Edyta Dyguda-Kazimierowicz

List of Publications by Citations

23 papers	484 citations	10 h-index	22 g-index
23 ext. papers	553 ext. citations	4.4 avg, IF	3.38 L-index

#	Paper	IF	Citations
23	Quantitative classification of covalent and noncovalent H-bonds. *Journal of Physical Chemistry B*, **2006**, 110, 6444-6	3.4	197
22	Rational Design of Orthogonal Multipolar Interactions with Fluorine in Protein-Ligand Complexes. *Journal of Medicinal Chemistry*, **2015**, 58, 7465-74	8.3	52
21	Alkaline hydrolysis of organophosphorus pesticides: the dependence of the reaction mechanism on the incoming group conformation. *Journal of Physical Chemistry B*, **2014**, 118, 7277-89	3.4	34
20	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, 9982-91	3.4	26
19	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, 11819-26	3.4	25
18	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. *Chemical Communications*, **2011**, 47, 2517-9	5.8	21
17	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, 677-83	2	19
16	Origins of the activity of PAL and LAP enzyme inhibitors: toward ab initio binding affinity prediction. *Journal of the American Chemical Society*, **2005**, 127, 1658-9	16.4	19
15	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	6.3	12
14	Exploiting the S4-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	8.3	11
13	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. *Journal of Physical Chemistry B*, **2013**, 117, 6656-66	3.4	10
12	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. *Journal of Physical Chemistry B*, **2014**, 118, 14727-36	3.4	8
11	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, 1797-9	3.5	8
10	Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-beta-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions. *Journal of Molecular Modeling*, **2007**, 13, 839-49	2	8
9	Theoretical models of inhibitory activity for inhibitors of protein-protein interactions: targeting menin-mixed lineage leukemia with small molecules. *MedChemComm*, **2017**, 8, 2216-2227	5	6
8	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductase1 inhibition. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 715-728	4.2	6
7	Tracking molecular charge distribution along reaction paths with atomic multipole moments. *Structural Chemistry*, **2016**, 27, 429-438	1.8	5

6	Revisiting the halogen bonding between phosphodiesterase type 5 and its inhibitors. *Journal of Molecular Modeling*, **2019**, 25, 29	2	4
5	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	4.2	4
4	Theoretical Model of EphA2-Ephrin A1 Inhibition. *Molecules*, **2018**, 23,	4.8	3
3	Interaction between DNA, Albumin and Apo-Transferrin and Iridium(III) Complexes with Phosphines Derived from Fluoroquinolones as a Potent Anticancer Drug. *Pharmaceuticals*, **2021**, 14,	5.2	2
2	Extension of an Atom-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	2.8	2
1	Validation of approximate nonempirical scoring model for menin-mixed lineage leukemia inhibitors. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	2