Edyta Dyguda-Kazimierowicz

List of Publications by Year
in descending order

23	581	840119 11	642321 23
papers	citations	h-index	g-index

23	23	23	772
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantitative Classification of Covalent and Noncovalent H-Bonds. Journal of Physical Chemistry B, 2006, 110, 6444-6446.	1.2	224
2	Rational Design of Orthogonal Multipolar Interactions with Fluorine in Proteinâ€“Ligand Complexes. Journal of Medicinal Chemistry, 2015, 58, 7465-7474.	2.9	70
3	Alkaline Hydrolysis of Organophosphorus Pesticides: The Dependence of the Reaction Mechanism on the Incoming Group Conformation. Journal of Physical Chemistry B, 2014, 118, 7277-7289.	1.2	43
4	Physical Nature of Intermolecular Interactions within cAMP-Dependent Protein Kinase Active Site: Differential Transition State Stabilization in Phosphoryl Transfer Reaction. Journal of Physical Chemistry B, 2008, 112, 11819-11826.	1.2	32
5	Gas-Phase Mechanisms of Degradation of Hazardous Organophosphorus Compounds: Do They Follow a Common Pattern of Alkaline Hydrolysis Reaction As in Phosphotriesterase?. Journal of Physical Chemistry B, 2008, 112, 9982-9991.	1.2	31
6	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. Chemical Communications, 2011, 47, 2517.	2.2	29
7	Origins of the Activity of PAL and LAP Enzyme Inhibitors:Â Toward Ab Initio Binding Affinity Prediction. Journal of the American Chemical Society, 2005, 127, 1658-1659.	6.6	20
8	The molecular basis of urokinase inhibition: from the nonempirical analysis of intermolecular interactions to the prediction of binding affinity. Journal of Molecular Modeling, 2007, 13, 677-683.	0.8	19
9	Exploiting the S4â€“S5 Specificity of Human Neutrophil Proteinase 3 to Improve the Potency of Peptidyl Di(chlorophenyl)-phosphonate Ester Inhibitors: A Kinetic and Molecular Modeling Analysis. Journal of Medicinal Chemistry, 2018, 61, 1858-1870.	2.9	14
10	The Mechanism of Phosphoryl Transfer Reaction and the Role of Active Site Residues on the Basis of Ribokinase-Like Kinases. International Journal of Molecular Sciences, 2004, 5, 141-153.	1.8	12
11	Nonempirical Energetic Analysis of Reactivity and Covalent Inhibition of Fatty Acid Amide Hydrolase. Journal of Physical Chemistry B, 2013, 117, 6656-6666.	1.2	11
12	Interaction between DNA, Albumin and Apo-Transferrin and Iridium(III) Complexes with Phosphines Derived from Fluoroquinolones as a Potent Anticancer Drug. Pharmaceuticals, 2021, 14, 685.	1.7	10
13	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. Journal of Physical Chemistry B, 2014, 118, 141210162534006.	1.2	9
14	Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-Î²-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions. Journal of Molecular Modeling, 2007, 13, 839-849.	0.8	8
15	Low cost prediction of relative stabilities of hydrogen bonded complexes from atomic multipole moments for overly short intermolecular distances. Journal of Computational Chemistry, 2013, 34, 1797-1799.	1.5	8
16	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductaseÂ1 inhibition. Journal of Computer-Aided Molecular Design, 2017, 31, 715-728.	1.3	8
17	Theoretical models of inhibitory activity for inhibitors of proteinâ€“protein interactions: targeting meninâ€“mixed lineage leukemia with small molecules. MedChemComm, 2017, 8, 2216-2227.	3.5	7
18	Synthesis, structural characterization, docking simulation and in vitro antiproliferative activity of the new gold(III) complex with 2-pyridineethanol. Journal of Inorganic Biochemistry, 2021, 215, 111311.	1.5	7

#	Article	IF	Citations
19	Tracking molecular charge distribution along reaction paths with atomic multipole moments. Structural Chemistry, 2016, 27, 429-438.	1.0	6
20	Theoretical Model of EphA2-Ephrin A1 Inhibition. Molecules, 2018, 23, 1688.	1.7	4
21	Revisiting the halogen bonding between phosphodiesterase type 5 and its inhibitors. Journal of Molecular Modeling, 2019, 25, 29.	0.8	4
22	Extension of an Atomâ€“Atom Dispersion Function to Halogen Bonds and Its Use for Rational Design of Drugs and Biocatalysts. Journal of Physical Chemistry A, 2021, 125, 1787-1799.	1.1	3
23	Validation of approximate nonempirical scoring model for menin-mixed lineage leukemia inhibitors. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2