

Tuning Photodynamic Properties of BODIPY Dyes, Porphyrins' Little Sisters

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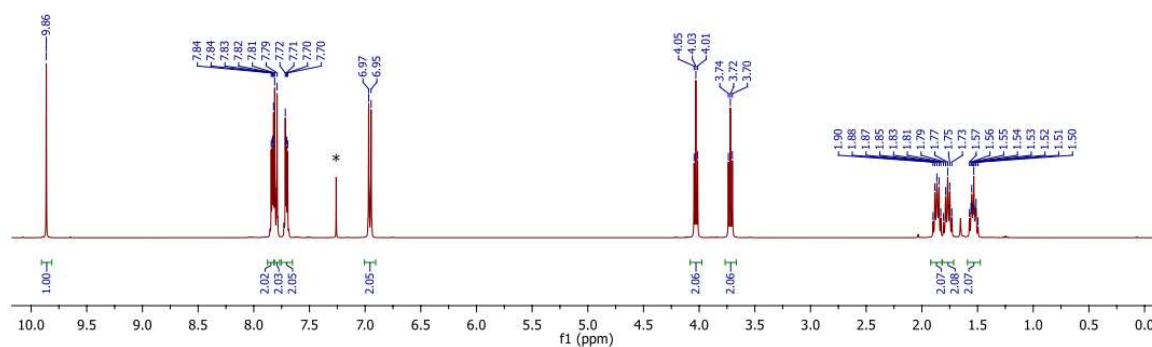
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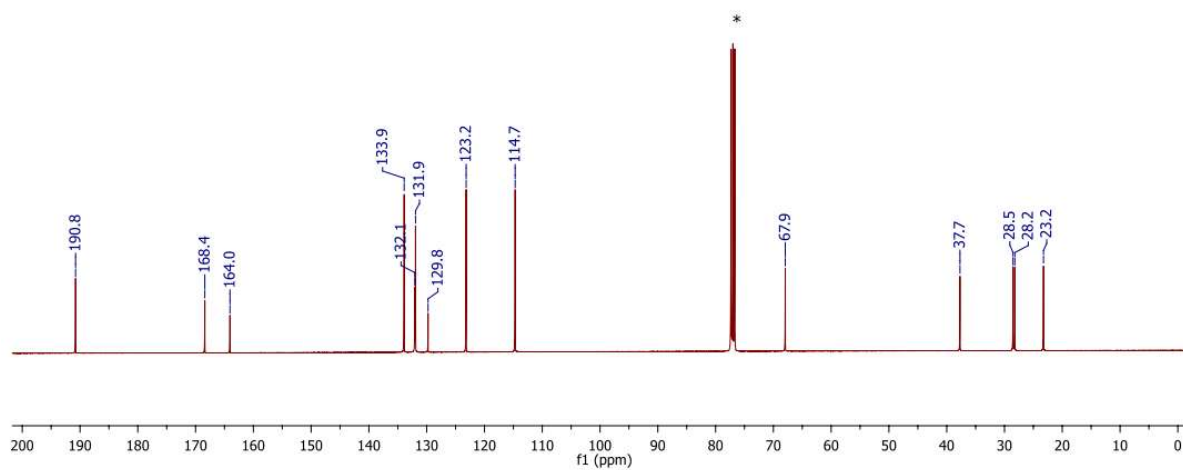
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NMR spectra

4-[5-(1,3-Dihydro-1,3-dioxo-2*H*-isoindol-2-yl)pentyloxy]benzaldehyde (**1a**)



¹H NMR spectrum of **1a** (400 MHz, CDCl₃). The symbol * indicates chloroform residual peak.



¹³C NMR spectrum of **1a** (100 MHz, CDCl₃). The symbol * indicates chloroform residual peak.

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

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.59-1.47	m	1.81-1.72, 1.91-1.82	23.2	28.2, 28.5, 67.9, 37.7
1.81-1.72	m	1.59-1.47, 3.72	28.2	23.2, 28.2, 28.5, 37.7
1.91-1.82	m	1.59-1.47, 4.03	28.5	23.2, 28.2, 28.5, 67.9
3.72	t (7)	1.81-1.72	37.7	23.2, 28.2, 28.5, 168.4
4.03	t (6)	1.91-1.82	67.9	23.2, 28.2, 28.5, 164.0
6.96	d (9)	7.80	114.7	129.8, 164.0
7.71	dd (3; 5)	7.83	133.9	123.2, 132.1, 168.4
7.80	d (9)	6.96	131.9	114.7, 164.0, 190.8
7.83	dd (3; 5)	7.71	123.2	132.1, 133.9, 168.4
9.86	s		190.8	131.9
δ_{C} [ppm] from ^{13}C NMR: 190.8, 168.4, 164.0, 133.9, 132.1, 131.9, 129.8, 123.2, 114.7, 67.9, 37.7, 28.5, 28.2, 23.2.				

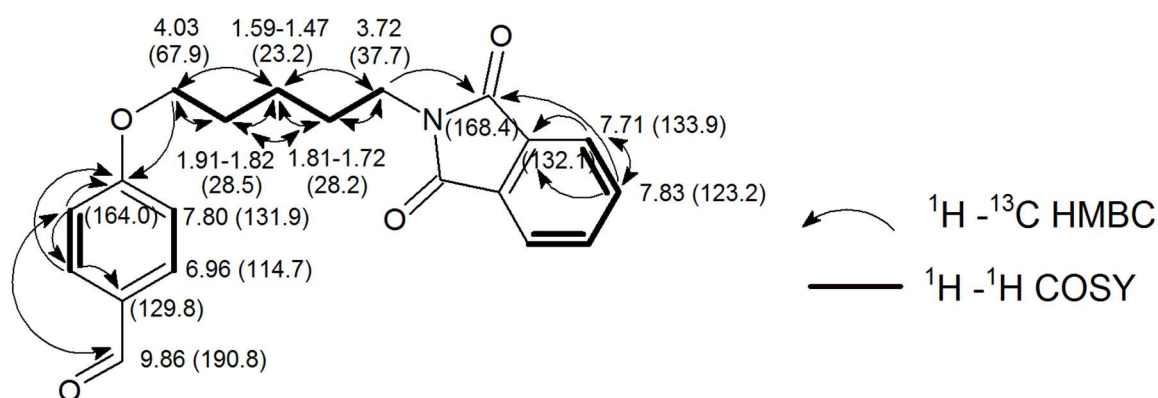
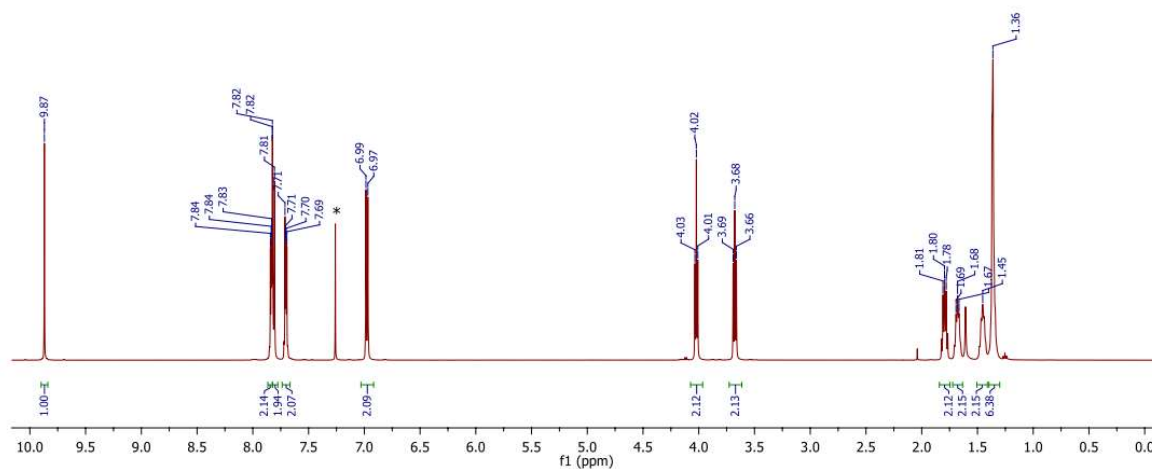
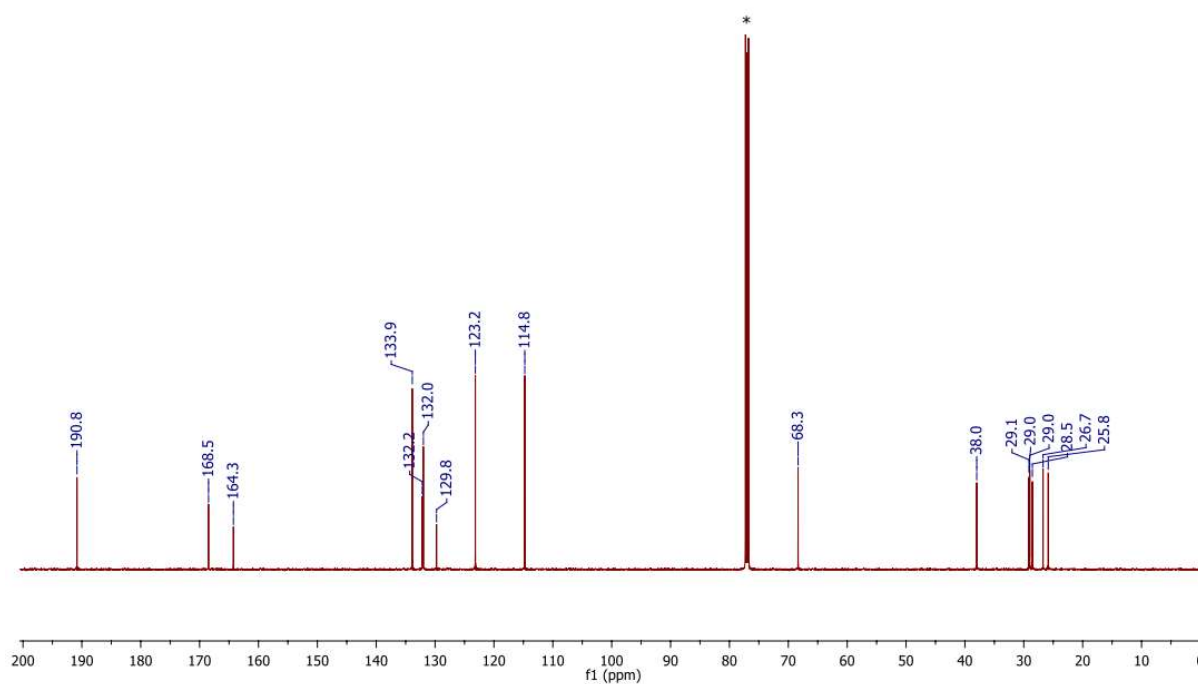


Fig. S1. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

4-[8-(1,3-Dihydro-1,3-dioxo-2*H*-isoindol-2-yl)octyloxy]benzaldehyde (**1b**)



¹H NMR spectrum of **1b** (500 MHz, CDCl₃). The symbol * indicates chloroform residual peak.



¹³C NMR spectrum of **1b** (126 MHz, CDCl₃). The symbol * indicates chloroform residual peak.

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

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.36	s	1.49-1.41, 1.72-1.65, 1.84-1.75,	26.7, 29.1	25.8, 28.5, 29.0, 38.0
1.49-1.41	m	1.36, 1.84-1.75	25.8	29.0, 68.3
1.72-1.65	m	1.36, 3.68	28.5	26.7, 38.0
1.84-1.75	m	1.36, 1.49-1.41, 4.02	29.0	25.8, 29.0, 68.3
3.68	t (7)	1.72-1.65	38.0	26.7, 28.5, 168.5,
4.02	t (7)	1.84-1.75	68.3	25.8, 29.0, 164.3,
6.98	d (9)	7.81	114.8	129.8, 164.3
7.70	dd (3; 5)	7.83	133.9	123.2, 132.2, 168.5
7.81	d (9)	6.98	132.0	114.8, 164.3, 190.8
7.83	dd (3; 5)	7.70	123.2	133.9, 168.4
9.87	s		190.8	132.0
δ_{C} [ppm] from ^{13}C NMR: 190.8, 168.5, 164.3, 133.9, 132.2, 132.0, 130.0, 129.8, 123.2, 114.8, 68.3, 38.0, 29.1, 29.0, 28.5, 26.7, 25.8				

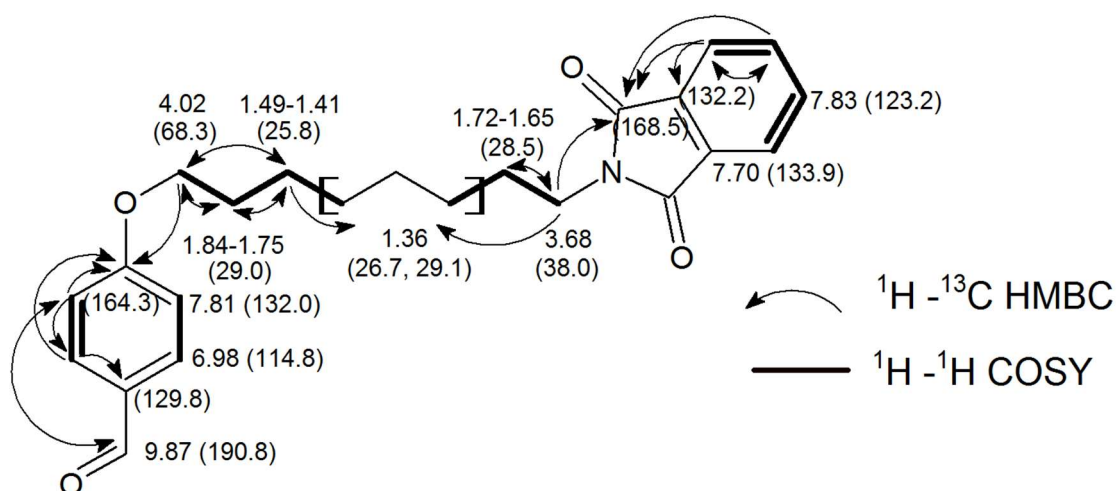
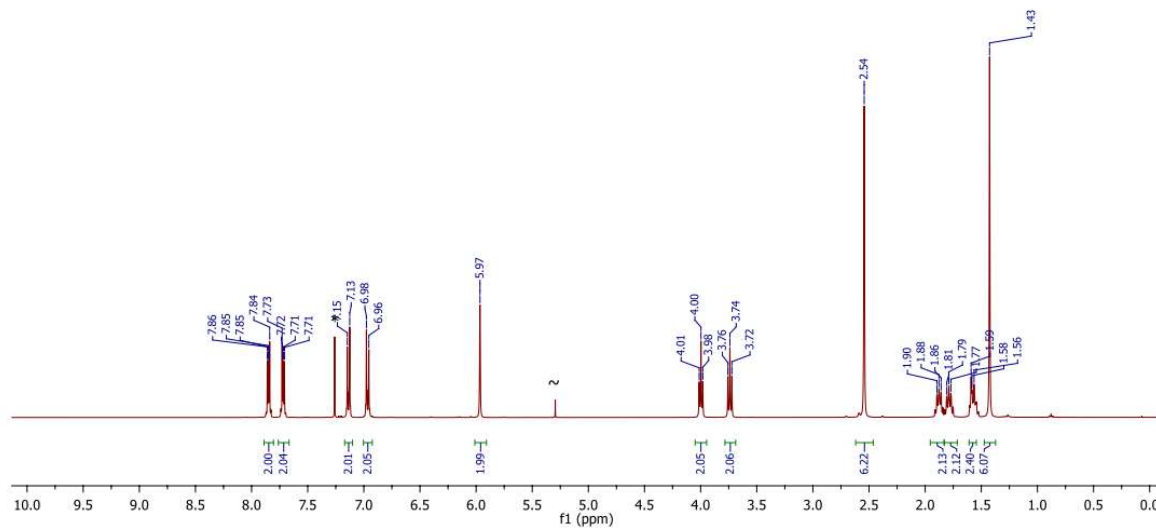
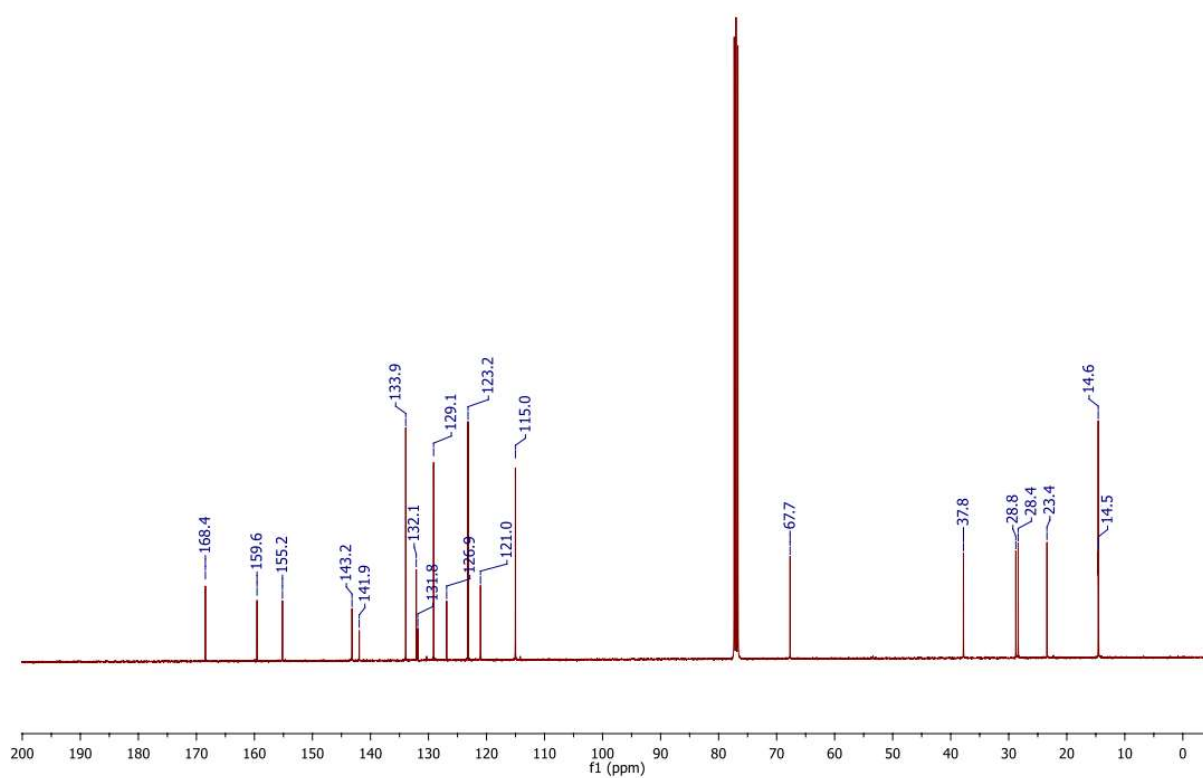


Fig. S2. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

1,3,5,7-Tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**2a**)



¹H NMR spectrum of **2a** (400 MHz, CDCl₃). The symbols * and ~ indicate residual peaks of chloroform and dichloromethane, respectively.



¹³C NMR spectrum of **2a** (100 MHz, CDCl₃).

Table S3. ^1H and ^{13}C NMR data obtained for **2a** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.43	s	2.54, 5.97	14.6/14.5	121.0, 131.8, 143.2, 155.2
1.61-1.52	m	1.83-1.74, 1.92-1.84	23.4	28.4, 28.8, 37.8, 67.7
1.83-1.74	m	1.61-1.52, 3.74	28.4	23.4, 28.8, 37.8
1.92-1.84	m	1.61-1.52, 4.00	28.8	23.4, 28.4, 67.7
2.54	s	1.43, 5.97	14.6/14.5	121.0, 143.2, 155.2
3.74	t (7)	1.83-1.74	37.8	23.4, 28.4, 168.4
4.00	t (6)	1.92-1.84	67.7	23.4, 28.8, 159.6
5.97	s	1.43, 2.54	121.0	14.6/14.5, 131.8, 143.2, 155.2,
6.97	d (9)	7.14	115.0	126.9, 129.1, 159.6
7.14	d (9)	6.97	129.1	115.0, 141.9, 159.6
7.72	dd (3, 5)	7.85	133.9	123.2, 132.1, 168.4
7.85	dd (3, 5)	7.72	123.2	132.1, 133.9, 168.4
δ_{C} [ppm] from ^{13}C NMR: 168.4, 159.6, 155.2, 143.2, 141.9, 133.9, 132.1, 131.8, 129.1, 126.9, 123.2, 121.0, 115.0, 67.7, 37.8, 28.8, 28.4, 23.4, 14.6, 14.5.				

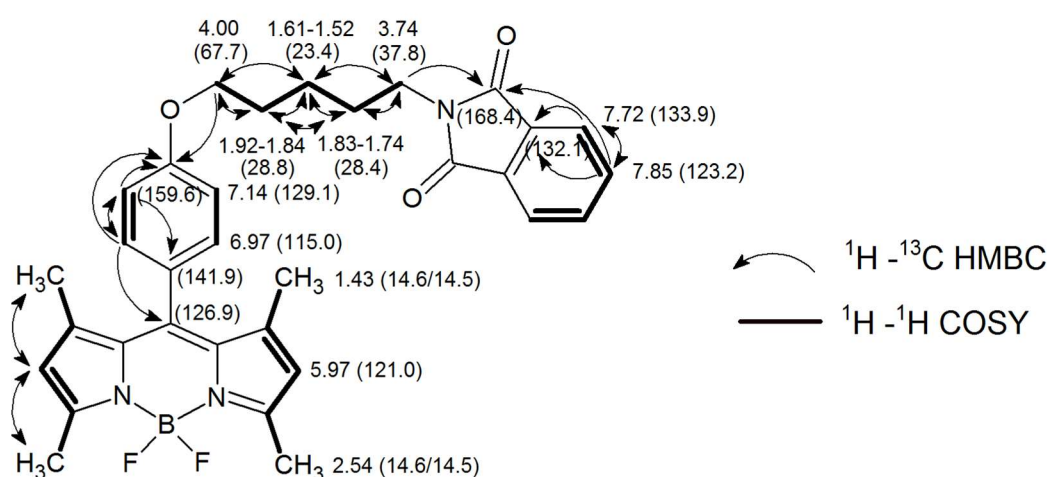
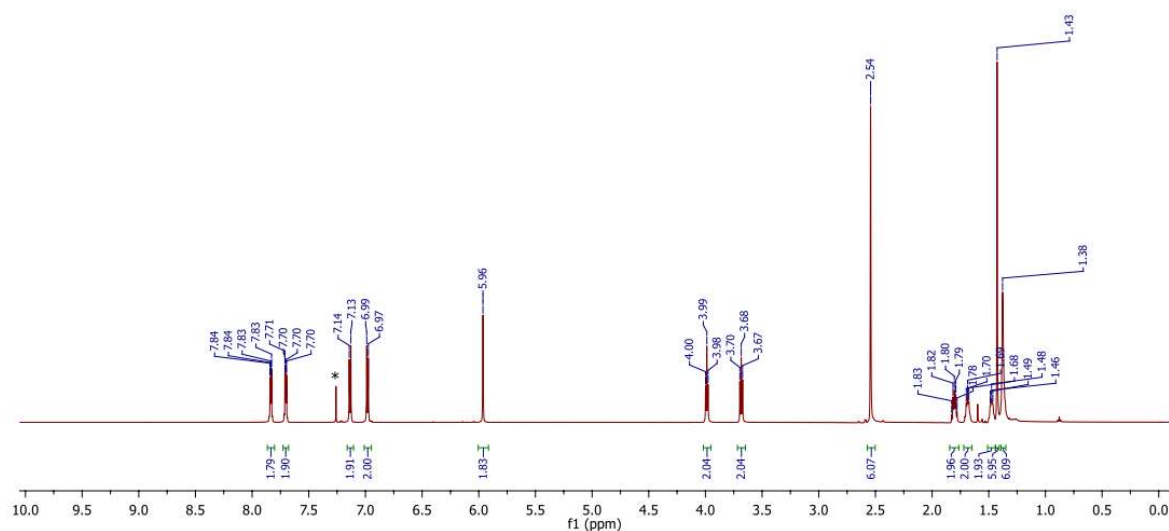
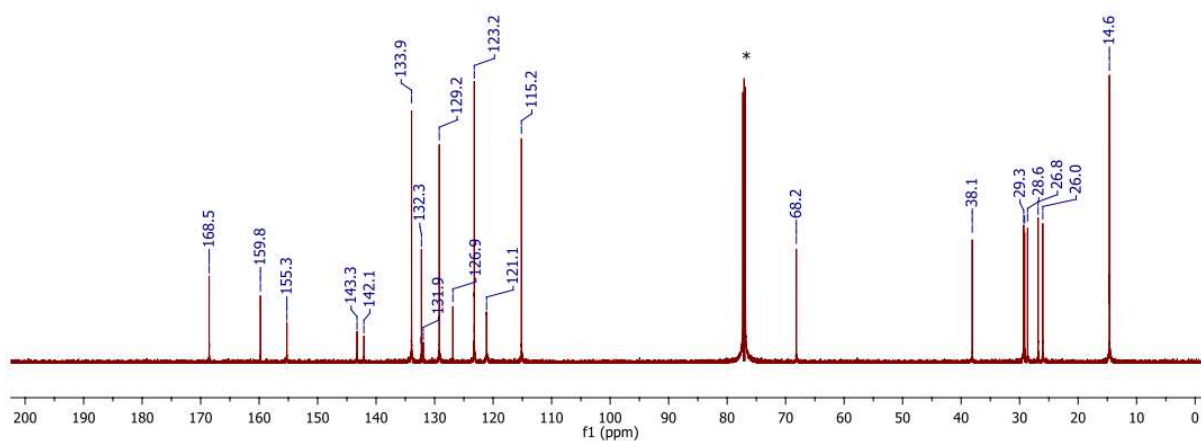


Fig. S3. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

1,3,5,7-Tetramethyl-8-{4-[8-(phthalimidyl)octyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**2b**)



¹H NMR spectrum of **2b** (600 MHz, CDCl₃). The symbol * indicates a chloroform residual peak.



¹³C NMR spectrum of **2b** (151 MHz, CDCl₃). The symbol * indicates a chloroform residual peak.

Table S4. ^1H and ^{13}C NMR data obtained for **2b** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.38	s	1.72-1.65, 1.83-1.74	26.8, 29.1	26.0, 38.1, 29.1
1.43	s	2.54, 5.96	14.6	121.1, 131.9, 143.3, 155.3
1.51-1.44	m	1.83-1.77	26.0	26.8, 29.1, 68.2
1.72-1.65	m	1.38, 3.68	28.6	26.8, 29.1, 38.1
1.83-1.77	m	1.51-1.44, 3.99	29.1	26.0, 29.3, 68.2
2.54	s	1.43	14.6	121.1, 131.9, 142.1, 143.3, 155.3
3.68	t (7)	1.72-1.65	38.1	26.8, 28.6, 168.5
3.99	t (7)	1.83-1.77	68.2	26.0, 29.1, 159.8
5.96	s	1.43	121.1	14.6, 131.9, 143.3, 155.3,
6.98	d (8.5)	7.14	115.2	126.9, 129.2, 159.8
7.14	d (9)	6.98	129.2	115.2, 142.1, 159.8
7.70	dd (3, 5)	7.84	133.9	123.2, 132.3, 168.5
7.84	dd (3, 5)	7.70	123.2	132.3, 133.9, 168.5
δ_{C} [ppm] from ^{13}C NMR: 168.5, 159.8, 155.3, 143.3, 142.1, 133.9, 132.3, 131.9, 129.2, 126.9, 123.2, 121.1, 115.2, 68.2, 38.1, 29.3, 29.1, 28.6, 26.8, 26.0, 14.6.				

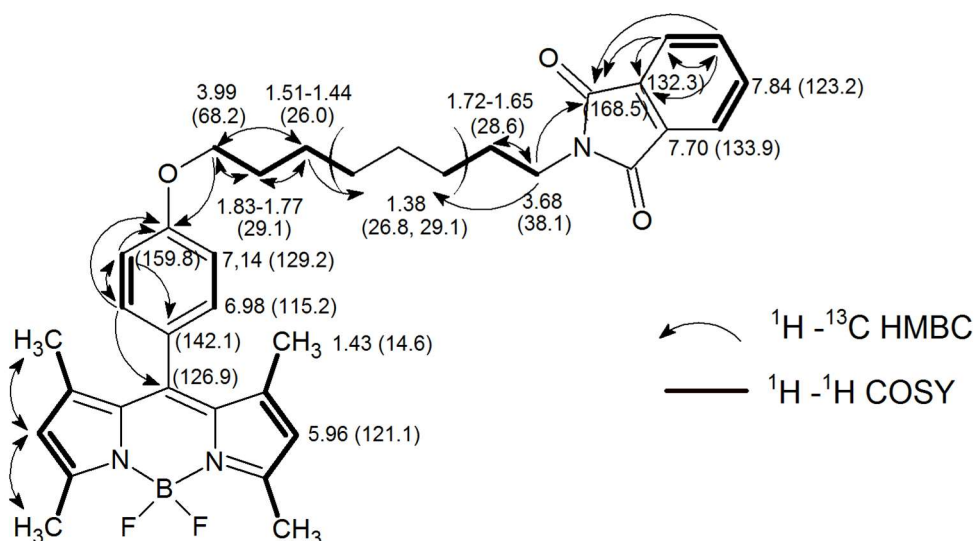
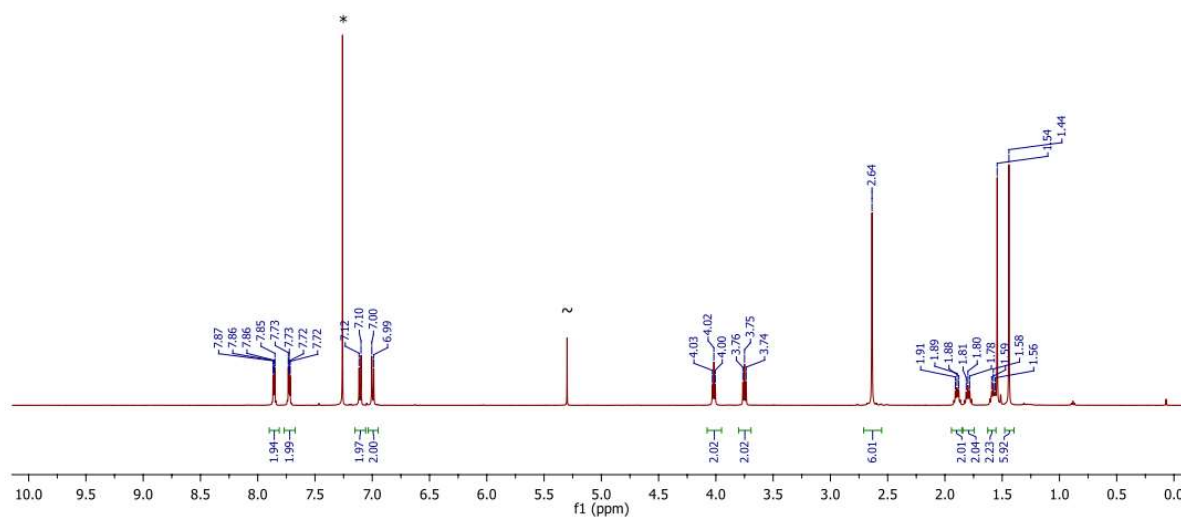
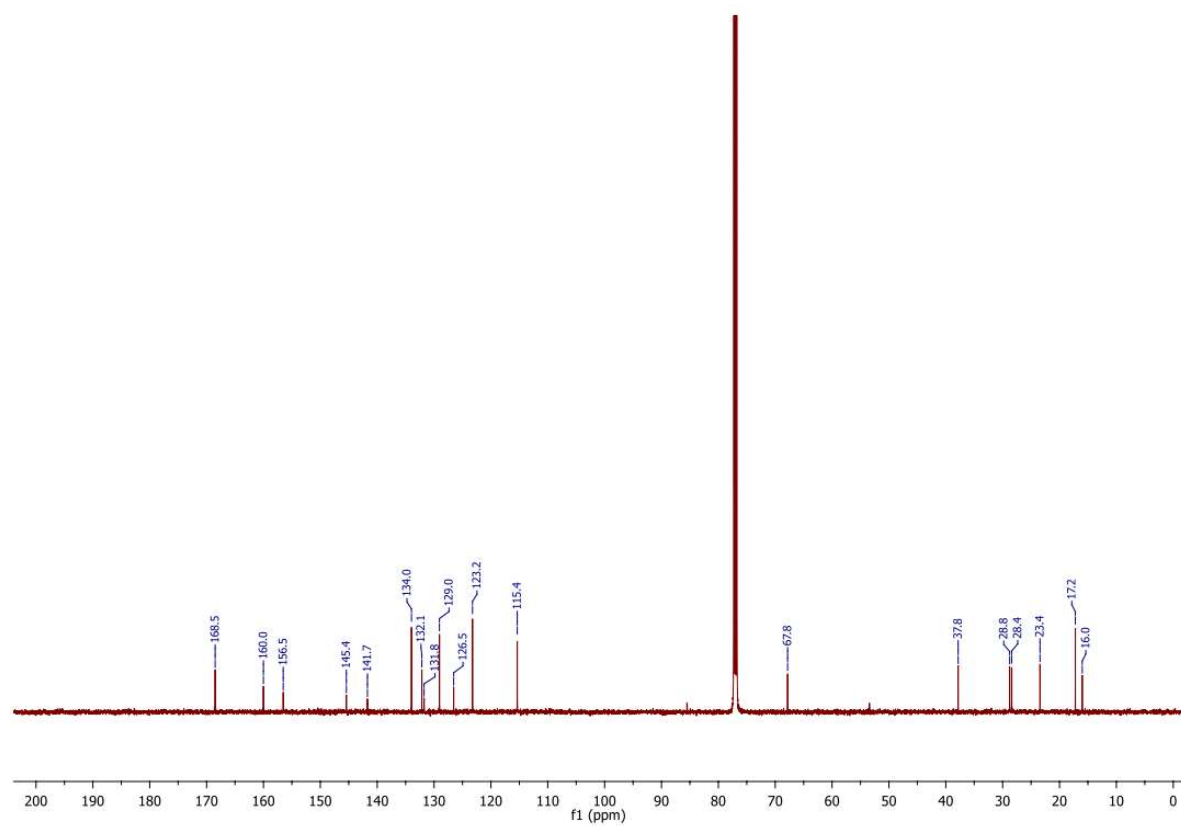


Fig. S4. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

2,6-Diiodo-1,3,5,7-tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**3a**)



¹H NMR spectrum of **3a** (500 MHz, CDCl₃). The symbol * and ~ indicate residual peaks of chloroform and dichloromethane, respectively.



¹³C NMR spectrum of **3a** (126 MHz, CDCl₃).

Table S5. ^1H and ^{13}C NMR data obtained for **3a** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.44	s	2.64	17.2	131.8, 145.4, 156.5
1.62-1.57	m	1.84-1.76, 1.93-1.86	23.4	28.4, 28.8, 37.8, 67.8
1.84-1.76	m	1.62-1.57, 3.75	28.4	23.4, 28.8, 37.8
1.93-1.86	m	1.62-1.57, 4.02	28.8	23.4, 28.4, 67.8
2.64	s	1.44	16.0	145.4, 156.5
3.75	t (7)	1.84-1.76	37.8	23.4, 28.4, 168.5
4.02	t (6)	1.93-1.86	67.8	23.4, 28.8, 160.0
7.00	d (9)	7.11	115.4	126.5, 160.0
7.11	d (9)	7.00	129.0	141.7, 160.0
7.73	dd (3, 5)	7.86	134.0	123.2, 132.1
7.86	dd (3, 5)	7.73	123.2	132.1, 134.0, 168.5
δ_{C} [ppm] from ^{13}C NMR: 168.5, 160.0, 156.5, 145.4, 141.7, 134.0, 132.1, 131.8, 129.0, 126.5, 123.2, 115.4, 67.8, 37.8, 28.8, 28.4, 23.4, 17.2, 16.0.				

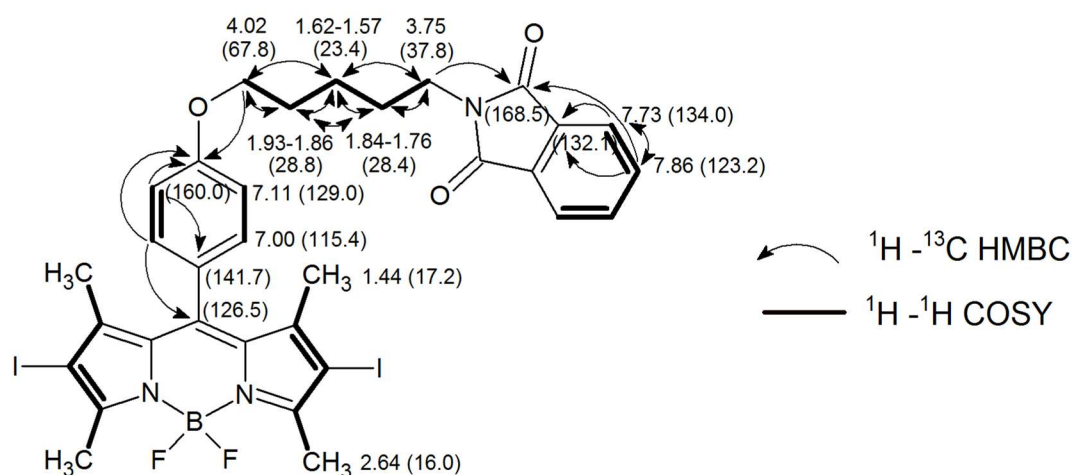
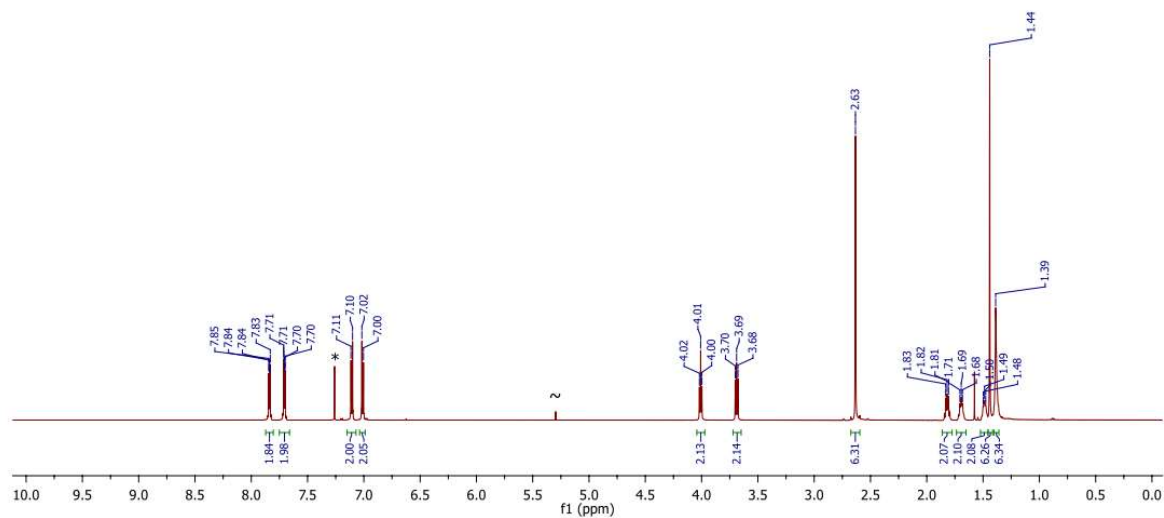
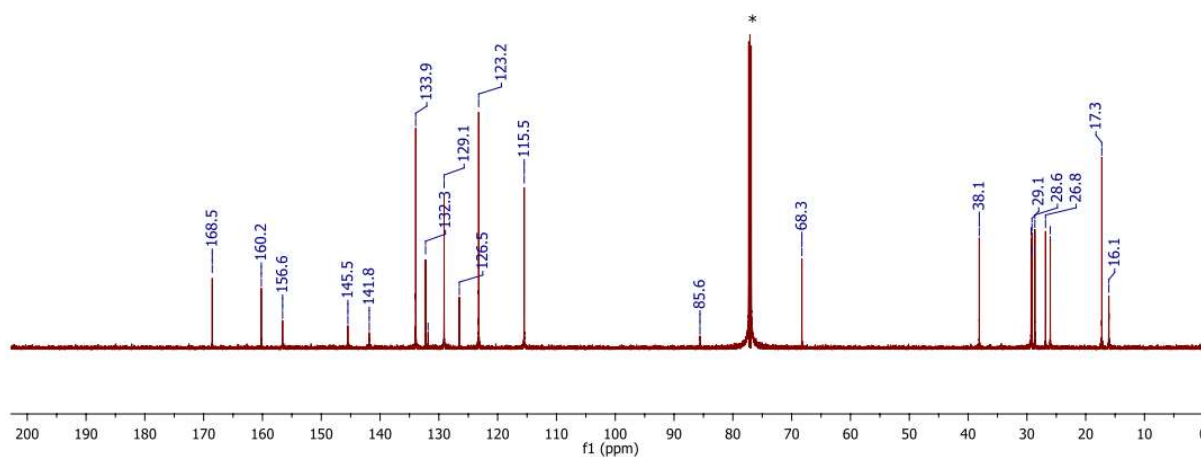


Fig. S5. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY. Arrows: ^1H - ^{13}C HMBC.

2,6-Diiodo-1,3,5,7-tetramethyl-8-{4-[8-(phthalimidyl)octyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**3b**)



¹H NMR spectrum of **3b** (600 MHz, CDCl₃). The symbol * and ~ indicate residual peaks of chloroform and dichloromethane, respectively.



¹³C NMR spectrum of **3b** (151 MHz, CDCl₃). The symbol * indicates a chloroform residual peak.

Table S6. ^1H and ^{13}C NMR data obtained for **3b** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.39	s	1.72-1.66	26.8, 29.2/29.3	26.0, 28.6, 29.1, 38.1
1.44	s	2.63	17.3	16.1, 85.6, 131.8, 141.8, 145.5 156.6
1.52-1.44	m	1.84-1.79	26.0	26.8, 29.1, 68.3
1.72-1.66	m	1.39, 3.69	28.6	26.8, 29.2/29.3, 38.1
1.84-1.79	m	1.52-1.44, 4.01	29.1	26.0, 68.3
2.63	s	1.44	16.1	17.3, 85.6, 131.8 145.5, 156.5
3.69	t (7)	1.72-1.66	38.1	26.8, 28.6, 168.5
4.01	t (7)	1.84-1.79	68.3	26.0, 29.1, 160.2
7.01	d (9)	7.11	115.5	126.5, 129.1, 160.2
7.11	d (9)	7.01	129.1	115.5, 141.8, 160.2
7.71	dd (3, 5)	7.84	133.9	123.2, 132.3, 168.5
7.84	dd (3, 5)	7.71	123.2	132.3, 133.9, 168.5
δ_{C} [ppm] from ^{13}C NMR: 168.5, 160.2, 156.6, 145.5, 141.8, 133.9, 132.3, 131.8, 129.1, 126.5, 123.2, 115.5, 85.6, 68.3, 38.1, 29.3, 29.2, 29.1, 28.6, 26.8, 26.0, 17.3, 16.1.				

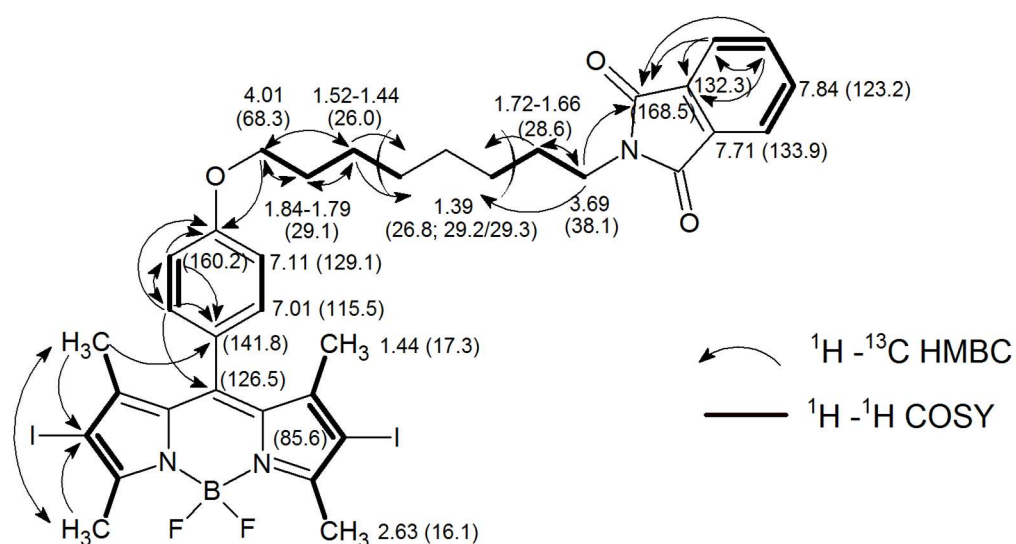
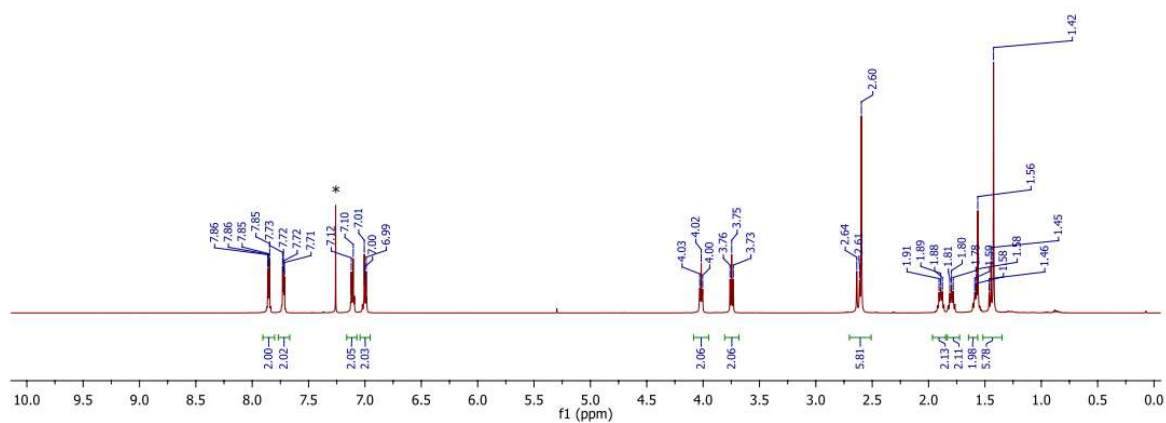
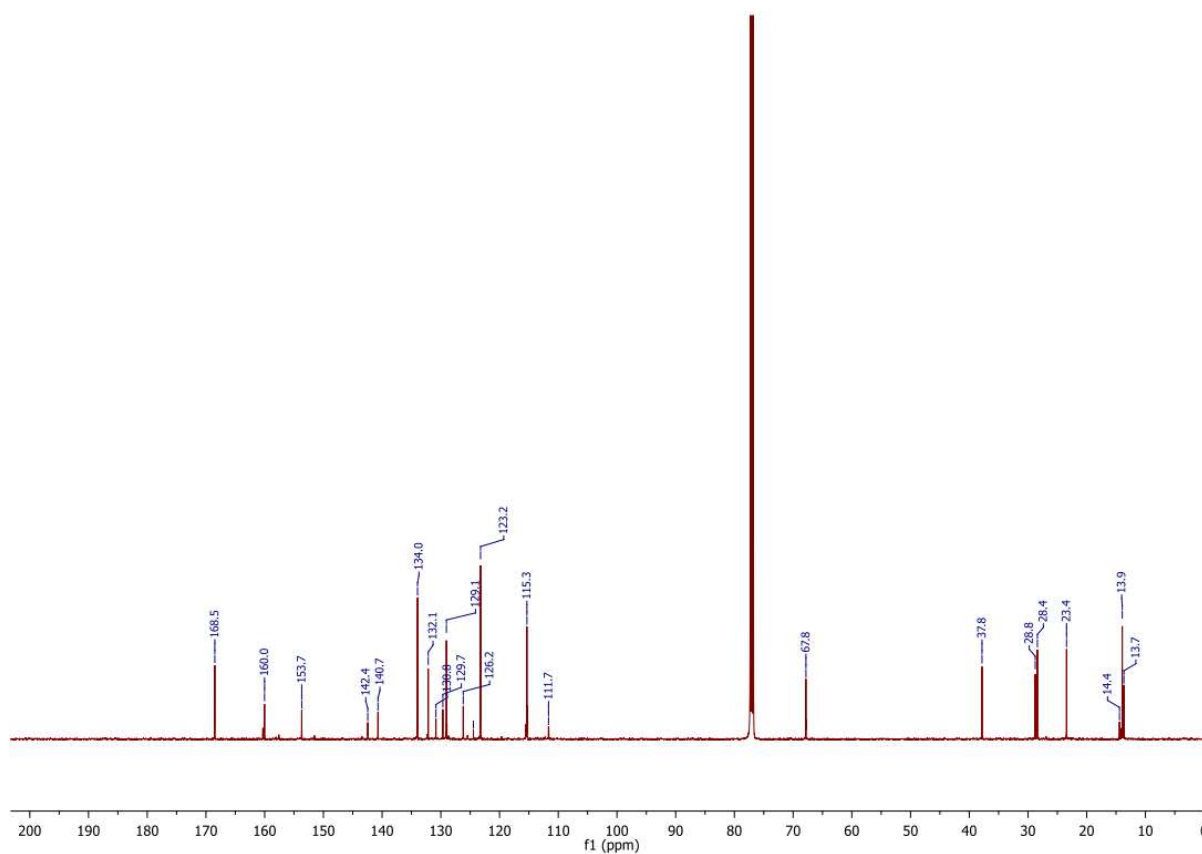


Fig. S6. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

2,6-Dibromo-1,3,5,7-tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**4a**)



¹H NMR spectrum of **4a** (500 MHz, CDCl₃). The symbol * indicates a chloroform residual peak.



¹³C NMR spectrum of **4a** (126 MHz, CDCl₃).

Table S7. ^1H and ^{13}C NMR data obtained for **4a** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.47-1.41	m	2.66-2.56	13.9	13.7, 111.7, 130.8, 140.7, 153.7
1.62-1.56	m	1.83-1.76, 1.93-1.86,	23.4	28.4, 37.8, 67.8
1.83-1.76	m	1.62-1.56, 3.75	28.4	23.4, 28.8, 37.8
1.93-1.86	m	1.62-1.56, 4.02	28.8	23.4, 28.4, 67.8
2.66-2.56	m	1.47-1.41	13.7	13.9, 111.7, 140.7, 142.4, 153.7
3.75	t (7)	1.86-1.73	37.8	23.4, 28.4, 168.5
4.02	t (6)	1.93-1.86	67.8	23.4, 28.8, 160.0
7.00	d (9)	7.11	115.3	124.4, 126.2, 160.0
7.11	d (9)	7.00	129.1	142.4, 160.0
7.72	dd (3, 5)	7.85	134.0	123.2, 132.1, 168.5
7.85	dd (3, 5)	7.72	123.2	132.1, 134.0, 168.5
δ_{C} [ppm] from ^{13}C NMR (126 MHz, CDCl_3) δ 168.5, 160.0, 153.7, 142.4, 140.7, 134.0, 132.1, 130.8, 129.7, 129.1, 126.2, 124.4, 123.2, 115.3, 111.7, 67.8, 37.8, 28.8, 28.4, 23.4, 14.4, 13.9, 13.7				

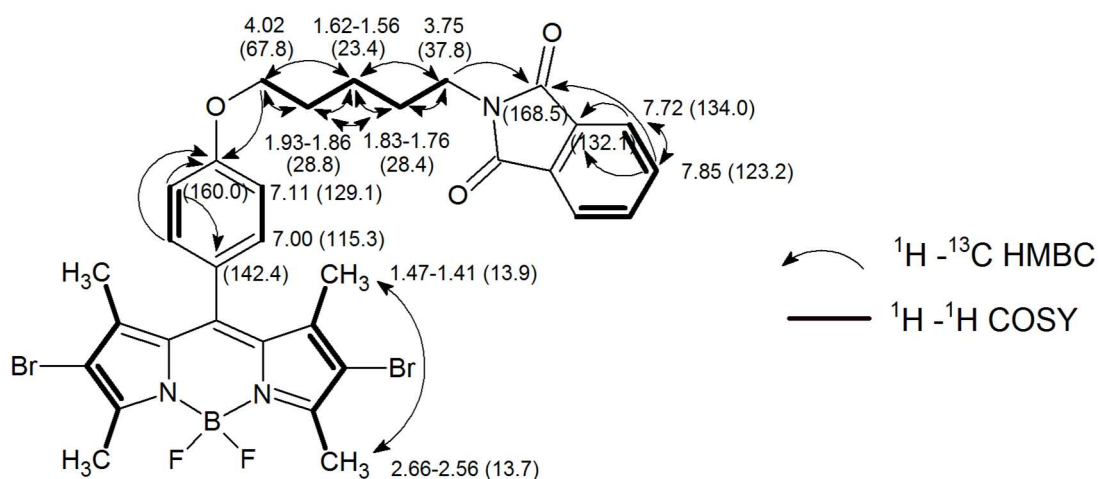
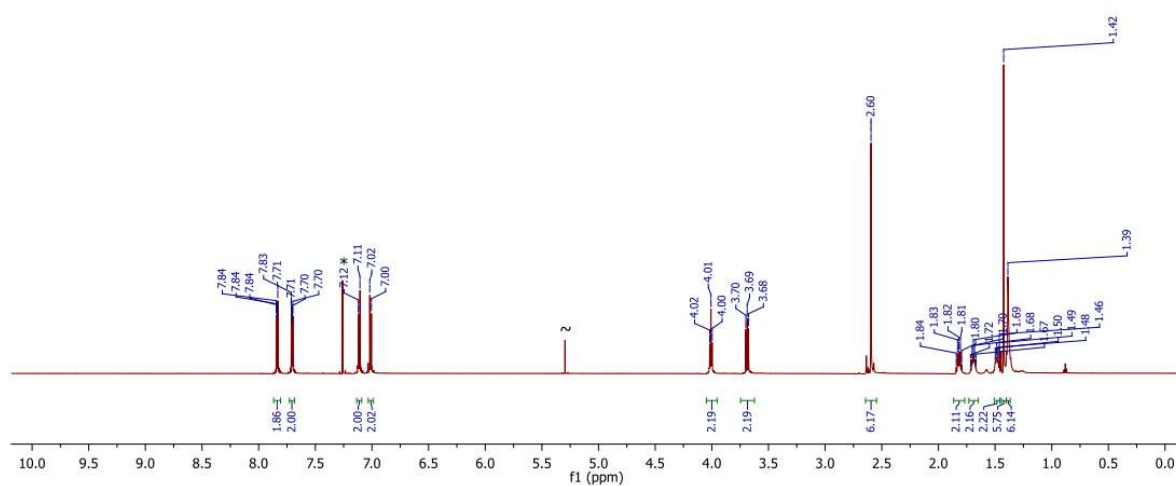
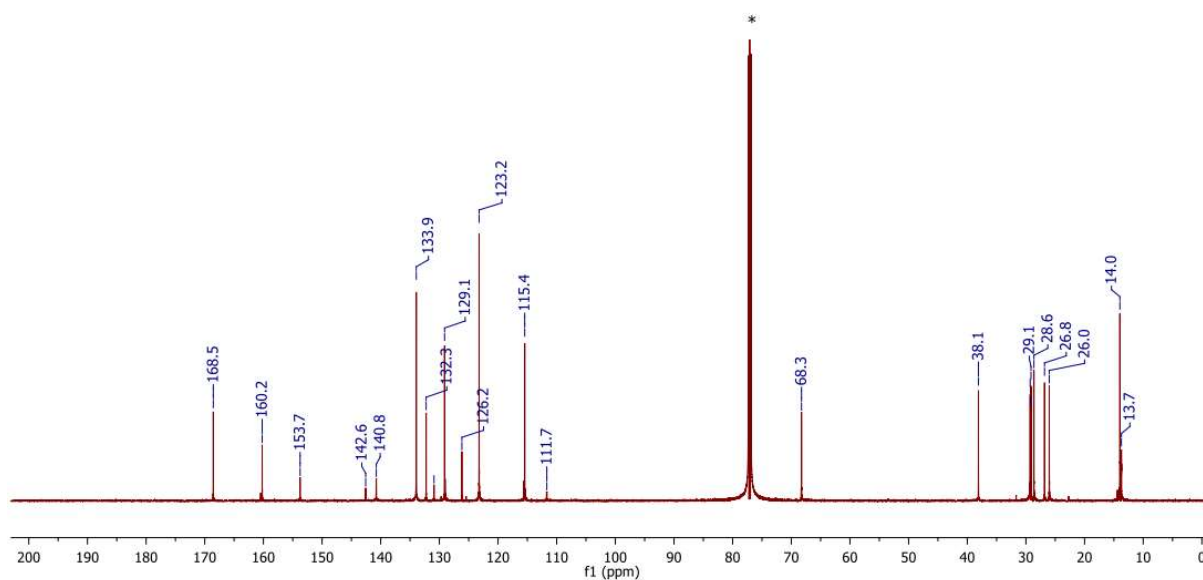


Fig. S7. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY. Arrows: ^1H - ^{13}C HMBC.

2,6-Dibromo-1,3,5,7-tetramethyl-8-{4-[8-(phthalimidyl)octyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**4b**)



¹H NMR spectrum of **4b** (600 MHz, CDCl₃). The symbol * and ~ indicate residual peaks of chloroform and dichloromethane, respectively.



¹³C NMR spectrum of **4b** (151 MHz, CDCl₃). The symbol * indicates a chloroform residual peak.

Table S8. ^1H and ^{13}C NMR data obtained for **4b** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.39	s	1.51-1.46, 1.72-1.66	26.8, 29.2/29.3	26.0, 28.6, 29.1, 38.1
1.42	s	2.60	14.0	111.7, 130.9, 140.8, 153.7
1.51-1.46	m	1.39, 1.85-1.79	26.0	26.8, 29.1, 29.2/29.3, 68.3
1.72-1.66	m	1.39, 3.69	28.6	26.8, 29.2/29.3, 38.1
1.85-1.79	m	1.51-1.46, 4.01	29.1	26.0, 29.2/29.3, 68.3
2.60	s	1.42	13.7	111.7, 130.9, 140.8, 153.7
3.69	t (7)	1.72-1.66	38.1	26.8, 28.6, 168.5
4.01	t (7)	1.85-1.79	68.3	26.0, 29.1, 160.2
7.01	d (9)	7.11	115.4	126.2, 129.1, 142.6, 160.2
7.11	d (9)	7.01	129.1	115.4, 142.6, 160.2
7.70	dd (3, 5)	7.84	133.9	123.2, 132.3, 133.9
7.84	dd (3, 5)	7.70	123.2	132.3, 133.9, 168.5
δ_{C} [ppm] from ^{13}C NMR: 168.5; 160.2; 153.7; 142.6; 140.8; 133.9; 132.3; 130.9; 129.1; 126.2; 123.2; 115.4; 111.7; 68.3; 38.1; 29.3; 29.2; 29.1; 28.6; 26.8; 26.0; 14.0; 13.7.				

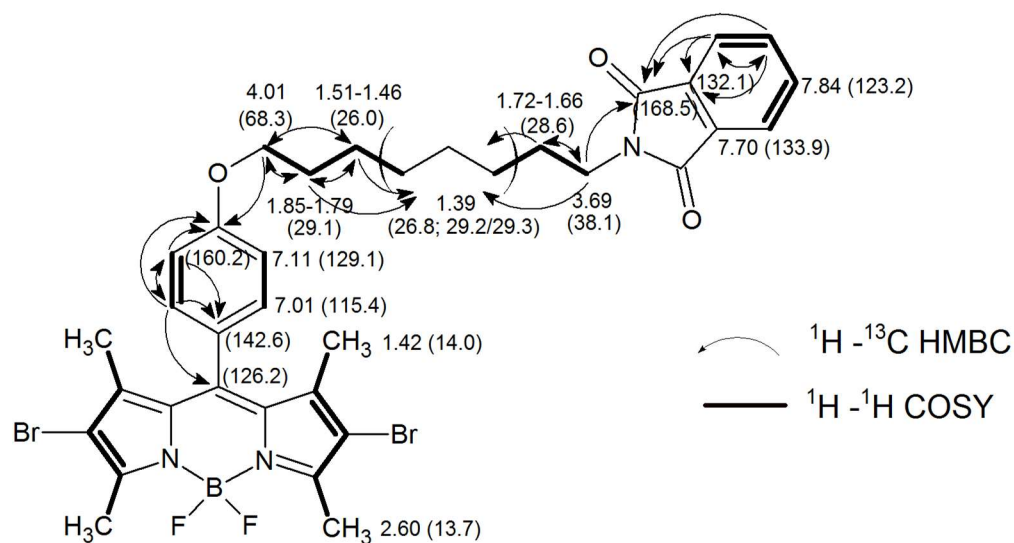
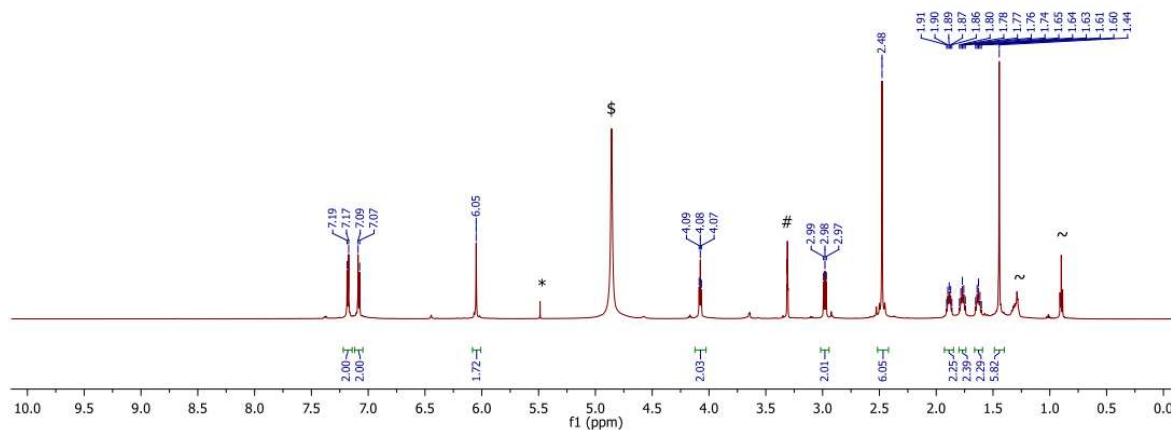
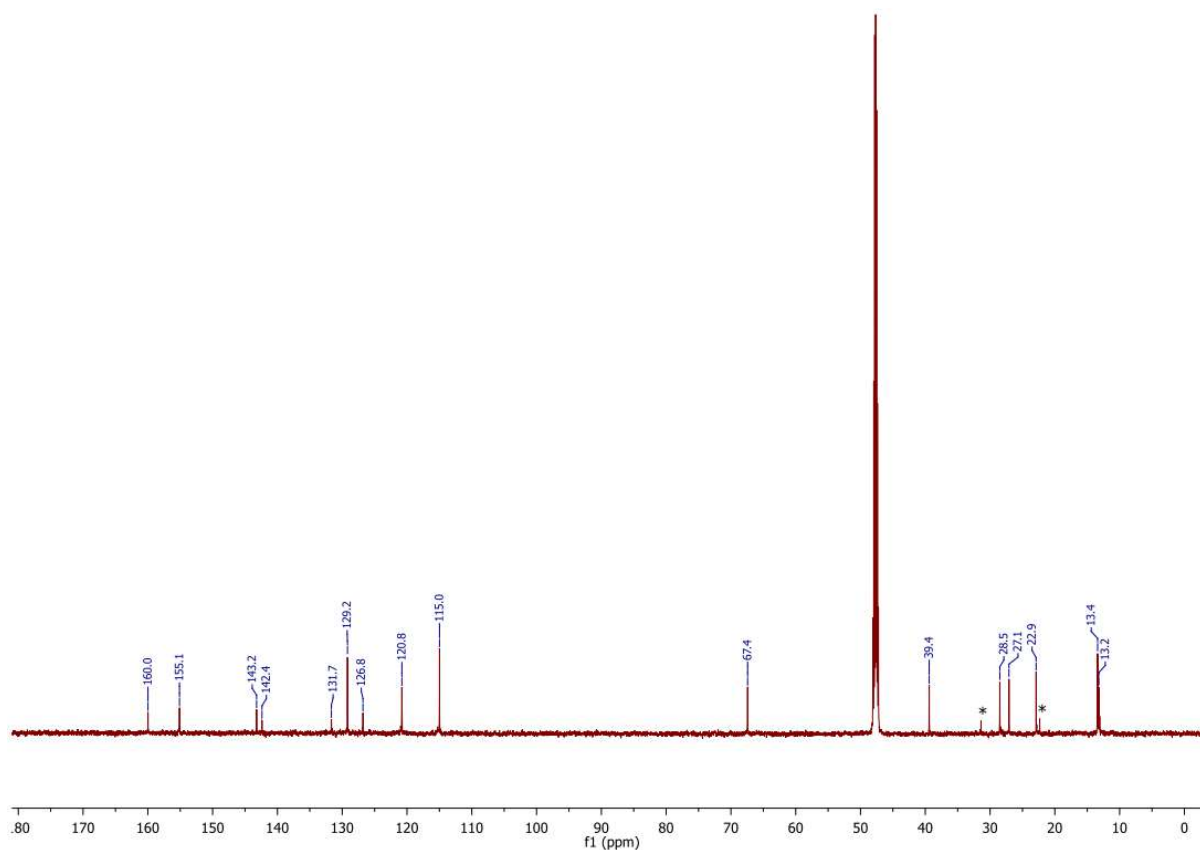


Fig. S8. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY, Arrows: ^1H - ^{13}C HMBC.

1,3,5,7-Tetramethyl-8-[4-(5-aminopentyloxy)phenyl]-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**5a**)



^1H NMR spectrum of **5a** (600 MHz, CD_3OD). The symbols *, \$, # and ~ indicate residual peaks of dichloromethane, water, methanol, and hexane, respectively.



^{13}C NMR spectrum of **5a** (151 MHz, MeOD). The symbol * indicates hexane residual peaks.

Table S9. ^1H and ^{13}C NMR data obtained for **5a** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^1H COSY δ_{H} [ppm]	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.44	s	2.48, 6.05	13.4	120.8, 131.7, 143.2, 155.1
1.66-1.60	m	1.80-1.74, 1.91-1.86	22.9	28.5, 39.4, 67.4
1.80-1.74	m	1.66-1.60, 3.01-2.95	27.1	22.9, 28.5, 39.4
1.91-1.86	m	1.66-1.60, 4.08	28.5	22.9, 27.1, 67.4
2.48	s	1.44, 6.05	13.2	120.8, 143.2, 155.1
3.01-2.95	m	1.80-1.74	39.4	22.9, 27.1
4.08	t (6)	1.91-1.86	67.4	22.9, 28.5, 160.0
6.05	s	1.44, 2.48	120.8	13.2, 13.4, 131.7, 143.2, 155.1
7.08	d (9)	7.18	115.0	126.8, 160.0
7.18	d (9)	7.08	129.2	142.4, 160.0
δ_{C} [ppm] from ^{13}C NMR: 160.0, 155.1, 143.2, 142.4, 131.7, 129.2, 126.8, 120.8, 115.0, 67.4, 39.4, 28.5, 27.1, 22.9, 13.4, 13.2.				

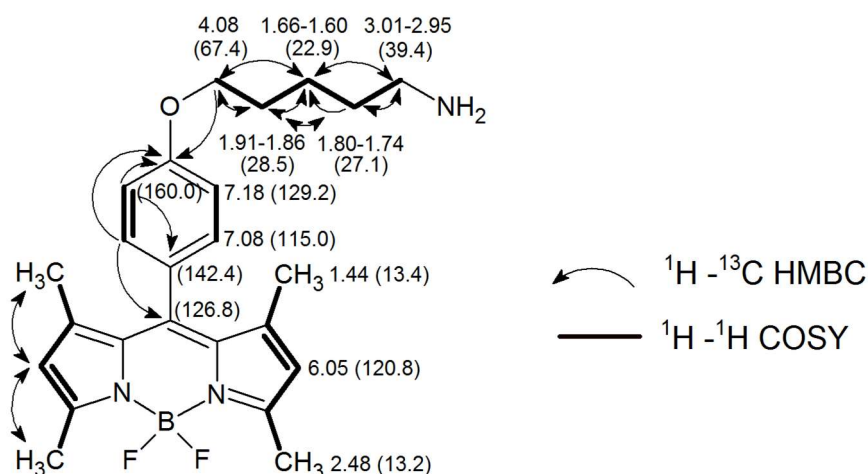
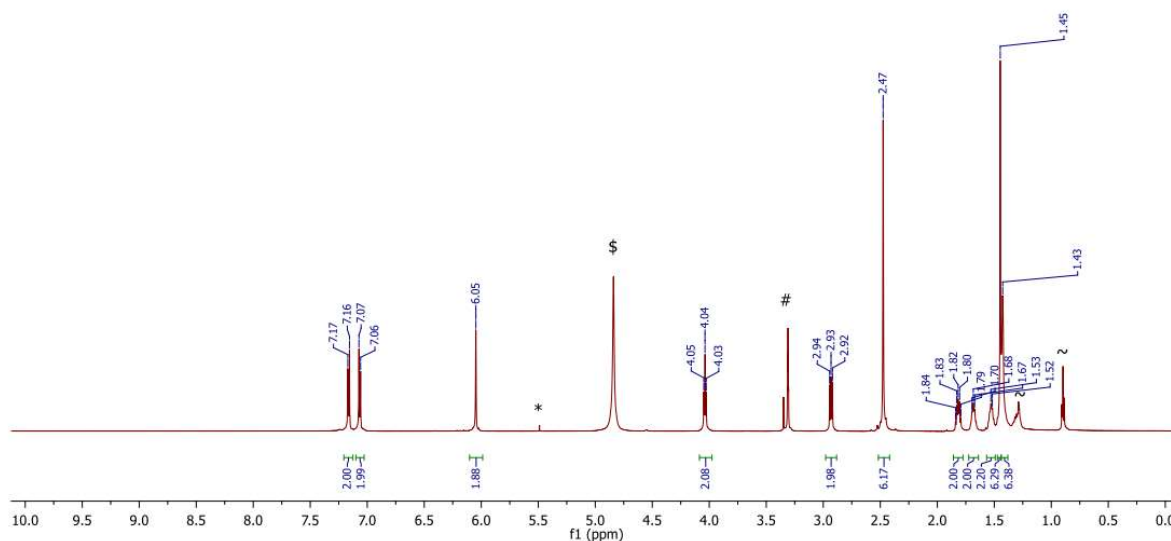
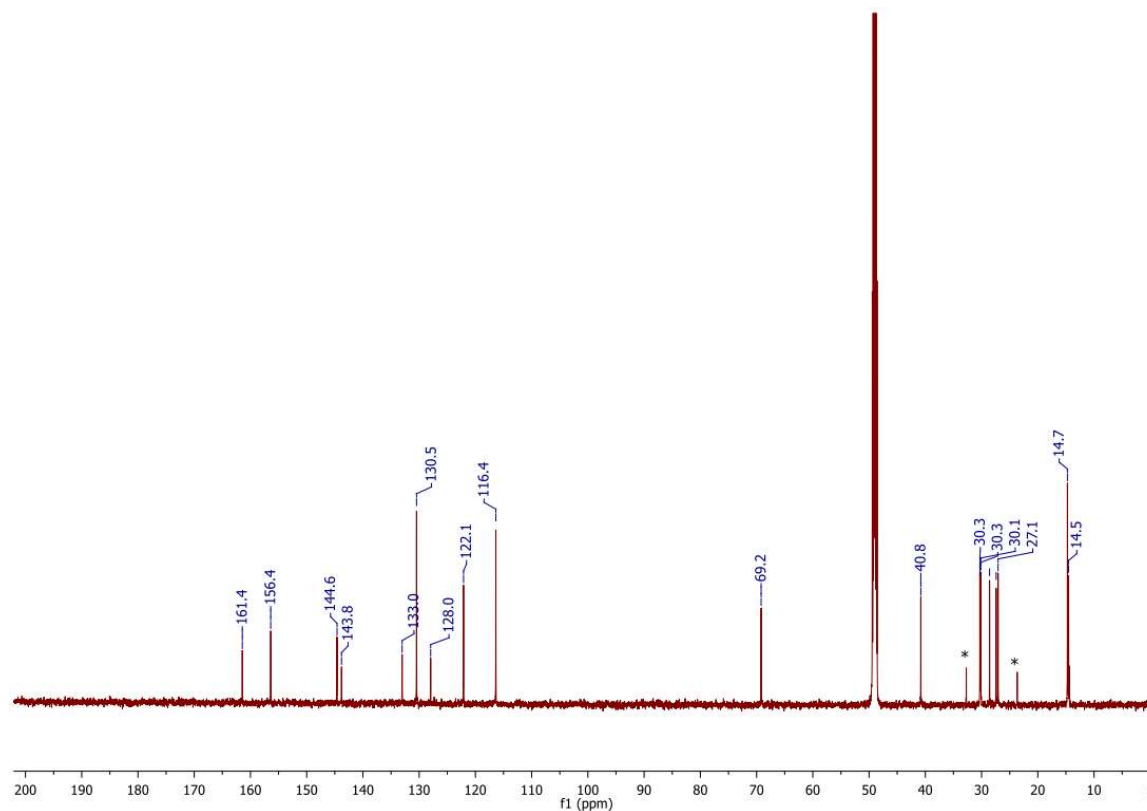


Fig. S9. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY. Arrows: ^1H - ^{13}C HMBC.

1,3,5,7-Tetramethyl-8-[4-(8-aminooctyloxy)phenyl]-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**5b**)



¹H NMR spectrum of **5b** (600 MHz, MeOD). The symbols *, \$, # and ~ indicate residual peaks of dichloromethane, water, methanol, and hexane, respectively.



¹³C NMR spectrum of **5b** (151 MHz, MeOD). The symbol * indicates hexane residual peaks.

Table S10. ^1H and ^{13}C NMR data obtained for **5b** including key correlations determined from ^1H - ^1H COSY, ^1H - ^{13}C HSQC and ^1H - ^{13}C HMBC spectra.

δ_{H} [ppm]	Multiplicity ($J_{\text{H-H}}$ w Hz)	^1H - ^{13}C HSQC δ_{C} [ppm]	^1H - ^{13}C HMBC δ_{C} [ppm]
1.43	s	27.4, 30.1	27.1, 28.6
1.45	s	14.7	122.1, 133.0, 143.8, 144.6, 156.4
1.56-1.49	m	27.1	30.1, 30.3
1.71-1.66	m	28.6	27.4, 40.8
1.85-1.78	m	30.3	27.1, 69.2
2.47	s	14.5	122.1, 133.0, 143.8, 144.6, 156.4
2.93	d (8)	40.8	27.4, 28.6
4.04	t (6)	69.2	27.1, 30.3, 161.4
6.05	s	122.1	14.5, 133.0, 143.8, 144.6, 156.5
7.06	d (9)	116.4	128.0, 130.5, 144.6, 161.4,
7.16	d (9)	130.5	116.4, 144.6, 161.4,
δ_{C} [ppm] from ^{13}C NMR: 161.4, 156.4, 144.6, 143.8, 133.0, 130.5, 128.0, 122.1, 116.4, 69.2, 40.8, 30.3, 30.1, 28.6, 27.4, 27.1, 14.7, 14.5			

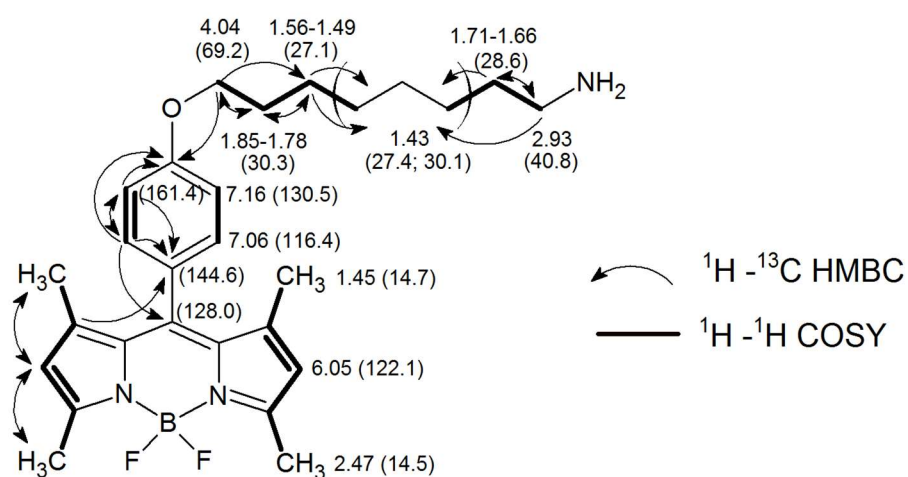


Fig.S10. ^1H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^1H - ^1H COSY. Arrows: ^1H - ^{13}C HMBC.

HRMS spectra

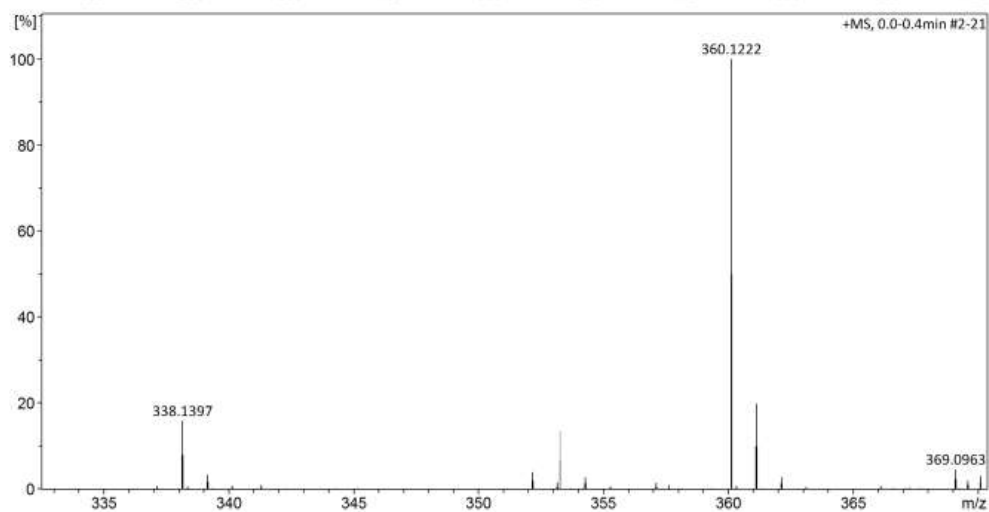
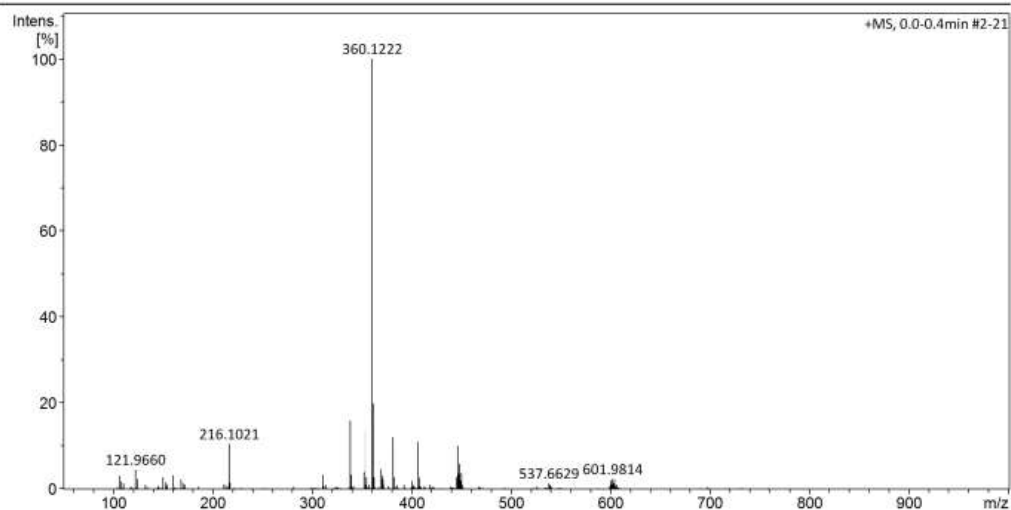
4-[5-(1,3-Dihydro-1,3-dioxo-2*H*-isoindol-2-yl)pentyl]oxy]benzaldehyde (**1a**)

Acquisition Parameter

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Scan End 1000 m/z

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Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.4 Bar
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Set APCI Heater 0 °C



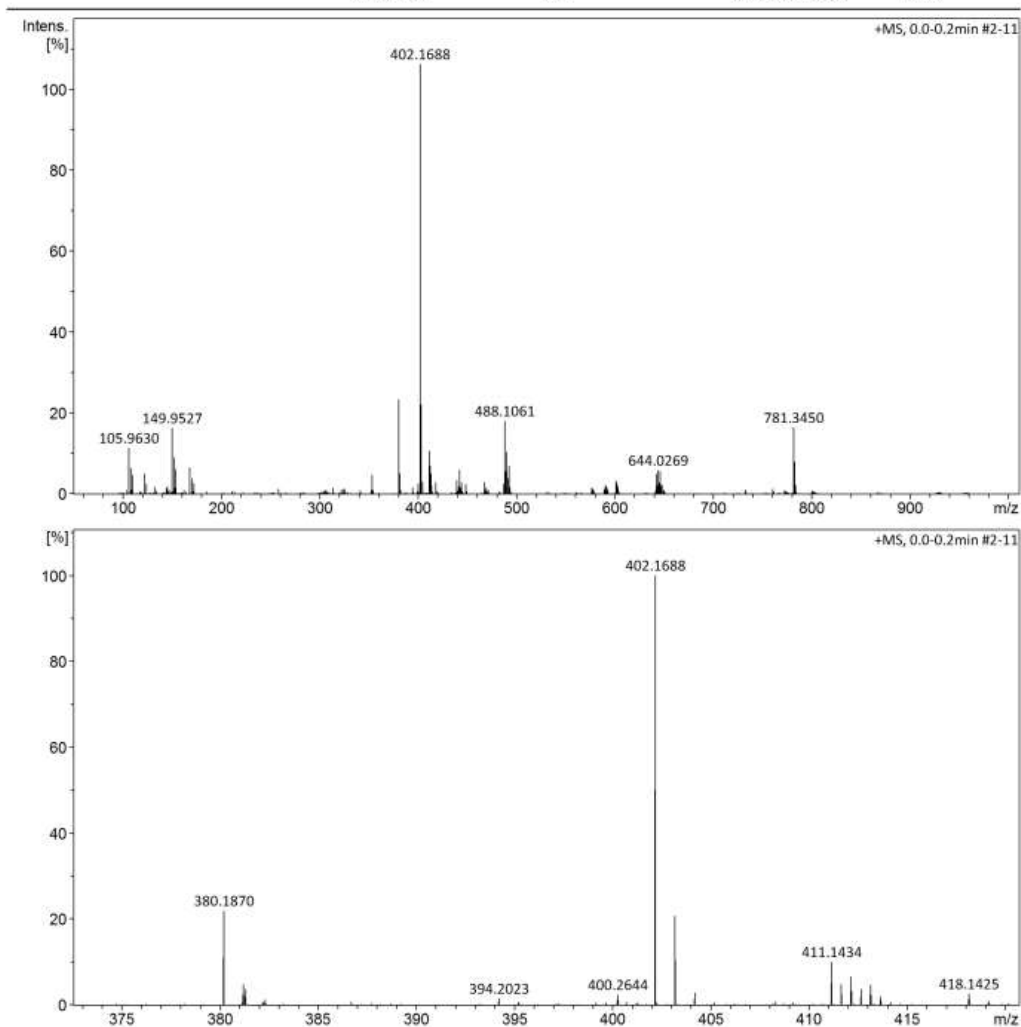
4-[8-(1,3-Dihydro-1,3-dioxo-2*H*-isoindol-2-yl)octyloxy]benzaldehyde (**1b**)

Acquisition Parameter

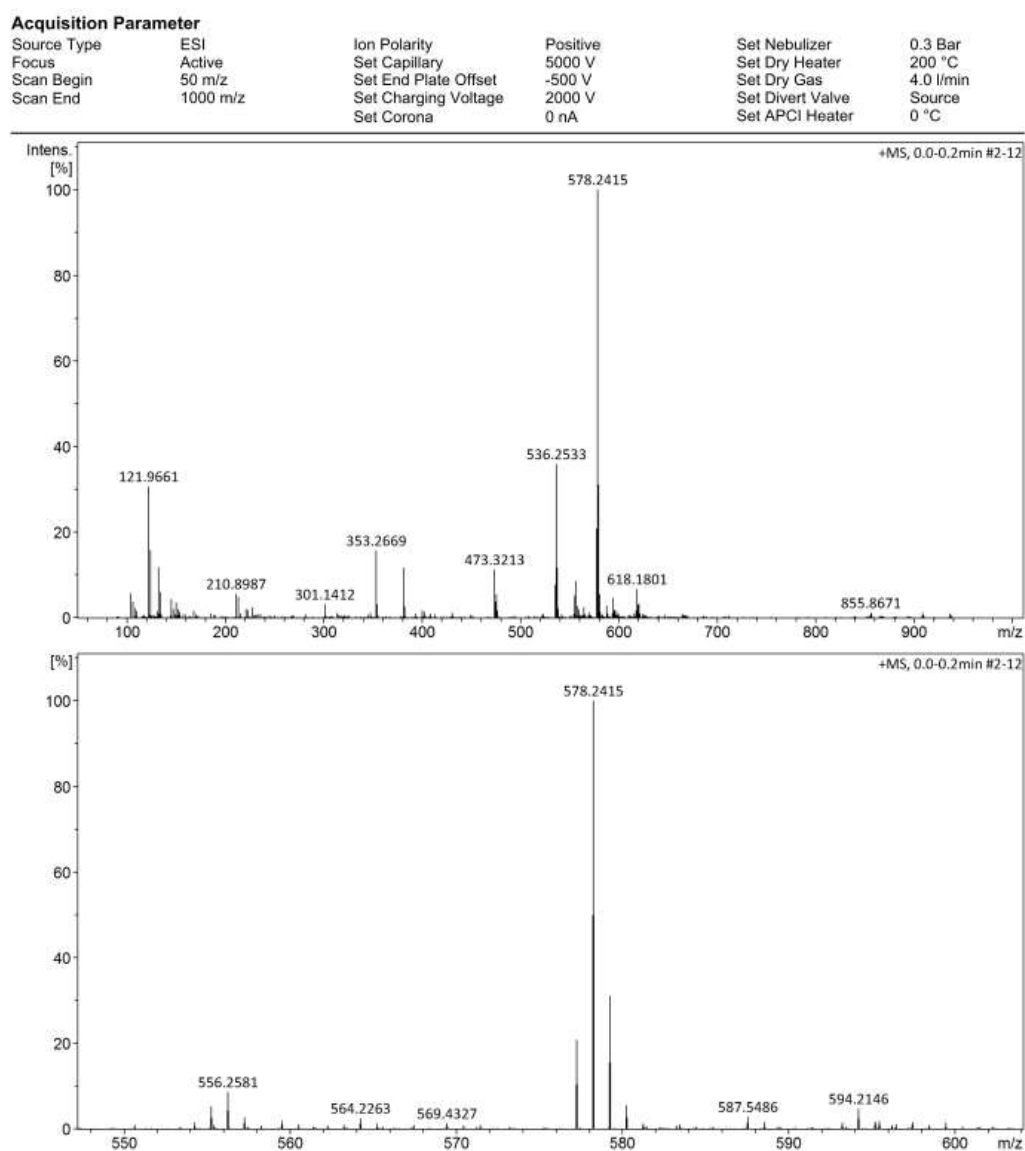
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Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Set APCI Heater 0 °C



1,3,5,7-Tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**2a**)



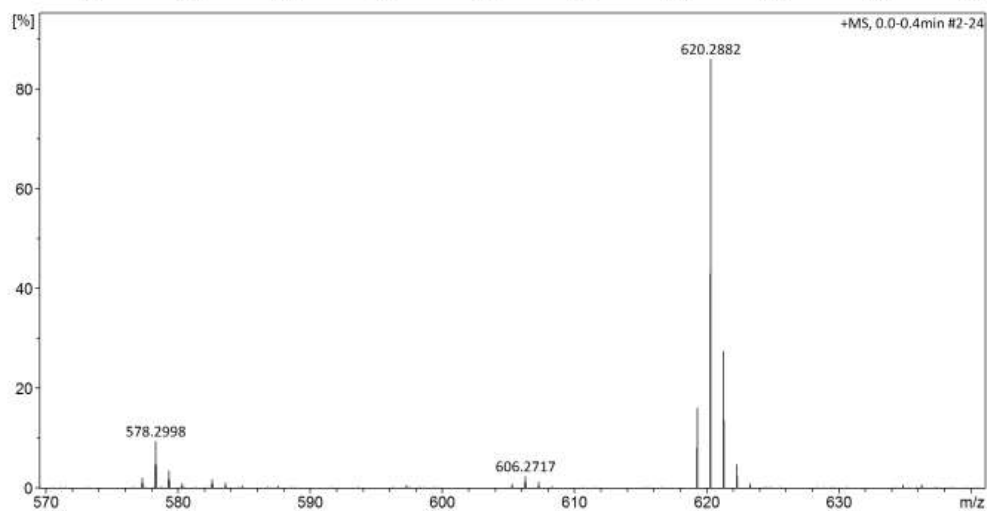
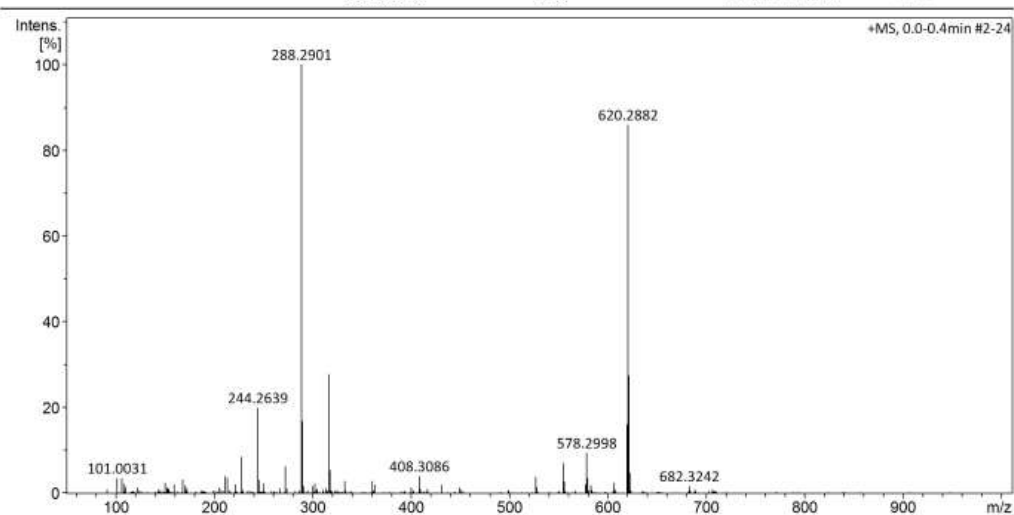
1,3,5,7-Tetramethyl-8-{4-[8-(phthalimidyl)octyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**2b**)

Acquisition Parameter

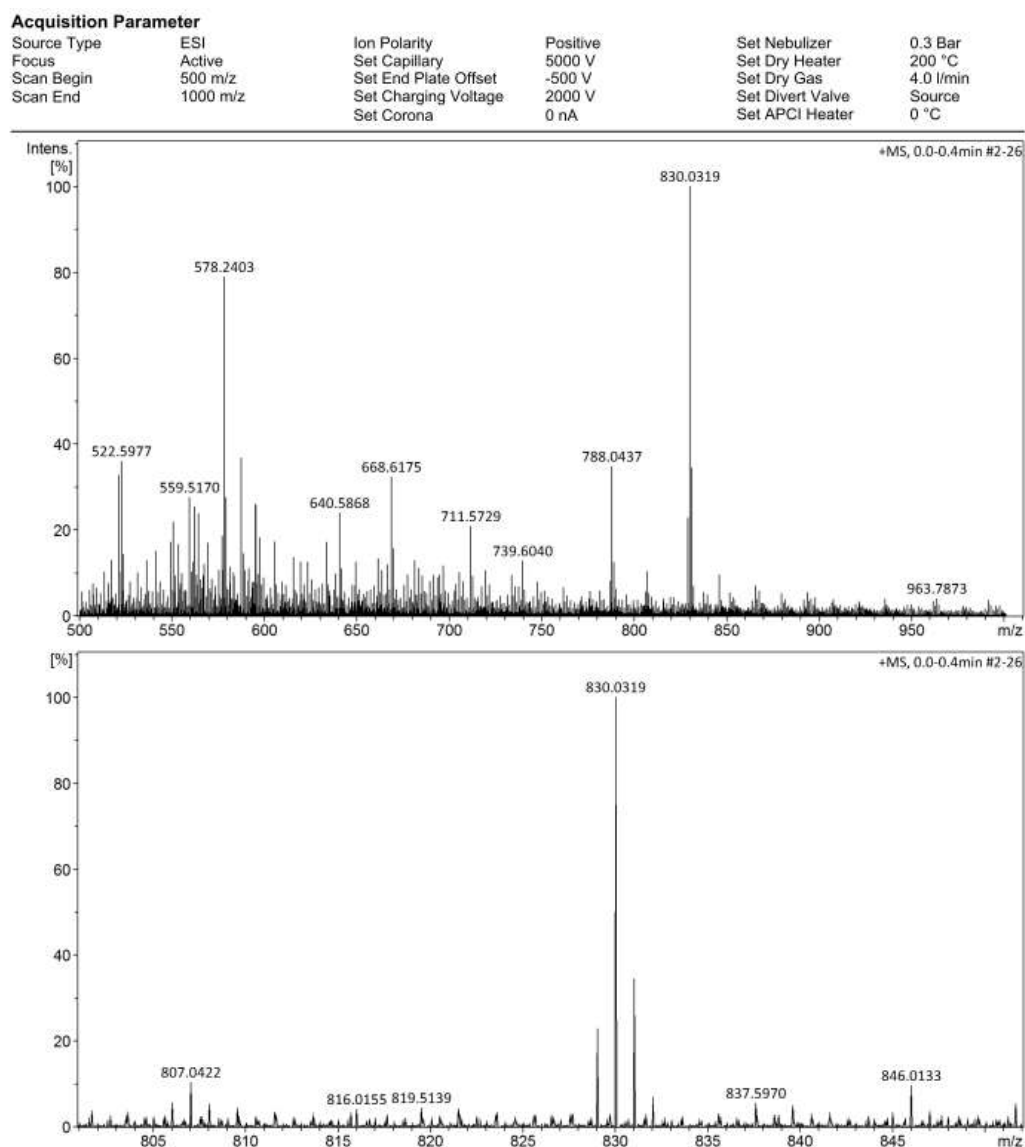
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Focus Active
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Ion Polarity Positive
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Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Set APCI Heater 0 °C



2,6-Diiodo-1,3,5,7-tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**3a**)



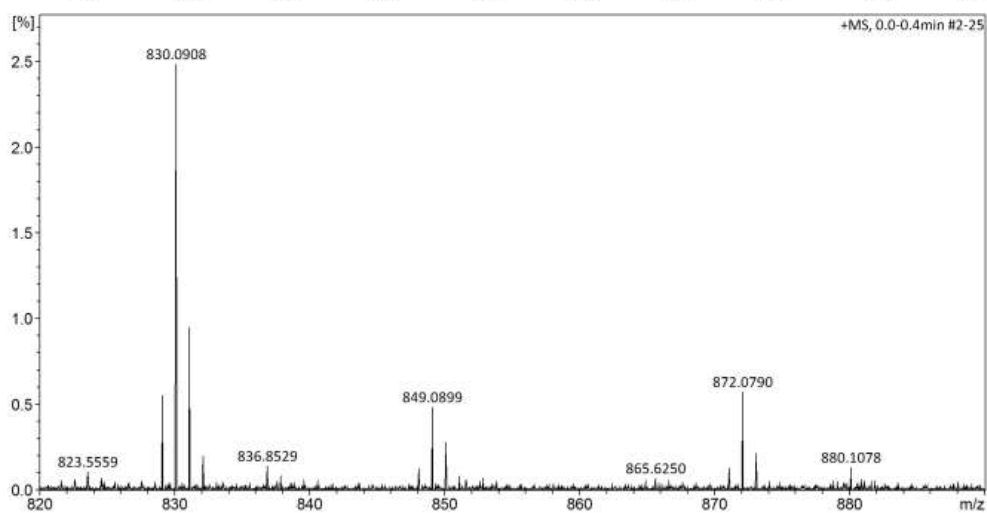
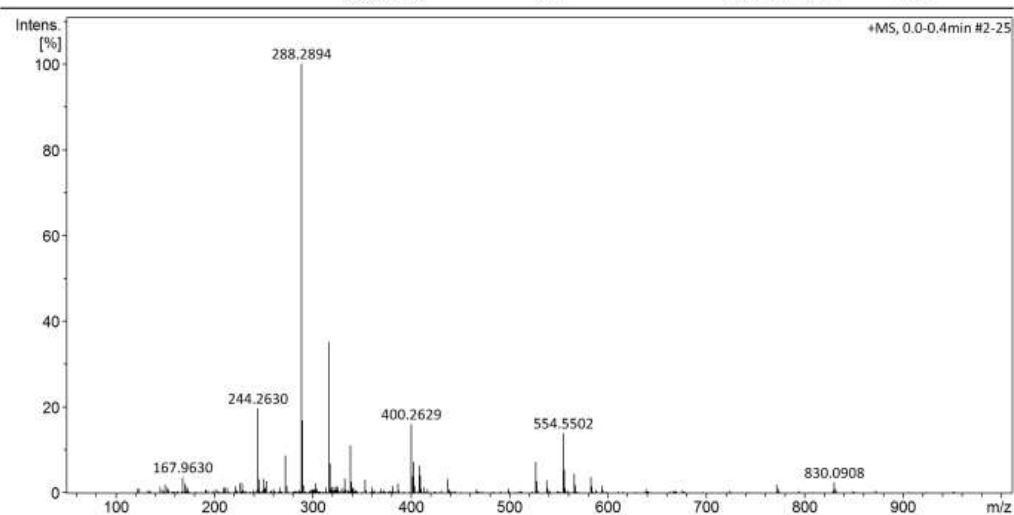
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Acquisition Parameter

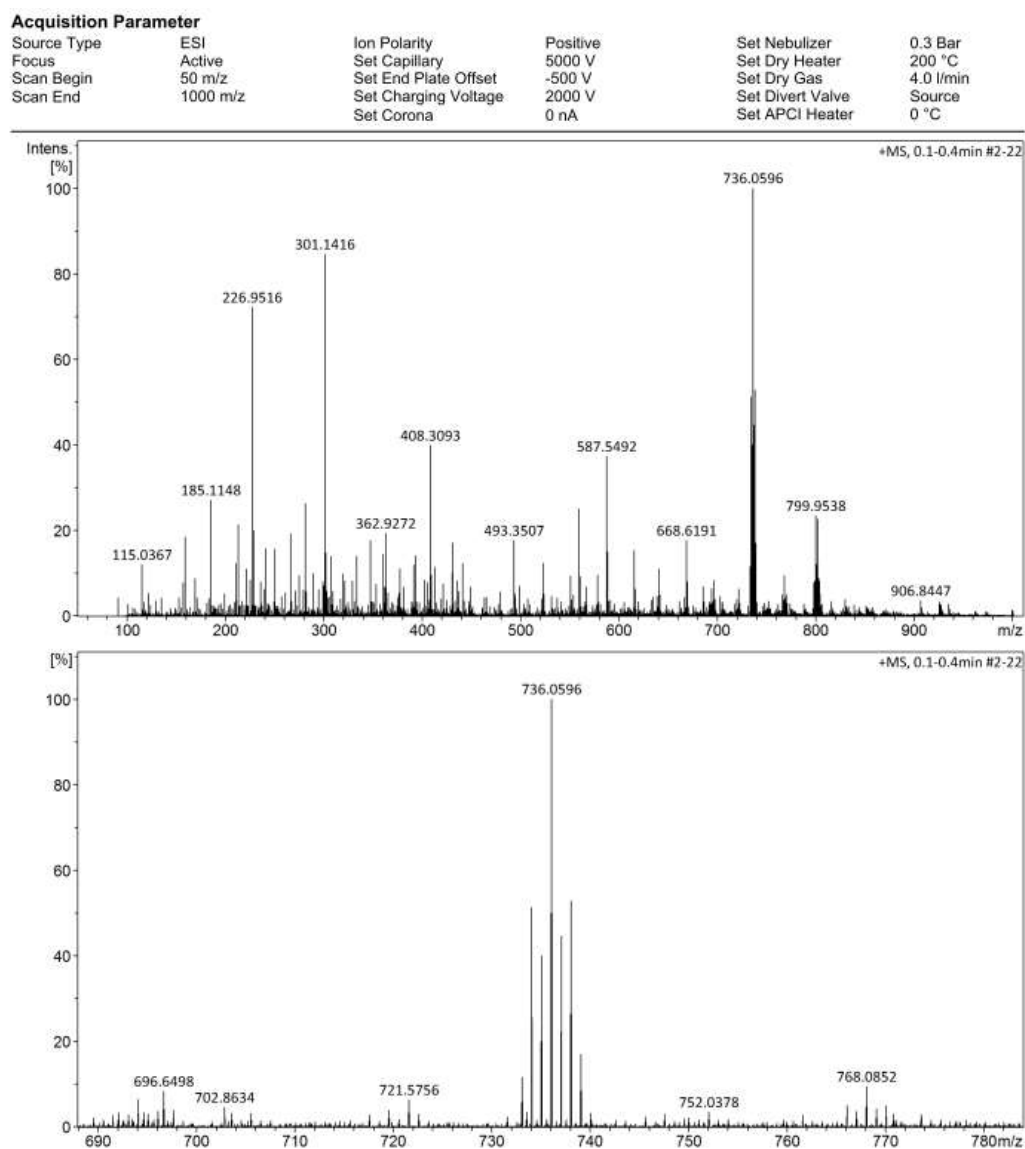
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Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Set APCI Heater 0 °C



2,6-Dibromo-1,3,5,7-tetramethyl-8-{4-[5-(phthalimidyl)pentyloxy]phenyl}-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**4a**)



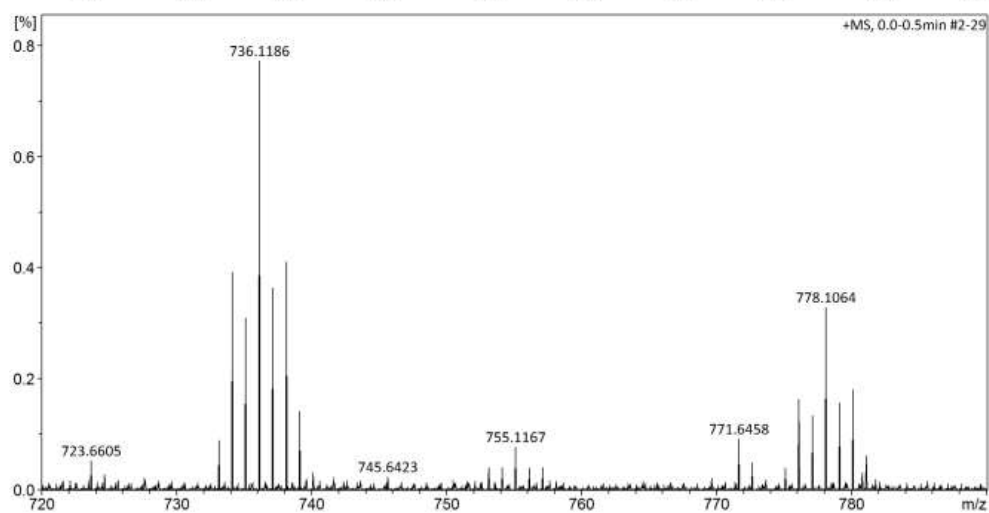
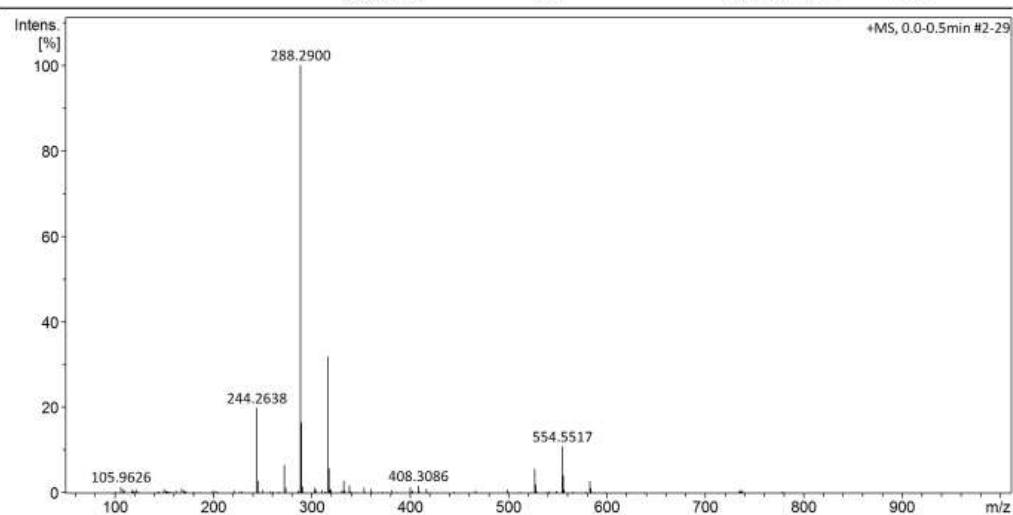
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Acquisition Parameter

Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 1000 m/z

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 200 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Set APCI Heater 0 °C



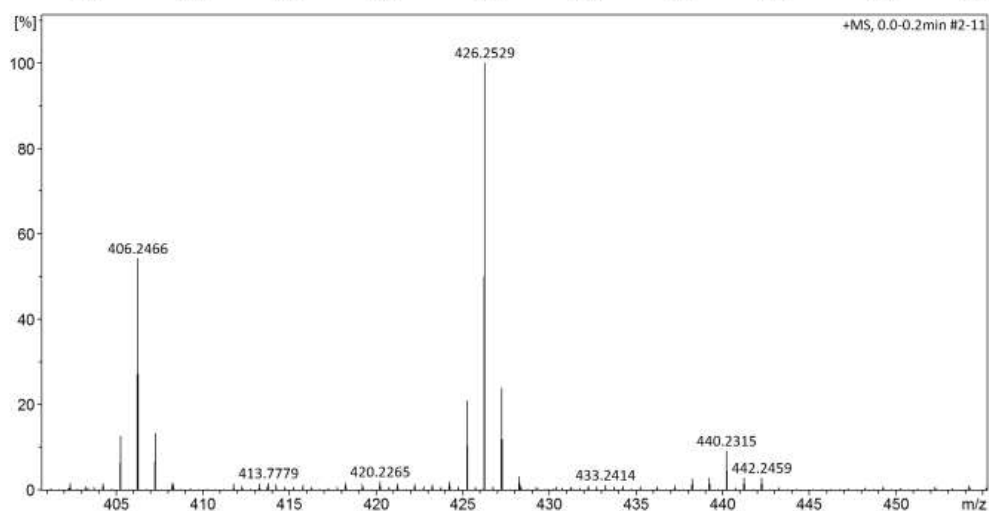
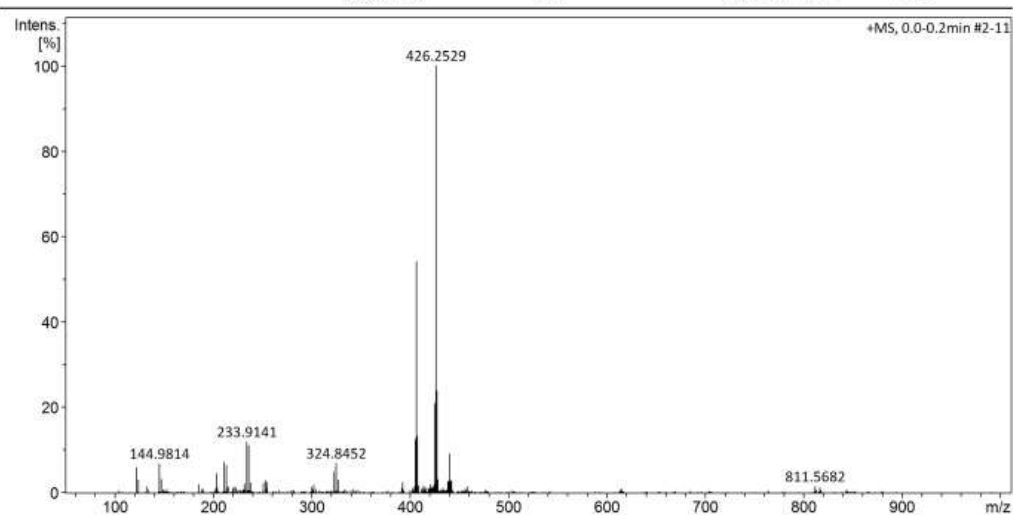
1,3,5,7-Tetramethyl-8-[4-(5-aminopentyloxy)phenyl]-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**5a**)

Acquisition Parameter

Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 1000 m/z

Ion Polarity Positive
Set Capillary 5000 V
Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 200 °C
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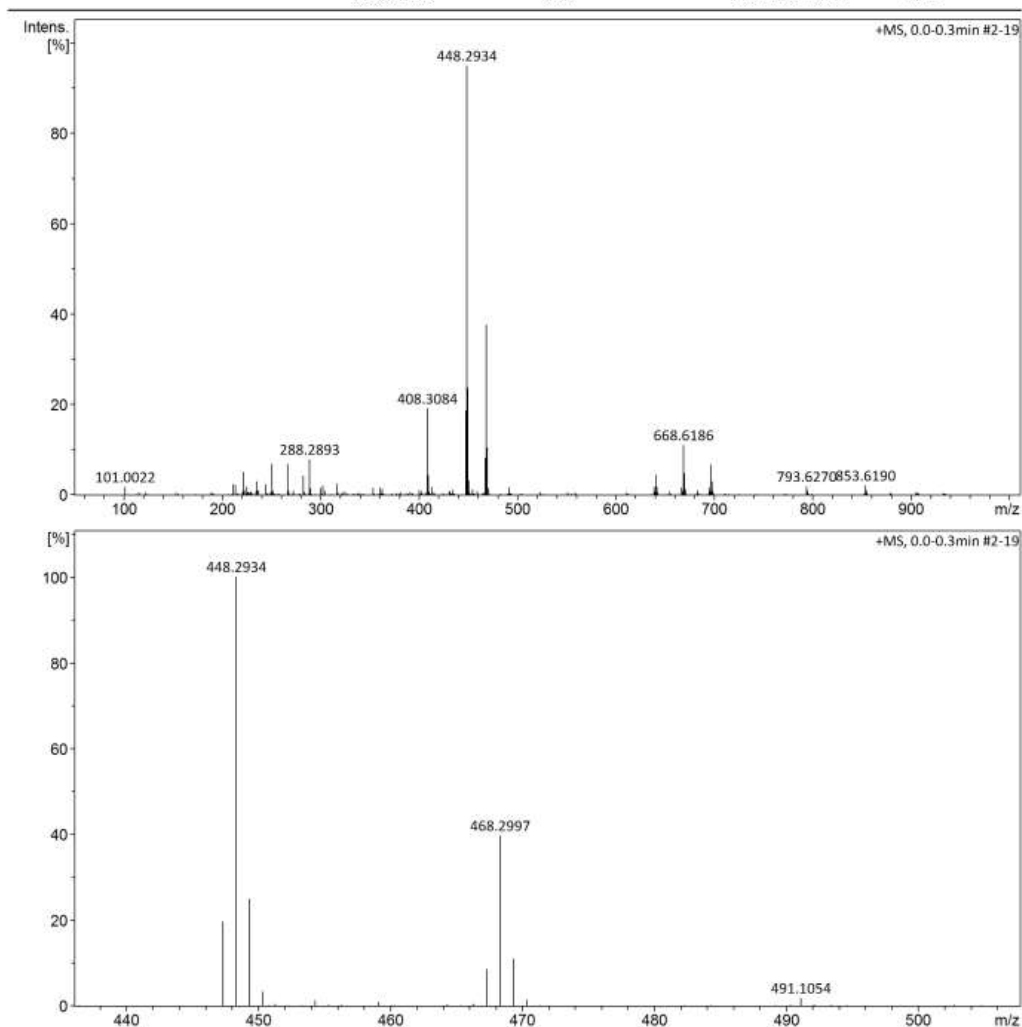
1,3,5,7-Tetramethyl-8-[4-(8-aminooctyloxy)phenyl]-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (**5b**)

Acquisition Parameter

Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 1000 m/z

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Charging Voltage 2000 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
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Set Dry Gas 4.0 l/min
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Absorption, emission, excitation spectra

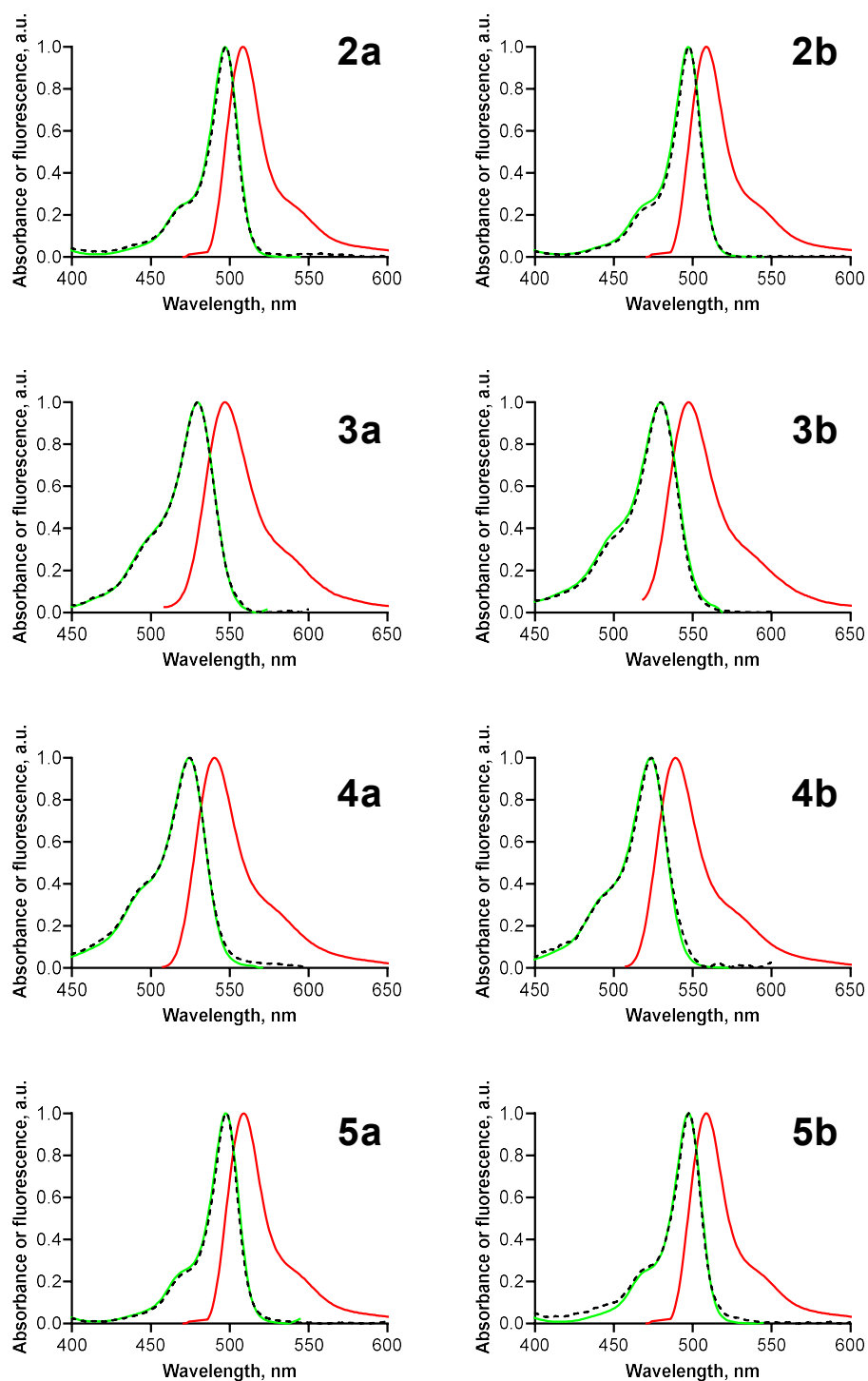


Fig. S11. Normalized absorption (black, dashed), emission (red), and excitation (green) spectra of **2a,b-5a,b** in MeOH ($c = 1 \mu\text{M}$).

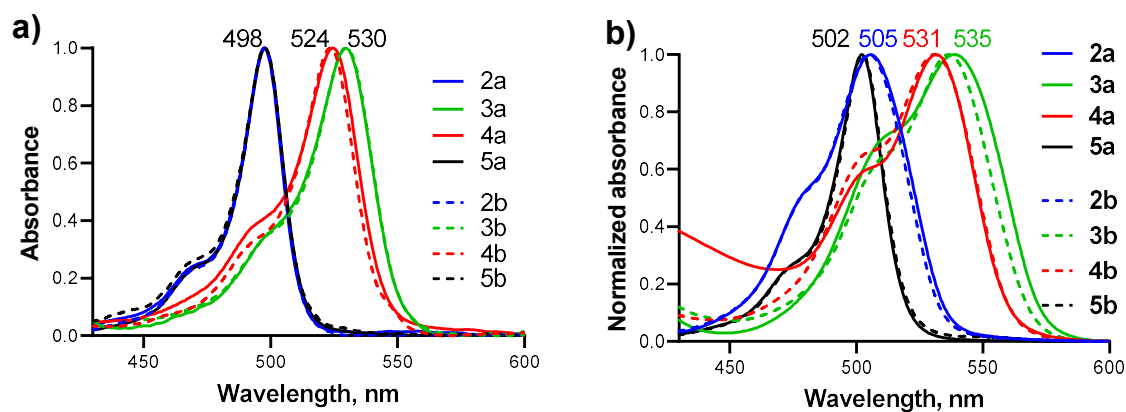


Fig. S12. Normalized absorption spectra of studied compounds in MeOH (a) and serum-containing cell culture medium (b).

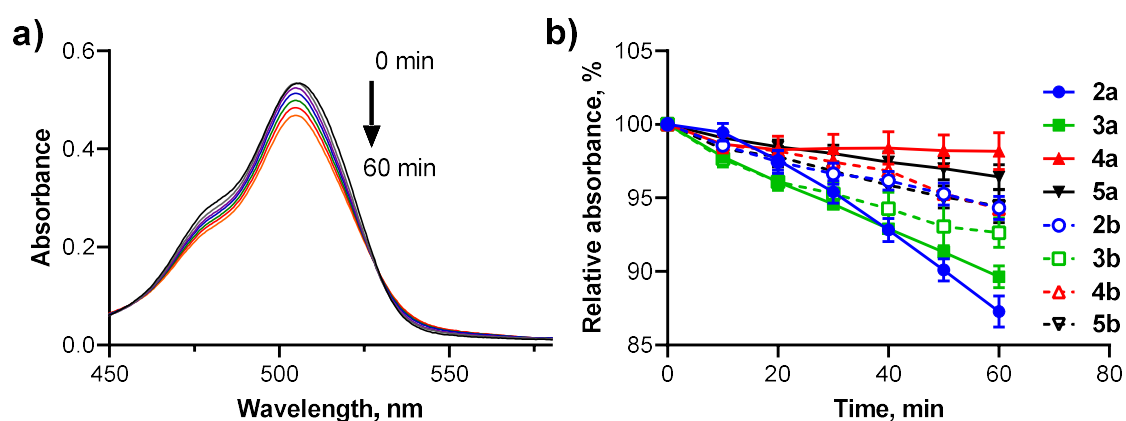


Fig. S13. a) Typical changes of absorption spectra of studied BODIPYs in time (example for 2a) during photobleaching experiment in serum-containing cell culture medium. b) Time-dependent changes in absorbance (relative to the non-irradiated sample) in absorption maximum of studied compounds (mean and standard deviation of three independent experiments are drawn).

Assessment of biological activity

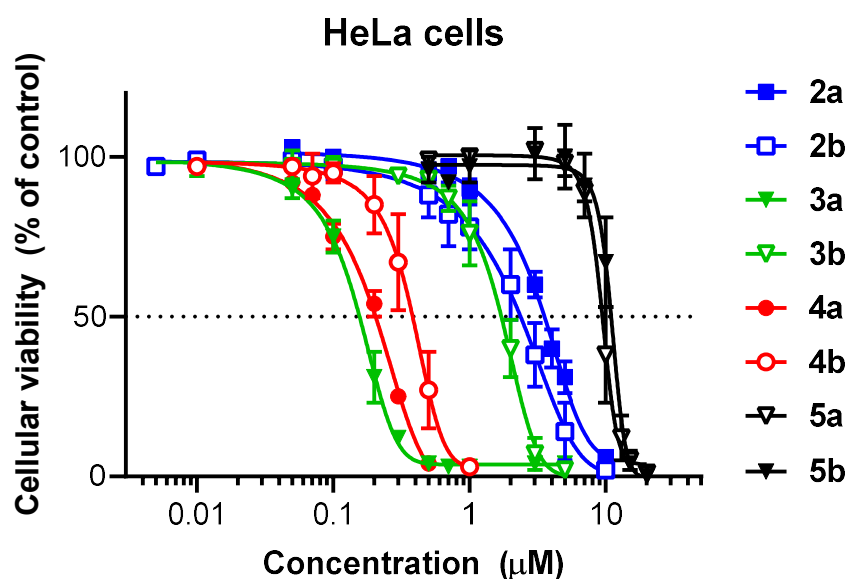


Figure S14. Photodynamic activity of studied compounds on HeLa cell line. At least four independent experiments each in triplicate were performed. Irradiation conditions: $\lambda > 455$ nm, 15.3 mW cm^{-2} , 15 min, 13.7 Jcm^{-2} .

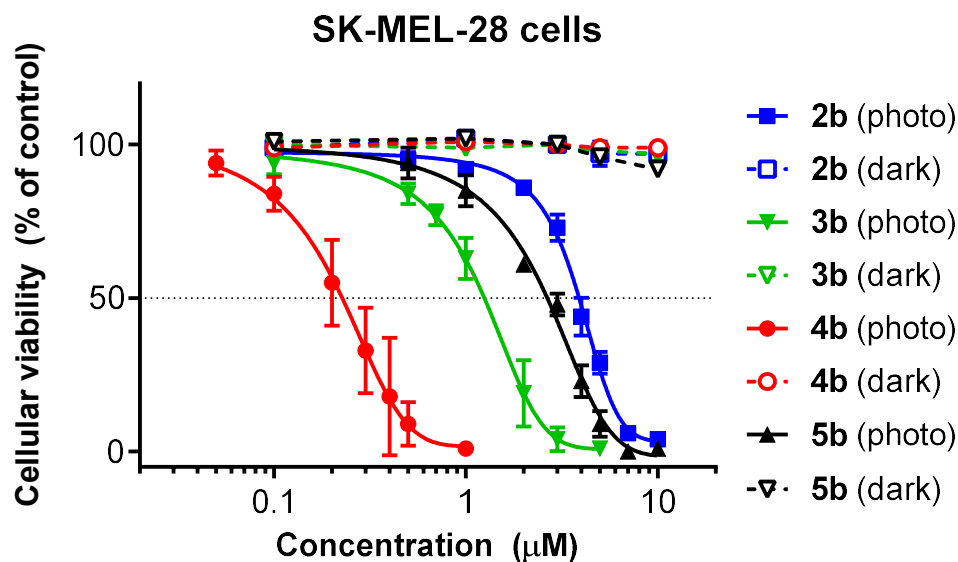


Figure S15. Photodynamic activity (full lines, full symbols) and dark toxicity (dashed lines, empty symbols) of **2b-5b** on SK-MEL-28 cell line. At least four independent experiments each in triplicate were performed. Irradiation conditions: $\lambda > 455$ nm, 15.3 mW cm^{-2} , 15 min, 13.7 Jcm^{-2} .

Subcellular localization

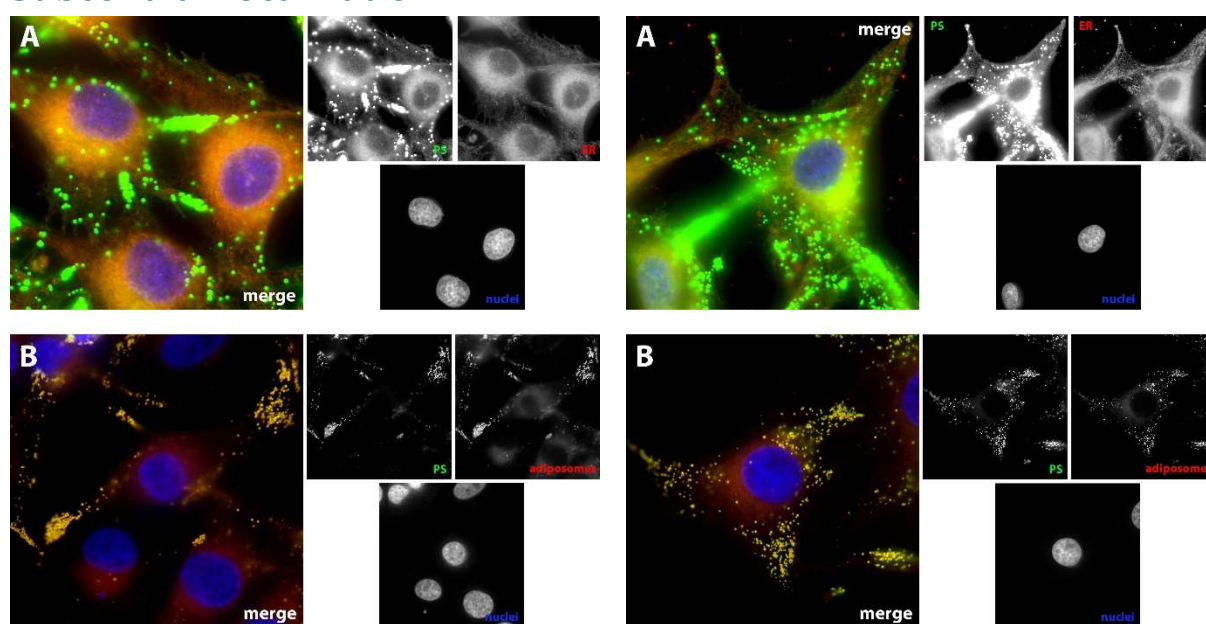


Figure S16. Subcellular localization of compounds **2a** (left) and **2b** (right). A) Intravital staining of nuclei (blue), endoplasmic reticulum (red - mesh) and **2a,b** (green - mesh). Colocalization of **2a,b** with lysosomes represents yellow/orange color in merge image. B) fixed specimen with **2a,b** (green - spots) stained for nuclei (blue) and adiposomes (red - spots). Colocalization of **2a,b** with adiposomes represents yellow/orange color in merge image. PS – photosensitizer (studied BODIPY); ER – endoplasmic reticulum

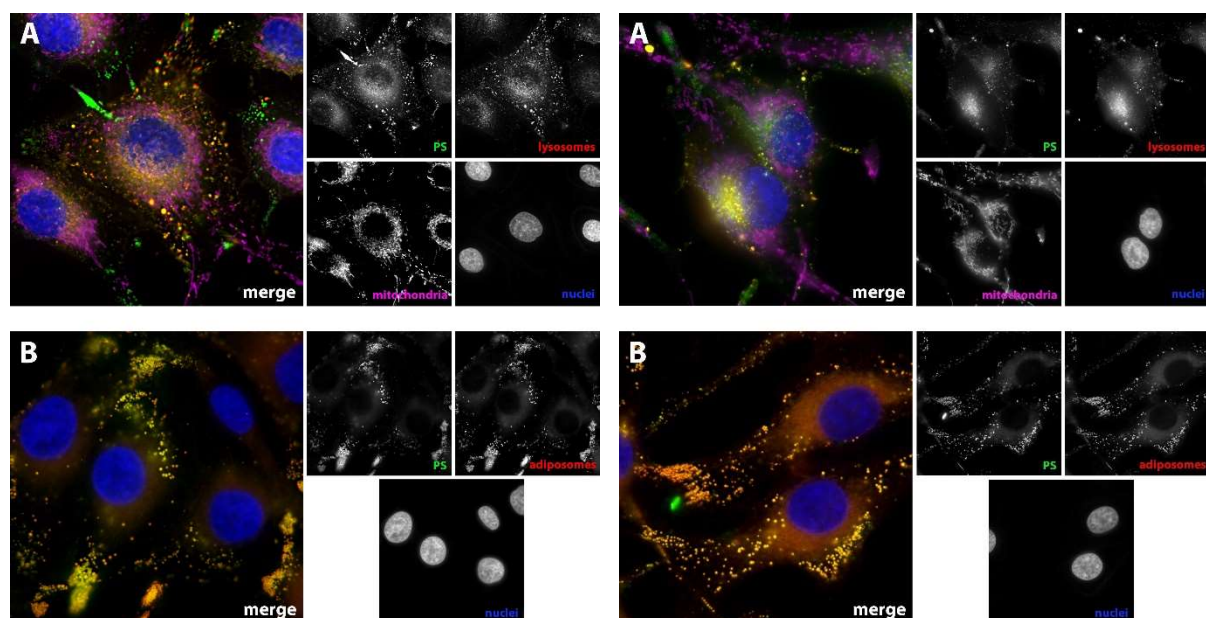


Figure S17 – Subcellular localization of compounds **3a** (left) and **3b** (right). A) Intravital staining of nuclei (blue), mitochondria (pink – rod-like shapes), lysosomes (red – dots) and **3a,b** (green – dots). Colocalization of **3a,b** with lysosomes represents yellow/orange color in merge image. B) fixed specimen with **3a,b** (green – spots) stained for nuclei (blue) and adiposomes (red – spots). Colocalization of **3a,b** with adiposomes represents yellow/orange color in merge image. PS – photosensitizer (studied BODIPY).

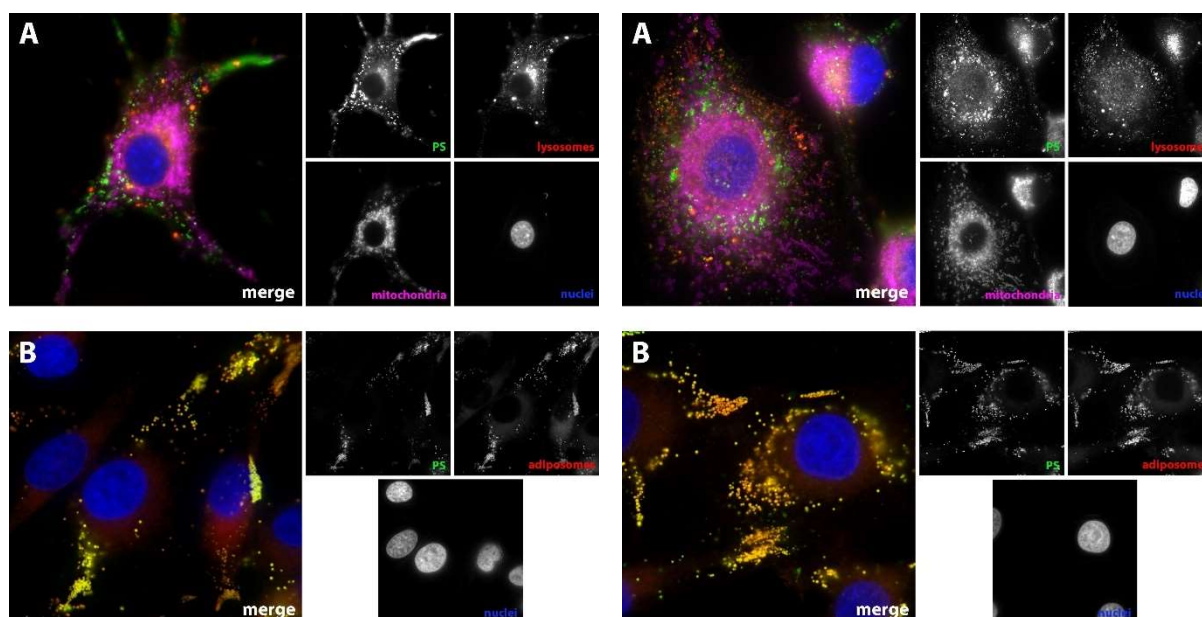


Figure S18 – Subcellular localization of compounds **4a** (left) and **4b** (right). A) Intravital staining of nuclei (blue), mitochondria (pink – rod-like shapes), lysosomes (red – dots) and **4a,b** (green – dots). Colocalization of **4a,b** with lysosomes represents yellow/orange color in merge image. B) fixed specimen with **4a,b** (green – spots) stained for nuclei (blue) and adiposomes (red – spots). Colocalization of **4a,b** with adiposomes represents yellow/orange color in merge image. PS – photosensitizer (studied BODIPY).

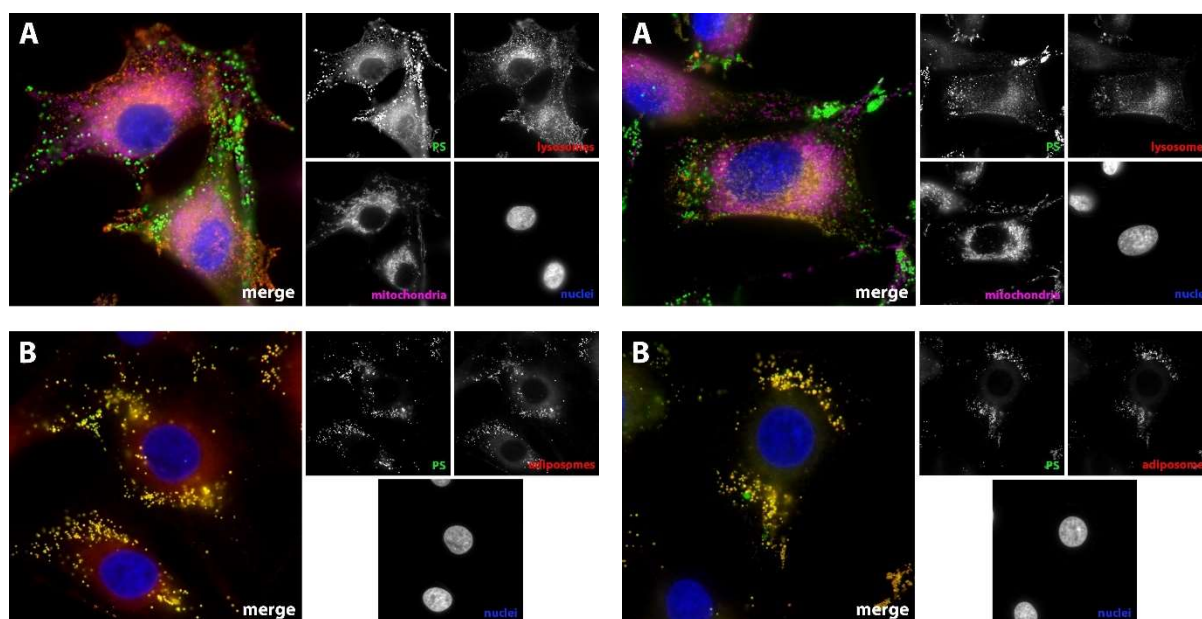


Figure S19 – Subcellular localization of compounds **5a** (left) and **5b** (right). A) Intravital staining of nuclei (blue), mitochondria (pink – rod-like shapes), lysosomes (red – dots) and **5a,b** (green – dots). Colocalization of **5a,b** with lysosomes represents yellow/orange color in merge image. B) fixed specimen with **5a,b** (green – spots) stained for nuclei (blue) and adiposomes (red – spots). Colocalization of **5a,b** with adiposomes represents yellow/orange color in merge image. PS – photosensitizer (studied BODIPY).

Assessment of cell death

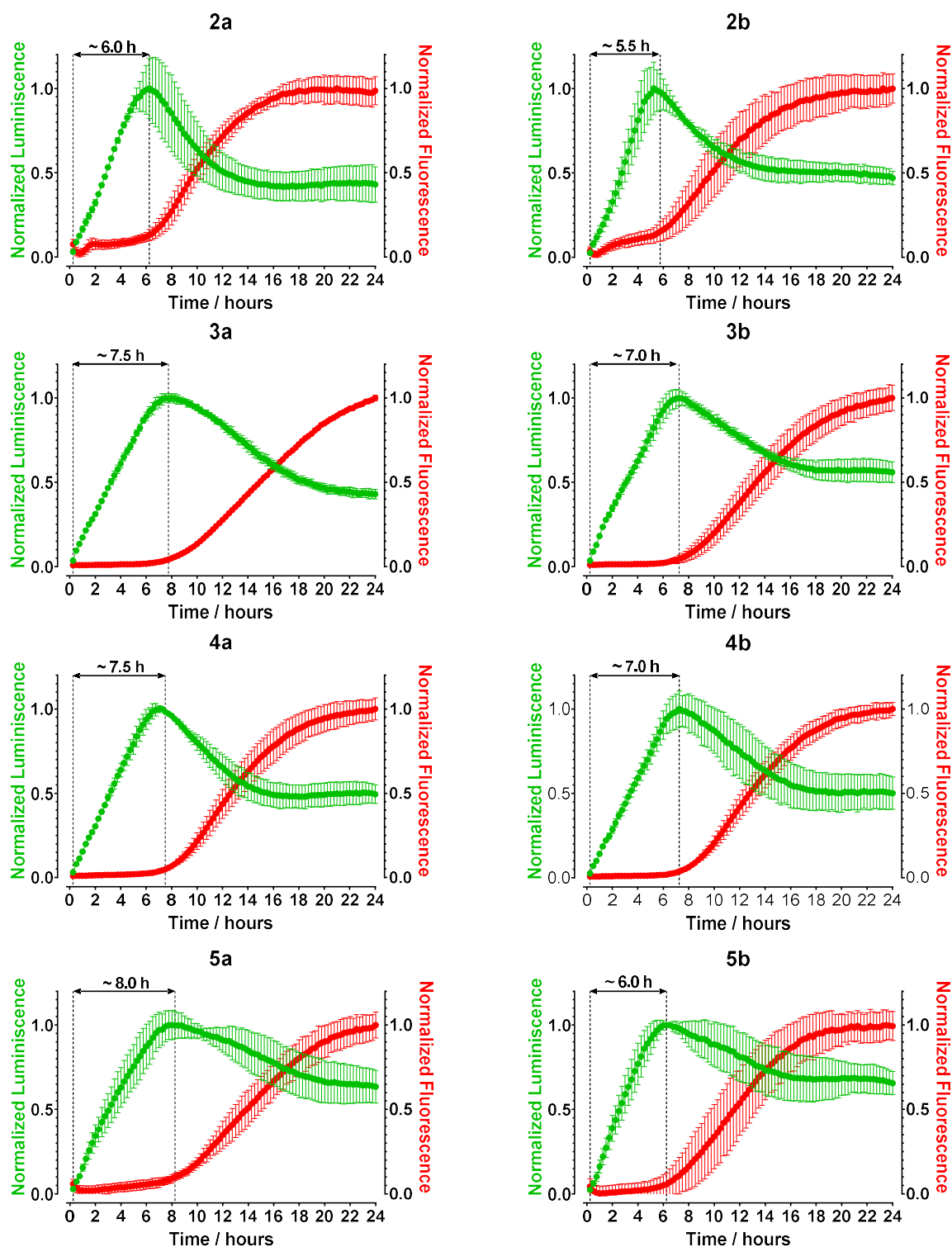


Figure S20. Cell death determination. Annexin V (green) and DNA-binding probe (red) binding profiles for all investigated compounds at their EC₈₅.

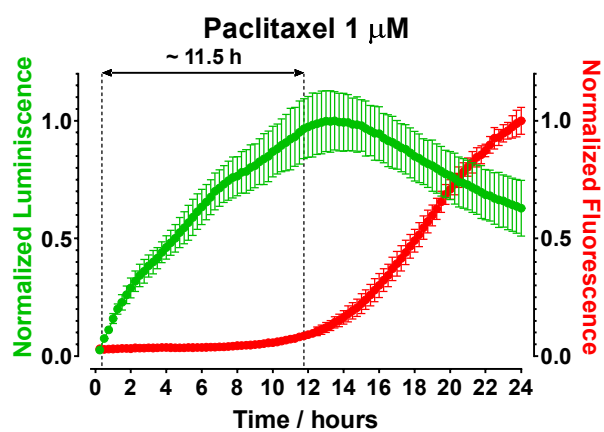


Figure S21. Cell death determination. Annexin V (green) and DNA-binding probe (red) binding profiles for paclitaxel (inducer of intrinsic-pathway apoptosis).