

International Centre for Diffraction Data
Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 14 March 2018
Fred Wireko, Chairman

1. Call to Order J. Deschamps
2. Appointment of Minutes Secretary
Megan Rost was appointed to record minutes.
3. Roll Call and Attendance
Attendance sheet on record at headquarters.
4. Approval of Minutes from March 2017
 - a. Motion moved by T. Fawcett
 - b. Second by L. Cook
 - c. 6- yes, 0- no, 0-abs
5. Review of Mission Statement – no changes R. Papoular
 - a. The mission of the Organic and Pharmaceutical Subcommittee shall be to increase the value and successful use of the organic section of the PDF by the diffraction community. To that end the subcommittee shall (1) provide technical support for all organic database products, and (2) support efforts demonstrating its capabilities.
6. Board of Directors Liaison Report
 - a. No report
7. Activities Update S. Gates-Rector
 - a. 2018 Organic Release
 - i. 13,288 processed/ 8,836 published.
 - ii. DOI link checker tool is now automated.
 - 1) 88,943 entries checked, took days instead of weeks to manually check.
 - iii. 2019 release still in production.
 - 1) 9,254 processed/~8,000 published.
 - b. Subfiles
 - i. Top Priority Subfiles New Entries 2018 Release: Bioactive-369, Forensics-1, Pharmaceutical-60, Pigment & Dye-21, Steroids-4, Micro & Mesoporous -291.
 - ii. Bioactive Subclass population for 2018 release- Narcotic-214, Depressant-883, Psychotropic-299, Pesticide & Antimicrobial-2863, Stimulant-112.
 - c. Excipients
 - i. Working to obtain data by: literature search, in house data collection, contributions.
 - ii. Top targeted excipients updated every year for member access.
 - d. 2-D Searching update
 - i. InChI based software has 53% success rate; The InChI code generation matches the formula from the data base for 53% of cases.
 - ii. Goal is to use atomic coordinates from PDF to generate InChI code for cost effectiveness.
 - 1) Issues: Formulas do not always match. Some of the formulas that did match did not have validated connectivity.
 - a. Compared InChI code from OSPIN to ICDD when formulas matched.
 - i. EXP-61.88% matched (Set 00 data)
 - ii. ORG-84.18% matched (Set 05 data)
 - e. Pharmaceuticals Project A. Gindhart

- a. Almost 100 entries of Top Pharmaceuticals complete.
- b. Start looking at top drugs by type (cardiovascular, neurological, antiviral, etc).
- c. 10 Compounds submitted for Appendix H. (ICDD Grant designation)
- d. In house scan screening for pharmaceuticals to check quality before sending it out APS for data collection on 11-BM.
- e. 9 Structures published in 2018-2019.
- f. Pharmaceuticals in PDJ publications.
 - i. 3 Published in PDJ publications.
 - ii. 5 in process for PDJ publications.

f. PPXRD Report Update

T. Maguire

- a. PPXRD-15 Aug 18-20 2017 Hyderabad, India (satellite of IUCr)
 - i. Symposium, Poster session, Workshop, Vendor exhibition.
 - 1. One day Workshop (not optional). Powder XRD applications for pharmaceutical product development.
 - 2. 5 vendors, 67 attendees/16 countries, 36 presentations.
 - 3. Reduced registrations fees.
- b. PPXRD-16 Spring 2019
 - i. No location chosen yet.

8. Future Tasks General

General

- a. Potential porphyrin classification.
- b. MOF- Vanessa Peterson is investigating MOF topography for the Micro and Meso subcommittee and will give her findings to the Micro and Meso subcommittee next year.
- c. GIA- Silvina Pagola offers to help with pharmaceutical structure solution.

9. Other Matters General

General

- a. No discussion

10. Adjournment

J. Deschamps

- a. Moved F. Wireko
- b. Second T. Fawcett