

PDF Editorial Staff Subcommittee Meeting Minutes
Wednesday, 14 March 2018
International Centre Headquarters
Conference Room A
9:00 a.m. – 10:00 a.m.
S. Kabekkodu, Chairman

Call to Order

The meeting was called to order at 9:00 a.m.

Appointment of Minutes Secretary

Lisa Lanno

Approval of Minutes from March 2017

Minutes from the March 20, 2017 PDF Editorial Staff Subcommittee were approved.

Review of Mission Statement

The PDF Editorial Staff shall be responsible for evaluating and recommending improvements in the editorial and bibliographic procedures of the ICDD.

Board of Directors' Liaison Report

D. Rafaja nothing to report from the Board – no motions.

S. Kabekkodu: Editorial Progress in PDF Release 2019

New Entries in the Current Release

Experimental	→	1,411
ICSD	→	4,376
LPF	→	10,414
Modulated	→	69
Total	→	16,270

Database Changes in the Current Release

WHIPPET used for data validations and database update
All new calculations done by ICDD_POWD (newly re-written)
Extended the ambient range, single unit for temperature and pressure of data collection

Amy Gindhart Experimental Report

Patterns Published in Experimental Set 68

Grants - 973
Pharmaceuticals Project – 2 In-house; 7 APS
Polymer Special Project – 12
Literature “BIBS” – 175
Writes/Contributed – 242
Total - 1,411

Miscellaneous Editorial Process Update:

Coming up on 1st full year with digital parcels for editing
Re-work of “Writes” program in progress which will include sending follow-up product email to those who publish via MailChimp.
Also a 2 month “trial” sending out “write” letters through MailChimp and tracking status on responses will be implemented and evaluated.
Using specialized lists to populate even more top drugs into the database
Amy also gave an update about the ongoing Pharmaceutical Project

Stacy Gates-Rector Organic Project Report

PDF-4/Organics Release 2018:
Processed → 13,288
Published → 8,836

PDF-4/Organics Release 2019:
Processed → 9,254
Published → in progress

2D Structure Searching:

C. Karumuhinzi is currently writing code to use the JNI-InChI Java library with a 53% success rate so far.

Other suggestions to convert 2-D structures:

- Using atomic coordinates from PDF database(s) to generate InChI code & 2D from InChI software
 - Advantages: bonds shown using numbers, cost saving, good accuracy when drawing compound
 - Disadvantages: display only, distorted image(s), cannot be incorporated in PDF products
- Using original bond tables and converting to InChI
 - Advantages: interactive 2-D structures, aesthetically pleasing
 - Disadvantages: doesn't support all InChI input

Using atomic coordinates and ICDD revised software to generate InChI and 2D would be cost efficient and interactive 2-D

InChI Update:

Manual reviews of entries that resulted in an incorrect formula revealed various types of errors in original table source

- misrepresented bonds
- no representation for metal bonding (thus detached ions)
- errors in chemical formulas
- misrepresentation of solvents

DOI Link Checker Tool:

- created by C. Karumuhinzi this year for experimental database
- 89,943 checked for REL2019 in few days vs few months

General Discussion

J. Kaduk (Zeolite Task Group per S. Quick) why all of her old patterns are not being deleted? S. Kabekkodu responded we are only deleting if they are from the same reference otherwise we don't delete – J. Kaduk will give Suri the list to review, he found 4 this past weekend.

New Business

None

Adjournment