CAChe Research
Computer-Aided Chemistry & Biochemistry

Chemical and physical property prediction from electronic properties of molecular surfaces

- **Cytochrome P450 drug metabolism prediction***
- **Ligand docking - improved accuracy****
- **3D QSAR & QSPR - novel electronic descriptors**
- **Chemical & physical property prediction…**

ParaSurf™ uses semiempirical methods to calculate electronic properties on the surface of molecules for use in QSPR, 3D-QSAR, ligand docking and reactivity prediction, such as Cytochrome P-450 drug metabolism.

ParaSurf™ is the basis module that uses output from a semiempirical molecular orbital program such as Cepos Mopac 6 or VAMP to construct molecular surfaces and calculate local properties and descriptors. Surfaces may be generated by shrink-wrap or marching-cube algorithms and the former may be fit to a spherical harmonic series. ParaSurf™ from Cepos InSilico was originally introduced in 2005.

ParaSurf™ can also generate local enthalpies and free energies of solvation and integrate them over the entire molecular surface. The application has the ability to read Surface-Integral Model (SIM) files that allow it to calculate properties such as the enthalpy and free energy of hydration plus the free energies of solvation in n-octanol and chloroform.

References:

*CypScore: Quantitative Prediction of Reactivity toward Cytochromes P450 Based on Semiempirical Molecular Orbital Theory, M. Hennemann *et al, ChemMedChem* **2009**, *4*, 657 – 669

*Search: http://scholar.google.com, keyword: “cypscore”

Discovery of Novel HIV Entry Inhibitors for the CXCR4 Receptor by Prospective Virtual Screening, Violeta I. Pérez-Nueno *et al*, *J. Chem. Inf. Model.* **2009, *49,* 810–823

**Search: http://scholar.google.com, keywords: “ParaSurf AND docking”

ParaFit™ from Cepos InSilico performs automatic 3-D superimpostion and similarity comparison of molecules and their electronic surface properties calculated by ParaSurf™.

ParaFit™ superimposes and compares molecules using the spherical harmonic (SH) expansions of the molecular surface and local surface properties calculated by ParaSurf™. By the special rotational properties of the spherical harmonic basis functions, computation times can be reduced by several orders of magnitude compared to conventional shape matching algorithms. Hence, the ParaFit™ module is an essential component of the ParaSurf™ suite for virtual high throughput screening studies where very large numbers of compounds need to be assessed.

ParaFit™ provides three main calculation modes. In the default "fitting" mode, ParaFit™ superimposes one or more "moving" molecules onto a single "fixed" reference molecule. The program can also perform

all-versus-all superimpositions in which each molecule is superimposed in turn onto all others. In this "matrix" mode, a table of distance scores can be written out in a format suitable for subsequent clustering analysis. In addition to superposing molecules, ParaFit™ may also be used to align molecules to the coordinate axes in order to place them in a standard or "canonical" orientation. This is often a useful first step in QSAR studies.

ParaFit™ can also apply arbitrary coordinate transformations to a given list of ParaSurf™, VAMP, or Mopac SDF files. These transformations could be supplied as part of a processing pipeline by other superposition programs that do not have the capability to rotate complex quantum mechanical (QM) properties such as quadrupole and octupole moments and atomic orbital charge density matrix elements. ParaFit™'s ability to rotate all of the orientation-dependent QM information in an SDF file eliminates the need to recalculate expensive QM quantities for new molecular orientations.

Cepos InSilico was created to make the science developed in the Parashift Project readily available and to support further research and development. (The Parashift Project was born at the 2002 EuroQSAR conference at Bournemouth in the UK, as a concerted attempt to break out of the mould of conventional atomistic modelling techniques with methods based on local molecular surface properties.) As a result, Cepos InSilico's surface-based modelling techniques provide in silico screening, modelling and simulation software designed to give accurate, generally applicable predictions of biological activity, reactivity, ecological impact, ADME and physical properties.

Researchers from the universities of Erlangen in Germany, Portsmouth in the UK and LORIA (Nancy, France) work together developing products marketed by Cepos InSilico Limited. The areas of expertise of the three research groups range from classical simulation and quantum mechanical techniques to analytical representations of irregular bodies and interpolation techniques for QSAR and QSPR. This expertise provides the uniquely powerful scientific background behind today's Cepos Insilico's technology.

Sales Information

CAChe Research is the authorized distributor for Cepos InSilico products in the Americas. For further information or price quotations please email CEPOS@CACheResearch.com

Annual lease price $USD per floating license token
Cepos products are available for annual lease for Windows and Linux, in both 32-bit and 64-bit versions. Only commercial and Government licenses include full support and updates. Cepos applications such as ParaSurf™ use a token licensing system. One application per token may run at any one time. CeposLM™ is installed on a central license server that must be available to all licensed users (this may be your PC hardrive if you have only a single-user license). ParaSurf™ pricing is as shown below, ParaFit™ pricing is 50% of prices shown, MOPAC6 is free.

ParaSurf™ annual lease pricing USD, (ParaFit™ is 50% of prices shown)

No. of Tokens	Commercial	Government	Academic
1	$16,000	$8,000	$1,600
2	$24,000	$12,000	$2,400
4	$32,000	$16,000	$3,200
8	$40,000	$20,000	$4,000

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