Iris Antes

List of Publications by Year
in descending order

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49 papers	1,381 citations	394421 19 h-index	345221 36 g-index
54 all docs	54 docs citations	54 times ranked	2415 citing authors

#	Article	IF	Citations
1	<scp>DynaBiS</scp>: A hierarchical sampling algorithm to identify flexible binding sites for large ligands and peptides. Proteins: Structure, Function and Bioinformatics, 2022, 90, 18-32.	2.6	3
2	The Q41R mutation in the HCV-protease enhances the reactivity towards MAVS by suppressing non-reactive pathways. Physical Chemistry Chemical Physics, 2022, 24, 2126-2138.	2.8	1
3	Investigation of the pH-dependent aggregation mechanisms of GCSF using low resolution protein characterization techniques and advanced molecular dynamics simulations. Computational and Structural Biotechnology Journal, 2022, 20, 1439-1455.	4.1	4
4	SenseNet, a tool for analysis of protein structure networks obtained from molecular dynamics simulations. PLoS ONE, 2022, 17, e0265194.	2.5	2
5	Structureâ€Guided Modulation of the Catalytic Properties of [2Feâ^'2S]â€Dependent Dehydratases. ChemBioChem, 2022, 23, .	2.6	6
6	Dynamic Docking of Macrocycles in Bound and Unbound Protein Structures with DynaDock. Journal of Chemical Information and Modeling, 2022, 62, 3426-3441.	5.4	0
7	Turning the Actin Nucleating Compound Miuraenamide into Nucleation Inhibitors. ACS Omega, 2021, 6, 22165-22172.	3.5	5
8	Functional analysis of peripheral and intratumoral neoantigen-specific TCRs identified in a patient with melanoma. , 2021, 9, e002754.		7
9	Acyldepsipeptide Probes Facilitate Specific Detection of Caseinolytic Proteaseâ€...P Independent of Its Oligomeric and Activity State. ChemBioChem, 2020, 21, 235-240.	2.6	5
10	Repurposing human kinase inhibitors to create an antibiotic active against drug-resistant Staphylococcus aureus, persisters and biofilms. Nature Chemistry, 2020, 12, 145-158.	13.6	78
11	Extended interaction networks with HCV protease NS3-4A substrates explain the lack of adaptive capability against protease inhibitors. Journal of Biological Chemistry, 2020, 295, 13862-13874.	3.4	10
12	Broad spectrum antibiotic-degrading metallo-Î²-lactamases are phylogenetically diverse. Protein and Cell, 2020, 11, 613-617.	11.0	21
13	Systematic analysis of the binding behaviour of UHRF1 towards different methyl- and carboxylcytosine modification patterns at CpG dyads. PLoS ONE, 2020, 15, e0229144.	2.5	11
14	A modular approach to the bisbenzylisoquinoline alkaloids tetrandrine and isotetrandrine. Organic and Biomolecular Chemistry, 2020, 18, 3047-3068.	2.8	17
15	Actin stabilizing compounds show specific biological effects due to their binding mode. Scientific Reports, 2019, 9, 9731.	3.3	30
16	Key Features Relevant to Select Antigens and TCR From the MHC-Mismatched Repertoire to Treat Cancer. Frontiers in Immunology, 2019, 10, 1485.	4.8	8
17	Predicting the bioactive conformations of macrocycles: a molecular dynamics-based docking procedure with DynaDock. Journal of Molecular Modeling, 2019, 25, 197.	1.8	13
18	Thiazoline-Specific Amidohydrolase PurAH Is the Gatekeeper of Bottromycin Biosynthesis. Journal of the American Chemical Society, 2019, 141, 9748-9752.	13.7	26

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19	A combined in silico and in vitro study on mouse Serpina1a antitrypsin-deficiency mutants. Scientific Reports, 2019, 9, 7486.	3.3	2
20	1,4-Disubstituted 1H-1,2,3-Triazole Containing Peptidotriazolamers: A New Class of Peptidomimetics With Interesting Foldamer Properties. Frontiers in Chemistry, 2019, 7, 155.	3.6	16
21	Identification of essential amino acids for glucose transporter 5 (GLUT5)-mediated fructose transport. Journal of Biological Chemistry, 2018, 293, 2115-2124.	3.4	11
22	Bap (Sil1) regulates the molecular chaperone BiP by coupling release of nucleotide and substrate. Nature Structural and Molecular Biology, 2018, 25, 90-100.	8.2	39
23	DynaDom: structure-based prediction of T cell receptor inter-domain and T cell receptor-peptide-MHC (class I) association angles. BMC Structural Biology, 2018, 17, 2.	2.3	16
24	Amber-Compatible Parametrization Procedure for Peptide-like Compounds: Application to 1,4- and 1,5-Substituted Triazole-Based Peptidomimetics. Journal of Chemical Information and Modeling, 2018, 58, 90-110.	5.4	11
25	1,5â€Disubstituted 1,2,3â€Triazoleâ€Containing Peptidotriazolamers: Design Principles for a Class of Versatile Peptidomimetics. Chemistry - A European Journal, 2018, 24, 953-961.	3.3	21
26	Ca2+ binding induced sequential allosteric activation of sortase A: An example for ion-triggered conformational selection. PLoS ONE, 2018, 13, e0205057.	2.5	7
27	Gliotoxin Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase GliJ. ACS Chemical Biology, 2017, 12, 1874-1882.	3.4	24
28	BiPPred: Combined sequenceâ€and structureâ€based prediction of peptide binding to the Hsp70 chaperone BiP. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1390-1407.	2.6	46
29	Multiple sclerosis. Neurology: Neuroimmunology and NeuroInflammation, 2016, 3, e241.	6.0	9
30	Naturstoffbasierte Aminoepoxybenzochinone inhibieren das Wachstum verschiedener Serovare des Gramâ€negativen Krankheitserregers Salmonella durch AbschwÃchen der bakteriellen Stressabwehr. Angewandte Chemie, 2016, 128, 15074-15079.	2.0	3
31	Naturalâ€Productâ€Inspired Aminoepoxybenzoquinones Kill Members of the Gramâ€Negative Pathogen Salmonella by Attenuating Cellular Stress Response. Angewandte Chemie - International Edition, 2016, 55, 14852-14857.	13.8	14
32	Sequential Inactivation of Gliotoxin by the S-Methyltransferase TmtA. ACS Chemical Biology, 2016, 11, 1082-1089.	3.4	22
33	Parameterization of the Hamiltonian Dielectric Solvent (HADES) Reactionâ€Field Method for the Solvation Free Energies of Amino Acid Sideâ€Chain Analogs. ChemPhysChem, 2015, 16, 1739-1749.	2.1	1
34	Prediction of VHâ€“VL domain orientation for antibody variable domain modeling. Proteins: Structure, Function and Bioinformatics, 2015, 83, 681-695.	2.6	47
35	Quantitative Analysis of the Association Angle between T-cell Receptor Vα/Vβ Domains Reveals Important Features for Epitope Recognition. PLoS Computational Biology, 2015, 11, e1004244.	3.2	10
36	Phenyl Esters Are Potent Inhibitors of Caseinolytic Protease P and Reveal a Stereogenic Switch for Deoligomerization. Journal of the American Chemical Society, 2015, 137, 8475-8483.	13.7	89

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37	MoFvAb: Modeling the Fv region of antibodies. MAbs, 2015, 7, 838-852.	5.2	21
38	Eine niedermolekulare Verbindung inhibiert die Proteindisulfidisomerase und sensibilisiert Krebszellen fÃ¼r die Chemotherapie. Angewandte Chemie, 2014, 126, 13174-13179.	2.0	5
39	A Small Molecule Inhibits Protein Disulfide Isomerase and Triggers the Chemosensitization of Cancer Cells. Angewandte Chemie - International Edition, 2014, 53, 12960-12965.	13.8	23
40	Regulation of the hepatitis C virus RNA replicase by endogenous lipid peroxidation. Nature Medicine, 2014, 20, 927-935.	30.7	130
41	Conformational Selection in Substrate Recognition by Hsp70 Chaperones. Journal of Molecular Biology, 2013, 425, 466-474.	4.2	38
42	Amythiamicinâ€…D and Related Thiopeptides as Inhibitors of the Bacterial Elongation Factor EFâ€Tu: Modification of the Amino Acid at Carbon Atom C2 of Ringâ€…C Dramatically Influences Activity. ChemMedChem, 2013, 8, 1954-1962.	3.2	18
43	Recognition of 5-Hydroxymethylcytosine by the Uhrf1 SRA Domain. PLoS ONE, 2011, 6, e21306.	2.5	159
44	Predicting MHC class I epitopes in large datasets. BMC Bioinformatics, 2010, 11, 90.	2.6	37
45	DynaDock: A new molecular dynamicsâ€based algorithm for proteinâ€“peptide docking including receptor flexibility. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1084-1104.	2.6	147
46	Docking and scoring with alternative sideâ€chain conformations. Proteins: Structure, Function and Bioinformatics, 2009, 74, 712-726.	2.6	38
47	IRECS: A new algorithm for the selection of most probable ensembles of side-chain conformations in protein models. Protein Science, 2007, 16, 1294-1307.	7.6	50
48	Improvement of the fungal enzyme pyranose 2-oxidase using protein engineering. Journal of Biotechnology, 2006, 124, 26-40.	3.8	14
49	DynaPred: A structure and sequence based method for the prediction of MHC class I binding peptide sequences and conformations. Bioinformatics, 2006, 22, e16-e24.	4.1	63