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Functionally important residues from mode coupling during short-time protein dynamics[1] ALKAN KABAKCIOGLU, Koc Univ, ONUR VAROL, Indiana Univ, DENIZ YURET, BURAK ERMAN, Koc Univ — Relevance of mode coupling to energy/information transfer during protein function, particularly in the context of allosteric interactions is widely accepted. However, existing evidence in favor of this hypothesis comes essentially from model systems. We here report a novel formal analysis of the near-native dynamics for proteins, which allows us to explore the impact of the interaction between possibly non-Gaussian vibrational modes on fluctutational dynamics. We show that, an information-theoretic measure based on mode coupling *alone* yields a ranking of residues with a statistically significant bias favoring the functionally critical locations identified by experiments on Myosin II and AncGR1,2.
Reference: O. Varol et al., Proteins: Structure, Function and Bioinformatics, 82(9), 1777 (2014).

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