CHEMISTRY
AN ASIAN JOURNAL

Supporting Information

Asymmetric Resolution in Ester Reduction by $NaBH_4$ at the Interface of Aqueous Aggregates of Amino Acid, Peptide, and Chiral Counter-ion based Cationic Surfactants

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Supporting Information

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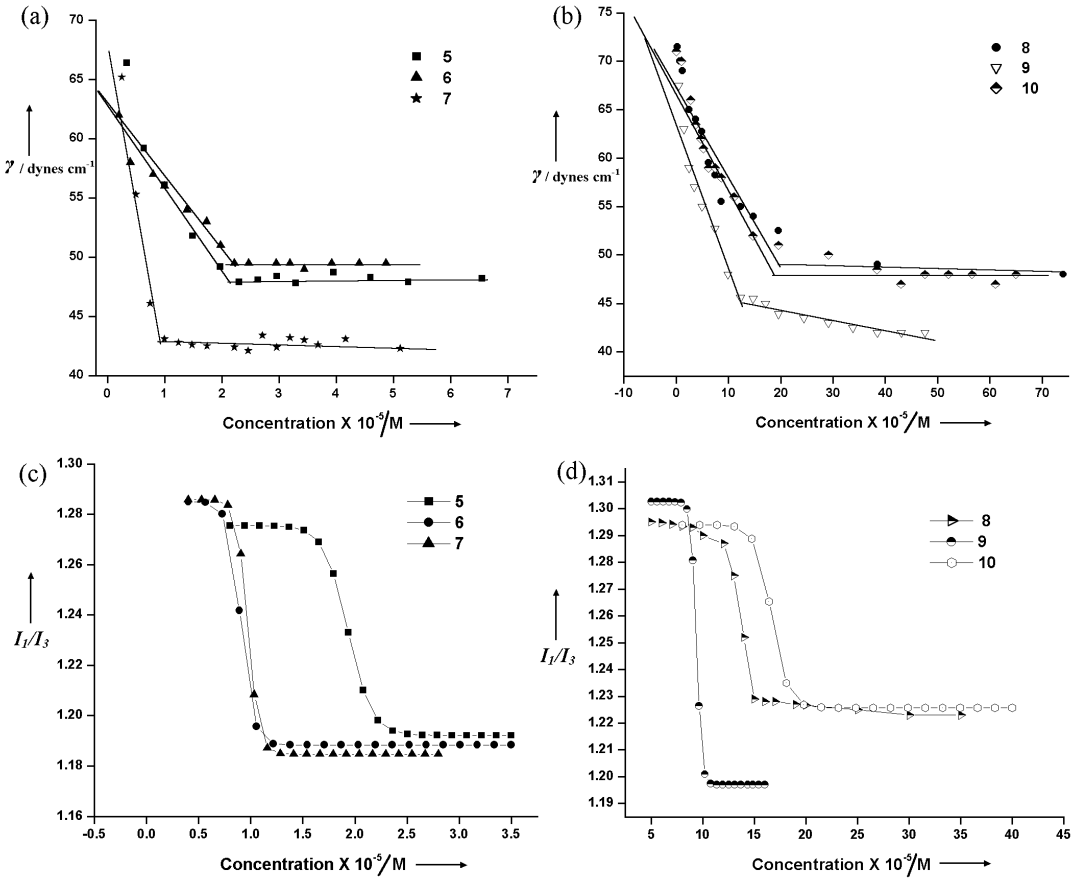

(a)
γ / dynes cm-1
Concentration X 10-5/M
5
6
7
(b)
γ / dynes cm-1
Concentration X 10-5/M
8
9
10
(c)
I1/I3
Concentration X 10-5/M
5
6
7
(d)
I1/I3
Concentration X 10-5/M
8
9
10

Figure 1

Syntheses of Esters [Hydroxy-phenyl-acetic acid hexyl ester (**I**), 2-Phenoxy-propionic acid hexyl ester (**II**), 2-Phenyl-propionic acid hexyl ester (**III**), 2-Phenyl-butyric acid hexyl ester (**IV**) and Methoxy-phenyl-acetic acid hexyl ester (**V**)]**:** The ester molecules were prepared following the usual *N, N*- dicyclohexylcarbodiimide (DCC) coupling of the corresponding acid and the *n*-hexanol in presence of 4-*N*,*N*-(dimethylamino)pyridine (DMAP). In brief, the acid (1 equivalent) was coupled with the alcohol (1 equivalent) in the presence of 1.1 equivalent of both DMAP and DCC in dry DCM under nitrogen atmosphere at ice-salt temperature and allowing the mixture to reach the room temperature. After overnight stirring, the reaction mixture was filtered and the concentrated filtrate was extracted with ether. The ether part was washed with water and dried over anhydrous sodium sulphate. Ether was concentrated in a rotary evaporator and the desired product was purified through a silica gel (60-120 mesh) column chromatography with acetone/hexane solvent mixture as elutant.

^{1}H NMR (300MHz, $CDCl_3$) and elemental analysis of the esters (I)-(V) :

^{1}H NMR of **(I)** : δ/ppm = 7.36 – 7.21 [m, 5H], 5.09 [d, ½ H], 4.08 [t, 2H), 3.43 [d, ½ H], 1.53 – 1.45 [m, 2H], 1.25 – 1.12 [m, 6H], 0.77 [t, 3H]. E.A: calculated for $C_{14}H_{20}O_3$ C, 71.16; H, 8.53. Found : C, 71.48; H, 8.40.

^{1}H NMR of **(II)**: δ/ppm = 7.23-7.29 [m, 2H], 6.96 [t, 1H], 6.85 [d, 2H], 4.71-4.78 [m, 1H], 4.1-4.18 [m, 2H], 1.54-1.63 [m, 5H], 1.23-1.99 [m, 6H], 0.86 [t, 3H]. E.A: calculated for $C_{15}H_{22}O_3$: C, 71.97; H, 8.86. Found : C, 71.72; H, 8.68.

^{1}H NMR of **(III)**: δ/ppm = 7.23-7.31 [m, 5H], 4.05 [t, 2H], 3.69-3.71 [m,1H], 1.48-1.63 [m, 5H], 1.17-1.37 [m, 6H], 0.85 [t, 3H]. E.A: calculated for $C_{15}H_{22}O_2$: C, 76.88; H, 9.46. Found : C, 76.72; H, 9.39.

^{1}H NMR of **(IV)**: δ/ppm = 7.23-7.31 [m, 5H], 4.02-4.09 [m, 2H], 3.43 [t, 1H], 1.74-1.84 [m, 2H], 1.51-1.58 [m, 2H], 1.24-1.33 [m, 6H], 0.85 [t, 6H]. E.A: calculated for $C_{16}H_{24}O_2$: C, 77.38; H, 9.74. Found : C, 77.26; H, 9.69.

^{1}H NMR of **(V)**: δ/ppm = 7.43-7.45 [m, 1H], 7.26-7.38 [m, 4H], 4.75 [s,1H], 4.11 [t, 2H], 3.41 [s, 3H], 1.54-1.61 [m, 2H], 1.21 [m, 6H], 0.84 [t, 3H]. E.A: calculated for $C_{15}H_{22}O_3$: C, 71.97; H, 8.86. Found : C, 71.88; H, 8.75.

^{1}H NMR (300MHz, $CDCl_3$) and elemental analysis of the alcohols produced by reduction of esters (I)-(V) :

^{1}H NMR of 2-Hydroxy-1-phenylethanol obtained from reduction of **I**: δ/ppm = 7.31-7.19 [m, 5H], 4.78 [br, 1H], 4.01 [br, 2H]. E.A: calculated for $C_8H_{10}O_2$: C, 69.54; H, 7.30. Found: C, 69.28; H, 7.50.

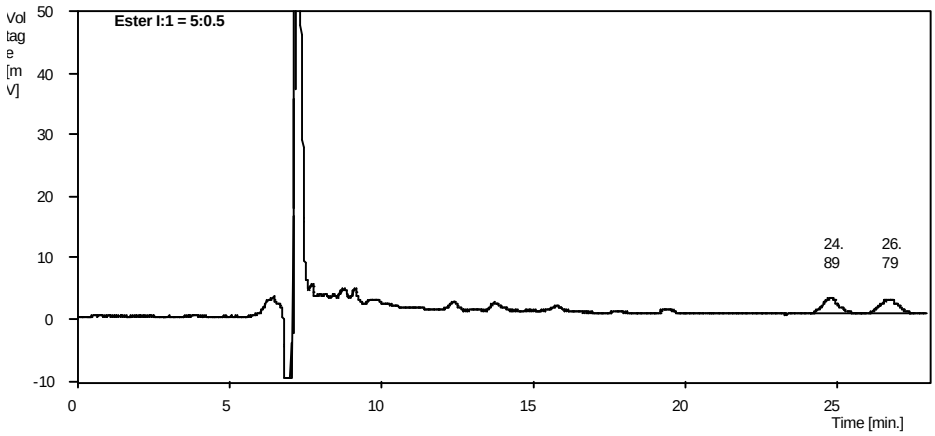
^{1}H NMR of 2-Phenoxy-propan-1-ol obtained from reduction of **II**: δ/ppm = 7.26-7.31[m, 3H], 6.86-6.99 [m, 2H], 4.48-4.53 [m, 1H], 3.74 [t, 2H], 1.58 [m, 3H]. E.A: calculated for $C_9H_{12}O_2$: C, 71.03; H, 7.95. Found: C, 71.24; H, 7.83.

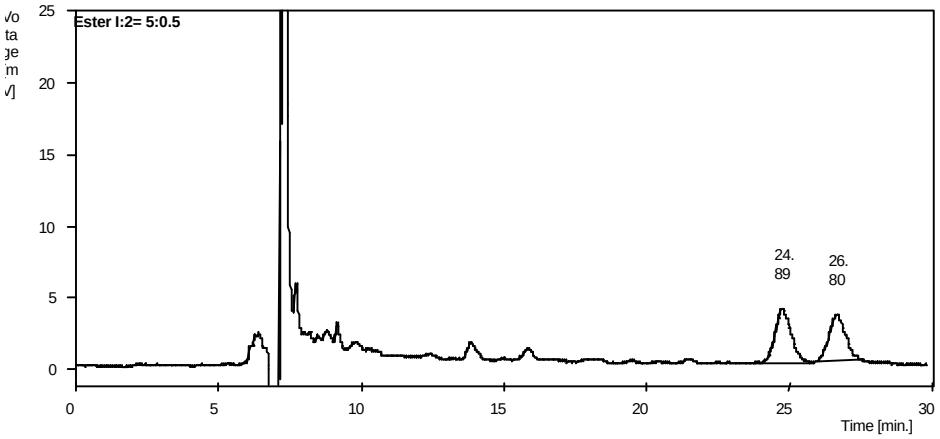
^{1}H NMR of 2-phenyl propan-1-ol obtained from reduction **III**: δ/ppm = 7.29-7.36 [m, 2H], 7.21-7.25 [m, 3H], 3.69 [t, 2H], 2.90-2.99 [m, 1H], 1.25-1.29 [m,3H]. E.A: calculated for $C_9H_{12}O$: C, 79.37; H, 8.88. Found: C, 79.32; H, 8.81.

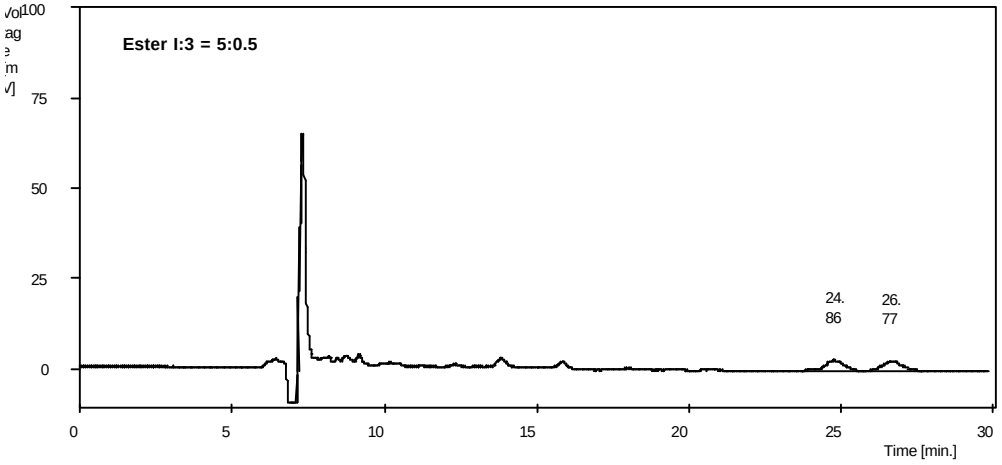
^{1}H NMR of 2-phenyl butan-1-ol obtained from reduction of **IV**: δ/ppm = 7.31-7.35 [m, 2H], 7.1-7.27 [m, 3H], 3.69-3.81[m, 2H], 2.64-2.72 [m, 1H], 1.53-1.69 [m, 2H], 0.83 (t, 3H). E.A: calculated for $C_{10}H_{14}O$: C, 79.96; H, 9.39. Found: C, 79.89; H, 9.51.

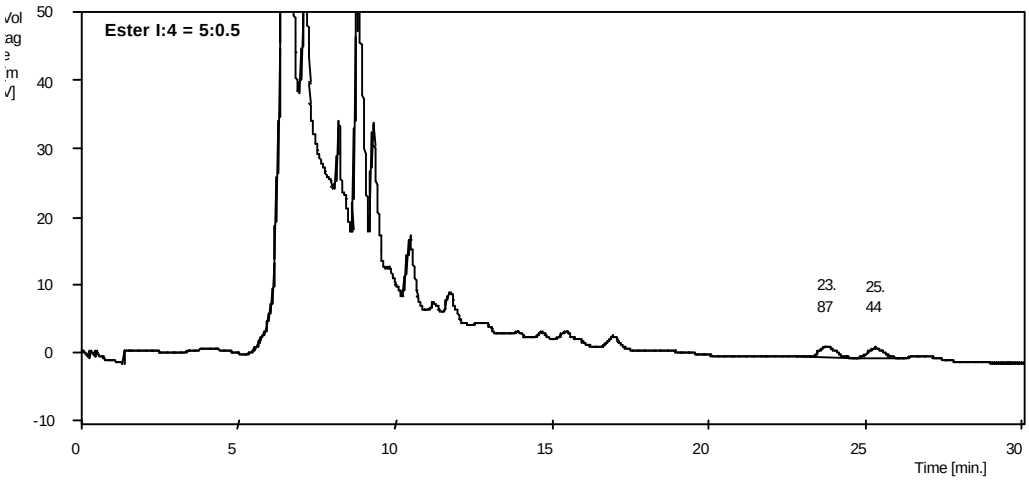
^{1}H NMR of 2-methoxy-2-phenyl-ethanol obtained from reduction of **V**: δ/ppm = 7.26-7.42 [m, 5H], 4.29-4.33 [m,1H], 3.58-3.71[m, 2H], 3.31 [s, 3H], E.A: calculated for $C_9H_{12}O_2$: C, 71.03; H, 7.95. Found: C, 71.15; H, 7.90.

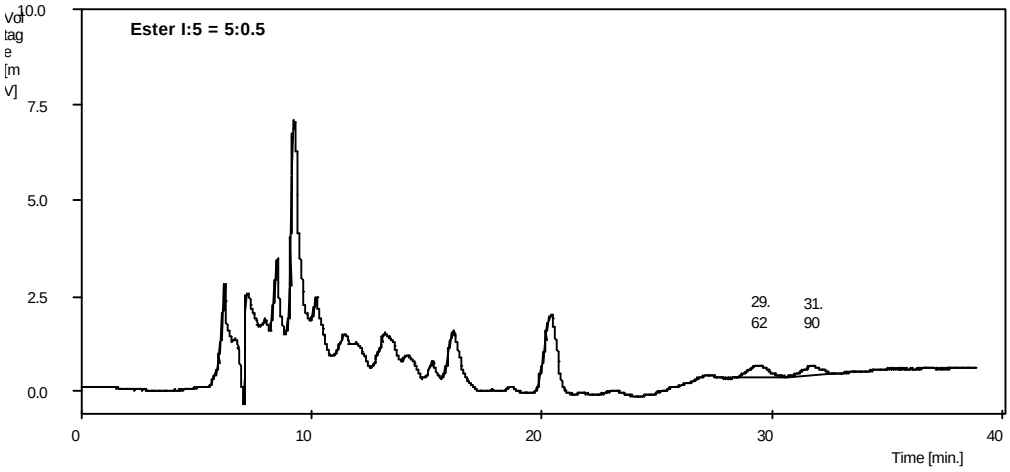
HPLC chromatograms for micelle mediated asymmetric reduction of esters (mobile phase: hexane/ethanol 95/5 for alcohol of I and hexane/isopropanol 95/5 for alcohols of II, v/v; λ = 254nm; flow rate: 0.5 mL/min) :

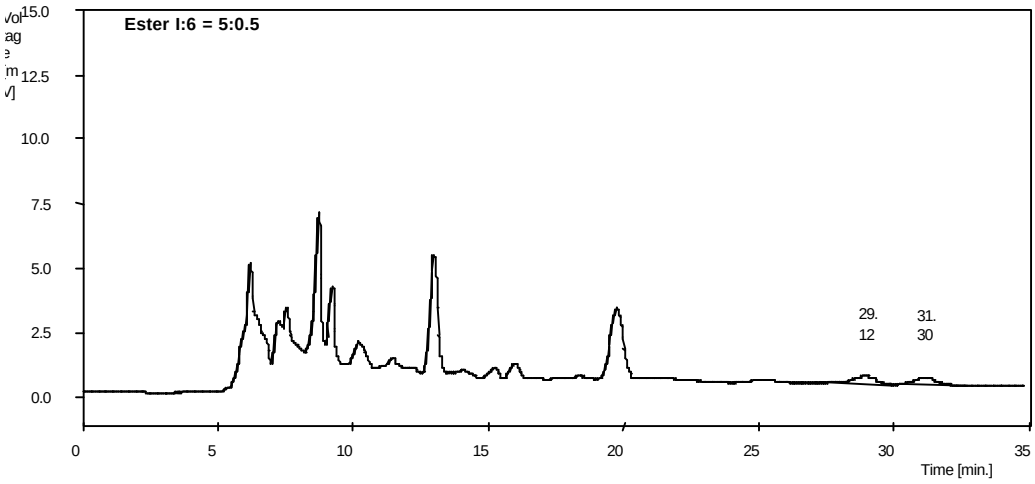


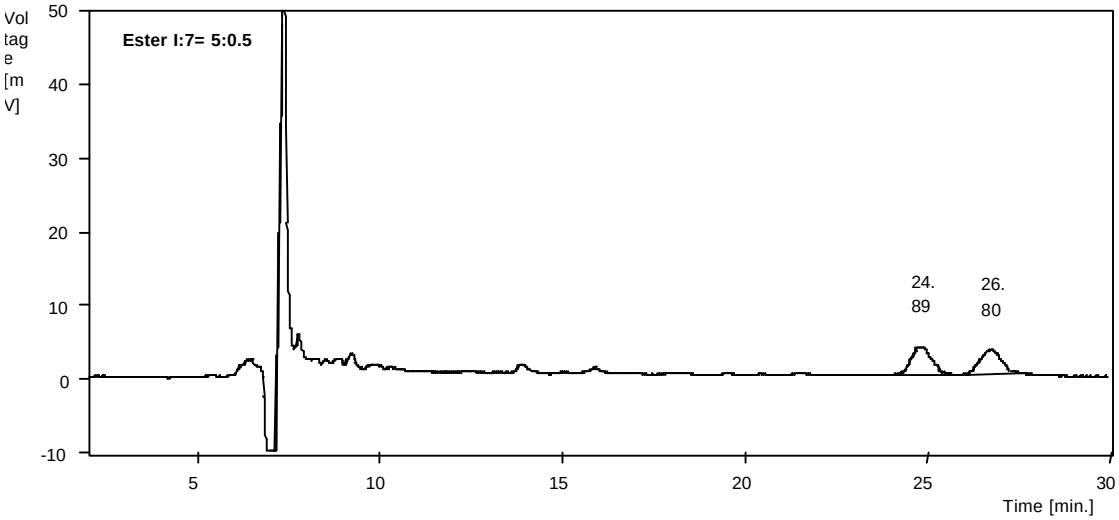

Ester I:2= 5:0.5
24.
89
26.
80
Time [min.]

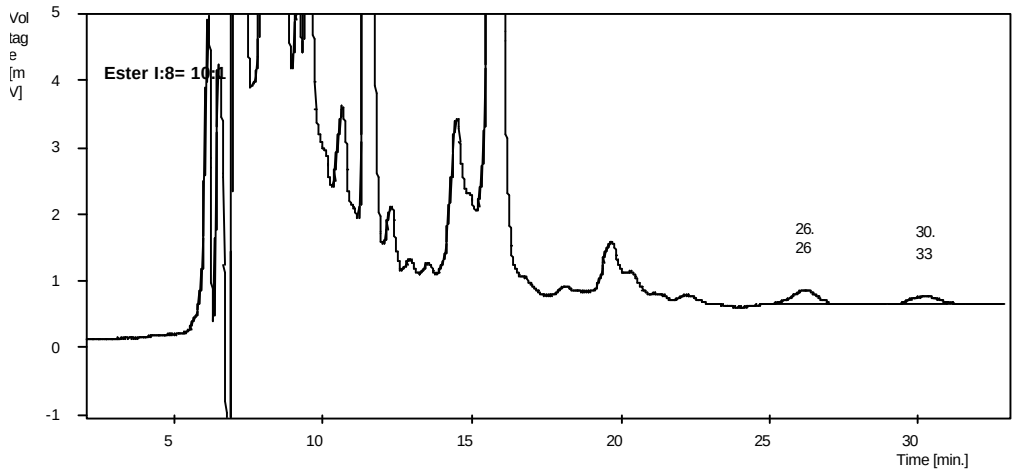

Ester I:3 = 5:0.5
24.
86
26.
77
Time [min.]

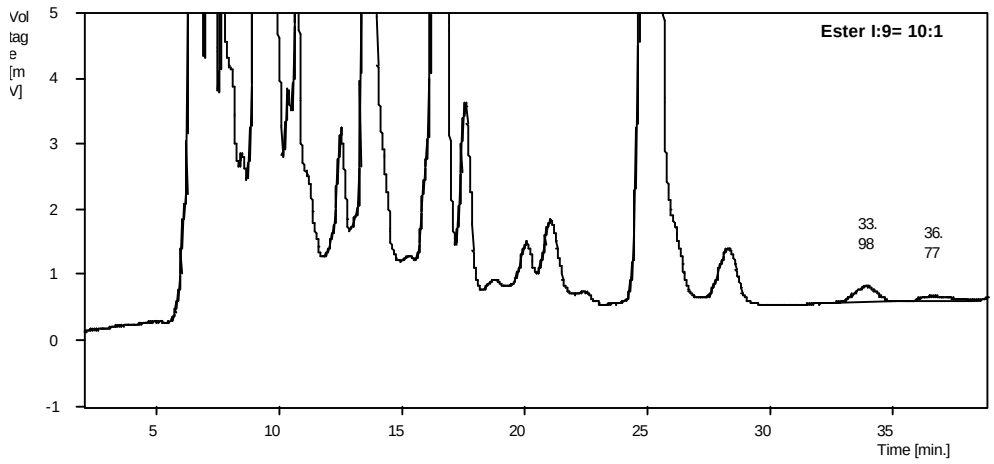

Ester I:4 = 5:0.5
Volt age [mV]
50
40
30
20
10
0
-10
0
5
10
15
20
25
30
Time [min.]
23. 87
25. 44

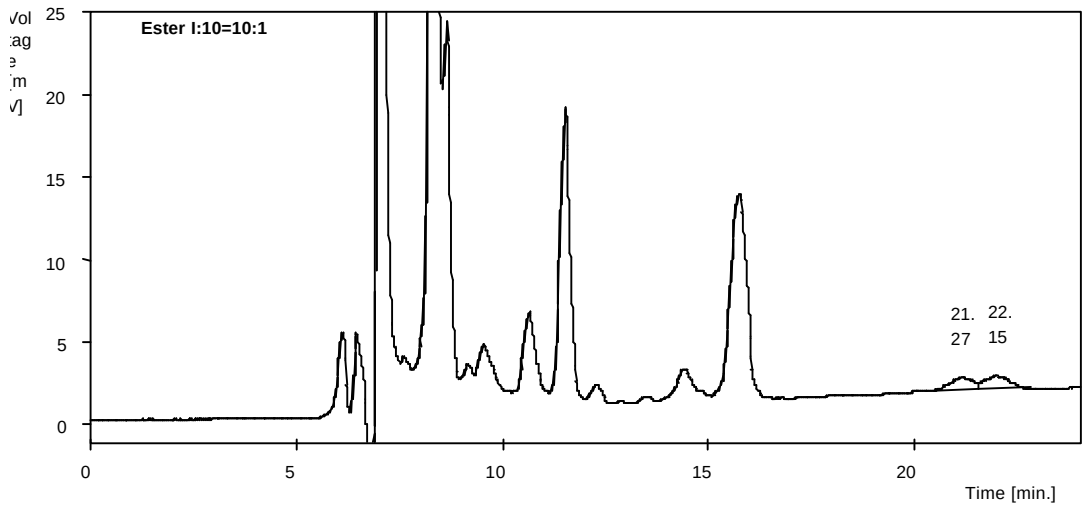

Ester I:5 = 5:0.5
Volt age [mV]
10.0
7.5
5.0
2.5
0.0
0
10
20
30
40
Time [min.]
29. 62
31. 90

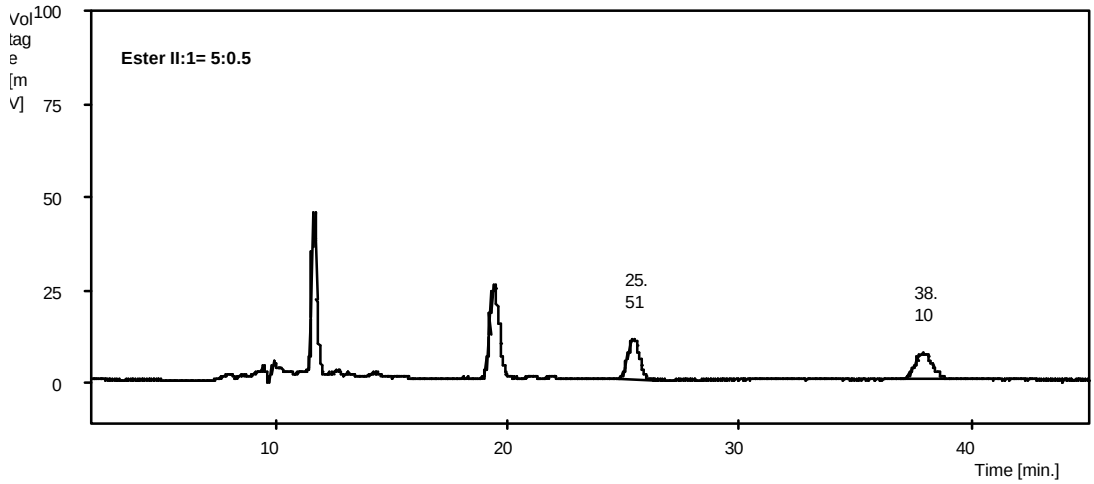

Ester I:6 = 5:0.5
Voltage [mV]
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20
25
30
35
Time [min.]
29.12
31.30

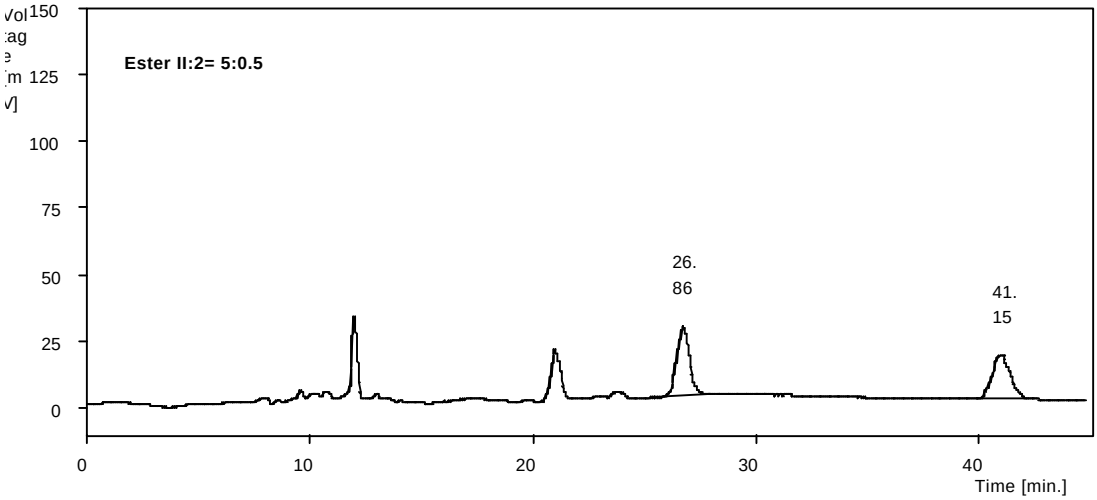

Ester I:7= 5:0.5
Voltage [mV]
50
40
30
20
10
0
-10
5
10
15
20
25
30
Time [min.]
24.89
26.80

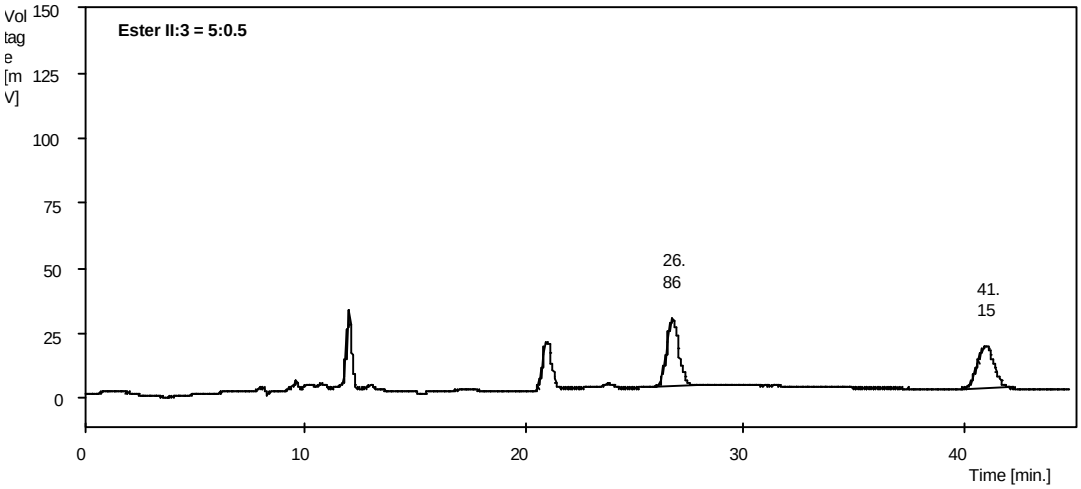

Voltage [mV]
Ester I:8= 10:1
26.26
30.33
Time [min.]

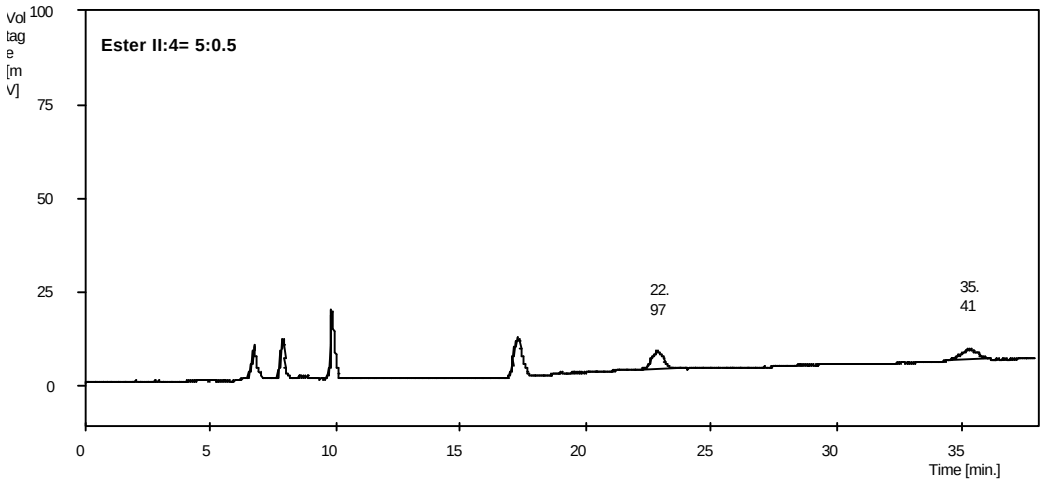

Voltage [mV]
Ester I:9= 10:1
33.98
36.77
Time [min.]

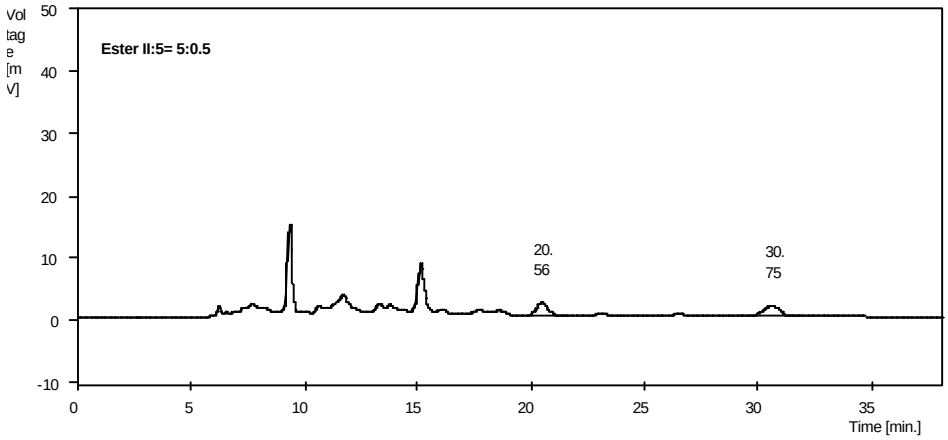

Ester I:10=10:1
25
20
15
10
5
0
0
5
10
15
20
Time [min.]
21.
27
22.
15

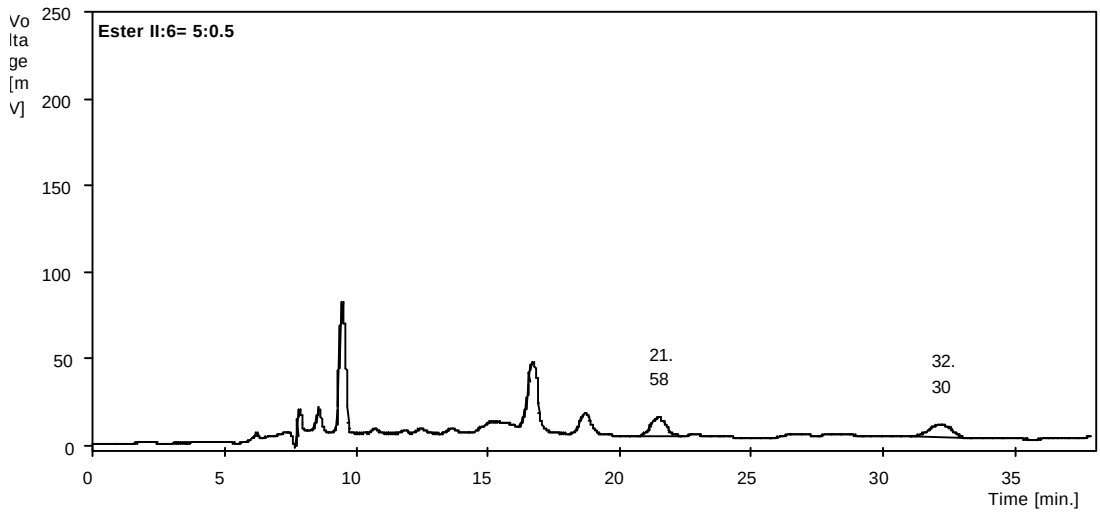

Ester II:1= 5:0.5
100
75
50
25
0
10
20
30
40
Time [min.]
25.
51
38.
10

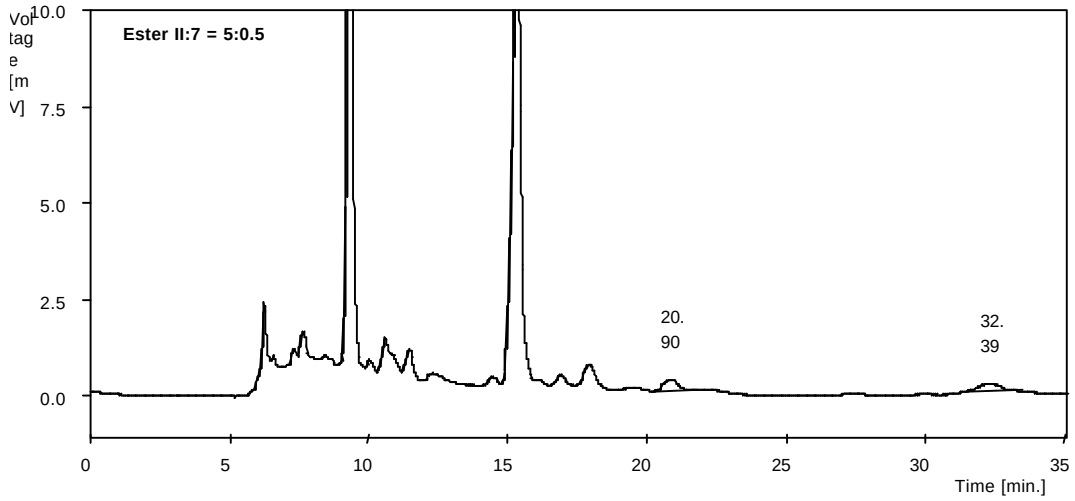

Ester II:2= 5:0.5
26.
86
41.
15
150
125
100
75
50
25
0
0
10
20
30
40
Time [min.]

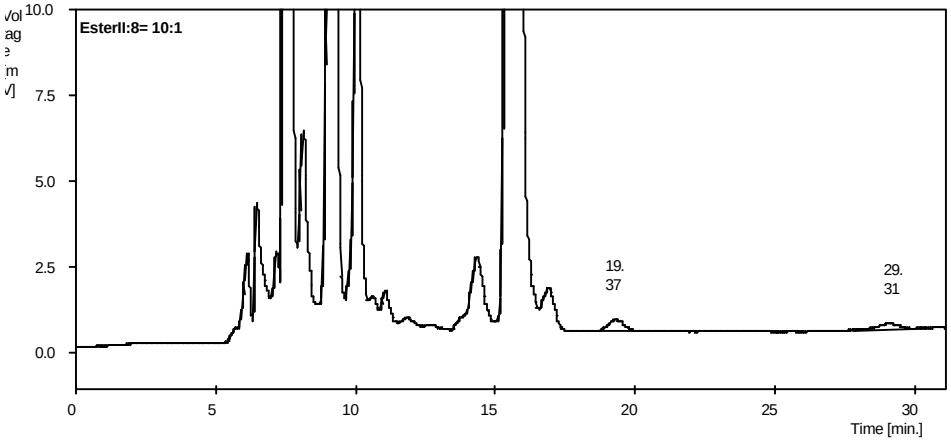

Ester II:3 = 5:0.5
26.
86
41.
15
150
125
100
75
50
25
0
0
10
20
30
40
Time [min.]

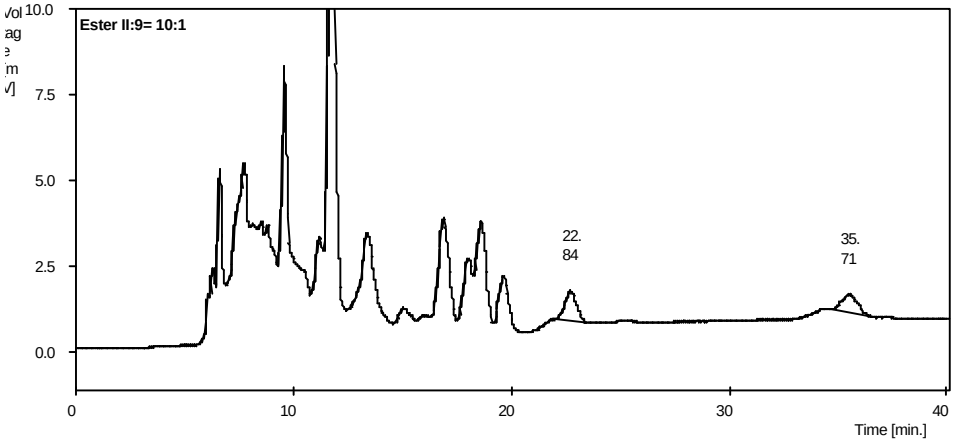

Voltage [mV]
Ester II:4= 5:0.5
22.
97
35.
41
Time [min.]

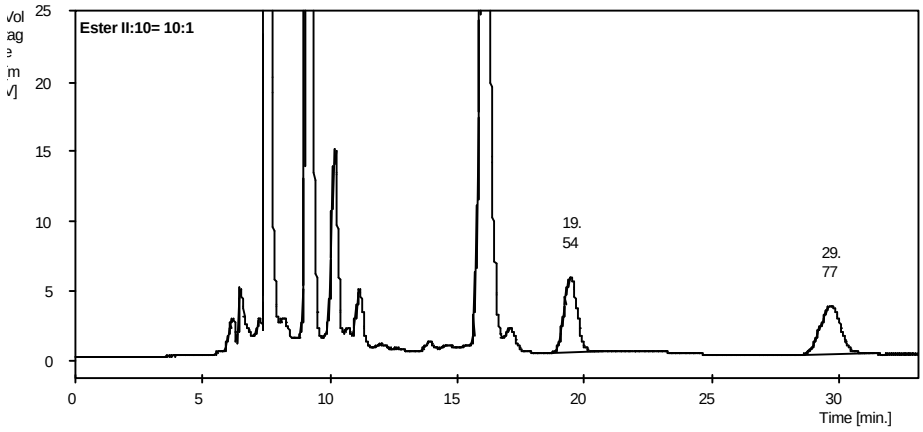

Voltage [mV]
Ester II:5= 5:0.5
20.
56
30.
75
Time [min.]


Ester II:6= 5:0.5
Voltage [mV]
250
200
150
100
50
0
0
5
10
15
20
25
30
35
Time [min.]
21.
58
32.
30


Ester II:7 = 5:0.5
Voltage [mV]
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20
25
30
35
Time [min.]
20.
90
32.
39


Vol
ag
e
[m
V]
10.0
7.5
5.0
2.5
0.0
EsterII:8= 10:1
19.
37
29.
31
0
5
10
15
20
25
30
Time [min.]


Vol
ag
e
[m
V]
10.0
7.5
5.0
2.5
0.0
Ester II:9= 10:1
22.
84
35.
71
0
10
20
30
40
Time [min.]


Ester II:10= 10:1
19.
54
29.
77
Time [min.]

Circular Dichroism Spectra of Surfactant 8, 9, and 10 (Scheme 1, in the manuscript)

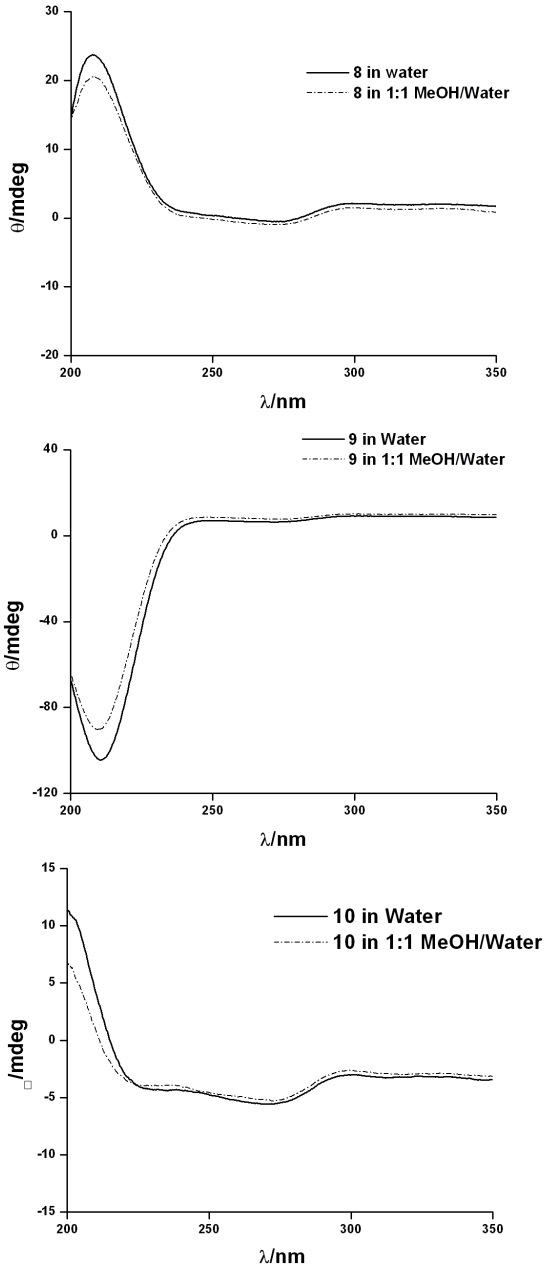


Figure 2