Amiram Goldblum

List of Publications by Year
in descending order

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62 papers	1,704 citations	279798 23 h-index	289244 40 g-index
63 all docs	63 docs citations	63 times ranked	2108 citing authors

#	Article	IF	Citations
1	Human-Based Immune Responsive In Vitro Infection Models for Validation of Novel TLR4 Antagonists Identified by Computational Discovery. Microorganisms, 2022, 10, 243.	3.6	2
2	Candidate Therapeutics by Screening for Multitargeting Ligands: Combining the CB2 Receptor With CB1, PPARÎ³ and 5-HT4 Receptors. Frontiers in Pharmacology, 2022, 13, 812745.	3.5	4
3	In silico Docking Analysis for Blocking JUNOâ€ŁZUMO1 Interaction Identifies Two Small Molecules that Block in vitro Fertilization. Frontiers in Cell and Developmental Biology, 2022, 10, 824629.	3.7	4
4	Computational design of substrate selective inhibition. PLoS Computational Biology, 2020, 16, e1007713.	3.2	4
5	Prediction and Experimental Confirmation of Novel Peripheral Cannabinoid-1 Receptor Antagonists. Journal of Chemical Information and Modeling, 2019, 59, 3996-4006.	5.4	7
6	Discovering highly selective and diverse PPAR-delta agonists by ligand based machine learning and structural modeling. Scientific Reports, 2019, 9, 1106.	3.3	36
7	New drug candidates for liposomal delivery identified by computer modeling of liposomes' remote loading and leakage. Journal of Controlled Release, 2017, 252, 18-27.	9.9	53
8	Computational Discovery and Experimental Confirmation of TLR9 Receptor Antagonist Leads. Journal of Chemical Information and Modeling, 2016, 56, 1835-1846.	5.4	21
9	Discovering Novel and Diverse Iron-Chelators in Silico. Journal of Chemical Information and Modeling, 2016, 56, 2476-2485.	5.4	9
10	Nano-mupirocin: enabling the parenteral activity of mupirocin. European Journal of Nanomedicine, 2016, 8, 139-149.	0.6	11
11	Structural basis of glycogen branching enzyme deficiency and pharmacologic rescue by rational peptide design. Human Molecular Genetics, 2015, 24, 5667-5676.	2.9	58
12	Iterative Stochastic Elimination for Solving Complex Combinatorial Problems in Drug Discovery. Israel Journal of Chemistry, 2014, 54, 1338-1357.	2.3	15
13	Computer-aided design of liposomal drugs: In silico prediction and experimental validation of drug candidates for liposomal remote loading. Journal of Controlled Release, 2014, 173, 125-131.	9.9	39
14	Effect of Solubilizing Agents on Mupirocin Loading into and Release from PEGylated Nanoliposomes. Journal of Pharmaceutical Sciences, 2014, 103, 2131-2138.	3.3	19
15	Indexing molecules for their hERG liability. European Journal of Medicinal Chemistry, 2013, 65, 304-314.	5.5	19
16	Quantitative structure - property relationship modeling of remote liposome loading of drugs. Journal of Controlled Release, 2012, 160, 147-157.	9.9	73
17	Molecular Properties from Conformational Ensembles. 1. Dipole Moments of Molecules with Multiple Internal Rotations. Journal of Physical Chemistry A, 2011, 115, 5794-5809.	2.5	1
18	Understanding drugâ€likeness. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 760-781.	14.6	152

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19	Flexible proteinâ€protein docking based on Bestâ€First search algorithm. Journal of Computational Chemistry, 2010, 31, 1929-1943.	3.3	3
20	Predicting Oral Druglikeness by Iterative Stochastic Elimination. Journal of Chemical Information and Modeling, 2010, 50, 437-445.	5.4	28
21	Liposome drugs' loading efficiency: A working model based on loading conditions and drug's physicochemical properties. Journal of Controlled Release, 2009, 139, 73-80.	9.9	277
22	High quality binding modes in docking ligands to proteins. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1373-1386.	2.6	39
23	A Model for the Structure of the C-Terminal Domain of Dragline Spider Silk and the Role of Its Conserved Cysteine. Biomacromolecules, 2007, 8, 2768-2773.	5.4	40
24	Constructing ensembles of flexible fragments in native proteins by iterative stochastic elimination is relevant to protein-protein interfaces. Proteins: Structure, Function and Bioinformatics, 2007, 68, 702-711.	2.6	3
25	Computational Protein Design: A Novel Path to Future Protein Drugs. Current Pharmaceutical Design, 2006, 12, 3973-3997.	1.9	41
26	Exploring the conformational space of cyclic peptides by a stochastic search method. Journal of Molecular Graphics and Modelling, 2004, 22, 319-333.	2.4	33
27	Stochastic Algorithm for Kinase Homology Model Construction. Current Medicinal Chemistry, 2004, 11, 675-692.	2.4	23
28	Inhibition of LDL oxidation by flavonoids in relation to their structure and calculated enthalpy. Phytochemistry, 2003, 62, 89-99.	2.9	136
29	Refined structure of bovine carboxypeptidase A at 1.25â€…Ã… resolution. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 323-333.	2.5	33
30	The â€œNearest Single Neighborâ€•MethodFinding Families of Conformations within a Sample. Journal of Chemical Information and Computer Sciences, 2003, 43, 208-217.	2.8	11
31	Anhydride formation is not a valid mechanism for peptide cleavage by carboxypeptidase-A: a semiempirical reaction pathway study. Molecular Physics, 2003, 101, 2715-2724.	1.7	11
32	Theoretical Studies of Catalysis by Carboxypeptidase A: Could Gas-Phase Calculations Support a Mechanism?. Collection of Czechoslovak Chemical Communications, 2003, 68, 2055-2079.	1.0	1
33	A stochastic algorithm for global optimization and for best populations: A test case of side chains in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 703-708.	7.1	44
34	Mechanism of action of zinc proteinases: A MNDO/d/H study of alternative general-acid general-base catalytic pathways for carboxypeptidase-A. International Journal of Quantum Chemistry, 2002, 88, 87-98.	2.0	20
35	Two cysteine residues in the DNA-binding domain of CREB control binding to CRE and CREB-mediated gene expression. Journal of Molecular Biology, 2001, 313, 695-709.	4.2	39
36	A novel energy-based stochastic method for positioning polar protons in protein structures from X-rays. Proteins: Structure, Function and Bioinformatics, 2000, 38, 273-287.	2.6	16

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37	Determining proton positions in an enzyme-inhibitor complex is a first step for theoretical mechanistic studies of aspartic proteinases. Theoretica Chimica Acta, 1993, 85, 231-247.	0.8	9
38	Extending crystallographic information with semiempirical quantum mechanics and molecular mechanics: A case of aspartic proteinases. Journal of Chemical Information and Computer Sciences, 1993, 33, 270-274.	2.8	8
39	Comments on the â€œSynthesis and Characterization of Some New Organophosphonates and Their Adducts with Some Metalsâ€•by Saad and Ramadan. Bulletin of the Chemical Society of Japan, 1991, 64, 1445-1446.	3.2	0
40	A molecular model for an anionic opiate Î¼-receptor: affinity and activation of morphine conformers. European Journal of Pharmacology, 1991, 206, 119-131.	2.6	10
41	Semiempirical MNDO/H calculations of opiates. Computational and Theoretical Chemistry, 1990, 207, 1-14.	1.5	12
42	Modulation of the affinity of aspartic proteases by the mutated residues in active site models. FEBS Letters, 1990, 261, 241-244.	2.8	12
43	Structure and Reactivity of 2-Hydroxyiminobenzyl-2-oxo-4,4,5,5-tetramethyl[1,3,2]dioxaphospholanes. Phosphorus, Sulfur and Silicon and the Related Elements, 1989, 41, 433-437.	1.6	4
44	Calculation of proton transfers in hydrogen bonding interactions with semi-empirical MNDO/H. Computational and Theoretical Chemistry, 1988, 179, 153-163.	1.5	6
45	Quantum mechanical modeling of aspartic proteinase interactions: Difference in binding of diastereomeric statine models. Biochemical and Biophysical Research Communications, 1988, 157, 450-456.	2.1	3
46	FRAGMENTATION OF ACYLPHOSPHONATES[sbnd]NEW PRECURSORS FOR DICOORDINATED PHOSPHORUS SPECIES. Phosphorous and Sulfur and the Related Elements, 1987, 33, 61-63.	0.2	4
47	Improvement of the hydrogen bonding correction to MNDO for calculations of biochemical interest. Journal of Computational Chemistry, 1987, 8, 835-849.	3.3	50
48	Geometrical analysis of Cysâ€Cys bridges in proteins and their prediction from incomplete structural information. International Journal of Peptide and Protein Research, 1987, 30, 784-793.	0.1	1
49	An improved approach to the analysis of drugâ€”protein binding by distance geometry. Computational and Theoretical Chemistry, 1986, 134, 415-428.	1.5	0
50	Quantum chemical studies of model cytochrome P450 oxidations of amines. 1. MNDO pathways for alkylamine reactions with singlet and triplet oxygen. Journal of the American Chemical Society, 1985, 107, 4265-4272.	13.7	24
51	Î²-adrenergic activity and conformation of the antihypertensive specific Î±2-agonist drug, guanabenz. Biochemical Pharmacology, 1985, 34, 491-498.	4.4	12
52	A NOVEL BASE-CATALYZED FRAGMENTATION OF ALIPHATIC ACYLPHOSPHONATES. Phosphorous and Sulfur and the Related Elements, 1984, 21, 119-120.	0.2	4
53	Fermentation and Post-Fermentation Changes in Israeli Wines. Journal of Food Science, 1984, 49, 251-256.	3.1	12
54	Electronic Structure and Reactivity of 2,2-ethano-1-methylene 1,2,3,4-tetrahydronaphthalene and 1,1-ethano-2-methylene 1,2,3,4-tetrahydronaphthalene. Israel Journal of Chemistry, 1982, 22, 71-75.	2.3	0

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55	Quantitative structure-activity relationship of phenyl N-methylcarbamate inhibition of acetylcholinesterase. Journal of Agricultural and Food Chemistry, 1981, 29, 277-288.	5.2	19
56	STRUCTURE, SPECTRA, AND FUNCTION OF MODEL CYTOCHROME P450. Annals of the New York Academy of Sciences, 1981, 367, 192-218.	3.8	19
57	Quantum chemical studies of anaerobic reductive metabolism of halothane by cytochrome P-450. Chemico-Biological Interactions, 1980, 32, 83-99.	4.0	14
58	Electronic spectrum of model cytochrome P450 complex with postulated carbene metabolite of halothane. Journal of the American Chemical Society, 1980, 102, 3657-3659.	13.7	23
59	Use of the overlap multipole expansion for approximating molecular electrostatic potentials. International Journal of Quantum Chemistry, 1979, 15, 121-129.	2.0	55
60	Study of anion binding to protonated nucleic acid bases using electrostatic molecular potentials. Theoretica Chimica Acta, 1978, 47, 345-347.	0.8	26
61	Hydration scheme of the complementary base-pairs of DNA. FEBS Letters, 1978, 91, 213-215.	2.8	42
62	Anion binding to nucleic acid bases. A quantum-mechanical exploration using electrostatic molecular potentials. Biochemical and Biophysical Research Communications, 1977, 77, 1166-1169.	2.1	10