Gran Widmalm

List of Publications by Citations

392 papers	8,648 citations	43 h-index	68 g-index
410 ext. papers	9,764 ext. citations	4.1 avg, IF	6.03 L-index

#	Paper	IF	Citations
392	Computer-assisted structural analysis of polysaccharides with an extended version of CASPER using 1H- and 13C-n.m.r. data. *Carbohydrate Research*, **1989**, 188, 169-91	2.9	453
391	The structures of Escherichia coli O-polysaccharide antigens. *FEMS Microbiology Reviews*, **2006**, 30, 382-403	15.1	296
390	Hydroxymethyl group conformation in saccharides: structural dependencies of (2)J(HH), (3)J(HH), and (1)J(CH) spin-spin coupling constants. *Journal of Organic Chemistry*, **2002**, 67, 949-58	4.2	154
389	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. *Journal of Chemical Theory and Computation*, **2019**, 15, 775-786	6.4	152
388	Structural analysis of glycans by NMR chemical shift prediction. *Analytical Chemistry*, **2011**, 83, 1514-7	7.8	148
387	Discrimination of epimeric glycans and glycopeptides using IM-MS and its potential for carbohydrate sequencing. *Nature Chemistry*, **2014**, 6, 65-74	17.6	146
386	Molecular dynamics and NMR spectroscopy studies of E. coli lipopolysaccharide structure and dynamics. *Biophysical Journal*, **2013**, 105, 1444-55	2.9	125
385	EUROCarbDB: An open-access platform for glycoinformatics. *Glycobiology*, **2011**, 21, 493-502	5.8	108
384	Brucellosis vaccines: assessment of Brucella melitensis lipopolysaccharide rough mutants defective in core and O-polysaccharide synthesis and export. *PLoS ONE*, **2008**, 3, e2760	3.7	102
383	E. coli outer membrane and interactions with OmpLA. *Biophysical Journal*, **2014**, 106, 2493-502	2.9	97
382	Molecular Properties Related to the Anomalous Solubility of Cyclodextrin. *Journal of Physical Chemistry B*, **2004**, 108, 4236-4238	3.4	87
381	Structure of the capsular polysaccharide of Vibrio cholerae O139 synonym Bengal containing D-galactose 4,6-cyclophosphate. *FEBS Journal*, **1995**, 232, 391-6		81
380	Structural studies of the O-antigen polysaccharides of Klebsiella O5 and Escherichia coli O8. *Carbohydrate Research*, **1985**, 145, 59-66	2.9	81
379	Structural studies of the exopolysaccharide produced by Lactobacillus rhamnosus strain GG (ATCC 53103). *Biomacromolecules*, **2002**, 3, 880-4	6.9	78
378	Sequence determination of oligosaccharides and regular polysaccharides using NMR spectroscopy and a novel Web-based version of the computer program CASPER. *Carbohydrate Research*, **2006**, 341, 1003-10	2.9	77
377	Phenotypic variation in molecular mimicry between Helicobacter pylori lipopolysaccharides and human gastric epithelial cell surface glycoforms. Acid-induced phase variation in Lewis(x) and Lewis(y) expression by H. Pylori lipopolysaccharides. *Journal of Biological Chemistry*, **2002**, 277, 5785-95	5.4	70
376	Structural studies of an extracellular polysaccharide (S-130) elaborated by Alcaligenes ATCC 31555. *Carbohydrate Research*, **1985**, 139, 217-223	2.9	66

375	Structural studies of the O-polysaccharide from the lipopolysaccharide of Moraxella (Branhamella) catarrhalis serotype A (strain ATCC 25238). *Carbohydrate Research*, **1994**, 257, 269-84	2.9	63
374	Chemoenzymatic synthesis of O-mannosylpeptides in solution and on solid phase. *Journal of the American Chemical Society*, **2012**, 134, 4521-4	16.4	62
373	Vibrio cholerae O139 Bengal possesses a capsular polysaccharide which may confer increased virulence. *Microbial Pathogenesis*, **1994**, 16, 235-41	3.8	61
372	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. *Biophysical Journal*, **2016**, 111, 1750-1760	3.7	60
371	Molecular dynamics simulations of an oligosaccharide using a force field modified for carbohydrates. *Carbohydrate Research*, **2003**, 338, 393-8	2.9	60
370	Separation, purification and characterisation of extracellular polysaccharides produced by slime-forming Lactococcus lactis ssp. cremoris strains. *International Dairy Journal*, **1999**, 9, 631-638	3.5	59
369	Conformational Flexibility of Carbohydrates: A Folded Conformer at the □Dihedral Angle of a Glycosidic Linkage. *Journal of the American Chemical Society*, **1997**, 119, 8695-8698	16.4	57
368	The structure of the exopolysaccharide produced by the halophilic Archaeon Haloferax mediterranei strain R4 (ATCC 33500). *Carbohydrate Research*, **1996**, 295, 147-56	2.9	56
367	A conformational study of alpha-L-Rhap-(1----2)-alpha-L-Rhap-(1----OMe) by NMR nuclear Overhauser effect spectroscopy (NOESY) and molecular dynamics calculations. *Carbohydrate Research*, **1992**, 229, 195-211	2.9	56
366	Advancing Solutions to the Carbohydrate Sequencing Challenge. *Journal of the American Chemical Society*, **2019**, 141, 14463-14479	16.4	55
365	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. *Biophysical Journal*, **2016**, 110, 930-8	2.9	54
364	CarbBuilder: Software for building molecular models of complex oligo- and polysaccharide structures. *Journal of Computational Chemistry*, **2016**, 37, 2098-105	3.5	53
363	Synthesis, NMR spectroscopy and conformational studies of the four anomeric methyl glycosides of the trisaccharide D-Glcp-(1->3)-[D-Glcp-(1->4)]-□D-Glcp. *Journal of the Chemical Society Perkin Transactions II*, **1998**, 639-648		50
362	NMR investigation of oligosaccharide conformation using dipolar couplings in an aqueous dilute liquid crystalline medium. *Magnetic Resonance in Chemistry*, **1998**, 36, 773-776	2.1	49
361	Distinguishing Anisotropy and Flexibility of the Pentasaccharide LNF-1 in Solution by Carbon-13 NMR Relaxation and Hydrodynamic Modeling. *Journal of the American Chemical Society*, **1999**, 121, 11847-11854	16.4	49
360	Structure and genetics of Escherichia coli O antigens. *FEMS Microbiology Reviews*, **2020**, 44, 655-683	15.1	49
359	Comparison of Langevin and molecular dynamics simulations. Equilibrium and dynamics of ethylene glycol in water. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 1747		48
358	A perspective on the primary and three-dimensional structures of carbohydrates. *Carbohydrate Research*, **2013**, 378, 123-32	2.9	46

357	Molecular Dynamics Simulations of the Ionic Liquid 1-n-Butyl-3-Methylimidazolium Chloride and Its Binary Mixtures with Ethanol. *Journal of Chemical Theory and Computation*, **2014**, 10, 4465-79	6.4	45
356	Long-range proton–carbon coupling constants in conformational analysis of oligosaccharides. *Magnetic Resonance in Chemistry*, **1998**, 36, 839-847	2.1	45
355	Molecular Dynamics Simulation of the α-d-Manp-(1 -> 3)- β-d-Glcp-OMe Disaccharide in Water and Water/DMSO Solution. *Journal of the American Chemical Society*, **1999**, 121, 5403-5412	16.4	45
354	Enabling adoption of 2D-NMR for the higher order structure assessment of monoclonal antibody therapeutics. *MAbs*, **2019**, 11, 94-105	6.6	45
353	Carbohydrates Exhibit a Distinct Preferential Solvation Pattern in Binary Aqueous Solvent Mixtures. *Angewandte Chemie - International Edition*, **2000**, 39, 140-142	16.4	44
352	Structural elucidation of the viscous exopolysaccharide produced by Lactobacillus helveticus Lb161. *Carbohydrate Research*, **2000**, 326, 113-9	2.9	44
351	Population distribution of flexible molecules from maximum entropy analysis using different priors as background information: application to the Φ,Ψ conformational space of the α-(1-->2)-linked mannose disaccharide present in N- and O-linked glycoproteins. *Organic and Biomolecular Chemistry*, **2010**, 8, 3684-95	3.9	43
350	Structure of the capsular polysaccharide from the Klebsiella K8 reference strain 1015. *Carbohydrate Research*, **1995**, 273, 197-205	2.9	43
349	Conformational properties of methyl α-maltoside and methyl α- and β-cellobioside disaccharides. *Journal of Physical Chemistry B*, **2011**, 115, 597-608	3.4	42
348	Conformational distribution function of a disaccharide in a liquid crystalline phase determined using NMR spectroscopy. *Journal of the American Chemical Society*, **2002**, 124, 5946-7	16.4	42
347	Dynamical Behavior of Carbohydrates As Studied by Carbon-13 and Proton Nuclear Spin Relaxation. *The Journal of Physical Chemistry*, **1996**, 100, 17103-17110		42
346	Structural studies on the short-chain lipopolysaccharide of Vibrio cholerae O139 Bengal. *FEBS Journal*, **1997**, 247, 402-10		41
345	Investigation of Carbohydrate Conformation in Solution and in Powders by Double-Quantum NMR. *Journal of the American Chemical Society*, **2000**, 122, 1102-1115	16.4	41
344	Hadamard Long-Range Proton–Carbon Coupling Constant Measurements with Pulsed Field Gradients. *Magnetic Resonance in Chemistry*, **1996**, 34, 377-382	2.1	41
343	Casper—a computerised approach to structure determination of polysaccharides using information from n.m.r. spectroscopy and simple chemical analyses. *Carbohydrate Research*, **1987**, 168, 67-77	2.9	41
342	Glycans Confer Specificity to the Recognition of Ganglioside Receptors by Botulinum Neurotoxin A. *Journal of the American Chemical Society*, **2017**, 139, 218-230	16.4	40
341	Direct evidence for hydrogen bonding in glycans: a combined NMR and molecular dynamics study. *Journal of Physical Chemistry B*, **2013**, 117, 4860-9	3.4	40
340	A molecular dynamics study of the effect of glycosidic linkage type in the hemicellulose backbone on the molecular chain flexibility. *Plant Journal*, **2016**, 88, 56-70	6.9	39

339	Molecular dynamics simulations of membrane-sugar interactions. *Journal of Physical Chemistry B*, **2013**, 117, 6667-73	3.4	39
338	Conformational properties of □or □(1->6)-linked oligosaccharides: Hamiltonian replica exchange MD simulations and NMR experiments. *Journal of Physical Chemistry B*, **2014**, 118, 2851-71	3.4	38
337	Complete (1)H and (13)C NMR chemical shift assignments of mono- to tetrasaccharides as basis for NMR chemical shift predictions of oligosaccharides using the computer program CASPER. *Carbohydrate Research*, **2013**, 380, 156-66	2.9	38
336	Caffeine and sugars interact in aqueous solutions: a simulation and NMR study. *Journal of Physical Chemistry B*, **2012**, 116, 11701-11	3.4	38
335	Automatic structure determination of regular polysaccharides based solely on NMR spectroscopy. *Biomacromolecules*, **2011**, 12, 3851-5	6.9	38
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333	A processive lipid glycosyltransferase in the small human pathogen Mycoplasma pneumoniae: involvement in host immune response. *Molecular Microbiology*, **2007**, 65, 1444-57	4.1	37
332	Multi-field carbon-13 NMR relaxation study of cyclodextrins. *The Journal of Physical Chemistry*, **1994**, 98, 28-34		37
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330	Hadamard long-range proton-carbon coupling constant measurements with band-selective proton decoupling. *Magnetic Resonance in Chemistry*, **1995**, 33, 596-599	2.1	36
329	Structural studies of the O-antigen oligosaccharides from two strains of Moraxella catarrhalis serotype C. *Carbohydrate Research*, **1995**, 266, 237-61	2.9	36
328	Development of the ECODAB into a relational database for Escherichia coli O-antigens and other bacterial polysaccharides. *Glycobiology*, **2015**, 25, 341-7	5.8	35
327	Structural analysis of the exopolysaccharide produced by Streptococcus thermophilus ST1 solely by NMR spectroscopy. *Journal of Biomolecular NMR*, **2010**, 47, 125-34	3	35
326	Structure of an atypical O-antigen polysaccharide of Helicobacter pylori containing a novel monosaccharide 3-C-methyl-D-mannose. *Biochemistry*, **2000**, 39, 4755-60	3.2	35
325	Structural elucidation of an extracellular polysaccharide produced by Lactobacillus helveticus. *Carbohydrate Research*, **1996**, 291, 155-64	2.9	35
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323	Glycosyltransferase functions of E. coli O-antigens. *Glycobiology*, **2010**, 20, 366-8	5.8	34
322	Conformational flexibility and dynamics of two (1-->6)-linked disaccharides related to an oligosaccharide epitope expressed on malignant tumour cells. *Chemistry - A European Journal*, **2009**, 15, 8886-94	4.8	34

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320	The lipopolysaccharide of moraxella catarrhalis structural relationships and antigenic properties. *FEBS Journal*, **1999**, 265, 524-9		34
319	CASPER: a computer program used for structural analysis of carbohydrates. *Journal of Chemical Information and Modeling*, **1991**, 31, 508-16	6.1	34
318	Syntheses and NMR Studies of Pyruvic Acid 4,6-Acetals of some Methyl Hexopyranosides.. *Acta Chemica Scandinavica*, **1993**, 47, 711-715		34
317	Databases and Associated Tools for Glycomics and Glycoproteomics. *Methods in Molecular Biology*, **2017**, 1503, 235-264	1.4	33
316	Glycan structure of a high-mannose glycoprotein from Raman optical activity. *Angewandte Chemie - International Edition*, **2011**, 50, 5349-51	16.4	33
315	Structural studies on lipopolysaccharides of serologically non-typable strains of Helicobacter pylori, AF1 and 007, expressing Lewis antigenic determinants. *FEBS Journal*, **1999**, 266, 123-31		33
314	Determination of the Conformational Flexibility of Methyl β-Cellobioside in Solution by NMR Spectroscopy and Molecular Simulations. *Journal of Physical Chemistry A*, **2004**, 108, 3932-3937	2.8	32
313	Oligosaccharides display both rigidity and high flexibility in water as determined by 13C NMR relaxation and 1H,1H NOE spectroscopy: evidence of anti-phi and anti-psi torsions in the same glycosidic linkage. *Chemistry - A European Journal*, **2001**, 7, 3069-77	4.8	32
312	A conformational study of the vicinally branched trisaccharide beta-D-glcp-(1 --> 2)[beta-D-glcp-(1 --> 3)]alpha-D-Manp-OMe by nuclear Overhauser effect spectroscopy (NOESY) and transverse rotating-frame Overhauser effect spectroscopy (TROESY) experiments: comparison to Monte Carlo and Langevin dynamics simulations. *Biopolymers*, **1999**, 50, 391-9	2.2	32
311	Structure of the O-specific polysaccharide of Proteus penneri strain 25 containing N-(L-alanyl) and multiple O-acetyl groups in a tetrasaccharide repeating unit. *Carbohydrate Research*, **1997**, 298, 229-35	2.9	31
310	Lipopolysaccharide membrane building and simulation. *Methods in Molecular Biology*, **2015**, 1273, 391-406	1.4	31
309	Discovery of glycerol phosphate modification on streptococcal rhamnose polysaccharides. *Nature Chemical Biology*, **2019**, 15, 463-471	11.7	30
308	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. *Biophysical Journal*, **2016**, 111, 1987-1999	2.9	29
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306	Computer-assisted structural analysis of oligo- and polysaccharides: an extension of CASPER to multibranched structures. *Carbohydrate Research*, **1998**, 306, 11-7	2.9	29
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304	The structure of the exopolysaccharide produced by the halophilic Archaeon Haloferax mediterranei strain R4 (ATCC 33500). *Carbohydrate Research*, **1996**, 295, 147-156	2.9	29

303	Structural Studies of Lipopolysaccharide-defective Mutants from Brucella melitensis Identify a Core Oligosaccharide Critical in Virulence. *Journal of Biological Chemistry*, **2016**, 291, 7727-41	5.4	28
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301	Structure of the phenol-soluble polysaccharide from Shewanella putrefaciens strain A6. *Carbohydrate Research*, **2002**, 337, 1119-27	2.9	28
300	Application of NMR, molecular simulation, and hydrodynamics to conformational analysis of trisaccharides. *Biopolymers*, **2003**, 69, 448-60	2.2	28
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297	Multiple-field carbon-13 NMR relaxation investigation on melezitose. *Magnetic Resonance in Chemistry*, **1995**, 33, 541-548	2.1	28
296	Carbon-13 relaxation study of motional properties of lacto-N-neotetraose in solution. *Magnetic Resonance in Chemistry*, **1992**, 30, 733-739	2.1	28
295	Delineating the conformational flexibility of trisaccharides from NMR spectroscopy experiments and computer simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 18776-94	3.6	28
294	Glycan flexibility: insights into nanosecond dynamics from a microsecond molecular dynamics simulation explaining an unusual nuclear Overhauser effect. *Carbohydrate Research*, **2010**, 345, 330-3	2.9	27
293	Modified GOESY in the analysis of disaccharide conformation. *Journal of Magnetic Resonance*, **2000**, 147, 266-72	3	27
292	Conformational investigation of a cyclic enterobacterial common antigen employing NMR spectroscopy and molecular dynamics simulations. *Biochemistry*, **2001**, 40, 3623-8	3.2	27
291	Structural studies of the O-antigen polysaccharide from the enteroinvasive Escherichia coli O164 cross-reacting with Shigella dysenteriae type 3. *FEBS Journal*, **1999**, 266, 460-6		27
290	Isolation and characterization of a trisulfide variant of recombinant human growth hormone formed during expression in Escherichia coli. *International Journal of Peptide and Protein Research*, **1996**, 47, 311-21		26
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288	A method for determination of the absolute configuration of chiral glycerol residues in natural products using TEMPO oxidation and characterization of the glyceric acids formed. *Analytical Biochemistry*, **1996**, 243, 228-33	3.1	26
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278	Structural studies of the O-antigenic polysaccharide from Escherichia coli O167. *FEBS Journal*, **1997**, 246, 565-73		24
277	Dynamics of the Escherichia coli O91 O-antigen polysaccharide in solution as studied by carbon-13 NMR relaxation. *Biomacromolecules*, **2004**, 5, 1015-20	6.9	24
276	Structural analysis of the O-antigen polysaccharide from Escherichia coli O152. *Carbohydrate Research*, **2005**, 340, 167-71	2.9	24
275	Analysis of Oligosaccharide Conformation by NMR Spectroscopy Utilizing1H,1H and1H,13C Residual Dipolar Couplings in a Dilute Liquid Crystalline Phase. *Journal of Physical Chemistry A*, **2001**, 105, 5119-5122	2.8	24
274	Structural studies of the Escherichia coli O26 O-antigen polysaccharide. *Carbohydrate Research*, **1996**, 281, 155-60	2.9	24
273	A 1H and 13C NMR study of oligosaccharides from human milk. Application of the computer program CASPER. *Carbohydrate Research*, **1992**, 235, 69-81	2.9	24
272	Rules for priming and inhibition of glycosaminoglycan biosynthesis; probing the β4GalT7 active site. *Chemical Science*, **2014**, 5, 3501-3508	9.4	23
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270	Glucose orientation and dynamics in alpha-, beta-, and gamma-cyclodextrins. *Journal of Physical Chemistry B*, **2008**, 112, 15151-7	3.4	23
269	Structural and immunochemical relationship between the O-antigenic polysaccharides from the enteroaggregative Escherichia coli strain 396/C-1 and Escherichia coli O126. *Carbohydrate Research*, **2004**, 339, 1491-6	2.9	23
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266	Brucella melitensis 16M produces a mannan and other extracellular matrix components typical of a biofilm. *FEMS Immunology and Medical Microbiology*, **2010**, 59, 364-77		22
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264	Structural Analysis of the Solution Conformation of Methyl 4-O-β-D-Glucopyranosyl-β-D-Glucopyranoside by Molecular Mechanics and ab Initio Calculation, Stochastic Dynamics Simulation, and NMR Spectroscopy. *The Journal of Physical Chemistry*, **1996**, 100, 9187-9192		22
263	Conformational analysis of a tetrasaccharide based on NMR spectroscopy and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2005**, 109, 17320-6	3.4	22
262	Structural determination and biosynthetic studies of the O-antigenic polysaccharide from the enterohemorrhagic Escherichia coli O91 using 13C-enrichment and NMR spectroscopy. *Biochemistry* , **1999**, 38, 12205-11	3.2	22
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257	Structural characterization of an all-aminosugar-containing capsular polysaccharide from Colwellia psychrerythraea 34H. *Antonie Van Leeuwenhoek*, **2017**, 110, 1377-1387	2.1	20
256	Molecular conformations in the pentasaccharide LNF-1 derived from NMR spectroscopy and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2011**, 115, 7109-21	3.4	20
255	Synthesis of cyclic beta-glucan using laminarinase 16A glycosynthase mutant from the basidiomycete Phanerochaete chrysosporium. *Journal of the American Chemical Society*, **2010**, 132, 1724-30	16.4	20
254	Structural analysis of the O-antigen polysaccharide from the Shiga toxin-producing Escherichia coli O172. *FEBS Journal*, **2001**, 268, 2239-45		20
253	Structural studies utilizing 13C-enrichment of the O-antigen polysaccharide from the enterotoxigenic Escherichia coli O159 cross-reacting with Shigella dysenteriae type 4. *FEBS Journal*, **1999**, 266, 246-51		20
252	Synthesis and NMR and conformational studies of the four anomeric methyl glycosides of the trisaccharide D-Glcp-(1->2)-D-Glcp-(1->3)-β-D-Glcp. *Journal of the Chemical Society Perkin Transactions II*, **1991**, 963-973		20
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250	The epitopic and structural characterization of Brucella suis biovar 2 O-polysaccharide demonstrates the existence of a new M-negative C-negative smooth Brucella serovar. *PLoS ONE*, **2013**, 8, e53941	3.7	20

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248	Structural Studies of the O-Acetyl-Containing O-Antigen from a Shigella flexneri Serotype 6 Strain and Synthesis of Oligosaccharide Fragments Thereof. *European Journal of Organic Chemistry*, **2013**, 2013, 4085-4106	3.2	19
247	NMR analysis of conformationally dependent (n)J(C, H) and (n)J(C, C) in the trisaccharide α-L-Rhap-(1 -> 2)[α-L-Rhap-(1 -> 3)]-α-L-Rhap-OMe and a site-specifically labeled isotopologue thereof. *Magnetic Resonance in Chemistry*, **2011**, 49, 117-24	2.1	19
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245	Structure determination of the O-antigenic polysaccharide from the enteroinvasive Escherichia coli O136. *FEBS Journal*, **1999**, 263, 656-61		19
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240	Exploration of conformational flexibility and hydrogen bonding of xylosides in different solvents, as a model system for enzyme active site interactions. *Organic and Biomolecular Chemistry*, **2013**, 11, 5465-72	3.9	18
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