

# Collection and Screening of QSAR Models for REACH



Chiara Milan, Emilio Benfenati, Alessandra Roncaglioni, Rodolfo Gonella Diaza,  
Antonio Cassano, Anna Lombardo, Azadi Golbamaki Bakhtyari  
Istituto di Ricerche Farmacologiche Mario Negri, Laboratory of Environmental Chemistry and Toxicology  
Via Giuseppe La Masa 19, 20156 Milan, ITALY



## Introduction and Main Objectives

**ANTARES** is an EC funded project, within the **LIFE+ programme**.

➔ It is dedicated to evaluate *the possible use of non-testing methods for REACH, checking models*.

➔ The web site of the project is: <http://www.antes-life.eu>

➔ These are the MAIN OBJECTIVES addressed here:

- **To LIST IMPLEMENTED QSAR MODELS FOR REACH**, considering models (commercial and free tools) which can be directly used by stakeholders;
- **To CHECK PERFORMANCE OF SOME OF THE MOST PROMISING MODELS**, using large sets of compounds.

## Results

ANTARES listed hundreds of models, both commercial and free, covering several endpoints relevant for REACH.

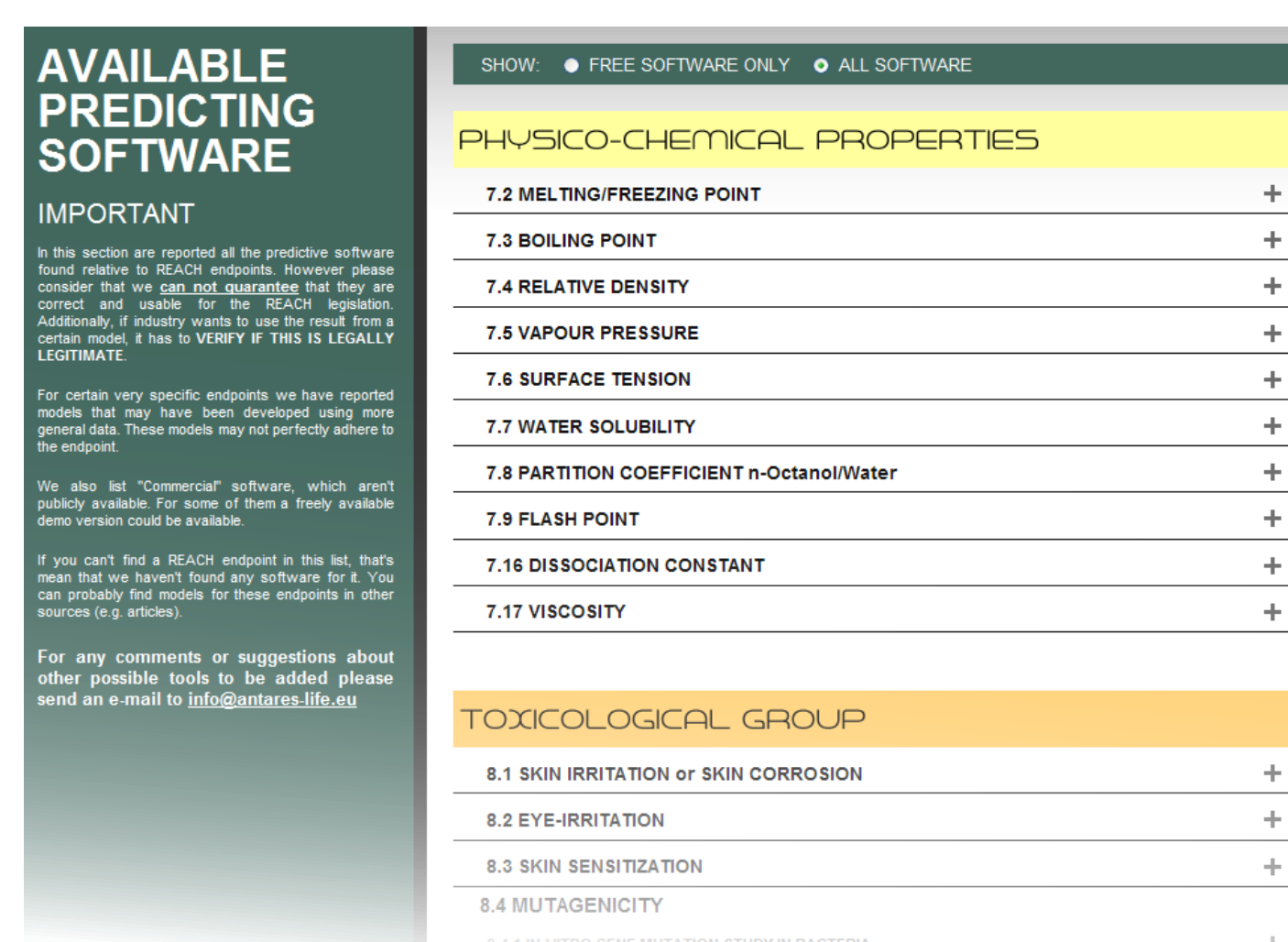
Models evaluated for REACH

38 endpoints covered

More than 250 software available

More than 70 are free

The full list of the QSAR models is available at the ANTARES website:

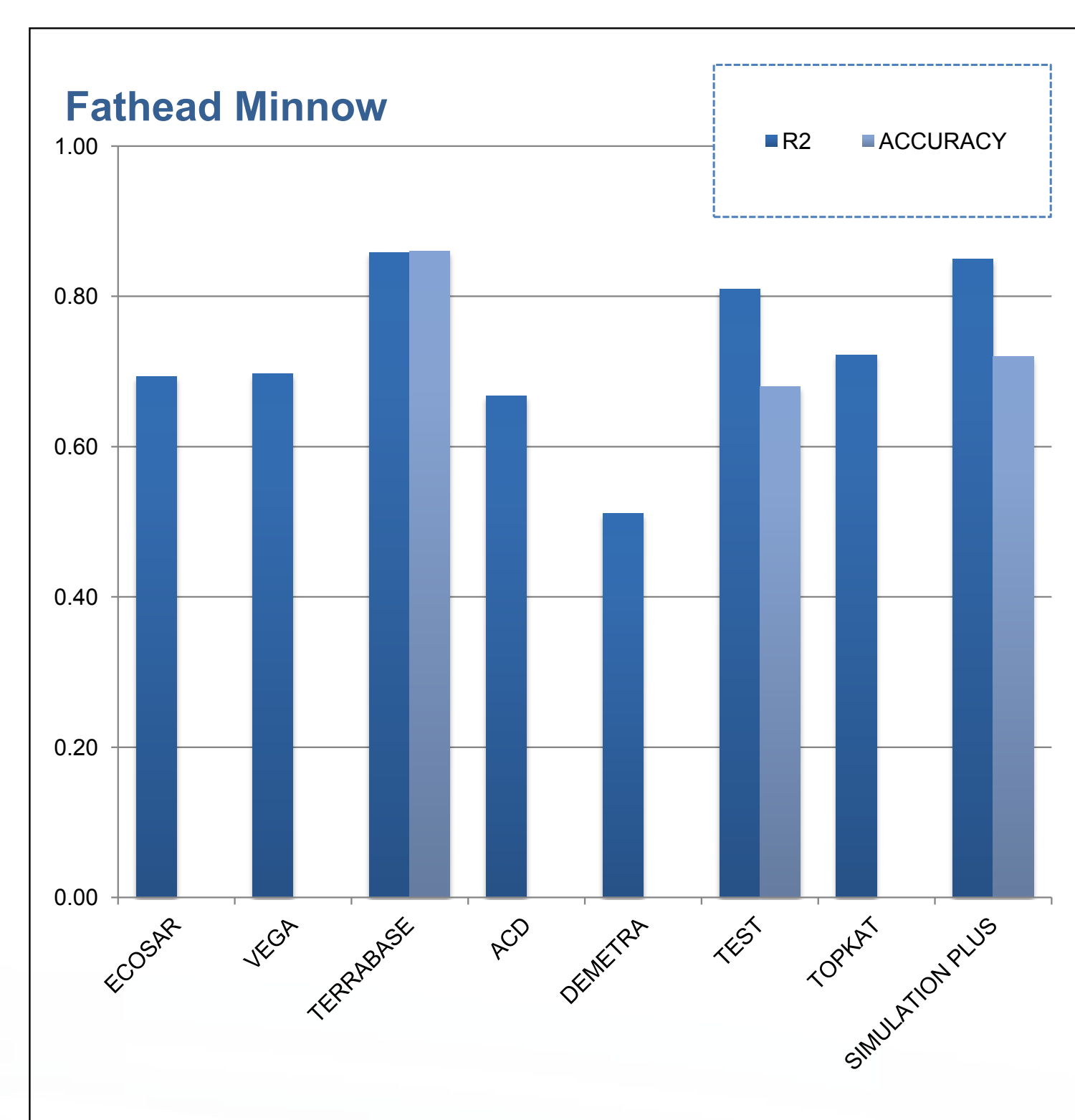
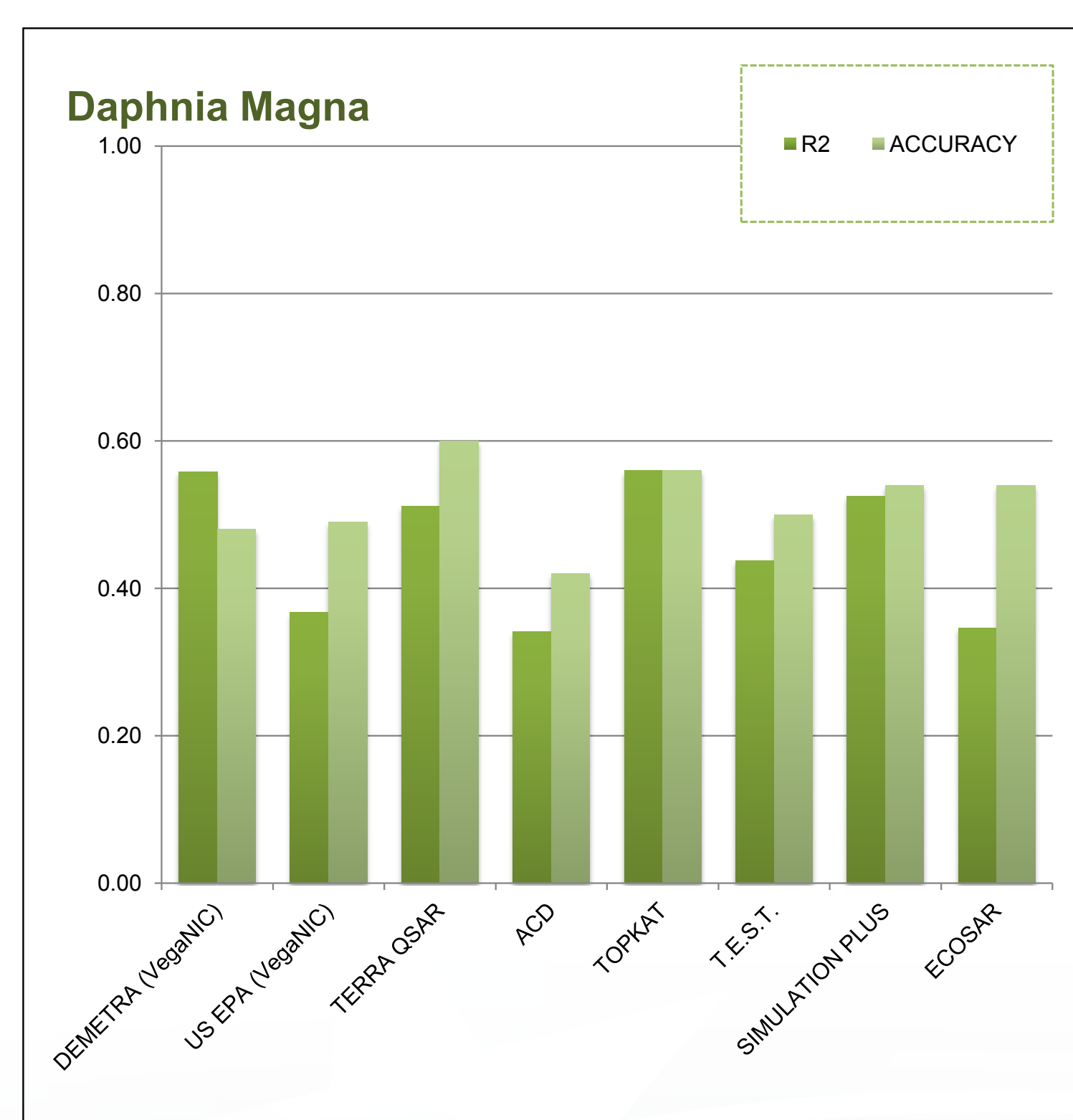
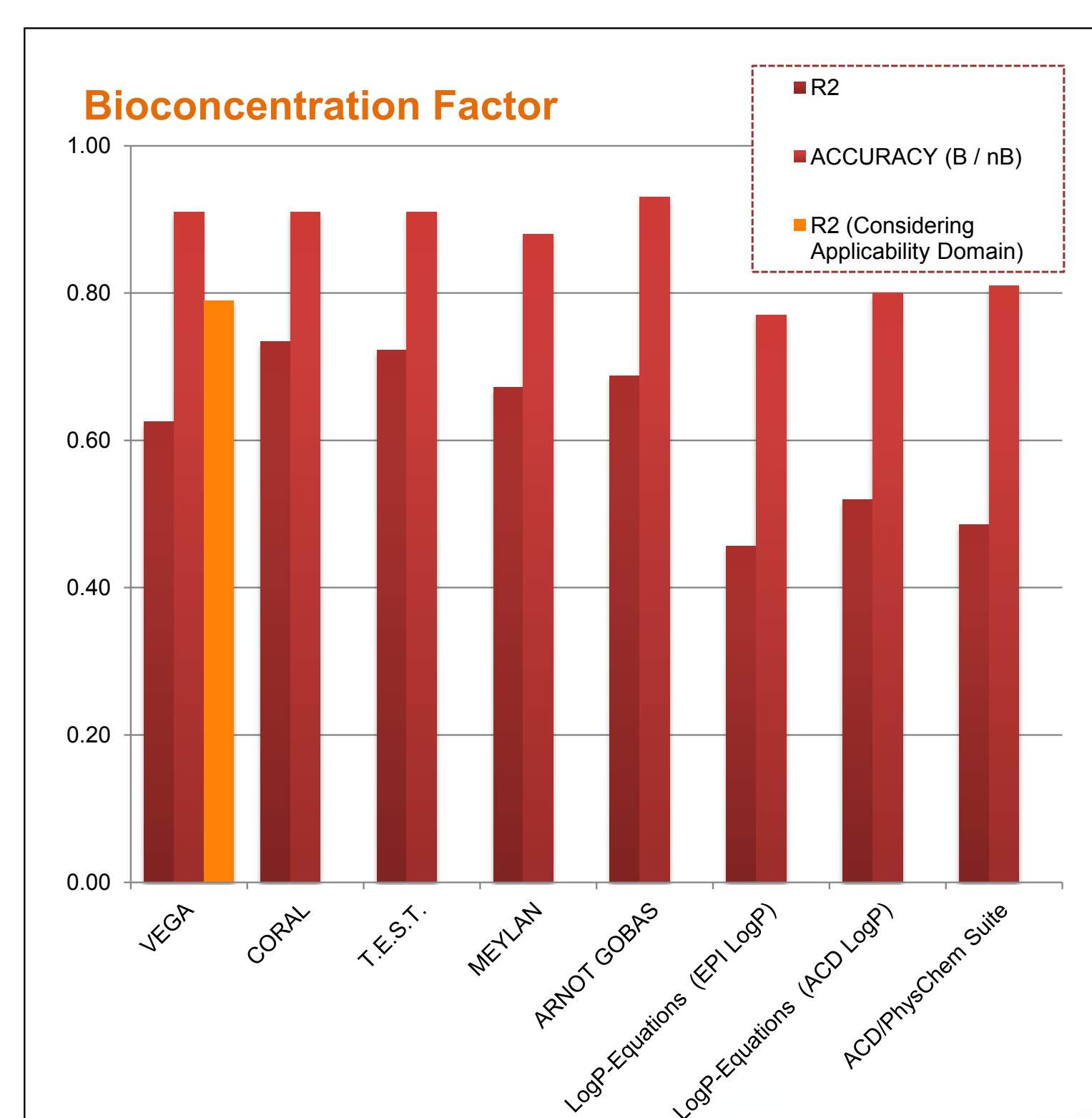


<http://www.antes-life.eu/software.php>

50 MODELS SELECTED because most PROMISING on the basis of their PERFORMANCES, covering 8 endpoints:

PHYSICO-CHEMICAL	Water solubility
ENVIRONMENTAL	Bioconcentration factor Ready biodegradability
ECOTOXICOLOGICAL	Short-term toxicity testing on invertebrates/Daphnia & fish
TOXICOLOGICAL	Carcinogenicity study In-Vitro gene mutation study in bacteria Acute toxicity by oral route

## BELOW WE FOCUS ON SOME OF THE RESULTS FOR THE ECOTOX AND ENVIRONMENTAL ENDPOINTS



## Conclusions

It appears that for some endpoints there are good models (BCF, mutagenicity, persistence), while for others (carcinogenicity and daphnia) more efforts are necessary. The results get worst on the test set, but improve when it is possible to keep into account the applicability domain.