Molecules to Organisms Working Group
Third Meeting Agenda

Monday, November 28, 2016
Working group members arrive.

Tuesday, November 29, 2016

8:00 – 9:00	Breakfast
9:00 – 9:10	Cheryl gives overview of progress
9:10 – 9:20	Roger presents overview of progress of other working group
9:20-9:50	Erik presents SETAC presentation and progress (there is time for discussion and questions)
9:50-10:10	Dina presents work on egg loading and release (there is time for discussion and questions)
10:10-10:30	Terry presents SETAC presentation and progress (there is time for discussion and questions)
10:30-10:45	Break
10:45-11:15	Phil and Andre presents overview of preliminary analyses with available data (there is time for discussion and questions)
11:15 – 12:00	General discussion on next steps/goals, grant applications
12:00-13:00	Lunch (with discussions) – time for a group photo.
13:00- 16:30	Work in subgroups (with coffee breaks)
16:30-17:00	Reconvene
17:00	Social at NIMBioS

Wednesday, November 30, 2016

8:00–9:00	Breakfast
9:00 – 12:00	Continue to work in groups to tackle objectives.
12:00 – 13:00	Lunch
13:00 – 17:00	Work in small groups or individually to make progress on tasks identified at the end of the morning's session.
17:00	Reconvene to discuss progress

Thursday, December 1, 2016

8:00 – 9:00	Breakfast

9:00 – 10:15 Discussion on connections to the other group
10:15-10:30 Break
10:30-11:30 Discussion on bringing everything together (Some talking points can include 1) how to classify AOPs along DEB parameters, 2) using DEBs to constrain AOPs, 3) other stressors and other contexts, 4) how to link molecular data quantitatively to DEB parameters', with sub-issues related to things like matching temporal scales of changes at the molecular and individual levels, 5) expectations of the AOP-DEB linkage - once we measure how a specific chemical exposure alters growth and reproduction (tox test data), how does inserting this information into a DEB model help us better understand or predict the ecological effects of chemical exposures? Or are we expecting that available tox test data is just 'training data' for the DEB model, which will permit DEB to be used to make predictions for chemicals not tested)

11:30 –noon Identify tasks remaining for workgroups

Noon - Pack lunch and excursion (Terry is looking into where)

15:00 - Work on tasks

Friday, December 2 2016
8:00 – 9:00 Breakfast

9:00 – 12:00 Report back on questions/tasks assigned the previous afternoon. Work in small groups or individually on model analyses, data gathering, and/or writing.

12:00 – 13:00 Lunch

13:00 – 14:00 Final session; assess progress achieved; develop plan for completing Meeting 3 Objectives; agree on next steps to be taken and deadlines to prepare for Meeting 4.

14:30 – working group member depart.

Reminder of Our First Three Objectives:
Objective 1 (October 2015): *Develop, and translate into mathematical terms, a conceptual model for each of the two case study species (Daphnia, rainbow trout) that focuses on the molecular to organism linkage.*
We will focus on sublethal effects of contaminants, and the first step will be to compile the data sources for our case studies, review the modeling tools and identify key processes that will allow for molecular and toxicokinetic data to be incorporated into DEB. We will decide on which contaminants, specific modes of action, and modeling platforms to use. We will address how molecular data, as it is measured and modeled currently within the AOP framework, can translate to behavior, reproduction, growth and reserve processes relevant to DEBs. We anticipate that this exercise will direct some ongoing studies with Daphnids at ORNL that will provide relevant data. After we compile all the available and the "wish-list" data, we will construct a conceptual model, and explore how each of the different types of quantitative tools can contribute or be modified to create

linkages between molecular responses and DEBs, with restrictions and limitations highlighted for both case study species which will be shared with the sister group. We anticipate that this conceptual model and review of the modeling tools will be written into 2 or more book chapters for a book titled "A Systems Biology Approach for Advancing Adverse Outcome Pathways for Risk Assessment", edited by Natalia Garcia-Reyero and Cheryl Murphy with publication date of February 2016.

Objective 2 (May 2016): *Refine conceptual model and mathematical implementations, conduct preliminary tests of model predictions, identify data gaps and further refine models.*
Portions of the conceptual model will be assigned to different teams of participants to refine mathematical and simulation models prior to the meeting. At the meeting and beyond, modeling efforts will be assembled, evaluated, refined and validated with existing data sets. Identified data gaps can inform activities at ORNL which can feed back to further refine model sets. We anticipate products from this objective will be prepared, submitted to scientific journals and will also be presented at national and international meetings.
Objective 3 (August 2016): *Meet with the Organism-Ecosystem Working Group, share progress to date, and agree on an approach for model integration and overall framework development.*

Our objective here is similar to the sister group, in that we will facilitate a coordinated meeting of the two working groups, where progress, challenges, key metrics and processes will be discussed. We will decide on a course of integration of the two sister groups and will assign tasks to participants to accomplish this goal between this meeting and the next.

Obviously we have diverged from Objective 3 because we were unable to find a time to meet with both working groups. I restate the objective though so we can prepare for the final meeting.b