Modelization of the supercritical carbon dioxide solubility of carotenoids and chlorophyll using Hansen theory

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Spinach (*Spinacia oleracea*), is a green leafy vegetable and is highly concentrated in phytochemicals. Phytochemicals are mainly lutein and chlorophyll, known to act as health benefit molecules according to their anti-oxidant, anti-inflammatory, and anti-genotoxic properties. Typically, petrochemical solvents which are non-renewable and often toxic are used to extract phytochemicals from spinach. However, in the present work, we explored the possibility of using supercritical carbon dioxide as a green solvent for extraction of phytochemicals. Optimizing a supercritical extraction process requires many experimental runs due to the numerous system parameters. Therefore, a simpler tool to obtain the optimum extraction conditions is essential. Hansen solubility parameters predict the solubility of natural bioactive compounds in different solvents or solvent combinations. Therefore, by applying the Hansen solubility theory we developed a predictive tool to ascertain and optimize solutes solubility's, with the example of lutein and chlorophyll, in supercritical carbon dioxide (SC-CO_2). The solubility distance (Ra) between the Hansen solubility parameters of SC-CO_2 at different pressures and the solutes were calculated and compared with experimental results from previous works. The developed tool predicted that the extraction yield of lutein with SC-CO_2 increases by rising pressure up to 500 bars. Furthermore, it is concluded that SC-CO_2 solely is not an efficient solvent for lutein and chlorophyll extraction and therefore, applying a modifier is suggested. Experimental results validated the results obtained by predictive tool and showed that the pressure and adding ethanol as modifier has a positive effect on lutein extraction yield. The predictive approach is then an efficient tool to determine the solubility of solutes in SC-CO_2 and can be used to estimate the optimum conditions for a SC-CO_2 extraction.