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Discovery of uracil-bearing DAPYs derivatives as novel HIV-1 NNRTIs *via* crystallographic overlay-based molecular hybridization

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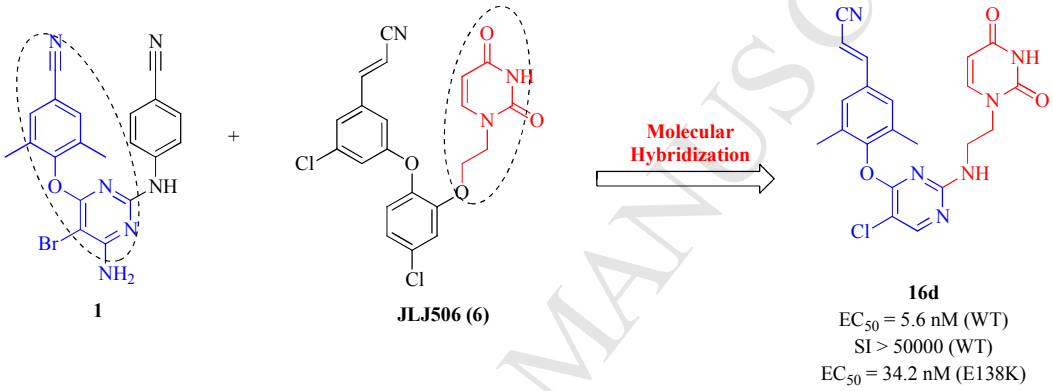
Graphical Abstract

Discovery of uracil-bearing DAPYs derivatives as novel HIV-1 NNRTIs via crystallographic overlay-based molecular hybridization

By structure-based molecular hybridization, a new HIV-1 NNRTI **16d** was discovered with excellent activity and high selectivity.



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JLJ506 (6)

16d
EC_{50} = 5.6 nM (WT)
SI > 50000 (WT)
EC_{50} = 34.2 nM (E138K)