

Quantifying the hydrogen-bond propensity of drugs and relationship to Lipinski's rule of five

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Supporting Information

Table of Contents

1. Table S1. MESP parameters of interacting atoms in the chemical motifs and interaction energies of the corresponding complexes.	–S2
2. Table S2. Cartesian coordinates of optimized geometry of rings in drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.	–S4
3. Table S3. Cartesian coordinates of optimized geometry of drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.	–S6
4. Table S4. Cartesian coordinates of optimized geometry of FDA approved drugs...H ₂ O at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.	–S16
5. The Python script for calculating the four Lipinski's parameters with description.	–S65
6. Table S5. Cartesian coordinates of optimized geometry of 193 FDA approved oral drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.	–S66

1. **Table S1.** MESP parameters of interacting atoms in the chemical motifs and interaction energies of the corresponding complexes.

Sl no	Name of the ring in drug	Motif	E_{int}	No of interactions	$\Delta V_{n(H)}$	$\Delta V_{n(A)}$
1	3,7-dihydro-1H-purine-2,6-dione	CO ⁻ HN	-9.8	6	7.1	-73.0
		CO ⁻ HN	-9.9		7.1	-75.8
		CO ⁻ HN	-10.9		16.5	-75.8
		CN ⁻ HN	-10.2		16.5	-26.8
		CN ⁻ HC	-6.1		-30.3	-26.8
		CO ⁻ HN	-14.5		30.8	-73.0
2	2-amino-1H-purin-6(9H)-one	CN ⁻ HN	-10.1	5	16.7	-34.8
		CN ⁻ HN	-9.9		3.1	-34.8
		CO ⁻ HC	-12.7		9.8	-86.6
		CO ⁻ NC	-9.1		-	-131.2
		CH ⁻ NC	-7.8		-47.4	-44.6
3	1,9-dihydro-6H-purin-6-one	CO ⁻ HN	-12.2	5	12.6	-82.4
		CH ⁻ NC	-7.5		-41.0	-38.2
		CO ⁻ NC	-8.5		-	-120.5
		CN ⁻ HN	-11.0		23.3	-25.8
		CN ⁻ HC	-5.9		-39.3	-25.8
4	1H-purin-6-one	CN ⁻ HN	-11.0	5	9.2	-30.3
		CN ⁻ HC	-5.9		-61.7	-30.3
		CO ⁻ HN	-12.2		4.2	-61.0
		CO ⁻ ON	-8.5		-	-87.5
		CN ⁻ HC	-7.5		-35.6	-26.6
5	1,5-naphthyridin-4(1H)-one	CN ⁻ HC	-9.6	2	-	-132.5
		CO ⁻ HC	-9.0		-62.5	-95.6
6	7H-purine	CN ⁻ HC	-6.6	5	-70.8	-36.3
		CN ⁻ HC	-5.9		-70.8	-35.0
		CN ⁻ HC	-7.1		-51.4	-35.0
		CN ⁻ HC	-7.4		-33.8	-36.6
		CN ⁻ NC	-7.6		-	-72.8
7	1,8-naphthyridin-4(1H)-one	CO ⁻ HC	-8.7	3	-60.9	-91.3
		CN ⁻ HN	-11.3		15.0	-29.5
		CO ⁻ HC	-8.7		-56.9	-91.3
8	[1,2,4]triazolo[4,3-a]pyridin-3(2H)one	CN ⁻ HN	-8.0	4	10.9	-21.7
		CN ⁻ HC	-7.0		-49.7	-21.7
		CO ⁻ HN	-10.7		10.9	-80.9
		CO ⁻ HC	-8.7		-40.9	-80.9
9	5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one	CN ⁻ HN	-10.4	3	-7.4	-34.8
		CO ⁻ HC	-6.7		-68.4	-80.9
		CO ⁻ HN	-11.0		-1.9	-80.9
10	phthalazin-1(2H)-one	CN ⁻ HC	-5.3	4	-53.6	-6.5
		CN ⁻ HN	-10.5		1.3	-6.5

		CO ⁻ HN	-10.5		1.3	-82.3
		CO ⁻ HC	-7.8		-59.5	-82.3
11	9H-purine	CN ⁻ HC	-6.4	5	-67.1	-36.4
		CN ⁻ HC	-6.5		-59.6	-36.4
		CN ⁻ HC	-6.7		-59.6	-33.3
		CN ⁻ HC	-6.8		-35.2	-33.3
		CN ⁻ HN	-11.7		25.8	-28.7
12	9H-purin-6-amine	CN ⁻ HN	-12.0	4	18.4	-42.5
		CN ⁻ HC	-6.3		-41.7	-37.9
		CN ⁻ HC	-11.7		-5.7	-37.9
		CN ⁻ HN	-10.9		-6.7	-45.7
13	1H-purin	CN ⁻ NC	-7.9	3	-	-80.5
		CN ⁻ HC	-7.5		-32.6	-31.6
		CN ⁻ HC	-10.5		-41.4	-28.2
14	2-Fluoropyridine	CN ⁻ FC	-5.9	2	-	-71.7
		CF ⁻ HC	-4.0		-49.4	-40.5
15	3,6,7,8-tetrahydroimidazo[4,5-d][1,3]diazepine	CN ⁻ HC	-8.7	2	-75.5	-58.7
		CN ⁻ HN	-11.1		1.4	-47.9
16	quinazoline	CN ⁻ HC	-6.8	3	-57.2	-34.7
		CN ⁻ HC	-6.1		-68.3	-34.7
		CN ⁻ HC	-7.4		-60.0	-35.8
17	2,3-dihydro-1,3,4-thiadiazole	CN ⁻ HC	-5.8	4	-45.7	-21.2
		CN ⁻ HN	-7.2		-15.8	-21.2
		CS ⁻ HC	-3.0		-45.7	-18.3
		CS ⁻ HC	-4.1		-62.9	-18.3
18	2H-benzo[d][1,2,3]triazole	CN ⁻ HC	-5.9	4	-60.7	-15.6
		CN ⁻ HN	-8.7		21.6	-15.6
		CN ⁻ HN	-8.7		21.6	-15.7
		CN ⁻ HC	-5.9		-60.7	-15.7
19	chlorobenzene	CCl ⁻ HC	-3.5	2	-59.1	-28.4
		CCl ⁻ HC	-3.5		-59.0	-28.4
20	5-bromo-2,3-dihydro-1H-pyrrole	CBr ⁻ HC	-2.9	2	-64.5	-16.6
		CBr ⁻ HC	-5.9		-19.3	-16.6

2. **Table S2.** Cartesian coordinates of optimized geometry of rings in drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

3,7-dihydro-1H-purin-2,6-dione (1)	2-amino-1H-purin-6(9H)-one (2)
6 0.275 1.440 0.000	6 0.199 1.473 0.003
6 -0.769 0.461 0.000	6 -0.853 0.499 0.007
7 1.528 0.791 0.000	7 1.467 0.791 0.000
1 2.337 1.398 0.000	6 -0.519 -0.852 -0.001
6 -0.545 -0.897 0.000	6 1.670 -0.560 -0.001
6 1.841 -0.571 0.000	7 2.971 -0.994 -0.075
8 2.979 -0.984 0.000	7 0.699 -1.440 0.008
7 0.730 -1.402 0.000	7 -2.218 0.675 0.007
8 0.172 2.652 0.000	7 -1.719 -1.506 -0.003
7 -2.140 0.582 0.000	6 -2.701 -0.537 0.001
7 -1.698 -1.608 0.000	1 -1.840 -2.508 -0.010
6 -2.640 -0.677 0.000	1 -3.749 -0.798 -0.001
1 -3.702 -0.874 0.000	8 0.179 2.684 -0.004
1 -2.652 1.452 -0.001	1 2.261 1.415 -0.064
1 0.898 -2.397 0.000	1 3.668 -0.428 0.384
	1 3.064 -1.980 0.120
1,9-dihydro-6H-purin-6-one (3)	1H-purin-6-one (4)
6 -1.159 -0.899 0.000	7 0.142 -1.880 0.000
6 0.243 -0.573 0.000	6 -0.629 -0.765 0.000
7 -1.912 0.324 -0.001	6 1.410 -1.587 0.000
1 -2.916 0.193 0.000	1 2.142 -2.391 0.001
6 0.629 0.765 0.000	6 -0.243 0.573 0.000
6 -1.410 1.587 0.000	7 1.912 -0.324 0.000
1 -2.142 2.391 0.000	1 2.916 -0.193 0.000
7 -0.142 1.880 0.000	6 1.159 0.899 0.000
8 -1.733 -1.965 0.001	7 -1.996 -0.735 0.000
7 1.335 -1.403 -0.001	7 -1.335 1.403 0.000
7 1.996 0.735 0.000	6 -2.360 0.591 -0.001
6 2.360 -0.591 0.000	1 -2.601 -1.542 0.000
1 2.601 1.542 0.000	8 1.733 1.966 0.000
1 3.398 -0.891 0.000	1 -3.398 0.891 0.000
1,5-naphthyridin-4(1H)-one (5)	7H-purine (6)
6 1.357 0.975 0.000	7 -0.912 -1.417 0.000
6 -0.061 0.508 0.000	6 0.219 -0.712 0.000
6 2.335 -0.104 0.000	6 -2.009 -0.665 0.000
1 3.384 0.164 0.000	1 -2.956 -1.199 0.000
6 -0.360 -0.873 0.000	6 0.233 0.700 0.000
6 1.974 -1.408 0.000	7 -2.107 0.677 0.000
1 2.694 -2.219 0.000	6 -0.975 1.377 0.000
7 0.664 -1.796 0.000	7 1.503 -1.212 0.000
1 0.435 -2.778 0.002	7 1.566 1.038 0.000
8 1.663 2.158 0.000	6 2.259 -0.147 0.000
7 -1.031 1.433 0.000	1 -1.053 2.463 0.000
6 -1.698 -1.281 0.000	1 1.964 1.965 0.000
6 -2.291 1.033 0.000	1 3.341 -0.155 0.000
6 -2.678 -0.314 0.000	
1 -3.047 1.816 0.000	
1 -3.728 -0.586 0.000	
1 -1.947 -2.339 0.000	
1,8-naphthyridin-4(1H)-one (7)	[1,2,4]triazolo[4,3-a]pyridin-3(2H)one (8)
6 -1.376 0.959 0.000	6 0.695 -1.441 0.000
6 0.036 0.514 0.000	7 -0.176 -0.385 0.000
6 -2.337 -0.129 0.000	6 2.026 -1.181 0.000
1 -3.391 0.114 0.000	6 0.225 0.951 0.000
6 0.380 -0.849 0.000	6 2.487 0.173 0.000
6 -1.942 -1.426 0.000	1 3.555 0.363 0.000
1 -2.646 -2.251 0.000	6 1.617 1.222 0.000
7 -0.627 -1.788 0.000	6 -1.588 -0.430 0.000
1 -0.345 -2.758 0.000	7 -0.804 1.767 0.000
8 -1.681 2.149 0.000	7 -1.881 0.910 0.000
6 1.092 1.426 0.000	1 -2.813 1.290 0.000
7 1.630 -1.325 0.000	1 0.235 -2.422 0.000
6 2.393 0.960 0.000	1 1.945 2.254 0.000
6 2.604 -0.422 0.000	1 2.730 -2.003 0.000
1 0.848 2.485 0.000	8 -2.299 -1.412 0.000
1 3.239 1.638 0.000	
1 3.616 -0.823 0.000	
5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one (9)	phthalazin-1(2H)-one (10)
6 3.518 -1.264 0.303	6 -1.342 -0.907 0.000
7 2.306 -1.640 -0.113	6 0.058 -0.480 0.000
6 3.842 0.053 0.584	7 -2.237 0.162 -0.001
1 4.832 0.322 0.934	6 0.361 0.897 0.000
6 1.374 -0.709 -0.292	7 -1.981 1.486 0.000
6 2.864 1.022 0.391	6 -0.729 1.829 0.000
1 3.078 2.072 0.573	6 1.084 -1.428 0.000
6 1.606 0.658 -0.072	6 1.707 1.300 0.000
1 4.251 -2.058 0.412	6 2.403 -1.014 0.000
7 0.156 -1.186 -0.780	6 2.713 0.353 0.000

7	0.675	1.651	-0.405	1	3.203	-1.746	0.000
6	-1.107	-0.826	-0.299	1	1.945	2.360	0.000
6	-0.697	1.723	-0.226	1	3.751	0.669	0.000
1	0.240	-2.184	-0.940	1	0.814	-2.479	0.000
1	1.060	2.582	-0.504	8	-1.745	-2.058	0.001
8	-1.225	2.821	-0.288	1	-3.221	-0.076	-0.001
6	-2.051	-1.856	-0.173	1	-0.541	2.899	0.001
6	-1.496	0.492	0.005				
6	-3.337	-1.605	0.270				
6	-2.803	0.717	0.459				
1	-4.039	-2.427	0.360				
1	-3.077	1.744	0.670				
6	-3.719	-0.308	0.607				
1	-4.721	-0.102	0.966				
1	-1.751	-2.869	-0.426				
9H-purine (11)				9H-purin-6-amine (12)			
6	0.990	1.374	0.000	6	1.222	-0.605	-0.004
6	-0.246	0.739	0.000	6	-0.179	-0.518	-0.004
7	2.112	0.653	0.000	7	1.944	0.526	0.006
6	-0.202	-0.668	0.000	6	-0.708	0.773	-0.004
6	2.000	-0.683	0.000	6	1.287	1.692	0.004
1	2.936	-1.237	0.000	1	1.919	2.578	0.011
7	0.887	-1.422	0.000	7	-0.027	1.920	-0.001
7	-1.551	1.193	0.000	7	-1.173	-1.476	0.001
7	-1.518	-1.058	0.000	7	-2.069	0.583	0.000
6	-2.263	0.099	0.000	6	-2.278	-0.776	0.004
1	-1.857	-2.008	-0.001	1	-2.767	1.311	0.002
1	-3.345	0.064	0.000	1	-3.277	-1.190	0.009
1	1.085	2.458	0.000	7	1.874	-1.793	-0.048
				1	2.862	-1.785	0.145
				1	1.356	-2.633	0.151
1H-purin (13)				2-Fluoropyridine (14)			
6	-0.864	1.392	0.000	6	0.000	0.890	0.000
6	0.331	0.733	0.000	7	-1.189	0.341	0.000
7	-1.982	0.606	0.000	6	1.214	0.215	0.000
1	-2.891	1.046	0.000	1	2.149	0.761	0.000
6	0.314	-0.724	0.000	6	-1.226	-0.997	0.000
6	-1.925	-0.763	0.000	6	1.153	-1.170	0.000
1	-2.889	-1.263	0.000	1	-2.219	-1.441	0.000
7	-0.825	-1.455	0.000	1	2.067	-1.754	0.000
1	-1.006	2.466	0.000	6	-0.092	-1.795	0.000
7	1.620	1.161	0.000	1	-0.180	-2.875	0.000
7	1.565	-1.171	0.000	9	0.024	2.230	0.000
6	2.274	-0.005	0.000				
1	3.359	-0.030	0.000				
3,6,7,8-tetrahydroimidazo[4,5-d][1,3]diazepine (15)				Quinazoline (16)			
6	0.538	0.666	0.004	6	-1.212	1.402	0.000
6	0.588	-0.712	0.130	6	0.020	0.712	0.000
7	-0.426	1.642	0.030	6	-2.388	0.695	0.000
6	-0.569	-1.633	0.264	1	-3.339	1.218	0.000
6	-1.678	1.362	0.109	6	0.040	-0.711	0.000
6	-1.808	-1.097	-0.442	6	-2.371	-0.717	0.000
1	-0.301	-2.600	-0.173	1	-3.313	-1.258	0.001
1	-1.590	-0.968	-1.511	6	-1.186	-1.413	0.000
7	-2.320	0.152	0.120	1	-1.157	-2.497	0.000
6	2.622	-0.077	-0.069	1	-1.211	2.489	0.000
7	1.862	1.047	-0.116	6	1.284	1.343	0.000
7	1.884	-1.156	0.075	7	1.215	-1.397	0.000
1	2.165	2.004	-0.215	7	2.419	0.682	0.000
1	3.699	-0.054	-0.147	6	2.310	-0.673	0.000
1	-3.325	0.226	0.133	1	1.343	2.434	0.000
1	-0.812	-1.829	1.316	1	3.254	-1.214	0.000
1	-2.623	-1.821	-0.369				
1	-2.364	2.202	0.221				
2,3-dihydro-1,3,4-thiadiazole (17)				2H-benzo[d][1,2,3]triazole (18)			
6	0.110	-1.232	0.169	6	0.924	1.439	0.000
7	1.297	-0.482	-0.251	6	-0.281	0.712	0.000
7	1.197	0.875	0.032	6	2.089	0.711	0.000
6	-0.024	1.236	0.098	6	-0.281	-0.712	0.000
16	-1.245	-0.035	-0.073	6	2.089	-0.711	0.000
1	0.142	-1.556	1.221	1	3.043	-1.228	0.000
1	2.156	-0.839	0.150	6	0.924	-1.439	0.000
1	-0.311	2.273	0.206	7	-1.562	1.143	0.000
1	-0.042	-2.100	-0.474	7	-1.562	-1.143	0.000
				7	-2.229	0.000	0.000
				1	0.922	2.523	0.000
				1	0.923	-2.523	0.000
				1	3.043	1.229	0.000
				1	-3.239	0.000	0.000

chlorobenzene (19)				5-bromo-2,3-dihydro-1H-pyrrole (20)			
6	-2.264	0.000	0.000	7	-0.972	-1.097	-0.221
6	-1.566	1.203	0.000	6	-2.364	-0.775	0.144
6	-1.566	-1.203	0.000	6	-0.266	0.091	-0.011
1	-2.104	2.146	0.000	6	-2.463	0.740	-0.088
1	-2.102	-2.147	0.000	6	-1.035	1.182	0.075
6	-0.175	1.212	0.000	1	-2.544	-1.004	1.204
6	-0.175	-1.212	0.000	1	-3.162	1.216	0.606
1	0.378	2.144	0.000	1	-3.066	-1.357	-0.456
1	0.379	-2.142	0.000	1	-2.825	0.962	-1.103
6	0.505	0.000	0.000	1	-0.685	2.202	0.102
17	2.250	0.000	0.000	1	-0.583	-1.904	0.252
1	-3.349	0.001	0.000	35	1.613	0.004	0.006

3. **Table S3.** Cartesian coordinates of optimized geometry of FDA approved drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

cefditoren pivoxil				Amlodipine			
16	0.883	-2.629	1.182	17	2.759	-2.612	-0.739
16	-3.926	-2.873	-1.598	8	-3.074	1.202	0.493
16	7.872	1.276	-2.002	8	-2.305	-0.927	-1.370
8	0.042	1.393	-0.258	8	3.831	0.341	-0.650
8	-2.792	0.360	-1.105	8	-0.311	-1.950	-1.561
8	-3.468	0.415	1.056	8	3.992	2.558	-0.276
8	4.007	-1.136	-1.761	7	-0.252	2.554	-0.149
8	-3.225	2.602	-0.840	7	-6.511	0.388	1.413
8	4.027	-1.296	2.034	6	1.166	0.138	-0.533
8	-5.197	2.968	0.214	6	-0.324	0.282	-0.806
7	-0.552	-0.905	-0.322	6	1.841	1.491	-0.377
7	2.669	-0.403	-0.081	6	-0.971	1.450	-0.562
7	5.186	-0.723	1.512	6	1.127	2.623	-0.141
7	7.326	0.538	0.423	6	1.381	-0.724	0.707
7	-5.864	-1.232	-2.017	6	-2.445	1.714	-0.659
7	9.405	1.628	0.234	6	-0.951	-0.958	-1.279
6	0.553	-1.846	-0.427	6	1.673	3.988	0.121
6	1.465	-0.646	-0.804	6	3.301	1.566	-0.420
6	0.257	0.229	-0.442	6	2.068	-1.942	0.717
6	-1.748	-1.116	0.359	6	0.855	-0.281	1.925
6	-0.832	-3.238	1.333	6	2.228	-2.677	1.889
6	-1.932	-2.234	1.104	6	1.004	-1.001	3.102
6	-2.769	-0.040	0.189	6	1.698	-2.206	3.082
6	-3.208	-2.585	1.719	6	-4.481	1.196	0.369
6	3.884	-0.710	-0.625	6	-2.903	-2.157	-1.818
6	5.081	-0.431	0.255	6	-5.060	0.453	1.552
6	-4.428	-2.551	1.154	6	5.254	0.288	-0.693
6	-3.706	1.409	-1.403	6	-4.396	-1.986	-1.757
6	-3.252	4.295	0.827	1	1.617	-0.395	-1.374
6	-4.763	-2.217	-0.221	1	-0.763	3.411	0.000
6	6.246	0.198	-0.364	1	-2.617	2.803	-0.736
6	-4.037	3.243	0.063	1	-2.863	1.255	-1.563
6	-4.235	5.227	1.529	1	2.367	3.985	0.961
6	-2.403	3.544	1.865	1	2.244	4.355	-0.733
6	-2.334	5.086	-0.108	1	0.863	4.693	0.331
6	-5.763	-1.372	-0.654	1	0.307	0.658	1.934
6	6.361	0.509	-1.694	1	2.767	-3.617	1.853
6	-6.668	-0.589	0.231	1	0.581	-0.625	4.027
6	8.247	1.104	-0.289	1	1.826	-2.785	3.991
6	-4.975	-1.957	-2.625	1	-4.767	0.695	-0.572
6	4.268	-1.656	3.390	1	-4.883	2.221	0.324
1	0.396	-2.610	-1.194	1	-2.551	-2.973	-1.179
1	1.703	-0.646	-1.870	1	-2.551	-2.375	-2.832
1	-0.962	-4.100	0.667	1	-4.822	0.999	2.470
1	-0.916	-3.631	2.351	1	-4.555	-0.524	1.629
1	2.619	-0.241	0.916	1	5.642	0.905	-1.507
1	-3.145	-2.934	2.749	1	5.683	0.642	0.246
1	-5.278	-2.778	1.795	1	5.503	-0.759	-0.856
1	-4.703	1.180	-1.023	1	-4.728	-1.794	-0.733
1	-3.696	1.490	-2.489	1	-4.729	-1.157	-2.387
1	-3.688	5.964	2.122	1	-4.893	-2.894	-2.107
1	-4.859	5.765	0.811	1	-6.760	-0.257	0.668
1	-4.901	4.674	2.194	1	-6.925	0.008	2.257
1	-1.845	4.267	2.466				
1	-1.687	2.874	1.383				
1	-3.030	2.952	2.537				
1	-1.810	5.857	0.465				
1	-2.898	5.588	-0.899				
1	-1.586	4.444	-0.576				
1	5.670	0.297	-2.493				
1	-6.449	0.482	0.170				
1	-7.710	-0.724	-0.066				
1	-6.554	-0.878	1.277				

1	-4.874	-2.016	-3.703				
1	5.057	-2.409	3.455				
1	4.548	-0.780	3.981				
1	3.326	-2.068	3.751				
1	9.600	1.281	1.163				
1	10.214	1.613	-0.369				
	Balsalazide				Acyclovir		
8	4.988	-1.999	0.786	8	2.351	0.128	-0.040
8	-7.445	-0.628	-0.813	8	-3.927	-1.539	0.832
8	7.312	1.574	-2.207	8	5.008	-0.557	0.883
8	5.847	2.395	-0.716	7	0.312	-0.667	-0.759
8	-5.668	2.750	0.912	7	-1.048	-2.334	-0.112
8	-7.607	1.838	0.241	7	-1.102	1.256	-0.386
7	4.910	0.252	1.045	7	-3.220	0.600	0.417
7	-1.271	-1.265	-0.160	7	-2.746	2.847	-0.014
7	-1.995	-0.279	0.157	6	-0.862	-0.074	-0.369
6	6.351	0.360	1.155	6	1.509	0.009	-1.157
6	2.856	-0.962	0.581	6	-1.689	-1.122	0.018
6	7.048	0.367	-0.196	6	0.134	-2.026	-0.565
6	4.333	-0.964	0.803	6	-3.019	-0.827	0.461
6	2.288	-2.110	0.024	6	3.538	0.831	-0.349
6	2.024	0.116	0.917	6	-2.316	1.541	0.016
6	0.100	-1.092	0.119	6	4.473	0.752	0.825
6	0.925	-2.173	-0.211	1	1.225	0.995	-1.552
6	0.661	0.058	0.692	1	2.004	-0.567	-1.954
6	-3.361	-0.447	-0.120	1	0.933	-2.722	-0.783
6	-5.567	0.591	-0.002	1	3.309	1.884	-0.579
6	-4.188	0.621	0.218	1	4.026	0.393	-1.235
6	-6.121	-0.567	-0.587	1	-4.160	0.883	0.663
6	-3.929	-1.593	-0.701	1	5.267	1.504	0.692
6	6.653	1.550	-1.030	1	3.919	1.006	1.739
6	-5.285	-1.643	-0.927	1	-1.986	3.503	-0.120
6	-6.411	1.745	0.373	1	-3.414	3.122	0.691
1	6.581	1.274	1.708	1	5.429	-0.677	1.736
1	6.703	-0.491	1.740				
1	6.814	-0.549	-0.750				
1	8.137	0.369	-0.083				
1	4.424	1.092	0.767				
1	2.942	-2.941	-0.213				
1	2.440	1.002	1.389				
1	0.467	-3.054	-0.649				
1	0.010	0.883	0.957				
1	-3.739	1.499	0.666				
1	-3.284	-2.423	-0.964				
1	-5.734	-2.526	-1.376				
1	-7.648	-1.482	-1.212				
1	7.000	2.354	-2.686				
1	-6.297	3.452	1.124				
	Cefprozil				Bumetanide		
16	0.157	0.604	-1.346	16	3.183	-1.019	-0.703
8	0.908	-2.034	2.011	8	0.216	-1.367	-0.849
8	-2.712	-3.029	-1.118	8	2.997	-1.434	-2.080
8	4.073	0.057	1.999	8	4.449	-0.501	-0.219
8	4.112	-2.040	1.177	8	0.808	4.651	0.921
8	-3.169	4.187	0.856	8	2.991	4.118	0.848
7	1.675	-1.249	-0.095	7	-1.728	0.517	-0.303
7	-1.569	-1.482	0.089	7	2.750	-2.289	0.314
7	-5.012	-1.636	-0.987	6	-2.781	1.512	-0.298
6	0.663	-1.131	-1.133	6	-4.132	0.861	-0.526
6	-0.278	-1.985	-0.240	6	-0.404	0.862	-0.189
6	0.809	-1.832	0.835	6	0.588	-0.114	-0.422
6	2.772	-0.406	0.078	6	1.936	0.203	-0.310
6	1.865	1.167	-1.657	6	-5.279	1.860	-0.507
6	2.921	0.705	-0.685	6	0.019	2.144	0.183
6	-2.712	-2.037	-0.412	6	1.376	2.442	0.313
6	3.727	-0.899	1.114	6	2.348	1.475	0.060
6	-4.018	-1.360	0.036	6	-6.630	1.209	-0.741
6	4.141	1.502	-0.696	6	-0.440	-2.211	0.034
6	-3.861	0.122	0.286	6	1.837	3.790	0.712
6	5.387	1.011	-0.680	6	-0.493	-1.987	1.404
6	-3.638	0.615	1.570	6	-1.026	-3.337	-0.536
6	-3.854	1.024	-0.783	6	-1.156	-2.906	2.209
6	6.623	1.833	-0.660	6	-1.681	-4.248	0.284
6	-3.402	1.968	1.791	6	-1.752	-4.036	1.657
6	-3.626	2.374	-0.578	1	-2.778	2.026	0.672
6	-3.393	2.851	0.713	1	-2.601	2.290	-1.060
1	0.973	-1.560	-2.090	1	-4.122	0.333	-1.490
1	-0.395	-3.004	-0.617	1	-4.292	0.090	0.239
1	-1.637	-0.606	0.591	1	-1.908	-0.301	-0.868
1	1.821	2.259	-1.636	1	-5.282	2.388	0.455
1	2.147	0.898	-2.682	1	-5.101	2.631	-1.267
1	-4.240	-1.840	1.010	1	-0.712	2.921	0.364
1	4.006	2.582	-0.770	1	3.400	1.712	0.158
1	5.520	-0.071	-0.678	1	-6.847	0.458	0.024

1	-5.945	-1.579	-0.597	1	-7.441	1.940	-0.723
1	-4.869	-2.583	-1.328	1	-6.665	0.703	-1.711
1	4.670	-0.369	2.632	1	3.556	-2.560	0.867
1	-3.646	-0.070	2.416	1	2.405	-3.072	-0.232
1	-4.040	0.644	-1.783	1	-0.013	-1.113	1.830
1	6.402	2.902	-0.700	1	-0.956	-3.482	-1.609
1	7.285	1.587	-1.496	1	-1.200	-2.736	3.280
1	7.203	1.646	0.251	1	-2.138	-5.127	-0.157
1	-3.233	2.339	2.798	1	-2.266	-4.748	2.294
1	-3.619	3.076	-1.404	1	1.213	5.492	1.172
1	-3.017	4.380	1.786				
Didanosine				Buspirone			
8	2.353	0.287	-1.012	8	3.658	2.120	1.297
8	4.092	-1.722	0.000	8	3.417	-1.870	-0.869
8	-4.028	-1.800	0.457	7	3.560	0.090	0.276
7	0.062	0.072	-0.587	7	-2.679	0.717	0.075
7	-1.013	-1.888	-0.320	7	-5.466	0.152	0.131
7	-1.761	1.630	-0.174	7	-7.157	-1.381	0.528
7	-3.750	0.475	0.337	7	-7.604	0.715	-0.562
6	1.160	1.005	-0.949	6	6.352	0.194	-0.226
6	1.366	2.074	0.109	6	6.741	-0.578	1.047
6	2.232	1.334	1.120	6	7.725	0.425	-0.863
6	3.073	0.410	0.243	6	7.850	-1.538	0.600
6	3.298	-0.944	0.869	6	8.487	-0.888	-0.651
6	-1.238	0.379	-0.273	6	5.598	1.483	0.055
6	0.123	-1.304	-0.617	6	5.461	-0.658	-1.128
6	-1.877	-0.849	-0.102	6	4.210	1.288	0.608
6	-3.271	-0.877	0.249	6	4.076	-0.893	-0.582
6	-3.025	1.606	0.133	6	2.207	-0.117	0.807
1	0.939	1.401	-1.945	6	1.135	0.436	-0.116
1	0.431	2.466	0.506	6	-0.262	0.216	0.442
1	1.918	2.900	-0.348	6	-1.338	0.740	-0.494
1	2.844	1.998	1.732	6	-3.166	-0.641	0.286
1	1.605	0.744	1.799	6	-3.611	1.427	-0.792
1	4.044	0.852	-0.011	6	-4.539	-0.635	0.927
1	2.324	-1.417	1.067	6	-4.993	1.492	-0.176
1	3.791	-0.787	1.842	6	-6.787	-0.180	0.036
1	1.043	-1.803	-0.881	6	-8.436	-1.701	0.378
1	4.201	-2.594	0.386	6	-8.873	0.347	-0.688
1	-3.565	2.543	0.238	6	-9.366	-0.871	-0.236
1	-4.731	0.554	0.573	1	5.896	-1.090	1.520
				1	7.126	0.137	1.783
				1	8.222	1.246	-0.331
				1	7.658	0.725	-1.914
				1	7.435	-2.520	0.354
				1	8.578	-1.710	1.396
				1	9.560	-0.719	-0.534
				1	8.378	-1.541	-1.522
				1	5.493	2.064	-0.873
				1	6.133	2.128	0.757
				1	5.887	-1.642	-1.336
				1	5.344	-0.166	-2.104
				1	2.167	0.374	1.780
				1	2.078	-1.192	0.943
				1	1.226	-0.044	-1.098
				1	1.312	1.508	-0.268
				1	-0.405	-0.855	0.629
				1	-0.365	0.714	1.414
				1	-1.301	0.179	-1.452
				1	-1.112	1.783	-0.746
				1	-2.475	-1.174	0.945
				1	-3.206	-1.199	-0.672
				1	-3.676	0.943	-1.788
				1	-3.235	2.444	-0.949
				1	-4.930	-1.646	1.018
				1	-4.467	-0.207	1.939
				1	-4.955	2.091	0.747
				1	-5.702	1.964	-0.854
				1	-8.731	-2.672	0.775
				1	-9.529	1.070	-1.173
				1	-10.406	-1.149	-0.345
Aminophylline				Atovaquone			
8	0.561	-2.706	0.000	17	-8.218	-0.483	0.000
8	2.312	1.552	0.000	8	2.665	-2.356	0.000
7	0.031	1.375	0.000	8	1.842	2.313	-0.001
7	1.426	-0.553	0.000	8	4.522	2.738	0.000
7	-2.176	-1.330	0.000	6	0.609	-0.274	0.000
7	-2.353	0.897	0.000	6	-2.254	0.521	0.000
6	-1.046	0.530	0.000	6	-0.078	0.263	-1.263
6	-0.890	-0.836	0.000	6	-0.079	0.264	1.264
6	0.370	-1.500	0.000	6	-1.570	-0.038	-1.253
6	1.321	0.848	0.001	6	-1.570	-0.037	1.254
6	-0.166	2.815	0.000	6	2.100	-0.032	0.000
6	2.793	-1.062	0.000	6	-3.740	0.269	0.000

6	-3.002	-0.258	0.000	6	3.013	-1.053	0.000
1	-2.426	-2.308	0.000	6	2.583	1.342	0.000
1	-0.726	3.118	-0.887	6	-4.648	1.328	-0.001
1	0.815	3.282	0.001	6	-4.254	-1.032	0.001
1	-0.728	3.118	0.885	6	4.465	-0.871	0.000
1	2.737	-2.147	0.000	6	4.108	1.599	0.000
1	3.327	-0.709	0.883	6	5.007	0.426	0.000
1	3.327	-0.708	-0.882	6	-6.021	1.112	-0.001
1	-4.077	-0.360	0.000	6	-5.622	-1.272	0.001
				6	5.329	-1.969	0.000
				6	-6.497	-0.192	0.000
				6	6.387	0.608	0.000
				6	6.706	-1.775	0.000
				6	7.239	-0.489	0.000
				1	0.412	-1.363	0.001
				1	-2.101	1.610	0.000
				1	0.393	-0.167	-2.154
				1	0.083	1.344	-1.313
				1	0.083	1.345	1.313
				1	0.393	-0.165	2.154
				1	-2.046	0.368	-2.152
				1	-1.732	-1.126	-1.290
				1	-1.732	-1.125	1.292
				1	-2.046	0.370	2.152
				1	-4.273	2.348	-0.001
				1	-3.574	-1.880	0.001
				1	-6.717	1.943	-0.001
				1	-6.010	-2.283	0.001
				1	4.917	-2.971	0.000
				1	1.701	-2.418	0.000
				1	6.767	1.624	0.000
				1	7.366	-2.636	0.000
				1	8.314	-0.345	0.000
	Methotrexate				Anileridine		
8	6.813	-0.750	0.970	8	-2.650	1.972	-0.140
8	2.952	-1.291	-2.134	8	-2.441	1.234	1.974
8	5.025	-1.474	2.125	7	0.659	-0.807	0.051
8	4.173	4.003	1.007	7	8.441	0.250	0.436
8	4.848	3.536	-1.086	6	-2.259	-0.362	0.142
7	-2.766	-3.204	0.045	6	-1.424	-0.277	-1.139
7	3.346	-1.049	0.082	6	-1.511	-1.281	1.123
7	-3.340	-0.526	0.044	6	0.008	0.138	-0.849
7	-5.107	0.689	1.871	6	-0.066	-0.858	1.317
7	-4.850	2.719	0.759	6	-3.677	-0.885	-0.093
7	-3.339	2.881	-1.136	6	2.055	-0.466	0.285
7	-2.163	1.037	-1.887	6	-2.435	1.018	0.785
7	-4.578	4.663	-0.418	6	2.953	-0.653	-0.936
6	4.733	-0.715	-0.151	6	-4.162	-1.200	-1.363
6	4.919	0.744	-0.588	6	-4.532	-1.051	1.003
6	-1.475	-2.754	-0.181	6	4.398	-0.420	-0.598
6	4.469	1.729	0.473	6	-5.456	-1.685	-1.531
6	-3.511	-2.676	1.169	6	-5.824	-1.531	0.836
6	1.177	-1.854	-0.654	6	-6.292	-1.854	-0.435
6	2.545	-1.390	-0.982	6	-2.908	3.293	0.382
6	-0.713	-2.151	0.841	6	4.961	0.856	-0.660
6	-0.871	-2.886	-1.448	6	5.216	-1.461	-0.153
6	5.504	-1.033	1.108	6	-3.125	4.209	-0.790
6	0.579	-1.720	0.605	6	6.281	1.088	-0.300
6	0.420	-2.441	-1.670	6	6.538	-1.245	0.209
6	-3.882	-1.214	1.033	6	7.093	0.038	0.142
6	-3.567	-3.589	-1.101	1	-1.873	0.420	-1.851
6	4.530	3.155	0.012	1	-1.409	-1.267	-1.608
6	-4.765	-0.580	1.937	1	-2.018	-1.289	2.090
6	-3.656	0.773	-0.031	1	-1.546	-2.299	0.721
6	-4.544	1.414	0.865	1	0.027	1.165	-0.423
6	-3.045	1.599	-1.039	1	0.569	0.181	-1.786
6	-4.245	3.357	-0.239	1	0.444	-1.571	1.973
1	5.126	-1.349	-0.957	1	-0.034	0.124	1.831
1	4.345	0.886	-1.506	1	2.161	0.572	0.663
1	5.967	0.912	-0.847	1	2.421	-1.117	1.089
1	5.066	1.651	1.391	1	2.651	0.032	-1.735
1	3.439	1.522	0.787	1	2.806	-1.668	-1.322
1	3.137	-1.408	1.005	1	-3.532	-1.071	-2.236
1	-4.418	-3.280	1.285	1	-4.180	-0.787	1.996
1	-2.949	-2.833	2.097	1	-5.811	-1.929	-2.528
1	-1.142	-1.990	1.822	1	-6.469	-1.652	1.700
1	-1.419	-3.329	-2.270	1	-7.300	-2.232	-0.567
1	1.109	-1.233	1.419	1	-2.056	3.595	0.999
1	0.871	-2.536	-2.653	1	-3.780	3.241	1.042
1	-4.548	-3.913	-0.753	1	4.351	1.690	-1.001
1	-3.111	-4.431	-1.628	1	4.807	-2.467	-0.091
1	-3.707	-2.765	-1.815	1	-3.975	3.884	-1.393
1	-5.211	-1.161	2.747	1	-2.244	4.243	-1.434
1	7.240	-0.980	1.807	1	-3.327	5.223	-0.439

1	4.230	4.897	0.641	1	6.696	2.091	-0.368
1	-1.631	1.630	-2.501	1	7.154	-2.077	0.541
1	-1.844	0.097	-1.699	1	8.840	-0.423	1.075
1	-3.981	5.220	-1.006	1	8.662	1.192	0.724
1	-5.076	5.116	0.330				
	Bupropion				Aspirin		
17	2.835	2.316	0.633	8	1.013	-1.045	-0.606
8	-0.341	-3.107	0.158	8	-0.557	2.835	0.137
7	-1.683	-0.135	-0.550	8	1.245	1.698	-0.558
6	-2.519	1.085	-0.377	8	1.679	-0.471	1.483
6	-1.444	-1.017	0.596	6	-0.307	-0.793	-0.304
6	-2.012	2.080	-1.418	6	-0.794	0.509	-0.102
6	-3.980	0.752	-0.681	6	-1.163	-1.885	-0.268
6	-2.403	1.708	1.015	6	-2.163	0.667	0.152
6	-2.652	-1.858	0.955	6	-2.517	-1.701	-0.027
6	-0.247	-1.901	0.243	6	-3.019	-0.421	0.189
6	1.070	-1.226	-0.001	6	0.088	1.691	-0.202
6	1.312	0.094	0.392	6	1.962	-0.749	0.353
6	2.087	-1.953	-0.625	6	3.321	-0.839	-0.247
6	2.552	0.666	0.147	1	-0.745	-2.872	-0.430
6	3.320	-1.365	-0.866	1	-2.544	1.668	0.313
6	3.564	-0.049	-0.484	1	-3.179	-2.560	-0.002
1	-0.790	0.158	-0.930	1	-4.075	-0.273	0.385
1	-1.138	-0.452	1.500	1	3.406	-1.698	-0.913
1	-2.044	1.641	-2.419	1	4.074	-0.885	0.536
1	-2.624	2.985	-1.426	1	3.479	0.060	-0.847
1	-0.978	2.378	-1.208	1	0.094	3.542	0.033
1	-4.403	0.054	0.043				
1	-4.068	0.300	-1.671				
1	-4.593	1.659	-0.659				
1	-1.366	1.960	1.260				
1	-2.983	2.633	1.065				
1	-2.786	1.046	1.797				
1	-2.380	-2.624	1.683				
1	-3.444	-1.246	1.390				
1	-3.046	-2.360	0.069				
1	0.549	0.678	0.895				
1	1.883	-2.978	-0.913				
1	4.106	-1.929	-1.357				
1	4.523	0.421	-0.668				
	Dantrolene				Cycloserine		
8	-0.270	-0.201	0.000	8	-1.763	-0.359	0.115
8	6.511	2.743	0.000	8	0.957	1.796	0.026
8	5.854	-1.807	0.000	7	-1.145	0.874	-0.240
8	-7.517	0.173	0.000	7	1.777	-0.974	-0.273
8	-6.728	2.199	0.001	6	0.540	-0.595	0.373
7	4.351	-0.013	0.000	6	-0.709	-1.303	-0.130
7	6.519	0.428	0.000	6	0.193	0.856	0.064
7	3.237	-0.761	0.000	1	0.569	-0.650	1.476
7	-6.593	0.980	0.000	1	-0.614	-1.505	-1.205
6	4.447	1.435	0.000	1	-0.988	-2.212	0.402
6	-1.302	-1.093	0.000	1	-1.743	1.655	-0.009
6	-2.639	-0.560	0.000	1	2.268	-1.677	0.265
6	0.891	-0.916	0.000	1	2.382	-0.156	-0.306
6	5.947	1.680	0.000				
6	5.602	-0.636	0.000				
6	-0.793	-2.372	0.000				
6	0.609	-2.261	0.000				
6	-3.747	-1.428	0.000				
6	-2.866	0.828	0.000				
6	2.099	-0.150	0.000				
6	-5.226	0.448	0.000				
6	-5.035	-0.931	0.000				
6	-4.153	1.332	0.000				
1	3.986	1.883	0.888				
1	3.986	1.883	-0.887				
1	-1.370	-3.284	0.000				
1	7.515	0.264	0.000				
1	1.343	-3.051	0.000				
1	-3.590	-2.501	0.000				
1	-2.020	1.504	0.000				
1	1.988	0.938	0.000				
1	-5.898	-1.585	0.000				
1	-4.348	2.398	0.000				
	Aminoglutethimide				Abacavir		
8	1.746	0.703	2.081	8	-4.932	2.189	0.032
8	2.306	-3.142	-0.222	7	3.564	-0.489	-0.251
7	2.008	-1.171	0.851	7	-0.868	-1.698	-0.022
7	-4.807	-0.382	0.191	7	1.251	-2.457	-0.202
6	0.827	0.754	-0.164	7	1.947	1.181	-0.104
6	1.430	0.166	-1.453	7	-0.426	0.701	0.047
6	0.979	2.287	-0.110	7	0.380	2.860	0.010
6	-0.660	0.401	-0.051	6	4.633	0.435	-0.456
6	1.310	-1.347	-1.485	6	5.154	1.199	0.721

6	1.564	0.138	1.023	6	5.964	0.084	0.130
6	1.914	-1.998	-0.271	6	-2.328	-1.735	0.092
6	2.397	2.811	-0.257	6	-3.047	-0.904	-0.995
6	-1.233	-0.130	1.106	6	-4.064	-0.004	-0.264
6	-1.516	0.652	-1.129	6	-2.834	-1.160	1.385
6	-2.591	-0.411	1.183	6	-3.772	-0.239	1.189
6	-2.872	0.377	-1.065	6	2.260	-0.116	-0.171
6	-3.436	-0.165	0.097	6	-0.061	-0.583	-0.027
1	2.487	0.449	-1.515	6	1.235	-1.079	-0.139
1	0.946	0.610	-2.328	6	-3.936	1.455	-0.667
1	0.557	2.623	0.842	6	-0.015	-2.779	-0.129
1	0.338	2.706	-0.895	6	0.643	1.508	-0.001
1	1.784	-1.791	-2.363	1	4.622	0.957	-1.411
1	0.255	-1.647	-1.517	1	4.664	1.019	1.669
1	2.444	-1.591	1.665	1	5.472	2.221	0.558
1	3.067	2.372	0.487	1	6.851	0.326	-0.443
1	2.815	2.615	-1.249	1	6.030	-0.841	0.692
1	2.422	3.893	-0.111	1	-2.582	-2.801	0.014
1	-0.618	-0.323	1.980	1	-3.520	-1.544	-1.741
1	-1.119	1.076	-2.048	1	-2.311	-0.289	-1.520
1	-3.004	-0.820	2.100	1	-5.096	-0.312	-0.486
1	-3.509	0.590	-1.920	1	3.724	-1.467	-0.448
1	-5.277	-0.531	-0.690	1	-2.452	-1.493	2.344
1	-5.083	-1.070	0.876	1	-4.292	0.306	1.968
				1	-4.068	1.548	-1.756
				1	-2.922	1.804	-0.420
				1	-0.410	-3.786	-0.148
				1	-4.829	3.118	-0.185
				1	1.162	3.434	0.284
				1	-0.503	3.114	0.425
	Diazepam				Anisindione		
17	0.512	4.219	-0.570	8	0.959	-2.371	0.760
8	2.472	-3.535	-0.121	8	0.959	2.377	0.744
7	2.102	-1.395	0.559	8	-4.990	-0.001	-0.373
7	-0.315	-1.960	-1.068	6	0.469	0.004	1.137
6	0.407	0.215	-0.229	6	1.278	-1.210	0.654
6	1.697	-0.078	0.263	6	1.278	1.215	0.646
6	-0.592	-0.848	-0.483	6	2.523	-0.698	0.034
6	1.045	-2.173	-1.509	6	2.523	0.698	0.029
6	1.940	-2.464	-0.322	6	-0.974	0.003	0.722
6	-1.995	-0.626	-0.059	6	3.590	-1.418	-0.495
6	0.063	1.550	-0.478	6	3.590	1.415	-0.505
6	2.579	0.979	0.527	6	-2.005	0.008	1.664
6	3.014	-1.617	1.674	6	-1.318	-0.004	-0.628
6	0.963	2.571	-0.237	6	4.655	-0.705	-1.029
6	2.225	2.293	0.282	6	4.655	0.697	-1.034
6	-2.318	0.230	1.000	6	-3.333	0.006	1.274
6	-3.027	-1.321	-0.702	6	-2.646	-0.005	-1.040
6	-3.638	0.387	1.406	6	-3.662	0.000	-0.083
6	-4.344	-1.156	-0.301	6	-5.356	-0.007	-1.737
6	-4.655	-0.300	0.754	1	0.527	0.008	2.233
1	1.448	-1.303	-2.051	1	3.578	-2.503	-0.485
1	1.084	-3.042	-2.165	1	3.578	2.500	-0.502
1	-0.926	1.779	-0.858	1	-1.761	0.013	2.722
1	3.566	0.763	0.919	1	-0.536	-0.008	-1.385
1	2.770	-0.928	2.483	1	5.503	-1.235	-1.452
1	4.062	-1.480	1.387	1	5.503	1.225	-1.460
1	2.896	-2.644	2.012	1	-4.134	0.010	2.004
1	2.922	3.099	0.479	1	-2.877	-0.010	-2.098
1	-1.529	0.762	1.523	1	-4.984	0.883	-2.259
1	-2.769	-1.990	-1.515	1	-6.445	-0.007	-1.760
1	-3.871	1.047	2.236	1	-4.985	-0.902	-2.251
1	-5.135	-1.693	-0.814				
1	-5.686	-0.172	1.066				
	Ethinamate				Fenoprofen		
8	-0.644	-0.448	-0.658	8	-1.682	1.659	0.195
8	-2.233	-0.408	0.984	8	3.609	-2.426	-0.464
7	-2.282	-1.943	-0.712	8	1.438	-1.972	-0.824
6	0.110	0.667	-0.076	6	2.786	-0.435	0.505
6	1.266	0.864	-1.066	6	1.883	0.720	0.154
6	0.658	0.296	1.310	6	0.506	0.624	0.353
6	2.191	-0.345	-1.116	6	2.683	-0.841	1.982
6	1.572	-0.920	1.249	6	2.417	1.896	-0.372
6	2.718	-0.706	0.267	6	-0.323	1.681	-0.004
6	-0.721	1.865	-0.029	6	2.498	-1.659	-0.344
6	-1.772	-0.868	-0.032	6	1.582	2.961	-0.696
6	-1.339	2.898	-0.017	6	0.210	2.860	-0.522
1	1.819	1.754	-0.742	6	-2.391	0.484	0.069
1	0.850	1.092	-2.051	6	-2.053	-0.514	-0.842
1	-0.173	0.150	2.001	6	-3.536	0.371	0.854
1	1.220	1.169	1.666	6	-2.867	-1.636	-0.949
1	3.018	-0.140	-1.804	6	-4.343	-0.752	0.728
1	1.645	-1.199	-1.535	6	-4.012	-1.762	-0.169
1	0.989	-1.801	0.950	1	3.823	-0.146	0.306

1	1.956	-1.135	2.251	1	0.075	-0.285	0.757
1	3.352	-1.597	0.214	1	2.915	0.013	2.621
1	3.360	0.106	0.635	1	1.674	-1.179	2.227
1	-1.910	3.793	0.012	1	3.380	-1.648	2.219
1	-1.999	-2.069	-1.671	1	3.489	1.975	-0.530
1	-3.236	-2.173	-0.491	1	2.004	3.876	-1.101
				1	-0.460	3.672	-0.780
				1	-1.161	-0.422	-1.451
				1	-3.776	1.169	1.548
				1	-2.599	-2.415	-1.656
				1	-5.235	-0.837	1.341
				1	3.350	-3.210	-0.969
				1	-4.641	-2.641	-0.260
	Acetazolamide				Carbamazepine		
16	2.808	-0.077	0.043	8	1.077	2.624	-0.983
16	-0.042	-1.290	0.155	7	0.008	0.788	-0.123
8	3.121	-0.647	1.334	7	-1.200	2.555	-1.070
8	3.238	-0.681	-1.196	6	1.244	0.157	0.203
8	-3.622	1.358	0.594	6	-1.201	0.120	0.229
7	-2.642	-0.539	-0.249	6	1.584	-1.058	-0.417
7	0.434	1.188	-0.325	6	-1.548	-1.083	-0.414
7	3.331	1.490	0.045	6	0.694	-1.766	-1.320
7	-0.911	1.078	-0.435	6	-0.656	-1.774	-1.328
6	1.018	0.062	-0.044	6	2.125	0.776	1.084
6	-1.323	-0.142	-0.219	6	-2.055	0.691	1.171
6	-3.743	0.252	0.140	6	2.848	-1.605	-0.140
6	-5.060	-0.435	-0.101	6	-2.803	-1.643	-0.123
1	-2.824	-1.501	-0.492	6	0.040	2.032	-0.756
1	3.033	1.983	-0.792	6	3.363	0.209	1.351
1	3.022	1.985	0.876	6	-3.284	0.110	1.453
1	-5.392	-0.219	-1.120	6	3.726	-0.987	0.734
1	-5.803	-0.033	0.585	6	-3.662	-1.059	0.794
1	-5.009	-1.520	0.011	1	1.191	-2.449	-2.006
				1	-1.142	-2.461	-2.017
				1	1.841	1.724	1.526
				1	-1.755	1.617	1.652
				1	3.128	-2.536	-0.625
				1	-3.090	-2.562	-0.627
				1	4.051	0.707	2.026
				1	-3.948	0.571	2.176
				1	4.697	-1.430	0.931
				1	-4.624	-1.515	1.001
				1	-1.141	3.305	-1.741
				1	-1.974	1.920	-1.207
	Acetaminophen				Clonidine		
8	3.963	-0.236	0.000	17	-0.321	2.436	-0.664
8	-2.509	-1.434	0.000	17	1.702	-2.572	-0.180
7	-1.537	0.639	0.000	7	-2.741	-1.021	-0.699
6	-0.161	0.340	0.000	7	-0.422	-0.569	-0.831
6	0.348	-0.961	0.000	7	-1.729	0.079	1.041
6	0.733	1.417	0.000	6	-3.864	-0.499	0.090
6	1.723	-1.161	0.000	6	-3.150	-0.022	1.371
6	2.102	1.213	0.000	6	-1.608	-0.461	-0.109
6	2.606	-0.086	0.000	6	0.761	-0.032	-0.308
6	-2.611	-0.220	0.000	6	0.935	1.353	-0.156
6	-3.953	0.470	0.000	6	1.853	-0.844	0.024
1	-0.332	-1.800	0.000	6	2.112	1.886	0.349
1	0.347	2.433	0.000	6	3.047	-0.327	0.504
1	-1.755	1.624	-0.001	6	3.166	1.045	0.680
1	2.111	-2.177	0.000	1	-4.614	-1.272	0.273
1	2.791	2.050	0.000	1	-4.356	0.332	-0.432
1	-4.517	0.147	0.877	1	-3.536	0.935	1.735
1	-4.517	0.145	-0.876	1	-3.276	-0.743	2.189
1	-3.900	1.560	-0.001	1	-2.806	-0.891	-1.701
1	4.171	-1.174	0.000	1	-0.300	-1.487	-1.241
				1	2.198	2.960	0.459
				1	3.861	-0.999	0.748
				1	4.089	1.461	1.067
	4-Aminosalicylic acid				Clomiphene		
8	-0.580	2.178	0.000	17	-4.954	1.159	0.789
8	-2.613	-1.488	0.003	8	2.728	-1.152	-0.857
8	-2.780	0.747	0.005	7	6.140	-0.362	0.203
7	3.570	-0.115	-0.062	6	5.071	-0.922	-0.613
6	-0.619	-0.238	-0.002	6	6.401	-1.202	1.374
6	0.065	1.006	-0.003	6	7.356	-0.128	-0.577
6	2.193	-0.148	-0.004	6	3.720	-0.485	-0.089
6	1.456	1.035	-0.003	6	7.092	-0.457	2.498
6	0.146	-1.418	-0.002	6	7.246	1.079	-1.485
6	1.519	-1.389	-0.004	6	-1.327	-0.468	-0.169
6	-2.064	-0.252	0.002	6	1.426	-0.889	-0.580
1	1.951	2.000	-0.006	6	-2.780	-0.268	0.035
1	-0.376	-2.369	0.000	6	-0.867	-1.358	-1.153
1	2.092	-2.311	-0.010	6	-0.371	0.178	0.618
1	4.055	-0.942	0.249	6	0.484	-1.561	-1.366

1	4.016	0.742	0.226	6	0.991	-0.021	0.424
1	-1.542	1.978	0.002	6	-3.601	-1.501	0.043
1	-3.570	-1.352	0.005	6	-3.291	0.972	0.233
				6	-2.596	2.258	0.052
				6	-3.172	-2.618	0.770
				6	-4.772	-1.610	-0.715
				6	-3.909	-3.796	0.767
				6	-5.499	-2.793	-0.732
				6	-1.794	2.471	-1.078
				6	-2.733	3.297	0.980
				6	-5.076	-3.888	0.015
				6	-1.128	3.675	-1.255
				6	-2.057	4.497	0.804
				6	-1.250	4.691	-0.312
				1	5.113	-2.026	-0.659
				1	5.172	-0.571	-1.643
				1	5.439	-1.577	1.736
				1	6.983	-2.101	1.089
				1	8.176	0.032	0.128
				1	7.631	-1.029	-1.160
				1	3.612	0.605	-0.182
				1	3.606	-0.737	0.975
				1	8.078	-0.087	2.206
				1	6.497	0.402	2.815
				1	7.237	-1.111	3.361
				1	6.451	0.970	-2.227
				1	7.036	1.980	-0.904
				1	8.178	1.235	-2.035
				1	-1.589	-1.892	-1.764
				1	-0.697	0.852	1.404
				1	0.837	-2.240	-2.134
				1	1.700	0.493	1.061
				1	-2.253	-2.554	1.344
				1	-5.105	-0.761	-1.303
				1	-3.568	-4.646	1.350
				1	-6.400	-2.861	-1.335
				1	-1.697	1.681	-1.816
				1	-3.372	3.153	1.845
				1	-5.648	-4.810	0.005
				1	-0.516	3.823	-2.140
				1	-2.167	5.287	1.541
				1	-0.728	5.633	-0.452
Angrelide				Diclofenac			
17	2.158	-2.119	0.000	17	1.343	-2.233	1.387
17	4.410	0.112	0.000	17	1.338	2.687	-0.905
8	-5.467	-0.313	0.000	8	-4.174	1.949	0.668
7	-1.978	-0.568	0.000	8	-1.996	2.390	0.353
7	-3.546	0.982	0.000	7	0.053	0.277	0.302
7	-1.303	1.720	0.000	6	-2.167	-0.677	0.145
6	-0.662	-1.164	0.000	6	-0.828	-0.652	-0.287
6	-3.219	-1.299	0.000	6	-2.632	0.242	1.246
6	-2.176	0.776	0.000	6	1.434	0.199	0.166
6	0.385	-0.083	0.000	6	-3.053	-1.574	-0.447
6	0.022	1.279	0.000	6	-0.410	-1.546	-1.275
6	-4.268	-0.195	0.000	6	-2.635	-2.461	-1.432
6	1.734	-0.432	0.000	6	-1.304	-2.445	-1.838
6	1.033	2.246	0.000	6	2.172	-0.914	0.613
6	2.733	0.545	0.000	6	2.185	1.267	-0.359
6	2.368	1.887	0.000	6	-2.865	1.633	0.722
1	-0.542	-1.820	-0.877	6	3.553	-0.978	0.497
1	-0.542	-1.819	0.878	6	3.568	1.230	-0.455
1	-3.336	-1.937	0.885	6	4.252	0.096	-0.039
1	-3.336	-1.937	-0.885	1	-1.854	0.310	2.015
1	-3.953	1.905	0.000	1	-3.545	-0.142	1.702
1	0.740	3.290	0.000	1	-0.317	1.225	0.314
1	3.146	2.642	0.000	1	-4.086	-1.584	-0.110
				1	0.623	-1.524	-1.605
				1	-3.337	-3.160	-1.871
				1	-0.960	-3.130	-2.606
				1	4.070	-1.861	0.852
				1	4.093	2.083	-0.868
				1	5.332	0.053	-0.121
				1	-4.230	2.837	0.285
Allopurinol				Flurbiprofen			
8	-1.752	1.958	0.000	9	0.733	1.936	0.898
7	1.983	-0.725	0.000	8	-3.966	-0.174	-1.902
7	-1.929	-0.330	0.000	8	-4.360	1.375	-0.319
7	-0.140	-1.871	0.000	6	-3.297	-0.712	0.305
7	2.483	0.536	0.000	6	-1.792	-0.556	0.204
6	0.224	0.585	0.000	6	1.029	-0.250	0.033
6	0.633	-0.753	0.000	6	-1.183	0.640	0.585
6	-1.179	0.889	0.000	6	-0.987	-1.592	-0.267
6	1.422	1.330	0.000	6	0.189	0.769	0.492
6	-1.408	-1.588	0.000	6	0.389	-1.439	-0.343

1	1.551	2.402	0.000	6	-3.807	-0.527	1.728
1	2.613	-1.512	0.000	6	2.495	-0.116	-0.050
1	-2.934	-0.210	0.000	6	-3.943	0.288	-0.631
1	-2.133	-2.398	0.000	6	3.107	1.065	-0.489
				6	3.314	-1.202	0.288
				6	4.490	1.151	-0.591
				6	4.696	-1.113	0.189
				6	5.290	0.065	-0.252
				1	-3.549	-1.713	-0.062
				1	-1.765	1.479	0.954
				1	-1.446	-2.524	-0.584
				1	0.998	-2.251	-0.729
				1	-3.322	-1.236	2.401
				1	-3.602	0.484	2.086
				1	-4.887	-0.680	1.783
				1	2.496	1.916	-0.767
				1	2.857	-2.117	0.653
				1	4.944	2.072	-0.942
				1	5.311	-1.964	0.465
				1	6.370	0.136	-0.328
				1	-4.338	0.534	-2.448
Amoxapine				Alprazolam			
17	-2.135	3.821	-1.109	17	1.313	4.211	-0.475
8	1.921	0.451	1.498	7	-2.202	-0.528	0.050
7	-1.447	-1.388	0.089	7	0.105	-1.869	-1.329
7	-3.955	-2.659	0.360	7	-3.174	-2.422	-0.535
7	0.827	-1.643	-0.154	7	-3.800	-1.938	0.596
6	-1.595	-2.809	-0.218	6	-1.347	0.589	-0.051
6	-2.422	-0.939	1.088	6	0.008	0.413	-0.394
6	-3.016	-3.082	-0.671	6	-2.229	-1.580	-0.845
6	-3.828	-1.230	0.606	6	0.626	-0.926	-0.631
6	-0.170	-0.855	0.081	6	-1.212	-1.658	-1.919
6	-0.089	0.621	0.190	6	-3.227	-0.810	0.935
6	0.967	1.226	0.878	6	-1.855	1.869	0.173
6	2.144	-1.219	-0.244	6	0.811	1.553	-0.518
6	-1.038	1.440	-0.432	6	1.964	-1.177	-0.038
6	2.715	-0.230	0.575	6	-1.045	2.986	0.058
6	1.054	2.609	0.981	6	0.288	2.818	-0.301
6	-0.938	2.818	-0.332	6	-3.585	0.007	2.116
6	0.095	3.415	0.384	6	2.385	-0.527	1.128
6	3.010	-1.903	-1.112	6	2.812	-2.125	-0.624
6	4.069	0.062	0.539	6	3.622	-0.816	1.693
6	4.363	-1.606	-1.167	6	4.050	-2.404	-0.066
6	4.902	-0.628	-0.334	6	4.460	-1.750	1.095
1	-1.351	-3.417	0.666	1	-1.452	-2.496	-2.572
1	-0.876	-3.066	-0.995	1	-1.233	-0.736	-2.521
1	-2.293	0.126	1.280	1	-2.904	1.989	0.417
1	-2.247	-1.475	2.034	1	1.856	1.441	-0.784
1	-3.184	-2.563	-1.633	1	-1.445	3.979	0.224
1	-3.139	-4.154	-0.849	1	-4.238	0.846	1.861
1	-4.547	-0.931	1.374	1	-4.124	-0.624	2.821
1	-4.027	-0.620	-0.296	1	-2.699	0.414	2.611
1	-4.903	-2.879	0.076	1	1.734	0.197	1.608
1	-1.850	0.985	-0.990	1	2.474	-2.634	-1.520
1	1.880	3.041	1.535	1	3.929	-0.312	2.603
1	0.150	4.494	0.461	1	4.701	-3.133	-0.536
1	2.584	-2.683	-1.733	1	5.428	-1.971	1.531
1	4.453	0.826	1.207				
1	5.004	-2.151	-1.851				
1	5.963	-0.405	-0.360				
Amodiaquine				Estradiol			
17	6.971	-0.204	0.845	8	-4.871	-1.233	0.198
8	-5.017	2.412	-0.302	8	5.962	-0.133	0.401
7	-3.617	-1.481	0.375	6	-2.529	-0.574	0.130
7	0.463	1.523	0.066	6	-1.851	0.708	-0.381
7	2.734	-1.678	-1.513	6	-0.387	0.796	0.012
6	-4.214	-0.155	0.314	6	0.353	-0.421	-0.573
6	-3.212	0.942	0.073	6	-3.947	-0.327	-0.390
6	-3.258	-1.949	-0.967	6	-1.808	-1.777	-0.469
6	-4.493	-2.432	1.058	6	-2.818	1.825	0.017
6	-1.844	0.726	0.175	6	-0.310	-1.743	-0.162
6	-0.923	1.749	-0.064	6	-4.210	1.160	-0.069
6	-3.663	2.233	-0.235	6	0.296	2.073	-0.454
6	-2.207	-3.040	-0.949	6	-2.559	-0.669	1.658
6	-4.522	-2.239	2.561	6	1.843	-0.358	-0.284
6	-1.390	3.024	-0.373	6	1.703	2.155	0.114
6	1.178	0.462	-0.440	6	2.477	0.865	0.004
6	-2.757	3.266	-0.443	6	2.640	-1.505	-0.338
6	2.562	0.324	-0.094	6	3.852	0.903	0.227
6	3.288	-0.758	-0.677	6	4.009	-1.468	-0.115
6	0.636	-0.492	-1.289	6	4.622	-0.251	0.171
6	3.235	1.192	0.793	1	-1.873	0.641	-1.484
6	4.662	-0.903	-0.374	1	-0.310	0.756	1.111
6	1.453	-1.519	-1.779	1	0.228	-0.338	-1.669

6	4.570	1.035	1.079	1	-3.934	-0.475	-1.483
6	5.277	-0.021	0.476	1	-1.951	-1.765	-1.559
1	-4.728	0.047	1.261	1	-2.249	-2.714	-0.110
1	-5.008	-0.096	-0.455	1	-2.730	2.702	-0.630
1	-4.158	-2.281	-1.520	1	-2.610	2.171	1.036
1	-2.870	-1.088	-1.522	1	-0.132	-1.916	0.907
1	-5.520	-2.390	0.644	1	0.171	-2.579	-0.678
1	-4.124	-3.437	0.838	1	-4.746	1.223	0.883
1	-1.505	-0.264	0.461	1	-4.852	1.628	-0.821
1	-1.306	-2.702	-0.429	1	-0.280	2.955	-0.155
1	-2.556	-3.947	-0.450	1	0.325	2.081	-1.553
1	-1.926	-3.321	-1.967	1	-3.133	-1.546	1.962
1	-3.516	-2.323	2.980	1	-1.558	-0.758	2.084
1	-4.921	-1.264	2.850	1	-3.034	0.202	2.118
1	-5.153	-2.996	3.033	1	1.643	2.430	1.177
1	1.005	2.324	0.349	1	2.272	2.963	-0.360
1	-0.687	3.830	-0.563	1	-5.731	-1.085	-0.202
1	-3.120	4.264	-0.677	1	2.186	-2.464	-0.564
1	-0.398	-0.433	-1.605	1	4.343	1.846	0.450
1	2.697	1.991	1.294	1	4.599	-2.380	-0.163
1	5.201	-1.725	-0.829	1	6.366	-1.001	0.323
1	-5.200	3.327	-0.536				
1	1.012	-2.254	-2.453				
1	5.078	1.700	1.767				
Diethylstilbestrol				Doxepin			
8	6.054	0.308	0.012	8	2.822	0.433	1.410
8	-6.036	-0.388	-0.121	7	-4.459	-0.555	0.443
6	0.454	-0.504	0.260	6	0.372	-0.323	-0.321
6	-0.455	0.501	0.261	6	0.414	1.157	-0.397
6	0.078	-1.964	0.336	6	1.670	-1.041	-0.220
6	-0.079	1.961	0.343	6	1.027	1.875	0.640
6	1.915	-0.255	0.198	6	-2.165	-0.458	-0.530
6	-1.916	0.252	0.193	6	-0.785	-1.009	-0.399
6	0.471	-2.755	-0.907	6	-3.125	-1.136	0.442
6	-0.465	2.755	-0.901	6	1.610	1.099	1.774
6	2.793	-0.829	1.129	6	2.773	-0.635	0.562
6	-2.795	0.824	1.119	6	-0.127	1.857	-1.477
6	2.482	0.512	-0.826	6	1.082	3.265	0.588
6	-2.480	-0.515	-0.836	6	1.845	-2.195	-1.005
6	4.163	-0.629	1.063	6	3.969	-1.361	0.528
6	-4.167	0.620	1.041	6	-0.069	3.245	-1.523
6	3.854	0.716	-0.911	6	0.534	3.953	-0.489
6	-3.847	-0.723	-0.932	6	3.024	-2.920	-1.030
6	4.700	0.147	0.038	6	4.100	-2.491	-0.256
6	-4.699	-0.156	0.013	6	-5.245	-1.099	1.532
1	0.590	-2.407	1.202	6	-5.146	-0.751	-0.819
1	-0.990	-2.075	0.534	1	-2.521	-0.611	-1.559
1	0.988	2.071	0.547	1	-2.182	0.623	-0.360
1	-0.595	2.402	1.206	1	-0.724	-2.095	-0.318
1	-0.035	-2.373	-1.799	1	-3.161	-2.226	0.225
1	0.213	-3.812	-0.806	1	-2.725	-1.042	1.458
1	1.547	-2.691	-1.094	1	1.895	1.752	2.601
1	-0.209	3.812	-0.796	1	0.894	0.356	2.154
1	-1.539	2.689	-1.096	1	-0.588	1.302	-2.289
1	0.048	2.375	-1.791	1	1.554	3.809	1.402
1	2.393	-1.432	1.938	1	1.021	-2.496	-1.644
1	-2.402	1.427	1.932	1	4.783	-1.008	1.151
1	1.832	0.945	-1.580	1	-0.493	3.775	-2.370
1	-1.824	-0.947	-1.586	1	0.579	5.037	-0.522
1	4.831	-1.066	1.797	1	3.110	-3.796	-1.663
1	-4.828	1.063	1.783	1	5.039	-3.035	-0.265
1	4.269	1.310	-1.721	1	-5.406	-2.191	1.446
1	-4.272	-1.313	-1.737	1	-6.226	-0.618	1.560
1	6.287	0.860	-0.741	1	-4.745	-0.908	2.485
1	-6.502	0.060	0.590	1	-6.149	-0.323	-0.760
				1	-5.249	-1.820	-1.090
				1	-4.62	-0.245	-1.632

4. Table S4. Cartesian coordinates of optimized geometry of FDA approved drugs...H₂O at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

cefditoren pivoxil motif 1, Eint = -7.6 kcal/mol				cefditoren pivoxil motif 2, Eint = -9.7 kcal/mol			
16	-0.454	-3.146	-0.994	16	0.849	-2.528	1.291
16	4.386	-2.531	1.713	16	-4.063	-3.014	-1.411
16	-7.262	1.780	1.668	16	7.797	0.557	-2.240
8	-0.132	1.048	0.204	8	-0.051	1.311	-0.518
8	2.786	0.461	1.040	8	-2.866	0.222	-1.212
8	3.426	0.478	-1.134	8	-3.480	0.473	0.954
8	-3.843	-1.210	1.932	8	3.889	-1.788	-1.390

8	2.839	2.718	0.622	8	-3.192	2.491	-1.112
8	-4.059	-2.197	-1.737	8	3.808	-0.917	2.177
8	4.706	3.331	-0.506	8	-5.099	3.030	-0.011
7	0.741	-1.147	0.369	7	-0.611	-0.985	-0.367
7	-2.500	-1.092	0.107	7	2.581	-0.375	-0.190
7	-5.110	-1.369	-1.330	7	4.983	-0.436	1.610
7	-7.111	0.228	-0.403	7	7.167	0.567	0.277
7	6.051	-0.587	1.977	7	-5.967	-1.351	-1.893
7	-9.086	1.514	-0.353	7	9.240	1.596	-0.163
6	-0.230	-2.219	0.552	6	0.511	-1.919	-0.384
6	-1.294	-1.127	0.854	6	1.398	-0.745	-0.891
6	-0.200	-0.131	0.448	6	0.177	0.130	-0.608
6	1.953	-1.237	-0.312	6	-1.799	-1.137	0.346
6	1.328	-3.522	-1.136	6	-0.854	-3.159	1.485
6	2.282	-2.365	-0.988	6	-1.967	-2.187	1.187
6	2.812	-0.019	-0.227	6	-2.814	-0.069	0.111
6	3.589	-2.575	-1.602	6	-3.229	-2.480	1.856
6	-3.717	-1.068	0.730	6	3.767	-0.964	-0.495
6	-4.906	-0.830	-0.171	6	4.943	-0.471	0.318
6	4.797	-2.326	-1.065	6	-4.465	-2.472	1.323
6	3.520	1.663	1.251	6	-3.747	1.282	-1.565
6	2.558	4.267	-1.158	6	-3.062	4.281	0.444
6	5.095	-1.853	0.276	6	-4.837	-2.234	-0.062
6	-5.949	0.065	0.324	6	6.122	-0.015	-0.408
6	3.519	3.420	-0.342	6	-3.933	3.230	-0.223
6	3.356	5.327	-1.911	6	-3.963	5.317	1.108
6	1.875	3.314	-2.154	6	-2.228	3.546	1.506
6	1.497	4.919	-0.269	6	-2.126	4.947	-0.567
6	5.959	-0.836	0.630	6	-5.827	-1.394	-0.528
6	-5.855	0.807	1.470	6	6.281	-0.113	-1.766
6	6.720	0.013	-0.327	6	-6.680	-0.521	0.324
6	-7.889	1.086	0.174	6	8.108	0.913	-0.543
6	5.292	-1.395	2.652	6	-5.118	-2.146	-2.472
6	-4.413	-2.799	-2.975	6	3.871	-0.766	3.586
1	0.034	-2.897	1.369	1	0.362	-2.753	-1.075
1	-1.560	-1.079	1.914	1	1.620	-0.868	-1.955
1	1.581	-4.314	-0.420	1	-0.973	-4.069	0.882
1	1.456	-3.964	-2.128	1	-0.933	-3.479	2.528
1	-2.469	-1.045	-0.902	1	2.491	0.215	0.639
1	3.566	-3.001	-2.604	1	-3.142	-2.755	2.906
1	5.664	-2.473	-1.708	1	-5.298	-2.644	2.003
1	4.537	1.576	0.863	1	-4.740	1.130	-1.137
1	3.509	1.813	2.329	1	-3.771	1.279	-2.654
1	2.685	5.917	-2.542	1	-3.352	6.056	1.635
1	3.862	6.010	-1.225	1	-4.574	5.846	0.372
1	4.118	4.874	-2.547	1	-4.640	4.853	1.827
1	1.200	3.887	-2.797	1	-1.595	4.267	2.033
1	1.290	2.552	-1.635	1	-1.586	2.790	1.049
1	2.609	2.811	-2.789	1	-2.866	3.051	2.242
1	0.842	5.543	-0.884	1	-1.539	5.720	-0.064
1	1.947	5.562	0.493	1	-2.682	5.429	-1.376
1	0.882	4.171	0.235	1	-1.436	4.226	-1.009
1	-5.049	0.834	2.185	1	5.625	-0.577	-2.483
1	6.308	1.027	-0.368	1	-6.411	0.534	0.204
1	7.764	0.098	-0.019	1	-7.732	-0.622	0.047
1	6.677	-0.388	-1.341	1	-6.565	-0.759	1.383
1	5.215	-1.394	3.733	1	-5.054	-2.288	-3.544
1	-5.298	-3.430	-2.860	1	4.707	-1.334	4.005
1	-4.604	-2.040	-3.738	1	3.970	0.288	3.863
1	-3.554	-3.408	-3.258	1	2.924	-1.156	3.958
1	-9.428	0.892	-1.073	1	9.405	1.540	0.833
1	-9.800	1.759	0.317	1	10.071	1.414	-0.707
8	-2.814	1.825	0.949	8	1.746	1.651	1.722
1	-3.152	2.689	0.706	1	2.292	2.399	1.975
1	-1.894	1.823	0.645	1	1.114	2.006	1.081
cefditoren pivoxil motif 3, Eint = -7.8 kcal/mol				cefditoren pivoxil motif 4, Eint = -8.3 kcal/mol			
16	1.013	-2.727	1.143	16	0.897	-2.602	1.387
16	-3.632	-2.965	-1.710	16	-3.588	-2.873	-1.484
16	7.910	1.443	-1.902	16	7.788	1.462	-1.966
8	0.107	1.355	-0.078	8	0.080	1.462	-0.095
8	-2.707	0.314	-1.001	8	-2.743	0.392	-0.916
8	-3.469	0.190	1.128	8	-3.543	0.439	1.202
8	4.083	-1.042	-1.751	8	3.977	-1.031	-1.707
8	-3.392	2.484	-0.617	8	-3.252	2.622	-0.717
8	4.157	-1.423	2.022	8	4.147	-1.396	2.067
8	-5.421	2.514	0.393	8	-5.272	2.951	0.255
7	-0.452	-0.941	-0.247	7	-0.532	-0.829	-0.040
7	2.762	-0.410	-0.017	7	2.693	-0.396	0.057
7	5.304	-0.806	1.522	7	5.276	-0.774	1.533
7	7.421	0.532	0.477	7	7.353	0.580	0.433
7	-5.665	-1.450	-2.151	7	-5.551	-1.330	-2.108
7	9.488	1.650	0.320	7	9.408	1.711	0.222
6	0.661	-1.864	-0.418	6	0.537	-1.795	-0.207

6	1.554	-0.633	-0.739	6	1.460	-0.617	-0.623
6	0.338	0.201	-0.322	6	0.282	0.288	-0.233
6	-1.652	-1.212	0.407	6	-1.734	-1.044	0.618
6	-0.692	-3.365	1.275	6	-0.826	-3.174	1.590
6	-1.813	-2.375	1.085	6	-1.926	-2.173	1.344
6	-2.713	-0.172	0.266	6	-2.776	-0.005	0.392
6	-3.091	-2.806	1.643	6	-3.229	-2.565	1.873
6	3.974	-0.679	-0.592	6	3.889	-0.663	-0.548
6	5.179	-0.439	0.286	6	5.116	-0.413	0.300
6	-4.286	-2.810	1.026	6	-4.394	-2.587	1.199
6	-3.704	1.287	-1.291	6	-3.677	1.410	-1.273
6	-3.692	4.052	1.153	6	-3.383	4.333	0.926
6	-4.579	-2.439	-0.348	6	-4.607	-2.276	-0.205
6	6.328	0.239	-0.310	6	6.246	0.268	-0.328
6	-4.305	2.946	0.315	6	-4.115	3.255	0.148
6	-4.718	4.490	2.194	6	-4.411	5.234	1.604
6	-2.430	3.516	1.843	6	-2.531	3.612	1.983
6	-3.327	5.231	0.241	6	-2.472	5.150	0.006
6	-5.620	-1.650	-0.793	6	-5.598	-1.482	-0.744
6	6.411	0.644	-1.617	6	6.301	0.656	-1.641
6	-6.619	-0.975	0.079	6	-6.639	-0.762	0.039
6	8.323	1.155	-0.213	6	8.236	1.199	-0.283
6	-4.697	-2.078	-2.746	6	-4.560	-2.000	-2.616
6	4.420	-1.862	3.350	6	4.450	-1.829	3.388
1	0.499	-2.585	-1.224	1	0.320	-2.539	-0.978
1	1.780	-0.573	-1.806	1	1.645	-0.627	-1.699
1	-0.814	-4.204	0.577	1	-0.985	-4.054	0.953
1	-0.768	-3.798	2.277	1	-0.898	-3.534	2.621
1	2.724	-0.314	0.990	1	2.686	-0.280	1.062
1	-3.050	-3.189	2.661	1	-3.238	-2.901	2.908
1	-5.151	-3.101	1.620	1	-5.291	-2.842	1.761
1	-4.693	0.936	-0.995	1	-4.680	1.154	-0.928
1	-3.631	1.452	-2.365	1	-3.629	1.466	-2.361
1	-4.297	5.286	2.813	1	-3.901	5.990	2.206
1	-5.628	4.867	1.724	1	-5.037	5.750	0.871
1	-5.002	3.662	2.846	1	-5.072	4.661	2.257
1	-2.003	4.301	2.474	1	-2.006	4.355	2.591
1	-1.668	3.212	1.122	1	-1.785	2.965	1.516
1	-2.659	2.657	2.479	1	-3.150	3.003	2.646
1	-2.946	6.053	0.853	1	-1.985	5.939	0.587
1	-4.202	5.602	-0.302	1	-3.036	5.631	-0.798
1	-2.553	4.971	-0.483	1	-1.695	4.530	-0.442
1	5.706	0.484	-2.415	1	5.581	0.476	-2.422
1	-6.431	0.103	0.133	1	-6.442	0.315	0.069
1	-7.627	-1.111	-0.316	1	-7.623	-0.898	-0.415
1	-6.581	-1.355	1.101	1	-6.674	-1.106	1.073
1	-4.542	-2.078	-3.819	1	-4.332	-2.041	-3.675
1	5.219	-2.608	3.360	1	5.250	-2.573	3.377
1	4.697	-1.021	3.990	1	4.744	-0.985	4.017
1	3.488	-2.308	3.698	1	3.530	-2.276	3.764
1	9.706	1.241	1.219	1	9.645	1.314	1.121
1	10.283	1.687	-0.299	1	10.192	1.737	-0.413
8	-0.873	3.495	-1.804	8	-0.854	-0.775	-2.972
1	-1.696	3.202	-1.396	1	-1.510	-0.392	-2.374
1	-0.214	2.999	1.307	1	-0.865	-0.204	-3.743
cefditoren pivoxil motif 5, Eint = -9.8 kcal/mol				cefditoren pivoxil motif 6, Eint = -9.2 kcal/mol			
16	1.088	-2.479	1.353	16	0.895	-2.228	1.591
16	-3.535	-3.127	-1.549	16	-3.915	-3.080	-1.128
16	8.122	1.184	-2.003	16	7.931	0.717	-2.019
8	0.222	1.365	-0.478	8	-0.117	1.470	-0.471
8	-2.544	0.234	-1.308	8	-2.892	0.215	-1.114
8	-3.356	0.386	0.792	8	-3.559	0.575	1.021
8	4.267	-1.231	-1.632	8	3.983	-1.417	-1.219
8	-3.168	2.452	-1.163	8	-3.345	2.464	-1.178
8	4.184	-1.017	2.160	8	3.763	-0.227	2.386
8	-5.203	2.625	-0.189	8	-5.310	2.970	-0.170
7	-0.330	-0.941	-0.356	7	-0.605	-0.832	-0.161
7	2.876	-0.353	-0.068	7	2.571	-0.126	0.002
7	5.352	-0.486	1.614	7	4.973	0.096	1.779
7	7.508	0.689	0.467	7	7.252	0.778	0.483
7	-5.519	-1.640	-2.239	7	-5.897	-1.564	-1.760
7	9.582	1.780	0.229	7	9.403	1.650	0.086
6	0.795	-1.864	-0.334	6	0.544	-1.729	-0.123
6	1.698	-0.685	-0.795	6	1.396	-0.562	-0.688
6	0.464	0.194	-0.551	6	0.146	0.300	-0.468
6	-1.541	-1.112	0.309	6	-1.794	-0.990	0.544
6	-0.619	-3.107	1.515	6	-0.787	-2.903	1.815
6	-1.730	-2.156	1.155	6	-1.932	-1.994	1.445
6	-2.582	-0.093	0.001	6	-2.852	0.014	0.226
6	-3.023	-2.482	1.749	6	-3.193	-2.302	2.110
6	4.110	-0.697	-0.547	6	3.798	-0.614	-0.309
6	5.279	-0.319	0.332	6	4.955	-0.072	0.495
6	-4.213	-2.554	1.124	6	-4.415	-2.387	1.554

6	-3.502	1.207	-1.722	6	-3.822	1.197	-1.555
6	-3.424	4.142	0.488	6	-3.371	4.384	0.222
6	-4.483	-2.382	-0.293	6	-4.765	-2.260	0.149
6	6.457	0.258	-0.314	6	6.182	0.269	-0.221
6	-4.067	3.014	-0.295	6	-4.154	3.227	-0.373
6	-4.512	4.922	1.218	6	-4.356	5.430	0.737
6	-2.471	3.494	1.507	6	-2.558	3.804	1.391
6	-2.631	5.060	-0.447	6	-2.416	4.999	-0.804
6	-5.496	-1.640	-0.865	6	-5.788	-1.509	-0.392
6	6.609	0.434	-1.664	6	6.364	0.156	-1.575
6	-6.487	-0.820	-0.117	6	-6.708	-0.630	0.382
6	8.446	1.191	-0.272	6	8.232	1.054	-0.316
6	-4.562	-2.373	-2.720	6	-4.990	-2.345	-2.266
6	4.392	-1.241	3.551	6	3.909	-0.099	3.797
1	0.678	-2.702	-1.028	1	0.447	-2.602	-0.771
1	1.964	-0.780	-1.851	1	1.630	-0.731	-1.742
1	-0.715	-4.034	0.934	1	-0.864	-3.851	1.269
1	-0.728	-3.399	2.564	1	-0.865	-3.159	2.876
1	2.797	-0.096	0.907	1	2.468	0.367	0.880
1	-3.001	-2.715	2.813	1	-3.116	-2.504	3.178
1	-5.088	-2.738	1.744	1	-5.255	-2.551	2.228
1	-4.509	0.908	-1.425	1	-4.813	1.018	-1.136
1	-3.395	1.259	-2.804	1	-3.821	1.117	-2.641
1	-4.059	5.735	1.791	1	-3.811	6.249	1.213
1	-5.232	5.359	0.521	1	-4.956	5.849	-0.075
1	-5.060	4.284	1.913	1	-5.044	5.002	1.468
1	-1.989	4.280	2.095	1	-2.008	4.611	1.884
1	-1.693	2.912	1.010	1	-1.838	3.062	1.041
1	-3.016	2.842	2.194	1	-3.209	3.330	2.131
1	-2.201	5.881	0.133	1	-1.895	5.848	-0.351
1	-3.269	5.499	-1.220	1	-2.952	5.370	-1.683
1	-1.815	4.527	-0.938	1	-1.668	4.278	-1.137
1	5.946	0.133	-2.458	1	5.691	-0.249	-2.312
1	-6.308	0.249	-0.274	1	-6.492	0.427	0.197
1	-7.501	-1.031	-0.465	1	-7.746	-0.806	0.089
1	-6.435	-0.994	0.958	1	-6.607	-0.792	1.456
1	-4.396	-2.535	-3.779	1	-4.891	-2.552	-3.325
1	5.184	-1.976	3.709	1	4.658	-0.800	4.171
1	4.650	-0.309	4.060	1	4.192	0.921	4.067
1	3.444	-1.625	3.926	1	2.930	-0.340	4.211
1	9.751	1.533	1.195	1	9.542	1.593	1.086
1	10.409	1.714	-0.344	1	10.230	1.415	-0.441
8	-5.461	1.437	2.537	8	2.053	-3.092	-2.446
1	-4.707	0.933	2.210	1	2.823	-2.621	-2.086
1	-5.735	1.916	1.746	1	2.424	-3.776	-3.006
cefditoren pivoxil motif 7, Eint = -7.1 kcal/mol				cefditoren pivoxil motif 8, Eint = -12.0 kcal/mol			
16	0.925	-2.754	1.152	16	0.663	-2.609	1.107
16	-3.855	-2.869	-1.660	16	-4.233	-2.905	-1.496
16	7.887	1.296	-1.898	16	7.614	1.166	-2.359
8	0.040	1.331	-0.247	8	-0.236	1.392	-0.351
8	-2.731	0.344	-0.990	8	-3.098	0.342	-1.086
8	-3.452	0.271	1.157	8	-3.703	0.422	1.095
8	4.037	-1.148	-1.731	8	3.680	-1.109	-1.977
8	-3.162	2.560	-0.567	8	-3.542	2.584	-0.837
8	4.037	-1.391	2.058	8	3.829	-1.191	1.854
8	-5.163	2.849	0.456	8	-5.483	2.949	0.272
7	-0.517	-0.972	-0.263	7	-0.830	-0.907	-0.365
7	2.685	-0.454	-0.044	7	2.396	-0.401	-0.245
7	5.195	-0.798	1.556	7	4.969	-0.650	1.263
7	7.331	0.505	0.508	7	7.089	0.492	0.083
7	-5.780	-1.197	-2.008	7	-6.194	-1.281	-1.874
7	9.403	1.613	0.353	7	9.203	1.486	-0.153
6	0.584	-1.910	-0.421	6	0.272	-1.848	-0.499
6	1.488	-0.696	-0.779	6	1.169	-0.652	-0.924
6	0.271	0.161	-0.408	6	-0.027	0.226	-0.529
6	-1.717	-1.213	0.401	6	-2.000	-1.111	0.361
6	-0.790	-3.373	1.282	6	-1.044	-3.218	1.331
6	-1.896	-2.365	1.092	6	-2.154	-2.219	1.127
6	-2.739	-0.131	0.275	6	-3.031	-0.042	0.212
6	-3.173	-2.755	1.677	6	-3.406	-2.565	1.791
6	3.906	-0.745	-0.587	6	3.594	-0.691	-0.835
6	5.095	-0.477	0.306	6	4.821	-0.404	-0.001
6	-4.388	-2.697	1.100	6	-4.645	-2.545	1.266
6	-3.626	1.422	-1.255	6	-4.031	1.379	-1.368
6	-3.235	4.128	1.209	6	-3.533	4.304	0.801
6	-4.708	-2.290	-0.258	6	-5.027	-2.233	-0.101
6	6.259	0.173	-0.293	6	5.981	0.177	-0.672
6	-3.999	3.130	0.354	6	-4.331	3.232	0.080
6	-4.235	4.986	1.977	6	-4.503	5.239	1.518
6	-2.376	3.312	2.188	6	-2.645	3.578	1.825
6	-2.327	5.006	0.343	6	-2.651	5.087	-0.174
6	-5.698	-1.416	-0.655	6	-6.047	-1.401	-0.514
6	6.379	0.513	-1.615	6	6.079	0.461	-2.008

6	-6.604	-0.672	0.262	6	-6.926	-0.609	0.390
6	8.253	1.092	-0.187	6	8.027	1.015	-0.654
6	-4.885	-1.889	-2.646	6	-5.321	-2.010	-2.501
6	4.274	-1.783	3.406	6	4.121	-1.507	3.210
1	0.409	-2.642	-1.214	1	0.088	-2.622	-1.250
1	1.730	-0.674	-1.844	1	1.370	-0.663	-1.997
1	-0.919	-4.209	0.583	1	-1.197	-4.090	0.682
1	-0.871	-3.805	2.283	1	-1.089	-3.596	2.356
1	2.630	-0.327	0.958	1	2.381	-0.235	0.753
1	-3.119	-3.159	2.687	1	-3.307	-2.898	2.823
1	-5.243	-2.961	1.719	1	-5.472	-2.764	1.939
1	-4.641	1.172	-0.942	1	-5.013	1.147	-0.952
1	-3.536	1.595	-2.325	1	-4.057	1.445	-2.455
1	-3.702	5.683	2.629	1	-3.944	5.992	2.080
1	-4.866	5.569	1.301	1	-5.155	5.759	0.811
1	-4.894	4.372	2.593	1	-5.141	4.692	2.214
1	-1.827	3.993	2.844	1	-2.077	4.316	2.397
1	-1.653	2.690	1.656	1	-1.938	2.908	1.331
1	-2.994	2.661	2.811	1	-3.245	2.990	2.524
1	-1.817	5.739	0.975	1	-2.118	5.872	0.370
1	-2.898	5.557	-0.411	1	-3.244	5.570	-0.956
1	-1.568	4.413	-0.170	1	-1.912	4.443	-0.653
1	5.695	0.312	-2.424	1	5.364	0.261	-2.789
1	-6.341	0.391	0.297	1	-6.707	0.462	0.314
1	-7.639	-0.741	-0.080	1	-7.976	-0.745	0.122
1	-6.538	-1.049	1.284	1	-6.784	-0.889	1.434
1	-4.769	-1.885	-3.723	1	-5.257	-2.085	-3.580
1	5.067	-2.533	3.456	1	4.924	-2.246	3.270
1	4.547	-0.921	4.020	1	4.404	-0.610	3.767
1	3.334	-2.210	3.753	1	3.198	-1.923	3.614
1	9.596	1.248	1.276	1	9.389	1.167	0.799
1	10.216	1.617	-0.245	1	9.998	1.494	-0.771
8	-1.096	2.206	-2.838	8	8.647	0.195	2.396
1	-0.857	2.116	-1.906	1	8.358	0.546	3.241
1	-0.827	3.100	-3.058	1	7.837	0.140	1.853
cefditoren pivoxil motif 9, Eint = -9.8 kcal/mol				Amlodipine motif 1, Eint = -6.4 kcal/mol			
16	1.235	-2.735	1.019	17	2.289	-2.303	-1.858
16	-3.868	-2.875	-1.606	8	-2.822	0.245	1.415
16	8.062	1.558	-1.991	8	-2.343	0.218	-1.378
8	0.239	1.336	-0.126	8	3.683	0.480	-0.985
8	-2.547	0.284	-1.019	8	-0.976	-1.576	-1.247
8	-3.195	0.184	1.149	8	4.084	2.420	0.093
8	4.263	-0.968	-1.848	7	0.042	2.189	1.396
8	-3.127	2.473	-0.613	7	-6.086	-1.334	1.077
8	4.342	-1.360	1.926	6	1.133	0.171	-0.264
8	-5.127	2.676	0.429	6	-0.356	0.429	-0.127
7	-0.276	-0.970	-0.358	6	1.916	1.391	0.201
7	2.932	-0.369	-0.110	6	-0.834	1.342	0.749
7	5.479	-0.725	1.427	6	1.372	2.311	1.045
7	7.571	0.657	0.391	6	1.554	-1.084	0.489
7	-5.808	-1.195	-1.685	6	-2.274	1.510	1.137
7	9.619	1.810	0.241	6	-1.229	-0.440	-0.927
6	0.863	-1.861	-0.532	6	2.069	3.479	1.658
6	1.727	-0.604	-0.833	6	3.315	1.525	-0.203
6	0.494	0.198	-0.400	6	2.080	-2.223	-0.125
6	-1.452	-1.259	0.329	6	1.412	-1.119	1.878
6	-0.458	-3.411	1.140	6	2.454	-3.344	0.611
6	-1.592	-2.426	1.007	6	1.776	-2.227	2.630
6	-2.496	-0.197	0.247	6	2.301	-3.345	1.991
6	-2.826	-2.845	1.663	6	-4.226	0.202	1.268
6	4.147	-0.613	-0.687	6	-3.269	-0.572	-2.151
6	5.349	-0.357	0.193	6	-4.670	-1.237	1.413
6	-4.089	-2.785	1.203	6	5.040	0.492	-1.421
6	-3.530	1.285	-1.248	6	-4.287	0.369	-2.737
6	-3.267	4.073	1.134	1	1.355	-0.004	-1.320
6	-4.551	-2.337	-0.100	1	-0.343	2.870	2.033
6	6.488	0.339	-0.401	1	-2.340	2.167	2.023
6	-3.977	3.020	0.303	1	-2.829	2.011	0.331
6	-4.309	4.908	1.870	1	2.978	3.175	2.177
6	-2.386	3.315	2.142	1	2.389	4.193	0.897
6	-2.384	4.961	0.253	1	1.411	3.994	2.363
6	-5.578	-1.454	-0.355	1	0.997	-0.245	2.374
6	6.574	0.736	-1.710	1	2.856	-4.207	0.094
6	-6.364	-0.722	0.675	1	1.649	-2.219	3.707
6	8.467	1.290	-0.297	1	2.592	-4.221	2.561
6	-4.993	-1.869	-2.443	1	-4.501	0.587	0.271
6	4.611	-1.799	3.253	1	-4.730	0.841	2.009
1	0.729	-2.577	-1.348	1	-3.720	-1.319	-1.488
1	1.948	-0.523	-1.900	1	-2.712	-1.119	-2.917
1	-0.568	-4.220	0.406	1	-4.534	-1.558	2.450
1	-0.514	-3.888	2.122	1	-4.001	-1.867	0.803
1	2.892	-0.272	0.896	1	5.245	1.377	-2.029
1	-2.686	-3.281	2.651	1	5.721	0.493	-0.568

1	-4.878	-3.082	1.892	1	5.167	-0.414	-2.010
1	-4.501	0.963	-0.874	1	-4.811	0.930	-1.958
1	-3.551	1.435	-2.326	1	-3.818	1.092	-3.408
1	-3.810	5.645	2.504	1	-5.030	-0.190	-3.310
1	-4.957	5.445	1.173	1	-6.213	-1.216	0.075
1	-4.946	4.286	2.500	1	-6.435	-2.261	1.294
1	-1.878	4.037	2.788	8	-1.844	3.104	-1.805
1	-1.627	2.715	1.635	1	-0.890	3.210	-1.849
1	-2.983	2.652	2.773	1	-1.963	2.145	-1.766
1	-1.911	5.728	0.873				
1	-2.968	5.472	-0.518				
1	-1.598	4.385	-0.237				
1	5.878	0.556	-2.512				
1	-6.270	-1.186	1.658				
1	-6.006	0.309	0.775				
1	-7.420	-0.680	0.398				
1	-5.001	-1.829	-3.525				
1	5.421	-2.533	3.260				
1	4.876	-0.956	3.896				
1	3.686	-2.260	3.598				
1	9.837	1.412	1.144				
1	10.419	1.854	-0.373				
8	-6.706	1.690	-1.995				
1	-6.596	0.729	-1.958				
1	-6.432	1.998	-1.122				
Amlodipine				Amlodipine			
motif 2, Eint = -6.7 kcal/mol				motif 3, Eint = -8.2 kcal/mol			
17	2.666	-2.602	0.079	17	2.666	-2.601	0.078
8	-3.196	1.268	0.342	8	-3.196	1.268	0.342
8	-2.304	-1.083	-1.167	8	-2.305	-1.083	-1.166
8	3.752	0.334	-0.547	8	3.752	0.334	-0.546
8	-0.281	-2.041	-1.331	8	-0.281	-2.041	-1.329
8	3.905	2.582	-0.444	8	3.905	2.582	-0.445
7	-0.346	2.564	-0.317	7	-0.346	2.564	-0.318
7	-6.661	0.467	1.163	7	-6.660	0.467	1.165
6	1.092	0.149	-0.305	6	1.092	0.149	-0.305
6	-0.376	0.230	-0.688	6	-0.376	0.230	-0.688
6	1.760	1.508	-0.370	6	1.760	1.508	-0.371
6	-1.043	1.410	-0.621	6	-1.043	1.410	-0.621
6	1.034	2.654	-0.312	6	1.034	2.655	-0.313
6	1.240	-0.469	1.080	6	1.240	-0.469	1.080
6	-2.509	1.640	-0.831	6	-2.510	1.640	-0.830
6	-0.956	-1.054	-1.091	6	-0.956	-1.054	-1.090
6	1.565	4.049	-0.269	6	1.565	4.049	-0.270
6	3.217	1.580	-0.454	6	3.217	1.580	-0.454
6	1.916	-1.662	1.350	6	1.917	-1.662	1.349
6	0.662	0.188	2.172	6	0.662	0.188	2.172
6	2.022	-2.169	2.643	6	2.023	-2.169	2.643
6	0.753	-0.301	3.466	6	0.754	-0.301	3.466
6	1.441	-1.487	3.702	6	1.442	-1.487	3.702
6	-4.593	1.200	0.142	6	-4.592	1.200	0.142
6	-2.861	-2.351	-1.569	6	-2.862	-2.351	-1.569
6	-5.224	0.599	1.377	6	-5.223	0.599	1.378
6	5.174	0.289	-0.621	6	5.175	0.289	-0.620
6	-4.359	-2.217	-1.541	6	-4.359	-2.216	-1.542
1	1.585	-0.511	-1.017	1	1.585	-0.511	-1.017
1	-0.866	3.428	-0.317	1	-0.866	3.428	-0.317
1	-2.687	2.707	-1.056	1	-2.688	2.707	-1.056
1	-2.872	1.064	-1.690	1	-2.873	1.064	-1.689
1	2.259	4.185	0.560	1	2.260	4.185	0.558
1	2.132	4.281	-1.171	1	2.131	4.282	-1.173
1	0.749	4.770	-0.172	1	0.749	4.771	-0.172
1	0.119	1.112	1.985	1	0.120	1.112	1.985
1	2.557	-3.097	2.806	1	2.558	-3.097	2.805
1	0.291	0.238	4.286	1	0.292	0.238	4.286
1	1.525	-1.887	4.708	1	1.527	-1.887	4.707
1	-4.809	0.572	-0.740	1	-4.809	0.572	-0.739
1	-5.016	2.197	-0.061	1	-5.016	2.197	-0.060
1	-2.499	-3.125	-0.886	1	-2.500	-3.124	-0.884
1	-2.484	-2.603	-2.565	1	-2.483	-2.604	-2.564
1	-5.058	1.269	2.226	1	-5.057	1.268	2.227
1	-4.699	-0.341	1.612	1	-4.698	-0.342	1.612
1	5.534	0.810	-1.511	1	5.534	0.809	-1.511
1	5.623	0.755	0.259	1	5.623	0.756	0.260
1	5.434	-0.767	-0.665	1	5.434	-0.767	-0.663
1	-4.711	-1.969	-0.536	1	-4.713	-1.967	-0.538
1	-4.703	-1.441	-2.229	1	-4.702	-1.440	-2.231
1	-4.824	-3.159	-1.839	1	-4.824	-3.158	-1.840
1	-6.846	-0.280	0.500	1	-6.846	-0.280	0.501
1	-7.118	0.193	2.025	1	-7.118	0.193	2.027
8	2.031	-1.633	-3.134	8	2.027	-1.634	-3.135
1	1.333	-1.962	-2.550	1	2.785	-1.559	-2.548
1	2.787	-1.558	-2.546	1	1.331	-1.963	-2.549
Amlodipine				Amlodipine			

motif 4, Eint = -10.7 kcal/mol				motif 5, Eint = -8.6 kcal/mol			
17	3.218	-2.502	-0.608	17	2.719	-2.497	-0.569
8	-3.143	0.936	0.206	8	-3.027	1.552	0.368
8	-2.003	-1.559	-1.156	8	-2.251	-0.843	-1.202
8	3.915	0.565	-0.623	8	3.867	0.471	-0.561
8	0.100	-2.285	-1.499	8	-0.246	-1.780	-1.600
8	3.793	2.804	-0.384	8	4.045	2.703	-0.297
7	-0.423	2.297	-0.463	7	-0.204	2.752	-0.327
7	-6.515	-0.158	1.095	7	-6.460	0.817	1.368
6	1.299	0.042	-0.590	6	1.204	0.307	-0.539
6	-0.192	-0.025	-0.888	6	-0.278	0.448	-0.855
6	1.792	1.478	-0.498	6	1.885	1.659	-0.422
6	-0.978	1.077	-0.785	6	-0.922	1.631	-0.692
6	0.931	2.523	-0.363	6	1.174	2.808	-0.271
6	1.595	-0.714	0.702	6	1.361	-0.501	0.746
6	-2.456	1.157	-1.026	6	-2.391	1.889	-0.843
6	-0.655	-1.376	-1.224	6	-0.906	-0.812	-1.260
6	1.294	3.955	-0.141	6	1.727	4.179	-0.062
6	3.231	1.730	-0.490	6	3.346	1.714	-0.415
6	2.421	-1.838	0.795	6	2.002	-1.740	0.835
6	0.998	-0.265	1.884	6	0.809	0.012	1.925
6	2.643	-2.479	2.012	6	2.095	-2.430	2.040
6	1.208	-0.891	3.105	6	0.891	-0.661	3.135
6	2.038	-2.005	3.167	6	1.540	-1.890	3.192
6	-4.520	0.658	0.000	6	-4.433	1.501	0.236
6	-2.439	-2.903	-1.429	6	-2.850	-2.120	-1.528
6	-5.120	0.206	1.312	6	-5.013	0.939	1.514
6	5.334	0.686	-0.612	6	5.289	0.400	-0.554
6	-3.931	-2.942	-1.241	6	-4.339	-1.963	-1.403
1	1.830	-0.477	-1.394	1	1.674	-0.266	-1.341
1	-1.061	3.059	-0.247	1	-0.711	3.620	-0.240
1	-2.713	2.155	-1.414	1	-2.555	2.957	-1.079
1	-2.772	0.414	-1.760	1	-2.805	1.307	-1.673
1	1.968	4.067	0.708	1	2.387	4.214	0.805
1	1.831	4.362	-1.000	1	2.338	4.491	-0.910
1	0.396	4.555	0.027	1	0.920	4.903	0.076
1	0.348	0.606	1.828	1	0.293	0.968	1.874
1	3.291	-3.348	2.039	1	2.603	-3.388	2.064
1	0.728	-0.512	4.001	1	0.449	-0.232	4.027
1	2.216	-2.509	4.111	1	1.614	-2.433	4.128
1	-4.617	-0.137	-0.756	1	-4.699	0.855	-0.619
1	-5.047	1.544	-0.387	1	-4.851	2.499	0.028
1	-1.917	-3.585	-0.750	1	-2.454	-2.875	-0.843
1	-2.140	-3.178	-2.445	1	-2.543	-2.405	-2.539
1	-5.086	1.033	2.030	1	-4.803	1.629	2.337
1	-4.486	-0.595	1.725	1	-4.488	0.000	1.750
1	5.678	1.310	-1.440	1	5.711	0.974	-1.382
1	5.678	1.131	0.324	1	5.692	0.794	0.381
1	5.716	-0.328	-0.715	1	5.531	-0.656	-0.659
1	-4.205	-2.648	-0.224	1	-4.618	-1.677	-0.385
1	-4.439	-2.273	-1.942	1	-4.722	-1.206	-2.092
1	-4.306	-3.953	-1.413	1	-4.833	-2.909	-1.633
1	-6.567	-1.025	0.567	1	-6.681	0.053	0.736
1	-6.970	-0.345	1.981	1	-6.880	0.570	2.257
8	-2.738	3.654	0.696	8	-0.444	-4.393	-0.492
1	-2.854	4.135	1.518	1	0.406	-4.636	-0.121
1	-2.992	2.736	0.890	1	-0.257	-3.569	-0.965
Amlodipine				Amlodipine			
motif 6, Eint = -8.2 kcal/mol				motif 7, Eint = -7.1 kcal/mol			
17	3.427	-2.385	-0.459	17	2.102	-3.017	-0.736
8	-2.893	0.675	0.261	8	-3.221	1.415	0.532
8	-1.777	-1.414	-1.444	8	-2.696	-0.666	-1.445
8	4.107	0.680	-0.597	8	3.532	-0.219	-0.635
8	0.334	-2.191	-1.443	8	-0.858	-1.957	-1.564
8	3.968	2.921	-0.399	8	3.964	1.952	-0.206
7	-0.242	2.371	-0.375	7	-0.236	2.469	-0.048
7	-6.256	-0.455	1.136	7	-6.743	0.980	1.385
6	1.486	0.141	-0.534	6	0.863	-0.093	-0.496
6	0.004	0.070	-0.868	6	-0.594	0.246	-0.773
6	1.977	1.578	-0.468	6	1.705	1.160	-0.317
6	-0.797	1.156	-0.728	6	-1.090	1.477	-0.493
6	1.115	2.620	-0.335	6	1.138	2.366	-0.045
6	1.756	-0.587	0.779	6	0.960	-0.994	0.731
6	-2.287	1.219	-0.890	6	-2.519	1.926	-0.577
6	-0.437	-1.269	-1.274	6	-1.367	-0.890	-1.292
6	1.471	4.060	-0.161	6	1.849	3.646	0.251
6	3.416	1.840	-0.480	6	3.159	1.045	-0.372
6	2.593	-1.700	0.912	6	1.491	-2.288	0.726
6	1.125	-0.125	1.938	6	0.483	-0.507	1.953
6	2.795	-2.314	2.146	6	1.551	-3.054	1.888
6	1.315	-0.725	3.174	6	0.534	-1.257	3.119
6	2.157	-1.826	3.277	6	1.074	-2.539	3.085
6	-4.285	0.515	0.089	6	-4.616	1.599	0.407
6	-2.193	-2.737	-1.824	6	-3.438	-1.793	-1.947

6	-4.826	-0.182	1.318	6	-5.298	0.836	1.521
6	5.525	0.811	-0.600	6	4.939	-0.464	-0.700
6	-3.697	-2.753	-1.841	6	-4.894	-1.413	-1.954
1	2.036	-0.392	-1.315	1	1.244	-0.666	-1.345
1	-0.865	3.160	-0.296	1	-0.637	3.376	0.136
1	-2.599	2.270	-1.022	1	-2.556	3.031	-0.577
1	-2.604	0.672	-1.786	1	-2.978	1.588	-1.513
1	2.141	4.205	0.686	1	2.536	3.534	1.090
1	2.008	4.442	-1.031	1	2.461	3.962	-0.595
1	0.571	4.664	-0.012	1	1.134	4.439	0.482
1	0.461	0.732	1.852	1	0.054	0.492	1.975
1	3.451	-3.175	2.205	1	1.970	-4.052	1.839
1	0.807	-0.337	4.051	1	0.154	-0.846	4.048
1	2.319	-2.310	4.235	1	1.124	-3.141	3.985
1	-4.477	-0.096	-0.811	1	-4.952	1.223	-0.575
1	-4.785	1.484	-0.059	1	-4.883	2.667	0.452
1	-1.777	-3.456	-1.112	1	-3.236	-2.659	-1.310
1	-1.764	-2.977	-2.803	1	-3.069	-2.043	-2.947
1	-4.712	0.475	2.185	1	-4.994	1.260	2.483
1	-4.221	-1.080	1.510	1	-4.929	-0.202	1.506
1	5.858	1.419	-1.444	1	5.401	0.120	-1.498
1	5.873	1.279	0.323	1	5.422	-0.205	0.244
1	5.912	-0.203	-0.683	1	5.038	-1.529	-0.899
1	-4.102	-2.536	-0.849	1	-5.249	-1.202	-0.942
1	-4.095	-2.016	-2.543	1	-5.072	-0.530	-2.572
1	-4.059	-3.737	-2.146	1	-5.493	-2.232	-2.357
1	-6.383	-1.131	0.387	1	-7.073	0.443	0.588
1	-6.628	-0.896	1.970	1	-7.210	0.589	2.195
8	-6.942	2.328	0.816	8	6.826	2.053	-0.270
1	-7.869	2.567	0.770	1	7.103	2.952	-0.086
1	-6.935	1.354	0.895	1	5.857	2.088	-0.231
Balsalazide				Balsalazide			
motif 1, Eint = -9.4 kcal/mol				motif 2, Eint = -7.5 kcal/mol			
8	-4.637	-1.862	-0.656	8	4.842	1.517	-0.938
8	7.825	-0.710	0.780	8	-7.640	0.735	0.866
8	-6.860	2.407	2.030	8	6.986	-2.062	2.252
8	-5.253	2.800	0.513	8	5.439	-2.834	0.820
8	6.096	2.652	-1.025	8	-6.045	-2.678	-0.967
8	8.022	1.727	-0.335	8	-7.930	-1.696	-0.243
7	-4.528	0.395	-0.909	7	4.628	-0.729	-1.021
7	1.631	-1.234	0.224	7	-1.452	1.098	0.153
7	2.372	-0.271	-0.125	7	-2.224	0.150	-0.172
6	-5.959	0.585	-1.061	6	6.058	-0.931	-1.146
6	-2.498	-0.853	-0.474	6	2.650	0.616	-0.625
6	-6.663	0.859	0.258	6	6.772	-0.922	0.197
6	-3.975	-0.823	-0.681	6	4.117	0.525	-0.866
6	-1.947	-2.005	0.091	6	2.140	1.793	-0.070
6	-1.646	0.203	-0.833	6	1.768	-0.428	-0.948
6	0.260	-1.036	-0.041	6	-0.093	0.865	-0.140
6	-0.583	-2.094	0.313	6	0.781	1.910	0.177
6	-0.283	0.118	-0.623	6	0.412	-0.311	-0.714
6	3.737	-0.460	0.139	6	-3.577	0.376	0.124
6	5.962	0.526	-0.039	6	-5.831	-0.552	0.003
6	4.581	0.580	-0.241	6	-4.458	-0.643	-0.232
6	6.500	-0.626	0.571	6	-6.323	0.616	0.623
6	4.288	-1.601	0.746	6	-4.083	1.532	0.740
6	-6.167	2.113	0.911	6	6.310	-2.038	1.087
6	5.646	-1.674	0.954	6	-5.433	1.641	0.982
6	6.825	1.651	-0.457	6	-6.734	-1.654	-0.390
1	-6.112	1.419	-1.751	1	6.221	-1.882	-1.657
1	-6.377	-0.312	-1.518	1	6.453	-0.132	-1.775
1	-6.537	0.020	0.949	1	6.607	0.030	0.713
1	-7.745	0.931	0.113	1	7.856	-1.002	0.072
1	-3.996	1.227	-0.694	1	4.094	-1.522	-0.696
1	-2.615	-2.819	0.349	1	2.811	2.612	0.167
1	-2.047	1.092	-1.312	1	2.143	-1.331	-1.420
1	-0.140	-2.978	0.758	1	0.369	2.812	0.617
1	0.382	0.925	-0.906	1	-0.276	-1.107	-0.970
1	4.145	1.454	-0.708	1	-4.056	-1.530	-0.706
1	3.630	-2.410	1.041	1	-3.396	2.323	1.016
1	6.083	-2.553	1.423	1	-5.834	2.532	1.459
1	8.016	-1.555	1.201	1	-7.798	1.586	1.289
1	-6.471	3.216	2.393	1	6.626	-2.794	2.772
1	6.736	3.336	-1.263	1	-6.710	-3.344	-1.188
8	-7.395	-2.116	-0.189	8	4.570	4.103	0.153
1	-6.440	-2.173	-0.369	1	4.842	4.794	-0.453
1	-7.694	-3.027	-0.172	1	4.760	3.276	-0.320
Balsalazide				Balsalazide			
motif 3, Eint = -7.6 kcal/mol				motif 4, Eint = -10.9 kcal/mol			
8	-5.512	-1.989	-0.774	8	-4.718	-2.267	-0.141
8	6.925	-0.658	0.770	8	7.771	-0.625	0.410
8	-7.818	1.602	2.224	8	-7.220	1.286	2.202
8	-6.350	2.410	0.729	8	-6.085	2.275	0.550
8	5.186	2.720	-0.911	8	5.727	2.971	-0.259

8	7.123	1.737	-0.372	8	7.747	2.036	0.039
7	-5.429	0.263	-1.032	7	-4.689	-0.143	-0.913
7	0.752	-1.276	0.143	7	1.594	-1.439	0.038
7	1.480	-0.294	-0.179	7	2.249	-0.362	-0.064
6	-6.870	0.375	-1.137	6	-6.128	-0.106	-1.058
6	-3.377	-0.958	-0.577	6	-2.586	-1.220	-0.339
6	-7.563	0.388	0.216	6	-6.852	-0.010	0.275
6	-4.855	-0.956	-0.793	6	-4.076	-1.266	-0.450
6	-2.810	-2.107	-0.022	6	-1.928	-2.428	-0.100
6	-2.543	0.117	-0.918	6	-1.835	-0.039	-0.444
6	-0.620	-1.097	-0.128	6	0.199	-1.287	-0.096
6	-1.447	-2.175	0.207	6	-0.549	-2.464	0.015
6	-1.179	0.054	-0.700	6	-0.457	-0.069	-0.323
6	2.846	-0.470	0.092	6	3.639	-0.514	0.068
6	5.057	0.548	-0.039	6	5.785	0.648	0.075
6	3.677	0.592	-0.252	6	4.393	0.651	-0.036
6	5.605	-0.613	0.548	6	6.431	-0.586	0.299
6	3.410	-1.620	0.671	6	4.298	-1.735	0.292
6	-7.160	1.570	1.046	6	-6.655	1.295	0.981
6	4.766	-1.684	0.893	6	5.669	-1.760	0.404
6	5.914	1.680	-0.434	6	6.550	1.907	-0.041
1	-7.099	1.288	-1.691	1	-6.375	0.749	-1.693
1	-7.227	-0.477	-1.719	1	-6.460	-1.015	-1.567
1	-7.330	-0.528	0.771	1	-6.535	-0.824	0.934
1	-8.652	0.394	0.107	1	-7.931	-0.150	0.145
1	-4.940	1.102	-0.755	1	-4.165	0.674	-1.204
1	-3.467	-2.936	0.220	1	-2.528	-3.327	-0.008
1	-2.958	1.004	-1.388	1	-2.322	0.918	-0.606
1	-0.990	-3.057	0.643	1	-0.020	-3.395	0.195
1	-0.527	0.876	-0.969	1	0.132	0.837	-0.398
1	3.232	1.472	-0.700	1	3.875	1.587	-0.208
1	2.758	-2.445	0.935	1	3.709	-2.641	0.373
1	5.210	-2.568	1.344	1	6.187	-2.701	0.577
1	7.181	-1.510	1.139	1	8.038	-1.539	0.559
1	-7.500	2.381	2.701	1	-7.061	2.157	2.593
1	5.826	3.403	-1.151	1	6.310	3.739	-0.320
8	9.557	0.123	0.309	8	-3.931	2.618	-1.232
1	10.176	0.788	0.002	1	-3.937	3.372	-1.824
1	8.689	0.522	0.156	1	-4.698	2.729	-0.649
Balsalazide				Balsalazide			
motif 5, Eint = -11.5 kcal/mol				motif 6, Eint = -3.9 kcal/mol			
8	-4.523	-2.660	-0.398	8	-5.185	-1.872	-1.086
8	7.757	-0.175	1.011	8	7.253	-1.036	0.806
8	-7.138	1.522	1.437	8	-7.498	1.208	2.460
8	-5.636	1.937	-0.185	8	-5.986	2.224	1.147
8	5.870	2.512	-1.590	8	5.567	2.593	-0.300
8	7.829	1.926	-0.662	8	7.351	1.680	0.719
7	-4.558	-0.552	-1.237	7	-5.069	0.388	-0.934
7	1.649	-1.319	0.441	7	1.063	-1.441	0.065
7	2.331	-0.411	-0.115	7	1.804	-0.419	-0.014
6	-5.998	-0.557	-1.399	6	-6.506	0.543	-1.044
6	-2.460	-1.475	-0.432	6	-3.042	-0.927	-0.669
6	-6.739	-0.200	-0.120	6	-7.224	0.343	0.281
6	-3.927	-1.627	-0.674	6	-4.516	-0.862	-0.908
6	-1.852	-2.393	0.427	6	-2.502	-2.170	-0.332
6	-1.674	-0.481	-1.034	6	-2.188	0.180	-0.782
6	0.282	-1.310	0.100	6	-0.299	-1.193	-0.196
6	-0.496	-2.308	0.696	6	-1.145	-2.302	-0.093
6	-0.319	-0.395	-0.776	6	-0.831	0.056	-0.550
6	3.694	-0.419	0.222	6	3.164	-0.665	0.228
6	5.847	0.674	-0.131	6	5.375	0.354	0.379
6	4.477	0.566	-0.375	6	3.996	0.451	0.188
6	6.440	-0.252	0.753	6	5.926	-0.918	0.634
6	4.300	-1.334	1.098	6	3.728	-1.927	0.478
6	-6.438	1.191	0.357	6	-6.818	1.361	1.305
6	5.649	-1.245	1.354	6	5.086	-2.042	0.679
6	6.645	1.732	-0.786	6	6.226	1.559	0.311
1	-6.251	0.147	-2.195	1	-6.709	1.540	-1.441
1	-6.290	-1.557	-1.721	1	-6.864	-0.192	-1.766
1	-6.484	-0.904	0.678	1	-7.019	-0.657	0.679
1	-7.823	-0.290	-0.251	1	-8.311	0.390	0.157
1	-4.124	0.358	-1.182	1	-4.572	1.159	-0.513
1	-2.470	-3.167	0.869	1	-3.174	-3.019	-0.267
1	-2.120	0.215	-1.738	1	-2.581	1.146	-1.084
1	-0.009	-3.009	1.366	1	-0.709	-3.259	0.176
1	0.298	0.363	-1.245	1	-0.164	0.905	-0.643
1	3.999	1.265	-1.050	1	3.541	1.420	0.018
1	3.690	-2.101	1.561	1	3.080	-2.796	0.506
1	6.127	-1.949	2.031	1	5.531	-3.016	0.868
1	7.990	-0.878	1.627	1	7.468	-1.966	0.937
1	-6.890	2.442	1.697	1	-7.176	1.889	3.067
1	6.470	3.166	-1.972	1	6.175	3.345	-0.281
8	-6.108	4.033	1.548	8	3.393	2.488	-2.435
1	-5.605	3.662	0.804	1	3.005	1.615	-2.342

1	-5.461	4.432	2.135	1	4.145	2.476	-1.832
Balsalazide				Balsalazide			
motif 7, Eint = -11.7 kcal/mol				motif 8, Eint = -6.9 kcal/mol			
8	-5.517	-1.775	-0.995	8	5.049	1.684	-1.227
8	6.952	-1.413	0.851	8	-7.401	0.383	0.532
8	-7.632	1.679	2.310	8	7.416	-1.271	2.391
8	-6.091	2.518	0.907	8	5.926	-2.342	1.097
8	5.438	2.229	-0.552	8	-5.424	-3.167	-0.488
8	7.286	1.135	0.120	8	-7.417	-2.250	-0.006
7	-5.286	0.481	-1.029	7	4.981	-0.574	-1.027
7	0.762	-1.562	0.074	7	-1.196	1.124	-0.069
7	1.554	-0.598	-0.128	7	-1.928	0.114	-0.280
6	-6.714	0.697	-1.140	6	6.421	-0.699	-1.129
6	-3.324	-0.909	-0.671	6	2.925	0.703	-0.793
6	-7.426	0.635	0.203	6	7.129	-0.455	0.195
6	-4.794	-0.790	-0.905	6	4.400	0.665	-1.028
6	-2.841	-2.144	-0.232	6	2.355	1.939	-0.485
6	-2.418	0.140	-0.885	6	2.097	-0.426	-0.880
6	-0.590	-1.270	-0.199	6	0.176	0.916	-0.329
6	-1.489	-2.322	0.008	6	0.996	2.048	-0.246
6	-1.066	-0.032	-0.654	6	0.737	-0.327	-0.655
6	2.901	-0.884	0.144	6	-3.297	0.285	-0.049
6	5.171	0.014	0.158	6	-5.448	-0.872	0.003
6	3.801	0.156	-0.071	6	-4.068	-0.869	-0.191
6	5.639	-1.234	0.621	6	-6.072	0.347	0.343
6	3.383	-2.120	0.606	6	-3.935	1.494	0.285
6	-6.960	1.709	1.140	6	6.741	-1.460	1.238
6	4.730	-2.282	0.837	6	-5.298	1.511	0.474
6	6.085	1.153	-0.081	6	-6.227	-2.120	-0.150
1	-6.874	1.670	-1.611	1	6.648	-1.700	-1.504
1	-7.116	-0.073	-1.799	1	6.765	0.029	-1.865
1	-7.263	-0.339	0.675	1	6.899	0.548	0.570
1	-8.511	0.724	0.084	1	8.217	-0.479	0.076
1	-4.748	1.255	-0.669	1	4.500	-1.344	-0.585
1	-3.553	-2.950	-0.089	1	3.006	2.806	-0.442
1	-2.767	1.095	-1.265	1	2.512	-1.391	-1.155
1	-1.097	-3.273	0.356	1	0.545	3.006	-0.003
1	-0.358	0.770	-0.824	1	0.089	-1.192	-0.728
1	3.420	1.106	-0.426	1	-3.566	-1.791	-0.458
1	2.682	-2.929	0.772	1	-3.365	2.410	0.394
1	5.113	-3.236	1.194	1	-5.799	2.443	0.726
1	7.087	-2.316	1.159	1	-7.656	1.286	0.751
1	-7.270	2.390	2.858	1	7.107	-1.947	3.010
1	6.105	2.942	-0.682	1	-6.012	-3.929	-0.567
8	7.704	3.747	-0.610	8	-1.633	3.717	1.288
1	8.255	3.999	-1.354	1	-1.454	2.838	0.908
1	8.031	2.878	-0.318	1	-1.361	3.644	2.205
Balsalazide				Acyclovir			
motif 9, Eint = -6.3 kcal/mol				motif 1, Eint = -10.8 kcal/mol			
8	-5.103	-2.189	-0.364	8	-2.024	0.683	-0.113
8	7.395	-0.847	0.565	8	3.997	-1.832	-0.860
8	-7.261	1.901	2.030	8	-4.606	-0.043	-1.084
8	-5.837	2.413	0.370	7	-0.131	-0.405	0.618
8	5.530	2.751	-0.474	7	0.985	-2.223	-0.082
8	7.506	1.745	-0.117	7	1.579	1.293	0.426
7	-5.007	-0.022	-1.026	7	3.607	0.362	-0.332
7	1.199	-1.444	0.148	7	3.467	2.626	0.229
7	1.904	-0.416	-0.065	6	1.137	0.019	0.314
6	-6.449	0.096	-1.099	6	-1.228	0.416	1.023
6	-2.951	-1.177	-0.441	6	1.812	-1.121	-0.108
6	-7.090	0.354	0.256	6	-0.158	-1.764	0.346
6	-4.436	-1.188	-0.596	6	3.190	-1.011	-0.478
6	-2.373	-2.221	0.285	6	-3.208	1.377	0.213
6	-2.120	-0.202	-1.011	6	2.841	1.408	0.094
6	-0.178	-1.282	-0.082	6	-4.134	1.298	-0.969
6	-1.001	-2.278	0.458	1	-0.820	1.343	1.449
6	-0.748	-0.247	-0.838	1	-1.826	-0.117	1.773
6	3.285	-0.597	0.115	1	-1.075	-2.319	0.487
6	5.477	0.469	0.055	1	-2.999	2.431	0.455
6	4.090	0.524	-0.088	1	-3.690	0.919	1.092
6	6.063	-0.763	0.416	1	4.592	0.507	-0.517
6	3.883	-1.817	0.471	1	-4.976	1.988	-0.824
6	-6.646	1.655	0.854	1	-3.593	1.600	-1.874
6	5.248	-1.889	0.619	1	2.810	3.383	0.348
6	6.303	1.675	-0.175	1	4.191	2.837	-0.443
1	-6.688	0.904	-1.794	1	-4.833	-0.218	-2.000
1	-6.837	-0.837	-1.511	8	-3.370	-1.804	0.836
1	-6.848	-0.455	0.952	1	-3.745	-1.317	0.085
1	-8.183	0.360	0.184	1	-4.080	-2.379	1.126
1	-4.494	0.843	-0.931				
1	-3.027	-2.982	0.696				
1	-2.542	0.584	-1.629				
1	-0.536	-3.083	1.017				
1	-0.114	0.499	-1.303				

1	3.621	1.463	-0.367				
1	3.255	-2.687	0.624				
1	5.721	-2.829	0.895				
1	7.621	-1.751	0.811				
1	-6.919	2.746	2.353				
1	6.142	3.485	-0.616				
8	1.351	2.458	-0.505				
1	0.935	2.868	0.256				
1	1.420	1.517	-0.272				
Acyclovir				Acyclovir			
motif 2, Eint = -12.9 kcal/mol				motif 3, Eint = -12.7 kcal/mol			
8	2.098	0.872	-0.087	8	2.821	0.143	0.025
8	-3.562	-2.107	0.384	8	-3.474	-1.603	0.525
8	4.318	-0.876	0.487	8	5.428	-0.505	1.104
7	0.239	0.026	-1.123	7	0.833	-0.674	-0.804
7	-0.690	-2.004	-0.859	7	-0.546	-2.354	-0.232
7	-1.486	1.445	-0.201	7	-0.630	1.230	-0.543
7	-3.345	0.172	0.497	7	-2.789	0.550	0.138
7	-3.360	2.501	0.653	7	-2.320	2.790	-0.285
6	-0.991	0.238	-0.545	6	-0.370	-0.092	-0.496
6	1.298	0.986	-1.240	6	2.043	0.013	-1.136
6	-1.550	-1.027	-0.404	6	-1.209	-1.148	-0.155
6	0.359	-1.348	-1.267	6	0.658	-2.035	-0.610
6	-2.861	-1.144	0.164	6	-2.560	-0.855	0.200
6	3.459	1.271	-0.240	6	4.016	0.858	-0.220
6	-2.687	1.354	0.318	6	-1.875	1.496	-0.218
6	4.287	0.501	0.765	6	4.883	0.798	1.006
1	0.849	1.982	-1.331	1	1.770	0.996	-1.548
1	1.892	0.765	-2.137	1	2.588	-0.558	-1.904
1	1.263	-1.781	-1.676	1	1.478	-2.722	-0.769
1	3.558	2.357	-0.092	1	3.788	1.907	-0.469
1	3.796	1.028	-1.258	1	4.558	0.422	-1.074
1	-4.290	0.174	0.860	1	-3.746	0.824	0.376
1	5.315	0.877	0.722	1	5.675	1.557	0.913
1	3.911	0.703	1.778	1	4.275	1.051	1.885
1	-2.762	3.314	0.689	1	-1.579	3.474	-0.315
1	-4.014	2.447	1.420	1	-3.105	3.046	0.294
1	3.522	-1.271	0.880	1	5.811	-0.610	1.977
8	1.761	-1.384	1.658	8	-5.495	0.222	0.849
1	1.539	-0.573	1.178	1	-6.067	0.193	1.618
1	1.114	-2.029	1.357	1	-5.037	-0.643	0.826
Acyclovir				Acyclovir			
motif 4, Eint = -10.8 kcal/mol				motif 5, Eint = -9.2 kcal/mol			
8	2.023	0.684	0.113	8	-2.646	0.077	0.006
8	-3.995	-1.833	0.861	8	3.845	-0.697	-0.610
8	4.605	-0.045	1.085	8	-5.100	-1.228	-0.773
7	0.131	-0.404	-0.619	7	-0.521	-0.287	0.805
7	-0.984	-2.222	0.082	7	1.070	-1.793	0.330
7	-1.580	1.293	-0.427	7	0.635	1.776	0.300
7	-3.607	0.361	0.332	7	2.850	1.351	-0.396
7	-3.469	2.625	-0.229	7	2.064	3.537	-0.171
6	-1.137	0.020	-0.315	6	0.573	0.430	0.392
6	1.228	0.418	-1.023	6	-1.815	0.244	1.121
6	-1.811	-1.121	0.108	6	1.548	-0.519	0.112
6	0.159	-1.763	-0.346	6	-0.158	-1.618	0.731
6	-3.190	-1.012	0.478	6	2.837	-0.080	-0.322
6	3.208	1.377	-0.212	6	-3.952	0.574	0.239
6	-2.841	1.407	-0.094	6	1.813	2.191	-0.098
6	4.134	1.297	0.971	6	-4.842	0.158	-0.898
1	0.820	1.344	-1.449	1	-1.686	1.305	1.381
1	1.826	-0.115	-1.773	1	-2.224	-0.290	1.993
1	1.076	-2.318	-0.488	1	-0.860	-2.399	0.986
1	3.000	2.432	-0.454	1	-3.933	1.672	0.323
1	3.690	0.919	-1.091	1	-4.351	0.172	1.184
1	-4.592	0.505	0.518	1	3.752	1.736	-0.646
1	4.976	1.987	0.826	1	-5.771	0.746	-0.848
1	3.593	1.599	1.875	1	-4.343	0.395	-1.847
1	-2.812	3.383	-0.348	1	1.224	4.097	-0.135
1	-4.193	2.835	0.443	1	2.726	3.847	-0.866
1	4.834	-0.219	2.000	1	-5.498	-1.539	-1.589
8	3.370	-1.803	-0.838	8	3.389	-3.647	-0.270
1	4.080	-2.380	-1.127	1	2.509	-3.329	-0.027
1	3.745	-1.316	-0.086	1	3.838	-2.816	-0.466
Acyclovir				Acyclovir			
motif 6, Eint = -7.6 kcal/mol				motif 7, Eint = -10.9 kcal/mol			
8	-2.452	-0.299	-0.046	8	2.096	-0.643	-0.071
8	3.938	0.727	0.890	8	-4.254	-0.768	0.932
8	-5.028	0.581	0.935	8	4.516	-0.650	1.514
7	-0.354	0.341	-0.743	7	0.014	-1.391	-0.697
7	1.167	1.831	-0.049	7	-1.802	-2.500	0.023
7	0.851	-1.729	-0.415	7	-0.704	0.896	-0.424
7	3.022	-1.320	0.414	7	-2.896	1.005	0.423
7	2.318	-3.490	-0.081	7	-1.698	2.955	-0.069
6	0.750	-0.383	-0.365	6	-0.906	-0.438	-0.348

6	-1.614	-0.196	-1.164	6	1.347	-1.127	-1.149
6	1.681	0.558	0.054	6	-2.021	-1.142	0.088
6	-0.041	1.666	-0.515	6	-0.588	-2.611	-0.435
6	2.968	0.116	0.495	6	-3.172	-0.408	0.524
6	-3.703	-0.874	-0.377	6	3.350	-0.127	-0.480
6	2.027	-2.150	-0.017	6	-1.746	1.593	-0.014
6	-4.619	-0.767	0.810	6	4.063	0.431	0.719
1	-1.426	-1.180	-1.619	1	1.313	-0.379	-1.959
1	-2.053	0.470	-1.922	1	1.766	-2.059	-1.557
1	-0.749	2.458	-0.717	1	-0.058	-3.536	-0.616
1	-3.572	-1.930	-0.661	1	3.203	0.671	-1.225
1	-4.152	-0.348	-1.234	1	3.960	-0.916	-0.946
1	3.925	-1.706	0.658	1	-3.680	1.587	0.692
1	-5.479	-1.435	0.650	1	4.904	1.048	0.367
1	-4.084	-1.115	1.705	1	3.373	1.084	1.268
1	1.497	-4.063	-0.210	1	-0.756	3.328	-0.172
1	2.956	-3.855	0.610	1	-2.290	3.464	0.568
1	-5.432	0.699	1.797	1	4.778	-0.307	2.370
8	1.224	4.713	-0.129	8	1.236	2.942	-0.507
1	1.457	3.779	0.005	1	1.552	3.127	-1.393
1	1.925	5.196	0.312	1	0.825	2.057	-0.564
Cefprozil				Cefprozil			
motif 1, Eint = -7.4 kcal/mol				motif 2, Eint = -11.2 kcal/mol			
16	0.493	0.589	-1.471	16	0.197	-0.524	-1.862
8	0.891	-1.608	2.246	8	0.884	-1.584	2.499
8	-2.854	-2.650	-0.538	8	-2.772	-3.078	-0.631
8	4.326	0.000	1.971	8	2.952	0.870	1.895
8	4.055	-2.179	1.468	8	4.139	-1.049	1.903
8	-2.310	4.812	0.555	8	-2.514	4.377	0.182
7	1.749	-1.250	0.061	7	1.603	-1.538	0.242
7	-1.496	-1.009	0.217	7	-1.576	-1.519	0.495
7	-4.934	-0.820	-0.771	7	-4.848	-1.422	-1.032
6	0.758	-1.150	-0.999	6	0.620	-1.916	-0.773
6	-0.286	-1.728	-0.008	6	-0.363	-2.262	0.386
6	0.816	-1.568	1.052	6	0.744	-1.769	1.323
6	2.953	-0.550	0.124	6	2.616	-0.599	0.097
6	2.260	0.865	-1.831	6	1.955	-0.205	-2.271
6	3.249	0.407	-0.789	6	2.842	0.035	-1.078
6	-2.721	-1.522	-0.083	6	-2.719	-1.992	-0.077
6	3.838	-1.016	1.232	6	3.346	-0.317	1.376
6	-3.918	-0.618	0.249	6	-3.961	-1.102	0.076
6	4.568	1.015	-0.902	6	3.932	0.984	-1.263
6	-3.547	0.842	0.358	6	-3.637	0.371	0.122
6	5.732	0.361	-0.805	6	5.171	0.873	-0.763
6	-3.288	1.428	1.596	6	-3.637	1.074	1.324
6	-3.388	1.622	-0.793	6	-3.271	1.049	-1.046
6	7.073	0.993	-0.893	6	6.246	1.883	-0.945
6	-2.872	2.752	1.692	6	-3.275	2.416	1.372
6	-2.979	2.942	-0.712	6	-2.903	2.383	-1.012
6	-2.714	3.511	0.534	6	-2.897	3.069	0.203
1	1.002	-1.752	-1.879	1	0.954	-2.762	-1.379
1	-0.546	-2.766	-0.228	1	-0.587	-3.331	0.435
1	-1.439	-0.052	0.543	1	-1.509	-0.560	0.829
1	2.365	1.946	-1.964	1	1.952	0.683	-2.908
1	2.498	0.418	-2.804	1	2.324	-1.028	-2.893
1	-4.222	-0.960	1.260	1	-4.369	-1.385	1.066
1	4.585	2.082	-1.131	1	3.705	1.843	-1.898
1	5.710	-0.718	-0.647	1	5.429	-0.018	-0.192
1	-5.764	-0.297	-0.513	1	-5.802	-1.169	-0.801
1	-5.211	-1.800	-0.811	1	-4.815	-2.425	-1.192
1	4.863	-0.408	2.666	1	3.412	0.973	2.741
1	-3.408	0.840	2.503	1	-3.918	0.564	2.243
1	-3.593	1.170	-1.759	1	-3.290	0.508	-1.988
1	7.004	2.065	-1.089	1	5.913	2.727	-1.553
1	7.682	0.538	-1.681	1	7.129	1.444	-1.421
1	7.632	0.857	0.039	1	6.587	2.276	0.019
1	-2.675	3.196	2.664	1	-3.272	2.950	2.318
1	-2.852	3.548	-1.603	1	-2.615	2.912	-1.914
1	-2.154	5.077	1.466	1	-2.513	4.713	1.083
8	-5.345	-3.891	-0.852	8	-0.154	1.061	1.068
1	-4.399	-3.680	-0.784	1	0.048	1.089	0.122
1	-5.492	-4.574	-0.196	1	0.709	1.109	1.497
Cefprozil				Cefprozil			
motif 3, Eint = -11.2 kcal/mol				motif 4, Eint = -12.2 kcal/mol			
16	0.265	-0.233	-1.754	16	-0.250	0.940	-1.353
8	0.878	-1.302	2.501	8	0.912	-2.207	1.415
8	-2.522	-3.188	-0.713	8	-2.912	-2.927	-1.470
8	3.609	0.931	1.874	8	3.963	0.063	1.544
8	4.139	-1.261	1.898	8	3.976	-1.869	0.381
8	-3.167	4.246	0.274	8	-3.617	3.907	1.541
7	1.688	-1.325	0.276	7	1.454	-1.001	-0.558
7	-1.536	-1.506	0.442	7	-1.745	-1.464	-0.182
7	-4.740	-1.744	-1.197	7	-5.266	-1.741	-0.925
6	0.733	-1.686	-0.763	6	0.356	-0.772	-1.484

6	-0.250	-2.116	0.367	6	-0.465	-1.825	-0.692
6	0.799	-1.550	1.330	6	0.702	-1.799	0.308
6	2.741	-0.424	0.150	6	2.520	-0.134	-0.318
6	2.004	0.151	-2.171	6	1.399	1.652	-1.680
6	2.951	0.254	-1.004	6	2.552	1.097	-0.884
6	-2.605	-2.103	-0.158	6	-2.897	-2.037	-0.638
6	3.584	-0.325	1.382	6	3.571	-0.734	0.557
6	-3.943	-1.360	-0.041	6	-4.188	-1.528	0.025
6	4.126	1.087	-1.227	6	3.726	1.959	-0.841
6	-3.793	0.138	0.058	6	-4.100	-0.085	0.466
6	5.375	0.795	-0.841	6	4.992	1.549	-0.993
6	-3.954	0.802	1.271	6	-3.766	0.245	1.778
6	-3.437	0.887	-1.068	6	-4.276	0.951	-0.456
6	6.553	1.674	-1.050	6	6.186	2.426	-0.907
6	-3.761	2.175	1.370	6	-3.596	1.571	2.166
6	-3.234	2.254	-0.983	6	-4.115	2.275	-0.084
6	-3.389	2.901	0.243	6	-3.767	2.589	1.231
1	1.096	-2.480	-1.422	1	0.609	-1.009	-2.521
1	-0.364	-3.203	0.401	1	-0.570	-2.768	-1.234
1	-1.583	-0.546	0.781	1	-1.813	-0.672	0.444
1	1.974	1.110	-2.696	1	1.302	2.720	-1.463
1	2.362	-0.583	-2.903	1	1.608	1.582	-2.754
1	-4.358	-1.717	0.922	1	-4.272	-2.150	0.938
1	3.958	2.003	-1.796	1	3.533	3.026	-0.718
1	5.558	-0.155	-0.338	1	5.176	0.491	-1.184
1	-5.724	-1.586	-1.010	1	-6.154	-1.809	-0.440
1	-4.604	-2.736	-1.367	1	-5.101	-2.620	-1.407
1	4.157	0.901	2.672	1	4.629	-0.434	2.079
1	-4.231	0.237	2.158	1	-3.633	-0.546	2.513
1	-3.330	0.376	-2.021	1	-4.550	0.696	-1.475
1	6.290	2.587	-1.589	1	5.912	3.472	-0.754
1	7.343	1.161	-1.609	1	6.802	2.360	-1.810
1	7.001	1.966	-0.094	1	6.832	2.123	-0.076
1	-3.883	2.680	2.325	1	-3.338	1.814	3.193
1	-2.952	2.838	-1.853	1	-4.249	3.081	-0.797
1	-3.260	4.554	1.180	1	-3.371	3.984	2.467
8	-0.522	1.164	1.204	8	5.657	-1.808	2.562
1	0.202	1.056	1.830	1	5.489	-2.329	3.351
1	-0.095	1.218	0.338	1	5.228	-2.291	1.834
Cefprozil				Cefprozil			
motif 5, Eint = -8.6 kcal/mol				motif 6, Eint = -7.2 kcal/mol			
16	-0.019	0.697	-1.281	16	-0.026	0.531	-1.102
8	0.794	-1.709	2.278	8	0.881	-2.706	1.675
8	-2.629	-3.170	-0.847	8	-2.995	-2.978	-1.318
8	3.955	0.511	2.173	8	4.033	-0.614	1.923
8	4.045	-1.589	1.379	8	4.035	-2.512	0.712
8	-3.744	4.142	0.497	8	-2.269	3.905	1.109
7	1.556	-0.935	0.170	7	1.539	-1.515	-0.270
7	-1.650	-1.423	0.225	7	-1.672	-1.741	0.057
7	-5.022	-1.938	-0.946	7	-5.166	-1.470	-0.863
6	0.604	-0.979	-0.924	6	0.480	-1.213	-1.223
6	-0.311	-1.847	-0.017	6	-0.427	-2.215	-0.452
6	0.713	-1.552	1.092	6	0.722	-2.275	0.568
6	2.609	-0.036	0.300	6	2.644	-0.710	0.010
6	1.656	1.373	-1.546	6	1.663	1.165	-1.349
6	2.715	1.028	-0.532	6	2.757	0.528	-0.532
6	-2.728	-2.115	-0.248	6	-2.873	-2.107	-0.477
6	3.611	-0.457	1.314	6	3.646	-1.384	0.886
6	-4.099	-1.504	0.090	6	-4.093	-1.363	0.109
6	3.916	1.850	-0.608	6	3.975	1.323	-0.441
6	-4.068	0.000	0.224	6	-3.756	0.075	0.430
6	5.167	1.370	-0.627	6	5.221	0.851	-0.576
6	-3.956	0.607	1.473	6	-3.397	0.460	1.721
6	-4.076	0.815	-0.913	6	-3.666	1.019	-0.597
6	6.395	2.202	-0.690	6	6.456	1.666	-0.456
6	-3.844	1.989	1.595	6	-2.915	1.739	1.981
6	-3.970	2.192	-0.807	6	-3.193	2.296	-0.353
6	-3.849	2.784	0.451	6	-2.796	2.647	0.935
1	1.016	-1.446	-1.821	1	0.743	-1.470	-2.253
1	-0.336	-2.892	-0.333	1	-0.605	-3.143	-1.000
1	-1.802	-0.506	0.625	1	-1.648	-0.925	0.655
1	1.533	2.460	-1.577	1	1.588	2.227	-1.100
1	2.002	1.079	-2.545	1	1.911	1.113	-2.417
1	-4.329	-1.922	1.090	1	-4.301	-1.884	1.062
1	3.762	2.925	-0.717	1	3.833	2.396	-0.302
1	5.306	0.289	-0.604	1	5.354	-0.211	-0.787
1	-5.974	-1.919	-0.599	1	-6.068	-1.413	-0.404
1	-4.795	-2.897	-1.196	1	-5.098	-2.375	-1.320
1	4.596	0.121	2.785	1	4.661	-1.148	2.431
1	-3.954	-0.009	2.370	1	-3.471	-0.258	2.535
1	-4.176	0.346	-1.887	1	-3.960	0.723	-1.599
1	6.163	3.267	-0.750	1	6.230	2.721	-0.285
1	7.016	1.935	-1.551	1	7.079	1.589	-1.353
1	7.022	2.045	0.195	1	7.077	1.316	0.376

1	-3.761	2.448	2.576	1	-2.620	2.022	2.988
1	-3.974	2.826	-1.686	1	-3.094	3.021	-1.154
1	-3.660	4.417	1.414	1	-2.068	4.035	2.041
8	3.546	-2.476	-1.366	8	0.066	3.967	-0.685
1	3.731	-2.425	-0.415	1	-0.045	4.718	-1.272
1	4.079	-3.212	-1.673	1	-0.693	4.019	-0.088
Cefprozil				Bumetanide			
motif 7, Eint = -9.1 kcal/mol				motif 1, Eint = -8.2 kcal/mol			
16	0.235	-0.072	-1.551	16	3.191	-1.085	-0.707
8	0.751	-0.566	2.721	8	0.242	-1.381	-0.630
8	-2.605	-2.962	-0.232	8	2.857	-1.531	-2.049
8	3.931	1.339	1.777	8	4.512	-0.589	-0.370
8	4.001	-0.870	2.211	8	1.046	4.655	1.000
8	-3.120	4.534	-0.141	8	3.211	4.071	0.827
7	1.663	-0.952	0.561	7	-1.641	0.582	-0.158
7	-1.577	-1.155	0.682	7	2.837	-2.312	0.388
7	-4.831	-1.568	-0.808	6	-2.653	1.620	-0.114
6	0.723	-1.432	-0.445	6	-4.028	1.024	-0.345
6	-0.268	-1.733	0.709	6	-0.309	0.897	-0.057
6	0.742	-1.006	1.605	6	0.654	-0.110	-0.286
6	2.751	-0.113	0.328	6	2.013	0.175	-0.245
6	1.963	0.274	-2.024	6	-5.137	2.064	-0.304
6	2.955	0.426	-0.899	6	0.165	2.168	0.294
6	-2.655	-1.812	0.190	6	1.534	2.431	0.376
6	3.633	0.048	1.521	6	2.472	1.441	0.087
6	-3.989	-1.054	0.259	6	-6.513	1.466	-0.539
6	4.179	1.128	-1.262	6	-0.434	-2.134	0.327
6	-3.824	0.445	0.170	6	2.044	3.769	0.747
6	5.418	0.753	-0.919	6	-0.316	-1.885	1.688
6	-3.793	1.233	1.319	6	-1.201	-3.188	-0.154
6	-3.621	1.064	-1.068	6	-0.991	-2.709	2.581
6	6.658	1.490	-1.271	6	-1.864	-4.006	0.753
6	-3.558	2.602	1.246	6	-1.766	-3.770	2.121
6	-3.390	2.426	-1.156	1	-2.618	2.108	0.869
6	-3.353	3.201	0.005	1	-2.453	2.411	-0.858
1	1.076	-2.295	-1.012	1	-4.038	0.510	-1.316
1	-0.340	-2.807	0.896	1	-4.212	0.246	0.407
1	-1.676	-0.171	0.899	1	-1.833	-0.139	-0.848
1	1.932	1.208	-2.594	1	-5.116	2.578	0.666
1	2.300	-0.497	-2.727	1	-4.936	2.840	-1.053
1	-4.366	-1.288	1.274	1	-0.537	2.969	0.489
1	4.058	2.000	-1.907	1	3.533	1.655	0.128
1	5.541	-0.160	-0.334	1	-6.753	0.713	0.217
1	-5.806	-1.377	-0.606	1	-7.298	2.226	-0.506
1	-4.711	-2.575	-0.861	1	-6.572	0.975	-1.515
1	4.484	1.332	2.571	1	3.695	-2.613	0.838
1	-3.953	0.771	2.291	1	2.383	-3.088	-0.084
1	-3.653	0.453	-1.965	1	0.301	-1.064	2.039
1	6.448	2.368	-1.886	1	-1.282	-3.345	-1.223
1	7.366	0.853	-1.811	1	-0.904	-2.520	3.646
1	7.181	1.829	-0.370	1	-2.468	-4.829	0.384
1	-3.540	3.205	2.150	1	-2.288	-4.408	2.825
1	-3.230	2.910	-2.113	1	1.482	5.487	1.229
1	-3.103	4.946	0.728	8	-1.543	-1.061	-2.778
8	-0.261	-4.274	-1.124	1	-1.488	-0.771	-3.691
1	-0.417	-5.138	-1.508	1	-0.639	-1.297	-2.535
1	-1.144	-3.941	-0.891				
Bumetanide				Bumetanide			
motif 2, Eint = -11.4 kcal/mol				motif 3, Eint = -5.6 kcal/mol			
16	-3.221	-0.369	0.436	16	3.541	0.012	-0.634
8	-0.375	-1.200	0.637	8	0.923	-1.408	-0.838
8	-3.153	-0.843	1.817	8	3.574	-0.474	-2.000
8	-4.380	0.363	-0.039	8	4.510	0.971	-0.135
8	0.079	4.948	-0.673	8	-0.797	4.488	0.702
8	-2.161	4.770	-0.716	8	1.428	4.763	0.666
7	1.873	0.389	0.321	7	-1.607	-0.351	-0.403
7	-2.958	-1.647	-0.601	7	3.566	-1.301	0.419
6	3.075	1.190	0.405	6	-2.943	0.215	-0.456
6	4.289	0.306	0.615	6	-3.985	-0.869	-0.639
6	0.627	0.945	0.185	6	-0.502	0.450	-0.278
6	-0.516	0.125	0.302	6	0.787	-0.097	-0.450
6	-1.790	0.664	0.168	6	1.920	0.699	-0.320
6	5.589	1.092	0.683	6	-5.399	-0.309	-0.671
6	0.428	2.301	-0.101	6	-0.594	1.809	0.051
6	-0.858	2.822	-0.257	6	0.553	2.592	0.196
6	-1.981	2.009	-0.116	6	1.822	2.044	0.005
6	6.802	0.206	0.904	6	-6.456	-1.383	-0.857
6	0.221	-2.056	-0.283	6	0.591	-2.416	0.053
6	-1.081	4.251	-0.567	6	0.484	4.025	0.536
6	0.373	-1.731	-1.625	6	0.361	-2.193	1.406
6	0.642	-3.283	0.216	6	0.536	-3.697	-0.486
6	0.975	-2.651	-2.475	6	0.059	-3.277	2.222
6	1.238	-4.192	-0.649	6	0.238	-4.770	0.345
6	1.413	-3.880	-1.994	6	-0.005	-4.566	1.701

1	3.189	1.759	-0.528	1	-3.132	0.763	0.474
1	3.004	1.937	1.214	1	-3.027	0.964	-1.260
1	4.160	-0.270	1.543	1	-3.787	-1.419	-1.570
1	4.338	-0.434	-0.194	1	-3.890	-1.604	0.171
1	1.903	-0.502	0.794	1	-1.466	-1.196	-0.940
1	5.712	1.667	-0.243	1	-5.587	0.246	0.257
1	5.521	1.837	1.486	1	-5.475	0.434	-1.475
1	1.280	2.963	-0.193	1	-1.574	2.247	0.185
1	-2.977	2.418	-0.230	1	2.711	2.653	0.114
1	6.911	-0.526	0.099	1	-6.424	-2.118	-0.048
1	7.726	0.786	0.948	1	-7.464	-0.962	-0.878
1	6.721	-0.353	1.841	1	-6.309	-1.927	-1.795
1	-3.773	-1.772	-1.191	1	4.403	-1.250	0.991
1	-2.721	-2.498	-0.081	1	3.535	-2.171	-0.103
1	0.018	-0.775	-1.996	1	0.426	-1.189	1.810
1	0.471	-3.514	1.261	1	0.730	-3.833	-1.545
1	1.096	-2.402	-3.525	1	-0.122	-3.109	3.278
1	1.566	-5.154	-0.265	1	0.195	-5.770	-0.072
1	1.880	-4.594	-2.664	1	-0.239	-5.405	2.346
1	-0.176	5.859	-0.872	1	-0.697	5.431	0.893
8	-2.266	-3.497	1.628	8	-3.539	3.351	0.708
1	-2.878	-4.114	2.036	1	-2.727	3.871	0.767
1	-2.477	-2.641	2.035	1	-4.062	3.636	1.461
Bumetanide				Bumetanide			
motif 4, Eint = -6.7 kcal/mol				motif 5, Eint = -9.8 kcal/mol			
16	2.792	-1.409	-0.943	16	2.973	-0.387	-0.951
8	-0.221	-1.458	-0.949	8	0.109	-1.220	-0.975
8	2.548	-1.919	-2.276	8	2.807	-0.775	-2.338
8	4.112	-0.956	-0.525	8	4.155	0.353	-0.514
8	1.176	4.529	0.542	8	-0.231	4.770	0.948
8	3.227	3.616	0.652	8	2.002	4.623	0.737
7	-1.922	0.640	-0.352	7	-2.092	0.287	-0.263
7	2.280	-2.550	0.174	7	2.831	-1.722	0.033
6	-2.871	1.732	-0.281	6	-3.298	1.083	-0.171
6	-4.291	1.214	-0.398	6	-4.527	0.212	-0.346
6	-0.567	0.848	-0.343	6	-0.842	0.852	-0.209
6	0.301	-0.236	-0.609	6	0.287	0.066	-0.523
6	1.678	-0.052	-0.612	6	1.566	0.607	-0.470
6	-5.332	2.319	-0.300	6	-5.827	0.995	-0.234
6	0.008	2.086	-0.028	6	-0.624	2.179	0.179
6	1.395	2.243	-0.006	6	0.668	2.704	0.246
6	2.235	1.184	-0.329	6	1.774	1.923	-0.085
6	-6.753	1.800	-0.424	6	-7.056	0.124	-0.417
6	-0.902	-2.191	0.013	6	-0.336	-2.189	-0.089
6	2.043	3.500	0.416	6	0.915	4.103	0.657
6	-0.837	-1.905	1.371	6	-0.341	-2.015	1.290
6	-1.643	-3.267	-0.464	6	-0.755	-3.383	-0.667
6	-1.539	-2.711	2.260	6	-0.785	-3.057	2.095
6	-2.335	-4.065	0.439	6	-1.192	-4.416	0.154
6	-2.290	-3.789	1.803	6	-1.213	-4.257	1.536
1	-2.744	2.249	0.680	1	-3.327	1.569	0.813
1	-2.674	2.484	-1.064	1	-3.299	1.897	-0.917
1	-4.406	0.686	-1.355	1	-4.483	-0.284	-1.326
1	-4.465	0.464	0.384	1	-4.507	-0.591	0.401
1	-2.231	-0.177	-0.861	1	-2.162	-0.541	-0.839
1	-5.210	2.845	0.655	1	-5.865	1.493	0.743
1	-5.139	3.068	-1.077	1	-5.829	1.803	-0.977
1	-0.625	2.932	0.208	1	-1.465	2.816	0.421
1	3.306	1.321	-0.346	1	2.774	2.336	-0.035
1	-6.982	1.075	0.362	1	-7.095	-0.670	0.335
1	-7.487	2.606	-0.350	1	-7.979	0.701	-0.332
1	-6.911	1.299	-1.383	1	-7.060	-0.359	-1.398
1	3.038	-2.780	0.808	1	3.686	-1.859	0.580
1	1.926	-3.375	-0.299	1	2.581	-2.539	-0.514
1	-0.236	-1.074	1.724	1	0.010	-1.084	1.720
1	-1.662	-3.464	-1.530	1	-0.728	-3.485	-1.746
1	-1.491	-2.493	3.322	1	-0.790	-2.927	3.173
1	-2.913	-4.906	0.071	1	-1.518	-5.349	-0.293
1	-2.832	-4.413	2.504	1	-1.555	-5.065	2.174
1	1.695	5.285	0.848	1	0.039	5.663	1.200
8	4.440	0.923	1.956	8	5.378	-1.294	1.378
1	4.537	0.354	1.183	1	6.273	-1.622	1.266
1	4.269	1.797	1.586	1	5.322	-0.510	0.811
Bumetanide				Didanosine			
motif 6, Eint = -12.0 kcal/mol				motif 1, Eint = -7.4 kcal/mol			
16	1.376	-3.043	-0.746	8	2.357	-0.302	0.532
8	-1.099	-1.367	-0.808	8	2.836	0.982	-1.903
8	0.890	-3.285	-2.090	8	-3.942	1.769	-0.652
8	2.697	-3.467	-0.318	7	0.058	0.057	0.895
8	3.388	2.837	0.558	7	-1.030	1.964	0.387
8	4.677	0.994	0.433	7	-1.699	-1.573	0.370
7	-1.304	1.349	-0.352	7	-3.649	-0.492	-0.389
7	0.277	-3.681	0.359	6	1.249	-0.732	1.287
6	-1.448	2.790	-0.398	6	1.142	-2.208	0.970

6	-2.906	3.174	-0.560	6	1.443	-2.225	-0.528
6	-0.072	0.745	-0.289	6	2.369	-1.020	-0.727
6	0.025	-0.650	-0.474	6	1.933	-0.106	-1.849
6	1.257	-1.290	-0.410	6	-1.200	-0.311	0.466
6	-3.120	4.680	-0.589	6	0.085	1.438	0.825
6	1.107	1.448	-0.012	6	-1.845	0.887	0.161
6	2.334	0.789	0.071	6	-3.199	0.870	-0.323
6	2.421	-0.586	-0.136	6	-2.926	-1.593	-0.061
6	-4.579	5.063	-0.762	1	1.471	-0.499	2.331
6	-2.089	-1.551	0.145	1	0.183	-2.651	1.223
6	3.582	1.528	0.367	1	1.932	-2.713	1.532
6	-1.909	-1.274	1.495	1	1.901	-3.158	-0.856
6	-3.289	-2.071	-0.331	1	0.515	-2.097	-1.096
6	-2.957	-1.516	2.375	1	3.414	-1.307	-0.885
6	-4.325	-2.311	0.564	1	0.902	0.233	-1.668
6	-4.166	-2.032	1.918	1	1.934	-0.682	-2.789
1	-1.055	3.214	0.536	1	0.984	1.984	1.091
1	-0.847	3.227	-1.212	1	2.485	1.637	-2.512
1	-3.296	2.731	-1.487	1	-3.433	-2.548	-0.176
1	-3.488	2.727	0.256	1	-4.601	-0.603	-0.716
1	-2.007	0.828	-0.859	8	3.189	2.342	1.162
1	-2.728	5.118	0.337	1	3.144	1.476	0.732
1	-2.522	5.116	-1.399	1	3.582	2.910	0.497
1	1.077	2.521	0.131				
1	3.376	-1.094	-0.078				
1	-5.193	4.668	0.052				
1	-4.715	6.146	-0.779				
1	-4.986	4.666	-1.697				
1	0.738	-4.400	0.906				
1	-0.530	-4.059	-0.129				
1	-0.959	-0.887	1.848				
1	-3.389	-2.282	-1.390				
1	-2.822	-1.302	3.430				
1	-5.261	-2.717	0.196				
1	-4.977	-2.218	2.613				
1	4.265	3.247	0.745				
8	6.039	3.327	0.916				
1	6.020	2.360	0.803				
1	6.544	3.490	1.715				
Didanosine				Didanosine			
motif 2, Eint = -9.1 kcal/mol				motif 3, Eint = -12.2 kcal/mol			
8	-2.623	-0.263	-0.980	8	2.893	0.253	-0.934
8	-3.960	2.100	-0.166	8	4.486	-1.838	0.148
8	4.045	0.859	0.208	8	-3.603	-1.662	0.154
7	-0.317	-0.402	-0.610	7	0.575	0.110	-0.647
7	1.070	1.364	-0.541	7	-0.577	-1.818	-0.485
7	1.239	-2.196	-0.072	7	-1.217	1.715	-0.275
7	3.403	-1.340	0.305	7	-3.269	0.612	0.109
6	-1.571	-1.166	-0.860	6	1.723	1.010	-0.930
6	-1.920	-2.075	0.305	6	1.902	2.058	0.154
6	-2.622	-1.106	1.245	6	2.679	1.274	1.203
6	-3.321	-0.142	0.289	6	3.537	0.330	0.364
6	-3.301	1.285	0.778	6	3.671	-1.040	0.981
6	0.921	-0.892	-0.284	6	-0.727	0.454	-0.387
6	-0.156	0.954	-0.768	6	0.589	-1.267	-0.712
6	1.759	0.220	-0.235	6	-1.415	-0.755	-0.280
6	3.145	0.049	0.096	6	-2.819	-0.733	0.005
6	2.498	-2.352	0.216	6	-2.497	1.718	-0.028
1	-1.447	-1.688	-1.814	1	1.575	1.426	-1.932
1	-1.053	-2.578	0.729	1	0.960	2.478	0.501
1	-2.614	-2.838	-0.061	1	2.510	2.868	-0.258
1	-3.319	-1.595	1.926	1	3.277	1.908	1.859
1	-1.889	-0.566	1.855	1	1.992	0.699	1.835
1	-4.358	-0.437	0.088	1	4.539	0.737	0.178
1	-2.257	1.600	0.935	1	2.669	-1.477	1.112
1	-3.800	1.311	1.761	1	4.110	-0.917	1.985
1	-0.988	1.575	-1.063	1	1.505	-1.791	-0.943
1	-3.932	3.009	0.144	1	4.544	-2.716	0.531
1	2.883	-3.350	0.404	1	-3.013	2.668	0.081
1	4.365	-1.557	0.538	1	-4.271	0.709	0.301
8	2.839	3.606	0.421	8	-5.877	-0.230	0.728
1	2.108	3.129	0.007	1	-6.708	-0.406	0.283
1	3.526	2.929	0.422	1	-5.316	-1.012	0.564
Didanosine				Didanosine			
motif 4, Eint = -7.8 kcal/mol				motif 5, Eint = -6.8 kcal/mol			
8	2.284	0.184	-0.839	8	1.848	0.285	-1.055
8	4.603	-1.485	-0.599	8	3.691	-1.682	-0.101
8	-4.064	-2.240	0.234	8	-4.512	-1.803	0.503
7	0.016	-0.171	-0.399	7	-0.434	0.067	-0.589
7	-0.998	-2.179	-0.332	7	-1.502	-1.892	-0.291
7	-1.886	1.292	-0.005	7	-2.258	1.625	-0.181
7	-3.857	0.045	0.301	7	-4.240	0.471	0.357
6	1.095	0.846	-0.526	6	0.657	1.003	-0.965
6	1.329	1.577	0.788	6	0.881	2.066	0.096

6	2.327	0.659	1.474	6	1.771	1.324	1.083
6	3.174	0.181	0.306	6	2.608	0.428	0.177
6	3.769	-1.189	0.501	6	2.885	-0.921	0.792
6	-1.308	0.067	-0.156	6	-1.732	0.374	-0.269
6	0.133	-1.537	-0.503	6	-0.370	-1.308	-0.603
6	-1.914	-1.188	-0.112	6	-2.367	-0.853	-0.079
6	-3.326	-1.285	0.143	6	-3.759	-0.880	0.280
6	-3.167	1.209	0.222	6	-3.520	1.602	0.134
1	0.811	1.514	-1.344	1	0.415	1.405	-1.954
1	0.408	1.751	1.344	1	-0.048	2.450	0.514
1	1.764	2.553	0.563	1	1.420	2.898	-0.366
1	2.919	1.157	2.243	1	2.387	1.985	1.693
1	1.817	-0.192	1.943	1	1.162	0.717	1.764
1	3.983	0.889	0.083	1	3.560	0.896	-0.098
1	2.955	-1.924	0.608	1	1.938	-1.436	1.001
1	4.332	-1.182	1.448	1	3.404	-0.760	1.749
1	1.088	-1.985	-0.734	1	0.549	-1.807	-0.870
1	4.942	-2.377	-0.493	1	3.770	-2.574	0.248
1	-3.743	2.120	0.361	1	-4.062	2.539	0.233
1	-4.852	0.075	0.483	1	-5.220	0.550	0.598
8	-0.353	3.717	-0.620	8	5.906	0.050	0.271
1	-0.802	4.247	-1.280	1	5.337	-0.658	-0.066
1	-0.971	2.990	-0.423	1	6.643	0.086	-0.341
Didanosine				Buspirone			
motif 6, Eint = -13.1 kcal/mol				motif 1, Eint = -8.3 kcal/mol			
8	-2.457	-0.727	-0.972	8	3.630	2.270	0.374
8	-3.014	1.806	0.176	8	3.370	-2.240	-0.168
8	3.776	1.656	0.264	7	3.514	0.005	0.180
7	-0.135	-0.534	-0.835	7	-2.732	0.577	-0.017
7	0.869	1.476	-0.810	7	-5.519	0.021	0.090
7	1.676	-1.923	0.034	7	-7.211	-1.493	0.557
7	3.573	-0.616	0.531	7	-7.665	0.570	-0.592
6	-1.285	-1.471	-1.019	6	6.299	-0.091	-0.388
6	-1.407	-2.492	0.098	6	6.719	-0.360	1.067
6	-2.155	-1.712	1.179	6	7.656	-0.105	-1.097
6	-2.869	-0.587	0.415	6	7.825	-1.418	0.967
6	-2.520	0.777	0.988	6	8.429	-1.259	-0.448
6	1.133	-0.736	-0.343	6	5.543	1.213	-0.570
6	-0.220	0.806	-1.111	6	5.392	-1.205	-0.908
6	1.731	0.523	-0.331	6	4.163	1.227	0.034
6	3.076	0.673	0.151	6	4.025	-1.227	-0.276
6	2.898	-1.793	0.461	6	2.169	-0.002	0.780
1	-1.199	-1.907	-2.018	6	1.074	0.222	-0.248
1	-0.451	-2.902	0.418	6	-0.305	0.180	0.392
1	-2.020	-3.311	-0.286	6	-1.391	0.579	-0.590
1	-2.846	-2.344	1.738	6	-3.219	-0.772	0.238
1	-1.453	-1.285	1.904	6	-3.670	1.259	-0.898
1	-3.957	-0.702	0.389	6	-4.583	-0.746	0.896
1	-1.430	0.855	1.118	6	-5.045	1.348	-0.270
1	-2.949	0.814	2.006	6	-6.842	-0.309	0.022
1	-1.145	1.233	-1.471	6	-8.492	-1.812	0.434
1	-2.398	2.553	0.252	6	-8.936	0.204	-0.689
1	3.442	-2.674	0.791	6	-9.428	-0.998	-0.193
1	4.524	-0.612	0.880	1	5.889	-0.668	1.710
8	-0.765	3.515	0.368	1	7.116	0.571	1.491
1	0.006	3.079	-0.039	1	8.160	0.850	-0.902
1	-0.612	4.456	0.269	1	7.565	-0.198	-2.184
				1	7.412	-2.422	1.099
				1	8.571	-1.294	1.754
				1	9.503	-1.064	-0.425
				1	8.302	-2.179	-1.026
				1	5.421	1.430	-1.641
				1	6.082	2.066	-0.149
				1	5.819	-2.200	-0.765
				1	5.246	-1.089	-1.991
				1	2.144	0.779	1.541
				1	2.050	-0.972	1.266
				1	1.154	-0.542	-1.032
				1	1.226	1.195	-0.730
				1	-0.486	-0.827	0.787
				1	-0.335	0.870	1.242
				1	-1.346	-0.070	-1.491
				1	-1.185	1.599	-0.935
				1	-2.520	-1.291	0.899
				1	-3.275	-1.355	-0.705
				1	-3.747	0.743	-1.877
				1	-3.294	2.269	-1.092
				1	-4.976	-1.753	1.021
				1	-4.498	-0.289	1.894
				1	-4.996	1.977	0.632
				1	-5.761	1.798	-0.955
				1	-8.786	-2.769	0.865
				1	-9.596	0.914	-1.186
				1	-10.470	-1.275	-0.280

				8	0.967	3.092	1.026
				1	1.899	2.921	0.823
				1	0.965	3.963	1.427
Buspirone				Buspirone			
motif 2, Eint = -8.2 kcal/mol				motif 3, Eint = -9.0 kcal/mol			
8	3.309	-2.573	-1.017	8	3.880	-2.515	-1.034
8	3.269	1.697	0.528	8	3.135	1.684	0.548
7	3.300	-0.423	-0.279	7	3.523	-0.384	-0.317
7	-2.955	-0.807	-0.010	7	-2.704	-1.012	-0.061
7	-5.724	-0.164	-0.119	7	-5.441	-0.243	-0.123
7	-7.369	1.379	-0.651	7	-7.023	1.383	-0.595
7	-7.876	-0.596	0.622	7	-7.612	-0.621	0.596
6	6.096	-0.546	0.195	6	6.289	-0.129	0.289
6	6.479	0.090	-1.152	6	6.667	0.482	-1.072
6	7.472	-0.728	0.841	6	7.643	-0.119	1.005
6	7.607	1.074	-0.816	6	7.656	1.605	-0.737
6	8.234	0.557	0.499	6	8.281	1.222	0.625
6	5.314	-1.842	0.063	6	5.677	-1.515	0.183
6	5.233	0.413	1.013	6	5.275	0.750	1.018
6	3.911	-1.679	-0.462	6	4.310	-1.546	-0.449
6	3.874	0.641	0.414	6	3.899	0.743	0.406
6	1.953	-0.238	-0.834	6	2.177	-0.404	-0.913
6	0.866	-0.628	0.154	6	1.117	-0.869	0.069
6	-0.525	-0.437	-0.431	6	-0.273	-0.827	-0.547
6	-1.614	-0.817	0.558	6	-1.354	-1.103	0.482
6	-3.401	0.541	-0.345	6	-3.090	0.371	-0.320
6	-3.906	-1.405	0.918	6	-3.673	-1.604	0.852
6	-4.776	0.519	-0.983	6	-4.463	0.442	-0.955
6	-5.291	-1.484	0.310	6	-5.064	-1.597	0.252
6	-7.035	0.215	-0.053	6	-6.735	0.184	-0.044
6	-8.637	1.750	-0.530	6	-8.276	1.798	-0.460
6	-9.133	-0.181	0.715	6	-8.851	-0.160	0.704
6	-9.590	1.007	0.156	6	-9.260	1.066	0.194
1	5.634	0.571	-1.659	1	5.803	0.829	-1.648
1	6.837	-0.702	-1.821	1	7.155	-0.292	-1.676
1	7.959	-1.598	0.383	1	8.245	-0.951	0.620
1	7.411	-0.928	1.916	1	7.552	-0.268	2.085
1	7.204	2.081	-0.677	1	7.140	2.567	-0.667
1	8.336	1.137	-1.627	1	8.407	1.725	-1.521
1	9.309	0.379	0.412	1	9.370	1.155	0.581
1	8.112	1.298	1.295	1	8.055	1.981	1.379
1	5.228	-2.329	1.045	1	5.576	-1.957	1.184
1	5.813	-2.564	-0.589	1	6.307	-2.202	-0.389
1	5.700	1.391	1.143	1	5.585	1.796	1.077
1	5.077	0.004	2.022	1	5.164	0.409	2.056
1	1.891	-0.853	-1.733	1	2.226	-1.068	-1.777
1	1.863	0.813	-1.112	1	1.958	0.607	-1.262
1	0.976	-0.027	1.065	1	1.140	-0.220	0.953
1	1.008	-1.676	0.445	1	1.359	-1.883	0.411
1	-0.638	0.608	-0.744	1	-0.423	0.164	-0.986
1	-0.641	-1.044	-1.337	1	-0.354	-1.555	-1.363
1	-1.553	-0.159	1.450	1	-1.225	-0.413	1.341
1	-1.424	-1.835	0.919	1	-1.227	-2.118	0.880
1	-2.697	0.991	-1.049	1	-2.361	0.833	-0.990
1	-3.423	1.184	0.559	1	-3.084	0.960	0.619
1	-3.955	-0.830	1.865	1	-3.690	-1.067	1.822
1	-3.562	-2.414	1.168	1	-3.375	-2.638	1.058
1	-5.137	1.529	-1.165	1	-4.782	1.474	-1.084
1	-4.719	-0.001	-1.952	1	-4.433	-0.030	-1.949
1	-5.274	-2.166	-0.555	1	-5.081	-2.243	-0.639
1	-6.013	-1.870	1.027	1	-5.799	-1.979	0.958
1	-8.903	2.690	-1.012	1	-8.504	2.767	-0.904
1	-9.810	-0.837	1.261	1	-9.555	-0.811	1.222
1	-10.621	1.326	0.240	1	-10.278	1.422	0.289
8	5.400	3.567	0.422	8	0.332	2.225	0.181
1	5.248	4.508	0.518	1	1.284	2.120	0.333
1	4.525	3.158	0.527	1	0.152	3.134	0.430
Buspirone				Buspirone			
motif 4, Eint = -6.7 kcal/mol				motif 5, Eint = -6.9 kcal/mol			
8	-3.978	-2.020	1.491	8	3.975	2.030	1.439
8	-3.651	1.718	-1.074	8	3.812	-1.823	-0.968
7	-3.839	-0.105	0.272	7	3.920	0.065	0.296
7	2.375	-0.946	0.139	7	-2.343	0.461	0.208
7	5.185	-0.463	0.100	7	-5.109	-0.228	0.185
7	6.947	1.053	0.190	7	-6.708	-1.895	0.342
7	7.294	-1.229	-0.466	7	-7.315	0.342	-0.278
6	-6.635	-0.189	-0.203	6	6.697	0.285	-0.241
6	-6.995	0.716	0.987	6	7.131	-0.549	0.976
6	-8.019	-0.448	-0.808	6	8.052	0.597	-0.885
6	-8.086	1.653	0.453	6	8.262	-1.445	0.456
6	-8.745	0.899	-0.725	6	8.856	-0.702	-0.764
6	-5.912	-1.463	0.201	6	5.911	1.532	0.127
6	-5.731	0.545	-1.192	6	5.817	-0.537	-1.181
6	-4.516	-1.248	0.725	6	4.539	1.260	0.690

6	-4.335	0.796	-0.681	6	4.449	-0.846	-0.630
6	-2.478	0.119	0.773	6	2.583	-0.216	0.833
6	-1.428	-0.569	-0.083	6	1.480	0.370	-0.031
6	-0.022	-0.330	0.445	6	0.098	0.051	0.519
6	1.030	-1.003	-0.419	6	-1.006	0.632	-0.348
6	2.907	0.411	0.159	6	-2.767	-0.933	0.201
6	3.280	-1.799	-0.619	6	-3.310	1.247	-0.545
6	4.284	0.452	0.788	6	-4.131	-1.088	0.839
6	4.663	-1.820	-0.004	6	-4.695	1.162	0.065
6	6.513	-0.206	-0.056	6	-6.416	-0.602	0.085
6	8.249	1.272	0.023	6	-7.970	-2.258	0.162
6	8.582	-0.959	-0.626	6	-8.568	-0.073	-0.453
6	9.141	0.292	-0.386	6	-8.968	-1.386	-0.259
1	-6.134	1.252	1.401	1	6.310	-1.114	1.429
1	-7.390	0.088	1.794	1	7.506	0.133	1.748
1	-8.532	-1.197	-0.192	1	8.533	1.398	-0.311
1	-7.968	-0.855	-1.823	1	7.959	0.958	-1.914
1	-7.651	2.597	0.112	1	7.873	-2.424	0.159
1	-8.804	1.918	1.232	1	9.008	-1.640	1.229
1	-9.822	0.772	-0.590	1	9.925	-0.509	-0.654
1	-8.623	1.459	-1.657	1	8.750	-1.306	-1.670
1	-5.828	-2.136	-0.664	1	5.771	2.163	-0.762
1	-6.457	-2.020	0.967	1	6.438	2.151	0.858
1	-6.133	1.515	-1.494	1	6.268	-1.495	-1.453
1	-5.635	-0.044	-2.115	1	5.670	0.007	-2.123
1	-2.447	-0.259	1.796	1	2.547	0.206	1.839
1	-2.316	1.199	0.786	1	2.485	-1.301	0.895
1	-1.509	-0.200	-1.113	1	1.577	-0.025	-1.050
1	-1.640	-1.644	-0.111	1	1.616	1.457	-0.097
1	0.160	0.750	0.499	1	-0.009	-1.037	0.599
1	0.067	-0.709	1.471	1	-0.005	0.446	1.537
1	1.005	-0.573	-1.442	1	-0.942	0.203	-1.370
1	0.773	-2.064	-0.530	1	-0.838	1.710	-0.461
1	2.242	1.055	0.741	1	-2.050	-1.535	0.764
1	2.956	0.831	-0.867	1	-2.793	-1.332	-0.834
1	3.354	-1.465	-1.675	1	-3.358	0.913	-1.602
1	2.875	-2.816	-0.630	1	-2.987	2.293	-0.551
1	4.679	1.464	0.752	1	-4.477	-2.117	0.774
1	4.210	0.156	1.845	1	-4.067	-0.819	1.905
1	4.613	-2.269	1.000	1	-4.692	1.636	1.059
1	5.350	-2.413	-0.603	1	-5.405	1.700	-0.560
1	8.584	2.288	0.228	1	-8.195	-3.304	0.370
1	9.201	-1.791	-0.961	1	-9.279	0.697	-0.752
1	10.197	0.489	-0.512	1	-9.992	-1.704	-0.403
8	5.720	3.669	0.589	8	-7.499	3.225	-0.637
1	5.552	3.988	-0.300	1	-7.371	2.275	-0.461
1	6.130	2.796	0.455	1	-7.458	3.633	0.229
Buspirone				Aminophylline			
motif 6, Eint = -7.4 kcal/mol				motif 1, Eint = -14.5 kcal/mol			
8	-3.477	2.023	-0.761	8	-1.469	-1.927	-0.007
8	-3.081	-2.325	0.467	8	3.012	-0.903	0.001
7	-3.313	-0.172	-0.225	7	1.562	0.852	0.000
7	2.904	0.623	0.076	7	0.775	-1.393	-0.002
7	5.707	0.175	-0.099	7	-1.925	1.117	-0.008
7	7.442	-1.189	-0.805	7	-0.192	2.538	-0.002
7	7.829	0.636	0.712	6	0.255	1.261	-0.003
6	-6.093	-0.287	0.328	6	-0.781	0.349	-0.007
6	-6.487	-0.806	-1.066	6	-0.593	-1.060	-0.006
6	-7.457	-0.239	1.023	6	1.865	-0.502	0.000
6	-7.551	-1.878	-0.799	6	2.666	1.799	0.005
6	-8.179	-1.512	0.567	6	1.144	-2.805	0.001
6	-5.397	1.063	0.297	6	-1.515	2.401	-0.005
6	-5.152	-1.266	1.027	1	-2.875	0.729	-0.014
6	-4.007	1.036	-0.275	1	2.244	2.801	0.007
6	-3.779	-1.336	0.413	1	3.290	1.656	-0.879
6	-1.960	-0.210	-0.798	1	3.287	1.650	0.889
6	-0.895	0.174	0.216	1	0.227	-3.386	0.011
6	0.502	0.128	-0.384	1	1.749	-3.031	0.880
6	1.569	0.475	0.640	1	1.735	-3.040	-0.885
6	3.433	-0.641	-0.424	1	-2.212	3.225	-0.004
6	3.819	1.161	1.075	8	-3.965	-0.743	0.084
6	4.802	-0.451	-1.047	1	-4.633	-1.100	-0.505
6	5.194	1.402	0.489	1	-3.215	-1.371	0.050
6	7.038	-0.132	-0.068				
6	8.730	-1.497	-0.719				
6	9.107	0.286	0.764				
6	9.636	-0.792	0.065				
1	-5.638	-1.181	-1.646				
1	-6.915	0.026	-1.637				
1	-7.993	0.652	0.674				
1	-7.374	-0.151	2.111				
1	-7.096	-2.872	-0.760				
1	-8.291	-1.918	-1.601				
1	-9.259	-1.364	0.502				

1	-8.028	-2.320	1.288				
1	-5.309	1.469	1.315				
1	-5.965	1.812	-0.262				
1	-5.540	-2.288	1.047				
1	-5.021	-0.970	2.077				
1	-1.951	0.477	-1.645				
1	-1.797	-1.227	-1.159				
1	-0.957	-0.508	1.073				
1	-1.107	1.181	0.594				
1	0.678	-0.873	-0.797				
1	0.576	0.826	-1.226				
1	1.561	-0.279	1.455				
1	1.311	1.432	1.111				
1	2.757	-1.041	-1.183				
1	3.498	-1.391	0.390				
1	3.907	0.477	1.944				
1	3.412	2.106	1.447				
1	5.225	-1.405	-1.355				
1	4.710	0.184	-1.942				
1	5.132	2.183	-0.285				
1	5.892	1.741	1.252				
1	9.053	-2.352	-1.313				
1	9.743	0.907	1.395				
1	10.683	-1.058	0.118				
8	-5.358	4.132	-0.554				
1	-5.183	4.934	-1.050				
1	-4.583	3.569	-0.712				
Aminophylline				Aminophylline			
motif 2, Eint = -6.5 kcal/mol				motif 3, Eint = -7.4 kcal/mol			
8	1.884	-1.311	0.002	8	-2.144	2.288	0.000
8	-0.106	2.843	-0.004	8	2.203	0.783	0.000
7	-1.488	1.028	0.004	7	0.568	-0.804	0.000
7	0.878	0.765	0.004	7	0.043	1.515	0.000
7	-0.972	-2.424	-0.001	7	-2.922	-0.673	0.000
7	-2.741	-1.056	-0.001	7	-1.371	-2.281	0.000
6	-1.590	-0.336	0.001	6	-0.779	-1.060	0.000
6	-0.474	-1.140	0.001	6	-1.700	-0.037	0.000
6	0.855	-0.640	0.003	6	-1.368	1.347	0.000
6	-0.234	1.637	0.000	6	1.012	0.506	0.000
6	-2.690	1.848	-0.003	6	1.555	-1.877	0.000
6	2.205	1.381	0.004	6	0.566	2.877	0.000
6	-2.322	-2.312	-0.002	6	-2.665	-2.002	0.000
1	-0.419	-3.268	-0.001	1	-3.820	-0.213	0.000
1	-3.247	1.695	-0.929	1	2.192	-1.810	0.882
1	-2.383	2.887	0.079	1	2.192	-1.810	-0.882
1	-3.330	1.573	0.837	1	1.015	-2.821	0.000
1	2.765	1.064	0.883	1	-0.286	3.552	0.000
1	2.075	2.458	0.007	1	1.183	3.043	-0.883
1	2.763	1.069	-0.880	1	1.183	3.043	0.884
1	-2.970	-3.177	-0.004	1	-3.454	-2.740	0.000
8	4.669	-0.625	-0.005	8	4.532	-0.882	0.000
1	3.750	-0.936	-0.003	1	3.811	-0.233	0.000
1	5.190	-1.429	-0.006	1	5.330	-0.352	-0.001
Aminophylline				Aminophylline			
motif 4, Eint = -7.1 kcal/mol				motif 5, Eint = -6.8 kcal/mol			
8	-0.447	-2.785	0.001	8	2.561	1.879	-0.001
8	2.035	1.104	0.003	8	1.339	-2.559	-0.001
7	-0.221	1.317	0.001	7	-0.359	-1.024	0.001
7	0.803	-0.830	0.002	7	1.930	-0.354	0.000
7	-2.884	-0.939	-0.002	7	-0.435	2.467	0.000
7	-2.659	1.284	-0.001	7	-1.944	0.826	0.001
6	-1.440	0.689	0.000	6	-0.687	0.301	0.001
6	-1.531	-0.683	-0.001	6	0.272	1.286	0.001
6	-0.413	-1.566	0.000	6	1.676	1.038	0.000
6	0.940	0.560	0.002	6	0.986	-1.398	0.000
6	-0.102	2.767	0.001	6	-1.398	-2.046	0.002
6	2.055	-1.584	0.003	6	3.321	-0.791	-0.001
6	-3.505	0.265	-0.002	6	-1.745	2.138	0.001
1	-3.305	-1.856	-0.002	1	-0.028	3.390	0.000
1	-1.108	3.182	-0.001	1	-2.031	-1.943	0.884
1	0.444	3.101	-0.881	1	-0.905	-3.014	0.005
1	0.439	3.101	0.887	1	-2.029	-1.948	-0.882
1	1.797	-2.639	0.004	1	3.944	0.099	0.001
1	2.647	-1.338	0.884	1	3.524	-1.396	-0.885
1	2.647	-1.341	-0.880	1	3.524	-1.400	0.880
1	-4.580	0.357	-0.003	1	-2.528	2.881	0.000
8	4.729	0.122	-0.006	8	-4.344	-0.897	-0.003
1	5.340	0.860	-0.004	1	-5.163	-0.398	-0.003
1	3.853	0.536	-0.003	1	-3.643	-0.224	-0.002
Aminophylline				Atovaquone			
motif 6, Eint = -6.3 kcal/mol				motif 1, Eint = -3.5 kcal/mol			
8	1.887	-2.441	0.009	17	-7.716	-1.069	0.007
8	2.225	2.150	0.005	8	3.185	-2.321	-0.008
7	0.113	1.270	-0.008	8	2.214	2.318	0.007

7	2.040	-0.127	0.008	8	4.879	2.829	0.010
7	-1.140	-1.989	-0.017	6	1.065	-0.306	0.003
7	-2.003	0.066	-0.029	6	-1.834	0.350	0.005
6	-0.646	0.132	-0.016	6	0.355	0.209	-1.258
6	-0.074	-1.117	-0.009	6	0.357	0.207	1.265
6	1.331	-1.355	0.003	6	-1.120	-0.165	-1.250
6	1.505	1.172	0.001	6	-1.118	-0.167	1.259
6	-0.520	2.578	-0.014	6	2.546	-0.017	0.002
6	3.498	-0.185	0.020	6	-3.301	0.001	0.006
6	-2.262	-1.237	-0.028	6	3.491	-1.008	-0.003
1	-1.072	-2.996	-0.014	6	2.985	1.372	0.005
1	-1.098	2.717	-0.930	6	-4.278	0.997	0.006
1	0.267	3.326	0.043	6	-3.724	-1.331	0.007
1	-1.191	2.674	0.842	6	4.937	-0.780	-0.005
1	3.782	-1.234	0.022	6	4.502	1.677	0.005
1	3.888	0.317	0.906	6	5.438	0.533	-0.001
1	3.902	0.317	-0.860	6	-5.637	0.693	0.007
1	-3.259	-1.653	-0.035	6	-5.072	-1.663	0.008
8	-4.854	0.338	0.095	6	5.834	-1.851	-0.010
1	-3.946	0.672	0.030	6	-6.013	-0.642	0.007
1	-5.399	1.022	-0.296	6	6.812	0.758	-0.002
				6	7.204	-1.613	-0.011
				6	7.698	-0.312	-0.007
				1	0.904	-1.401	0.002
				1	-1.750	1.447	0.006
				1	0.847	-0.192	-2.152
				1	0.467	1.297	-1.299
				1	0.469	1.295	1.308
				1	0.850	-0.195	2.158
				1	-1.616	0.223	-2.146
				1	-1.226	-1.259	-1.296
				1	-1.224	-1.261	1.303
				1	-1.612	0.220	2.157
				1	-3.974	2.040	0.004
				1	-2.989	-2.132	0.008
				1	-6.386	1.478	0.007
				1	-5.393	-2.699	0.008
				1	5.454	-2.865	-0.013
				1	2.224	-2.414	-0.007
				1	7.160	1.786	0.002
				1	7.891	-2.453	-0.015
				1	8.768	-0.134	-0.008
				8	-8.591	2.174	-0.107
				1	-9.241	2.508	0.515
				1	-8.715	1.218	-0.091
Atovaquone				Atovaquone			
motif 2, Eint = -3.6 kcal/mol				motif 3, Eint = -3.2 kcal/mol			
17	7.833	-0.190	-0.007	17	-8.375	0.649	0.041
8	-2.891	2.353	0.000	8	2.531	1.987	0.288
8	-2.401	-2.362	-0.001	8	1.564	-2.623	-0.216
8	-5.104	-2.596	0.005	8	4.227	-3.132	-0.312
6	-0.988	0.131	0.006	6	0.420	-0.012	0.065
6	1.818	-0.849	0.005	6	-2.475	-0.676	-0.034
6	-0.337	-0.449	-1.258	6	-0.298	-0.664	1.257
6	-0.340	-0.460	1.267	6	-0.277	-0.381	-1.253
6	1.171	-0.245	-1.247	6	-1.775	-0.297	1.277
6	1.168	-0.255	1.261	6	-1.754	-0.017	-1.216
6	-2.492	-0.004	0.003	6	1.901	-0.303	0.046
6	3.316	-0.681	0.006	6	-3.945	-0.346	-0.011
6	-3.330	1.079	0.001	6	2.851	0.675	0.160
6	-3.071	-1.341	0.001	6	2.338	-1.686	-0.109
6	4.164	-1.789	-0.013	6	-4.910	-1.347	-0.136
6	3.900	0.589	0.022	6	-4.387	0.973	0.131
6	-4.792	1.000	-0.002	6	4.296	0.448	0.164
6	-4.611	-1.489	0.002	6	3.855	-1.990	-0.155
6	-5.424	-0.255	-0.002	6	4.791	-0.859	0.003
6	5.547	-1.647	-0.016	6	-6.269	-1.055	-0.121
6	5.279	0.762	0.020	6	-5.739	1.288	0.149
6	-5.575	2.157	-0.006	6	5.198	1.502	0.333
6	6.086	-0.369	0.000	6	-6.673	0.266	0.022
6	-6.814	-0.338	-0.004	6	6.163	-1.092	0.001
6	-6.962	2.061	-0.008	6	6.567	1.254	0.330
6	-7.586	0.816	-0.008	6	7.054	-0.038	0.162
1	-0.714	1.203	0.011	1	0.257	1.076	0.187
1	1.602	-1.927	0.001	1	-2.378	-1.765	-0.155
1	-0.779	0.012	-2.149	1	0.185	-0.361	2.193
1	-0.570	-1.518	-1.309	1	-0.182	-1.749	1.180
1	-0.573	-1.529	1.308	1	-0.159	-1.456	-1.418
1	-0.784	-0.007	2.160	1	0.221	0.122	-2.090
1	1.620	-0.680	-2.146	1	-2.275	-0.783	2.121
1	1.402	0.830	-1.283	1	-1.888	0.785	1.440
1	1.398	0.820	1.306	1	-1.867	1.075	-1.137
1	1.615	-0.697	2.157	1	-2.239	-0.303	-2.155
1	3.734	-2.787	-0.026	1	-4.592	-2.380	-0.248

1	3.268	1.473	0.036	1	-3.663	1.777	0.231
1	6.197	-2.513	-0.032	1	-7.009	-1.840	-0.219
1	5.720	1.753	0.034	1	-6.072	2.313	0.260
1	-5.093	3.127	-0.006	1	4.840	2.516	0.468
1	-1.925	2.348	0.001	1	1.569	2.065	0.338
1	-7.265	-1.325	-0.004	1	6.506	-2.113	-0.127
1	-7.560	2.966	-0.011	1	7.255	2.082	0.462
1	-8.668	0.749	-0.010	1	8.123	-0.223	0.161
8	7.567	3.160	-0.073	8	3.788	4.511	-0.579
1	7.985	2.291	-0.088	1	3.323	3.668	-0.521
1	8.096	3.666	0.547	1	3.928	4.645	-1.518
Atovaquone				Atovaquone			
motif 4, Eint = -8.8 kcal/mol				motif 5, Eint = -6.8 kcal/mol			
17	-8.188	-0.707	0.000	17	-8.590	-0.180	-0.014
8	2.686	-2.495	-0.002	8	2.143	-2.675	-0.032
8	1.905	2.181	0.002	8	1.637	2.036	0.056
8	4.567	2.578	0.004	8	4.312	2.290	-0.005
6	0.639	-0.419	0.002	6	0.228	-0.462	-0.007
6	-2.230	0.331	0.000	6	-2.582	0.508	0.014
6	-0.055	0.103	-1.266	6	-0.422	0.153	-1.255
6	-0.055	0.106	1.267	6	-0.425	0.089	1.270
6	-1.542	-0.225	-1.252	6	-1.929	-0.056	-1.254
6	-1.542	-0.222	1.254	6	-1.933	-0.119	1.254
6	2.130	-0.172	0.001	6	1.731	-0.321	-0.001
6	-3.712	0.064	0.000	6	-4.080	0.336	0.008
6	3.042	-1.199	-0.001	6	2.576	-1.399	-0.013
6	2.626	1.190	0.002	6	2.306	1.014	0.025
6	-4.625	1.120	-0.002	6	-4.931	1.442	0.035
6	-4.221	-1.239	0.002	6	-4.661	-0.935	-0.026
6	4.496	-1.028	-0.001	6	4.037	-1.312	-0.002
6	4.152	1.440	0.002	6	3.846	1.167	0.010
6	5.046	0.265	0.001	6	4.670	-0.054	0.012
6	-5.997	0.897	-0.002	6	-6.314	1.297	0.029
6	-5.588	-1.485	0.002	6	-6.039	-1.103	-0.032
6	5.351	-2.132	-0.002	6	4.820	-2.468	-0.005
6	-6.467	-0.409	0.000	6	-6.857	0.020	-0.005
6	6.427	0.439	0.001	6	6.062	0.031	0.027
6	6.730	-1.946	-0.002	6	6.208	-2.372	0.008
6	7.271	-0.663	-0.001	6	6.830	-1.128	0.025
1	0.451	-1.509	0.003	1	-0.041	-1.535	-0.035
1	-2.080	1.417	-0.001	1	-2.369	1.587	0.042
1	0.426	-0.326	-2.152	1	0.024	-0.279	-2.157
1	0.078	1.187	-1.329	1	-0.193	1.223	-1.274
1	0.077	1.190	1.327	1	-0.195	1.157	1.343
1	0.425	-0.320	2.155	1	0.018	-0.389	2.150
1	-2.022	0.176	-2.151	1	-2.378	0.403	-2.141
1	-1.684	-1.316	-1.291	1	-2.156	-1.131	-1.321
1	-1.684	-1.313	1.295	1	-2.160	-1.196	1.267
1	-2.023	0.181	2.151	1	-2.383	0.295	2.162
1	-4.250	2.140	-0.003	1	-4.503	2.441	0.061
1	-3.538	-2.084	0.004	1	-4.027	-1.818	-0.047
1	-6.697	1.725	-0.003	1	-6.965	2.163	0.050
1	-5.973	-2.498	0.004	1	-6.480	-2.093	-0.059
1	4.933	-3.131	-0.003	1	4.338	-3.437	-0.018
1	1.721	-2.552	-0.002	1	1.177	-2.673	-0.038
1	6.813	1.453	0.002	1	6.538	1.007	0.042
1	7.385	-2.811	-0.003	1	6.805	-3.278	0.005
1	8.347	-0.526	0.000	1	7.912	-1.058	0.036
8	-0.703	3.329	-0.008	8	7.027	3.172	-0.111
1	-0.631	4.285	-0.005	1	7.206	4.027	0.283
1	0.216	3.020	-0.005	1	6.064	3.082	-0.080
Atovaquone				Methotrexate			
motif 6, Eint = -7.7 kcal/mol				motif 1, Eint = -9.0 kcal/mol			
17	8.371	-0.448	-0.002	8	-6.832	-0.470	0.300
8	-2.439	-2.688	-0.005	8	-2.674	-1.351	2.461
8	-1.781	2.000	0.007	8	-5.513	-1.368	-1.268
8	-4.462	2.333	0.007	8	-3.870	3.884	-1.676
6	-0.455	-0.538	0.000	8	-4.036	3.975	0.564
6	2.378	0.358	0.002	7	2.772	-3.225	-0.332
6	0.213	0.021	1.266	7	-3.254	-0.911	0.313
6	0.212	0.027	-1.262	7	3.427	-0.578	-0.070
6	1.714	-0.228	1.254	7	5.067	0.811	-1.890
6	1.714	-0.222	-1.253	7	4.941	2.709	-0.545
6	-1.953	-0.350	0.001	7	3.587	2.676	1.472
6	3.872	0.155	0.001	7	2.437	0.773	2.108
6	-2.833	-1.402	-0.001	7	4.803	4.512	0.858
6	-2.487	0.998	0.004	6	-4.519	-0.346	0.709
6	4.744	1.245	0.003	6	-4.481	1.191	0.789
6	4.428	-1.127	-0.002	6	1.514	-2.767	0.031
6	-4.291	-1.271	-0.001	6	-4.180	1.838	-0.551
6	-4.018	1.204	0.005	6	3.459	-2.591	-1.437
6	-4.877	0.007	0.002	6	-1.064	-1.844	0.785
6	6.124	1.073	0.002	6	-2.379	-1.359	1.270
6	5.803	-1.322	-0.002	6	0.706	-2.037	-0.864

6	-5.116	-2.397	-0.004	6	0.992	-3.019	1.316
6	6.642	-0.214	-0.001	6	-5.631	-0.804	-0.202
6	-6.263	0.144	0.002	6	-0.551	-1.594	-0.494
6	-6.500	-2.248	-0.004	6	-0.262	-2.560	1.676
6	-7.077	-0.982	-0.001	6	3.873	-1.158	-1.170
1	-0.221	-1.619	-0.002	6	3.634	-3.751	0.709
1	2.188	1.441	0.005	6	-4.028	3.327	-0.452
1	-0.243	-0.427	2.155	6	4.694	-0.438	-2.068
1	0.014	1.096	1.319	6	3.776	0.700	0.122
1	0.014	1.102	-1.310	6	4.602	1.426	-0.769
1	-0.244	-0.417	-2.154	6	3.261	1.415	1.259
1	2.175	0.194	2.154	6	4.430	3.238	0.563
1	1.914	-1.309	1.290	1	-4.730	-0.725	1.715
1	1.914	-1.303	-1.294	1	-3.712	1.462	1.517
1	2.174	0.205	-2.150	1	-5.430	1.560	1.188
1	4.336	2.252	0.005	1	-4.953	1.625	-1.300
1	3.777	-1.998	-0.003	1	-3.256	1.438	-0.988
1	6.791	1.927	0.004	1	-3.031	-0.984	-0.674
1	6.225	-2.321	-0.005	1	4.342	-3.194	-1.676
1	-4.671	-3.384	-0.006	1	2.837	-2.635	-2.339
1	-1.473	-2.718	-0.005	1	1.073	-1.783	-1.851
1	-6.678	1.146	0.004	1	1.578	-3.563	2.046
1	-7.131	-3.131	-0.006	1	-1.122	-1.017	-1.215
1	-8.156	-0.874	-0.001	1	-0.647	-2.742	2.675
8	-2.675	4.805	-0.014	1	4.578	-4.063	0.262
1	-2.363	3.889	-0.003	1	3.184	-4.631	1.176
1	-3.627	4.684	-0.009	1	3.849	-3.011	1.493
				1	5.061	-0.930	-2.972
				1	-7.498	-0.762	-0.338
				1	-3.765	4.835	-1.535
				1	1.957	1.305	2.815
				1	2.080	-0.132	1.839
				1	4.261	5.007	1.546
				1	5.245	5.040	0.124
				8	-3.149	-0.909	-2.686
				1	-2.808	-1.541	-3.322
				1	-4.044	-1.219	-2.476
Methotrexate				Methotrexate			
motif 2, Eint = -11.8 kcal/mol				motif 3, Eint = -13.5 kcal/mol			
8	6.553	-0.423	0.370	8	5.996	-0.930	0.850
8	2.523	-1.031	-2.504	8	2.010	-2.141	-2.049
8	4.877	-1.308	1.586	8	4.370	-1.766	2.160
8	3.691	4.173	0.801	8	1.784	2.941	0.740
8	4.232	3.837	-1.355	8	2.938	2.788	-1.187
7	-2.956	-3.267	-0.041	7	-3.781	-2.441	0.328
7	3.061	-0.868	-0.310	7	2.673	-2.041	0.113
7	-3.604	-0.611	0.112	7	-2.828	0.092	-0.236
7	-5.243	0.482	2.125	7	-3.331	2.334	1.385
7	-5.113	2.565	1.090	7	-1.728	3.544	0.208
7	-3.758	2.843	-0.907	7	-0.446	2.461	-1.539
7	-2.611	1.060	-1.829	7	-0.830	0.264	-2.135
7	-4.971	4.564	-0.015	7	0.024	4.598	-0.852
6	4.412	-0.450	-0.618	6	3.915	-1.363	-0.179
6	4.494	1.034	-0.996	6	3.698	0.086	-0.657
6	-1.698	-2.762	-0.329	6	-2.415	-2.616	0.144
6	4.072	1.945	0.140	6	2.823	0.880	0.295
6	-3.642	-2.812	1.150	6	-4.211	-1.342	1.176
6	0.882	-1.738	-0.933	6	0.362	-2.565	-0.394
6	2.204	-1.198	-1.332	6	1.736	-2.260	-0.856
6	-0.889	-2.178	0.668	6	-1.494	-2.181	1.116
6	-1.175	-2.815	-1.638	6	-1.897	-3.158	-1.050
6	5.290	-0.782	0.566	6	4.754	-1.398	1.077
6	0.367	-1.685	0.367	6	-0.141	-2.143	0.843
6	0.081	-2.310	-1.923	6	-0.539	-3.112	-1.311
6	-4.052	-1.354	1.109	6	-3.644	0.014	0.799
6	-3.818	-3.629	-1.150	6	-4.658	-2.742	-0.787
6	4.020	3.391	-0.256	6	2.555	2.283	-0.164
6	-4.873	-0.780	2.108	6	-3.895	1.160	1.588
6	-3.950	0.682	0.121	6	-2.203	1.258	-0.430
6	-4.776	1.263	1.113	6	-2.425	2.397	0.375
6	-3.434	1.564	-0.892	6	-1.140	1.342	-1.397
6	-4.600	3.259	0.078	6	-0.798	3.488	-0.732
1	4.778	-1.027	-1.479	1	4.455	-1.899	-0.968
1	3.850	1.187	-1.866	1	3.229	0.045	-1.643
1	5.512	1.267	-1.315	1	4.668	0.570	-0.792
1	4.741	1.862	1.006	1	3.238	0.926	1.310
1	3.081	1.666	0.518	1	1.845	0.395	0.420
1	2.934	-1.273	0.608	1	2.460	-2.181	1.091
1	-4.525	-3.443	1.292	1	-5.305	-1.318	1.162
				1	-3.947	-1.545	2.222
				1	-1.844	-1.770	2.055
				1	-2.562	-3.547	-1.810
				1	0.510	-1.691	1.587
				1	-0.157	-3.447	-2.270

1	-3.020	-2.997	2.034	1	-5.692	-2.600	-0.473
1	-1.255	-2.079	1.682	1	-4.549	-3.785	-1.090
1	-1.760	-3.243	-2.442	1	-4.468	-2.104	-1.663
1	0.933	-1.215	1.166	1	-4.596	1.097	2.423
1	0.468	-2.342	-2.936	1	6.466	-0.958	1.695
1	-4.763	-4.002	-0.755	1	1.470	3.768	0.318
1	-3.370	-4.429	-1.743	1	0.041	0.259	-2.644
1	-4.031	-2.779	-1.814	1	-1.228	-0.627	-1.867
1	-5.241	-1.406	2.924	1	0.496	4.667	-1.744
1	7.070	-0.665	1.177	1	-0.397	5.457	-0.525
1	3.673	5.083	0.473	8	-0.146	1.211	2.134
1	-2.136	1.692	-2.452	1	0.467	1.870	1.777
1	-2.260	0.121	-1.708	1	-0.796	1.743	2.601
1	-4.429	5.159	-0.619				
1	-5.414	4.973	0.791				
8	7.345	-1.228	2.826				
1	6.421	-1.524	2.856				
1	7.876	-1.971	3.121				
Methotrexate				Methotrexate			
motif 4, Eint = -11.5 kcal/mol				motif 5, Eint = -11.6 kcal/mol			
8	-6.428	-1.818	-1.086	8	7.082	-0.017	1.164
8	-2.602	-1.844	2.109	8	3.439	-1.243	-2.014
8	-4.539	-2.328	-2.194	8	5.352	-0.878	2.313
8	-4.417	3.222	-1.111	8	3.857	4.349	0.760
8	-5.000	2.672	0.994	8	4.677	3.827	-1.268
7	3.359	-3.062	0.092	7	-2.105	-3.666	0.099
7	-2.972	-1.684	-0.119	7	3.719	-0.819	0.192
7	3.592	-0.335	-0.010	7	-2.956	-1.068	-0.060
7	5.201	1.023	-1.882	7	-4.917	0.034	1.633
7	4.666	3.048	-0.863	7	-4.827	2.022	0.426
7	3.129	3.090	1.017	7	-3.271	2.257	-1.423
7	2.203	1.140	1.848	7	-1.889	0.511	-2.041
7	4.124	4.989	0.222	7	-4.664	3.955	-0.790
6	-4.395	-1.519	0.079	6	5.062	-0.326	-0.021
6	-4.766	-0.090	0.496	6	5.080	1.110	-0.560
6	2.017	-2.773	0.279	6	-0.863	-3.089	-0.111
6	-4.419	0.934	-0.566	6	4.466	2.102	0.410
6	4.053	-2.489	-1.043	6	-2.943	-3.168	1.169
6	-0.737	-2.202	0.677	6	1.688	-1.921	-0.554
6	-2.159	-1.907	0.967	6	3.004	-1.318	-0.871
6	1.207	-2.302	-0.774	6	-0.209	-2.353	0.898
6	1.407	-2.943	1.539	6	-0.202	-3.219	-1.350
6	-5.091	-1.940	-1.192	6	5.814	-0.454	1.281
6	-0.133	-2.029	-0.575	6	1.034	-1.791	0.677
6	0.066	-2.659	1.724	6	1.038	-2.643	-1.558
6	4.228	-0.987	-0.967	6	-3.463	-1.763	0.944
6	4.179	-3.299	1.264	6	-2.817	-4.194	-1.049
6	-4.648	2.350	-0.126	6	4.363	3.487	-0.156
6	5.030	-0.282	-1.894	6	-4.446	-1.187	1.779
6	3.734	0.996	0.009	6	-3.403	0.182	-0.215
6	4.538	1.710	-0.912	6	-4.390	0.764	0.614
6	3.010	1.777	0.977	6	-2.850	1.020	-1.249
6	3.971	3.642	0.102	6	-4.251	2.690	-0.582
1	-4.727	-2.190	0.884	1	5.565	-0.960	-0.766
1	-4.233	0.129	1.424	1	4.530	1.113	-1.504
1	-5.833	-0.051	0.733	1	6.108	1.393	-0.798
1	-4.985	0.779	-1.493	1	5.031	2.166	1.349
1	-3.366	0.847	-0.861	1	3.459	1.785	0.707
1	-2.699	-2.021	-1.033	1	3.519	-1.137	1.132
1	5.032	-2.975	-1.118	1	-3.783	-3.860	1.290
1	3.535	-2.757	-1.971	1	-2.401	-3.217	2.121
1	1.633	-2.117	-1.752	1	-0.687	-2.192	1.856
1	1.988	-3.289	2.385	1	-0.667	-3.763	-2.162
1	-0.702	-1.638	-1.414	1	1.477	-1.207	1.478
1	-0.392	-2.782	2.700	1	1.533	-2.737	-2.519
1	5.201	-3.503	0.944	1	-3.770	-4.605	-0.715
1	3.826	-4.175	1.814	1	-2.254	-5.006	-1.515
1	4.195	-2.439	1.949	1	-3.018	-3.427	-1.810
1	5.556	-0.833	-2.677	1	-4.864	-1.773	2.601
1	-6.803	-2.106	-1.930	1	7.499	-0.131	2.029
1	-4.571	4.129	-0.758	1	3.813	5.214	0.329
1	1.586	1.685	2.426	1	-1.402	1.123	-2.674
1	2.010	0.161	1.697	1	-1.486	-0.382	-1.799
1	3.445	5.485	0.775	1	-4.306	4.448	-1.589
				1	-5.440	4.320	-0.245
				8	-6.802	3.894	1.138
				1	-6.274	3.071	1.171
				1	-6.920	4.156	2.053

1	4.557	5.469	-0.548				
8	-4.909	5.373	0.496				
1	-5.099	4.621	1.082				
1	-5.665	5.960	0.564				
Methotrexate				Anileridine			
motif 6, Eint = -9.3 kcal/mol				motif 1, Eint = -7.6 kcal/mol			
8	-6.975	-0.556	-0.745	8	-2.484	2.030	-0.127
8	-3.020	-1.038	2.246	8	-2.357	1.013	1.861
8	-5.321	-1.591	-1.863	7	0.810	-0.757	-0.246
8	-3.949	3.869	-1.583	7	8.580	0.135	0.550
8	-4.364	3.746	0.623	6	-2.111	-0.320	-0.176
7	2.458	-3.596	0.122	6	-1.238	-0.042	-1.406
7	-3.506	-1.059	0.034	6	-1.391	-1.389	0.663
7	3.133	-0.958	-0.140	6	0.186	0.312	-1.012
7	4.870	0.023	-2.129	6	0.043	-1.006	0.971
7	4.705	2.157	-1.210	6	-3.528	-0.783	-0.529
7	3.261	2.541	0.706	6	2.197	-0.460	0.084
7	2.080	0.798	1.676	6	-2.307	0.954	0.649
7	4.470	4.227	-0.269	6	3.133	-0.445	-1.123
6	-4.844	-0.565	0.272	6	-4.012	-0.768	-1.838
6	-4.871	0.952	0.504	6	-4.378	-1.222	0.493
6	1.200	-3.055	0.335	6	4.568	-0.292	-0.707
6	-4.397	1.730	-0.709	6	-5.305	-1.198	-2.123
6	3.198	-3.208	-1.061	6	-5.670	-1.647	0.207
6	-1.369	-1.931	0.786	6	-6.139	-1.639	-1.103
6	-2.681	-1.322	1.103	6	-2.763	3.268	0.564
6	0.434	-2.530	-0.726	6	5.139	0.968	-0.517
6	0.637	-3.006	1.627	6	5.366	-1.406	-0.436
6	-5.705	-0.976	-0.897	6	-2.937	4.338	-0.477
6	-0.817	-1.987	-0.500	6	6.449	1.116	-0.082
6	-0.612	-2.451	1.838	6	6.677	-1.274	-0.002
6	3.619	-1.753	-1.075	6	7.241	-0.006	0.183
6	3.272	-3.909	1.281	1	-1.659	0.762	-2.014
6	-4.248	3.199	-0.444	1	-1.219	-0.949	-2.021
6	4.490	-1.235	-2.062	1	-1.924	-1.588	1.594
6	3.487	0.331	-0.201	1	-1.402	-2.318	0.083
6	4.360	0.859	-1.182	1	0.192	1.265	-0.436
6	2.935	1.262	0.746	1	0.774	0.495	-1.915
6	4.151	2.917	-0.268	1	0.531	-1.815	1.525
1	-5.249	-1.041	1.176	1	0.058	-0.118	1.637
1	-4.231	1.164	1.364	1	2.286	0.503	0.630
1	-5.882	1.256	0.784	1	2.541	-1.233	0.782
1	-5.067	1.608	-1.569	1	2.861	0.371	-1.801
1	-3.424	1.356	-1.052	1	2.991	-1.377	-1.682
1	-3.376	-1.554	-0.839	1	-3.381	-0.425	-2.650
1	4.079	-3.853	-1.134	1	-4.031	-1.235	1.523
1	2.611	-3.433	-1.960	1	-5.660	-1.185	-3.149
1	0.830	-2.515	-1.733	1	-6.311	-1.987	1.014
1	1.188	-3.389	2.477	1	-7.147	-1.974	-1.326
1	-1.350	-1.565	-1.347	1	-1.934	3.477	1.248
1	-1.028	-2.401	2.839	1	-3.659	3.127	1.177
1	4.220	-4.328	0.945	1	4.544	1.856	-0.717
1	2.783	-4.660	1.906	1	4.951	-2.402	-0.572
1	3.483	-3.024	1.900	1	-3.764	4.103	-1.150
1	4.893	-1.904	-2.826	1	-2.032	4.457	-1.077
1	-7.465	-0.855	-1.525	1	-3.152	5.294	0.004
1	-3.857	4.801	-1.338	1	6.870	2.110	0.047
1	1.580	1.443	2.264	1	7.279	-2.158	0.189
1	1.749	-0.153	1.589	1	8.955	-0.648	1.067
1	4.154	4.828	0.484	1	8.797	1.006	1.012
1	5.181	4.531	-0.911	8	-2.866	-1.086	3.688
8	3.052	4.990	2.158	1	-2.625	-0.281	3.204
1	2.189	5.403	2.225	1	-3.111	-0.781	4.564
1	2.880	4.075	1.866				
Anileridine				Anileridine			
motif 2, Eint = -7.0 kcal/mol				motif 3, Eint = -9.1 kcal/mol			
8	-2.551	1.504	-0.911	8	-2.721	2.072	-0.351
8	-2.402	1.473	1.333	8	-2.439	1.643	1.837
7	0.829	-0.936	0.208	7	0.645	-0.612	0.206
7	8.561	0.476	0.373	7	8.429	0.424	0.512
6	-2.103	-0.603	0.103	6	-2.281	-0.192	0.241
6	-1.234	-0.896	-1.124	6	-1.451	-0.277	-1.043
6	-1.354	-1.129	1.339	6	-1.524	-0.963	1.336
6	0.175	-0.354	-0.957	6	-0.022	0.190	-0.824
				6	-0.084	-0.500	1.472

6	0.071	-0.609	1.411	6	-3.694	-0.758	0.087
6	-3.497	-1.230	0.022	6	2.040	-0.215	0.396
6	2.207	-0.485	0.344	6	-2.465	1.261	0.691
6	-2.346	0.901	0.262	6	2.930	-0.464	-0.820
6	3.144	-1.015	-0.740	6	-4.161	-1.295	-1.113
6	-3.933	-1.949	-1.091	6	-4.557	-0.741	1.188
6	-4.378	-1.077	1.099	6	4.378	-0.234	-0.490
6	4.572	-0.634	-0.468	6	-5.450	-1.814	-1.205
6	-5.204	-2.515	-1.120	6	-5.844	-1.255	1.096
6	-5.648	-1.637	1.070	6	-6.295	-1.798	-0.103
6	-6.066	-2.364	-0.041	6	-2.995	3.449	-0.013
6	-2.866	2.920	-0.856	6	4.955	1.033	-0.595
6	5.099	0.577	-0.921	6	5.184	-1.269	-0.012
6	5.405	-1.450	0.298	6	-3.260	4.186	-1.296
6	-3.068	3.392	-2.267	6	6.278	1.262	-0.246
6	6.400	0.960	-0.629	6	6.509	-1.056	0.340
6	6.710	-1.083	0.598	6	7.078	0.218	0.229
6	7.229	0.133	0.138	1	-1.909	0.311	-1.841
1	-1.685	-0.483	-2.029	1	-1.421	-1.321	-1.374
1	-1.174	-1.983	-1.249	1	-2.031	-0.849	2.297
1	-1.888	-0.851	2.250	1	-1.550	-2.027	1.074
1	-1.344	-2.223	1.281	1	0.001	1.265	-0.551
1	0.148	0.756	-0.881	1	0.535	0.086	-1.758
1	0.760	-0.589	-1.849	1	0.437	-1.110	2.217
1	0.584	-1.054	2.269	1	-0.061	0.541	1.843
1	0.057	0.486	1.585	1	2.109	0.849	0.697
1	2.270	0.623	0.375	1	2.428	-0.794	1.242
1	2.572	-0.834	1.318	1	2.636	0.196	-1.643
1	2.844	-0.627	-1.720	1	2.770	-1.490	-1.170
1	3.037	-2.104	-0.788	1	-3.522	-1.317	-1.988
1	-3.281	-2.076	-1.949	1	-4.217	-0.308	2.125
1	-4.065	-0.500	1.965	1	-5.791	-2.232	-2.147
1	-5.521	-3.076	-1.994	1	-6.496	-1.231	1.963
1	-6.314	-1.505	1.916	1	-7.300	-2.202	-0.178
1	-7.057	-2.804	-0.066	1	-2.136	3.850	0.533
1	-2.046	3.439	-0.352	1	-3.850	3.473	0.670
1	-3.758	3.052	-0.237	1	4.354	1.862	-0.964
1	4.475	1.238	-1.519	1	4.765	-2.268	0.080
1	5.025	-2.400	0.668	1	-4.117	3.764	-1.824
1	-3.889	2.858	-2.750	1	-2.396	4.145	-1.962
1	-2.167	3.248	-2.867	1	-3.476	5.236	-1.085
1	-3.308	4.456	-2.267	1	6.704	2.257	-0.349
1	6.787	1.904	-1.003	1	7.117	-1.884	0.696
1	7.340	-1.744	1.186	1	8.824	-0.233	1.170
1	8.962	0.055	1.199	1	8.664	1.372	0.767
1	8.747	1.469	0.351	8	0.516	-3.092	-1.254
8	-2.837	4.237	2.009	1	0.577	-2.349	-0.618
1	-2.722	4.382	2.949	1	0.375	-3.869	-0.710
1	-2.687	3.287	1.893				
Anileridine				Anileridine			
motif 4, Eint = -7.3 kcal/mol				motif 5, Eint = -9.1 kcal/mol			
8	-2.658	1.750	-0.522	8	-2.721	2.072	-0.351
8	-2.325	1.375	1.669	8	-2.439	1.643	1.837
7	0.660	-0.967	0.076	7	0.645	-0.612	0.206
7	8.438	0.148	0.329	7	8.429	0.424	0.512
6	-2.257	-0.502	0.117	6	-2.281	-0.192	0.241
6	-1.431	-0.625	-1.167	6	-1.451	-0.277	-1.043
6	-1.509	-1.270	1.221	6	-1.524	-0.963	1.336
6	0.000	-0.164	-0.950	6	-0.022	0.190	-0.824
6	-0.057	-0.844	1.340	6	-0.084	-0.500	1.472
6	-3.684	-1.035	-0.021	6	-3.694	-0.758	0.087
6	2.052	-0.582	0.258	6	2.040	-0.215	0.396
6	-2.397	0.967	0.527	6	-2.465	1.261	0.691
6	2.950	-0.899	-0.935	6	2.930	-0.464	-0.820
6	-4.178	-1.558	-1.216	6	-4.161	-1.295	-1.113
6	-4.535	-0.998	1.090	6	-4.557	-0.741	1.188
6	4.395	-0.629	-0.623	6	4.378	-0.234	-0.490
6	-5.479	-2.046	-1.296	6	-5.450	-1.814	-1.205
6	-5.835	-1.480	1.010	6	-5.844	-1.255	1.096
6	-6.312	-2.010	-0.185	6	-6.295	-1.798	-0.103
6	-2.846	3.161	-0.240	6	-2.995	3.449	-0.013
6	4.956	0.634	-0.818	6	4.955	1.033	-0.595
6	5.214	-1.618	-0.073	6	5.184	-1.269	-0.012
6	-3.273	3.820	-1.521	6	-3.260	4.186	-1.296
				6	6.278	1.262	-0.246
				6	6.509	-1.056	0.340
				6	7.078	0.218	0.229

6	6.276	0.904	-0.486	1	-1.909	0.311	-1.841
6	6.536	-1.364	0.263	1	-1.421	-1.321	-1.374
6	7.089	-0.094	0.062	1	-2.031	-0.849	2.297
1	-1.886	-0.052	-1.978	1	-1.550	-2.027	1.074
1	-1.417	-1.678	-1.470	1	0.001	1.265	-0.551
1	-2.007	-1.128	2.183	1	0.535	0.086	-1.758
1	-1.561	-2.336	0.977	1	0.437	-1.110	2.217
1	0.017	0.914	-0.679	1	-0.061	0.541	1.843
1	0.556	-0.260	-1.885	1	2.109	0.849	0.697
1	0.452	-1.467	2.083	1	2.428	-0.794	1.242
1	-0.009	0.198	1.717	1	2.636	0.196	-1.643
1	2.142	0.497	0.506	1	2.770	-1.490	-1.170
1	2.431	-1.125	1.133	1	-3.522	-1.317	-1.988
1	2.648	-0.304	-1.803	1	-4.217	-0.308	2.125
1	2.804	-1.950	-1.208	1	-5.791	-2.232	-2.147
1	-3.548	-1.590	-2.099	1	-6.496	-1.231	1.963
1	-4.175	-0.576	2.024	1	-7.300	-2.202	-0.178
1	-5.842	-2.453	-2.234	1	-2.136	3.850	0.533
1	-6.478	-1.440	1.884	1	-3.850	3.473	0.670
1	-7.327	-2.390	-0.249	1	4.354	1.862	-0.964
1	-1.901	3.559	0.139	1	4.765	-2.268	0.080
1	-3.594	3.255	0.552	1	-4.117	3.764	-1.824
1	4.345	1.427	-1.244	1	-2.396	4.145	-1.962
1	4.807	-2.612	0.093	1	-3.476	5.236	-1.085
1	-4.210	3.399	-1.892	1	6.704	2.257	-0.349
1	-2.514	3.703	-2.297	1	7.117	-1.884	0.696
1	-3.424	4.888	-1.355	1	8.824	-0.233	1.170
1	6.690	1.894	-0.659	1	8.664	1.372	0.767
1	7.153	-2.156	0.679	8	0.516	-3.092	-1.254
1	8.839	-0.454	1.033	1	0.577	-2.349	-0.618
1	8.659	1.116	0.516	1	0.375	-3.869	-0.710
8	0.043	3.017	1.465				
1	-0.697	2.515	1.835				
1	0.823	2.594	1.830				
Anileridine				Bupropion			
motif 6, Eint = -4.9 kcal/mol				motif 1, Eint = -4.9 kcal/mol			
8	-2.670	1.761	0.271	17	2.914	-2.109	0.089
8	-2.338	0.709	2.235	8	-0.478	3.156	-0.629
7	0.762	-0.934	0.006	7	-1.753	0.354	0.659
7	8.536	0.131	0.516	6	-2.572	-0.889	0.725
6	-2.165	-0.574	0.174	6	-1.502	0.980	-0.645
6	-1.336	-0.273	-1.079	6	-2.047	-1.664	1.932
6	-1.391	-1.621	0.994	6	-4.035	-0.518	0.974
6	0.086	0.129	-0.724	6	-2.453	-1.763	-0.524
6	0.046	-1.206	1.250	6	-2.722	1.689	-1.198
6	-3.572	-1.085	-0.140	6	-0.347	1.962	-0.454
6	2.154	-0.608	0.287	6	0.982	1.406	-0.034
6	-2.368	0.682	1.029	6	1.281	0.044	-0.147
6	3.043	-0.557	-0.953	6	1.950	2.286	0.454
6	-4.051	-1.219	-1.444	6	2.537	-0.404	0.234
6	-4.420	-1.433	0.918	6	3.196	1.815	0.840
6	4.489	-0.376	-0.589	6	3.503	0.461	0.732
6	-5.334	-1.703	-1.684	1	-0.861	0.152	1.097
6	-5.702	-1.912	0.679	1	-1.152	0.246	-1.400
6	-6.163	-2.053	-0.627	1	-2.073	-1.042	2.831
6	-3.015	2.972	0.999	1	-2.652	-2.554	2.120
6	5.034	0.895	-0.392	1	-1.013	-1.990	1.769
6	5.326	-1.473	-0.378	1	-4.464	0.039	0.139
6	-3.769	3.876	0.064	1	-4.123	0.102	1.868
6	6.355	1.069	-0.006	1	-4.641	-1.419	1.115
6	6.650	-1.316	0.007	1	-1.414	-2.028	-0.743
6	7.187	-0.038	0.200	1	-3.014	-2.692	-0.386
1	-1.813	0.502	-1.687	1	-2.864	-1.270	-1.410
1	-1.295	-1.180	-1.691	1	-2.452	2.284	-2.072
1	-1.894	-1.793	1.949	1	-3.490	0.975	-1.501
1	-1.410	-2.562	0.435	1	-3.147	2.361	-0.450
1	0.082	1.074	-0.134	1	0.560	-0.658	-0.552
1	0.642	0.339	-1.642	1	1.698	3.339	0.522
1	0.574	-2.006	1.777	1	3.944	2.499	1.227
1	0.063	-0.322	1.918	1	4.474	0.080	1.027
1	2.242	0.349	0.843	8	0.591	-2.186	-2.323
1	2.540	-1.382	0.961	1	0.457	-2.752	-3.086
1	2.729	0.261	-1.610	1	1.430	-2.476	-1.948
1	2.901	-1.485	-1.519				

1	-3.426	-0.948	-2.287
1	-4.073	-1.315	1.940
1	-5.684	-1.804	-2.707
1	-6.342	-2.175	1.515
1	-7.163	-2.429	-0.816
1	-2.082	3.423	1.353
1	-3.599	2.684	1.875
1	4.408	1.771	-0.545
1	4.932	-2.477	-0.521
1	-4.687	3.398	-0.285
1	-3.167	4.152	-0.803
1	-4.045	4.793	0.589
1	6.755	2.070	0.131
1	7.282	-2.188	0.152
1	8.954	-0.653	0.997
1	8.750	0.998	0.988
8	-0.987	3.285	-1.629
1	-0.348	2.842	-2.191
1	-1.448	2.568	-1.176
Bupropion			
motif 2, Eint = -3.6 kcal/mol			
17	2.703	-1.699	-0.782
8	-1.331	3.093	-0.103
7	-2.119	-0.079	0.574
6	-2.730	-1.423	0.394
6	-2.068	0.851	-0.558
6	-2.027	-2.332	1.400
6	-4.218	-1.360	0.740
6	-2.545	-1.992	-1.014
6	-3.412	1.477	-0.868
6	-1.031	1.923	-0.217
6	0.388	1.484	-0.024
6	0.843	0.231	-0.450
6	1.285	2.364	0.588
6	2.170	-0.116	-0.246
6	2.607	1.993	0.784
6	3.069	0.745	0.370
1	-1.179	-0.214	0.930
1	-1.695	0.362	-1.482
1	-2.107	-1.922	2.411
1	-2.471	-3.330	1.405
1	-0.963	-2.440	1.158
1	-4.776	-0.734	0.042
1	-4.357	-0.947	1.742
1	-4.662	-2.360	0.713
1	-1.486	-2.052	-1.290
1	-2.953	-3.005	-1.069
1	-3.061	-1.396	-1.772
1	-3.296	2.290	-1.587
1	-4.100	0.745	-1.296
1	-3.861	1.889	0.038
1	0.177	-0.468	-0.944
1	0.916	3.334	0.903
1	3.298	2.676	1.267
1	4.101	0.446	0.520
8	5.781	-1.055	0.394
1	5.155	-1.617	-0.074
1	6.618	-1.203	-0.052
Bupropion			
motif 3, Eint = -6.0 kcal/mol			
17	3.786	-1.306	-0.736
8	-1.207	2.458	0.033
7	-1.297	-0.821	0.593
6	-1.611	-2.260	0.371
6	-1.436	0.126	-0.518
6	-0.736	-3.027	1.361
6	-3.080	-2.521	0.704
6	-1.301	-2.737	-1.048
6	-2.880	0.445	-0.847
6	-0.661	1.381	-0.128
6	0.817	1.263	0.066
6	1.535	0.150	-0.386
6	1.494	2.304	0.708
6	2.906	0.090	-0.179
6	2.865	2.226	0.908
6	3.583	1.119	0.468
1	-0.351	-0.769	0.953
1	-0.947	-0.244	-1.444
1	-0.906	-2.671	2.381
1	-0.959	-4.096	1.335
1	0.328	-2.901	1.127
1	-3.756	-2.007	0.020
1	-3.306	-2.177	1.716
1	-3.303	-3.591	0.645
1	-0.252	-2.566	-1.313
1	-1.487	-3.811	-1.136
1	-1.926	-2.242	-1.797
1	-2.944	1.268	-1.561
1	-3.377	-0.417	-1.294
1	-3.431	0.733	0.050
1	1.041	-0.664	-0.903
1	0.922	3.160	1.044
1	3.388	3.032	1.413
1	4.653	1.048	0.621
8	-3.896	3.528	-0.301
1	-3.014	3.158	-0.148
1	-3.797	4.457	-0.086
Bupropion			
motif 4, Eint = -6.6 kcal/mol			
17	1.740	-3.439	-0.547
8	0.412	2.721	-0.422
7	-1.738	0.353	0.525
6	-2.913	-0.557	0.446
6	-1.274	1.041	-0.684
6	-2.701	-1.596	1.544
6	-4.190	0.229	0.748
6	-3.042	-1.268	-0.903
6	-2.178	2.187	-1.093
6	0.146	1.532	-0.408
6	1.197	0.511	-0.118
6	1.003	-0.840	-0.435
6	2.399	0.913	0.474
6	1.999	-1.761	-0.152
6	3.382	-0.027	0.752
6	3.193	-1.370	0.444
Bupropion			
motif 5, Eint = -9.1 kcal/mol			
17	3.435	-2.169	-0.194
8	-0.474	2.763	-0.711
7	-1.521	-0.158	0.236
6	-2.334	-1.412	0.246
6	-1.211	0.504	-1.045
6	-1.993	-2.086	1.573
6	-3.826	-1.077	0.236
6	-1.985	-2.343	-0.914
6	-2.428	1.118	-1.709
6	-0.184	1.584	-0.691
6	1.181	1.144	-0.264
6	1.623	-0.174	-0.420
6	2.035	2.091	0.310
6	2.898	-0.524	0.001
6	3.306	1.724	0.726
6	3.749	0.413	0.576

1	-0.967	-0.177	0.915	1	-0.640	-0.381	0.691
1	-1.184	0.351	-1.549	1	-0.734	-0.190	-1.761
1	-2.561	-1.110	2.513	1	-2.203	-1.416	2.410
1	-3.562	-2.265	1.623	1	-2.583	-2.996	1.710
1	-1.818	-2.212	1.339	1	-0.934	-2.367	1.614
1	-4.403	0.979	-0.015	1	-4.156	-0.662	-0.716
1	-4.100	0.744	1.706	1	-4.067	-0.355	1.019
1	-5.052	-0.444	0.796	1	-4.410	-1.985	0.414
1	-2.141	-1.842	-1.144	1	-0.919	-2.596	-0.918
1	-3.880	-1.970	-0.882	1	-2.544	-3.279	-0.832
1	-3.229	-0.569	-1.723	1	-2.235	-1.903	-1.884
1	-1.711	2.778	-1.883	1	-2.116	1.811	-2.491
1	-3.133	1.817	-1.470	1	-3.057	0.355	-2.169
1	-2.371	2.845	-0.244	1	-3.028	1.675	-0.987
1	0.089	-1.178	-0.911	1	0.992	-0.929	-0.877
1	2.557	1.958	0.717	1	1.675	3.107	0.420
1	4.312	0.287	1.215	1	3.966	2.459	1.175
1	3.957	-2.108	0.658	1	4.740	0.116	0.899
8	2.742	4.189	0.364	8	-2.745	1.954	1.879
1	2.502	5.037	0.741	1	-2.318	1.244	1.364
1	1.914	3.840	0.002	1	-2.419	2.759	1.468
Aspirin				Aspirin			
motif 1, Eint = -4.8 kcal/mol				motif 2, Eint = -3.5 kcal/mol			
8	1.156	-0.222	-0.115	8	-1.787	0.347	-0.753
8	-2.250	2.280	-0.506	8	1.626	-1.953	0.258
8	-0.031	2.158	-0.798	8	-0.568	-2.029	-0.175
8	0.996	1.011	1.782	8	-2.348	-0.121	1.393
6	-0.146	-0.668	0.015	6	-0.594	0.906	-0.348
6	-1.246	0.184	-0.163	6	0.507	0.114	0.021
6	-0.319	-2.019	0.275	6	-0.494	2.288	-0.387
6	-2.527	-0.369	-0.051	6	1.699	0.763	0.371
6	-1.600	-2.547	0.366	6	0.701	2.908	-0.046
6	-2.708	-1.719	0.209	6	1.798	2.145	0.340
6	-1.071	1.611	-0.511	6	0.417	-1.357	0.019
6	1.624	0.707	0.812	6	-2.573	-0.241	0.223
6	2.963	1.194	0.386	6	-3.682	-0.997	-0.419
1	0.562	-2.639	0.405	1	-1.365	2.861	-0.683
1	-3.383	0.281	-0.182	1	2.559	0.174	0.667
1	-1.732	-3.604	0.568	1	0.771	3.991	-0.075
1	-3.710	-2.125	0.286	1	2.731	2.623	0.616
1	3.609	0.362	0.101	1	-4.106	-0.445	-1.258
1	3.417	1.775	1.185	1	-4.450	-1.229	0.315
1	2.829	1.828	-0.494	1	-3.267	-1.929	-0.812
1	-2.036	3.191	-0.751	1	1.445	-2.903	0.280
8	3.230	-1.962	-1.120	8	4.434	-1.209	-0.255
1	2.468	-1.377	-1.027	1	3.522	-1.524	-0.250
1	3.349	-2.056	-2.067	1	4.630	-1.064	-1.183
Aspirin				Aspirin			
motif 3, Eint = -6.9 kcal/mol				motif 4, Eint = -11.5 kcal/mol			
8	0.822	-1.116	-0.117	8	0.471	1.612	-0.611
8	-0.685	2.771	0.508	8	-1.261	-2.177	0.228
8	1.081	1.675	-0.317	8	-1.678	-0.092	-0.493
8	1.089	-0.289	1.980	8	-0.375	1.728	1.489
6	-0.523	-0.809	-0.119	6	1.195	0.477	-0.311
6	-0.999	0.509	-0.028	6	0.585	-0.766	-0.081
6	-1.403	-1.873	-0.252	6	2.576	0.605	-0.308
6	-2.384	0.715	-0.053	6	1.416	-1.867	0.166
6	-2.772	-1.642	-0.300	6	3.378	-0.504	-0.073
6	-3.265	-0.345	-0.194	6	2.796	-1.744	0.170
6	-0.081	1.663	0.034	6	-0.883	-0.949	-0.136
6	1.578	-0.762	0.995	6	-0.372	2.117	0.356
6	3.008	-1.075	0.737	6	-1.223	3.186	-0.239
1	-0.997	-2.875	-0.312	1	3.004	1.584	-0.491
1	-2.755	1.729	0.027	1	0.951	-2.828	0.347
1	-3.453	-2.479	-0.410	1	4.457	-0.395	-0.073
1	-4.333	-0.161	-0.222	1	3.416	-2.613	0.360
1	3.126	-2.131	0.487	1	-0.636	3.854	-0.869
1	3.604	-0.832	1.613	1	-1.723	3.746	0.548
1	3.348	-0.504	-0.131	1	-1.970	2.707	-0.876
1	-0.018	3.471	0.488	1	-2.244	-2.221	0.163
8	2.502	0.140	-2.358	8	-3.906	-1.677	-0.176
1	2.005	-0.679	-2.291	1	-3.492	-0.819	-0.372
1	2.037	0.720	-1.739	1	-4.567	-1.501	0.497
Aspirin				Dantrolene			
motif 5, Eint = -6.4 kcal/mol				motif 1, Eint = -8.1 kcal/mol			
8	0.457	-0.832	-1.119	8	-0.538	-0.426	0.000
8	-1.253	2.794	0.290	8	6.384	2.148	-0.001
8	0.468	1.895	-0.828	8	5.501	-2.360	0.000
8	1.582	-0.383	0.783	8	-7.756	0.333	0.000
6	-0.754	-0.756	-0.460	8	-6.864	2.315	0.000
6	-1.293	0.467	-0.030	7	4.085	-0.496	0.001
6	-1.455	-1.941	-0.299	7	6.269	-0.158	0.000
6	-2.555	0.450	0.578	7	2.931	-1.184	0.001
6	-2.708	-1.931	0.299	7	-6.793	1.091	0.000

6	-3.258	-0.733	0.744	6	4.250	0.947	0.000
6	-0.580	1.744	-0.243	6	-1.618	-1.259	0.000
6	1.592	-0.532	-0.413	6	-2.924	-0.654	0.000
6	2.762	-0.435	-1.324	6	0.581	-1.205	0.000
1	-1.002	-2.862	-0.648	6	5.756	1.111	-0.001
1	-2.977	1.388	0.914	6	5.297	-1.179	0.000
1	-3.251	-2.862	0.423	6	-1.181	-2.565	0.000
1	-4.234	-0.720	1.216	6	0.224	-2.532	0.000
1	2.741	-1.226	-2.074	6	-4.076	-1.462	0.000
1	3.688	-0.462	-0.753	6	-3.078	0.744	0.000
1	2.688	0.520	-1.851	6	1.830	-0.507	0.001
1	-0.717	3.575	0.096	6	-5.455	0.488	0.000
8	4.324	-0.375	1.585	6	-5.336	-0.899	0.000
1	4.569	0.166	2.337	6	-4.337	1.315	0.000
1	3.358	-0.306	1.538	1	3.811	1.428	0.881
				1	3.810	1.427	-0.881
				1	-1.809	-3.443	0.000
				1	7.256	-0.369	-0.001
				1	0.913	-3.361	0.000
				1	-3.976	-2.542	-0.001
				1	-2.197	1.376	0.001
				1	1.783	0.585	0.001
				1	-6.232	-1.506	-0.001
				1	-4.474	2.389	0.000
				8	4.133	3.838	0.000
				1	5.072	3.595	0.000
				1	4.121	4.797	0.005
Dantrolene				Dantrolene			
motif 2, Eint = -5.7 kcal/mol				motif 3, Eint = -5.7 kcal/mol			
8	0.061	-0.452	0.006	8	0.187	-0.053	0.016
8	6.638	2.917	0.052	8	7.111	2.529	-0.056
8	6.275	-1.665	-0.038	8	6.218	-1.980	0.017
8	-7.189	-0.588	0.065	8	-7.048	0.710	-0.008
8	-6.582	1.492	0.019	8	-6.132	2.672	0.043
7	4.661	0.027	-0.001	7	4.811	-0.111	-0.005
7	6.795	0.607	0.005	7	6.999	0.217	-0.021
7	3.596	-0.789	-0.014	7	3.659	-0.798	0.010
7	-6.331	0.285	0.038	7	-6.064	1.451	0.019
6	4.663	1.479	0.027	6	4.982	1.331	-0.028
6	-0.912	-1.407	-0.010	6	-0.891	-0.890	0.032
6	-2.280	-0.964	0.004	6	-2.199	-0.291	0.030
6	1.265	-1.092	-0.012	6	1.308	-0.828	0.021
6	6.144	1.820	0.031	6	6.493	1.497	-0.038
6	5.948	-0.513	-0.015	6	6.028	-0.797	0.000
6	-0.322	-2.652	-0.038	6	-0.449	-2.194	0.048
6	1.069	-2.452	-0.039	6	0.956	-2.157	0.041
6	-3.326	-1.905	-0.010	6	-3.347	-1.103	0.047
6	-2.603	0.404	0.031	6	-2.358	1.107	0.010
6	2.422	-0.251	0.000	6	2.556	-0.128	0.005
6	-4.929	-0.132	0.027	6	-4.735	0.837	0.024
6	-4.643	-1.497	0.002	6	-4.613	-0.551	0.044
6	-3.920	0.826	0.042	6	-3.619	1.670	0.008
1	4.175	1.878	0.924	1	4.549	1.815	0.854
1	4.171	1.913	-0.851	1	4.541	1.788	-0.921
1	-0.841	-3.598	-0.056	1	-1.074	-3.074	0.062
1	7.800	0.508	0.001	1	7.985	0.001	-0.022
1	1.852	-3.193	-0.058	1	1.648	-2.984	0.049
1	-3.098	-2.965	-0.031	1	-3.244	-2.182	0.063
1	-1.807	1.139	0.043	1	-1.482	1.743	-0.005
1	2.242	0.828	0.021	1	2.503	0.965	-0.011
1	-5.459	-2.209	-0.008	1	-5.490	-1.188	0.060
1	-4.157	1.884	0.064	1	-3.760	2.743	-0.007
8	-4.995	3.914	-0.182	8	-7.447	-2.158	-0.217
1	-5.327	4.686	0.280	1	-7.586	-1.203	-0.194
1	-5.724	3.281	-0.153	1	-8.206	-2.524	0.241
Dantrolene				Dantrolene			
motif 4, Eint = -9.3 kcal/mol				motif 5, Eint = -10.1 kcal/mol			
8	-0.471	0.014	-0.005	8	-0.807	0.263	0.003
8	6.196	-3.201	0.007	8	6.073	-2.432	0.020
8	5.683	1.369	-0.024	8	5.254	2.088	0.006
8	-7.726	-0.109	-0.002	8	-8.038	-0.352	-0.006
8	-7.008	-2.160	0.026	8	-7.185	-2.351	-0.001
7	4.138	-0.374	-0.003	7	3.819	0.242	0.010
7	6.287	-0.887	-0.009	7	6.005	-0.121	0.008
7	3.059	0.432	-0.007	7	2.679	0.947	0.007
7	-6.832	-0.947	0.010	7	-7.090	-1.129	-0.003
6	4.177	-1.823	0.005	6	3.967	-1.201	0.013
6	-1.471	0.939	-0.015	6	-1.870	1.119	-0.001
6	-2.825	0.452	-0.009	6	-3.188	0.540	-0.001
6	0.713	0.696	-0.013	6	0.328	1.019	0.003
6	5.669	-2.120	0.002	6	5.472	-1.378	0.014
6	5.403	0.199	-0.013	6	5.050	0.908	0.007
6	-0.919	2.202	-0.030	6	-1.406	2.415	-0.003
6	0.479	2.051	-0.029	6	-0.001	2.353	-0.001

6	-3.901	1.359	-0.021	6	-4.323	1.371	-0.004
6	-3.101	-0.926	0.009	6	-3.369	-0.854	0.001
6	1.889	-0.116	-0.006	6	1.563	0.296	0.007
6	-5.446	-0.463	0.003	6	-5.740	-0.552	-0.003
6	-5.206	0.908	-0.015	6	-5.594	0.832	-0.005
6	-4.405	-1.385	0.016	6	-4.639	-1.401	0.001
1	3.698	-2.259	-0.880	1	3.525	-1.668	-0.875
1	3.703	-2.249	0.896	1	3.523	-1.665	0.900
1	-1.467	3.132	-0.040	1	-2.014	3.306	-0.006
1	7.288	-0.758	-0.014	1	7.014	0.035	0.007
1	1.240	2.820	-0.036	1	0.706	3.168	-0.002
1	-3.706	2.425	-0.036	1	-4.202	2.449	-0.006
1	-2.279	-1.632	0.019	1	-2.501	-1.503	0.004
1	1.733	-1.199	0.000	1	1.491	-0.796	0.009
1	-6.045	1.592	-0.025	1	-6.479	1.457	-0.008
1	-4.637	-2.443	0.030	1	-4.797	-2.472	0.002
8	3.310	3.433	0.097	8	8.564	-1.142	-0.096
1	4.138	3.908	0.007	1	8.020	-1.941	-0.025
1	3.576	2.503	0.063	1	9.418	-1.360	0.280
Dantrolene				Cycloserine			
motif 6, Eint = -10.5 kcal/mol				motif 1, Eint = -5.8 kcal/mol			
8	-0.766	-0.141	0.004	8	-1.065	-0.087	1.174
8	5.917	3.012	0.004	8	1.453	-1.559	-0.706
8	5.397	-1.551	0.019	7	-0.206	-1.184	0.854
8	-8.021	0.017	-0.008	7	1.934	1.285	-0.316
8	-7.293	2.065	-0.007	6	0.612	0.697	-0.249
7	3.845	0.192	0.013	6	-0.192	1.048	0.993
7	6.003	0.697	0.009	6	0.695	-0.817	-0.126
7	2.757	-0.594	0.013	1	-0.011	0.872	-1.141
7	-7.122	0.851	-0.006	1	0.471	1.154	1.861
6	3.897	1.643	0.004	1	-0.845	1.916	0.903
6	-1.771	-1.064	0.003	1	-0.745	-2.037	0.769
6	-3.124	-0.571	0.000	1	1.930	2.105	-0.911
6	0.416	-0.822	0.007	1	2.557	0.613	-0.760
6	5.391	1.929	0.005	8	-2.442	0.241	-1.274
6	5.115	-0.377	0.014	1	-2.328	0.094	-0.325
6	-1.225	-2.328	0.005	1	-3.390	0.240	-1.417
6	0.174	-2.175	0.007				
6	-4.205	-1.471	-0.001				
6	-3.392	0.810	0.000				
6	1.600	-0.020	0.008				
6	-5.739	0.359	-0.004				
6	-5.507	-1.013	-0.004				
6	-4.694	1.276	-0.003				
1	3.420	2.080	0.889				
1	3.424	2.069	-0.887				
1	-1.775	-3.256	0.005				
1	7.008	0.515	0.008				
1	0.931	-2.943	0.009				
1	-4.016	-2.539	-0.001				
1	-2.567	1.511	0.001				
1	1.455	1.065	0.004				
1	-6.350	-1.693	-0.005				
1	-4.919	2.335	-0.003				
8	8.156	-1.042	-0.113				
1	8.867	-1.466	0.370				
1	7.391	-1.634	-0.041				
Cycloserine				Cycloserine			
motif 2, Eint = -6.8 kcal/mol				motif 3, Eint = -10.4 kcal/mol			
8	-0.888	-0.975	-0.143	8	-0.388	1.814	0.107
8	0.913	1.990	-0.026	8	0.808	-1.452	0.060
7	-0.700	0.401	-0.485	7	0.592	0.833	-0.159
7	2.659	-0.315	-0.026	7	-2.068	-1.359	-0.299
6	1.288	-0.387	0.427	6	-1.340	-0.303	0.370
6	0.449	-1.495	-0.186	6	-1.612	1.102	-0.145
6	0.508	0.847	-0.018	6	0.153	-0.417	0.093
1	1.176	-0.411	1.526	1	-1.431	-0.320	1.471
1	0.760	-1.667	-1.225	1	-1.817	1.065	-1.223
1	0.429	-2.437	0.362	1	-2.397	1.656	0.371
1	-1.581	0.892	-0.343	1	1.558	1.140	-0.067
1	3.285	-0.762	0.633	1	-2.899	-1.613	0.221
1	2.928	0.667	-0.060	1	-1.475	-2.186	-0.325
8	-3.388	0.216	0.311	8	3.202	-0.025	-0.104
1	-4.256	0.150	-0.092	1	2.629	-0.811	-0.060
1	-3.032	-0.679	0.293	1	3.984	-0.243	0.405
Cycloserine				Cycloserine			
motif 4, Eint = -8.7 kcal/mol				motif 5, Eint = -7.7 kcal/mol			
8	2.341	-0.189	0.288	8	-1.734	-0.976	-0.293
8	-0.847	-1.451	-0.226	8	-0.066	2.070	-0.207
7	1.426	-1.153	-0.207	7	-1.331	0.254	-0.875
7	-0.722	1.532	-0.508	7	1.323	0.082	1.326
6	0.190	0.739	0.288	6	-0.100	-0.029	1.058
6	1.655	1.042	0.015	6	-0.568	-1.349	0.465
6	0.132	-0.743	-0.066	6	-0.486	0.942	-0.053

1	0.001	0.770	1.379	1	-0.738	0.238	1.919
1	1.781	1.322	-1.039	1	0.200	-1.761	-0.201
1	2.110	1.792	0.662	1	-0.905	-2.096	1.183
1	1.732	-2.094	0.002	1	-2.083	0.681	-1.398
1	-0.730	2.484	-0.157	1	1.558	-0.326	2.224
1	-1.674	1.184	-0.375	1	1.550	1.073	1.386
8	-3.178	-0.023	0.323	8	2.197	-0.740	-1.352
1	-3.997	-0.302	-0.091	1	2.126	-0.462	-0.422
1	-2.537	-0.725	0.117	1	2.098	0.077	-1.847
Aminoglutethimide motif 1, Eint = -9.1 kcal/mol				Aminoglutethimide motif 2, Eint = -7.4 kcal/mol			
8	-1.769	0.137	-1.743	8	0.630	2.281	1.713
8	-2.156	-2.120	2.156	8	2.973	-1.541	1.273
7	-1.957	-0.916	0.249	7	1.775	0.364	1.398
7	4.908	-1.062	-0.493	7	-4.681	-1.764	0.201
6	-0.430	1.028	0.060	6	0.253	1.142	-0.401
6	-0.796	1.195	1.545	6	1.291	0.440	-1.288
6	-0.472	2.373	-0.693	6	-0.157	2.510	-0.984
6	0.972	0.424	-0.084	6	-1.018	0.305	-0.208
6	-0.794	-0.140	2.266	6	1.762	-0.881	-0.704
6	-1.440	0.072	-0.567	6	0.880	1.353	0.975
6	-1.685	-1.154	1.601	6	2.233	-0.750	0.713
6	-1.787	3.130	-0.609	6	0.982	3.477	-1.265
6	1.248	-0.695	-0.872	6	-1.849	0.506	0.899
6	2.051	1.022	0.574	6	-1.448	-0.613	-1.170
6	2.535	-1.201	-0.992	6	-3.041	-0.186	1.049
6	3.340	0.528	0.462	6	-2.639	-1.310	-1.032
6	3.606	-0.600	-0.325	6	-3.457	-1.112	0.086
1	-1.789	1.650	1.622	1	2.154	1.105	-1.404
1	-0.103	1.894	2.023	1	0.892	0.298	-2.296
1	-0.227	2.171	-1.739	1	-0.863	2.967	-0.284
1	0.344	2.992	-0.301	1	-0.723	2.312	-1.902
1	-1.111	-0.060	3.307	1	2.568	-1.338	-1.282
1	0.218	-0.564	2.282	1	0.953	-1.622	-0.694
1	-2.594	-1.576	-0.208	1	2.123	0.474	2.345
1	-2.627	2.516	-0.945	1	1.593	3.646	-0.374
1	-2.005	3.477	0.404	1	1.638	3.128	-2.066
1	-1.760	4.015	-1.249	1	0.591	4.448	-1.575
1	0.450	-1.189	-1.418	1	-1.564	1.225	1.661
1	1.887	1.900	1.193	1	-0.850	-0.796	-2.058
1	2.715	-2.072	-1.616	1	-3.662	-0.006	1.921
1	4.156	1.020	0.984	1	-2.943	-2.015	-1.800
1	5.541	-0.837	0.260	1	-4.749	-2.636	-0.302
1	4.983	-2.033	-0.758	1	-5.027	-1.855	1.144
8	-3.597	-1.951	-1.860	8	3.598	-3.470	-0.711
1	-3.053	-1.231	-2.219	1	3.506	-2.951	0.105
1	-3.592	-2.641	-2.526	1	4.349	-4.044	-0.551
Aminoglutethimide motif 3, Eint = -9.4 kcal/mol				Abacavir motif 1, Eint = -6.6 kcal/mol			
8	-1.458	0.794	-2.000	8	-4.517	1.942	0.340
8	-2.616	-2.009	1.353	7	4.002	-0.362	-0.367
7	-2.014	-0.552	-0.277	7	-0.350	-1.799	0.031
7	4.807	-1.518	-0.297	7	1.791	-2.443	-0.278
6	-0.267	1.179	0.075	7	2.316	1.219	-0.071
6	-0.835	1.159	1.503	7	-0.021	0.616	0.175
6	-0.023	2.618	-0.422	7	0.680	2.813	0.190
6	1.053	0.404	-0.012	6	5.012	0.622	-0.592
6	-1.099	-0.259	1.975	6	5.559	1.368	0.584
6	-1.286	0.498	-0.838	6	6.389	0.317	-0.092
6	-1.971	-1.027	1.022	6	-1.802	-1.912	0.196
6	-1.225	3.546	-0.361	6	-2.600	-1.088	-0.839
6	1.363	-0.430	-1.089	6	-3.612	-0.237	-0.044
6	2.033	0.567	0.971	6	-2.285	-1.400	1.524
6	2.585	-1.082	-1.175	6	-3.262	-0.509	1.389
6	3.258	-0.077	0.895	6	2.688	-0.058	-0.205
6	3.556	-0.920	-0.183	6	0.401	-0.645	0.033
1	-1.772	1.727	1.520	6	1.713	-1.072	-0.159
1	-0.159	1.677	2.189	6	-3.522	1.233	-0.412
1	0.340	2.551	-1.451	6	0.547	-2.830	-0.159
1	0.804	3.030	0.169	6	1.005	1.476	0.109
1	-1.574	-0.299	2.956	1	4.923	1.176	-1.524
1	-0.157	-0.816	2.064	1	5.132	1.129	1.550
1	-2.643	-1.057	-0.911	1	5.819	2.410	0.444
1	-2.079	3.131	-0.903	1	7.230	0.624	-0.702
1	-1.542	3.753	0.664	1	6.530	-0.623	0.429
1	-0.989	4.508	-0.821	1	-2.004	-2.986	0.095
1	0.644	-0.572	-1.890	1	-3.092	-1.733	-1.569
1	1.846	1.216	1.822	1	-1.914	-0.444	-1.394
1	2.794	-1.722	-2.028	1	-4.642	-0.559	-0.248
1	3.999	0.076	1.675	1	4.198	-1.323	-0.608
1	5.295	-1.657	0.576	1	-1.861	-1.750	2.458
1	4.831	-2.350	-0.868	1	-3.772	-0.011	2.206
8	-3.971	-2.502	-1.022	1	-3.702	1.357	-1.489
1	-3.987	-3.355	-1.460	1	-2.516	1.607	-0.181

1	-3.685	-2.678	-0.110	1	0.200	-3.855	-0.201
				1	-4.394	2.882	0.188
				1	1.450	3.412	0.445
				1	-0.186	3.006	0.667
				8	-6.733	0.780	-1.009
				1	-6.138	1.261	-0.413
				1	-7.572	0.753	-0.545
Abacavir				Abacavir			
motif 2, Eint = -11.8 kcal/mol				motif 3, Eint = -12.4 kcal/mol			
8	5.366	-1.897	-0.081	8	5.578	-1.298	-0.393
7	-3.346	-0.071	-0.238	7	-3.815	0.551	-0.297
7	0.957	1.595	0.062	7	0.602	1.745	0.145
7	-1.214	2.156	-0.090	7	-1.511	2.508	-0.072
7	-1.558	-1.543	-0.119	7	-2.207	-1.129	-0.189
7	0.752	-0.830	0.046	7	0.160	-0.658	0.071
7	0.169	-3.057	-0.058	7	-0.651	-2.812	-0.107
6	-4.287	-1.136	-0.376	6	-4.881	-0.358	-0.576
6	-4.799	-1.826	0.852	6	-5.431	-1.181	0.546
6	-5.680	-0.875	0.095	6	-6.225	-0.034	-0.004
6	2.409	1.759	0.172	6	2.055	1.791	0.275
6	3.191	1.049	-0.956	6	2.807	1.192	-0.927
6	4.294	0.217	-0.273	6	4.065	0.533	-0.340
6	2.976	1.174	1.434	6	2.602	1.016	1.444
6	3.996	0.357	1.191	6	3.704	0.351	1.108
6	-2.017	-0.284	-0.148	6	-2.516	0.169	-0.196
6	0.254	0.409	0.016	6	-0.201	0.631	0.049
6	-1.084	0.779	-0.079	6	-1.492	1.130	-0.082
6	4.300	-1.228	-0.741	6	4.441	-0.754	-1.051
6	0.018	2.595	-0.005	6	-0.252	2.830	0.063
6	-0.231	-1.739	-0.028	6	-0.908	-1.473	-0.060
1	-4.154	-1.751	-1.262	1	-4.847	-0.827	-1.557
1	-4.396	-1.494	1.801	1	-4.964	-1.054	1.514
1	-5.003	-2.888	0.790	1	-5.748	-2.192	0.320
1	-6.500	-1.272	-0.491	1	-7.098	-0.242	-0.610
1	-5.877	0.094	0.540	1	-6.303	0.860	0.605
1	2.563	2.846	0.143	1	2.289	2.859	0.395
1	3.594	1.764	-1.674	1	3.018	1.931	-1.703
1	2.511	0.392	-1.505	1	2.172	0.418	-1.373
1	5.291	0.630	-0.485	1	4.930	1.212	-0.404
1	-3.678	0.889	-0.324	1	-3.968	1.539	-0.439
1	2.574	1.425	2.410	1	2.154	1.069	2.430
1	4.572	-0.172	1.942	1	4.322	-0.236	1.780
1	4.432	-1.258	-1.834	1	4.662	-0.540	-2.109
1	3.325	-1.681	-0.508	1	3.595	-1.452	-1.011
1	0.314	3.635	0.011	1	0.141	3.837	0.113
1	5.350	-2.820	-0.341	1	5.711	-2.191	-0.719
1	-0.551	-3.717	0.192	1	-1.447	-3.412	0.029
1	1.074	-3.234	0.350	1	0.249	-3.128	0.235
8	-3.932	2.796	-0.409	8	2.180	-2.553	0.663
1	-2.961	2.846	-0.284	1	2.707	-2.420	1.453
1	-4.304	3.333	0.293	1	1.707	-1.704	0.533
Abacavir				diazepam			
motif 4, Eint = -11.2 kcal/mol				motif 1, Eint = -5.4 kcal/mol			
8	-4.957	2.401	0.088	17	-0.648	4.083	-0.317
7	3.290	-1.002	-0.312	8	3.670	-2.675	-0.321
7	-1.225	-1.813	-0.046	7	2.718	-0.757	0.449
7	0.817	-2.754	-0.257	7	0.467	-2.033	-1.024
7	1.828	0.807	-0.152	6	0.548	0.251	-0.154
7	-0.576	0.537	0.026	6	1.899	0.371	0.234
7	0.412	2.618	-0.010	6	-0.086	-1.064	-0.385
6	4.458	-0.187	-0.405	6	1.792	-1.810	-1.561
6	4.977	0.471	0.840	6	2.822	-1.817	-0.449
6	5.704	-0.697	0.247	6	-1.461	-1.281	0.129
6	-2.681	-1.723	0.094	6	-0.225	1.409	-0.322
6	-3.344	-0.830	-0.978	6	2.422	1.648	0.482
6	-4.272	0.146	-0.228	6	3.739	-0.695	1.488
6	-3.113	-1.112	1.397	6	0.328	2.656	-0.095
6	-3.976	-0.118	1.219	6	1.650	2.785	0.321
6	2.028	-0.515	-0.225	6	-1.925	-0.629	1.276
6	-0.324	-0.772	-0.060	6	-2.316	-2.168	-0.536
6	0.921	-1.381	-0.193	6	-3.214	-0.852	1.745
6	-4.033	1.592	-0.628	6	-3.609	-2.378	-0.077
6	-0.471	-2.964	-0.166	6	-4.064	-1.720	1.066
6	0.552	1.258	-0.032	1	1.862	-0.853	-2.102
1	4.569	0.366	-1.337	1	2.049	-2.618	-2.245
1	4.406	0.304	1.746	1	-1.262	1.319	-0.634
1	5.400	1.463	0.749	1	3.454	1.750	0.794
1	6.647	-0.525	-0.258	1	3.357	-0.129	2.337
1	5.638	-1.647	0.764	1	4.666	-0.231	1.131
1	-3.026	-2.763	0.018	1	3.976	-1.712	1.793
1	-3.879	-1.425	-1.720	1	2.071	3.767	0.505
1	-2.569	-0.274	-1.513	1	-1.270	0.055	1.806
1	-5.329	-0.076	-0.432	1	-1.945	-2.676	-1.420
1	3.367	-1.996	-0.476	1	-3.556	-0.346	2.642

1	-2.743	-1.479	2.348	1	-4.267	-3.058	-0.609
1	-4.435	0.466	2.009	1	-5.074	-1.888	1.426
1	-4.173	1.700	-1.715	8	-3.360	1.017	-1.311
1	-2.991	1.858	-0.395	1	-3.632	0.155	-0.976
1	-0.953	-3.932	-0.181	1	-4.012	1.624	-0.951
1	-4.779	3.320	-0.122				
1	1.244	3.163	0.186				
1	-0.463	2.955	0.354				
8	3.334	3.221	0.022				
1	3.605	3.499	-0.855				
1	3.060	2.287	-0.090				
diazepam motif 2, Eint = -3.7 kcal/mol				diazepam motif 3, Eint = -6.8 kcal/mol			
17	-2.951	-2.495	-0.734	17	3.333	-2.979	-1.012
8	1.210	4.322	-0.070	8	-3.907	0.050	0.591
7	-0.090	2.558	0.545	7	-1.914	-0.976	0.927
7	2.056	1.237	-1.027	7	-1.152	1.371	-0.719
6	-0.035	0.231	-0.269	6	0.263	-0.534	-0.147
6	-0.741	1.353	0.215	6	-0.666	-1.419	0.438
6	1.431	0.258	-0.474	6	-0.026	0.911	-0.303
6	1.275	2.366	-1.480	6	-2.187	0.418	-1.067
6	0.819	3.197	-0.297	6	-2.772	-0.169	0.199
6	2.234	-0.908	-0.033	6	1.039	1.889	0.025
6	-0.743	-0.944	-0.551	6	1.493	-1.038	-0.587
6	-2.121	1.243	0.438	6	-0.317	-2.766	0.599
6	-0.605	3.354	1.653	6	-2.466	-1.606	2.121
6	-2.109	-1.009	-0.349	6	1.803	-2.379	-0.443
6	-2.813	0.076	0.162	6	0.904	-3.251	0.165
6	1.809	-1.739	1.010	6	2.049	1.595	0.949
6	3.470	-1.166	-0.638	6	1.015	3.159	-0.565
6	2.600	-2.800	1.437	6	3.010	2.545	1.273
6	4.253	-2.230	-0.217	6	1.980	4.102	-0.248
6	3.821	-3.052	0.822	6	2.982	3.798	0.672
1	0.390	2.055	-2.057	1	-1.802	-0.404	-1.691
1	1.893	3.008	-2.107	1	-2.989	0.923	-1.604
1	-0.207	-1.809	-0.925	1	2.211	-0.364	-1.041
1	-2.667	2.096	0.824	1	-1.023	-3.447	1.060
1	-0.956	2.690	2.442	1	-1.654	-1.858	2.803
1	-1.423	4.014	1.344	1	-3.035	-2.511	1.883
1	0.203	3.981	2.025	1	-3.146	-0.903	2.596
1	-3.883	0.010	0.332	1	1.155	-4.298	0.283
1	0.863	-1.543	1.505	1	2.072	0.622	1.431
1	3.798	-0.512	-1.439	1	0.224	3.382	-1.273
1	2.262	-3.429	2.255	1	3.781	2.305	1.998
1	5.205	-2.423	-0.701	1	1.955	5.078	-0.720
1	4.435	-3.884	1.150	1	3.736	4.538	0.920
8	-5.829	-1.122	0.299	8	-5.389	1.247	-1.519
1	-5.312	-1.866	-0.027	1	-5.047	0.899	-0.680
1	-6.516	-1.521	0.837	1	-5.889	2.026	-1.271
diazepam motif 4, Eint = -7.3 kcal/mol				diazepam motif 5, Eint = -7.4 kcal/mol			
17	-2.093	3.995	-0.423	17	-3.348	-2.909	-0.942
8	3.487	-1.745	-0.474	8	0.225	4.165	0.275
7	2.145	-0.098	0.339	7	-0.987	2.289	0.711
7	0.233	-1.758	-1.207	7	1.363	1.200	-0.729
6	-0.174	0.467	-0.290	6	-0.687	0.005	-0.179
6	1.118	0.847	0.128	6	-1.512	1.052	0.287
6	-0.523	-0.948	-0.553	6	0.782	0.145	-0.271
6	1.488	-1.247	-1.717	6	0.534	2.287	-1.206
6	2.477	-1.070	-0.586	6	-0.068	3.029	-0.030
6	-1.817	-1.468	-0.051	6	1.633	-0.982	0.175
6	-1.152	1.457	-0.453	6	-1.277	-1.211	-0.551
6	1.377	2.195	0.405	6	-2.892	0.828	0.399
6	3.091	0.122	1.432	6	-1.643	2.991	1.808
6	-0.863	2.786	-0.199	6	-2.644	-1.394	-0.458
6	0.401	3.163	0.245	6	-3.460	-0.378	0.031
6	-2.446	-0.910	1.068	6	1.209	-1.848	1.192
6	-2.408	-2.575	-0.674	6	2.901	-1.172	-0.390
6	-3.636	-1.442	1.551	6	2.033	-2.874	1.636
6	-3.599	-3.098	-0.196	6	3.716	-2.204	0.050
6	-4.218	-2.533	0.917	6	3.287	-3.058	1.063
1	1.366	-0.282	-2.235	1	-0.276	1.931	-1.861
1	1.916	-1.965	-2.415	1	1.150	2.993	-1.763
1	-2.146	1.172	-0.776	1	-0.646	-2.017	-0.911
1	2.366	2.489	0.738	1	-3.530	1.621	0.769
1	2.579	0.633	2.246	1	-1.991	2.267	2.544
1	3.963	0.702	1.119	1	-2.489	3.597	1.465
1	3.453	-0.844	1.781	1	-0.917	3.664	2.261
1	0.618	4.205	0.450	1	-4.530	-0.530	0.111
1	-1.992	-0.065	1.576	1	0.236	-1.704	1.651
1	-1.909	-3.009	-1.533	1	3.240	-0.506	-1.176
1	-4.106	-1.004	2.425	1	1.695	-3.530	2.432
1	-4.051	-3.950	-0.694	1	4.692	-2.344	-0.403
1	-5.151	-2.945	1.289	1	3.928	-3.864	1.405

8	5.946	-0.966	0.768	8	4.090	1.844	-1.494
1	6.686	-1.503	0.481	1	3.224	1.653	-1.092
1	5.180	-1.345	0.309	1	4.516	2.441	-0.876
Anisindione motif 1, Eint = -7.9 kcal/mol				Anisindione motif 2, Eint = -7.9 kcal/mol			
8	0.945	2.014	-0.612	8	-0.582	-2.689	-1.096
8	0.585	-2.687	-1.108	8	-0.945	2.011	-0.596
8	-5.101	0.429	0.489	8	5.105	0.447	0.490
6	0.268	-0.260	-1.186	6	-0.267	-0.262	-1.173
6	1.175	0.821	-0.586	6	-0.980	-1.574	-0.842
6	0.981	-1.572	-0.853	6	-1.177	0.818	-0.575
6	2.353	0.154	0.003	6	-2.248	-1.234	-0.159
6	2.244	-1.231	-0.161	6	-2.359	0.151	0.005
6	-1.166	-0.145	-0.739	6	1.168	-0.142	-0.728
6	3.458	0.722	0.637	6	-3.242	-2.093	0.296
6	3.236	-2.090	0.301	6	-3.468	0.718	0.631
6	-1.995	0.825	-1.314	6	1.975	0.867	-1.267
6	-1.684	-0.933	0.284	6	1.710	-0.966	0.253
6	4.445	-0.140	1.099	6	-4.348	-1.532	0.921
6	4.338	-1.528	0.933	6	-4.458	-0.145	1.086
6	-3.299	0.995	-0.886	6	3.279	1.041	-0.843
6	-2.996	-0.775	0.725	6	3.023	-0.805	0.690
6	-3.809	0.193	0.139	6	3.813	0.204	0.141
6	-5.649	-0.367	1.520	6	5.676	-0.384	1.479
1	0.312	-0.135	-2.278	1	-0.312	-0.136	-2.265
1	3.537	1.798	0.765	1	-3.143	-3.165	0.162
1	3.138	-3.162	0.166	1	-3.548	1.794	0.759
1	-1.607	1.458	-2.106	1	1.567	1.527	-2.025
1	-1.070	-1.701	0.744	1	1.116	-1.767	0.682
1	5.319	0.266	1.599	1	-5.142	-2.173	1.289
1	5.130	-2.169	1.307	1	-5.335	0.261	1.580
1	-3.945	1.742	-1.333	1	3.908	1.819	-1.262
1	-3.369	-1.413	1.517	1	3.416	-1.470	1.448
1	-5.648	-1.430	1.252	1	5.138	-0.307	2.431
1	-6.676	-0.031	1.650	1	6.698	-0.035	1.616
1	-5.104	-0.237	2.462	1	5.693	-1.434	1.163
8	2.827	3.863	0.466	8	-2.840	3.861	0.459
1	2.074	3.387	0.079	1	-2.473	4.677	0.802
1	2.454	4.678	0.806	1	-2.083	3.385	0.082
Anisindione motif 3, Eint = -5.1 kcal/mol				Anisindione motif 4, Eint = -5.1 kcal/mol			
8	1.103	2.379	-0.091	8	1.124	2.367	-0.321
8	1.699	-2.173	-1.287	8	1.746	-2.270	-1.111
8	-4.528	-0.480	0.446	8	-4.522	-0.434	0.316
6	0.903	0.132	-1.057	6	0.946	0.046	-1.095
6	1.574	1.283	-0.284	6	1.597	1.258	-0.404
6	1.873	-1.039	-0.901	6	1.910	-1.108	-0.813
6	2.899	0.801	0.168	6	2.906	0.816	0.127
6	3.074	-0.536	-0.194	6	3.089	-0.546	-0.115
6	-0.531	-0.103	-0.667	6	-0.498	-0.156	-0.724
6	3.889	1.496	0.856	6	3.877	1.567	0.784
6	4.247	-1.217	0.120	6	4.250	-1.198	0.291
6	-1.505	0.823	-1.057	6	-1.457	0.747	-1.200
6	-0.922	-1.181	0.121	6	-0.916	-1.177	0.124
6	5.059	0.817	1.171	6	5.036	0.917	1.190
6	5.236	-0.525	0.806	6	5.220	-0.451	0.946
6	-2.827	0.677	-0.677	6	-2.788	0.632	-0.841
6	-2.249	-1.344	0.513	6	-2.253	-1.307	0.495
6	-3.201	-0.411	0.114	6	-3.190	-0.397	0.012
6	-4.959	-1.588	1.214	6	-4.979	-1.465	1.174
1	0.939	0.425	-2.117	1	1.011	0.248	-2.175
1	3.739	2.534	1.133	1	3.722	2.625	0.967
1	4.371	-2.256	-0.167	1	4.380	-2.258	0.097
1	-1.218	1.676	-1.665	1	-1.150	1.555	-1.855
1	-0.195	-1.925	0.428	1	-0.202	-1.903	0.497
1	5.851	1.328	1.708	1	5.813	1.472	1.706
1	6.163	-1.026	1.068	1	6.137	-0.928	1.277
1	-3.585	1.389	-0.987	1	-3.532	1.325	-1.218
1	-2.523	-2.199	1.119	1	-2.548	-2.118	1.150
1	-4.772	-2.531	0.690	1	-4.809	-2.452	0.732
1	-6.030	-1.461	1.356	1	-6.048	-1.301	1.299
1	-4.463	-1.615	2.191	1	-4.487	-1.417	2.152
8	-6.064	1.960	0.040	8	-6.272	1.881	0.424
1	-5.609	1.122	0.196	1	-5.767	2.569	0.860
1	-5.702	2.547	0.707	1	-5.643	1.153	0.331
Ethinamate motif 1, Eint = -8.0 kcal/mol				Ethinamate motif 2, Eint = -6.6 kcal/mol			
8	0.691	0.224	-0.063	8	0.164	0.585	0.979
8	1.760	-1.273	1.296	8	2.170	0.393	-0.095
7	2.555	0.850	0.979	7	2.002	0.301	2.178
6	-0.407	-0.705	-0.355	6	-0.611	0.712	-0.268
6	-1.305	0.103	-1.304	6	-2.051	0.852	0.243
6	-1.182	-1.065	0.920	6	-0.485	-0.544	-1.140
6	-1.907	1.330	-0.629	6	-2.522	-0.402	0.970

6	-1.762	0.171	1.596	6	-0.936	-1.795	-0.399
6	-2.657	0.955	0.643	6	-2.366	-1.649	0.107
6	0.108	-1.889	-1.033	6	-0.199	1.915	-0.981
6	1.694	-0.181	0.786	6	1.501	0.437	0.918
6	0.469	-2.860	-1.646	6	0.070	2.920	-1.585
1	-2.098	-0.571	-1.646	1	-2.684	1.048	-0.631
1	-0.726	0.374	-2.194	1	-2.115	1.735	0.885
1	-0.536	-1.632	1.589	1	0.530	-0.646	-1.518
1	-1.992	-1.737	0.610	1	-1.131	-0.373	-2.011
1	-2.571	1.839	-1.334	1	-3.565	-0.271	1.277
1	-1.113	2.045	-0.385	1	-1.942	-0.521	1.893
1	-0.946	0.813	1.949	1	-0.255	-1.988	0.440
1	-2.319	-0.132	2.488	1	-0.837	-2.658	-1.062
1	-3.049	1.852	1.132	1	-2.671	-2.539	0.667
1	-3.530	0.340	0.382	1	-3.046	-1.580	-0.754
1	0.811	-3.726	-2.158	1	0.336	3.798	-2.121
1	2.537	1.647	0.352	1	1.428	0.564	2.962
1	3.418	0.618	1.442	1	2.999	0.385	2.275
8	1.656	2.629	-1.194	8	2.505	-2.236	-1.152
1	1.118	1.825	-1.168	1	3.256	-2.359	-1.735
1	1.946	2.709	-2.105	1	2.576	-1.315	-0.863
Ethinamate motif 3, Eint = -10.2 kcal/mol				Fenoprofen motif 1, Eint = -4.9 kcal/mol			
8	-0.155	-0.197	-0.783	8	-1.724	0.956	0.321
8	-1.849	0.134	0.705	8	4.366	-1.721	-0.552
7	-2.097	-1.223	-1.116	8	2.138	-1.803	-0.829
6	0.765	0.682	-0.049	6	3.125	0.009	0.469
6	2.029	0.665	-0.919	6	1.958	0.914	0.160
6	1.072	0.113	1.344	6	0.652	0.488	0.399
6	2.661	-0.720	-0.987	6	3.173	-0.413	1.945
6	1.694	-1.274	1.264	6	2.174	2.186	-0.368
6	2.952	-1.272	0.403	6	-0.412	1.318	0.076
6	0.223	2.033	0.020	6	3.109	-1.246	-0.383
6	-1.411	-0.372	-0.314	6	1.098	3.021	-0.655
6	-0.146	3.178	0.056	6	-0.205	2.592	-0.443
1	2.731	1.383	-0.480	6	-2.152	-0.346	0.140
1	1.775	1.039	-1.914	6	-1.581	-1.215	-0.786
1	0.163	0.121	1.945	6	-3.260	-0.727	0.891
1	1.774	0.812	1.816	6	-2.127	-2.484	-0.941
1	3.578	-0.670	-1.583	6	-3.798	-1.996	0.717
1	1.984	-1.399	-1.517	6	-3.232	-2.882	-0.195
1	0.963	-1.979	0.847	1	4.054	0.540	0.239
1	1.917	-1.629	2.275	1	0.463	-0.499	0.807
1	3.373	-2.279	0.334	1	3.214	0.470	2.585
1	3.718	-0.650	0.888	1	2.283	-0.985	2.219
1	-0.503	4.178	0.101	1	4.051	-1.030	2.149
1	-1.733	-1.414	-2.035	1	3.189	2.523	-0.557
1	-3.097	-1.274	-0.958	1	1.274	4.012	-1.059
8	-4.521	-0.538	0.267	1	-1.059	3.222	-0.669
1	-3.740	-0.161	0.710	1	-0.718	-0.912	-1.368
1	-5.052	-0.916	0.970	1	-3.683	-0.024	1.601
Fenoprofen motif 2, Eint = -4.9 kcal/mol				Fenoprofen motif 3, Eint = -10.3 kcal/mol			
8	-2.262	1.551	0.254	8	-1.408	2.007	0.246
8	3.341	-2.056	-0.659	8	3.226	-1.620	-1.539
8	1.150	-1.732	-1.014	8	1.318	-2.329	-0.605
6	2.394	-0.118	0.331	6	2.691	-0.713	0.585
6	1.370	0.952	0.046	6	1.995	0.609	0.309
6	0.018	0.720	0.292	6	0.609	0.687	0.428
6	2.408	-0.549	1.806	6	2.321	-1.312	1.938
6	1.772	2.188	-0.459	6	2.719	1.732	-0.092
6	-0.919	1.706	0.002	6	-0.042	1.877	0.123
6	2.178	-1.347	-0.524	6	2.319	-1.650	-0.543
6	0.829	3.180	-0.716	6	2.056	2.927	-0.358
6	-0.520	2.944	-0.495	6	0.673	3.008	-0.260
6	-2.861	0.316	0.134	6	-2.206	0.922	-0.039
6	-2.479	-0.624	-0.820	6	-1.966	0.096	-1.136
6	-3.946	0.077	0.973	6	-3.311	0.713	0.779
6	-3.188	-1.816	-0.916	6	-2.839	-0.952	-1.403
6	-4.649	-1.115	0.859	6	-4.178	-0.337	0.500
6	-4.273	-2.069	-0.082	6	-3.945	-1.178	-0.586
1	3.392	0.268	0.096	1	3.771	-0.545	0.526
1	-0.312	-0.235	0.683	1	0.034	-0.177	0.750
1	2.598	0.321	2.438	1	2.590	-0.619	2.737
1	1.447	-0.979	2.101	1	1.250	-1.512	2.007
1	3.194	-1.281	1.997	1	2.848	-2.253	2.109
1	2.825	2.373	-0.648	1	3.798	1.670	-0.194

1	1.147	4.142	-1.103	1	2.622	3.803	-0.659
1	-1.272	3.697	-0.699	1	0.139	3.926	-0.477
1	-1.633	-0.433	-1.471	1	-1.100	0.271	-1.765
1	-4.223	0.832	1.700	1	-3.471	1.371	1.625
1	-2.887	-2.550	-1.657	1	-2.652	-1.595	-2.256
1	-5.494	-1.300	1.514	1	-5.036	-0.505	1.143
1	3.120	-2.851	-1.164	1	2.892	-2.199	-2.240
1	-4.820	-3.002	-0.165	1	-4.621	-1.999	-0.796
8	5.589	-0.708	0.600	8	-0.935	-2.270	1.238
1	6.486	-0.773	0.267	1	-0.289	-2.432	0.536
1	5.085	-1.343	0.078	1	-1.757	-2.093	0.770
Fenoprofen motif 4, Eint = -11.5 kcal/mol				Acetazolamide motif 1, Eint = -11.9 kcal/mol			
8	-2.265	1.505	-0.038	16	2.584	-0.563	-0.001
8	3.873	-1.220	0.069	16	-0.367	-1.503	0.026
8	1.659	-1.408	-0.288	8	2.676	-1.933	0.457
6	2.538	0.608	0.736	8	3.131	-0.109	-1.259
6	1.416	1.440	0.167	8	-3.697	1.370	0.746
6	0.087	1.053	0.343	7	-2.895	-0.509	-0.298
6	2.423	0.420	2.255	7	0.312	0.949	-0.262
6	1.698	2.609	-0.539	7	3.188	0.415	1.164
6	-0.936	1.815	-0.209	7	-1.037	0.967	-0.369
6	2.618	-0.768	0.100	6	0.808	-0.238	-0.076
6	0.665	3.382	-1.061	6	-1.546	-0.232	-0.245
6	-0.656	2.988	-0.907	6	-3.919	0.332	0.183
6	-2.678	0.192	0.001	6	-5.294	-0.206	-0.109
6	-2.063	-0.822	-0.731	1	-3.162	-1.424	-0.629
6	-3.816	-0.070	0.759	1	3.081	1.411	0.915
6	-2.595	-2.105	-0.687	1	2.858	0.179	2.092
6	-4.339	-1.356	0.787	1	-5.608	0.139	-1.097
6	-3.731	-2.381	0.068	1	-5.995	0.189	0.623
1	3.489	1.109	0.527	1	-5.341	-1.297	-0.106
1	-0.151	0.145	0.884	8	2.494	2.892	-0.086
1	2.398	1.392	2.752	1	2.960	2.892	-0.927
1	1.507	-0.114	2.517	1	1.623	2.516	-0.296
1	3.272	-0.145	2.647				
1	2.731	2.914	-0.679				
1	0.892	4.293	-1.604				
1	-1.476	3.568	-1.314				
1	-1.175	-0.613	-1.317				
1	-4.276	0.742	1.311				
1	-2.116	-2.895	-1.257				
1	-5.227	-1.558	1.378				
1	3.859	-2.135	-0.300				
1	-4.139	-3.386	0.095				
8	3.145	-3.592	-1.057				
1	3.053	-4.469	-0.680				
1	2.287	-3.152	-0.929				
Acetazolamide motif 2, Eint = -11.8 kcal/mol				Acetazolamide motif 3, Eint = -8.8 kcal/mol			
16	-2.582	-0.550	-0.197	16	-3.072	0.001	0.004
16	0.355	-1.504	0.039	16	-0.348	-1.450	0.302
8	-2.992	0.101	-1.419	8	-3.503	-1.012	-0.930
8	-2.707	-1.975	0.029	8	-3.475	0.004	1.390
8	3.761	1.364	-0.712	8	3.263	0.206	-1.468
7	2.881	-0.501	0.300	7	2.335	-0.859	0.335
7	-0.310	0.969	0.041	7	-0.578	1.061	-0.189
7	-3.324	0.234	1.034	7	-3.461	1.474	-0.634
7	1.036	0.992	0.178	7	0.753	0.855	-0.065
6	-0.812	-0.228	-0.028	6	-1.273	-0.023	-0.008
6	1.538	-0.216	0.189	6	1.048	-0.394	0.193
6	3.940	0.321	-0.142	6	3.421	-0.425	-0.455
6	5.290	-0.245	0.205	6	4.748	-0.824	0.117
1	3.124	-1.415	0.652	1	2.529	-1.464	1.119
1	-3.100	-0.155	1.943	1	-3.085	2.237	-0.079
1	-3.194	1.255	0.969	1	-3.168	1.555	-1.602
1	5.557	0.061	1.220	1	5.015	-0.086	0.880
1	6.034	0.163	-0.475	1	5.503	-0.808	-0.665
1	5.322	-1.336	0.168	1	4.730	-1.808	0.589
8	-2.482	2.885	0.371	8	3.231	2.205	0.884
1	-1.604	2.527	0.152	1	2.359	2.012	0.506
1	-2.854	3.140	-0.478	1	3.706	2.591	0.144
Acetazolamide motif 4, Eint = -7.2 kcal/mol				Acetazolamide motif 5, Eint = -8.1 kcal/mol			
16	3.310	0.142	0.133	16	2.590	-0.417	-0.010
16	0.606	-1.356	0.369	16	-0.140	1.091	0.031
8	3.585	-0.067	1.536	8	2.998	0.053	-1.318
8	3.889	-0.684	-0.902	8	3.090	0.199	1.203
8	-3.248	0.877	0.060	8	-3.991	-1.268	-0.581
7	-2.026	-1.022	-0.292	7	-2.795	0.519	0.228
7	0.845	1.009	-0.604	7	0.117	-1.466	0.145
7	3.668	1.715	-0.222	7	2.950	-2.027	0.067
7	-0.472	0.721	-0.743	7	-1.221	-1.266	0.220
6	1.527	0.043	-0.067	6	0.799	-0.363	0.056

6	-0.761	-0.468	-0.290	6	-1.517	0.007	0.173
6	-3.226	-0.317	-0.132	6	-3.981	-0.153	-0.133
6	-4.450	-1.179	-0.231	6	-5.211	0.673	0.132
1	-2.086	-2.028	-0.337	1	-2.879	1.492	0.482
1	3.389	1.957	-1.168	1	2.612	-2.437	0.933
1	3.247	2.353	0.446	1	2.559	-2.527	-0.726
1	-4.970	-0.937	-1.161	1	-5.526	0.524	1.169
1	-5.137	-0.920	0.576	1	-6.016	0.332	-0.515
1	-4.239	-2.249	-0.217	1	-5.053	1.743	-0.017
8	-5.998	1.384	0.547	8	2.346	2.762	-0.209
1	-6.294	2.237	0.869	1	2.795	2.352	-0.956
1	-5.046	1.492	0.398	1	2.867	2.466	0.545
Acetazolamide motif 6, Eint = -9.7 kcal/mol				Carbamazepine motif 1, Eint = -8.1 kcal/mol			
16	-3.032	0.132	0.001	8	-1.440	1.954	1.163
16	-0.072	1.035	0.007	7	0.078	0.567	0.151
8	-3.340	0.760	1.266	7	0.755	2.536	1.207
8	-3.342	0.760	-1.264	6	-0.930	-0.387	-0.188
8	3.328	-2.132	0.010	6	1.422	0.288	-0.237
7	2.427	-0.013	-0.003	6	-0.897	-1.661	0.408
7	-0.813	-1.426	-0.008	6	2.112	-0.782	0.363
7	-3.735	-1.366	0.000	6	0.179	-2.107	1.273
7	0.543	-1.488	-0.010	6	1.475	-1.726	1.264
6	-1.273	-0.213	0.000	6	-1.963	-0.022	-1.041
6	1.087	-0.300	-0.003	6	2.054	1.110	-1.169
6	3.484	-0.938	0.003	6	-1.964	-2.534	0.137
6	4.837	-0.272	-0.001	6	3.470	-0.946	0.039
1	2.665	0.975	-0.005	6	-0.281	1.696	0.870
1	-3.479	-1.891	-0.831	6	-3.005	-0.903	-1.292
1	-3.481	-1.890	0.832	6	3.392	0.916	-1.484
1	5.390	-0.609	-0.880	6	-3.004	-2.164	-0.701
1	5.396	-0.610	0.873	6	4.103	-0.113	-0.869
1	4.798	0.818	-0.001	1	-0.084	-2.924	1.942
8	2.775	2.869	-0.004	1	2.153	-2.264	1.922
1	2.626	3.435	-0.766	1	-1.976	0.976	-1.464
1	2.632	3.435	0.759	1	1.488	1.921	-1.615
				1	-1.960	-3.516	0.601
				1	4.020	-1.757	0.508
				1	-3.830	-0.588	-1.921
				1	3.880	1.569	-2.200
				1	-3.820	-2.854	-0.885
				1	5.152	-0.266	-1.102
				1	0.506	3.203	1.920
				1	1.692	2.164	1.265
				8	-3.893	2.234	-0.294
				1	-3.117	2.067	0.265
				1	-4.254	3.050	0.058
Carbamazepine motif 2, Eint = -10.6 kcal/mol				Acetaminophen motif 1, Eint = -5.0 kcal/mol			
8	-1.308	2.274	0.008	8	3.252	1.044	-0.063
7	-0.028	0.400	-0.230	8	-3.326	1.156	0.045
7	0.958	2.491	0.120	7	-2.028	-0.730	-0.012
6	-1.187	-0.426	-0.332	6	-0.721	-0.209	-0.021
6	1.250	-0.224	-0.334	6	-0.434	1.158	0.021
6	-1.437	-1.390	0.660	6	0.337	-1.124	-0.073
6	1.682	-1.103	0.677	6	0.891	1.581	0.008
6	-0.520	-1.661	1.753	6	1.655	-0.703	-0.082
6	0.824	-1.531	1.767	6	1.930	0.661	-0.044
6	-2.082	-0.232	-1.379	6	-3.228	-0.057	0.019
6	2.082	0.083	-1.410	6	-4.440	-0.958	0.020
6	-2.633	-2.122	0.574	1	-1.242	1.873	0.062
6	2.992	-1.603	0.594	1	0.121	-2.189	-0.101
6	-0.191	1.765	-0.019	1	-2.082	-1.737	-0.034
6	-3.250	-0.978	-1.448	1	1.109	2.645	0.038
6	3.368	-0.436	-1.476	1	2.474	-1.414	-0.114
6	-3.527	-1.925	-0.464	1	-5.066	-0.708	-0.838
6	3.826	-1.277	-0.463	1	-5.031	-0.754	0.915
1	-0.977	-2.118	2.628	1	-4.210	-2.024	-0.012
1	1.346	-1.895	2.650	1	3.306	1.997	0.047
1	-1.867	0.535	-2.114	8	4.911	-1.315	0.187
1	1.716	0.763	-2.173	1	4.559	-0.417	0.124
1	-2.845	-2.859	1.344	1	5.629	-1.335	-0.448
1	3.343	-2.268	1.378				
1	-3.951	-0.809	-2.258				
1	4.013	-0.179	-2.309				
1	-4.443	-2.504	-0.507				
1	4.833	-1.679	-0.503				
1	0.813	3.430	0.478				
1	1.810	2.022	0.385				
8	-0.615	4.745	1.028				
1	-1.153	4.007	0.682				
1	-0.963	5.531	0.604				
Acetaminophen motif 2, Eint = -6.8 kcal/mol				Acetaminophen motif 3, Eint = -7.9 kcal/mol			

8	4.023	0.192	-0.087	8	4.458	-0.768	0.000
8	-2.418	0.804	-0.214	8	-2.116	-0.786	-0.001
7	-1.363	-1.183	0.202	7	-0.796	1.075	0.000
6	-0.006	-0.786	0.149	6	0.505	0.532	0.000
6	0.413	0.480	0.553	6	0.773	-0.839	0.000
6	0.941	-1.708	-0.302	6	1.576	1.433	0.000
6	1.754	0.824	0.468	6	2.090	-1.281	0.000
6	2.285	-1.375	-0.362	6	2.886	0.988	0.001
6	2.695	-0.096	0.013	6	3.151	-0.380	0.000
6	-2.466	-0.400	-0.007	6	-2.004	0.435	0.000
6	-3.780	-1.134	0.050	6	-3.202	1.346	0.000
1	-0.296	1.205	0.926	1	-0.045	-1.544	-0.001
1	0.621	-2.698	-0.617	1	1.377	2.501	0.001
1	-1.527	-2.177	0.266	1	-0.833	2.084	0.000
1	2.062	1.825	0.759	1	2.291	-2.350	-0.001
1	3.023	-2.087	-0.712	1	3.713	1.689	0.001
1	-4.325	-0.957	-0.878	1	-3.821	1.122	0.871
1	-4.384	-0.719	0.858	1	-3.821	1.123	-0.872
1	-3.683	-2.210	0.205	1	-2.951	2.407	0.000
1	4.163	1.105	0.182	1	4.498	-1.729	0.000
8	-0.879	3.233	-0.327	8	-4.894	-1.286	0.001
1	-1.544	3.923	-0.344	1	-5.153	-2.209	0.002
1	-1.392	2.416	-0.421	1	-3.921	-1.305	0.000
Clonidine motif 1, Eint = -8.4 kcal/mol				Clonidine motif 2, Eint = -3.4 kcal/mol			
17	-0.259	2.451	-0.100	17	-0.785	-1.908	-0.758
17	1.842	-2.523	-0.502	17	0.370	3.348	-0.119
7	-2.615	-1.044	-0.263	7	3.173	-0.389	-0.659
7	-0.350	-0.476	-0.678	7	0.991	0.510	-0.833
7	-1.332	-0.260	1.474	7	1.670	-0.803	1.023
6	-3.590	-0.735	0.790	6	3.800	-1.466	0.118
6	-2.675	-0.489	2.008	6	2.904	-1.504	1.373
6	-1.412	-0.569	0.237	6	1.901	-0.252	-0.105
6	0.888	-0.005	-0.210	6	-0.298	0.728	-0.326
6	1.068	1.347	0.112	6	-1.232	-0.311	-0.214
6	2.008	-0.836	-0.095	6	-0.740	2.008	0.031
6	2.284	1.837	0.561	6	-2.515	-0.103	0.271
6	3.242	-0.361	0.328	6	-2.025	2.248	0.494
6	3.370	0.978	0.668	6	-2.905	1.183	0.626
1	-4.294	-1.558	0.936	1	4.846	-1.239	0.338
1	-4.167	0.161	0.529	1	3.767	-2.416	-0.432
1	-3.003	0.358	2.618	1	2.693	-2.525	1.706
1	-2.649	-1.363	2.671	1	3.380	-0.990	2.217
1	-2.840	-0.697	-1.192	1	3.189	-0.502	-1.665
1	-0.267	-1.320	-1.236	1	1.412	1.346	-1.223
1	2.375	2.888	0.806	1	-3.202	-0.938	0.347
1	4.080	-1.043	0.402	1	-2.317	3.257	0.758
1	4.326	1.358	1.011	1	-3.908	1.355	0.999
8	-2.205	0.692	-2.672	8	-3.745	-3.169	0.248
1	-2.454	1.588	-2.908	1	-2.825	-3.183	-0.041
1	-1.398	0.790	-2.147	1	-4.202	-3.720	-0.392
Clonidine motif 3, Eint = -8.4 kcal/mol				Clonidine motif 4, Eint = -3.2 kcal/mol			
17	-0.254	-2.556	-0.946	17	-1.526	2.402	-0.430
17	-1.339	2.610	0.316	17	1.935	-1.763	-0.640
7	2.771	0.293	-0.359	7	-2.783	-1.616	-0.687
7	0.416	0.356	-0.612	7	-0.734	-0.457	-0.927
7	1.453	-0.796	1.182	7	-1.968	-0.428	1.098
6	3.706	-0.575	0.377	6	-3.922	-1.541	0.238
6	2.840	-1.042	1.563	6	-3.250	-0.994	1.514
6	1.500	-0.093	0.117	6	-1.814	-0.792	-0.116
6	-0.880	-0.008	-0.233	6	0.279	0.372	-0.427
6	-1.320	-1.339	-0.318	6	0.043	1.723	-0.135
6	-1.820	0.937	0.198	6	1.592	-0.085	-0.254
6	-2.608	-1.707	0.045	6	1.050	2.548	0.345
6	-3.121	0.592	0.538	6	2.622	0.725	0.198
6	-3.507	-0.739	0.472	6	2.334	2.047	0.511
1	4.600	-0.026	0.679	1	-4.386	-2.520	0.377
1	4.022	-1.419	-0.247	1	-4.689	-0.854	-0.142
1	2.999	-2.098	1.804	1	-3.864	-0.242	2.020
1	3.069	-0.475	2.474	1	-3.068	-1.794	2.242
1	2.846	0.228	-1.369	1	-2.989	-1.416	-1.658
1	0.538	1.304	-0.971	1	-0.389	-1.244	-1.463
1	-2.900	-2.747	-0.031	1	0.821	3.584	0.567
1	-3.808	1.362	0.866	1	3.618	0.315	0.324
1	-4.516	-1.023	0.748	1	3.122	2.694	0.879
8	1.857	2.852	-1.231	8	5.013	-1.496	0.684
1	1.670	3.669	-0.763	1	5.344	-1.925	1.477
1	2.474	2.365	-0.664	1	4.228	-2.002	0.449
Clonidine motif 5, Eint = -6.4 kcal/mol				Clonidine motif 6, Eint = -9.8 kcal/mol			
17	-0.746	-2.695	-0.520	17	-0.275	2.160	-1.291
17	-0.988	2.714	-0.371	17	1.610	-2.728	0.101
7	2.662	-0.132	-0.854	7	-2.765	-1.219	-0.703

7	0.303	0.084	-0.958	7	-0.446	-0.823	-0.940
7	1.410	-0.722	0.978	7	-1.726	0.138	0.813
6	3.602	-0.882	-0.004	6	-3.873	-0.557	-0.004
6	2.807	-1.000	1.311	6	-3.143	0.111	1.177
6	1.419	-0.294	-0.224	6	-1.618	-0.589	-0.237
6	-0.966	0.006	-0.361	6	0.756	-0.230	-0.520
6	-1.569	-1.230	-0.091	6	0.967	1.152	-0.627
6	-1.705	1.155	-0.054	6	1.818	-1.000	-0.028
6	-2.830	-1.312	0.485	6	2.160	1.736	-0.224
6	-2.976	1.093	0.498	6	3.027	-0.436	0.353
6	-3.530	-0.148	0.776	6	3.187	0.941	0.263
1	4.545	-0.341	0.107	1	-4.632	-1.278	0.309
1	3.819	-1.865	-0.439	1	-4.356	0.185	-0.652
1	2.909	-1.984	1.775	1	-3.511	1.119	1.385
1	3.149	-0.263	2.049	1	-3.263	-0.468	2.101
1	2.670	-0.377	-1.838	1	-2.842	-1.278	-1.711
1	0.450	0.940	-1.482	1	-0.346	-1.789	-1.225
1	-3.257	-2.286	0.685	1	2.269	2.811	-0.297
1	-3.509	2.010	0.718	1	3.820	-1.073	0.725
1	-4.518	-0.211	1.217	1	4.121	1.396	0.571
8	2.775	2.612	0.419	8	0.075	1.773	2.427
1	2.033	2.380	0.984	1	-0.512	1.213	1.885
1	2.867	1.843	-0.161	1	0.813	1.194	2.630
4-aminosalicylic acid motif 1, Eint = -6.0 kcal/mol				4-aminosalicylic acid motif 2, Eint = -3.9 kcal/mol			
8	0.070	1.840	-0.128	8	-0.741	-2.524	-0.299
8	-3.330	-0.582	0.072	8	2.626	-0.097	0.343
8	-2.511	1.501	-0.028	8	1.841	-2.170	0.030
7	2.840	-2.012	-0.087	7	-3.558	1.277	-0.071
6	-0.992	-0.325	-0.007	6	0.288	-0.373	0.115
6	0.161	0.496	-0.075	6	-0.843	-1.202	-0.117
6	1.585	-1.452	-0.027	6	-2.303	0.722	0.027
6	1.430	-0.066	-0.084	6	-2.117	-0.647	-0.160
6	-0.810	-1.718	0.047	6	0.075	1.006	0.308
6	0.443	-2.281	0.038	6	-1.185	1.551	0.265
6	-2.300	0.289	0.009	6	1.598	-0.973	0.153
1	2.292	0.593	-0.131	1	-2.960	-1.305	-0.344
1	-1.688	-2.351	0.100	1	0.924	1.653	0.494
1	0.565	-3.359	0.076	1	-1.327	2.617	0.411
1	2.938	-2.953	0.258	1	-3.692	2.180	0.356
1	3.618	-1.412	0.142	1	-4.345	0.657	0.042
1	-0.889	2.067	-0.097	1	0.210	-2.756	-0.225
1	-4.133	-0.045	0.078	1	3.426	-0.639	0.381
8	2.724	2.914	0.204	8	2.998	2.731	-0.394
1	2.913	3.715	-0.289	1	2.935	1.776	-0.266
1	1.769	2.793	0.111	1	2.861	2.851	-1.336
4-aminosalicylic acid motif 3, Eint = -11.5 kcal/mol				Clomiphene motif 1, Eint = -4.7 kcal/mol			
8	0.106	2.231	-0.001	17	-4.720	0.918	1.096
8	-2.099	-1.333	0.003	8	2.968	-1.123	-0.876
8	-2.155	0.914	0.000	7	6.393	-0.273	0.095
7	4.138	-0.263	-0.057	6	5.312	-0.845	-0.698
6	-0.054	-0.182	-0.003	6	6.705	-1.122	1.247
6	0.691	1.026	-0.003	6	7.581	-0.007	-0.717
6	2.761	-0.229	-0.001	6	3.968	-0.447	-0.126
6	2.081	0.989	0.000	6	7.411	-0.375	2.360
6	0.654	-1.397	-0.004	6	7.423	1.209	-1.607
6	2.027	-1.435	-0.003	6	-1.075	-0.560	-0.033
6	-1.501	-0.142	-0.001	6	1.670	-0.899	-0.550
1	2.623	1.929	-0.003	6	-2.524	-0.407	0.226
1	0.085	-2.320	-0.004	6	-0.628	-1.417	-1.052
1	2.555	-2.383	-0.010	6	-0.109	0.096	0.733
1	4.580	-1.113	0.255	6	0.718	-1.578	-1.317
1	4.624	0.570	0.236	6	1.249	-0.063	0.487
1	-0.864	2.076	-0.004	6	-3.320	-1.656	0.197
1	-3.074	-1.185	0.001	6	-3.056	0.809	0.491
8	-4.618	-0.289	-0.076	6	-2.419	2.124	0.330
1	-4.060	0.506	-0.026	6	-2.895	-2.771	0.927
1	-5.260	-0.206	0.633	6	-4.460	-1.770	-0.608
				6	-3.610	-3.961	0.885
				6	-5.163	-2.968	-0.662
				6	-1.696	2.408	-0.837
				6	-2.533	3.119	1.308
				6	-4.747	-4.063	0.089
				6	-1.078	3.640	-1.001
				6	-1.908	4.348	1.144
				6	-1.174	4.612	-0.009
				1	5.377	-1.946	-0.762
				1	5.374	-0.476	-1.724
				1	5.762	-1.523	1.631
				1	7.299	-2.003	0.935
				1	8.418	0.161	-0.034
				1	7.856	-0.895	-1.319
				1	3.834	0.641	-0.196

				1	3.892	-0.720	0.936	
				1	8.379	0.023	2.045	
				1	6.805	0.466	2.705	
				1	7.596	-1.036	3.210	
				1	6.608	1.093	-2.327	
				1	7.211	2.099	-1.010	
				1	8.335	1.389	-2.180	
				1	-1.359	-1.954	-1.650	
				1	-0.424	0.743	1.546	
				1	1.061	-2.231	-2.112	
				1	1.967	0.457	1.109	
				1	-1.997	-2.696	1.534	
				1	-4.776	-0.924	-1.210	
				1	-3.276	-4.813	1.469	
				1	-6.037	-3.046	-1.301	
				1	-1.633	1.655	-1.615	
				1	-3.113	2.918	2.204	
				1	-5.302	-4.995	0.047	
				1	-0.528	3.845	-1.914	
				1	-1.996	5.104	1.917	
				1	-0.691	5.575	-0.140	
				8	-5.006	1.275	-2.175	
				1	-5.151	1.518	-1.253	
				1	-5.547	1.894	-2.670	
	Clomiphene motif 2, Eint = -5.9 kcal/mol				Clomiphene motif 3, Eint = -5.9 kcal/mol			
17	-4.825	1.148	0.561	17	-5.137	1.031	0.870	
8	2.875	-1.142	-0.961	8	2.625	-0.756	-1.037	
7	6.250	-0.374	0.228	7	5.992	-0.001	0.160	
6	5.209	-0.917	-0.636	6	4.968	-0.428	-0.783	
6	6.466	-1.234	1.393	6	6.224	-1.031	1.178	
6	7.493	-0.130	-0.503	6	7.231	0.391	-0.510	
6	3.842	-0.484	-0.152	6	3.600	-0.083	-0.234	
6	7.115	-0.509	2.554	6	6.811	-0.470	2.457	
6	7.420	1.094	-1.393	6	7.125	1.735	-1.201	
6	-1.197	-0.472	-0.393	6	-1.448	-0.343	-0.232	
6	1.565	-0.883	-0.721	6	1.311	-0.575	-0.724	
6	-2.656	-0.282	-0.216	6	-2.906	-0.240	0.015	
6	-0.707	-1.355	-1.368	6	-0.963	-1.156	-1.268	
6	-0.269	0.174	0.429	6	-0.513	0.320	0.566	
6	0.649	-1.552	-1.541	6	0.393	-1.265	-1.521	
6	1.099	-0.023	0.275	6	0.853	0.212	0.334	
6	-3.472	-1.516	-0.195	6	-3.650	-1.519	-0.004	
6	-3.163	0.960	-0.021	6	-3.481	0.961	0.272	
6	-2.462	2.242	-0.183	6	-2.863	2.289	0.122	
6	-3.025	-2.632	0.526	6	-3.138	-2.632	0.675	
6	-4.665	-1.629	-0.920	6	-4.830	-1.675	-0.740	
6	-3.764	-3.808	0.553	6	-3.801	-3.852	0.647	
6	-5.393	-2.811	-0.909	6	-5.484	-2.899	-0.783	
6	-1.691	2.475	-1.330	6	-2.109	2.587	-1.021	
6	-2.545	3.246	0.788	6	-3.026	3.283	1.093	
6	-4.952	-3.901	-0.165	6	-4.977	-3.990	-0.083	
6	-1.007	3.672	-1.489	6	-1.511	3.830	-1.170	
6	-1.853	4.439	0.630	6	-2.419	4.523	0.946	
6	-1.081	4.656	-0.508	6	-1.656	4.801	-0.184	
1	5.250	-2.020	-0.698	1	5.022	-1.511	-0.993	
1	5.349	-0.550	-1.656	1	5.108	0.079	-1.741	
1	5.490	-1.613	1.713	1	5.265	-1.513	1.396	
1	7.058	-2.128	1.115	1	6.869	-1.835	0.775	
1	8.288	0.015	0.234	1	8.014	0.444	0.252	
1	7.787	-1.021	-1.092	1	7.559	-0.389	-1.225	
1	3.739	0.606	-0.237	1	3.430	1.001	-0.264	
1	3.693	-0.748	0.904	1	3.507	-0.416	0.809	
1	8.111	-0.134	2.306	1	7.784	0.002	2.296	
1	6.508	0.345	2.864	1	6.147	0.282	2.889	
1	7.228	-1.178	3.411	1	6.956	-1.263	3.194	
1	6.651	1.001	-2.165	1	6.364	1.738	-1.986	
1	7.191	1.985	-0.804	1	6.864	2.517	-0.485	
1	8.371	1.257	-1.906	1	8.073	2.004	-1.673	
1	-1.410	-1.887	-2.003	1	-1.667	-1.701	-1.889	
1	-0.622	0.843	1.208	1	-0.859	0.933	1.392	
1	1.028	-2.224	-2.302	1	0.765	-1.879	-2.334	
1	1.787	0.489	0.937	1	1.548	0.732	0.981	
1	-2.085	-2.571	1.068	1	-2.212	-2.529	1.234	
1	-5.012	-0.784	-1.506	1	-5.228	-0.828	-1.291	
1	-3.408	-4.654	1.131	1	-3.397	-4.698	1.193	
1	-6.309	-2.882	-1.486	1	-6.393	-3.002	-1.367	
1	-1.632	1.706	-2.094	1	-1.994	1.832	-1.793	
1	-3.142	3.075	1.678	1	-3.630	3.073	1.970	
1	-5.526	-4.822	-0.153	1	-5.493	-4.945	-0.113	
1	-0.420	3.839	-2.386	1	-0.936	4.044	-2.066	
1	-1.916	5.201	1.399	1	-2.546	5.277	1.716	
1	-0.545	5.592	-0.633	1	-1.188	5.773	-0.302	
8	-2.756	0.313	3.165	8	3.331	-3.139	0.514	

1	-2.337	-0.389	2.658	1	3.000	-2.633	-0.239
1	-3.593	0.442	2.704	1	2.553	-3.591	0.850
Clomiphene motif 4, Eint = -5.3 kcal/mol				Angrelide motif 1, Eint = -3.5 kcal/mol			
17	-5.141	1.260	0.665	17	1.406	2.589	0.040
8	2.616	-1.069	-0.501	17	3.956	0.728	-0.032
7	5.979	-0.036	0.514	8	-5.866	-0.318	-0.025
6	4.948	-0.723	-0.251	7	-2.449	0.436	-0.177
6	6.257	-0.737	1.769	7	-3.777	-1.318	0.039
6	7.195	0.172	-0.274	7	-1.451	-1.715	0.105
6	3.573	-0.287	0.208	6	-1.253	1.214	0.074
6	6.901	0.150	2.816	6	-3.783	0.980	-0.094
6	7.043	1.265	-1.312	6	-2.453	-0.917	0.003
6	-1.475	-0.408	-0.021	6	-0.050	0.313	0.034
6	1.290	-0.809	-0.299	6	-0.204	-1.088	0.051
6	-2.937	-0.215	0.119	6	-4.663	-0.261	-0.027
6	-0.967	-1.359	-0.919	6	1.232	0.858	0.016
6	-0.559	0.312	0.750	6	0.937	-1.896	0.027
6	0.394	-1.554	-1.070	6	2.360	0.033	-0.007
6	0.811	0.123	0.621	6	2.207	-1.348	-0.005
6	-3.741	-1.453	0.225	1	-1.323	1.733	1.047
6	-3.463	1.034	0.178	1	-1.169	2.005	-0.682
6	-2.770	2.299	-0.116	1	-4.048	1.598	-0.959
6	-3.309	-2.493	1.058	1	-3.929	1.590	0.808
6	-4.899	-1.648	-0.537	1	-4.046	-2.289	0.095
6	-4.029	-3.676	1.153	1	0.802	-2.972	0.038
6	-5.609	-2.838	-0.455	1	3.088	-1.982	-0.024
6	-1.940	2.399	-1.241	8	5.343	-2.337	0.017
6	-2.934	3.428	0.696	1	6.028	-2.609	-0.597
6	-5.183	-3.854	0.396	1	5.369	-1.374	-0.005
6	-1.272	3.581	-1.526				
6	-2.257	4.607	0.414				
6	-1.421	4.688	-0.695				
1	5.036	-1.824	-0.173				
1	5.052	-0.485	-1.313				
1	5.305	-1.111	2.159				
1	6.879	-1.634	1.586				
1	7.994	0.450	0.420				
1	7.523	-0.772	-0.750				
1	3.423	0.780	-0.001				
1	3.447	-0.436	1.290				
1	7.876	0.527	2.498				
1	6.267	1.012	3.035				
1	7.059	-0.405	3.744				
1	6.272	1.031	-2.051				
1	6.772	2.211	-0.838				
1	7.977	1.410	-1.859				
1	-1.658	-1.946	-1.517				
1	-0.926	1.039	1.468				
1	0.784	-2.272	-1.785				
1	1.490	0.696	1.240				
1	-2.400	-2.362	1.638				
1	-5.233	-0.862	-1.206				
1	-3.686	-4.465	1.815				
1	-6.499	-2.975	-1.062				
1	-1.823	1.538	-1.892				
1	-3.595	3.370	1.554				
1	-5.742	-4.781	0.462				
1	-0.639	3.641	-2.406				
1	-2.387	5.468	1.061				
1	-0.899	5.613	-0.919				
8	3.277	-2.679	-2.831				
1	3.730	-3.471	-2.535				
1	3.117	-2.180	-2.019				
Angrelide motif 2, Eint = -5.1 kcal/mol				Angrelide motif 3, Eint = -10.3 kcal/mol			
17	2.101	1.995	-0.518	17	-2.825	-1.989	0.085
17	4.332	-0.245	-0.306	17	-4.811	0.478	-0.032
8	-5.532	0.300	-0.088	8	4.944	-1.050	-0.057
7	-2.048	0.472	-0.412	7	1.450	-0.901	-0.196
7	-3.624	-1.006	0.053	7	3.190	0.458	-0.005
7	-1.388	-1.758	0.127	7	1.042	1.437	0.054
6	-0.735	1.074	-0.299	6	0.100	-1.341	0.084
6	-3.276	1.230	-0.367	6	2.600	-1.767	-0.101
6	-2.257	-0.827	-0.060	6	1.807	0.409	-0.034
6	0.308	-0.007	-0.242	6	-0.834	-0.164	0.024
6	-0.063	-1.349	-0.021	6	-0.323	1.150	0.011
6	-4.335	0.164	-0.124	6	3.758	-0.787	-0.055
6	1.659	0.321	-0.331	6	-2.213	-0.362	0.020
6	0.940	-2.320	0.084	6	-1.218	2.224	-0.032
6	2.651	-0.657	-0.216	6	-3.096	0.720	-0.022
6	2.278	-1.981	-0.013	6	-2.585	2.014	-0.051
1	-0.667	1.704	0.605	1	0.045	-1.835	1.072
1	-0.563	1.735	-1.158	1	-0.193	-2.104	-0.647

1	-3.477	1.774	-1.296	1	2.696	-2.450	-0.952
1	-3.284	1.959	0.455	1	2.590	-2.378	0.814
1	-4.037	-1.906	0.245	1	3.748	1.310	0.037
1	0.640	-3.348	0.251	1	-0.811	3.228	-0.045
1	3.049	-2.737	0.071	1	-3.274	2.849	-0.084
8	0.865	1.132	2.714	8	5.679	1.642	0.186
1	1.085	0.198	2.655	1	6.400	2.105	-0.244
1	1.637	1.569	2.340	1	5.863	0.695	0.077
Angrelide motif 4, Eint = -11.6 kcal/mol				Diclofenac motif 1, Eint = -3.6 kcal/mol			
17	-2.668	-2.067	0.076	17	-1.730	-1.642	-1.017
17	-4.618	0.429	-0.041	17	-0.045	3.209	0.725
8	5.119	-1.251	-0.024	8	4.824	0.627	-1.030
7	1.626	-1.050	-0.149	8	2.920	1.761	-0.676
7	3.385	0.288	0.003	7	0.333	0.418	-0.274
7	1.250	1.294	0.048	6	2.155	-1.168	-0.103
6	0.260	-1.468	0.082	6	0.929	-0.676	0.383
6	2.764	-1.934	-0.071	6	2.790	-0.558	-1.327
6	2.009	0.248	-0.021	6	-0.989	0.794	-0.064
6	-0.651	-0.273	0.023	6	2.764	-2.236	0.550
6	-0.121	1.033	0.008	6	0.337	-1.289	1.490
6	3.947	-0.972	-0.030	6	2.172	-2.843	1.651
6	-2.034	-0.450	0.015	6	0.950	-2.365	2.113
6	-1.000	2.119	-0.039	6	-2.070	-0.061	-0.348
6	-2.901	0.645	-0.028	6	-1.330	2.086	0.378
6	-2.370	1.930	-0.059	6	3.482	0.734	-0.988
1	0.170	-1.982	1.055	6	-3.392	0.314	-0.162
1	-0.028	-2.209	-0.675	6	-2.645	2.493	0.543
1	2.840	-2.608	-0.931	6	-3.675	1.598	0.287
1	2.749	-2.551	0.837	1	2.012	-0.326	-2.063
1	3.877	1.184	0.035	1	3.502	-1.253	-1.773
1	-0.583	3.120	-0.059	1	0.975	1.195	-0.419
1	-3.046	2.776	-0.095	1	3.713	-2.606	0.170
8	3.450	3.070	0.011	1	-0.609	-0.908	1.862
1	2.510	2.815	0.072	1	2.657	-3.681	2.139
1	3.579	3.763	0.662	1	0.474	-2.825	2.973
				1	-4.186	-0.390	-0.387
				1	-2.849	3.500	0.886
				1	-4.706	1.903	0.428
				1	5.181	1.486	-0.761
				8	-4.966	-2.511	-0.807
				1	-5.389	-2.984	-1.527
				1	-4.023	-2.638	-0.961
Diclofenac motif 2, Eint = -11.7 kcal/mol				Diclofenac motif 3, Eint = -3.4 kcal/mol			
17	2.318	1.891	-1.317	17	-0.082	-2.853	-1.231
17	0.680	-2.819	0.831	17	-1.856	1.997	0.424
8	-4.264	-0.282	-0.814	8	3.702	2.959	-0.773
8	-2.347	-1.397	-0.449	8	1.478	2.685	-0.655
7	0.266	-0.088	-0.313	7	0.225	0.036	-0.409
6	-1.522	1.536	-0.160	6	2.605	-0.107	0.008
6	-0.275	1.065	0.289	6	1.293	-0.476	0.353
6	-2.238	0.848	-1.295	6	2.860	0.780	-1.185
6	1.594	-0.468	-0.168	6	-1.066	-0.478	-0.340
6	-2.080	2.659	0.446	6	3.668	-0.588	0.769
6	0.390	1.749	1.309	6	1.086	-1.341	1.431
6	-1.416	3.337	1.462	6	3.459	-1.446	1.842
6	-0.174	2.878	1.886	6	2.160	-1.825	2.163
6	2.661	0.354	-0.578	6	-1.361	-1.811	-0.682
6	1.950	-1.736	0.328	6	-2.168	0.324	0.006
6	-2.942	-0.394	-0.820	6	2.578	2.221	-0.857
6	3.986	-0.039	-0.455	6	-2.654	-2.313	-0.637
6	3.268	-2.157	0.430	6	-3.472	-0.147	0.029
6	4.290	-1.297	0.050	6	-3.707	-1.480	-0.282
1	-1.508	0.541	-2.052	1	2.185	0.494	-2.000
1	-2.960	1.525	-1.755	1	3.890	0.672	-1.526
1	-0.397	-0.858	-0.367	1	0.276	1.043	-0.542
1	-3.045	3.014	0.096	1	4.678	-0.294	0.497
1	1.352	1.382	1.652	1	0.072	-1.625	1.694
1	-1.862	4.217	1.913	1	4.300	-1.820	2.414
1	0.358	3.394	2.679	1	1.977	-2.494	2.998
1	4.768	0.636	-0.782	1	-2.825	-3.349	-0.905
1	3.480	-3.145	0.819	1	-4.282	0.521	0.302
1	5.323	-1.611	0.137	1	-4.718	-1.868	-0.255
1	-4.643	-1.123	-0.457	1	3.430	3.854	-0.521
8	-4.647	-2.791	0.144	8	-5.121	2.514	1.056
1	-4.906	-3.095	1.016	1	-4.191	2.757	0.997
1	-3.677	-2.746	0.151	1	-5.587	3.266	0.684
Diclofenac motif 4, Eint = -5.2 kcal/mol				Allopurinol motif 1, Eint = -7.8 kcal/mol			
17	-1.589	-2.275	-1.374	8	1.470	-1.723	-0.028
17	-1.818	2.679	0.834	7	-1.287	1.962	0.001
8	3.784	2.019	-0.301	7	-0.803	-1.937	-0.001
8	1.590	2.471	-0.279	7	-2.384	-0.186	0.016

7	-0.415	0.284	-0.268	7	-0.035	2.489	-0.013
6	1.820	-0.613	0.011	6	0.064	0.235	-0.010
6	0.461	-0.614	0.376	6	-1.285	0.613	0.004
6	2.315	0.309	-1.078	6	0.385	-1.159	-0.015
6	-1.799	0.171	-0.198	6	0.786	1.451	-0.020
6	2.703	-1.480	0.651	6	-2.074	-1.446	0.014
6	0.019	-1.504	1.358	1	1.859	1.590	-0.031
6	2.254	-2.364	1.626	1	-2.088	2.574	0.009
6	0.907	-2.375	1.971	1	-0.657	-2.938	-0.001
6	-2.486	-0.967	-0.662	1	-2.865	-2.191	0.023
6	-2.601	1.228	0.272	8	3.607	0.139	0.073
6	2.483	1.699	-0.537	1	3.002	-0.620	0.030
6	-3.870	-1.064	-0.611	1	4.444	-0.196	-0.254
6	-3.986	1.158	0.301				
6	-4.620	0.000	-0.128				
1	1.570	0.362	-1.879				
1	3.258	-0.059	-1.483				
1	-0.073	1.241	-0.282				
1	3.749	-1.463	0.357				
1	-1.030	-1.503	1.640				
1	2.951	-3.043	2.106				
1	0.543	-3.058	2.732				
1	-4.346	-1.965	-0.976				
1	-4.552	2.003	0.673				
1	-5.702	-0.069	-0.098				
1	3.784	2.902	0.097				
8	5.540	-0.259	-0.741				
1	6.491	-0.205	-0.849				
1	5.260	0.637	-0.521				
Allopurinol				Allopurinol			
motif 2, Eint = -9.9 kcal/mol				motif 3, Eint = -6.0 kcal/mol			
8	3.132	0.221	-0.007	8	1.901	2.332	-0.023
7	-1.399	1.041	0.009	7	0.512	-2.051	0.014
7	1.610	-1.495	-0.001	7	-0.330	1.794	0.020
7	-0.737	-1.282	0.011	7	-1.237	-0.382	0.046
7	-0.840	2.273	0.005	7	1.867	-2.132	-0.013
6	0.772	0.691	0.003	6	1.207	0.030	-0.003
6	-0.477	0.059	0.008	6	0.065	-0.776	0.021
6	1.964	-0.105	-0.002	6	1.061	1.457	-0.005
6	0.470	2.068	0.001	6	2.288	-0.877	-0.023
6	0.348	-1.999	0.005	6	-1.365	0.916	0.044
1	1.149	2.908	-0.003	1	3.347	-0.664	-0.045
1	-2.408	0.904	0.010	1	-0.036	-2.897	0.021
1	2.396	-2.133	-0.006	1	-0.529	2.787	0.018
1	0.269	-3.082	0.005	1	-2.368	1.336	0.060
8	-3.546	-0.741	-0.081	8	-4.107	-0.332	-0.108
1	-4.233	-1.150	0.448	1	-3.254	-0.786	-0.029
1	-2.775	-1.329	-0.016	1	-4.731	-0.893	0.356
Allopurinol				Flurbiprofen			
motif 4, Eint = -8.6 kcal/mol				motif 1, Eint = -7.6 kcal/mol			
8	2.675	-1.656	-0.017	9	-0.861	1.986	-0.304
7	-1.472	0.340	0.030	8	3.582	-1.622	1.667
7	2.451	0.628	-0.012	8	4.121	0.462	1.053
7	0.420	1.835	0.013	6	2.981	-0.991	-0.534
7	-1.734	-0.992	0.028	6	1.486	-0.756	-0.397
6	0.492	-0.646	0.006	6	-1.306	-0.331	-0.115
6	-0.150	0.600	0.016	6	0.968	0.539	-0.405
6	1.926	-0.701	-0.008	6	0.612	-1.831	-0.241
6	-0.552	-1.591	0.014	6	-0.396	0.719	-0.264
6	1.717	1.776	-0.001	6	-0.752	-1.618	-0.109
1	-0.490	-2.669	0.009	6	3.605	-0.241	-1.703
1	-2.266	0.974	0.032	6	-2.762	-0.130	0.015
1	3.461	0.687	-0.023	6	3.632	-0.612	0.779
1	2.289	2.700	-0.006	6	-3.301	0.907	0.787
8	-4.230	0.318	-0.107	6	-3.645	-1.012	-0.621
1	-3.807	-0.552	-0.056	6	-4.676	1.049	0.921
1	-5.000	0.259	0.462	6	-5.020	-0.866	-0.490
				6	-5.542	0.166	0.283
				1	3.130	-2.069	-0.655
				1	1.604	1.413	-0.520
				1	1.006	-2.843	-0.214
				1	-1.418	-2.465	0.025
				1	3.138	-0.558	-2.637
				1	3.475	0.838	-1.610
				1	4.677	-0.442	-1.771
				1	-2.638	1.597	1.297
				1	-3.245	-1.808	-1.242
				1	-5.074	1.855	1.529
				1	-5.685	-1.555	-1.000
				1	-6.615	0.284	0.385
				1	3.960	-1.291	2.494
				8	3.405	2.834	-0.361
				1	3.808	2.165	0.213
				1	3.456	3.653	0.135

<p style="text-align: center;">Flurbiprofen motif 2, Eint = -4.9 kcal/mol</p>				<p style="text-align: center;">Flurbiprofen motif 3, Eint = -5.8 kcal/mol</p>			
9	-0.634	1.772	0.785	9	-1.222	-2.301	0.111
8	4.342	-1.387	1.193	8	3.735	0.339	-1.565
8	4.539	0.854	1.169	8	4.018	-1.740	-0.764
6	3.517	-0.265	-0.723	6	3.047	-0.045	0.680
6	2.020	-0.329	-0.495	6	1.540	0.000	0.493
6	-0.786	-0.434	-0.070	6	-1.279	0.069	0.159
6	1.348	0.757	0.068	6	0.813	-1.183	0.366
6	1.285	-1.463	-0.839	6	0.859	1.216	0.444
6	-0.016	0.682	0.265	6	-0.558	-1.128	0.202
6	-0.086	-1.507	-0.635	6	-0.519	1.239	0.286
6	3.922	0.901	-1.615	6	3.465	-0.868	1.892
6	-2.246	-0.489	0.127	6	-2.745	0.127	0.004
6	4.197	-0.167	0.629	6	3.659	-0.607	-0.582
6	-2.854	0.003	1.289	6	-3.433	-0.722	-0.871
6	-3.061	-1.050	-0.865	6	-3.481	1.077	0.724
6	-4.233	-0.062	1.449	6	-4.810	-0.617	-1.023
6	-4.440	-1.110	-0.705	6	-4.858	1.177	0.575
6	-5.032	-0.613	0.453	6	-5.529	0.330	-0.302
1	3.822	-1.214	-1.174	1	3.393	0.988	0.783
1	1.874	1.662	0.354	1	1.297	-2.154	0.395
1	1.796	-2.322	-1.265	1	1.418	2.144	0.511
1	-0.641	-2.403	-0.897	1	-1.034	2.194	0.233
1	3.406	0.844	-2.575	1	3.002	-0.468	2.796
1	3.674	1.855	-1.147	1	3.165	-1.911	1.784
1	4.999	0.899	-1.800	1	4.549	-0.852	2.023
1	-2.242	0.429	2.076	1	-2.885	-1.458	-1.448
1	-2.606	-1.414	-1.781	1	-2.967	1.727	1.425
1	-4.685	0.322	2.358	1	-5.324	-1.279	-1.713
1	-5.054	-1.537	-1.491	1	-5.410	1.914	1.150
1	-6.109	-0.655	0.577	1	-6.605	0.406	-0.420
1	4.729	-1.245	2.069	1	4.071	-0.109	-2.355
8	-2.958	2.486	-1.205	8	3.457	3.043	-0.489
1	-2.384	2.398	-0.438	1	4.038	3.737	-0.809
1	-3.480	1.679	-1.183	1	3.586	2.308	-1.102
<p style="text-align: center;">Amoxapine motif 1, Eint = -4.7 kcal/mol</p>				<p style="text-align: center;">Amoxapine motif 2, Eint = -3.6 kcal/mol</p>			
17	2.360	3.539	0.694	17	4.013	0.289	-1.112
8	-2.236	0.571	-1.474	8	-0.839	-1.781	1.495
7	1.053	-1.579	-0.326	7	-0.921	2.059	0.088
7	3.460	-3.015	-0.643	7	-0.895	4.870	0.363
7	-1.204	-1.610	0.121	7	-2.197	0.159	-0.153
6	1.129	-2.985	0.055	6	-2.112	2.845	-0.223
6	1.997	-1.244	-1.397	6	-0.078	2.716	1.093
6	2.554	-3.312	0.460	6	-1.698	4.233	-0.673
6	3.409	-1.593	-0.972	6	0.314	4.099	0.615
6	-0.160	-0.930	-0.225	6	-1.037	0.679	0.081
6	-0.107	0.546	-0.361	6	0.235	-0.073	0.190
6	-1.157	1.250	-0.956	6	0.288	-1.289	0.876
6	-2.459	-1.057	0.312	6	-2.427	-1.205	-0.244
6	0.975	1.265	0.160	6	1.400	0.394	-0.430
6	-3.005	-0.025	-0.473	6	-1.811	-2.169	0.573
6	-1.117	2.635	-1.070	6	1.477	-2.002	0.980
6	0.998	2.644	0.046	6	2.574	-0.332	-0.325
6	-0.030	3.344	-0.577	6	2.638	-1.525	0.388
6	-3.310	-1.644	1.263	6	-3.435	-1.657	-1.110
6	-4.317	0.396	-0.326	6	-2.176	-3.505	0.535
6	-4.619	-1.219	1.428	6	-3.795	-2.994	-1.167
6	-5.133	-0.202	0.627	6	-3.174	-3.925	-0.337
1	0.812	-3.625	-0.782	1	-2.768	2.908	0.658
1	0.432	-3.153	0.876	1	-2.669	2.326	-1.003
1	1.918	-0.186	-1.643	1	0.807	2.111	1.288
1	1.734	-1.820	-2.298	1	-0.640	2.806	2.036
1	2.797	-2.738	1.374	1	-1.155	4.143	-1.632
1	2.626	-4.376	0.704	1	-2.592	4.836	-0.854
1	4.095	-1.395	-1.800	1	0.905	4.598	1.388
1	3.697	-0.945	-0.126	1	0.952	3.996	-0.284
1	4.407	-3.268	-0.382	1	-0.651	5.813	0.080
1	1.787	0.733	0.648	1	1.372	1.324	-0.986
1	-1.944	3.145	-1.551	1	1.480	-2.933	1.535
1	0.016	4.423	-0.664	1	3.572	-2.071	0.466
1	-2.907	-2.456	1.860	1	-3.933	-0.918	-1.729
1	-4.682	1.187	-0.972	1	-1.672	-4.199	1.200
1	-5.247	-1.694	2.174	1	-4.577	-3.311	-1.850
1	-6.162	0.122	0.739	1	-3.465	-4.969	-0.365
8	3.745	0.670	1.897	8	5.803	-2.275	0.102
1	3.729	0.553	2.849	1	5.682	-1.473	-0.418
1	3.635	1.620	1.773	1	6.402	-2.812	-0.422
<p style="text-align: center;">Amoxapine motif 3, Eint = -6.4 kcal/mol</p>				<p style="text-align: center;">Amoxapine motif 4, Eint = -8.1 kcal/mol</p>			
17	-1.738	3.968	-1.406	17	3.205	3.321	1.117
8	1.874	0.078	1.128	8	-1.616	1.193	-1.495
7	-1.887	-1.183	0.201	7	1.153	-1.490	-0.113

7	-4.543	-1.936	0.797	7	3.274	-3.340	-0.356
7	0.265	-1.872	-0.229	7	-1.114	-1.144	0.115
6	-2.319	-2.568	0.033	6	0.949	-2.899	0.225
6	-2.660	-0.486	1.235	6	2.217	-1.304	-1.107
6	-3.805	-2.600	-0.270	6	2.262	-3.506	0.680
6	-4.137	-0.542	0.903	6	3.506	-1.928	-0.613
6	-0.545	-0.898	0.027	6	0.064	-0.646	-0.102
6	-0.191	0.542	-0.003	6	0.369	0.802	-0.194
6	1.021	0.989	0.527	6	-0.485	1.674	-0.875
6	1.616	-1.704	-0.487	6	-2.270	-0.377	0.229
6	-1.034	1.478	-0.613	6	1.504	1.330	0.431
6	2.443	-0.785	0.181	6	-2.558	0.738	-0.574
6	1.380	2.330	0.494	6	-0.195	3.030	-0.971
6	-0.671	2.815	-0.649	6	1.782	2.685	0.338
6	0.524	3.255	-0.088	6	0.948	3.542	-0.373
6	2.246	-2.584	-1.382	6	-3.280	-0.821	1.097
6	3.811	-0.727	-0.026	6	-3.785	1.381	-0.519
6	3.613	-2.530	-1.606	6	-4.505	-0.174	1.167
6	4.403	-1.607	-0.925	6	-4.767	0.924	0.352
1	-2.102	-3.147	0.944	1	0.549	-3.448	-0.639
1	-1.740	-3.010	-0.776	1	0.206	-2.960	1.020
1	-2.322	0.547	1.318	1	2.352	-0.243	-1.312
1	-2.490	-0.976	2.207	1	1.918	-1.794	-2.047
1	-3.972	-2.128	-1.256	1	2.557	-3.032	1.635
1	-4.136	-3.640	-0.340	1	2.114	-4.572	0.871
1	-4.708	-0.059	1.700	1	4.278	-1.821	-1.381
1	-4.312	0.028	-0.030	1	3.847	-1.376	0.285
1	-5.539	-1.994	0.616	1	4.138	-3.788	-0.071
1	-1.968	1.148	-1.053	1	2.164	0.670	0.984
1	2.323	2.635	0.937	1	-0.873	3.672	-1.520
1	0.784	4.307	-0.119	1	1.186	4.597	-0.445
1	1.624	-3.315	-1.889	1	-3.073	-1.693	1.709
1	4.393	0.006	0.525	1	-3.954	2.230	-1.173
1	4.068	-3.221	-2.308	1	-5.265	-0.537	1.852
1	5.474	-1.571	-1.089	1	-5.729	1.423	0.391
8	3.869	1.574	2.527	8	-2.116	-3.922	0.054
1	3.178	0.931	2.317	1	-2.999	-3.840	-0.310
1	4.044	1.453	3.462	1	-1.762	-3.016	0.020
Alprazolam motif 1, Eint = -9.0 kcal/mol				Alprazolam motif 2, Eint = -7.3 kcal/mol			
17	2.706	3.843	-0.078	17	-0.293	4.556	-0.883
7	-1.878	0.102	-0.352	7	-2.049	-1.005	0.160
7	0.207	-1.698	-1.550	7	0.653	-1.630	-0.972
7	-3.181	-1.465	-1.200	7	-2.282	-3.174	-0.181
7	-3.814	-0.894	-0.118	7	-3.103	-2.802	0.865
6	-0.773	0.977	-0.261	6	-1.610	0.316	-0.069
6	0.534	0.486	-0.450	6	-0.255	0.575	-0.356
6	-2.032	-0.865	-1.327	6	-1.665	-2.101	-0.588
6	0.840	-0.950	-0.720	6	0.793	-0.486	-0.402
6	-0.927	-1.138	-2.274	6	-0.616	-1.950	-1.620
6	-3.044	0.042	0.383	6	-2.969	-1.514	1.059
6	-0.988	2.331	-0.001	6	-2.531	1.364	-0.022
6	1.595	1.397	-0.385	6	0.127	1.899	-0.602
6	1.989	-1.555	0.001	6	2.097	-0.187	0.237
6	0.074	3.217	0.068	6	-2.135	2.669	-0.260
6	1.365	2.740	-0.137	6	-0.801	2.927	-0.560
6	-3.360	0.862	1.573	6	-3.654	-0.734	2.114
6	2.401	-1.091	1.255	6	2.180	0.659	1.350
6	2.650	-2.654	-0.562	6	3.265	-0.793	-0.241
6	3.447	-1.710	1.930	6	3.399	0.889	1.974
6	3.701	-3.262	0.107	6	4.483	-0.552	0.378
6	4.103	-2.792	1.355	6	4.554	0.288	1.486
1	-1.269	-1.857	-3.018	1	-0.510	-2.888	-2.166
1	-0.646	-0.210	-2.796	1	-0.899	-1.166	-2.338
1	-2.001	2.694	0.124	1	-3.573	1.147	0.179
1	2.609	1.043	-0.531	1	1.165	2.120	-0.824
1	-0.096	4.269	0.260	1	-2.854	3.479	-0.232
1	-3.753	1.846	1.299	1	-4.537	-0.210	1.736
1	-4.133	0.354	2.151	1	-3.989	-1.422	2.890
1	-2.478	1.019	2.198	1	-2.993	0.012	2.562
1	1.888	-0.253	1.716	1	1.281	1.125	1.742
1	2.318	-3.015	-1.529	1	3.211	-1.454	-1.099
1	3.747	-1.346	2.907	1	3.446	1.537	2.843
1	4.211	-4.106	-0.346	1	5.382	-1.022	-0.009
1	4.925	-3.270	1.879	1	5.509	0.473	1.969
8	-6.026	-1.003	1.685	8	2.460	-3.842	-1.550
1	-5.422	-1.163	0.936	1	2.282	-4.610	-1.004
1	-6.474	-1.840	1.819	1	1.859	-3.156	-1.209
Alprazolam motif 3, Eint = -8.4 kcal/mol				Alprazolam motif 4, Eint = -3.9 kcal/mol			
17	3.261	3.232	-1.062	17	2.586	-3.148	-0.549
7	-1.882	0.683	0.396	7	0.313	2.293	0.042
7	-0.606	-1.686	-0.935	7	-2.040	0.993	-1.303
7	-3.649	-0.606	0.172	7	-0.839	4.094	-0.507

7	-3.848	0.211	1.263	7	-0.083	4.381	0.611
6	-0.641	1.274	0.072	6	0.838	0.989	-0.076
6	0.439	0.469	-0.337	6	-0.008	-0.086	-0.409
6	-2.480	-0.320	-0.335	6	-0.597	2.855	-0.831
6	0.364	-1.021	-0.423	6	-1.478	0.061	-0.622
6	-1.760	-0.961	-1.459	6	-1.201	2.026	-1.900
6	-2.797	0.982	1.389	6	0.606	3.313	0.929
6	-0.502	2.661	0.141	6	2.203	0.776	0.124
6	1.638	1.102	-0.682	6	0.565	-1.356	-0.545
6	1.519	-1.795	0.100	6	-2.365	-0.969	-0.022
6	0.695	3.271	-0.194	6	2.759	-0.487	-0.004
6	1.759	2.481	-0.616	6	1.923	-1.542	-0.351
6	-2.598	1.981	2.462	6	1.514	3.199	2.092
6	2.332	-1.302	1.127	6	-2.005	-1.662	1.139
6	1.776	-3.074	-0.409	6	-3.617	-1.221	-0.596
6	3.376	-2.068	1.632	6	-2.874	-2.584	1.712
6	2.826	-3.831	0.087	6	-4.477	-2.149	-0.031
6	3.629	-3.332	1.110	6	-4.109	-2.834	1.126
1	-2.436	-1.656	-1.959	1	-1.813	2.663	-2.537
1	-1.450	-0.193	-2.185	1	-0.406	1.581	-2.521
1	-1.349	3.267	0.437	1	2.844	1.618	0.359
1	2.483	0.502	-1.003	1	-0.066	-2.199	-0.802
1	0.799	4.348	-0.148	1	3.821	-0.649	0.144
1	-2.846	2.996	2.136	1	2.564	3.342	1.816
1	-3.257	1.734	3.293	1	1.256	3.977	2.809
1	-1.565	1.991	2.819	1	1.430	2.225	2.579
1	2.137	-0.320	1.546	1	-1.046	-1.467	1.609
1	1.134	-3.453	-1.197	1	-3.894	-0.671	-1.489
1	3.991	-1.678	2.436	1	-2.585	-3.104	2.619
1	3.021	-4.817	-0.324	1	-5.440	-2.342	-0.492
1	4.450	-3.927	1.498	1	-4.785	-3.558	1.568
8	-4.778	-2.275	-1.865	8	5.638	-1.909	0.112
1	-4.643	-1.780	-1.037	1	6.418	-2.243	0.559
1	-5.249	-3.066	-1.598	1	5.115	-2.692	-0.086
Amodiaquine motif 1, Eint = -2.7 kcal/mol				Amodiaquine motif 2, Eint = -8.2 kcal/mol			
17	-6.571	-0.526	1.014	17	-6.688	-0.640	1.129
8	5.559	-2.114	-0.484	8	5.399	-2.144	-0.741
7	3.883	1.622	0.414	7	3.782	1.495	0.568
7	0.039	-1.671	0.049	7	-0.104	-1.711	-0.053
7	-2.512	1.394	-1.364	7	-2.645	1.503	-1.060
6	4.578	0.352	0.273	6	4.461	0.239	0.290
6	3.657	-0.807	0.001	6	3.523	-0.878	-0.082
6	3.451	2.124	-0.893	6	3.336	2.129	-0.676
6	4.701	2.605	1.123	6	4.623	2.394	1.357
6	2.280	-0.703	0.145	6	2.150	-0.778	0.101
6	1.434	-1.782	-0.122	6	1.288	-1.816	-0.261
6	4.197	-2.044	-0.378	6	4.041	-2.073	-0.600
6	2.317	3.125	-0.795	6	2.217	3.128	-0.460
6	4.785	2.344	2.614	6	4.728	1.985	2.812
6	1.989	-3.002	-0.502	6	1.821	-2.994	-0.778
6	-0.768	-0.651	-0.402	6	-0.910	-0.647	-0.370
6	3.368	-3.134	-0.615	6	3.195	-3.125	-0.933
6	-2.152	-0.638	-0.027	6	-2.288	-0.669	0.027
6	-2.975	0.401	-0.557	6	-3.113	0.428	-0.363
6	-0.321	0.375	-1.221	6	-0.465	0.463	-1.078
6	-2.732	-1.589	0.839	6	-2.865	-1.712	0.783
6	-4.353	0.425	-0.231	6	-4.485	0.423	-0.016
6	-1.228	1.351	-1.656	6	-1.366	1.486	-1.384
6	-4.069	-1.552	1.155	6	-4.197	-1.702	1.119
6	-4.867	-0.538	0.598	6	-5.001	-0.627	0.701
1	5.134	0.146	1.195	1	5.027	-0.064	1.178
1	5.352	0.392	-0.519	1	5.224	0.349	-0.505
1	4.306	2.556	-1.449	1	4.187	2.603	-1.202
1	3.118	1.263	-1.483	1	2.982	1.334	-1.342
1	5.716	2.664	0.684	1	5.631	2.488	0.907
1	4.249	3.587	0.962	1	4.179	3.392	1.302
1	1.874	0.243	0.485	1	1.762	0.131	0.548
1	1.459	2.688	-0.277	1	1.365	2.653	0.033
1	2.604	4.030	-0.254	1	2.527	3.974	0.158
1	1.990	3.435	-1.791	1	1.875	3.536	-1.415
1	3.787	2.327	3.059	1	3.739	1.935	3.272
1	5.267	1.391	2.845	1	5.202	1.008	2.938
1	5.367	3.125	3.108	1	5.329	2.707	3.371
1	-0.433	-2.526	0.297	1	-0.577	-2.578	0.150
1	1.345	-3.850	-0.715	1	1.163	-3.809	-1.065
1	3.800	-4.088	-0.905	1	3.611	-4.048	-1.330
1	0.708	0.412	-1.556	1	0.558	0.529	-1.425
1	-2.120	-2.358	1.303	1	-2.255	-2.535	1.141
1	-4.972	1.213	-0.649	1	-5.100	1.260	-0.331
1	5.805	-3.000	-0.765	1	5.631	-2.998	-1.117
1	-0.861	2.145	-2.306	1	-1.007	2.346	-1.950
1	-4.507	-2.278	1.828	1	-4.632	-2.502	1.706
8	-7.104	2.285	-0.737	8	-4.832	3.302	-1.611

1	-7.281	1.587	-0.096	1	-4.659	4.161	-1.222
1	-7.263	3.098	-0.252	1	-3.999	2.806	-1.490
Amodiaquine motif 3, Eint = -5.0 kcal/mol				Estradiol motif 1, Eint = -6.8 kcal/mol			
17	7.241	-0.153	0.624	8	4.706	0.420	-0.040
8	-4.838	2.257	0.215	8	-6.192	0.672	0.444
7	-3.320	-1.639	0.561	6	2.282	0.071	-0.007
7	0.672	1.474	0.281	6	1.443	-1.170	-0.364
7	2.914	-1.588	-1.590	6	-0.010	-1.041	0.053
6	-3.946	-0.330	0.661	6	-0.618	0.190	-0.644
6	-2.984	0.808	0.441	6	3.641	-0.406	-0.523
6	-3.055	-1.976	-0.842	6	1.690	1.283	-0.720
6	-4.127	-2.666	1.220	6	2.281	-2.346	0.143
6	-1.608	0.618	0.456	6	0.208	1.457	-0.381
6	-0.720	1.676	0.243	6	3.738	-1.873	-0.060
6	-3.471	2.107	0.245	6	-0.849	-2.268	-0.273
6	-2.004	-3.057	-0.998	6	2.368	0.321	1.502
6	-4.049	-2.604	2.732	6	-2.096	0.335	-0.325
6	-1.227	2.960	0.051	6	-2.242	-2.128	0.316
6	1.378	0.453	-0.320	6	-2.861	-0.770	0.092
6	-2.600	3.174	0.062	6	-2.753	1.559	-0.479
6	2.779	0.328	-0.053	6	-4.225	-0.621	0.340
6	3.495	-0.704	-0.734	6	-4.110	1.708	-0.231
6	0.809	-0.463	-1.192	6	-4.854	0.606	0.183
6	3.481	1.158	0.848	1	1.446	-1.225	-1.468
6	4.886	-0.835	-0.512	1	-0.057	-0.884	1.143
6	1.618	-1.444	-1.780	1	-0.534	-0.017	-1.727
6	4.832	1.014	1.055	1	3.625	-0.355	-1.623
6	5.527	0.012	0.355	1	1.794	1.136	-1.805
1	-4.386	-0.220	1.658	1	2.244	2.194	-0.471
1	-4.796	-0.231	-0.040	1	2.063	-3.276	-0.388
1	-3.990	-2.256	-1.362	1	2.074	-2.536	1.202
1	-2.711	-1.064	-1.340	1	0.087	1.755	0.668
1	-5.181	-2.614	0.884	1	-0.185	2.290	-0.970
1	-3.755	-3.639	0.887	1	4.309	-1.912	0.873
1	-1.239	-0.383	0.652	1	4.280	-2.489	-0.783
1	-1.077	-2.772	-0.492	1	-0.373	-3.179	0.106
1	-2.324	-4.017	-0.585	1	-0.904	-2.380	-1.366
1	-1.778	-3.222	-2.055	1	2.980	1.206	1.697
1	-3.014	-2.697	3.069	1	1.386	0.502	1.942
1	-4.445	-1.668	3.134	1	2.820	-0.516	2.039
1	-4.628	-3.415	3.179	1	-2.190	-2.306	1.400
1	1.215	2.278	0.553	1	-2.912	-2.903	-0.071
1	-0.551	3.793	-0.117	1	5.521	0.145	-0.468
1	-2.995	4.175	-0.091	1	-2.195	2.430	-0.805
1	-0.241	-0.410	-1.452	1	-4.817	-1.473	0.663
1	2.954	1.914	1.422	1	-4.590	2.675	-0.360
1	5.415	-1.617	-1.042	1	-6.493	1.571	0.288
1	-5.049	3.192	0.133	8	4.380	3.220	0.461
1	1.156	-2.151	-2.469	1	4.710	3.345	1.353
1	5.362	1.649	1.754	1	4.537	2.279	0.281
8	-4.477	1.026	-2.594				
1	-4.918	1.322	-1.790				
1	-3.560	1.273	-2.444				
Estradiol motif 2, Eint = -5.0 kcal/mol				Diethylstilbestrol motif 1, Eint = -4.7 kcal/mol			
8	-5.409	-0.846	0.311	8	5.538	0.590	-0.525
8	5.480	-0.843	0.299	8	-6.498	-0.547	0.178
6	-3.016	-0.430	0.172	6	0.002	-0.465	0.064
6	-2.224	0.756	-0.405	6	-0.932	0.501	0.240
6	-0.752	0.712	-0.041	6	-0.322	-1.938	0.014
6	-0.148	-0.597	-0.585	6	-0.594	1.957	0.449
6	-4.413	-0.062	-0.331	6	1.446	-0.154	-0.081
6	-2.433	-1.723	-0.388	6	-2.386	0.206	0.256
6	-3.066	1.980	-0.038	6	-0.009	-2.581	-1.333
6	-0.932	-1.828	-0.109	6	-1.101	2.862	-0.669
6	-4.519	1.455	-0.070	6	2.410	-0.778	0.724
6	0.046	1.892	-0.574	6	-3.207	0.643	1.301
6	-3.021	-0.459	1.703	6	1.905	0.727	-1.065
6	1.346	-0.673	-0.322	6	-3.006	-0.468	-0.806
6	1.466	1.858	-0.035	6	3.765	-0.519	0.581
6	2.103	0.492	-0.095	6	-4.574	0.398	1.303
6	2.021	-1.896	-0.341	6	3.258	0.993	-1.231
6	3.480	0.403	0.107	6	-4.370	-0.714	-0.823
6	3.392	-1.988	-0.139	6	4.186	0.370	-0.404
6	4.120	-0.827	0.088	6	-5.162	-0.282	0.239
1	-2.277	0.646	-1.503	1	0.271	-2.447	0.786
1	-0.655	0.710	1.058	1	-1.367	-2.108	0.282
1	-0.285	-0.546	-1.682	1	0.483	2.085	0.582
1	-4.440	-0.254	-1.418	1	-1.052	2.285	1.392
1	-2.597	-1.739	-1.475	1	-0.598	-2.129	-2.137
1	-2.957	-2.595	0.018	1	-0.225	-3.652	-1.324
1	-2.905	2.816	-0.724	1	1.046	-2.456	-1.596
1	-2.801	2.344	0.961	1	-0.869	3.911	-0.470

1	-0.750	-1.977	0.964	1	-2.185	2.777	-0.787
1	-0.550	-2.728	-0.599	1	-0.651	2.598	-1.631
1	-5.025	1.612	0.888	1	2.092	-1.467	1.500
1	-5.127	1.955	-0.830	1	-2.769	1.170	2.143
1	-0.433	2.840	-0.305	1	1.184	1.204	-1.723
1	0.052	1.851	-1.673	1	-2.398	-0.793	-1.645
1	-3.676	-1.258	2.055	1	4.503	-0.988	1.224
1	-2.025	-0.634	2.114	1	-5.188	0.736	2.135
1	-3.392	0.474	2.134	1	3.592	1.676	-2.008
1	1.458	2.185	1.014	1	-4.839	-1.230	-1.654
1	2.104	2.579	-0.555	1	5.690	1.267	-1.190
1	-6.261	-0.618	-0.069	1	-6.921	-0.196	0.968
1	1.469	-2.812	-0.521	8	6.963	-0.709	1.648
1	4.070	1.301	0.273	1	6.675	-0.196	0.881
1	3.888	-2.955	-0.157	1	7.653	-1.280	1.305
1	5.806	-1.740	0.178				
8	6.575	1.847	0.259				
1	7.075	1.981	1.066				
1	6.379	0.901	0.258				
Diethylstilbestrol				Doxepin			
motif 2, Eint = -4.7 kcal/mol				motif 1, Eint = -6.0 kcal/mol			
8	6.489	0.056	0.368	8	2.604	-0.027	1.237
8	-5.588	-0.183	-0.497	7	-4.765	-0.032	0.557
6	0.893	0.356	-0.449	6	0.014	-0.530	-0.372
6	0.051	-0.691	-0.275	6	0.258	0.923	-0.537
6	0.436	1.725	-0.891	6	1.203	-1.417	-0.268
6	0.519	-2.096	0.016	6	0.995	1.606	0.440
6	2.356	0.243	-0.230	6	-2.522	-0.320	-0.492
6	-1.423	-0.548	-0.368	6	-1.227	-1.051	-0.371
6	0.670	2.809	0.157	6	-3.521	-0.787	0.562
6	0.078	-2.609	1.384	6	1.503	0.822	1.604
6	3.274	0.646	-1.210	6	2.380	-1.131	0.455
6	-2.182	-1.376	-1.201	6	-0.212	1.629	-1.646
6	2.877	-0.214	0.985	6	1.242	2.970	0.307
6	-2.117	0.378	0.423	6	1.189	-2.626	-0.988
6	4.643	0.572	-1.005	6	3.463	-2.013	0.433
6	-3.566	-1.268	-1.266	6	0.038	2.991	-1.776
6	4.246	-0.287	1.210	6	0.763	3.665	-0.799
6	-3.499	0.496	0.380	6	2.256	-3.507	-1.002
6	5.135	0.103	0.212	6	3.409	-3.192	-0.287
6	-4.221	-0.331	-0.474	6	-5.566	-0.370	1.717
1	0.993	1.997	-1.798	6	-5.528	-0.238	-0.659
1	-0.616	1.702	-1.184	1	-2.942	-0.495	-1.492
1	1.604	-2.166	-0.083	1	-2.382	0.761	-0.404
1	0.105	-2.764	-0.752	1	-1.314	-2.129	-0.226
1	0.111	2.601	1.075	1	-3.709	-1.875	0.437
1	0.357	3.790	-0.207	1	-3.070	-0.669	1.554
1	1.727	2.875	0.430	1	1.913	1.472	2.379
1	0.403	-3.639	1.548	1	0.714	0.199	2.047
1	-1.011	-2.583	1.485	1	-0.770	1.101	-2.413
1	0.491	-1.996	2.191	1	1.816	3.482	1.073
1	2.909	1.009	-2.166	1	0.308	-2.844	-1.583
1	-1.684	-2.109	-1.829	1	4.340	-1.747	1.013
1	2.192	-0.505	1.775	1	-0.333	3.526	-2.644
1	-1.554	1.011	1.103	1	0.957	4.728	-0.899
1	5.344	0.872	-1.775	1	2.198	-4.420	-1.585
1	-4.135	-1.911	-1.933	1	4.263	-3.861	-0.291
1	4.625	-0.639	2.167	1	-5.874	-1.433	1.734
1	-4.028	1.204	1.009	1	-6.472	0.241	1.734
1	6.689	-0.283	1.245	1	-5.002	-0.169	2.631
1	-5.970	-0.856	-1.067	1	-6.461	0.328	-0.605
8	-6.429	1.587	1.646	1	-5.785	-1.302	-0.828
1	-6.352	0.971	0.906	1	-4.977	0.120	-1.531
1	-7.001	2.283	1.317	8	4.494	2.146	0.899
				1	4.055	1.288	0.975
				1	4.279	2.426	0.006

Doxepin			
motif 2, Eint = -10.3 kcal/mol			
8	2.541	0.768	1.542
7	-3.914	-1.049	0.312
6	0.644	-0.489	-0.532
6	0.367	0.962	-0.652
6	2.044	-0.887	-0.236
6	0.630	1.789	0.449
6	-1.764	-1.172	-0.936
6	-0.312	-1.421	-0.705
6	-2.597	-1.681	0.243
6	1.166	1.144	1.684
6	2.882	-0.255	0.707
6	-0.141	1.530	-1.822
6	0.371	3.154	0.373
6	2.598	-1.950	-0.970
6	4.204	-0.681	0.869
6	-0.401	2.895	-1.891
6	-0.148	3.711	-0.792
6	3.904	-2.379	-0.801
6	4.715	-1.730	0.126
6	-4.595	-1.439	1.538
6	-4.732	-1.358	-0.849
1	-2.092	-1.659	-1.865
1	-1.958	-0.102	-1.056
1	-0.025	-2.464	-0.567
1	-2.683	-2.785	0.208
1	-2.076	-1.432	1.174
1	1.156	1.830	2.532
1	0.570	0.261	1.950
1	-0.329	0.893	-2.681
1	0.567	3.782	1.238
1	1.971	-2.420	-1.721
1	4.808	-0.167	1.609
1	-0.797	3.323	-2.807
1	-0.350	4.776	-0.844
1	4.290	-3.195	-1.401
1	5.745	-2.040	0.271
1	-4.778	-2.526	1.595
1	-5.558	-0.928	1.605
1	-3.992	-1.146	2.401
1	-5.705	-0.872	-0.751
1	-4.901	-2.443	-0.970
1	-4.262	-0.983	-1.760
8	-2.531	1.299	1.366
1	-2.175	1.917	0.722
1	-3.127	0.724	0.853

5. The Python script for calculating the four Lipinski's parameters with description.

```
import pandas as pd
from rdkit import Chem
from rdkit.Chem import rdMolDescriptors, Lipinski
```

This imports necessary libraries for working with chemical structures and data analysis. pandas is for data manipulation, and rdkit is a cheminformatics toolkit.

<pre> csv_file_path = r"Path/to/input.csv" data = pd.read_csv(csv_file_path) </pre>	<p>This reads the CSV file containing chemical information (SMILES representations) into a Pandas DataFrame.</p>
<pre> def validate_lipinski_rule_of_five(molecule_smiles): molecule = Chem.MolFromSmiles(molecule_smiles) if molecule is None: return False, "Invalid SMILES representation of the molecule." mw = rdMolDescriptors.CalcExactMolWt(molecule) logp = rdMolDescriptors.CalcCrippenDescriptors(molecule)[0] hbd = Lipinski.NumHDonors(molecule) hba = Lipinski.NumHAcceptors(molecule) criteria_violated = 0 if mw > 500: criteria_violated += 1 if logp >= 5: criteria_violated += 1 if hbd >= 5: criteria_violated += 1 if hba >= 10: criteria_violated += 1 return criteria_violated <= 1, criteria_violated, mw, logp, hbd, hba </pre>	<p>The function, validate_lipinski_rule_of_five, takes SMILES representation of a molecule as input, converts it to an RDKit molecule object, and calculates various molecular descriptors. It checks if the molecule violates Lipinski's Rule of Five and returns a tuple with a boolean indicating pass/fail, the number of violations, and the calculated descriptors.</p>

<pre> pass_results = [] violations_results = [] mw_results = [] logp_results = [] hbd_results = [] hba_results = [] for index, row in data.iterrows(): compound_smiles = row['SMILES'] is_pass, violations, mw, logp, hbd, hba = validate_lipinski_rule_of_five(compound_smiles) pass_results.append(is_pass) violations_results.append(violations) mw_results.append(mw) logp_results.append(logp) hbd_results.append(hbd) hba_results.append(hba) </pre>	<p>This loop iterates through each row of the DataFrame (data), extracts the SMILES string for each compound, and applies the <code>validate_lipinski_rule_of_five</code> function. The results are then appended to lists.</p>
<pre> data['Pass_Lipinski'] = pass_results data['Violations'] = violations_results data['MW'] = mw_results data['LogP'] = logp_results data['HBD'] = hbd_results data['HBA'] = hba_results </pre>	<p>These lines add new columns to the original DataFrame (data) to store the results.</p>
<pre> output_csv_path = r"Path/to/output.csv" data.to_csv(output_csv_path, index=False) print(f"Results saved to {output_csv_path}") </pre>	<p>The final DataFrame, now containing the results, is saved as a new CSV file at the specified path and prints a message indicating where the results are saved.</p>

6. Table S5. Cartesian coordinates of optimized geometry of 193 FDA approved oral drugs at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

	cefditoren pivoxil					etoposide			
16	0.883	-2.629	1.182		8	-1.589	0.468	-0.738	
16	-3.926	-2.873	-1.598		8	0.505	-2.971	-1.362	
16	7.872	1.276	-2.002		8	-3.125	-0.940	0.201	
8	0.042	1.393	-0.258		8	-6.748	-0.692	0.431	

8	-2.792	0.360	-1.105	8	2.192	-2.526	-2.770
8	-3.468	0.415	1.056	8	-3.537	2.415	-1.227
8	4.007	-1.136	-1.761	8	-6.029	-2.503	1.723
8	-3.225	2.602	-0.840	8	-6.157	1.314	-1.531
8	4.027	-1.296	2.034	8	0.402	5.155	0.809
8	-5.197	2.968	0.214	8	2.407	5.135	-0.327
7	-0.552	-0.905	-0.322	8	6.331	-2.481	-0.799
7	2.669	-0.403	-0.081	8	4.552	-0.202	2.971
7	5.186	-0.723	1.512	8	6.525	-1.893	1.742
7	7.326	0.538	0.423	6	0.331	-0.936	-0.217
7	-5.864	-1.232	-2.017	6	1.099	-0.725	-1.507
7	9.405	1.628	0.234	6	-0.439	0.318	0.137
6	0.553	-1.846	-0.427	6	2.239	0.274	-1.316
6	1.465	-0.646	-0.804	6	0.429	1.549	-0.022
6	0.257	0.229	-0.442	6	1.642	1.540	-0.724
6	-1.748	-1.116	0.359	6	-0.407	-2.228	-0.516
6	-0.832	-3.238	1.333	6	1.384	-2.133	-1.972
6	-1.932	-2.234	1.104	6	-2.822	0.416	-0.117
6	-2.769	-0.040	0.189	6	3.384	-0.275	-0.477
6	-3.208	-2.585	1.719	6	-3.832	1.045	-1.077
6	3.884	-0.710	-0.625	6	-5.461	-0.548	-0.150
6	5.081	-0.431	0.255	6	-5.244	0.900	-0.540
6	-4.428	-2.551	1.154	6	-4.395	-1.022	0.826
6	-3.706	1.409	-1.403	6	-0.068	2.746	0.539
6	-3.252	4.295	0.827	6	2.390	2.727	-0.858
6	-4.763	-2.217	-0.221	6	-4.705	-2.452	1.215
6	6.246	0.198	-0.364	6	0.679	3.884	0.389
6	-4.037	3.243	0.063	6	1.889	3.873	-0.296
6	-4.235	5.227	1.529	6	3.491	-0.017	0.885
6	-2.403	3.544	1.865	6	4.332	-1.105	-1.088
6	-2.334	5.086	-0.108	6	-6.979	-2.047	0.782
6	-5.763	-1.372	-0.654	6	5.347	-1.656	-0.325
6	6.361	0.509	-1.694	6	4.521	-0.564	1.656
6	-6.668	-0.589	0.231	6	1.585	5.905	0.548
6	8.247	1.104	-0.289	6	5.471	-1.383	1.046
6	-4.975	-1.957	-2.625	6	-8.343	-2.157	1.394
6	4.268	-1.656	3.390	6	6.239	-2.875	-2.158
1	0.396	-2.610	-1.194	6	4.943	-1.177	3.931
1	1.703	-0.646	-1.870	1	1.060	-1.115	0.585
1	-0.962	-4.100	0.667	1	0.402	-0.311	-2.254
1	-0.916	-3.631	2.351	1	-0.819	0.264	1.167
1	2.619	-0.241	0.916	1	2.648	0.519	-2.304
1	-3.145	-2.934	2.749	1	-1.334	-2.053	-1.067
1	-5.278	-2.778	1.795	1	-0.623	-2.849	0.354
1	-4.703	1.180	-1.023	1	-2.814	0.998	0.828
1	-3.696	1.490	-2.489	1	-3.765	0.510	-2.039
1	-3.688	5.964	2.122	1	-5.399	-1.176	-1.058
1	-4.859	5.765	0.811	1	-5.339	1.527	0.365
1	-4.901	4.674	2.194	1	-4.422	-0.384	1.727
1	-1.845	4.267	2.466	1	-1.016	2.762	1.068
1	-1.687	2.874	1.383	1	3.336	2.725	-1.387
1	-3.030	2.952	2.537	1	-4.044	-2.823	2.001
1	-1.810	5.857	0.465	1	-4.598	-3.104	0.333
1	-2.898	5.588	-0.899	1	2.783	0.631	1.391
1	-1.586	4.444	-0.576	1	4.247	-1.329	-2.143
1	5.670	0.297	-2.493	1	-6.874	-2.655	-0.138
1	-6.449	0.482	0.170	1	-2.631	2.470	-1.551
1	-7.710	-0.724	-0.066	1	-7.039	1.155	-1.180
1	-6.554	-0.878	1.277	1	1.319	6.848	0.063
1	-4.874	-2.016	-3.703	1	2.122	6.084	1.491
1	5.057	-2.409	3.455	1	-9.101	-1.813	0.690
1	4.548	-0.780	3.981	1	-8.393	-1.543	2.295
1	3.326	-2.068	3.751	1	-8.551	-3.192	1.663
1	9.600	1.281	1.163	1	7.030	-2.428	1.115
1	10.214	1.613	-0.369	1	7.057	-3.572	-2.330
				1	6.347	-2.015	-2.826
				1	5.283	-3.369	-2.362
				1	4.519	-2.158	3.693
				1	4.540	-0.834	4.885
				1	6.028	-1.270	4.003
	candesartan cilexetil				dipyridamole		
8	2.564	-1.930	-0.115	8	-5.738	1.219	-1.641
8	0.571	-2.742	-0.161	8	-4.942	-0.945	2.535
8	1.928	-3.122	-1.942	8	5.738	-1.219	-1.641
8	-1.622	-3.239	-0.101	8	4.941	0.945	2.535
8	-5.219	2.454	-0.719	7	-0.079	3.054	-0.302
8	-2.133	-1.778	-1.754	7	0.079	-3.054	-0.303
7	-4.113	0.426	-0.617	7	-1.868	1.614	-0.102
7	-6.023	0.672	0.586	7	1.868	-1.614	-0.103
7	4.034	3.067	-0.723	7	-1.668	-0.774	-0.086
7	2.003	3.745	-0.071	7	1.668	0.774	-0.086
7	3.538	4.046	-1.465	7	-3.712	0.262	0.201
7	2.332	4.472	-1.101	7	3.712	-0.262	0.201
6	3.912	-1.781	-0.648	6	-1.003	4.166	-0.099

6	4.817	-1.618	0.554	6	1.048	3.408	-1.169
6	3.990	-0.583	-1.575	6	1.003	-4.166	-0.101
6	6.256	-1.352	0.125	6	-1.048	-3.408	-1.170
6	5.428	-0.350	-2.025	6	-0.267	5.352	0.509
6	6.343	-0.159	-0.820	6	1.843	4.553	-0.566
6	1.715	-2.637	-0.857	6	0.267	-5.352	0.507
6	-4.305	-0.778	0.051	6	-1.843	-4.553	-0.567
6	-2.960	0.923	-1.356	6	0.943	5.757	-0.324
6	-0.430	-3.586	-0.767	6	-0.943	-5.757	-0.325
6	-5.497	-0.590	0.794	6	-0.559	1.769	-0.228
6	-3.579	-1.978	0.142	6	0.559	-1.770	-0.229
6	-5.170	1.222	-0.231	6	-0.326	-0.623	-0.206
6	-1.684	0.938	-0.557	6	0.326	0.623	-0.206
6	-5.986	-1.592	1.623	6	-2.359	0.357	0.007
6	-2.396	-2.270	-0.681	6	2.359	-0.357	0.007
6	-4.084	-2.956	1.014	6	-4.523	1.453	0.386
6	-1.671	1.010	0.833	6	-4.352	-1.040	0.237
6	-0.464	0.904	-1.235	6	4.524	-1.453	0.386
6	-0.139	-5.035	-0.502	6	4.352	1.040	0.237
6	-5.263	-2.775	1.728	6	-4.913	2.123	-0.913
6	0.756	1.060	0.852	6	-4.234	-1.728	1.580
6	-0.467	1.060	1.527	6	4.913	-2.123	-0.913
6	0.733	0.976	-0.545	6	4.234	1.728	1.580
6	2.023	1.104	1.613	1	-1.815	3.827	0.543
6	-6.341	3.244	-0.264	1	-1.461	4.452	-1.063
6	3.111	1.927	1.256	1	0.643	3.720	-2.148
6	2.168	0.279	2.735	1	1.669	2.530	-1.318
6	4.295	1.885	2.003	1	1.815	-3.828	0.541
6	-6.231	4.595	-0.912	1	1.461	-4.452	-1.064
6	3.336	0.261	3.484	1	-0.644	-3.719	-2.149
6	3.042	2.889	0.153	1	-1.669	-2.530	-1.319
6	4.411	1.064	3.114	1	-0.964	6.189	0.617
1	4.150	-2.696	-1.204	1	0.059	5.079	1.520
1	4.443	-0.773	1.143	1	2.283	4.213	0.379
1	4.749	-2.503	1.194	1	2.672	4.811	-1.233
1	3.317	-0.725	-2.426	1	0.964	-6.189	0.616
1	3.648	0.300	-1.019	1	-0.059	-5.080	1.519
1	6.660	-2.243	-0.377	1	-2.283	-4.213	0.379
1	6.880	-1.192	1.010	1	-2.673	-4.811	-1.233
1	5.475	0.520	-2.688	1	0.601	6.149	-1.292
1	5.773	-1.208	-2.618	1	1.492	6.569	0.161
1	7.377	-0.001	-1.142	1	-0.601	-6.149	-1.294
1	6.038	0.752	-0.286	1	-1.492	-6.570	0.160
1	-2.824	0.328	-2.261	1	-3.984	2.171	1.009
1	-3.223	1.938	-1.663	1	-5.421	1.154	0.933
1	-0.496	-3.338	-1.828	1	-3.914	-1.683	-0.531
1	-6.904	-1.433	2.177	1	-5.406	-0.896	-0.015
1	-3.537	-3.886	1.103	1	5.421	-1.154	0.933
1	-2.606	1.028	1.386	1	3.984	-2.171	1.008
1	-0.458	0.800	-2.316	1	5.405	0.896	-0.015
1	-5.620	-3.571	2.373	1	3.914	1.683	-0.532
1	0.807	-5.312	-0.969	1	-5.453	3.057	-0.690
1	-0.928	-5.657	-0.926	1	-4.007	2.380	-1.477
1	-0.082	-5.220	0.572	1	-4.662	-2.740	1.506
1	-0.476	1.128	2.611	1	-3.174	-1.825	1.847
1	1.667	0.936	-1.096	1	5.453	-3.057	-0.690
1	-6.306	3.295	0.829	1	4.007	-2.379	-1.477
1	-7.263	2.719	-0.534	1	4.661	2.740	1.506
1	1.349	-0.385	2.995	1	3.173	1.825	1.847
1	5.116	2.532	1.710	1	-5.852	1.563	-2.529
1	-7.062	5.226	-0.594	1	-4.726	-1.271	3.411
1	-6.263	4.516	-2.001	1	5.853	-1.563	-2.529
1	-5.300	5.093	-0.633	1	4.726	1.271	3.411
1	3.414	-0.394	4.346				
1	5.331	1.053	3.688				
1	4.037	4.443	-2.250				
Cefpodoxime proxetil				Auranofin			
16	-1.940	-3.007	0.963	16	2.370	-3.244	-0.576
16	3.819	1.587	-1.379	8	-0.038	-2.187	-0.805
8	-0.356	-0.276	-2.338	8	-1.522	1.135	-1.052
8	-2.542	1.611	-0.325	8	1.112	1.730	-0.169
8	-5.924	-0.724	1.265	8	1.759	-0.761	0.916
8	-3.281	1.083	-2.401	8	-2.661	-1.623	0.387
8	2.328	-3.015	-2.040	8	-2.061	1.745	1.062
8	-1.427	3.469	0.285	8	2.664	2.221	-1.736
8	2.889	-3.919	1.151	8	3.544	0.613	1.139
8	0.450	3.375	1.346	8	-4.392	-0.214	0.002
8	0.363	2.518	-0.755	6	-0.620	0.137	-0.559
7	-2.116	-1.492	-1.306	6	0.801	0.536	-0.888
7	0.720	-2.565	-0.489	6	-0.941	-1.183	-1.257
7	3.486	-2.662	1.045	6	1.769	-0.581	-0.509
7	4.473	-0.086	0.497	6	1.308	-1.889	-1.137
7	5.631	1.965	0.636	6	-2.353	-1.657	-1.012
6	-1.780	-2.843	-0.837	6	-2.200	1.875	-0.127

6	-0.366	-2.648	-1.428	6	2.127	2.481	-0.691
6	-0.852	-1.251	-1.851	6	2.705	-0.098	1.632
6	-3.024	-0.620	-0.715	6	-3.146	2.806	-0.807
6	-3.770	-0.986	0.343	6	2.459	3.613	0.221
6	-3.653	-2.346	0.962	6	-3.701	-0.838	0.772
6	-4.708	-0.042	1.019	6	2.528	-0.383	3.088
6	-2.983	0.769	-1.279	6	-3.827	-0.833	2.259
6	2.013	-2.602	-0.943	1	-0.750	0.030	0.521
6	3.022	-2.024	0.025	1	0.900	0.732	-1.964
6	-2.274	2.978	-0.726	1	-0.822	-1.047	-2.349
6	-6.837	0.079	1.974	1	2.780	-0.323	-0.836
6	3.494	-0.681	-0.271	1	1.405	-1.786	-2.230
6	-3.532	3.794	-0.735	1	-3.064	-1.027	-1.551
6	3.016	0.066	-1.317	1	-2.453	-2.692	-1.345
6	4.749	1.092	0.031	1	2.036	-4.075	-1.577
6	-0.131	3.058	0.198	1	-4.064	2.250	-1.018
6	1.882	3.060	1.429	1	-3.391	3.634	-0.145
6	3.477	-4.614	2.239	1	-2.747	3.171	-1.752
6	2.182	2.854	2.892	1	1.578	3.978	0.749
6	2.668	4.185	0.799	1	2.935	4.415	-0.339
1	-2.388	-3.607	-1.330	1	3.168	3.241	0.965
1	-0.082	-3.325	-2.235	1	1.608	0.091	3.438
1	-3.958	-2.305	2.009	1	3.371	0.011	3.650
1	-4.309	-3.080	0.483	1	2.422	-1.454	3.261
1	0.541	-2.072	0.378	1	-3.170	-0.047	2.642
1	-4.889	0.860	0.414	1	-4.849	-0.593	2.544
1	-4.280	0.302	1.979	1	-3.514	-1.781	2.694
1	-1.757	2.940	-1.689				
1	-7.736	-0.514	2.138				
1	-7.104	0.982	1.407				
1	-6.429	0.391	2.947				
1	-4.002	3.776	0.250				
1	-4.223	3.393	-1.478				
1	-3.303	4.829	-0.994				
1	2.251	-0.180	-2.041				
1	2.033	2.133	0.867				
1	4.546	-4.775	2.072				
1	3.334	-4.069	3.177				
1	2.962	-5.573	2.286				
1	6.248	1.485	1.278				
1	6.140	2.569	0.006				
1	1.567	2.059	3.316				
1	3.231	2.574	3.009				
1	2.005	3.770	3.463				
1	2.416	4.298	-0.257				
1	3.737	3.971	0.875				
1	2.471	5.129	1.315				
cefuroxime axetil				Bosentan			
16	-0.825	-2.464	-0.698	16	0.915	3.397	1.013
8	-0.439	1.265	1.512	8	0.307	4.546	0.365
8	3.445	0.243	0.665	8	1.639	3.515	2.256
8	3.606	-1.683	-1.613	8	-2.431	0.880	0.038
8	2.369	0.230	2.656	8	-2.008	-1.846	-0.298
8	-4.578	-0.637	2.002	8	-4.322	1.441	-1.661
8	4.871	1.894	0.041	8	-4.152	-3.623	-0.075
8	-5.777	2.295	-1.257	7	-0.447	2.347	1.240
8	-5.823	-1.780	-0.528	7	0.818	0.403	1.540
8	5.752	-1.348	-0.923	7	0.080	-1.692	0.676
8	2.928	3.051	-0.085	7	3.056	-0.801	2.481
7	0.238	-1.014	1.328	7	2.607	-2.645	1.026
7	-2.871	-0.481	0.497	6	3.748	-0.545	-2.613
7	-5.918	-0.432	-0.849	6	3.162	0.572	-1.754
7	4.977	-0.505	-2.904	6	4.078	-0.007	-4.012
6	-0.834	-1.959	1.050	6	2.700	-1.664	-2.726
6	-1.844	-0.845	1.418	6	5.020	-1.135	-2.008
6	-0.622	0.084	1.468	6	2.006	1.240	-2.188
6	1.552	-1.127	0.878	6	3.694	0.927	-0.512
6	1.901	-2.096	0.004	6	1.901	2.468	-0.138
6	0.909	-3.020	-0.646	6	1.374	2.183	-1.396
6	3.322	-2.366	-0.376	6	3.062	1.856	0.307
6	2.482	-0.150	1.519	6	-0.314	0.971	1.125
6	-4.175	-0.338	0.899	6	-1.334	0.228	0.528
6	-5.069	0.261	-0.165	6	-1.064	-1.130	0.320
6	4.379	1.221	1.182	6	0.970	-0.889	1.273
6	-4.952	1.679	-0.365	6	-3.689	0.389	0.331
6	4.862	-1.182	-1.725	6	2.290	-1.488	1.623
6	5.522	0.547	1.877	6	-1.785	-3.262	-0.456
6	-4.104	2.599	0.200	6	-4.703	0.710	-0.586
6	-4.431	3.851	-0.380	6	-3.971	-0.349	1.468
6	-5.447	3.609	-1.251	6	-5.997	0.259	-0.337
6	4.027	2.822	-0.510	6	-3.088	-3.806	-0.982
6	4.693	3.497	-1.666	6	-5.269	-0.796	1.707
6	-6.809	-2.498	-1.255	6	-6.277	-0.493	0.803
1	-0.807	-2.839	1.699	6	4.242	-1.334	2.762

1	-5.722	1.431	1.744		
1	-6.297	0.533	3.142		
1	-4.615	0.361	2.621		
1	-5.739	0.887	-2.986		
1	-9.539	-2.961	0.023		
1	-9.838	-1.208	-0.086		
1	-9.614	-1.970	1.504		
1	-3.034	2.116	-0.981		
1	-0.630	2.481	-0.418		
1	-7.415	4.049	0.661		
1	-9.013	4.155	1.269		
1	-2.518	-2.659	-2.609		
1	-3.454	-2.612	-1.121		
1	-1.790	-3.245	-1.118		
1	3.785	-1.586	-0.233		
1	2.640	1.832	0.162		
1	6.525	1.766	0.649		
1	5.343	-2.362	0.536		
1	8.760	2.335	1.305		
1	9.887	1.100	1.843		
1	7.660	-3.030	0.910		
1	9.362	1.892	-1.095		
1	9.787	-2.313	1.221		
1	12.645	-0.218	0.185		
1	13.065	1.423	0.634		
1	11.773	0.572	1.496		
1	12.675	2.170	-1.835		
1	12.242	0.528	-2.267		
1	11.099	1.845	-2.574		
	adefovir dipivoxil				
15	0.059	2.263	-0.607		
8	0.118	0.530	1.351		
8	-3.576	1.356	-0.742		
8	3.138	0.523	-1.168		
8	-1.373	1.726	-1.149		
8	0.898	1.070	-1.309		
8	-2.958	0.859	1.371		
8	2.963	2.016	0.502		
8	0.411	3.650	-0.963		
7	-0.114	-2.071	1.388		
7	1.749	-2.844	0.374		
7	-1.402	-1.445	-0.588		
7	-0.176	-1.849	-2.628		
7	1.935	-2.816	-2.686		
6	-4.773	-0.394	0.342		
6	4.499	0.175	0.790		
6	-4.906	-1.015	-1.048		
6	-4.521	-1.487	1.375		
6	-6.057	0.376	0.697		
6	5.746	1.061	0.923		
6	3.934	-0.128	2.182		
6	4.848	-1.125	0.071		
6	-3.646	0.626	0.408		
6	3.457	1.006	0.060		
6	-0.852	-1.338	2.402		
6	-0.232	0.036	2.626		
6	0.058	1.922	1.184		
6	-0.328	-1.940	0.032		
6	-2.579	2.351	-0.789		
6	2.165	1.288	-1.869		
6	0.830	-2.430	-0.568		
6	1.152	-2.595	1.513		
6	0.873	-2.361	-1.968		
6	-1.226	-1.435	-1.910		
1	-5.735	-1.728	-1.047		
1	-5.106	-0.265	-1.814		
1	-3.997	-1.555	-1.319		
1	-5.377	-2.166	1.412		
1	-3.639	-2.073	1.103		
1	-4.371	-1.072	2.374		
1	-6.261	1.168	-0.028		
1	-5.991	0.826	1.691		
1	-6.907	-0.311	0.694		
1	6.511	0.536	1.501		
1	5.511	1.999	1.431		
1	6.173	1.299	-0.056		
1	4.677	-0.667	2.776		
1	3.671	0.793	2.708		
1	3.039	-0.752	2.110		
1	5.625	-1.651	0.634		
1	3.983	-1.788	-0.002		
1	5.234	-0.939	-0.935		
1	-1.870	-1.217	2.033		
1	-0.878	-1.915	3.331		
	estramustine phosphate				
17	7.504	-3.652	-0.299		
17	8.617	3.240	1.035		
15	-8.074	-0.281	0.750		
8	-6.732	0.566	0.645		
8	-7.532	-1.650	1.401		
8	-8.800	0.420	1.998		
8	-8.887	-0.433	-0.469		
8	4.110	-0.688	0.180		
8	4.429	1.549	-0.194		
7	6.189	0.138	0.160		
6	-4.339	0.366	0.111		
6	-3.624	0.298	-1.250		
6	-2.120	0.453	-1.126		
6	-1.582	-0.673	-0.222		
6	-5.774	0.216	-0.386		
6	-3.826	-0.763	0.996		
6	-4.425	1.251	-2.143		
6	-2.303	-0.715	1.133		
6	-5.872	1.135	-1.611		
6	-1.391	0.419	-2.461		
6	-4.176	1.720	0.807		
6	-0.068	-0.626	-0.115		
6	0.082	0.736	-2.266		
6	0.707	0.014	-1.099		
6	0.599	-1.251	0.945		
6	2.100	0.016	-0.997		
6	1.981	-1.243	1.052		
6	2.723	-0.600	0.074		
6	4.862	0.444	0.026		
6	6.676	-1.191	0.501		
6	7.147	1.217	-0.028		
6	6.827	-2.052	-0.738		
6	7.363	1.981	1.264		
1	-3.800	-0.724	-1.631		
1	-1.898	1.421	-0.646		
1	-1.840	-1.614	-0.743		
1	-5.941	-0.832	-0.671		
1	-4.119	-1.723	0.547		
1	-4.297	-0.731	1.985		
1	-4.051	2.276	-2.046		
1	-4.347	0.991	-3.201		
1	-1.999	0.156	1.728		
1	-1.979	-1.589	1.704		
1	-6.267	2.103	-1.294		
1	-6.573	0.740	-2.348		
1	-1.514	-0.579	-2.907		
1	-1.836	1.128	-3.166		
1	-4.491	2.554	0.175		
1	-4.789	1.748	1.711		
1	-3.142	1.906	1.100		
1	0.653	0.523	-3.176		
1	0.197	1.816	-2.100		
1	0.028	-1.760	1.714		
1	2.693	0.517	-1.753		

1	0.666	-0.023	3.263	1	2.487	-1.730	1.879
1	-0.964	0.688	3.120	1	-8.150	-2.373	1.257
1	0.913	2.444	1.631	1	-9.422	1.093	1.705
1	-0.872	2.335	1.604	1	5.996	-1.670	1.207
1	-2.889	3.045	-1.572	1	7.643	-1.084	1.001
1	-2.503	2.863	0.179	1	6.778	1.895	-0.801
1	2.425	2.351	-1.856	1	8.091	0.789	-0.378
1	2.164	0.882	-2.881	1	5.862	-2.226	-1.215
1	1.575	-2.786	2.491	1	7.508	-1.600	-1.462
1	-2.048	-1.018	-2.491	1	6.446	2.484	1.575
1	1.983	-2.525	-3.650	1	7.706	1.328	2.068
1	2.808	-2.946	-2.200				
	Bacampicillin				Dasatinib		
16	1.388	-1.170	1.013	17	-6.746	2.424	0.628
8	0.261	1.283	-2.018	16	-1.993	-1.401	0.963
8	-3.334	-0.826	0.390	8	11.746	-0.741	-0.164
8	-2.575	-2.169	-1.266	8	-4.982	-1.896	0.873
8	4.539	-0.899	-2.720	7	8.042	-0.609	0.189
8	-5.520	-0.256	0.604	7	5.285	0.119	0.062
8	-6.377	1.702	0.323	7	3.717	1.803	-0.194
8	-5.075	0.854	-1.332	7	1.362	1.400	-0.115
7	-0.066	-0.887	-1.131	7	0.546	-0.743	0.332
7	3.087	0.083	-1.274	7	-1.238	0.300	-0.856
7	6.691	-0.056	-1.342	7	-5.499	-0.057	-0.402
6	1.181	-1.559	-0.761	6	7.016	-1.597	-0.106
6	-0.460	-1.285	1.240	6	7.627	0.672	-0.374
6	-1.049	-0.689	-0.088	6	5.683	-1.206	0.503
6	1.934	-0.612	-1.731	6	6.321	1.132	0.234
6	0.612	0.170	-1.742	6	9.340	-1.035	-0.312
6	-0.865	-0.462	2.451	6	3.965	0.498	0.044
6	-0.847	-2.751	1.425	6	10.497	-0.265	0.303
6	-2.384	-1.324	-0.433	6	2.909	-0.406	0.228
6	4.329	-0.138	-1.793	6	1.623	0.119	0.126
6	5.461	0.697	-1.168	6	2.442	2.177	-0.265
6	-4.679	-1.303	0.172	6	2.170	3.622	-0.535
6	5.209	1.044	0.282	6	-0.781	-0.515	0.057
6	-4.953	-2.513	1.013	6	-3.207	-0.598	0.016
6	4.625	2.264	0.628	6	-6.897	-0.142	-0.266
6	5.490	0.119	1.290	6	-2.593	0.256	-0.866
6	4.315	2.554	1.954	6	-7.601	-1.298	-0.648
6	5.183	0.408	2.614	6	-4.618	-0.931	0.223
6	-5.603	0.790	-0.254	6	-7.615	0.967	0.202
6	4.593	1.624	2.950	6	-8.988	-1.308	-0.493
6	-6.562	2.918	-0.444	6	-6.904	-2.477	-1.248
6	-5.389	3.850	-0.285	6	-8.994	0.950	0.332
1	1.212	-2.634	-0.955	6	-9.681	-0.208	-0.007
1	-1.205	0.390	0.035	1	7.327	-2.562	0.304
1	2.176	-1.093	-2.682	1	6.889	-1.727	-1.199
1	-1.952	-0.489	2.572	1	7.520	0.598	-1.475
1	-0.556	0.581	2.348	1	8.392	1.425	-0.171
1	-0.418	-0.865	3.363	1	5.750	-1.243	1.602
1	-1.923	-2.845	1.608	1	4.937	-1.936	0.189
1	-0.325	-3.173	2.285	1	6.468	1.332	1.307
1	-0.605	-3.355	0.548	1	5.976	2.053	-0.231
1	2.999	0.660	-0.447	1	9.391	-0.961	-1.420
1	5.436	1.642	-1.745	1	9.472	-2.095	-0.071
1	-4.799	-1.476	-0.900	1	10.395	0.815	0.123
1	6.654	-0.521	-2.246	1	10.500	-0.409	1.386
1	7.489	0.567	-1.342	1	3.058	-1.457	0.437
1	-4.307	-3.332	0.693	1	11.799	-0.562	-1.107
1	-4.769	-2.294	2.067	1	0.770	-1.630	0.756
1	-5.992	-2.825	0.896	1	3.096	4.193	-0.577
1	4.411	2.993	-0.152	1	1.517	4.035	0.236
1	5.959	-0.820	1.015	1	1.637	3.730	-1.483
1	3.865	3.508	2.208	1	-3.125	0.858	-1.597
1	5.405	-0.319	3.389	1	-5.144	0.876	-0.565
1	4.356	1.848	3.985	1	-9.533	-2.201	-0.787
1	-7.482	3.341	-0.040	1	-7.590	-3.046	-1.878
1	-6.724	2.646	-1.490	1	-6.511	-3.140	-0.475
1	-5.583	4.782	-0.819	1	-6.051	-2.168	-1.858
1	-5.219	4.092	0.766	1	-9.509	1.828	0.700
1	-4.480	3.410	-0.698	1	-10.760	-0.242	0.096
	Cefdinir				Erlotinib		
16	1.883	-1.785	0.390	8	2.500	1.262	-0.103
16	-6.190	1.223	0.656	8	3.573	-1.041	0.186
8	1.541	2.244	-1.135	8	3.655	3.698	0.935
8	5.489	1.621	-1.462	8	6.086	-1.759	-1.032
8	4.404	2.888	0.048	7	-2.659	0.409	-0.119
8	-1.887	0.238	1.826	7	-0.710	-3.200	0.418
8	-1.368	-2.185	-1.038	7	-2.710	-1.898	0.213
7	2.636	0.798	0.404	6	-0.574	-0.788	0.101
7	-0.546	0.141	-0.003	6	0.024	-2.060	0.275
7	-2.692	-1.729	-0.952	6	1.625	0.240	0.008
7	-5.183	-0.672	-0.801	6	2.227	-1.048	0.172

7	-7.461	-0.270	-1.248	6	0.253	0.353	-0.028
6	1.771	-0.126	1.119	6	-2.006	-0.785	0.069
6	0.563	0.738	0.662	6	1.433	-2.162	0.305
6	1.579	1.472	-0.222	6	1.969	2.564	-0.283
6	3.946	0.558	0.001	6	-4.020	0.729	-0.193
6	3.690	-1.863	0.608	6	4.229	-2.294	0.340
6	4.498	-0.683	0.127	6	-2.011	-3.037	0.381
6	4.625	1.810	-0.442	6	3.114	3.533	-0.353
6	-1.717	-0.088	0.663	6	5.710	-2.057	0.290
6	5.913	-0.924	-0.093	6	-5.061	-0.186	-0.021
6	-2.820	-0.720	-0.155	6	-4.326	2.074	-0.452
6	6.541	-2.100	0.054	6	-6.391	0.249	-0.111
6	-4.167	-0.169	-0.017	6	-5.643	2.496	-0.539
6	-4.518	0.847	0.832	6	-6.684	1.594	-0.371
6	-6.292	-0.048	-0.560	6	4.793	4.522	0.926
1	1.974	-0.165	2.193	6	7.453	-1.450	-1.133
1	0.183	1.348	1.485	6	-7.446	-0.688	0.065
1	-0.403	-0.306	-0.899	6	-8.348	-1.476	0.213
1	3.993	-2.750	0.047	1	-0.176	1.340	-0.146
1	3.918	-2.075	1.660	1	1.853	-3.151	0.436
1	6.507	-0.065	-0.384	1	-2.056	1.203	-0.257
1	7.608	-2.177	-0.112	1	1.308	2.826	0.555
1	6.037	-3.016	0.341	1	1.382	2.605	-1.212
1	5.850	2.495	-1.670	1	3.949	-2.747	1.301
1	-3.907	1.352	1.562	1	3.927	-2.978	-0.464
1	-1.455	-2.937	-1.634	1	-2.618	-3.933	0.499
1	-7.451	-1.147	-1.751	1	3.877	3.158	-1.053
1	-8.317	-0.122	-0.734	1	2.748	4.497	-0.748
				1	5.980	-1.231	0.968
				1	6.231	-2.961	0.649
				1	-4.836	-1.223	0.176
				1	-3.517	2.789	-0.586
				1	-5.857	3.540	-0.741
				1	-7.717	1.915	-0.438
				1	5.148	4.600	1.954
				1	4.562	5.532	0.553
				1	5.593	4.099	0.303
				1	7.714	-0.570	-0.528
				1	8.085	-2.291	-0.809
				1	7.664	-1.235	-2.180
				1	-9.138	-2.174	0.343
Delavirdine				Darunavir			
16	7.301	-1.449	0.294	16	4.040	0.026	-1.027
8	-0.182	3.604	-1.739	8	-5.249	-2.037	2.055
8	8.670	-1.333	-0.168	8	-5.080	-0.420	3.704
8	6.968	-2.007	1.588	8	-3.318	-0.535	0.385
7	-3.787	0.756	0.090	8	0.638	-2.691	-1.523
7	-1.329	1.924	-0.695	8	-3.206	-1.300	-1.753
7	1.271	1.233	0.469	8	3.267	0.604	-2.118
7	-4.840	-1.708	-0.525	8	5.356	-0.556	-1.220
7	-5.363	1.039	1.824	7	-1.311	-0.762	-0.563
7	6.691	0.127	0.239	7	3.069	-1.190	-0.397
6	-3.604	2.206	0.118	7	4.333	4.056	3.341
6	-2.514	0.079	0.367	6	-5.349	0.257	1.437
6	-2.591	2.617	-0.932	6	-5.726	-0.781	2.528
6	-1.491	0.471	-0.677	6	-4.758	-0.587	0.303
6	-4.869	0.270	0.866	6	-4.396	1.197	2.178
6	-0.170	2.548	-1.127	6	-5.257	-1.980	0.641
6	1.106	1.924	-0.722	6	-3.921	0.332	3.335
6	-5.397	-1.006	0.531	6	-0.453	-0.544	-1.734
6	2.312	1.978	-1.376	6	0.866	-1.291	-1.551
6	3.268	1.308	-0.564	6	-2.669	-0.896	-0.750
6	2.590	0.874	0.605	6	1.647	-0.850	-0.309
6	-5.559	-2.802	-1.179	6	-0.287	0.950	-2.052
6	-6.446	-1.475	1.321	6	3.626	-2.006	0.685
6	4.634	1.020	-0.700	6	3.224	-3.474	0.559
6	3.248	0.209	1.638	6	-1.613	1.612	-2.301
6	-6.392	0.579	2.548	6	4.169	1.268	0.235
6	5.291	0.369	0.334	6	3.740	-4.068	-0.743
6	-6.941	-0.677	2.348	6	3.731	-4.240	1.773
6	4.604	-0.027	1.501	6	-2.241	1.504	-3.544
6	-6.835	-2.338	-1.874	6	-2.291	2.264	-1.269
6	-4.610	-3.483	-2.148	6	5.111	1.121	1.255
6	6.351	-2.352	-0.927	6	3.299	2.357	0.239
1	-3.276	2.545	1.113	6	-3.513	2.025	-3.746
1	-4.568	2.681	-0.075	6	-3.567	2.783	-1.465
1	-2.672	-1.002	0.354	6	-4.183	2.661	-2.705
1	-2.147	0.354	1.373	6	5.176	2.055	2.274
1	-2.967	2.380	-1.938	6	3.366	3.293	1.258
1	-2.399	3.689	-0.900	6	4.303	3.154	2.293
1	-0.534	-0.013	-0.489	1	-6.231	0.780	1.063
1	-1.843	0.136	-1.667	1	-6.797	-0.858	2.753
1	2.467	2.449	-2.335	1	-5.051	-0.256	-0.695
1	0.584	1.219	1.207	1	-4.947	2.061	2.560

1	-4.385	-1.076	-1.179	1	-3.582	1.558	1.548
1	-5.821	-3.522	-0.392	1	-4.622	-2.776	0.252
1	-6.891	-2.444	1.121	1	-6.274	-2.120	0.239
1	5.176	1.318	-1.593	1	-3.599	0.887	4.218
1	2.724	-0.101	2.535	1	-3.115	-0.345	3.023
1	-6.776	1.245	3.315	1	-0.981	-1.024	-2.564
1	-7.761	-1.024	2.967	1	1.492	-1.103	-2.427
1	5.159	-0.520	2.289	1	1.238	-1.361	0.570
1	-6.595	-1.658	-2.697	1	1.526	0.228	-0.127
1	-7.387	-3.184	-2.292	1	-1.080	-0.213	0.258
1	-7.500	-1.809	-1.188	1	0.227	1.450	-1.222
1	-5.095	-4.327	-2.643	1	0.375	1.044	-2.919
1	-4.293	-2.786	-2.932	1	3.319	-1.602	1.665
1	-3.716	-3.848	-1.640	1	4.716	-1.933	0.627
1	7.139	0.623	-0.524	1	2.126	-3.523	0.546
1	6.687	-3.388	-0.891	1	-0.111	-2.834	-0.930
1	5.296	-2.290	-0.662	1	3.354	-3.522	-1.605
1	6.536	-1.927	-1.912	1	3.438	-5.113	-0.844
				1	4.834	-4.028	-0.780
				1	3.434	-5.291	1.730
				1	4.825	-4.214	1.824
				1	3.347	-3.825	2.711
				1	-1.731	0.991	-4.355
				1	-1.811	2.361	-0.297
				1	5.806	0.289	1.228
				1	2.600	2.482	-0.582
				1	-3.987	1.928	-4.718
				1	-4.079	3.285	-0.648
				1	5.915	1.946	3.062
				1	2.698	4.149	1.253
				1	-5.178	3.066	-2.863
				1	3.944	4.967	3.152
				1	5.198	4.107	3.857
Amprenavir				Diltiazem			
16	3.565	0.017	-1.222	16	-0.534	-0.496	-2.114
8	0.404	-2.990	-0.719	8	0.851	-2.175	1.269
8	-3.408	-0.897	1.453	8	0.102	0.396	1.733
8	-6.207	0.652	1.319	8	5.774	0.766	-0.731
8	2.606	0.298	-2.281	8	-0.786	-2.445	2.795
8	4.911	-0.456	-1.488	7	-1.863	0.127	0.619
8	-3.436	-2.145	-0.446	7	-2.209	3.852	0.780
7	2.833	-1.148	-0.260	6	0.565	-1.449	-0.966
7	-1.538	-1.043	0.244	6	-0.118	-1.591	0.399
7	3.809	4.822	2.281	6	-0.594	-0.260	0.979
6	0.497	-1.603	-1.003	6	-2.331	1.415	1.134
6	-0.898	-0.983	-1.075	6	-2.665	-0.570	-0.319
6	1.413	-0.908	0.008	6	1.921	-0.797	-0.929
6	3.625	-1.726	0.829	6	-2.164	-0.956	-1.577
6	-0.914	0.441	-1.649	6	-1.899	2.550	0.214
6	3.361	-3.222	0.991	6	-3.991	-0.864	0.008
6	-4.801	-1.237	1.663	6	-3.006	-1.625	-2.471
6	-2.304	1.002	-1.757	6	2.096	0.568	-0.720
6	4.124	-3.739	2.203	6	3.061	-1.594	-1.076
6	3.730	-3.978	-0.276	6	-4.819	-1.510	-0.898
6	-5.190	-0.610	2.988	6	-4.329	-1.890	-2.144
6	3.678	1.485	-0.229	6	3.366	1.131	-0.645
6	-5.705	-0.517	0.666	6	4.332	-1.052	-1.006
6	-2.858	-1.421	0.332	6	-1.277	4.207	1.837
6	-5.528	0.806	2.557	6	-2.219	4.880	-0.243
6	-3.139	0.652	-2.820	6	4.491	0.318	-0.786
6	-2.812	1.845	-0.765	6	0.380	-2.519	2.495
6	4.713	1.621	0.698	6	1.499	-2.959	3.380
6	2.701	2.475	-0.334	6	5.971	2.145	-0.497
6	-4.439	1.137	-2.894	1	0.679	-2.459	-1.374
6	-4.114	2.332	-0.833	1	-0.970	-2.273	0.315
6	4.766	2.735	1.515	1	-3.419	1.393	1.220
6	2.756	3.591	0.483	1	-1.914	1.536	2.134
6	3.786	3.737	1.423	1	-2.427	2.450	-0.742
6	-4.931	1.980	-1.901	1	-0.820	2.439	-0.012
1	0.962	-1.527	-1.990	1	-4.361	-0.590	0.990
1	-1.504	-1.634	-1.715	1	-2.607	-1.922	-3.435
1	1.195	-1.294	1.010	1	1.228	1.211	-0.612
1	1.214	0.173	0.045	1	2.945	-2.662	-1.240
1	3.424	-1.193	1.773	1	-5.845	-1.731	-0.623
1	4.681	-1.577	0.584	1	-4.970	-2.400	-2.854
1	-0.305	1.098	-1.017	1	3.465	2.196	-0.477
1	-0.418	0.419	-2.625	1	5.216	-1.669	-1.121
1	2.285	-3.357	1.167	1	-1.271	3.450	2.623
1	-1.299	-0.293	0.883	1	-1.575	5.157	2.287
1	-4.901	-2.323	1.618	1	-0.240	4.311	1.465
1	-6.081	-1.110	3.378	1	-2.498	5.839	0.200
1	-4.395	-0.681	3.731	1	-1.236	5.009	-0.734
1	3.848	-3.207	3.119	1	-2.953	4.635	-1.014
1	3.932	-4.802	2.367	1	1.108	-3.516	4.228

1	5.204	-3.621	2.065	1	2.231	-3.552	2.832
1	3.161	-3.614	-1.133	1	2.013	-2.068	3.750
1	3.529	-5.047	-0.168	1	7.048	2.300	-0.480
1	4.796	-3.858	-0.504	1	5.532	2.756	-1.295
1	-0.236	-3.081	-0.002	1	5.545	2.455	0.464
1	-5.159	-0.245	-0.243				
1	-6.555	-1.144	0.377				
1	-4.609	1.402	2.427				
1	-6.191	1.340	3.241				
1	-2.764	-0.012	-3.595				
1	-2.175	2.126	0.072				
1	5.487	0.862	0.753				
1	1.925	2.375	-1.085				
1	-5.073	0.854	-3.729				
1	-4.496	2.976	-0.048				
1	5.577	2.846	2.229				
1	2.002	4.368	0.392				
1	-5.949	2.350	-1.951				
1	3.311	5.642	1.970				
1	4.706	5.048	2.685				
	Colchicine				Balsalazide		
8	0.973	-1.779	1.295	8	4.988	-1.999	0.786
8	3.686	-1.652	1.008	8	-7.445	-0.628	-0.813
8	4.787	-0.381	-1.236	8	7.312	1.574	-2.207
8	-5.062	-1.970	-0.069	8	5.847	2.395	-0.716
8	-5.016	0.721	0.573	8	-5.668	2.750	0.912
8	-0.885	2.854	2.046	8	-7.607	1.838	0.241
7	0.422	2.249	0.297	7	4.910	0.252	1.045
6	-0.693	2.121	-0.637	7	-1.271	-1.265	-0.160
6	-0.211	2.278	-2.086	7	-1.995	-0.279	0.157
6	0.326	0.988	-2.719	6	6.351	0.360	1.155
6	-1.513	0.842	-0.429	6	2.856	-0.962	0.581
6	1.222	0.234	-1.780	6	7.048	0.367	-0.196
6	0.641	-0.435	-0.687	6	4.333	-0.964	0.803
6	-0.831	-0.418	-0.482	6	2.288	-2.110	0.024
6	1.484	-1.085	0.226	6	2.024	0.116	0.917
6	2.605	0.257	-1.924	6	0.100	-1.092	0.119
6	-2.845	1.053	-0.180	6	0.925	-2.173	-0.211
6	-1.446	-1.649	-0.368	6	0.661	0.058	0.692
6	2.876	-1.058	0.079	6	-3.361	-0.447	-0.120
6	3.440	-0.381	-1.009	6	-5.567	0.591	-0.002
6	-3.984	0.210	0.122	6	-4.188	0.621	0.218
6	0.224	2.606	1.601	6	-6.121	-0.567	-0.587
6	-2.796	-2.008	-0.248	6	-3.929	-1.593	-0.701
6	-3.934	-1.243	-0.114	6	6.653	1.550	-1.030
6	1.481	2.697	2.432	6	-5.285	-1.643	-0.927
6	0.618	-0.949	2.397	6	-6.411	1.745	0.373
6	3.721	-3.075	0.919	1	6.581	1.274	1.708
6	5.573	0.287	-0.253	1	6.703	-0.491	1.740
6	-6.346	-1.403	-0.361	1	6.814	-0.549	-0.750
1	-1.356	2.957	-0.401	1	8.137	0.369	-0.083
1	0.558	3.058	-2.101	1	4.424	1.092	0.767
1	-1.044	2.652	-2.690	1	2.942	-2.941	-0.213
1	-0.522	0.352	-2.998	1	2.440	1.002	1.389
1	0.856	1.227	-3.645	1	0.467	-3.054	-0.649
1	1.347	1.984	-0.006	1	0.010	0.883	0.957
1	3.063	0.764	-2.769	1	-3.739	1.499	0.666
1	-3.139	2.097	-0.088	1	-3.284	-2.423	-0.964
1	-0.773	-2.499	-0.437	1	-5.734	-2.526	-1.376
1	-2.999	-3.076	-0.280	1	-7.648	-1.482	-1.212
1	2.337	2.185	1.986	1	7.000	2.354	-2.686
1	1.288	2.280	3.421	1	-6.297	3.452	1.124
1	1.743	3.749	2.572				
1	-0.131	-0.200	2.109				
1	1.504	-0.445	2.802				
1	0.193	-1.603	3.158				
1	4.385	-3.418	1.713				
1	2.725	-3.502	1.067				
1	4.122	-3.390	-0.050				
1	6.609	0.198	-0.577				
1	5.304	1.350	-0.205				
1	5.455	-0.166	0.734				
1	-6.761	-0.892	0.505				
1	-6.291	-0.703	-1.196				
1	-6.962	-2.258	-0.640				
	Bicalutamide				Cinoxacin		
16	-2.441	-0.497	-0.665	8	4.020	0.599	-0.052
9	-6.644	3.421	0.469	8	3.734	-1.677	0.169
9	4.524	1.202	2.409	8	-1.387	-2.549	0.006
9	6.168	0.768	1.070	8	-3.944	-1.693	0.753
9	4.970	2.545	0.770	8	-4.546	-0.041	-0.649
8	-2.034	-3.594	0.357	7	-0.771	1.424	-0.305
8	-2.992	-1.515	-1.552	7	-2.010	0.964	-0.245
8	-1.220	0.230	-1.003	6	0.353	0.621	-0.176

8	0.008	-2.772	-1.082	6	0.167	-0.769	-0.044
7	0.900	-1.476	0.585	6	2.695	0.306	-0.085
7	6.253	1.535	-2.293	6	1.652	1.185	-0.196
6	-1.304	-2.536	0.911	6	2.515	-1.076	0.045
6	-2.172	-1.255	0.965	6	1.272	-1.637	0.068
6	-0.950	-2.953	2.334	6	-0.682	2.887	-0.391
6	-0.057	-2.288	0.028	6	-1.182	-1.340	-0.029
6	-3.721	0.701	-0.326	6	-2.232	-0.319	-0.093
6	2.002	-0.888	-0.041	6	4.700	-0.660	-0.055
6	-3.363	2.002	0.014	6	-0.471	3.532	0.964
6	-5.054	0.310	-0.411	6	-3.688	-0.647	-0.055
6	2.885	-0.163	0.768	1	1.829	2.247	-0.288
6	-4.357	2.931	0.288	1	1.090	-2.700	0.168
6	-6.052	1.234	-0.138	1	0.113	3.142	-1.096
6	2.238	-0.971	-1.417	1	-1.626	3.203	-0.834
6	3.986	0.472	0.227	1	5.441	-0.672	0.749
6	-5.681	2.525	0.207	1	5.177	-0.809	-1.033
6	4.234	0.394	-1.156	1	-1.301	3.294	1.633
6	3.343	-0.333	-1.953	1	0.453	3.194	1.439
6	4.914	1.247	1.120	1	-0.419	4.618	0.863
6	5.352	1.028	-1.765	1	-4.899	-1.837	0.708
1	-3.153	-1.520	1.368				
1	-1.728	-0.468	1.582				
1	-1.864	-3.229	2.863				
1	-0.467	-2.156	2.906				
1	-0.294	-3.824	2.318				
1	0.756	-1.203	1.546				
1	-1.937	-3.535	-0.606				
1	-2.315	2.282	0.042				
1	-5.300	-0.705	-0.707				
1	2.708	-0.094	1.836				
1	-4.125	3.957	0.548				
1	-7.102	0.975	-0.200				
1	1.558	-1.522	-2.048				
1	3.527	-0.391	-3.020				
	Cyclacillin				Chloramphenicol		
16	1.199	1.447	0.224	17	4.592	1.525	-0.190
8	1.332	-2.528	1.081	17	5.582	-1.239	-0.473
8	5.600	-0.443	0.407	8	-0.096	-1.413	1.812
8	-2.626	-1.058	-1.386	8	0.569	2.384	0.155
8	4.706	-1.113	-1.550	8	2.738	-1.404	-1.137
7	2.119	-0.896	-0.442	8	-6.415	0.972	-0.579
7	-1.109	-0.697	0.265	8	-6.326	-1.166	-0.948
7	-2.949	-0.459	2.115	7	1.953	-0.014	0.501
6	1.074	0.020	-0.907	7	-5.835	-0.106	-0.584
6	0.020	-1.051	-0.520	6	0.580	0.029	-0.006
6	3.259	-0.314	0.232	6	-0.375	-0.174	1.188
6	3.052	1.242	0.257	6	-1.815	-0.169	0.756
6	1.194	-1.719	0.206	6	0.361	1.321	-0.769
6	-3.446	-0.221	0.749	6	-2.536	1.027	0.748
6	3.656	1.913	-0.973	6	-2.429	-1.347	0.325
6	3.598	1.857	1.536	6	2.936	-0.617	-0.243
6	-3.571	1.304	0.573	6	-3.851	1.058	0.309
6	-4.808	-0.889	0.487	6	-3.745	-1.333	-0.113
6	-2.378	-0.722	-0.239	6	-4.435	-0.128	-0.117
6	4.568	-0.689	-0.436	6	4.347	-0.212	0.227
6	-4.219	1.705	-0.745	1	0.471	-0.820	-0.688
6	-5.520	-0.443	-0.787	1	-0.217	0.658	1.894
6	-5.601	1.076	-0.880	1	-0.653	1.348	-1.190
1	1.147	0.317	-1.956	1	1.078	1.369	-1.599
1	-0.330	-1.605	-1.396	1	2.223	0.830	0.999
1	3.281	-0.693	1.262	1	-2.055	1.939	1.090
1	-1.011	-0.439	1.241	1	-1.870	-2.275	0.354
1	3.395	2.972	-0.990	1	0.863	-1.471	1.898
1	4.749	1.838	-0.958	1	-4.432	1.971	0.297
1	3.306	1.460	-1.904	1	-4.246	-2.232	-0.449
1	3.419	2.935	1.554	1	0.623	3.211	-0.330
1	3.135	1.416	2.421	1	4.437	-0.268	1.313
1	4.678	1.697	1.595				
1	-2.585	1.765	0.699				
1	-4.193	1.672	1.403				
1	-5.438	-0.640	1.354				
1	-4.685	-1.978	0.499				
1	-3.587	1.382	-1.582				
1	-4.281	2.796	-0.804				
1	-6.524	-0.880	-0.809				
1	-4.984	-0.833	-1.655				
1	-6.249	1.463	-0.080				
1	-6.067	1.374	-1.824				
1	-3.047	-1.445	2.348				
1	-3.540	0.041	2.773				
1	6.411	-0.676	-0.068				
	Eplerenone				Aprepitant		
8	0.685	-0.045	-1.439	9	0.359	4.710	-0.162

8	-4.467	-1.108	0.133	9	4.641	2.752	0.834
8	2.260	2.287	-0.569	9	3.228	2.876	-0.797
8	0.237	3.168	-0.118	9	2.522	2.936	1.250
8	-6.544	-1.390	-0.663	9	5.317	-3.402	-0.199
8	6.406	-0.742	-0.456	9	5.635	-1.971	-1.793
6	0.862	-0.616	-0.137	9	6.606	-1.688	0.117
6	0.202	0.207	0.961	8	-1.058	-2.775	-0.779
6	-2.040	-0.680	0.186	8	-0.416	-1.170	0.775
6	-1.232	0.558	0.605	8	-8.523	-0.988	0.298
6	0.014	-1.276	-1.144	7	-2.995	-0.705	-0.477
6	2.270	-1.156	0.193	7	-6.385	-0.656	-0.645
6	-1.499	-1.235	-1.129	7	-5.544	0.754	0.831
6	-3.456	-0.067	0.173	7	-6.818	0.378	1.171
6	1.095	1.419	1.303	6	-1.694	-0.436	-1.096
6	-2.066	1.216	1.718	6	-0.654	-1.442	-0.582
6	-3.506	0.710	1.499	6	-3.374	-2.102	-0.664
6	3.122	-0.048	0.801	6	-2.307	-3.029	-0.137
6	2.462	0.903	1.757	6	-1.203	0.968	-0.854
6	-1.965	-1.793	1.241	6	-4.023	0.181	-1.024
6	2.960	-1.698	-1.068	6	0.745	-1.820	1.297
6	-3.815	0.843	-1.011	6	-5.305	0.108	-0.271
6	2.105	-2.285	1.230	6	-1.439	1.620	0.360
6	1.129	2.397	0.146	6	-0.434	1.607	-1.825
6	4.427	-2.031	-0.851	6	2.008	-1.147	0.806
6	-5.324	0.691	-1.089	6	0.624	-1.762	2.806
6	4.442	0.058	0.556	6	-0.919	2.885	0.597
6	-5.571	-0.701	-0.552	6	0.101	2.872	-1.602
6	5.206	-0.874	-0.272	6	3.102	-1.907	0.400
6	2.298	3.056	-1.776	6	2.106	0.244	0.804
1	0.181	-0.405	1.874	6	-0.153	3.487	-0.390
1	-1.208	1.234	-0.257	6	4.285	-1.285	0.013
1	0.446	-2.121	-1.681	6	3.296	0.859	0.430
1	-1.806	-0.632	-1.988	6	-7.418	-0.493	0.286
1	-1.890	-2.244	-1.304	6	4.391	0.100	0.029
1	0.619	1.960	2.128	6	3.417	2.355	0.435
1	-1.991	2.305	1.671	6	5.457	-2.092	-0.460
1	-1.700	0.921	2.708	1	-1.746	-0.608	-2.192
1	-3.822	0.033	2.296	1	0.269	-1.336	-1.170
1	-4.243	1.517	1.465	1	-3.554	-2.321	-1.737
1	2.300	0.373	2.708	1	-4.310	-2.289	-0.128
1	3.145	1.726	1.981	1	-2.199	-2.910	0.949
1	-2.128	-1.427	2.257	1	-2.552	-4.070	-0.354
1	-2.716	-2.559	1.040	1	-3.658	1.208	-0.970
1	-0.984	-2.276	1.222	1	-4.215	-0.040	-2.093
1	2.869	-0.943	-1.855	1	0.747	-2.868	0.963
1	2.433	-2.590	-1.424	1	-2.037	1.121	1.116
1	-3.358	0.490	-1.938	1	-0.247	1.110	-2.773
1	-3.478	1.869	-0.851	1	-0.284	-2.270	3.135
1	1.653	-1.935	2.161	1	1.484	-2.236	3.282
1	1.469	-3.079	0.828	1	0.576	-0.722	3.141
1	3.072	-2.723	1.489	1	-1.095	3.407	1.531
1	4.910	-2.347	-1.779	1	0.708	3.375	-2.345
1	4.541	-2.874	-0.156	1	-6.471	-1.228	-1.470
1	-5.754	0.801	-2.083	1	3.034	-2.990	0.390
1	-5.849	1.396	-0.435	1	1.249	0.844	1.101
1	5.013	0.868	1.002	1	5.318	0.584	-0.257
1	2.158	4.117	-1.562	1	-7.257	0.773	1.985
1	1.512	2.718	-2.454				
1	3.280	2.878	-2.210				
	chlorphenesin carbamate				Dexamethasone		
17	6.108	-0.580	0.031	9	1.475	-0.064	-1.291
8	0.396	0.801	-0.178	8	-2.779	0.418	-1.821
8	-1.995	1.502	0.942	8	0.424	-2.108	1.492
8	-4.287	0.259	-0.206	8	-4.765	-0.408	0.978
8	-5.408	-1.666	0.236	8	-5.662	-2.297	-0.605
7	-6.501	0.241	-0.417	8	6.180	-0.305	-1.853
6	-1.934	0.540	-0.093	6	-1.631	-0.145	0.309
6	-0.609	-0.197	-0.064	6	-0.751	1.090	0.061
6	-3.073	-0.428	0.098	6	0.642	0.978	0.666
6	1.700	0.406	-0.118	6	1.339	-0.275	0.111
6	2.112	-0.919	0.019	6	-2.942	0.350	-0.403
6	2.652	1.424	-0.210	6	-1.640	2.265	0.459
6	3.470	-1.219	0.066	6	-0.945	-1.351	-0.328
6	4.002	1.124	-0.164	6	-3.080	1.805	0.118
6	4.407	-0.201	-0.026	6	0.485	-1.565	0.177
6	-5.405	-0.500	-0.082	6	2.815	-0.425	0.632
1	-2.041	1.027	-1.076	6	1.462	2.234	0.373
1	-0.534	-0.912	-0.894	6	-1.909	-0.388	1.796
1	-0.492	-0.742	0.884	6	2.920	2.107	0.808
1	-3.101	-0.791	1.131	6	3.529	0.859	0.256
1	-2.966	-1.296	-0.562	6	-4.160	-0.499	-0.074
1	-1.212	2.055	0.854	6	-3.817	2.718	-0.846
1	1.392	-1.724	0.089	6	2.914	-0.583	2.170
1	2.315	2.449	-0.320	6	3.458	-1.635	0.020

8	-2.170	-2.825	0.673	8	2.675	0.558	-0.041
8	-5.192	-0.401	-1.062	8	3.545	1.638	-1.839
7	2.404	-1.062	0.708	7	-3.786	-1.176	-0.920
7	-0.826	-1.093	0.058	7	-0.964	0.510	-1.303
7	-4.502	0.814	-0.981	6	-2.482	-1.290	-0.261
6	1.624	-1.700	-0.355	6	-4.422	-0.796	1.400
6	3.367	0.023	-1.251	6	-4.931	-0.893	-0.082
6	3.393	-0.082	0.314	6	-1.845	-0.592	-1.491
6	0.380	-1.644	0.569	6	-3.299	-0.268	-1.864
6	1.256	-0.711	1.425	6	-4.464	-2.150	2.102
6	4.353	-0.944	-1.901	6	-5.193	0.251	2.187
6	3.615	1.449	-1.717	6	-6.017	-1.942	-0.228
6	4.777	-0.433	0.825	6	0.353	0.448	-1.660
6	-2.050	-1.698	0.215	6	1.163	1.727	-1.413
6	-3.193	-0.895	-0.256	6	0.626	2.674	-0.364
6	-3.319	0.508	-0.502	6	2.608	1.322	-1.162
6	-4.413	-1.398	-0.623	6	7.386	-3.154	0.192
6	-2.324	1.575	-0.299	6	6.543	-2.512	-0.920
6	-4.991	-2.754	-0.627	6	7.471	-2.086	1.293
6	-1.771	1.840	0.963	6	5.672	-1.545	-0.170
6	-1.873	2.327	-1.388	6	6.203	-1.300	1.101
6	-0.774	2.795	1.126	6	4.509	-0.916	-0.589
6	-0.888	3.293	-1.232	6	3.895	-0.036	0.295
6	-0.333	3.517	0.024	6	0.371	4.005	-0.699
1	1.988	-2.676	-0.682	6	0.368	2.248	0.945
1	3.105	0.885	0.747	6	5.571	-0.418	1.968
1	0.148	-2.602	1.041	6	4.402	0.221	1.560
1	4.215	-1.970	-1.551	6	-0.130	4.894	0.246
1	4.230	-0.935	-2.985	6	-0.137	3.135	1.887
1	5.385	-0.653	-1.680	6	-0.386	4.461	1.542
1	3.564	1.516	-2.806	1	-2.165	-2.308	-0.023
1	2.882	2.140	-1.295	1	-5.348	0.075	-0.387
1	4.613	1.773	-1.409	1	-1.362	-1.303	-2.166
1	-0.780	-0.154	-0.317	1	-3.996	-2.079	3.085
1	6.450	0.385	1.085	1	-5.499	-2.478	2.248
1	-5.525	-2.944	-1.560	1	-3.948	-2.927	1.533
1	-4.204	-3.491	-0.482	1	-5.126	1.235	1.717
1	-5.707	-2.864	0.192	1	-6.247	-0.031	2.247
1	-2.306	2.129	-2.363	1	-4.810	0.329	3.207
1	-0.354	2.958	2.111	1	-1.310	1.328	-0.819
1	-0.550	3.863	-2.090	1	1.179	2.249	-2.376
1	0.445	4.262	0.154	1	-7.838	-2.171	0.174
				1	6.860	-4.032	0.581
				1	8.365	-3.495	-0.153
				1	5.977	-3.239	-1.509
				1	7.178	-1.966	-1.631
				1	8.343	-1.435	1.142
				1	7.572	-2.509	2.296
				1	4.072	-1.095	-1.566
				1	0.568	4.345	-1.712
				1	0.563	1.216	1.220
				1	5.975	-0.225	2.957
				1	3.876	0.911	2.211
				1	-0.321	5.925	-0.033
				1	-0.340	2.788	2.895
				1	-0.779	5.152	2.280
	Capecitabine				Felbamate		
9	-0.022	2.653	-0.447	8	-2.372	-0.738	-0.506
8	-4.569	1.002	-0.800	8	2.372	-0.737	-0.506
8	-4.775	-2.284	0.438	8	-3.708	-1.964	0.863
8	-6.827	-0.762	-0.146	8	3.709	-1.963	0.863
8	-2.165	-2.220	-0.300	7	-4.578	-0.554	-0.722
8	3.764	0.269	-0.052	7	4.579	-0.553	-0.722
8	2.510	-1.625	-0.029	6	0.000	-0.637	-0.419
7	-2.453	0.027	-0.465	6	0.000	0.842	-0.105
7	-0.278	-0.933	-0.252	6	-1.235	-1.337	0.123
7	1.580	0.502	-0.201	6	1.235	-1.337	0.123
6	-4.541	-0.917	0.604	6	0.000	1.293	1.216
6	-5.883	-0.196	0.730	6	-0.001	1.785	-1.131
6	-3.915	-0.217	-0.625	6	0.000	2.653	1.504
6	-5.548	1.205	0.255	6	-0.001	3.148	-0.848
6	-4.995	2.114	1.332	6	-0.001	3.586	0.471
6	-1.935	1.275	-0.513	6	-3.570	-1.155	-0.023
6	-1.624	-1.120	-0.334	6	3.571	-1.154	-0.023
6	-0.594	1.427	-0.410	6	0.000	-0.756	-1.510
6	0.225	0.275	-0.284	1	-1.220	-2.410	-0.098
6	7.453	-0.377	0.209	1	-1.323	-1.231	1.210
6	6.142	0.386	0.090	1	1.221	-2.410	-0.098
6	8.673	0.532	0.239	1	1.323	-1.230	1.210
6	4.953	-0.539	0.063	1	0.000	0.575	2.033
6	2.609	-0.434	-0.087	1	-0.001	1.444	-2.162
6	9.979	-0.234	0.356	1	0.000	2.986	2.537
1	-3.915	-0.717	1.488	1	-0.001	3.868	-1.661
1	-6.248	-0.199	1.769	1	-0.001	4.648	0.695

1	-4.025	-0.847	-1.517	1	-4.361	0.280	-1.243
1	-6.417	1.655	-0.233	1	-5.489	-0.602	-0.297
1	-5.759	2.329	2.082	1	4.361	0.281	-1.244
1	-4.669	3.064	0.904	1	5.489	-0.601	-0.298
1	-4.141	1.661	1.845				
1	-3.920	-2.664	0.170				
1	-6.639	-1.710	-0.168				
1	-2.629	2.096	-0.640				
1	7.545	-1.083	-0.628				
1	7.438	-0.997	1.115				
1	6.037	1.085	0.929				
1	6.144	0.998	-0.819				
1	1.874	1.468	-0.238				
1	8.577	1.236	1.076				
1	8.684	1.151	-0.667				
1	4.989	-1.233	-0.784				
1	4.879	-1.145	0.973				
1	10.007	-0.835	1.270				
1	10.114	-0.919	-0.486				
1	10.843	0.434	0.377				
Cephradine				Dyphylline			
16	0.098	0.990	-0.637	8	-3.184	-1.185	0.919
8	1.919	-2.207	1.540	8	-0.250	2.020	-0.706
8	-2.176	-2.226	-1.525	8	-4.741	1.025	1.086
8	5.107	0.446	1.095	8	4.026	0.904	0.580
8	4.702	-1.563	0.164	7	-0.792	-1.000	-0.730
7	2.112	-0.787	-0.360	7	2.567	-0.827	0.243
7	-0.941	-1.728	0.312	7	1.898	1.436	-0.059
7	-4.522	-2.048	-0.171	7	0.819	-2.461	-0.173
6	0.882	-0.587	-1.105	6	0.336	-0.260	-0.430
6	0.304	-1.831	-0.378	6	-2.103	-0.459	-1.046
6	1.560	-1.743	0.496	6	1.293	-1.194	-0.102
6	3.112	0.174	-0.155	6	-2.841	-0.014	0.201
6	1.587	1.959	-1.036	6	0.562	1.144	-0.433
6	2.905	1.466	-0.499	6	-0.445	-2.295	-0.545
6	-2.122	-1.856	-0.365	6	2.912	0.521	0.277
6	-3.355	-1.432	0.435	6	-4.075	0.793	-0.147
6	3.943	2.541	-0.459	6	3.554	-1.838	0.581
6	4.371	-0.421	0.361	6	2.301	2.836	-0.008
6	-3.355	0.084	0.504	1	-1.968	0.384	-1.727
6	-3.552	0.825	-0.787	1	-2.676	-1.241	-1.551
6	-3.152	0.714	1.665	1	-2.173	0.625	0.802
6	-3.077	2.197	1.817	1	-1.161	-3.092	-0.687
6	-3.492	2.309	-0.633	1	-4.713	0.223	-0.840
6	-3.278	2.925	0.528	1	-3.777	1.733	-0.631
1	1.008	-0.646	-2.189	1	4.482	-1.327	0.823
1	0.284	-2.700	-1.040	1	3.705	-2.514	-0.263
1	-0.952	-1.261	1.209	1	3.213	-2.425	1.436
1	1.397	2.959	-0.634	1	1.440	3.435	-0.290
1	1.657	2.087	-2.125	1	3.131	3.014	-0.694
1	-3.235	-1.807	1.462	1	2.633	3.096	0.998
1	4.962	2.162	-0.460	1	-3.769	-0.905	1.632
1	3.825	3.157	0.440	1	-5.588	1.440	0.911
1	3.818	3.210	-1.316				
1	-4.510	0.531	-1.243				
1	-2.803	0.495	-1.524				
1	-3.023	0.117	2.569				
1	-4.375	-2.114	-1.176				
1	-5.349	-1.485	-0.007				
1	-2.107	2.474	2.259				
1	-3.812	2.538	2.563				
1	-3.630	2.900	-1.536				
1	-3.247	4.011	0.563				
1	5.889	-0.048	1.380				
Busulfan				Clavulanate			
16	4.470	0.173	0.000	8	0.330	-0.903	1.030
16	-4.470	-0.173	0.000	8	-2.378	-1.498	-1.736
8	2.994	-0.538	0.000	8	0.039	2.973	-0.780
8	-2.994	0.538	0.001	8	-1.151	2.449	1.065
8	4.656	0.874	1.253	8	3.787	-1.370	-0.553
8	4.657	0.872	-1.254	7	-1.583	-0.127	0.033
8	-4.656	-0.874	1.253	6	-1.094	-0.882	1.178
8	-4.656	-0.871	-1.255	6	-0.520	0.705	-0.486
6	0.620	-0.441	0.000	6	-1.801	-2.133	0.654
6	-0.620	0.441	0.000	6	-2.030	-1.307	-0.608
6	1.882	0.384	0.000	6	0.716	0.015	0.091
6	-1.882	-0.384	0.001	6	-0.613	2.125	0.040
6	5.401	-1.339	0.001	6	1.990	0.244	-0.228
6	-5.401	1.339	0.002	6	3.155	-0.475	0.362
1	0.621	-1.097	0.878	1	-1.342	-0.480	2.163
1	0.621	-1.097	-0.878	1	-0.518	0.698	-1.579
1	-0.621	1.096	-0.879	1	-2.703	-2.434	1.190
1	-0.621	1.097	0.878	1	-1.152	-2.996	0.509
1	1.946	1.022	-0.890	1	2.173	0.997	-0.990

1	1.946	1.022	0.890	1	2.835	-1.094	1.200
1	-1.946	-1.022	0.891	1	3.888	0.249	0.751
1	-1.947	-1.023	-0.889	1	0.005	3.849	-0.369
1	5.158	-1.900	0.901	1	4.065	-0.862	-1.319
1	5.159	-1.902	-0.898				
1	6.452	-1.054	0.001				
1	-6.452	1.054	0.001				
1	-5.158	1.900	0.902				
1	-5.158	1.902	-0.897				
	Halofantrine				Ambrisentan		
17	-3.942	-4.045	-0.353	8	2.165	-0.360	-1.814
17	-6.884	0.402	0.235	8	-0.709	0.062	0.366
9	0.132	4.829	-0.414	8	-0.297	-1.607	-2.742
9	-1.795	4.751	0.581	8	-0.802	-2.482	-0.728
9	0.036	4.625	1.734	7	-2.675	0.048	-0.818
8	0.917	-3.544	-0.149	7	-2.576	0.383	1.552
7	3.699	-0.855	-0.836	6	1.466	-0.041	-0.605
6	3.094	-1.927	-1.631	6	-0.062	-0.179	-0.873
6	1.577	-1.831	-1.634	6	1.905	-1.085	0.415
6	0.976	-2.126	-0.259	6	1.842	1.370	-0.157
6	4.977	-1.258	-0.254	6	1.698	-0.865	1.778
6	3.788	0.381	-1.611	6	3.176	1.587	0.202
6	-0.370	-1.460	-0.089	6	2.481	-2.286	0.002
6	4.808	-2.161	0.957	6	0.972	2.458	-0.174
6	4.089	1.619	-0.777	6	-0.437	-1.556	-1.400
6	-0.429	-0.036	0.110	6	2.024	0.545	-2.892
6	-1.691	0.617	0.193	6	2.058	-1.830	2.710
6	-1.523	-2.179	-0.171	6	3.627	2.855	0.540
6	-2.911	-0.162	0.110	6	2.847	-3.248	0.938
6	-2.806	-1.571	-0.067	6	1.421	3.732	0.169
6	6.136	-2.617	1.545	6	2.637	-3.025	2.293
6	3.699	2.909	-1.488	6	2.747	3.934	0.527
6	0.751	0.736	0.220	6	-2.053	0.162	0.351
6	-1.713	2.017	0.351	6	-4.013	0.147	-0.777
6	-0.546	2.743	0.439	6	-3.908	0.481	1.585
6	-4.183	0.432	0.201	6	-4.677	0.363	0.425
6	0.698	2.097	0.387	6	-4.731	0.007	-2.077
6	-4.007	-2.317	-0.142	6	-4.525	0.722	2.922
6	5.969	-3.501	2.769	1	-0.383	0.561	-1.614
6	3.951	4.151	-0.651	1	1.246	0.064	2.108
6	-5.317	-0.345	0.120	1	3.860	0.743	0.209
6	-5.249	-1.731	-0.053	1	2.646	-2.459	-1.055
6	-0.557	4.231	0.585	1	-0.070	2.330	-0.447
1	3.483	-1.921	-2.665	1	2.361	1.554	-2.628
1	3.381	-2.891	-1.201	1	0.995	0.593	-3.269
1	1.264	-0.837	-1.970	1	2.659	0.158	-3.690
1	1.145	-2.545	-2.343	1	1.888	-1.646	3.766
1	1.668	-1.734	0.502	1	4.666	3.002	0.816
1	5.625	-1.748	-1.008	1	3.298	-4.177	0.603
1	5.512	-0.355	0.058	1	0.727	4.566	0.156
1	4.522	0.288	-2.436	1	2.921	-3.778	3.022
1	2.815	0.527	-2.097	1	3.095	4.926	0.796
1	4.206	-3.041	0.694	1	-0.514	-2.512	-3.005
1	4.227	-1.620	1.716	1	-5.757	0.440	0.460
1	3.552	1.541	0.178	1	-5.808	0.134	-1.965
1	5.153	1.662	-0.511	1	-4.361	0.740	-2.798
1	-1.464	-3.249	-0.334	1	-4.538	-0.979	-2.509
1	6.708	-3.151	0.776	1	-4.282	-0.100	3.601
1	6.740	-1.737	1.802	1	-4.113	1.628	3.372
1	4.245	2.981	-2.437	1	-5.610	0.818	2.862
1	2.637	2.860	-1.764				
1	1.720	0.248	0.168				
1	-2.655	2.548	0.400				
1	0.708	-3.765	0.763				
1	-4.294	1.499	0.338				
1	1.611	2.677	0.474				
1	5.431	-2.979	3.565				
1	5.400	-4.404	2.531				
1	6.931	-3.818	3.177				
1	3.378	4.128	0.282				
1	3.667	5.063	-1.181				
1	5.007	4.242	-0.377				
1	-6.150	-2.326	-0.114				
	Enalapril				cortisone acetate		
8	1.570	-1.691	-0.439	8	-2.238	1.412	-1.984
8	4.799	-2.324	-1.931	8	0.683	-2.254	0.240
8	4.685	-2.189	0.315	8	-4.384	0.956	0.768
8	0.016	1.776	-0.480	8	-5.376	-0.987	-0.816
8	-1.299	2.045	1.331	8	6.994	-0.983	-1.082
7	2.964	-0.002	0.080	8	-3.896	-2.037	0.516
7	-0.305	-0.849	1.456	6	-0.127	1.678	-0.101
6	3.824	-0.367	-1.032	6	-1.226	0.613	0.051
6	4.882	0.742	-1.037	6	1.207	1.254	0.490
6	4.990	1.123	0.436	6	1.666	-0.075	-0.161

6	3.553	1.030	0.936	6	-2.431	1.398	-0.560
6	1.867	-0.781	0.320	6	3.041	-0.596	0.349
6	1.097	-0.480	1.603	6	-0.780	2.958	0.415
6	4.456	-1.725	-0.773	6	-0.799	-0.647	-0.701
6	-1.026	-0.174	0.378	6	-2.272	2.797	0.056
6	-2.502	-0.523	0.455	6	2.274	2.322	0.289
6	1.707	-1.308	2.730	6	0.540	-1.119	-0.160
6	-3.317	0.061	-0.699	6	-1.507	0.256	1.513
6	-0.830	1.333	0.473	6	4.048	0.545	0.277
6	-4.781	-0.250	-0.574	6	3.619	1.867	0.836
6	-5.341	-1.355	-1.218	6	3.505	-1.751	-0.558
6	-5.606	0.535	0.236	6	-3.771	0.745	-0.252
6	0.356	3.177	-0.414	6	2.957	-1.058	1.817
6	-6.688	-1.665	-1.063	6	4.977	-2.094	-0.405
6	-6.952	0.229	0.393	6	5.293	0.390	-0.215
6	-7.498	-0.874	-0.256	6	5.863	-0.894	-0.633
6	1.339	3.453	-1.518	6	-4.290	-0.219	-1.309
1	3.258	-0.421	-1.965	6	-5.038	-1.856	0.169
1	5.826	0.419	-1.478	6	-6.251	-2.514	0.737
1	4.514	1.584	-1.631	1	0.027	1.797	-1.185
1	5.428	2.110	0.596	1	1.086	1.097	1.572
1	5.609	0.393	0.966	1	1.800	0.168	-1.232
1	3.018	1.983	0.815	1	-0.341	3.857	-0.025
1	3.500	0.755	1.992	1	-0.650	3.048	1.499
1	1.220	0.595	1.838	1	-0.691	-0.415	-1.767
1	-0.601	-0.524	-0.568	1	-1.515	-1.465	-0.582
1	-0.776	-0.644	2.335	1	-2.918	2.872	0.933
1	-2.597	-1.613	0.473	1	-2.623	3.559	-0.649
1	-2.905	-0.153	1.407	1	1.968	3.256	0.773
1	1.601	-2.369	2.498	1	2.363	2.540	-0.785
1	2.770	-1.096	2.863	1	-0.615	-0.163	1.988
1	1.197	-1.106	3.676	1	-1.829	1.116	2.104
1	-3.177	1.149	-0.726	1	-2.286	-0.505	1.581
1	-2.930	-0.327	-1.648	1	3.533	1.768	1.929
1	5.216	-3.166	-1.698	1	4.396	2.616	0.659
1	-4.711	-1.976	-1.851	1	3.323	-1.459	-1.602
1	-5.181	1.398	0.745	1	2.886	-2.629	-0.371
1	0.767	3.388	0.580	1	3.945	-1.341	2.188
1	-0.561	3.766	-0.510	1	2.586	-0.266	2.474
1	-7.106	-2.526	-1.575	1	2.293	-1.917	1.912
1	-7.578	0.854	1.023	1	-2.603	2.234	-2.323
1	-8.550	-1.113	-0.136	1	5.282	-2.895	-1.082
1	0.903	3.245	-2.497	1	5.184	-2.460	0.610
1	2.232	2.832	-1.410	1	5.971	1.240	-0.258
1	1.647	4.500	-1.499	1	-3.477	-0.856	-1.671
				1	-4.675	0.337	-2.166
				1	-6.967	-2.768	-0.044
				1	-6.741	-1.810	1.413
				1	-5.966	-3.400	1.299
Cisapride				Ezetimibe			
17	-8.081	-1.459	0.290	9	7.314	-0.707	-1.770
9	9.862	-0.488	-1.643	9	-7.772	1.183	-0.785
8	0.001	1.156	-1.631	8	2.150	-2.621	2.155
8	5.479	0.776	1.383	8	-2.792	-2.703	-1.072
8	-3.086	-2.317	-0.856	8	1.104	5.390	0.733
8	-3.209	1.796	-0.264	7	2.296	-0.950	0.483
7	1.474	-0.692	1.147	6	0.363	-1.059	1.264
7	-1.812	-0.502	-0.405	6	1.055	-0.238	0.136
7	-7.970	1.521	0.452	6	-0.800	-1.946	0.871
6	-0.587	-1.118	-0.886	6	1.713	-1.736	1.460
6	0.479	-0.023	-0.997	6	1.088	1.255	0.265
6	-0.077	-2.226	0.035	6	-2.048	-1.143	0.532
6	0.969	0.429	0.370	6	3.570	-0.891	-0.086
6	0.414	-1.676	1.358	6	-3.222	-2.008	0.097
6	2.043	-0.259	2.418	6	0.364	2.056	-0.615
6	3.288	0.601	2.263	6	1.813	1.878	1.285
6	-3.013	-1.134	-0.538	6	4.607	-1.682	0.426
6	4.313	-0.038	1.356	6	3.810	-0.040	-1.168
6	-0.458	0.953	-2.949	6	-4.462	-1.183	-0.153
6	-4.246	-0.338	-0.249	6	0.347	3.439	-0.480
6	-4.352	1.064	-0.119	6	1.811	3.255	1.430
6	-5.424	-1.077	-0.128	6	1.072	4.042	0.546
6	6.528	0.398	0.605	6	5.869	-1.618	-0.146
6	-5.579	1.668	0.130	6	5.075	0.024	-1.739
6	-6.640	-0.481	0.125	6	-5.431	-1.037	0.839
6	-6.751	0.911	0.261	6	-4.634	-0.511	-1.365
6	6.546	-0.745	-0.196	6	6.084	-0.767	-1.217
6	7.646	1.237	0.639	6	-6.551	-0.238	0.639
6	-3.286	3.207	-0.211	6	-5.748	0.288	-1.588
6	7.676	-1.043	-0.956	6	-6.687	0.411	-0.576
6	8.769	0.942	-0.116	1	0.105	-0.421	2.119
6	8.767	-0.198	-0.906	1	0.692	-0.526	-0.862
1	-0.785	-1.558	-1.873	1	-1.011	-2.642	1.692
1	1.328	-0.437	-1.566	1	-0.519	-2.566	0.012

1	0.748	-2.744	-0.468	1	-2.358	-0.540	1.394
1	-0.877	-2.953	0.185	1	-1.836	-0.430	-0.277
1	1.761	1.168	0.220	1	-3.439	-2.731	0.903
1	0.142	0.951	0.895	1	-0.197	1.592	-1.423
1	0.817	-2.481	1.979	1	2.400	1.272	1.971
1	-0.432	-1.230	1.919	1	4.408	-2.341	1.262
1	1.295	0.280	3.033	1	3.009	0.577	-1.560
1	2.300	-1.168	2.975	1	-0.223	4.051	-1.174
1	-1.821	0.507	-0.336	1	2.379	3.741	2.216
1	3.041	1.599	1.884	1	-3.510	-3.273	-1.361
1	3.731	0.759	3.251	1	6.685	-2.222	0.232
1	4.555	-1.057	1.696	1	5.282	0.678	-2.577
1	3.934	-0.123	0.328	1	-5.311	-1.560	1.785
1	0.289	0.426	-3.559	1	-3.886	-0.629	-2.144
1	-0.633	1.938	-3.382	1	-7.314	-0.121	1.399
1	-1.398	0.385	-2.977	1	-5.899	0.811	-2.525
1	-5.347	-2.152	-0.244	1	0.561	5.814	0.062
1	-5.655	2.745	0.215				
1	5.693	-1.410	-0.236				
1	7.615	2.121	1.267				
1	-8.705	0.923	0.803				
1	-7.953	2.435	0.875				
1	-2.272	3.567	-0.381				
1	-3.634	3.553	0.769				
1	-3.948	3.599	-0.990				
1	7.709	-1.926	-1.584				
1	9.643	1.583	-0.099				
	Dutasteride				Felodipine		
9	-3.442	3.962	1.236	17	-1.985	-0.789	-1.544
9	-2.645	2.345	2.436	17	-4.195	-1.244	0.627
9	-1.758	2.803	0.519	8	-0.703	2.047	-1.257
9	-7.723	-0.372	-1.795	8	0.571	-2.525	-1.072
9	-6.011	-1.504	-2.490	8	0.507	3.753	-0.394
9	-6.906	-1.966	-0.577	8	2.603	-3.243	-0.411
8	-2.384	-2.313	0.466	7	3.393	0.803	0.613
8	8.635	1.818	-1.001	6	0.860	0.053	-0.435
7	7.190	0.131	-0.476	6	1.316	1.496	-0.276
7	-2.297	-0.050	0.851	6	2.005	-0.924	-0.213
6	1.957	-1.556	1.112	6	-0.291	-0.229	0.533
6	0.713	-1.051	0.358	6	2.521	1.815	0.264
6	3.249	-1.398	0.323	6	3.191	-0.531	0.324
6	3.434	0.101	-0.012	6	0.379	2.565	-0.626
6	4.765	0.363	-0.762	6	3.039	3.190	0.534
6	0.902	0.431	0.045	6	4.358	-1.408	0.640
6	-0.371	-1.388	1.422	6	1.809	-2.332	-0.552
6	2.201	0.663	-0.729	6	-1.582	-0.599	0.134
6	1.543	-2.933	1.621	6	-0.044	-0.084	1.899
6	4.450	-1.969	1.073	6	-2.580	-0.806	1.095
6	0.042	-2.775	1.948	6	-1.031	-0.291	2.850
6	5.902	-0.210	0.109	6	-2.308	-0.652	2.449
6	5.761	-1.700	0.349	6	-1.800	2.945	-1.504
6	0.432	-1.841	-0.924	6	0.258	-3.870	-1.424
6	4.753	-0.246	-2.174	6	-2.722	2.981	-0.309
6	5.060	1.836	-0.915	1	0.469	-0.086	-1.446
6	-1.783	-1.341	0.878	1	4.303	1.071	0.954
6	6.310	2.313	-0.920	1	2.993	3.815	-0.357
6	7.494	1.435	-0.794	1	4.073	3.150	0.886
6	-3.528	0.395	0.368	1	2.432	3.700	1.284
6	-3.882	1.757	0.504	1	4.744	-1.892	-0.258
6	-4.434	-0.467	-0.258	1	4.076	-2.219	1.312
6	-5.646	0.022	-0.730	1	5.162	-0.828	1.100
6	-5.100	2.219	0.023	1	0.957	0.205	2.209
6	-2.952	2.722	1.167	1	-0.812	-0.170	3.906
6	-5.994	1.360	-0.599	1	-3.101	-0.817	3.168
6	-6.576	-0.950	-1.398	1	-1.403	3.935	-1.740
1	2.053	-0.901	1.996	1	-2.295	2.537	-2.387
1	3.150	-1.958	-0.620	1	0.329	-4.525	-0.553
1	3.515	0.624	0.958	1	0.941	-4.239	-2.193
1	0.937	0.997	0.989	1	-0.763	-3.846	-1.800
1	0.056	0.828	-0.529	1	-3.569	3.644	-0.502
1	-0.276	-0.639	2.221	1	-3.114	1.985	-0.088
1	2.115	0.205	-1.722	1	-2.197	3.352	0.574
1	2.321	1.735	-0.908				
1	2.128	-3.252	2.487				
1	1.700	-3.692	0.845				
1	4.313	-3.044	1.231				
1	4.491	-1.517	2.075				
1	-0.566	-3.541	1.463				
1	-0.155	-2.856	3.020				
1	5.808	0.291	1.091				
1	6.609	-2.062	0.942				
1	5.798	-2.240	-0.605				
1	-0.437	-1.426	-1.446				
1	1.271	-1.809	-1.622				

1	0.207	-2.890	-0.723				
1	4.099	0.324	-2.838				
1	5.757	-0.226	-2.604				
1	4.405	-1.282	-2.178				
1	4.227	2.513	-1.096				
1	7.990	-0.439	-0.233				
1	6.527	3.364	-1.079				
1	-1.691	0.650	1.253				
1	-4.179	-1.511	-0.363				
1	-5.347	3.267	0.140				
1	-6.943	1.723	-0.972				
	Aripiprazole				Clindamycin		
17	6.666	-1.830	-0.531	17	0.835	2.997	-0.832
17	9.654	-0.845	-0.451	16	4.774	0.920	-1.195
8	-4.236	-0.674	0.047	8	3.083	0.452	0.912
-8	11.163	-1.569	0.006	8	1.558	-2.019	1.178
7	1.898	-0.287	0.608	8	3.076	-3.355	-0.685
7	4.646	0.286	0.071	8	5.513	-1.897	-0.537
7	-8.950	-1.160	-0.250	8	-1.496	-0.227	2.116
6	2.948	-1.263	0.874	7	-3.088	-1.908	0.243
6	2.304	0.577	-0.494	7	-0.481	0.340	0.161
6	4.254	-0.573	1.193	6	-5.167	-0.800	0.160
6	3.611	1.277	-0.180	6	-2.756	-0.503	0.077
6	0.634	-0.961	0.344	6	-4.040	0.203	0.509
6	-0.561	-0.025	0.278	6	-4.406	-2.025	-0.355
6	5.975	0.737	0.073	6	1.954	0.132	0.086
6	-1.874	-0.791	0.206	6	0.751	0.774	0.773
6	-3.065	0.130	0.097	6	1.856	-1.375	-0.060
6	7.027	-0.175	-0.164	6	-6.185	-0.269	-0.839
6	6.306	2.085	0.252	6	3.149	-1.949	-0.643
6	-8.010	1.061	-0.272	6	-1.538	-0.122	0.905
6	-9.408	1.573	-0.452	6	4.362	-1.468	0.152
6	-7.823	-0.330	-0.197	6	4.328	0.053	0.360
6	-5.435	-0.041	-0.054	6	0.860	2.293	0.863
6	8.352	0.266	-0.167	6	-2.096	-2.811	-0.293
6	7.626	2.514	0.221	6	-7.064	0.845	-0.290
-6	10.406	0.705	0.305	6	-0.239	2.929	1.674
6	-6.552	-0.878	-0.091	6	-8.057	1.376	-1.309
6	8.657	1.610	0.026	6	4.636	2.608	-0.558
6	-6.884	1.868	-0.218	6	-5.693	-1.073	1.082
6	-5.597	1.343	-0.111	1	-2.550	-0.285	-0.997
-6	10.250	-0.767	0.004	1	-4.163	1.163	-0.002
1	2.639	-1.881	1.723	1	-3.995	0.399	1.583
1	3.101	-1.939	0.009	1	-4.347	-1.993	-1.465
1	2.417	0.000	-1.434	1	-4.870	-2.979	-0.083
1	1.532	1.332	-0.662	1	2.106	0.574	-0.911
1	4.138	0.036	2.107	1	0.703	0.408	1.807
1	5.033	-1.311	1.380	1	1.028	-1.636	-0.727
1	3.913	1.897	-1.028	1	-6.822	-1.095	-1.184
1	3.461	1.943	0.690	1	-5.654	0.087	-1.736
1	0.687	-1.562	-0.588	1	3.268	-1.605	-1.678
1	0.477	-1.680	1.158	1	4.314	-1.925	1.157
1	-0.548	0.629	1.158	1	-0.621	0.525	-0.823
1	-0.482	0.634	-0.595	1	5.059	0.355	1.120
1	-1.871	-1.470	-0.654	1	1.849	2.551	1.248
1	-1.993	-1.423	1.094	1	-1.156	-2.705	0.255
1	-3.000	0.753	-0.808	1	-1.898	-2.636	-1.369
1	-3.116	0.812	0.960	1	-2.433	-3.844	-0.177
1	5.514	2.801	0.436	1	-7.599	0.475	0.594
1	-9.483	2.615	-0.132	1	-6.433	1.666	0.074
1	-9.666	1.565	-1.521	1	-0.221	2.527	2.691
-1	11.441	0.979	0.100	1	-0.118	4.012	1.722
-1	10.256	0.820	1.387	1	-1.221	2.711	1.248
1	7.855	3.564	0.368	1	2.054	-1.567	1.872
1	-6.407	-1.952	-0.029	1	2.661	-3.621	0.145
1	-7.011	2.946	-0.271	1	-7.545	1.783	-2.187
1	9.693	1.925	0.010	1	-8.682	2.171	-0.896
1	-4.745	2.010	-0.073	1	-8.724	0.584	-1.664
1	-8.816	-2.157	-0.347	1	6.292	-1.578	-0.071
				1	4.985	3.276	-1.345
				1	5.268	2.743	0.323
				1	3.603	2.862	-0.320
	Bisoprolol				Clofazimine		
8	2.747	-0.859	0.864	17	-6.896	-2.380	0.209
8	5.207	-1.298	2.223	17	8.558	0.654	0.294
8	-3.253	-0.913	-0.964	7	-2.156	1.178	-0.055
8	-5.502	0.268	0.393	7	0.124	2.798	-0.185
7	5.103	1.215	-0.504	7	2.923	-1.101	-0.215
6	5.098	0.722	0.865	7	0.850	-2.639	-0.228
6	5.127	-0.803	0.895	6	-0.908	0.583	-0.120
6	4.413	2.494	-0.715	6	0.241	1.486	-0.162
6	3.903	-1.405	0.247	6	-2.305	2.561	-0.066
6	4.845	3.059	-2.055	6	-0.738	-0.776	-0.154
6	2.908	2.280	-0.670	6	0.564	-1.371	-0.187

6	1.536	-1.196	0.348	6	-1.127	3.346	-0.144
6	-1.056	-1.742	-0.579	6	1.729	-0.448	-0.180
6	-2.442	-2.067	-1.041	6	1.539	0.908	-0.192
6	-5.896	1.588	0.762	6	-3.314	0.336	0.011
6	0.426	-0.598	0.955	6	-3.560	3.177	0.004
6	1.347	-2.067	-0.725	6	-0.223	-3.620	-0.232
6	-4.604	-1.183	-1.252	6	-1.257	4.746	-0.166
6	-5.421	0.053	-0.997	6	-4.021	0.041	-1.149
6	-0.850	-0.872	0.498	6	-3.705	-0.203	1.232
6	0.055	-2.323	-1.178	6	-3.650	4.559	-0.017
6	-5.678	1.691	2.254	6	-2.498	5.348	-0.106
6	-7.334	1.884	0.368	6	4.227	-0.630	-0.091
1	5.939	1.109	1.468	6	0.306	-4.920	-0.818
1	4.185	1.051	1.367	6	-0.750	-3.831	1.186
1	5.991	-1.154	0.302	6	-5.130	-0.793	-1.093
1	4.686	3.222	0.074	6	-4.809	-1.041	1.298
1	6.059	1.296	-0.833	6	-5.513	-1.329	0.133
1	3.915	-2.497	0.361	6	5.255	-1.389	-0.667
1	3.914	-1.152	-0.821	6	4.566	0.522	0.629
1	4.599	2.361	-2.861	6	6.580	-1.005	-0.547
1	4.341	4.005	-2.263	6	5.893	0.914	0.745
1	5.923	3.245	-2.087	6	6.894	0.154	0.153
1	2.580	1.843	0.275	1	-1.602	-1.426	-0.149
1	2.598	1.599	-1.469	1	2.364	1.604	-0.258
1	2.377	3.227	-0.800	1	-4.457	2.572	0.076
1	5.921	-0.835	2.670	1	-1.059	-3.275	-0.864
1	-2.421	-2.461	-2.072	1	-0.343	5.326	-0.229
1	-2.887	-2.861	-0.414	1	2.779	-2.105	-0.329
1	-5.229	2.299	0.242	1	-3.700	0.467	-2.095
1	0.593	0.080	1.785	1	-3.136	0.031	2.126
1	2.190	-2.539	-1.214	1	-4.627	5.027	0.038
1	-4.947	0.916	-1.493	1	-2.581	6.429	-0.123
1	-6.420	-0.078	-1.443	1	0.681	-4.769	-1.833
1	-4.723	-1.494	-2.304	1	-0.476	-5.684	-0.853
1	-4.973	-2.009	-0.622	1	1.131	-5.303	-0.211
1	-1.709	-0.399	0.964	1	-1.547	-4.580	1.199
1	-0.083	-2.994	-2.022	1	-1.145	-2.905	1.611
1	-6.323	0.985	2.783	1	0.055	-4.181	1.839
1	-4.642	1.461	2.511	1	-5.693	-1.031	-1.987
1	-5.909	2.697	2.612	1	-5.126	-1.469	2.242
1	-8.013	1.164	0.834	1	5.003	-2.288	-1.221
1	-7.482	1.842	-0.713	1	3.801	1.094	1.137
1	-7.623	2.885	0.698	1	7.367	-1.596	-1.000
				1	6.151	1.803	1.308
	Chlorotrianisene				Doxycycline		
17	-0.675	-2.951	-0.629	8	0.341	-2.812	-0.530
8	-6.368	-0.179	-0.148	8	1.761	0.723	2.372
8	1.547	4.873	0.260	8	-0.267	2.272	1.503
8	5.615	-1.596	0.725	8	1.987	2.676	0.224
6	-0.722	-0.291	-0.114	8	-2.716	2.206	1.019
6	-2.199	-0.316	-0.114	8	3.089	-1.227	-2.126
6	-0.101	1.053	-0.046	8	-5.212	2.091	0.711
6	0.057	-1.400	-0.200	8	4.727	1.205	-2.247
6	1.507	-1.486	0.017	7	3.774	-1.065	1.159
6	-2.920	0.602	-0.893	7	3.123	2.807	-2.328
6	-0.583	2.015	0.856	6	1.306	-0.992	0.772
6	-2.928	-1.192	0.693	6	-1.195	-1.148	0.386
6	0.949	1.426	-0.889	6	0.197	-1.444	-0.187
6	-4.302	0.621	-0.895	6	1.235	0.512	1.059
6	-0.014	3.272	0.942	6	2.688	-1.400	0.239
6	-4.318	-1.177	0.717	6	-2.305	-1.736	-0.512
6	1.527	2.688	-0.823	6	-1.322	0.323	0.678
6	2.112	-0.785	1.075	6	-0.197	1.072	1.082
6	2.330	-2.268	-0.797	6	2.042	1.341	0.048
6	-5.013	-0.273	-0.088	6	-3.577	-0.919	-0.607
6	1.051	3.617	0.105	6	2.887	-0.653	-1.077
6	3.475	-0.840	1.286	6	-2.570	0.959	0.631
6	3.705	-2.327	-0.602	6	2.787	0.814	-0.955
6	4.286	-1.607	0.442	6	-3.740	0.319	0.057
6	-7.116	-1.069	0.654	6	-2.658	-3.150	-0.029
6	2.632	5.249	-0.563	6	-4.621	-1.427	-1.374
6	6.461	-2.369	-0.101	6	3.686	-1.811	2.399
1	-2.378	1.310	-1.514	6	5.067	-1.279	0.523
1	-1.415	1.760	1.506	6	-5.010	0.953	0.013
1	-2.400	-1.896	1.327	6	3.641	1.620	-1.886
1	1.326	0.710	-1.613	6	-5.840	-0.768	-1.448
1	-4.856	1.321	-1.509	6	-6.045	0.401	-0.737
1	-0.379	4.009	1.649	1	1.120	-1.487	1.736
1	-4.846	-1.865	1.365	1	-1.254	-1.680	1.353
1	2.335	2.940	-1.499	1	0.291	-0.912	-1.146
1	1.494	-0.190	1.739	1	2.684	-2.477	-0.004
1	1.885	-2.841	-1.604	1	-1.902	-1.824	-1.531
1	3.937	-0.306	2.108	1	-3.115	-3.107	0.964
1	4.309	-2.940	-1.261	1	-1.762	-3.765	0.026

1	-6.907	-0.925	1.720	1	-3.361	-3.652	-0.694
1	-6.917	-2.115	0.390	1	0.518	-3.306	0.277
1	-8.164	-0.845	0.461	1	1.456	1.591	2.665
1	2.359	5.228	-1.625	1	-4.479	-2.352	-1.922
1	2.889	6.268	-0.279	1	2.797	-1.526	2.963
1	3.501	4.599	-0.406	1	3.678	-2.908	2.243
1	6.203	-3.434	-0.059	1	4.552	-1.571	3.020
1	7.470	-2.229	0.282	1	5.214	-2.322	0.189
1	6.421	-2.034	-1.145	1	5.184	-0.627	-0.347
				1	5.858	-1.034	1.235
				1	1.229	2.878	0.813
				1	-1.818	2.518	1.327
				1	-6.643	-1.177	-2.053
				1	-7.006	0.908	-0.765
				1	2.411	3.260	-1.774
				1	3.779	3.411	-2.801
				1	-6.120	2.376	0.564
	Chlorothiazide				Bendroflumethiazide		
17	2.641	2.205	0.083	16	-0.783	2.896	-0.113
16	-2.778	-0.962	0.090	16	3.906	0.322	0.585
16	2.669	-1.076	-0.175	9	1.479	-3.312	-0.825
8	-3.026	-1.225	1.495	9	3.127	-2.289	-1.763
8	-2.773	-2.040	-0.871	9	3.107	-2.588	0.388
8	2.248	-2.462	-0.113	8	-0.105	3.950	-0.837
8	3.467	-0.549	-1.263	8	-1.134	3.053	1.283
7	-2.439	2.009	-0.017	8	4.736	-0.411	-0.349
7	-3.912	0.172	-0.388	8	4.126	1.725	0.881
7	3.433	-0.712	1.272	7	-2.189	2.561	-0.984
6	-1.239	-0.082	-0.034	7	-1.770	0.229	-1.341
6	-1.237	1.315	0.016	7	3.875	-0.456	2.074
6	1.169	-0.099	-0.060	6	-2.736	1.217	-0.852
6	-0.039	-0.779	-0.089	6	0.120	1.367	-0.289
6	-0.023	2.004	0.049	6	-0.486	0.226	-0.846
6	1.169	1.301	0.018	6	-3.224	0.912	0.571
6	-3.639	1.421	-0.308	6	1.442	1.338	0.133
1	-0.037	-1.863	-0.147	6	0.297	-0.937	-0.935
1	-0.006	3.088	0.090	6	2.202	0.183	0.032
1	-2.398	3.017	-0.036	6	1.611	-0.976	-0.508
1	-4.440	2.135	-0.507	6	-3.893	-0.432	0.624
1	3.563	-1.558	1.817	6	2.343	-2.286	-0.681
1	4.315	-0.241	1.100	6	-5.225	-0.584	0.234
				6	-3.175	-1.570	1.005
				6	-5.827	-1.838	0.229
				6	-3.773	-2.826	0.999
				6	-5.102	-2.962	0.609
				1	-3.596	1.170	-1.530
				1	-2.008	2.794	-1.957
				1	-2.162	-0.692	-1.488
				1	-3.906	1.713	0.870
				1	-2.380	0.947	1.265
				1	1.902	2.233	0.539
				1	-0.152	-1.834	-1.347
				1	-5.799	0.292	-0.057
				1	-2.140	-1.463	1.322
				1	4.321	-1.365	2.013
				1	4.339	0.135	2.757
				1	-6.867	-1.936	-0.068
				1	-3.203	-3.697	1.305
				1	-5.572	-3.940	0.608
	Ciprofloxacin				Entecavir		
9	-2.104	-2.790	-0.505	8	-2.795	2.691	-0.230
8	2.859	-2.624	-0.295	8	-4.620	-1.681	0.407
8	5.379	-1.628	0.048	8	4.501	-1.960	-0.459
8	5.591	0.586	0.320	7	0.187	-0.388	0.002
7	1.574	1.244	0.228	7	1.381	-2.244	-0.436
7	-3.070	-0.231	-0.088	7	1.951	1.231	0.309
7	-5.749	0.538	0.404	7	4.070	0.235	0.037
6	1.148	2.607	0.443	7	3.868	2.525	0.453
6	1.898	3.715	-0.220	6	-0.950	0.512	0.121
6	0.522	3.358	-0.693	6	-3.403	0.346	0.144
6	0.624	0.224	0.074	6	-2.930	1.418	-0.853
6	2.888	0.933	0.262	6	-1.525	0.976	-1.221
6	1.078	-1.093	-0.102	6	-2.138	-0.079	0.858
6	-0.745	0.510	0.116	6	-4.079	-0.818	-0.573
6	-1.702	-0.493	-0.054	6	1.504	-0.019	0.046
6	-3.919	-0.980	0.851	6	-2.063	-0.866	1.927
6	-3.480	1.164	-0.183	6	0.185	-1.736	-0.302
6	3.405	-0.325	0.100	6	2.225	-1.181	-0.220
6	2.511	-1.462	-0.118	6	3.656	-1.117	-0.245
6	-5.372	-0.869	0.442	6	3.257	1.304	0.284
6	-4.942	1.245	-0.579	1	-0.579	1.388	0.665
6	0.121	-2.100	-0.275	1	-4.141	0.761	0.842
6	-1.214	-1.802	-0.264	1	-3.594	1.487	-1.728
6	4.877	-0.387	0.167	1	-0.943	1.775	-1.685

1	0.754	2.787	1.440	1	-1.568	0.135	-1.921
1	2.729	3.449	-0.862	1	-4.868	-0.427	-1.235
1	2.042	4.628	0.343	1	-3.349	-1.345	-1.208
1	-0.305	4.021	-0.470	1	-1.104	-1.160	2.343
1	0.442	2.833	-1.638	1	-2.954	-1.254	2.404
1	3.567	1.763	0.426	1	-3.648	2.942	0.134
1	-1.072	1.523	0.299	1	-0.745	-2.283	-0.383
1	-3.794	-0.568	1.867	1	-4.916	-2.486	-0.024
1	-3.608	-2.022	0.867	1	5.071	0.372	-0.028
1	-2.865	1.658	-0.942	1	3.239	3.223	0.821
1	-3.330	1.694	0.775	1	4.768	2.522	0.911
1	-5.504	-1.373	-0.533				
1	-5.995	-1.389	1.175				
1	-5.250	2.294	-0.611				
1	-5.051	0.831	-1.598				
1	0.466	-3.114	-0.445				
1	-6.732	0.626	0.170				
1	6.339	-1.519	0.111				
Clorazepate				Acamprosate			
17	3.942	-2.247	-1.171	16	-2.265	-0.190	0.172
8	-3.516	-1.038	1.569	8	-2.922	-1.149	-0.990
8	-4.200	-1.045	-1.427	8	-3.117	0.978	0.294
8	-4.080	1.171	-1.026	8	-1.957	-1.023	1.307
7	-1.299	-1.521	1.493	8	3.078	0.179	1.309
7	-1.429	0.871	-0.195	7	2.269	0.353	-0.794
6	0.503	-0.603	0.103	6	0.137	1.119	0.226
6	-0.167	0.714	-0.001	6	-0.741	0.252	-0.657
6	-0.067	-1.659	0.842	6	1.438	1.499	-0.473
6	-2.250	-0.293	-0.375	6	3.065	-0.225	0.159
6	0.654	1.942	0.124	6	3.907	-1.383	-0.310
6	-2.465	-0.978	0.978	1	-0.400	2.031	0.503
6	1.745	-0.808	-0.513	1	0.375	0.591	1.154
6	0.639	-2.859	0.990	1	-1.037	0.759	-1.580
6	2.410	-2.014	-0.380	1	-0.258	-0.695	-0.913
6	1.871	-3.042	0.391	1	1.236	2.044	-1.401
6	1.856	1.958	0.842	1	2.011	2.160	0.183
6	0.195	3.134	-0.451	1	2.323	0.029	-1.746
6	-3.601	0.075	-0.964	1	-3.776	-0.764	-1.229
6	2.583	3.135	0.977	1	4.956	-1.165	-0.107
6	0.927	4.304	-0.323	1	3.648	-2.269	0.272
6	2.124	4.309	0.390	1	3.793	-1.614	-1.371
1	-1.782	-1.044	-1.036				
1	-1.457	-2.099	2.309				
1	2.189	-0.007	-1.093				
1	0.201	-3.660	1.577				
1	2.408	-3.977	0.504				
1	2.215	1.049	1.316				
1	-0.745	3.116	-0.992				
1	3.507	3.134	1.546				
1	0.565	5.218	-0.781				
1	2.695	5.226	0.490				
1	-5.080	-0.786	-1.733				
Cefaclor				Emtricitabine			
17	4.489	1.984	-0.460	16	3.250	-0.820	0.639
16	0.288	1.071	-1.123	9	-2.536	2.408	0.277
8	1.092	-2.049	1.739	8	1.433	-0.075	-1.149
8	-2.585	-2.623	-1.360	8	2.305	2.136	0.480
8	3.958	-2.175	0.731	8	-1.281	-2.759	-0.205
8	4.847	-0.247	1.489	7	-0.601	-0.577	-0.178
7	1.832	-0.976	-0.253	7	-2.913	-1.155	-0.117
7	-1.417	-1.209	-0.021	7	-4.490	0.501	0.131
7	-4.913	-1.350	-0.931	6	0.788	-0.994	-0.287
6	0.792	-0.678	-1.223	6	1.498	-0.976	1.059
6	-0.135	-1.654	-0.450	6	2.792	0.164	-0.862
6	0.976	-1.675	0.609	6	2.993	1.654	-0.655
6	2.970	-0.199	-0.006	6	-0.886	0.743	0.001
6	1.982	1.696	-1.368	6	-1.621	-1.591	-0.167
6	3.048	1.035	-0.551	6	-2.177	1.114	0.119
6	-2.572	-1.731	-0.532	6	-3.194	0.121	0.031
6	-3.870	-1.157	0.060	1	0.771	-2.003	-0.711
6	4.031	-0.830	0.824	1	1.150	-0.133	1.664
6	-3.738	0.293	0.472	1	1.327	-1.905	1.603
6	-3.417	0.630	1.788	1	3.417	-0.199	-1.687
6	-3.865	1.310	-0.477	1	2.582	2.187	-1.517
6	-3.214	1.959	2.151	1	4.070	1.873	-0.605
6	-3.666	2.636	-0.114	1	-0.051	1.437	0.025
6	-3.337	2.964	1.199	1	2.709	1.706	1.244
1	1.065	-0.941	-2.248	1	-5.191	-0.191	-0.079
1	-0.263	-2.604	-0.976	1	-4.733	1.475	0.057
1	-1.475	-0.425	0.616				
1	1.945	2.756	-1.107				
1	2.248	1.651	-2.431				
1	-4.020	-1.752	0.982				
1	-5.823	-1.380	-0.485				

1	-4.758	-2.241	-1.394				
1	-3.329	-0.157	2.534				
1	-4.130	1.040	-1.494				
1	4.625	-2.527	1.336				
1	-2.968	2.206	3.179				
1	-3.767	3.419	-0.859				
1	-3.183	4.001	1.480				
	Diflunisal				Dihydrocodeine		
9	-1.990	-2.104	0.952	8	1.504	0.982	1.372
9	-5.380	0.954	-0.058	8	1.491	2.386	-0.945
8	4.135	-1.335	-0.304	8	3.764	-0.620	0.626
8	2.750	2.545	0.481	7	-3.098	-1.012	0.486
8	4.573	1.244	0.320	6	-0.746	0.612	0.722
6	0.059	-0.448	-0.163	6	-1.899	0.972	-0.220
6	-1.372	-0.094	-0.140	6	0.262	1.708	1.110
6	1.025	0.531	0.059	6	-2.504	-0.363	-0.695
6	0.506	-1.749	-0.433	6	-1.348	-0.089	1.953
6	2.398	0.267	0.020	6	0.201	-0.317	0.028
6	-2.353	-0.926	0.405	6	-1.462	1.931	-1.314
6	-1.826	1.126	-0.659	6	0.512	2.770	0.008
6	2.819	-1.049	-0.256	6	-1.507	-1.237	-1.501
6	1.857	-2.038	-0.480	6	-0.798	3.149	-0.681
6	-3.698	-0.600	0.448	6	-2.136	-1.320	1.539
6	-3.162	1.497	-0.639	6	-0.100	-1.234	-0.960
6	-4.078	0.619	-0.084	6	1.469	-0.087	0.524
6	3.372	1.346	0.279	6	-3.909	-2.164	0.162
1	0.715	1.543	0.293	6	0.971	-2.010	-1.413
1	-0.209	-2.540	-0.624	6	2.540	-0.872	0.097
1	-1.099	1.795	-1.110	6	2.252	-1.841	-0.878
1	2.187	-3.050	-0.701	6	4.842	-1.391	0.142
1	-4.418	-1.274	0.892	1	-2.685	1.469	0.366
1	-3.498	2.439	-1.053	1	-0.006	2.209	2.045
1	4.235	-2.273	-0.501	1	-3.349	-0.140	-1.360
1	3.462	3.177	0.647	1	-2.006	0.620	2.472
				1	-0.554	-0.375	2.651
				1	-2.323	2.229	-1.921
				1	-0.763	1.443	-2.009
				1	0.948	3.654	0.484
				1	-1.490	-0.876	-2.539
				1	-1.900	-2.259	-1.569
				1	-0.582	3.919	-1.426
				1	-1.484	3.596	0.051
				1	-1.439	-2.125	1.234
				1	-2.696	-1.714	2.395
				1	-3.331	-3.045	-0.173
				1	-4.622	-1.909	-0.627
				1	-4.477	-2.470	1.045
				1	0.823	-2.749	-2.195
				1	1.243	1.534	-1.321
				1	3.057	-2.461	-1.255
				1	4.988	-1.249	-0.935
				1	4.700	-2.459	0.345
				1	5.727	-1.041	0.672
	Carvedilol				Cefadroxil		
8	2.483	0.138	-0.079	16	0.510	0.820	-1.384
8	4.713	2.130	0.394	8	1.643	-1.596	1.974
8	-1.241	1.896	-0.306	8	-1.851	-3.221	-0.978
8	-1.059	-0.357	-1.518	8	5.060	0.709	1.405
7	-0.207	-3.404	1.055	8	4.670	-1.475	1.032
7	1.212	2.933	-0.248	8	-3.393	3.893	0.897
6	1.192	-1.743	0.431	7	2.284	-0.828	-0.184
6	0.289	-1.219	1.417	7	-0.913	-1.454	0.097
6	0.853	-3.097	0.224	7	-4.338	-2.219	-0.756
6	-0.583	-2.278	1.768	6	1.233	-0.842	-1.184
6	2.195	-1.162	-0.357	6	0.428	-1.784	-0.249
6	3.574	2.244	-0.452	6	1.510	-1.462	0.793
6	3.175	0.905	-1.055	6	3.307	0.125	-0.078
6	2.498	2.866	0.422	6	2.121	1.599	-1.722
6	1.488	-3.890	-0.732	6	3.273	1.258	-0.815
6	0.104	0.037	1.996	6	-1.974	-2.210	-0.310
6	2.813	-1.930	-1.342	6	4.372	2.270	-0.881
6	-1.629	-2.105	2.668	6	4.400	-0.320	0.823
6	2.462	-3.278	-1.507	6	-3.349	-1.735	0.192
6	0.198	3.489	0.632	6	-3.429	-0.238	0.379
6	-0.941	0.217	2.890	6	-3.182	0.345	1.624
6	-1.798	-0.841	3.220	6	-3.677	0.601	-0.709
6	-1.189	3.262	0.073	6	-3.168	1.724	1.788
6	-2.425	1.345	-0.668	6	-3.672	1.980	-0.558
6	-2.324	0.084	-1.295	6	-3.412	2.546	0.690
6	-3.673	1.912	-0.456	1	1.554	-1.237	-2.152
6	-3.483	-0.596	-1.650	1	0.445	-2.819	-0.598
6	-4.831	1.224	-0.827	1	-1.093	-0.591	0.593
6	-4.736	-0.026	-1.411	1	1.938	2.677	-1.662
6	-0.925	-1.596	-2.184	1	2.406	1.405	-2.764

1	3.788	2.916	-1.299	1	5.341	1.880	-0.585
1	-0.670	-4.296	1.092	1	4.150	3.123	-0.229
1	4.082	0.387	-1.394	1	4.451	2.666	-1.899
1	2.524	1.047	-1.930	1	-3.432	-2.200	1.194
1	2.818	3.879	0.689	1	-5.242	-2.308	-0.305
1	2.463	2.292	1.366	1	-4.052	-3.141	-1.074
1	1.219	-4.930	-0.882	1	5.736	0.304	1.967
1	0.769	0.853	1.736	1	-2.996	-0.294	2.485
1	3.573	-1.503	-1.983	1	-3.884	0.152	-1.675
1	-2.295	-2.922	2.925	1	-2.981	2.176	2.755
1	0.910	1.986	-0.472	1	-3.867	2.624	-1.412
1	2.970	-3.855	-2.273	1	-3.586	4.338	0.066
1	0.246	3.047	1.645				
1	0.364	4.565	0.757				
1	-1.103	1.193	3.340				
1	-2.610	-0.673	3.919				
1	-1.938	3.491	0.842				
1	-1.391	3.889	-0.807				
1	5.462	1.855	-0.141				
1	-3.751	2.891	0.001				
1	-3.416	-1.567	-2.125				
1	-5.800	1.678	-0.652				
1	-5.631	-0.569	-1.698				
1	-1.363	-2.414	-1.598				
1	-1.400	-1.572	-3.173				
1	0.144	-1.771	-2.296				
	Albendazole				Chlormezanone		
16	3.734	-1.078	0.085	17	4.975	0.110	-0.348
8	-5.935	-0.346	-0.180	16	-1.854	-1.506	-0.072
8	-4.628	1.246	0.783	8	-2.888	-1.975	0.841
7	-1.484	-1.369	-0.018	8	-0.875	-2.427	-0.640
7	-1.862	0.819	-0.396	8	-2.341	2.808	-0.638
7	-3.749	-0.661	-0.189	7	-1.684	1.095	0.717
6	-0.233	-0.780	-0.072	6	-0.931	-0.130	0.842
6	-0.499	0.585	-0.306	6	-2.625	-0.578	-1.425
6	2.110	-0.392	-0.071	6	-1.849	0.701	-1.684
6	1.047	-1.294	0.050	6	0.536	-0.052	0.513
6	0.569	1.468	-0.430	6	-1.965	1.658	-0.514
6	-2.398	-0.349	-0.198	6	-1.795	1.914	1.914
6	4.817	0.378	0.035	6	1.358	-1.147	0.797
6	1.862	0.973	-0.313	6	1.115	1.098	-0.024
6	6.261	-0.053	0.240	6	2.718	-1.106	0.532
6	7.212	1.132	0.196	6	2.477	1.156	-0.290
6	-4.754	0.208	0.196	6	3.269	0.048	-0.016
6	-7.081	0.416	0.205	1	-1.061	-0.492	1.867
1	1.229	-2.347	0.237	1	-3.656	-0.382	-1.126
1	-1.694	-2.298	0.312	1	-2.616	-1.259	-2.277
1	0.392	2.522	-0.614	1	-2.241	1.214	-2.563
1	4.511	1.079	0.818	1	-0.797	0.471	-1.889
1	4.705	0.883	-0.931	1	-0.811	2.245	2.261
1	2.692	1.661	-0.414	1	-2.278	1.341	2.708
1	6.353	-0.573	1.200	1	-2.395	2.789	1.674
1	6.537	-0.784	-0.528	1	0.930	-2.049	1.220
1	6.975	1.863	0.974	1	0.508	1.976	-0.227
1	8.247	0.818	0.345	1	3.351	-1.959	0.747
1	7.161	1.649	-0.766	1	2.923	2.053	-0.702
1	-4.049	-1.498	-0.668				
1	-7.129	0.522	1.290				
1	-7.941	-0.139	-0.160				
1	-7.051	1.410	-0.245				
	Clonazepam				Azathioprine		
17	-0.967	-0.551	2.204	16	0.186	-0.515	1.183
8	0.668	4.706	0.229	8	2.175	-2.516	-0.031
8	3.526	-3.235	-0.261	8	3.812	-1.919	-1.340
8	1.576	-3.444	-1.198	7	1.918	1.552	0.653
7	1.322	2.577	0.635	7	-3.041	-1.267	0.987
7	-1.108	2.097	-0.999	7	3.629	0.643	-0.448
7	2.434	-2.801	-0.608	7	-0.800	1.058	-0.801
6	0.579	0.444	-0.316	7	-4.580	-0.390	-0.399
6	1.569	1.254	0.285	7	2.923	-1.683	-0.541
6	-0.795	0.936	-0.552	7	-3.086	1.128	-1.561
6	-1.916	-0.011	-0.313	6	1.621	0.214	0.523
6	0.888	-0.887	-0.599	6	-2.379	-0.339	0.218
6	2.811	0.696	0.628	6	-1.077	0.134	0.110
6	-0.039	3.010	-1.345	6	2.714	-0.302	-0.154
6	2.134	-1.398	-0.288	6	3.120	1.747	0.046
6	0.653	3.548	-0.112	6	-3.359	0.195	-0.642
6	3.100	-0.623	0.348	6	1.090	2.567	1.274
6	-2.065	-0.761	0.861	6	-4.345	-1.244	0.561
6	-2.891	-0.161	-1.306	6	-1.813	1.492	-1.580
6	-3.124	-1.646	1.028	1	3.578	2.726	0.001
6	-3.948	-1.045	-1.154	1	0.241	2.803	0.631
6	-4.059	-1.794	0.012	1	0.723	2.205	2.236
1	0.145	-1.541	-1.042	1	1.695	3.458	1.434

1	1.918	2.976	1.349	1	-2.647	-1.877	1.687
1	3.552	1.323	1.114	1	-5.085	-1.894	1.009
1	-0.449	3.860	-1.889	1	-1.534	2.243	-2.316
1	0.723	2.523	-1.976				
1	4.057	-1.063	0.600				
1	-2.788	0.437	-2.205				
1	-3.212	-2.201	1.954				
1	-4.683	-1.150	-1.945				
1	-4.881	-2.491	0.142				
	Betamethasone				Dolasetron		
9	1.525	-0.331	-1.273	8	0.454	0.867	0.089
8	-2.693	-0.045	-2.001	8	-6.600	-0.928	0.154
8	0.403	-1.732	1.861	8	1.150	-1.290	0.168
8	-4.658	-0.355	0.948	7	-3.611	0.889	-0.764
8	-5.809	-2.221	-0.463	7	4.432	1.920	-0.080
8	6.238	-0.662	-1.686	6	-2.886	-0.315	-1.220
6	-1.614	-0.087	0.232	6	-3.235	1.190	0.632
6	-0.726	1.076	-0.240	6	-4.255	-1.115	0.743
6	0.654	1.095	0.407	6	-3.258	-1.548	-0.345
6	1.361	-0.245	0.138	6	-3.618	0.010	1.573
6	-2.906	0.227	-0.608	6	-1.392	-0.014	-1.238
6	-1.630	2.289	-0.086	6	-1.753	1.548	0.678
6	-0.909	-1.395	-0.120	6	-0.913	0.409	0.140
6	-3.018	1.793	-0.551	6	-5.048	0.641	-0.833
6	0.503	-1.491	0.460	6	-5.462	-0.533	0.044
6	2.827	-0.279	0.707	6	1.407	-0.105	0.104
6	1.482	2.267	-0.118	6	2.745	0.457	0.039
6	-1.930	-0.010	1.729	6	3.978	-0.282	0.039
6	2.932	2.235	0.362	6	3.075	1.793	-0.035
6	3.550	0.902	0.089	6	5.022	0.669	-0.037
6	-4.135	-0.532	-0.136	6	4.302	-1.643	0.095
6	-4.162	2.405	0.239	6	6.366	0.309	-0.059
6	2.896	-0.117	2.247	6	5.639	-2.006	0.073
6	3.481	-1.587	0.370	6	6.659	-1.044	-0.003
6	4.648	0.755	-0.669	1	-3.213	-0.493	-2.250
6	-4.726	-1.580	-1.055	1	-3.811	2.078	0.915
6	4.574	-1.714	-0.386	1	-4.560	-1.956	1.369
6	5.242	-0.545	-0.983	1	-2.371	-1.979	0.135
1	-0.565	0.924	-1.315	1	-3.690	-2.344	-0.958
1	0.544	1.193	1.496	1	-4.309	0.344	2.353
1	-1.669	2.615	0.962	1	-2.740	-0.389	2.093
1	-1.299	3.151	-0.672	1	-0.832	-0.891	-1.574
1	-0.793	-1.474	-1.207	1	-1.201	0.803	-1.942
1	-1.469	-2.273	0.224	1	-1.583	2.439	0.064
1	-3.151	2.070	-1.602	1	-1.453	1.789	1.702
1	1.000	-2.339	-0.030	1	-0.942	-0.450	0.820
1	1.010	3.208	0.180	1	-5.344	0.441	-1.869
1	1.466	2.241	-1.214	1	-5.598	1.537	-0.521
1	-2.586	0.827	1.967	1	2.429	2.656	-0.058
1	-2.433	-0.915	2.071	1	4.928	2.794	-0.139
1	-1.020	0.084	2.321	1	3.513	-2.383	0.153
1	2.959	2.438	1.442	1	7.152	1.055	-0.117
1	3.517	3.024	-0.117	1	5.907	-3.057	0.116
1	-4.120	2.154	1.301	1	7.695	-1.365	-0.017
1	-4.113	3.494	0.151				
1	-5.141	2.091	-0.130				
1	2.208	0.640	2.624				
1	2.676	-1.047	2.771				
1	3.911	0.176	2.527				
1	-2.402	-0.956	-2.106				
1	3.038	-2.476	0.820				
1	1.159	-2.257	2.133				
1	5.145	1.624	-1.093				
1	-3.936	-2.307	-1.316				
1	-5.008	-1.097	-2.001				
1	5.024	-2.682	-0.582				
1	-5.902	-1.809	0.412				
	Carbinoxamine				Cetirizine		
17	5.583	-1.494	-0.338	17	-6.346	-3.293	-0.509
8	-0.984	-0.775	0.130	8	5.781	-0.628	-0.120
7	-4.574	-1.406	-0.234	8	9.243	0.108	0.105
7	-0.334	1.715	-1.119	8	8.187	-1.573	-0.967
6	-0.113	0.159	0.736	7	-0.632	0.239	0.225
6	-2.353	-0.493	0.352	7	2.162	-0.444	0.436
6	-3.142	-1.659	-0.204	6	-0.183	-1.017	0.826
6	1.302	-0.288	0.481	6	0.395	1.252	0.464
6	-0.327	1.572	0.211	6	1.133	-1.453	0.221
6	2.282	-0.119	1.455	6	1.716	0.821	-0.136
6	1.658	-0.828	-0.755	6	-1.937	0.648	0.752
6	-0.485	2.643	1.087	6	3.435	-0.880	-0.115
6	-5.137	-1.300	1.099	6	-3.007	-0.384	0.447
6	-5.254	-2.443	-0.986	6	-2.376	1.986	0.186
6	3.602	-0.483	1.214	6	4.596	-0.049	0.389
6	2.970	-1.202	-1.011	6	-3.024	-1.075	-0.766

6	-2.569	0.521	0.333	7	4.040	0.908	-0.629
6	-0.286	1.133	-0.563	6	-0.464	-0.071	0.728
6	-3.220	-0.656	-0.011	6	0.809	0.501	1.357
6	-2.907	-0.992	-1.424	6	1.818	1.082	0.356
6	0.453	-0.039	-0.423	6	3.199	0.454	0.472
6	-2.703	1.072	1.596	1	1.276	-0.306	1.938
6	0.348	2.359	-0.381	1	0.490	1.252	2.086
6	1.806	0.008	-0.115	1	1.471	0.919	-0.673
6	-4.025	-1.329	0.897	1	1.907	2.165	0.484
6	-3.512	0.403	2.514	1	3.664	0.766	1.415
6	1.701	2.415	-0.071	1	3.080	-0.640	0.520
6	2.435	1.244	0.060	1	-1.193	-1.340	2.044
6	-4.163	-0.785	2.171	1	-1.556	-1.110	-1.786
1	-1.646	0.024	-2.759	1	0.494	-3.334	0.797
1	-0.011	-1.012	-0.552	1	-2.876	0.574	1.042
1	-2.195	1.993	1.865	1	-0.177	2.934	-0.666
1	-0.220	3.275	-0.489	1	3.706	0.480	-1.489
1	-4.523	-2.250	0.611	1	4.988	0.571	-0.505
1	-3.141	2.316	-1.374				
1	2.197	3.368	0.070				
1	-3.635	0.808	3.513				
1	-4.782	-1.285	2.908				
1	2.987	-2.421	2.004				
1	4.254	-1.413	1.572				
	Codeine				Amiloride		
8	1.623	1.032	1.058	17	2.683	-2.303	0.022
8	1.865	3.356	-0.204	8	-2.091	1.646	0.048
8	3.701	-0.827	0.544	7	2.114	1.632	-0.012
7	-3.349	-0.418	0.407	7	0.596	-0.684	0.004
6	-0.724	0.731	0.601	7	0.231	2.926	-0.065
6	-1.674	1.040	-0.572	7	-2.096	-0.687	0.013
6	-2.524	-0.226	-0.796	7	4.048	0.378	-0.051
6	0.370	1.777	0.887	7	-3.926	-2.040	-0.149
6	-1.553	0.410	1.852	7	-4.295	0.232	0.106
6	0.117	-0.431	0.163	6	-0.025	0.505	-0.007
6	-1.679	-1.462	-1.208	6	0.770	1.691	-0.023
6	-2.549	-0.705	1.592	6	2.691	0.439	-0.010
6	-0.289	-1.491	-0.629	6	1.886	-0.729	-0.004
6	0.564	2.808	-0.243	6	-1.500	0.540	0.019
6	-0.881	1.489	-1.763	6	-3.405	-0.782	-0.002
6	1.431	-0.199	0.493	1	0.851	3.713	0.027
6	0.184	2.275	-1.600	1	-0.774	3.003	0.023
6	-4.400	-1.395	0.228	1	4.545	1.230	0.151
6	0.697	-2.425	-0.958	1	4.493	-0.494	0.188
6	2.425	-1.122	0.177	1	-3.241	-2.769	-0.019
6	2.018	-2.257	-0.536	1	-4.833	-2.227	0.250
6	4.700	-1.755	0.181	1	-3.876	1.157	0.045
1	-2.377	1.832	-0.270	1	-5.246	0.090	-0.194
1	-3.231	-0.023	-1.610				
1	0.223	2.298	1.836				
1	-2.089	1.318	2.155				
1	-0.887	0.132	2.677				
1	-1.591	-1.481	-2.301				
1	-2.236	-2.373	-0.957				
1	-2.018	-1.674	1.503				
1	-3.231	-0.808	2.442				
1	-0.116	3.643	-0.016				
1	-1.183	1.157	-2.754				
1	0.776	2.628	-2.439				
1	-4.040	-2.436	0.128				
1	-4.984	-1.154	-0.664				
1	-5.072	-1.369	1.090				
1	0.449	-3.284	-1.576				
1	2.754	-3.002	-0.814				
1	2.454	2.630	0.040				
1	4.524	-2.737	0.636				
1	5.641	-1.352	0.553				
1	4.763	-1.875	-0.908				
	Ampicillin				Cephaloglycin		
16	-0.713	0.859	0.896	16	0.098	0.990	-0.637
8	-1.106	-1.654	-2.278	8	1.919	-2.207	1.540
8	-5.146	0.539	-0.904	8	-2.176	-2.226	-1.525
8	-4.804	-1.344	0.288	8	5.107	0.446	1.095
8	2.383	-2.932	0.841	8	4.702	-1.563	0.164
7	-2.027	-1.125	-0.164	7	2.112	-0.787	-0.360
7	1.271	-1.263	-0.228	7	-0.941	-1.728	0.312
7	4.686	-1.539	0.899	7	-4.522	-2.048	-0.171
6	-1.021	-0.941	0.885	6	0.882	-0.587	-1.105
6	-2.517	1.158	0.531	6	0.304	-1.831	-0.378
6	-2.908	-0.011	-0.442	6	1.560	-1.743	0.496
6	-0.032	-1.773	0.026	6	3.112	0.174	-0.155
6	-1.079	-1.585	-1.081	6	1.587	1.959	-1.036
6	-3.307	1.096	1.835	6	2.905	1.466	-0.499
6	-2.672	2.514	-0.136	6	-2.122	-1.856	-0.365

6	-4.369	-0.390	-0.296	6	-3.355	-1.432	0.435
6	2.399	-1.877	0.233	6	3.943	2.541	-0.459
6	3.722	-1.174	-0.124	6	4.371	-0.421	0.361
6	3.574	0.325	-0.258	6	-3.355	0.084	0.504
6	3.359	0.907	-1.508	6	-3.552	0.825	-0.787
6	3.576	1.140	0.877	6	-3.152	0.714	1.665
6	3.137	2.276	-1.626	6	-3.077	2.197	1.817
6	3.357	2.506	0.759	6	-3.492	2.309	-0.633
6	3.134	3.079	-0.491	6	-3.278	2.925	0.528
1	-1.297	-1.320	1.871	1	1.008	-0.646	-2.189
1	-2.740	0.308	-1.478	1	0.284	-2.700	-1.040
1	0.065	-2.803	0.379	1	-0.952	-1.261	1.209
1	-3.239	0.116	2.313	1	1.397	2.959	-0.634
1	-2.935	1.844	2.537	1	1.657	2.087	-2.125
1	-4.368	1.305	1.656	1	-3.235	-1.807	1.462
1	-2.368	3.316	0.540	1	4.962	2.162	-0.460
1	-2.071	2.584	-1.045	1	3.825	3.157	0.440
1	-3.719	2.682	-0.402	1	3.818	3.210	-1.316
1	1.351	-0.345	-0.647	1	-4.510	0.531	-1.243
1	3.967	-1.575	-1.127	1	-2.803	0.495	-1.524
1	-6.065	0.269	-0.766	1	-3.023	0.117	2.569
1	5.629	-1.466	0.536	1	-4.375	-2.114	-1.176
1	4.523	-2.507	1.160	1	-5.349	-1.485	-0.007
1	3.365	0.278	-2.397	1	-2.107	2.474	2.259
1	3.760	0.682	1.844	1	-3.812	2.538	2.563
1	2.974	2.715	-2.605	1	-3.630	2.900	-1.536
1	3.359	3.130	1.648	1	-3.247	4.011	0.563
1	2.965	4.147	-0.579	1	5.889	-0.048	1.380
Acetohexamide				Chlorpropamide			
16	-0.643	2.514	-0.151	17	4.297	2.184	0.057
8	0.826	0.416	1.437	16	-0.129	-2.242	-0.096
8	-0.653	3.133	1.152	8	-0.257	-2.808	1.225
8	-0.837	3.262	-1.380	8	0.077	-3.050	-1.284
8	-4.993	-2.496	-1.207	8	-1.534	0.007	1.332
7	2.665	0.418	0.082	7	-1.573	-1.425	-0.466
7	0.878	1.806	-0.394	7	-3.219	0.178	-0.195
6	3.420	-0.524	0.919	6	-3.907	1.237	0.536
6	3.016	-1.967	0.610	6	1.124	-0.981	-0.047
6	4.914	-0.315	0.692	6	-3.335	2.619	0.252
6	3.454	-2.393	-0.786	6	-2.078	-0.370	0.314
6	5.358	-0.753	-0.701	6	1.436	-0.374	1.165
6	4.953	-2.196	-0.981	6	1.781	-0.637	-1.225
6	1.424	0.833	0.466	6	-3.466	3.035	-1.202
6	-1.794	1.151	-0.131	6	2.419	0.605	1.197
6	-2.153	0.588	1.088	6	2.762	0.343	-1.195
6	-2.319	0.694	-1.337	6	3.068	0.955	0.017
6	-3.592	-0.951	-0.105	1	-3.845	1.013	1.604
6	-3.058	-0.464	1.092	1	-4.963	1.193	0.249
6	-3.215	-0.362	-1.317	1	-3.848	3.338	0.901
6	-4.568	-2.086	-0.144	1	-2.284	2.628	0.561
6	-5.001	-2.697	1.162	1	-1.815	-1.494	-1.446
1	3.164	-0.297	1.960	1	-3.723	-0.322	-0.910
1	1.935	-2.073	0.739	1	0.905	-0.665	2.063
1	3.485	-2.617	1.360	1	1.536	-1.148	-2.150
1	5.449	-0.911	1.441	1	-4.514	3.067	-1.517
1	5.180	0.730	0.884	1	-3.041	4.025	-1.378
1	2.909	-1.797	-1.531	1	-2.945	2.335	-1.862
1	3.174	-3.435	-0.968	1	2.683	1.094	2.126
1	6.440	-0.625	-0.804	1	3.294	0.626	-2.096
1	4.912	-0.099	-1.465				
1	5.498	-2.859	-0.295				
1	5.254	-2.488	-1.992				
1	3.182	0.991	-0.567				
1	1.191	1.871	-1.355				
1	-1.719	0.971	2.003				
1	-2.036	1.176	-2.267				
1	-3.344	-0.908	2.040				
1	-3.651	-0.748	-2.233				
1	-5.463	-1.948	1.811				
1	-4.143	-3.102	1.708				
1	-5.713	-3.497	0.971				
Captopril				Budesonide			
16	-3.435	0.659	-1.157	8	-2.537	0.716	-0.266
8	-0.475	-1.323	-0.882	8	-2.776	1.064	1.934
8	3.165	-1.379	-1.272	8	1.465	-2.373	-1.493
8	2.308	-1.355	0.811	8	-3.952	-2.422	0.411
7	0.423	0.537	0.011	8	-5.012	-2.131	-1.986
6	1.629	0.347	-0.777	8	6.097	2.549	-1.016
6	2.432	1.619	-0.491	6	-0.970	-1.137	0.039
6	2.044	1.954	0.946	6	-0.194	-0.372	1.129
6	0.563	1.597	1.012	6	1.292	-0.698	1.168
6	-0.563	-0.397	-0.086	6	-2.408	-0.586	0.298
6	-1.740	-0.280	0.870	6	1.897	-0.378	-0.215
6	2.368	-0.893	-0.300	6	-1.050	-0.556	2.375

1	5.016	-2.267	1.168	1	-4.119	2.022	1.353
1	-6.184	-1.874	1.390	1	-1.496	-1.931	0.728
1	6.184	1.874	1.390	1	-1.457	-2.566	-0.897
1	-6.673	0.522	1.814	1	-1.912	2.958	-0.242
1	6.673	-0.522	1.814	1	-1.543	2.102	-1.730
1	-0.875	-2.264	-0.889	1	-6.305	1.344	-0.659
1	0.875	2.264	-0.889	1	-6.438	1.330	1.081
				1	-2.715	-0.774	2.163
				1	-4.214	0.104	2.452
				1	-4.245	-1.649	2.276
				1	0.222	2.477	0.730
				1	0.566	3.009	-0.894
				1	0.533	-2.422	-1.082
				1	2.771	1.922	-0.416
				1	3.000	-2.296	-1.062
				1	6.933	-0.747	-0.379
	Anastrozole				Cyclophosphamide		
7	-3.249	1.271	-0.272	17	-3.473	-2.252	-0.451
7	-4.032	0.292	-0.790	17	-1.228	4.007	-0.069
7	2.284	-3.733	-1.140	15	0.993	-0.698	0.873
7	4.109	0.848	2.126	8	2.202	0.383	0.855
7	-4.751	0.882	1.280	8	0.673	-1.143	2.242
6	0.270	-2.630	0.141	7	-0.194	0.103	-0.025
6	2.924	1.646	-0.081	7	1.424	-1.926	-0.173
6	0.292	-1.122	-0.126	6	2.187	-1.561	-1.376
6	1.562	0.951	-0.182	6	3.342	-0.615	-1.074
6	1.494	-0.428	-0.002	6	2.853	0.654	-0.401
6	-0.818	0.968	-0.617	6	-1.259	-0.691	-0.643
6	-0.864	-0.414	-0.440	6	-0.622	1.411	0.484
6	0.392	1.644	-0.485	6	-2.109	-1.429	0.376
6	-2.068	1.731	-0.981	6	-0.570	2.438	-0.630
6	-1.023	-3.309	-0.328	1	1.495	-1.084	-2.082
6	0.465	-2.877	1.651	1	2.536	-2.480	-1.853
6	2.824	3.175	-0.034	1	4.076	-1.111	-0.430
6	3.797	1.224	-1.279	1	3.856	-0.343	-2.002
6	1.395	-3.243	-0.579	1	1.795	-2.725	0.326
6	3.581	1.197	1.155	1	3.675	1.331	-0.161
6	-3.689	1.596	0.961	1	2.152	1.184	-1.060
6	-4.914	0.105	0.181	1	-0.821	-1.409	-1.341
1	2.401	-0.977	0.245	1	-1.890	-0.016	-1.232
1	-1.816	-0.922	-0.555	1	0.029	1.723	1.304
1	0.409	2.722	-0.616	1	-1.638	1.359	0.896
1	-1.940	2.797	-0.772	1	-1.534	-2.194	0.899
1	-2.293	1.633	-2.047	1	-2.539	-0.755	1.119
1	-1.219	-3.123	-1.385	1	0.455	2.617	-0.958
1	-1.873	-2.945	0.253	1	-1.164	2.131	-1.493
1	-0.954	-4.388	-0.179				
1	1.398	-2.439	2.010				
1	-0.362	-2.418	2.199				
1	0.478	-3.946	1.869				
1	2.188	3.516	0.786				
1	2.419	3.556	-0.974				
1	3.814	3.612	0.102				
1	3.922	0.141	-1.321				
1	3.316	1.548	-2.206				
1	4.785	1.685	-1.219				
1	-3.214	2.353	1.570				
1	-5.710	-0.619	0.083				
	Acrivastine				Atropine		
8	-5.774	1.125	0.401	8	0.104	0.170	0.441
8	-6.471	-1.017	0.382	8	0.515	1.891	-0.958
7	0.464	3.112	-0.603	8	2.511	3.521	0.240
7	-1.413	-1.238	-0.248	7	-3.900	-0.560	0.906
6	1.171	4.380	-0.724	6	-3.621	0.762	0.314
6	0.105	3.045	0.811	6	-3.228	-1.453	-0.056
6	0.313	5.349	0.086	6	-3.887	0.590	-1.202
6	-0.404	4.450	1.116	6	-3.622	-0.910	-1.452
6	1.247	1.974	-1.053	6	-2.158	1.095	0.602
6	0.449	0.720	-0.951	6	-1.724	-1.352	0.195
6	0.863	-0.491	-0.530	6	-1.256	0.068	-0.064
6	2.270	-0.786	-0.179	6	-5.324	-0.829	1.008
6	-0.132	-1.586	-0.411	6	0.879	1.117	-0.095
6	3.324	-0.433	-1.026	6	2.271	1.093	0.506
6	2.590	-1.424	1.027	6	2.965	-0.222	0.241
6	0.262	-2.934	-0.493	6	3.095	2.269	-0.031
6	4.644	-0.696	-0.677	6	3.586	-0.926	1.271
6	3.907	-1.678	1.375	6	3.037	-0.729	-1.060
6	4.963	-1.319	0.529	6	4.264	-2.113	1.011
6	-2.344	-2.200	-0.164	6	3.712	-1.915	-1.321
6	-0.701	-3.926	-0.406	6	4.328	-2.610	-0.286
6	-2.029	-3.562	-0.236	1	-4.270	1.513	0.772
6	6.383	-1.593	0.917	1	-3.562	-2.482	0.104
6	-3.731	-1.787	0.020	1	-3.247	1.241	-1.804
6	-4.144	-0.517	0.128	1	-4.919	0.854	-1.446

6	-5.567	-0.215	0.312	1	-4.520	-1.412	-1.822
1	1.286	4.660	-1.776	1	-2.839	-1.085	-2.195
1	2.189	4.307	-0.289	1	-1.906	2.097	0.242
1	0.996	2.807	1.428	1	-1.995	1.069	1.684
1	-0.631	2.255	0.989	1	-1.518	-1.617	1.236
1	-0.411	5.851	-0.559	1	-1.172	-2.049	-0.443
1	0.918	6.128	0.553	1	-1.209	0.268	-1.141
1	-0.194	4.740	2.148	1	-5.779	-0.118	1.702
1	-1.488	4.502	0.985	1	-5.476	-1.833	1.413
1	2.196	1.888	-0.488	1	-5.876	-0.766	0.053
1	1.529	2.162	-2.100	1	2.149	1.217	1.588
1	-0.605	0.825	-1.198	1	3.262	2.127	-1.110
1	3.102	0.037	-1.980	1	4.077	2.263	0.451
1	1.789	-1.713	1.703	1	3.534	-0.541	2.286
1	1.307	-3.184	-0.638	1	2.555	-0.190	-1.873
1	5.444	-0.418	-1.359	1	1.712	3.561	-0.299
1	4.127	-2.163	2.323	1	4.741	-2.650	1.825
1	-0.419	-4.972	-0.475	1	3.758	-2.297	-2.336
1	-2.814	-4.307	-0.157	1	4.855	-3.537	-0.489
1	7.074	-1.362	0.104				
1	6.683	-0.995	1.783				
1	6.530	-2.641	1.194				
1	-4.480	-2.575	0.075				
1	-3.438	0.305	0.082				
1	-6.727	1.243	0.520				
Baclofen				Enoxacin			
17	4.402	0.163	-0.144	9	1.927	-2.788	-0.496
8	-2.497	2.618	-0.990	8	-3.077	-2.375	-0.211
8	-1.926	2.031	1.104	8	-5.508	-1.135	-0.023
7	-3.321	-2.549	0.164	8	-5.526	1.088	0.266
6	-1.566	-0.700	0.307	7	2.902	-0.171	-0.003
6	-0.077	-0.474	0.192	7	5.603	0.600	0.325
6	-2.348	0.308	-0.532	7	-1.463	1.378	0.279
6	-1.941	-2.149	-0.060	7	0.692	0.532	0.159
6	0.674	-0.067	1.295	6	3.273	1.242	0.059
6	0.589	-0.673	-1.021	6	3.853	-1.025	0.720
6	-2.217	1.715	-0.022	6	4.688	1.421	-0.456
6	2.046	0.131	1.204	6	5.254	-0.807	0.188
6	1.960	-0.482	-1.134	6	1.557	-0.473	0.004
6	2.679	-0.081	-0.014	6	-0.617	0.281	0.120
1	-1.847	-0.537	1.356	6	-1.182	-0.988	-0.044
1	-2.055	0.274	-1.587	6	1.064	-1.785	-0.221
1	-3.420	0.071	-0.513	6	-0.276	-2.040	-0.230
1	-1.294	-2.824	0.511	6	-0.906	2.733	0.387
1	-1.705	-2.335	-1.115	6	-2.636	-1.241	-0.064
1	0.170	0.116	2.240	6	-2.799	1.190	0.258
1	0.033	-0.984	-1.902	6	-3.427	-0.020	0.104
1	-3.957	-2.030	-0.432	6	-0.553	3.317	-0.966
1	-3.596	-2.355	1.122	6	-4.900	0.054	0.127
1	2.621	0.451	2.065	1	3.197	1.612	1.094
1	2.470	-0.640	-2.077	1	2.568	1.814	-0.544
1	-2.418	3.493	-0.582	1	3.568	-2.068	0.620
				1	3.829	-0.761	1.789
				1	4.704	1.168	-1.532
				1	4.975	2.472	-0.358
				1	5.957	-1.411	0.769
				1	5.294	-1.158	-0.859
				1	6.555	0.753	0.013
				1	-0.660	-3.039	-0.408
				1	-1.658	3.339	0.897
				1	-0.026	2.676	1.029
				1	-3.406	2.082	0.381
				1	0.192	2.700	-1.472
				1	-1.434	3.385	-1.609
				1	-0.142	4.321	-0.850
				1	-6.456	-0.941	0.009
Atovaquone				Carbidopa			
17	-8.218	-0.483	0.000	8	-1.095	1.104	1.573
8	2.665	-2.356	0.000	8	-2.159	1.964	-0.206
8	1.842	2.313	-0.001	8	3.105	1.948	-0.391
8	4.522	2.738	0.000	8	4.451	-0.149	0.555
6	0.609	-0.274	0.000	7	-3.273	-0.542	-0.730
6	-2.254	0.521	0.000	7	-4.306	-0.050	0.132
6	-0.078	0.263	-1.263	6	-1.969	-0.441	-0.062
6	-0.079	0.264	1.264	6	-0.916	-0.727	-1.160
6	-1.570	-0.038	-1.253	6	0.516	-0.618	-0.721
6	-1.570	-0.037	1.254	6	-1.897	-1.451	1.070
6	2.100	-0.032	0.000	6	-1.766	1.000	0.411
6	-3.740	0.269	0.000	6	1.173	0.615	-0.772
6	3.013	-1.053	0.000	6	1.204	-1.727	-0.232
6	2.583	1.342	0.000	6	2.483	0.741	-0.336
6	-4.648	1.328	-0.001	6	2.522	-1.611	0.205
6	-4.254	-1.032	0.001	6	3.158	-0.382	0.156
6	4.465	-0.871	0.000	1	-1.130	-1.733	-1.535

6	4.108	1.599	0.000	1	-1.102	-0.031	-1.988
6	5.007	0.426	0.000	1	-2.027	-2.456	0.662
6	-6.021	1.112	-0.001	1	-2.695	-1.265	1.789
6	-5.622	-1.272	0.001	1	-0.939	-1.399	1.589
6	5.329	-1.969	0.000	1	-3.227	0.035	-1.571
6	-6.497	-0.192	0.000	1	0.669	1.497	-1.155
6	6.387	0.608	0.000	1	0.710	-2.693	-0.192
6	6.706	-1.775	0.000	1	3.056	-2.479	0.581
6	7.239	-0.489	0.000	1	-4.436	0.952	-0.008
1	0.412	-1.363	0.001	1	-5.166	-0.514	-0.136
1	-2.101	1.610	0.000	1	-0.991	2.051	1.748
1	0.393	-0.167	-2.154	1	4.004	1.827	-0.059
1	0.083	1.344	-1.313	1	4.846	-0.967	0.869
1	0.083	1.345	1.313				
1	0.393	-0.165	2.154				
1	-2.046	0.368	-2.152				
1	-1.732	-1.126	-1.290				
1	-1.732	-1.125	1.292				
1	-2.046	0.370	2.152				
1	-4.273	2.348	-0.001				
1	-3.574	-1.880	0.001				
1	-6.717	1.943	-0.001				
1	-6.010	-2.283	0.001				
1	4.917	-2.971	0.000				
1	1.701	-2.418	0.000				
1	6.767	1.624	0.000				
1	7.366	-2.636	0.000				
1	8.314	-0.345	0.000				
	Ergotamine				Cephalexin		
8	1.509	1.916	1.123	16	0.405	1.046	-1.272
8	2.100	1.322	-1.056	8	1.388	-1.726	1.849
8	6.175	0.772	-1.244	8	-2.283	-2.724	-1.228
8	2.665	-1.227	2.207	8	4.965	0.350	1.408
8	-1.562	1.530	1.609	8	4.403	-1.760	0.864
7	4.792	2.345	-0.398	7	2.059	-0.832	-0.251
7	3.206	0.482	0.759	7	-1.171	-1.213	0.051
7	0.079	-0.008	1.212	7	-4.651	-1.502	-0.876
7	-3.673	-2.383	0.716	6	0.996	-0.678	-1.226
7	-9.135	-0.525	-0.888	6	0.130	-1.627	-0.355
6	3.561	2.793	0.257	6	1.251	-1.483	0.686
6	2.555	1.651	0.240	6	3.155	0.026	-0.087
6	3.213	4.068	-0.495	6	2.068	1.719	-1.581
6	4.438	-0.036	0.183	6	3.202	1.216	-0.728
6	5.415	3.414	-1.182	6	-2.303	-1.795	-0.441
6	4.591	4.643	-0.819	6	4.376	2.141	-0.733
6	1.172	0.702	1.837	6	4.221	-0.574	0.755
6	5.215	1.059	-0.548	6	-3.626	-1.242	0.119
6	2.430	-0.168	1.663	6	-3.546	0.223	0.484
6	4.184	-1.247	-0.744	6	-3.243	0.612	1.790
6	0.910	1.054	3.282	6	-3.704	1.206	-0.496
6	-2.146	-0.450	0.361	6	-3.086	1.957	2.113
6	-4.879	-1.574	0.503	6	-3.551	2.548	-0.173
6	-1.206	0.483	1.104	6	-3.239	2.928	1.130
6	5.324	-2.226	-0.779	1	1.268	-1.016	-2.230
6	-2.626	-1.572	1.309	1	0.053	-2.627	-0.790
6	-4.589	-0.199	-0.116	1	-1.258	-0.394	0.639
6	-5.971	-2.379	-0.225	1	1.974	2.800	-1.433
6	-3.337	0.281	-0.172	1	2.322	1.588	-2.642
6	-5.768	0.585	-0.504	1	5.315	1.655	-0.483
6	-7.168	-1.519	-0.441	1	4.228	2.956	-0.015
6	-6.970	-0.125	-0.601	1	4.477	2.607	-1.719
6	-3.197	-3.091	-0.462	1	-3.767	-1.811	1.058
6	6.150	-2.349	-1.895	1	-5.563	-1.555	-0.437
6	5.569	-3.037	0.333	1	-4.456	-2.401	-1.309
6	-8.202	0.489	-0.885	1	5.614	-0.151	1.923
6	-8.508	-1.736	-0.615	1	-3.130	-0.149	2.560
6	-5.845	1.961	-0.718	1	-3.954	0.896	-1.505
6	-8.270	1.864	-1.102	1	-2.853	2.244	3.133
6	7.196	-3.264	-1.905	1	-3.675	3.304	-0.942
6	6.617	-3.950	0.327	1	-3.121	3.978	1.380
6	-7.072	2.572	-1.017				
6	7.434	-4.067	-0.794				
1	3.750	3.020	1.316				
1	2.575	4.735	0.087				
1	2.691	3.823	-1.427				
1	5.061	-0.373	1.023				
1	5.353	3.165	-2.249				
1	6.476	3.503	-0.938				
1	4.570	5.383	-1.619				
1	5.007	5.132	0.068				
1	3.292	-1.753	-0.361				
1	3.945	-0.886	-1.748				
1	1.540	2.045	-1.360				
1	0.324	-0.790	0.620				

1	0.048	1.712	3.360				
1	0.724	0.137	3.844				
1	1.786	1.551	3.704				
1	-1.583	-0.918	-0.464				
1	-5.279	-1.361	1.509				
1	-1.791	-2.219	1.601				
1	-3.022	-1.112	2.222				
1	-6.185	-3.286	0.350				
1	-5.592	-2.710	-1.200				
1	-3.162	1.275	-0.574				
1	-2.224	-3.532	-0.233				
1	-3.869	-3.911	-0.719				
1	-3.079	-2.456	-1.359				
1	5.981	-1.704	-2.752				
1	4.924	-2.951	1.205				
1	-9.089	-2.646	-0.582				
1	-4.959	2.581	-0.623				
-1	10.124	-0.412	-1.029				
1	-9.203	2.372	-1.323				
1	7.832	-3.347	-2.780				
1	6.794	-4.576	1.197				
1	-7.094	3.647	-1.171				
1	8.251	-4.781	-0.801				
	Cervastatin				Alfuzosin		
9	3.888	5.196	0.327	8	-3.302	-3.018	-0.217
8	4.731	-1.231	0.688	8	-4.554	-0.787	0.788
8	-2.011	3.742	-1.108	8	4.614	-2.105	-0.184
8	-4.002	1.079	1.444	8	2.165	-3.124	0.377
8	-7.355	-1.003	-0.073	7	-2.567	0.203	1.301
8	-5.434	-1.345	1.036	7	-0.712	3.338	-0.373
7	0.680	-2.532	-0.172	7	0.183	1.236	-0.012
6	1.992	-2.353	-0.333	7	1.586	3.131	-0.496
6	-0.125	-1.484	0.018	7	3.850	2.970	-0.769
6	2.580	-1.079	-0.314	6	-2.523	-1.879	0.055
6	0.361	-0.165	0.039	6	-2.044	-1.406	-1.318
6	1.747	0.031	-0.100	6	-3.313	-1.612	-2.142
6	-1.587	-1.821	0.237	6	-3.968	-2.825	-1.473
6	2.787	-3.632	-0.494	6	-3.335	-0.781	0.755
6	4.053	-0.915	-0.522	6	-3.156	1.442	1.786
6	2.313	1.400	0.001	6	-2.225	2.601	1.480
6	-0.539	0.982	0.281	6	-2.011	2.791	-0.026
6	-2.338	2.611	-0.288	6	0.390	2.526	-0.287
6	-1.753	-2.994	1.198	6	-0.581	4.779	-0.391
6	-2.266	-2.122	-1.100	6	2.586	0.949	-0.297
6	2.658	-4.478	0.772	6	1.290	0.444	-0.028
6	2.317	-4.406	-1.723	6	2.656	2.359	-0.507
6	-3.796	2.293	-0.585	6	3.688	0.071	-0.313
6	-1.432	1.460	-0.586	6	1.145	-0.937	0.224
6	-4.244	0.990	0.046	6	3.536	-1.272	-0.073
6	1.919	2.416	-0.876	6	2.233	-1.786	0.193
6	3.259	1.699	0.988	6	5.035	-2.717	1.030
6	-5.707	0.682	-0.242	6	0.884	-3.688	0.602
6	2.450	3.697	-0.778	1	-1.707	-2.196	0.717
6	3.792	2.977	1.108	1	-1.663	-0.381	-1.322
6	3.374	3.954	0.221	1	-1.237	-2.060	-1.666
6	6.122	-1.074	0.551	1	-3.110	-1.774	-3.202
6	-6.115	-0.649	0.316	1	-3.961	-0.735	-2.060
1	-2.072	-0.943	0.677	1	-3.841	-3.747	-2.051
1	3.845	-3.382	-0.618	1	-5.037	-2.668	-1.295
1	4.413	-1.575	-1.328	1	-3.350	1.379	2.863
1	4.296	0.113	-0.828	1	-4.133	1.562	1.303
1	-0.462	1.470	1.256	1	-1.252	2.407	1.948
1	-2.235	2.871	0.775	1	-2.610	3.518	1.939
1	-4.423	3.122	-0.239	1	-1.587	0.264	1.026
1	-3.921	2.228	-1.673	1	-2.122	1.830	-0.536
1	-1.302	-3.900	0.785	1	-2.770	3.461	-0.443
1	-1.272	-2.796	2.160	1	-1.435	5.207	-0.921
1	-2.813	-3.186	1.382	1	0.336	5.063	-0.901
1	-1.789	-2.980	-1.584	1	-0.556	5.208	0.621
1	-2.201	-1.275	-1.790	1	4.689	0.420	-0.546
1	-3.323	-2.361	-0.951	1	0.149	-1.314	0.417
1	3.225	-5.408	0.677	1	3.838	3.977	-0.706
1	3.034	-3.940	1.647	1	4.698	2.526	-0.456
1	1.610	-4.731	0.953	1	5.332	-1.959	1.764
1	2.442	-3.824	-2.641	1	4.254	-3.352	1.456
1	2.879	-5.337	-1.836	1	5.901	-3.330	0.779
1	1.257	-4.656	-1.629	1	0.210	-3.499	-0.241
1	-1.512	1.025	-1.585	1	1.039	-4.760	0.707
1	-3.637	0.171	-0.375	1	0.430	-3.294	1.519
1	1.198	2.196	-1.657				
1	3.584	0.913	1.663				
1	-5.918	0.691	-1.317				
1	-6.355	1.449	0.199				
1	2.165	4.486	-1.464				

1	4.519	3.221	1.874				
1	-1.109	3.997	-0.891				
1	-4.180	0.201	1.803				
1	6.528	-1.729	-0.235				
1	6.388	-0.035	0.304				
1	6.580	-1.341	1.504				
1	-7.546	-1.858	0.340				
	Disopyramide				Clofibrate		
8	0.773	-1.031	-2.363	17	-4.603	0.832	0.340
7	-2.246	-0.563	0.359	8	0.745	-1.182	-1.091
7	2.937	-1.113	1.173	8	2.398	0.874	-0.116
7	1.065	-2.620	-0.774	8	1.821	0.045	1.896
6	0.937	-0.301	-0.028	6	1.737	-1.412	-0.055
6	0.166	-0.796	1.228	6	1.289	-2.487	0.916
6	-1.249	-1.369	1.071	6	2.983	-1.822	-0.818
6	-3.106	-1.374	-0.536	6	1.981	-0.100	0.709
6	-3.039	0.309	1.258	6	-0.489	-0.715	-0.701
6	0.441	1.097	-0.399	6	2.589	2.165	0.504
6	2.456	-0.269	0.255	6	-0.744	0.656	-0.712
6	0.892	-1.324	-1.190	6	-1.513	-1.607	-0.387
6	-4.183	-0.519	-1.198	6	-2.008	1.135	-0.391
6	-2.310	-2.050	-1.646	6	-2.779	-1.135	-0.065
6	-4.046	-0.443	2.132	6	2.964	3.136	-0.580
6	-2.165	1.198	2.128	6	-3.015	0.235	-0.064
6	0.885	2.175	0.375	1	2.076	-2.686	1.644
6	-0.515	1.352	-1.383	1	0.403	-2.183	1.474
6	3.298	0.531	-0.526	1	1.075	-3.409	0.370
6	0.404	3.463	0.175	1	3.821	-1.973	-0.133
6	-1.002	2.640	-1.585	1	2.797	-2.759	-1.345
6	4.666	0.480	-0.311	1	3.256	-1.057	-1.544
6	-0.547	3.702	-0.811	1	1.662	2.442	1.017
6	4.257	-1.146	1.378	1	3.363	2.072	1.273
6	5.163	-0.368	0.673	1	0.050	1.337	-0.996
1	0.173	0.036	1.937	1	-1.315	-2.673	-0.409
1	0.761	-1.575	1.713	1	-2.217	2.199	-0.402
1	-1.593	-1.621	2.090	1	-3.581	-1.822	0.178
1	-1.162	-2.332	0.566	1	3.115	4.131	-0.155
1	-3.612	-2.173	0.045	1	3.887	2.837	-1.079
1	-3.595	0.983	0.597	1	2.178	3.207	-1.335
1	-4.954	-0.170	-0.509				
1	-4.684	-1.101	-1.974				
1	-3.731	0.356	-1.676				
1	-2.982	-2.671	-2.244				
1	-1.859	-1.311	-2.314				
1	-1.511	-2.698	-1.287				
1	-4.764	-1.021	1.546				
1	-4.615	0.261	2.746				
1	-3.545	-1.134	2.818				
1	-1.653	0.629	2.910				
1	-2.792	1.936	2.635				
1	-1.421	1.734	1.540				
1	1.615	2.002	1.163				
1	-0.887	0.541	-1.992				
1	2.875	1.177	-1.287				
1	1.304	-3.279	-1.500				
1	1.486	-2.780	0.133				
1	0.767	4.277	0.796				
1	-1.747	2.811	-2.356				
1	5.336	1.090	-0.907				
1	-0.930	4.704	-0.974				
1	4.601	-1.840	2.142				
1	6.225	-0.435	0.880				
	Diphenoxylate				Carphenazine		
8	4.398	-1.735	-0.779	16	4.555	1.359	-1.048
8	5.024	-1.669	1.382	8	-7.540	0.058	-0.999
7	0.124	-0.722	1.695	8	-1.871	2.069	0.747
7	-4.013	2.085	2.299	7	-1.643	-2.275	0.292
6	2.926	-0.634	0.723	7	-4.413	-1.672	-0.177
6	2.537	-0.718	2.209	7	2.284	-0.575	-0.349
6	1.773	-1.271	-0.065	6	-2.595	-3.306	-0.098
6	1.188	-0.079	2.467	6	-2.345	-1.248	1.056
6	0.433	-0.638	0.268	6	-3.713	-2.707	-0.924
6	-1.141	-0.058	1.991	6	-3.460	-0.644	0.232
6	3.241	0.807	0.294	6	-0.516	-2.834	1.024
6	4.225	-1.409	0.515	6	0.668	-1.880	1.095
6	-2.364	-0.765	1.398	6	-5.504	-1.127	-0.968
6	-3.326	0.180	0.626	6	1.175	-1.525	-0.303
6	2.739	1.375	-0.879	6	-6.430	-0.238	-0.163
6	4.112	1.577	1.073	6	1.975	0.792	-0.238
6	-2.583	0.768	-0.585	6	3.585	-1.062	-0.127
6	-4.609	-0.524	0.162	6	2.952	1.785	-0.472
6	3.065	2.677	-1.242	6	4.716	-0.253	-0.345
6	4.445	2.877	0.709	6	0.685	1.227	0.067
6	-3.717	1.252	1.550	6	3.814	-2.381	0.290

6	3.915	3.437	-0.448	6	0.354	2.584	0.149
6	5.644	-2.394	-1.090	6	2.634	3.136	-0.361
6	-2.050	2.056	-0.580	6	5.999	-0.734	-0.110
6	-4.763	-1.908	0.205	6	1.343	3.545	-0.062
6	-2.360	-0.050	-1.694	6	5.103	-2.868	0.483
6	-5.644	0.252	-0.365	6	6.204	-2.047	0.297
6	5.663	-2.655	-2.570	6	-1.051	2.936	0.486
6	-1.283	2.508	-1.651	6	-1.443	4.399	0.500
6	-5.929	-2.504	-0.272	6	-2.905	4.623	0.822
6	-1.591	0.397	-2.760	1	-3.025	-3.811	0.789
6	-6.807	-0.339	-0.836	1	-2.067	-4.067	-0.685
6	-1.043	1.678	-2.739	1	-1.653	-0.451	1.340
6	-6.953	-1.724	-0.792	1	-2.763	-1.676	1.989
1	3.299	-0.258	2.839	1	-4.431	-3.487	-1.199
1	2.501	-1.775	2.495	1	-3.288	-2.304	-1.866
1	1.734	-2.336	0.191	1	-3.024	-0.127	-0.646
1	1.951	-1.223	-1.142	1	-3.969	0.117	0.828
1	0.932	-0.161	3.529	1	-0.809	-3.148	2.045
1	1.237	1.005	2.236	1	-0.207	-3.748	0.500
1	-0.348	-1.151	-0.297	1	0.399	-0.970	1.640
1	0.409	0.418	-0.066	1	1.463	-2.343	1.687
1	-1.105	0.996	1.649	1	-6.097	-1.963	-1.355
1	-1.240	-0.007	3.080	1	-5.137	-0.566	-1.850
1	-2.043	-1.548	0.706	1	0.354	-1.116	-0.895
1	-2.931	-1.267	2.187	1	1.494	-2.430	-0.829
1	2.079	0.806	-1.525	1	-6.739	-0.769	0.749
1	4.549	1.149	1.970	1	-5.919	0.685	0.145
1	2.649	3.097	-2.154	1	-0.122	0.526	0.231
1	5.122	3.451	1.333	1	2.982	-3.049	0.461
1	4.168	4.454	-0.731	1	3.415	3.870	-0.535
1	5.709	-3.314	-0.501	1	6.843	-0.071	-0.276
1	6.467	-1.749	-0.767	1	-8.103	0.682	-0.537
1	-2.228	2.710	0.269	1	1.121	4.604	0.005
1	-3.979	-2.538	0.610	1	5.233	-3.899	0.795
1	-2.786	-1.051	-1.717	1	7.210	-2.417	0.459
1	-5.533	1.333	-0.402	1	-1.179	4.835	-0.472
1	5.594	-1.723	-3.135	1	-0.797	4.918	1.221
1	4.833	-3.298	-2.869	1	-3.160	4.212	1.800
1	6.594	-3.153	-2.850	1	-3.148	5.687	0.824
1	-0.867	3.510	-1.626	1	-3.548	4.127	0.092
1	-6.034	-3.583	-0.231				
1	-1.422	-0.254	-3.612				
1	-7.602	0.280	-1.237				
1	-0.441	2.027	-3.572				
1	-7.862	-2.189	-1.159				
	Anileridine				Estazolam		
8	-2.650	1.972	-0.140	17	1.199	4.171	-0.464
8	-2.441	1.234	1.974	7	-2.384	-0.462	0.371
7	0.659	-0.807	0.051	7	-0.233	-1.904	-1.145
7	8.441	0.250	0.436	7	-3.498	-2.309	-0.095
6	-2.259	-0.362	0.142	7	-4.043	-1.747	1.044
6	-1.424	-0.277	-1.139	6	-1.505	0.624	0.192
6	-1.511	-1.281	1.123	6	-0.194	0.409	-0.271
6	0.008	0.138	-0.849	6	0.370	-0.949	-0.534
6	-0.066	-0.858	1.317	6	-2.519	-1.535	-0.482
6	-3.677	-0.885	-0.093	6	-1.591	-1.687	-1.626
6	2.055	-0.466	0.285	6	1.755	-1.215	-0.068
6	-2.435	1.018	0.785	6	-1.955	1.914	0.480
6	2.953	-0.653	-0.936	6	0.624	1.529	-0.466
6	-4.162	-1.200	-1.363	6	-3.380	-0.653	1.298
6	-4.532	-1.051	1.003	6	-1.128	3.008	0.295
6	4.398	-0.420	-0.598	6	0.159	2.805	-0.196
6	-5.456	-1.685	-1.531	6	2.294	-0.568	1.050
6	-5.824	-1.531	0.836	6	2.530	-2.175	-0.730
6	-6.292	-1.854	-0.435	6	3.574	-0.873	1.495
6	-2.908	3.293	0.382	6	3.812	-2.469	-0.292
6	4.961	0.856	-0.660	6	4.339	-1.819	0.822
6	5.216	-1.461	-0.153	1	-1.904	-2.545	-2.222
6	-3.125	4.209	-0.790	1	-1.646	-0.791	-2.265
6	6.281	1.088	-0.300	1	-2.972	2.055	0.828
6	6.538	-1.245	0.209	1	1.638	1.390	-0.825
6	7.093	0.038	0.142	1	-3.542	0.012	2.133
1	-1.873	0.420	-1.851	1	-1.479	4.010	0.508
1	-1.409	-1.267	-1.608	1	1.701	0.165	1.588
1	-2.018	-1.289	2.090	1	2.101	-2.682	-1.587
1	-1.546	-2.299	0.721	1	3.974	-0.372	2.371
1	0.027	1.165	-0.423	1	4.406	-3.207	-0.821
1	0.569	0.181	-1.786	1	5.342	-2.052	1.164
1	0.444	-1.571	1.973				
1	-0.034	0.124	1.831				
1	2.161	0.572	0.663				
1	2.421	-1.117	1.089				
1	2.651	0.032	-1.735				
1	2.806	-1.668	-1.322				

1	-3.532	-1.071	-2.236				
1	-4.180	-0.787	1.996				
1	-5.811	-1.929	-2.528				
1	-6.469	-1.652	1.700				
1	-7.300	-2.232	-0.567				
1	-2.056	3.595	0.999				
1	-3.780	3.241	1.042				
1	4.351	1.690	-1.001				
1	4.807	-2.467	-0.091				
1	-3.975	3.884	-1.393				
1	-2.244	4.243	-1.434				
1	-3.327	5.223	-0.439				
1	6.696	2.091	-0.368				
1	7.154	-2.077	0.541				
1	8.840	-0.423	1.075				
1	8.662	1.192	0.724				
	Diazoxide				Entacapone		
17	4.136	-0.274	-0.001	8	-2.793	1.679	-1.044
16	-1.185	-1.377	0.000	8	3.220	-2.893	-0.177
8	-1.133	-2.104	-1.252	8	5.002	-1.005	0.070
8	-1.136	-2.101	1.255	8	3.839	2.855	0.631
7	-1.459	1.630	0.001	8	5.411	1.595	-0.184
7	-2.570	-0.464	-0.002	7	-3.991	0.142	0.117
6	0.140	-0.185	0.000	7	4.264	1.798	0.180
6	-0.142	1.182	0.001	7	-1.685	-2.766	-0.576
6	-2.568	0.825	-0.001	6	-5.192	0.958	-0.110
6	1.454	-0.642	-0.001	6	-4.051	-0.801	1.235
6	0.916	2.095	0.001	6	-2.836	0.621	-0.432
6	2.489	0.279	0.000	6	-5.761	0.759	-1.501
6	2.225	1.649	0.001	6	-3.967	-0.109	2.585
6	-3.874	1.550	-0.001	6	0.968	0.042	-0.149
1	-1.608	2.628	0.001	6	-1.573	-0.203	-0.307
1	1.657	-1.707	-0.001	6	-0.404	0.485	-0.218
1	0.707	3.161	0.002	6	1.951	1.024	-0.008
1	3.046	2.355	0.001	6	1.385	-1.306	-0.210
1	-3.969	2.180	0.888	6	3.299	0.696	0.050
1	-4.689	0.832	-0.011	6	2.720	-1.623	-0.140
1	-3.961	2.197	-0.879	6	3.723	-0.636	-0.014
				6	-1.633	-1.610	-0.439
				1	-4.943	2.011	0.054
				1	-5.922	0.670	0.651
				1	-3.258	-1.541	1.139
				1	-4.989	-1.358	1.139
				1	-5.036	1.060	-2.258
				1	-6.026	-0.287	-1.672
				1	-6.660	1.363	-1.636
				1	-3.011	0.408	2.699
				1	-4.763	0.631	2.709
				1	-4.058	-0.834	3.396
				1	-0.537	1.566	-0.201
				1	1.684	2.072	0.058
				1	0.663	-2.107	-0.315
				1	2.506	-3.531	-0.269
				1	5.024	-1.973	0.040
	Cycloserine				Chlorzoxazone		
8	-1.763	-0.359	0.115	17	3.458	-0.512	0.000
8	0.957	1.796	0.026	8	-2.172	0.972	0.000
7	-1.145	0.874	-0.240	8	-3.946	-0.467	0.000
7	1.777	-0.974	-0.273	7	-1.732	-1.200	0.000
6	0.540	-0.595	0.373	6	-0.507	-0.557	0.000
6	-0.709	-1.303	-0.130	6	-0.813	0.803	0.000
6	0.193	0.856	0.064	6	0.802	-1.003	0.000
1	0.569	-0.650	1.476	6	0.160	1.776	0.000
1	-0.614	-1.505	-1.205	6	1.788	-0.014	0.000
1	-0.988	-2.212	0.402	6	-2.766	-0.283	0.000
1	-1.743	1.655	-0.009	6	1.489	1.346	0.000
1	2.268	-1.677	0.265	1	-1.905	-2.191	0.000
1	2.382	-0.156	-0.306	1	1.063	-2.054	0.000
				1	-0.093	2.829	0.000
				1	2.296	2.068	0.000
	estradiol acetate				Armodafinil		
8	-5.789	-1.084	0.602	16	-0.783	-1.147	0.405
8	5.058	-0.507	-0.321	8	-0.651	-2.520	-0.210
8	5.226	0.832	1.508	8	-4.549	-0.684	0.533
6	-3.446	-0.519	0.270	7	-3.503	-2.537	-0.284
6	-2.781	0.694	-0.402	6	0.421	-0.038	-0.543
6	-1.285	0.758	-0.150	6	1.824	-0.495	-0.242
6	-0.638	-0.527	-0.699	6	0.126	1.404	-0.252
6	-4.898	-0.261	-0.137	6	-2.325	-0.419	-0.302
6	-2.820	-1.791	-0.292	6	2.736	-0.593	-1.295
6	-3.673	1.874	-0.010	6	-0.413	2.216	-1.254
6	-1.299	-1.789	-0.125	6	2.256	-0.801	1.050
6	-5.087	1.255	0.086	6	0.333	1.953	1.017
6	-0.610	1.969	-0.776	6	4.053	-0.968	-1.062

6	-3.336	-0.494	1.797	6	-0.733	3.543	-0.999
6	0.873	-0.499	-0.553	6	3.572	-1.182	1.284
6	0.845	2.042	-0.346	6	0.006	3.278	1.275
6	1.564	0.718	-0.418	6	4.476	-1.261	0.230
6	1.622	-1.680	-0.589	6	-0.527	4.078	0.268
6	2.957	0.722	-0.318	6	-3.570	-1.222	0.051
6	3.005	-1.679	-0.485	1	0.187	-0.262	-1.590
6	3.664	-0.467	-0.344	1	-2.435	0.593	0.087
6	5.744	0.184	0.640	1	-2.184	-0.389	-1.388
6	7.213	-0.011	0.433	1	2.406	-0.371	-2.306
1	-2.907	0.541	-1.489	1	-0.580	1.798	-2.244
1	-1.108	0.800	0.938	1	1.556	-0.767	1.880
1	-0.858	-0.525	-1.783	1	0.759	1.341	1.806
1	-4.992	-0.493	-1.212	1	4.748	-1.038	-1.892
1	-3.063	-1.858	-1.363	1	-1.144	4.161	-1.791
1	-3.252	-2.680	0.180	1	3.889	-1.426	2.292
1	-3.620	2.693	-0.731	1	0.170	3.689	2.265
1	-3.360	2.290	0.954	1	5.502	-1.561	0.414
1	-1.028	-1.885	0.934	1	-0.780	5.113	0.471
1	-0.894	-2.680	-0.613	1	-4.263	-3.125	0.021
1	-5.529	1.412	1.074	1	-2.597	-2.961	-0.463
1	-5.782	1.687	-0.640				
1	-1.129	2.892	-0.497				
1	-0.684	1.892	-1.870				
1	-3.906	-1.322	2.223				
1	-2.303	-0.588	2.136				
1	-3.738	0.427	2.227				
1	0.895	2.402	0.692				
1	1.392	2.787	-0.934				
1	-6.680	-0.928	0.280				
1	1.117	-2.633	-0.703				
1	3.483	1.663	-0.209				
1	3.576	-2.600	-0.516				
1	7.465	-1.070	0.512				
1	7.769	0.554	1.176				
1	7.500	0.310	-0.570				
Efavirenz				Atenolol			
17	-2.714	3.498	0.187	8	0.959	-1.007	0.327
9	0.496	-0.047	2.313	8	2.926	-3.061	0.446
9	-0.333	-1.997	1.852	8	-6.556	0.576	-0.068
9	1.802	-1.671	1.723	7	3.974	0.393	-0.409
8	0.591	-1.912	-0.752	7	-5.049	-1.085	0.246
8	-0.244	-3.876	-1.381	6	3.777	-0.778	0.431
7	-1.706	-2.231	-0.812	6	3.069	-1.888	-0.340
6	3.494	1.823	-0.987	6	4.019	1.677	0.303
6	4.887	1.255	-1.162	6	1.694	-1.467	-0.800
6	4.586	2.094	0.028	6	4.624	2.719	-0.619
6	0.440	-0.687	0.017	6	2.616	2.076	0.734
6	2.421	0.951	-0.647	6	-0.276	-0.493	0.110
6	-0.922	-0.059	-0.185	6	-2.849	0.630	-0.126
6	1.525	0.196	-0.357	6	-0.942	-0.005	1.239
6	-1.975	-0.890	-0.567	6	-0.897	-0.419	-1.138
6	0.614	-1.108	1.504	6	-2.206	0.545	1.116
6	-1.147	1.293	0.038	6	-2.170	0.138	-1.239
6	-3.259	-0.363	-0.708	6	-4.241	1.178	-0.241
6	-0.449	-2.758	-0.994	6	-5.398	0.205	-0.013
6	-2.430	1.806	-0.100	1	3.151	-0.511	1.285
6	-3.489	0.982	-0.468	1	4.719	-1.177	0.851
1	3.229	2.651	-1.638	1	3.644	-2.108	-1.258
1	5.486	1.676	-1.960	1	4.655	1.602	1.207
1	4.999	0.187	-1.021	1	4.827	0.284	-0.948
1	4.492	1.603	0.988	1	1.801	-0.658	-1.533
1	4.974	3.104	0.067	1	1.178	-2.316	-1.267
1	-0.323	1.936	0.327	1	5.645	2.456	-0.913
1	-2.458	-2.851	-1.073	1	4.661	3.697	-0.136
1	-4.076	-1.009	-1.011	1	4.025	2.815	-1.530
1	-4.484	1.396	-0.575	1	2.633	3.020	1.284
				1	1.972	2.197	-0.142
				1	2.153	1.326	1.379
				1	3.785	-3.276	0.819
				1	-0.445	-0.066	2.201
				1	-0.403	-0.787	-2.028
				1	-2.710	0.921	2.003
				1	-2.645	0.189	-2.216
				1	-4.412	1.612	-1.230
				1	-4.402	1.996	0.468
				1	-5.780	-1.758	0.408
				1	-4.086	-1.378	0.300
Caffeine				Acitretin			
8	-0.552	-2.534	0.000	8	-6.964	1.029	-0.320
8	3.070	0.304	0.000	8	8.685	1.898	-0.782
7	0.999	1.277	0.000	8	8.760	-0.220	-0.032
7	-2.267	0.013	0.000	6	-4.062	-1.138	-0.230
7	1.257	-1.087	0.000	6	-3.029	-0.248	0.176

1	-3.663	1.901	2.807	1	0.034	0.131	-2.761
1	-5.558	-1.822	-1.136	1	1.355	-1.825	-1.967
1	-1.261	-0.489	1.368				
1	-4.050	-3.644	-1.977				
1	0.944	-1.210	2.136				
1	1.713	-2.644	1.469				
1	-1.340	-4.456	-1.685				
1	0.723	-3.821	-0.474				
1	1.516	0.082	0.068				
1	2.272	-1.369	-0.630				
1	3.560	2.387	0.709				
1	5.357	-1.093	-1.023				
1	4.656	3.820	-1.018				
1	6.457	0.331	-2.755				
1	6.097	2.780	-2.742				
	Etodolac				Cabergoline		
8	2.309	0.936	0.823	8	2.475	1.687	-0.163
8	4.296	-1.697	-0.574	8	2.332	-2.437	1.589
8	4.486	0.364	-1.451	7	-1.588	2.354	0.419
7	-0.791	-0.737	-0.289	7	-5.888	-1.274	-1.658
6	1.642	-0.192	0.253	7	2.613	-0.204	1.071
6	0.202	0.162	0.048	7	1.382	-0.893	2.948
6	-0.334	1.410	0.198	7	5.996	-0.099	-1.592
6	0.529	2.578	0.532	6	-1.820	-0.085	0.236
6	1.803	-1.320	1.279	6	-2.314	1.290	-0.296
6	2.288	-0.558	-1.115	6	-0.310	-0.223	0.105
6	-1.743	1.292	-0.027	6	0.398	0.958	0.763
6	1.974	2.197	0.245	6	-3.842	1.458	-0.160
6	-2.002	-0.071	-0.318	6	-0.148	2.249	0.178
6	-3.280	-0.568	-0.586	6	-2.559	-1.236	-0.405
6	1.090	-1.046	2.591	6	-3.864	-0.965	-0.807
6	-2.813	2.196	-0.014	6	-4.547	0.273	-0.727
6	3.788	-0.545	-1.082	6	-2.041	3.703	0.071
6	-3.516	-2.031	-0.831	6	1.902	0.878	0.547
6	-4.313	0.364	-0.558	6	-4.704	-1.925	-1.393
6	-4.087	1.721	-0.280	6	-2.100	-2.529	-0.618
6	-3.496	-2.858	0.454	6	-5.788	0.056	-1.264
1	0.258	3.459	-0.062	6	-4.246	3.228	-1.595
1	0.413	2.867	1.585	6	-2.941	-3.500	-1.200
1	2.873	-1.468	1.448	6	-1.401	4.753	0.919
1	1.443	-2.254	0.829	6	3.925	-0.470	0.453
1	1.923	-1.540	-1.428	6	2.096	-1.273	1.858
1	1.976	0.171	-1.865	6	3.793	-1.058	-0.943
1	2.156	2.174	-0.840	6	-0.853	5.873	0.457
1	2.682	2.905	0.679	6	5.141	-1.280	-1.607
1	-0.675	-1.736	-0.350	6	0.719	-1.878	3.791
1	1.427	-0.102	3.022	6	5.388	1.027	-2.278
1	0.006	-0.979	2.459	6	7.290	-0.410	-2.160
1	1.288	-1.838	3.316	6	-0.533	-2.448	3.151
1	-2.647	3.247	0.203	1	-2.060	-0.084	1.314
1	-4.479	-2.162	-1.334	1	-2.067	1.328	-1.380
1	-2.762	-2.419	-1.530	1	-0.034	-0.263	-0.959
1	-5.325	0.023	-0.761	1	0.011	-1.173	0.540
1	-4.928	2.406	-0.276	1	0.147	0.953	1.829
1	-2.550	-2.748	0.993	1	-4.170	2.369	-0.667
1	-3.642	-3.921	0.250	1	-4.077	1.593	0.906
1	-4.287	-2.534	1.135	1	0.085	2.295	-0.902
1	5.258	-1.589	-0.566	1	0.349	3.109	0.631
				1	-1.878	3.933	-1.001
				1	-3.119	3.756	0.244
				1	-1.089	-2.815	-0.345
				1	-6.625	0.723	-1.410
				1	-6.698	-1.681	-2.095
				1	-4.865	-3.998	-2.043
				1	-2.550	-4.501	-1.350
				1	-1.433	4.565	1.993
				1	4.474	0.472	0.424
				1	4.462	-1.156	1.111
				1	3.173	-0.392	-1.553
				1	3.263	-2.013	-0.880
				1	-0.443	6.626	1.121
				1	-0.797	6.078	-0.608
				1	5.683	-2.077	-1.082
				1	4.981	-1.644	-2.643
				1	1.388	0.075	3.223
				1	0.488	-1.386	4.739
				1	1.431	-2.681	4.007
				1	4.474	1.345	-1.771
				1	5.141	0.801	-3.334
				1	6.082	1.872	-2.272
				1	7.233	-0.712	-3.224
				1	7.755	-1.230	-1.605
				1	7.948	0.461	-2.094
				1	-1.010	-3.174	3.813

				1	-0.285	-2.962	2.219
				1	-1.261	-1.664	2.927
	Darifenacin			Cimetidine			
8	-1.906	-1.063	2.288	16	0.821	-1.805	-0.621
8	8.218	-0.152	0.149	7	4.328	1.076	-0.371
7	0.610	-1.297	-0.855	7	-1.932	-0.508	0.021
7	-1.932	1.186	2.340	7	3.888	-0.606	0.994
6	-1.637	-0.644	-0.610	7	-2.878	1.613	0.162
6	-2.725	0.028	0.289	7	-4.248	-0.315	-0.091
6	-1.536	-2.185	-0.472	7	-0.639	2.595	0.641
6	-0.191	-0.169	-0.399	6	2.716	-0.137	0.442
6	-0.053	-2.456	-0.261	6	1.411	-0.754	0.780
6	2.012	-1.212	-0.497	6	-0.654	-2.575	0.140
6	-4.019	-0.795	0.184	6	-1.969	-1.931	-0.257
6	-3.074	1.453	-0.160	6	2.961	0.908	-0.419
6	-2.171	-0.008	1.736	6	2.071	1.738	-1.262
6	2.744	-0.065	-1.188	6	4.833	0.146	0.490
6	-4.592	-0.952	-1.083	6	-3.093	0.211	0.005
6	-4.147	2.106	0.466	6	-5.405	0.534	0.043
6	-4.677	-1.355	1.279	6	-1.699	2.160	0.428
6	-2.402	2.139	-1.173	1	1.536	-1.398	1.653
6	4.215	-0.071	-0.877	1	0.651	0.000	1.008
6	-5.772	-1.660	-1.256	1	-0.515	-2.541	1.224
6	-4.517	3.395	0.111	1	-0.657	-3.626	-0.157
6	-5.867	-2.060	1.107	1	-2.796	-2.362	0.313
6	-2.776	3.431	-1.538	1	-2.188	-2.119	-1.318
6	4.693	0.493	0.314	1	4.852	1.770	-0.882
6	5.126	-0.687	-1.739	1	-1.113	-0.052	-0.373
6	-6.417	-2.221	-0.157	1	2.007	2.772	-0.910
6	-3.829	4.068	-0.896	1	2.398	1.755	-2.307
6	6.044	0.444	0.608	1	1.058	1.335	-1.243
6	6.924	-0.171	-0.278	1	5.889	0.073	0.705
6	6.837	0.896	1.800	1	-3.693	2.209	0.151
6	6.491	-0.747	-1.460	1	-5.421	1.102	0.987
6	8.272	0.740	1.285	1	-6.308	-0.077	0.027
1	-1.914	-0.417	-1.645	1	-5.502	1.256	-0.783
1	-2.130	-2.563	0.359				
1	-1.901	-2.665	-1.384				
1	0.058	0.735	-0.961				
1	0.007	0.050	0.669				
1	0.301	-3.378	-0.731				
1	0.170	-2.523	0.821				
1	2.138	-1.118	0.603				
1	2.488	-2.159	-0.777				
1	2.579	-0.145	-2.268				
1	2.306	0.890	-0.874				
1	-4.110	-0.500	-1.947				
1	-4.705	1.582	1.238				
1	-4.256	-1.263	2.273				
1	-1.581	1.670	-1.701				
1	-2.146	2.070	1.910				
1	-1.526	1.169	3.262				
1	-6.193	-1.771	-2.251				
1	-5.353	3.872	0.614				
1	-6.361	-2.489	1.974				
1	-2.237	3.938	-2.332				
1	3.995	0.969	1.000				
1	4.757	-1.126	-2.663				
1	-7.341	-2.774	-0.288				
1	-4.120	5.073	-1.182				
1	6.622	1.922	2.109				
1	6.643	0.252	2.666				
1	7.191	-1.219	-2.140				
1	8.966	0.310	2.007				
1	8.680	1.697	0.937				
	Escitalopram			Chlordiazepoxide			
9	-1.197	5.330	-0.281	17	-2.808	3.494	-0.244
8	0.135	-0.450	1.737	8	1.296	-2.707	-0.270
7	-4.521	-1.908	-0.433	7	1.071	-1.452	-0.858
7	6.702	-1.770	-0.665	7	2.538	1.022	0.202
6	0.139	-0.114	0.332	7	4.064	-0.797	0.203
6	-0.793	-1.085	-0.413	6	0.027	-0.760	-0.352
6	1.576	-0.356	-0.071	6	0.074	0.649	-0.230
6	2.224	-1.050	0.944	6	2.269	-0.813	-1.367
6	-2.251	-0.979	0.004	6	1.291	1.432	0.019
6	-0.264	1.342	0.180	6	-1.170	-1.544	-0.004
6	1.253	-1.268	2.059	6	3.023	-0.173	-0.222
6	-3.088	-2.091	-0.606	6	-1.182	1.339	-0.292
6	2.237	-0.020	-1.243	6	1.101	2.849	0.200
6	3.547	-1.432	0.812	6	-1.622	-2.575	-0.837
6	-0.696	1.837	-1.053	6	-1.873	-1.267	1.173
6	-0.157	2.226	1.253	6	-1.267	2.686	-0.125
6	3.567	-0.390	-1.391	6	-0.109	3.462	0.132
6	4.224	-1.094	-0.370	6	-2.754	-3.302	-0.505

6	-1.008	3.181	-1.220	6	-3.000	-2.004	1.510
6	-0.472	3.572	1.107	6	-3.445	-3.022	0.672
6	-0.890	4.026	-0.131	6	4.709	-0.259	1.379
6	-4.910	-1.928	0.965	1	2.886	-1.569	-1.855
6	-5.251	-2.917	-1.174	1	1.939	-0.072	-2.102
6	5.589	-1.465	-0.533	1	-2.079	0.772	-0.506
1	-0.685	-0.935	-1.495	1	2.002	3.419	0.397
1	-0.420	-2.100	-0.223	1	-1.088	-2.785	-1.759
1	-2.300	-1.009	1.097	1	-1.520	-0.475	1.826
1	-2.666	-0.011	-0.300	1	-0.201	4.534	0.266
1	0.955	-2.326	2.136	1	-3.104	-4.088	-1.166
1	1.634	-0.963	3.040	1	-3.531	-1.786	2.430
1	-2.896	-2.137	-1.686	1	1.572	-3.274	-1.002
1	-2.756	-3.070	-0.196	1	-4.328	-3.595	0.932
1	1.734	0.536	-2.029	1	4.312	-0.737	2.283
1	4.067	-1.974	1.595	1	5.777	-0.489	1.343
1	-0.803	1.169	-1.903	1	4.568	0.823	1.494
1	0.165	1.847	2.216				
1	4.114	-0.135	-2.292				
1	-1.348	3.572	-2.172				
1	-0.399	4.265	1.937				
1	-4.449	-1.100	1.507				
1	-4.631	-2.871	1.474				
1	-5.993	-1.813	1.043				
1	-5.045	-3.946	-0.820				
1	-4.986	-2.867	-2.233				
1	-6.326	-2.741	-1.084				
	Dexmethylphenidate				Diethylcarbamazine		
8	0.126	2.255	0.632	8	0.737	0.565	1.684
8	-0.605	2.541	-1.480	7	-0.271	-0.884	0.219
7	2.339	0.377	-0.416	7	-2.996	-0.157	-0.284
6	1.115	-0.281	0.042	7	1.753	0.170	-0.341
6	1.235	-1.781	-0.209	6	-0.808	-0.858	-1.141
6	-0.090	0.304	-0.712	6	-1.319	-1.131	1.204
6	2.480	-2.356	0.454	6	-1.949	0.141	-1.248
6	3.721	-1.585	0.027	6	-2.451	-0.129	1.071
6	3.525	-0.103	0.291	6	0.737	-0.005	0.602
6	-1.398	-0.325	-0.277	6	-4.101	0.768	-0.417
6	-0.216	1.811	-0.604	6	2.692	1.251	-0.024
6	-1.845	-0.218	1.043	6	2.369	-1.026	-0.926
6	-2.170	-1.042	-1.192	6	2.062	2.618	-0.190
6	-3.032	-0.824	1.438	6	3.335	-1.726	0.017
6	-3.358	-1.648	-0.798	1	-1.169	-1.863	-1.392
6	-3.792	-1.542	0.519	1	-0.021	-0.590	-1.845
6	-0.057	3.661	0.834	1	-0.878	-1.080	2.198
1	0.958	-0.123	1.128	1	-1.703	-2.144	1.034
1	1.283	-1.946	-1.294	1	-1.542	1.165	-1.099
1	0.334	-2.287	0.151	1	-2.380	0.108	-2.255
1	0.052	0.107	-1.779	1	-3.255	-0.372	1.774
1	2.580	-3.421	0.221	1	-2.075	0.879	1.333
1	2.371	-2.289	1.545	1	-4.890	0.510	0.294
1	4.608	-1.945	0.557	1	-4.519	0.708	-1.426
1	3.901	-1.735	-1.044	1	-3.807	1.819	-0.232
1	2.252	1.376	-0.251	1	3.536	1.140	-0.714
1	3.448	0.058	1.384	1	3.087	1.136	0.994
1	4.387	0.474	-0.057	1	2.882	-0.719	-1.845
1	-1.258	0.347	1.761	1	1.583	-1.720	-1.224
1	-1.831	-1.127	-2.220	1	1.224	2.746	0.498
1	-3.366	-0.734	2.467	1	1.696	2.759	-1.211
1	-3.946	-2.204	-1.521	1	2.790	3.405	0.022
1	-4.719	-2.014	0.829	1	2.823	-2.042	0.931
1	-1.105	3.933	0.699	1	4.162	-1.074	0.307
1	0.546	4.234	0.127	1	3.762	-2.615	-0.454
1	0.261	3.859	1.855				
	Betaxolol				Dicyclomine		
8	-4.048	0.464	-0.234	8	-0.473	0.172	-0.004
8	1.749	-1.717	0.066	8	0.391	1.115	-1.851
8	4.530	-2.141	-0.345	7	-4.062	-0.556	-0.280
7	3.241	1.324	-0.042	6	1.842	0.706	0.072
6	-2.742	2.394	-0.681	6	2.265	-0.792	0.195
6	-1.506	3.208	-0.447	6	2.882	1.561	-0.668
6	-1.525	2.170	-1.530	6	1.598	1.306	1.470
6	-3.128	1.376	0.343	6	2.227	-1.552	-1.136
6	-4.453	-0.574	0.643	6	3.634	-0.996	0.852
6	-3.915	-1.922	0.175	6	2.526	3.045	-0.705
6	-2.416	-1.942	0.104	6	1.193	2.774	1.405
6	3.861	-0.949	-0.727	6	2.540	-3.032	-0.947
6	3.903	0.100	0.382	6	3.931	-2.477	1.065
6	2.533	2.076	1.000	6	2.257	3.598	0.689
6	2.442	-1.301	-1.103	6	3.879	-3.242	-0.251
6	-1.637	-2.175	1.244	6	0.536	0.719	-0.720
6	-1.751	-1.646	-1.082	6	-1.734	0.075	-0.687
6	0.394	-1.793	0.005	6	-2.733	-0.478	0.307
6	2.178	3.441	0.436	6	-4.734	0.742	-0.246

1	0.080	0.043	3.847				
1	3.850	-0.926	1.552				
1	3.402	0.845	-2.341				
	Dexchlorpheniramine				Chlorpheniramine		
17	-5.557	-0.189	-0.080	17	-5.557	-0.189	-0.080
7	3.089	-1.757	-0.107	7	3.089	-1.757	-0.107
7	1.000	1.784	0.908	7	1.000	1.784	0.908
6	0.490	-0.389	-0.065	6	0.490	-0.389	-0.065
6	1.033	-1.145	1.156	6	1.033	-1.145	1.156
6	2.551	-1.252	1.151	6	2.551	-1.252	1.151
6	-1.022	-0.323	-0.059	6	-1.022	-0.323	-0.059
6	1.126	0.983	-0.160	6	1.126	0.983	-0.160
6	-1.751	-0.870	-1.115	6	-1.751	-0.870	-1.115
6	-1.726	0.270	0.993	6	-1.726	0.270	0.993
6	1.834	1.367	-1.300	6	1.834	1.367	-1.300
6	2.730	-3.144	-0.333	6	2.730	-3.144	-0.333
6	4.526	-1.580	-0.160	6	4.526	-1.580	-0.160
6	-3.141	-0.836	-1.134	6	-3.141	-0.837	-1.134
6	-3.114	0.316	0.992	6	-3.114	0.316	0.992
6	2.419	2.625	-1.340	6	2.420	2.625	-1.340
6	-3.811	-0.241	-0.074	6	-3.811	-0.240	-0.074
6	1.563	2.991	0.854	6	1.564	2.991	0.854
6	2.281	3.462	-0.239	6	2.282	3.462	-0.239
1	0.795	-0.940	-0.961	1	0.795	-0.940	-0.961
1	0.728	-0.622	2.068	1	0.727	-0.622	2.068
1	0.565	-2.135	1.199	1	0.565	-2.135	1.198
1	2.883	-1.872	2.008	1	2.883	-1.873	2.008
1	2.980	-0.256	1.309	1	2.980	-0.256	1.309
1	-1.222	-1.335	-1.944	1	-1.222	-1.335	-1.943
1	-1.176	0.717	1.814	1	-1.176	0.718	1.814
1	1.930	0.675	-2.130	1	1.930	0.675	-2.131
1	1.645	-3.257	-0.389	1	1.645	-3.257	-0.389
1	3.099	-3.819	0.463	1	3.099	-3.819	0.463
1	3.150	-3.484	-1.283	1	3.150	-3.484	-1.283
1	4.770	-0.519	-0.055	1	4.770	-0.519	-0.055
1	4.909	-1.924	-1.124	1	4.909	-1.924	-1.124
1	5.062	-2.134	0.634	1	5.062	-2.134	0.634
1	-3.699	-1.266	-1.958	1	-3.699	-1.266	-1.957
1	-3.655	0.778	1.809	1	-3.655	0.779	1.808
1	2.977	2.946	-2.214	1	2.977	2.946	-2.214
1	1.438	3.615	1.737	1	1.438	3.615	1.737
1	2.721	4.453	-0.223	1	2.721	4.453	-0.223
	Desloratadine				Chlorpromazine		
17	-5.371	0.282	-0.161	17	4.929	0.566	-0.798
7	3.061	3.360	0.493	16	-0.383	-1.679	1.667
7	1.795	-1.640	-1.596	7	-0.189	0.120	-0.710
6	1.400	1.262	-0.511	7	-2.187	2.250	0.628
6	0.649	0.146	-0.406	6	-0.313	1.399	-1.400
6	2.892	1.234	-0.688	6	0.010	2.569	-0.474
6	0.869	2.656	-0.325	6	-0.763	2.478	0.835
6	3.581	2.001	0.438	6	1.054	-0.251	-0.181
6	1.636	3.365	0.791	6	-1.214	-0.839	-0.811
6	-0.830	0.162	-0.259	6	1.120	-1.143	0.904
6	1.258	-1.212	-0.447	6	-1.396	-1.778	0.216
6	-0.916	-1.334	1.869	6	2.247	0.255	-0.705
6	-1.535	-0.526	0.748	6	-2.066	-0.895	-1.918
6	0.606	-1.401	1.959	6	2.351	-1.527	1.424
6	1.231	-1.982	0.728	6	-2.403	-2.734	0.135
6	-1.569	0.854	-1.234	6	-2.862	3.434	0.138
6	-2.933	-0.468	0.753	6	-2.825	1.741	1.825
6	1.784	-3.256	0.679	6	3.462	-0.111	-0.139
6	-2.952	0.908	-1.225	6	-3.096	-1.827	-1.976
6	-3.628	0.238	-0.213	6	3.536	-1.002	0.921
6	2.335	-3.715	-0.511	6	-3.271	-2.749	-0.952
6	2.318	-2.869	-1.613	1	0.295	1.435	-2.316
1	3.276	0.215	-0.742	1	-1.356	1.485	-1.703
1	3.144	1.722	-1.639	1	-0.217	3.497	-1.010
1	1.005	3.229	-1.252	1	1.080	2.611	-0.245
1	-0.197	2.657	-0.092	1	-0.576	3.382	1.446
1	3.422	1.451	1.387	1	-0.381	1.628	1.412
1	4.660	2.041	0.264	1	2.235	0.932	-1.550
1	1.296	4.401	0.882	1	-1.921	-0.207	-2.742
1	1.405	2.858	1.749	1	2.380	-2.226	2.253
1	-1.308	-0.950	2.819	1	-2.515	-3.452	0.940
1	-1.304	-2.359	1.795	1	-3.917	3.212	-0.043
1	0.876	-2.001	2.834	1	-2.810	4.284	0.845
1	1.008	-0.395	2.131	1	-2.427	3.763	-0.810
1	3.560	3.892	1.196	1	-2.331	0.818	2.139
1	-1.025	1.351	-2.031	1	-3.874	1.513	1.617
1	-3.485	-0.986	1.532	1	-2.796	2.454	2.671
1	1.790	-3.879	1.570	1	-3.753	-1.838	-2.839
1	-3.498	1.446	-1.990	1	4.494	-1.276	1.345
1	2.774	-4.705	-0.584	1	-4.069	-3.482	-0.998
1	2.746	-3.190	-2.560				

	Brompheniramine				Chlorprothixene		
35	-5.074	-0.105	-0.049	17	1.770	4.024	-1.100
7	3.710	-1.783	-0.113	16	-2.655	0.479	1.592
7	1.675	1.784	0.910	7	4.152	-1.776	0.667
6	1.129	-0.381	-0.060	6	-0.522	-0.590	-0.372
6	1.668	-1.144	1.159	6	2.007	-1.004	-0.336
6	3.184	-1.271	1.148	6	-0.465	0.850	-0.066
6	-0.381	-0.297	-0.048	6	-1.870	-1.179	-0.488
6	1.782	0.983	-0.159	6	0.571	-1.370	-0.508
6	-1.122	-0.841	-1.098	6	2.780	-2.130	0.343
6	-1.074	0.310	1.004	6	-1.384	1.432	0.826
6	2.486	1.358	-1.304	6	-2.909	-0.767	0.364
6	3.331	-3.164	-0.338	6	0.485	1.681	-0.671
6	5.149	-1.625	-0.171	6	-2.154	-2.176	-1.429
6	-2.512	-0.792	-1.110	6	-1.291	2.786	1.151
6	-2.462	0.371	1.008	6	-4.165	-1.374	0.303
6	3.087	2.608	-1.348	6	0.562	3.024	-0.339
6	-3.173	-0.183	-0.052	6	-3.399	-2.783	-1.490
6	2.253	2.984	0.852	6	4.755	-2.802	1.495
6	2.969	3.446	-0.247	6	4.956	-1.544	-0.517
1	1.424	-0.936	-0.957	6	-0.311	3.587	0.586
1	1.372	-0.617	2.072	6	-4.406	-2.387	-0.613
1	1.187	-2.128	1.203	1	2.118	-0.086	0.250
1	3.511	-1.896	2.003	1	2.458	-0.793	-1.316
1	3.627	-0.280	1.304	1	2.275	-2.389	1.281
1	-0.602	-1.317	-1.926	1	2.736	-3.041	-0.292
1	-0.515	0.755	1.820	1	0.389	-2.426	-0.712
1	2.567	0.666	-2.136	1	1.160	1.274	-1.414
1	2.244	-3.262	-0.390	1	-1.373	-2.468	-2.124
1	3.694	-3.844	0.457	1	-2.004	3.220	1.845
1	3.742	-3.510	-1.289	1	-4.952	-1.040	0.972
1	5.409	-0.568	-0.067	1	-3.589	-3.556	-2.227
1	5.524	-1.974	-1.137	1	4.825	-3.782	0.987
1	5.680	-2.187	0.620	1	4.169	-2.937	2.408
1	-3.073	-1.221	-1.932	1	5.766	-2.501	1.782
1	-2.989	0.846	1.827	1	4.988	-2.422	-1.192
1	3.642	2.922	-2.227	1	5.982	-1.313	-0.221
1	2.143	3.609	1.737	1	4.579	-0.692	-1.084
1	3.421	4.432	-0.234	1	-0.241	4.639	0.836
				1	-5.386	-2.850	-0.657
	Acebutolol				Carprofen		
16	-0.783	-1.147	0.405	17	5.649	-0.991	-0.204
8	-0.651	-2.520	-0.210	8	-4.643	-0.746	-1.767
8	-4.549	-0.684	0.533	8	-4.834	1.268	-0.784
7	-3.503	-2.537	-0.284	7	0.489	1.760	0.142
6	0.421	-0.038	-0.543	6	0.372	-0.506	0.168
6	1.824	-0.495	-0.242	6	-0.383	0.691	0.213
6	0.126	1.404	-0.252	6	1.756	-0.121	0.067
6	-2.325	-0.419	-0.302	6	-2.420	-0.543	0.364
6	2.736	-0.593	-1.295	6	1.787	1.295	0.053
6	-0.413	2.216	-1.254	6	-3.933	-0.588	0.488
6	2.256	-0.801	1.050	6	-1.769	0.688	0.310
6	0.333	1.953	1.017	6	-0.298	-1.728	0.220
6	4.053	-0.968	-1.062	6	-1.682	-1.737	0.313
6	-0.733	3.543	-0.999	6	2.951	-0.836	-0.012
6	3.572	-1.182	1.284	6	2.981	2.001	-0.039
6	0.006	3.278	1.275	6	-4.429	0.059	1.775
6	4.476	-1.261	0.230	6	4.135	-0.122	-0.103
6	-0.527	4.078	0.268	6	-4.527	0.103	-0.720
6	-3.570	-1.222	0.051	6	4.163	1.277	-0.118
1	0.187	-0.262	-1.590	1	-4.238	-1.639	0.450
1	-2.435	0.593	0.087	1	-2.337	1.614	0.331
1	-2.184	-0.389	-1.388	1	0.218	2.729	0.147
1	2.406	-0.371	-2.306	1	0.254	-2.662	0.184
1	-0.580	1.798	-2.244	1	-2.214	-2.683	0.348
1	1.556	-0.767	1.880	1	2.964	-1.920	-0.004
1	0.759	1.341	1.806	1	3.000	3.085	-0.050
1	4.748	-1.038	-1.892	1	-3.974	-0.425	2.642
1	-1.144	4.161	-1.791	1	-4.171	1.119	1.799
1	3.889	-1.426	2.292	1	-5.515	-0.018	1.866
1	0.170	3.689	2.265	1	5.115	1.788	-0.190
1	5.502	-1.561	0.414	1	-4.973	-0.224	-2.512
1	-0.780	5.113	0.471				
1	-4.263	-3.125	0.021				
1	-2.597	-2.961	-0.463				
	Carteolol				Exemestane		
8	0.328	-1.393	-0.514	8	-4.887	-1.233	-0.895
8	2.553	-2.337	-2.150	8	5.385	-0.606	-1.330
8	-4.509	2.556	-0.881	6	-1.953	0.610	-0.423
7	2.885	0.141	0.584	6	-0.580	0.725	0.218
7	-3.936	0.572	0.049	6	-2.744	-0.602	0.089
6	2.984	1.610	0.750	6	0.207	-0.572	-0.073
6	2.864	-0.354	-0.783	6	-1.996	-1.873	-0.273
6	2.641	-1.864	-0.813	6	-0.578	-1.839	0.301

6	3.025	1.859	2.254	6	1.644	-0.516	0.556
6	4.275	2.109	0.111	6	-2.946	1.771	-0.345
6	1.777	2.340	0.147	6	0.179	1.949	-0.291
6	-1.770	-0.435	-0.211	6	-4.091	-0.380	-0.589
6	1.365	-2.276	-0.110	6	-4.257	1.124	-0.811
6	-1.491	0.567	-1.290	6	-3.044	-0.542	1.597
6	-0.856	-1.431	0.155	6	2.341	0.718	0.020
6	-3.012	-0.411	0.427	6	1.609	1.988	0.169
6	-2.191	1.889	-1.003	6	1.581	-0.392	2.097
6	-3.647	1.733	-0.639	6	2.409	-1.769	0.257
6	-1.173	-2.381	1.128	6	3.545	0.666	-0.583
6	-3.346	-1.354	1.403	6	3.603	-1.804	-0.345
6	-2.423	-2.331	1.739	6	2.188	3.084	0.669
1	2.096	0.106	-1.426	6	4.280	-0.581	-0.800
1	3.836	-0.146	-1.247	1	-1.779	0.421	-1.499
1	2.013	-0.135	1.030	1	-0.711	0.830	1.305
1	3.468	-2.360	-0.280	1	0.360	-0.598	-1.166
1	2.122	1.476	2.740	1	-1.949	-1.960	-1.366
1	3.089	2.928	2.475	1	-2.531	-2.760	0.081
1	3.886	1.359	2.704	1	-0.625	-1.937	1.392
1	4.253	2.030	-0.979	1	-0.037	-2.721	-0.053
1	5.133	1.540	0.479	1	-2.654	2.621	-0.966
1	4.435	3.162	0.355	1	-3.027	2.143	0.682
1	1.715	2.203	-0.936	1	-0.334	2.873	-0.007
1	1.830	3.416	0.336	1	0.172	1.914	-1.393
1	0.846	1.968	0.589	1	-4.433	1.280	-1.880
1	1.505	-2.221	0.978	1	-5.156	1.485	-0.305
1	1.115	-3.312	-0.370	1	-3.657	-1.402	1.880
1	-0.415	0.715	-1.403	1	-2.133	-0.568	2.200
1	-1.837	0.166	-2.254	1	-3.594	0.359	1.879
1	-2.128	2.584	-1.841	1	1.065	-1.246	2.543
1	-1.712	2.387	-0.149	1	2.592	-0.362	2.509
1	-4.884	0.502	0.395	1	1.073	0.523	2.409
1	-0.470	-3.159	1.396	1	1.967	-2.694	0.620
1	-4.317	-1.314	1.886	1	4.005	1.572	-0.969
1	-2.676	-3.070	2.491	1	4.132	-2.739	-0.507
1	3.340	-2.048	-2.621	1	1.640	4.016	0.767
				1	3.221	3.077	1.001
	Fenofibrate				Diphenhydramine		
17	-7.717	-2.016	0.076	8	0.840	0.334	-0.201
8	2.353	-0.008	-0.828	7	3.662	0.468	-0.164
8	5.692	-0.145	0.313	6	-0.339	0.003	0.515
8	4.636	-1.118	-1.432	6	-1.470	0.956	0.198
8	-3.182	2.859	0.243	6	-0.660	-1.447	0.218
6	3.376	0.234	0.159	6	1.447	1.531	0.232
6	3.597	1.726	0.370	6	2.824	1.636	-0.381
6	3.049	-0.468	1.474	6	-2.101	1.683	1.204
6	4.618	-0.428	-0.449	6	-1.943	-1.948	0.445
6	6.944	-0.793	-0.067	6	-1.885	1.127	-1.125
6	1.079	0.407	-0.558	6	0.337	-2.313	-0.235
6	0.169	-0.480	0.018	6	3.770	0.094	1.230
6	0.655	1.681	-0.948	6	4.966	0.674	-0.757
6	-1.585	1.179	-0.178	6	-3.139	2.562	0.902
6	8.044	0.058	0.517	6	-2.226	-3.292	0.227
6	6.939	-2.216	0.447	6	-2.913	2.008	-1.431
6	-1.153	-0.098	0.198	6	0.049	-3.655	-0.460
6	-0.659	2.065	-0.741	6	-3.546	2.725	-0.417
6	-2.969	1.669	0.062	6	-1.230	-4.150	-0.228
6	-4.104	0.700	0.077	1	-0.120	0.093	1.598
6	-5.245	1.032	0.816	1	0.850	2.410	-0.058
6	-4.110	-0.475	-0.681	1	1.502	1.541	1.334
6	-6.352	0.199	0.831	1	2.731	1.780	-1.464
6	-5.221	-1.308	-0.696	1	3.292	2.559	0.023
6	-6.329	-0.968	0.072	1	-1.776	1.557	2.235
1	2.699	2.186	0.789	1	-2.727	-1.279	0.788
1	3.834	2.223	-0.573	1	-1.389	0.562	-1.910
1	4.421	1.890	1.064	1	1.331	-1.920	-0.419
1	2.898	-1.540	1.318	1	2.800	-0.232	1.616
1	2.141	-0.050	1.915	1	4.145	0.911	1.877
1	3.866	-0.333	2.184	1	4.460	-0.748	1.324
1	6.984	-0.792	-1.162	1	5.568	-0.233	-0.662
1	0.509	-1.469	0.307	1	5.530	1.506	-0.291
1	1.365	2.349	-1.421	1	4.859	0.900	-1.821
1	7.977	0.087	1.608	1	-3.624	3.121	1.696
1	7.995	1.082	0.143	1	-3.228	-3.667	0.407
1	9.019	-0.356	0.250	1	-3.229	2.134	-2.461
1	6.841	-2.231	1.536	1	0.830	-4.318	-0.820
1	6.120	-2.789	0.010	1	-4.352	3.411	-0.657
1	7.875	-2.715	0.185	1	-1.452	-5.198	-0.405
1	-1.850	-0.790	0.660				
1	-0.999	3.057	-1.019				
1	-5.244	1.960	1.378				
1	-3.250	-0.729	-1.292				
1	-7.230	0.446	1.416				

1	-5.234	-2.209	-1.297				
	aminocaproic acid				Dydrogesterone		
8	-3.978	-0.687	0.000	8	-5.426	-0.193	0.145
8	-3.019	1.346	0.000	8	6.192	-0.389	-0.438
7	4.688	0.293	0.000	6	-2.132	-0.125	0.327
6	0.906	-0.545	0.000	6	-1.180	0.985	-0.159
6	-0.387	0.255	0.000	6	0.027	1.188	0.762
6	2.153	0.325	0.000	6	0.832	-0.112	1.008
6	-1.622	-0.626	0.000	6	-3.227	-0.001	-0.777
6	3.449	-0.477	0.000	6	-1.344	-1.430	0.355
6	-2.908	0.146	0.000	6	-2.100	2.172	-0.426
1	0.926	-1.211	0.874	6	-0.105	-1.314	1.253
1	0.926	-1.211	-0.874	6	2.000	-0.362	0.004
1	-0.417	0.920	0.871	6	-3.396	1.521	-0.953
1	-0.417	0.921	-0.870	6	-2.747	0.174	1.698
1	2.139	0.990	0.875	6	0.894	2.313	0.313
1	2.139	0.989	-0.876	6	2.860	0.893	-0.058
1	-1.635	-1.297	-0.869	6	2.864	-1.527	0.522
1	-1.635	-1.298	0.867	6	-4.513	-0.733	-0.444
1	3.468	-1.142	-0.873	6	1.532	-0.671	-1.427
1	3.468	-1.141	0.873	6	2.186	2.173	-0.022
1	4.707	0.908	0.809	6	4.189	-1.679	-0.210
1	4.707	0.908	-0.809	6	4.208	0.842	-0.207
1	-4.764	-0.124	0.001	6	4.979	-0.392	-0.289
				6	-4.589	-2.175	-0.873
				1	-0.806	0.643	-1.133
				1	-0.388	1.496	1.736
				1	1.358	0.054	1.960
				1	-2.803	-0.450	-1.686
				1	-1.062	-1.694	-0.672
				1	-1.961	-2.258	0.728
				1	-1.669	2.883	-1.135
				1	-2.284	2.729	0.500
				1	-0.454	-1.252	2.290
				1	0.460	-2.248	1.208
				1	-4.274	1.852	-0.393
				1	-3.583	1.769	-2.001
				1	-1.990	0.336	2.468
				1	-3.395	1.053	1.677
				1	-3.369	-0.664	2.029
				1	0.445	3.304	0.299
				1	2.307	-2.467	0.458
				1	3.062	-1.359	1.590
				1	0.996	0.169	-1.872
				1	2.386	-0.878	-2.078
				1	0.881	-1.548	-1.450
				1	2.778	3.048	-0.276
				1	4.027	-2.018	-1.241
				1	4.820	-2.442	0.252
				1	4.779	1.765	-0.283
				1	-4.712	-2.215	-1.960
				1	-3.660	-2.709	-0.652
				1	-5.435	-2.677	-0.406
	Difenoxin				Alosetron		
8	4.250	2.409	0.364	8	0.125	-1.864	1.199
8	3.522	1.843	-1.682	7	1.080	0.208	0.932
7	0.728	-0.121	0.708	7	-2.674	1.519	-0.183
7	-3.380	-0.292	3.208	7	2.805	-0.838	-1.190
6	3.594	0.131	0.051	7	4.952	-0.346	-1.383
6	3.039	0.192	1.478	6	-1.374	1.241	0.157
6	2.596	-0.666	-0.805	6	-0.275	2.212	0.368
6	1.618	0.723	1.498	6	-1.221	-0.111	0.359
6	1.176	-0.141	-0.683	6	1.043	1.468	0.194
6	-0.647	0.345	0.829	6	-2.494	-0.724	0.130
6	4.984	-0.504	-0.032	6	-3.381	0.324	-0.217
6	-1.650	-0.653	0.273	6	0.024	-0.698	0.841
6	3.752	1.532	-0.539	6	2.401	-0.325	1.224
6	-3.121	-0.291	0.593	6	-3.244	2.810	-0.474
6	5.680	-0.936	1.098	6	-2.978	-2.035	0.175
6	5.590	-0.659	-1.284	6	-4.719	0.103	-0.525
6	-4.121	-1.319	0.037	6	3.287	-0.394	0.022
6	-3.441	1.098	0.019	6	-4.313	-2.261	-0.128
6	6.936	-1.523	0.978	6	-5.173	-1.209	-0.475
6	6.845	-1.241	-1.404	6	4.620	-0.070	-0.070
6	-3.275	-0.287	2.054	6	5.607	0.437	0.913
6	7.523	-1.679	-0.271	6	3.826	-0.798	-2.007
6	-5.481	-1.124	0.294	1	-0.311	3.046	-0.341
6	-3.635	2.218	0.823	1	-0.345	2.652	1.374
6	-3.731	-2.418	-0.724	1	1.219	1.279	-0.876
6	-3.497	1.241	-1.369	1	1.875	2.085	0.549
6	-6.430	-2.006	-0.200	1	2.231	-1.322	1.642
6	-3.876	3.464	0.248	1	2.877	0.285	2.002
6	-4.685	-3.302	-1.225	1	-2.486	3.582	-0.353

6	-3.732	2.483	-1.942	1	-3.621	2.851	-1.501
6	-6.034	-3.100	-0.966	1	-4.072	3.032	0.206
6	-3.922	3.601	-1.133	1	-2.310	-2.845	0.445
1	3.037	-0.824	1.889	1	-5.385	0.918	-0.793
1	3.675	0.808	2.118	1	-4.704	-3.273	-0.096
1	2.898	-0.644	-1.854	1	-6.212	-1.422	-0.707
1	2.631	-1.710	-0.473	1	5.862	-0.224	-1.800
1	1.602	1.772	1.133	1	6.362	-0.313	1.173
1	1.242	0.747	2.526	1	6.139	1.320	0.546
1	0.508	-0.786	-1.262	1	5.105	0.719	1.839
1	1.109	0.870	-1.132	1	3.818	-1.073	-3.052
1	-0.783	1.331	0.341				
1	-0.848	0.499	1.896				
1	-1.423	-1.646	0.675				
1	-1.567	-0.717	-0.817				
1	5.246	-0.819	2.085				
1	5.075	-0.306	-2.174				
1	4.374	3.244	-0.109				
1	7.458	-1.856	1.870				
1	7.295	-1.350	-2.385				
1	8.503	-2.136	-0.362				
1	-5.792	-0.268	0.887				
1	-3.596	2.121	1.904				
1	-2.684	-2.601	-0.933				
1	-3.368	0.368	-2.004				
1	-7.481	-1.840	0.012				
1	-4.027	4.327	0.887				
1	-4.366	-4.153	-1.817				
1	-3.773	2.579	-3.022				
1	-6.775	-3.791	-1.355				
1	-4.109	4.572	-1.580				
	Chlorambucil				Cilostazol		
17	3.317	3.932	-0.303	8	-0.562	2.482	0.668
17	4.321	-3.231	-0.769	8	6.045	-1.110	-0.472
8	-5.266	-0.365	-2.465	7	-3.064	-1.296	0.052
8	-5.942	1.083	-0.885	7	-3.785	-2.407	0.336
7	2.157	0.080	0.048	7	-5.159	-0.757	-0.085
6	0.863	-0.136	0.516	7	-5.029	-2.063	0.256
6	-3.198	-0.783	1.947	7	4.392	0.413	-0.744
6	-1.785	-0.576	1.476	6	-1.599	-1.314	-0.045
6	-4.235	-0.060	1.085	6	-1.161	-1.487	-1.499
6	2.856	1.317	0.317	6	-1.007	-2.403	0.842
6	2.856	-0.931	-0.714	6	0.359	-1.490	-1.601
6	0.149	0.875	1.186	6	0.514	-2.420	0.726
6	0.217	-1.372	0.339	6	0.965	-2.576	-0.722
6	-1.138	0.649	1.650	6	-3.929	-0.294	-0.216
6	-1.075	-1.572	0.809	6	-3.533	1.095	-0.551
6	-4.234	-0.542	-0.354	6	-3.355	1.975	0.689
6	2.502	2.385	-0.705	6	-2.747	3.338	0.375
6	3.535	-1.940	0.198	6	-1.361	3.245	-0.228
6	-5.237	0.163	-1.216	6	2.604	0.734	0.849
1	-3.300	-0.438	2.982	6	3.429	-0.054	1.823
1	-3.421	-1.857	1.962	6	3.144	0.972	-0.426
1	-4.047	1.019	1.103	6	4.230	-1.141	1.119
1	-5.233	-0.192	1.515	6	0.656	2.045	0.244
1	2.634	1.675	1.327	6	1.362	1.259	1.160
1	3.934	1.130	0.293	6	4.996	-0.636	-0.082
1	2.170	-1.444	-1.396	6	2.454	1.767	-1.333
1	3.606	-0.446	-1.347	6	1.216	2.317	-1.004
1	0.594	1.850	1.347	1	-1.257	-0.331	0.316
1	0.720	-2.193	-0.159	1	-1.573	-2.435	-1.870
1	-1.654	1.457	2.164	1	-1.594	-0.695	-2.120
1	-1.541	-2.543	0.654	1	-1.421	-3.368	0.530
1	-3.247	-0.407	-0.815	1	-1.326	-2.254	1.877
1	-4.424	-1.620	-0.419	1	0.663	-1.618	-2.644
1	1.428	2.578	-0.724	1	0.745	-0.511	-1.285
1	2.823	2.100	-1.708	1	0.917	-1.480	1.127
1	2.817	-2.422	0.863	1	0.921	-3.223	1.349
1	4.312	-1.471	0.804	1	2.058	-2.549	-0.792
1	-5.923	0.143	-2.961	1	0.659	-3.563	-1.095
				1	-2.603	1.065	-1.129
				1	-4.297	1.520	-1.209
				1	-2.716	1.460	1.414
				1	-4.327	2.102	1.175
				1	-2.699	3.933	1.292
				1	-3.385	3.894	-0.322
				1	-0.917	4.239	-0.376
				1	-1.388	2.753	-1.210
				1	4.121	0.632	2.333
				1	2.798	-0.482	2.608
				1	3.556	-1.928	0.757
				1	4.943	-1.628	1.785
				1	0.917	1.074	2.134
				1	4.850	0.700	-1.598

				1	2.881	1.961	-2.313
				1	0.705	2.943	-1.724
	Drospirenone			Clidinium			
8	-4.201	-0.625	0.628	8	0.593	-1.257	-0.640
8	-6.301	-1.391	0.462	8	-0.650	-1.632	1.197
8	6.664	-0.754	-0.879	8	-1.516	-0.531	-2.033
6	-0.955	0.818	-0.322	7	3.222	0.132	0.772
6	-1.857	2.033	-0.293	6	2.890	-1.745	-0.946
6	-3.267	1.498	-0.222	6	2.110	-0.794	1.213
6	-1.767	-0.362	0.273	6	1.744	-1.740	0.062
6	0.473	0.878	0.206	6	4.494	-0.675	0.628
6	-3.192	-0.023	-0.239	6	2.850	0.714	-0.583
6	-2.700	2.312	0.908	6	4.191	-1.948	-0.166
6	1.235	2.069	-0.355	6	2.938	-0.381	-1.643
6	1.179	-0.447	-0.156	6	3.393	1.227	1.764
6	2.725	1.928	-0.569	6	-0.548	-1.174	0.089
6	-1.094	-1.627	-0.266	6	-1.555	-0.257	-0.635
6	2.170	2.828	0.521	6	-0.953	1.130	-0.404
6	2.646	-0.488	0.369	6	-2.961	-0.422	-0.096
6	0.357	-1.689	0.222	6	-0.756	1.588	0.903
6	-3.577	-0.549	-1.629	6	-3.804	0.677	0.072
6	3.411	0.651	-0.300	6	-0.536	1.918	-1.475
6	-1.787	-0.483	1.816	6	-3.469	-1.707	0.118
6	3.297	-1.824	-0.035	6	-0.148	2.818	1.133
6	-5.088	-0.654	-1.534	6	-5.128	0.495	0.458
6	2.710	-0.351	1.900	6	0.066	3.153	-1.241
6	-5.321	-0.948	-0.069	6	-4.791	-1.887	0.502
6	4.688	0.505	-0.725	6	0.269	3.604	0.060
6	4.804	-1.852	0.154	6	-5.623	-0.786	0.676
6	5.494	-0.695	-0.531	1	2.743	-2.544	-1.674
1	-0.857	0.580	-1.396	1	1.270	-0.165	1.511
1	-1.622	2.860	-0.957	1	2.471	-1.330	2.094
1	-4.062	1.953	-0.806	1	1.540	-2.736	0.464
1	0.433	0.981	1.297	1	4.863	-0.874	1.636
1	-2.462	1.869	1.863	1	5.212	-0.019	0.128
1	-3.097	3.318	0.986	1	3.532	1.549	-0.761
1	0.714	2.641	-1.118	1	1.837	1.111	-0.466
1	1.257	-0.447	-1.257	1	5.019	-2.160	-0.844
1	3.149	2.475	-1.405	1	4.107	-2.808	0.504
1	-1.093	-1.624	-1.363	1	2.109	-0.268	-2.342
1	-1.635	-2.527	0.052	1	3.866	-0.297	-2.216
1	2.270	2.509	1.552	1	3.550	0.793	2.751
1	2.296	3.894	0.371	1	4.257	1.829	1.480
1	0.372	-1.837	1.308	1	2.492	1.841	1.760
1	0.828	-2.578	-0.205	1	-2.302	-1.044	-2.248
1	-3.151	-1.542	-1.788	1	-1.104	0.986	1.740
1	-3.217	0.102	-2.429	1	-3.428	1.680	-0.103
1	-1.893	-1.535	2.093	1	-0.696	1.559	-2.485
1	-0.870	-0.121	2.283	1	-2.825	-2.574	-0.002
1	-2.628	0.026	2.277	1	-0.026	3.177	2.151
1	3.065	-2.015	-1.092	1	-5.773	1.357	0.587
1	2.840	-2.639	0.535	1	0.369	3.769	-2.081
1	-5.544	-1.423	-2.157	1	-5.171	-2.889	0.672
1	-5.593	0.289	-1.772	1	0.727	4.571	0.238
1	2.187	-1.180	2.385	1	-6.654	-0.926	0.979
1	3.746	-0.366	2.248				
1	2.267	0.575	2.267				
1	5.189	1.330	-1.226				
1	5.243	-2.783	-0.212				
1	5.066	-1.801	1.219				
	Acetophenazine			Citalopram			
16	2.123	0.509	-2.185	9	-1.197	5.330	-0.281
8	-6.291	-0.489	-1.293	8	0.135	-0.450	1.737
8	-3.042	3.613	0.783	7	-4.521	-1.908	-0.432
7	-0.242	-2.049	0.299	7	6.702	-1.770	-0.665
7	-3.040	-1.740	-0.175	6	0.139	-0.114	0.332
7	1.886	0.097	0.791	6	-0.793	-1.085	-0.413
6	-1.220	-2.594	1.224	6	1.576	-0.356	-0.071
6	-0.772	-2.064	-1.052	6	2.224	-1.050	0.944
6	-2.484	-1.761	1.169	6	-2.251	-0.979	0.003
6	-2.040	-1.238	-1.116	6	-0.264	1.342	0.180
6	1.080	-2.636	0.416	6	1.253	-1.268	2.059
6	1.782	-2.198	1.699	6	-3.088	-2.091	-0.607
6	-4.258	-0.946	-0.200	6	2.237	-0.020	-1.243
6	1.574	-0.709	1.967	6	3.547	-1.432	0.812
6	-5.004	-1.043	-1.515	6	-0.696	1.837	-1.053
6	0.918	0.956	0.246	6	-0.157	2.227	1.253
6	3.206	0.108	0.312	6	3.567	-0.390	-1.391
6	0.934	1.267	-1.125	6	4.224	-1.095	-0.370
6	3.470	0.352	-1.046	6	-1.008	3.181	-1.220
6	-0.093	1.520	1.028	6	-0.472	3.572	1.107
6	4.293	-0.135	1.159	6	-0.890	4.027	-0.131
6	-0.034	2.105	-1.679	6	-4.910	-1.928	0.965
6	-1.093	2.323	0.469	6	-5.251	-2.916	-1.174

6	4.776	0.389	-1.523	6	5.589	-1.465	-0.533
6	-1.055	2.615	-0.896	1	-0.685	-0.935	-1.495
6	5.594	-0.136	0.669	1	-0.420	-2.100	-0.224
6	5.844	0.133	-0.670	1	-2.300	-1.009	1.097
6	-2.207	2.881	1.285	1	-2.666	-0.011	-0.300
6	-2.284	2.507	2.745	1	0.955	-2.326	2.136
1	-1.456	-3.652	0.992	1	1.634	-0.964	3.040
1	-0.813	-2.570	2.241	1	-2.896	-2.137	-1.687
1	-0.020	-1.635	-1.723	1	-2.756	-3.070	-0.196
1	-0.983	-3.096	-1.398	1	1.734	0.536	-2.029
1	-3.239	-2.168	1.851	1	4.067	-1.974	1.595
1	-2.241	-0.733	1.515	1	-0.803	1.170	-1.903
1	-1.793	-0.179	-0.903	1	0.165	1.847	2.216
1	-2.450	-1.284	-2.130	1	4.114	-0.135	-2.292
1	1.064	-3.741	0.350	1	-1.348	3.572	-2.172
1	1.660	-2.282	-0.445	1	-0.399	4.265	1.937
1	1.412	-2.752	2.569	1	-4.449	-1.101	1.508
1	2.847	-2.442	1.621	1	-4.630	-2.872	1.473
1	-4.060	0.120	0.032	1	-5.993	-1.814	1.043
1	-4.923	-1.319	0.587	1	-5.045	-3.945	-0.821
1	0.520	-0.550	2.189	1	-4.986	-2.866	-2.233
1	2.137	-0.379	2.849	1	-6.326	-2.741	-1.083
1	-5.063	-2.099	-1.820				
1	-4.476	-0.494	-2.308				
1	-0.105	1.323	2.093				
1	4.120	-0.326	2.211				
1	0.013	2.330	-2.739				
1	4.947	0.597	-2.574				
1	-6.732	-0.403	-2.141				
1	-1.832	3.245	-1.315				
1	6.416	-0.338	1.348				
1	6.858	0.141	-1.054				
1	-1.389	2.832	3.284				
1	-2.353	1.421	2.867				
1	-3.159	2.974	3.193				
	Chenodiol				Diphenidol		
8	2.192	2.216	-1.281	8	1.362	-0.302	1.975
8	6.044	-0.765	-2.244	7	-3.497	-0.790	0.130
8	-7.732	-0.146	0.686	6	-3.843	0.565	-0.292
8	-5.972	1.243	0.553	6	-4.504	-1.738	-0.335
6	-0.148	0.828	-0.229	6	-2.178	-1.187	-0.339
6	-1.053	-0.353	0.179	6	-5.196	0.987	0.255
6	1.168	0.900	0.531	6	-5.880	-1.406	0.215
6	1.955	-0.410	0.327	6	-6.282	0.010	-0.169
6	3.298	-0.401	1.112	6	-1.034	-0.409	0.289
6	-2.283	-0.075	-0.726	6	0.314	-0.993	-0.100
6	4.139	0.817	0.647	6	1.512	-0.278	0.546
6	-0.264	-1.632	-0.110	6	1.522	1.189	0.137
6	1.087	-1.642	0.608	6	2.852	-0.921	0.187
6	1.994	2.131	0.137	6	1.784	1.524	-1.193
6	-1.078	2.035	-0.199	6	3.992	-0.485	0.870
6	-2.424	1.471	-0.689	6	1.242	2.206	1.047
6	3.364	2.129	0.796	6	2.997	-1.907	-0.788
6	4.124	-1.678	0.871	6	1.761	2.849	-1.609
6	-1.463	-0.285	1.654	6	5.240	-1.024	0.592
6	-3.605	-0.782	-0.402	6	1.222	3.534	0.631
6	4.710	0.642	-0.766	6	4.250	-2.449	-1.070
6	3.060	-0.315	2.625	6	1.478	3.861	-0.695
6	4.636	-1.838	-0.553	6	5.374	-2.011	-0.382
6	5.498	-0.645	-0.933	1	-3.852	0.633	-1.402
6	-4.688	-0.369	-1.411	1	-3.067	1.251	0.057
6	-3.480	-2.301	-0.361	1	-4.194	-2.741	-0.024
6	-6.106	-0.653	-0.947	1	-4.546	-1.751	-1.447
6	-6.550	0.259	0.162	1	-2.112	-1.118	-1.447
1	0.104	0.631	-1.286	1	-2.059	-2.252	-0.099
1	0.936	1.025	1.599	1	-5.425	2.003	-0.085
1	2.203	-0.435	-0.746	1	-5.138	1.023	1.350
1	-1.990	-0.378	-1.746	1	-5.857	-1.501	1.307
1	5.004	0.872	1.329	1	-6.608	-2.136	-0.154
1	-0.102	-1.700	-1.196	1	-7.247	0.279	0.274
1	-0.823	-2.529	0.172	1	-6.414	0.066	-1.259
1	0.918	-1.739	1.687	1	-1.145	-0.413	1.378
1	1.629	-2.547	0.314	1	-1.067	0.642	-0.019
1	1.450	3.031	0.468	1	0.425	-0.961	-1.192
1	-0.724	2.869	-0.815	1	0.356	-2.056	0.177
1	-1.157	2.429	0.821	1	1.473	-1.216	2.255
1	-3.247	1.759	-0.026	1	2.023	0.738	-1.907
1	-2.683	1.866	-1.674	1	3.884	0.287	1.627
1	3.216	2.345	1.860	1	1.037	1.948	2.079
1	3.950	2.962	0.393	1	2.134	-2.266	-1.339
1	3.557	-2.560	1.186	1	1.970	3.093	-2.646
1	4.992	-1.638	1.545	1	6.113	-0.672	1.133
1	-0.602	-0.272	2.327	1	1.004	4.318	1.350
1	-2.061	0.603	1.873	1	4.343	-3.217	-1.832

1	-2.067	-1.155	1.928	1	1.463	4.898	-1.017
1	-3.930	-0.428	0.588	1	6.349	-2.434	-0.602
1	3.900	0.657	-1.505				
1	5.347	1.500	-1.010				
1	4.016	-0.223	3.150				
1	2.446	0.537	2.925				
1	2.573	-1.218	3.005				
1	5.215	-2.761	-0.657				
1	3.799	-1.916	-1.262				
1	6.378	-0.626	-0.274				
1	-4.612	0.700	-1.625				
1	-4.506	-0.889	-2.360				
1	1.332	2.356	-1.688				
1	-3.001	-2.679	-1.272				
1	-2.890	-2.648	0.489				
1	-4.457	-2.787	-0.284				
1	5.317	-0.663	-2.866				
1	-6.826	-0.526	-1.764				
1	-6.245	-1.688	-0.616				
1	-7.965	0.497	1.370				
Doxylamine				Cevimeline			
8	0.496	-0.956	0.249	16	2.441	-1.153	-0.266
7	4.159	-0.974	0.201	8	0.904	0.837	0.517
7	-0.987	2.229	0.909	7	-2.344	0.401	0.897
6	-0.607	-0.190	0.744	6	0.001	-0.275	0.386
6	-1.867	-0.867	0.215	6	-0.710	-0.255	-0.982
6	-0.540	1.223	0.153	6	-1.089	-0.090	1.461
6	-0.621	-0.169	2.269	6	-1.898	-1.222	-0.932
6	1.774	-0.549	0.705	6	-1.259	1.156	-1.215
6	2.788	-1.146	-0.250	6	-2.931	-0.661	0.072
6	-3.112	-0.292	0.483	6	-2.061	1.563	0.043
6	-1.813	-2.042	-0.533	6	0.883	-1.503	0.603
6	-0.067	1.408	-1.149	6	2.012	0.672	-0.323
6	-4.280	-0.884	0.023	6	3.137	1.556	0.143
6	-2.986	-2.635	-0.994	1	-0.010	-0.550	-1.771
6	-0.046	2.690	-1.675	1	-1.291	-1.041	1.966
6	-4.221	-2.061	-0.718	1	-0.718	0.613	2.214
6	4.561	0.421	0.198	1	-1.567	-2.224	-0.639
6	5.062	-1.760	-0.616	1	-2.332	-1.326	-1.932
6	-0.968	3.458	0.384	1	-1.898	1.146	-2.105
6	-0.507	3.745	-0.893	1	-0.453	1.868	-1.411
1	0.230	0.388	2.668	1	-3.798	-0.236	-0.444
1	-0.590	-1.194	2.644	1	-3.310	-1.446	0.735
1	-1.523	0.317	2.638	1	-1.497	2.281	0.645
1	1.842	0.549	0.721	1	-3.012	2.034	-0.222
1	1.967	-0.908	1.726	1	1.072	-1.651	1.670
1	2.586	-2.219	-0.331	1	0.431	-2.411	0.200
1	2.629	-0.718	-1.262	1	1.742	0.894	-1.367
1	-3.160	0.635	1.051	1	4.018	1.423	-0.487
1	-0.850	-2.489	-0.746	1	2.835	2.606	0.090
1	0.274	0.551	-1.720	1	3.406	1.319	1.173
1	-5.239	-0.425	0.241				
1	-2.931	-3.552	-1.572				
1	0.318	2.866	-2.683				
1	-5.134	-2.526	-1.079				
1	3.960	1.002	0.901				
1	4.468	0.890	-0.801				
1	5.604	0.502	0.511				
1	6.083	-1.664	-0.239				
1	5.064	-1.450	-1.679				
1	4.781	-2.815	-0.574				
1	-1.341	4.254	1.026				
1	-0.511	4.764	-1.264				
Clemastine				Bromodiphenhydramine			
17	-2.359	4.820	-0.467	35	5.263	-0.894	-0.156
8	0.112	-1.315	0.107	8	-1.533	-0.730	0.056
7	4.730	-0.250	-0.940	7	-5.029	-1.799	-0.213
6	3.647	-0.112	0.035	6	-0.765	0.282	0.684
6	4.268	-0.684	1.313	6	0.698	-0.032	0.467
6	5.784	-0.471	1.147	6	-1.126	1.665	0.177
6	5.916	0.192	-0.220	6	-2.918	-0.638	0.340
6	2.366	-0.797	-0.406	6	-3.576	-1.867	-0.251
6	1.267	-0.679	0.627	6	1.664	0.791	1.049
6	4.521	0.485	-2.167	6	1.113	-1.114	-0.305
6	-1.125	-0.987	0.754	6	-1.561	2.657	1.051
6	-1.438	0.488	0.500	6	-1.033	1.952	-1.186
6	-2.188	-1.855	0.085	6	-5.604	-2.879	-0.989
6	-1.058	-1.339	2.240	6	-5.541	-1.826	1.145
6	-1.880	1.360	1.491	6	3.018	0.542	0.874
6	-1.290	0.980	-0.800	6	2.467	-1.373	-0.495
6	-3.537	-1.620	0.364	6	-1.892	3.924	0.577
6	-1.850	-2.897	-0.776	6	-1.371	3.211	-1.663
6	-2.169	2.692	1.204	6	3.411	-0.544	0.097
6	-1.567	2.304	-1.106	6	-1.798	4.202	-0.781

6	-4.527	-2.413	-0.200	1	-0.971	0.260	1.771
6	-2.844	-3.689	-1.345	1	-3.063	-0.579	1.431
6	-2.008	3.153	-0.094	1	-3.354	0.272	-0.098
6	-4.183	-3.453	-1.059	1	-3.267	-1.943	-1.298
1	3.434	0.970	0.194	1	-3.191	-2.773	0.260
1	4.030	-1.750	1.393	1	1.354	1.646	1.644
1	3.867	-0.201	2.208	1	0.368	-1.758	-0.757
1	6.214	0.146	1.939	1	-1.644	2.432	2.112
1	6.314	-1.427	1.165	1	-0.696	1.176	-1.869
1	5.924	1.297	-0.117	1	-6.693	-2.791	-0.997
1	6.824	-0.087	-0.764	1	-5.349	-3.881	-0.593
1	2.000	-0.364	-1.343	1	-5.251	-2.826	-2.022
1	2.575	-1.855	-0.606	1	-5.206	-0.950	1.705
1	1.570	-1.150	1.574	1	-5.229	-2.730	1.703
1	1.061	0.382	0.843	1	-6.633	-1.805	1.124
1	4.367	1.567	-1.990	1	3.762	1.184	1.331
1	3.653	0.101	-2.706	1	2.785	-2.216	-1.098
1	5.391	0.370	-2.819	1	-2.229	4.690	1.268
1	-0.360	-0.695	2.782	1	-1.297	3.425	-2.724
1	-0.735	-2.376	2.348	1	-2.058	5.187	-1.154
1	-2.039	-1.246	2.710				
1	-2.006	1.012	2.511				
1	-0.946	0.307	-1.579				
1	-3.813	-0.798	1.020				
1	-0.806	-3.079	-0.998				
1	-2.512	3.366	1.980				
1	-1.449	2.681	-2.115				
1	-5.570	-2.215	0.026				
1	-2.566	-4.496	-2.016				
1	-4.956	-4.071	-1.505				
Buclizine				Duloxetine			
17	-7.767	-2.307	0.071	16	2.370	2.128	0.389
7	-1.387	-0.089	0.001	8	-0.266	-0.796	0.089
7	1.187	-1.370	0.110	7	4.172	-2.560	0.317
6	-1.166	-1.432	-0.536	6	1.056	-0.369	0.437
6	-0.142	0.668	-0.128	6	1.945	-1.568	0.137
6	-0.051	-2.126	0.215	6	3.414	-1.324	0.426
6	0.978	-0.020	0.620	6	1.439	0.861	-0.335
6	-2.505	0.579	-0.670	6	-1.333	-0.046	0.482
6	2.281	-2.041	0.796	6	-2.596	-0.540	0.038
6	-3.801	-0.191	-0.491	6	-3.777	0.165	0.419
6	-2.705	1.992	-0.153	6	1.168	1.144	-1.646
6	3.620	-1.414	0.518	6	-1.257	1.094	1.253
6	7.529	0.316	-0.362	6	-2.711	-1.700	-0.761
6	6.168	-0.291	-0.023	6	-3.668	1.329	1.219
6	3.970	-1.021	-0.776	6	-2.436	1.774	1.620
6	4.554	-1.230	1.531	6	-5.028	-0.328	-0.022
6	-4.739	-0.232	-1.520	6	1.714	2.381	-2.071
6	-4.110	-0.816	0.719	6	2.397	3.025	-1.080
6	-2.923	3.042	-1.043	6	5.594	-2.355	0.518
6	-2.722	2.255	1.218	6	-3.943	-2.149	-1.172
6	5.216	-0.472	-1.036	6	-5.112	-1.457	-0.799
6	5.808	-0.682	1.266	1	1.092	-0.156	1.517
6	8.430	0.435	0.866	1	1.807	-1.837	-0.918
6	8.236	-0.572	-1.397	1	1.593	-2.417	0.731
6	7.329	1.718	-0.954	1	3.537	-0.946	1.452
6	-5.961	-0.874	-1.359	1	3.802	-0.526	-0.235
6	-5.323	-1.467	0.898	1	0.576	0.486	-2.271
6	-3.158	4.332	-0.576	1	4.018	-2.957	-0.605
6	-2.950	3.542	1.687	1	-0.301	1.486	1.575
6	-6.242	-1.488	-0.145	1	-1.808	-2.230	-1.042
6	-3.172	4.586	0.791	1	-4.572	1.859	1.502
1	-0.910	-1.385	-1.613	1	-2.352	2.669	2.228
1	-2.086	-2.014	-0.445	1	-5.926	0.210	0.268
1	0.141	0.779	-1.194	1	1.604	2.782	-3.071
1	-0.287	1.672	0.276	1	2.913	3.973	-1.121
1	-0.356	-2.257	1.273	1	6.131	-3.294	0.370
1	0.112	-3.125	-0.203	1	5.772	-2.034	1.549
1	1.906	0.548	0.504	1	6.040	-1.593	-0.144
1	0.735	-0.040	1.702	1	-4.018	-3.041	-1.785
1	-2.310	0.651	-1.760	1	-6.081	-1.820	-1.128
1	2.283	-3.085	0.452				
1	2.113	-2.082	1.891				
1	3.244	-1.142	-1.575				
1	4.299	-1.516	2.549				
1	-4.512	0.249	-2.469				
1	-3.377	-0.805	1.520				
1	-2.905	2.846	-2.112				
1	-2.538	1.441	1.913				
1	5.455	-0.176	-2.054				
1	6.504	-0.557	2.088				
1	9.393	0.869	0.581				
1	7.994	1.082	1.632				
1	8.632	-0.539	1.321				

1	7.655	-0.662	-2.318				
1	9.212	-0.152	-1.660				
1	8.397	-1.581	-1.007				
1	8.293	2.168	-1.209				
1	6.725	1.692	-1.865				
1	6.826	2.378	-0.242				
1	-6.686	-0.905	-2.163				
1	-5.559	-1.958	1.835				
1	-3.325	5.140	-1.281				
1	-2.954	3.735	2.755				
1	-3.352	5.591	1.158				
	Dexbrompheniramine				Bethanechol		
35	-5.074	-0.105	-0.049	8	1.381	0.446	-0.520
7	3.712	-1.781	-0.114	8	1.529	-1.101	1.144
7	1.672	1.783	0.910	7	-1.685	-0.312	-0.077
6	1.129	-0.383	-0.061	7	2.996	-1.083	-0.609
6	1.668	-1.146	1.158	6	-0.977	1.015	-0.320
6	3.184	-1.270	1.147	6	0.422	1.201	0.241
6	-0.381	-0.298	-0.049	6	-1.688	-0.664	1.383
6	1.781	0.982	-0.159	6	-3.100	-0.143	-0.544
6	-1.122	-0.837	-1.101	6	-1.063	-1.435	-0.856
6	-1.074	0.303	1.006	6	0.808	2.663	0.136
6	2.486	1.358	-1.303	6	1.959	-0.621	0.115
6	3.336	-3.163	-0.338	1	-0.977	1.164	-1.403
6	5.150	-1.620	-0.172	1	-1.630	1.771	0.124
6	-2.512	-0.787	-1.113	1	0.471	0.867	1.281
6	-2.462	0.365	1.010	1	-2.107	0.171	1.944
6	3.087	2.608	-1.346	1	-2.311	-1.548	1.517
6	-3.173	-0.183	-0.052	1	-0.666	-0.877	1.695
6	2.249	2.984	0.853	1	-3.096	0.118	-1.602
6	2.966	3.446	-0.245	1	-3.633	-1.080	-0.395
1	1.424	-0.937	-0.958	1	-3.574	0.650	0.034
1	1.372	-0.620	2.071	1	-0.937	-1.121	-1.891
1	1.189	-2.130	1.201	1	-0.110	-1.696	-0.406
1	3.513	-1.895	2.002	1	-1.734	-2.292	-0.804
1	3.626	-0.279	1.304	1	0.769	3.010	-0.900
1	-0.602	-1.309	-1.932	1	1.825	2.804	0.500
1	-0.515	0.745	1.825	1	0.145	3.288	0.737
1	2.569	0.666	-2.135	1	3.386	-0.524	-1.351
1	2.249	-3.263	-0.391	1	3.561	-1.810	-0.204
1	3.700	-3.842	0.456				
1	3.748	-3.507	-1.290				
1	5.408	-0.562	-0.067				
1	5.526	-1.968	-1.138				
1	5.683	-2.180	0.620				
1	-3.073	-1.212	-1.938				
1	-2.989	0.836	1.832				
1	3.642	2.923	-2.224				
1	2.137	3.609	1.737				
1	3.417	4.432	-0.231				
	Bexarotene				Acetaminophen		
8	-5.965	-1.557	-1.883	8	3.963	-0.236	0.000
8	-7.132	-0.469	-0.298	8	-2.509	-1.434	0.000
6	3.571	1.272	-0.958	7	-1.537	0.639	0.000
6	3.845	-1.589	0.132	6	-0.161	0.340	0.000
6	4.900	0.522	-0.793	6	0.348	-0.961	0.000
6	4.742	-0.975	-0.952	6	0.733	1.417	0.000
6	2.468	0.568	-0.170	6	1.723	-1.161	0.000
6	2.589	-0.742	0.320	6	2.102	1.213	0.000
6	3.778	2.706	-0.460	6	2.606	-0.086	0.000
6	3.173	1.321	-2.440	6	-2.611	-0.220	0.000
6	3.491	-3.015	-0.305	6	-3.953	0.470	0.000
6	4.603	-1.660	1.466	1	-0.332	-1.800	0.000
6	1.263	1.243	0.049	1	0.347	2.433	0.000
6	1.519	-1.277	1.049	1	-1.755	1.624	-0.001
6	0.191	0.693	0.747	1	2.111	-2.177	0.000
6	0.325	-0.605	1.277	1	2.791	2.050	0.000
6	-1.045	1.493	0.934	1	-4.517	0.147	0.877
6	-0.754	-1.249	2.097	1	-4.517	0.145	-0.876
6	-2.330	0.911	0.493	1	-3.900	1.560	-0.001
6	-0.983	2.735	1.440	1	4.171	-1.174	0.000
6	-3.537	1.232	1.131				
6	-2.369	0.023	-0.591				
6	-4.736	0.700	0.694				
6	-3.568	-0.509	-1.037				
6	-4.765	-0.175	-0.397				
6	-6.069	-0.720	-0.819				
1	5.315	0.747	0.198				
1	5.623	0.917	-1.516				
1	4.315	-1.199	-1.937				
1	5.718	-1.475	-0.929				
1	3.977	2.728	0.616				
1	4.636	3.158	-0.969				
1	2.915	3.348	-0.654				

1	3.938	1.839	-3.029				
1	3.040	0.321	-2.861				
1	2.229	1.857	-2.573				
1	4.405	-3.574	-0.528				
1	2.953	-3.570	0.467				
1	2.873	-3.011	-1.208				
1	5.501	-2.280	1.367				
1	4.912	-0.671	1.814				
1	3.978	-2.099	2.248				
1	1.135	2.244	-0.355				
1	1.625	-2.273	1.473				
1	-1.232	-0.534	2.773				
1	-1.552	-1.667	1.473				
1	-0.351	-2.066	2.699				
1	-0.040	3.157	1.770				
1	-1.863	3.365	1.524				
1	-3.521	1.887	1.997				
1	-1.440	-0.244	-1.087				
1	-5.671	0.937	1.190				
1	-3.586	-1.188	-1.882				
1	-6.865	-1.852	-2.077				
	Almotriptan				Diethylpropion		
16	2.097	0.036	0.791	8	-0.251	2.591	-0.087
8	2.292	0.997	1.862	7	1.462	-0.367	0.243
8	1.204	-1.103	0.917	6	1.247	0.801	-0.619
7	3.601	-0.571	0.428	6	1.426	-0.048	1.673
7	-3.617	2.923	0.111	6	2.646	-1.149	-0.094
7	-3.483	-3.017	0.010	6	-0.130	1.402	-0.317
6	3.726	-1.620	-0.604	6	2.333	1.867	-0.569
6	4.744	0.359	0.383	6	0.899	-1.206	2.500
6	4.901	-1.154	-1.452	6	2.648	-1.677	-1.514
6	5.767	-0.404	-0.445	6	-1.318	0.500	-0.302
6	1.578	0.966	-0.699	6	-1.323	-0.764	-0.903
6	0.220	1.558	-0.518	6	-2.480	0.961	0.324
6	-2.171	1.300	-0.433	6	-2.470	-1.546	-0.879
6	-0.906	0.759	-0.676	6	-3.620	0.170	0.367
6	-3.494	0.751	-0.477	6	-3.616	-1.085	-0.237
6	-2.279	2.660	-0.053	1	1.178	0.418	-1.648
6	0.083	2.903	-0.120	1	2.421	0.264	2.039
6	-3.823	-0.673	-0.771	1	0.773	0.819	1.819
6	-1.159	3.473	0.106	1	3.578	-0.581	0.095
6	-4.341	1.771	-0.136	1	2.674	-1.996	0.600
6	-3.369	-1.604	0.354	1	3.303	1.449	-0.849
6	-3.413	-3.838	1.205	1	2.104	2.688	-1.250
6	-2.445	-3.419	-0.923	1	2.417	2.296	0.432
1	2.795	-1.738	-1.166	1	-0.115	-1.468	2.188
1	3.927	-2.582	-0.119	1	1.520	-2.100	2.397
1	5.077	0.599	1.394	1	0.877	-0.947	3.561
1	4.473	1.306	-0.108	1	1.723	-2.216	-1.736
1	4.553	-0.465	-2.231	1	2.764	-0.883	-2.257
1	5.418	-1.978	-1.947	1	3.480	-2.370	-1.659
1	6.308	-1.114	0.189	1	-0.426	-1.135	-1.385
1	6.504	0.257	-0.906	1	-2.463	1.948	0.775
1	2.348	1.725	-0.861	1	-2.470	-2.521	-1.356
1	1.612	0.239	-1.516	1	-4.513	0.531	0.866
1	-0.795	-0.285	-0.958	1	-4.507	-1.704	-0.208
1	-4.897	-0.803	-0.935				
1	-3.337	-0.968	-1.709				
1	0.979	3.501	0.021				
1	-1.248	4.512	0.407				
1	-5.418	1.774	-0.048				
1	-4.009	3.803	0.398				
1	-3.996	-1.419	1.234				
1	-2.334	-1.350	0.660				
1	-4.218	-3.566	1.891				
1	-2.453	-3.733	1.745				
1	-3.534	-4.891	0.939				
1	-2.559	-4.478	-1.167				
1	-1.427	-3.267	-0.516				
1	-2.522	-2.857	-1.856				
	Calcitriol				Altretamine		
8	8.391	-2.064	-0.133	7	2.086	1.658	-0.098
8	-8.452	0.679	-0.098	7	-2.480	0.974	-0.099
8	-5.430	-1.433	1.966	7	0.395	-2.633	0.102
6	0.854	1.266	0.294	7	-0.205	1.365	-0.051
6	2.176	0.473	0.446	7	1.285	-0.505	0.000
6	0.076	0.305	-0.652	7	-1.080	-0.859	0.000
6	1.712	-1.003	0.538	6	1.016	0.808	-0.042
6	0.284	-1.069	-0.036	6	-1.208	0.475	-0.042
6	0.951	2.622	-0.411	6	0.192	-1.283	0.023
6	3.132	0.850	1.585	6	1.911	3.087	0.022
6	-1.295	0.805	-0.978	6	3.435	1.169	0.067
6	0.146	1.403	1.644	6	-3.626	0.110	0.065
6	-0.427	3.162	-0.795	6	-2.734	2.390	0.026

6	-1.249	2.164	-1.618	6	-0.705	-3.561	-0.027
6	4.338	-0.100	1.651	6	1.719	-3.196	-0.024
6	3.593	2.304	1.531	1	2.064	3.431	1.054
6	-2.418	0.101	-0.717	1	0.907	3.363	-0.288
6	5.237	-0.112	0.420	1	2.642	3.595	-0.614
6	6.429	-1.039	0.599	1	3.776	1.254	1.108
6	-3.774	0.533	-0.941	1	4.111	1.758	-0.558
6	7.381	-1.145	-0.591	1	3.487	0.124	-0.229
6	-4.901	-0.198	-0.775	1	-4.448	0.479	-0.555
6	-6.261	0.422	-0.948	1	-3.974	0.086	1.108
6	6.694	-1.728	-1.820	1	-3.372	-0.903	-0.236
6	8.032	0.193	-0.921	1	-2.985	2.670	1.058
6	-4.923	-1.620	-0.391	1	-3.578	2.665	-0.613
6	-7.178	0.131	0.231	1	-1.854	2.950	-0.278
6	-5.889	-1.972	0.719	1	-0.526	-4.426	0.617
6	-7.262	-1.370	0.479	1	-0.813	-3.923	-1.059
6	-4.177	-2.571	-0.964	1	-1.632	-3.076	0.267
1	2.716	0.609	-0.505	1	2.462	-2.465	0.282
1	0.651	0.330	-1.596	1	1.936	-3.502	-1.058
1	2.401	-1.666	0.005	1	1.797	-4.082	0.612
1	1.726	-1.336	1.582				
1	0.147	-1.877	-0.760				
1	-0.444	-1.245	0.763				
1	1.466	3.361	0.210				
1	1.562	2.500	-1.317				
1	2.582	0.709	2.528				
1	-0.902	1.690	1.528				
1	0.632	2.162	2.265				
1	0.160	0.466	2.210				
1	-0.984	3.423	0.113				
1	-0.317	4.096	-1.355				
1	-0.772	2.057	-2.605				
1	-2.248	2.563	-1.809				
1	4.944	0.174	2.525				
1	3.993	-1.123	1.846				
1	2.790	2.999	1.787				
1	4.410	2.482	2.237				
1	3.954	2.579	0.534				
1	-2.298	-0.889	-0.282				
1	4.655	-0.421	-0.458				
1	5.584	0.907	0.206				
1	7.019	-0.721	1.467				
1	6.078	-2.052	0.832				
1	-3.918	1.572	-1.233				
1	-6.752	0.011	-1.843				
1	-6.180	1.502	-1.099				
1	5.921	-1.060	-2.211				
1	7.417	-1.891	-2.626				
1	6.232	-2.690	-1.583				
1	8.785	0.072	-1.706				
1	7.303	0.922	-1.283				
1	8.528	0.607	-0.039				
1	-6.774	0.621	1.129				
1	-5.965	-3.068	0.792				
1	-7.902	-1.583	1.343				
1	-7.721	-1.846	-0.395				
1	9.027	-2.178	-0.845				
1	-4.251	-3.608	-0.647				
1	-3.492	-2.351	-1.777				
1	-9.024	0.576	0.667				
1	-4.501	-1.666	2.060				
	Clotrimazole				Ethchlorvynol		
17	1.491	-0.026	2.366	17	-3.103	-0.265	-0.183
7	-0.785	-0.069	-1.670	8	0.930	0.118	1.535
7	-1.952	-0.962	-3.352	6	0.994	-0.081	0.119
6	-0.221	0.030	-0.289	6	1.714	1.107	-0.559
6	0.816	-1.094	-0.088	6	1.040	2.440	-0.298
6	-1.433	-0.112	0.647	6	-0.422	-0.195	-0.388
6	0.505	1.388	-0.168	6	1.718	-1.321	-0.183
6	1.630	-1.174	1.054	6	-1.479	-0.158	0.410
6	1.028	-2.066	-1.070	6	2.343	-2.322	-0.425
6	-2.545	0.710	0.427	1	2.748	1.114	-0.194
6	-0.012	2.477	0.531	1	1.776	0.899	-1.634
6	-1.516	-1.080	1.646	1	0.038	2.474	-0.733
6	1.762	1.524	-0.767	1	1.619	3.258	-0.730
6	-0.344	0.535	-2.830	1	0.940	2.624	0.773
6	-1.746	-0.967	-2.055	1	-0.532	-0.299	-1.463
6	-1.081	-0.023	-3.840	1	1.806	-0.058	1.891
6	2.586	-2.172	1.210	1	-1.411	-0.058	1.485
6	1.980	-3.068	-0.927	1	2.881	-3.214	-0.634
6	-3.686	0.596	1.208				
6	0.698	3.671	0.615				
6	-2.663	-1.199	2.428				
6	2.470	2.716	-0.688				

6	2.763	-3.124	0.217				
6	-3.747	-0.359	2.219				
6	1.939	3.799	0.005				
1	0.439	-2.036	-1.979				
1	-2.521	1.431	-0.384				
1	-0.958	2.394	1.052				
1	-0.694	-1.765	1.815				
1	2.197	0.680	-1.294				
1	0.401	1.311	-2.828				
1	-2.256	-1.593	-1.337				
1	-1.040	0.215	-4.893				
1	3.185	-2.188	2.113				
1	2.108	-3.799	-1.718				
1	-4.535	1.245	1.016				
1	0.278	4.501	1.175				
1	-2.705	-1.962	3.198				
1	3.444	2.794	-1.161				
1	3.512	-3.899	0.342				
1	-4.641	-0.455	2.827				
1	2.492	4.729	0.076				
	Albuterol				Cycrimine		
8	0.454	3.201	0.075	8	-2.067	0.146	1.867
8	-3.340	-1.787	0.732	7	2.291	-1.119	0.161
8	-4.547	-0.098	-1.025	6	-2.183	-0.860	-0.346
7	2.590	0.196	0.488	6	-1.326	-0.061	0.650
6	2.872	-0.966	-0.380	6	-2.528	-2.284	0.133
6	2.058	1.395	-0.137	6	-3.546	-0.190	-0.657
6	0.888	1.980	0.670	6	-3.915	-2.554	-0.439
6	3.508	-2.019	0.522	6	-4.613	-1.211	-0.256
6	1.556	-1.505	-0.936	6	-0.024	-0.804	0.998
6	3.829	-0.621	-1.527	6	0.876	-1.130	-0.193
6	-0.275	1.031	0.712	6	-0.978	1.337	0.153
6	-1.224	1.026	-0.306	6	2.782	0.253	0.283
6	-0.384	0.078	1.724	6	3.083	-1.848	-0.825
6	-2.259	0.093	-0.342	6	4.231	0.280	0.738
6	-2.356	-0.850	0.695	6	4.545	-1.908	-0.418
6	-1.415	-0.850	1.722	6	5.109	-0.507	-0.225
6	-3.200	0.052	-1.504	6	-0.949	1.675	-1.201
1	2.824	2.179	-0.268	6	-0.590	2.304	1.085
1	1.683	1.174	-1.143	6	-0.534	2.939	-1.613
1	3.431	0.422	1.008	6	-0.178	3.566	0.676
1	1.237	2.159	1.701	6	-0.144	3.888	-0.677
1	4.448	-1.655	0.950	1	-1.605	-0.958	-1.273
1	3.732	-2.931	-0.037	1	-2.591	-2.320	1.230
1	2.836	-2.274	1.345	1	-1.778	-3.024	-0.158
1	1.059	-0.784	-1.591	1	-3.621	0.039	-1.725
1	0.864	-1.748	-0.126	1	-3.657	0.757	-0.123
1	1.737	-2.409	-1.526	1	-4.428	-3.390	0.044
1	3.407	0.145	-2.184	1	-3.839	-2.796	-1.507
1	4.042	-1.498	-2.145	1	-5.539	-1.115	-0.829
1	4.782	-0.245	-1.142	1	-4.874	-1.079	0.801
1	-1.155	1.770	-1.096	1	0.520	-0.190	1.720
1	0.352	0.065	2.522	1	-0.276	-1.732	1.527
1	1.227	3.759	-0.045	1	0.682	-0.426	-1.027
1	-1.515	-1.583	2.515	1	0.633	-2.126	-0.580
1	-3.102	0.969	-2.098	1	2.146	0.799	0.986
1	-2.956	-0.798	-2.161	1	2.685	0.781	-0.691
1	-4.055	-1.481	0.151	1	2.999	-1.373	-1.827
1	-5.127	-0.211	-1.783	1	2.666	-2.856	-0.919
				1	-2.108	-0.699	2.325
				1	4.296	-0.157	1.741
				1	4.569	1.318	0.819
				1	5.114	-2.460	-1.173
				1	4.627	-2.471	0.520
				1	5.133	0.009	-1.195
				1	6.144	-0.547	0.130
				1	-1.252	0.953	-1.951
				1	-0.625	2.055	2.140
				1	-0.519	3.179	-2.672
				1	0.116	4.303	1.418
				1	0.178	4.873	-0.999
	Diphenylpyraline				Dronabinol		
8	0.145	-0.935	0.263	8	-0.734	1.871	-0.647
7	4.296	-0.954	-0.233	8	-0.501	-2.598	1.037
6	1.477	-0.431	0.195	6	-2.848	0.885	-0.094
6	2.082	-0.501	-1.200	6	-2.203	-0.371	0.500
6	2.300	-1.259	1.161	6	-1.962	2.112	0.100
6	3.549	-0.108	-1.153	6	-4.278	0.989	0.419
6	3.759	-0.842	1.117	6	-0.743	-0.435	0.115
6	-0.822	-0.232	-0.500	6	-5.102	-0.178	-0.117
6	5.705	-0.625	-0.257	6	-3.042	-1.564	0.104
6	-2.155	-0.922	-0.314	6	-4.349	-1.479	-0.169
6	-0.902	1.232	-0.110	6	-0.109	0.677	-0.461
6	-3.228	-0.552	-1.127	6	-2.542	3.352	-0.554

6	-0.754	2.237	-1.063	6	-1.601	2.382	1.554
6	-2.350	-1.897	0.662	6	0.067	-1.554	0.355
6	-1.123	1.588	1.222	6	1.222	0.628	-0.885
6	-4.474	-1.145	-0.971	6	-5.154	-2.674	-0.565
6	-0.832	3.579	-0.699	6	1.979	-0.521	-0.704
6	-3.599	-2.491	0.820	6	1.393	-1.611	-0.058
6	-1.194	2.924	1.590	6	3.425	-0.562	-1.110
6	-4.663	-2.119	0.007	6	4.370	-0.149	0.019
6	-1.051	3.924	0.629	6	5.835	-0.185	-0.383
1	1.484	0.623	0.529	6	6.783	0.225	0.734
1	1.555	0.166	-1.891	6	8.244	0.187	0.322
1	1.980	-1.523	-1.582	1	-2.896	0.736	-1.185
1	2.209	-2.315	0.883	1	-2.252	-0.289	1.601
1	1.902	-1.152	2.174	1	-4.741	1.937	0.127
1	4.000	-0.198	-2.147	1	-4.270	0.970	1.517
1	3.637	0.962	-0.864	1	-5.461	0.053	-1.132
1	3.863	0.198	1.496	1	-6.017	-0.308	0.477
1	4.357	-1.476	1.779	1	-2.556	-2.532	0.061
1	-0.563	-0.280	-1.572	1	-2.868	3.141	-1.575
1	6.102	-0.751	-1.268	1	-3.395	3.731	0.013
1	6.256	-1.293	0.410	1	-1.786	4.138	-0.593
1	5.910	0.416	0.060	1	-1.002	3.293	1.633
1	-3.084	0.214	-1.886	1	-2.503	2.516	2.157
1	-0.574	1.963	-2.101	1	-1.023	1.562	1.985
1	-1.514	-2.190	1.287	1	1.649	1.513	-1.345
1	-1.236	0.803	1.966	1	-5.627	-2.527	-1.544
1	-5.298	-0.849	-1.612	1	-5.971	-2.858	0.142
1	-0.717	4.352	-1.451	1	-4.545	-3.578	-0.619
1	-3.739	-3.251	1.582	1	1.976	-2.510	0.133
1	-1.365	3.192	2.628	1	3.689	-1.573	-1.445
1	-5.636	-2.585	0.131	1	3.585	0.098	-1.971
1	-1.110	4.969	0.918	1	4.206	-0.804	0.885
				1	4.102	0.860	0.359
				1	0.166	-3.282	1.148
				1	6.095	-1.196	-0.729
				1	5.992	0.469	-1.253
				1	6.624	-0.430	1.601
				1	6.520	1.234	1.078
				1	8.437	0.859	-0.520
				1	8.908	0.484	1.137
				1	8.541	-0.818	0.007
Cinacalcet				Chlorphentermine			
9	-7.114	1.304	0.405	17	4.122	0.010	0.389
9	-5.233	2.017	1.212	7	-4.070	0.049	-0.414
9	-5.689	2.311	-0.880	6	-2.718	0.010	0.172
7	1.434	-1.468	1.092	6	-1.750	-0.023	-1.033
6	2.880	-1.464	0.878	6	-2.507	-1.209	1.072
6	0.664	-1.299	-0.131	6	-2.540	1.289	0.980
6	3.390	-0.060	0.604	6	-0.288	-0.018	-0.696
6	-0.825	-1.275	0.158	6	0.412	1.183	-0.545
6	-1.665	-1.087	-1.105	6	0.418	-1.209	-0.510
6	4.634	0.143	-0.068	6	1.760	1.204	-0.212
6	3.565	-2.049	2.109	6	1.767	-1.214	-0.177
6	5.103	1.482	-0.271	6	2.428	-0.001	-0.027
6	-3.138	-1.073	-0.815	1	-1.984	-0.918	-1.624
6	2.679	1.034	1.048	1	-1.995	0.837	-1.666
6	5.444	-0.920	-0.543	1	-1.506	-1.228	1.514
6	4.330	2.569	0.199	1	-3.230	-1.206	1.893
6	3.143	2.348	0.848	1	-2.643	-2.140	0.512
6	-3.793	0.115	-0.503	1	-1.547	1.342	1.433
6	6.334	1.692	-0.936	1	-3.274	1.335	1.791
6	-3.878	-2.260	-0.800	1	-2.685	2.170	0.349
6	-5.151	0.119	-0.188	1	-4.757	0.076	0.335
6	6.637	-0.681	-1.183	1	-4.247	-0.821	-0.912
6	7.089	0.637	-1.384	1	-0.109	2.124	-0.699
6	-5.231	-2.258	-0.486	1	-0.097	-2.158	-0.634
6	-5.877	-1.066	-0.177	1	2.293	2.141	-0.101
6	-5.802	1.427	0.137	1	2.305	-2.144	-0.039
1	3.134	-2.094	0.006				
1	0.890	-2.078	-0.885				
1	0.965	-0.347	-0.588				
1	-1.042	-0.474	0.874				
1	-1.124	-2.209	0.654				
1	1.175	-2.347	1.530				
1	-1.374	-0.150	-1.595				
1	-1.436	-1.889	-1.817				
1	4.651	-2.031	2.003				
1	3.259	-3.087	2.276				
1	3.302	-1.466	2.995				
1	1.739	0.858	1.563				
1	5.121	-1.945	-0.402				
1	4.698	3.579	0.038				
1	2.554	3.184	1.211				
1	-3.242	1.052	-0.509				

1	6.673	2.714	-1.083				
1	-3.382	-3.196	-1.043				
1	7.235	-1.515	-1.537				
1	8.032	0.815	-1.890				
1	-5.789	-3.188	-0.485				
1	-6.933	-1.053	0.065				
	Bepridil				Dextromethorphan		
8	-1.949	1.415	-0.546	8	-4.054	0.120	0.653
7	-2.789	-1.128	0.625	7	2.681	-1.422	0.510
7	0.806	-0.705	-0.349	6	0.773	0.755	0.735
6	-1.686	-0.955	-0.312	6	1.930	0.754	-0.286
6	-4.129	-0.970	0.071	6	2.238	-0.685	-0.684
6	-2.816	-2.449	1.247	6	1.232	-0.072	1.952
6	-5.035	-1.475	1.188	6	0.519	2.206	1.168
6	-4.178	-2.516	1.935	6	1.640	1.667	-1.476
6	-0.383	-0.762	0.481	6	-0.457	0.084	0.128
6	-1.889	0.204	-1.269	6	1.036	-1.288	-1.425
6	1.355	0.602	-0.631	6	1.678	-1.470	1.567
6	1.509	-1.855	-0.673	6	0.224	3.130	-0.006
6	-2.027	2.548	-1.384	6	1.360	3.094	-1.022
6	-1.940	3.806	-0.538	6	-0.310	-0.910	-0.858
6	2.423	1.098	0.321	6	-1.733	0.382	0.600
6	2.794	-1.788	-1.248	6	3.191	-2.740	0.208
6	0.964	-3.134	-0.443	6	-1.452	-1.549	-1.337
6	-0.627	3.854	0.234	6	-2.864	-0.268	0.110
6	-2.113	5.034	-1.420	6	-2.727	-1.246	-0.873
6	3.084	2.295	0.036	6	-5.217	-0.520	0.178
6	2.753	0.411	1.487	1	2.816	1.143	0.237
6	3.482	-2.945	-1.584	1	3.098	-0.691	-1.368
6	1.671	-4.280	-0.779	1	0.423	-0.128	2.689
6	2.934	-4.203	-1.356	1	2.070	0.454	2.426
6	4.048	2.799	0.899	1	1.426	2.555	1.680
6	3.721	0.913	2.353	1	-0.277	2.253	1.919
6	4.370	2.108	2.064	1	0.768	1.295	-2.030
1	-1.583	-1.854	-0.957	1	2.483	1.640	-2.176
1	-4.318	0.073	-0.197	1	1.128	-2.380	-1.464
1	-4.263	-1.583	-0.844	1	1.081	-0.966	-2.475
1	-2.730	-3.242	0.475	1	2.128	-1.972	2.431
1	-1.981	-2.584	1.939	1	0.803	-2.087	1.277
1	-5.967	-1.891	0.798	1	0.059	4.152	0.350
1	-5.305	-0.652	1.852	1	-0.711	2.819	-0.491
1	-4.093	-2.263	2.994	1	1.129	3.732	-1.882
1	-4.599	-3.522	1.883	1	2.268	3.513	-0.563
1	-0.273	-1.555	1.226	1	-1.884	1.134	1.367
1	-0.467	0.175	1.039	1	2.419	-3.463	-0.116
1	-1.043	0.224	-1.976	1	3.671	-3.159	1.098
1	-2.799	0.068	-1.873	1	3.944	-2.676	-0.583
1	0.520	1.313	-0.618	1	-1.341	-2.316	-2.100
1	1.742	0.624	-1.659	1	-3.587	-1.770	-1.273
1	-2.966	2.528	-1.963	1	-5.192	-1.600	0.368
1	-1.199	2.529	-2.119	1	-5.362	-0.353	-0.897
1	-2.767	3.767	0.184	1	-6.052	-0.081	0.723
1	3.269	-0.828	-1.411				
1	-0.026	-3.237	-0.014				
1	0.226	3.879	-0.455				
1	-0.508	2.982	0.882				
1	-0.566	4.748	0.859				
1	-1.309	5.102	-2.161				
1	-2.086	5.952	-0.828				
1	-3.062	5.018	-1.963				
1	2.838	2.836	-0.875				
1	2.257	-0.528	1.712				
1	4.472	-2.855	-2.022				
1	1.218	-5.248	-0.590				
1	3.480	-5.102	-1.618				
1	4.552	3.731	0.662				
1	3.971	0.365	3.256				
1	5.125	2.497	2.739				
	Danazol				Biperiden		
8	-5.062	-1.185	0.629	8	-1.712	0.358	1.862
8	5.684	0.255	-0.613	7	2.426	-1.276	0.170
7	6.168	-1.050	-0.435	6	-1.961	-0.482	-0.430
6	-2.101	0.756	-0.233	6	-2.589	-1.861	-0.047
6	-2.748	-0.444	0.472	6	-4.358	-0.706	-0.790
6	-0.684	1.043	0.238	6	-3.206	0.337	-0.859
6	0.181	-0.216	0.027	6	-3.609	-1.985	-1.189
6	1.669	-0.034	0.456	6	-1.041	0.175	0.609
6	-1.911	-1.685	0.188	6	-3.525	-1.661	1.125
6	-4.165	-0.403	-0.165	6	-4.587	-0.983	0.678
6	-0.463	-1.474	0.631	6	0.136	-0.743	0.970
6	-3.153	1.865	-0.137	6	-0.492	1.523	0.130
6	-0.075	2.224	-0.505	6	1.021	-1.155	-0.203
6	-4.503	1.118	-0.148	6	-0.377	1.878	-1.216
6	2.227	1.274	-0.119	6	-0.008	2.419	1.089

6	-2.901	-0.232	1.982	6	3.038	0.045	0.315
6	1.348	2.485	-0.037	6	3.161	-2.061	-0.816
6	2.458	-1.285	-0.026	6	4.478	-0.065	0.786
6	1.821	0.080	1.985	6	4.607	-2.259	-0.394
6	-4.173	-0.905	-1.539	6	5.293	-0.917	-0.177
6	3.508	1.390	-0.526	6	0.203	3.087	-1.592
6	3.915	-1.021	-0.163	6	0.573	3.625	0.718
6	4.353	0.239	-0.447	6	0.683	3.964	-0.628
6	5.101	-1.780	-0.176	1	-1.346	-0.669	-1.319
6	-4.240	-1.309	-2.673	1	-1.858	-2.666	0.052
1	-2.023	0.472	-1.297	1	-5.240	-0.439	-1.374
1	-0.710	1.292	1.311	1	-3.091	0.739	-1.870
1	0.208	-0.368	-1.067	1	-3.399	1.198	-0.208
1	-1.935	-1.892	-0.889	1	-4.229	-2.881	-1.110
1	-2.336	-2.564	0.685	1	-3.155	-1.936	-2.185
1	-0.420	-1.423	1.724	1	-3.297	-1.928	2.149
1	0.121	-2.357	0.353	1	-5.406	-0.582	1.265
1	-3.069	2.587	-0.953	1	0.733	-0.221	1.724
1	-3.029	2.431	0.794	1	-0.265	-1.627	1.476
1	-0.685	3.123	-0.362	1	0.911	-0.441	-1.045
1	-0.084	2.011	-1.583	1	0.695	-2.126	-0.593
1	-5.085	1.314	0.756	1	-2.571	0.759	1.684
1	-5.131	1.392	-0.998	1	2.446	0.636	1.021
1	-3.498	0.649	2.223	1	3.000	0.592	-0.652
1	-3.397	-1.093	2.434	1	3.133	-1.569	-1.813
1	-1.931	-0.109	2.468	1	2.656	-3.026	-0.928
1	1.306	2.810	1.014	1	-0.739	1.210	-1.991
1	1.809	3.311	-0.586	1	-0.100	2.155	2.138
1	2.057	-1.606	-0.999	1	4.908	0.936	0.885
1	2.269	-2.114	0.663	1	4.492	-0.519	1.784
1	1.264	0.926	2.395	1	4.626	-2.838	0.537
1	1.474	-0.825	2.488	1	5.133	-2.851	-1.149
1	2.874	0.218	2.248	1	5.376	-0.394	-1.140
1	3.911	2.342	-0.858	1	6.316	-1.055	0.189
1	-5.855	-1.344	0.109	1	0.280	3.341	-2.645
1	5.243	-2.840	-0.007	1	0.941	4.303	1.481
1	-4.289	-1.673	-3.670	1	1.136	4.906	-0.921
Atomoxetine				Chlophedianol			
8	0.662	1.126	0.220	17	0.612	0.577	2.207
7	-4.045	1.954	0.059	8	0.029	-0.397	-2.221
6	-0.521	0.556	-0.348	7	-3.326	-1.751	-0.138
6	-1.660	1.429	0.161	6	0.176	-0.340	-0.786
6	-0.686	-0.895	0.036	6	-0.903	-1.236	-0.156
6	-3.016	1.033	-0.391	6	-2.315	-0.740	-0.420
6	1.883	0.683	-0.206	6	-0.046	1.125	-0.413
6	-0.348	-1.329	1.318	6	1.601	-0.782	-0.459
6	-1.227	-1.809	-0.867	6	0.109	1.616	0.889
6	2.976	1.201	0.512	6	-0.452	2.043	-1.386
6	-0.548	-2.654	1.688	6	2.660	0.031	-0.875
6	-1.435	-3.133	-0.498	6	1.896	-1.987	0.177
6	2.079	-0.198	-1.267	6	-3.363	-2.100	1.270
6	-1.096	-3.558	0.782	6	-4.629	-1.290	-0.575
6	-5.355	1.624	-0.468	6	-0.124	2.949	1.207
6	4.254	0.819	0.122	6	-0.692	3.377	-1.083
6	2.738	2.133	1.657	6	3.977	-0.343	-0.649
6	3.373	-0.561	-1.632	6	3.217	-2.366	0.403
6	4.465	-0.055	-0.943	6	-0.528	3.835	0.218
1	-0.470	0.634	-1.446	6	4.261	-1.545	-0.005
1	-1.434	2.467	-0.112	1	-0.720	-1.324	0.918
1	-1.679	1.390	1.255	1	-0.803	-2.244	-0.579
1	-3.288	0.029	-0.038	1	-2.404	-0.461	-1.476
1	-2.965	0.957	-1.497	1	-2.505	0.183	0.166
1	0.088	-0.622	2.019	1	0.332	-1.269	-2.493
1	-1.482	-1.477	-1.872	1	-0.575	1.683	-2.400
1	-3.794	2.895	-0.228	1	2.439	0.968	-1.379
1	-0.275	-2.983	2.685	1	1.097	-2.634	0.521
1	-1.855	-3.835	-1.212	1	-4.157	-2.829	1.447
1	1.235	-0.614	-1.805	1	-3.552	-1.224	1.922
1	-1.250	-4.592	1.071	1	-2.421	-2.554	1.583
1	-6.085	2.373	-0.152	1	-4.606	-1.064	-1.644
1	-5.677	0.660	-0.064	1	-4.966	-0.380	-0.043
1	-5.395	1.548	-1.569	1	-5.376	-2.071	-0.408
1	5.103	1.216	0.672	1	0.014	3.279	2.230
1	2.213	3.038	1.337	1	-1.005	4.057	-1.868
1	2.106	1.673	2.422	1	4.785	0.305	-0.972
1	3.679	2.430	2.123	1	3.427	-3.304	0.907
1	3.517	-1.249	-2.459	1	-0.710	4.874	0.469
1	5.473	-0.339	-1.224	1	5.289	-1.838	0.177
Clomipramine				Azatadine			
17	3.650	-2.739	-0.961	7	-3.935	-0.367	0.086
7	-0.651	-0.001	-0.615	7	0.824	2.053	-1.564
7	1.587	3.706	-0.108	6	-1.171	-0.199	-0.730
6	-0.152	0.749	-1.769	6	-2.123	0.943	-0.942
6	0.229	-0.878	0.061	6	-1.884	-1.519	-0.653

6	-2.055	-0.228	-0.575	6	-3.241	0.912	0.094
6	-1.074	-0.859	2.323	6	-3.010	-1.451	0.375
6	-1.962	0.290	1.860	6	0.148	-0.033	-0.507
6	0.053	-1.276	1.406	6	1.098	-1.162	-0.320
6	-2.740	-0.070	0.637	6	0.762	1.322	-0.444
6	1.007	1.674	-1.419	6	1.989	-1.276	0.766
6	0.700	2.556	-0.218	6	2.088	-0.317	1.933
6	1.348	-1.357	-0.642	6	1.124	0.866	1.987
6	-2.761	-0.543	-1.739	6	1.250	1.765	0.796
6	1.008	-2.129	1.964	6	-5.037	-0.364	1.023
6	-4.119	-0.268	0.660	6	1.146	-2.137	-1.331
6	2.274	-2.187	-0.036	6	2.861	-2.371	0.800
6	-4.139	-0.718	-1.700	6	1.836	3.024	0.848
6	2.122	-2.592	1.281	6	2.018	-3.212	-1.278
6	-4.822	-0.587	-0.497	6	2.885	-3.333	-0.197
6	2.967	3.305	0.097	6	1.917	3.787	-0.311
6	1.150	4.570	0.970	6	1.394	3.258	-1.484
1	0.119	0.099	-2.616	1	-1.616	1.908	-0.915
1	-0.995	1.355	-2.113	1	-2.574	0.848	-1.939
1	-1.714	-1.731	2.515	1	-2.323	-1.758	-1.631
1	-0.634	-0.606	3.295	1	-1.206	-2.333	-0.393
1	-2.647	0.560	2.669	1	-2.814	1.123	1.099
1	-1.343	1.172	1.656	1	-3.971	1.702	-0.110
1	1.207	2.309	-2.290	1	-3.571	-2.392	0.382
1	1.919	1.097	-1.241	1	-2.568	-1.334	1.388
1	0.729	1.944	0.708	1	1.982	-0.897	2.858
1	-0.327	2.935	-0.299	1	3.115	0.073	1.960
1	1.488	-1.097	-1.682	1	1.318	1.432	2.904
1	-2.225	-0.661	-2.675	1	0.094	0.496	2.058
1	0.875	-2.427	3.001	1	-4.711	-0.208	2.070
1	-4.649	-0.143	1.601	1	-5.570	-1.318	0.977
1	-4.675	-0.967	-2.610	1	-5.742	0.432	0.769
1	2.851	-3.236	1.754	1	0.483	-2.021	-2.183
1	-5.898	-0.725	-0.460	1	3.540	-2.461	1.645
1	3.340	2.745	-0.764	1	2.217	3.407	1.792
1	3.099	2.675	0.998	1	2.028	-3.944	-2.079
1	3.593	4.193	0.211	1	3.578	-4.166	-0.134
1	1.790	5.455	1.022	1	2.368	4.774	-0.306
1	1.178	4.072	1.959	1	1.430	3.828	-2.410
1	0.124	4.901	0.791				
	Bethanidine				Dapsone		
7	0.939	-0.950	0.603	16	0.000	1.631	0.000
7	2.879	-0.546	-0.621	8	0.000	2.337	-1.279
7	1.858	1.186	0.630	8	0.000	2.336	1.279
6	-0.194	-0.519	1.413	7	-4.643	-2.096	0.000
6	-1.419	-0.167	0.610	7	4.643	-2.097	0.000
6	-1.396	0.906	-0.288	6	-1.406	0.539	0.000
6	-2.591	-0.914	0.733	6	1.406	0.539	0.000
6	1.887	-0.025	0.194	6	-1.949	0.108	1.208
6	-2.520	1.216	-1.043	6	1.950	0.109	-1.208
6	-3.719	-0.603	-0.021	6	-1.950	0.109	-1.208
6	-3.686	0.463	-0.912	6	1.950	0.109	1.208
6	2.818	-1.860	-1.217	6	-3.035	-0.750	1.209
6	2.974	2.026	0.281	6	3.035	-0.749	-1.209
1	0.155	0.344	1.985	6	-3.035	-0.749	-1.209
1	-0.436	-1.319	2.121	6	3.035	-0.749	1.209
1	0.707	-1.652	-0.085	6	-3.594	-1.192	0.000
1	-0.487	1.494	-0.371	6	3.594	-1.192	0.000
1	-2.618	-1.748	1.430	1	-1.529	0.471	2.141
1	-2.493	2.055	-1.732	1	1.530	0.472	-2.141
1	-4.623	-1.194	0.088	1	-1.530	0.473	-2.141
1	-4.563	0.709	-1.502	1	1.530	0.472	2.141
1	3.379	0.153	-1.147	1	-3.466	-1.081	2.149
1	1.988	-1.991	-1.927	1	3.466	-1.080	-2.149
1	2.732	-2.624	-0.441	1	-3.467	-1.079	-2.149
1	3.746	-2.048	-1.757	1	3.467	-1.080	2.149
1	3.946	1.607	0.586	1	-5.204	-2.119	0.838
1	2.869	2.996	0.771	1	-5.205	-2.118	-0.838
1	3.042	2.234	-0.803	1	5.205	-2.118	-0.838
				1	5.205	-2.118	0.837
	Doxercalciferol				Calcifediol		
8	-8.272	-0.062	1.145	8	-7.984	-2.360	0.140
8	-4.753	-2.360	1.577	8	6.940	-0.901	2.077
6	0.841	1.622	0.001	6	-0.677	1.448	-0.278
6	2.200	1.028	-0.439	6	-1.976	0.621	-0.458
6	-0.083	1.006	-1.091	6	0.250	0.367	0.342
6	1.851	-0.415	-0.888	6	-1.477	-0.767	-0.918
6	0.332	-0.456	-1.142	6	-0.001	-0.882	-0.491
6	0.703	3.145	-0.087	6	-0.771	2.650	0.691
6	3.372	1.043	0.557	6	-3.064	1.190	-1.376
6	-1.516	1.397	-0.917	6	1.647	0.869	0.523
6	0.457	1.118	1.394	6	-0.131	1.901	-1.635
6	-0.752	3.591	0.055	6	0.376	2.690	1.710
6	-1.688	2.890	-0.937	6	1.713	2.258	1.116

6	3.740	2.441	1.052	6	-4.242	0.217	-1.538
6	4.572	0.399	-0.075	6	-3.549	2.569	-0.939
6	-2.510	0.497	-0.762	6	2.734	0.161	0.148
6	5.159	-0.723	0.335	6	-4.983	-0.147	-0.256
6	-3.903	0.786	-0.532	6	-6.160	-1.072	-0.527
6	6.341	-1.383	-0.310	6	4.099	0.600	0.290
6	-4.922	-0.104	-0.472	6	-6.955	-1.521	0.697
6	7.535	-1.472	0.666	6	5.209	-0.019	-0.179
6	-6.318	0.338	-0.123	6	6.585	0.513	0.128
6	5.924	-2.754	-0.847	6	-7.602	-0.344	1.419
6	-4.780	-1.552	-0.702	6	-6.104	-2.342	1.659
6	-6.928	-0.510	0.982	6	5.203	-1.274	-0.959
6	-5.451	-2.436	0.326	6	7.445	-0.566	0.786
6	-6.873	-1.986	0.609	6	6.138	-2.340	-0.442
6	7.955	-0.086	1.142	6	7.526	-1.792	-0.119
6	8.725	-2.200	0.054	6	4.455	-1.448	-2.054
6	-4.131	-2.095	-1.739	1	-2.405	0.519	0.552
1	2.518	1.603	-1.325	1	-0.167	0.181	1.348
1	0.258	1.476	-2.031	1	-2.094	-1.569	-0.501
1	2.143	-1.130	-0.110	1	-1.570	-0.856	-2.007
1	2.427	-0.698	-1.773	1	0.214	-1.801	0.062
1	0.067	-0.932	-2.090	1	0.657	-0.891	-1.367
1	-0.176	-1.025	-0.357	1	-1.724	2.631	1.230
1	1.094	3.474	-1.061	1	-0.774	3.583	0.115
1	1.310	3.647	0.672	1	-2.618	1.295	-2.376
1	3.086	0.429	1.424	1	-0.063	1.077	-2.351
1	0.651	0.047	1.508	1	0.870	2.333	-1.540
1	1.032	1.634	2.169	1	-0.774	2.668	-2.077
1	-0.604	1.274	1.607	1	0.140	2.033	2.556
1	-0.823	4.676	-0.080	1	0.461	3.695	2.135
1	-1.098	3.393	1.076	1	2.016	2.975	0.338
1	-1.444	3.245	-1.950	1	2.498	2.316	1.879
1	-2.723	3.187	-0.755	1	-3.892	-0.706	-2.016
1	3.911	3.125	0.213	1	-4.958	0.657	-2.245
1	4.657	2.413	1.646	1	-2.760	3.321	-1.006
1	2.957	2.875	1.678	1	-4.379	2.908	-1.565
1	4.981	0.918	-0.947	1	-3.902	2.565	0.098
1	-2.242	-0.557	-0.800	1	2.584	-0.820	-0.293
1	4.748	-1.241	1.207	1	-4.289	-0.627	0.446
1	-4.166	1.825	-0.344	1	-5.332	0.766	0.243
1	6.657	-0.758	-1.160	1	-6.861	-0.587	-1.218
1	7.194	-2.048	1.541	1	-5.809	-1.975	-1.043
1	-6.332	1.393	0.164	1	4.263	1.522	0.849
1	-6.974	0.239	-1.001	1	6.521	1.391	0.777
1	6.709	-3.217	-1.449	1	7.080	0.827	-0.801
1	5.031	-2.671	-1.472	1	-8.247	-0.697	2.230
1	5.686	-3.439	-0.025	1	-6.855	0.319	1.865
1	-6.360	-0.352	1.910	1	-8.215	0.241	0.729
1	-5.449	-3.474	-0.039	1	-5.311	-1.743	2.115
1	-7.491	-2.148	-0.282	1	-6.718	-2.739	2.474
1	-7.290	-2.603	1.414	1	-5.645	-3.187	1.141
1	8.790	-0.145	1.846	1	8.452	-0.176	0.967
1	8.283	0.529	0.296	1	5.710	-2.758	0.481
1	7.136	0.446	1.632	1	6.198	-3.168	-1.153
1	9.038	-1.718	-0.880	1	-8.528	-2.677	0.867
1	9.584	-2.183	0.731	1	8.134	-2.562	0.364
1	8.510	-3.247	-0.171	1	8.041	-1.510	-1.047
1	-4.076	-3.173	-1.861	1	4.490	-2.375	-2.618
1	-3.659	-1.486	-2.503	1	3.800	-0.667	-2.425
1	-8.651	-0.533	1.892	1	5.976	-0.895	2.022
1	-3.815	-2.476	1.396				
	Desogestrel				Benztropine		
8	-4.460	0.476	0.222	8	0.221	-0.978	-0.265
6	-1.966	0.276	-0.141	7	-3.819	-1.384	0.334
6	-1.117	-1.011	-0.115	6	-3.221	-0.314	1.153
6	0.287	-0.853	-0.679	6	-3.424	-0.959	-1.022
6	1.011	0.258	0.123	6	-3.560	1.002	0.409
6	-3.282	-0.285	0.501	6	-3.704	0.563	-1.063
6	-2.047	-2.076	-0.695	6	-1.714	-0.559	1.211
6	-1.214	1.356	0.645	6	-1.940	-1.273	-1.189
6	-3.444	-1.662	-0.197	6	-1.114	-0.479	-0.191
6	2.498	0.439	-0.245	6	-5.260	-1.461	0.493
6	1.069	-2.158	-0.640	6	1.176	-0.271	0.512
6	0.171	1.521	0.070	6	2.525	-0.920	0.299
6	-2.263	0.729	-1.590	6	1.207	1.205	0.161
6	2.483	-1.951	-1.164	6	3.592	-0.545	1.118
6	3.209	-0.893	-0.389	6	0.963	2.177	1.128
6	3.213	1.324	0.781	6	2.740	-1.858	-0.708
6	-2.788	2.145	-1.777	6	1.455	1.604	-1.154
6	-3.151	-0.443	1.950	6	4.852	-1.099	0.937
6	4.722	1.300	0.605	6	0.968	3.529	0.793
6	4.421	-1.123	0.130	6	4.005	-2.412	-0.890
6	0.555	2.665	-0.499	6	1.454	2.949	-1.493
6	5.255	-0.106	0.840	6	5.063	-2.036	-0.072

6	-3.079	-0.546	3.149	6	1.211	3.917	-0.519
1	-0.984	-1.256	0.953	1	-3.645	-0.346	2.161
1	0.233	-0.531	-1.731	1	-4.009	-1.513	-1.763
1	0.991	-0.088	1.173	1	-2.786	1.762	0.551
1	-1.773	-3.084	-0.375	1	-4.493	1.430	0.786
1	-2.002	-2.072	-1.790	1	-4.711	0.762	-1.438
1	-1.137	1.033	1.692	1	-3.013	1.087	-1.730
1	-1.749	2.312	0.644	1	-1.246	0.180	1.870
1	2.534	0.930	-1.234	1	-1.525	-1.553	1.631
1	-4.156	-1.529	-1.015	1	-1.777	-2.342	-1.018
1	-3.885	-2.388	0.487	1	-1.603	-1.044	-2.206
1	0.551	-2.923	-1.229	1	-1.105	0.578	-0.505
1	1.105	-2.531	0.394	1	-5.498	-1.744	1.522
1	-2.976	0.031	-2.041	1	-5.658	-2.238	-0.165
1	-1.344	0.630	-2.177	1	-5.801	-0.524	0.271
1	2.415	-1.644	-2.219	1	0.922	-0.356	1.582
1	3.055	-2.884	-1.150	1	3.431	0.192	1.901
1	2.966	0.951	1.786				
1	2.832	2.346	0.741	1	0.765	1.869	2.153
1	-3.698	2.327	-1.203	1	1.909	-2.155	-1.337
1	-2.047	2.896	-1.495	1	1.643	0.844	-1.909
1	-3.030	2.319	-2.829	1	5.672	-0.800	1.583
1	-4.488	1.214	0.840	1	0.778	4.277	1.556
1	5.203	2.015	1.279	1	4.162	-3.144	-1.676
1	4.974	1.618	-0.415	1	1.647	3.250	-2.518
1	4.852	-2.116	0.001	1	6.047	-2.470	-0.215
1	1.532	2.802	-0.950	1	1.213	4.969	-0.784
1	-0.109	3.524	-0.528				
1	5.278	-0.325	1.919				
1	6.298	-0.188	0.512				
1	-3.017	-0.646	4.206				
	Desipramine				Ergocalciferol		
7	-0.004	0.062	-0.033	8	-7.317	-0.215	-1.444
7	4.265	0.726	0.426	6	0.646	1.574	0.093
6	-2.096	0.616	1.757	6	1.945	0.917	-0.435
6	-2.721	-0.674	1.241	6	-0.408	0.818	-0.760
6	-0.765	1.243	-0.250	6	1.569	-0.570	-0.627
6	-0.616	-1.207	-0.211	6	0.033	-0.639	-0.714
6	1.434	0.180	-0.258	6	0.508	3.095	-0.157
6	-1.800	1.561	0.639	6	3.226	1.089	0.396
6	-1.865	-1.551	0.356	6	-1.806	1.184	-0.372
6	2.242	-0.634	0.746	6	0.450	1.261	1.580
6	-0.458	2.116	-1.297	6	-0.848	3.481	-0.762
6	0.056	-2.180	-0.974	6	-2.006	2.672	-0.185
6	-2.528	2.732	0.438	6	3.604	2.552	0.621
6	-2.372	-2.830	0.107	6	4.360	0.363	-0.265
6	3.726	-0.627	0.436	6	-2.774	0.266	-0.168
6	-1.183	3.289	-1.472	6	5.015	-0.681	0.239
6	-0.469	-3.443	-1.190	6	-4.131	0.563	0.212
6	-2.227	3.598	-0.607	6	6.125	-1.432	-0.432
6	-1.704	-3.779	-0.651	6	-5.102	-0.324	0.540
6	5.691	0.755	0.161	6	7.426	-1.369	0.398
1	-1.170	0.383	2.297	6	-6.508	0.133	0.825
1	-2.778	1.085	2.472	6	5.673	-2.868	-0.702
1	-3.642	-0.417	0.700	6	-4.917	-1.788	0.587
1	-3.049	-1.284	2.092	6	-7.504	-0.591	-0.081
1	1.733	-0.084	-1.287	6	-5.952	-2.578	-0.176
1	1.689	1.235	-0.147	6	-7.375	-2.101	0.106
1	1.886	-1.668	0.773	6	7.876	0.073	0.601
1	2.062	-0.230	1.751	6	8.548	-2.187	-0.229
1	0.348	1.870	-1.981	6	-3.932	-2.377	1.275
1	1.011	-1.935	-1.422	1	2.134	1.361	-1.426
1	3.897	-1.056	-0.562	1	-0.247	1.177	-1.792
1	4.259	-1.290	1.143	1	1.943	-1.161	0.218
1	-3.329	2.975	1.132	1	2.058	-0.988	-1.511
1	-3.332	-3.084	0.551	1	-0.322	-1.207	-1.578
1	-0.937	3.955	-2.293	1	-0.386	-1.132	0.170
1	0.087	-4.158	-1.789	1	1.307	3.446	-0.820
1	-2.798	4.511	-0.741	1	0.647	3.634	0.788
1	-2.134	-4.762	-0.807	1	3.057	0.616	1.374
1	4.084	1.154	1.330	1	1.184	1.794	2.190
1	6.289	0.125	0.843	1	-0.542	1.565	1.926
1	6.064	1.779	0.226	1	0.556	0.194	1.796
1	5.878	0.400	-0.857	1	-0.824	3.332	-1.848
				1	-1.028	4.550	-0.617
				1	-2.951	2.994	-0.637
				1	-2.109	2.896	0.887
				1	3.745	3.072	-0.333
				1	4.541	2.630	1.178
				1	2.837	3.094	1.180
				1	4.654	0.741	-1.249
				1	-2.525	-0.783	-0.302
				1	4.718	-1.059	1.222
				1	-4.418	1.615	0.222

1	-6.861	-3.130	2.523				
1	-5.776	-3.512	1.184				
1	8.152	0.061	0.953				
1	5.505	-2.628	0.526				
1	6.009	-3.058	-1.098				
1	7.920	-2.349	0.406				
1	7.792	-1.333	-1.029				
1	4.279	-2.358	-2.585				
1	3.526	-0.672	-2.429				
1	5.704	-0.724	2.026				
	Cyclobenzaprine				Cyproheptadine		
7	-2.617	-1.993	0.549	7	-3.896	0.000	0.094
6	0.305	-0.086	-0.733	6	-1.129	0.000	-0.731
6	1.694	-0.514	-0.453	6	-1.967	1.245	-0.794
6	-0.053	1.330	-0.485	6	-1.967	-1.245	-0.794
6	-2.019	-0.763	-1.527	6	-3.080	1.195	0.247
6	-0.571	-0.975	-1.235	6	-3.080	-1.195	0.247
6	-2.892	-1.831	-0.871	6	0.203	0.000	-0.517
6	2.271	-0.374	0.829	6	0.990	-1.250	-0.391
6	0.077	1.920	0.793	6	0.990	1.250	-0.391
6	1.611	0.277	1.946	6	-4.995	0.000	1.037
6	0.673	1.248	1.933	6	1.630	-1.574	0.825
6	2.428	-1.149	-1.460	6	1.630	1.574	0.825
6	-0.584	2.094	-1.530	6	1.071	-2.145	-1.462
6	3.545	-0.923	1.054	6	1.071	2.145	-1.462
6	-0.403	3.227	0.980	6	1.670	-0.675	1.967
6	3.698	-1.660	-1.223	6	1.670	0.675	1.967
6	-1.020	3.397	-1.332	6	2.261	-2.824	0.939
6	4.258	-1.551	0.046	6	2.261	2.824	0.939
6	-0.940	3.964	-0.063	6	1.731	-3.360	-1.341
6	-3.401	-3.080	1.096	6	1.731	3.361	-1.341
6	-2.830	-0.773	1.302	6	2.320	-3.707	-0.126
1	-2.203	-0.806	-2.609	6	2.320	3.707	-0.126
1	-2.338	0.236	-1.215	1	-1.370	2.146	-0.644
1	-0.211	-1.995	-1.377	1	-2.429	1.323	-1.788
1	-3.960	-1.591	-1.055	1	-2.429	-1.323	-1.788
1	-2.705	-2.801	-1.348	1	-1.370	-2.146	-0.644
1	2.002	-0.002	2.923	1	-2.630	1.241	1.261
1	0.394	1.664	2.900	1	-3.730	2.071	0.148
1	1.979	-1.242	-2.444	1	-3.730	-2.071	0.148
1	-0.661	1.640	-2.513	1	-2.630	-1.241	1.261
1	3.973	-0.840	2.049	1	-5.618	-0.885	0.884
1	-0.329	3.666	1.971	1	-5.618	0.885	0.884
1	4.243	-2.150	-2.024	1	-4.657	0.000	2.091
1	-1.433	3.963	-2.161	1	0.585	-1.880	-2.396
1	5.244	-1.955	0.248	1	0.585	1.880	-2.396
1	-1.291	4.975	0.111	1	1.835	-1.162	2.926
1	-3.189	-4.004	0.551	1	1.835	1.162	2.926
1	-4.492	-2.898	1.043	1	2.726	-3.085	1.886
1	-3.139	-3.238	2.146	1	2.726	3.085	1.886
1	-3.868	-0.394	1.224	1	1.773	-4.042	-2.184
1	-2.152	0.014	0.964	1	1.773	4.042	-2.184
1	-2.617	-0.956	2.358	1	2.825	-4.661	-0.015
				1	2.825	4.661	-0.015
	Benzphetamine				Amitriptyline		
7	0.714	-0.435	0.275	7	-2.439	-1.477	0.709
6	-0.684	-0.484	-0.182	6	1.524	0.954	1.876
6	-1.627	-0.033	0.943	6	0.009	0.786	1.795
6	1.664	-0.472	-0.827	6	0.471	-0.407	-0.747
6	-1.119	-1.823	-0.774	6	2.375	0.266	0.830
6	-3.021	0.246	0.456	6	-0.565	1.435	0.574
6	1.050	-1.428	1.281	6	1.901	-0.360	-0.341
6	3.039	0.004	-0.433	6	-0.319	0.848	-0.675
6	-3.294	1.402	-0.282	6	-0.068	-1.559	-1.182
6	-4.066	-0.649	0.691	6	-1.492	-1.799	-1.565
6	3.198	1.088	0.433	6	3.751	0.236	1.089
6	4.178	-0.611	-0.952	6	-1.325	2.602	0.641
6	-4.572	1.655	-0.768	6	2.832	-0.978	-1.194
6	-5.347	-0.401	0.207	6	-0.832	1.447	-1.828
6	4.466	1.548	0.765	6	-2.295	-2.401	-0.408
6	5.449	-0.149	-0.626	6	4.656	-0.379	0.239
6	-5.603	0.753	-0.526	6	-1.842	3.188	-0.509
6	5.597	0.933	0.234	6	4.189	-0.996	-0.917
1	-0.748	0.274	-0.975	6	-1.593	2.609	-1.749
1	-1.195	0.864	1.400	6	-2.793	-2.169	1.931
1	-1.665	-0.801	1.724	6	-3.394	-0.420	0.430
1	1.270	0.178	-1.620	1	1.865	0.606	2.858
1	1.754	-1.480	-1.278	1	1.758	2.028	1.858
1	-2.120	-1.749	-1.205	1	-0.441	1.221	2.694
1	-1.150	-2.606	-0.009	1	-0.254	-0.279	1.789
1	-0.441	-2.155	-1.565	1	0.569	-2.445	-1.164
1	0.359	-1.370	2.124	1	-1.540	-2.498	-2.408
1	2.054	-1.228	1.663	1	-1.975	-0.879	-1.904
1	1.042	-2.464	0.897	1	4.111	0.708	2.000

1	-2.494	2.114	-0.470	1	-1.522	3.048	1.613
1	-3.869	-1.553	1.262	1	2.463	-1.431	-2.109
1	2.310	1.553	0.851	1	-0.627	0.993	-2.793
1	4.064	-1.464	-1.616	1	-3.281	-2.747	-0.777
1	-4.764	2.561	-1.334	1	-1.774	-3.291	-0.037
1	-6.145	-1.109	0.404	1	5.715	-0.377	0.475
1	4.575	2.391	1.441	1	-2.435	4.095	-0.438
1	6.325	-0.640	-1.038	1	4.878	-1.477	-1.604
1	-6.601	0.951	-0.903	1	-1.986	3.063	-2.654
1	6.588	1.293	0.495	1	-2.038	-2.925	2.165
				1	-3.777	-2.673	1.881
				1	-2.828	-1.457	2.761
				1	-3.425	0.276	1.273
				1	-4.419	-0.806	0.266
				1	-3.096	0.153	-0.451
Diphemanil							
7	-3.632	-0.120	0.184				
6	-2.824	1.166	0.063				
6	-2.707	-1.257	0.595				
6	-1.626	1.011	-0.851				
6	-1.516	-1.423	-0.334				
6	-0.744	-0.138	-0.448				
6	-4.319	-0.437	-1.106				
6	-4.672	0.062	1.241				
6	0.585	-0.026	-0.209				
6	1.461	-1.204	-0.005				
6	1.269	1.290	-0.142				
6	2.390	-1.208	1.044				
6	2.420	1.522	-0.904				
6	1.426	-2.303	-0.871				
6	0.822	2.300	0.718				
6	3.228	-2.297	1.244				
6	3.079	2.743	-0.838				
6	2.278	-3.385	-0.682				
6	1.491	3.516	0.798				
6	3.174	-3.388	0.382				
6	2.616	3.743	0.013				
1	-2.510	1.407	1.083				
1	-3.525	1.934	-0.274				
1	-3.331	-2.153	0.648				
1	-2.375	-1.007	1.606				
1	-1.089	1.960	-0.854				
1	-1.974	0.864	-1.885				
1	-1.856	-1.786	-1.314				
1	-0.904	-2.225	0.083				
1	-4.983	0.389	-1.359				
1	-3.585	-0.574	-1.895				
1	-4.896	-1.352	-0.977				
1	-5.250	-0.857	1.333				
1	-4.181	0.287	2.186				
1	-5.326	0.886	0.957				
1	2.449	-0.348	1.705				
1	2.794	0.737	-1.555				
1	0.751	-2.291	-1.722				
1	-0.037	2.111	1.357				
1	3.933	-2.289	2.069				
1	3.962	2.911	-1.445				
1	2.251	-4.221	-1.373				
1	1.142	4.282	1.483				
1	3.839	-4.232	0.531				
1	3.140	4.691	0.074				