

# The Twelfth International Conference on Properties and Phase Equilibria for Product and Process Design

## PPEPPD 2010



## Book of abstracts



<http://www.ppeppd2010.cn/>

May 16-21, 2010 Suzhou, China

**1-15 Poster****High-Pressure Modeling of Multifunctional Associating Molecules with the CPA EoS**

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Molecules containing different and/or multiple associating groups in their structure are well known in biological systems, as well as are important products in the pharmaceutical, chemical and food industries.

This presentation follows previous works where the study of the low pressure phase equilibria of multifunctional associating molecules in water and organic solvents has been addressed and where the CPA EoS was successfully used with a predictive scheme for the pure component parameters using solely the molecular structure (Ind. Eng. Chem. Res. 47, 2008, 5182-5189 and J. Phys. Chem. B. 113, 2009, 3469-3476).

We will show here how this same scheme can be used for the high pressure phase equilibria of phenolic compounds. The focus will be on the CO<sub>2</sub> phase equilibria, due to its importance for supercritical fluid extraction.

**Keywords:** High Pressure, Phenolics, Associating Compounds, CPA EoS.