Aneta Jezierska

List of Publications by Year
in descending order

61	888	516561 16	526166 27
papers	citations	h-index	g-index

62	62	62	980
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Biological Evaluation and Molecular Docking Studies of Novel 1,3,4-Oxadiazole Derivatives of 4,6-Dimethyl-2-sulfanylpyridine-3-carboxamide. International Journal of Molecular Sciences, 2022, 23, 549.	1.8	6
2	Exploring Intra- and Intermolecular Interactions in Selected N-Oxidesâ€"The Role of Hydrogen Bonds. Molecules, 2022, 27, 792.	1.7	3
3	Inside out Approach to Rotator State in Hydrogen-Bonded Systemâ€"Experimental and Theoretical Cross-Examination in n-Octanol. International Journal of Molecular Sciences, 2022, 23, 2138.	1.8	2
4	Intermolecular Interactions and Spectroscopic Signatures of the Hydrogen-Bonded Systemâ€"n-Octanol in Experimental and Theoretical Studies. Molecules, 2022, 27, 1225.	1.7	1
5	Interactions between Artificial Channel Protein, Water Molecules, and Ions Based on Theoretical Approaches. Symmetry, 2022, 14, 691.	1.1	2
6	Revealing Intra- and Intermolecular Interactions Determining Physico-Chemical Features of Selected Quinolone Carboxylic Acid Derivatives. Molecules, 2022, 27, 2299.	1.7	0
7	Structure-Property Relationship in Selected Naphtho- and Anthra-Quinone Derivatives on the Basis of Density Functional Theory and Carâ€"Parrinello Molecular Dynamics. Symmetry, 2021, 13, 564.	1.1	5
8	Sensitivity of Intra- and Intermolecular Interactions of Benzo[h]quinoline from Carâ€"Parrinello Molecular Dynamics and Electronic Structure Inspection. International Journal of Molecular Sciences, 2021, 22, 5220.	1.8	2
9	Competition of Intra- and Intermolecular Forces in Anthraquinone and Its Selected Derivatives. Molecules, 2021, 26, 3448.	1.7	6
10	On the nature of inter- and intramolecular interactions involving benzo[h]quinoline and 10-hydroxybenzo[h]quinoline: Electronic ground state vs excited state study. Journal of Molecular Structure, 2021, 1234, 130126.	1.8	7
11	Non-Covalent Forces in Naphthazarinâ€"Cooperativity or Competition in the Light of Theoretical Approaches. International Journal of Molecular Sciences, 2021, 22, 8033.	1.8	6
12	Naphthazarin Derivatives in the Light of Intra- and Intermolecular Forces. Molecules, 2021, 26, 5642.	1.7	5
13	How Substitution Combines with Non-Covalent Interactions to Modulate 1,4-Naphthoquinone and Its Derivatives Molecular Featuresâ€"Multifactor Studies. International Journal of Molecular Sciences, 2021, 22, 10357.	1.8	3
14	Microsolvation of Histidineâ€"A Theoretical Study of Intermolecular Interactions Based on AIM and SAPT Approaches. Symmetry, 2020, 12, 1153.	1.1	3
15	Symmetry/Asymmetry of the NHN Hydrogen Bond in Protonated 1,8-Bis(dimethylamino)naphthalene. Symmetry, 2020, 12, 1924.	1.1	8
16	Inter- vs. Intramolecular Hydrogen Bond Patterns and Proton Dynamics in Nitrophthalic Acid Associates. Molecules, 2020, 25, 4720.	1.7	13
17	New anticandidal Cu(<scp>i</scp>) complexes with neocuproine and ketoconazole derived diphenyl(aminomethyl)phosphane: luminescence properties for detection in fungal cells. Dalton Transactions, 2020, 49, 8528-8539.	1.6	7
18	Theoretical study of intramolecular hydrogen bond in selected symmetric â€œproton spongesâ€•on the basis of DFT and CPMD methods. Journal of Molecular Modeling, 2020, 26, 37.	0.8	8

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19	Fluconazole and Lipopeptide Surfactin Interplay During Candida albicans Plasma Membrane and Cell Wall Remodeling Increases Fungal Immune System Exposure. Pharmaceutics, 2020, 12, 314.	2.0	22
20	New diphenylphosphane derivatives of ketoconazole are promising antifungal agents. Scientific Reports, 2019, 9, 16214.	1.6	14
21	Intramolecular Hydrogen Bonds in Selected Aromatic Compounds: Recent Developments. Catalysts, 2019, 9, 909.	1.6	14
22	Cooperativity of hydrogen bonding network in microsolvated biotin, the ligand of avidin class proteins. Journal of Molecular Modeling, 2019, 25, 361.	0.8	8
23	A molecular roundabout: triple cyclically arranged hydrogen bonds in light of experiment and theory. New Journal of Chemistry, 2018, 42, 19467-19477.	1.4	10
24	N-oxide Derivatives: Carâ€“Parrinello Molecular Dynamics and Electron Localization Function Study on Intramolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2018, 122, 6605-6614.	1.1	6
25	Hydrogen bonds in quinoline N-oxide derivatives: first-principle molecular dynamics and metadynamics ground state study. Structural Chemistry, 2016, 27, 65-75.	1.0	12
26	Correlations of NBO energies of individual hydrogen bonds in nucleic acid base pairs with some QTAIM parameters. Structural Chemistry, 2016, 27, 367-376.	1.0	25
27	Nâ€“Hâ‹¯O versus Oâ€“Hâ‹¯O: density functional calculation and first principle molecular dynamics study on a quinoline-2-carboxamide N-oxide. Journal of Molecular Modeling, 2015, 21, 47.	0.8	2
28	Hydrogen bridges of polycyclic aromatic systems with O-HÂ·Â·Â·O bonds â€" a gas-phase vs. solid-state Car-Parrinello study. Journal of Molecular Modeling, 2015, 21, 15.	0.8	4
29	â€œZwitterionic Proton Spongeâ€•Hydrogen Bonding Investigations on the Basis of Carâ€“Parrinello Molecular Dynamics. Journal of Chemical Information and Modeling, 2015, 55, 1148-1157.	2.5	12
30	Molecular reorganization of selected quinoline derivatives in the ground and excited statesâ€"Investigations via static DFT. Journal of Chemical Physics, 2015, 143, 034301.	1.2	7
31	A complex study of 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole monohydrate: A new low-molecular-weight immune response modifier. Journal of Molecular Structure, 2011, 999, 60-67.	1.8	8
32	pâ€Nitrobenzoic Acid Adsorption on Nanostructured Gold Surfaces Investigated by Combined Experimental and Computational Approaches. ChemPhysChem, 2011, 12, 2485-2495.	1.0	8
33	Quantitative and qualitative models for carcinogenicity prediction for non-congeneric chemicals using CP ANN method for regulatory uses. Molecular Diversity, 2010, 14, 581-594.	2.1	45
34	A combined experimental and theoretical study of benzoxaborole derivatives by Raman and IR spectroscopy, static DFT, and firstâ€principle molecular dynamics. Journal of Physical Organic Chemistry, 2010, 23, 451-460.	0.9	14
35	Investigations of an Oï£¿H Â· Â· Â· S hydrogen bond via Carâ€Parrinello and path integral molecular dynamics. Journal of Computational Chemistry, 2009, 30, 1241-1250.	1.5	13
36	Effects of tryptophan residue fluorination on streptavidin stability and biotinâ€“streptavidin interactions via molecular dynamics simulations. Journal of Molecular Modeling, 2009, 15, 257-266.	0.8	8

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37	Structural and electronic structure differences due to the Oâ€“HÂ·Â·Â·O and Oâ€“HÂ·Â·Â·S bond formation in selected benzamide derivatives: a first-principles molecular dynamics study. Theoretical Chemistry Accounts, 2009, 124, 319-330.	0.5	15
38	Interrelations between the Mesomeric and Electronegativity Effects in Para-Substituted Derivatives of Phenol/Phenolate and Aniline/Anilide H-Bonded Complexes: A DFT-Based Computational Study. Journal of Physical Chemistry A, 2009, 113, 5800-5805.	1.1	5
39	Impact of intermolecular hydrogen bond on structural properties of phenylboronic acid: quantum chemical and Xâ€ray study. Journal of Physical Organic Chemistry, 2008, 21, 472-482.	0.9	80
40	Spectroscopic Properties of a Strongly Anharmonic Mannich Base Nâ€oxide. ChemPhysChem, 2008, 9, 839-846.	1.0	24
41	Structural property investigations of 1-[2-(2-methoxyphenyl)ethyl]piperidinium chloride: An experimental and computational study. Journal of Molecular Structure, 2008, 891, 184-191.	1.8	3
42	First-Principle Molecular Dynamics Study of Selected Schiff and Mannich Bases:â€‰ Application of Two-Dimensional Potential of Mean Force to Systems with Strong Intramolecular Hydrogen Bonds. Journal of Chemical Theory and Computation, 2008, 4, 375-384.	2.3	21
43	H-Bonded Complexes of Aniline with HF/F^{â^'}and Anilide with HF in Terms of Symmetry-Adapted Perturbation, Atoms in Molecules, and Natural Bond Orbitals Theories. Journal of Physical Chemistry A, 2008, 112, 9895-9905.	1.1	27
44	Structural and spectroscopic properties of an aliphatic boronic acid studied by combination of experimental and theoretical methods. Journal of Chemical Physics, 2008, 128, 124512.	1.2	22
45	Car-Parrinello simulation of an Oâ€“H stretching envelope and potential of mean force of an intramolecular hydrogen bonded system: Application to a Mannich base in solid state and in vacuum. Journal of Chemical Physics, 2007, 126, 205101.	1.2	61
46	On the Oligomeric State of DJ-1 Protein and Its Mutants Associated with Parkinson Disease. Journal of Biological Chemistry, 2007, 282, 24905-24914.	1.6	30
47	Molecular Properties Investigation of a Substituted Aromatic Mannich Base:â€‰ Dynamic and Static Models. Journal of Chemical Information and Modeling, 2007, 47, 818-831.	2.5	7
48	Symmetry-Adapted Perturbation Theory Analysis of the NÂ·Â·Â·HX Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 650-655.	1.1	22
49	Carâ^'Parrinello Molecular Dynamics Study of Anharmonic Systems:Â A Mannich Base in Solution. Journal of Physical Chemistry B, 2007, 111, 5243-5248.	1.2	20
50	Synthesis, X-ray crystal structure and DFT study of potential ligands of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylâ€alkâ€•2-en-1-one type. Journal of Molecular Structure, 2007, 839, 33-40.	1.8	6
51	Solvent influence on the rotational isomerism in terephthalaldehyde. Structural Chemistry, 2006, 17, 177-188.	1.0	4
52	Molecular Modeling Study of Leflunomide and Its Active Metabolite Analogues.. ChemInform, 2005, 36, no.	0.1	0
53	Synthesis, analgesic activity and computational study of new isothiazolopyridines of Mannich base type. Il Farmaco, 2005, 60, 961-968.	0.9	55
54	Molecular Modeling Study of Leflunomide and Its Active Metabolite Analogues. Journal of Chemical Information and Modeling, 2005, 45, 39-48.	2.5	22

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55	Kohonen Network Study of Aromatic Compounds Based on Electronic and Nonelectronic Structure Descriptors. Journal of Chemical Information and Modeling, 2005, 45, 264-272.	2.5	15
56	Counter-propagation artificial neural network as a tool for the independent variable selection: Structure-mutagenicity study on aromatic amines. Molecular Diversity, 2004, 8, 371-377.	2.1	16
57	Structure/Activity Investigations of 5-Substituted 3-Methylisoxazole[5, 4-d]1, 2, 3-triazin-4-one Derivatives. Archiv Der Pharmazie, 2004, 337, 81-89.	2.1	12
58	Density Functional Calculation of the 2D Potential Surface and Deuterium Isotope Effect on13C Chemical Shifts in Picolinic AcidN-Oxide. Comparison with Experiment. Journal of the American Chemical Society, 2004, 126, 4437-4443.	6.6	42
59	An experimental and theoretical structural study of 5-amino-3-methylisoxazolo-4-carboxylic acid p -chlorophenylamide. Journal of Molecular Modeling, 2003, 9, 159-163.	0.8	4
60	DFT study of a novel lead structure in the isoxazole heterocyclic system. Computational and Theoretical Chemistry, 2003, 636, 203-214.	1.5	8
61	Modeling Toxicity by Using Supervised Kohonen Neural Networks. Journal of Chemical Information and Computer Sciences, 2003, 43, 485-492.	2.8	46