STUDY ON OPTIMIZATION OF ENZYMATIC SYNTHESIS OF HEXYL ESTERS BY RESPONSE SURFACE METHODOLOGY

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ABSTRACT

LOW MOLECULAR WEIGHT ESTERS (LMWE) REPRESENT AN IMPORTANT CLASS OF FLAVORING MATERIALS, RESPONSIBLE FOR THE FLAVORS OF MANY FOODS AND FRAGRANCES. HEXYL ESTER IS AN EXTREMELY ARO -MATIC COMPOUND WITH GREEN NOTE FLAVOR AND WIDELY USED IN THE FOODS, BEVERAGES, COSMETICS AND PHARMACEUTICAL INDUSTRIES. TRADITIONALLY, IT HAS BEEN ISOLATED FROM NATURAL SOURCES OR PRODUCED BY CHEMICAL SYNTHESIS. HOWEVER,THIS STEADILY GROWING DEMAND HAS LEFT NATURAL COMP -OUNDS IN INCREASINGLY SHORT SUPPLY. THEREFORE, THE BIOSYNTHESIS OF SUCH ESTERS BY LIPASE -CATALYZED CHEMICAL REACTIONS UNDER MILD CONDITIONS HAS BECOME OF MUCH CURRENT COMMERCIAL INTEREST. THE PRESENT WORK FOCUSES ON THE ABILITY FOR IMMOBILIZED LIPASE FROM RHIZOMUCOR MIEHEI(LI -POZYME IM-77) TO CATALYZED THE TRANS- OR DIRECT- ESTERIFICATION OF C-6 ALCOHOL (HEXANOL; CIS-3-HEXEN-1-OL) WITH ACYL DONOR (TRACETIN; TRIBUTYRIN AND BUTYRIC ACID). RESPONSE SURFA -CE METHODOLOGY (RSM) AND FIVE-LEVEL-FIVE-FACTOR CENTRAL COMPOSITE ROTATABLE DESIGN (CCRD) WERE ADOPTED TO EVALUATE THE EFFECTS OF SYNTHESIS VARIABLES, SUCH AS REACTION TIME (2-10 H), TEMPERATURE (25-65 oC), SUBSTRATE MOLAR RATIO (1:1-3:1), ENZYME AMOUNT (10-50%; 0.02- 0.1 BAUN), ADDED WATER CONTENT (0-20%) ON PERCENTAGE MOLAR CONVERSION OF HEXYL ESTERS. THE RESULTS SHOWED THAT HEXYL ESTERS HAVE BEEN SUCCESSFULLY SYNTHESIZED BY LIPOZYME IM- 77 IN N-HEXANE.FOR TRANSESTERIFICATION, THE OPTIMUM MOLAR CONVERSION OF HEXYL BUTYRATE (96%) WAS HIGHER THAN HEXYL ACETATE (88.9%). THE OPTIMUM MOLAR CONVERSION OF CIS-3-HEXENYL ACETATE WAS 80%. FOR DIRECT-ESTERIFICATION, THE OPTIMUM MOLAR CONVERSION OF HEXYL BUTYRATE WAS 98.2%.

Keywords : CONTOUR PLOTS, HEXYL ESTER, LIPASE, OPTIMIZATION, RESPONSE SURFACE METHOD.

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