SILCSBIO
FREE ENERGY BASED LIGAND DESIGN

# SINGLE STEP FEP

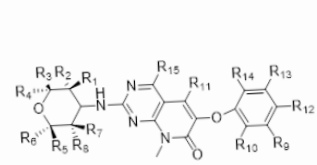
Evaluate Thousands of Ligands per Hour with Single Step FEP!

Rapid free energy calculations by Single Step Free Energy Perturbation minimize lead optimization times in drug discovery.

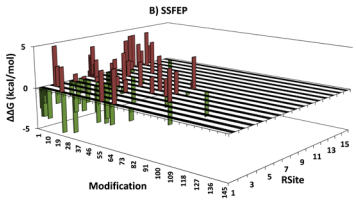
Free Energy Perturbation (FEP) is the standard approach to calculate relative free energies. but it is often impractical due to its large computational burden. SilcsBio offers Single Step Free Energy Perturbation (SSFEP). an alternative that is 1.000-fold faster than FEP. while maintaining comparable accuracy. After a conditioning step involving the target and ligand. SSFEP uses an automated ligand scanning approach to calculate relative free energies for thousands of ligand transformations per hour to determine which will best enhance binding.

## SSFEP CAN BE USED WITH DIVERSE PROTEIN TARGETS

Single Step FEP methodology can be employed during lead optimization in any structure-based drug discovery project. It is well validated across diverse gene family targets including but not limited to traditional targets like Kinases. Proteases. and Nuclear Hormone Receptors and also on novel epigenetic targets like Methyl Transferases and Bromodomains.



Ligand R sites undergo hundreds of modifications to produce chemically diverse ligand derivatives.




Relative binding free energies for new ligands are calculated in SSFEP.

Figures from Raman et al. Estimation of relative free energies of binding using precomputed ensembles based on the single-step free energy perturbation and the site-identification by ligand competitive saturation approaches. J Comput Chem. In press.

## BEST FOR

Single (-H to -CH3. -Cl. etc.) & small functional group (-ethyl. -cycloproply. etc.) changes.

## QUICK SET-UP

Target conditioning step requires only 30 minutes of set-up time & 3 hours of computer time (on 12 cores + 1 GPU node).

## FAST

SSFEP evaluates 1000 ligand modifications per hour.

## CONTACT US

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Find out how SILCS can improve and accelerate your computational drug design efforts.

## MORE INFO

www.silcsbio.com

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