

Optimizing Drug Design

Workshop, July 20 - 23, 2009 Leiden, The Netherlands

**Scientific
Organizers**

- Michael Emmerich, Leiden
- Andreas Bender, Leiden

**Keynote
Speakers**

- Nathan Brown, London
- Christos Nicolaou, Nicosia
- Ian Parmee, Bristol
- Carlo Poloni, Trieste
- Matt Seagall, Saffron Walden

Topics

- Problem definitions in drug design
Which objectives are we talking about?
- Algorithmic approaches to perform multicriteria optimization of compounds
- Trade-offs in virtual screening:
Finding many vs. diverse active compounds
- The role of the expert; interactive and semi-automatic optimization
- Case studies in multicriteria drug design
Where we fail, and where we succeed

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