Igor Tvaroska

List of Publications by Year in Descending Order

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	Glycosyltransferases as targets for therapeutic intervention in cancer and inflammation: molecular modeling insights. *Chemical Papers*, **2022**, 76, 1953	1.9	0
148	The catalytic reaction mechanism of tyrosylprotein sulfotransferase-1. *Physical Chemistry Chemical Physics*, **2021**, 23, 23850-23860	3.6	0
147	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. *Glycobiology*, **2021**, 31, 975-987	5.8	6
146	Selectins-The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Molecules-A Review. *Molecules*, **2020**, 25,	4.8	19
145	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. *ACS Omega*, **2020**, 5, 21374-21384	3.9	1
144	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. *Nature Communications*, **2019**, 10, 2222	17.4	8
143	Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain. *Scientific Reports*, **2019**, 9, 18918	4.9	2
142	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. *Chemistry - A European Journal*, **2018**, 24, 7051-7059	4.8	7
141	Automated Training of ReaxFF Reactive Force Fields for Energetics of Enzymatic Reactions. *Journal of Chemical Theory and Computation*, **2018**, 14, 291-302	6.4	19
140	First-Principles Interaction Analysis Assessment of the Manganese Cation in the Catalytic Activity of Glycosyltransferases. *Journal of Physical Chemistry B*, **2017**, 121, 6148-6162	3.4	13
139	Different QM/MM Approaches To Elucidate Enzymatic Reactions: Case Study on ppGalNAcT2. *Journal of Chemical Theory and Computation*, **2016**, 12, 6062-6076	6.4	8
138	Using DFT methodology for more reliable predictive models: Design of inhibitors of Golgi α-Mannosidase II. *Journal of Molecular Graphics and Modelling*, **2016**, 66, 47-57	2.8	5
137	Three-dimensional homology model of GlcNAc-TV glycosyltransferase. *Glycobiology*, **2016**, 26, 757-771	5.8	3
136	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, 18501-13	3.6	5
135	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	5	16
134	Exploring reaction pathways for O-GlcNAc transferase catalysis. A string method study. *Journal of Physical Chemistry B*, **2015**, 119, 4371-81	3.4	23
133	Molecular simulations of hevein/(GlcNAc)3 complex with weakened OH/O and CH/π hydrogen bonds: implications for their role in complex stabilization. *Carbohydrate Research*, **2015**, 408, 1-7	2.9	8

132	Atomistic insight into the catalytic mechanism of glycosyltransferases by combined quantum mechanics/molecular mechanics (QM/MM) methods. *Carbohydrate Research*, **2015**, 403, 38-47	2.9	26
131	Development of transition state analogue inhibitors for N-acetylglycosyltransferases bearing D-psicoor D-tagatofuranose scaffolds. *Chemical Papers*, **2015**, 69,	1.9	3
130	Molecular dynamic studies of amyloid-beta interactions with curcumin and Cu2+ ions. *Chemical Papers*, **2015**, 69,	1.9	11
129	Synthesis of potential inhibitors of glycosyltransferases representing UDP-GlcNAc. *Chemical Papers*, **2015**, 69,	1.9	3
128	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	5.8	21
127	QM/MM methods for studying enzymatic reactions of glycosyltransferases. *Methods in Molecular Biology*, **2015**, 1273, 489-99	1.4	2
126	A theoretical study on the catalytic mechanism of the retaining □1,2-mannosyltransferase Kre2p/Mnt1p: the impact of different metal ions on catalysis. *Organic and Biomolecular Chemistry*, **2014**, 12, 4201-10	3.9	27
125	Structure□Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. *ChemPlusChem*, **2014**, 79, 1558-1568	2.8	3
124	Carbohydrate-protein interactions: molecular modeling insights. *Advances in Carbohydrate Chemistry and Biochemistry*, **2014**, 71, 9-136	3.7	34
123	Structure□Activity Relationships of Glycogen Phosphorylase Inhibitor FR258900 and Its Analogues: A Combined Synthetic, Enzyme Kinetics, and Computational Study. *ChemPlusChem*, **2014**, 79, 1536-1536	2.8	
122	A QM/MM investigation of the catalytic mechanism of metal-ion-independent core 2 □1,6-N-acetylglucosaminyltransferase. *Chemistry - A European Journal*, **2013**, 19, 8153-62	4.8	14
121	Toward an accurate conformational modeling of iduronic acid. *Journal of Physical Chemistry B*, **2013**, 117, 1003-9	3.4	17
120	N-(4-Substituted-benzoyl)-N□(□-d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 1801-16	3.4	13
119	PEGylated nanoparticles bind to and alter amyloid-beta peptide conformation: toward engineering of functional nanomedicines for Alzheimer□ disease. *ACS Nano*, **2012**, 6, 5897-908	16.7	141
118	Binding of □amyloid (1-42) peptide to negatively charged phospholipid membranes in the liquid-ordered state: modeling and experimental studies. *Biophysical Journal*, **2012**, 103, 453-463	2.9	53
117	Substrate-assisted catalytic mechanism of O-GlcNAc transferase discovered by quantum mechanics/molecular mechanics investigation. *Journal of the American Chemical Society*, **2012**, 134, 15563-71	10.4	33
116	Conformational free energy modeling of druglike molecules by metadynamics in the WHIM space. *Journal of Chemical Information and Modeling*, **2012**, 52, 804-13	6.1	4
115	The binding properties of the H5N1 influenza virus neuraminidase as inferred from molecular modeling. *Journal of Molecular Modeling*, **2011**, 17, 1445-56	2	15

114	□D-mannose derivatives as models designed for selective inhibition of Golgi □mannosidase II. *European Journal of Medicinal Chemistry*, **2011**, 46, 944-52	6.8	22
113	QM/MM Insight on Enzymatic Reactions of Glycosyltransferases. *Mini-Reviews in Organic Chemistry*, **2011**, 8, 263-269	1.7	7
112	Binding of □D-glucosides and □D-mannosides by rice and barley □D-glycosidases with distinct substrate specificities. *Biochemistry*, **2010**, 49, 8779-93	3.2	12
111	Modelling of beta-D-glucopyranose ring distortion in different force fields: a metadynamics study. *Carbohydrate Research*, **2010**, 345, 530-7	2.9	57
110	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. *Carbohydrate Research*, **2009**, 344, 1575-81	2.9	24
109	Synthesis of saccharide precursors for preparation of potential inhibitors of glycosyltranferases. *Chemical Papers*, **2009**, 63,	1.9	3
108	Comparative DFT study on the □glycosidic bond in reactive species of galactosyl diphosphates. *Chemical Papers*, **2009**, 63,	1.9	24
107	Conformational free energy surface of alpha-N-acetylneuraminic acid: an interplay between hydrogen bonding and solvation. *Journal of Physical Chemistry B*, **2009**, 113, 9589-94	3.4	29
106	Hybrid quantum mechanical/molecular mechanical investigation of the beta-1,4-galactosyltransferase-I mechanism. *Journal of Physical Chemistry B*, **2009**, 113, 11314-9	3.4	31
105	Molecular Basis for the Biosynthesis of Oligo- and Polysaccharides **2008**, 2265-2323		1
104	Elucidation of the Au-S bond in a passivated gold cluster through density functional theory calculations (abstract only). *Journal of Physics Condensed Matter*, **2008**, 20, 064214	1.8	
103	DFT and Docking Study of Potential Transition State Analogue Inhibitors of Glycosyltransferases. *Collection of Czechoslovak Chemical Communications*, **2008**, 73, 591-607		5
102	DFT calculations of the anomeric and exo-anomeric effect of the hydroperoxy and peroxy groups. *Carbohydrate Research*, **2008**, 343, 1463-72	2.9	13
101	Continuous metadynamics in essential coordinates as a tool for free energy modelling of conformational changes. *Journal of Molecular Modeling*, **2008**, 14, 995-1002	2	21
100	Enantioselective epoxidation of electrophilic olefins by using glycosyl hydroperoxides. *Chemistry - A European Journal*, **2008**, 14, 6087-97	4.8	15
99	Resolution of Racemic N-Benzyl □Amino Acids by Liquid-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	3.2	35
98	Step by step towards understanding gold glyconanoparticles as elements of the nanoworld. *Chemical Papers*, **2007**, 61,	1.9	13
97	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, 147-54	1.1	1

96	Catalytic mechanism of glycosyltransferases: hybrid quantum mechanical/molecular mechanical study of the inverting N-acetylglucosaminyltransferase I. *Journal of the American Chemical Society*, **2006**, 128, 16921-7	16.4	37
95	DFT Study on 3-Substituted Tetrahydropyran-2-yl Radicals. *Collection of Czechoslovak Chemical Communications*, **2006**, 71, 1453-1469		2
94	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	3.5	7
93	Potential transition-state analogs for glycosyltransferases. Design and DFT calculations of conformational behavior. *Carbohydrate Research*, **2005**, 340, 1051-7	2.9	24
92	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	0.1	15
91	Electrospray ionization ion-trap multistage mass spectrometric study of sodium cationized aldobiuronic and pseudoaldobiuronic acid derivatives. *Journal of Mass Spectrometry*, **2004**, 39, 1554-61	2.2	3
90	Synthesis and conformational analysis of novel N(OCH3)-linked disaccharide analogues. *Chemistry - A European Journal*, **2004**, 10, 1433-44	4.8	49
89	Molecular modeling insights into the catalytic mechanism of the retaining galactosyltransferase LgtC. *Carbohydrate Research*, **2004**, 339, 1007-14	2.9	33
88	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, 559-66	5.8	20
87	On the reaction pathways and determination of transition-state structures for retaining alpha-galactosyltransferases. *Carbohydrate Research*, **2003**, 338, 865-77	2.9	24
86	Highly conserved cysteines of mouse core 2 beta1,6-N-acetylglucosaminyltransferase I form a network of disulfide bonds and include a thiol that affects enzyme activity. *Journal of Biological Chemistry*, **2003**, 278, 45864-81	5.4	16
85	Quantum mechanical and NMR spectroscopy studies on the conformations of the hydroxymethyl and methoxymethyl groups in aldohexosides. *Carbohydrate Research*, **2002**, 337, 353-67	2.9	103
84	Structure of bovine alpha-1,3-galactosyltransferase and its complexes with UDP and DPGal inferred from molecular modeling. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 428-34	4.2	6
83	Effects of the Complexation by the Mg2+ Cation on the Stereochemistry of the Sugar□Diphosphate Linkage. Ab Initio Modeling on Nucleotide□Sugars. *Journal of Physical Chemistry A*, **2000**, 104, 4609-4617	2.8	13
82	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. *Journal of the American Chemical Society*, **2000**, 122, 8762-8776	16.4	59
81	Ab initio studies of conformational properties of dimethyl diphosphate dianion and its complex with magnesium. *Computational and Theoretical Chemistry*, **1999**, 469, 103-114		8
80	Ab Initio Molecular Orbital Study of the Conformational Behavior of the Sugar□Phosphate Linkage. Toward an Understanding of the Catalytic Mechanism of Glycosyltransferases. *Journal of Physical Chemistry B*, **1999**, 103, 2560-2569	3.4	15
79	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	2.9	40

78	Studies on the conformational behaviour of GlcNAc-Man3-GlcNAc2 oligosaccharides using molecular dynamics simulations. *Glycoconjugate Journal*, **1998**, 15, 187-91	3	11
77	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	3.4	42
76	Ab initio molecular orbital calculation of carbohydrate model compounds 4. Flexibility of Φ type glycosidic bonds in carbohydrates. *Computational and Theoretical Chemistry*, **1997**, 395-396, 1-13		14
75	Conformational statistics of pectin substances in solution by a Metropolis Monte Carlo study. *Carbohydrate Polymers*, **1997**, 32, 255-266	10.3	23
74	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		39
73	Molecular and Crystal Structures of Inulin from Electron Diffraction Data. *Macromolecules*, **1996**, 29, 4626-4635	5.5	56
72	The role of chemical structure on the stereochemistry of the Φ(1→4) diaxial glycosidic linkage. *Journal of Molecular Structure*, **1995**, 344, 157-170	3.4	5
71	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		22
70	Conformation and dynamics of a cyclic (1-->2)-beta-D-glucan. *International Journal of Biological Macromolecules*, **1995**, 17, 189-98	7.9	30
69	Carbon-proton coupling constants in the conformational analysis of sugar molecules. *Advances in Carbohydrate Chemistry and Biochemistry*, **1995**, 51, 15-61	3.7	115
68	Angular dependence of vicinal carbon-proton coupling constants for conformational studies of the hydroxymethyl group in carbohydrates. *Carbohydrate Research*, **1995**, 271, 151-162	2.9	43
67	Hydration of alpha-maltose and amylose: molecular modelling and thermodynamics study. *Carbohydrate Research*, **1995**, 278, 27-41	2.9	56
66	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		25
65	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		59
64	Computer modelling of kappa carrageenan-mannan interactions. *Journal of Molecular Recognition*, **1994**, 7, 243-50	2.6	5
63	Conformational analysis of ester and ether linkages in lignin-arabinoxylan complexes. *Carbohydrate Research*, **1994**, 261, 91-102	2.9	8
62	Conformational study of digalacturonic acid and sodium digalacturonate in solution. *Carbohydrate Research*, **1994**, 261, 187-202	2.9	15
61	The conformational analysis of methyl beta-xylobioside: effect of choice of potential functions. *Carbohydrate Research*, **1993**, 247, 71-81	2.9	14

60	Theoretical aspects of structure and conformation of oligosaccharides. *Current Opinion in Structural Biology*, **1992**, 2, 661-665	8.1	13
59	Karplus-type equation for vicinal carbon-proton coupling constants for the C?S?C?H pathway in 1-thioglycosides. *Carbohydrate Research*, **1992**, 229, 225-231	2.9	15
58	One-bond carbon-proton coupling constants: Angular dependence in □-linked oligosaccharides. *Journal of Biomolecular NMR*, **1992**, 2, 421-430	3	31
57	PCILO quantum-mechanical relaxed conformational energy map of methyl 4-thio-alpha-maltoside in solution. *Carbohydrate Research*, **1992**, 225, 27-41	2.9	18
56	Computer modeling of polysaccharide-polysaccharide interactions: an approach to the kappa-carrageenan-mannan case. *Biopolymers*, **1992**, 32, 551-60	2.2	13
55	Nuclear Overhauser effects and the flexibility of saccharides: methyl beta-xylobioside. *Carbohydrate Research*, **1991**, 210, 13-20	2.9	7
54	One-bond carbon-proton coupling constants: angular dependence in alpha-linked oligosaccharides. *Carbohydrate Research*, **1991**, 221, 83-94	2.9	23
53	Solution behavior of methyl beta-xylobioside: conformational flexibility revealed by n.m.r. measurements and theoretical calculations. *Carbohydrate Research*, **1990**, 198, 193-203	2.9	23
52	Theoretical studies on the conformation of saccharides. XIV. Structure and conformational properties of the glycosylamines. *Biopolymers*, **1990**, 29, 1531-9	2.2	3
51	Solvent effect on the stability of isomaltose conformers. *Biopolymers*, **1990**, 30, 369-379	2.2	20
50	Conformational dependence of the one-bond carbon□proton coupling constants in oligosaccharides. *Magnetic Resonance in Chemistry*, **1990**, 28, 862-866	2.1	26
49	Dependence on saccharide conformation of the one-bond and three-bond carbon?proton coupling constants. *Carbohydrate Research*, **1990**, 206, 55-64	2.9	29
48	RAMM □A new procedure for theoretical conformational analysis of carbohydrates. *Carbohydrate Research*, **1990**, 204, 29-36	2.9	23
47	Oligosaccharides in Solution. *ACS Symposium Series*, **1990**, 162-176	0.4	8
46	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	1.7	20
45	An attempt to derive a new Karplus-type equation of vicinal proton-carbon coupling constants for C?O?C?H segments of bonded atoms. *Carbohydrate Research*, **1989**, 189, 359-362	2.9	235
44	Conformational analysis of oligosaccharides in solution. *International Journal of Quantum Chemistry* , **1989**, 35, 141-151	2.1	3
43	Anomeric and Exo-Anomeric Effects in Carbohydrate Chemistry. *Advances in Carbohydrate Chemistry and Biochemistry*, **1989**, 47, 45-123	3.7	266

42	Computational methods for studying oligo- and polysaccharide conformations. *Pure and Applied Chemistry*, **1989**, 61, 1201-1216	2.1	20
41	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. *Holzforschung*, **1987**, 41, 371-377	2	1
40	Multidisciplinary Approaches to the Structures of Model Compounds for Cellulose II. *ACS Symposium Series*, **1987**, 38-67	0.4	7
39	Stereochemistry of nonreducing disaccharides in solution. *Carbohydrate Research*, **1987**, 160, 137-149	2.9	37
38	Solvent effect on the stability of mannobiose conformers. *Biopolymers*, **1987**, 26, 1499-1508	2.2	12
37	Conformational-energy calculations for oligosaccharides: a comparison of methods and a strategy of calculation. *Carbohydrate Research*, **1986**, 149, 389-410	2.9	121
36	Theoretical studies on the conformation of saccharides. *Theoretica Chimica Acta*, **1986**, 70, 99-114		37
35	Effect of the electric field on molecular structure in the MNDO approximation. *Collection of Czechoslovak Chemical Communications*, **1986**, 51, 1803-1818		8
34	Electron impact, chemical ionization and collisional activation mass spectrometry of methyl O-acetyl-β-D-xylopyranosides. *Biological Mass Spectrometry*, **1985**, 12, 49-58		15
33	Theoretical studies on the conformation of saccharides. *Computational and Theoretical Chemistry*, **1985**, 123, 141-154		4
32	An attempt to derive the potential function for evaluation of the energy associated with the exo-anomeric effect. *Carbohydrate Research*, **1984**, 125, 155-160	2.9	27
31	Theoretical studies on the conformation of saccharides. VIII. Solvent effect on the stability of β-cellobiose conformers. *Biopolymers*, **1984**, 23, 1951-1960	2.2	21
30	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		5
29	Electrostatic effects on conformational equilibria: Solvation enthalpies and the reaction field theory. *Collection of Czechoslovak Chemical Communications*, **1984**, 49, 2050-2069		5
28	Theoretical studies on the conformation of saccharides. V. Hydration of the acetal segment in glycosides. *International Journal of Quantum Chemistry*, **1983**, 23, 765-778	2.1	14
27	Mass spectrometry of the positionally isomeric, monobenzyl ethers of methyl glycopyranosides. *Carbohydrate Research*, **1983**, 119, 13-24	2.9	1
26	Regioselective enhancement of the nucleophilicity of the hydroxyl groups in methyl β-rhamnopyranoside by complexation with tin(II) chloride. *Carbohydrate Research*, **1983**, 118, 21-28	2.9	4
25	Crystalline conformation and structure of lichenan and barley β-glucan. *Canadian Journal of Chemistry*, **1983**, 61, 1608-1616	0.9	48

24	Acid-catalyzed hydrolysis of 2-methoxypropenal. *Carbohydrate Research*, **1983**, 115, 85-94	2.9	1
23	Theoretical studies on the conformation of saccharides. IV. Solvent effect on the stability of maltose conformers. *Biopolymers*, **1982**, 21, 1887-1897	2.2	44
22	Non-planar conformations of methylacetamide: Solvent effect and chiroptical properties. *Collection of Czechoslovak Chemical Communications*, **1982**, 47, 17-28		7
21	MNDO conformations of chloromethyloxirane and solvent effect. *Collection of Czechoslovak Chemical Communications*, **1982**, 47, 3199-3205		6
20	The conformational properties of the glycosidic linkage. *Carbohydrate Research*, **1981**, 90, 173-185	2.9	30
19	Conformational dependence of solvation energy of phosphates. *Collection of Czechoslovak Chemical Communications*, **1981**, 46, 1722-1733		2
18	Study of the kinetics and mechanism of the acid-base-catalyzed enolization of hydroxyacetaldehyde and methoxyacetaldehyde. *Carbohydrate Research*, **1980**, 87, 35-50	2.9	16
17	Kinetics and mechanism of the acid-catalyzed reactions of methylated trioses. *Carbohydrate Research*, **1980**, 87, 51-62	2.9	10
16	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	3.4	10
15	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	16.4	84
14	Calculation of solvent effect on conformation stability and anomeric effect in dimethoxymethane. *Collection of Czechoslovak Chemical Communications*, **1980**, 45, 1883-1895		13
13	Theoretical studies on the conformation of saccharides. *Theoretica Chimica Acta*, **1979**, 53, 9-19		13
12	Lone pair interactions in dimethoxymethane and anomeric effect. *Canadian Journal of Chemistry*, **1979**, 57, 424-435	0.9	30
11	Incorporation of lone pairs into the electrostatic term in the empirical intra- and intermolecular energy calculations. *Biopolymers*, **1979**, 18, 2537-2547	2.2	13
10	Conformational analysis of (1 -> 6)-D-glucan. *Carbohydrate Research*, **1978**, 61, 97-106	2.9	55
9	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		8
8	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		2
7	Synthesis of methyl (methyl L-altropyranosid)uronate and some of its derivatives. *Collection of Czechoslovak Chemical Communications*, **1976**, 41, 3804-3811		3

6	On Thermal Dehydrochlorination of Model Compounds for PVC IV. MO Study of the Catalytic Effect of Hydrogen Chloride. *Polymer Journal*, **1975**, 7, 34-43	2.7	7
5	Saturated irregular structures in poly(vinyl chloride). *European Polymer Journal*, **1975**, 11, 411-416	5.2	21
4	Molecular orbitals studies of the conformations of dimethoxymethane. *Journal of Molecular Structure*, **1975**, 24, 249-259	3.4	32
3	On thermal dehydrochlorination of model compounds for poly(vinyl chloride)□. *Tetrahedron*, **1974**, 30, 3275-3280	2.4	14
2	Irregular structures in polyvinylchloride II. Unsaturated structures. *Angewandte Makromolekulare Chemie*, **1972**, 23, 173-187		8
1	On thermal dehydrochlorination of model compounds for polyvinylchloride□ *European Polymer Journal*, **1971**, 7, 41-54	5.2	10