Supplemental Material

Cucurbit[7]uril Complexations of Bis(isoquinolinium)alkane Dications in Aqueous Solution

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Table S1. The ESI-MS molecular ion peaks for the 1:1 and 2:1 host-guest complexes formed between cucurbit[7]uril and the isoquinolinium cationic and dicationic guests in aqueous solution.

Guest	CB[7]•G ²⁺ <i>m/z</i> (obs)	CB[7]•G ²⁺ <i>m/z</i> (calc)	CB[7] ₂ •G ²⁺ <i>m/z</i> (obs)	CB[7] ₂ •G ²⁺ <i>m/z</i> (calc)
Iq(CH ₂) ₂ Iq ²⁺	724.2441	724.2447 for C ₆₂ H ₆₀ N ₃₀ O ₁₄ ²⁺		
Iq(CH ₂) ₄ Iq ²⁺	738.2623	738.2604 for C ₆₄ H ₆₄ N ₃₀ O ₁₄ ²⁺	1319.4406	1319.4327 for C ₁₀₆ H ₁₀₆ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₅ Iq ²⁺	745.2694	745.2682 for C ₆₅ H ₆₆ N ₃₀ O ₁₄ ²⁺	1326.4469	1326.4405 for C ₁₀₇ H ₁₀₈ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₆ Iq ²⁺	752.2775	752.2760 for C ₆₆ H ₆₈ N ₃₀ O ₁₄ ²⁺	1333.4454	1333.4483 for C ₁₀₈ H ₁₁₀ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₈ Iq ²⁺	766.2902	766.2917 for C ₆₈ H ₇₂ N ₃₀ O ₁₄ ²⁺	1347.4659	1347.4639 for C ₁₁₀ H ₁₁₄ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₉ Iq ²⁺	773.2986	773.2995 for C ₆₉ H ₇₄ N ₃₀ O ₁₄ ²⁺	1354.4706	1354.4718 for C ₁₁₁ H ₁₁₆ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₁₀ Iq ²⁺	780.3061	780.3073 for C ₇₀ H ₇₆ N ₃₀ O ₁₄ ²⁺	1361.4818	1361.4796 for C ₁₁₂ H ₁₁₈ N ₅₈ O ₂₈ ²⁺
Iq(CH ₂) ₁₂ Iq ²⁺	794.3220	794.3230 for C ₇₂ H ₈₀ N ₃₀ O ₁₄ ²⁺	1375.4980	1375.4953 for C ₁₁₄ H ₁₂₂ N ₅₈ O ₂₈ ²⁺
Iq(<i>p</i> -xyl)Iq ²⁺	762.2604	762.2609 for C ₆₈ H ₆₄ N ₃₀ O ₁₄ ²⁺	1343.4401	1343.4327 for C ₁₁₀ H ₁₀₆ N ₅₈ O ₂₈ ²⁺