Traian Sulea

List of Publications by Year
in descending order

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75 papers	2,666 citations	201575 27 h-index	197736 49 g-index
76 all docs	76 docs citations	76 times ranked	3501 citing authors

#	Article	IF	Citations
1	Solvated Interaction Energy (SIE) for Scoring Proteinâ"Ligand Binding Affinities. 1. Exploring the Parameter Space. Journal of Chemical Information and Modeling, 2007, 47, 122-133.	2.5	358
2	The Papain-Like Protease from the Severe Acute Respiratory Syndrome Coronavirus Is a Deubiquitinating Enzyme. Journal of Virology, 2005, 79, 15199-15208.	1.5	323
3	Molecular Dynamicsâ€"Solvated Interaction Energy Studies of Proteinâ€"Protein Interactions: The MP1â€"p14 Scaffolding Complex. Journal of Molecular Biology, 2008, 379, 787-802.	2.0	135
4	Human Cathepsin X:Â A Cysteine Protease with Unique Carboxypeptidase Activityâ€. Biochemistry, 1999, 38, 12648-12654.	1.2	126
5	Deubiquitination, a New Function of the Severe Acute Respiratory Syndrome Coronavirus Papain-Like Protease?. Journal of Virology, 2005, 79, 4550-4551.	1.5	95
6	The Structure of Chondroitin B Lyase Complexed with Glycosaminoglycan Oligosaccharides Unravels a Calcium-dependent Catalytic Machinery. Journal of Biological Chemistry, 2004, 279, 32882-32896.	1.6	91
7	Full-Length cDNA of Human Cathepsin F Predicts the Presence of a Cystatin Domain at the N-terminus of the Cysteine Protease Zymogen. Biochemical and Biophysical Research Communications, 1999, 257, 313-318.	1.0	70
8	Design of Noncovalent Inhibitors of Human Cathepsin L. From the 96-Residue Proregion to Optimized Tripeptides. Journal of Medicinal Chemistry, 2002, 45, 5321-5329.	2.9	68
9	Characterization of a Pseudomonad 2-Nitrobenzoate Nitroreductase and Its Catabolic Pathway-Associated 2-Hydroxylaminobenzoate Mutase and a Chemoreceptor Involved in 2-Nitrobenzoate Chemotaxis. Journal of Bacteriology, 2007, 189, 3502-3514.	1.0	64
10	Improvement of the Thermostability and Activity of a Pectate Lyase by Single Amino Acid Substitutions, Using a Strategy Based on Melting-Temperature-Guided Sequence Alignment. Applied and Environmental Microbiology, 2008, 74, 1183-1189.	1.4	57
11	Solvated Interaction Energy (SIE) for Scoring Proteinâ€"Ligand Binding Affinities. 2. Benchmark in the CSAR-2010 Scoring Exercise. Journal of Chemical Information and Modeling, 2011, 51, 2066-2081.	2.5	51
12	High incidence of ubiquitin-like domains in human ubiquitin-specific proteases. Proteins: Structure, Function and Bioinformatics, 2007, 69, 1-7.	1.5	49
13	Structure-based engineering of pH-dependent antibody binding for selective targeting of solid-tumor microenvironment. MAbs, 2020, 12, 1682866.	2.6	47
14	Cathepsins X and B Can Be Differentiated through Their Respective Mono- and Dipeptidyl Carboxypeptidase Activitiesâ€. Biochemistry, 2001, 40, 2702-2711.	1.2	41
15	Evolutionary Reshaping of Fungal Mating Pathway Scaffold Proteins. MBio, 2011, 2, e00230-10.	1.8	41
16	The crystal structure of the formiminotransferase domain of formiminotransferase-cyclodeaminase: implications for substrate channeling in a bifunctional enzyme. Structure, 2000, 8, 35-46.	1.6	40
17	Catalytic Mechanism of Heparinase II Investigated by Site-directed Mutagenesis and the Crystal Structure with Its Substrate. Journal of Biological Chemistry, 2010, 285, 20051-20061.	1.6	39
18	Structure and Function of the Glycopeptide N-methyltransferase MtfA, a Tool for the Biosynthesis of Modified Glycopeptide Antibiotics. Chemistry and Biology, 2009, 16, 401-410.	6.2	37

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19	Small-Molecule Inhibitors of the Pseudaminic Acid Biosynthetic Pathway: Targeting Motility as a Key Bacterial Virulence Factor. Antimicrobial Agents and Chemotherapy, 2014, 58, 7430-7440.	1.4	36
20	Application of Assisted Design of Antibody and Protein Therapeutics (ADAPT) improves efficacy of a Clostridium difficile toxin A single-domain antibody. Scientific Reports, 2018, 8, 2260.	1.6	36
21	An engineered transforming growth factor Î² (TGF-Î²) monomer that functions as a dominant negative to block TGF-Î² signaling. Journal of Biological Chemistry, 2017, 292, 7173-7188.	1.6	34
22	Optimizing Ligand Charges for Maximum Binding Affinity. A Solvated Interaction Energy Approach. Journal of Physical Chemistry B, 2001, 105, 889-899.	1.2	33
23	Restoring Charge Asymmetry in Continuum Electrostatics Calculations of Hydration Free Energies. Journal of Physical Chemistry B, 2009, 113, 8206-8209.	1.2	32
24	Modeling of the bacterial luciferase-flavin mononucleotide complex combining flexible docking with structure-activity data. Protein Science, 2001, 10, 1563-1571.	3.1	31
25	A Conserved Î±-Helix at the Amino Terminus of Prosomatostatin Serves as a Sorting Signal for the Regulated Secretory Pathway. Journal of Biological Chemistry, 2001, 276, 26308-26316.	1.6	31
26	Rapid Prediction of Solvation Free Energy. 2. The First-Shell Hydration (FiSH) Continuum Model. Journal of Chemical Theory and Computation, 2010, 6, 1622-1637.	2.3	31
27	Assisted Design of Antibody and Protein Therapeutics (ADAPT). PLoS ONE, 2017, 12, e0181490.	1.1	31
28	The Solvated Interaction Energy Method for Scoring Binding Affinities. Methods in Molecular Biology, 2012, 819, 295-303.	0.4	29
29	A Different Method for Steric Field Evaluation in CoMFA Improves Model Robustness. Journal of Chemical Information and Computer Sciences, 1997, 37, 1162-1170.	2.8	27
30	Crystal Structure of TDP-Fucosamine Acetyltransferase (WecD) from Escherichia coli , an Enzyme Required for Enterobacterial Common Antigen Synthesis. Journal of Bacteriology, 2006, 188, 5606-5617.	1.0	27
31	On the transferability of hydration-parametrized continuum electrostatics models to solvated binding calculations. Journal of Computational Chemistry, 2003, 24, 954-962.	1.5	26
32	Prediction of SAMPL-1 Hydration Free Energies Using a Continuum Electrostatics-Dispersion Model. Journal of Physical Chemistry B, 2009, 113, 4511-4520.	1.2	26
33	Exhaustive docking and solvated interaction energy scoring: lessons learned from the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 417-427.	1.3	26
34	Serum albuminâ€binding V _H Hs with variable pH sensitivities enable tailored halfâ€life extension of biologics. FASEB Journal, 2020, 34, 8155-8171.	0.2	26
35	A Rational Engineering Strategy for Designing Protein A-Binding Camelid Single-Domain Antibodies. PLoS ONE, 2016, 11, e0163113.	1.1	24
36	Assessment of Solvated Interaction Energy Function for Ranking Antibodyâ€“Antigen Binding Affinities. Journal of Chemical Information and Modeling, 2016, 56, 1292-1303.	2.5	23

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37	Profiling Charge Complementarity and Selectivity for Binding at the Protein Surface. Biophysical Journal, 2003, 84, 2883-2896.	0.2	22
38	Crystal Structure of StaL, a Glycopeptide Antibiotic Sulfotransferase from Streptomyces toyocaensis. Journal of Biological Chemistry, 2007, 282, 13073-13086.	1.6	22
39	ProPOSE: Direct Exhaustive Proteinâ€“Protein Docking with Side Chain Flexibility. Journal of Chemical Theory and Computation, 2018, 14, 4938-4947.	2.3	22
40	Binding site-based classification of coronaviral papain-like proteases. Proteins: Structure, Function and Bioinformatics, 2005, 62, 760-775.	1.5	21
41	Structural and Functional Analysis of Campylobacter jejuni PseG. Journal of Biological Chemistry, 2009, 284, 20989-21000.	1.6	21
42	Structural aspects of recently discovered viral deubiquitinating activities. Biological Chemistry, 2006, 387, 853-862.	1.2	20
43	The propeptide of cruzipainâ€ƒâ€”â€ƒa potent selective inhibitor of the trypanosomal enzymes cruzipain and brucipain, and of the human enzyme cathepsinâ€ƒF. FEBS Journal, 2007, 274, 1224-1234.	2.2	20
44	Carboxy-monopeptidase substrate specificity of human cathepsin X. Biochemical and Biophysical Research Communications, 2005, 329, 445-452.	1.0	18
45	Rapid prediction of solvation free energy. 3. Application to the SAMPL2 challenge. Journal of Computer-Aided Molecular Design, 2010, 24, 373-383.	1.3	18
46	Exhaustive search and solvated interaction energy (SIE) for virtual screening and affinity prediction. Journal of Computer-Aided Molecular Design, 2012, 26, 617-633.	1.3	18
47	Engineering and Therapeutic Application of Single-Chain Bivalent TGF-Î² Family Traps. Molecular Cancer Therapeutics, 2012, 11, 1477-1487.	1.9	17
48	Brain Delivery of IGF1R5, a Single-Domain Antibody Targeting Insulin-like Growth Factor-1 Receptor. Pharmaceutics, 2022, 14, 1452.	2.0	16
49	Bridging structural biology and genetics by computational methods: An investigation into how the R774C mutation in the AR gene can result in complete androgen insensitivity syndrome. Human Mutation, 2003, 22, 465-475.	1.1	15
50	Rapid Prediction of Solvation Free Energy. 1. An Extensive Test of Linear Interaction Energy (LIE). Journal of Chemical Theory and Computation, 2010, 6, 1608-1621.	2.3	14
51	Sulfonation of glycopeptide antibiotics by sulfotransferase StaL depends on conformational flexibility of aglycone scaffold. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11824-11829.	3.3	14
52	Mapping of putative binding sites on the ectodomain of the type II TGF-Î² receptor by scanning-deletion mutagenesis and knowledge-based modeling. FEBS Letters, 1999, 456, 79-84.	1.3	13
53	Binding symmetry and surface flexibility mediate antibody self-association. MAbs, 2019, 11, 1300-1318.	2.6	10
54	Coupled atomic charge selectivity for optimal ligand-charge distributions at protein binding sites. Journal of Computational Chemistry, 2006, 27, 1899-1907.	1.5	9

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55	Selective Inhibition of USP7. Chemistry and Biology, 2012, 19, 437-438.	6.2	9
56	Evaluation of the Wilma-SIE Virtual Screening Method in Community Structureâ€“Activity Resource 2013 and 2014 Blind Challenges. Journal of Chemical Information and Modeling, 2016, 56, 955-964.	2.5	9
57	Binding and functional profiling of antibody mutants guides selection of optimal candidates as antibody drug conjugates. PLoS ONE, 2019, 14, e0226593.	1.1	8
58	Humanization of Camelid Single-Domain Antibodies. Methods in Molecular Biology, 2022, 2446, 299-312.	0.4	8
59	Identification of a functional site on the type I TGF-Î² receptor by mutational analysis of its ectodomain. FEBS Letters, 2002, 513, 147-152.	1.3	7
60	An accurate TMT-based approach to quantify and model lysine susceptibility to conjugation via N-hydroxysuccinimide esters in a monoclonal antibody. Scientific Reports, 2018, 8, 17680.	1.6	7
61	Structure-based dual affinity optimization of a SARS-CoV-1/2 cross-reactive single-domain antibody. PLoS ONE, 2022, 17, e0266250.	1.1	7
62	Site-directed mutagenesis of the type II TGF-Î² receptor indicates a ligand-binding site distinct from that of the type II activin receptor. FEBS Letters, 2002, 515, 13-19.	1.3	6
63	Predicting hydration free energies of polychlorinated aromatic compounds from the SAMPL-3 data set with FiSH and LIE models. Journal of Computer-Aided Molecular Design, 2012, 26, 661-667.	1.3	6
64	Solvation Models: Theory and Validation. Current Pharmaceutical Design, 2014, 20, 3266-3280.	0.9	5
65	Human Cathepsin X. , 2000, 477, 317-322.		4
66	Hydrogen-deuterium exchange mass spectrometry reveals three unique binding responses of mAbs directed to the catalytic domain of hCAIX. MAbs, 2021, 13, 1997072.	2.6	4
67	Antibody mutations favoring <scp>pH</scp>â€dependent binding in solid tumor microenvironments: Insights from largeâ€scale structureâ€based calculations. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1538-1546.	1.5	4
68	Role of the nonâ€hypervariable FR3 Dâ€E loop in singleâ€domain antibody recognition of haptens and carbohydrates. Journal of Molecular Recognition, 2019, 32, e2805.	1.1	3
69	Redesigning an antibody H3 loop by virtual screening of a small library of human germline-derived sequences. Scientific Reports, 2021, 11, 21362.	1.6	3
70	Structure determination and prediction: A study on human Tom20. Computational and Theoretical Chemistry, 1999, 468, 127-134.	1.5	2
71	Binding mechanism of a de novo coiled coil complex elucidated from surface forces measurements. Journal of Colloid and Interface Science, 2021, 581, 218-225.	5.0	2
72	Comparative molecular field analysis of protein tyrosine phosphatase low-molecular-weight substrates. Computational and Theoretical Chemistry, 1998, 434, 139-153.	1.5	1

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73	Combinatorial Synthesis of Alkaloid-like Compounds In Search of Chemical Probes of Protein-Protein Interactions. , 0, , 521-540.		0
74	Cathepsin X. , 2013, , 1839-1844.		0
75	Probing the acylâ€binding pocket of aminoacylaseâ€1. FASEB Journal, 2006, 20, A906.	0.2	0