**Global Health Compound Design Webinars**

During 2016 we are running a series of webinars on the subject of compound design. The programme for future meetings is available below (the agenda will develop through the year) and links to recordings & other information is provided on the next page.

The aim is to share experiences of compound design in global health projects (malaria, TB, NTD), covering a range of topics including the use of freely available design tools, quality criteria such as target candidate profiles, screen sequences and case histories. If you are interested in making a presentation, please contact mark.gardner@amgconsultants.co.uk

**Programme for remainder of 2016 (links to recordings of previous sessions below)**

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| **Date** | **Agenda** | **Registration**  |
| 24th May 2016Two hours earlier than usual, ie 8am East Coast US, 1pm UK, 2pm CET etc | **MMV open source malaria workshop, with Paul Willis & Mat Todd** – [link to 1 page flyer including structures](https://www.dropbox.com/s/wnopbeetpxq0ne8/OSM%20Webinar%20Initial%20Flyer.pdf?dl=0)Project background & scientific objectives (5)Overview of project information sources - ie what's where  (5)Data sources & summary of analyses (5-10)SAR overview, questions for the audience (20)Discussion (10-15)Final guidance on what's required from the audience & how to submit your suggestions & what happens next (5) | [Registration](https://attendee.gotowebinar.com/register/7722880987090170883) |

## Previous meetings: recordings, questions & answers from session

Please note, to view recordings please download the file to your machine or it is likely to stop part way through

**[Link to Recording - 21](https://goo.gl/RDOmhB)[st](https://goo.gl/RDOmhB) [Jan 2016](https://goo.gl/RDOmhB)**

0:00 – introduction to meetings, Mark Gardner

4:04 - **Application of PK Tools in the optimisation of a series for the treatment of leishmaniasis, Gavin Whitlock, Sandexis**, working with DNDi

32:51 - **Hints and tips to working with DataWarrior, Isabelle Giraud, Actelion**, slides

38:18 - Isabelle Giraud, DataWarrior demonstration

**[Link to Recording 25](https://goo.gl/7qqiCL)[th](https://goo.gl/7qqiCL) [Feb 2016](https://goo.gl/7qqiCL)**

0:00 - **Visceral leishmaniasis Target Candidate Profile & screen sequence, Charlie Mowbrary, DNDi** (recording starts at Charlie’s slide 5 – [full slides here](https://goo.gl/MN9Jhs)),

16:45 – Q&A1-How would you determine therapeutic Index if efficacy was driven by Cmax rather than AUC?

19:02 – Q&A2 Any general guide to the level of potency you would look for in phenotypic hits?

Additional Q&A by text: Do you think that some of the response variability between Africa and India is due to fake medicines on the market? Or is it genetic differences?

There are clear differences in response in well controlled clinical trials conducted by DNDi and other groups. We suspect that both subtle parasite and/or host differences (including immune status, nutritional status, genetics,...) contribute to these striking differences. Fake medicines may contribute to some treatment failures and toxicity but that is I think a seprate, albeit important topic.,You can also see the big regional differences within Africa e.g. http://journals.plos.org/plosntds/article?id=10.1371/journal.pntd.0000709

21:52 – Poll results “Would you prioritize phenotypic or target based approaches for new malaria targets?”

22:45 – **Malaria Target Candidate Profiles, stage gates and implications for successful malaria drug discovery, Paul Willis, MMV**

45:20 – Q&A - Given the desire for very-long-half-life agents, do you consider biologics?

[**Link to Recording 17th March 2016**](https://goo.gl/DfKryW)

**0:00** - **DataWarrior advanced data analysis, Isabelle Giraud, Actelion – introduction**

03:05 - Demonstration of SAR analysis by R group analysis

09:00 – BoxPlots & statistics

12:20 – changing the order of items (eg R groups) in charts

14:18 – property calculation eg clogP

15:25 – adding new compounds (eg by sketching)

22:00 – Q1 – Is it possible to script Datawarrior perhaps using python (DataWarrior has it’s own macro language which can be edited, but not in Python. However, KNIME integration is coming)

22:42 – Q2 – Can you plot 2 properities say activity and solubility and then colour code the data point by R group. Say R1 red, R2 blue etc (yes, demo in video)

**26:46 - Using the RSC Medicinal Chemistry Toolkit in Drug Discovery Projects, Andy Davis, AZ**

32:33 – Case Study 1 – Understanding the impact of ATP concentration on correlation between enzyme binding and whole cell assay using the Cheng Prusoff calculator

35:40 – Case Study 2 – Understanding a drop-off between cell assay & using an app to calculate the impact of plasma protein binding on assays

38:38 – Case Study 3 – Dose to Man app & illustrating the relatively minor impact of plasma protein binding on dose prediction

43:23 – Chemical sketching, property calculation including ligand efficiency, lipophilic ligand efficiency & AZ ‘structural alerts’

46:38 - Q1 - Is there any way to add further medchem filters? (Yes in principle, but will require additional funding)

47:45 – Q2 - Is the toolkit only available on the UK appstore? I can't see it in Switzerland. (It should be available on the world AppStore but you won’t see it from an iPhone, you need to search from an iPad)

48:35 – Poll Question: Currently RSC Medicinal Chemistry Toolkit is only available on Apple platforms, will that prevent you from using it?

[**Link to Recording 21st April 2016**](https://goo.gl/XsvxZD)

0:00 – Introduction, agenda for this meeting & that on 24th May

1:41 – Poll “What is your experience with KNIME?”

2:01 - **An introduction to the open-source workflow tool** [**KNIME**](https://www.knime.org/) **and applications in drug discovery, Greg Landrum, KNIME**

15:19 – Q&A - Given that Java is no longer preinstalled on any of the major platforms, and not available on mobile devices is this a concern for the future?

16:37 – Q&A - Nodes from Vernalis, Indigo etc are they open source or commercial?

17:29 - **KNIME use case: Property calculation and chemical space diagrams in DNDi's Drug Booster project, Ben Perry, DNDi**

36:14 – Q&A - How can I get the Workflow shown in this demo? ([Workflow](https://goo.gl/3e9BQh), [PDF documentation](https://goo.gl/CaiW9N))

37:53 – Q&A – Where’s a good place to go for workflow examples (KNIME forums are a good source)?

39:24 – Q&A - Does [DataWarrior](https://goo.gl/Kzid6b) come with KNIME?

40:27 – Q&A - Are the demos available on KNIME?

41:10 – Q&A - Can DataWarrior be integrated into the knime node workflow though?

41:49 - **KNIME use case: ‘Know Your Molecule’ searching ChEMBL with KNIME & interpreting the data, Mark Gardner, AMG (**[**Guide & workflow**](https://goo.gl/oY8eYg)**)**

53:18 – Comments, George Papadatos, EBI/ChEMBL – 1. [ChEMBL](https://www.google.co.uk/url?sa=t&rct=j&q=&esrc=s&source=web&cd=1&cad=rja&uact=8&ved=0ahUKEwjVx6TO-KnMAhWBrRoKHU8oBM4QFggcMAA&url=https%3A%2F%2Fwww.ebi.ac.uk%2Fchembl%2F&usg=AFQjCNGnnkFVSRh6hrmUCYQ6_K4bdi9P6w&sig2=xk5PjpEgBg7Tir2qF0anOg&bvm=bv.120551593,d.d2s), KNIME & DataWarrior, 2. Workflow data access examples on KNIME server

54:50 – Accessing ChEMBL directly through DataWarrior

55:45 – Q&A – Is KNIME connected to Pubchem?

56:13 – George Papadatos – Unichem, access through webservices to multiple repositories including Pubchem

56:59 – Conclusion

57:37 - End