Supporting Information

Title: Synthesis of [1]Rotaxane via Covalent Bond Formation and Its Unique Fluorescent Response by Energy Transfer in the Presence of Lithium Ion

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Content

Assignments of ^{1}H NMR and ^{13}C NMR, and ESI-MS data for [1]rotaxane **7**, crownophane **8**, and Li^{+} complex of [1]rotaxane **7**.

Mili-Mass data for [1]rotaxane **7** and crownophane **8**

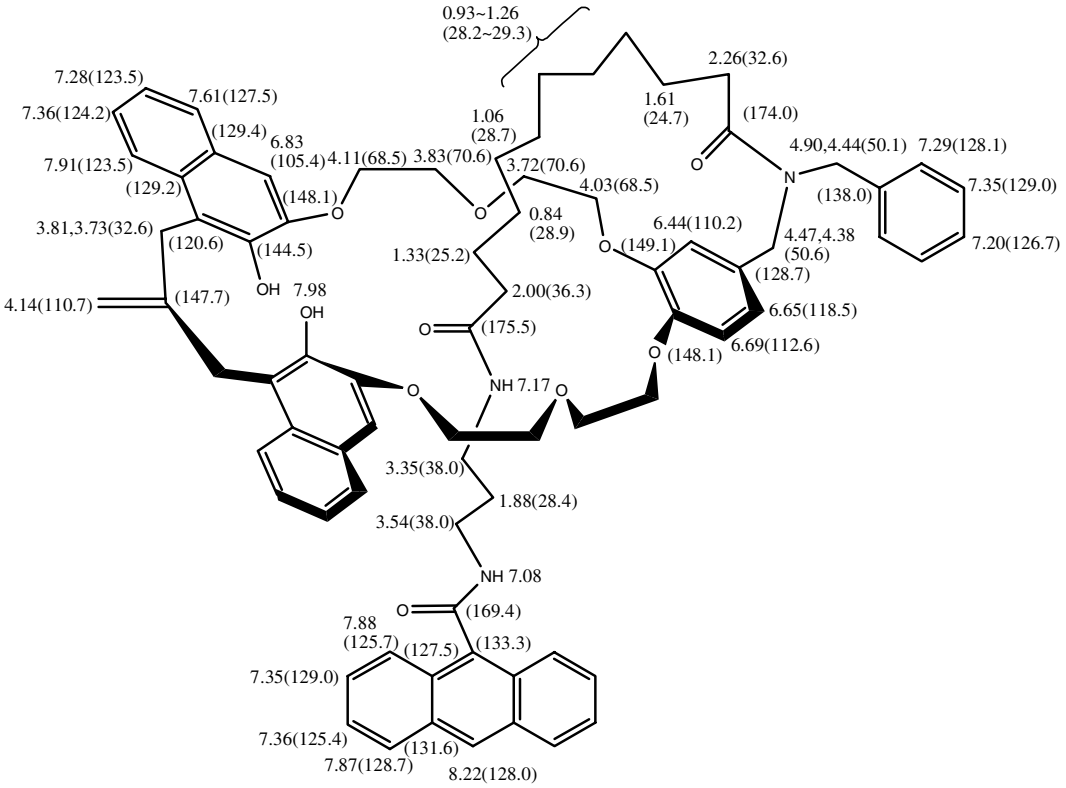
Spectroscopic data

[1]Rataxane **7**: IR (KBr, cm^{-1}) 3395, 3061, 2925, 2857, 1644, 1510, 1447, 1264, 740; ESI-MS (CH_3CN) Found: m/z = 1214.7 (H^+), 1236.7 (Na^+); Calcd: 1213.60 for $C_{76}H_{83}N_3O_{11}$. Mili-Mass Found: 1214.6273, Calcd: 1214.6100 for $C_{76}H_{83}N_3O_{11} + H^+$.

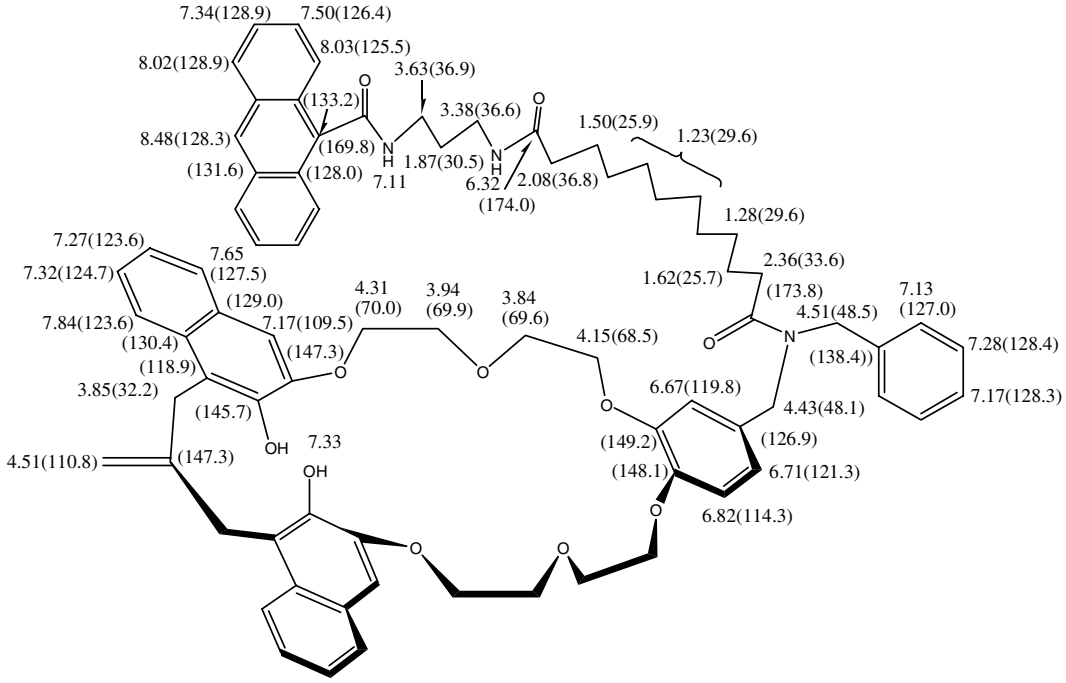
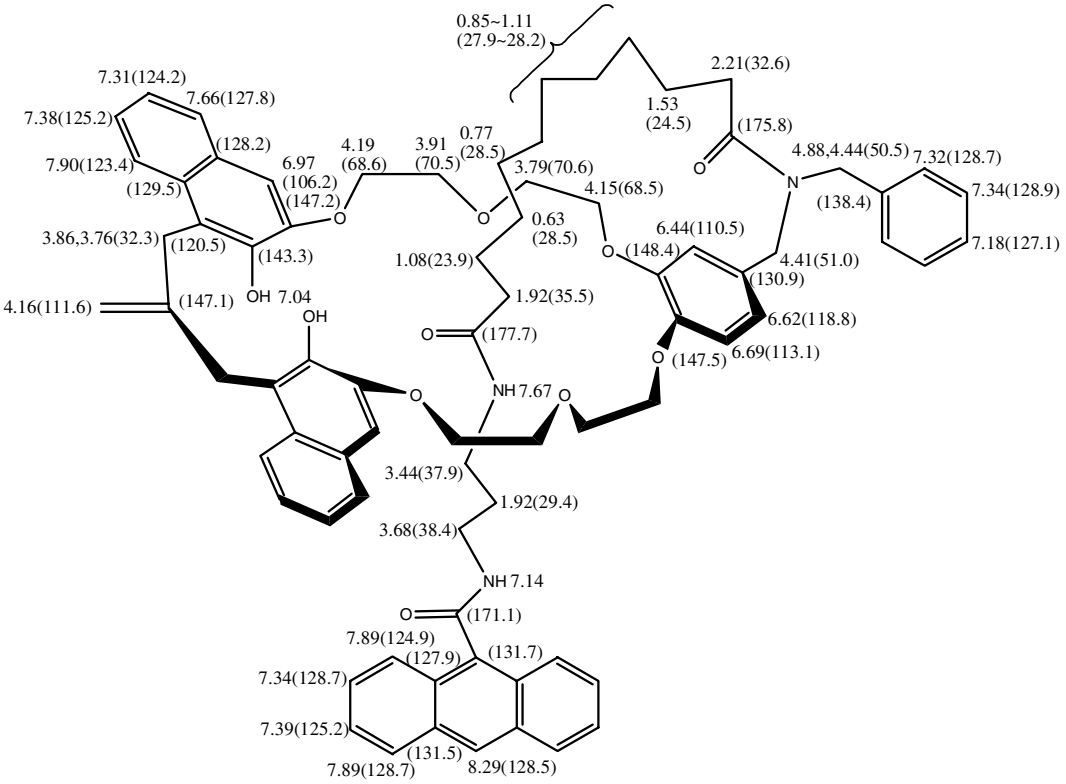
Crownophane **8**: IR (KBr, cm^{-1}) 3428, 2925, 2852, 1639, 1511, 1448, 1265, 742; ESI-MS (CH_3CN) Found: m/z = 1214.7 (H^+), 1236.7 (Na^+); Calcd: 1213.60 for $C_{76}H_{83}N_3O_{11}$. Mili-Mass Found: 1236.6079, Calcd: 1236.5920 for $C_{76}H_{83}N_3O_{11} + Na^+$.

Li^+ complex of [1]Rotaxane **7**: ESI-MS (CH_3CN) Found: m/z = 1220.4 ($^6Li^+$), 1221.5 ($^7Li^+$); Calcd: 1220.62 for $C_{76}H_{83}N_3O_{11} + Li^+$.

^{1}H and ^{13}C NMR Assignments of 7 (Values in parentheses for ^{13}C)



^{1}H and ^{13}C NMR Assignments of 8 (Values in parentheses for ^{13}C)



^{1}H and ^{13}C NMR Assignments of 7+$LiClO_4$ (Values in parentheses for ^{13}C)