PK/PD analyses & statistical evaluation
Regulatory aspects for evaluation of clinical trials
Computational chemistry in drug development

Wednesday, September 08, 2004 (08:00 AM – 01:30 PM)

The participant of the 08:00 to 10:45 AM session should gain insight in the standard PK/PD analysis techniques as most often applied in clinical studies. The participants should see how professional and easy to learn software can be applied to analyze pharmacokinetic studies, derive summary statistics and generate reports automatically.

The application of different kinds of models and non-compartmental analysis in the process of clinical drug development will be the focus of the next workshop lecture. Regulatory aspects will also be covered from an industry perspective.

The third lecture will concentrate on the optimization of clinical trials by use of computer assisted trial design. This technique allows an ideal use of prior knowledge for saving time and other resources in the drug development process.

Time	Topic	Level / Prerequisites
08:00 - 09:00 AM	*Pharmacokinetic analysis as applied in practice:* **From analytical concentration-time raw data to the final statistical results within minutes (even for beginners)** - Visualization and presentation of PK raw data and results - Introduction to application of non-compartmental analysis, the method of choice for standard PK analyses, in case rich data are available - Demos via use of WinNonlin Pro - A 21CFR11 compliant database (PKS) - Report automation (scripting & reporter) **Abid Sattar**	**Beginner – intermediate** *Prerequisite(s):* Basic knowledge in PK/PD (e.g. workshops on Monday and Tuesday)
09:00 - 10:00 AM	**Role of PK/PD in drug development – A regulatory point of view** - Background and Introduction to Modeling – When, how and when not to apply models - PK/PD modeling and non-compartment analysis and their place within the drug development process - Relevant FDA Guidances - Modeling of rich datasets - Population PK/PD modeling **Dan Weiner**	**Beginner – intermediate – advanced** *Prerequisite(s):* Basic knowledge in PK and PD models (e.g. workshops on Monday and Tuesday)
10:00 - 10:45 AM	**Optimizing drug development: Use of Computer Assisted Trial Design to optimally design clinical trials** - Theoretical background - Presentation of several case studies - Use of the Trial Simulator (TS2) software **Dan Weiner**	**Intermediate – advanced** *Prerequisite(s):* Some background in PK models and basic statistics
	Coffee break, 10:45 - 11:00 AM	

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This session will discuss several strategies of assessing bioequivalence. Bioequivalence studies are very frequently used for evaluation of food-effects, interactions, generic vs. originator bioequivalence and other issues in healthy volunteer studies.

The next two talks will introduce a computational chemistry approach to optimize the drug development process by direct incorporation of computational chemistry to predict pharmacokinetic and affinity / activity data.

Time	Topic	Level / Prerequisites
11:00 AM - 12:00 PM	**Strategies for assessment of bioequivalence (BE)** - Theoretical background for different types of bioequivalence (average vs. individual bioequivalence) - Demonstrations on how bioequivalence statistics are applied in practice - Discussion of problems and pitfalls associated with bioequivalence evaluation - See how non-professional statisticians can run bioequivalence statistics **Dan Weiner**	**Beginner – intermediate – advanced** *Prerequisite(s):* Some basic knowledge in statistics and design of clinical studies
12:00 - 12:30 PM	**Quantitative Structure Pharmacokinetics Relationships (QSPKR): How to estimate pharmacokinetic parameters** - when there are no plasma concentrations for a drug - when the drug has never been synthesized before - by use of the 2D chemical structure of a molecule solely(?) o Predicting a complete set of PK parameters and plasma concentration time curves *in silico* o How computational chemistry may optimize pharmacokinetic characteristics in drug development o Proof of concept for quinolone antibiotics in humans **Jürgen Bulitta**	**Beginner – intermediate** *Prerequisite(s):* Basic knowledge non-compartmental analysis and statistics Prior knowledge in computational chemistry is not required.
12:30 – 01:30 PM	**Exploring structure and function of peptides and proteins with homology modeling and molecular dynamics simulations** - Generating protein structures by homology to experimentally known systems - Visualization and modeling the interaction between ligands and hosts in dynamic systems - How can a ligand be optimized by use of computational chemistry? - How to determine the “ideal” ligand? **Harald Lanig**	**Beginner – intermediate** *Prerequisite(s):* Basic knowledge in ligand / host interactions Prior knowledge in computational chemistry is not required.
01:30 – 01:45 PM	**Discussion**	**All**

Speakers:

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