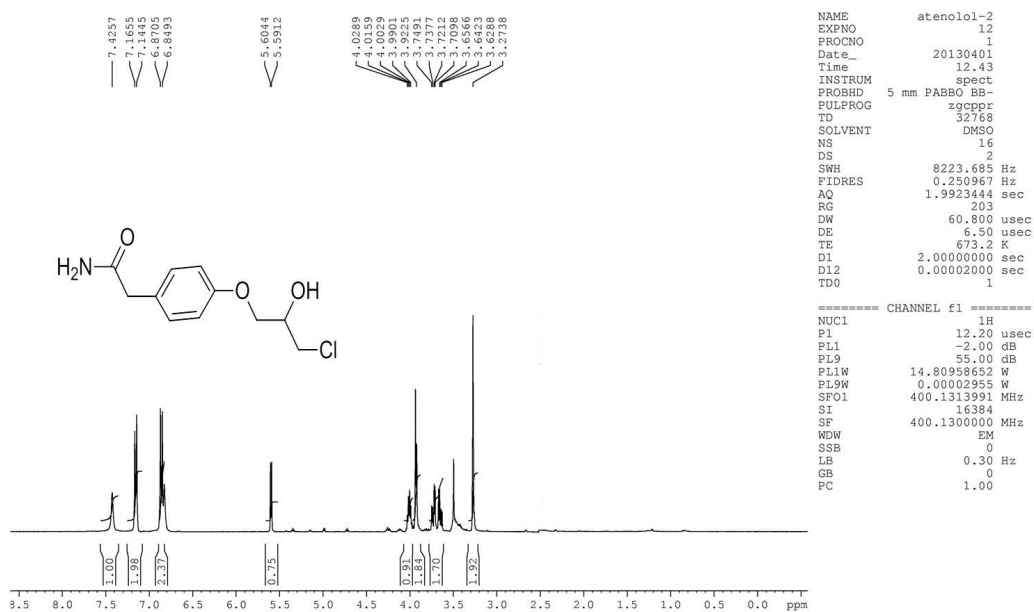


Supporting information

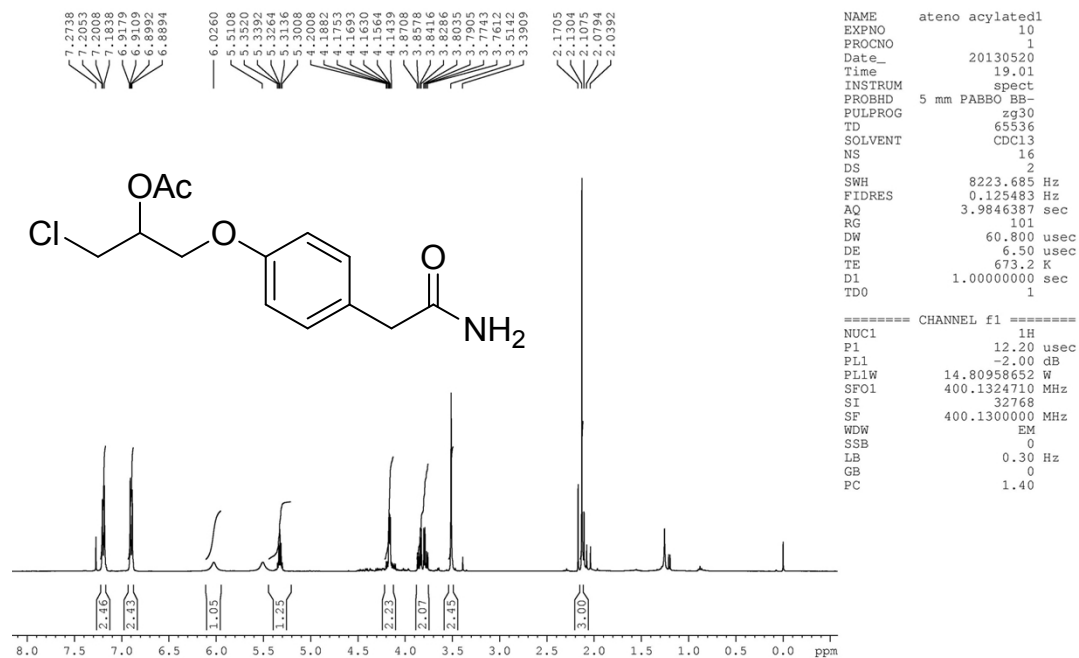
Lipase Catalyzed Green Synthesis of Enantiopure Atenolol

Bharat Prasad Dwivedee, Saptarshi Ghosh, Jayeeta Bhaumik, Linga Banoth
and Uttam Chand Banerjee*

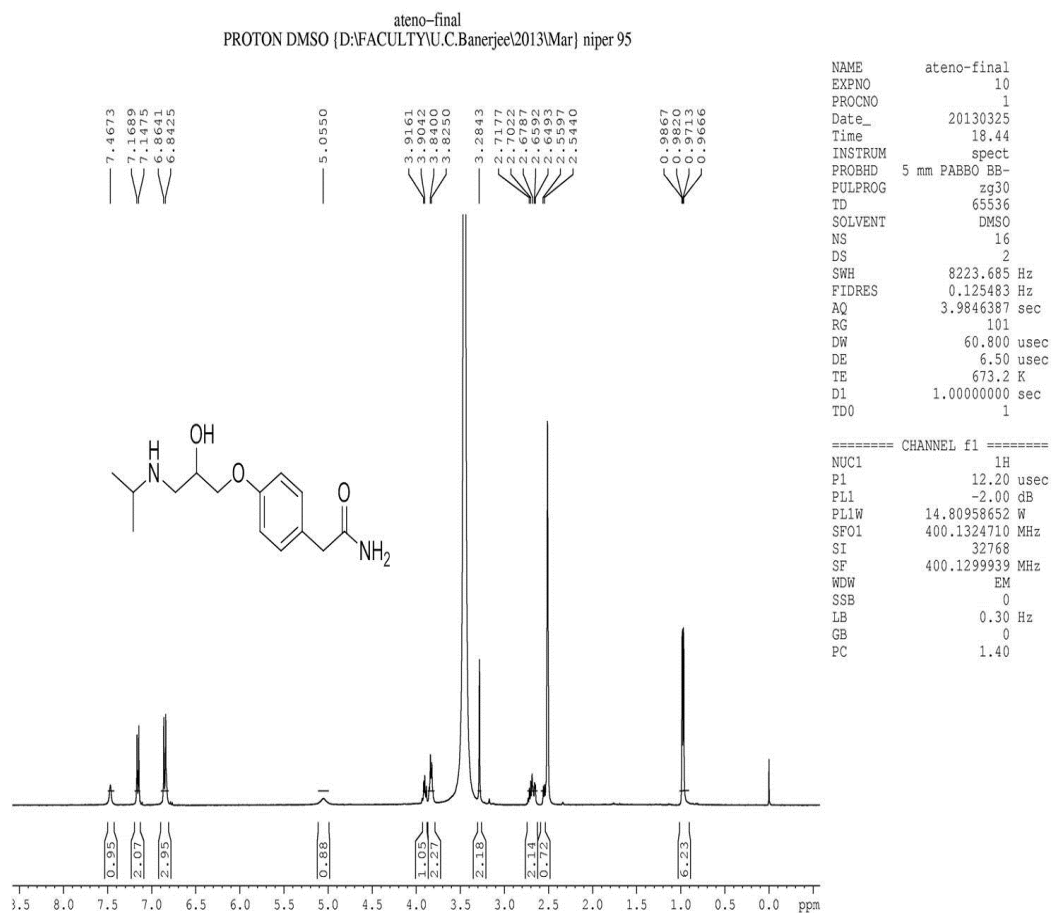
1. ¹H NMR Spectra of (*RS*)-2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide



2. ¹H NMR Spectra of (RS)-1-(4-(2-amino-2-oxoethyl)phenoxy)-3-chloropropan-2-yl acetate



3. ¹H NMR Spectra of atenolol



4. Mass Spectra of (RS)-2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide

Mass Spectrum List Report

Analysis Info

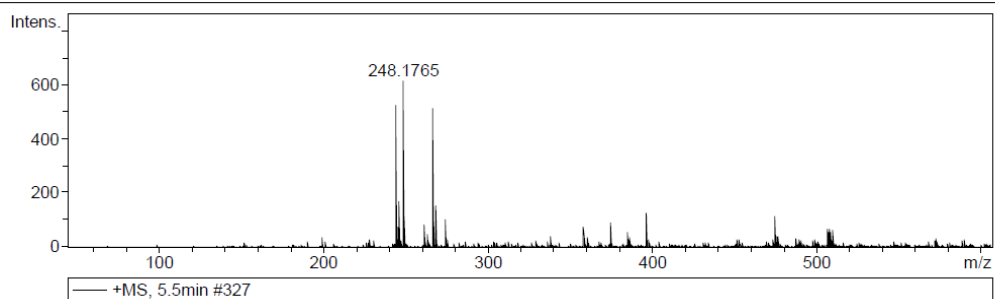
Analysis Name D:\Data\Dr. UCB\at-z_1-A_1_01_743.d
Method HIGH FLOW DIRECT INJECTION LOW MASS.m
Sample Name at-z
Comment

Acquisition Date 7/2/2014 11:10:31 AM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



5. Mass spectra of atenolol

Mass Spectrum List Report

Analysis Info

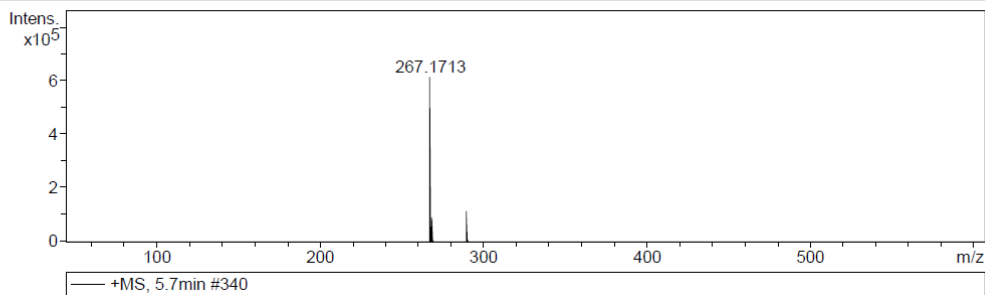
Analysis Name D:\Data\Dr. UCB\at-f_1-A,2_01_744.d
Method HIGH FLOW DIRECT INJECTION LOW MASS.m
Sample Name at-f
Comment

Acquisition Date 7/2/2014 11:27:11 AM

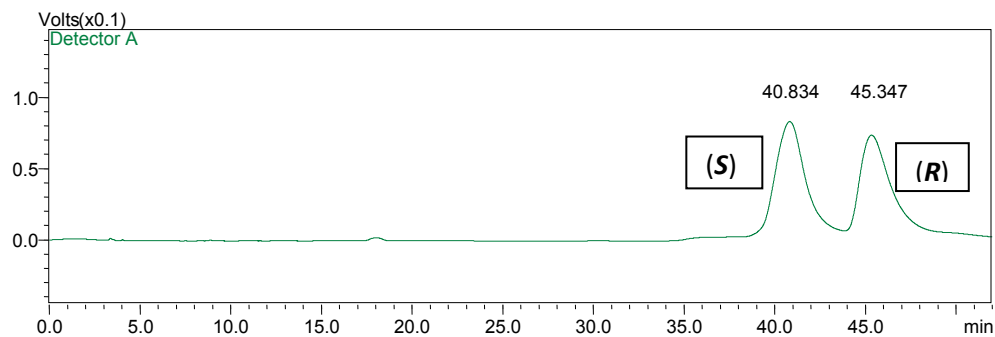
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

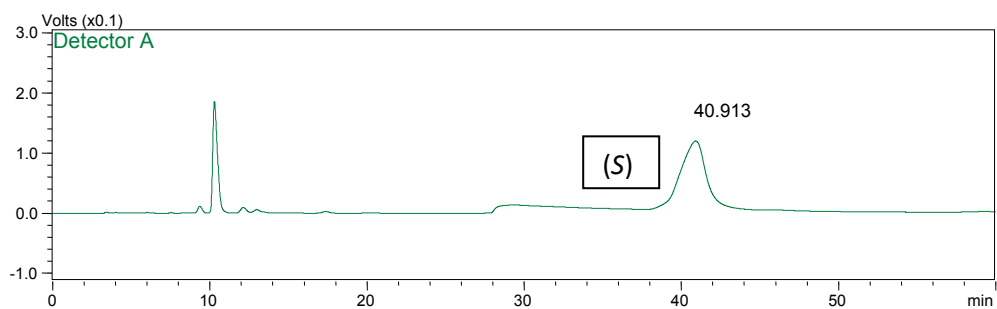


6. HPLC chromatogram of (RS)-2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide

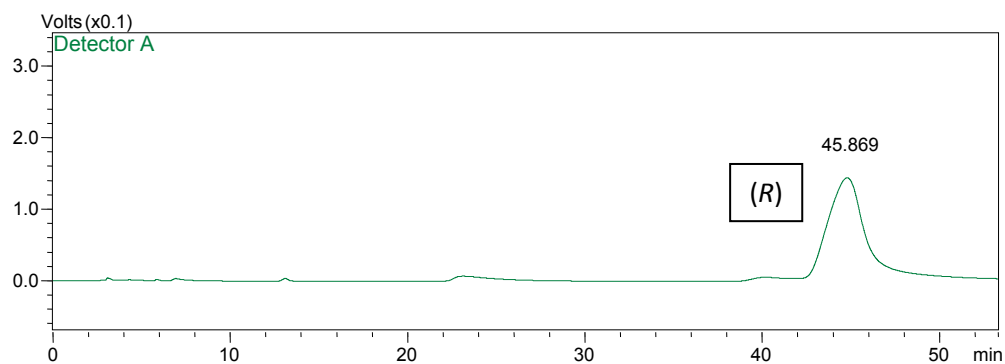


7. Chromatogram of enantiopure alcohol.

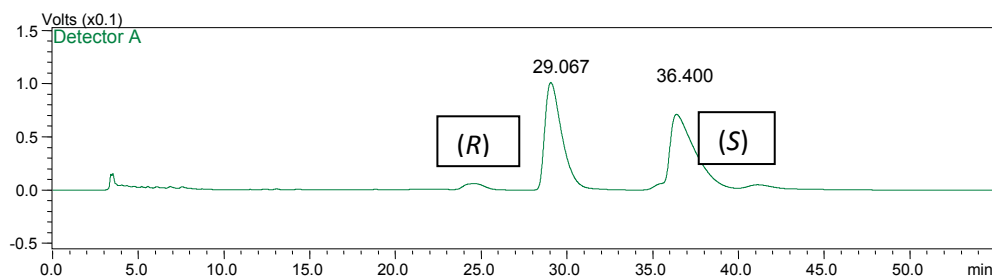
a) (S)-(2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide)



b) Chromatogram of (R)-(2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide)

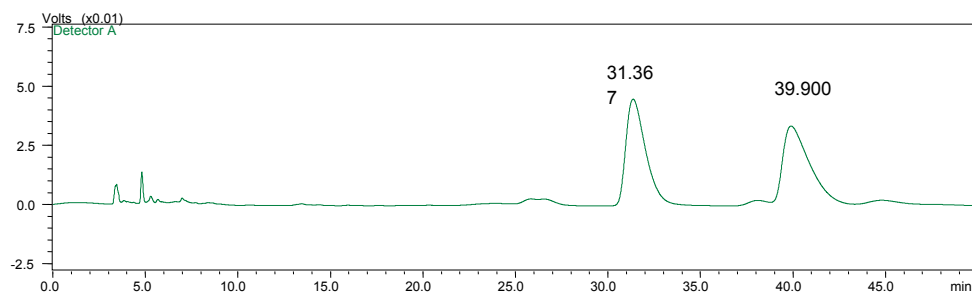


8. Chromatogram of (RS)-1-(4-(2-amino-2-oxoethyl) phenoxy)-3-chloropropan-2-yl acetate

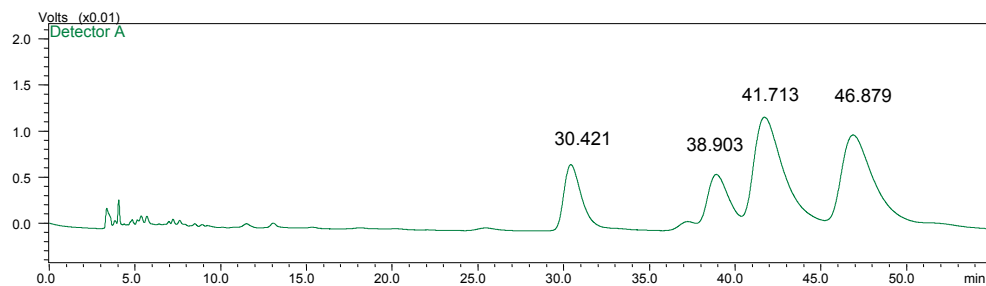


9. Selective HPLC chromatograms from lipase screening

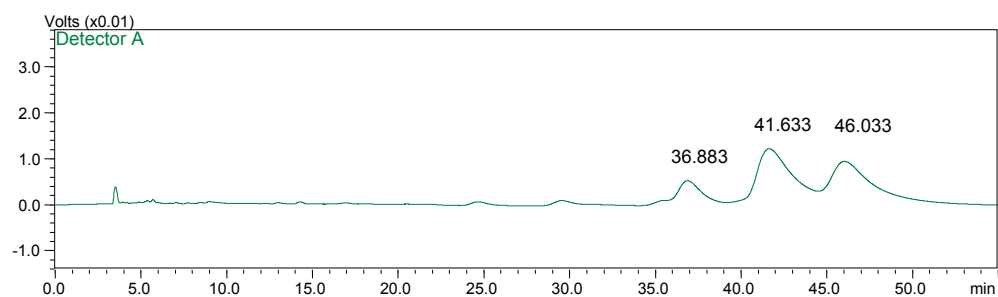
Candida antarctica Lipase-A CLEA (maximum enantioselectivity observed)



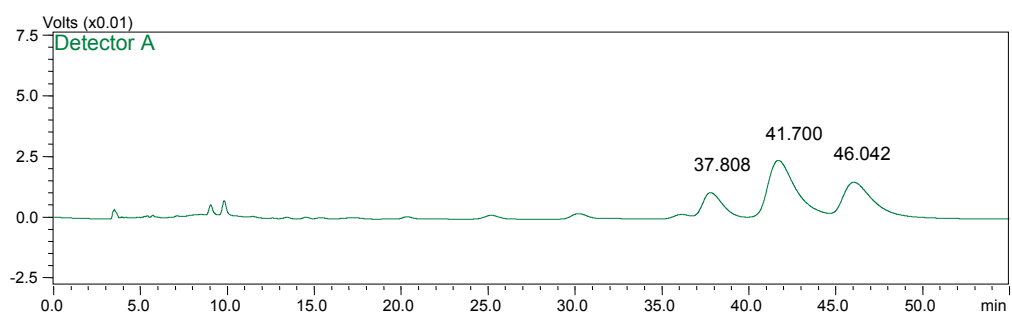
Candida cylindracea (non selective)



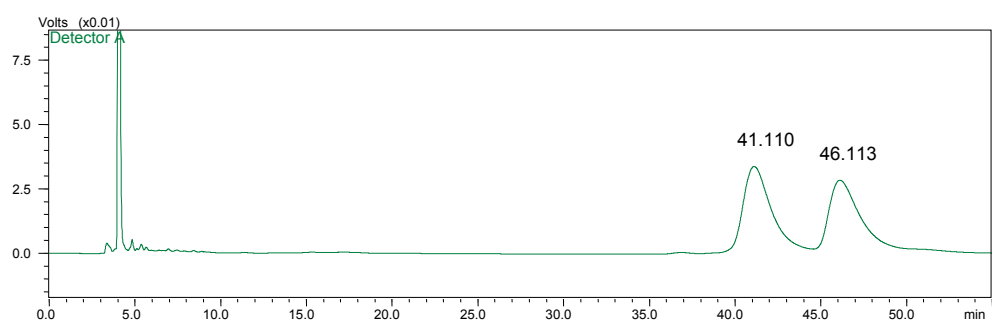
***Candida rugosa* (62316) (non selectivity)**



AMANO (non selectivity)

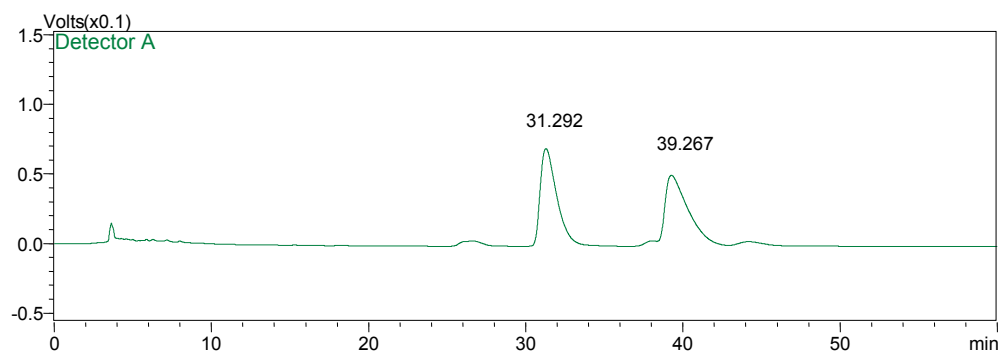


Porcine pancreas lipase (no reactivity)

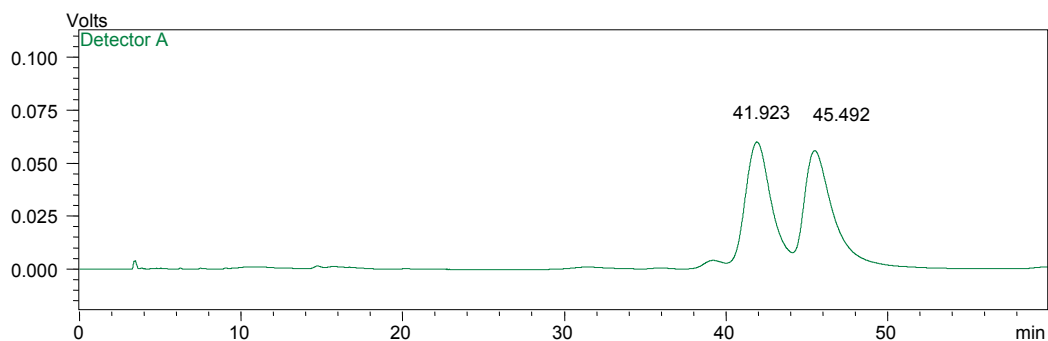


10. Selective HPLC chromatograms of solvent screening

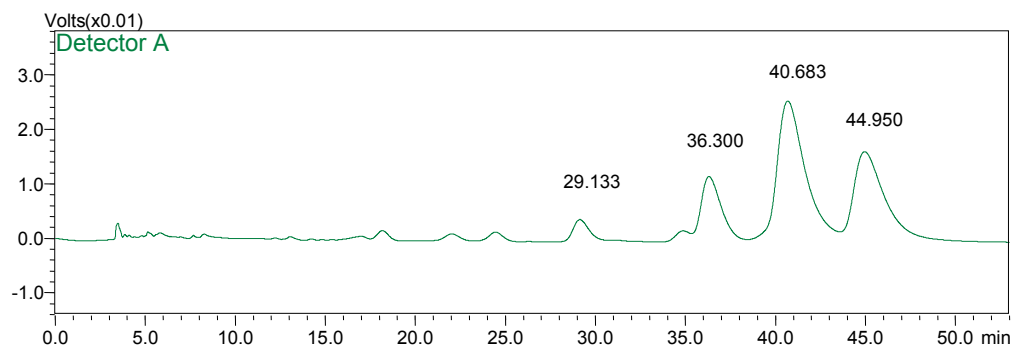
Toluene (enantioselective)



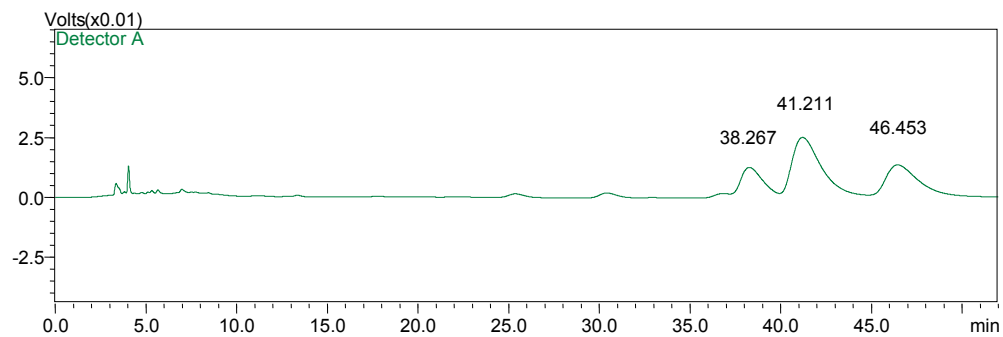
Acetonitrile (no reactivity)



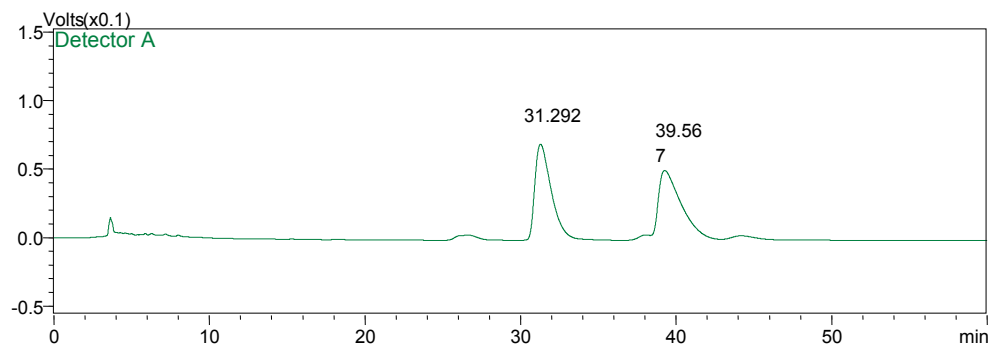
TBME (non selective)



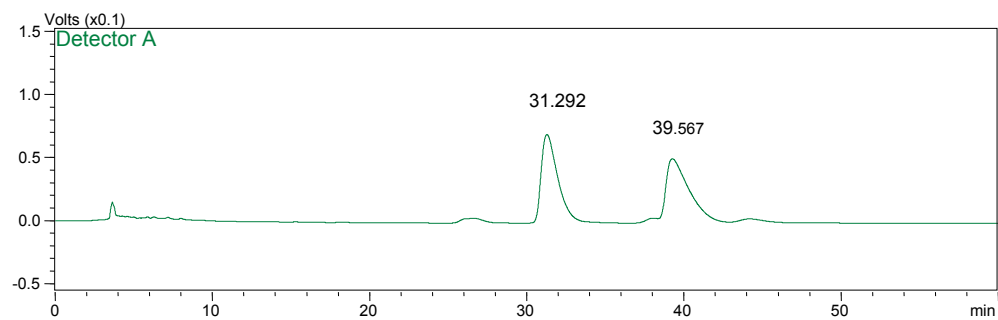
Benzene (non selective)



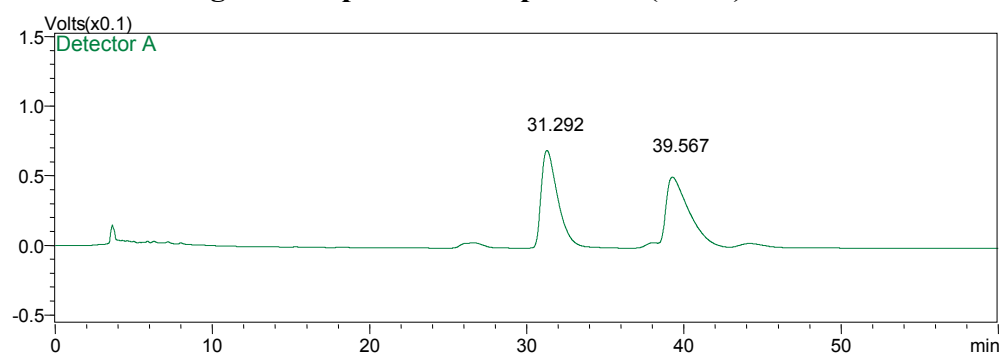
11. HPLC chromatogram at optimized time period (18 h).



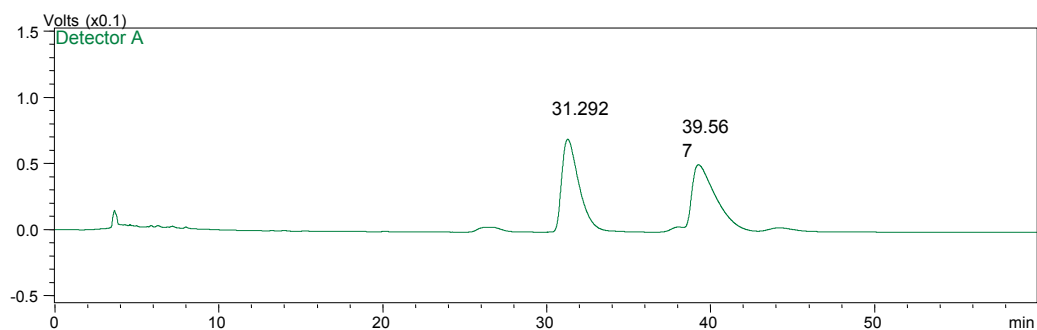
12. HPLC chromatogram using best acyl donor (Vinyl acetate)



13. HPLC chromatogram at optimized temperature (30 °C)



14. HPLC chromatogram at optimized enzyme concentration (15 mg/ml).



15. HPLC chromatogram at the optimized substrate concentration (20 mM)

