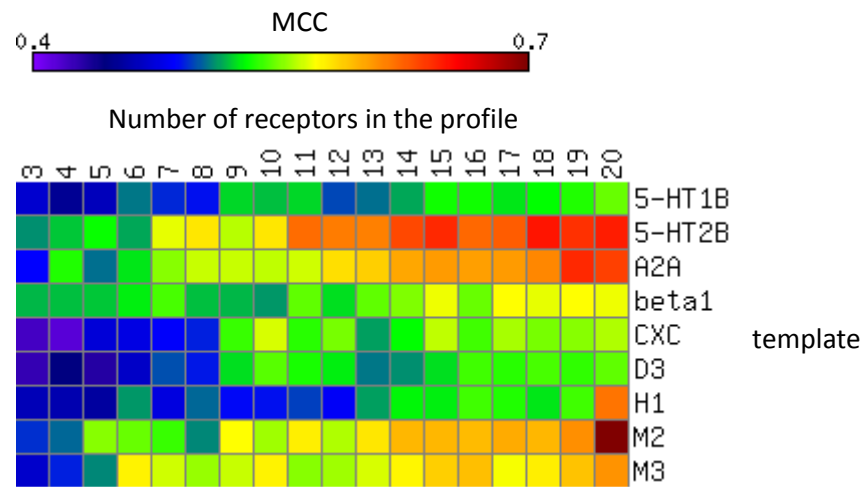
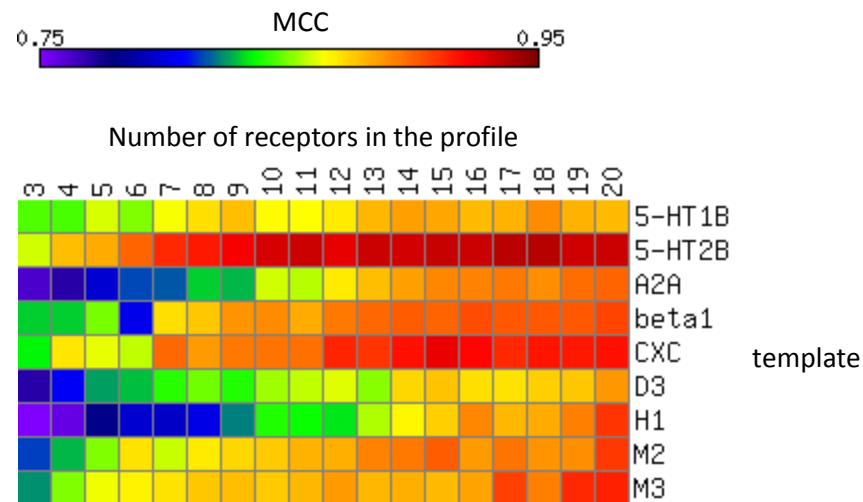


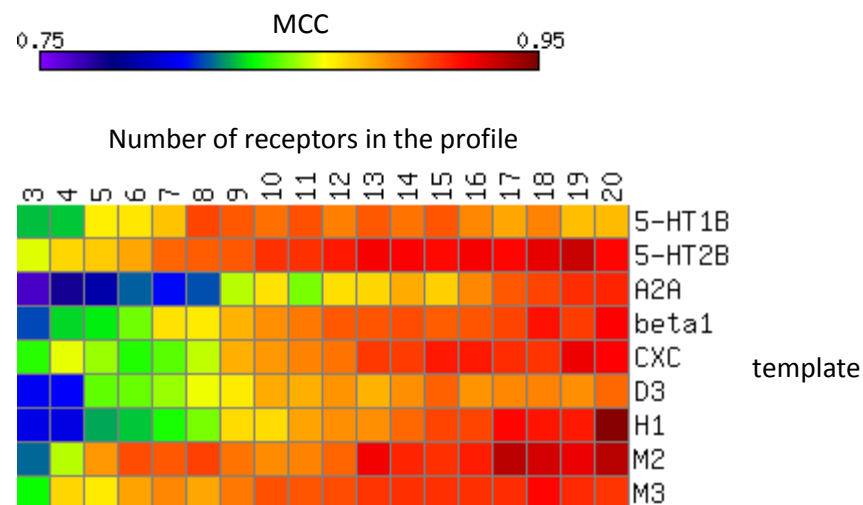
Figure S2. MCC values obtained for various numbers of models included in the SIFt profile for models built on various templates for a) actives/true inactives, b) actives/DUDs, and c) actives/ZINC discrimination



a)



b)



c)