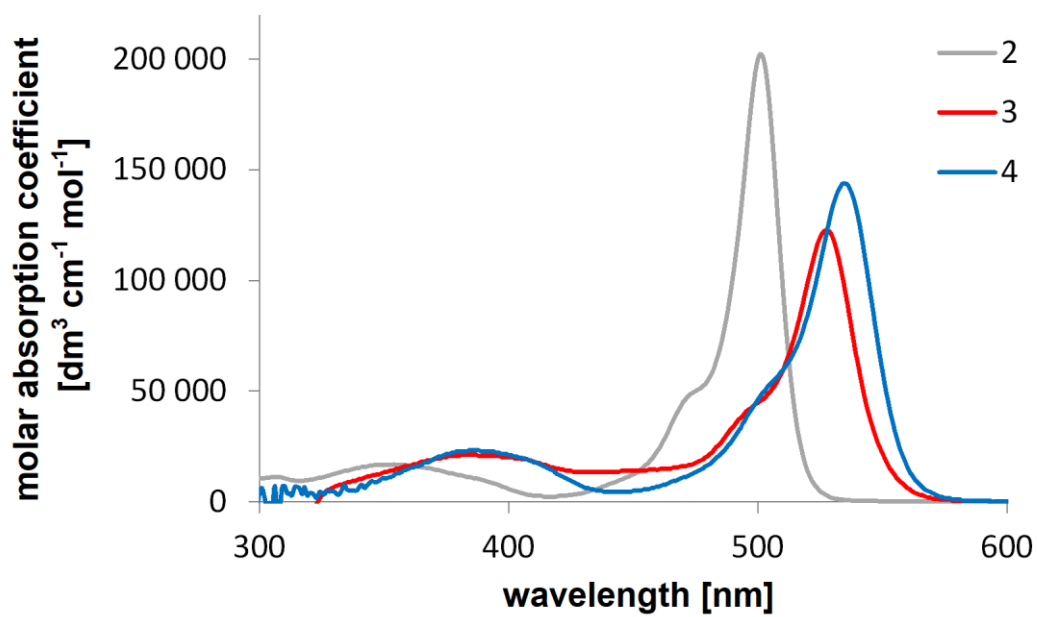


Fig S15. Absorption spectra of compounds **2-4** in DMF.

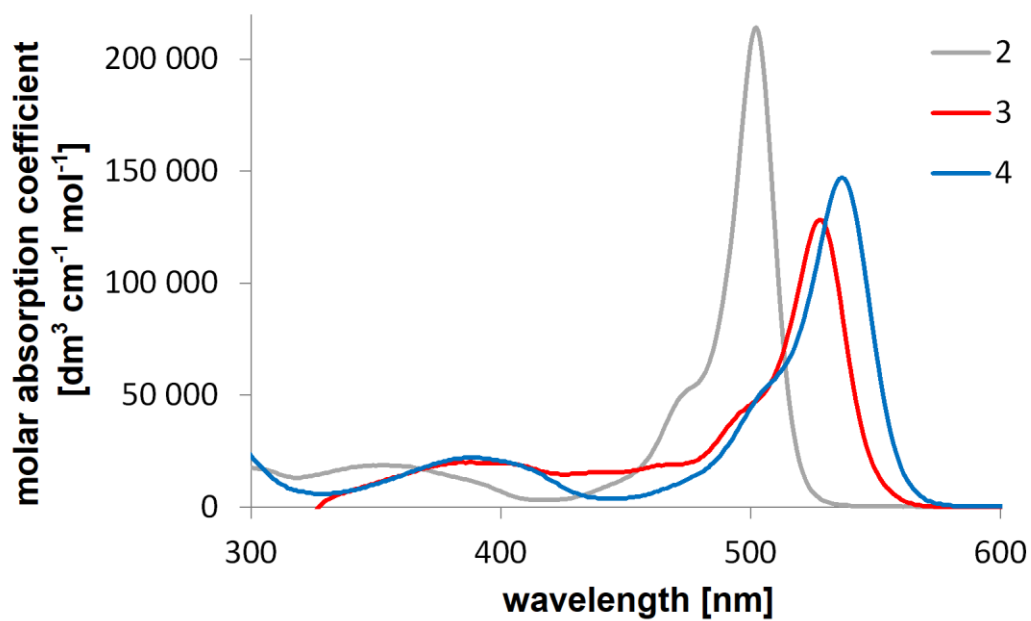


Fig S16. Absorption spectra of compounds **2-4** in DMSO.

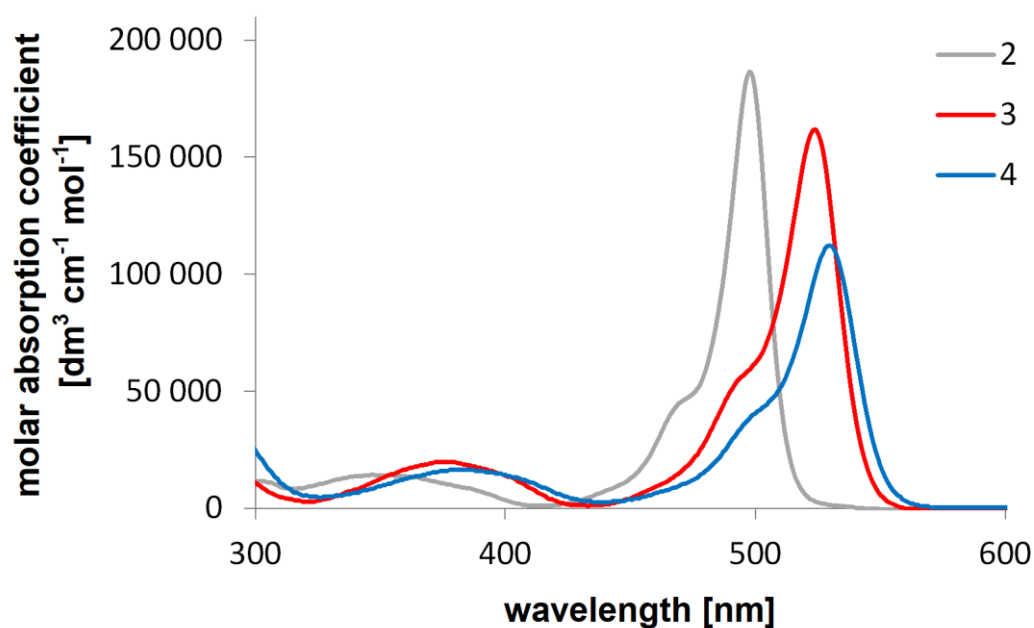


Fig S17. Absorption spectra of compounds **2-4** in acetonitrile.

Table S4. UV-Vis absorption maxima (λ_{Abs}) and logarithms of molar absorption coefficients ($\log \epsilon$) of compounds **2-4** in various solvents

BODIPY	solvent	BODIPY					
		CH₂Cl₂	CH₃OH	C₂H₅OH	DMF	DMSO	CH₃CN
2	λ_1 ($\log \epsilon$)	347 (4.31)	345 (4.23)	346 (4.17)	354 (4.23)	353 (4.28)	347 (4.16)
	λ_2 ($\log \epsilon$)	502 (5.32)	499 (5.31)	500 (5.33)	501 (5.31)	502 (5.33)	498 (5.27)
3	λ_1 ($\log \epsilon$)	378 (4.32)	376 (4.35)	377 (4.31)	384 (4.33)	387 (4.31)	376 (4.30)
	λ_2 ($\log \epsilon$)	529 (5.24)	525 (5.23)	526 (5.25)	527 (5.09)	528 (5.11)	524 (5.21)
4	λ_1 ($\log \epsilon$)	386 (4.21)	383 (4.26)	384 (4.28)	386 (4.37)	388 (4.35)	382 (4.22)
	λ_2 ($\log \epsilon$)	535 (5.20)	531 (5.12)	532 (5.10)	535 (5.16)	536 (5.17)	530 (5.05)