

Minutes of the Subcommittee Drug Discovery and Development Telecon

Held on December 10, 2021

List of participants: Balu, Helmut Buschmann, Mukund Chorgade, Michael Liebman, Helle Møller Johannessen, John Proudfoot, Roland Pieters, Janos Fischer, Tom Perun, Robin Ganellin, Jan Heeres and Gerd Schnorrenberg; Paul Erhardt, Vincenzo Abbate, Hassan Ibraim (excused)

Jonathan Baell and Toshi Kobayashi (unable to attend due to time zone issue)

1) Welcome and Introduction

Gerd and Balu welcomed the participants.

Gerd welcomed the new Division VII President Helle Møller Johannessen and congratulated her for her new role. He wished her much success in the name of the whole D3 Subcommittee in leading the Division VII in the future. On behalf of the D3Sc, Gerd expressed many thanks to Rita Cornelis for her strong support of our Subcommittee during her tenure as President.

Helle Møller Johannessen introduced herself and introduced her goals for the presidency. According to the newly defined strategy of IUPAC which has not been published yet she wants to strengthen the role of IUPAC on chemistry organizations and to take respective action on chemistry organizations related to human health. She also stated that budget for new projects' funding is secured.

2) IUPAC Richter Prize

Janos Fischer presented the overview on the objectives of the prize, the organization related to Medchem conferences, the nomination process and the selection of the awardee by a committee. He raised several questions with respect to future continuation (presentation attached). The SC D3 members suggested to build a small working group to find answers to the questions raised and to present them at the next telecon. The group members will be Janos, Balu and Gerd. In addition 2-3 SC D3 members should join.

Action all: SC D3 members are asked to indicate their interest to join.

3) Project updates

Book Series Successful Drug Discovery

Janos Fischer reported on the completion of Volume 5 in the first half of 2022. He reported on discussions with Wiley on their wish to refocus the series. They would like to change topics and create a new series with focus on new technologies/new therapeutic modalities, e.g. mRNA vaccines, and therapeutic areas, e.g. CNS and oncology as examples. Open questions are: Who will be the new editors? Will there be the still a link to IUPAC? As the

book series has been a cornerstone of SC D3 activities and contributed to the income of IUPAC via royalties it is important to take a well aligned decision how to proceed. A small team of SC D3 members aligning with IUPAC management needs to work out a proposal. Janos will be important member.

Action all: Indicate interest to join the team.

Analysis of Drug Failure

Michael Liebman reported on the progress made in the pilot study in Multiple Sclerosis Drugs (presentation attached). Good progress has been made, one of the first conclusions is that deficiencies in diagnosis of the MS subtypes and in selection of respective subpopulations is often connected to failures in reaching predefined endpoints. It was discussed whether results in MS will translate also to other indications and Michael responded that he would be confident that this will be a general root cause of failures.

Newsletter

After the release of the first edition positive responses were collected by SC D3 members. However, we need to improve the breadth of distribution. We need to define distribution channels, including social media and need to define among the SC members who does what. It is planned to start work on the second edition with the aim to publish it end of first half of 2022, scientific topics could be continuation of the AI topic from new perspectives, new drugs against multi drug resistant bacterial strains, new therapeutic modalities like PROTACs or antisense oligonucleotides.

Action all: Please make proposals how to improve distribution and indicate your links to respective channels. Please indicate your commitment to contribute to the second edition, e.g. as moderator.

Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development

In absence of the project leader Paul Erhardt, Gerd presented Paul's update giving evidence for the successful completion and the ongoing publications of the glossary giving evidence for the importance for scientists and the general interest (presentation attached).

Human Drug Metabolism Database (hDMdb)

In absence of the project leader Paul Erhardt, Gerd presented his update. As similar tools that have evolved over the last several years for use across the pharmaceutical enterprise within companies and for academics in general, the need and focus of the hDMdb needs to be reassessed (presentation attached). Accordingly, Paul has generated a short questionnaire (attached) which should help him to focus on the needs of scientists in the field.

Action all: Please distribute questionnaire via your links to respective organizations, please align with Paul to coordinate distribution.

4) Next Telecon on Current Topics

Due to the positive feedback from the last Current Topics telecon we want to continue by planning the next one.

Action all: Please nominate new topics to be distributed (e.g. reviews), shortly presented and discussed. Please also indicate your interest to moderate the discussion.

5) Planning of next face to face meeting of SC D3

Tom Perun has made contacts to the organizers of the ACS National Medicinal Chemistry Symposium in New York on June 26-28, 2022. **As the IUPAC Richter Prize Award Ceremony will take place on the evening of Tuesday, June 28, we plan to have the next meeting in the afternoon of the same day.** A room will be provided by the Symposium organizers, thanks to Tom.

Before the next face to face meeting we will have a telecon end of first quarter 2022.

Gerd and Balu would like to thank all participants and all members contributing to our telecon.

We would like to remind all SC D3 members to respond to the action points by email as soon as possible, deadline end of December 2021, as many actions are time-critical.