超临界 CO_2 中植物油溶解度预测的研究

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摘要：本文选择两种常见的大豆油、菜籽油进行植物油在超临界 CO_2 中溶解度预测研究。方法：首先通过甘油三酯组成细化法得出每种植物油经简化后的甘油三酯组成，然后用我们自己建立的遗传算法（GA）优化的支持向量机（SVM）定量结构-性质关系(QSPR)模型对植物油组成的每种甘油三酯在对应条件下超临界 CO_2 中的溶解度进行了预测计算，以计算得到的各甘油三酯溶解度为初值和其在植物油中组成的摩尔比作为权重，计算菜籽油和大豆油所有组成甘油三酯溶解度的加权平均值作为对应条件下的溶解度并与文献值进行了比较。结果表明：菜籽油溶解度的绝对平均偏差（AARD）为 36.45%，大豆油的 AARD 为 33.41%，小于已有文献中提到的 40%，因此该方法可以用来估计植物油在超临界 CO_2 中的溶解度。

关键词：超临界 CO_2；溶解度；预测；GA-SVM；植物油；组成细化

A Study on Prediction for the Solubility of Vegetable Oils in Supercritical CO_2

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Abstract: A study on prediction for the solubility of vegetable oil in supercritical CO_2 was investigated. Common soybean oil and rapeseed oil were selected as materials. Method: First, the triglyceride composition of each vegetable oil was obtained by triglyceride composition refinement method. Then, the solubility value of each triglyceride of composition for the vegetable oil under corresponding supercritical CO_2 condition was calculated by the quantitative structure-property relationship (QSPR) model of support vector machine (SVM) based on genetic algorithm (GA), which was established by ourselves. With the solubility value of each triglyceride as the initial value, and the molar ratio of this triglyceride in triglyceride composition of this vegetable oil as weights, we calculated the weighted average solubility values as the solubility prediction values both for rapeseed oil and soybean oil according to their triglyceride composition respectively. Those solubility prediction values were compared with the reference values in same condition of supercritical CO_2.

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