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APPENDICES

ศูนย์วิทยทรัพยากร
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Appendix A

Glossary

Correlation coefficient (R^2) is a number between 0 and 1, which indicates the degree of linear relationship between two variables.

Distribution constant (K) is defined as the concentration ratio of a compound in a stationary phase and in a mobile phase. K is related to retention factor according to the equation shown below.

$$K = \frac{C_s}{C_m} \\ = k' \cdot \frac{V_M}{V_s} = k' \cdot \beta$$

C_s, C_m = concentration of a solute in stationary phase and mobile phase, respectively

V_s, V_M = volume of stationary phase and mobile phase, respectively

Number of theoretical plates (N) is one of the factors used to express column efficiency. It is calculated according to the equation

$$N = 16 \left[\frac{t_R}{w_b} \right]^2 = 5.545 \left[\frac{t_R}{w_h} \right]^2$$

t_R = retention time of a peak

w_b = peak width at base (in the same unit as t_R)

w_h = peak width at half height (in the same unit as t_R)

Phase ratio (β) is a measure of the openness of the column defined as the volume ratio of mobile phase to stationary phase in a column or can be calculated from the following equation.

$$\beta = \frac{r_c}{2d_f}$$

r_c = capillary column radius

d_f = stationary phase film thickness

Retention factor or capacity factor (k') is defined as the number of mole of a compound in a stationary phase to that in mobile phase. It is equal to the ratio of the total time spent in the stationary phase (t'_R) to the time spent in the mobile phase (t_M). The retention factor is calculated using the equation below.

$$k' = \frac{t_R - t_M}{t_M} = \frac{t'_R}{t_M}$$

Separation factor or selectivity (α) is a measure of the quality of peak separation expressed as a relative adjusted retention. It is calculated from the ratio of the retention factors of the two adjacent peaks.

$$\alpha = \frac{k'_2}{k'_1} = \frac{t_{R,2} - t_M}{t_{R,1} - t_M}$$

Separation number (SN) or Trennzahl (TZ) is another term used for a measure of separation efficiency of a column. SN can be explained as the number of peaks that can be placed close together between the two peaks of homologous series differing by one carbon. The higher the number, the greater the column efficiency. It is calculated using the equation below.

$$SN = \left[\frac{t_{R,2} - t_{R,1}}{w_{h,1} + w_{h,2}} \right] - 1$$

$t_{R,1}, t_{R,2}$ = retention time of the first and second eluted peaks, respectively.

$w_{h,1}, w_{h,2}$ = peak width at half height of the first and second eluted peaks, respectively.

Appendix B

NMR Spectra

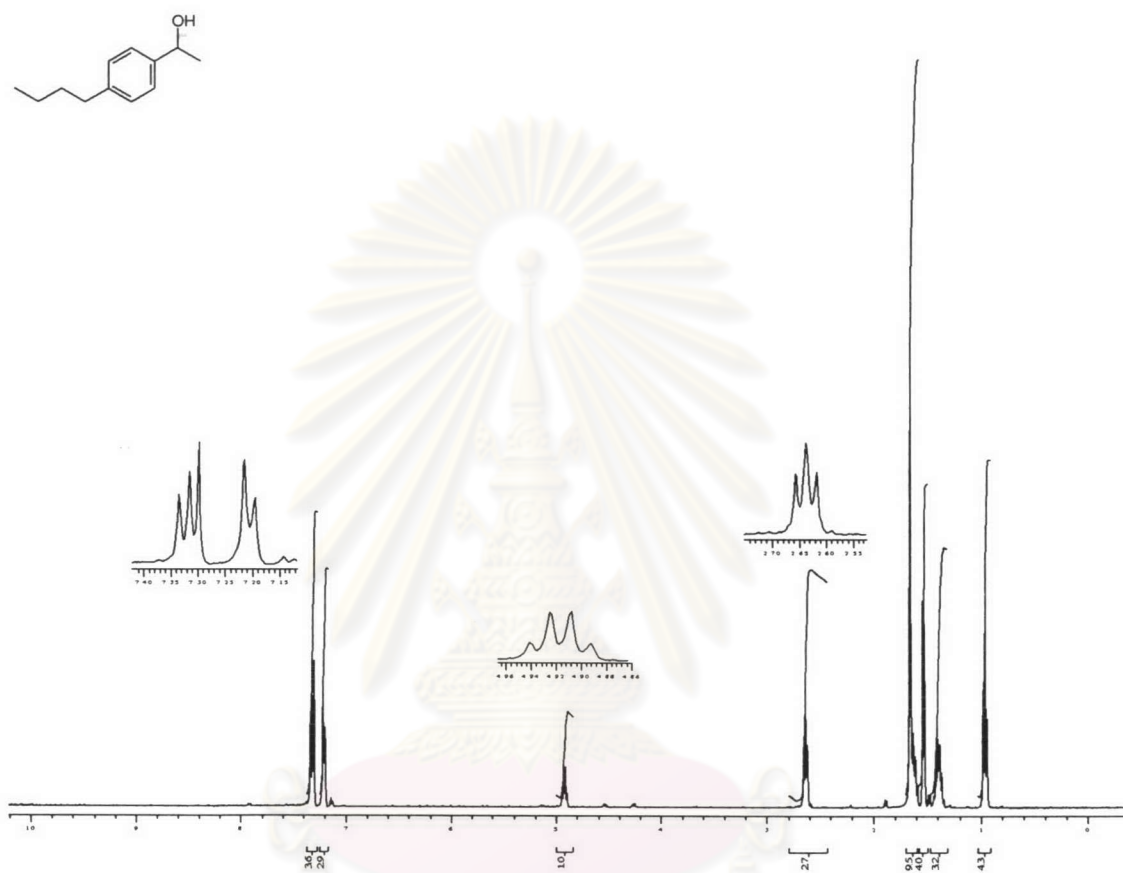


Figure B1 NMR spectrum of **4Bu**, ¹H NMR (CDCl₃, 400 MHz): δ 0.95 (3H, t, CH₂CH₃), 1.40 (2H, s, CH₃CH₂), 1.54 (3H, d, CHCH₃), 1.62 (2H, m, CH₂CH₂CH₂), 1.65 (1H, s, CHOH), 2.62 (2H, t, CH₂(CH₂)CH₂), 4.92 (1H, q, CHOH) 7.22 (2H, d, ArH), 7.32 (2H, d, ArH)

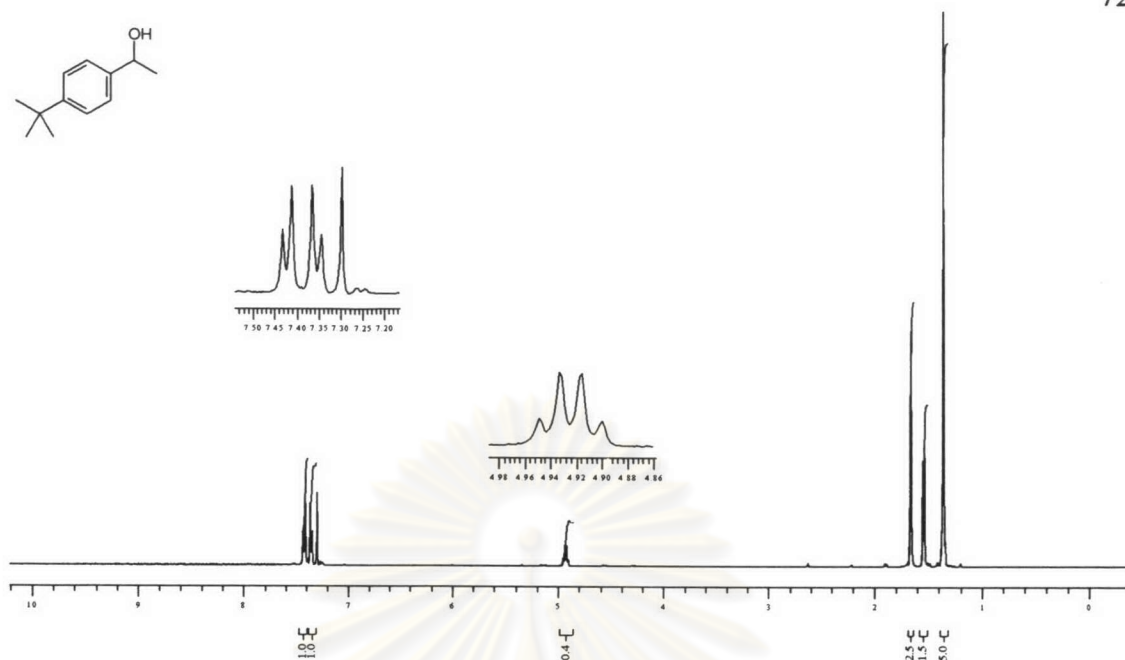


Figure B2 NMR spectrum of **4tBu**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.35 (9H, s, $3(\text{CH}_3)$), 1.54 (3H, d, CHCH_3), 1.66 (1H, m, CHOH), 4.94 (1H, q, CHOH), 7.35 (2H, d, ArH), 7.44 (2H, d, ArH)

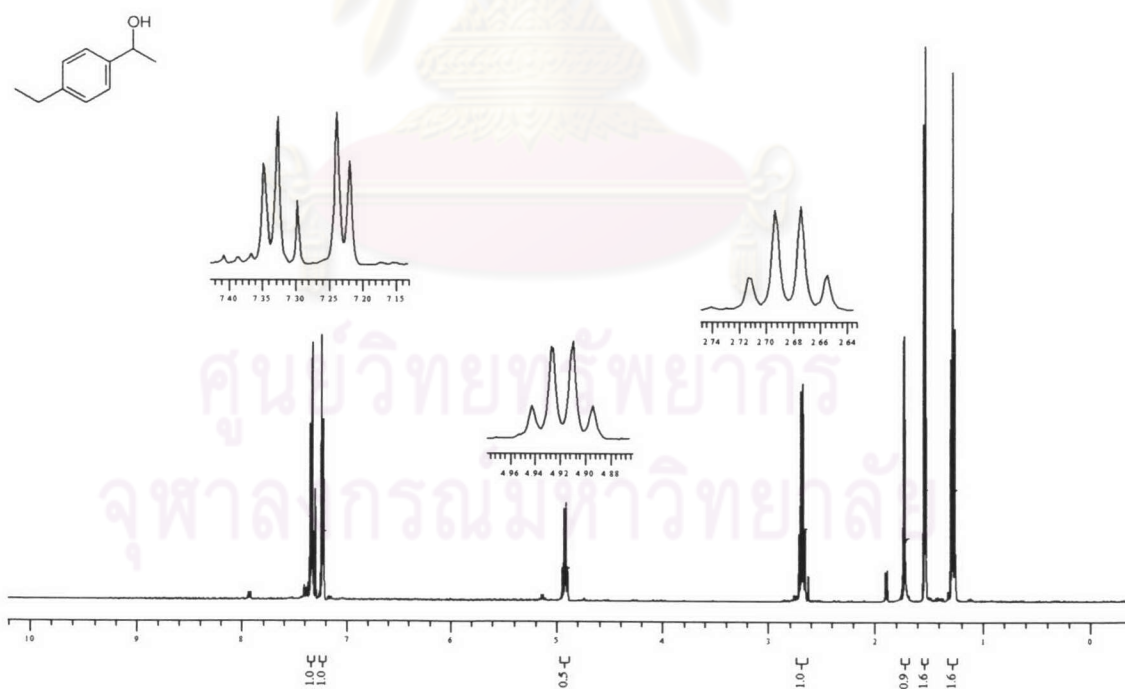


Figure B3 NMR spectrum of **4Et**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.30 (3H, t, CH_3CH_2), 1.54 (3H, d, CHCH_3), 1.74 (1H, s, CHOH), 2.68 (2H, q, CH_3CH_2), 4.90 (1H, q, CHOH), 7.22 (2H, d, ArH), 7.34 (2H, d, ArH)

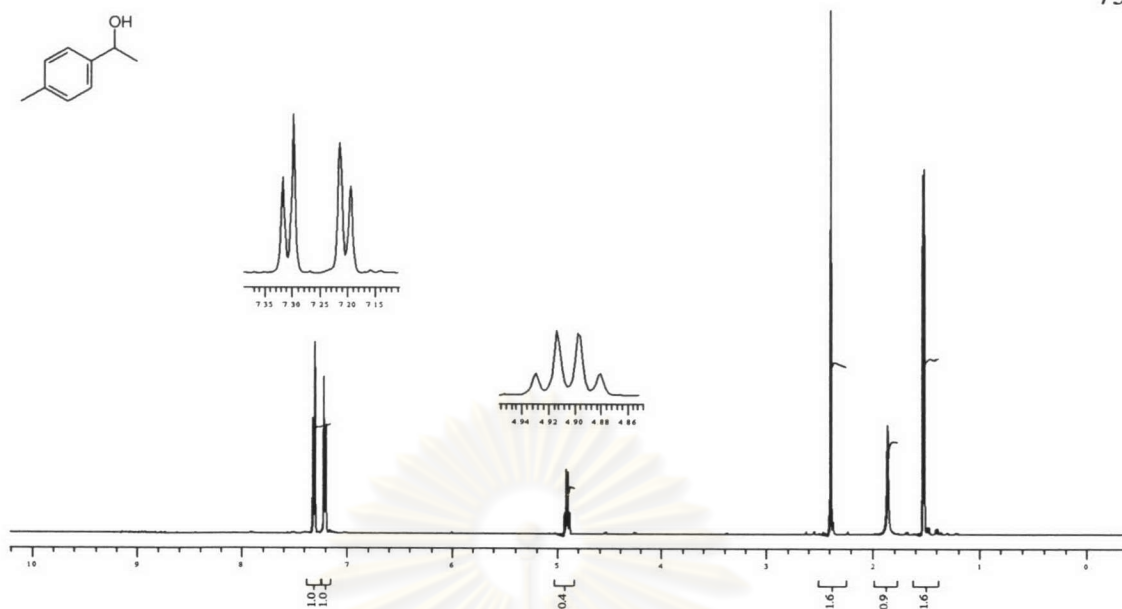


Figure B4 NMR spectrum of **4Me**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.54 (3H, d, CHCH_3), 1.85 (1H, s, CHOH), 2.40 (3H, s, CCH_3), 4.90 (1H, q, CHOH), 7.20 (2H, d, ArH), 7.30 (2H, d, ArH)

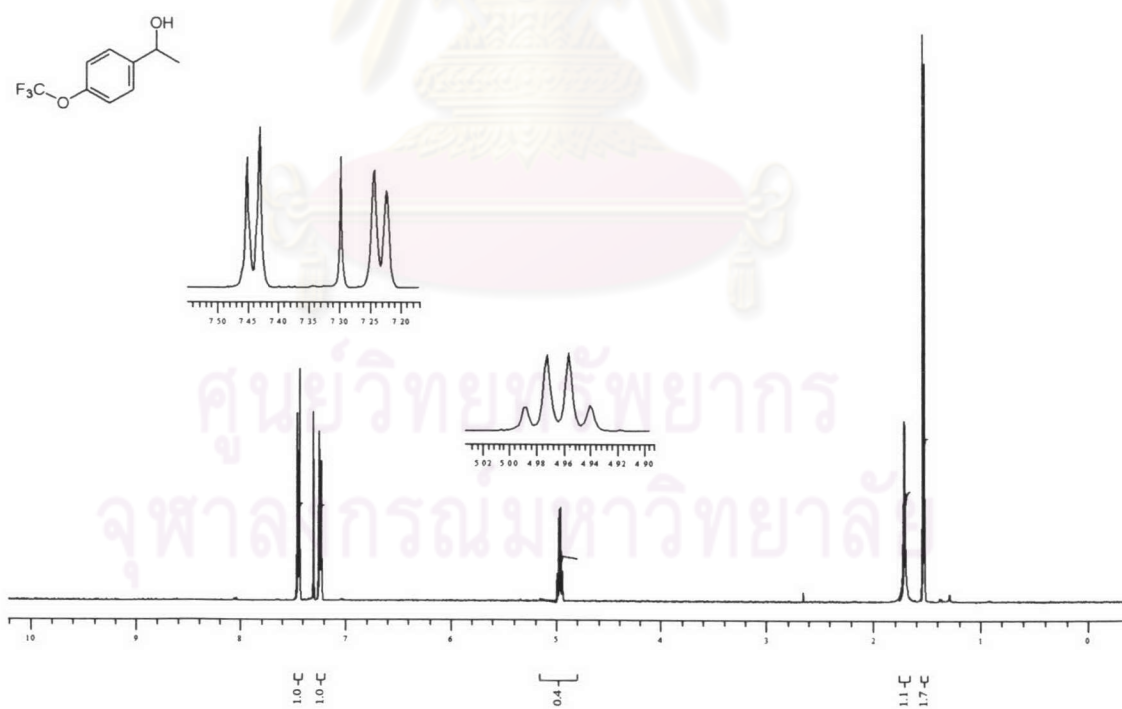


Figure B5 NMR spectrum of **4OCF₃**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.54 (3H, d, CHCH_3), 1.72 (1H, s, CHOH), 4.95 (1H, q, CHOH), 7.24 (2H, d, ArH), 7.44 (2H, d, ArH)

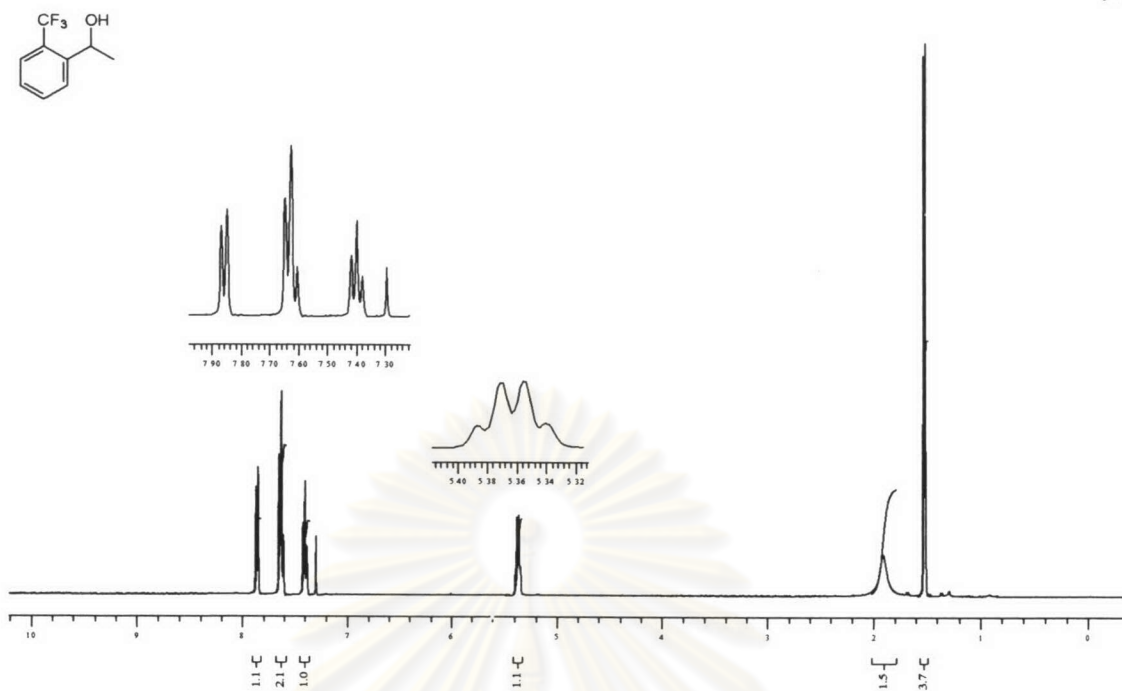


Figure B6 NMR spectrum of **2CF₃**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.50 (3H, d, CHCH_3), 1.90 (1H, s, CHOH), 5.35 (1H, q, CHOH), 7.40 (1H, t, ArH), 7.62 (2H, t, ArH), 7.85 (1H, d, ArH)

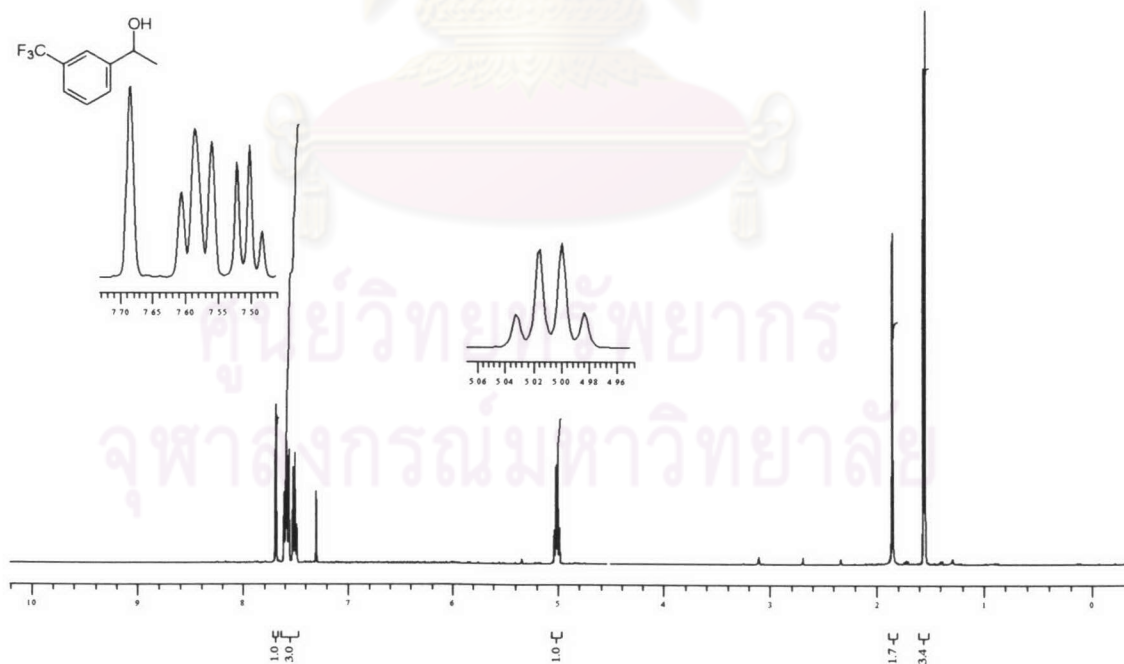


Figure B7 NMR spectrum of **3CF₃**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.55 (3H, d, CHCH_3), 1.82 (1H, s, CHOH), 5.00 (1H, q, CHOH), 7.52 (3H, m, ArH), 7.70 (1H, s, ArH)

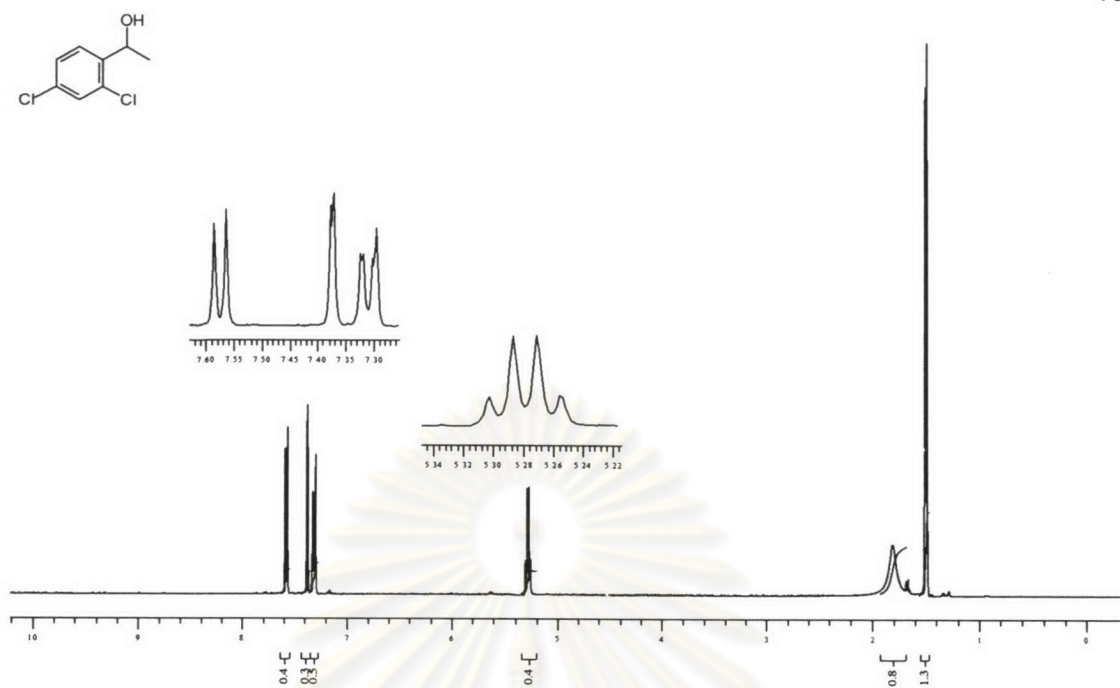


Figure B8 NMR spectrum of **24Cl**; ^1H NMR (CDCl_3 , 400MHz): δ 1.50 (3H, d, CHCH_3), 1.80 (1H, s, CHOH), 5.18 (1H, q, CHOH), 7.30 (1H, d, ArH), 7.37 (1H, s, ArH), 7.58 (1H, d, ArH)

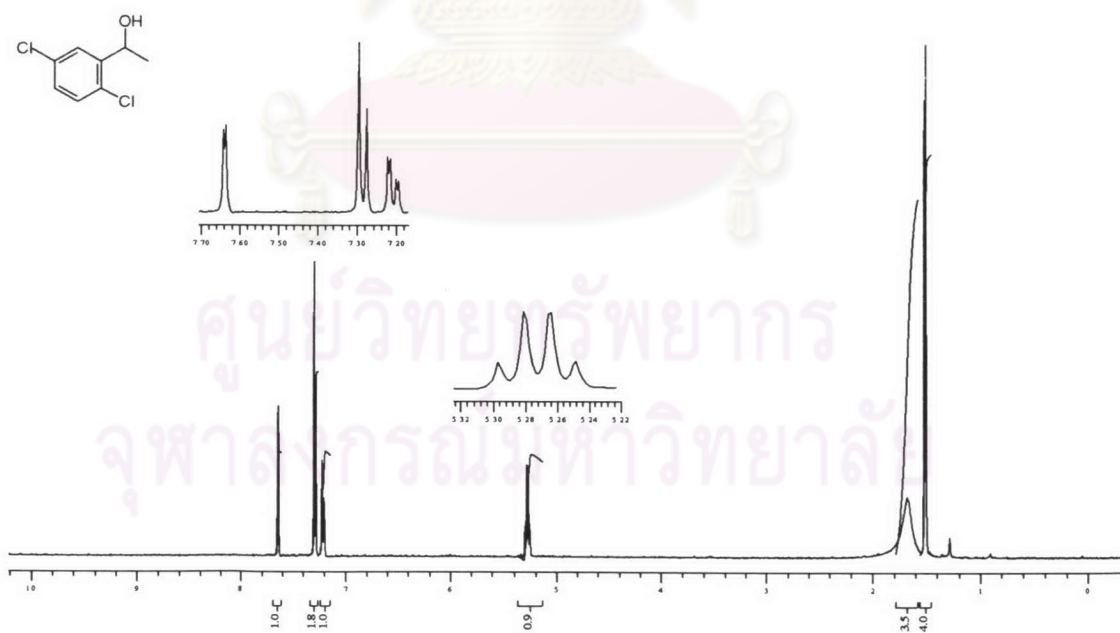


Figure B9 NMR spectrum of **25Cl**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.50 (3H, d, CHCH_3), 1.70 (1H, s, CHOH), 5.28 (1H, q, CHOH), 7.22 (1H, d, ArH), 7.30 (1H, s, ArH), 7.65 (1H, d, ArH)

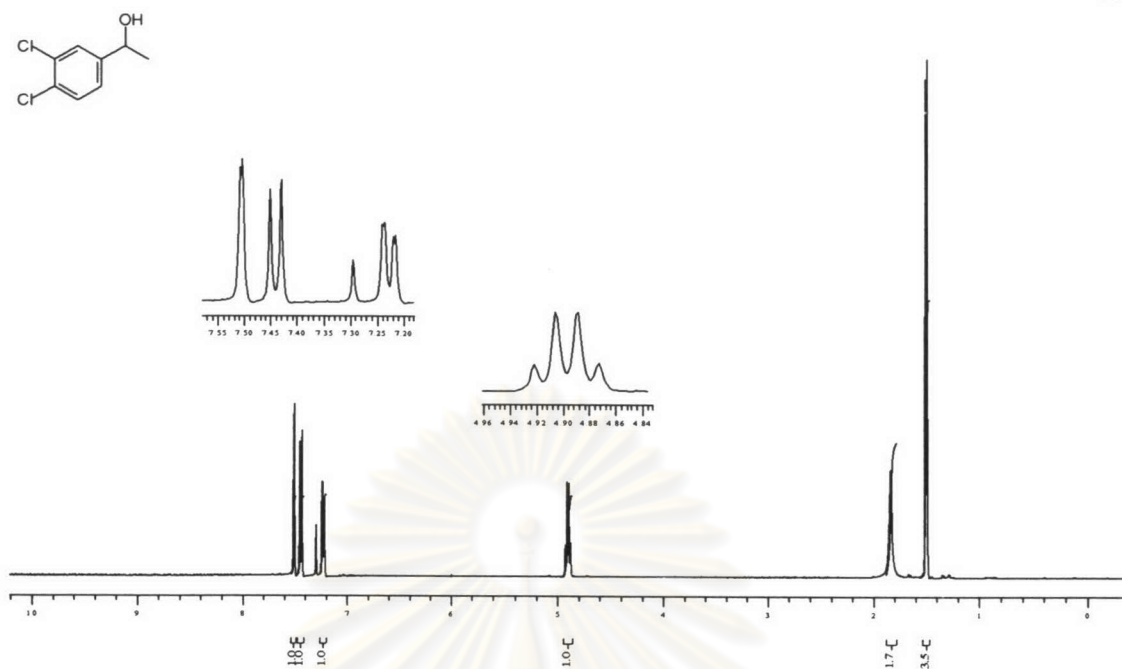


Figure B10 NMR spectrum of **34Cl**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.50 (3H, d, CHCH_3), 1.85 (1H, s, CHOH), 4.90 (1H, q, CHOH), 7.22 (1H, d, ArH), 7.45 (1H, d, ArH), 7.52 (1H, s, ArH)

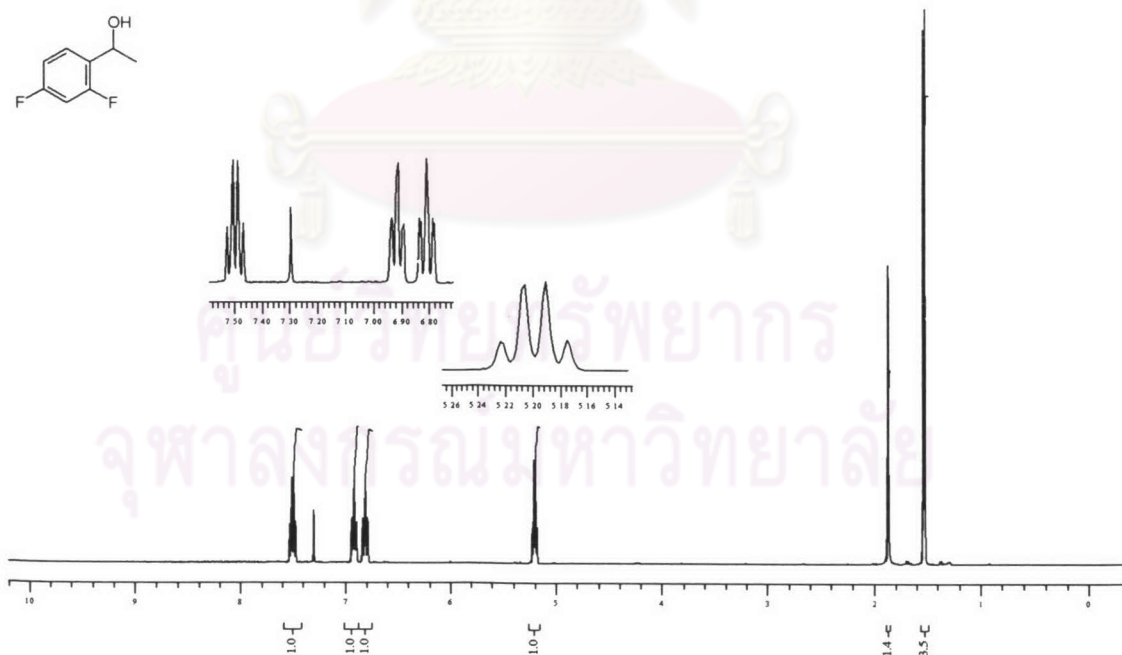


Figure B11 NMR spectrum of **24F**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.54 (3H, d, CHCH_3), 1.88 (1H, s, CHOH), 5.20 (1H, q, CHOH), 6.80 (1H, t, ArH), 6.94 (1H, t, ArH), 7.50 (1H, q, ArH)

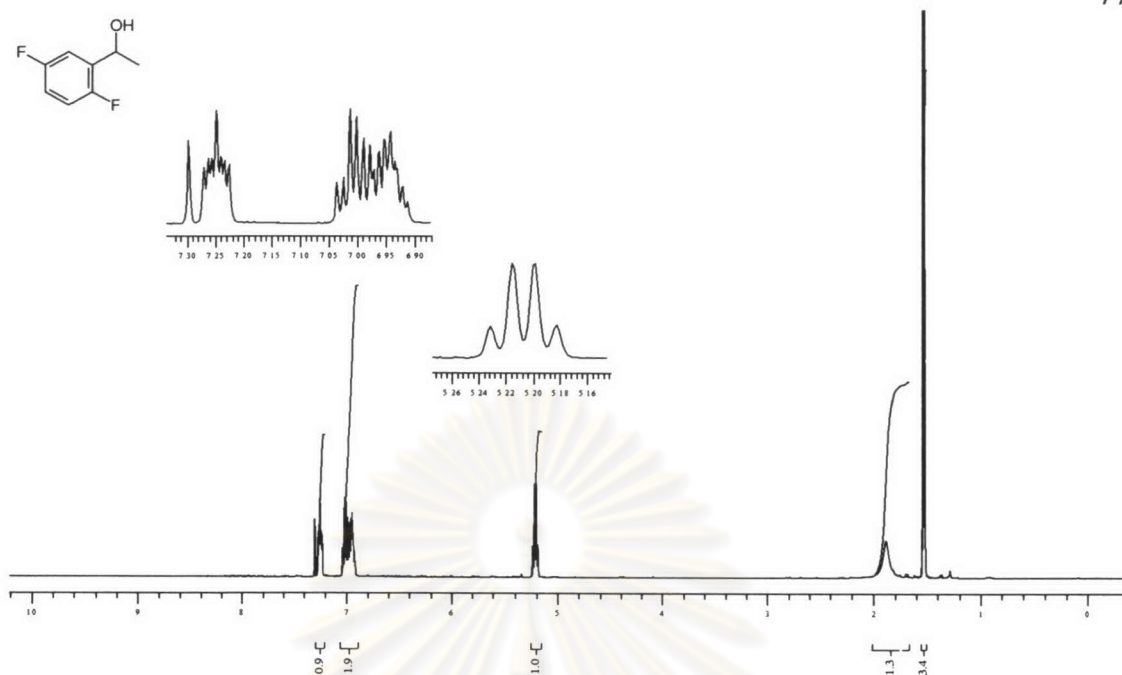


Figure B12 NMR spectrum of **25F**; ¹H NMR (CDCl₃, 400 MHz): δ 1.55 (3H, d, CHCH₃), 1.90 (1H, s, CHOH), 5.24 (1H, q, CHOH), 7.00 (2H, m, ArH), 7.24 (1H, m, ArH)

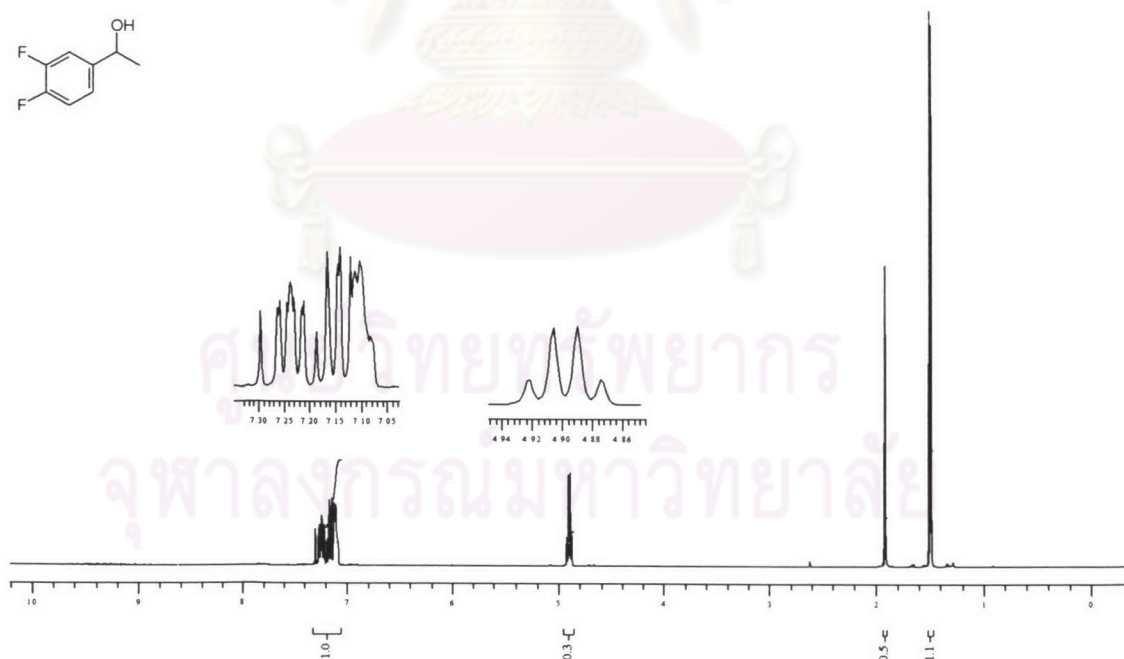


Figure B13 NMR spectrum of **34F**; ¹H NMR (CDCl₃, 400 MHz): δ 1.50 (3H, d, CHCH₃), 1.90 (1H, s, CHOH), 4.90 (1H, q, CHOH), 7.10 (1H, d, ArH), 7.15 (1H, d, ArH), 7.24 (1H, t, ArH)

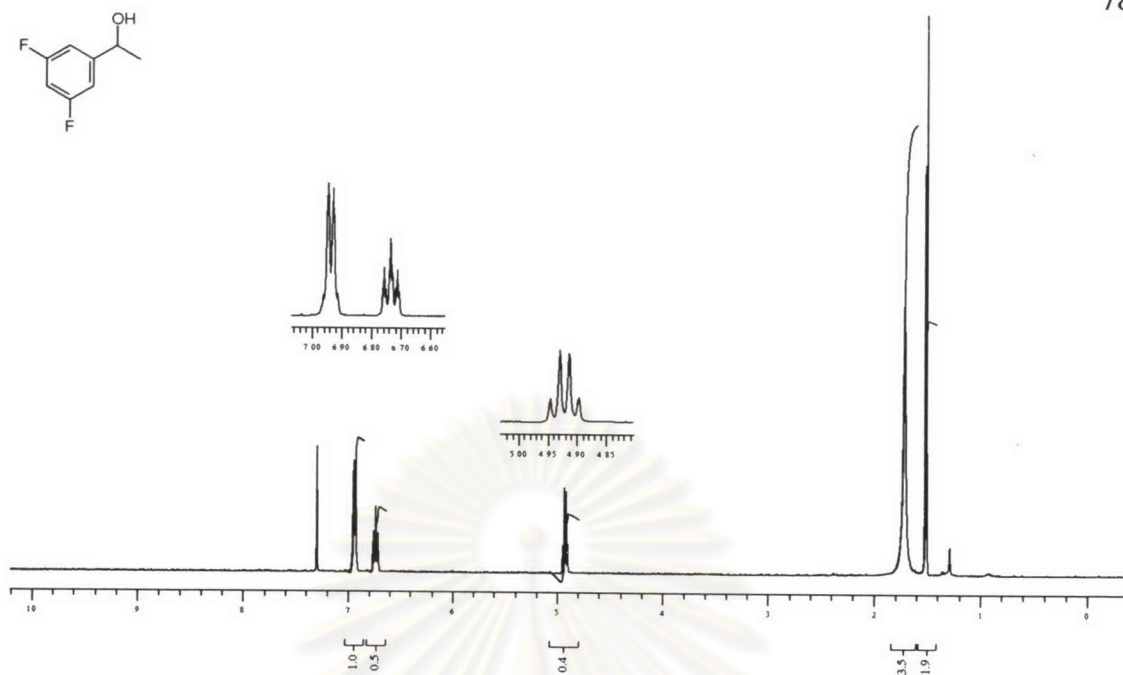


Figure B14 NMR spectrum of **35F**; $^1\text{H NMR}$ (CDCl₃, 400 MHz): δ 1.50 (3H, d, CHCH₃), 1.70 (1H, s, CHOH), 4.92 (1H, q, CHOH), 6.74 (2H, t, ArH), 6.94 (2H, d, ArH)

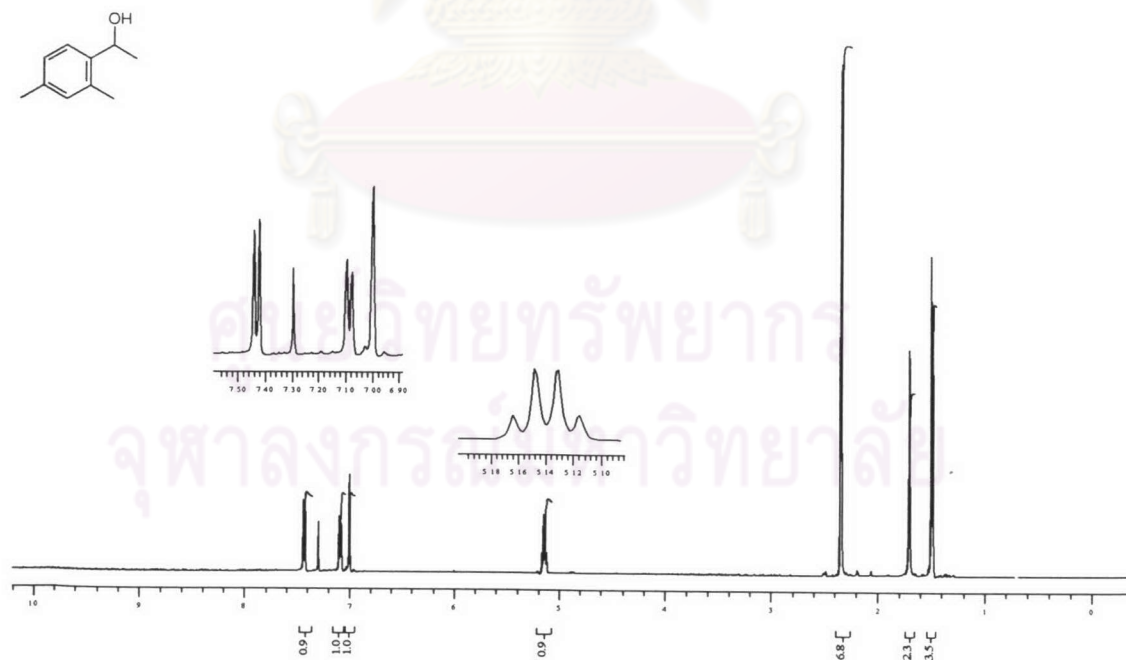


Figure B15 NMR spectrum of **24Me**; $^1\text{H NMR}$ (CDCl₃, 400 MHz): δ 1.47 (3H, d, CHCH₃), 1.70 (1H, s, CHOH), 2.35 (6H, d, 2(CCH₃)), 5.12 (1H, q, CHOH), 7.00 (1H, s, ArH), 7.10 (1H, d, ArH), 7.44 (1H, d, ArH)

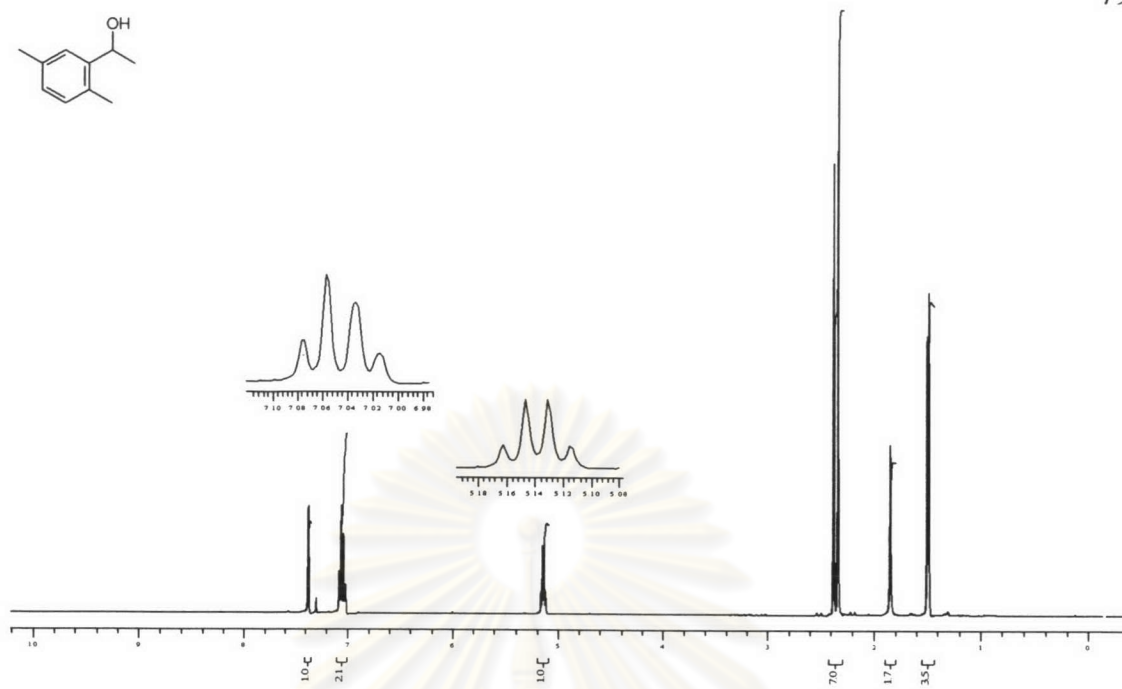


Figure B16 NMR spectrum of **25Me**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.50 (3H, d, CHCH_3), 1.85 (1H, s, CHOH), 2.35 (6H, d, $2(\text{C}_6\text{H}_5\text{CH}_3)$), 5.15 (1H, q, CHOH), 7.05 (2H, q, ArH), 7.38 (1H, d, ArH)

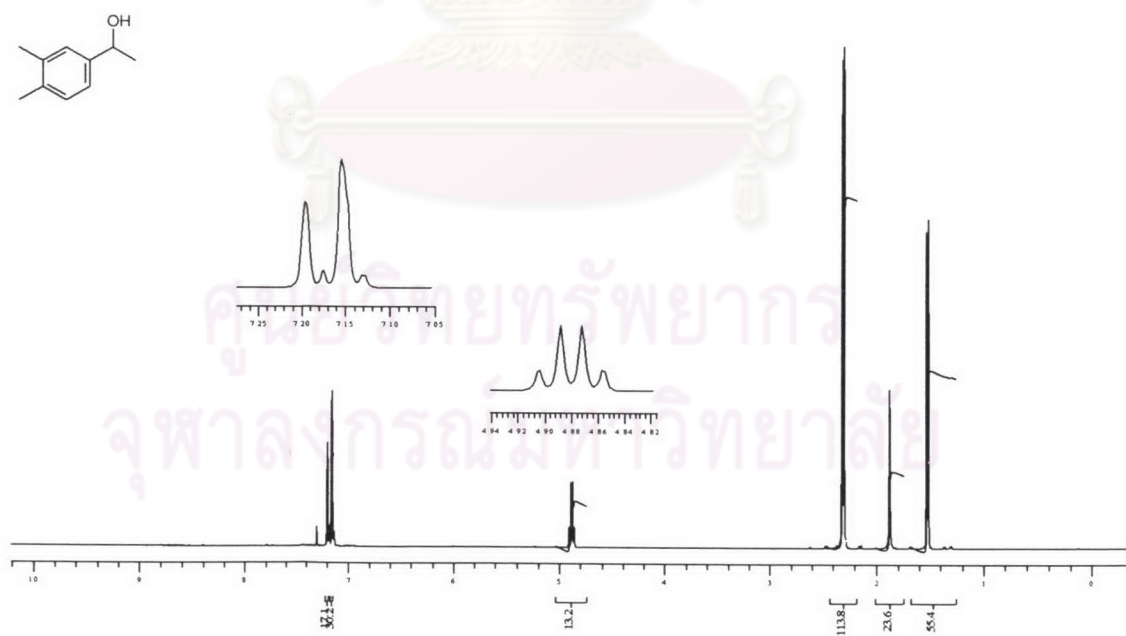


Figure B17 NMR spectrum of **34Me**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.52 (3H, d, CHCH_3), 1.87 (1H, s, CHOH), 2.30 (6H, d, $2(\text{CH}_3\text{C})$), 4.88 (1H, q, CHOH), 7.15 (2H, d, ArH), 7.18 (1H, s, ArH)

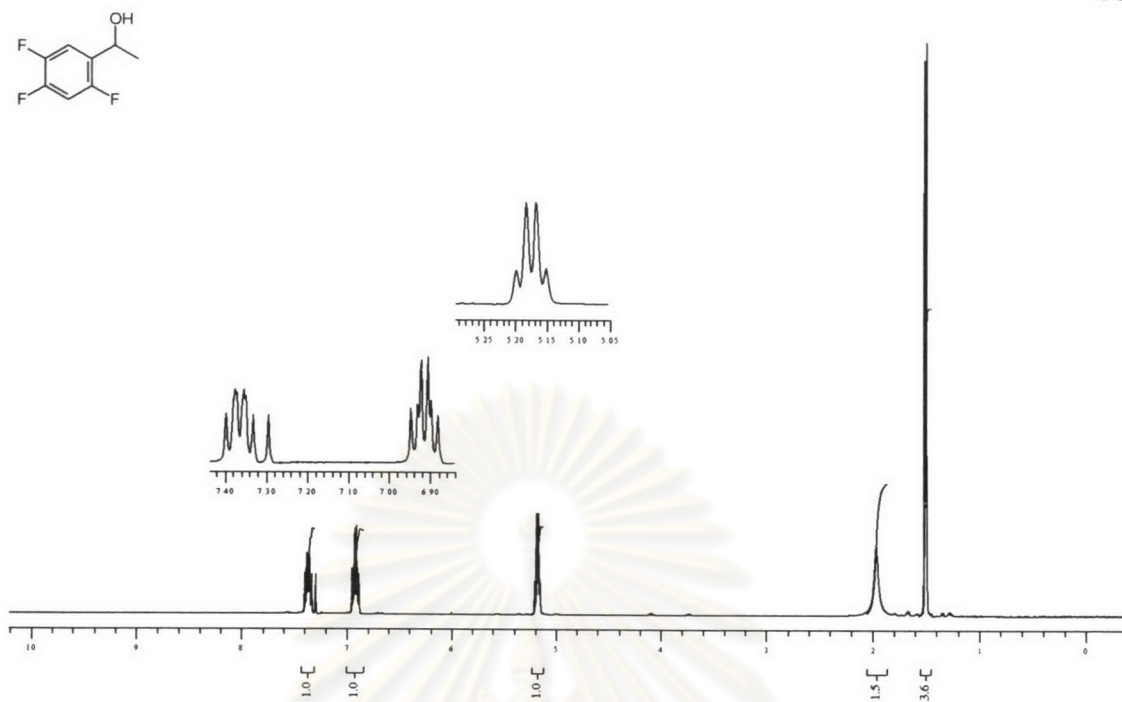


Figure B18 NMR spectrum of **triF**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.52 (3H, d, CHCH_3), 1.95 (1H, s, CHOH), 5.18 (1H, q, CHOH), 6.90 (1H, q, ArH), 7.37 (1H, q, ArH)

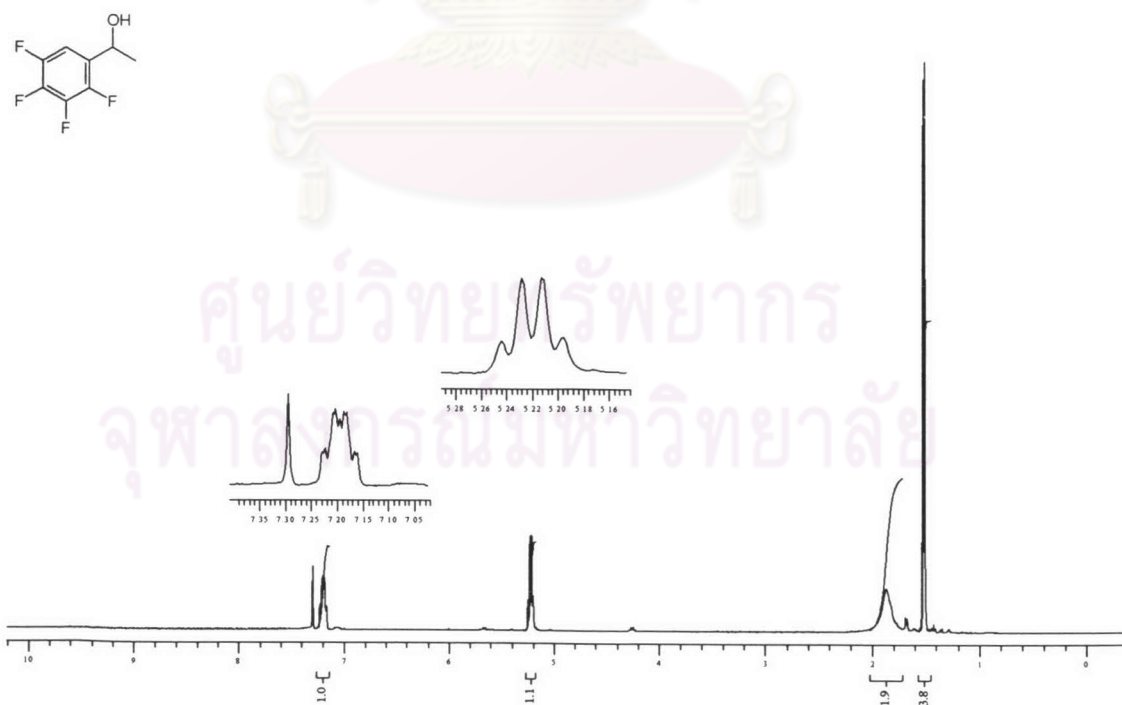


Figure B19 NMR spectrum of **tetraF**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.50 (3H, d, CHCH_3), 1.85 (1H, s, CHOH), 5.22 (1H, q, CHOH), 7.85 (1H, q, ArH)

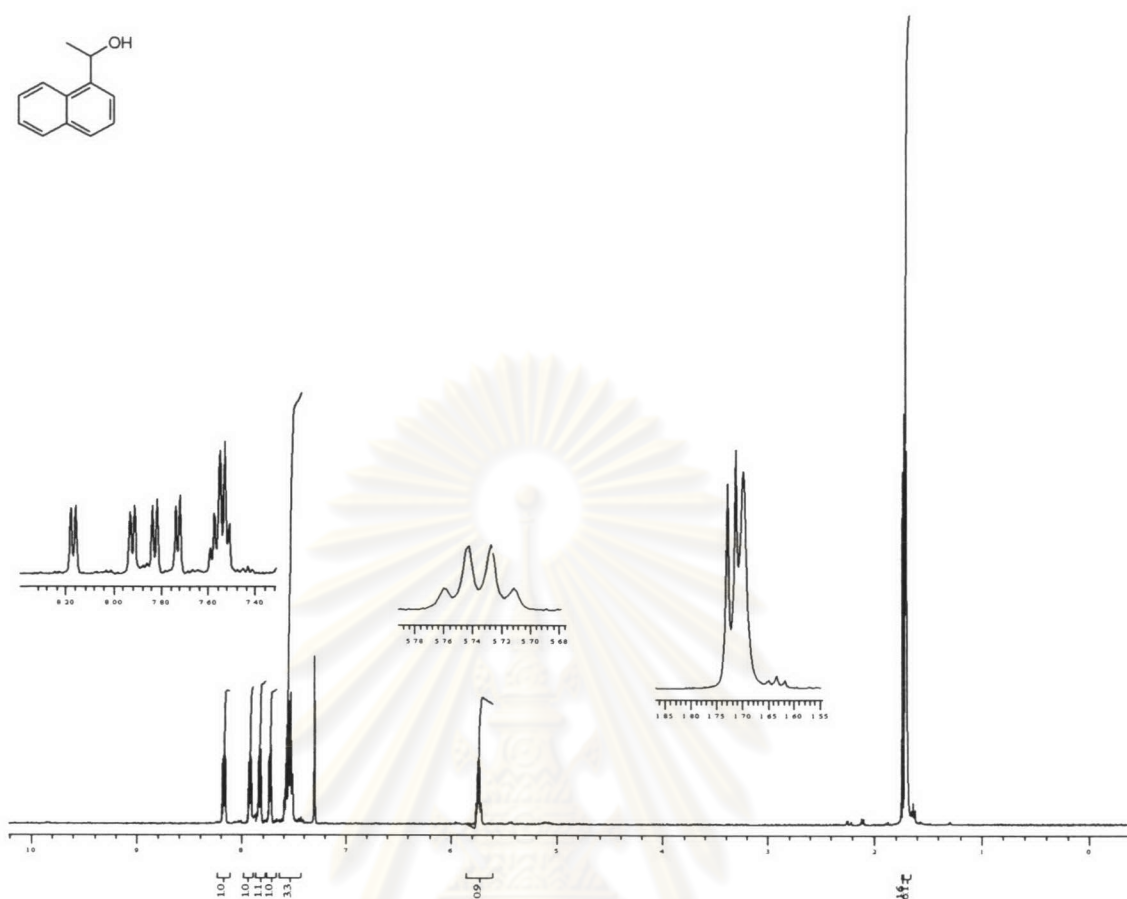


Figure B20 NMR spectrum of **3**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.70 (3H, d, CHCH_3), 1.74 (1H, s, CHOH), 5.74 (1H, q, CHOH), 7.56 (3H, m, ArH), 7.77 (1H, d, ArH), 7.84 (1H, d, ArH), 7.92 (1H, d, ArH), 8.15 (1H, d, ArH)

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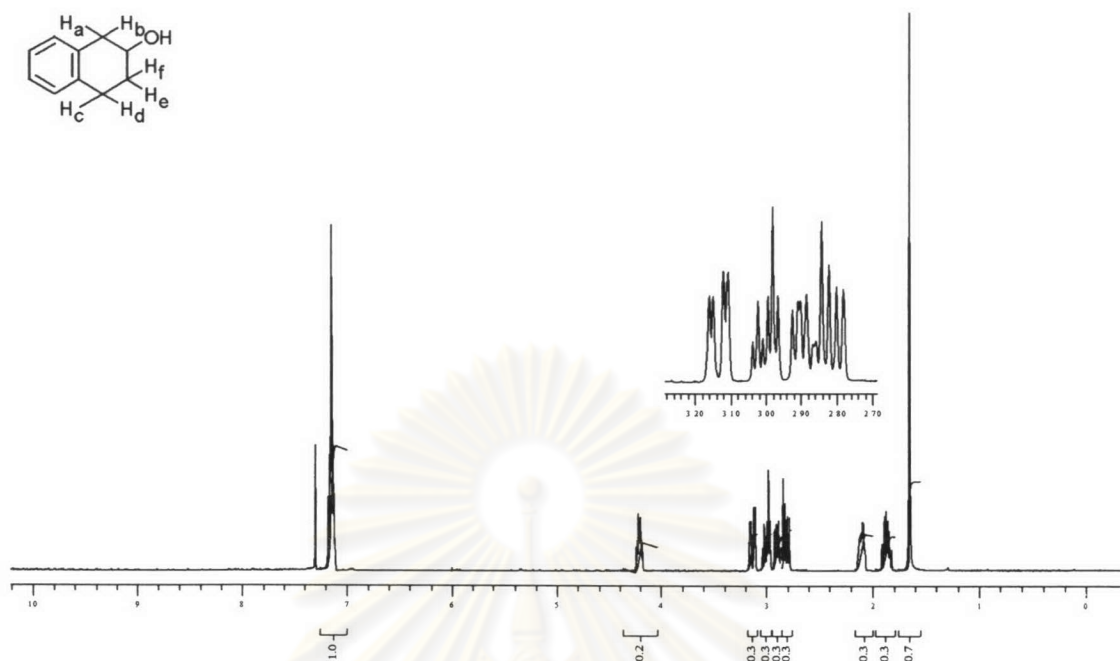


Figure B21 NMR spectrum of **5**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.64 (1H, s, CHOH), 1.88 (1H, m, H_f), 2.10 (1H, m, H_e), 2.80 (1H, m, H_c), 2.88 (1H, m, H_b), 2.98 (1H, m, H_d), 3.14 (1H, m, H_a), 4.20 (1H, m, CHOH), 7.14 (4H, d, ArH)

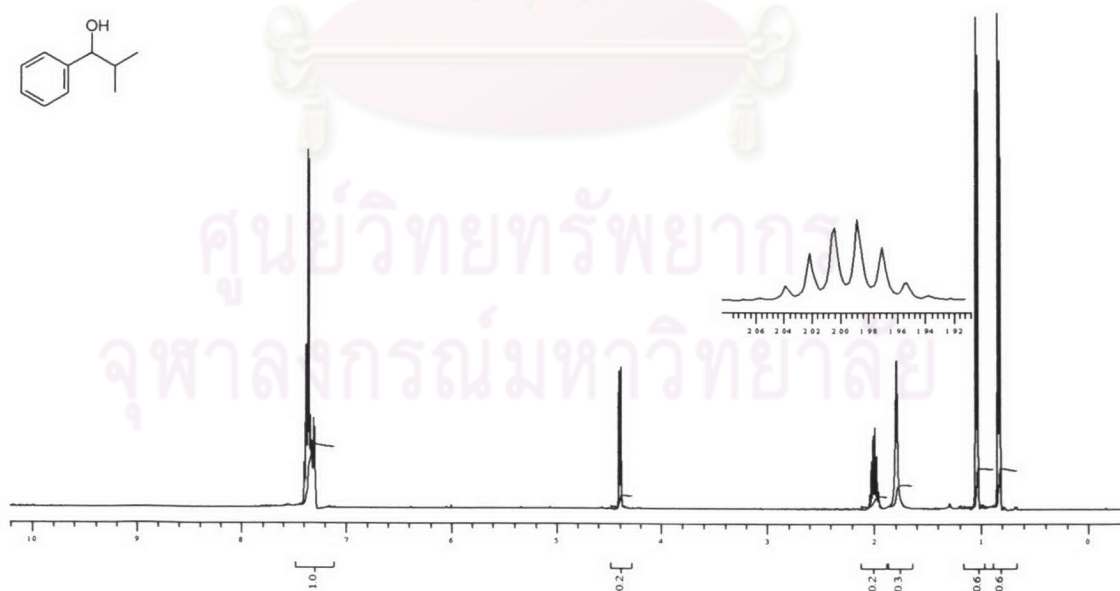


Figure B22 NMR spectrum of **8**; ^1H NMR (CDCl_3 , 400 MHz): δ 0.82 (3H, d, CHCH_3), 1.02 (3H, d, CHCH_3), 1.78 (1H, s, CHOH), 2.00 (1H, m, $\text{CH}(\text{CH}_3)_2$), 4.40 (1H, d, CHOH), 7.37 (5H, m, C_6H_5)

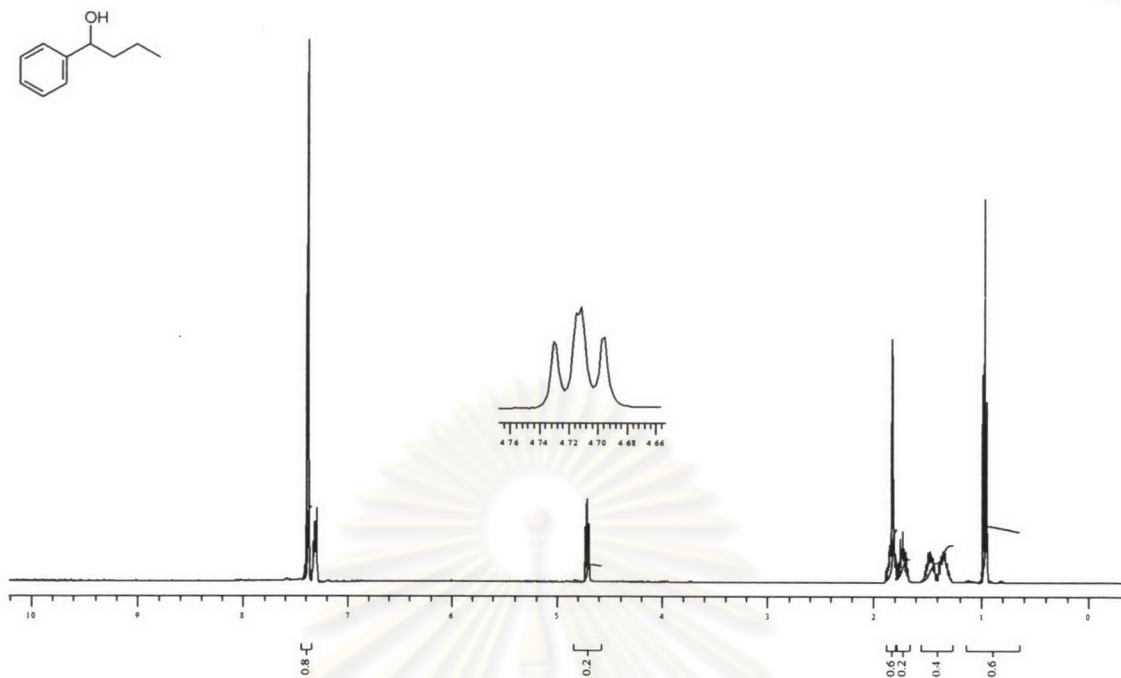


Figure B23 NMR spectrum of **10**; ^1H NMR (CDCl_3 , 400 MHz): δ 0.95 (3H, t, CH_2CH_3), 1.40 (2H, m, CHOH), 1.76 (2H, q, $\text{CH}_2\text{CH}_2\text{CH}_3$), 1.82 (1H, s, CHOH), 4.70 (1H, t, CHOH), 7.30-7.35 (5H, d, C_6H_5)

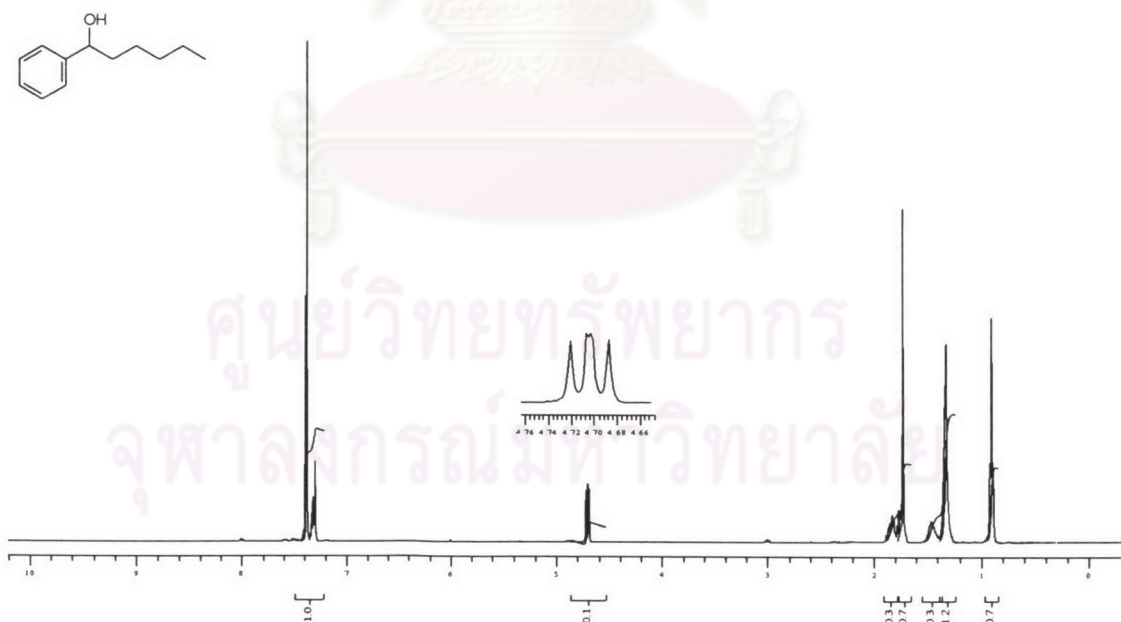


Figure B24 NMR spectrum of **11**; ^1H NMR (CDCl_3 , 400 MHz): δ 0.92 (3H, t, CH_2CH_3), 1.32 (4H, m, $2(\text{CH}_2)\text{CH}_2\text{CH}_3$), 1.46 (2H, m, CH_2CH_3), 1.75 (1H, s, CHOH), 1.84 (2H, m, $\text{CHCH}_2\text{3}(\text{CH}_2)\text{CH}_3$), 4.70 (1H, t, CHOH), 7.30-7.40 (5H, d, C_6H_5)

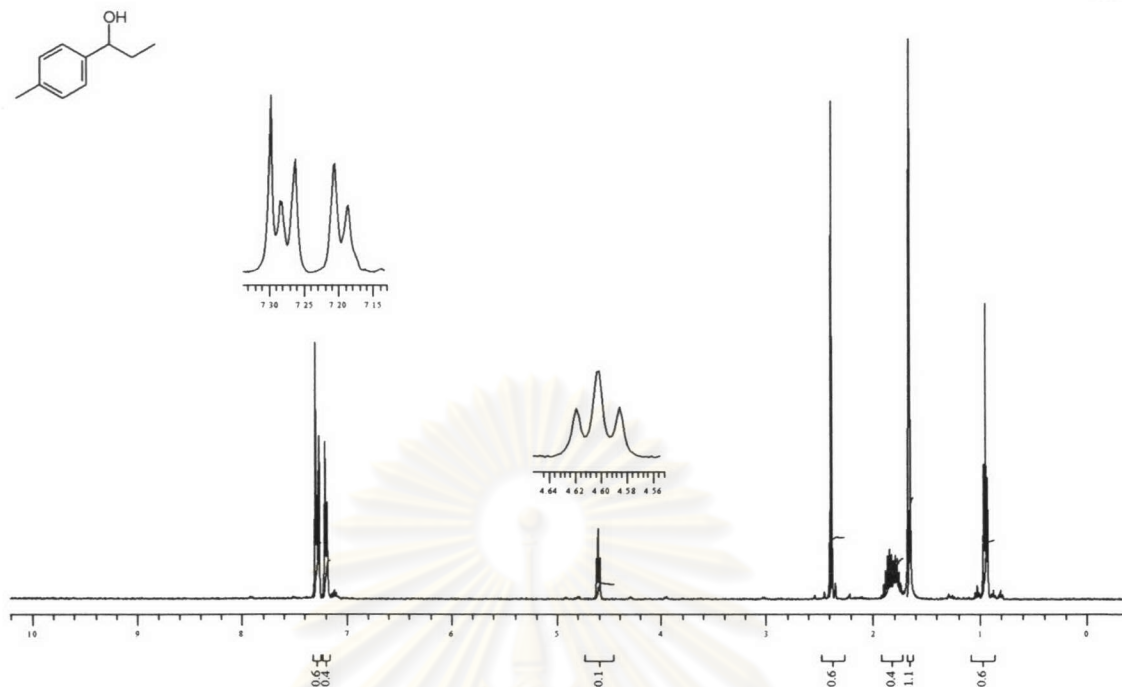


Figure B25 NMR spectrum of **12**; ^1H NMR (CDCl_3 , 400 MHz): δ 0.95 (3H, t, CH_2CH_3), 1.66 (1H, s, CHOH), 1.80 (2H, m, CHCH_2CH_3), 2.40 (3H, s, $\text{C}_6\text{H}_5\text{CH}_3$), 4.60 (1H, t, CHOH), 7.20 (2H, d, ArH), 7.28 (2H, d, ArH)

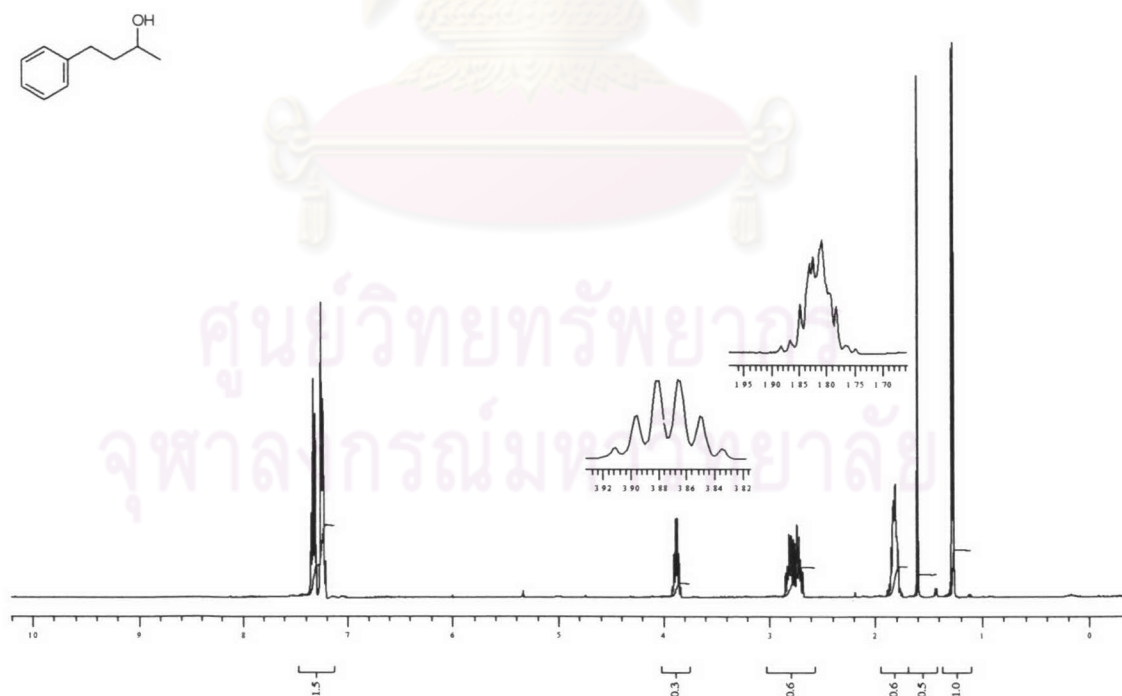


Figure B26 NMR spectrum of **18**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.28 (3H, d, CHCH_3), 1.60 (1H, s, CHOH), 1.80 (2H, q, $\text{CH}_2\text{CH}_2\text{CH}$), 2.75 (2H, m, $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2$), 3.88 (1H, q, CHOH), 7.28 (5H, m, C_6H_5)

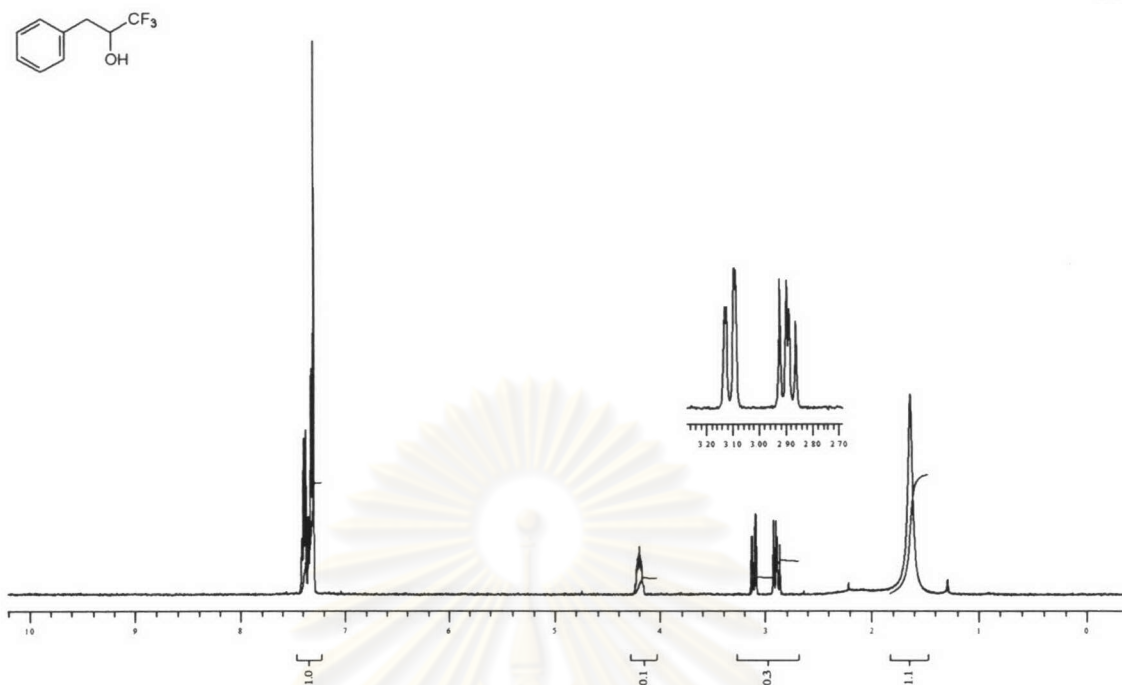


Figure B27 NMR spectrum of **20**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.60 (3H, d, CHOH), 2.88-3.12 (2H, s, CH_2CHCF_3), 4.20 (1H, m, CHOH), 7.35 (5H, d, C_6H_5)

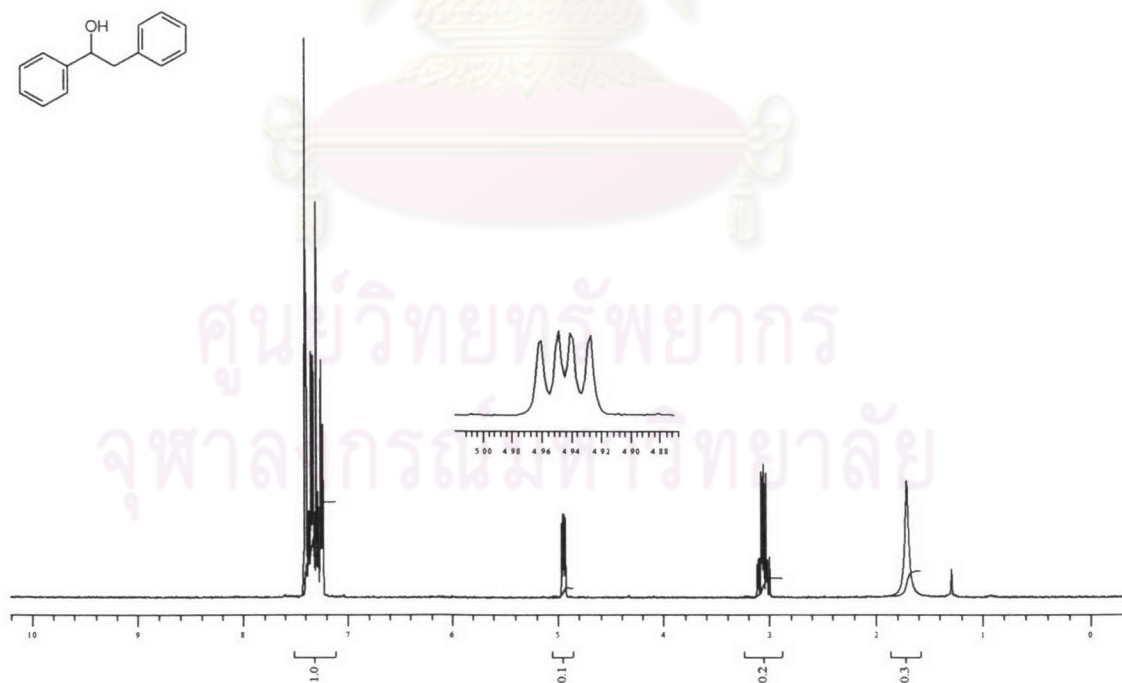


Figure B28 NMR spectrum of **22**; ^1H NMR (CDCl_3 , 400 MHz): δ 1.70 (1H, s, CHOH), 3.05 (2H, m, $\text{C}_6\text{H}_5\text{CH}_2\text{CH}$), 4.95 (1H, q, CHOH), 7.30 (10H, m, $2(\text{C}_6\text{H}_5)$)

Appendix C

Thermodynamic Studies

Table 1 Equations and correlation coefficients of all analytes obtained from $\ln k'$ vs. $1/T$ plots on OV-1701 column

analytes	Equations $\ln k' = m(1/T)+c$		R^2
	m	c	
1	5525.1	-13.366	0.9995
2	7064.6	-14.168	0.9991
3	7004.6	-14.053	0.9992
4	6309.8	-13.684	0.9996
5	6629.2	-14.252	0.9998
6	5273.9	-13.037	0.9992
7	5781.8	-13.531	0.9995
8	5957.7	-13.705	0.9995
9	6054.8	-13.672	0.9999
10	6123.0	-13.885	0.9998
11	6772.6	-14.464	0.9991
12	6123.0	-13.890	0.9999
13	5867.7	-13.664	0.9995
14	5868.7	-13.594	0.9995
15	6076.3	-13.721	0.9998
16	5627.7	-13.258	0.9995
17	5895.4	-13.428	0.9999
18	6192.3	-13.940	0.9998
19	6241.0	-13.954	0.9999
20	6345.8	-14.839	0.9991
21	6281.3	-14.946	0.9993

analytes	Equations $\ln k' = m(1/T)+c$		R^2
	M	c	
22	7309.5	-14.390	0.9992
23	6053.8	-13.659	0.9999
2Br	6053.1	-13.226	0.9986
3Br	6302.5	-13.563	0.9988
4Br	6455.7	-13.917	0.9992
F4Br	7183.7	-15.449	0.9988
4Bu	6786.6	-14.493	0.9993
4tBu	6637.3	-14.474	0.9997
2Cl	5850.8	-13.180	0.9986
3Cl	6080.5	-13.494	0.9989
4Cl	6223.2	-13.857	0.9997
F4Cl	7020.9	-15.552	0.9994
3CN	6963.4	-14.409	0.9990
4CN	6832.0	-14.084	0.9990
4Et	6158.8	-13.933	0.9999
2F	5364.5	-12.931	0.9978
3F	5528.1	-13.153	0.9984
4F	5699.1	-13.644	0.9995
F4F	6504.1	-15.339	0.9993
2OMe	6097.2	-13.562	0.9990
3OMe	6212.9	-13.649	0.9989
4OMe	6130.2	-13.838	0.9999
2Me	5651.8	-13.039	0.9989
3Me	5569.4	-12.975	0.9986
4Me	5831.6	-13.606	0.9996
2NO₂	6818.8	-14.222	0.9988
3NO₂	7192.6	-14.472	0.9991

analytes	Equations $\ln k' = m(1/T)+c$		R^2
	M	c	
4NO₂	7226.6	-14.462	0.9991
4OCF₃	6034.9	-14.339	0.9994
2CF₃	5765.9	-13.948	0.9995
3CF₃	6045.5	-14.334	0.9995
4CF₃	6051.6	-14.293	0.9995
24Cl	6529.7	-13.924	0.9990
25Cl	6650.9	-14.125	0.9990
34Cl	6751.2	-14.012	0.9989
24F	5.712.2	-13.883	0.9996
25F	5866.6	-14.085	0.9995
26F	5403.4	-13.275	0.9994
34F	5933.0	-13.976	0.9995
35F	5902.1	-14.124	0.9994
triF	5963.0	-14.312	0.9995
tetraF	6119.6	-14.532	0.9995
pentaF	5823.5	-14.209	0.9995
24Me	6224.8	-13.994	0.9997
25Me	6249.0	-14.069	0.9997
34Me	6204.6	-13.883	0.9998
2oct	5363.8	-13.703	0.9992
3oct	5362.7	-13.760	0.9989
4oct	5346.2	-13.760	0.9989

Table 2 Equations and correlation coefficients of all analytes obtained from $\ln k'$ vs. $1/T$ plots on BSiMe column

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		m	c	
1	7100.6	-16.151	0.9996	7314.0	-16.631	0.9996
2	8474.2	-16.642	0.9987	8579.2	-16.861	0.9985
3	8674.8	-17.057	0.9979	8987.0	-17.665	0.9977
4	8178.5	-17.111	0.9995	8291.1	-17.364	0.9994
5	8312.4	-17.296	0.9995	8328.1	-17.332	0.9995
6	7015.1	-16.339	0.9998	7073.0	-16.480	0.9999
7	7790.9	-17.374	1.0000	7876.1	-17.574	0.9999
8	8172.6	-18.044	0.9999	8141.1	-17.955	0.9999
9	8235.8	-17.983	0.9999	8330.6	-18.168	0.9999
10	7845.2	-17.121	0.9996	7958.7	-17.358	0.9996
11	8287.7	-17.233	0.9986	8466.2	-17.597	0.9986
12	7782.6	-17.014	0.9998	7999.1	-17.503	0.9998
13	7237.9	-16.283	0.9998	7398.8	-16.653	0.9998
14	7478.5	-16.636	0.9998	7571.1	-16.830	0.9998
15	7594.8	-16.667	0.9998	7693.8	-16.896	0.9998
16	7044.9	-15.895	0.9998	7150.6	-16.124	0.9998
17	7216.9	-15.863	0.9997	7374.1	-16.203	0.9997
18	7498.8	-16.310	0.9997	7589.6	-16.517	0.9997
19	7779.7	-16.897	0.9996	7819.0	-16.986	0.9996
20	8521.5	-18.881	0.9994	8873.4	-19.596	0.9994
21	8330.5	-18.708	0.9994	8375.6	-18.795	0.9994
22	8955.7	-17.417	0.9991	8993.9	-17.496	0.9990
23	7637.5	-16.532	0.9997	-	-	-

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		m	c	
2Br	8050.3	-16.950	0.9977	9142.1	-19.169	0.9957
3Br	8046.0	-16.762	0.9982	8118.3	-16.914	0.9979
4Br	8072.3	-16.714	0.9990	8208.6	-17.009	0.9989
F4Br	9050.7	-18.702	0.9990	-		
4Bu	8105.7	-16.783	0.9990	8236.2	-17.064	0.9988
4tBu	8291.2	-17.475	0.9994	8359.4	-17.626	0.9994
2Cl	7767.5	-16.760	0.9978	8687.3	-18.654	0.9961
3Cl	7801.1	-16.655	0.9983	7907.2	-16.878	0.9979
4Cl	7865.1	-16.739	0.9994	8054.6	-17.154	0.9993
F4Cl	8888.2	-18.833	0.9994	-		
3CN	8720.4	-17.557	0.9981	8782.7	-17.685	0.9980
4CN	8593.1	-17.213	0.9987	8788.4	-17.612	0.9984
4Et	7564.8	-16.420	0.9996	7731.8	-16.793	0.9996
2F	7560.8	-17.317	0.9999	8137.7	-18.612	0.9997
3F	7702.8	-17.431	0.9999	7870.9	-17.805	0.9999
4F	7296.0	-16.433	0.9995	7518.6	-16.943	0.9995
F4F	8363.5	-18.622	0.9995	8392.0	-18.659	0.9995
2OMe	7610.6	-16.440	0.9978	8285.3	-17.827	0.9969
3OMe	7777.8	-16.585	0.9982	7949.9	-16.951	0.9979
4OMe	6635.4	-14.653	0.9996	6735.1	-14.873	0.9995
2Me	8000.8	-17.657	0.9992	8476.9	-18.701	0.9989
3Me	7635.6	-17.039	0.9994	7871.5	-17.557	0.9993
4Me	7144.2	-15.894	0.9996	7398.2	-16.456	0.9995
2NO₂	8514.6	-17.264	0.9984	9642.2	-19.492	0.9969
3NO₂	8736.8	-17.214	0.9990	8758.7	-17.260	0.9988

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		M	c	
4NO₂	8865.6	-17.300	0.9993	8997.7	-17.571	0.9992
4OCF₃	7423.6	-16.726	0.9994	7683.0	-17.299	0.9994
2CF₃	7749.7	-17.750	0.9997	9008.3	-20.503	0.9990
3CF₃	7889.1	-17.882	0.9998	8037.6	-18.217	0.9998
4CF₃	7501.0	-16.758	0.9995	7745.0	-17.296	0.9994
24Cl	8280.5	-16.999	0.9983	9243.8	-18.940	0.9968
25Cl	8956.0	-18.308	0.9977	10136	-20.646	0.9967
34Cl	8363.4	-16.864	0.9987	8467.7	-17.080	0.9985
24F	7466.4	-17.067	0.9997	8364.5	-19.037	0.9993
25F	8190.7	-18.481	0.9996	8713.8	-19.608	0.9994
26F	6694.5	-15.636	0.9997	7328.9	-17.050	0.9994
34F	7497.1	-16.748	0.9995	7747.1	-17.296	0.9994
35F	7892.8	-17.879	0.9998	-		
triF	7688.8	-17.449	0.9996	9103.6	-20.456	0.9994
tetraF	7590.6	-17.197	0.9997	7828.7	-17.737	0.9997
pentaF	7030.0	-16.382	0.9998	7449.3	-17.316	0.9998
24Me	8142.2	-17.552	0.9994	8746.0	-18.858	0.9989
25Me	8301.2	-17.933	0.9993	8887.5	-19.174	0.9990
34Me	7886.3	-16.993	0.9995	7959.5	-17.157	0.9995
2oct	6368.2	-15.415	0.9998	-		
3oct	6426.5	-15.585	0.9996	-		
4oct	6437.8	-15.654	0.9996	-		

Table 3 Equations and correlation coefficients of all analytes obtained from $\ln k'$ vs. $1/T$ plots on GSiMe column

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		m	c	
1	6131.6	-14.487	0.9992	6170.6	-14.583	0.9991
2	7574.3	-15.039	0.9987	-		
3	7620.8	-15.139	0.9988	7651.3	-15.205	0.9986
4	6817.9	-14.582	0.9998	6852.0	-14.661	0.9998
5	6965.9	-14.734	0.9994	-		
6	5967.6	-14.515	0.9990	5991.5	-14.578	0.9988
7	6430.8	-14.744	0.9998	6476.6	-14.854	0.9997
8	6725.4	-15.182	0.9997	6756.4	-15.256	0.9997
9	6911.7	-15.335	0.9997	6924.2	-15.365	0.9996
10	6872.6	-15.339	0.9997	-		
11	7335.9	-15.464	0.9986	73507	-15.497	0.9984
12	6747.5	-15.065	0.9996	6834.7	-15.270	0.9995
13	6417.2	-14.693	0.9996	6544.7	-14.989	0.9997
14	6497.6	-14.773	0.9998	6560.7	-14.925	0.9997
15	6839.1	-15.215	0.9996	6922.9	-15.414	0.9995
16	6219.0	-14.427	0.9991	6251.3	-14.505	0.9991
17	6433.5	-14.468	0.9998	6521.7	-14.673	0.9998
18	6815.6	-15.176	0.9996	7011.7	-15.618	0.9994
19	7119.3	-15.715	0.9995	7284.4	-16.097	0.9994
20	7228.4	-16.514	0.9994	7480.2	-17.044	0.9993
21	7109.9	-16.433	0.9998	-		
22	7900.2	-15.410	0.9982	7985.2	-15.589	0.9982
23	6592.5	-14.635	0.9996	6668.2	-14.812	0.9996

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		m	c	
2Br	7154.9	-15.427	0.9997	7340.9	-15.827	0.9997
3Br	7354.8	-15.679	0.9997	-		
4Br	7146.0	-15.218	0.9998	7194.0	-15.328	0.9997
F4Br	8080.9	-17.062	0.9993	8122.7	-17.155	0.9993
4Bu	7320.7	-15.467	0.9994	7375.4	-15.589	0.9993
4tBu	7115.4	-15.282	0.9992	-		
2Cl	6873.5	-15.245	0.9998	7055.2	-15.641	0.9997
3Cl	6993.4	-15.318	0.9997	-		
4Cl	6884.2	-15.097	0.9998	6940.5	-15.228	0.9998
F4Cl	7894.4	-17.121	0.9997	7903.7	-17.142	0.9997
3CN	7615.2	-15.638	0.9988	7624.7	-15.659	0.9987
4CN	7527.2	-15.407	0.9989	7588.5	-15.540	0.9987
4Et	6790.1	-15.129	0.9997	6899.8	-15.378	0.9997
2F	6269.6	-14.803	0.9991	6416.5	-15.148	0.9990
3F	6423.3	-15.007	0.9992	-		
4F	63057	-14.780	0.9992	6360.9	-14.915	0.9991
F4F	7269.1	-16.668	0.9998	-		
2OMe	6891.8	-15.192	0.9997	6939.3	-15.301	0.9997
3OMe	7231.7	-15.736	0.9997	7303.6	-15.900	0.9997
4OMe	6311.6	-14.143	0.9999	6425.7	-14.412	0.9998
2Me	6477.1	-14.695	0.9997	6557.4	-14.882	0.9997
3Me	6592.9	-15.090	0.9997	-		
4Me	6339.3	-14.516	0.9997	6445.0	-14.761	0.9998
2NO₂	7524.9	-15.528	0.9987	7787.6	-16.072	0.9984
3NO₂	7933.6	-15.875	0.9983	-		

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = m(1/T)+c$		R^2	Equation: $\ln k' = m(1/T)+c$		R^2
	m	c		m	c	
4NO₂	7916.3	-15.747	0.9984	7930.7	-15.778	0.9984
4OCF₃	6545.2	-15.266	0.9998	6619.0	-15.440	0.9997
2CF₃	6452.1	-15.263	0.9993	6653.9	-15.729	0.9991
3CF₃	6677.5	-15.526	0.9997	6729.0	-15.649	0.9996
4CF₃	6519.8	-15.104	0.9998	6585.3	-15.258	0.9998
24Cl	7259.8	-15.230	0.9986	7542.9	-15.819	0.9982
25Cl	7439.6	-15.552	0.9984	7604.1	-15.886	0.9984
34Cl	7469.6	-15.338	0.9987	-		
24F	6375.5	-15.118	0.9992	6555.0	-15.531	0.9991
25F	6614.3	-15.504	0.9992	6720.9	-15.749	0.9992
26F	5959.7	-14.376	0.9996	6157.8	-14.847	0.9995
34F	6599.0	-15.266	0.9992	6634.9	-15.354	0.9992
35F	6676.5	-15.659	0.9994	-		
triF	6471.3	-15.155	0.9996	6610.8	-15.461	0.9997
tetraF	6602.4	-15.357	0.9997	6709.8	-15.606	0.9998
pentaF	6338.5	-15.206	0.9992	6472.8	-15.524	0.9992
24Me	6861.3	-15.184	0.9997	7030.7	-15.557	0.9997
25Me	6867.3	-15.222	0.9997	6974.9	-15.459	0.9997
34Me	6948.4	-15.339	0.9996	7031.4	-15.530	0.9997
2oct	6011.8	-15.130	0.9987	-		
3oct	5865.9	-14.805	0.9988	5944.5	-15.008	0.9988
4oct	5819.2	-14.731	0.9989	5858.2	-14.834	0.9987

Table4 Thermodynamic parameters of all alcohols calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on OV-1701 column

compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)	compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)
1	10.98	15.59	20	12.61	18.52
2	14.04	17.18	21	12.48	18.73
3	13.92	16.95	22	14.53	17.62
4	12.54	16.22	23	12.03	16.17
5	13.17	17.35	2Br	12.03	15.31
6	10.48	14.93	3Br	12.52	15.98
7	11.49	15.92	4Br	12.83	16.68
8	11.84	16.26	F4Br	14.28	19.73
9	12.03	16.20	4Bu	13.49	17.83
10	12.17	16.62	4tBu	13.19	17.79
11	13.46	17.77	2Cl	11.63	15.22
12	12.17	16.63	3Cl	12.08	15.84
13	11.66	16.18	4Cl	12.37	16.56
14	11.66	16.04	F4Cl	13.95	19.93
15	12.07	16.29	3CN	13.84	17.66
16	11.18	15.37	4CN	13.58	17.02
17	11.72	15.71	4Et	12.24	16.72
18	12.31	16.73	2F	10.66	14.72
19	12.40	16.76	3F	10.99	15.17

compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)	compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)
4F	11.33	16.14	25Cl	13.22	17.10
F4F	12.92	19.51	34Cl	13.42	16.87
2OMe	12.12	15.98	24F	11.35	16.62
3OMe	12.35	16.15	25F	11.66	17.02
4OMe	12.18	16.53	26F	10.74	15.41
2Me	11.23	14.94	34F	11.79	16.80
3Me	11.07	14.81	35F	11.73	17.09
4Me	11.59	16.07	triF	11.85	17.47
2NO₂	13.55	17.29	tetraF	12.16	17.91
3NO₂	14.29	17.79	pentaF	11.57	17.26
4NO₂	14.36	17.77	24Me	12.37	16.84
4OCF₃	11.99	17.52	25Me	12.42	16.99
2CF₃	11.46	16.75	34Me	12.33	16.62
3CF₃	12.01	17.51	2oct	10.66	16.26
4CF₃	12.03	17.43	3oct	10.66	16.37
24Cl	12.98	16.70	4oct	10.62	16.37

Table5 Thermodynamic parameters of all alcohols calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on BSiMe column

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
1	11.11	14.53	0.42	21.12	22.08	0.95
2	16.84	17.05	0.21	22.10	22.53	0.44
3	17.24	17.86	0.62	22.92	24.13	1.21
4	16.25	16.48	0.22	23.03	23.53	0.50
5	16.52	16.55	0.03	23.40	23.47	0.07
6	13.94	14.06	0.12	21.50	21.78	0.28
7	15.48	15.65	0.17	23.55	23.95	0.40
8	16.24	16.18	-0.06	24.88	24.71	-0.18
9	16.37	16.55	.019	24.76	25.13	0.37
10	15.59	15.82	0.23	23.05	23.52	0.47
11	16.47	16.82	0.35	23.27	24.00	0.72
12	15.47	15.90	0.43	22.84	23.81	0.97
13	14.38	14.70	0.32	21.39	22.12	0.74
14	14.86	15.05	0.18	22.09	22.47	0.39
15	15.09	15.29	0.18	22.15	22.60	0.46
16	14.00	14.21	0.21	20.61	21.07	0.46
17	14.34	14.65	0.31	20.55	21.23	0.68
18	14.90	15.09	0.18	21.44	21.85	0.41
19	15.46	15.54	0.08	22.61	22.78	0.18

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
20	16.93	17.63	0.70	26.55	27.97	1.42
21	16.55	16.64	0.09	26.20	26.38	0.17
22	17.80	17.87	0.08	23.64	23.80	0.16
23	15.46	15.46	0.00	22.58	22.58	0.00
2Br	16.00	18.17	2.17	22.71	27.12	4.41
3Br	15.99	16.13	0.14	22.34	22.64	0.30
4Br	16.04	16.31	0.27	22.24	22.83	0.59
F4Br	17.99	17.99	0.00	26.19	26.19	0.00
4Bu	16.11	16.37	0.26	22.38	22.94	0.56
4tBu	16.48	16.61	0.14	23.75	24.05	0.30
2Cl	15.44	17.26	1.83	22.33	26.10	3.76
3Cl	15.50	15.71	0.21	22.12	22.57	0.44
4Cl	15.63	16.01	0.38	22.29	23.12	0.82
F4Cl	17.66	17.66	0.00	26.45	26.45	0.00
3CN	17.33	17.45	0.12	23.92	24.17	0.25
4CN	17.08	17.46	0.39	23.23	24.03	0.79
4Et	15.03	15.36	0.33	21.66	22.40	0.74
2F	15.02	16.17	1.15	23.44	26.01	2.57
3F	15.31	15.64	0.33	23.67	24.41	0.74
4F	14.50	14.94	0.44	21.68	22.70	1.01
F4F	16.62	16.68	0.06	26.03	26.11	0.07

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
2OMe	15.12	16.46	1.34	21.70	24.45	2.76
3OMe	15.46	15.80	0.34	21.99	22.71	0.73
4OMe	13.19	13.38	0.20	18.15	18.58	0.44
2Me	15.90	16.85	0.95	24.12	26.19	2.07
3Me	15.17	15.64	0.47	22.89	23.92	1.03
4Me	14.20	14.70	0.50	20.61	21.73	1.12
2NO₂	16.92	19.16	2.24	23.33	27.76	4.43
3NO₂	17.36	17.41	0.04	23.24	23.33	0.09
4NO₂	17.62	17.88	0.26	23.41	23.94	0.54
4OCF₃	14.75	15.27	0.52	22.27	23.40	1.14
2CF₃	15.40	17.90	2.50	24.30	29.77	5.47
3CF₃	15.68	15.97	0.30	24.56	25.23	0.67
4CF₃	14.91	15.39	0.48	22.33	23.40	1.07
24Cl	16.46	18.37	1.91	22.81	26.67	3.86
25Cl	17.80	20.14	2.34	25.41	30.06	4.65
34Cl	16.62	16.83	0.21	22.54	22.97	0.43
24F	14.84	16.62	1.78	22.94	26.86	3.91
25F	16.28	17.32	1.04	25.75	27.99	2.24
26F	13.30	14.56	1.26	20.10	22.91	2.81
34F	14.90	15.40	0.50	22.31	23.40	1.09
35F	15.68	15.68	0.00	24.56	24.56	0.00

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
triF	15.28	18.09	2.81	23.70	29.68	5.98
tetraF	15.08	15.56	0.47	23.20	24.27	1.07
pentaF	13.97	14.80	0.83	21.58	23.44	1.86
24Me	16.18	17.38	1.20	23.91	26.50	2.60
25Me	16.50	17.66	1.17	24.66	27.13	2.47
34Me	15.67	15.82	0.15	22.80	23.12	0.33
2oct	12.65	12.65	0.00	19.66	19.66	0.00
3oct	12.77	12.77	0.00	20.00	20.00	0.00
4oct	12.79	12.79	0.00	20.14	20.14	0.00

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Table6 Thermodynamic parameters of all alcohols calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on GSiMe column

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
1	12.18	12.26	0.08	17.82	18.01	0.19
2	15.05	15.05	0.00	18.91	18.91	0.00
3	15.14	15.20	0.06	19.11	19.24	0.13
4	13.55	13.62	0.07	18.01	18.16	0.16
5	13.84	13.84	0.00	18.31	18.31	0.00
6	11.86	11.91	0.05	17.87	18.00	0.13
7	12.78	12.87	0.09	18.33	18.55	0.22
8	13.36	13.43	0.06	19.20	19.34	0.15
9	13.73	13.76	0.02	19.50	19.56	0.06
10	13.66	13.66	0.00	19.51	19.51	0.00
11	14.58	14.61	0.03	19.76	19.82	0.07
12	13.41	13.58	0.17	18.96	19.37	0.41
13	12.75	13.01	0.25	18.23	18.81	0.59
14	12.91	13.04	0.13	18.38	18.69	0.30
15	13.59	13.76	0.17	19.26	19.66	0.40
16	12.36	12.42	0.06	17.70	17.85	0.16
17	12.78	12.96	0.18	17.78	18.19	0.41
18	13.54	13.93	0.39	19.19	20.06	0.88
19	14.15	14.48	0.33	20.26	21.02	0.76

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
20	14.36	14.86	0.50	21.84	22.90	1.05
21	14.13	14.13	0.00	21.68	21.68	0.00
22	15.70	15.87	0.17	19.65	20.01	0.36
23	13.10	13.25	0.15	18.11	18.46	0.35
2Br	14.22	14.59	0.37	19.68	20.48	0.79
3Br	14.62	14.62	0.00	20.19	20.19	0.00
4Br	14.20	14.30	0.10	19.27	19.49	0.22
F4Br	16.06	16.14	0.08	22.93	23.12	0.18
4Bu	14.55	14.66	0.11	19.76	20.01	0.24
4tBu	14.14	14.14	0.00	19.40	19.40	0.00
2Cl	13.66	14.02	0.36	19.32	20.11	0.79
3Cl	13.90	13.90	0.00	19.47	19.47	0.00
4Cl	13.68	13.79	0.11	19.03	19.29	0.26
F4Cl	15.69	15.71	0.02	23.05	23.09	0.04
3CN	15.13	15.15	0.02	20.10	20.15	0.04
4CN	14.96	15.08	0.12	19.64	19.91	0.26
4Et	13.49	13.71	0.22	19.09	19.59	0.49
2F	12.46	12.75	0.29	18.44	19.13	0.69
3F	12.76	12.76	0.00	18.85	18.85	0.00
4F	12.53	12.64	0.11	18.40	18.67	0.27
F4F	14.45	14.45	0.00	22.15	22.15	0.00

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
2OMe	13.70	13.79	0.09	19.22	19.43	0.22
3OMe	14.37	14.51	0.14	20.30	20.62	0.33
4OMe	12.54	12.77	0.23	17.13	17.67	0.53
2Me	12.87	13.03	0.16	18.23	18.60	0.37
3Me	13.10	13.10	0.00	19.01	19.01	0.00
4Me	12.60	12.81	0.21	17.87	18.36	0.49
2NO₂	14.95	15.48	0.52	19.89	20.97	1.08
3NO₂	15.77	15.77	0.00	20.57	20.57	0.00
4NO₂	15.73	15.76	0.03	20.32	20.38	0.06
4OCF₃	13.01	13.15	0.15	19.36	19.71	0.35
2CF₃	12.82	13.22	0.40	19.36	20.28	0.93
3CF₃	13.27	13.37	0.10	19.88	20.13	0.24
4CF₃	12.96	13.09	0.13	19.04	19.35	0.31
24Cl	14.43	14.99	0.56	19.29	20.46	1.17
25Cl	14.78	15.11	0.33	19.93	20.60	0.66
34Cl	14.84	14.84	0.00	19.51	19.51	0.00
24F	12.67	13.03	0.36	19.07	19.89	0.82
25F	13.14	13.36	0.21	19.84	20.32	0.49
26F	11.84	12.24	0.39	17.60	18.53	0.94
34F	13.11	13.18	0.07	19.36	19.54	0.17
35F	13.27	13.27	0.00	20.15	20.15	0.00

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
triF	12.86	13.14	0.28	19.14	19.75	0.61
tetraF	13.12	13.33	0.21	19.55	20.04	0.49
pentaF	12.60	12.86	0.27	19.25	19.88	0.63
24Me	13.63	13.97	0.34	19.20	19.94	0.74
25Me	13.65	13.86	0.21	19.28	19.75	0.47
34Me	13.81	13.97	0.16	19.51	19.89	0.38
2oct	11.95	11.95	0.00	19.09	19.09	0.00
3oct	11.66	11.81	0.16	18.45	18.85	0.40
4oct	11.56	11.64	0.08	18.30	18.51	0.20

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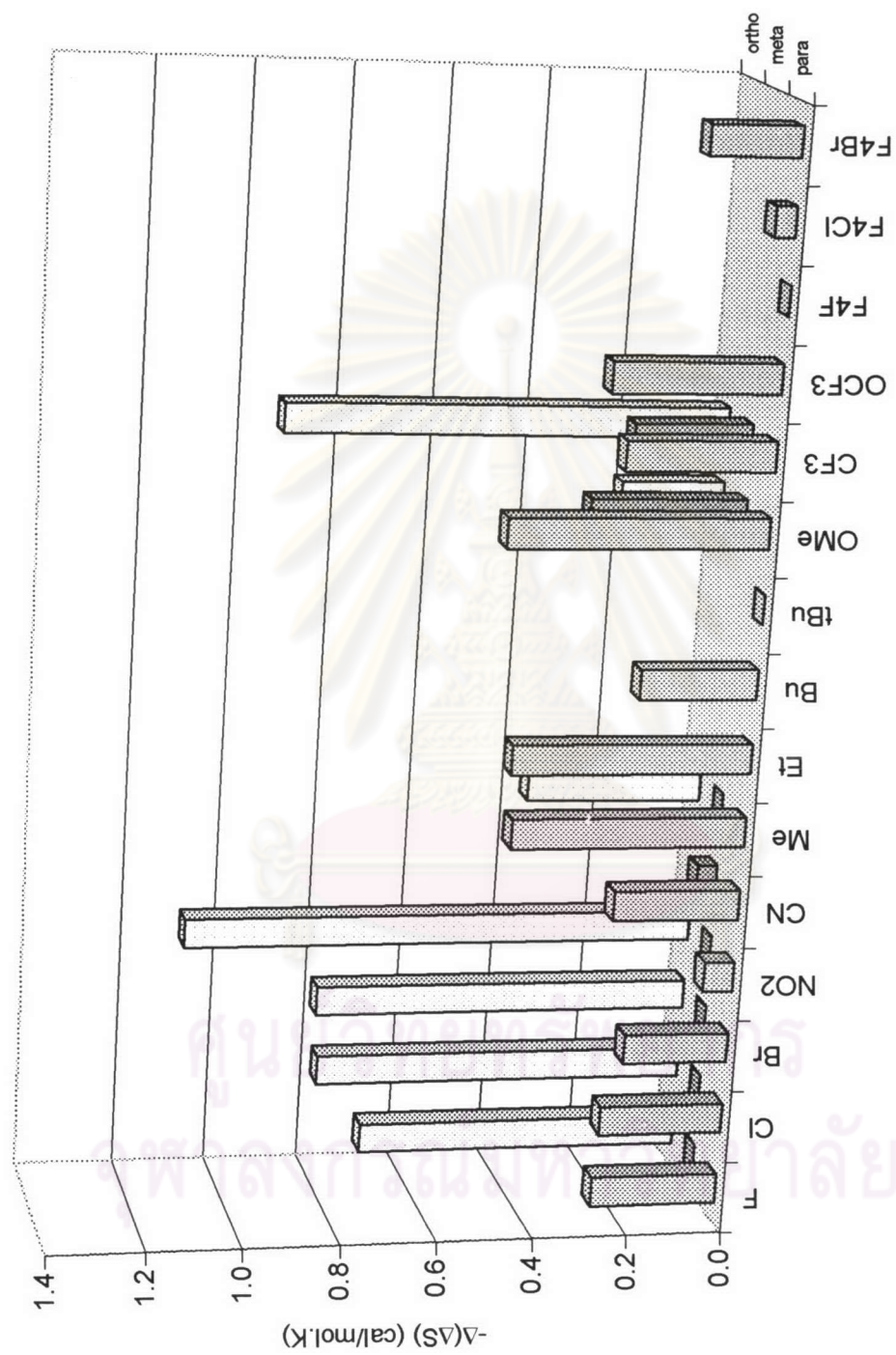


Figure C1 Difference in entropy values ($-\Delta(\Delta S)$, cal/mol \cdot K) of the enantiomers of mono-substituted 1-phenylethanol derivatives on GSiMe column.

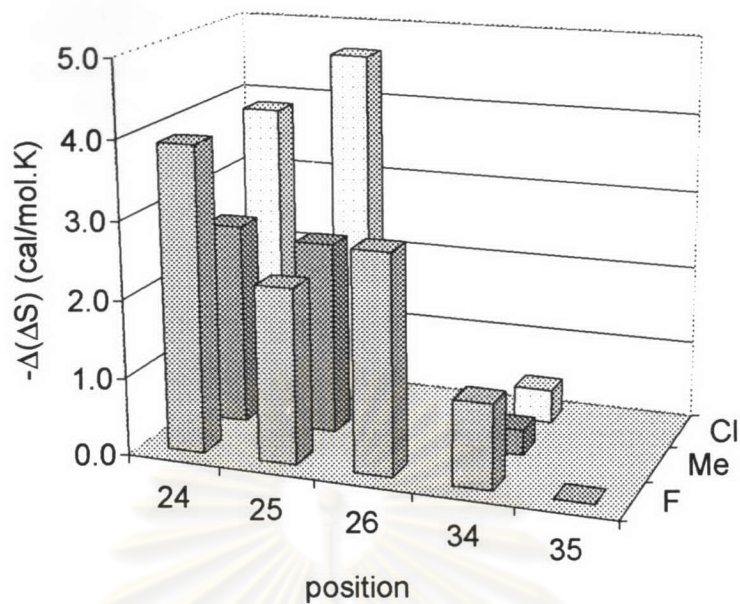


Figure C2 Difference in enthalpy values ($-\Delta(\Delta S)$, cal/mol.K) of the enantiomers of di-substituted 1-phenylethanol derivatives on BSiMe column.

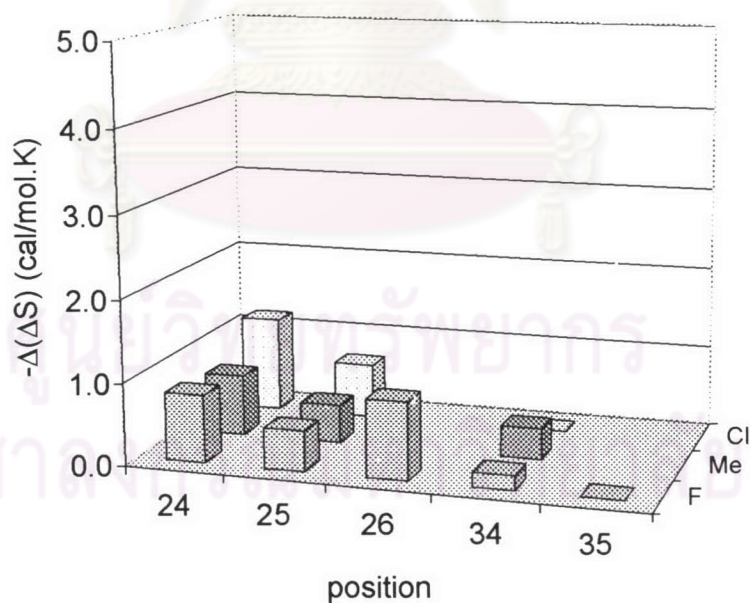


Figure C3 Difference in enthalpy values ($-\Delta(\Delta S)$, cal/mol.K) of the enantiomers of di-substituted 1-phenylethanol derivatives on GSiMe column.

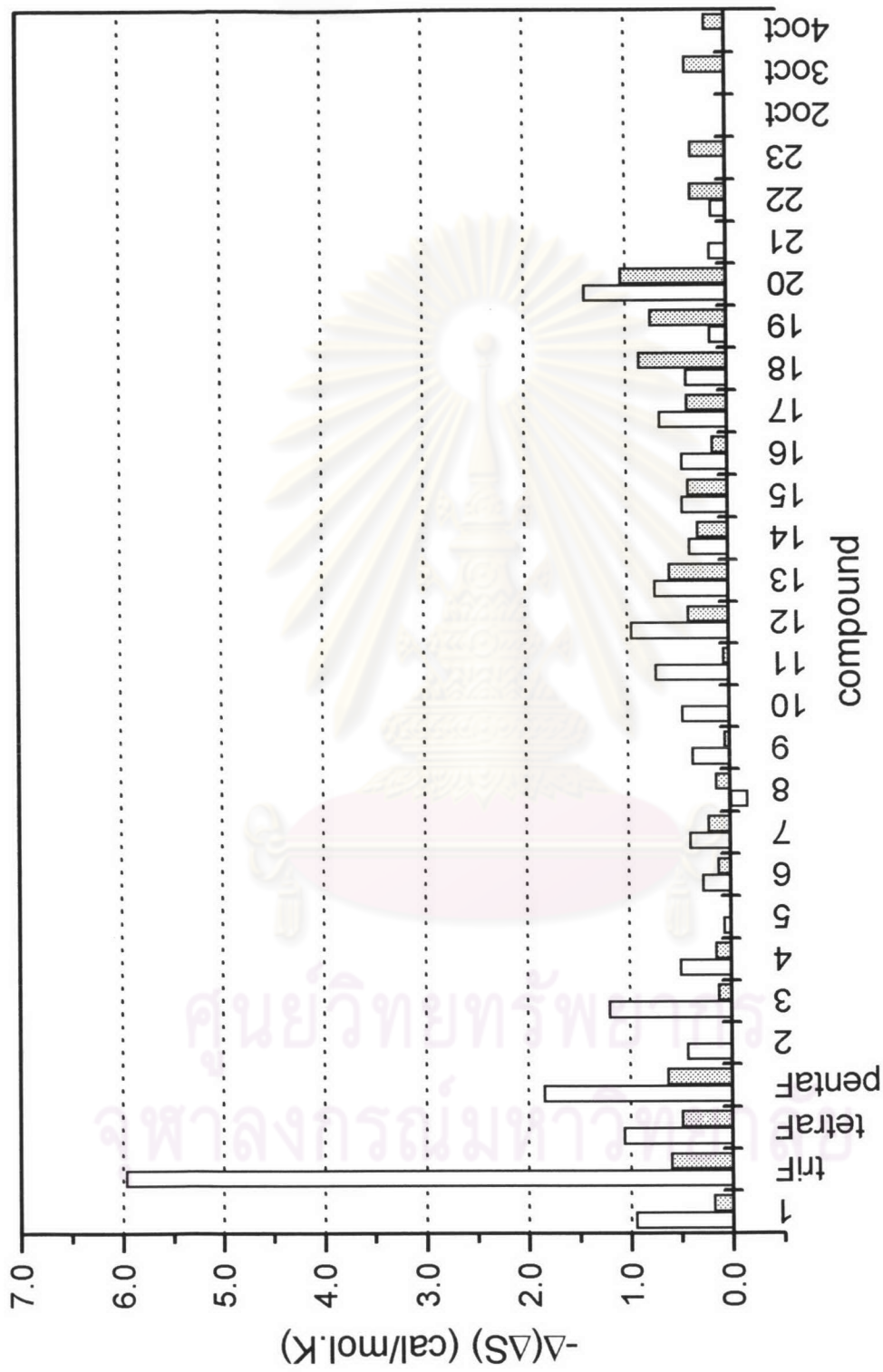


Figure C4 Difference in enthalpy values ($-\Delta(\Delta S)$, cal/mol·K) of the enantiomers of alcohols in series 3 on BSiMe (white bar) and GSiMe (gray bar) columns.

VITA

Miss Ornuma Konghuirob was born on Thursday 2nd November, 1978 in Uthaithani, Thailand. She moved to Bangkok in 1990 to study in Prathom 6 at Samsane Kindergarten School. From 1991 to 1996, she entered secondary school at Horwang School. Majoring in chemistry, the author completed her undergraduate study from the Faculty of Science, Kasetsart University in 2000. After graduation, she had worked as a chemist at International Laboratories Co., Ltd. for 2 years. Since 2002, she has been a graduate student of Chemistry Department, Chulalongkorn University. Her current address is 90/522 Moo 2 Soi Phoopansomnuk 2, Ladplakao Road, Anusaovaree, Bangkok, Bangkok 10220.



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