Correlations between secondary structure- and protein-protein interface-mimicry: The Interface Mimicry Hypothesis

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A. EKO Procedures

The QMD was performed according to the procedure described before. After energy minimization in the QMD process, all conformers within 3.0 kcal/mol of the lowest energy conformer were clustered into families with similar RMSDs (< 0.5 Å) based on Cα – Cβ coordinates. The conformer having lowest energy in each family was selected as a representative. These representatives were systematically aligned on the Cα – Cβ coordinates of interface residues on > 240,000 protein-protein complexes recorded in the PDB, and the results were sorted based on RMSDs of Cα – Cβ coordinates.
B. EKOS, EKO, and DSSP/STRIDE data for chemotype 2
Figure S1. (a) RMSD (Å) of the overlays of mimics 2 on each of the ideal secondary structures, organized by stereochemistry. Statistical distribution of secondary structures at PPI interfaces derived by DSSP and STRIDE calculations; (b) the best 115 overlays of DDD-2; and, (c) 287 overlays of LDD-2.
c. EKOS, EKO, and DSSP/STRIDE data for chemotype 3

![Diagram showing helical and extended structures with corresponding RMSD values for different configurations: LLL, LLD, LDL, DLL, LDD, DLD, DDL, and DDD.](image)
Figure S2. (a) RMSD (Å) of the overlays of mimics 3 on each of the ideal secondary structures, organized by stereochemistry. Statistical distribution of secondary structures at PPI interfaces derived by DSSP and STRIDE calculations; (b) the best 288 overlays of DDD-3.
D. EKOS, EKO, and DSSP/STRIDE data for chemotype 4
Figure S2. (a) RMSD (Å) of the overlays of mimics 4 on each of the ideal secondary structures, organized by stereochemistry. Statistical distribution of secondary structures at PPI interfaces derived by DSSP and STRIDE calculations; (b) the best 369 overlays of LDL-4; (c) the best 308 overlays of LLL-4.
E. Reference