- Eris

Protein stability analysis and design

Eris

- Eris server calculates the change of the protein stability induced by mutations $(\Delta \Delta G)$ utilizing the recently developed Medusa modeling suite.
- The Δ Δ G values of a large dataset (>500), calculated and compared with the experimental data, feature significant correlations (~0.8).



Yin, Ding & Dokholyan, Nature Methods 4: 466-467 (2007)

Eris

- Eris allows refinement of the protein structure when high-resolution structures are not available.
- Compared with many other stability prediction servers, Eris is not trained using protein stability data and is valid for a wide range of proteins.
- Eris models backbone flexibility, which turns out to be crucial for $\Delta \Delta G$ estimation of small-to-large mutations.

Structural refinement improves $\Delta \Delta G$ estimation. original NMR structure pre-relaxed structure 8 6 -10 -× \times × ×× х х -20 2 2 3 4 4 Experimental $\Delta\Delta G$ Experimental $\Delta\Delta G$ Core mutant × Trans-helix mutant

Yin, Ding & Dokholyan, Structure, 15: 1567-1576 (2007)

Eris

Eris stand-alone package is commercially available and includes the following functions:

- [ddg] Estimates the changes in protein stability upon point mutations, using either fixed or flexible backbone method.
- [fixed backbone design] For a given protein backbone conformation, identifies an amino sequence that minimizes energy of this conformation (fixed-backbone redesign).
- [flexible backbone design] For a given protein backbone conformation, identifies an amino sequence that minimizes energy of this conformation with the ability to locally perturb this conformation (flexible-backbone redesign).
- [scan] For a given protein conformation and a given amino acid position, identifies a substitute amino acid that minimizes this conformation.

