



CALIFORNIA STATE SCIENCE FAIR  
2006 PROJECT SUMMARY

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<b>Project Title</b> <b>A New Quantum Mechanical Approach in Determining the Octanol Water Partition Coefficients of Organic Aromatic Compounds</b>	
<b>Abstract</b> <b>Objectives/Goals</b> The octanol-water partition coefficient ( $K_{ow}$ ) measures a solute's distribution between competing organic and aqueous phases, determining its environmental fate and safety. Current experimental methods to determine $K_{ow}$ are subject to human error and require many resources. How can quantum computational modeling be used to determine the $K_{ow}$ of organic aromatic compounds? The objective is to develop a new efficient and practical method to predict $K_{ow}$ . <b>Methods/Materials</b> The calculations were run with the Gaussian 98 program. The project considers two organic families, chlorophenol and chlorobenzene. Four probe molecules simulate the aqueous and organic phase. A water molecule represents immersion in water. Argon, neon, and benzene represent the organic phase because octanol itself is too large and inefficient. First, I optimized the geometry and vibrational frequencies of all molecules. Second, I added a probe molecule above the center of the ring. Next, I calculated the zero-point energy of the complex using the counterpoise method. Finally, I plotted the various energy parameters versus experimental $\log K_{ow}$ and assessed the strength of linear correlation. The procedures are repeated for different probe molecules, probe distances, and molecular geometries. <b>Results</b> There is a moderately strong linear correlation between $\log K_{ow}$ and Electron Correlation energy, or pure dispersion forces, of the octanol probe-solute complex ( $r^2=0.95$ ). Stronger correlations were found between $\log K_{ow}$ and the Hartree-Fock energy, or pure dipole-dipole interactions of the water-solute complex ( $r^2=0.98$ ). Finally, the strongest linear correlations were found when plotting $\log K_{ow}$ with the difference of the dispersion and electrostatic contributions ( $r^2=0.99$ ). The strengths of the linear correlations are statistically acceptable for the extrapolation of $\log K_{ow}$ of similar compounds. <b>Conclusions/Discussion</b> The results confirm that $K_{ow}$ can be derived from computational methods. Also, the $\log K_{ow}$ of four chlorophenol congeners were predicted from the linear correlations. Because the water probe correlations are strong enough, dipole-dipole interactions can be used solely to predict $K_{ow}$ . Overall, the project successfully validated a new method to determine $K_{ow}$ , which can be applied to other organic compounds with limited experimental data. The computational approach saves many resources and diminishes the chance of human error.	
<b>Summary Statement</b> A new computational method is developed to accurately predict the octanol-water partition coefficient ( $K_{ow}$ ) of organic pollutants, and is subsequently used to predict the $K_{ow}$ of 4 chlorophenol congeners with uncertain experimental data.	
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