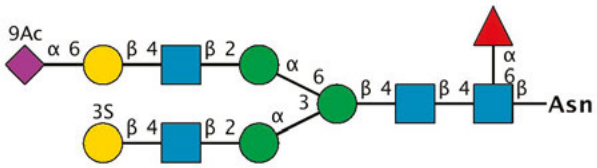


Neu5Ac(a6 -U "9Ac")Gal(b4)GlcNAc(b2)Man(a6)
[Gal(b4 -U "3S")GlcNAc(b2)Man(a3)]Man(b4)
GlcNAc(b4)[Fuc(a6)]GlcNAc(b)Asn(-CHAR)

Example of structure generated using DrawGlycan-SNFG shown with the IUPAC string used to generate it; from <http://www.virtualglycome.org/DrawGlycan/>

antibodies, other oligonucleotides and therapeutic proteins. HELM has been developed and supported by the Pistoia Alliance since 2013 through an active user community and member organizations. As of 2021, HELM is a mature digital motif with demonstrated efficacy and applicability in informatics and structure representation. The HELM notation is now jointly stewarded by IUPAC and the Pistoia Alliance.

The scope of HELM monomers presently includes only amino acids and nucleic acids. However, carbohydrates are branching biopolymers and are difficult to represent using a linear notation. Thus, rules are needed to ensure that they are represented uniquely.

The introduction of monosaccharides as monomers to HELM notation would provide a standardized representation of glycoconjugates, including glycoproteins and glycolipids in addition to glycosides. Such molecules can be used to represent substrates for glycosyltransferase enzymes, for example, as can be seen in the Gene Ontology, Reactome, and other pathway databases.

The initial set of monomers identified by the Pistoia Alliance is based on the well-established convention for the pictorial display of structures: Symbol Nomenclature For Glycans (SNFG), recommended for submission to major journal and other publications. The SNFG system was originally released in 2015, building on earlier symbolic notation in coordination with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) and other community resources [1]. The approach to represent glycans in HELM outlined by the Pistoia Alliance describes the use of SNFG for nomenclature and display.

The project will work through several objectives, including:

- Update HELM notation to include appropriate methodology to properly represent glycan moieties
- Establish a set of commonly used glycan monomers (e.g., found in public databases)
- Establish a validation data set to ensure appropriate implementation of the IUPAC HELM glycan extensions
- Represent glycan-containing structures using the newly established HELM glycan extensions
- Work with the stakeholder communities to adopt HELM glycan extensions

Addition of glycan monomers by HELM would provide critical support for machine readable large molecule representation and extend the utility of the HELM line notation. Furthermore, this effort would be able to better inform the IUPAC InChI large molecule initiative.

References

1. Symbol Nomenclature for Graphical Representation of Glycans, *Glycobiology* 25: 1323-1324, 2015. https://doi.org/10.1093/glycob/cwv091

For more information and comment, contact Task Group Chairs Kiyoko Aoki-Kinoshita or Evan Bolton <bolton@ncbi.nlm.nih.gov> | https://iupac.org/project/2024-011-1-024/

Molecular Machine Terminology

Artificial molecular machines (AMMs) are molecular-scale "devices" that, despite disagreements on how best to define them, dissipate energy and convert inputs to outputs in general, often in service of some prescribed function. The field of research on AMMs is reaching unprecedented levels of complexity with regard to the diversity of AMMs reported in the literature. As yet, there appears to be no consensus on the exact meaning of "molecular machine" and many associated words such as "molecular motor" and "molecular pump."

The objective of the project is therefore to identify, review, and summarize the terminology that is used in the literature to discuss artificial molecular machines, including terms such as artificial molecular machine, molecular switch, molecular motor, molecular pump, and numerous others (pulleys, gates, transporters, walkers, muscles, drills, *etc*). There may be a need to consolidate and rectify terminological discrepancies in the literature associated with these frequently-used words because it leads to frequent confusion and unproductive debate among researchers in the field (see, for example, https://cen.acs.org/materials/Chemists-debate-fuel-molecular-machines/101/i5 and https://doi.org/10.1038/s41565-022-01247-5).

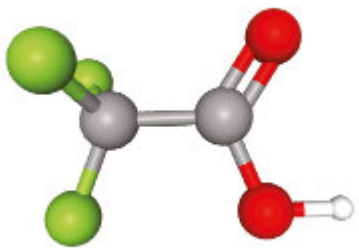
The major outcome of the project will be a Technical Report, with an overview of the terminology employed in the chemical literature on artificial molecular machines, potentially identifying the need for a unified nomenclature, and highlighting differences and similarities with the field of biological molecular machines. The Technical Report to be published in *Pure and Applied Chemistry* will provide the background for a prospective IUPAC Recommendation.

For more information and comment, contact Task Group Chair Carson J. Bruns <carson.bruns@colorado.edu> | https://iupac.org/project/2024-004-2-100/

Terminology and Classification of Per- and Poly-Fluoroalkyl Substances (PFAS)

Per- and poly-fluoroalkyl substances (PFAS) have become an issue of global concern. PFAS are a large and diverse set of compounds with a wide variety of physical, chemical, and toxicological properties. Some PFAS are persistent, bioaccumulate, and are highly toxic, others are not. Many commercially important agrochemicals, pharmaceuticals, polymers, and chlorofluorocarbon (CFC) replacements are PFAS. The European Commission is considering a proposal to ban all PFAS which has led to concerns being raised by industry. Several definitions of PFAS are in use. The European Chemical Agency (ECHA) defines PFAS as "substances containing at least one aliphatic CF2 or CF3 element." The U.S. Environmental Protection Agency defines PFAS as "per- and polyfluorinated substances that structurally contain the unit R–(CF2)–C(F)(R1)R2. Both the CF2 and CF moieties are saturated carbons and none of the R groups (R, R1, or R2) can be hydrogen."

Different definitions of PFAS lead to confusion in technical, regulatory, and public discussions. For example, it has been shown that trifluoroacetic acid (CF3C(O)OH) is a potential degradation product of many agrochemicals, pharmaceuticals, polymers, and CFC replacements. This leads to the question of do these chemicals degrade to give PFAS? Using ECHA definition the answer is "yes," while using the U.S. EPA definition the answer is "no." IUPAC has initiated a project to collect, and critically analyze existing information, providing a rigorous definition for PFAS, and standardizing terminology, classification, and nomenclature. The outcomes will benefit the global scientific, regulatory, and industrial communities, by means of a common terminology and a harmonized communication on PFAS. It will align with the IUPAC mission of providing a common language for chemistry and promoting free exchange of scientific information. These findings are expected to help national and global regulation and policy decisions, by filling information gaps and allowing targeted education campaigns.



Is trifluoroacetic acid a PFAS? (Structure from PUBCHEM)

For more information and comment, contact Task Group Chair T. J. Wallington <twalling@umich.edu> or P. Metrangolo <pierangelo.metrangolo@polimi.it> | https://iupac.org/project/2024-006-3-100/

Chemistry Entrepreneurship

The world benefits when the research output of a chemistry student is commercialized to give a useful product. This requires an entrepreneurial mindset and understanding of the requirements of starting and running a business unit. The objective of a project recently initiated by the Committee on Chemistry and Industry is to create awareness about "Chemistry Entrepreneurship" and motivate chemistry students to become entrepreneurs. The project will help create more awareness of the opportunities and challenges in entrepreneurship and build bridges between academia and industry.

To achieve this objective, a series of webinars with successful entrepreneurs sharing their learnings and experiences is being planned. The first of such webinars, **"Catalyzing Chemistry Entrepreneurship"** took place on September 10 and featured Javier García Martínez and was moderated by Miguel Jimenez. The abstract of the main presentation is reproduced on the following pages.

A second webinar titled "**From Lab to Market**" was staged on 22 November and featured Vladimir Gubala, current President of the Chemistry and Human Health Division and Chief Scientific Officer and co-founder of