Glen E Kellogg

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	3D Interaction Homology: Hydropathic Analyses of the "π–Cation―and "π–π―Interaction Motifs i Phenylalanine, Tyrosine, and Tryptophan Residues. Journal of Chemical Information and Modeling, 2021, 61, 2937-2956.	n 2.5	11
2	Structural understanding of 5-(4-hydroxy-phenyl)-N-(2-(5-methoxy-1H-indol-3-yl)-ethyl)-3-oxopentanamide as a neuroprotectant for Alzheimer's disease. Bioorganic and Medicinal Chemistry Letters, 2021, 43, 128081.	1.0	1
3	FOSL1 promotes metastasis of head and neck squamous cell carcinoma through super-enhancer-driven transcription program. Molecular Therapy, 2021, 29, 2583-2600.	3.7	39
4	3D interaction homology: Hydropathic interaction environments of serine and cysteine are strikingly different and their roles adapt in membrane proteins. Current Research in Structural Biology, 2021, 3, 239-256.	1.1	10
5	3D Interaction Homology: Computational Titration of Aspartic Acid, Glutamic Acid and Histidine Can Create pH-Tunable Hydropathic Environment Maps. Frontiers in Molecular Biosciences, 2021, 8, 773385.	1.6	4
6	Systematized Analysis of Secondary Structure Dependence of Key Structural Features of Residues in Soluble and Membrane-Bound Proteins. Journal of Structural Biology: X, 2021, 5, 100055.	0.7	1
7	Synthesis of novel 5-substituted-2-aminotetralin analogs: 5-HT1A and 5-HT7 G protein-coupled receptor affinity, 3D-QSAR and molecular modeling. Bioorganic and Medicinal Chemistry, 2020, 28, 115262.	1.4	14
8	3D interaction homology: The hydropathic interaction environments of even alanine are diverse and provide novel structural insight. Journal of Structural Biology, 2019, 207, 183-198.	1.3	8
9	Functional diversification of the chemical landscapes of yeast Sec14-like phosphatidylinositol transfer protein lipid-binding cavities. Journal of Biological Chemistry, 2019, 294, 19081-19098.	1.6	17
10	Inhibiting Pneumococcal Surface Antigen A (PsaA) with Small Molecules Discovered through Virtual Screening: Steps toward Validating a Potential Target forStreptococcus pneumoniae. Chemistry and Biodiversity, 2018, 15, e1800234.	1.0	8
11	Exploring the binding mechanisms of diaminopimelic acid analogs to meso-diaminopimelate dehydrogenase by molecular modeling. Journal of Molecular Graphics and Modelling, 2018, 83, 100-111.	1.3	3
12	Ortho group activation of a bromopyrrole ester in Suzuki-Miyaura cross-coupling reactions: Application to the synthesis of new microtubule depolymerizing agents with potent cytotoxic activities. Bioorganic and Medicinal Chemistry, 2017, 25, 3206-3214.	1.4	4
13	The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. Journal of Medicinal Chemistry, 2017, 60, 6781-6827.	2.9	111
14	Diaminopimelic acid (DAP) analogs bearing isoxazoline moiety as selective inhibitors against meso-diaminopimelate dehydrogenase (m-Ddh) from Porphyromonas gingivalis. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3840-3844.	1.0	6
15	Design, synthesis, and biological evaluation of substrate-competitive inhibitors of C-terminal Binding Protein (CtBP). Bioorganic and Medicinal Chemistry, 2016, 24, 2707-2715.	1.4	21
16	Crystal structure of carbonmonoxy sickle hemoglobin in R-state conformation. Journal of Structural Biology, 2016, 194, 446-450.	1.3	30
17	Biological Characterization of an Improved Pyrrole-Based Colchicine Site Agent Identified through Structure-Based Design. Molecular Pharmacology, 2016, 89, 287-296.	1.0	9
18	3d interaction homology: The structurally known rotamers of tyrosine derive from a surprisingly limited set of information-rich hydropathic interaction environments described by maps. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1118-1136.	1.5	10

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19	Understanding Water and Its Many Roles in Biological Structure: Ways to Exploit a Resource for Drug Discovery. Methods in Pharmacology and Toxicology, 2015, , 85-110.	0.1	0
20	Molecular basis of E. coli l-threonine aldolase catalytic inactivation at low pH. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 278-283.	1.1	7
21	Anti-cytomegalovirus activity of the anthraquinone atanyl blue PRL. Antiviral Research, 2015, 114, 86-95.	1.9	17
22	Design, syntheses, and pharmacological characterization of 17-cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6α-(isoquinoline-3′-carboxamido)morphinan analogues as opioid receptor ligands. Bioorganic and Medicinal Chemistry, 2015, 23, 1701-1715.	1.4	19
23	Identification of Small-Molecule Inhibitors against Meso-2, 6-Diaminopimelate Dehydrogenase from Porphyromonas gingivalis. PLoS ONE, 2015, 10, e0141126.	1.1	13
24	Formyl group activation of a bromopyrrole ester in Suzuki cross-coupling reactions: application to a formal synthesis of Polycitone AÂand B and Polycitrin A. Tetrahedron, 2014, 70, 2738-2745.	1.0	4
25	Intuitive, but not simple: Including explicit water molecules in protein–protein docking simulations improves model quality. Proteins: Structure, Function and Bioinformatics, 2014, 82, 916-932.	1.5	18
26	Predicting the molecular interactions of CRIP1a–cannabinoid 1 receptor with integrated molecular modeling approaches. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1158-1165.	1.0	13
27	Targeting Cystalysin, a Virulence Factor of <i>Treponema denticolaâ€</i> Supported Periodontitis. ChemMedChem, 2014, 9, 1501-1511.	1.6	26
28	Binding mode characterization of 6α- and 6β-N-heterocyclic substituted naltrexamine derivatives via docking in opioid receptor crystal structures and site-directed mutagenesis studies: Application of the â€~message–address' concept in development of mu opioid receptor selective antagonists. Bioorganic and Medicinal Chemistry, 2013, 21, 6405-6413.	1.4	20
29	Unintended consequences? Water molecules at biological and crystallographic protein–protein interfaces. Computational Biology and Chemistry, 2013, 47, 126-141.	1.1	14
30	How to Deal with Low-Resolution Target Structures: Using SAR, Ensemble Docking, Hydropathic Analysis, and 3D-QSAR to Definitively Map the αβ-Tubulin Colchicine Site. Journal of Medicinal Chemistry, 2013, 56, 7382-7395.	2.9	37
31	Developing novel C-4 analogues of pyrrole-based antitubulin agents: weak but critical hydrogen bonding in the colchicine site. MedChemComm, 2013, 4, 417.	3.5	17
32	Fine tuning of the active site modulates specificity in the interaction of O-acetylserine sulfhydrylase isozymes with serine acetyltransferase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 169-181.	1.1	35
33	Structure–Activity Relationships of Retro-dihydrochalcones Isolated from Tacca sp Journal of Natural Products, 2013, 76, 2189-2194.	1.5	12
34	Identification of quercitrin as an inhibitor of the p90 S6 ribosomal kinase (RSK): structure of its complex with the N-terminal domain of RSK2 at 1.8â€Ã resolution. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 266-275.	2.5	15
35	lsozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. PLoS ONE, 2013, 8, e77558.	1.1	43
36	Biological Characterization of 3-(2-amino-ethyl)-5-[3-(4-butoxyl-phenyl)-propylidene]-thiazolidine-2,4-dione (K145) as a Selective Sphingosine Kinase-2 Inhibitor and Anticancer Agent. PLoS ONE, 2013, 8, e56471.	1.1	67

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37	Correct Protonation States and Relevant Waters = Better Computational Simulations?. Current Pharmaceutical Design, 2013, 19, 4291-4309.	0.9	7
38	Structural modelling and mutagenesis of human cytomegalovirus alkaline nuclease UL98. Journal of General Virology, 2012, 93, 130-138.	1.3	7
39	Pyrrole-Based Antitubulin Agents: Two Distinct Binding Modalities Are Predicted for C-2 Analogues in the Colchicine Site. ACS Medicinal Chemistry Letters, 2012, 3, 53-57.	1.3	20
40	On the Specificity of Heparin/Heparan Sulfate Binding to Proteins. Anion-Binding Sites on Antithrombin and Thrombin Are Fundamentally Different. PLoS ONE, 2012, 7, e48632.	1.1	45
41	3,5-Disubstituted-thiazolidine-2,4-dione analogs as anticancer agents: Design, synthesis and biological characterization. European Journal of Medicinal Chemistry, 2012, 47, 125-137.	2.6	77
42	Computational analysis of structure-based interactions and ligand properties can predict efflux effects on antibiotics. European Journal of Medicinal Chemistry, 2012, 52, 98-110.	2.6	10
43	Regio- and Stereoselective Syntheses of the Natural Product CCR5 Antagonist Anibamine and its Three Olefin Isomers. Journal of Organic Chemistry, 2011, 76, 7945-7952.	1.7	16
44	Editorial [Hot topic: Applying Induced Fit in Drug Discovery: Square Pegs and Round Holes? (Guest) Tj ETQq0 0 (Medicinal Chemistry, 2011, 11, 131-132.) rgBT /Ov 1.0	erlock 10 Tf 5 2
45	Applying an Empirical Hydropathic Forcefield in Refinement May Improve Low-Resolution Protein X-Ray Crystal Structures. PLoS ONE, 2011, 6, e15920.	1.1	13
46	Factors influencing protein tyrosine nitration—structure-based predictive models. Free Radical Biology and Medicine, 2011, 50, 749-762.	1.3	40
47	Premature Activation of the Paramyxovirus Fusion Protein before Target Cell Attachment with Corruption of the Viral Fusion Machinery. Journal of Biological Chemistry, 2011, 286, 37945-37954.	1.6	34
48	Using Active Site Mapping and Receptor-Based Pharmacophore Tools: Prelude to Docking and De Novo/Fragment-Based Ligand Design. Methods in Molecular Biology, 2011, 716, 39-54.	0.4	8
49	Bound Water at Protein-Protein Interfaces: Partners, Roles and Hydrophobic Bubbles as a Conserved Motif. PLoS ONE, 2011, 6, e24712.	1.1	57
50	A novel and efficient tool for locating and characterizing protein cavities and binding sites. Proteins: Structure, Function and Bioinformatics, 2010, 78, 825-842.	1.5	53
51	Hydrophobicity - Shake Flasks, Protein Folding and Drug Discovery. Current Topics in Medicinal Chemistry, 2010, 10, 67-83.	1.0	111
52	Nitration of the Tumor Suppressor Protein p53 at Tyrosine 327 Promotes p53 Oligomerization and Activation. Biochemistry, 2010, 49, 5331-5339.	1.2	51
53	Design of <i>O</i> -Acetylserine Sulfhydrylase Inhibitors by Mimicking Nature. Journal of Medicinal Chemistry, 2010, 53, 345-356.	2.9	75
54	Hydropathic analysis and biological evaluation of stilbene derivatives as colchicine site microtubule inhibitors with anti-leukemic activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 1237-1244.	2.5	10

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55	Web application for studying the free energy of binding and protonation states of protein–ligand complexes based on HINT. Journal of Computer-Aided Molecular Design, 2009, 23, 621-632.	1.3	26
56	Development of water soluble derivatives of cis-3, 4′, 5-trimethoxy-3′-aminostilbene for optimization and use in cancer therapy. Investigational New Drugs, 2009, 27, 41-52.	1.2	10
57	Design, synthesis and biological evaluation of novel stilbene-based antitumor agents. Bioorganic and Medicinal Chemistry, 2009, 17, 512-522.	1.4	27
58	Synthesis, structure–affinity relationships, and modeling of AMDA analogs at 5-HT2A and H1 receptors: Structural factors contributing to selectivity. Bioorganic and Medicinal Chemistry, 2009, 17, 6496-6504.	1.4	22
59	Structure–activity relationship (SAR) studies of 3-(2-amino-ethyl)-5-(4-ethoxy-benzylidene)-thiazolidine-2,4-dione: Development of potential substrate-specific ERK1/2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6042-6046.	1.0	39
60	Comparative Docking Study of Anibamine as the First Natural Product CCR5 Antagonist in CCR5 Homology Models. Journal of Chemical Information and Modeling, 2009, 49, 120-132.	2.5	34
61	Energyâ€based prediction of amino acidâ€nucleotide base recognition. Journal of Computational Chemistry, 2008, 29, 1955-1969.	1.5	44
62	Stilbene derivatives that are colchicine site microtubule inhibitors have antileukemic activity and minimal systemic toxicity. American Journal of Hematology, 2008, 83, 390-397.	2.0	21
63	Docking and hydropathic scoring of polysubstituted pyrrole compounds with antitubulin activity. Bioorganic and Medicinal Chemistry, 2008, 16, 2235-2242.	1.4	42
64	Novel inhibitors of anthrax edema factor. Bioorganic and Medicinal Chemistry, 2008, 16, 7225-7233.	1.4	38
65	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
66	Robust Classification of "Relevant―Water Molecules in Putative Protein Binding Sites. Journal of Medicinal Chemistry, 2008, 51, 1063-1067.	2.9	93
67	Molecular Modeling: Considerations for the Design of Pharmaceuticals and Biopharmaceuticals. , 2008, , 267-291.		0
68	A LC-Electrospray Tandem MS Method for the Analysis of Naltrexone in Canine Plasma Employing a Molecular Model to Demonstrate the Absence of Internal Standard Deuterium Isotope Effects. Journal of Chromatographic Science, 2007, 45, 694-700.	0.7	14
69	A Second Receptor Binding Site on Human Parainfluenza Virus Type 3 Hemagglutinin-Neuraminidase Contributes to Activation of the FusionMechanism. Journal of Virology, 2007, 81, 3216-3228.	1.5	87
70	Tyrosine Nitration of lκBα:  A Novel Mechanism for NF-κB Activation [,] . Biochemistry, 2007, 46, 11671-11683.	1.2	88
71	Complexity in Modeling and Understanding Protonation States: Computational Titration of HIVâ€l â€Protease–Inhibitor Complexes. Chemistry and Biodiversity, 2007, 4, 2564-2577.	1.0	10
72	Hydropathic Analysis and Comparison of KcsA and Shaker Potassium Channels. Chemistry and Biodiversity, 2007, 4, 2578-2592.	1.0	4

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73	The consequences of scoring docked ligand conformations using free energy correlations. European Journal of Medicinal Chemistry, 2007, 42, 921-933.	2.6	58
74	Energetics of the protein-DNA-water interaction. BMC Structural Biology, 2007, 7, 4.	2.3	57
75	Autophagic cell death, polyploidy and senescence induced in breast tumor cells by the substituted pyrrole JG-03-14, a novel microtubule poison. Biochemical Pharmacology, 2007, 74, 981-991.	2.0	72
76	Mapping the Energetics of Water–Protein and Water–Ligand Interactions with the "Natural―HINT Forcefield: Predictive Tools for Characterizing the Roles of Water in Biomolecules. Journal of Molecular Biology, 2006, 358, 289-309.	2.0	85
77	Water: How to evaluate its contribution in protein-ligand interactions. International Journal of Quantum Chemistry, 2006, 106, 647-651.	1.0	12
78	Tools for building a comprehensive modeling system for virtual screening under real biological conditions: The Computational Titration algorithm. Journal of Molecular Graphics and Modelling, 2006, 24, 434-439.	1.3	18
79	Paramyxovirus Receptor-Binding Molecules: Engagement of One Site on the Hemagglutinin-Neuraminidase Protein Modulates Activity at the Second Site. Journal of Virology, 2006, 80, 1204-1213.	1.5	57
80	A computational tool to optimize ligand selectivity between two similar biomacromolecular targets. Journal of Computer-Aided Molecular Design, 2005, 19, 69-82.	1.3	12
81	A molecular model to explain paclitaxel and docetaxel sensitivity changes through adduct formation with primary amines in electrospray ionization mass spectrometry. Rapid Communications in Mass Spectrometry, 2005, 19, 1221-1226.	0.7	14
82	Homology Model of the CDK1/cyclin B Complex. Journal of Biomolecular Structure and Dynamics, 2005, 22, 493-502.	2.0	37
83	Free Energy of Ligand Binding to Protein: Evaluation of the Contribution of Water Molecules by Computational Methods. Current Medicinal Chemistry, 2004, 11, 3093-3118.	1.2	89
84	Evaluation of Deuterium Isotope Effects in Normal-Phase LC-MS-MS Separations Using a Molecular Modeling Approach. Journal of Chromatographic Science, 2004, 42, 383-387.	0.7	60
85	The Importance of Being Exhaustive. Optimization of Bridging Structural Water Molecules and Water Networks in Models of Biological Systems. Chemistry and Biodiversity, 2004, 1, 98-105.	1.0	40
86	Getting it right: modeling of pH, solvent and "nearly―everything else in virtual screening of biological targets. Journal of Molecular Graphics and Modelling, 2004, 22, 479-486.	1.3	32
87	1,2-Dithiole-3-Ones as Potent Inhibitors of the Bacterial 3-Ketoacyl Acyl Carrier Protein Synthase III (FabH). Antimicrobial Agents and Chemotherapy, 2004, 48, 3093-3102.	1.4	88
88	ComputationalÂTitrationÂAnalysisÂofÂaÂMultiproticÂHIV-1ÂProteaseâ^`LigandÂComplex. Journal of the American Chemical Society, 2004, 126, 11764-11765.	6.6	34
89	A Computational Model for Anthracycline Binding to DNA:Â Tuning Groove-Binding Intercalators for Specific Sequences. Journal of Medicinal Chemistry, 2004, 47, 1360-1374.	2.9	47
90	Simple, Intuitive Calculations of Free Energy of Binding for Proteinâ^Ligand Complexes. 3. The Free Energy Contribution of Structural Water Molecules in HIV-1 Protease Complexes. Journal of Medicinal Chemistry, 2004, 47, 4507-4516.	2.9	112

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91	3D QSAR in modern drug design. , 2003, , 223-241.		14
92	Simple, Intuitive Calculations of Free Energy of Binding for Proteinâ^'Ligand Complexes. 2. Computational Titration and pH Effects in Molecular Models of Neuraminidaseâ^'Inhibitor Complexes. Journal of Medicinal Chemistry, 2003, 46, 4487-4500.	2.9	77
93	Hydropathic analysis of the free energy differences in anthracycline antibiotic binding to DNA. Nucleic Acids Research, 2003, 31, 4410-4416.	6.5	24
94	Simple, Intuitive Calculations of Free Energy of Binding for Proteinâ^'Ligand Complexes. 1. Models without Explicit Constrained Water. Journal of Medicinal Chemistry, 2002, 45, 2469-2483.	2.9	131
95	Which aminoglycoside ring is most important for binding? a hydropathic analysis of gentamicin, paromomycin, and analogues. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 119-122.	1.0	23
96	Computationally accessible method for estimating free energy changes resulting from site-specific mutations of biomolecules: Systematic model building and structural/hydropathic analysis of deoxy and oxy hemoglobins. Proteins: Structure, Function and Bioinformatics, 2001, 42, 355-377.	1.5	45
97	Very empirical treatment of solvation and entropy: a force field derived from log Po/w. Journal of Computer-Aided Molecular Design, 2001, 15, 381-393.	1.3	54
98	HINT predictive analysis of binding between retinol binding protein and hydrophobic ligands. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2129-2132.	1.0	13
99	Hydrophobicity: is LogPo/w more than the sum of its parts?. European Journal of Medicinal Chemistry, 2000, 35, 651-661.	2.6	236
100	Computational Methodology for Estimating Changes in Free Energies of Biomolecular Association upon Mutation. The Importance of Bound Water in Dimerâ^'Tetramer Assembly for β37 Mutant Hemoglobinsâ€. Biochemistry, 2000, 39, 1622-1633.	1.2	42
101	Use of 3D QSAR Methodology for Data Mining the National Cancer Institute Repository of Small Molecules: Application to HIV-1 Reverse Transcriptase Inhibition. Methods, 1998, 14, 255-263.	1.9	18
102	Identification and hydropathic characterization of structural features affecting sequence specificity for doxorubicin intercalation into DNA double-stranded polynucleotides. Nucleic Acids Research, 1998, 26, 4721-4732.	6.5	64
103	All-Atom Models for the Non-Nucleoside Binding Site of HIV-1 Reverse Transcriptase Complexed with Inhibitors: A 3D QSAR Approachâ€. Journal of Medicinal Chemistry, 1996, 39, 1645-1650.	2.9	53
104	E-state fields: Applications to 3D QSAR. Journal of Computer-Aided Molecular Design, 1996, 10, 513-520.	1.3	86
105	Differences in hydropathic properties of ligand binding at four independent sites in wheat germ agglutininâ€oligosaccharide crystal complexes. Protein Science, 1996, 5, 1466-1476.	3.1	91
106	The effect of physical organic properties on hydrophobic fields. Journal of Computer-Aided Molecular Design, 1994, 8, 41-49.	1.3	33
107	Evaluating docked complexes with the HINT exponential function and empirical atomic hydrophobicities. Journal of Computer-Aided Molecular Design, 1994, 8, 299-306.	1.3	52
108	Effect of distamycin on chlorambucil-induced mutagenesis in pZ189: evidence of a role for minor groove alkylation at adenine N-3. Mutagenesis, 1994, 9, 133-139.	1.0	15

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109	Allosteric modifiers of hemoglobin. 2. Crystallographically determined binding sites and hydrophobic binding/interaction analysis of novel hemoglobin oxygen effectors. Journal of Medicinal Chemistry, 1991, 34, 758-767.	2.9	123
110	HINT: A new method of empirical hydrophobic field calculation for CoMFA. Journal of Computer-Aided Molecular Design, 1991, 5, 545-552.	1.3	303
111	Molecular metals with widely tunable band filling. Structure/stoichiometry/counterion relationships in the electrochemistry of a cofacially joined polymeric phthalocyanine metal. Journal of the American Chemical Society, 1989, 111, 5259-5271.	6.6	38
112	Molecular metals with widely tunable band filling. Response of the collective properties of a phthalocyanine molecular metal to drastic excursions in partial oxidation state and charge-compensating counterions. Journal of the American Chemical Society, 1989, 111, 5271-5284.	6.6	20
113	Additions and Corrections. Electronic Structure Factors of Carbon-Hydrogen Bond Activation. The Photoelectron Spectroscopy of (Cyclohexenyl) manganese Tricarbonyl. Journal of the American Chemical Society, 1986, 108, 7134-7134.	6.6	0
114	Ligand additivity in the valence photoelectron spectroscopy of phosphine-substituted molybdenum carbonyls. Inorganic Chemistry, 1984, 23, 4361-4365.	1.9	29