

1st MuTaLig COST Action Training School

Computational Approaches to Polypharmacology

8 - 10 February 2017

Vienna, Austria

Scientific Program Day 1

Wednesday, 8th February 2017

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08:00 - 08:55 **Arrival / Registration.** (Pharmaziezentrum UZA 2, University of Vienna).

08:55 – 09:00 **Move to Lecture Hall 5 (Hörsaal 5).**

09:00 - 09:15 **Welcome.** **Sharon Bryant**, (Local Organizing Chair) Inte:Ligand GmbH, Austria.

09:15 - 09:30 **Initiatives of the MuTaLig Cost Action CA15135.** **Stefano Alcaro**, (Chair, MuTaLig COST Action) University "Magna Græcia" di Catanzaro, Italy.

Lectures

Session Chair, Fernanda Borges (Vice Chair, MuTaLig COST Action, University of Porto, Portugal)

09:30 - 10:00 **Pharmacophore Approaches for Polypharmacological Profiling of Compound Libraries.**
Thierry Langer, University of Vienna, Austria.

10:10 – 10:30 **Coffee Break**

10:30 – 11:00 **Navigation in Chemical Space Towards Biological Activity.**
Peter Ertl, Novartis, Switzerland.

11:10 - 11:40 **Smart Screening Libraries and Successful Medicinal Chemistry.**
Marie-Louise Jung, Prestwick Chemical, France.

11:50 – 13:45 **Lunch (on your own).**

13:45 -14:00 **Move to Training Sessions (Pharmaziezentrum UZA 2).**

Training Sessions

Group 1 to Room 2F363

Group 2 to Room 2D313

Time	Group 1	Group 2
14:00 - 15:45	Workshop 1 (Room 2F363) Finding Hit Compounds Using Structure-Based Pharmacophore Modeling and Virtual Screening. Sharon Bryant, Gökhan Ibis	Workshop 2 (Room-2D313) Data Mining and Machine Learning Tools for Drug Design. Hanoch Senderowitz, Abraham Yosipof
15:45 – 16:00	<i>Coffee Break</i>	<i>Coffee Break</i>
16:00- 17:45	Workshop 3 (Room 2F363) Ligand-Based Pharmacophore Modeling and Parallel Virtual Screening Strategies to Find Multi Target Ligands. Sharon Bryant, Gökhan Ibis	Workshop 4 (Room- 2D313) In Silico Fragment-Based Design and Profiling of Diverse or Focused Compound Libraries. Thierry Langer, Riccardo Martini

Scientific Program Day 2

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Thursday, 9th February 2017

08:15 - 08:45 **Registration** (*Sign-in all participants*). Pharmaziezentrum UZA 2, University of Vienna.

08:45 - 08:50 **Move to Lecture Hall 5** (Hörsaal 5).

08:50 – 09:00 **Brief Welcome & Announcements**. **Sharon Bryant**, Inte:Ligand GmbH, Austria.

Lectures

Session Chair, Rita Guedes (University of Lisbon).

09:00 – 09:30 **Exploiting Semantically Integrated Life Science Data – from Transporter Profiling to Toxicity Prediction**. **Gerhard Ecker**, University of Vienna, Austria.

09:40 – 10:10 **Building Compound Archives and Triaging Hit Lists for the Future**.

Richard Lewis, Novartis, Switzerland.

10:20 – 10: 40 **Coffee Break**

Session Chair, Marie-Louise Jung (Prestwick Chemical).

10:40 – 11:10 **An Optimized Approved Drug Library for Combinatorial Screening**.

Stefan Kubicek, CeMM, Austria.

11:20 – 11:50 **Optimization Algorithms in Chemoinformatics: Theory and Applications**.

Hanoch Senderowitz, Bar Ilan University, Israel.

11:50 – 13:45 **Lunch** (on your own).

13:45 - 14:00 **Move to Training Sessions** (Pharmaziezentrum UZA 2).

Training Sessions

Group 2 to Room 2F363

Group 1 to Room 2D313

Time	Group 2	Group 1
14:00 - 15:45	Workshop 1 (Room 2F363) Finding Hit Compounds Using Structure-Based Pharmacophore Modeling and Virtual Screening. Sharon Bryant, Gökhan Ibis	Workshop 2 (Room-2D313) Data Mining and Machine Learning Tools for Drug Design. Hanoch Senderowitz, Abraham Yosipof
15:45 – 16:00	<i>Coffee Break</i>	<i>Coffee Break</i>
16:00- 17:45	Workshop 3 (Room 2F363) Ligand-Based Pharmacophore Modeling and Parallel Virtual Screening Strategies to Find Multi Target Ligands. Sharon Bryant, Riccardo Martini	Workshop 4 (Room- 2D313) In Silico Fragment-Based Design and Profiling of Diverse or Focused Compound Libraries. Thierry Langer, Gökhan Ibis

Scientific Program Day 3 Friday, 10th February 2017

08:30 - 08:45 Registration (*Sign-in all participants*). Pharmaziezentrum UZA 2, University of Vienna.

08:45 – 08:50 Move to Lecture Hall 5 (Hörsaal 5).

08:50 – 09:00 Brief Welcome. **Sharon Bryant**, Inte:Ligand GmbH, Austria.

Lectures

Session Chair, Thierry Langer (University of Vienna).

09:00 – 09:30 **Phenotypic Screening of Annotated Libraries: The Published Kinase Inhibitor Set (PKIS).** **Peter Ettmayer**, Boehringer-Ingelheim, Austria.

09:40 – 10:10 **Multiscale Approach for the Study of Ghrelin and Toll Like 7 Receptor Ligands Proposed by Pharmaceutical Companies.** **Andrea Danani**, IDSIA, Switzerland.

10:20 – 10:50 **Virtual Screening Strategies in Drug Discovery: Some Theory ... Some Applications.** **Rita Guedes**, University of Lisbon, Portugal.

11:00 – 11:30 Coffee Break.

Session Chair, Hanoch Senderowitz (Bar Ilan University).

11:30 – 12:00 **Molecular Databases: Useful tools for Medicinal Chemists. Do We Need Something More?** **Francesco Ortuso**, University Magna Græcia di Catanzaro, Italy.

Searching the Chemotheca - Interactive Session

12:00 – 13:00 **MuTaLig Virtual Chemotheca Updates: What it Can Do for Us, What We Can Do for It.** Bring your computer and experiment with the first prototype of the MuTaLig Chemotheca. **Francesco Ortuso & Stefano Alcaro**. University Magna Græcia di Catanzaro, Italy.

Closing Session

13:00 – 13:20 **MuTaLig COST Action: Next Steps for a Successful Future.** **Fernanda Borges**, (Vice Chair, MuTaLig COST Action) University of Porto, Portugal.

13:20 – 13:30 Closing Remarks. **Sharon Bryant**, Inte:Ligand GmbH, Austria.

13:30 Training School Closes.

Acknowledgements

Local Organizing Committee

Sharon D. Bryant (Inte:Ligand GmbH)
Thierry Langer (Universität Wien)
Goekhan Ibis (Inte:Ligand GmbH)
Daniela Krizan (Universität Wien)

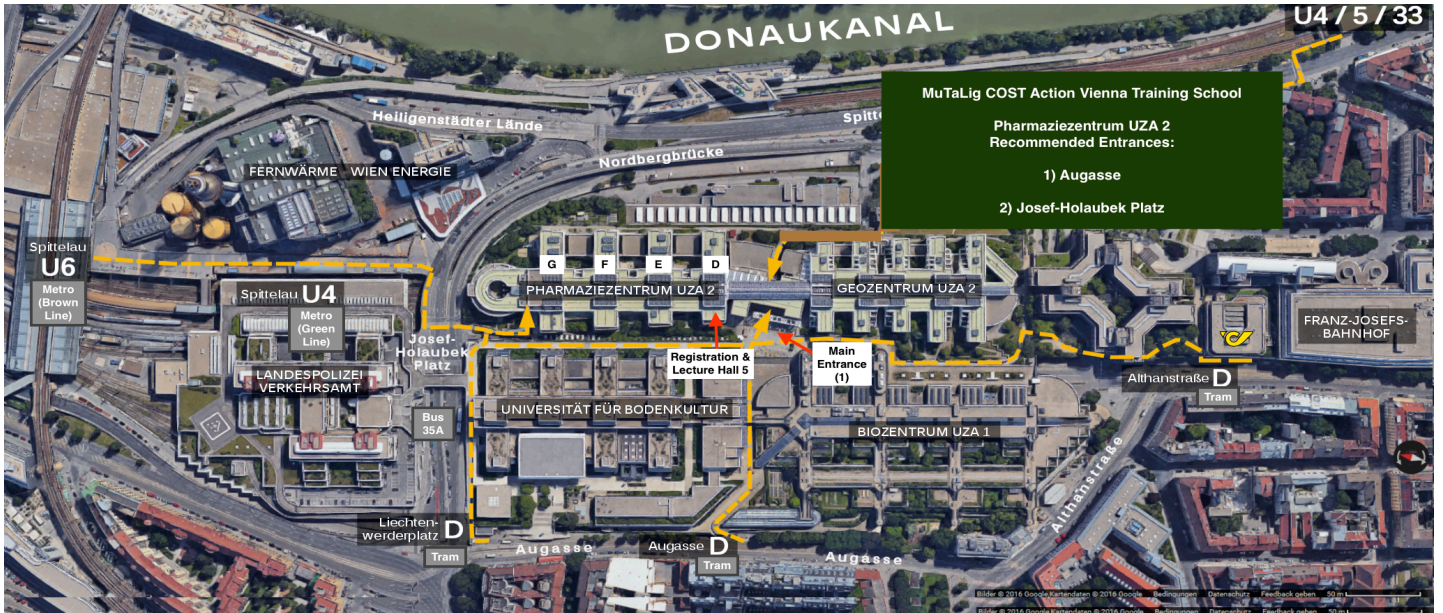
Riccardo Martini (Inte:Ligand GmbH)
Patrick Penner (Universität Wien)
Clara Van Hoey (Universität Wien)
Doris Schuetz (Universität Wien)

MuTaLig COST Action (CA 15135) Committee

Stefano Alcaro, Chair (Italy)
Fernanda Borges, Vice Chair (Portugal)
João Carlos Ferreira Ribeiro (Portugal)
Danijel Kikelj (Slovenia)
Eugenio Gaudio (Switzerland)
Sharon D. Bryant (Austria)
Hanoeh Senderowitz (Israel)
Maria Laura Bolognesi (Italy)

Maurizio Botta, (Italy)
Rita Guedes (Portugal)
Anna Artese (Italy)
Holger Stark (Germany)
Claire Schoemake (Malta)
Christa Muller (Germany)
Joana Abrantes (Portugal)
Lucia Forzi (COST-Belgium)
Svetlana Voinova (COST-Belgium)

Pharmaziezentrum (Pharmacy Center) UZA 2 Site Map



Registration and Lecture Hall 5 is located in section D of the Pharmaziezentrum UZA 2

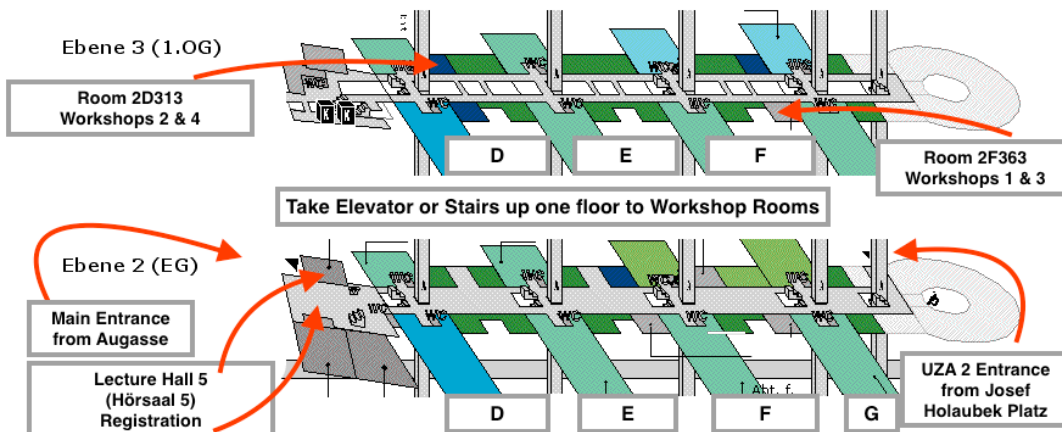
U6- Metro Line (Brown) – Exit Spittelau.

U4- Metro Line (Green) – Exit Spittelau.

Tram D – **(1) Augasse stop (Recommended)**, (2) Lichtenwerderplatz stop (enter UZA 2 from Josef Hoflaubek Platz- go up the stairs and walk straight to the Main Entrance), or (3) Althanstrasse stop (*not recommended for 1st time visitors*-enter the Biozentrum UZA 1 building then exit and cross over into Pharmaziezentrum UZA 2).

Workshop and Lecture Hall Locations

Pharmaziezentrum UZA 2 Site Map
Locations for MuTaLig Vienna Training School Registration and Sessions



Nearby Restaurants

1. Fly's American Fifties Restaurant*

Heiligenstädter Str. 29-31, 1190
flys.at

2. Brandauers Bierbögen*

Heiligenstädter Str. 31, 1190
bierig.at

3. Anker Bakery (Sandwiches & Pastries)

Augasse 2-6, 1090
06 :30 - 18 :00

4. Gasthaus Grabmüller

Lichtenwerder Pl. 3, 1190
<http://www.gasthausgrabmueller.at/>

5. Jasmin Al Sham Restaurant

Heiligenstädter Str. 9, 1190
jasmin.al.sham

6. The Roast

Augasse 21, 1090
TheRoast

7. Café Blau Stern

Döblinger Gürtel 2, 1190
www.blaustern.at

8. Lichtenthaler Bräu – Craft Beer Pub

Lichtensteinstraße 108, 1090
lichtenthalerbraeu.at

9. Restaurant Mediterraneo

Althanstrasse 47, 1090
RestaurantMediterrano

10. Tokyo Nudel

Althanstraße 37, 1090
TokyoNudelRestaurant

11. Ristorante Trattoria Antica

Althanstraße 15, 1090
trattoria-antica.at

12. Akakiko (Japanese)

Julius-Tandler-Platz 4, 1090
akakiko.at



1-2. Tram D (Radelmayergasse-stop)

3-6, 8-11. Very Close (6 minutes walk or less)

7. Walk 10 min

10. Tram D (Franz Josefs Bahnhof (Alserbachstraße)-Stop)