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Supporting Information to: On the ionophoric selectivity of nonactin and related macrotetrolide derivatives†

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Figure S1: Low-energy conformers of the Nonactin complexes with K^+ in chloroform predicted by the computation survey and DFT/6-31+G* optimization approach of this study. A: non-hydrated complexes; B: complexes hydrated by six water molecules (highlighted in yellow for better visualization). The relative energy of each conformer is indicated in kJ/mol. Chloroform is in all cases treated as an implicit solvent with the PCM method (see manuscript text for details).