Title: Solubilities prediction of ginger bioactive compounds in liquid phase of water by the COSMO-RS method

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Abstract: The solubilities in water of four main ginger bioactive compounds, 6-gingerol, 6-shogaol, 8-gingerol and 10-gingerol, were predicted using a conductorlike screening model for real solvent (COSMO-RS) calculations. This study was conducted since no experimental data are available for ginger bioactive compounds solubilities in liquid phase of water. The s-profiles of these selected molecules were calculated using Gaussian software and the solubilities were calculated using the COSMO-RS method. The solubilities of these ginger bioactive compounds were calculated at 50–200 °C. In order to validate the accuracy of the COSMO-RS method, the solubilities of five hydrocarbon molecules were calculated using the COSMO-RS method and compared with the experimental data in the literature. The selected hydrocarbon molecules were 3-pentanone, 1-hexanol, benzene, 3-methylphenol and 2-hydroxy-5-methylbenzaldehyde. The calculated results of the hydrocarbon molecules are in good agreement with the data in the literature. These results confirm that the solubilities of ginger bioactive compounds can be predicted using the COSMORS method. The solubilities of the ginger bioactive compounds are lower than 1.0 × 10-4 at temperatures lower than 130 °C. At 130–200 °C, the solubilities increase dramatically with the highest being 6-shogaol, which is 3.7 × 10-4 mole fraction, and the lowest is 10-gingerol, which is 0.39 × 10-4 mole fraction at 200 °C.