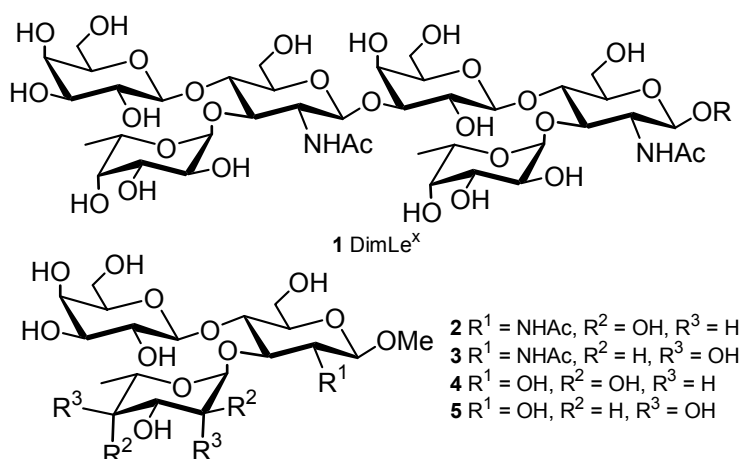


## SYNTHESIS AND CONFORMATIONAL ANALYSIS OF LEWIS X TRISACCHARIDE ANALOGUES

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A combination of synthetic carbohydrate chemistry and molecular modeling experiments are used to design anti-tumor vaccines based on the tumor associated carbohydrate antigen DimLe<sup>x</sup> (1). Biased stochastic conformational searches [1] were applied to Le<sup>x</sup> (2) and analogues 3-5. The conformations generated randomly were first minimized using the PEFSAC95 force field and those found within 10 kcal of the global minimum were re-minimized using CHARMM22 and AMBER94. Syntheses of 2-5 will be described and the results of NMR experiments acquired to support the conformations identified in the stochastic searches will be presented. The global minimum identified for Le<sup>x</sup> is in agreement with conformations described in the literature [2].



### Acknowledgements:

F.-I.A. is grateful for financial support from NSERC, CFI, OIT and PREA. A.A. acknowledges the World Bank for a fellowship under the DUE program.

**References:** [1] F.-I. Auzanneau *et al.*, *Can. J. Chem.*, **80** (2002) 1088. [2] H. Thogersen *et al.* *Can. J. Chem.*, **60** (1982), 44; K. E. Miller *et al.* *Biochemistry*, **31** (1992) 6703; A. Imberty *et al.*, *Glycoconj. J.*, **12** (1995) 331; S. Pérez *et al.* *Glycobiol.*, **6** (1996) 537; G. I. Csonka *et al.* *J. Phys. Chem.*, **104** (2000) 3381; T. Haselhorst *et al.*, *J. Am. Chem. Soc.*, **123** (2001) 10705.