Solvation Free Energy Prediction Model Across Different Surfaces

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WSAS is a model that focuses on predicting Solvation free energy using Weighted Solvent Accessible Surface area (SASA)[1]. In this model, the surface elements of the molecule are assigned to an atom type depending on the closest atom. The atom type surfaces are then multiplied by a factor unique to each atom type. The sum of the resulting values is the solvation energy. The training of this model revolves around finding the optimal atom types and factors.

To form a more robust dataset we added to the original Kollman dataset, molecules from two other publicly available databases (MNSOL[2] & FREESOLV0.51[3]) resulting in a dataset with 826 molecules. We applied this model to several surface types which included Iso-density surfaces [4], Hirshfeld surfaces [5], and the SASA [6]. The best model remained the SASA with RMSE of 1.42 kcal/mol and a Pearson Correlation of 0.9169. Surfaces and energy values are computed in software MoproViewer[7]. Figure 1 represents the scatter plot of the experimental values and the predicted values of our best fitted surfaces (SASA & Hirshfeld)..

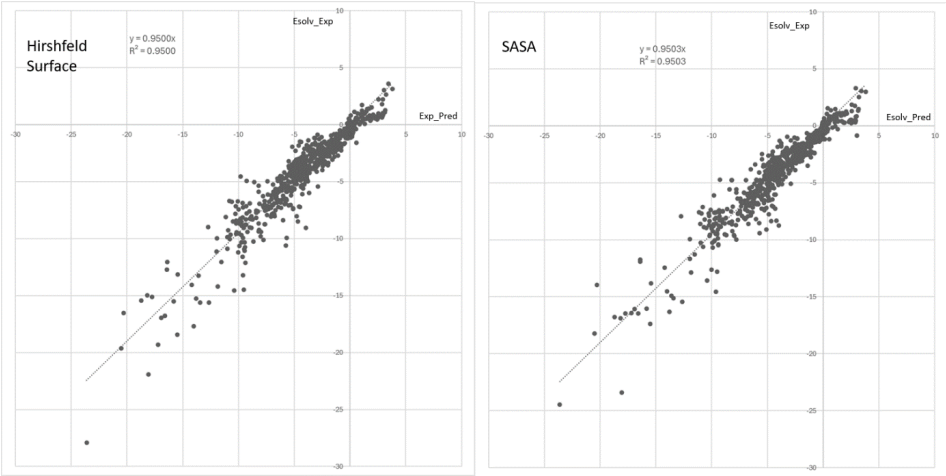

Figure 1 – Experimental vs Predicted values of the Model using the SASA and Hirshfeld surfaces.

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