Supporting Materials to

A General and Efficient Method for the Selective Synthesis of β -Hydroxy Sulfides and β -Hydroxy Sulfoxides Catalyzed by Gallium(III) Triflate

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General Experimental Details

General: Column chromatography was performed using EM Silica gel 60 (300-400 mesh). ^1H NMR and ^{13}C NMR were recorded on a 300 MHz or 400 MHz spectrometer. Chemical shifts were reported in ppm downfield from tetramethylsilane with the solvent resonance as the internal standard.

General procedure for the $\text{Ga}(\text{OTf})_3$ catalyzed ring-opening of epoxides (Table 2): To a mixture of epoxides (5 mmol) and thiophenols (5 mmol), $\text{Ga}(\text{OTf})_3$ 0.0258 g (0.05 mmol, 1 mol%) was added. The mixture was stirred at 30 °C for 30 min. After completion of the reaction, as indicated by TLC or HPLC, water was added, and the product was extracted with diethyl ether (3×10 mL). The organic layer was dried (MgSO_4) and evaporated, the crude product was purified by flash column chromatography (ethyl acetate/hexane, 1: 15 to 1:5) to provide the corresponding products. The catalyst in the aqueous phase was concentrated in vacuo to give a crystalline residue, which was finally heated at 180 °C for 48 h in vacuo to afford $\text{Ga}(\text{OTf})_3$ as colorless crystal. The recovered $\text{Ga}(\text{OTf})_3$ could be reused in the next batch reaction.

Typical procedure for the oxidation of 1h to 3a (Table 4, entry 1): To a mixture of 1h 0.42g (2 mmol) and H_2O_2 (0.5 mL of 30% wt aq solution, 4 mmol), $\text{Ga}(\text{OTf})_3$ 0.01g (0.02 mmol, 1 mol %) was added under stirring at 30 °C. After 25 min the reaction was completed, as indicated by TLC or HPLC, the reaction mixture was extracted with diethyl ether (3×10 mL). Then the organic layer was dried (MgSO_4) and evaporated, an off-white solid (4a) was obtained which did not need further purification. yield: 0.4 g (89%).

General one-pot synthesis of β -hydroxy sulfoxides starting from epoxides and thiophenols (Table 4):

Method A: To a mixture of epoxides (5 mmol) and thiophenols (5 mmol), $\text{Ga}(\text{OTf})_3$ 0.0258 g (0.05 mmol, 1 mol %) and H_2O_2 1.2 mL (30% wt aq solution, 10 mmol) was added and stirred at 30 °C. The progress of the reaction was monitored by TLC or HPLC. After completion of the reaction, the excess amount of H_2O_2 was destroyed by the addition of a saturated aqueous solution of Na_2SO_3 to the reaction mixture. If the products are solid, they were obtained through simple filtering which did not need further purification. If the products are liquid, the reaction mixture was extracted with diethyl ether (3×10 mL). The organic layer was dried (MgSO_4) and evaporated, the crude product was purified by flash column chromatography to provide the corresponding products.

Method B: To a mixture of epoxides (5 mmol), thiophenols (5 mmol) and $\text{Ga}(\text{OTf})_3$ 0.0258 g (0.05 mmol, 1 mol %) was stirred at 30 °C. After the ring-opening reaction was completed and H_2O_2 1.2 mL (30% wt aq solution, 10 mmol) was added. Then the mixture continued to be stirred at 30 °C. The progress of the reaction was monitored by TLC or HPLC. After completion of the reaction, the excess amount of H_2O_2 was destroyed by the addition of a saturated aqueous solution of Na_2SO_3 to the reaction mixture. If the products are solid, they were obtained through simple filtering which did not need further purification. If the products are liquid, the reaction mixture was extracted with diethyl ether (3×10 mL). The organic layer was dried (MgSO_4) and evaporated,

the crude product was purified by flash column chromatography to provide the corresponding products.

TABLE 1. Thiolysis of 1, 2-Epoxy-3-phenoxypropane by Thiophenol under Different Reaction Conditions^a

entry	solvent	catalyst (mol %)	yield (%) ^b	entry	solvent	catalyst (mol %)	yield (%) ^b
1	none	none	23 (34) ^c	12	none	In(OTf) ₃ (5)	90
2	H ₂ O	TfOH (5)	32	13	none	Sc(OTf) ₃ (5)	87
3	H ₂ O	Ga(OTf) ₃ (5)	70	14	none	Y(OTf) ₃ (5)	86
4	CH ₃ CN	Ga(OTf) ₃ (5)	73	15	none	La(OTf) ₃ (5)	89
5	CH ₃ NO ₂	Ga(OTf) ₃ (5)	84	16	none	Sm(OTf) ₃ (5)	85
6	C ₂ H ₅ NO ₂	Ga(OTf) ₃ (5)	79	17	none	Eu(OTf) ₃ (5)	85
7	CH ₂ Cl ₂	Ga(OTf) ₃ (5)	67	18	none	Yb(OTf) ₃ (5)	90
8	none	InCl ₃ (5)	53	19	none	Ga(OTf) ₃ ^e (1)	95, 92, 91
9	none	Cu(OTf) ₂ (5)	74	20	none	Ga(OTf) ₃ (2.5)	96
10	none	Mg(OTf) ₂ (5)	72	21	none	Ga(OTf) ₃ (5)	95
11	none	Bi(OTf) ₃ ^d (5)	71	22	none	Ga(OTf) ₃ (10)	97

^a At 30 °C for 30 min. ^b Isolated total yield. ^c At 50 °C for 12 h. ^d The mixture became yellow when Bi(OTf)₃ was added. ^e Catalyst was reused three times.

TABLE 2. Optimization of One-pot Protocol Using Cyclohexene Oxide and Thiophenol in the Presence of Various Metal Triflates under Different Reaction Conditions^a

entry	catalyst	time (h)	yield (%) ^b	entry	catalyst	time (h)	yield (%) ^b
1	none	24	trace	9	Sm(OTf) ₃	1.5	72
2	TfOH	5	trace	10	Eu(OTf) ₃	1.5	71
3	Cu(OTf) ₂	2	73	11	Yb(OTf) ₃	1.5	75
4	Mg(OTf) ₂	3	63	12	Ga(OTf) ₃	0.5	83

5	Bi(OTf) ₃	0.2	34 (trace) ^c	13	Ga(OTf) ₃ ^e	0.5	88, 82, 75
6	Sc(OTf) ₃	1.5	44 (trace) ^d	14	Ga(OTf) ₃	1	81 ^f
7	Y(OTf) ₃	1.5	76	15	Ga(OTf) ₃	1	85 ^g
8	La(OTf) ₃	1.5	74				

^a General reaction procedure: To a mixture of cyclohexene oxide (5 mmol) were added thiophenol (5 mmol), catalyst (1 mol %), and 30% H₂O₂ (10 mmol) simultaneously at 30 °C. ^b Isolated total yield. ^c 20% of 2-(phenylsulfonyl)cyclohexanol was found and 42% of diphenyldisulfide was formed after 25 min. ^d 46% of diphenyldisulfide was formed after 12 h. ^e Ga(OTf)₃ was reused three times. ^f 2 mL of CH₂Cl₂ was added. ^g 2 mL of CH₃NO₂ was added.

Analytical data

● β-Hydroxy Sulfoxides

1a (Lit.¹): Oil, *R*_f = 0.35 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.40 (d, *J* = 7.6 Hz, 2 H, ArH), 7.30 - 7.25 (m, 4 H), 7.20 (t, *J* = 7.2 Hz, 1 H, ArH), 6.96 (t, *J* = 7.2 Hz, 1 H, ArH), 6.88 (d, *J* = 8.4 Hz, 2 H, ArH), 4.14 - 4.02 (m, 3 H), 3.25 (dd, *J* = 13.6, 5.4 Hz, 1 H), 3.15 (dd, *J* = 13.6, 6.6 Hz, 1 H), 2.73 (br s, 1 H, OH).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 158.3, 135.0, 129.8, 129.5, 129.1, 126.6, 121.2, 114.5, 70.0, 68.5, 37.5.

MS (EI) *m/z*: 260 (M⁺, 100), 167 (63), 109 (6).

1b (Lit.²): Oil, *R*_f = 0.35 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.32 - 7.24 (m, 4 H, ArH), 7.08 (d, *J* = 8.4 Hz, 2 H, ArH), 6.95 (t, *J* = 7.2 Hz, 1 H, ArH), 6.86 (t, *J* = 8.4 Hz, 2 H, ArH), 4.06 - 3.99 (m, 3 H), 3.19 (dd, *J* = 14.0, 5.6 Hz, 1 H), 3.09 (dd, *J* = 14.0, 6.8 Hz, 1 H), 2.82 (br s, 1 H, OH), 2.30 (s, 3 H).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 158.6, 137.2, 131.5, 130.9, 130.2, 129.7, 121.4, 114.8, 70.3, 68.8, 38.6, 21.3.

MS (EI) *m/z*: 274 (M⁺, 100), 257 (34), 181 (38), 163 (39).

1c (Lit.³): Oil, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.39 (t, J = 8.4 Hz, 2 H, ArH), 7.27 (t, J = 8.4 Hz, 2 H, ArH), 7.00 – 6.94 (m, 3 H, ArH), 6.86 (d, J = 8.4 Hz, 2 H, ArH), 4.11 – 3.97 (m, 3 H), 3.18 (dd, J = 14.0, 5.2 Hz, 1 H), 3.07 (dd, J = 14.0, 6.4 Hz, 1 H), 2.85 (br s, 1 H, OH).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 162.0 (d, $^1J_{CF}$ = 246.2 Hz), 158.2, 132.7 (d, $^3J_{CF}$ = 8.4 Hz), 129.9, 129.5, 121.2, 116.2 (d, $^2J_{CF}$ = 22.0 Hz), 114.4, 69.8, 68.4, 38.7.

IR_{max} (neat): 3424, 3064, 3040, 2927, 2874, 1589, 1492, 1397, 1243 cm⁻¹.

MS (EI) m/z : 278 (M⁺, 100), 185 (54), 167 (37), 141 (54), 133 (55), 127 (15).

1d (Lit.³): Oil, R_f = 0.3 (petroleum ether / EtOAc = 2 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.30 – 7.26 (m, 2 H, ArH), 7.13 (t, J = 8.0 Hz, 1 H, ArH), 6.99 – 6.88 (m, 5 H, ArH), 6.68 (ddd, J = 8.4, 2.4, 0.8 Hz, 1 H, ArH), 5.98 (br s, 1 H, ArOH), 4.15 – 4.02 (m, 3 H), 3.24 (dd, J = 14.0, 5.6 Hz, 1 H), 2.85 (dd, J = 14.0, 7.2 Hz, 1 H), 2.86 (br s, 1 H, OH).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 158.3, 156.3, 136.5, 130.1, 129.5, 121.5, 121.3, 116.1, 114.5, 113.8, 69.9, 68.6, 37.1.

IR_{max} (neat): 3355, 3063, 2926, 1587, 1496, 1431, 1244 cm⁻¹.

MS (EI) m/z : 276 (M⁺, 100), 259 (52), 183 (46).

1e: Oil, R_f = 0.3 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.43 – 7.40 (m, 2 H, ArH), 7.31 – 7.20 (m, 4 H, ArH), 6.82 – 6.78 (m, 2 H, ArH), 4.12 – 4.06 (m, 1 H), 4.02 – 3.97 (m, 2 H), 3.24 (dd, J = 13.8, 5.7 Hz, 1 H), 3.14 (dd, J = 13.8, 6.9 Hz, 1 H), 2.12 (br s, 1 H, OH).

¹³C NMR (75 MHz, CDCl₃): δ (ppm) 156.9, 134.8, 129.9, 129.3, 129.0, 126.7, 126.1, 115.7, 70.4, 68.4, 37.6.

IR_{max} (neat): 3431, 2926, 1582, 1492, 1244, 1092, 1025, 823, 740, 691 cm⁻¹.

MS (EI) m/z : 296 ([M=2]⁺, 66), 294 (M⁺, 25), 160 (100), 149 (39), 135 (28), 123 (74).

Anal. Calcd for C₁₅H₁₅ClO₂S: C, 61.11; H, 5.13. Found: C, 60.98.77; H, 5.24.

1f (Lit.⁴): Oil, R_f = 0.35 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.37 – 7.35 (m, 2 H, ArH), 7.32 – 7.23 (m, 7 H, ArH), 7.21 – 7.17 (m, 1 H, ArH), 4.66 (dd, J = 3.6 Hz, 1 H, CHOH), 3.25 (dd, J = 13.6,

3.6 Hz, 1 H), 3.13 (br s, 1 H, OH), 3.05 (dd, $J = 13.6, 9.2$ Hz, 1 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 142.4, 135.3, 130.2, 129.3, 128.7, 128.1, 126.8, 126.1, 71.9, 43.9.

IR ν_{max} (neat): 3425, 3060, 3030, 2922, 1583, 1480, 1439, 1056 cm^{-1} .

MS (EI) m/z : 230 (M^+ , 57), 213 (100), 196 (16), 124 (26).

2f (Lit.⁴): Oil, $R_f = 0.3$ (petroleum ether / EtOAc = 6 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.37 – 7.29 (m, 2 H, ArH), 7.28 – 7.20 (m, 8 H, ArH), 4.27 (t, $J = 6.8$ Hz, 1 H), 3.87 (dd, $J = 11.2, 5.6$ Hz, 1 H), 3.82 (dd, $J = 11.2, 6.8$ Hz, 1 H), 2.41 (br s, 1 H, OH).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 138.8, 133.6, 132.3, 128.8, 128.5, 127.9, 127.6, 127.3, 67.2, 55.6.

IR ν_{max} (neat): 3405, 3059, 3028, 2927, 2872, 1583, 1480, 1438, 1055 cm^{-1} .

MS (EI) m/z : 230 (M^+ , 100), 213 (39), 199 (48), 121 (36).

1g (Lit.³): Oil, $R_f = 0.3$ (petroleum ether / EtOAc = 2 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.34 – 7.25 (m, 5 H, ArH), 7.17 – 7.10 (m, 1 H, ArH), 7.01 – 6.93 (m, 1 H, ArH), 6.87 (t, $J = 2.0$ Hz, 1 H, ArH), 6.69 – 6.64 (m, 1 H, ArH), 5.89 (br s, 1 H, ArOH), 4.66 (dd, $J = 9.6, 3.6$ Hz, 1 H, CHOH), 3.46 (dd, $J = 13.6, 3.6$ Hz, 1 H), 3.13 (br s, 1 H, OH), 3.05 (dd, $J = 13.6, 9.2$ Hz, 1 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 156.0, 141.7, 136.1, 130.1, 128.5, 128.0, 125.8, 122.0, 116.6, 113.9, 71.8, 43.3.

IR ν_{max} (neat): 3355, 3062, 2922, 1583, 1476, 1493, 1250 cm^{-1} .

MS (EI) m/z : 246 (M^+ , 100), 229 (92), 140 (12).

2g (Lit.³): Oil, $R_f = 0.25$ (petroleum ether / EtOAc = 2 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) = 7.32 – 7.24 (m, 5 H, ArH), 7.07 (t, $J = 7.6$ Hz, 1 H, ArH), 6.86 – 6.82 (m, 2 H, ArH), 6.69 – 6.66 (m, 1 H, ArH), 5.98 (br s, 1 H, ArOH), 4.30 (t, $J = 6.8$ Hz, 1 H), 3.92 (dd, $J = 11.6, 6.8$ Hz, 1 H), 3.87 (dd, $J = 11.6, 7.2$ Hz, 1 H), 2.64 (br s, 1 H, OH).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 156.4, 141.5, 135.8, 130.3, 128.5, 128.0, 124.2, 123.1, 115.2, 113.4, 68.3, 50.1.

IR ν_{max} (neat): 3345, 3061, 3028, 2928, 1584, 1440, 1251, 1053 cm^{-1} .

MS (EI) m/z : 246 (M^+ , 100), 229 (70), 215 (79), 121 (42), 91 (24).

1h (Lit.³): Oil, $R_f = 0.4$ (petroleum ether / EtOAc = 6 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.47 (d, $J = 5.6$ Hz, 2 H, ArH), 7.31 – 7.26 (m, 3 H, ArH), 3.36 – 3.30 (m, 1 H, CHOH), 2.98 (br s, 1 H, OH), 2.80 – 2.75 (m, 1 H), 2.14 – 2.08 (m, 2 H), 1.73 – 1.66 (m, 2 H), 1.37 – 1.25 (m, 4 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 133.7, 132.5, 128.8, 127.7, 72.0, 56.4, 33.7, 32.6, 26.1, 24.2.

MS (EI) m/z : 209 ($[\text{M}+1]^+$, 30), 208 (M^+ , 100), 191 (35), 110 (75), 81 (40).

1i (Lit.⁵): Oil, $R_f = 0.4$ (petroleum ether / EtOAc = 6 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.49 – 7.44 (m, 2 H, ArH), 7.04 – 6.99 (m, 2 H, ArH), 3.31 – 3.26 (m, 1 H, CHOH), 3.03 (br s, 1 H, OH), 2.71 – 2.65 (m, 1 H), 2.16 – 2.04 (m, 2 H), 1.73 – 1.64 (m, 2 H), 1.38 – 1.53 (m, 4 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 163.0 (d, $^1J_{\text{CF}} = 246.4$ Hz), 136.8 (d, $^3J_{\text{CF}} = 8.3$ Hz), 127.3, 116.2 (d, $^2J_{\text{CF}} = 22.0$ Hz), 71.9, 56.9, 34.0, 32.6, 26.3, 24.5.

IR_{max} (neat): 3440, 3066, 2934, 2858, 1589, 1550, 1449, 1224, 1068 cm^{-1} .

MS (EI) m/z : 226 (M^+ , 100), 209 (85).

1j: mp: 160.9 – 162.7 $^{\circ}\text{C}$; $R_f = 0.35$ (petroleum ether / EtOAc = 6 : 1).

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 7.97 (d, $J = 8.4$ Hz, 2 H, ArH), 7.05 (d, $J = 8.4$ Hz, 2 H, ArH), 6.10 (s, 2 H, NH_2), 5.17 (d, $J = 5.6$ Hz, 1 H, OH), 4.09 (q, $J = 7.2$ Hz, 2 H, CH_2CH_3), 3.34 – 3.30 (m, 1 H), 3.25 – 3.22 (m, 1 H), 2.12 – 2.09 (m, 1 H), 1.92 – 1.90 (m, 1 H), 1.65 – 1.60 (m, 2 H), 1.51 – 1.42 (m, 1 H), 1.36 (t, $J = 7.2$ Hz, 3 H, CH_3CH_2), 1.30 – 1.21 (m, 3 H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ (ppm) 160.3, 154.1, 152.1, 130.1, 120.2, 115.1, 72.4, 64.0, 54.4, 35.7, 32.7, 25.8, 24.4, 15.4.

IR_{max} (KBr): 3424, 3299, 2931, 2849, 1617, 1475, 1248, 1116 cm^{-1} .

MS (ESI) m/z : 335 ($[\text{M}+1]^+$, 100).

Anal. Calcd for $\text{C}_{16}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$: C, 57.46; H, 6.63. Found: C, 57.61; H, 6.52.

1k (Lit.³): Oil, $R_f = 0.4$ (petroleum ether / EtOAc = 6 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) = 7.41 – 7.38 (m, 2 H, ArH), 7.00 (t, J = 8.4 Hz, 2 H, ArH), 3.85 – 3.77 (m, 1 H, CHOH), 3.04 (dd, J = 13.6, 3.6 Hz, 1 H), 2.81 (dd, J = 13.6, 8.4 Hz, 1 H), 2.67 (br s, 1 H, OH), 1.25 (d, J = 6.4 Hz, 3 H).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 162.0 (d, $^1J_{\text{CF}}$ = 245.7 Hz), 133.0 (d, $^3J_{\text{CF}}$ = 8.3 Hz), 130.0, 116.1 (d, $^2J_{\text{CF}}$ = 21.2 Hz), 65.4, 44.7, 21.8.
 IR_{max} (neat): 3404, 2971, 2926, 1590, 1491, 1456, 1228, 1157, 1090 cm^{-1} .
 MS (EI) m/z : 186 (M^+ , 100), 169 (77), 141 (13).

1l (Lit.³): Oil, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1).
 ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.41 (t, J = 6.4 Hz, 2 H, ArH), 7.02 (t, J = 8.4 Hz, 2 H, ArH), 3.90 – 3.87 (m, 1 H, CHOH), 3.70 – 3.63 (m, 2 H, CH_2Cl), 3.11 (dd, J = 14.0, 5.6 Hz, 1 H), 3.02 (dd, J = 14.0, 7.2 Hz, 1 H), 2.77 (br s, 1 H, OH).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 162.1 (d, $^1J_{\text{CF}}$ = 246.5 Hz), 133.0 (d, $^3J_{\text{CF}}$ = 8.3 Hz), 129.4, 116.3 (d, $^2J_{\text{CF}}$ = 22.0 Hz), 69.3, 47.8, 39.3.
 IR_{max} (neat): 3367, 2935, 2912, 1555, 1457, 1408, 1235 cm^{-1} .
 MS (EI) m/z : 222 ($[\text{M}+2]^+$, 20), 220 (M^+ , 57), 205 (5), 203 (18), 141 (72), 84 (100).

1m (Lit.³): Oil, R_f = 0.3 (petroleum ether / EtOAc = 2 : 1).
 ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.14 (t, J = 7.6 Hz, 1 H, ArH), 6.92 – 6.87 (m, 2 H, ArH), 6.70 (dd, J = 8.4, 2.4 Hz, 1 H, ArH), 6.62 (br s, 1 H, ArOH), 3.99 – 3.94 (m, 1 H, CHOH), 3.69 (dd, J = 11.2, 4.4 Hz, 1 H), 3.65 (dd, J = 11.2, 5.2 Hz, 1 H), 3.15 (br s, 1 H, OH), 3.13 (dd, J = 14.4, 5.6 Hz, 1 H), 3.11 (dd, J = 14.4, 7.2 Hz, 1 H).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 156.1, 135.8, 130.2, 121.7, 116.2, 114.1, 69.5, 47.8, 37.5.
 IR_{max} (neat): 3362, 2955, 2924, 1583, 1476, 1437, 1042, 775, 686 cm^{-1} .
 MS (EI) m/z : 220 ($[\text{M}+2]^+$, 46), 218 (M^+ , 100), 184 (72), 183 (28), 182 (22), 167 (30).

1n (Lit.⁶): mp: 138.3 – 140.1 $^\circ\text{C}$, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1).
 ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.45 (d, J = 8.0 Hz, 1 H, ArH), 7.34 (t, J = 8.0 Hz, 1 H, ArH), 7.12 – 7.17 (m, 2 H, ArH), 4.21 (dd, J = 15.2, 6.8 Hz, 1 H), 4.12 (dd, J = 15.2, 6.0 Hz, 1 H), 3.25 – 3.19 (m, 1 H), 2.53 (dd, J = 6.0, 1.2 Hz, 1 H), 2.47 (dd, J = 6.0, 1.6 Hz, 1 H), 1.74 (br s, 1 H, OH).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 170.5, 137.1, 126.7, 123.7, 123.1, 122.9, 111.1, 48.2, 30.9,

24.3.

IR_{max} (KBr): 3375, 2925, 2853, 1591, 1471 cm⁻¹.

MS (EI) m / z: 261 ([M+2]⁺, 28), 259 (M⁺, 70), 223 (100), 190 (36).

1o (Lit.⁷): Oil, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1)。

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.30 (d, 2 H, ArH), 7.11 (d, 2 H, ArH), 3.89 -3.87 (m, 1 H, CHOH), 3.68 – 3.61 (m, 2 H), 3.10 (dd, *J* = 13.6, 4.8 Hz, 1 H), 3.01 (dd, *J* = 13.6, 7.2 Hz, 1 H), 2.80 (br s, 1 H, OH), 2.32 (s, 3 H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 137.2, 130.8, 130.7, 129.9, 69.4, 47.9, 38.8, 21.0.

IR_{max} (neat): 3422, 3020, 2954, 2921, 1493, 1425, 1043 cm⁻¹.

MS (EI) m / z: 218 ([M+2]⁺, 35), 216 (M⁺, 100), 199 (33), 190 (50).

[α]_D²⁰ +26.4 (*c* 0.99 in CHCl₃), R; 96% ee [*t*_R(S) 39.50 min and *t*_R(R) 41.63 min].

1p (Lit.⁷): Oil, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1)。

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.30 (d, 2 H, ArH), 7.11 (d, 2 H, ArH), 3.89 -3.87 (m, 1 H, CHOH), 3.68 – 3.61 (m, 2 H), 3.10 (dd, *J* = 13.6, 4.8 Hz, 1 H), 3.01 (dd, *J* = 13.6, 7.2 Hz, 1 H), 2.80 (br s, 1 H, OH), 2.32 (s, 3 H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 137.2, 130.8, 130.7, 129.9, 69.4, 47.9, 38.8, 21.0.

IR_{max} (neat): 3422, 3020, 2954, 2921, 1493, 1425, 1043 cm⁻¹.

MS (EI) m / z: 218 ([M+2]⁺, 35), 216 (M⁺, 100), 199 (33), 190 (50).

[α]_D²⁰ -25.9 (*c* 0.99 in CHCl₃), S; 94% ee [*t*_S(S) 39.56 min and *t*_S(R) 42.56 min].

1q (Lit.³): Oil, R_f = 0.4 (petroleum ether / EtOAc = 6 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.44 (t, *J* = 7.6 Hz, 1 H, ArH), 7.26 – 7.23 (m, 1 H, ArH), 7.11 – 7.05 (m, 2 H, ArH), 3.61 – 3.60 (m, 1 H, CHOH), 3.12 (dd, *J* = 13.2, 2.8 Hz, 1 H), 2.80 (dd, *J* = 13.2, 8.8 Hz, 1 H), 2.48 (br s, 1 H, OH), 1.52 – 1.26 (m, 10 H), 0.87 (t, *J* = 6.0 Hz, 3 H).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 161.9 (d, ¹*J*_{CF} = 244.2 Hz, CF), 133.3, 129.1 (d, ³*J*_{CF} = 7.5 Hz, CH_{Ar}), 124.6 (d, ³*J*_{CF} = 3.8 Hz, CH_{Ar}), 121.9 (d, ²*J*_{CF} = 16.5 Hz, CSCH₂), 115.8 (d, ²*J*_{CF} = 22.8 Hz, CH_{Ar}), 69.5, 41.9, 35.4, 31.7, 29.2, 25.6, 22.5, 14.0.

IR_{max} (neat): 3392, 2935, 2847, 1587, 1461, 1240 cm⁻¹.

MS (EI) m/z : 256 (M^+ , 100), 239 (76), 142 (64).

1r: Oil, R_f = 0.5 (petroleum ether / EtOAc = 6 : 1).

^1H NMR (300 MHz, CDCl_3): δ (ppm) 7.40 – 7.21 (m, 5 H, ArH), 5.82 – 5.76 (m, 1 H, $\text{CH}_2=\text{CH}-\text{C}$), 5.02 – 4.91 (m, 2 H, $\text{CH}_2=\text{C}$), 3.68 – 3.66 (m, 1 H, CHOH) 3.15 (dd, J = 13.6, 3.50 Hz, 1 H), 2.85 (dd, J = 13.6, 8.65 Hz, 1 H), 2.39 -2.68 (m, 1 H), 2.05 – 2.00 (m, 2 H, $\text{CH}_2=\text{CH}-\text{CH}_2$), 1.54 - 1.29 (m, 9 H).

^{13}C NMR (75 MHz, CDCl_3): δ (ppm) 139.0, 135.3, 129.9, 129.0, 126.4, 114.1, 69.3, 42.1, 36.0, 33.6, 29.3, 28.9, 28.7, 25.5.

IR_{max} (neat): 3418, 2927, 2854, 1584, 1439, 1025, 737, 691 cm^{-1} .

MS (EI) m/z : 264 (M^+ , 78), 247 (30), 124 (100).

Anal. Calcd for $\text{C}_{16}\text{H}_{24}\text{OS}$: C, 72.67; H, 9.15. Found: C, 72.77; H, 9.02.

1s (Lit.⁸): Oil, R_f = 0.6 (petroleum ether / EtOAc = 4 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.34 – 7.24 (m, 5 H, ArH), 3.83 – 3.78 (m, 2 H, CHOH), 3.32 – 3.31 (m, 1 H), 2.81 (br s, 1 H, OH), 2.41 – 2.39 (m, 1 H), 2.10 – 2.98 (m, 2 H), 1.74 – 1.66 (m, 2 H), 1.45 -1.18 (m, 4 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 138.4, 128.4, 128.3, 127.0, 72.2, 53.0, 34.6, 33.8, 32.5, 26.0, 24.2.

IR_{max} (neat): 3346, 3032, 2935, 1562, 1468 cm^{-1} .

MS (ESI) m/z : 223 ($[\text{M}+1]^+$, 100).

1t (Lit.⁹): Oil, R_f = 0.5 (petroleum ether / EtOAc = 4 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.25 – 7.20 (m, 2 H, ArH), 6.89 – 6.81 (m, 2 H, ArH), 3.93 – 3.81 (m, 1 H, CHOH), 3.73 (s, 3 H, OCH_3), 3.68 (s, 2 H, SCH_2Ar), 3.64 – 3.53 (m, 2 H, ClCH_2), 3.08 (br s, 1 H, OH), 2.63 (dd, J = 12.0, 4.0 Hz, 1 H, CH_2S), 2.55 (dd, J = 12.0, 8.0 Hz, 1 H, CH_2S).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 158.6, 129.9, 129.6, 113.9, 69.8, 55.1, 48.0, 35.8, 35.0.

IR_{max} (neat): 3422, 3025, 2933, 1523, 1456 cm^{-1} .

1u (Lit.¹⁰): Oil, R_f = 0.5 (petroleum ether / EtOAc = 4 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.30 – 7.24 (m, 4 H, ArH), 3.91 – 3.87 (m, 1 H, CHOH), 3.72 (s, 2 H, SCH₂Ar), 3.64 – 3.57 (m, 2 H, ClCH₂), 2.66 (dd, J = 16.0, 4.0 Hz, 2 H), 2.57 (dd, J = 12.0, 8.0 Hz, 1 H).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 136.3, 132.8, 130.2, 128.6, 70.0, 48.0, 35.8, 35.0.

IR_{max} (neat): 3372, 3023, 2846, 1581, 1460, 1237 cm⁻¹.

1v (Lit.¹¹): Oil, R_f = 0.5 (petroleum ether / EtOAc = 4 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.28 – 7.24 (m, 2 H, ArH), 6.96 – 6.89 (m, 2 H, ArH), 4.09 – 4.00 (m, 3 H, CHOH and PhOCH₂), 3.26 (br s, 1 H, OH), 2.87 (dd, J = 12.0, 8.0 Hz, 1 H, CH₂S), 2.70 (dd, J = 12.0, 8.0 Hz, 1 H, CH₂S), 2.53 (t, J = 8.0 Hz, 2 H, SCH₂CH₂), 1.58 – 1.52 (m, 2 H, SCH₂CH₂), 1.40 – 1.35 (m, 2 H), 0.89 (t, J = 8.0 Hz, 2 H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 158.3, 129.5, 121.1, 114.5, 70.2, 68.6, 35.7, 32.2, 31.6, 21.8, 13.6.

IR_{max} (neat): 3363, 3008, 2852, 1565, 1448, 1240 cm⁻¹.

MS (ESI) m/z : 241 ([M+1]⁺, 100).

● β -Hydroxy Sulfoxides

3a (Lit.¹²): mp: 152.5 – 154.1 °C; R_f = 0.25 - 0.30 (petroleum ether / EtOAc = 1 : 1).

¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.74 – 7.67 (m, 2 H, ArH), 7.64 – 7.48 (m, 3 H, ArH), 5.05 (br s, 1 H, OH), 4.15 – 4.09; 3.94 – 3.88 (m, 1 H, CHOH), 2.79 – 2.69 (m, 1 H), 2.15 – 2.05 (m, 1 H), 1.76 – 1.69 (m, 2 H), 1.48 – 1.05 (br m, 5 H).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.3, 142.1, 131.9, 129.2, 128.9, 125.4, 124.9, 72.0, 68.4, 35.5, 34.6, 24.5, 23.6, 21.1.

IR_{max} (KBr): 3308, 2932, 2854, 1476, 1440, 1010 (SO st) cm⁻¹.

MS (EI) m/z : 225 ([M+1]⁺, 75), 126 (100), 81 (43), 78 (55).

A mixture of two diastereoisomers were isolated by flash column chromatography (ethyl acetate / hexane, 1 : 15 to 1 : 2) to provide major isomers and minor isomers.

Major isomer (83%): mp: 155.3 – 156.2 °C; R_f = 0.30 (petroleum ether / EtOAc = 1 : 1). ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.74 – 7.72 (m, 2 H, ArH), 7.56 – 7.55 (m, 3 H, ArH), 5.09 (br s, 1 H, OH), 4.15 – 4.10 (m, 1 H, CHOH), 2.76 – 2.74 (m, 1 H), 2.17 – 2.12 (m, 1 H), 1.76 – 1.69 (m, 2 H), 1.47 – 1.24 (m, 4 H), 1.12 – 1.08 (m, 1 H).

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 142.5, 131.9, 129.3, 125.5, 72.2, 68.5, 34.6, 24.7, 23.9, 23.7.

Minor isomer (17%): mp: 152.8 -153.2 °C; R_f = 0.25 (petroleum ether / EtOAc = 1 : 1). ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.62 – 7.50 (m, 5 H, ArH), 3.95 – 3.88 (m, 1 H, CHOH), 2.72 – 2.70 (br m 2 H including OH), 2.11 – 2.05 (m, 1 H), 1.71 - 1.68 (m, 2 H), 1.48 – 1.12 (m, 5 H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 142.1, 131.0, 129.0, 125.2, 69.4, 68.4, 35.5, 24.8, 23.6, 21.1.

3b (Lit.¹³): mp: 144.3 - 145.0 °C; R_f = 0.2 (petroleum ether / EtOAc = 1 : 1). ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.62 (d, J = 8 Hz, 2 H, ArH), 7.35 (d, J = 8 Hz, 2 H, ArH), 5.28 (br s, 1 H, OH), 4.11 – 4.09 (m, 1 H, CHOH), 2.75 – 2.69 (m, 1 H), 2.43 (s, 3 H, CH_3), 2.14 – 2.12 (m, 1 H), 1.75 – 1.68 (m, 2 H), 1.42 – 1.07 (m, 5 H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 142.7, 139.1, 130.0, 125.6, 72.3, 68.4, 34.6, 24.7, 23.8, 23.7, 21.5. IR_{max} (KBr): 3316, 2932, 2853, 1454, 1028 (SO st) cm^{-1} . MS (EI) m/z : 239 ($[\text{M}+1]^+$, 87), 220 (14), 140 (100), 92 (47), 81 (27).

3c: mp: 175.1 – 176.0 °C; R_f = 0.23 (petroleum ether / EtOAc = 1 : 1). ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.76 – 7.72 (m, 2 H, ArH), 7.27 – 7.23 (m, 2 H, ArH), 4.26 (br s, 1 H, OH), 4.15 – 4.06 (m, 1 H, CHOH), 2.76 – 2.70 (m, 1 H), 2.18 – 2.12 (m, 1 H), 1.78 – 1.71 (m, 2 H), 1.46 – 1.06 (m, 5 H). ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 164.8 (d, $^1J_{\text{CF}}$ = 251.8 Hz), 137.7, 127.8 (d, $^3J_{\text{CF}}$ = 9.1 Hz), 116.7 (d, $^2J_{\text{CF}}$ = 22.7 Hz), 72.1, 68.6, 34.6, 24.6, 23.6. IR_{max} (KBr): 3362, 3060, 2933, 1588, 1493, 1022 (SO st) cm^{-1} . MS (EI) m/z : 243 ($[\text{M}+1]^+$, 25), 242 (M^+ , 4), 144 (100), 96 (44), 81 (50). Anal. Calcd for $\text{C}_{12}\text{H}_{15}\text{FO}_2\text{S}$: C, 59.48; H, 6.24. Found: C, 59.22; H, 6.35.

3d: Oil, R_f = 0.2 (petroleum ether / EtOAc = 1 : 1). ^1H NMR (300 MHz, CDCl_3): δ (ppm) 7.70 – 7.65 (m, 2 H, ArH), 7.54 – 7.51 (m, 3 H, ArH), 7.27 – 7.24 (m, 2 H, ArH), 6.90 – 6.83 (m, 3 H, ArH), 4.62 – 4.57 (m, 1 H, CHOH), 4.01 – 3.96 (m, 2 H), 3.19 – 3.15 (m, 2 H). ^{13}C NMR (75 MHz, CDCl_3): δ (ppm) 158.1, 143.3, 131.4, 129.4, 129.3, 123.9, 121.2, 114.5, 70.73, 67.0, 59.9.

IR_{max} (neat): 3338, 2927, 2855, 1440, 1020 (SO st) cm⁻¹.

MS (EI) *m/z*: 277 ([M+1]⁺, 54), 133 (100), 125 (36), 43 (77).

Anal. Calcd for C₁₅H₁₆O₃S: C, 65.19; H, 5.84. Found: C, 65.04; H, 6.01.

3e: mp: 107.9 – 109.0 °C; *R_f* = 0.2 (petroleum ether / EtOAc = 1 : 1).

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.70 – 7.67 (m, 2 H, ArH), 7.56 – 7.54 (m, 3 H, ArH), 7.26 – 7.20 (m, 2 H, ArH), 6.84 – 6.79 (m, 2 H, ArH), 4.65 – 4.58 (m, 1 H, *CHOH*), 4.11 (dd, *J* = 9.6, 5.2 Hz, 1 H), 3.95 (dd, *J* = 9.6, 5.4 Hz, 1 H), 3.13 – 3.06 (m, 2 H), 2.74 (br s, 1 H, OH).

¹³C NMR (75 MHz, CDCl₃): δ (ppm) 156.7, 143.3, 131.4, 129.4, 129.3, 126.2, 123.8, 115.7, 70.8, 67.2, 59.4.

IR_{max} (KBr): 3338, 3065, 2929, 2873, 1578, 1492, 1035 (SO st) cm⁻¹.

MS (EI) *m/z*: 313 ([M+2]⁺, 58), 311 (M⁺, 22), 218 (69), 183 (100), 169 (24), 128 (34), 125 (40).

Anal. Calcd for C₁₅H₁₅ClO₃S: C, 57.97; H, 4.86. Found: C, 57.88; H, 4.95.

3f (Lit.¹⁴): mp: 89.5 – 90.1 °C; *R_f* = 0.2 (petroleum ether / EtOAc = 1 : 1).

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.66 – 7.63 (m, 2 H, ArH), 7.55 – 7.52 (m, 3 H, ArH), 7.33 – 7.26 (m, 5 H, ArH), 4.51 (s, 1 H), 4.42 – 4.39 (m, 1 H, *CHOH*), 3.55 (dd, *J* = 9.6, 4.8 Hz, 1 H),

3.46 (dd, *J* = 9.6, 5.7 Hz, 1 H), 3.12 – 3.05 (m, 2 H).

¹³C NMR (75 MHz, CDCl₃): δ (ppm) 142.8, 137.5, 131.1, 129.3, 128.3, 127.7, 127.6, 123.9, 73.3, 72.9, 65.7, 59.4.

IR_{max} (KBr): 3330, 2908, 2800, 1443, 1027 (SO st) cm⁻¹.

MS (EI) *m/z*: 291 ([M+1]⁺, 35), 167 (30), 125 (28), 91 (100).

3g: mp: 119.2 – 120.3 °C; *R_f* = 0.2 (petroleum ether / EtOAc = 1 : 1).

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.78 – 7.71 (m, 5 H, ArH), 7.58 – 7.55 (m, 3 H, ArH), 7.45 – 7.35 (m, 2 H, ArH), 7.15 – 7.08 (m, 2 H, ArH), 4.71 – 4.68 (m, 1 H, *CHOH*), 4.28 (dd, *J* = 9.6, 5.1 Hz, 1 H), 4.11 (dd, *J* = 9.6, 5.4 Hz, 1 H), 3.23 – 3.17 (m, 2 H), 2.01 (br s, 1 H, OH).

¹³C NMR (75 MHz, CDCl₃): δ (ppm) 155.8, 143.3, 134.2, 134.0, 129.5, 129.3, 129.2, 127.9, 127.5, 126.7, 126.4, 123.9, 118.3, 107.1, 70.0, 65.0, 59.4.

IR_{max} (KBr): 3417, 2932, 2862, 1579, 1022 (SO st) cm⁻¹.

MS (EI) m/z : 327 ($[M+1]^+$, 15), 326 (M^+ , 25), 183 (100), 127 (35).

Anal. Calcd for $C_{19}H_{18}O_3S$: C, 69.91; H, 5.56. Found: C, 70.02; H, 5.47.

3h (Lit.¹⁵): Oil, R_f = 0.2 (petroleum ether / EtOAc = 1 : 1).

1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.65 – 7.50 (m, 5 H, ArH), 4.40 – 4.31 (m, 1 H, $CHOH$), 3.14 – 3.06 (m, 1 H), 2.68 – 2.64 (m, 1 H), 2.46 (br s, 1 H, OH), 1.24 (d, J = 6.3 Hz, 3 H).

^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 142.6, 131.0, 129.4, 123.9, 62.9, 62.2, 23.1.

IR_{max} (neat): 3352, 2968, 2929, 1444, 1043 (SO st) cm^{-1} .

MS (EI) m/z : 185 ($[M+1]^+$, 100), 168 (16), 126 (20).

3i (Lit.¹⁶): mp: 103.3 – 103.9 °C; R_f = 0.25 (petroleum ether / EtOAc = 1 : 1).

1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.66 (d, J = 6.4 Hz, 2 H, ArH), 7.56 (d, J = 6.4 Hz, 2 H, ArH), 4.43 – 4.41 (m, 1 H, $CHOH$), 4.02 (br s, 1 H, OH), 3.63 – 3.54 (m, 2H), 3.15 – 3.09 (m, 1 H), 2.92 – 2.89 (m, 1 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 142.3, 131.4, 129.5, 123.9, 66.7, 59.1, 48.0.

IR_{max} (KBr): 3241, 1444, 1089, 1039 (SO st) cm^{-1} .

MS (EI) m/z : 239 ($[M+3]^+$, 37), 238 ($[M+2]^+$, 19), 237 ($[M+1]^+$, 90), 236 (M^+ , 31), 202 (28), 126 (100), 125 (93), 97 (36), 78 (76).

3j (Lit.¹⁷): mp: 124.4 – 126.3 °C; R_f = 0.25 (petroleum ether / EtOAc = 1 : 1).

1H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.69 – 7.65 (m, 2 H, ArH), 7.29 – 7.25 (m, 2 H, ArH), 4.45 – 4.41 (m, 1 H, $CHOH$), 3.75 (br s, 1 H, OH), 3.62 (dd, J = 11.2, 5.2 Hz, 1 H), 3.57 (dd, J = 11.2, 5.2 Hz, 1 H), 3.13 – 3.06 (m, 1 H), 2.89 (dd, J = 13.6, 1.6 Hz, 1 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 164.5 (d, $^1J_{CF}$ = 250.3 Hz), 137.9, 126.3 (d, $^3J_{CF}$ = 9.1 Hz), 117.0 (d, $^2J_{CF}$ = 22.8 Hz), 66.5, 59.8, 48.0.

IR_{max} (KBr): 3258, 3063, 2941, 1590, 1493, 1030 (SO st) cm^{-1} .

MS (EI) m/z : 239 ($[M+3]^+$, 35), 238 ($[M+2]^+$, 11), 237 ($[M+1]^+$, 100), 236 (M^+ , 23), 220 (33), 144 (65), 143 (75), 96 (40).

3k: Oil, $R_f = 0.2$ (petroleum ether / EtOAc = 1 : 1).

^1H NMR (300 MHz, CDCl_3): δ (ppm) 7.68 – 7.63 (m, 2 H, ArH), 7.58 – 7.53 (m, 3 H, ArH), 5.84 – 5.73 (m, 1 H, $\text{CH}_2=\text{CH}-\text{C}$), 5.00 – 4.90 (m, 2 H, $\text{CH}_2=\text{C}$), 4.32 – 4.30 (m, 1 H, CHOH), 3.04 – 2.70 (m, 3 H, $\text{CH}_2\text{S}(\text{O})$ and OH), 2.06 – 1.99 (m, 2 H, $\text{CH}_2=\text{CH}-\text{CH}_2$), 1.58 – 1.25 (m, 10 H).

^{13}C NMR (75 MHz, CDCl_3): δ (ppm) 143.8, 138.9, 131.3, 129.4, 123.9, 68.7, 62.3, 36.9, 33.7, 29.1, 28.8, 28.6, 24.8.

IR_{max} (KBr): 3373, 2927, 2855, 1444, 1020(SO st) cm^{-1} .

MS (EI) m/z : 281 ($[\text{M}+1]^+$, 85), 263 (42), 126 (100).

Anal. Calcd for $\text{C}_{16}\text{H}_{24}\text{O}_2\text{S}$: C, 68.53; H, 8.63. Found: C, 68.48; H, 8.71.

3l (Lit.¹⁸): mp: 113.4 – 114.7 °C; $R_f = 0.3$ (petroleum ether / EtOAc = 2 : 3).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.39 – 7.27 (m, 5 H, ArH), 4.48 – 4.45 (m, 1 H, CHOH), 3.95 (s, 2 H, $\text{S}(\text{O})\text{CH}_2\text{Ph}$), 3.22 (br s, 1 H, OH), 2.77 – 2.74 (m, 1 H, $\text{CH}_2\text{S}(\text{O})$), 2.61 – 2.58 (m, 1 H, $\text{CH}_2\text{S}(\text{O})$), 1.30 (d, $J = 4.0$ Hz, 3 H, CH_3).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 129.9, 129.4, 128.9, 128.3, 62.4, 57.9, 57.1, 23.3.

IR_{max} (KBr): 3345, 2936, 2927, 1438, 1029(SO st) cm^{-1} .

MS (ESI) m/z : 257 ($[\text{M}+1]^+$, 100).

3m (Lit.¹⁹): mp: 122.8 – 123.2 °C; $R_f = 0.3$ (petroleum ether / EtOAc = 2 : 3).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.30 – 7.27 (m, 2 H, ArH), 6.98 – 6.90 (m, 3 H, ArH), 4.65 – 4.61 (m, 2 H, CHOH and OH), 4.06 (d, $J = 4.0$ Hz, 2 H, PhOCH_2), 3.05 – 2.97 (m, 2 H, $\text{S}(\text{O})\text{CH}_2\text{CH}_3$), 2.96 – 2.73 (m, 2 H, $\text{CH}_2\text{S}(\text{O})$), 1.58 – 1.25 (m, 10 H).

^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 158.2, 129.4, 121.1, 114.4, 70.8, 64.3, 55.5, 52.2, 24.5, 21.9, 13.5.

IR_{max} (KBr): 3263, 2941, 1548, 1025(SO st) cm^{-1} .

MS (ESI) m/z : 199 ($[\text{M}+1]^+$, 100).

● Other Compounds

4a (Lit.²⁰): mp: 108.3 – 109.4 °C; $R_f = 0.35$ (petroleum ether / EtOAc = 2 : 1).

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.91 (d, $J = 7.6$ Hz, 2 H, ArH), 7.70 (d, $J = 7.6$ Hz, 1 H,

ArH), 7.60 (d, $J = 7.6$ Hz, 2 H, ArH), 3.95 – 3.89 (m, 1 H, *CHOH*), 3.01 – 2.96 (m, 1 H), 2.16 – 2.12 (m, 1 H), 1.92 – 1.89 (m, 1 H), 1.73 – 1.71 (m, 1 H), 1.39 – 1.18 (m, 4 H).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 136.7, 134.1, 129.2, 129.0, 68.9, 68.2, 34.1, 25.7, 24.5, 23.5.
 IR_{max} (KBr): 3417, 2934, 2853, 1448, 12952 (SO_2 st as), 1143 (SO_2 st sy) cm^{-1} .
MS (EI) m/z : 241 ($[\text{M}+1]^+$, 73), 240 (28), 143 (47), 99 (70), 81 (100).

Diphenyldisulfide (Lit.²¹) : mp: 61.2 – 62.5 °C; R_f = 0.85 (petroleum).
 ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.50 – 7.48 (m, 2 H, ArH), 7.73 – 7.22 (m, 3 H, ArH).
 ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 137.0, 129.1, 127.5, 127.1.

X-Ray crystal structure of 3c, 3j, 4a

X-Ray crystal structure of 4a.

X-Ray crystal structure of 3c.

X-Ray crystal structure of 3j.

Copies of NMR, MS, IR and HPLC spectra for all compounds

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ESI

CHEN_051214150845 #19 RT: 0.26 AV: 1 NL: 3.20E7

T: +c ESI ms [50.00-750.00]

CHEN_051214150845 #19 RT: 0.26 AV: 1 NL: 3.20E7

T: +c ESI ms [50.00-750.00]

Eurochrom HPLC Software, Version 2.05.

Wed Feb 22 20:07:27 2006

Operator: Unknown

Base: cmj

DOS path: d:\progra~1\euroch~1\cmj.bnw

Object name: CJX02183_Chn1 - Created: 22-02-2006, 20:02

Object type: Peak Report Table

Path: >cmj>样品分析>手性药物>OJ

	Ret.time [min]	Start [min]	End [min]	Height [mAU]	Area [mAU*min]	% Area	Width [min]	T-fact.	N-plates	Type	Compound
1	37.863	36.46	39.46	583.332	667.459	49.5557	3.001	-1.000	6816.7	BP	
2	40.447	39.46	45.28	497.172	679.427	50.4443	5.819	-1.000	5731.2	PB	

	Units	Selectivity	Capacity Factor	Resolution
1		-1.000	17.931	-1.000
2		-1.000	19.223	1.305

Wed Feb 22 20:05:42 2006

Eurochrom HPLC Software. Version 2.05.

Operator: Unknown

Base: cmj

DOS path: d:\progra~1\euroch~1\cmj.bnw

Object name: CJX02183_Chn1 - Created: 22-02-2006, 19:15

Object type: Curve

Path: >cmj>样品分析>手性药物>OJ

Page 1

Eurochrom HPLC Software, Version 2.05.

Wed Feb 22 21:58:43 2006

Operator: Unknown

Base: cmj

DOS path: d:\progra~1\euroch~1\cmj.bnw

Object name: CJX02181_Ch1 - Created: 22-02-2006, 20:52

Object type: Peak Report Table

Path: >cmj>样品分析>手性药物>OJ

	Ret.time [min]	Start [min]	End [min]	Height [mAU]	Area [mAU*min]	% Area	Width [min]	T-fact.	N-plates	Type	Compound
1	39.496	38.10	40.45	12.5832	14.1826	1.5062	2.351	-1.000	-1.0	BP	
2	41.630	40.45	46.95	665.297	927.406	98.4938	6.502	1.713	5791.7	PB	

	Units	Selectivity	Capacity Factor	Resolution
1		-1.000	18.748	-1.000
2		-1.000	19.815	1.042

Eurochrom HPLC Software, Version 2.05.

Operator: Unknown

Base: cmj

DOS path: d:\progra~1\euroch~1\cmj.bnw

Object name: CJX02181_Ch11 - Created: 22-02-2006, 20:03

Object type: Curve

Path: >cmj>样品分析>手性药物>OJ

Wed Feb 22 21:58:21 2006

Page 1

Eurochrom HPLC Software, Version 2.05.

Wed Feb 22 21:56:22 2006

Operator: Unknown

Base: cmj

DOS path: d:\progra~1\euroch~1\cmj.bnw

Object name: CJX02182 Chn1 - Created: 22-02-2006, 21:51

Object type: Peak Report Table

Path: >cmj>样品分析>手性药物>OJ

	Ret.time [min]	Start [min]	End [min]	Height [mAU]	Area [mAU*min]	% Area	Width [min]	T-fact.	N-plates	Type	Compound
1	4.968	4.70	5.63	17.8088	9.0902	1.0134	0.934	1.695	376.7	BB	
2	39.560	37.83	47.28	641.843	869.066	96.8863	9.453	1.802	5925.0	BB	
3	42.561	41.81	43.94	18.3022	18.84	2.1003	2.134	1.548	8580.9	SS	

	Units	Selectivity	Capacity Factor	Resolution
1		-1.000	1.484	-1.000
2		-1.000	18.780	22.525
3		-1.000	20.281	1.546

Eurochrom HPLC Software, Version 2.05.

Operator: Unknown

Base: cmj

DOS path: d:\progra-1\euroch-1\cmj.bnw

Object name: CJX02182_Ch11 - Created: 22-02-2006, 20:53

Object type: Curve

Path: >cmj>样品分析>手性药物>OJ

Wed Feb 22 21:53:25 2006

1p

Page 1

13C:070207-CJX072

Current Data Parameters
NAME 070207-CJX072
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070208
Time 9.19
INSTRUM spect
PROBHD 5 mm F400 MM-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 512
DS 4
SWH 26881.721 Hz
FIDRES 0.205091 Hz
AQ 2.4379852 sec
RG 26008
DW 18.600 usec
DE 60.00 usec
TE 294.5 K
d11 0.03000000 sec
D1 3.00000000 sec
DELTA 2.90000010 sec
TD0 4

===== CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
PL1 -1.00 dB
SFO1 100.6263395 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1320010 MHz

F2 - Processing parameters
SI 131072
SF 100.6127870 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.40

1H Sample: 070208-CJX076

Current Data Parameters
NAME 070208-CJX076
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070208
Time 14.35
INSTRUM spect
PROBHD 5 mm F400 MM-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.828 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 12.7
DW 62.400 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 -1.00 dB
SFO1 400.1324010 MHz

F2 - Processing parameters
SI 16384
SF 400.1305300 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

ch3oh:water=35:65

Injection Date : 12/08/2006 11:41:45 PM
Sample Name : cjk
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 12/08/2006 11:30:00 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 14/08/2006 16:41:00 PM by chen
Z-CHO

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.160	BP	0.5513	4280.43115	120.83621	83.4344
2	21.056	BB	0.5725	849.86359	22.30773	16.5656

Totals : 5130.29474 143.14394

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 10:59:58 PM
Sample Name : cjk-03
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 13:54:41 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	51.824	BB	1.2668	7744.06104	84.84647	68.1487
2	58.175	BB	1.2216	3619.41089	35.61562	31.8513

Totals : 1.13635e4 120.46209

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 08:55:08 PM
Sample Name : cjkx-01
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 14/08/2006 16:41:00 PM by chen
Z-CHO

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.983	BB	0.5921	5613.41748	146.15689	85.2276
2	24.205	BB	0.6151	972.97076	23.79466	14.7724

Totals : 6586.38824 169.95155

Results obtained with enhanced integrator!

*** End of Report ***

CHEN051220 #148 RT: 1.32 AV: 1 NL: 1.45E5
T: + c Full ms [50.00-300.00]

C18B4

Injection Date : 16/08/2006 12:15:10 PM
Sample Name : cjkx-04
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 13:54:41 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.158	BB	0.2761	9836.60840	546.27167	100.0000

Totals : 9836.60840 546.27167

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 13:02:05 PM
Sample Name : cjkx-05
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 14/08/2006 16:41:00 PM by chen
Z-CHO

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.928	BB	1.4601	9.01193e4	904.70087	46.6105
2	14.468	BB	1.0698	1768.62793	19.39726	0.9148
3	27.706	BB	1.8733	1.01457e5	774.00281	52.4747

Totals : 1.93345e5 1698.10093

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 19:23:27 PM
Sample Name : cjx-6
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 16:14:05 PM by chen
(modified after loading)

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.056	BB	0.2992	252.73444	12.75323	40.3250
2	10.646	BB	0.3269	374.00922	17.53035	59.6750

Totals : 626.74365 30.28358

Results obtained with enhanced integrator!

*** End of Report ***

Data File D:\DATA\06081614.D

Injection Date : 16/08/2006 16:38:13 PM
Sample Name : cfx-09
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 16:14:05 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.798	VV	0.2216	2.25130e4	1548.54761	44.4615
2	6.649	VV	0.2557	2.81219e4	1676.47522	55.5385

Totals : 5.06349e4 3225.02283

Results obtained with enhanced integrator!

*** End of Report ***

Instrument 1 16/08/2006 17:14:10 PM chen

Page 1 of 1

Injection Date : 16/08/2006 15:36:01 PM
Sample Name : cjk-08
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 18/08/2006 20:28:47 PM by chen
(modified after loading)

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.650	BV	0.1994	2.34082e4	1827.47864	38.9617
2	5.190	VB	0.2337	3.57458e4	2294.80225	59.4968
3	16.554	BB	0.4522	926.17029	30.85735	1.5416

Totals : 6.00801e4 4153.13824

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 18:06:02 PM
Sample Name : cjk-12
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 16:14:05 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.973	BP	0.2599	702.37903	40.18214	2.7342
2	8.291	PB	0.2710	2.49867e4	1435.92029	97.2658

Totals : 2.56890e4 1476.10243

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 18:59:04 PM
Sample Name : cjkx-10
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 16:14:05 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.743	BV	0.3094	834.79742	40.34034	4.0008
2	10.677	VB	0.3582	2.00311e4	852.37439	95.9992

Totals : 2.08659e4 892.71473

Results obtained with enhanced integrator!

*** End of Report ***

Injection Date : 16/08/2006 10:31:38 PM
Sample Name : cjk-
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 14/08/2006 16:41:00 PM by chen
Z-CHO

Location : Vial 1

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.633	BB	0.5591	9662.60254	247.73116	58.7592
2	20.387	BP	0.5126	837.69043	24.51554	5.0941
3	22.298	BB	0.5800	5944.11963	156.88579	36.1467

Totals : 1.64444e4 429.13248

Results obtained with enhanced integrator!

*** End of Report ***

13C 070208-CJX078

Current Data Parameters
NAME 070208-CJX078
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070208
Time 11.49
INSTRUM spect
PROBHD 5 mm PABBO MM-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 384
DS 4
SWH 26881.721 Hz
FIDRES 0.205091 Hz
AQ 2.4378892 sec
RG 26008
DW 19.600 usec
DE 62.00 usec
TE 294.2 K
d11 0.03000000 sec
D1 3.00000000 sec
DELTA 2.90000010 sec
TD0 3

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -1.00 dB
SFO1 100.626395 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.132010 MHz

F2 - Processing parameters
SI 131072
SF 100.6127870 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

1H Sample: 070208-CJX0710

Current Data Parameters
NAME 070208-CJX0710
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070208
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO MM-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 6
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 37
DW 62.400 usec
DE 1.00 usec
TE 294.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 -1.00 dB
SFO1 400.1324010 MHz

F2 - Processing parameters
SI 16384
SF 400.1300058 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Injection Date : 16/08/2006 18:32:42 PM
Sample Name : cjkx-13
Acq. Operator : chen
Acq. Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 08:39:52 PM by chen
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\WK0713.M
Last changed : 16/08/2006 16:14:05 PM by chen
(modified after loading)

Location : Vial 1

Z-CHO

DAD1 A, Sig=206,4 Ref=360,100 (06081619.D)

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.487	BB	0.4346	1.17544e4	417.30231	100.0000

Totals : 1.17544e4 417.30231

Results obtained with enhanced integrator!

*** End of Report ***

References

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