

Reverse fragment based drug discovery approach *via* simple estimation of fragment contributions

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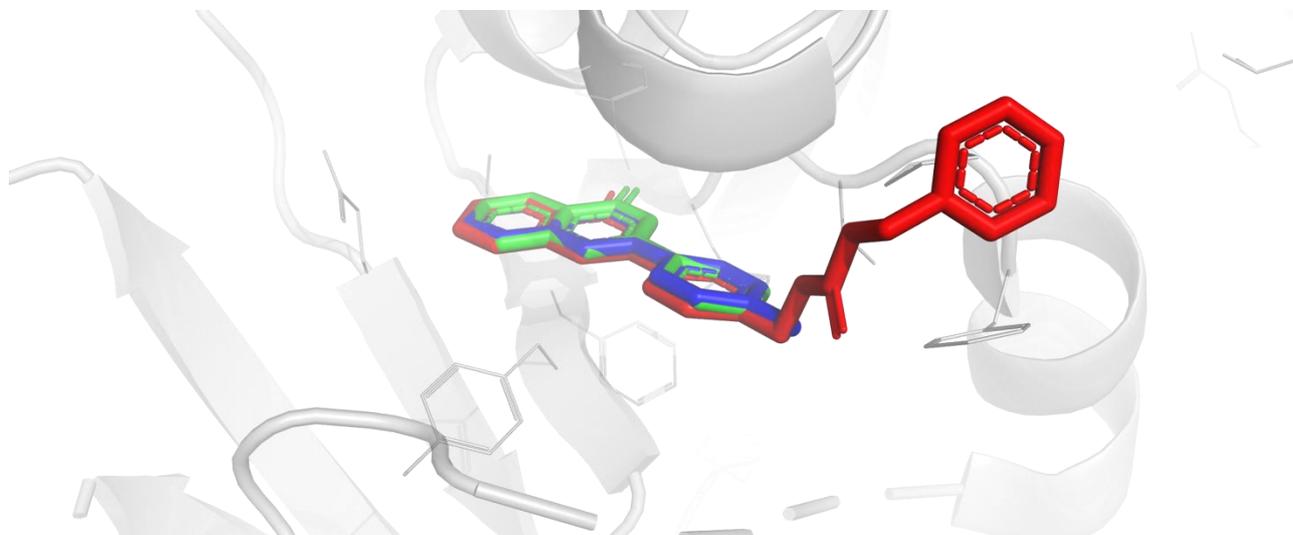


Figure S1 Alignment of 3D complexes. Red ligand from 4BU3 (**1**), cyan from 4UHG (**2**), blue from 4UI4 (**3**).

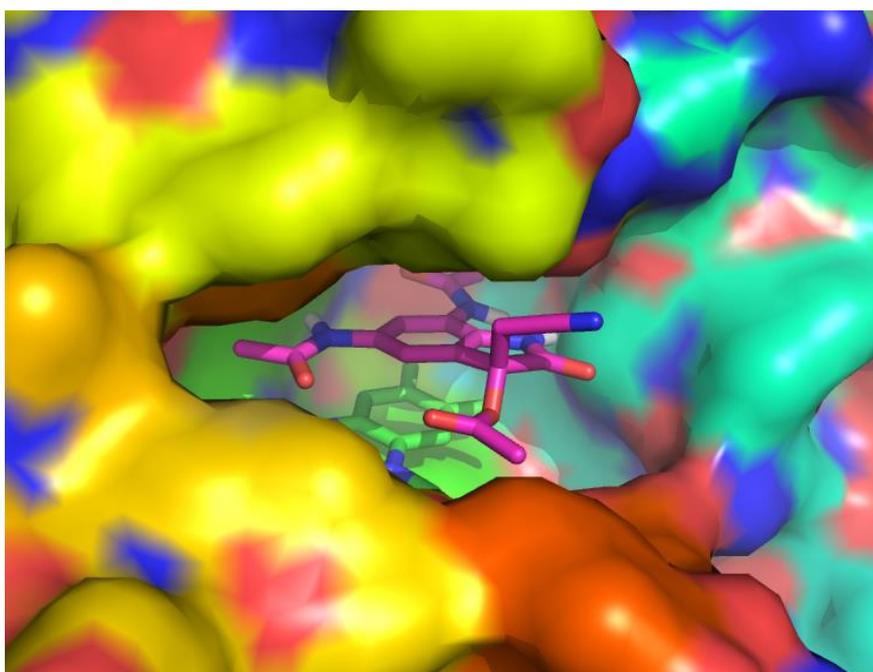


Figure S2 The docked position of structure **4** to MT3/QR2 receptor (PDB:2QWX), showing the substitution at position 3 prevents ligand penetration into the flat site cavity.