

Organic and Pharmaceutical Subcommittee Meeting Minutes
Wednesday, 13 March 2019
Fred Wireko, Chairman

1. Call to Order F. Wireko
Appointment of Minutes Secretary
Megan Rost was appointed to record minutes.
2. Roll Call and Attendance
Attendance sheet on record at headquarters.
3. Approval of Minutes from March 2018
 - A. Motion moved by T. Fawcett
 - B. Second by G. Delgado
 - C. 6- yes, 0 - no, 0 -abs
4. Review of Mission Statement – no changes
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.
5. Board of Directors Liaison Report J. Kaduk
 - A. Board Members request advice about merging PDF-4+ and PDF-4/Organics.
 - i. Many of the entries are calculated from CCDC at low temp single crystal data.
 - ii. Marketing/business impacts of one single product for organics/inorganics.
6. Activities Update S. Gates-Rector
 - A. 2019 PDF-4/Organics
 - i. 9,254 processing/8319 published 2019 product
 - ii. 2,149 processing/in progress for 2020 product
 - a. No interns during the 2020 product year abstracting
 - B. Subfiles in 2019 PDF-4/Organics Release
 - i. New 05- Entries: Bioactive-201, Forensic-6, Pharmaceutical-49, Pigment & Dye-25, Steroid-10, Micro & Mesoporous-339.
 - ii. Bioactive subclass population for 2019 release– Narcotic-216, Depressant-883, Stimulant-112, Psycotropic-303, Pesticide & Antimicrobial-2,892
 - C. 2-D Searching update
 - i. InChI Java library had 53% success rate (2017)
 - ii. SMILES (Simplified Molecular Input Line Entry System) notation(2018) had ~72% success rate and is currently in PDF-4/Organics Prototype for inhouse testing
 - a. Not all bond types are supported in SMILES, working on solution.
 - b. Can draw or import SMILES code into product to do structure search
 - 1) Substructure as well as exact structure
 - D. Pharmaceuticals Project A. Gindhart
 - i. Three new pharmaceuticals in set 69
 - ii. Eleven sent to 11-BM February 2019 collection, another 2 sets of ~ 10 to be sent out in the remainder of 2019
 - iii. Working on for next year product release, using software to extract full raw powder data from patents for API. ~ 40 patterns being reviewed by David Rendle
 - iv. Publications
 - a. 9- 2018
 - b. 4- 2019 (in progress)

- E. PPXRD Report Update T. Maguire
- i. No PPXRD in 2018, last one with IUCR in 2017
 - ii. PPXRD-16 Spring 2019 May 9-12 in Switzerland
 - a. Partnering with SPS-XRPD (Spring Pharmaceutical Synchrotron X-ray Powder Diffraction Workshop)
 - b. One day workshop
 - c. Three days of Sessions
 - 1) Plenaries, vendor exhibition, posters
 - 2) More pharmaceutical companies are sending speakers
 - iii. PPXRD is helping pharmaceutical companies utilize PXRD
Pharmaceutical analysis review paper to be published by T. Fawcett, will go a long way to educate in the utility of the PDF excipient subfile
7. Future Tasks F. Wireko
Nothing to report
8. Other Matters F. Wireko
Nothing to report
9. Adjournment F. Wireko

Organic and Pharmaceutical Subcommittee

Attendance Sheet

Wednesday, 13 March 2019

Time: 4:00 - 5:00 p.m.

Conference Room A

Fred Wireko, Chairman

Jim Kaduk, BoD Liaison

Stacy Gates-Rector, Staff Liaison

Name of Member	Signature	Name of Member	Signature
Aflori, Magdalena		Kan, Wang Hay (SA)	
Antipov, Evgeny		Kern, Arnt	
Armas, Hector Novoa de		King, Danny	
Benard-Rocherulle, Patricia		Leoni, Matteo	
Bernstein, Lawrence		Lin, Shao-Fan	
Blanton, Justin++		Miller, Stephen	
Blanton, Tom		Myer, George	
Blatov, Vladislav		Pagola, Silvina	
Boldyreva, Elena		Papoular, Robert	<i>R Papoular</i>
Bosnic, Vesna++		Peterson, Vanessa	
Boughzala, Habib		Pikus, Stanislaw	
Brittain, Harry G.		Poellmann, Herbert	
Carr, Michael++		Proserpio, Davide	
Chernyshev, Vladimir		Rendle, David	
Cook, Lawrence	<i>Lawrence A. Cook</i>	Rizzi, Rosanna	
Crowder, Cyrus		Rodriguez, Mark	
Cuffini, Silvia		Rost, Megan++	<i>Megan RA</i>
de Delgado, Graciela C. D.	<i>Graciela C. D. Delgado</i>	Sagnella, Diane++	
Delgado, Jose Miguel	<i>J. Delgado</i>	Saikia, Binoy Kumar	
Deschamps, Jeffrey		Stephens, Peter	
Dey, Archan		Stephenson, Gregory	
DiNunno, Antonio		Thakral, Naveen	
Dugarte, Analio (SA)		Thakral, Seema	
Ely, Thomas	<i>Tom Ely</i>	Toro, Robert	
Fawcett, Timothy	<i>Timothy Fawcett</i>	Tremayne, Maryjane	
Ferreira, Fabio		Urban, Jennifer (SA)	
Foris, C.	<i>C. Foris</i>	Varlashkin, Peter	
Garvey, Roy		Wireko, Fred	<i>Fred Wireko</i>
Gates-Rector, Stacy++	<i>Stacy Rector</i>	Yin, Shawn	
Gindhart, Amy++	<i>Amy Gindhart</i>	Zavalij, Peter	
Johnson, Jr., Gerald G.		Zheng, Jimin	
Kabekkodu, Soorya		Zheng, Shao-Liang	
Kaduk, James	<i>James G. Kaduk</i>		

(SA) Student Affiliate, Non-voting

** Associate Member, Non-voting

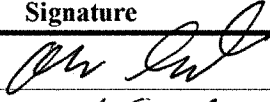
++ Staff Consultant - Non-voting

Guest List
Attendance Sheet

Name (Please print)

Signature

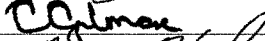
ALAN COELHO



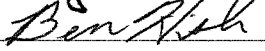
Nick Ernst Boris



CHRIS SIMONE

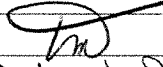


Ben Hish

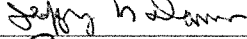


~~CHRIS SIMONE~~

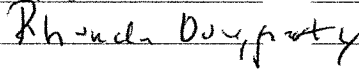
MAGUIRE J.



Jeffrey Dann



Rhonda Dufferty



Name (Please print)

Signature

Blank lined area for additional guest names and signatures.