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APPENDICES

Appendix A

NMR Spectra

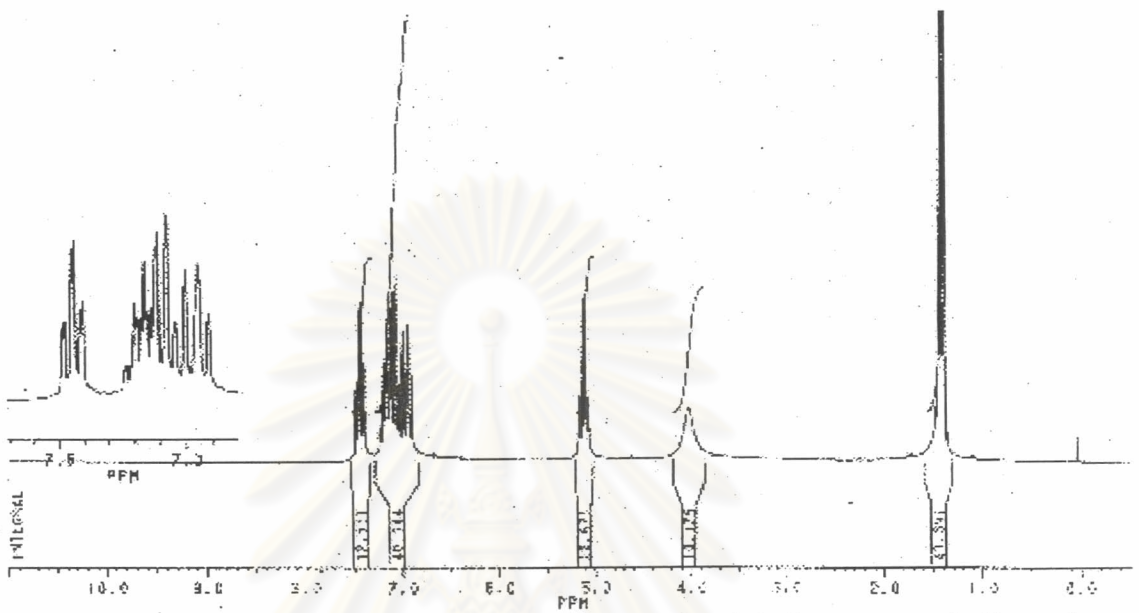

Figure A1 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 2-fluoro-α-methylbenzyl alcohol (**2F**), δ (ppm) 1.44 (d, 3H, J=6.51 Hz) CH_3, 4.03 (s, 1H) OH, 5.11 (q, 1H, J=6.51 Hz) CH, 6.91-7.49 (m,4H) Ar.

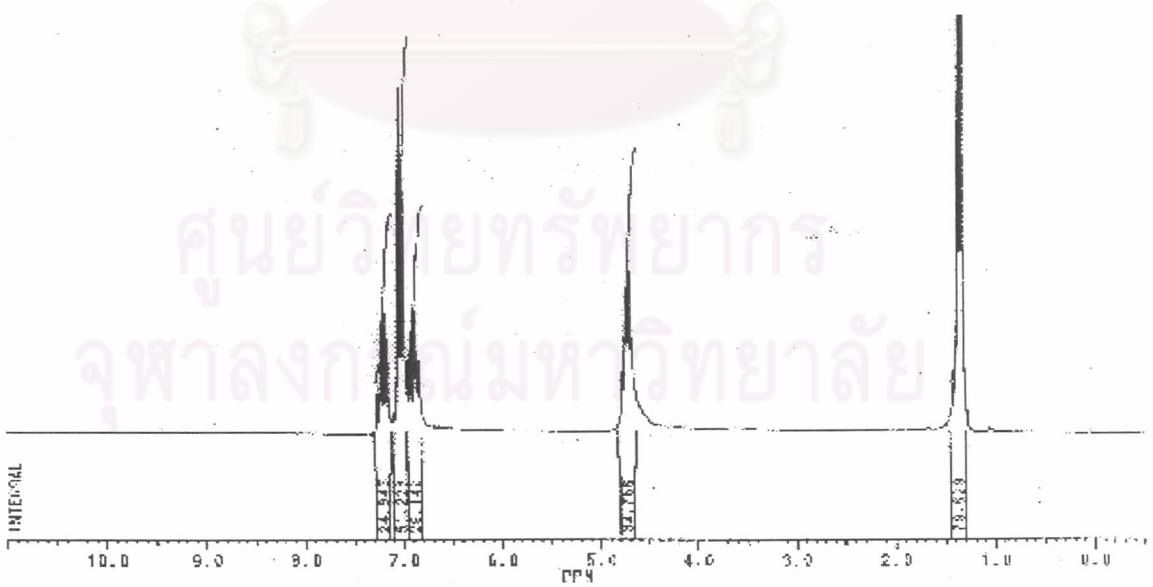

Figure A2 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-fluoro-α-methylbenzyl alcohol (**3F**), δ (ppm) 1.35 (d, 3H, J=6.43 Hz) CH_3, 4.75 (q, 1H, J=6.43 Hz) CH, 6.85-7.27 (m, 4H) Ar.

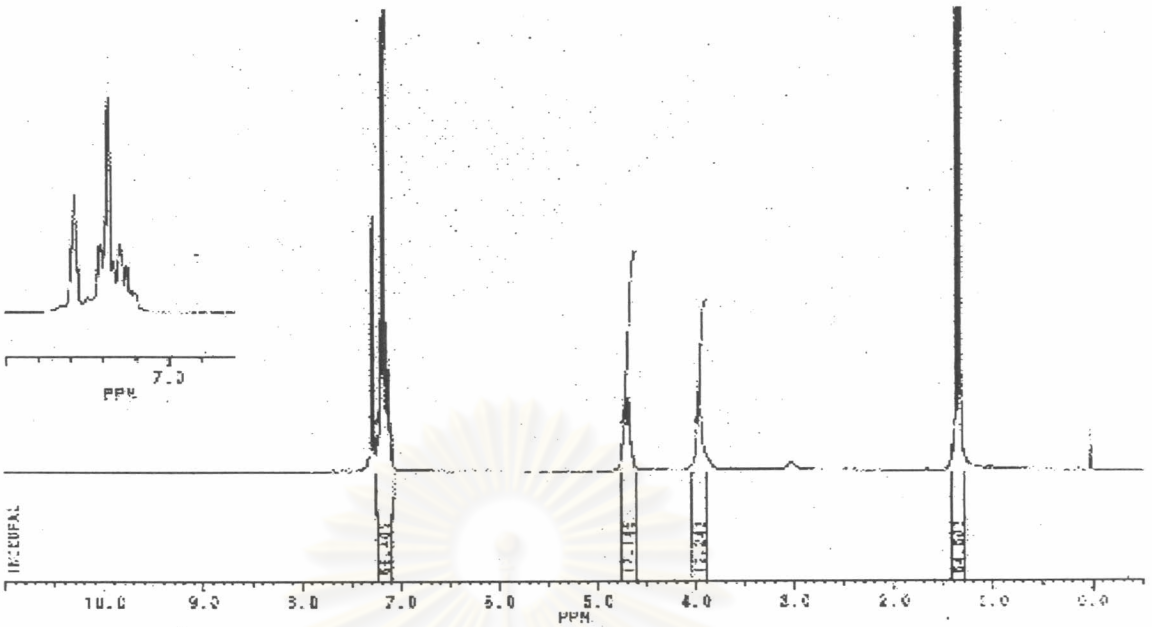

Figure A3 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 1-(2-chlorophenyl)ethanol (**2Cl**), δ (ppm) 1.40 (d, 3H, J=5.12 Hz) CH_3, 4.63 (s, 1H) OH, 5.25 (q, 1H, J=5.12 Hz) CH, 7.08-7.57 (m, 4H) Ar.

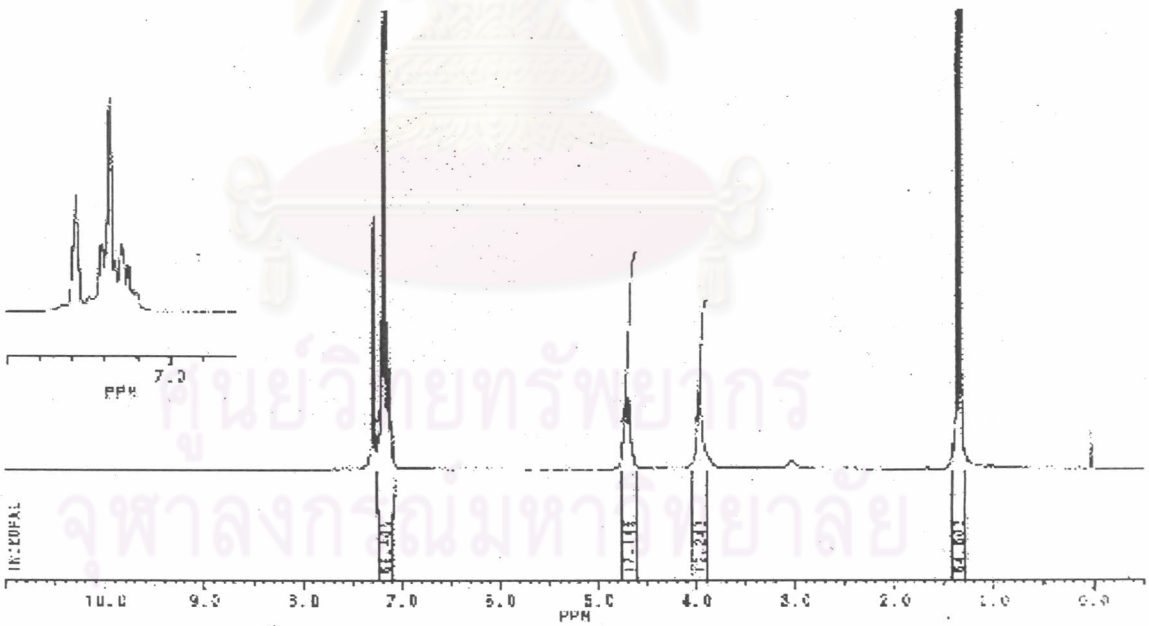

Figure A4 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 1-(3-chlorophenyl) ethanol (**3Cl**), δ (ppm) 1.35 (d, 3H, J=6.49 Hz) CH_3, 3.95 (s, 1H) OH, 4.64 (q, 1H, J= 6.49 Hz) CH, 7.09-7.28 (m, 4H) Ar

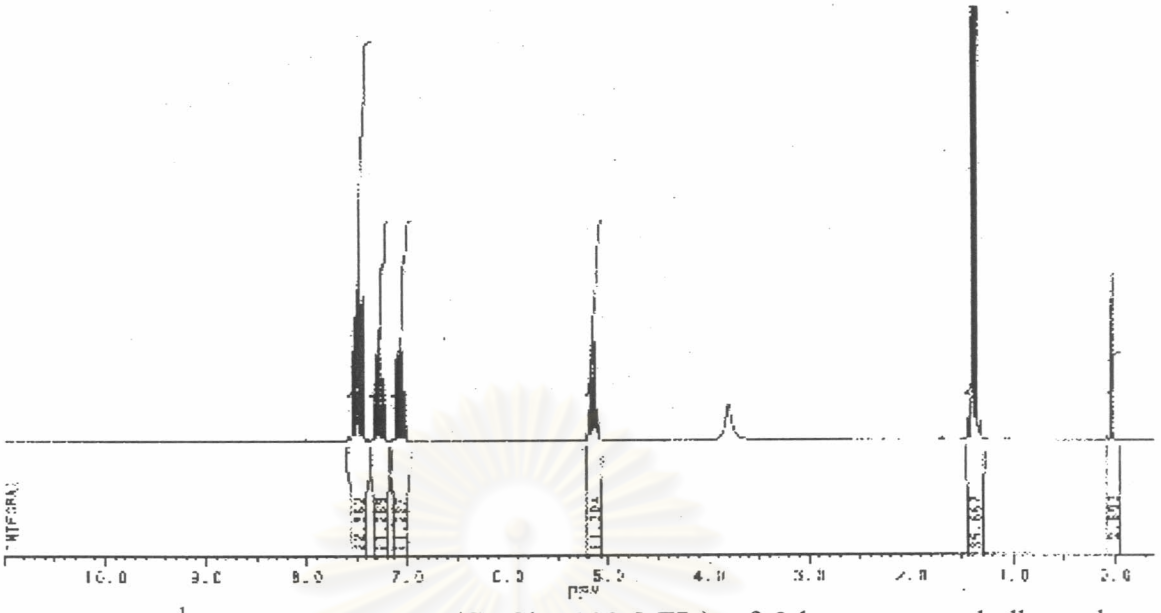

Figure A5 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 2-bromo-α-methylbenzyl alcohol (**2Br**), δ (ppm) 1.35 (d, 3H, J=6.40 Hz) CH_3, 4.25 (s, 1H) OH, 4.65 (q, 1H, J= 6.40 Hz) CH, 7.01-7.53 (m, 4H) Ar

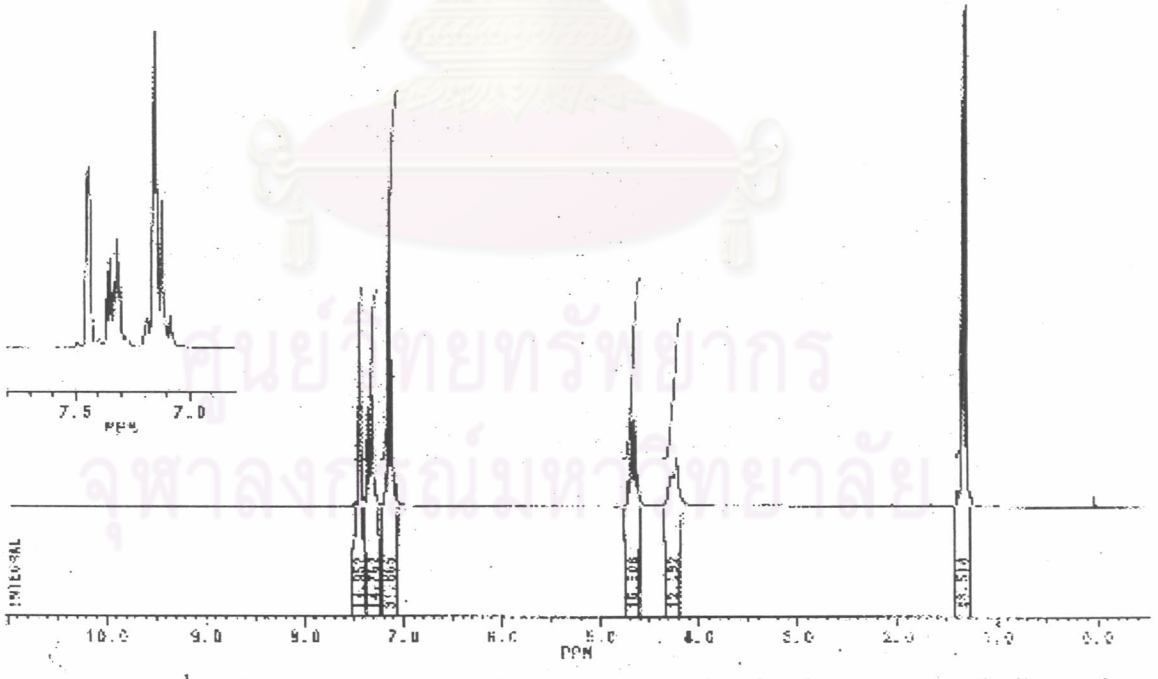

Figure A6 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-bromo-α-methylbenzyl alcohol (**3Br**), δ (ppm) 1.35 (d, 3H, J=6.49 Hz) CH_3, 4.25(s, 1H) OH, 4.65 (q, 1H, J=6.49 Hz) CH, 7.08-7.44 (m, 4H) Ar

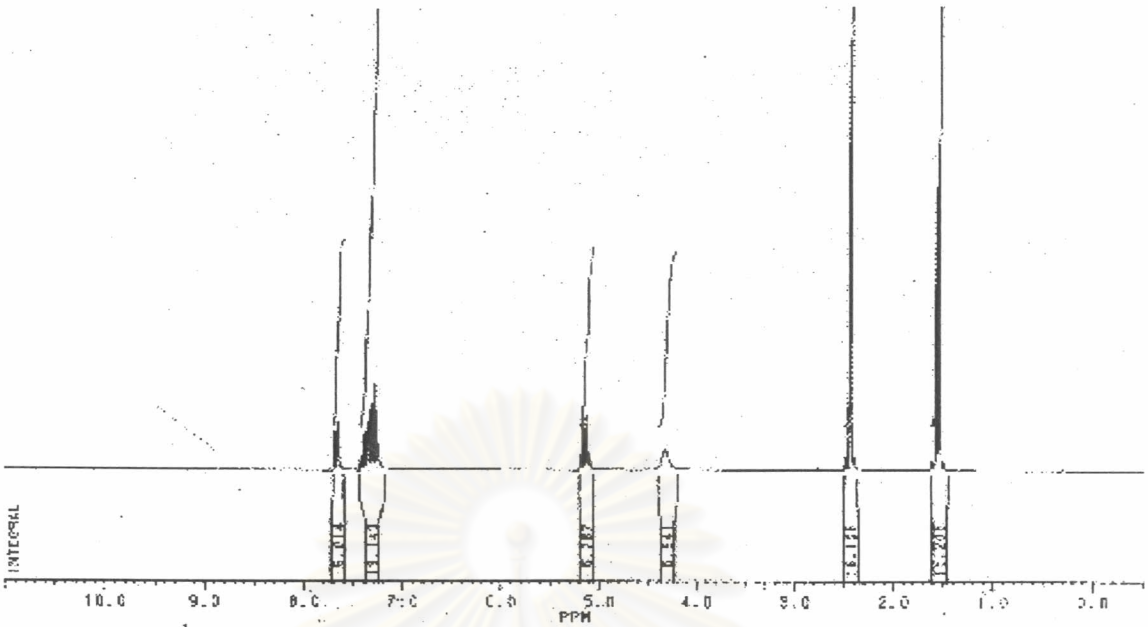

Figure A7 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 2-methyl-α-methylbenzyl alcohol (**2Me**), δ (ppm) 1.55 (d, 3H, J=6.42 Hz) $C\underline{H}_3$-CH, 2.44 (s, 3H) $C\underline{H}_3$-Ar, 4.31 (s, 1H) OH, 5.10 (q, 1H, J=4.62 Hz) CH, 7.23-7.69 (m, 4H)

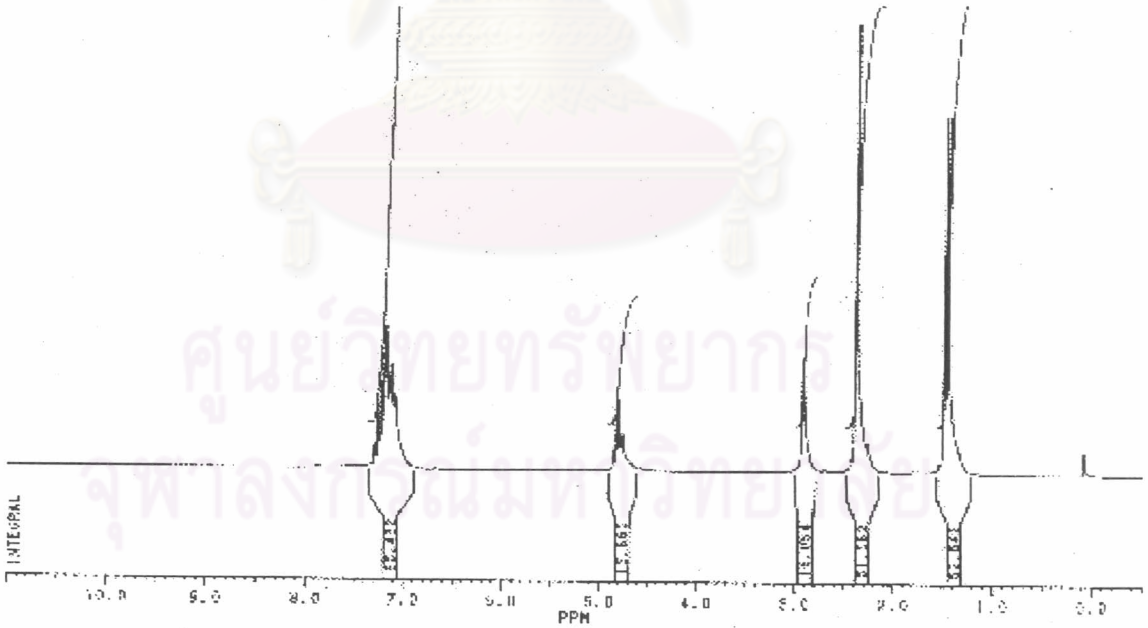

Figure A8 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-methyl-α-methylbenzyl alcohol (**3Me**), δ (ppm) 1.45 (d, 3H, J=6.42 Hz) $C\underline{H}_3$-CH, 2.39 (s, 3H) $C\underline{H}_3$-Ar, 2.92 (s, 1H) OH, 4.80 (q, 1H, J=6.42 Hz) CH, 7.09-7.30 (m, 4H) Ar

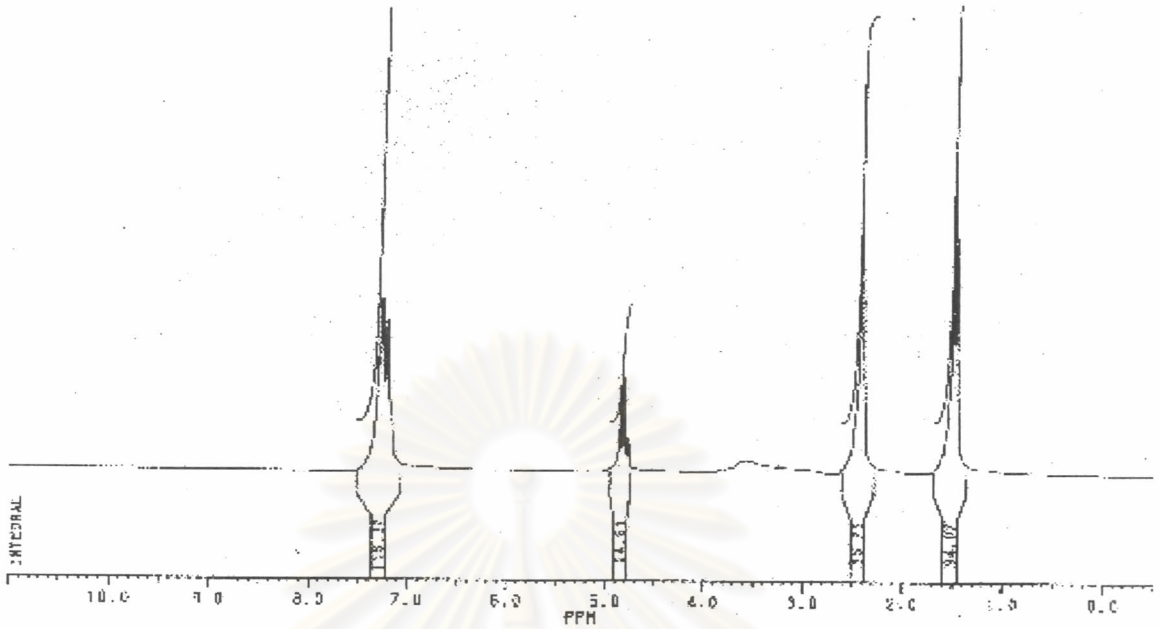

Figure A9 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-methyl-α-methylbenzyl alcohol (**4Me**), δ (ppm) 1.46 (d, 3H, J=6.46 Hz) $C\underline{H}_3$-CH, 2.40 (s, 3H) $C\underline{H}_3$-Ar, 4.28 (q, 1H, J=6.46 Hz) CH, 7.16- 7.29 (m, 4H) Ar

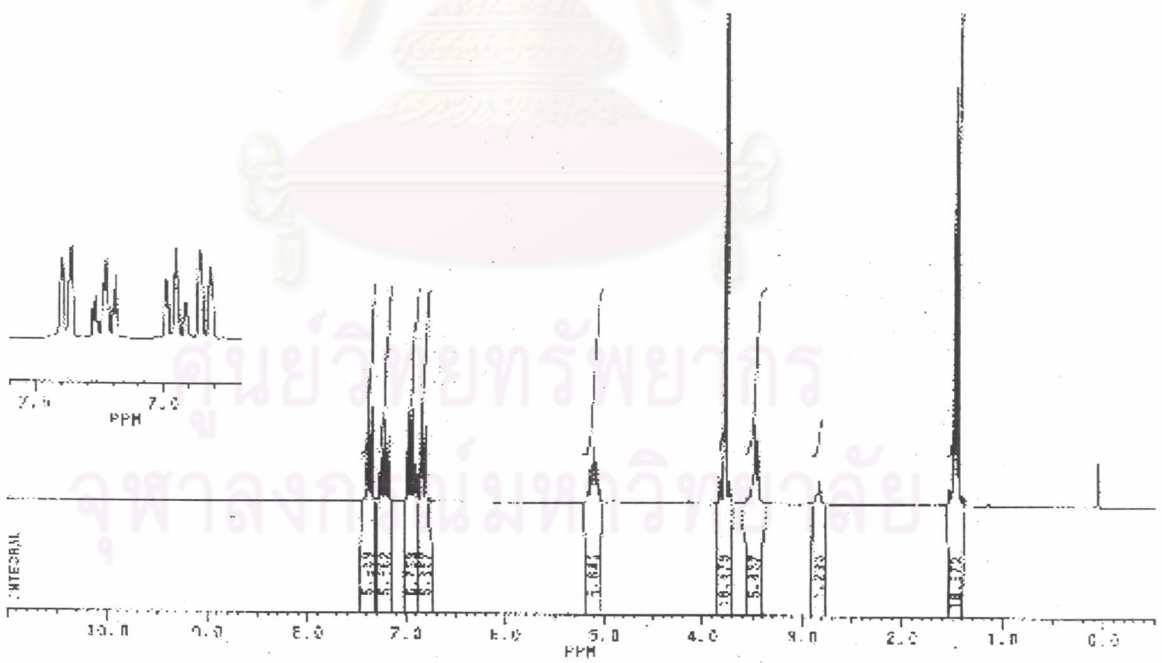

Figure A10 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 2-methoxy-α-methylbenzyl alcohol (**2OMe**), δ (ppm) 1.45 (d, 3H,J=6.00 Hz) CH_3, 3.45 (s, 1H) OH, 3.78 (s, 3H) OCH_3, 5.11 (q, 1H, J=6.00 Hz) CH, 6.81-7.39 (m, 4H) Ar

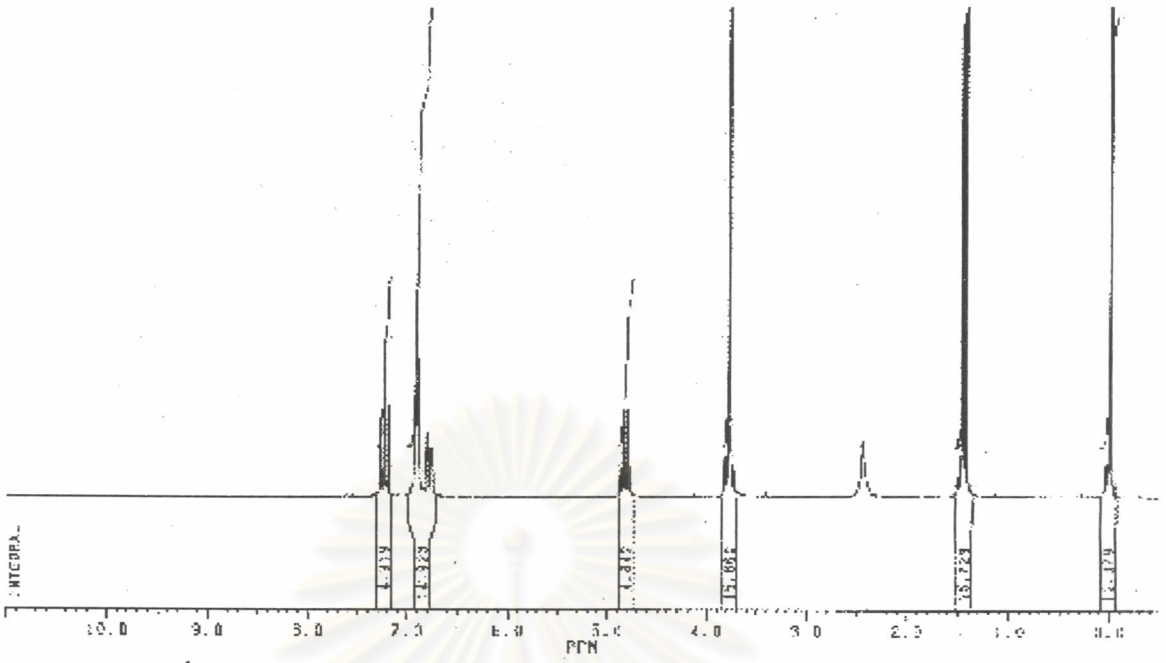

Figure A11 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-methoxy-α-methylbenzyl alcohol (**3OMe**), δ (ppm) 1.45 (d, 3H, J=6.45 Hz) CH_3, 2.45 (s, 1H) OH, 3.77 (s, 3H) OCH_3, 4.80 (q, 1H, J=6.45 Hz) CH, 6.75-7.27 (m, 4H) Ar

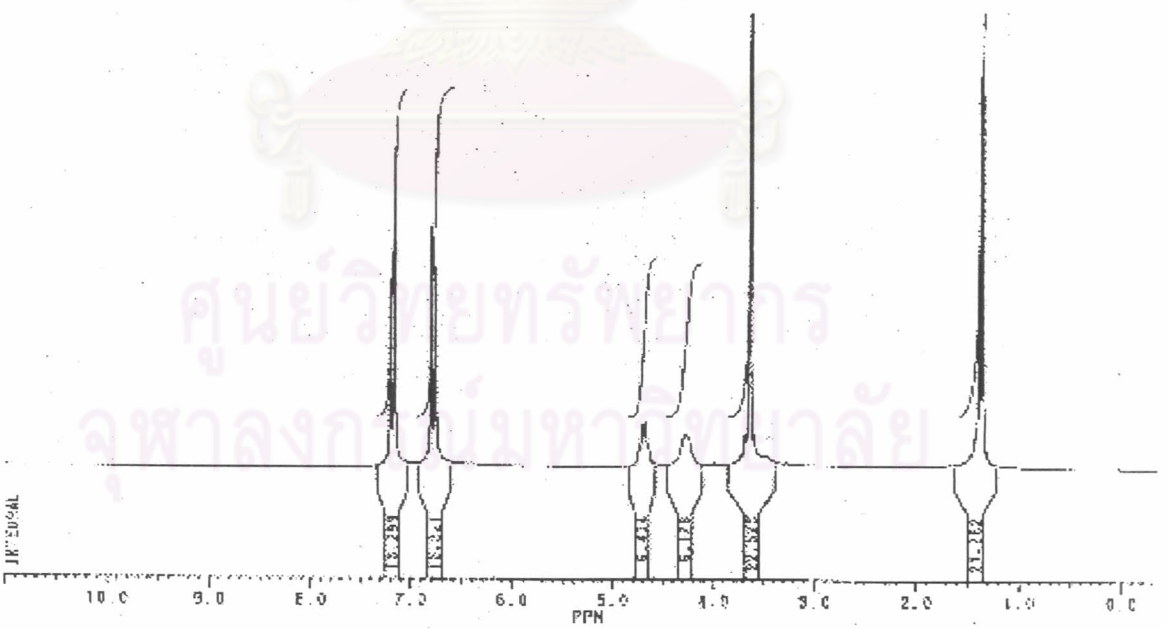

Figure A12 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-methoxy-α-methylbenzyl alcohol (**4OMe**), δ (ppm) 1.35 (d, 3H, J=6.08 Hz) CH_3, 3.64 (s, 3H) OCH_3, 4.28 (s, 1H) OH, 4.70 (q, 1H, J=6.08 Hz) CH, 6.76-7.22 (m, 4H) Ar

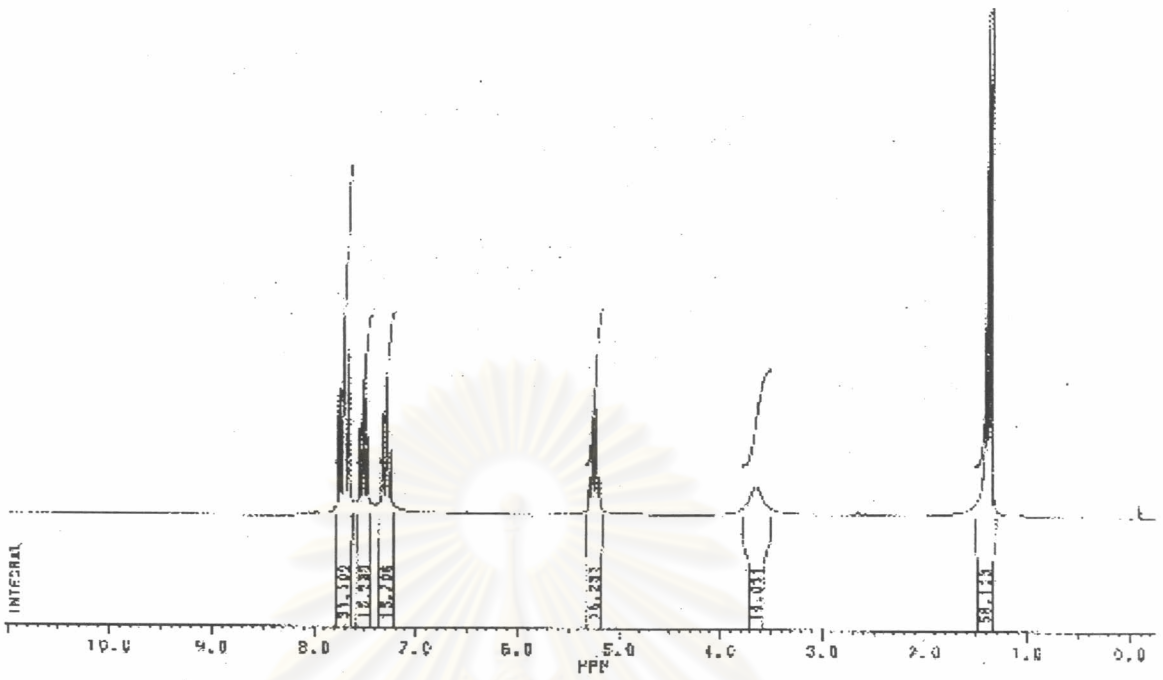

Figure A13 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 2-nitro-α-methylbenzyl alcohol (**2N**), δ (ppm) 1.40 (d, 3H, J=6.33 Hz) CH_3 3.66 (s, 1H) OH, 5.25 (q, 1H, J=6.33 Hz) CH, 7.25-7.76 (m, 4H) Ar

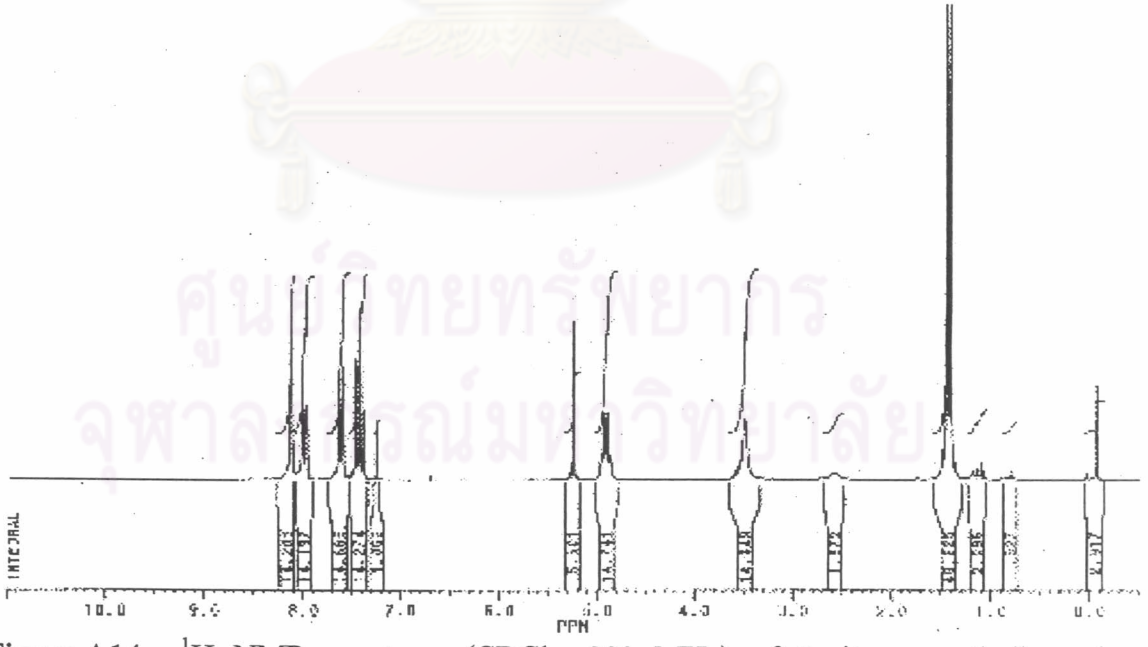

Figure A14 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-nitro-α-methylbenzyl alcohol (**3N**), δ (ppm) 1.40 (d, 3H, J=6.45 Hz) CH_3, 3.48 (s, 1H) OH, 4.90 (q, 1H, J=6.45 Hz) CH, 7.37-8.12 (m, 4H) Ar

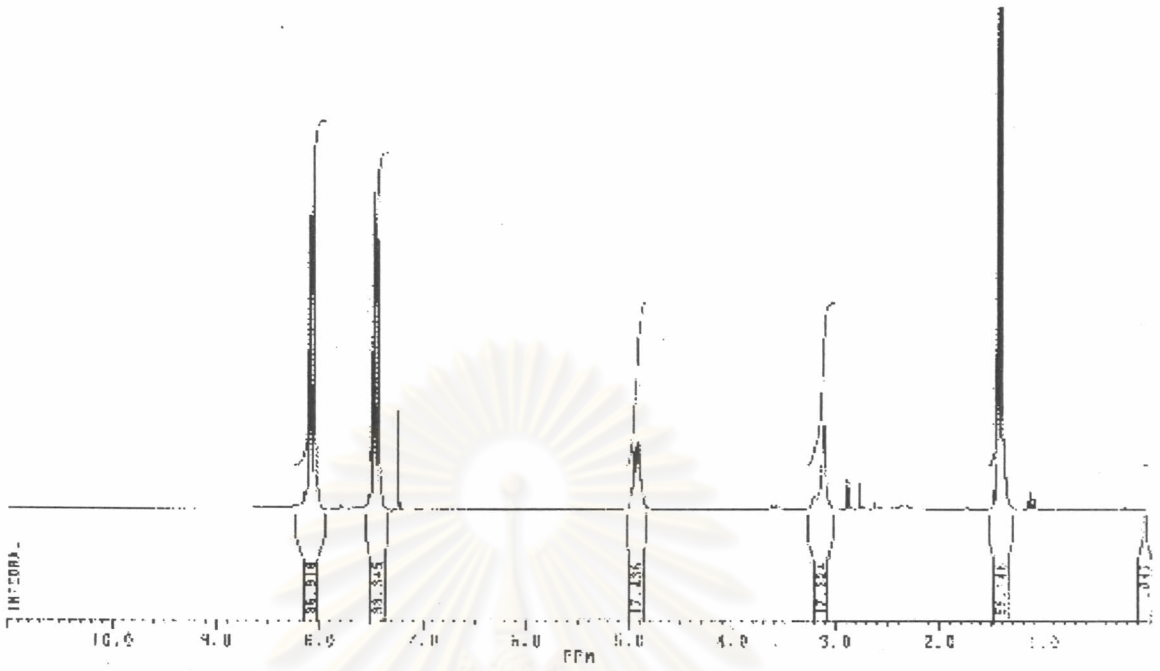

Figure A15 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-nitro-α-methylbenzyl alcohol (**4N**), δ (ppm) 1.45 (d, 3H, J=6.42 Hz) CH_3, 3.11 (s, 1H) OH, 4.95 (q, 1H, J=6.42 Hz) CH, 7.40-8.20 (m, 4H) Ar

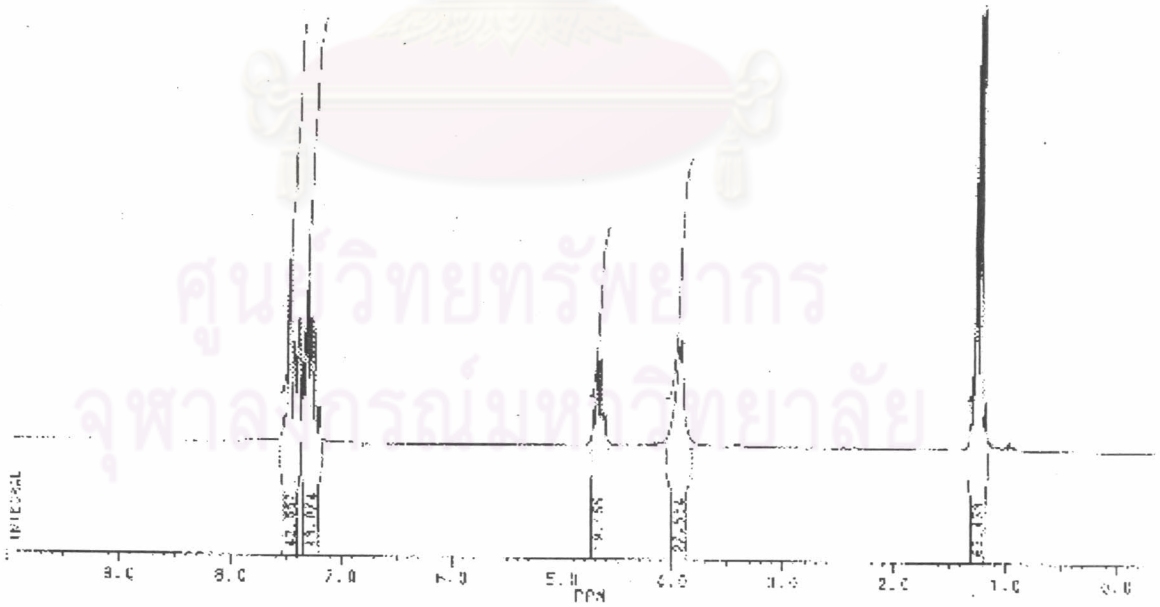

Figure A16 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 3-cyano-α-methylbenzyl alcohol (**3CN**), δ (ppm) 1.24 (d, 3H, J=6.44 Hz) CH_3, 3.93 (s, 1H) OH, 4.69 (q, 1H, J=6.44 Hz) CH, 7.20-7.52 (m, 4H) Ar

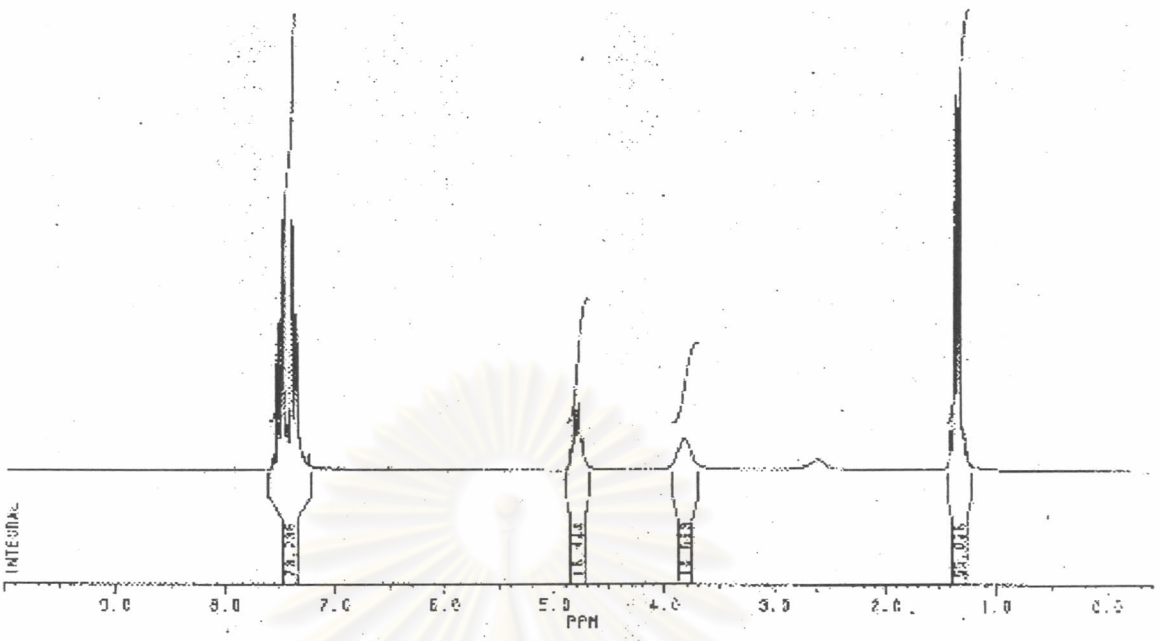

Figure A17 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-cyano-α-methylbenzyl alcohol (**4CN**), δ (ppm) 1.34 (d, 3H, J=6.48 Hz) CH_3, 3.82 (s, 1H) OH, 4.78 (q, 1H, J=6.48 Hz) CH, 7.30-7.52 (m, 4H) Ar

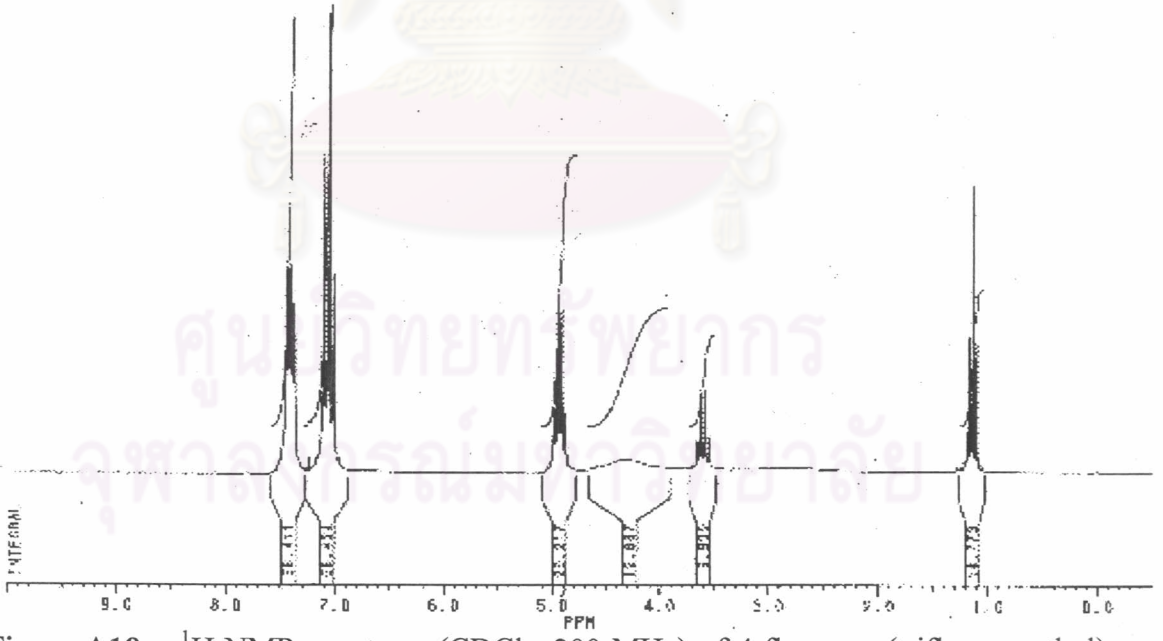

Figure A18 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-fluoro-α-(trifluoromethyl) benzyl alcohol (**F-TF**), δ (ppm) 4.40 (s, 1H) OH, 4.90 (q, 1H) CH, 7.02-7.48 (m, 4H) Ar

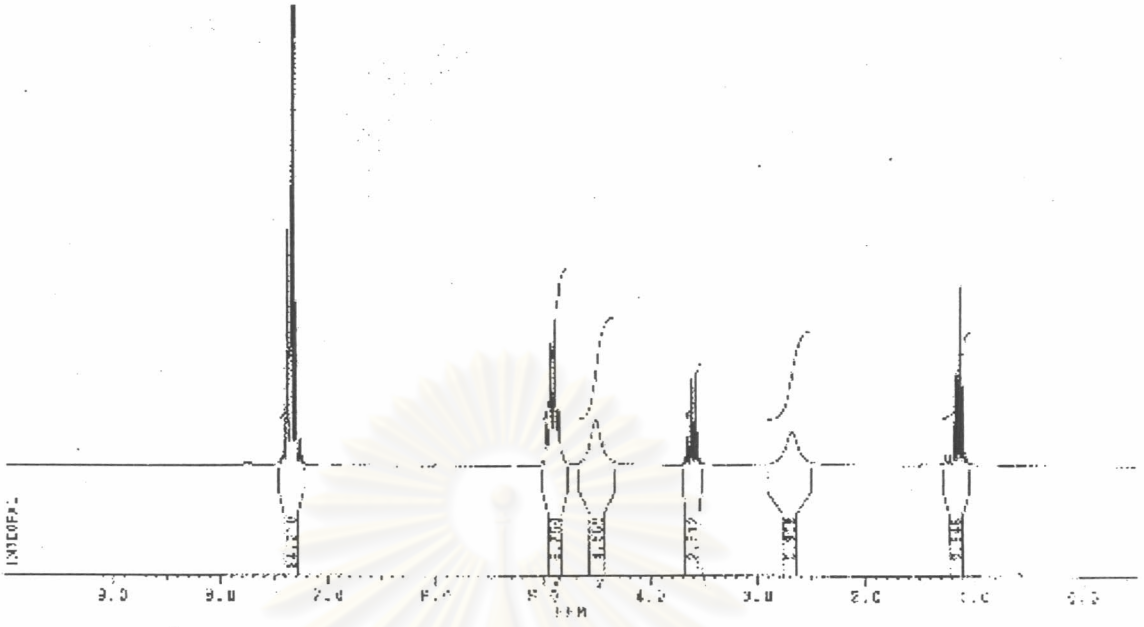

Figure A19 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-chloro-α-(trifluoromethyl) benzyl alcohol (**Cl-TF**), δ (ppm) 4.51 (s, 1H) OH, 4.92 (q, 1H) CH, 7.26-7.39 (m, 4H) Ar

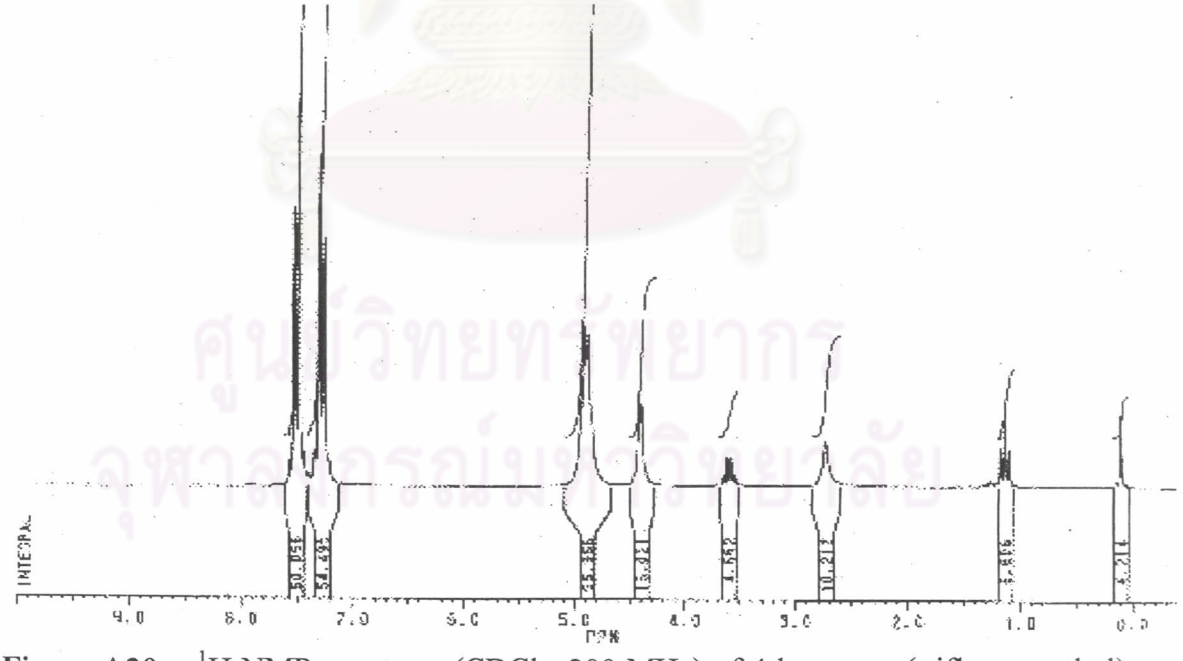

Figure A20 ^{1}H NMR spectrum ($CDCl_3$, 200 MHz) of 4-bromo-α-(trifluoromethyl) benzyl alcohol (**Br-TF**), δ (ppm) 4.86 (s, 1H) OH, 4.88 (s, 1H) CH, 7.21-7.57 (m, 4H) Ar

Appendix B

Thermodynamic Data

Table B1 Retention factors (k′) and separation factors (α) of 1-phenylethanol and its derivatives on OV-1701, BSiMe, and BMe columns at 150 °C

analyte	OV-1701	BSiMe		BMe	
	k′	k′2	α	k′2	α
H	0.76	1.64	1.016	1.87	1.026
2F	0.76	1.69	1.040	1.87	1.022
3F	0.89	2.02	1.017	2.28	1.036
4F	0.86	2.07	1.013	2.25	1.036
2Cl	1.87	5.84	1.257	5.81	1.131
3Cl	2.35	5.52	1.024	6.19	1.046
4Cl	2.33	5.57	1.025	6.56	1.059
2Br	2.93	10.73	1.404	10.29	1.210
3Br	3.76	9.00	1.020	10.09	1.047
4Br	3.76	9.24	1.024	11.03	1.061
2Me	1.36	3.35	1.056	3.59	1.079
3Me	1.19	2.39	1.024	2.76	1.027
4Me	1.21	2.39	1.024	2.75	1.037
2OMe	2.29	5.16	1.180	5.23	1.039
3OMe	2.80	5.62	1.034	6.77	1.036
4OMe	2.86	5.53	1.019	5.84	1.031
2N	6.56	30.50	1.647	25.55	1.174
3N	12.80	31.80	1.021	39.52	1.054
4N	13.90	40.4	1.059	55.39	1.115
3CN	7.71	20.81	1.021	24.16	1.050
4CN	8.01	22.40	1.075	30.14	1.126
F-TF	1.04	2.73	1.024	3.58	1.037
Cl-TF	2.78	7.31	1.000	10.10	1.053
Br-TF	4.49	12.35	1.000	17.05	1.056

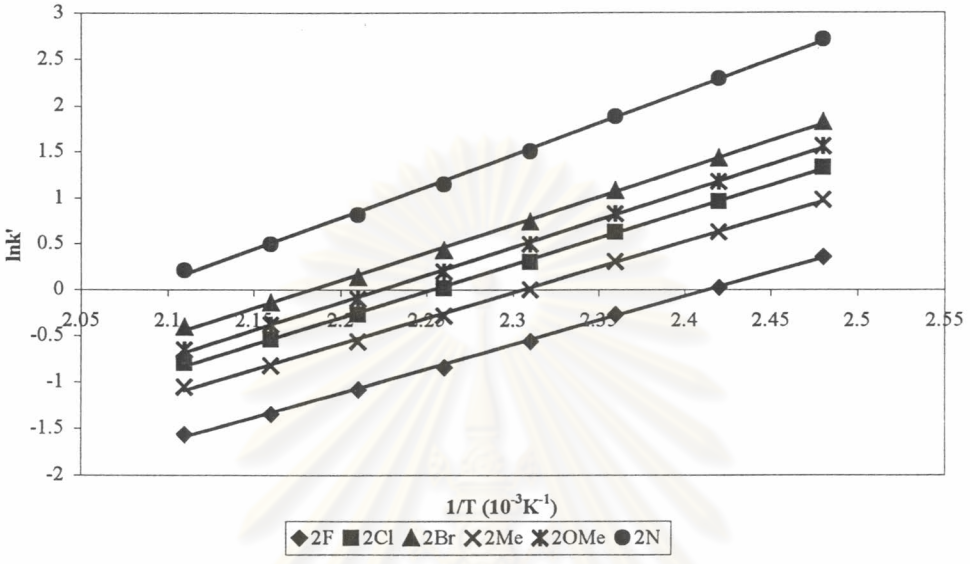

Figure B1 Plots of ln k′ vs. 1/T of *ortho*-substituted analytes on OV-1701 column

Table B2 Equations, correlation coefficients, and thermodynamic values of all analytes obtained from ln k′ vs. 1/T plots on OV-1701 column

analyte	Equation: $\ln k' = a\frac{1}{T} + b$		R^2	-ΔH (kcal/mol)	-ΔS (cal/mol.K)
	a	b			
H	4942.3	-11.94	0.9977	9.82	12.75
2F	5173.3	-12.49	0.9991	10.28	13.85
3F	5312.7	-12.66	0.9991	10.56	14.19
4F	5265.3	-12.58	0.9992	10.46	14.03
2Cl	5783.9	-13.04	0.9990	11.49	14.94
3Cl	6006.6	-13.33	0.9990	11.93	15.52
4Cl	5967.7	-13.25	0.9990	11.86	15.36
2Br	6091.6	-13.31	0.9990	12.10	15.48
3Br	6343.7	-13.66	0.9990	12.60	16.17
4Br	6295.9	-13.55	0.9991	12.51	15.95
2Me	5553.9	-12.81	0.9990	11.03	14.48
3Me	5480.9	-12.77	0.9990	10.89	14.40
4Me	5482.7	-12.76	0.9991	10.89	14.38
2OMe	6013.6	-13.37	0.9990	11.95	15.60
3OMe	6237.3	-13.70	0.9990	12.39	16.25
4OMe	6202.0	-13.60	0.9990	12.32	16.05
2N	6847.9	-14.29	0.9989	13.61	17.42
3N	7360.2	-14.84	0.9990	14.62	18.52
4N	7395.2	-14.83	0.9990	14.69	18.50
3CN	6972.4	-14.43	0.9991	13.85	17.70
4CN	7000.2	-14.45	0.9990	13.91	17.74
F-TF	5873.4	-12.83	0.9980	11.67	14.52
Cl-TF	6614.1	-14.59	0.9983	13.14	18.02
Br-TF	6973.3	-14.96	0.9985	13.85	18.76

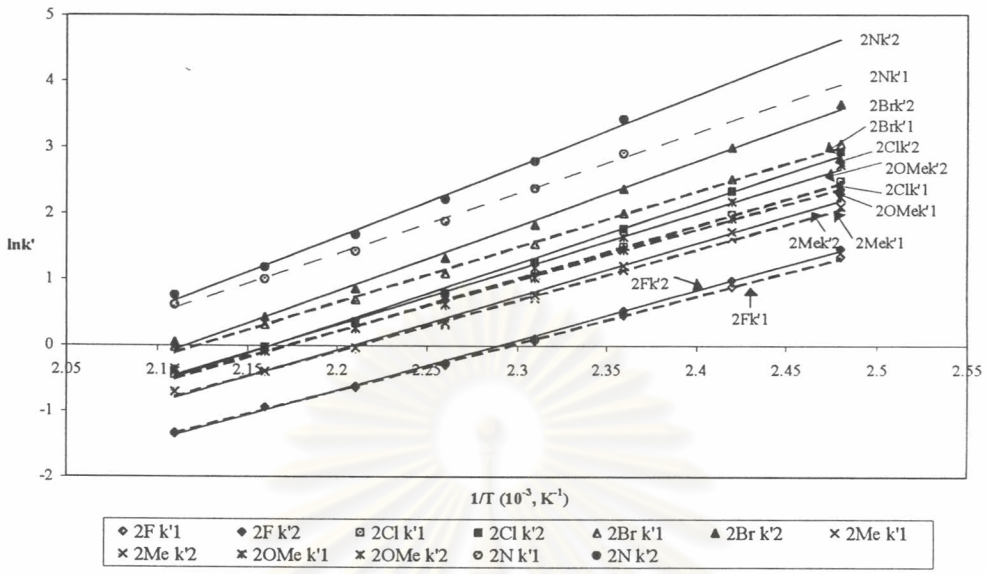

Figure B2 Plots of ln k′ vs. 1/T of *ortho*-substituted analytes on BSiMe column

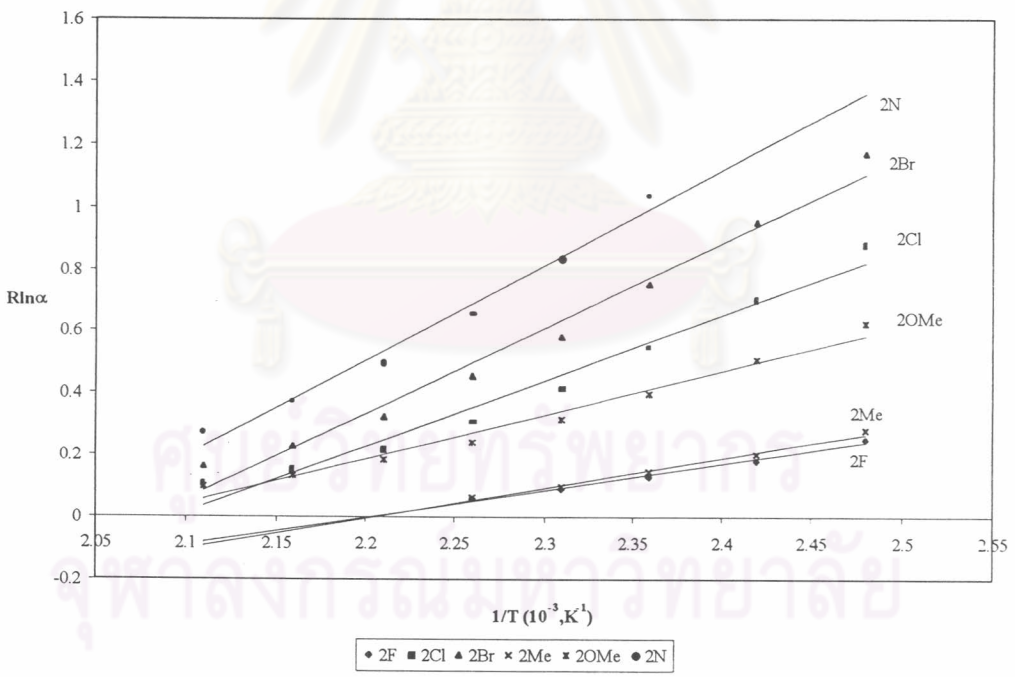

Figure B3 Plots of R ln α vs. 1/T of *ortho*-substituted analytes on BSiMe column

Table B3 Equations and correlation coefficients of all analytes obtained from ln k′ vs. 1/T plots on BSiMe column

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation : $\ln k' = a\frac{1}{T} + b$		R^2	Equation: $\ln k' = a\frac{1}{T} + b$		R^2
	a	b		a	b	
H	6591.7	-15.08	0.9982	6719.8	-15.37	0.9978
2F	6857.5	-15.71	0.9993	7191.0	-16.43	0.9988
3F	6940.9	-15.70	0.9986	7062.5	-15.96	0.9982
4F	6880.5	-15.57	0.9982	6987.3	-15.80	0.9978
2Cl	7612.9	-16.51	0.9985	8626.5	-18.63	0.9972
3Cl	7551.1	-16.18	0.9975	7683.3	-16.47	0.9973
4Cl	7419.5	-15.87	0.9990	7570.1	-16.20	0.9988
2Br	8015.6	-16.98-	0.9985	9332.7	-19.71	0.9974
3Br	7988.7	16.74	0.9987	8094.4	-16.97	0.9985
4Br	7748.0	-16.16	0.9992	7884.4	-16.46	0.9990
2Me	7364.3	-16.25	0.9986	7740.2	-17.07	0.9978
3Me	6689.7	-14.98	0.9995	6863.2	-15.32	0.9994
4Me	6639.5	-14.83	0.9991	6813.3	-15.21	0.9988
2OMe	7356.5	-15.95	0.9983	8040.2	-17.36	0.9975
3OMe	7515.5	-16.09	0.9985	7702.9	-16.49	0.9984
4OMe	7166.2	-15.23	0.9977	7277.3	-15.50	0.9975
2N	8770.6	-17.93	0.9969	10252	-20.95	0.9957
3N	8495.1	-16.75	0.9846	8580.7	-16.93	0.9847
4N	8894.1	-17.50	0.9976	9085.7	-17.90	0.9973
3CN	8681.5	-17.60	0.9974	8776.7	-17.81	0.9970
4CN	8454.5	-17.04	0.9979	8691.8	-17.53	0.9976
F-TF	7726.6	-17.27	0.9980	7829.8	-17.49	0.9984
Cl-TF	8691.0	-18.54	0.9993	---	---	---
Br-TF	9094.8	-18.98	0.9995	---	---	---

Table B4 Thermodynamic values of all analytes obtained from ln k′ vs. 1/T plots on BSiMe column

analyte	Enthalpic term			Entropic term		
	-ΔH1	-ΔH2	-Δ(ΔH)	-ΔS1	-ΔS2	-Δ(ΔS)
H	13.10	13.35	0.25	18.99	19.56	0.57
2F	13.62	14.29	0.67	20.22	21.68	1.46
3F	13.79	14.03	0.24	20.24	21.68	1.44
4F	13.67	13.88	0.21	19.96	20.74	0.78
2Cl	15.13	17.14	2.01	21.83	26.04	4.21
3Cl	15.00	15.27	0.27	21.18	21.75	0.57
4Cl	14.74	15.04	0.30	20.56	21.21	0.65
2Br	15.93	18.54	2.61	22.76	28.20	5.44
3Br	15.87	16.08	0.21	22.30	22.75	0.45
4Br	15.39	15.67	0.28	21.14	21.73	0.59
2Me	14.63	15.38	0.75	21.32	22.94	1.62
3Me	13.29	13.64	0.35	18.73	19.47	0.74
4Me	13.19	13.54	0.35	18.50	19.25	075
2OMe	14.62	15.97	1.35	20.72	23.53	2.81
3OMe	14.93	15.30	0.37	21.00	21.79	0.79
4OMe	14.24	14.46	0.22	19.36	19.83	0.47
2N	17.43	20.37	2.94	24.66	30.65	5.99
3N	16.88	17.05	0.14	22.31	22.67	0.30
4N	17.67	18.05	0.38	23.81	24.60	0.79
3CN	17.25	17.44	0.19	24.00	24.42	0.42
4CN	16.80	17.27	0.47	22.89	23.87	0.98
F-TF	15.35	15.58	0.23	23.34	23.77	0.43
Cl-TF	17.27	---	0.00	25.87	---	0.00
Br-TF	18.07	---	0.00	26.74	---	0.00

-ΔH1, -ΔH2 are enthalpy of less retained enantiomer and more retained enantiomer

-ΔS1, -ΔS2 are entropy of less retained and more retained enantiomer

Table B5 Equations, correlation coefficients, and thermodynamic differences of all analytes obtained from R ln α vs. 1/T plots on BSiMe column

analytes	Equation: $R\ln\alpha = a \cdot \frac{1}{T} + b$		R^2	-Δ(ΔH) (kcal/mol)	-Δ(ΔS) (cal/mol.K)
	a	b			
H	322.0	-0.71	0.9930	0.32	0.70
2F	864.3	-1.90	0.9851	0.86	1.90
3F	276.3	-0.60	0.9984	0.24	0.60
4F	362.5	-0.82	0.9935	0.36	0.82
2Cl	2121.6	-4.44	0.9728	2.12	4.44
3Cl	290.9	-0.63	0.9936	0.29	0.63
4Cl	384.0	-0.84	0.9892	0.38	0.84
2Br	2760.7	-5.74	0.9809	2.76	5.74
3Br	239.5	-0.52	0.9956	0.24	0.52
4Br	353.1	-0.78	0.9884	0.35	0.78
2Me	979.1	-2.16	0.9888	0.98	2.16
3Me	377.1	-0.81	0.9684	0.38	0.81
4Me	430.6	-0.94	0.9896	0.43	0.94
2OMe	1433.2	-2.97	0.9773	1.43	2.97
3OMe	430.8	-0.93	0.9827	0.43	0.93
4OMe	271.2	-0.59	0.9918	0.27	0.59
2N	3064.9	-6.24	0.9857	3.06	6.24
3N	185.1	-0.40	0.9620	0.18	0.40
4N	396.1	-0.83	0.9683	0.40	0.83
3CN	136.0	-0.28	0.9914	0.14	0.28
4CN	491.0	-1.02	0.9631	0.47	1.02
F-TF Cl-TF* Br-TF*	118.2	-0.22	0.9676	0.12	0.22

* not separated in this temperature range (130-200 °C)

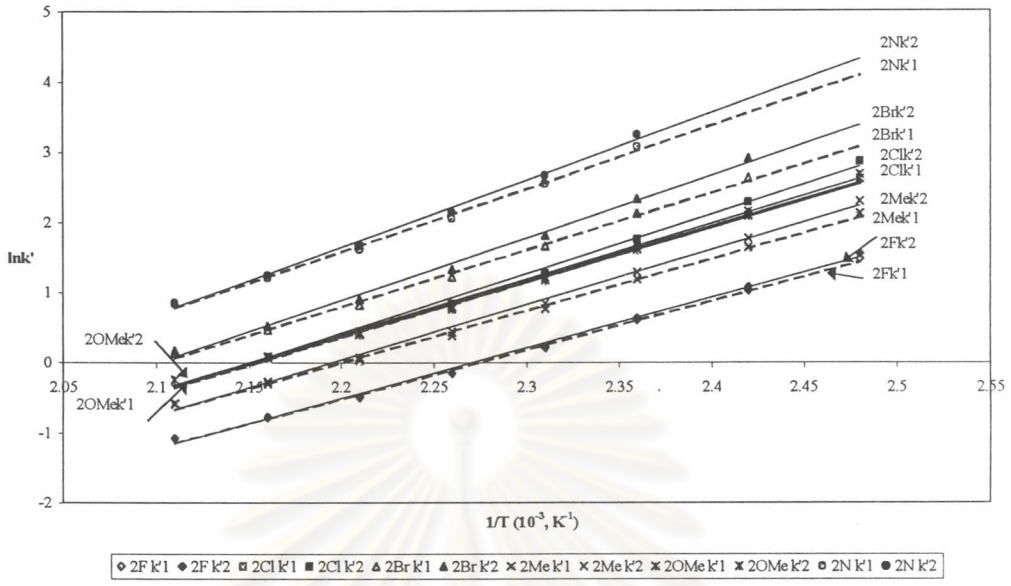

Figure B4 Plots of ln k′ vs. 1/T of *ortho*-substituted analytes on BMe column

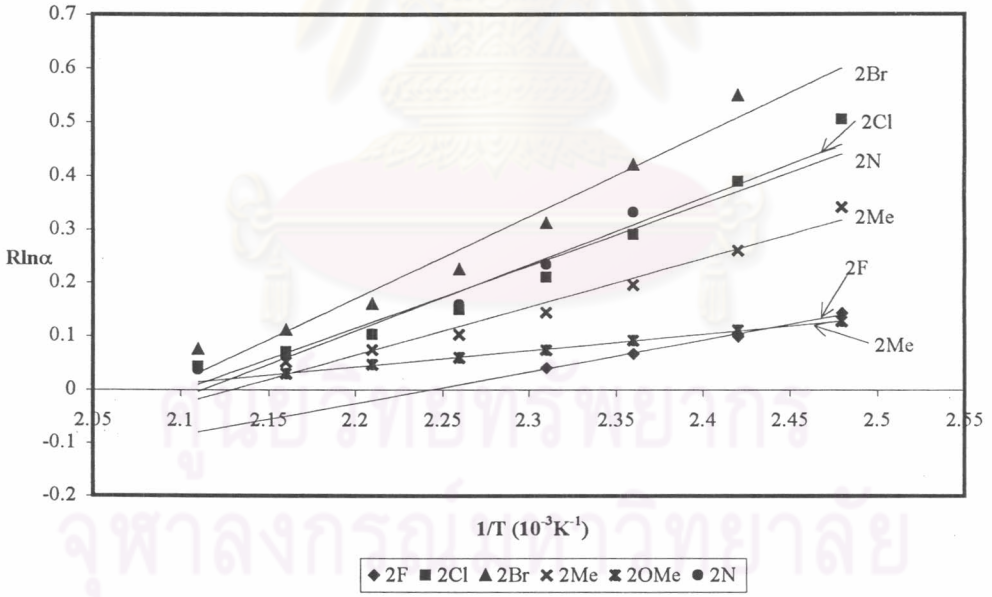

Figure B5 Plots of R ln α vs. 1/T of *ortho*-substituted analytes on BMe column

Table B6 Equations and correlation coefficients of all analytes obtained from ln k′ vs. 1/T plots on BMe column

enantiomer	less retained enantiomer			more retained enantiomer		
	Equation: $\ln k' = a\frac{1}{T} + b$		R^2	Equation: $\ln k' = a\frac{1}{T} + b$		R^2
	a	b		a	b	
H	6634.4	-15.06	0.9978	6819.5	-15.46	0.9976
2F	6784.8	-15.41	0.9978	6981.2	-15.84	0.9969
3F	6853.5	-15.40	0.9975	7077.4	-15.87	0.9975
4F	6815.2	-15.32	0.9979	7064.0	-15.86	0.9977
2Cl	7670.6	-16.51	0.9975	8282.6	-17.80	0.9963
3Cl	7623.9	-16.25	0.9978	7839.6	-16.70	0.9977
4Cl	7627.5	-16.24	0.9980	7891.3	-16.77	0.9980
2Br	7964.4	-16.73	0.9970	8719.6	-18.31	0.9956
3Br	7841.0	-16.30	0.9971	8034.2	-16.71	0.9972
4Br	7627.5	-16.39	0.9976	8127.1	-16.84	0.9973
2Me	7208.9	-15.84	0.9973	7640.0	-16.75	0.9969
3Me	6997.8	-15.53	0.9976	7168.8	-15.90	0.9974
4Me	6785.2	-15.05	0.9979	7010.8	-15.54	0.9978
2OMe	7592.3	-16.32	0.9969	7754.1	-16.66	0.9972
3OMe	7746.2	-16.43	0.9974	7935.2	-16.84	0.9973
4OMe	7610.4	-16.10	0.9978	7765.5	-16.43	0.9978
2N	8769.8	-17.73	0.9962	9341.8	-18.93	0.9948
3N	8891.4	-17.48	0.9967	9055.0	-17.81	0.9964
4N	9244.5	-18.04	0.9967	9564.2	-18.69	0.9963
3CN	8590.8	-17.25	0.9967	8744.2	-17.56	0.9965
4CN	8734.6	-17.44	0.9967	9090.6	-18.17	0.9962
F-TF	7879.7	-17.38	0.9979	8116.1	-17.89	0.9975
Cl-TF	8615.1	-18.11	0.9979	8854.7	-18.62	0.9978
Br-TF	8881.3	-18.25	0.9972	9098.3	-18.71	0.9973

Table B7 Thermodynamic values of all analytes obtained from ln k′ vs. 1/T plots on BMe column

analyte	Enthalpic term			Entropic term		
	-ΔH1	-ΔH2	-Δ(ΔH)	-ΔS1	-ΔS2	-Δ(ΔS)
H	13.18	13.55	0.37	18.96	19.75	0.79
2F	13.48	13.87	0.39	19.95	20.5	0.55
3F	13.62	14.06	0.44	19.62	20.57	0.95
4F	13.54	14.04	0.50	19.48	20.54	1.06
2Cl	15.24	16.46	1.22	21.83	24.40	2.57
3Cl	15.15	15.58	0.43	21.31	22.21	0.90
4Cl	15.16	15.68	0.52	21.25	22.35	1.10
2Br	15.82	17.32	1.50	22.27	25.41	3.14
3Br	15.58	15.96	0.38	21.42	22.23	0.81
4Br	15.72	16.15	0.43	21.60	22.50	0.90
2Me	14.32	15.18	0.86	20.50	22.32	1.82
3Me	13.90	14.24	0.34	19.89	20.63	0.74
4Me	13.48	13.93	0.45	18.94	19.90	0.96
2OMe	15.08	15.41	0.33	21.46	22.13	0.67
3OMe	15.09	15.77	0.68	21.68	22.48	0.80
4OMe	15.12	15.43	0.31	21.02	21.68	0.66
2N	17.42	18.56	1.14	24.26	26.65	2.39
3N	17.67	17.99	0.32	23.76	24.43	0.67
4N	18.37	19.00	0.63	24.87	26.17	1.30
3CN	17.35	18.06	0.71	23.68	25.13	1.45
4CN	17.07	17.37	0.30	23.30	23.92	0.62
F-TF	15.66	16.13	0.47	23.56	24.58	1.02
Cl-TF	17.12	17.59	0.47	25.02	26.03	1.01
Br-TF	17.65	18.08	0.43	25.30	26.20	0.90

Table B8 Equations, correlation coefficients, and thermodynamic differences of all analytes obtained from R ln α vs. 1/T plots on BMe column

analyte	Equation: $R\ln\alpha = a \cdot \frac{1}{T} + b$		R^2	-Δ(ΔH) (kcal/mol)	-Δ(ΔS) (cal/mol.K)
	a	b			
H	394.6	-0.85	0.9938	0.39	0.85
2F	593.1	-1.33	0.9931	0.39	0.55
3F	456.1	-0.97	0.9945	0.46	0.97
4F	521.3	-1.12	0.9929	0.52	1.12
2Cl	1246.7	-3.21	0.9592	1.25	2.64
3Cl	438.8	-0.79	0.9785	0.44	0.92
4Cl	532.2	-0.91	0.9788	0.53	1.12
2Br	1536.0	-3.21	0.9638	1.54	3.21
3Br	379.2	-0.79	0.9863	0.38	0.79
4Br	441.6	-0.91	0.9725	0.44	0.91
2Me	906.9	-1.93	0.9711	0.91	1.93
3Me	370.0	-0.80	0.9961	0.37	0.80
4Me	483.1	-1.04	0.9889	0.48	1.04
2OMe	307.1	-0.63	0.9990	0.31	0.63
3OMe	408.8	-0.88	0.9868	0.68	0.88
4OMe	316.5	-0.67	0.9890	0.32	0.67
2N	116.1.6	-2.44	0.9508	1.16	2.44
3N	332.1	-0.68	0.9683	0.33	0.68
4N	647.3	-1.32	0.9724	0.65	1.32
3CN	311.4	-0.64	0.9841	0.31	0.64
4CN	722.5	-1.48	0.9697	0.72	1.48
F-TF	562.2	-1.23	0.9918	0.56	1.23
Cl-TF	493.3	-1.04	0.9794	0.49	1.04
Br-TF	429.9	-0.90	0.9818	0.43	0.90

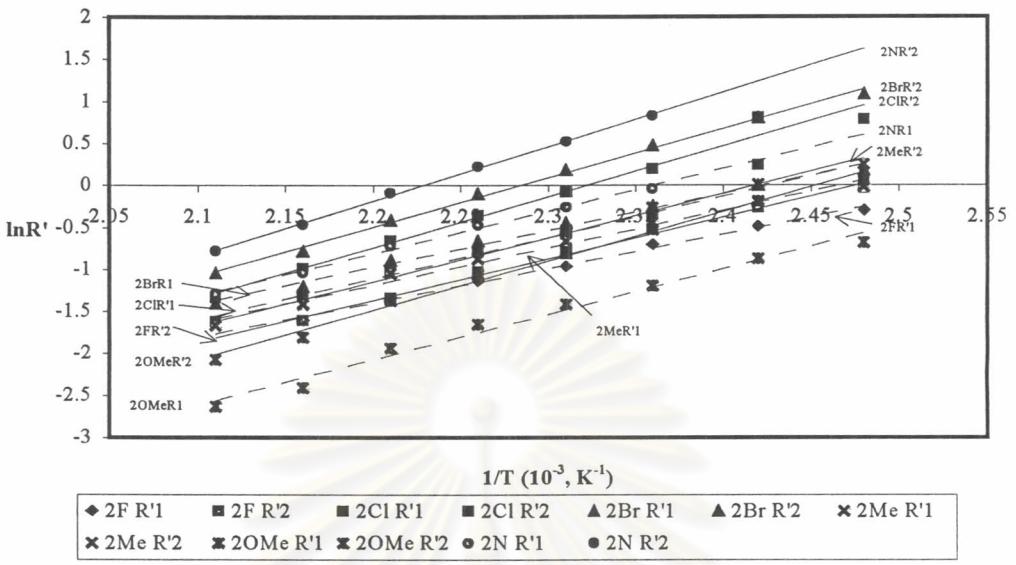

Figure B6 Plots of ln R′ vs. 1/T of *ortho*-substituted analytes on BSiMe column

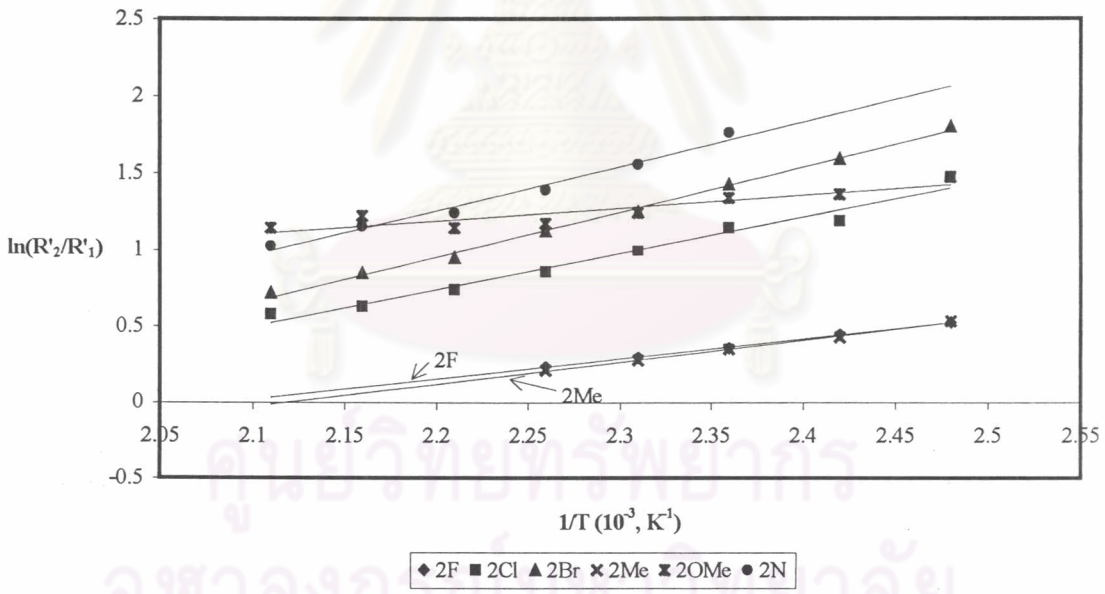

Figure B7 Plots of R ln (R'_2/R'_1) vs. 1/T of *ortho*-substituted analytes on BSiMe column

Table B9 Equations and correlation coefficients of all analytes obtained from ln R′ vs. 1/T plots on BSiMe column

analyte	Less retained enantiomer			More retained enantiomer		
	Equation: $\ln R' = a \cdot \frac{1}{T} + b$		R^2	Equation: $\ln R' = a \cdot \frac{1}{T} + b$		R^2
	a	b		a	b	
H	4691.5	-11.92	0.9748	5052.2	-12.70	0.9802
2F	4073.7	-10.36	0.9950	4943.7	-12.24	0.9948
3F	4168.6	-10.44	0.9790	4465.3	-11.08	0.9854
4F	3882.7	-69.69	0.9693	4133.7	-10.24	0.9771
2Cl	4886.1	-11.86	0.9538	6049.5	-14.05	0.9812
3Cl	3591.7	-8.98	0.9852	3893.1	-9.62	0.9852
4Cl	3237.0	-8.10	0.9837	3582.7	-8.85	0.9888
2Br	4373.8	-10.60	0.9926	5855.7	-13.38	0.9972
3Br	3930.7	-9.72	0.9905	4021.7	-9.90	0.9830
4Br	3106.4	-7.71	0.9838	3257.3	-8.03	0.9770
2Me	4449.0	-10.98	0.9871	5244.8	-12.68	0.9931
3Me	3324.1	-8.81	0.9440	3858.8	-9.95	0.9582
4Me	3091.7	-8.32	0.9800	3641.3	-9.49	0.9901
2OMe	5402.4	-13.96	0.9831	5858.2	-14.38	0.9918
3OMe	4000.2	-10.44	0.9793	4535.2	-11.57	0.9780
4OMe	2201.8	-6.26	0.8782	2583.6	-7.09	0.9012
2N	5052.0	-11.93	0.9944	6475.0	-14.43	0.9987
3N	4392.0	-10.62	0.9887	4608.0	-11.09	0.9906
4N	3478.9	-8.25	0.9921	3831.7	-8.97	0.9949
3CN	4358.9	-10.39	0.9946	4577.7	-10.86	0.9948
4CN	3537.1	-8.48	0.9875	3972.0	-9.36	0.9932
F-TF	3742.2	-9.13	0.9917	3934.1	-9.52	0.9891
Cl-TF	3458.8	-8.39	0.9911	---	---	---
Br-TF	3346.5	-8.04	0.9909	---	---	---

Table B10 Thermodynamic values of all analytes obtained from ln R′ vs. 1/T plots on BSiMe column

analyte	Enthalpic term			Entropic term		
	-ΔH1	-ΔH2	-Δ(ΔH)	-ΔS1	-ΔS2	-Δ(ΔS)
H	9.32	10.04	0.72	20.05	21.60	1.55
2F	8.09	9.82	1.73	16.95	20.69	3.74
3F	8.28	8.87	0.59	17.11	18.39	1.28
4F	7.71	8.21	0.50	15.63	16.72	1.09
2Cl	9.71	12.02	2.31	19.94	24.29	4.35
3Cl	7.14	7.73	0.59	14.21	15.49	1.28
4Cl	6.43	7.12	0.69	12.46	13.98	1.52
2Br	8.69	11.63	2.94	17.43	22.96	5.53
3Br	7.81	7.99	0.18	15.68	16.04	0.36
4Br	6.17	6.47	0.30	11.69	12.32	0.63
2Me	8.84	10.42	1.58	18.17	21.57	3.40
3Me	6.60	7.67	1.07	13.86	16.14	2.28
4Me	6.14	7.23	1.09	12.89	15.23	2.34
2OMe	10.73	11.64	0.91	24.11	24.93	0.82
3OMe	7.95	9.01	1.06	17.11	19.35	2.24
4OMe	4.37	5.13	0.76	8.81	10.45	1.64
2N	10.04	12.87	2.83	20.07	25.04	4.97
3N	8.73	9.16	0.43	17.48	18.40	0.92
4N	6.91	7.61	0.70	12.76	14.19	1.43
3CN	8.66	9.09	0.43	17.02	17.95	0.93
4CN	7.03	7.89	0.86	13.22	14.96	1.74
F-TF	7.44	7.82	0.38	14.52	15.28	0.76
Cl-TF	6.87	---	0.00	13.04	---	0.00
Br-TF	6.65	---	0.00	12.33	---	0.00

Table B11 Equations, correlation coefficients, and thermodynamic differences of all analytes obtained from R ln (R'_2/R'_1) vs. 1/T plots on BSiMe column

analytes	Equation $R\ln\left(\frac{R'_2}{R'_1}\right) = a \cdot \frac{1}{T} + b$		R^2	-Δ(ΔH) (kcal/mol)	-Δ(ΔS) (cal/mol.K)
	a	b			
H	525.2	-1.08	0.9652	0.53	1.08
2F	1326.3	-2.77	0.9997	1.33	2.77
3F	371.0	-0.74	0.9969	0.37	0.74
4F	683.3	-1.52	0.9998	0.68	1.52
2Cl	2380.2	-4.50	0.9777	2.38	4.50
3Cl	418.7	-0.85	0.9988	0.42	0.85
4Cl	687.3	-1.48	0.9963	0.69	1.47
2Br	2944.0	-5.53	0.9964	2.94	5.53
3Br	351.1	-0.72	0.9982	0.35	0.72
4Br	624.9	-1.35	0.9980	0.62	1.35
2Me	1447.3	-3.07	0.9981	1.45	3.07
3Me	799.9	-1.64	0.9766	0.80	1.64
4Me	970.1	-2.04	0.9969	0.97	2.04
2OMe	851.8	-0.69	0.8261	0.85	0.69
3OMe	655.7	-1.37	0.9974	0.86	1.75
4OMe	716.7	-1.52	0.9863	0.72	1.52
2N	2894.9	-5.11	0.9834	2.89	5.11
3N	918.6	-2.04	0.8651	0.43	0.92
4N	699.4	-1.43	0.9867	0.70	1.43
3CN	140.0	-0.24	0.9735	0.43	0.93
4CN	860.0	-1.73	0.9746	0.86	1.74
F-TF[a]					
Cl-TF[b]					
Br-TF[b]					

[a] correlation was not linear, [b] not separated in this temperature rang (130-200 °C)

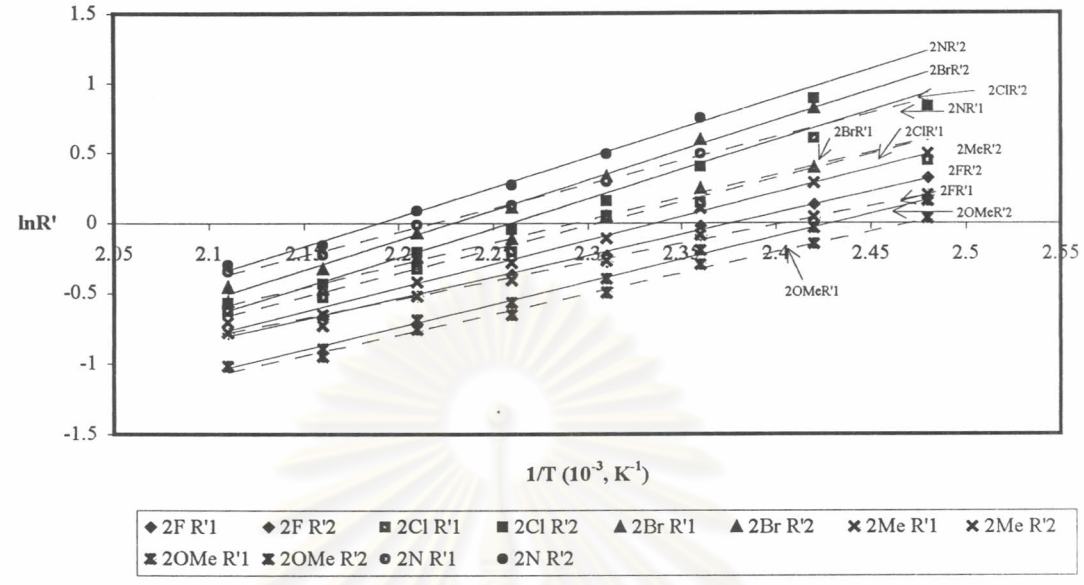

Figure B8 Plots of ln R′ vs. 1/T of *ortho*-substituted analytes on BMe column

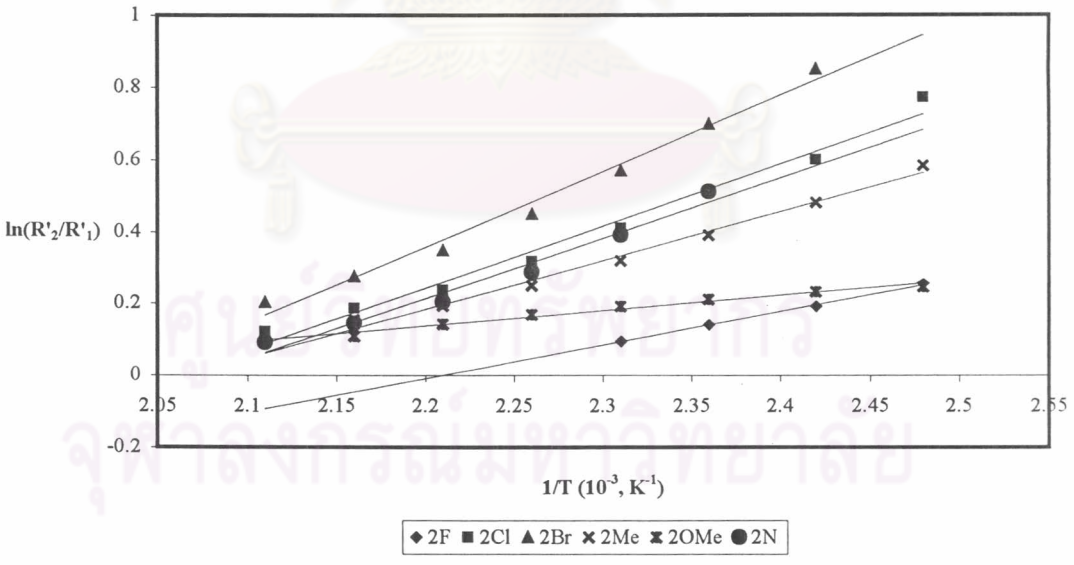

Figure B9 Plots of $R\ln(R'_2/R'_1)$ vs. 1/T of *ortho*-substituted analytes on BMe column

Table B12 Equations and correlation coefficients of all analytes obtained from ln R′ vs. 1/T plots on BMe column

analyte	Less retained enantiomer			More retained enantiomer		
	Equation: $\ln R' = a \cdot \frac{1}{T} + b$		R^2	Equation: $\ln R' = a \cdot \frac{1}{T} + b$		R^2
	a	b		a	b	
H	2862.7	-6.93	0.9794	2986.6	-7.18	0.9649
2F	2658.7	-6.39	0.9973	3032.5	-7.21	0.9975
3F	2400.4	-5.76	0.9944	2813.4	-6.64	0.9947
4F	2369.6	-5.65	0.9917	2732.1	-6.43	0.9841
2Cl	3365.5	-7.76	0.9450	4198.8	-9.48	0.9946
3Cl	2560.5	-6.08	0.9946	2926.6	-6.84	0.9968
4Cl	2517.7	-5.88	0.9946	2945.9	-6.77	0.9969
2Br	3194.2	-7.32	0.9946	4253.9	-9.48	0.9958
3Br	2598.4	-6.13	0.9918	2942.2	-6.84	0.9958
4Br	2664.4	-6.13	0.9930	2995.0	-6.80	0.9953
2Me	2758.7	-6.63	0.9935	3378.4	-7.89	0.9938
3Me	2631.5	-6.48	0.9940	2981.4	-7.23	0.9960
4Me	2029.1	-5.17	0.9547	2627.0	-6.43	0.9965
2OMe	2937.6	-7.26	0.9948	3228.7	-7.84	0.9977
3OMe	2510.0	-6.11	0.9949	2872.5	-6.88	0.9946
4OMe	2203.9	-5.40	0.9943	2509.5	-6.05	0.9938
2N	3379.1	-7.50	0.9955	4222.4	-9.25	0.9948
3N	2766.5	-6.24	0.9921	3020.3	-6.76	0.9935
4N	3006.6	-6.49	0.9961	3429.4	-7.33	0.9964
3CN	2884.1	-6.50	0.9939	3114.5	-6.96	0.9949
4CN	2896.4	-6.34	0.9938	3381.2	-7.30	0.9950
F-TF	2454.8	-5.36	0.9734	2817.0	-6.14	0.9767
Cl-TF	2270.7	-4.85	0.9742	2625.1	-5.59	0.9828
Br-TF	2422.9	-5.14	0.9445	2736.5	-5.79	0.9622

Table B13 Thermodynamic values of all analytes obtained from ln R′ vs. 1/T plots on BMe column

analyte	Enthalpic term			Entropic term		
	-ΔH1	-ΔH2	-Δ(ΔH)	-ΔS1	-ΔS2	-Δ(ΔS)
H	5.69	5.93	0.24	9.94	10.45	0.51
2F	5.28	6.02	0.74	8.88	10.50	1.62
3F	4.77	5.59	0.82	7.63	9.36	1.73
4F	4.71	5.43	0.72	7.40	8.95	1.55
2Cl	6.69	8.34	1.65	11.59	15.02	3.43
3Cl	5.09	5.81	0.72	8.26	9.77	1.51
4Cl	5.00	5.85	0.85	7.86	9.62	1.76
2Br	6.35	8.45	2.10	10.73	15.01	4.28
3Br	5.16	5.85	0.69	8.35	9.77	1.42
4Br	5.29	5.95	0.66	8.36	9.68	1.32
2Me	5.48	6.71	1.23	9.36	11.86	2.50
3Me	5.23	5.92	0.69	9.05	10.54	1.49
4Me	4.03	5.22	1.19	6.44	8.95	2.51
2OMe	5.84	6.41	0.57	10.60	11.76	1.16
3OMe	4.99	5.71	0.72	8.31	9.84	1.53
4OMe	4.38	4.99	0.61	6.91	8.19	1.28
2N	6.71	8.39	1.68	11.08	14.55	3.47
3N	5.50	6.00	0.50	8.58	9.60	1.02
4N	5.97	6.81	0.84	9.08	10.74	1.66
3CN	5.73	6.19	0.46	9.01	10.00	0.99
4CN	5.75	6.72	0.97	8.77	10.68	1.91
F-TF	4.88	5.60	0.72	6.83	8.38	1.55
Cl-TF	4.51	5.22	0.71	5.81	7.29	1.48
Br-TF	4.81	5.44	0.63	6.39	7.68	1.29

Table B14 Equations, correlation coefficients, and thermodynamic differences of all analytes obtained from R ln (R'_2/R'_1) vs. 1/T plots on BMe column

analytes	Equation $R\ln\left(\frac{R'_2}{R'_1}\right) = a \cdot \frac{1}{T} + b$		R^2	-Δ(ΔH) (kcal/mol)	-Δ(ΔS) (cal/mol.K)
	a	b			
H	598.6	-1.25	0.9965	0.24	0.51
2F	934.7	-2.07	0.9977	0.93	2.07
3F	692.7	-1.43	0.9969	0.69	1.43
4F	758.4	-1.58	0.9966	0.76	1.58
2Cl	1725.5	-3.55	0.9834	1.72	3.55
3Cl	655.6	-1.34	0.9921	0.66	1.34
4Cl	762.8	-1.55	0.9898	0.76	1.55
2Br	2106.9	-4.28	0.9862	2.11	4.28
3Br	580.5	-1.17	0.9964	0.58	1.17
4Br	657.6	-1.32	0.9874	0.66	1.32
2Me	1361.9	-2.81	0.9891	1.36	2.81
3Me	577.3	-1.20	0.9996	0.58	1.20
4Me	857.9	-1.80	0.9979	0.86	1.79
2OMe	427.1	-0.80	0.9751	0.43	0.80
3OMe	330.1	-0.69	0.9974	0.66	1.37
4OMe	520.1	-1.07	0.9960	0.52	1.07
2N	1677.3	-3.48	0.9756	1.68	3.48
3N	504.9	-1.02	0.9817	0.50	1.02
4N	839.8	-1.66	0.9845	0.84	1.66
3CN	458.6	-0.91	0.9953	0.46	0.91
4CN	964.2	-1.91	0.9811	0.96	1.91
F-TF	741.3	-1.60	0.9951	0.74	1.60
Cl-TF	650.7	-1.35	0.9908	0.65	1.35
Br-TF	554.8	-1.14	0.9894	0.55	1.14

VITA

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