K Anton Feenstra

List of Publications by Year
in descending order

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59	2,488	279701	206029
papers	citations	23 h-index	48 g-index

67	67	67	3616
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improving efficiency of large time-scale molecular dynamics simulations of hydrogen-rich systems. Journal of Computational Chemistry, 1999, 20, 786-798.	1.5	779
2	Cytochrome P450 in Silico:Â An Integrative Modeling Approach. Journal of Medicinal Chemistry, 2005, 48, 2725-2755.	2.9	205
3	Dynamic Conformations of Flavin Adenine Dinucleotide:â€‰ Simulated Molecular Dynamics of the Flavin Cofactor Related to the Time-Resolved Fluorescence Characteristics. Journal of Physical Chemistry B, 2002, 106, 8858-8869.	1.2	130
4	Interaction of 14-3-3 proteins with the Estrogen Receptor Alpha F domain provides a drug target interface. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8894-8899.	3.3	114
5	PRALINEâ„¢: a strategy for improved multiple alignment of transmembrane proteins. Bioinformatics, 2008, 24, 492-497.	1.8	108
6	Multi-RELIEF: a method to recognize specificity determining residues from multiple sequence alignments using a Machine-Learning approach for feature weighting. Bioinformatics, 2008, 24, 18-25.	1.8	83
7	Hard-wired heterogeneity in blood stem cells revealed using a dynamic regulatory network model. Bioinformatics, 2013, 29, i80-i88.	1.8	83
8	Seeing the trees through the forest: sequence-based homo- and heteromeric protein-protein interaction sites prediction using random forest. Bioinformatics, 2017, 33, 1479-1487.	1.8	66
9	Metabolic Regio- and Stereoselectivity of Cytochrome P450 2D6 towards 3,4-Methylenedioxy-N-alkylamphetamines:Â in Silico Predictions and Experimental Validation. Journal of Medicinal Chemistry, 2005, 48, 6117-6127.	2.9	64
10	Sequence comparison by sequence harmony identifies subtype-specific functional sites. Nucleic Acids Research, 2006, 34, 6540-6548.	6.5	64
11	Altering the Regioselectivity of Cytochrome P450 CYP102A3 of Bacillus subtilis by Using a New Versatile Assay System. ChemBioChem, 2006, 7, 345-350.	1.3	51
12	Multi-Harmony: detecting functional specificity from sequence alignment. Nucleic Acids Research, 2010, 38, W35-W40.	6.5	51
13	Executing multicellular differentiation: quantitative predictive modelling of C.elegans vulval development. Bioinformatics, 2009, 25, 2049-2056.	1.8	45
14	In vitro evolution of styrene monooxygenase from Pseudomonas putida CA-3 for improved epoxide synthesis. Applied Microbiology and Biotechnology, 2010, 85, 995-1004.	1.7	43
15	Coarse-grained versus atomistic simulations: realistic interaction free energies for real proteins. Bioinformatics, 2014, 30, 326-334.	1.8	40
16	The potential use of big data in oncology. Oral Oncology, 2019, 98, 8-12.	0.8	40
17	HIV-1 envelope glycoprotein signatures that correlate with the development of cross-reactive neutralizing activity. Retrovirology, 2013, 10, 102.	0.9	39
18	Aurora kinase A (AURKA) interaction with Wnt and Ras-MAPK signalling pathways in colorectal cancer. Scientific Reports, 2018, 8, 7522.	1.6	38

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19	Sequence harmony: detecting functional specificity from alignments. Nucleic Acids Research, 2007, 35, W495-W498.	6.5	34
20	Combining substrate dynamics, binding statistics, and energy barriers to rationalize regioselective hydroxylation of octane and lauric acid by CYP102A1 and mutants. Protein Science, 2007, 16, 420-431.	3.1	33
21	A comparison of methods for calculating NMR cross-relaxation rates (NOESY and ROESY intensities) in small peptides. Journal of Biomolecular NMR, 2002, 23, 181-194.	1.6	30
22	Multiple Sequence Alignment. Methods in Molecular Biology, 2017, 1525, 167-189.	0.4	29
23	Enantioselective Substrate Binding in a Monooxygenase Protein Model by Molecular Dynamics and Docking. Biophysical Journal, 2006, 91, 3206-3216.	0.2	26
24	SeRenDIP: SEquential REmasteriNg to DerIve profiles for fast and accurate predictions of PPI interface positions. Bioinformatics, 2019, 35, 4794-4796.	1.8	21
25	CLUB-MARTINI: Selecting Favourable Interactions amongst Available Candidates, a Coarse-Grained Simulation Approach to Scoring Docking Decoys. PLoS ONE, 2016, 11, e0155251.	1.1	20
26	Molecular modeling of the RNA binding N-terminal part of cowpea chlorotic mottle virus coat protein in solution with phosphate ions. Biophysical Journal, 1996, 71, 2920-2932.	0.2	18
27	Sequence specificity between interacting and non-interacting homologs identifies interface residues â€“ a homodimer and monomer use case. BMC Bioinformatics, 2015, 16, 325.	1.2	18
28	SeRenDIP-CE: sequence-based interface prediction for conformational epitopes. Bioinformatics, 2021, 37, 3421-3427.	1.8	18
29	Construction and Experimental Validation of a Petri Net Model of Wnt/Î²-Catenin Signaling. PLoS ONE, 2016, 11, e0155743.	1.1	16
30	What Can Formal Methods Bring to Systems Biology?. Lecture Notes in Computer Science, 2009, , 16-22.	1.0	15
31	BioASF: a framework for automatically generating executable pathway models specified in BioPAX. Bioinformatics, 2016, 32, i60-i69.	1.8	14
32	The meaning of alignment: lessons from structural diversity. BMC Bioinformatics, 2008, 9, 556.	1.2	13
33	HIV-1 Replication Fitness of HLA-B*57/58:01 CTL Escape Variants Is Restored by the Accumulation of Compensatory Mutations in Gag. PLoS ONE, 2013, 8, e81235.	1.1	13
34	Bioinformatics and Systems Biology: bridging the gap between heterogeneous student backgrounds. Briefings in Bioinformatics, 2013, 14, 589-598.	3.2	12
35	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	0.8	12
36	Predicting the relationships between gut microbiota and mental disorders with knowledge graphs. Health Information Science and Systems, 2021, 9, 3.	3.4	11

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37	Design Issues for Qualitative Modelling of Biological Cells with Petri Nets. , 2008, , 48-62.		11
38	Influence of Gut Microbiota on Mental Health via Neurotransmitters: A Review. Journal of Artificial Intelligence for Medical Sciences, 2020, 1, 1-14.	1.3	10
39	PIPENN: protein interface prediction from sequence with an ensemble of neural nets. Bioinformatics, 2022, 38, 2111-2118.	1.8	10
40	Petri Nets Are a Biologistâ€™s Best Friend. Lecture Notes in Computer Science, 2014, , 102-116.	1.0	8
41	Motif-Aware PRALINE: Improving the alignment of motif regions. PLoS Computational Biology, 2018, 14, e1006547.	1.5	7
42	On defining the dynamics of hydrophobic patches on protein surfaces. Proteins: Structure, Function and Bioinformatics, 2008, 72, 105-114.	1.5	5
43	Training for translation between disciplines: a philosophy for life and data sciences curricula. Bioinformatics, 2018, 34, i4-i12.	1.8	5
44	Enabling grandâ€canonical Monte Carlo: Extending the flexibility of GROMACS through the GromPy python interface module. Journal of Computational Chemistry, 2012, 33, 1207-1214.	1.5	4
45	Tailor-made multiple sequence alignments using the PRALINE 2 alignment toolkit. Bioinformatics, 2019, 35, 5315-5317.	1.8	4
46	The ability of transcription factors to differentially regulate gene expression is a crucial component of the mechanism underlying inversion, a frequently observed genetic interaction pattern. PLoS Computational Biology, 2019, 15, e1007061.	1.5	4
47	Multi-task learning to leverage partially annotated data for PPI interface prediction. Scientific Reports, 2022, 12, .	1.6	4
48	Executing multicellular differentiation: quantitative predictive modelling of C.elegans vulval development. Bioinformatics, 2009, 25, 2624-2624.	1.8	3
49	A framework for exhaustive modelling of genetic interaction patterns using Petri nets. Bioinformatics, 2020, 36, 2142-2149.	1.8	3
50	A Feature Selection Algorithm for Detecting Subtype Specific Functional Sites from Protein Sequences for Smad Receptor Binding. , 2006, , .		2
51	Multiple alignment of transmembrane protein sequences. , 2010, , 103-122.		2
52	Cytochrome P450 in Silico: An Integrative Modeling Approach. ChemInform, 2005, 36, no.	0.1	1
53	Structure and function analysis of flexible alignment regions in proteins. BMC Bioinformatics, 2009, 10, .	1.2	1
54	Online biophysical predictions for SARS-CoV-2 proteins. BMC Molecular and Cell Biology, 2021, 22, 23.	1.0	1

#	Article	IF	Citations
55	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	0.5	0
56	Explaining disease using big data: How valid is your pathway?. , 2015, , .		0
57	Deep sequencing identifies hepatitis B virus core protein signatures in chronic hepatitis B patients. Antiviral Research, 2018, 158, 213-225.	1.9	0
58	Impact of pathogenic mutations of the GLUT1 glucose transporter on channel dynamics using ConsDYN enhanced sampling. F1000Research, 0, 8, 322.	0.8	0
59	Impact of pathogenic mutations of the GLUT1 glucose transporter on solute carrier dynamics using ComDYN enhanced sampling. F1000Research, 0, 8, 322.	0.8	0