**Objective**
The main objective of the MEMOBIOL project (2009 – 2013) is to evaluate different predictive tools for calculating the thermodynamic phase equilibria and the properties required by the chemical industry for the design of new chemicals and processes involved in the conversion of the lignocellulosic raw material.

**Main Deliverables**
- STI delivers (reports, publications, conferences)
  - Evaluation of existing predictive thermodynamic models
  - Development of new models
- Databases
  - Inventory of available experimental data for high-value oxygenated molecules and their mixtures
  - New experimental data for high-value oxygenated compounds
  - New molecular parameters / descriptions for existing models
- Software
  - New release of Simulis® Thermodynamics providing the new PPC-SAFT EOS
  - New release of Medea-Gibbs® with new functionalities

**Technical Scope**
- Experimental measurements
  - COSMO: Conduct-like Molecular Model
  - SAFT EOS: (Statistical Associating Fluid Theory)
- Process simulation software
  - COSMO: Simulation software
  - SAFT EOS: (Statistical Associating Fluid Theory)

**Molecules**
A thorough evaluation and comparison of COSMO-SAC and COSMO-RR approaches in the context of multifunctional oxygen-bearing molecules
- An extension of the AUA4 force field to furans and organic acids
- A thorough evaluation of the AUA4 force field to reproduce VLE/EEL of oxygenated molecules via Monte Carlo Molecular Simulation and a comparison with other force fields
- Good prediction of hydrogen solubility in oxygen-bearing solvents using Monte Carlo Molecular Simulation
- Recommendations on the most convenient frequencies for the different Monte Carlo moves
- An evaluation of the use of the group contribution PPC-SAFT equation to reproduce VLE/EEL of oxygenated molecules
- A new version of the associating term in the SAFT theory for acid-like association
- New and original VLE/EEL/SLE experimental data for different binary and ternary systems containing high added-value oxygenated molecules and different solvents

**Organization**
- Project management
- Research
- Development of models & methods
- Computer-based models, methods
- Process simulation software
- Experimental measurements
- Molecules

**Publications**

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