Igor Tvaroska

List of Publications by Year in descending order

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154 papers	4,001 citations	126858 33 h-index	155592 55 g-index
158 all docs	158 docs citations	158 times ranked	2941 citing authors

#	Article	IF	Citations
1	Anomeric and Exo-Anomeric Effects in Carbohydrate Chemistry. Advances in Carbohydrate Chemistry and Biochemistry, 1989, 47, 45-123.	0.4	293
2	An attempt to derive a new Karplus-type equation of vicinal proton-carbon coupling constants for Cî—¸Oî—¸Cî—¸H segments of bonded atoms. Carbohydrate Research, 1989, 189, 359-362.	1.1	260
3	PEGylated Nanoparticles Bind to and Alter Amyloid-Beta Peptide Conformation: Toward Engineering of Functional Nanomedicines for Alzheimerâ€™s Disease. ACS Nano, 2012, 6, 5897-5908.	7.3	164
4	Carbon-Proton Coupling Constants In The Conformational Analysis of Sugar Molecules. Advances in Carbohydrate Chemistry and Biochemistry, 1995, 51, 15-61.	0.4	134
5	Conformational-energy calculations for oligosaccharides: a comparison of methods and a strategy of calculation. Carbohydrate Research, 1986, 149, 389-410.	1.1	128
6	Quantum mechanical and NMR spectroscopy studies on the conformations of the hydroxymethyl and methoxymethyl groups in aldohexosides. Carbohydrate Research, 2002, 337, 353-367.	1.1	105
7	Theoretical studies on the conformation of saccharides. 3. Conformational properties of the glycosidic linkage in solution and their relation to the anomeric and exoanomeric effects. Journal of the American Chemical Society, 1980, 102, 6929-6936.	6.6	94
8	Binding of Î²-Amyloid (1â€“42) Peptide to Negatively Charged Phospholipid Membranes in the Liquid-Ordered State: Modeling and Experimental Studies. Biophysical Journal, 2012, 103, 453-463.	0.2	65
9	Hydration of Î±-maltose and amylose: molecular modelling and thermodynamics study. Carbohydrate Research, 1995, 278, 27-41.	1.1	64
10	Ab Initio Molecular Orbital Study of the Catalytic Mechanism of Glycosyltransferases:Â Description of Reaction Pathways and Determination of Transition-State Structures for InvertingN-Acetylglucosaminyltransferases. Journal of the American Chemical Society, 2000, 122, 8762-8776.	6.6	63
11	Modelling of Î²-d-glucopyranose ring distortion in different force fields: a metadynamics study. Carbohydrate Research, 2010, 345, 530-537.	1.1	61
12	Conformational analysis of (1 â† 6)-Î±-D-glucan. Carbohydrate Research, 1978, 61, 97-106.	1.1	60
13	Ab initio molecular orbital calculation of carbohydrate model compounds. 2. Conformational analysis of axial and equatorial 2-methoxytetrahydropyrans. The Journal of Physical Chemistry, 1994, 98, 9477-9485.	2.9	60
14	Molecular and Crystal Structures of Inulin from Electron Diffraction Data. Macromolecules, 1996, 29, 4626-4635.	2.2	60
15	Carbohydrateâ€“Protein Interactions. Advances in Carbohydrate Chemistry and Biochemistry, 2014, 71, 9-136.	0.4	60
16	Crystalline conformation and structure of lichenan and barley Î²-glucan. Canadian Journal of Chemistry, 1983, 61, 1608-1616.	0.6	56
17	Synthesis and Conformational Analysis of Novel N(OCH3)-linked Disaccharide Analogues. Chemistry - A European Journal, 2004, 10, 1433-1444.	1.7	53
18	Theoretical studies on the conformation of saccharides. IV. Solvent effect on the stability of ?-maltose conformers. Biopolymers, 1982, 21, 1887-1897.	1.2	48

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19	Angular dependence of vicinal carbon-proton coupling constants for conformational studies of the hydroxymethyl group in carbohydrates. Carbohydrate Research, 1995, 271, 151-162.	1.1	47
20	Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. 6. The Gauche Effect and Conformations of the Hydroxymethyl and Methoxymethyl Groups. Journal of Physical Chemistry B, 1997, 101, 2992-2999.	1.2	45
21	The anomeric and exo-anomeric effects of a hydroxyl group and the stereochemistry of the hemiacetal linkage11Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. Part 7. For Part 6, see ref[1].. Carbohydrate Research, 1998, 309, 1-9.	1.1	44
22	Ab InitioMolecular Orbital Calculation of Carbohydrate Model Compounds. 5. Anomeric,Exo-Anomeric, and Reverse Anomeric Effects inC-,N-, andS-Glycosyl Compounds. The Journal of Physical Chemistry, 1996, 100, 11305-11313.	2.9	43
23	Theoretical studies on the conformation of saccharides. Theoretica Chimica Acta, 1986, 70, 99-114.	0.9	40
24	Molecular modeling insights into the catalytic mechanism of the retaining galactosyltransferase LgtC. Carbohydrate Research, 2004, 339, 1007-1014.	1.1	40
25	Catalytic Mechanism of Glycosyltransferases:Â Hybrid Quantum Mechanical/Molecular Mechanical Study of the InvertingN-Acetylglucosaminyltransferase I. Journal of the American Chemical Society, 2006, 128, 16921-16927.	6.6	40
26	Stereochemistry of nonreducing disaccharides in solution. Carbohydrate Research, 1987, 160, 137-149.	1.1	39
27	Substrate-Assisted Catalytic Mechanism of O-GlcNAc Transferase Discovered by Quantum Mechanics/Molecular Mechanics Investigation. Journal of the American Chemical Society, 2012, 134, 15563-15571.	6.6	39
28	Resolution of Racemic Nâ€Benzyl Îąâ€Amino Acids by Liquidâ€Liquid Extraction: A Practical Method Using a Lipophilic Chiral Cobalt(III) Salen Complex and Mechanistic Studies. European Journal of Organic Chemistry, 2008, 2008, 1253-1264.	1.2	38
29	Selectinsâ€”The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Moleculesâ€”A Review. Molecules, 2020, 25, 2835.	1.7	38
30	Molecular orbitals studies of the conformations of dimethoxymethane. Journal of Molecular Structure, 1975, 24, 249-259.	1.8	34
31	Lone pair interactions in dimethoxymethane and anomeric effect. Canadian Journal of Chemistry, 1979, 57, 424-435.	0.6	34
32	The conformational properties of the glycosidic linkage. Carbohydrate Research, 1981, 90, 173-185.	1.1	33
33	Hybrid Quantum Mechanical/Molecular Mechanical Investigation of the Î²-1,4-Galactosyltransferase-I Mechanism. Journal of Physical Chemistry B, 2009, 113, 11314-11319.	1.2	33
34	A theoretical study on the catalytic mechanism of the retaining Îą-1,2-mannosyltransferase Kre2p/Mnt1p: the impact of different metal ions on catalysis. Organic and Biomolecular Chemistry, 2014, 12, 4201.	1.5	33
35	One-bond carbon-proton coupling constants: Angular dependence in Î²-linked oligosaccharides. Journal of Biomolecular NMR, 1992, 2, 421-430.	1.6	32
36	Conformational Free Energy Surface of Îą-N-Acetylneuraminic Acid: An Interplay Between Hydrogen Bonding and Solvation. Journal of Physical Chemistry B, 2009, 113, 9589-9594.	1.2	32

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37	Atomistic insight into the catalytic mechanism of glycosyltransferases by combined quantum mechanics/molecular mechanics (QM/MM) methods. Carbohydrate Research, 2015, 403, 38-47.	1.1	32
38	An attempt to derive the potential function for evaluation of the energy associated with the exo-anomeric effect. Carbohydrate Research, 1984, 125, 155-160.	1.1	31
39	Conformational dependence of the one-bond carbon-proton coupling constants in oligosaccharides. Magnetic Resonance in Chemistry, 1990, 28, 862-866.	1.1	30
40	Dependence on saccharide conformation of the one-bond and three-bond carbonî—¸proton coupling constants. Carbohydrate Research, 1990, 206, 55-64.	1.1	30
41	Conformation and dynamics of a cyclic (1 â†' 2)-Î²-d-glucan. International Journal of Biological Macromolecules, 1995, 17, 189-198.	3.6	30
42	Conformational statistics of pectin substances in solution by a Metropolis Monte Carlo study. Carbohydrate Polymers, 1997, 32, 255-266.	5.1	29
43	RAMM â€" A new procedure for theoretical conformational analysis of carbohydrates. Carbohydrate Research, 1990, 204, 29-36.	1.1	28
44	On the reaction pathways and determination of transition-state structures for retaining Î±-galactosyltransferases. Carbohydrate Research, 2003, 338, 865-877.	1.1	28
45	Exploring Reaction Pathways for O-GlcNAc Transferase Catalysis. A String Method Study. Journal of Physical Chemistry B, 2015, 119, 4371-4381.	1.2	28
46	Automated Training of ReaxFF Reactive Force Fields for Energetics of Enzymatic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 291-302.	2.3	28
47	Ab Initio Molecular Orbital Calculation on Carbohydrate Model Compounds. 1. The Anomeric Effect in Fluoro and Chloro Derivatives of Tetrahydropyran. The Journal of Physical Chemistry, 1994, 98, 6452-6458.	2.9	27
48	Solution behavior of methyl Î²-xylobioside: Conformational flexibility revealed by n.m.r. measurements and theoretical calculations. Carbohydrate Research, 1990, 198, 193-203.	1.1	26
49	Potential transition-state analogs for glycosyltransferases. Design and DFT calculations of conformational behavior. Carbohydrate Research, 2005, 340, 1051-1057.	1.1	26
50	One-bond carbon-proton coupling constants: angular dependence in Î±-linked oligosaccharides. Carbohydrate Research, 1991, 221, 83-94.	1.1	25
51	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. Carbohydrate Research, 2009, 344, 1575-1581.	1.1	25
52	Comparative DFT study on the Î±-glycosidic bond in reactive species of galactosyl diphosphates. Chemical Papers, 2009, 63, .	1.0	25
53	Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. 3. Effect of the Electric Field on Conformations about the Glycosidic Linkage. The Journal of Physical Chemistry, 1995, 99, 6234-6241.	2.9	24
54	Î±-d-Mannose derivatives as models designed for selective inhibition of Golgi Î±-mannosidase II. European Journal of Medicinal Chemistry, 2011, 46, 944-952.	2.6	24

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55	Saturated irregular structures in poly(vinyl chloride). European Polymer Journal, 1975, 11, 411-416.	2.6	23
56	Study of the kinetics and mechanism of the acid-base-catalyzed enolization of hydroxyacetaldehyde and methoxyacetaldehyde. Carbohydrate Research, 1980, 87, 35-50.	1.1	22
57	Determination of Long Range Proton Carbon Coupling Constants by Modified Semi-Selective Two-Dimensional Inept: An Application in Stereochemical Analysis of Saccharides. Journal of Carbohydrate Chemistry, 1989, 8, 389-394.	0.4	22
58	Solvent effect on the stability of isomaltose conformers. Biopolymers, 1990, 30, 369-379.	1.2	22
59	PCILO quantum-mechanical relaxed conformational energy map of methyl 4-thio-Î±-maltoside in solution. Carbohydrate Research, 1992, 225, 27-41.	1.1	22
60	Continuous metadynamics in essential coordinates as a tool for free energy modelling of conformational changes. Journal of Molecular Modeling, 2008, 14, 995-1002.	0.8	22
61	Theoretical study of enzymatic catalysis explains why the trapped covalent intermediate in the E303C mutant of glycosyltransferase GTB was not detected in the wild-type enzyme. Glycobiology, 2015, 25, 3-7.	1.3	22
62	Theoretical studies on the conformation of saccharides. VIII. Solvent effect on the stability of Î²-cellobiose conformers. Biopolymers, 1984, 23, 1951-1960.	1.2	21
63	Catalytic mechanism of the inverting N-acetylglucosaminyltransferase I: DFT quantum mechanical model of the reaction pathway and determination of the transition state structure. Glycobiology, 2003, 13, 559-566.	1.3	21
64	Stepwise Catalytic Mechanism via Short-Lived Intermediate Inferred from Combined QM/MM MERP and PES Calculations on Retaining Glycosyltransferase ppGalNAcT2. PLoS Computational Biology, 2015, 11, e1004061.	1.5	21
65	Computational methods for studying oligo- and polysaccharide conformations. Pure and Applied Chemistry, 1989, 61, 1201-1216.	0.9	21
66	Toward an Accurate Conformational Modeling of Iduronic Acid. Journal of Physical Chemistry B, 2013, 117, 1003-1009.	1.2	20
67	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	5.8	20
68	Structural Insights into the Catalytic Mechanism and Transition State of Glycosyltransferases Using ab initio Molecular Modeling. Trends in Glycoscience and Glycotechnology, 2005, 17, 177-190.	0.0	19
69	Conformational study of digalacturonic acid and sodium digalacturonate in solution. Carbohydrate Research, 1994, 261, 187-202.	1.1	18
70	Highly Conserved Cysteines of Mouse Core 2 Î²1,6-N-Acetylglucosaminyltransferase I Form a Network of Disulfide Bonds and Include a Thiol That Affects Enzyme Activity. Journal of Biological Chemistry, 2003, 278, 45864-45881.	1.6	18
71	Enantioselective Epoxidation of Electrophilic Olefins by Using Glycosyl Hydroperoxides. Chemistry - A European Journal, 2008, 14, 6087-6097.	1.7	17
72	The binding properties of the H5N1 influenza virus neuraminidase as inferred from molecular modeling. Journal of Molecular Modeling, 2011, 17, 1445-1456.	0.8	17

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73	Theoretical aspects of structure and conformation of oligosaccharides. Current Opinion in Structural Biology, 1992, 2, 661-665.	2.6	16
74	Ab Initio Molecular Orbital Study of the Conformational Behavior of the Sugarâ^'Phosphate Linkage. Toward an Understanding of the Catalytic Mechanism of Glycosyltransferases. Journal of Physical Chemistry B, 1999, 103, 2560-2569.	1.2	16
75	Molecular dynamic studies of amyloid-beta interactions with curcumin and Cu2+ ions. Chemical Papers, 2015, 69, .	1.0	16
76	On thermal dehydrochlorination of model compounds for poly(vinyl chloride)â€"II. Tetrahedron, 1974, 30, 3275-3280.	1.0	15
77	Theoretical studies on the conformation of saccharides. Theoretica Chimica Acta, 1979, 53, 9-19.	0.9	15
78	Theoretical studies on the conformation of saccharides. V. Hydration of the acetal segment in glycosides. International Journal of Quantum Chemistry, 1983, 23, 765-778.	1.0	15
79	Electron impact, chemical ionization and collisional activation mass spectrometry of methylO-acetyl-Î²-D-xylopyranosides. Biological Mass Spectrometry, 1985, 12, 49-58.	0.5	15
80	Karplus-type equation for vicinal carbon-proton coupling constants for the Cî—¸Sî—¸Cî—¸H pathway in 1-thioglycosides. Carbohydrate Research, 1992, 229, 225-231.	1.1	15
81	Computer modeling of polysaccharide-polysaccharide interactions: An approach to the ?-carrageenan-mannan case. Biopolymers, 1992, 32, 551-560.	1.2	15
82	The conformational analysis of methyl Î²-xylobioside: effect of choice of potential functions. Carbohydrate Research, 1993, 247, 71-81.	1.1	15
83	Binding of Î²-<scp>d</scp>-Glucosides and Î²-<scp>d</scp>-Mannosides by Rice and Barley Î²-<scp>d</scp>-Glycosidases with Distinct Substrate Specificities. Biochemistry, 2010, 49, 8779-8793.	1.2	15
84	A QM/MM Investigation of the Catalytic Mechanism of Metalâ€Ionâ€Independent Core 2 Î²1,6â€Nâ€Acetylglucosaminyltransferase. Chemistry - A European Journal, 2013, 19, 8153-8162.	1.7	15
85	Calculation of solvent effect on conformation stability and anomeric effect in dimethoxymethane. Collection of Czechoslovak Chemical Communications, 1980, 45, 1883-1895.	1.0	15
86	Ab initio molecular orbital calculation of carbohydrate model compounds 4. Flexibility of Î¨-type glycosidic bonds in carbohydrates. Computational and Theoretical Chemistry, 1997, 395-396, 1-13.	1.5	14
87	Effects of the Complexation by the Mg2+ Cation on the Stereochemistry of the Sugarâ^'Diphosphate Linkage. Ab Initio Modeling on Nucleotideâ^'Sugars. Journal of Physical Chemistry A, 2000, 104, 4609-4617.	1.1	14
88	DFT calculations of the anomeric and exo-anomeric effect of the hydroperoxy and peroxy groups. Carbohydrate Research, 2008, 343, 1463-1472.	1.1	14
89	On thermal dehydrochlorination of model compounds for polyvinylchlorideâ€"I. European Polymer Journal, 1971, 7, 41-54.	2.6	13
90	Incorporation of lone pairs into the electrostatic term in the empirical intra- and intermolecular energy calculations. Biopolymers, 1979, 18, 2537-2547.	1.2	13

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91	Step by step towards understanding gold glyconanoparticles as elements of the nanoworld. Chemical Papers, 2007, 61, .	1.0	13
92	N-(4-Substituted-benzoyl)-Nâ€²-(Î²-d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. Bioorganic and Medicinal Chemistry, 2012, 20, 1801-1816.	1.4	13
93	First-Principles Interaction Analysis Assessment of the Manganese Cation in the Catalytic Activity of Glycosyltransferases. Journal of Physical Chemistry B, 2017, 121, 6148-6162.	1.2	13
94	Solvent effect on the stability of mannobiose conformers. Biopolymers, 1987, 26, 1499-1508.	1.2	12
95	Studies on the conformational behaviour of GlcNAc-Man3-GlcNAc2 oligosaccharides using molecular dynamics simulations. Glycoconjugate Journal, 1998, 15, 187-191.	1.4	12
96	Irregular structures in polyvinylchloride II. Unsaturated structures. Angewandte Makromolekulare Chemie, 1972, 23, 173-187.	0.3	11
97	Kinetics and mechanism of the acid-catalyzed reactions of methylated trioses. Carbohydrate Research, 1980, 87, 51-62.	1.1	11
98	Change of the molecular surface and volume during internal rotation and its effect on conformational equilibrium in solution. Journal of Molecular Structure, 1980, 68, 189-198.	1.8	11
99	Different QM/MM Approaches To Elucidate Enzymatic Reactions: Case Study on ppGalNAcT2. Journal of Chemical Theory and Computation, 2016, 12, 6062-6076.	2.3	11
100	Molecular simulations of hevein/(GlcNAc)3 complex with weakened OH/O and CH/Ï€ hydrogen bonds: implications for their role in complex stabilization. Carbohydrate Research, 2015, 408, 1-7.	1.1	10
101	Ab initio modelling of the anomeric and exo anomeric effects in 2-methoxytetrahydropyran and 2-methoxythiane corrected for intramolecular BSSE. Physical Chemistry Chemical Physics, 2015, 17, 18501-18513.	1.3	9
102	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. Glycobiology, 2021, 31, 975-987.	1.3	9
103	Non-planar conformations of methylacetamide: Solvent effect and chiroptical properties. Collection of Czechoslovak Chemical Communications, 1982, 47, 17-28.	1.0	9
104	QM/MM Insight on Enzymatic Reactions of Glycosyltransferases. Mini-Reviews in Organic Chemistry, 2011, 8, 263-269.	0.6	9
105	Nuclear overhauser effects and the flexibility of saccharides: methyl Î²-xylobioside. Carbohydrate Research, 1991, 210, 13-20.	1.1	8
106	Conformational analysis of ester and ether linkages in lignin-arabinoxylan complexes. Carbohydrate Research, 1994, 261, 91-102.	1.1	8
107	Ab initio studies of conformational properties of dimethyl diphosphate dianion and its complex with magnesium. Computational and Theoretical Chemistry, 1999, 469, 103-114.	1.5	8
108	Positive electrospray ion trap multistage mass spectrometric fragmentation of synthetic analogs of saccharide part of lipopolysaccharides of Vibrio cholerae O:1. Journal of the American Society for Mass Spectrometry, 2006, 17, 749-756.	1.2	8

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109	Oligosaccharides in Solution. ACS Symposium Series, 1990, , 162-176.	0.5	8
110	Role of electrostatic interactions in determination of anomeric effect in molecular-mechanical calculations of acetal conformation. Collection of Czechoslovak Chemical Communications, 1978, 43, 922-931.	1.0	8
111	Effect of the electric field on molecular structure in the MNDO approximation. Collection of Czechoslovak Chemical Communications, 1986, 51, 1803-1818.	1.0	8
112	On Thermal Dehydrochlorination of Model Compounds for PVC IV. MO Study of the Catalytic Effect of Hydrogen Chloride. Polymer Journal, 1975, 7, 34-43.	1.3	7
113	Multidisciplinary Approaches to the Structures of Model Compounds for Cellulose II. ACS Symposium Series, 1987, , 38-67.	0.5	7
114	Computer modelling of kappa carrageenam-mannan interactions. Journal of Molecular Recognition, 1994, 7, 243-250.	1.1	7
115	How Mycobacterium tuberculosis Galactofuranosyl Transferaseâ€…2 (GlfT2) Generates Alternating Î²â€(1â€“6) and Î²â€(1â€“5) Linkages: Aâ€‰QM/MM Molecular Dynamics Study of the Chemical Steps. Chemistry - A European Journal, 2018, 24, 7051-7059.	3.7	7
116	The role of chemical structure on the stereochemistry of the Î±-(1â€“4) diaxial glycosidic linkage. Journal of Molecular Structure, 1995, 344, 157-170.	1.8	6
117	Structure of bovine ?-1,3-galactosyltransferase and its complexes with UDP and DPGal inferred from molecular modeling. Proteins: Structure, Function and Bioinformatics, 2001, 44, 428-434.	1.5	6
118	Synthesis of saccharide precursors for preparation of potential inhibitors of glycosyltranferases. Chemical Papers, 2009, 63, .	1.0	6
119	Using DFT methodology for more reliable predictive models: Design of inhibitors of Golgi Î±-Mannosidase II. Journal of Molecular Graphics and Modelling, 2016, 66, 47-57.	1.3	6
120	Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain. Scientific Reports, 2019, 9, 18918.	1.6	6
121	MNDO conformations of chloromethyloxirane and solvent effect. Collection of Czechoslovak Chemical Communications, 1982, 47, 3199-3205.	1.0	6
122	Electrostatic effects on conformational equilibria: Solvation enthalpies and the reaction field theory. Collection of Czechoslovak Chemical Communications, 1984, 49, 2050-2069.	1.0	6
123	DFT and Docking Study of Potential Transition State Analogue Inhibitors of Glycosyltransferases. Collection of Czechoslovak Chemical Communications, 2008, 73, 591-607.	1.0	5
124	Conformational Free Energy Modeling of Druglike Molecules by Metadynamics in the WHIM Space. Journal of Chemical Information and Modeling, 2012, 52, 804-813.	2.5	5
125	Theoretical study of stereochemistry of methoxy(methylthio)methane as a model of thioacetal segment in thiosaccharides. Collection of Czechoslovak Chemical Communications, 1984, 49, 345-354.	1.0	5
126	Regioselective enhancement of the nucleophilicity of the hydroxyl groups in methyl Î±-l-rhamnopyranoside by complexation with tin(II) chloride. Carbohydrate Research, 1983, 118, 21-28.	1.1	4

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127	Theoretical studies on the conformation of saccharides. Computational and Theoretical Chemistry, 1985, 123, 141-154.	1.5	4
128	Electrospray ionization ion-trap multistage mass spectrometric study of sodium cationized aldobiuronic and pseudoaldobiuronic acid derivatives. Journal of Mass Spectrometry, 2004, 39, 1554-1561.	0.7	4
129	Development of transition state analogue inhibitors for N-acetylglycosyltransferases bearing D-psicoor D-tagatofuranose scaffolds. Chemical Papers, 2015, 69, .	1.0	4
130	Three-dimensional homology model of GlcNAc-TV glycosyltransferase. Glycobiology, 2016, 26, 757-771.	1.3	4
131	Purdie reagent-induced C(5)-epimerization of D-galacturonic acid derivatives in the presence of methyl sulphide. Collection of Czechoslovak Chemical Communications, 1976, 41, 3119-3130.	1.0	4
132	Synthesis of methyl (methyl Î±-L-altropyranosid)uronate and some of its derivatives. Collection of Czechoslovak Chemical Communications, 1976, 41, 3804-3811.	1.0	4
133	Glycosyltransferases as targets for therapeutic intervention in cancer and inflammation: molecular modeling insights. Chemical Papers, 2022, 76, 1953-1988.	1.0	4
134	Conformational analysis of oligosaccharides in solution. International Journal of Quantum Chemistry, 1989, 35, 141-151.	1.0	3
135	Theoretical studies on the conformation of saccharides. XIV. Structure and conformational properties of the glycosylamines. Biopolymers, 1990, 29, 1531-1539.	1.2	3
136	Structureâ€“Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. ChemPlusChem, 2014, 79, 1558-1568.	1.3	3
137	Synthesis of potential inhibitors of glycosyltransferases representing UDP-GlcNAc. Chemical Papers, 2015, 69, .	1.0	3
138	Conformational dependence of solvation energy of phosphates. Collection of Czechoslovak Chemical Communications, 1981, 46, 1722-1733.	1.0	3
139	The catalytic reaction mechanism of tyrosylprotein sulfotransferase-1. Physical Chemistry Chemical Physics, 2021, 23, 23850-23860.	1.3	3
140	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. ACS Omega, 2020, 5, 21374-21384.	1.6	3
141	DFT Study on 3-Substituted Tetrahydropyran-2-yl Radicals. Collection of Czechoslovak Chemical Communications, 2006, 71, 1453-1469.	1.0	2
142	Elimination of Isocyanate and Isothiocyanate Molecules at the Electrospray Ionization Ion Trap, Electrospray Ionization Quadrupole Time-of-Flight and Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Tandem Mass Spectrometry Fragmentation of Sodium Cationized Brassitin, Brassinin and Their Glycosides. European Journal of Mass Spectrometry, 2007, 13, 147-154.	0.5	2
143	Molecular Basis for the Biosynthesis of Oligo- and Polysaccharides. , 2008, , 2265-2323.		2
144	QM/MM Methods for Studying Enzymatic Reactions of Glycosyltransferases. Methods in Molecular Biology, 2015, 1273, 489-499.	0.4	2

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145	Acid-catalyzed hydrolysis of 2-methoxypropenal. Carbohydrate Research, 1983, 115, 85-94.	1.1	1
146	Mass spectrometry of the positionally isomeric, monobenzyl ethers of methyl glycopyranosides. Carbohydrate Research, 1983, 119, 13-24.	1.1	1
147	Molecular Orbital Investigations on Lignin Model Compounds. XXI. Solvent Effect on the Stability of Î²-Aryl Ether and Benzyl Aryl Ether Dimeric Units of Lignin. Holzforschung, 1987, 41, 371-377.	0.9	1
148	Conformational analysis of carbohydrates inferred from carbon-proton coupling constants. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1994, 91, 798-805.	0.2	1
149	The anomeric effect and associated Stereoelectronic effects. Carbohydrate Research, 1995, 267, C9-C10.	1.1	0
150	Elucidation of the Auâ€“S bond in a passivated gold cluster through density functional theory calculations (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064214.	0.7	0
151	Binding of Î²-Amyloid (1-42) Peptide to Negatively Charged Phospholipid Membranes in the Liquid-Ordered State. Biophysical Journal, 2013, 104, 94a.	0.2	0
152	Structure-Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. ChemPlusChem, 2014, 79, 1536-1536.	1.3	0
153	Conformational analysis of 2-acetamido-1,3-propanediol as a model of 3-acetamido-3-deoxyhexopyranoses. Collection of Czechoslovak Chemical Communications, 1977, 42, 1002-1012.	1.0	0
154	Effect of temperature on chiroptical and conformational properties of acyclic ketoses. Collection of Czechoslovak Chemical Communications, 1980, 45, 475-481.	1.0	0