Mario Vazdar

List of Publications by Year
in descending order

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74 papers	2,264 citations	218381 26 h-index	223531 46 g-index
77 all docs	77 docs citations	77 times ranked	3256 citing authors

#	Article	IF	Citations
1	Chemistry and Reactivity of 4-hydroxy-2-nonenal (HNE) in Model Biological Systems. Mini-Reviews in Medicinal Chemistry, 2021, 21, 1394-1405.	1.1	3
2	ANT1 Activation and Inhibition Patterns Support the Fatty Acid Cycling Mechanism for Proton Transport. International Journal of Molecular Sciences, 2021, 22, 2490.	1.8	25
3	Computation and volumetric insight into (p,T) effect on aqueous guanidinium chloride. Journal of Chemical Thermodynamics, 2021, 158, 106450.	1.0	5
4	Mitochondrial Uncoupling Proteins (UCP1-UCP3) and Adenine Nucleotide Translocase (ANT1) Enhance the Protonophoric Action of 2,4-Dinitrophenol in Mitochondria and Planar Bilayer Membranes. Biomolecules, 2021, 11, 1178.	1.8	16
5	Molecular Dynamics Simulations of Mitochondrial Uncoupling Protein 2. International Journal of Molecular Sciences, 2021, 22, 1214.	1.8	8
6	Mechanism of Cell Penetration by Permeabilization of Late Endosomes: Interplay between a Multivalent TAT Peptide and Bis(monoacylglycero)phosphate. Cell Chemical Biology, 2020, 27, 1296-1307.e5.	2.5	23
7	Molecular Dynamics Simulations of the Elusive Matrixâ€Open State of Mitochondrial ADP/ATP Carrier. Israel Journal of Chemistry, 2020, 60, 735-743.	1.0	11
8	Molecular dynamics study of functionally relevant interdomain and active site interactions in the autotransporter esterase EstA from Pseudomonas aeruginosa. Molecular Simulation, 2020, 46, 743-756.	0.9	0
9	Desaturase specificity is controlled by the physicochemical properties of a single amino acid residue in the substrate binding tunnel. Computational and Structural Biotechnology Journal, 2020, 18, 1202-1209.	1.9	8
10	Surface Propensity of Aqueous Atmospheric Bromine at the Liquidâ€“Gas Interface. Journal of Physical Chemistry Letters, 2020, 11, 3422-3429.	2.1	22
11	Vibrational spectroscopy combined with molecular dynamics simulations as a tool for studying behavior of reactive aldehydes inserted in phospholipid bilayers. Chemistry and Physics of Lipids, 2019, 225, 104793.	1.5	3
12	Covalent modification of phosphatidylethanolamine by 4-hydroxy-2-nonenal increases sodium permeability across phospholipid bilayer membranes. Free Radical Biology and Medicine, 2019, 143, 433-440.	1.3	13
13	Calculation of apparent pKa values of saturated fatty acids with different lengths in DOPC phospholipid bilayers. Physical Chemistry Chemical Physics, 2019, 21, 10052-10060.	1.3	16
14	Membrane Lipids Alter Uncoupling Effect of 2,4 Dinitrophenol. Biophysical Journal, 2019, 116, 511a.	0.2	0
15	A Computational Insight into Reaction Between Different Amino Acids with Reactive Aldehydes 4-hydroxy-2-nonenal and 4-oxo-2-nonenal. Croatica Chemica Acta, 2019, 92, 229-239.	0.1	0
16	Revisited Mechanism of Reaction between a Model Lysine Amino Acid Side Chain and 4-Hydroxynonenal in Different Solvent Environments. Journal of Organic Chemistry, 2019, 84, 526-535.	1.7	14
17	How cardiolipin peroxidation alters the properties of the inner mitochondrial membrane?. Chemistry and Physics of Lipids, 2018, 214, 15-23.	1.5	35
18	Photocyclization of Tetra- and Pentapeptides Containing Adamantylphthalimide and Phenylalanines: Reaction Efficiency and Diastereoselectivity. Journal of Organic Chemistry, 2018, 83, 14905-14922.	1.7	10

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19	Coarse-grained model of titrating peptides interacting with lipid bilayers. Journal of Chemical Physics, 2018, 149, 244108.	1.2	4
20	Synthesis of Glycomimetics by Diastereoselective Passerini Reaction. Journal of Organic Chemistry, 2018, 83, 13146-13156.	1.7	17
21	Arginine â€œMagicâ€• Guanidinium Like-Charge Ion Pairing from Aqueous Salts to Cell Penetrating Peptides. Accounts of Chemical Research, 2018, 51, 1455-1464.	7.6	128
22	Mechanism of Long-Chain Free Fatty Acid Protonation at the Membrane-Water Interface. Biophysical Journal, 2018, 114, 2142-2151.	0.2	57
23	Anomalous surface behavior of hydrated guanidinium ions due to ion pairing. Journal of Chemical Physics, 2018, 148, 144508.	1.2	10
24	Distributions of therapeutically promising neurosteroids in cellular membranes. Chemistry and Physics of Lipids, 2017, 203, 78-86.	1.5	3
25	Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2017, , 1697-1739.		1
26	Metal-induced supramolecular chirality inversion of small self-assembled molecules in solution. Chemical Communications, 2017, 53, 1945-1948.	2.2	28
27	Reaction Mechanism of Covalent Modification of Phosphatidylethanolamine Lipids by Reactive Aldehydes 4-Hydroxy-2-nonenal and 4-Oxo-2-nonenal. Chemical Research in Toxicology, 2017, 30, 840-850.	1.7	19
28	Anomalous Proteinâ€“Protein Interactions in Multivalent Salt Solution. Journal of Physical Chemistry B, 2017, 121, 3000-3006.	1.2	23
29	A surface-stabilized ozonide triggers bromide oxidation at the aqueous solution-vapour interface. Nature Communications, 2017, 8, 700.	5.8	59
30	Self-association of a highly charged arginine-rich cell-penetrating peptide. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11428-11433.	3.3	63
31	The Antiferromagnetic Spin Coupling in Nonâ€kekulÃ© Acenesâ€”Impressive Polyradical Character Revealed by Highâ€Level Multireference Methods. ChemPhysChem, 2016, 17, 2013-2021.	1.0	4
32	Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers. Journal of Physical Chemistry B, 2016, 120, 9287-9296.	1.2	76
33	Unraveling the weak hydrogen bonds of ethynylpyridines and ethynylbenzene with trimethylphosphate â€” A combined FT-Raman spectroscopic and quantum-chemical study. Journal of Molecular Liquids, 2016, 218, 499-507.	2.3	4
34	Guanidinium Pairing Facilitates Membrane Translocation. Journal of Physical Chemistry B, 2016, 120, 143-153.	1.2	22
35	Temperature-induced release of crystal water in the Co, Mo and Pt complexes of N,N-diacetatedithiocarbamate. FTIR spectroscopy and quantum chemical study. Journal of Molecular Structure, 2016, 1103, 245-253.	1.8	4
36	Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2016, , 1-43.		0

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37	Cholesterol under oxidative stressâ€"How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. Free Radical Biology and Medicine, 2015, 84, 30-41.	1.3	57
38	High pressure promoted exchange of guests from hemicarceplexes. Tetrahedron, 2015, 71, 550-553.	1.0	6
39	Ab Initio Study of the Reaction of Ozone with Bromide Ion. Journal of Physical Chemistry A, 2015, 119, 4482-4488.	1.1	13
40	The molecular mechanism behind reactive aldehyde action on transmembrane translocations of proton and potassium ions. Free Radical Biology and Medicine, 2015, 89, 1067-1076.	1.3	39
41	Synthesis of new 2-aminoimidazolones with antiproliferative activity via base promoted amino-Î²-lactam rearrangement. Tetrahedron, 2015, 71, 9202-9215.	1.0	14
42	A computational study of regioselectivity in Î²-lactam iminothiazolidinone formation. Tetrahedron Letters, 2015, 56, 6908-6911.	0.7	2
43	The exploration of hydrogen bonding properties of 2,6- and 3,5-diethynylpyridine by IR spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1912-1923.	2.0	3
44	Multireference Configuration Interaction Methods â€" An Application to the Valence Isomerism in Cyclobutadieno-p-benzoquinone and its Diprotonated Form. Croatica Chemica Acta, 2015, 88, 495-503.	0.1	0
45	Does fluoride disrupt hydrogen bond network in cationic lipid bilayer? Time-dependent fluorescence shift of Laurdan and molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 22D516.	1.2	6
46	Acetamide as the model of the peptide bond: Nonadiabatic photodynamical simulations in the gas phase and in the argon matrix. Computational and Theoretical Chemistry, 2014, 1040-1041, 136-143.	1.1	4
47	Accurate Determination of the Orientational Distribution of a Fluorescent Molecule in a Phospholipid Membrane. Journal of Physical Chemistry B, 2014, 118, 855-863.	1.2	30
48	The study of hydrogen bonding and Ï€â‹¯Ï€ interactions in phenolâ‹¯ethynylbenzene complex by IR spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 6-14.	2.0	31
49	Interactions of monovalent salts with cationic lipid bilayers. Faraday Discussions, 2013, 160, 341-358.	1.6	17
50	Aggregation of Oligoarginines at Phospholipid Membranes: Molecular Dynamics Simulations, Time-Dependent Fluorescence Shift, and Biomimetic Colorimetric Assays. Journal of Physical Chemistry B, 2013, 117, 11530-11540.	1.2	34
51	Aqueous Guanidiniumâ€"Carbonate Interactions by Molecular Dynamics and Neutron Scattering: Relevance to Ionâ€"Protein Interactions. Journal of Physical Chemistry B, 2013, 117, 1844-1848.	1.2	33
52	Overcharging in Biological Systems: Reversal of Electrophoretic Mobility of Aqueous Polyaspartate by Multivalent Cations. Physical Review Letters, 2012, 108, 186101.	2.9	61
53	Behavior of 4-Hydroxynonenal in Phospholipid Membranes. Journal of Physical Chemistry B, 2012, 116, 6411-6415.	1.2	31
54	QM/MM non-adiabatic decay dynamics of formamide in polar and non-polar solvents. Physical Chemistry Chemical Physics, 2012, 14, 13262.	1.3	11

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55	Like-Charge Ion Pairing in Water: An Ab Initio Molecular Dynamics Study of Aqueous Guanidinium Cations. Journal of Physical Chemistry Letters, 2012, 3, 2021-2024.	2.1	58
56	Ions at Hydrophobic Aqueous Interfaces: Molecular Dynamics with Effective Polarization. Journal of Physical Chemistry Letters, 2012, 3, 2087-2091.	2.1	89
57	Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2012, , 1175-1213.		3
58	Thermal reaction of [3,4]-benzo-8-substituted-3Z,5Z,7E-octatetraenes and quantum-chemical study of the (8Ï€,6Ï€)-electrocyclisation. Organic and Biomolecular Chemistry, 2011, 9, 6771.	1.5	11
59	Orientational Dependence of the Affinity of Guanidinium Ions to the Water Surface. Journal of Physical Chemistry B, 2011, 115, 12521-12526.	1.2	44
60	Like-Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations. Journal of Physical Chemistry A, 2011, 115, 11193-11201.	1.1	53
61	Absorption and Fluorescence of PRODAN in Phospholipid Bilayers: A Combined Quantum Mechanics and Classical Molecular Dynamics Study. Journal of Physical Chemistry A, 2011, 115, 11428-11437.	1.1	43
62	Ab initioquantum dynamical study of the multi-state nonadiabatic photodissociation of pyrrole. Journal of Chemical Physics, 2011, 135, 154310.	1.2	27
63	Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond. Challenges and Advances in Computational Chemistry and Physics, 2010, , 77-106.	0.6	7
64	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. Physical Chemistry Chemical Physics, 2010, 12, 12719.	1.3	29
65	Zwitterionic structures of strained cis-pyramidalized disilenes: fact or artifact. Theoretical Chemistry Accounts, 2009, 124, 421-430.	0.5	8
66	The Isomerization Barrier in Cyanocyclobutadienes: An ab Initio Multireference Average Quadratic Coupled Cluster Study. Journal of Physical Chemistry A, 2009, 113, 8351-8358.	1.1	11
67	Excited-state non-adiabatic dynamics simulations of pyrrole. Molecular Physics, 2009, 107, 845-854.	0.8	65
68	The effect of protonation on the photodissociation processes in formamide â€“ An ab initio surface hopping dynamics study. Chemical Physics, 2008, 349, 308-318.	0.9	20
69	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 228-240.	2.0	422
70	The nonadiabatic deactivation paths of pyrrole. Journal of Chemical Physics, 2006, 125, 164323.	1.2	101
71	Automerization reaction of cyclobutadiene and its barrier height: Anab initiobenchmark multireference average-quadratic coupled cluster study. Journal of Chemical Physics, 2006, 125, 064310.	1.2	101
72	Magnetic domain states in nano-sized Co nuclei electrodeposited onto monocrystalline silicon. Materials Letters, 2004, 58, 3518-3522.	1.3	17

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73	Electrodeposition of nano-sized nuclei of magnetic Coâ€“Ni alloys onto n-Si (100). Electrochemistry Communications, 2001, 3, 159-163.	2.3	26
74	Mechanism of Cell Penetration by Permeabilization of Late Endosomes: Interplay between a Multivalent TAT-Like Cell-Penetrating Peptide and the Lipid Bis(Monoacylglycerol)Phosphate. SSRN Electronic Journal, 0, , .	0.4	0