

Piotr Paneth

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3875956/publications.pdf>

Version: 2024-02-01

176
papers

3,420
citations

159525

30
h-index

206029

48
g-index

178
all docs

178
docs citations

178
times ranked

3279
citing authors

#	ARTICLE	IF	CITATIONS
1	Physical and chemical basis of carbon isotope fractionation in plants. <i>Plant, Cell and Environment</i> , 1992, 15, 1099-1104.	2.8	194
2	ISOEFF98. A program for studies of isotope effects using Hessian modifications. <i>Journal of Mathematical Chemistry</i> , 1999, 26, 75-86.	0.7	144
3	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
4	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
5	Coupling of hydrogenic tunneling to active-site motion in the hydrogen radical transfer catalyzed by a coenzyme B12-dependent mutase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 10774-10779.	3.3	77
6	Carbon isotope effect on dehydration of bicarbonate ion catalyzed by carbonic anhydrase. <i>Biochemistry</i> , 1985, 24, 5143-5147.	1.2	75
7	Solvent-Dependent Transition States for Decarboxylations. <i>Journal of the American Chemical Society</i> , 2001, 123, 7683-7686.	6.6	73
8	Binding Isotope Effects. <i>Chemical Reviews</i> , 2013, 113, 7851-7879.	23.0	72
9	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
10	Investigation of the enzymic mechanism of yeast orotidine-5'-monophosphate decarboxylase using carbon-13 kinetic isotope effects. <i>Biochemistry</i> , 1991, 30, 6216-6223.	1.2	65
11	Synthesis, Cytotoxic Effect, and Structure-Activity Relationship of Pd(II) Complexes with Coumarin Derivatives. <i>Inorganic Chemistry</i> , 2006, 45, 9688-9695.	1.9	61
12	Altered Transition State for the Reaction of an RNA Model Catalyzed by a Dinuclear Zinc(II) Catalyst. <i>Journal of the American Chemical Society</i> , 2008, 130, 17858-17866.	6.6	59
13	H-Bonding in Alcohols Is Reflected in the C-H Bond Strength: Variation of C-D Vibrational Frequency and Fractionation Factor. <i>Journal of the American Chemical Society</i> , 2000, 122, 11660-11669.	6.6	56
14	DFT and ONIOM(DFT:MM) Studies on Co-C Bond Cleavage and Hydrogen Transfer in B ₁₂ -Dependent Methylmalonyl-CoA Mutase. Stepwise or Concerted Mechanism?. <i>Journal of the American Chemical Society</i> , 2009, 131, 5115-5125.	6.6	53
15	Chlorine Kinetic Isotope Effects on the Haloalkane Dehalogenase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 4550-4555.	6.6	49
16	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
17	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
18	Isotope Effects. , 2009, , .		41

#	ARTICLE	IF	CITATIONS
19	Carbon kinetic isotope effects on the spontaneous and antibody-catalyzed decarboxylation of 5-nitro-3-carboxybenzisoxazole. <i>Journal of the American Chemical Society</i> , 1993, 115, 1410-1413.	6.6	38
20	Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. <i>ACS Catalysis</i> , 2017, 7, 5294-5307.	5.5	38
21	Isotopic Analysis of Oxidative Pollutant Degradation Pathways Exhibiting Large H Isotope Fractionation. <i>Environmental Science & Technology</i> , 2013, 47, 13459-13468.	4.6	37
22	RNA-Inspired and Accelerated Degradation of Polylactide in Seawater. <i>Journal of the American Chemical Society</i> , 2021, 143, 16673-16681.	6.6	37
23	Chlorine Kinetic Isotope Effects on Enzymatic Dehalogenations. <i>Accounts of Chemical Research</i> , 2003, 36, 120-126.	7.6	36
24	Modeling of Isotope Effects on Binding Oxamate to Lactic Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12782-12789.	1.2	36
25	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
26	Nitrogen and deuterium isotope effects on quaternization of N,N-dimethyl-p-toluidine. <i>Journal of the American Chemical Society</i> , 1991, 113, 1691-1693.	6.6	35
27	A New Method of Determining Chlorine Kinetic Isotope Effects. <i>Analytical Chemistry</i> , 1998, 70, 3548-3552.	3.2	35
28	Kinetic Isotope Effects on Dehalogenations at an Aromatic Carbon. <i>Environmental Science & Technology</i> , 2008, 42, 7744-7750.	4.6	34
29	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
30	Equilibrium Isotope Effect on Ternary Complex Formation of [1- ^{18}O]Oxamate with NADH and Lactate Dehydrogenase. <i>Biochemistry</i> , 1995, 34, 6050-6058.	1.2	33
31	The Effect of Solvent on the Structure of the Transition State for the $\text{S}_{\text{N}}2$ 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
32	A DFT Study of the <i>cis</i> -Dihydroxylation of Nitroaromatic Compounds Catalyzed by Nitrobenzene Dioxygenase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3245-3256.	1.2	30
33	A Theoretical Investigation of $\delta^{13}\text{C}$ -Carbon Kinetic Isotope Effects and Their Relationship to the Transition-State Structure of $\text{S}_{\text{N}}2$ Reactions. <i>Journal of Organic Chemistry</i> , 2005, 70, 4022-4027.	1.7	29
34	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
35	DFT Study of Trichloroethene Reaction with Permanganate in Aqueous Solution. <i>Environmental Science & Technology</i> , 2011, 45, 3006-3011.	4.6	29
36	Biological and docking studies of topoisomerase IV inhibition by thiosemicarbazides. <i>Journal of Molecular Modeling</i> , 2011, 17, 2297-2303.	0.8	29

#	ARTICLE	IF	CITATIONS
37	Assessing Molecular Docking Tools for Relative Biological Activity Prediction: A Case Study of Triazole HIV-1 NNRTIs. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 3326-3342.	2.5	29
38	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
39	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2246-2254.	2.3	27
40	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
41	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
42	Thiol-thione tautomeric forms recognition on the example of 4-((3-(2-methylfuran-3-yl)acetyl)thioacetyl)-2,4-triazolin-4-yl]acetic acid. <i>Heteroatom Chemistry</i> , 2008, 19, 337-344.	0.4	26
43	Modeling excitation properties of iridium complexes. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 845-856.	0.9	26
44	Structural Aspects and Rearrangement of Radical Cations Generated from NADH Analogues. <i>Journal of the American Chemical Society</i> , 1996, 118, 691-692.	6.6	24
45	Structure-cytotoxic activity relationship of 3-arylidene flavanone and chromanone (E,Z isomers) and 3-arylflavones. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 4102-4106.	1.0	24
46	1,4-Disubstituted Thiosemicarbazide Derivatives are Potent Inhibitors of <i>Toxoplasma gondii</i> Proliferation. <i>Molecules</i> , 2014, 19, 9926-9943.	1.7	24
47	The Assignment of the Absolute Configuration of Diethyl Hydroxy- and Aminophosphonates by ¹ H and ³¹ P NMR Using Naproxen as a Reliable Chiral Derivatizing Agent. <i>Journal of Organic Chemistry</i> , 2007, 72, 878-887.	1.7	23
48	Extending Limits of Chlorine Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2012, 77, 5120-5124.	1.7	23
49	Kinetic Isotope Effects on Substrate Association: Reactions of Phosphoenolpyruvate with Phosphoenolpyruvate Carboxylase and Pyruvate Kinase. <i>Biochemistry</i> , 1995, 34, 2577-2583.	1.2	22
50	Synthesis, crystal structure, theoretical calculation and cytotoxic effect of new Pt(ii), Pd(ii) and Cu(ii) complexes with pyridine-pyrazoles derivatives. <i>New Journal of Chemistry</i> , 2008, 32, 2238.	1.4	22
51	Theoretical calculations of heavy-atom isotope effects. <i>Computers & Chemistry</i> , 1995, 19, 231-240.	1.2	20
52	A DFT Study of the Kinetic Isotope Effects on the Competing S _N 2 and E2 Reactions between Hypochlorite Anion and Ethyl Chloride. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 33-36.	2.3	20
53	Nitrogen and deuterium kinetic isotope effects on the Menshutkin reaction. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 35-40.	0.9	19
54	Measurements of Heavy-Atom Isotope Effects Using ¹ H NMR Spectroscopy. <i>Journal of Organic Chemistry</i> , 2011, 76, 8033-8035.	1.7	19

#	ARTICLE	IF	CITATIONS
55	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
56	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
57	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
58	Phosphorus-sulfur bond order in phosphothioate anions. <i>Journal of the American Chemical Society</i> , 1986, 108, 1720-1722.	6.6	17
59	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
60	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
61	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
62	On the application of the steady state to kinetic isotope effects. <i>Journal of the American Chemical Society</i> , 1985, 107, 7070-7071.	6.6	16
63	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
64	Differences and similarities in binding of pyruvate and l-lactate in the active site of M4 and H4 isoforms of human lactate dehydrogenase. <i>Archives of Biochemistry and Biophysics</i> , 2011, 505, 33-41.	1.4	16
65	Theoretical evaluation of isotopic fractionation factors in oxidation reactions of benzene, phenol and chlorophenols. <i>Journal of Molecular Modeling</i> , 2011, 17, 2285-2296.	0.8	16
66	DFT Studies of S _N 2 Dechlorination of Polychlorinated Biphenyls. <i>Environmental Science & Technology</i> , 2016, 50, 6293-6298.	4.6	16
67	Importance of the Lactate Dehydrogenase Quaternary Structure in Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3393-3397.	1.2	15
68	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
69	Antibacterial Activity of Fluorobenzoylthiosemicarbazides and Their Cyclic Analogues with 1,2,4-Triazole Scaffold. <i>Molecules</i> , 2021, 26, 170.	1.7	15
70	Progress in understanding the N-demethylation of alkaloids by exploiting isotopic techniques. <i>Phytochemistry Reviews</i> , 2007, 6, 51-63.	3.1	14
71	Elucidation of the mechanism of N-demethylation catalyzed by cytochrome P450 monooxygenase is facilitated by exploiting nitrogen-15 heavy isotope effects. <i>Archives of Biochemistry and Biophysics</i> , 2011, 510, 35-41.	1.4	14
72	Cytochrome P450-Catalyzed Degradation of Nicotine: Fundamental Parameters Determining Hydroxylation by Cytochrome P450 2A6 at the 5- ² -Carbon or the <i>i</i> -Methyl Carbon. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7827-7840.	1.2	14

#	ARTICLE	IF	CITATIONS
73	A DFT and ONIOM study of C-H hydroxylation catalyzed by nitrobenzene 1,2-dioxygenase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13889-13899.	1.3	14
74	Comparison of quantitative NMR and IRMS for the authentication of "Polish Vodk"™. <i>Journal of the Science of Food and Agriculture</i> , 2019, 99, 263-268.	1.7	14
75	Kinetic isotope effects on the Menshutkin reaction: Theory versus experiment. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 41-49.	0.9	13
76	Isotope effects on binding. <i>Journal of Molecular Structure</i> , 1996, 378, 35-43.	1.8	13
77	Preparation of ¹⁸ O-labelled nicotinamide. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 2002, 45, 1005-1010.	0.5	13
78	Mechanism of 4-methyl-1,2,4-triazol-3-thiole reaction with formaldehyde. A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1043-1049.	0.9	13
79	Binding Ligands and Cofactor to Lactate Dehydrogenase from Human Skeletal and Heart Muscles. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6366-6376.	1.2	13
80	Cytotoxic effect and molecular docking of 4-ethoxycarbonylmethyl-1-(piperidin-4-ylcarbonyl)-thiosemicarbazide a novel topoisomerase II inhibitor. <i>Journal of Molecular Modeling</i> , 2013, 19, 1319-1324.	0.8	13
81	Binding modes of DL-2-haloacid dehalogenase revealed by crystallography, modeling and isotope effects studies. <i>Archives of Biochemistry and Biophysics</i> , 2013, 540, 26-32.	1.4	13
82	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
83	2- OMe -lysophosphatidylcholine analogues are GPR119 ligands and activate insulin secretion from β TC-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
84	Some analytical aspects of the measurement of heavy-atom kinetic isotope effects. <i>Talanta</i> , 1987, 34, 877-883.	2.9	12
85	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
86	Investigation of the mechanism of nicotine demethylation in <i>Nicotiana</i> through ² H and ¹⁵ N heavy isotope effects: Implication of cytochrome P450 oxidase and hydroxyl ion transfer. <i>Archives of Biochemistry and Biophysics</i> , 2007, 458, 175-183.	1.4	12
87	Synthesis and antibacterial activity of 1,4-dibenzoylthiosemicarbazide derivatives. <i>Biomedicine and Pharmacotherapy</i> , 2017, 88, 1235-1242.	2.5	12
88	Evolved <i>Fusarium oxysporum</i> laccase expressed in <i>Saccharomyces cerevisiae</i> . <i>Scientific Reports</i> , 2020, 10, 3244.	1.6	12
89	RNA-inspired intramolecular transesterification accelerates the hydrolysis of polyethylene-like polyphosphoesters. <i>Chemical Science</i> , 2021, 12, 16054-16064.	3.7	12
90	Semiempirical calculations of the oxygen equilibrium isotope effect on binding of oxamate to lactate dehydrogenase. <i>European Biophysics Journal</i> , 1994, 23, 353-60.	1.2	11

#	ARTICLE	IF	CITATIONS
91	¹³ C and ¹⁵ N Kinetic Isotope Effects on the Decarboxylation of 3-Carboxybenzisoxazole. Theory vs Experiment. <i>Journal of Organic Chemistry</i> , 1997, 62, 7305-7309.	1.7	11
92	Validation of semiempirical methods for modeling of corrinoid systems. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 1078-1086.	1.5	11
93	Chlorine Isotope Effects on Chemical Reactions. <i>Current Organic Chemistry</i> , 2005, 9, 75-88.	0.9	11
94	Synthesis and pharmacological properties of 3-(2-methyl-furan-3-yl)-4-substituted-1 ^H -2,1,2,4-triazoline-5-thiones. <i>Open Chemistry</i> , 2008, 6, 47-53.	1.0	11
95	Tautomeric forms study of 1H-(2- ² -pyridyl)-3-methyl-5-hydroxypyrazole and 1H-(2- ² -pyridyl)-3-phenyl-5-hydroxypyrazole. Synthesis, structure, and cytotoxic activity of their complexes with palladium(II) ions. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009, 24, 1257-1268.	2.5	11
96	Pharmacological and Structure-Activity Relationship Evaluation of 4-aryl-1-Diphenylacetyl(thio)semicarbazides. <i>Molecules</i> , 2014, 19, 4745-4759.	1.7	11
97	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
98	Isotopic fractionation - chemical v. environmental perspective. <i>Environmental Chemistry</i> , 2012, 9, 67.	0.7	10
99	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
100	Analogues of NADP ⁺ as inhibitors and coenzymes for NADP ⁺ malic enzyme from maize leaves. <i>Photosynthesis Research</i> , 1991, 28, 69-76.	1.6	10
101	Sulfur-34, sulfur-36, and oxygen-18 isotope effects on phosphorus-31 chemical shifts in thiophosphate anhydrides. <i>Journal of the American Chemical Society</i> , 1985, 107, 1409-1411.	6.6	9
102	Heavy atom isotope effects on enzymatic reactions. <i>Journal of Molecular Structure</i> , 1994, 321, 35-44.	1.8	9
103	¹³ C NMR and ¹ H- ¹ H NOEs of Coenzyme-A: Conformation of the Pantoic Acid Moiety. <i>Bioorganic Chemistry</i> , 1995, 23, 169-181.	2.0	9
104	Chlorine Kinetic Isotope Effect on the Fluoroacetate Dehalogenase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 9192-9193.	6.6	9
105	Computational studies of the cyclization of thiosemicarbazides. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 463-468.	0.9	9
106	Chemical and Pharmacological Properties of 3-(Thiophen-2-yl)-4-substituted-1 ^H -2,1,2,4-triazoline-5-thiones. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2008, 183, 2669-2677.	0.8	9
107	Enzyme mechanisms from molecular modeling and isotope effects. <i>Archives of Biochemistry and Biophysics</i> , 2008, 474, 274-282.	1.4	9
108	Valence anions of N-acetylproline in the gas phase: Computational and anion photoelectron spectroscopic studies. <i>Journal of Chemical Physics</i> , 2011, 135, 114301.	1.2	9

#	ARTICLE	IF	CITATIONS
109	Isotope effect evidence for the zinc hydroxide mechanism of carbonic anhydrase catalysis. <i>Biochemistry</i> , 1987, 26, 1728-1731.	1.2	8
110	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
111	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. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 59-67.	2.3	8
112	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
113	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
114	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
115	Lipophilicity Studies on Thiosemicarbazide Derivatives. <i>Molecules</i> , 2017, 22, 952.	1.7	8
116	4-Arylthiosemicarbazide derivatives as a new class of tyrosinase inhibitors and anti-Toxoplasma gondii agents. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1145-1164.	2.5	8
117	Thiosemicarbazide Derivatives Decrease the ATPase Activity of Staphylococcus aureus Topoisomerase IV, Inhibit Mycobacterial Growth, and Affect Replication in Mycobacterium smegmatis. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3881.	1.8	8
118	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
119	Relative sulfur-36-sulfur-34 kinetic isotope effects. <i>Journal of the American Chemical Society</i> , 1985, 107, 1407-1408.	6.6	7
120	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
121	Influence of the Solvent Description on the Predicted Mechanism of SN2 Reactions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12414-12419.	1.2	7
122	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
123	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
124	Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. <i>Molecules</i> , 2018, 23, 2981.	1.7	7
125	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
126	Photochemical and radiolytic cleavage of 10-methylacridine dimer in solutions and cryogenic glasses. <i>Journal of Physical Organic Chemistry</i> , 1993, 6, 254-256.	0.9	6

#	ARTICLE	IF	CITATIONS
127	Theoretical calculations of heavy-atom isotope effects. <i>Computers & Chemistry</i> , 1995, 19, 11-20.	1.2	6
128	Are mutated enzymes good models for interpretation of intrinsic isotope effects?. <i>Computational and Theoretical Chemistry</i> , 1998, 454, 69-75.	1.5	6
129	Cytochrome P450 Monooxygenaseâ€Catalyzed Ring Opening of the Bicyclic Amine, Nortropine: An Experimental and DFT Computational Study. <i>ChemCatChem</i> , 2012, 4, 530-539.	1.8	6
130	A DFT study of permanganate oxidation of toluene and its ortho-nitroderivatives. <i>Journal of Molecular Modeling</i> , 2014, 20, 2091.	0.8	6
131	Rhabdomyosarcoma in children in the light of isotope ratio mass spectrometry. <i>Polish Journal of Pathology</i> , 2015, 4, 383-388.	0.1	6
132	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
133	Measurement and Prediction of Chlorine Kinetic Isotope Effects in Enzymatic Systems. <i>Methods in Enzymology</i> , 2017, 596, 179-215.	0.4	6
134	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
135	Assessment of Nonnucleoside Inhibitors Binding to HIV-1 Reverse Transcriptase Using HYDE Scoring. <i>Pharmaceuticals</i> , 2019, 12, 64.	1.7	6
136	Docking and QSAR of Aminothiureas at the SARS-CoV-2 S-Proteinâ€Human ACE2 Receptor Interface. <i>Molecules</i> , 2020, 25, 4645.	1.7	6
137	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
138	1,3,4-Thiadiazoles Effectively Inhibit Proliferation of <i>Toxoplasma gondii</i> . <i>Cells</i> , 2021, 10, 1053.	1.8	6
139	Deuterium kinetic isotope effect on quaternization of N,N-dimethylaniline. <i>Journal of Molecular Structure</i> , 1994, 321, 97-99.	1.8	5
140	Mechanism of 4-methyl-1,2,4-triazol-3-thione reaction with formaldehyde. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 345-348.	0.9	5
141	Synthesis and theoretical characterization of some new 4-substituted-1,3-diphenyl-5-thioxo-4,5-dihydro-1,2,4-triazoles with potential pharmacological activity. <i>Heteroatom Chemistry</i> , 2008, 19, 713-718.		5
142	Micropreparative isolation of Cu(II) complexes of isoniazid and ethambutol and determination of their structures. <i>Journal of Planar Chromatography - Modern TLC</i> , 2009, 22, 83-88.	0.6	5
143	Does dehydrocyclization of 4-benzoylthiosemicarbazides in acetic acid lead to s-triazoles or thiadiazoles?. <i>Structural Chemistry</i> , 2012, 23, 1441-1448.	1.0	5
144	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

#	ARTICLE	IF	CITATIONS
145	Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6638-6645.	1.1	5
146	Characteristic of Oral Squamous Cell Carcinoma Tissues Using Isotope Ratio Mass Spectrometry. <i>Journal of Clinical Medicine</i> , 2020, 9, 3760.	1.0	5
147	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
148	Direct mass spectrometric analysis of the ¹⁸ O/ ¹⁶ O ratio in sulfur-containing organophosphorus compounds. <i>Organic Mass Spectrometry</i> , 1980, 15, 302-303.	1.3	4
149	Semiempirical SCF-MO calculations of kinetic isotope effects. <i>Journal of Physical Organic Chemistry</i> , 1991, 4, 635-638.	0.9	4
150	Significance of the cis-trans isomerization of early intermediates in the carotene biosynthetic pathway. <i>Journal of Physical Organic Chemistry</i> , 1992, 5, 783-786.	0.9	4
151	³⁶ S and ¹⁸ O isotope effects in infrared spectra of monothiopyrophosphates. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1985, 41, 513-514.	0.1	3
152	Mechanisms of Isomerization of Sym-Monothiopyrophosphates. <i>Phosphorous and Sulfur and the Related Elements</i> , 1987, 30, 257-260.	0.2	3
153	Numerical evaluation of the time-dependence of concentrations, rates and kinetic isotope effects. <i>Computers & Chemistry</i> , 1991, 15, 347-349.	1.2	3
154	Dependence of isotope effects on conformation in decarboxylation of 3-carboxybenzisoxazoles. <i>Computational and Theoretical Chemistry</i> , 1996, 370, 237-243.	1.5	3
155	A Search for Dual Action HIV-1 Reverse Transcriptase, Bacterial RNA Polymerase Inhibitors. <i>Molecules</i> , 2017, 22, 1808.	1.7	3
156	Quantum approach to the mechanism of monothiopyrophosphate isomerization. <i>Journal of Molecular Modeling</i> , 2019, 25, 286.	0.8	3
157	Machine Learning augmented docking studies of aminothiureas at the SARS-CoV-2 ACE2 interface. <i>PLoS ONE</i> , 2021, 16, e0256834.	1.1	3
158	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
159	Nitrogen Kinetic Isotope Effects on the Decarboxylation of 4-Pyridylacetic Acid. <i>Journal of Organic Chemistry</i> , 2001, 66, 5534-5536.	1.7	2
160	Analysis of Conformer Stability for 1,3,8-Trihydroxynaphthalene: A Natural Substrate of Fungal Trihydroxynaphthalene Reductase. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8314-8320.	1.2	2
161	Carbon and secondary deuterium kinetic isotope effects on S _N 2 methyl transfer reactions. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1114-1120.	0.9	2
162	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

#	ARTICLE	IF	CITATIONS
163	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
164	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
165	Isotopic Consequences of Host–Guest Interactions; Noncovalent Chlorine Isotope Effects. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1874-1880.	1.2	2
166	Substrate-Enzyme Interactions from Modeling and Isotope Effects. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 341-363.	0.6	2
167	Isotope Effect Evidence for Charge Localization in Phosphothioates. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1990, 51, 405-405.	0.8	1
168	Hydrogen Atom Transfers in B12 Enzymes. , 0, , 1473-1495.		1
169	Chlorine Kinetic Isotope Effects on Biological Systems. , 2005, , 875-892.		1
170	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
171	Synthesis of N,N-dimethyl[2- ¹⁴ C] morpholinium chloride. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 1982, 19, 309-312.	0.5	0
172	Mass spectra of isomeric monothiopyrophosphates. <i>Organic Mass Spectrometry</i> , 1986, 21, 419-423.	1.3	0
173	Evaluation of normal frequencies for isotopic nonlinear X-Y-Z molecules by a programmable calculator. <i>Computers & Chemistry</i> , 1986, 10, 21-26.	1.2	0
174	Synthetic route to isotopically labelled-oxamate. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 2011, 54, 344-344.	0.5	0
175	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
176	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