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生物化学工程与技术

绿原酸分子修饰产物的制备、表征及量子化学计算

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摘要 绿原酸（CGA）是一种天然酚类抗氧化剂，已应用于医药保健、食品、日用化工等行业中。然而，其易溶于水难溶于油的特性使其应用受到了限制。本研究对CGA进行了分子修饰，即在非水相中，以三乙胺（TEA）为催化剂，对其进行月桂酰氯（LC）酰化，制备了脂溶性的绿原酸月桂酸酯（CGL）。探讨了原料配比、温度及反应时间对CGL收率的影响，得出制备CGL的最佳工艺条件为：以N, N-二甲基甲酰胺（DMF）作为溶解、稀释剂，n CGA：n LC：n TEA＝1：1：1.5，温度控制在35±1 ℃，反应时间8 h。在此条件下，可得到微黄色粉状固体产物绿原酸月桂酸酯，其产率为81.24 %。通过UV-Vis、IR、ESI －MS、1HNMR对CGL的结构进行了表征。同时，在理论上，采用量子化学计算的方法论证了该分子修饰的可行性和合理性。

关键词

分子修饰 绿原酸月桂酸酯 脂溶性 量子化学计算

分类号

Preparation,characterization and quantum chemistry calculation for modified chlorogenic acid

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Abstract

Chlorogenic acid (CGA) is a natural antioxidant, and nowadays it has been used in medicine, food processing and cosmetic industry.However, to a certain extent its application is restricted because it is only soluble in water but is lipo-insoluble.In this research, liposoluble chlorogenic laurate(CGL) was synthesized by acylation with lauroyl chloride (LC) in the presence of triethylamine (TEA) in non-water phase.It was found that the optimized synthesis conditions were as follows: with dimethylformamide (DMF) as the dissolution agent and thinner, n CGA∶n LC∶n TEA＝1∶1∶1.5, temperature(35±1)℃ and reaction time 8 h.Under these conditions a light yellowish powder was obtained and the yield of CGL was 81.24 %.The structure of CGL was characterized by UV-Vis, IR, ESI-MS and H NMR. Theoretically, the method of quantum chemistry calculation was used to demonstrate the feasibility and rationality of molecular modification for CGA.Meanwhile, the result of the test of the use of CGL on Guangdong-type sausage showed that 0.05% of CGL could increase the antioxidant ability of the products.

Key words

molecular modification chlorogenic laurate liposoluble quantum chemistry calculation

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