Electronic Supplementary Material (ESI) for RSC Advances.

In silico studies of ASEM analogues targeting α7-nAChR and experimental verification

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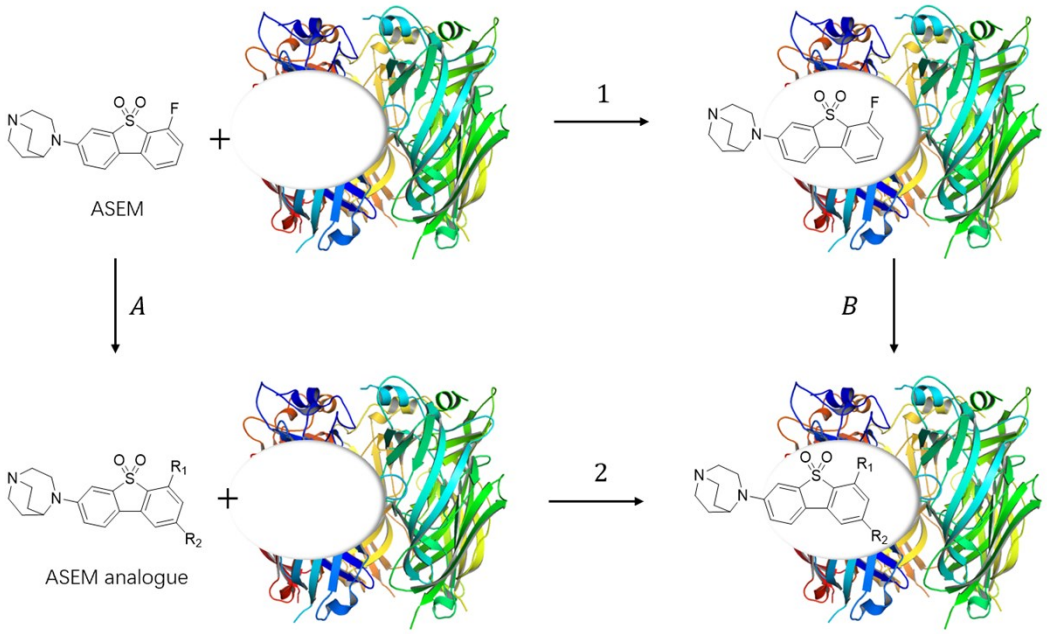
Supporting Information



$$\Delta\Delta G = \Delta G_2\text{-}\Delta G_1 = \Delta G_B - \Delta G_A$$

Figure S1. Illustration of the thermodynamic cycle, together with the perturbation pathways, used by an FEP+ calculation. The perturbation pathways are represented by arrows A and B. The difference in the binding free energy ($\Delta\Delta G$) between an ASEM analogue (ΔG_2) and ASEM (ΔG_1) is related to the free energy of transforming ASEM to its analogue in the solvent (ΔG_A) and in α7-AChBP (ΔG_B).