Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Deciphering the Shape Selective Conformational Equilibrium of *E*- and *Z*-Locked Azobenzene-Tetraethyl Ammonium Ion in Regulating Photo-switchable K^+-ion Channel Blocking

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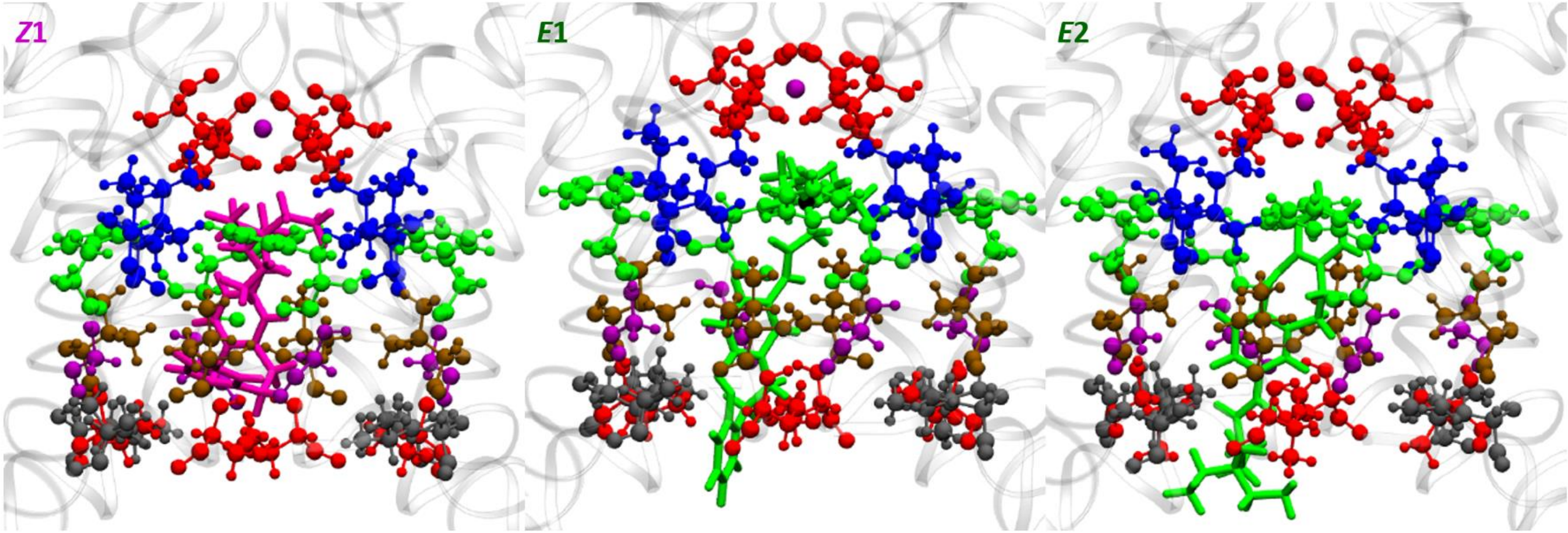

The representative structures used for SAPT0 calculation are shown. The protein and LAB-TEA are represented as the ribbon and stick (*Z*: magenta and *E*: green), respectively, and the interacting residues THR-75 (red), ILE-100 (blue), PHE-103 (green), GLY-104 (purple), VAL-106 (ochre), THR-107 (red), and LEU-110 (grey) from the extracellular to intracellular region are shown as a ball and stick model.