Piotr Paneth

List of Publications by Year in Descending Order

175 papers	2,934 citations	29 h-index	44 g-index
178 ext. papers	3,159 ext. citations	5.8 avg, IF	5.1 L-index

#	Paper	IF	Citations
175	Unprecedently large Cl/Cl equilibrium isotopic fractionation on nano-confinement of chloride anion.. *Scientific Reports*, **2022**, 12, 1768	4.9	1
174	13C Natural Isotope Abundance in Urothelium as a New Marker in the Follow-Up of Patients with Bladder Cancer. *Cancers*, **2022**, 14, 2423	6.6	
173	RNA-inspired intramolecular transesterification accelerates the hydrolysis of polyethylene-like polyphosphoesters.. *Chemical Science*, **2021**, 12, 16054-16064	9.4	1
172	RNA-Inspired and Accelerated Degradation of Polylactide in Seawater. *Journal of the American Chemical Society*, **2021**, 143, 16673-16681	16.4	5
171	1,3,4-Thiadiazoles Effectively Inhibit Proliferation of. *Cells*, **2021**, 10,	7.9	1
170	Thiosemicarbazide Derivatives Decrease the ATPase Activity of Topoisomerase IV, Inhibit Mycobacterial Growth, and Affect Replication in. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
169	4-Arylthiosemicarbazide derivatives as a new class of tyrosinase inhibitors and anti- agents. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 1145-1164	5.6	0
168	New organometallic ruthenium(ii) complexes with purine analogs - a wide perspective on their biological application. *Dalton Transactions*, **2021**, 50, 5557-5573	4.3	0
167	Intramolecular non-covalent isotope effects at natural abundance associated with the migration of paracetamol in solid matrices during liquid chromatography. *Journal of Chromatography A*, **2021**, 1639, 461932	4.5	3
166	Isotopic Consequences of Host-Guest Interactions; Noncovalent Chlorine Isotope Effects. *Journal of Physical Chemistry B*, **2021**, 125, 1874-1880	3.4	2
165	Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computational-Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate. *Environmental Science & Technology*, **2021**, 55, 14037-14050	10.3	2
164	Machine Learning augmented docking studies of aminothioureas at the SARS-CoV-2-ACE2 interface. *PLoS ONE*, **2021**, 16, e0256834	3.7	1
163	Docking and QSAR of Aminothioureas at the SARS-CoV-2 S-Protein-Human ACE2 Receptor Interface. *Molecules*, **2020**, 25,	4.8	4
162	Evolved Fusarium oxysporum laccase expressed in Saccharomyces cerevisiae. *Scientific Reports*, **2020**, 10, 3244	4.9	9
161	The influence of experimental parameters on quantitative deuterium measurements for ethyl alcohols of different origin. *Journal of the Science of Food and Agriculture*, **2020**, 100, 1812-1815	4.3	
160	Antibacterial Activity of Fluorobenzoylthiosemicarbazides and Their Cyclic Analogues with 1,2,4-Triazole Scaffold. *Molecules*, **2020**, 26,	4.8	5
159	Characteristic of Oral Squamous Cell Carcinoma Tissues Using Isotope Ratio Mass Spectrometry. *Journal of Clinical Medicine*, **2020**, 9,	5.1	3

158	Computational Investigations of Position-Specific Vapor Pressure Isotope Effects in Ethanol-Toward More Powerful Isotope Models for Food Forensics. *ACS Omega*, **2020**, 5, 18499-18506	3.9	2
157	Quantum approach to the mechanism of monothiopyrophosphate isomerization. *Journal of Molecular Modeling*, **2019**, 25, 286	2	3
156	Assessment of Nonnucleoside Inhibitors Binding to HIV-1 Reverse Transcriptase Using HYDE Scoring. *Pharmaceuticals*, **2019**, 12,	5.2	3
155	Comparison of quantitative NMR and IRMS for the authentication of 'Polish Vodka'. *Journal of the Science of Food and Agriculture*, **2019**, 99, 263-268	4.3	8
154	2-OMe-lysophosphatidylcholine analogues are GPR119 ligands and activate insulin secretion from MIN6C-3 pancreatic cells: Evaluation of structure-dependent biological activity. *Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids*, **2018**, 1863, 91-103	5	6
153	Diaryl ethers with carboxymethoxyphenacyl motif as potent HIV-1 reverse transcriptase inhibitors with improved solubility. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 9-16	5.6	6
152	Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. *Molecules*, **2018**, 23,	4.8	7
151	Non-statistical isotope fractionation as a novel "retro-biosynthetic" approach to understanding alkaloid metabolic pathways. *Phytochemistry Letters*, **2017**, 20, 499-506	1.9	7
150	Synthesis and antibacterial activity of 1,4-dibenzoylthiosemicarbazide derivatives. *Biomedicine and Pharmacotherapy*, **2017**, 88, 1235-1242	7.5	8
149	The cytotoxic effect of spiroflavanone derivatives, their binding ability to human serum albumin (HSA) and a DFT study on the mechanism of their synthesis. *Journal of Molecular Structure*, **2017**, 1137, 267-276	3.4	6
148	What do docking and QSAR tell us about the design of HIV-1 reverse transcriptase nonnucleoside inhibitors?. *Journal of Molecular Modeling*, **2017**, 23, 317	2	6
147	Measurement and Prediction of Chlorine Kinetic Isotope Effects in Enzymatic Systems. *Methods in Enzymology*, **2017**, 596, 179-215	1.7	5
146	Lipophilicity Studies on Thiosemicarbazide Derivatives. *Molecules*, **2017**, 22,	4.8	6
145	Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. *Journal of Physical Chemistry A*, **2017**, 121, 6638-6645	2.8	4
144	Oxygen binding isotope effects of triazole-based HIV-1 reverse transcriptase inhibitors indicate the actual binding site. *Archives of Biochemistry and Biophysics*, **2017**, 635, 87-95	4.1	2
143	Insights into the role of methionine synthase in the universal C depletion in O- and N-methyl groups of natural products. *Archives of Biochemistry and Biophysics*, **2017**, 635, 60-65	4.1	9
142	Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. *ACS Catalysis*, **2017**, 7, 5294-5307	13.1	26
141	A Search for Dual Action HIV-1 Reverse Transcriptase, Bacterial RNA Polymerase Inhibitors. *Molecules*, **2017**, 22,	4.8	2

140	Design, synthesis and biological evaluation of 4-benzoyl-1-dichlorobenzoylthiosemicarbazides as potent Gram-positive antibacterial agents. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 434-40	5.6	5
139	Searching for novel scaffold of triazole non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 481-9	5.6	7
138	DFT Studies of SN2 Dechlorination of Polychlorinated Biphenyls. *Environmental Science & Technology*, **2016**, 50, 6293-8	10.3	11
137	Non-statistical 13C Fractionation Distinguishes Co-incident and Divergent Steps in the Biosynthesis of the Alkaloids Nicotine and Tropine. *Journal of Biological Chemistry*, **2016**, 291, 16620-9	5.4	12
136	Biological evaluation and molecular modelling study of thiosemicarbazide derivatives as bacterial type IIA topoisomerases inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 14-22	5.6	14
135	Theoretical studies of energetics and binding isotope effects of binding a triazole-based inhibitor to HIV-1 reverse transcriptase. *Physical Chemistry Chemical Physics*, **2016**, 18, 310-7	3.6	4
134	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. *Oncotarget*, **2016**, 7, 76726-76734	3.3	6
133	Hepatoblastoma Biology Using Isotope Ratio Mass Spectrometry: Utility of a Unique Technique for the Analysis of Oncological Specimens. *Postepy Higieny I Medycyny Doswiadczalnej*, **2016**, 70, 797-802	0.3	3
132	Carbon, Nitrogen and Sulphur concentration and δ13C, δ15N values in Hypogymnia physodes within the montane area – preliminary data. *Geoscience Records*, **2016**, 2, 24-32		1
131	Substrate and Enzyme Specificity of the Kinetic Isotope Effects Associated with the Dioxygenation of Nitroaromatic Contaminants. *Environmental Science & Technology*, **2016**, 50, 6708-16	10.3	23
130	Analyzing sites of OH radical attack (ring vs. side chain) in oxidation of substituted benzenes via dual stable isotope analysis (δ(13)C and δ(2)H). *Science of the Total Environment*, **2016**, 542, 484-94	10.2	25
129	Search for human DNA topoisomerase II poisons in the group of 2,5-disubstituted-1,3,4-thiadiazoles. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2015**, 30, 1021-6	5.6	9
128	Binding isotope effects as a tool for distinguishing hydrophobic and hydrophilic binding sites of HIV-1 RT. *Journal of Physical Chemistry B*, **2015**, 119, 917-27	3.4	30
127	The first protocol of stable isotope ratio assessment in tumor tissues based on original research. *Polish Journal of Pathology*, **2015**, 66, 288-95	0.9	4
126	Rhabdomyosarcoma in children in the light of isotope ratio mass spectrometry. *Polish Journal of Pathology*, **2015**, 66, 383-8	0.9	5
125	A DFT study of permanganate oxidation of toluene and its ortho-nitroderivatives. *Journal of Molecular Modeling*, **2014**, 20, 2091	2	6
124	A DFT study of the cis-dihydroxylation of nitroaromatic compounds catalyzed by nitrobenzene dioxygenase. *Journal of Physical Chemistry B*, **2014**, 118, 3245-56	3.4	25
123	A DFT and ONIOM study of C-H hydroxylation catalyzed by nitrobenzene 1,2-dioxygenase. *Physical Chemistry Chemical Physics*, **2014**, 16, 13889-99	3.6	11

122	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 2246-2254	6.4	20
121	Pharmacological and structure-activity relationship evaluation of 4-aryl-1-diphenylacetyl(thio)semicarbazides. *Molecules*, **2014**, 19, 4745-59	4.8	10
120	1,4-Disubstituted thiosemicarbazide derivatives are potent inhibitors of Toxoplasma gondii proliferation. *Molecules*, **2014**, 19, 9926-43	4.8	22
119	Triazole-based compound as a candidate to develop novel medicines to treat toxoplasmosis. *Antimicrobial Agents and Chemotherapy*, **2014**, 58, 7583-5	5.9	16
118	Binding isotope effects. *Chemical Reviews*, **2013**, 113, 7851-79	68.1	58
117	Cytotoxic effect and molecular docking of 4-ethoxycarbonylmethyl-1-(piperidin-4-ylcarbonyl)-thiosemicarbazide--a novel topoisomerase II inhibitor. *Journal of Molecular Modeling*, **2013**, 19, 1319-24	2	10
116	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, 3326-42	6.1	23
115	Binding modes of DL-2-haloacid dehalogenase revealed by crystallography, modeling and isotope effects studies. *Archives of Biochemistry and Biophysics*, **2013**, 540, 26-32	4.1	12
114	Structure-cytotoxic activity relationship of 3-arylideneflavanone and chromanone (E,Z isomers) and 3-arylflavones. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 4102-6	2.9	19
113	Isotopic analysis of oxidative pollutant degradation pathways exhibiting large H isotope fractionation. *Environmental Science & Technology*, **2013**, 47, 13459-68	10.3	31
112	Cytochrome P450-catalyzed degradation of nicotine: fundamental parameters determining hydroxylation by cytochrome P450 2A6 at the 5'-carbon or the n-methyl carbon. *Journal of Physical Chemistry B*, **2012**, 116, 7827-40	3.4	12
111	Extending limits of chlorine kinetic isotope effects. *Journal of Organic Chemistry*, **2012**, 77, 5120-4	4.2	23
110	Does dehydrocyclization of 4-benzoylthiosemicarbazides in acetic acid lead to s-triazoles or thiadiazoles?. *Structural Chemistry*, **2012**, 23, 1441-1448	1.8	5
109	Cytochrome P450 Monooxygenase-Catalyzed Ring Opening of the Bicyclic Amine, Nortropine: An Experimental and DFT Computational Study. *ChemCatChem*, **2012**, 4, 530-539	5.2	6
108	Isotopic fractionation - chemical v. environmental perspective. *Environmental Chemistry*, **2012**, 9, 67	3.2	10
107	Binding ligands and cofactor to L-lactate dehydrogenase from human skeletal and heart muscles. *Journal of Physical Chemistry B*, **2011**, 115, 6366-76	3.4	11
106	DFT study of trichloroethene reaction with permanganate in aqueous solution. *Environmental Science & Technology*, **2011**, 45, 3006-11	10.3	25
105	Measurements of heavy-atom isotope effects using 1H NMR spectroscopy. *Journal of Organic Chemistry*, **2011**, 76, 8033-5	4.2	17

104	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	4.1	15
103	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	4.1	13
102	Biological and docking studies of topoisomerase IV inhibition by thiosemicarbazides. *Journal of Molecular Modeling*, **2011**, 17, 2297-303	2	27
101	Theoretical evaluation of isotopic fractionation factors in oxidation reactions of benzene, phenol and chlorophenols. *Journal of Molecular Modeling*, **2011**, 17, 2285-96	2	13
100	Synthetic route to isotopically labelled-oxamate. *Journal of Labelled Compounds and Radiopharmaceuticals*, **2011**, 54, 344-344	1.9	
99	Valence anions of N-acetylproline in the gas phase: computational and anion photoelectron spectroscopic studies. *Journal of Chemical Physics*, **2011**, 135, 114301	3.9	9
98	Importance of the lactate dehydrogenase quaternary structure in theoretical calculations. *Journal of Physical Chemistry B*, **2010**, 114, 3393-7	3.4	15
97	Antimicrobial Properties of 4-Aryl-3-(2-methyl-furan-3-yl)-Δ2-1,2,4-triazoline-5-thiones. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2009**, 184, 3149-3159	1	7
96	Modeling excitation properties of iridium complexes. *Journal of Physical Organic Chemistry*, **2009**, 22, 845-856	2.1	24
95	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, 1257-68	5.6	11
94	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	6.4	8
93	Isotope Effects **2009**,		34
92	Modeling of isotope effects on binding oxamate to lactic dehydrogenase. *Journal of Physical Chemistry B*, **2009**, 113, 12782-9	3.4	30
91	A DFT Study of the Kinetic Isotope Effects on the Competing SN2 and E2 Reactions between Hypochlorite Anion and Ethyl Chloride. *Journal of Chemical Theory and Computation*, **2009**, 5, 33-6	6.4	17
90	DFT and ONIOM(DFT:MM) studies on Co-C bond cleavage and hydrogen transfer in B12-dependent methylmalonyl-CoA mutase. Stepwise or concerted mechanism?. *Journal of the American Chemical Society*, **2009**, 131, 5115-25	16.4	44
89	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	0.9	4
88	Chemical and Pharmacological Properties of 3-(Thiophen-2-yl)-4-substituted-Δ2-1,2,4-triazoline-5-thiones. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2008**, 183, 2669-2677	1	6
87	Enzyme mechanisms from molecular modeling and isotope effects. *Archives of Biochemistry and Biophysics*, **2008**, 474, 274-82	4.1	8

86	Kinetic isotope effects on dehalogenations at an aromatic carbon. *Environmental Science & Technology*, **2008**, 42, 7744-50	10.3	32
85	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	3.6	19
84	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, 17858-66	16.4	59
83	Influence of the solvent description on the predicted mechanism of SN2 reactions. *Journal of Physical Chemistry B*, **2008**, 112, 12414-9	3.4	6
82	Mechanism of 4-methyl-1,2,4-triazol-3-thione reaction with formaldehyde. *Journal of Physical Organic Chemistry*, **2008**, 21, 345-348	2.1	5
81	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	1.2	26
80	Synthesis and theoretical characterization of some new 4-substituted-1,3-diphenyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazoles with potential pharmacological activity. *Heteroatom Chemistry*, **2008**, 19, 713-718	1.2	3
79	Synthesis and pharmacological properties of 3-(2-methyl-furan-3-yl)-4-substituted-□2-1,2,4-triazoline-5-thiones. *Open Chemistry*, **2008**, 6, 47-53	1.6	8
78	Analysis of conformer stability for 1,3,8-trihydroxynaphthalene: natural substrate of fungal trihydroxynaphthalene reductase. *Journal of Physical Chemistry B*, **2007**, 111, 8314-20	3.4	2
77	Computational studies of the cyclization of thiosemicarbazides. *Journal of Physical Organic Chemistry*, **2007**, 20, 463-468	2.1	9
76	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	2.1	13
75	Carbon and secondary deuterium kinetic isotope effects on SN2 methyl transfer reactions. *Journal of Physical Organic Chemistry*, **2007**, 20, 1114-1120	2.1	2
74	Progress in understanding the N-demethylation of alkaloids by exploiting isotopic techniques. *Phytochemistry Reviews*, **2007**, 6, 51-63	7.7	13
73	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, 10774-9	11.5	74
72	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, 175-83	4.1	12
71	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, 878-87	4.2	21
70	Substrate-Enzyme Interactions from Modeling and Isotope Effects. *Challenges and Advances in Computational Chemistry and Physics*, **2007**, 341-363	0.7	2
69	Quantum catalysis in B12-dependent methylmalonyl-CoA mutase: experimental and computational insights. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 1333-9	5.8	15

68	Synthesis, cytotoxic effect, and structure-activity relationship of Pd(II) complexes with coumarin derivatives. *Inorganic Chemistry*, **2006**, 45, 9688-95	5.1	53
67	Computational insights into the mechanism of radical generation in B12-dependent methylmalonyl-CoA mutase. *Journal of the American Chemical Society*, **2006**, 128, 1287-92	16.4	68
66	The effect of solvent on the structure of the transition state for the S(N)2 reaction between cyanide ion and ethyl chloride in DMSO and THF probed with six different kinetic isotope effects. *Journal of Organic Chemistry*, **2006**, 71, 4742-7	4.2	29
65	Mechanism of the reaction catalyzed by DL-2-haloacid dehalogenase as determined from kinetic isotope effects. *Biochemistry*, **2006**, 45, 6012-7	3.2	16
64	A theoretical investigation of alpha-carbon kinetic isotope effects and their relationship to the transition-state structure of S(N)2 reactions. *Journal of Organic Chemistry*, **2005**, 70, 4022-7	4.2	26
63	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. *Journal of the American Chemical Society*, **2005**, 127, 5414-22	16.4	29
62	Chlorine Isotope Effects on Chemical Reactions. *Current Organic Chemistry*, **2005**, 9, 75-88	1.7	11
61	Chlorine Kinetic Isotope Effects on Biological Systems **2005**, 875-892		1
60	Correlating biological activity with calculated geometric motifs in cyclolinopeptide A analogs. *Journal of Physical Organic Chemistry*, **2004**, 17, 625-630	2.1	7
59	Validation of semiempirical methods for modeling of corrinoid systems. *Journal of Inorganic Biochemistry*, **2004**, 98, 1078-86	4.2	10
58	A new interpretation of chlorine leaving group kinetic isotope effects; a theoretical approach. *Journal of Organic Chemistry*, **2004**, 69, 4900-5	4.2	26
57	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. *Journal of Physical Chemistry A* , **2004**, 108, 2475-2486	2.8	63
56	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. *Chemistry - A European Journal*, **2003**, 9, 2696-709	4.8	44
55	Calculations of substituent and solvent effects on the kinetic isotope effects of Menshutkin reactions. *Journal of Organic Chemistry*, **2003**, 68, 8232-5	4.2	11
54	Chlorine kinetic isotope effects on enzymatic dehalogenations. *Accounts of Chemical Research*, **2003**, 36, 120-6	24.3	34
53	Preparation of 18O-labelled nicotinamide. *Journal of Labelled Compounds and Radiopharmaceuticals* , **2002**, 45, 1005-1010	1.9	9
52	Borderline between E1cB and E2 mechanisms. Chlorine isotope effects in base-promoted elimination Reactions. *Journal of Organic Chemistry*, **2002**, 67, 177-81	4.2	17
51	Determination of the chlorine kinetic isotope effect on the 4-chlorobenzoyl-CoA dehalogenase-catalyzed nucleophilic aromatic substitution. *Archives of Biochemistry and Biophysics*, **2002**, 398, 249-52	4.1	10

50	How Well Does Microsolvation Represent Macrosolvation? A Test Case: Dynamics of Decarboxylation of 4-Pyridylacetic Acid Zwitterion. *Journal of Physical Chemistry B*, **2002**, 106, 2708-2713	3.4	42
49	Theoretical evaluation of the hydrogen kinetic isotope effect on the first step of the methylmalonyl-CoA mutase reaction. *Journal of Inorganic Biochemistry*, **2001**, 86, 681-9	4.2	25
48	Chlorine kinetic isotope effect on the fluoroacetate dehalogenase reaction. *Journal of the American Chemical Society*, **2001**, 123, 9192-3	16.4	8
47	Solvent-dependent transition states for decarboxylations. *Journal of the American Chemical Society*, **2001**, 123, 7683-6	16.4	65
46	Nitrogen kinetic isotope effects on the decarboxylation of 4-pyridylacetic acid. *Journal of Organic Chemistry*, **2001**, 66, 5534-6	4.2	2
45	Chlorine kinetic isotope effects on the haloalkane dehalogenase reaction. *Journal of the American Chemical Society*, **2001**, 123, 4550-5	16.4	46
44	H-Bonding in Alcohols Is Reflected in the C–H Bond Strength: Variation of C–D Vibrational Frequency and Fractionation Factor. *Journal of the American Chemical Society*, **2000**, 122, 11660-11669	16.4	48
43	ISOEFF98. A program for studies of isotope effects using Hessian modifications. *Journal of Mathematical Chemistry*, **1999**, 26, 75-86	2.1	141
42	Tritium secondary kinetic isotope effect on phenylalanine ammonia-lyase-catalyzed reaction. *Archives of Biochemistry and Biophysics*, **1999**, 370, 216-21	4.1	16
41	Are mutated enzymes good models for interpretation of intrinsic isotope effects?. *Computational and Theoretical Chemistry*, **1998**, 454, 69-75		6
40	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. *Journal of Organic Chemistry*, **1998**, 63, 4248-4255	4.2	100
39	A new method of determining chlorine kinetic isotope effects. *Analytical Chemistry*, **1998**, 70, 3548-52	7.8	32
38	13C and (15)N Kinetic Isotope Effects on the Decarboxylation of 3-Carboxybenzisoxazole. Theory vs Experiment. *Journal of Organic Chemistry*, **1997**, 62, 7305-7309	4.2	9
37	Structural Aspects and Rearrangement of Radical Cations Generated from NADH Analogues. *Journal of the American Chemical Society*, **1996**, 118, 691-692	16.4	22
36	Dependence of isotope effects on conformation in decarboxylation of 3-carboxybenzisoxazoles. *Computational and Theoretical Chemistry*, **1996**, 370, 237-243		3
35	Nitrogen and deuterium kinetic isotope effects on the Menshutkin reaction. *Journal of Physical Organic Chemistry*, **1996**, 9, 35-40	2.1	18
34	Kinetic isotope effects on the Menshutkin reaction: Theory versus experiment. *Journal of Physical Organic Chemistry*, **1996**, 9, 41-49	2.1	12
33	Isotope effects on binding. *Journal of Molecular Structure*, **1996**, 378, 35-43	3.4	12

32	Theoretical calculations of heavy-atom isotope effects. *Computers & Chemistry*, **1995**, 19, 11-20		5
31	Theoretical calculations of heavy-atom isotope effects. *Computers & Chemistry*, **1995**, 19, 231-40		20
30	Kinetic isotope effects on substrate association: reactions of phosphoenolpyruvate with phosphoenolpyruvate carboxylase and pyruvate kinase. *Biochemistry*, **1995**, 34, 2577-83	3.2	21
29	Equilibrium isotope effect on ternary complex formation of [1-18O]oxamate with NADH and lactate dehydrogenase. *Biochemistry*, **1995**, 34, 6050-8	3.2	33
28	13C NMR and 1H-1H NOEs of Coenzyme-A: Conformation of the Pantoic Acid Moiety. *Bioorganic Chemistry*, **1995**, 23, 169-181	5.1	9
27	Semiempirical calculations of the oxygen equilibrium isotope effect on binding of oxamate to lactate dehydrogenase. *European Biophysics Journal*, **1994**, 23, 353-60	1.9	10
26	Deuterium kinetic isotope effect on quaternization of N,N-dimethylaniline. *Journal of Molecular Structure*, **1994**, 321, 97-99	3.4	5
25	Heavy atom isotope effects on enzymatic reactions. *Journal of Molecular Structure*, **1994**, 321, 35-44	3.4	9
24	Carbon kinetic isotope effects on the spontaneous and antibody-catalyzed decarboxylation of 5-nitro-3-carboxybenzisoxazole. *Journal of the American Chemical Society*, **1993**, 115, 1410-1413	16.4	33
23	Photochemical and radiolytic cleavage of 10-methylacridine dimer in solutions and cryogenic glasses. *Journal of Physical Organic Chemistry*, **1993**, 6, 254-256	2.1	5
22	Significance of the cis□trans isomerization of early intermediates in the carotene biosynthetic pathway. *Journal of Physical Organic Chemistry*, **1992**, 5, 783-786	2.1	4
21	Physical and chemical basis of carbon isotope fractionation in plants. *Plant, Cell and Environment*, **1992**, 15, 1099-1104	8.4	175
20	Numerical evaluation of the time-dependence of concentrations, rates and kinetic isotope effects. *Computers & Chemistry*, **1991**, 15, 347-349		3
19	Semiempirical SCF-MO calculations of kinetic isotope effects. *Journal of Physical Organic Chemistry*, **1991**, 4, 635-638	2.1	3
18	Nitrogen and deuterium isotope effects on quaternization of N,N-dimethyl-p-toluidine. *Journal of the American Chemical Society*, **1991**, 113, 1691-1693	16.4	30
17	Investigation of the enzymatic mechanism of yeast orotidine-5'-monophosphate decarboxylase using 13C kinetic isotope effects. *Biochemistry*, **1991**, 30, 6216-23	3.2	62
16	Analogues of NADP(+) as inhibitors and coenzymes for NADP(+) malic enzyme from maize leaves. *Photosynthesis Research*, **1991**, 28, 69-76	3.7	6
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