Attila Gursoy

List of Publications by Year in descending order

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130 papers	8,956 citations	81743 39 h-index	43802 91 g-index
138 all docs	138 docs citations	138 times ranked	9135 citing authors

#	Article	IF	Citations
1	Artificial intelligence based methods for hot spot prediction. Current Opinion in Structural Biology, 2022, 72, 209-218.	2.6	16
2	Artificial intelligence approaches to human-microbiome proteinâ€“protein interactions. Current Opinion in Structural Biology, 2022, 73, 102328.	2.6	13
3	Is Persistent Post-COVID Headache Associated With Protein-Protein Interactions Between Antibodies Against Viral Spike Protein and CGRP Receptor?: A Case Report. Frontiers in Pain Research, 2022, 3, 858709.	0.9	4
4	SARS-CoV-2 Interactome 3D: A Web interface for 3D visualization and analysis of SARS-CoV-2â€“human mimicry and interactions. Bioinformatics, 2022, 38, 1455-1457.	1.8	3
5	Inhibition of Nonfunctional Ras. Cell Chemical Biology, 2021, 28, 121-133.	2.5	23
6	Neuropsychiatric Symptoms of COVID-19 Explained by SARS-CoV-2 Proteinsâ€™ Mimicry of Human Protein Interactions. Frontiers in Human Neuroscience, 2021, 15, 656313.	1.0	41
7	Mechanistic Differences of Activation of Rac1^{P29S} and Rac1^{A159V}. Journal of Physical Chemistry B, 2021, 125, 3790-3802.	1.2	9
8	The structural basis of Akt PH domain interaction with calmodulin. Biophysical Journal, 2021, 120, 1994-2008.	0.2	10
9	Normal Mode Analysis of KRas4B Reveals Partner Specific Dynamics. Journal of Physical Chemistry B, 2021, 125, 5210-5221.	1.2	7
10	Interactome analysis of Bag-1 isoforms reveals novel interaction partners in endoplasmic reticulum-associated degradation. PLoS ONE, 2021, 16, e0256640.	1.1	3
11	Examining the stability of binding modes of the co-crystallized inhibitors of human HDAC8 by molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1-10.	2.0	12
12	Identification of potential inhibitors of human methionine aminopeptidase (type II) for cancer therapy: Structure-based virtual screening, ADMET prediction and molecular dynamics studies. Computational Biology and Chemistry, 2020, 86, 107244.	1.1	15
13	HMI-PRED: A Web Server for Structural Prediction of Host-Microbe Interactions Based on Interface Mimicry. Journal of Molecular Biology, 2020, 432, 3395-3403.	2.0	34
14	Oncogenic K-Ras4B Dimerization Enhances Downstream Mitogen-activated Protein Kinase Signaling. Journal of Molecular Biology, 2020, 432, 1199-1215.	2.0	16
15	Beyond the heterodimer model for mineralocorticoid and glucocorticoid receptor interactions in nuclei and at DNA. PLoS ONE, 2020, 15, e0227520.	1.1	36
16	Embedding Alternative Conformations of Proteins in Proteinâ€“Protein Interaction Networks. Methods in Molecular Biology, 2020, 2074, 113-124.	0.4	9
17	Androgen receptor-binding sites are highly mutated in prostate cancer. Nature Communications, 2020, 11, 832.	5.8	44
18	Mutational effects on proteinâ€“protein interactions. , 2020, , 109-143.		3

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19	Intelligent Edge Computing: State-of-the-art Techniques and Applications. , 2020, , .		0
20	Head and Neck Cancers Promote an Inflammatory Transcriptome through Coactivation of Classic and Alternative NF-Î²B Pathways. Cancer Immunology Research, 2019, 7, 1760-1774.	1.6	17
21	3D spatial organization and network-guided comparison of mutation profiles in Glioblastoma reveals similarities across patients. PLoS Computational Biology, 2019, 15, e1006789.	1.5	11
22	Cryptochrome deletion in p53 mutant mice enhances apoptotic and anti-tumorigenic responses to UV damage at the transcriptome level. Functional and Integrative Genomics, 2019, 19, 729-742.	1.4	9
23	Developments in integrative modeling with dynamical interfaces. Current Opinion in Structural Biology, 2019, 56, 11-17.	2.6	14
24	Methods for Discovering and Targeting Druggable Protein-Protein Interfaces and Their Application to Repurposing. Methods in Molecular Biology, 2019, 1903, 1-21.	0.4	29
25	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.	1.6	36
26	Analysis of single amino acid variations in singlet hot spots of proteinâ€“protein interfaces. Bioinformatics, 2018, 34, i795-i801.	1.8	22
27	Arl2-Mediated Allosteric Release of Farnesylated KRas4B from Shuttling Factor PDEÎ´. Journal of Physical Chemistry B, 2018, 122, 7503-7513.	1.2	12
28	Abstract 3412: Androgen receptor binding sites are highly mutated in prostate cancer. , 2018, , .		0
29	PDEÎ´ Binding to Ras Isoforms Provides a Route to Proper Membrane Localization. Journal of Physical Chemistry B, 2017, 121, 5917-5927.	1.2	26
30	Relation between Protein Intrinsic Normal Mode Weights and Pre-Existing Conformer Populations. Journal of Physical Chemistry B, 2017, 121, 3686-3700.	1.2	6
31	Enriching Traditional Protein-protein Interaction Networks with Alternative Conformations of Proteins. Scientific Reports, 2017, 7, 7180.	1.6	15
32	Topological, functional, and structural analyses of protein-protein interaction networks of breast cancer lung and brain metastases. , 2017, , .		1
33	Prediction of Protein Interactions by Structural Matching: Prediction of PPI Networks and the Effects of Mutations on PPIs that Combines Sequence and Structural Information. Methods in Molecular Biology, 2017, 1558, 255-270.	0.4	6
34	TRAF3 signaling: Competitive binding and evolvability of adaptive viral molecular mimicry. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2646-2655.	1.1	30
35	Predicting Proteinâ€“Protein Interactions from the Molecular to the Proteome Level. Chemical Reviews, 2016, 116, 4884-4909.	23.0	289
36	PRISM-EM: template interface-based modelling of multi-protein complexes guided by cryo-electron microscopy density maps. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1137-1148.	1.1	17

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37	The potential impact of recent developments in three-dimensional quantitative interaction proteomics on structural biology. Expert Review of Proteomics, 2016, 13, 447-449.	1.3	2
38	Membrane-associated Ras dimers are isoform-specific: K-Ras dimers differ from H-Ras dimers. Biochemical Journal, 2016, 473, 1719-1732.	1.7	92
39	Ras Conformational Ensembles, Allostery, and Signaling. Chemical Reviews, 2016, 116, 6607-6665.	23.0	290
40	K-Ras4B/calmodulin/PI3KÎ±: A promising new adenocarcinoma-specific drug target?. Expert Opinion on Therapeutic Targets, 2016, 20, 831-842.	1.5	29
41	Abstract 81: RNA-seq, exome-seq, functional RNAi screening and bioinformatics analyses identify molecules promoting aberrant activation of classical and alternative NF-kB pathways in head and neck cell lines. , 2016, , .		0
42	The Architecture of the TIR Domain Signalosome in the Toll-like Receptor-4 Signaling Pathway. Scientific Reports, 2015, 5, 13128.	1.6	98
43	Plasma membrane regulates Ras signaling networks. Cellular Logistics, 2015, 5, e1136374.	0.9	35
44	GTP-Dependent K-Ras Dimerization. Structure, 2015, 23, 1325-1335.	1.6	187
45	The Key Role of Calmodulin in KRAS-Driven Adenocarcinomas. Molecular Cancer Research, 2015, 13, 1265-1273.	1.5	72
46	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, 669-682.	1.3	37
47	A Structural View of Negative Regulation of the Toll-like Receptor-Mediated Inflammatory Pathway. Biophysical Journal, 2015, 109, 1214-1226.	0.2	62
48	Structural Modeling of GR Interactions with the SWI/SNF Chromatin Remodeling Complex and C/EBP. Biophysical Journal, 2015, 109, 1227-1239.	0.2	31
49	Advances in template-based protein docking by utilizing interfaces towards completing structural interactome. Current Opinion in Structural Biology, 2015, 35, 87-92.	2.6	24
50	Taming Oncogenic Signaling at Protein Interfaces: Challenges and Opportunities. Current Topics in Medicinal Chemistry, 2015, 15, 2005-2018.	1.0	8
51	Abstract 1111: Altered inflammatory and death pathways in head and neck cell lines model genomic and expression signatures identified in The Cancer Genome Atlas. , 2015, , .		0
52	Structural Pathways of Cytokines May Illuminate Their Roles in Regulation of Cancer Development and Immunotherapy. Cancers, 2014, 6, 663-683.	1.7	18
53	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.	1.5	63
54	PRISM: a web server and repository for prediction of proteinâ€“protein interactions and modeling their 3D complexes. Nucleic Acids Research, 2014, 42, W285-W289.	6.5	187

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55	Hot spots in proteinâ€“protein interfaces: Towards drug discovery. Progress in Biophysics and Molecular Biology, 2014, 116, 165-173.	1.4	140
56	Modeling Protein Assemblies in the Proteome. Molecular and Cellular Proteomics, 2014, 13, 887-896.	2.5	18
57	The structural network of Interleukin-10 and its implications in inflammation and cancer. BMC Genomics, 2014, 15, S2.	1.2	58
58	Non-Redundant Unique Interface Structures as Templates for Modeling Protein Interactions. PLoS ONE, 2014, 9, e86738.	1.1	66
59	Network-Based Strategies Can Help Mono- and Poly-pharmacology Drug Discovery: A Systems Biology View. Current Pharmaceutical Design, 2014, 20, 1201-1207.	0.9	38
60	Modeling Structural Protein Interaction Networks for Betweenness Analysis. , 2014, , 367-376.		1
61	Abstract 3170: Alternative NF-Î²B pathway activation enhanced by deficient TRAF3 in human papillomavirus (HPV)-associated head and neck cancer. , 2014, , .		0
62	Abstract 3435: Genome-wide RNA and DNA high throughput sequencing reveals proinflammatory and death gene signatures in head and neck squamous cell carcinoma lines with different HPV status. , 2014, , .		0
63	Structural and functional analysis of perforin mutations in association with clinical data of familial hemophagocytic lymphohistiocytosis type 2 (FHL2) patients. Protein Science, 2013, 22, 823-839.	3.1	28
64	Exploiting Conformational Ensembles in Modeling Proteinâ€“Protein Interactions on the Proteome Scale. Journal of Proteome Research, 2013, 12, 2641-2653.	1.8	45
65	The structural network of inflammation and cancer: Merits and challenges. Seminars in Cancer Biology, 2013, 23, 243-251.	4.3	62
66	Identification of Interconnected Markers for T-Cell Acute Lymphoblastic Leukemia. BioMed Research International, 2013, 2013, 1-20.	0.9	5
67	Integrating Structure to Protein-Protein Interaction Networks That Drive Metastasis to Brain and Lung in Breast Cancer. PLoS ONE, 2013, 8, e81035.	1.1	38
68	Emerging Role of the Ubiquitin-proteasome System as Drug Targets. Current Pharmaceutical Design, 2013, 19, 3175-3189.	0.9	16
69	HotRegion: a database of predicted hot spot clusters. Nucleic Acids Research, 2012, 40, D829-D833.	6.5	90
70	Protein-protein Interfaces Integrated into Interaction Networks: Implications on Drug Design. Current Pharmaceutical Design, 2012, 18, 4697-4705.	0.9	17
71	Enriching the human apoptosis pathway by predicting the structures of proteinâ€“protein complexes. Journal of Structural Biology, 2012, 179, 338-346.	1.3	27
72	Human Proteome-scale Structural Modeling of E2â€“E3 Interactions Exploiting Interface Motifs. Journal of Proteome Research, 2012, 11, 1196-1207.	1.8	46

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73	A Strategy Based on Proteinâ€“Protein Interface Motifs May Help in Identifying Drug Off-Targets. Journal of Chemical Information and Modeling, 2012, 52, 2273-2286.	2.5	30
74	Structural Bioinformatics of Proteins: Predicting the Tertiary and Quaternary Structure of Proteins from Sequence. , 2012, , .		1
75	Fast and accurate modeling of proteinâ€“protein interactions by combining templateâ€interfaceâ€based docking with flexible refinement. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1239-1249.	1.5	43
76	Constructing structural networks of signaling pathways on the proteome scale. Current Opinion in Structural Biology, 2012, 22, 367-377.	2.6	61
77	Expanding the Conformational Selection Paradigm in Protein-Ligand Docking. Methods in Molecular Biology, 2012, 819, 59-74.	0.4	11
78	Prediction of Protein-Protein Interactions at Genome Scale. Biophysical Journal, 2011, 100, 386a.	0.2	0
79	Predicting protein-protein interactions on a proteome scale by matching evolutionary and structural similarities at interfaces using PRISM. Nature Protocols, 2011, 6, 1341-1354.	5.5	253
80	Transient protein-protein interactions. Protein Engineering, Design and Selection, 2011, 24, 635-648.	1.0	213
81	Prediction of proteinâ€“protein interactions: unifying evolution and structure at protein interfaces. Physical Biology, 2011, 8, 035006.	0.8	58
82	Structural cooperativity in histone H3 tail modifications. Protein Science, 2011, 20, 1982-1990.	3.1	4
83	Molecular Recognition of H3/H4 Histone Tails by the Tudor Domains of JMJD2A: A Comparative Molecular Dynamics Simulations Study. PLoS ONE, 2011, 6, e14765.	1.1	27
84	A Comparative Molecular Dynamics Study of Methylation State Specificity of JMJD2A. PLoS ONE, 2011, 6, e24664.	1.1	13
85	Analysis of Hot Region Organization in Hub Proteins. Annals of Biomedical Engineering, 2010, 38, 2068-2078.	1.3	37
86	Interaction prediction and classification of PDZ domains. BMC Bioinformatics, 2010, 11, 357.	1.2	44
87	Analysis and network representation of hotspots in protein interfaces using minimum cut trees. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2283-2294.	1.5	58
88	VitAL: Viterbi Algorithm for de novo Peptide Design. PLoS ONE, 2010, 5, e10926.	1.1	32
89	Interaction prediction of PDZ domains using a machine learning approach. , 2010, , .		0
90	Determination of the correspondence between mobility (rigidity) and conservation of the interface residues. , 2010, , .		0

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91	Computational analysis of the binding free energy of H3K9me3 peptide to the tandem tudor domains of JMJD2A. , 2010, , .		0
92	HotPoint: hot spot prediction server for protein interfaces. Nucleic Acids Research, 2010, 38, W402-W406.	6.5	185
93	Allostery and population shift in drug discovery. Current Opinion in Pharmacology, 2010, 10, 715-722.	1.7	176
94	Relation between kinetic conversion rates and ANM mode frequencies. , 2010, , .		0
95	Conformational ensembles, signal transduction and residue hot spots: application to drug discovery. Current Opinion in Drug Discovery & Development, 2010, 13, 527-37.	1.9	34
96	Human Cancer Protein-Protein Interaction Network: A Structural Perspective. PLoS Computational Biology, 2009, 5, e1000601.	1.5	202
97	Conformational energies and entropies of peptides, and the peptideâ€“protein binding problem. Physical Biology, 2009, 6, 036014.	0.8	10
98	Combining Protein-protein Interaction Networks with Structures. Biophysical Journal, 2009, 96, 649a.	0.2	0
99	Towards inferring time dimensionality in proteinâ€“protein interaction networks by integrating structures: the p53 example. Molecular BioSystems, 2009, 5, 1770.	2.9	76
100	Identification of computational hot spots in protein interfaces: combining solvent accessibility and inter-residue potentials improves the accuracy. Bioinformatics, 2009, 25, 1513-1520.	1.8	239
101	Large Scale Prediction of Computational Hot Spots in Protein Interfaces. Biophysical Journal, 2009, 96, 650a-651a.	0.2	0
102	Probing Protein Folding Dynamics Using Multivariate Statistical Techniques. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2009, 42, 171-176.	0.4	0
103	Architectures and Functional Coverage of Proteinâ€“Protein Interfaces. Journal of Molecular Biology, 2008, 381, 785-802.	2.0	106
104	Principles of Proteinâˆ’Protein Interactions: What are the Preferred Ways For Proteins To Interact?. Chemical Reviews, 2008, 108, 1225-1244.	23.0	568
105	A survey of available tools and web servers for analysis of protein-protein interactions and interfaces. Briefings in Bioinformatics, 2008, 10, 217-232.	3.2	140
106	Characterization and Prediction of Protein Interfaces to Infer Protein-Protein Interaction Networks. Current Pharmaceutical Biotechnology, 2008, 9, 67-76.	0.9	28
107	Topological properties of protein interaction networks from a structural perspective. Biochemical Society Transactions, 2008, 36, 1398-1403.	1.6	152
108	Prism: Protein-Protein Interaction Prediction by Structural Matching. Methods in Molecular Biology, 2008, 484, 505-521.	0.4	70

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109	A Novel Economic-Based Scheduling Heuristic for Computational Grids. International Journal of High Performance Computing Applications, 2007, 21, 21-29.	2.4	25
110	Towards Drugs Targeting Multiple Proteins in a Systems Biology Approach. Current Topics in Medicinal Chemistry, 2007, 7, 943-951.	1.0	51
111	Learning Gene Regulation from Microarray Data via Hidden Markov Models. , 2007, , .		0
112	HotSprint: database of computational hot spots in protein interfaces. Nucleic Acids Research, 2007, 36, D662-D666.	6.5	102
113	Relationships between unfolded configurations of proteins and dynamics of folding to the native state. Journal of Polymer Science, Part B: Polymer Physics, 2006, 44, 3667-3678.	2.4	3
114	Computational basis of knowledge-based conformational probabilities derived from local- and long-range interactions in proteins. Proteins: Structure, Function and Bioinformatics, 2006, 66, 29-40.	1.5	15
115	Extracting Gene Regulation Information from Microarray Time-Series Data Using Hidden Markov Models. Lecture Notes in Computer Science, 2006, , 144-153.	1.0	2
116	Comparison of Pricing Policies for a Computational Grid Market. Lecture Notes in Computer Science, 2006, , 766-773.	1.0	1
117	PHR: A Parallel Hierarchical Radiosity System with Dynamic Load Balancing. Journal of Supercomputing, 2005, 31, 249-263.	2.4	1
118	Prediction of protein-protein interactions by combining structure and sequence conservation in protein interfaces. Bioinformatics, 2005, 21, 2850-2855.	1.8	176
119	PRISM: protein interactions by structural matching. Nucleic Acids Research, 2005, 33, W331-W336.	6.5	196
120	Folding Dynamics of Proteins from Denatured to Native State: Principal Component Analysis. Journal of Computational Biology, 2004, 11, 1149-1168.	0.8	14
121	Relationships between amino acid sequence and backbone torsion angle preferences. Proteins: Structure, Function and Bioinformatics, 2004, 55, 992-998.	1.5	42
122	Performance and modularity benefits of message-driven execution. Journal of Parallel and Distributed Computing, 2004, 64, 461-480.	2.7	18
123	Data Decomposition for Parallel K-means Clustering. Lecture Notes in Computer Science, 2004, , 241-248.	1.0	13
124	Parallel Pruning for K-Means Clustering on Shared Memory Architectures. Lecture Notes in Computer Science, 2001, , 321-325.	1.0	4
125	Neighbourhood Preserving Load Balancing: A Self-Organizing Approach. Lecture Notes in Computer Science, 2000, , 234-241.	1.0	6
126	NAMD2: Greater Scalability for Parallel Molecular Dynamics. Journal of Computational Physics, 1999, 151, 283-312.	1.9	2,222

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127	Avoiding Algorithmic Obfuscation in a Message-Driven Parallel MD Code. Lecture Notes in Computational Science and Engineering, 1999, , 472-482.	0.1	5
128	NAMD: a Parallel, Object-Oriented Molecular Dynamics Program. International Journal of High Performance Computing Applications, 1996, 10, 251-268.	1.6	356
129	MDScope â€" a visual computing environment for structural biology. Computer Physics Communications, 1995, 91, 111-133.	3.0	45
130	Androgen receptor binding sites are highly mutated in prostate cancer. Oncology Abstracts, 0, , .	0.0	0