

Piotr Paneth

List of Publications by Year in descending order

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176
papers

3,420
citations

159525

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206029

48
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178
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178
docs citations

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times ranked

3279
citing authors

#	ARTICLE	IF	CITATIONS
1	Unprecedentedly large ³⁷ Cl/ ³⁵ Cl equilibrium isotopic fractionation on nano-confinement of chloride anion. <i>Scientific Reports</i> , 2022, 12, 1768.	1.6	1
2	¹³ C Natural Isotope Abundance in Urothelium as a New Marker in the Follow-Up of Patients with Bladder Cancer. <i>Cancers</i> , 2022, 14, 2423.	1.7	5
3	Influence of Association on Binding of Disaccharides to YKL-39 and hHyal-1 Enzymes. <i>International Journal of Molecular Sciences</i> , 2022, 23, 7705.	1.8	0
4	4-Arylthiosemicarbazide derivatives as a new class of tyrosinase inhibitors and anti- <i>Toxoplasma gondii</i> agents. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1145-1164.	2.5	8
5	New organometallic ruthenium(ii) complexes with purine analogs – a wide perspective on their biological application. <i>Dalton Transactions</i> , 2021, 50, 5557-5573.	1.6	7
6	Intramolecular non-covalent isotope effects at natural abundance associated with the migration of paracetamol in solid matrices during liquid chromatography. <i>Journal of Chromatography A</i> , 2021, 1639, 461932.	1.8	6
7	Isotopic Consequences of Host-Guest Interactions; Noncovalent Chlorine Isotope Effects. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1874-1880.	1.2	2
8	1,3,4-Thiadiazoles Effectively Inhibit Proliferation of <i>Toxoplasma gondii</i> . <i>Cells</i> , 2021, 10, 1053.	1.8	6
9	Thiosemicarbazide Derivatives Decrease the ATPase Activity of <i>Staphylococcus aureus</i> Topoisomerase IV, Inhibit Mycobacterial Growth, and Affect Replication in <i>Mycobacterium smegmatis</i> . <i>International Journal of Molecular Sciences</i> , 2021, 22, 3881.	1.8	8
10	Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computational-Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate. <i>Environmental Science & Technology</i> , 2021, 55, 14037-14050.	4.6	19
11	Machine Learning augmented docking studies of aminothiureas at the SARS-CoV-2-ACE2 interface. <i>PLoS ONE</i> , 2021, 16, e0256834.	1.1	3
12	Antibacterial Activity of Fluorobenzoylthiosemicarbazides and Their Cyclic Analogues with 1,2,4-Triazole Scaffold. <i>Molecules</i> , 2021, 26, 170.	1.7	15
13	RNA-Inspired and Accelerated Degradation of Polylactide in Seawater. <i>Journal of the American Chemical Society</i> , 2021, 143, 16673-16681.	6.6	37
14	RNA-inspired intramolecular transesterification accelerates the hydrolysis of polyethylene-like polyphosphoesters. <i>Chemical Science</i> , 2021, 12, 16054-16064.	3.7	12
15	Characteristic of Oral Squamous Cell Carcinoma Tissues Using Isotope Ratio Mass Spectrometry. <i>Journal of Clinical Medicine</i> , 2020, 9, 3760.	1.0	5
16	Computational Investigations of Position-Specific Vapor Pressure Isotope Effects in Ethanol – Toward More Powerful Isotope Models for Food Forensics. <i>ACS Omega</i> , 2020, 5, 18499-18506.	1.6	2
17	Docking and QSAR of Aminothiureas at the SARS-CoV-2 S-Protein-Human ACE2 Receptor Interface. <i>Molecules</i> , 2020, 25, 4645.	1.7	6
18	Evolved <i>Fusarium oxysporum</i> laccase expressed in <i>Saccharomyces cerevisiae</i> . <i>Scientific Reports</i> , 2020, 10, 3244.	1.6	12

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19	The influence of experimental parameters on quantitative deuterium measurements for ethyl alcohols of different origin. <i>Journal of the Science of Food and Agriculture</i> , 2020, 100, 1812-1815.	1.7	0
20	Comparison of quantitative NMR and IRMS for the authentication of "Polish Vodka". <i>Journal of the Science of Food and Agriculture</i> , 2019, 99, 263-268.	1.7	14
21	Quantum approach to the mechanism of monothiopyrophosphate isomerization. <i>Journal of Molecular Modeling</i> , 2019, 25, 286.	0.8	3
22	Assessment of Nonnucleoside Inhibitors Binding to HIV-1 Reverse Transcriptase Using HYDE Scoring. <i>Pharmaceuticals</i> , 2019, 12, 64.	1.7	6
23	2- OMe -lysophosphatidylcholine analogues are GPR119 ligands and activate insulin secretion from Î²TC-3 pancreatic cells: Evaluation of structure-dependent biological activity. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2018, 1863, 91-103.	1.2	13
24	Diaryl ethers with carboxymethoxyphenacyl motif as potent HIV-1 reverse transcriptase inhibitors with improved solubility. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 9-16.	2.5	6
25	Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. <i>Molecules</i> , 2018, 23, 2981.	1.7	7
26	Non-statistical isotope fractionation as a novel "retro-biosynthetic" approach to understanding alkaloid metabolic pathways. <i>Phytochemistry Letters</i> , 2017, 20, 499-506.	0.6	8
27	Synthesis and antibacterial activity of 1,4-dibenzoylthiosemicarbazide derivatives. <i>Biomedicine and Pharmacotherapy</i> , 2017, 88, 1235-1242.	2.5	12
28	The cytotoxic effect of spiroflavanone derivatives, their binding ability to human serum albumin (HSA) and a DFT study on the mechanism of their synthesis. <i>Journal of Molecular Structure</i> , 2017, 1137, 267-276.	1.8	8
29	What do docking and QSAR tell us about the design of HIV-1 reverse transcriptase nonnucleoside inhibitors?. <i>Journal of Molecular Modeling</i> , 2017, 23, 317.	0.8	7
30	Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6638-6645.	1.1	5
31	Oxygen binding isotope effects of triazole-based HIV-1 reverse transcriptase inhibitors indicate the actual binding site. <i>Archives of Biochemistry and Biophysics</i> , 2017, 635, 87-95.	1.4	2
32	Insights into the role of methionine synthase in the universal ¹³ C depletion in O - and N -methyl groups of natural products. <i>Archives of Biochemistry and Biophysics</i> , 2017, 635, 60-65.	1.4	10
33	Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. <i>ACS Catalysis</i> , 2017, 7, 5294-5307.	5.5	38
34	A Search for Dual Action HIV-1 Reverse Transcriptase, Bacterial RNA Polymerase Inhibitors. <i>Molecules</i> , 2017, 22, 1808.	1.7	3
35	Measurement and Prediction of Chlorine Kinetic Isotope Effects in Enzymatic Systems. <i>Methods in Enzymology</i> , 2017, 596, 179-215.	0.4	6
36	Lipophilicity Studies on Thiosemicarbazide Derivatives. <i>Molecules</i> , 2017, 22, 952.	1.7	8

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37	Searching for novel scaffold of triazole non-nucleoside inhibitors of HIV-1 reverse transcriptase. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 1-9.	2.5	8
38	Carbon, Nitrogen and Sulphur concentration and $\delta^{13}\text{C}$, $\delta^{15}\text{N}$ values in <i>Hypogymnia physodes</i> within the montane area – preliminary data. <i>Geoscience Records</i> , 2016, 2, 24-32.	0.0	2
39	Substrate and Enzyme Specificity of the Kinetic Isotope Effects Associated with the Dioxygenation of Nitroaromatic Contaminants. <i>Environmental Science & Technology</i> , 2016, 50, 6708-6716.	4.6	27
40	Analyzing sites of OH radical attack (ring vs. side chain) in oxidation of substituted benzenes via dual stable isotope analysis ($\delta^{13}\text{C}$ and $\delta^2\text{H}$). <i>Science of the Total Environment</i> , 2016, 542, 484-494.	3.9	36
41	DFT Studies of S_2N_2 Dechlorination of Polychlorinated Biphenyls. <i>Environmental Science & Technology</i> , 2016, 50, 6293-6298.	4.6	16
42	Non-statistical ^{13}C Fractionation Distinguishes Co-incident and Divergent Steps in the Biosynthesis of the Alkaloids Nicotine and Tropine. <i>Journal of Biological Chemistry</i> , 2016, 291, 16620-16629.	1.6	15
43	Biological evaluation and molecular modelling study of thiosemicarbazide derivatives as bacterial type IIA topoisomerases inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 14-22.	2.5	18
44	Theoretical studies of energetics and binding isotope effects of binding a triazole-based inhibitor to HIV-1 reverse transcriptase. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 310-317.	1.3	5
45	The first investigation of Wilms' tumour atomic structure-nitrogen and carbon isotopic composition as a novel biomarker for the most individual approach in cancer disease. <i>Oncotarget</i> , 2016, 7, 76726-76734.	0.8	8
46	Hepatoblastoma Biology Using Isotope Ratio Mass Spectrometry: Utility of a Unique Technique for the Analysis of Oncological Specimens. <i>Postepy Higieny i Medycyny Doswiadczalnej</i> , 2016, 70, 797-802.	0.1	3
47	The first protocol of stable isotope ratio assessment in tumor tissues based on original research. <i>Polish Journal of Pathology</i> , 2015, 3, 288-295.	0.1	7
48	Rhabdomyosarcoma in children in the light of isotope ratio mass spectrometry. <i>Polish Journal of Pathology</i> , 2015, 4, 383-388.	0.1	6
49	Search for human DNA topoisomerase II poisons in the group of 2,5-disubstituted-1,3,4-thiadiazoles. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2015, 30, 1021-1026.	2.5	13
50	Design, synthesis and biological evaluation of 4-benzoyl-1-dichlorobenzoylthiosemicarbazides as potent Gram-positive antibacterial agents. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2015, 31, 1-7.	2.5	6
51	Binding Isotope Effects as a Tool for Distinguishing Hydrophobic and Hydrophilic Binding Sites of HIV-1 RT. <i>Journal of Physical Chemistry B</i> , 2015, 119, 917-927.	1.2	34
52	Pharmacological and Structure-Activity Relationship Evaluation of 4-aryl-1-Diphenylacetyl(thio)semicarbazides. <i>Molecules</i> , 2014, 19, 4745-4759.	1.7	11
53	1,4-Disubstituted Thiosemicarbazide Derivatives are Potent Inhibitors of <i>Toxoplasma gondii</i> Proliferation. <i>Molecules</i> , 2014, 19, 9926-9943.	1.7	24
54	Triazole-Based Compound as a Candidate To Develop Novel Medicines To Treat Toxoplasmosis. <i>Antimicrobial Agents and Chemotherapy</i> , 2014, 58, 7583-7585.	1.4	17

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55	A DFT study of permanganate oxidation of toluene and its ortho-nitroderivatives. Journal of Molecular Modeling, 2014, 20, 2091.	0.8	6
56	A DFT Study of the <i>cis</i> -Dihydroxylation of Nitroaromatic Compounds Catalyzed by Nitrobenzene Dioxygenase. Journal of Physical Chemistry B, 2014, 118, 3245-3256.	1.2	30
57	A DFT and ONIOM study of C-H hydroxylation catalyzed by nitrobenzene 1,2-dioxygenase. Physical Chemistry Chemical Physics, 2014, 16, 13889-13899.	1.3	14
58	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2246-2254.	2.3	27
59	Binding Isotope Effects. Chemical Reviews, 2013, 113, 7851-7879.	23.0	72
60	Cytotoxic effect and molecular docking of 4-ethoxycarbonylmethyl-1-(piperidin-4-ylcarbonyl)-thiosemicarbazide—a novel topoisomerase II inhibitor. Journal of Molecular Modeling, 2013, 19, 1319-1324.	0.8	13
61	Assessing Molecular Docking Tools for Relative Biological Activity Prediction: A Case Study of Triazole HIV-1 NNRTIs. Journal of Chemical Information and Modeling, 2013, 53, 3326-3342.	2.5	29
62	Binding modes of DL-2-haloacid dehalogenase revealed by crystallography, modeling and isotope effects studies. Archives of Biochemistry and Biophysics, 2013, 540, 26-32.	1.4	13
63	Structure-cytotoxic activity relationship of 3-arylidene flavanone and chromanone (E,Z isomers) and 3-arylflavones. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4102-4106.	1.0	24
64	Isotopic Analysis of Oxidative Pollutant Degradation Pathways Exhibiting Large H Isotope Fractionation. Environmental Science & Technology, 2013, 47, 13459-13468.	4.6	37
65	Isotopic fractionation - chemical v. environmental perspective. Environmental Chemistry, 2012, 9, 67.	0.7	10
66	Cytochrome P450-Catalyzed Degradation of Nicotine: Fundamental Parameters Determining Hydroxylation by Cytochrome P450 2A6 at the 5 ^α -Carbon or the <i>N</i> -Methyl Carbon. Journal of Physical Chemistry B, 2012, 116, 7827-7840.	1.2	14
67	Extending Limits of Chlorine Kinetic Isotope Effects. Journal of Organic Chemistry, 2012, 77, 5120-5124.	1.7	23
68	Does dehydrocyclization of 4-benzoylthiosemicarbazides in acetic acid lead to <i>s</i> -triazoles or thiadiazoles?. Structural Chemistry, 2012, 23, 1441-1448.	1.0	5
69	Cytochrome P450 Monooxygenase-Catalyzed Ring Opening of the Bicyclic Amine, Nortropine: An Experimental and DFT Computational Study. ChemCatChem, 2012, 4, 530-539.	1.8	6
70	Binding Ligands and Cofactor to L-Lactate Dehydrogenase from Human Skeletal and Heart Muscles. Journal of Physical Chemistry B, 2011, 115, 6366-6376.	1.2	13
71	DFT Study of Trichloroethene Reaction with Permanganate in Aqueous Solution. Environmental Science & Technology, 2011, 45, 3006-3011.	4.6	29
72	Measurements of Heavy-Atom Isotope Effects Using ¹ H NMR Spectroscopy. Journal of Organic Chemistry, 2011, 76, 8033-8035.	1.7	19

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73	Differences and similarities in binding of pyruvate and l-lactate in the active site of M4 and H4 isoforms of human lactate dehydrogenase. Archives of Biochemistry and Biophysics, 2011, 505, 33-41.	1.4	16
74	Elucidation of the mechanism of N-demethylation catalyzed by cytochrome P450 monooxygenase is facilitated by exploiting nitrogen-15 heavy isotope effects. Archives of Biochemistry and Biophysics, 2011, 510, 35-41.	1.4	14
75	Biological and docking studies of topoisomerase IV inhibition by thiosemicarbazides. Journal of Molecular Modeling, 2011, 17, 2297-2303.	0.8	29
76	Theoretical evaluation of isotopic fractionation factors in oxidation reactions of benzene, phenol and chlorophenols. Journal of Molecular Modeling, 2011, 17, 2285-2296.	0.8	16
77	Synthetic route to isotopically labelled-oxamate. Journal of Labelled Compounds and Radiopharmaceuticals, 2011, 54, 344-344.	0.5	0
78	Valence anions of N-acetylproline in the gas phase: Computational and anion photoelectron spectroscopic studies. Journal of Chemical Physics, 2011, 135, 114301.	1.2	9
79	Importance of the Lactate Dehydrogenase Quaternary Structure in Theoretical Calculations. Journal of Physical Chemistry B, 2010, 114, 3393-3397.	1.2	15
80	Antimicrobial Properties of 4-Aryl-3-(2-methyl-furan-3-yl)-1,2,4-triazoline-5-thiones. Phosphorus, Sulfur and Silicon and the Related Elements, 2009, 184, 3149-3159.	0.8	8
81	Modeling excitation properties of iridium complexes. Journal of Physical Organic Chemistry, 2009, 22, 845-856.	0.9	26
82	Tautomeric forms study of 1H-(2-pyridyl)-3-methyl-5-hydroxypyrazole and 1H-(2-pyridyl)-3-phenyl-5-hydroxypyrazole. Synthesis, structure, and cytotoxic activity of their complexes with palladium(II) ions. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 1257-1268.	2.5	11
83	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. Journal of Chemical Theory and Computation, 2009, 5, 59-67.	2.3	8
84	Isotope Effects. , 2009, , .		41
85	Modeling of Isotope Effects on Binding Oxamate to Lactic Dehydrogenase. Journal of Physical Chemistry B, 2009, 113, 12782-12789.	1.2	36
86	A DFT Study of the Kinetic Isotope Effects on the Competing S _N 2 and E2 Reactions between Hypochlorite Anion and Ethyl Chloride. Journal of Chemical Theory and Computation, 2009, 5, 33-36.	2.3	20
87	DFT and ONIOM(DFT:MM) Studies on Co ^{III} -C Bond Cleavage and Hydrogen Transfer in B ₁₂ -Dependent Methylmalonyl-CoA Mutase. Stepwise or Concerted Mechanism?. Journal of the American Chemical Society, 2009, 131, 5115-5125.	6.6	53
88	Micropreparative isolation of Cu(II) complexes of isoniazid and ethambutol and determination of their structures. Journal of Planar Chromatography - Modern TLC, 2009, 22, 83-88.	0.6	5
89	Mechanism of 4-methyl-1,2,4-triazolin-5-thione reaction with formaldehyde. Journal of Physical Organic Chemistry, 2008, 21, 345-348.	0.9	5
90	Thiol-thione tautomeric forms recognition on the example of 4-(3-(2-methyl-furan-3-yl)-5-thioxo-1,2,4-triazolin-4-yl)acetic acid. Heteroatom Chemistry, 2008, 19, 337-344.	0.4	26

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91	Synthesis and theoretical characterization of some new 4-substituted-1,3-diphenyl-5-thioxo-4,5-dihydro-1 <i>H</i> -1,2,4-triazoles with potential pharmacological activity. Heteroatom Chemistry, 2008, 19, 713-718.	0.6	5
92	Synthesis and pharmacological properties of 3-(2-methyl-furan-3-yl)-4-substituted-1 ² -1,2,4-triazoline-5-thiones. Open Chemistry, 2008, 6, 47-53.	1.0	11
93	Chemical and Pharmacological Properties of 3-(Thiophen-2-yl)-4-substituted-1 ² -1,2,4-triazoline-5-thiones. Phosphorus, Sulfur and Silicon and the Related Elements, 2008, 183, 2669-2677.	0.8	9
94	Enzyme mechanisms from molecular modeling and isotope effects. Archives of Biochemistry and Biophysics, 2008, 474, 274-282.	1.4	9
95	Kinetic Isotope Effects on Dehalogenations at an Aromatic Carbon. Environmental Science & Technology, 2008, 42, 7744-7750.	4.6	34
96	Synthesis, crystal structure, theoretical calculation and cytotoxic effect of new Pt(ii), Pd(ii) and Cu(ii) complexes with pyridine-pyrazoles derivatives. New Journal of Chemistry, 2008, 32, 2238.	1.4	22
97	Altered Transition State for the Reaction of an RNA Model Catalyzed by a Dinuclear Zinc(II) Catalyst. Journal of the American Chemical Society, 2008, 130, 17858-17866.	6.6	59
98	Influence of the Solvent Description on the Predicted Mechanism of SN2 Reactions. Journal of Physical Chemistry B, 2008, 112, 12414-12419.	1.2	7
99	Coupling of hydrogenic tunneling to active-site motion in the hydrogen radical transfer catalyzed by a coenzyme B12-dependent mutase. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 10774-10779.	3.3	77
100	Investigation of the mechanism of nicotine demethylation in Nicotiana through 2H and 15N heavy isotope effects: Implication of cytochrome P450 oxidase and hydroxyl ion transfer. Archives of Biochemistry and Biophysics, 2007, 458, 175-183.	1.4	12
101	The Assignment of the Absolute Configuration of Diethyl Hydroxy- and Aminophosphonates by 1H and 31P NMR Using Naproxen as a Reliable Chiral Derivatizing Agent. Journal of Organic Chemistry, 2007, 72, 878-887.	1.7	23
102	Analysis of Conformer Stability for 1,3,8-Trihydroxynaphthalene: A Natural Substrate of Fungal Trihydroxynaphthalene Reductase. Journal of Physical Chemistry B, 2007, 111, 8314-8320.	1.2	2
103	Computational studies of the cyclization of thiosemicarbazides. Journal of Physical Organic Chemistry, 2007, 20, 463-468.	0.9	9
104	Mechanism of 4-methyl-1,2,4-triazol-3-thiole reaction with formaldehyde. A DFT study. Journal of Physical Organic Chemistry, 2007, 20, 1043-1049.	0.9	13
105	Carbon and secondary deuterium kinetic isotope effects on S _N 2 methyl transfer reactions. Journal of Physical Organic Chemistry, 2007, 20, 1114-1120.	0.9	2
106	Progress in understanding the N-demethylation of alkaloids by exploiting isotopic techniques. Phytochemistry Reviews, 2007, 6, 51-63.	3.1	14
107	Substrate-Enzyme Interactions from Modeling and Isotope Effects. Challenges and Advances in Computational Chemistry and Physics, 2007, , 341-363.	0.6	2
108	Synthesis, Cytotoxic Effect, and Structure-Activity Relationship of Pd(II) Complexes with Coumarin Derivatives. Inorganic Chemistry, 2006, 45, 9688-9695.	1.9	61

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109	Computational Insights into the Mechanism of Radical Generation in B12-Dependent Methylmalonyl-CoA Mutase. <i>Journal of the American Chemical Society</i> , 2006, 128, 1287-1292.	6.6	83
110	The Effect of Solvent on the Structure of the Transition State for the SN2 Reaction between Cyanide Ion and Ethyl Chloride in DMSO and THF Probed with Six Different Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2006, 71, 4742-4747.	1.7	32
111	Mechanism of the Reaction Catalyzed by dl-2-Haloacid Dehalogenase As Determined from Kinetic Isotope Effects. <i>Biochemistry</i> , 2006, 45, 6012-6017.	1.2	16
112	Quantum catalysis in B 12 -dependent methylmalonyl-CoA mutase: experimental and computational insights. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2006, 361, 1333-1339.	1.8	17
113	Chlorine Isotope Effects on Chemical Reactions. <i>Current Organic Chemistry</i> , 2005, 9, 75-88.	0.9	11
114	A Theoretical Investigation of $\delta^{13}\text{C}$ -Carbon Kinetic Isotope Effects and Their Relationship to the Transition-State Structure of SN2 Reactions. <i>Journal of Organic Chemistry</i> , 2005, 70, 4022-4027.	1.7	29
115	Dependence of Transition State Structure on Substrate: The Intrinsic C-13 Kinetic Isotope Effect Is Different for Physiological and Slow Substrates of the Ornithine Decarboxylase Reaction Because of Different Hydrogen Bonding Structures. <i>Journal of the American Chemical Society</i> , 2005, 127, 5414-5422.	6.6	29
116	Chlorine Kinetic Isotope Effects on Biological Systems. , 2005, , 875-892.		1
117	Correlating biological activity with calculated geometric motifs in cyclolinopeptide A analogs. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 625-630.	0.9	7
118	Validation of semiempirical methods for modeling of corrinoid systems. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 1078-1086.	1.5	11
119	A New Interpretation of Chlorine Leaving Group Kinetic Isotope Effects; A Theoretical Approach. <i>Journal of Organic Chemistry</i> , 2004, 69, 4900-4905.	1.7	27
120	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2475-2486.	1.1	70
121	Experimental and Theoretical Multiple Kinetic Isotope Effects for an SN2 Reaction. An Attempt to Determine Transition-State Structure and the Ability of Theoretical Methods to Predict Experimental Kinetic Isotope Effects. <i>Chemistry - A European Journal</i> , 2003, 9, 2696-2709.	1.7	47
122	Calculations of Substituent and Solvent Effects on the Kinetic Isotope Effects of Menshutkin Reactions. <i>Journal of Organic Chemistry</i> , 2003, 68, 8232-8235.	1.7	12
123	Chlorine Kinetic Isotope Effects on Enzymatic Dehalogenations. <i>Accounts of Chemical Research</i> , 2003, 36, 120-126.	7.6	36
124	Borderline between E1cB and E2 Mechanisms. Chlorine Isotope Effects in Base-Promoted Elimination Reactions. <i>Journal of Organic Chemistry</i> , 2002, 67, 177-181.	1.7	18
125	Determination of the Chlorine Kinetic Isotope Effect on the 4-Chlorobenzoyl-CoA Dehalogenase-Catalyzed Nucleophilic Aromatic Substitution. <i>Archives of Biochemistry and Biophysics</i> , 2002, 398, 249-252.	1.4	10
126	How Well Does Microsolvation Represent Macrosolvation? A Test Case: Dynamics of Decarboxylation of 4-Pyridylacetic Acid Zwitterion. <i>Journal of Physical Chemistry B</i> , 2002, 106, 2708-2713.	1.2	46

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127	Preparation of ^{18}O -labelled nicotinamide. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 2002, 45, 1005-1010.	0.5	13
128	Chlorine Kinetic Isotope Effect on the Fluoroacetate Dehalogenase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 9192-9193.	6.6	9
129	Solvent-Dependent Transition States for Decarboxylations. <i>Journal of the American Chemical Society</i> , 2001, 123, 7683-7686.	6.6	73
130	Nitrogen Kinetic Isotope Effects on the Decarboxylation of 4-Pyridylacetic Acid. <i>Journal of Organic Chemistry</i> , 2001, 66, 5534-5536.	1.7	2
131	Chlorine Kinetic Isotope Effects on the Haloalkane Dehalogenase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 4550-4555.	6.6	49
132	Theoretical evaluation of the hydrogen kinetic isotope effect on the first step of the methylmalonyl-CoA mutase reaction. <i>Journal of Inorganic Biochemistry</i> , 2001, 86, 681-689.	1.5	26
133	H-Bonding in Alcohols Is Reflected in the $\text{C}\text{--}\text{H}$ Bond Strength: δ Variation of $\text{C}\text{--}\text{D}$ Vibrational Frequency and Fractionation Factor. <i>Journal of the American Chemical Society</i> , 2000, 122, 11660-11669.	6.6	56
134	ISOEFF98. A program for studies of isotope effects using Hessian modifications. <i>Journal of Mathematical Chemistry</i> , 1999, 26, 75-86.	0.7	144
135	Tritium Secondary Kinetic Isotope Effect on Phenylalanine Ammonia-Lyase-Catalyzed Reaction. <i>Archives of Biochemistry and Biophysics</i> , 1999, 370, 216-221.	1.4	17
136	Are mutated enzymes good models for interpretation of intrinsic isotope effects?. <i>Computational and Theoretical Chemistry</i> , 1998, 454, 69-75.	1.5	6
137	A Study on the Activation of Carboxylic Acids by Means of 2-Chloro-4,6-dimethoxy-1,3,5-triazine and 2-Chloro-4,6-diphenoxy-1,3,5-triazine. <i>Journal of Organic Chemistry</i> , 1998, 63, 4248-4255.	1.7	115
138	A New Method of Determining Chlorine Kinetic Isotope Effects. <i>Analytical Chemistry</i> , 1998, 70, 3548-3552.	3.2	35
139	^{13}C and ^{15}N Kinetic Isotope Effects on the Decarboxylation of 3-Carboxybenzoxazole. Theory vs Experiment. <i>Journal of Organic Chemistry</i> , 1997, 62, 7305-7309.	1.7	11
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