

Training School

Risk assessment approaches for water T&O Rome, 16-18/10/2023

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This TS represents an introduction to risk assessment applied to T&O compounds and their degradation products, for those professionals who are not familiar with these procedures; since most T&O compounds and degradation products are generally data-poor compounds, examples of *in silico* approaches such as TTC, read across and QSAR methods will be presented. Training includes theory and practical computer-based exercises on specific case studies. **Trainees are asked to have their own laptop to carry out the exercise** and to **pre-install** the software QSAR Toolbox (v4.6), as a standalone version (installation package 3.2 GB).

QSAR Toolbox is a free application software, downloadable from the QSAR Toolbox homepage ([QSAR Toolbox](#)); registration to the web account is required. For the installation, please consider the minimum system requirements and instructions in the attached Installation Manual.

Trainees will receive a training certificate.

Trainers: Emanuela Testai, Cecilia Bossa, Chiara Laura Battistelli, Simona Scardala, Maura Manganelli, Olga Tcheremenskaia (Dept. of Environment and Health-Istituto Superiore di Sanità- Rome Italy)

Meeting point 9.00 AM just inside ISS, after document control, at the main entrance on Viale Regina Elena 299, Rome

Training school program

Monday 16.10.2023 – Marotta Room

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| 09:00 – 10:00 | Welcome – Introductions |
| 10.00 – 12:00 | Fundamentals of the risk assessment procedure for single chemicals: hazard identification, dose-response relationship, exposure assessment, risk characterization (Trainers: Dr. Emanuela Testai, Dr. Maura Manganelli) |
| 12.00 – 13:00 | Methodologies to apply to data-poor and data-rich chemicals: some case studies (Trainers: Dr. Emanuela Testai, Dr. Simona Scardala) |
| 13.00 – 14:30 | Lunch |
| 14.30 – 16:30 | Practical exercise in working group: case studies to be evaluated by trainees on the basis of information provided by the trainers (Trainers: Dr. Maura Manganelli, Dr. Simona Scardala; Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia) |
| 16.30 – 17:00 | Discussion of exercises |

COST is funded by the EU Framework Programme Horizon 2020

20:00 – 22:00 Social program, TBA

Tuesday 17.10.2023 – Marotta Room

- 9:00 – 10:00 Q&A Case studies of the previous day (Trainers: Dr. Emanuela Testai, Dr. Maura Manganelli, Dr. Simona Scardala Scardala)
- 10.00 – 11.30 Introduction to *in silico* methods: QSAR, read across, TTC, and the related tools (QSAR Toolbox) characterization (Trainers: Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia)
- 11.30 – 13.00 Presentation of tool functioning (Trainers: Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia)
- 13.00 – 14:30 Lunch
- 14.30 – 16:30 Practical exercise on case studies, in working groups with QSAR Toolbox software (Trainers: Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia)
- 16.30 – 17:00 Discussion of exercises

20:00 – 22:00 Social program, TBA

Wednesday 18.10.2023 –Marotta Room

- 9:00 – 10:00 Q&A Case studies results (Trainers: Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia)
- 10.00 – 11:30 Introduction to risk assessment procedure for combined exposure (Trainers: Dr. Emanuela Testai, Dr. Maura Manganelli, Dr. Simona Scardala Scardala)
- 11.30 – 13:00 Introduction to new perspective in Risk Assessment (Trainers: Dr. Chiara Battistelli, Dr. Cecilia Bossa, Dr. Olga Tcheremenskaia)
- 13.00 – 14:30 Lunch
- 14.30 – 16:30 Questions by the trainees and discussion
- 16.30 – 17:00 Closing remarks