Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

One-Pot Route to β-Adrenergic Blockers *via* Enantioselective Organocatalysed Epoxidation of Terminal Alkenes as a Key Step

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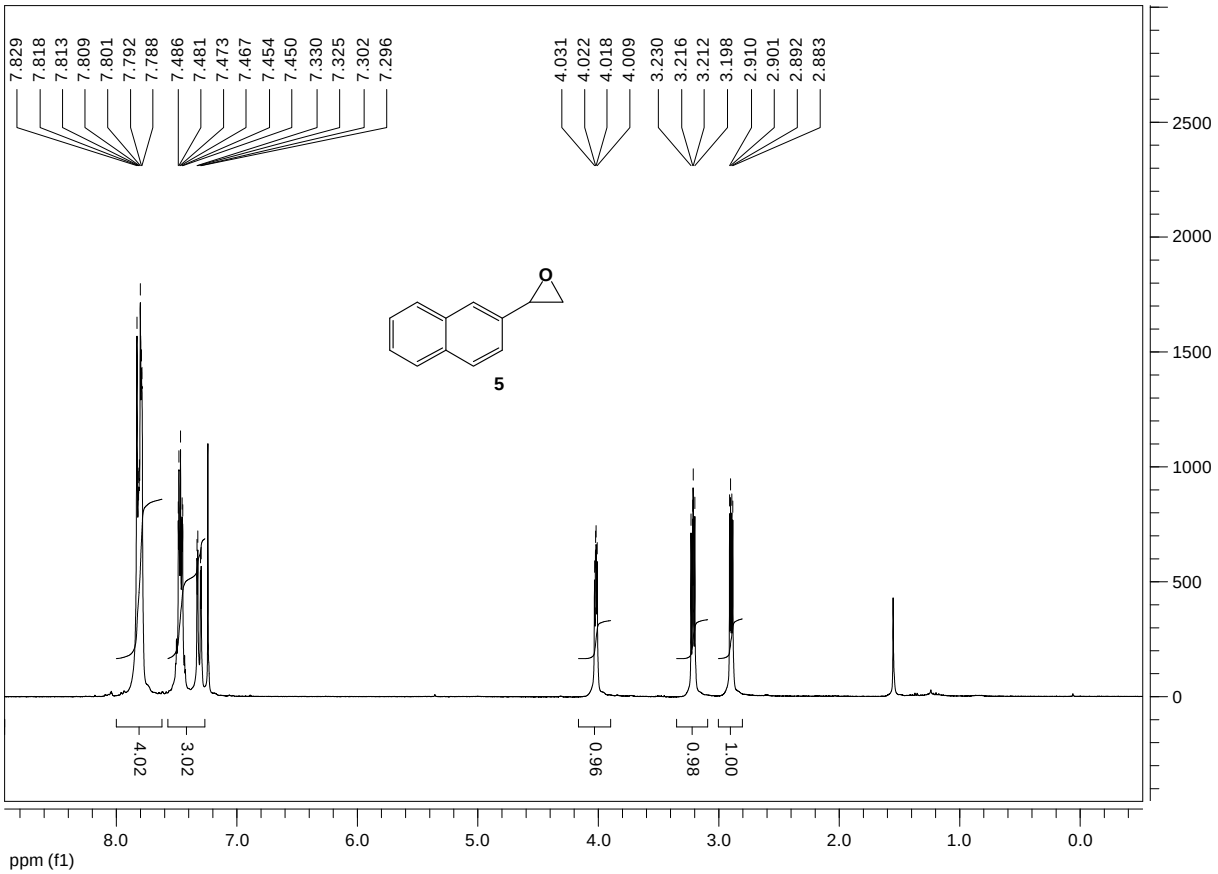
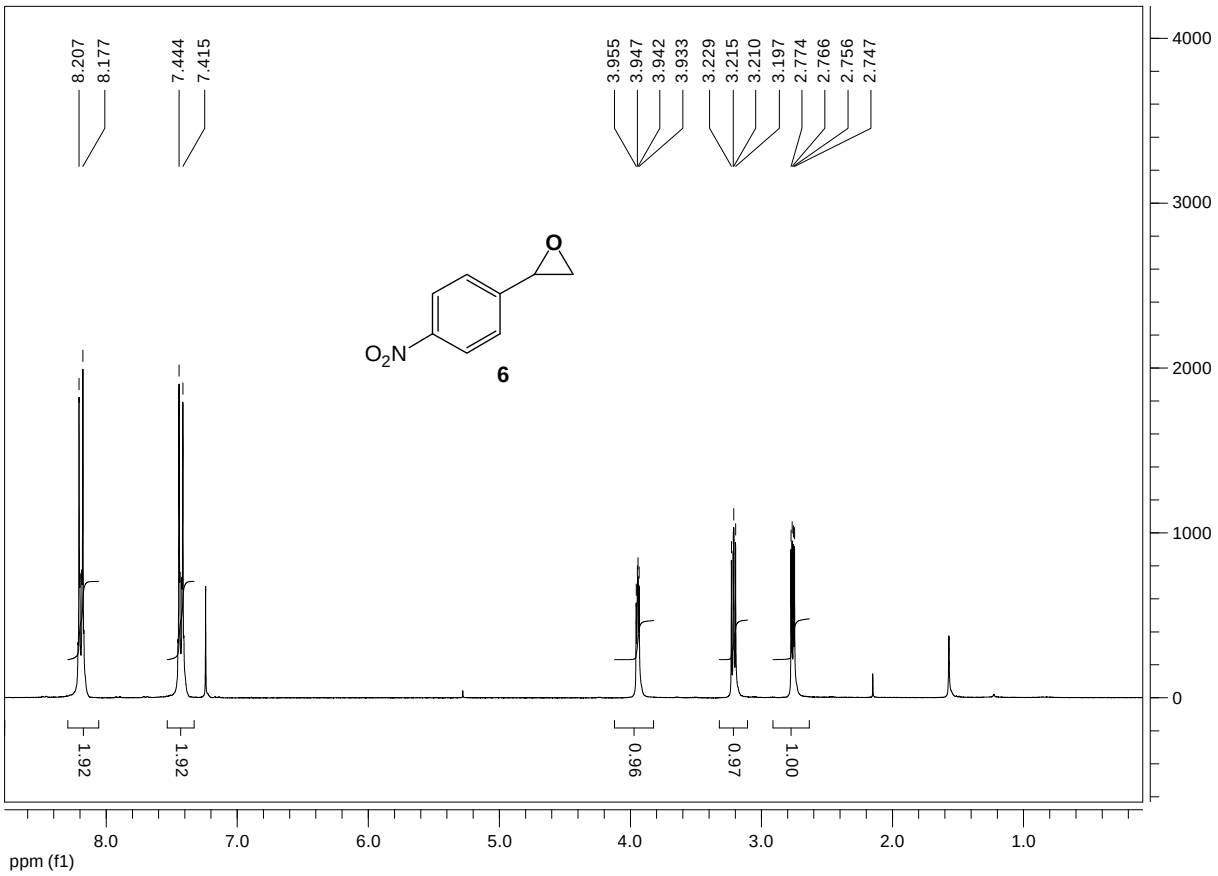
1. NMR Spectra of Products:

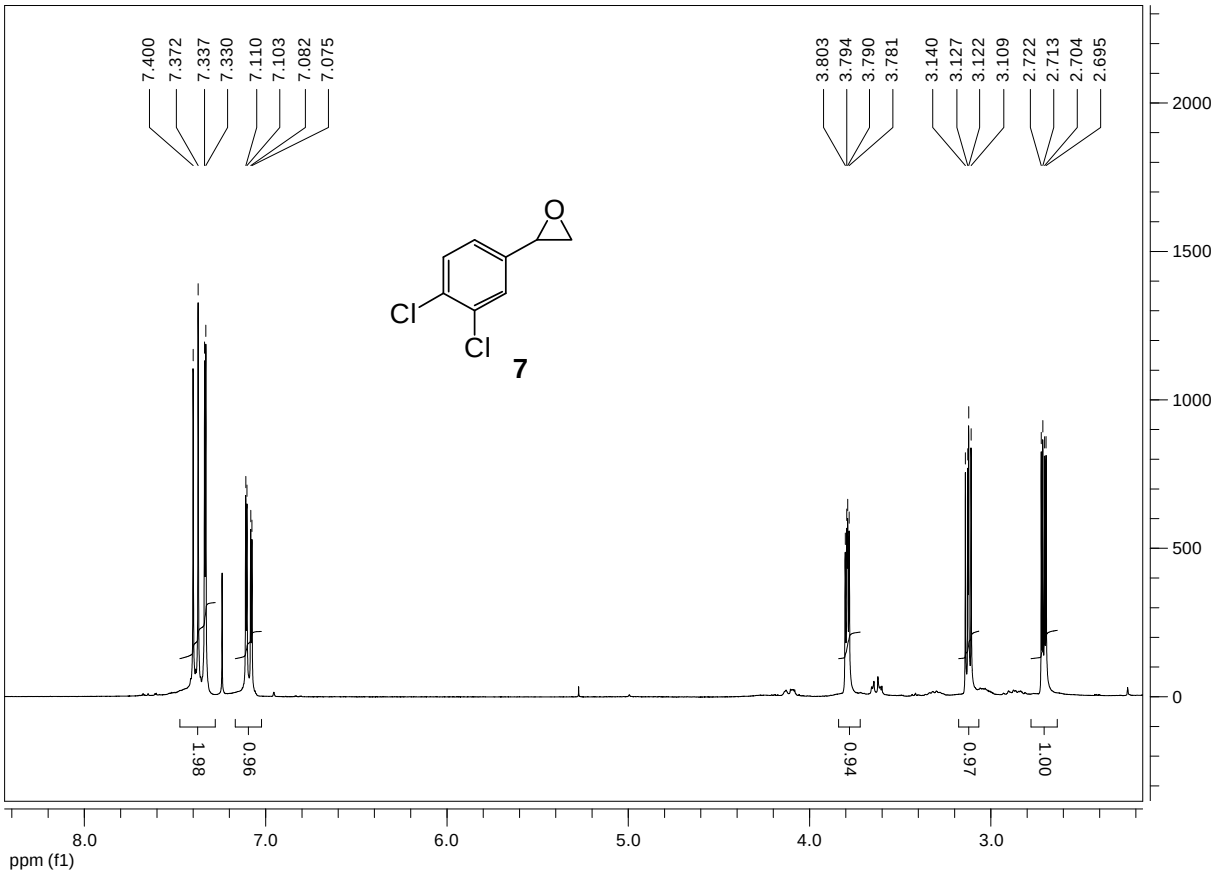
2-Naphthalen-2-yl-oxirane: ^{1}H-NMR (300 MHz, $CDCl_3$)



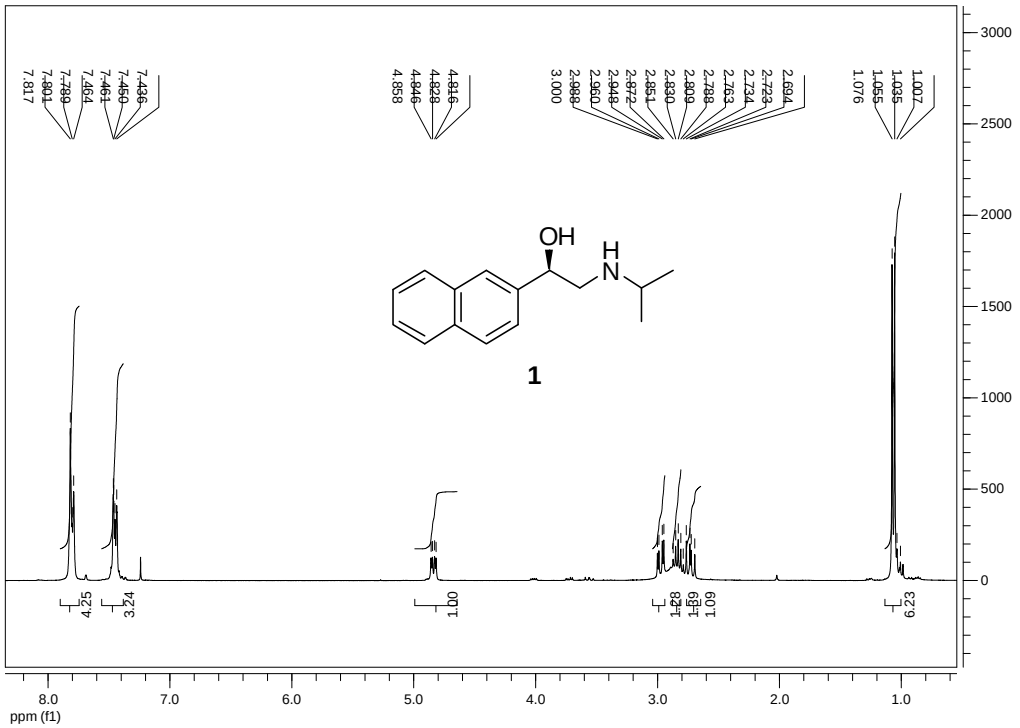
2-(4-Nitro-phenyl)-oxirane: ^{1}H-NMR (300 MHz, $CDCl_3$)



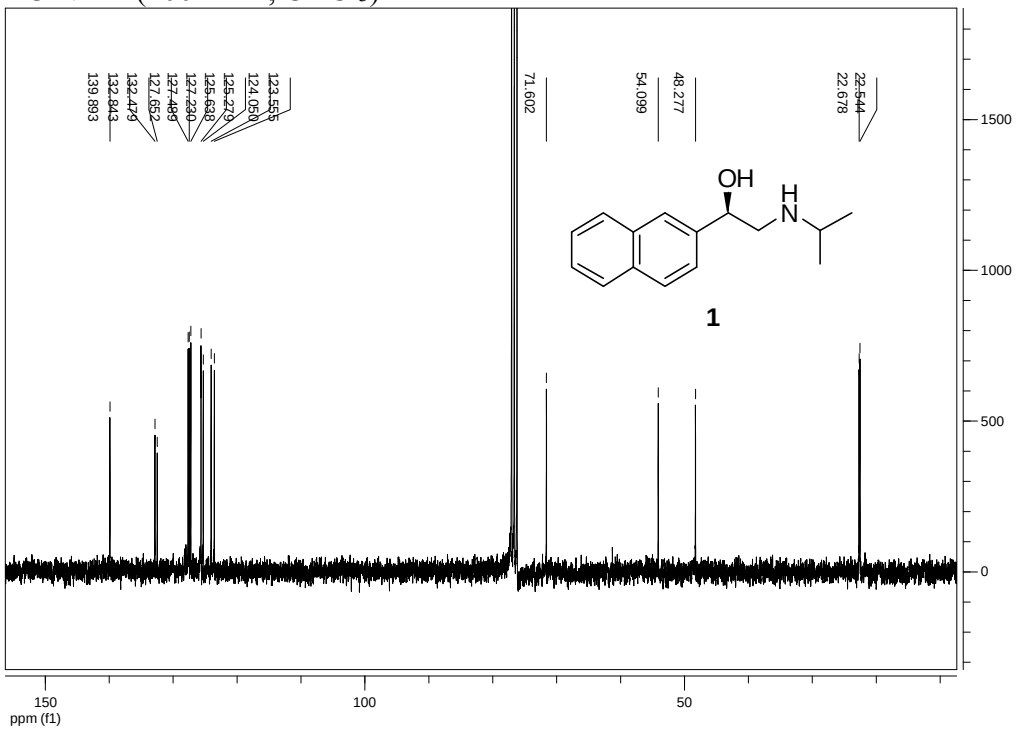
2-(3,4-Dichloro-phenyl)-oxirane: ^{1}H-NMR (300 MHz, $CDCl_3$)



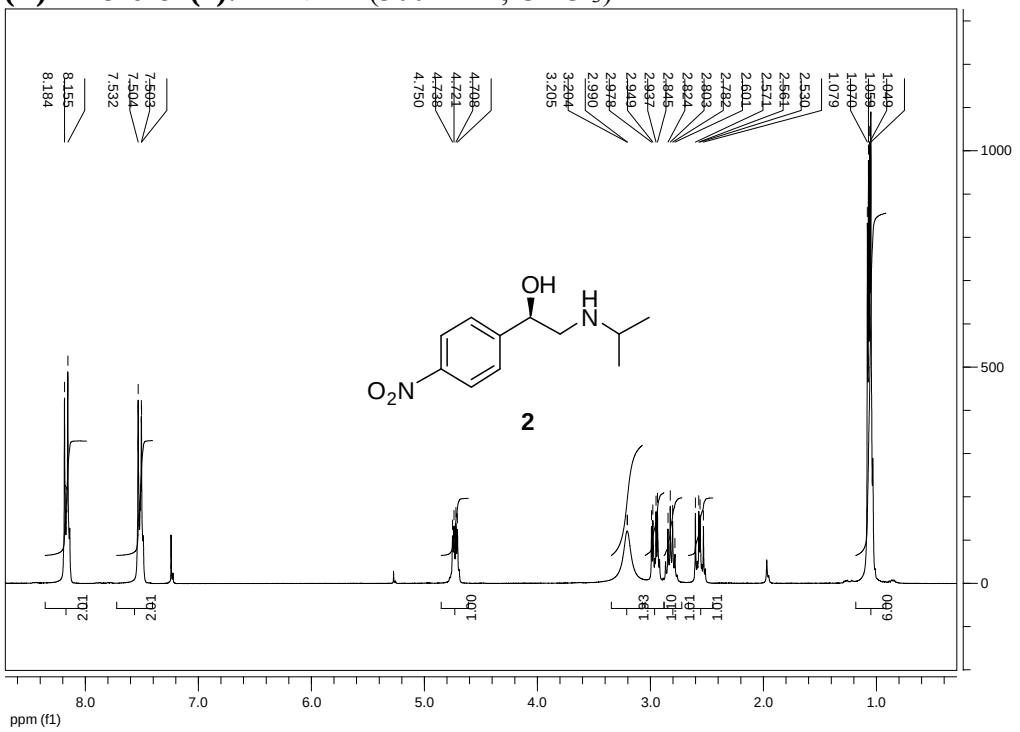
(*R*)-Pronethalol (1): ^{1}H NMR (300 MHz, $CDCl_3$)



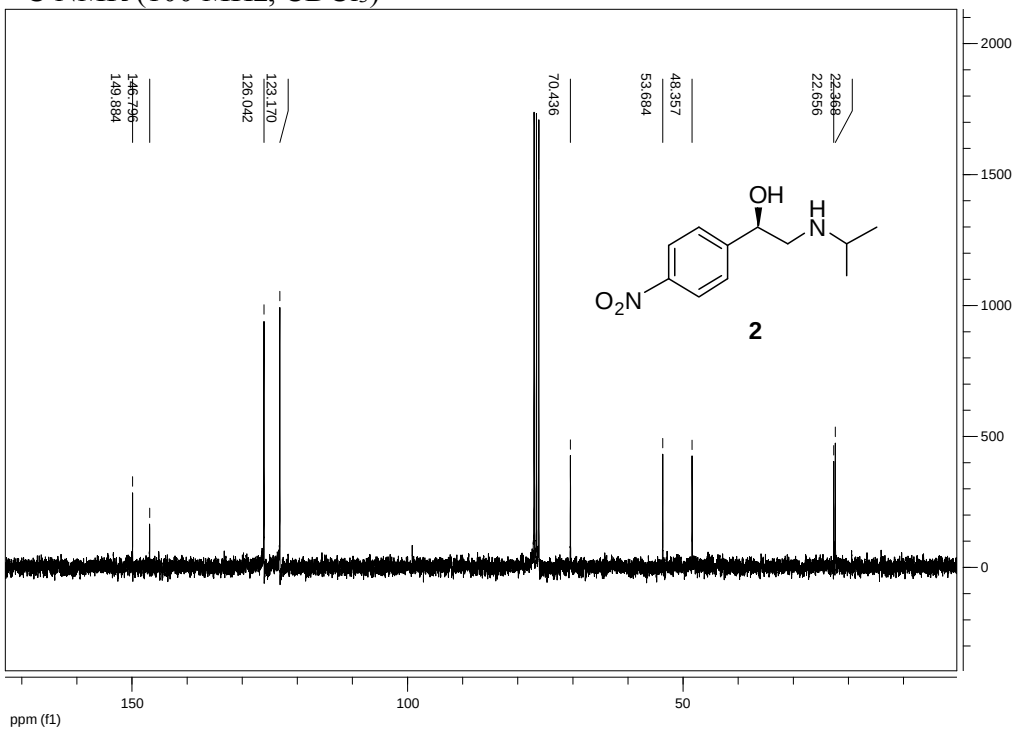
^{13}C NMR (100 MHz, $CDCl_3$)



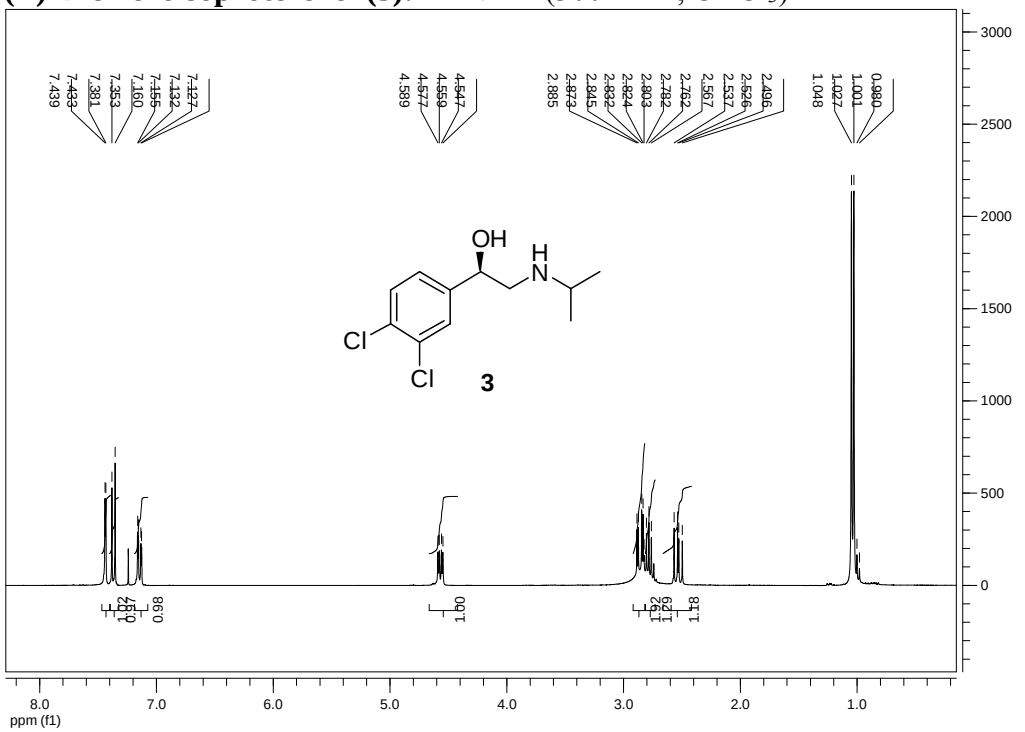
(*R*)-Nifenalol (2): ^{1}H NMR (300 MHz, $CDCl_3$)



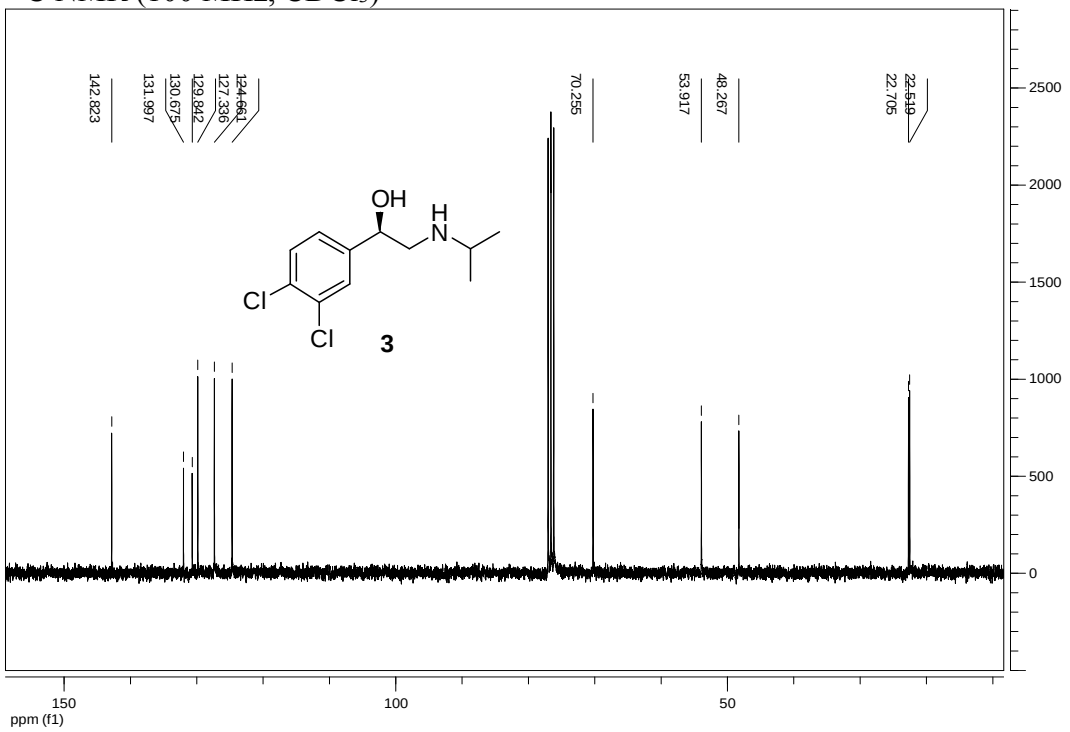
^{13}C NMR (100 MHz, $CDCl_3$)



(*R*)-Dichloroisoproterenol (3): ^{1}H NMR (300 MHz, $CDCl_3$)

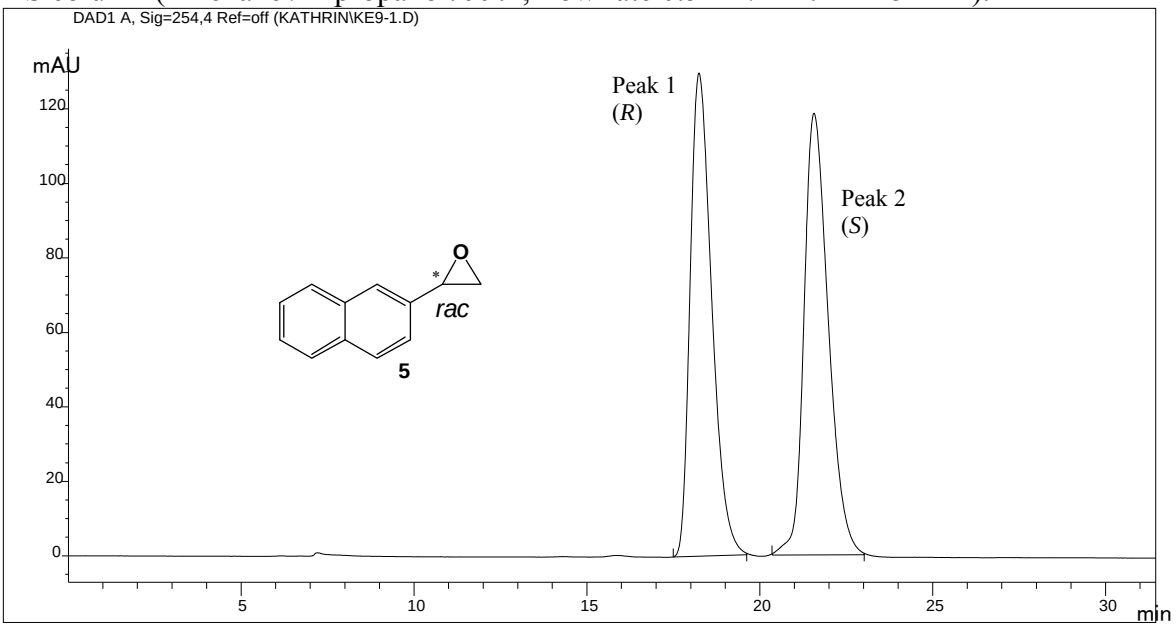


^{13}C NMR (100 MHz, $CDCl_3$)



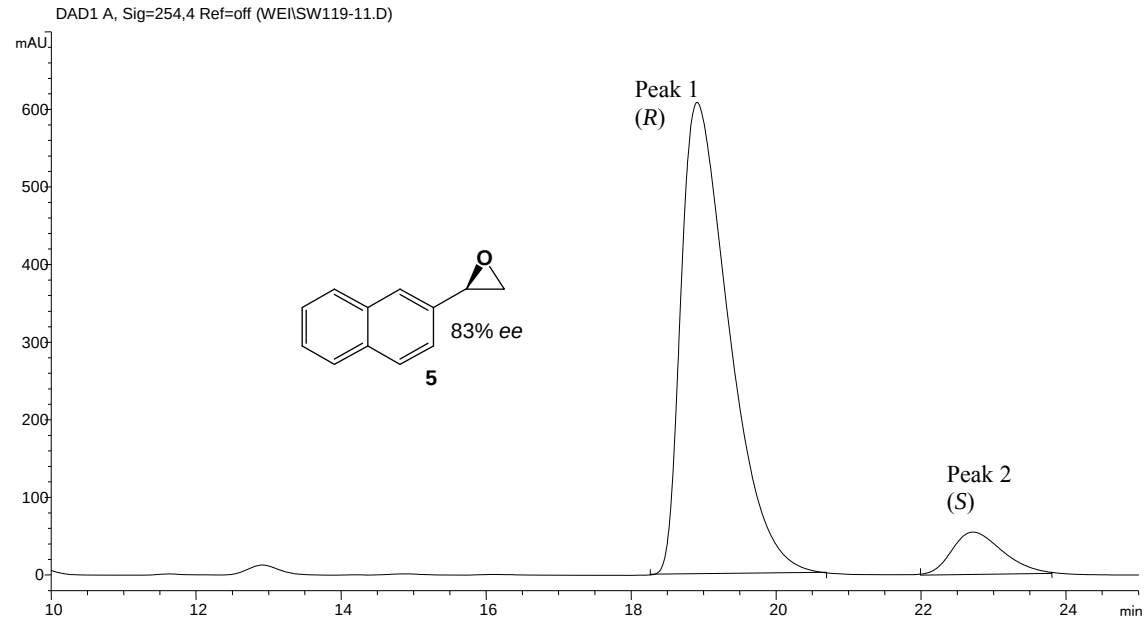
2. HPLC chromatograms

Table 1,
***rac*-2-Naphthalen-2-yl-oxirane**
AS column (*n*-hexane / 2-propanol: 99:1, flow rate 0.5 ml /min. λ = 254 nm).



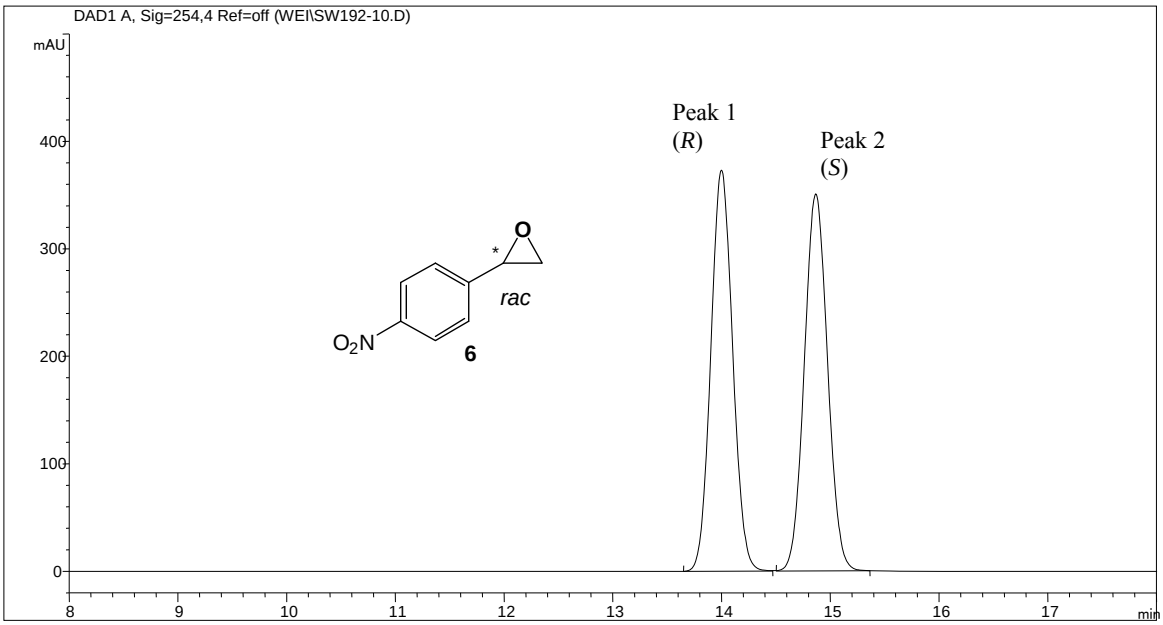
Peak	t_R	Area	Area (%)
1	18.236	5621.8	49.24
2	21.563	5796	50.76

Table 1, Entry 4
***(R)*-2-Naphthalen-2-yl-oxirane**
AS column (*n*-hexane / 2-propanol: 99:1, flow rate 0.5 ml /min. λ = 254 nm).



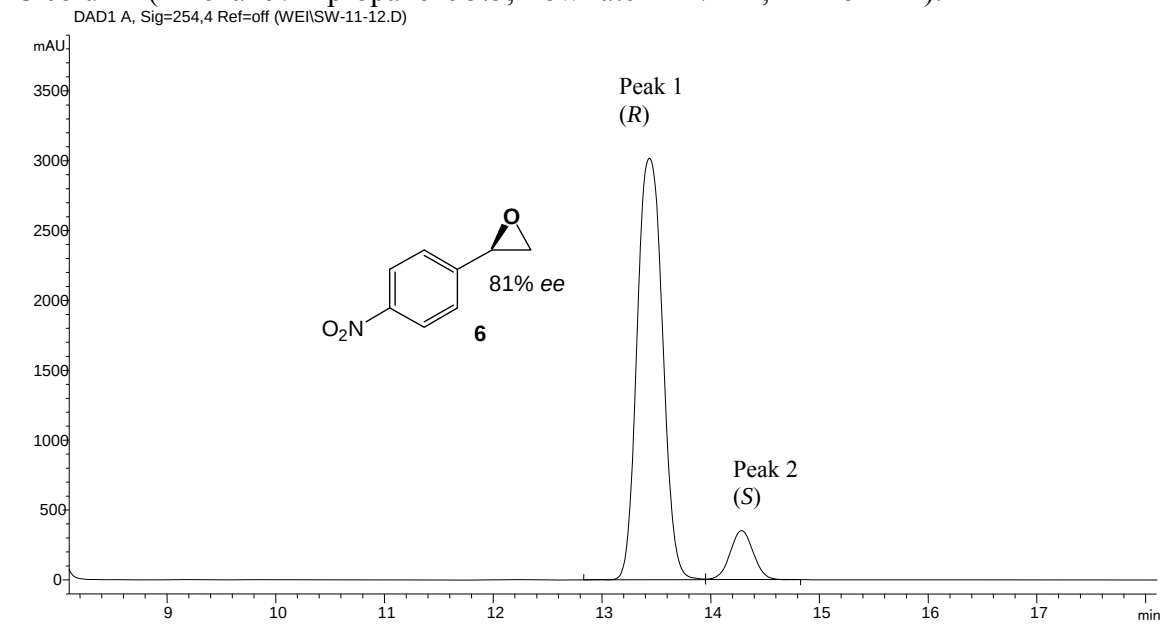
Peak	t_R	Area	Area (%)
1	18.909	610.975	91.43
2	22.716	54.791	8.56

Table 1
***rac*-2-(4-Nitro-phenyl)-oxirane**
IC column (*n*-hexane / 2-propanol 95:5, flow rate 1 ml/min, λ = 254 nm).



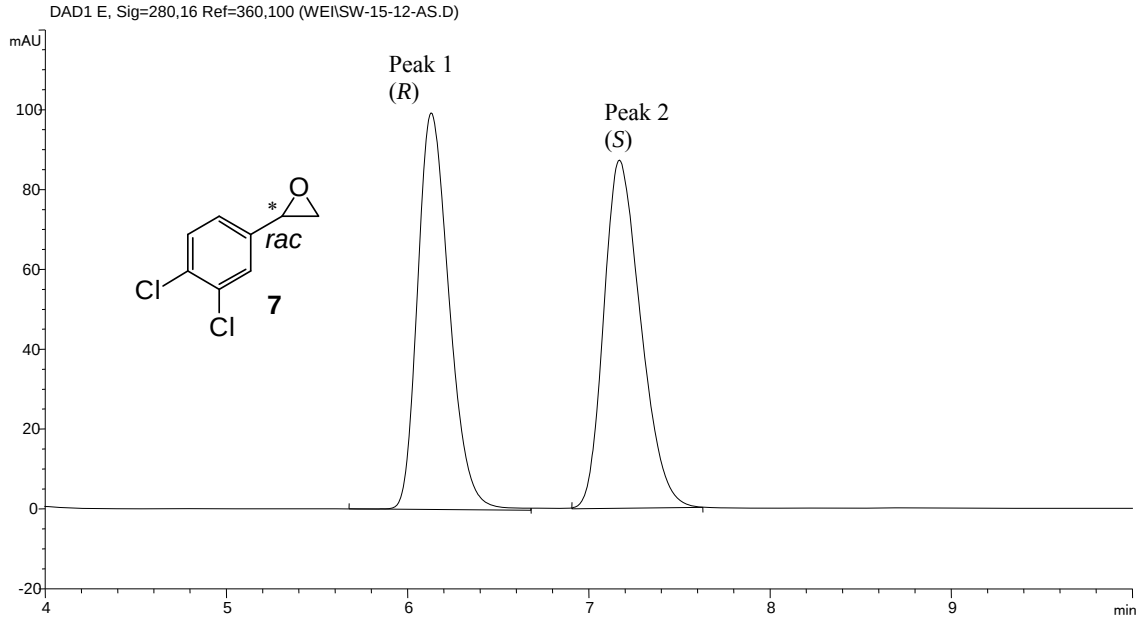
Peak	t_R	Area	Area (%)
1	13.998	360.44	49.94
2	14.865	339.40	50.06

Table 1, Entry 8
***(R)*-2-(4-Nitro-phenyl)-oxirane**
IC column (*n*-hexane / 2-propanol 95:5, flow rate 1 ml/min, λ = 254 nm).



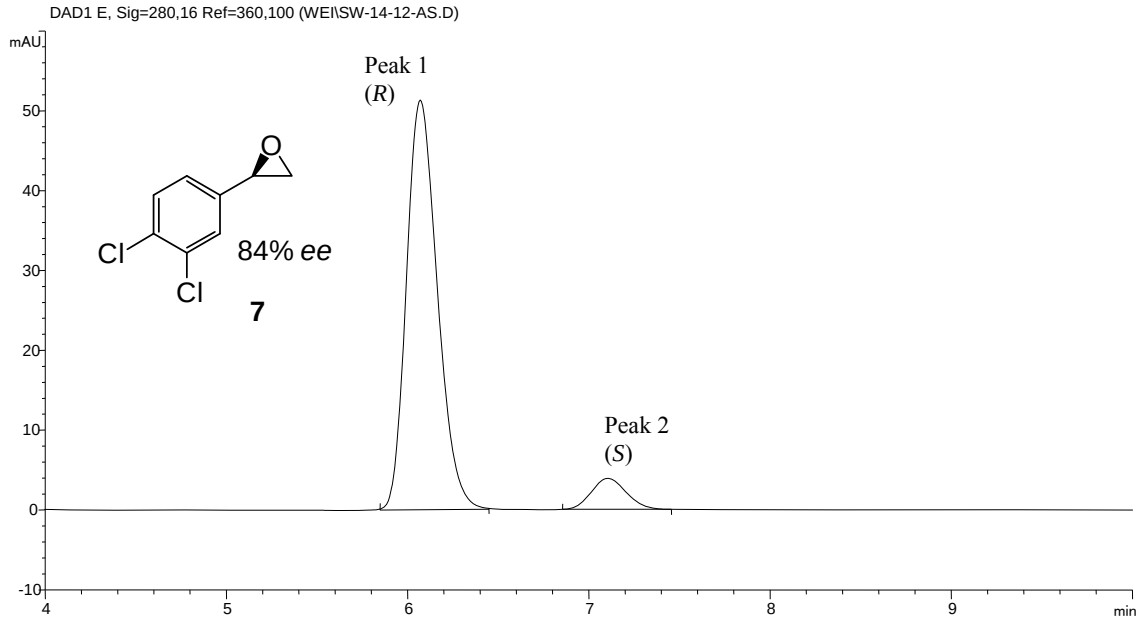
Peak	t_R	Area	Area (%)
1	13.436	3016.79	90.63
2	14.283	348.84	9.37

Table 1
***rac*-2-(3,4-Dichloro-phenyl)-oxirane**
AS column (*n*-hexane / 2-propanol 98:2, flow rate 1 ml/min. λ = 280 nm).



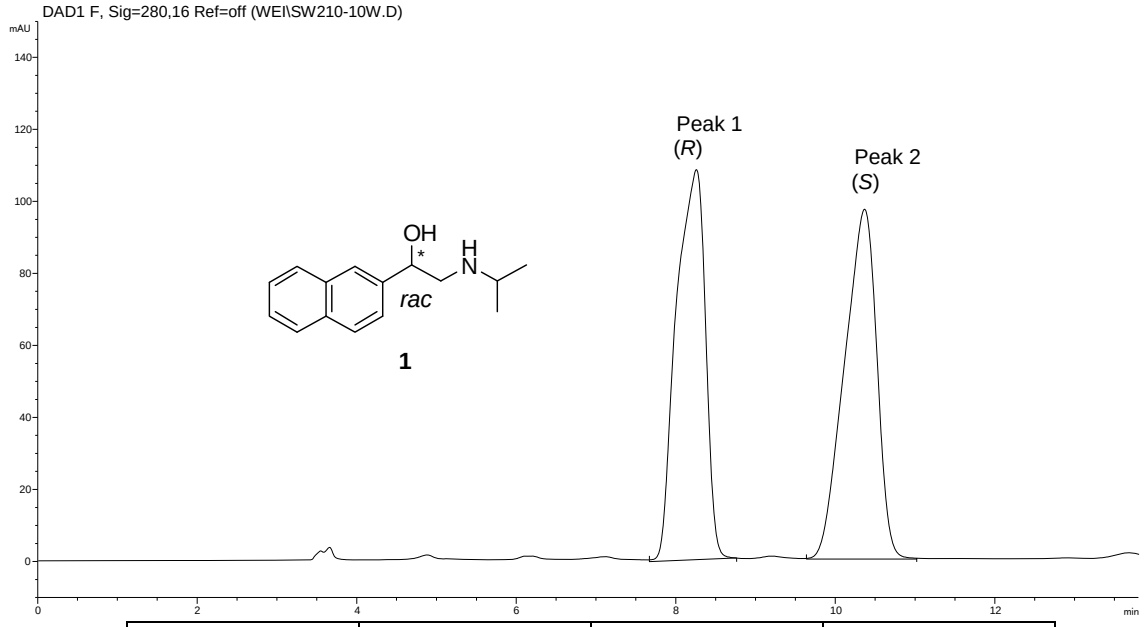
Peak	t_R	Area	Area (%)
1	6.130	99.3	49.237
2	7.168	87	50.763

Table 1, Entry 9
***(R)*-2-(3,4-Dichloro-phenyl)-oxirane**
AS column (*n*-hexane / 2-propanol 98:2, flow rate 1 ml/min. λ = 280 nm).



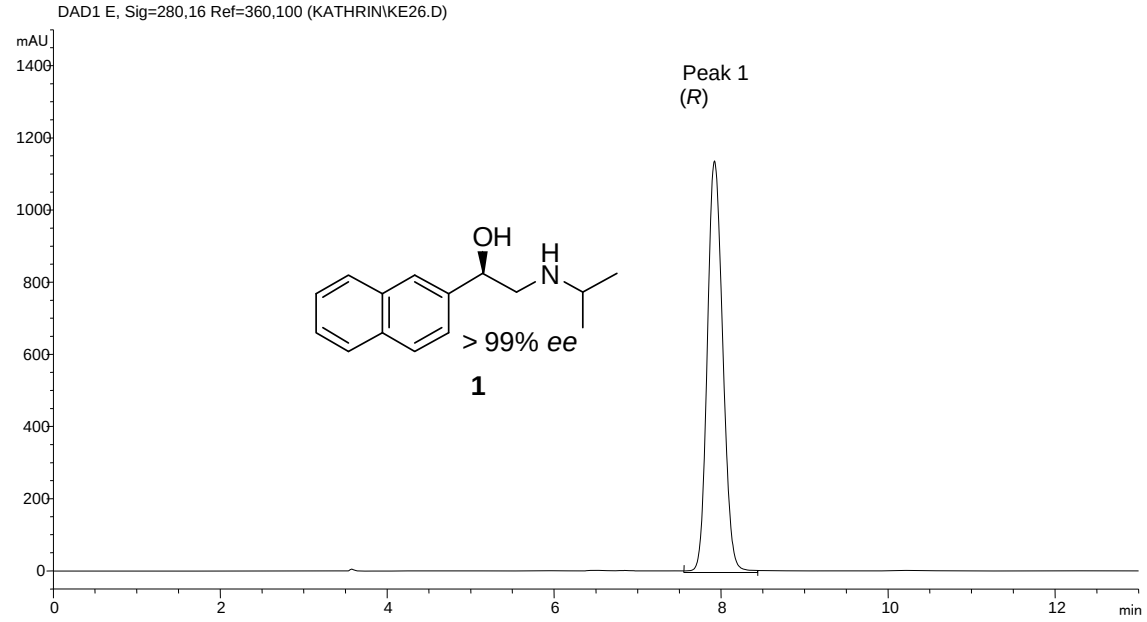
Peak	t_R	Area	Area (%)
1	6.069	611.2	91.992
2	7.105	53.2	8.008

Table 2
***rac*-Pronethalol (1)**
IC column (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 1ml/min, λ = 280 nm).



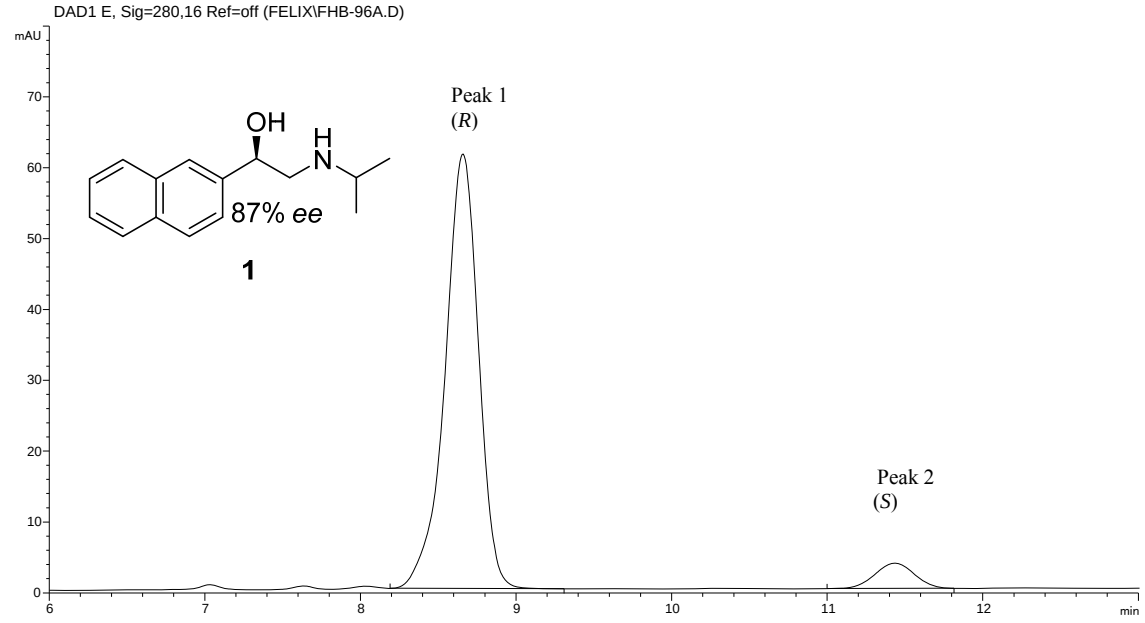
Peak	t_R	Area	Area (%)
1	8.257	2126.5	49.758
2	10.364	2147,2	50.242

Table 2, Entry 1 (recrystallized product)
***(R)*-Pronethalol (1)**
IC column (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 1ml/min, λ = 280 nm).



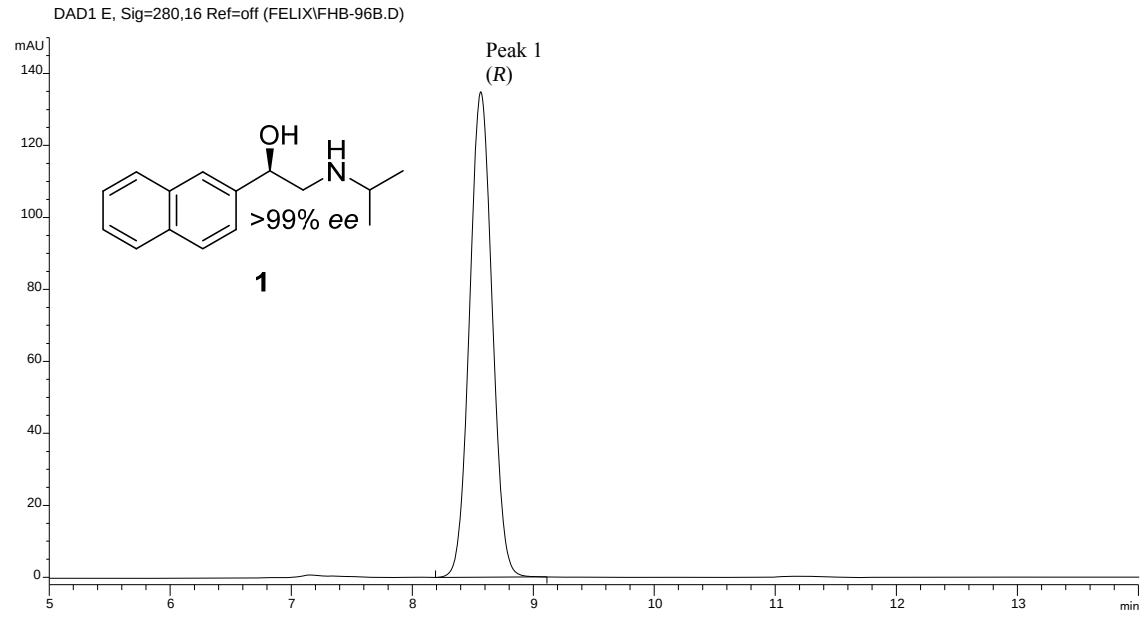
Peak	t_R	Area	Area (%)
1	7.95	2361.50	100
2	-	-	0

Table 2, Entry 6
***(R)*-Pronethalol (1)**
IC column (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 1ml/min, λ = 280 nm).



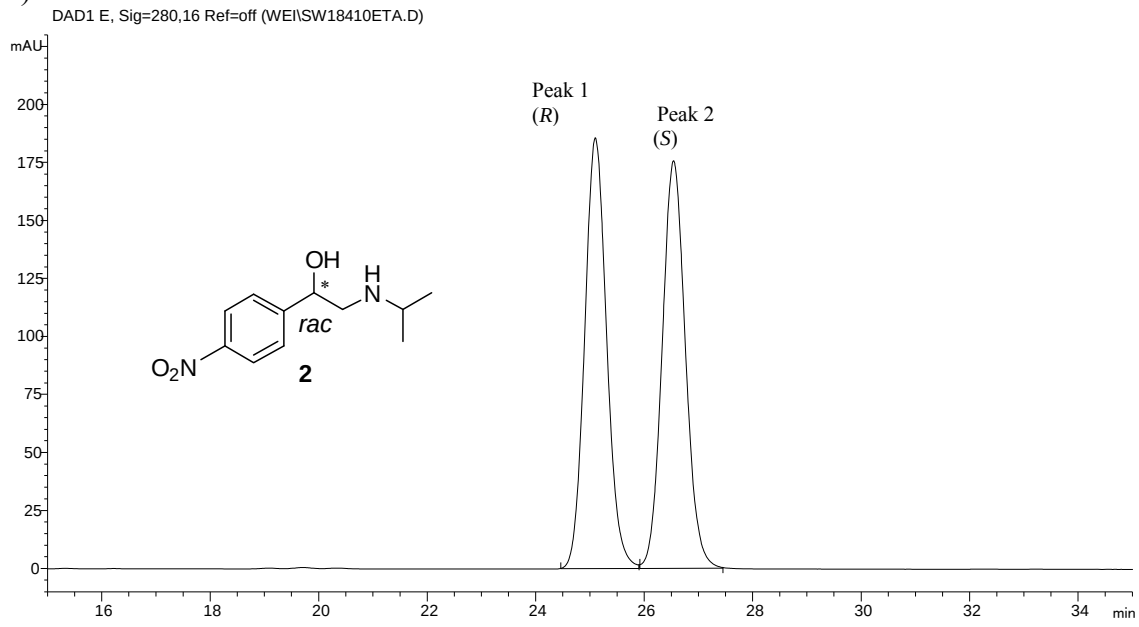
Peak	t_R	Area	Area (%)
1	8.657	912.2	93.523
2	11.434	63.2	6.477

Table 2, Entry 6 (recrystallized product):
***(R)*-Pronethalol (1)**
IC column (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 1ml/min, λ = 280 nm).



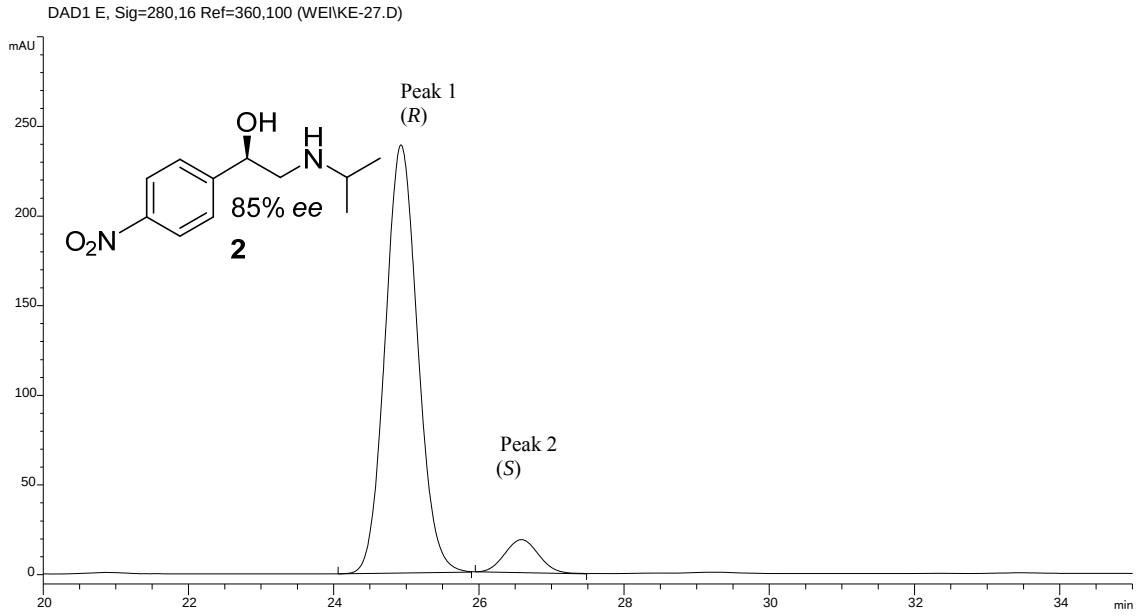
Peak	t_R	Area	Area (%)
1	8.564	1763.6	100
2	-	-	-

Table 2
***rac*-Nifenalol (2)**
IC column (*n*-hexane / 2-propanol / triethylamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).



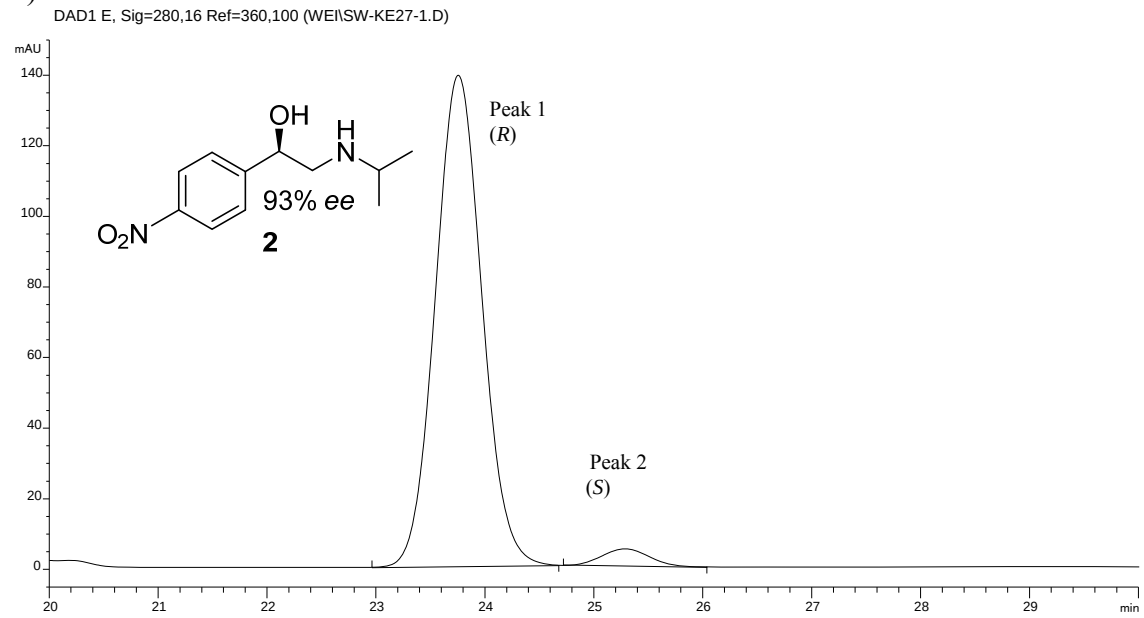
Peak	t_R	Area	Area (%)
1	25.097	5369.39	50.04
2	26.538	5361.83	49.96

Table 2, Entry 10:
***(R)*-Nifenalol (2)**
IC column (*n*-hexane / 2-propanol / triethylamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).



Peak	t_R	Area	Area (%)
1	24.924	7431	92.484
2	26.583	603.9	7.516

Table 2, Entry 10 (recrystallized product):
***(R)*-Nifenalol (2)**
IC column (*n*-hexane / 2-propanol / triethylamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).

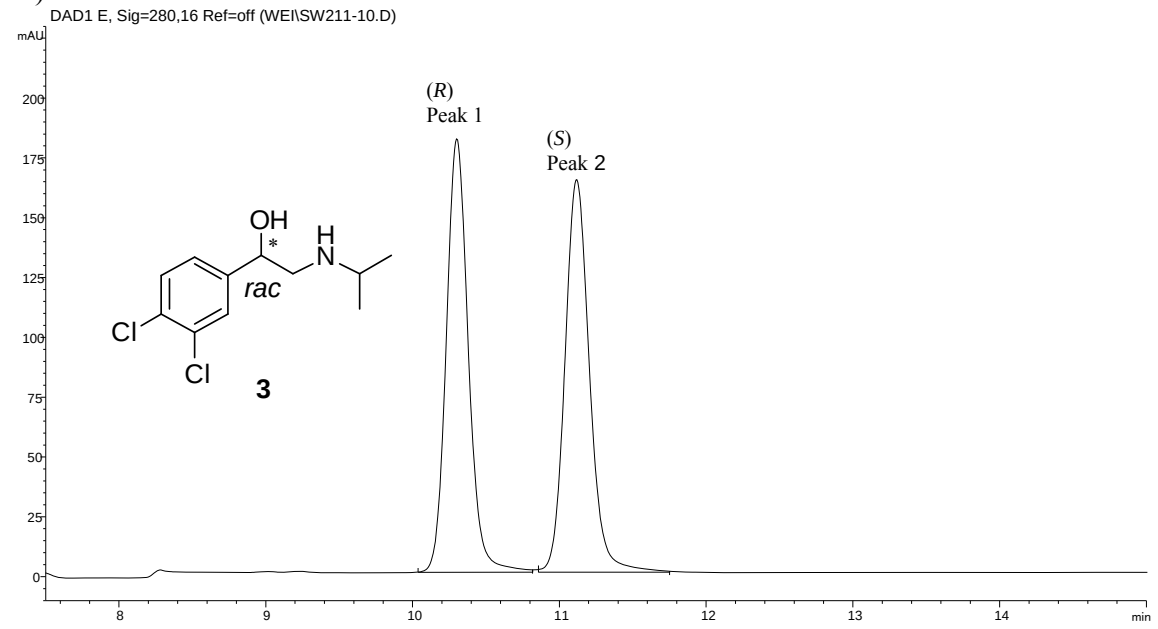


Peak	t_R	Area	Area (%)
1	23.754	4154.5	96.489
2	25.292	151.2	3.511

Table 2

***rac*-Dichloroisoproterenol (3)**

IC column, (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).

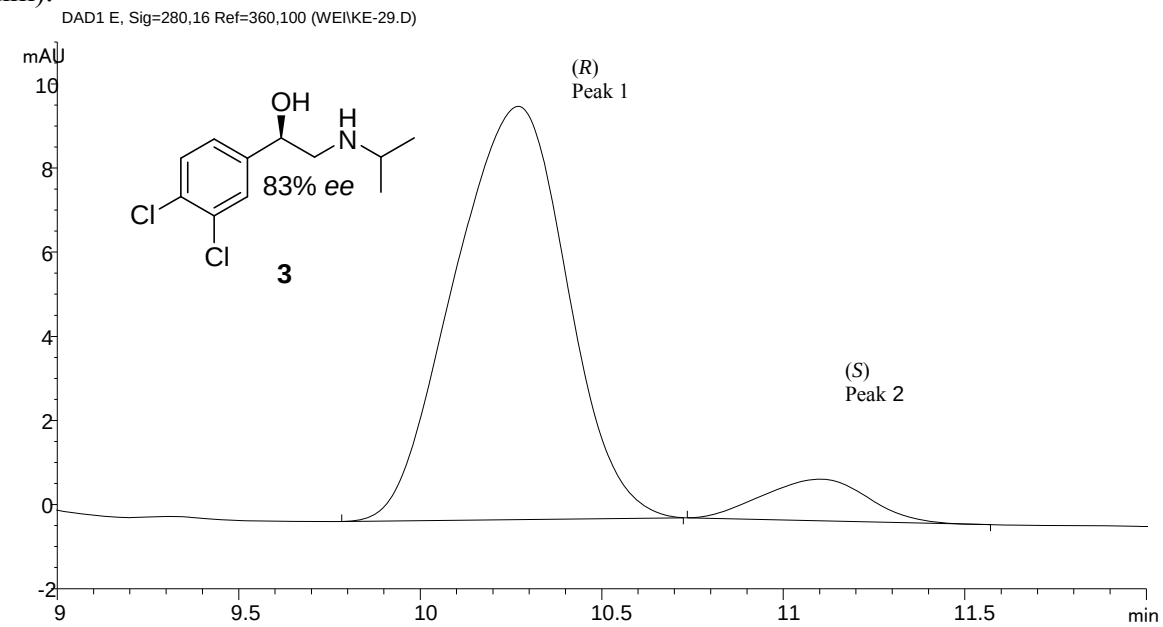


Peak	t_R	Area	Area (%)
1	10.300	1893.2	49.823
2	11.116	1906.7	50.177

Table 2, Entry 12

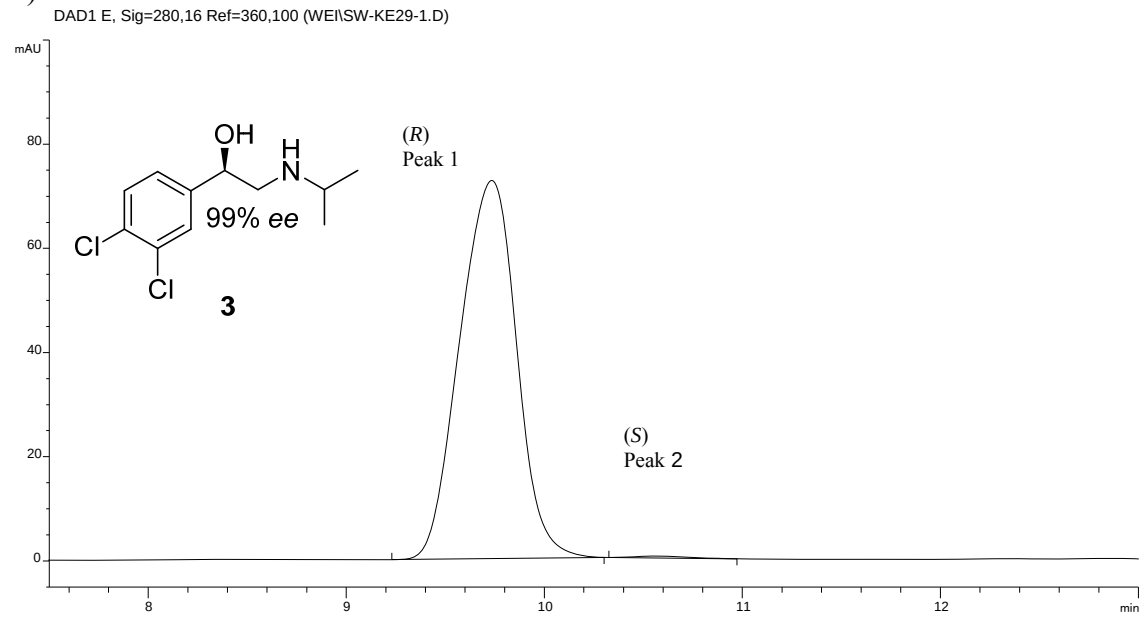
***(R)*-Dichloroisoproterenol (3)**

IC column, (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).



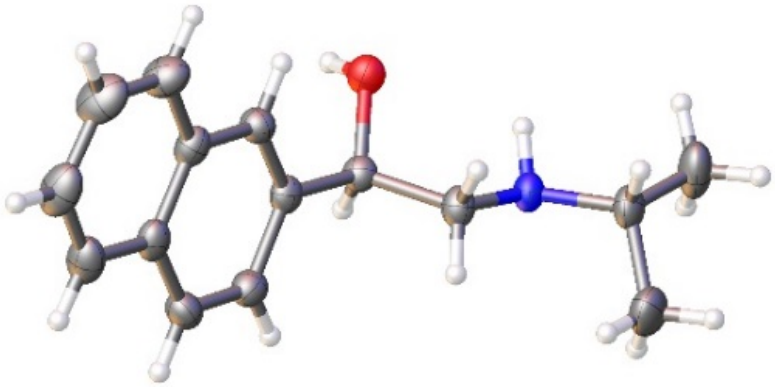
Peak	t_R	Area	Area (%)
1	10.269	213.1	91.376
2	11.104	20.1	8.624

Table 2, Entry 12 (recrystallized product)
***(R)*-Dichloroisoproterenol (3)**
IC column, (*n*-hexane / 2-propanol / ethanolamine 94.9:5:0.1, flow rate 0.5 ml/min, λ = 280 nm).



Peak	t_R	Area	Area (%)
1	9.734	1448.7	99.455
2	10.587	7.9	0.545

*X-ray crystal structure of the (R)-pronethalol (**1**)*:



CCDC-994083 data can be obtained free of charge from The Cambridge Crystallographic Data Center *via* www.ccdc.cam.ac.uk/data_request/cif.