

Supporting Information

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1. Photophysical Data

1.1 Absorption spectra

a.

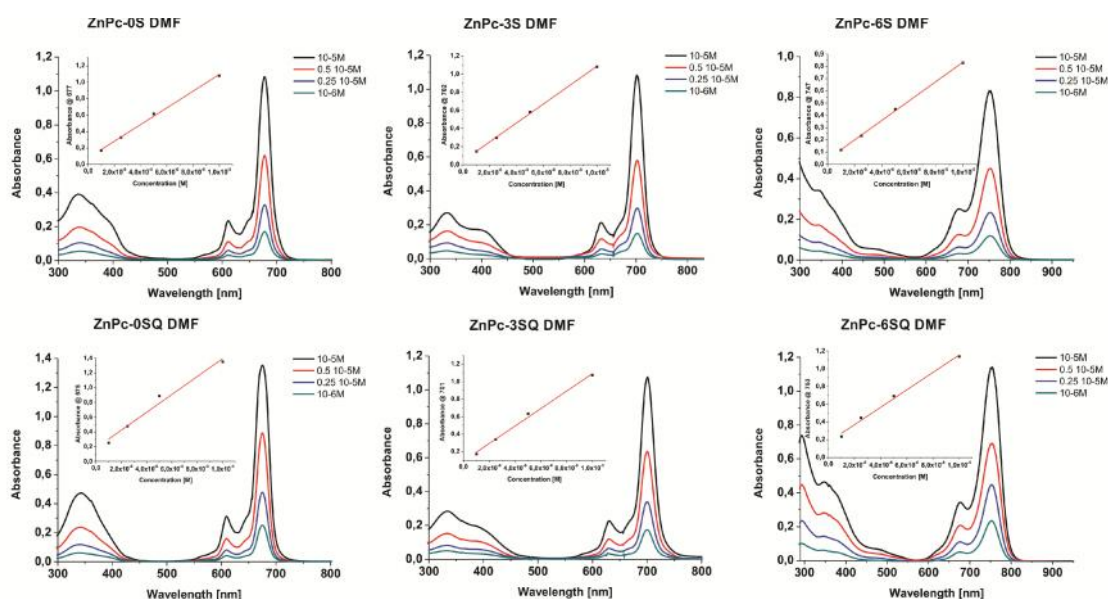


Figure S1. a. UV-Visible spectra of Zn(II)Pcs in DMF at different concentrations $1\mu\text{M}$ to $10\mu\text{M}$. The inset of each spectrum plots the Q-band absorbance vs the concentration of the photosensitizer, and the line represents the best-fitted straight line.

1.2 Singlet oxygen quantum yields

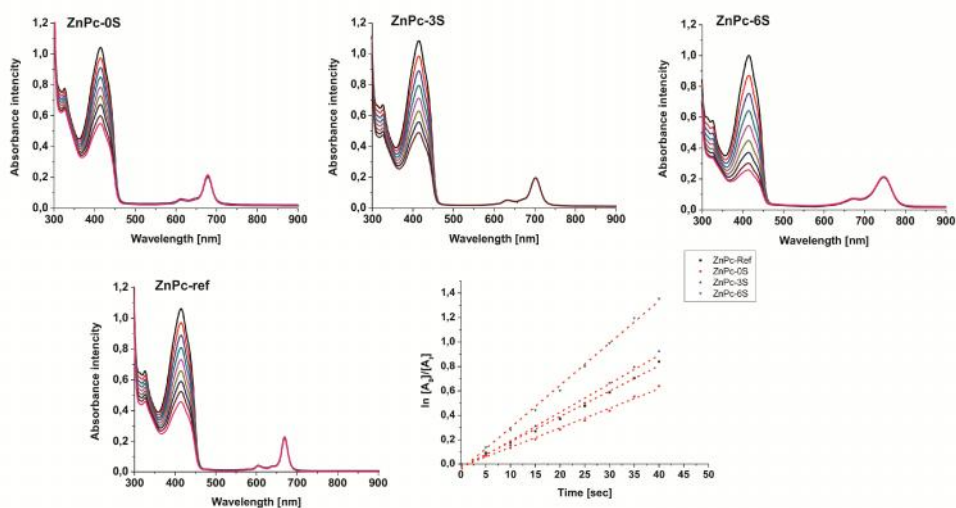


Figure S2. Time-dependent decomposition of DPBF photosensitized by ZnPc-0S, ZnPc-3S and ZnPc-6S in DMF upon irradiation with light from projector lamp filtered through a cut-off filter for $\lambda > 610$ nm and corresponding first-order plots.

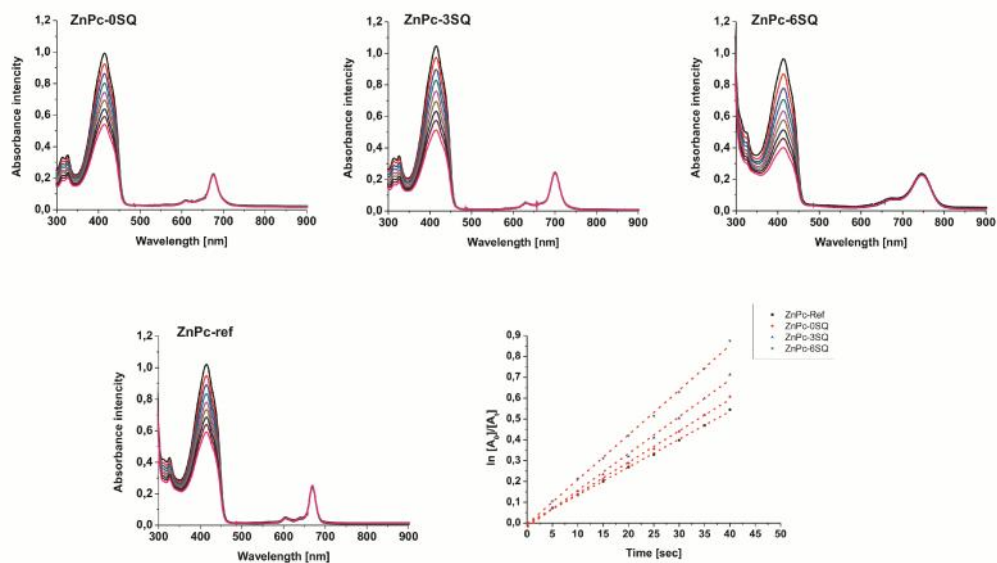


Figure S3. Time-dependent decomposition of DPBF photosensitized by ZnPc-0SQ, ZnPc-3SQ and ZnPc-6SQ in DMF upon irradiation with light from projector lamp filtered through a cut-off filter for $\lambda > 610$ nm and corresponding first-order plots.

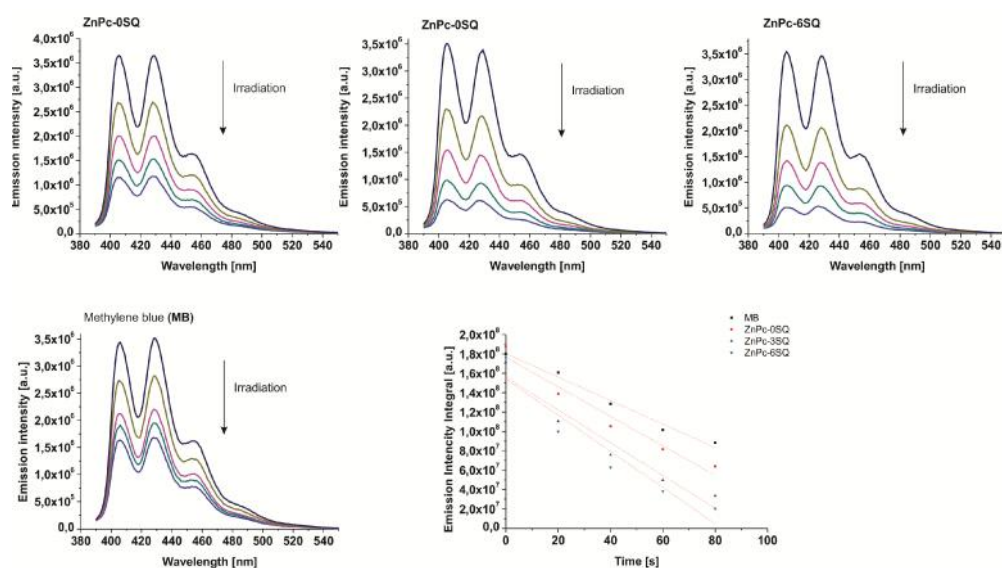


Figure S4. Emission spectra of ADMADM at different irradiation times in double distilled water with ZnPc-0SQ, ZnPc-3SQ, ZnPc-6SQ and MB (0 s, 20 s, 40s, 60s and 80 s) and corresponding decays.

1.3 Photodegradation

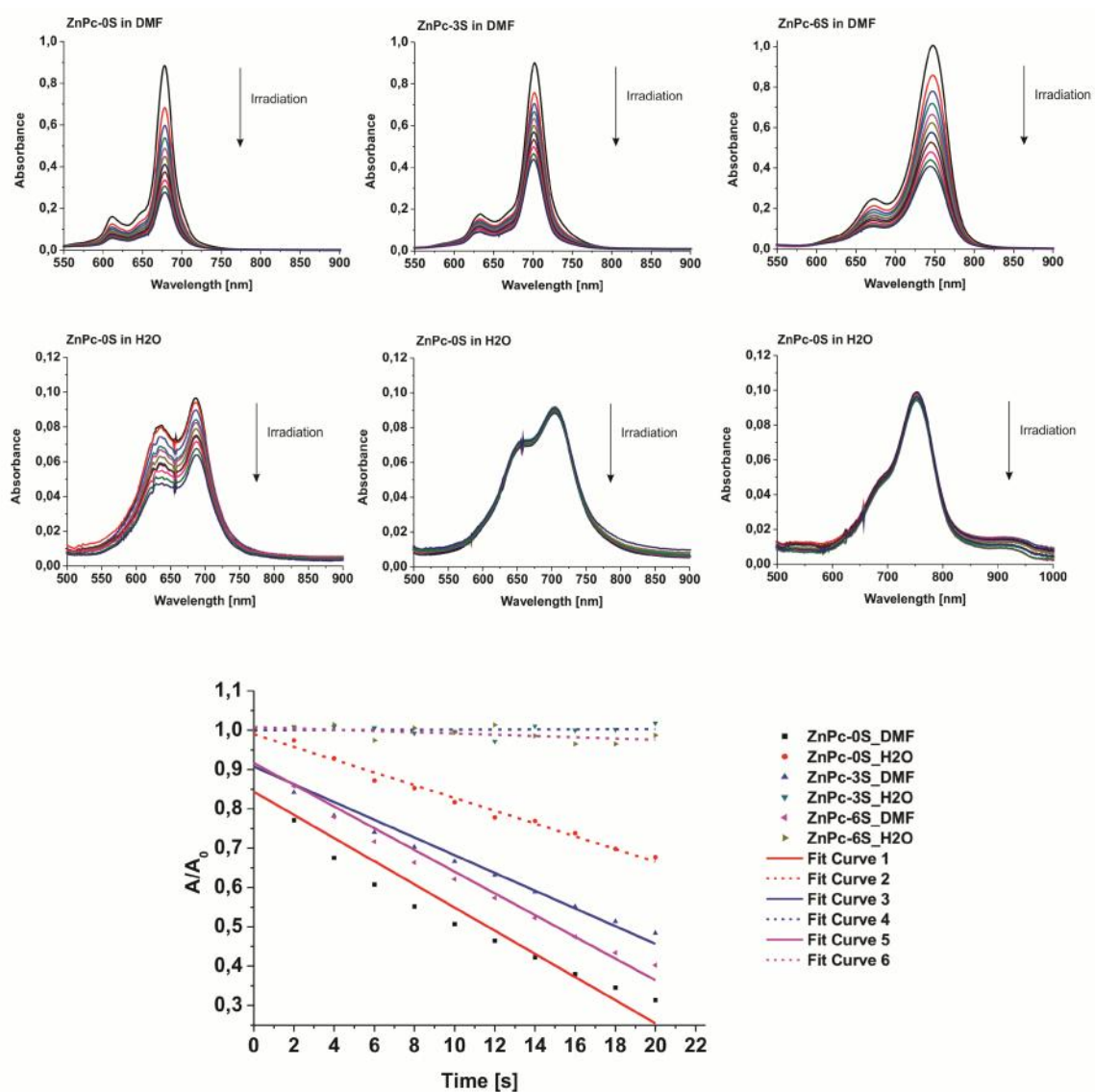


Figure S5. Changes of optical density of Pcs at the absorption maximum wavelength during irradiation with red light ($>610\text{nm}$, 30mW/cm^2) and corresponding decays.

2. DFT calculations

2.1 Cartesian coordinates

ZnPc-0S

0	1		
6	-0.677275000	-4.175688000	0.065399000
6	-0.568952000	-5.565562000	0.067899000
6	0.688390000	-6.198520000	0.046984000
6	1.869440000	-5.458185000	0.022988000
6	1.763541000	-4.066990000	0.020385000
6	2.762898000	-3.001435000	-0.001405000
7	4.074440000	-3.219158000	-0.024443000
6	4.992730000	-2.256703000	-0.043984000
6	6.430925000	-2.509957000	-0.068583000
6	7.178730000	-3.687835000	-0.078081000
6	8.567799000	-3.574727000	-0.102898000
6	9.196078000	-2.315021000	-0.117837000
6	8.450932000	-1.137063000	-0.108344000
6	7.060325000	-1.247985000	-0.083562000
6	5.992797000	-0.251467000	-0.067809000
7	4.782756000	-0.900043000	-0.044466000
7	6.207832000	1.060949000	-0.075303000
6	5.245333000	1.978427000	-0.060615000
6	5.498040000	3.416847000	-0.068571000
6	6.675784000	4.164663000	-0.091325000
6	6.562683000	5.553903000	-0.092612000
6	5.303160000	6.182416000	-0.071627000
6	4.125440000	5.437220000	-0.048824000
6	4.236436000	4.046427000	-0.047549000
6	3.239615000	2.979030000	-0.027186000
7	3.888207000	1.768621000	-0.035840000
7	1.928195000	3.194791000	-0.003933000
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6	-2.531036000	3.601656000	0.078475000
6	-3.189154000	2.361706000	0.094317000
6	-2.466268000	1.163247000	0.083732000
6	-1.062725000	1.234816000	0.056721000
6	-0.001627000	0.231858000	0.039477000
7	1.213099000	0.877724000	0.015051000
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1	0.735498000	-7.283550000	0.049586000
1	9.179358000	-4.472155000	-0.110912000
1	7.459972000	6.165469000	-0.110087000
1	5.252046000	7.267233000	-0.073300000
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1	-9.025312000	-0.934202000	1.277049000
7	-5.248815000	0.121147000	-3.530499000
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1	-10.749576000	-1.685251000	-1.246075000
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1	-6.069211000	1.793173000	-2.560524000
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E(B3LYP) = -4272.5132019

ZPVE = 0.802077

ZnPc-3S

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6	6.698124000	-0.308055000	1.358844000
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6	10.290634000	-0.958960000	0.204937000
1	10.653603000	-0.910413000	1.250811000
1	10.443866000	-1.994961000	-0.125121000
6	6.015298000	-0.240129000	-2.422191000
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1	5.130372000	0.413476000	-2.334161000
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1	6.096195000	-1.305109000	-4.851529000
1	5.303020000	0.280539000	-5.022348000
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1	10.078575000	1.659610000	-0.145951000
6	12.423472000	-0.621716000	-0.875974000
1	12.958648000	0.002758000	-1.598505000
1	13.020415000	-0.645746000	0.056877000
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6	6.070740000	-0.162964000	5.063097000
1	5.077602000	0.303462000	5.209801000
1	5.946346000	-1.248807000	5.121561000
1	6.712912000	0.150013000	5.892551000
6	6.958004000	1.631841000	3.732197000
1	6.034278000	2.239501000	3.780633000
1	7.604227000	1.927502000	4.564740000
1	7.474716000	1.874125000	2.799898000

E(B3LYP) = -6160.2387958

ZPVE = 1.046688

ZnPc-6S

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6	-1.650296000	4.656158000	-0.100058000
6	-1.370647000	3.283647000	0.033860000
6	-0.126641000	2.505367000	0.081707000
7	1.098979000	3.031040000	0.118525000
6	2.234957000	2.329711000	0.103728000
6	3.567547000	2.934625000	0.112467000
6	4.012500000	4.255451000	0.301751000
6	5.386177000	4.484704000	0.155844000
6	6.276964000	3.458916000	-0.152120000
6	5.857391000	2.131083000	-0.299445000
6	4.486631000	1.875801000	-0.113872000
6	3.700324000	0.641342000	-0.105738000
7	2.369269000	0.966750000	-0.000056000
7	4.234790000	-0.581910000	-0.124893000
6	3.540159000	-1.719901000	-0.078442000
6	4.130160000	-3.065266000	-0.035460000
6	5.448384000	-3.548223000	0.065373000
6	5.612787000	-4.939901000	0.059177000
6	4.533953000	-5.823047000	-0.010894000

6	3.213292000	-5.365588000	-0.069077000
6	3.039648000	-3.971809000	-0.077318000
6	1.833998000	-3.164186000	-0.091975000
7	2.171820000	-1.837488000	-0.090444000
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6	-1.831751000	-3.618534000	-0.026881000
6	-2.213218000	-4.958427000	-0.077901000
6	-3.578628000	-5.230189000	-0.059786000
6	-4.531903000	-4.202082000	0.006976000
6	-4.140386000	-2.859499000	0.059188000
6	-2.766016000	-2.563525000	0.042144000
6	-1.990899000	-1.323878000	0.072827000
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7	-2.509830000	-0.102597000	0.126956000
6	-1.804534000	1.024785000	0.130996000
7	-0.441419000	1.169640000	0.115707000
6	-2.427022000	2.339440000	0.112384000
16	6.818119000	-2.417363000	0.215954000
16	-5.068590000	1.490630000	0.256846000
1	-5.053916000	4.458017000	0.040964000
1	-3.264681000	6.075872000	-0.173061000
1	5.777370000	5.486967000	0.282684000
1	6.610813000	-5.356806000	0.119553000
1	4.738339000	-6.886891000	-0.010014000
1	-3.925789000	-6.258630000	-0.098277000
30	0.861298000	-0.335936000	0.018506000
16	-0.329623000	5.836181000	-0.305656000
6	-1.206139000	7.341258000	-0.752905000
6	-1.380729000	8.351936000	0.200695000
6	-1.627839000	7.553619000	-2.073035000
6	-1.978212000	9.560916000	-0.161841000
1	-1.046360000	8.186693000	1.219828000
6	-2.231744000	8.759344000	-2.428207000
1	-1.478836000	6.773821000	-2.812971000
6	-2.406390000	9.764807000	-1.474094000
1	-2.109307000	10.341160000	0.582274000
1	-2.558378000	8.917100000	-3.452004000
1	-2.871225000	10.705426000	-1.754726000
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6	5.501812000	9.013737000	2.216846000
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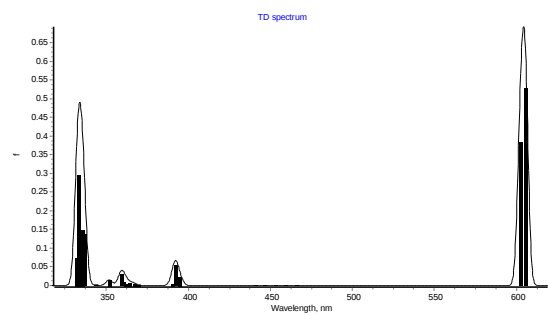
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E(B3LYP) = -8047.9476283

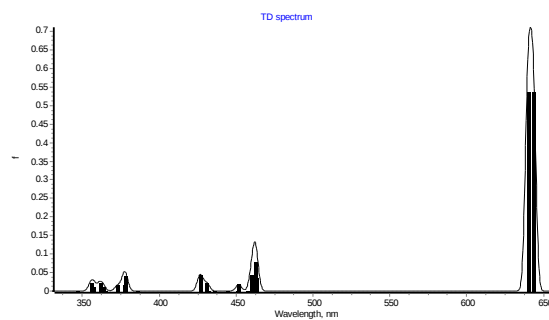
ZPVE = 1.290852

2.2 Calculated UV-Vis spectra

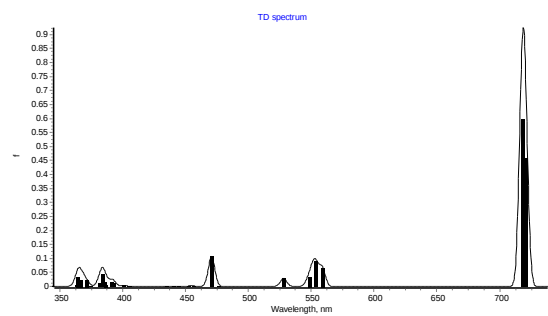
ZnPc-0S



ZnPc-3S



ZnPc-6S



3. Photobiological studies

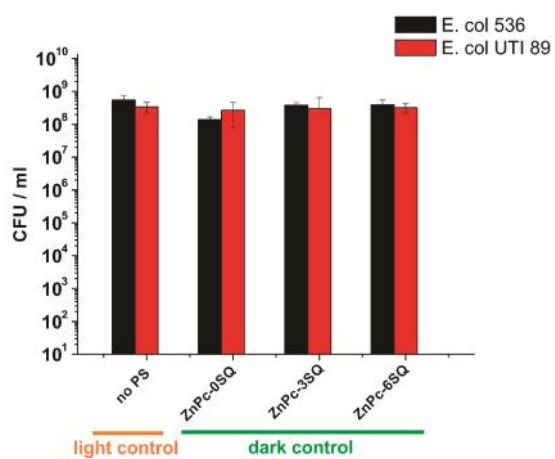
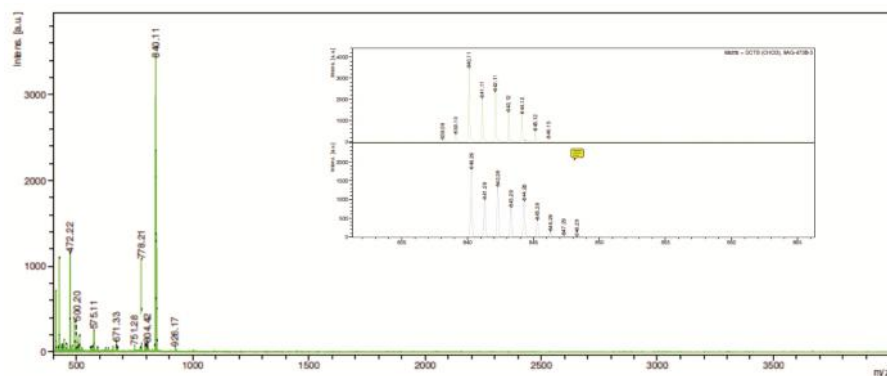
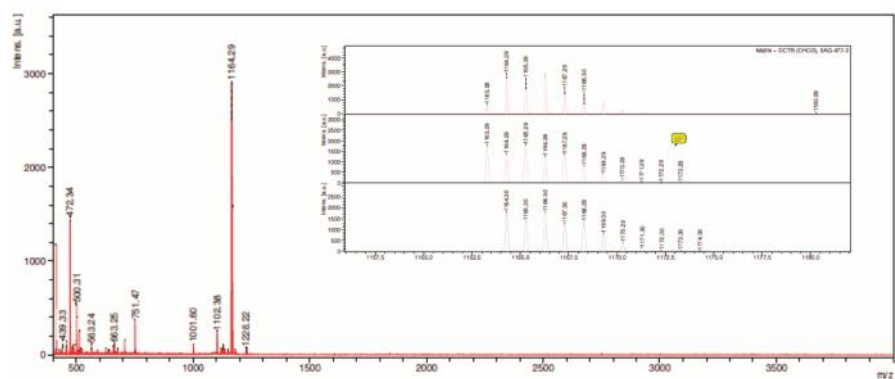


Figure S6. Viability of bacterial cells upon irradiation - light control (30 min - 19 J/cm^2) and upon incubation with ZnPc-0SQ, ZnPc-3SQ, ZnPc-6SQ - dark control ($10 \mu\text{M}$, 30 min).

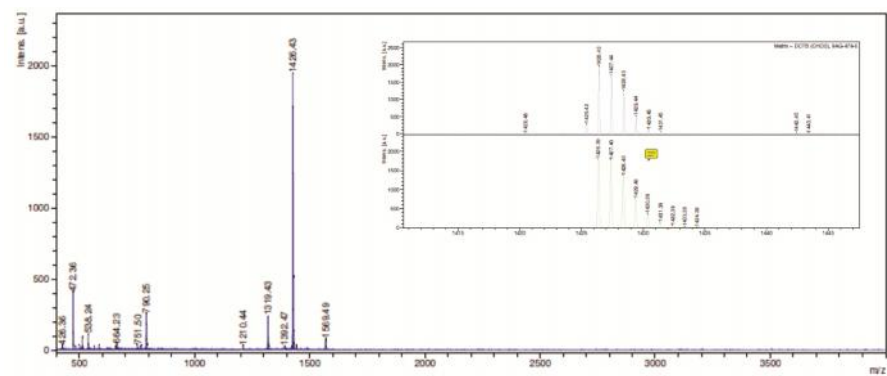
ZnPc-0S



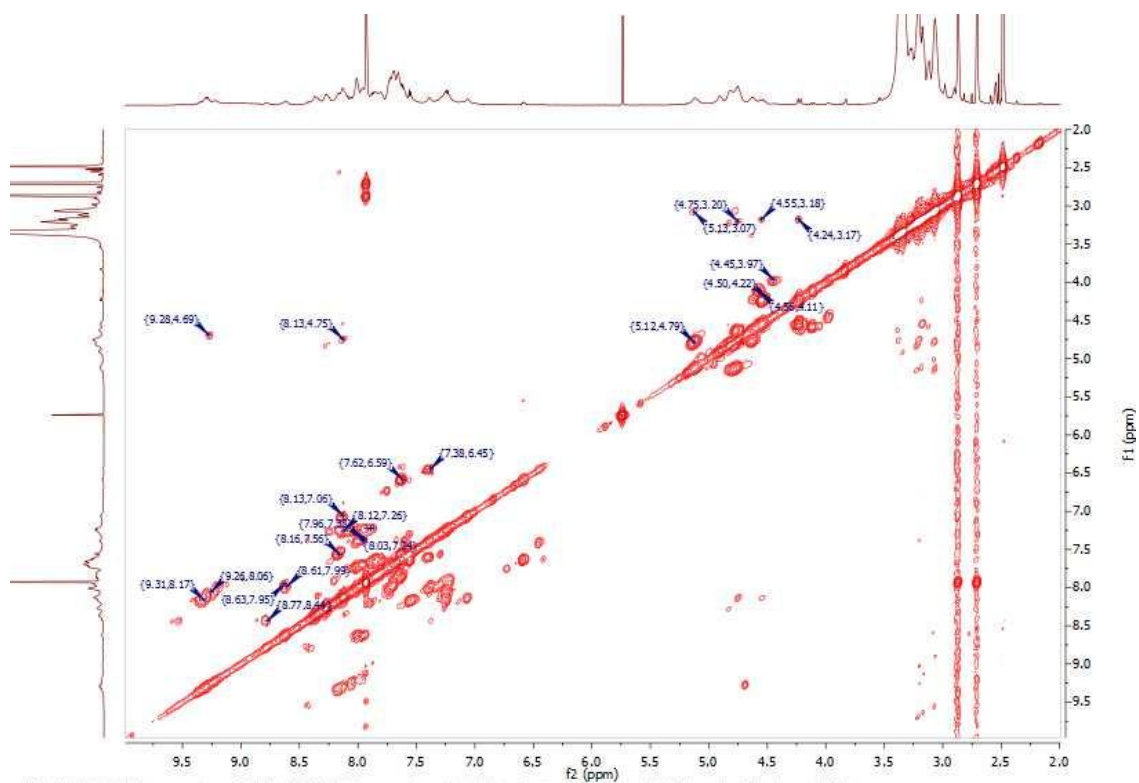
ZnPc-3S



ZnPc-6S



ZnPc-3SQ



ZnPc-6SQ

