



TECHNOLOGY EVALUATION CONSORTIUM™

Quantitative Medicine Meeting with Lundbeck
Tuesday, August 20, 2013
Webinar

Cambridge Healthtech Associates

Dawn Van Dam (General Manager)
Amid Zand (Project Manager)
Ernie Bush (Scientific Director)

Quantitative Medicine

John King
Scott Bodine
Geoff Hoare
Joshua Kangas
Robert Murphy
David Demosthenes
Jim Parrino (not on call)
Jamie Grooms (not on call)

Lundbeck

Jorrit Hornberg (Head of *In vitro*
Exploratory Toxicology)
Ulf Norinder

Agenda

- I) Opening Remarks: CHA – Ernie
 - II) One on One Discussion: Quantitative Medicine Slides
 - III) Q&A: Quantitative Medicine and Lundbeck
 - IV) Closing and Action Items
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I) Opening Remarks

Ernie briefly explained the slight difference in the nature of this project, given the likelihood that interactions would be one on one versus the conventional group format.

Roles and responsibilities of the meeting participants were discussed in brief.

Amid Zand (Project Manager) and Dawn Van Dam (General Manager) were involved in a meeting in Boston and therefore were listening in but were not likely to actively participate.

Ernie Bush: provides most of the management and/or oversight for all of the projects. Ernie's background is in pharmaceutical research and development.

Jorrit Hornberg: head of *in vitro* exploratory toxicology at Lundbeck. Jorrit's background is in molecular cell biology and he holds a Ph.D. in systems biology. His group's role is to assess the potential safety liabilities of their novel drug candidates and integrate toxicology into the drug discovery process to identify potential liabilities very early on.

Ulf Norinder: computational chemist with a special interest in pattern recognition and machine learning. He has extensive experience with machine learning and *in silico* modeling.

II) One on One Discussion: Quantitative Medicine's Presentation

John King of Quantitative Medicine welcomed the Lundbeck team and introduced himself and the members of Quantitative Medicine participating in the meeting. John

briefly described the origins of the Quantitative Medicine system and turned the meeting over to Joshua Kangas.

Josh presented Quantitative Medicine's slides intended to cover several major topics:

1. Comparison with Current Experimental Approaches

The Lundbeck team asked how the initial batch of experiments was chosen. Josh's response to Lundbeck: the initial batch was chosen at random.

Lundbeck expressed an interest in learning more about how the predictive model is updated in the AFRS system.

Josh briefly described several methods of updating the model. Josh and the Lundbeck team discussed uncertainty sampling and utilizing the system to discover new chemistries.

Lundbeck asked how Quantitative Medicine assesses the applicability domain of their model.

Josh explained the assessment.

The Lundbeck team and Josh discussed some specifics of the PubChem data simulation and of the Quantitative Medicine system.

- AFRS across several campaigns simultaneously was discussed
- Immediate and long term benefits of AFRS were discussed

2. AFRS Use Cases: Situation, Action, Results

Lundbeck expressed interest in how the hypothetical accuracy percentage in the use cases may differ as the assays differ.

Ernie explained that he noticed many of the questions directed toward Quantitative Medicine involved inquiries about things they had or had not tried. Given that, he thought it appropriate to highlight the fact that this particular project differed from the conventional projects the group was used to seeing in that Quantitative Medicine was essentially looking for a partner to help evaluate the validity of their system in a real world setting. He further explained the potential for a one-on-one collaboration between Lundbeck and Quantitative Medicine.

Josh expressed interest in possibly using the system to integrate toxicology into early stage drug development as the Lundbeck team had mentioned earlier in the meeting.

Ernie expressed an interest in using a system like that of Quantitative Medicine to provide a sort of architecture for choosing and weighting assays in the drug development process.

The Lundbeck team expressed further interest, of a more exclusive nature, in the Quantitative Medicine machine learning technology.

John suggested a polypharmacological application.

The Lundbeck team suggested using time stamp data to show differences in time usage.

Confidentiality concerns were discussed.

III) Q&A: Quantitative Medicine and Lundbeck

The Lundbeck team inquired about the size of the data set required for a potential project. They also requested whatever possible information could be disclosed, specifically concerning the Quantitative Medicine machine learning technology.

Lundbeck inquired as to the end goals of a project.

John explained that Quantitative Medicine is most interested in exploring the technology with Lundbeck and further progression of the collaboration which would benefit Lundbeck would simply be an added benefit.

IV) Closing Remarks and Action Items

Lundbeck intends to verify that all matters of confidentiality are addressed properly. They are also going to have an internal discussion about a potential project proposal.

Quantitative Medicine requested contact information for Lundbeck team from Amid to send the information requested by Lundbeck.

Further correspondence will be arranged through CHA to assist in project proposal and execution.
