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

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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 ($\Delta G_A$) and ASEM ($\Delta G_B$) is related to the free energy of transforming ASEM to its analogue in the solvent ($\Delta G_A$) and in $\alpha_7$-AChBP ($\Delta G_B$).