

以反應曲面法研究酵素合成己醇酯類之最優化

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摘要

具水果芳香之低分子量酯類(LOW MOLECULAR WEIGHT ESTERS; LMWE)為目前食品與化粧品工業上之重要香味原料。己醇酯類(HEXYL ESTERS)主要是由帶"青味"(GREEN NOTES)之C-6醇類衍生而來之短鏈芳香酯類，可廣泛的應用在食品、飲料、化粧品及製藥工業上。傳統之香料來源-直接萃取法，大部分已被低成本之化學合成法所取代，但仍無法符合消費市場對"天然"香料之需求，進而發展出以酵素等生成方式來生產安全性高之天然香料，成為香料工業未來之主要發展趨勢。故本研究主要是選用脂解酵素IM-77催化不同結構之醇類(HEXANOL; CIS-3-HEXEN-1-OL)與醯基供給者(TRIACETIN; TRIBUTYRIN; BUTYRIC ACID)進行酯化反應，合成己醇酯類，並利用反應曲面法(RESPONSE SURFACE METHODOLOGY; RSM)及五階層五變數之中心混層實驗設計法(CENTRAL COMPOSITE ROTATABLE DESIGN; CCD)，分別探討反應時間(2-10 H)、反應溫度(25-65 oC)、莫耳數比(1:1-3:1)、酵素用量(10-50%; 0.02-0.1 BAUN; BATCH ACIDOLYSIS UNIT OF NOVO)及水分添加量(0-20%)等反應參數對莫耳轉換率之影響及求得己醇酯類之最優化合成條件。研究結果顯示，在有機系統下，脂解酵素IM-77可成功地催化己醇酯類之合成。在轉酯化反應方面，丁酸己酯之最優化莫耳轉換率(96%)高於乙酸己酯(88.9%)。順-3-乙酸己烯酯可獲得約82%之最優化莫耳轉換率。而直接酯化反應方面，丁酸己酯之最優化莫耳轉換率為98.2%。

關鍵詞：己醇酯類、反應曲面法、脂解酵素、最優化、等高線圖

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