Manifesto of the Chemistry GO FAIR Implementation Network

Introduction:
We will coordinate our investments in and support of the technological, organisational and social developments in the distributed management and analysis of machine-readable Chemistry data.

The Chemistry community needs to create a FAIR culture which is supported by standards and infrastructure development promoting machine readability of chemical data and other digital resources. Hence, the ChIN commits to the following guiding principles:

- Effecting a change in culture around FAIR data stewardship and data sharing practice
- Findable chemistry data
- Reusable code and data – validation, compilation/aggregation, incorporation into future work, data mining
- The use of standards at source and throughout the information lifecycle (interoperability)
- Availability and accessibility of tools and infrastructure
- The use of persistent identifiers and machine readability at the core
- Governance of standards
- Use of general data standards outside of chemistry where appropriate and FAIR in their implementation
- Enable and promote use of chemical data standards in other disciplines that work with chemical data

Purpose in the Implementation Network:
The Chemistry IN will draw from the three GO FAIR pillars of GO CHANGE and GO BUILD and GO TRAIN. The goals of this Implementation Network are:

- To enhance the open, FAIR and effective communication of chemical knowledge within the chemical sciences and between chemistry and other disciplines
- To enable chemists and chemistry to contribute to the achievement of the UN Global Sustainable Development goals.

Overarching Principle of Operation
We commit to comply with the Rules of Engagement of GO FAIR Implementation Networks. ChIN will operate in tandem with the Chemistry Research Data Interest Group (CRDIG) of the Research Data Alliance.

Deliverables (elements of the IFDS):

1. Governance structure for Chemistry FAIR standards in IUPAC organisation
2. FAIRsharing resource with chemistry-centric personas
3. Maps and Gaps analyses
4. Sets of aggregated standards
5. Development of Chemistry FAIR data tools and resources, and professional FAIR Data Stewardship training mechanisms.

The primary objectives/tasks include:

1. Complete the execution plan & roadmap as part of the process becoming a GO FAIR Implementation Network (within 3 months)

Phase 1: Creating a GO FAIR Chemistry culture

2. Establishing a ChIN working group focussing on implementation and community engagement, which works in tandem with CRDIG and the IUPAC Colour Book project (which are the main drivers of standards development)
3. Collaborative ChIN-CRDIG promotion through stakeholders
4. Create a group of recognised chemistry leaders who will champion GO FAIR in the sub-disciplines by example
5. Develop a map of existing GO FAIR Chemistry resources, bodies, approaches and ensure these are curated by the FAIRsharing organisation
6. Create a clear chemistry GO FAIR web/digital/social media presence in order to make GO FAIR Chemistry more digestible by chemists. This will be done by creating chemistry-centric personas that provide guidance and links to FAIRsharing resources to all chemists (young and established), chemistry support staff and non-specialists wishing to use or create chemistry data
7. Identifying gaps (based on coverage from above) and recommending priorities.

Phase 2: Building Chemistry standards and infrastructure

8. Governance: Establish a clear governance structure for Chemistry FAIR standards through IUPAC (specifically the Cheminformatics Colour Book project), that will serve to highlight to the wider chemistry community the on-going relevance of IUPAC in the digital world and create a definitive single point of chemical reference
9. Standards: Add impetus to, and an audience for, the IUPAC Cheminformatics Colour Book project to aggregate current standards. Collaborate on a GAP analysis, addressing gaps where possible in the short term, establishing a programme for those gaps that need more work, e.g.
    - Chemical structure representation / structure normalization (file formats and identifiers e.g. mol/InChI)
    - Representations/descriptors of molecular structure in ambiguous/unknown/complicated situations
    - Encoding of representations into standardised formats
    - Chemical semantics e.g. the IUPAC recommended terms being repurposed as an ontology, CHEMINF, RXNO, RXNO, CAO
    - Chemical representation standards
        - chemical instrumentation data standards
        - online/standalone validation tools to support the standards
        - reference implementations of standards
10. Tools: Identify tools (ala ELN) or services (eg format converters, structure to picture) to manipulate data/information and interface to repository (pre “publication”, for publication and post-publication)
11. Resources: Undertake an analysis of the data repository needs in chemistry and suggest a sustainable pathway forward
12. Workflows: Establish agreement on workflows for stakeholders that support FAIR management of chemical data across the information life-cycle.

Membership list:

We consider this Manifesto to be one way by which the undersigned stakeholders can **speak with one voice** on a number of critical issues that are of generic importance to the objectives of FAIR, and on which we feel we have reached consensus.

- The IUPAC member directory will provide the initial route to wider engagement; general outreach will cascade out from the IUPAC member network once it is formalised.
- An initial workshop was held in Amsterdam with participation of a diverse representation of backgrounds, and the effort will continue to be highlighted in data and chemistry venues globally, such as the International Data week in Botswana in Fall 2018
- Engage across broad range of stakeholders and organizations globally, including major international chemical societies, Research Data Alliance (Chemistry Data Interest Group), US Federal Drug Administration (FDA), US Environmental Protection Agency (EPA), European Chemical Industry Council (CEFIC), Society of Chemical Industry (SCI), National Institute of Science and Technology Policy (NISTEP), InChI Trust, Pistoia Alliance, Allotrope Foundation and recognised/active experts in the field of chemical informatics (eg NCBI and EBI).
- Other stakeholders will be directly invited to join - specifically publishers, learned societies, industry members and funding agencies.

Date:
4th January 2019