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Lipid vesicles loaded *meso*-substituted chlorins of high *in vitro* antimicrobial photodynamic activity

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Supplementary Data

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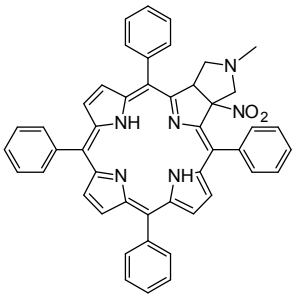
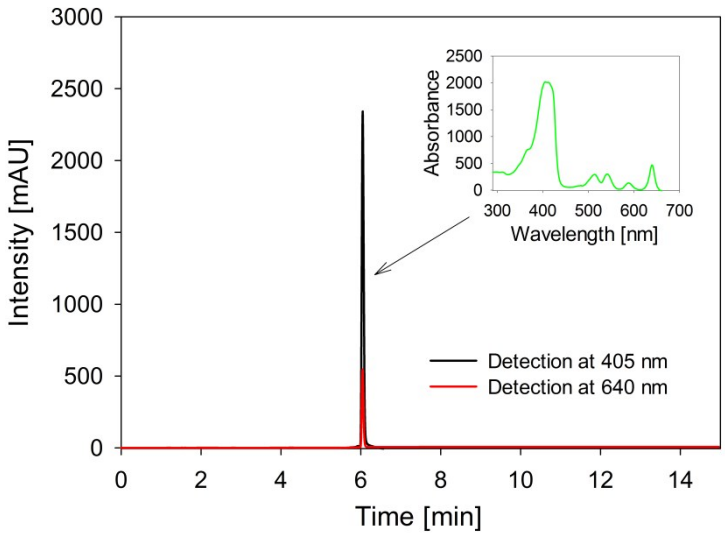
HPLC purity assessment

Analytical HPLC was carried out on an Agilent 1200 instrument equipped with a DAD detector.

Compound 1



Phases configuration 1



Mobile phase [%]

Time	MeOH	CH_2Cl_2
0	100	0
3	100	0
4	0	100
15	0	100

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

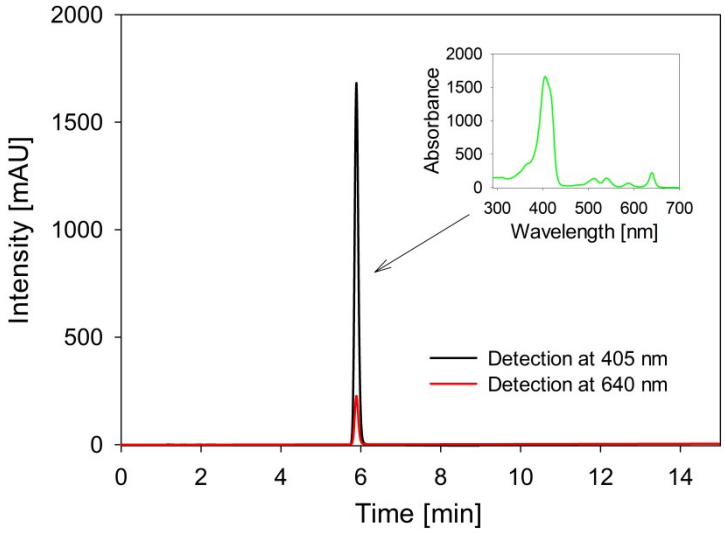
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.59	6.4	0.07
2	4.27	17.1	0.20
3	5.94	162.2	1.86
4	6.05	8548.8	97.87

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.05	1672.4	100.00

Phases configuration 2



Mobile phase [%]

Time	MeOH	CH_2Cl_2
0	100	0
15	0	100

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

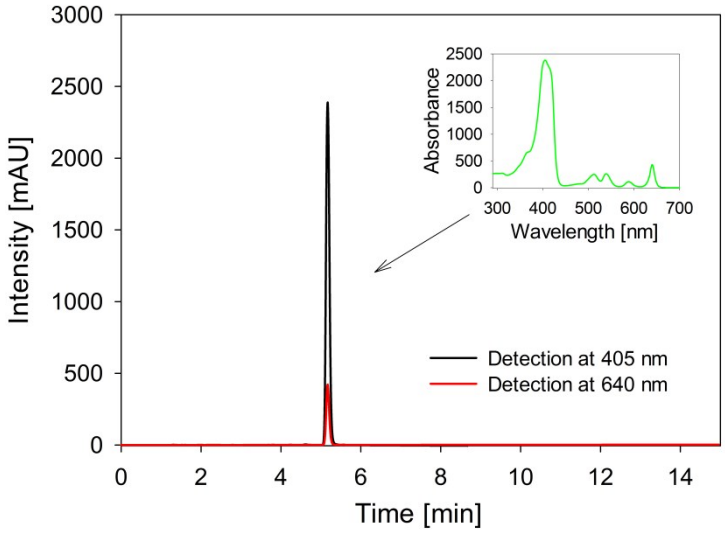
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.59	6.8	0.06
2	3.94	9.3	0.08
3	5.06	27.0	0.24
4	5.89	11383.1	99.32
5	6.37	34.5	0.30

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	5.89	1486.4	100.00

Phases configuration 3



Mobile phase [%]

Time	MeOH	THF
0	100	0
15	0	100

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

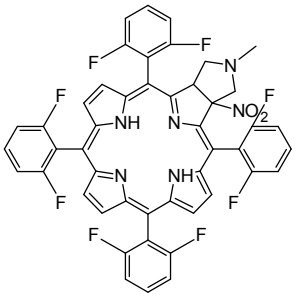
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.31	14.9	0.10
2	1.52	5.6	0.04
3	1.59	7.3	0.05
4	3.69	8.7	0.06
5	3.81	15.8	0.11
6	4.24	25.7	0.17
7	4.62	62.6	0.42
8	5.17	14556.7	98.79
9	5.57	38.4	0.26

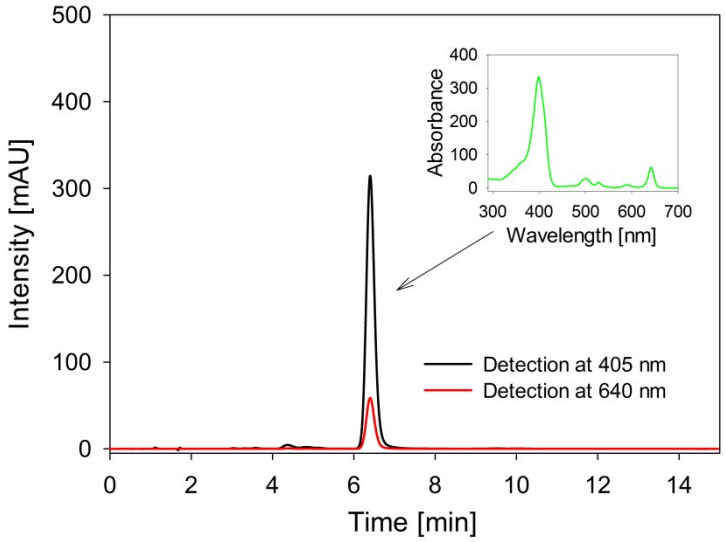
Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	5.89	1486.4	100.00

Compound 2



Phases configuration 1



Mobile phase [%]

MeOH	H_2O
90	10

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

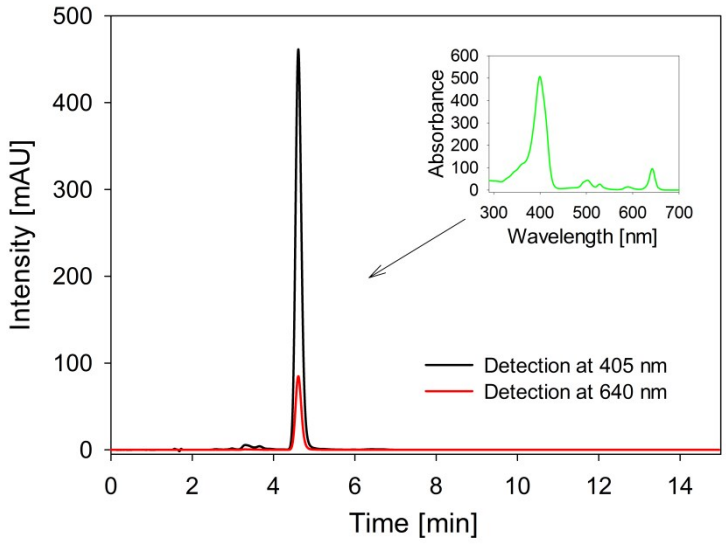
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.11	6.9	0.14
2	1.72	9.4	0.2
3	4.37	74.8	1.56
4	4.82	49.2	1.03
5	6.4	4656.1	97.08

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.4	857.6	100

Phases configuration 2



Mobile phase [%]

MeOH	H_2O	THF
85	10	5

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

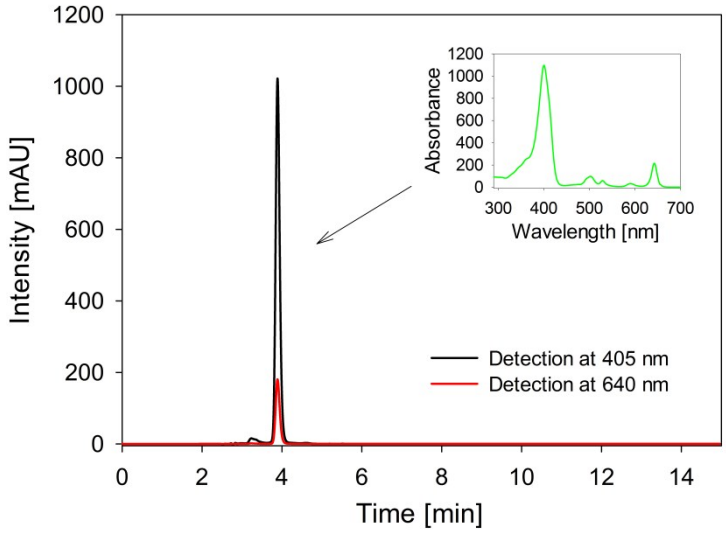
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.57	15.3	0.30
2	1.73	9.6	0.19
3	2.98	12.6	0.25
4	3.31	80.9	1.61
5	3.66	52.8	1.05
6	4.61	4867.6	96.60

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	4.61	891.4	100.00

Phases configuration 3



Mobile phase [%]

MeOH	H_2O	THF
70	10	20

Flow	0.6 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

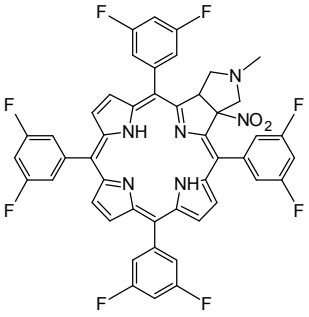
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	2.58	7.6	0.09
2	2.73	16.0	0.20
3	2.84	20.7	0.26
4	2.98	37.5	0.46
5	3.23	298.9	3.70
6	3.89	7655.4	94.74
7	4.60	44.7	0.55

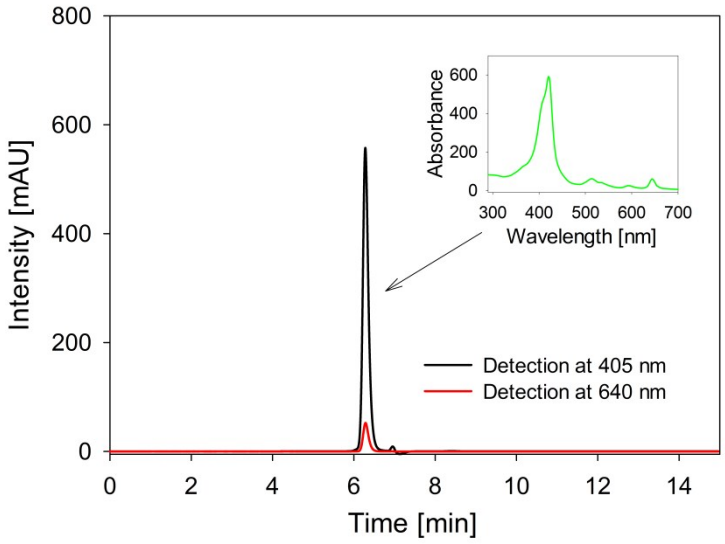
Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	3.23	19.4	1.44
2	3.89	1322.8	98.56

Compound 3



Phases configuration 1



Mobile phase [%]

THF
100

Flow	0.2 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

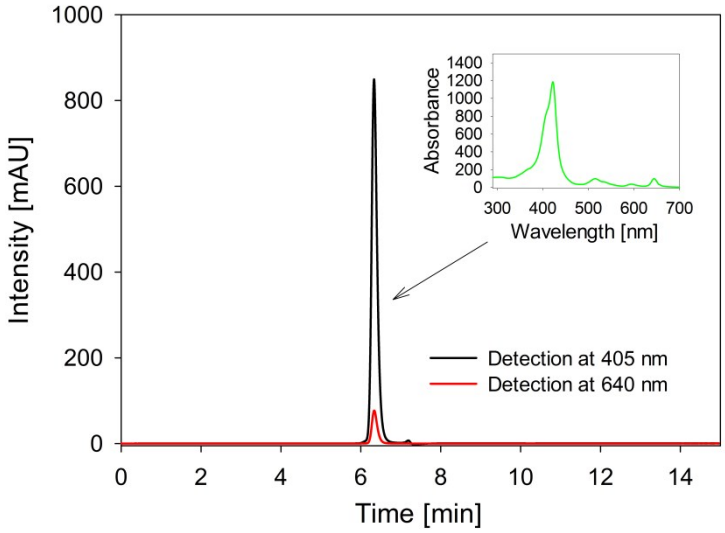
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	6.28	5640.1	98.04
2	6.95	112.5	1.96

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.29	507.7	100.00

Phases configuration 2



Mobile phase [%]

THF	CH_2Cl_2
50	50

Flow	0.2 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

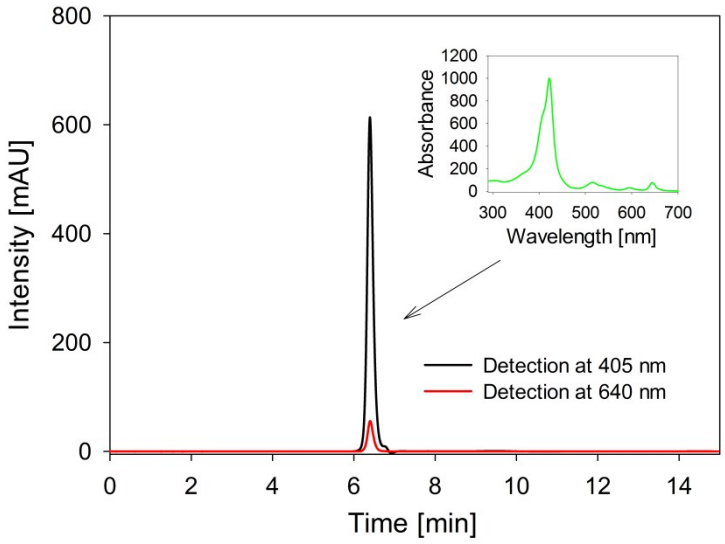
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	6.33	8599.3	99.13
2	7.19	75.1	0.87

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.34	754.6	100.00

Phases configuration 3



Mobile phase [%]

THF	CH_2Cl_2	MeOH
45	45	10

Flow	0.4 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

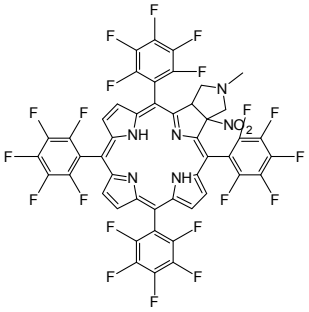
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	6.40	6687.7	100.00

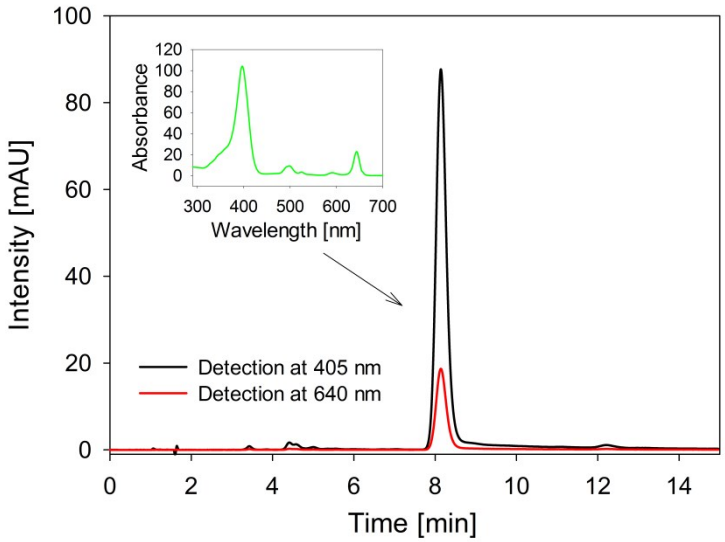
Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.40	585.2	100.00

Compound 4



Phases configuration 1



Mobile phase [%]

MeOH	H_2O
95	5

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

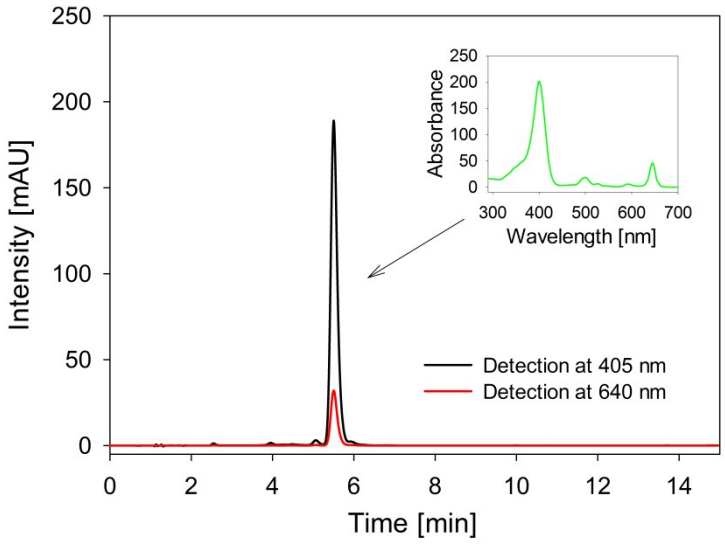
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	1.65	7.4	0.46
2	4.41	25.1	1.56
3	8.14	1574.9	97.98

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	8.14	333.4	100.00

Phases configuration 2



Mobile phase [%]

THF	H_2O
70	30

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

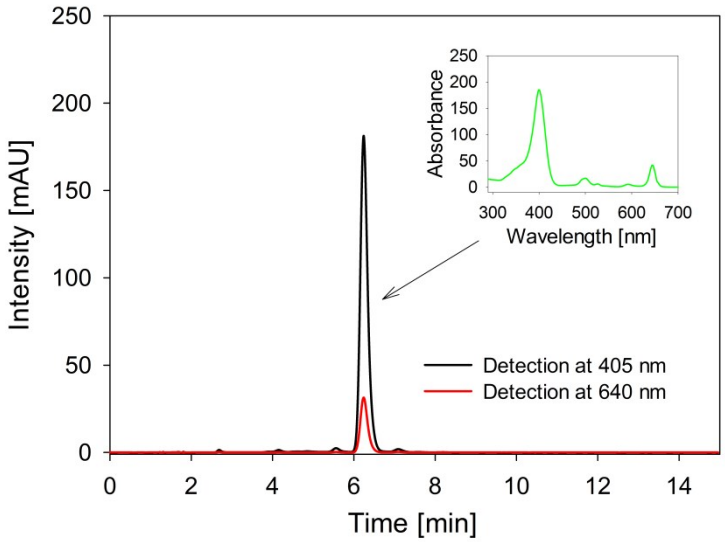
Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	2.55	8.5	0.38
2	3.96	11.1	0.50
3	5.06	26.2	1.18
4	5.51	2173.4	97.93

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	5.51	362.1	100.00

Phases configuration 3



Mobile phase [%]

THF	H_2O	MeOH
65	25	10

Flow	1.0 ml/min
Temperature	25°C
Column	Agilent, Eclipse XDB-C18 150 mm · 4.6 mm, 5 µm

Detection at λ = 405 nm

Signal	Retention time [min]	Area	Content [%]
1	2.69	10.0	0.41
2	4.15	10.9	0.45
3	5.56	25.7	1.06
4	6.24	2350.8	97.03
5	7.09	25.5	1.05

Detection at λ = 640 nm

Signal	Retention time [min]	Area	Content [%]
1	6.24	404.7	100.00

Spectral properties

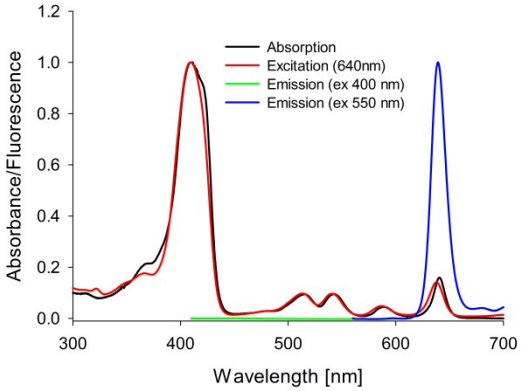


Figure 1S. Absorption, emission, excitation spectra of **1** in DMSO.

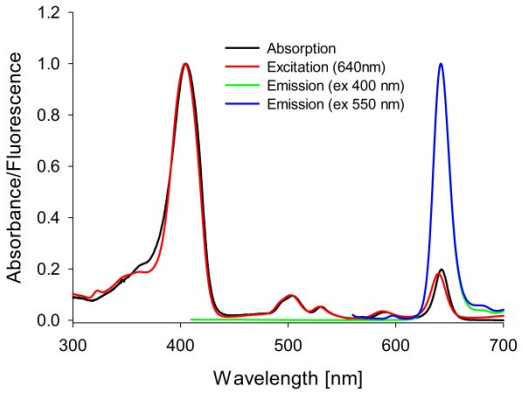
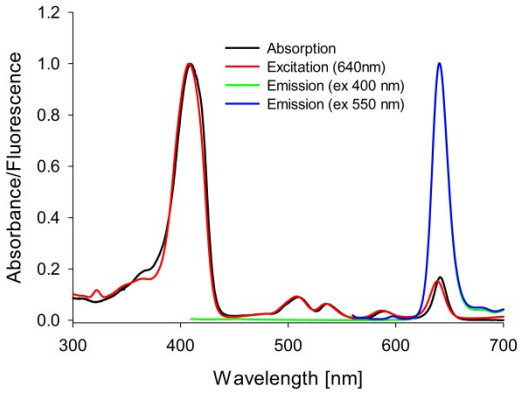


Figure 2S. Absorption, emission, excitation spectra of **2** in DMSO



S

Figure 3S. Absorption, emission, excitation spectra of **3** in DMSO

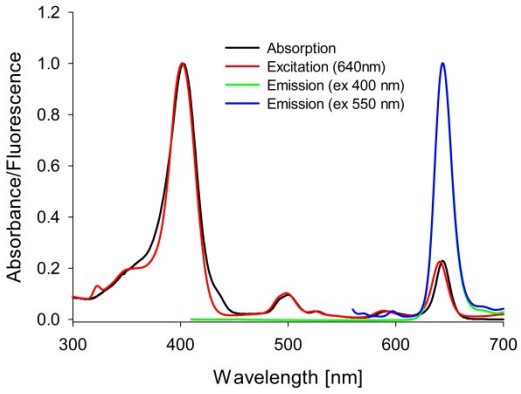


Figure 4S. Absorption, emission, excitation spectra of **4** in DMSO

In vitro photodynamic activity against bacteria and fungi

Table 1S. Log reduction values of *S. aeruginos*, *T. mentagrophytes* and *C. albicans* obtained for studied compounds

			log reduction of bacterial growth	
	1			
Bacteria strain	ATCC	conditions	100 µM	10 µM
Pseudomonas aeruginosa	6749	light	-0.23	0.00
		dark	-0.12	-0.08
Trichophyton mentagrophytes	9533	light	1.43	-0.01
		dark	-0.16	-0.23
Candida albicans	10231	light	-0.22	-0.08
		dark	-0.10	0.08
	2			
Bacteria strain	ATCC	conditions	100 µM	10 µM
Pseudomonas aeruginosa	6749	light	0.85	-0.14
		dark	-	-0.02
Trichophyton mentagrophytes	9533	light	-0.24	0.14
		dark	0.03	-0.35
Candida albicans	10231	light	0.04	0.17
		dark	0.02	0.02
	3			
Bacteria strain	ATCC	conditions	100 µM	10 µM
Pseudomonas aeruginosa	6749	light	-0.24	-0.04
		dark	-0.15	-0.10
Trichophyton mentagrophytes	9533	light	-0.17	-0.27
		dark	-0.25	-0.3

Candida albicans	10231	light	-0.18	-0.06
		dark	0.01	-0.05

4

Bacteria strain	ATCC	conditions	100 µM	10 µM
Pseudomonas aeruginosa	6749	light	-0.09	-0.02
		dark	-	-0.10
Trichophyton mentagrophytes	9533	light	-0.29	-0.14
		dark	-0.22	0.73
Candida albicans	10231	light	-0.15	0.27
		dark	0.47	0.57