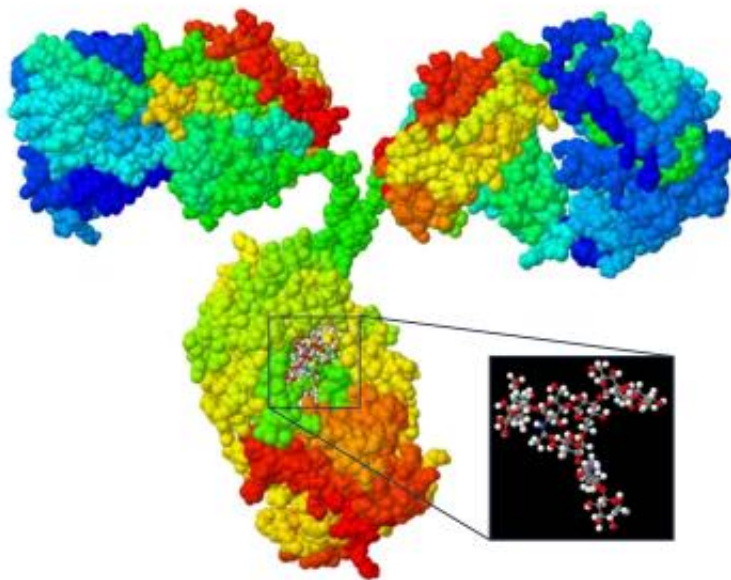


New web tool makes working with glycan sugars a lot sweeter

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This image shows immunoglobulin G (IgG) antibody molecule with glycan attached. The inset shows glycan structure. Credit: RCSB Protein Data Bank

When researchers at the National Institute of Standards and Technology (NIST) need a special tool to do their work more effectively, they often prove that necessity is truly the mother of invention. Such was the case recently for M. Lorna De Leoz and Stephen Stein, NIST chemists working in the growing specialization of glycomics. Glycomics is the study of the abundant, often-branched sugar chains called glycans that are attached to proteins and lipids and influence cellular processes,

including immunity, protein folding and, sometimes, changes associated with cancer.

Like their fellow scientists in the glycomics field, De Leoz and Stein rely heavily on mass spectral (MS) analyses that yield "[chemical fingerprints](#)" used to characterize the mass, composition and organization of individual glycan molecules. The human body produces thousands of different glycans and, unfortunately, MS analysis is slow and laborious, involving lots of number crunching by hand. Out of their frustration with this low-tech system for calculating high-tech MS data, the NIST duo came up with a tool that automates most of the process.

Their new Glyco MS Calculator automatically determines the mass of individual glycan components and breaks them down element-by-element. Designed in a spreadsheet format, the user inputs the number of residues (the individual units that make up a polymer; in this case, the monosaccharide sugars in the polysaccharide chain) in the glycan and the program calculates the masses and elemental composition within the molecule. It also provides mass and composition for glycans that are chemically modified. Finally, the calculator generates the mass of molecules formed as byproducts of mass spectrometry so that they can be considered when interpreting the MS data.

More information: www.nist.gov/customcf/glyco-mass-calc

Provided by National Institute of Standards and Technology

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