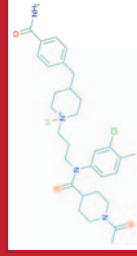


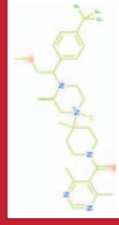
# Finding the Bioactive Conformation of Inhibitors of CCR5 using FieldTemplater and FieldScreen

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TAK-220, IC50 3.5 nM



SCH-417690, Virciviroc, Ki 1.6nM

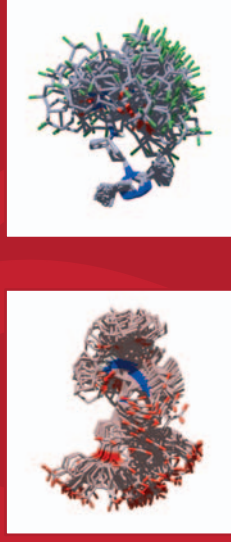


ONO-4128, Aplaviroc, IC50 0.5nM



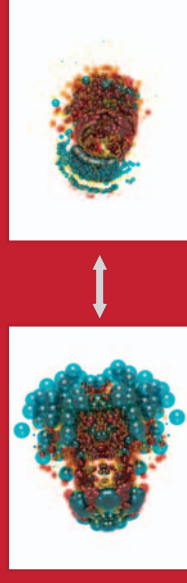
UK-427857, Maraviroc, IC50 1nM

Populate conformation space

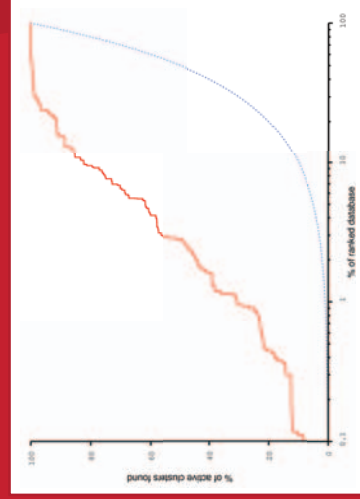


Add Molecular Interaction Fields to each conformation

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

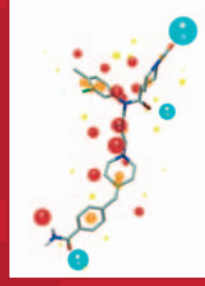


Search for common Field Pattern

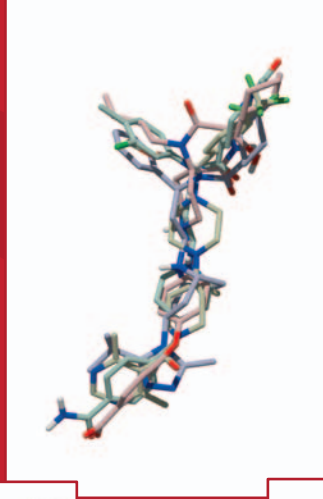


fieldscreen™

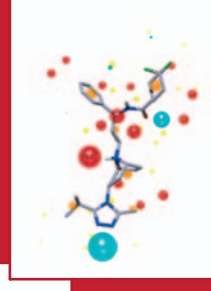
fieldtemplater™



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



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



Virtual Screening for new Chemotypes

