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APPENDICES

Appendix A

Glossary

Adjusted retention time (t'_R) is the absolute retention of a compound on a stationary phase. This value is calculated by subtracting the time of unretained compound (t_M) from the compound's retention time (t_R), according to:

$$t'_R = t_R - t_M$$

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

Distribution coefficient (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 by the following equation.

$$\begin{aligned} K &= \frac{C_S}{C_M} \\ &= k' \cdot \frac{V_M}{V_S} = k' \cdot \beta \end{aligned}$$

C_S, C_M = concentration of a solute in stationary phase and in mobile phase, respectively

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

Number of theoretical plate (N) is used as a measure of column efficiency. It is defined as the square of the ratio of the retention of analyte divided by peak broadening.

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

- 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 defined as the ratio of the volume of mobile phase (V_M) to the volume of stationary phase (V_S) in the column. It is a unitless value and can be calculated from column dimension by the following equation.

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

- r_c = capillary column radius
 d_f = stationary phase film thickness (in the same unit as r_c)

Retention factor or capacity factor (k') is defined as the ratio of analyte masses in the stationary phase and mobile phase. It is equivalent to the ratio of time of analyte molecules spend in stationary phase (t'_R) to the time that they spend in that mobile phase (t_M). The retention factor is calculated from:

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

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, when $k'_2 \geq k'_1$.

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

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

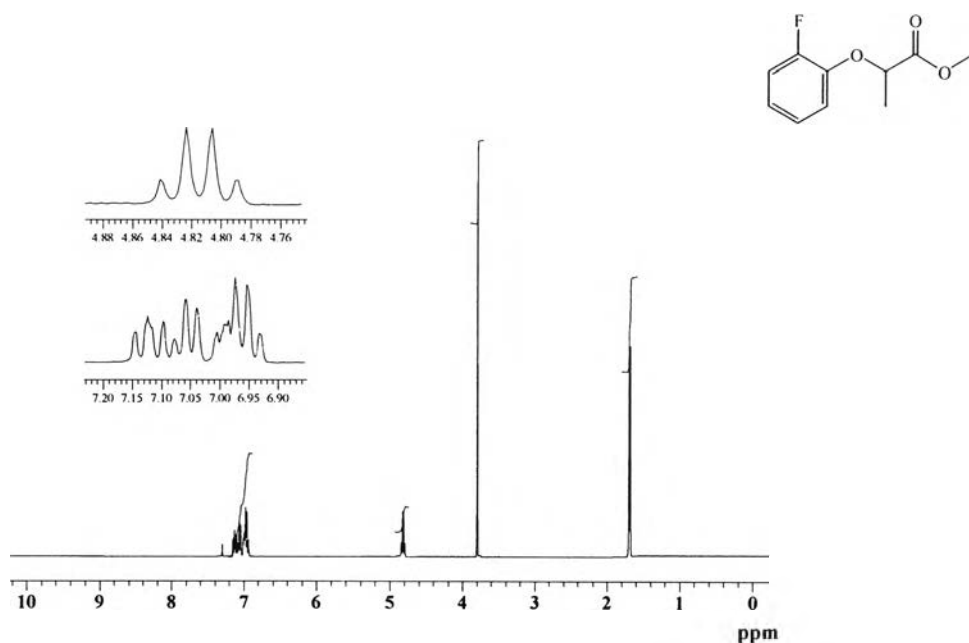


Figure B1 NMR spectrum of **2F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.69 (3H, d, $J=7.02$ Hz, CHCH_3), 3.79 (3H, s, OCH_3), 4.78-4.84
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.93-7.16 (4H, m, ArH)

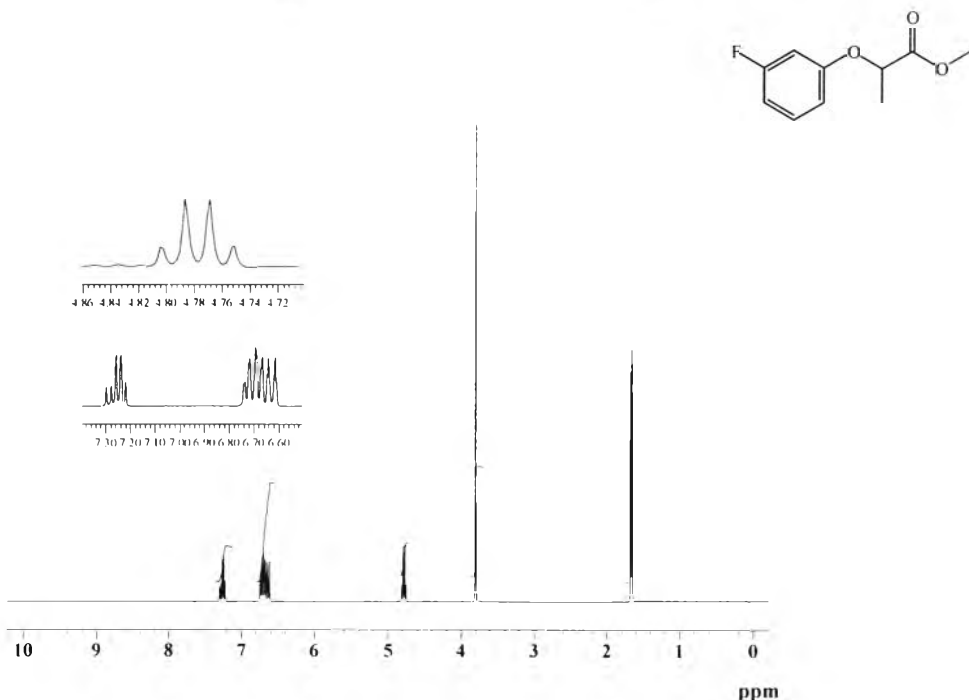


Figure B2 NMR spectrum of **3F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.72 (3H, d, $J=6.24$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.74-4.80
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.60-6.75 (3H, m, ArH), 7.20-7.30
 (1H, m, ArH)



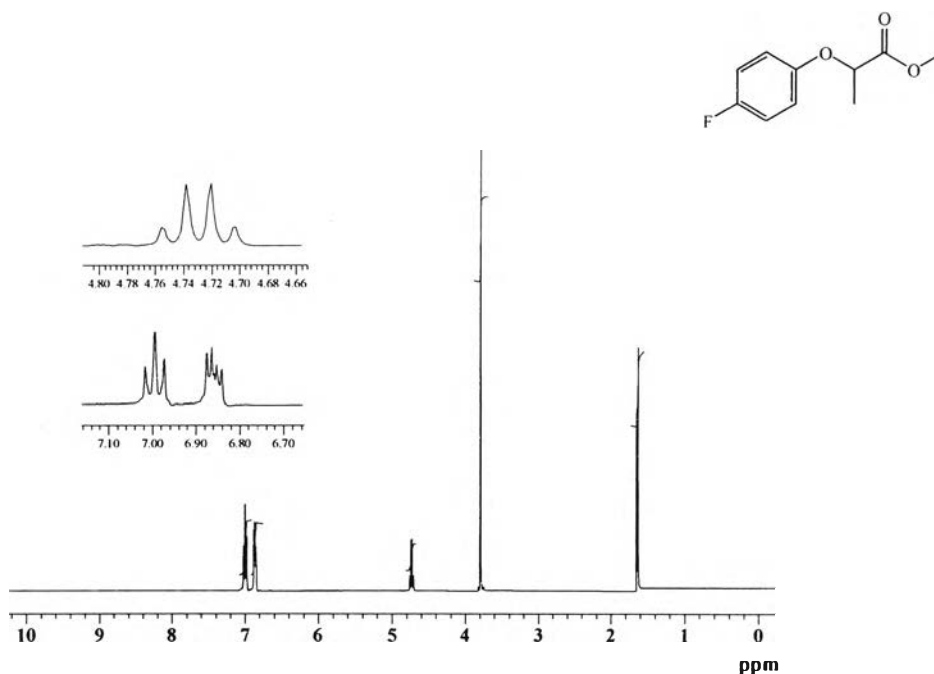


Figure B3 NMR spectrum of **4F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.63 (3H, d, $J=6.24$ Hz, CHCH_3), 3.82 (3H, s, OCH_3), 4.70-4.76
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.84-6.90 (2H, m, ArH), 6.96-7.04
 (2H, m, ArH)

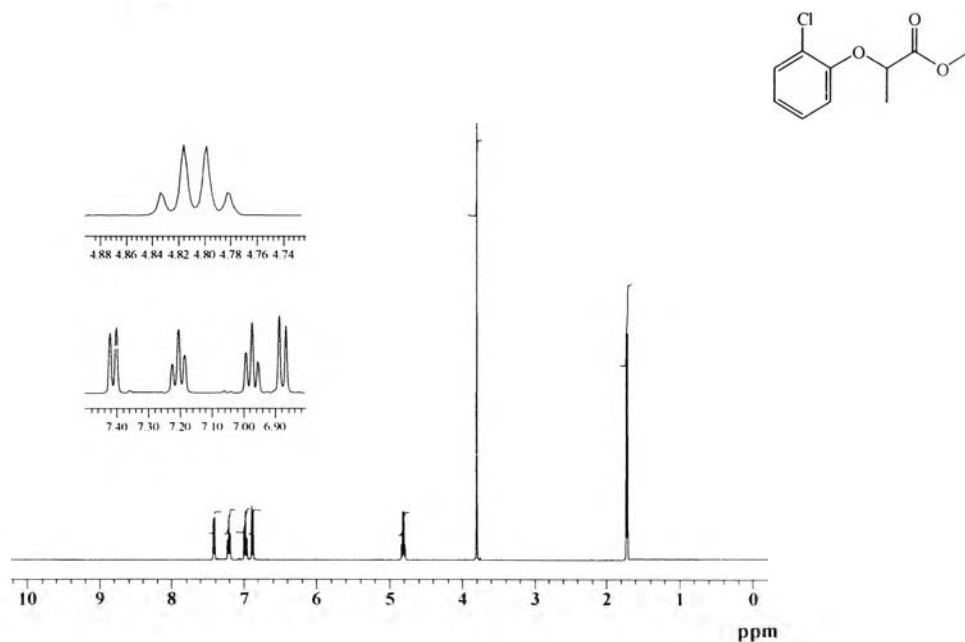


Figure B4 NMR spectrum of **2Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.77 (3H, d, $J=7.02$ Hz, CHCH_3), 3.77 (3H, s, OCH_3), 4.77-4.84
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.87 (1H, d, $J=8.58$ Hz, ArH), 6.97
 (1H, t, $J=7.80$ Hz, ArH), 7.22 (1H, t, $J=7.80$ Hz, ArH), 7.44
 (1H, d, $J=7.80$ Hz, ArH)

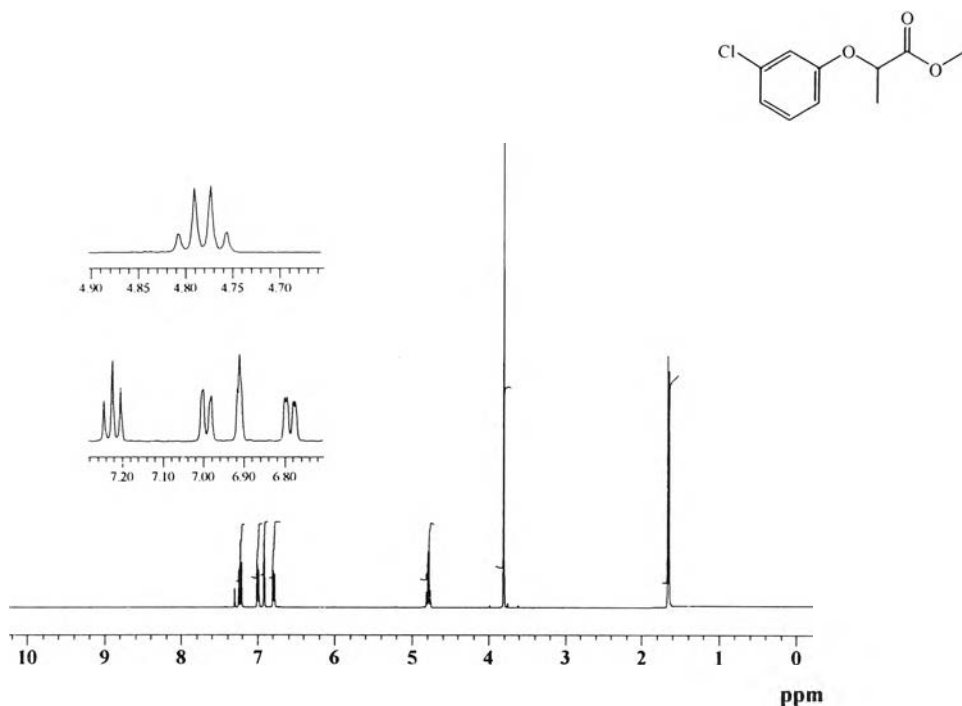


Figure B5 NMR spectrum of **3Cl**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.66 (3H, d, *J*=7.02 Hz, CHCH₃), 3.80 (3H, s, OCH₃), 4.75-4.82
 (1H, q, *J*=7.02 Hz, CHCH₃), 6.79 (1H, d, *J*=6.24 Hz, ArH), 6.91
 (1H, s, ArH), 7.00 (1H, d, *J*=7.80 Hz, ArH), 7.22 (1H, t, *J*=8.58 Hz, ArH)

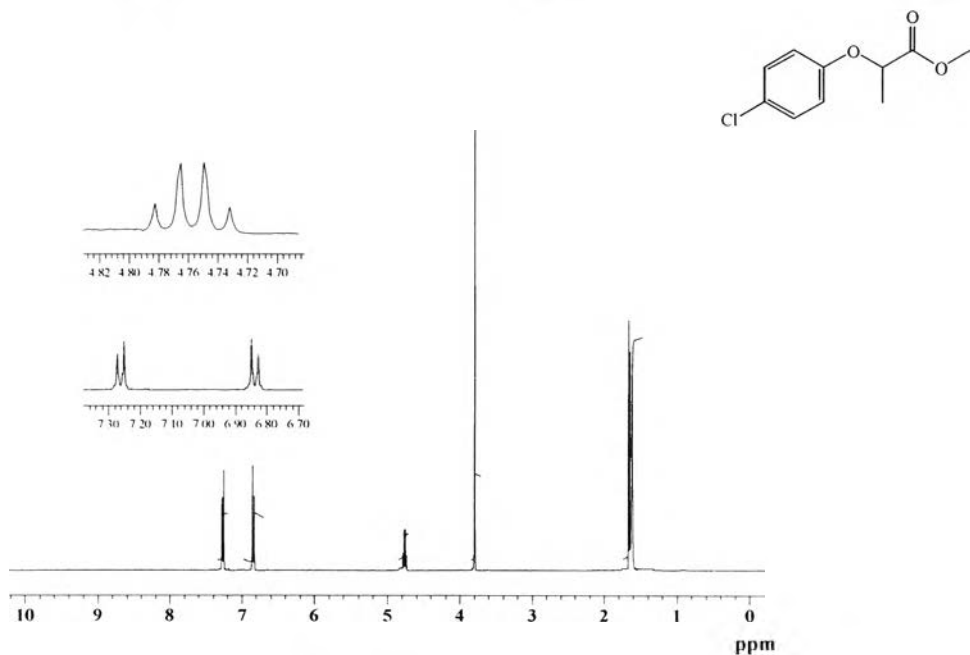


Figure B6 NMR spectrum of **4Cl**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.64 (3H, d, *J*=7.02 Hz, CHCH₃), 3.80 (3H, s, OCH₃), 4.72-4.79
 (1H, q, *J*=6.24 Hz, CHCH₃), 6.83 (2H, d, *J*=8.58 Hz, ArH),
 7.27 (2H, d, *J*=8.58 Hz, ArH)

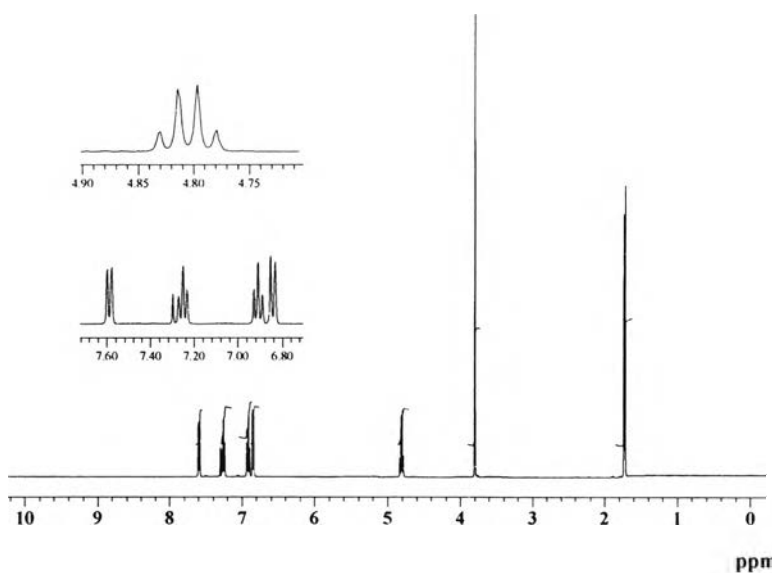
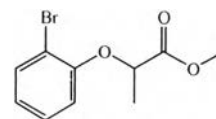


Figure B7 NMR spectrum of **2Br**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.71 (3H, d, $J=6.24$ Hz, CHCH_3), 3.83 (3H, s, OCH_3), 4.77-4.84 (1H, q, $J=7.02$ Hz, CHCH_3), 6.83 (1H, d, $J=7.80$ Hz, ArH), 6.93 (1H, t, $J=7.02$ Hz, ArH), 7.23 (1H, t, $J=7.80$ Hz, ArH), 7.58 (1H, d, $J=7.80$ Hz, ArH)

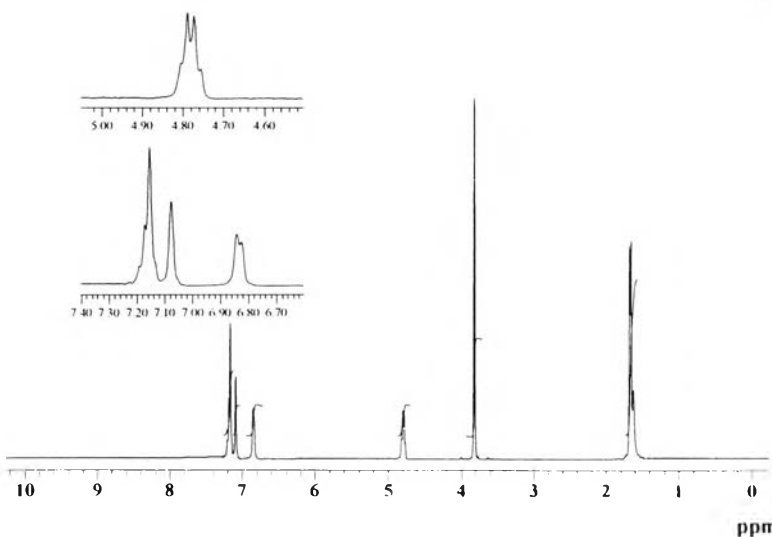
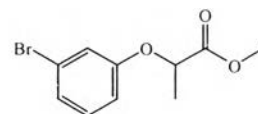


Figure B8 NMR spectrum of **3Br**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.64 (3H, d, $J=6.24$ Hz, CHCH_3), 3.81 (3H, s, OCH_3), 4.74-4.82 (1H, q, $J=6.24$ Hz, CHCH_3), 6.82 (1H, d, $J=7.02$ Hz, ArH), 7.07 (1H, s, ArH), 7.12-7.19 (2H, m, ArH)

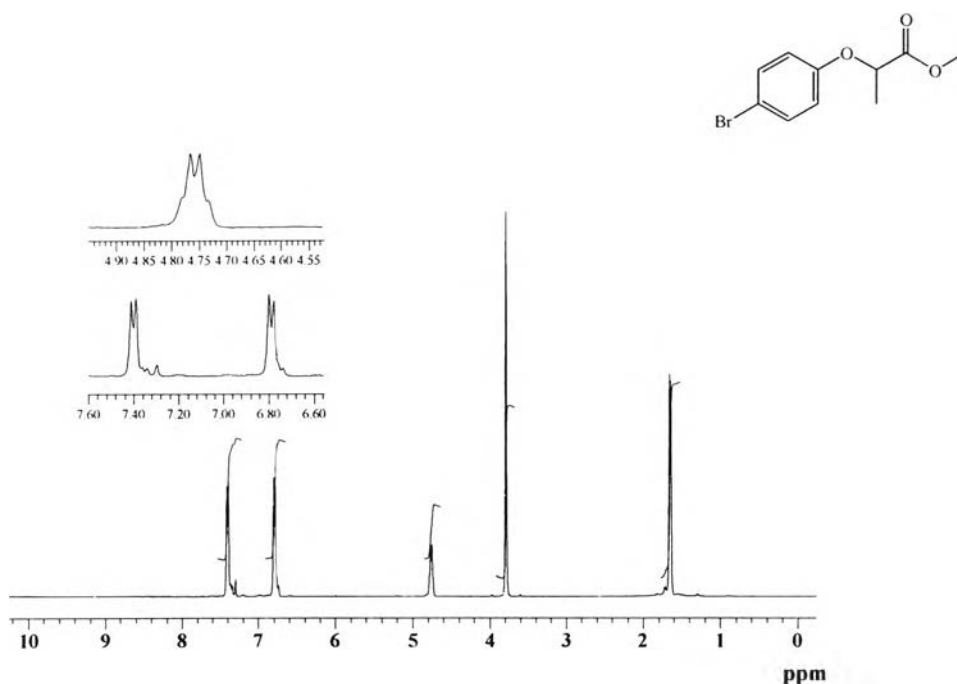


Figure B9 NMR spectrum of **4Br**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.64 (3H, d, $J=7.02$ Hz, CHCH₃), 3.79 (3H, s, OCH₃), 4.71-4.80
 (1H, q, $J=7.02$ Hz, CHCH₃), 6.80 (2H, d, $J=8.58$ Hz, ArH), 7.42
 (2H, d, $J=8.58$ Hz, ArH)

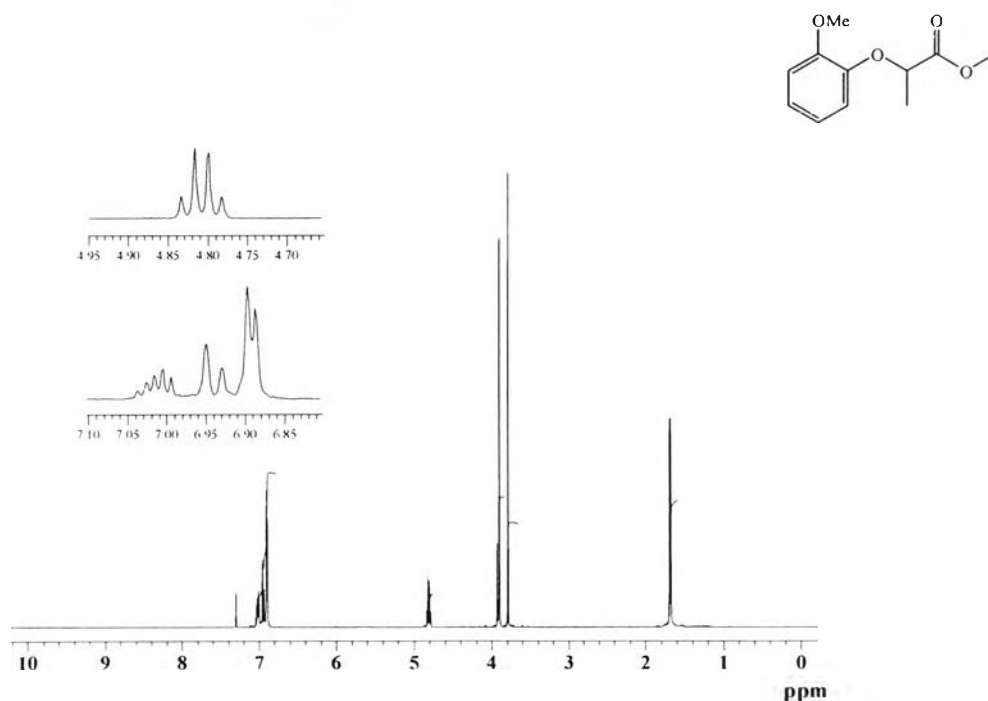


Figure B10 NMR spectrum of **2OMe**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.69 (3H, d, $J=6.24$ Hz, CHCH₃), 3.79 (3H, s, OCH₃), 3.93
 (3H, s, ArOCH₃), 4.78-4.84 (1H, q, $J=7.02$ Hz, CHCH₃),
 6.86-7.04 (4H, m, ArH)

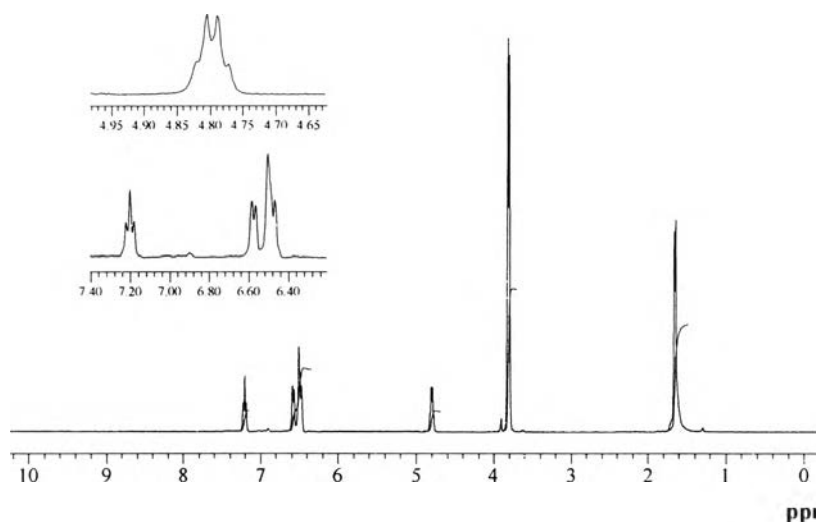
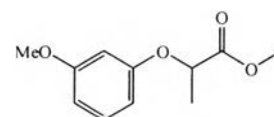


Figure B11 NMR spectrum of **3OMe**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.64 (3H, d, $J=6.24$ Hz, CHCH_3), 3.79 (3H, s, OCH_3), 3.81
 (3H, s, ArOCH_3), 4.75-4.85 (1H, q, $J=6.24$ Hz, CHCH_3),
 6.45-6.60 (3H, m, ArH), 7.22 (1H, t, $J=7.80$ Hz, ArH)

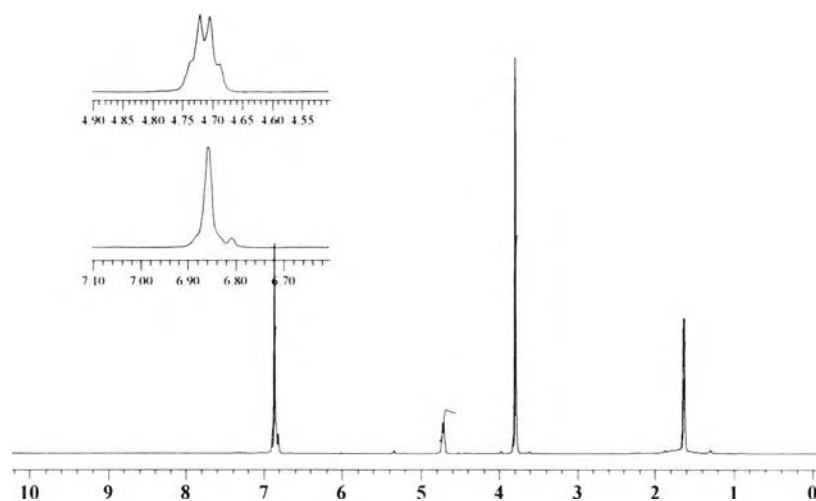
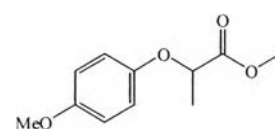


Figure B12 NMR spectrum of **4OMe**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.62 (3H, d, $J=7.02$ Hz, CHCH_3), 3.80 (6H, s, OCH_3 , ArOCH_3),
 4.66-4.76 (1H, q, $J=6.24$ Hz, CHCH_3), 6.80-6.90 (4H, m, ArH)

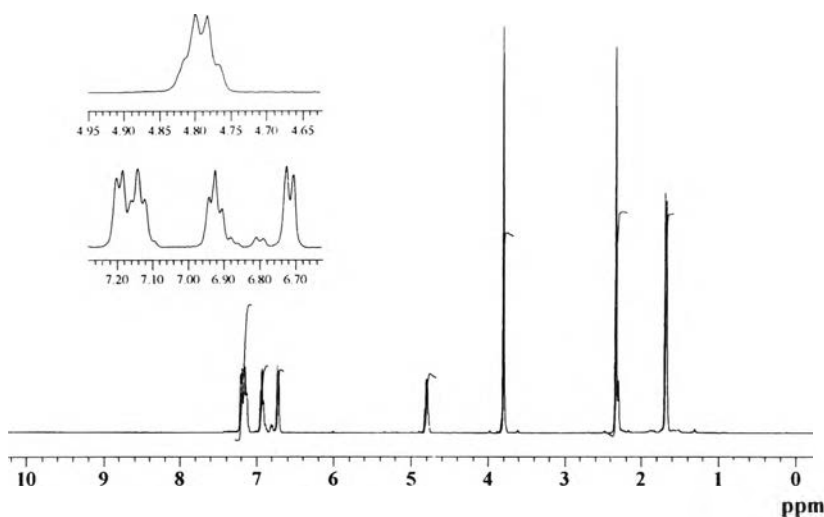
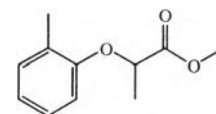


Figure B13 NMR spectrum of **2Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.67 (3H, d, $J=6.24$ Hz, CHCH_3), 2.32 (3H, s, ArCH_3), 3.79 (3H, s, OCH_3), 4.75-4.85 (1H, q, $J=7.02$ Hz, CHCH_3), 6.71 (1H, d, $J=7.80$ Hz ArH), 6.88-6.96 (1H, m, ArH), 7.10-7.22 (2H, m, ArH)

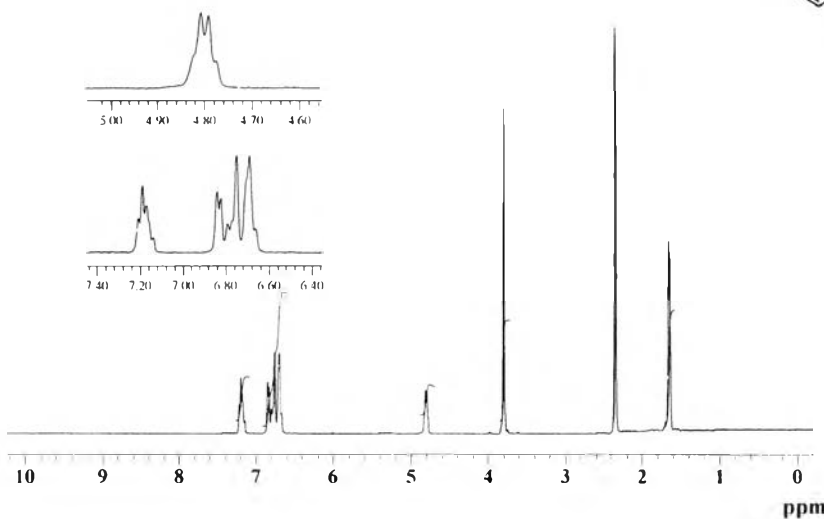
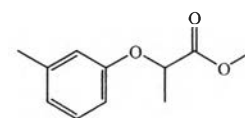


Figure B14 NMR spectrum of **3Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.64 (3H, d, $J=6.24$ Hz, CHCH_3), 2.35 (3H, s, ArCH_3), 3.80 (3H, s, OCH_3), 4.78-4.83 (1H, q, $J=6.24$ Hz, CHCH_3), 6.62-6.84 (3H, m, ArH), 7.10-7.24 (1H, m, ArH)

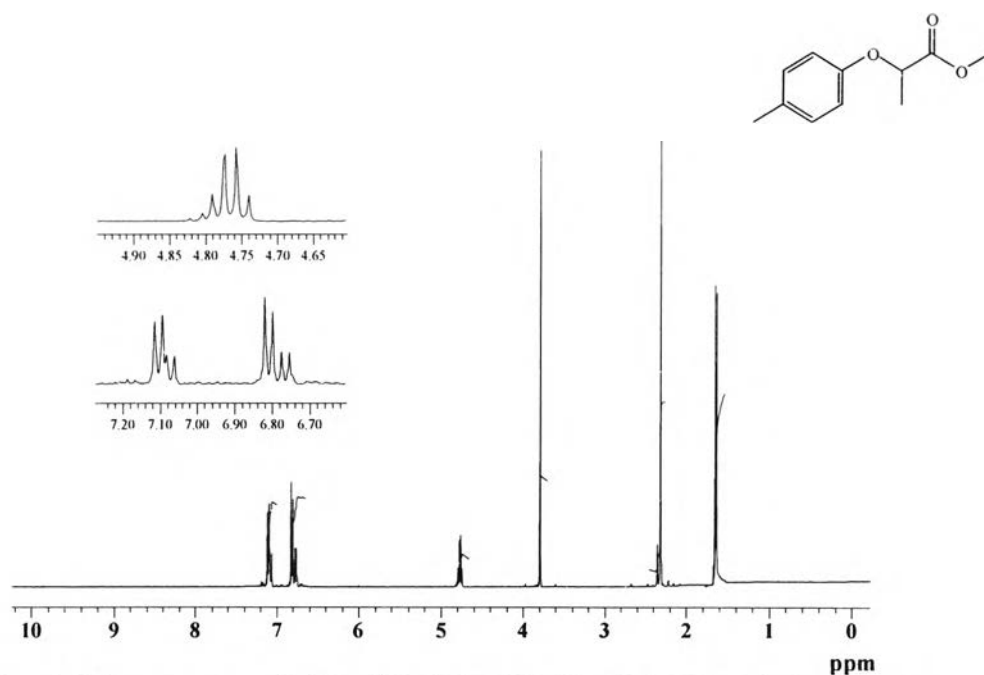


Figure B15 NMR spectrum of **4Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.84 (3H, d, $J=7.02$ Hz, CHCH_3), 2.31 (3H, s, ArCH_3), 3.79 (3H, s, OCH_3), 4.74-4.80 (1H, q, $J=6.24$ Hz, CHCH_3), 6.74-6.84 (2H, m, ArH), 7.06-7.14 (2H, m, ArH)

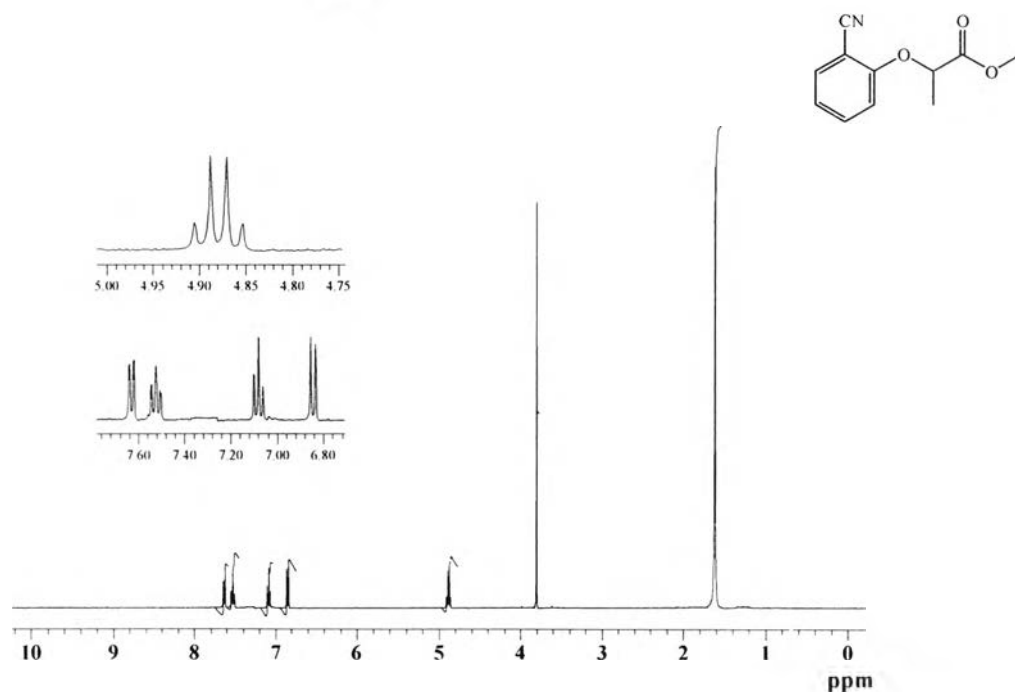


Figure B16 NMR spectrum of **2CN**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm): 1.61 (3H, d, $J=7.02$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.85-4.91 (1H, q, $J=7.02$ Hz, CHCH_3), 6.82 (1H, d, $J=8.58$ Hz, ArH), 7.08 (1H, t, $J=7.80$ Hz, ArH), 7.54 (1H, t, $J=7.02$ Hz, ArH), 7.62 (1H, d, $J=6.24$ Hz, ArH)

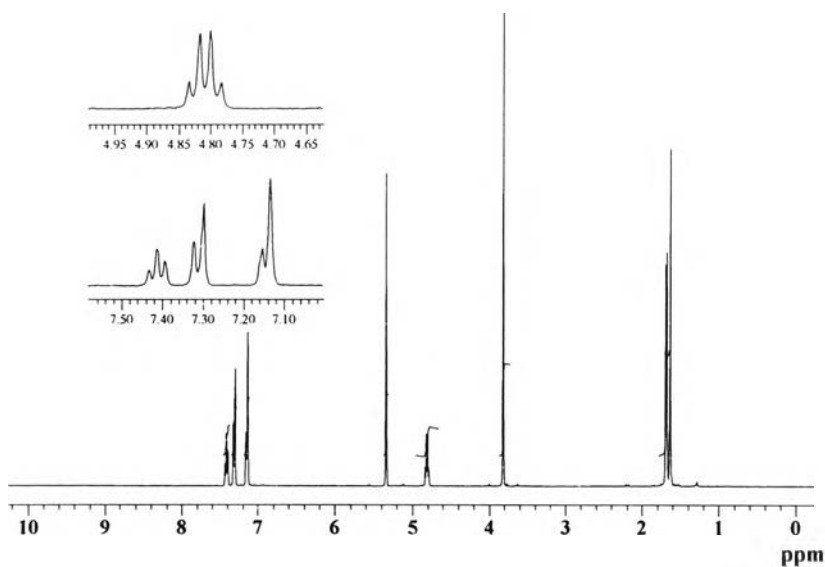
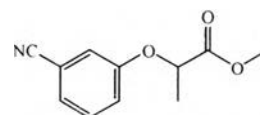


Figure B17 NMR spectrum of **3CN**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.69 (3H, d, $J=7.02$ Hz, CHCH_3), 3.82 (3H, s, OCH_3), 4.77-4.85
 (1H, q, $J=6.24$ Hz, CHCH_3), 7.12-7.18 (2H, m, ArH), 7.32
 (1H, d, $J=8.58$ Hz, ArH), 7.42 (1H, t, $J=7.80$ Hz, ArH)

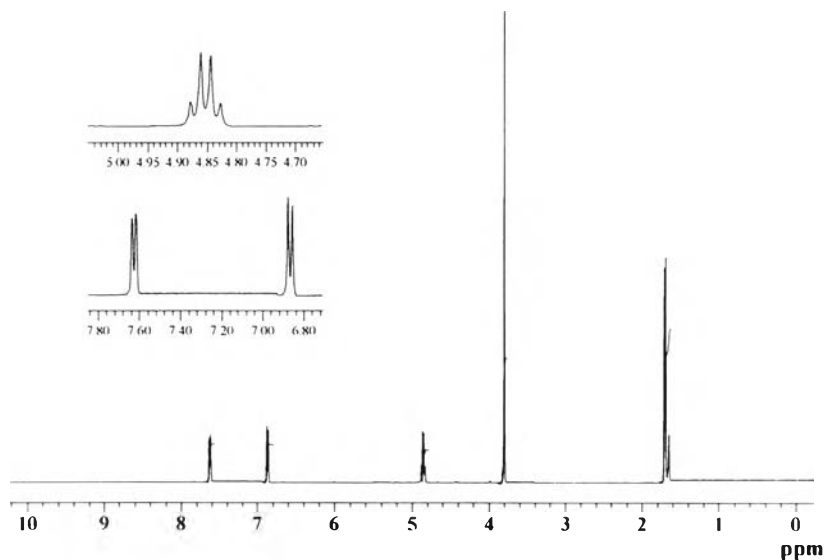
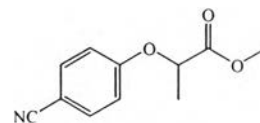


Figure B18 NMR spectrum of **4CN**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.69 (3H, d, $J=6.24$ Hz, CHCH_3), 3.79 (3H, s, OCH_3), 4.81-4.90
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.85 (2H, d, $J=8.58$ Hz, ArH), 7.62
 (2H, d, $J=7.80$ Hz, ArH)

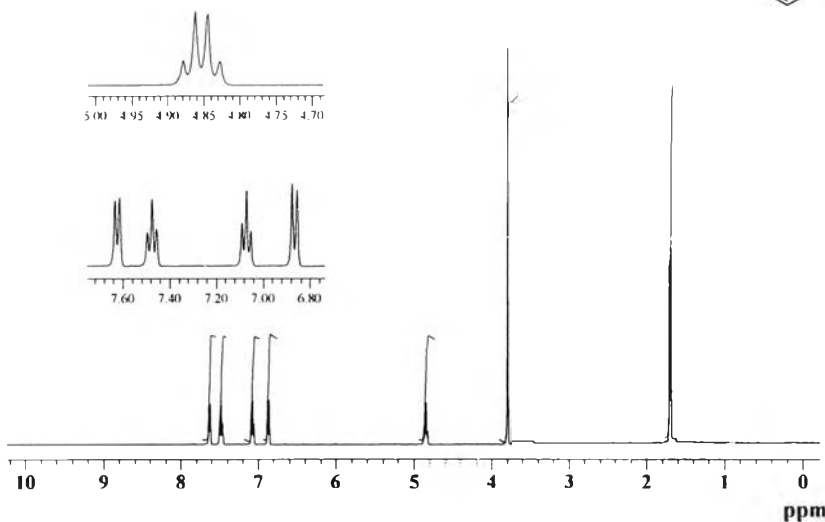
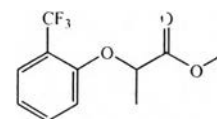


Figure B19 NMR spectrum of **2CF₃**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.70 (3H, d, *J*=6.24 Hz, CHCH₃), 3.80 (3H, s, OCH₃), 4.81-4.89
 (1H, q, *J*=7.02 Hz, CHCH₃), 6.85 (1H, d, *J*=7.80 Hz, ArH), 7.09
 (1H, t, *J*=7.02 Hz, ArH), 7.48 (1H, t, *J*=7.80 Hz, ArH),
 7.63 (1H, d, *J*=7.80 Hz, ArH)

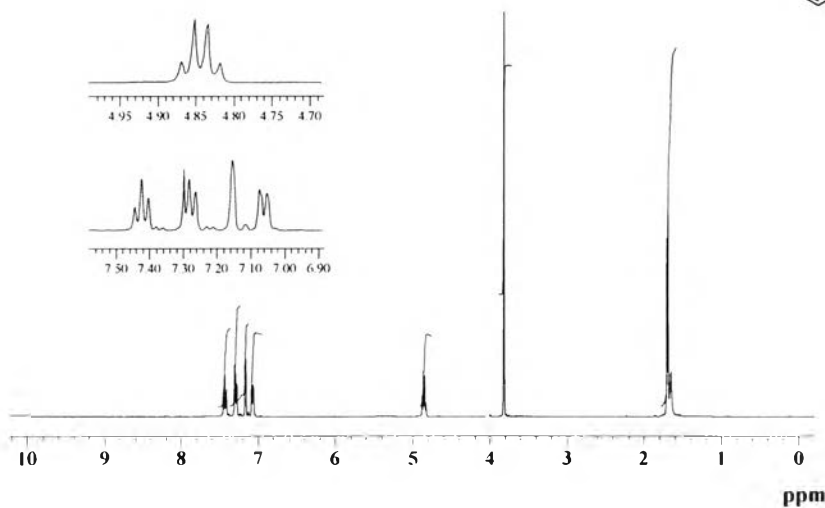
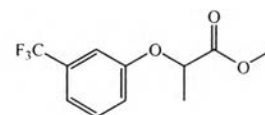


Figure B20 NMR spectrum of **3CF₃**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.69 (3H, d, *J*=7.02 Hz, CHCH₃), 3.81 (3H, s, OCH₃), 4.82-4.88
 (1H, q, *J*=7.02 Hz, CHCH₃), 7.07 (1H, d, *J*=8.58 Hz, ArH), 7.15
 (1H, s, ArH), 7.25-7.32 (1H, m, ArH), 7.44 (1H, t, *J*=7.80 Hz, ArH)

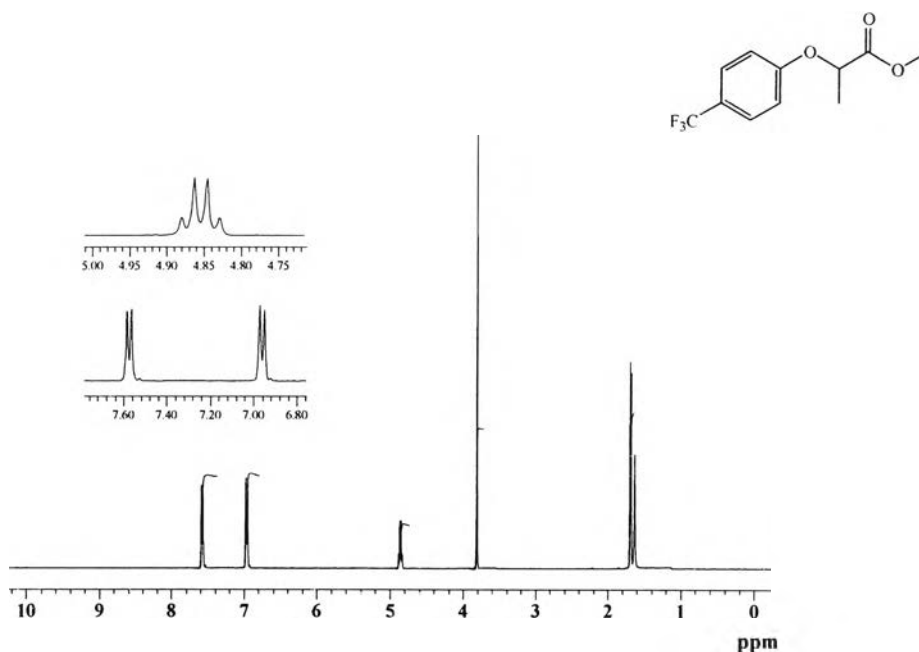


Figure B21 NMR spectrum of **4CF₃**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.69 (3H, d, *J*=6.24 Hz, CHCH₃), 3.81 (3H, s, OCH₃), 4.82-4.89
 (1H, q, *J*=7.02 Hz, CHCH₃), 6.97 (2H, d, *J*=8.58 Hz, ArH),
 7.59 (2H, d, *J*=8.58 Hz, ArH)

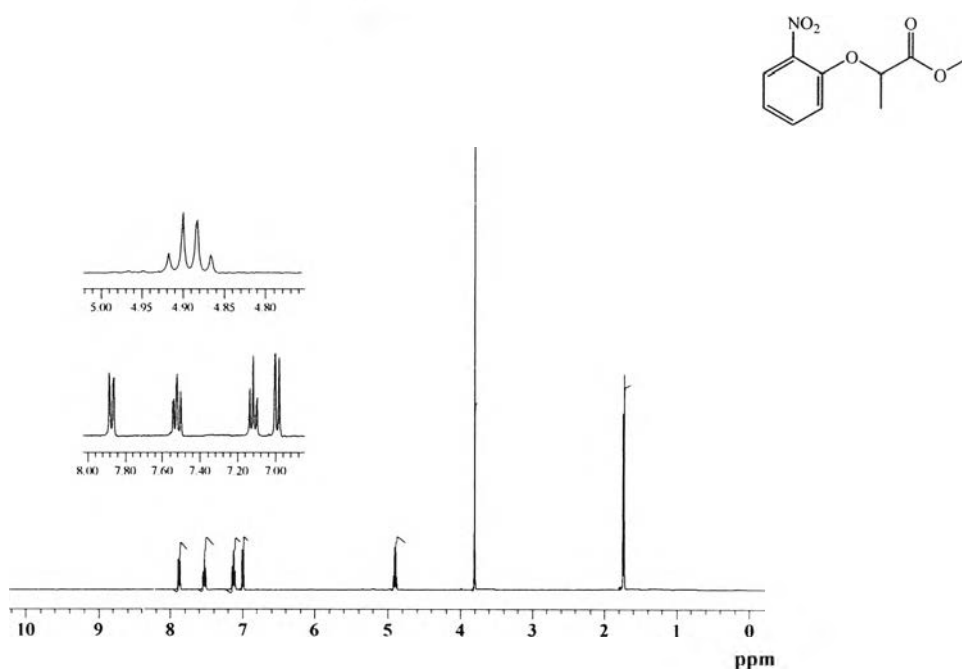


Figure B22 NMR spectrum of **2NO₂**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.72 (3H, d, *J*=7.02 Hz, CHCH₃), 3.80 (3H, s, OCH₃), 4.86-4.92
 (1H, q, *J*=7.02 Hz, CHCH₃), 6.99 (1H, d, *J*=7.80 Hz, ArH),
 7.12 (1H, t, *J*=7.02 Hz, ArH), 7.52 (1H, t, *J*=7.02 Hz, ArH),
 7.88 (1H, d, *J*=7.02 Hz, ArH)

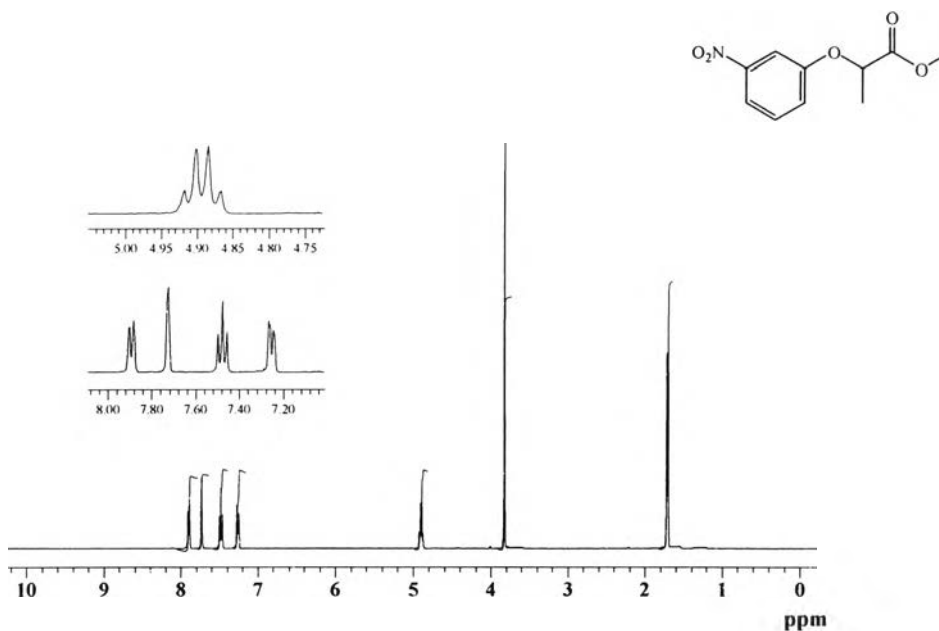


Figure B23 NMR spectrum of 3NO₂; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.70 (3H, d, *J*=6.24 Hz, CHCH₃), 3.86 (3H, s, OCH₃), 4.86-4.92
 (1H, q, *J*=7.02 Hz, CHCH₃), 7.28 (1H, d, *J*=8.58 Hz, ArH),
 7.46 (1H, t, *J*=8.58 Hz, ArH), 7.72 (1H, s, ArH), 7.90
 (1H, d, *J*=8.58 Hz, ArH)

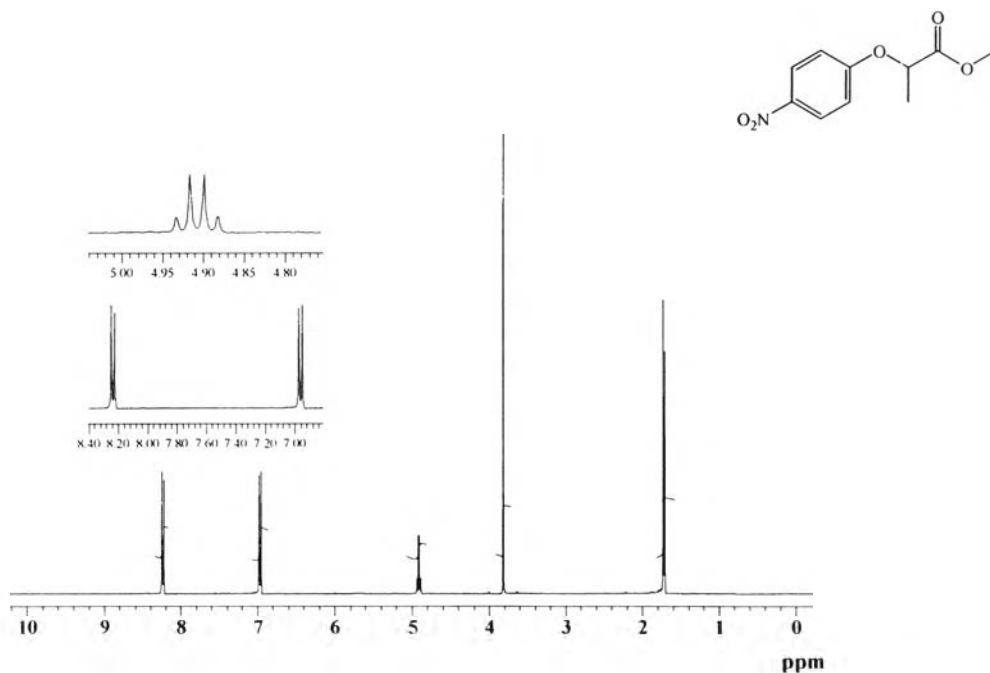


Figure B24 NMR spectrum of 4NO₂; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
 1.71 (3H, d, *J*=7.02 Hz, CHCH₃), 3.82 (3H, s, OCH₃), 4.87-4.94
 (1H, q, *J*=7.02 Hz, CHCH₃), 6.97 (2H, d, *J*=8.38 Hz, ArH),
 8.22 (2H, d, *J*=8.38 Hz, ArH)

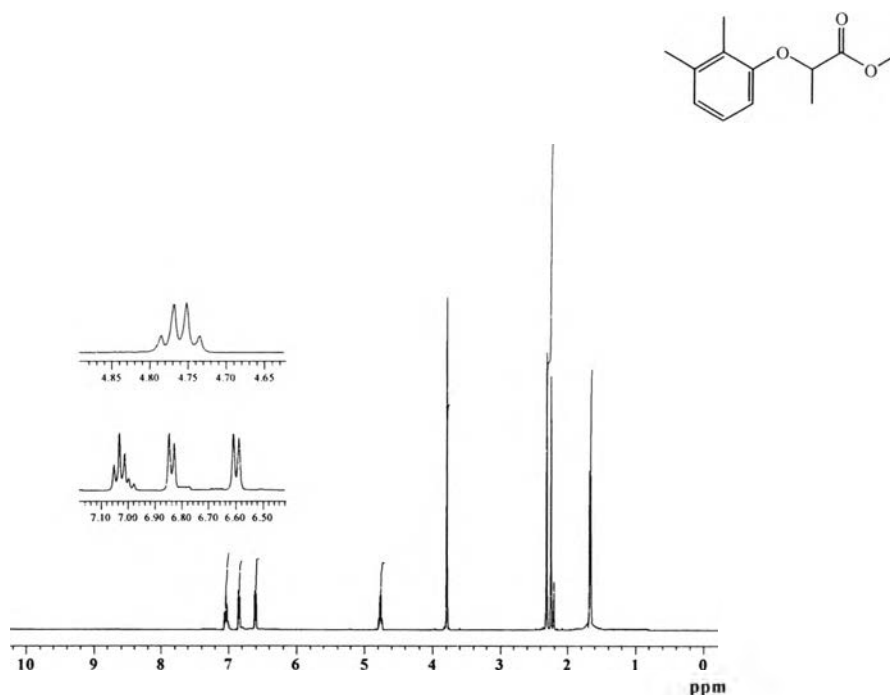


Figure B25 NMR spectrum of **2,3Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.67 (3H, d, $J=6.24$ Hz, CHCH_3), 2.31 (3H, s, ArCH_3), 2.33 (3H, s, ArCH_3), 3.78 (3H, s, OCH_3), 4.72-4.80 (1H, q, $J=6.24$ Hz, CHCH_3),
 6.59 (1H, d, $J=8.58$ Hz, ArH), 6.83 (1H, d, $J=7.02$ Hz, ArH),
 6.98-7.06 (1H, m, ArH)

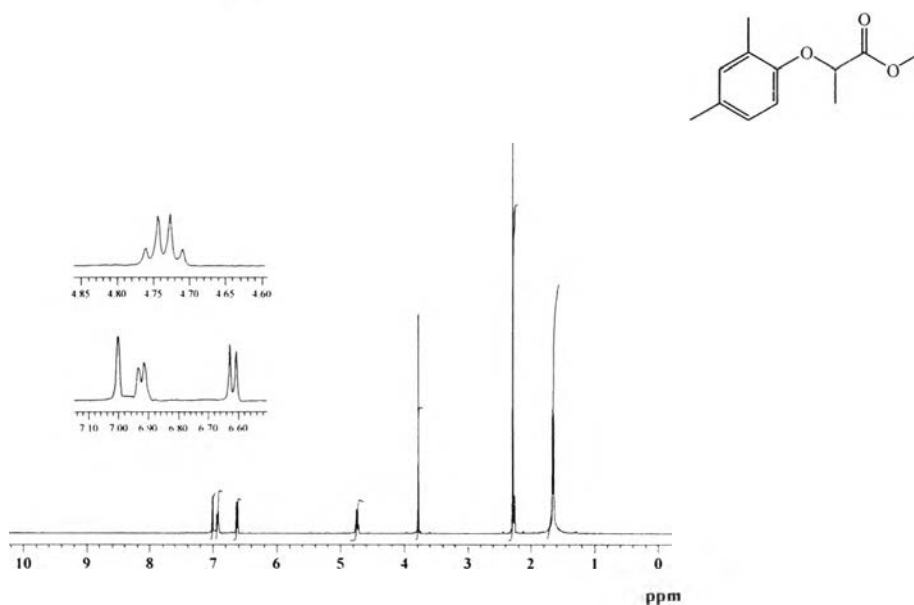


Figure B26 NMR spectrum of **2,4Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.64 (3H, d, $J=6.24$ Hz, CHCH_3), 2.28 (6H, s, 2ArCH_3), 3.78
 (3H, s, OCH_3), 4.71-4.76 (1H, q, $J=7.02$ Hz, CHCH_3), 6.63
 (1H, d, $J=8.58$ Hz, ArH), 6.93 (1H, d, $J=7.80$ Hz, ArH),
 7.00 (1H, s, ArH)

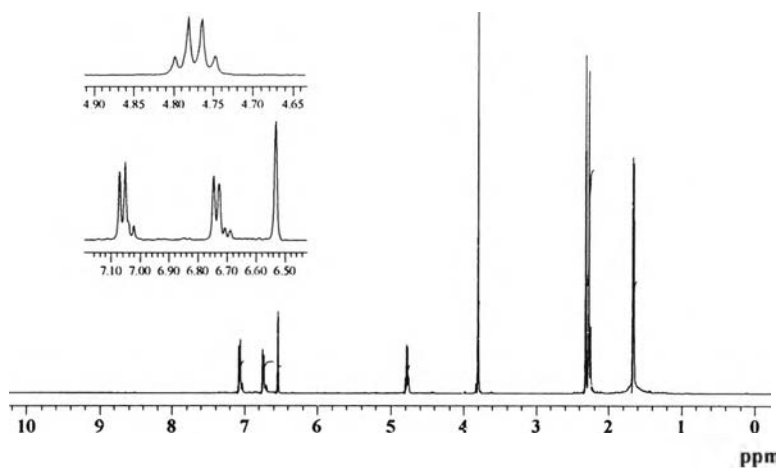
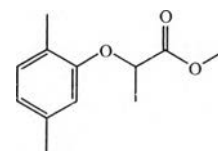


Figure B27 NMR spectrum of **2,5Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.70 (3H, d, $J=7.02$ Hz, CHCH_3), 2.28 (3H, m, ArCH_3), 2.30
 (3H, m, ArCH_3), 3.81 (3H, s, OCH_3), 4.74-5.82 (1H, q, $J=7.02$ Hz,
 CHCH_3), 6.55 (1H, s, ArH), 6.73 (1H, d, $J=7.02$ Hz, ArH), 7.06
 (1H, d, $J=7.02$ Hz, ArH)

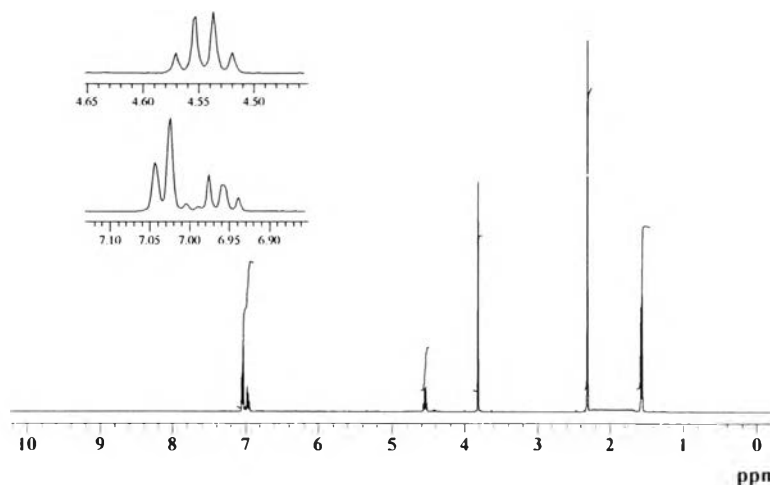
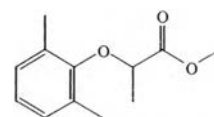


Figure B28 NMR spectrum of **2,6Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.59 (3H, d, $J=7.02$ Hz, CHCH_3), 2.31 (6H, s, 2ArCH_3), 3.82
 (3H, s, OCH_3), 4.51-4.58 (1H, q, $J=6.24$ Hz, CHCH_3),
 6.93-7.06 (3H, m, ArH)

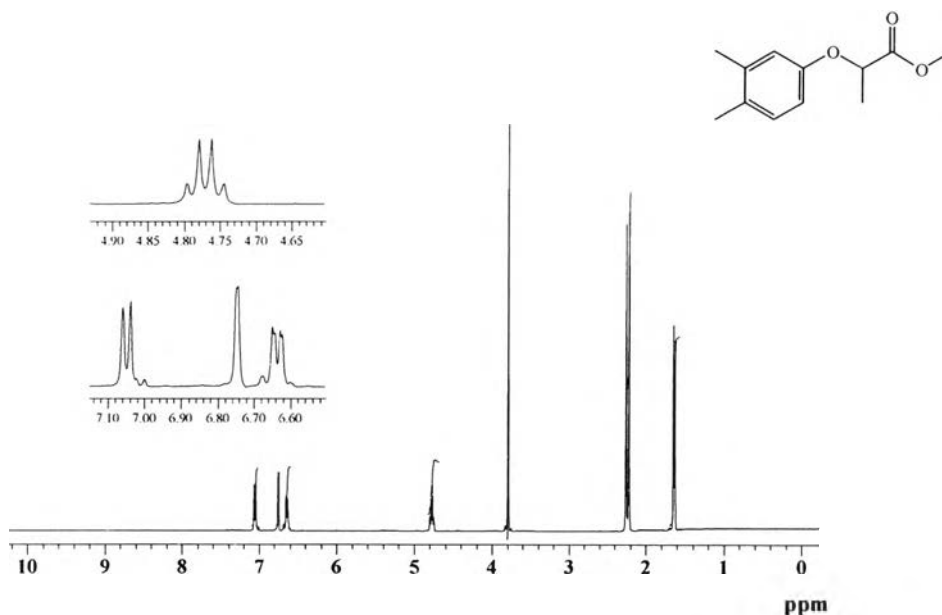


Figure B29 NMR spectrum of **3,4Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.69 (3H, d, $J=7.02$ Hz, CHCH_3), 2.22 (3H, m, ArCH_3), 2.24
 (3H, m, ArCH_3), 3.80 (3H, s, OCH_3), 4.74-4.81 (1H, q, $J=7.02$ Hz,
 CHCH_3), 6.64 (1H, d, $J=8.58$ Hz, ArH), 6.75 (1H, s, ArH), 7.06
 (2H, d, $J=8.58$ Hz, ArH)

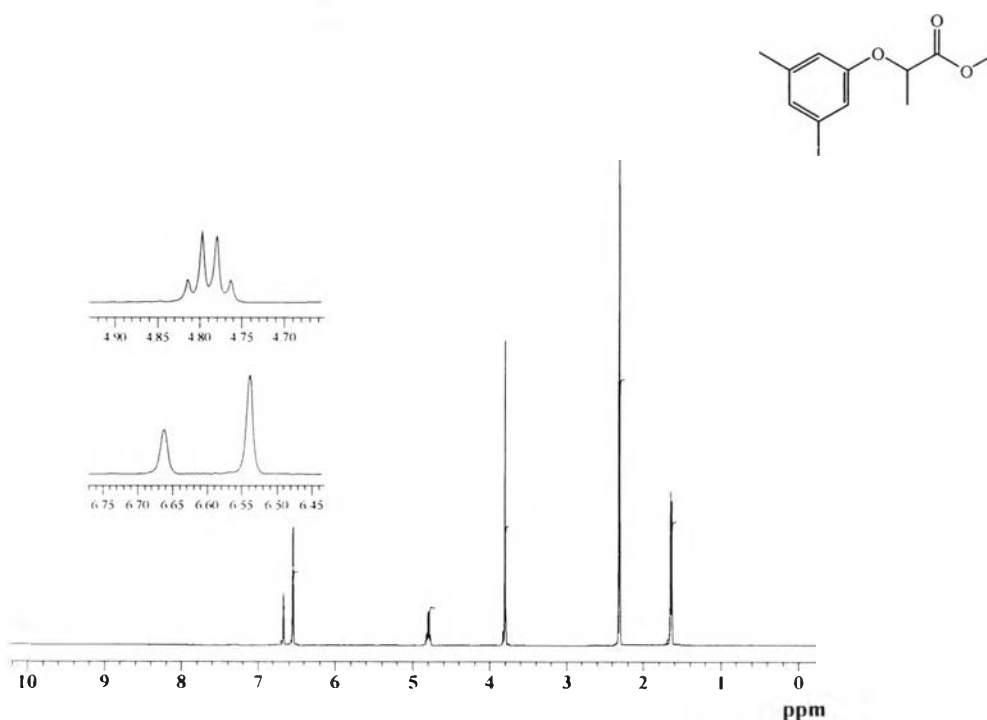


Figure B30 NMR spectrum of **3,5Me**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.65 (3H, d, $J=7.02$ Hz, CHCH_3), 2.31 (6H, s, 2ArCH_3), 3.80
 (3H, s, OCH_3), 4.75-4.82 (1H, q, $J=7.02$ Hz, CHCH_3), 6.54
 (2H, s, ArH), 6.67 (1H, s, ArH)

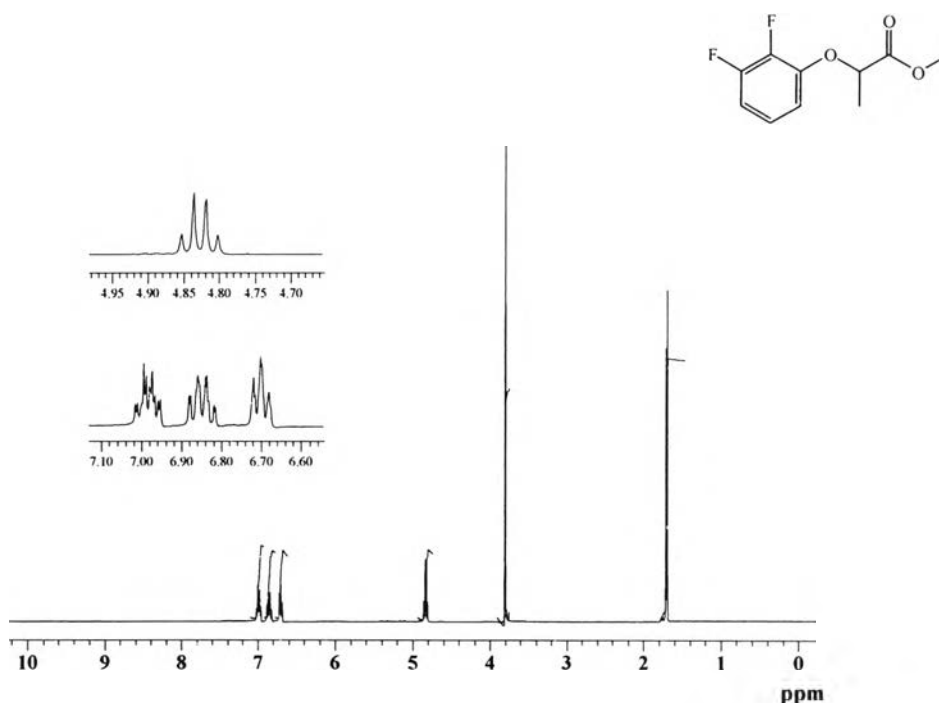


Figure B31 NMR spectrum of **2,3F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.66 (3H, d, $J=7.02$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.80-4.86
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.70 (1H, t, $J=7.02$ Hz, ArH),
 6.80-6.90 (1H, m, ArH), 6.94-7.03 (1H, m, ArH)

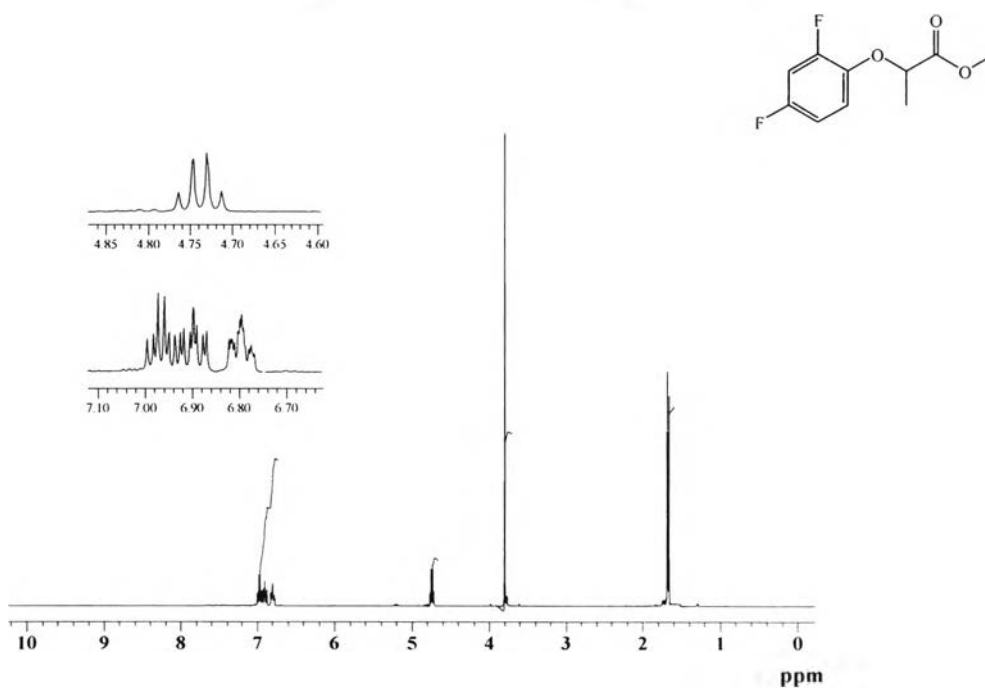


Figure B32 NMR spectrum of **2,4F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.69 (3H, d, $J=7.02$ Hz, CHCH_3), 3.85 (3H, s, OCH_3), 4.70-4.78
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.76-6.83 (1H, m, ArH), 6.87-7.02
 (2H, m, ArH)

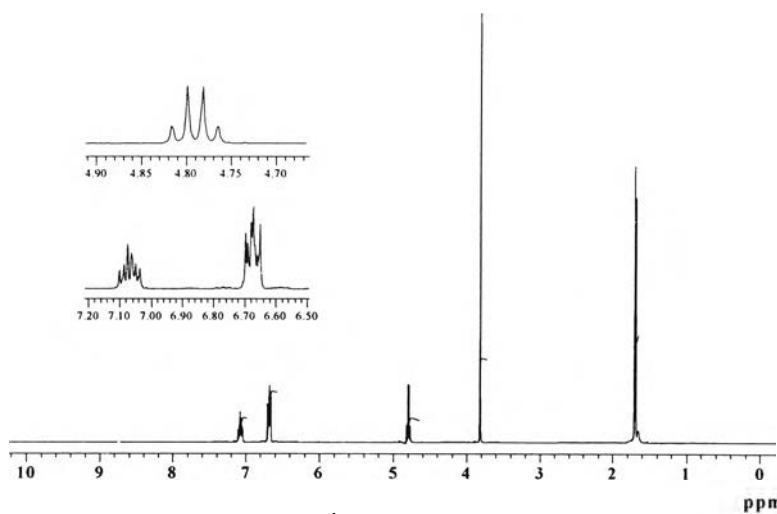
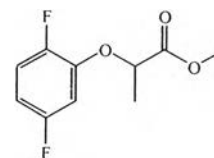


Figure B33 NMR spectrum of **2,5F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.70 (3H, d, $J=6.24$ Hz, CHCH_3), 3.81 (3H, s, OCH_3), 4.76-4.82
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.64-6.72 (2H, m, ArH), 7.02-7.11
 (1H, m, ArH)

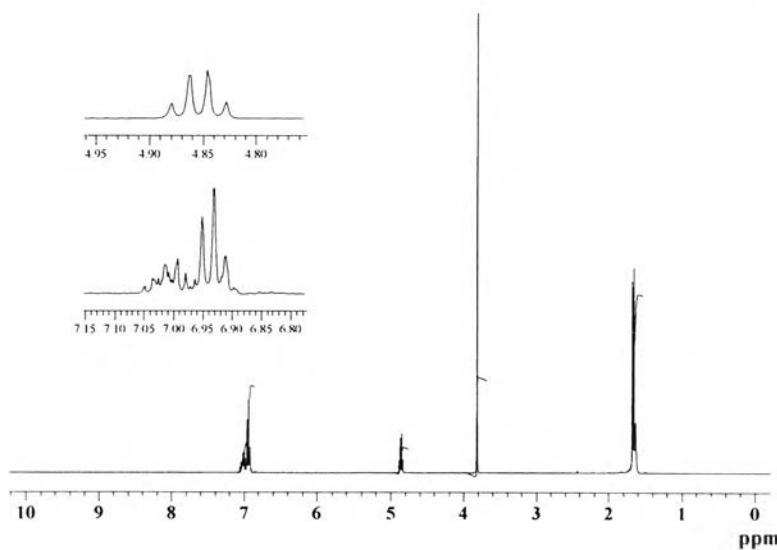
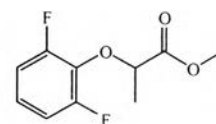


Figure B34 NMR spectrum of **2,6F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.67 (3H, d, $J=7.02$ Hz, CHCH_3), 3.81 (3H, s, OCH_3), 4.82-4.89
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.89-7.06 (3H, m, ArH)

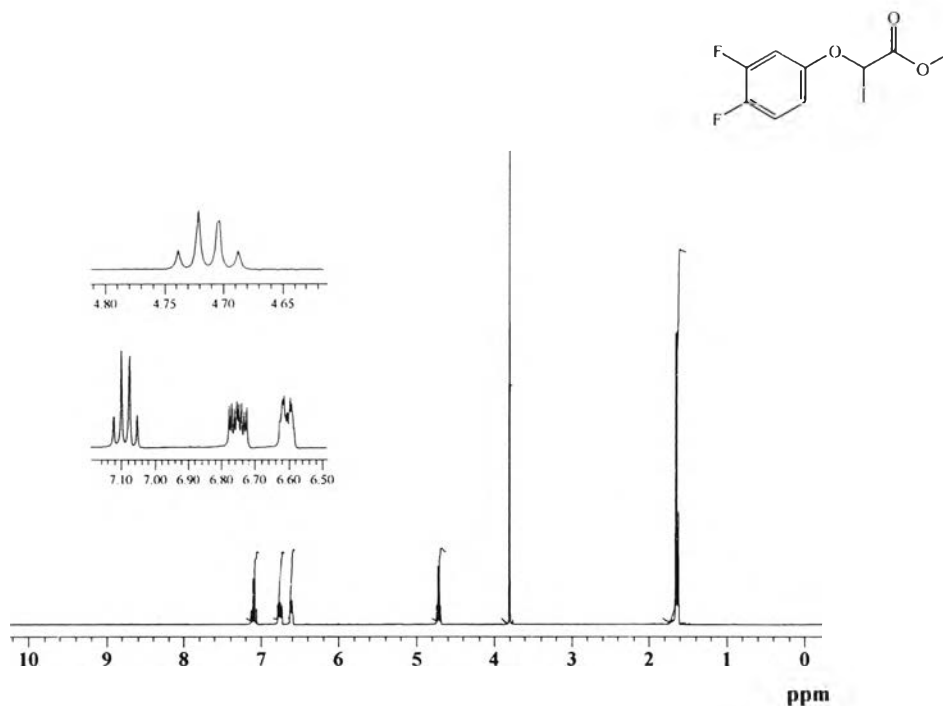


Figure B35 NMR spectrum of **3,4F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.62 (3H, d, $J=6.24$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.68-4.75
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.58-6.64 (1H, m, ArH),
 6.72-6.78 (1H, m, ArH), 7.06-7.14 (1H, m, ArH)

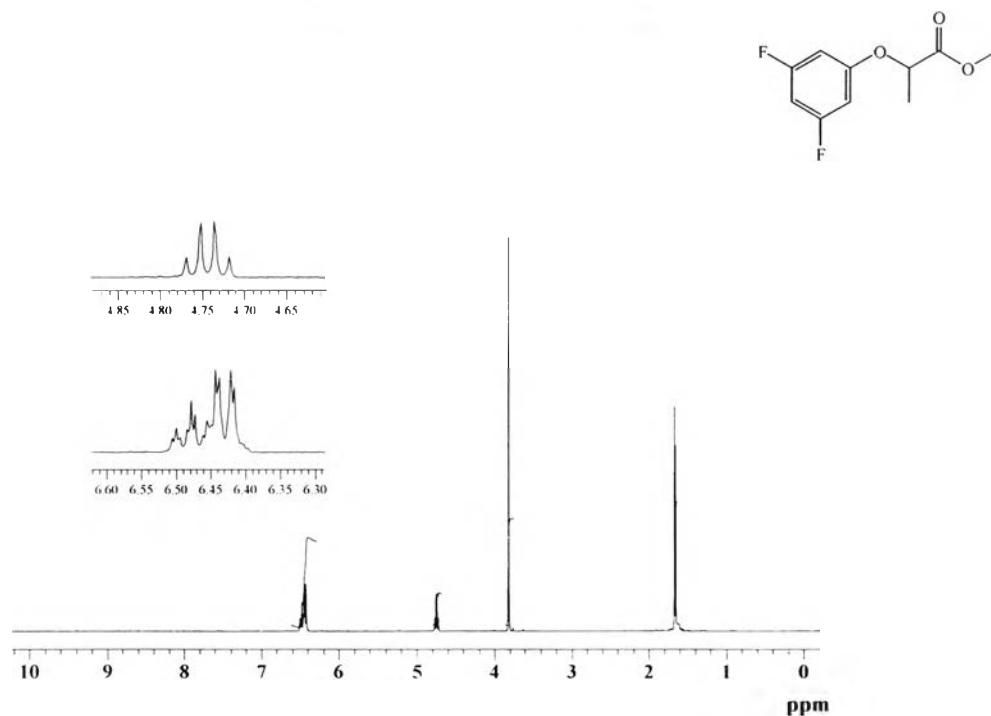


Figure B36 NMR spectrum of **3,5F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.67 (3H, d, $J=7.02$ Hz, CHCH_3), 3.84 (3H, s, OCH_3), 4.71-4.78
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.40-6.52 (3H, m, ArH)

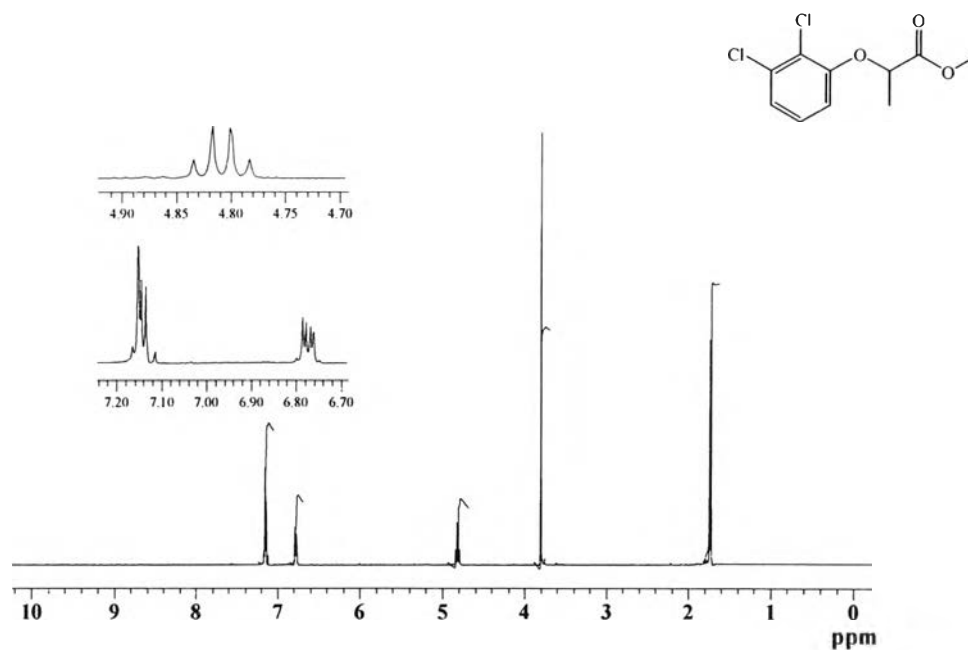


Figure B37 NMR spectrum of **2,3Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.74 (3H, d, $J=7.02$ Hz, CHCH_3), 3.82 (3H, s, OCH_3), 4.78-4.84
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.75-6.80 (1H, m, ArH), 7.12-7.18
 (2H, m, ArH)

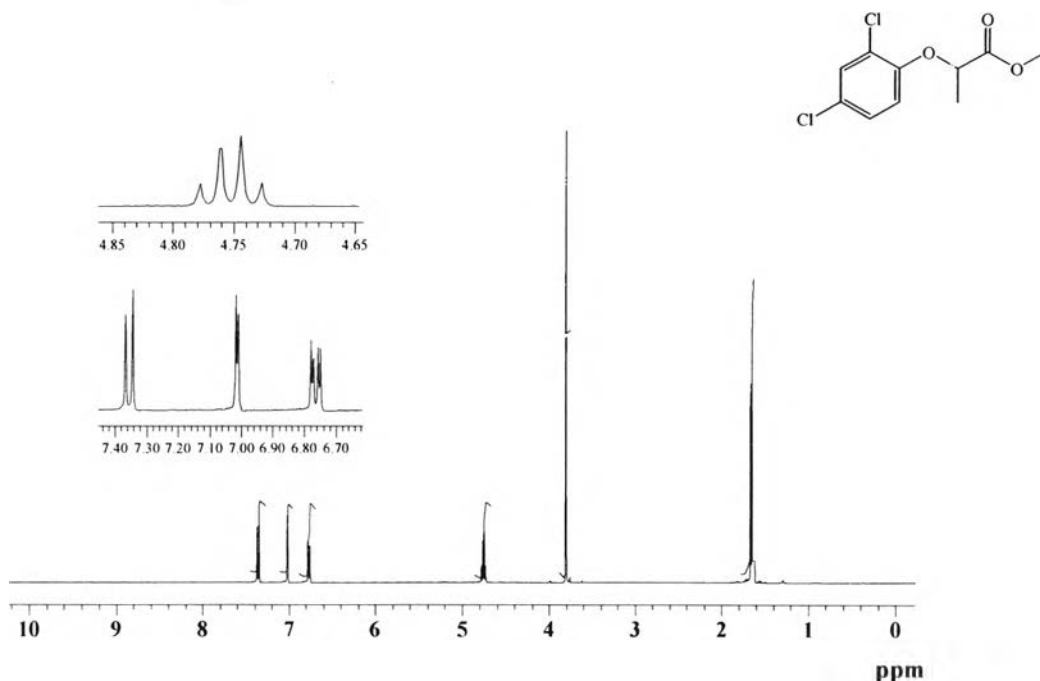


Figure B38 NMR spectrum of **2,4Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.62 (3H, d, $J=6.24$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.72-4.79
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.76 (1H, d, $J=6.24$ Hz, ArH), 7.02
 (1H, s, ArH), 7.36 (1H, d, $J=6.24$ Hz, ArH)

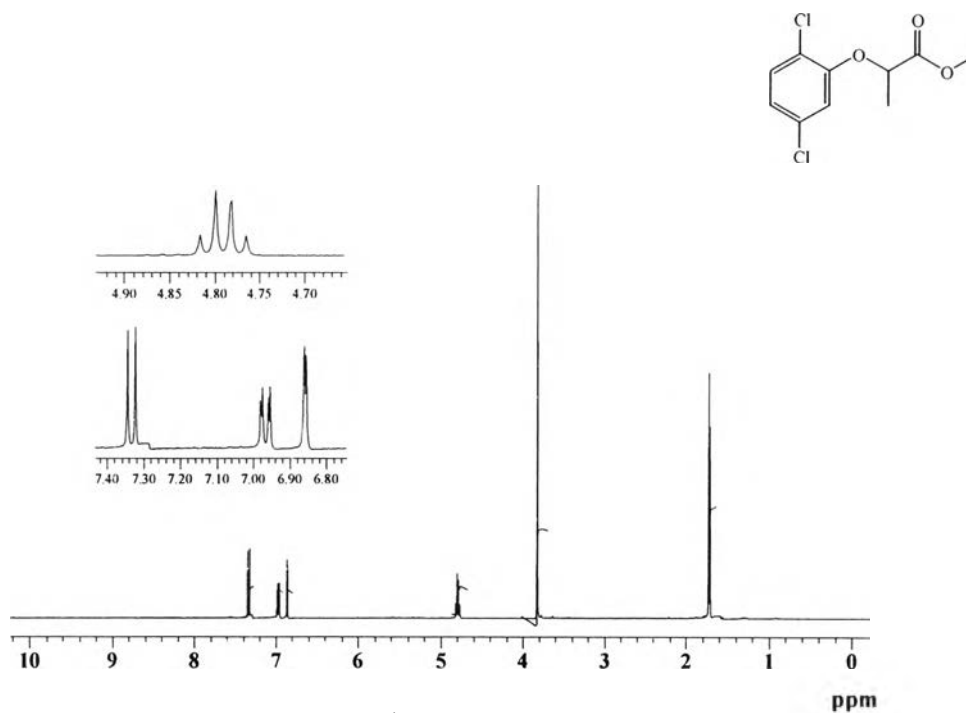


Figure B39 NMR spectrum of **2,5Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.73 (3H, d, $J=7.02$ Hz, CHCH_3), 3.82 (3H, s, OCH_3), 4.76-4.82 (1H, q, $J=7.02$ Hz, CHCH_3), 6.86 (1H, s, ArH), 6.96 (1H, d, $J=6.24$ Hz, ArH), 7.33 (1H, d, $J=8.58$ Hz, ArH)

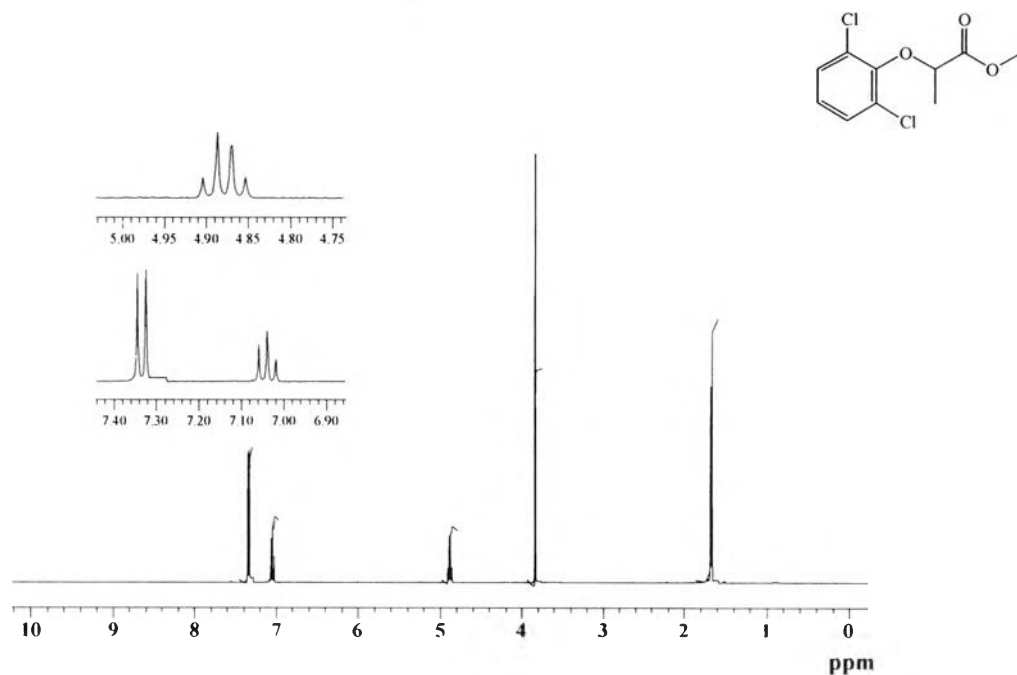


Figure B40 NMR spectrum of **2,6Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.66 (3H, d, $J=7.02$ Hz, CHCH_3), 3.83 (3H, s, OCH_3), 4.85-4.92 (1H, q, $J=7.02$ Hz, CHCH_3), 7.05 (1H, t, $J=7.81$ Hz, ArH), 7.34 (2H, d, $J=7.81$ Hz, ArH)

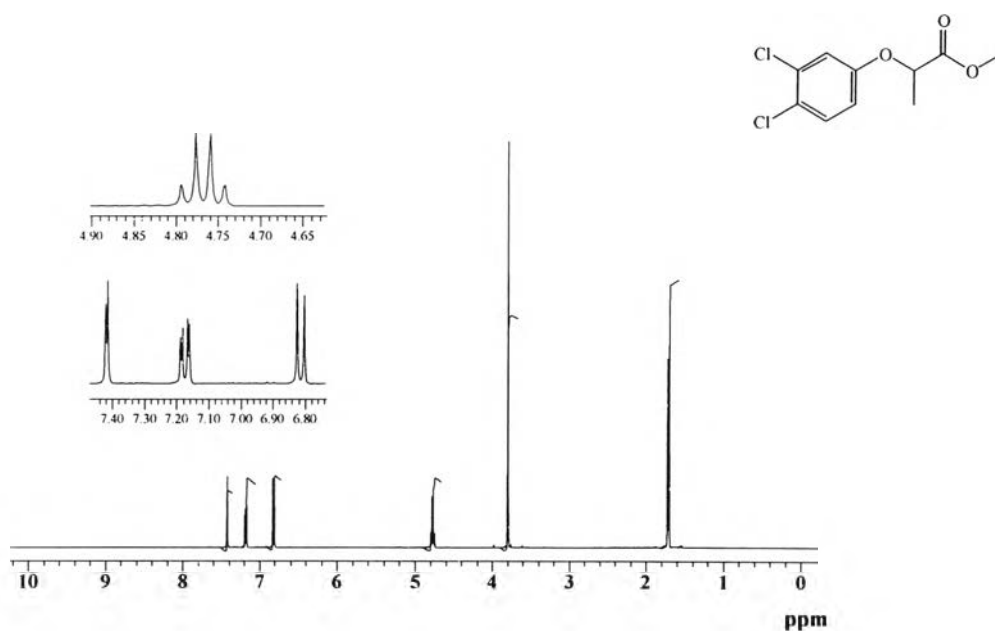


Figure B41 NMR spectrum of **3,4Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.70 (3H, d, $J=6.24$ Hz, CHCH_3), 3.80 (3H, s, OCH_3), 4.74-4.81
 (1H, q, $J=7.02$ Hz, CHCH_3), 6.83 (1H, d, $J=8.58$ Hz, ArH),
 7.17 (1H, d, $J=6.24$ Hz, ArH), 7.45 (1H, s, ArH)

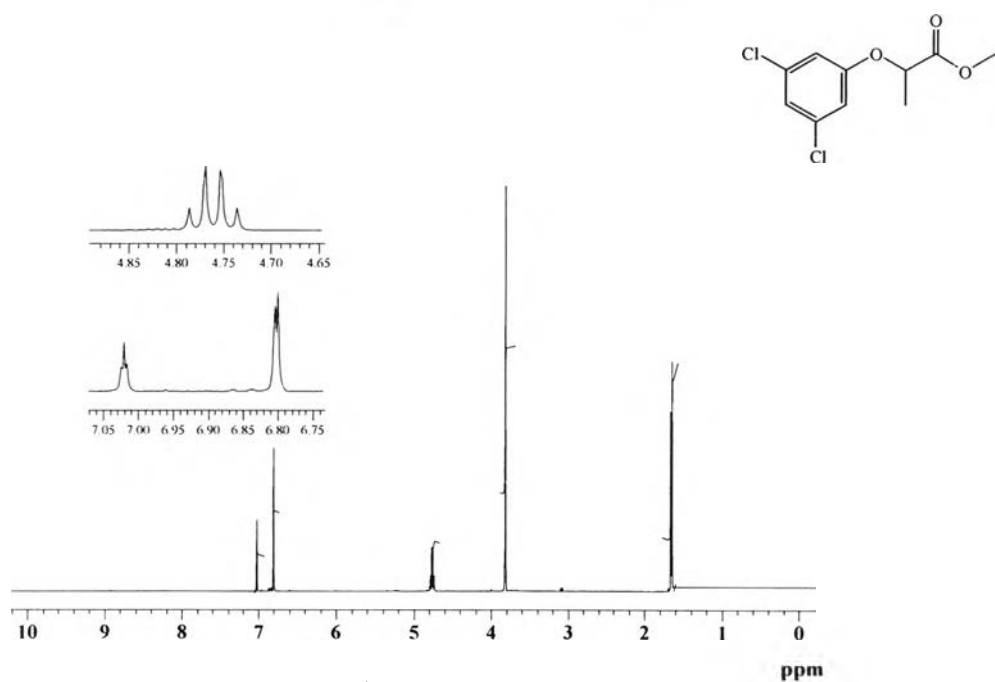


Figure B42 NMR spectrum of **3,5Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.70 (3H, d, $J=7.02$ Hz, CHCH_3), 3.85 (3H, s, OCH_3), 4.73-4.79 (1H, q,
 $J=6.24$ Hz, CHCH_3), 6.80 (2H, s, ArH), 7.01-7.04 (1H, m, ArH)

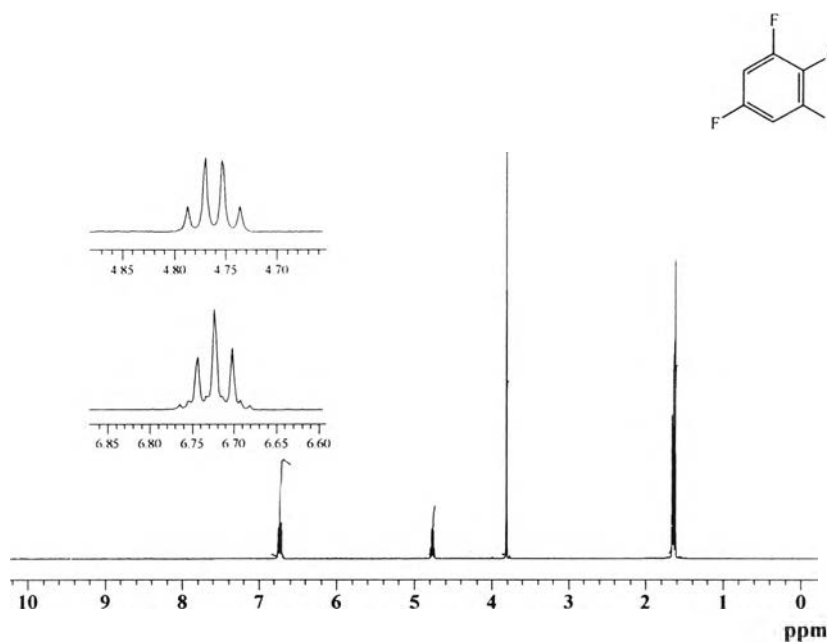


Figure B43 NMR spectrum of **2,4,6F**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.64 (3H, d, $J=7.02$ Hz, CHCH_3), 3.81 (3H, s, OCH_3), 4.74-4.79
 (1H, q, $J=6.24$ Hz, CHCH_3), 6.73 (2H, t, $J=7.80$ Hz, ArH)

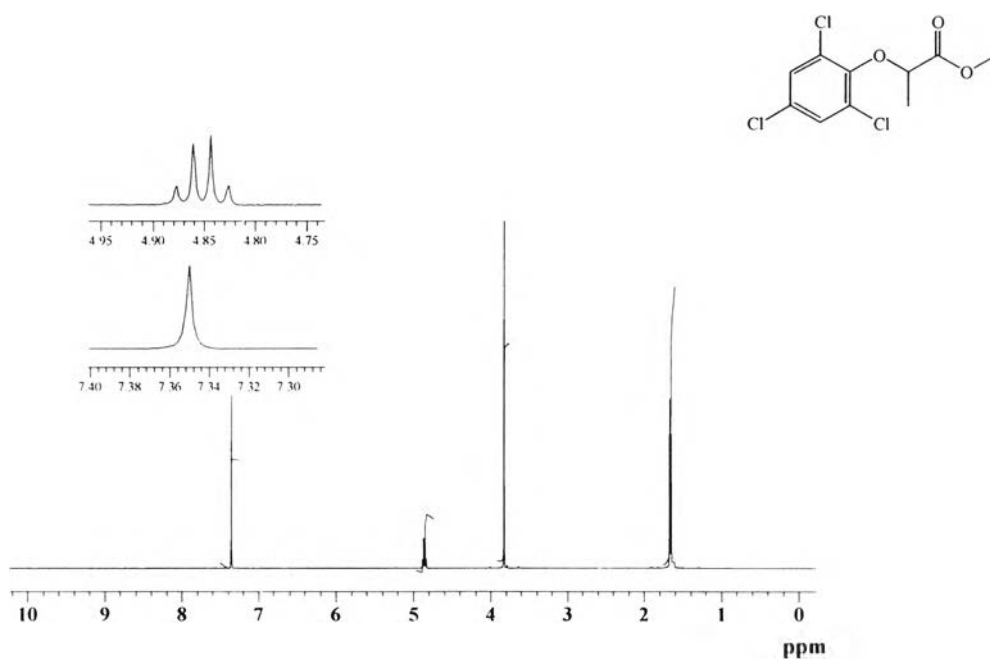


Figure B44 NMR spectrum of **2,4,6Cl**; ^1H NMR (CDCl_3 , 400 MHz), δ (ppm):
 1.67 (3H, d, $J=6.24$ Hz, CHCH_3), 3.83 (3H, s, OCH_3), 4.82-4.89
 (1H, q, $J=7.02$ Hz, CHCH_3), 7.35 (2H, s, ArH)

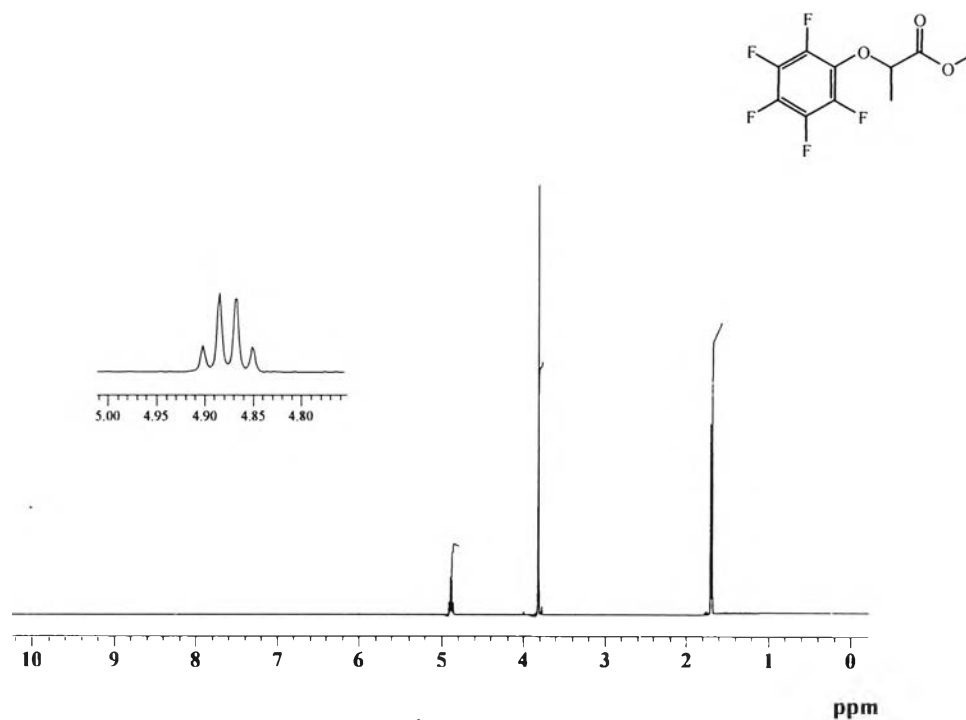


Figure B45 NMR spectrum of **pentaF**; ¹H NMR (CDCl₃, 400 MHz), δ (ppm):
1.69 (3H, d, $J=7.02$ Hz, CHCH₃), 3.81 (3H, s, OCH₃), 4.85-4.92
(1H, q, $J=7.02$ Hz, CHCH₃)

Appendix C

Thermodynamic Studies

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

analytes	Equation :		R^2
	$\ln k' = m (1/T) + c$		
	m	c	
1	6344.80	-14.22	0.9998
2F	6394.60	-14.33	0.9997
3F	6368.80	-14.32	0.9998
4F	6409.30	-14.38	0.9998
2Cl	6734.80	-14.29	0.9997
3Cl	6748.90	-14.34	0.9996
4Cl	6822.30	-14.42	0.9997
2Br	7142.90	-14.82	0.9981
3Br	6983.10	-14.47	0.9998
4Br	7066.60	-14.54	0.9998
2OMe	6995.60	-14.76	0.9998
3OMe	7164.10	-14.92	0.9998
4OMe	7182.30	-14.91	0.9998
2Me	6497.00	-14.32	0.9998
3Me	6714.80	-14.67	0.9998

analytes	Equation :		R ²
	ln k' = m (1/T) + c		
	m	c	
4Me	6740.00	-14.67	0.9998
2CN	7407.20	-14.90	0.9998
3CN	7314.10	-14.77	0.9998
4CN	7531.10	-14.98	0.9998
2CF ₃	6540.20	-14.61	0.9998
3CF ₃	6470.50	-14.70	0.9998
4CF ₃	6637.90	-14.89	0.9998
2NO ₂	7536.80	-14.89	0.9999
3NO ₂	7508.70	-14.82	0.9999
4NO ₂	7830.70	-15.16	0.9999
2,3Me	6898.90	-14.65	0.9998
2,4Me	6805.00	-14.59	0.9997
2,5Me	6742.50	-14.53	0.9997
2,6Me	6651.80	-14.28	0.9998
3,4Me	7105.10	-14.96	0.9998
3,5Me	6995.70	-14.93	0.9998
2,3F	6525.70	-14.57	0.9998
2,4F	6290.10	-14.29	0.9998
2,5F	6423.00	-14.51	0.9997
2,6F	6278.80	-14.18	0.9997
3,4F	6463.90	-14.49	0.9998

analytes	Equation :		R ²
	ln k' = m (1/T) + c		
	m	c	
3,5F	6260.70	-14.32	0.9998
2,3Cl	7278.80	-14.63	0.9998
2,4Cl	7256.90	-14.64	0.9998
2,5Cl	7054.20	-14.44	0.9998
2,6Cl	6908.10	-14.12	0.9998
3,4Cl	7190.30	-14.51	0.9998
3,5Cl	7031.70	-14.44	0.9998
2,4,6F	6136.40	-14.21	0.9997
2,4,6Cl	7315.50	-14.60	0.9999
penta F	6203.10	-14.48	0.9994

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

analytes	less retained enantiomer			more retained enantiomer		
	equation :		R^2	equation :		R^2
	$\ln k' = m (1/T) + c$			$\ln k' = m (1/T) + c$		
m	c		m	c		
1	6853.30	-15.16	0.9993	7038.00	-15.57	0.9993
2F	6862.20	-15.27	0.9997	7081.50	-15.75	0.9994
3F	7164.30	-15.94	0.9995	7345.50	-16.35	0.9994
4F	7307.00	-16.62	0.9996	7644.30	-16.91	0.9993
2Cl	6840.40	-14.39	0.9993	6994.80	-14.71	0.9992
3Cl	7119.60	-14.96	0.9993	7212.20	-15.16	0.9990
4Cl	7447.80	-15.51	0.9991	7558.20	-15.72	0.9992
2Br	7056.20	-14.50	0.9995	7185.40	-14.76	0.9994
3Br	7344.30	-15.06	0.9994	7434.10	-15.25	0.9992
4Br	7741.50	-15.71	0.9992	7986.50	-16.21	0.9992
2OMe	7274.50	-15.25	0.9992	7363.00	-15.43	0.9990
3OMe	7344.20	-15.17	0.9993	7440.30	-15.37	0.9993
4OMe	7517.20	-15.45	0.9994	7664.10	-15.75	0.9993
2Me	6957.30	-15.23	0.9997	7241.20	-15.85	0.9996
3Me	7419.30	-16.11	0.9997	7573.60	-16.44	0.9995
4Me	7551.90	-16.30	0.9997	7767.90	-16.77	0.9995
2CN	7620.80	-15.30	0.9994	7764.00	-15.59	0.9994
3CN	7918.50	-15.91	0.9994	7993.30	-16.07	0.9991

analytes	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	
4CN	8226.70	-16.19	0.9992	8462.50	-16.65	0.9991
2CF ₃	6891.10	-15.33	0.9996	7109.20	-15.80	0.9995
3CF ₃	7082.00	-15.94	0.9995	7432.60	-16.72	0.9992
4CF ₃	7749.90	-17.13	0.9996	8463.90	-18.68	0.9992
2NO ₂	7849.60	-15.50	0.9996	7984.70	-15.78	0.9995
3NO ₂	8066.80	-15.88	0.9995	8187.30	-16.13	0.9994
4NO ₂	8609.20	-16.53	0.9994	8822.50	-16.94	0.9993
2,3Me	7472.40	-15.79	0.9998	7644.10	-16.16	0.9996
2,4Me	7304.40	-15.56	0.9998	7535.40	-16.05	0.9997
2,5Me	7151.70	-15.33	0.9998	7213.60	-15.47	0.9997
2,6Me	7220.40	-15.44	0.9997	7220.40	-15.44	0.9997
3,4Me	7992.80	-16.75	0.9996	8132.00	-17.05	0.9996
3,5Me	7476.10	-15.87	0.9997	7590.50	-16.12	0.9997
2,3F	6999.80	-15.54	0.9997	7286.10	-16.16	0.9994
2,4F	6922.50	-15.55	0.9997	7206.30	-16.16	0.9996
2,5F	6947.90	-15.57	0.9997	7102.70	-15.90	0.9996
2,6F	6554.50	-14.71	0.9997	6663.20	-14.96	0.9998
3,4F	7468.80	-16.58	0.9996	7511.50	-16.63	0.9990
3,5F	6927.50	-15.64	0.9997	7112.50	-16.07	0.9995
2,3Cl	7661.80	-15.33	0.9997	7790.30	-15.50	0.9996

analytes	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	
2,4Cl	7941.80	-15.90	0.9992	8092.10	-16.21	0.9992
2,5Cl	7554.90	-15.38	0.9992	7637.60	-15.55	0.9991
2,6Cl	7163.80	-14.57	0.9995	7164.10	-14.57	0.9995
3,4Cl	7577.90	-15.30	0.9994	7815.80	-15.78	0.9994
3,5Cl	7622.70	-15.56	0.9992	7653.00	-15.62	0.9991
2,4,6F	6494.80	-14.89	0.9996	6627.90	-15.18	0.9997
2,4,6Cl	7619.40	-15.11	0.9995	7619.80	-15.11	0.9995
pentaF	6349.70	-14.76	0.9995	6523.50	-15.14	0.9996

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

analytes	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	6294.00	-14.75	0.9983	6942.60	-15.45	0.9964
2F	6845.10	-15.27	0.9993	7062.10	-15.78	0.9988
3F	6848.20	-15.30	0.9984	7149.90	-16.00	0.9979
4F	6975.00	-15.56	0.9992	7215.50	-16.11	0.9987
2Cl	6870.90	-14.49	0.9993	6884.00	-14.52	0.9991
3Cl	6923.00	-14.62	0.9992	7037.70	-14.86	0.9987
4Cl	7173.20	-15.04	0.9991	7315.00	-15.34	0.9985
2Br	7033.10	-14.49	0.9994	7033.10	-14.49	0.9994
3Br	7113.50	-14.64	0.9994	7211.20	-14.85	0.9990
4Br	7413.40	-15.15	0.9992	7544.10	-15.42	0.9987
2OMe	6979.20	-14.65	0.9995	6979.20	-14.65	0.9995
3OMe	6979.20	-14.65	0.9992	7509.50	-15.53	0.9987
4OMe	7560.10	-15.58	0.9985	7606.60	-15.68	0.9987
2Me	6596.80	-14.49	0.9997	6596.80	-14.49	0.9997
3Me	7035.60	-15.32	0.9993	7320.10	-15.96	0.9987
4Me	7213.80	-15.65	0.9991	7650.20	-16.62	0.9982
2CN	7514.50	-15.02	0.9995	7514.50	-15.02	0.9995
3CN	7825.50	-15.71	0.9992	7845.80	-15.75	0.9991

analytes	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	
4CN	8569.90	-16.88	0.9989	8595.40	-16.93	0.9988
2CF ₃	6481.00	-14.40	0.9998	6658.90	-14.82	0.9976
3CF ₃	7024.60	-15.89	0.9981	7156.30	-16.18	0.9974
4CF ₃	7583.80	-16.90	0.9988	7918.20	-17.66	0.9982
2NO ₂	7776.00	-15.25	0.9997	7776.00	-15.25	0.9997
3NO ₂	7957.00	-15.63	0.9996	8014.70	-15.75	0.9994
4NO ₂	9510.30	-18.33	0.9986	9579.90	-18.47	0.9984
2,3Me	7090.00	-15.05	0.9990	7090.00	-15.05	0.9990
2,4Me	7073.00	-15.14	0.9994	7073.00	-15.14	0.9994
2,5Me	6845.00	-14.73	0.9997	6845.00	-14.73	0.9997
2,6Me	6740.50	-14.45	0.9998	6740.50	-14.45	0.9998
3,4Me	7563.40	-15.92	0.9991	7945.20	-16.76	0.9983
3,5Me	7238.10	-15.42	0.9996	7314.90	-15.59	0.9993
2,3F	6976.30	-15.50	0.9992	7195.00	-16.01	0.9986
2,4F	6793.70	-15.34	0.9995	6882.40	-15.54	0.9989
2,5F	6937.30	-15.58	0.9992	7057.90	-15.86	0.9987
2,6F	6851.20	-15.42	0.9989	6876.80	-15.48	0.9988
3,4F	7308.00	-16.28	0.9989	7472.90	-16.66	0.9985
3,5F	6892.50	-15.66	0.9987	7103.40	-16.14	0.9985
2,3Cl	7401.10	-14.81	0.9998	7401.10	-14.81	0.9998

analytes	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	
2,4Cl	7581.60	-15.22	0.9996	7692.20	-15.45	0.9993
2,5Cl	7200.50	-14.68	0.9998	7200.50	-14.68	0.9998
2,6Cl	6984.30	-14.23	0.9999	6984.30	-14.23	0.9999
3,4Cl	7400.70	-15.00	0.9996	7425.60	-15.05	0.9995
3,5Cl	7330.50	-14.99	0.9996	7387.60	-15.11	0.9994
2,4,6F	6481.50	-14.92	0.9993	6550.10	-15.08	0.9990
2,4,6Cl	7402.00	-14.71	0.9998	7402.10	-14.71	0.9998
pentaF	6605.70	-15.33	0.9989	6759.70	-15.69	0.9986

Table 4 Thermodynamic parameters of all analytes calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on OV-1701 column

analytes	enthalpy term (kcal/mol)	entropy term (cal/mol·K)
	$-\Delta H$	$-\Delta S$
1	12.61	17.29
2F	12.71	17.50
3F	12.65	17.49
4F	12.74	17.60
2Cl	13.38	17.42
3Cl	13.41	17.53
4Cl	13.56	17.67
2Br	14.19	18.48
3Br	13.88	17.77
4Br	14.04	17.93
2OMe	13.90	18.35
3OMe	14.24	18.67
4OMe	14.27	18.66
2Me	12.91	17.48
3Me	13.34	18.17
4Me	13.39	18.19
2CN	14.72	18.63
3CN	14.53	18.37
4CN	14.96	18.79

analytes	enthalpy term (kcal/mol)	entropy term (cal/mol·K)
	$-\Delta H$	$-\Delta S$
2CF ₃	13.00	18.07
3CF ₃	12.86	18.23
4CF ₃	13.19	18.61
2NO ₂	14.98	18.62
3NO ₂	14.92	18.48
4NO ₂	15.56	19.15
2,3Me	13.71	18.14
2,4Me	13.52	18.02
2,5Me	13.40	17.90
2,6Me	13.22	17.41
3,4Me	14.12	18.76
3,5Me	13.90	18.69
2,3F	12.97	17.98
2,4F	12.50	17.41
2,5F	12.76	17.85
2,6F	12.48	17.20
3,4F	12.84	17.82
3,5F	12.44	17.47
2,3Cl	14.46	18.10
2,4Cl	14.42	18.11
2,5Cl	14.02	17.72
2,6Cl	13.73	17.09

analytes	enthalpy term (kcal/mol)	entropy term (cal/mol·K)
	$-\Delta H$	$-\Delta S$
3,4Cl	14.29	17.87
3,5Cl	13.97	17.72
2,4,6F	12.19	17.27
2,4,6Cl	14.54	18.03
pentaF	12.33	17.79

Table 5 Thermodynamic parameters of all analytes calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on BSiMe column

analytes	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	13.62	13.98	0.37	19.16	19.96	0.80
2F	13.64	14.07	0.44	19.37	20.32	0.94
3F	14.24	14.60	0.36	20.71	21.51	0.80
4F	14.52	15.19	0.67	22.05	22.63	0.57
2Cl	13.59	13.90	0.31	17.63	18.26	0.63
3Cl	14.15	14.33	0.18	18.76	19.15	0.39
4Cl	14.80	15.02	0.22	19.84	20.26	0.43
2Br	14.02	14.28	0.26	17.84	18.36	0.53
3Br	14.59	14.77	0.18	18.96	19.32	0.37
4Br	15.38	15.87	0.49	20.25	21.24	1.00
2OMe	14.45	14.63	0.18	19.32	19.69	0.37
3OMe	14.59	14.78	0.19	19.16	19.56	0.40
4OMe	14.94	15.23	0.29	19.72	20.32	0.60
2Me	13.82	14.39	0.56	19.29	20.53	1.23
3Me	14.74	15.05	0.31	21.04	21.70	0.66
4Me	15.01	15.43	0.43	21.42	22.36	0.94
2CN	15.14	15.43	0.28	19.43	20.00	0.58
3CN	15.73	15.88	0.15	20.64	20.96	0.31
4CN	16.35	16.81	0.47	21.20	22.11	0.92
2CF ₃	13.69	14.13	0.43	19.48	20.42	0.94

analytes	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
3CF ₃	14.07	14.77	0.70	20.71	22.24	1.54
4CF ₃	15.40	16.82	1.42	23.07	26.15	3.08
2NO ₂	15.60	15.87	0.27	19.82	20.38	0.56
3NO ₂	16.03	16.27	0.24	20.59	21.09	0.50
4NO ₂	17.11	17.53	0.42	21.87	22.69	0.83
2,3Me	14.85	15.19	0.34	20.41	21.14	0.73
2,4Me	14.51	14.97	0.46	19.95	20.92	0.98
2,5Me	14.21	14.33	0.12	19.50	19.78	0.28
2,6Me	14.35	14.35	0.00	19.70	19.70	0.00
3,4Me	15.88	16.16	0.28	22.32	22.90	0.59
3,5Me	14.86	15.08	0.23	20.56	21.06	0.50
2,3F	13.91	14.48	0.57	19.90	21.15	1.25
2,4F	13.76	14.32	0.56	19.92	21.15	1.22
2,5F	13.81	14.11	0.31	19.97	20.63	0.66
2,6F	13.02	13.24	0.22	18.26	18.75	0.48
3,4F	14.84	14.93	0.08	21.98	22.07	0.10
3,5F	13.76	14.13	0.37	20.10	20.96	0.86
2,3Cl	15.22	15.48	0.26	19.49	19.82	0.33
2,4Cl	15.78	16.08	0.30	20.62	21.23	0.61
2,5Cl	15.01	15.18	0.16	19.59	19.93	0.34
2,6Cl	14.23	14.24	0.00	17.98	17.98	0.00
3,4Cl	15.06	15.53	0.47	19.42	20.39	0.97

analytes	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
3,5Cl	15.15	15.21	0.06	19.93	20.06	0.13
2,4,6F	12.91	13.17	0.26	18.61	19.19	0.58
2,4,6Cl	15.14	15.14	0.00	19.05	19.05	0.00
pentaF	12.62	12.96	0.35	18.35	19.12	0.76

Table 6 Thermodynamic parameters of all analytes calculated from van't Hoff plots of $\ln k'$ vs. $1/T$ on BSiAc column

analytes	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	13.17	13.79	0.62	18.34	19.72	1.38
2F	13.60	14.03	0.43	19.37	20.37	1.00
3F	13.61	14.21	0.60	19.44	20.81	1.38
4F	13.86	14.34	0.48	19.94	21.04	1.10
2Cl	13.65	13.68	0.03	17.83	18.07	0.24
3Cl	13.76	13.98	0.23	18.07	18.56	0.48
4Cl	14.25	14.53	0.28	18.91	19.51	0.60
2Br	13.97	13.97	0.00	17.81	17.81	0.00
3Br	14.13	14.33	0.19	18.12	18.53	0.41
4Br	14.73	14.99	0.26	19.13	19.67	0.55
2OMe	13.87	13.87	0.00	18.13	18.13	0.00
3OMe	14.68	14.92	0.24	19.40	19.89	0.50
4OMe	15.02	15.11	0.09	19.99	20.18	0.19
2Me	13.11	13.11	0.00	17.83	17.83	0.00
3Me	13.98	14.55	0.57	19.46	20.74	1.27
4Me	14.33	15.20	0.87	20.12	22.06	1.94
2CN	14.93	14.93	0.00	18.87	18.87	0.00
3CN	15.55	15.59	0.04	20.25	20.33	0.09
4CN	17.03	17.08	0.05	22.57	22.68	0.11
2CF ₃	12.84	13.23	0.39	17.64	18.47	0.83

analytes	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
3CF ₃	13.96	14.22	0.26	20.60	21.19	0.58
4CF ₃	15.07	15.73	0.66	22.61	24.12	1.51
2NO ₂	15.45	15.45	0.00	19.33	19.33	0.00
3NO ₂	15.81	15.93	0.11	20.08	20.32	0.24
4NO ₂	18.90	19.04	0.14	25.44	25.73	0.29
2,3Me	14.09	14.09	0.00	18.92	18.92	0.00
2,4Me	14.05	14.05	0.00	19.11	19.11	0.00
2,5Me	13.60	13.60	0.00	18.30	18.30	0.00
2,6Me	13.39	13.39	0.00	17.74	17.74	0.00
3,4Me	15.03	15.79	0.76	20.66	22.33	1.68
3,5Me	14.38	14.53	0.15	19.66	20.00	0.34
2,3F	13.86	14.30	0.43	19.84	20.84	1.01
2,4F	13.50	13.68	0.18	19.51	19.91	0.40
2,5F	13.78	14.02	0.24	19.98	20.54	0.56
2,6F	13.61	13.66	0.05	19.67	19.79	0.12
3,4F	14.52	14.85	0.33	21.37	22.13	0.76
3,5F	13.70	14.11	0.42	20.14	21.10	0.96
2,3Cl	14.71	14.71	0.00	18.46	18.46	0.00
2,4Cl	15.06	15.28	0.22	19.27	19.73	0.46
2,5Cl	14.31	14.31	0.00	18.20	18.20	0.00
2,6Cl	13.88	13.88	0.00	17.30	17.30	0.00
3,4Cl	14.71	14.75	0.05	18.82	18.93	0.11

analytes	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta(\Delta H)$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta(\Delta S)$
3,5Cl	14.57	14.68	0.11	18.82	19.06	0.24
2,4,6F	12.88	13.02	0.14	18.68	19.00	0.32
2,4,6Cl	14.71	14.71	0.00	18.26	18.26	0.00
pentaF	13.13	13.43	0.31	19.50	20.20	0.71



VITA

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