Karel Berka

List of Publications by Year
in descending order

91 papers	4,746 citations	134610 34 h-index	120465 65 g-index
101 all docs	101 docs citations	101 times ranked	8466 citing authors

#	Article	IF	Citations
1	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
2	Antitumour drugs targeting tau R3 VQIVYK and Cys322 prevent seeding of endogenous tau aggregates by exogenous seeds. FEBS Journal, 2022, 289, 1929-1949.	2.2	7
3	OverProt: secondary structure consensus for protein families. Bioinformatics, 2022, 38, 3648-3650.	1.8	1
4	CATH: increased structural coverage of functional space. Nucleic Acids Research, 2021, 49, D266-D273.	6.5	270
5	In silico screening of drug candidates for thermoresponsive liposome formulations. Molecular Systems Design and Engineering, 2021, 6, 368-380.	1.7	4
6	Mol* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures. Nucleic Acids Research, 2021, 49, W431-W437.	6.5	515
7	Uncovering of cytochrome P450 anatomy by SecStrAnnotator. Scientific Reports, 2021, 11, 12345.	1.6	9
8	Optimized SQE atomic charges for peptides accessible via a web application. Journal of Cheminformatics, 2021, 13, 45.	2.8	2
9	2DProts: database of family-wide protein secondary structure diagrams. Bioinformatics, 2021, 37, 4599-4601.	1.8	3
10	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
11	Novel thiazolidinedione-hydroxamates as inhibitors of Mycobacterium tuberculosis virulence factor Zmp1. European Journal of Medicinal Chemistry, 2020, 185, 111812.	2.6	12
12	Cytokinin fluoroprobe reveals multiple sites of cytokinin perception at plasma membrane and endoplasmic reticulum. Nature Communications, 2020, 11, 4285.	5.8	64
13	Atomic Charge Calculator II: web-based tool for the calculation of partial atomic charges. Nucleic Acids Research, 2020, 48, W591-W596.	6.5	26
14	Visualization and Analysis of Protein Structures with LiteMol Suite. Methods in Molecular Biology, 2020, 2112, 1-13.	0.4	3
15	High-performance macromolecular data delivery and visualization for the web. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1167-1173.	1.1	3
16	MolMeDB: Molecules on Membranes Database. Database: the Journal of Biological Databases and Curation, 2019, 2019, .	1.4	9
17	In vitro testing of flash-frozen sublingual membranes for storage and reproducible permeability studies of macromolecular drugs from solution or nanofiber mats. International Journal of Pharmaceutics, 2019, 572, 118711.	2.6	3
18	Synthesis of novel galeterone derivatives and evaluation of their inÂvitro activity against prostate cancer cell lines. European Journal of Medicinal Chemistry, 2019, 179, 483-492.	2.6	13

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19	Automated Family-Wide Annotation of Secondary Structure Elements. Methods in Molecular Biology, 2019, 1958, 47-71.	0.4	5
20	Membrane-attached mammalian cytochromes P450: An overview of the membrane's effects on structure, drug binding, and interactions with redox partners. Journal of Inorganic Biochemistry, 2018, 183, 117-136.	1.5	117
21	Discovery of N²-(4-Amino-cyclohexyl)-9-cyclopentyl-N⁶-(4-morpholin-4-ylmethyl-phenyl)-9H-purine-2,6 as a Potent FLT3 Kinase Inhibitor for Acute Myeloid Leukemia with FLT3 Mutations. Journal of Medicinal Chemistry, 2018, 61, 3855-3869.	2.9	36
22	Secondary Structure Elements - Annotations and Schematic 2D Visualizations Stable for Individual Protein Families. Biophysical Journal, 2018, 114, 46a-47a.	0.2	1
23	ChannelsDB: database of biomacromolecular tunnels and pores. Nucleic Acids Research, 2018, 46, D399-D405.	6.5	30
24	Structural patterns of the human ABCC4/MRP4 exporter in lipid bilayers rationalize clinically observed polymorphisms. Pharmacological Research, 2018, 133, 318-327.	3.1	19
25	Interactive 3D Macromolecular Structure Data Mining with MolQL and Litemol Suite. Biophysical Journal, 2018, 114, 47a.	0.2	0
26	Channelsdb and Moleonline - Database and Tool for Analysis of Biomacromolecular Tunnels and Pores. Biophysical Journal, 2018, 114, 342a-343a.	0.2	1
27	MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update). Nucleic Acids Research, 2018, 46, W368-W373.	6.5	208
28	ALK5 kinase inhibitory activity and synthesis of 2,3,4-substituted 5,5-dimethyl-5,6-dihydro-4H-pyrrolo[1,2-b]pyrazoles. European Journal of Medicinal Chemistry, 2017, 127, 632-642.	2.6	8
29	Real-Time Interactive Visualisation of Large Macromolecular Assemblies and Molecular Machines at Atomic Resolution. Biophysical Journal, 2017, 112, 178a.	0.2	1
30	RH421 binds into the ATP-binding site on the Na+/K+-ATPase. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2113-2122.	1.4	3
31	Molecular insights into the role of a distal F240A mutation that alters CYP1A1 activity towards persistent organic pollutants. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2852-2860.	1.1	12
32	LiteMol suite: interactive web-based visualization of large-scale macromolecular structure data. Nature Methods, 2017, 14, 1121-1122.	9.0	137
33	Surface properties of MoS₂ probed by inverse gas chromatography and their impact on electrocatalytic properties. Nanoscale, 2017, 9, 19236-19244.	2.8	19
34	Acetylated deoxycholic (DCA) and cholic (CA) acids are potent ligands of pregnane X (PXR) receptor. Toxicology Letters, 2017, 265, 86-96.	0.4	25
35	LiteMol: web-based three-dimensional visualization of macromolecular structure data. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C669-C669.	0.0	1
36	Arabidopsis histidine kinase 4 cytokinin receptor â€“ The object of interest in ligand-receptor study. New Biotechnology, 2016, 33, S165.	2.4	2

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37	In silico pharmacology: Drug membrane partitioning and crossing. Pharmacological Research, 2016, 111, 471-486.	3.1	50
38	Ion Pathways in the Na⁺/K⁺-ATPase. Journal of Chemical Information and Modeling, 2016, 56, 2434-2444.	2.5	21
39	Biomacromolecular Fragments and Patterns. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 7-15.	0.3	0
40	Detection of Channels. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 59-69.	0.3	1
41	Effect of Lipid Charge on Membrane Immersion of Cytochrome P450 3A4. Journal of Physical Chemistry B, 2016, 120, 11205-11213.	1.2	24
42	Design, synthesis and biological activities of new brassinosteroid analogues with a phenyl group in the side chain. Organic and Biomolecular Chemistry, 2016, 14, 8691-8701.	1.5	21
43	Exponential repulsion improves structural predictability of molecular docking. Journal of Computational Chemistry, 2016, 37, 2485-2494.	1.5	8
44	Novel thidiazuron-derived inhibitors of cytokinin oxidase/dehydrogenase. Plant Molecular Biology, 2016, 92, 235-248.	2.0	43
45	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. Drug Metabolism and Disposition, 2016, 44, 576-590.	1.7	39
46	Tools and data services registry: a community effort to document bioinformatics resources. Nucleic Acids Research, 2016, 44, D38-D47.	6.5	113
47	Role of Enzyme Flexibility in Ligand Access and Egress to Active Site: Bias-Exchange Metadynamics Study of 1,3,7-Trimethyluric Acid in Cytochrome P450 3A4. Journal of Chemical Theory and Computation, 2016, 12, 2101-2109.	2.3	44
48	Synthesis, biological evaluation and molecular modeling of a novel series of 7-azaindole based tri-heterocyclic compounds as potent CDK2/Cyclin E inhibitors. European Journal of Medicinal Chemistry, 2016, 108, 701-719.	2.6	33
49	Structural Bioinformatics Databases of General Use. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 17-30.	0.3	0
50	Channel Characteristics. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 81-90.	0.3	0
51	Characterization of a Pyrazolo[4,3â€d]pyrimidine Inhibitor of Cyclinâ€Dependent Kinases 2 and 5 and Aurora A With Proâ€Apoptotic and Antiâ€Angiogenic Activity In Vitro. Chemical Biology and Drug Design, 2015, 86, 1528-1540.	1.5	16
52	Coarse-Grain Simulations of Skin Ceramide NS with Newly Derived Parameters Clarify Structure of Melted Phase. Journal of Physical Chemistry B, 2015, 119, 3988-3998.	1.2	26
53	Effect of Cholesterol on the Structure of Membrane-Attached Cytochrome P450 3A4. Journal of Chemical Information and Modeling, 2015, 55, 628-635.	2.5	25
54	Chrysin, baicalein and galangin are indirect activators of the human constitutive androstane receptor (CAR). Toxicology Letters, 2015, 233, 68-77.	0.4	37

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55	2,6,9-Trisubstituted purines as CRK3 kinase inhibitors with antileishmanial activity in vitro. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2298-2301.	1.0	11
56	Structural Changes in Ceramide Bilayers Rationalize Increased Permeation through Stratum Corneum Models with Shorter Acyl Tails. Journal of Physical Chemistry B, 2015, 119, 9811-9819.	1.2	46
57	Lipocarbazole, an efficient lipid peroxidation inhibitor anchored in the membrane. Bioorganic and Medicinal Chemistry, 2015, 23, 4866-4870.	1.4	13
58	Synergism of antioxidant action of vitamins E, C and quercetin is related to formation of molecular associations in biomembranes. Chemical Communications, 2015, 51, 7713-7716.	2.2	62
59	Rationalization of Reduced Penetration of Drugs through Ceramide Gel Phase Membrane. Langmuir, 2014, 30, 13942-13948.	1.6	28
60	Anatomy of enzyme channels. BMC Bioinformatics, 2014, 15, 379.	1.2	89
61	PDBsum additions. Nucleic Acids Research, 2014, 42, D292-D296.	6.5	279
62	Photoluminescence effects of graphitic core size and surface functional groups in carbon dots: COOâ^' induced red-shift emission. Carbon, 2014, 70, 279-286.	5.4	240
63	Synthesis and kinase inhibitory activity of new sulfonamide derivatives of pyrazolo[4,3-e][1,2,4]triazines. European Journal of Medicinal Chemistry, 2014, 78, 217-224.	2.6	27
64	Amphiphilic Drug-Like Molecules Accumulate in a Membrane below the Head Group Region. Journal of Physical Chemistry B, 2014, 118, 1030-1039.	1.2	89
65	Benchmarking of Force Fields for Moleculeâ€"Membrane Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4143-4151.	2.3	73
66	Biological activities of new monohydroxylated brassinosteroid analogues with a carboxylic group in the side chain. Steroids, 2014, 85, 58-64.	0.8	20
67	A Novel Series of Highly Potent 2,6,9-Trisubstituted Purine Cyclin-Dependent Kinase Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 6234-6247.	2.9	45
68	Behavior of Human Cytochromes P450 on Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11556-11564.	1.2	94
69	MOLE 2.0: advanced approach for analysis of biomacromolecular channels. Journal of Cheminformatics, 2013, 5, 39.	2.8	262
70	Molecular Insight into Affinities of Drugs and Their Metabolites to Lipid Bilayers. Journal of Physical Chemistry B, 2013, 117, 2403-2410.	1.2	50
71	Lipid Bilayer Membrane Affinity Rationalizes Inhibition of Lipid Peroxidation by a Natural Lignan Antioxidant. Journal of Physical Chemistry B, 2013, 117, 5043-5049.	1.2	22
72	Fluorone dyes have binding sites on both cytoplasmic and extracellular domains of Na,K-ATPase. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 568-576.	1.4	5

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73	Antiallergic Effects of Pigments Isolated from Green Sea Urchin (Strongylocentrotus droebachiensis) Shells. Planta Medica, 2013, 79, 1698-1704.	0.7	33
74	MOLEonline 2.0: interactive web-based analysis of biomacromolecular channels. Nucleic Acids Research, 2012, 40, W222-W227.	6.5	123
75	Is There a Relationship Between the Substrate Preferences and Structural Flexibility of Cytochromes P450?. Current Drug Metabolism, 2012, 13, 130-142.	0.7	60
76	Dynamics and Hydration of the Active Sites of Mammalian Cytochromes P450 Probed by Molecular Dynamics Simulations. Current Drug Metabolism, 2012, 13, 177-189.	0.7	49
77	Positioning of Antioxidant Quercetin and Its Metabolites in Lipid Bilayer Membranes: Implication for Their Lipid-Peroxidation Inhibition. Journal of Physical Chemistry B, 2012, 116, 1309-1318.	1.2	119
78	Convergence of Free Energy Profile of Coumarin in Lipid Bilayer. Journal of Chemical Theory and Computation, 2012, 8, 1200-1211.	2.3	102
79	Binding of quinidine radically increases the stability and decreases the flexibility of the cytochrome P450 2D6 active site. Journal of Inorganic Biochemistry, 2012, 110, 46-50.	1.5	19
80	Membrane Position of Ibuprofen Agrees with Suggested Access Path Entrance to Cytochrome P450 2C9 Active Site. Journal of Physical Chemistry A, 2011, 115, 11248-11255.	1.1	128
81	Novel Covalent Bond in Proteins: Calculations on Model Systems Question the Bond Stability. ChemPhysChem, 2011, 12, 3449-3457.	1.0	5
82	Insenstivity to Close Contacts and Inability to Predict Protein Foldability. Journal of Biomolecular Structure and Dynamics, 2011, 28, 633-634.	2.0	2
83	On the Reliability of the AMBER Force Field and its Empirical Dispersion Contribution for the Description of Noncovalent Complexes. ChemPhysChem, 2010, 11, 2399-2408.	1.0	30
84	Energy Matrix of Structurally Important Side-Chain/Side-Chain Interactions in Proteins. Journal of Chemical Theory and Computation, 2010, 6, 2191-2203.	2.3	33
85	Analysis of Energy Stabilization inside the Hydrophobic Core of Rubredoxin. ChemPhysChem, 2009, 10, 543-548.	1.0	4
86	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlatedab InitioQuantum Chemical and Empirical Potential Procedures. Journal of Chemical Theory and Computation, 2009, 5, 982-992.	2.3	89
87	Another role of proline: stabilization interactions in proteins and protein complexes concerning proline and tryptophane. Physical Chemistry Chemical Physics, 2008, 10, 6350.	1.3	80
88	Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270.	1.0	144
89	The Stabilization Energy of the GLU-LYS Salt Bridge in the Protein/Water Environment: Correlated Quantum Chemical ab initio, DFT and Empirical Potential Studies. Collection of Czechoslovak Chemical Communications, 2008, 73, 921-936.	1.0	2
90	Ligand binding to the human MT2 melatonin receptor: The role of residues in transmembrane domains 3, 6, and 7. Biochemical and Biophysical Research Communications, 2005, 332, 726-734.	1.0	27

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91	Molecular modeling of human MT2 melatonin receptor: the role of Val204, Leu272 and Tyr298 in ligand binding. Journal of Neurochemistry, 2004, 91, 836-842.	2.1	33