

International Centre for Diffraction Data
Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 15 March 2017
Fred Wireko, Chairman

1. Call to Order F. Wireko
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 2015
 - a. Motion moved by J. Deschamps
 - b. Second by D. Rendle
 - c. 3- yes, 0- no, 0-abs
5. Review of Mission Statement – no changes
6. Board of Directors Liaison Report R. Papoular
 - a. No report
7. Activities Update S. Gates-Rector
 - a. New Subclasses for Bioactive Subfile
 - i. Stimulants- Substances that work on the central nervous system to increase signal or decrease inhibitors.
 - ii. Depressants- Substances that lowers neurotransmission.
 - iii. Pesticides & Antimicrobial- Substance used for destroying insects or other organisms harmful to cultivated plants or animals.
 - iv. Suggestion to separate Antimicrobial and Pesticides into different subclasses. EPA states that anti-microbial falls under pesticides therefore they will remain as one subclass.
 - v. Headquarters requests lists of compounds or information for new subclasses.
 - vi. Headquarters request data for Narcotic and Psychotropic subclasses.
 - b. Excipients
 - i. Target list of Excipients is available on members' website.
 - c. 2D Structure Update
 - i. InChI based code is being evaluated in house by software engineer having a 53% success rate.
 - ii. Substructure searching is not currently possible.
 - iii. Other suggestions for implementing 2D structure searching are needed.
 - d. 2018 Organic Release
 - i. ~15,000 in editorial process for 2018 PDF-4/Organics Release.
 - ii. ~9,500 have names.
 - e. MOF Nomenclature
 - i. Headquarters reached out to IUCPAC for help about MOF naming.
 - ii. Possibility of publishing unnamed without a name.
 - iii. Suggestion to use multiplicity, composition and components for MOF naming.
 - f. Top Pharmaceutical Project A. Gindhart
 - i. 12 compounds Submitted for appendix G.
 - ii. 7 structures published in 2016-2017.
 - iii. New proposal- 42 compounds if no previous literature is published or entries in database.

- 8. PPXRD Report Update T. Maguire
 - a. PPXRD-14 held 6-9 June 2016, Fort Myers, Florida. (during hurricane)
 - i. Workshop – 16 attendees
 - ii. Symposium-34 attendees/ 10 countries
 - iii. Poster Session
 - b. PPXRD-15 Aug 18-20 2017, India (satellite of IUCr)
 - i. Workshop, Symposium, Vendor exhibition and Poster session.

- 9. Future Tasks General General
 - a. Bioactive subclasses- open to suggestions.
 - b. Possible to have joint task group with Micro and Meso Subcommittee.

- 10. Other Matters General General

No discussion.

- 11. Adjournment F. Wireko
 - a. Moved J. Deschamps
 - b. Second R. Garvey