Electronic Supplementary Information

Binding of toluidine blue-myristic acid derivative to cucurbit[7]uril and human serum albumin: computational and biophysical insights towards a biosupramolecular assembly

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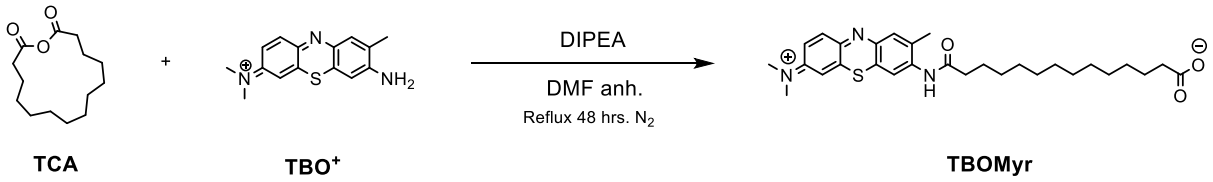
Synthesis and Characterization of TBOMyr by 1H-NMR spectroscopy and mass spectrometry



Synthesis of TBOMyr. To a solution containing dissolving 23 mg (0.095 mmol) of the TCA in 2 mL of dry DMF under atmosphere of N_2. Then 25 mg (0.082 mmol) of TBO dissolved in a minimal anhydrous DMF were added. Finally, 17 µL of DIPEA were added. The mixture was left to react under atmosphere of N_2 and away from light for 48 hours. The product was extracted with ethyl acetate and purified by column chromatography with acetonitrile as the eluent and further by semipreparative HPLC using methanol as eluent. The product was dried under vacuum at 40 ºC overnight. ^{1}H NMR δH (400 MHz, $CDCl_3$-d_3): 6.94-6.35 (5H, m); 2.26-2.15 (3H, m); 2.00-1.98 (4H, m); 1.55-1.46 (4H, m); 1.33-1.15 (16H, m). HRMS $[M+H]^+$: m/z 510,2785 calculated and 510,2770 detected.

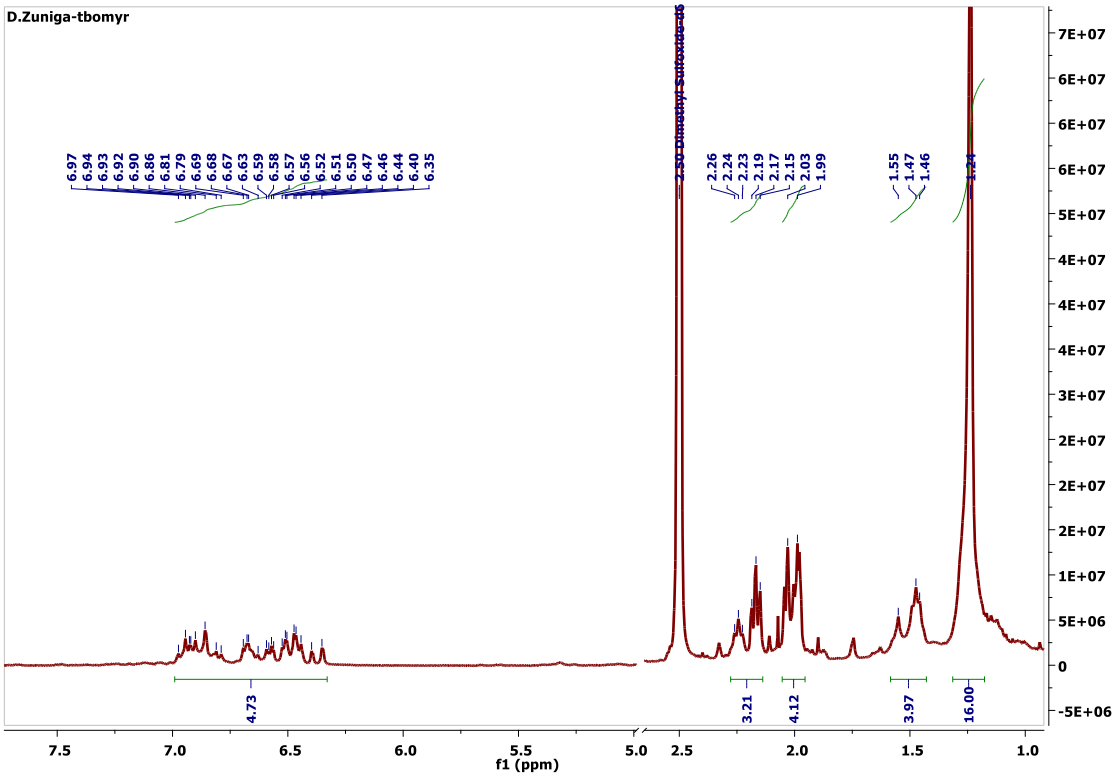


Figure S1. ^{1}H NMR spectrum of TBOMyr in DMSO-d_6.

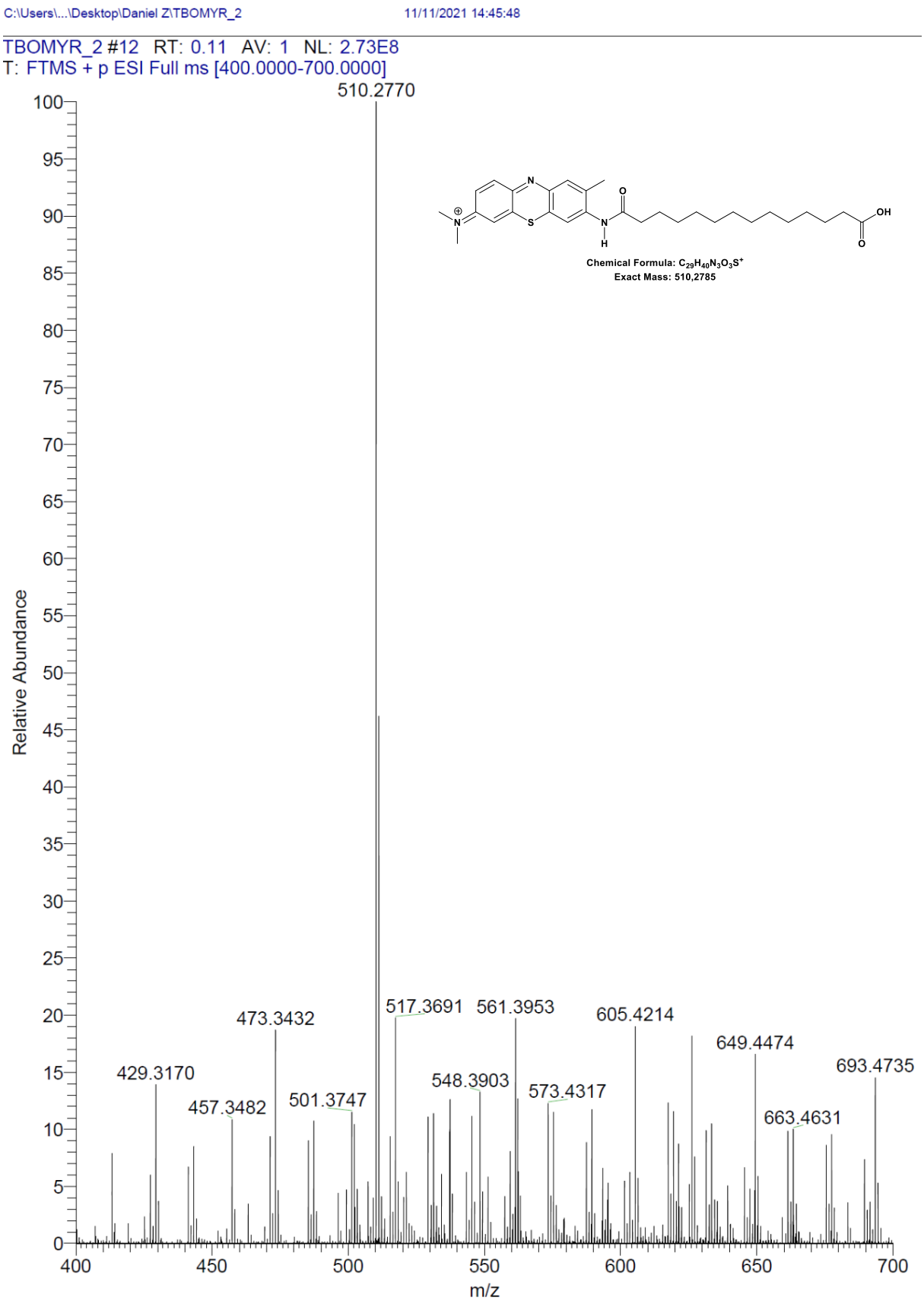


Figure S2. HRMS spectrum of TBOMyr.

Molecular orbital and electronic absorption spectra of TBOMyr.

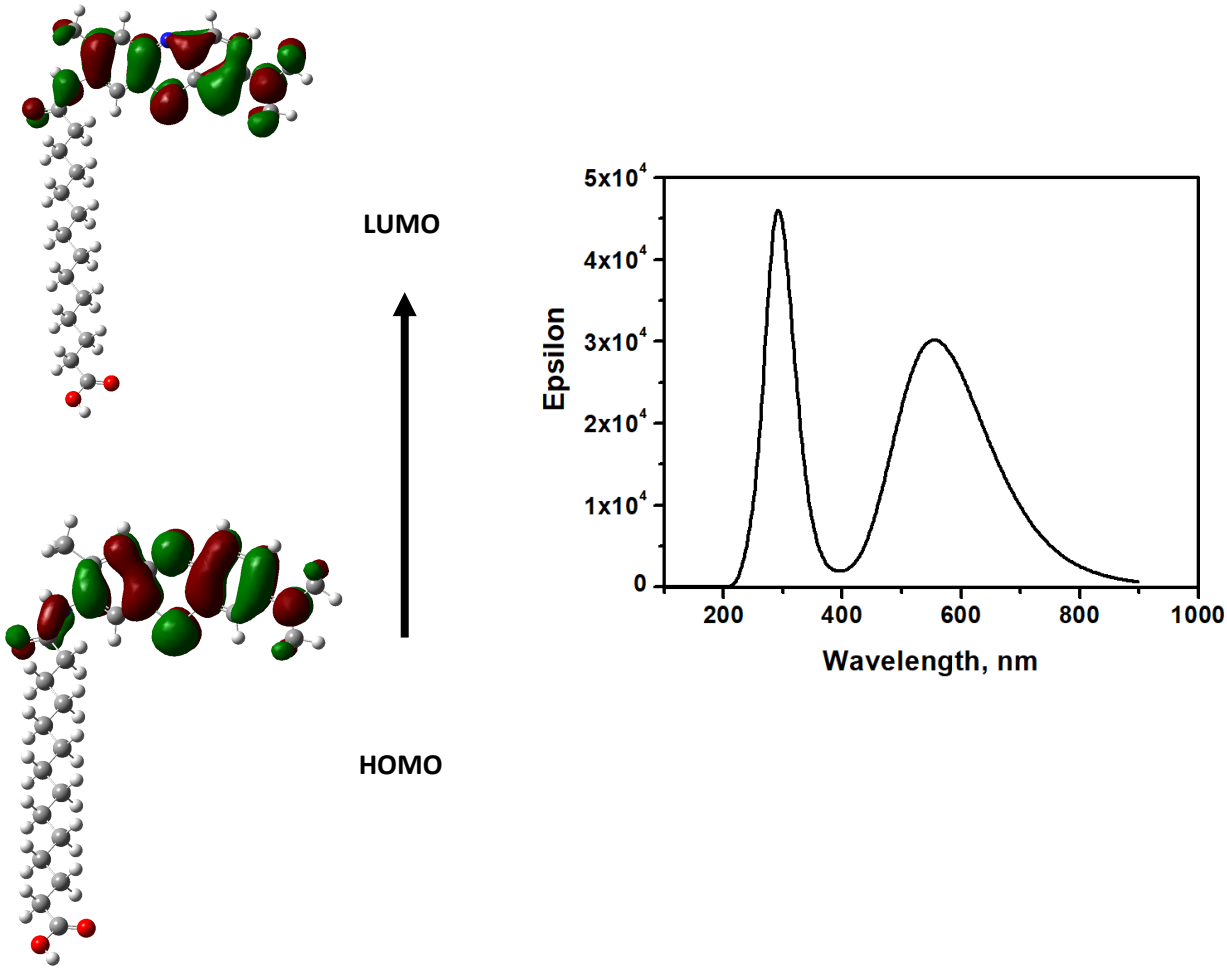


Figure S3. Molecular orbital surfaces involved in the electronic transitions of TBOMyr calculated at the B3LYP/6-311++G (d, p) level of theory. (B) Electronic absorption spectra for TBO-C6 in water using B97D/6-311++G (d, p). The solvent was modeled using C-PCM model solvent.

Stern Volmer plots of Trp214 fluorescence quenching of HSA with TBO.

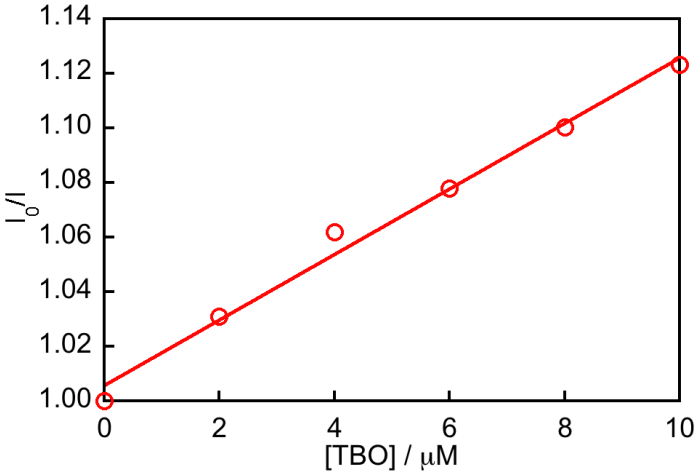


Figure S4. Stern-Volmer plots of Trp214 fluorescence quenching in HSA by TBO. Ka = (1.0 ± 0.2) x 10^4 M^{-1}.