Analysis of Correlations between Energy and Residue Fluctuations in Native Proteins and Determination of Specific Sites for Binding

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The Gaussian network model is used to derive the correlations between energy and residue fluctuations in native proteins. Residues are identified that respond strongly to energy fluctuations and that display correlations with the remaining residues of the protein at the highest modes. We postulate that these residues are located at specific sites for drug binding. We test the validity of this postulate on a data set of 33 structurally distinct proteins in the unbound state. Detailed results are presented for drug binding to the HIV protease.

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