## Supporting Information

## GAME OF LIGANDS: TUNING PHOTODYNAMIC ACTIVITY OF P(V) PORPHYRINS IN AQUEOUS MEDIA

I.A. Efimova<sup>*a*</sup>, E.A. Safonova<sup>*a*</sup>, M.A. Polovkova<sup>*a*</sup>, E.V. Gorshkov<sup>*a,b,c*</sup>, T.E. Egorova<sup>*d*</sup>, R.A. Akasov<sup>*d*</sup>, A. Yu. Tsivadze<sup>*a,c*</sup>, Yu. G. Gorbunova<sup>*a,b,c*</sup>

<sup>a</sup> Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninsky pr., 31, building 4, Moscow, 119071, Russia

<sup>b</sup> Lomonosov Moscow State University, Faculty of fundamental physical and chemical engineering, Leninskie Gory, 1, building. 51, Moscow, 119991, Russia

<sup>c</sup> Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninsky pr., 31, Moscow, 119991, Russia

<sup>d</sup> Moscow State Pedagogical University, Malaya Pirogovskaya St., 1, building 1, Moscow, 119435, Russia

| Figure S1. Normalized UV-Vis spectrum of complex <b>1b-3b</b> , <b>1c-3c</b> , <b>2d</b> in EtOH2 |
|---|
| Figure S2. <sup>1</sup> H NMR spectrum (CDCl <sub>3</sub> , 600 MHz) of <b>2d</b>                 |
| Figure S3. <sup>13</sup> C NMR spectrum (CDCl <sub>3</sub> , 151 MHz) of <b>2d</b>                |
| Figure S4. <sup>31</sup> P NMR spectrum (CDCl <sub>3</sub> , 162 MHz) of <b>2d</b>                |
| Figure S5. ESI HRMS spectra of 2d: experimental (top), calculated (bottom)                        |
| Figure S6. <sup>1</sup> H NMR spectrum (CDCl <sub>3</sub> , 600 MHz) of $3c$ 4                    |
| Figure S7. <sup>13</sup> C NMR spectrum (CDCl <sub>3</sub> , 151 MHz) of <b>3c.</b>               |
| Figure S8. <sup>31</sup> P NMR spectrum (CDCl <sub>3</sub> , 162 MHz) of <b>3c</b>                |
| Figure S9. ESI HRMS spectra of <b>3c</b> : experimental <i>(top)</i> , calculated <i>(bottom)</i> |
| Figure S10. Emission spectra of complexes 1b-3b, 1c-3c, 2d in PBS (black) and A-549 cell lysate   |
| (after incubation this complexes in cells medium) without FBS (light red) and in presence FBS     |
| (dark red)  |
| Figure S11. Cell viability of human breast adenocarcinoma MCF-7 cells in dark and light (450 nm,  |
| 3.5 J/cm2) conditions, 72 h, MTT assay. Non-treated cells were taken as controls (100%)7          |
| Table S1. Fluorescence images of human lung adenocarcinoma A-549 cells incubated with 20 $\mu M$  |
| of tested compounds, 1 h incubation, excitation with 405 nm, 488 nm, 543 nm, and 640 nm8          |



Figure S1. Normalized UV-Vis spectrum of complex 1b-3b, 1c-3c, 2d in EtOH.



Figure S2. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 600 MHz) of 2d.



Figure S3. <sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>, 151 MHz) of **2d**.



Figure S4. <sup>31</sup>P NMR spectrum (CDCl<sub>3</sub>, 162 MHz) of **2d**.



Figure S5. ESI HRMS spectra of 2d: experimental (top), calculated (bottom).



Figure S6. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 600 MHz) of **3c**.



Figure S7. <sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>, 151 MHz) of **3c.** 



Figure S8. <sup>31</sup>P NMR spectrum (CDCl<sub>3</sub>, 162 MHz) of **3c**.



Figure S9. ESI HRMS spectra of 3c: experimental (top), calculated (bottom).



Figure S10. Emission spectra of complexes **1b-3b**, **1c-3c**, **2d** in PBS (black) and A-549 cell lysate (after incubation this complexes in cells medium) without FBS (light red) and in presence FBS (dark red).



Figure S11. Cell viability of human breast adenocarcinoma MCF-7 cells in dark and light (450 nm, 3.5 J/cm2) conditions, 72 h, MTT assay. Non-treated cells were taken as controls (100%).

| $[(TPP)P(OH)_2]^+(1b)$   | $[(MPyP)P(OH)_2]^+(\mathbf{2b})$ | $[(t-DPyP)P(OH)_2]^+(\mathbf{3b})$ |
|--------------------------|----------------------------------|------------------------------------|
|                          |                                  |                                    |
| $[(TPP)P(OEt)_2]^+ (1c)$ | $[(MPyP)P(OEt)_2]^+(2c)$         | $[(t-DPyP)P(OEt)_2]^+(3c)$         |
|                          |                                  |                                    |
|                          | $[(MPyP)P(OPrOH)_2]^+(2d)$       | Control (unstained cells)          |
|                          |                                  |                                    |

Table S1. Fluorescence images of human lung adenocarcinoma A-549 cells incubated with 20  $\mu$ M of tested compounds, 1 h incubation, excitation with 405 nm, 488 nm, 543 nm, and 640 nm.