

Minutes of the Subcommittee Drug Discovery and Development Telecon

Held on Octoberber 28, 2020

List of participants: Balu, Helmut Buschmann, Mukund Chorgade, Michael Liebman, John Proudfoot, Hassan Ibraim, Roland Pieters, Vincenzo Abbate, Rita Cornelis, Janos Fischer, Jan Heeres, Tom Perun and Gerd Schnorrenberg

1) Welcome and Introduction

Gerd and Balu welcomed the participants.

Gerd acknowledged the online *IUPAC Richter Prize Award* presentation and award lecture given by John Macor. The current chairman of the selection committee, Janos Fischer, introduced the awardee. The idea for the online award presentation was appraised and John's presentation was well received.

2) Minutes of last telecon

The minutes have been uploaded to the IUPAC/Division VII/Subcommittee D3 homepage, please give any proposals for changes to Balu and Gerd within the next two weeks, Balu would then upload a revised version.

3) Impact of Covid-19 pandemic on SC D3

There is reason to assume that physical meetings of the SC D3 for the next 6 months will not be feasible. The question arises how to structure our SC work during this time. There was support for Gerd's proposal to have every 3 months a SC D3 telecon where we would exchange information and get informal updates on project progression and collect and discuss new project proposals. Michael Liebman suggested to combine this with a discussion on current topics in drug discovery and development. Respective literature could be sent out before the telecon and be discussed during the telecon. The regular updates on projects should continue to be given in a 6 months interval. We would like to ask the project leaders to give their updates in the formal standardized templates and add during the meeting their comments. Mukund suggested to put more focus on chemical development where synthetic routes for upscaling have increased importance as recent shortfalls of API's led to issues with respect to drug supply in the US and in Europe. Mukund also suggested that D3 SC should be able to reach out to pharma and biotech companies to attract funding for the division. It needs to be clarified, if such fund raising is in line with IUPAC policy.

We finally agreed to have telecons every 3 months, the next telecon to be planned for early 2021. Balu and Gerd will send out invitations and ask for topics to be discussed.

4) Project updates

Janos Fischer reported on Volume 4 of *Successful Drug Discovery* which received a very positive review. Vol 5 is already well advanced and going into the proof reading process currently. Publication is expected in the first half of 2021.

Balu reported on the *Medicinal Chemistry Training Course in India*. Due to the current pandemic the next course is only planned for 2022. A project proposal that includes the

emerging technologies in Drug Discovery and Development will be submitted in the first half of 2021 for funding. Balu also reported on Wayne Childers *Advanced Training Course for Medicinal Chemists*, the current status is open.

Michael Liebman reported on his project on *Failure Analysis of MS Drugs* both in clinical development and market. He has made good progress in getting access to relevant databases being prerequisite for starting the analysis phase.

Michael Liebman's project on the *Newsletter* has also made progress. His article/critique on Artificial Intelligence in Drug Discovery and Development has so far focused on the translational clinical aspects and will be complemented by a part on AI in drug discovery and development. Goal is to have a first edition of the Newsletter end of this year.

Helmut Buschmann is currently working on a critique on New Anti-infectives for the Newsletter.

From contacts with Paul Erhardt and Ganesan we learnt that after submission of their papers on a *Drug Metabolism Glossary and Tutorial / Glossary and Terms in Combinatorial Chemistry* to IUPAC/PAC for release/publication. No response was given so far. The SC members and authors expressed their concern about the delays of progression. Rita Cornelis will take this topic up at the planned online IUPAC Division heads telecon.

5) New Project Proposals

Mukund Chorgade will prepare a project proposal on measures how to improve API supply for drug substance production.

Balu and Bill Greenlee will be submitting a proposal on Medicinal Chemistry training course that includes a focus on new technologies.

Janos Fischer has prepared a project proposal as joint project with the SC Toxicology on high dose Paracetamol toxicity (see attached slides). The structure of the joint project will be discussed with Vincenzo Abbate beginning of November.

Hassan Ibraim will send a project proposal on Natural Products based drugs.

Helmut Buschmann has sent a document (see attachment) with ideas for future Newsletter Topics. In addition ideas on Annual Publications, future Glossaries and other Topics of Potential Relevance were given. We will discuss these ideas at our next upcoming SC D3 telecon early 2021.

Rita Cornelis reported on available funds within IUPAC for new project proposals and stimulated fast submission of proposals.

6) Terms and Glossary updates

The SC discussed about the current status of Glossaries and Terms, one cornerstone of IUPAC's mission. In many cases – including Glossaries and Terms from the SC D3 - that the documents are outdated. This leads to decreased acceptance by the scientific community as binding guidance for terminology. There is an urgent need to discuss measures how to update Glossaries and Terms according to technology advances regularly. As another measure to increase acceptance we suggest to publish these documents and their updates online. Balu and Gerd will make a practical proposal how to update the documents regularly.

7) Miscellaneous

Tom Perun reported on the upcoming election of new Titular Members for the Division in early 2021. Ten TMs will be elected for the 2022-2023 term. Three of these include the incoming President, Helle Moller Johannessen, the Past President, Rita Cornelis , and the current Secretary, Vladimir Gubala. Of the current TMs, Gerd Schnorrenberg and Sharon Teh will finish their eligibility. Gerd will remain on the DC as chair of the SC D3. The Nominating Committee chaired by Tom will include one additional member of the current DC and three non-members. Candidates for the election will be selected from the nominations sent by the NAOs at the beginning of 2021.

The high number of participants in the SC D3 telecon was acknowledged and suggests telecons as valuable communication tool in the future. This will not substitute our plan to have at least one face to face meeting per year. Tom Perun reported that the ACS MEDI Symposium in New York is planned now for June 2021 being a perfect opportunity to have a meeting of our SC back to back, if the pandemic situation allows.

The next meeting will be in the month of Jan/Feb 2021.

Gerd Schnorrenberg and Balu