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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, which indicates the degree of linear relationship between two variables.

Distribution constant (K) is defined as the concentration ratio of a compound in a stationary phase (C_S) and in a mobile phase(C_M). K is related to retention factor by the following equation

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

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

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

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 mol ratio of analyte in the stationary phase and in the 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

Details of thermodynamic data

Table B1 Linear equation and correlation coefficient of aliphatic epoxides obtained from ln k′ vs. 1/T plots on OV-1701 column.

analyte	ln k′ = m(1/T) + c		R^2
	m	c	
hexa	4453.2	−12.718	0.9999
5hexe	4443.2	−12.720	0.9999
octa	5261.6	−13.514	0.9998
deca	5959.0	−14.084	0.9998
9dece	5956.6	−14.061	0.9998
dodec	6582.4	−14.539	0.9998

Table B2 Thermodynamic parameters of aliphatic epoxides calculated from van't Hoff plots of ln k′ vs. 1/T on OV-1701 column.

analyte	−ΔH (kcal/mol)	−ΔS (cal/mol·K)
hexa	8.85	14.30
5hexe	8.83	14.30
octa	10.45	15.88
deca	11.84	17.01
9dece	11.84	16.97
dodec	13.08	17.92

Table B3 Linear equation and correlation coefficient of all epoxides obtained from van't Hoff plots of ln k′ vs. 1/T on GSiMe column.

analyte	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	5585.4	−13.539	0.9997	5585.4	−13.539	0.9997
2Br	6151.5	−13.695	0.9998	6235.3	−13.886	0.9998
3Br	6518.0	−14.250	0.9998	6518.0	−14.250	0.9998
4Br	6596.7	−14.461	0.9999	6634.9	−14.549	0.9999
2Cl	5888.5	−13.528	0.9998	5985.6	−13.749	0.9997
3Cl	6380.6	−14.484	1.0000	6413.0	−14.560	1.0000
4Cl	6300.7	−14.253	0.9999	6341.2	−14.346	0.9999
2F	5488.6	−13.466	0.9999	5561.3	−13.635	0.9999
3F	5644.3	−13.708	0.9999	5703.1	−13.844	0.9999
4F	5835.3	−14.203	0.9999	5875.6	−14.301	0.9998
2Me	6096.0	−14.322	0.9999	6161.5	−14.492	0.9997
3Me	6137.1	−14.378	0.9998	6211.2	−14.557	0.9998
4Me	6017.6	−14.074	0.9999	6064.2	−14.181	0.9999
4Et	6402.0	−14.512	0.9998	6460.2	−14.649	0.9999
2CF	5609.9	−14.002	0.9999	5681.8	−14.186	0.9999
3CF	6234.4	−15.286	0.9997	6306.0	−15.489	0.9997
4CF	6817.1	−15.859	0.9998	6853.2	−15.943	0.9998
3OMe	7016.3	−14.509	0.9999	7091.7	−14.672	0.9999
3CN	6777.4	−14.330	0.9998	6849.7	−14.482	0.9998
4CN	6939.4	−14.684	0.9999	6985.0	−14.785	0.9999
2NO	6630.0	−14.098	0.9999	6703.0	−14.252	0.9999
3NO	7103.6	−14.595	0.9999	7103.6	−14.595	0.9999
4NO	7232.2	−14.834	0.9998	7270.8	−14.927	0.9998
24Cl	6287.5	−13.677	0.9998	6375.1	−13.869	0.9998
25Cl	6634.1	−14.504	0.9999	6685.3	−14.635	0.9999
34Cl	6760.1	−14.298	0.9998	6760.1	−14.298	0.9998

Table B3 (continued)

analyte	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	
24F	5447.5	−13.548	0.9998	5563.4	−13.818	0.9997
25F	5537.0	−13.657	0.9998	5537.0	−13.657	0.9998
26F	5777.9	−13.953	0.9998	5865.9	−14.157	0.9997
34F	5956.3	−14.468	0.9999	6000.1	−14.584	0.9999
24Me	6391.2	−14.476	0.9999	6453.1	−14.619	0.9999
25Me	6370.6	−14.473	0.9999	6427.7	−14.605	0.9999
34Me	6522.2	−14.606	0.9999	6563.0	−14.712	0.9999
triF	5509.5	−13.722	0.9998	5509.5	−13.722	0.9998
tetraF	5462.7	−13.678	0.9998	5462.7	−13.678	0.9998
pentaF	5729.4	−14.328	0.9999	5760.4	−14.412	0.9999
cis−2	5991.8	−14.474	0.9999	6067.2	−14.663	0.9998
trans−2	6045.6	−14.542	0.9999	6159.3	−14.823	0.9998
cis−3	6303.8	−14.747	0.9998	6397.2	−14.977	0.9998
trans−3	6271.6	−14.538	0.9998	6360.9	−14.754	0.9998
4	6114.8	−14.757	0.9999	6191.0	−14.956	0.9999
cis−5	6179.2	−14.355	0.9998	6233.9	−14.484	0.9998
trans−5	6248.8	−14.418	0.9999	6248.8	−14.418	0.9999
6	6076.7	−14.230	0.9998	6076.7	−14.230	0.9998
7	6888.9	−15.427	0.9999	6918.9	−15.505	0.9998
8	6983.8	−15.267	0.9999	7020.0	−15.359	0.9998
hexa	4463.3	−12.660	0.9999	4463.3	−12.660	0.9999
5hexe	4459.2	−12.677	0.9999	4459.2	−12.677	0.9999
octa	5391.9	−13.767	0.9998	5391.9	−13.767	0.9998
deca	6000.5	−14.082	0.9998	6000.5	−14.082	0.9998
9dece	6002.2	−14.065	0.9998	6002.2	−14.065	0.9998
dodec	6718.8	−14.754	0.9998	6718.8	−14.754	0.9998

Table B4 Linear equation and correlation coefficient of all epoxides obtained from van't Hoff plots of ln k′ vs. 1/T on GSiAc column.

analyte	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	6231.3	−14.961	0.9992	6341.3	−15.216	0.9991
2Br	6238.5	−13.735	0.9996	6486.4	−14.274	0.9993
3Br	6638.4	−14.316	0.9996	6724.5	−14.497	0.9996
4Br	6653.1	−14.331	0.9997	6642.3	−14.293	0.9998
2Cl	6116.0	−13.885	0.9996	6456.3	−14.639	0.9993
3Cl	6469.2	−14.400	0.9995	6578.3	−14.632	0.9995
4Cl	6374.1	−14.152	0.9996	6403.4	−14.206	0.9997
2F	5925.0	−14.276	0.9995	6329.8	−15.211	0.9991
3F	6134.6	−14.604	0.9997	6343.3	--15.074	0.9994
4F	5949.9	−14.147	0.9995	6124.2	−14.542	0.9996
2Me	6388.3	−14.776	0.9996	6644.8	−15.356	0.9995
3Me	6600.9	−15.436	0.9997	6845.4	−16.062	0.9995
4Me	6281.2	−14.610	0.9998	6321.3	−14.704	0.9998
4Et	6493.2	−14.620	0.9999	6531.5	−14.715	0.9999
2CF	5807.2	−14.257	0.9996	6262.8	−15.341	0.9992
3CF	6519.1	−15.581	0.9996	6946.5	−16.674	0.9990
4CF	6409.1	−15.267	0.9998	6740.6	−16.126	0.9996
3OMe	6963.0	−14.235	0.9999	7103.9	−14.529	0.9998
3CN	7423.9	−15.278	0.9996	7584.4	−15.598	0.9995
4CN	7982.5	−16.482	0.9998	8204.7	−16.988	0.9997
2NO	7416.9	−15.402	0.9993	7795.3	−16.169	0.9990
3NO	8176.7	−16.464	0.9995	8173.3	−16.441	0.9996
4NO	8235.6	−16.448	0.9997	8536.2	−17.087	0.9995
24Cl	6634.8	−14.388	0.9998	6791.0	−14.746	0.9997
25Cl	6830.8	−14.788	0.9998	6971.0	−15.126	0.9999
34Cl	7443.1	−15.633	0.9999	7637.9	−16.099	0.9997

Table B4 (continued)

analyte	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	
24F	5912.0	−14.433	0.9995	6173.7	−15.054	0.9993
25F	6053.4	−14.657	0.9995	6244.4	−15.117	0.9994
26F	6492.5	−15.345	0.9993	6668.1	−15.748	0.9992
34F	6508.7	−15.324	0.9995	6501.4	−15.276	0.9996
24Me	6539.1	−14.703	0.9996	6607.5	−14.854	0.9996
25Me	6634.5	−14.946	0.9997	6634.5	−14.946	0.9997
34Me	6449.6	−14.300	0.9999	6449.6	−14.300	0.9999
triF	5955.2	−14.488	0.9997	6085.2	−14.797	0.9997
tetraF	6132.7	−14.924	0.9997	6435.4	−15.644	0.9995
pentaF	6336.5	−15.312	0.9996	6826.5	−16.474	0.9992
cis−2	5956.9	−14.191	0.9995	6536.4	−15.557	0.9988
trans−2	5923.2	−14.017	0.9996	6201.8	−14.671	0.9992
cis−3	5992.6	−13.897	0.9998	6340.6	−14.688	0.9994
trans−3	6074.8	−13.903	0.9998	6218.1	−14.226	0.9998
4	5909.6	−14.002	0.9998	5909.6	−14.002	0.9998
cis−5	6154.4	−14.184	0.9997	6439.3	−14.852	0.9994
trans−5	6302.5	−14.377	0.9998	6334.1	−14.440	0.9998
6	6748.6	−15.714	0.9998	6835.9	−15.930	0.9998
7	7374.3	−16.304	0.9998	7483.7	−16.573	0.9998
8	7271.0	−15.741	0.9998	7382.0	−16.007	0.9999
hexa	4937.7	−13.752	0.9998	4937.7	−13.752	0.9998
5hexe	5163.3	−14.306	0.9997	5262.1	−14.560	0.9997
octa	5426.8	−13.755	0.9997	5426.8	−13.755	0.9997
deca	6046.2	−14.153	0.9998	6046.2	−14.153	0.9998
9dece	6115.3	−14.264	0.9998	6115.3	−14.264	0.9998
dodec	6758.0	−14.857	0.9999	6758.0	−14.857	0.9999

Table B5 Thermodynamic parameters of all epoxides calculated from van't Hoff plots of ln k′ vs. 1/T 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	11.10	11.10	0.00	15.93	15.93	0.00
2Br	12.22	12.39	0.17	16.24	16.62	0.38
3Br	12.95	12.95	0.00	17.34	17.34	0.00
4Br	13.11	13.18	0.08	17.76	17.94	0.17
2Cl	11.70	11.89	0.19	15.91	16.35	0.44
3Cl	12.68	12.74	0.06	17.81	17.96	0.15
4Cl	12.52	12.60	0.08	17.35	17.53	0.18
2F	10.91	11.05	0.14	15.79	16.12	0.34
3F	11.22	11.33	0.12	16.27	16.54	0.27
4F	11.59	11.67	0.08	17.25	17.44	0.19
2Me	12.11	12.24	0.13	17.49	17.82	0.34
3Me	12.19	12.34	0.15	17.60	17.95	0.36
4Me	11.96	12.05	0.09	16.99	17.21	0.21
4Et	12.72	12.84	0.12	17.86	18.14	0.27
2CF	11.15	11.29	0.14	16.85	17.22	0.37
3CF	12.39	12.53	0.14	19.40	19.81	0.40
4CF	13.55	13.62	0.07	20.54	20.71	0.17
3OMe	13.94	14.09	0.15	17.86	18.18	0.32
3CN	13.47	13.61	0.14	17.50	17.80	0.30
4CN	13.79	13.88	0.09	18.21	18.41	0.20
2NO	13.17	13.32	0.15	17.04	17.35	0.31
3NO	14.11	14.11	0.00	18.03	18.03	0.00
4NO	14.37	14.45	0.08	18.50	18.69	0.18
24Cl	12.49	12.67	0.17	16.21	16.59	0.38
25Cl	13.18	13.28	0.10	17.85	18.11	0.26
34Cl	13.43	13.43	0.00	17.44	17.44	0.00

Table B5 (continued)

analyte	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta\Delta H$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta\Delta S$
24F	10.82	11.05	0.23	15.95	16.49	0.54
25F	11.00	11.00	0.00	16.17	16.17	0.00
26F	11.48	11.66	0.17	16.75	17.16	0.41
34F	11.84	11.92	0.09	17.78	18.01	0.23
24Me	12.70	12.82	0.12	17.79	18.08	0.28
25Me	12.66	12.77	0.11	17.79	18.05	0.26
34Me	12.96	13.04	0.08	18.05	18.26	0.21
triF	10.95	10.95	0.00	16.29	16.29	0.00
tetraF	10.85	10.85	0.00	16.21	16.21	0.00
pentaF	11.38	11.45	0.06	17.50	17.67	0.17
cis–2	11.91	12.06	0.15	17.79	18.16	0.38
trans–2	12.01	12.24	0.23	17.92	18.48	0.56
cis–3	12.53	12.71	0.19	18.33	18.79	0.46
trans–3	12.46	12.64	0.18	17.92	18.35	0.43
4	12.15	12.30	0.15	18.35	18.75	0.40
cis–5	12.28	12.39	0.11	17.55	17.81	0.26
trans–5	12.42	12.42	0.00	17.68	17.68	0.00
6	12.07	12.07	0.00	17.30	17.30	0.00
7	13.69	13.75	0.06	19.68	19.84	0.15
8	13.88	13.95	0.07	19.36	19.55	0.18
hexa	8.87	8.87	0.00	14.18	14.18	0.00
5hexe	8.86	8.86	0.00	14.22	14.22	0.00
octa	10.71	10.71	0.00	16.38	16.38	0.00
deca	11.92	11.92	0.00	17.01	17.01	0.00
9dece	11.93	11.93	0.00	16.98	16.98	0.00
dodec	13.35	13.35	0.00	18.35	18.35	0.00

Table B6 Thermodynamic parameters of all epoxides calculated from van't Hoff plots of ln k′ vs. 1/T on GSiAc 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	12.38	12.60	0.22	18.76	19.26	0.51
2Br	12.40	12.89	0.49	16.32	17.39	1.07
3Br	13.19	13.36	0.17	17.47	17.83	0.36
4Br	13.22	13.20	−0.02	17.50	17.43	−0.08
2Cl	12.15	12.83	0.68	16.62	18.12	1.50
3Cl	12.85	13.07	0.22	17.64	18.10	0.46
4Cl	12.67	12.72	0.06	17.15	17.26	0.11
2F	11.77	12.58	0.80	17.40	19.25	1.86
3F	12.19	12.60	0.41	18.05	18.98	0.93
4F	11.82	12.17	0.35	17.14	17.92	0.78
2Me	12.69	13.20	0.51	18.39	19.54	1.15
3Me	13.12	13.60	0.49	19.70	20.94	1.24
4Me	12.48	12.56	0.08	18.06	18.25	0.19
4Et	12.90	12.98	0.08	18.08	18.27	0.19
2CF	11.54	12.44	0.91	17.36	19.51	2.15
3CF	12.95	13.80	0.85	19.99	22.16	2.17
4CF	12.73	13.39	0.66	19.36	21.07	1.71
3OMe	13.84	14.12	0.28	17.31	17.90	0.58
3CN	14.75	15.07	0.32	19.39	20.02	0.64
4CN	15.86	16.30	0.44	21.78	22.78	1.01
2NO	14.74	15.49	0.75	19.63	21.16	1.52
3NO	16.25	16.24	−0.01	21.74	21.70	−0.05
4NO	16.36	16.96	0.60	21.71	22.98	1.27
24Cl	13.18	13.49	0.31	17.62	18.33	0.71
25Cl	13.57	13.85	0.28	18.41	19.08	0.67
34Cl	14.79	15.18	0.39	20.09	21.02	0.93

Table B6 (continued)

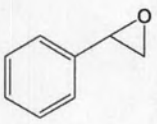
analyte	enthalpy term (kcal/mol)			entropy term (cal/mol·K)		
	$-\Delta H_1$	$-\Delta H_2$	$-\Delta\Delta H$	$-\Delta S_1$	$-\Delta S_2$	$-\Delta\Delta S$
24F	11.75	12.27	0.52	17.71	18.94	1.23
25F	12.03	12.41	0.38	18.15	19.07	0.91
26F	12.90	13.25	0.35	19.52	20.32	0.80
34F	12.93	12.92	−0.01	19.48	19.38	−0.10
24Me	12.99	13.13	0.14	18.24	18.54	0.30
25Me	13.18	13.18	0.00	18.73	18.73	0.00
34Me	12.82	12.82	0.00	17.44	17.44	0.00
triF	11.83	12.09	0.26	17.82	18.43	0.61
tetraF	12.19	12.79	0.60	18.68	20.11	1.43
pentaF	12.59	13.56	0.97	19.45	21.76	2.31
cis−2	11.84	12.99	1.15	17.23	19.94	2.71
trans−2	11.77	12.32	0.55	16.88	18.18	1.30
cis−3	11.91	12.60	0.69	16.64	18.21	1.57
trans−3	12.07	12.36	0.28	16.65	17.30	0.64
4	11.74	11.74	0.00	16.85	16.85	0.00
cis−5	12.23	12.79	0.57	17.21	18.54	1.33
trans−5	12.52	12.59	0.06	17.60	17.72	0.13
6	13.41	13.52	0.11	20.25	20.53	0.27
7	14.65	14.87	0.22	21.42	21.96	0.53
8	14.45	14.67	0.22	20.31	20.83	0.53
hexa	9.81	9.81	0.00	16.35	16.35	0.00
5hexe	10.26	10.46	0.20	17.45	17.96	0.50
octa	10.78	10.78	0.00	16.36	16.36	0.00
deca	12.01	12.01	0.00	17.15	17.15	0.00
9dece	12.15	12.15	0.00	17.37	17.37	0.00
dodec	13.43	13.43	0.00	18.55	18.55	0.00

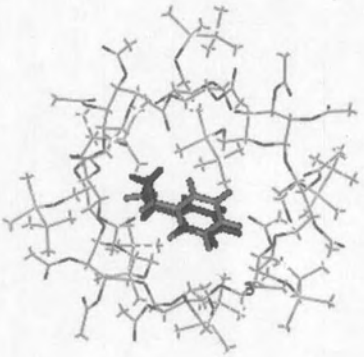
Appendix C

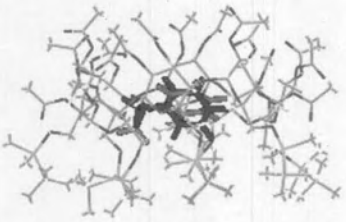
Molecular model of the docked configurations

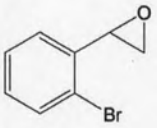
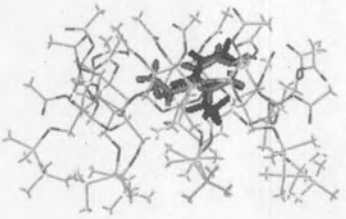
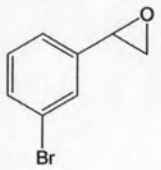
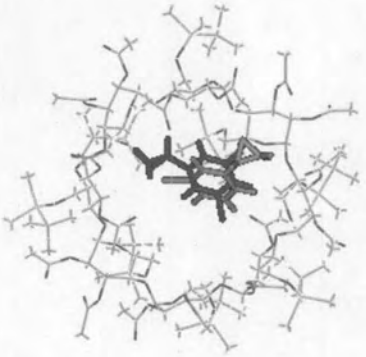
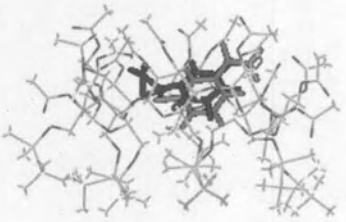
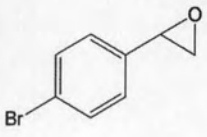
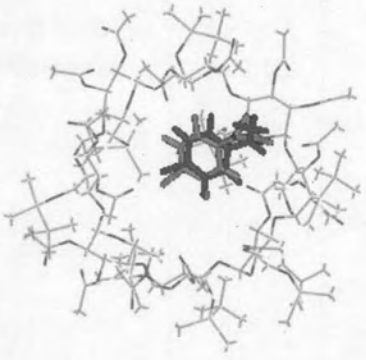
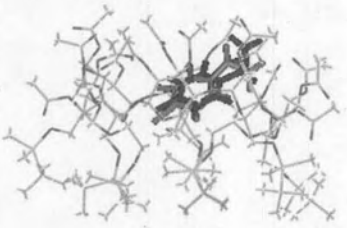
Figure C1 Docking configuration between GSiAc and *R*-enantiomer (green) and *S*-enantiomer (pink) of analytes.

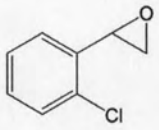
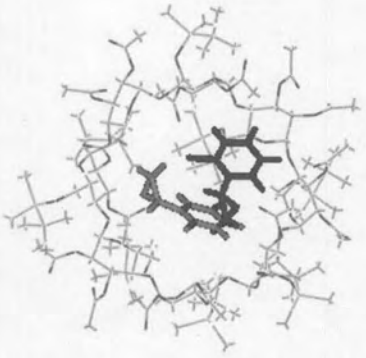
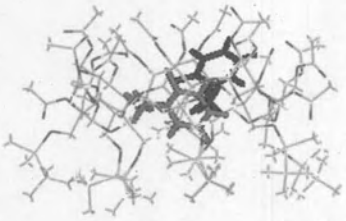
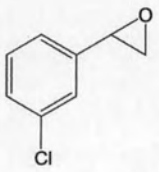
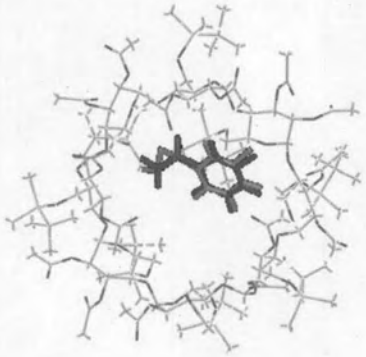
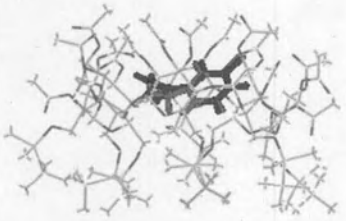
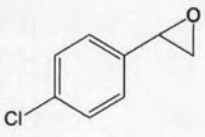
analyte **top view** **side view**

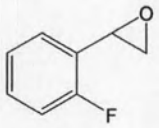
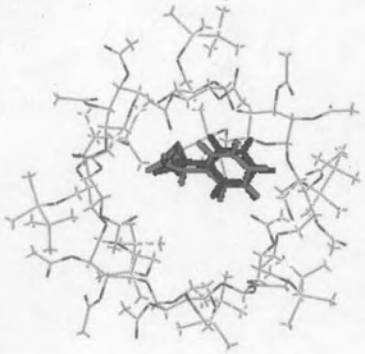
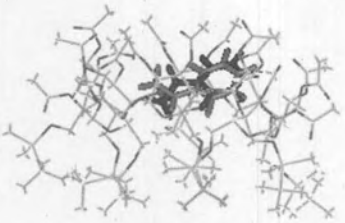
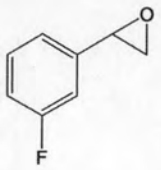
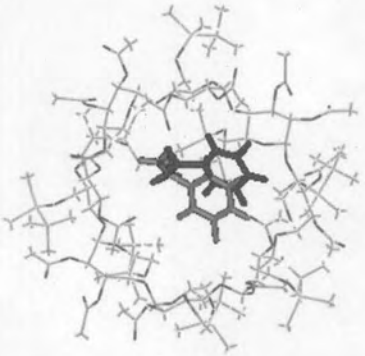
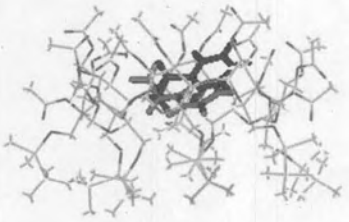
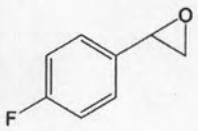
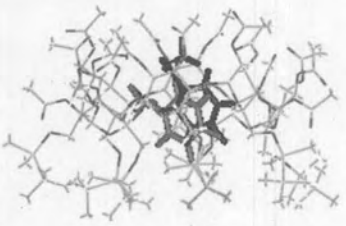


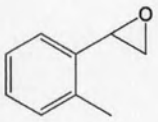
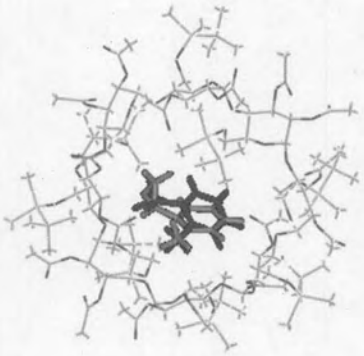
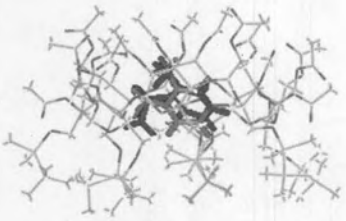
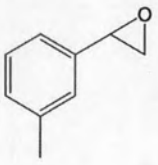
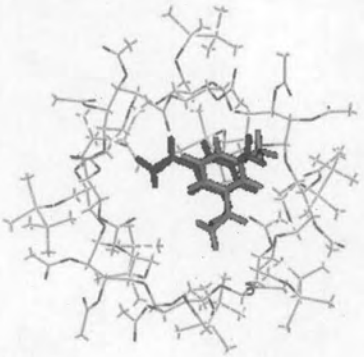
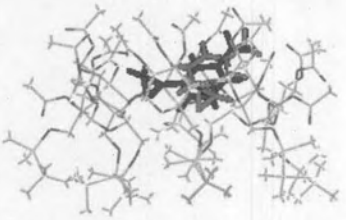
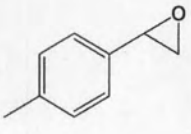
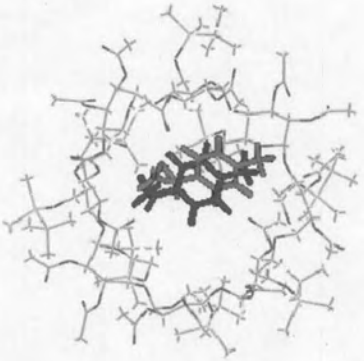
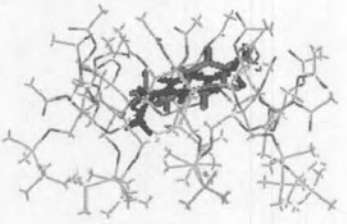




analyte	top view	side view
		
		
		

analyte	top view	side view
		
		
		

analyte	top view	side view
		
		
		

analyte	top view	side view
		
		
		

Appendix D

Example of input and output files

Input files

D1. Grid parameter file (.gpf)

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gridfld HOST.maps.fld                # grid_data_file
spacing 0.375                        # spacing (Å)
receptor_types C H OA SI             # receptor atom types
ligand_types A H OA                  # ligand atom types
receptor HOST.pdbqt                  # macromolecule
gridcenter 0.0 0.0 0.0               # xyz-coordinates or auto
smooth 0.5                           # store minimum energy w/in rad (Å)
map HOST.A.map                       # atom-specific affinity map
map HOST.H.map                       # atom-specific affinity map
map HOST.OA.map                      # atom-specific affinity map
elecmap HOST.e.map                   # electrostatic potential map
dsolvmap HOST.d.map                  # desolvation potential map
dielectric -0.1465                   # <0, AD4 distance-dep.diel;>0, constant
```

D2. Docking parameter file (.dpf)

```
outlev 1                        # diagnostic output level
intelec                         # calculate internal electrostatics
seed pid time                   # seeds for random generator
ligand_types A H OA             # atoms types in ligand
fld host.maps.fld               # grid_data_file
map host.A.map                  # atom-specific affinity map
map host.H.map                  # atom-specific affinity map
map host.OA.map                 # atom-specific affinity map
elecmap host.e.map              # electrostatics map
desolvmap host.d.map            # desolvation map
move guest.pdbqt                # small molecule
about 0.0956 0.0638 -0.0947     # small molecule center
tran0  0.096  0.064  0.095      # initial coordinates/ Å or random
quat0 random                    # initial quaternion
ndihe 1                         # number of active torsions
dihe0 random                    # initial dihedrals (relative) or random
tstep 2.0                       # translation step/ Å
qstep 50.0                      # quaternion step/deg
dstep 50.0                      # torsion step/deg
torsdof 1 0.274000              # torsional degrees of freedom and coefficient
rmstol 2.0                      # cluster_tolerance/ Å
extnrg 1000.0                   # external grid energy
e0max 0.0 10000                 # max initial energy; max number of retries
ga_pop_size 300                 # number of individuals in population
ga_num_evals 2500000            # maximum number of energy evaluations
ga_num_generations 27000        # maximum number of generations
ga_elitism 1                    # number of top individuals to survive to next
                                  generation
ga_mutation_rate 0.02           # rate of gene mutation
ga_crossover_rate 0.8           # rate of crossover
ga_window_size 10               #
ga_cauchy_alpha 0.0             # Alpha parameter of Cauchy distribution
```

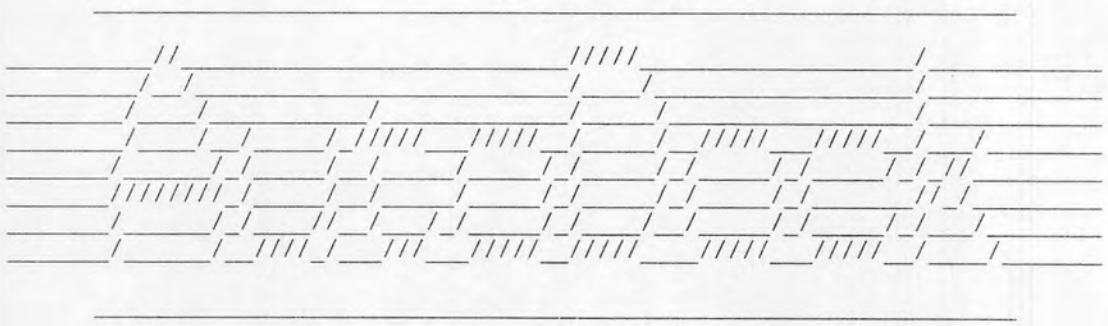
D2. Docking parameter file (.dpf) (continued)

```
ga_cauchy_beta 1.0                # Beta parameter Cauchy distribution
set_ga                            # set the above parameters for GA or LGA
sw_max_its 300                    # iterations of Solis & Wets local search
sw_max_succ 4                     # consecutive successes before changing rho
sw_max_fail 4                     # consecutive failures before changing rho
sw_rho 1.0                        # size of local search space to sample
sw_lb_rho 0.01                    # lower bound on rho
ls_search_freq 0.06               # probability of performing local search on
                                    individual

set_sw1                           # set the above Solis & Wets parameters
compute_unbound_extended          # compute extended ligand energy
ga_run 100                        # do this many hybrid GA-LS runs
analysis                          # perform a ranked cluster analysis
```

Output file

D3. Docking log file (.dlg)



```
                    AutoDock 4.00

                    (c) 1991-2007
            The Scripps Research Institute

               Garrett M. Morris, TSRI
                    Ruth Huey, TSRI
                 William E. Hart, Sandia
                 William Lindstrom, TSRI
                 Alexander Gillet, TSRI
                David S. Goodsell, TSRI
                 Arthur J. Olson, TSRI

        Automated Docking of Flexible Ligand
          to Flexible Macromolecular Receptor

AutoDock comes with ABSOLUTELY NO WARRANTY; for details
type 'warranty'.  This is free software, and you are welcome
to redistribute it under certain conditions; type 'copyright'
for details.

      ..........................................................
      ..........................................................

------------------------------------------------------------------

                SETTING UP DEFAULT PARAMETER LIBRARY

------------------------------------------------------------------

      ..........................................................
      ..........................................................
```

```
INPUT LIGAND PDBQT FILE:
________________________

                .....................................................
                .....................................................

Determining Atom Types and Parameters for the Moving Atoms
__________________________________________________________

                .....................................................
                .....................................................

      BEGINNING COMPUTATION OF UNBOUND EXTENDED STATE USING LGA
      _________________________________________________________

                .....................................................
                .....................................................

_____________________________________________________________________________

      BEGINNING LAMARCKIAN GENETIC ALGORITHM DOCKING

Run:   1 / 100
Date:  Fri Feb 29 13:52:28 2008
Output level is set to 1.


Creating an initial population of 300 individuals.

Assigning a random translation, a random orientation and 1 random torsions
to each of the 300 individuals.

Beginning Lamarckian Genetic Algorithm (LGA), with a maximum of 2500000
energy evaluations.

Generation: 100   Oldest's energy: -4.440    Lowest energy: -4.440
Num.evals.: 230838   Timing: Real= 0.00s,  CPU= 0.00s,  System= 0.00s
Generation: 200   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 466066   Timing: Real= 0.01s,  CPU= 0.00s,  System= 0.00s
Generation: 300   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 696619   Timing: Real= 0.00s,  CPU= 0.00s,  System= 0.00s
Generation: 400   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 928060   Timing: Real= 0.00s,  CPU= 0.01s,  System= 0.00s
Generation: 500   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 1160246   Timing: Real= 0.00s,  CPU= 0.00s,  System= 0.00s
Generation: 600   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 1389750   Timing: Real= 0.01s,  CPU= 0.01s,  System= 0.00s
Generation: 700   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 1629122   Timing: Real= 0.01s,  CPU= 0.00s,  System= 0.00s
Generation: 800   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 1856361   Timing: Real= 0.01s,  CPU= 0.00s,  System= 0.00s
Generation: 900   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 2087494   Timing: Real= 0.01s,  CPU= 0.00s,  System= 0.00s
Generation: 1000   Oldest's energy: -4.447    Lowest energy: -4.447
Num.evals.: 2318092   Timing: Real= 0.00s,  CPU= 0.00s,  System= 0.00s
Final-Value: -4.449

Run completed;  time taken for this run:
Real= 19.63s,  CPU= 19.61s,  System= 0.01s

1:52 48" p.m., 02/29/2008
Total number of Energy Evaluations: 2502345
Total number of Generations:        1080
```

FINAL LAMARCKIAN GENETIC ALGORITHM DOCKED STATE

```
State: -0.567 -1.400 0.310  -0.401 0.812 -0.424 -114.059   -172.31

DOCKED: MODEL        1
DOCKED: USER    Run = 1
DOCKED: USER    DPF = DR1.dpf
DOCKED: USER
DOCKED: USER    Estimated Free Energy of Binding    =   -4.17 kcal/mol
[=(1)+(2)+(3)-(4)]
DOCKED: USER    Estimated Inhibition Constant, Ki   =  871.27 uM
(micromolar)  [Temperature = 298.15 K]
DOCKED: USER
DOCKED: USER    (1) Final Intermolecular Energy     =   -4.44 kcal/mol
DOCKED: USER        vdW + Hbond + desolv Energy     =   -4.41 kcal/mol
DOCKED: USER        Electrostatic Energy            =   -0.03 kcal/mol
DOCKED: USER    (2) Final Total Internal Energy     =   -0.10 kcal/mol
DOCKED: USER    (3) Torsional Free Energy           =   +0.27 kcal/mol
DOCKED: USER    (4) Unbound System's Energy         =   -0.10 kcal/mol
DOCKED: USER
DOCKED: USER
DOCKED: USER    NEWDPF move DR1.pdbqt
DOCKED: USER    NEWDPF about 0.095600 0.063800 0.094700
DOCKED: USER    NEWDPF tran0 -0.566909 -1.399859 0.309755
DOCKED: USER    NEWDPF quaternion0 -0.336813 0.680994 -0.355869 -0.544207
DOCKED: USER    NEWDPF axisangle0 -0.401469 0.811721 -0.424184 -114.059074
DOCKED: USER    NEWDPF quat0 -0.401469 0.811721 -0.424184 -114.059074 #
deprecated
DOCKED: USER    NEWDPF dihe0 -172.31
DOCKED: USER
DOCKED: REMARK  1 active torsions:
DOCKED: REMARK  status: ('A' for Active; 'I' for Inactive)
DOCKED: REMARK    1  A    between atoms: C_1  and  C_12
DOCKED: USER                              x       y       z     vdW  Elec
q    Type
DOCKED: USER                           _______ _______ _______ _____ _____
_____ ____
DOCKED: ROOT
DOCKED: ATOM      1  C   Inh     1      -0.773  -1.080   0.319 -0.47 -0.00
DOCKED: ATOM      2  C   Inh     1      -0.229  -1.860   1.332 -0.49 +0.00
DOCKED: ATOM      3  C   Inh     1       1.098  -2.261   1.269 -0.54 -0.00
DOCKED: ATOM      4  C   Inh     1       1.893  -1.885   0.195 -0.55 -0.01
DOCKED: ATOM      5  C   Inh     1       1.356  -1.101  -0.815 -0.49 -0.01
DOCKED: ATOM      6  C   Inh     1       0.031  -0.697  -0.749 -0.41 -0.01
DOCKED: ATOM      7  H   Inh     1      -0.841  -2.137   2.170 +0.04 -0.02
DOCKED: ATOM      8  H   Inh     1       1.511  -2.861   2.060 -0.01 -0.00
DOCKED: ATOM      9  H   Inh     1       2.921  -2.196   0.150 +0.00 +0.01
DOCKED: ATOM     10  H   Inh     1       1.966  -0.799  -1.647 +0.04 +0.02
DOCKED: ATOM     11  H   Inh     1      -0.377  -0.081  -1.534 +0.05 +0.02
DOCKED: ENDROOT
DOCKED: BRANCH   1  12
DOCKED: ATOM     12  C   Inh     1      -2.205  -0.651   0.351 -0.49 -0.00
DOCKED: ATOM     13  O   Inh     1      -2.767  -0.183  -0.845 -0.46 +0.01
DOCKED: ATOM     14  C   Inh     1      -2.607   0.744   0.198 -0.65 -0.00
DOCKED: ATOM     15  H   Inh     1      -1.853   1.494   0.033 +0.03 -0.00
DOCKED: ATOM     16  H   Inh     1      -3.524   1.092   0.644 -0.02 +0.00
DOCKED: ATOM     17  H   Inh     1      -2.858  -1.298   0.916 +0.01 -0.02
DOCKED: ENDBRANCH   1  12
DOCKED: TORSDOF 1
DOCKED: TER
DOCKED: ENDMDL
```

.....

.....

CLUSTER ANALYSIS OF CONFORMATIONS

Number of conformations = 100

RMSD cluster analysis will be performed using the ligand atoms only (17 / 17 total atoms).

STATE VARIABLES:

```
Translation x,y,z          = -0.567 -1.400 0.310
Quaternion x,y,z,w         = -0.337 0.681 -0.356 -0.544
Axis-Angle nx,ny,nz,angle  = -0.401 0.812 -0.424 -114.059
Number of Torsions         = 1
Torsions (degrees)         = -172.31
```

. . . . . .
. . . . . .

CLUSTERING HISTOGRAM

Cluster Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-4.18	2	-4.18	100	##########

Number of multi-member conformational clusters found = 1, out of 100 runs.

RMSD TABLE

. . . . . .
. . . . . .

INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING

Information entropy for this clustering = 0.00 (rmstol = 2.00 Angstrom)

STATISTICAL MECHANICAL ANALYSIS

```
Partition function, Q =   100.71            at Temperature, T = 298.15 K
Free energy,        A ~ -2732.65 kcal/mol   at Temperature, T = 298.15 K
Internal energy,    U =    -4.18 kcal/mol   at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K
```

LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER

```
Keeping original residue number (specified in the input PDBQ file) for
outputting.

MODEL        2
USER    Run = 2
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 2.089 A
USER
USER    Estimated Free Energy of Binding    =   -4.18 kcal/mol
[=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  857.32 uM (micromolar)
[Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.45 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.42 kcal/mol
USER        Electrostatic Energy            =   -0.03 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.10 kcal/mol
USER    (3) Torsional Free Energy           =   +0.27 kcal/mol
USER    (4) Unbound System's Energy         =   -0.10 kcal/mol
USER
USER
USER
USER    DPF = guest.dpf
USER    NEWDPF move guest.pdbqt
USER    NEWDPF about       0.095600 0.063800 0.094700
USER    NEWDPF tran0       -0.418413 -0.933889 0.289710
USER    NEWDPF axisangle0  -0.750409 -0.228709 -0.620144 119.195652
USER    NEWDPF quaternion0 -0.647224 -0.197260 -0.534871 0.506066
USER    NEWDPF ndihe       1
USER    NEWDPF dihe0       6.52
USER
USER                                 x       y       z    vdW   Elec       q
RMS
ATOM      1  C   Inh     1      -0.767  -1.087   0.302 -0.47 -0.00    -0.027
ATOM      2  C   Inh     1       0.045  -0.718  -0.764 -0.41 -0.01    -0.074
ATOM      3  C   Inh     1       1.373  -1.114  -0.800 -0.49 -0.01    -0.082
ATOM      4  C   Inh     1       1.904  -1.885   0.225 -0.55 -0.01    -0.083
ATOM      5  C   Inh     1       1.096  -2.262   1.287 -0.54 -0.00    -0.082
ATOM      6  C   Inh     1      -0.233  -1.869   1.322 -0.49 +0.00    -0.074
ATOM      7  H   Inh     1      -0.370  -0.134  -1.565 +0.05 +0.02    +0.084
ATOM      8  H   Inh     1       1.992  -0.826  -1.631 +0.04 +0.02    +0.083
ATOM      9  H   Inh     1       2.933  -2.192   0.193 +0.00 +0.01    +0.083
ATOM     10  H   Inh     1       1.496  -2.865   2.083 -0.01 -0.00    +0.083
ATOM     11  H   Inh     1      -0.857  -2.172   2.146 +0.04 -0.02    +0.084
ATOM     12  C   Inh     1      -2.196  -0.656   0.378 -0.49 -0.00    +0.084
ATOM     13  O   Inh     1      -2.785  -0.157  -0.792 -0.47 +0.01    -0.376
ATOM     14  C   Inh     1      -2.599   0.743   0.270 -0.65 -0.00    +0.048
ATOM     15  H   Inh     1      -1.846   1.495   0.107 +0.03 -0.00    +0.078
ATOM     16  H   Inh     1      -3.504   1.081   0.746 -0.02 +0.00    +0.078
ATOM     17  H   Inh     1      -2.838  -1.316   0.941 +0.01 -0.02    +0.094
TER
ENDMDL
                .....................................................
                .....................................................

>>> Closing the docking parameter file (DPF)...

This docking finished at:                2:26 49" p.m., 02/29/2008

-------------------------------------------------------------------------
autodock4: Successful Completion on "ewald"

Real= 34m 27.54s,  CPU= 34m 24.35s,  System= 1.51s

-------------------------------------------------------------------------
```

VITA

Mr. Natthapol Assavachartthongchai was born on May 30, 1983 in Bangkok, Thailand. After completing his secondary school from Suankularb Wittayalai School, he entered the Department of Chemistry, Faculty of Science, Chulalongkorn University in 2001. He received his Bachelor of Science Degree in March 2005. He then continued his graduate study at the same university and worked in analytical chemistry, focusing on the chromatographic separation. His current address is 95/71 Tripetch Road, Wangburapapirom, Phranakorn, Bangkok, 10200 Thailand.