

Minutes of the IUPAC Division VII Drug Discovery & Development Telecon March 27, 2019

Participants

Vincenzo Abbate, Balu (secretary), Helmut Buschmann, Paul Erhardt, Janos Fischer, Robin Ganellin, Michael Liebman, Tom Perun, John Proudfoot, Gerd Schnorrenberg (chair)

Agenda

- Short Project Updates, ongoing Projects (Balu, Janos Fischer, Paul Erhardt)
- Project Proposal (Michael Liebman)
- Proposal on a Newsletter of the SC D3 (Michael Liebman)
- Preparation of the D3 SC Meeting in Paris, planning of joint meetings with other Subcommittees of Division

Updates on ongoing projects

The updates provided by the project leaders are attached.

- 1) Ganesan's Project on ***Glossaries and Terms of Combinatorial Chemistry*** is in the final review phase and will be concluded end of 2019, feedback given by A. Ganesan by email. Gerd Schnorrenberg was asked to contact A. Ganesan and ask him to send the draft document to Gerd for information. **Action: Gerd Schnorrenberg**
- 2) Balu reported on the project ***Medicinal Chemistry in Drug Discovery and Development India 2019*** (MCADDI2019-see attached project update). The residential training course was held in the first week of March 2019 in Bangalore with a total of 106 participants, 98 from industry and 8 from academia. Focus was given on all aspects of medicinal chemistry contributions from early hit finding up to clinical candidate upscaling and beyond. Funding was complemented by other organizations like, ACS, ANS MEDI division and local Pharma/CRO industries. Discussions during the telecon centered mainly on the question of how the substantial effort to prepare and organize this course could bring benefit to a larger territorial area. Balu reported on the limited interest in the course from East Asia countries. The question was raised whether online training courses would help to enlarge the outreach. This however was an issue for industry presenters. This topic will be discussed in more detail at the upcoming Paris SC D3 Meeting.
- 3) The current status of Wayne Childers' training course was asked for. **Action: Balu and Gerd to contact Wayne.**
- 4) Janos Fischer reported on the status of the ***Book Series "Successful Drug Discovery", Volume 4*** (see attached project update) being in the final review and editing phase. Vol 4 will have

three parts, Part I General Aspects (peptide therapeutics, physicochemical parameters), Part II Drug Class Studies (antibody conjugates, dopamine agonists) and Part III Case Studies with 5 chapters. Publication is planned for the second half of 2019. Janos was congratulated for the quick progress made. Janos also reported on his experience with the attempt to hand over more responsibility to section editors. He mentioned that due to the heterogeneity of the section topics, the need to have individual experts for the sections is leading to issues with respect to continuity. As we need to make sure that the Book Series on Successful Drug Discovery continues successfully, this topic will have high priority at the Paris SC D3 Meeting.

- 5) Paul Erhard's project on ***Drug Metabolism Terms*** will need some final editing before finalizing and PAC publication in 2019. Paul reiterated that the review process is too slow and the harmonization of different feedback on one aspect is tedious. Paul's project on ***Human Drug Metabolism Database*** has received very positive feedback. Medicinal chemists see the database as an important source to predict metabolic pathways of designed compounds. As there is potential to secure US grants (big data initiative), the initiation and progression of the project IUPAC funding will no longer be necessary. Paul stated, however, that the link to IUPAC as initial sponsor of the concept will be kept. The SC members acknowledged this attitude and wished Paul every success with the project. **Action: Paul to prepare more detailed information at Paris Meeting**

- 6) Vincenzo Abbate gave a short update (see attached project update, detailed update to be given at the Paris SC D3 Meeting) on the Project on ***Psychoactive Substances Part II*** being ready for submission end of 2019. **Action: Vincent to prepare update at Paris Meeting**

Update on new Project Proposals

- 1) Michael Liebman gave a short summary of his project proposal on a ***Systematic Analysis of Clinical Trial Failures*** (see attached Project Proposal). The participants of the telecon unanimously supported the proposal. Michael explained the concept of sponsoring an initial "proof of concept" study on multiple sclerosis trials. A respective database and a search algorithm should be established leading to publications. Longer term external funding should then be searched for in a second step. Gerd reported on the unsuccessful attempts to initiate a joint project with the Toxicology sub-committee. John Duffus explained to Gerd that the current change in the SC compromising active contributions for the time being. The telecon participants reiterated that the project would be a perfect opportunity for a joint project with the Division VII SC Toxicology. **Action: Tom Perun suggested that Gerd should contact Michael Schwenk and ask for support.**

- 2) Michael Liebman presented a second proposal on a ***D3 SC Newsletter*** (see attached proposal) with the aim to increase scientific community awareness on D3 SC, to promote communication among D3 members and scientists outside D3 and to attract new members to D3 SC. The idea is to distribute online, also beyond D3 members, the newsletter should include D3 news and an "expert analysis" section. The idea was positively discussed in the telecon, it was mentioned that both the updating was seen as a possibility to attract interest to D3 as well as the online analysis of hot topics in D3 would potentially attract younger

medicinal chemists to D3 and thereby help to find new members. The participants of the telecon unanimously supported the proposal. The team emphasized the need for an editorial group to make sure that the articles are relevant to D3 SC. They saw the newsletter as being complementary to any other publication including IUPAC publications. The participants suggested to run it as project with yearly funding and yearly review. The discussion centered around the channels of distribution to maximize the reader audience (links in other newsletters from IUPAC, ACS, accounts in Linked In, YouTube, Twitter etc.). Michael was asked to serve as project leader, support will be given by other D3 SC members (Balu and Gerd to continue support). **Action: Michael, Balu and Gerd to refine proposal, to present outline for first Newsletter at Paris Meeting and to prepare a distribution concept.**

Next D3 SC Meeting Paris July 8, 2019

Balu and Gerd would like to thank all participants of the telecon for active contributions and very good discussion points.

Signed

Gerd and Balu