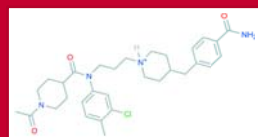


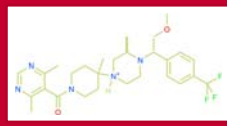
Finding the Bioactive Conformation of inhibitors of CCR5 using FieldTemplater and FieldScreen

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TAK-220, IC50 3.5 nM



SCH-417690, Vicriviroc, Ki 1.6nM

4 CCR5 Actives in 2D

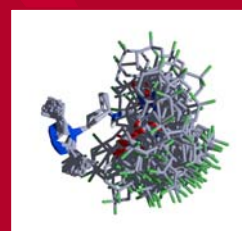
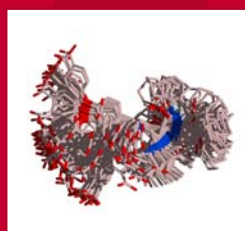
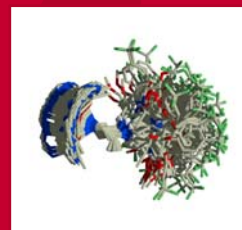
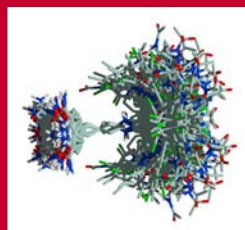


ONO-4128, Aplaviroc, IC50 0.5nM



UK-427857, Maraviroc, IC50 1nM

Populate conformation space

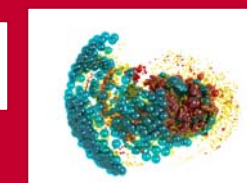


Add Molecular interaction Fields to each conformation

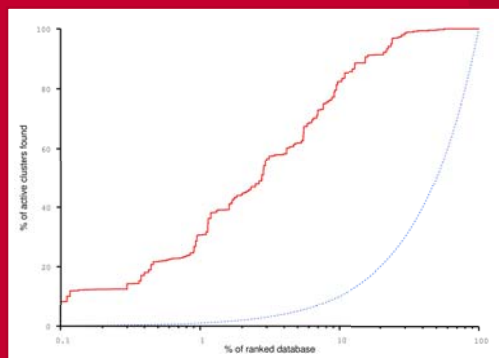
Blue: Negative
Red: Positive
Yellow: Steric
Gold:Hydrophobic



Search for common Field Pattern



fieldscreen™

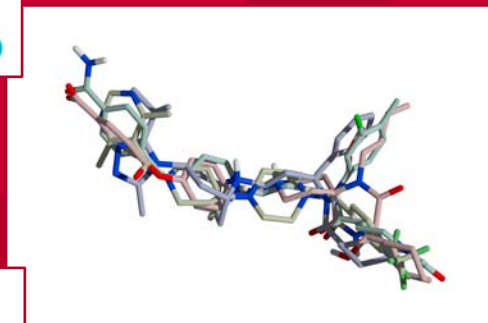


Virtual Screening for new Chemotypes



Chemotype retrieved at position 19 as aligned to Maraviroc and as 2D

fieldtemplater™



Blue: Negative
Red: Positive
Yellow: Steric
Gold:Hydrophobic

