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Assembly of protein tertiary structures from fragments with similar local sequences using simulated annealing and Bayesian scoring functions

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|------|---|-----|-----------|
| 1202 | Rosetta Protein Structure Prediction from Hydroxyl Radical Protein Footprinting Mass Spectrometry Data. | | |
| 1201 | Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. | | |
| 1200 | Using Local States To Drive the Sampling of Global Conformations in Proteins. | | |
| 1199 | Folding dynamics of the src SH3 domain. 1997 , 36, 15685-92 | | 174 |
| 1198 | Contrasting roles for symmetrically disposed beta-turns in the folding of a small protein. <i>Journal of Molecular Biology</i> , 1997 , 274, 588-96 | 6.5 | 82 |
| 1197 | Blind predictions of local protein structure in CASP2 targets using the I-sites library. 1997 , 29, 167-171 | | 22 |
| 1196 | Accuracy of side-chain prediction upon near-native protein backbones generated by Ab initio folding methods. 1998 , 33, 204-17 | | 39 |
| 1195 | Distance geometry generates native-like folds for small helical proteins using the consensus distances of predicted protein structures. 1998 , 7, 1998-2003 | | 22 |
| 1194 | An all-atom distance-dependent conditional probability discriminatory function for protein structure prediction. <i>Journal of Molecular Biology</i> , 1998 , 275, 895-916 | 6.5 | 383 |
| 1193 | Fold assembly of small proteins using monte carlo simulations driven by restraints derived from multiple sequence alignments. <i>Journal of Molecular Biology</i> , 1998 , 277, 419-48 | 6.5 | 79 |
| 1192 | The single helix in protein L is largely disrupted at the rate-limiting step in folding. <i>Journal of Molecular Biology</i> , 1998 , 284, 807-15 | 6.5 | 49 |
| 1191 | Clustering of low-energy conformations near the native structures of small proteins. 1998 , 95, 11158-62 | | 229 |
| 1190 | Analysis and algorithms for protein sequence-structure alignment. 1998 , 32, 227-283 | | 10 |
| 1189 | Experiment and theory highlight role of native state topology in SH3 folding. 1999 , 6, 1016-24 | | 323 |
| 1188 | Progress in protein structure prediction: assessment of CASP3. 1999 , 9, 368-73 | | 105 |
| 1187 | Structure prediction: The state of the art. 1999 , 9, R205-9 | | 11 |
| 1186 | Ab initio protein structure prediction of CASP III targets using ROSETTA. 1999 , 37, 171-176 | | 334 |

| | | | |
|------|--|-----|-----|
| 1185 | Ab initio protein structure prediction using a combined hierarchical approach. 1999 , 37, 194-198 | | 64 |
| 1184 | Improved recognition of native-like protein structures using a combination of sequence-dependent and sequence-independent features of proteins. 1999 , 34, 82-95 | | 337 |
| 1183 | De novo design and structural characterization of proteins and metalloproteins. 1999 , 68, 779-819 | | 529 |
| 1182 | Prediction of protein tertiary structure to low resolution: performance for a large and structurally diverse test set. <i>Journal of Molecular Biology</i> , 1999 , 288, 725-42 | 6.5 | 50 |
| 1181 | Ab initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions. <i>Journal of Molecular Biology</i> , 1999 , 290, 267-81 | 6.5 | 76 |
| 1180 | Application of Reduced Models to Protein Structure Prediction. 1999 , 397-440 | | 2 |
| 1179 | Derivation of protein-specific pair potentials based on weak sequence fragment similarity. 2000 , 38, 3-16 | | 84 |
| 1178 | Distance-dependent, pair potential for protein folding: Results from linear optimization. 2000 , 41, 40-46 | | 155 |
| 1177 | Bayesian probabilistic approach for predicting backbone structures in terms of protein blocks. 2000 , 41, 271-87 | | 212 |
| 1176 | Effective energy functions for protein structure prediction. 2000 , 10, 139-45 | | 361 |
| 1175 | De novo protein structure determination using sparse NMR data. 2000 , 18, 311-8 | | 138 |
| 1174 | Computational tools for protein modeling. 2000 , 1, 1-21 | | 49 |
| 1173 | Protein Structure Prediction. 2000 , | | 6 |
| 1172 | Constructing side chains on near-native main chains for ab initio protein structure prediction. 2000 , 13, 453-7 | | 28 |
| 1171 | Scoring functions for ab initio protein structure prediction. 2000 , 143, 223-45 | | 8 |
| 1170 | Extracting knowledge-based energy functions from protein structures by error rate minimization: Comparison of methods using lattice model. 2000 , 113, 9318-9330 | | 24 |
| 1169 | NMR characterization of residual structure in the denatured state of protein L. <i>Journal of Molecular Biology</i> , 2000 , 299, 1341-51 | 6.5 | 105 |
| 1168 | Ab initio construction of protein tertiary structures using a hierarchical approach. <i>Journal of Molecular Biology</i> , 2000 , 300, 171-85 | 6.5 | 148 |

| | | | |
|------|--|-----|-----|
| 1167 | Protein tertiary structure prediction. 2001 , Chapter 2, Unit2.7 | | 2 |
| 1166 | Ab initio protein structure prediction: progress and prospects. 2001 , 30, 173-89 | | 236 |
| 1165 | Convergent evolution of protein structure prediction and computer chess tournaments: CASP, Kasparov, and CAFASP. 2001 , 40, 410-425 | | 10 |
| 1164 | A novel method for sampling alpha-helical protein backbones. <i>Journal of Molecular Biology</i> , 2001 , 305, 191-201 | 6.5 | 28 |
| 1163 | Prospects for ab initio protein structural genomics. <i>Journal of Molecular Biology</i> , 2001 , 306, 1191-9 | 6.5 | 152 |
| 1162 | Functional inferences from blind ab initio protein structure predictions. 2001 , 134, 186-90 | | 28 |
| 1161 | Solvation Model Based on Weighted Solvent Accessible Surface Area. 2001 , 105, 5055-5067 | | 100 |
| 1160 | . 2001 , | | 3 |
| 1159 | Comparative Protein Structure Modeling. 2001 , | | 5 |
| 1158 | Determination, prediction, and understanding of structures, using the energy landscapes of chemical systems [Part II. 2001 , 216, 361-383 | | 50 |
| 1157 | Protein Structure Prediction. 2001 , 237-313 | | |
| 1156 | Application of PROSPECT in CASP4: characterizing protein structures with new folds. 2001 , Suppl 5, 140-8 | | 15 |
| 1155 | CAFASP2: the second critical assessment of fully automated structure prediction methods. 2001 , Suppl 5, 171-83 | | 93 |
| 1154 | A distance-dependent atomic knowledge-based potential for improved protein structure selection. 2001 , 44, 223-32 | | 252 |
| 1153 | Computer simulations aimed at structure prediction of supersecondary motifs in proteins. 2001 , 45, 159-66 | | 45 |
| 1152 | Rosetta in CASP4: progress in ab initio protein structure prediction. 2001 , Suppl 5, 119-26 | | 204 |
| 1151 | Modeling the third loop of short-chain snake venom neurotoxins: roles of the short-range and long-range interactions. 2001 , 42, 6-16 | | 3 |
| 1150 | Identification and ab initio simulations of early folding units in proteins. 2001 , 42, 164-76 | | 14 |

| | | | |
|------|--|-----|-----|
| 1149 | Improving the performance of Rosetta using multiple sequence alignment information and global measures of hydrophobic core formation. 2001 , 43, 1-11 | | 71 |
| 1148 | New energy terms for reduced protein models implemented in an off-lattice force field. 2001 , 22, 1229-1242 | | 102 |
| 1147 | Protein structure similarities. 2001 , 11, 348-53 | | 139 |
| 1146 | Sequence-based detection of distantly related proteins with the same fold. 2001 , 14, 455-8 | | 5 |
| 1145 | Statistical mechanical refinement of protein structure prediction schemes: Cumulant expansion approach. 2002 , 117, 4602-4615 | | 49 |
| 1144 | In silico identification, structure prediction and phylogenetic analysis of the 2'-O-ribose (cap 1) methyltransferase domain in the large structural protein of ssRNA negative-strand viruses. 2002 , 15, 101-8 | | 65 |
| 1143 | Toward predicting protein topology: an approach to identifying beta hairpins. 2002 , 99, 11157-62 | | 41 |
| 1142 | Improved recognition of native-like protein structures using a family of designed sequences. 2002 , 99, 691-6 | | 17 |
| 1141 | De novo determination of protein backbone structure from residual dipolar couplings using Rosetta. 2002 , 124, 2723-9 | | 153 |
| 1140 | On the Hamiltonian replica exchange method for efficient sampling of biomolecular systems: Application to protein structure prediction. 2002 , 116, 9058-9067 | | 598 |
| 1139 | Fully automated ab initio protein structure prediction using I-SITES, HMMSTR and ROSETTA. 2002 , 18 Suppl 1, S54-61 | | 100 |
| 1138 | Protein structure prediction constrained by solution X-ray scattering data and structural homology identification. <i>Journal of Molecular Biology</i> , 2002 , 316, 173-87 | 6.5 | 41 |
| 1137 | Contact order and ab initio protein structure prediction. 2002 , 11, 1937-44 | | 88 |
| 1136 | . 2002 , 17, 48-54 | | 1 |
| 1135 | De novo prediction of three-dimensional structures for major protein families. <i>Journal of Molecular Biology</i> , 2002 , 322, 65-78 | 6.5 | 206 |
| 1134 | Evaluation of C-H cdots, three dots, centered O hydrogen bonds in native and misfolded proteins. <i>Journal of Molecular Biology</i> , 2002 , 322, 497-503 | 6.5 | 23 |
| 1133 | Ab Initio Protein Structure Prediction Using a Size-dependent Tertiary Folding Potential. 2002 , 223-263 | | 1 |
| 1132 | . 2002 , | | 8 |

| | | |
|------|--|-----|
| 1131 | Ab initio protein structure prediction. 2002 , 12, 176-81 | 147 |
| 1130 | A comprehensive analysis of 40 blind protein structure predictions. 2002 , 2, 3 | 42 |
| 1129 | Use of structure comparison methods for the refinement of protein structure predictions. I. Identifying the structural family of a protein from low-resolution models. 2002 , 46, 72-84 | 3 |
| 1128 | A critical analysis of continuum electrostatics: the screened Coulomb potential--implicit solvent model and the study of the alanine dipeptide and discrimination of misfolded structures of proteins. 2002 , 47, 45-61 | 55 |
| 1127 | Distributions of beta sheets in proteins with application to structure prediction. 2002 , 48, 85-97 | 64 |
| 1126 | Prediction of protein secondary structures from conformational biases. 2002 , 48, 558-65 | 5 |
| 1125 | Distinguishing native conformations of proteins from decoys with an effective free energy estimator based on the OPLS all-atom force field and the Surface Generalized Born solvent model. 2002 , 48, 404-22 | 117 |
| 1124 | Natural coordinate representation for the protein backbone structure. 2002 , 49, 206-15 | 2 |
| 1123 | FROST: a filter-based fold recognition method. 2002 , 49, 493-509 | 36 |
| 1122 | Exact solutions for chemical bond orientations from residual dipolar couplings. 2002 , 22, 137-51 | 28 |
| 1121 | Design of an optimal Chebyshev-expanded discrimination function for globular proteins. 2002 , 11, 2010-21 | 20 |
| 1120 | Amino acid empirical contact energy definitions for fold recognition in the space of contact maps. 2003 , 4, 8 | 74 |
| 1119 | Protein decoy assembly using short fragments under geometric constraints. 2003 , 68, 278-85 | 32 |
| 1118 | Optimization of protein force-field parameters with the Protein Data Bank. 2003 , 382, 626-636 | 30 |
| 1117 | Ab initio construction of polypeptide fragments: efficient generation of accurate, representative ensembles. 2003 , 51, 41-55 | 123 |
| 1116 | Protein local structure prediction from sequence. 2003 , 50, 572-9 | 21 |
| 1115 | 3D-SHOTGUN: a novel, cooperative, fold-recognition meta-predictor. 2003 , 51, 434-41 | 143 |
| 1114 | Conserved residue clustering and protein structure prediction. 2003 , 52, 225-35 | 53 |

| | | |
|------|---|-----|
| 1113 | Assembly of protein tertiary structures from secondary structures using optimized potentials. 2003 , 52, 155-65 | 13 |
| 1112 | Fold recognition with minimal gaps. 2003 , 51, 531-43 | 4 |
| 1111 | Deciphering a novel thioredoxin-like fold family. 2003 , 52, 323-31 | 12 |
| 1110 | Optimizing physical energy functions for protein folding. 2004 , 54, 88-103 | 76 |
| 1109 | How well can we predict native contacts in proteins based on decoy structures and their energies?. 2003 , 52, 598-608 | 21 |
| 1108 | An improved protein decoy set for testing energy functions for protein structure prediction. 2003 , 53, 76-87 | 140 |
| 1107 | ProVal: a protein-scoring function for the selection of native and near-native folds. 2004 , 54, 289-302 | 10 |
| 1106 | Automated prediction of CASP-5 structures using the Robetta server. 2003 , 53 Suppl 6, 524-33 | 241 |
| 1105 | LiveBench-6: large-scale automated evaluation of protein structure prediction servers. 2003 , 53 Suppl 6, 542-7 | 50 |
| 1104 | Predicting interresidue contacts using templates and pathways. 2003 , 53 Suppl 6, 497-502 | 59 |
| 1103 | Combining local-structure, fold-recognition, and new fold methods for protein structure prediction. 2003 , 53 Suppl 6, 491-6 | 246 |
| 1102 | Assembling novel protein folds from super-secondary structural fragments. 2003 , 53 Suppl 6, 480-5 | 68 |
| 1101 | Application of 3D-Jury, GRDB, and Verify3D in fold recognition. 2003 , 53 Suppl 6, 418-23 | 45 |
| 1100 | Novel use of a genetic algorithm for protein structure prediction: searching template and sequence alignment space. 2003 , 53 Suppl 6, 424-9 | 27 |
| 1099 | Rosetta predictions in CASP5: successes, failures, and prospects for complete automation. 2003 , 53 Suppl 6, 457-68 | 142 |
| 1098 | CASP5 assessment of fold recognition target predictions. 2003 , 53 Suppl 6, 395-409 | 82 |
| 1097 | Strand-loop-strand motifs: prediction of hairpins and diverging turns in proteins. 2004 , 54, 282-8 | 39 |
| 1096 | Can correct protein models be identified?. 2003 , 12, 1073-86 | 551 |

| | | | |
|------|--|-----|-----|
| 1095 | Evaluation of Models of Electrostatic Interactions in Proteins. 2003 , 107, 2075-2090 | | 46 |
| 1094 | Combining inference from evolution and geometric probability in protein structure evaluation. <i>Journal of Molecular Biology</i> , 2003 , 331, 263-79 | 6.5 | 41 |
| 1093 | Protein-protein docking with simultaneous optimization of rigid-body displacement and side-chain conformations. <i>Journal of Molecular Biology</i> , 2003 , 331, 281-99 | 6.5 | 858 |
| 1092 | ASTRO-FOLD: a combinatorial and global optimization framework for Ab initio prediction of three-dimensional structures of proteins from the amino acid sequence. 2003 , 85, 2119-46 | | 92 |
| 1091 | Mining residue contacts in proteins using local structure predictions. 2003 , 33, 789-801 | | 11 |
| 1090 | Assigning function to yeast proteins by integration of technologies. 2003 , 12, 1353-65 | | 236 |
| 1089 | 3D-Jury: a simple approach to improve protein structure predictions. 2003 , 19, 1015-8 | | 655 |
| 1088 | Coupled prediction of protein secondary and tertiary structure. 2003 , 100, 12105-10 | | 148 |
| 1087 | Associative memory Hamiltonians for structure prediction without homology: alpha/beta proteins. 2003 , 100, 1679-84 | | 38 |
| 1086 | Small-angle scattering: a view on the properties, structures and structural changes of biological macromolecules in solution. 2003 , 36, 147-227 | | 427 |
| 1085 | A reversible fragment assembly method for de novo protein structure prediction. 2003 , 119, 6895-6903 | | 43 |
| 1084 | Using protein design for homology detection and active site searches. 2003 , 100, 11361-6 | | 24 |
| 1083 | Rapid protein fold determination using unassigned NMR data. 2003 , 100, 15404-9 | | 103 |
| 1082 | Funnel sculpting for in silico assembly of secondary structure elements of proteins. 2003 , 100, 10700-5 | | 31 |
| 1081 | A novel approach to fold recognition using sequence-derived properties from sets of structurally similar local fragments of proteins. 2003 , 19 Suppl 2, ii81-91 | | 20 |
| 1080 | Efficient Energy Computation for Monte Carlo Simulation of Proteins. 2003 , 354-373 | | 3 |
| 1079 | Novel Fold and Ab Initio Methods for Protein Structure Generation. 2003 , 251-276 | | |
| 1078 | Algorithm and data structures for efficient energy maintenance during Monte Carlo simulation of proteins. 2004 , 11, 902-32 | | 15 |

| | | |
|------|---|------|
| 1077 | Contact-based sequence alignment. 2004 , 32, 2464-73 | 16 |
| 1076 | Developing optimal non-linear scoring function for protein design. 2004 , 20, 3080-98 | 28 |
| 1075 | Wurst: a protein threading server with a structural scoring function, sequence profiles and optimized substitution matrices. 2004 , 32, W532-5 | 38 |
| 1074 | The Yeast Resource Center Public Data Repository. 2005 , 33, D378-82 | 25 |
| 1073 | Protein Structure Prediction with Stochastic Optimization Methods: Folding and Misfolding the Villin Headpiece. 2004 , 454-464 | 8 |
| 1072 | PROTEIN FORCE-FIELD PARAMETERS OPTIMIZED WITH THE PROTEIN DATA BANK I: FORCE-FIELD OPTIMIZATIONS. 2004 , 03, 339-358 | 17 |
| 1071 | 10 residue folded peptide designed by segment statistics. 2004 , 12, 1507-18 | 230 |
| 1070 | Development of novel statistical potentials for protein fold recognition. 2004 , 14, 225-32 | 104 |
| 1069 | Protein structure prediction and analysis using the Robetta server. 2004 , 32, W526-31 | 1239 |
| 1068 | Oriental potentials extracted from protein structures improve native fold recognition. 2004 , 13, 862-74 | 79 |
| 1067 | Some fundamental aspects of building protein structures from fragment libraries. 2004 , 13, 1636-50 | 34 |
| 1066 | Reduced models of proteins and their applications. 2004 , 45, 511-524 | 159 |
| 1065 | Single-body residue-level knowledge-based energy score combined with sequence-profile and secondary structure information for fold recognition. 2004 , 55, 1005-13 | 165 |
| 1064 | Prediction of protein tertiary structure using PROFESY, a novel method based on fragment assembly and conformational space annealing. 2004 , 56, 704-14 | 64 |
| 1063 | Combining evolutionary and structural information for local protein structure prediction. 2004 , 56, 782-94 | 21 |
| 1062 | Accurate prediction of solvent accessibility using neural networks-based regression. 2004 , 56, 753-67 | 205 |
| 1061 | Fold recognition by combining sequence profiles derived from evolution and from depth-dependent structural alignment of fragments. 2005 , 58, 321-8 | 195 |
| 1060 | Ab initio prediction of the three-dimensional structure of a de novo designed protein: a double-blind case study. 2005 , 58, 560-70 | 46 |

| | | |
|------|---|--------|
| 1059 | Distinguish protein decoys by using a scoring function based on a new AMBER force field, short molecular dynamics simulations, and the generalized born solvent model. 2004 , 55, 620-34 | 239 |
| 1058 | Modeling structurally variable regions in homologous proteins with rosetta. 2004 , 55, 656-77 | 264 |
| 1057 | Improved protein structure selection using decoy-dependent discriminatory functions. 2004 , 4, 8 | 49 |
| 1056 | Peptide backbone reconstruction using dead-end elimination and a knowledge-based forcefield. 2004 , 25, 16-27 | 20 |
| 1055 | Continuous anisotropic representation of coarse-grained potentials for proteins by spherical harmonics synthesis. 2004 , 22, 441-50 | 24 |
| 1054 | Automated structure determination of proteins by NMR spectroscopy. 2004 , 44, 33-96 | 91 |
| 1053 | Orientation-dependent coarse-grained potentials derived by statistical analysis of molecular structural databases. 2004 , 45, 597-608 | 23 |
| 1052 | Protein folding mechanisms and energy landscape of src SH3 domain studied by a structure prediction toolbox. 2004 , 307, 157-162 | 18 |
| 1051 | Protein decoy sets for evaluating energy functions. 2004 , 21, 725-36 | 20 |
| 1050 | On the transferability of folding and threading potentials and sequence-independent filters for protein folding simulations. 2004 , 102, 1291-1305 | 6 |
| 1049 | An accurate, residue-level, pair potential of mean force for folding and binding based on the distance-scaled, ideal-gas reference state. 2004 , 13, 400-11 | 144 |
| 1048 | The dependence of all-atom statistical potentials on structural training database. 2004 , 86, 3349-58 | 39 |
| 1047 | Database-derived potentials dependent on protein size for in silico folding and design. 2004 , 87, 171-81 | 16 |
| 1046 | An all-atom force field for tertiary structure prediction of helical proteins. 2004 , 87, 3100-9 | 54 |
| 1045 | Analysis of anisotropic side-chain packing in proteins and application to high-resolution structure prediction. <i>Journal of Molecular Biology</i> , 2004 , 342, 651-64 | 6.5 40 |
| 1044 | Protein structure prediction using Rosetta. 2004 , 383, 66-93 | 1142 |
| 1043 | Informatics (Computational Biology). 2004 , | |
| 1042 | Ab initio methods. 2003 , 44, 547-57 | 7 |

| | | |
|------|--|-----|
| 1041 | Ab initio structure prediction. 2005 , | |
| 1040 | Ab initio Modeling. 2005 , 137-161 | |
| 1039 | Recent progress in the study of biomolecular structure and dynamics in solution from residual dipolar couplings. 2005 , 46, 23-61 | 247 |
| 1038 | Photochemical surface mapping of C14S-Sml1p for constrained computational modeling of protein structure. 2005 , 340, 201-12 | 34 |
| 1037 | A coarse-grained langevin molecular dynamics approach to protein structure reproduction. 2005 , 402, 102-106 | 7 |
| 1036 | Characterization and study of a kappa-casein-like chymosin-sensitive linkage. 2005 , 1749, 75-80 | 3 |
| 1035 | Folding of small helical proteins assisted by small-angle X-ray scattering profiles. 2005 , 13, 1587-97 | 29 |
| 1034 | Identification of a new family of putative PD-(D/E)XK nucleases with unusual phylogenomic distribution and a new type of the active site. 2005 , 6, 21 | 35 |
| 1033 | Evolutionary method for the assembly of rigid protein fragments. 2005 , 26, 131-41 | 6 |
| 1032 | Practical conversion from torsion space to Cartesian space for in silico protein synthesis. 2005 , 26, 1063-8 | 52 |
| 1031 | Research challenges, opportunities and synergism in systems engineering and computational biology. 2005 , 51, 1872-1884 | 27 |
| 1030 | The fumarate sensor DcuS: progress in rapid protein fold elucidation by combining protein structure prediction methods with NMR spectroscopy. 2005 , 173, 310-6 | 22 |
| 1029 | Protein structure prediction based on fragment assembly and parameter optimization. 2005 , 115, 209-14 | 35 |
| 1028 | Progress and challenges in high-resolution refinement of protein structure models. 2005 , 59, 15-29 | 130 |
| 1027 | An amino acid has two sides: a new 2D measure provides a different view of solvent exposure. 2005 , 59, 38-48 | 95 |
| 1026 | Inferring ideal amino acid interaction forms from statistical protein contact potentials. 2005 , 59, 49-57 | 55 |
| 1025 | Sequence-structure-function relationships of a tRNA (m7G46) methyltransferase studied by homology modeling and site-directed mutagenesis. 2005 , 59, 482-8 | 27 |
| 1024 | Prediction of the conformation and geometry of loops in globular proteins: testing ArchDB, a structural classification of loops. 2005 , 60, 746-57 | 17 |

| | | |
|------|---|-----|
| 1023 | Progress in protein-protein docking: atomic resolution predictions in the CAPRI experiment using RosettaDock with an improved treatment of side-chain flexibility. 2005 , 60, 187-94 | 87 |
| 1022 | A new catalog of protein beta-sheets. 2005 , 61, 545-58 | 16 |
| 1021 | Assessment of CASP6 predictions for new and nearly new fold targets. 2005 , 61 Suppl 7, 67-83 | 44 |
| 1020 | TASSER: an automated method for the prediction of protein tertiary structures in CASP6. 2005 , 61 Suppl 7, 91-8 | 161 |
| 1019 | FRankenStein becomes a cyborg: the automatic recombination and realignment of fold recognition models in CASP6. 2005 , 61 Suppl 7, 106-13 | 63 |
| 1018 | Prediction of novel and analogous folds using fragment assembly and fold recognition. 2005 , 61 Suppl 7, 143-51 | 71 |
| 1017 | Prediction of CASP6 structures using automated Robetta protocols. 2005 , 61 Suppl 7, 157-66 | 114 |
| 1016 | Automated prediction of domain boundaries in CASP6 targets using Ginzu and RosettaDOM. 2005 , 61 Suppl 7, 193-200 | 72 |
| 1015 | CASP6 assessment of contact prediction. 2005 , 61 Suppl 7, 214-24 | 72 |
| 1014 | SimFold energy function for de novo protein structure prediction: consensus with Rosetta. 2006 , 62, 381-98 | 43 |
| 1013 | Assessing a novel approach for predicting local 3D protein structures from sequence. 2006 , 62, 865-80 | 36 |
| 1012 | Multipass membrane protein structure prediction using Rosetta. 2006 , 62, 1010-25 | 260 |
| 1011 | Recent developments in structural proteomics for protein structure determination. 2005 , 5, 2056-68 | 57 |
| 1010 | Score functions for structure prediction. 2005 , | |
| 1009 | Molecular simulations in structure prediction. 2005 , | |
| 1008 | Protein Threading. 2005 , 921-938 | 4 |
| 1007 | Less is more: towards an optimal universal description of protein folds. 2005 , 21 Suppl 2, ii66-71 | 15 |
| 1006 | Density guided importance sampling: application to a reduced model of protein folding. 2005 , 21, 2839-43 | 8 |

1005 Overview of Structural Bioinformatics. **2005**, 15-44

1004 HCPM--program for hierarchical clustering of protein models. **2005**, 21, 3179-80 29

1003 Building native protein conformation from highly approximate backbone torsion angles. **2005**, 102, 16227-32 47

1002 Protein structure estimation from minimal restraints using Rosetta. **2005**, 394, 244-60 27

1001 How effective for fold recognition is a potential of mean force that includes relative orientations between contacting residues in proteins?. **2005**, 122, 024901 50

1000 GEMSCORE: A New Empirical Energy Function for Protein Folding. **2005**,

999 A new approach to prediction of short-range conformational propensities in proteins. **2005**, 21, 981-7 6

998 Conkunitzin-S1 is the first member of a new Kunitz-type neurotoxin family. Structural and functional characterization. **2005**, 280, 23766-70 78

997 Release of long-range tertiary interactions potentiates aggregation of natively unstructured alpha-synuclein. **2005**, 102, 1430-5 612

996 Triticum durum metallothionein. Isolation of the gene and structural characterization of the protein using solution scattering and molecular modeling. **2005**, 280, 13701-11 52

995 Linear regression models for solvent accessibility prediction in proteins. **2005**, 12, 355-69 84

994 Development of a Grid-based statistical potential for protein structure prediction. **2005**, 2005, 6064-7 1

993 Mva1269I: a monomeric type IIS restriction endonuclease from *Micrococcus varians* with two EcoRI- and FokI-like catalytic domains. **2005**, 280, 41584-94 24

992 Prediction of contact map integrated PNN with conformational energy. 1

991 Progress in modeling of protein structures and interactions. **2005**, 310, 638-42 244

990 The Proteomics Protocols Handbook. **2005**, 204

989 SCRATCH: a protein structure and structural feature prediction server. **2005**, 33, W72-6 678

988 Structural Determinants of Transmembrane EBarrels. **2005**, 1, 716-22 28

| | | | |
|-----|---|-----|-----|
| 987 | An atomic environment potential for use in protein structure prediction. <i>Journal of Molecular Biology</i> , 2005 , 352, 986-1001 | 6.5 | 53 |
| 986 | Global optimization and folding pathways of selected alpha-helical proteins. 2005 , 123, 234901 | | 89 |
| 985 | Chapter 11 Protein bioinformatics. 2005 , 487-500 | | |
| 984 | Data Mining in Bioinformatics. 2005 , | | 5 |
| 983 | Bioinformatics Technologies. 2005 , | | 10 |
| 982 | Reconstructing protein structure from solvent exposure using tabu search. 2006 , 1, 20 | | 9 |
| 981 | Evaluation of molecular models for the affinity maturation of antibodies: roles of cytosine deamination by AID and DNA repair. 2006 , 106, 700-19 | | 25 |
| 980 | Characterization of the hydrodynamic properties of the folding transition state of an SH3 domain by magnetization transfer NMR spectroscopy. 2006 , 45, 6434-45 | | 6 |
| 979 | Parallelization and performance characterization of protein 3D structure prediction of Rosetta. 2006 , | | |
| 978 | Molecular analysis of capsid protein of Homalodisca coagulata Virus-1, a new leafhopper-infecting virus from the glassy-winged sharpshooter, Homalodisca coagulata. 2006 , 6, 1-10 | | 14 |
| 977 | Computer-based design of novel protein structures. 2006 , 35, 49-65 | | 107 |
| 976 | Structural diversity of protein segments follows a power-law distribution. 2006 , 91, 1213-23 | | 14 |
| 975 | A new generation of statistical potentials for proteins. 2006 , 90, 4010-7 | | 78 |
| 974 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1553-1553 | | |
| 973 | A multi-objective evolutionary approach to the protein structure prediction problem. 2006 , 3, 139-51 | | 85 |
| 972 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1576-1576 | | |
| 971 | Bayesian segmental models with multiple sequence alignment profiles for protein secondary structure and contact map prediction. 2006 , 3, 98-113 | | 22 |
| 970 | Protein Structure Prediction: The Next Generation. 2006 , 2, 705-16 | | 36 |

| | | | |
|-----|--|-----|------|
| 969 | Characterization of prmt7alpha and beta isozymes from Chinese hamster cells sensitive and resistant to topoisomerase II inhibitors. 2006 , 1760, 1646-56 | | 27 |
| 968 | Protein structure prediction using mutually orthogonal Latin squares and a genetic algorithm. 2006 , 342, 424-33 | | 12 |
| 967 | A unique amino acid substitution, T126I, in human genotype C of hepatitis B virus S gene and its possible influence on antigenic structural change. 2006 , 383, 43-51 | | 22 |
| 966 | Nucleotide channel of RNA-dependent RNA polymerase used for intermolecular uridylylation of protein primer. <i>Journal of Molecular Biology</i> , 2006 , 357, 665-75 | 6.5 | 26 |
| 965 | Recapitulation and design of protein binding peptide structures and sequences. <i>Journal of Molecular Biology</i> , 2006 , 357, 917-27 | 6.5 | 48 |
| 964 | Minimalist representations and the importance of nearest neighbor effects in protein folding simulations. <i>Journal of Molecular Biology</i> , 2006 , 363, 835-57 | 6.5 | 37 |
| 963 | A fast algorithm for low-resolution protein structure prediction. 2006 , 2006, 5826-9 | | 2 |
| 962 | Sequence-dependent enhancement of hydrolytic deamination of cytosines in DNA by the restriction enzyme PspGI. 2006 , 34, 3762-70 | | 12 |
| 961 | The Challenges of Making Useful Protein-Ligand Free Energy Predictions for Drug Discovery. 2006 , 321-351 | | 3 |
| 960 | A general method for the unbiased improvement of solution NMR structures by the use of related X-ray data, the AUREMOL-ISIC algorithm. 2006 , 6, 14 | | 5 |
| 959 | Empirical potential function for simplified protein models: combining contact and local sequence-structure descriptors. 2006 , 63, 949-60 | | 31 |
| 958 | Nearest-neighbor effects and structural preferences in dipeptides are a function of the electronic properties of amino acid side-chains. 2006 , 63, 939-48 | | 8 |
| 957 | Novel approach for alpha-helical topology prediction in globular proteins: generation of interhelical restraints. 2006 , 65, 930-52 | | 14 |
| 956 | Prediction of peptide structure: how far are we?. 2006 , 65, 889-97 | | 54 |
| 955 | Advances in protein structure prediction and de novo protein design: A review. 2006 , 61, 966-988 | | 175 |
| 954 | Statistical potential for assessment and prediction of protein structures. 2006 , 15, 2507-24 | | 1714 |
| 953 | What is a desirable statistical energy function for proteins and how can it be obtained?. 2006 , 46, 165-74 | | 44 |
| 952 | Threading with environment-specific score by artificial neural networks. 2006 , 10, 305-314 | | 1 |

| | | |
|-----|---|-----|
| 951 | Analysis of HIV-2 Vpx by modeling and insertional mutagenesis. 2006 , 348, 165-74 | 13 |
| 950 | High-resolution protein-protein docking. 2006 , 16, 183-93 | 152 |
| 949 | Local protein structure prediction using discriminative models. 2006 , 7, 14 | 51 |
| 948 | Novel knowledge-based mean force potential at the profile level. 2006 , 7, 324 | 23 |
| 947 | Molecular phylogenetics and comparative modeling of HEN1, a methyltransferase involved in plant microRNA biogenesis. 2006 , 6, 6 | 39 |
| 946 | Protein-structure prediction by recombination of fragments. 2006 , 7, 19-27 | 65 |
| 945 | Modelling sequential protein folding under kinetic control. 2006 , 22, e203-10 | 23 |
| 944 | A supersecondary structure library and search algorithm for modeling loops in protein structures. 2006 , 34, 2085-97 | 67 |
| 943 | HARMONY: a server for the assessment of protein structures. 2006 , 34, W231-4 | 30 |
| 942 | Homology modeling using parametric alignment ensemble generation with consensus and energy-based model selection. 2006 , 34, e112 | 85 |
| 941 | A knowledge-based scoring function based on residue triplets for protein structure prediction. 2006 , 19, 187-93 | 15 |
| 940 | Protein folding using fragment assembly and physical energy function. 2006 , 125, 194908 | 9 |
| 939 | A NEW MEMBER OF THE GROWTH-PROMOTING GLYCOPROTEINS FROM DIAPREPES ROOT WEEVIL (COLEOPTERA: CURCULIONIDAE). 2006 , 89, 223-232 | 2 |
| 938 | Sampling realistic protein conformations using local structural bias. 2006 , 2, e131 | 66 |
| 937 | Structure modeling of all identified G protein-coupled receptors in the human genome. 2006 , 2, e13 | 159 |
| 936 | A simple approach for protein structure discrimination based on the network pattern of conserved hydrophobic residues. 2006 , 19, 265-75 | 27 |
| 935 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1415-1415 | |
| 934 | Physically realistic homology models built with ROSETTA can be more accurate than their templates. 2006 , 103, 5361-6 | 138 |

| | | |
|-----|---|-----|
| 933 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1359-1362 | |
| 932 | Oligomerization of hantavirus nucleocapsid protein: analysis of the N-terminal coiled-coil domain. 2006 , 80, 9073-81 | 22 |
| 931 | Complete cap 4 formation is not required for viability in <i>Trypanosoma brucei</i> . 2006 , 5, 905-15 | 27 |
| 930 | Shaping up the protein folding funnel by local interaction: lesson from a structure prediction study. 2006 , 103, 3141-6 | 57 |
| 929 | Structure and function of the voltage sensor of sodium channels probed by a beta-scorpion toxin. 2006 , 281, 21332-21344 | 115 |
| 928 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1533-1537 | |
| 927 | HYPLOSP: a knowledge-based approach to protein local structure prediction. 2006 , 4, 1287-307 | 4 |
| 926 | Protein structure evaluation using an all-atom energy based empirical scoring function. 2006 , 23, 385-406 | 26 |
| 925 | Proteases and Inhibitors. 2005 , 1469-1473 | |
| 924 | Graph theoretic properties of networks formed by the Delaunay tessellation of protein structures. 2006 , 73, 041925 | 20 |
| 923 | Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. 2005 , 1449-1449 | |
| 922 | CONSTANS and the CCAAT box binding complex share a functionally important domain and interact to regulate flowering of <i>Arabidopsis</i> . 2006 , 18, 2971-84 | 415 |
| 921 | JSSPrediction: a Framework to Predict Protein Secondary Structures Using Integration. 2006 , | 1 |
| 920 | Comparison of properties of particles of Cucumber mosaic virus and Tomato aspermy virus based on the analysis of molecular surfaces of capsids. 2006 , 87, 2073-2083 | 8 |
| 919 | Effective optimization algorithms for fragment-assembly based protein structure prediction. 2007 , 5, 335-52 | 2 |
| 918 | Automated de novo prediction of native-like RNA tertiary structures. 2007 , 104, 14664-9 | 334 |
| 917 | Superfamily assignments for the yeast proteome through integration of structure prediction with the gene ontology. 2007 , 5, e76 | 42 |
| 916 | Draft crystal structure of the vault shell at 9-A resolution. 2007 , 5, e318 | 36 |

| | | | |
|-----|---|-----|-----|
| 915 | An extremal optimization search method for the protein folding problem. 2007 , | | 2 |
| 914 | Hypergraph model of multi-residue interactions in proteins: sequentially-constrained partitioning algorithms for optimization of site-directed protein recombination. 2007 , 14, 777-90 | | 17 |
| 913 | Prediction of the structure of symmetrical protein assemblies. 2007 , 104, 17656-61 | | 142 |
| 912 | High-resolution design of a protein loop. 2007 , 104, 17668-73 | | 97 |
| 911 | In vivo oligomerization of the F conjugative coupling protein TraD. 2007 , 189, 6626-34 | | 16 |
| 910 | Consensus Data Mining (CDM) Protein Secondary Structure Prediction Server: combining GOR V and Fragment Database Mining (FDM). 2007 , 23, 2628-30 | | 23 |
| 909 | Homology Modeling in Biology and Medicine. 297-349 | | 1 |
| 908 | Role of the C-terminal domains of rice (<i>Oryza sativa</i> L.) bZIP proteins RF2a and RF2b in regulating transcription. 2007 , 405, 243-9 | | 10 |
| 907 | Pathogenic proline mutation in the linker between spectrin repeats: disease caused by spectrin unfolding. 2007 , 109, 3538-43 | | 30 |
| 906 | Mapping early conformational changes in alpha11b and beta3 during biogenesis reveals a potential mechanism for alpha11bbeta3 adopting its bent conformation. 2007 , 109, 3725-32 | | 26 |
| 905 | Jaburetox-2Ec: an insecticidal peptide derived from an isoform of urease from the plant <i>Canavalia ensiformis</i> . 2007 , 28, 2042-50 | | 60 |
| 904 | Truncation of the caspase-related subunit (Gpi8p) of <i>Saccharomyces cerevisiae</i> GPI transamidase: dimerization revealed. 2007 , 462, 83-93 | | 10 |
| 903 | Density-based score for selecting near-native atomic models of unknown structures. 2007 , 158, 188-95 | | 7 |
| 902 | Structural model of human endoglin, a transmembrane receptor responsible for hereditary hemorrhagic telangiectasia. <i>Journal of Molecular Biology</i> , 2007 , 365, 694-705 | 6.5 | 74 |
| 901 | Improved structural characterizations of the drkN SH3 domain unfolded state suggest a compact ensemble with native-like and non-native structure. <i>Journal of Molecular Biology</i> , 2007 , 367, 1494-510 | 6.5 | 99 |
| 900 | Role of the intracellular domains of the human FSH receptor in G(alphaS) protein coupling and receptor expression. 2007 , 260-262, 153-62 | | 42 |
| 899 | Protein Interactions. 2007 , | | 5 |
| 898 | Bioinformatics. 2007 , | | 1 |

| | | |
|-----|--|-----|
| 897 | LOMETS: a local meta-threading-server for protein structure prediction. 2007 , 35, 3375-82 | 626 |
| 896 | Assessment of Semiempirical Quantum Mechanical Methods for the Evaluation of Protein Structures. 2007 , 3, 1609-1619 | 23 |
| 895 | Decoy Discrimination Using Contact Potentials Based on Delaunay Tessellation of Hydrated Proteins. 2007 , | 1 |
| 894 | Statistical estimation of statistical mechanical models: helix-coil theory and peptide helicity prediction. 2007 , 14, 1287-310 | 6 |
| 893 | Protein Secondary Structure Prediction using Bayesian Inference method on Decision fusion algorithms. 2007 , | 0 |
| 892 | Data Mining in Biomedicine. 2007 , | 27 |
| 891 | Protein structure determination from NMR chemical shifts. 2007 , 104, 9615-20 | 440 |
| 890 | Assessment of Detection and Refinement Strategies for de novo Protein Structures Using Force Field and Statistical Potentials. 2007 , 3, 312-24 | 23 |
| 889 | Computational Methods for Protein Structure Prediction and Modeling. 2007 , | 5 |
| 888 | A free-rotating and self-avoiding chain model for deriving statistical potentials based on protein structures. 2007 , 92, 3868-77 | 8 |
| 887 | Ab initio protein structure prediction using chunk-TASSER. 2007 , 93, 1510-8 | 78 |
| 886 | Elucidation of Protein-Protein and Protein-Ligand Interactions by NMR Spectroscopy. 2007 , 189-229 | |
| 885 | Protein Structure Prediction using String Kernels. 145-168 | 1 |
| 884 | Bioinformatics. 2007 , 315-347 | 1 |
| 883 | Computational methods in protein structure prediction. 2007 , 97, 207-13 | 93 |
| 882 | An object-oriented library for computational protein design. 2007 , 28, 2378-88 | 32 |
| 881 | Protein structure prediction aided by geometrical and probabilistic constraints. 2007 , 28, 1943-52 | 5 |
| 880 | Protein structure prediction by all-atom free-energy refinement. 2007 , 7, 12 | 17 |

| | | |
|-----|--|-----|
| 879 | Scoring predictive models using a reduced representation of proteins: model and energy definition. 2007 , 7, 15 | 20 |
| 878 | Type II restriction endonuclease R.Eco29ki is a member of the GIY-YIG nuclease superfamily. 2007 , 7, 48 | 27 |
| 877 | Ab initio modeling of small proteins by iterative TASSER simulations. 2007 , 5, 17 | 378 |
| 876 | Benchmarking of TASSER in the ab initio limit. 2007 , 68, 48-56 | 6 |
| 875 | Library of local descriptors models the core of proteins accurately. 2007 , 69, 499-510 | 4 |
| 874 | Scoring function accuracy for membrane protein structure prediction. 2007 , 68, 67-75 | 13 |
| 873 | A model of restriction endonuclease MvaI in complex with DNA: a template for interpretation of experimental data and a guide for specificity engineering. 2007 , 68, 324-36 | 12 |
| 872 | A tetrapeptide fragment-based design method results in highly stable artificial proteins. 2007 , 68, 839-49 | 14 |
| 871 | A coarse-grained protein force field for folding and structure prediction. 2007 , 69, 394-408 | 160 |
| 870 | Ideal amino acid exchange forms for approximating substitution matrices. 2007 , 69, 379-93 | 11 |
| 869 | Modeling the structure of mAb 14B7 bound to the anthrax protective antigen. 2008 , 70, 218-30 | 28 |
| 868 | Structure prediction for CASP7 targets using extensive all-atom refinement with Rosetta@home. 2007 , 69 Suppl 8, 118-28 | 158 |
| 867 | Assessment of predictions submitted for the CASP7 domain prediction category. 2007 , 69 Suppl 8, 137-51 | 36 |
| 866 | Template-based modeling and free modeling by I-TASSER in CASP7. 2007 , 69 Suppl 8, 108-17 | 368 |
| 865 | Incorporating biochemical information and backbone flexibility in RosettaDock for CAPRI rounds 6-12. 2007 , 69, 793-800 | 37 |
| 864 | Straightening and sequential buckling of the pore-lining helices define the gating cycle of MscS. 2007 , 14, 1141-9 | 86 |
| 863 | High-resolution structure prediction and the crystallographic phase problem. 2007 , 450, 259-64 | 262 |
| 862 | Worth the effort. An account of the Seventh Meeting of the Worldwide Critical Assessment of Techniques for Protein Structure Prediction. 2007 , 274, 1651-4 | 6 |

| | | |
|-----|--|-----|
| 861 | An adaptive bin framework search method for a beta-sheet protein homopolymer model. 2007 , 8, 136 | 3 |
| 860 | Potential energy functions for protein design. 2007 , 17, 199-204 | 118 |
| 859 | Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007 , 15, 727-40 | 41 |
| 858 | Molecular modeling of the complex between the xWNT8 protein and the CRD domain of the mFZD8 receptor. 2007 , 412, 8-11 | 3 |
| 857 | OPUS-Ca: a knowledge-based potential function requiring only C α positions. 2007 , 16, 1449-63 | 65 |
| 856 | Reduced C(beta) statistical potentials can outperform all-atom potentials in decoy identification. 2007 , 16, 2123-39 | 35 |
| 855 | Constraint Programming in Structural Bioinformatics. 2008 , 13, 3-20 | 13 |
| 854 | The sequence and model structure analysis of three Polish peanut stunt virus strains. 2008 , 36, 221-9 | 11 |
| 853 | Direct methods and residue type specific isotope labeling in NMR structure determination and model-driven sequential assignment. 2008 , 42, 111-27 | 4 |
| 852 | Tip-alpha (hp0596 gene product) is a highly immunogenic Helicobacter pylori protein involved in colonization of mouse gastric mucosa. 2008 , 56, 279-86 | 20 |
| 851 | The twists and turns of beta-peptides. 1999 , 54, 206-17 | 148 |
| 850 | Type II restriction endonuclease R.Hpy188I belongs to the GIY-YIG nuclease superfamily, but exhibits an unusual active site. 2008 , 8, 48 | 14 |
| 849 | SELECTpro: effective protein model selection using a structure-based energy function resistant to BLUNDERS. 2008 , 8, 52 | 21 |
| 848 | Residue contact-count potentials are as effective as residue-residue contact-type potentials for ranking protein decoys. 2008 , 8, 53 | 8 |
| 847 | Stochastic reconstruction of protein structures from effective connectivity profiles. 2008 , 1, 5 | 6 |
| 846 | Molecular replacement using ab initio polyalanine models generated with ROSETTA. 2008 , 64, 1288-91 | 29 |
| 845 | Using the Rosetta algorithm and selected inter-residue distances to predict protein structure. 2008 , 108, 2793-2802 | 2 |
| 844 | Using distances between β -carbons to predict protein structure. 2008 , 108, 2782-2792 | 3 |

| | | |
|-----|--|-----|
| 843 | Distance dependent centroid to centroid force fields using high resolution decoys. 2008 , 70, 950-70 | 40 |
| 842 | Local interactions in protein folding determined through an inverse folding model. 2008 , 71, 278-99 | 4 |
| 841 | Crystal structure of a novel non-Pfam protein AF1514 from <i>Archeoglobus fulgidus</i> DSM 4304 solved by S-SAD using a Cr X-ray source. 2008 , 71, 2109-13 | 6 |
| 840 | Discriminative learning for protein conformation sampling. 2008 , 73, 228-40 | 30 |
| 839 | Constructing templates for protein structure prediction by simulation of protein folding pathways. 2008 , 73, 380-94 | 8 |
| 838 | Time-averaged predictions of folded and misfolded peptides using a reduced physicochemical model. 2008 , 29, 1177-85 | 4 |
| 837 | Soft energy function and generic evolutionary method for discriminating native from nonnative protein conformations. 2008 , 29, 1364-73 | |
| 836 | Modeling and experimental analyses reveal a two-domain structure and amino acids important for the activity of aminoglycoside resistance methyltransferase Sgm. 2008 , 1784, 582-90 | 14 |
| 835 | A historical perspective of template-based protein structure prediction. 2008 , 413, 3-42 | 17 |
| 834 | Aligning sequences to structures. 2008 , 413, 61-90 | 2 |
| 833 | Scoring functions for de novo protein structure prediction revisited. 2008 , 413, 243-81 | 8 |
| 832 | Scoring functions in protein folding and design. 2000 , 9, 812-9 | 14 |
| 831 | Macromolecular modeling with rosetta. 2008 , 77, 363-82 | 693 |
| 830 | Bioinformatic analysis and molecular modelling of human ameloblastin suggest a two-domain intrinsically unstructured calcium-binding protein. 2008 , 116, 124-34 | 37 |
| 829 | Validation of protein models by a neural network approach. 2008 , 9, 66 | 22 |
| 828 | Using neural networks and evolutionary information in decoy discrimination for protein tertiary structure prediction. 2008 , 9, 94 | 10 |
| 827 | Progress and challenges in protein structure prediction. 2008 , 18, 342-8 | 382 |
| 826 | De novo high-resolution protein structure determination from sparse spin-labeling EPR data. 2008 , 16, 181-95 | 102 |

| | | | |
|-----|--|-----|-----|
| 825 | Structure prediction of domain insertion proteins from structures of individual domains. 2008 , 16, 513-27 | | 17 |
| 824 | Iterative assembly of helical proteins by optimal hydrophobic packing. 2008 , 16, 1257-66 | | 10 |
| 823 | Template-Free Predictions of Three-Dimensional Protein Structures: From First Principles to Knowledge-Based Potentials. 2008 , 117-141 | | 1 |
| 822 | Generalized pattern search algorithm for Peptide structure prediction. 2008 , 95, 4988-99 | | 28 |
| 821 | Fragment-HMM: a new approach to protein structure prediction. 2008 , 17, 1925-34 | | 48 |
| 820 | Protein structure prediction. Preface. 2008 , 413, v-vii | | 8 |
| 819 | Protein sequence and structure alignments within one framework. 2008 , 3, 4 | | 9 |
| 818 | Machine learning methods for protein structure prediction. 2008 , 1, 41-9 | | 70 |
| 817 | Modern Genome Annotation. 2008 , | | 3 |
| 816 | Practical Bioinformatics. 2008 , | | |
| 815 | Packing of transmembrane helices in bacteriorhodopsin folding: structure and thermodynamics. 2008 , 162, 237-47 | | 8 |
| 814 | Three-dimensional architecture of membrane-embedded MscS in the closed conformation. <i>Journal of Molecular Biology</i> , 2008 , 378, 55-70 | 6.5 | 71 |
| 813 | HsdR subunit of the type I restriction-modification enzyme EcoR124I: biophysical characterisation and structural modelling. <i>Journal of Molecular Biology</i> , 2008 , 376, 438-52 | 6.5 | 22 |
| 812 | OPUS-PSP: an orientation-dependent statistical all-atom potential derived from side-chain packing. <i>Journal of Molecular Biology</i> , 2008 , 376, 288-301 | 6.5 | 141 |
| 811 | Backrub-like backbone simulation recapitulates natural protein conformational variability and improves mutant side-chain prediction. <i>Journal of Molecular Biology</i> , 2008 , 380, 742-56 | 6.5 | 232 |
| 810 | Conformer selection and induced fit in flexible backbone protein-protein docking using computational and NMR ensembles. <i>Journal of Molecular Biology</i> , 2008 , 381, 1068-87 | 6.5 | 128 |
| 809 | The nature of the transition state ensemble and the mechanisms of protein folding: a review. 2008 , 469, 34-45 | | 24 |
| 808 | Amino Acids, Peptides and Proteins. 2008 , 251-296 | | 1 |

| | | |
|-----|---|-----|
| 807 | Mutational analysis and a structural model of methyl-directed restriction enzyme Mrr. 2008 , 377, 862-6 | 11 |
| 806 | A stochastic method for the reconstruction of protein structures from one-dimensional structural profiles. 2008 , 422, 47-51 | 6 |
| 805 | Analyzing protein interaction networks using structural information. 2008 , 77, 415-41 | 71 |
| 804 | In silico chaperonin-like cycle helps folding of proteins for structure prediction. 2008 , 94, 2558-65 | 3 |
| 803 | Advances in Rosetta protein structure prediction on massively parallel systems. 2008 , 52, 7-17 | 14 |
| 802 | A generative, probabilistic model of local protein structure. 2008 , 105, 8932-7 | 84 |
| 801 | Protein Folding Pathways Revealed by Essential Dynamics Sampling. 2008 , 4, 1940-8 | 12 |
| 800 | Deuterated protein folds obtained directly from unassigned nuclear overhauser effect data. 2008 , 130, 3797-805 | 8 |
| 799 | Stimulus-specific modulation of the cation channel TRPV4 by PACSIN 3. 2008 , 283, 6272-80 | 94 |
| 798 | Sequence analysis of GerM and SpoVS, uncharacterized bacterial 'sporulation' proteins with widespread phylogenetic distribution. 2008 , 24, 1793-7 | 25 |
| 797 | Evolutionary Algorithm for Protein Structure Prediction. 2008 , | 3 |
| 796 | A GLOBAL OPTIMIZATION SCHEME: KERNEL REPLICA EXCHANGE SIMULATION METHOD FOR PROTEIN FOLDING. 2008 , 07, 177-187 | 2 |
| 795 | Inference of the solvation energy parameters of amino acids using maximum entropy approach. 2008 , 129, 035102 | 3 |
| 794 | CS23D: a web server for rapid protein structure generation using NMR chemical shifts and sequence data. 2008 , 36, W496-502 | 177 |
| 793 | TMBpro: secondary structure, beta-contact and tertiary structure prediction of transmembrane beta-barrel proteins. 2008 , 24, 513-20 | 67 |
| 792 | The YqfN protein of Bacillus subtilis is the tRNA: m1A22 methyltransferase (TrmK). 2008 , 36, 3252-62 | 23 |
| 791 | Designing succinct structural alphabets. 2008 , 24, i182-9 | 8 |
| 790 | Conformational distributions of unfolded polypeptides from novel NMR techniques. 2008 , 128, 052204 | 83 |

| | | |
|-----|---|-----|
| 789 | Chapter 1. Target selection in structural genomics projects to increase knowledge of protein structure and function space. 2008 , 75, 1-52 | 1 |
| 788 | Fragment replica-exchange method for efficient protein conformation sampling. 2008 , 34, 267-275 | 2 |
| 787 | Simulating virtual protein Calpha traces with applications. 2008 , 15, 1209-20 | 1 |
| 786 | Comparison of the structural features of botulinum neurotoxin and NTN1, a non-toxic accessory protein of the progenitor complex. 2008 , 1, 116 | 6 |
| 785 | The Impact of Structural Proteomics on the Prediction of Protein-Protein Interactions. 2008 , 251-267 | |
| 784 | . 2008 , | 6 |
| 783 | Protein Structure Determination. 671-692 | |
| 782 | Biomolecular Structures by Solution Nuclear Magnetic Resonance. 2009 , 963-987 | |
| 781 | A probabilistic model of RNA conformational space. 2009 , 5, e1000406 | 68 |
| 780 | Neural Network: A Machine Learning Technique for Tertiary Structure Prediction of Proteins from Peptide Sequences. 2009 , | 2 |
| 779 | Optimizing energy potential for protein fold recognition with parametric evaluation function. 2009 , 16, 427-42 | 2 |
| 778 | Probabilistic models and machine learning in structural bioinformatics. 2009 , 18, 505-26 | 13 |
| 777 | Generalized ensemble methods for de novo structure prediction. 2009 , 106, 1415-20 | 45 |
| 776 | Enhanced Bounding Techniques to Reduce the Protein Conformational Search Space. 2009 , 24, 837-855 | 4 |
| 775 | Simultaneous prediction of protein folding and docking at high resolution. 2009 , 106, 18978-83 | 127 |
| 774 | An ab Initio structural model of a nucleoside permease predicts functionally important residues. 2009 , 284, 19067-76 | 22 |
| 773 | Alteration of enzyme specificity by computational loop remodeling and design. 2009 , 106, 9215-20 | 104 |
| 772 | Folding energy landscape and network dynamics of small globular proteins. 2009 , 106, 73-8 | 60 |

| | | |
|-----|--|-----|
| 771 | Calculation of Isothermal Intrinsic Compressibility and Compression of GvpA Protein in Halobacterium sp. NRC-1 Using Molecular Modeling and Dynamics. 2009 , | |
| 770 | Predicting peptide structures in native proteins from physical simulations of fragments. 2009 , 5, e1000281 | 27 |
| 769 | Knowledge-based instantiation of full atomic detail into coarse-grain RNA 3D structural models. 2009 , 25, 3259-66 | 45 |
| 768 | Encyclopedia of Optimization. 2008 , 2938-2953 | 4 |
| 767 | Computation of conformational coupling in allosteric proteins. 2009 , 5, e1000484 | 46 |
| 766 | Artefacts and biases affecting the evaluation of scoring functions on decoy sets for protein structure prediction. 2009 , 25, 1271-9 | 21 |
| 765 | GeNMR: a web server for rapid NMR-based protein structure determination. 2009 , 37, W670-7 | 44 |
| 764 | Understanding Membrane Proteins. How to Design Inhibitors of Transmembrane Protein-Protein Interactions. 2009 , 315-337 | 0 |
| 763 | Progress and challenges in the automated construction of Markov state models for full protein systems. 2009 , 131, 124101 | 303 |
| 762 | Data Mining and Inorganic Crystallography. 2009 , 59-87 | 4 |
| 761 | The structure of M.EcoKI Type I DNA methyltransferase with a DNA mimic antirestriction protein. 2009 , 37, 762-70 | 61 |
| 760 | Restriction versus guidance in protein structure prediction. 2009 , 106, 15302-7 | 32 |
| 759 | Functional analysis of MmeI from methanol utilizer Methylophilus methylotrophus, a subtype IIC restriction-modification enzyme related to type I enzymes. 2009 , 75, 212-23 | 17 |
| 758 | EM-fold: De novo folding of alpha-helical proteins guided by intermediate-resolution electron microscopy density maps. 2009 , 17, 990-1003 | 64 |
| 757 | Predicting continuous local structure and the effect of its substitution for secondary structure in fragment-free protein structure prediction. 2009 , 17, 1515-27 | 89 |
| 756 | Ab initio and homology based prediction of protein domains by recursive neural networks. 2009 , 10, 195 | 11 |
| 755 | Structural building blocks: construction of protein 3-D structures using a structural variant of mountain clustering method. 2009 , 28, 38-44 | 8 |
| 754 | A graph theoretic approach to protein structure selection. 2009 , 45, 229-37 | 4 |

| | | |
|-----|---|-----|
| 753 | Ab initio protein modelling reveals novel human MIT domains. 2009 , 583, 872-8 | 14 |
| 752 | Modeling of Escherichia coli Endonuclease V structure in complex with DNA. 2009 , 15, 173-82 | 4 |
| 751 | Solvent accessible surface area approximations for rapid and accurate protein structure prediction. 2009 , 15, 1093-108 | 122 |
| 750 | Consistent Sets of Secondary Structures in Proteins. 2009 , 53, 16-34 | 1 |
| 749 | Backbone flexibility in computational protein design. 2009 , 20, 420-8 | 84 |
| 748 | Computation of 3D queries for ROCS based virtual screens. 2009 , 23, 853-68 | 23 |
| 747 | 4D prediction of protein (1)H chemical shifts. 2009 , 45, 413-26 | 31 |
| 746 | Automated structure determination from NMR spectra. 2009 , 38, 129-43 | 189 |
| 745 | Simulated tempering yields insight into the low-resolution Rosetta scoring functions. 2009 , 74, 777-88 | 22 |
| 744 | Evaluating the absolute quality of a single protein model using structural features and support vector machines. 2009 , 75, 638-47 | 76 |
| 743 | Local descriptors of protein structure: a systematic analysis of the sequence-structure relationship in proteins using short- and long-range interactions. 2009 , 75, 870-84 | 15 |
| 742 | Toward high-resolution homology modeling of antibody Fv regions and application to antibody-antigen docking. 2009 , 74, 497-514 | 149 |
| 741 | All-atom chain-building by optimizing MODELLER energy function using conformational space annealing. 2009 , 75, 1010-23 | 37 |
| 740 | Simulating protein folding initiation sites using an alpha-carbon-only knowledge-based force field. 2009 , 76, 331-42 | 3 |
| 739 | REMO: A new protocol to refine full atomic protein models from C-alpha traces by optimizing hydrogen-bonding networks. 2009 , 76, 665-76 | 97 |
| 738 | X-ray vs. NMR structures as templates for computational protein design. 2009 , 77, 97-110 | 33 |
| 737 | Template-free protein structure prediction and quality assessment with an all-atom free-energy model. 2009 , 77, 330-41 | 9 |
| 736 | A distance-dependent atomic knowledge-based potential and force for discrimination of native structures from decoys. 2009 , 77, 454-63 | 12 |

| | | |
|-----|---|-----|
| 735 | Structural understanding of stabilization patterns in engineered bispecific Ig-like antibody molecules. 2009 , 77, 832-41 | 32 |
| 734 | Free-energy function based on an all-atom model for proteins. 2009 , 77, 950-61 | 29 |
| 733 | Motif-directed flexible backbone design of functional interactions. 2009 , 18, 1293-305 | 24 |
| 732 | Analyses on hydrophobicity and attractiveness of all-atom distance-dependent potentials. 2009 , 18, 1906-15 | 2 |
| 731 | EDM-DEDM and protein crystal structure solution. 2009 , 65, 477-84 | 8 |
| 730 | Universal partitioning of the hierarchical fold network of 50-residue segments in proteins. 2009 , 9, 34 | |
| 729 | QMEANclust: estimation of protein model quality by combining a composite scoring function with structural density information. 2009 , 9, 35 | 114 |
| 728 | Ab initio and template-based prediction of multi-class distance maps by two-dimensional recursive neural networks. 2009 , 9, 5 | 35 |
| 727 | Splitting statistical potentials into meaningful scoring functions: testing the prediction of near-native structures from decoy conformations. 2009 , 9, 71 | 7 |
| 726 | Discriminating the native structure from decoys using scoring functions based on the residue packing in globular proteins. 2009 , 9, 76 | 7 |
| 725 | Computer-aided design of functional protein interactions. 2009 , 5, 797-807 | 131 |
| 724 | Natural computing methods in bioinformatics: A survey. 2009 , 10, 211-216 | 17 |
| 723 | Computer simulation of proteins: thermodynamics and structure prediction. 2009 , 51, 33-40 | 3 |
| 722 | Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction. 2002 , 11, 2714-26 | 717 |
| 721 | Extension of a local backbone description using a structural alphabet: a new approach to the sequence-structure relationship. 2002 , 11, 2871-86 | 44 |
| 720 | Beta edge strands in protein structure prediction and aggregation. 2003 , 12, 2348-59 | 39 |
| 719 | RosettaAntibody: antibody variable region homology modeling server. 2009 , 37, W474-9 | 123 |
| 718 | A Transferable Coarse Grain Non-bonded Interaction Model For Amino Acids. 2009 , 5, 2115-2124 | 106 |

| | | |
|-----|--|--------|
| 717 | Integrating ELF4 into the circadian system through combined structural and functional studies. 2009 , 3, 350-66 | 81 |
| 716 | A dual-scale approach toward structure prediction of retinal proteins. 2009 , 165, 37-46 | 7 |
| 715 | Fold prediction of VP24 protein of Ebola and Marburg viruses using de novo fragment assembly. 2009 , 167, 136-44 | 10 |
| 714 | Sampling bottlenecks in de novo protein structure prediction. <i>Journal of Molecular Biology</i> , 2009 , 393, 249-60 | 6.5 80 |
| 713 | Backbone structure of transmembrane domain IX of the Na ⁺ /proline transporter PutP of <i>Escherichia coli</i> . 2009 , 96, 217-25 | 36 |
| 712 | Selecting high quality protein structures from diverse conformational ensembles. 2009 , 97, 1728-36 | 15 |
| 711 | Ab Initio Protein Structure Prediction. 2009 , 3-25 | 46 |
| 710 | A novel semi-biosynthetic route for artemisinin production using engineered substrate-promiscuous P450(BM3). 2009 , 4, 261-7 | 167 |
| 709 | The basic concepts of molecular modeling. 2009 , 467, 307-334 | 13 |
| 708 | Probabilistic cross-link analysis and experiment planning for high-throughput elucidation of protein structure. 2004 , 13, 3298-313 | 13 |
| 707 | Encyclopedia of Optimization. 2008 , 3008-3012 | |
| 706 | Protein Engineering. 2009 , | 3 |
| 705 | Probing hot spots on protein-protein interfaces with all-atom free-energy simulation. 2009 , 131, 034114 | 11 |
| 704 | Bioinformatics. 2009 , | 7 |
| 703 | Interaction of the disordered <i>Yersinia</i> effector protein YopE with its cognate chaperone SycE. 2009 , 48, 11158-60 | 5 |
| 702 | A Web-Accessible Protein Structure Prediction Pipeline. 2009 , | |
| 701 | Explicit orientation dependence in empirical potentials and its significance to side-chain modeling. 2009 , 42, 1087-96 | 13 |
| 700 | Scatter search algorithm for protein structure prediction. 2009 , 5, 501-15 | 6 |

| | | |
|-----|--|-----|
| 699 | Molecular biology, genetics and biochemistry of the repulsive guidance molecule family. 2009 , 422, 393-403 | 48 |
| 698 | Proteins: sequence to structure and function--current status. 2010 , 11, 498-514 | 47 |
| 697 | The role of quantum mechanics in structure-based drug design. 120-136 | |
| 696 | Basic protein structure prediction for the biologist: A review. 2010 , 62, 857-871 | 18 |
| 695 | Hybrid Methods for Protein Structure Prediction. 2010 , 265-277 | 2 |
| 694 | Modeling and Validation of Transmembrane Protein Structures. 2010 , 369-401 | 4 |
| 693 | The solution structures of the cucumber mosaic virus and tomato aspermy virus coat proteins explored with molecular dynamics simulations. 2010 , 28, 569-76 | 7 |
| 692 | Trm13p, the tRNA:XM4 modification enzyme from <i>Saccharomyces cerevisiae</i> is a member of the Rossmann-fold MTase superfamily: prediction of structure and active site. 2010 , 16, 599-606 | 7 |
| 691 | Structure prediction and validation of an affibody engineered for cell-specific nucleic acid targeting. 2010 , 4, 293-7 | 9 |
| 690 | An improved hybrid global optimization method for protein tertiary structure prediction. 2010 , 45, 377-413 | 16 |
| 689 | Protein Structure Prediction Using Bee Colony Optimization Metaheuristic. 2010 , 9, 181-194 | 15 |
| 688 | Recognizing protein substructure similarity using segmental threading. 2010 , 18, 858-67 | 26 |
| 687 | Using NMR chemical shifts as structural restraints in molecular dynamics simulations of proteins. 2010 , 18, 923-33 | 121 |
| 686 | A pairwise residue contact area-based mean force potential for discrimination of native protein structure. 2010 , 11, 16 | 16 |
| 685 | Directionality in protein fold prediction. 2010 , 11, 172 | 15 |
| 684 | Calibur: a tool for clustering large numbers of protein decoys. 2010 , 11, 25 | 53 |
| 683 | Calculation of accurate small angle X-ray scattering curves from coarse-grained protein models. 2010 , 11, 429 | 41 |
| 682 | Mining metagenomic data for novel domains: BACON, a new carbohydrate-binding module. 2010 , 584, 2421-6 | 32 |

| | | |
|-----|---|------|
| 681 | Prediction of the parallel/antiparallel orientation of beta-strands using amino acid pairing preferences and support vector machines. 2010 , 263, 360-8 | 24 |
| 680 | Structure-oriented methods for protein NMR data analysis. 2010 , 56, 311-28 | 5 |
| 679 | Prediction of structures of zinc-binding proteins through explicit modeling of metal coordination geometry. 2010 , 19, 494-506 | 36 |
| 678 | Amino acid interaction preferences in proteins. 2010 , 19, 603-16 | 36 |
| 677 | Efficient identification of near-native conformations in ab initio protein structure prediction using structural profiles. 2010 , 78, 249-58 | 5 |
| 676 | MUFOLD: A new solution for protein 3D structure prediction. 2010 , 78, 1137-52 | 60 |
| 675 | Improving threading algorithms for remote homology modeling by combining fragment and template comparisons. 2010 , 78, 2041-8 | 15 |
| 674 | Computational modeling of laminin N-terminal domains using sparse distance constraints from disulfide bonds and chemical cross-linking. 2010 , 78, 3409-27 | 28 |
| 673 | Protein loop modeling by using fragment assembly and analytical loop closure. 2010 , 78, 3428-36 | 77 |
| 672 | Structure-based prediction of protein-peptide specificity in Rosetta. 2010 , 78, 3437-49 | 34 |
| 671 | Designing artificial enzymes by intuition and computation. 2010 , 2, 15-24 | 193 |
| 670 | I-TASSER: a unified platform for automated protein structure and function prediction. 2010 , 5, 725-38 | 4448 |
| 669 | Tasser-Based Protein Structure Prediction. 2010 , 219-242 | 2 |
| 668 | MULTICOM: a multi-level combination approach to protein structure prediction and its assessments in CASP8. 2010 , 26, 882-8 | 82 |
| 667 | Insights into the structure, function and evolution of the radical-SAM 23S rRNA methyltransferase Cfr that confers antibiotic resistance in bacteria. 2010 , 38, 1652-63 | 67 |
| 666 | Introduction to Protein Structure Prediction. 2010 , 1-13 | 0 |
| 665 | Contact Map Prediction by Machine Learning. 2010 , 137-163 | 1 |
| 664 | A probabilistic and continuous model of protein conformational space for template-free modeling. 2010 , 17, 783-98 | 14 |

| | | |
|-----|--|-----|
| 663 | Fragment-free approach to protein folding using conditional neural fields. 2010 , 26, i310-7 | 25 |
| 662 | Structural Bioinformatics of Membrane Proteins. 2010 , | 6 |
| 661 | Unique gating properties of <i>C. elegans</i> ClC anion channel splice variants are determined by altered CBS domain conformation and the R-helix linker. 2010 , 4, 289-301 | 8 |
| 660 | Network models for molecular kinetics and their initial applications to human health. 2010 , 20, 622-30 | 41 |
| 659 | How do amino acid mismatches affect the outcome of hematopoietic cell transplants?. 2010 , | 1 |
| 658 | BCL::contact-low confidence fold recognition hits boost protein contact prediction and de novo structure determination. 2010 , 17, 153-68 | 4 |
| 657 | Practically useful: what the Rosetta protein modeling suite can do for you. 2010 , 49, 2987-98 | 298 |
| 656 | Integrative structure modeling of macromolecular assemblies from proteomics data. 2010 , 9, 1689-702 | 58 |
| 655 | Prediction and Calculation of Protein-Protein Binding Affinities and Mutation Effects. 2010 , 295-317 | |
| 654 | In vitro effects of recombinant otoconin 90 upon calcite crystal growth. Significance of tertiary structure. 2010 , 268, 172-83 | 19 |
| 653 | Characterization of two linear cationic antimalarial peptides in the scorpion <i>Mesobuthus eupeus</i> . 2010 , 92, 350-9 | 64 |
| 652 | Multiscale methods for protein folding simulations. 2010 , 52, 106-14 | 26 |
| 651 | Incremental Mountain Clustering Method to find building blocks for constructing structures of proteins. 2010 , 9, 278-88 | 2 |
| 650 | Effects of side-chain packing on the formation of secondary structures in protein folding. 2010 , 132, 065105 | 39 |
| 649 | Conformational optimization with natural degrees of freedom: a novel stochastic chain closure algorithm. 2010 , 17, 993-1010 | 23 |
| 648 | Genetic algorithm feature-based resampling for protein structure prediction. 2010 , | 2 |
| 647 | Novel nonlinear knowledge-based mean force potentials based on machine learning. 2011 , 8, 476-86 | 6 |
| 646 | Recursive protein modeling: A divide and conquer strategy for protein structure prediction and its case study in CASP9. 2011 , | 4 |

| | | |
|-----|--|--------|
| 645 | Computational design of the sequence and structure of a protein-binding peptide. 2011 , 133, 4190-2 | 41 |
| 644 | Determination of the structures of symmetric protein oligomers from NMR chemical shifts and residual dipolar couplings. 2011 , 133, 6288-98 | 55 |
| 643 | Backbones of folded proteins reveal novel invariant amino acid neighborhoods. 2011 , 28, 443-54 | 33 |
| 642 | GOAP: a generalized orientation-dependent, all-atom statistical potential for protein structure prediction. 2011 , 101, 2043-52 | 192 |
| 641 | Improving the physical realism and structural accuracy of protein models by a two-step atomic-level energy minimization. 2011 , 101, 2525-34 | 600 |
| 640 | A hybrid genetic algorithm for the 3-D protein structure prediction problem using a path-relinking strategy. 2011 , | 5 |
| 639 | Protein Structure Prediction: From Recognition of Matches with Known Structures to Recombination of Fragments. 2011 , 231-254 | 2 |
| 638 | Genome-Wide Protein Structure Prediction. 2011 , 255-279 | 2 |
| 637 | Predicting antibody complementarity determining region structures without classification. 2011 , 7, 3327-34 | 35 |
| 636 | Ab initio modeling led annotation suggests nucleic acid binding function for many DUFs. 2011 , 15, 431-8 | 16 |
| 635 | Prediction of calcite morphology from computational and experimental studies of mutations of a de novo-designed peptide. 2011 , 27, 11520-7 | 8 |
| 634 | Data-driven high-throughput prediction of the 3-D structure of small molecules: review and progress. 2011 , 51, 760-76 | 19 |
| 633 | ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. 2011 , 487, 545-74 | 1216 |
| 632 | Statistical mechanics analysis of sparse data. 2011 , 173, 541-8 | 14 |
| 631 | RosettaEPR: an integrated tool for protein structure determination from sparse EPR data. 2011 , 173, 506-14 | 93 |
| 630 | Algorithm for selection of optimized EPR distance restraints for de novo protein structure determination. 2011 , 173, 549-57 | 34 |
| 629 | Computational protein design using flexible backbone remodeling and resurfacing: case studies in structure-based antigen design. <i>Journal of Molecular Biology</i> , 2011 , 405, 284-97 | 6.5 51 |
| 628 | Statistical potential for modeling and ranking of protein-ligand interactions. 2011 , 51, 3078-92 | 61 |

| | | |
|-----|---|-----|
| 627 | Contributions of Structure Comparison Methods to the Protein Structure Prediction Field. 2011 , | |
| 626 | Basic Principles and Practices of Computer-Aided Drug Design. 259-278 | |
| 625 | Incorporation of local structural preference potential improves fold recognition. 2011 , 6, e17215 | 12 |
| 624 | Four small puzzles that Rosetta doesn't solve. 2011 , 6, e20044 | 54 |
| 623 | Neural network pairwise interaction fields for protein model quality assessment and ab initio protein folding. 2011 , 12, 549-62 | 2 |
| 622 | A framework for direct locating and conformational sampling of protein structural motifs. 2011 , 18, 488-97 | 1 |
| 621 | Towards structure-based protein drug design. 2011 , 39, 1382-6, suppl 1 p following 1386 | 22 |
| 620 | Structure and function of ameloblastin as an extracellular matrix protein: adhesion, calcium binding, and CD63 interaction in human and mouse. 2011 , 119 Suppl 1, 270-9 | 24 |
| 619 | Improving protein structure prediction using multiple sequence-based contact predictions. 2011 , 19, 1182-91 | 55 |
| 618 | Generative probabilistic models extend the scope of inferential structure determination. 2011 , 213, 182-6 | 15 |
| 617 | Protein design with fragment databases. 2011 , 21, 452-9 | 22 |
| 616 | Uncoupled binding and folding of immune signaling-related intrinsically disordered proteins. 2011 , 106, 525-36 | 23 |
| 615 | Tridimensional model structure and patterns of molecular evolution of Pepino mosaic virus TGBp3 protein. 2011 , 8, 318 | 2 |
| 614 | Theoretical and computational protein design. 2011 , 62, 129-49 | 119 |
| 613 | Effect of substrate features and mutagenesis of active site tyrosine residues on the reaction course catalysed by Trypanosoma brucei sterol C-24-methyltransferase. 2011 , 439, 413-22 | 7 |
| 612 | Force fields for homology modeling. 2012 , 857, 83-106 | 9 |
| 611 | RNA and protein 3D structure modeling: similarities and differences. 2011 , 17, 2325-36 | 67 |
| 610 | Trends in template/fragment-free protein structure prediction. 2011 , 128, 3-16 | 41 |

| | | |
|-----|--|-----|
| 609 | Accelerating ab initio phasing with de novo models. 2011 , 67, 804-12 | 13 |
| 608 | DECK: Distance and environment-dependent, coarse-grained, knowledge-based potentials for protein-protein docking. 2011 , 12, 280 | 40 |
| 607 | LoCo: a novel main chain scoring function for protein structure prediction based on local coordinates. 2011 , 12, 368 | 5 |
| 606 | Incorporating Ab Initio energy into threading approaches for protein structure prediction. 2011 , 12 Suppl 1, S54 | 4 |
| 605 | Absolute quality evaluation of protein model structures using statistical potentials with respect to the native and reference states. 2011 , 79, 1550-63 | 2 |
| 604 | Protein structure prediction using a docking-based hierarchical folding scheme. 2011 , 79, 1759-73 | 3 |
| 603 | Free-energy function for discriminating the native fold of a protein from misfolded decoys. 2011 , 79, 2161-71 | 26 |
| 602 | Statistical mechanics-based method to extract atomic distance-dependent potentials from protein structures. 2011 , 79, 2648-61 | 43 |
| 601 | Computed structures of point deletion mutants and their enzymatic activities. 2011 , 79, 2844-60 | 5 |
| 600 | Automated protein structure modeling in CASP9 by I-TASSER pipeline combined with QUARK-based ab initio folding and FG-MD-based structure refinement. 2011 , 79 Suppl 10, 147-60 | 111 |
| 599 | Constraining local structure can speed up folding by promoting structural polarization of the folding pathway. 2011 , 20, 959-69 | 2 |
| 598 | Calculation of Structures from NMR Restraints. 2011 , 159-192 | |
| 597 | Protein structure predictions by parallel simulated annealing molecular dynamics using genetic crossover. 2011 , 32, 1353-60 | 15 |
| 596 | A versatile method for systematic conformational searches: application to CheY. 2011 , 32, 2369-85 | 3 |
| 595 | Loop simulations. 2012 , 857, 207-29 | 6 |
| 594 | Fast Algorithm for Clustering a Large Number of Protein Structural Decoys. 2011 , | 4 |
| 593 | What's in a likelihood? Simple models of protein evolution and the contribution of structurally viable reconstructions to the likelihood. 2011 , 60, 161-74 | 11 |
| 592 | Analysis and modeling of the variable region of camelid single-domain antibodies. 2011 , 186, 6357-67 | 57 |

| | | |
|-----|---|----|
| 591 | A chimeric HIV-1 envelope glycoprotein trimer with an embedded granulocyte-macrophage colony-stimulating factor (GM-CSF) domain induces enhanced antibody and T cell responses. 2011 , 286, 22250-61 | 13 |
| 590 | Log-linear modelling of protein dipeptide structure reveals interesting patterns of side-chain-backbone interactions. 2011 , 10, Article 8 | 1 |
| 589 | The core domain as the force sensor of the yeast mechanosensitive TRP channel. 2011 , 138, 627-40 | 13 |
| 588 | HHfrag: HMM-based fragment detection using HHpred. 2011 , 27, 3110-6 | 23 |
| 587 | A single zinc ion is sufficient for an active Trypanosoma brucei tRNA editing deaminase. 2011 , 286, 20366-74 | 13 |
| 586 | Improvement of a potential anthrax therapeutic by computational protein design. 2011 , 286, 32586-92 | 9 |
| 585 | Fast geometric consensus approach for protein model quality assessment. 2011 , 18, 1807-18 | 9 |
| 584 | BriX: a database of protein building blocks for structural analysis, modeling and design. 2011 , 39, D435-42 | 37 |
| 583 | Characterization of C- and N-terminal domains of Aquifex aeolicus MutL endonuclease: N-terminal domain stimulates the endonuclease activity of C-terminal domain in a zinc-dependent manner. 2011 , 31, 309-22 | 23 |
| 582 | A conditional random fields method for RNA sequence-structure relationship modeling and conformation sampling. 2011 , 27, i102-10 | 10 |
| 581 | Catalytic residues and a predicted structure of tetrahydrobiopterin-dependent alkylglycerol mono-oxygenase. 2012 , 443, 279-86 | 16 |
| 580 | A scoring function based on solvation thermodynamics for protein structure prediction. 2012 , 8, 127-38 | 1 |
| 579 | Application of Hydration Thermodynamics to the Evaluation of Protein Structures and Protein-Ligand Binding. 2012 , 14, 1443-1468 | 6 |
| 578 | Fast large-scale clustering of protein structures using Gauss integrals. 2012 , 28, 510-5 | 21 |
| 577 | Towards Creating Complete Proteomic Structural Databases of Whole Organisms. 2012 , 7, 424-435 | 4 |
| 576 | Clustering 100,000 protein structure decoys in minutes. 2012 , 9, 765-73 | 7 |
| 575 | Recursive protein modeling: a divide and conquer strategy for Protein Structure Prediction and its case study in CASP9. 2012 , 10, 1242003 | 8 |
| 574 | Computational Biology. 2012 , | 1 |

| | | |
|-----|---|--------|
| 573 | A simple and efficient statistical potential for scoring ensembles of protein structures. 2012 , 2, | 42 |
| 572 | Principles for designing ideal protein structures. 2012 , 491, 222-7 | 391 |
| 571 | Membrane protein structural bioinformatics. 2012 , 179, 327-37 | 33 |
| 570 | Molecular cloning, sequence analysis and expression of Fein-Penaeidin from the haemocytes of Indian white shrimp <i>Fenneropenaeus indicus</i> . 2012 , 2, 35-43 | 19 |
| 569 | Using the unfolded state as the reference state improves the performance of statistical potentials. 2012 , 103, 1950-9 | 4 |
| 568 | TRPV4 mutations in children with congenital distal spinal muscular atrophy. 2012 , 13, 195-203 | 24 |
| 567 | Structure refinement of protein low resolution models using the GNEIMO constrained dynamics method. 2012 , 116, 2365-75 | 18 |
| 566 | Protein structure determination from pseudocontact shifts using ROSETTA. <i>Journal of Molecular Biology</i> , 2012 , 416, 668-77 | 6.5 89 |
| 565 | Novel protein-protein interactions between <i>Entamoeba histolytica</i> -phosphoglycerate dehydrogenase and phosphoserine aminotransferase. 2012 , 94, 1676-86 | 5 |
| 564 | The MULTICOM toolbox for protein structure prediction. 2012 , 13, 65 | 23 |
| 563 | Template-based protein structure modeling using the RaptorX web server. 2012 , 7, 1511-22 | 1115 |
| 562 | Role of computational methods in pharmaceutical sciences. 2012 , 929, 21-48 | 8 |
| 561 | AMPLE: a cluster-and-truncate approach to solve the crystal structures of small proteins using rapidly computed ab initio models. 2012 , 68, 1622-31 | 89 |
| 560 | Self-complementarity within proteins: bridging the gap between binding and folding. 2012 , 102, 2605-14 | 17 |
| 559 | Coarse-grained simulations of protein-protein association: an energy landscape perspective. 2012 , 103, 837-45 | 44 |
| 558 | Structure Prediction for Alternatively Spliced Proteins. 2012 , 582-591 | |
| 557 | Protein Structure Prediction. 2012 , | 2 |
| 556 | Protein structure prediction: challenging targets for CASP10. 2012 , 30, 607-15 | 12 |

| | | |
|-----|--|-----|
| 555 | Identification of residues defining phospholipid flippase substrate specificity of type IV P-type ATPases. 2012 , 109, E290-8 | 88 |
| 554 | Functional Genomics. 2012 , | 2 |
| 553 | Bayesian Methods in Structural Bioinformatics. 2012 , | 18 |
| 552 | A predictive model of intein insertion site for use in the engineering of molecular switches. 2012 , 7, e37355 | 12 |
| 551 | BCL::Score--knowledge based energy potentials for ranking protein models represented by idealized secondary structure elements. 2012 , 7, e49242 | 37 |
| 550 | Predicting nucleic acid binding interfaces from structural models of proteins. 2012 , 80, 482-9 | 8 |
| 549 | The dual role of fragments in fragment-assembly methods for de novo protein structure prediction. 2012 , 80, 490-504 | 33 |
| 548 | Geofold: topology-based protein unfolding pathways capture the effects of engineered disulfides on kinetic stability. 2012 , 80, 920-34 | 14 |
| 547 | AutoMatch: target-binding protein design and enzyme design by automatic pinpointing potential active sites in available protein scaffolds. 2012 , 80, 1078-94 | 18 |
| 546 | Distance-dependent atomic knowledge-based force in protein fold recognition. 2012 , 80, 683-90 | 7 |
| 545 | Ab initio protein structure assembly using continuous structure fragments and optimized knowledge-based force field. 2012 , 80, 1715-35 | 607 |
| 544 | Comparative modeling and protein-like features of hydrophobic-polar models on a two-dimensional lattice. 2012 , 80, 1683-93 | 14 |
| 543 | What is the best reference state for designing statistical atomic potentials in protein structure prediction?. 2012 , 80, 2311-22 | 21 |
| 542 | Bioinformatics and variability in drug response: a protein structural perspective. 2012 , 9, 1409-37 | 57 |
| 541 | Introduction. 2012 , 1-3 | |
| 540 | Why Can't We Predict RNA Structure At Atomic Resolution?. 2012 , 43-65 | 7 |
| 539 | Template-Based and Template-Free Modeling of RNA 3D Structure: Inspirations from Protein Structure Modeling. 2012 , 67-90 | 8 |
| 538 | ASTRO-FOLD 2.0: an Enhanced Framework for Protein Structure Prediction. 2012 , 58, 1619-1637 | 18 |

| | | |
|-----|--|-----|
| 537 | Accurate de novo structure prediction of large transmembrane protein domains using fragment-assembly and correlated mutation analysis. 2012 , 109, E1540-7 | 158 |
| 536 | Ligand-based virtual screening approach using a new scoring function. 2012 , 52, 963-74 | 58 |
| 535 | Statistical energy potential: reduced representation of Dehouck-Gilis-Rooman function by selecting against decoy datasets. 2012 , 42, 2353-61 | |
| 534 | A new approach for investigating protein flexibility based on Constraint Logic Programming. The first application in the case of the estrogen receptor. 2012 , 49, 127-40 | 5 |
| 533 | A position-specific distance-dependent statistical potential for protein structure and functional study. 2012 , 20, 1118-26 | 48 |
| 532 | Protein Structure Idealization: How accurately is it possible to model protein structures with dihedral angles?. 2013 , 8, 5 | 1 |
| 531 | How to design a drug for the disordered proteins?. 2013 , 18, 910-5 | 64 |
| 530 | Computational Protein Design for Synthetic Biology. 2013 , 101-122 | 3 |
| 529 | Iterative Molecular Dynamics-Rosetta Protein Structure Refinement Protocol to Improve Model Quality. 2013 , 9, 3843-3847 | 30 |
| 528 | Segment assembly, structure alignment and iterative simulation in protein structure prediction. 2013 , 11, 44 | 11 |
| 527 | Secondary structural analysis of proteins based on (13)C chemical shift assignments in unresolved solid-state NMR spectra enhanced by fragmented structure database. 2013 , 55, 189-200 | 7 |
| 526 | The loop hypothesis: contribution of early formed specific non-local interactions to the determination of protein folding pathways. 2013 , 5, 85-98 | 15 |
| 525 | Statistical approaches to three key challenges in protein structural bioinformatics. 2013 , 62, 487-514 | 15 |
| 524 | Extracting knowledge from protein structure geometry. 2013 , 81, 841-51 | 3 |
| 523 | Perspective: Coarse-grained models for biomolecular systems. 2013 , 139, 090901 | 532 |
| 522 | Advanced Technologies for Managing Insect Pests. 2013 , | 1 |
| 521 | De Novo Computational Protein Design. 2013 , 467-493 | |
| 520 | Mining tertiary structural motifs for assessment of designability. 2013 , 523, 21-40 | 16 |

| | | |
|-----|---|-----|
| 519 | The scoring of poses in protein-protein docking: current capabilities and future directions. 2013 , 14, 286 | 75 |
| 518 | Improved chemical shift based fragment selection for CS-Rosetta using Rosetta3 fragment picker. 2013 , 57, 117-27 | 34 |
| 517 | Scientific benchmarks for guiding macromolecular energy function improvement. 2013 , 523, 109-43 | 164 |
| 516 | Ratio of mutated versus wild-type coat protein sequences in Pepino mosaic virus determines the nature and severity of yellowing symptoms on tomato plants. 2013 , 14, 923-33 | 26 |
| 515 | Fast algorithm for population-based protein structural model analysis. 2013 , 13, 221-9 | 17 |
| 514 | Toward optimal fragment generations for ab initio protein structure assembly. 2013 , 81, 229-39 | 156 |
| 513 | Capturing native/native like structures with a physico-chemical metric (pcSM) in protein folding. 2013 , 1834, 1520-31 | 18 |
| 512 | Finding short structural motifs for re-construction of proteins 3D structure. 2013 , 13, 1214-1221 | 1 |
| 511 | BCL::MP-fold: folding membrane proteins through assembly of transmembrane helices. 2013 , 21, 1107-17 | 31 |
| 510 | Accounting for receptor flexibility and enhanced sampling methods in computer-aided drug design. 2013 , 81, 41-9 | 90 |
| 509 | Flexible backbone sampling methods to model and design protein alternative conformations. 2013 , 523, 61-85 | 36 |
| 508 | Coarse- and fine-grained models for proteins: evaluation by decoy discrimination. 2013 , 81, 754-73 | 1 |
| 507 | Design of chimeric proteins by combination of subdomain-sized fragments. 2013 , 523, 389-405 | 7 |
| 506 | Membrane protein native state discrimination by implicit membrane models. 2013 , 34, 731-8 | 23 |
| 505 | Computational enzyme design. 2013 , 52, 5700-25 | 351 |
| 504 | Theoretical prediction of the protein-protein interaction between Arabidopsis thaliana COP1 and UVR8. 2013 , 132, 1 | 6 |
| 503 | Small-molecule ligand docking into comparative models with Rosetta. 2013 , 8, 1277-98 | 116 |
| 502 | A simple probabilistic model of multibody interactions in proteins. 2013 , 81, 1340-50 | 5 |

| | | |
|-----|--|----|
| 501 | Detecting repetitions and periodicities in proteins by tiling the structural space. 2013 , 117, 12887-97 | 25 |
| 500 | PaLaCe: A Coarse-Grain Protein Model for Studying Mechanical Properties. 2013 , 9, 785-93 | 37 |
| 499 | Detection of orexin A neuropeptide in biological fluids using a zinc oxide field effect transistor. 2013 , 4, 444-53 | 13 |
| 498 | An analytical method for computing atomic contact areas in biomolecules. 2013 , 34, 105-20 | 7 |
| 497 | Combining coarse-grained nonbonded and atomistic bonded interactions for protein modeling. 2013 , 81, 81-92 | 21 |
| 496 | How the "folding funnel" depends on size and structure of proteins? a view from the scoring function perspective. 2013 , 18, 462-468 | 2 |
| 495 | Using the RosettaSurface algorithm to predict protein structure at mineral surfaces. 2013 , 532, 343-66 | 20 |
| 494 | Recurrent structural motifs in non-homologous protein structures. 2013 , 14, 7795-814 | 3 |
| 493 | Advanced Screening to Identify Novel Pesticides. 2013 , 135-163 | 2 |
| 492 | An evolution-based approach to De Novo protein design and case study on Mycobacterium tuberculosis. 2013 , 9, e1003298 | 39 |
| 491 | Optimized atomic statistical potentials: assessment of protein interfaces and loops. 2013 , 29, 3158-66 | 88 |
| 490 | A TRPV4 channel C-terminal folding recognition domain critical for trafficking and function. 2013 , 288, 10427-39 | 31 |
| 489 | Using physical potentials and learned models to distinguish native binding interfaces from de novo designed interfaces that do not bind. 2013 , 81, 1919-30 | 4 |
| 488 | Assessing protein conformational sampling methods based on bivariate lag-distributions of backbone angles. 2013 , 14, 724-36 | 10 |
| 487 | GRID: a high-resolution protein structure refinement algorithm. 2013 , 34, 445-50 | 7 |
| 486 | A homology/ab initio hybrid algorithm for sampling near-native protein conformations. 2013 , 34, 1925-36 | 14 |
| 485 | Ab Initio Protein Structure Prediction: Methods and challenges. 2013 , 703-724 | 5 |
| 484 | The activity of prolactin releasing peptide correlates with its helicity. 2013 , 99, 314-25 | 6 |

| | | |
|-----|---|----|
| 483 | Computerbasiertes Enzymdesign. 2013 , 125, 5810-5836 | 37 |
| 482 | A sampling approach for protein backbone fragment conformations. 2013 , 7, 180-95 | 1 |
| 481 | Validating a Coarse-Grained Potential Energy Function through Protein Loop Modelling. 2013 , 8, e65770 | 12 |
| 480 | The PyRosetta Toolkit: a graphical user interface for the Rosetta software suite. 2013 , 8, e66856 | 23 |
| 479 | Efficient sampling in fragment-based protein structure prediction using an estimation of distribution algorithm. 2013 , 8, e68954 | 20 |
| 478 | Cold adaptation, Ca^{2+} dependency and autolytic stability are related features in a highly active cold-adapted trypsin resistant to autoproteolysis engineered for biotechnological applications. 2013 , 8, e72355 | 7 |
| 477 | Principles for Designing Ideal Protein Structures. 2013 , 53, 190-193 | 3 |
| 476 | De novo structure prediction of globular proteins aided by sequence variation-derived contacts. 2014 , 9, e92197 | 81 |
| 475 | Structural basis for the recognition in an idiotype-anti-idiotype antibody complex related to celiac disease. 2014 , 9, e102839 | 9 |
| 474 | N-terminal hydrophobic amino acids of activating transcription factor 5 (ATF5) protein confer interleukin 1[IL-1]-induced stabilization. 2014 , 289, 3888-900 | 6 |
| 473 | Dynameomics: data-driven methods and models for utilizing large-scale protein structure repositories for improving fragment-based loop prediction. 2014 , 23, 1584-95 | 5 |
| 472 | Fast protein loop sampling and structure prediction using distance-guided sequential chain-growth Monte Carlo method. 2014 , 10, e1003539 | 38 |
| 471 | Fast closure of long loops at the initiation of the folding transition of globular proteins studied by time-resolved FRET-based methods. 2014 , 10, | 2 |
| 470 | Molecular basis for the fold organization and sarcomeric targeting of the muscle atrogenin MuRF1. 2014 , 4, 130172 | 15 |
| 469 | Modeling the spatial conformation and allosteric phenomenon of protein alpha helix's tertiary structure. 2014 , | |
| 468 | Protein structure prediction: assembly of secondary structure elements by basin-hopping. 2014 , 15, 3378-90 | 1 |
| 467 | SSThread: Template-free protein structure prediction by threading pairs of contacting secondary structures followed by assembly of overlapping pairs. 2014 , 35, 644-56 | 7 |
| 466 | Pancreatic polypeptide is recognized by two hydrophobic domains of the human Y4 receptor binding pocket. 2014 , 289, 5846-59 | 24 |

| | | |
|-----|---|----|
| 465 | Improving the orientation-dependent statistical potential using a reference state. 2014 , 82, 2383-93 | 8 |
| 464 | Centenary Award and Sir Frederick Gowland Hopkins Memorial Lecture. Protein folding, structure prediction and design. 2014 , 42, 225-9 | 25 |
| 463 | Computational design of metalloproteins. 2014 , 1216, 233-49 | 4 |
| 462 | The role of nucleobase interactions in RNA structure and dynamics. 2014 , 42, 13306-14 | 75 |
| 461 | From local structure to a global framework: recognition of protein folds. 2014 , 11, 20131147 | 8 |
| 460 | Protein Design. 2014 , | |
| 459 | ROTAS: a rotamer-dependent, atomic statistical potential for assessment and prediction of protein structures. 2014 , 15, 307 | 14 |
| 458 | SVR_CAF: an integrated score function for detecting native protein structures among decoys. 2014 , 82, 556-64 | 15 |
| 457 | Physics-Based Modeling of Side Chain - Side Chain Interactions in the UNRES Force Field. 2014 , 81-107 | 1 |
| 456 | Interplay of I-TASSER and QUARK for template-based and ab initio protein structure prediction in CASP10. 2014 , 82 Suppl 2, 175-87 | 91 |
| 455 | MOIRAE: A computational strategy to extract and represent structural information from experimental protein templates. 2014 , 18, 773-795 | 2 |
| 454 | Formulation of probabilistic models of protein structure in atomic detail using the reference ratio method. 2014 , 82, 288-99 | 8 |
| 453 | Toward an accurate prediction of inter-residue distances in proteins using 2D recursive neural networks. 2014 , 15, 6 | 33 |
| 452 | Fingerprinting protein structures effectively and efficiently. 2014 , 30, 949-55 | 5 |
| 451 | Improving fragment quality for de novo structure prediction. 2014 , 82, 2240-52 | 9 |
| 450 | CDKN2A unclassified variants in familial malignant melanoma: combining functional and computational approaches for their assessment. 2014 , 35, 828-40 | 13 |
| 449 | Delaunay-based nonlocal interactions are sufficient and accurate in protein fold recognition. 2014 , 82, 415-23 | 7 |
| 448 | Protein NMR structures refined with Rosetta have higher accuracy relative to corresponding X-ray crystal structures. 2014 , 136, 1893-906 | 47 |

| | | |
|-----|---|-----|
| 447 | Quinary lattice model of secondary structures of polymers. 2014 , 393, 86-95 | 2 |
| 446 | Predicting backbone C α angles and dihedrals from protein sequences by stacked sparse auto-encoder deep neural network. 2014 , 35, 2040-6 | 110 |
| 445 | A distance- and orientation-dependent energy function of amino acid key blocks. 2014 , 101, 681-92 | 4 |
| 444 | The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. 2014 , 43, 4871-93 | 118 |
| 443 | Retro operation on the Trp-cage miniprotein sequence produces an unstructured molecule capable of folding similar to the original only upon 2,2,2-trifluoroethanol addition. 2014 , 27, 463-72 | 3 |
| 442 | Formation of ceramophilic chitin and biohybrid materials enabled by a genetically engineered bifunctional protein. 2014 , 50, 7348-51 | 12 |
| 441 | Three-dimensional protein structure prediction: Methods and computational strategies. 2014 , 53PB, 251-276 | 107 |
| 440 | Equilibrium simulations of proteins using molecular fragment replacement and NMR chemical shifts. 2014 , 111, 13852-7 | 26 |
| 439 | Application of information theory to a three-body coarse-grained representation of proteins in the PDB: insights into the structural and evolutionary roles of residues in protein structure. 2014 , 82, 3450-65 | 1 |
| 438 | A physics-based scoring function for protein structural decoys: Dynamic testing on targets of CASP-ROLL. 2014 , 610-611, 135-140 | 7 |
| 437 | A local landscape mapping method for protein structure prediction in the HP model. 2014 , 13, 309-319 | 1 |
| 436 | Designing and evaluating the MULTICOM protein local and global model quality prediction methods in the CASP10 experiment. 2014 , 14, 13 | 39 |
| 435 | Recent Advances in De Novo Protein Design. 2014 , 207-232 | |
| 434 | Detecting local residue environment similarity for recognizing near-native structure models. 2014 , 82, 3255-72 | 7 |
| 433 | Utilizing Markov Chains to Model Ion Channel Sequence Variation and Kinetics. 2015 , 123-132 | |
| 432 | Proteins, physics and probability kinematics: a Bayesian formulation of the protein folding problem. 2015 , 356-376 | 2 |
| 431 | Protolfold II: Enhanced Model and Implementation for Kinetostatic Protein Folding1. 2015 , 6, | 7 |
| 430 | Solution study of the Escherichia coli DNA polymerase III clamp loader reveals the location of the dynamic heterodimer. 2015 , 2, 054701 | 5 |

| | | |
|-----|---|-------|
| 429 | De novo protein conformational sampling using a probabilistic graphical model. 2015 , 5, 16332 | 15 |
| 428 | A large-scale conformation sampling and evaluation server for protein tertiary structure prediction and its assessment in CASP11. 2015 , 16, 337 | 14 |
| 427 | Rapid search for tertiary fragments reveals protein sequence-structure relationships. 2015 , 24, 508-24 | 50 |
| 426 | CASP10-BCL::Fold efficiently samples topologies of large proteins. 2015 , 83, 547-63 | 5 |
| 425 | The NESH/Abi-3-based WAVE2 complex is functionally distinct from the Abi-1-based WAVE2 complex. 2015 , 13, 41 | 12 |
| 424 | General overview on structure prediction of twilight-zone proteins. 2015 , 12, 15 | 47 |
| 423 | Selective refinement and selection of near-native models in protein structure prediction. 2015 , 83, 1823-35 | 3 |
| 422 | Structural modeling of the N-terminal signal-receiving domain of IRE1. 2015 , 2, 32 | 5 |
| 421 | Integrating solid-state NMR and computational modeling to investigate the structure and dynamics of membrane-associated ghrelin. 2015 , 10, e0122444 | 12 |
| 420 | RNA folding: structure prediction, folding kinetics and ion electrostatics. 2015 , 827, 143-83 | 12 |
| 419 | An empirical energy function for structural assessment of protein transmembrane domains. 2015 , 115, 155-61 | 10 |
| 418 | Decomposing the space of protein quaternary structures with the interface fragment pair library. 2015 , 16, 14 | 6 |
| 417 | Customised fragments libraries for protein structure prediction based on structural class annotations. 2015 , 16, 136 | 14 |
| 416 | A bioinformatic approach to check the spatial epitope structure of an immunogenic protein coded by DNA vaccine plasmids. 2015 , 380, 315-20 | 2 |
| 415 | Large-scale model quality assessment for improving protein tertiary structure prediction. 2015 , 31, i116-23 | 42 |
| 414 | Rational design of β helical tandem repeat proteins with closed architectures. 2015 , 528, 585-8 | 85 |
| 413 | ICOSA: A Distance-Dependent, Orientation-Specific Coarse-Grained Contact Potential for Protein Structure Modeling. <i>Journal of Molecular Biology</i> , 2015 , 427, 2562-2576 | 6.5 9 |
| 412 | Assessing protein conformational sampling and structural stability via de novo design and molecular dynamics simulations. 2015 , 103, 351-61 | 5 |

| | | |
|-----|--|----|
| 411 | Molecular evolution of Pepino mosaic virus during long-term passaging in different hosts and its impact on virus virulence. 2015 , 166, 389-401 | 12 |
| 410 | Improved cryoEM-Guided Iterative Molecular Dynamics--Rosetta Protein Structure Refinement Protocol for High Precision Protein Structure Prediction. 2015 , 11, 1337-46 | 29 |
| 409 | Quality Assessment of Predicted Protein Models Using Energies Calculated by the Fragment Molecular Orbital Method. 2015 , 34, 97-104 | 12 |
| 408 | Quality assessment of modeled protein structure using physicochemical properties. 2015 , 13, 1550005 | 14 |
| 407 | Annotating RNA motifs in sequences and alignments. 2015 , 43, 691-8 | 18 |
| 406 | Optimized distance-dependent atom-pair-based potential DOOP for protein structure prediction. 2015 , 83, 881-90 | 8 |
| 405 | Exploring the speed and performance of molecular replacement with AMPLE using QUARK ab initio protein models. 2015 , 71, 338-43 | 21 |
| 404 | Tertiary structural propensities reveal fundamental sequence/structure relationships. 2015 , 23, 961-971 | 17 |
| 403 | Chimeric peptides as implant functionalization agents for titanium alloy implants with antimicrobial properties. 2015 , 67, 754-766 | 53 |
| 402 | Broadening the Spectrum of Ehlers Danlos Syndrome in Patients With Congenital Adrenal Hyperplasia. 2015 , 100, E1143-52 | 41 |
| 401 | Combination of Differential Evolution and Fragment-based Replacements for Protein Structure Prediction. 2015 , | 2 |
| 400 | Design of symmetric TIM barrel proteins from first principles. 2015 , 16, 18 | 21 |
| 399 | Amplitude spectrum distance: measuring the global shape divergence of protein fragments. 2015 , 16, 256 | |
| 398 | Prediction Enhancement of Residue Real-Value Relative Accessible Surface Area in Transmembrane Helical Proteins by Solving the Output Preference Problem of Machine Learning-Based Predictors. 2015 , 55, 2464-74 | 14 |
| 397 | Experimental Protein Structure Verification by Scoring with a Single, Unassigned NMR Spectrum. 2015 , 23, 1958-1966 | 7 |
| 396 | Structure-based pKa prediction provides a thermodynamic basis for the role of histidines in pH-induced conformational transitions in dengue virus. 2015 , 4, 375-385 | 10 |
| 395 | Molecular basis for structural heterogeneity of an intrinsically disordered protein bound to a partner by combined ESI-IM-MS and modeling. 2015 , 26, 472-81 | 39 |
| 394 | Finding All Longest Common Segments in Protein Structures Efficiently. 2015 , 12, 644-55 | 1 |

| | | |
|-----|--|-----|
| 393 | Homology modeling: an important tool for the drug discovery. 2015 , 33, 1780-93 | 33 |
| 392 | Multiphase Simulated Annealing Based on Boltzmann and Bose-Einstein Distribution Applied to Protein Folding Problem. 2016 , 2016, 7357123 | 2 |
| 391 | GP0.4 from bacteriophage T7: in silico characterisation of its structure and interaction with E. coli FtsZ. 2016 , 9, 343 | 2 |
| 390 | Comparison of Algorithms for Prediction of Protein Structural Features from Evolutionary Data. 2016 , 11, e0150769 | 1 |
| 389 | Computational methods in drug discovery. 2016 , 12, 2694-2718 | 271 |
| 388 | Protein structure prediction (RMSD & 5 Å) using machine learning models. 2016 , 14, 71 | 7 |
| 387 | UniCon3D: de novo protein structure prediction using united-residue conformational search via stepwise, probabilistic sampling. 2016 , 32, 2791-9 | 29 |
| 386 | sDFIRE: Sequence-specific statistical energy function for protein structure prediction by decoy selections. 2016 , 37, 1119-24 | 10 |
| 385 | CASP11 refinement experiments with ROSETTA. 2016 , 84 Suppl 1, 314-22 | 18 |
| 384 | Integration of QUARK and I-TASSER for Ab Initio Protein Structure Prediction in CASP11. 2016 , 84 Suppl 1, 76-86 | 47 |
| 383 | Massive integration of diverse protein quality assessment methods to improve template based modeling in CASP11. 2016 , 84 Suppl 1, 247-59 | 22 |
| 382 | Constrained cyclic coordinate descent for cryo-EM images at medium resolutions: beyond the protein loop closure problem. 2016 , 34, 1777-1790 | 7 |
| 381 | Mutational analysis and interactions of HBV preS1 with asialoglycoprotein receptor. 2016 , 11, 761-774 | 1 |
| 380 | Protein Secondary Structure Prediction Using Deep Convolutional Neural Fields. 2016 , 6, 18962 | 285 |
| 379 | Zinc and p53 Misfolding. 2016 , 207-222 | 1 |
| 378 | Model of protein fragments and statistical potentials. 2016 , 8, 325-337 | 3 |
| 377 | A Stochastic Point Cloud Sampling Method for Multi-Template Protein Comparative Modeling. 2016 , 6, 25687 | 7 |
| 376 | DeepQA: improving the estimation of single protein model quality with deep belief networks. 2016 , 17, 495 | 120 |

| | | |
|-----|--|-----|
| 375 | Discriminate protein decoys from native by using a scoring function based on ubiquitous Phi and Psi angles computed for all atom. 2016 , 398, 112-21 | 7 |
| 374 | Toward a detailed understanding of search trajectories in fragment assembly approaches to protein structure prediction. 2016 , 84, 411-26 | 14 |
| 373 | EGFR Fusions as Novel Therapeutic Targets in Lung Cancer. 2016 , 6, 601-11 | 65 |
| 372 | Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. 2016 , 45, 253-78 | 54 |
| 371 | A Derived Allosteric Switch Underlies the Evolution of Conditional Cooperativity between HOXA11 and FOXO1. 2016 , 15, 2097-2108 | 17 |
| 370 | Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. 2016 , 55, 4748-63 | 118 |
| 369 | Recent advances in sequence-based protein structure prediction. 2017 , 18, 1021-1032 | 16 |
| 368 | Pushing the Backbone in Protein-Protein Docking. 2016 , 24, 1821-1829 | 33 |
| 367 | The coming of age of de novo protein design. 2016 , 537, 320-7 | 697 |
| 366 | Structural Diversity in the Type IV Pili of Multidrug-resistant Acinetobacter. 2016 , 291, 22924-22935 | 31 |
| 365 | Structural and mechanistic insights into human splicing factor SF3b complex derived using an integrated approach guided by the cryo-EM density maps. 2016 , 13, 1025-1040 | 4 |
| 364 | 3D structure determination of a protein in living cells using paramagnetic NMR spectroscopy. 2016 , 52, 10237-40 | 72 |
| 363 | Solution structure of the microtubule-targeting COS domain of MID1. 2016 , 283, 3089-102 | 8 |
| 362 | Solution structure of the isolated histone H2A-H2B heterodimer. 2016 , 6, 24999 | 16 |
| 361 | LRFragLib: an effective algorithm to identify fragments for de novo protein structure prediction. 2017 , 33, 677-684 | 3 |
| 360 | Translational Biomedical Informatics. 2016 , | 1 |
| 359 | Tertiary alphabet for the observable protein structural universe. 2016 , 113, E7438-E7447 | 34 |
| 358 | Exploring Human Diseases and Biological Mechanisms by Protein Structure Prediction and Modeling. 2016 , 939, 39-61 | 2 |

| | | |
|-----|--|-----|
| 357 | Design and engineering of artificial oxygen-activating metalloenzymes. 2016 , 45, 5020-54 | 128 |
| 356 | An Atomistic Statistically Effective Energy Function for Computational Protein Design. 2016 , 12, 4146-68 | 9 |
| 355 | Blind Evaluation of Hybrid Protein Structure Analysis Methods based on Cross-Linking. 2016 , 41, 564-567 | 17 |
| 354 | GNAO1 encephalopathy: further delineation of a severe neurodevelopmental syndrome affecting females. 2016 , 11, 38 | 23 |
| 353 | FRAGSION: ultra-fast protein fragment library generation by IOHMM sampling. 2016 , 32, 2059-61 | 5 |
| 352 | RNA folding pathways in stop motion. 2016 , 44, 5883-91 | 29 |
| 351 | Evaluation of free modeling targets in CASP11 and ROLL. 2016 , 84 Suppl 1, 51-66 | 60 |
| 350 | Using Local States To Drive the Sampling of Global Conformations in Proteins. 2016 , 12, 1368-79 | 12 |
| 349 | Generating, Maintaining, and Exploiting Diversity in a Memetic Algorithm for Protein Structure Prediction. 2016 , 24, 577-607 | 28 |
| 348 | 3D protein structure prediction using Imperialist Competitive algorithm and half sphere exposure prediction. 2016 , 391, 81-7 | 4 |
| 347 | 3DRobot: automated generation of diverse and well-packed protein structure decoys. 2016 , 32, 378-87 | 87 |
| 346 | Computational de novo design of antibodies binding to a peptide with high affinity. 2017 , 114, 1331-1342 | 19 |
| 345 | Computational Prediction of the Heterodimeric and Higher-Order Structure of gpE1/gpE2 Envelope Glycoproteins Encoded by Hepatitis C Virus. 2017 , 91, | 24 |
| 344 | Improving prediction of helix-helix packing in membrane proteins using predicted contact numbers as restraints. 2017 , 85, 1212-1221 | 6 |
| 343 | Computational tools for exploring sequence databases as a resource for antimicrobial peptides. 2017 , 35, 337-349 | 71 |
| 342 | The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. 2017 , 13, 3031-3048 | 486 |
| 341 | Protein structural motifs in prediction and design. 2017 , 44, 161-167 | 21 |
| 340 | ClusPro PeptiDock: efficient global docking of peptide recognition motifs using FFT. 2017 , 33, 3299-3301 | 54 |

| | | | |
|-----|---|-----|----|
| 339 | EpiSweep: Computationally Driven Reengineering of Therapeutic Proteins to Reduce Immunogenicity While Maintaining Function. 2017 , 1529, 375-398 | | 17 |
| 338 | Structural studies of RNA-protein complexes: A hybrid approach involving hydrodynamics, scattering, and computational methods. 2017 , 118-119, 146-162 | | 23 |
| 337 | Role of Bioinformatics in the Study of Ionic Channels. 2017 , 227, 17-37 | | 1 |
| 336 | Volunteer computing for computational materials design. 2017 , 38, 926-930 | | 2 |
| 335 | The soluble domains of Gpi8 and Gaa1, two subunits of glycosylphosphatidylinositol transamidase (GPI-T), assemble into a complex. 2017 , 633, 58-67 | | 5 |
| 334 | Double estimation of distribution guided sampling algorithm for de-novo protein structure prediction. 2017 , | | 0 |
| 333 | Improving protein fold recognition by extracting fold-specific features from predicted residue-residue contacts. 2017 , 33, 3749-3757 | | 31 |
| 332 | A natural ligand for the orphan receptor GPR15 modulates lymphocyte recruitment to epithelia. 2017 , 10, | | 35 |
| 331 | Convergent and divergent genetic changes in the genome of Chinese and European pigs. 2017 , 7, 8662 | | 12 |
| 330 | OPUS-DOSP: A Distance- and Orientation-Dependent All-Atom Potential Derived from Side-Chain Packing. <i>Journal of Molecular Biology</i> , 2017 , 429, 3113-3120 | 6.5 | 18 |
| 329 | Small-Angle X-ray Scattering Data in Combination with RosettaDock Improves the Docking Energy Landscape. 2017 , 57, 2463-2475 | | 7 |
| 328 | Analysis of positive and negative allosteric modulation in metabotropic glutamate receptors 4 and 5 with a dual ligand. 2017 , 7, 4944 | | 11 |
| 327 | Probing Medin Monomer Structure and its Amyloid Nucleation Using C-Direct Detection NMR in Combination with Structural Bioinformatics. 2017 , 7, 45224 | | 8 |
| 326 | Crowd sourcing difficult problems in protein science. 2017 , 26, 2118-2125 | | 1 |
| 325 | Conformational Space Sampling Method Using Multi-Subpopulation Differential Evolution for De novo Protein Structure Prediction. 2017 , 16, 618-633 | | 5 |
| 324 | Heterologous expression of abaecin peptide from <i>Apis mellifera</i> in <i>Pichia pastoris</i> . 2017 , 16, 76 | | 14 |
| 323 | Protein Engineering Techniques. 2017 , | | 7 |
| 322 | Paramagnetic restraints for structure and dynamics of biomolecules. 2017 , 277-312 | | |

| | | |
|-----|---|----|
| 321 | Honey Bee Deformed Wing Virus Structures Reveal that Conformational Changes Accompany Genome Release. 2017 , 91, | 22 |
| 320 | Feature importance calculation and protein quality assessment on the decoy discrimination problem. 2017 , | |
| 319 | On heuristic bias in fragment-assembly methods for protein structure prediction. 2017 , | |
| 318 | Optimal Tilt Angle and Orientation of Photovoltaic Modules Using HS Algorithm in Different Climates of China. 2017 , 7, 1028 | 26 |
| 317 | Geometry Analysis for Protein Secondary Structures Matching Problem. 2017 , | |
| 316 | High-resolution global peptide-protein docking using fragments-based PIPER-FlexPepDock. 2017 , 13, e1005905 | 58 |
| 315 | An efficient algorithm for improving structure-based prediction of transcription factor binding sites. 2017 , 18, 342 | 6 |
| 314 | Protein Structure Prediction and Homology Modeling. 2017 , 120-144 | |
| 313 | Molecular Recognition by a Short Partial Peptide of the Adrenergic Receptor: A Bottom-Up Approach. 2018 , 57, 5626-5629 | 18 |
| 312 | Protein homology model refinement by large-scale energy optimization. 2018 , 115, 3054-3059 | 49 |
| 311 | Protein Tertiary Structure by Crosslinking/Mass Spectrometry. 2018 , 43, 157-169 | 54 |
| 310 | New Knowledge-Based Scoring Function with Inclusion of Backbone Conformational Entropies from Protein Structures. 2018 , 58, 724-732 | 5 |
| 309 | Hydrophobic residues can identify native protein structures. 2018 , 86, 467-474 | 3 |
| 308 | Data-assisted protein structure modeling by global optimization in CASP12. 2018 , 86 Suppl 1, 240-246 | 3 |
| 307 | OPUS-CSF: A C-atom-based scoring function for ranking protein structural models. 2018 , 27, 286-292 | 12 |
| 306 | Protein structure prediction. 2018 , 32, | 28 |
| 305 | Molecular Recognition by a Short Partial Peptide of the Adrenergic Receptor: A Bottom-Up Approach. 2018 , 130, 5728-5731 | 3 |
| 304 | Chemical shift-based methods in NMR structure determination. 2018 , 106-107, 1-25 | 24 |

| | | |
|-----|--|-------|
| 303 | Principal component analysis in protein tertiary structure prediction. 2018 , 16, 1850005 | 4 |
| 302 | Accurately Predicting Disordered Regions of Proteins Using Rosetta ResidueDisorder Application. 2018 , 122, 3920-3930 | 10 |
| 301 | Guiding exploration in conformational feature space with Lipschitz underestimation for ab-initio protein structure prediction. 2018 , 73, 105-119 | 4 |
| 300 | Shikimate Induced Transcriptional Activation of Protocatechuate Biosynthesis Genes by QuiR, a LysR-Type Transcriptional Regulator, in <i>Listeria monocytogenes</i> . <i>Journal of Molecular Biology</i> , 2018 , 430, 1265-1283 | 6.5 4 |
| 299 | A Memetic Algorithm for 3-D Protein Structure Prediction Problem. 2018 , 15, 690-704 | 14 |
| 298 | DynaDom: structure-based prediction of T cell receptor inter-domain and T cell receptor-peptide-MHC (class I) association angles. 2017 , 17, 2 | 8 |
| 297 | Finding the needle in the haystack: towards solving the protein-folding problem computationally. 2018 , 53, 1-28 | 23 |
| 296 | Integration of molecular dynamics simulation and hotspot residues grafting for de novo scFv design against <i>Salmonella Typhi</i> TolC protein. 2018 , 31, e2695 | 3 |
| 295 | Three-dimensional protein structure prediction based on memetic algorithms. 2018 , 91, 160-177 | 11 |
| 294 | Predicting Protein Interactions Using a Deep Learning Method-Stacked Sparse Autoencoder Combined with a Probabilistic Classification Vector Machine. 2018 , 2018, 1-12 | 15 |
| 293 | Replacement, Refinement, and Reduction in Animal Studies With Biohazardous Agents. 2018 , 59, 177-194 | 10 |
| 292 | THE-DB: a threading model database for comparative protein structure analysis of the <i>E. coli</i> K12 and human proteomes. 2018 , 2018, | 5 |
| 291 | Systematic Comparison of Amber and Rosetta Energy Functions for Protein Structure Evaluation. 2018 , 14, 6015-6025 | 13 |
| 290 | Bioinformatics: Sequences, Structures, Phylogeny. 2018 , | |
| 289 | Structural Bioinformatics: Life Through The 3D Glasses. 2018 , 191-253 | |
| 288 | Generation of Pairwise Potentials Using Multidimensional Data Mining. 2018 , 14, 5045-5067 | 8 |
| 287 | Improved fragment-based protein structure prediction by redesign of search heuristics. 2018 , 8, 13694 | 6 |
| 286 | Analytical Approaches to Improve Accuracy in Solving the Protein Topology Problem. 2018 , 23, | 4 |

| | | |
|-----|--|-----|
| 285 | Quality Estimation Of Protein Structure Using Machine Learning Approaches : A Survey. 2018, | |
| 284 | To the Final Goal: Can We Predict and Suggest Mutations for Protein to Develop Desired Phenotype?. 2018, 23, 134-143 | 5 |
| 283 | A Novel Method for Drug Screen to Regulate G Protein-Coupled Receptors in the Metabolic Network of Alzheimer's Disease. 2018, 2018, 5486403 | 2 |
| 282 | A random forest learning assisted "divide and conquer" approach for peptide conformation search. 2018, 8, 8796 | 2 |
| 281 | Computer-aided design of amino acid-based therapeutics: a review. 2018, 12, 1239-1254 | 19 |
| 280 | Contact Potential for Structure Prediction of Proteins and Protein Complexes from Potts Model. 2018, 115, 809-821 | 12 |
| 279 | MyPMFs: a simple tool for creating statistical potentials to assess protein structural models. 2018, 151, 37-41 | 3 |
| 278 | Rosetta Protein Structure Prediction from Hydroxyl Radical Protein Footprinting Mass Spectrometry Data. 2018, 90, 7721-7729 | 33 |
| 277 | Loop modelling 1.0. 2018, 84, 64-68 | 4 |
| 276 | Studies on a landscape of perfluoroaromatic-reactive peptides. 2019, 17, 1862-1868 | 6 |
| 275 | Protein Structural Bioinformatics: An Overview. 2019, 445-459 | 9 |
| 274 | Protein Design. 2019, 644-651 | 1 |
| 273 | Advances in protein structure prediction and design. 2019, 20, 681-697 | 215 |
| 272 | Improved fragment sampling for ab initio protein structure prediction using deep neural networks. 2019, 1, 347-355 | 15 |
| 271 | Discrimination power of knowledge-based potential dictated by the dominant energies in native protein structures. 2019, 51, 1029-1038 | 1 |
| 270 | Protein structure prediction using sparse NOE and RDC restraints with Rosetta in CASP13. 2019, 87, 1341-1350 | 4 |
| 269 | Tracing the GSAP-APP C-99 Interaction Site in the β Amyloid Pathway Leading to Alzheimer's Disease. 2019, 10, 3868-3879 | 8 |
| 268 | OPUS-SSF: A side-chain-inclusive scoring function for ranking protein structural models. 2019, 28, 1157-1162 | 4 |

| | | |
|-----|---|-----|
| 267 | Loop Enhanced Conformational Resampling Method for Protein Structure Prediction. 2019 , 18, 567-577 | |
| 266 | Protein structure prediction using multiple deep neural networks in the 13th Critical Assessment of Protein Structure Prediction (CASP13). 2019 , 87, 1141-1148 | 145 |
| 265 | Detecting distant-homology protein structures by aligning deep neural-network based contact maps. 2019 , 15, e1007411 | 25 |
| 264 | Reliable Generation of Native-Like Decoys Limits Predictive Ability in Fragment-Based Protein Structure Prediction. 2019 , 9, | |
| 263 | Can Conformational Changes of Proteins Be Represented in Torsion Angle Space? A Study with Rescaled Ridge Regression. 2019 , 59, 4929-4941 | 6 |
| 262 | Differences in protein structural regions that impact functional specificity in GT2 family β glucan synthases. 2019 , 14, e0224442 | 5 |
| 261 | An Integrated Approach for Determining a Protein-Protein Binding Interface in Solution and an Evaluation of Hydrogen-Deuterium Exchange Kinetics for Adjudicating Candidate Docking Models. 2019 , 91, 15709-15717 | 17 |
| 260 | Liraglutide exhibits anti-inflammatory activity through the activation of the PKA/CREB pathway. 2019 , 16, 21 | 3 |
| 259 | rawMSA: End-to-end Deep Learning using raw Multiple Sequence Alignments. 2019 , 14, e0220182 | 27 |
| 258 | Integrative Protein Modeling in RosettaNMR from Sparse Paramagnetic Restraints. 2019 , 27, 1721-1734.e5 | 13 |
| 257 | Computational design of structured loops for new protein functions. 2019 , 400, 275-288 | 16 |
| 256 | Decoding the Structural Keywords in Protein Structure Universe. 2019 , 34, 3-15 | 2 |
| 255 | Molecular simulation of peptides coming of age: Accurate prediction of folding, dynamics and structures. 2019 , 664, 76-88 | 14 |
| 254 | LPS-squalene interaction on D-galactose intestinal absorption. 2019 , 75, 329-340 | 3 |
| 253 | Atomic Motif Recognition in (Bio)Polymers: Benchmarks From the Protein Data Bank. 2019 , 6, 24 | 8 |
| 252 | Integrating Bonded and Nonbonded Potentials in the Knowledge-Based Scoring Function for Protein Structure Prediction. 2019 , 59, 3080-3090 | 7 |
| 251 | Integrative Structure Modeling: Overview and Assessment. 2019 , 88, 113-135 | 29 |
| 250 | Structural, magnetic and electronic properties of CuNi_{55}B ($n = 0\text{B}5$) nanoparticles: Combination artificial bee colony algorithm with DFT. 2019 , 1154, 11-16 | 7 |

| | | |
|-----|---|----|
| 249 | A new benchmark illustrates that integration of geometric constraints inferred from enzyme reaction chemistry can increase enzyme active site modeling accuracy. 2019 , 14, e0214126 | 5 |
| 248 | A global map of the protein shape universe. 2019 , 15, e1006969 | 12 |
| 247 | Constructing effective energy functions for protein structure prediction through broadening attraction-basin and reverse Monte Carlo sampling. 2019 , 20, 135 | 0 |
| 246 | Utility of Covalent Labeling Mass Spectrometry Data in Protein Structure Prediction with Rosetta. 2019 , 15, 3410-3424 | 18 |
| 245 | Advances in Protein Super-Secondary Structure Prediction and Application to Protein Structure Prediction. 2019 , 1958, 15-45 | 4 |
| 244 | Conformational Stabilization and Rapid Labeling of a 29-Residue Peptide by a Small Molecule Reaction Partner. 2019 , 58, 1343-1353 | 7 |
| 243 | Random Forest Refinement of the KECSA2 Knowledge-Based Scoring Function for Protein Decoy Detection. 2019 , 59, 1919-1929 | 9 |
| 242 | What has de novo protein design taught us about protein folding and biophysics?. 2019 , 28, 678-683 | 81 |
| 241 | Protein structure predictions by enhanced conformational sampling methods. 2019 , 16, 344-366 | 3 |
| 240 | Consistency principle for protein design. 2019 , 16, 304-309 | 5 |
| 239 | 3D Structure Determination and Validation of mTORC2 using Computational Modeling Techniques. 2019 , | |
| 238 | On the possible origin of protein homochirality, structure, and biochemical function. 2019 , | 16 |
| 237 | CS-ROSETTA. 2019 , 614, 321-362 | 10 |
| 236 | Computational Intelligence Tools for Protein Modeling. 2019 , 949-956 | 0 |
| 235 | Sampling Native-like Structures of RNA-Protein Complexes through Rosetta Folding and Docking. 2019 , 27, 140-151.e5 | 18 |
| 234 | Rapid determination of quaternary protein structures in complex biological samples. 2019 , 10, 192 | 31 |
| 233 | Statistical force-field for structural modeling using chemical cross-linking/mass spectrometry distance constraints. 2019 , 35, 3005-3012 | 11 |
| 232 | Contribution of Cotranslational Folding Defects to Membrane Protein Homeostasis. 2019 , 141, 204-215 | 13 |

| | | |
|-----|---|----|
| 231 | Modeling of Protein Tertiary and Quaternary Structures Based on Evolutionary Information. 2019 , 1851, 301-316 | 6 |
| 230 | Secondary Structure and Contact Guided Differential Evolution for Protein Structure Prediction. 2020 , 17, 1068-1081 | 18 |
| 229 | Two-Stage Distance Feature-based Optimization Algorithm for De novo Protein Structure Prediction. 2020 , 17, 2119-2130 | 2 |
| 228 | Comparison of Rosetta flexible-backbone computational protein design methods on binding interactions. 2020 , 88, 206-226 | 20 |
| 227 | The characterization of pc-polylines representing protein backbones. 2020 , 88, 307-318 | 1 |
| 226 | Structural complementarity of distance constraints obtained from chemical cross-linking and amino acid coevolution. 2020 , 88, 625-632 | 2 |
| 225 | Using NMR Chemical Shifts and Cryo-EM Density Restraints in Iterative Rosetta-MD Protein Structure Refinement. 2020 , 60, 2522-2532 | 11 |
| 224 | CGLFold: a contact-assisted de novo protein structure prediction using global exploration and loop perturbation sampling algorithm. 2020 , 36, 2443-2450 | 9 |
| 223 | Modeling beta-sheet peptide-protein interactions: Rosetta FlexPepDock in CAPRI rounds 38-45. 2020 , 88, 1037-1049 | 8 |
| 222 | Computational reconstruction of atomistic protein structures from coarse-grained models. 2020 , 18, 162-176 | 24 |
| 221 | CATHER: a novel threading algorithm with predicted contacts. 2020 , 36, 2119-2125 | 6 |
| 220 | SPOT-Fold: Fragment-Free Protein Structure Prediction Guided by Predicted Backbone Structure and Contact Map. 2020 , 41, 745-750 | 6 |
| 219 | The Last Secret of Protein Folding: The Real Relationship Between Long-Range Interactions and Local Structures. 2020 , 39, 422-433 | 3 |
| 218 | Tightening the Crosslinking Distance Restraints for Better Resolution of Protein Structure and Dynamics. 2020 , 28, 1160-1167.e3 | 4 |
| 217 | Deep Learning in Proteomics. 2020 , 20, e1900335 | 27 |
| 216 | Allosteric cooperation in a de novo-designed two-domain protein. 2020 , 117, 33246-33253 | 15 |
| 215 | De Novo Protein Design Using the Blueprint Builder in Rosetta. 2020 , 102, e116 | 0 |
| 214 | Structural insights into the mechanism of rhodopsin phosphodiesterase. 2020 , 11, 5605 | 15 |

| | | |
|-----|--|------|
| 213 | An information gain-based approach for evaluating protein structure models. 2020 , 18, 2228-2236 | 2 |
| 212 | Better together: Elements of successful scientific software development in a distributed collaborative community. 2020 , 16, e1007507 | 15 |
| 211 | Modeled structure-based computational redesign of a glycosyltransferase for the synthesis of rebaudioside D from rebaudioside A. 2020 , 159, 107626 | 10 |
| 210 | FARFAR2: Improved De Novo Rosetta Prediction of Complex Global RNA Folds. 2020 , 28, 963-976.e6 | 37 |
| 209 | A Unified De Novo Approach for Predicting the Structures of Ordered and Disordered Proteins. 2020 , 124, 5538-5548 | 5 |
| 208 | Structural Insight of the Full-Length Ros Protein: A Prototype of the Prokaryotic Zinc-Finger Family. 2020 , 10, 9283 | 3 |
| 207 | Performance of human and server prediction in CAPRI rounds 38-45. 2020 , 88, 1110-1120 | 1 |
| 206 | Neighborhood Preference of Amino Acids in Protein Structures and its Applications in Protein Structure Assessment. 2020 , 10, 4371 | 2 |
| 205 | SphereCon-a method for precise estimation of residue relative solvent accessible area from limited structural information. 2020 , 36, 3372-3378 | 1 |
| 204 | De novo Protein Structure Prediction by Coupling Contact with Distance Profile. 2020 , PP, | 1 |
| 203 | Pair Potentials as Machine Learning Features. 2020 , 16, 5385-5400 | 1 |
| 202 | Structural proteomics, electron cryo-microscopy and structural modeling approaches in bacteria-human protein interactions. 2020 , 209, 265-275 | 8 |
| 201 | Dynamic Evolution of the Cthrc1 Genes, a Newly Defined Collagen-Like Family. 2020 , 12, 3957-3970 | 4 |
| 200 | Improved protein structure prediction using potentials from deep learning. 2020 , 577, 706-710 | 1007 |
| 199 | Experimentally-driven protein structure modeling. 2020 , 220, 103777 | 14 |
| 198 | ProtFold-DFG: protein fold recognition by combining Directed Fusion Graph and PageRank algorithm. 2021 , 22, | 25 |
| 197 | Protein Structure Prediction Using Population-Based Algorithm Guided by Information Entropy. 2021 , 18, 697-707 | 1 |
| 196 | Computationally grafting an IgE epitope onto a scaffold: Implications for a pan anti-allergy vaccine design. 2021 , 19, 4738-4750 | 0 |

| | | |
|-----|--|----|
| 195 | Computational Methods for the Elucidation of Protein Structure and Interactions. 2021 , 2305, 23-52 | 0 |
| 194 | Geometrical Features of Epidermal Growth Factor Receptor-Related Dimers Reveal the Mechanisms of Drug Resistance in Lung Cancer Patients. 2021 , 9, 5704-5715 | 0 |
| 193 | Recent advances in de novo protein design: Principles, methods, and applications. 2021 , 296, 100558 | 29 |
| 192 | Representations of protein structure for exploring the conformational space: A speed-accuracy trade-off. 2021 , 19, 2618-2625 | 0 |
| 191 | Mapping the Promiscuous Binding Interface of HOX-A11 with KIX by Experimentally Guided in-silico docking. | |
| 190 | Aromaphilicity Index of Amino Acids: Molecular Dynamics Simulations of the Protein Binding Affinity for Carbon Nanomaterials. 2021 , 4, 2486-2495 | 12 |
| 189 | Defining a novel domain that provides an essential contribution to site-specific interaction of Rep protein with DNA. 2021 , 49, 3394-3408 | 2 |
| 188 | Protein Structure Prediction from NMR Hydrogen-Deuterium Exchange Data. 2021 , 17, 2619-2629 | 4 |
| 187 | Protein sequence design by conformational landscape optimization. 2021 , 118, | 29 |
| 186 | APPTTEST is an innovative new method for the automatic prediction of peptide tertiary structures. | 1 |
| 185 | Extension of a de novo TIM barrel with a rationally designed secondary structure element. 2021 , 30, 982-989 | 4 |
| 184 | Construction of a neural network energy function for protein physics. | 1 |
| 183 | Effects of pH on an IDP conformational ensemble explored by molecular dynamics simulation. 2021 , 271, 106552 | 6 |
| 182 | Docking Paradigm in Drug Design. 2021 , 21, 507-546 | 7 |
| 181 | Decoding microbiome and protein family linkage to improve protein structure prediction. | |
| 180 | Plausible blockers of Spike RBD in SARS-CoV2-molecular design and underlying interaction dynamics from high-level structural descriptors. 2021 , 27, 191 | 1 |
| 179 | Step-by-step design of proteins for small molecule interaction: A review on recent milestones. 2021 , 30, 1502-1520 | 1 |
| 178 | Synthesis and Modeling of Ezetimibe Analogues. 2021 , 26, | 1 |

| | | |
|-----|---|----|
| 177 | Protein shape sampled by ion mobility mass spectrometry consistently improves protein structure prediction. | 1 |
| 176 | Genotype-determined EGFR-RTK heterodimerization and its effects on drug resistance in lung Cancer treatment revealed by molecular dynamics simulations. 2021 , 22, 34 | 0 |
| 175 | Genome editing in mammalian cells using the CRISPR type I-D nuclease. 2021 , 49, 6347-6363 | 7 |
| 174 | Role of backbone strain in de novo design of complex $\alpha\beta$ protein structures. 2021 , 12, 3921 | 9 |
| 173 | Efficient Generative Modelling of Protein Structure Fragments using a Deep Markov Model. | |
| 172 | Complementing sequence-derived features with structural information extracted from fragment libraries for protein structure prediction. 2021 , 22, 351 | 0 |
| 171 | A secondary structure-based position-specific scoring matrix applied to the improvement in protein secondary structure prediction. 2021 , 16, e0255076 | 2 |
| 170 | The influence of dataset homology and a rigorous evaluation strategy on protein secondary structure prediction. 2021 , 16, e0254555 | 2 |
| 169 | Toward the solution of the protein structure prediction problem. 2021 , 297, 100870 | 12 |
| 168 | Accurately positioning functional residues with robotics-inspired computational protein design. | |
| 167 | APPTTEST is a novel protocol for the automatic prediction of peptide tertiary structures. 2021 , 22, | 7 |
| 166 | Improving fragment-based ab initio protein structure assembly using low-accuracy contact-map predictions. 2021 , 12, 5011 | 6 |
| 165 | Precise estimation of residue relative solvent accessible area from C α atom distance matrix using a deep learning method. 2021 , | 2 |
| 164 | On the Potential of Machine Learning to Examine the Relationship Between Sequence, Structure, Dynamics and Function of Intrinsically Disordered Proteins. <i>Journal of Molecular Biology</i> , 2021 , 433, 167198 | 7 |
| 163 | PatchMAN docking: Modeling peptide-protein interactions in the context of the receptor surface. | 1 |
| 162 | Green biomanufacturing promoted by automatic retrobiosynthesis planning and computational enzyme design. 2021 , 41, 6-6 | |
| 161 | Structure-based protein design with deep learning. 2021 , 65, 136-144 | 3 |
| 160 | Computational Modeling of Protein Three-Dimensional Structure: Methods and Resources. 2021 , 155-178 | 1 |

| | | |
|-----|---|----|
| 159 | Molecular flexibility in computational protein design: an algorithmic perspective. 2021 , 34, | 6 |
| 158 | <i>Listeria monocytogenes</i> upregulates mitochondrial calcium signalling to inhibit LC3-associated phagocytosis as a survival strategy. 2021 , 6, 366-379 | 12 |
| 157 | MO4: A Many-objective Evolutionary Algorithm for Protein Structure Prediction. 2021 , 1-1 | 2 |
| 156 | Ab initio protein structure prediction of CASP III targets using ROSETTA. 1999 , 37, 171-176 | 82 |
| 155 | Hypergraph Model of Multi-residue Interactions in Proteins: Sequentially Constrained Partitioning Algorithms for Optimization of Site-Directed Protein Recombination. 2006 , 15-29 | 4 |
| 154 | Integrating Web Resources to Model Protein Structure and Function. 2006 , 184-196 | 2 |
| 153 | A Historical Perspective and Overview of Protein Structure Prediction. 2007 , 1-43 | 5 |
| 152 | Computational Methods for Protein Fold Prediction: an Ab-initio Topological Approach. 2007 , 391-429 | 4 |
| 151 | Protein Structure Prediction. 2009 , 225-242 | 3 |
| 150 | Coarse-Grained Models of Proteins: Theory and Applications. 2011 , 35-83 | 10 |
| 149 | Annotation of Alternatively Spliced Proteins and Transcripts with Protein-Folding Algorithms and Isoform-Level Functional Networks. 2017 , 1558, 415-436 | 2 |
| 148 | Flexible Backbone Methods for Predicting and Designing Peptide Specificity. 2017 , 1561, 173-187 | 3 |
| 147 | Protein structure prediction. 2008 , 453, 33-85 | 3 |
| 146 | Protein structure modeling. 2010 , 673, 63-72 | 5 |
| 145 | Prediction of protein tertiary structures using MUFOLD. 2012 , 815, 3-13 | 8 |
| 144 | Bayesian Multiple Protein Structure Alignment. 2014 , 326-339 | 2 |
| 143 | Construction of Protein Backbone Fragments Libraries on Large Protein Sets Using a Randomized Spectral Clustering Algorithm. 2017 , 108-119 | 2 |
| 142 | Physics-Based Modeling of Side Chain-Side Chain Interactions in the UNRES Force Field. 2019 , 89-115 | 2 |

| | | |
|-----|--|----|
| 141 | Finding Largest Well-Predicted Subset of Protein Structure Models. 2008 , 44-55 | 10 |
| 140 | Analytically Tuned Simulated Annealing Applied to the Protein Folding Problem. 2007 , 370-377 | 6 |
| 139 | Computational Methods for Protein Structure Prediction and Fold Recognition. 2008 , 1-21 | 6 |
| 138 | MetaApproaches to Protein Structure Prediction. 2008 , 23-34 | 4 |
| 137 | Modeling Protein Folding Pathways. 2008 , 97-122 | 1 |
| 136 | Protein Decoy Generation Using Branch and Bound with Efficient Bounding. 2008 , 382-393 | 3 |
| 135 | Investigations into the Effect of Multiobjectivization in Protein Structure Prediction. 2008 , 702-711 | 22 |
| 134 | A Probabilistic Graphical Model for Ab Initio Folding. 2009 , 5541, 59-73 | 7 |
| 133 | Data Mining for Protein Secondary Structure Prediction. 2009 , 135-167 | 1 |
| 132 | Ab Initio Protein Structure Prediction. 2017 , 3-35 | 34 |
| 131 | A glance into the evolution of template-free protein structure prediction methodologies. 2020 , 175, 85-92 | 9 |
| 130 | Epitope and Paratope Mapping of PD-1/Nivolumab by Mass Spectrometry-Based Hydrogen-Deuterium Exchange, Cross-linking, and Molecular Docking. 2020 , 92, 9086-9094 | 12 |
| 129 | Hybrid methods for combined experimental and computational determination of protein structure. 2020 , 153, 240901 | 13 |
| 128 | The Rosetta all-atom energy function for macromolecular modeling and design. | 3 |
| 127 | High-resolution global peptide-protein docking using fragments-based PIPER-FlexPepDock. | 2 |
| 126 | A Unified De Novo Approach for Predicting the Structures of Ordered and Disordered Proteins. | 1 |
| 125 | Structural insights into the mechanism of rhodopsin phosphodiesterase. | 2 |
| 124 | Sampling native-like structures of RNA-protein complexes through Rosetta folding and docking. | 1 |

| | | |
|-----|---|-----|
| 123 | rawMSA: End-to-end Deep Learning Makes Protein Sequence Profiles and Feature Extraction obsolete. | 5 |
| 122 | Structural Learning of Proteins Using Graph Convolutional Neural Networks. | 18 |
| 121 | FARFAR2: Improved de novo Rosetta prediction of complex global RNA folds. | 4 |
| 120 | Routine phasing of coiled-coil protein crystal structures with AMPLE. 2015 , 2, 198-206 | 18 |
| 119 | Residue contacts predicted by evolutionary covariance extend the application of ab initio molecular replacement to larger and more challenging protein folds. 2016 , 3, 259-70 | 12 |
| 118 | Extending the scope of coiled-coil crystal structure solution by AMPLE through improved ab initio modelling. 2020 , 76, 272-284 | 4 |
| 117 | An estimate of the numbers and density of low-energy structures (or decoys) in the conformational landscape of proteins. 2009 , 4, e5148 | 3 |
| 116 | The roles of entropy and kinetics in structure prediction. 2009 , 4, e5840 | 7 |
| 115 | PSPP: a protein structure prediction pipeline for computing clusters. 2009 , 4, e6254 | 12 |
| 114 | Potentials of mean force for protein structure prediction vindicated, formalized and generalized. 2010 , 5, e13714 | 51 |
| 113 | A novel side-chain orientation dependent potential derived from random-walk reference state for protein fold selection and structure prediction. 2010 , 5, e15386 | 172 |
| 112 | The 2010 Rosetta developers meeting: macromolecular prediction and design meets reproducible publishing. 2011 , 6, e22431 | 6 |
| 111 | Benchmarking and analysis of protein docking performance in Rosetta v3.2. 2011 , 6, e22477 | 190 |
| 110 | CARD8 and NLRP1 undergo autoproteolytic processing through a ZU5-like domain. 2011 , 6, e27396 | 112 |
| 109 | BCL::Fold--de novo prediction of complex and large protein topologies by assembly of secondary structure elements. 2012 , 7, e49240 | 38 |
| 108 | Improvements to robotics-inspired conformational sampling in rosetta. 2013 , 8, e63090 | 115 |
| 107 | On the importance of the distance measures used to train and test knowledge-based potentials for proteins. 2014 , 9, e109335 | 7 |
| 106 | A Framework to Simplify Combined Sampling Strategies in Rosetta. 2015 , 10, e0138220 | 10 |

| | | |
|-----|---|----|
| 105 | Improving Loop Modeling of the Antibody Complementarity-Determining Region 3 Using Knowledge-Based Restraints. 2016 , 11, e0154811 | 18 |
| 104 | Critical Features of Fragment Libraries for Protein Structure Prediction. 2017 , 12, e0170131 | 12 |
| 103 | Sequence statistics of tertiary structural motifs reflect protein stability. 2017 , 12, e0178272 | 11 |
| 102 | Knowledge-based prediction of protein backbone conformation using a structural alphabet. 2017 , 12, e0186215 | 10 |
| 101 | A computer-based approach for developing linamarase inhibitory agents. 2020 , 5, | 1 |
| 100 | Sequence analysis of the gliding protein Gli349 in. 2005 , 1, 33-43 | 32 |
| 99 | Rosetta and the Journey to Predict Proteins Structures, 20 Years on. 2020 , 15, 611-628 | 5 |
| 98 | MHCII3D-Robust Structure Based Prediction of MHC II Binding Peptides. 2020 , 22, | 2 |
| 97 | RosettaTMH: a method for membrane protein structure elucidation combining EPR distance restraints with assembly of transmembrane helices. 2015 , 3, 1-26 | 1 |
| 96 | Multi-Agent Systems in Three-Dimensional Protein Structure Prediction. 2017 , 241-278 | 1 |
| 95 | Molecular Dynamics Simulations for Biological Systems. 2017 , 1044-1071 | 1 |
| 94 | Multiple Sequence Alignment Optimization Using Meta-Heuristic Techniques. 2017 , 409-423 | 4 |
| 93 | HLA mismatches and hematopoietic cell transplantation: structural simulations assess the impact of changes in peptide binding specificity on transplant outcome. 2011 , 7, 4 | 6 |
| 92 | Molecular docking studies shows tivozanib and lapatinib as potential inhibitors of EML4-ALK translocation mediated fusion protein in non small cell lung cancer. 2014 , 10, 658-63 | 2 |
| 91 | Protein structure prediction. 2016 , 65, 178701 | 2 |
| 90 | Learning protein constitutive motifs from sequence data. 2019 , 8, | 42 |
| 89 | Hierarchical Parallel Simulated Annealing and Its Applications. 2005 , 293-300 | |
| 88 | What We can Learn about Protein Folding from Recent Progress in Structure Prediction. 2007 , 149-155 | |

- 87 Protein Structure Prediction as a Systems Problem. **2007**, 177-206
- 86 Structure prediction of globular proteins. **2008**, 283-307
- 85 Neural Network Pairwise Interaction Fields for Protein Model Quality Assessment. **2009**, 235-248
- 84 New Insights into the Mechanism of Protein Folding by Single Molecule Detection. **2009**, 49, 282-286
- 83 Chapter Binary and Bayesian Networks as Static Models of Regulatory Pathways. **2009**, 97-100
- 82 Novel Perspectives on Protein Structure Prediction. **2010**, 179-207
- 81 Transmembrane beta-barrel protein structure prediction. **2010**, 83-102
- 80 Prediction of three-dimensional transmembrane helical protein structures. **2010**, 231-249
- 79 Recent Advances in De Novo Protein Design. 207-232
- 78 A Filtering Technique for Fragment Assembly- Based Proteins Loop Modeling with Constraints. **2012**, 850-866
- 77 How Accurately Can We Model Protein Structures with Dihedral Angles?. **2012**, 274-287
- 76 Finding Longest Common Segments in Protein Structures in Nearly Linear Time. **2012**, 334-348
- 75 The RosettaCon 2012 Special Collection: Code Writ on Water, Documentation Writ in Stone. **2013**, 8, e73775 1
- 74 Computational analyses of protein coded by rice (*Oryza sativa japonica*) cDNA (GI: 32984786) indicate lectin like Ca(2+) binding properties for Eicosapenta Peptide Repeats (EPRs). **2014**, 10, 63-7 1
- 73 Molecular Dynamics Simulations for Biological Systems. **2016**, 286-313 2
- 72 Generating the Fancy Protein Basket with De Novo and Combinatorial Approaches. **2017**, 85-102
- 71 PB-kPRED: knowledge-based prediction of protein backbone conformation using a structural alphabet.
- 70 OPUS-CSF: A C-atom-based Scoring Function for Ranking Protein Structural Models.

- 69 Approaches to ab initio molecular replacement of helical transmembrane proteins. **2017**, 73, 985-996 3
- 68 NEPRE: a Scoring Function for Protein Structures based on Neighbourhood Preference.
- 67 Multi-Agent Systems in Three-Dimensional Protein Structure Prediction. **2019**, 1031-1068
- 66 Integrative protein modeling in RosettaNMR from sparse paramagnetic restraints. 0
- 65 Protein structure prediction using sparse NOE and RDC restraints with Rosetta in CASP13.
- 64 Comparison of Rosetta flexible-backbone computational protein design methods on binding interactions.
- 63 Consistency Principle for Protein Design. **2020**, 60, 325-330
- 62 MBius Transformation-Induced Distributions Provide Better Modelling for Protein Architecture. **2021**, 9, 2749
- 61 PolyFold: An interactive visual simulator for distance-based protein folding. **2020**, 15, e0243331
- 60 A Study on Protein Structure Prediction. **2020**, 95-118 0
- 59 Multiple Sequence Alignment Optimization Using Meta-Heuristic Techniques. **2020**, 565-579 1
- 58 Protein structure prediction using residue-resolved protection factors from hydrogen-deuterium exchange NMR. **2021**, 0
- 57 Supercomputers in Modeling of Biological Systems. 201-222
- 56 Exact Energy Landscapes of Proteins Using a Coarse-Grained Model. **2008**, 247-268 2
- 55 Extension of a de novo TIM barrel with a rationally designed secondary structure element. 0
- 54 Computationally Grafting an IgE Epitope onto a Scaffold: Implications for a Pan Anti-Allergy Vaccine Design.
- 53 Constraint-based assembly of tertiary protein structures from secondary structure elements. **2000**, 9, 1935-46 15
- 52 Structural and functional analysis of protein. **2022**, 189-206

- 51 Seq-SetNet: directly exploiting multiple sequence alignment for protein secondary structure prediction. **2021**, 0
- 50 The SPICA Coarse-Grained Force Field for Proteins and Peptides.
- 49 Artificial Intelligence in Medicine: Biochemical 3D Modeling and Drug Discovery. **2021**, 1-12
- 48 Lipid-Protein Interactions in Plasma Membrane Organization and Function.. **2022**, 0
- 47 An inductive transfer learning force field (ITLFF) protocol builds protein force fields in seconds.. **2022**, 0
- 46 Designing synthetic transcription factors: A structural perspective.. **2022**, 130, 245-287 0
- 45 Decoding the link of microbiome niches with homologous sequences enables accurately targeted protein structure prediction. **2021**, 118, 2
- 44 Artificial Intelligence in Medicine: Biochemical 3D Modeling and Drug Discovery. **2022**, 661-672
- 43 Modeling of protein conformational changes with Rosetta guided by limited experimental data. 0
- 42 Benchmarking Peptide Structure Prediction with AlphaFold2. 0
- 41 Accurate positioning of functional residues with robotics-inspired computational protein design.. **2022**, 119, e2115480119 0
- 40 Molecular Modeling is an Enabling Approach to Complement and Enhance Channelopathy Research.. **2022**, 12, 3141-3166
- 39 State-of-the-Art Estimation of Protein Model Accuracy using AlphaFold. 4
- 38 Predictive Method for Interhelical Contacts in Alpha-Helical Proteins. **2008**, 3023-3031
- 37 Data_Sheet_1.pdf. **2019**,
- 36 Matching protein surface structural patches for high-resolution blind peptide docking.. **2022**, 119, e2121153119
- 35 Finding protein sites using machine learning methods. **2003**, 23, 5-11
- 34 Different methods, techniques and their limitations in protein structure prediction: A review.. **2022**, 2

| | | |
|----|--|---|
| 33 | De Novo RNA Tertiary Structure Prediction at Atomic Resolution Using Geometric Potentials from Deep Learning. | 2 |
| 32 | Deep learning geometrical potential for high-accuracy ab initio protein structure prediction. 2022 , 25, 104425 | 0 |
| 31 | Combination of genetic algorithm and generalised-ensemble algorithms for biomolecular simulations. 2022 , 93-109 | |
| 30 | Modeling of protein conformational changes with Rosetta guided by limited experimental data. 2022 , | 0 |
| 29 | Understanding the interactions between bone mineral crystals and their binding peptides derived from filamentous phage. 2022 , 15, 100263 | 0 |
| 28 | Protein shape sampled by ion mobility mass spectrometry consistently improves protein structure prediction. 2022 , 13, | 2 |
| 27 | Construction of a Deep Neural Network Energy Function for Protein Physics. | 1 |
| 26 | Modeling protein structure as a stable static equilibrium. 2022 , 106, | |
| 25 | I-TASSER-MTD: a deep-learning-based platform for multi-domain protein structure and function prediction. | 2 |
| 24 | Protein Design: From the Aspect of Water Solubility and Stability. | 7 |
| 23 | StarMap: a user-friendly workflow for Rosetta-driven molecular structure refinement. | 0 |
| 22 | Modeling and simulation of peptides. 2023 , 35-56 | 0 |
| 21 | Cyclic Peptide Screening Methods for Preclinical Drug Discovery. 2022 , 65, 11913-11926 | 1 |
| 20 | Folding Coarse-Grained Oligomer Models with PyRosetta. | 0 |
| 19 | Fast and accurate Ab Initio Protein structure prediction using deep learning potentials. 2022 , 18, e1010539 | 0 |
| 18 | Pseudocontact shift NMR data obtained from a non-canonical amino acid-linked lanthanide tag improves integral membrane protein structure prediction. | 0 |
| 17 | Prediction of Intrinsic Disorder Using Rosetta ResidueDisorder and AlphaFold2. 2022 , 126, 8439-8446 | 2 |
| 16 | ProteinProtein Interaction Modelling with the Fragment Molecular Orbital Method. 2023 , 295-305 | 0 |

| | | |
|----|---|---|
| 15 | In Silico Protein Folding Prediction of COVID-19 Mutations and Variants. 2022 , 12, 1665 | 0 |
| 14 | CADD, AI and ML in Drug Discovery: A Comprehensive Review. 2022 , 106324 | 2 |
| 13 | Prediction of protein structure and intrinsic disorder in the era of deep learning. 2023 , 199-224 | 0 |
| 12 | A Peptides Prediction Methodology with Fragments and CNN for Tertiary Structure Based on GRSA2. 2022 , 11, 729 | 0 |
| 11 | Artificial intelligence for template-free protein structure prediction: a comprehensive review. | 0 |
| 10 | Illuminating protein space with a programmable generative model. | 1 |
| 9 | The buckling-condensation mechanism driving gas vesicle collapse. | 0 |
| 8 | Critical Assessment of Methods for Predicting the 3D Structure of Proteins and Protein Complexes. 2023 , 52, | 0 |
| 7 | A probabilistic view of protein stability, conformational specificity, and design. | 0 |
| 6 | Protein Structure Determination using Sparse NMR Data. 2012 , 84-110 | 0 |
| 5 | Sparse pseudocontact shift NMR data obtained from a non-canonical amino acid-linked lanthanide tag improves integral membrane protein structure prediction. | 0 |
| 4 | Network of hotspot interactions cluster tau amyloid folds. 2023 , 14, | 0 |
| 3 | Computational strategies and tools for protein tertiary structure prediction. 2023 , 225-242 | 0 |
| 2 | Protein Structure Prediction: Challenges, Advances, and the Shift of Research Paradigms. 2023 , | 0 |
| 1 | Recent Advances in NMR Protein Structure Prediction with ROSETTA. 2023 , 24, 7835 | 0 |