

Putting a “C₆₀ ball” and Chain to Chlorin e6 Improves Its Cellular Uptake and Photodynamic Performances

Manuele Di Sante,^{1,†} Alena Kaltenbrunner,^{2,†} Marco Lombardo,¹ Alberto Danielli,² Paolo Emidio Costantini,^{2,*} Matteo Di Giosia,^{1,*} Matteo Calvaresi^{1,*}

¹ Dipartimento di Chimica “Giacomo Ciamician”, Alma Mater Studiorum—Università di Bologna, Via Francesco Selmi 2, 40126 Bologna, Italy

² Dipartimento di Farmacia e Biotecnologie, Alma Mater Studiorum—Università di Bologna, Via Francesco Selmi 3, 40126 Bologna, Italy

* Correspondence: paolo.costantini4@unibo.it (P.E.C.); matteo.digiosia2@unibo.it (M.D.G.); matteo.calvaresi3@unibo.it (M.C.)

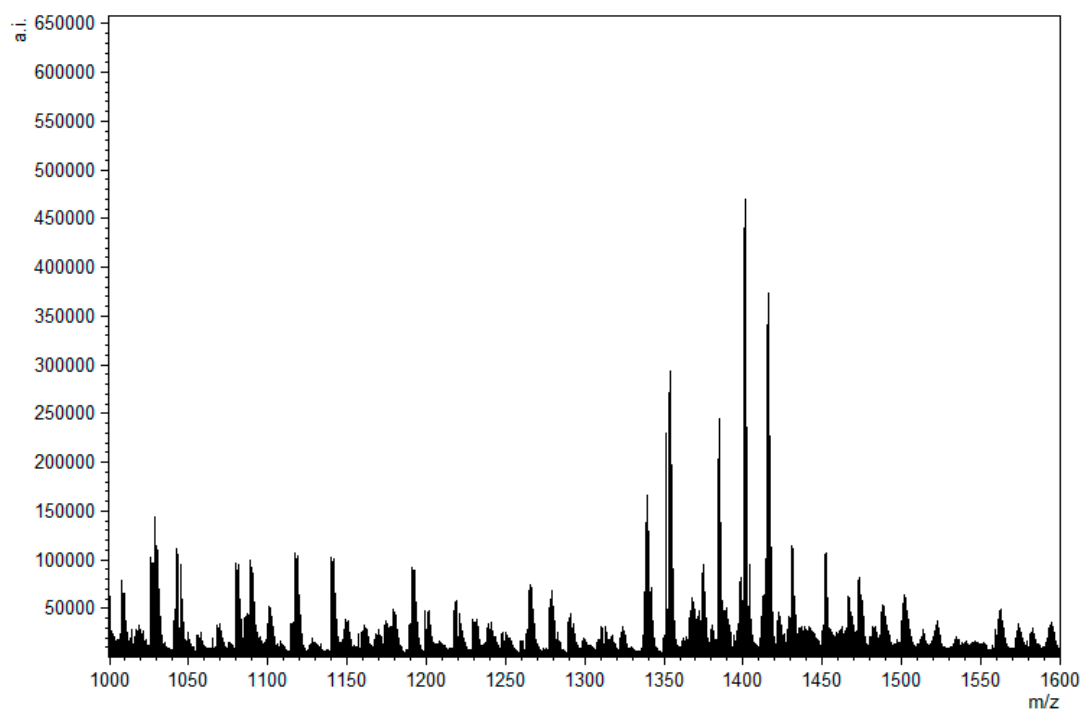


Figure S1. HR ESI-MS of compound Ce6-C₆₀ (MeOH, negative mode, range: 1000-1600 m/z)

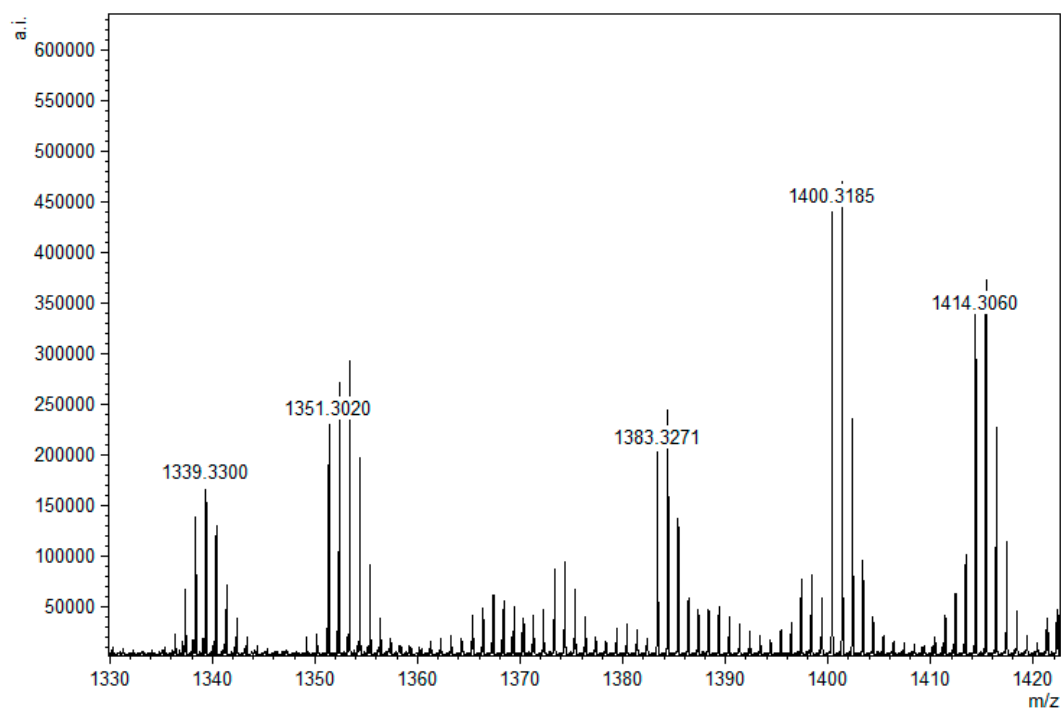


Figure S2. HR ESI-MS of compound Ce6-C₆₀ (MeOH, negative mode, range: 1330-1420 m/z)

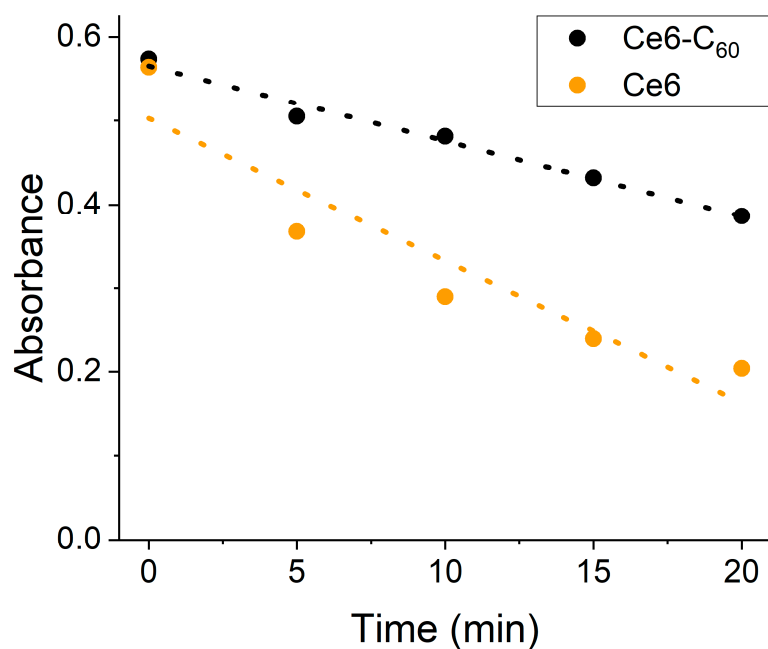


Figure S3. Absorbance at 401 nm of ABMDMA vs. irradiation time, under red light irradiation (irradiance 6.32 mW/cm^2), in the presence of Ce6-C₆₀ (black dots) and Ce6 (gold dots) at $0.5 \mu\text{M}$ concentration. Curve fitting equations (represented as dotted lines) are used to calculate the quantum yield.

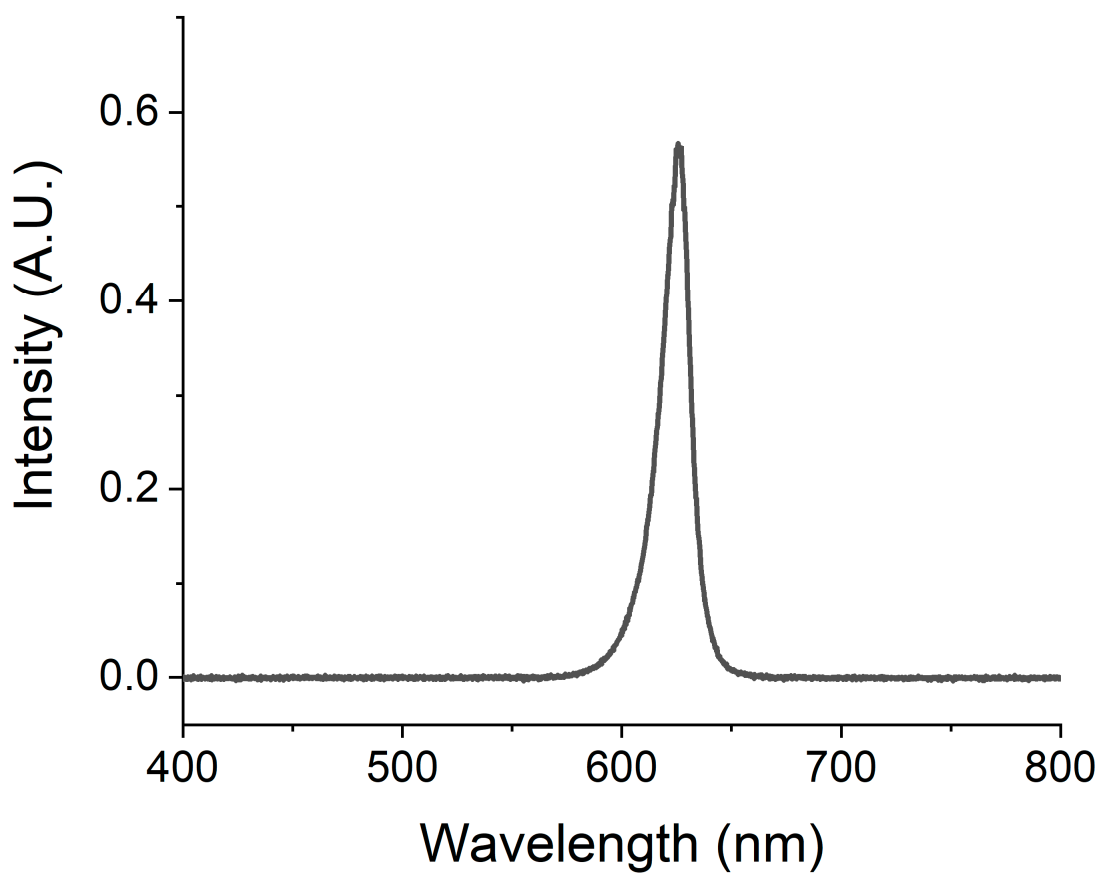


Figure S4. Spectral profile of the red light lamp (LED SMD 50W RGB)

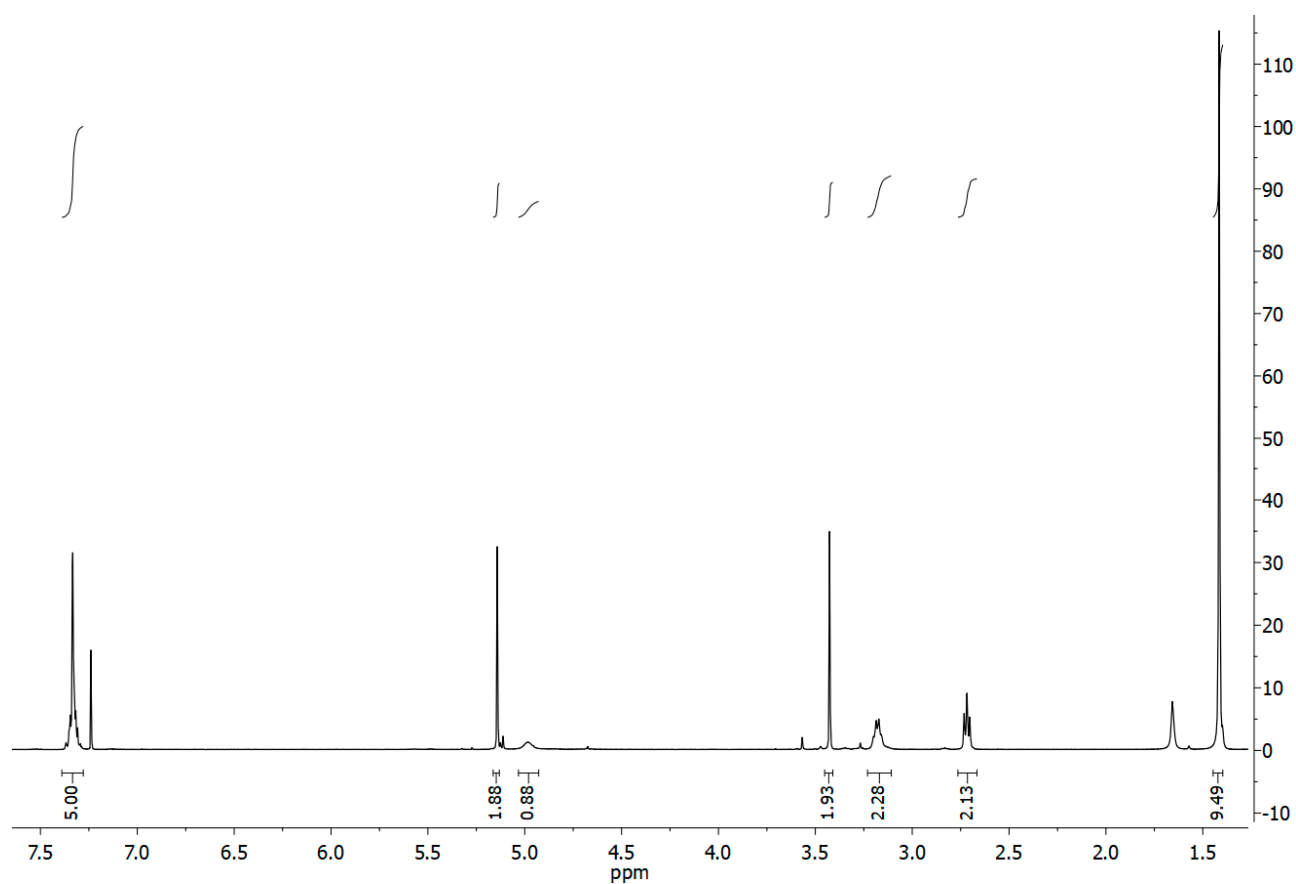


Figure S5. ^1H NMR of compound **2** (400 MHz, Chloroform-*d*)

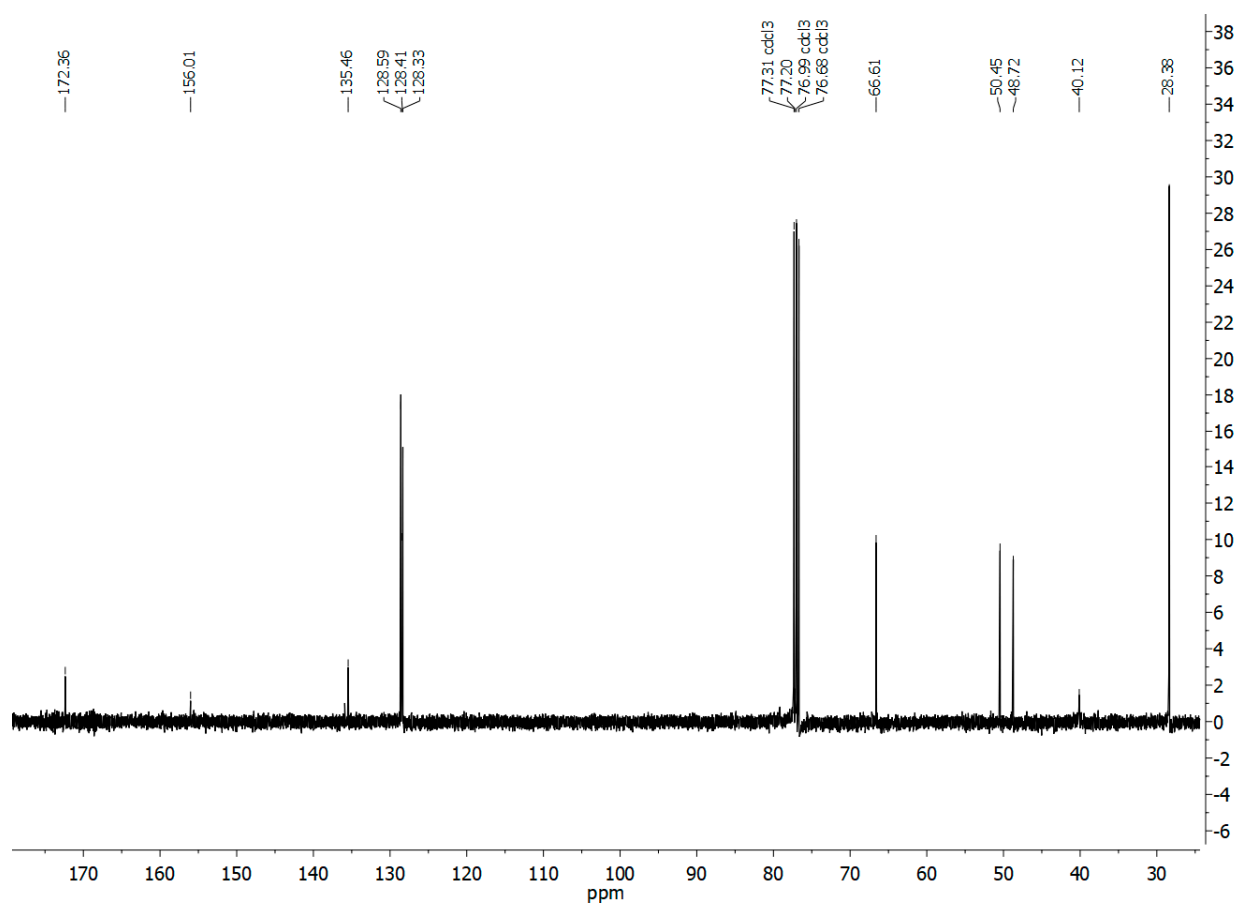


Figure S6. ^{13}C NMR of compound **2** (100 MHz, Chloroform-*d*)

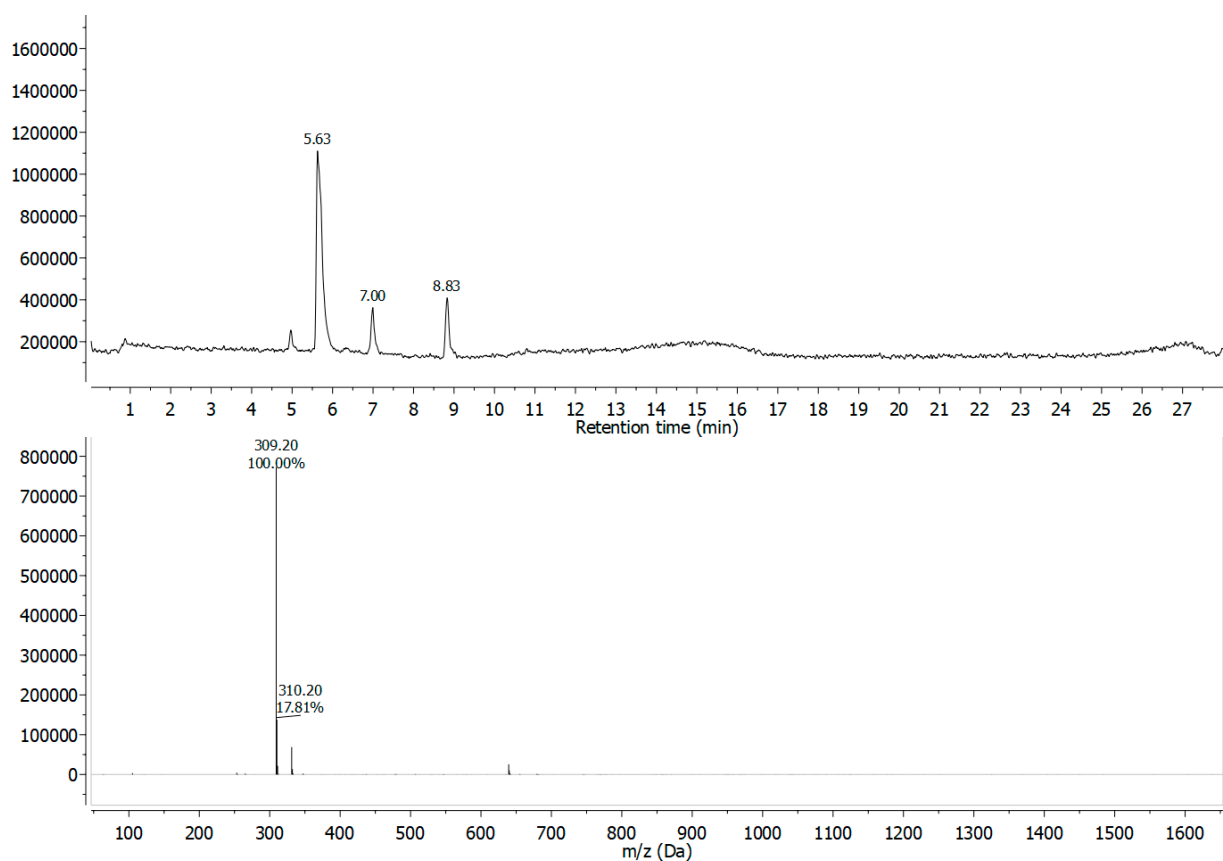


Figure S7. HPLC-MS of compound **2** (Acetonitrile)

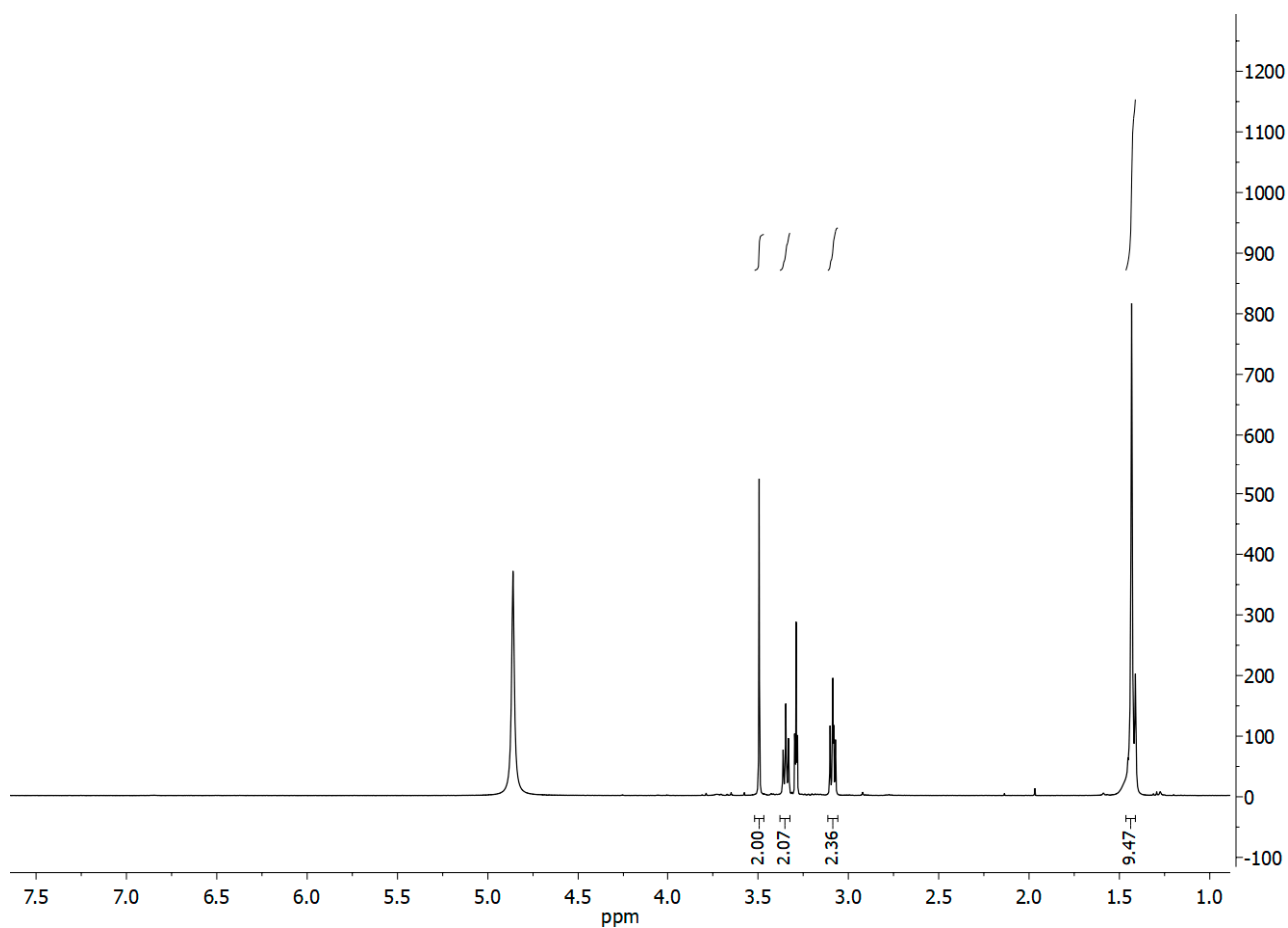


Figure S8. ¹H NMR of compound **3** (400 MHz, CD₃OD)

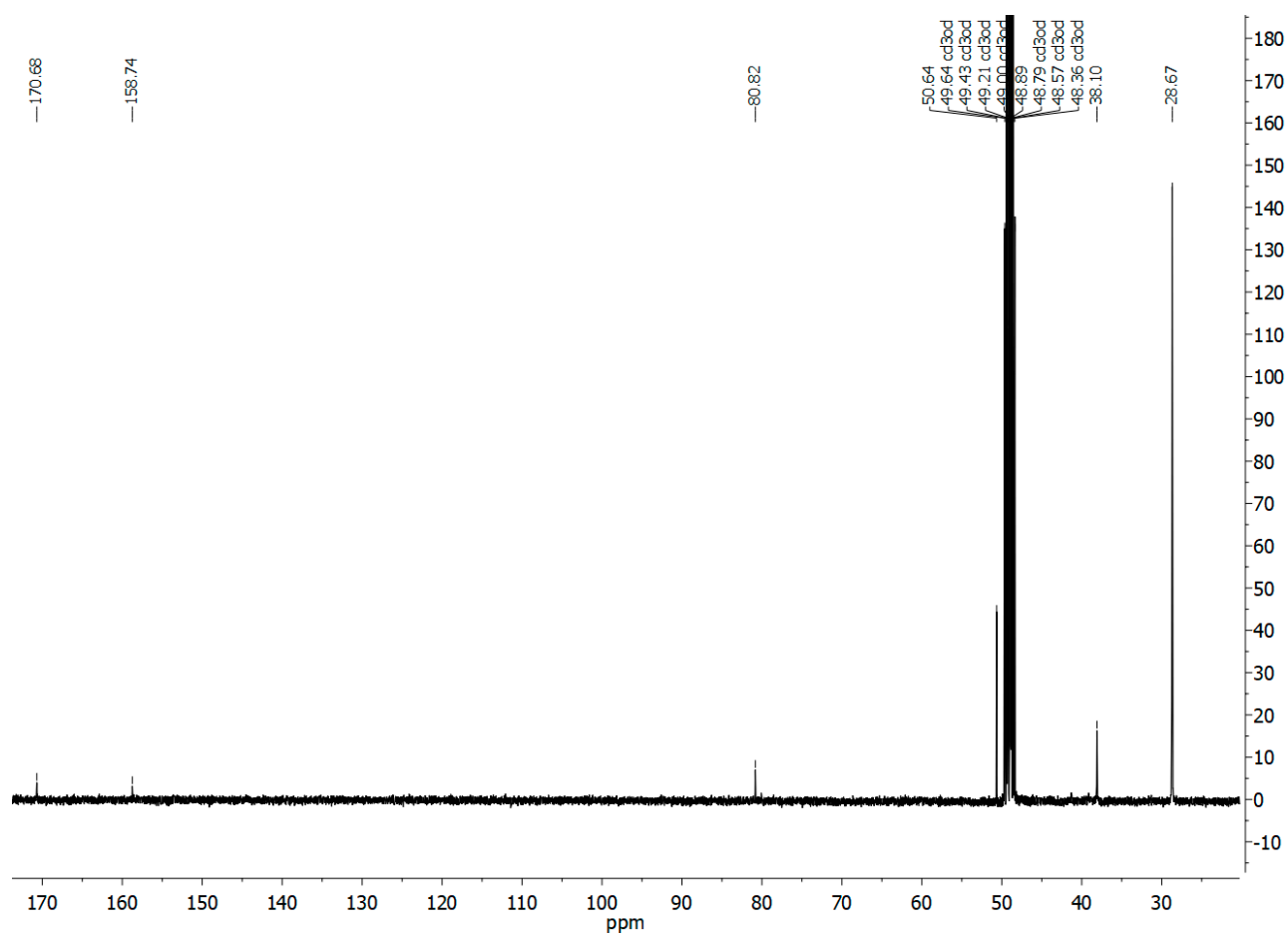


Figure S9. ¹³C NMR of compound **3** (100 MHz, CD₃OD)

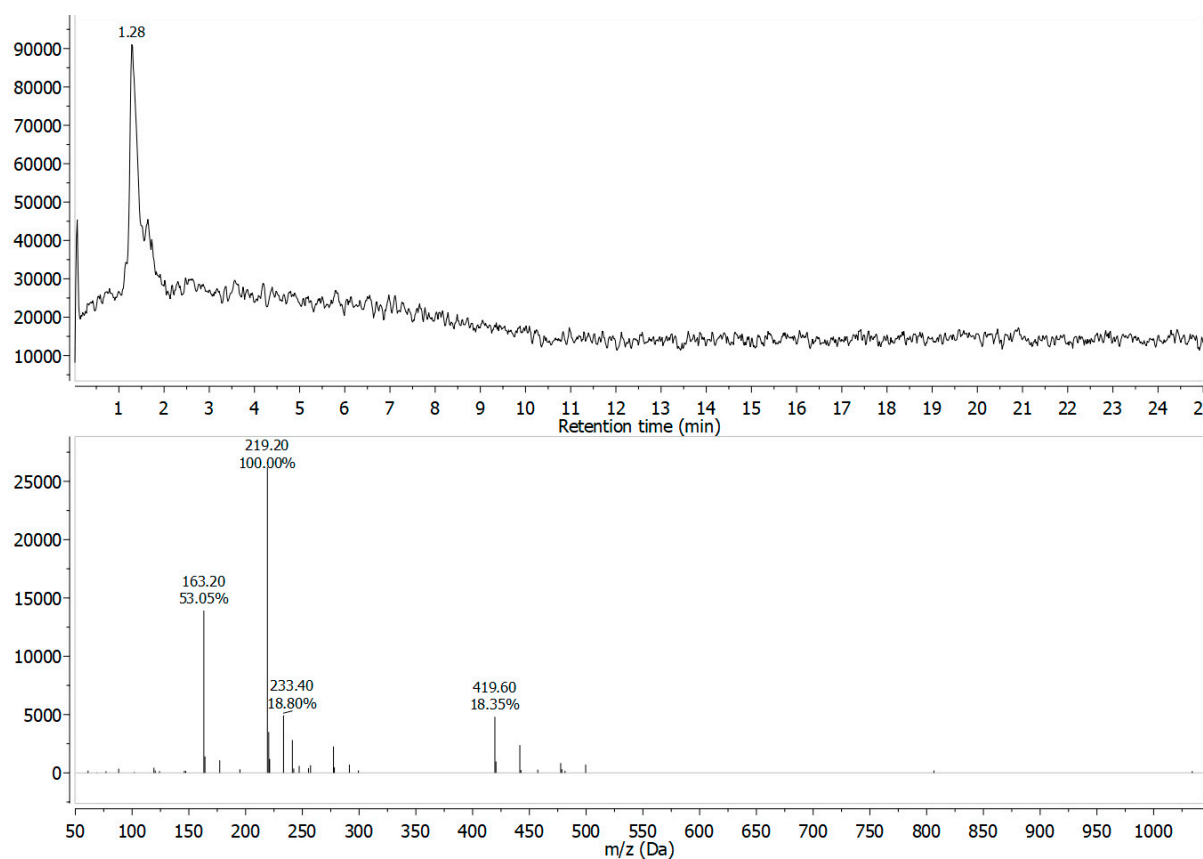


Figure S10. HPLC-MS of compound **3** (Acetonitrile)

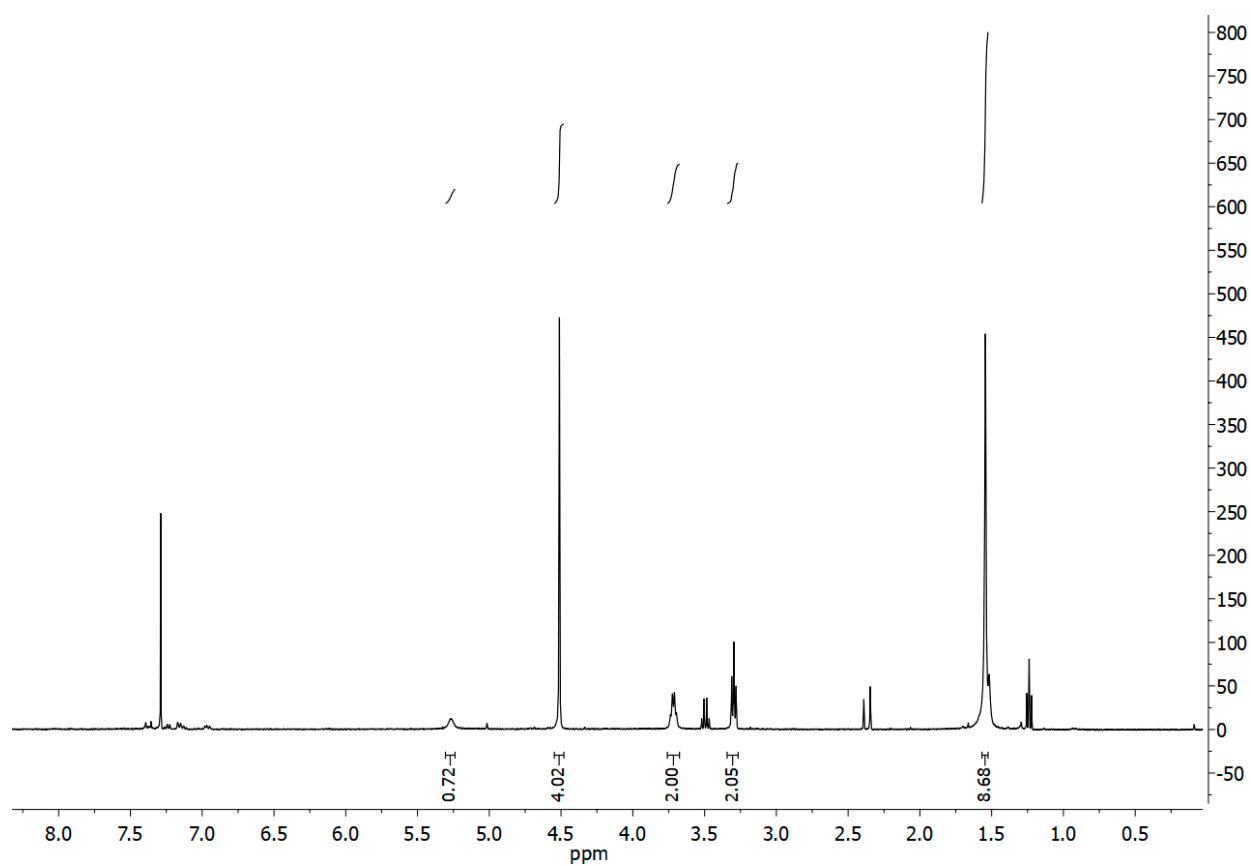


Figure S11. ¹H NMR of compound **4** (400 MHz, Chloroform-d:CS₂ 1:1)

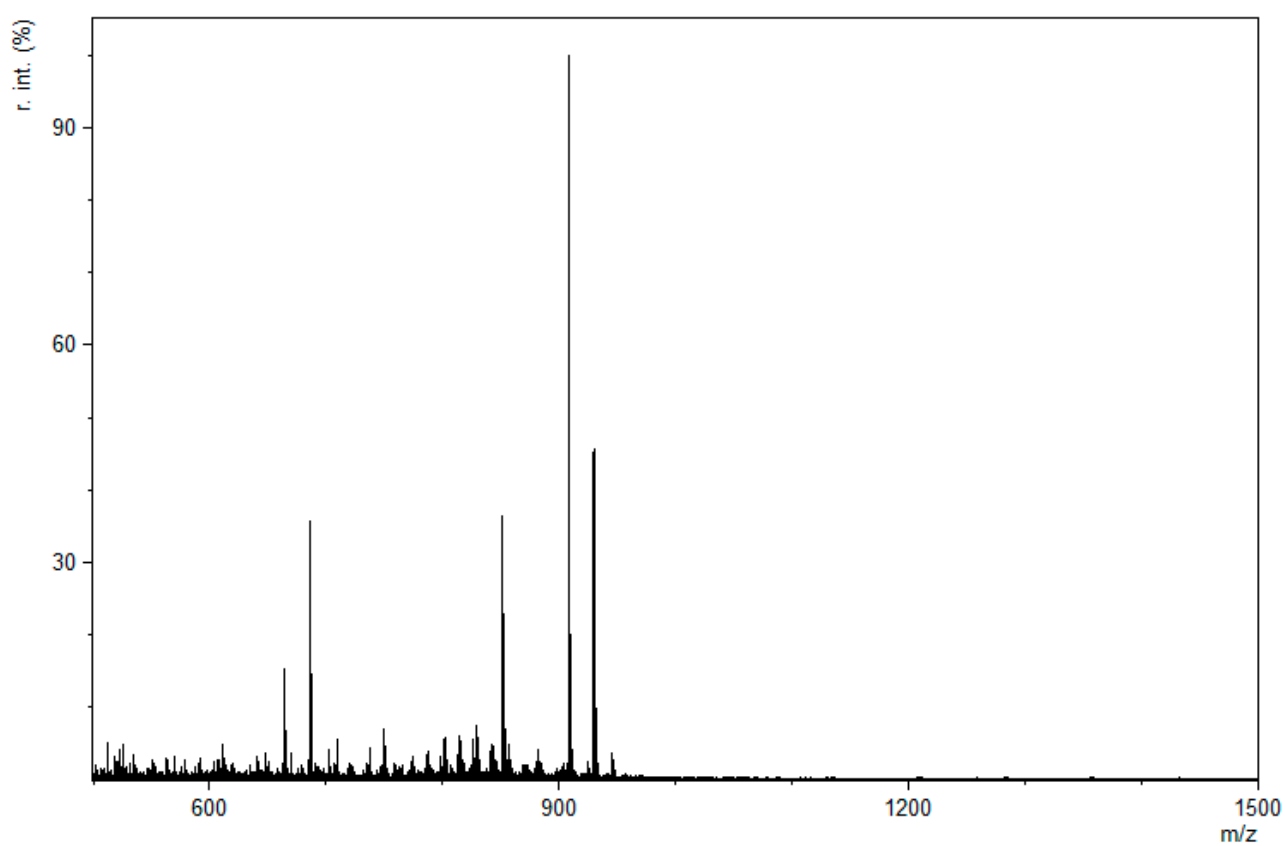


Figure S12. HR ESI-MS of compound **4** (MeOH, range: 500-1500 m/z)

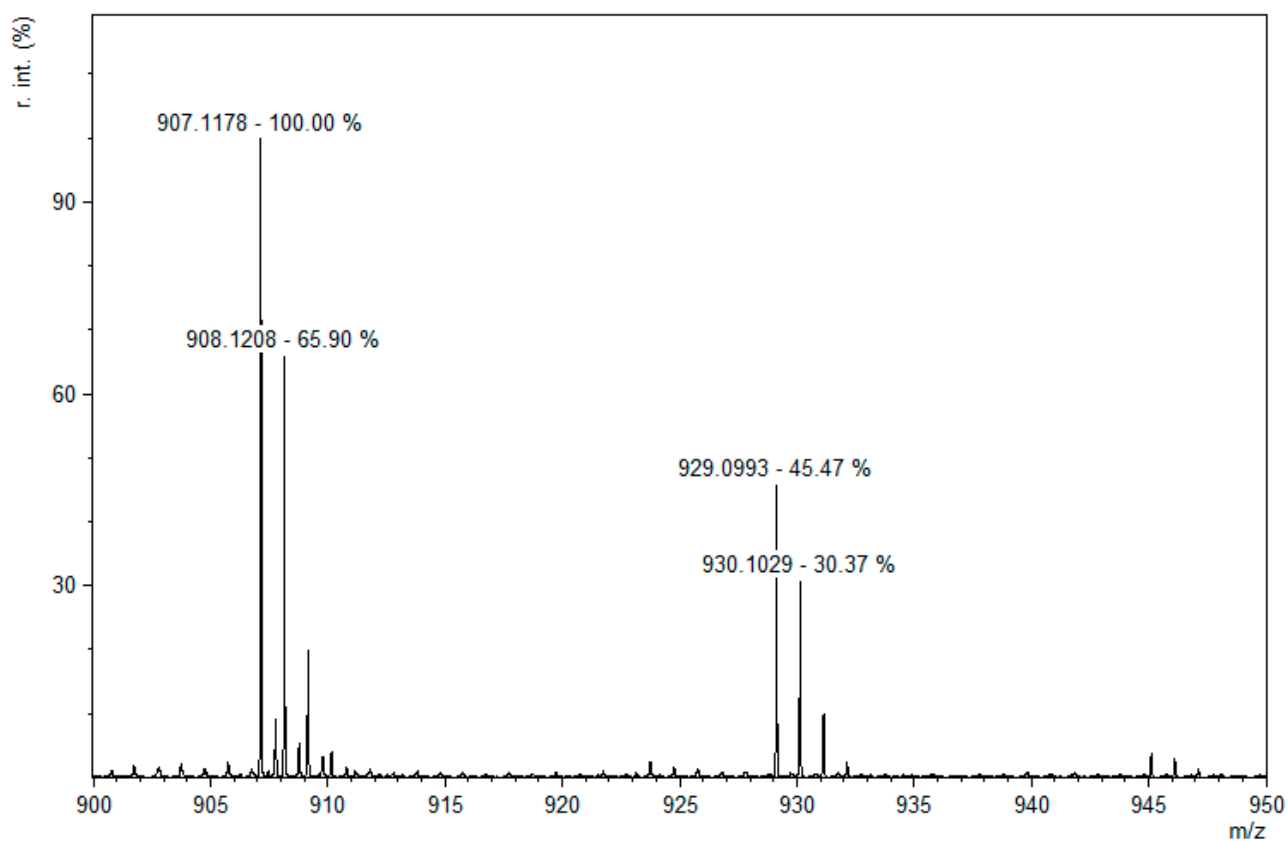


Figure S13. HR ESI-MS of compound 4 (MeOH, range: 900-950 m/z)

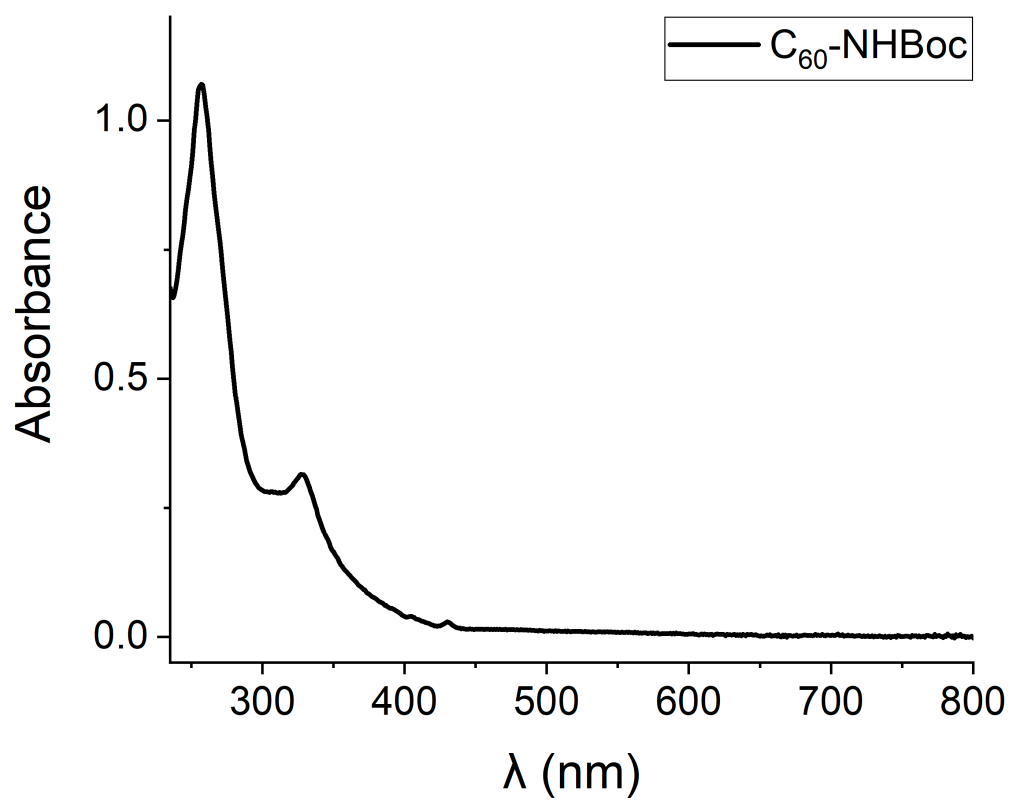


Figure S14. UV-Vis spectrum of compound 4 (Dichloromethane, 230-800 nm)

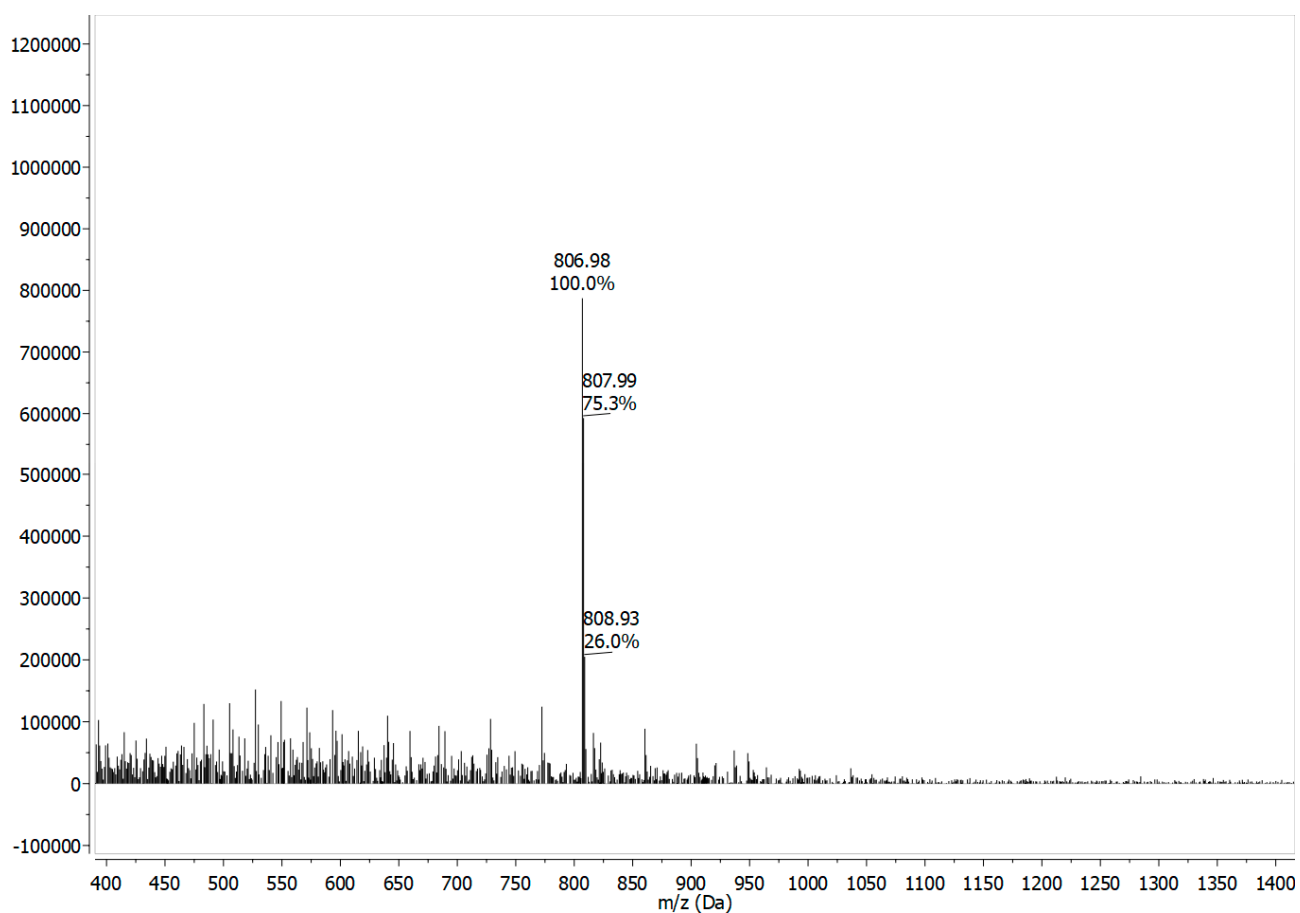


Figure S15. ESI-MS of compound **5** (MeOH, range: 400-1400 m/z)

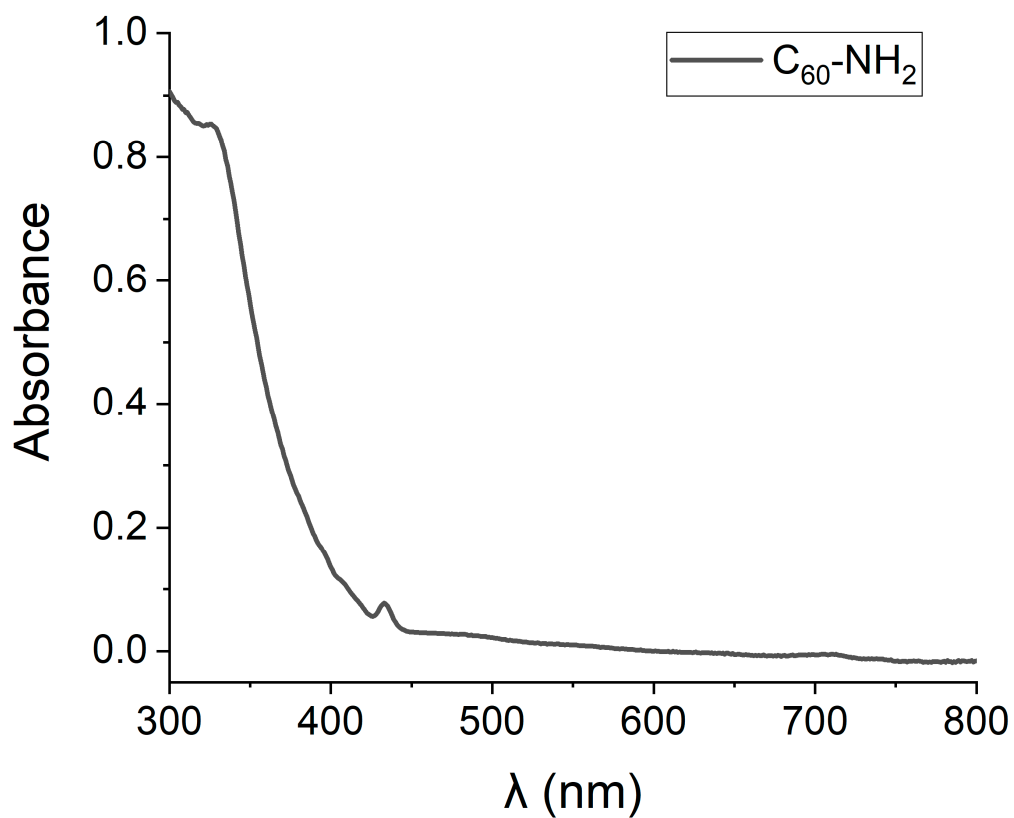


Figure S16. UV-Vis spectrum of compound **5** (DMSO, 300-800 nm).