Day 1: Friday, March 29, 2019

Welcome & Introductions

7:30 AM – 8:00 AM
Coffee and Continental Breakfast

8:15 AM – 8:30 AM
(If available) Beth Plale, NSF OAC, Science Advisor for Public Access
Welcome

8:30 AM – 9:00 AM
Leah McEwen and Vincent Scalfani
Premise for workshop and review of goals and outcomes

Chemical Data Reuse Case Studies

9:00 AM – 9:15 AM
Damien Jeannerat
NMReData and reuse of spectral data

9:15 AM – 9:30 AM
Jonathan Bisson
The NMR raw data initiative

9:30 AM – 9:45 AM
Pall Thordarson
Opendatafit project and supramolecular.org

9:45 AM – 10:00 AM
Henry Rzepa
Mpublish and persistent identifiers

10:00 AM – 10:15 AM
Matthew Donahue
Researcher story: Data reuse challenges

10:15 AM – 10:30 AM
Paul Rupar
Researcher story: Open Science Framework

10:30 AM – 11:00 AM
Coffee Break
Day 1: Friday, March 29, 2019

Background Presentations

11:00 AM – 11:10 AM  Angie Hunter
                      Current journal spectral and chemical structure review practices

11:10 AM – 11:20 AM  Martin Hicks
                      Addressing the F in FAIR: Freeing up meta-data in journal publications

11:20 AM – 11:30 AM  Dave Martinsen
                      Progress on data model and metadata for spectral data files

11:30 AM – 11:40 AM  Pierre Tremouilhac
                      Chemotion IR

11:40 AM – 11:50 AM  Sajjan Singh Mehta
                      MoNA database

12:00 PM – 12:10 PM  Ian Bruno
                      CCDC workflow

12:10 PM – 12:20 PM  Evan Bolton
                      PubChem data repository capabilities

12:20 PM – 12:30 PM  Guy Jones
                      ChemSpider data repository capabilities

12:30 PM – 1:30 PM    Lunch

Work-group Breakouts

1:30 PM – 4:30 PM    Pierre Tremouilhac and Ian Bruno, Facilitators
                      Track A1 – Publishing Work-flow and Data Deposit Hack

                      Henry Rzepa and Dave Martinsen, Facilitators
                      Track B1 – FAIR Criteria/Metadata Profiles for Spectra and Chemical Structures

                      Jeff Lang, Stuart Chalk, and Elsa Alvardo, Facilitators
                      Track C1 – Value Propositions for Stakeholders

3:00 PM              Coffee Available

4:30 PM – 5:30 PM    Work-group Breakout Report and Discussion

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Day 2: Saturday, March 30, 2019

**Welcome and Debrief**

7:30 AM – 8:30 AM  Coffee and Continental Breakfast

8:30 AM – 9:00 AM  Leah McEwen and Vincent Scalfani  
Day 1 debrief and review goals

**Work-group Breakouts**

9:00 AM – 12:00 PM  Martin Hicks and Angie Hunter, Facilitators  
Track A2 – Plan Work-flow Implementation Pilots

Guy Jones and Ye Li, Facilitators  
Track B2 – Draft Harmonized Guidelines for Publishing Machine-readable Data

Donna Wrublewski and Richard Hartshorn, Facilitators  
Track C2 – Community Support and Engagement

10:00 AM  Coffee Available

12:00 PM – 1:00 PM  Lunch

1:00 PM – 2:00 PM  Work-group Breakout Report and Discussion

**Next Steps: Community Structures for Moving Forward**

2:00 PM – 2:15 PM  Richard Hartshorn  
IUPAC community

2:15 PM – 2:30 PM  Simon Coles  
GO FAIR Chemistry Implementation Network (ChIN)

2:30 PM – 3:00 PM  Final Discussion

3:00 PM – 3:30 PM  Goodbyes and Coffee

3:30 PM  Workshop Adjourns

3:30 PM – 5:00 PM  Organizing Team Debrief and Planning

**Workshop Nominal Cosponsors**

ACS Division of Chemical Information  
IUPAC Committee on Publications and Cheminformatics Data Standards  
GO FAIR Chemistry Implementation Network