



Supporting Information

for

Synthesis of a new water-soluble hexacarboxylated tribenzotriquinacene derivative and its competitive host–guest interaction for drug delivery

Man-Ping Li, Nan Yang and Wen-Rong Xu

Beilstein J. Org. Chem. **2022**, *18*, 539–548. [doi:10.3762/bjoc.18.56](https://doi.org/10.3762/bjoc.18.56)

Copies of NMR and mass spectra and fluorescence spectra of TBTQ–CB6 with MV and DOX, respectively, at different ratios

Table of contents

Figure S1:	^1H NMR spectrum of compound 2	S1
Figure S2:	^{13}C NMR spectrum of compound 2	S1
Figure S3:	(+)-ESI mass spectrum of compound 2	S2
Figure S4:	^1H NMR spectrum of compound 3	S2
Figure S5:	^{13}C NMR spectrum of compound 3	S3
Figure S6:	MALDI-TOF mass spectrum of compound 3	S3
Figure S7:	^1H NMR spectrum of compound TBTQ-CB6	S4
Figure S8:	^{13}C NMR spectrum of compound TBTQ-CB6	S4
Figure S9:	MALDI-TOF mass spectrum of compound TBTQ-CB6	S5
Figure S10:	Fluorescence spectra of the mixture of TBTQ-CB6 and MV in different molar ratios at a constant total concentration of 10 μM	S5
Figure S11:	Fluorescence spectra of the mixture of TBTQ-CB6 and DOX in different molar ratios at a constant total concentration of 10 μM	S6

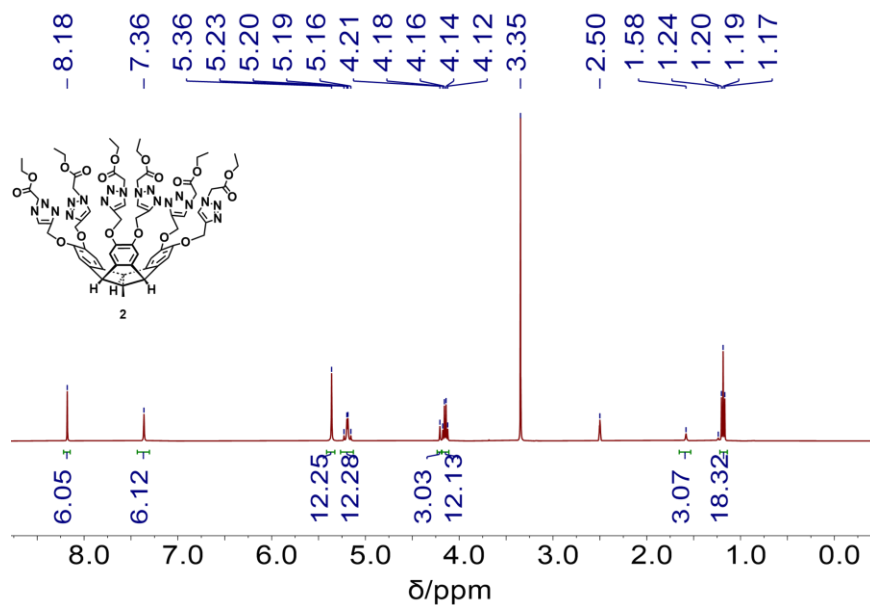


Figure S1: ¹H NMR spectrum of compound **2** (400 MHz, DMSO-*d*₆, 25 °C).

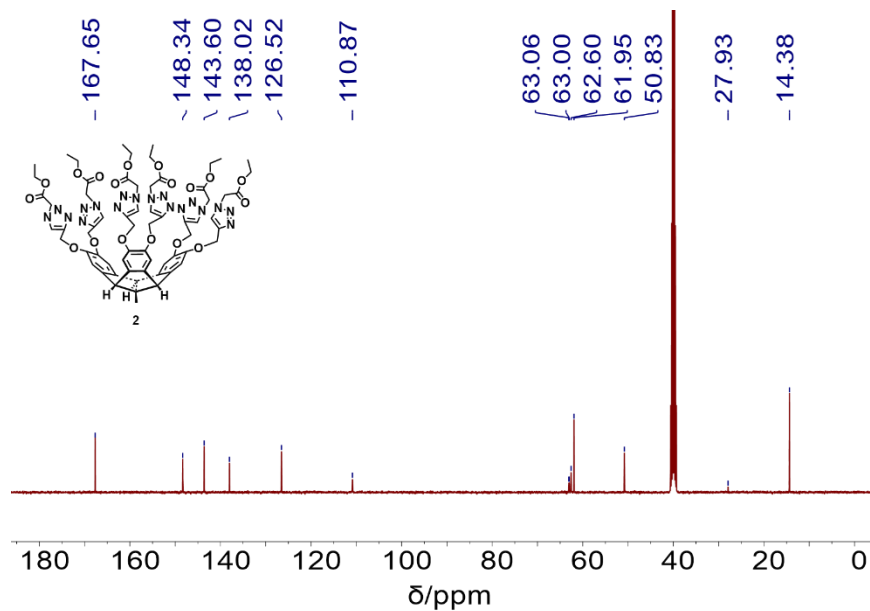


Figure S2: ¹³C NMR spectrum of compound **2** (100 MHz, DMSO-*d*₆, 25 °C).

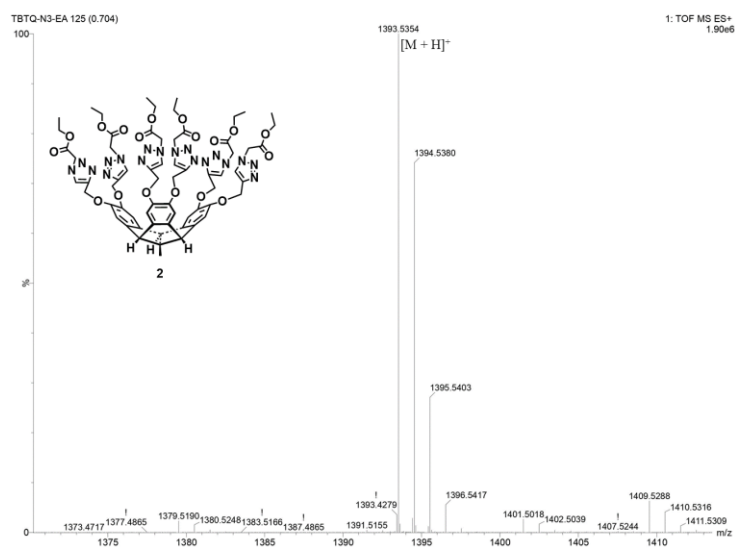


Figure S3: (+)-ESI mass spectrum of compound **2**.

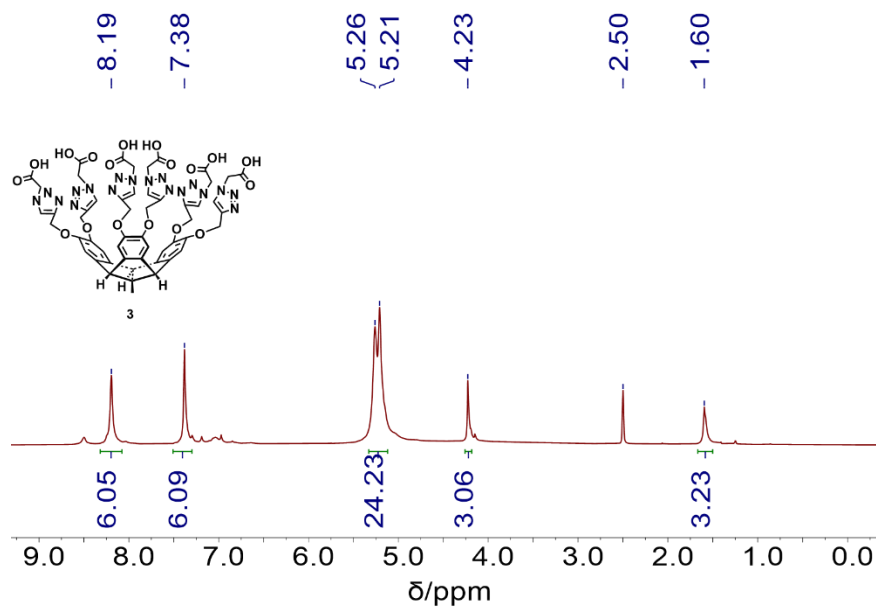


Figure S4: ¹H NMR spectrum of compound **3** (400 MHz, DMSO-*d*₆, 25 °C).

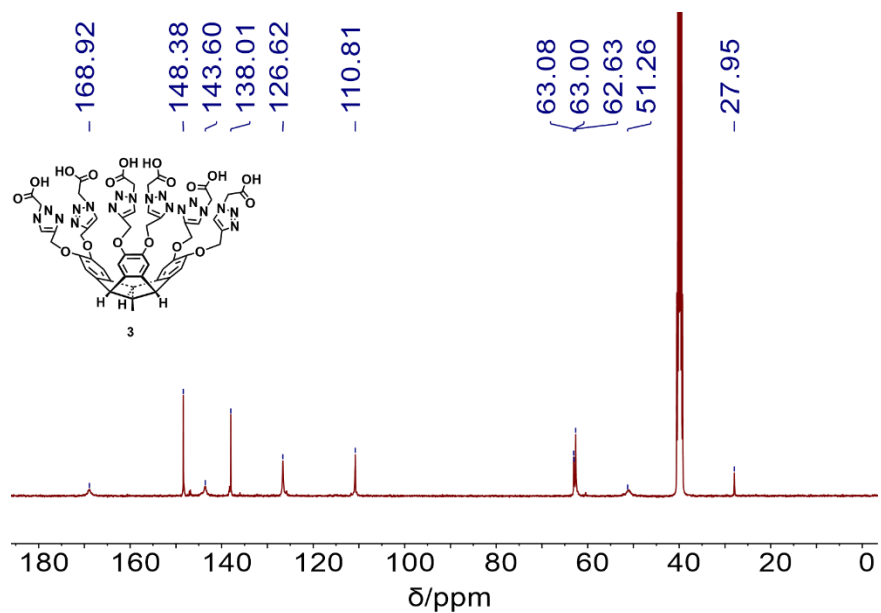


Figure S5: ^{13}C NMR spectrum of compound **3** (100 MHz, $\text{DMSO-}d_6$, 25 °C).

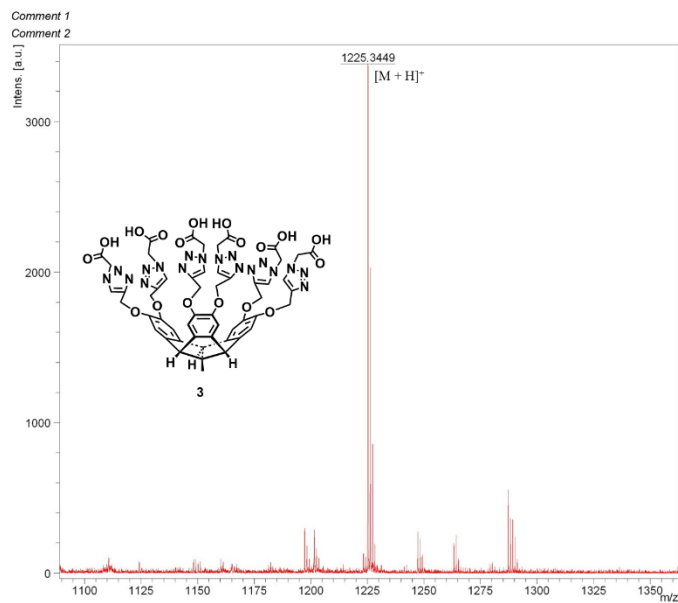


Figure S6: MALDI-TOF mass spectrum of compound **3**.

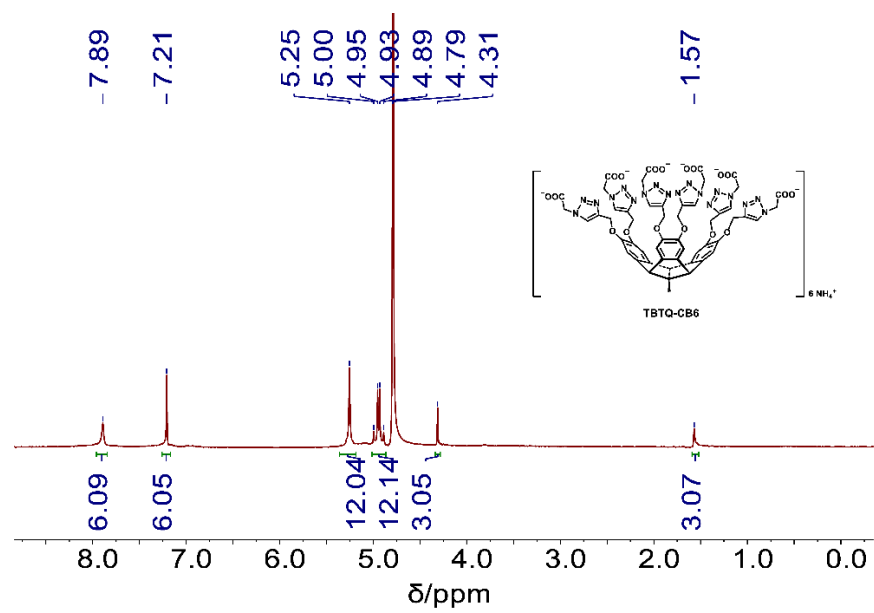


Figure S7: ^1H NMR spectrum of compound **TBTQ-CB6** (400 MHz, D_2O , 25 °C).

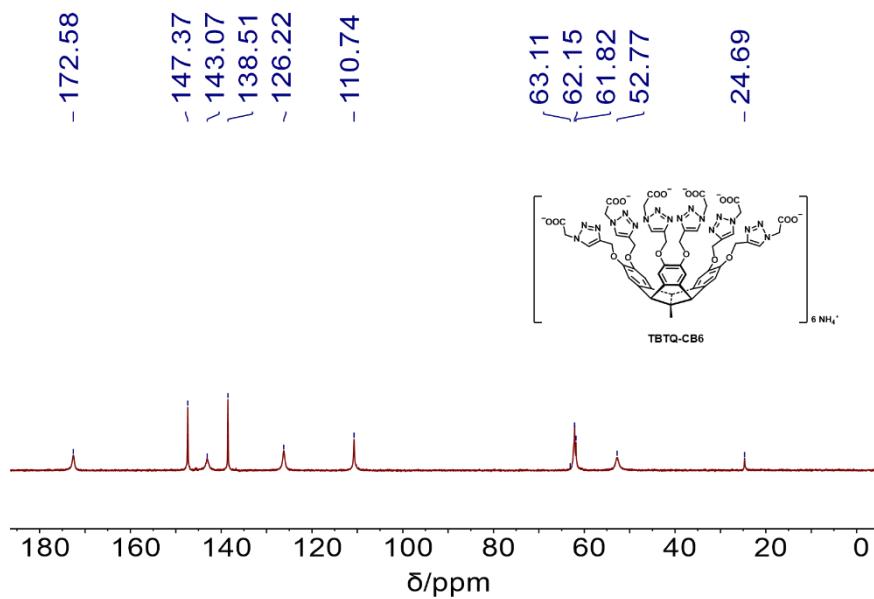


Figure S8: ^{13}C NMR spectrum of compound **TBTQ-CB6** (100 MHz, D_2O , 25 °C).

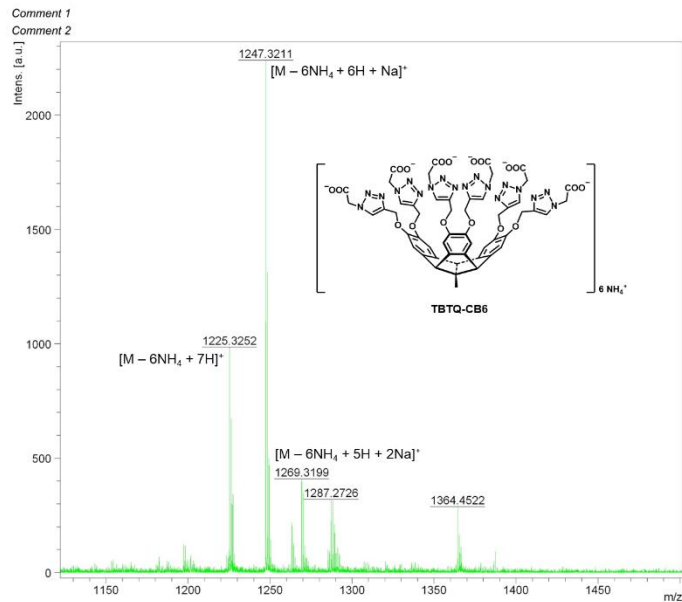


Figure S9: MALDI-TOF mass spectrum of compound TBTQ-CB6.

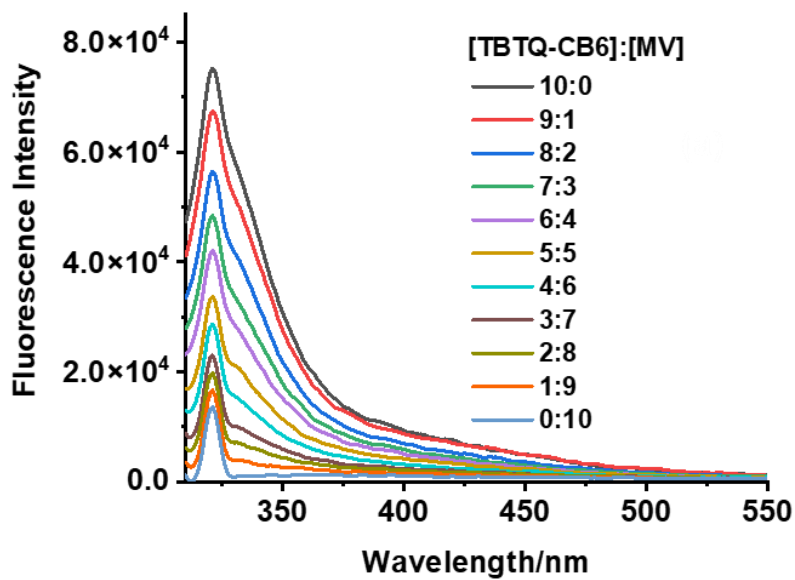


Figure S10: Fluorescence spectra of the mixture of TBTQ-CB6 and MV in different molar ratios at a constant total concentration of 10 μM.

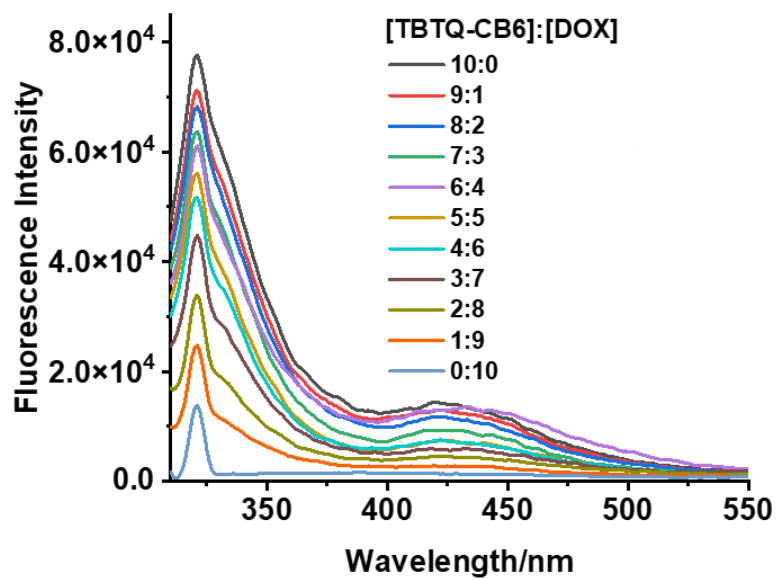


Figure S11: Fluorescence spectra of the mixture of TBTQ-CB6 and DOX in different molar ratios at a constant total concentration of 10 μM .