Very Strong Binding for a Neutral Calix[4]pyrrole Receptor Displaying Positive Allosteric Binding

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Résumé en anglais	The dual-analyte responsive behavior of tetraTTF-calix[4]pyrrole receptor 1 has been shown to complex electron-deficient planar guests in a 2:1 fashion by adopting a so-called 1,3-alternate conformation. However, stronger 1:1 complexes have been demonstrated with tetraalkylammonium halide salts that defer receptor 1 to its cone conformation. Herein, we report the complexation of an electron-deficient planar guest, 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA, 2) that champions the complexation with 1, resulting in a high association constant Ka = 3 × 1010 M–2. The tetrathiafulvalene (TTF) subunits in the tetraTTF-calix[4]pyrrole receptor 1 present a near perfect shape and electronic complementarity to the NTCDA guest, which was confirmed by X-ray crystal structure analysis, DFT calculations, and electron density surface mapping. Moreover, the complexation of these species results in the formation of a charge transfer complex (22⊂1) as visualized by a readily apparent color change from yellow to brown.
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