

Igor Tvaroska

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149
papers

3,535
citations

31
h-index

51
g-index

158
ext. papers

3,718
ext. citations

3.7
avg, IF

5.27
L-index

#	Paper	IF	Citations
149	Anomeric and Exo-Anomeric Effects in Carbohydrate Chemistry. <i>Advances in Carbohydrate Chemistry and Biochemistry</i> , 1989 , 47, 45-123	3.7	266
148	An attempt to derive a new Karplus-type equation of vicinal proton-carbon coupling constants for C?O?C?H segments of bonded atoms. <i>Carbohydrate Research</i> , 1989 , 189, 359-362	2.9	235
147	PEGylated nanoparticles bind to and alter amyloid-beta peptide conformation: toward engineering of functional nanomedicines for Alzheimer's disease. <i>ACS Nano</i> , 2012 , 6, 5897-908	16.7	141
146	Conformational-energy calculations for oligosaccharides: a comparison of methods and a strategy of calculation. <i>Carbohydrate Research</i> , 1986 , 149, 389-410	2.9	121
145	Carbon-proton coupling constants in the conformational analysis of sugar molecules. <i>Advances in Carbohydrate Chemistry and Biochemistry</i> , 1995 , 51, 15-61	3.7	115
144	Quantum mechanical and NMR spectroscopy studies on the conformations of the hydroxymethyl and methoxymethyl groups in aldohexosides. <i>Carbohydrate Research</i> , 2002 , 337, 353-67	2.9	103
143	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. <i>Journal of the American Chemical Society</i> , 1980 , 102, 6929-6936	16.4	84
142	Ab Initio Molecular Orbital Study of the Catalytic Mechanism of Glycosyltransferases: Description of Reaction Pathways and Determination of Transition-State Structures for Inverting N-Acetylglucosaminyltransferases. <i>Journal of the American Chemical Society</i> , 2000 , 122, 8762-8776	16.4	59
141	Ab initio molecular orbital calculation of carbohydrate model compounds. 2. Conformational analysis of axial and equatorial 2-methoxytetrahydropyrans. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 9477-9485		59
140	Modelling of beta-D-glucopyranose ring distortion in different force fields: a metadynamics study. <i>Carbohydrate Research</i> , 2010 , 345, 530-7	2.9	57
139	Molecular and Crystal Structures of Inulin from Electron Diffraction Data. <i>Macromolecules</i> , 1996 , 29, 4626-4635	5.5	56
138	Hydration of alpha-maltose and amylose: molecular modelling and thermodynamics study. <i>Carbohydrate Research</i> , 1995 , 278, 27-41	2.9	56
137	Conformational analysis of (1 -> 6)-D-glucan. <i>Carbohydrate Research</i> , 1978 , 61, 97-106	2.9	55
136	Binding of Amyloid (1-42) peptide to negatively charged phospholipid membranes in the liquid-ordered state: modeling and experimental studies. <i>Biophysical Journal</i> , 2012 , 103, 453-463	2.9	53
135	Synthesis and conformational analysis of novel N(OCH3)-linked disaccharide analogues. <i>Chemistry - A European Journal</i> , 2004 , 10, 1433-44	4.8	49
134	Crystalline conformation and structure of lichenan and barley D-glucan. <i>Canadian Journal of Chemistry</i> , 1983 , 61, 1608-1616	0.9	48
133	Theoretical studies on the conformation of saccharides. IV. Solvent effect on the stability of D-maltose conformers. <i>Biopolymers</i> , 1982 , 21, 1887-1897	2.2	44

132	Angular dependence of vicinal carbon-proton coupling constants for conformational studies of the hydroxymethyl group in carbohydrates. <i>Carbohydrate Research</i> , 1995 , 271, 151-162	2.9	43
131	Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. 6. The Gauche Effect and Conformations of the Hydroxymethyl and Methoxymethyl Groups. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 2992-2999	3.4	42
130	The anomeric and exo-anomeric effects of a hydroxyl group and the stereochemistry of the hemiacetal linkage Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. Part 7. For Part 6, see ref[1]. <i>Carbohydrate Research</i> , 1998 , 309, 1-9	2.9	40
129	Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. 5. Anomeric, Exo-Anomeric, and Reverse Anomeric Effects in C-, N-, and S-Glycosyl Compounds. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 11305-11313		39
128	Catalytic mechanism of glycosyltransferases: hybrid quantum mechanical/molecular mechanical study of the inverting N-acetylglucosaminyltransferase I. <i>Journal of the American Chemical Society</i> , 2006 , 128, 16921-7	16.4	37
127	Theoretical studies on the conformation of saccharides. <i>Theoretica Chimica Acta</i> , 1986 , 70, 99-114		37
126	Stereochemistry of nonreducing disaccharides in solution. <i>Carbohydrate Research</i> , 1987 , 160, 137-149	2.9	37
125	Resolution of Racemic N-Benzyl α -Amino Acids by Liquid-Liquid Extraction: A Practical Method Using a Lipophilic Chiral Cobalt(III) Salen Complex and Mechanistic Studies. <i>European Journal of Organic Chemistry</i> , 2008 , 2008, 1253-1264	3.2	35
124	Carbohydrate-protein interactions: molecular modeling insights. <i>Advances in Carbohydrate Chemistry and Biochemistry</i> , 2014 , 71, 9-136	3.7	34
123	Substrate-assisted catalytic mechanism of O-GlcNAc transferase discovered by quantum mechanics/molecular mechanics investigation. <i>Journal of the American Chemical Society</i> , 2012 , 134, 15563-71	16.4	33
122	Molecular modeling insights into the catalytic mechanism of the retaining galactosyltransferase LgtC. <i>Carbohydrate Research</i> , 2004 , 339, 1007-14	2.9	33
121	Molecular orbitals studies of the conformations of dimethoxymethane. <i>Journal of Molecular Structure</i> , 1975 , 24, 249-259	3.4	32
120	Hybrid quantum mechanical/molecular mechanical investigation of the beta-1,4-galactosyltransferase-I mechanism. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 11314-9	3.4	31
119	One-bond carbon-proton coupling constants: Angular dependence in linked oligosaccharides. <i>Journal of Biomolecular NMR</i> , 1992 , 2, 421-430	3	31
118	Conformation and dynamics of a cyclic (1 \rightarrow 2)-beta-D-glucan. <i>International Journal of Biological Macromolecules</i> , 1995 , 17, 189-98	7.9	30
117	Lone pair interactions in dimethoxymethane and anomeric effect. <i>Canadian Journal of Chemistry</i> , 1979 , 57, 424-435	0.9	30
116	The conformational properties of the glycosidic linkage. <i>Carbohydrate Research</i> , 1981 , 90, 173-185	2.9	30
115	Conformational free energy surface of alpha-N-acetylneuraminic acid: an interplay between hydrogen bonding and solvation. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 9589-94	3.4	29

114	Dependence on saccharide conformation of the one-bond and three-bond carbon-proton coupling constants. <i>Carbohydrate Research</i> , 1990 , 206, 55-64	2.9	29
113	A theoretical study on the catalytic mechanism of the retaining α ,2-mannosyltransferase Kre2p/Mnt1p: the impact of different metal ions on catalysis. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 4201-10	3.9	27
112	An attempt to derive the potential function for evaluation of the energy associated with the exo-anomeric effect. <i>Carbohydrate Research</i> , 1984 , 125, 155-160	2.9	27
111	Atomistic insight into the catalytic mechanism of glycosyltransferases by combined quantum mechanics/molecular mechanics (QM/MM) methods. <i>Carbohydrate Research</i> , 2015 , 403, 38-47	2.9	26
110	Conformational dependence of the one-bond carbon-proton coupling constants in oligosaccharides. <i>Magnetic Resonance in Chemistry</i> , 1990 , 28, 862-866	2.1	26
109	Ab Initio Molecular Orbital Calculation on Carbohydrate Model Compounds. 1. The Anomeric Effect in Fluoro and Chloro Derivatives of Tetrahydropyran. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 6452-6458		25
108	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. <i>Carbohydrate Research</i> , 2009 , 344, 1575-81	2.9	24
107	Comparative DFT study on the glycosidic bond in reactive species of galactosyl diphosphates. <i>Chemical Papers</i> , 2009 , 63,	1.9	24
106	On the reaction pathways and determination of transition-state structures for retaining alpha-galactosyltransferases. <i>Carbohydrate Research</i> , 2003 , 338, 865-77	2.9	24
105	Potential transition-state analogs for glycosyltransferases. Design and DFT calculations of conformational behavior. <i>Carbohydrate Research</i> , 2005 , 340, 1051-7	2.9	24
104	Exploring reaction pathways for O-GlcNAc transferase catalysis. A string method study. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4371-81	3.4	23
103	Conformational statistics of pectin substances in solution by a Metropolis Monte Carlo study. <i>Carbohydrate Polymers</i> , 1997 , 32, 255-266	10.3	23
102	One-bond carbon-proton coupling constants: angular dependence in alpha-linked oligosaccharides. <i>Carbohydrate Research</i> , 1991 , 221, 83-94	2.9	23
101	Solution behavior of methyl beta-xylobioside: conformational flexibility revealed by n.m.r. measurements and theoretical calculations. <i>Carbohydrate Research</i> , 1990 , 198, 193-203	2.9	23
100	RAMM: A new procedure for theoretical conformational analysis of carbohydrates. <i>Carbohydrate Research</i> , 1990 , 204, 29-36	2.9	23
99	α -mannose derivatives as models designed for selective inhibition of Golgi α mannosidase II. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 944-52	6.8	22
98	Ab Initio Molecular Orbital Calculation of Carbohydrate Model Compounds. 3. Effect of the Electric Field on Conformations about the Glycosidic Linkage. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 6234-6241		22
97	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. <i>Glycobiology</i> , 2015 , 25, 3-7	5.8	21

96	Continuous metadynamics in essential coordinates as a tool for free energy modelling of conformational changes. <i>Journal of Molecular Modeling</i> , 2008 , 14, 995-1002	2	21
95	Theoretical studies on the conformation of saccharides. VIII. Solvent effect on the stability of β -cellobiose conformers. <i>Biopolymers</i> , 1984 , 23, 1951-1960	2.2	21
94	Saturated irregular structures in poly(vinyl chloride). <i>European Polymer Journal</i> , 1975 , 11, 411-416	5.2	21
93	Catalytic mechanism of the inverting N-acetylglucosaminyltransferase I: DFT quantum mechanical model of the reaction pathway and determination of the transition state structure. <i>Glycobiology</i> , 2003 , 13, 559-66	5.8	20
92	Determination of Long Range Proton Carbon Coupling Constants by Modified Semi-Selective Two-Dimensional Inept: An Application in Stereochemical Analysis of Saccharides. <i>Journal of Carbohydrate Chemistry</i> , 1989 , 8, 389-394	1.7	20
91	Solvent effect on the stability of isomaltose conformers. <i>Biopolymers</i> , 1990 , 30, 369-379	2.2	20
90	Computational methods for studying oligo- and polysaccharide conformations. <i>Pure and Applied Chemistry</i> , 1989 , 61, 1201-1216	2.1	20
89	Selectins-The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Molecules-A Review. <i>Molecules</i> , 2020 , 25,	4.8	19
88	Automated Training of ReaxFF Reactive Force Fields for Energetics of Enzymatic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 291-302	6.4	19
87	PCILO quantum-mechanical relaxed conformational energy map of methyl 4-thio- α -maltoside in solution. <i>Carbohydrate Research</i> , 1992 , 225, 27-41	2.9	18
86	Toward an accurate conformational modeling of iduronic acid. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 1003-9	3.4	17
85	Stepwise catalytic mechanism via short-lived intermediate inferred from combined QM/MM MERP and PES calculations on retaining glycosyltransferase ppGalNAcT2. <i>PLoS Computational Biology</i> , 2015 , 11, e1004061	5	16
84	Highly conserved cysteines of mouse core 2 β 1,6-N-acetylglucosaminyltransferase I form a network of disulfide bonds and include a thiol that affects enzyme activity. <i>Journal of Biological Chemistry</i> , 2003 , 278, 45864-81	5.4	16
83	Study of the kinetics and mechanism of the acid-base-catalyzed enolization of hydroxyacetaldehyde and methoxyacetaldehyde. <i>Carbohydrate Research</i> , 1980 , 87, 35-50	2.9	16
82	The binding properties of the H5N1 influenza virus neuraminidase as inferred from molecular modeling. <i>Journal of Molecular Modeling</i> , 2011 , 17, 1445-56	2	15
81	Enantioselective epoxidation of electrophilic olefins by using glycosyl hydroperoxides. <i>Chemistry - A European Journal</i> , 2008 , 14, 6087-97	4.8	15
80	Ab Initio Molecular Orbital Study of the Conformational Behavior of the Sugar-Phosphate Linkage. Toward an Understanding of the Catalytic Mechanism of Glycosyltransferases. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 2560-2569	3.4	15
79	Conformational study of digalacturonic acid and sodium digalacturonate in solution. <i>Carbohydrate Research</i> , 1994 , 261, 187-202	2.9	15

78	Karplus-type equation for vicinal carbon-proton coupling constants for the C ² S ² C ² H pathway in 1-thioglycosides. <i>Carbohydrate Research</i> , 1992 , 229, 225-231	2.9	15
77	Electron impact, chemical ionization and collisional activation mass spectrometry of methyl O-acetyl- β -xylopyranosides. <i>Biological Mass Spectrometry</i> , 1985 , 12, 49-58		15
76	Structural Insights into the Catalytic Mechanism and Transition State of Glycosyltransferases Using ab initio Molecular Modeling. <i>Trends in Glycoscience and Glycotechnology</i> , 2005 , 17, 177-190	0.1	15
75	A QM/MM investigation of the catalytic mechanism of metal-ion-independent core 2 β ,6-N-acetylglucosaminyltransferase. <i>Chemistry - A European Journal</i> , 2013 , 19, 8153-62	4.8	14
74	Ab initio molecular orbital calculation of carbohydrate model compounds 4. Flexibility of β -type glycosidic bonds in carbohydrates. <i>Computational and Theoretical Chemistry</i> , 1997 , 395-396, 1-13		14
73	The conformational analysis of methyl beta-xylobioside: effect of choice of potential functions. <i>Carbohydrate Research</i> , 1993 , 247, 71-81	2.9	14
72	Theoretical studies on the conformation of saccharides. V. Hydration of the acetal segment in glycosides. <i>International Journal of Quantum Chemistry</i> , 1983 , 23, 765-778	2.1	14
71	On thermal dehydrochlorination of model compounds for poly(vinyl chloride) β . <i>Tetrahedron</i> , 1974 , 30, 3275-3280	2.4	14
70	First-Principles Interaction Analysis Assessment of the Manganese Cation in the Catalytic Activity of Glycosyltransferases. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 6148-6162	3.4	13
69	N-(4-Substituted-benzoyl)-N α - β -glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. <i>Bioorganic and Medicinal Chemistry</i> , 2012 , 20, 1801-16	3.4	13
68	Step by step towards understanding gold glyconanoparticles as elements of the nanoworld. <i>Chemical Papers</i> , 2007 , 61,	1.9	13
67	DFT calculations of the anomeric and exo-anomeric effect of the hydroperoxy and peroxy groups. <i>Carbohydrate Research</i> , 2008 , 343, 1463-72	2.9	13
66	Effects of the Complexation by the Mg ²⁺ Cation on the Stereochemistry of the Sugar β Diphosphate Linkage. Ab Initio Modeling on Nucleotide β ugars. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 4609-4617	2.8	13
65	Theoretical aspects of structure and conformation of oligosaccharides. <i>Current Opinion in Structural Biology</i> , 1992 , 2, 661-665	8.1	13
64	Computer modeling of polysaccharide-polysaccharide interactions: an approach to the kappa-carrageenan-mannan case. <i>Biopolymers</i> , 1992 , 32, 551-60	2.2	13
63	Theoretical studies on the conformation of saccharides. <i>Theoretica Chimica Acta</i> , 1979 , 53, 9-19		13
62	Incorporation of lone pairs into the electrostatic term in the empirical intra- and intermolecular energy calculations. <i>Biopolymers</i> , 1979 , 18, 2537-2547	2.2	13
61	Calculation of solvent effect on conformation stability and anomeric effect in dimethoxymethane. <i>Collection of Czechoslovak Chemical Communications</i> , 1980 , 45, 1883-1895		13

60	Binding of D-glucosides and D-mannosides by rice and barley D-glycosidases with distinct substrate specificities. <i>Biochemistry</i> , 2010 , 49, 8779-93	3.2	12
59	Solvent effect on the stability of mannobiose conformers. <i>Biopolymers</i> , 1987 , 26, 1499-1508	2.2	12
58	Molecular dynamic studies of amyloid-beta interactions with curcumin and Cu ²⁺ ions. <i>Chemical Papers</i> , 2015 , 69,	1.9	11
57	Studies on the conformational behaviour of GlcNAc-Man ₃ -GlcNAc ₂ oligosaccharides using molecular dynamics simulations. <i>Glycoconjugate Journal</i> , 1998 , 15, 187-91	3	11
56	Kinetics and mechanism of the acid-catalyzed reactions of methylated trioses. <i>Carbohydrate Research</i> , 1980 , 87, 51-62	2.9	10
55	Change of the molecular surface and volume during internal rotation and its effect on conformational equilibrium in solution. <i>Journal of Molecular Structure</i> , 1980 , 68, 189-198	3.4	10
54	On thermal dehydrochlorination of model compounds for polyvinylchloride. <i>European Polymer Journal</i> , 1971 , 7, 41-54	5.2	10
53	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. <i>Nature Communications</i> , 2019 , 10, 2222	17.4	8
52	Molecular simulations of hevein/(GlcNAc) ₃ complex with weakened OH/O and CH/Hydrogen bonds: implications for their role in complex stabilization. <i>Carbohydrate Research</i> , 2015 , 408, 1-7	2.9	8
51	Different QM/MM Approaches To Elucidate Enzymatic Reactions: Case Study on ppGalNAcT2. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 6062-6076	6.4	8
50	Ab initio studies of conformational properties of dimethyl diphosphate dianion and its complex with magnesium. <i>Computational and Theoretical Chemistry</i> , 1999 , 469, 103-114		8
49	Conformational analysis of ester and ether linkages in lignin-arabinoxylan complexes. <i>Carbohydrate Research</i> , 1994 , 261, 91-102	2.9	8
48	Irregular structures in polyvinylchloride II. Unsaturated structures. <i>Angewandte Makromolekulare Chemie</i> , 1972 , 23, 173-187		8
47	Role of electrostatic interactions in determination of anomeric effect in molecular-mechanical calculations of acetal conformation. <i>Collection of Czechoslovak Chemical Communications</i> , 1978 , 43, 922-931		8
46	Effect of the electric field on molecular structure in the MNDO approximation. <i>Collection of Czechoslovak Chemical Communications</i> , 1986 , 51, 1803-1818		8
45	Oligosaccharides in Solution. <i>ACS Symposium Series</i> , 1990 , 162-176	0.4	8
44	How Mycobacterium tuberculosis Galactofuranosyl Transferase 2 (GlFT2) Generates Alternating β(1-6) and β(1-5) Linkages: A QM/MM Molecular Dynamics Study of the Chemical Steps. <i>Chemistry - A European Journal</i> , 2018 , 24, 7051-7059	4.8	7
43	Positive electrospray ion trap multistage mass spectrometric fragmentation of synthetic analogs of saccharide part of lipopolysaccharides of Vibrio cholerae O:1. <i>Journal of the American Society for Mass Spectrometry</i> , 2006 , 17, 749-756	3.5	7

42	Nuclear Overhauser effects and the flexibility of saccharides: methyl beta-xylobioside. <i>Carbohydrate Research</i> , 1991 , 210, 13-20	2.9	7
41	Multidisciplinary Approaches to the Structures of Model Compounds for Cellulose II. <i>ACS Symposium Series</i> , 1987 , 38-67	0.4	7
40	On Thermal Dehydrochlorination of Model Compounds for PVC IV. MO Study of the Catalytic Effect of Hydrogen Chloride. <i>Polymer Journal</i> , 1975 , 7, 34-43	2.7	7
39	Non-planar conformations of methylacetamide: Solvent effect and chiroptical properties. <i>Collection of Czechoslovak Chemical Communications</i> , 1982 , 47, 17-28		7
38	QM/MM Insight on Enzymatic Reactions of Glycosyltransferases. <i>Mini-Reviews in Organic Chemistry</i> , 2011 , 8, 263-269	1.7	7
37	Structure of bovine alpha-1,3-galactosyltransferase and its complexes with UDP and DPGal inferred from molecular modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , 44, 428-34	4.2	6
36	MNDO conformations of chloromethyloxirane and solvent effect. <i>Collection of Czechoslovak Chemical Communications</i> , 1982 , 47, 3199-3205		6
35	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. <i>Glycobiology</i> , 2021 , 31, 975-987	5.8	6
34	Ab initio modelling of the anomeric and exo anomeric effects in 2-methoxytetrahydropyran and 2-methoxythiane corrected for intramolecular BSSE. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 18501-13	2.6	5
33	Using DFT methodology for more reliable predictive models: Design of inhibitors of Golgi β -Mannosidase II. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 66, 47-57	2.8	5
32	DFT and Docking Study of Potential Transition State Analogue Inhibitors of Glycosyltransferases. <i>Collection of Czechoslovak Chemical Communications</i> , 2008 , 73, 591-607		5
31	The role of chemical structure on the stereochemistry of the β (1 β) diaxial glycosidic linkage. <i>Journal of Molecular Structure</i> , 1995 , 344, 157-170	3.4	5
30	Computer modelling of kappa carrageenan-mannan interactions. <i>Journal of Molecular Recognition</i> , 1994 , 7, 243-50	2.6	5
29	Theoretical study of stereochemistry of methoxy(methylthio)methane as a model of thioacetal segment in thiosaccharides. <i>Collection of Czechoslovak Chemical Communications</i> , 1984 , 49, 345-354		5
28	Electrostatic effects on conformational equilibria: Solvation enthalpies and the reaction field theory. <i>Collection of Czechoslovak Chemical Communications</i> , 1984 , 49, 2050-2069		5
27	Conformational free energy modeling of druglike molecules by metadynamics in the WHIM space. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 804-13	6.1	4
26	Regioselective enhancement of the nucleophilicity of the hydroxyl groups in methyl β -rhamnopyranoside by complexation with tin(II) chloride. <i>Carbohydrate Research</i> , 1983 , 118, 21-28	2.9	4
25	Theoretical studies on the conformation of saccharides. <i>Computational and Theoretical Chemistry</i> , 1985 , 123, 141-154		4

24	Three-dimensional homology model of GlcNAc-TV glycosyltransferase. <i>Glycobiology</i> , 2016 , 26, 757-771	5.8	3
23	Structure-Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. <i>ChemPlusChem</i> , 2014 , 79, 1558-1568	2.8	3
22	Development of transition state analogue inhibitors for N-acetylglycosyltransferases bearing D-psicor D-tagatofuranose scaffolds. <i>Chemical Papers</i> , 2015 , 69,	1.9	3
21	Synthesis of potential inhibitors of glycosyltransferases representing UDP-GlcNAc. <i>Chemical Papers</i> , 2015 , 69,	1.9	3
20	Synthesis of saccharide precursors for preparation of potential inhibitors of glycosyltransferases. <i>Chemical Papers</i> , 2009 , 63,	1.9	3
19	Electrospray ionization ion-trap multistage mass spectrometric study of sodium cationized aldobiuronic and pseudoaldobiuronic acid derivatives. <i>Journal of Mass Spectrometry</i> , 2004 , 39, 1554-61	2.2	3
18	Conformational analysis of oligosaccharides in solution. <i>International Journal of Quantum Chemistry</i> , 1989 , 35, 141-151	2.1	3
17	Theoretical studies on the conformation of saccharides. XIV. Structure and conformational properties of the glycosylamines. <i>Biopolymers</i> , 1990 , 29, 1531-9	2.2	3
16	Synthesis of methyl (methyl β -D-altropyranosid)uronate and some of its derivatives. <i>Collection of Czechoslovak Chemical Communications</i> , 1976 , 41, 3804-3811		3
15	DFT Study on 3-Substituted Tetrahydropyran-2-yl Radicals. <i>Collection of Czechoslovak Chemical Communications</i> , 2006 , 71, 1453-1469		2
14	Purdie reagent-induced C(5)-epimerization of D-galacturonic acid derivatives in the presence of methyl sulphide. <i>Collection of Czechoslovak Chemical Communications</i> , 1976 , 41, 3119-3130		2
13	Conformational dependence of solvation energy of phosphates. <i>Collection of Czechoslovak Chemical Communications</i> , 1981 , 46, 1722-1733		2
12	QM/MM methods for studying enzymatic reactions of glycosyltransferases. <i>Methods in Molecular Biology</i> , 2015 , 1273, 489-99	1.4	2
11	Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain. <i>Scientific Reports</i> , 2019 , 9, 18918	4.9	2
10	Molecular Basis for the Biosynthesis of Oligo- and Polysaccharides 2008 , 2265-2323		1
9	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. <i>European Journal of Mass Spectrometry</i> , 2007 , 13, 147-54	1.1	1
8	Molecular Orbital Investigations on Lignin Model Compounds. XXI. Solvent Effect on the Stability of β -Aryl Ether and Benzyl Aryl Ether Dimeric Units of Lignin. <i>Holzforschung</i> , 1987 , 41, 371-377	2	1
7	Mass spectrometry of the positionally isomeric, monobenzyl ethers of methyl glycopyranosides. <i>Carbohydrate Research</i> , 1983 , 119, 13-24	2.9	1

6	Acid-catalyzed hydrolysis of 2-methoxypropenal. <i>Carbohydrate Research</i> , 1983 , 115, 85-94	2.9	1
5	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. <i>ACS Omega</i> , 2020 , 5, 21374-21384	3.9	1
4	Glycosyltransferases as targets for therapeutic intervention in cancer and inflammation: molecular modeling insights. <i>Chemical Papers</i> , 2022 , 76, 1953	1.9	0
3	The catalytic reaction mechanism of tyrosylprotein sulfotransferase-1. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 23850-23860	3.6	0
2	Structure-Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. <i>ChemPlusChem</i> , 2014 , 79, 1536-1536 ^{2.8}		
1	Elucidation of the Au-S bond in a passivated gold cluster through density functional theory calculations (abstract only). <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 064214	1.8	