Arvi Rauk

List of Publications by Year
in descending order

86 papers	5,335 citations	201575 27 h-index	88593 70 g-index
91 all docs	91 docs citations	91 times ranked	5145 citing authors

#	Article	IF	Citations
1	Pseudopeptide Amyloid Aggregation Inhibitors: In Silico, Single Molecule and Cell Viability Studies. International Journal of Molecular Sciences, 2021, 22, 1051.	1.8	12
2	Pseudopeptide Designed to Inhibit Oligomerization and Redox Chemistry in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2019, 123, 5206-5215.	1.2	3
3	Exploring Amyloid-Î² Dimer Structure Using Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 4658-4670.	1.1	13
4	New Orbital Symmetry-Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives. Journal of Physical Chemistry A, 2019, 123, 1749-1757.	1.1	17
5	Î²-N-Methylamino-l-alanine (BMAA) Not Involved in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2018, 122, 4472-4480.	1.2	12
6	d-Amino Acid Pseudopeptides as Potential Amyloid-Beta Aggregation Inhibitors. Molecules, 2018, 23, 2387.	1.7	9
7	Copper(I) Chelators for Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2017, 121, 11304-11310.	1.2	10
8	Interaction of the N-AcAÎ²(13â€“23)NH2 segment of the beta amyloid peptide with beta-sheet-blocking peptides: site and edge specificity. Canadian Journal of Chemistry, 2016, 94, 583-592.	0.6	5
9	Molecular dynamics studies of a Î²-sheet blocking peptide with the full-length amyloid beta peptide of Alzheimerâ€™s disease. Canadian Journal of Chemistry, 2016, 94, 833-841.	0.6	6
10	Molecular dynamics study of the monomers and dimers of N-AcAÎ²(13â€“23)NH2: on the effect of pH on the aggregation of the amyloid beta peptide of Alzheimerâ€™s disease. Canadian Journal of Chemistry, 2016, 94, 273-281.	0.6	9
11	Testing synthetic amyloid-Î² aggregation inhibitor using single molecule atomic force spectroscopy. Biosensors and Bioelectronics, 2014, 54, 492-498.	5.3	26
12	Fe(III)â€“Heme Complexes with the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations of Binding and Redox Properties of Heme Bound to the His Residues of AÎ²(1â€“42). Journal of Chemical Theory and Computation, 2013, 9, 4233-4242.	2.3	7
13	The Binding of Fe(II)â€“Heme to the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations. Journal of Chemical Theory and Computation, 2012, 8, 5150-5158.	2.3	10
14	Measurement of the interaction of aqueous copper(II) with a model amyloid-Î² protein fragmentÂâ€” Interference from buffers. Canadian Journal of Chemistry, 2011, 89, 1429-1444.	0.6	8
15	The Structures and Stabilities of the Complexes of Biologically Available Ligands with Fe(III)â^'Porphine: An Ab Initio Study. Journal of Physical Chemistry B, 2011, 115, 569-579.	1.2	15
16	On the Involvement of Copper Binding to the N-Terminus of the Amyloid Beta Peptide of Alzheimer's Disease: A Computational Study on Model Systems. International Journal of Alzheimer's Disease, 2011, 2011, 1-15.	1.1	18
17	Structures and Stabilities of Fe2+/3+Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	1.1	27
18	Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane, and selenane. Canadian Journal of Chemistry, 2010, 88, 831-838.	0.6	5

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19	Can copper binding to the prion protein generate a misfolded form of the protein?. BioMetals, 2009, 22, 159-175.	1.8	21
20	The chemistry of Alzheimerâ€™s disease. Chemical Society Reviews, 2009, 38, 2698.	18.7	391
21	Mechanism of Hydrogen Peroxide Production by Copper-Bound Amyloid Beta Peptide: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 1202-1209.	1.2	64
22	Molecular dynamics study of the interaction of AÎ²(13-23) with Î²-sheet inhibitors. Arkivoc, 2009, 2009, 116-134.	0.3	6
23	Why is the amyloid beta peptide of Alzheimer's disease neurotoxic?. Dalton Transactions, 2008, , 1273.	1.6	122
24	The a Priori Calculation of Vibrational Circular Dichroism Intensities. Reviews in Computational Chemistry, 2007, , 261-301.	1.5	4
25	Molecular Dynamics Study of the Beta Amyloid Peptide of Alzheimer's Disease and Its Divalent Copper Complexes. Journal of Physical Chemistry B, 2007, 111, 3789-3799.	1.2	77
26	Ab initio modelling of the structure and redox behaviour of copper(I) bound to a Hisâ€“His model peptide: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2007, 12, 147-164.	1.1	48
27	One-electron oxidation of methionine peptides â€” Stability of the three-electron Sâ€”N(amide) bond. Canadian Journal of Chemistry, 2006, 84, 893-904.	0.6	24
28	Effect of Side Chains on Competing Pathways for Î²-Scission Reactions of Peptide-Backbone Alkoxyl Radicals. Journal of Physical Chemistry A, 2006, 110, 10316-10323.	1.1	19
29	Ab initio model studies of copper binding to peptides containing a Hisâ€“His sequence: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2005, 10, 887-902.	1.1	54
30	Computational Studies of Cu(II)/Met and Cu(I)/Met Binding Motifs Relevant for the Chemistry of Alzheimer's Disease. Journal of Physical Chemistry A, 2005, 109, 5498-5508.	1.1	20
31	Binding Affinities for Models of Biologically Available Potential Cu(II) Ligands Relevant to Alzheimer's Disease:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 8361-8370.	1.1	36
32	Dialkyl sulphur radical cations: competition between proton and methyl cation transfers to sulphur nucleophiles: anab initiostudy. Molecular Physics, 2005, 103, 1201-1209.	0.8	2
33	Modeling Î²-Scission Reactions of Peptide Backbone Alkoxy Radicals:Â Backbone Câ^'C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	2.3	6
34	Alzheimerâ€™s disease and the â€˜ABSENTâ€™ hypothesis: mechanism for amyloid Î² endothelial and neuronal toxicity. Medical Hypotheses, 2005, 65, 123-137.	0.8	33
35	Structure and reactions of the peroxy radicals of glycine and alanine in peptides: anab initiostudy. Journal of Physical Organic Chemistry, 2004, 17, 777-786.	0.9	17
36	One-Electron Oxidation of Methionine in Peptide Environments:Â The Effect of Three-Electron Bonding on the Reduction Potential of the Radical Cation. Journal of Physical Chemistry A, 2004, 108, 11032-11041.	1.1	46

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37	Entropies in Solution from Entropies in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 2720-2725.	1.1	98
38	Reactions of One-Electron-Oxidized Methionine with Oxygen:Â An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 6222-6230.	1.1	32
39	Computational studies of Cu(II)[peptide] binding motifs: Cu[HGGG] and Cu[HG] as models for Cu(II) binding to the prion protein octarepeat region. Journal of Biological Inorganic Chemistry, 2003, 8, 53-65.	1.1	65
40	H-Atom abstraction by C-centered radicals from cyclic and acyclic dipeptides. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3278-3288.	1.3	14
41	H-atom abstraction by thiyl radicals from peptides and cyclic dipeptides. A theoretical study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3994-3999.	1.3	34
42	Alkoxy radicals in the gaseous phase: Î²-scission reactions and formation by radical addition to carbonyl compounds. Canadian Journal of Chemistry, 2003, 81, 431-442.	0.6	58
43	A computational investigation of the structure of the novel anomeric amide N-azido-N-methoxyformamide and its concerted decomposition to methyl formate and nitrogen. Perkin Transactions II RSC, 2002, , 1740-1746.	1.1	24
44	H-atom abstraction from thiols by C-centered radicals. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2002, 4, 2965-2974.	1.3	32
45	The radical model of Alzheimer's disease: Specific recognition of Gly29 and Gly33 by Met35 in a Î²-sheet model of AÎ²: An ONIOM study. Journal of Alzheimer's Disease, 2002, 4, 283-289.	1.2	25
46	Tertiary cyclohexyl cations. Definitive evidence for the existence of isomeric structures (hyperconjomers). Perkin Transactions II RSC, 2001, , 869-874.	1.1	38
47	Influence of Î²-Sheet Structure on the Susceptibility of Proteins to Backbone Oxidative Damage:â€‰ Preference for Î±C-Centered Radical Formation at Glycine Residues of Antiparallel Î²-Sheets. Journal of the American Chemical Society, 2000, 122, 4185-4192.	6.6	54
48	Is Oxidative Damage by Î²-Amyloid and Prion Peptides Mediated by Hydrogen Atom Transfer from Glycine Î±-Carbon to Methionine Sulfur within Î²-Sheets?. Journal of the American Chemical Society, 2000, 122, 9761-9767.	6.6	89
49	Cheletropic Decomposition of Cyclic Nitrosoamines Revisited:â€‰ The Nature of the Transition States and a Critical Role of the Ring Strain. Journal of Organic Chemistry, 2000, 65, 3612-3619.	1.7	4
50	Conformational Stereochemistry of the HERON Amide,N-Methoxy-N-dimethylaminoformamide:Â A Theoretical Study. Journal of Organic Chemistry, 1999, 64, 2340-2345.	1.7	46
51	Mechanism of Dioxirane Oxidation of CH Bonds:Â Application to Homo- and Heterosubstituted Alkanes as a Model of the Oxidation of Peptides. Journal of Organic Chemistry, 1998, 63, 5413-5422.	1.7	59
52	Regioselective Preparation of 2,4-, 3,4-, and 2,3,4-Substituted Furan Rings. 2.1Regioselective Lithiation of 2-Silylated-3-substituted Furan Rings. Journal of Organic Chemistry, 1997, 62, 8750-8759.	1.7	22
53	Rearrangement of Protonated Propene Oxide to Protonated Propanal. Journal of the American Chemical Society, 1997, 119, 4712-4718.	6.6	47
54	A Computational Investigation of the Stereoisomerism in Heteroatom-Substituted Amides. Journal of Organic Chemistry, 1996, 61, 2337-2345.	1.7	52

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55	Ring Opening of Bicyclo[n.1.0]alkanones to 2-Cycloalkanone-1,3-diyls. Why Does Oxyallyl Diradical Formation Require Less Energy from Bicyclo[3.1.0]hexan-6-ones than from Bicyclo[1.1.0]butan-2-ones?. Journal of the American Chemical Society, 1996, 118, 4159-4166.	6.6	20
56	The lifetimes of gas phase CO2?? and N2O?? calculated from the transition probability of the autodetachment processA? ?A +e?. International Journal of Chemical Kinetics, 1994, 26, 7-24.	1.0	9
57	Vibrational circular dichroism intensities by ab initio secondâ€order Mo/llerâ€“Plesset vibronic coupling theory. Journal of Chemical Physics, 1994, 100, 7995-8002.	1.2	22
58	The transition probability of electron loss from anions in the gas phase: The lifetime of O2â€‰â‹…â^'. Journal of Chemical Physics, 1992, 97, 5522-5531.	1.2	3
59	Vibrational circular dichroism intensities: Ab initio vibronic coupling theory using the distributed origin gauge. Journal of Chemical Physics, 1992, 97, 6517-6534.	1.2	43
60	Structures, barriers for internal rotation and inversion, vibrational frequencies, and thermodynamic functions of CH2FCHF, CHF2CHF, and CF3CHF radicals: An ab initio study. Journal of Chemical Physics, 1991, 94, 7299-7310.	1.2	16
61	Structures, barriers for internal rotation and inversion, vibrational frequencies, and thermodynamic functions of CH2FCF2, CHF2CF2, and CF3CF2 radicals: An ab initio study. Journal of Chemical Physics, 1991, 95, 2774-2786.	1.2	15
62	Structures, barriers for rotation and inversion, vibrational frequencies, and thermodynamic functions of ethyl, Î±â€fluoroethyl, and Î±,Î±â€difluoroethyl radicals: An ab inito study. Journal of Chemical Physics, 1990, 93, 1187-1195.	1.2	28
63	Structures, barriers for internal rotation, vibrational frequencies, and thermodynamic functions of CH2FCH2, CHF2CH2, and CF3CH2radicals: Anabinitiostudy. Journal of Chemical Physics, 1990, 93, 6620-6629.	1.2	27
64	Implementation and applications of Gaussian 82 on a CDC Cyber 205. Journal of Computational Chemistry, 1987, 8, 324-332.	1.5	3
65	The electronic structure and optical activity of conjugated dienes: 1,3-Butadiene and ?- and ?-phellandrene. Journal of Computational Chemistry, 1980, 1, 240-256.	1.5	16
66	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.9	2,151
67	On the calculation of multiplet energies by the hartree-fock-slater method. Theoretica Chimica Acta, 1977, 43, 261-271.	0.9	912
68	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.9	55
69	Magnetic dipole moment integrals over Slater orbitals. Journal of Chemical Physics, 1973, 59, 5720-5724.	1.2	10
70	Appendix B: Exercises. , 0, , 247-312.		0
71	References and Notes. , 0, , 313-324.		0
72	Nucleophilic Substitution Reactions. , 0, , 129-136.		0

#	Article	IF	Citations
73	Appendix A: Derivation of Hartreeâ€“Fock Theory. , 0, , 218-246.		0
74	Symmetry and Stereochemistry. , 0, , 1-19.		0
75	Molecular Orbital Theory. , 0, , 20-33.		0
76	Orbital Interaction Theory. , 0, , 34-71.		0
77	Sigma Bonds and Orbital Interaction Theory. , 0, , 72-85.		0
78	Simple HÃ¼ckel Molecular Orbital Theory. , 0, , 86-97.		0
79	Reactions and Properties of Ï€ Bonds. , 0, , 98-104.		0
80	Reactive Intermediates. , 0, , 105-120.		0
81	Carbonyl Compounds. , 0, , 121-128.		0
82	Aromatic Compounds. , 0, , 150-160.		0
83	Pericyclic Reactions. , 0, , 161-174.		0
84	Organometallic Compounds. , 0, , 175-195.		0
85	Orbital and State Correlation Diagrams. , 0, , 196-208.		0
86	Bonds to Hydrogen. , 0, , 137-149.		0