



WORKSHOP ON  
QSAR MODELS  
FOR REACH

Mario Negri Institute, Milan, Italy - March 10-11, 2009



# WORKSHOP ON QSAR MODELS FOR REACH

Mario Negri Institute, Milan, Italy - March 10-11, 2009



**Emilio BENFENATI**

**Istituto di Ricerche Farmacologiche Mario Negri**

INTRODUCTION

the **Project** and the **Workshop**

<http://www.caesar-project.eu/>



# Computer Assisted Evaluation of industrial chemical Substances According to Regulations



<http://www.caesar-project.eu/>



# THE CONSORTIUM OF THE CAESAR PROJECT



1 Istituto di Ricerche Farmacologiche Mario Negri  
coordinator



2 Central Science Laboratory



3 BioChemics Consulting SAS



4 Politecnico di Milano



5 KnowledgeMiner Software Frank Lemke



6 Liverpool John Moores University



7 Helmholtz-Zentrum für Umweltforschung - UFZ



8 Kemijski inštitut Ljubljana Slovenija



9 TNO - Nederlandse Organisatie voor  
Toegepast Natuurwetenschappelijk Onderzoek





# THE COORDINATOR



The *Mario Negri Institute for Pharmacological Research* is a **not-for-profit biomedical research organization**. It was founded in 1961, and started work in Milan on 1 February 1963. There are now research units in Bergamo, at Ranica – near Bergamo – and at Santa Maria Imbaro, near Chieti.

**The Institute's main aim is to help defend human health and life**



<http://www.marionegri.it>

# THE ADVISORY COMMITTEE



**Andrew WORTH**

European Commission Joint Research Centre - EC JRC - IHCP



**Betty HAKKERT**

Rijksinstituut voor Volksgezondheid en Milieu - RIVM



**Carlo ZAGHI**

Ministero dell'Ambiente e della Tutela del Territorio e del Mare



**Kevin HARRADINE**

Syngenta Ltd



# COLLABORATIONS



## US EPA



Dr. Ann M. Richard - US EPA - NCCT : validation of toxicity data

Dr. Douglas Young & Dr. Todd Martin - US EPA - NRMRL : chemical descriptors



## OSIRIS

Intelligent Testing Strategy



## CHEMPREDICT

SMILES and InChI



## CHEMOMENTUM

automatic QSAR models





# THE CAESAR ENDPOINTS



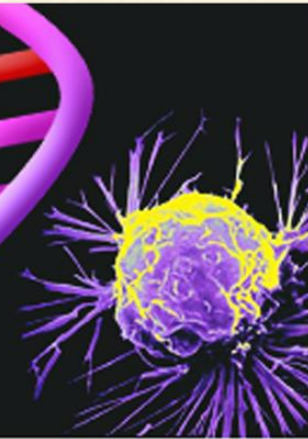
*Bioconcentration*



*Mutagenicity*



*Skin Sensitization*



*Carcinogenicity*

*Developmental  
Toxicity*







# WORKSHOP ON QSAR MODELS FOR REACH

Mario Negri Institute, Milan, Italy - March 10-11, 2009

## PROGRAMME OF THE CAESAR WORKSHOP

Speakers and Oral Presentations

# PROGRAMME

Tuesday, March 10<sup>th</sup>

- 
- 15:50 - 16:00**     **Introduction**  
*Emilio Benfenati* *coordinator of the CAESAR project*  
Istituto Mario Negri - Laboratory of Environmental Chemistry and Toxicology  
Milan, Italy
- 
- 16:00 - 16:30**     **The second phase of the (Q)SAR Application Toolbox**  
*Doris Hirmann*  
European Chemicals Agency (ECHA)  
Helsinki, Finland
- 
- 16:30 - 17:00**     **Computational tools and guidance developed by the JRC**  
*Klaus Daginnus*  
European Commission Joint Research Centre (EC JRC)  
Ispra, Italy
- 
- 17:00 - 17:30**     **Use of QSAR models for REACH and the CAESAR approach**  
*Emilio Benfenati*  
Istituto Mario Negri - Laboratory of Environmental Chemistry and Toxicology  
Milan, Italy
- 

**19:30**     **Social Dinner**  
*Osteria dei Vecchi Sapori - Via Carmagnola 3, Milan*





# Wednesday, March 11<sup>th</sup>

**08:45** REGISTRATION Opening

**09:30 - 10:00** **Technical aspects behind the CAESAR models**

**Emilio Benfenati**

Istituto Mario Negri - Laboratory of Environmental Chemistry and Toxicology  
Milan, Italy

**10:00 - 10:30** **The model for bioconcentration in fish**

**Alessandra Roncaglioni**

Istituto Mario Negri - Laboratory of Environmental Chemistry and Toxicology  
Milan, Italy

coffee break



**11:00 - 11:30** **The model for skin sensitization**

**Qasim Chaudhry**

Central Science Laboratory  
York, United Kingdom

**11:30 - 12:00** **The model for mutagenicity**

**Giuseppina Gini**

Department of Electronics and Information, Politecnico di Milano  
Milan, Italy

lunch break



**13:30 - 14:00** **The model for carcinogenicity**

**Marjana Novič**

Kemijski institut Ljubljana Slovenija  
Ljubljana, Slovenia



**14:00 - 14:30**    **The model for developmental toxicity**

***Qasim Chaudhry***

Central Science Laboratory  
York, United Kingdom

**14:30 - 15:00**    **The local models for skin sensitization and developmental toxicity**

***Steven J. Enoch***

Liverpool John Moores University, School of Pharmacy and Chemistry  
Liverpool, United Kingdom

**15:00 - 15:30**    **The applicability domain of the CAESAR models**

***Gerrit Schüürmann***

Helmholtz-Zentrum für Umweltforschung UFZ  
Leipzig, Germany

coffee break



**16:00 - 16:30**    **Enhancing CAESAR models**

***Frank Lemke***

KnowledgeMiner Software Frank Lemke  
Panketal, Germany

**16:30 - 17:00**    **The use of the models for risk assessment and classification**

***Tialda Bouwman***

N. O. voor Toegepast Natuurwetenschappelijk Onderzoek - TNO  
Zeist, The Netherlands

**17:00**

**Discussion & Conclusions**

***Emilio Benfenati***

Istituto Mario Negri - Laboratory of Environmental Chemistry and Toxicology  
Milan, Italy



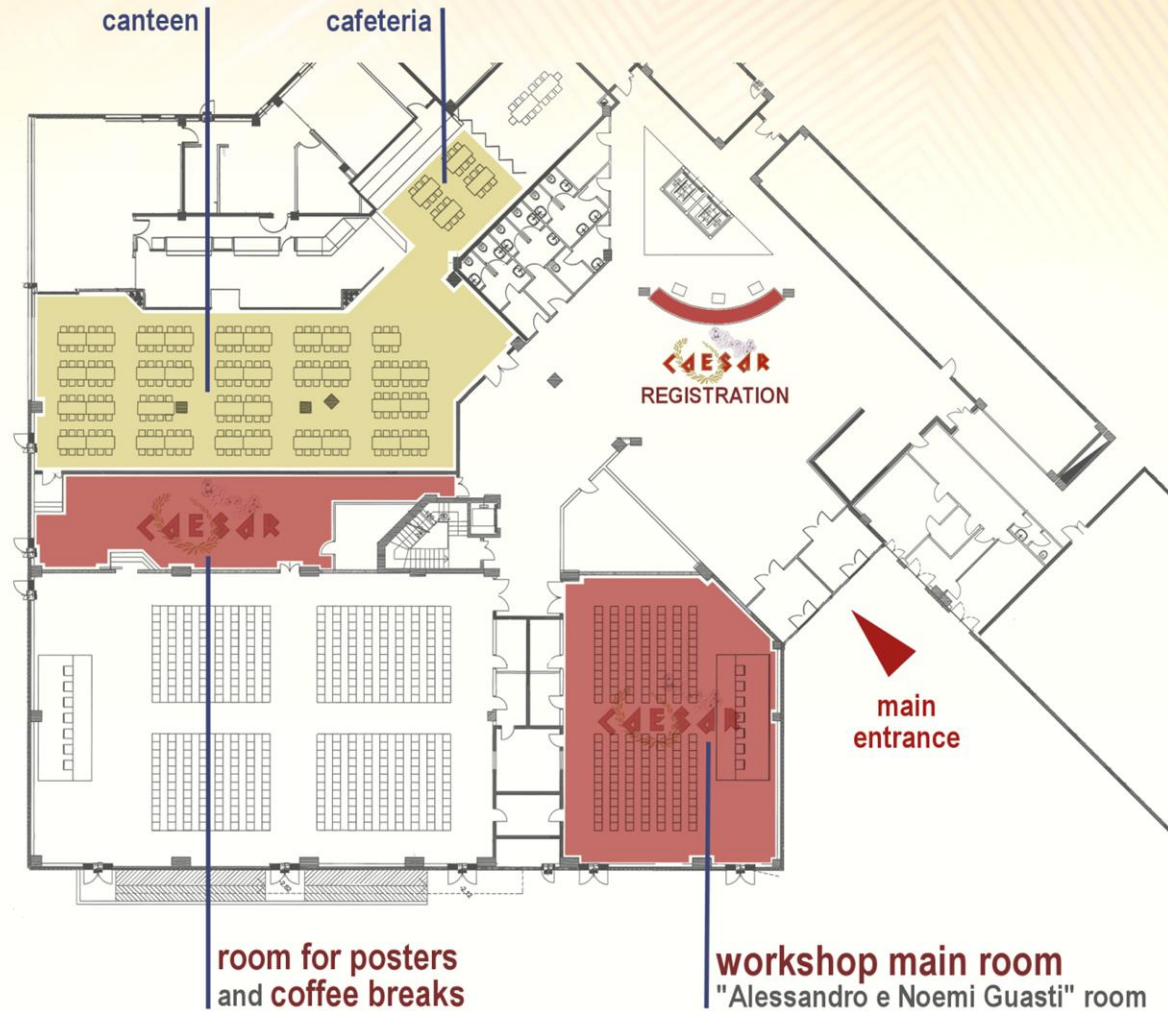


# PRACTICAL INFORMATION



WORKSHOP ON  
QSAR MODELS  
FOR REACH

Mario Negri Institute, Milan, Italy - March 10-11, 2009



## Main details about access to the Mario Negri Institute

- 1 At the end of the session on **March 10**, please remember to **SIGN** the *attendance register* before leaving the Institute.
- 2 Please keep with you the **identification badge** at the end of the session on March 10.
- 3 On **March 11**, the **registration will re-open at 8:45** and each participant will have to **SIGN** the *attendance register*.
- 4 At the **end of the workshop**, please remember to **SIGN** the *attendance register* before leaving the Institute.
- 5 If you have a **car** in the Institute park , please ask the reception for a **coin** to get out.

**During registration on March 11**  
please remind to take **TICKETS for LUNCH**



badge for  
REGISTERED PARTICIPANTS



badge for  
CAESAR CONSORTIUM MEMBERS





# PRACTICAL INFORMATION

## MARCH 10



WORKSHOP ON  
QSAR MODELS  
FOR REACH

Mario Negri Institute, Milan, Italy - March 10-11, 2009

19:30

**Social Dinner**

***Osteria dei Vecchi Sapori - Via Carmagnola 3, Milan***



The restaurant is near to the *Porta Garibaldi Railway Station* and to the stop *Garibaldi FS* of the *subway line 2 (green line)*

It can be reached from the Institute, with trains (*line S10*) starting from *Bovisa* to *Porta Garibaldi* at 19:06, 19:10 and 19:25

To return to Bovisa, there will be trains from *Porta Garibaldi* every 30 minutes (22:09, 22:39, 23:09 until 23:39)



EXITS from the *Porta Garibaldi Station* near to the Restaurant