# MODELLING&SIMULATION: RESEARCH METHODOLOGIES FOR SMALL POPULATIONS IN RARE DISEASES

Hotel Excelsior Bari, Italy

4-5 July 2022

**AGENDA**

**4 July 2022**

| Time | Speaker and Affiliation | Session name/Topic |
|---|---|---|
| **09.00 – 09.10** | D. Bonifazi, CVBF | Welcome address |
| **09.10 – 10.00** | A. De Luca, University of Bari 'Aldo Moro' | Developmental pharmacology and toxicology in drug discovery: what is needed for translational pre-clinical studies |
| **10.00 – 10.50** | S. Lorenzetti, Italian National Institute of Health | In utero exposure to chemicals: the case of hepatoblastoma |
| **10.50 – 11.10** | *Coffee Break* | |
| **11.10 – 11.50** | C. D. Altomare, University of Bari 'Aldo Moro' | QSAR in designing and repurposing drugs for small populations |
| **11.50 – 12.30** | O. Nicolotti, University of Bari 'Aldo Moro' | Data and models of human health endpoints in predictive toxicology |
| **12.30 – 13.00** | M. Lettieri - S-IN Soluzioni Informatiche | Machine learning in early prediction of metabolism of drugs for rare diseases |
| **13.00 – 14.00** | *Lunch Break* | |
| **14.00 - 15.30** | F. Ciriaco, University of Bari 'Aldo Moro' | Practical session: A web platform for in-silico ADMETox profiling |
| **15.30 – 15.40** | *Coffee Break* | |
| **15.40 – 17.10** | N. Amoroso, University of Bari 'Aldo Moro' | Practical session: Machine learning approach for prediction of developmental toxicity of chemicals |
| **17.10 – 17.40** | Q&A session | |
| **17.40 – 18.00** | Conclusions | |



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**5 July 2022**

| Time | Speaker and Affiliation | Session name/Topic |
|---|---|---|
| **09.00 – 09.50** | O. Della Pasqua, University College London | PK/PD modelling and simulation: utility in drug development |
| **09.50 – 10.40** | O. Della Pasqua, University College London | Off-label use of medicinal products |
| **10.40 – 11.00** | *Coffee Break* | |
| **11.00 – 11.30** | G. Migliaccio, CVBF | Use of Experimental medicinal products: the regulatory point of view |
| **11.30 – 12.00** | V. Giannuzzi, Gianni Benzi Foundation | How to implement innovative research methodologies in the EU regulatory framework |
| **12.00 – 12.50** | A. Gissi, ECHA, Helsinki, Finland | Regulatory use of QSAR models: the perspective of the European Chemicals Agency (ECHA) |
| **13.00 – 14.00** | *Lunch Break* | |
| **14.00 – 15.30** | Case study: Dose rational and prediction of therapeutic exposure from preclinical models (O. Della Pasqua)* | |
| **15.30- 16.50** | *Coffee Break* | |
| **15.50 – 17.10** | Case study: Clinical Trials simulations: protocol optimisation for small populations (O. Della Pasqua)* | |
| **17.10 – 17.40** | Q&A session | |
| **17.40 – 18.00** | Conclusions | |

** to be able to execute the case studies please Install on your pc the following softwares R: https://cran.r-project.org/. R Studio: https://www.rstudio.com/products/rstudio/download/.*



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