

With the contribution of the LIFE Programme of the European Union



LIFE15 ENV/ES/416 COMBASE

COMputational tool for the assessment and substitution of Biocidal Active substances of Ecotoxicological concern

THIRD INTERNATIONAL WORKSHOP OF THE LIFE-COMBASE PROJECT

Use of computational tools for prediction of toxicity of biocides and its degradation products for the aquatic environment and substitute's proposal

24th September 2019

Salón de Actos, Ministerio para la Transición Ecológica – Plaza San Juan de la Cruz s/n; 28003 Madrid

Organizers

María Luisa Fernández-Cruz. Researcher. Instituto Nacional de Investigación y Tecnología Agraria y Alimentaria (INIA), Madrid, Spain

María Blázquez. LIFE-COMBASE Project coordinator. INKOA Sistemas S.L., Bilbao, Spain

PROGRAMME

8:30-9:00 Registration

9:00 Opening

9:15 LIFE-COMBASE project, objectives and outputs

María Blázquez. INKOA Sistemas S.L., Bilbao, Spain

9:30 Regulatory background and needs of extrapolation for industrial chemicals and biocidal products

Simón Gutierrez Alonso. European Chemicals Agency (ECHA), Helsinki, Finland

9:50 Human risk assessment of biocides and metabolites. Use of predictive models

María Luisa González Márquez. Ministerio de Sanidad, Consumo y Bienestar Social, Madrid, Spain

10:05 Environmental risk assessment of Biocides. Application of BPR Regulation

Inmaculada Izquierdo Moya. Ministerio para la Transición Ecológica, Madrid, Spain

10:20 Use of computational toxicology in regulation around the world

Emilio Benfenati. Istituto di Recherche Farmacologiche Mario Negri (IRFMN), Milan, Italy

10:30 Acute fish toxicity testing and 3Rs approaches

Marlies Halder. Joint Research Centre (JRC), Ispra, Italy

11:00-11:30 Coffee break



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11:30 The use of in silico models: lights and shadows, problems and opportunities

Emilio Benfenati. Istituto di Recherche Farmacologiche Mario Negri (IRFMN), Milan, Italy

11:45 Computer aided design for the discovery of new chemicals. Uses in the design of biocidal active substances

Rafael Gozalbes. ProtoQSAR SL, Valencia, Spain

12:05 Predictive models developed in the frame of the LIFE-COMBASE for acute toxicity for algae and microorganisms

Sergi Gómez. ProtoQSAR SL, Valencia, Spain

12:25 Predictive models developed in the frame of the LIFE-COMBASE for *Daphnia* and fish

Emilio Benfenati. Istituto di Recherche Farmacologiche Mario Negri (IRFMN), Milan, Italy

12:45 Comparison of in vitro/in vivo/in silico fish acute toxicity studies

María Luisa Fernández-Cruz. Instituto Nacional de Investigación y Tecnología Agraria y Alimentaria (INIA), Madrid, Spain

13:00 Ecotoxicological impacts of biocidal active substances and environmentally relevant metabolites in *Daphnia*, algae and microorganisms

Oscar Andreu-Sánchez. Xenobiotics SL, Valencia, Spain

13:10 Introduction to mobile APP for the sustainable use of biocidal products

Carlos Fito. Instituto Tecnológico del Embalaje, Transporte y Logística (ITENE), Valencia, Spain

13:20 Break

13:30 Introduction to LIFE-COMBASE Decision Support System: data base of ecotoxicological impacts corresponding to biocidal active substances and metabolites and predictive information for metabolites and ecotoxicological effects on fish, *Daphnia*, algae and microorganisms

María Blázquez. INKOA Sistemas S.L., Bilbao, Spain

14:00 Discussion

14:45 Workshop closure



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The access to the event is free. The programme can be downloaded from the link:

<https://drive.google.com/file/d/1Go-nsczB2JgPrnUGBZQGibopgTMSIDiT/view?usp=sharing>

Registration:

To participate in the event it is necessary to register in the following link:

<https://forms.gle/oZMr2N9yXBExBLj16>

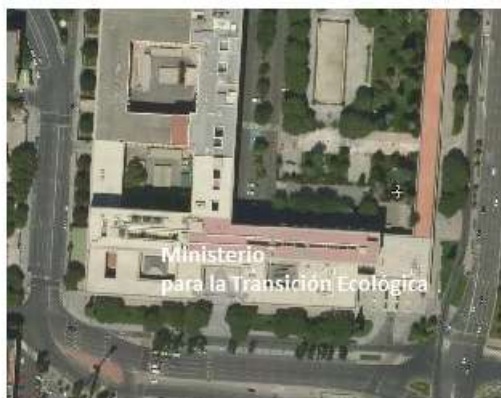
Registrations are on a first-come, first-served basis, so an early registration, ideally before the 31st August 2019, is recommended.

Venue:

Salón de Actos, Ministerio Para la Transición Ecológica

Plaza de San Juan de la Cruz, s/n

28071 Madrid



How to get

- Metro: Nuevos Ministerios (lines 6, 8 and 10)
- Train Renfe Cercanías: Nuevos Ministerios
- Buses: 7, 14, 27, 40, 147 and 150

If you need additional information, please, send an email to life.combase@gmail.com

Media partners:

