Partition coefficient of ions (Na^+, K^+, Mg^{++}, Ca^{++}, Cl^-) in solid/liquid system

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Thermodynamic equilibrium (partition) of the migration process can be defined as an exchange of mass and energy between two systems. Several studies reported partition coefficient values for migrants in food system and involved finding factors that affected the partitioning behavior. Additional data are needed on the food ingredients, solvent chemical structures and properties as related to partitioning behavior.
Objective of this work is to determine the partition coefficient of ions (Na^+, K^+, Ca^{++}, Mg^{++}, Cl^-) in solid/liquid system. We studied the relationship between structure and properties of molecule and main type of molecular descriptors used in quantitative structure-property relationship (QSPR). The main objectives of this study are to better understand which parameters influence the partition coefficient and to identify the main existing methods to evaluate and predict partition coefficient. Four types of salt in osmotic solution (NaCl, KCl, $CaCl_2$ $6H_2O$, $MgCl_2$ $6H_2O$) with one salt concentration level (200g/L) are used. The ratio of sample (eggplant)/salt solution is 1:2; the thickness of sample is 20mm. Equilibrium time between eggplant and solution at 5°C is after 15 days. Partition coefficient of each ion is calculated by analyzing the ion concentration in both phases.The molecular descriptors for each system were obtained from database of the Molecular Modelling Pro version 5, 2002 (ChemSW Software Inc.). We demonstrated that the molecular descriptors drived from the constitutional and quantum chemically calculated have wide applicability for determination of partition coefficient. Factors that affected partition coefficient including polarity, ionic strength, water activity of solution, total energy and significant functional groups of ions, food and solution. We validated these results with Molecular Dynamics (MD) simulation. Molecular Dynamics determine the chemical bonds, bond angles, and bond dihedrals, and non-bonded forces associated with van der Waals forces and electrostatic charge.