

**QSAR APPLICATION TOOLBOX  
TRAINING WORKSHOPS  
for OECD MEMBER COUNTRIES and STAKEHOLDERS**

**BARCELONA, SPAIN  
BASIC TRAINING: 3-4 JUNE 2013  
ADVANCED TRAINING\*: 5-6 JUNE 2013  
PRACTICUM SESSION\*: 7 JUNE 2013**

***[\*NOTE: BASIC COURSE IS PREREQUISITE TO REGISTER FOR ADVANCED COURSE. BASIC AND ADVANCED COURSES PREREQUISITE FOR PRACTICUM]***

**BACKGROUND**

The QSAR Application Toolbox was developed under the aegis of OECD to facilitate the use of the category approach and QSAR methods to fill data gaps in classification and labeling. Use of the Toolbox will save resources, reduce the need for animal testing, and greatly accelerate the hazard assessment process.

The Toolbox provides the ability to:

- Make estimates of the relevant endpoints for single chemicals, linked to the CAS number or the chemical structure. Obtain summary information on the validation processes and results of the model so that the user can decide for which regulatory purpose the estimate can be used.
- Obtain a list of analogues for a chemical, together with their experimental, or estimated environmental, toxic or health effects.
- Obtain estimates for metabolite activation/detoxification information for the chemical.
- Interface with IUCLID 5 with ability for automated submission of estimated values for registration purposes

New features of QSAR Toolbox 3.1 include:

- New database for observed rat in vivo metabolism;
- Updated auto oxidation, rat liver metabolism, skin metabolism and microbial metabolism simulators;
- Updated DNA binding profiler;
- Additional ways of expressing mixtures composition (fraction, mass concentration, volume concentration).
- Interface improvement, list of last entered substances, list of last opened files, hint windows, warning messages, etc.
- Improved search functionalities (query search tool) and minor functionality updates.

**WHO SHOULD TAKE THIS OFFICIAL TRAINING?**

QSAR Toolbox training is offered at two levels: Basic and Advanced. The Basic Training Course, which requires some knowledge of chemical structure, provides an overview of the Toolbox databases, modeling system, and use of QSAR methods for managing data and modeling, plus a hands-on introduction to filling data gaps for hazard assessment. The Advanced Training Course, for which the Basic Training Course is a prerequisite, is intended to provide the capability to make advanced hazard assessments for a wide variety of chemicals, along with documentation of the process in a form suitable for submission to regulatory

agencies. Practicum training is offered for those who have completed the Basic and Advanced Training courses and wish to have additional practical work in applying the acquired skills to specific chemicals.

The Training Courses are designed for those charged with developing safety assessments for chemical manufacturers and distributors as well as for those charged with evaluating submitted assessments for new chemicals or those already in use in commerce. Those interested in or conducting research on QSAR tools and database development would also find the training useful.

### **WHO IS CONDUCTING THE TRAINING?**

Instructors are selected from those who were original developers of the Toolbox (please see <http://oasis-lmc.org/>). Limited follow-up assistance will be provided by the instructors, or trainees can subscribe to paid support services. If you would like to see a training session in your area, contact the Toolbox Training Coordinator, Dr. Rosemarie Russo, at [russo@qsari.org](mailto:russo@qsari.org).

### **FEES AND REQUIREMENTS**

Course registration fee for each course is €1815 (includes 21% VAT) for industry trainees and €1210 (includes 21% VAT) for government and university trainees. Registration fee for Practicum is €907.50 (includes 21% VAT) for industry trainees and €605 (includes 21% VAT) for government and university trainees. This includes installation of the OECD Toolbox on each trainee's laptop computer, all course materials, lunches, coffee breaks, and a Course Certificate. Language of the course is English. Trainees must provide their own laptop computers. The Toolbox requires Microsoft Windows 2000, XP or Vista. It needs a PC or laptop with a processor running at 2GHz or faster, 3GB of hard disc space for storage and 1 GB (2GB for Vista) of RAM to operate. NOTE: UK and non-EU trainees should bring their own adaptor for the EU electrical plug. Registrants are responsible for their own transportation and lodging arrangements; it is recommended you purchase refundable airline tickets in the event of course cancellation. Registration is limited and is on a first-come first-served basis. A waiting list will be maintained in event of cancellation(s). Registrants canceling with 30 days or more advance notice will receive a full refund of registration fee; canceling by fewer than 30 days is nonrefundable. Venue for the training sessions is the Barcelona World Trade Center, located on the Mediterranean Sea at the end of the Barcelona Wharf in the historic center of Barcelona. It is 15-20 minutes from the airport and easily reached by city bus and city metro. Address: World Trade Center, Moll de Barcelona s/n, Edificio Sur, 1<sup>st</sup> floor, 08039 Barcelona; telephone 34 93 508 8000, <http://www.wtcbarcelona.com/>.

### **HOW TO REGISTER**

Local arrangements are being made by local coordinator Dr. Gemma Falcó Alay, REACH Monitor SLNE. REACH Monitor is affiliated with the University of Barcelona, with activity in the field of toxicology, specially focused on REACH regulation. To register, please go to <http://reachmonitor.org/index.php?lang=2&aptd=4&id=38> and complete the registration form for the specific course (BASIC and/or ADVANCED and/or PRACTICUM) you are planning to attend. Payment is due upon notification of acceptance of registration form and will be made by funds transfer to REACH Monitor. Credit cards are not accepted. Registration is not complete until payment is received. Government/academic registrants must provide written proof of employer.

### **QUESTIONS?**

Please direct questions to Dr. Rosemarie Russo, Training Coordinator, at [russo@qsari.org](mailto:russo@qsari.org).