# Piotr Paneth

## List of Publications by Citations



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| 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 | Physical and chemical basis of carbon isotope fractionation in plants. *Plant, Cell and Environment*, **1992**, 15, 1099-1104 | 8.4 | 175 |
| 174 | ISOEFF98. A program for studies of isotope effects using Hessian modifications. *Journal of Mathematical Chemistry*, **1999**, 26, 75-86 | 2.1 | 141 |
| 173 | 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 |
| 172 | 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 |
| 171 | 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 |
| 170 | Solvent-dependent transition states for decarboxylations. *Journal of the American Chemical Society*, **2001**, 123, 7683-6 | 16.4 | 65 |
| 169 | Carbon isotope effect on dehydration of bicarbonate ion catalyzed by carbonic anhydrase. *Biochemistry*, **1985**, 24, 5143-7 | 3.2 | 65 |
| 168 | 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 |
| 167 | Investigation of the enzymatic mechanism of yeast orotidine-5'-monophosphate decarboxylase using 13C kinetic isotope effects. *Biochemistry*, **1991**, 30, 6216-23 | 3.2 | 62 |
| 166 | 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 |
| 165 | Binding isotope effects. *Chemical Reviews*, **2013**, 113, 7851-79 | 68.1 | 58 |
| 164 | Synthesis, cytotoxic effect, and structure-activity relationship of Pd(II) complexes with coumarin derivatives. *Inorganic Chemistry*, **2006**, 45, 9688-95 | 5.1 | 53 |
| 163 | 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 |
| 162 | Chlorine kinetic isotope effects on the haloalkane dehalogenase reaction. *Journal of the American Chemical Society*, **2001**, 123, 4550-5 | 16.4 | 46 |
| 161 | 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 |
| 160 | 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 |
| 159 | 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 |

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| 158 | Isotope Effects **2009**, | | 34 |
| 157 | Chlorine kinetic isotope effects on enzymatic dehalogenations. *Accounts of Chemical Research*, **2003**, 36, 120-6 | 24.3 | 34 |
| 156 | Equilibrium isotope effect on ternary complex formation of [1-18O]oxamate with NADH and lactate dehydrogenase. *Biochemistry*, **1995**, 34, 6050-8 | 3.2 | 33 |
| 155 | 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 |
| 154 | A new method of determining chlorine kinetic isotope effects. *Analytical Chemistry*, **1998**, 70, 3548-52 | 7.8 | 32 |
| 153 | Kinetic isotope effects on dehalogenations at an aromatic carbon. *Environmental Science & Technology*, **2008**, 42, 7744-50 | 10.3 | 32 |
| 152 | Isotopic analysis of oxidative pollutant degradation pathways exhibiting large H isotope fractionation. *Environmental Science & Technology*, **2013**, 47, 13459-68 | 10.3 | 31 |
| 151 | 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 |
| 150 | Modeling of isotope effects on binding oxamate to lactic dehydrogenase. *Journal of Physical Chemistry B*, **2009**, 113, 12782-9 | 3.4 | 30 |
| 149 | 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 |
| 148 | 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 |
| 147 | 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 |
| 146 | Biological and docking studies of topoisomerase IV inhibition by thiosemicarbazides. *Journal of Molecular Modeling*, **2011**, 17, 2297-303 | 2 | 27 |
| 145 | Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. *ACS Catalysis*, **2017**, 7, 5294-5307 | 13.1 | 26 |
| 144 | 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 |
| 143 | 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 |
| 142 | A new interpretation of chlorine leaving group kinetic isotope effects; a theoretical approach. *Journal of Organic Chemistry*, **2004**, 69, 4900-5 | 4.2 | 26 |
| 141 | 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 |

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| 140 | DFT study of trichloroethene reaction with permanganate in aqueous solution. *Environmental Science & Technology*, **2011**, 45, 3006-11 | 10.3 | 25 |
| 139 | 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 |
| 138 | Analyzing sites of OH radical attack (ring vs. side chain) in oxidation of substituted benzenes via dual stable isotope analysis (δ13C and δ2H). *Science of the Total Environment*, **2016**, 542, 484-94 | 10.2 | 25 |
| 137 | Modeling excitation properties of iridium complexes. *Journal of Physical Organic Chemistry*, **2009**, 22, 845-856 | 2.1 | 24 |
| 136 | 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 |
| 135 | Extending limits of chlorine kinetic isotope effects. *Journal of Organic Chemistry*, **2012**, 77, 5120-4 | 4.2 | 23 |
| 134 | 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 |
| 133 | 1,4-Disubstituted thiosemicarbazide derivatives are potent inhibitors of Toxoplasma gondii proliferation. *Molecules*, **2014**, 19, 9926-43 | 4.8 | 22 |
| 132 | Structural Aspects and Rearrangement of Radical Cations Generated from NADH Analogues. *Journal of the American Chemical Society*, **1996**, 118, 691-692 | 16.4 | 22 |
| 131 | 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 |
| 130 | Kinetic isotope effects on substrate association: reactions of phosphoenolpyruvate with phosphoenolpyruvate carboxylase and pyruvate kinase. *Biochemistry*, **1995**, 34, 2577-83 | 3.2 | 21 |
| 129 | Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 2246-2254 | 6.4 | 20 |
| 128 | Theoretical calculations of heavy-atom isotope effects. *Computers & Chemistry*, **1995**, 19, 231-40 | | 20 |
| 127 | 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 |
| 126 | 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 |
| 125 | Nitrogen and deuterium kinetic isotope effects on the Menshutkin reaction. *Journal of Physical Organic Chemistry*, **1996**, 9, 35-40 | 2.1 | 18 |
| 124 | Measurements of heavy-atom isotope effects using 1H NMR spectroscopy. *Journal of Organic Chemistry*, **2011**, 76, 8033-5 | 4.2 | 17 |
| 123 | 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 |

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| 122 | 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 |
| 121 | Triazole-based compound as a candidate to develop novel medicines to treat toxoplasmosis. *Antimicrobial Agents and Chemotherapy*, **2014**, 58, 7583-5 | 5.9 | 16 |
| 120 | Mechanism of the reaction catalyzed by DL-2-haloacid dehalogenase as determined from kinetic isotope effects. *Biochemistry*, **2006**, 45, 6012-7 | 3.2 | 16 |
| 119 | Tritium secondary kinetic isotope effect on phenylalanine ammonia-lyase-catalyzed reaction. *Archives of Biochemistry and Biophysics*, **1999**, 370, 216-21 | 4.1 | 16 |
| 118 | Phosphorus-sulfur bond order in phosphothioate anions. *Journal of the American Chemical Society*, **1986**, 108, 1720-1722 | 16.4 | 16 |
| 117 | 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 |
| 116 | Importance of the lactate dehydrogenase quaternary structure in theoretical calculations. *Journal of Physical Chemistry B*, **2010**, 114, 3393-7 | 3.4 | 15 |
| 115 | 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 |
| 114 | On the application of the steady state to kinetic isotope effects. *Journal of the American Chemical Society*, **1985**, 107, 7070-7071 | 16.4 | 15 |
| 113 | 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 |
| 112 | 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 |
| 111 | Theoretical evaluation of isotopic fractionation factors in oxidation reactions of benzene, phenol and chlorophenols. *Journal of Molecular Modeling*, **2011**, 17, 2285-96 | 2 | 13 |
| 110 | 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 |
| 109 | Progress in understanding the N-demethylation of alkaloids by exploiting isotopic techniques. *Phytochemistry Reviews*, **2007**, 6, 51-63 | 7.7 | 13 |
| 108 | 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 |
| 107 | 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 |
| 106 | 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 |
| 105 | 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 |

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| 104 | Kinetic isotope effects on the Menshutkin reaction: Theory versus experiment. *Journal of Physical Organic Chemistry*, **1996**, 9, 41-49 | 2.1 | 12 |
| 103 | Isotope effects on binding. *Journal of Molecular Structure*, **1996**, 378, 35-43 | 3.4 | 12 |
| 102 | DFT Studies of SN2 Dechlorination of Polychlorinated Biphenyls. *Environmental Science & Technology*, **2016**, 50, 6293-8 | 10.3 | 11 |
| 101 | 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 |
| 100 | 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 |
| 99 | 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 |
| 98 | 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 |
| 97 | Chlorine Isotope Effects on Chemical Reactions. *Current Organic Chemistry*, **2005**, 9, 75-88 | 1.7 | 11 |
| 96 | Some analytical aspects of the measurement of heavy-atom kinetic isotope effects. *Talanta*, **1987**, 34, 877-83 | 6.2 | 11 |
| 95 | 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 |
| 94 | Pharmacological and structure-activity relationship evaluation of 4-aryl-1-diphenylacetyl(thio)semicarbazides. *Molecules*, **2014**, 19, 4745-59 | 4.8 | 10 |
| 93 | Isotopic fractionation - chemical v. environmental perspective. *Environmental Chemistry*, **2012**, 9, 67 | 3.2 | 10 |
| 92 | Validation of semiempirical methods for modeling of corrinoid systems. *Journal of Inorganic Biochemistry*, **2004**, 98, 1078-86 | 4.2 | 10 |
| 91 | 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 |
| 90 | 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 |
| 89 | 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 |
| 88 | Evolved Fusarium oxysporum laccase expressed in Saccharomyces cerevisiae. *Scientific Reports*, **2020**, 10, 3244 | 4.9 | 9 |
| 87 | 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 |

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| 86 | 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 |
| 85 | 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 |
| 84 | Computational studies of the cyclization of thiosemicarbazides. *Journal of Physical Organic Chemistry*, **2007**, 20, 463-468 | 2.1 | 9 |
| 83 | Preparation of 18O-labelled nicotinamide. *Journal of Labelled Compounds and Radiopharmaceuticals* , **2002**, 45, 1005-1010 | 1.9 | 9 |
| 82 | Heavy atom isotope effects on enzymatic reactions. *Journal of Molecular Structure*, **1994**, 321, 35-44 | 3.4 | 9 |
| 81 | 13C NMR and 1H-1H NOEs of Coenzyme-A: Conformation of the Pantoic Acid Moiety. *Bioorganic Chemistry*, **1995**, 23, 169-181 | 5.1 | 9 |
| 80 | Synthesis and antibacterial activity of 1,4-dibenzoylthiosemicarbazide derivatives. *Biomedicine and Pharmacotherapy*, **2017**, 88, 1235-1242 | 7.5 | 8 |
| 79 | 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 |
| 78 | 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 |
| 77 | Enzyme mechanisms from molecular modeling and isotope effects. *Archives of Biochemistry and Biophysics*, **2008**, 474, 274-82 | 4.1 | 8 |
| 76 | Synthesis and pharmacological properties of 3-(2-methyl-furan-3-yl)-4-substituted-Δ2-1,2,4-triazoline-5-thiones. *Open Chemistry*, **2008**, 6, 47-53 | 1.6 | 8 |
| 75 | Chlorine kinetic isotope effect on the fluoroacetate dehalogenase reaction. *Journal of the American Chemical Society*, **2001**, 123, 9192-3 | 16.4 | 8 |
| 74 | Sulfur-34, sulfur-36, and oxygen-18 isotope effects on phosphorus-31 chemical shifts in thiophosphate anhydrides. *Journal of the American Chemical Society*, **1985**, 107, 1409-1411 | 16.4 | 8 |
| 73 | Non-statistical isotope fractionation as a novel "retro-biosynthetic" approach to understanding alkaloid metabolic pathways. *Phytochemistry Letters*, **2017**, 20, 499-506 | 1.9 | 7 |
| 72 | 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 |
| 71 | 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 |
| 70 | Correlating biological activity with calculated geometric motifs in cyclolinopeptide A analogs. *Journal of Physical Organic Chemistry*, **2004**, 17, 625-630 | 2.1 | 7 |
| 69 | Isotope effect evidence for the zinc hydroxide mechanism of carbonic anhydrase catalysis. *Biochemistry*, **1987**, 26, 1728-31 | 3.2 | 7 |

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| 68 | Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. *Molecules*, **2018**, 23, | 4.8 | 7 |
| 67 | 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 |
| 66 | 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 |
| 65 | Lipophilicity Studies on Thiosemicarbazide Derivatives. *Molecules*, **2017**, 22, | 4.8 | 6 |
| 64 | 2-OMe-lysophosphatidylcholine analogues are GPR119 ligands and activate insulin secretion from IT C-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 |
| 63 | A DFT study of permanganate oxidation of toluene and its ortho-nitroderivatives. *Journal of Molecular Modeling*, **2014**, 20, 2091 | 2 | 6 |
| 62 | 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 |
| 61 | Are mutated enzymes good models for interpretation of intrinsic isotope effects?. *Computational and Theoretical Chemistry*, **1998**, 454, 69-75 | | 6 |
| 60 | Chemical and Pharmacological Properties of 3-(Thiophen-2-yl)-4-substituted- 2-1,2,4-triazoline-5-thiones. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2008**, 183, 2669-2677 | 1 | 6 |
| 59 | Influence of the solvent description on the predicted mechanism of SN2 reactions. *Journal of Physical Chemistry B*, **2008**, 112, 12414-9 | 3.4 | 6 |
| 58 | 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 |
| 57 | 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 |
| 56 | Analogues of NADP(+) as inhibitors and coenzymes for NADP(+) malic enzyme from maize leaves. *Photosynthesis Research*, **1991**, 28, 69-76 | 3.7 | 6 |
| 55 | 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 |
| 54 | Measurement and Prediction of Chlorine Kinetic Isotope Effects in Enzymatic Systems. *Methods in Enzymology*, **2017**, 596, 179-215 | 1.7 | 5 |
| 53 | Rhabdomyosarcoma in children in the light of isotope ratio mass spectrometry. *Polish Journal of Pathology*, **2015**, 66, 383-8 | 0.9 | 5 |
| 52 | Does dehydrocyclization of 4-benzoylthiosemicarbazides in acetic acid lead to s-triazoles or thiadiazoles?. *Structural Chemistry*, **2012**, 23, 1441-1448 | 1.8 | 5 |
| 51 | 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 |

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| 50 | Theoretical calculations of heavy-atom isotope effects. *Computers & Chemistry*, **1995**, 19, 11-20 | | 5 |
| 49 | Deuterium kinetic isotope effect on quaternization of N,N-dimethylaniline. *Journal of Molecular Structure*, **1994**, 321, 97-99 | 3.4 | 5 |
| 48 | 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 |
| 47 | Relative sulfur-36-sulfur-34 kinetic isotope effects. *Journal of the American Chemical Society*, **1985**, 107, 1407-1408 | 16.4 | 5 |
| 46 | Antibacterial Activity of Fluorobenzoylthiosemicarbazides and Their Cyclic Analogues with 1,2,4-Triazole Scaffold. *Molecules*, **2020**, 26, | 4.8 | 5 |
| 45 | RNA-Inspired and Accelerated Degradation of Polylactide in Seawater. *Journal of the American Chemical Society*, **2021**, 143, 16673-16681 | 16.4 | 5 |
| 44 | Docking and QSAR of Aminothioureas at the SARS-CoV-2 S-Protein-Human ACE2 Receptor Interface. *Molecules*, **2020**, 25, | 4.8 | 4 |
| 43 | 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 |
| 42 | Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. *Journal of Physical Chemistry A*, **2017**, 121, 6638-6645 | 2.8 | 4 |
| 41 | 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 |
| 40 | 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 |
| 39 | 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 |
| 38 | Quantum approach to the mechanism of monothiopyrophosphate isomerization. *Journal of Molecular Modeling*, **2019**, 25, 286 | 2 | 3 |
| 37 | Assessment of Nonnucleoside Inhibitors Binding to HIV-1 Reverse Transcriptase Using HYDE Scoring. *Pharmaceuticals*, **2019**, 12, | 5.2 | 3 |
| 36 | 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 |
| 35 | Dependence of isotope effects on conformation in decarboxylation of 3-carboxybenzisoxazoles. *Computational and Theoretical Chemistry*, **1996**, 370, 237-243 | | 3 |
| 34 | Numerical evaluation of the time-dependence of concentrations, rates and kinetic isotope effects. *Computers & Chemistry*, **1991**, 15, 347-349 | | 3 |
| 33 | Semiempirical SCF-MO calculations of kinetic isotope effects. *Journal of Physical Organic Chemistry*, **1991**, 4, 635-638 | 2.1 | 3 |

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| 32 | Mechanisms of Isomerization of Sym-Monothiopyrophosphates. *Phosphorous and Sulfur and the Related Elements*, **1987**, 30, 257-260 | | 3 |
| 31 | 36S and 18O isotope effects in infrared spectra of monothiopyrophosphates. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1985**, 41, 513-514 | | 3 |
| 30 | 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 |
| 29 | Characteristic of Oral Squamous Cell Carcinoma Tissues Using Isotope Ratio Mass Spectrometry. *Journal of Clinical Medicine*, **2020**, 9, | 5.1 | 3 |
| 28 | 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 |
| 27 | 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 |
| 26 | A Search for Dual Action HIV-1 Reverse Transcriptase, Bacterial RNA Polymerase Inhibitors. *Molecules*, **2017**, 22, | 4.8 | 2 |
| 25 | 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 |
| 24 | Carbon and secondary deuterium kinetic isotope effects on SN2 methyl transfer reactions. *Journal of Physical Organic Chemistry*, **2007**, 20, 1114-1120 | 2.1 | 2 |
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