Supporting Information

Inverted methoxypyridinium phthalocyanines for PDI of pathogenic bacteria

Leandro M. O. Lourenço,[a] Andreina Sousa,[b] Maria C. Gomes,[a,b] Maria A. F. Faustino,[a] Adelaide Almeida,[b] Artur M. S. Silva,[a] Maria G. P. M. S. Neves,[a] José A. S. Cavaleiro,[a] Ângela Cunha,[b] João P. C. Tomé[a,c*]

[a]*Department of Chemistry & QOPNA, University of Aveiro, 3810-193 Aveiro, Portugal.*

[b]*Department of Biology and CESAM, University of Aveiro, 3810-193 Aveiro, Portugal.*

[c]*Department of Organic and Macromolecular Chemistry, Ghent University, B-9000 Gent, Belgium.*

Contents

1 Experimental section

1.1 NMR spectra of phthalonitrile and phthalocyanine derivatives

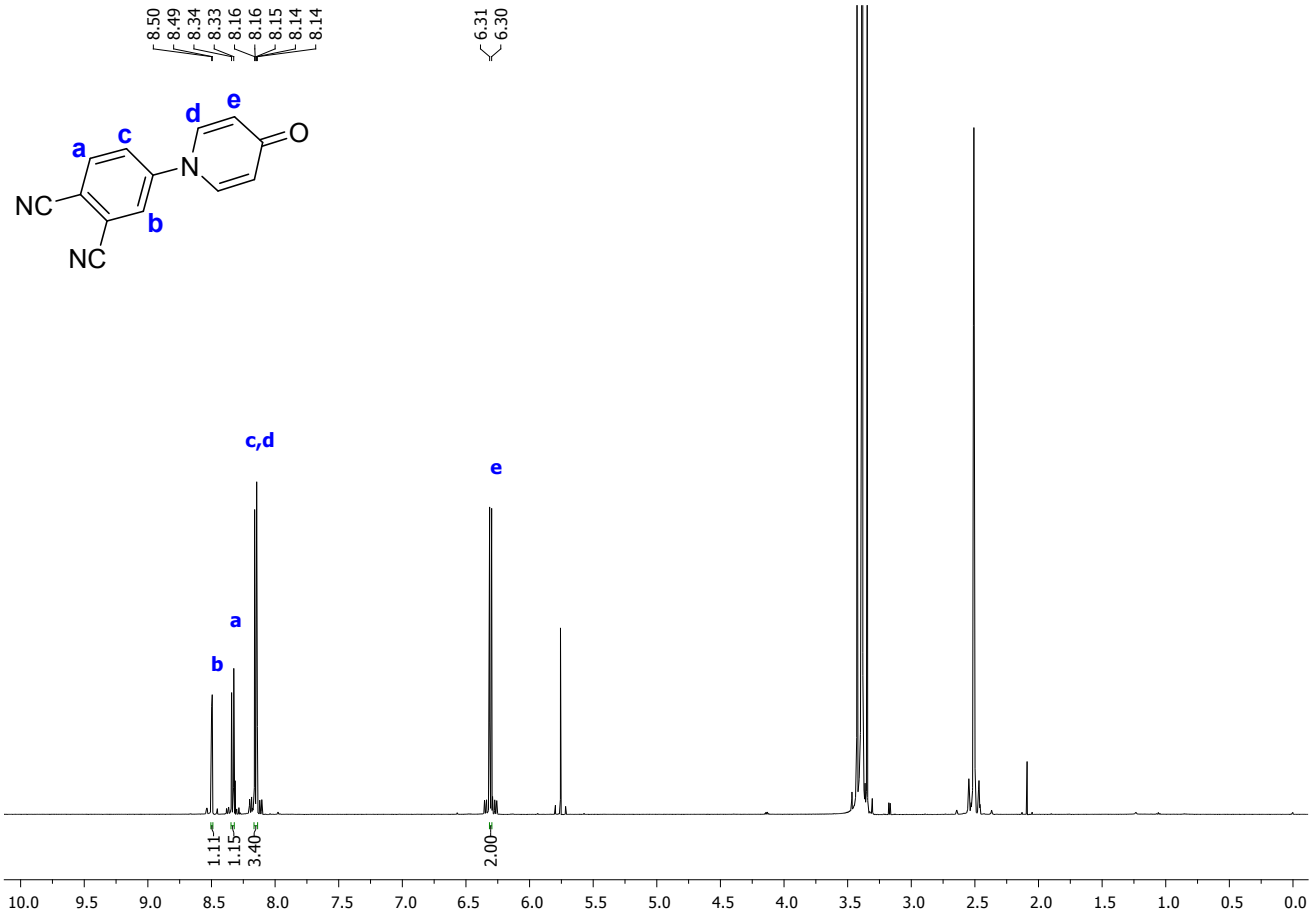

Figure SI 1 – ^{1}H NMR spectrum of compound **1** in DMSO-d_6.

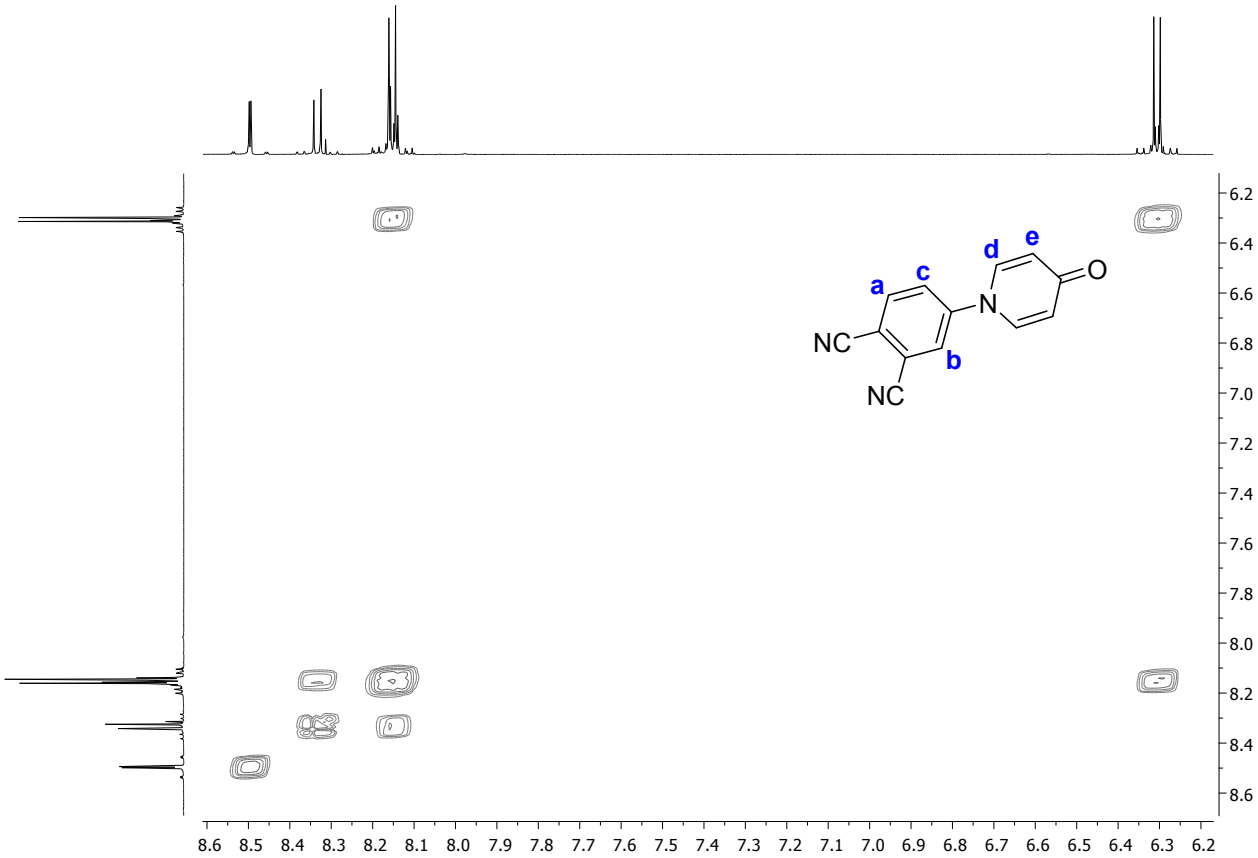

Figure SI 2 – COSY 2D ^{1}H-^{1}H NMR spectrum of compound **1** in DMSO-d_6.

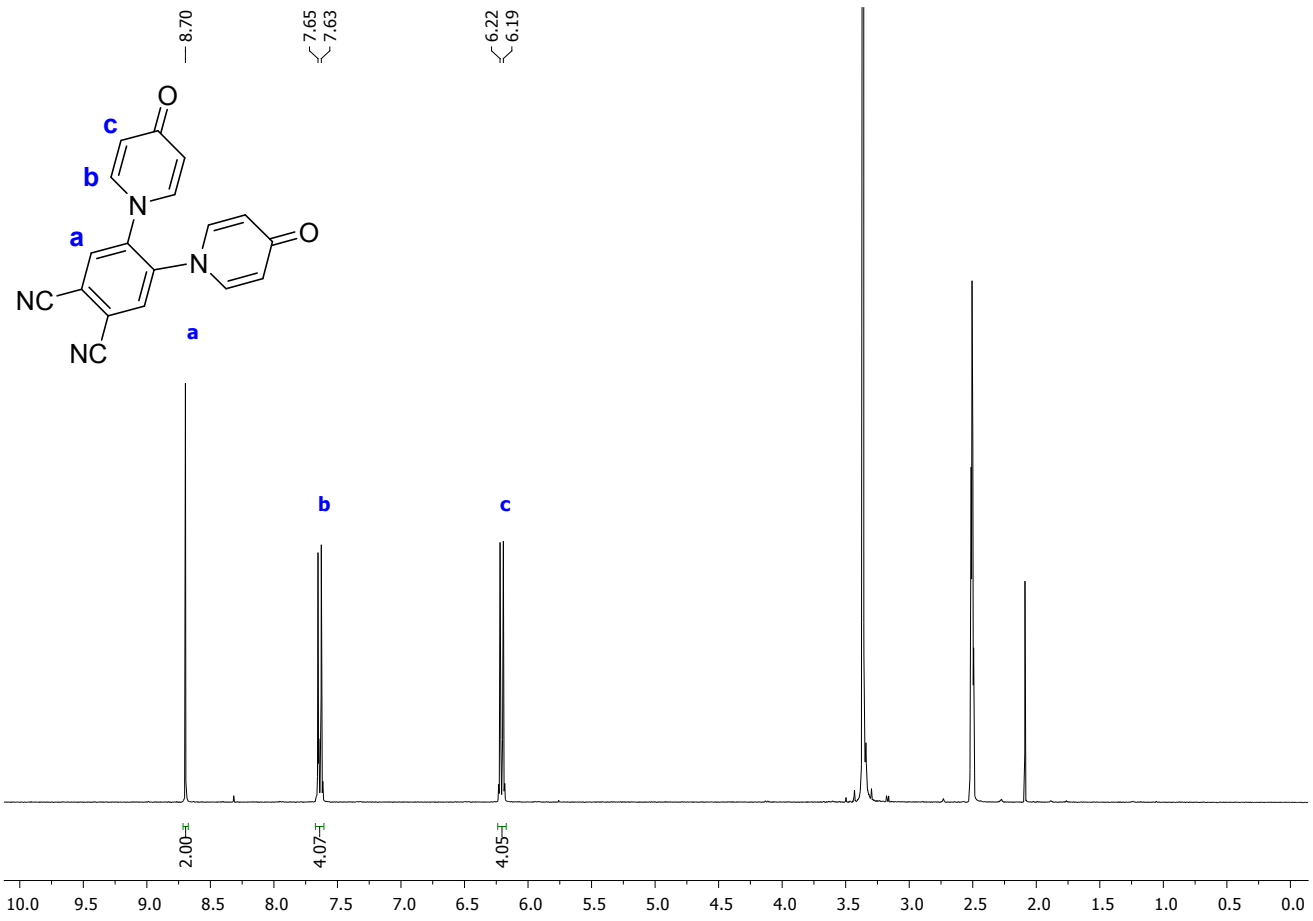

Figure SI 3 – ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

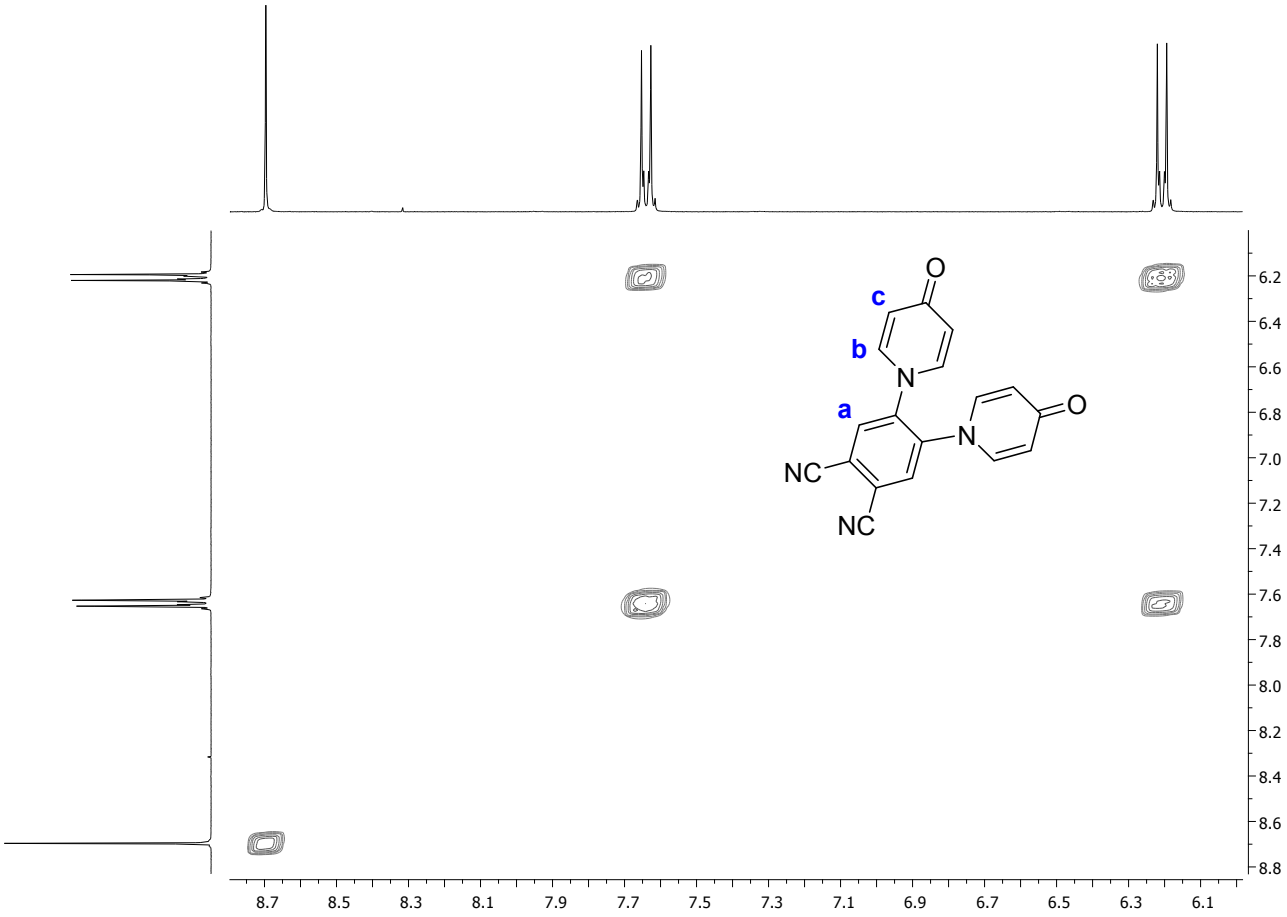

Figure SI 4 – COSY 2D ^{1}H-^{1}H NMR spectrum of compound **2** in DMSO-d_6.

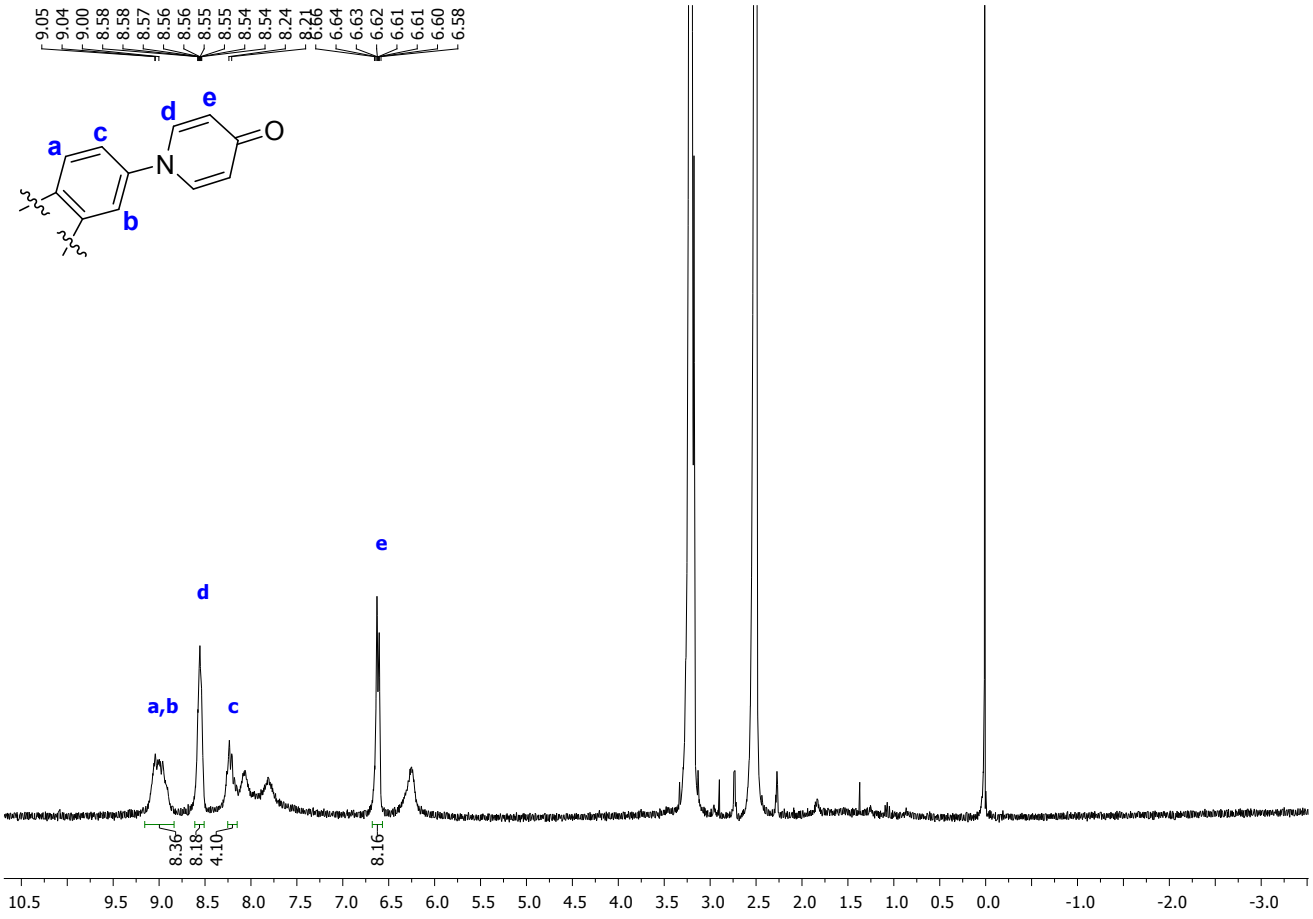

Figure SI 5 – ^{1}H NMR spectrum of compound **3** in DMSO-d_6.

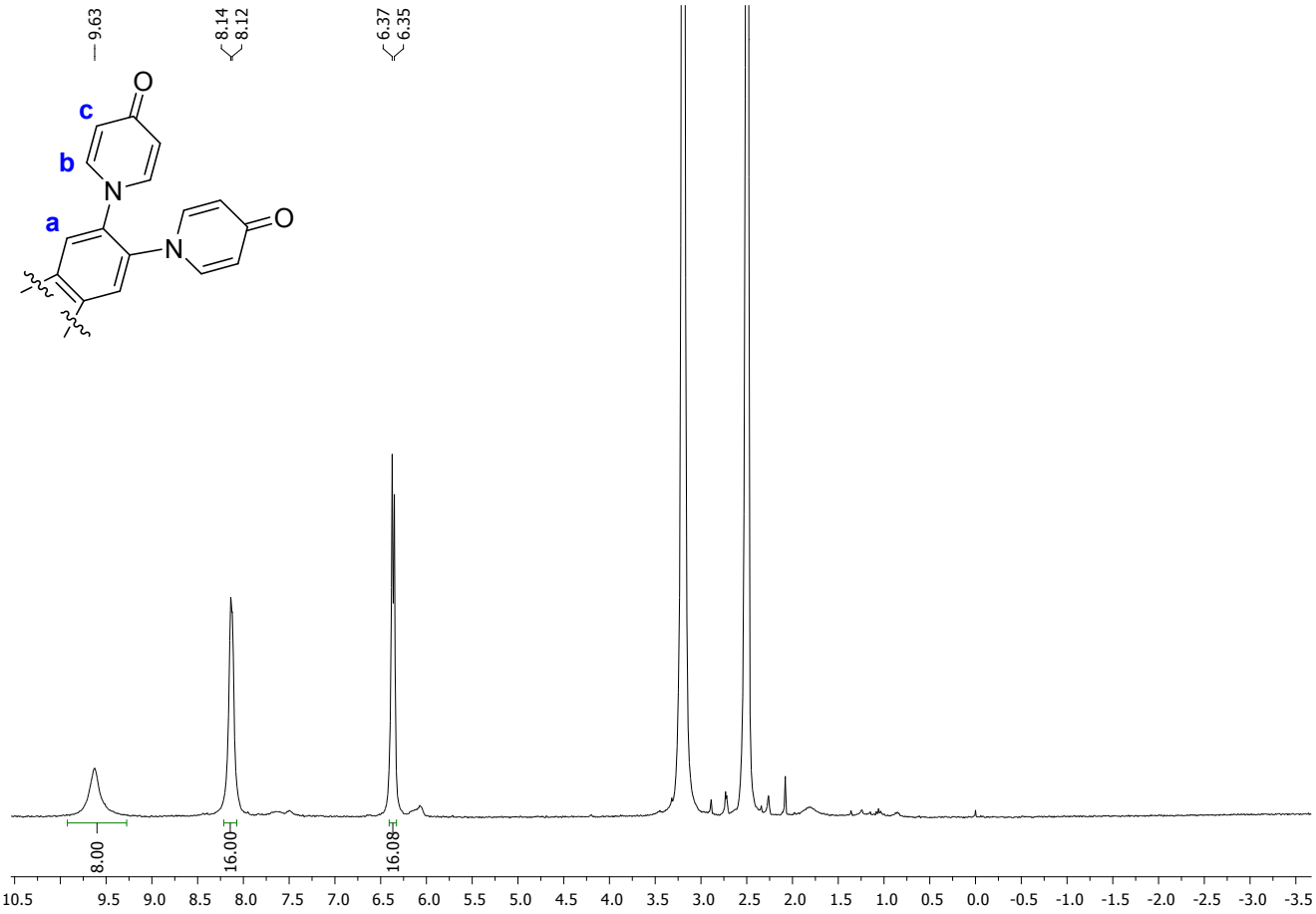

Figure SI 6 – ^{1}H NMR spectrum of compound **4** in DMSO-d_6.

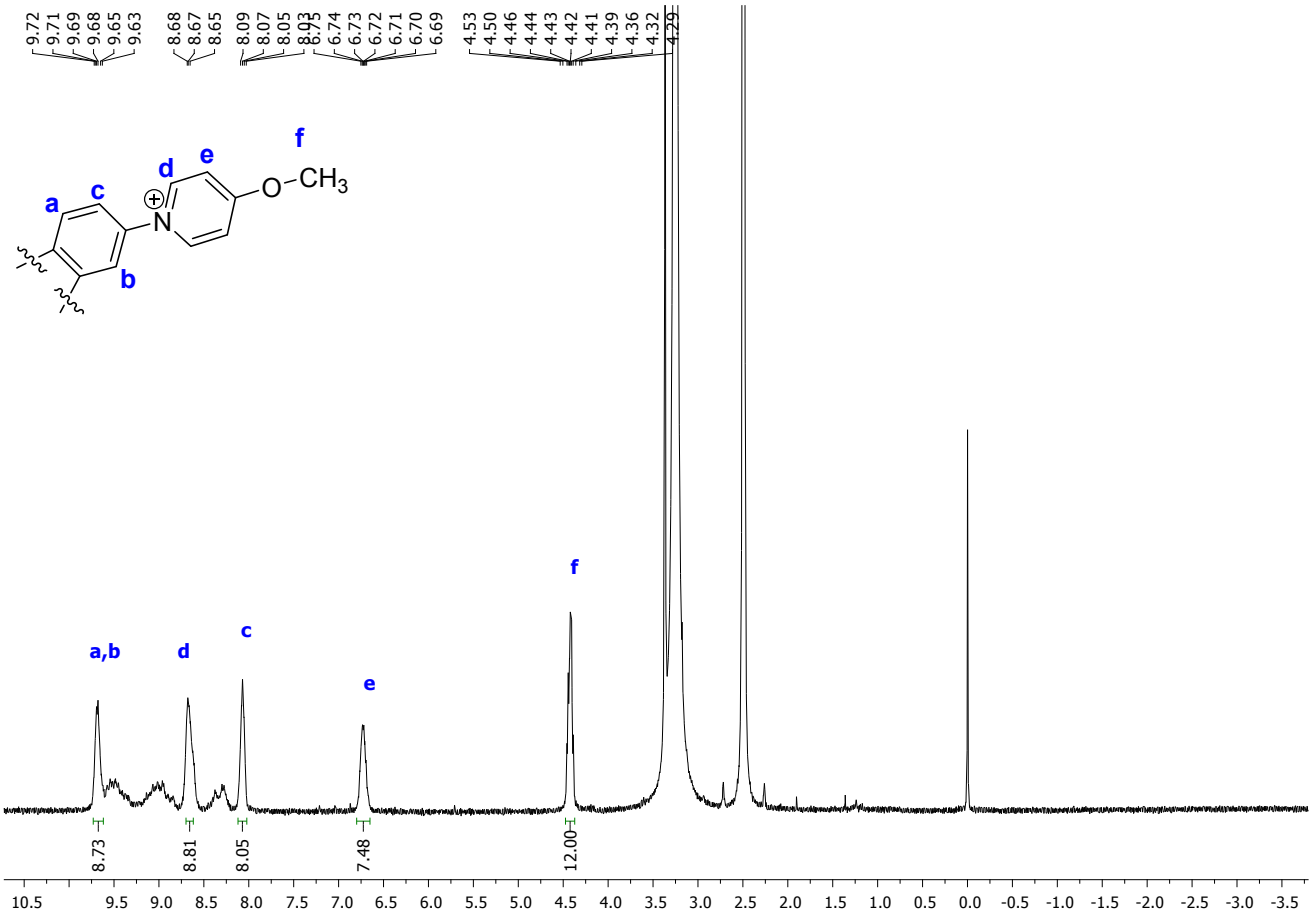

Figure SI 7 – ^{1}H NMR spectrum of compound **5** in DMSO-d_6.

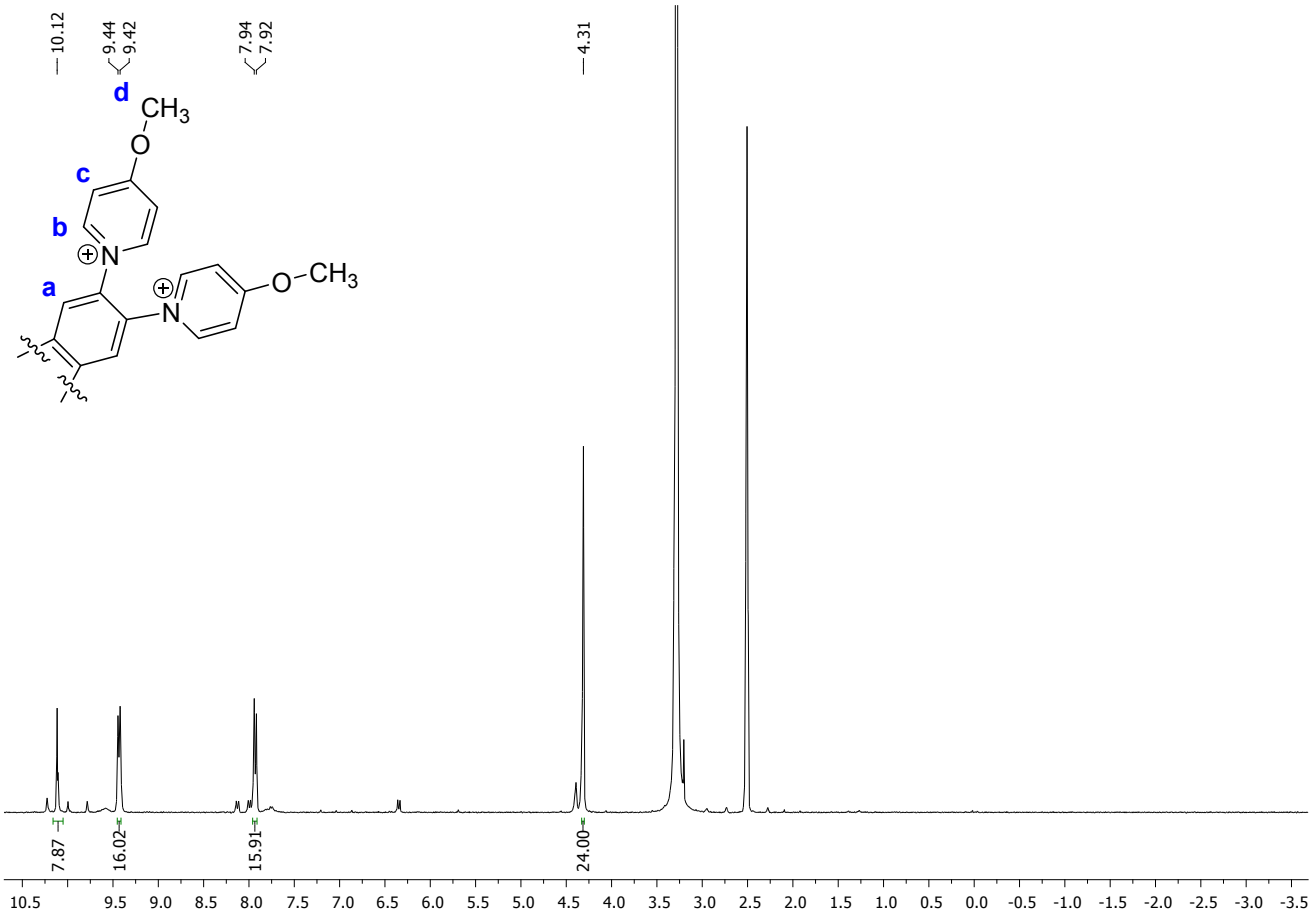

Figure SI 8 – ^{1}H NMR spectrum of compound **6** in DMSO-d_6.

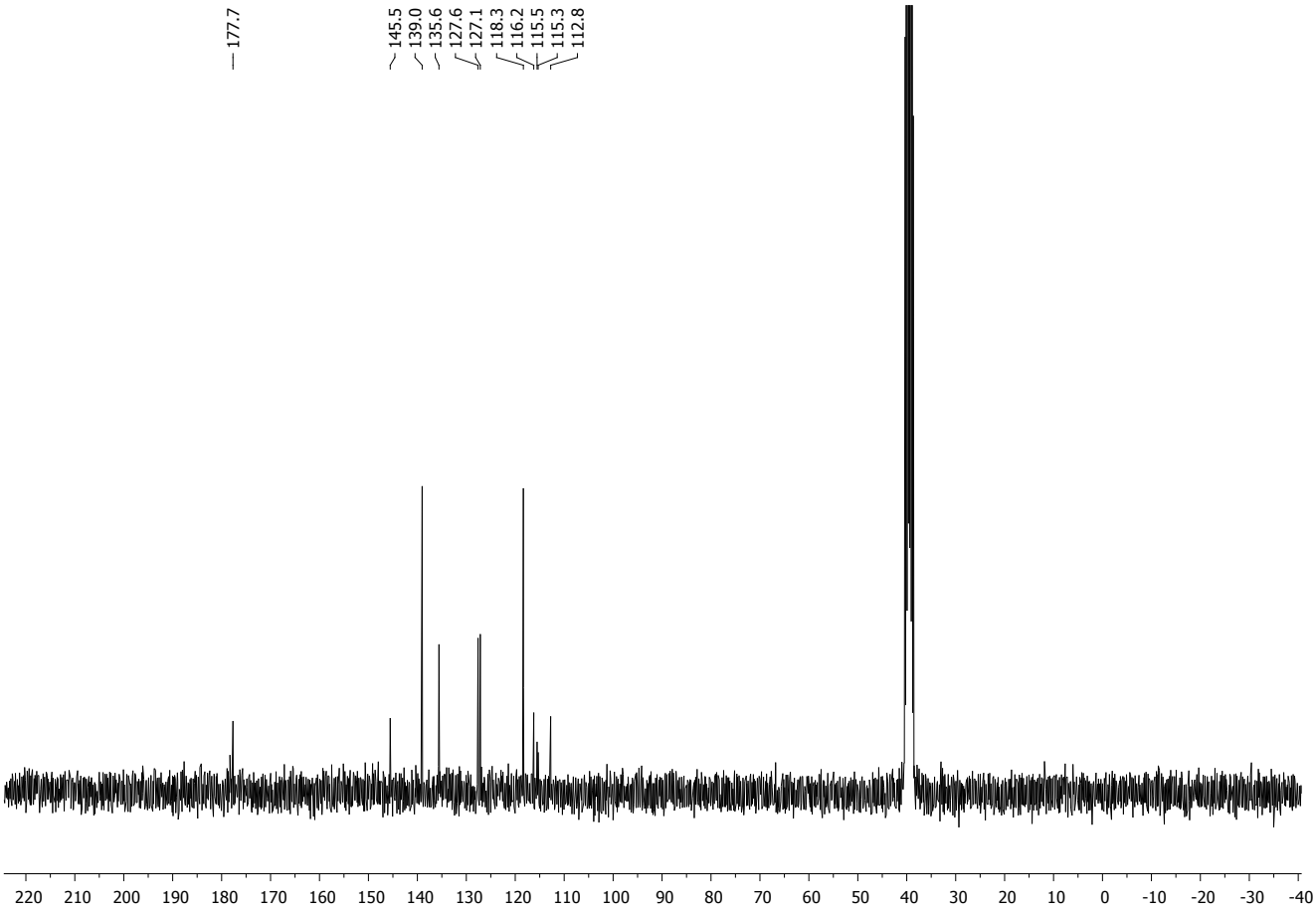

Figure SI 9 – ^{13}C NMR spectrum of compound **1** in DMSO-d_6.

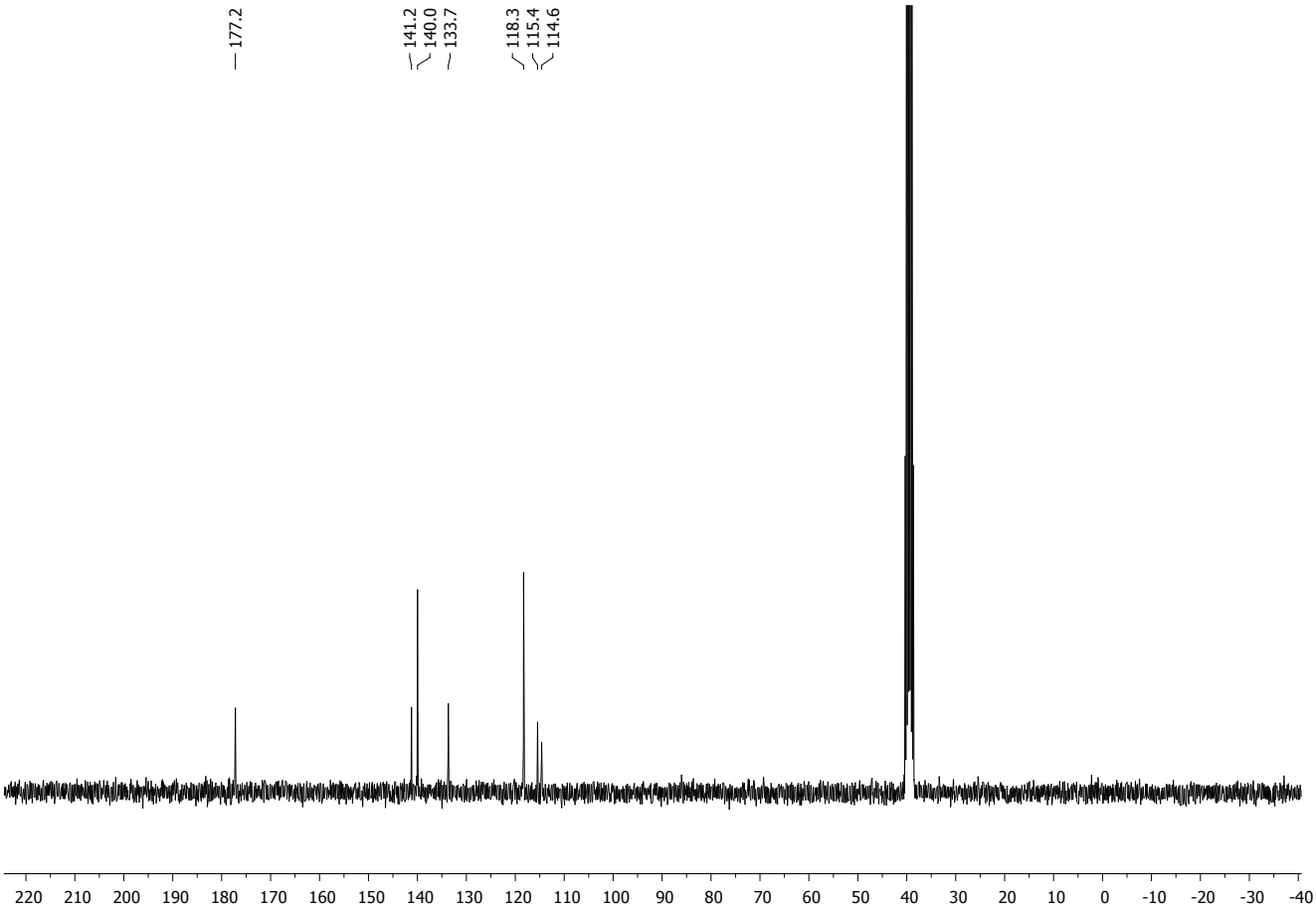

Figure SI 10 – ^{13}C NMR spectrum of compound **2** in DMSO-d_6.

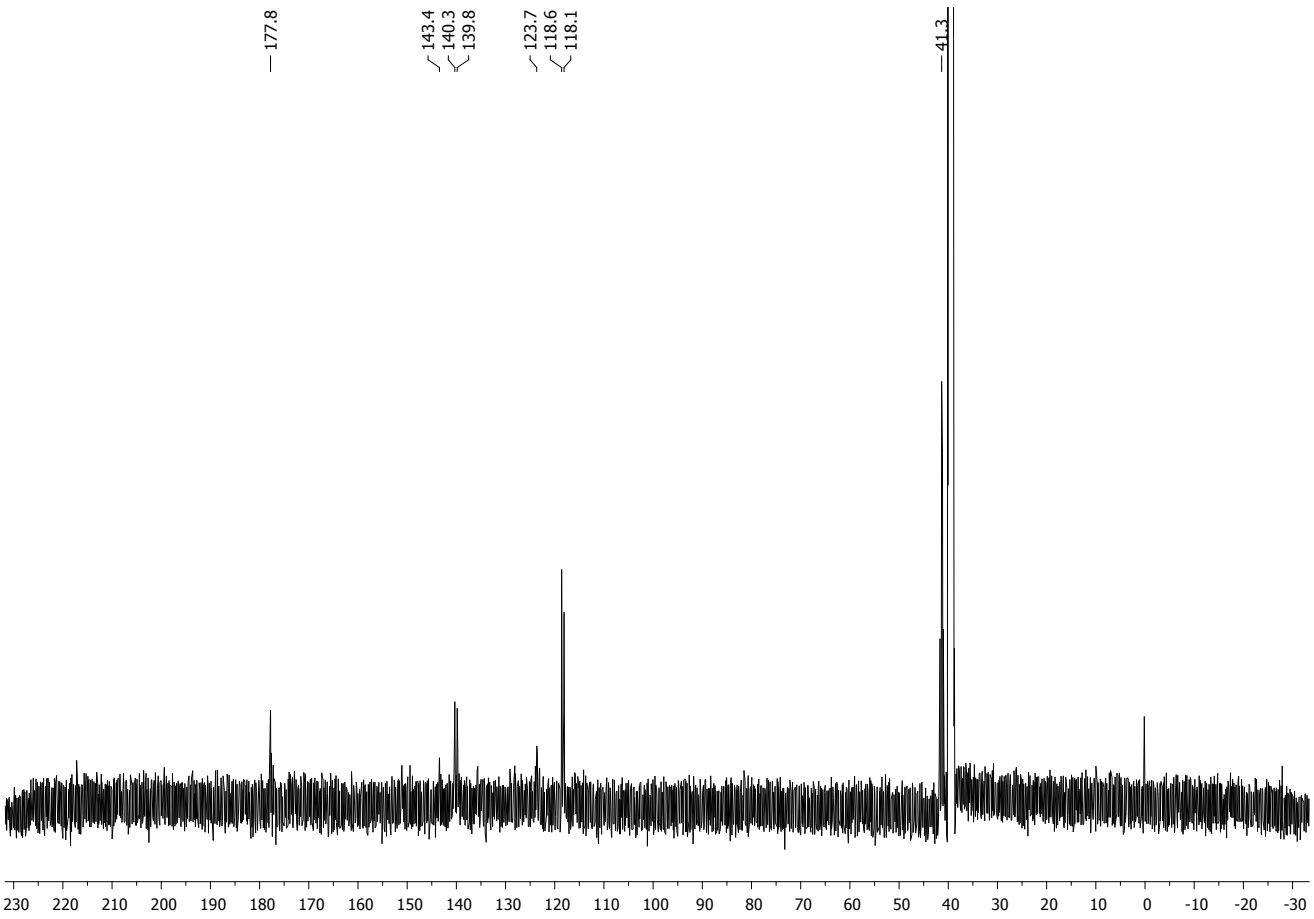

Figure SI 11 – ^{13}C NMR spectrum of compound **3** in DMSO-d_6.

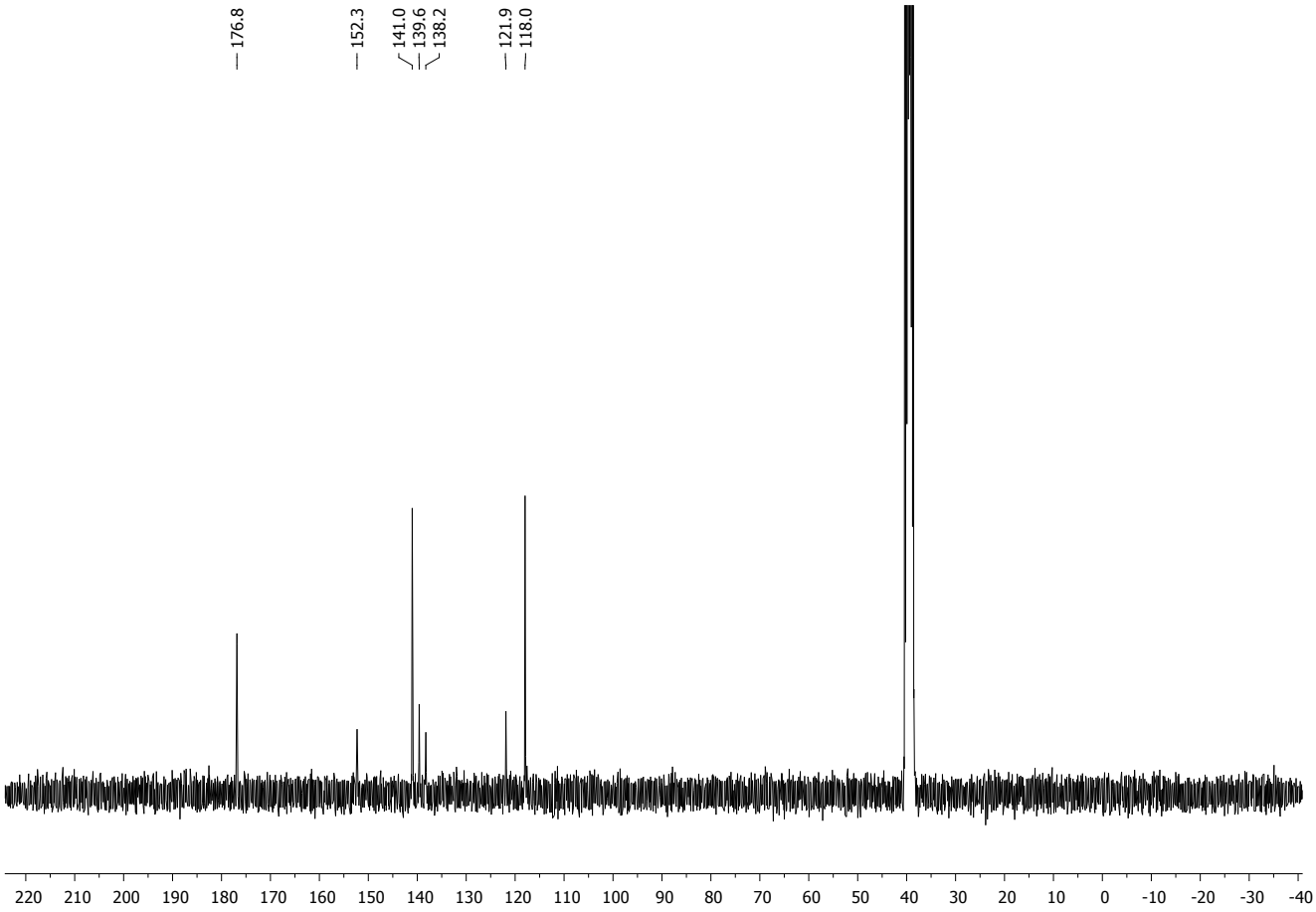

Figure SI 12 – ^{13}C NMR spectrum of compound **4** in DMSO-d_6.

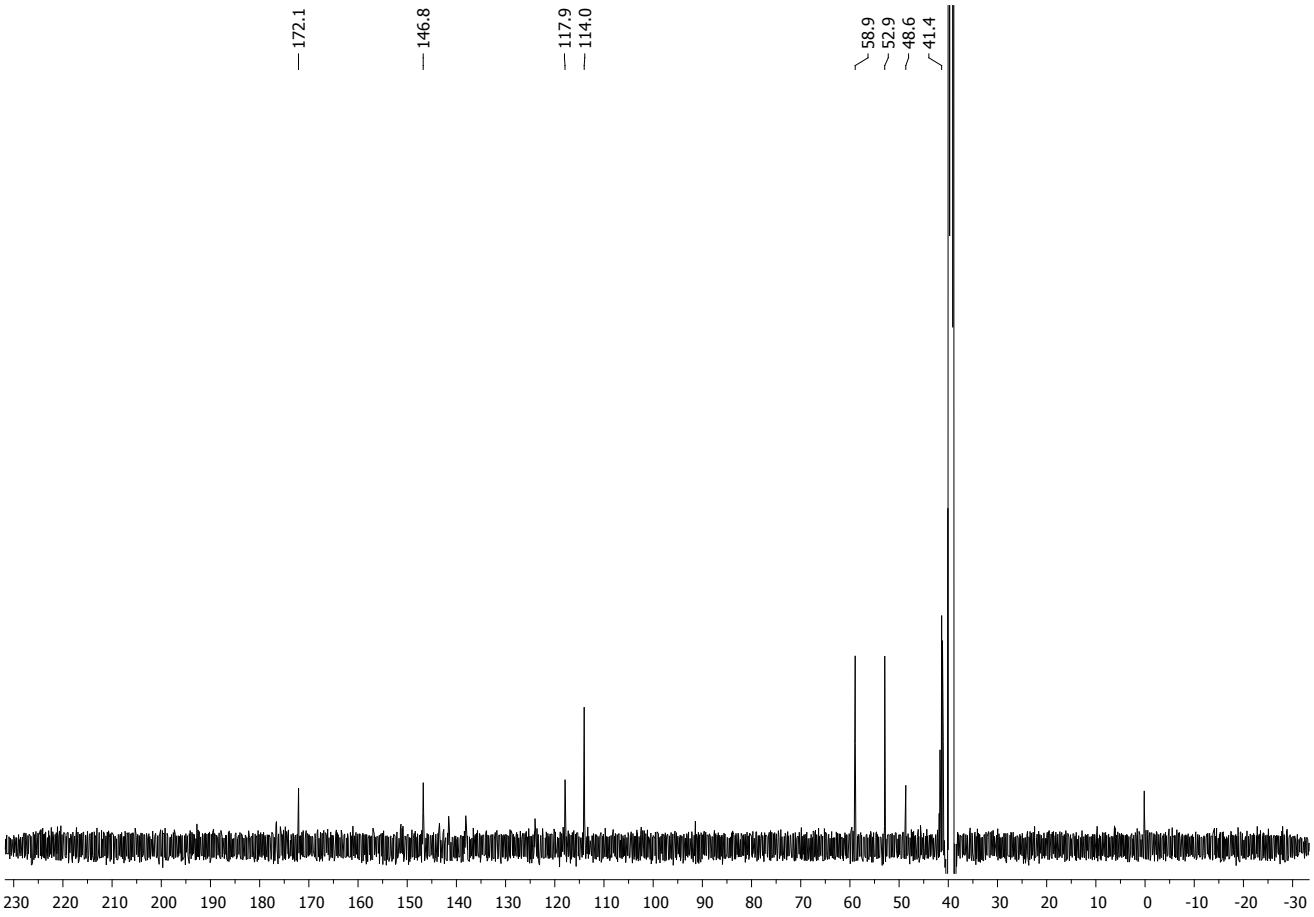

Figure SI 13 – ^{13}C NMR spectrum of compound **5** in DMSO-d_6.

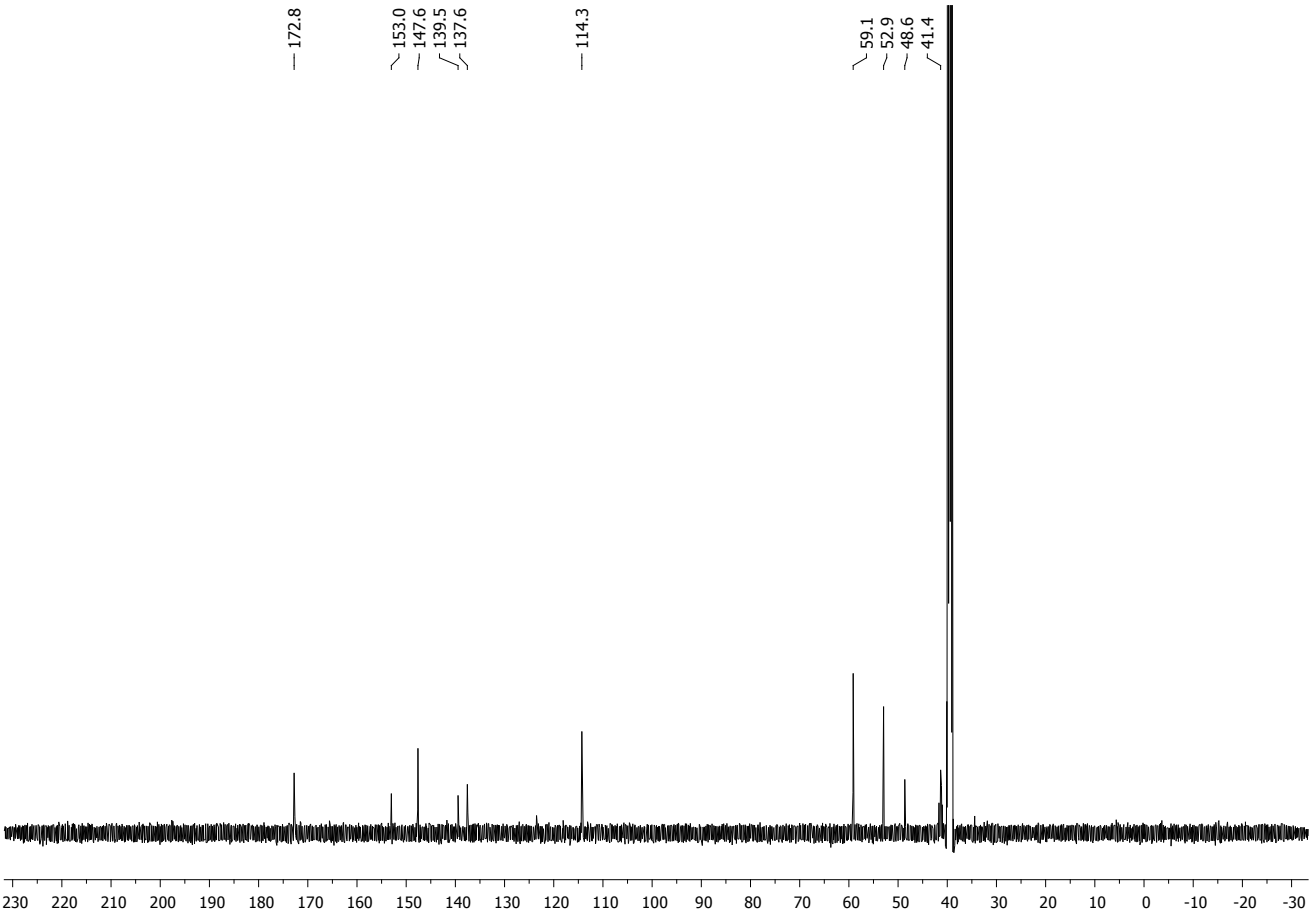

Figure SI 14 – ^{13}C NMR spectrum of compound **6** in DMSO-d_6.

1.2 Mass spectra of phthalonitrile and phthalocyanine derivatives

1.2.1 ESI-MS spectra

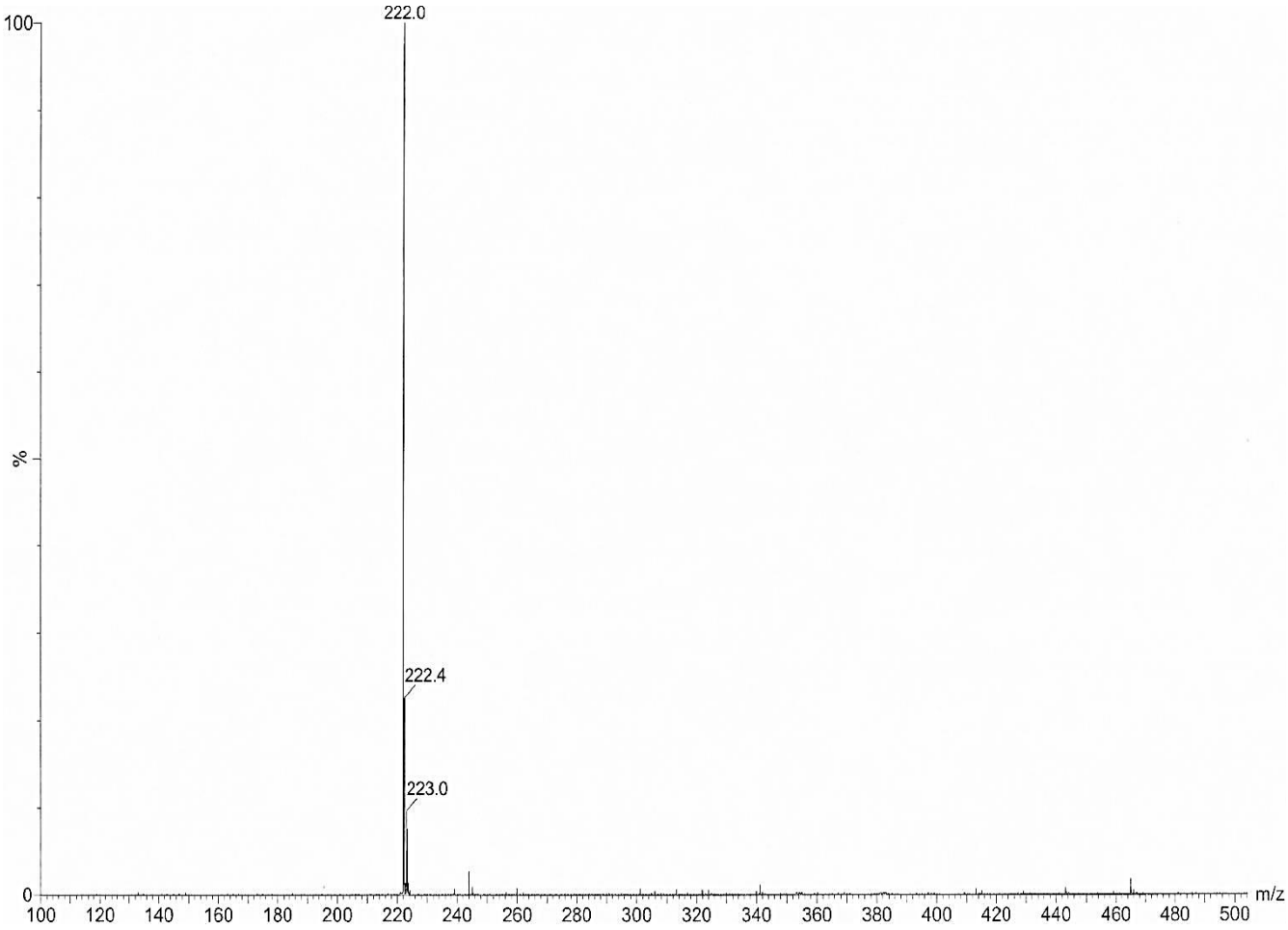

Figure SI 15 – ESI-MS spectrum of compound **1**.

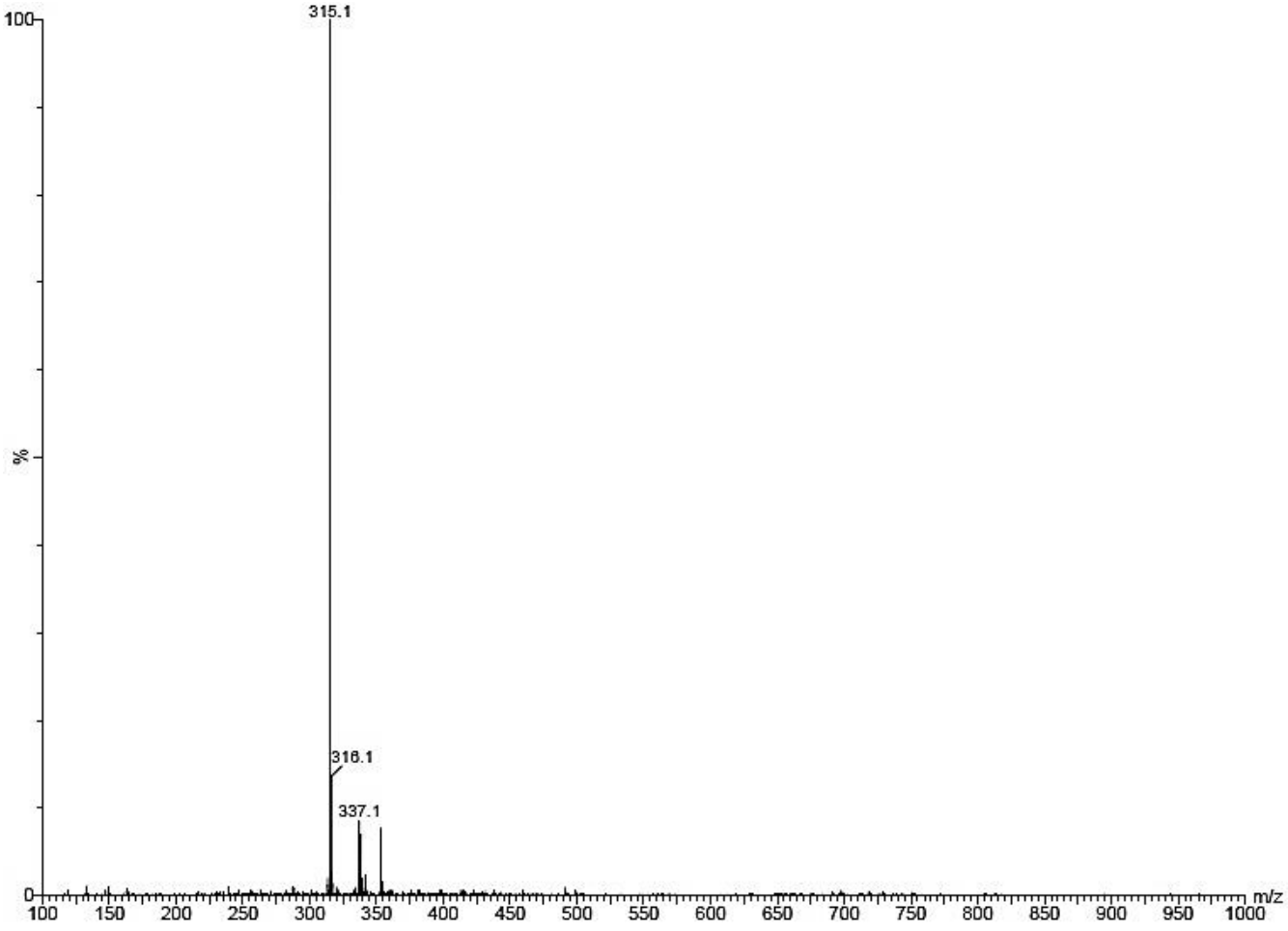

Figure SI 16 – ESI-MS spectrum of compound **2**.

1.2.2 ESI-HRMS spectra

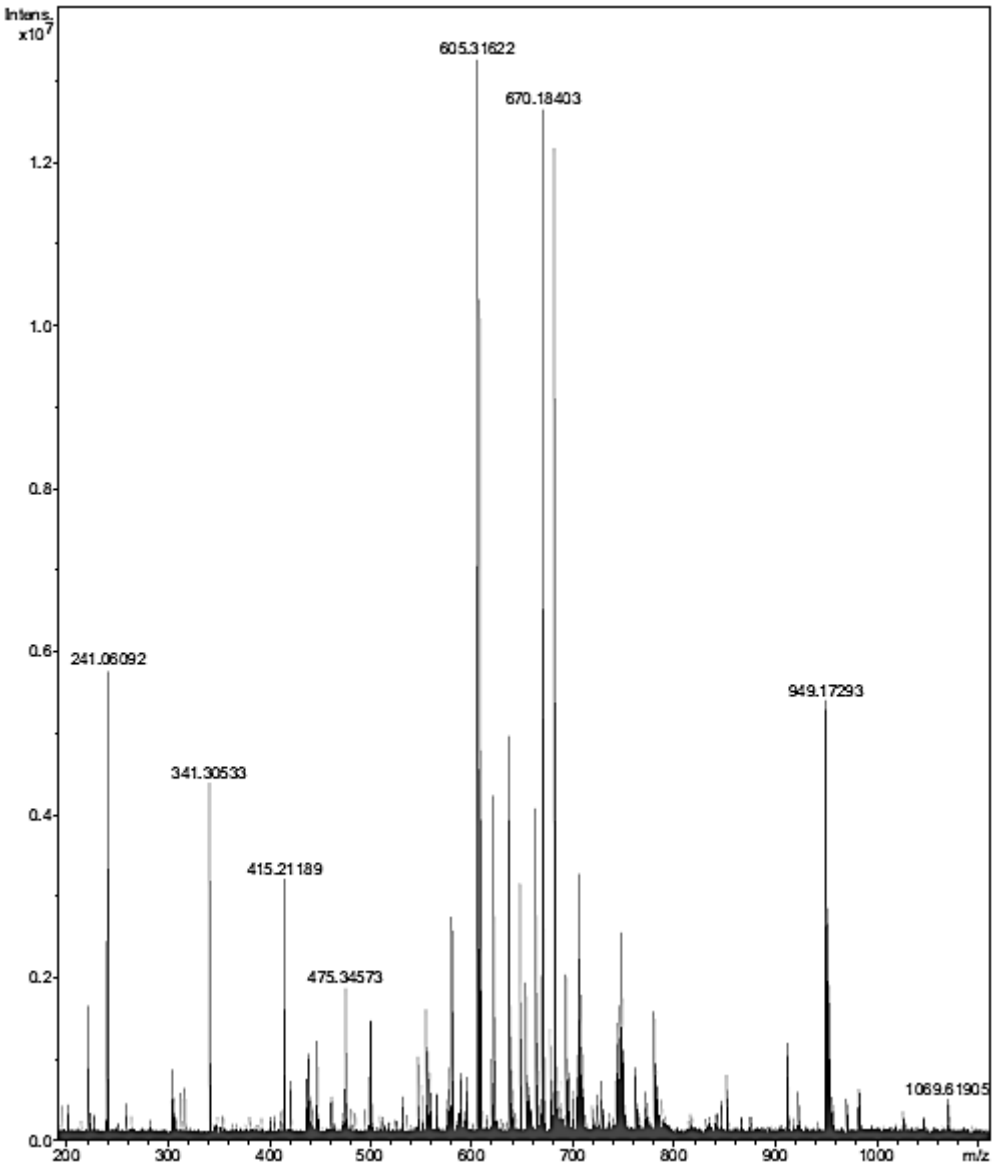

Figure SI 17 – ESI-HRMS spectrum of compound **3**.

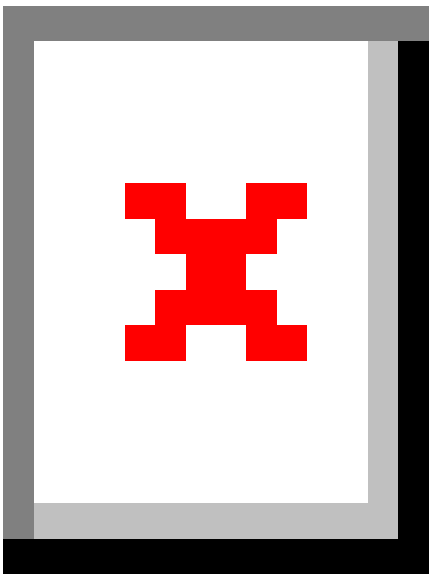

Figure SI 18 – ESI-HRMS spectrum of compound **4**.

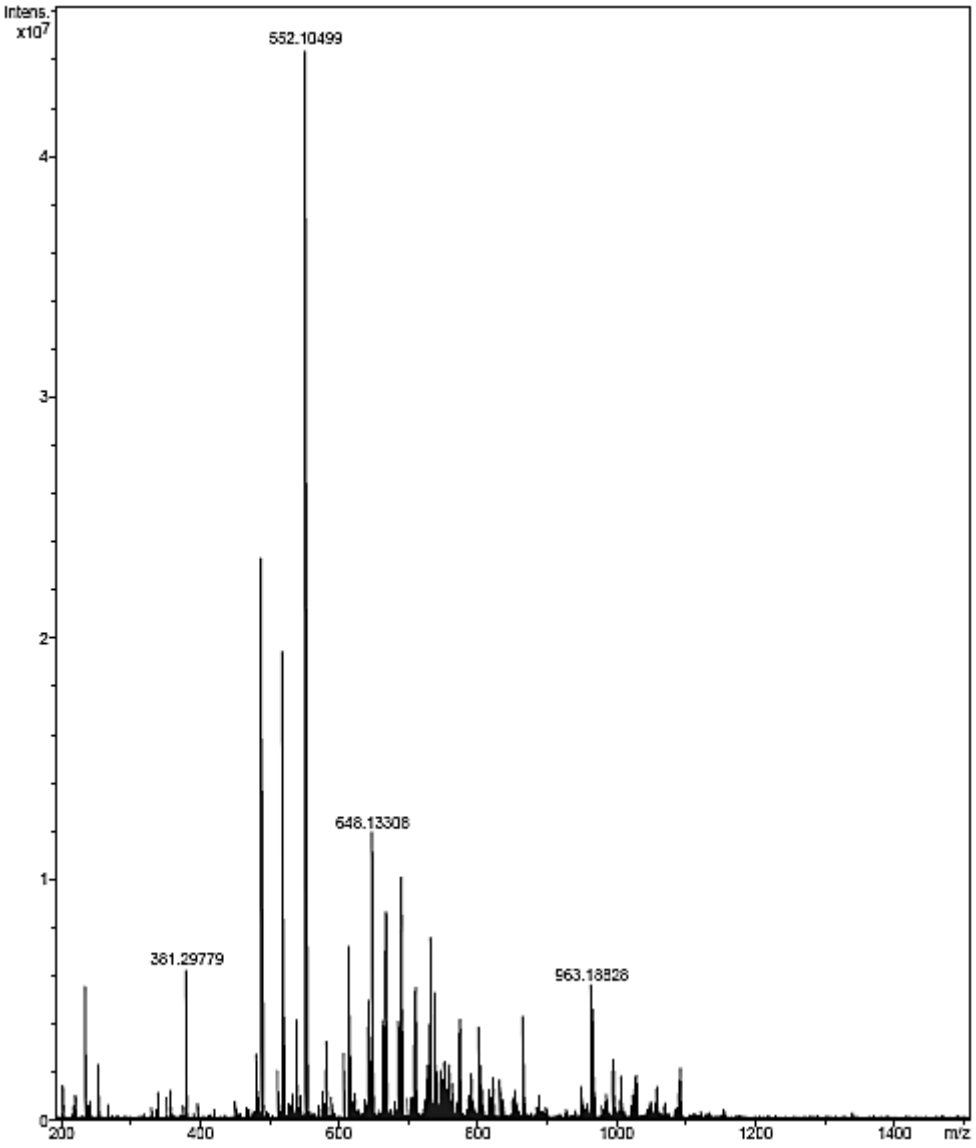

Figure SI 19 – ESI-HRMS spectrum of compound **5**.

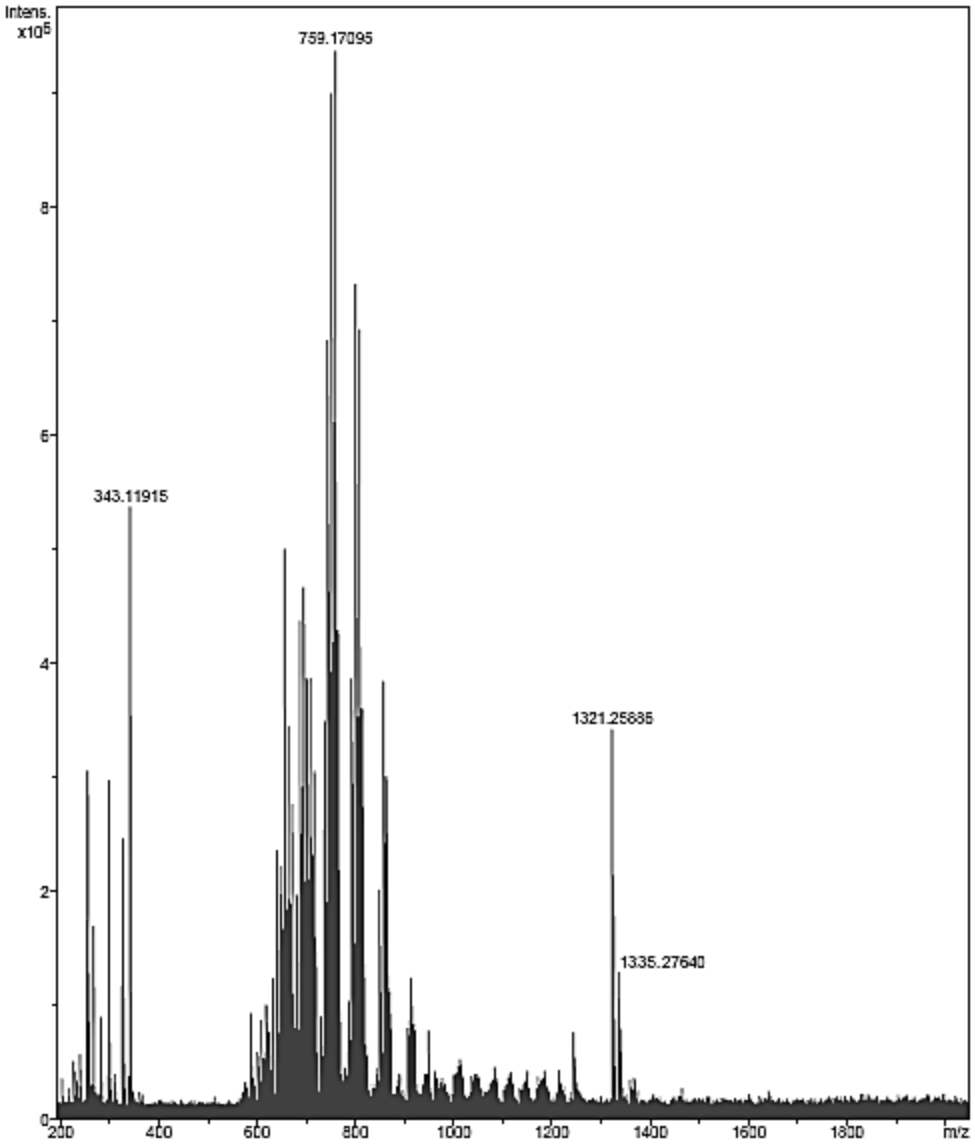

Figure SI 20 – ESI-HRMS spectrum of compound **6**.

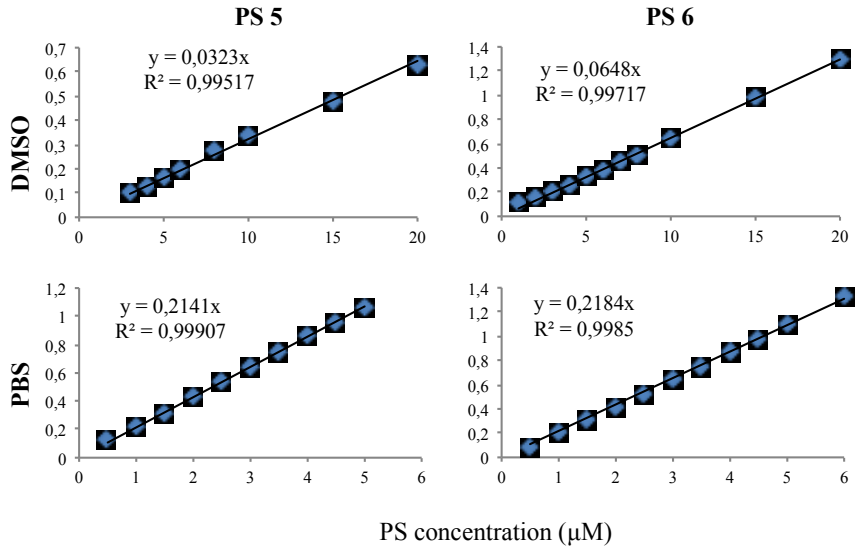

Figure SI 21 – Linear regression graphics of Pcs **5** and **6** plotted the Q-band absorbance *versus* the concentrations in PBS and DMSO.

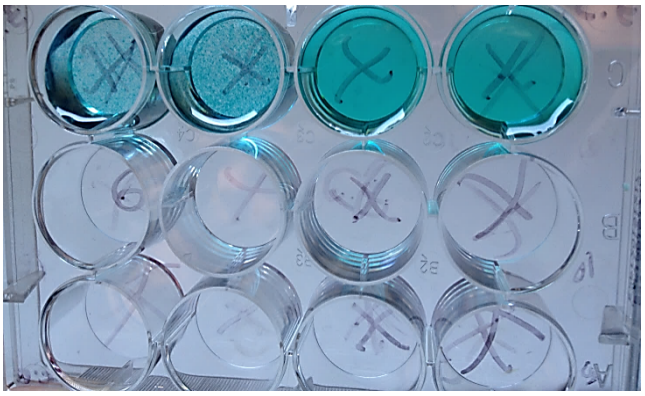

Figure SI 22 – 12-well plate prepared for PDI studies with 20 μM of **5**, two left wells, and **6**, two right wells, after 15 min of pre-incubation in the dark, under gentle shaking conditions.