ParaSurf´10 Release Notes

Release date: 1st July 2010

Changes relative to ParaSurf´09™

ParaSurf'10™ has been enhanced relative to its predecessor in order to provide improved flexibility and a more comprehensive range of descriptors and features. The changes are outlined below:

1. Local electron affinity for AM1* and other Hamiltonians with d-orbitals as polarisation functions

Calculating the local electron affinity with AM1* led to spurious results with ParaSurf'09™ because the d-polarisation functions dominated the summation. A new technique [1] has been introduced to fix this problem in ParaSurf'10™. A new command-line option requests that the local electron affinity be calculated exactly as in ParaSurf'09™ to ensure continuity.

2. The PM6 Hamiltonian

ParaSurf'10™ can be used with PM6. [2] This was also the case with paraSurf'09 if the post-release Vhamil.par file were used. PM6 is available for 70 elements.

3. Second generation surface-integral models; local hydrophobicity

The binned surface descriptors for local hydrophobicity and the logPOW models associated with them are now available in ParaSurf'10™. [3, 4] The descriptors can be written to a comma-separated table for model generation.

4. Molecular fragments

ParaSurf'10™ can now divide molecules up into predefined fragments and output their surfaces and the descriptors derived from them.

5. Atom-centered descriptors

Since ParaSurf'09™ release B1, ParaSurf™ has been able to calculate and output a new series of descriptors that relate to the properties of single atoms. These properties have proven to be useful in models of H-bonding and chemical reactivity. [5, 6]

1 T. Clark, *The Local Electron Affinity for Non-Minimal Basis Sets*, *J. Mol. Model.*, **2010**, *16*, 1231-1238.

2 J. J. P. Stewart, *J. Mol. Model.*, **2007**, *13*, 1173-1213.

3 C. Kramer, B. Beck and T. Clark, *A* Surface-*Integral Model for logP*OW, *J. Chem. Inf. Model.*, **2010**, *50*, 429-436.

4 C. Kramer, T. Heinisch, T. Fligge, B. Beck, and T. Clark, *A Consistent Kinetic Solubility Dataset for Earlyphase Drug Discovery*, *ChemMedChem*, **2009**, *4*, 1529-1536.

5 M. Hennemann and T. Clark, *A QSPR-Approach to the Estimation of the pKHB of Six-Membered Nitrogen-Heterocycles using Quantum Mechanically Derived Descriptors*, *J. Mol. Model.* **2002**, *8*, 95-101.

6 M. Hennemann, A. Friedl, M. Lobell, J. Keldenich, A. Hillisch, T. Clark and A. H. Göller, *CypScore: Quantitative Prediction of Reactivity toward Cytochromes P450 Based on Semiempirical Molecular Orbital Theory*, *ChemMedChem*, **2009**, *4*, 657-669.

