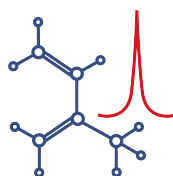


Agenda

March 29–30, Orlando, FL
Orange County Convention Center
Rooms W312B and W312C
Limited Attendance Workshop



FAIR Chemical Data
Publishing Guidelines Workshop
Chemical Structures and Spectra

#FAIRchemDATA

Workshop Chairs: Leah McEwen and Vincent Scalfani

Advisors: Angie Hunter, Ian Bruno, Guy Jones, and Dave Martinsen

NSF OAC – Award No. [1838958](#) and [1838960](#)

Updates and Supporting Material – osf.io/psq7k

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**
NMRData 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 Rugar**
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 Alvaro, Facilitators Track C1 – Value Propositions for Stakeholders |
| 3:00 PM | Coffee Available |
| 4:30 PM – 5:30 PM | Work-group Breakout Report and Discussion |

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