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APPENDICES

Appendix A

Glossary

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

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 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 $k'_2 \geq k'_1$.

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

Appendix B

Thermodynamic data

Table B1 Equation and correlation coefficient of all phenoxy acid methyl esters obtained from plots of ln k′ vs. 1/T on ASiMe column.

analyte	temparature range (°C)	less retained enantiomer			more retained enantiomer		
		ln k′ = m (1/T) + c		R^2	ln k′ = m (1/T) + c		R^2
		m	c		m	c	
1	100–170	6640.70	-14.949	0.9998	6640.70	-14.949	0.9998
2F	70–130	6955.30	-15.769	0.9999	7020.70	-15.917	0.9999
3F	80-140	6923.00	-15.706	0.9999	7041.70	-15.978	0.9999
4F	90-150	7243.90	-16.318	0.9998	7356.90	-16.568	0.9998
2Cl	100-160	7339.50	-15.760	0.9998	7447.30	-15.998	0.9998
3Cl	110-170	7586.00	-16.274	0.9996	7790.90	-16.726	0.9995
4Cl	110-170	8509.40	-18.135	0.9994	8661.50	-18.460	0.9994
2Br	110-170	7529.70	-15.779	0.9997	7636.60	-16.013	0.9997
3Br	110-170	8032.90	-16.861	0.9995	8250.50	-17.341	0.9994
4Br	120-180	8734.70	-18.160	0.9993	8872.50	-18.452	0.9992
2OMe	90-130	7889.70	-16.992	1.0000	7949.90	-17.132	1.0000
3OMe	130-190	7527.00	-15.792	0.9998	7527.00	-15.792	0.9998
4OMe	100-140	8190.70	-17.305	0.9999	8253.00	-17.450	1.0000
2Me	90-140	7029.90	-15.644	0.9999	7096.30	-15.793	0.9999
3Me	90-130	7486.70	-16.537	1.0000	7560.50	-16.708	1.0000
4Me	100-140	7671.60	-16.837	0.9999	7739.30	-16.987	0.9999
2CN	120-180	8089.50	-16.536	0.9997	8211.70	-16.794	0.9997
3CN	130-190	8601.90	-17.583	0.9994	8829.00	-18.056	0.9993
4CN	150-220	8974.10	-17.891	0.9990	9171.60	-18.281	0.9990
$2CF_3$	90-170	6832.60	-15.363	0.9997	7050.40	-15.839	0.9996
$3CF_3$	70-110	7058.80	-16.272	0.9999	7117.30	-16.415	0.9999
$4CF_3$	100-170	6907.40	-15.575	0.9997	6907.40	-15.575	0.9997
$2NO_2$	120-180	8278.40	-16.658	0.9997	8376.80	-16.867	0.9997
$3NO_2$	150-220	7792.60	-15.503	0.9996	7792.60	-15.503	0.9996
$4NO_2$	130-170	9057.60	-17.906	0.9999	9144.00	-18.090	0.9999

Table B1 (continued)

analyte	temparature range (°C)	less retained enantiomer			more retained enantiomer		
		ln k′ = m (1/T) + c		R^2	ln k′ = m (1/T) + c		R^2
		m	c		m	c	
2,3Me	80-120	7827.20	-16.947	1.0000	7875.40	-17.060	1.0000
2,4Me	100-160	7898.80	-17.078	0.9997	7990.60	-17.279	0.9997
2,5Me	90-130	7432.00	-16.242	1.0000	7475.60	-16.344	1.0000
2,6Me	120-180	6842.20	-14.795	0.9998	6842.20	-14.795	0.9998
3,4Me	130-190	7469.80	-15.797	0.9996	7469.80	-15.797	0.9996
3,5Me	100-160	7965.10	-17.149	0.9998	8114.60	-17.481	0.9997
2,3F	100-170	6682.00	-15.017	0.9998	6682.00	-15.017	0.9998
2,4F	90-150	7268.10	-16.549	0.9998	7399.30	-16.843	0.9998
2,5F	100-160	6720.40	-15.270	0.9998	6720.40	-15.270	0.9998
2,6F	100-160	6556.60	-14.902	0.9998	6556.60	-14.902	0.9998
3,4F	100-170	6676.30	-15.054	0.9998	6676.30	-15.054	0.9998
3,5F	100-160	6877.10	-15.756	0.9997	7080.00	-16.205	0.9997
2,3Cl	140-210	7454.60	-15.096	0.9996	7454.60	-15.096	0.9996
2,4Cl	140-210	7526.70	-15.281	0.9996	7526.70	-15.281	0.9996
2,5Cl	100-140	8106.60	-16.935	0.9999	8152.00	-17.036	1.0000
2,6Cl	140-200	7122.60	-14.678	0.9998	7122.60	-14.678	0.9998
3,4Cl	140-190	8640.60	-17.734	0.9993	8869.60	-18.210	0.9991
3,5Cl	130-190	8126.20	-16.822	0.9994	8428.80	-17.461	0.9991
2,4,6F	70-110	7504.00	-17.485	0.9999	7562.70	-17.628	1.0000
2,4,6Cl	120-160	9194.90	-18.799	0.9997	9282.70	-18.990	0.9997
pentaF	90-150	6345.20	-14.958	0.9999	6345.20	-14.958	0.9999

Table B2 Equation and correlation coefficient of all phenoxy acid methyl esters obtained from plots of ln k′ vs. 1/T on GSiMe column.

analyte	temperature range (°C)	less retained enantiomer			more retained enantiomer		
		ln k′ = m (1/T) + c		R^2	ln k′ = m (1/T) + c		R^2
		m	c		m	c	
1	110-170	6396.8	-14.256	0.9998	6396.8	-14.256	0.9998
2F	110-170	6428.4	-14.335	0.9998	6428.4	-14.335	0.9998
3F	80-120	6910.3	-15.474	0.9999	6968.2	-15.610	0.9999
4F	110-170	6494.7	-14.476	0.9998	6494.7	-14.476	0.9998
2Cl	130-190	6834.8	-14.430	0.9998	6834.8	-14.430	0.9998
3Cl	100-140	7333.9	-15.525	0.9999	7401.1	-15.679	0.9999
4Cl	110-190	6959.5	-14.614	0.9998	6959.5	-14.614	0.9998
2Br	130-200	7045.5	-14.508	0.9997	7045.5	-14.508	0.9997
3Br	100-140	7662.6	-15.854	0.9999	7730.2	-16.007	0.9999
4Br	130-200	7208.4	-14.733	0.9997	7208.4	-14.733	0.9997
2OMe	130-190	7123.4	-14.981	0.9997	7123.4	-14.981	0.9997
3OMe	100-140	7855.6	-16.361	0.9999	7932.0	-16.536	0.9999
4OMe	130-200	7267.9	-15.009	0.9997	7267.9	-15.009	0.9997
2Me	110-170	6597.4	-14.462	0.9998	6597.4	-14.462	0.9998
3Me	90-130	7164.1	-15.569	0.9999	7236.0	-15.738	0.9999
4Me	120-180	6720.0	-14.530	0.9998	6720.0	-14.530	0.9998
2CN	110-150	8159.7	-16.504	0.9998	8256.5	-16.723	0.9998
3CN	110-150	8035.0	-16.271	0.9999	8108.2	-16.436	0.9999
4CN	110-140	8379.9	-16.770	0.9999	8446.0	-16.921	0.9999
$2CF_3$	70-110	7141.3	-15.982	0.9999	7184.9	-16.085	0.9999
$3CF_3$	70-100	7163.5	-16.296	0.9999	7222.9	-16.449	0.9999
$4CF_3$	80-120	7228.6	-16.153	0.9999	7289.1	-16.298	0.9999
$2NO_2$	150-220	7574.0	-14.927	0.9997	7574.0	-14.927	0.9997
$3NO_2$	150-220	7560.6	-14.871	0.9998	7560.6	-14.871	0.9998
$4NO_2$	160-220	7920.6	-15.262	0.9998	7920.6	-15.262	0.9998
2,3Me	130-190	6890.1	-14.533	0.9998	6890.1	-14.533	0.9998
2,4Me	120-180	6916.1	-14.750	0.9998	6916.1	-14.750	0.9998
2,5Me	120-180	6820.5	-14.636	0.9998	6820.5	-14.636	0.9998

Table B2 (continued)

analyte	temparature range (°C)	less retained enantiomer			more retained enantiomer		
		ln k′ = m (1/T) + c		R^2	ln k′ = m (1/T) + c		R^2
		m	c		m	c	
2,6Me	120-180	6761.0	-14.440	0.9998	6761.0	-14.440	0.9998
3,4Me	90-120	7732.5	-16.293	1.0000	7779.9	-16.405	1.0000
3,5Me	90-120	7593.6	-16.198	1.0000	7645.8	-16.320	0.9999
2,3F	110-170	6544.0	-14.550	0.9998	6544.0	-14.550	0.9998
2,4F	70-100	7038.9	-15.999	0.9999	7103.8	-16.166	0.9999
2,5F	100-160	6637.7	-14.819	0.9998	6637.7	-14.819	0.9998
2,6F	100-160	6456.8	-14.403	0.9998	6456.8	-14.403	0.9998
3,4F	110-170	6598.6	-14.588	0.9997	6598.6	-14.588	0.9997
3,5F	90-140	6621.9	-14.991	0.9999	6710.7	-15.196	0.9999
2,3Cl	140-210	7404.3	-14.813	0.9997	7404.3	-14.813	0.9997
2,4Cl	110-140	8075.4	-16.314	0.9999	8127.5	-16.431	0.9999
2,5Cl	130-200	7305.1	-14.906	0.9997	7305.1	-14.906	0.9997
2,6Cl	130-200	7135.9	-14.527	0.9997	7135.9	-14.527	0.9997
3,4Cl	130-200	7410.2	-15.024	0.9997	7410.2	-15.024	0.9997
3,5Cl	110-160	7680.7	-15.714	0.9998	7770.1	-15.912	0.9998
2,4,6F	110-150	8054.1	-16.069	0.9999	8054.1	-16.069	0.9999
2,4,6Cl	140-200	7517.8	-14.924	0.9998	7517.8	-14.924	0.9998
pentaF	90-150	6300.1	-14.593	0.9998	6300.1	-14.593	0.9998

Table B3 Thermodynamic parameters of all phenoxy acid methyl esters on ASiMe column.

analyte	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	13.20	13.20	0.00	18.73	18.73	0.00
2F	13.82	13.95	0.13	20.36	20.66	0.29
3F	13.76	13.99	0.24	20.24	20.78	0.54
4F	14.39	14.62	0.22	21.45	21.95	0.50
2Cl	14.58	14.80	0.21	20.34	20.82	0.47
3Cl	15.07	15.48	0.41	21.37	22.26	0.90
4Cl	16.91	17.21	0.30	25.06	25.71	0.65
2Br	14.96	15.17	0.21	20.38	20.85	0.46
3Br	15.96	16.39	0.43	22.53	23.49	0.95
4Br	17.36	17.63	0.27	25.11	25.69	0.58
2OMe	15.68	15.80	0.12	22.79	23.07	0.28
3OMe	14.96	14.96	0.00	20.41	20.41	0.00
4OMe	16.27	16.40	0.12	23.41	23.70	0.29
2Me	13.97	14.10	0.13	20.11	20.41	0.30
3Me	14.88	15.02	0.15	21.89	22.23	0.34
4Me	15.24	15.38	0.13	22.48	22.78	0.30
2CN	16.07	16.32	0.24	21.89	22.40	0.51
3CN	17.09	17.54	0.45	23.97	24.91	0.94
4CN	17.83	18.22	0.39	24.58	25.35	0.77
$2CF_3$	13.58	14.01	0.43	19.56	20.50	0.95
$3CF_3$	14.03	14.14	0.12	21.36	21.65	0.28
$4CF_3$	13.73	13.73	0.00	19.98	19.98	0.00
$2NO_2$	16.45	16.64	0.20	22.13	22.54	0.42
$3NO_2$	15.48	15.48	0.00	19.83	19.83	0.00
$4NO_2$	18.00	18.17	0.17	24.61	24.97	0.37
2,3Me	15.55	15.65	0.10	22.70	22.93	0.22
2,4Me	15.69	15.88	0.18	22.96	23.36	0.40
2,5Me	14.77	14.85	0.09	21.30	21.50	0.20
2,6Me	13.60	13.60	0.00	18.43	18.43	0.00

Table B3 (continued)

analyte	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta\Delta H$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta\Delta S$
3,4Me	14.84	14.84	0.00	20.42	20.42	0.00
3,5Me	15.83	16.12	0.30	23.10	23.76	0.66
2,3F	13.28	13.28	0.00	18.87	18.87	0.00
2,4F	14.44	14.70	0.26	21.91	22.50	0.58
2,5F	13.35	13.35	0.00	19.37	19.37	0.00
2,6F	13.03	13.03	0.00	18.64	18.64	0.00
3,4F	13.27	13.27	0.00	18.94	18.94	0.00
3,5F	13.66	14.07	0.40	20.34	21.23	0.89
2,3Cl	14.81	14.81	0.00	19.02	19.02	0.00
2,4Cl	14.96	14.96	0.00	19.39	19.39	0.00
2,5Cl	16.11	16.20	0.09	22.68	22.88	0.20
2,6Cl	14.15	14.15	0.00	18.19	18.19	0.00
3,4Cl	17.17	17.62	0.46	24.27	25.21	0.95
3,5Cl	16.15	16.75	0.60	22.45	23.72	1.27
2,4,6F	14.91	15.03	0.12	23.77	24.06	0.28
2,4,6Cl	18.27	18.44	0.17	26.38	26.76	0.38
pentaF	12.61	12.61	0.00	18.75	18.75	0.00

Table B4 Thermodynamic parameters of all phenoxy acid methyl esters on GSiMe column.

analyte	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta\Delta H$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta\Delta S$
1	12.71	12.71	0.00	17.36	17.36	0.00
2F	12.77	12.77	0.00	17.51	17.51	0.00
3F	13.73	13.85	0.12	19.78	20.05	0.27
4F	12.90	12.90	0.00	17.79	17.79	0.00
2Cl	13.58	13.58	0.00	17.70	17.70	0.00
3Cl	14.57	14.71	0.13	19.88	20.18	0.31
4Cl	13.83	13.83	0.00	18.07	18.07	0.00
2Br	14.00	14.00	0.00	17.86	17.86	0.00
3Br	15.23	15.36	0.13	20.53	20.83	0.30
4Br	14.32	14.32	0.00	18.30	18.30	0.00
2OMe	14.15	14.15	0.00	18.80	18.80	0.00
3OMe	15.61	15.76	0.15	21.54	21.89	0.35
4OMe	14.44	14.44	0.00	18.85	18.85	0.00
2Me	13.11	13.11	0.00	17.76	17.76	0.00
3Me	14.24	14.38	0.14	19.96	20.30	0.34
4Me	13.35	13.35	0.00	17.90	17.90	0.00
2CN	16.21	16.41	0.19	21.82	22.26	0.44
3CN	15.97	16.11	0.15	21.36	21.69	0.33
4CN	16.65	16.78	0.13	22.35	22.65	0.30
$2CF_3$	14.19	14.28	0.09	20.79	20.99	0.20
$3CF_3$	14.23	14.35	0.12	21.41	21.71	0.30
$4CF_3$	14.36	14.48	0.12	21.12	21.41	0.29
$2NO_2$	15.05	15.05	0.00	18.69	18.69	0.00
$3NO_2$	15.02	15.02	0.00	18.58	18.58	0.00
$4NO_2$	15.74	15.74	0.00	19.35	19.35	0.00
2,3Me	13.69	13.69	0.00	17.91	17.91	0.00
2,4Me	13.74	13.74	0.00	18.34	18.34	0.00
2,5Me	13.55	13.55	0.00	18.11	18.11	0.00
2,6Me	13.43	13.43	0.00	17.72	17.72	0.00

Table B4 (continued)

analyte	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta\Delta H$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta\Delta S$
3,4Me	15.36	15.46	0.09	21.40	21.63	0.22
3,5Me	15.09	15.19	0.10	21.21	21.46	0.24
2,3F	13.00	13.00	0.00	17.94	17.94	0.00
2,4F	13.99	14.12	0.13	20.82	21.15	0.33
2,5F	13.19	13.19	0.00	18.47	18.47	0.00
2,6F	12.83	12.83	0.00	17.65	17.65	0.00
3,4F	13.11	13.11	0.00	18.02	18.02	0.00
3,5F	13.16	13.33	0.18	18.82	19.22	0.41
2,3Cl	14.71	14.71	0.00	18.46	18.46	0.00
2,4Cl	16.05	16.15	0.10	21.44	21.68	0.23
2,5Cl	14.52	14.52	0.00	18.65	18.65	0.00
2,6Cl	14.18	14.18	0.00	17.89	17.89	0.00
3,4Cl	14.72	14.72	0.00	18.88	18.88	0.00
3,5Cl	15.26	15.44	0.18	20.25	20.65	0.39
2,4,6F	16.00	16.00	0.00	20.96	20.96	0.00
2,4,6Cl	14.94	14.94	0.00	18.68	18.68	0.00
pentaF	12.52	12.52	0.00	18.03	18.03	0.00

VITA

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