

CARB

DIVISION OF CARBOHYDRATE CHEMISTRY

N. Snyder, *Program Chair*

SUNDAY MORNING

Section A

Venue

Placeholder

Glycomimetics as Antibiotic-Sparing Therapeutics for Infectious Disease (Oral)

Targeting *P. Aeruginosa* Bacterial Lectins & Other Anti-Virulence Strategies

Cosponsored by MEDI

Financially supported by Glycomimetics and Carbosynth

J. W. Janetka, *Organizer*

M. Anderluh, J. L. Magnani, A. Titz, *Presiding*

8:30 Introductory Remarks-Preface honoring Nathan Sharon, 1925-2011.

8:45 . Glycomimetic antagonist (GMI-1387) of PA-IL and PA-III virulence factors of *Pseudomonas aeruginosa* promotes survival in an acute lung infection model. W.E. Fogler, T. Grandjean, B. Guery, **J.L. Magnani**

9:15 . Carbohydrate-binding proteins as targets for anti-infectives: *Pseudomonas aeruginosa* and its Lectin LecB. **A. Titz**

9:45 . Blocking bacterial toxins and lectins with multivalent carbohydrates. **R.J. Pieters**

10:15 . Glycopeptide dendrimers as *Pseudomonas aeruginosa* biofilm inhibitors. **T. Darbre**

10:45 Intermission.

11:00 . Human milk oligosaccharides exhibit antimicrobial and anti-biofilm properties against Group B *Streptococcus*. **D.L. Ackerman**, S.D. Townsend

11:30 . Understanding the Molecular Recognition of Carbohydrates by the *C. albicans* Adenylyl Cyclase, CYR1p. **J. Burch**, D. Wykoff, C.L. Grimes

12:00 Concluding remarks.

Section B

Venue
Placeholder

Carbohydrate-Based Vaccines & Adjuvants (Oral)

Cosponsored by CELL
Financially supported by Pfizer
A. Prasad, *Organizer*

8:30 Introductory Remarks.

8:35 . Entirely Carbohydrate-based Immunotherapies Targeting Cancer. **P.R. Andreana**

9:05 . Defining carbohydrate antigenicity - How are flexible molecules recognized by the immune system?. **R.J. Woods**

9:35 . Exploring the capsule biosynthesis machinery of *Neisseria meningitidis*: suitability for *in vitro* vaccine production. **F. Berti**

10:05 Intermission.

10:20 . Therapeutic and prophylactic approaches for pneumococcal infection. **F. Avci**

10:50 . Biochemical Assay Development for a *Neisseria meningitidis* Capsule Polymerase. **P.C. McCarthy**

11:20 . Multicomponent glycoconjugate vaccines: Development challenges. **A. Prasad**

11:50 Concluding Remarks.

Recent Advances towards the Bioeconomy (Oral)

Sponsored by CELL, Cosponsored by AGFD, CARB, ENFL and ENVR

SUNDAY AFTERNOON

Section A

Venue
Placeholder

Glycomimetics as Antibiotic-Sparing Therapeutics for Infectious Disease (Oral)

Targeting Uropathogenic E. Coli Bacterial Adhesins & Other Anti-Virulence Strategies

Cosponsored by MEDI

Financially supported by Fimbrion and Carbosynth

J. W. Janetka, *Organizer, Presiding*

B. Ernst, R. J. Pieters, *Presiding*

1:30 Introductory Remarks.

1:35 . Rational design and optimization of C-glycoside bacterial lectin antagonists as oral therapeutics for Urinary Tract Infection. **L. McGrane**

2:05 . Biophysical basis and glycomimetic inhibition of receptor recognition by uropathogenic *E. coli* adhesins

. **V. Kalas**, J.W. Janetka, S.J. Hultgren

2:35 . Conformational variability of the bacterial lectin FimH – Which conformation represents the therapeutic target?. **B. Ernst**

3:05 . E.coli antiadhesives as potential therapeutics for Crohn's disease. d. alvarez-dorta, t. chalopin, a. sivignon, d. deniaud, n. barnich, j. bouckaert, **s.g. gouin**

3:35 Intermission.

3:50 . Highs and lows of DC-SIGN inhibitors design. **M. Anderluh**

4:20 . Seeking antibiotic leads from glycan biosynthesis inhibitors. **L.L. Kiessling**

4:50 . Glycomimetics of maltose-1-phosphate as inhibitors of the glycoside hydrolase-like enzyme *Streptomyces coelicolor* GlgEI-V279S. S. Kapil, C. Petit, D.R. Ronning, **S.J. Suheck**

5:20 Concluding remarks.

Section B

Venue

Placeholder

Carbohydrate-Based Vaccines & Adjuvants (Oral)

Cosponsored by CELL

A. Prasad, *Organizer*

1:30 Introductory Remarks.

1:35 . Toward a bivalent synthetic carbohydrate-based vaccine candidate against shigellosis. Z. Hu, J. Cornil, c. Ligeour, F. Thouron, S. Hoos, C. Guerreiro, A. Phalipon, **L.A. Mulard**

2:05 . Small but Bright: μ SEC-MALS characterizes conjugated proteins with light scattering and UHPLC
. **E. Seymour**

2:35 . Synthesis of multi-component anti-tumor vaccine using strain promoted azide alkyne cycloaddition (SPAAC) and enhancement of immune response using human anti-rhamnose antibodies. **a. vartak**, S.J. Sucheck, K.A. Wall

3:05 . Preclinical studies on new proteins as carrier for glycoconjugate vaccines
. **M. Romano**

3:35 Concluding Remarks.

Recent Advances towards the Bioeconomy (Oral)

Sponsored by CELL, Cosponsored by AGFD, CARB, ENFL and ENVR

MONDAY MORNING

Section A

Venue
Placeholder

Derek Horton Award in Industrial Carbohydrate Chemistry (Oral)

L. Wang, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 . Derek Horton: His impact on carbohydrate science. **D.C. Baker**

9:40 . Banded paper – An important example of contemporary industrial carbohydrate chemistry.
J.H. Lauterbach, A. Rahman

10:10 Intermission.

10:30 . Recent trends in the design of carbohydrate-based conjugate vaccines. **F. Berti**

11:15 Concluding Remarks.

Sustainable Design of Polymers from Xylochemicals (Oral)

Strategic Design of Complex Polymers from the Combination of Xylochemicals

Sponsored by CELL, Cosponsored by CARB, PMSE and POLY

MONDAY AFTERNOON

Section A

Venue

Placeholder

Frontiers in Carbohydrate Synthesis (Oral)

Cosponsored by CELL

M. A. Walczak, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 . Chemical Promoters for Controlling Selectivity in Glycosylation Reactions

. **C. Bennett**

1:55 . Synthesis of the *O*-linked pentasaccharide containig β -D-Galf-(1 \rightarrow 2)- β -D-Galf in *Trypanosoma cruzi* mucins. **C. Gallo-Rodriguez**, C.R. Cori, G. Kashiwagi, R.M. Lederkremer

2:15 . 4-Aryl-3-butenylthioglycosides: versatile donors for *O*-glycosylation. **J.R. Ragains**

2:35 . Remote Activation of O/S-Benzyl Glycosides *via* Interrupted Pummerer Reaction

. **Q. Wan**

2:55 Intermission.

3:10 . Studies toward chemical synthesis of homogeneously glycosylated interferon gamma. **S. Dong**

3:30 . Chemoenzymatic synthesis of novel heparan sulfate and heparin oligosaccharides. **X. Zhang**, R.J. Linhardt, L. Lin, V.L. Schultz, J. Liu, Y. Xu, P. Hsieh

3:50 . Chemoselective strategy for the synthesis of functionalized heparan sulfate oligosaccharides utilizing a [2.2.2] iduronic lactone. **R. Jeanneret**, C. Dalton, G. Jayson, J. Gardiner

4:10 . Stereoselective 1,2-Cis Glycosylation. H.M. Nguyen

4:30 Concluding Remarks.

MONDAY EVENING

Section A

Venue

Placeholder

General Posters (Poster)

N. L. Snyder, *Organizer*

8:00 - 10:00

. Development and study of the substrate specificities of lipid II analogues against MurJ flippase via an *in vitro* liposome-based assay. **C. Guo**, w. cheng

. Important of Carbohydrate in Animal Production. **T.O. AKINMUSIRE**

. Fabrication of well-defined superparamagnetic amylose microparticles. **K. LUO**, k. jeong, J. Lee, Y. Kim

. Cytotoxicity β -glucanase NCBG Purified from *Bacillus* sp. Screened from Antarctic sea. **L. Zheng**, D. Kang, F. Zhang, R.J. Linhardt

. Effects of chondroitin sulfate and hyaluronic acid supplementation in the chondrogenic differentiation of bone marrow/synovial – derived mesenchymal stem cells on poly (ϵ -caprolactone) scaffolds towards cartilage repair. **J.C. Silva**, C. Moura, G. Borrecho, A. Alves de Matos, J. Sampaio Cabral, R.J. Linhardt, F. Ferreira

. Glycosaminoglycan change in differentiating ReN cells. **F. Ferreira Garrudo**, J. Fernandes da Silva, P. Mikael, F. Ferreira, R.J. Linhardt

. Nanocellulose templated growth of ultra-small bismuth nanoparticles for enhanced radiation therapy. **L. Jiao**, M. Su, J. Deng

. Synthesis and gelation properties of a series of 4,6-O-alkylidene protected monosaccharides. **K.E. Bashaw**, L. Samakumara, G. Wang

. Synthesis and study of sugar derived molecular gelators and their applications for enzyme immobilization. **J.Y. Morris**, G. Wang

- . Enzymatic hydrolysis and ion exchange fractionation of sulfated polysaccharides extracted from *Ulva lactuca* and evaluation of their antioxidant and antitumor activities. **M.M. El-Sayed**, D. Fleita, D. Rifaat, N. Abou El Azm
- . Development of Photodegradable Nanoarchitectures for Drug/DNA Loading and Release. **b. singh**, a. prasad
- . Preparation of cross-linked chitosan hydrogel as a drug delivery carrier of podophyllotoxin. **S. Sedaghat**
- . Developing an HPLC based fluorescent assay for *Neisseria meningitidis* serogroup W capsule polymerase. **S. Ghimire**, A. Sharyan, P. McCarthy
- . Synthesis and solution structure study of cADPR and three of its analogues. **S. Saatori**, S.M. Graham
- . Replacement of endogenous isoprenoids with fluorescent probes in bacteria. **C. George**, J.M. Troutman
- . Targeting cancer cell metabolism using carbohydrate-based small molecules. **F. Ndombera**
- . Stereospecific deuteration of C6 position on the 2-amino-2-deoxy and 2,6-diamino-2,6-dideoxy glucopyranosides derivatives for their side chain conformational analysis. **T. Kato**, D. Crich
- . Synthesis of multivalent lactose-based dendrimers and their antitumor activity by targeting galectin-3. p. wang, Y. Pan, **X. Zhang**, F. Zhang, R.J. Linhardt
- . Synthesis and inhibition studies of substrate and suicide analogs for *Mycobacterium tuberculosis* for trehalose phosphate phosphatase (TPP2). **S. Kapil**, S.J. Sucheck, D.R. Ronning, S. Thanna
- . Development of a multifunctional neoglycoside linker for applications in glycomic research. **T. Cheewawisuttichai**, A. Yu, M. Brichacek
- . Characterization of the Degree of Substitution of Sodium Carboxymethyl Cellulose by Conductimetric Titration. H. Jacobs, **Z.J. Wiczak**, T. Hodle
- . Thio-click functionalization of carbohydrate exo-cyclic enones *via* thiol enone Michael addition (TEMA). W. McLay, **Z.J. Wiczak**, R. Bielski
- . Stereoselective thio-click functionalization of conjugated heterocyclic chalcone synthons with 1-thio-sugars. E. Kweiba-Yamoah, S. Jang, **Z.J. Wiczak**
- . Synthesis of novel exo-cyclic carbohydrate enones from dihydrolevoglucosenone via direct aldol condensation with aromatic aldehydes. R. Hohol, **Z.J. Wiczak**, D.E. Mencer

- . Antioxidant activities of diatom polysaccharides. **S. Lai**, Y. Tian, S.P. Wang, M. Wang
- . Creation of artificial pectin substrates. **D.T. De Silva**, L. Kent, M. Williams
- . Characterizing oligosaccharides by SEC with on-line viscometry detection. **A.M. Striegel**, M.J. Morris
- . Apramycin produced by *Streptoalloteichus tenebrarius* NRRL B-3816. **P. Manitchotipist**, M. Bowman, D. Crich, N.P. Price
- . Antibacterial liamocins with alternative carbohydrate headgroups. **T. Leathers**, N.P. Price, C.D. Skory
- . Complex formation of sucrose and calcium additives for durable sawdust pellet. **Y. Song**, J. Seo
- . Site saturation mutagenesis of *Streptococcus pyogenes* endoglycosidase S and S2 leads to discovery of novel glycosynthases for antibody Fc glycan remodeling. **X. Tong**, L. Wang
- . C-Glycosyl compounds in the synthesis of analogs of the phytotoxin diplopyrone. **R.M. Giuliano**, R. Rosano, N. Lazzara
- . Sequence determination of decorin glycosaminoglycan chains. **Y. Yu**, H. Zhang, F. Zhang, R.J. Linhardt
- . Evidence for the mechanisms of cancer, HIV-AIDS and Parkinson's disease by binding significant proteins to a 3'-sialyl lactose-6'-phosphate, from bovine milk, carbohydrate affinity column. **M.A. Madson**, J. Christus
- . Utilization of mycobacteria carbohydrate metabolic pathways to develop chemical reporters for detecting and identifying O-mycoloylated proteins in mycobacteria. **H.W. Kavunja**, B. Piligian, T. Fiolek, H. Foley, T. Nathan, B. Swarts
- . Glycosaminoglycan composition analysis of human fetal neural cells and their binding interactions with Zika virus envelope protein. **S.Y. Kim**, G. Nierode, Y. Yu, J.S. Dordick, R.J. Linhardt
- . Synthesis of human milk oligosaccharides and determination of their localization in Group B *Streptococcus*. **K.M. Craft**, S.D. Townsend
- . Multivalent glucosamine conjugates for targeted image-guided therapy of cancer. **I. Tworowska**, N. Wagh, E. Delpassand

Venue
Placeholder

Sci-Mix

N. L. Snyder, *Organizer*

8:00 - 10:00

TUESDAY MORNING

Section A

Venue
Placeholder

Advances in Glycan Structure & Dynamics (Oral)

Host-Pathogen Interactions, Glycan-Based Vaccine Design and Glycan-Protein Interactions

Cosponsored by CELL
D. I. Freedberg, *Organizer*
R. J. Woods, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 . Attachment of histo blood group antigens to human norovirus coat protein - NMR reveals unexpected complexity of the carbohydrate binding process. **T. Peters**, A. Mallagaray

9:05 . Beyond Sweet attractions: Structural insights into host-cell glycan interactions of human pathogens. **T. Haselhorst**

9:25 . Investigating serotype cross-protection in carbohydrate vaccines: A molecular modelling approach. **M. Kuttel**, N. Ravenscroft

9:45 . Structural analysis of peptide and carbohydrate epitopes cleaved by the *Cryptococcus neoformans* catalytic monoclonal antibody 18B7. **M. Wear**, A. Bowen, R. Cordero, A. Casadevall

10:05 Intermission.

10:25 . Bound geometry of glycans using proteins with paramagnetic tags. **J.H. Prestegard**

10:55 . Protein crystallography and molecular dynamics simulations reveal an NOE-silent conformation of the GM1 glycan. **B.S. Blaum**, M. Frank, T. Stehle

11:15 . Molecular basis of Siglec-carbohydrate interaction. **M. Schubert**

11:35 . Substrate presentation and activation in neuraminidase NEU2. **O.C. Grant**, S. Makeneni, B.L. Foley, R.J. Woods

11:55 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Venue
Placeholder

Advances in Glycan Structure & Dynamics (Oral)

Glycosaminoglycan structure

Cosponsored by CELL
D. I. Freedberg, *Organizer*
R. J. Woods, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 . Insights into the interactions between synthetic GAG and Growth Factors (FGF-1 and Midkine). M. García-Jiménez, S. Gil-Caballero, J. Muñoz-García, J. de Paz, **P.M. Nieto**

2:05 . GAGs glycomics/interactome research using SPR. **F. Zhang**, S. Kim, J. Zhao, R.J. Linhardt

2:25 . High-resolution NMR and theoretical insights into the structure and NMR spin-spin coupling constants in heparin oligosaccharides. **M. Hricovini**

2:45 Intermission.

3:05 . Protein-Induced changes in glycosaminoglycan dynamics: A study in pleiotrophin-glycosaminoglycan interactions. **X. Wang**

3:25 . Analysis of the 3D structure of fucosylated chondroitin sulfate from *H. forskali* and its interaction with selectins. **C. Panagos**, C. Moss, C. Bavington, B. Mulloy, T. Feizi, W. Chai, R.J. Woods, D. Uhrin

3:45 . Is there a structural role for 3-O-sulfation in heparan sulfate?. **A. Green**, C. Larive, R. Young, L.J. Mueller

4:05 Concluding Remarks.

WEDNESDAY MORNING

Section A

Venue

Placeholder

Advances in Glycan Structure & Dynamics (Oral)

Glycoproteins

Cosponsored by CELL

R. J. Woods, *Organizer*

D. I. Freedberg, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 . Invisible glycoproteins with unusually high carbohydrate content in animal gametic cells.
K. Kitajima

9:05 . Characterizing asparagine-linked glycoprotein glycans with a rapid NMR-based approach.
A.W. Barb

9:25 . Unlocking the secrets of asialo-APF: Combining NMR spectroscopy and molecular dynamics to refine the complex structure-activity relationship of a (seemingly) simple antiproliferative glycopeptide. **K.M. Adams**, S.S. Mallajosyula, A.D. Mackerell, J.J. Barchi

9:45 . Separation of oligosaccharide and glycopeptide isomers using ion mobility-mass spectrometry. J. Hofmann, H. Hahm, H. Hinneburg, W.B. Struwe, D. Kolarich, P.H. Seeberger,
K. Pagel

10:05 Intermission.

10:25 . Modeling the conformational heterogeneity of complex carbohydrates: Enhanced sampling, methods of analyses and towards a polarizable force field. **A.D. Mackerell**, M. Yang, A. Aytenfisu

10:55 . Routine microsecond molecular dynamics simulations of carbohydrates and glycoproteins – prospects and limitations. **M. Frank**, R. Walker, P. Nyholm

11:15 . Effects of exocyclic C–O bond conformation on NMR *J*-couplings in saccharides. **A.S. Serianni**

11:35 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Venue

Placeholder

Advances in Glycan Structure & Dynamics (Oral)

Glycan Conformational Analysis and Less Common Approaches to Structure Determination

Cosponsored by CELL

R. J. Woods, *Organizer*

D. I. Freedberg, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 . Conformational Aspects of Oligosaccharides and Their Interactions with Proteins. **G. Widmalm**

2:05 . Characterization of the distinct structural motif of $\alpha(2-8)$ -polysialic acid at the reducing end. **H. Azurmendi**, M. Battistel, D.I. Freedberg

2:25 . NMR studies on cADPR and cADPR analogs: conformational analysis and thermodynamics of the N/S equilibrium. **S.M. Graham**, S. Saatori

2:45 . Structure, conformation and dynamics of marine sulfated glycans. I.N. Queiroz, P.A. Soares, **V.H. Pomin**

3:05 . NMR methodology for OH/OH hydrogen bond detection: Diols, networks, and stereochemical assignments. **D.J. O'Leary**

3:25 Intermission.

3:45 . Mannosylated surfaces exhibit self-adhesive and water-structuring properties; model for pathogen surface. **K. Perera**, P. Chandran

4:15 . Atomic-level structure characterization of carbohydrate pre and post lignin treatment by dynamic nuclear polarization - enhanced solid state NMR. **H. Luo**

4:35 . Simple methods for *de novo* structural determination of glucose-containing underivatized oligosaccharides. **C.K. Ni**

4:55 Concluding Remarks.