BIOGRAPHICAL SKETCH

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NAME
Robert J. Woods

POSITION TITLE
Professor of Biochemistry & Molecular Biology

eRA COMMONS USER NAME
RJWOODS

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
Queen's University, Kingston, Ontario, Canada	B.Sc.	1985	Engineering Chemistry
Queen's University, Kingston, Ontario, Canada	Ph.D.	1990	Computational & Synthetic Carbohydrate Chemistry
University of North Carolina, Chapel Hill	Post-doc	1990-1991	Molecular Modeling
Glycobiology Institute, University of Oxford, UK	Post-doc	1991-1994	Force Field Development
Institute for Biological Sciences, National Research Council of Canada	Term Scientist	1994-1995	Carbohydrate Conformational Analysis

A. Positions and Honors

Professional Experience:

2008-Present Professor and Chair of Computational Glycosciences, Department of Chemistry, National University of Ireland, Galway, Ireland
2007-Present Professor, Complex Carbohydrate Research Center and Department of Biochemistry and Molecular Biology, University of Georgia, Athens
2002-2007 Associate Professor, Complex Carbohydrate Research Center and Department of Biochemistry and Molecular Biology, University of Georgia, Athens
1996-Present Adjunct Professor, Department of Chemistry, University of Georgia, Athens
1995-2002 Assistant Professor, Complex Carbohydrate Research Center and Department of Biochemistry and Molecular Biology, University of Georgia, Athens

Editorial Boards/Committees/Memberships:

2003-Present *Carbohydrate Research,* Editorial Board
2008-Present *International Journal of Carbohydrate Chemistry*, Editorial Board
2007-Present President, Glycosensors and Diagnostics, LLC.
2008-Present Subgroup leader of 3-D Structural Glycobiology, Consortium for Functional Glycomics
2008-Present Faculty of Infectious Diseases, University of Georgia, Athens
2004-Present *Ad hoc* reviewer: NIH Review Panel for Biophysics Fellowships

2006-Present *Ad hoc* reviewer: NIH Macromolecular Structure and Function B study section

Ad hoc reviewer: Biochemistry, Bioinformatics, Biophys. J., Biopolymers, Can. J. Chem., Carbohydr. Res., Glycobiology, Eur. J. Org. Chem., Int. J. Quant. Chem., J. Am. Chem. Soc., J. Biol. Chem., J. Comput. Chem., J. Mol. Biol., J. Phys. Chem., Nucl. Acids Res., Proteins

B. Selected Publications

Edited Books:

NMR Spectroscopy and Computer Modeling of Carbohydrates. Recent Advances. (**R.J. Woods**, and J.F.G Vliegenthart, eds.), ACS Symposium Series 930, 2005.

Book Chapters:

Tschampel, S.M., K. Kirschner, **R.J. Woods**. 2006. Incorporation of Carbohydrates into Macromolecular Force Fields. In: *NMR Spectroscopy and Computer Modeling of Carbohydrates. Recent Advances* (J.F.G. Vliegenthart and R.J. Woods, Eds) Chapter 13, ACS Symposium Series 930. American Chemical Society, Washington, DC.

Dyekjær, J.D., **R.J. Woods**. 2006. Predicting the 3D structures of anti-carbohydrate antibodies: Combining comparative modeling and MD simulations. In: *NMR Spectroscopy and Computer Modeling of Carbohydrates. Recent Advances* (J.F.G. Vliegenthart and R.J. Woods, eds) ACS Symposium Series 930, Chapter 11, American Chemical Society, Washington, DC.

Weimar, T. and **R.J. Woods**. 2002. Combining NMR and Simulation Methods in Oligosaccharide Conformational Analysis, In *NMR of Glycoconjugates*, (J. Jiménez-Barbero, T. Peters, eds.) Chapter 6, Wiley-VCH: Weinheim.

Woods, R.J. 1998. Carbohydrate force fields. In: Encyclopedia of Computational Chemistry (P.V.R. Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner, eds.), Vol. 1, pp 220-233. Chichester: John Wiley & Sons.

Woods, R.J. 1996. The application of molecular modeling techniques to the determination of oligosaccharide solution conformations. In: *Reviews in Computational Chemistry*, (K. Lipkowitz and D.B. Boyd, eds.) Vol. 9, Chapter 3. VCH Publishers, New York.

Woods, R.J., C.J. Edge, and R.A. Dwek. 1994. The Role of Nonbonded Interactions in Determining the Solution Conformations of Oligosaccharides. In: *Modeling the Hydrogen Bond*, (D. Smith, ed), ACS Symposium Series 569, Chapter 16. American Chemical Society: Washington, D.C.

Peer-reviewed Publications:

49. Kadirvelraj, R., B.L. Foley, J.D. Dyekjær and **R.J. Woods**. 2008. Involvement of Water in Carbohydrate-Protein Binding: Concanavalin A Revisited. *J. Am. Chem. Soc.* In Press.
48. Yongye, A.B., J. González-Outeriño, J.Glushka, V. Schutlheis, and **R.J. Woods**. 2008. The Conformational Properties of Methyl a-(2,8)- di/trisialoside. Implications for anti-*Neisseria meningitidis* Vaccine Design. *Biochemistry*, In Press.
47. Charvátová, O., B.L. Foley, M. Bern, J. Sharp, R. Orlando and **R.J. Woods**. 2008. Quantifying Protein Interface Footprinting by Hydroxyl Radical Oxidation and Molecular Dynamics Simulation: Application to Galectin-1. *J. Am. Soc. Mass Spectrom*. doi:10.1016/j.jasms.2008.07.013
46. DeMarco, M.L. and **R. J. Woods**. 2008. Bridging Structural Biology and Glycobiology: A Game of Snakes and Ladders. (Invited Review) *Glycobiology*, **18,** 426.
45. Yongye, A.B., B.L. Foley and **R.J. Woods**. 2008. On achieving experimental accuracy from molecular dynamics simulations of flexible molecules: aqueous glycerol. *J. Phys. Chem. B,* **112**, 2634 -2639.
44. Seo, M., N. Castillo, R. Ganzynkowicz, C.R. Daniels, **R.J. Woods**, P.-N. Roy and T. L. Lowary. 2008. An approach for the simulation and modeling of flexible rings. Application to the a-D-arabinofuranoside ring, a key constituent of polysaccharides from Mycobacterium tuberculosis. *J. Chem. Theory Comput.,* **4**, 184-191.

43. Pedatella, S., De Nisco, M., Ernst, B., Guaragna, A., Wagner, B., **Woods, R.J.**, Palumbo, G. 2007. New Sialyl Lewis^x Mimic Containing an a-Substituted ß^3-Amino Acid Spacer. *Carb. Res*., **343**, 31-38.
42. Tessier, M.B., M.L. DeMarco, A.B. Yongye and **R. J. Woods**, 2007, Extension of the GLYCAM06 Biomolecular Force Field to Lipids, Lipid Bilayers and Glycolipids. *Molecular Simulation*, **34**, 349-364.
41. Kirschner, K.N., A.B. Yongye, S.M. Tschampel, J. Gonzalez Outeriño, C.R. Daniels, B.L. Foley and **R. J. Woods**. 2008. GLYCAM06: A Generalizable Biomolecular Force Field. Carbohydrates. *J. Comput. Chem.,* **29**, 622-655.
40. Tschampel, S. M., M. R. Kennerty and **R. J**. **Woods,** 2007. A TIP5P-Consistent Treatment of Electrostatics for Biomolecular Simulations. *J. Chem. Theory Comput.***, 3**, 1721-1733.
39. Seyfried, N. T., J. A. Atwood, III, A. Almond, A. J. Day, R. Orlando, **R. J. Woods**. 2007. Fourier transform mass spectrometry to monitor hyaluronan–protein interactions: use of hydrogen/deuterium amide exchange, *Rapid Commun. Mass Spectrom.* **21,** 121-131.
38. Elking, D., T. Darden and R.J. Woods. 2006. Gaussian induced dipole polarization model. *J. Comput. Chem.* **28,** 1261-1274.
37. Kadirvelraj, R., M.L. Beckham, M. G. Ford Gonzalez Outeriño, J. and **R.J. Woods**. 2006. Understanding the bacterial polysaccharide antigenicity of *Streptococcus agalactiae* versus *Streptococcus pneumoniae*. *Proc. Natl. Acad. Sci. USA.* **103**, 8149-8154.
36. Kawatkar, S.P., Kuntz, D.A., **Woods, R.J.**, Rose, D.R., Boons, G.J. 2006. Structural basis of the inhibition of golgi a-mannosidase II by mannostatin A and the role of the thiomethyl moiety in ligand-protein interactions. *J. Am. Chem. Soc.* **128**, 8310-8319.
35. Gonzalez-Outeiriño, J., K.N. Kirschner, S. Thobhani, and **R.J. Woods**. 2006. Reconciling solvent effects on rotamer populations in carbohydrates: a joint MD and NMR analysis. *Can. J. Chem.* **84**, 569-579.
34. Case, D.A., T. Cheatham, T. Darden, H. Gohlke, R. Luo, K.H. Merz, Jr., A. Onufriev, C. Simmerling, B. Wang, **R.J. Woods**. 2005. The AMBER biomolecular simulation programs. *J. Comput. Chem.* **26**, 1668-1688.
33. Gonzalez Outeriño, J., R. Kadirvelraj and **R. J. Woods**. 2005. Structural elucidation of type III group B Streptococcus capsular polysaccharide using molecular dynamics simulations: the role of sialic acid. *Carbohydr. Res.* **340**, 1007-1018.
32. Li, B., S. Kawatkar, S. George, H. Strachan, **R.J. Woods**, A. Siriwardena, K.W. Moremen, G.-J. Boons. 2005. Inhibition of golgi mannosidase II with mannostatin A analogues: synthesis, biological evaluation, and structure activity relationship studies. *Chembiochem* **5**: 1220-1227.
31. Bosques, C., S.M. Tschampel, **R.J. Woods** and B. Imperiali. 2004. Effects of glycosylation on peptide conformation: a synergistic experimental and computational study. *J. Am. Chem. Soc.* **126**: 8421-8425.
30. Gonzalez Outeriño, J., J. Glushka, A. Siriwardena, and **R.J. Woods**. 2004. The structure and conformational behavior of sulfonium salt glycosidase inhibitors in solution: a combined quantum mechanical-NMR approach. *J. Am. Chem. Soc.* **126**: 6866-6867.
29. Corzana, F., M. S. Motawia, C. Hervé du Penhoat, S. Perez, S. M. Tschampel, **R. J. Woods** and S. B. Engelsen. 2004. A hydration study of (1-4) and (1-6) linked a-glucans by comparative 10 ns molecular dynamics simulations and 500 MHz NMR. *J. Comput. Chem.* **25:** 573-586.
28. Tschampel, S.M. and **R.J. Woods**. 2003. Quantifying the role of water in protein-ligand interactions. *J. Phys. Chem. A.* **107:** 9175-9181.
27. Ford, M.G., T. Weimar, T. Köhli, and **R.J. Woods**. 2003. MD simulations of galectin-1 -- Oligosaccharide complexes reveal the molecular basis for ligand diversity. *Proteins: Structure, Function and Genetics* **53:** 229-240.
26. Tempel, W., S. Tschampel, and **R.J. Woods**. 2002. The xenograft antigen bound to Griffonia simplicifolia isolectin 1-B$_4$: X-ray crystal structure of the complex and molecular dynamics characterization of the binding site. *J. Biol. Chem.* **277:** 6615-6621.
25. Tempel, W., L.A. Lipscomb, J.P. Rose, and **R.J. Woods**. 2001.The xenograft antigen in complex with a GS-1-B$_4$ lectin: crystallization and preliminary X-ray analysis. *Acta Crystallog.* **D57:** 1639-1642.
24. Clarke, C., **R.J. Woods**, A. Cooper, MA. Nutley, and G.-J. Boons. 2001. The involvement of water in carbohydrate-protein binding. *J. Am. Chem. Soc.* **123:** 12238-12247.
23. Kirschner, K. and **R.J. Woods**. 2001. Solvent interactions determine carbohydrate conformation. *Proc. Natl. Acad. Sci. USA* **98**: 10541-10545.
22. Basma, M., S. Sundara, D. Calgan, T. Varnali, and **R.J. Woods**. 2001. Solvated ensemble averaging in the calculation of partial atomic charges. *J. Comput. Chem.* **22:** 1125-1137.

21. Bukowski, R., L. Morris, **R.J. Woods**, and T. Weimar. 2001. Synthesis and conformational analysis of the T-antigen disaccharide. *Eur. J. Org. Chem.* pp. 2697-2705.
20. Kirschner, K.N. and **R.J. Woods**. 2001. A quantum mechanical study of the non-bonded forces in water-methanol complexes. *J. Phys. Chem. A* **105:** 4150-4155.
19. **Woods, R.J.** and R. Chappelle. 2000. RESP-partial charges for condensed phase MD simulations. *J. Mol. Struct. (THEOCHEM).* **527:** 149-156.
18. Pathiaseril, A. and **R.J. Woods**. 2000. Relative energies of binding for antibody carbohydrate-antigen complexes computed from free energy simulations. *J. Am. Chem. Soc.* **122**: 331-338.
17. **Woods, R.J.**, A. Pathiaseril, M.R. Wormald, C.J. Edge, and R.A. Dwek. 1998. The high degree of internal flexibility observed for an oligomannose oligosaccharide does not alter the overall topology of the molecule. *Eur. J. Biochem*. **258:** 372-386.
16. **Woods, R.J.** 1998. Computational carbohydrate chemistry: What theoretical methods can tell us. *Glycoconj. J.* **15:** 209-216.
15. Brisson, J.-R., S. Uhrinova, **R.J. Woods**, M. Van der Zwan, H.C. Jarrell, L.C. Paoletti, D.L. Kasper, and H.J. Jennings. 1997. NMR and molecular dynamics studies of the conformational epitope of the type-III Group-B *Streptococcus* capsular polysaccharide and derivatives. *Biochemistry* **36:** 3278-3292.
14. **Woods, R.J.** 1995. 3-Dimensional structures of oligosaccharides. *Curr. Opin. Struct. Biol.* **5:** 591-598.
13. Rudd, P.M., **R.J. Woods**, M.R. Wormald, G. Opdenakker, A.K. Downing, I.D. Campbell, and R.A. Dwek. 1995. The effects of variable glycosylation on the functional activities of ribonuclease, plasminogen and tissue plasminogen activator. *Biochim. Biophys. Acta* **1248:** 1-10.
12. **Woods, R.J.**, R.A. Dwek, C.J. Edge, and B. Fraser-Reid. 1995. Molecular mechanical and molecular dynamical simulations of glycoproteins and oligosaccharides. 1. GLYCAM_93 parameter development. *J. Phys. Chem.* **99**: 3832-3846.
11. **Woods, R.J.**, C.J. Edge, and R.A. Dwek. 1994. Protein surface oligosaccharides and protein function. *Nature, Struct. Biol.* **1:** 499-501.
10. Edge, C.J., H.C. Joao, **R.J. Woods**, and M.R. Wormald. 1993. The conformational effects of *N*-linked glycosylation. *Biochem. Soc. Trans.* **21:** 452-455.
9. **Woods, R.J.**, C.W. Andrews, and J.P. Bowen. 1992. A molecular mechanical investigation of the properties of oxocarbenium ions. II. Application to glycoside hydrolysis. *J. Am. Chem. Soc.* **114:** 859-864.
8. **Woods, R.J.**, C.W. Andrews, and J.P. Bowen. 1992. A molecular mechanical investigation of the properties of oxocarbenium ions I. Parameter development. *J. Am. Chem. Soc.* **114:** 850-858.
7. **Woods, R.J.**, W.A. Szarek, and V.H. Smith, Jr. 1991. A comparison of the semiempirical and *ab initio* methods for the study of structural features of relevance in carbohydrate chemistry. *J. Chem. Soc., Chem. Commun.* 334-337.
6. **Woods, R.J.**, W.A. Szarek, and V.H. Smith, Jr. 1991. The proton affinities and deprotonation enthalpies of ß-D-fructopyraonse and a-L-sorbopyranose: An examination using the semiempirical molecular orbital method, AM1. *Can. J. Chem.* **69:** 1917-1928.
5. **Woods, R.J.**, W.A. Szarek, and V.H. Smith, Jr. 1990. An investigation of the relationship between sweetness and intra-molecular hydrogen-bonding networks in hexuloses using the semi-empirical molecular orbital method, AM1. *J. Am. Chem. Soc.* **112:** 4732-4741.
4. Khalil, M., **R.J. Woods**, D.F. Weaver, and V.H. Smith, Jr. 1990. An examination of *inter*molecular and *intra*molecular hydrogen bonding in biomolecules by AM1 and MNDO/M semiempirical methodologies. *J. Comput. Chem.* **12:** 584-593.
3. **Woods, R.J.**, M. Khalil, W. Pell, S.H. Moffat, and V.H. Smith, Jr. 1990. Derivation of net atomic charges from molecular electrostatic potentials. *J. Comput. Chem.* **11:** 297-310.
2. **Woods, R.J.**, K.A. Watson, S. Fortier, and W.A. Szarek. 1989. The conformation of 6-thio-ß-D-fructopyranose in the crystalline state. *Carbohydrate Res.* **193:** 1-7.
1. **Woods, R.J.**, V.H. Smith, Jr., W.A. Szarek, and A. Farazdel. 1987. *Ab initio* LCAO-MO calculations on a-D-glucopyranose, ßD-fructopyranose, and their thiopyranoid-ring analogues. Application to a theory of sweetness. *J. Chem. Soc., Chem. Commun.* 937-939.

C. Research Support

Research Projects Ongoing:

Science Foundation of Ireland 07/RP1/B1321	04/01/08-04-01/10	$1,439,000
Title:	Characterizing Molecular Interactions in Glycoscience	
Role on Project:	Principal Investigator	
Georgia Research Alliance.VAC08.E	09/30/2007-06/30/2008	$100,000
Title:	Defining the Structural Basis of Lipid A Variants as Vaccine Adjuvants	
Role on Project:	Co-PI with David S. Stephens (Emory)	
NIH/NCRR 5P41RR005351	09/30/97-01/31/10	$1,383,112
Title:	Research Resource for Integrated Glycotechnology	
Role on Project:	Senior Investigator (James H. Prestegard, PI)	
NIH U54 GM62116	09/01/08-08/31/09	$65,635
Title:	Carbohydrate Interactions in Cell Communication	
Role on Project:	Participating Investigator (James Paulson, PI)	