

## REFERENCES

1. N. M. Maier, P. Franco, and W. Lindner, "Separation of Enantiomers: Needs, Challenges, Perspectives", *J. Chromatogr. A*, 906 (2001) 3-33.
2. J. Szymura-Oleksiak, J. Bojarski, and H. Y. Aboul-Enein, "Recent Applications of Stereoselective Chromatography", *Chirality*, 14 (2002) 417-435.
3. A. C. Sewell, M. Heil, F. Podebrad, and A. Mosandl, "Chiral Compounds in Metabolism: A Look in the Molecular Mirror", *Eur. J. Pediatr.*, 157 (1998) 185-191.
4. A. N. Collins, G. N. Sheldrake, and J. Crosby, Chirality in Industrial II: Developments in The Manufacture and Applications of Optically Active Compounds, Wiley, Chichester, 1997, p. 226.
5. E. R. Francotte, "Enantioselective Chromatography as A Powerful Alternative for The Preparation of Drug Enantiomers", *J. Chromatogr. A*, 906 (2001) 379-397.
6. V. Schurig, "Separation of Enantiomers by Gas Chromatography", *J. Chromatogr. A*, 906 (2001) 275-299.
7. A. Venema, H. Henderiks, and R. V. Geest, "The Enantioselectivity of Modified Cyclodextrins: Studies on Interaction Mechanisms", *J. High Resolut. Chromatogr.*, 14 (1991) 676-680.
8. I. D. Smith and C. F. Simpson, "Investigation into The GC Separation of Enantiomers on A Trifluoroacetylated Cyclodextrin: Effect of Analyte Structure on Stereoselectivity for Alcohols", *J. High Resolut. Chromatogr.*, 15 (1992) 800-806.
9. I. D. Smith and C. F. Simpson, "Investigation into The GC Separation of Enantiomers on A Trifluoroacetylated Cyclodextrin, Part II: Effect of Derivatization on Stereoselectivity towards Alcohols", *J. High Resolut. Chromatogr.*, 16 (1993) 530-535.
10. A. Berthod, W. Li, and D. W. Armstrong, "Multiple Enantioselective Retention Mechanisms on Derivatized Cyclodextrin Gas Chromatographic Chiral Stationary Phases", *Anal. Chem.*, 64 (1992) 873-879.

11. R. Reinhardt, W. Engewald, O. Goj, and G. Haufe, "Enantiomer Separation of Side-chain Fluorinated Alkylbenzenes by Capillary Gas Chromatography on Cyclodextrin Phases", *Chromatographia*, 39 (1994) 192-199.
12. K. Jaques, W. M. Buda, A. Venema, and P. Sandra, "Enantioselective Separations by Capillary Gas Chromatography on Derivatized Cyclodextrins III. Separation of Some Racemic 2,2-Dialkyl-4-alkoxycarbonyl-1,3-dioxolane Derivatives on 2,3-di-*O*-acetyl-6-*O*-*tert*-butyldimethylsilyl- $\beta$ - and  $\gamma$ -Cyclodextrins", *J. Chromatogr. A*, 666 (1994) 131-136.
13. K. Jaques, W. M. Buda, A. Venema, and P. Sandra, "Enantioselective Separations by Capillary Gas Chromatography on Derivatized Cyclodextrins. Part IV: Enantioselective Interaction Model of 2,2-Dialkyl-4-alkoxycarbonyl-1,3-dioxolane Derivatives on Some Substituted Cyclodextrins", *J. Microcol. Sep.*, 7 (1995) 145-151.
14. I. Spanik, P. Oswald, J. Krupcik, E. Benicka, P. Sandra, and D. W. Armstrong, "Evaluation of Non-polar Interactions in Chiral Recognition by Alkylated  $\beta$ - and  $\gamma$ -Cyclodextrin Chiral Stationary Phases", *J. Sep. Sci.*, 25 (2002) 45-52.
15. H.-G. Schmarr and A. Mosandl, "Influence of Derivatization on The Chiral Selectivity of Cyclodextrins: Alkylated/Acylated Cyclodextrins and  $\gamma$ - $\delta$ -Lactones as An Example", *J. Microcol. Sep.*, 3 (1991) 395-402.
16. A. Dietrich, B. Maas, V. Karl, P. Kreis, D. Lehmann, B. Weber, and A. Mosandl, "Stereoisomeric Flavor Compounds, Part LV: Stereodifferentiation of Some Chiral Volatiles on Heptakis(2,3-di-*O*-acetyl-6-*O*-*tert*-butyldimethylsilyl)- $\beta$ -cyclodextrin", *J. High Resolut. Chromatogr.*, 15 (1992) 176-179.
17. A. Dietrich, B. Maas, W. Messer, G. Bruche, V. Karl, A. Kaunzinger, and A. Mosandl, "Stereoisomeric Flavor Compounds, Part LVIII: The Use of Heptakis(2,3-di-*O*-acetyl-6-*O*-*tert*-butyldimethylsilyl)- $\beta$ -cyclodextrin as A Chiral Stationary Phase in Flavor Analysis", *J. High Resolut. Chromatogr.*, 15 (1992) 590-593.
18. F. Kobor and G. Schomburg, "6-*tert*-Butyldimethylsilyl-2,3-dimethyl- $\alpha$ -,  $\beta$ -, and  $\gamma$ -cyclodextrins, Dissolved in Polysiloxanes, as Chiral Selectors for Gas Chromatography", *J. High Resolut. Chromatogr.*, 16 (1993) 693-699.

19. B. Maas, A. Dietrich, and A. Mosandl, "Comparison of Different 6-*tert*-Butyldimethyl-Silylated Cyclodextrins as Chiral Stationary Phases in GC", *J. Microcol. Sep.*, 8 (1996) 47-56.
20. Z. Juvancz and J. Szejtli, "The Role of Cyclodextrins in Chiral Selective Chromatography", *Trends Anal. Chem.*, 21 (2002) 379-388.
21. S. Allenmark and V. Schurig, "Chromatography on Chiral Stationary Phases", *J. Mater. Chem.*, 7 (1997) 1955-1963.
22. V. Schurig, "Enantiomer Separation by Gas Chromatography on Chiral Stationary Phases", *J. Chromatogr. A*, 666 (1994) 111-129.
23. V. Schurig and H.-P. Nowotny, "Gas Chromatographic Separation of Enantiomers on Cyclodextrin Derivatives", *Angew. Chem. Int. Ed. Engl.*, 29 (1990) 939-957.
24. W. A. Konig, "Enantioselective Gas Chromatography", *Trends Anal. Chem.*, 12 (1993) 130-137.
25. D. W. Armstrong, W. Li, and A. M. Stalcup, "Capillary Gas Chromatographic Separation of Enantiomers with Stable Dipentyl- $\alpha$ -,  $\beta$ -, and  $\gamma$ -Cyclodextrin Derivatized Stationary Phases", *Anal. Chim. Acta*, 234 (1990) 365-380.
26. B. E. Kim, K.-P. Lee, K.-S. Park, S. H. Lee, and J. H. Park, "Enantioselectivity of 6-*O*-Alkyldimethylsilyl-2,3-di-*O*-methyl- $\beta$ -cyclodextrins as Chiral Stationary Phases in Capillary GC", *Chromatographia*, 46 (1997) 145-150.
27. B. Maas, A. Dietrich, T. Beck, S. Borner, and A. Mosandl, "Di-*tert*-butyldimethylsilylated Cyclodextrins as Chiral Stationary Phases: Thermodynamic Investigations", *J. Microcol. Sep.*, 7 (1995) 65-73.
28. W. A. Konig, D. Icheln, T. Runge, I. Pforr, and A. Krebs, "Cyclodextrins as Chiral Stationary Phases in Capillary Gas Chromatography, Part VII: Cyclodextrins with An Inverse Substitution Pattern - Synthesis and Enantioselectivity", *J. High Resolut. Chromatogr.*, 13 (1990) 702-707.
29. T. Beck, J.-M. Liepe, J. Nandzik, S. Rohn, and A. Mosandl, "Comparison of Different Di-*tert*-butyldimethyl-silylated Cyclodextrins as Chiral Stationary Phases in Capillary Gas Chromatography", *J. High Resolut. Chromatogr.*, 23 (2000) 569-575.

30. C. Bicchi, G. Cravotto, A. D'Amato, P. Rubiolo, A. Galli, and M. Galli, "Cyclodextrin Derivatives in Gas Chromatographic Separation of Racemates with Different Volatility. Part XV: 6-*O*-*t*-Butyldimethylsilyl versus 6-*O*-*t*-Hexyldimethylsilyl- $\beta$  and - $\gamma$  Derivatives", *J. Microcol. Sep.*, 11 (1999) 487-500.
31. M.-Y. Nie, L.-M. Zhou, X.-L. Liu, Q.-H. Wang, and D.-Q. Zhu, "Gas Chromatographic Enantiomer Separation on Long-chain Alkylated  $\beta$ -Cyclodextrin Chiral Stationary Phases", *Anal. Chim. Acta*, 408 (2000) 279-284.
32. B. Maas, A. Dietrich, V. Karl, A. Kaunzinger, D. Lehmann, T. Kopke, and A. Mosandl, "*tert*-Butyldimethylsilyl-substituted Cyclodextrin Derivatives as Versatile Chiral Stationary Phases in Capillary GC", *J. Microcol. Sep.*, 5 (1993) 421-427.
33. M. Jung and V. Schurig, "Enantiomeric Separation by GC on Chirasil-Dex: Systematic Study of Cyclodextrin Concentration, Polarity, Immobilization, and Column Stability", *J. Microcol. Sep.*, 5 (1993) 11-22.
34. A. Dietrich, B. Maas, and A. Mosandl, "Diluted Modified Cyclodextrins as Chiral Stationary Phases – Influence of the Polysiloxane Solvent: Heptakis(2,3-di-*O*-acetyl-6-*O*-*tert*-butyldimethylsilyl)- $\beta$ -Cyclodextrin", *J. High Resolut. Chromatogr.*, 18 (1995) 152-156.
35. A. Dietrich, B. Maas, and A. Mosandl, "Diluted Modified Cyclodextrins as Chiral Capillary Gas Chromatographic Stationary Phases: Influence of the Polysiloxane Solvents on Enantioselectivity and Column Efficiency", *J. Microcol. Sep.*, 6 (1994) 33-42.
36. T. Beck, J. Nandzik, and A. Mosandl, "Diluted Modified Cyclodextrins as Chiral Stationary Phases in Capillary Gas Chromatography - Octakis(2,3-di-*O*-propionyl-6-*O*-*tert*-butyldimethylsilyl)- $\gamma$ -cyclodextrin," *J. Microcol. Sep.*, 12 (2000) 482-492.
37. M. Jung, D. Schmalzing, and V. Schurig, "Theoretical Approach to The Gas Chromatographic Separation of Enantiomers on Dissolved Cyclodextrin Derivatives", *J. Chromatogr.*, 552 (1991) 43-57.

38. V. Schurig and M. Juza, "Approach to the Thermodynamics of Enantiomer Separation by Gas Chromatography - Enantioselectivity Between The Chiral Inhalation Anesthetics Enflurane, Isoflurane and Desflurane and A Diluted  $\gamma$ -Cyclodextrin Derivative", *J. Chromatogr. A*, 757 (1997) 119-135.
39. I. Spanik, J. Krupcik, and V. Schurig, "Comparison of Two Methods for The Gas Chromatographic Determination of Thermodynamic Parameters of Enantioselectivity", *J. Chromatogr. A*, 843 (1999) 123-128.
40. K. Grob, Making and Manipulating Capillary Columns for Gas Chromatography, Heidelberg: Huthig, 1986.
41. K. Grob, Jr., G. Grob, and K. Grob, "Comprehensive, Standardized Quality Test for Glass Capillary Columns", *J. Chromatogr.*, 156 (1978) 1-20.
42. G. Grob, K. Grob, and K. Grob, Jr., "Testing Capillary Gas Chromatographic Columns", *J. Chromatogr.*, 219 (1981) 13-20.
43. T. Beier and H.-D. Holtje, "Modified Cyclodextrins as Chiral Selectors: Molecular Modelling Investigations on The Enantioselective Binding Properties of Heptakis(2,3-di-*O*-methyl-6-*O*-*tert*-butyldimethylsilyl)- $\beta$ -Cyclodextrin", *J. Chromatogr. B*, 708 (1998) 1-20.
44. J. A. Dean, *Handbook of Organic Chemistry*, McGraw-Hill, Inc, 1987, p.3-29.



## **APPENDICES**

คุณย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย

## Appendix A

### Glossary

**Adjusted retention time ( $t'_R$ )** is the absolute retention of a compound on a stationary phase. This value is calculated from subtracting retention time ( $t_R$ ) with the time of unretained compound ( $t_M$ ), according to the following equation.

$$t'_R = t_R - t_M$$

**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 ratio of the concentrations of a compound in a stationary phase and a mobile phase.  $K$  is related to retention factor by the following equation.

$$K = k' \cdot \frac{V_M}{V_S} = k' \cdot \beta$$

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

$$N = 16 \left( \frac{t_R}{W_b} \right)^2 = 5.545 \left( \frac{t_R}{W_h} \right)^2$$

where  $W_b$  and  $W_h$  are peak width at base and at half height, respectively.

**Phase ratio ( $\beta$ )** is defined as the ratio of the volume of the mobile phase to the stationary phase in a column or can be calculated from the following equation.

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

where  $r_c$  and  $d_f$  is the capillary column radius and stationary phase film thickness, respectively.

**Retention factor or capacity factor ( $k'$ )** is defined as mole of a compound in a stationary phase to that in mobile phase. It is equivalent to the ratio of the time that a compound spends in a stationary phase ( $t'_R$ ) to the time that it spends in a mobile phase ( $t_M$ ). The retention factor is calculated using the below equation.

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

**Separation factor or selectivity ( $\alpha$ )** is a measure of the quantity of peak separation. It is calculated from the ratio of the retention factors of the two adjacent peaks.

$$\alpha = \frac{k'_2}{k'_1}$$

**Trennzahl (TZ) or separation number** is another term used for a measure of separation efficiency of a column, which is calculated using the equation below. TZ can be explained as the numbers of peaks which can be placed close together between the two peaks of homologous series differing in one carbon. The higher the number, the more efficient the column.

$$TZ = \left( \frac{t_{R2} - t_{R1}}{W_{h1} + W_{h2}} \right) - 1$$

$t_{R1}, t_{R2}$  = the retention times of the first and second peaks, respectively.

$W_{h1}$  and  $W_{h2}$  = the peak width at half height of the first and second peaks, respectively.

จุฬาลงกรณ์มหาวิทยาลัย

## Appendix B

### NMR Spectra

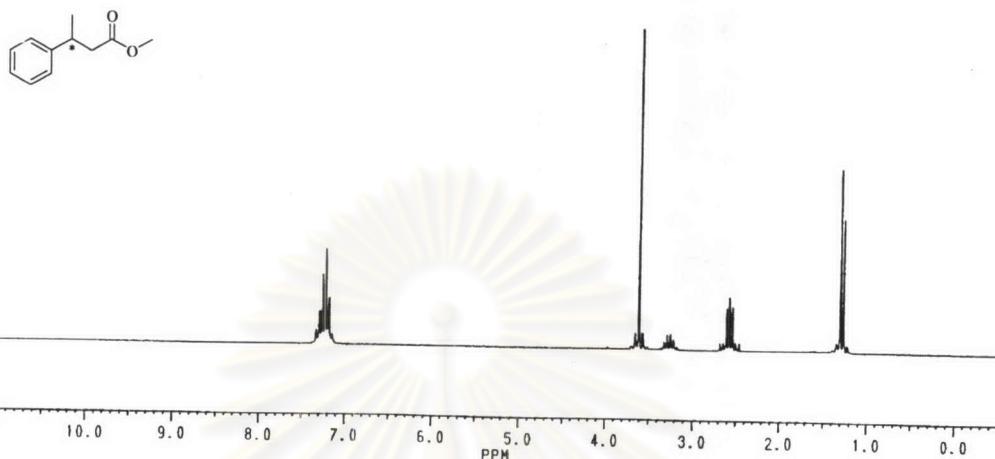


Figure B1 NMR spectrum of **P3-Me**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz):  $\delta$  1.29 (3H, d, CHCH<sub>3</sub>), 2.57 (2H, m, CHCH<sub>2</sub>), 3.25 (1H, m, CHPh), 3.61 (3H, s, OCH<sub>3</sub>), 7.22 (5H, m, ArH)

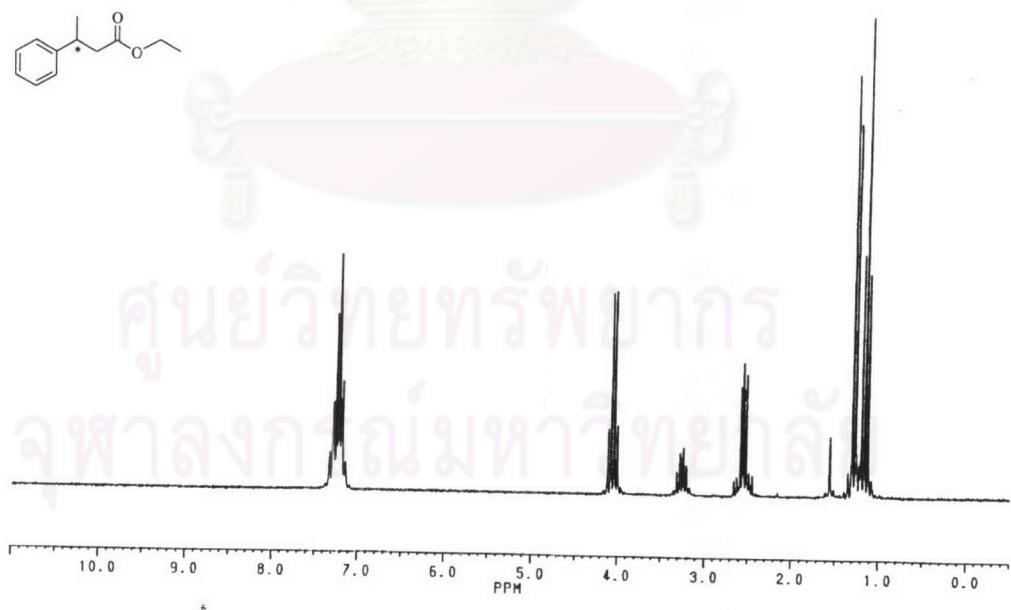


Figure B2 NMR spectrum of **P3-Et**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz):  $\delta$  1.16 (3H, t, CH<sub>2</sub>CH<sub>3</sub>), 1.29 (3H, d, CHCH<sub>3</sub>), 2.56 (2H, m, CHCH<sub>2</sub>), 3.24 (1H, m, CHCH<sub>3</sub>), 4.06 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 7.24 (5H, m, ArH)

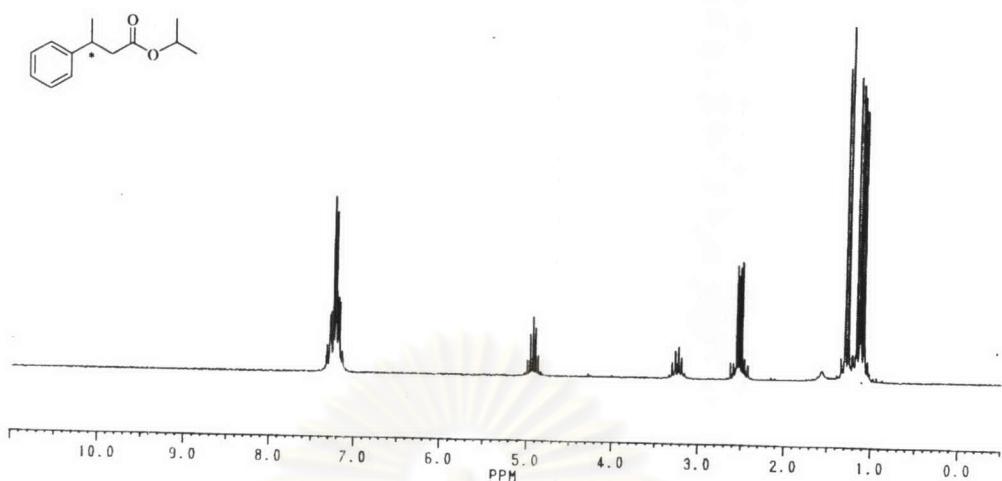


Figure B3 NMR spectrum of P3-iPr; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz): δ 1.08 (3H, d, OCHCH<sub>3</sub>), 1.15 (3H, d, OCHCH<sub>3</sub>), 2.52 (2H, m, CHCH<sub>2</sub>), 3.23 (1H, m, CHCH<sub>3</sub>), 4.93 (1H, m, OCH), 7.22 (5H, m, ArH)

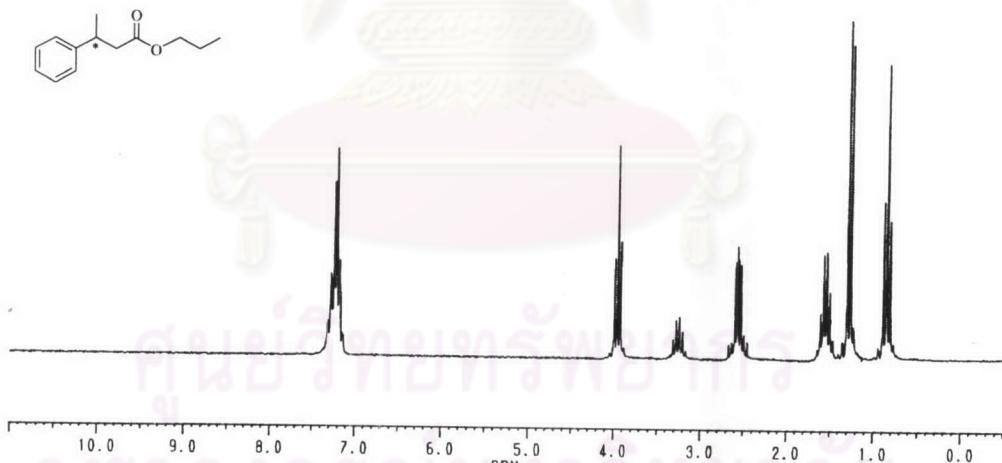


Figure B4 NMR spectrum of P3-nPr; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz): δ 0.85 (3H, t, CH<sub>2</sub>CH<sub>3</sub>), 1.28 (3H, d, CHCH<sub>3</sub>), 1.54 (2H, m, CH<sub>2</sub>CH<sub>3</sub>), 2.56 (2H, m, CHCH<sub>2</sub>), 3.26 (1H, m, CHCH<sub>3</sub>), 3.96 (2H, t, OCH<sub>2</sub>), 7.23 (5H, m, ArH)

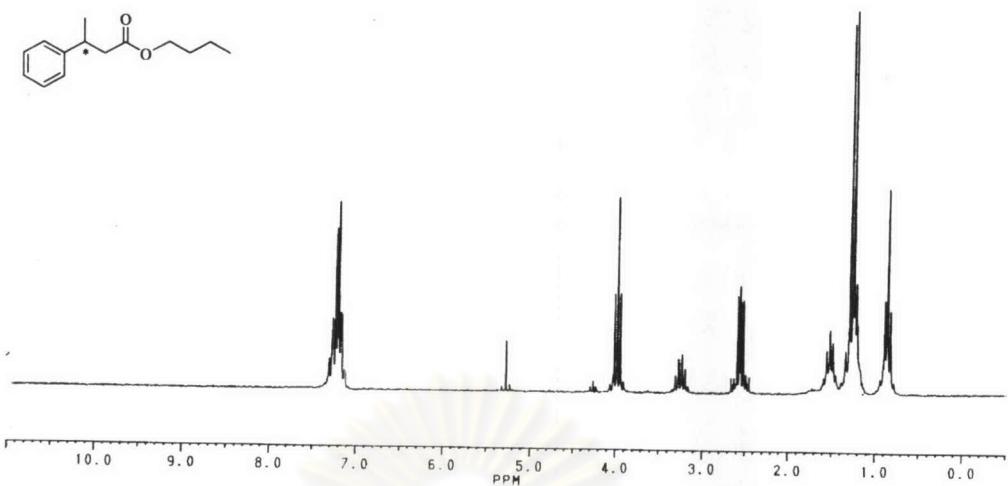


Figure B5 NMR spectrum of **P3-nBu**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz): δ 0.87 (3H, t, CH<sub>2</sub>CH<sub>3</sub>), 1.27 (5H, m, CH<sub>2</sub>CH<sub>3</sub>, CHCH<sub>3</sub>), 1.49 (2H, m, CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>), 2.53 (2H, m, CHCH<sub>2</sub>), 3.24 (1H, m, CHCH<sub>3</sub>), 3.99 (2H, t, OCH<sub>2</sub>), 7.25 (5H, m, ArH)

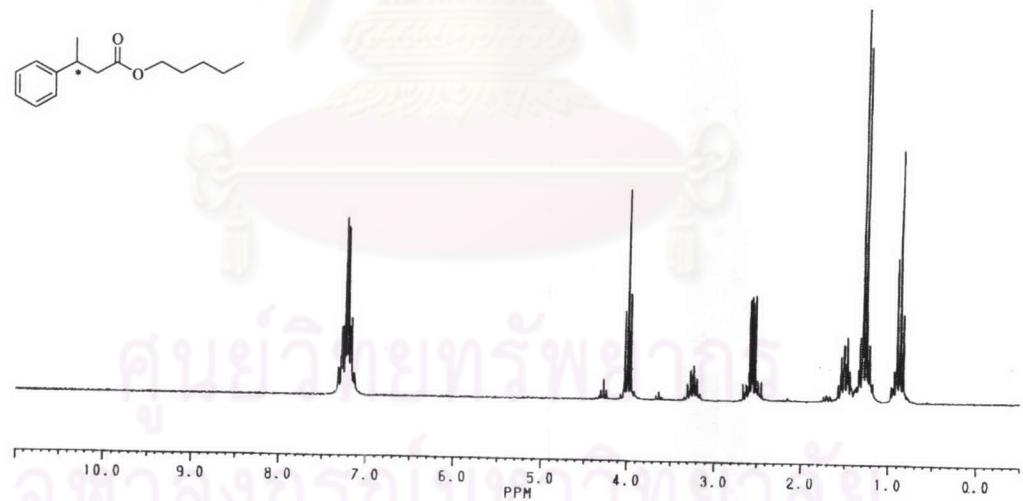


Figure B6 NMR spectrum of **P3-nPen**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz): δ 0.83-1.55 (12H, m, (CH<sub>2</sub>)CH<sub>3</sub>, CHCH<sub>3</sub>), 2.56 (2H, m, CHCH<sub>2</sub>), 3.24 (1H, m, CHCH<sub>3</sub>), 4.00 (2H, t, OCH<sub>2</sub>), 7.22 (5H, m, ArH)

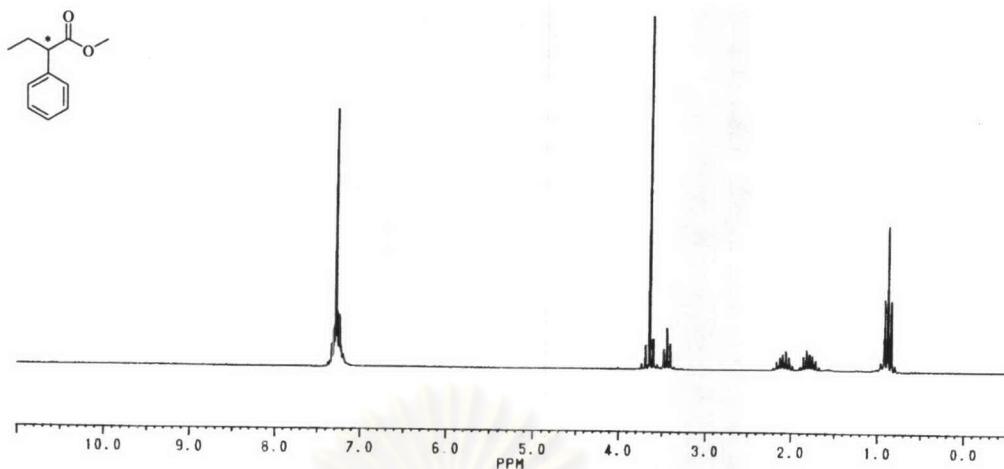


Figure B7 NMR spectrum of **P4-Me**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  0.87 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 1.92 (2H, m,  $\text{CH}_2\text{CH}_3$ ), 3.44 (1H, t, CHPh), 3.64 (3H, s, OCH<sub>3</sub>), 7.28 (5H, m, ArH)

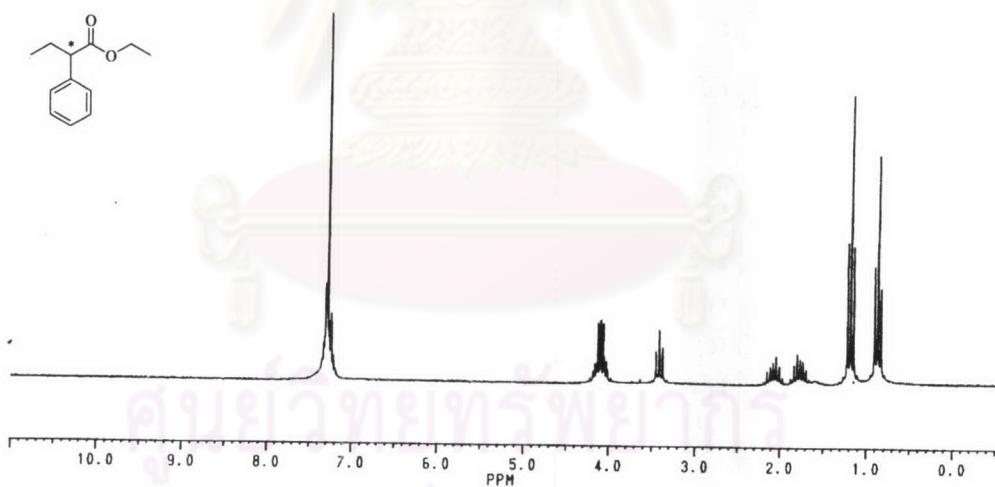


Figure B8 NMR spectrum of **P4-Et**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  0.88 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 1.21 (3H, t, OCH<sub>2</sub>CH<sub>3</sub>) 1.93 (2H, m,  $\text{CH}_2\text{CH}_3$ ), 3.42 (1H, t, CHPh), 4.10 (2H, m, OCH<sub>2</sub>CH<sub>3</sub>), 7.27 (5H, m, ArH)

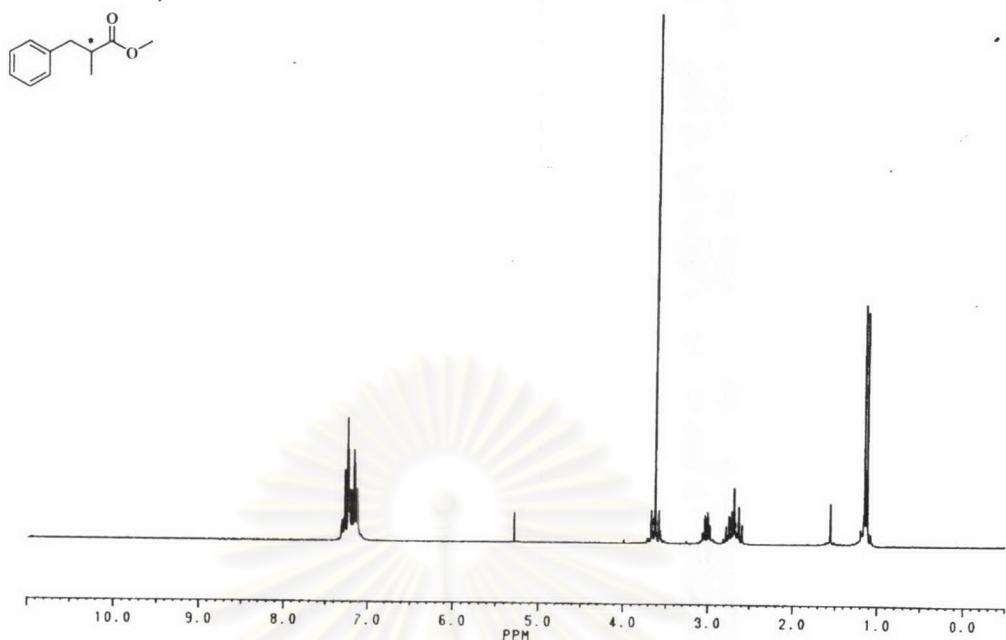


Figure B9 NMR spectrum of **M6-Me**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.13 (3H, d,  $\text{CHCH}_3$ ), 2.70 (2H, m,  $\text{CH}_2\text{Ph}$ ), 3.01 (1H, m,  $\text{CHCH}_3$ ), 3.62 (3H, s,  $\text{OCH}_3$ ), 7.22 (5H, m,  $\text{ArH}$ )

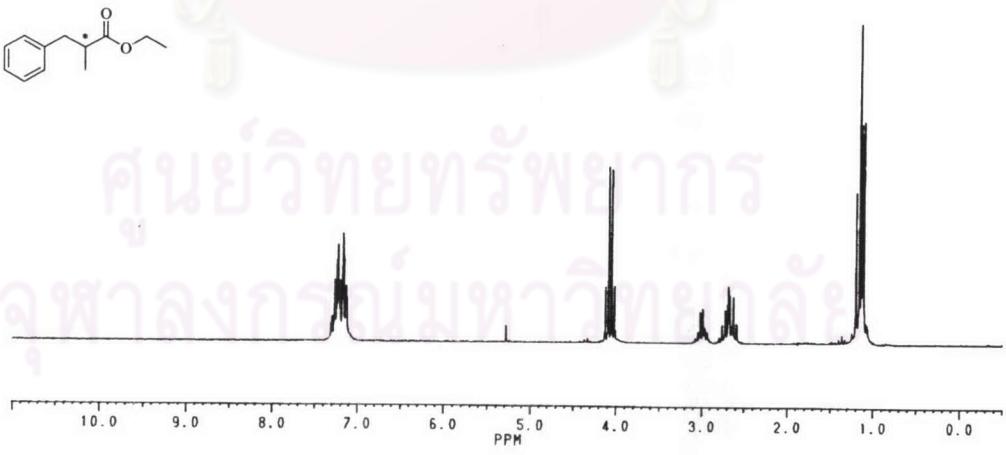


Figure B10 NMR spectrum of **M6-Et**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.15 (3H, d,  $\text{CHCH}_3$ ), 1.17 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 2.69 (2H, m,  $\text{CH}_2\text{Ph}$ ), 2.99 (1H, m,  $\text{CHCH}_3$ ), 4.07 (2H, q,  $\text{CH}_2\text{CH}_3$ ), 7.22 (5H, m,  $\text{ArH}$ )

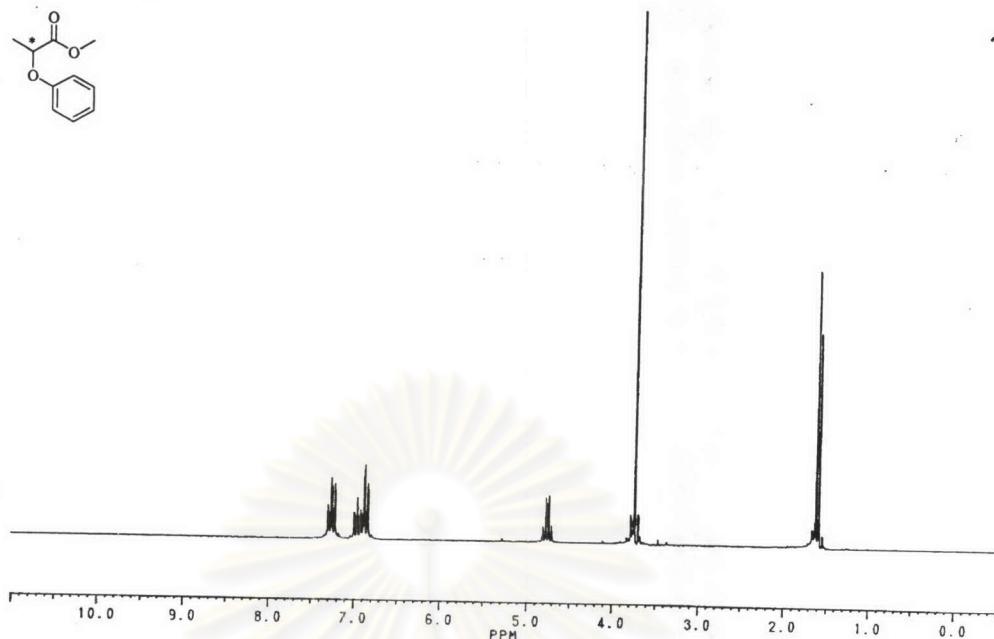


Figure B11 NMR spectrum of **P2-Me**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.61 (3H, d,  $\text{CHCH}_3$ ), 3.74 (3H, s,  $\text{OCH}_3$ ), 4.76 (1H, q,  $\text{CHCH}_3$ ), 7.07 (5H, m, ArH)

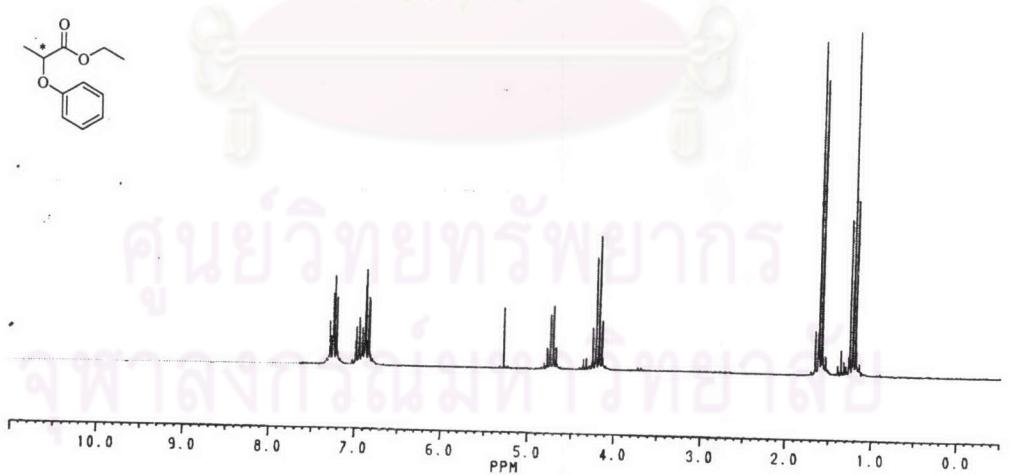


Figure B12 NMR spectrum of **P2-Et**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.28 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 1.54 (3H, d,  $\text{CHCH}_3$ ), 4.20 (2H, q,  $\text{CH}_2\text{CH}_3$ ), 4.73 (1H, q,  $\text{CHCH}_3$ ), 7.07 (5H, m, ArH)

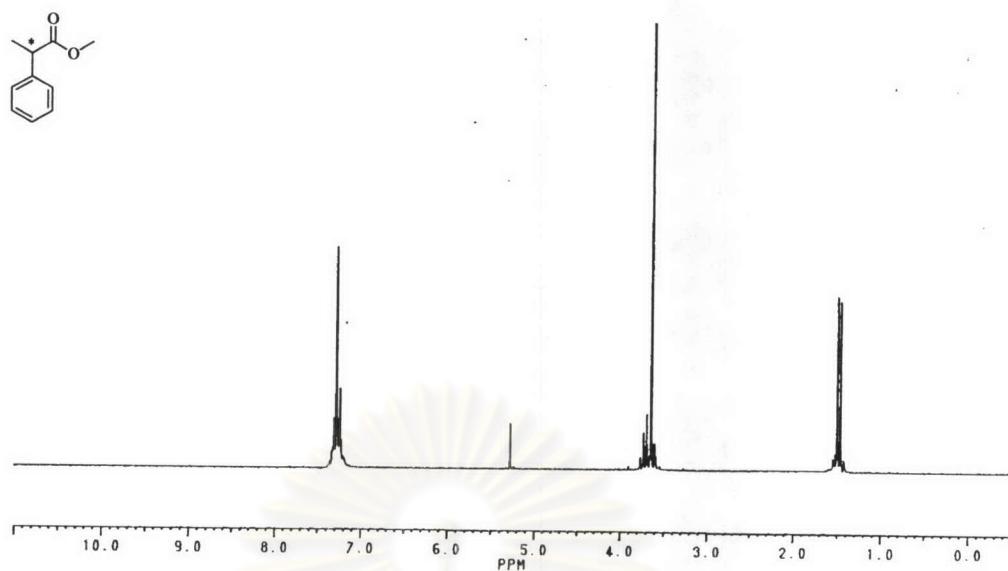


Figure B13 NMR spectrum of **P13-Me**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.49 (3H, d,  $\text{CHCH}_3$ ), 3.66 (3H, s,  $\text{OCH}_3$ ), 7.28 (5H, m,  $\text{ArH}$ )

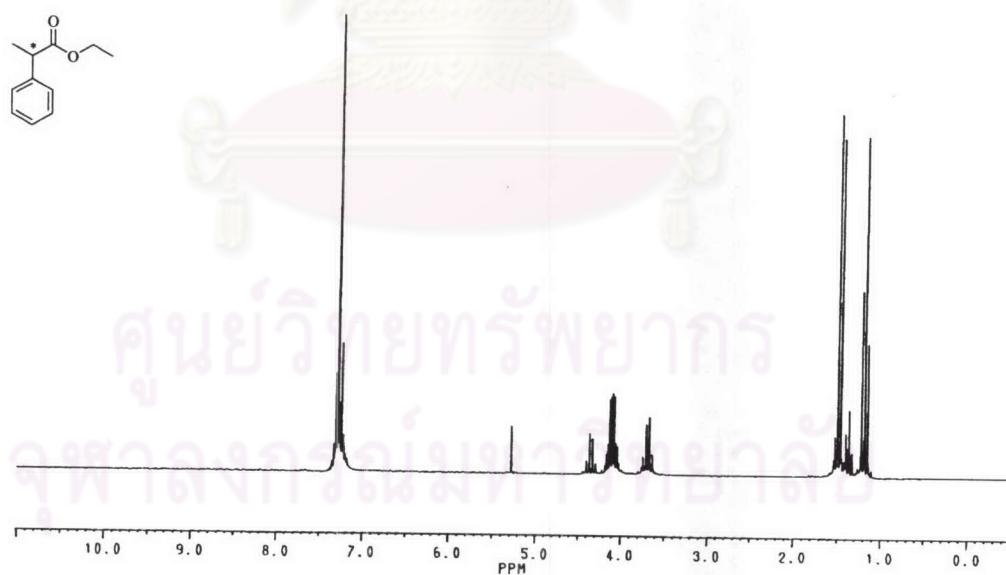


Figure B14 NMR spectrum of **P13-Et**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.19 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 1.48 (3H, d,  $\text{CHCH}_3$ ), 3.69 (1H, q,  $\text{CHCH}_3$ ), 4.09 (2H, m,  $\text{CH}_2\text{CH}_3$ ), 7.29 (5H, m,  $\text{ArH}$ )

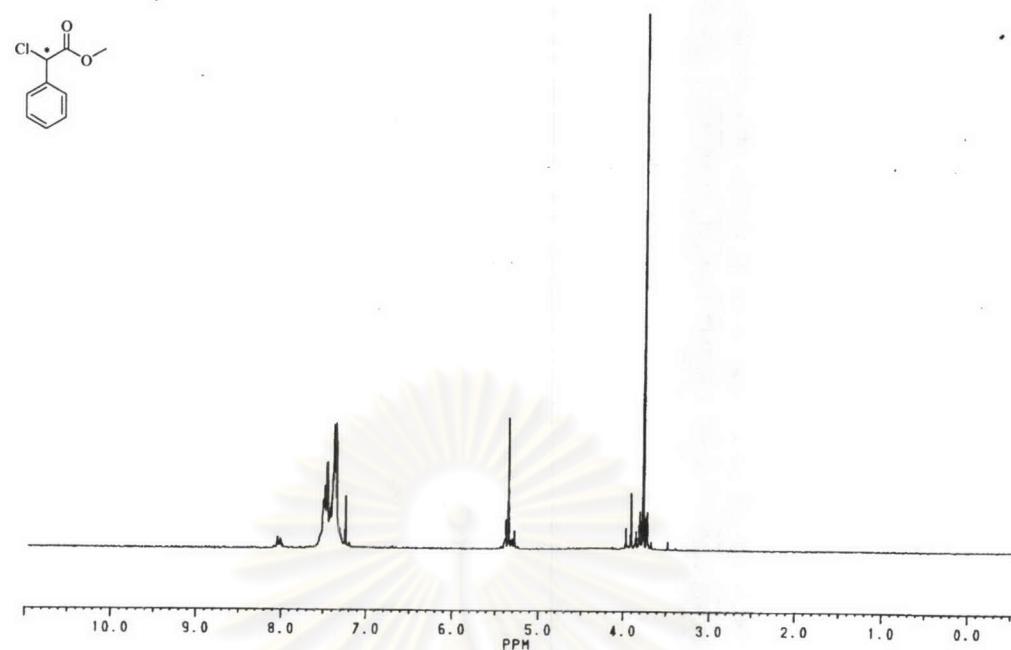


Figure B15 NMR spectrum of **C8-Me**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz):  $\delta$  3.76 (3H, s, OCH<sub>3</sub>), 5.35 (1H, s, CHPh), 7.39 (5H, m, ArH)

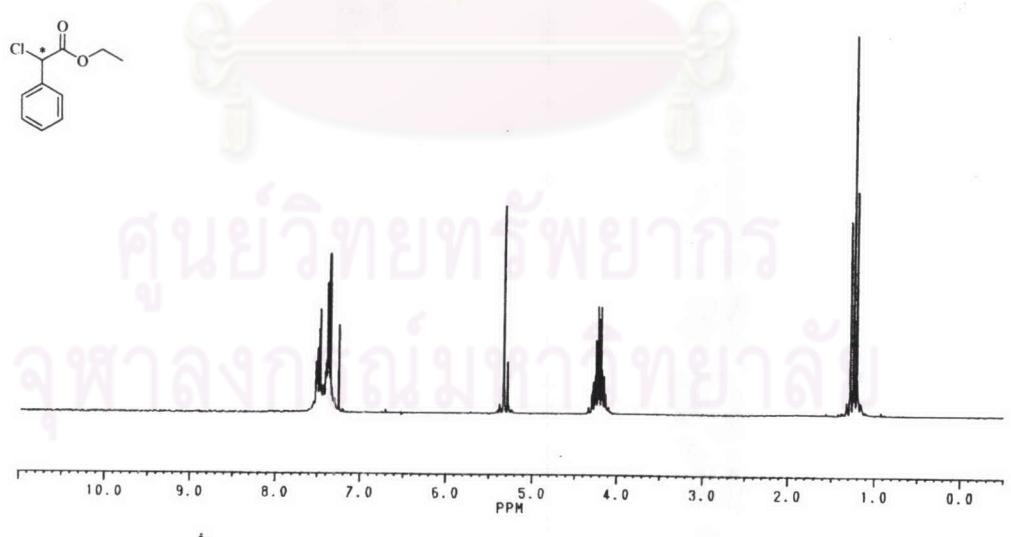


Figure B16 NMR spectrum of **C8-Et**; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 200MHz):  $\delta$  1.24 (3H, t, CH<sub>2</sub>CH<sub>3</sub>), 4.21 (2H, m, CH<sub>2</sub>CH<sub>3</sub>), 5.34 (1H, s, CHPh), 7.40 (5H, m, ArH)

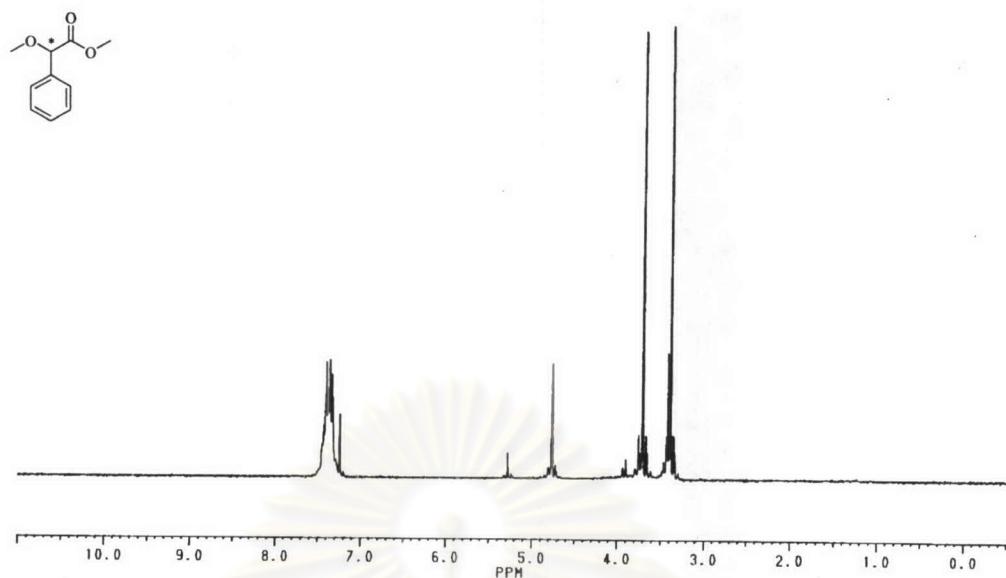


Figure B17 NMR spectrum of **M20-Me**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  3.39 (3H, s,  $\text{CHOCH}_3$ ), 3.71 (3H, s,  $\text{OCH}_3$ ), 4.76 (1H, s,  $\text{CHPh}$ ), 7.37 (5H, m,  $\text{ArH}$ )

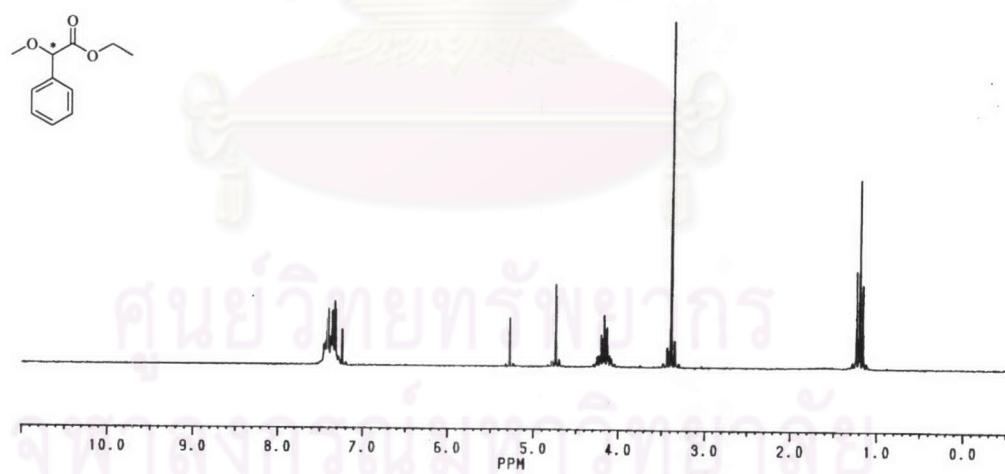


Figure B18 NMR spectrum of **M20-Et**;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200MHz):  $\delta$  1.20 (3H, t,  $\text{CH}_2\text{CH}_3$ ), 3.39 (3H, s,  $\text{CHOCH}_3$ ), 4.17 (2H, m,  $\text{CH}_2\text{CH}_3$ ), 4.74 (1H, s,  $\text{CHPh}$ ), 7.38 (5H, m,  $\text{ArH}$ )

## Appendix C

### Thermodynamic Studies

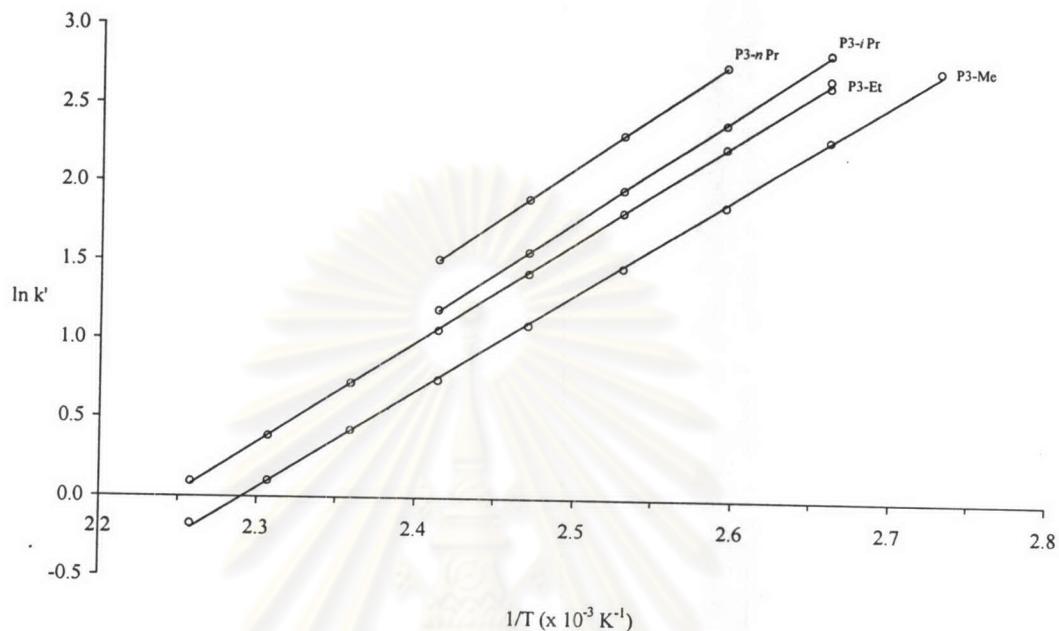


Figure C1 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 1) on OV-1701 column

Table C1 Equation and correlation coefficient for the relationship in figure C1

compound	equation	$R^2$
P3-Me	$\ln k' = 6.1547(1/T) - 13.790$	0.9997
P3-Et	$\ln k' = 6.3710 (1/T) - 13.988$	0.9998
P3-iPr	$\ln k' = 6.6635 (1/T) - 14.568$	0.9999
P3-nPr	$\ln k' = 6.8565 (1/T) - 14.700$	1.0000

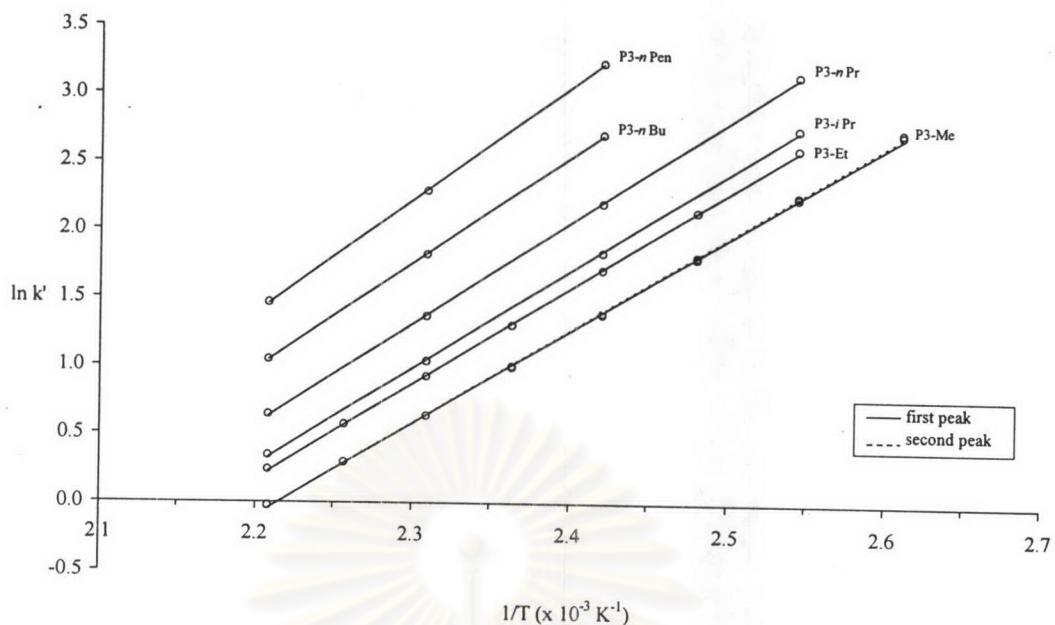


Figure C2 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 1) on BSiMe column

Table C2 Equation and correlation coefficient for the relationship in figure C2

compound	equation	$R^2$	equation	$R^2$
<b>P3-Me</b>	$\ln k'_1 = 6.7889 (1/T) - 15.035$	0.9997	$\ln k'_2 = 6.8381 (1/T) - 15.145$	0.9997
<b>P3-Et</b>	$\ln k'_1 = 7.0067 (1/T) - 15.245$	0.9998	—	—
<b>P3-iPr</b>	$\ln k'_1 = 7.1437 (1/T) - 15.445$	0.9998	—	—
<b>P3-nPr</b>	$\ln k'_1 = 7.4190 (1/T) - 15.752$	0.9998	—	—
<b>P3-nBu</b>	$\ln k'_1 = 7.7691 (1/T) - 16.110$	0.9999	—	—
<b>P3-nPen</b>	$\ln k'_1 = 8.2802 (1/T) - 16.823$	0.9999	—	—

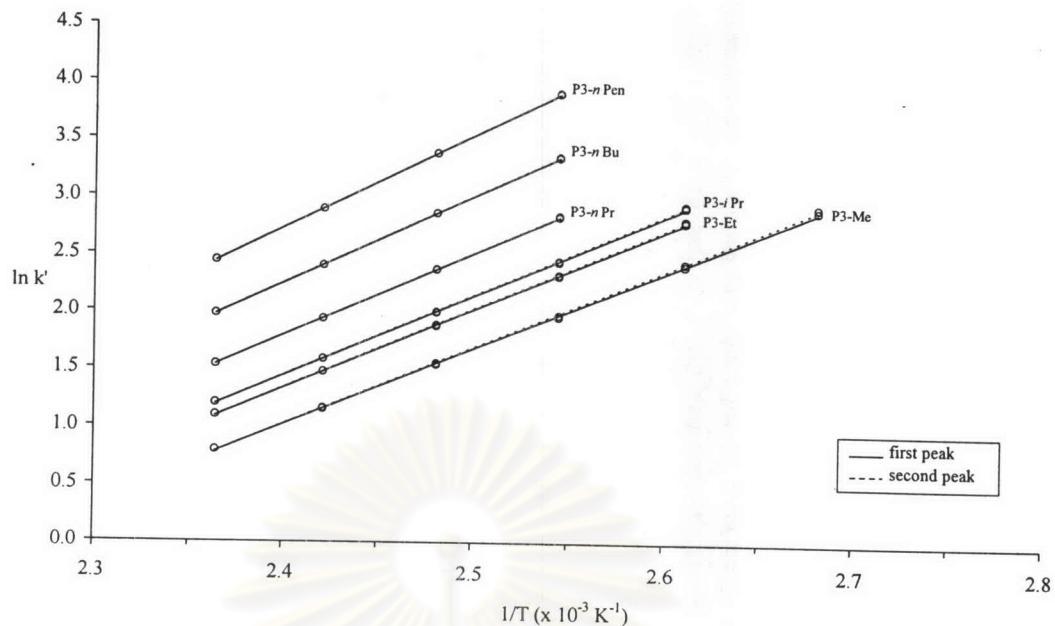


Figure C3 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 1) on BSiAc column

Table C3 Equation and correlation coefficient for the relationship in figure C3

compound	equation	$R^2$	equation	$R^2$
P3-Me	$\ln k'_1 = 6.5946 (1/T) - 14.811$	0.9997	$\ln k'_2 = 6.6888 (1/T) - 15.034$	0.9997
P3-Et	$\ln k'_1 = 6.8104 (1/T) - 15.012$	0.9998	$\ln k'_2 = 6.8870 (1/T) - 15.195$	0.9998
P3-iPr	$\ln k'_1 = 6.9120 (1/T) - 15.146$	0.9998	$\ln k'_2 = 6.9814 (1/T) - 15.312$	0.9998
P3-nPr	$\ln k'_1 = 7.1175 (1/T) - 15.290$	1.0000	$\ln k'_2 = 7.1696 (1/T) - 15.415$	0.9999
P3-nBu	$\ln k'_1 = 7.5203 (1/T) - 15.800$	1.0000	$\ln k'_2 = 7.5648 (1/T) - 15.907$	0.9999
P3-nPen	$\ln k'_1 = 7.9834 (1/T) - 16.431$	1.0000	$\ln k'_2 = 8.0128 (1/T) - 16.502$	0.9999

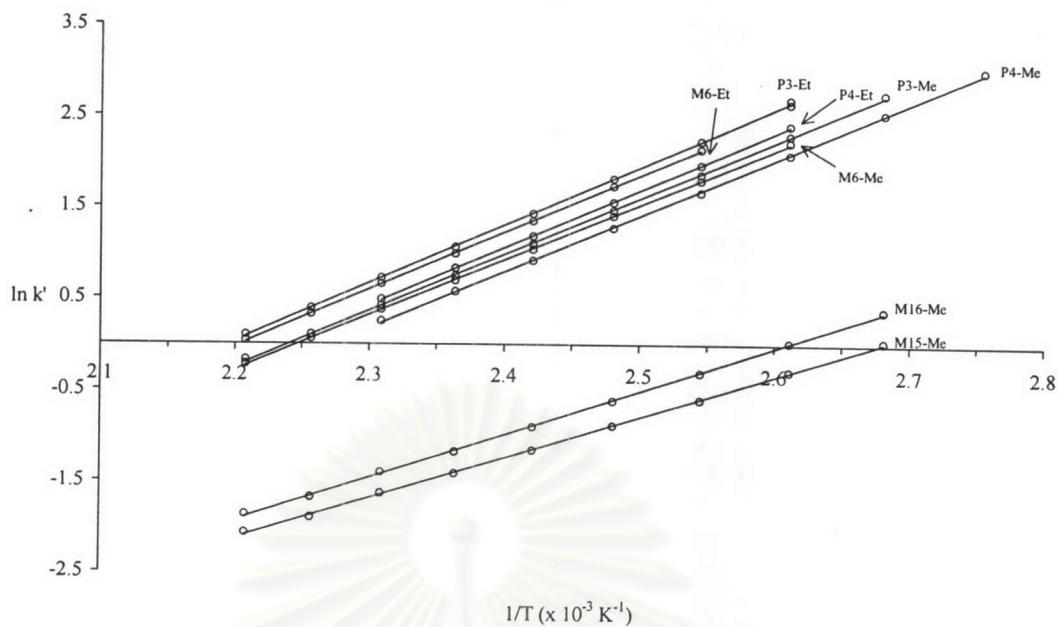


Figure C4 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 2) on OV-1701 column

Table C4 Equation and correlation coefficient for the relationship in figure C4

compound	equation	$R^2$
<b>P4-Me</b>	$\ln k' = 6.1587 (1/T) - 13.992$	0.9997
<b>P4-Et</b>	$\ln k' = 6.3093 (1/T) - 14.089$	0.9999
<b>P3-Me</b>	$\ln k' = 6.1547 (1/T) - 13.790$	0.9997
<b>P3-Et</b>	$\ln k' = 6.3710 (1/T) - 13.988$	0.9998
<b>M6-Me</b>	$\ln k' = 6.0296 (1/T) - 13.550$	0.9998
<b>M6-Et</b>	$\ln k' = 6.2542 (1/T) - 13.787$	0.9999
<b>M15-Me</b>	$\ln k' = 4.4650 (1/T) - 11.950$	0.9995
<b>M16-Me</b>	$\ln k' = 4.7408 (1/T) - 12.360$	0.9995

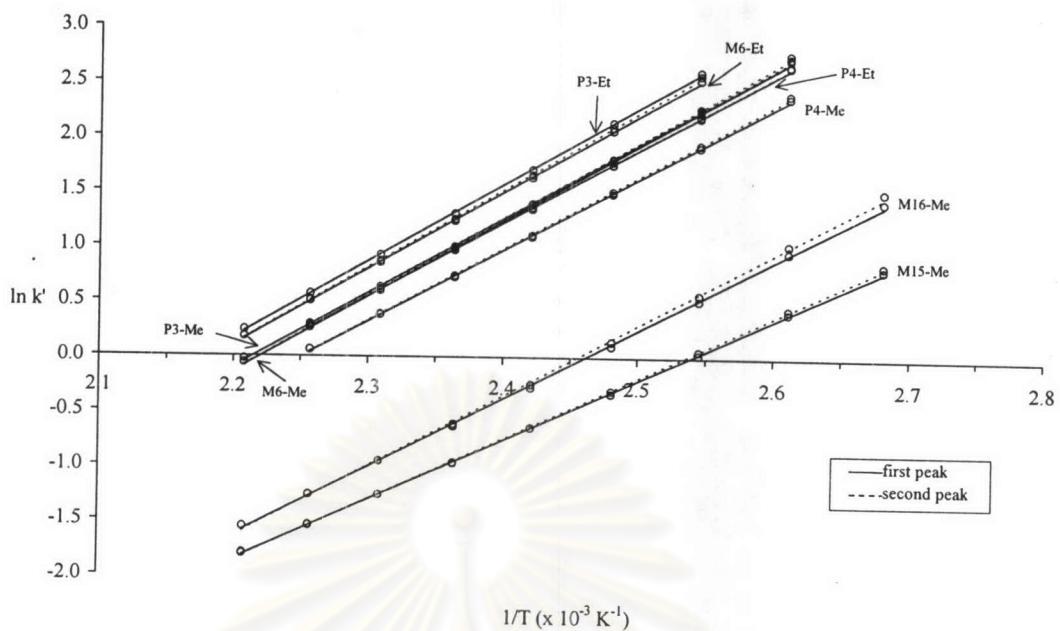


Figure C5 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 2) on BSiMe column

Table C5 Equation and correlation coefficient for the relationship in figure C5

compound	equation	$R^2$	equation	$R^2$
<b>P4-Me</b>	$\ln k'_1 = 6.5063 (1/T) - 14.643$	0.9996	$\ln k'_2 = 6.5854 (1/T) - 14.820$	0.9997
<b>P4-Et</b>	$\ln k'_1 = 6.6832 (1/T) - 14.821$	0.9997	$\ln k'_2 = 6.7248 (1/T) - 14.917$	0.9997
<b>P3-Me</b>	$\ln k'_1 = 6.7889 (1/T) - 15.035$	0.9997	$\ln k'_2 = 6.8381 (1/T) - 15.145$	0.9997
<b>P3-Et</b>	$\ln k'_1 = 7.0067 (1/T) - 15.245$	0.9998	$\ln k'_2 = 7.0067 (1/T) - 15.245$	0.9998
<b>M6-Me</b>	$\ln k'_1 = 6.8766 (1/T) - 15.268$	0.9996	$\ln k'_2 = 6.9878 (1/T) - 15.514$	0.9996
<b>M6-Et</b>	$\ln k'_1 = 6.9739 (1/T) - 15.238$	0.9997	$\ln k'_2 = 7.0832 (1/T) - 15.478$	0.9997
<b>M15-Me</b>	$\ln k'_1 = 5.5077 (1/T) - 13.975$	0.9998	$\ln k'_2 = 5.6009 (1/T) - 14.188$	0.9998
<b>M16-Me</b>	$\ln k'_1 = 6.2867 (1/T) - 15.468$	0.9994	$\ln k'_2 = 6.4836 (1/T) - 15.913$	0.9993

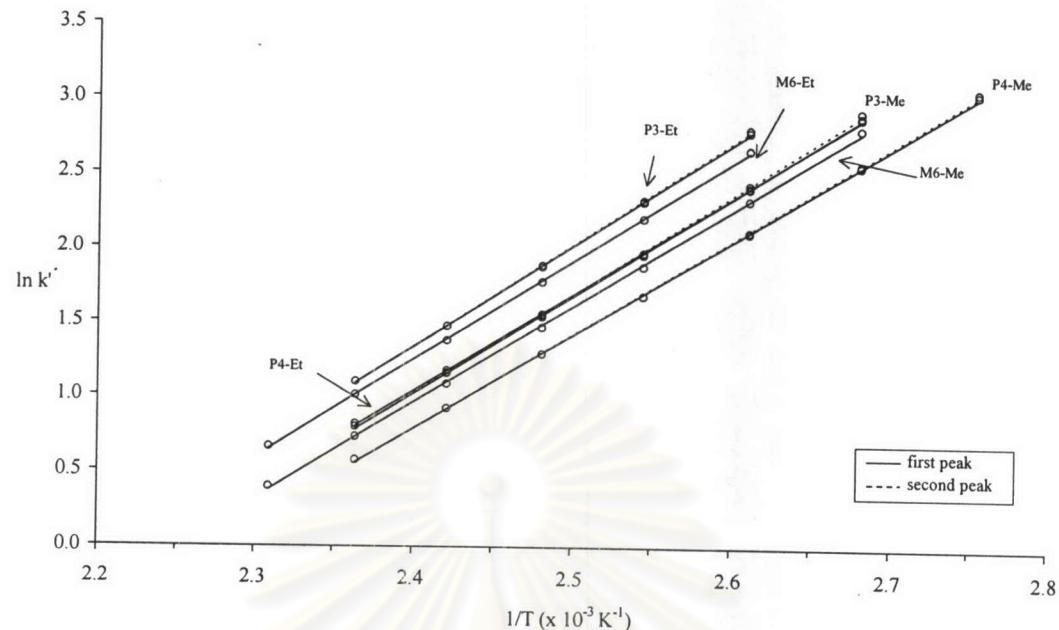


Figure C6 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of 1 esters (series 2) on BSiAc column

Table C6 Equation and correlation coefficient for the relationship in figure C6

compound	equation	$R^2$	equation	$R^2$
<b>P4-Me</b>	$\ln k'_1 = 6.3003 (1/T) - 14.330$	0.9998	$\ln k'_2 = 6.3543 (1/T) - 14.46$	0.9997
<b>P4-Et</b>	$\ln k'_1 = 6.5084 (1/T) - 14.582$	0.9998	$\ln k'_2 = 6.5084 (1/T) - 14.582$	0.9998
<b>P3-Me</b>	$\ln k'_1 = 6.5946 (1/T) - 14.811$	0.9997	$\ln k'_2 = 6.6888 (1/T) - 15.034$	0.9997
<b>P3-Et</b>	$\ln k'_1 = 6.8104 (1/T) - 15.012$	0.9998	$\ln k'_2 = 6.8870 (1/T) - 15.195$	0.9998
<b>M6-Me</b>	$\ln k'_1 = 6.4672 (1/T) - 14.561$	0.9996	$\ln k'_2 = 6.4672 (1/T) - 14.561$	0.9996
<b>M6-Et</b>	$\ln k'_1 = 6.6187 (1/T) - 14.636$	0.9997	$\ln k'_2 = 6.6187 (1/T) - 14.636$	0.9997

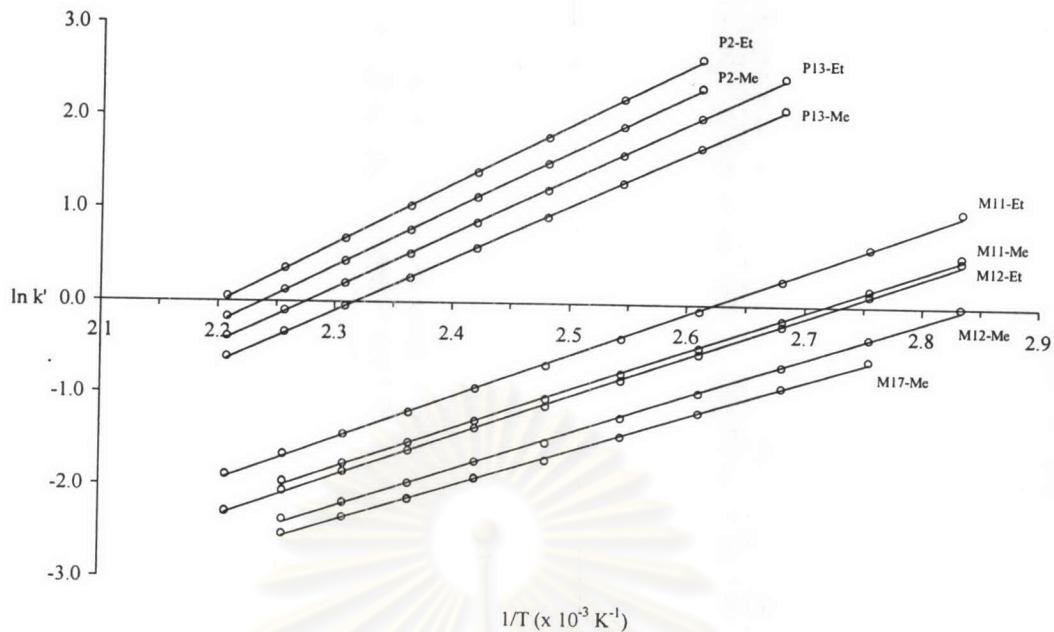


Figure C7 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 3) on OV-1701 column

Table C7 Equation and correlation coefficient for the relationship in figure C7

compound	equation	$R^2$
<b>M11-Me</b>	$\ln k' = 4.3501 (1/T) - 11.814$	0.9994
<b>M11-Et</b>	$\ln k' = 4.6302 (1/T) - 12.139$	0.9994
<b>M12-Me</b>	$\ln k' = 4.1103 (1/T) - 11.684$	0.9992
<b>M12-Et</b>	$\ln k' = 4.4076 (1/T) - 12.034$	0.9995
<b>M17-Me</b>	$\ln k' = 3.8798 (1/T) - 11.309$	0.9993
<b>P2-Me</b>	$\ln k' = 6.2384 (1/T) - 13.960$	0.9998
<b>P2-Et</b>	$\ln k' = 6.4661 (1/T) - 14.241$	0.9998
<b>P13-Me</b>	$\ln k' = 5.7490 (1/T) - 13.318$	0.9997
<b>P13-Et</b>	$\ln k' = 6.0054 (1/T) - 13.664$	0.9997

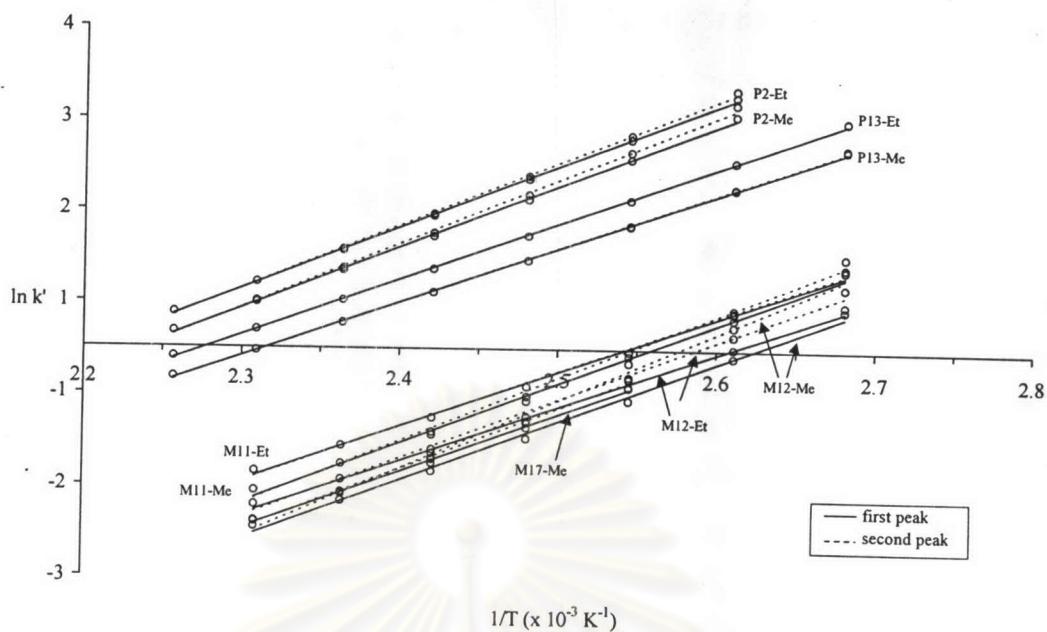


Figure C9 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 3) on BSiAc column

Table C9 Equation and correlation coefficient for the relationship in figure C9

compound	equation	$R^2$	equation	$R^2$
<b>M11-Me</b>	$\ln k'_1 = 6.5448 (1/T) - 16.740$	0.9953	$\ln k'_2 = 6.9412 (1/T) - 17.669$	0.9949
<b>M11-Et</b>	$\ln k'_1 = 5.9828 (1/T) - 15.208$	0.9974	$\ln k'_2 = 6.0541 (1/T) - 15.379$	0.9966
<b>M12-Me</b>	$\ln k'_1 = 6.4386 (1/T) - 16.887$	0.9958	$\ln k'_2 = 7.4640 (1/T) - 19.222$	0.9944
<b>M12-Et</b>	$\ln k'_1 = 5.9188 (1/T) - 15.432$	0.9964	$\ln k'_2 = 6.4549 (1/T) - 16.688$	0.9955
<b>M17-Me</b>	$\ln k'_1 = 6.2685 (1/T) - 16.388$	0.9975	$\ln k'_2 = 6.6647 (1/T) - 17.308$	0.9979
<b>P2-Me</b>	$\ln k'_1 = 6.7714 (1/T) - 15.138$	0.9991	$\ln k'_2 = 7.1006 (1/T) - 15.891$	0.9984
<b>P2-Et</b>	$\ln k'_1 = 6.7794 (1/T) - 14.940$	0.9995	$\ln k'_2 = 6.9812 (1/T) - 15.404$	0.9992
<b>P13-Me</b>	$\ln k'_1 = 5.9592 (1/T) - 13.796$	0.9996	$\ln k'_2 = 6.0022 (1/T) - 13.897$	0.9995
<b>P13-Et</b>	$\ln k'_1 = 6.1816 (1/T) - 14.078$	0.9997	$\ln k'_2 = 6.1932 (1/T) - 14.106$	0.9996

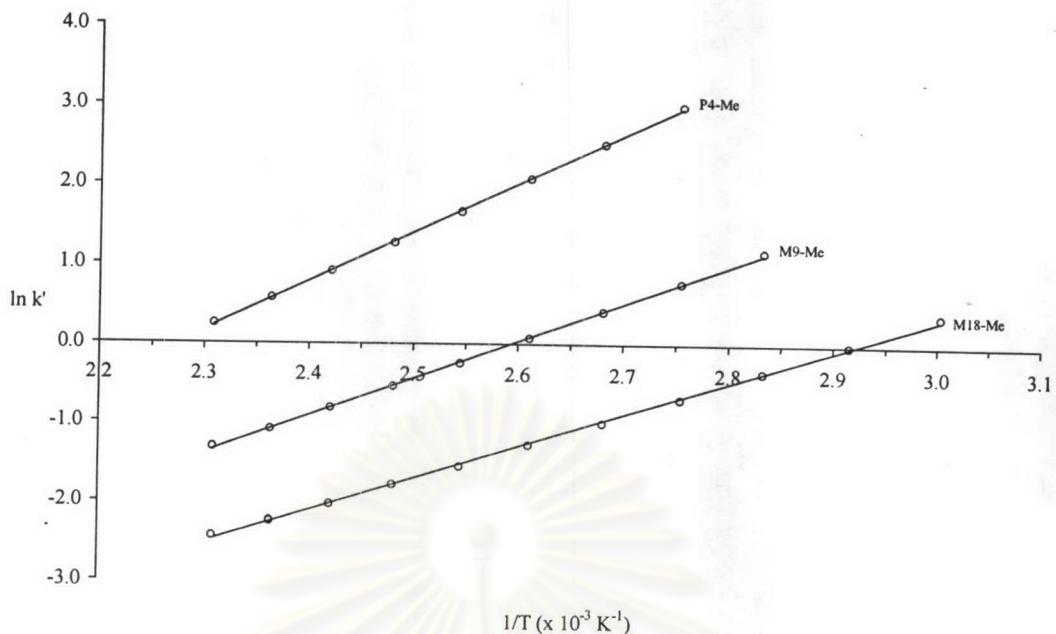


Figure C10 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 4) on OV-1701 column

Table C10 Equation and correlation coefficient for the relationship in figure C10

compound	equation	$R^2$
<b>M9-Me</b>	$\ln k' = 4.7483 (1/T) - 12.312$	0.9996
<b>P4-Me</b>	$\ln k' = 6.1587 (1/T) - 13.992$	0.9997
<b>M18-Me</b>	$\ln k' = 4.0553 (1/T) - 11.845$	0.9992

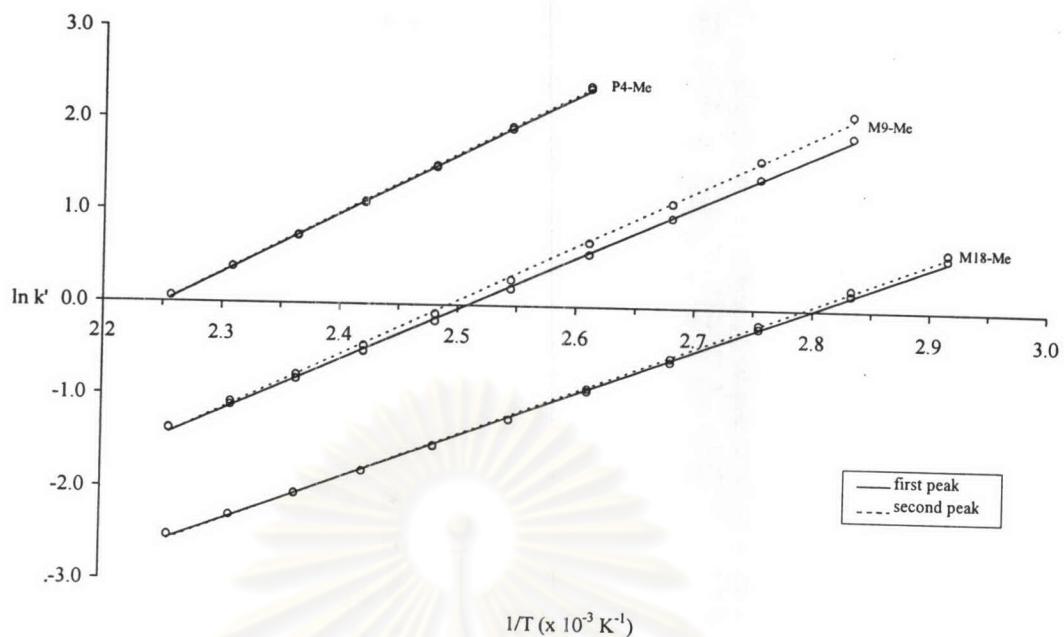


Figure C11 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 4) on BSiMe column

Table C11 Equation and correlation coefficient for the relationship in figure C11

compound	equation	$R^2$	equation	$R^2$
<b>M9-Me</b>	$\ln k'_1 = 5.6550 (1/T) - 14.181$	0.9994	$\ln k'_2 = 6.0432 (1/T) - 15.058$	0.9992
<b>P4-Me</b>	$\ln k'_1 = 6.5063 (1/T) - 14.643$	0.9996	$\ln k'_2 = 6.5854 (1/T) - 14.820$	0.9997
<b>M18-Me</b>	$\ln k'_1 = 4.7116 (1/T) - 13.194$	0.9995	$\ln k'_2 = 4.8201 (1/T) - 13.451$	0.9991

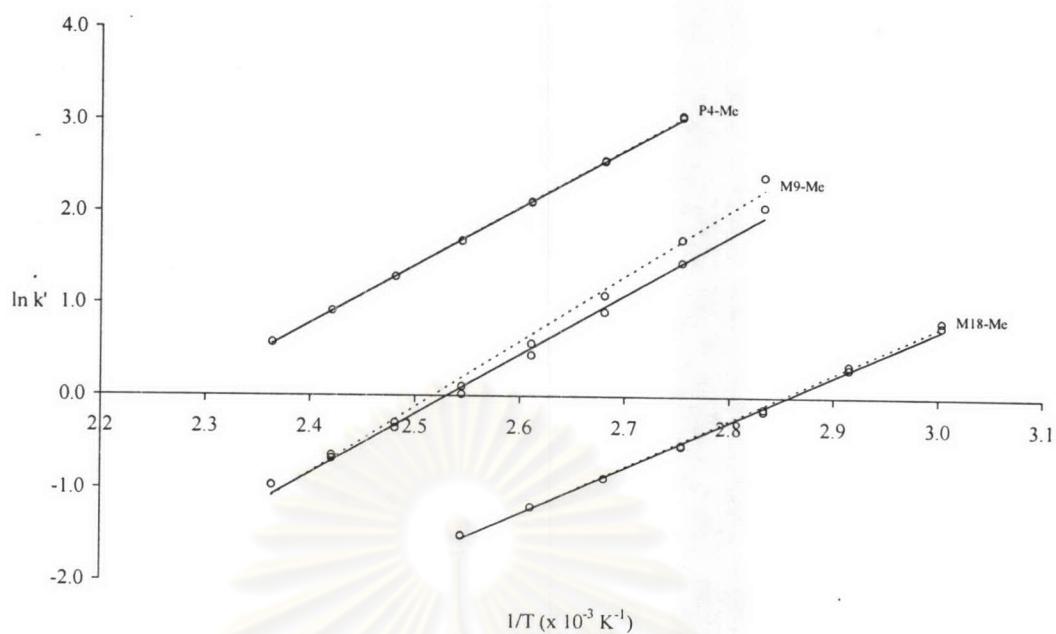


Figure C12 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 4) on BSiAc column

Table C12 Equation and correlation coefficient for the relationship in figure C12

compound	equation	$R^2$	equation	$R^2$
<b>M9-Me</b>	$\ln k'_1 = 6.4294 (1/T) - 16.266$	0.9995	$\ln k'_2 = 7.1128 (1/T) - 17.901$	0.9935
<b>P4-Me</b>	$\ln k'_1 = 6.3003 (1/T) - 14.336$	0.9998	$\ln k'_2 = 6.3543 (1/T) - 14.468$	0.9997
<b>M18-Me</b>	$\ln k'_1 = 4.9599 (1/T) - 14.160$	0.9984	$\ln k'_2 = 5.0759 (1/T) - 14.463$	0.9982

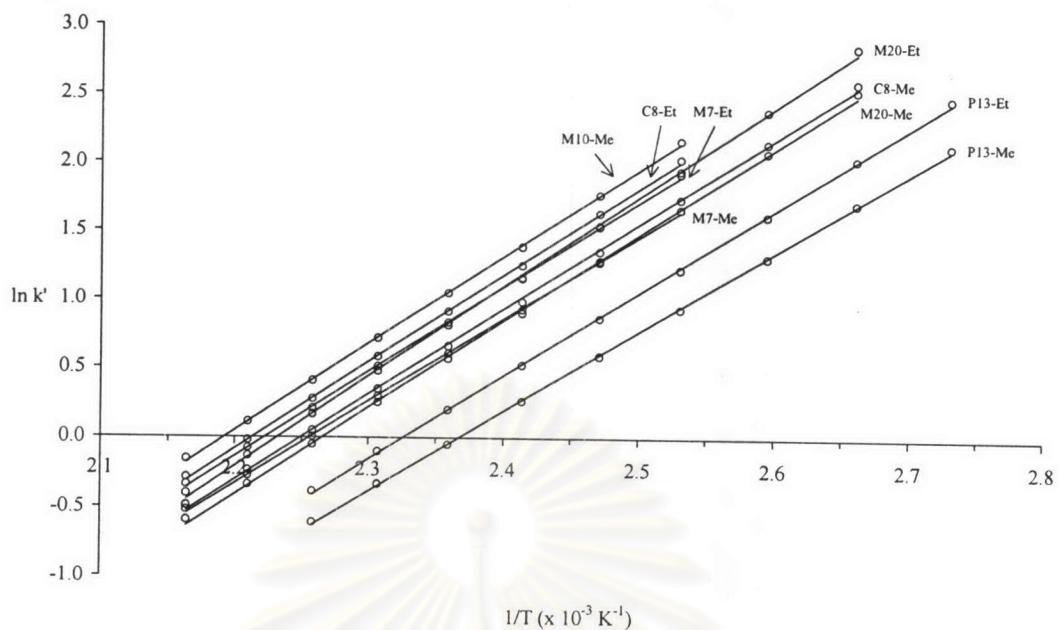


Figure C13 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 5) on oV-1701 column

Table C13 Equation and correlation coefficient for the relationship in figure C13

compound	equation	$R^2$
<b>P13-Me</b>	$\ln k' = 5.7490 (1/T) - 13.318$	0.9997
<b>P13-Et</b>	$\ln k' = 6.0054 (1/T) - 13.664$	0.9997
<b>M10-Me</b>	$\ln k' = 6.3174 (1/T) - 13.534$	0.9997
<b>C8-Me</b>	$\ln k' = 6.1756 (1/T) - 13.583$	0.9995
<b>C8-Et</b>	$\ln k' = 6.3017 (1/T) - 13.631$	0.9997
<b>M20-Me</b>	$\ln k' = 6.2706 (1/T) - 13.891$	0.9994
<b>M20-Et</b>	$\ln k' = 6.5152 (1/T) - 14.216$	0.9994
<b>M7-Me</b>	$\ln k' = 5.9402 (1/T) - 13.102$	0.9996
<b>M7-Et</b>	$\ln k' = 6.1485 (1/T) - 13.357$	0.9996

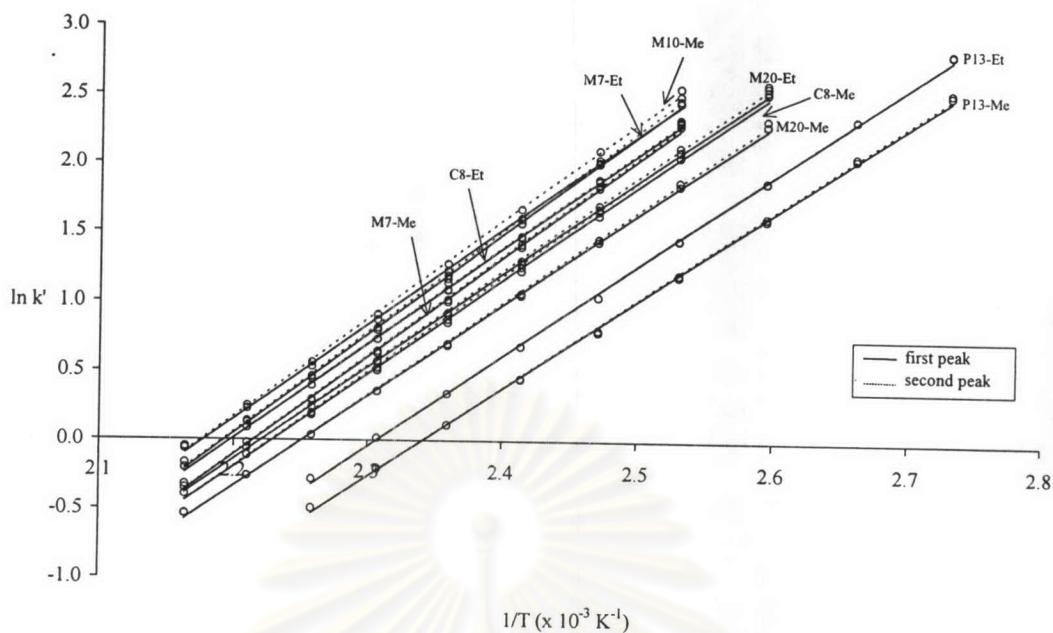


Figure C14 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 5) on BSiMe column

Table C14 Equation and correlation coefficient for the relationship in figure C14

compound	equation	$R^2$	equation	$R^2$
<b>P13-Me</b>	$\ln k'_1 = 6.3766 (1/T) - 14.607$	0.9994	$\ln k'_2 = 6.4282 (1/T) - 14.723$	0.9994
<b>P13-Et</b>	$\ln k'_1 = 6.5614 (1/T) - 14.805$	0.9994	$\ln k'_2 = 6.5736 (1/T) - 14.834$	0.9994
<b>M10-Me</b>	$\ln k'_1 = 6.8858 (1/T) - 14.653$	0.9995	$\ln k'_2 = 7.1328 (1/T) - 15.168$	0.9992
<b>C8-Me</b>	$\ln k'_1 = 6.7883 (1/T) - 14.790$	0.9991	$\ln k'_2 = 6.9020 (1/T) - 15.031$	0.9992
<b>C8-Et</b>	$\ln k'_1 = 6.8792 (1/T) - 14.777$	0.9994	$\ln k'_2 = 6.9260 (1/T) - 14.878$	0.9993
<b>M20-Me</b>	$\ln k'_1 = 6.5767 (1/T) - 14.473$	0.9995	$\ln k'_2 = 6.6717 (1/T) - 14.681$	0.9993
<b>M20-Et</b>	$\ln k'_1 = 6.7336 (1/T) - 14.615$	0.9996	$\ln k'_2 = 6.8461 (1/T) - 14.860$	0.9994
<b>M7-Me</b>	$\ln k'_1 = 7.1355 (1/T) - 15.448$	0.9991	$\ln k'_2 = 7.1943 (1/T) - 15.570$	0.9993
<b>M7-Et</b>	$\ln k'_1 = 7.2120 (1/T) - 15.458$	0.9989	$\ln k'_2 = 7.3011 (1/T) - 15.640$	0.9992

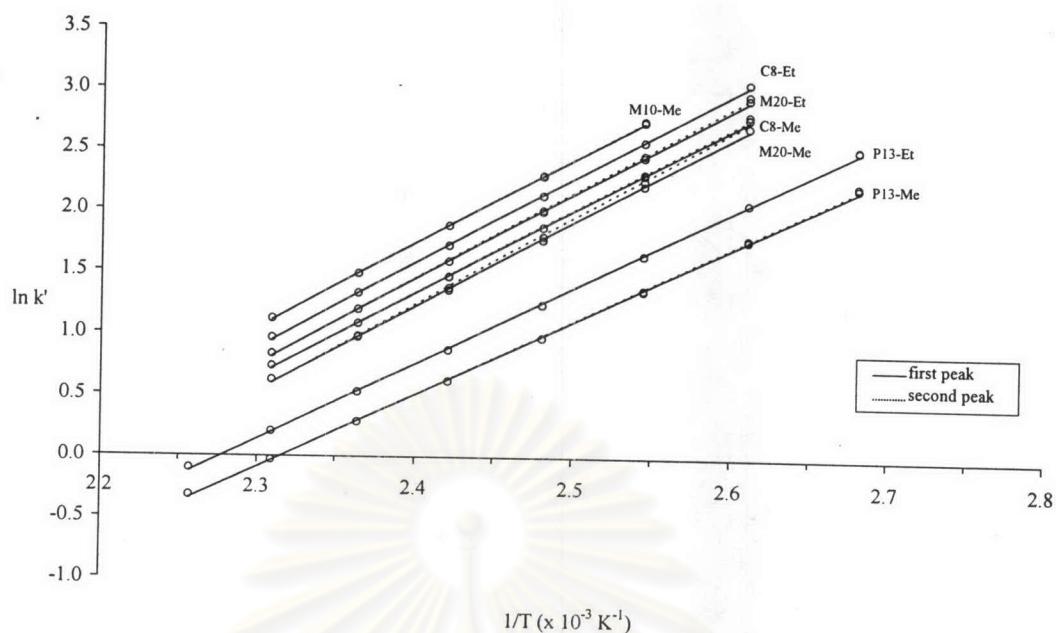


Figure C15 Plots of  $\ln$  (capacity factor) versus reciprocal of temperature of esters (series 5) on BSiAc column

Table C15 Equation and correlation coefficient for the relationship in figure C15

compound	equation	$R^2$	equation	$R^2$
<b>P13-Me</b>	$\ln k'_1 = 5.9592 (1/T) - 13.796$	0.9996	$\ln k'_2 = 6.0022 (1/T) - 13.897$	0.9995
<b>P13-Et</b>	$\ln k'_1 = 6.1816 (1/T) - 14.078$	0.9997	$\ln k'_2 = 6.1932 (1/T) - 14.106$	0.9996
<b>M10-Me</b>	$\ln k'_1 = 6.8772 (1/T) - 14.769$	0.9999	$\ln k'_2 = 6.9293 (1/T) - 14.892$	0.9998
<b>C8-Me</b>	$\ln k'_1 = 6.7413 (1/T) - 14.848$	0.9996	$\ln k'_2 = 6.8186 (1/T) - 15.031$	0.9993
<b>C8-Et</b>	$\ln k'_1 = 6.9308 (1/T) - 15.055$	0.9997	$\ln k'_2 = 6.9308 (1/T) - 15.056$	0.9997
<b>M20-Me</b>	$\ln k'_1 = 6.8839 (1/T) - 15.297$	0.9994	$\ln k'_2 = 7.1138 (1/T) - 15.832$	0.9990
<b>M20-Et</b>	$\ln k'_1 = 6.9385 (1/T) - 15.203$	0.9997	$\ln k'_2 = 7.0474 (1/T) - 15.460$	0.9995

Table C16 Thermodynamic parameters of all esters calculated from van't Hoff plots of  $\ln k'$  versus  $1/T$  on OV-1701 column

compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)	compound	$-\Delta H$ (kcal/mol)	$-\Delta S$ (cal/mol.K)
<b>P3-Me</b>	12.23	16.43	<b>M17-Me</b>	7.71	11.50
<b>P3-Et</b>	12.66	16.83	<b>P2-Me</b>	12.40	16.77
<b>P3-iPr</b>	13.24	17.98	<b>P2-Et</b>	12.85	17.33
<b>P3-nPr</b>	13.62	18.24	<b>P13-Me</b>	11.42	15.49
<b>P4-Me</b>	12.24	16.83	<b>P13-Et</b>	11.93	16.18
<b>P4-Et</b>	12.54	17.03	<b>M9-Me</b>	9.43	13.50
<b>M6-Me</b>	11.98	15.96	<b>M18-Me</b>	8.06	12.57
<b>M6-Et</b>	12.43	16.43	<b>M10-Me</b>	12.55	15.92
<b>M15-Me</b>	8.87	12.78	<b>C8-Me</b>	12.27	16.02
<b>M16-Me</b>	9.42	13.59	<b>C8-Et</b>	12.52	16.12
<b>M11-Me</b>	8.64	12.51	<b>M20-Me</b>	12.46	16.63
<b>M11-Et</b>	9.20	13.15	<b>M20-Et</b>	12.95	17.28
<b>M12-Me</b>	8.17	12.25	<b>M7-Me</b>	11.80	15.07
<b>M12-Et</b>	8.76	12.94	<b>M7-Et</b>	12.22	15.57

Table C17 Thermodynamic parameters of all esters calculated from van't Hoff plots  
of  $\ln k'$  versus  $1/T$  on BSiMe column

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
<b>P3-Me</b>	13.49	13.59	0.10	18.91	19.12	0.22
<b>P3-Et</b>	13.92	—	0.00	19.32	—	0.00
<b>P3-iPr</b>	14.19	—	0.00	19.72	—	0.00
<b>P3-nPr</b>	14.74	—	0.00	20.33	—	0.00
<b>P3-nBu</b>	15.44	—	0.00	21.04	—	0.00
<b>P3-nPen</b>	16.45	—	0.00	22.46	—	0.00
<b>P4-Me</b>	12.93	13.09	0.16	18.13	18.48	0.35
<b>P4-Et</b>	13.28	13.36	0.08	18.48	18.67	0.19
<b>M6-Me</b>	13.66	13.88	0.22	19.37	19.86	0.49
<b>M6-Et</b>	13.86	14.07	0.22	19.31	19.79	0.48
<b>M15-Me</b>	10.94	11.13	0.19	16.80	17.22	0.42
<b>M16-Me</b>	12.49	12.88	0.39	19.77	20.65	0.88
<b>M11-Me</b>	10.63	11.58	0.95	16.64	18.76	2.12
<b>M11-Et</b>	11.03	11.74	0.70	17.07	18.67	1.61
<b>M12-Me</b>	10.17	10.74	0.56	16.47	17.77	1.30
<b>M12-Et</b>	11.25	11.62	0.36	17.87	18.70	0.82
<b>M17-Me</b>	10.47	11.15	0.68	17.15	18.73	1.58
<b>P2-Me</b>	13.70	14.09	0.39	19.40	20.27	0.87
<b>P2-Et</b>	14.07	14.35	0.27	19.82	20.44	0.62

compound	enthalpy term (kcal/mol)			entrolpny term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
<b>P13-Me</b>	12.67	12.77	0.10	18.06	18.29	0.23
<b>P13-Et</b>	13.04	13.06	0.02	18.45	18.51	0.06
<b>M9-Me</b>	11.24	12.01	0.77	17.21	18.95	1.74
<b>M18-Me</b>	9.36	9.58	0.22	15.25	15.76	0.51
<b>M10-Me</b>	13.68	14.17	0.49	18.15	19.17	1.02
<b>C8-Me</b>	13.49	13.71	0.23	18.42	18.90	0.48
<b>C8-Et</b>	13.67	13.76	0.09	18.39	18.59	0.20
<b>M20-Me</b>	13.07	13.26	0.19	17.79	18.20	0.41
<b>M20-Et</b>	13.38	13.60	0.22	18.07	18.56	0.49
<b>M7-Me</b>	14.18	14.30	0.12	19.73	19.97	0.24
<b>M7-Et</b>	14.33	14.51	0.18	19.75	20.11	0.36

ศูนย์วิทยาศาสตร์  
จุฬาลงกรณ์มหาวิทยาลัย

Table C18 Thermodynamic parameters of all esters calculated from van't Hoff plots  
of  $\ln k'$  versus  $1/T$  on BSiAc column

compound	enthalpy term (kcal/mol)			entropy term (cal/mol.K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
<b>P3-Me</b>	13.10	13.29	0.19	18.46	18.90	0.44
<b>P3-Et</b>	13.53	13.68	0.15	18.86	19.22	0.36
<b>P3-iPr</b>	13.73	13.87	0.14	19.13	19.46	0.33
<b>P3-nPr</b>	14.14	14.25	0.10	19.41	19.66	0.25
<b>P3-nBu</b>	14.94	15.03	0.09	20.43	20.64	0.21
<b>P3-nPen</b>	15.86	15.92	0.06	21.68	21.82	0.14
<b>P4-Me</b>	12.52	12.63	0.11	17.52	17.78	0.26
<b>P4-Et</b>	12.93	—	0.00	18.01	—	0.00
<b>M6-Me</b>	12.85	—	0.00	17.96	—	0.00
<b>M6-Et</b>	13.15	—	0.00	18.11	—	0.00
<b>M11-Me</b>	13.00	13.79	0.79	22.30	24.14	1.84
<b>M11-Et</b>	11.89	12.03	0.14	19.25	19.59	0.34
<b>M12-Me</b>	12.79	14.83	2.04	22.59	27.23	4.64
<b>M12-Et</b>	11.76	12.83	1.07	19.70	22.19	2.50
<b>M17-Me</b>	12.46	13.24	0.79	21.59	23.42	1.83
<b>P2-Me</b>	13.45	14.11	0.65	19.11	20.61	1.50
<b>P2-Et</b>	13.47	13.87	0.40	18.72	19.64	0.92
<b>P13-Me</b>	11.84	11.93	0.09	16.44	16.65	0.20
<b>P13-Et</b>	12.28	12.31	0.02	17.00	17.06	0.06

compound	enthalpy term (kcal/mol)			entrolpay term (cal/mol.K)		
	-ΔH <sub>1</sub>	-ΔH <sub>2</sub>	-Δ(ΔH)	-ΔS <sub>1</sub>	-ΔS <sub>2</sub>	-Δ(ΔS)
<b>M9-Me</b>	12.77	14.13	1.36	21.35	24.60	3.25
<b>M18-Me</b>	9.86	10.09	0.23	17.17	17.77	0.60
<b>M10-Me</b>	13.66	13.77	0.10	18.38	18.62	0.24
<b>C8-Me</b>	13.39	13.55	0.15	18.53	18.90	0.36
<b>C8-Et</b>	13.77	—	0.00	18.95	—	0.00
<b>M20-Me</b>	13.68	14.14	0.46	19.43	20.49	1.06
<b>M20-Et</b>	13.79	14.00	0.22	19.24	19.75	0.51

ศูนย์วิทยาศาสตร์  
จุฬาลงกรณ์มหาวิทยาลัย

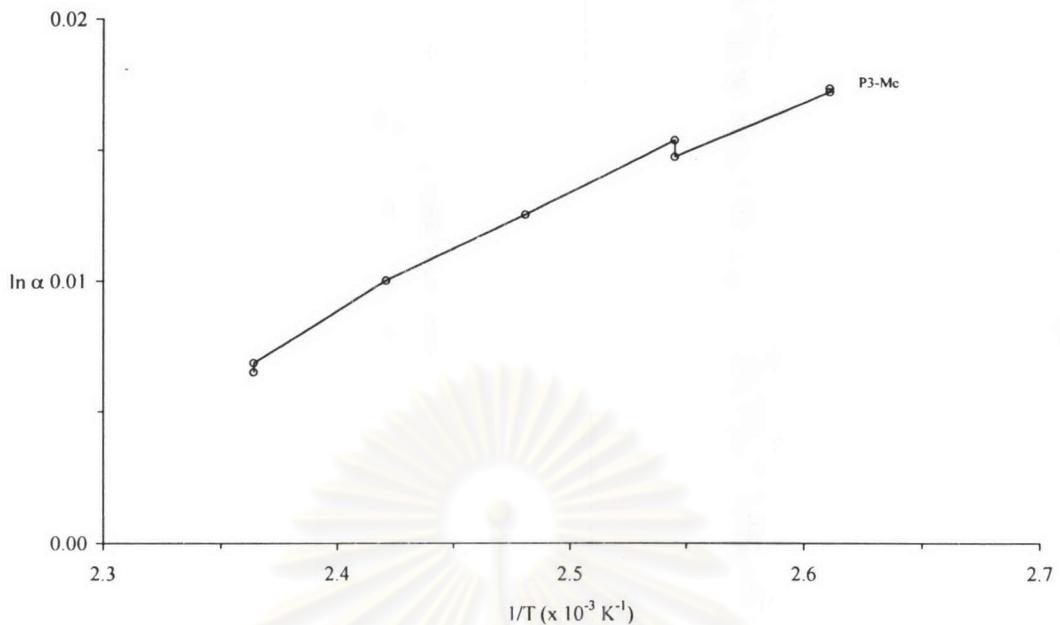


Figure C16 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 1) on BSiMe column

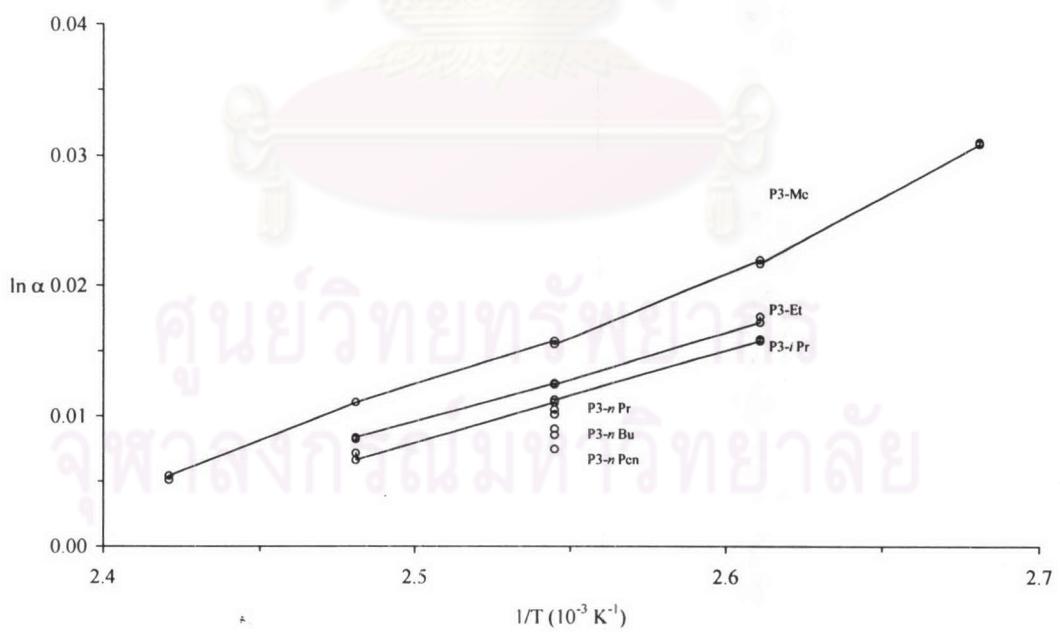


Figure C17 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 1) on BSiAc column

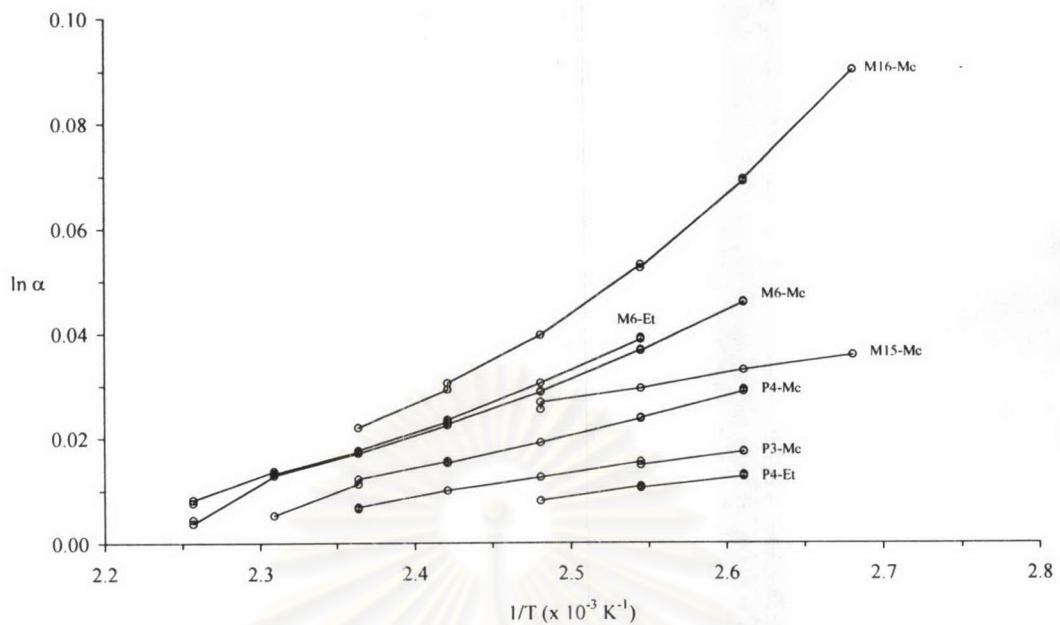


Figure C18 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 2) on BSiMe column

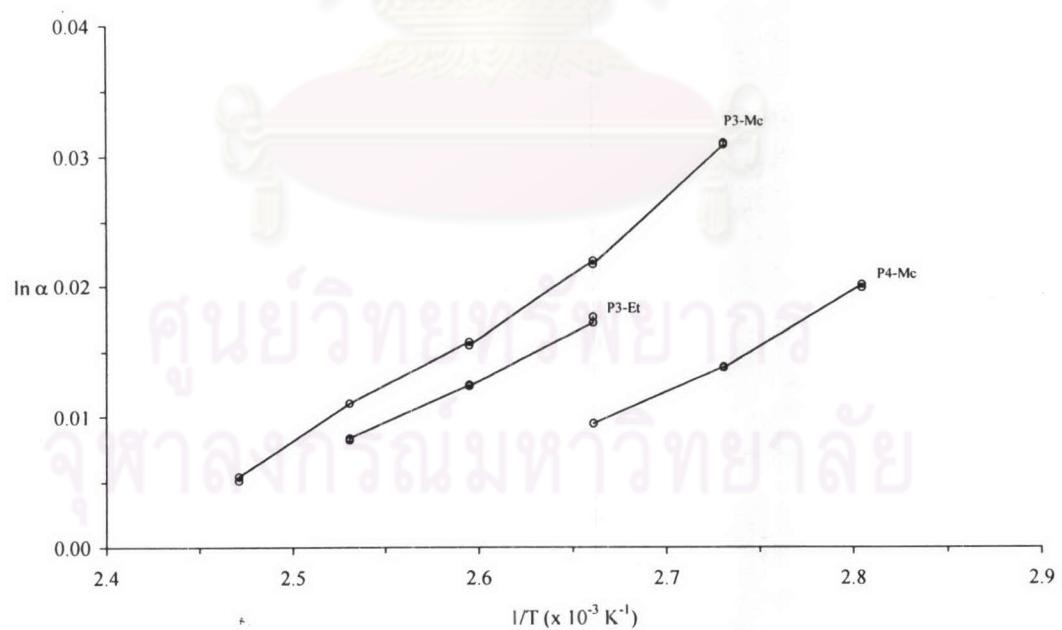


Figure C19 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 2) on BSiAc column

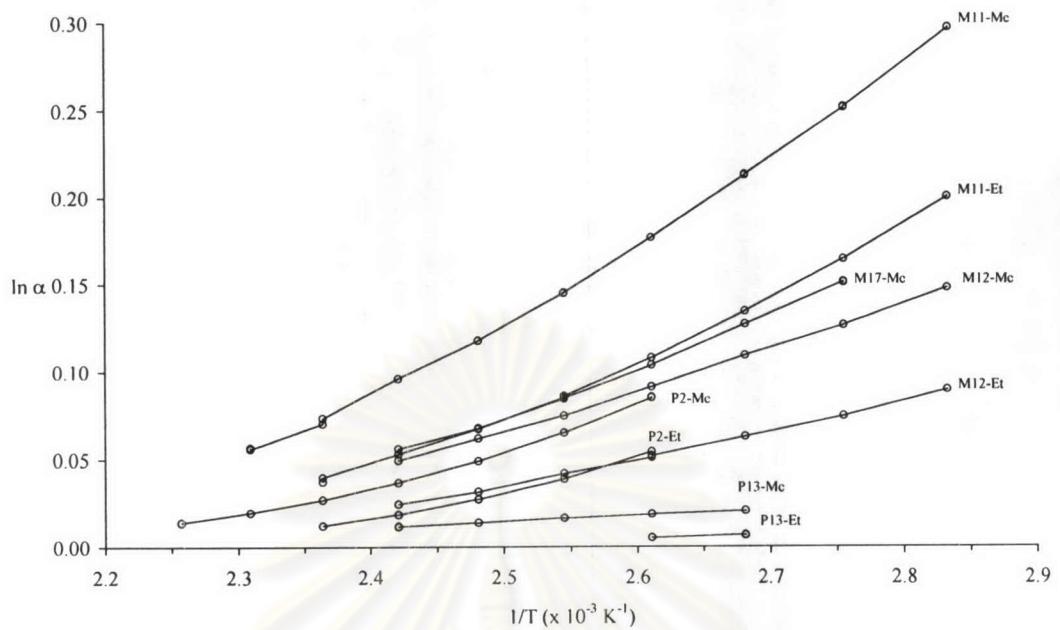


Figure C20 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 3) on BSiMe column

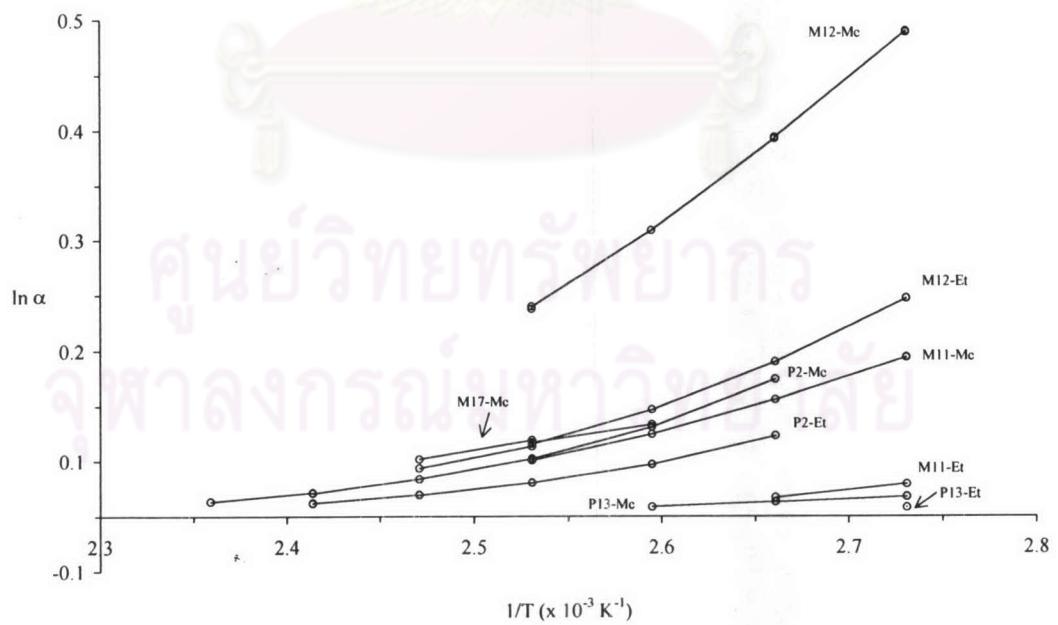


Figure C21 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 3) on BSiAc column

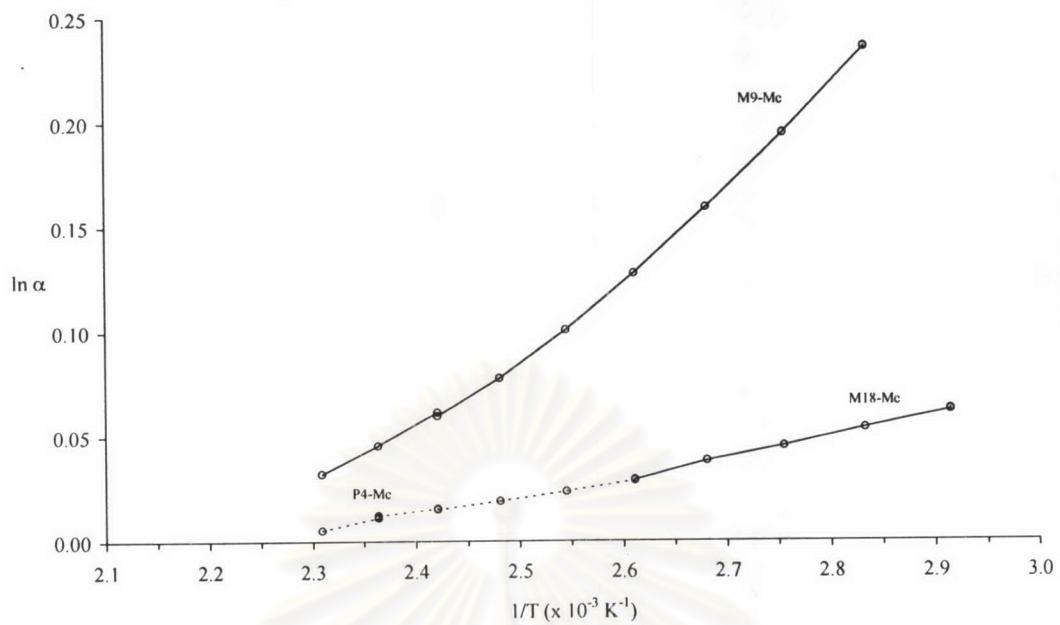


Figure C22 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 4) on BSiMe column

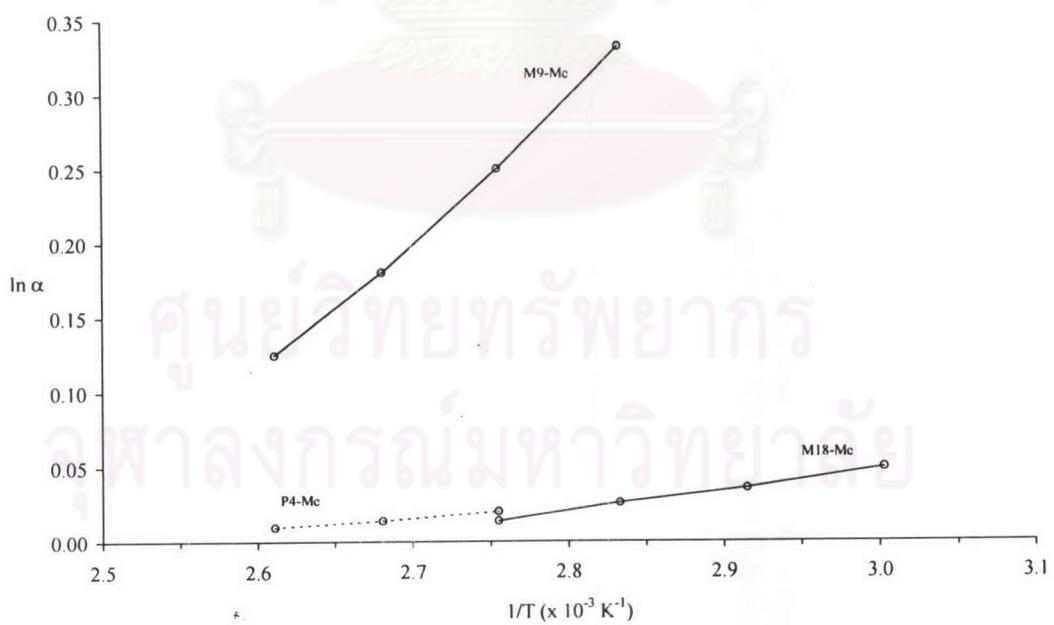


Figure C23 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 4) on BSiAc column

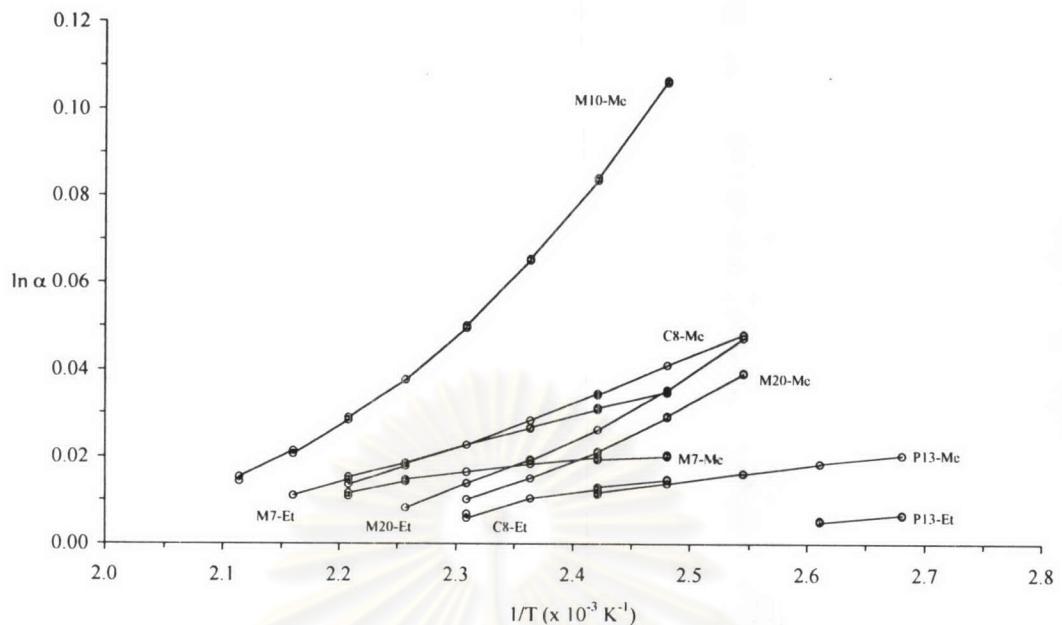


Figure C24 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 5) on BSiMe column

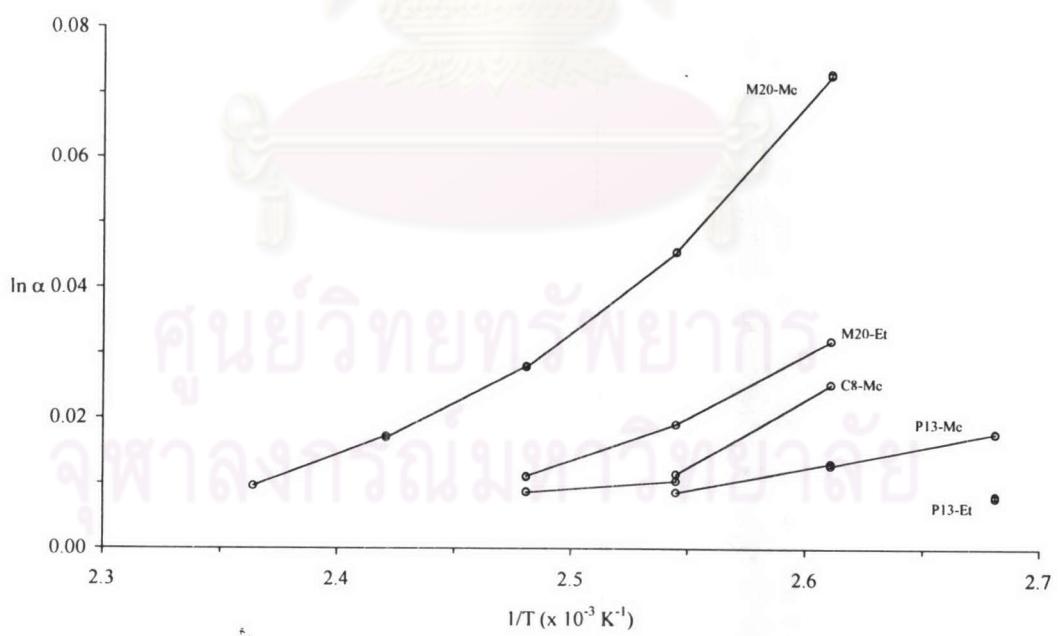


Figure C25 Plots of  $\ln$  (separation factor) versus reciprocal of temperature of esters (series 5) on BSiAc column

Table C19 Plots of  $\log t'$  versus n (number of C atoms) for the homologous series of n-alkane on OV-1701 column

temperature (°C)	equation	$R^2$
160	$\log t' = 0.2023n - 2.7335$	0.9998
150	$\log t' = 0.2124n - 2.7273$	0.9998
140	$\log t' = 0.2231n - 2.7137$	0.9999
130	$\log t' = 0.2346n - 2.7071$	0.9999
120	$\log t' = 0.2479n - 2.7115$	1.0000
110	$\log t' = 0.2640n - 2.7408$	0.9999
100	$\log t' = 0.2811n - 2.7640$	1.0000
90	$\log t' = 0.2964n - 2.7588$	1.0000
80	$\log t' = 0.3123n - 2.7563$	1.0000
70	$\log t' = 0.3378n - 2.8194$	0.9999
60	$\log t' = 0.3561n - 2.8142$	0.9999

คุณวิทยากร  
จุฬาลงกรณ์มหาวิทยาลัย

Table C20 Plots of  $\log t'$  versus n (number of C atoms) for the homologous series of n-alkane on BSiMe column

temperature (°C)	equation	$R^2$
160	$\log t' = 0.2093n - 2.6712$	0.9999
150	$\log t' = 0.2224n - 2.6792$	0.9999
140	$\log t' = 0.2346n - 2.6671$	0.9999
130	$\log t' = 0.2496n - 2.6815$	0.9999
120	$\log t' = 0.2701n - 2.7445$	1.0000
110	$\log t' = 0.2850n - 2.7303$	1.0000
100	$\log t' = 0.3012n - 2.7227$	1.0000
90	$\log t' = 0.3223n - 2.7563$	0.9999
80	$\log t' = 0.3386n - 2.7232$	1.0000
70	$\log t' = 0.3581n - 2.7214$	1.0000

ศูนย์วิทยทรัพยากร  
จุฬาลงกรณ์มหาวิทยาลัย

Table C21 Plots of  $\log t'$  versus  $n$  (number of C atoms) for the homologous series of n-alkane on BSiAc column

temperature (°C)	equation	$R^2$
160	$\log t' = 0.2002n - 2.7348$	0.9999
150	$\log t' = 0.2103n - 2.7258$	0.9999
140	$\log t' = 0.2241n - 2.7581$	0.9999
130	$\log t' = 0.2359n - 2.7508$	1.0000
120	$\log t' = 0.2502n - 2.7667$	0.9999
110	$\log t' = 0.2690n - 2.8123$	0.9999
100	$\log t' = 0.2835n - 2.8029$	0.9999
90	$\log t' = 0.2992n - 2.7929$	1.0000
80	$\log t' = 0.3161n - 2.7903$	1.0000
70	$\log t' = 0.3461n - 2.8989$	0.9998
60	$\log t' = 0.3597n - 2.8152$	0.9999

คุณวิทยากร  
จุฬาลงกรณ์มหาวิทยาลัย

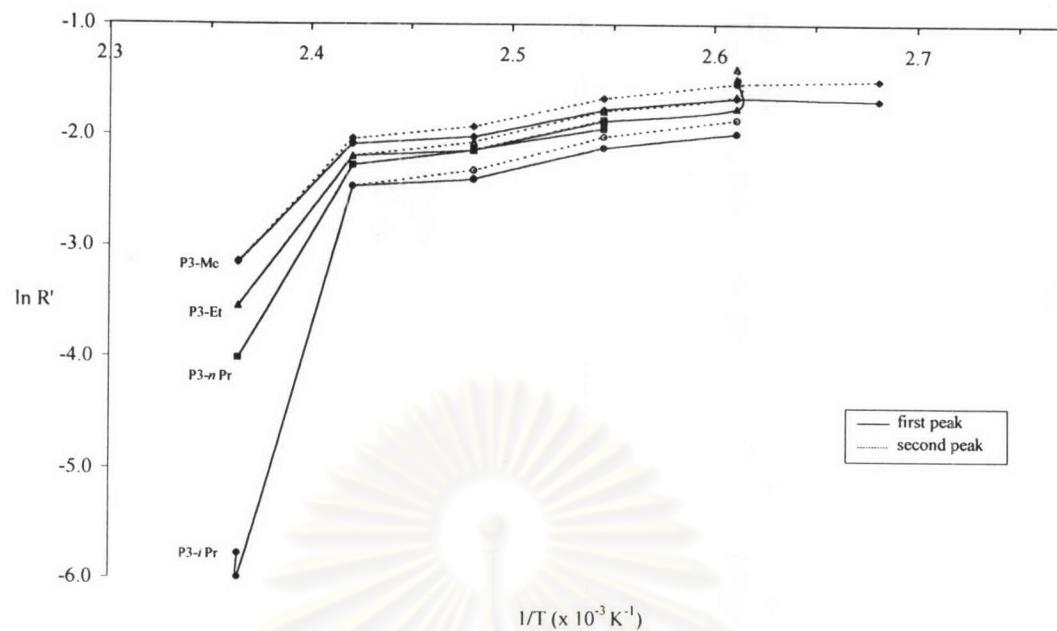


Figure C26 Plots of  $\ln$  (retention increment) versus reciprocal of temperature of esters with different ester chain length (series 1) on BSiAc column

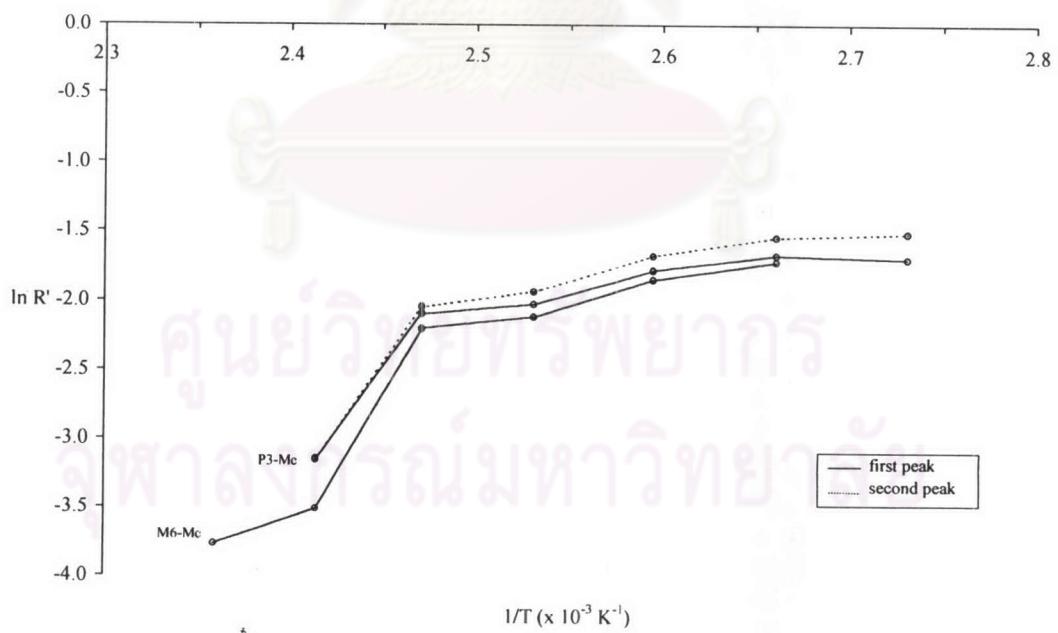


Figure C27 Plots of  $\ln$  (retention increment) versus reciprocal of temperature of esters with different position of substituent (series 2) on BSiAc column

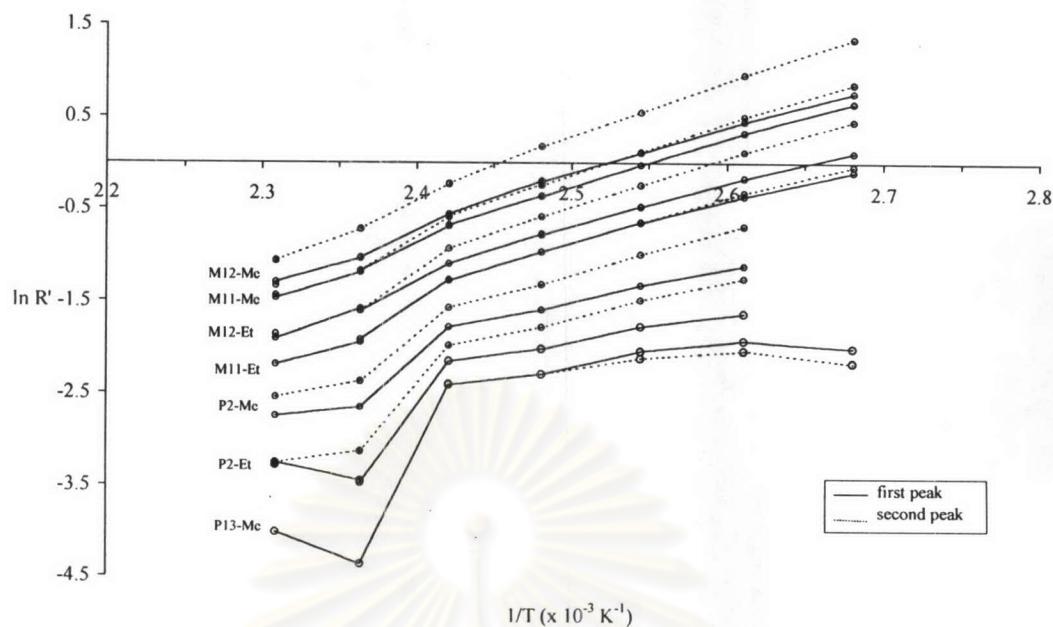


Figure C28 Plots of  $\ln$  (retention increment) versus reciprocal of temperature of esters with different position of substituent (series 3) on BSiAc column

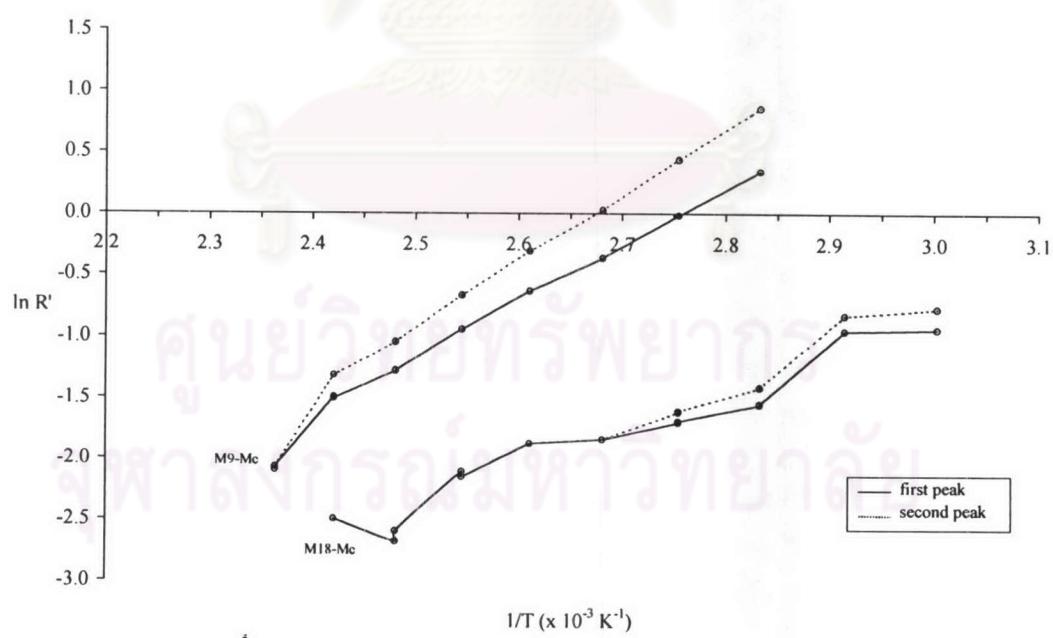


Figure C29 Plots of  $\ln$  (retention increment) versus reciprocal of temperature of esters with different position of substituent (series 4) on BSiAc column

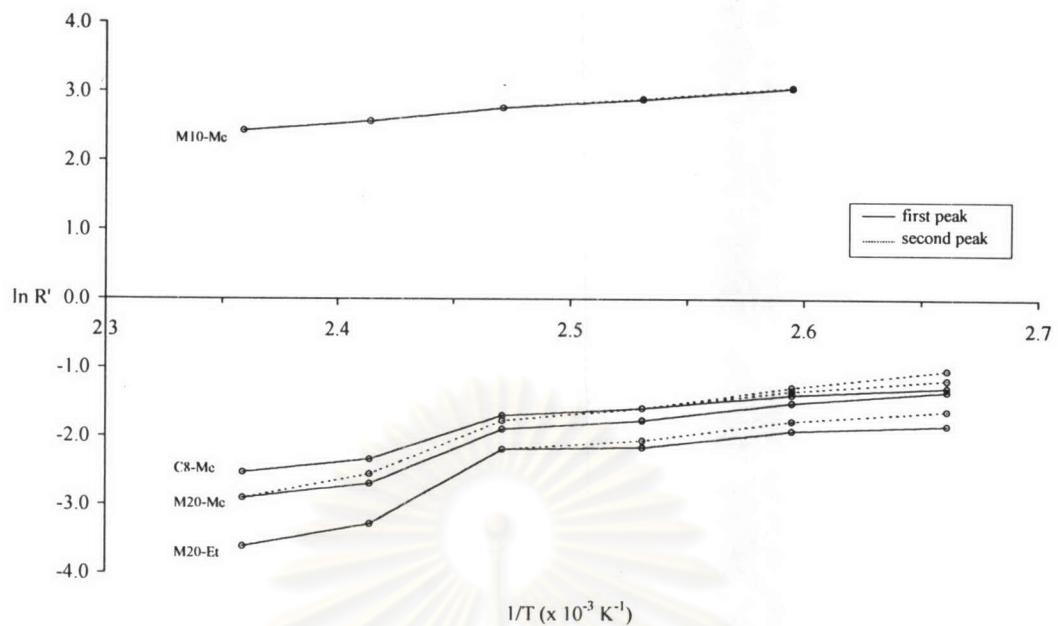


Figure C30 Plots of  $\ln$  (retention increment) versus reciprocal of temperature of esters with different position of substituent (series 5) on BSiAc column

Table C22 Equation and correlation coefficient for the relationships in figures  
C26-C30 (only linear part)

compound	equation	R <sup>2</sup>	equation	R <sup>2</sup>
<b>P3-Me</b>	$\ln R'_1 = 1.7474 (1/T) - 6.300$	0.8639	$\ln R'_2 = 2.2316 (1/T) - 7.423$	0.9310
<b>P3-Et</b>	$\ln R'_1 = 3.1493 (1/T) - 9.881$	0.8722	$\ln R'_2 = 3.6501 (1/T) - 11.073$	0.9289
<b>P3-iPr</b>	$\ln R'_1 = 2.7179 (1/T) - 9.080$	0.9505	$\ln R'_2 = 3.3349 (1/T) - 10.555$	0.9788
<b>P3-nPr</b>	$\ln R'_1 = 2.7006 (1/T) - 8.827$	0.9931	$\ln R'_2 = 3.3512 (1/T) - 10.416$	0.9703
<b>M6-Me</b>	$\ln R'_1 = 2.7201 (1/T) - 8.806$	0.9654	$\ln R'_2 = 2.7201 (1/T) - 8.806$	0.9654
<b>M11-Me</b>	$\ln R'_1 = 5.1621 (1/T) - 13.170$	0.9991	$\ln R'_2 = 5.6039 (1/T) - 14.146$	0.9994
<b>M11-Et</b>	$\ln R'_1 = 4.5343 (1/T) - 12.223$	0.9955	$\ln R'_2 = 4.7842 (1/T) - 12.839$	0.9979
<b>M12-Me</b>	$\ln R'_1 = 5.0566 (1/T) - 12.769$	0.9978	$\ln R'_2 = 6.0797 (1/T) - 14.925$	0.9990
<b>M12-Et</b>	$\ln R'_1 = 4.6265 (1/T) - 12.268$	0.9972	$\ln R'_2 = 5.3361 (1/T) - 13.832$	0.9990
<b>P2-Me</b>	$\ln R'_1 = 3.5665 (1/T) - 10.425$	0.9964	$\ln R'_2 = 4.6985 (1/T) - 12.958$	0.9983
<b>P2-Et</b>	$\ln R'_1 = 2.7998 (1/T) - 8.934$	0.9873	$\ln R'_2 = 3.8818 (1/T) - 11.388$	0.9956
<b>P13-Me</b>	$\ln R'_1 = 2.0005 (1/T) - 7.242$	0.9808	$\ln R'_2 = 2.6311 (1/T) - 8.782$	0.9729
<b>M9-Me</b>	$\ln R'_1 = 4.4976 (1/T) - 12.402$	0.9989	$\ln R'_2 = 5.3072 (1/T) - 14.183$	0.9994
<b>M18-Me</b>	$\ln R'_1 = 3.2357 (1/T) - 10.451$	0.9568	$\ln R'_2 = 2.9119 (1/T) - 9.636$	0.9407
<b>M10-Me</b>	$\ln R'_1 = 2.6812 (1/T) - 3.755$	0.9956	$\ln R'_2 = 2.7359 (1/T) - 3.884$	0.9966
<b>C8-Me</b>	$\ln R'_1 = 2.2590 (1/T) - 7.168$	0.9846	$\ln R'_2 = 2.8760 (1/T) - 8.678$	0.9813
<b>M20-Me</b>	$\ln R'_1 = 3.0277 (1/T) - 9.239$	0.9871	$\ln R'_2 = 3.9969 (1/T) - 11.466$	0.9933
<b>M20-Et</b>	$\ln R'_1 = 2.4276 (1/T) - 8.148$	0.9135	$\ln R'_2 = 3.2795 (1/T) - 10.166$	0.9666

Table C23 Thermodynamic parameters calculated by *Schurig approach* (from equation in table C22) for ester analytes separated on BSiAc column

compound	enthalpy term (kcal/mol)			entrolpny term (cal/mol.K)		
	-ΔH <sub>1</sub>	-ΔH <sub>2</sub>	-Δ(ΔH)	-ΔS <sub>1</sub>	-ΔS <sub>2</sub>	-Δ(ΔS)
<b>P3-Me</b>	3.47	4.43	0.96	9.02	11.25	2.23
<b>P3-Et</b>	6.26	7.25	1.00	16.13	18.50	2.37
<b>P3-iPr</b>	5.40	6.63	1.23	14.54	17.47	2.93
<b>P3-nPr</b>	5.37	6.66	1.29	14.04	17.20	3.16
<b>M6-Me</b>	5.40	—	0.00	14.00	—	0.00
<b>M11-Me</b>	10.26	11.13	0.88	22.67	24.61	1.94
<b>M11-Et</b>	9.01	9.51	0.50	20.79	22.01	1.22
<b>M12-Me</b>	10.05	12.08	2.03	21.87	26.16	4.28
<b>M12-Et</b>	9.19	10.60	1.41	20.88	23.99	3.11
<b>P2-Me</b>	7.09	9.34	2.25	17.22	22.25	5.03
<b>P2-Et</b>	5.56	7.71	2.15	14.25	19.13	4.88
<b>P13-Me</b>	3.97	5.23	1.25	10.89	13.95	3.06
<b>M9-Me</b>	8.94	10.55	1.61	21.14	24.68	3.54
<b>M18-Me</b>	5.79	6.43	0.64	15.65	17.27	1.62
<b>M10-Me</b>	5.33	5.44	0.11	3.96	4.22	0.26
<b>C8-Me</b>	4.49	5.71	1.23	10.74	13.74	3.00
<b>M20-Me</b>	6.02	7.94	1.93	14.86	19.28	4.43
<b>M20-Et</b>	4.82	6.52	1.69	12.69	16.70	4.01

## VITA

Miss Pattama Changseeplag was born on Saturday 22<sup>nd</sup> July, 1978 and brought up in Bangkok, the capital city of Thailand. Majoring in chemistry, the author completed her undergraduate study from the Faculty of Science, Chulalongkorn University in 2000. After graduation, the author continued studying for a Master of Science degree in analytical chemistry at the same university. Her current address is 6 Moo 2 Soi Ramintra 8, Ramintra Road, Bangkhen, Bangkok 10220.

คุณย์วิทยากร  
จุฬาลงกรณ์มหาวิทยาลัย