Supporting Information

An insight into the synthesis of cationic porphyrin-imidazole derivatives and their photodynamic inactivation ability against *Escherichia coli*

Xavier Moreira,^a Patrícia Santos,^b M. Amparo F. Faustino,^a M. Manuela M. Raposo,^c Susana P. G. Costa,^c Nuno M. M. Moura,^{a,*} Ana T. P. C. Gomes,^{b,*} Adelaide Almeida,^b M. G. P. M. S. Neves^{a,*}

^aLAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

^bCESAM and Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal.

^cCentro de Química, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal.

NMR and mass spectra of compounds **2a-d** and **3a-d**

Figure S1. ^1H NMR spectrum of compound **2a** in CHCl_3 .

Figure S2. COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **2a** in CHCl_3 .

Figure S3. ¹³C NMR spectrum of compound **2a** in CHCl₃.

Figure S4. MS-ESI(+) spectrum of compound **2a**.

NM-XM1 #20-36 RT: 0.81-1.38 AV: 17 NL: 3.78E6
T: FTMS + p ESI Full ms [700.0000-1000.0000]

Figure S5. HRMS-ESI(+) spectrum of compound **2a**.

Figure S6. ^1H NMR spectrum of compound **2b** in DMSO-d_6 .

Figure S7. COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **2b** in DMSO-d_6 .

Figure S8. ¹³C NMR spectrum of compound **2b** in DMSO-d₆.

Figure S9. MS-ESI(+) spectrum of compound **2b**.

NM-XM2 #22-44 RT: 0.88-1.64 AV: 23 NL: 1.11E6
T: FTMS + p ESI Full ms [800.0000-1200.0000]

Figure S10. HRMS-ESI(+) spectrum of compound **2b**.

Figure S11. MS-ESI(+) spectrum of compound **2c** in DMSO-d₆.

Figure S12. Partial COSY (¹H/¹H) spectrum of compound **2c** in DMSO-d₆.

Figure S13. ^{13}C NMR spectrum of compound **2C** in DMSO-d_6 .

Figure S14. MS-ESI(+) spectrum of compound **2C**.

NM-XM3 #20-36 RT: 0.81-1.35 AV: 17 NL: 3.37E6
T: FTMS + p ESI Full ms [700.0000-1000.0000]

Figure S15. HRMS-ESI(+) spectrum of compound **2C**.

Figure S16. ¹H NMR spectrum of compound **2d** in DMSO-d₆.

Figure S17. Partial COSY (¹H/¹H) spectrum of compound **2d** in DMSO-d₆.

Figure S18. ^{13}C NMR spectrum of compound **2d** in DMSO-d_6 .

Figure S19. MS-ESI(+) spectrum of compound **2d**.

NM-XM4_190225153548 #2-51 RT: 0.08-2.04 AV: 50 NL: 1.46E5
T: FTMS + p ESI Full ms [700.0000-1000.0000]

Figure S20. HRMS-ESI(+) spectrum of compound **2d**.

Figure S23. ¹³C NMR spectrum of compound **3a** in DMSO-d₆.

Figure S24. MS-ESI(+) spectrum of compound **3a**.

NM-XM1-MAIS #19-41 RT: 0.77-1.44 AV: 23 NL: 4.22E7
T: FTMS + p ESI Full ms [700.0000-1000.0000]

Figure S25. HRMS-ESI(+) spectrum of compound **3a**.

Figure 26. ¹H NMR spectrum of compound **3b** in DMSO-d₆.

Figure S27. ¹³C NMR spectrum of compound **3b** in DMSO-d₆.

NM-XM2-MAIS #19-39 RT: 0.73-1.40 AV: 21 NL: 6.68E5

T: FTMS + p ESI Full ms [800.0000-1200.0000]

Figure S28. HRMS-ESI(+) spectrum of compound **3b**.

Figure S29. ¹H NMR spectrum of compound **3c** in DMSO-d₆.

Figure S30. Partial COSY (¹H/¹H) spectrum of compound **3c** in DMSO-d₆.

Figure S31. ^{13}C NMR spectrum of compound **3c** in DMSO-d_6 .

Figure S32. MS-ESI(+) spectrum of compound **3c**.

NM-XM3-MAIS #21-44 RT: 0.82-1.55 AV: 24 NL: 7.02E6
T: FTMS + p ESI Full ms [800.0000-1200.0000]

Figure S33. HRMS-ESI(+) spectrum of compound **3c**.

Figure S36. MS-ESI(+) spectrum of compound **3d**.

NM-856_190325103145 #20-35 RT: 0.67-1.17 AV: 16 NL: 9.09E4
T: FTMS + p ESI Full ms [800.0000-900.0000]

Figure S37. HRMS-ESI(+) spectrum of compound 3d.