

**International Centre for Diffraction Data
Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 16 March 2016
Fred Wireko, Chairman**

1. 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 Jeffrey Deschamps.
 - b. Second by Graciela Delgado.
5. Review of Mission Statement – No changes.
6. Board of Directors Liaison Report R. Papoular
 - a. Report on motion to evaluate the ability of 2D chemical structure data and fragment search capability
 - i. IUPAC International Chemical Identifier (InChI) programs do not give a consistent code output.
 - ii. Problem is that no programs have been acceptable for large scale processing of data.
 - iii. The Engineering and Design department are looking into it.
 - iv. Net: the previous year's motion on 2D-fragment search capability was not implemented due to technical challenges.
 - b. 2D Structure Search In-House Response S. Gates-Rector
 - i. In House evaluation for 2D enhancement
 - 1) Manually converted images to code using commercially available software.
 - a. Resulted in variations in code
 - b. Limited on max amount of atoms
 - c. Limited on type of molecules that can be named
 - 2) 2D Enhancement Plan
 - a. Improve 2D structures
 - b. Incorporate structure search feature
 - c. Use one program or create in-house software
 - 3) Suggestions S. Kabekkodu
 - a. Roy Garvey knows about InChI.
 - b. Form a task group
 - c. New Narcotic and Psychotropic subclass for Bioactive Subfile S. Gates-Rector
 - i. New Subclasses are defined as listed by International Narcotics Control Board, including polymorphic or chemically modified forms.
 - ii. 15-20% of compounds are covered in PDF-4/Organics, PDF-4+ 2016 release.

ACTION ITEM #1
Request for data to obtain missing controlled substances either by references, contributed data, or possibly by Grant-in-Aid (GiA).

 - d. Top Pharmaceutical Project A. Gindhart
88 more patterns published in 2016 PDF products.
 - e. Organic excipients entries reviewed T. Blanton

In-house review

ACTION ITEM #2

Full excipient list will be displayed on FTP site by headquarters. Request for data, references, or samples (legal and/or non-toxic) from missing items on the list to be contributed.

7. PPXRD Report Update T. Maguire
 - a. Review of PPXRD-13, held in Black Forest Germany, was successful. 41 people attended the pharmaceutical symposium. 18 people attended the workshops.
 - b. PPXRD-14 will be held 6-9 June 2016, Fort Myers, Florida.
 - i. Workshop
 - ii. Symposium
 - iii. Poster Session
 - c. ICCOSS XXII- held in Niigata, Japan July 12-17 2015 G. Delgado
Grant-in-Aid- New proposal
 - d. ICCOSS XXIII- April 3-7, 2017
8. Update—Energetic Materials Database J. Deschamps
 - a. Proposed subcategories
 - i. Explosive, Common
 - ii. Explosive, Ingredients
 - iii. Explosive, Exotic/Experimental
 - iv. Explosive, Residue
 - b. Current Status
 - i. ~924 current entries reviewed and submitted to Soorya Kabekkodu.
 - ii. New entries will be reviewed annually.
9. Future Tasks General General
 - a. Need Task Group for database transfer into InChI for Organics
 - i. Ask Winnie Wong-Ng to facilitate contact with InChI at NIST.
 - ii. Tell developers about problems with InChI Code.
 - iii. Headquarters (S. Gates-Rector) to follow-up with InChI developers about resolution of current limitation and/or transfer our tables into their format.
 - b. Discussion on using Z-matrix for naming
10. Other Matters General General

No discussion
11. Adjournment F. Wireko