

Discussion questions for

Calculation of the Relative Change in Binding Free Energy of a Protein-Inhibitor Complex

Kollman et al.

**Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with Sustiva
through Computation of Resistance Profiles**

Jorgensen et al.

GIBBS

- Kollman paper: system, methods, results

SANGER

- Jorgensen paper: system, methods, results
- Resistance mutations: why so many in HIV, why is sustiva less so, etc.

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- Compare and contrast two papers
- Sources of errors in both papers
- Limitations of each paper
- Prospects for the future, generality of methods, prospective applications in drug discovery