Arvi Rauk

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1782583/publications.pdf

Version: 2024-02-01

86	5,335	201674	88630
papers	citations	27 h-index	70 g-index

91	91	91	5145
all docs	docs citations	times ranked	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.	4.1	12
2	Pseudopeptide Designed to Inhibit Oligomerization and Redox Chemistry in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2019, 123, 5206-5215.	2.6	3
3	Exploring Amyloid-Î² Dimer Structure Using Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 4658-4670.	2.5	13
4	New Orbital Symmetry-Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives. Journal of Physical Chemistry A, 2019, 123, 1749-1757.	2.5	17
5	Î²-N-Methylamino-l-alanine (BMAA) Not Involved in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2018, 122, 4472-4480.	2.6	12
6	d-Amino Acid Pseudopeptides as Potential Amyloid-Beta Aggregation Inhibitors. Molecules, 2018, 23, 2387.	3.8	9
7	Copper(I) Chelators for Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2017, 121, 11304-11310.	2.6	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.	1.1	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.	1.1	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.	1.1	9
11	Testing synthetic amyloid-Î² aggregation inhibitor using single molecule atomic force spectroscopy. Biosensors and Bioelectronics, 2014, 54, 492-498.	10.1	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.	5.3	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.	5.3	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.	1.1	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.	2.6	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.	2.0	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.	2.5	27
18	Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane, and selenane. Canadian Journal of Chemistry, 2010, 88, 831-838.	1.1	5

#	Article	IF	Citations
19	Can copper binding to the prion protein generate a misfolded form of the protein?. BioMetals, 2009, 22, 159-175.	4.1	21
20	The chemistry of Alzheimerâ€™s disease. Chemical Society Reviews, 2009, 38, 2698.	38.1	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.	2.6	64
22	Molecular dynamics study of the interaction of AÎ²(13-23) with Î²-sheet inhibitors. Arkivoc, 2009, 2009, 116-134.	0.5	6
23	Why is the amyloid beta peptide of Alzheimer's disease neurotoxic?. Dalton Transactions, 2008, , 1273.	3.3	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.	2.6	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.	2.6	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.	1.1	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.	2.5	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.	2.6	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.	2.5	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.	2.5	36
32	Dialkyl sulphur radical cations: competition between proton and methyl cation transfers to sulphur nucleophiles: anab initiostudy. Molecular Physics, 2005, 103, 1201-1209.	1.7	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.	5.3	6
34	Alzheimerâ€™s disease and the â€˜ABSENTâ€™ hypothesis: mechanism for amyloid Î² endothelial and neuronal toxicity. Medical Hypotheses, 2005, 65, 123-137.	1.5	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.	1.9	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.	2.5	46

#	Article	IF	Citations
37	Entropies in Solution from Entropies in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 2720-2725.	2.5	98
38	Reactions of One-Electron-Oxidized Methionine with Oxygen:Â An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 6222-6230.	2.5	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.	2.6	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.	2.8	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.	2.8	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.	1.1	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.	2.8	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.	2.6	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.	13.7	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.	13.7	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.	3.2	4
50	Conformational Stereochemistry of the HERON Amide,N-Methoxy-N-dimethylaminoformamide:Â A Theoretical Study. Journal of Organic Chemistry, 1999, 64, 2340-2345.	3.2	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.	3.2	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.	3.2	22
53	Rearrangement of Protonated Propene Oxide to Protonated Propanal. Journal of the American Chemical Society, 1997, 119, 4712-4718.	13.7	47
54	A Computational Investigation of the Stereoisomerism in Heteroatom-Substituted Amides. Journal of Organic Chemistry, 1996, 61, 2337-2345.	3.2	52

#	Article	IF	Citations
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.	13.7	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.	1.6	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.	3.0	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.	3.0	3
59	Vibrational circular dichroism intensities: Ab initio vibronic coupling theory using the distributed origin gauge. Journal of Chemical Physics, 1992, 97, 6517-6534.	3.0	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.	3.0	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.	3.0	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.	3.0	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.	3.0	27
64	Implementation and applications of Gaussian 82 on a CDC Cyber 205. Journal of Computational Chemistry, 1987, 8, 324-332.	3.3	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.	3.3	16
66	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.8	2,151
67	On the calculation of multiplet energies by the hartree-fock-slater method. Theoretica Chimica Acta, 1977, 43, 261-271.	0.8	912
68	On the calculation of bonding energies by the Hartree Fock Slater method. Theoretica Chimica Acta, 1977, 46, 1-10.	0.8	55
69	Magnetic dipole moment integrals over Slater orbitals. Journal of Chemical Physics, 1973, 59, 5720-5724.	3.0	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