

Electronic Supplementary Information

Polybenzofulvene Derivatives Bearing Dynamic Binding Sites as Potential Anticancer Drug Delivery Systems

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Contents: ¹H NMR spectrum of poly-6-BAUP-TM-**BF3k** compared with those of **DOXO** and of their mixtures.

Selection of the Small Drug Molecule to be Loaded in the Newly-Synthesized Polybenzofulvene Derivatives.

The potential ability of **BAUP** present in the newly-synthesized polybenzofulvene derivatives to interact with therapeutically relevant **DOXO** was evaluated by NMR spectroscopic studies.

Poly-6-BAUP-TM-**BF3k** (ca. 13 mg, 0.0145 mmol in monomeric unit) was dissolved in CDCl₃ (ca. 0.6 mL) at room temperature. The same amount (ca. 0.6 mL) of DMSO-d₆ was then added and the resulting solution was analyzed by NMR measurements (i. e. standard ¹H NMR and NOESY experiments). The ¹H NMR spectrum of the polymer shows the presence of a low amount of monomer 6-BAUP-TM-**BF3k**, which was judged to not interfere with the interaction studies. Thus, the resulting poly-6-BAUP-TM-**BF3k** was treated with doxorubicin hydrochloride (ca. 1 mg, 0.0017 mmol) and the resulting solution was analyzed by NMR measurements (i. e. standard ¹H NMR and NOESY experiments). The resulting poly-6-BAUP-TM-**BF3k** was treated again with doxorubicin hydrochloride (ca. 1 mg, 0.0017 mmol) and the resulting solution was analyzed by NMR measurements (i. e. standard ¹H NMR and NOESY experiments). The ¹H NMR spectra obtained are shown in Figure ESI-1.

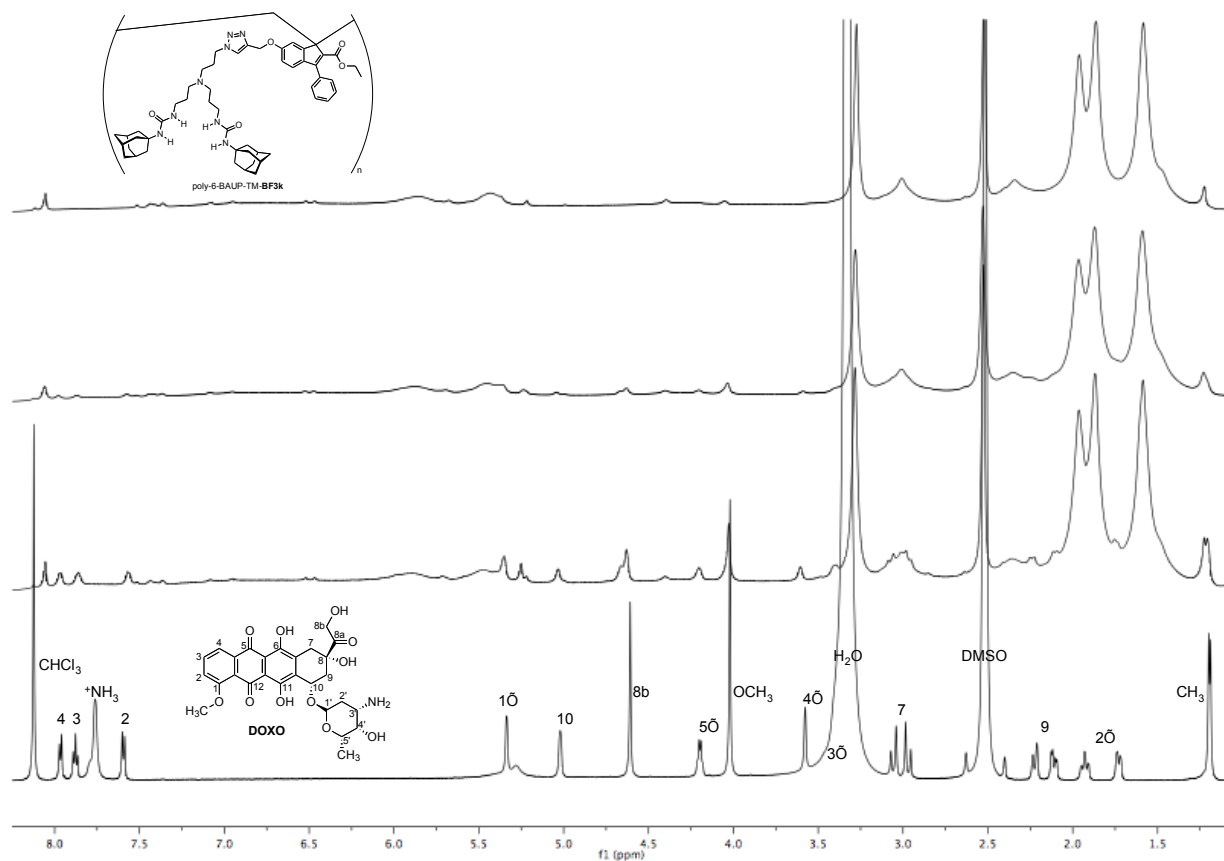


Figure ESI-1. ^1H NMR spectrum [600 MHz, CDCl_3 - DMSO-d_6 (1:1)] of poly-6-BAUP-TM-BF3k (top trace) compared with those of **DOXO** (bottom trace) and of their mixtures (middle traces).