Electronic Supplementary Material

Optically Pure Bulky (hetero)Arylalkyl Carbinols *via* Kinetic Resolution

Bin Hu, Meng Meng, John S. Fossey, Weimin Mo, Xinquan Hu, Wei-Ping Deng*

General Information

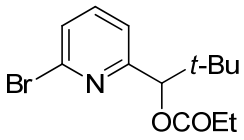
THF and toluene were distilled from sodium prior to use. All reagents were obtained commercially and propionate anhydride was distilled from anhydrous $CaCl_2$ prior to use. Catalyst **Fc-PIP** was prepared as previously described.[1] The substrates **1-8**, **14-15** were prepared by the addition of pivaldehyde with corresponding aromatic lithiums *in situ* generating from halo-lithium exchanges of aromatic halides. The substrates **9-11** were prepared by the aldol reaction of benzaldehyde with corresponding ketones or silyl ketene acetal.[2-4] The substrates **12-13** were prepared by the addition of pivaldehyde with corresponding aromatic organolithiums *in situ* generating from deprotonation of furan or thiophene with 1 equiv. *n*-BuLi.

^{1}H NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data are reported as (s = single, d = doublet, t = triple, q = quartet, m = multiple, br s = broad single, coupling constant(s) in Hz, integration). ^{13}C NMR spectra were recorded on a Bruker DPX 100 MHz spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

Methods used for kinetic resolution experiments determination of ee's and calculation of conversions and selectivities were adopted from previously published work.[1] Enantiomeric ratios were determined by HPLC, using a Diacel CHIRALPAK AD-H column, a Diacel CHIRALCEL OD-H column, a Diacel AS-H column and a Diacel OJ-H column with hexane and *i*-PrOH as eluents

Spectral data for new substrates and esters

Propionate of **1:**



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (dt, J_1 = 0.6 Hz, J_2 = 7.8 Hz; 1H), 7.26 (d, J = 7.9 Hz, 1H), 7.14 (d, J = 7.6 Hz, 1H), 5.42 (s, 1H), 2.30-2.37 (m, 2H), 1.07 (dt, J_1 = 1.3 Hz, J_2 = 7.6 Hz; 3H), 0.88 (d, J = 1.3 Hz, 9H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 173.3, 160.0, 140.6, 138.2, 126.8, 120.6, 82.4, 35.0, 27.7, 26.0, 9.1;

HRMS (EI, m/z): Calcd for $C_{14}H_{19}BrO_2$: 298.0568, found: 298.0571.

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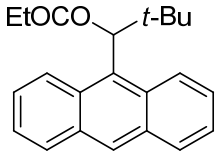
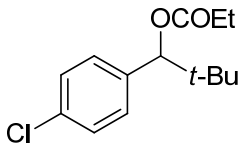
Propionate of **3**:



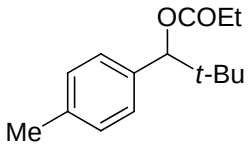
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.87-8.90 (m, 1H), 8.54 (d, *J* = 9.1 Hz, 1H), 8.40 (s, 1H), 7.94-7.98 (m, 2H), 7.50-7.54 (m, 1H), 7.37-7.44 (m, 3H), 7.30 (s, 1H), 2.36-2.55 (m, 2H), 1.13 (t, *J* = 7.6 Hz, 3H), 1.04 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.8, 132.2, 131.7, 131.4, 130.7, 130.0, 129.5, 129.4, 129.2, 128.7, 126.2, 124.8 (d), 124.7, 124.6, 79.3, 38.5, 28.5, 27.9, 9.3.
HRMS (EI, m/z): Calcd for $C_{22}H_{24}O_2$: 320.1776, found: 320.1777.

Propionate of **5**:



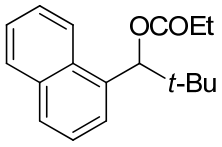
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.29 (m, 2H), 7.19-7.21 (m, 2H), 5.45 (s, 1H), 2.30-2.46 (m, 2H), 1.15 (t, *J* = 7.6 Hz, 3H), 0.91 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.2, 137.2, 133.3, 129.0, 127.8, 81.9, 35.0, 27.8, 25.9, 9.1.
HRMS (EI, m/z): Calcd for $C_{14}H_{19}ClO_2$: 254.1074, found: 254.1075.

Propionate of **6**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.46 (s, 1H), 2.32-2.43 (m, 2H), 1.15 (t, *J* = 7.6 Hz, 3H), 0.92 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.3, 137.0, 135.8, 128.4, 127.7, 82.5, 35.1, 27.9, 26.1, 21.1, 9.3.
HRMS (EI, m/z): Calcd for $C_{15}H_{22}O_2$: 234.1620, found: 234.1621.

Propionate of **7**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40-8.42 (m, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.65-7.68 (m, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.51-7.56 (m, 2H), 6.71 (s, 1H), 2.40-2.57 (m, 2H), 1.24 (t, *J* = 7.6 Hz, 3H), 1,13 (s, 9H);

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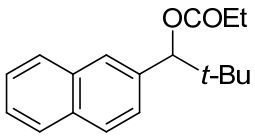
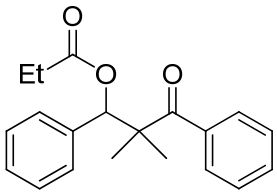
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.5, 135.5, 133.6, 132.2, 128.9, 128.3, 126.1, 125.5, 124.8, 123.9, 76.7, 36.5, 28.0, 26.7, 9.3.
HRMS (EI, m/z): Calcd for $C_{18}H_{22}O_2$: 270.1620, found: 270.1619.

Propionate of **8**:



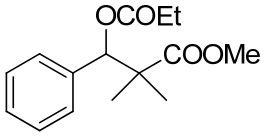
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90-7.95 (m, 4H), 7.53-7.60 (m, 3H), 5.87 (s, 1H), 2.49-2.61 (m, 2H), 1.31 (t, *J* = 7.6 Hz, 3H), 1.14 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.4, 136.5, 133.1, 133.0, 128.2, 127.8, 127.4, 127.0, 126.2, 126.1, 126.0, 82.8, 35.5, 28.0, 26.4, 9.4.
HRMS (EI, m/z): Calcd for $C_{18}H_{22}O_2$: 270.1620, found: 270.1615.

Propionate of **9**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.8 Hz, 2H), 7.45-7.49 (m, 1H), 7.39-7.42 (m, 2H), 7.26-7.33 (m, 5H), 6.31 (s, 1H), 2.30 (q, *J* = 7.6 Hz, 2H), 1.31 (s, 3H), 1.25 (s, 3H), 1.07 (t, *J* = 7.6 Hz, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 172.7, 139.4, 137.1, 130.9, 128.2, 128.0, 127.9, 127.7, 127.2, 79.1, 51.9, 27.6, 23.5, 21.0, 9.0.
HRMS (EI, m/z): Calcd for $C_{20}H_{22}O_3$: 310.1569, found: 310.1566.

Propionate of **10**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.23 (m, 5H), 6.07 (s, 1H), 3.66 (s, 3H), 2.40-2.29 (m, 2H), 1.21 (s, 3H), 1.14-1.10 (m, 6H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 175.8, 172.6, 136.9, 128.0, 127.9, 127.5, 78.8, 51.8, 47.1, 27.7, 21.9, 19.9, 9.1.
HRMS (EI, m/z): Calcd for $C_{15}H_{20}O_4$: 264.1362, found: 264.1359.

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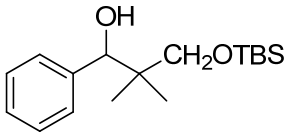
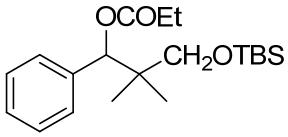
Alcohol **11**:



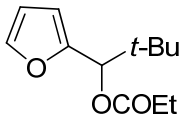
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.27 (m, 5H), 4.62 (d, J = 3.3 Hz, 1H), 4.49 (d, J = 3.4 Hz, 1H), 3.50 (q, J = 9.8 Hz, 2H), 0.96 (s, 9H), 0.86 (s, 3H), 0.83 (s, 3H), 0.12 (s, 6H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 141.7, 127.8, 127.5, 127.1, 82.2, 73.0, 39.0, 25.9, 22.9, 19.3, 18.2, -5.6.
HRMS (EI, m/z): Calcd for $C_{17}H_{30}O_2Si$: 294.2015, found: 294.2020.

Propionate of **11**:



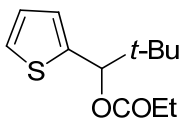
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.30 (m, 5H), 5.77 (s, 1H), 3.35 (d, J = 9.5 Hz, 1H), 3.18 (d, J = 9.5 Hz, 1H), 2.31-2.42 (m, 2H), 1.14 (t, J = 7.6 Hz, 3H), 0.92 (s, 9H), 0.04 (s, 3H), 0.03 (s, 3H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.1, 138.5, 127.7, 127.6, 127.4, 78.5, 69.2, 39.9, 27.9, 26.0, 20.5, 18.3, 9.2, -5.5, -5.6.
HRMS (EI, m/z): Calcd for $C_{20}H_{34}O_3Si$: 350.2277, found: 350.2278.

Propionate of **12**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (m, 1H), 6.31-6.32 (m, 1H), 6.23 (d, J = 3.2 Hz, 1H), 5.57 (s, 1H), 2.34-2.40 (m, 2H), 1.15 (t, J = 7.5 Hz, 3H), 9.7 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.2, 152.3, 141.7, 109.9, 108.3, 76.0, 35.1, 27.6, 25.9, 9.0.
HRMS (EI, m/z): Calcd for $C_{12}H_{18}O_3$: 210.1256, found: 210.1255.

Propionate of **13**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.22 (dd, J_1 = 1.5 Hz, J_2 = 4.7 Hz; 1H), 6.94-6.96 (m, 2H), 5.81 (s, 1H), 2.32-2.42 (m, 2H), 1.15 (t, J = 7.6 Hz, 3H), 0.98 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.2, 141.2, 126.5, 126.1, 124.5, 78.8, 35.2, 27.8, 26.0, 9.1.
HRMS (EI, m/z): Calcd for $C_{12}H_{18}O_2S$: 226.1028, found: 226.1023.

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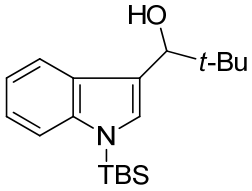
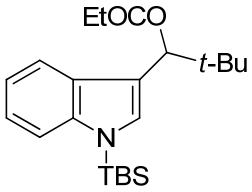
Alcohol of **14**:



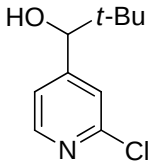
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 8.1 Hz, 1H), 7.16-7.08 (m, 3H), 4.80 (d, *J* = 2.1 Hz, 1H), 1.75 (d, *J* = 2.2 Hz, 1H), 1.00 (s, 9H), 0.92 (s, 9H), 0.60 (d, *J* = 4.2 Hz, 6H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 141.1, 130.5, 129.1, 121.4, 120.3, 120.1, 119.6, 113.9, 76.7, 36.5, 26.4, 26.3, 19.5, 3.8.
HRMS (EI, m/z): Calcd for $C_{19}H_{31}NOSi$: 317.2175, found: 317.2175.

Propionate of **14**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78-7.81 (m, 1H), 7.50-7.52 (m, 1H), 7.13-7.18 (m, 2H), 7.09 (s, 1H), 5.99 (s, 1H), 2.36-2.48 (m, 2H), 1.18 (t, *J* = 7.6 Hz, 3H), 1.05 (s, 9H), 0.95 (s, 9H), 0.64 (s, 6H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.6, 141.1, 130.4, 129.7, 121.3, 120.7, 119.7, 116.1, 113.9, 77.9, 36.1, 28.0, 26.5, 26.3, 19.3, 9.3, 3.9.
HRMS (EI, m/z): Calcd for $C_{22}H_{35}NO_2Si$: 373.2437, found: 373.2442.

Alcohol of **15**:



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29-8.23 (m, 1H), 7.28 (m, 1H), 7.16 (m, 1H), 4.36 (s, 1H), 2.72-2.40 (m, 1H), 0.92 (d, J = 2.3 Hz, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 155.6, 150.6, 148.2, 123.3, 121.9, 80.2, 35.5, 25.7.
HRMS (EI, m/z): Calcd for $C_{10}H_{14}ClNO$: 199.0764, found: 199.0769.

Propionate of **15**:

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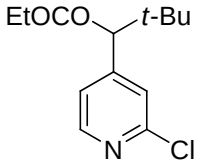
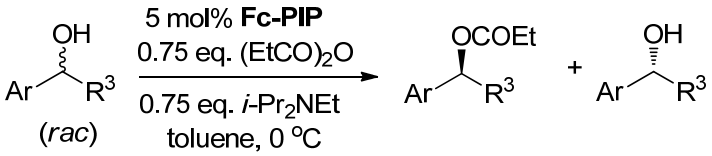


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, J = 5.2 Hz, 1H), 7.15 (m, 1H), 7.05 (dd, J_1 = 1.3 Hz, J_2 = 5.1 Hz; 1H), 2.28-2.43 (m, 2H), 1.09 (t, J = 7.5 Hz, 3H), 0.86 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.2, 151.2, 150.9, 149.0, 123.0, 121.5, 80.7, 34.9, 27.6, 25.8, 9.0.
HRMS (EI, m/z): Calcd for $C_{13}H_{18}ClNO_2$: 255.1026, found: 255.1034.

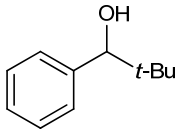
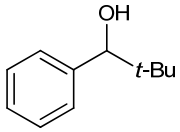
Kinetic resolution experiment



General procedure for the kinetic resolution of alcohols by reaction with propionyl anhydride and catalyst Fc-PIP.

Fc-PIP catalyst (0.02 mmol) , bulky alcohols (0.4 mmol), toluene (1.0 mL) and of *N*,*N*-diisopropylethylamine (0.3 mmol, 0.052 mL) were sequentially added to a 10 mL flask cooled to 0 °C (ice bath), resulting in a red-orange solution. After stirring at 0 °C for 5 min, the reaction mixture was treated with 0.3 mmol of propionyl anhydride (0.039 mL), the resulting green solution was stirred at 0 °C for the specified period, at the end of which it was quenched by rapid addition of 0.5 mL of methanol. The solution was allowed to warm up to room temperature and stirred for 1 h, during which time the solution returned to a red-orange colour. The solvent was removed *in vacuo*, and the residue purified by silca gel chromatography (5% - 10% EtOAc/petroleum) to separate the ester from the unreacted alcohol

Table 1

entry[a]	Substrate	t (h)	ee_E (%)[b]	ee_A (%)[c]	C_{HPLC}(%)[d]	*d*
1	 **4**	11	> **99.0**	93.2	48.5	690
2	 **4**	24	98.2	> **99.0**	50.4	683

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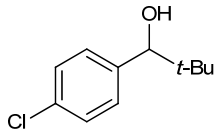
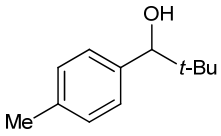
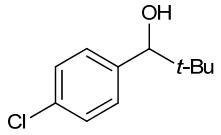
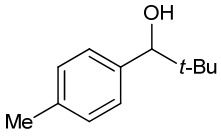
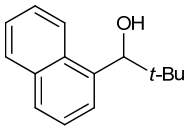
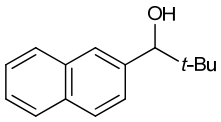
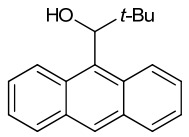
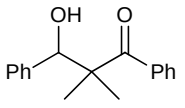
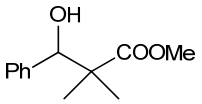
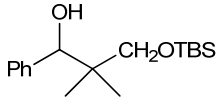
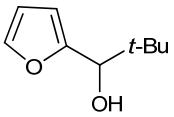
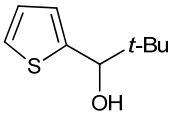
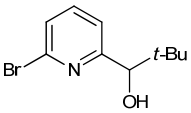
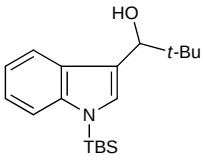
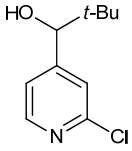
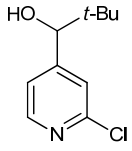
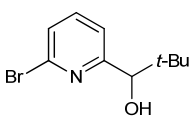
3	 **5**	7	92.5	98.0	51.4	118
4	 **6**	10.5	88.0	96.0	52.2	61
5	 **5**	11	91.6	> **99.0**	51.9	120
6	 **6**	93	79.8	> **99.0**	55.6	59
7	 **7**	48	85.2	> **99.0**	53.8	71
8	 **8**	19	92.6	> **99.0**	51.7	142
9	 **3**	96	75.8	> **99.0**	56.6	37
10	 **9**	93	83.8	> **99.0**	54.3	68
11	 **10**	36	85.4	> **99.0**	53.9	85
12	 **11**	93	88.6	> **99.0**	52.8	86

Electronic Supplementary Material

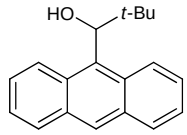
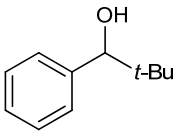
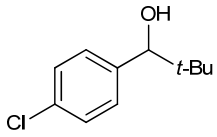
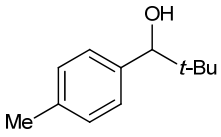
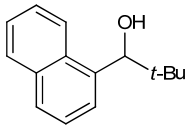
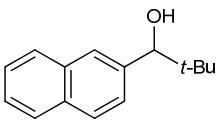
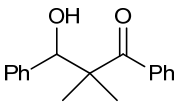
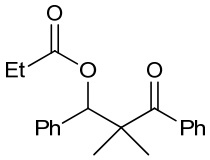
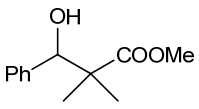
13	 **12**	93	80.6	> **99.0**	55.1	48
14	 **13**	48	86.2	> **99.0**	53.5	73
15[e]	 **1**	78	76.8	> **99.0**	56.3	39
16[f]	 **14**	72	75.6	> **99.0**	56.7	37
17	 **15**	15.5	86.8	> **99.0**	53.7	74
18[g]	 **15**	48	53.6	97.6	64.6	13

[a] The reaction was carried out using 0.4 M of substrates.
[b] The ee value of the ester. [c] The ee value of the unreacted alcohol, and was tested at least three times for the ees >99.0%. [d] Calculated from the ee of the ester and unreacted alcohol. [e] Using 15 mol% catalyst Fc-PIP instead. [f] The reaction was conducted at rt. [g] Using 5 mol% catalyst Cl-PIQ .

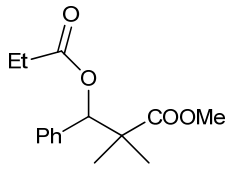
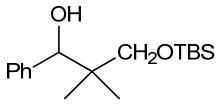
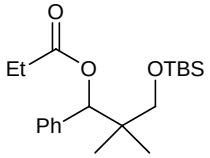
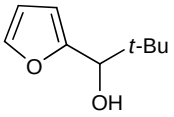
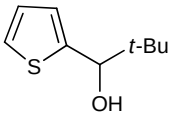
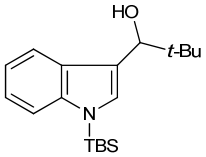
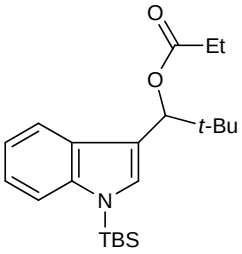
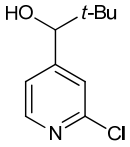
Table 2: Methods used to Assay Enantiomeric Excess

Substrate	HPLC conditions[a]	Retention time of (*R*) isomer (min)[c]	Retention time of (*S*) isomer (min)
	AD-H column, 254nm Hexane/*i*-PrOH = 40/1, 1.0 mL/min	14.39	12.09

Electronic Supplementary Material

	AD-H column, 254nm Hexane/*i*-PrOH = 40/1, 1.0 mL/min	32.53	26.07
	OD-H column, 254nm Hexane/*i*-PrOH = 60/1, 1.0 mL/min	12.77	9.78
	OD-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	23.93	20.87
	OD-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	22.75	17.94
	OD-H column, 254nm Hexane/*i*-PrOH = 95/5, 1.0 mL/min	27.72	15.77
	OD-H column, 254nm Hexane/*i*-PrOH = 95/5, 1.0 mL/min	21.24	16.16
	OD-H column,220nm, Hexane/*i*-PrOH = 95/5, 1.0 mL/min	14.88	20.87
	OD-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min[b]	19.38	18.07
	OJ-H column,220nm, Hexane/*i*-PrOH = 95/5, 1.0 mL/min	28.75	22.87

Electronic Supplementary Material

	OD-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 0.5 mL/min[b]	21.87	19.18
	AD-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	10.48	13.26
	OD-H column, 220nm Hexane 1.0 mL/min[b]	14.47	9.03
	AS-H column, 220nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	12.60	15.70
	OD-H column, 254nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	32.38	21.57
	AD-H column, 254nm Hexane/*i*-PrOH = 99.5/0.5, 1.0 mL/min	13.26	10.48
	OD-H column, 254nm Hexane/*i*-PrOH = 99.5/0.5, 0.5 mL/min[b]	12.67	7.80
	AD-H column, 254nm Hexane/*i*-PrOH = 40/1, 1.0 mL/min	22.27	19.89

a) Unless otherwise specified, HPLC separation of enantiomers was achieved using free alcohols with isopropanol/hexane eluent at the concentration indicated;

b) HPLC separation of enatiomers was achieved using the propionated of the alcohols;

c) The absolute configurations were assigned by comparison of the signs of optical rotation with literatures.

Electronic Supplementary Material

Procedure for preparative scale reaction:

Alcohol **15** (800 mg, 4.0 mmol, 1 equiv.), **Fc-PIP** (88 mg, 0.12 mmol, 0.03 equiv), toluene (8.0 mL) and *N*,*N*-diisopropylethylamine (0.52 mL, 3.0 mmol, 0.75 equiv) was added in turn to a 25 mL flask, resulting in a red-orange solution. After stirring at 0 ^{o}C for 15 min, the reaction mixture was treated with propionic anhydride (0.39 mL, 3.0 mmol, 0.75 equiv), the resulting green solution wasstirred at 0 ≡C for 24 h, the reaction was then quenched by methanol (5.0 mL). The solution was allowed to warm up to room temperature slowly and stirred for a further hour at room temperature, during which time the solution turnedto a red-orange colour once again. The solvent was removed *in vacuo*, and the residue was purified by silica gel chromatography (EtOAc/petroleum = 1/20 to EtOAc/petroleum/Et_3N = 19/86/5). The ester was eluted first (567 mg, 2.22 mmol, 55.4%), followed by the unreacted alcohol (354 mg, 1.77 mmol, 44.3%) and finally **Fc-PIP** (83 mg, 95% recovery). The enantiomeric excess of the ester was determined by HPLC to be 79.2%, and that of the alcohol was > 99.0%. Based on these ee values, the conversion was calculated to be 55.6% (cf. 55.4% conversion based on the isolated materials), and the selectivity factor was 46.

Electronic Supplementary Material

X-Ray Crystal Data of (*R, Rp*)-Fc-PIP

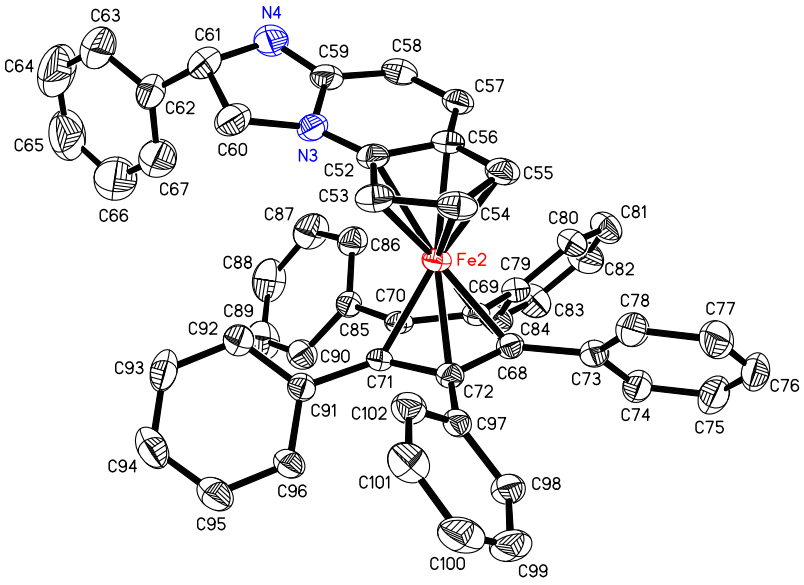


Table 3. Crystal data and structure refinement for cd201500.

Identification code	cd201500
Empirical formula	C51 H38 Fe N2
Formula weight	734.68
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 11.8838(7) A alpha = 90 deg. b = 21.2674(13) A beta = 104.1870(10) deg. c = 15.6935(10) A gamma = 90 deg.
Volume	3845.4(4) A^3
Z, Calculated density	4, 1.269 Mg/m^3
Absorption coefficient	0.431 mm^-1
F(000)	1536
Crystal size	0.422 x 0.357 x 0.116 mm
Theta range for data collection	2.01 to 26.00 deg.
Limiting indices	-13<=h<=14, -25<=k<=26, -19<=l<=12
Reflections collected / unique	21150 / 14472 [R(int) = 0.0325]
Completeness to theta = 26.00	99.7 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.57355
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14472 / 1 / 973

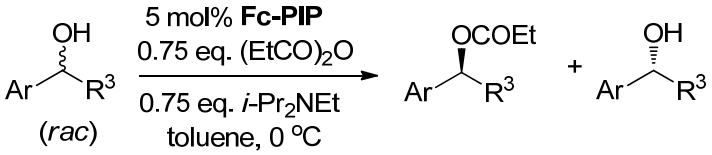
Goodness-of-fit on F^2	0.951
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.0930
R indices (all data)	R1 = 0.0525, wR2 = 0.0974
Absolute structure parameter	-0.005(11)
Largest diff. peak and hole	0.397 and -0.262 e.A^-3

References:

1. B. Hu, M. Meng, Z. Wang, W-T. Du, J. S. Fossey, X-Q. Hu, W-P. Deng, *J. Am. Chem. Soc.*, 2010, **132**, 17041-17044.
2. L. A. Paquette, G. D. Parker, T. Tei, S-Z. Dong, *J. Org. Chem.*, 2007, **72**, 7125-7134.
3. S. Kobayashi, K. Seki, M. Ueno, *Org. Biomol. Chem.*, 2007, **5**, 1347-1350.
4. X-M. Hu, R. M. Kellogg, *Synthesis*, 1995, 533-538.

Electronic Supplementary Material

HPLC Data

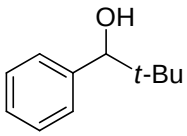


entry	substrate	t (h)	ee_E (%)[a]	ee_A (%)[b]	C_{HPLC}(%)[c]	S^c
1	**4**	11	> **99.0**	93.2	48.5	690
2	**4**	24	98.2	> **99.0**	50.4	683
3	**5**	7	92.5	98.0	51.4	118
4	**6**	10.5	88.0	96.0	52.2	61
5	**5**	11	91.6	> **99.0**	51.9	120
6	**6**	93	79.8	> **99.0**	55.6	59
7	**7**	48	85.2	> **99.0**	53.8	71
8	**8**	19	92.6	> **99.0**	51.7	142
9	**3**	96	75.8	> **99.0**	56.6	37
10	**9**	93	83.8	> **99.0**	54.3	68
11	**10**	36	85.4	> **99.0**	53.9	85
12	**11**	93	88.6	> **99.0**	52.8	86
13	**12**	93	80.6	> **99.0**	55.1	48
14	**13**	48	86.2	> **99.0**	53.5	73
15	**1**[d]	78	76.8	> **99.0**	56.3	39
16	**14**[e]	72	75.6	> **99.0**	56.7	37
17	**15**	15.5	86.8	> **99.0**	53.7	74
18	**15**[f]	48	53.6	97.6	64.6	13

[a] The ee value of the ester. [b] The ee value of the unreacted alcohol, which was tested at least three times for the ees >99.0% [c] Calculated from the ee of the ester and unreacted alcohol. [d] Using 15 mol% catalyst Fc-PIP instead. [e] The reaction was conducted at rt. [f] Using 5 mol% catalyst Cl-PIQ.

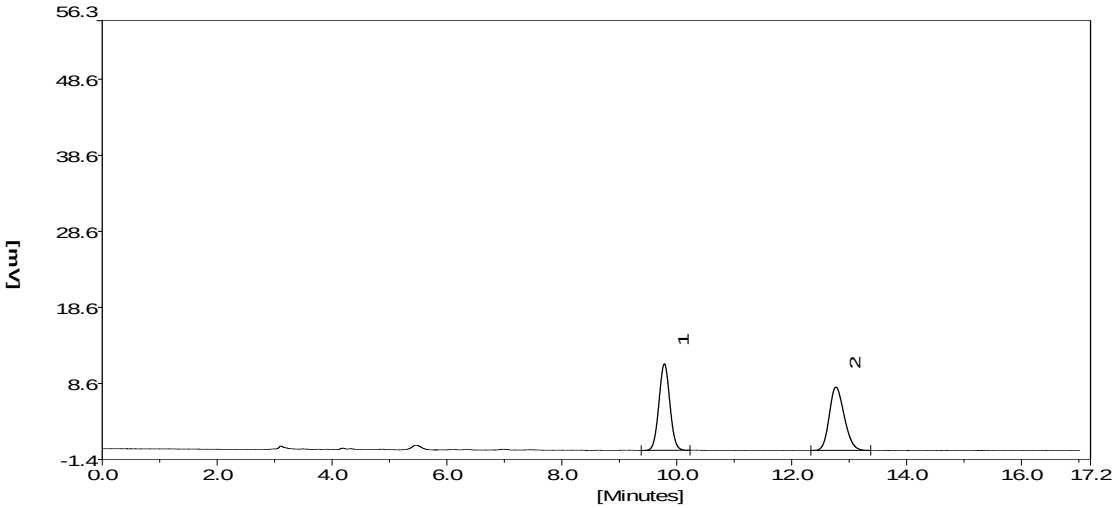
Electronic Supplementary Material

Entry 1:



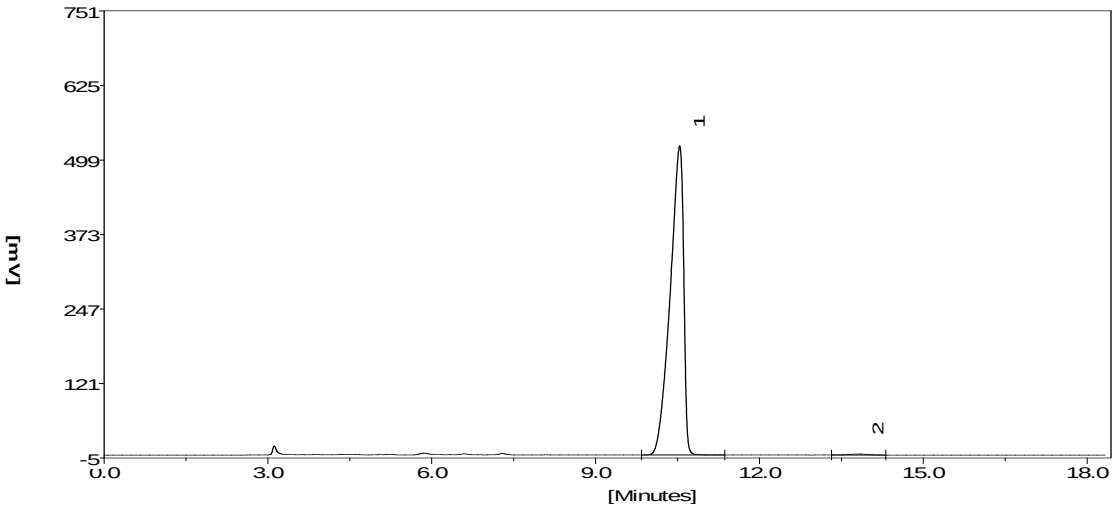
4

(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	9.78417	11.37	150.64	50.0344
2	12.77	8.34	150.43	49.9656

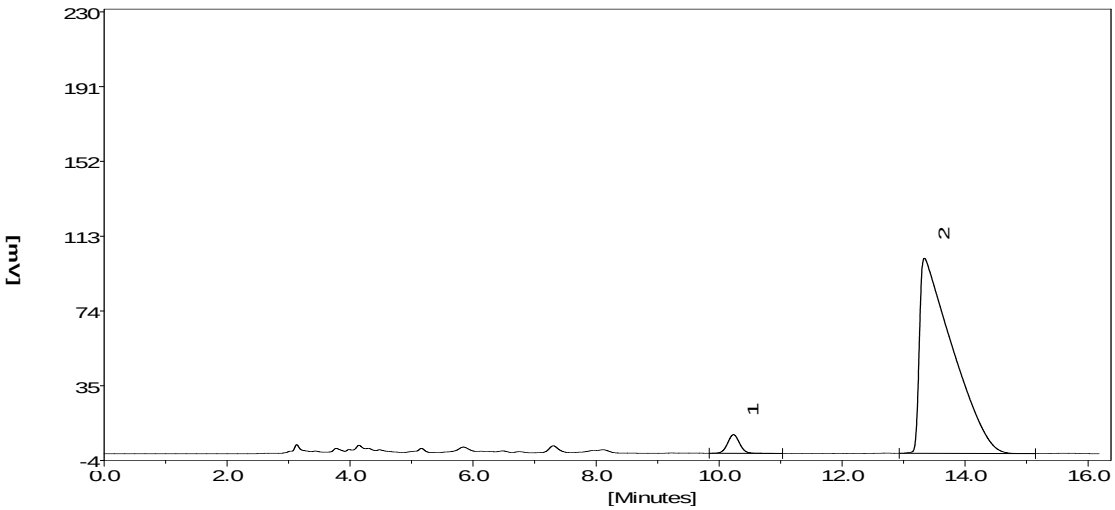
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	10.54	522.62	8952.83	99.5388
2	13.81333	1.78	41.48	0.4612

Electronic Supplementary Material

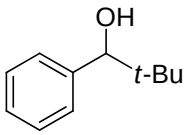
Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	10.235	9.72	133.3	3.3883
2	13.33833	101.79	3800.7	96.6117

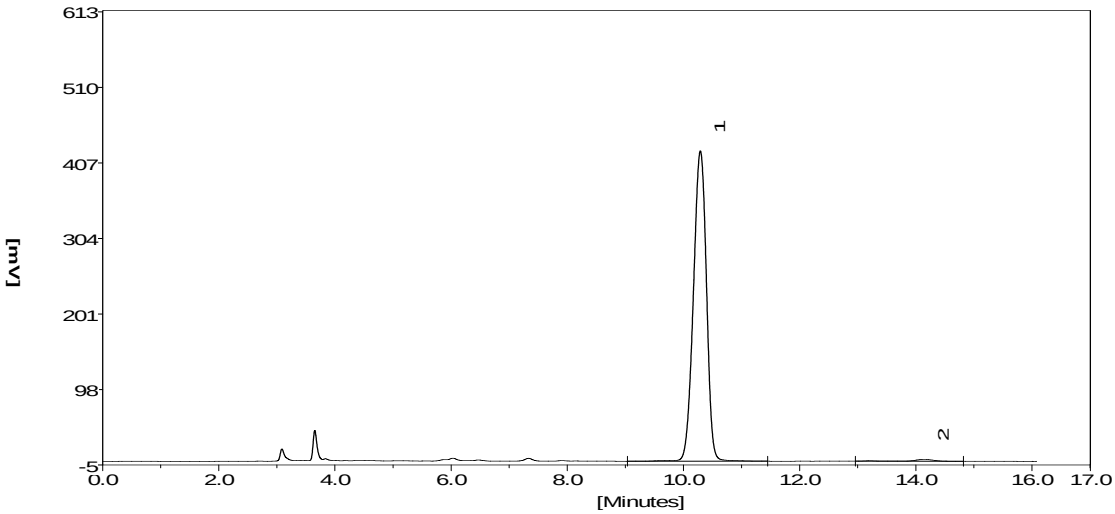
S = 690

Entry 2:



4

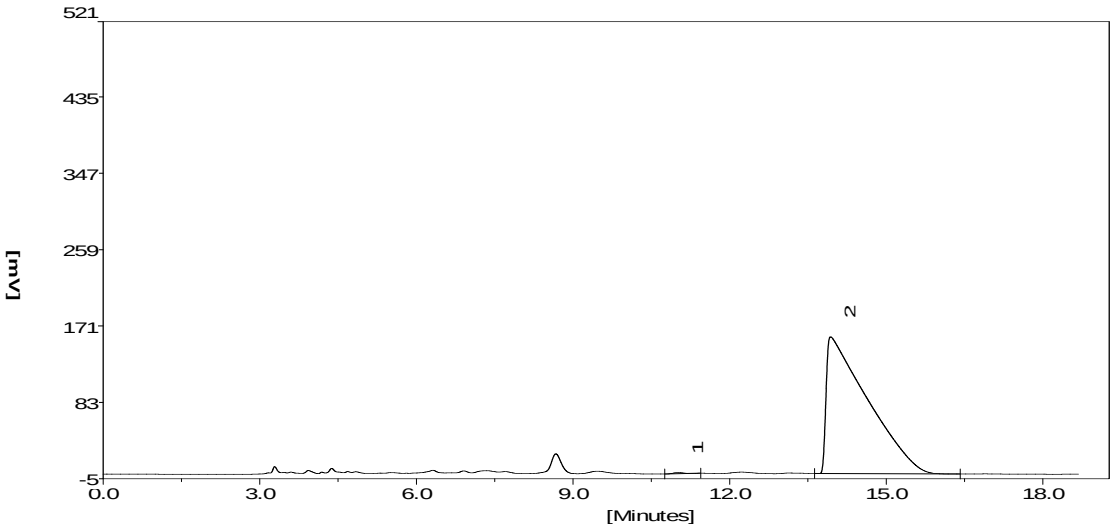
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	10.29083	423.32	6615.04	99.0706
2	14.14167	2.57	62.06	0.9294

Electronic Supplementary Material

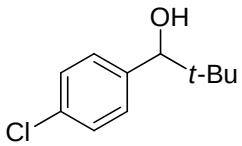
Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	11.0175	1.4	18.99	0.2184
2	13.93333	157.72	8675.85	99.7816

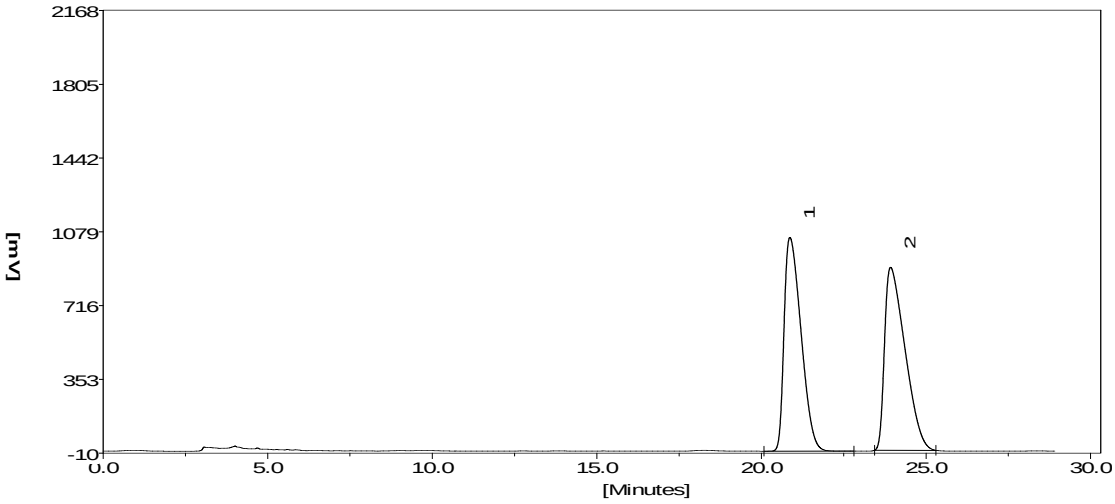
S = 683

Entry 5:



5

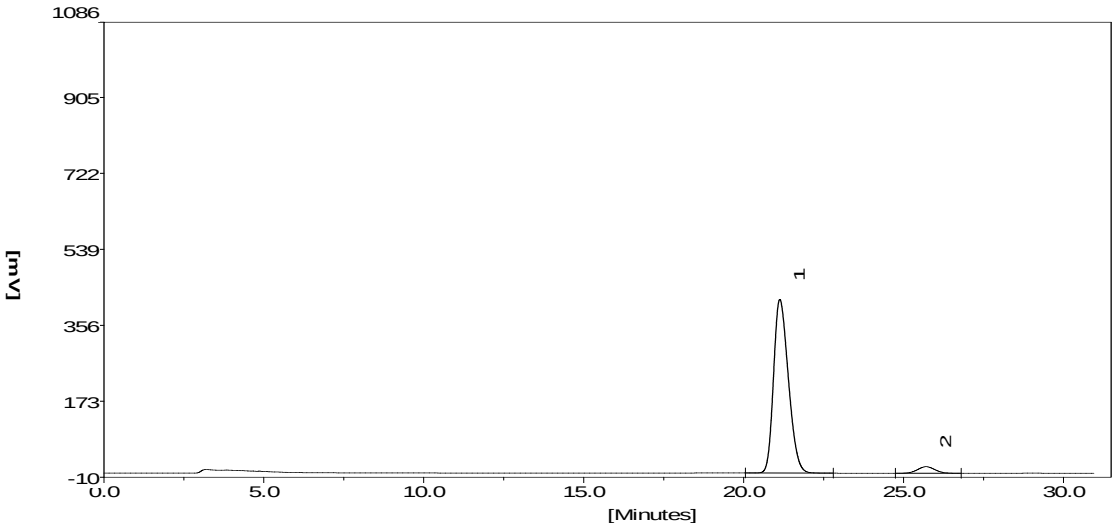
(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	20.865	1052.39	37593.86	49.2223
2	23.925	900.84	38781.81	50.7777

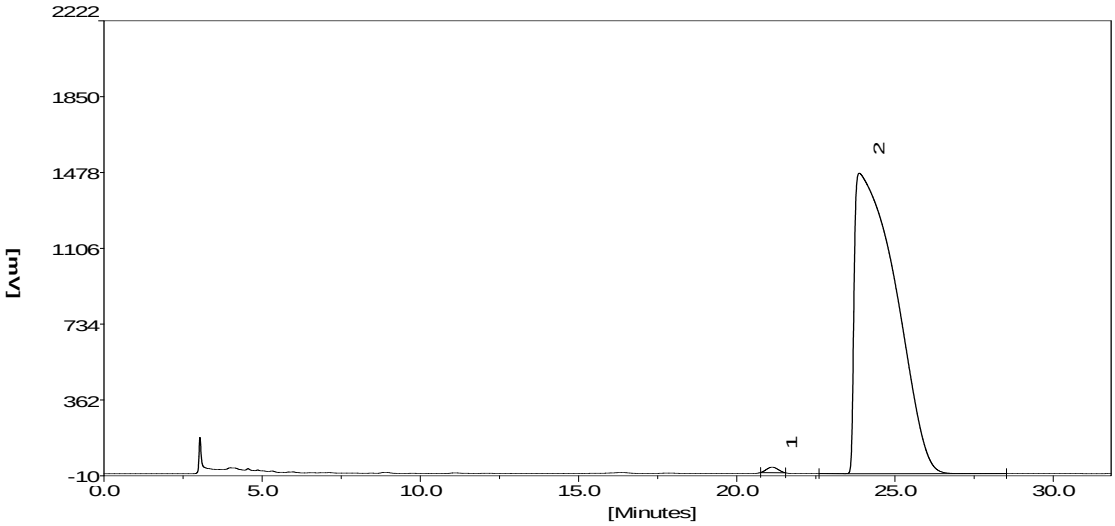
Electronic Supplementary Material

Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	21.1325	418.43	13469.73	95.7847
2	25.70333	15.73	592.78	4.2153

Alcohol:

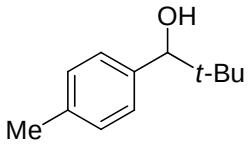


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	21.11833	27.17	682.09	0.473
2	23.87167	1474.01	132276.67	99.527

$S = 120$

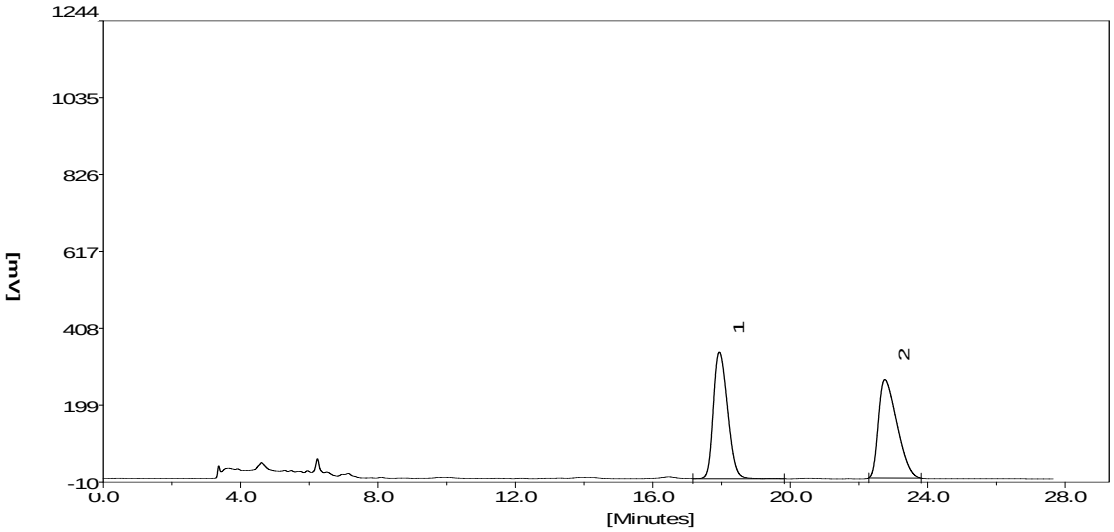
Electronic Supplementary Material

Entry 6:



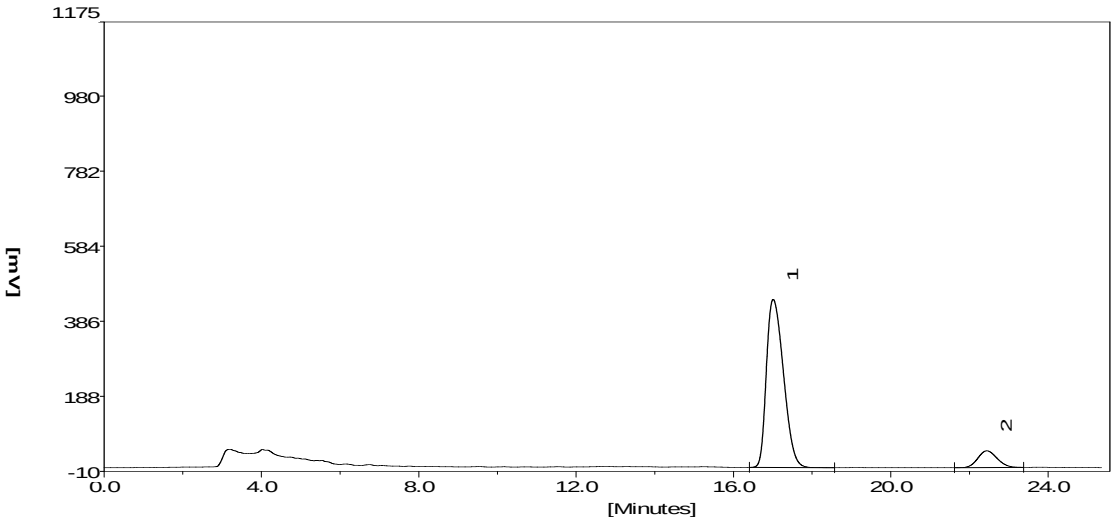
6

(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	17.93667	344.45	9897.66	49.8016
2	22.75417	267.62	9976.51	50.1984

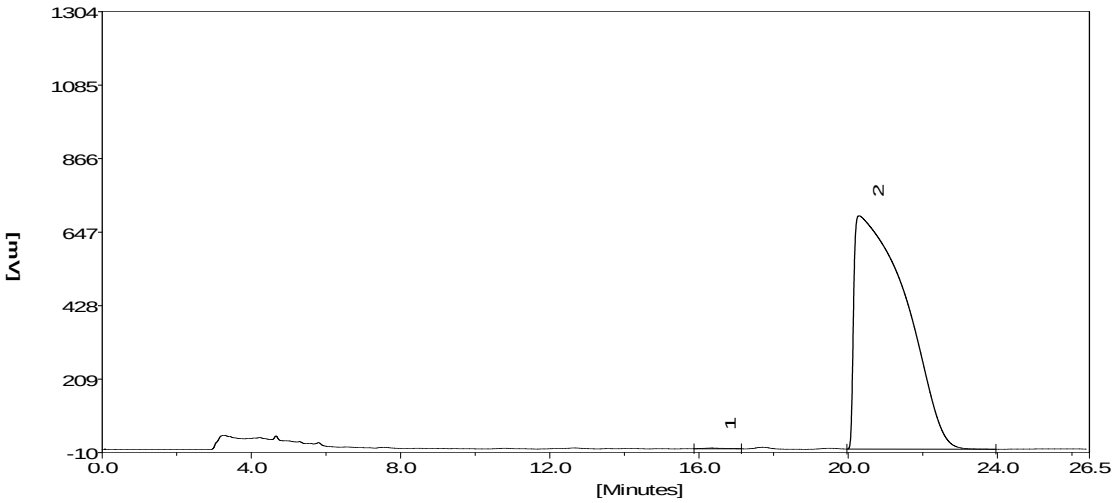
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	17.01083	443.35	13333.39	89.9131
2	22.44	44.14	1495.81	10.0869

Electronic Supplementary Material

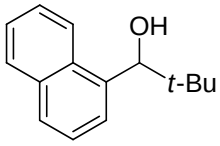
Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	16.325	2.17	81.35	0.1217
2	20.29083	695.42	66769.05	99.8783

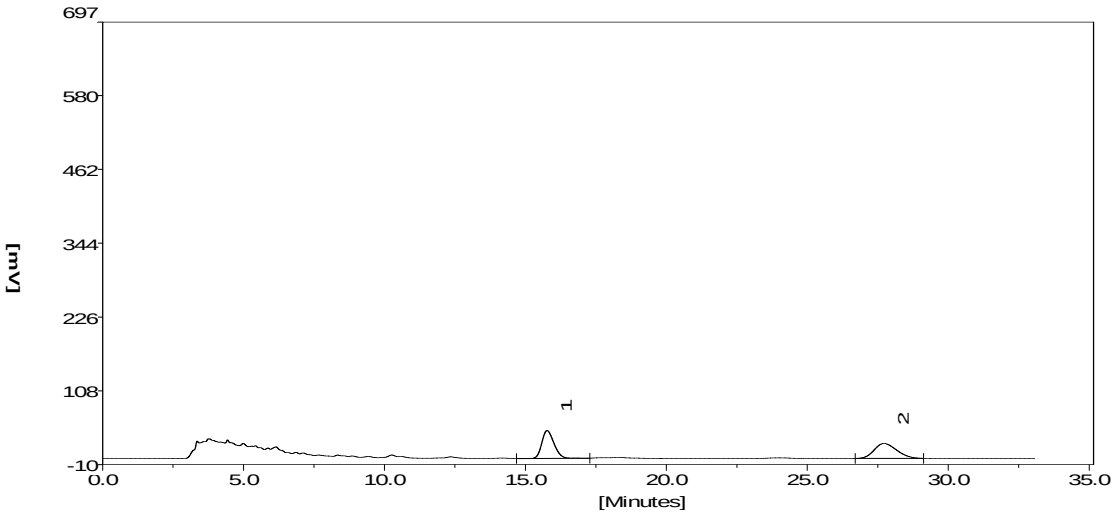
S = 59

Entry 7:



7

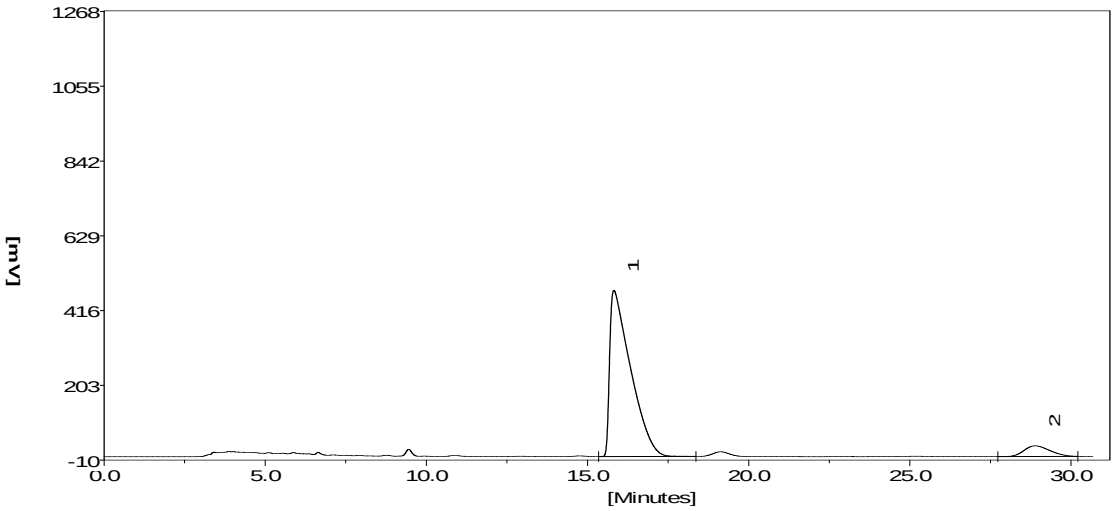
(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	15.7675	44.47	1323.48	50.0199
2	27.72	23.82	1322.43	49.9801

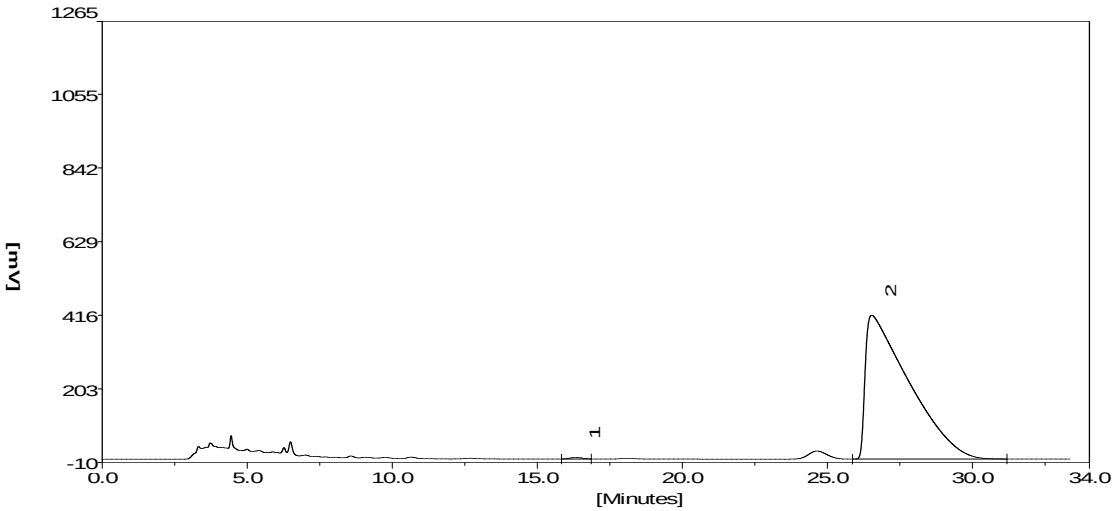
Electronic Supplementary Material

Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	15.8175	473.86	21333.47	92.6064
2	28.88083	30.52	1703.25	7.3936

Alcohol:

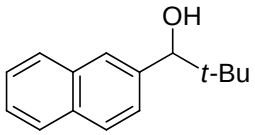


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	16.32167	4.39	128.51	0.2944
2	26.5275	415.93	43529.32	99.7056

S = 71

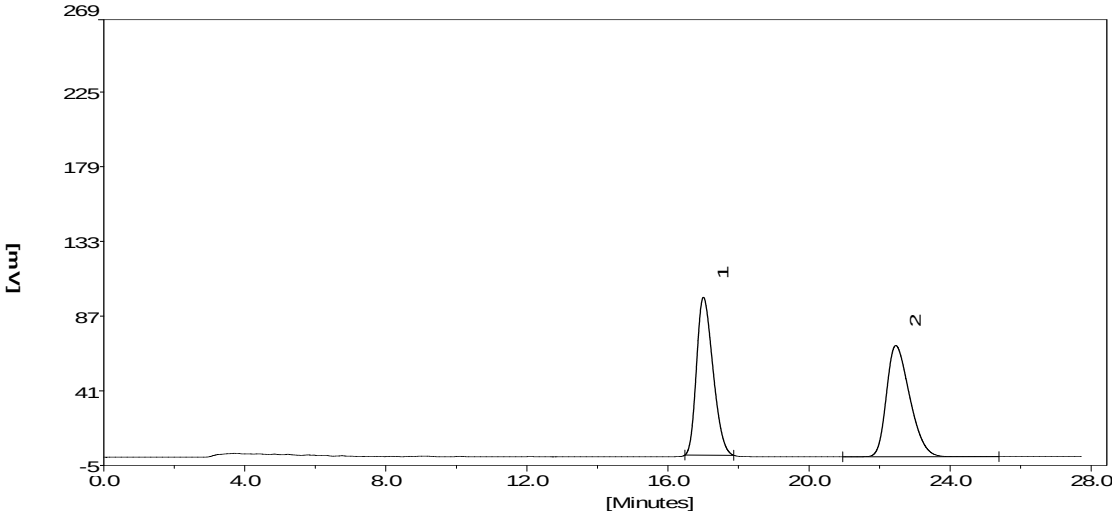
Electronic Supplementary Material

Entry 8:



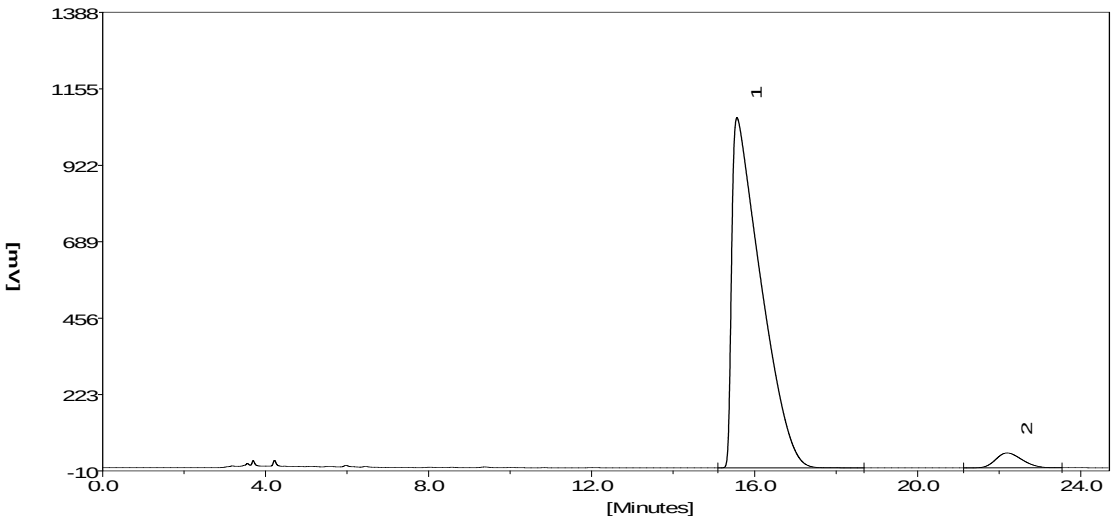
8

(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	17.00583	97.3	3140.41	50.0278
2	22.46083	68.52	3136.92	49.9722

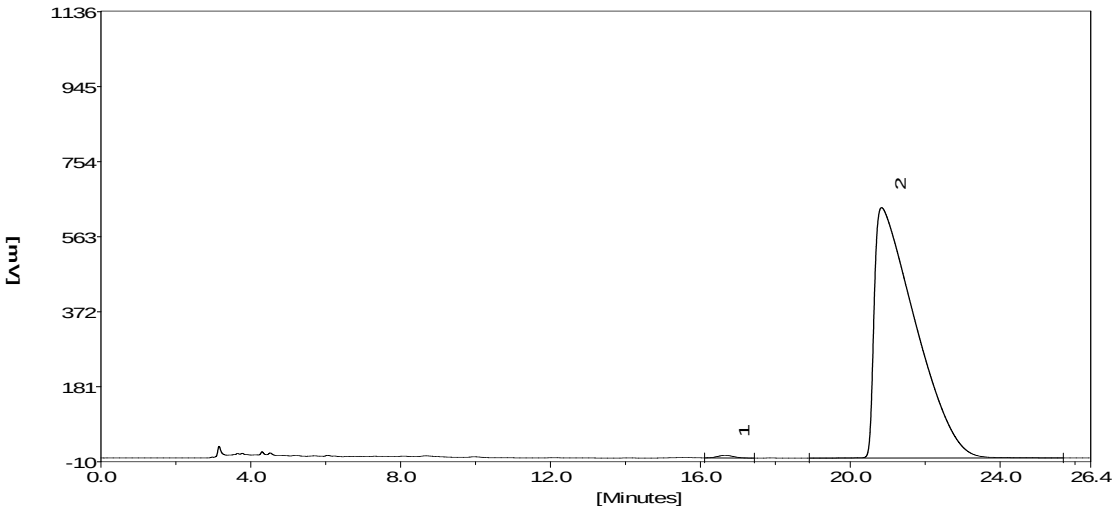
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	15.56667	1067.49	52763.99	96.2569
2	22.20167	45.64	2051.78	3.7431

Electronic Supplementary Material

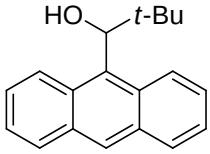
Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	16.66167	6.65	195.8	0.4036
2	20.83583	637.56	48314.84	99.5964

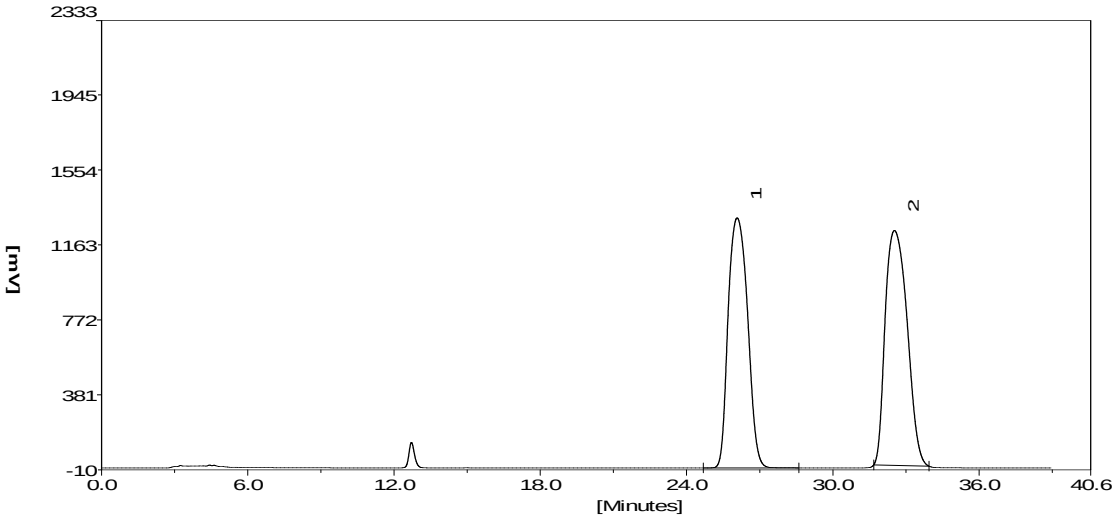
S = 142

Entry 9:



3

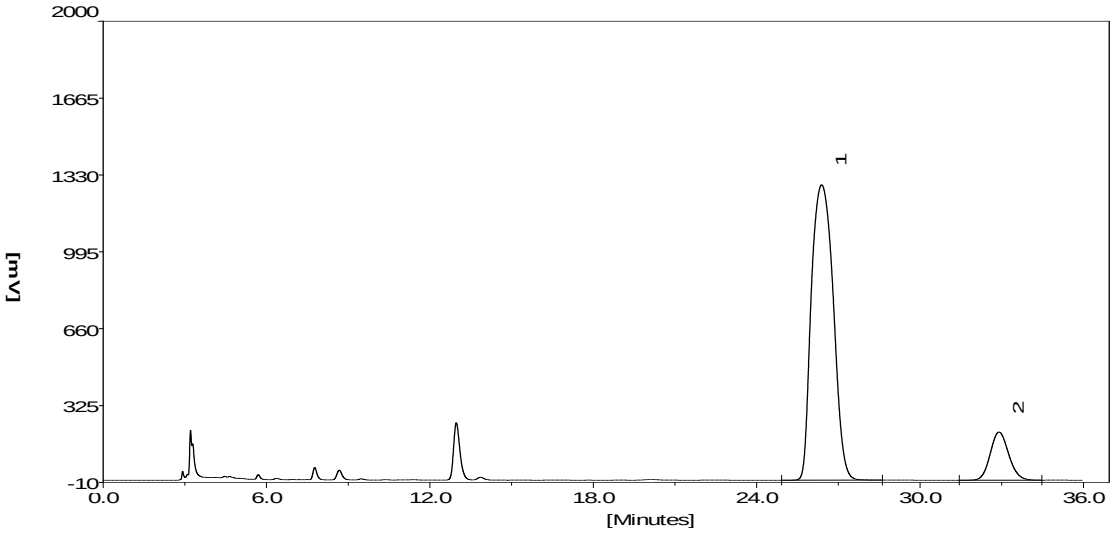
(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	26.07417	1304.29	72171.97	49.4943
2	32.52833	1224.81	76653.75	50.5057

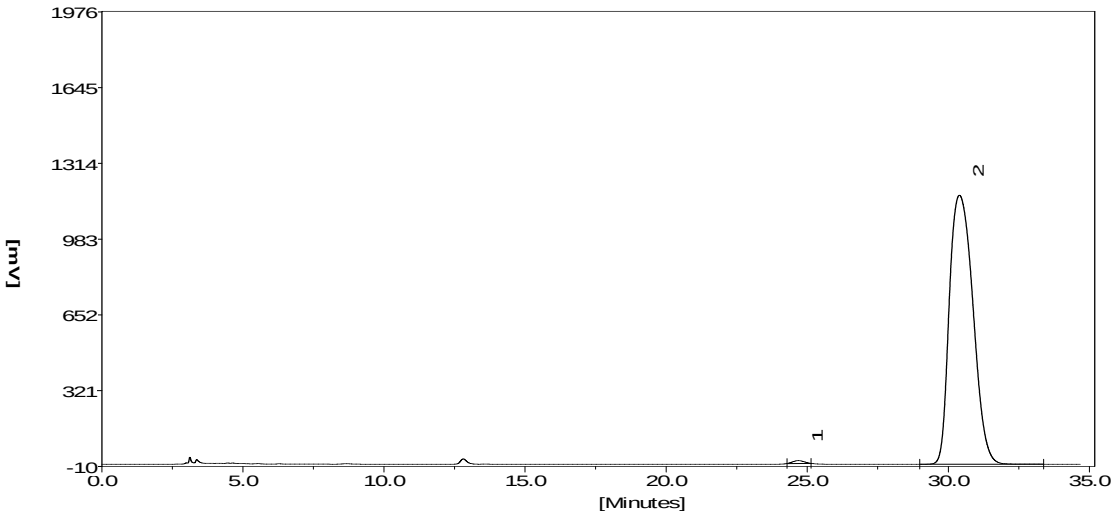
Electronic Supplementary Material

Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	26.38833	1287.2	71799.97	87.9359
2	32.90083	209.94	9850.38	12.0641

Alcohol:

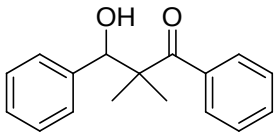


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	24.68583	12.49	346.52	0.4847
2	30.395	1175.25	68315.41	99.5153

S = 37

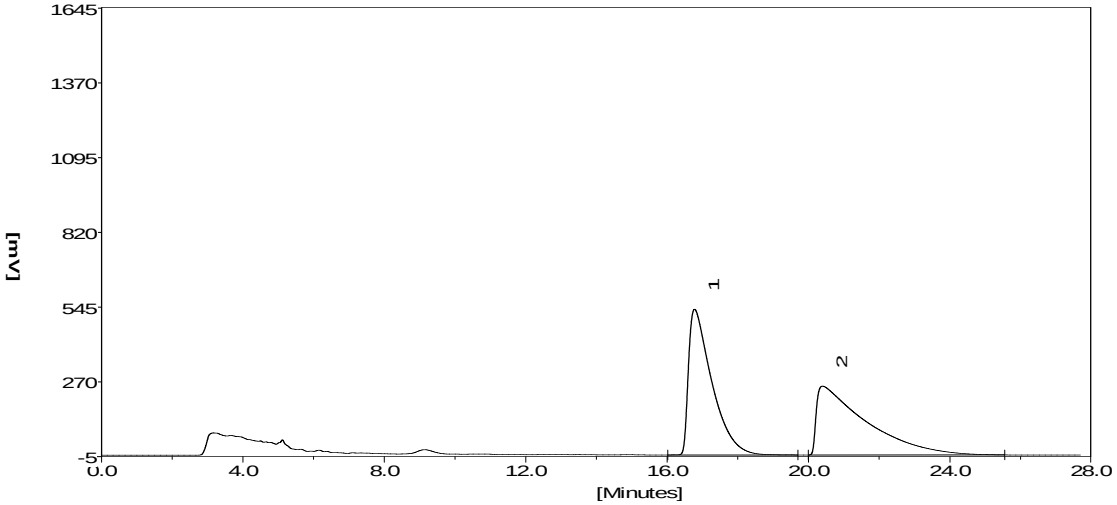
Electronic Supplementary Material

Entry 10



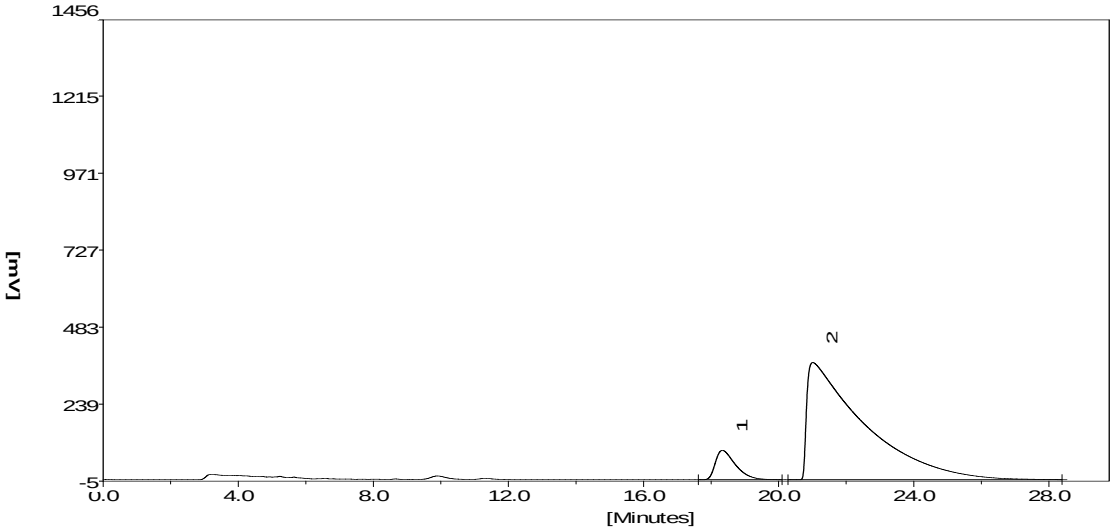
9

Racemate of ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	16.77833	536.29	24513.49	49.9368
2	20.39833	253.4	24575.51	50.0632

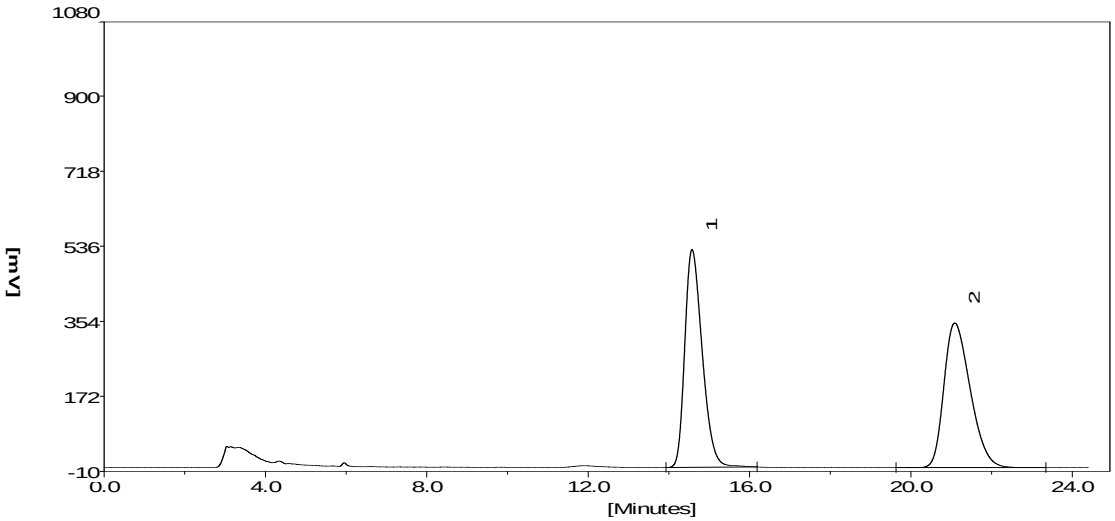
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	18.33583	93.14	3850.63	8.1104
2	21.01083	371.25	43627.26	91.8896

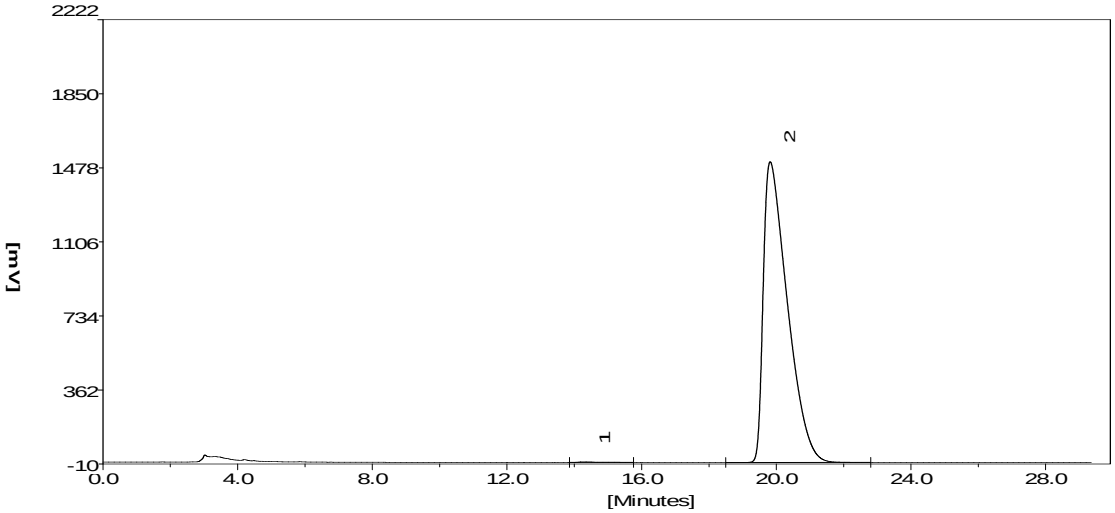
Electronic Supplementary Material

Racemate of alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	14.57417	527.93	15848.11	49.9903
2	21.0875	350.55	15854.26	50.0097

Alcohol:

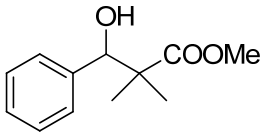


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	14.32667	3.03	128.33	0.1712
2	19.81833	1510.83	74827.81	99.8288

S = 68

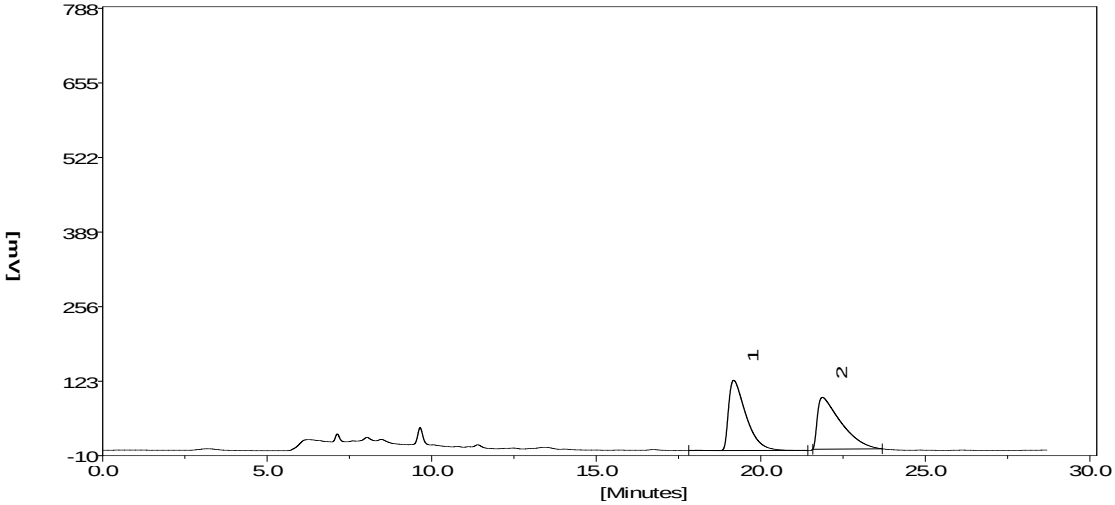
Electronic Supplementary Material

Entry 11:



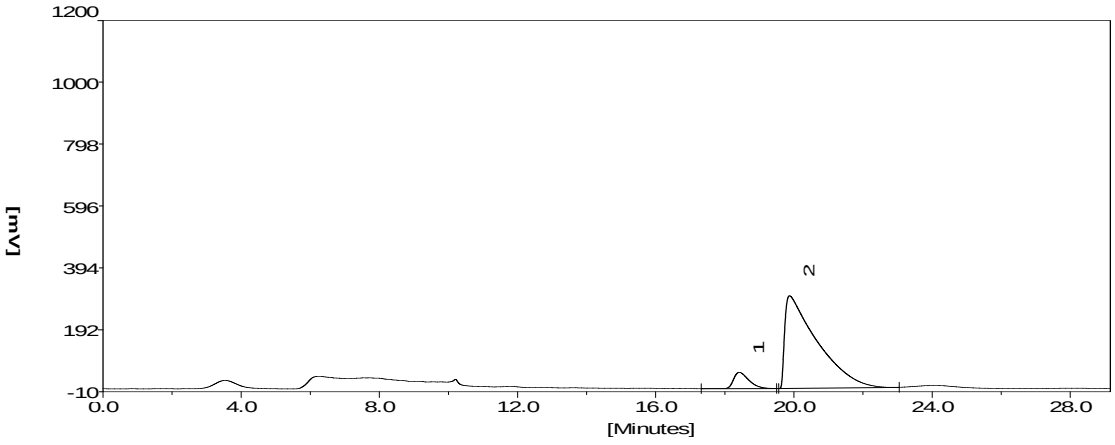
10

Racemate of ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	19.17833	125.37	4593.01	50.0032
2	21.8725	92.65	4592.43	49.9968

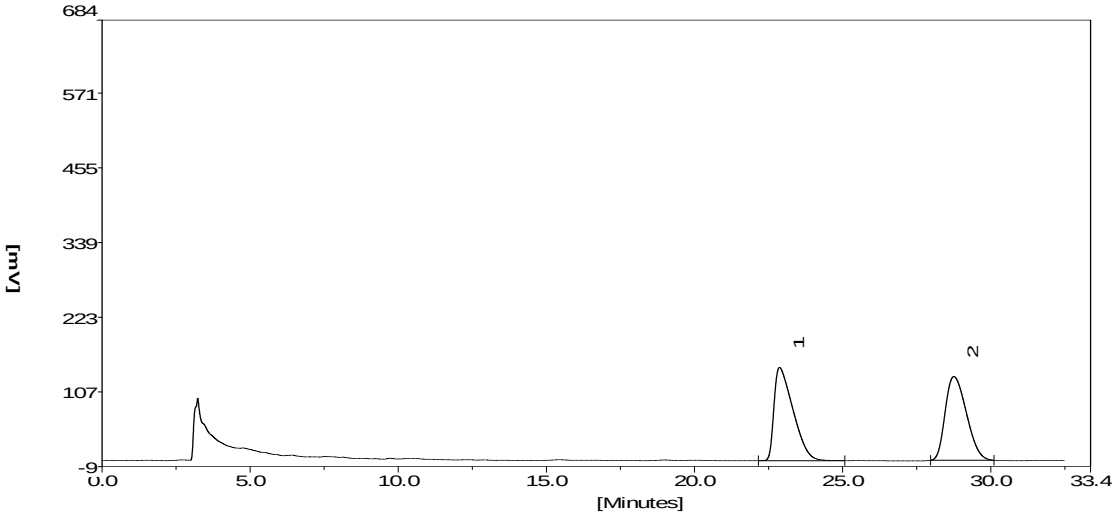
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	18.42	52.35	1539.63	7.3308
2	19.87583	300.91	19462.56	92.6692

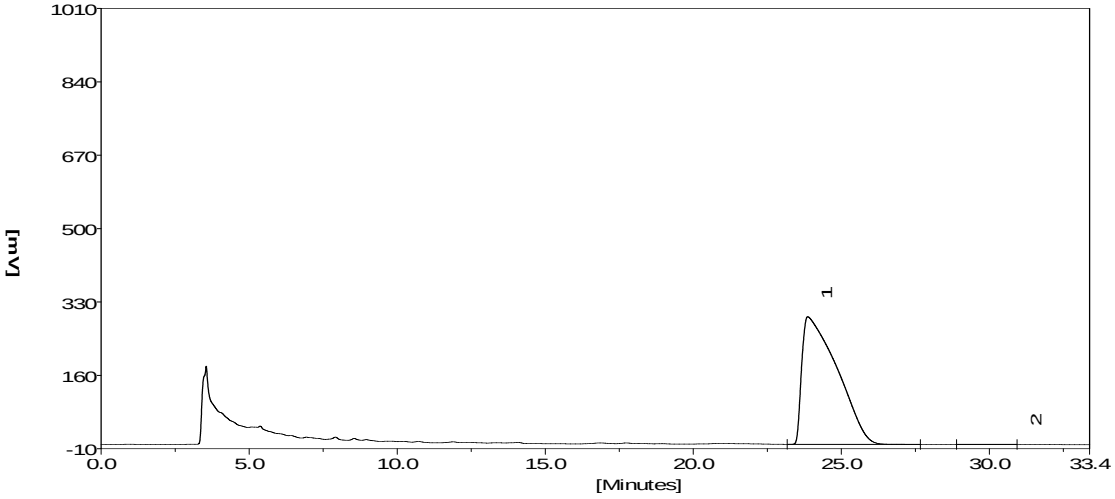
Electronic Supplementary Material

Racemate of alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	22.8675	144.73	6437.43	49.8832
2	28.75167	130.04	6467.58	50.1168

Alcohol:

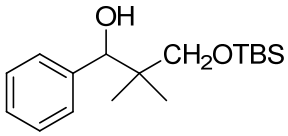


1	23.86917	295.76	24362.41	99.9030
2	30.93583	0.01	23.65	0.0970

S = 85

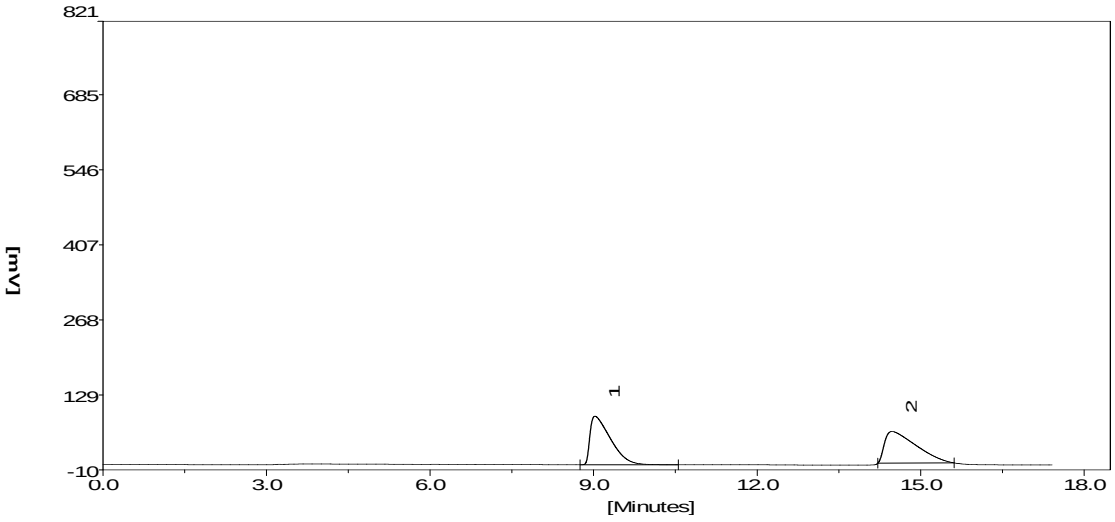
Electronic Supplementary Material

Entry 12:



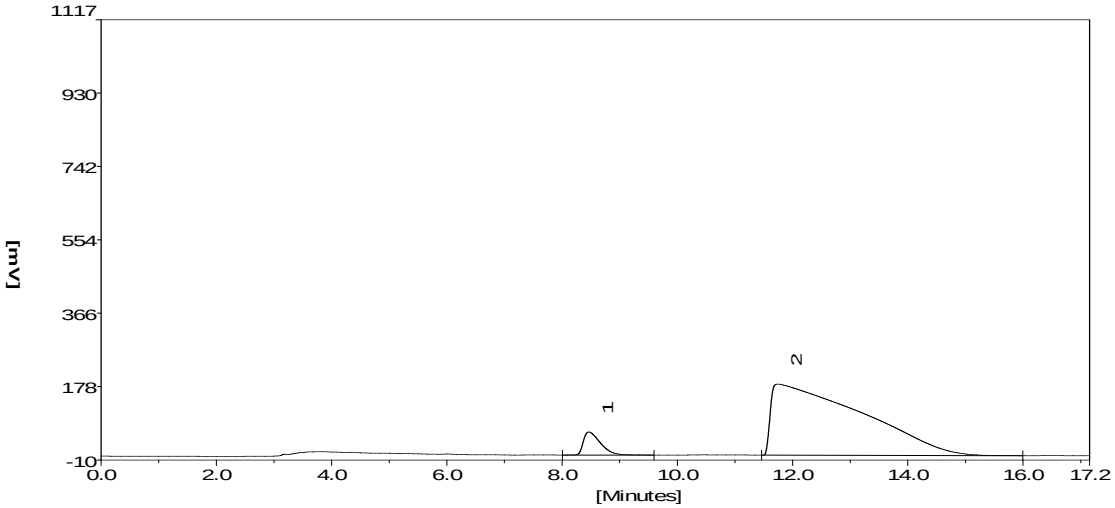
11

Racemate of ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	9.02583	89.96	2348.99	49.9785
2	14.4725	58.7	2351.01	50.0215

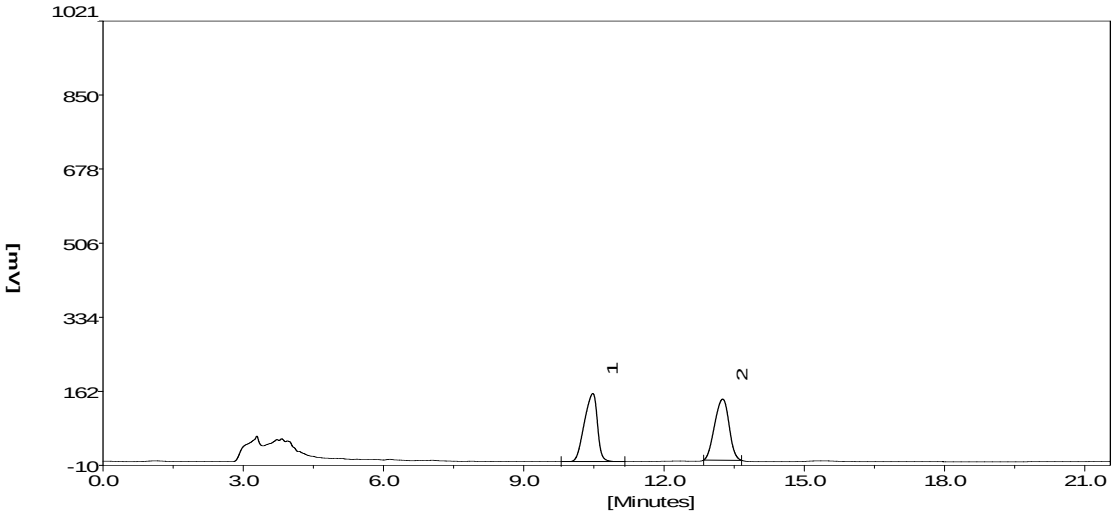
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	8.46417	59.24	1218.52	5.7407
2	11.74	182.02	20007.53	94.2593

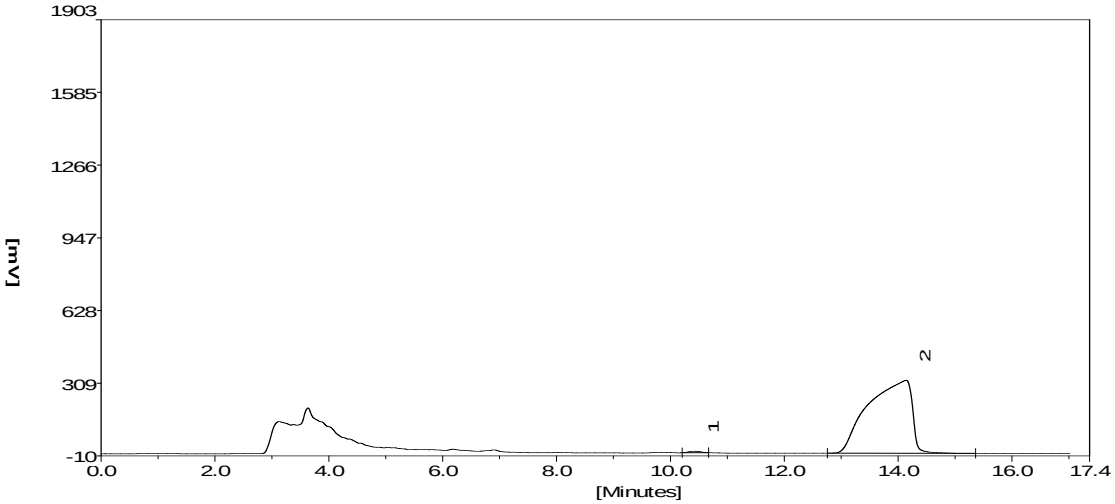
Electronic Supplementary Material

Racemate of alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	10.47917	158.21	3057.06	50.1891
2	13.25583	142.08	3034.03	49.8109

Alcohol:

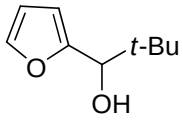


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	10.42	6.14	90.24	0.4861
2	14.14167	320.65	17064.39	99.5139

S = 86

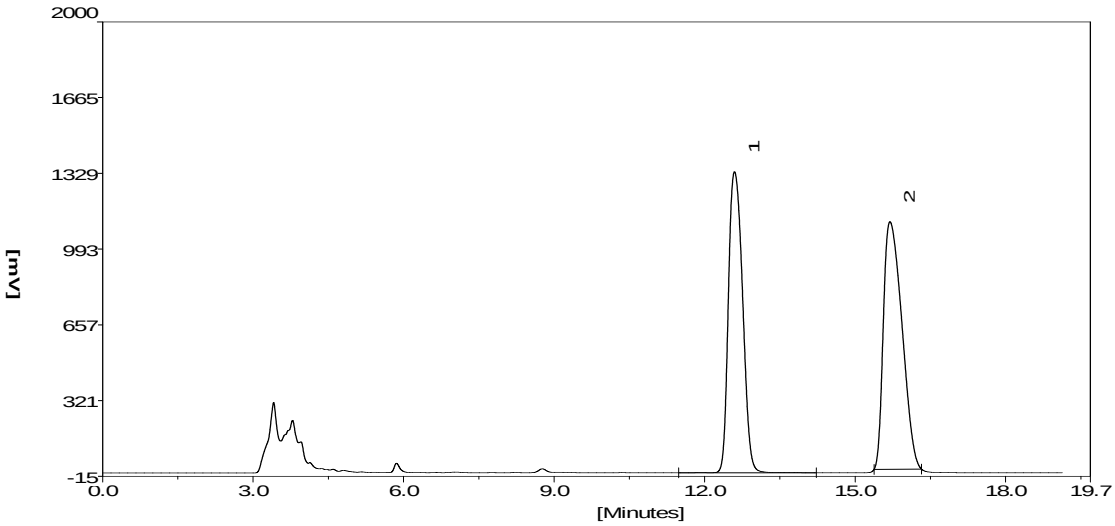
Electronic Supplementary Material

Entry 13:



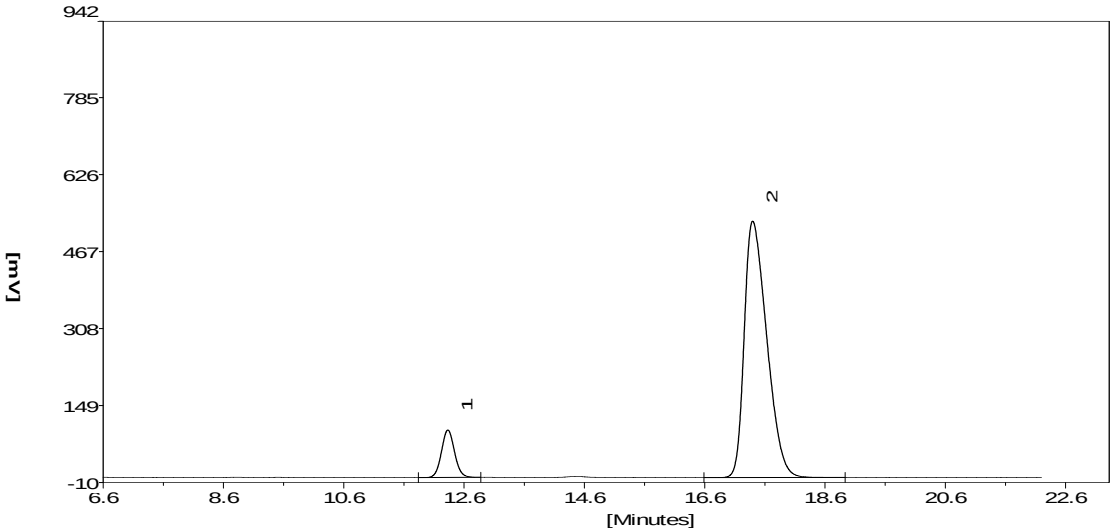
12

(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.59583	1335.39	26222.24	48.2104
2	15.695	1098.05	28169.07	51.7896

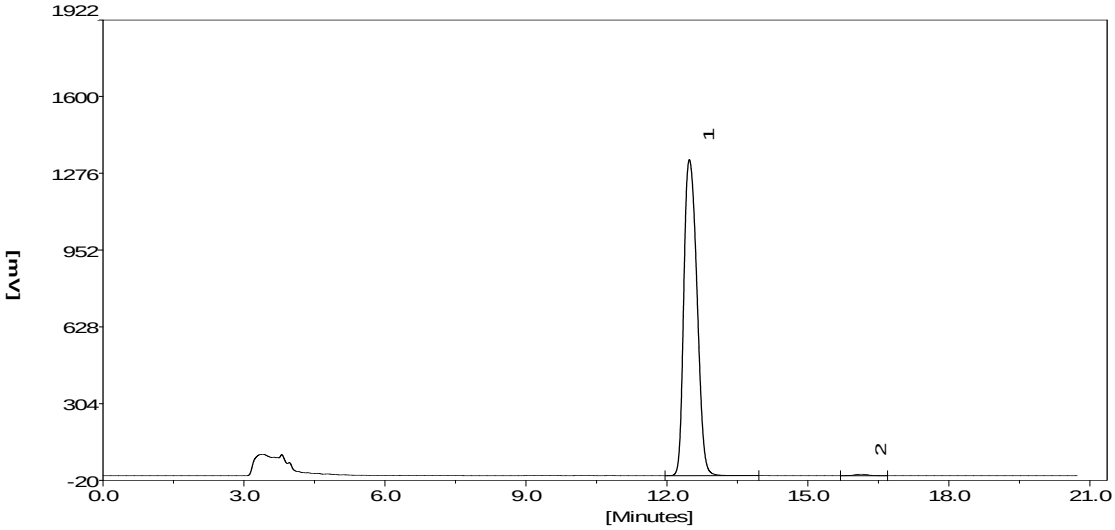
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.34417	98.08	1474.31	9.6779
2	17.4125	529.56	13759.51	90.3221

Electronic Supplementary Material

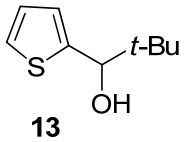
Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.47833	1333.33	25850.56	99.5367
2	16.13917	6.23	120.32	0.4633

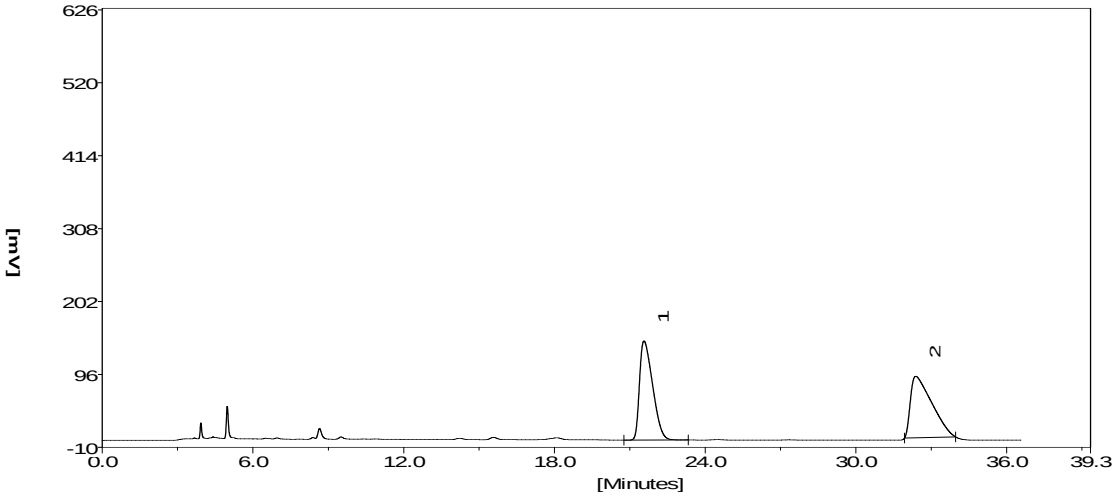
S = 48

Entry 14:



13

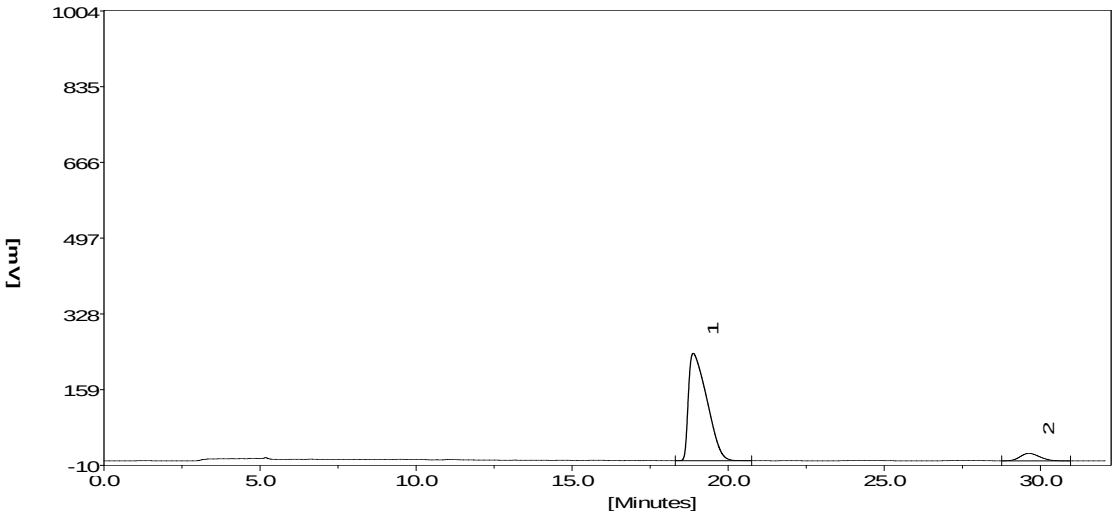
(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	21.56667	144.26	5201.94	49.7172
2	32.38	89.59	5261.13	50.2828

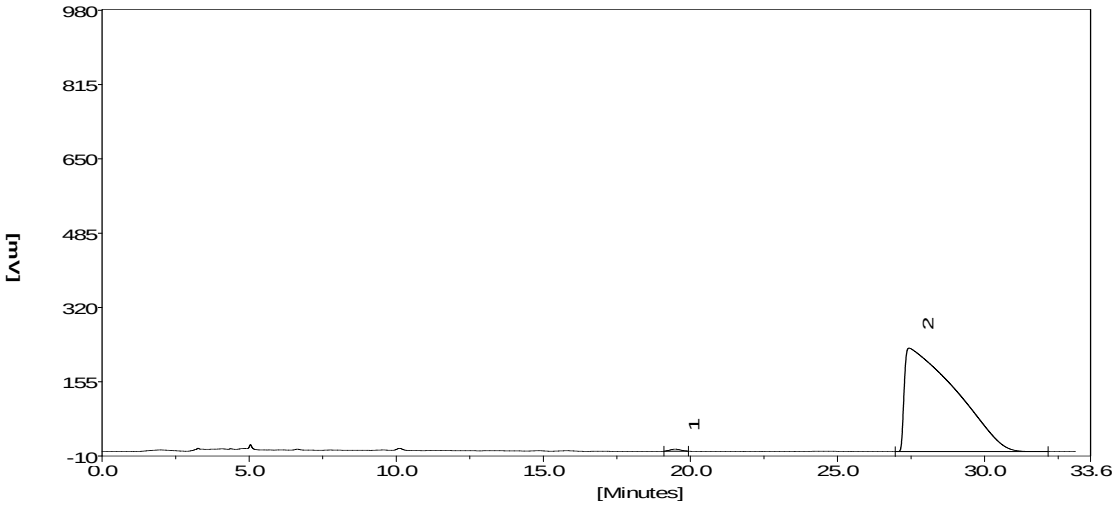
Electronic Supplementary Material

Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	18.87917	239.86	9789.98	93.1408
2	29.63417	16.64	720.97	6.8592

Alcohol:

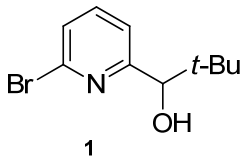


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	19.47667	4.54	113.35	0.4093
2	27.43083	229.93	27579.08	99.5907

S = 73

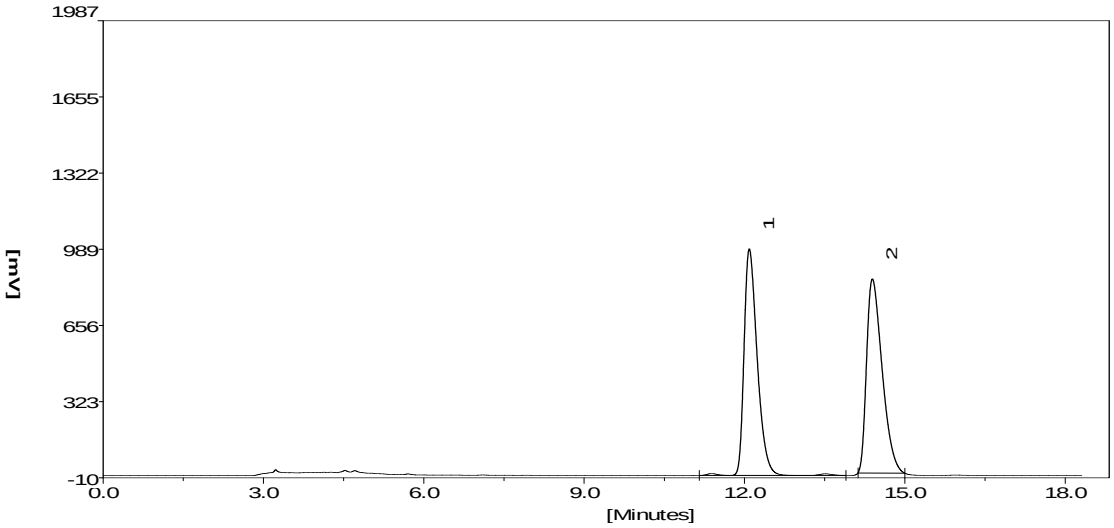
Electronic Supplementary Material

Entry 15:



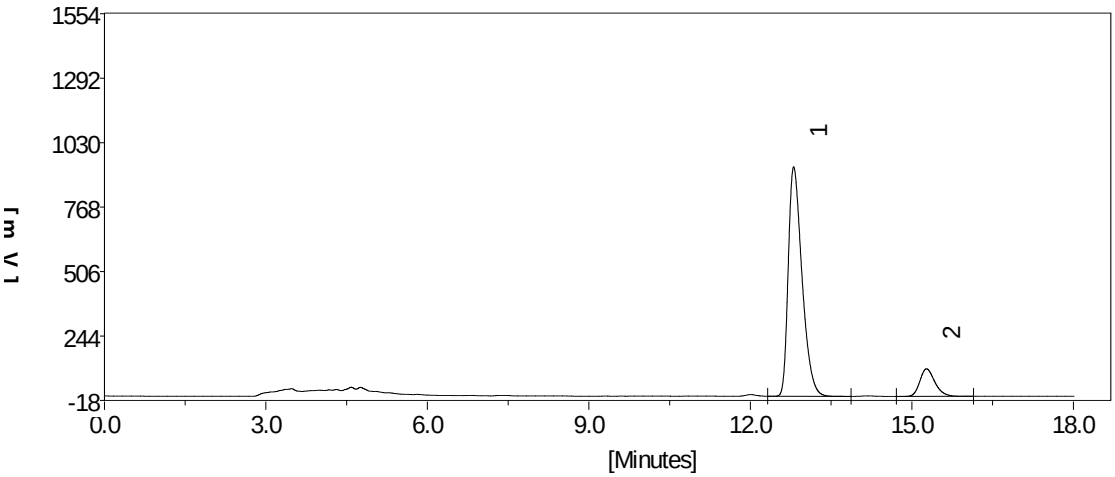
1

(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.09	990.57	17052.55	49.3048
2	14.39333	855.44	17533.45	50.6952

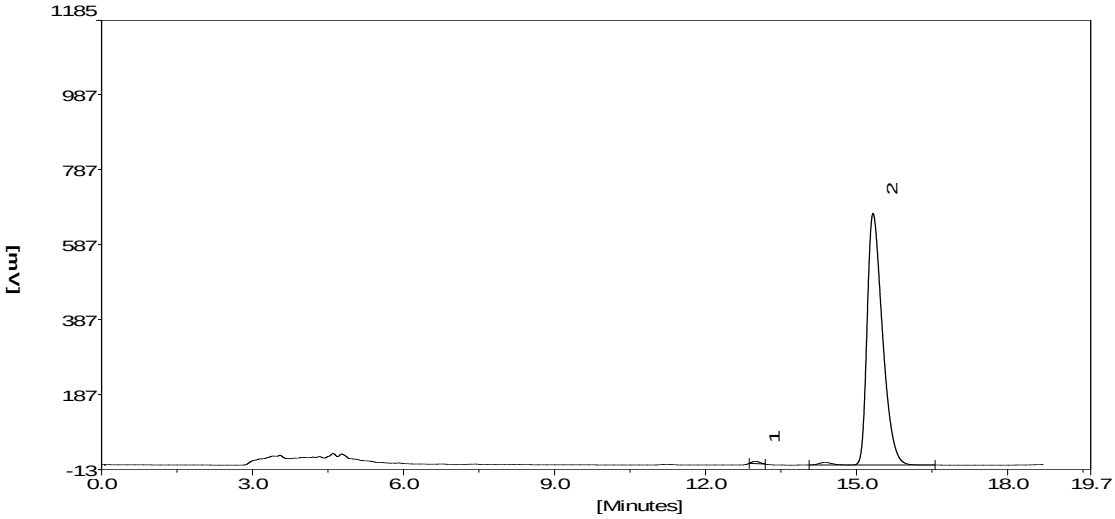
Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.805	932.75	16546.38	88.3905
2	15.27333	112.27	2173.27	11.6095

Alcohol:

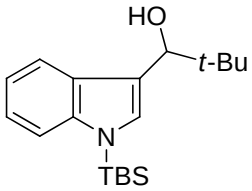
Electronic Supplementary Material



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.98917	6.24	67.50	0.4704
2	15.32833	670.93	14282.37	99.5296

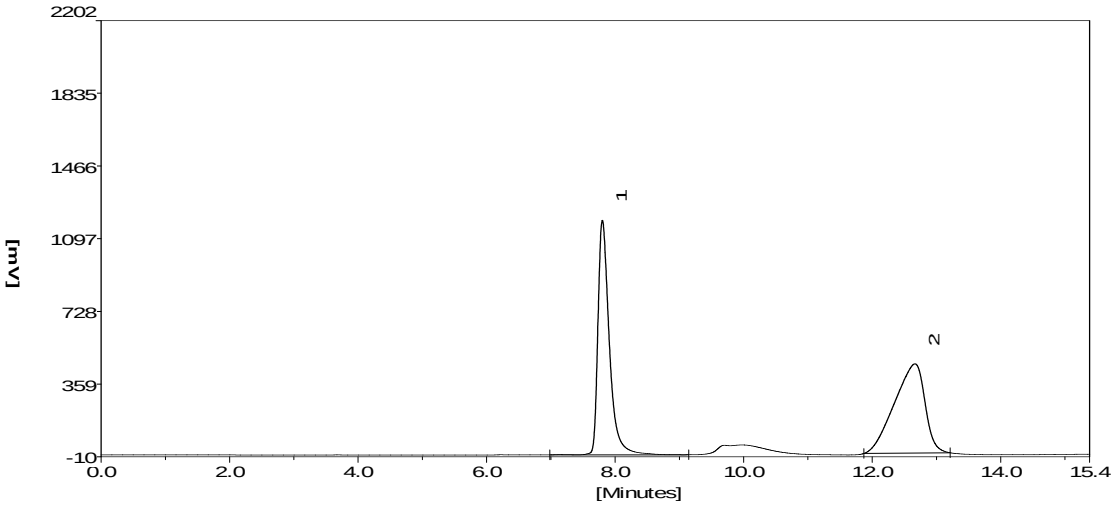
S = 39

Entry 16:



14

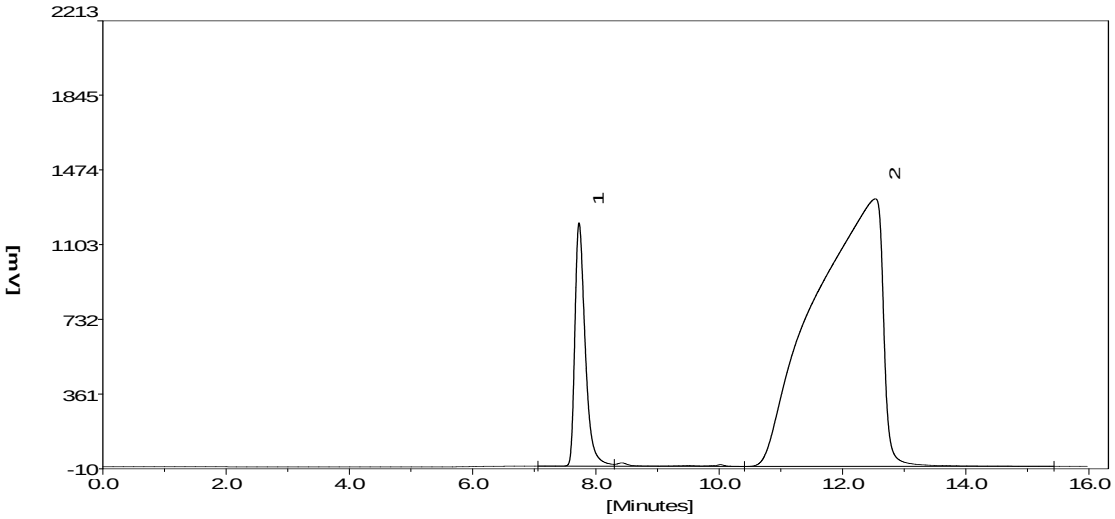
Racemate of ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	7.80167	1190.24	14659.78	49.5604
2	12.66583	452.56	14919.82	50.4396

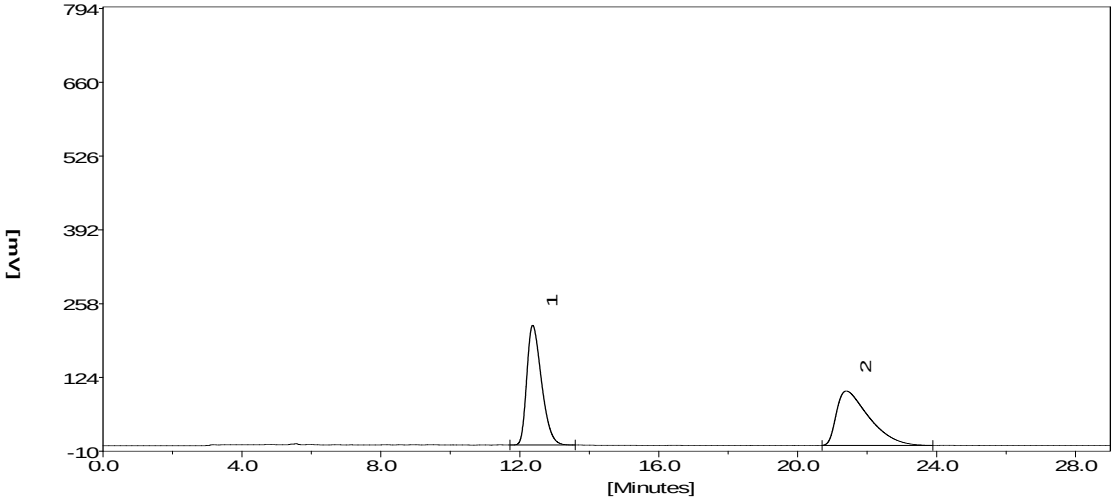
Ester:

Electronic Supplementary Material



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	7.72583	1207.46	14098.9	12.2136
2	12.53417	1327.55	101337.5	87.7864

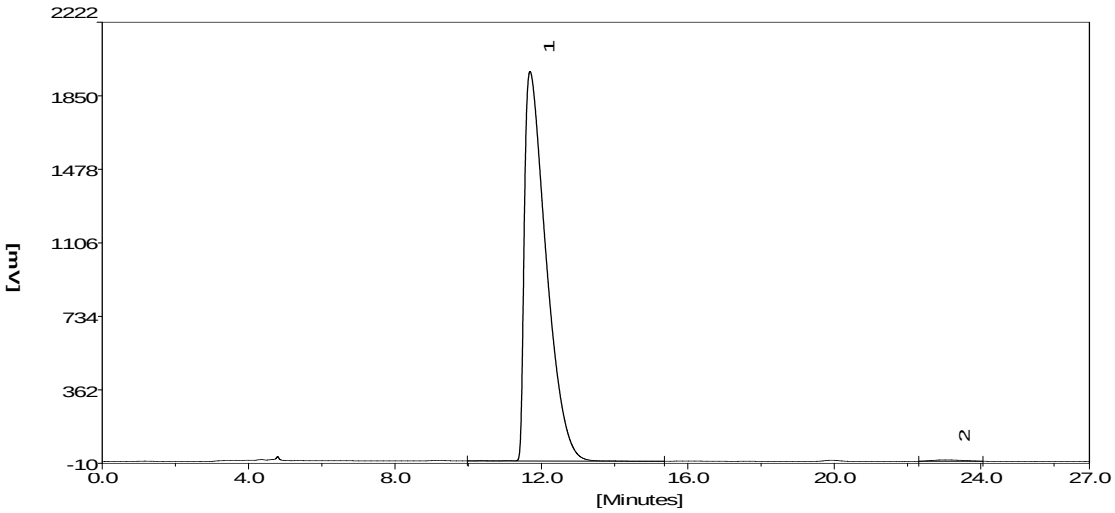
Racemate of alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	12.37333	217.52	6402.74	50.0152
2	21.3975	98.81	6398.85	49.9848

Alcohol:

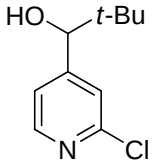
Electronic Supplementary Material



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	11.68667	1971.31	81117.52	99.5155
2	23.02667	6.96	394.91	0.4845

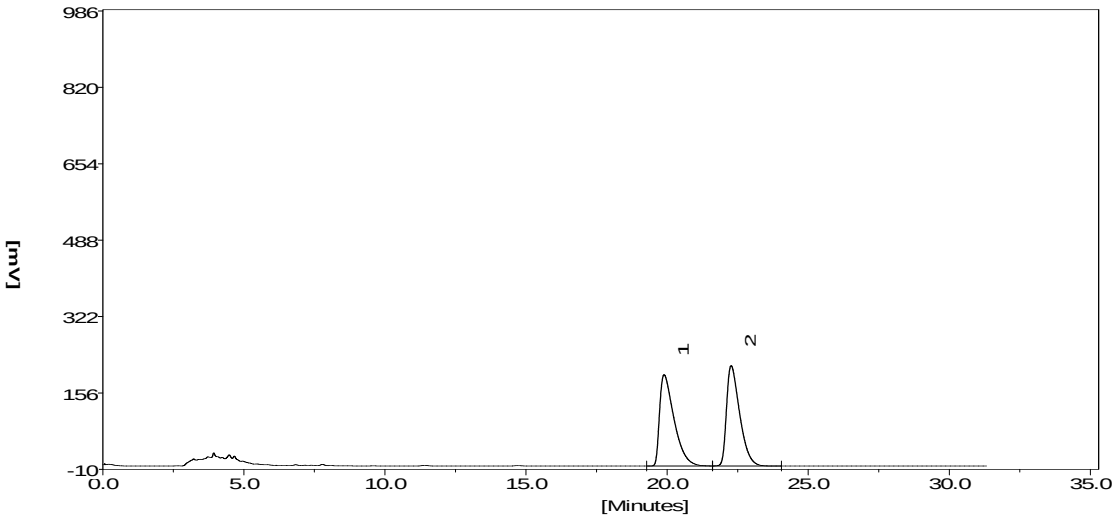
S = 37

Entry 17:



15

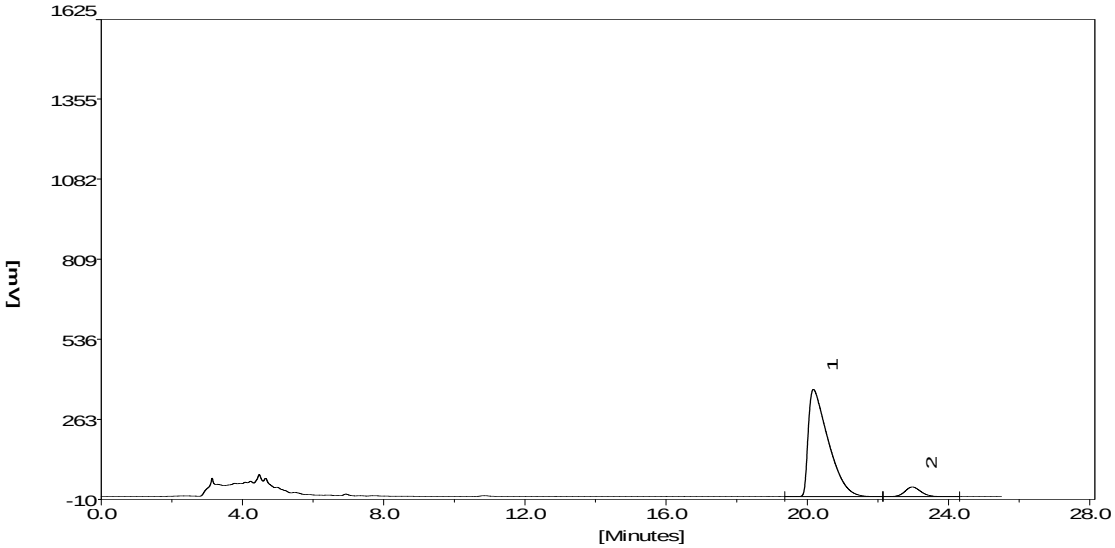
(rac)



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	19.89333	198.48	7069.49	50.007
2	22.27083	218.26	7067.53	49.993

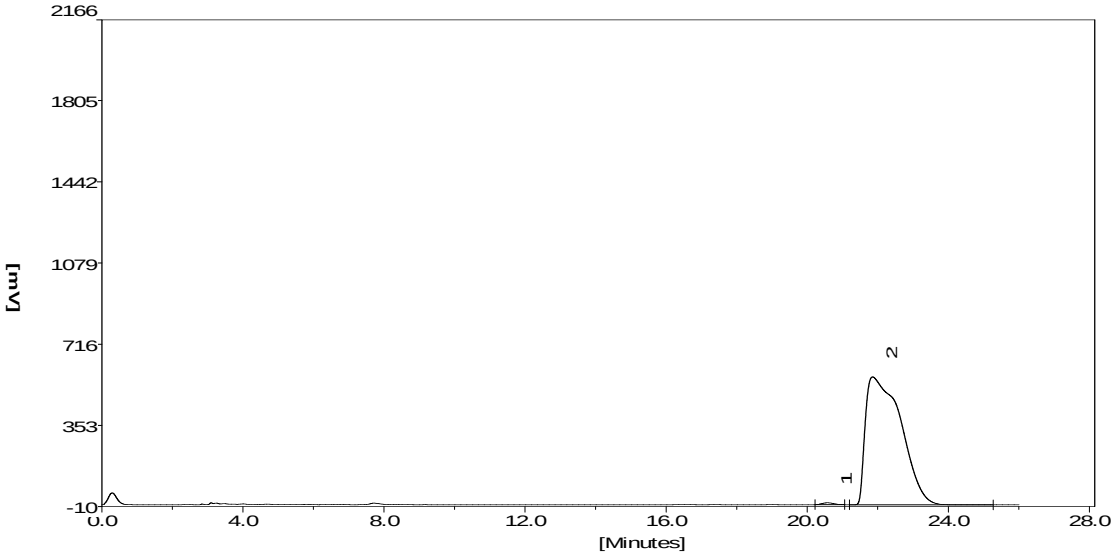
Ester:

Electronic Supplementary Material



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	20.17333	365.12	14294.88	93.3559
2	22.97333	32.67	1017.36	6.6441

Alcohol:

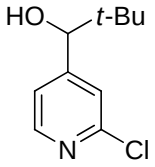


Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	20.57083	8.60	199.61	0.4985
2	21.85333	571.86	39839.89	99.5015

S = 74

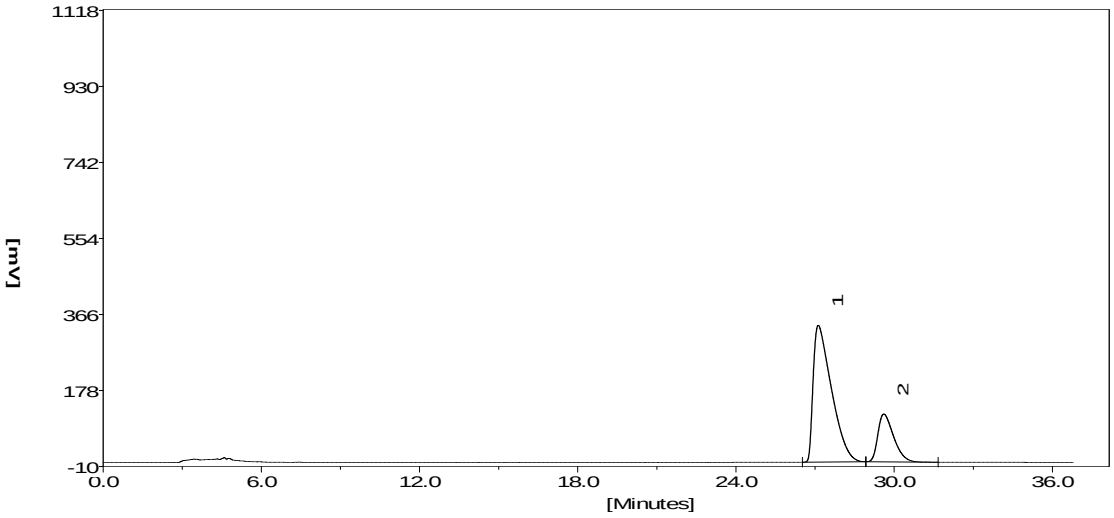
Entry 18:

Electronic Supplementary Material



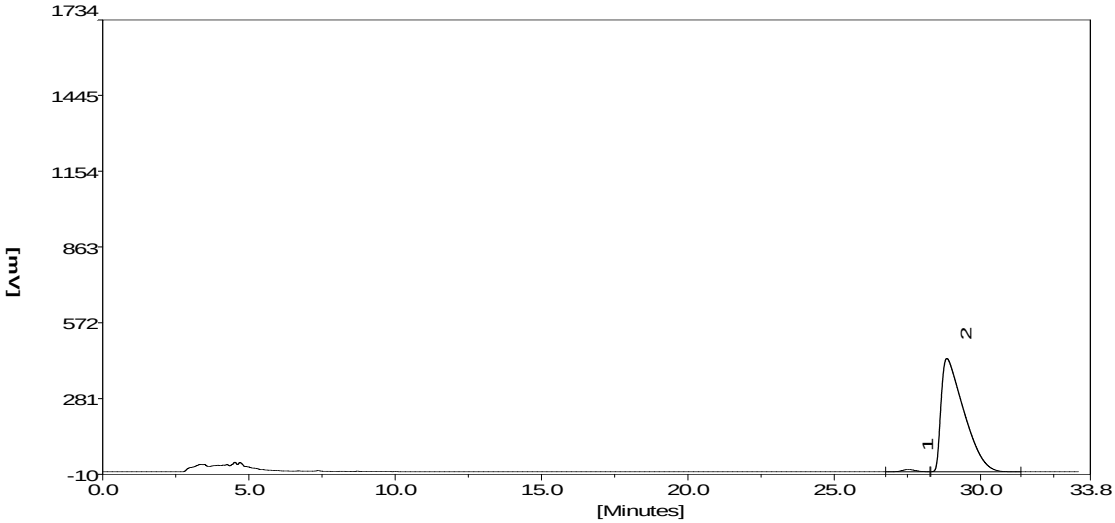
15

Ester:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	27.12250	338.48	16273.06	76.8176
2	29.60750	118.56	4910.97	23.1824

Alcohol:



Peak #	Time (min)	Hight(mV)	Area(mV.sec)	Area(%)
1	27.53250	8.85	281.40	1.1838
2	28.84917	435.21	23488.63	98.8162

S = 13