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Measured Octanol/Water Distribution Coefficients and Abraham Summation Hydrogen Bonding Acidities for the Catechol-Flavones[1]
TARYN GIBBS, DR. LANCE WHALEY, Tarleton State University — Flavonoids are a class of diverse organic molecules present broadly in plants. They are claimed to have a wide range of bioactive effects including anti-cancer, anti-inflammatory, anti-aging, and anti-neurodegenerative properties. Information is sparce, however, on correlations between chemical structure and biological absorption. One sub-group of flavonoids is characterized by containing one or more *ortho* hydroxyl pairs called catechol groups. These catechol flavonoids are of special interest as the presence of the catechol groups changes the physical properties of these compounds in terms of their intermolecular interactions. In this study, a set of catechol flavones, a simple sub-group of flavonoids, were examined for their octanol/water partition coefficients (LogP_{oct}) at various standard pH values within the human digestive system to predict their possible mode and extent of absorption in the body. Using NMR techniques, Abraham summation, and methods of chemical approximation, the hydrogen bonding acidities were also calculated for the catechol-flavones to further assess and confirm their permissibility through the body. Through further research and development, these naturally produced compounds could prove to be viable medical treatments for many neurodegenerative and cancerous diseases.

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