# Ruth Nussinov

## List of Publications by Citations



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|---|---|---|---|
| 291 papers | 23,721 citations | 74 h-index | 147 g-index |
| 323 ext. papers | 27,816 ext. citations | 8.1 avg, IF | 7.54 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 291 | PatchDock and SymmDock: servers for rigid and symmetric docking. *Nucleic Acids Research*, **2005**, 33, W363-7 | 20.1 | 1963 |
| 290 | The role of dynamic conformational ensembles in biomolecular recognition. *Nature Chemical Biology*, **2009**, 5, 789-96 | 11.7 | 1420 |
| 289 | Is allostery an intrinsic property of all dynamic proteins?. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 433-43 | 4.2 | 669 |
| 288 | Induced fit, conformational selection and independent dynamic segments: an extended view of binding events. *Trends in Biochemical Sciences*, **2010**, 35, 539-46 | 10.3 | 617 |
| 287 | Structure and dynamics of molecular networks: a novel paradigm of drug discovery: a comprehensive review. *Pharmacology & Therapeutics*, **2013**, 138, 333-408 | 13.9 | 604 |
| 286 | Folding funnels, binding funnels, and protein function. *Protein Science*, **1999**, 8, 1181-90 | 6.3 | 571 |
| 285 | A[1-42) fibril structure illuminates self-recognition and replication of amyloid in Alzheimer's disease. *Nature Structural and Molecular Biology*, **2015**, 22, 499-505 | 17.6 | 550 |
| 284 | Folding and binding cascades: dynamic landscapes and population shifts. *Protein Science*, **2000**, 9, 10-9 | 6.3 | 474 |
| 283 | FireDock: a web server for fast interaction refinement in molecular docking. *Nucleic Acids Research*, **2008**, 36, W229-32 | 20.1 | 469 |
| 282 | FireDock: fast interaction refinement in molecular docking. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 139-59 | 4.2 | 468 |
| 281 | Principles of protein-protein interactions: what are the preferred ways for proteins to interact?. *Chemical Reviews*, **2008**, 108, 1225-44 | 68.1 | 463 |
| 280 | Folding funnels and binding mechanisms. *Protein Engineering, Design and Selection*, **1999**, 12, 713-20 | 1.9 | 451 |
| 279 | Allostery in disease and in drug discovery. *Cell*, **2013**, 153, 293-305 | 56.2 | 447 |
| 278 | Hot regions in protein--protein interactions: the organization and contribution of structurally conserved hot spot residues. *Journal of Molecular Biology*, **2005**, 345, 1281-94 | 6.5 | 394 |
| 277 | Multiple diverse ligands binding at a single protein site: a matter of pre-existing populations. *Protein Science*, **2002**, 11, 184-97 | 6.3 | 321 |
| 276 | Studies of protein-protein interfaces: a statistical analysis of the hydrophobic effect. *Protein Science*, **1997**, 6, 53-64 | 6.3 | 313 |
| 275 | The origin of allosteric functional modulation: multiple pre-existing pathways. *Structure*, **2009**, 17, 1042-50 | 5.2 | 309 |

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| 274 | Folding and binding cascades: shifts in energy landscapes. *Proceedings of the National Academy of Sciences of the United States of America*, **1999**, 96, 9970-2 | 11.5 | 307 |
| 273 | Protein allostery, signal transmission and dynamics: a classification scheme of allosteric mechanisms. *Molecular BioSystems*, **2009**, 5, 207-16 | | 278 |
| 272 | A unified view of "how allostery works". *PLoS Computational Biology*, **2014**, 10, e1003394 | 5 | 262 |
| 271 | Polymorphism in Alzheimer Abeta amyloid organization reflects conformational selection in a rugged energy landscape. *Chemical Reviews*, **2010**, 110, 4820-38 | 68.1 | 239 |
| 270 | Efficient detection of three-dimensional structural motifs in biological macromolecules by computer vision techniques. *Proceedings of the National Academy of Sciences of the United States of America*, **1991**, 88, 10495-9 | 11.5 | 225 |
| 269 | Conservation of polar residues as hot spots at protein interfaces **2000**, 39, 331-342 | | 224 |
| 268 | Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. *Chemical Reviews*, **2016**, 116, 6516-51 | 68.1 | 221 |
| 267 | The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. *Chemical Reviews*, **2016**, 116, 6391-423 | 68.1 | 213 |
| 266 | Ras Conformational Ensembles, Allostery, and Signaling. *Chemical Reviews*, **2016**, 116, 6607-65 | 68.1 | 199 |
| 265 | deepDR: a network-based deep learning approach to in silico drug repositioning. *Bioinformatics*, **2019**, 35, 5191-5198 | 7.2 | 194 |
| 264 | Artificial intelligence in COVID-19 drug repurposing. *The Lancet Digital Health*, **2020**, 2, e667-e676 | 14.4 | 188 |
| 263 | Structured disorder and conformational selection. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 418-27 | 4.2 | 173 |
| 262 | Dynamic allostery: linkers are not merely flexible. *Structure*, **2011**, 19, 907-17 | 5.2 | 171 |
| 261 | Allostery and population shift in drug discovery. *Current Opinion in Pharmacology*, **2010**, 10, 715-22 | 5.1 | 163 |
| 260 | Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578 | 5.2 | 158 |
| 259 | Allosteric effects of the oncogenic RasQ61L mutant on Raf-RBD. *Structure*, **2015**, 23, 505-516 | 5.2 | 156 |
| 258 | Allosteric post-translational modification codes. *Trends in Biochemical Sciences*, **2012**, 37, 447-55 | 10.3 | 152 |
| 257 | GTP-Dependent K-Ras Dimerization. *Structure*, **2015**, 23, 1325-35 | 5.2 | 145 |

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| 256 | Allostery without a conformational change? Revisiting the paradigm. *Current Opinion in Structural Biology*, **2015**, 30, 17-24 | 8.1 | 137 |
| 255 | The underappreciated role of allostery in the cellular network. *Annual Review of Biophysics*, **2013**, 42, 169-89 | 21.1 | 137 |
| 254 | Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67 | 5.2 | 131 |
| 253 | A set of van der Waals and coulombic radii of protein atoms for molecular and solvent-accessible surface calculation, packing evaluation, and docking. *Proteins: Structure, Function and Bioinformatics* , **1998**, 32, 111-127 | 4.2 | 131 |
| 252 | Electrostatic strengths of salt bridges in thermophilic and mesophilic glutamate dehydrogenase monomers. *Proteins: Structure, Function and Bioinformatics*, **2000**, 38, 368-83 | 4.2 | 128 |
| 251 | Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. *Chemical Reviews*, **2021**, 121, 2545-2647 | 68.1 | 128 |
| 250 | PRISM: a web server and repository for prediction of protein-protein interactions and modeling their 3D complexes. *Nucleic Acids Research*, **2014**, 42, W285-9 | 20.1 | 126 |
| 249 | Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. *PLoS Computational Biology*, **2016**, 12, e1004619 | 5 | 124 |
| 248 | Similar binding sites and different partners: implications to shared proteins in cellular pathways. *Structure*, **2007**, 15, 341-54 | 5.2 | 114 |
| 247 | A computer vision based technique for 3-D sequence-independent structural comparison of proteins. *Protein Engineering, Design and Selection*, **1993**, 6, 279-88 | 1.9 | 114 |
| 246 | Allo-network drugs: harnessing allostery in cellular networks. *Trends in Pharmacological Sciences*, **2011**, 32, 686-93 | 13.2 | 113 |
| 245 | Thermodynamic differences among homologous thermophilic and mesophilic proteins. *Biochemistry*, **2001**, 40, 14152-65 | 3.2 | 113 |
| 244 | Shape complementarity at protein-protein interfaces. *Biopolymers*, **1994**, 34, 933-40 | 2.2 | 113 |
| 243 | Drugging Ras GTPase: a comprehensive mechanistic and signaling structural view. *Chemical Society Reviews*, **2016**, 45, 4929-52 | 58.5 | 113 |
| 242 | Protein-protein interaction networks: how can a hub protein bind so many different partners?. *Trends in Biochemical Sciences*, **2009**, 34, 594-600 | 10.3 | 111 |
| 241 | Topological properties of protein interaction networks from a structural perspective. *Biochemical Society Transactions*, **2008**, 36, 1398-403 | 5.1 | 111 |
| 240 | Hydrophobic folding units at protein-protein interfaces: implications to protein folding and to protein-protein association. *Protein Science*, **1997**, 6, 1426-37 | 6.3 | 101 |
| 239 | Examination of shape complementarity in docking of Unbound proteins **1999**, 36, 307-317 | | 101 |

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| 238 | An integrated suite of fast docking algorithms. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3197-204 | 4.2 | 100 |
| 237 | Unraveling structural mechanisms of allosteric drug action. *Trends in Pharmacological Sciences*, **2014**, 35, 256-64 | 13.2 | 97 |
| 236 | Principles of allosteric interactions in cell signaling. *Journal of the American Chemical Society*, **2014**, 136, 17692-701 | 16.4 | 97 |
| 235 | Flexible docking allowing induced fit in proteins: Insights from an open to closed conformational isomers. *Proteins: Structure, Function and Bioinformatics*, **1998**, 32, 159-174 | 4.2 | 96 |
| 234 | The Structural Basis of Oncogenic Mutations G12, G13 and Q61 in Small GTPase K-Ras4B. *Scientific Reports*, **2016**, 6, 21949 | 4.9 | 95 |
| 233 | Molecular surface representations by sparse critical points. *Proteins: Structure, Function and Bioinformatics*, **1994**, 18, 94-101 | 4.2 | 94 |
| 232 | Protein-protein interfaces: architectures and interactions in protein-protein interfaces and in protein cores. Their similarities and differences. *Critical Reviews in Biochemistry and Molecular Biology*, **1996**, 31, 127-52 | 8.7 | 92 |
| 231 | Target identification among known drugs by deep learning from heterogeneous networks. *Chemical Science*, **2020**, 11, 1775-1797 | 9.4 | 91 |
| 230 | Mutations in LZTR1 drive human disease by dysregulating RAS ubiquitination. *Science*, **2018**, 362, 1177-1182 | 37.5 | 87 |
| 229 | Synergistic interactions between repeats in tau protein and A□amyloids may be responsible for accelerated aggregation via polymorphic states. *Biochemistry*, **2011**, 50, 5172-81 | 3.2 | 83 |
| 228 | Mechanisms of membrane binding of small GTPase K-Ras4B farnesylated hypervariable region. *Journal of Biological Chemistry*, **2015**, 290, 9465-77 | 5.4 | 81 |
| 227 | Mechanism and evolution of protein dimerization. *Protein Science*, **1998**, 7, 533-44 | 6.3 | 81 |
| 226 | Multiple conformational selection and induced fit events take place in allosteric propagation. *Biophysical Chemistry*, **2014**, 186, 22-30 | 3.5 | 78 |
| 225 | Three-dimensional, sequence order-independent structural comparison of a serine protease against the crystallographic database reveals active site similarities: potential implications to evolution and to protein folding. *Protein Science*, **1994**, 3, 769-78 | 6.3 | 78 |
| 224 | The design of covalent allosteric drugs. *Annual Review of Pharmacology and Toxicology*, **2015**, 55, 249-67 | 17.9 | 76 |
| 223 | The different ways through which specificity works in orthosteric and allosteric drugs. *Current Pharmaceutical Design*, **2012**, 18, 1311-6 | 3.3 | 74 |
| 222 | Hydrophobic folding units derived from dissimilar monomer structures and their interactions. *Protein Science*, **1997**, 6, 24-42 | 6.3 | 74 |
| 221 | Allosteric effects in the marginally stable von Hippel-Lindau tumor suppressor protein and allostery-based rescue mutant design. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 901-6 | 11.5 | 74 |

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| 220 | A New View of Ras Isoforms in Cancers. *Cancer Research*, **2016**, 76, 18-23 | 10.1 | 71 |
| 219 | Towards inferring time dimensionality in protein-protein interaction networks by integrating structures: the p53 example. *Molecular BioSystems*, **2009**, 5, 1770-8 | | 70 |
| 218 | Folding funnels and conformational transitions via hinge-bending motions. *Cell Biochemistry and Biophysics*, **1999**, 31, 141-64 | 3.2 | 70 |
| 217 | An efficient automated computer vision based technique for detection of three dimensional structural motifs in proteins. *Journal of Biomolecular Structure and Dynamics*, **1992**, 9, 769-89 | 3.6 | 69 |
| 216 | Membrane-associated Ras dimers are isoform-specific: K-Ras dimers differ from H-Ras dimers. *Biochemical Journal*, **2016**, 473, 1719-32 | 3.8 | 68 |
| 215 | The Architecture of the TIR Domain Signalosome in the Toll-like Receptor-4 Signaling Pathway. *Scientific Reports*, **2015**, 5, 13128 | 4.9 | 67 |
| 214 | Selective molecular recognition in amyloid growth and transmission and cross-species barriers. *Journal of Molecular Biology*, **2012**, 421, 172-84 | 6.5 | 66 |
| 213 | Structural motifs at protein-protein interfaces: protein cores versus two-state and three-state model complexes. *Protein Science*, **1997**, 6, 1793-805 | 6.3 | 66 |
| 212 | The Key Role of Calmodulin in KRAS-Driven Adenocarcinomas. *Molecular Cancer Research*, **2015**, 13, 1265-73 | 6.6 | 65 |
| 211 | Oncogenic Ras Isoforms Signaling Specificity at the Membrane. *Cancer Research*, **2018**, 78, 593-602 | 10.1 | 65 |
| 210 | Structural Insight into Tau Protein's Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. *Journal of Physical Chemistry Letters*, **2014**, 5, 3026-3031 | 6.4 | 65 |
| 209 | Amylin-A□bligomers at atomic resolution using molecular dynamics simulations: a link between Type 2 diabetes and Alzheimer's disease. *Physical Chemistry Chemical Physics*, **2016**, 18, 2330-8 | 3.6 | 63 |
| 208 | Pathogenic Autoreactive T and B Cells Cross-React with Mimotopes Expressed by a Common Human Gut Commensal to Trigger Autoimmunity. *Cell Host and Microbe*, **2019**, 26, 100-113.e8 | 23.4 | 63 |
| 207 | The molecular basis of targeting protein kinases in cancer therapeutics. *Seminars in Cancer Biology*, **2013**, 23, 235-42 | 12.7 | 63 |
| 206 | Surface motifs by a computer vision technique: searches, detection, and implications for protein-ligand recognition. *Proteins: Structure, Function and Bioinformatics*, **1993**, 16, 278-92 | 4.2 | 63 |
| 205 | GTP Binding and Oncogenic Mutations May Attenuate Hypervariable Region (HVR)-Catalytic Domain Interactions in Small GTPase K-Ras4B, Exposing the Effector Binding Site. *Journal of Biological Chemistry*, **2015**, 290, 28887-900 | 5.4 | 60 |
| 204 | How similar are protein folding and protein binding nuclei? Examination of vibrational motions of energy hot spots and conserved residues. *Biophysical Journal*, **2005**, 88, 1552-9 | 2.9 | 60 |
| 203 | The structural basis of ATP as an allosteric modulator. *PLoS Computational Biology*, **2014**, 10, e1003831 | 5 | 59 |

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| 202 | Network-based prediction of drug-target interactions using an arbitrary-order proximity embedded deep forest. *Bioinformatics*, **2020**, 36, 2805-2812 | 7.2 | 58 |
| 201 | Transition-state ensemble in enzyme catalysis: possibility, reality, or necessity?. *Journal of Theoretical Biology*, **2000**, 203, 383-97 | 2.3 | 58 |
| 200 | The higher level of complexity of K-Ras4B activation at the membrane. *FASEB Journal*, **2016**, 30, 1643-55 | 0.9 | 58 |
| 199 | MUSTA--a general, efficient, automated method for multiple structure alignment and detection of common motifs: application to proteins. *Journal of Computational Biology*, **2001**, 8, 93-121 | 1.7 | 57 |
| 198 | High-Affinity Interaction of the K-Ras4B Hypervariable Region with the Ras Active Site. *Biophysical Journal*, **2015**, 109, 2602-2613 | 2.9 | 56 |
| 197 | Conformational basis for asymmetric seeding barrier in filaments of three- and four-repeat tau. *Journal of the American Chemical Society*, **2012**, 134, 10271-8 | 16.4 | 56 |
| 196 | Cross-seeding and conformational selection between three- and four-repeat human Tau proteins. *Journal of Biological Chemistry*, **2012**, 287, 14950-9 | 5.4 | 54 |
| 195 | Allo-network drugs: extension of the allosteric drug concept to protein- protein interaction and signaling networks. *Current Topics in Medicinal Chemistry*, **2013**, 13, 64-77 | 3 | 54 |
| 194 | Contribution of salt bridges toward protein thermostability. *Journal of Biomolecular Structure and Dynamics*, **2000**, 17 Suppl 1, 79-85 | 3.6 | 54 |
| 193 | Computational network biology: Data, models, and applications. *Physics Reports*, **2020**, 846, 1-66 | 27.7 | 54 |
| 192 | Non-redundant unique interface structures as templates for modeling protein interactions. *PLoS ONE*, **2014**, 9, e86738 | 3.7 | 53 |
| 191 | The structural network of inflammation and cancer: merits and challenges. *Seminars in Cancer Biology*, **2013**, 23, 243-51 | 12.7 | 52 |
| 190 | Protein folding: binding of conformationally fluctuating building blocks via population selection. *Critical Reviews in Biochemistry and Molecular Biology*, **2001**, 36, 399-433 | 8.7 | 52 |
| 189 | An overview of recent advances in structural bioinformatics of protein-protein interactions and a guide to their principles. *Progress in Biophysics and Molecular Biology*, **2014**, 116, 141-50 | 4.7 | 51 |
| 188 | Automated multiple structure alignment and detection of a common substructural motif. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 235-45 | 4.2 | 51 |
| 187 | 'Latent drivers' expand the cancer mutational landscape. *Current Opinion in Structural Biology*, **2015**, 32, 25-32 | 8.1 | 50 |
| 186 | 'Pathway drug cocktail': targeting Ras signaling based on structural pathways. *Trends in Molecular Medicine*, **2013**, 19, 695-704 | 11.5 | 49 |
| 185 | A New View of Pathway-Driven Drug Resistance in Tumor Proliferation. *Trends in Pharmacological Sciences*, **2017**, 38, 427-437 | 13.2 | 47 |

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| 184 | The Mechanism of ATP-Dependent Allosteric Protection of Akt Kinase Phosphorylation. *Structure*, **2015**, 23, 1725-1734 | 5.2 | 47 |
| 183 | Fluctuations in ion pairs and their stabilities in proteins. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 433-54 | 4.2 | 47 |
| 182 | PI3K inhibitors: review and new strategies. *Chemical Science*, **2020**, 11, 5855-5865 | 9.4 | 46 |
| 181 | Raf-1 Cysteine-Rich Domain Increases the Affinity of K-Ras/Raf at the Membrane, Promoting MAPK Signaling. *Structure*, **2018**, 26, 513-525.e2 | 5.2 | 46 |
| 180 | Inhibitors of Ras-SOS Interactions. *ChemMedChem*, **2016**, 11, 814-21 | 3.7 | 46 |
| 179 | The mechanism of PI3K activation at the atomic level. *Chemical Science*, **2019**, 10, 3671-3680 | 9.4 | 45 |
| 178 | Review: Precision medicine and driver mutations: Computational methods, functional assays and conformational principles for interpreting cancer drivers. *PLoS Computational Biology*, **2019**, 15, e1006658 | 5 | 45 |
| 177 | Calmodulin and PI3K Signaling in Cancers. *Trends in Cancer*, **2017**, 3, 214-224 | 12.5 | 43 |
| 176 | Allosteric conformational barcodes direct signaling in the cell. *Structure*, **2013**, 21, 1509-21 | 5.2 | 43 |
| 175 | Oncogenic KRAS signaling and YAP1/ catenin: Similar cell cycle control in tumor initiation. *Seminars in Cell and Developmental Biology*, **2016**, 58, 79-85 | 7.5 | 43 |
| 174 | A 3D sequence-independent representation of the protein data bank. *Protein Engineering, Design and Selection*, **1995**, 8, 981-97 | 1.9 | 42 |
| 173 | A broad view of scaffolding suggests that scaffolding proteins can actively control regulation and signaling of multienzyme complexes through allostery. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2013**, 1834, 820-9 | 4 | 41 |
| 172 | The structural pathway of interleukin 1 (IL-1) initiated signaling reveals mechanisms of oncogenic mutations and SNPs in inflammation and cancer. *PLoS Computational Biology*, **2014**, 10, e1003470 | 5 | 40 |
| 171 | Phosphorylated Calmodulin Promotes PI3K Activation by Binding to the SH Domains. *Biophysical Journal*, **2017**, 113, 1956-1967 | 2.9 | 39 |
| 170 | Mechanisms of recognition of amyloid- [A] monomer, oligomer, and fibril by homologous antibodies. *Journal of Biological Chemistry*, **2017**, 292, 18325-18343 | 5.4 | 38 |
| 169 | A Structural View of Negative Regulation of the Toll-like Receptor-Mediated Inflammatory Pathway. *Biophysical Journal*, **2015**, 109, 1214-26 | 2.9 | 37 |
| 168 | Hydrophobic interactions in the major groove can influence DNA local structure. *Journal of Biomolecular Structure and Dynamics*, **1986**, 4, 41-8 | 3.6 | 37 |
| 167 | The disordered hypervariable region and the folded catalytic domain of oncogenic K-Ras4B partner in phospholipid binding. *Current Opinion in Structural Biology*, **2016**, 36, 10-7 | 8.1 | 35 |

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| 166 | Amplification of signaling via cellular allosteric relay and protein disorder. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 6887-8 | 11.5 | 35 |
| 165 | Structural host-microbiota interaction networks. *PLoS Computational Biology*, **2017**, 13, e1005579 | 5 | 35 |
| 164 | Flexible-body motions of calmodulin and the farnesylated hypervariable region yield a high-affinity interaction enabling K-Ras4B membrane extraction. *Journal of Biological Chemistry*, **2017**, 292, 12544-12559 | 5.4 | 34 |
| 163 | Intrinsic protein disorder in oncogenic KRAS signaling. *Cellular and Molecular Life Sciences*, **2017**, 74, 3245-3261 | 6.3 | 34 |
| 162 | Al Stretching-and-Packing Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. *Journal of Physical Chemistry Letters*, **2015**, 6, 3276-3282 | 6.4 | 34 |
| 161 | Comparison of the Conformations of KRAS Isoforms, K-Ras4A and K-Ras4B, Points to Similarities and Significant Differences. *Journal of Physical Chemistry B*, **2016**, 120, 667-79 | 3.4 | 34 |
| 160 | The free energy landscape in translational science: how can somatic mutations result in constitutive oncogenic activation?. *Physical Chemistry Chemical Physics*, **2014**, 16, 6332-41 | 3.6 | 34 |
| 159 | The spatial structure of cell signaling systems. *Physical Biology*, **2013**, 10, 045004 | 3 | 34 |
| 158 | Oligomerization and nanocluster organization render specificity. *Biological Reviews*, **2015**, 90, 587-98 | 13.5 | 34 |
| 157 | Principles of docking: An overview of search algorithms and a guide to scoring functions **2002**, 47, 409 | | 34 |
| 156 | Pathogen mimicry of host protein-protein interfaces modulates immunity. *Seminars in Cell and Developmental Biology*, **2016**, 58, 136-45 | 7.5 | 33 |
| 155 | Single mutations in tau modulate the populations of fibril conformers through seed selection. *Angewandte Chemie - International Edition*, **2014**, 53, 1590-3 | 16.4 | 33 |
| 154 | The structural basis for cancer treatment decisions. *Oncotarget*, **2014**, 5, 7285-302 | 3.3 | 33 |
| 153 | Gene-specific transcription activation via long-range allosteric shape-shifting. *Biochemical Journal*, **2011**, 439, 15-25 | 3.8 | 32 |
| 152 | Principles of K-Ras effector organization and the role of oncogenic K-Ras in cancer initiation through G1 cell cycle deregulation. *Expert Review of Proteomics*, **2015**, 12, 669-82 | 4.2 | 31 |
| 151 | Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. *PLoS Computational Biology*, **2015**, 11, e1004470 | 5 | 31 |
| 150 | Molecular insights into the reversible formation of tau protein fibrils. *Chemical Communications*, **2013**, 49, 3582-4 | 5.8 | 31 |
| 149 | Energetic redistribution in allostery to execute protein function. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7480-7482 | 11.5 | 30 |

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| 148 | A disulphide-reinforced structural scaffold shared by small proteins with diverse functions. *Nature Structural Biology*, **1995**, 2, 835-7 | | 30 |
| 147 | Antigen binding allosterically promotes Fc receptor recognition. *MAbs*, **2019**, 11, 58-74 | 6.6 | 30 |
| 146 | Personal Mutanomes Meet Modern Oncology Drug Discovery and Precision Health. *Pharmacological Reviews*, **2019**, 71, 1-19 | 22.5 | 30 |
| 145 | Is Nanoclustering essential for all oncogenic KRas pathways? Can it explain why wild-type KRas can inhibit its oncogenic variant?. *Seminars in Cancer Biology*, **2019**, 54, 114-120 | 12.7 | 30 |
| 144 | Conformational ensembles, signal transduction and residue hot spots: application to drug discovery. *Current Opinion in Drug Discovery & Development*, **2010**, 13, 527-37 | | 30 |
| 143 | K-Ras4B/calmodulin/PI3K□A promising new adenocarcinoma-specific drug target?. *Expert Opinion on Therapeutic Targets*, **2016**, 20, 831-42 | 6.4 | 29 |
| 142 | Does Ras Activate Raf and PI3K Allosterically?. *Frontiers in Oncology*, **2019**, 9, 1231 | 5.3 | 29 |
| 141 | Autoinhibition in Ras effectors Raf, PI3K□and RASSF5: a comprehensive review underscoring the challenges in pharmacological intervention. *Biophysical Reviews*, **2018**, 10, 1263-1282 | 3.7 | 29 |
| 140 | The structural basis for Ras activation of PI3K□lipid kinase. *Physical Chemistry Chemical Physics*, **2019**, 21, 12021-12028 | 3.6 | 28 |
| 139 | Peptide-MHC (pMHC) binding to a human antiviral T cell receptor induces long-range allosteric communication between pMHC- and CD3-binding sites. *Journal of Biological Chemistry*, **2018**, 293, 15991-16005 | 5.4 | 27 |
| 138 | Dimerization of the SP1 Region of HIV-1 Gag Induces a Helical Conformation and Association into Helical Bundles: Implications for Particle Assembly. *Journal of Virology*, **2016**, 90, 1773-87 | 6.6 | 26 |
| 137 | The role of allostery in the ubiquitin-proteasome system. *Critical Reviews in Biochemistry and Molecular Biology*, **2013**, 48, 89-97 | 8.7 | 26 |
| 136 | Plasma membrane regulates Ras signaling networks. *Cellular Logistics*, **2015**, 5, e1136374 | | 26 |
| 135 | Fluctuations between stabilizing and destabilizing electrostatic contributions of ion pairs in conformers of the c-Myc-Max leucine zipper. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 485-497 | 4.2 | 26 |
| 134 | Precision medicine review: rare driver mutations and their biophysical classification. *Biophysical Reviews*, **2019**, 11, 5-19 | 3.7 | 26 |
| 133 | The quaternary assembly of KRas4B with Raf-1 at the membrane. *Computational and Structural Biotechnology Journal*, **2020**, 18, 737-748 | 6.8 | 26 |
| 132 | Familial Mutations May Switch Conformational Preferences in □Synuclein Fibrils. *ACS Chemical Neuroscience*, **2017**, 8, 837-849 | 5.7 | 25 |
| 131 | Protein ensembles link genotype to phenotype. *PLoS Computational Biology*, **2019**, 15, e1006648 | 5 | 25 |

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| 130 | Free energy diagrams for protein function. *Chemistry and Biology*, **2014**, 21, 311-8 | | 25 |
| 129 | Flexible structural comparison allowing hinge-bending, swiveling motions. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 232-54 | 4.2 | 25 |
| 128 | Harnessing endophenotypes and network medicine for Alzheimer's drug repurposing. *Medicinal Research Reviews*, **2020**, 40, 2386-2426 | 14.4 | 25 |
| 127 | Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. *Journal of Biological Chemistry*, **2018**, 293, 17336-17348 | 5.4 | 25 |
| 126 | Structural Modeling of GR Interactions with the SWI/SNF Chromatin Remodeling Complex and C/EBP. *Biophysical Journal*, **2015**, 109, 1227-39 | 2.9 | 24 |
| 125 | Unraveling the molecular mechanism of interactions of the Rho GTPases Cdc42 and Rac1 with the scaffolding protein IQGAP2. *Journal of Biological Chemistry*, **2018**, 293, 3685-3699 | 5.4 | 24 |
| 124 | RASSF5: An MST activator and tumor suppressor in vivo but opposite in vitro. *Current Opinion in Structural Biology*, **2016**, 41, 217-224 | 8.1 | 24 |
| 123 | Dynamic multiprotein assemblies shape the spatial structure of cell signaling. *Progress in Biophysics and Molecular Biology*, **2014**, 116, 158-64 | 4.7 | 24 |
| 122 | A Systems Pharmacology Approach Uncovers Wogonoside as an Angiogenesis Inhibitor of Triple-Negative Breast Cancer by Targeting Hedgehog Signaling. *Cell Chemical Biology*, **2019**, 26, 1143-1158.e6 | 8.2 | 23 |
| 121 | How Does Hyperphopsphorylation Promote Tau Aggregation and Modulate Filament Structure and Stability?. *ACS Chemical Neuroscience*, **2016**, 7, 565-75 | 5.7 | 23 |
| 120 | Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 1818-1825 | 3.8 | 22 |
| 119 | Promiscuous and specific recognition among ephrins and Eph receptors. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2014**, 1844, 1729-40 | 4 | 22 |
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