

Supporting information for:

QM/MM Modeling of Regioselectivity of Drug Metabolism in Cytochrome P450 2C9

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Contents

- A. Additional CHARMM topology and parameters for *S*-warfarin
- B. QM calculations
 - i. Absolute energies
 - ii. Mulliken charges and spin densities
 - iii. Cartesian coordinates
- C. QM/MM calculations
 - i. Absolute energies
 - ii. Mulliken charges and spin densities
 - iii. Cartesian coordinates of QM region
 - iv. Details of the supplementary PDB files

A. Additional CHARMM topology and parameters for S-warfarin

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GROUP
ATOM C3 CA -0.115 !
ATOM H1 HP 0.115 !
GROUP !
ATOM C4 CA -0.115 !
ATOM H2 HP 0.115 !
GROUP !
ATOM C5 CA -0.115 !
ATOM H3 HP 0.115 !
GROUP !
ATOM C6 CA -0.115 !
ATOM H4 HP 0.115 !
GROUP !
ATOM
C1CPT 0.35 !
ATOM O1 OS -0.315 !
ATOM C12 C 0.61 !
ATOM O3 O -0.51 !
ATOM C10 CA -0.115 !
ATOM C8 CA 0.11 !
ATOM O2 OH1 -0.54 !
ATOM H8 H 0.43 !
ATOM C2 CPT -0.02 !
GROUP !
ATOM C13 CA -0.115 !
ATOM H7 HA 0.09 !
GROUP !
ATOM C14 CT1 -0.09 !
ATOM H11 HA 0.09 !
GROUP !
ATOM C15 CA 0 !
GROUP !
ATOM C16 CT2 -0.18 !
ATOM H5 HA 0.09 !
ATOM H6 HA 0.09 !
GROUP !
ATOM C17 CA -0.115 !
ATOM H15 HP 0.115 !
GROUP !
ATOM C18 C 0.51 !
ATOM O4 O -0.51 !
GROUP !
ATOM C7 CT3 -0.27 !
ATOM H12 HA 0.09 !
ATOM H14 HA 0.09 !
ATOM H10 HA 0.09 !
GROUP !
ATOM C19 CA -0.115 !
ATOM H16 HP 0.115 !
GROUP !
ATOM C9 CA -0.115 !
ATOM H9 HP 0.115 !

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The diagram illustrates the chemical structure of S-warfarin with atom numbering and connectivity. The structure consists of a coumarin ring system (atoms C1-C8, O1, O2) fused to a benzofuran ring system (atoms C9-C19, O3, O4). The atoms are numbered as follows: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19; O1, O2, O3, O4; H1, H2, H3, H4, H5, H6, H7, H8, H9, H10, H11, H12, H13, H14, H15, H16. The connectivity is shown with lines and symbols: /, \, //, and ||.

```

GROUP
ATOM C11 CA -0.115
ATOM H11 HP 0.115
GROUP
ATOM C13 CA -0.115
ATOM H13 HP 0.115

```

```

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
CPT  OS      340.0      1.381
CA   C        450.0      1.389
CA   CT1      230.0      1.490
C    OS       340.0      1.381

```

```

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types      Ktheta      Theta0
CA   CPT  OS      55.0      118.4
OS   CPT  CPT      55.0      118.4
CPT  OS   C        40.0      122.6
OS   C    O        90.0      115.6
OS   C    CA       55.0      116.8
O    C    CA       80.0      127.3
C    CA   CA       40.0      122.2
C    CA   CT1      45.8      120.3
CA   CA   CT1      45.8      122.3
OH1  CA   CPT      55.0      118.5
CA   CPT  CA       40.0      120.0
CA   CT1  HA       29.0      120.0
CA   CT1  CA       52.0      108.0
CA   CT1  CT2      52.0      108.0
CT1  CT2  C        50.0      109.0
CT2  C    CT3      70.0      121.5

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DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees

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!
!atom types          Kchi    n    delta
CA    CPT  CA    CA    3.1    1    0.0
CA    CPT  CA    OH1   3.1    1   180.0
HP    CA    CPT  CA    3.5    1   180.0
CA    CA    CPT  OS    3.1    1    0.0
CA    CPT  OS    C     3.1    1    0.0
HP    CA    CPT  OS    0.1    1   180.0
CPT   OS    C     O     3.1    1    0.0
CPT   OS    C     CA    3.1    1   180.0
CPT   CPT   CA    OH1   3.1    1    0.0
OS    C     CA    CA    3.1    1   180.0
OS    C     CA    CT1   3.1    1    0.0
C     OS    CPT  CPT   3.1    1   180.0
C     CA    CA    OH1   3.1    1    0.0
C     CA    CA    CPT   3.1    1   180.0
C     CA    CT1  HA    4.2    3    0.0
C     CA    CT1  CA    3.1    3    0.0
C     CA    CT1  CT2   3.1    3    0.0
O     C     CA    CA    3.1    1    0.0
O     C     CA    CT1   3.1    1   180.0
CA    CT1  CA    CA    4.2    1    0.0
CA    CA    CT1  HA    0.3    3    0.0
CA    CA    CT1  CT2   4.2    3    0.0
OH1   CA    CA    CT1   4.2    1   180.0
H     OH1  CA    CPT   0.1    1    0.0
CPT   CA    CA    CT1   4.2    1    0.0
CT1   CA    CA    HP    4.2    1   180.0
CT1   CA    CA    CA    4.2    1    0.0
CT1   CT2  C     O     0.3    1    0.0
CT1   CT2  C     CT3   0.3    1    0.0
CT2   C     CT3  HA    0.3    3    0.0
HA    CT2  C     CT3   0.3    3    0.0

```

B. QM Calculations

i) Absolute energies [in atomic units] of reactant complexes and transition states, calculated at the B3LYP-D level. Energies calculated at with the LANL2DZ/6-31G basis set combination are shown in bold, with energies calculated at the SDD/VTZ(d,p) level shown in regular typeface.

Table S1 Energies of individual reactants

		Quartet	Doublet	Singlet
Compound I	BSI	-1584.878528	-1584.878393	-
	BSII	-1585.647078	-1585.647272	-
Diclofenac	BSI	-	-	-1664.957067
	BSII	-	-	-1665.511463
Ibuprofen	BSI	-	-	-656.1592195
	BSII	-	-	-656.5687707
Warfarin	BSI	-	-	-571.7788991
	BSII	-	-	-572.1481413

Table S2 Energies of reactant complexes (RC) and transition states (TS) for hydrogen abstraction from C2 and C3 of ibuprofen

			Quartet	Doublet
C2	RC	BSI	-2241.06786	-2241.067706
		BSII	-2242.239048	-2242.239329
	TS	BSI	-2241.042855	-2241.039498
		BSII	-2242.215529	-2242.213424
C3	RC	BSI	-2241.067121	-2241.066908
		BSII	-2242.237856	-2242.237995
	TS	BSI	-2241.02662	-2241.029079
		BSII	-2242.197836	-2242.202071

Table S3 Energies of reactant complexes (RC) and transition states (TS) for C-O bond formation to C6 and C7 of warfarin

			Quartet	Doublet
C6	RC	BSI	-2156.683588	-2156.683085
		BSII	-2157.816	-2157.815932
	TS	BSI	-2156.660675	-2156.664002
		BSII	-2157.792537	-2157.795576
C7	RC	BSI	-2156.683588	-2156.683085
		BSII	-2157.816	-2157.815932
	TS	BSI	-2156.658322	-2156.663595
		BSII	-2157.79048	-2157.794707

Table S4 Energies of reactant complexes (RC) and transition states (TS) for C-O bond formation to C4' and C5 of diclofenac

			Quartet	Doublet
C5	RC	BSI	-3249.859295	-3249.859187
		BSII	-3251.175314	-3251.175465
	TS	BSI	-3249.834017	-3249.838194
		BSII	-3251.15068	-3251.15407
C4'	RC	BSI	-3249.85964	-3249.859568
		BSII	-3251.177803	-3251.178005
	TS	BSI	-3249.838463	-3249.839691
		BSII	-3251.156516	-3251.157498

ii) Mulliken charges and spin densities (calculated with BSII)

Table S5 Ibuprofen

		TS					
		RC		C2		C3	
		Doublet	Quartet	Doublet	Quartet	Doublet	Quartet
Fe	Charge	0.36	0.35	0.32	0.26	0.31	0.26
	Spin	1.35	1.21	1.13	1.57	2.13	1.55
O	Charge	-0.31	-0.31	-0.38	-0.37	-0.36	-0.32
	Spin	0.78	0.85	0.48	0.62	0.16	0.62
SH	Charge	-0.08	-0.09	-0.14	-0.09	-0.10	-0.11
	Spin	-0.61	0.54	-0.42	0.30	-0.52	0.36
Por	Charge	0.02	0.03	-0.04	-0.07	0.02	0.06
	Spin	-0.52	0.38	-0.55	-0.01	-0.40	0.14
Sub	Charge	0.01	0.01	0.24	0.26	0.12	0.12
	Spin	0.01	0.01	0.36	0.51	-0.37	0.33

Table S6 Warfarin

		TS					
		RC		C6		C7	
		Doublet	Quartet	Doublet	Quartet	Doublet	Quartet
Fe	Charge	0.39	0.38	0.31	0.31	0.31	0.30
	Spin	1.30	1.18	1.84	1.58	1.87	1.49
O	Charge	-0.31	-0.31	-0.35	-0.34	-0.35	-0.33
	Spin	0.81	0.89	0.04	0.63	0.09	0.62
SH	Charge	-0.07	-0.08	-0.16	-0.11	-0.15	-0.10
	Spin	-0.63	0.56	-0.19	0.28	-0.25	0.33
Por	Charge	0.00	0.01	-0.03	-0.06	0.03	0.01
	Spin	-0.50	0.35	-0.27	0.00	-0.34	0.12
Sub	Charge	-0.01	0.00	0.23	0.21	0.16	0.11
	Spin	0.00	0.02	-0.41	0.52	-0.37	0.44

Table S7 Diclofenac

		c4'				c5			
		rc		ts		rc		ts	
		Doublet	Quartet	Doublet	Quartet	Doublet	Quartet	Doublet	Quartet
Fe	Charge	0.39	0.38	0.31	0.33	0.39	0.38	0.31	0.31
	Spin	1.33	1.21	1.81	1.38	1.31	1.19	1.70	1.62
O	Charge	-0.33	-0.33	-0.38	-0.33	-0.32	-0.31	-0.35	-0.35
	Spin	0.79	0.86	0.02	0.75	0.81	0.88	0.15	0.64
SH	Charge	-0.07	-0.07	-0.19	-0.11	-0.08	-0.09	-0.21	-0.16
	Spin	-0.62	0.57	-0.13	0.43	-0.62	0.56	-0.18	0.23
Por	Charge	0.31	0.32	0.19	0.19	0.30	0.31	0.21	0.17
	Spin	-0.50	0.36	-0.23	0.10	-0.51	0.37	-0.26	-0.06
Sub	Charge	-0.30	-0.30	0.07	-0.08	-0.29	-0.29	0.04	0.03
	Spin	0.00	0.01	-0.47	0.35	0.01	0.01	-0.41	0.57

iii) Cartesian coordinates of optimized reactant complexes (RC) and transition states (TS)

Ibuprofen RC Quartet

H	8.128581	23.676368	-2.173737
S	7.702558	23.871585	-0.873825
O	5.012082	26.923476	-1.813775
Fe	6.017241	25.658647	-1.447384
N	5.750926	24.782571	-3.236582
N	4.513406	24.565741	-0.683660
N	6.455518	26.336703	0.397701
N	7.692285	26.533573	-2.142126
C	6.465322	25.013559	-4.396392
C	5.902068	24.255977	-5.490327
C	4.836206	23.564144	-4.987249
C	4.743292	23.896258	-3.584058
C	3.674289	23.710707	-1.373897
C	2.658433	23.185731	-0.488356
C	2.886541	23.731393	0.743533
C	4.044472	24.588577	0.614446
C	5.724995	26.121112	1.557634
C	6.304995	26.863055	2.655488
C	7.386507	27.531677	2.157005
C	7.478931	27.199820	0.752287
C	8.559881	27.362140	-1.442161
C	9.572926	27.888525	-2.327413
C	9.316077	27.389904	-3.570553
C	8.147595	26.546146	-3.459012
C	7.574894	25.844446	-4.501357
H	8.032173	25.941194	-5.480307
C	3.784137	23.395175	-2.719465
H	3.054529	22.704567	-3.130848
C	4.606155	25.313415	1.657226
H	4.131775	25.235785	2.630092
C	8.455686	27.685688	-0.102583
H	9.185466	28.384280	0.293179

C	6.837275	29.736755	-4.218445
C	6.446495	29.455983	-2.900498
C	7.031418	30.133007	-1.826276
C	8.023508	31.097063	-2.037014
C	8.415574	31.391372	-3.354639
C	7.819874	30.724302	-4.427178
H	8.128067	30.957661	-5.443882
H	9.193146	32.129140	-3.531345
H	6.728950	29.884757	-0.813288
H	5.712467	28.687064	-2.690860
C	8.686986	31.788508	-0.843614
C	10.127323	31.326769	-0.793733
O	10.981959	32.132424	-1.515807
O	10.534796	30.300301	-0.231018
H	8.223865	31.395800	0.068500
C	8.535434	33.320941	-0.887509
H	8.983481	33.723823	-1.800324
H	9.024836	33.792237	-0.026575
H	7.470363	33.576176	-0.874573
C	6.284150	28.972789	-5.408580
C	4.994913	28.158059	-5.173472
C	3.804940	29.062282	-4.802635
C	4.664032	27.349711	-6.441675
H	4.381258	28.034279	-7.254903
H	3.823742	26.668966	-6.259014
H	5.522379	26.750474	-6.768693
H	3.597154	29.765172	-5.623023
H	4.008326	29.641692	-3.896026
H	2.905168	28.458197	-4.629712
H	5.166658	27.457714	-4.346621
H	7.063199	28.275843	-5.759051
H	6.107970	29.675726	-6.238567
H	6.282329	24.268001	-6.501390
H	4.165973	22.890011	-5.501527
H	1.883772	22.493856	-0.787928
H	2.339054	23.577684	1.662450
H	5.921349	26.856873	3.665901
H	8.076456	28.184120	2.672986
H	10.350447	28.564058	-2.005507
H	9.848262	27.570840	-4.493175
H	11.891711	31.760734	-1.505983

*

Ibuprofen RC Doublet

H	8.123134	23.665273	-2.205484
S	7.748345	23.875396	-0.892302
O	5.036089	26.934265	-1.810954
Fe	6.004183	25.647545	-1.440727
N	5.742567	24.768064	-3.229524
N	4.512743	24.545903	-0.675819
N	6.449800	26.320402	0.405801
N	7.685329	26.522207	-2.136277
C	6.456138	25.002764	-4.389488
C	5.893127	24.245655	-5.483812
C	4.827058	23.552990	-4.981891
C	4.734394	23.882944	-3.578282
C	3.672864	23.690254	-1.365942
C	2.665086	23.156284	-0.477317
C	2.898505	23.695667	0.756525
C	4.050361	24.559887	0.625586
C	5.722337	26.101924	1.566753

C	6.297327	26.851357	2.662173
C	7.373540	27.526404	2.160925
C	7.466677	27.192786	0.756554
C	8.546106	27.359383	-1.438221
C	9.553425	27.893250	-2.325591
C	9.297823	27.393029	-3.568304
C	8.135397	26.540671	-3.454973
C	7.562522	25.837793	-4.496159
H	8.015997	25.938599	-5.476388
C	3.776848	23.380069	-2.713128
H	3.045799	22.690891	-3.124278
C	4.609856	25.285976	1.668545
H	4.138191	25.203588	2.642308
C	8.440285	27.683718	-0.099336
H	9.167174	28.386053	0.295201
C	6.847832	29.745404	-4.225994
C	6.452748	29.468714	-2.908507
C	7.035233	30.147639	-1.834088
C	8.028768	31.110306	-2.044413
C	8.426355	31.399285	-3.361543
C	7.833108	30.730158	-4.434330
H	8.145080	30.960301	-5.450622
H	9.205710	32.135406	-3.537591
H	6.729157	29.901666	-0.821630
H	5.721049	28.698271	-2.697457
C	8.688757	31.805219	-0.851114
C	10.125870	31.335082	-0.789821
O	10.991884	32.136265	-1.503153
O	10.521332	30.304893	-0.225389
H	8.218081	31.420027	0.060417
C	8.545531	33.338035	-0.904828
H	9.000865	33.732973	-1.817526
H	9.032500	33.812210	-0.044148
H	7.481714	33.598716	-0.899738
C	6.293512	28.979847	-5.414655
C	4.995527	28.178799	-5.176459
C	3.814015	29.099431	-4.820855
C	4.664781	27.356487	-6.433870
H	4.451152	28.027932	-7.278887
H	3.785186	26.722875	-6.266202
H	5.502804	26.706528	-6.714913
H	3.617148	29.795400	-5.649860
H	4.020624	29.686939	-3.920126
H	2.906821	28.507431	-4.644881
H	5.161841	27.486517	-4.341176
H	7.066833	28.274031	-5.760085
H	6.125128	29.680001	-6.248610
H	6.272461	24.261186	-6.495111
H	4.156863	22.879771	-5.497405
H	1.891924	22.462205	-0.775738
H	2.357370	23.533694	1.677782
H	5.914593	26.845022	3.672938
H	8.058855	28.185361	2.674832
H	10.326225	28.574216	-2.003886
H	9.825699	27.579365	-4.492293
H	11.899037	31.758505	-1.485936
*			
Ibuprofen C2 TS Quartet			
H	6.716551	22.793184	-1.679988
S	7.646709	23.778392	-1.411158

O	5.085239	26.909257	-2.155837
Fe	6.162270	25.575836	-1.750848
N	5.993679	24.842188	-3.644262
N	4.616616	24.455166	-1.183505
N	6.368762	26.269649	0.095672
N	7.816352	26.589773	-2.314784
C	6.861542	25.056798	-4.701654
C	6.400871	24.335161	-5.866676
C	5.248487	23.690851	-5.508637
C	5.004199	24.003945	-4.118878
C	3.796279	23.685972	-2.001623
C	2.745221	23.085189	-1.211257
C	2.929950	23.491022	0.080289
C	4.087864	24.356635	0.091880
C	5.600249	25.936523	1.200107
C	6.045631	26.684290	2.355587
C	7.087536	27.467691	1.949537
C	7.300865	27.199813	0.544232
C	8.569016	27.443862	-1.535296
C	9.660911	27.992269	-2.305293
C	9.567793	27.459499	-3.559639
C	8.418494	26.582443	-3.564960
C	7.985580	25.867050	-4.668009
H	8.567583	25.953363	-5.579759
C	3.962503	23.487209	-3.360524
H	3.245482	22.847011	-3.863967
C	4.553516	25.031843	1.208232
H	4.039422	24.864702	2.148563
C	8.322077	27.750717	-0.205527
H	8.982356	28.470786	0.266590
C	6.621373	29.739450	-3.742305
C	6.412201	29.662761	-2.356116
C	7.143019	30.471409	-1.481794
C	8.110629	31.361294	-1.960285
C	8.328024	31.444308	-3.345625
C	7.580003	30.652789	-4.220556
H	7.753895	30.724925	-5.292020
H	9.089581	32.114283	-3.733003
H	6.983316	30.379494	-0.411322
H	5.721092	28.935388	-1.949455
C	8.966354	32.154927	-0.970591
C	10.304491	31.446908	-0.898697
O	11.245817	31.976223	-1.755934
O	10.546732	30.445673	-0.211101
H	8.522087	32.033995	0.024382
C	9.071210	33.651278	-1.312318
H	9.522904	33.792907	-2.297931
H	9.688683	34.179418	-0.576400
H	8.068263	34.091805	-1.316382
C	5.912258	28.832308	-4.735458
C	4.611744	28.165496	-4.293735
C	3.528074	29.099061	-3.771507
C	4.085118	27.152156	-5.299260
H	3.653977	27.678694	-6.168085
H	3.294293	26.538083	-4.851745
H	4.877418	26.489757	-5.657755
H	3.132990	29.701993	-4.607037
H	3.906126	29.784860	-3.007944
H	2.697780	28.522512	-3.346544
H	4.927927	27.449484	-3.256176

H	6.609377	28.039233	-5.041692
H	5.695838	29.413410	-5.651571
H	6.904094	24.335242	-6.823321
H	4.616881	23.053743	-6.111728
H	1.976834	22.438363	-1.611738
H	2.342269	23.248589	0.954269
H	5.605097	26.603092	3.339288
H	7.683873	28.155677	2.532063
H	10.380174	28.690220	-1.904876
H	10.202712	27.633867	-4.416945
H	12.074869	31.449939	-1.720355

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Ibuprofen C2 TS Doublet

H	8.498120	23.946339	-2.132486
S	7.628451	23.845223	-1.062776
O	4.984743	26.927283	-2.083506
Fe	6.111747	25.588627	-1.818075
N	5.991364	24.822283	-3.658485
N	4.550865	24.476510	-1.212307
N	6.307385	26.301915	0.068774
N	7.779057	26.566894	-2.362679
C	6.846404	25.028411	-4.729178
C	6.397175	24.280196	-5.880741
C	5.264330	23.613934	-5.503334
C	5.021844	23.944418	-4.117665
C	3.772202	23.660067	-2.008602
C	2.699306	23.078973	-1.228685
C	2.834646	23.554028	0.045075
C	3.986339	24.431995	0.045688
C	5.498259	26.027680	1.157936
C	5.936099	26.791934	2.308952
C	7.012666	27.529468	1.909067
C	7.245793	27.215104	0.513071
C	8.541697	27.409170	-1.567214
C	9.657183	27.935360	-2.319377
C	9.574665	27.409424	-3.576894
C	8.408046	26.557662	-3.602389
C	7.972642	25.840238	-4.703127
H	8.556496	25.916297	-5.614982
C	3.986192	23.420756	-3.357726
H	3.296512	22.748049	-3.858352
C	4.430173	25.147066	1.150937
H	3.884565	25.016272	2.080030
C	8.283189	27.732813	-0.245527
H	8.953121	28.448909	0.220340
C	6.601453	29.697825	-3.700430
C	6.387993	29.654350	-2.313539
C	7.136198	30.464571	-1.455093
C	8.124932	31.321635	-1.950239
C	8.345385	31.372087	-3.336815
C	7.580881	30.579555	-4.196205
H	7.757940	30.625162	-5.268661
H	9.122029	32.016828	-3.737078
H	6.973000	30.399533	-0.382960
H	5.682469	28.946911	-1.895773
C	8.999847	32.115766	-0.977833
C	10.327648	31.387904	-0.905286
O	11.284710	31.914968	-1.745788
O	10.549208	30.373795	-0.229249
H	8.560380	32.016241	0.021759

C	9.123790	33.605322	-1.341798
H	9.568544	33.726649	-2.333286
H	9.756316	34.134182	-0.619320
H	8.127573	34.060726	-1.342979
C	5.873069	28.787814	-4.676587
C	4.571708	28.140268	-4.214891
C	3.497259	29.099161	-3.717606
C	4.029794	27.117086	-5.203565
H	3.584011	27.633948	-6.070493
H	3.246761	26.508052	-4.735607
H	4.816392	26.450784	-5.568443
H	3.103713	29.680533	-4.568664
H	3.884699	29.802454	-2.974874
H	2.665410	28.541085	-3.271727
H	4.855478	27.452945	-3.169391
H	6.559738	27.986352	-4.985147
H	5.652964	29.362779	-5.595738
H	6.895460	24.274270	-6.839929
H	4.646084	22.949619	-6.090680
H	1.954833	22.400043	-1.620874
H	2.223985	23.345316	0.912079
H	5.470067	26.751066	3.283373
H	7.616634	28.214182	2.487606
H	10.384223	28.616922	-1.904912
H	10.228407	27.573256	-4.422150
H	12.106737	31.377858	-1.707669
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Ibuprofen C3 TS Quartet			
H	7.859067	23.527615	-1.467543
S	7.321380	24.051287	-0.309141
O	5.292421	27.115125	-2.218489
Fe	6.134555	25.844985	-1.413553
N	5.739736	24.530220	-2.893071
N	4.482662	25.271164	-0.444442
N	6.630697	27.013634	0.134364
N	7.901319	26.271120	-2.300908
C	6.490942	24.297889	-4.035063
C	5.816671	23.339808	-4.881543
C	4.657503	22.991582	-4.246473
C	4.614140	23.735359	-3.007590
C	3.535928	24.359943	-0.888504
C	2.461914	24.255706	0.075040
C	2.762112	25.104355	1.101737
C	4.022202	25.735132	0.775114
C	5.875396	27.264877	1.268978
C	6.538075	28.250070	2.095645
C	7.696530	28.596032	1.459552
C	7.756002	27.816789	0.243239
C	8.850449	27.176178	-1.856974
C	9.929132	27.271444	-2.812424
C	9.636562	26.412012	-3.834032
C	8.371395	25.791818	-3.515617
C	7.714031	24.880904	-4.324982
H	8.192396	24.603396	-5.258292
C	3.590383	23.653634	-2.076040
H	2.768650	22.979871	-2.295159
C	4.664005	26.668377	1.572097
H	4.183489	26.950229	2.502878
C	8.780053	27.903421	-0.680408
H	9.568246	28.619643	-0.477671

C	7.344270	30.019196	-3.235273
C	6.770812	30.000364	-1.949683
C	7.184268	30.903773	-0.968482
C	8.194732	31.836698	-1.232384
C	8.761732	31.877703	-2.516567
C	8.330980	30.985426	-3.504550
H	8.791732	31.007595	-4.488841
H	9.557449	32.585615	-2.732297
H	6.760954	30.842056	0.029420
H	6.054406	29.229567	-1.695672
C	8.725985	32.731994	-0.113164
C	10.119714	32.256016	0.247572
O	10.092127	31.054227	0.949945
O	11.185463	32.800835	-0.046329
H	8.094832	32.574462	0.769955
C	8.743086	34.223417	-0.488283
H	9.413002	34.394680	-1.336704
H	9.099701	34.833699	0.349483
H	7.732808	34.544074	-0.762721
C	7.010193	28.955932	-4.257452
C	5.577075	28.944882	-4.863180
C	4.488352	28.844725	-3.804688
C	5.475274	27.759813	-5.842622
H	6.259926	27.809306	-6.609682
H	4.498558	27.747710	-6.343117
H	5.590943	26.818492	-5.288595
H	4.380053	29.741223	-3.184501
H	4.858149	27.953723	-2.977787
H	3.522784	28.505114	-4.196597
H	5.437685	29.889140	-5.421069
H	7.137842	27.978268	-3.785408
H	7.727054	29.017546	-5.086956
H	6.196622	22.991261	-5.830933
H	3.893194	22.298646	-4.569339
H	1.601243	23.612002	-0.039656
H	2.198996	25.299573	2.003508
H	6.147420	28.617524	3.033601
H	8.443604	29.324885	1.740340
H	10.785619	27.920256	-2.698992
H	10.206602	26.209037	-4.729766
H	11.009216	30.760220	1.144840

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Ibuprofen	C3	TS	Doublet	
H	7.948732	23.557484		-1.480340
S	7.373206	24.023460		-0.313957
O	5.185684	27.115807		-2.220865
Fe	6.146716	25.887347		-1.469094
N	5.792638	24.530836		-2.914410
N	4.531410	25.234203		-0.456151
N	6.642380	27.043254		0.100849
N	7.898262	26.330947		-2.343607
C	6.534668	24.319034		-4.067196
C	5.887388	23.327759		-4.895314
C	4.753437	22.937406		-4.239831
C	4.695915	23.688047		-3.006166
C	3.613403	24.290608		-0.883487
C	2.546796	24.164374		0.086152
C	2.823154	25.037752		1.098975
C	4.062255	25.702331		0.757916
C	5.885218	27.274933		1.238180

C	6.543565	28.251389	2.078974
C	7.704335	28.605748	1.451309
C	7.763480	27.845527	0.223131
C	8.845358	27.241082	-1.892459
C	9.913818	27.359745	-2.854635
C	9.623386	26.510580	-3.885643
C	8.370595	25.869208	-3.566639
C	7.731208	24.945039	-4.374865
H	8.207833	24.684537	-5.313844
C	3.685556	23.575111	-2.066006
H	2.887895	22.869413	-2.273192
C	4.684353	26.658074	1.543624
H	4.201426	26.933868	2.475103
C	8.783172	27.948879	-0.705482
H	9.570445	28.664622	-0.498070
C	7.281130	30.024152	-3.216408
C	6.717520	30.014545	-1.926579
C	7.163985	30.901904	-0.944951
C	8.200051	31.805343	-1.212225
C	8.759080	31.835672	-2.500184
C	8.293876	30.962158	-3.488979
H	8.747462	30.975324	-4.476774
H	9.575300	32.519329	-2.717719
H	6.746687	30.848209	0.055911
H	5.984230	29.260041	-1.670649
C	8.766337	32.680968	-0.094201
C	10.161460	32.182383	0.226002
O	10.134812	30.990911	0.946045
O	11.226955	32.700098	-0.114467
H	8.152413	32.521944	0.800387
C	8.794835	34.175980	-0.454803
H	9.445412	34.345987	-1.318320
H	9.180471	34.772829	0.379970
H	7.782465	34.512933	-0.700420
C	6.908371	28.976561	-4.240807
C	5.467100	29.001427	-4.823866
C	4.394815	28.909664	-3.747516
C	5.327140	27.826921	-5.811601
H	6.097408	27.870722	-6.593418
H	4.340803	27.833862	-6.292857
H	5.439066	26.879876	-5.266449
H	4.321753	29.794760	-3.106897
H	4.753475	27.982582	-2.955071
H	3.413213	28.605871	-4.129079
H	5.336278	29.953345	-5.370338
H	7.018811	27.993295	-3.776210
H	7.614996	29.027251	-5.079779
H	6.267358	22.986316	-5.847260
H	4.014114	22.210512	-4.545867
H	1.707050	23.491424	-0.015601
H	2.258029	25.227482	2.000658
H	6.151857	28.603458	3.022412
H	8.452106	29.328347	1.745463
H	10.764077	28.016296	-2.739041
H	10.190527	26.324711	-4.786897
H	11.051981	30.680507	1.113520
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Warfarin RC Doublet			
H	1.964654	-1.801399	-1.087084
S	1.512707	-1.232044	0.087817

O	-0.705844	1.780109	-1.806233
Fe	0.071841	0.542953	-1.041123
N	-0.025547	-0.663230	-2.643620
N	-1.621879	-0.255582	-0.325425
N	0.320864	1.549598	0.684859
N	1.918262	1.122580	-1.613762
C	0.824707	-0.668989	-3.732321
C	0.346944	-1.597454	-4.733651
C	-0.795856	-2.161072	-4.239744
C	-1.030777	-1.568530	-2.941465
C	-2.406960	-1.218783	-0.928998
C	-3.597019	-1.457011	-0.141623
C	-3.533378	-0.619052	0.936385
C	-2.296876	0.122666	0.817982
C	-0.620675	1.698881	1.693435
C	-0.114027	2.586565	2.716862
C	1.145964	2.958049	2.333593
C	1.405052	2.319815	1.062011
C	2.790890	1.966244	-0.932329
C	3.953636	2.244190	-1.745551
C	3.780863	1.584355	-2.927631
C	2.517633	0.883405	-2.846877
C	1.997762	0.069693	-3.836482
H	2.569843	-0.030054	-4.752965
C	-2.123056	-1.843673	-2.135071
H	-2.833227	-2.582856	-2.492139
C	-1.842708	1.050529	1.745995
H	-2.480768	1.254664	2.599709
C	2.559321	2.507797	0.315074
H	3.319618	3.162157	0.726981
C	2.228716	5.204257	-1.387698
C	1.349674	5.418100	-0.305984
C	-0.024855	5.157765	-0.496133
C	-0.486172	4.665820	-1.709542
C	0.416063	4.438388	-2.767172
C	1.770765	4.718968	-2.615715
C	1.937582	5.853358	0.944774
C	3.274730	6.099596	1.057034
C	4.185303	5.908195	-0.045024
O	3.592969	5.426249	-1.262864
O	1.157949	6.021340	2.069783
O	5.406171	6.065696	-0.044872
H	-0.732415	5.334647	0.308411
H	-1.531365	4.414920	-1.835059
H	0.051693	4.015304	-3.695572
H	2.489582	4.539688	-3.404904
H	0.341000	5.484091	2.035611
H	0.838965	-1.785822	-5.677065
H	-1.435008	-2.902580	-4.697992
H	-4.368824	-2.168766	-0.398246
H	-4.239106	-0.507484	1.747481
H	-0.647257	2.844736	3.621282
H	1.846578	3.598880	2.848438
H	4.761971	2.895518	-1.447100
H	4.438455	1.558702	-3.785072
H	3.695872	6.421214	1.999286
*			
Warfarin RC Quartet			
H	1.990545	-1.751498	-1.090382
S	1.491949	-1.222487	0.084179

O	-0.720111	1.773057	-1.799891
Fe	0.081340	0.544008	-1.038481
N	-0.023207	-0.654374	-2.644693
N	-1.620326	-0.245624	-0.328653
N	0.326517	1.551538	0.687474
N	1.922327	1.126918	-1.614688
C	0.826897	-0.660377	-3.734810
C	0.349100	-1.590472	-4.734782
C	-0.791521	-2.155898	-4.238882
C	-1.026720	-1.562485	-2.940878
C	-2.406669	-1.207807	-0.932713
C	-3.601075	-1.439291	-0.149399
C	-3.538845	-0.599514	0.926608
C	-2.298366	0.136869	0.812907
C	-0.615169	1.701476	1.695096
C	-0.106473	2.584763	2.721021
C	1.154481	2.954841	2.338844
C	1.412825	2.317932	1.066670
C	2.797567	1.964346	-0.929119
C	3.961935	2.240544	-1.740759
C	3.788599	1.582802	-2.923952
C	2.522255	0.886900	-2.845745
C	2.000375	0.076302	-3.838014
H	2.573402	-0.023706	-4.753865
C	-2.119776	-1.836993	-2.135452
H	-2.829257	-2.576940	-2.492263
C	-1.841098	1.058896	1.743871
H	-2.479116	1.263675	2.597471
C	2.565960	2.506342	0.318149
H	3.326124	3.161592	0.729030
C	2.219832	5.188259	-1.388358
C	1.343343	5.401252	-0.304158
C	-0.030499	5.134614	-0.489110
C	-0.494272	4.638238	-1.700072
C	0.405576	4.412641	-2.760814
C	1.759662	4.698846	-2.613953
C	1.933461	5.845521	0.942739
C	3.269631	6.099860	1.048732
C	4.177293	5.908781	-0.055597
O	3.583054	5.418236	-1.269389
O	1.157653	6.015410	2.069578
O	5.397378	6.071494	-0.060522
H	-0.737110	5.309281	0.316717
H	-1.539433	4.385851	-1.821863
H	0.039482	3.990298	-3.688816
H	2.476853	4.521943	-3.405216
H	0.341420	5.476894	2.040926
H	0.840313	-1.778904	-5.678615
H	-1.429890	-2.899037	-4.695586
H	-4.374839	-2.148249	-0.407909
H	-4.247642	-0.483489	1.734429
H	-0.640302	2.843105	3.625068
H	1.855784	3.594329	2.854452
H	4.771253	2.889941	-1.440844
H	4.446481	1.556691	-3.781134
H	3.692049	6.428161	1.988114
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Warfarin C7 TS Quartet			
H	2.076578	-1.571899	-0.947216
S	1.316504	-1.155093	0.127805

O	-0.486643	1.960924	-1.863728
Fe	0.230337	0.610085	-1.057161
N	0.150786	-0.518916	-2.696590
N	-1.566447	-0.056462	-0.494873
N	0.385917	1.636499	0.674140
N	2.100711	1.178785	-1.545567
C	1.058113	-0.526936	-3.748091
C	0.603724	-1.430405	-4.781510
C	-0.570423	-1.977964	-4.347532
C	-0.857848	-1.398550	-3.054363
C	-2.347352	-0.995405	-1.146482
C	-3.604646	-1.160311	-0.450235
C	-3.586485	-0.305772	0.615190
C	-2.308573	0.372978	0.592723
C	-0.615156	1.834802	1.609386
C	-0.123067	2.665347	2.686538
C	1.180117	2.961679	2.400711
C	1.492659	2.317761	1.144403
C	2.985502	1.911310	-0.763515
C	4.221923	2.115209	-1.485317
C	4.073838	1.529778	-2.709850
C	2.752542	0.940684	-2.741989
C	2.253364	0.171551	-3.783300
H	2.871642	0.063865	-4.668110
C	-2.007081	-1.643959	-2.321260
H	-2.715984	-2.359975	-2.723583
C	-1.879595	1.270065	1.557949
H	-2.568528	1.506981	2.361937
C	2.710005	2.429245	0.488163
H	3.494004	2.994941	0.980907
C	1.788516	4.697709	-1.384753
C	1.189255	5.159959	-0.179664
C	-0.202390	4.925336	0.008970
C	-0.946983	4.270367	-0.940122
C	-0.327900	3.758210	-2.148818
C	1.059325	4.051939	-2.363691
C	2.038827	5.837057	0.762651
C	3.379257	5.996389	0.531237
C	4.010494	5.518117	-0.672475
O	3.139674	4.902854	-1.630958
O	1.538721	6.364147	1.937637
O	5.197642	5.626039	-0.984028
H	-0.685249	5.221490	0.936595
H	-1.993543	4.049494	-0.770733
H	-0.952752	3.678680	-3.033225
H	1.558105	3.729841	-3.268500
H	0.564943	6.376837	1.972541
H	1.133914	-1.616361	-5.704733
H	-1.203603	-2.698089	-4.846534
H	-4.387751	-1.838914	-0.757266
H	-4.348501	-0.146278	1.365302
H	-0.710982	2.968191	3.541513
H	1.875362	3.565907	2.966320
H	5.073044	2.656191	-1.098224
H	4.782474	1.485564	-3.524625
H	4.000658	6.513781	1.248704
*			
Warfarin C7 TS Doublet			
H	2.024583	-1.576414	-0.903607
S	1.171563	-1.214974	0.120288

O	-0.527541	1.903796	-1.960968
Fe	0.263577	0.693003	-1.016809
N	0.189341	-0.483098	-2.649097
N	-1.553713	0.027564	-0.456793
N	0.401072	1.717042	0.688572
N	2.113746	1.240264	-1.500495
C	1.088663	-0.490755	-3.700301
C	0.638920	-1.410689	-4.723447
C	-0.529770	-1.961156	-4.279424
C	-0.818218	-1.366965	-2.991110
C	-2.323692	-0.923243	-1.102814
C	-3.597176	-1.062795	-0.428153
C	-3.598472	-0.178225	0.612476
C	-2.314892	0.491919	0.598614
C	-0.611286	1.934450	1.614200
C	-0.101854	2.712779	2.719034
C	1.230249	2.928832	2.477246
C	1.532948	2.319432	1.203496
C	3.015256	1.942838	-0.712207
C	4.237769	2.174200	-1.447633
C	4.074344	1.611709	-2.680506
C	2.760722	1.007175	-2.705328
C	2.272112	0.229054	-3.743114
H	2.892333	0.126234	-4.626914
C	-1.971850	-1.596488	-2.260127
H	-2.679391	-2.318461	-2.654430
C	-1.889682	1.406066	1.549781
H	-2.582984	1.667284	2.342196
C	2.759296	2.413869	0.560836
H	3.554545	2.945178	1.070656
C	1.745079	4.695817	-1.503685
C	1.147275	5.065083	-0.269696
C	-0.241520	4.835573	-0.095613
C	-0.982698	4.227021	-1.083034
C	-0.349041	3.748339	-2.287799
C	1.027772	4.062513	-2.500889
C	2.001357	5.659601	0.729337
C	3.315989	5.930262	0.473343
C	3.937316	5.575181	-0.778668
O	3.081485	4.974698	-1.755321
O	1.510844	5.963088	1.981828
O	5.128029	5.691446	-1.075728
H	-0.732654	5.157410	0.816264
H	-2.041871	4.044825	-0.949268
H	-0.968095	3.584897	-3.161859
H	1.524645	3.793209	-3.423504
H	0.751799	5.392317	2.222106
H	1.167081	-1.602747	-5.646490
H	-1.159493	-2.691378	-4.767931
H	-4.377582	-1.745177	-0.734032
H	-4.375846	0.005950	1.340789
H	-0.685112	2.998045	3.583909
H	1.954217	3.445132	3.091802
H	5.075992	2.746246	-1.076865
H	4.769522	1.594412	-3.507648
H	3.945990	6.364109	1.237229
*			
Warfarin C6 TS Quartet			
H	2.003940	-1.531819	-1.034412
S	1.310890	-1.159152	0.100146

O	-0.623520	2.025679	-1.632825
Fe	0.164081	0.640372	-0.922804
N	-0.030664	-0.406079	-2.604825
N	-1.589264	-0.040534	-0.274883
N	0.443793	1.597147	0.830760
N	1.997308	1.253207	-1.525611
C	0.799948	-0.362467	-3.715730
C	0.276183	-1.225888	-4.752597
C	-0.860136	-1.801291	-4.260032
C	-1.057338	-1.278898	-2.925116
C	-2.407065	-0.961785	-0.902522
C	-3.613107	-1.160529	-0.126278
C	-3.527829	-0.342280	0.963119
C	-2.257730	0.347721	0.877846
C	-0.492645	1.763529	1.831529
C	0.078058	2.534280	2.913690
C	1.379210	2.801698	2.570087
C	1.598761	2.228710	1.262841
C	2.933488	1.948947	-0.779007
C	4.106623	2.213657	-1.583486
C	3.872154	1.678222	-2.817786
C	2.560000	1.068796	-2.773744
C	1.987527	0.343606	-3.808707
H	2.541065	0.273853	-4.739029
C	-2.148701	-1.564608	-2.122624
H	-2.880767	-2.270462	-2.500466
C	-1.766816	1.209099	1.840905
H	-2.398192	1.417141	2.698174
C	2.761789	2.381458	0.524581
H	3.580976	2.922105	0.985953
C	2.147579	4.907523	-1.540881
C	1.207691	4.950969	-0.479032
C	-0.076577	4.450037	-0.692984
C	-0.426251	3.819029	-1.932525
C	0.552002	3.853104	-2.999715
C	1.814543	4.362363	-2.795087
C	1.647555	5.572451	0.759607
C	2.893716	6.111118	0.880297
C	3.863816	6.058101	-0.184337
O	3.419918	5.415923	-1.398675
O	0.798656	5.658771	1.837980
O	5.024417	6.462569	-0.167472
H	-0.835471	4.529153	0.077584
H	-1.473768	3.835324	-2.215759
H	0.278926	3.426824	-3.957367
H	2.570591	4.358518	-3.569611
H	0.202846	4.881949	1.907757
H	0.740382	-1.368760	-5.718039
H	-1.523289	-2.505564	-4.742392
H	-4.411399	-1.834912	-0.402174
H	-4.237704	-0.214681	1.768350
H	-0.441363	2.787973	3.827329
H	2.123064	3.350627	3.128780
H	4.969870	2.764817	-1.240246
H	4.517526	1.677943	-3.684812
H	3.201703	6.570708	1.808979
*			
Warfarin C7 TS Doublet			
H	1.987254	-1.547929	-1.045926
S	1.186684	-1.263022	0.042207

O	-0.665570	1.951747	-1.713485
Fe	0.215053	0.691254	-0.926589
N	0.003817	-0.392228	-2.613035
N	-1.556457	-0.010155	-0.261156
N	0.481016	1.649032	0.799195
N	2.024654	1.265425	-1.527693
C	0.821316	-0.352095	-3.726330
C	0.286217	-1.213753	-4.760473
C	-0.850211	-1.780514	-4.258560
C	-1.033444	-1.254884	-2.921273
C	-2.376306	-0.924988	-0.892940
C	-3.590006	-1.109242	-0.123391
C	-3.505141	-0.284969	0.961777
C	-2.228451	0.394169	0.876816
C	-0.456753	1.813021	1.808159
C	0.128161	2.557507	2.899528
C	1.436407	2.800377	2.564603
C	1.648596	2.243568	1.251200
C	2.977606	1.943238	-0.784177
C	4.146712	2.197434	-1.594805
C	3.896094	1.675530	-2.831978
C	2.581064	1.076239	-2.784609
C	2.009552	0.355636	-3.820445
H	2.563330	0.289179	-4.750756
C	-2.123802	-1.528386	-2.114022
H	-2.863282	-2.227755	-2.489653
C	-1.732036	1.268467	1.828179
H	-2.357768	1.487609	2.686780
C	2.819374	2.372375	0.521809
H	3.651327	2.887706	0.988590
C	2.096664	4.860895	-1.517535
C	1.153981	4.911268	-0.458646
C	-0.134229	4.419098	-0.679964
C	-0.486218	3.824483	-1.927284
C	0.491914	3.837332	-2.985196
C	1.764971	4.321813	-2.773366
C	1.589066	5.539390	0.778056
C	2.836619	6.073839	0.902125
C	3.813602	6.004393	-0.154439
O	3.368850	5.363927	-1.371675
O	0.730444	5.646396	1.846790
O	4.978348	6.394785	-0.133490
H	-0.892847	4.499514	0.090693
H	-1.534937	3.797543	-2.195530
H	0.215387	3.417092	-3.944340
H	2.526441	4.302415	-3.541969
H	0.142277	4.865383	1.932441
H	0.742278	-1.360360	-5.729180
H	-1.522253	-2.480530	-4.734797
H	-4.392506	-1.777743	-0.401356
H	-4.219394	-0.145183	1.761086
H	-0.387348	2.806041	3.816877
H	2.190044	3.323827	3.134387
H	5.019039	2.735431	-1.253779
H	4.535705	1.673660	-3.703230
H	3.140098	6.541007	1.828463
*			
Diclofenac C4' RC Quartet			
H	0.167354	-0.853409	2.682073
S	0.091414	0.452360	2.236966

O	0.056626	-0.566796	-1.813571
Fe	-0.029106	-0.151339	-0.215473
N	-0.835569	-1.920361	0.302760
N	-1.865575	0.637282	-0.401769
N	0.775774	1.672918	-0.487660
N	1.791065	-0.862408	0.276743
C	-0.161192	-3.090784	0.601546
C	-1.100157	-4.174126	0.787348
C	-2.350486	-3.652231	0.605734
C	-2.181032	-2.249426	0.300739
C	-3.071247	-0.031034	-0.288678
C	-4.168004	0.866605	-0.577346
C	-3.618423	2.082687	-0.870366
C	-2.184074	1.932380	-0.758178
C	0.104030	2.832914	-0.846821
C	1.048239	3.906260	-1.066836
C	2.293659	3.393765	-0.841230
C	2.119034	2.005166	-0.477078
C	3.000657	-0.176070	0.224555
C	4.088353	-1.059255	0.567733
C	3.547008	-2.289897	0.807114
C	2.119798	-2.171255	0.619166
C	1.215313	-3.208046	0.745943
H	1.610265	-4.187921	0.992236
C	-3.219101	-1.369238	0.040946
H	-4.229583	-1.762838	0.086765
C	-1.268206	2.953989	-0.970390
H	-1.660859	3.925264	-1.252550
C	3.154681	1.144599	-0.148303
H	4.165134	1.535204	-0.189749
C	4.977062	-2.813049	-2.996549
C	4.307087	-1.580065	-2.835403
C	2.926504	-1.478574	-2.706925
C	2.147358	-2.641016	-2.748745
C	2.759632	-3.885904	-2.923512
C	4.146627	-3.951930	-3.035438
Cl	5.277649	-0.030489	-2.831481
H	2.448065	-0.516524	-2.582193
H	1.073365	-2.547481	-2.641579
H	2.173310	-4.796119	-2.963547
Cl	4.920516	-5.597967	-3.232678
C	9.104076	-1.684896	-0.153510
C	9.492848	-1.735536	-1.496925
C	8.590960	-2.116487	-2.499937
C	7.273430	-2.483124	-2.143358
C	6.884999	-2.432364	-0.793025
C	7.789430	-2.028838	0.191237
H	9.812439	-1.378300	0.609040
H	10.503007	-1.455758	-1.783125
N	6.369304	-2.902197	-3.142142
H	5.873735	-2.717002	-0.531595
H	7.472913	-2.000482	1.230325
H	6.733156	-3.572953	-3.816217
C	9.005141	-2.075254	-3.962322
H	9.907662	-1.473430	-4.084857
H	8.185127	-1.629906	-4.543473
C	9.245459	-3.455851	-4.520079
O	8.378250	-4.331035	-4.661813
O	10.559492	-3.680610	-4.848334
H	-0.821306	-5.188939	1.032779

H	-3.306137	-4.153104	0.668081
H	-5.211001	0.584072	-0.555390
H	-4.117632	3.003306	-1.136851
H	0.773696	4.911021	-1.354344
H	3.251006	3.890813	-0.905015
H	5.126861	-0.764261	0.579239
H	4.051577	-3.207478	1.074409
H	10.681290	-4.596414	-5.184869
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Diclofenac C4' RC Doublet			
H	0.162323	-0.854225	2.689111
S	0.087871	0.454001	2.250616
O	0.092757	-0.564809	-1.813406
Fe	-0.039874	-0.146962	-0.221631
N	-0.847486	-1.915387	0.296951
N	-1.871897	0.643716	-0.404856
N	0.770314	1.677122	-0.483890
N	1.783653	-0.859433	0.282706
C	-0.173879	-3.085048	0.600713
C	-1.113645	-4.168364	0.782536
C	-2.363360	-3.647365	0.592582
C	-2.192525	-2.244863	0.287442
C	-3.079192	-0.023003	-0.293090
C	-4.174492	0.880398	-0.567562
C	-3.622915	2.098157	-0.851005
C	-2.188662	1.943041	-0.747986
C	0.101090	2.838640	-0.842155
C	1.047886	3.908886	-1.066484
C	2.292418	3.392153	-0.845932
C	2.114953	2.004408	-0.479156
C	2.994703	-0.177558	0.223208
C	4.081609	-1.064560	0.560704
C	3.537120	-2.292831	0.804748
C	2.109211	-2.169303	0.622889
C	1.202026	-3.203570	0.750440
H	1.594470	-4.184105	0.998161
C	-3.229251	-1.363137	0.026984
H	-4.240243	-1.755790	0.069340
C	-1.271262	2.963506	-0.959578
H	-1.662977	3.936818	-1.235936
C	3.150004	1.142829	-0.151039
H	4.160996	1.531518	-0.196826
C	4.986819	-2.826844	-2.999871
C	4.311530	-1.597198	-2.835050
C	2.932283	-1.504256	-2.693877
C	2.158784	-2.671236	-2.730283
C	2.775889	-3.912536	-2.913146
C	4.162412	-3.970131	-3.035306
Cl	5.272924	-0.042000	-2.838022
H	2.442236	-0.548904	-2.562479
H	1.086081	-2.580732	-2.608008
H	2.194970	-4.826384	-2.949819
Cl	4.944732	-5.611592	-3.239391
C	9.106173	-1.673754	-0.159235
C	9.496524	-1.725915	-1.502084
C	8.597435	-2.112819	-2.505306
C	7.281118	-2.484309	-2.149252
C	6.891177	-2.432147	-0.799108
C	7.792656	-2.022462	0.185170
H	9.812504	-1.362142	0.603161

H	10.505645	-1.442066	-1.787917
N	6.379252	-2.908244	-3.148215
H	5.879992	-2.719852	-0.540100
H	7.474838	-1.993398	1.223828
H	6.746083	-3.578551	-3.821070
C	9.012405	-2.071124	-3.967497
H	9.913141	-1.466578	-4.089745
H	8.191342	-1.628652	-4.549368
C	9.257434	-3.451246	-4.524429
O	8.392128	-4.327548	-4.670790
O	10.572681	-3.672767	-4.849955
H	-0.835917	-5.182616	1.031550
H	-3.319111	-4.148539	0.650718
H	-5.218249	0.600979	-0.542310
H	-4.121149	3.022766	-1.105170
H	0.775574	4.914356	-1.353580
H	3.251156	3.885924	-0.914072
H	5.120771	-0.771888	0.569762
H	4.039618	-3.211727	1.071235
H	10.697122	-4.587916	-5.187317

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Diclofenac C4' TS Quartet

H	-1.392868	-0.398107	1.811586
S	-0.077933	-0.548615	2.206391
O	1.477482	-0.512119	-1.609739
Fe	0.864023	-0.445822	-0.020806
N	0.126969	-2.334582	-0.156266
N	-0.906256	0.262372	-0.681734
N	1.536885	1.414490	0.210295
N	2.540282	-1.158465	0.808966
C	0.765913	-3.499219	0.231283
C	-0.062145	-4.642867	-0.077029
C	-1.205128	-4.164782	-0.656814
C	-1.086722	-2.723074	-0.696663
C	-1.979435	-0.477908	-1.159888
C	-3.019463	0.411023	-1.628281
C	-2.570452	1.687968	-1.436727
C	-1.248659	1.589004	-0.859141
C	0.860588	2.588483	-0.088734
C	1.709550	3.730599	0.180014
C	2.896642	3.245553	0.645601
C	2.783079	1.801937	0.672043
C	3.653548	-0.432766	1.194921
C	4.687302	-1.324811	1.671391
C	4.193751	-2.594030	1.576618
C	2.855161	-2.490543	1.039988
C	2.032773	-3.572177	0.784992
H	2.421939	-4.557701	1.012035
C	-2.059425	-1.861271	-1.180261
H	-2.964879	-2.303665	-1.582431
C	-0.431972	2.673804	-0.570563
H	-0.832304	3.664562	-0.758451
C	3.771021	0.946487	1.128151
H	4.699369	1.387740	1.474471
C	3.960152	-2.491172	-3.221669
C	3.540625	-1.315951	-3.904658
C	2.223649	-0.917826	-3.957578
C	1.245229	-1.670712	-3.254229
C	1.586416	-2.969063	-2.795468
C	2.917531	-3.335544	-2.766822

Cl	4.771472	-0.297136	-4.790100
H	1.949178	0.003862	-4.453005
H	0.200196	-1.400137	-3.331467
H	0.825813	-3.633919	-2.411376
Cl	3.363663	-4.972912	-2.079127
C	7.964403	-0.046428	-1.190513
C	8.449092	-1.069071	-2.014076
C	7.575289	-1.968339	-2.639663
C	6.187390	-1.851302	-2.409381
C	5.698961	-0.825779	-1.579469
C	6.583263	0.072975	-0.983433
H	8.654102	0.650285	-0.724944
H	9.516266	-1.163533	-2.197157
N	5.299098	-2.785273	-3.001004
H	4.631627	-0.745882	-1.400281
H	6.185802	0.858942	-0.349245
H	5.570675	-3.763376	-2.909143
C	8.113581	-3.018951	-3.597791
H	9.128968	-2.766698	-3.908369
H	7.463230	-3.054055	-4.483567
C	8.106040	-4.398486	-2.986555
O	7.092156	-5.009014	-2.613822
O	9.361312	-4.937146	-2.859626
H	0.215910	-5.667411	0.123558
H	-2.060615	-4.717773	-1.018150
H	-3.962254	0.082672	-2.042307
H	-3.068248	2.619263	-1.666379
H	1.413563	4.758625	0.025734
H	3.774869	3.793507	0.956367
H	5.660991	-1.002790	2.009768
H	4.677064	-3.526696	1.828671
H	9.317657	-5.828420	-2.446696

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Diclofenac C4' TS Doublet

H	0.146133	-1.487677	2.550866
S	-0.107179	-0.196470	2.130900
O	1.807866	-0.592801	-1.469945
Fe	0.899042	-0.475249	-0.012070
N	0.197979	-2.340396	-0.099432
N	-0.763141	0.197262	-0.901906
N	1.554909	1.422027	0.195666
N	2.550064	-1.140743	0.946577
C	0.875211	-3.499098	0.259824
C	0.052738	-4.651008	-0.018218
C	-1.127823	-4.189490	-0.535204
C	-1.032392	-2.749882	-0.592032
C	-1.868562	-0.549763	-1.281018
C	-2.855964	0.310149	-1.894065
C	-2.344845	1.577660	-1.882922
C	-1.045141	1.507387	-1.252901
C	0.960786	2.562420	-0.310842
C	1.765873	3.721970	0.012498
C	2.842967	3.274218	0.721912
C	2.712718	1.835306	0.827932
C	3.580495	-0.373689	1.457323
C	4.618931	-1.235439	1.983736
C	4.215062	-2.522650	1.775525
C	2.918586	-2.460489	1.134770
C	2.145637	-3.560535	0.808088
H	2.555301	-4.543254	1.011149

C	-2.002024	-1.918993	-1.130796
H	-2.919959	-2.378111	-1.481430
C	-0.239190	2.605497	-0.999768
H	-0.592663	3.574608	-1.334669
C	3.647983	1.009132	1.428251
H	4.514224	1.478538	1.882598
C	3.828242	-2.436584	-3.304451
C	3.451575	-1.201867	-3.914094
C	2.165402	-0.726802	-3.872467
C	1.191060	-1.458345	-3.119731
C	1.459232	-2.832574	-2.819616
C	2.755384	-3.279169	-2.899485
Cl	4.710291	-0.210081	-4.786627
H	1.916120	0.237435	-4.294323
H	0.166038	-1.110615	-3.095008
H	0.677068	-3.474120	-2.439032
Cl	3.144863	-4.979286	-2.354615
C	7.786013	-0.144002	-1.063662
C	8.283534	-1.095938	-1.961359
C	7.419094	-1.954856	-2.653344
C	6.032610	-1.862328	-2.416805
C	5.527669	-0.911765	-1.511272
C	6.404299	-0.053419	-0.846263
H	8.468988	0.520931	-0.544532
H	9.352083	-1.166551	-2.146901
N	5.146124	-2.767586	-3.070036
H	4.457716	-0.854132	-1.328041
H	5.999012	0.673138	-0.149879
H	5.400762	-3.752531	-2.991795
C	7.967038	-2.938683	-3.674320
H	8.983899	-2.665180	-3.961026
H	7.325032	-2.917696	-4.566681
C	7.958899	-4.356180	-3.154933
O	6.949652	-4.977168	-2.786267
O	9.208586	-4.918151	-3.110086
H	0.355881	-5.671809	0.164424
H	-1.988857	-4.756467	-0.859752
H	-3.809009	-0.029897	-2.273286
H	-2.795539	2.489441	-2.248285
H	1.517288	4.734727	-0.271376
H	3.661909	3.843816	1.137883
H	5.536065	-0.880196	2.430923
H	4.728102	-3.440240	2.024864
H	9.167000	-5.834876	-2.756883

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Diclofenac C5 RC Doublet

H	-0.427618	0.332529	2.501710
S	-0.086952	0.902202	1.290281
O	0.099735	-2.776150	-0.704800
Fe	-0.086708	-1.301554	0.013984
N	-1.411588	-2.003657	1.353584
N	-1.591210	-0.727037	-1.180298
N	1.221920	-0.346756	-1.184352
N	1.401086	-1.619459	1.341169
C	-1.130814	-2.640304	2.548267
C	-2.352834	-3.104326	3.165899
C	-3.378476	-2.744996	2.336808
C	-2.786828	-2.066270	1.205780
C	-2.941191	-0.961853	-0.988867
C	-3.697146	-0.484107	-2.125775

C	-2.795810	0.037585	-3.009984
C	-1.487071	-0.113240	-2.412951
C	0.949291	0.233085	-2.415436
C	2.169280	0.733997	-3.009472
C	3.182756	0.450226	-2.139802
C	2.588865	-0.221409	-1.005565
C	2.750620	-1.338722	1.171869
C	3.509015	-1.858941	2.285763
C	2.622457	-2.465051	3.129232
C	1.309747	-2.320493	2.541061
C	0.137035	-2.798889	3.094084
H	0.209486	-3.327807	4.038475
C	-3.498105	-1.573514	0.123233
H	-4.576907	-1.692277	0.139463
C	-0.304926	0.328695	-2.991601
H	-0.372589	0.800056	-3.966225
C	3.302395	-0.690890	0.083823
H	4.378474	-0.566790	0.067853
C	7.476692	-2.442353	-3.360445
C	7.929266	-1.553267	-2.356997
C	9.275305	-1.376253	-2.048033
C	10.250948	-2.065941	-2.774931
C	9.860958	-2.924459	-3.808683
C	8.507519	-3.102150	-4.073333
C1	6.737839	-0.498685	-1.460033
H	9.554242	-0.682735	-1.263597
H	11.301682	-1.927310	-2.546526
H	10.596159	-3.463427	-4.393548
C1	8.054679	-4.266003	-5.412972
C	3.051509	-3.762027	-1.010353
C	2.750539	-3.189949	-2.249403
C	3.764931	-2.782775	-3.126451
C	5.114757	-2.980453	-2.757741
C	5.416950	-3.556281	-1.512115
C	4.391516	-3.936375	-0.642564
H	2.239162	-4.020705	-0.342431
H	1.711516	-3.014887	-2.506685
N	6.137112	-2.634885	-3.681562
H	6.455949	-3.709153	-1.238990
H	4.640610	-4.367584	0.322192
H	5.935370	-2.910489	-4.640138
C	3.395233	-2.097415	-4.433303
H	4.126390	-1.307350	-4.647731
H	2.404250	-1.650113	-4.343332
C	3.360075	-3.047133	-5.603780
O	4.644722	-3.487523	-5.925748
O	2.374613	-3.427589	-6.231539
H	-2.399884	-3.628932	4.109407
H	-4.438151	-2.919979	2.459349
H	-4.772365	-0.550436	-2.216936
H	-2.979223	0.489105	-3.974351
H	2.221503	1.231549	-3.967453
H	4.238846	0.650798	-2.241234
H	4.581295	-1.766111	2.384217
H	2.817875	-2.966331	4.066422
H	4.633042	-4.147274	-6.650853
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Diclofenac C5 RC Quartet			
H	-0.371341	0.359774	2.479953
S	-0.115502	0.912567	1.239767

O	0.085877	-2.775352	-0.721417
Fe	-0.072182	-1.307561	0.022199
N	-1.400045	-2.012653	1.354788
N	-1.576763	-0.742869	-1.184593
N	1.238120	-0.353436	-1.177168
N	1.408763	-1.623268	1.348920
C	-1.124273	-2.639951	2.555826
C	-2.348004	-3.104039	3.169872
C	-3.369999	-2.753827	2.332638
C	-2.774565	-2.080289	1.200378
C	-2.925546	-0.987245	-1.000612
C	-3.678322	-0.519299	-2.144230
C	-2.775790	0.007758	-3.023643
C	-1.469422	-0.130406	-2.417106
C	0.965011	0.234535	-2.404462
C	2.183152	0.750122	-2.989709
C	3.196418	0.464576	-2.120416
C	2.603680	-0.219912	-0.993441
C	2.757939	-1.336292	1.185019
C	3.512710	-1.840954	2.308350
C	2.624141	-2.441017	3.154152
C	1.314592	-2.309315	2.556789
C	0.141151	-2.788033	3.109172
H	0.211540	-3.306762	4.059320
C	-3.483438	-1.596504	0.112097
H	-4.561620	-1.721093	0.124769
C	-0.287315	0.323547	-2.986185
H	-0.353274	0.799844	-3.958564
C	3.313669	-0.689941	0.097496
H	4.389447	-0.561498	0.087268
C	7.464754	-2.440796	-3.358677
C	7.921505	-1.561023	-2.348744
C	9.268504	-1.392591	-2.038495
C	10.241105	-2.081568	-2.769847
C	9.847170	-2.930284	-3.810249
C	8.493114	-3.099368	-4.076657
Cl	6.737024	-0.502516	-1.446966
H	9.550272	-0.705581	-1.249372
H	11.292461	-1.949457	-2.540399
H	10.579887	-3.468275	-4.399149
Cl	8.036012	-4.251621	-5.425033
C	3.029614	-3.759227	-1.025367
C	2.732824	-3.179606	-2.261805
C	3.750870	-2.772942	-3.135078
C	5.099313	-2.975799	-2.764313
C	5.396828	-3.560479	-1.521586
C	4.368373	-3.941867	-0.656567
H	2.217542	-4.019882	-0.358146
H	1.695173	-2.998479	-2.520697
N	6.124825	-2.626156	-3.682715
H	6.434763	-3.718199	-1.247335
H	4.613574	-4.379787	0.306191
H	5.924142	-2.892041	-4.644315
C	3.385437	-2.084864	-4.442008
H	4.121071	-1.299376	-4.656804
H	2.397023	-1.632169	-4.351216
C	3.343596	-3.037215	-5.610101
O	4.627319	-3.473193	-5.941688
O	2.354075	-3.425320	-6.226631
H	-2.398689	-3.622572	4.116532

H	-4.429697	-2.931800	2.450401
H	-4.752272	-0.595089	-2.242400
H	-2.956580	0.455491	-3.990243
H	2.234856	1.256975	-3.942843
H	4.251077	0.673828	-2.217579
H	4.583779	-1.740876	2.412647
H	2.816521	-2.929916	4.098432
H	4.612848	-4.136566	-6.663398

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Diclofenac C5 TS Quartet

H	0.483217	0.120127	2.299811
S	0.363517	0.739612	1.070898
O	0.524132	-2.747870	-1.107317
Fe	0.403030	-1.284710	-0.181182
N	-0.578441	-2.218307	1.280724
N	-1.317851	-0.822940	-1.071519
N	1.403932	-0.221922	-1.575295
N	2.150313	-1.655881	0.772059
C	-0.027046	-2.980791	2.300862
C	-1.083416	-3.548191	3.111291
C	-2.268468	-3.118363	2.585178
C	-1.951151	-2.301694	1.433187
C	-2.590671	-1.093875	-0.604992
C	-3.574691	-0.635801	-1.564036
C	-2.888956	-0.100034	-2.616209
C	-1.478753	-0.204891	-2.301935
C	0.879714	0.328802	-2.726593
C	1.922826	1.004505	-3.467128
C	3.077442	0.868094	-2.745640
C	2.751060	0.090348	-1.570301
C	3.393909	-1.145255	0.452469
C	4.389843	-1.680325	1.354614
C	3.741361	-2.528806	2.208870
C	2.338596	-2.495366	1.852180
C	1.325855	-3.139435	2.549843
H	1.611799	-3.764583	3.389476
C	-2.890974	-1.754526	0.574698
H	-3.938423	-1.900979	0.816917
C	-0.461001	0.306414	-3.087406
H	-0.738263	0.780320	-4.023106
C	3.673838	-0.317445	-0.620607
H	4.699674	0.003058	-0.753387
C	6.670535	-2.392618	-2.388087
C	7.434524	-1.261952	-2.025463
C	8.639561	-1.346252	-1.335538
C	9.130551	-2.606418	-0.975453
C	8.434650	-3.759075	-1.353981
C	7.244304	-3.644756	-2.070220
Cl	6.841929	0.399518	-2.502710
H	9.177778	-0.442093	-1.079361
H	10.060446	-2.689604	-0.424683
H	8.824400	-4.743106	-1.124045
Cl	6.492118	-5.180354	-2.688670
C	1.717949	-3.915966	-1.963248
C	1.908335	-3.264045	-3.229173
C	3.109294	-2.679977	-3.583746
C	4.229958	-2.799130	-2.703594
C	4.070863	-3.469744	-1.464703
C	2.866700	-4.037335	-1.111189
H	0.936583	-4.664164	-1.887289

H	1.060311	-3.185894	-3.900039
N	5.453724	-2.244746	-3.070891
H	4.910411	-3.528007	-0.784797
H	2.764639	-4.541467	-0.158143
H	5.480952	-1.648464	-3.889368
C	3.203532	-1.900311	-4.888096
H	3.546399	-0.878358	-4.695748
H	2.201124	-1.835712	-5.320806
C	4.098685	-2.553918	-5.915705
O	5.339580	-1.920206	-5.975330
O	3.829623	-3.521601	-6.622674
H	-0.917759	-4.179760	3.972883
H	-3.272880	-3.333837	2.921164
H	-4.643699	-0.730138	-1.432685
H	-3.280132	0.343563	-3.521048
H	1.768981	1.525821	-4.401683
H	4.064542	1.245101	-2.968670
H	5.441802	-1.433616	1.315211
H	4.150983	-3.109818	3.023463
H	5.931573	-2.369855	-6.617305

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Diclofenac C5 TS Doublet

H	-0.140690	0.177725	2.195137
S	0.272386	0.755602	1.011578
O	0.401646	-2.768414	-1.087797
Fe	0.477679	-1.298006	-0.221644
N	-0.526690	-2.211611	1.271375
N	-1.280848	-0.830176	-1.104515
N	1.450053	-0.231850	-1.592808
N	2.200110	-1.674597	0.713720
C	0.023221	-2.977175	2.283220
C	-1.030726	-3.555229	3.089596
C	-2.216934	-3.134115	2.558099
C	-1.899902	-2.311754	1.409460
C	-2.548011	-1.121301	-0.640055
C	-3.538526	-0.670784	-1.598888
C	-2.858331	-0.119693	-2.646085
C	-1.446477	-0.211111	-2.326867
C	0.910604	0.342828	-2.733031
C	1.940507	1.054440	-3.454342
C	3.097818	0.926210	-2.735414
C	2.790140	0.113987	-1.581160
C	3.442215	-1.148537	0.414277
C	4.434736	-1.678300	1.321723
C	3.786317	-2.533368	2.168668
C	2.385689	-2.507621	1.805970
C	1.379858	-3.141429	2.517309
H	1.673158	-3.763863	3.356435
C	-2.841128	-1.782398	0.540801
H	-3.887503	-1.943844	0.778756
C	-0.425950	0.315202	-3.100959
H	-0.699778	0.801847	-4.031154
C	3.718950	-0.296107	-0.638863
H	4.738568	0.047323	-0.757056
C	6.668936	-2.416187	-2.344395
C	7.414776	-1.269809	-1.996105
C	8.600451	-1.325415	-1.270047
C	9.090084	-2.571348	-0.862267
C	8.416001	-3.740129	-1.230263
C	7.244825	-3.654279	-1.981576

Cl	6.831726	0.370275	-2.548515
H	9.125661	-0.410568	-1.025168
H	10.004817	-2.631715	-0.283641
H	8.808110	-4.714123	-0.964760
Cl	6.523448	-5.211138	-2.583432
C	1.733595	-3.972111	-1.997165
C	1.907460	-3.262316	-3.220808
C	3.110292	-2.666003	-3.561015
C	4.232992	-2.821289	-2.689956
C	4.063346	-3.500584	-1.458028
C	2.854844	-4.078508	-1.125414
H	0.912272	-4.668778	-1.901215
H	1.057785	-3.157786	-3.885974
N	5.465351	-2.295461	-3.059925
H	4.894352	-3.562789	-0.768805
H	2.747736	-4.599056	-0.181708
H	5.520249	-1.775934	-3.928654
C	3.193065	-1.832472	-4.833459
H	3.626214	-0.850814	-4.616796
H	2.177636	-1.670576	-5.203604
C	3.977753	-2.502782	-5.936148
O	5.303873	-2.068994	-5.938896
O	3.566640	-3.334781	-6.740605
H	-0.863833	-4.189670	3.948811
H	-3.221341	-3.360981	2.886566
H	-4.606395	-0.779131	-1.468944
H	-3.252819	0.325261	-3.548770
H	1.775790	1.595196	-4.375919
H	4.076226	1.329965	-2.949137
H	5.484422	-1.420885	1.292619
H	4.193031	-3.109994	2.987784
H	5.827284	-2.537174	-6.625148

*

C. QM/MM calculations

i) Absolute energies [in atomic units] of reactant complexes and transition states, calculated at the B3LYP-D/CHARMM level. Energies calculated at with the LACVP* basis set are shown in bold, with energies calculated at the LACV3P++**//LACVP level shown in regular typeface.

Table S8 Ibuprofen

		RC		TS	
		doublet	quartet	doublet	quartet
2-1	BSI	-2286.955355	-2286.521954	-2286.910578	-2286.476634
	BSII	-2287.515009	-2287.502268	-2287.473023	-2287.457494
2-2	BSI	-2287.043379	-2286.608058	-2287.604303	-2286.55545
	BSII	-2286.985999	-2287.591834	-2287.554257	-2287.540055
2-3	BSI	-2287.024093	-2286.590105	-2286.977048	-2286.542246
	BSII	-2287.583164	-2287.570744	-2287.541497	-2287.523461
3-1	BSI	-2286.416476	-2286.40992	-2286.384964	-2286.376522
	BSII	-2287.403479	-2295.430582	-2287.374527	-2295.401698
3-2	BSI	-2286.860355	-2286.428147	-2286.823007	-2286.393763
	BSII	-2287.424246	-2287.41099	-2287.392628	-2287.381282
3-3	BSI	-2286.904600	-2286.469328	-2286.86455	-2286.430798
	BSII	-2287.468958	-2287.453727	-2287.433062	-2287.419681
3-4	BSI	-2286.860751	-2286.427416	-2286.825046	-2286.392653
	BSII	-2287.423835	-2287.411053	-2287.391643	-2287.37970
3-5	BSI	-2286.879387	-2286.447364	-2286.841048	-2286.412373
	BSII	-2287.445561	-2287.433607	-2287.412326	-2287.40171
3-6	BSI	-2286.812164	-2286.379916	-2286.769279	-2286.339058
	BSII	-2287.371834	-2287.359169	-2287.332635	-2287.32341

Table S9 Warfarin

		RC		TS	
		doublet	quartet	doublet	quartet
6-1	BSI	-2202.392585	-2202.385102	-2202.358276	-2202.348133
	BSII	-2202.918713	-2202.911372	-2202.88278	-2202.875347
6-2	BSI	-2202.364383	-2202.357988	-2202.326595	-2202.31771
	BSII	-2202.890529	-2202.883129	-2202.85135	-2202.844846
6-3	BSI	-2202.382826	-2202.375396	-2202.347411	-2202.33789
	BSII	-2202.909296	-2202.901866	-2202.872383	-2202.865954
6-4	BSI	-2202.445216	-2202.438855	-2202.410457	-2202.401058
	BSII	-2202.971914	-2202.965043	-2202.935472	-2202.928054
6-5	BSI	-2202.280828	-2202.273439	-2202.23819	-2202.230446
	BSII	-2202.807494	-2202.799501	-2202.763219	-2202.757555
6-6	BSI	-2202.315557	-2202.308816	-2202.27922	-2202.269786
	BSII	-2202.841112	-2202.83381	-2202.803113	-2202.796459
6-7	BSI	-2202.363564	-2202.356474	-2202.328087	-2202.318658
	BSII	-2202.889813	-2202.883307	-2202.852665	-2202.845962
6-8	BSI	-2202.405586	-2202.399203	-2202.372868	-2202.362962
	BSII	-2202.932485	-2202.925761	-2202.89844	-2202.89105
6-9	BSI	-2202.474279	-2202.467601	-2202.439651	-2202.430155
	BSII	-2203.001004	-2202.993417	-2202.964637	-2202.957421
6-10	BSI	-2202.067967	-2202.061043	-2202.029947	-2202.021019
	BSII	-2202.595319	-2202.588081	-2202.555965	-2202.549263
7-1	BSI	-2202.348455	-2202.342585	-2202.318252	-2202.310651
	BSII	-2202.872546	-2202.866241	-2202.840791	-2202.836174
7-2	BSI	-2202.429379	-2202.423091	-2202.403411	-2202.395973
	BSII	-2202.952839	-2202.946445	-2202.925423	-2202.920714
7-3	BSI	-2202.171704	-2202.16535	-2202.146833	-2202.14002
	BSII	-2202.69559	-2202.688837	-2202.669034	-2202.665906
7-4	BSI	-2202.237821	-2202.231734	-2202.202903	-2202.195485
	BSII	-2202.761703	-2202.755236	-2202.725099	-2202.719995
7-5	BSI	-2202.525743	-2202.518398	-2202.494409	-2202.486709
	BSII	-2203.049975	-2203.041633	-2203.017144	-2203.012251
7-6	BSI	-2202.412531	-2202.4062	-2202.387847	-2202.38064
	BSII	-2202.936516	-2202.929492	-2202.911053	-2202.906257
7-7	BSI	-2202.463566	-2202.457326	-2202.439105	-2202.431333
	BSII	-2202.988041	-2202.981107	-2202.962034	-2202.956927
7-8	BSI	-2202.157169	-2202.150975	-2202.133097	-2202.125106
	BSII	-2202.680427	-2202.673767	-2202.655574	-2202.650477
7-9	BSI	-2202.215698	-2202.208695	-2202.191679	-2202.184385
	BSII	-2202.737061	-2202.730942	-2202.714501	-2202.709348
7-10	BSI	-2202.412531	-2202.4062	-2202.387847	-2202.38064
	BSII	-2202.936516	-2202.929492	-2202.911053	-2202.906257

Table S10 Diclofenac

		RC		TS	
		doublet	quartet	doublet	quartet
4'-1	BSI	-3298.292122	-3298.285393	-3298.262233	-3298.253394
	BSII	-3298.948266	-3298.940974	-3298.918288	-3298.909853
4'-2	BSI	-3298.265319	-3298.253606	-3298.235087	-3298.22453
	BSII	-3298.921329	-3298.909139	-3298.892236	-3298.881474
4'-3	BSI	-3298.303822	-	-3298.269364	-
	BSII	-3298.96073	-	-3298.925186	-
4'-4	BSI	-3298.818899	-	-3298.775636	-
	BSII	-3299.475896	-	-3299.432545	-
4'-5	BSI	-3299.104651	-	-3299.071813	-
	BSII	-3299.760286	-	-3299.727779	-
5-1	BSI	-3297.934156	-	-3297.905164	-
	BSII	-3298.591075	-	-3298.561209	-
5-2	BSI	-3298.112906	-	-3298.093736	-
	BSII	-3298.763581	-	-3298.74464	-
5-3	BSI	-3298.660293	-3298.653803	-3298.641555	-3298.627358
	BSII	-3299.31126	-3299.304474	-3299.292531	-3299.279393

ii) Mulliken charges and spin densities (calculated with BSI)

Table S11 Ibuprofen C2 Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Ibu	Fe	O	S	Por	Ibu
2-1	SPIN	1.15	0.79	0.50	0.55	0.01	1.41	0.46	0.34	0.59	0.18
	CHARGE	0.53	-0.36	-0.39	0.53	-1.11	0.63	-0.54	-0.52	-0.34	-0.92
2-2	SPIN	1.13	0.82	0.57	0.47	0.01	1.50	0.23	0.11	0.17	0.96
	CHARGE	0.47	-0.36	-0.33	0.53	-1.10	0.46	-0.58	-0.53	-0.24	-0.75
2-3	SPIN	1.15	0.79	0.52	0.53	0.01	1.37	0.47	0.39	0.62	0.15
	CHARGE	0.53	-0.36	-0.36	0.50	-1.11	0.65	-0.53	-0.49	-0.38	-0.95

Table S12 Ibuprofen C2 Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Ibu	Fe	O	S	Por	Ibu
2-1	SPIN	1.24	0.86	-0.57	-0.55	0.00	1.17	0.68	-0.54	-0.59	0.23
	CHARGE	0.47	-0.41	-0.29	0.48	-1.12	0.50	-0.54	-0.35	0.47	-0.96
2-2	SPIN	1.22	0.87	-0.64	-0.48	0.00	1.54	0.53	-0.53	-0.58	0.01
	CHARGE	0.44	-0.41	-0.22	0.47	-1.11	0.53	-0.55	-0.31	0.47	-0.99
2-3	SPIN	1.23	0.86	-0.57	-0.55	0.00	1.02	0.55	-0.56	-0.54	0.50
	CHARGE	0.50	-0.41	-0.27	0.44	-1.12	0.47	-0.60	-0.36	0.43	-0.83

Table S13 Ibuprofen C3 Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Ibu	Fe	O	S	Por	Ibu
3-1	SPIN	1.13	0.81	0.57	0.47	0.01	0.93	0.50	0.58	0.41	0.58
	CHARGE	0.50	-0.36	-0.33	0.51	-1.13	0.47	-0.54	-0.38	-0.37	-0.86
3-2	SPIN	1.15	0.79	0.51	0.54	0.01	0.93	0.51	0.54	0.45	0.56
	CHARGE	0.53	-0.36	-0.37	0.53	-1.12	0.48	-0.53	-0.42	-0.34	-0.86
3-3	SPIN	1.15	0.79	0.55	0.50	0.01	0.93	0.50	0.59	0.41	0.58
	CHARGE	0.55	-0.36	-0.34	0.47	-1.13	0.49	-0.54	-0.39	-0.39	-0.86
3-4	SPIN	1.15	0.78	0.51	0.54	0.01	0.92	0.50	0.53	0.46	0.58
	CHARGE	0.55	-0.36	-0.36	0.50	-1.12	0.48	-0.53	-0.41	-0.37	-0.85
3-5	SPIN	1.15	0.79	0.54	0.51	0.00	0.92	0.51	0.60	0.40	0.57
	CHARGE	0.54	-0.35	-0.34	0.48	-1.13	0.47	-0.54	-0.38	-0.38	-0.85
3-6	SPIN	1.13	0.81	0.58	0.46	0.01	1.00	0.47	0.48	0.41	0.64
	CHARGE	0.50	-0.36	-0.31	0.50	-1.16	0.46	-0.55	-0.43	-0.33	-0.85

Table S14 Ibuprofen C3 Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Ibu	Fe	O	S	Por	Ibu
3-1	SPIN	1.21	0.89	-0.64	-0.50	0.00	1.04	0.56	-0.69	-0.38	0.47
	CHARGE	0.49	-0.35	-0.30	0.49	-1.13	0.46	-0.53	-0.34	-0.39	-0.87
3-2	SPIN	1.24	0.86	-0.57	-0.55	0.00	1.03	0.53	-0.63	-0.44	0.51
	CHARGE	0.49	-0.41	-0.27	0.47	-1.12	0.40	-0.61	-0.30	-0.36	-0.81
3-3	SPIN	1.23	0.87	-0.64	-0.48	0.00	0.99	0.20	-0.75	-0.33	0.88
	CHARGE	0.49	-0.41	-0.22	0.41	-1.14	0.35	-0.67	-0.24	-0.40	-0.73
3-4	SPIN	1.24	0.86	-0.58	-0.54	0.00	0.99	0.34	-0.65	-0.42	0.74
	CHARGE	0.51	-0.41	-0.26	0.44	-1.13	0.38	-0.65	-0.28	-0.40	-0.73
3-5	SPIN	1.22	0.87	-0.61	-0.50	0.00	1.02	0.51	-0.69	-0.39	0.53
	CHARGE	0.49	-0.40	-0.24	0.42	-1.13	0.39	-0.61	-0.27	0.42	-0.80
3-6	SPIN	1.23	0.87	-0.66	-0.47	0.00	0.99	0.15	-0.70	-0.37	0.93
	CHARGE	0.46	-0.42	-0.21	0.43	-1.16	0.35	-0.67	-0.25	-0.38	-0.76

Table S15 Warfarin C6 Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Warf	Fe	O	S	Por	Warf
6-1	SPIN	1.11	0.83	0.35	0.67	0.03	1.32	0.57	0.31	0.38	0.43
	CHARGE	0.43	-0.40	-0.10	0.15	-0.09	0.49	-0.49	-0.07	-0.04	0.12
6-2	SPIN	1.12	0.83	0.34	0.68	0.03	1.29	0.57	0.32	0.42	0.39
	CHARGE	0.43	-0.41	-0.11	0.17	-0.09	0.48	-0.49	-0.06	0.00	0.08
6-3	SPIN	1.12	0.83	0.36	0.66	0.03	1.34	0.57	0.27	0.35	0.47
	CHARGE	0.41	-0.41	-0.05	0.14	-0.09	0.45	-0.50	-0.01	-0.06	0.12
6-4	SPIN	1.12	0.83	0.39	0.62	0.03	1.26	0.57	0.37	0.45	0.34
	CHARGE	0.43	-0.41	-0.05	0.12	-0.09	0.48	-0.48	-0.04	0.00	0.04
6-5	SPIN	1.13	0.82	0.38	0.64	0.03	1.31	0.57	0.35	0.39	0.38
	CHARGE	0.43	-0.41	-0.07	0.14	-0.09	0.48	-0.49	-0.05	-0.03	0.09
6-6	SPIN	1.11	0.84	0.36	0.66	0.03	1.32	0.56	0.30	0.37	0.44
	CHARGE	0.43	-0.40	-0.09	0.15	-0.09	0.48	-0.49	-0.06	-0.05	0.12
6-7	SPIN	1.11	0.84	0.36	0.67	0.03	1.33	0.57	0.29	0.36	0.46
	CHARGE	0.43	-0.40	-0.10	0.16	-0.08	0.48	-0.50	-0.07	-0.06	0.14
6-8	SPIN	1.11	0.84	0.35	0.67	0.03	1.30	0.58	0.30	0.41	0.41
	CHARGE	0.42	-0.40	-0.07	0.15	-0.10	0.46	-0.49	-0.04	-0.02	0.08
6-9	SPIN	1.12	0.83	0.39	0.63	0.03	1.28	0.57	0.37	0.45	0.34
	CHARGE	0.44	-0.40	-0.07	0.12	-0.08	0.49	-0.49	-0.05	0.00	0.04
6-10	SPIN	1.12	0.82	0.39	0.63	0.03	1.25	0.58	0.38	0.48	0.32
	CHARGE	0.43	-0.41	-0.08	0.13	-0.08	0.49	-0.48	-0.06	0.03	0.03

Table S16 Warfarin C6 Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Warf	Fe	O	S	Por	Warf
6-1	SPIN	1.17	0.90	-0.36	-0.72	0.00	1.07	0.54	-0.33	-0.59	0.31
	CHARGE	0.42	-0.40	-0.11	0.18	-0.09	0.42	-0.49	-0.09	0.02	0.14
6-2	SPIN	1.19	0.90	-0.34	-0.74	-0.01	1.08	0.56	-0.34	-0.63	0.32
	CHARGE	0.42	-0.40	-0.12	0.19	-0.10	0.42	-0.49	-0.09	0.06	0.10
6-3	SPIN	1.18	0.89	-0.37	-0.70	0.00	1.08	0.53	-0.31	-0.59	0.29
	CHARGE	0.40	-0.40	-0.06	0.16	-0.10	0.38	-0.49	-0.04	0.02	0.12
6-4	SPIN	1.18	0.89	-0.41	-0.66	-0.01	1.08	0.58	-0.40	-0.60	0.33
	CHARGE	0.42	-0.40	-0.06	0.14	-0.09	0.43	-0.48	-0.05	0.03	0.08
6-5	SPIN	1.20	0.89	-0.39	-0.69	0.00	1.11	0.58	-0.42	-0.58	0.31
	CHARGE	0.42	-0.40	-0.08	0.16	-0.09	0.45	-0.49	-0.08	0.02	0.09
6-6	SPIN	1.18	0.90	-0.38	-0.70	-0.01	1.08	0.55	-0.36	-0.59	0.32
	CHARGE	0.43	-0.40	-0.10	0.16	-0.09	0.43	-0.49	-0.08	0.02	0.13
6-7	SPIN	1.18	0.90	-0.37	-0.71	-0.01	1.07	0.54	-0.34	-0.59	0.31
	CHARGE	0.43	-0.39	-0.12	0.17	-0.09	0.43	-0.49	-0.10	0.01	0.14
6-8	SPIN	1.18	0.90	-0.36	-0.71	-0.01	1.08	0.54	-0.31	-0.59	0.29
	CHARGE	0.41	-0.40	-0.09	0.17	-0.10	0.40	-0.48	-0.06	0.03	0.11
6-9	SPIN	1.18	0.90	-0.40	-0.67	-0.01	1.07	0.58	-0.39	-0.60	0.34
	CHARGE	0.43	-0.40	-0.08	0.14	-0.09	0.43	-0.48	-0.07	0.03	0.08
6-10	SPIN	1.19	0.89	-0.40	-0.68	-0.01	1.10	0.59	-0.40	-0.60	0.31
	CHARGE	0.42	-0.40	-0.09	0.15	-0.08	0.44	-0.48	-0.08	0.05	0.07

Table S17 Warfarin C7 Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Warf	Fe	O	S	Por	Warf
7-1	SPIN	1.12	0.82	0.41	0.62	0.03	1.25	0.51	0.29	0.40	0.55
	CHARGE	0.44	-0.41	-0.07	0.12	-0.08	0.44	-0.49	-0.04	0.00	0.09
7-2	SPIN	1.12	0.82	0.44	0.58	0.04	1.23	0.51	0.32	0.40	0.54
	CHARGE	0.46	-0.40	-0.08	0.09	-0.08	0.46	-0.49	-0.06	-0.01	0.10
7-3	SPIN	1.11	0.83	0.42	0.60	0.04	1.29	0.49	0.28	0.33	0.60
	CHARGE	0.45	-0.40	-0.08	0.11	-0.08	0.46	-0.49	-0.06	-0.05	0.14
7-4	SPIN	1.13	0.82	0.37	0.65	0.03	1.29	0.51	0.27	0.40	0.54
	CHARGE	0.43	-0.42	-0.10	0.17	-0.08	0.45	-0.49	-0.06	0.09	0.02
7-5	SPIN	1.11	0.84	0.35	0.67	0.03	1.29	0.51	0.24	0.37	0.58
	CHARGE	0.43	-0.41	-0.07	0.14	-0.09	0.43	-0.50	-0.02	0.00	0.08
7-6	SPIN	1.11	0.84	0.35	0.67	0.03	1.29	0.51	0.24	0.37	0.58
	CHARGE	0.42	-0.40	-0.07	0.16	-0.10	0.43	-0.50	-0.02	-0.01	0.10
7-7	SPIN	1.12	0.83	0.35	0.67	0.03	1.26	0.52	0.27	0.48	0.55
	CHARGE	0.41	-0.41	-0.06	0.16	-0.10	0.43	-0.50	-0.03	0.07	0.03
7-8	SPIN	1.12	0.83	0.36	0.66	0.03	1.28	0.51	0.26	0.41	0.55
	CHARGE	0.42	-0.41	-0.08	0.15	-0.09	0.44	-0.50	-0.04	0.01	0.09
7-9	SPIN	1.12	0.82	0.42	0.60	0.03	1.18	0.52	0.34	0.49	0.47
	CHARGE	0.43	-0.41	-0.06	0.12	-0.09	0.44	-0.49	-0.03	0.06	0.02
7-10	SPIN	1.11	0.84	0.35	0.67	0.03	1.29	0.51	0.24	0.37	0.58
	CHARGE	0.42	-0.40	-0.07	0.16	-0.10	0.43	-0.50	-0.02	-0.01	0.10

Table S18 Warfarin C7 Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Warf	Fe	O	S	Por	Warf
7-1	SPIN	1.20	0.89	-0.40	-0.68	-0.01	1.05	0.51	-0.35	-0.67	0.46
	CHARGE	0.43	-0.40	-0.09	0.15	-0.09	0.40	-0.49	-0.08	0.09	0.08
7-2	SPIN	1.19	0.89	-0.46	-0.62	-0.01	1.05	0.51	-0.41	-0.62	0.46
	CHARGE	0.45	-0.39	-0.09	0.12	-0.08	0.43	-0.49	-0.09	0.05	0.10
7-3	SPIN	1.18	0.91	-0.42	-0.65	-0.01	1.05	0.50	-0.38	-0.63	0.46
	CHARGE	0.44	-0.39	-0.10	0.13	-0.08	0.42	-0.49	-0.10	0.05	0.11
7-4	SPIN	1.20	0.88	-0.35	-0.74	0.00	1.08	0.53	-0.33	-0.72	0.43
	CHARGE	0.42	-0.41	-0.12	0.21	-0.09	0.42	-0.50	-0.10	0.15	0.04
7-5	SPIN	1.21	0.88	-0.38	-0.70	0.00	1.06	0.50	-0.32	-0.69	0.44
	CHARGE	0.42	-0.41	-0.09	0.17	-0.10	0.38	-0.50	-0.07	0.11	0.07
7-6	SPIN	1.18	0.90	-0.35	-0.73	0.00	1.05	0.49	-0.28	-0.69	0.43
	CHARGE	0.41	-0.40	-0.09	0.19	-0.11	0.37	-0.49	-0.07	0.10	0.09
7-7	SPIN	1.19	0.89	-0.34	-0.73	0.00	1.07	0.51	-0.30	-0.72	0.43
	CHARGE	0.40	-0.41	-0.09	0.20	-0.10	0.38	-0.50	-0.07	0.14	0.04
7-8	SPIN	1.19	0.89	-0.35	-0.73	0.00	1.05	0.49	-0.30	-0.70	0.45
	CHARGE	0.41	-0.41	-0.10	0.19	-0.10	0.38	-0.50	-0.08	0.11	0.08
7-9	SPIN	1.19	0.89	-0.43	-0.65	-0.01	1.07	0.53	-0.40	-0.64	0.44
	CHARGE	0.43	-0.40	-0.08	0.14	-0.09	0.43	-0.49	-0.07	0.09	0.05
7-10	SPIN	1.18	0.90	-0.35	-0.73	0.00	1.05	0.49	-0.28	-0.69	0.43
	CHARGE	0.41	-0.40	-0.09	0.19	-0.11	0.37	-0.49	-0.07	0.10	0.09

Table S19 Diclofenac C4' Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Dicl	Fe	O	S	Por	Dicl
4'-1	SPIN	1.14	0.80	0.66	0.38	0.01	1.23	0.65	0.44	0.35	0.33
	CHARGE	0.47	-0.42	-0.21	0.42	-0.31	0.49	-0.47	-0.35	0.42	-0.12
4'-2	SPIN	1.13	0.81	0.66	0.37	0.02	1.23	0.64	0.45	0.35	0.33
	CHARGE	0.48	-0.40	-0.20	0.38	-0.24	0.49	-0.47	-0.35	0.40	-0.06

Table S20 Diclofenac C4' Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Dicl	Fe	O	S	Por	Dicl
4'-1	SPIN	1.22	0.88	-0.72	-0.39	0.00	1.22	0.58	-0.49	-0.32	0.00
	CHARGE	0.46	-0.41	-0.18	0.40	-0.31	0.43	-0.46	-0.36	0.40	-0.04
4'-2	SPIN	1.18	0.90	-0.75	-0.36	0.00	1.18	0.46	-0.39	-0.20	-0.05
	CHARGE	0.43	-0.39	-0.17	0.38	-0.25	0.38	-0.46	-0.41	0.38	0.12
4'-3	SPIN	1.21	0.90	-0.75	-0.38	0.00	1.22	0.65	-0.55	-0.41	0.06
	CHARGE	0.46	-0.39	-0.17	0.34	-0.17	0.47	-0.45	-0.32	0.37	0.01
4'-4	SPIN	1.22	0.88	-0.72	-0.39	0.00	1.09	0.35	-0.47	-0.25	0.26
	CHARGE	0.46	-0.41	-0.18	0.40	-0.31	0.38	-0.50	-0.42	0.39	0.11
4'-5	SPIN	1.19	0.90	-0.73	-0.38	0.00	1.19	0.57	-0.52	-0.29	0.04
	CHARGE	0.42	-0.39	-0.19	0.41	-0.25	0.40	-0.46	-0.36	0.41	0.01

Table S21 Diclofenac C5 Quartet

		QUARTET									
		reactant complex					transition state				
		Fe	O	S	Por	Dicl	Fe	O	S	Por	Dicl
5-3	SPIN	1.12	0.81	0.60	0.38	0.08	1.40	0.59	0.14	0.19	0.68
	CHARGE	0.47	-0.40	-0.23	0.38	-0.28	0.47	-0.50	-0.54	0.35	0.17

Table S22 Diclofenac C5 Doublet

		DOUBLET									
		reactant complex					transition state				
		Fe	O	S	Por	Dicl	Fe	O	S	Por	Dicl
5-1	SPIN	1.19	0.90	-0.82	-0.29	0.00	1.14	0.53	-0.47	-0.24	0.03
	CHARGE	0.43	-0.39	-0.14	0.34	-0.33	0.38	-0.46	-0.42	0.39	0.02
5-2	SPIN	1.18	0.90	-0.67	-0.35	-0.08	1.19	0.39	-0.13	-0.09	-0.37
	CHARGE	0.43	-0.39	-0.21	0.35	-0.25	0.38	-0.47	-0.57	0.33	0.27
5-3	SPIN	1.18	0.90	-0.68	-0.37	-0.05	1.23	0.39	-0.14	-0.10	-0.39
	CHARGE	0.43	-0.39	-0.20	0.37	-0.27	0.39	-0.47	-0.56	0.33	0.26

iii) Cartesian coordinates of QM region

Diclofenac 4'-1 Reactant Complex Doublet

C1	-1.984816	0.077129	2.971950
S2	-1.291004	1.191700	1.707387
H3	-3.028195	0.375748	3.124001
H4	-1.978108	-0.948441	2.593088
O5	1.096838	-0.531957	-1.204658
Fe6	0.101145	0.010575	-0.020968
N7	-0.252331	-1.866502	0.682618
N8	-1.536604	-0.126609	-1.196050
N9	0.304159	1.977864	-0.502308
N10	1.593428	0.205548	1.332971
C11	0.562107	-2.589894	1.516506
C12	0.123259	-3.961573	1.591764
C13	-0.969627	-4.060505	0.783000
C14	-1.184856	-2.750262	0.209043
C15	-2.297192	-1.239925	-1.413917
C16	-3.288577	-0.977411	-2.438903
C17	-3.120887	0.319949	-2.826511
C18	-2.021039	0.833448	-2.028787
C19	-0.468501	2.659370	-1.396899
C20	-0.030690	4.031615	-1.489739
C21	1.012864	4.180378	-0.626546
C22	1.222780	2.876629	-0.019738
C23	2.376518	1.310986	1.519396
C24	3.430073	1.023579	2.463652
C25	3.293230	-0.281617	2.824191
C26	2.144997	-0.785026	2.106095
C27	1.677641	-2.088497	2.173839
H28	2.239503	-2.785762	2.782749
C29	-2.152144	-2.450235	-0.747762
H30	-2.841370	-3.243337	-1.002097
C31	-1.534311	2.135301	-2.114882
H32	-1.997689	2.802257	-2.829213
C33	2.218641	2.534476	0.884889
H34	2.988710	3.259483	1.097394
C35	5.012032	-3.195252	-3.435778
C36	4.849699	-2.701993	-2.124756
C37	3.607041	-2.609367	-1.510980
C38	2.467334	-3.003722	-2.209541
C39	2.583626	-3.480156	-3.510343
C40	3.837930	-3.576187	-4.100183
C141	6.262759	-2.121642	-1.263657
H42	3.522906	-2.191651	-0.515461
H43	1.494686	-2.895246	-1.746195
H44	1.716781	-3.775021	-4.085399
C145	3.921802	-4.190003	-5.752914
C46	9.164431	-6.078943	-2.824944
C47	9.555640	-4.851935	-3.369184
C48	8.621944	-3.873276	-3.725548
C49	7.253976	-4.190397	-3.590893
C50	6.856976	-5.413077	-3.031124
C51	7.808208	-6.348203	-2.629113
H52	9.912285	-6.814473	-2.548309
H53	10.605270	-4.624321	-3.510933
N54	6.282728	-3.250028	-4.025925
H55	5.798482	-5.630319	-2.930832

H56	7.488257	-7.289590	-2.194743
H57	6.308060	-3.025015	-5.007676
C58	9.013958	-2.476793	-4.202068
H59	8.255027	-1.777582	-3.847895
H60	9.013512	-2.438905	-5.299436
C61	10.401080	-2.012848	-3.732110
O62	11.385058	-2.626345	-4.221299
O63	10.459382	-1.070244	-2.905868
H64	-1.504115	0.053379	3.963486
H65	0.602905	-4.759681	2.161766
H66	-1.537338	-4.964394	0.572324
H67	-4.011334	-1.723326	-2.764901
H68	-3.626759	0.957605	-3.564958
H69	-0.510429	4.799053	-2.093803
H70	1.497394	5.149366	-0.459623
H71	4.172235	1.746710	2.786923
H72	3.892051	-0.865416	3.514699

Diclofenac 4'-1 Reactant Complex Quartet

C1	-1.957065	0.077094	2.962298
S2	-1.248478	1.186934	1.702396
H3	-2.999917	0.383961	3.105628
H4	-1.954512	-0.947696	2.582435
O5	1.116557	-0.557449	-1.235987
Fe6	0.141915	-0.002606	-0.046834
N7	-0.221453	-1.872701	0.662379
N8	-1.514362	-0.134053	-1.205994
N9	0.333753	1.968212	-0.518364
N10	1.626264	0.198001	1.306608
C11	0.589280	-2.595568	1.499910
C12	0.136042	-3.960584	1.592398
C13	-0.961826	-4.057271	0.790116
C14	-1.165138	-2.752138	0.202028
C15	-2.278989	-1.244256	-1.418334
C16	-3.276269	-0.981319	-2.437691
C17	-3.106186	0.315902	-2.827833
C18	-2.001377	0.825786	-2.036111
C19	-0.447292	2.648559	-1.407776
C20	-0.020023	4.021807	-1.497597
C21	1.024341	4.176162	-0.636506
C22	1.245746	2.871165	-0.034551
C23	2.404986	1.307503	1.499903
C24	3.449452	1.020905	2.454444
C25	3.309194	-0.284759	2.816912
C26	2.171134	-0.790578	2.086285
C27	1.706194	-2.094420	2.155471
H28	2.265082	-2.788363	2.771124
C29	-2.136223	-2.452904	-0.750728
H30	-2.830790	-3.243356	-1.000455
C31	-1.514220	2.127400	-2.123517
H32	-1.975725	2.794769	-2.838019
C33	2.246396	2.532279	0.869180
H34	3.014058	3.259547	1.081323
C35	4.984922	-3.105141	-3.362135
C36	4.817083	-2.607405	-2.053373
C37	3.570251	-2.483644	-1.451833
C38	2.428051	-2.858877	-2.155830
C39	2.553549	-3.358421	-3.449138

C40	3.810158	-3.472165	-4.032467
C141	6.236520	-2.060077	-1.182853
H42	3.484643	-2.057209	-0.460127
H43	1.453281	-2.747680	-1.701937
H44	1.690082	-3.658561	-4.024690
C145	3.900444	-4.087864	-5.685867
C46	9.113397	-6.055425	-2.813646
C47	9.514930	-4.829010	-3.351383
C48	8.590786	-3.836875	-3.694272
C49	7.219278	-4.127835	-3.531789
C50	6.813831	-5.350319	-2.976963
C51	7.755556	-6.306753	-2.605781
H52	9.853860	-6.805721	-2.560103
H53	10.565643	-4.615961	-3.504467
N54	6.257740	-3.169683	-3.950108
H55	5.753487	-5.552851	-2.859530
H56	7.427270	-7.253013	-2.188128
H57	6.276789	-2.953640	-4.934529
C58	9.009551	-2.464713	-4.215659
H59	8.257030	-1.738052	-3.906772
H60	9.030890	-2.479941	-5.313202
C61	10.397453	-2.007516	-3.737847
O62	11.381043	-2.626754	-4.223457
O63	10.457365	-1.068894	-2.908763
H64	-1.486518	0.051722	3.958752
H65	0.613549	-4.755877	2.166197
H66	-1.539299	-4.957072	0.584479
H67	-4.002326	-1.726332	-2.760288
H68	-3.610446	0.954219	-3.565251
H69	-0.509860	4.785984	-2.098204
H70	1.500622	5.146662	-0.469388
H71	4.188749	1.743360	2.781766
H72	3.899925	-0.869445	3.514021

Diclofenac 4'-1 Transition State Doublet

C1	-1.829916	0.042108	2.878601
S2	-1.112434	1.140487	1.600813
H3	-2.880373	0.330996	2.994478
H4	-1.801794	-0.989536	2.517864
O5	1.343950	-0.594358	-1.328778
Fe6	0.281209	-0.072607	-0.068984
N7	-0.093508	-1.910645	0.637998
N8	-1.374202	-0.202577	-1.257704
N9	0.485195	1.903473	-0.600040
N10	1.756804	0.138649	1.266323
C11	0.690584	-2.626966	1.516908
C12	0.216027	-3.980814	1.623460
C13	-0.882981	-4.073996	0.821299
C14	-1.062327	-2.783756	0.200051
C15	-2.167538	-1.298056	-1.439720
C16	-3.193716	-1.021761	-2.430559
C17	-3.017417	0.271643	-2.828111
C18	-1.880388	0.765601	-2.071745
C19	-0.326063	2.581880	-1.459972
C20	0.053744	3.969571	-1.523818
C21	1.104497	4.138816	-0.673176
C22	1.367819	2.823833	-0.095542
C23	2.518879	1.261130	1.455815

C24	3.551829	0.991567	2.428383
C25	3.407161	-0.307680	2.813929
C26	2.277051	-0.826684	2.083207
C27	1.802622	-2.128230	2.176156
H28	2.345476	-2.815609	2.811606
C29	-2.032966	-2.497009	-0.756047
H30	-2.740835	-3.281718	-0.983885
C31	-1.403544	2.064448	-2.159401
H32	-1.889938	2.741137	-2.845065
C33	2.349268	2.491851	0.833434
H34	3.092881	3.230526	1.084701
C35	4.744503	-2.533608	-2.942196
C36	4.753055	-2.141612	-1.579048
C37	3.608910	-2.001514	-0.822043
C38	2.325739	-2.236578	-1.397537
C39	2.309055	-2.670071	-2.751804
C40	3.463742	-2.766836	-3.495577
C141	6.301280	-1.768347	-0.864677
H42	3.687736	-1.691860	0.210230
H43	1.531014	-2.591114	-0.755502
H44	1.374304	-2.970842	-3.196276
C145	3.364817	-3.315538	-5.172495
C46	8.643990	-5.783096	-2.770155
C47	9.106395	-4.593221	-3.333618
C48	8.252433	-3.517918	-3.608657
C49	6.877964	-3.689734	-3.337663
C50	6.412168	-4.886464	-2.771624
C51	7.286878	-5.925924	-2.474052
H52	9.338097	-6.592408	-2.566877
H53	10.158844	-4.463545	-3.555762
N54	5.928192	-2.671975	-3.664930
H55	5.349348	-4.999332	-2.587093
H56	6.902459	-6.845060	-2.044935
H57	5.858524	-2.451684	-4.648005
C58	8.791428	-2.208239	-4.176754
H59	8.107940	-1.401327	-3.910015
H60	8.829032	-2.275237	-5.271432
C61	10.218909	-1.864743	-3.691498
O62	11.157535	-2.561247	-4.165286
O63	10.343368	-0.928960	-2.866007
H64	-1.385436	0.032753	3.892592
H65	0.699234	-4.769897	2.196204
H66	-1.505722	-4.949662	0.652323
H67	-3.944930	-1.755600	-2.717583
H68	-3.530560	0.923430	-3.553247
H69	-0.489554	4.719943	-2.098932
H70	1.539455	5.129058	-0.510313
H71	4.282346	1.723823	2.755950
H72	3.976529	-0.888362	3.528738

Diclofenac 4'-1 Transition State Quartet

C1	-1.840721	0.038490	2.896794
S2	-1.102161	1.122145	1.623832
H3	-2.888668	0.338807	3.007243
H4	-1.821657	-0.993923	2.536115
O5	1.325515	-0.748034	-1.299530
Fe6	0.287724	-0.056544	-0.132693
N7	-0.128055	-1.898364	0.630913
N8	-1.374818	-0.189434	-1.290047

N9	0.479098	1.898737	-0.626910
N10	1.757478	0.154411	1.228851
C11	0.669019	-2.612214	1.491595
C12	0.197338	-3.967424	1.603975
C13	-0.905432	-4.062906	0.805887
C14	-1.088298	-2.770657	0.187543
C15	-2.175085	-1.287496	-1.462485
C16	-3.202870	-1.009128	-2.449924
C17	-3.030692	0.283362	-2.846534
C18	-1.890703	0.780608	-2.096948
C19	-0.341018	2.588509	-1.482573
C20	0.043406	3.975016	-1.534020
C21	1.093251	4.139394	-0.682377
C22	1.361206	2.826076	-0.110374
C23	2.515165	1.271594	1.433932
C24	3.535427	0.999273	2.419852
C25	3.385860	-0.300008	2.797953
C26	2.265780	-0.817285	2.049914
C27	1.784372	-2.113159	2.147570
H28	2.323446	-2.798577	2.788590
C29	-2.055573	-2.480631	-0.771165
H30	-2.773542	-3.258046	-0.994660
C31	-1.418449	2.080574	-2.177502
H32	-1.912943	2.763971	-2.853204
C33	2.341861	2.503129	0.814720
H34	3.076294	3.249668	1.070618
C35	4.789073	-2.608873	-2.975050
C36	4.738272	-2.258780	-1.602088
C37	3.569103	-2.175081	-0.875229
C38	2.306242	-2.391496	-1.497101
C39	2.348254	-2.780306	-2.867565
C40	3.532810	-2.838978	-3.574479
C141	6.252976	-1.879300	-0.825021
H42	3.612225	-1.925469	0.175844
H43	1.485080	-2.758301	-0.904110
H44	1.445446	-3.101716	-3.359581
C145	3.495260	-3.337716	-5.268937
C46	8.734632	-5.822305	-2.775333
C47	9.188974	-4.629864	-3.346373
C48	8.327934	-3.562397	-3.622957
C49	6.952392	-3.734697	-3.349272
C50	6.495392	-4.937485	-2.780737
C51	7.378653	-5.968545	-2.480241
H52	9.433824	-6.625465	-2.566999
H53	10.240673	-4.496886	-3.568518
N54	6.006635	-2.716722	-3.656045
H55	5.434579	-5.056732	-2.596957
H56	6.998774	-6.887742	-2.044858
H57	6.010541	-2.378962	-4.605732
C58	8.858336	-2.249297	-4.194370
H59	8.172416	-1.446202	-3.922067
H60	8.893315	-2.314039	-5.289244
C61	10.282403	-1.891935	-3.708967
O62	11.230340	-2.571805	-4.179246
O63	10.389824	-0.954023	-2.880502
H64	-1.397733	0.029541	3.912163
H65	0.681435	-4.756242	2.177692
H66	-1.519901	-4.944308	0.632259
H67	-3.949504	-1.747561	-2.741032
H68	-3.544221	0.935261	-3.571293

H69	-0.489405	4.733299	-2.112190
H70	1.533051	5.130432	-0.517777
H71	4.263396	1.729171	2.756621
H72	3.954091	-0.882794	3.513958

Diclofenac 4'-2 Reactant Complex Doublet

C1	-1.930812	0.114312	3.121564
S2	-1.328084	1.231170	1.814260
H3	-2.957591	0.422689	3.354038
H4	-1.961112	-0.907994	2.736508
O5	1.106966	-0.432917	-1.073304
Fe6	0.092240	0.042189	0.121655
N7	-0.215370	-1.839177	0.835610
N8	-1.528544	-0.165922	-1.073537
N9	0.260120	1.992576	-0.397159
N10	1.571167	0.280011	1.474778
C11	0.610272	-2.545762	1.672211
C12	0.222052	-3.935531	1.729726
C13	-0.873882	-4.054240	0.926652
C14	-1.123525	-2.748290	0.365075
C15	-2.256082	-1.299156	-1.285795
C16	-3.209890	-1.098605	-2.355600
C17	-3.047440	0.185003	-2.786007
C18	-1.999851	0.751720	-1.959414
C19	-0.516724	2.625808	-1.317636
C20	-0.107632	3.997923	-1.456310
C21	0.943183	4.195283	-0.612039
C22	1.175755	2.915197	0.048764
C23	2.364346	1.385465	1.615801
C24	3.428897	1.113795	2.560595
C25	3.258804	-0.166405	2.993556
C26	2.113121	-0.684324	2.287010
C27	1.683560	-2.000473	2.360451
H28	2.255105	-2.674892	2.986072
C29	-2.090993	-2.492315	-0.596274
H30	-2.747449	-3.311688	-0.848406
C31	-1.546779	2.061286	-2.058144
H32	-2.011158	2.703606	-2.793638
C33	2.184789	2.598620	0.954637
H34	2.946577	3.336046	1.153833
C35	4.601801	-2.707257	-2.966656
C36	4.469947	-2.501125	-1.580112
C37	3.274981	-2.681674	-0.901930
C38	2.144565	-3.081376	-1.606679
C39	2.216954	-3.262802	-2.982922
C40	3.428927	-3.082586	-3.641611
Cl41	5.864734	-1.958990	-0.668987
H42	3.224477	-2.483551	0.161483
H43	1.205215	-3.210213	-1.083325
H44	1.341870	-3.568221	-3.544490
Cl45	3.490608	-3.359050	-5.388183
C46	8.813023	-5.413699	-2.722299
C47	9.146286	-4.060587	-2.769233
C48	8.189824	-3.080850	-3.053846
C49	6.872376	-3.497720	-3.307311
C50	6.536659	-4.856022	-3.260719
C51	7.498239	-5.817698	-2.965714
H52	9.573042	-6.154224	-2.500301
H53	10.163013	-3.737032	-2.576510

N54	5.844201	-2.530810	-3.598237
H55	5.509941	-5.145991	-3.459706
H56	7.227935	-6.867050	-2.944691
H57	5.765482	-2.304818	-4.577811
C58	8.550926	-1.601436	-3.017411
H59	8.499005	-1.265077	-1.977279
H60	7.808725	-1.042269	-3.581772
C61	9.952626	-1.306708	-3.553463
O62	10.069152	-0.947953	-4.746184
O63	10.914991	-1.469051	-2.744794
H64	-1.397859	0.066782	4.081426
H65	0.748796	-4.726719	2.270656
H66	-1.462149	-4.938506	0.693361
H67	-3.895941	-1.878456	-2.683663
H68	-3.502581	0.766357	-3.592712
H69	-0.626397	4.706474	-2.098941
H70	1.417676	5.175148	-0.506488
H71	4.225774	1.806784	2.807630
H72	3.824760	-0.750559	3.717227

Diclofenac 4'-2 Reactant Complex Quartet

C1	-1.957547	0.130544	3.120208
S2	-1.267331	1.213386	1.820993
H3	-2.985249	0.472422	3.291356
H4	-1.998439	-0.896135	2.747363
O5	1.083874	-0.564750	-1.148077
Fe6	0.105500	-0.000225	0.032450
N7	-0.249978	-1.864650	0.760125
N8	-1.541693	-0.148236	-1.138089
N9	0.287973	1.965414	-0.469439
N10	1.578126	0.213701	1.388440
C11	0.570305	-2.590993	1.585750
C12	0.154292	-3.972549	1.633877
C13	-0.935781	-4.070622	0.821820
C14	-1.167246	-2.755524	0.273582
C15	-2.289079	-1.270617	-1.355926
C16	-3.256719	-1.035193	-2.405045
C17	-3.081199	0.250913	-2.818636
C18	-2.010400	0.791440	-2.005104
C19	-0.487022	2.632877	-1.376205
C20	-0.072109	4.011075	-1.467638
C21	0.963574	4.178743	-0.594267
C22	1.189265	2.878513	0.017959
C23	2.358664	1.325098	1.564320
C24	3.410678	1.044824	2.514941
C25	3.261130	-0.250432	2.904037
C26	2.120866	-0.764983	2.184078
C27	1.670485	-2.074187	2.256875
H28	2.236308	-2.760759	2.873361
C29	-2.131132	-2.474948	-0.686420
H30	-2.791433	-3.286001	-0.950383
C31	-1.533676	2.093549	-2.107278
H32	-2.001359	2.745131	-2.834212
C33	2.187665	2.546691	0.929996
H34	2.943090	3.284457	1.151113
C35	4.790313	-2.845264	-3.026793
C36	4.600156	-2.550303	-1.662945
C37	3.357411	-2.579392	-1.045104
C38	2.231854	-2.931809	-1.782878

C39	2.374845	-3.268842	-3.124961
C40	3.630122	-3.214594	-3.726954
C141	5.986978	-2.063429	-0.709236
H42	3.268482	-2.294870	-0.004224
H43	1.258686	-2.961439	-1.311020
H44	1.523231	-3.585070	-3.712662
C145	3.746289	-3.625554	-5.443533
C46	9.161701	-5.444938	-2.824422
C47	9.410774	-4.073614	-2.786715
C48	8.399270	-3.137894	-3.024142
C49	7.110826	-3.616286	-3.319769
C50	6.856744	-4.993840	-3.344751
C51	7.872534	-5.910786	-3.096873
H52	9.967182	-6.150221	-2.654427
H53	10.407871	-3.701332	-2.579508
N54	6.047906	-2.695013	-3.638257
H55	5.852164	-5.332473	-3.578546
H56	7.669504	-6.975102	-3.140778
H57	5.976027	-2.517455	-4.626732
C58	8.696738	-1.647221	-2.914624
H59	8.726457	-1.380434	-1.853952
H60	7.886977	-1.087780	-3.379023
C61	10.043360	-1.287197	-3.547796
O62	10.079386	-0.981042	-4.756684
O63	11.059619	-1.363563	-2.788045
H64	-1.470668	0.084451	4.111043
H65	0.662419	-4.775240	2.170845
H66	-1.518719	-4.954679	0.571218
H67	-3.978967	-1.775086	-2.744004
H68	-3.553108	0.837947	-3.612674
H69	-0.554708	4.763607	-2.091878
H70	1.426227	5.156709	-0.434501
H71	4.171757	1.760676	2.806573
H72	3.840233	-0.830933	3.614084

Diclofenac 4'-2 Transition State Doublet

C1	-1.849302	0.081345	3.014957
S2	-1.169546	1.159529	1.695545
H3	-2.885013	0.398981	3.177051
H4	-1.862033	-0.950251	2.654966
O5	1.231184	-0.570439	-1.218788
Fe6	0.188045	-0.072753	0.085776
N7	-0.152600	-1.912464	0.799715
N8	-1.439570	-0.244910	-1.136621
N9	0.403818	1.880788	-0.513789
N10	1.681983	0.146976	1.393611
C11	0.645873	-2.627015	1.670344
C12	0.227999	-4.005910	1.719878
C13	-0.862348	-4.110219	0.905763
C14	-1.088770	-2.807584	0.330898
C15	-2.199276	-1.358683	-1.330426
C16	-3.174374	-1.133091	-2.379214
C17	-2.997144	0.149271	-2.807494
C18	-1.912080	0.689486	-2.011672
C19	-0.397239	2.530754	-1.404913
C20	-0.027052	3.920121	-1.488680
C21	1.014211	4.113893	-0.631071
C22	1.281605	2.811558	-0.022237
C23	2.446141	1.273308	1.550818

C24	3.481228	1.023743	2.528933
C25	3.315616	-0.255228	2.970054
C26	2.187724	-0.792347	2.249104
C27	1.728590	-2.101588	2.354917
H28	2.271425	-2.772715	3.007312
C29	-2.049237	-2.550135	-0.633163
H30	-2.722028	-3.359796	-0.872328
C31	-1.442948	1.985957	-2.127434
H32	-1.913301	2.634614	-2.852618
C33	2.266101	2.494342	0.910432
H34	3.006655	3.240531	1.152178
C35	4.515987	-2.559400	-2.773338
C36	4.499529	-2.214252	-1.395501
C37	3.344216	-2.062992	-0.667268
C38	2.071017	-2.271550	-1.275604
C39	2.067650	-2.713821	-2.633258
C40	3.235454	-2.806851	-3.348764
C141	6.018642	-1.879269	-0.607465
H42	3.401971	-1.756245	0.365442
H43	1.256346	-2.610665	-0.650472
H44	1.132744	-3.021714	-3.080505
C145	3.180026	-3.357758	-5.028744
C46	8.758896	-5.393111	-2.715870
C47	9.068969	-4.035060	-2.759237
C48	8.091945	-3.060954	-2.999476
C49	6.768450	-3.502203	-3.182565
C50	6.453141	-4.864435	-3.126879
C51	7.441710	-5.816659	-2.898764
H52	9.544647	-6.121906	-2.548074
H53	10.088676	-3.701817	-2.609215
N54	5.684635	-2.595081	-3.513045
H55	5.423244	-5.164111	-3.292421
H56	7.190884	-6.870979	-2.886205
H57	5.523098	-2.540965	-4.511397
C58	8.458230	-1.583731	-3.006612
H59	8.398807	-1.213368	-1.978796
H60	7.715531	-1.043416	-3.590408
C61	9.873452	-1.296107	-3.534121
O62	10.001011	-0.914436	-4.718005
O63	10.829294	-1.484327	-2.723521
H64	-1.370822	0.053165	4.014351
H65	0.745151	-4.799036	2.258123
H66	-1.468418	-4.981368	0.665478
H67	-3.898440	-1.879789	-2.696081
H68	-3.468431	0.748440	-3.596447
H69	-0.569106	4.651394	-2.090472
H70	1.441256	5.109783	-0.486405
H71	4.237731	1.750280	2.805205
H72	3.870418	-0.819202	3.710446

Diclofenac 4'-2 Transition State Quartet

C1	-1.878170	0.102875	3.066524
S2	-1.170688	1.165364	1.755365
H3	-2.910092	0.439677	3.215342
H4	-1.905901	-0.928629	2.704507
O5	1.217065	-0.773036	-1.178107
Fe6	0.200222	-0.051758	-0.011923
N7	-0.204154	-1.885179	0.779316
N8	-1.444356	-0.210862	-1.184173

N9	0.389478	1.890417	-0.543602
N10	1.665920	0.180249	1.348651
C11	0.609519	-2.600011	1.623379
C12	0.194997	-3.979533	1.677450
C13	-0.897419	-4.084319	0.865045
C14	-1.122840	-2.778571	0.297827
C15	-2.215465	-1.326896	-1.369489
C16	-3.198843	-1.092141	-2.406839
C17	-3.020586	0.190669	-2.833855
C18	-1.928231	0.727077	-2.047321
C19	-0.418563	2.560652	-1.426727
C20	-0.047916	3.949031	-1.489962
C21	0.991881	4.133168	-0.627433
C22	1.264091	2.829812	-0.034592
C23	2.431279	1.296542	1.525532
C24	3.455950	1.038718	2.512784
C25	3.287004	-0.245796	2.934859
C26	2.165273	-0.774565	2.197053
C27	1.700378	-2.076034	2.302415
H28	2.245345	-2.750199	2.949547
C29	-2.079037	-2.514768	-0.674215
H30	-2.754562	-3.319758	-0.916127
C31	-1.463963	2.026808	-2.153585
H32	-1.941622	2.683894	-2.865407
C33	2.253756	2.519724	0.888736
H34	2.988894	3.270756	1.128182
C35	4.588861	-2.630768	-2.837749
C36	4.508629	-2.332411	-1.454111
C37	3.331003	-2.270421	-0.746874
C38	2.080698	-2.475966	-1.394734
C39	2.144656	-2.879221	-2.759574
C40	3.340878	-2.909525	-3.447029
C141	5.997545	-1.987379	-0.609540
H42	3.351112	-2.031817	0.305264
H43	1.243329	-2.834673	-0.820319
H44	1.244765	-3.226521	-3.250352
C145	3.341840	-3.433694	-5.139429
C46	8.856687	-5.425471	-2.778260
C47	9.163799	-4.065832	-2.789437
C48	8.187225	-3.090973	-3.025924
C49	6.865608	-3.523453	-3.244995
C50	6.556637	-4.889473	-3.233092
C51	7.543897	-5.844399	-3.002871
H52	9.638687	-6.156461	-2.602020
H53	10.180389	-3.733572	-2.612091
N54	5.798246	-2.587790	-3.534389
H55	5.532577	-5.190042	-3.428758
H56	7.295862	-6.899478	-3.019121
H57	5.677744	-2.422295	-4.523873
C58	8.556723	-1.613243	-2.982993
H59	8.525659	-1.285686	-1.939339
H60	7.803700	-1.046495	-3.526988
C61	9.958202	-1.316923	-3.540363
O62	10.061184	-0.960755	-4.735399
O63	10.932799	-1.474969	-2.745311
H64	-1.406825	0.068770	4.069982
H65	0.713178	-4.773600	2.213297
H66	-1.496043	-4.958975	0.622315
H67	-3.928203	-1.833292	-2.726249
H68	-3.490660	0.786615	-3.621626

H69	-0.570732	4.691372	-2.097479
H70	1.427055	5.126909	-0.474304
H71	4.212992	1.759750	2.801366
H72	3.845357	-0.818794	3.666282

Diclofenac 4'-3 Reactant Complex Doublet

C1	-2.105625	0.200934	3.178028
S2	-1.362513	1.235220	1.857941
H3	-3.116627	0.586627	3.344800
H4	-2.192915	-0.829522	2.821398
O5	1.032836	-0.590560	-1.074902
Fe6	0.041224	0.020657	0.078024
N7	-0.323071	-1.835339	0.809092
N8	-1.601898	-0.121904	-1.102369
N9	0.234937	1.983420	-0.428138
N10	1.528176	0.242944	1.425120
C11	0.499310	-2.554734	1.637638
C12	0.098954	-3.940675	1.678993
C13	-0.980407	-4.049729	0.851870
C14	-1.221545	-2.734319	0.303737
C15	-2.342772	-1.245340	-1.331258
C16	-3.319118	-1.003928	-2.375062
C17	-3.157070	0.291508	-2.773658
C18	-2.077529	0.819985	-1.961106
C19	-0.541526	2.652201	-1.329864
C20	-0.120113	4.026417	-1.434866
C21	0.925698	4.191913	-0.576505
C22	1.151679	2.893379	0.041243
C23	2.336342	1.337403	1.570435
C24	3.402088	1.049112	2.503275
C25	3.228440	-0.235714	2.917014
C26	2.066216	-0.734640	2.222402
C27	1.600466	-2.038519	2.305148
H28	2.164867	-2.728196	2.919570
C29	-2.172529	-2.455602	-0.672079
H30	-2.820470	-3.268703	-0.957302
C31	-1.590325	2.119026	-2.061046
H32	-2.034640	2.769510	-2.800580
C33	2.168741	2.557576	0.925256
H34	2.939782	3.288460	1.118799
C35	4.872160	-2.846147	-3.467341
C36	4.659183	-2.684283	-2.083875
C37	3.401057	-2.750406	-1.497412
C38	2.291156	-3.027400	-2.291958
C39	2.463582	-3.262929	-3.652698
C40	3.728102	-3.149817	-4.224702
Cl41	6.032216	-2.306674	-1.056675
H42	3.287935	-2.548530	-0.440379
H43	1.303595	-3.047073	-1.850184
H44	1.626694	-3.530840	-4.285428
Cl45	3.875337	-3.388306	-5.964807
C46	9.095114	-5.646259	-3.496627
C47	9.398473	-4.308466	-3.248075
C48	8.438288	-3.296953	-3.381537
C49	7.150062	-3.662016	-3.804548
C50	6.836822	-5.008627	-4.034989
C51	7.797833	-6.005011	-3.879529
H52	9.863772	-6.408170	-3.397290
H53	10.404254	-4.021100	-2.956005

N54	6.147821	-2.655373	-4.027610
H55	5.830289	-5.256757	-4.354684
H56	7.541477	-7.041860	-4.067469
H57	6.127961	-2.345340	-4.991397
C58	8.800754	-1.864581	-3.026466
H59	9.081667	-1.828334	-1.970141
H60	7.922814	-1.234514	-3.170986
C61	9.957134	-1.332567	-3.881412
O62	9.727480	-1.001446	-5.045682
O63	11.110650	-1.270692	-3.315625
H64	-1.601528	0.150294	4.164058
H65	0.618891	-4.734535	2.221652
H66	-1.540831	-4.944136	0.588732
H67	-4.005173	-1.764438	-2.740219
H68	-3.644357	0.909238	-3.542023
H69	-0.600008	4.769782	-2.072939
H70	1.403619	5.164894	-0.430030
H71	4.194405	1.743587	2.763707
H72	3.808435	-0.822091	3.620946

Diclofenac 4'-3 Transition State Doublet

C1	-1.978502	0.188933	3.068911
S2	-1.206090	1.214518	1.753260
H3	-3.002567	0.557275	3.195532
H4	-2.029715	-0.843204	2.711579
O5	1.217314	-0.672814	-1.240444
Fe6	0.183434	-0.080292	-0.002508
N7	-0.199037	-1.899707	0.746582
N8	-1.483305	-0.212163	-1.168501
N9	0.373628	1.895615	-0.539230
N10	1.648656	0.163012	1.343992
C11	0.593856	-2.608316	1.618694
C12	0.168079	-3.982696	1.687441
C13	-0.911390	-4.094069	0.859868
C14	-1.126769	-2.794793	0.269444
C15	-2.246211	-1.325348	-1.374106
C16	-3.255516	-1.069812	-2.384701
C17	-3.102369	0.228269	-2.775587
C18	-1.991149	0.744861	-1.997417
C19	-0.452324	2.571128	-1.390248
C20	-0.081500	3.961362	-1.459902
C21	0.982302	4.135002	-0.625530
C22	1.260950	2.822397	-0.050482
C23	2.437044	1.274551	1.493482
C24	3.477030	1.011340	2.462337
C25	3.294248	-0.263571	2.906670
C26	2.155993	-0.786137	2.192023
C27	1.683849	-2.086293	2.298571
H28	2.226500	-2.763417	2.945014
C29	-2.083476	-2.527291	-0.700424
H30	-2.757882	-3.331485	-0.952045
C31	-1.525214	2.046558	-2.086563
H32	-2.015833	2.716556	-2.777583
C33	2.264962	2.495894	0.853771
H34	3.013768	3.239226	1.080575
C35	4.541463	-2.570233	-2.913638
C36	4.516218	-2.305765	-1.522651
C37	3.357109	-2.212746	-0.777999
C38	2.089346	-2.383806	-1.393226

C39	2.100285	-2.796208	-2.754093
C40	3.273173	-2.831992	-3.485401
C141	6.046755	-2.013720	-0.733895
H42	3.419530	-1.976322	0.275377
H43	1.257705	-2.712174	-0.788337
H44	1.182414	-3.131628	-3.214398
C145	3.208332	-3.310331	-5.187203
C46	8.766747	-5.426022	-3.442184
C47	9.089948	-4.083240	-3.256570
C48	8.118071	-3.073991	-3.284994
C49	6.783318	-3.455759	-3.512243
C50	6.455048	-4.807267	-3.682720
C51	7.434805	-5.795603	-3.649474
H52	9.549868	-6.177826	-3.436826
H53	10.123224	-3.786844	-3.100244
N54	5.722983	-2.480858	-3.657715
H55	5.418172	-5.064853	-3.874580
H56	7.164228	-6.835847	-3.805284
H57	5.558358	-2.246191	-4.628767
C58	8.548906	-1.636514	-3.028336
H59	8.765576	-1.528198	-1.961654
H60	7.723999	-0.968093	-3.273589
C61	9.798179	-1.247490	-3.842201
O62	9.652055	-0.901895	-5.013392
O63	10.931657	-1.320397	-3.236694
H64	-1.509031	0.152241	4.078363
H65	0.676597	-4.765945	2.249209
H66	-1.511075	-4.971135	0.631564
H67	-3.961601	-1.822323	-2.727481
H68	-3.611350	0.861317	-3.520276
H69	-0.614816	4.703126	-2.058110
H70	1.425645	5.123806	-0.473986
H71	4.256561	1.720237	2.725006
H72	3.846984	-0.829960	3.646172

Diclofenac 4'-4 Reactant Complex Doublet

C1	-2.048853	0.237620	3.077026
S2	-1.343649	1.270967	1.751854
H3	-3.058904	0.617564	3.273773
H4	-2.139289	-0.791253	2.717576
O5	1.098156	-0.565259	-1.105689
Fe6	0.077201	0.017791	0.036439
N7	-0.293359	-1.842954	0.756195
N8	-1.543209	-0.125245	-1.167634
N9	0.280690	1.981132	-0.461443
N10	1.536478	0.227815	1.421640
C11	0.520690	-2.570611	1.585408
C12	0.108360	-3.952867	1.624564
C13	-0.974872	-4.050300	0.802288
C14	-1.201218	-2.733157	0.253422
C15	-2.301213	-1.239120	-1.387162
C16	-3.280417	-0.986600	-2.425417
C17	-3.100303	0.303173	-2.831281
C18	-2.010388	0.822637	-2.026008
C19	-0.484892	2.656766	-1.367772
C20	-0.065835	4.034152	-1.448280
C21	0.968065	4.190733	-0.571819
C22	1.181273	2.888862	0.040243
C23	2.330478	1.328253	1.594605

C24	3.392631	1.034010	2.529532
C25	3.233584	-0.261738	2.917950
C26	2.078996	-0.758856	2.206982
C27	1.618352	-2.064621	2.267479
H28	2.175984	-2.761029	2.881091
C29	-2.151278	-2.448193	-0.721710
H30	-2.811488	-3.257862	-0.997526
C31	-1.525078	2.122364	-2.116523
H32	-1.976828	2.779944	-2.846986
C33	2.169086	2.552169	0.958641
H34	2.928781	3.284381	1.185182
C35	4.634611	-3.065847	-3.264740
C36	4.498143	-2.707231	-1.909289
C37	3.281893	-2.721622	-1.238936
C38	2.144297	-3.145559	-1.918589
C39	2.241176	-3.560287	-3.242745
C40	3.466999	-3.499120	-3.904027
C141	5.922046	-2.172358	-1.030132
H42	3.218095	-2.381830	-0.212633
H43	1.185520	-3.142855	-1.414184
H44	1.367160	-3.905854	-3.782088
C145	3.511407	-3.972858	-5.594897
C46	8.777863	-5.866818	-2.903868
C47	9.155887	-4.527504	-3.023653
C48	8.244108	-3.525950	-3.371051
C49	6.895991	-3.901157	-3.599323
C50	6.525797	-5.251656	-3.486188
C51	7.449518	-6.227031	-3.134608
H52	9.509512	-6.620695	-2.635020
H53	10.179212	-4.230000	-2.836176
N54	5.889481	-2.975630	-3.939288
H55	5.494375	-5.522604	-3.683783
H56	7.131455	-7.261224	-3.057393
H57	6.176069	-2.019646	-4.099423
C58	8.668953	-2.058165	-3.432762
H59	8.443331	-1.594391	-2.464547
H60	8.089228	-1.533402	-4.192865
C61	10.146341	-1.797852	-3.769317
O62	10.390856	-1.277236	-4.873854
O63	11.027837	-2.122421	-2.905345
H64	-1.526351	0.186472	4.048120
H65	0.619034	-4.748022	2.171382
H66	-1.559838	-4.930495	0.547882
H67	-3.994944	-1.733851	-2.762450
H68	-3.589358	0.922235	-3.594547
H69	-0.538598	4.790532	-2.076564
H70	1.452036	5.158382	-0.410109
H71	4.174094	1.736776	2.798581
H72	3.819719	-0.850229	3.619324

Diclofenac 4'-4 Transition State Doublet

C1	-1.934508	0.203121	2.982977
S2	-1.200538	1.228684	1.657392
H3	-2.957247	0.567482	3.136835
H4	-1.996525	-0.831104	2.632774
O5	1.281612	-0.746676	-1.301591
Fe6	0.214809	-0.095778	-0.031397
N7	-0.197003	-1.897161	0.719062
N8	-1.420250	-0.209431	-1.235295

N9	0.437530	1.890126	-0.574069
N10	1.646184	0.142644	1.353999
C11	0.578392	-2.617714	1.599252
C12	0.138864	-3.986235	1.657542
C13	-0.938099	-4.081826	0.826920
C14	-1.130951	-2.780007	0.239239
C15	-2.213065	-1.304490	-1.427030
C16	-3.218236	-1.033799	-2.436835
C17	-3.027665	0.252701	-2.845728
C18	-1.904387	0.749781	-2.073312
C19	-0.370161	2.575395	-1.434799
C20	-0.009506	3.971072	-1.470028
C21	1.028301	4.137131	-0.603715
C22	1.293609	2.818590	-0.036678
C23	2.421721	1.260246	1.537798
C24	3.449721	0.989557	2.516512
C25	3.274717	-0.295011	2.936708
C26	2.147061	-0.811374	2.201911
C27	1.666252	-2.110048	2.292418
H28	2.189947	-2.791571	2.949138
C29	-2.080916	-2.500460	-0.738677
H30	-2.770772	-3.296658	-0.979207
C31	-1.426282	2.049742	-2.160566
H32	-1.910485	2.722845	-2.853860
C33	2.260173	2.488226	0.908016
H34	2.990794	3.235487	1.178034
C35	4.497257	-2.736391	-2.883819
C36	4.504900	-2.328034	-1.528438
C37	3.372007	-2.155544	-0.762282
C38	2.072099	-2.368890	-1.332522
C39	2.065046	-2.931547	-2.659855
C40	3.221612	-3.060816	-3.400975
C141	6.060563	-1.983048	-0.806898
H42	3.453276	-1.825326	0.263794
H43	1.310414	-2.771135	-0.676298
H44	1.127564	-3.286060	-3.069105
C145	3.125962	-3.742263	-5.024115
C46	8.524454	-5.823771	-2.969696
C47	8.950656	-4.498915	-3.070954
C48	8.065531	-3.444223	-3.312147
C49	6.682200	-3.748584	-3.432793
C50	6.264084	-5.085408	-3.348447
C51	7.167036	-6.118698	-3.115687
H52	9.242392	-6.615791	-2.786653
H53	10.000070	-4.257468	-2.951032
N54	5.687966	-2.772256	-3.670194
H55	5.211935	-5.303527	-3.499894
H56	6.816493	-7.144243	-3.074593
H57	5.986905	-1.862413	-4.003142
C58	8.571269	-2.004497	-3.406829
H59	8.369623	-1.503870	-2.452481
H60	8.012703	-1.475433	-4.180411
C61	10.064596	-1.820233	-3.748238
O62	10.334389	-1.337948	-4.863402
O63	10.931647	-2.158919	-2.873256
H64	-1.452655	0.167469	3.980863
H65	0.651180	-4.769776	2.207512
H66	-1.548427	-4.943726	0.579484
H67	-3.953687	-1.768767	-2.752655
H68	-3.519470	0.888176	-3.594807

H69	-0.528902	4.724475	-2.067815
H70	1.472638	5.122460	-0.433757
H71	4.222459	1.701967	2.788481
H72	3.832858	-0.872664	3.665130

Diclofenac 4'-5 Reactant Complex Doublet

C1	-1.914183	0.204244	3.146755
S2	-1.353667	1.284105	1.793588
H3	-2.950167	0.491248	3.365654
H4	-1.914002	-0.833834	2.805120
O5	1.064217	-0.379009	-1.087573
Fe6	0.074509	0.103093	0.124316
N7	-0.255821	-1.765460	0.847396
N8	-1.559411	-0.075766	-1.056455
N9	0.275562	2.048564	-0.392649
N10	1.568148	0.318666	1.472224
C11	0.554151	-2.477005	1.693409
C12	0.140522	-3.855868	1.768930
C13	-0.955866	-3.965575	0.965975
C14	-1.181031	-2.662316	0.386863
C15	-2.309029	-1.196913	-1.258972
C16	-3.284437	-0.968077	-2.306109
C17	-3.111643	0.319023	-2.727656
C18	-2.027186	0.856133	-1.927680
C19	-0.470317	2.691290	-1.336323
C20	-0.012201	4.049031	-1.490449
C21	1.017373	4.228202	-0.616535
C22	1.210671	2.950120	0.051537
C23	2.389783	1.405527	1.599053
C24	3.465866	1.115707	2.523258
C25	3.277168	-0.158148	2.960431
C26	2.104751	-0.651756	2.280918
C27	1.642922	-1.953552	2.374147
H28	2.198330	-2.634484	3.006549
C29	-2.146903	-2.394185	-0.576218
H30	-2.805778	-3.210463	-0.828822
C31	-1.522874	2.146310	-2.055586
H32	-1.960103	2.781499	-2.813855
C33	2.227455	2.618114	0.941368
H34	3.019859	3.333041	1.109345
C35	4.595749	-2.622398	-2.943131
C36	4.478387	-2.377805	-1.561846
C37	3.289867	-2.555202	-0.866262
C38	2.166448	-3.013771	-1.546380
C39	2.227617	-3.245866	-2.917325
C40	3.428126	-3.046693	-3.594417
Cl41	5.877173	-1.791033	-0.689295
H42	3.238849	-2.310812	0.187046
H43	1.233745	-3.131221	-1.010874
H44	1.353958	-3.583055	-3.460132
Cl45	3.478681	-3.360503	-5.331711
C46	8.564185	-5.624429	-2.915675
C47	9.006601	-4.302249	-2.879539
C48	8.143561	-3.226327	-3.115248
C49	6.792735	-3.508995	-3.392923
C50	6.351119	-4.841388	-3.435133
C51	7.223882	-5.898097	-3.197863
H52	9.259762	-6.436403	-2.732869
H53	10.042369	-4.070445	-2.663906

N54	5.843631	-2.452706	-3.575655
H55	5.308410	-5.035847	-3.656539
H56	6.862142	-6.918331	-3.247883
H57	5.804659	-2.036771	-4.497811
C58	8.659042	-1.795375	-3.019915
H59	8.639499	-1.490302	-1.969892
H60	7.989889	-1.136983	-3.571251
C61	10.092119	-1.670189	-3.562600
O62	10.249896	-1.386570	-4.762162
O63	11.030766	-1.919917	-2.737872
H64	-1.373564	0.223142	4.108690
H65	0.676759	-4.639200	2.312896
H66	-1.560826	-4.840595	0.741331
H67	-3.980626	-1.731991	-2.648611
H68	-3.586832	0.924391	-3.507319
H69	-0.498463	4.782555	-2.128590
H70	1.494235	5.197761	-0.467860
H71	4.275709	1.799917	2.754108
H72	3.844562	-0.751405	3.671772

Diclofenac 4'-5 Transition State Doublet

C1	-1.839240	0.162970	3.073142
S2	-1.242128	1.222820	1.705652
H3	-2.888550	0.430841	3.243290
H4	-1.806400	-0.881648	2.754024
O5	1.186838	-0.564385	-1.187879
Fe6	0.159654	-0.008551	0.091777
N7	-0.206650	-1.831168	0.823918
N8	-1.482769	-0.150328	-1.113392
N9	0.389451	1.946414	-0.495793
N10	1.644222	0.213730	1.415668
C11	0.584209	-2.546582	1.694684
C12	0.157419	-3.919554	1.755680
C13	-0.931224	-4.021538	0.939424
C14	-1.142985	-2.720458	0.354558
C15	-2.257011	-1.256856	-1.301254
C16	-3.255134	-1.007252	-2.325004
C17	-3.078072	0.281453	-2.739279
C18	-1.963071	0.797396	-1.966383
C19	-0.383223	2.607282	-1.405774
C20	0.035218	3.982748	-1.515440
C21	1.059219	4.160778	-0.634059
C22	1.283830	2.862966	-0.010338
C23	2.442811	1.319462	1.551684
C24	3.497623	1.049714	2.502770
C25	3.314472	-0.223592	2.948330
C26	2.154950	-0.734128	2.258962
C27	1.678307	-2.032140	2.373112
H28	2.218712	-2.708953	3.021245
C29	-2.102292	-2.452222	-0.614943
H30	-2.773314	-3.261027	-0.859174
C31	-1.457882	2.081436	-2.101833
H32	-1.920028	2.733090	-2.828558
C33	2.279707	2.536708	0.907121
H34	3.047989	3.265616	1.113521
C35	4.517325	-2.444806	-2.782292
C36	4.506266	-2.093162	-1.410939
C37	3.356547	-1.996640	-0.660462
C38	2.087931	-2.248723	-1.252611

C39	2.083834	-2.699313	-2.603285
C40	3.248597	-2.746619	-3.339148
C141	6.030915	-1.700818	-0.658236
H42	3.418164	-1.699264	0.376619
H43	1.285926	-2.601604	-0.619936
H44	1.156734	-3.047037	-3.038661
C145	3.184171	-3.315492	-5.013581
C46	8.458476	-5.598342	-2.832330
C47	8.905568	-4.279564	-2.816589
C48	8.042794	-3.197235	-3.039904
C49	6.682795	-3.484988	-3.266061
C50	6.233589	-4.811253	-3.281105
C51	7.110323	-5.873701	-3.070792
H52	9.159487	-6.411220	-2.668210
H53	9.949958	-4.053621	-2.632227
N54	5.708695	-2.447392	-3.513689
H55	5.183388	-4.997775	-3.479755
H56	6.747617	-6.893871	-3.109794
H57	5.597848	-2.197834	-4.487067
C58	8.582457	-1.772906	-2.998502
H59	8.573663	-1.430899	-1.960194
H60	7.914520	-1.127156	-3.567601
C61	10.022046	-1.667112	-3.541819
O62	10.184891	-1.358557	-4.735826
O63	10.955798	-1.944524	-2.721694
H64	-1.341548	0.202282	4.063804
H65	0.686897	-4.701169	2.299717
H66	-1.548532	-4.886043	0.708701
H67	-3.973007	-1.751924	-2.662100
H68	-3.566667	0.900477	-3.504071
H69	-0.474603	4.730914	-2.121069
H70	1.503908	5.143401	-0.461305
H71	4.277333	1.759222	2.758519
H72	3.875500	-0.801432	3.671099

Diclofenac 5-1 Reactant Complex Doublet

C1	-2.032900	-0.385908	2.793425
S2	-1.484143	0.850878	1.577876
H3	-3.021889	-0.079302	3.156664
H4	-2.138506	-1.353647	2.294033
O5	1.241071	-0.592936	-1.179291
Fe6	0.136381	-0.163062	-0.040878
N7	-0.137634	-2.061558	0.610339
N8	-1.465402	-0.382343	-1.264816
N9	0.207086	1.820009	-0.452374
N10	1.564608	0.096380	1.377323
C11	0.690153	-2.749161	1.457236
C12	0.327428	-4.140845	1.510664
C13	-0.747958	-4.289836	0.688783
C14	-1.019874	-2.986643	0.125411
C15	-2.217905	-1.506661	-1.450358
C16	-3.270852	-1.259876	-2.415231
C17	-3.138757	0.036824	-2.816729
C18	-2.016907	0.570716	-2.061293
C19	-0.573293	2.462786	-1.366719
C20	-0.194438	3.848862	-1.457438
C21	0.825621	4.047951	-0.575840
C22	1.075000	2.759101	0.053500
C23	2.321725	1.219751	1.561350

C24	3.362921	0.963247	2.534479
C25	3.199039	-0.321249	2.962589
C26	2.107416	-0.863702	2.188761
C27	1.727465	-2.196982	2.187646
H28	2.310713	-2.881056	2.788609
C29	-2.021050	-2.717962	-0.802663
H30	-2.697578	-3.528874	-1.042480
C31	-1.599019	1.895826	-2.112343
H32	-2.097754	2.558047	-2.807157
C33	2.097223	2.446394	0.945876
H34	2.823976	3.209995	1.172289
C35	8.067858	-1.477570	-4.600244
C36	8.827782	-1.238981	-5.784266
C37	9.944016	-1.973567	-6.139357
C38	10.432611	-2.975558	-5.302653
C39	9.764058	-3.201434	-4.101728
C40	8.621289	-2.482420	-3.755423
C141	8.344515	0.038222	-6.901260
H42	10.400175	-1.771216	-7.098672
H43	11.290159	-3.572213	-5.586997
H44	10.105302	-3.968334	-3.418023
C145	7.920104	-2.920381	-2.204599
C46	3.932412	-1.345132	-1.450673
C47	3.800910	-1.906864	-2.716997
C48	4.765010	-1.713060	-3.715903
C49	5.906315	-0.969966	-3.379611
C50	6.027621	-0.356823	-2.129059
C51	5.044618	-0.547318	-1.161374
H52	3.175844	-1.515814	-0.699323
H53	2.933185	-2.514559	-2.948566
N54	6.936990	-0.736512	-4.363937
H55	6.891079	0.264742	-1.928371
H56	5.134190	-0.053570	-0.199337
H57	6.598930	-0.217996	-5.167328
C58	4.505806	-2.217188	-5.116796
H59	5.391781	-2.100163	-5.747480
H60	3.733944	-1.597011	-5.584278
C61	4.067728	-3.689517	-5.256914
O62	3.437128	-3.963691	-6.310674
O63	4.401429	-4.497487	-4.362244
H64	-1.392446	-0.565307	3.664793
H65	0.829471	-4.890383	2.116773
H66	-1.280794	-5.207904	0.460618
H67	-4.002353	-2.029530	-2.658359
H68	-3.672523	0.664839	-3.541288
H69	-0.708661	4.580183	-2.076298
H70	1.281341	5.033480	-0.439944
H71	4.157978	1.653937	2.799272
H72	3.702361	-0.850442	3.775851

Diclofenac 5-1 Transition State Doublet

C1	-1.881155	-0.454791	2.693562
S2	-1.345465	0.800021	1.489352
H3	-2.906148	-0.205811	2.995243
H4	-1.901203	-1.432813	2.202417
O5	1.384148	-0.396004	-1.374839
Fe6	0.251163	-0.167656	-0.073636
N7	0.039749	-2.085265	0.489600
N8	-1.354666	-0.380627	-1.325587

N9	0.277271	1.831539	-0.471227
N10	1.678512	0.062714	1.309757
C11	0.818683	-2.775955	1.392658
C12	0.405546	-4.151831	1.474407
C13	-0.654282	-4.287370	0.629353
C14	-0.876151	-2.996105	0.020533
C15	-2.100811	-1.506395	-1.519162
C16	-3.177550	-1.249648	-2.458308
C17	-3.062496	0.054837	-2.838949
C18	-1.931256	0.585653	-2.092875
C19	-0.510940	2.470706	-1.381489
C20	-0.156000	3.863184	-1.449501
C21	0.843723	4.073423	-0.549856
C22	1.112613	2.775079	0.068697
C23	2.388013	1.215007	1.536255
C24	3.417661	0.962846	2.522878
C25	3.274463	-0.333667	2.931822
C26	2.212192	-0.889802	2.132489
C27	1.836415	-2.225776	2.145134
H28	2.390838	-2.899373	2.782722
C29	-1.882575	-2.726134	-0.896912
H30	-2.559711	-3.535692	-1.134718
C31	-1.533914	1.911623	-2.128912
H32	-2.044663	2.579117	-2.808876
C33	2.129541	2.458116	0.970141
H34	2.825315	3.233474	1.249480
C35	7.330074	-1.541523	-4.130088
C36	8.128835	-1.336982	-5.298015
C37	9.321249	-2.003490	-5.538225
C38	9.811987	-2.931548	-4.623229
C39	9.044335	-3.202396	-3.490387
C40	7.839004	-2.542096	-3.262007
C141	7.612345	-0.245091	-6.575235
H42	9.823760	-1.824003	-6.481010
H43	10.728724	-3.475453	-4.820642
H44	9.346838	-3.968038	-2.790705
C145	6.956795	-3.063709	-1.844854
C46	2.856499	-1.604372	-1.366290
C47	2.928358	-2.103653	-2.702290
C48	3.980128	-1.809243	-3.561598
C49	5.067793	-1.075215	-3.049037
C50	5.034256	-0.560087	-1.736534
C51	3.970079	-0.830866	-0.900483
H52	2.283984	-2.180606	-0.648052
H53	2.131809	-2.751429	-3.053301
N54	6.193631	-0.778222	-3.910823
H55	5.868515	0.040761	-1.389822
H56	3.966753	-0.450765	0.113960
H57	5.912532	-0.221519	-4.712486
C58	3.961310	-2.309178	-4.987767
H59	4.882283	-2.031919	-5.508993
H60	3.149908	-1.841291	-5.549730
C61	3.832476	-3.835766	-5.138106
O62	3.256608	-4.228308	-6.183863
O63	4.336053	-4.558651	-4.252455
H64	-1.291231	-0.587997	3.608595
H65	0.867150	-4.905347	2.108416
H66	-1.236326	-5.184655	0.434728
H67	-3.920115	-2.010516	-2.691687
H68	-3.608731	0.688690	-3.551996

H69	-0.683512	4.575310	-2.080436
H70	1.271660	5.067171	-0.407480
H71	4.192411	1.670725	2.798285
H72	3.757068	-0.876211	3.748924

Diclofenac 5-2 Reactant Complex Doublet

C1	-1.962277	-0.533220	3.076824
S2	-1.364561	0.570791	1.754001
H3	-3.008006	-0.262256	3.270994
H4	-1.942094	-1.566238	2.718446
O5	0.869236	-1.026233	-1.334815
Fe6	-0.069307	-0.532072	-0.085555
N7	-0.364287	-2.395411	0.648083
N8	-1.778255	-0.702723	-1.159343
N9	0.098105	1.422053	-0.626088
N10	1.482783	-0.304757	1.174864
C11	0.498122	-3.104727	1.441701
C12	0.092712	-4.483284	1.539148
C13	-1.054307	-4.594843	0.812164
C14	-1.321169	-3.289766	0.251082
C15	-2.574408	-1.801219	-1.269562
C16	-3.655356	-1.557536	-2.201822
C17	-3.485834	-0.293753	-2.678952
C18	-2.313768	0.229905	-1.995538
C19	-0.732960	2.064898	-1.489511
C20	-0.282319	3.414829	-1.704587
C21	0.864162	3.581389	-0.985281
C22	1.087445	2.317350	-0.288382
C23	2.278476	0.798919	1.285587
C24	3.354091	0.542302	2.220215
C25	3.180686	-0.731074	2.682343
C26	2.031129	-1.257637	1.993583
C27	1.602648	-2.570857	2.081459
H28	2.195104	-3.252092	2.676245
C29	-2.369765	-3.005802	-0.609089
H30	-3.070101	-3.803837	-0.805876
C31	-1.838077	1.522296	-2.129927
H32	-2.338394	2.170249	-2.837455
C33	2.100505	2.002643	0.611492
H34	2.850082	2.744657	0.832881
C35	7.459000	-3.556934	-2.881559
C36	8.129338	-2.571195	-2.131222
C37	9.281386	-2.847743	-1.402201
C38	9.827885	-4.131004	-1.437564
C39	9.211150	-5.131029	-2.190484
C40	8.032858	-4.841686	-2.875846
Cl41	7.486216	-0.949079	-2.084601
H42	9.730652	-2.067779	-0.803555
H43	10.724436	-4.353112	-0.871334
H44	9.611843	-6.137474	-2.217920
Cl45	7.213032	-6.156607	-3.706656
C46	2.599731	-3.345447	-1.474560
C47	2.648141	-3.116347	-2.854233
C48	3.848791	-3.034411	-3.557525
C49	5.050473	-3.246321	-2.839152
C50	5.006644	-3.427682	-1.447899
C51	3.790397	-3.465989	-0.767252
H52	1.645520	-3.386988	-0.968777
H53	1.725402	-2.976084	-3.398909

N54	6.258377	-3.276872	-3.544298
H55	5.932895	-3.534119	-0.901758
H56	3.780036	-3.583001	0.312126
H57	6.173519	-3.589448	-4.520638
C58	3.834402	-2.629650	-5.025010
H59	4.512366	-1.779888	-5.156244
H60	2.827325	-2.309374	-5.283624
C61	4.269298	-3.698554	-6.048182
O62	5.509468	-3.970827	-6.095106
O63	3.387918	-4.204585	-6.763010
H64	-1.452730	-0.533589	4.056741
H65	0.622425	-5.256721	2.095618
H66	-1.654177	-5.480079	0.639086
H67	-4.409467	-2.309694	-2.408718
H68	-4.029369	0.310981	-3.414994
H69	-0.827227	4.137916	-2.311331
H70	1.407981	4.532796	-1.030506
H71	4.167532	1.235156	2.409173
H72	3.735786	-1.302401	3.423090

Diclofenac 5-2 Transition State Doublet

C1	-1.906490	-0.568940	2.970981
S2	-1.300869	0.523515	1.626779
H3	-2.961641	-0.318150	3.133021
H4	-1.853112	-1.608711	2.634722
O5	1.084370	-0.944788	-1.382439
Fe6	0.022700	-0.587822	-0.070961
N7	-0.263330	-2.449450	0.602196
N8	-1.675254	-0.773742	-1.215193
N9	0.183566	1.366492	-0.667503
N10	1.552996	-0.365569	1.177059
C11	0.561877	-3.151255	1.452793
C12	0.137673	-4.525528	1.544276
C13	-0.994862	-4.632476	0.794554
C14	-1.237806	-3.337981	0.206240
C15	-2.490074	-1.859112	-1.307665
C16	-3.590865	-1.598850	-2.215644
C17	-3.415864	-0.335469	-2.693311
C18	-2.221417	0.172347	-2.035600
C19	-0.656793	2.003238	-1.527779
C20	-0.229060	3.364569	-1.717409
C21	0.909787	3.540326	-0.989386
C22	1.152650	2.267184	-0.306935
C23	2.330724	0.752353	1.280302
C24	3.389260	0.511006	2.234486
C25	3.208648	-0.753863	2.720701
C26	2.063058	-1.293408	2.036220
C27	1.627880	-2.610427	2.142818
H28	2.191185	-3.281358	2.777827
C29	-2.291381	-3.063595	-0.647890
H30	-3.003010	-3.854694	-0.827414
C31	-1.756790	1.463929	-2.173124
H32	-2.261416	2.108452	-2.875308
C33	2.154013	1.959814	0.609694
H34	2.888797	2.711317	0.846462
C35	7.119821	-3.521778	-2.684523
C36	7.876694	-2.519626	-2.050138
C37	9.080561	-2.795675	-1.407531
C38	9.601067	-4.084458	-1.433540

C39	8.911735	-5.096932	-2.101768
C40	7.688572	-4.811742	-2.703848
C141	7.333665	-0.866002	-2.082873
H42	9.597365	-1.995472	-0.893533
H43	10.541117	-4.302226	-0.937974
H44	9.301204	-6.106577	-2.141746
C145	6.841427	-6.128860	-3.489875
C46	2.182546	-2.606184	-1.479974
C47	2.328106	-2.743879	-2.895915
C48	3.538413	-2.796039	-3.541683
C49	4.726208	-2.899653	-2.732299
C50	4.616267	-2.654632	-1.333019
C51	3.395181	-2.486405	-0.729070
H52	1.310735	-3.026138	-0.991595
H53	1.433264	-2.798757	-3.493650
N54	5.891732	-3.264101	-3.330805
H55	5.519012	-2.623642	-0.737725
H56	3.354376	-2.320212	0.336021
H57	5.812787	-3.582189	-4.327665
C58	3.579458	-2.611764	-5.053421
H59	4.193272	-1.725464	-5.254694
H60	2.568787	-2.391057	-5.387319
C61	4.131902	-3.727011	-5.960755
O62	5.367649	-4.017908	-5.837576
O63	3.350044	-4.232755	-6.775853
H64	-1.430568	-0.549330	3.977821
H65	0.652061	-5.302400	2.106204
H66	-1.625462	-5.502239	0.629475
H67	-4.380051	-2.319441	-2.404874
H68	-3.975601	0.281181	-3.412491
H69	-0.795079	4.097874	-2.292547
H70	1.428684	4.502240	-1.023246
H71	4.185870	1.222304	2.423710
H72	3.762539	-1.318763	3.461927

Diclofenac 5-3 Reactant Complex Doublet

C1	-1.990740	-0.456018	3.063474
S2	-1.444640	0.685512	1.748752
H3	-3.052457	-0.241437	3.237970
H4	-1.908220	-1.483967	2.701058
O5	0.950113	-0.846621	-1.252394
Fe6	-0.062636	-0.361225	-0.059272
N7	-0.328564	-2.230263	0.658367
N8	-1.740391	-0.572748	-1.170573
N9	0.067785	1.596887	-0.598730
N10	1.426287	-0.074824	1.261759
C11	0.538093	-2.910444	1.472206
C12	0.188432	-4.305107	1.539662
C13	-0.933103	-4.454738	0.782854
C14	-1.242146	-3.157316	0.231832
C15	-2.530436	-1.676915	-1.266001
C16	-3.627848	-1.442226	-2.179593
C17	-3.464251	-0.186545	-2.678545
C18	-2.292757	0.349823	-2.007246
C19	-0.753978	2.214182	-1.487824
C20	-0.337722	3.573944	-1.698619
C21	0.779210	3.780902	-0.946069
C22	1.017966	2.525543	-0.235788
C23	2.177695	1.056793	1.404169

C24	3.211655	0.840754	2.392036
C25	3.065103	-0.436709	2.849663
C26	1.969461	-1.006897	2.109264
C27	1.585515	-2.334276	2.170018
H28	2.163669	-2.993644	2.805640
C29	-2.302538	-2.888368	-0.624844
H30	-2.993991	-3.694678	-0.835101
C31	-1.835298	1.650548	-2.150314
H32	-2.332581	2.292685	-2.863846
C33	1.997296	2.249331	0.710580
H34	2.701954	3.022457	0.970774
C35	7.518740	-3.373633	-2.809273
C36	8.158573	-2.392860	-2.025726
C37	9.315557	-2.658546	-1.300843
C38	9.899923	-3.922539	-1.373322
C39	9.310369	-4.918492	-2.152385
C40	8.122914	-4.643196	-2.830041
C141	7.480720	-0.786595	-1.941993
H42	9.743523	-1.884177	-0.678474
H43	10.805109	-4.133405	-0.815367
H44	9.735620	-5.914810	-2.202714
C145	7.327569	-5.966065	-3.667801
C46	2.632983	-3.198584	-1.457841
C47	2.701037	-2.917373	-2.825218
C48	3.907819	-2.854481	-3.520654
C49	5.098920	-3.117304	-2.803889
C50	5.034112	-3.404656	-1.432810
C51	3.812633	-3.433688	-0.760643
H52	1.672448	-3.221930	-0.960659
H53	1.785755	-2.735503	-3.370627
N54	6.322519	-3.101992	-3.485461
H55	5.950590	-3.625983	-0.904297
H56	3.793245	-3.647170	0.303458
H57	6.262275	-3.396176	-4.468452
C58	3.914468	-2.442200	-4.986336
H59	4.600295	-1.597071	-5.102842
H60	2.912439	-2.117407	-5.262225
C61	4.354715	-3.530564	-5.989535
O62	5.601154	-3.772598	-6.056242
O63	3.475238	-4.091475	-6.665429
H64	-1.497234	-0.428838	4.057057
H65	0.743549	-5.061556	2.093522
H66	-1.488832	-5.361842	0.582092
H67	-4.420814	-2.170858	-2.287314
H68	-4.003521	0.401923	-3.430188
H69	-0.888303	4.249508	-2.350403
H70	1.299319	4.748278	-0.974193
H71	3.995304	1.562714	2.597158
H72	3.622338	-0.994852	3.600932

Diclofenac 5-3 Reactant Complex Quartet

C1	-2.040494	-0.463863	3.089597
S2	-1.420871	0.671609	1.798641
H3	-3.106274	-0.229241	3.219527
H4	-1.964757	-1.497525	2.729640
O5	0.961599	-0.832522	-1.282581
Fe6	-0.042046	-0.320490	-0.110780
N7	-0.302887	-2.175247	0.616938
N8	-1.730618	-0.540246	-1.206276

N9	0.050899	1.647361	-0.633349
N10	1.427951	-0.004619	1.215190
C11	0.582249	-2.853302	1.414463
C12	0.245962	-4.249322	1.482647
C13	-0.891545	-4.405002	0.747219
C14	-1.215028	-3.110761	0.198053
C15	-2.520625	-1.650952	-1.307410
C16	-3.616250	-1.417192	-2.226191
C17	-3.450456	-0.157836	-2.724331
C18	-2.288635	0.379750	-2.046008
C19	-0.785010	2.266293	-1.514060
C20	-0.401337	3.636192	-1.708692
C21	0.716799	3.855269	-0.956569
C22	0.983923	2.597040	-0.265233
C23	2.156434	1.142521	1.378225
C24	3.175073	0.944177	2.382775
C25	3.050047	-0.341194	2.830650
C26	1.982942	-0.929635	2.064833
C27	1.628656	-2.268252	2.108763
H28	2.225488	-2.923926	2.733063
C29	-2.281532	-2.855239	-0.656088
H30	-2.960753	-3.676239	-0.858139
C31	-1.856203	1.688691	-2.179183
H32	-2.373275	2.323854	-2.887864
C33	1.963523	2.336145	0.687108
H34	2.654791	3.124640	0.951175
C35	7.627246	-3.799713	-2.715260
C36	8.204653	-2.715704	-2.009391
C37	9.415770	-2.831212	-1.330986
C38	10.125605	-4.031683	-1.383433
C39	9.617650	-5.114478	-2.103521
C40	8.377470	-4.996299	-2.732307
C41	7.405949	-1.163009	-2.025863
H42	9.799325	-1.978920	-0.781557
H43	11.071925	-4.127517	-0.857730
H44	10.154940	-6.056788	-2.150075
C45	7.716227	-6.409558	-3.542544
C46	2.758790	-2.991573	-1.392797
C47	2.932460	-2.636712	-2.732698
C48	4.126328	-2.843045	-3.423713
C49	5.200515	-3.447733	-2.727345
C50	5.028091	-3.830497	-1.386575
C51	3.825211	-3.597121	-0.723226
H52	1.811802	-2.818554	-0.901043
H53	2.119305	-2.144857	-3.247946
N54	6.412985	-3.688122	-3.377754
H55	5.846789	-4.342652	-0.888428
H56	3.716657	-3.908313	0.313331
H57	6.396716	-3.748319	-4.412345
C58	4.281740	-2.324428	-4.840722
H59	5.089400	-1.583321	-4.832312
H60	3.354399	-1.824383	-5.133080
C61	4.632244	-3.373264	-5.925157
O62	5.879070	-3.645189	-6.062250
O63	3.702407	-3.877745	-6.583406
H64	-1.588811	-0.449025	4.109330
H65	0.805389	-5.002821	2.031434
H66	-1.443363	-5.319860	0.569054
H67	-4.428439	-2.118630	-2.379273
H68	-3.990291	0.423575	-3.482279

H69	-0.961958	4.327161	-2.337505
H70	1.203781	4.837245	-0.981781
H71	3.936885	1.684416	2.606447
H72	3.606637	-0.887968	3.590639

Diclofenac 5-3 Transition State Doublet

C1	-1.925955	-0.490328	2.969260
S2	-1.356181	0.641186	1.639306
H3	-2.995994	-0.299170	3.110787
H4	-1.807510	-1.523193	2.630413
O5	1.125369	-0.779116	-1.322953
Fe6	0.037688	-0.418083	-0.041215
N7	-0.217316	-2.278806	0.630665
N8	-1.639716	-0.635391	-1.200867
N9	0.164904	1.541162	-0.633788
N10	1.531330	-0.144623	1.243625
C11	0.621090	-2.955409	1.488174
C12	0.259276	-4.347411	1.545733
C13	-0.851368	-4.493988	0.768770
C14	-1.146272	-3.201935	0.201266
C15	-2.438713	-1.732502	-1.286887
C16	-3.553265	-1.483383	-2.180195
C17	-3.393035	-0.225718	-2.671412
C18	-2.205445	0.303512	-2.020293
C19	-0.672439	2.152484	-1.514731
C20	-0.277001	3.521952	-1.707294
C21	0.833498	3.738960	-0.949283
C22	1.097607	2.474623	-0.254841
C23	2.259824	1.001925	1.378101
C24	3.274433	0.807829	2.386779
C25	3.121531	-0.461342	2.872018
C26	2.036474	-1.048829	2.130422
C27	1.644104	-2.380941	2.217783
H28	2.205788	-3.033817	2.872314
C29	-2.208381	-2.944613	-0.651121
H30	-2.899101	-3.752078	-0.855888
C31	-1.758281	1.598362	-2.165674
H32	-2.268798	2.246235	-2.865340
C33	2.076132	2.200217	0.692204
H34	2.782333	2.971829	0.952987
C35	7.164659	-3.318548	-2.576593
C36	7.893095	-2.313422	-1.915746
C37	9.096120	-2.572012	-1.264036
C38	9.651026	-3.847134	-1.314903
C39	8.994858	-4.858195	-2.013733
C40	7.769242	-4.593319	-2.620489
Cl41	7.328247	-0.667930	-1.936564
H42	9.585902	-1.769989	-0.730608
H43	10.594167	-4.050235	-0.819002
H44	9.409750	-5.857623	-2.076964
Cl45	6.975259	-5.917641	-3.442281
C46	2.187792	-2.464504	-1.441922
C47	2.356017	-2.611150	-2.855458
C48	3.581033	-2.640724	-3.477728
C49	4.756449	-2.729592	-2.648744
C50	4.617878	-2.489732	-1.252771
C51	3.385508	-2.335330	-0.669826
H52	1.305864	-2.878796	-0.970692
H53	1.471731	-2.702035	-3.466262

N54	5.938185	-3.078656	-3.232377
H55	5.510972	-2.443189	-0.642021
H56	3.319095	-2.163124	0.394063
H57	5.882345	-3.388989	-4.230547
C58	3.653991	-2.451645	-4.987969
H59	4.275110	-1.566267	-5.171377
H60	2.650810	-2.229380	-5.341723
C61	4.227329	-3.571409	-5.878926
O62	5.469881	-3.823866	-5.764707
O63	3.448659	-4.123040	-6.669721
H64	-1.467693	-0.445705	3.985381
H65	0.797650	-5.105829	2.109884
H66	-1.432041	-5.391866	0.579680
H67	-4.370856	-2.186479	-2.280960
H68	-3.948863	0.371200	-3.408110
H69	-0.856980	4.198683	-2.333315
H70	1.320738	4.719064	-0.959670
H71	4.023575	1.559692	2.605907
H72	3.666433	-1.002296	3.638807

Diclofenac 5-3 Transition State Quartet

C1	-1.943098	-0.504869	2.981689
S2	-1.329603	0.614728	1.664592
H3	-3.012821	-0.299781	3.099030
H4	-1.829308	-1.539213	2.643709
O5	1.179185	-1.051355	-1.254919
Fe6	0.061175	-0.392031	-0.106848
N7	-0.254029	-2.247402	0.639118
N8	-1.623519	-0.613048	-1.250083
N9	0.187814	1.538115	-0.686061
N10	1.554665	-0.108212	1.192096
C11	0.602809	-2.919295	1.472063
C12	0.245568	-4.312834	1.536234
C13	-0.869859	-4.462091	0.766178
C14	-1.169250	-3.168117	0.202494
C15	-2.437769	-1.708083	-1.315814
C16	-3.554721	-1.455363	-2.206168
C17	-3.386951	-0.202074	-2.707760
C18	-2.191973	0.321008	-2.069247
C19	-0.662016	2.161972	-1.556039
C20	-0.286673	3.535962	-1.719763
C21	0.822601	3.755579	-0.958286
C22	1.104168	2.490720	-0.283883
C23	2.271321	1.035830	1.349254
C24	3.271544	0.843762	2.373484
C25	3.124423	-0.432051	2.842280
C26	2.052793	-1.021107	2.076927
C27	1.642834	-2.342690	2.180821
H28	2.202439	-2.993347	2.839448
C29	-2.225382	-2.911166	-0.663122
H30	-2.920943	-3.715525	-0.861769
C31	-1.746737	1.616939	-2.214775
H32	-2.259759	2.268338	-2.908074
C33	2.077944	2.236525	0.671438
H34	2.756137	3.025121	0.951421
C35	7.227014	-3.415213	-2.601691
C36	7.927804	-2.404818	-1.916468
C37	9.139986	-2.643506	-1.274210
C38	9.730391	-3.901697	-1.356347

C39	9.102232	-4.915533	-2.078119
C40	7.866966	-4.671073	-2.675564
C141	7.311371	-0.776115	-1.912624
H42	9.611958	-1.839736	-0.725335
H43	10.679057	-4.091455	-0.864519
H44	9.545697	-5.900827	-2.163422
C145	7.104328	-5.998592	-3.525115
C46	2.186132	-2.644543	-1.499074
C47	2.406998	-2.671068	-2.919577
C48	3.651198	-2.686164	-3.506611
C49	4.803013	-2.869373	-2.667629
C50	4.624795	-2.782649	-1.259109
C51	3.379653	-2.660645	-0.693069
H52	1.306711	-3.132964	-1.099934
H53	1.544589	-2.704275	-3.565173
N54	6.001124	-3.181955	-3.254827
H55	5.498292	-2.861799	-0.624809
H56	3.282417	-2.644017	0.383046
H57	5.963280	-3.449720	-4.262180
C58	3.782615	-2.414190	-4.998876
H59	4.469491	-1.568961	-5.112895
H60	2.808516	-2.107328	-5.372321
C61	4.308189	-3.533917	-5.918667
O62	5.550845	-3.806144	-5.842830
O63	3.496514	-4.070492	-6.682925
H64	-1.500518	-0.461883	4.006131
H65	0.792490	-5.070713	2.093556
H66	-1.442446	-5.362385	0.571169
H67	-4.384328	-2.144867	-2.313834
H68	-3.946425	0.392272	-3.444368
H69	-0.872688	4.222177	-2.330041
H70	1.298757	4.743005	-0.961578
H71	4.006244	1.604778	2.607770
H72	3.664733	-0.975650	3.613697

Ibuprofen 2-1 Reactant Complex Doublet

C1	6.478607	21.213755	-2.447482
S2	6.322747	22.250017	-0.940983
H3	5.984092	20.267559	-2.200825
H4	5.939922	21.677935	-3.273212
O5	5.598610	26.353632	-1.551186
Fe6	5.757644	24.744793	-1.287494
N7	5.534308	24.211997	-3.212131
N8	3.781812	24.448528	-0.961266
N9	6.045890	24.916483	0.724290
N10	7.755040	24.775349	-1.545664
C11	6.507528	24.137003	-4.172946
C12	5.925963	23.829871	-5.456233
C13	4.582955	23.749711	-5.259559
C14	4.346096	23.978719	-3.853449
C15	2.831554	24.200370	-1.908217
C16	1.511718	24.178072	-1.309952
C17	1.680762	24.422289	0.021952
C18	3.106784	24.596359	0.217317
C19	5.059647	24.987016	1.665922
C20	5.621187	25.235276	2.966747
C21	6.969017	25.324227	2.815429
C22	7.223570	25.152811	1.394045
C23	8.685869	25.106972	-0.599198

C24	9.989572	25.224445	-1.204399
C25	9.838006	24.950566	-2.529252
C26	8.435141	24.683134	-2.736425
C27	7.855937	24.383555	-3.958247
H28	8.504137	24.358281	-4.825995
C29	3.093456	23.981424	-3.256469
H30	2.249419	23.790991	-3.904088
C31	3.699127	24.854977	1.442612
H32	3.062345	24.989067	2.308095
C33	8.446352	25.288907	0.752852
H34	9.303253	25.601299	1.332062
C35	7.642458	30.443615	-4.371429
C36	8.519813	30.381910	-3.284813
C37	8.934332	31.541211	-2.629168
C38	8.469696	32.800177	-3.025165
C39	7.587124	32.865350	-4.108236
C40	7.188756	31.704896	-4.776840
H41	6.506638	31.775091	-5.618494
H42	7.182011	33.817672	-4.423741
H43	9.604011	31.464864	-1.778199
H44	8.878095	29.412815	-2.955400
C45	8.881791	34.026524	-2.231889
C46	10.025987	34.862495	-2.841194
O47	10.123505	35.101816	-4.052291
O48	10.860449	35.331253	-1.987242
H49	9.260882	33.674032	-1.268486
C50	7.685074	34.956311	-1.928310
H51	7.250127	35.345556	-2.850296
H52	8.007674	35.796598	-1.309716
H53	6.911623	34.393000	-1.397971
C54	7.136884	29.181082	-5.021208
C55	6.167264	28.375027	-4.126762
C56	5.017926	29.243115	-3.606025
C57	5.615658	27.187624	-4.918907
H58	4.987032	27.540652	-5.746373
H59	5.014325	26.550296	-4.269739
H60	6.420358	26.582507	-5.342250
H61	4.446671	29.658687	-4.445778
H62	5.376473	30.075138	-2.993893
H63	4.341997	28.634600	-3.001120
H64	6.722506	27.987875	-3.266099
H65	7.977280	28.530092	-5.292584
H66	6.613391	29.436583	-5.949592
H67	7.496868	20.947737	-2.821593
H68	6.470299	23.752692	-6.397809
H69	3.798080	23.607640	-5.996702
H70	0.602734	23.980808	-1.871825
H71	0.983934	24.472097	0.872391
H72	5.032108	25.290067	3.878152
H73	7.638414	25.464067	3.668508
H74	10.873999	25.507810	-0.642752
H75	10.568689	24.936944	-3.323831

Ibuprofen 2-1 Reactant Complex Quartet

C1	6.477402	21.196217	-2.434499
S2	6.323035	22.224826	-0.902000
H3	5.975378	20.240225	-2.218024
H4	5.939165	21.684476	-3.254702
O5	5.571041	26.373222	-1.554832

Fe6	5.747520	24.798709	-1.289157
N7	5.528118	24.217390	-3.218069
N8	3.763716	24.468916	-0.958134
N9	6.039612	24.943959	0.737209
N10	7.757913	24.779040	-1.541943
C11	6.494887	24.142793	-4.172392
C12	5.916894	23.838782	-5.454980
C13	4.580347	23.759282	-5.258561
C14	4.347435	23.989345	-3.856066
C15	2.822751	24.218141	-1.897999
C16	1.506088	24.184139	-1.303457
C17	1.673369	24.425655	0.022767
C18	3.096174	24.608115	0.213287
C19	5.059589	25.003931	1.673974
C20	5.619865	25.237708	2.974289
C21	6.962526	25.325417	2.823028
C22	7.211947	25.164391	1.404349
C23	8.684682	25.104839	-0.601243
C24	9.986019	25.221064	-1.201236
C25	9.835145	24.951497	-2.522656
C26	8.434667	24.685916	-2.727023
C27	7.858681	24.388675	-3.964973
H28	8.505994	24.368903	-4.835280
C29	3.077952	23.992287	-3.262255
H30	2.234073	23.796912	-3.909245
C31	3.686079	24.864945	1.457779
H32	3.048738	24.987398	2.326032
C33	8.452117	25.291724	0.765256
H34	9.314196	25.593924	1.343898
C35	7.652550	30.441571	-4.373089
C36	8.521386	30.376382	-3.283049
C37	8.929626	31.532460	-2.622399
C38	8.462617	32.788634	-3.019659
C39	7.585161	32.855762	-4.103566
C40	7.194511	31.698901	-4.776926
H41	6.513493	31.769317	-5.627929
H42	7.181965	33.817300	-4.416334
H43	9.600582	31.457683	-1.763323
H44	8.881080	29.399411	-2.954737
C45	8.868473	34.022805	-2.231258
C46	10.034622	34.870465	-2.857776
O47	10.127093	35.091812	-4.036778
O48	10.836522	35.320281	-1.997313
H49	9.258149	33.680601	-1.269035
C50	7.669698	34.953016	-1.930029
H51	7.231609	35.342671	-2.851354
H52	7.990946	35.793628	-1.309162
H53	6.896678	34.387353	-1.398688
C54	7.149835	29.173332	-5.025962
C55	6.171272	28.375592	-4.132191
C56	5.022600	29.249077	-3.618329
C57	5.617093	27.184654	-4.917393
H58	4.981114	27.536049	-5.741516
H59	5.019881	26.547530	-4.262502
H60	6.417872	26.574994	-5.345472
H61	4.449644	29.663104	-4.459312
H62	5.380935	30.084189	-3.007085
H63	4.347653	28.643058	-3.007926
H64	6.719908	27.993715	-3.262218
H65	7.994306	28.522547	-5.290632

H66	6.633679	29.427267	-5.959896
H67	7.496846	20.936143	-2.819418
H68	6.464762	23.760862	-6.398600
H69	3.793724	23.611218	-5.998073
H70	0.593988	23.979543	-1.865114
H71	0.977307	24.472583	0.876095
H72	5.029188	25.292618	3.888678
H73	7.635792	25.466588	3.677747
H74	10.873396	25.506659	-0.637099
H75	10.569799	24.940545	-3.319022

Ibuprofen 2-1 Transition State Doublet

C1	6.500987	21.308755	-2.459032
S2	6.367272	22.390491	-0.971566
H3	5.971503	20.385382	-2.198424
H4	5.977450	21.770986	-3.297439
O5	5.737801	26.656259	-1.762247
Fe6	5.845093	24.960485	-1.464528
N7	5.618307	24.349562	-3.351715
N8	3.859676	24.655259	-1.125564
N9	6.116266	25.146660	0.566617
N10	7.827156	24.902379	-1.688988
C11	6.595422	24.212058	-4.304000
C12	6.018319	23.831048	-5.568567
C13	4.673599	23.755335	-5.368226
C14	4.434871	24.064955	-3.981495
C15	2.909506	24.350825	-2.058793
C16	1.597024	24.275725	-1.448597
C17	1.769009	24.524154	-0.117751
C18	3.187489	24.760641	0.059781
C19	5.131078	25.161885	1.510906
C20	5.687819	25.325155	2.826320
C21	7.037030	25.402355	2.687292
C22	7.293940	25.304980	1.256744
C23	8.758894	25.206924	-0.731355
C24	10.070295	25.274276	-1.320938
C25	9.923109	24.993940	-2.646933
C26	8.518112	24.768819	-2.867970
C27	7.945027	24.446965	-4.087844
H28	8.602459	24.368540	-4.944320
C29	3.176864	24.081936	-3.395002
H30	2.339197	23.834726	-4.032710
C31	3.776387	25.002124	1.288568
H32	3.142145	25.073004	2.161896
C33	8.524171	25.389432	0.622184
H34	9.395004	25.642657	1.206372
C35	7.541723	30.095565	-3.909393
C36	8.588993	30.187054	-2.993725
C37	9.049830	31.421381	-2.522792
C38	8.490257	32.625715	-2.959044
C39	7.473824	32.545688	-3.925548
C40	7.011868	31.305495	-4.389670
H41	6.230074	31.278108	-5.143223
H42	7.018724	33.451829	-4.307313
H43	9.837046	31.439129	-1.774427
H44	9.053955	29.269332	-2.655141
C45	8.899288	33.926143	-2.263597
C46	10.039285	34.783580	-2.864547
O47	10.147299	35.029368	-4.074062

O48	10.842866	35.290916	-2.000674
H49	9.264880	33.633702	-1.275049
C50	7.694518	34.867021	-2.029536
H51	7.289323	35.225880	-2.977964
H52	8.008427	35.729489	-1.437362
H53	6.902074	34.332590	-1.497672
C54	7.050277	28.742008	-4.404960
C55	5.752626	28.128776	-3.794832
C56	4.748942	29.170926	-3.324779
C57	5.121272	27.202188	-4.829620
H58	4.751578	27.792416	-5.683422
H59	4.281037	26.656518	-4.399501
H60	5.842628	26.481130	-5.215517
H61	4.469043	29.834488	-4.157223
H62	5.135666	29.803138	-2.522397
H63	3.835849	28.676774	-2.985513
H64	5.920478	27.365991	-2.778342
H65	7.860759	28.010264	-4.325334
H66	6.849946	28.854571	-5.481401
H67	7.509919	20.998958	-2.834148
H68	6.562461	23.716898	-6.499904
H69	3.875785	23.584166	-6.081903
H70	0.690369	24.044220	-1.999330
H71	1.085329	24.542046	0.745024
H72	5.096167	25.319938	3.737500
H73	7.688028	25.477772	3.560740
H74	10.953380	25.531820	-0.747994
H75	10.653290	24.937527	-3.431669

Ibuprofen 2-1 Transition State Quartet

C1	6.493808	21.250750	-2.505611
S2	6.343683	22.327713	-1.004042
H3	5.964781	20.315980	-2.264809
H4	5.972083	21.723040	-3.348187
O5	5.725123	26.653932	-1.872841
Fe6	5.825645	24.989819	-1.428449
N7	5.596024	24.324697	-3.336132
N8	3.829556	24.677039	-1.097192
N9	6.096331	25.165364	0.590506
N10	7.824283	24.922900	-1.657816
C11	6.569003	24.206959	-4.280138
C12	5.995587	23.836330	-5.547239
C13	4.656665	23.761689	-5.348682
C14	4.421675	24.062007	-3.961544
C15	2.887214	24.369726	-2.032267
C16	1.577000	24.294136	-1.422878
C17	1.744892	24.541528	-0.098820
C18	3.160071	24.783569	0.079307
C19	5.112534	25.184413	1.534680
C20	5.673966	25.341484	2.844250
C21	7.018546	25.413213	2.704262
C22	7.275685	25.318675	1.279512
C23	8.750261	25.222619	-0.714036
C24	10.058503	25.285092	-1.305554
C25	9.905816	25.002796	-2.623020
C26	8.500708	24.781599	-2.834860
C27	7.933028	24.451659	-4.071185
H28	8.591496	24.381571	-4.929546
C29	3.143945	24.092999	-3.379192

H30	2.305628	23.856306	-4.022320
C31	3.745343	25.032850	1.323603
H32	3.108959	25.115134	2.195789
C33	8.521572	25.408487	0.656232
H34	9.390038	25.671585	1.243756
C35	7.511959	30.084772	-3.940331
C36	8.555453	30.179498	-3.022016
C37	9.013665	31.416715	-2.558039
C38	8.451453	32.613864	-3.004735
C39	7.442807	32.528709	-3.976185
C40	6.985998	31.289234	-4.434403
H41	6.201343	31.252820	-5.194686
H42	6.985165	33.438369	-4.365166
H43	9.798859	31.442632	-1.799806
H44	9.017504	29.257745	-2.669822
C45	8.840983	33.923695	-2.304555
C46	10.017065	34.791621	-2.897812
O47	10.126659	35.029522	-4.072102
O48	10.790147	35.265208	-2.019784
H49	9.187916	33.638942	-1.307509
C50	7.624556	34.858738	-2.105536
H51	7.231278	35.200712	-3.066296
H52	7.914354	35.733535	-1.517446
H53	6.827670	34.320951	-1.581323
C54	6.996228	28.728060	-4.405666
C55	5.660653	28.201012	-3.818047
C56	4.694959	29.264246	-3.333387
C57	5.000359	27.248149	-4.804849
H58	4.643549	27.820667	-5.677670
H59	4.143405	26.738324	-4.356931
H60	5.697250	26.489264	-5.169481
H61	4.426810	29.938375	-4.161156
H62	5.104359	29.885931	-2.530783
H63	3.768722	28.796870	-2.987414
H64	5.840287	27.401761	-2.764211
H65	7.776972	27.970784	-4.257724
H66	6.839906	28.790970	-5.494032
H67	7.509654	20.958388	-2.872711
H68	6.541658	23.721094	-6.484642
H69	3.858688	23.591075	-6.070836
H70	0.667693	24.055774	-1.974994
H71	1.055877	24.552930	0.766437
H72	5.082739	25.335150	3.760983
H73	7.677528	25.487861	3.578891
H74	10.950319	25.538245	-0.735286
H75	10.639427	24.943252	-3.414571

Ibuprofen 2-2 Reactant Complex Doublet

C1	6.390206	20.994236	-2.143478
S2	6.254053	22.097372	-0.685763
H3	5.883238	20.068091	-1.853418
H4	5.858925	21.430738	-2.989839
O5	5.613842	26.128150	-1.572277
Fe6	5.745207	24.524557	-1.241774
N7	5.498325	23.980808	-3.157671
N8	3.764108	24.247315	-0.907164
N9	6.050486	24.718090	0.760110
N10	7.746067	24.552264	-1.515550
C11	6.457987	23.953898	-4.131840

C12	5.861796	23.728367	-5.422361
C13	4.519821	23.633869	-5.216027
C14	4.303053	23.797040	-3.798545
C15	2.803303	24.027413	-1.849494
C16	1.485786	24.012641	-1.242033
C17	1.669401	24.215793	0.093744
C18	3.102560	24.357199	0.278489
C19	5.072551	24.724100	1.708534
C20	5.632778	24.959354	3.010209
C21	6.976460	25.105201	2.853124
C22	7.230684	24.956025	1.427861
C23	8.680868	24.901075	-0.579966
C24	9.968732	25.075449	-1.207227
C25	9.800865	24.827100	-2.535996
C26	8.406738	24.502966	-2.718530
C27	7.806840	24.211718	-3.931464
H28	8.429867	24.239409	-4.816018
C29	3.051238	23.813862	-3.197111
H30	2.202506	23.643414	-3.840912
C31	3.712286	24.558395	1.503788
H32	3.088508	24.640026	2.383764
C33	8.450193	25.081581	0.776374
H34	9.315403	25.390520	1.341610
C35	7.836183	30.596813	-4.199193
C36	8.653915	30.623753	-3.065255
C37	9.079780	31.830602	-2.507673
C38	8.696202	33.056827	-3.062936
C39	7.888505	33.035481	-4.203916
C40	7.467693	31.826030	-4.763038
H41	6.846635	31.834053	-5.653183
H42	7.575519	33.973240	-4.645473
H43	9.709859	31.817042	-1.624036
H44	8.966167	29.687088	-2.618887
C45	9.093210	34.353438	-2.382549
C46	10.022782	35.293390	-3.200337
O47	10.863463	35.942465	-2.475236
O48	9.915424	35.372699	-4.425611
H49	9.649151	34.099964	-1.475596
C50	7.843620	35.148176	-1.932567
H51	7.251571	34.549508	-1.232830
H52	7.219133	35.379403	-2.799868
H53	8.140544	36.080020	-1.444383
C54	7.379074	29.281897	-4.791574
C55	6.453785	28.421480	-3.896048
C56	5.187940	29.182213	-3.494508
C57	6.091945	27.143122	-4.659751
H58	5.513081	27.389236	-5.558146
H59	5.502626	26.477033	-4.027853
H60	6.991560	26.603654	-4.973180
H61	5.395730	30.099205	-2.932647
H62	4.554586	28.549081	-2.868256
H63	4.619931	29.448905	-4.395235
H64	6.983000	28.122131	-2.982350
H65	8.255733	28.676475	-5.054659
H66	6.845306	29.481359	-5.731607
H67	7.395930	20.688909	-2.507810
H68	6.405538	23.718262	-6.362312
H69	3.722260	23.518398	-5.943172
H70	0.575130	23.874185	-1.817009
H71	0.982860	24.278169	0.951112

H72	5.025022	24.975683	3.908993
H73	7.629741	25.284477	3.709022
H74	10.855206	25.391654	-0.665713
H75	10.522803	24.879755	-3.340977

Ibuprofen 2-2 Reactant Complex Quartet

C1	6.371805	20.946670	-2.123454
S2	6.259779	22.066587	-0.665651
H3	5.877246	20.011068	-1.820781
H4	5.820752	21.376199	-2.968685
O5	5.522597	26.084194	-1.512955
Fe6	5.734518	24.512337	-1.226931
N7	5.495606	23.955495	-3.160118
N8	3.748349	24.190177	-0.889807
N9	6.045289	24.693958	0.787019
N10	7.748100	24.547217	-1.505952
C11	6.448620	23.937744	-4.127942
C12	5.857394	23.728035	-5.420242
C13	4.521782	23.632463	-5.214799
C14	4.307184	23.778236	-3.798501
C15	2.796876	23.985323	-1.829836
C16	1.479633	23.985954	-1.231450
C17	1.659462	24.193430	0.097374
C18	3.089453	24.320460	0.283446
C19	5.070606	24.717176	1.725394
C20	5.626231	24.969017	3.021744
C21	6.965810	25.102272	2.866456
C22	7.218105	24.936262	1.447442
C23	8.676380	24.890930	-0.575267
C24	9.962416	25.069471	-1.197851
C25	9.797187	24.821706	-2.521209
C26	8.407130	24.493610	-2.701952
C27	7.813400	24.195106	-3.930832
H28	8.439727	24.215820	-4.815101
C29	3.041387	23.786247	-3.196966
H30	2.187999	23.633108	-3.844094
C31	3.696817	24.549437	1.524066
H32	3.068006	24.657575	2.400203
C33	8.452110	25.067915	0.796555
H34	9.318171	25.377471	1.364380
C35	7.859587	30.615398	-4.261617
C36	8.640949	30.635376	-3.105328
C37	9.040960	31.837092	-2.525611
C38	8.658575	33.061057	-3.083291
C39	7.873429	33.045087	-4.237378
C40	7.482572	31.840904	-4.821626
H41	6.869813	31.843751	-5.724217
H42	7.547127	33.989866	-4.670017
H43	9.644639	31.826097	-1.615828
H44	8.934529	29.690058	-2.649825
C45	9.040981	34.355498	-2.387367
C46	10.006533	35.301692	-3.207572
O47	10.832524	35.903441	-2.470552
O48	9.897511	35.376567	-4.405685
H49	9.592713	34.096189	-1.479134
C50	7.784657	35.141289	-1.938881
H51	7.200636	34.532591	-1.239102
H52	7.154825	35.365934	-2.805206
H53	8.067107	36.078170	-1.448437

C54	7.403631	29.297668	-4.854227
C55	6.493132	28.470876	-3.919445
C56	5.225816	29.238204	-3.535291
C57	6.128828	27.153384	-4.607223
H58	5.529331	27.353983	-5.505783
H59	5.554470	26.517223	-3.931204
H60	7.026485	26.607226	-4.916234
H61	5.428708	30.163092	-2.984878
H62	4.584014	28.616069	-2.905976
H63	4.665027	29.492993	-4.445726
H64	7.056497	28.241217	-3.003837
H65	8.276119	28.684036	-5.115192
H66	6.859935	29.485889	-5.790722
H67	7.380181	20.654520	-2.497176
H68	6.404350	23.725858	-6.364225
H69	3.722943	23.528039	-5.949358
H70	0.565120	23.867022	-1.813600
H71	0.971250	24.269874	0.954457
H72	5.012848	25.008018	3.920704
H73	7.624855	25.291788	3.721796
H74	10.851945	25.390967	-0.654996
H75	10.524682	24.882023	-3.328243

Ibuprofen 2-2 Transition State Doublet

C1	6.404352	21.098811	-2.135388
S2	6.271153	22.223797	-0.685895
H3	5.859151	20.193929	-1.848505
H4	5.889269	21.552514	-2.983968
O5	5.716117	26.420645	-1.710445
Fe6	5.812446	24.751016	-1.348225
N7	5.550094	24.129425	-3.230319
N8	3.823057	24.436295	-0.993778
N9	6.114631	24.885174	0.673323
N10	7.796738	24.689605	-1.601697
C11	6.507486	24.072621	-4.209285
C12	5.905584	23.781098	-5.484260
C13	4.567015	23.673848	-5.263684
C14	4.354557	23.900026	-3.858231
C15	2.855999	24.169022	-1.922361
C16	1.548620	24.097314	-1.297952
C17	1.741468	24.296309	0.036145
C18	3.168322	24.496266	0.203513
C19	5.138336	24.838287	1.627895
C20	5.703998	24.982977	2.938438
C21	7.048855	25.125648	2.789755
C22	7.302007	25.048988	1.356053
C23	8.741028	24.987327	-0.656566
C24	10.032623	25.127829	-1.280307
C25	9.857057	24.902223	-2.612948
C26	8.456359	24.626921	-2.802892
C27	7.855244	24.337801	-4.019099
H28	8.480906	24.339174	-4.900661
C29	3.100098	23.922966	-3.261894
H30	2.253961	23.705761	-3.897243
C31	3.782582	24.669270	1.428223
H32	3.164346	24.703929	2.315407
C33	8.524035	25.136942	0.708014
H34	9.405151	25.384611	1.277450
C35	7.781584	30.196656	-3.511538

C36	8.828473	30.435242	-2.616881
C37	9.259922	31.729753	-2.304050
C38	8.677129	32.856920	-2.886932
C39	7.651768	32.631653	-3.820607
C40	7.216078	31.332984	-4.121664
H41	6.425038	31.202055	-4.852651
H42	7.179786	33.474614	-4.312482
H43	10.052470	31.853797	-1.571720
H44	9.332896	29.595871	-2.160872
C45	9.068911	34.240575	-2.368066
C46	9.988045	35.175971	-3.218869
O47	10.817681	35.849924	-2.498033
O48	9.885771	35.262457	-4.447579
H49	9.633793	34.071796	-1.447097
C50	7.815250	35.054218	-1.969463
H51	7.214284	34.488804	-1.249876
H52	7.202210	35.255243	-2.852218
H53	8.113471	36.003812	-1.518771
C54	7.383674	28.771383	-3.901789
C55	6.002728	28.153337	-3.484800
C56	4.926244	29.192680	-3.201214
C57	5.542050	27.229180	-4.615431
H58	5.267031	27.827000	-5.500998
H59	4.672996	26.644003	-4.310664
H60	6.333401	26.539212	-4.913766
H61	5.126546	29.888687	-2.379718
H62	3.973508	28.694232	-3.012563
H63	4.781112	29.804594	-4.106901
H64	6.011164	27.316304	-2.506087
H65	8.187784	28.090354	-3.605051
H66	7.384984	28.763022	-5.003819
H67	7.400961	20.756509	-2.502531
H68	6.440903	23.736797	-6.424139
H69	3.760376	23.508257	-5.971595
H70	0.635058	23.916536	-1.858114
H71	1.061824	24.321648	0.903572
H72	5.094564	24.931894	3.838490
H73	7.693985	25.261451	3.661133
H74	10.926834	25.411346	-0.733816
H75	10.577899	24.916126	-3.414220

Ibuprofen 2-2 Transition State Quartet

C1	6.414703	21.079203	-2.139109
S2	6.311747	22.214559	-0.681607
H3	5.859685	20.174805	-1.851282
H4	5.899332	21.542997	-2.990414
O5	5.732591	26.462923	-1.821464
Fe6	5.786128	24.821634	-1.343857
N7	5.525660	24.131956	-3.228297
N8	3.792439	24.464936	-0.979914
N9	6.089226	24.924933	0.691427
N10	7.786839	24.714696	-1.585060
C11	6.481648	24.068163	-4.195807
C12	5.887871	23.771287	-5.469800
C13	4.554135	23.673571	-5.255604
C14	4.339361	23.908923	-3.854025
C15	2.832962	24.191576	-1.905901
C16	1.528835	24.109865	-1.285417
C17	1.718184	24.303574	0.043905

C18	3.141127	24.511483	0.210128
C19	5.120663	24.865863	1.645211
C20	5.687815	25.002813	2.951828
C21	7.026787	25.146360	2.801274
C22	7.274005	25.081648	1.371929
C23	8.725264	25.010879	-0.648215
C24	10.017146	25.130770	-1.269505
C25	9.842457	24.892511	-2.593280
C26	8.441182	24.630541	-2.780544
C27	7.845131	24.329509	-4.008425
H28	8.475345	24.319369	-4.890473
C29	3.068908	23.937767	-3.260153
H30	2.220199	23.718434	-3.893686
C31	3.751018	24.685563	1.454869
H32	3.132281	24.713387	2.342280
C33	8.513255	25.172792	0.727454
H34	9.393751	25.423969	1.300647
C35	7.757332	30.227843	-3.683434
C36	8.768871	30.424891	-2.744305
C37	9.200478	31.700915	-2.375131
C38	8.648598	32.848867	-2.947909
C39	7.660358	32.665334	-3.925638
C40	7.224167	31.385103	-4.281866
H41	6.455769	31.279025	-5.049260
H42	7.218104	33.536848	-4.409444
H43	9.970347	31.799050	-1.606764
H44	9.245636	29.553735	-2.300001
C45	9.035108	34.219957	-2.385974
C46	9.983662	35.178670	-3.225968
O47	10.792295	35.805227	-2.484281
O48	9.876888	35.273712	-4.424811
H49	9.594995	34.031139	-1.465681
C50	7.777593	35.028151	-1.981024
H51	7.176686	34.451242	-1.268542
H52	7.164262	35.238219	-2.863168
H53	8.068865	35.974653	-1.515834
C54	7.336015	28.820634	-4.116160
C55	5.988783	28.187436	-3.625900
C56	4.904997	29.218704	-3.351813
C57	5.523406	27.200216	-4.699399
H58	5.196176	27.753791	-5.596499
H59	4.687592	26.594336	-4.341959
H60	6.328249	26.524363	-5.002346
H61	5.115905	29.933733	-2.546685
H62	3.957024	28.721138	-3.130216
H63	4.749385	29.801763	-4.274823
H64	6.030276	27.382662	-2.601454
H65	8.161338	28.126974	-3.914163
H66	7.244434	28.860971	-5.214844
H67	7.410114	20.733217	-2.510071
H68	6.427608	23.724539	-6.414778
H69	3.749422	23.511758	-5.973344
H70	0.612020	23.924458	-1.847555
H71	1.034683	24.325736	0.912512
H72	5.080950	24.951376	3.858532
H73	7.680312	25.277371	3.674480
H74	10.917856	25.412559	-0.723982
H75	10.569649	24.903459	-3.397808

Ibuprofen 2-3 Reactant Complex Doublet

C1	6.525043	21.131728	-2.197115
S2	6.481291	22.273944	-0.762000
H3	5.895554	20.284942	-1.911918
H4	6.066808	21.625551	-3.055322
O5	5.546656	26.341867	-1.478648
Fe6	5.756892	24.744412	-1.224137
N7	5.522127	24.207548	-3.141012
N8	3.779119	24.406850	-0.892268
N9	6.054525	24.898497	0.780014
N10	7.759841	24.803299	-1.501268
C11	6.484406	24.187175	-4.112623
C12	5.893118	23.919487	-5.399125
C13	4.555510	23.801884	-5.199310
C14	4.329552	23.989172	-3.786139
C15	2.825389	24.195397	-1.842167
C16	1.504837	24.168286	-1.249883
C17	1.670564	24.361668	0.088588
C18	3.101886	24.521411	0.290113
C19	5.072088	24.891105	1.727497
C20	5.638029	25.098287	3.031579
C21	6.984906	25.252355	2.876182
C22	7.233198	25.138563	1.447092
C23	8.693275	25.135413	-0.556867
C24	9.990791	25.279585	-1.175721
C25	9.835864	25.017795	-2.504072
C26	8.431495	24.734833	-2.700293
C27	7.832169	24.456649	-3.912997
H28	8.462993	24.479129	-4.792437
C29	3.081726	23.999075	-3.192803
H30	2.234652	23.834406	-3.842388
C31	3.709417	24.735789	1.515413
H32	3.075466	24.814134	2.390179
C33	8.450190	25.299438	0.797392
H34	9.305554	25.611485	1.376078
C35	7.375224	30.494484	-4.437727
C36	8.347155	30.393396	-3.437504
C37	8.922660	31.536904	-2.878960
C38	8.543040	32.815819	-3.307134
C39	7.556119	32.920095	-4.290958
C40	6.984183	31.773836	-4.847386
H41	6.233559	31.879517	-5.621462
H42	7.261950	33.900207	-4.640096
H43	9.676278	31.436166	-2.104160
H44	8.660843	29.409597	-3.103140
C45	9.169235	34.042295	-2.673487
C46	9.859914	35.019585	-3.653773
O47	9.332563	35.406317	-4.688965
O48	11.016414	35.443039	-3.244502
H49	9.943923	33.702073	-1.982337
C50	8.121523	34.834743	-1.851978
H51	7.312649	35.173703	-2.500772
H52	8.573722	35.710873	-1.377859
H53	7.683249	34.191179	-1.081354
C54	6.750559	29.251981	-5.027923
C55	5.942299	28.417284	-4.013438
C56	4.827237	29.238721	-3.360827
C57	5.351578	27.194177	-4.714935
H58	4.823567	26.566827	-3.996489
H59	6.132764	26.595161	-5.185855

H60	4.648047	27.505668	-5.496845
H61	5.203537	30.160864	-2.908866
H62	4.344416	28.640091	-2.587277
H63	4.074442	29.509273	-4.112371
H64	6.617777	28.069188	-3.224183
H65	7.530511	28.611544	-5.458729
H66	6.084682	29.533700	-5.851859
H67	7.488070	20.688661	-2.546018
H68	6.443950	23.871979	-6.327517
H69	3.771233	23.648457	-5.937029
H70	0.603871	24.007728	-1.837213
H71	0.963882	24.384834	0.933813
H72	5.033457	25.090826	3.933932
H73	7.649496	25.421563	3.731457
H74	10.882690	25.577909	-0.630593
H75	10.586658	25.012326	-3.295331

Ibuprofen 2-3 Reactant Complex Quartet

C1	6.522529	21.125606	-2.196573
S2	6.490805	22.272730	-0.752413
H3	5.892818	20.271733	-1.915191
H4	6.063711	21.627349	-3.057010
O5	5.533337	26.347506	-1.478747
Fe6	5.751396	24.777879	-1.227219
N7	5.520749	24.205014	-3.151201
N8	3.766880	24.408262	-0.890873
N9	6.054493	24.903722	0.790932
N10	7.766933	24.803370	-1.500815
C11	6.476745	24.182280	-4.114375
C12	5.889563	23.917177	-5.400044
C13	4.558190	23.802407	-5.200762
C14	4.335938	23.989147	-3.792225
C15	2.822503	24.197381	-1.833638
C16	1.503520	24.168755	-1.247990
C17	1.667674	24.361379	0.085632
C18	3.096541	24.521274	0.284366
C19	5.078415	24.893390	1.731546
C20	5.640283	25.098572	3.032885
C21	6.981125	25.250409	2.878014
C22	7.226472	25.138020	1.454347
C23	8.695835	25.134041	-0.562377
C24	9.989064	25.278331	-1.178722
C25	9.835487	25.016878	-2.500682
C26	8.435571	24.732791	-2.694512
C27	7.840351	24.452890	-3.923449
H28	8.470833	24.478212	-4.805156
C29	3.069701	23.996175	-3.201848
H30	2.221164	23.832986	-3.848583
C31	3.699251	24.735934	1.527109
H32	3.065944	24.813317	2.403717
C33	8.461460	25.302203	0.806036
H34	9.318108	25.617207	1.383802
C35	7.375672	30.496318	-4.437226
C36	8.344345	30.392287	-3.435898
C37	8.916604	31.533904	-2.875644
C38	8.534077	32.810486	-3.302875
C39	7.551323	32.918815	-4.288528
C40	6.983250	31.774445	-4.845571
H41	6.230634	31.879605	-5.627784

H42	7.265163	33.906168	-4.645907
H43	9.679795	31.435361	-2.101761
H44	8.663284	29.402254	-3.103551
C45	9.163942	34.037988	-2.668410
C46	9.861715	35.030470	-3.671549
O47	9.335025	35.392179	-4.673144
O48	10.993163	35.433881	-3.244976
H49	9.945558	33.702832	-1.982760
C50	8.119794	34.837372	-1.849399
H51	7.313074	35.178843	-2.501700
H52	8.572875	35.712200	-1.370186
H53	7.680302	34.190422	-1.082076
C54	6.751205	29.249134	-5.028677
C55	5.942346	28.415349	-4.012638
C56	4.826430	29.239226	-3.361660
C57	5.352822	27.192212	-4.715109
H58	4.824774	26.564562	-3.995511
H59	6.134071	26.588782	-5.184747
H60	4.649362	27.505089	-5.498655
H61	5.200042	30.163944	-2.908292
H62	4.341325	28.643254	-2.585833
H63	4.074139	29.506769	-4.116380
H64	6.616997	28.065951	-3.220470
H65	7.530538	28.608069	-5.462868
H66	6.082466	29.532500	-5.850665
H67	7.487500	20.684217	-2.548759
H68	6.442671	23.870525	-6.330708
H69	3.770912	23.648451	-5.940566
H70	0.600111	24.007250	-1.837538
H71	0.958955	24.384601	0.932379
H72	5.031405	25.095582	3.936168
H73	7.648239	25.421774	3.734443
H74	10.882761	25.576352	-0.629477
H75	10.588397	25.011894	-3.294292

Ibuprofen 2-3 Transition State Doublet

C1	6.587490	21.337520	-2.268652
S2	6.566588	22.474277	-0.822674
H3	5.880210	20.541523	-2.024229
H4	6.206437	21.869926	-3.142046
O5	5.684063	26.714701	-1.529909
Fe6	5.859926	24.956910	-1.339400
N7	5.597821	24.481204	-3.260677
N8	3.873636	24.621303	-0.996028
N9	6.157333	25.116592	0.678038
N10	7.843937	24.982625	-1.626246
C11	6.554252	24.426163	-4.238409
C12	5.961158	24.083253	-5.505295
C13	4.628920	23.931476	-5.283289
C14	4.412174	24.182462	-3.881735
C15	2.913739	24.358644	-1.930290
C16	1.606309	24.261920	-1.314770
C17	1.787790	24.451900	0.023069
C18	3.211994	24.680586	0.197402
C19	5.187824	25.043792	1.630432
C20	5.761664	25.148144	2.943644
C21	7.105523	25.304369	2.790239
C22	7.342306	25.277547	1.350447
C23	8.787755	25.254221	-0.669519

C24	10.088098	25.367200	-1.284539
C25	9.924865	25.140028	-2.618346
C26	8.514566	24.915272	-2.823499
C27	7.909665	24.671867	-4.044758
H28	8.543346	24.662359	-4.921407
C29	3.163838	24.145213	-3.278552
H30	2.324614	23.900687	-3.913540
C31	3.825472	24.873914	1.423142
H32	3.201585	24.891537	2.306127
C33	8.563670	25.387213	0.692515
H34	9.443503	25.618306	1.269407
C35	7.504146	30.060253	-3.893730
C36	8.616229	30.161803	-3.059257
C37	9.171763	31.402001	-2.723388
C38	8.647506	32.598801	-3.228175
C39	7.538719	32.505255	-4.086914
C40	6.981171	31.260833	-4.406954
H41	6.132020	31.225036	-5.081600
H42	7.128179	33.408572	-4.522945
H43	10.022858	31.436977	-2.051602
H44	9.063306	29.248592	-2.684534
C45	9.211415	33.923510	-2.721119
C46	9.850435	34.933673	-3.715471
O47	9.292460	35.318178	-4.735216
O48	10.988824	35.410591	-3.307845
H49	10.004083	33.675117	-2.011485
C50	8.116837	34.700106	-1.946505
H51	7.288990	34.945882	-2.614269
H52	8.517725	35.632749	-1.539661
H53	7.723803	34.087163	-1.128710
C54	6.933603	28.699627	-4.279699
C55	5.613493	28.244056	-3.620533
C56	4.808072	29.328716	-2.946845
C57	4.777976	27.380000	-4.542451
H58	3.971640	26.889535	-3.993429
H59	5.376002	26.616580	-5.041448
H60	4.324959	28.012520	-5.322957
H61	5.347449	29.815829	-2.133027
H62	3.877865	28.916072	-2.562222
H63	4.551043	30.110219	-3.677239
H64	5.820869	27.308685	-2.529927
H65	7.696956	27.925728	-4.134978
H66	6.739473	28.724326	-5.361997
H67	7.531218	20.823524	-2.587030
H68	6.509587	23.976250	-6.425641
H69	3.835057	23.704146	-5.987993
H70	0.702245	24.057519	-1.879779
H71	1.099321	24.431490	0.884682
H72	5.160305	25.048561	3.844524
H73	7.764281	25.417327	3.658206
H74	10.982577	25.635102	-0.730558
H75	10.669839	25.088942	-3.405063

Ibuprofen 2-3 Transition State Quartet

C1	6.591852	21.244205	-2.264889
S2	6.595359	22.400253	-0.829436
H3	5.895302	20.439117	-1.999158
H4	6.185503	21.765208	-3.142561
O5	5.706480	26.682291	-1.718155

Fe6	5.816803	25.021576	-1.334021
N7	5.561596	24.401553	-3.243684
N8	3.823303	24.659877	-0.984296
N9	6.114436	25.136670	0.688396
N10	7.822282	24.950453	-1.593328
C11	6.517609	24.352345	-4.208703
C12	5.928047	24.026091	-5.478002
C13	4.598408	23.894860	-5.265039
C14	4.380712	24.142410	-3.866230
C15	2.870629	24.385063	-1.916546
C16	1.566873	24.286328	-1.303412
C17	1.743657	24.481417	0.027705
C18	3.161964	24.724982	0.200840
C19	5.142806	25.079141	1.641111
C20	5.718488	25.173667	2.949378
C21	7.060363	25.313981	2.797693
C22	7.298567	25.285047	1.365202
C23	8.759306	25.236859	-0.650708
C24	10.055833	25.342746	-1.264045
C25	9.892191	25.098168	-2.589297
C26	8.485687	24.865690	-2.788326
C27	7.886064	24.604088	-4.021423
H28	8.520855	24.599639	-4.900321
C29	3.111619	24.148199	-3.273605
H30	2.266163	23.927759	-3.911491
C31	3.768886	24.930980	1.444019
H32	3.140213	24.976582	2.324566
C33	8.537953	25.393872	0.722705
H34	9.411694	25.646502	1.303561
C35	7.431258	30.087197	-3.938634
C36	8.539534	30.168986	-3.099469
C37	9.097340	31.400583	-2.740966
C38	8.578818	32.601917	-3.232145
C39	7.475364	32.529781	-4.096203
C40	6.914646	31.295245	-4.437399
H41	6.063897	31.269917	-5.120385
H42	7.073179	33.448288	-4.523676
H43	9.948123	31.424224	-2.057330
H44	8.979709	29.240093	-2.736820
C45	9.146050	33.923107	-2.710656
C46	9.810967	34.945746	-3.721004
O47	9.277624	35.304554	-4.717808
O48	10.925399	35.395082	-3.281856
H49	9.937677	33.670109	-2.001179
C50	8.051254	34.706202	-1.939948
H51	7.226042	34.958199	-2.610300
H52	8.453886	35.636193	-1.525369
H53	7.650453	34.090682	-1.125921
C54	6.845731	28.735114	-4.332180
C55	5.547154	28.259481	-3.625637
C56	4.686237	29.367482	-3.051032
C57	4.747838	27.355484	-4.554316
H58	3.935786	26.858371	-4.018312
H59	5.376514	26.588337	-5.011210
H60	4.305436	27.953883	-5.370121
H61	5.175733	29.923203	-2.245957
H62	3.754276	28.947716	-2.672051
H63	4.425217	30.095343	-3.835534
H64	5.777001	27.454227	-2.613097
H65	7.616053	27.960340	-4.234119

H66	6.607590	28.786481	-5.406960
H67	7.538552	20.746237	-2.591709
H68	6.479969	23.930392	-6.403085
H69	3.804968	23.685072	-5.982417
H70	0.660796	24.066692	-1.868064
H71	1.051389	24.451162	0.891613
H72	5.119992	25.077375	3.858411
H73	7.721628	25.424461	3.670706
H74	10.954680	25.619473	-0.712496
H75	10.641573	25.056480	-3.379580

Ibuprofen 3-1 Reactant Complex Doublet

C1	6.483136	21.210433	-2.283718
S2	6.387633	22.229893	-0.750771
H3	5.875647	20.313449	-2.102324
H4	6.042333	21.760361	-3.122322
O5	5.474750	26.255815	-1.380716
Fe6	5.704701	24.661187	-1.222924
N7	5.478557	24.201315	-3.188207
N8	3.719796	24.283198	-0.916597
N9	6.000386	24.793608	0.791265
N10	7.722731	24.752673	-1.506249
C11	6.441841	24.196192	-4.150390
C12	5.864593	23.954037	-5.449907
C13	4.528444	23.837522	-5.251137
C14	4.300004	23.982096	-3.835159
C15	2.776573	24.066449	-1.863700
C16	1.455853	24.035369	-1.269131
C17	1.624807	24.245157	0.061814
C18	3.051355	24.395464	0.255302
C19	5.014120	24.831247	1.716457
C20	5.555372	25.114278	3.010641
C21	6.896436	25.232944	2.872153
C22	7.164330	25.054011	1.457518
C23	8.640117	25.078851	-0.558402
C24	9.941052	25.217121	-1.156858
C25	9.802454	24.951685	-2.481418
C26	8.401285	24.680198	-2.692012
C27	7.811258	24.421280	-3.934088
H28	8.452735	24.422431	-4.808585
C29	3.032936	23.903586	-3.236315
H30	2.190746	23.699800	-3.888326
C31	3.644324	24.639913	1.499236
H32	3.003290	24.742873	2.365973
C33	8.398369	25.234507	0.813579
H34	9.246277	25.563825	1.398696
C35	8.214345	31.058994	-2.674220
C36	9.042449	31.395182	-1.597856
C37	9.448890	32.717419	-1.379380
C38	9.021550	33.745521	-2.228580
C39	8.178484	33.415270	-3.294826
C40	7.788118	32.097340	-3.513205
H41	7.139674	31.872671	-4.362275
H42	7.853883	34.204585	-3.973373
H43	10.105566	32.949248	-0.539469
H44	9.385366	30.612042	-0.919087
C45	9.448569	35.200052	-1.993369
C46	10.090285	35.751047	-3.317704
O47	11.312890	35.541422	-3.451158

O48	9.348285	36.290572	-4.116536
H49	10.230480	35.201113	-1.227384
C50	8.264166	36.060483	-1.515222
H51	7.492823	36.082956	-2.288970
H52	8.587169	37.087646	-1.307580
H53	7.828601	35.640132	-0.604056
C54	7.860282	29.601850	-2.959813
C55	6.423638	29.321111	-3.446874
C56	5.404710	29.572284	-2.326180
C57	6.323678	27.876946	-3.962777
H58	7.031599	27.693850	-4.780051
H59	5.313476	27.656914	-4.325365
H60	6.534763	27.172537	-3.154676
H61	5.541537	30.564400	-1.878657
H62	5.517791	28.804614	-1.552350
H63	4.378359	29.500588	-2.704521
H64	6.203295	30.000034	-4.282460
H65	8.047493	29.001579	-2.061568
H66	8.550524	29.220992	-3.725190
H67	7.478079	20.847446	-2.618868
H68	6.423883	23.889256	-6.392076
H69	3.737203	23.710196	-5.991244
H70	0.540426	23.882289	-1.843310
H71	0.926082	24.315562	0.916107
H72	4.949850	25.189665	3.907879
H73	7.549756	25.392875	3.736984
H74	10.822869	25.517365	-0.586761
H75	10.571250	24.951513	-3.259947

Ibuprofen 3-1 Reactant Complex Quartet

C1	6.485724	21.198986	-2.303961
S2	6.392490	22.239089	-0.732921
H3	5.875044	20.313860	-2.105196
H4	6.040289	21.765006	-3.124470
O5	5.452632	26.270416	-1.384860
Fe6	5.709786	24.651869	-1.218674
N7	5.481327	24.205528	-3.172033
N8	3.736085	24.284925	-0.918926
N9	6.000545	24.791163	0.776033
N10	7.705243	24.749076	-1.501021
C11	6.459900	24.198874	-4.155816
C12	5.870548	23.954295	-5.457107
C13	4.520289	23.836065	-5.255303
C14	4.282610	23.981576	-3.834318
C15	2.770025	24.063644	-1.881888
C16	1.448515	24.033610	-1.273691
C17	1.620186	24.246147	0.071503
C18	3.051469	24.398434	0.274052
C19	4.998239	24.831493	1.721414
C20	5.547830	25.121860	3.017652
C21	6.903565	25.238114	2.879810
C22	7.185195	25.056128	1.460715
C23	8.644104	25.081463	-0.539078
C24	9.946410	25.219705	-1.149417
C25	9.806650	24.951694	-2.486776
C26	8.400903	24.675570	-2.707813
C27	7.813154	24.420232	-3.935015
H28	8.454808	24.420781	-4.808269
C29	3.031050	23.903470	-3.236950

H30	2.190941	23.697591	-3.890447
C31	3.644819	24.639996	1.500403
H32	3.002766	24.743163	2.365066
C33	8.402354	25.234542	0.818226
H34	9.250612	25.565423	1.401013
C35	8.213811	31.057740	-2.674769
C36	9.048181	31.394708	-1.594051
C37	9.452931	32.720170	-1.376495
C38	9.021443	33.751153	-2.227294
C39	8.176753	33.422121	-3.301574
C40	7.785278	32.098665	-3.520122
H41	7.139993	31.873426	-4.363146
H42	7.854887	34.206999	-3.977914
H43	10.106160	32.954108	-0.539138
H44	9.388862	30.613530	-0.919888
C45	9.446102	35.202929	-1.993508
C46	10.084968	35.743502	-3.292777
O47	11.349512	35.534683	-3.451385
O48	9.318145	36.314907	-4.153488
H49	10.228265	35.204193	-1.223371
C50	8.262552	36.066410	-1.515896
H51	7.489443	36.090187	-2.291231
H52	8.590732	37.096020	-1.313161
H53	7.827801	35.649439	-0.601029
C54	7.863016	29.604759	-2.958077
C55	6.422165	29.322822	-3.443727
C56	5.401843	29.575102	-2.320766
C57	6.323903	27.874874	-3.960130
H58	7.036904	27.695053	-4.776072
H59	5.313564	27.653856	-4.324480
H60	6.534063	27.170454	-3.150042
H61	5.544692	30.566839	-1.871674
H62	5.512294	28.804290	-1.547718
H63	4.375319	29.507982	-2.703652
H64	6.199993	30.002209	-4.282441
H65	8.049138	29.002429	-2.057997
H66	8.549535	29.218511	-3.727540
H67	7.480441	20.843803	-2.625018
H68	6.425078	23.889866	-6.394184
H69	3.733652	23.709881	-5.991587
H70	0.536570	23.881977	-1.842538
H71	0.922883	24.317409	0.919289
H72	4.948103	25.201313	3.910776
H73	7.550436	25.397363	3.740877
H74	10.823180	25.519920	-0.582743
H75	10.572615	24.952243	-3.260307

Ibuprofen 3-1 Transition State Doublet

C1	6.456761	21.242047	-2.306312
S2	6.361222	22.282646	-0.779326
H3	5.843744	20.352459	-2.111013
H4	6.017183	21.783888	-3.151172
O5	5.576699	26.432110	-1.409436
Fe6	5.767922	24.659361	-1.304057
N7	5.523972	24.275980	-3.272320
N8	3.760174	24.361030	-0.998825
N9	6.038150	24.844099	0.717869
N10	7.764048	24.779215	-1.592021
C11	6.486967	24.224800	-4.234274

C12	5.905775	23.964418	-5.528045
C13	4.569114	23.869392	-5.326310
C14	4.343584	24.051704	-3.914445
C15	2.814214	24.142928	-1.942963
C16	1.495790	24.079172	-1.342420
C17	1.669088	24.267051	-0.009238
C18	3.094477	24.435903	0.177424
C19	5.060171	24.833409	1.646335
C20	5.601249	25.058802	2.953600
C21	6.940349	25.198523	2.815378
C22	7.203665	25.075437	1.389381
C23	8.676429	25.097046	-0.636293
C24	9.982773	25.219784	-1.226680
C25	9.848592	24.953134	-2.552072
C26	8.448150	24.693093	-2.769933
C27	7.860229	24.428496	-4.015205
H28	8.506133	24.403991	-4.886069
C29	3.072625	23.984636	-3.315770
H30	2.231720	23.775950	-3.967946
C31	3.690247	24.643136	1.425432
H32	3.052101	24.710899	2.297341
C33	8.435391	25.249593	0.739218
H34	9.292401	25.556549	1.324548
C35	8.173002	30.833988	-2.606182
C36	9.030081	31.200310	-1.563092
C37	9.450469	32.523617	-1.398099
C38	9.013307	33.531286	-2.265925
C39	8.145693	33.173999	-3.304325
C40	7.737659	31.848638	-3.471575
H41	7.060785	31.602642	-4.290521
H42	7.800887	33.946095	-3.993571
H43	10.122880	32.775899	-0.574468
H44	9.377400	30.438097	-0.863235
C45	9.432026	34.992064	-2.042181
C46	10.060441	35.593862	-3.353080
O47	11.284661	35.396179	-3.499820
O48	9.317095	36.173959	-4.120473
H49	10.223314	34.991884	-1.285452
C50	8.247759	35.835249	-1.534085
H51	7.472711	35.878507	-2.302884
H52	8.569657	36.857138	-1.299745
H53	7.819602	35.387555	-0.632408
C54	7.793566	29.365308	-2.806280
C55	6.356569	29.079172	-3.292409
C56	5.300316	29.603130	-2.304267
C57	6.159069	27.599341	-3.574132
H58	7.027458	27.061747	-3.957727
H59	5.236848	27.350227	-4.101097
H60	5.910958	26.949689	-2.378583
H61	5.478737	30.653822	-2.049506
H62	5.329429	28.997812	-1.393813
H63	4.292513	29.508879	-2.723843
H64	6.217526	29.606550	-4.253286
H65	7.958559	28.822636	-1.869783
H66	8.485594	28.920207	-3.535045
H67	7.448915	20.864399	-2.641591
H68	6.464512	23.881223	-6.465879
H69	3.771878	23.722719	-6.055978
H70	0.577975	23.907402	-1.906892
H71	0.977180	24.306688	0.853063

H72	4.991672	25.062362	3.852854
H73	7.587918	25.337001	3.687343
H74	10.863356	25.507593	-0.649551
H75	10.613038	24.938651	-3.328514

Ibuprofen 3-1 Transition State Quartet

C1	6.459453	21.224735	-2.318906
S2	6.376216	22.306643	-0.771110
H3	5.848785	20.346060	-2.093768
H4	6.010989	21.771979	-3.150528
O5	5.520793	26.430719	-1.494549
Fe6	5.758102	24.675432	-1.287471
N7	5.522408	24.256156	-3.248198
N8	3.770059	24.370863	-0.989545
N9	6.024863	24.866056	0.699080
N10	7.739982	24.792664	-1.579068
C11	6.500441	24.213290	-4.230700
C12	5.907986	23.954938	-5.525432
C13	4.556809	23.853787	-5.321468
C14	4.323120	24.030298	-3.903916
C15	2.804941	24.139886	-1.953152
C16	1.483483	24.080136	-1.342572
C17	1.656156	24.274284	0.003847
C18	3.085729	24.449388	0.202270
C19	5.030402	24.854501	1.652559
C20	5.585320	25.081027	2.960928
C21	6.939018	25.218616	2.819700
C22	7.213819	25.098107	1.389444
C23	8.674920	25.115675	-0.613962
C24	9.984135	25.226902	-1.215395
C25	9.846057	24.954966	-2.551842
C26	8.440212	24.694894	-2.779354
C27	7.856709	24.424161	-4.007601
H28	8.502785	24.400497	-4.877457
C29	3.067945	23.968784	-3.305107
H30	2.227758	23.753188	-3.954574
C31	3.680195	24.660593	1.433951
H32	3.042639	24.723993	2.305740
C33	8.430271	25.269246	0.746253
H34	9.285912	25.572693	1.333768
C35	8.179061	30.886202	-2.624539
C36	9.034588	31.246756	-1.567309
C37	9.452438	32.572698	-1.389926
C38	9.016301	33.589643	-2.255753
C39	8.151343	33.238914	-3.308479
C40	7.745693	31.910817	-3.488830
H41	7.078673	31.670548	-4.311355
H42	7.815333	34.013501	-3.991670
H43	10.117837	32.820916	-0.564980
H44	9.377613	30.482143	-0.876417
C45	9.436114	35.045408	-2.029508
C46	10.064388	35.628925	-3.316778
O47	11.332528	35.444244	-3.480537
O48	9.294202	36.228527	-4.155418
H49	10.227133	35.045402	-1.267920
C50	8.250686	35.892037	-1.525848
H51	7.476490	35.932544	-2.299238
H52	8.572964	36.917111	-1.295370
H53	7.819864	35.447587	-0.621992

C54	7.813664	29.421718	-2.843141
C55	6.370006	29.130412	-3.321522
C56	5.322047	29.619601	-2.301499
C57	6.180962	27.651999	-3.644369
H58	7.057270	27.132897	-4.045974
H59	5.258682	27.418494	-4.182422
H60	5.908903	26.941706	-2.448847
H61	5.495808	30.669496	-2.034246
H62	5.376227	28.997912	-1.401722
H63	4.307663	29.520266	-2.705491
H64	6.213023	29.695280	-4.261474
H65	7.991754	28.863227	-1.915661
H66	8.500209	28.992911	-3.590349
H67	7.453383	20.858625	-2.641729
H68	6.462122	23.876897	-6.458518
H69	3.765837	23.715888	-6.050322
H70	0.571918	23.908444	-1.904663
H71	0.967750	24.314928	0.860445
H72	4.983842	25.087563	3.857187
H73	7.583593	25.350738	3.687326
H74	10.861620	25.510825	-0.643219
H75	10.607029	24.940830	-3.322959

Ibuprofen 3-2 Reactant Complex Doublet

C1	6.459291	21.153081	-2.350573
S2	6.337786	22.206785	-0.855665
H3	5.823563	20.280134	-2.165687
H4	6.053481	21.696532	-3.205870
O5	5.512908	26.303055	-1.457786
Fe6	5.690921	24.690972	-1.245672
N7	5.466953	24.223307	-3.183403
N8	3.712953	24.345818	-0.940137
N9	5.972096	24.826337	0.759638
N10	7.693690	24.755781	-1.503673
C11	6.435074	24.249016	-4.152475
C12	5.856489	24.002035	-5.450783
C13	4.519780	23.837502	-5.252013
C14	4.285965	23.970311	-3.833860
C15	2.769008	24.073024	-1.886648
C16	1.447696	24.027459	-1.289758
C17	1.610892	24.280215	0.041563
C18	3.033395	24.475183	0.236155
C19	4.975344	24.899360	1.689345
C20	5.522233	25.160806	2.990187
C21	6.875666	25.225570	2.857305
C22	7.144995	25.050507	1.440225
C23	8.619625	25.066927	-0.544495
C24	9.922238	25.219119	-1.144367
C25	9.775971	24.988898	-2.478993
C26	8.374105	24.718677	-2.698071
C27	7.785344	24.490285	-3.930184
H28	8.425276	24.518238	-4.802564
C29	3.036907	23.873043	-3.235830
H30	2.204965	23.627949	-3.882546
C31	3.620100	24.734313	1.462356
H32	2.976586	24.845504	2.323371
C33	8.372517	25.207133	0.810502
H34	9.219763	25.517005	1.403314
C35	8.096937	31.020931	-2.701332

C36	8.908715	31.123982	-1.567300
C37	9.422495	32.360076	-1.153898
C38	9.115761	33.531173	-1.853688
C39	8.277507	33.438658	-2.972491
C40	7.789742	32.202706	-3.392671
H41	7.162988	32.157100	-4.277223
H42	8.035556	34.335496	-3.532102
H43	10.063962	32.407780	-0.278345
H44	9.153136	30.231609	-0.999037
C45	9.670036	34.882322	-1.396275
C46	10.238776	35.618808	-2.627947
O47	11.451727	35.401226	-2.947661
O48	9.461124	36.346439	-3.269024
H49	10.489625	34.689145	-0.698212
C50	8.579853	35.720460	-0.698817
H51	8.985809	36.656104	-0.295592
H52	8.133684	35.159870	0.127241
H53	7.796064	35.965077	-1.416061
C54	7.594742	29.676962	-3.200488
C55	6.073345	29.606725	-3.452131
C56	5.297097	29.792621	-2.144330
C57	5.691457	28.274460	-4.114554
H58	5.870260	27.444016	-3.422969
H59	6.266979	28.105157	-5.031062
H60	4.626877	28.265394	-4.371826
H61	5.595100	30.712990	-1.632467
H62	5.483231	28.934218	-1.488303
H63	4.219957	29.835132	-2.337534
H64	5.810246	30.424687	-4.134641
H65	7.872909	28.890986	-2.489189
H66	8.106208	29.441234	-4.143082
H67	7.463106	20.769076	-2.646433
H68	6.413844	23.961319	-6.383198
H69	3.740581	23.699767	-5.994579
H70	0.538964	23.842295	-1.857072
H71	0.911701	24.333018	0.889233
H72	4.924684	25.222887	3.889035
H73	7.532262	25.332038	3.721979
H74	10.807041	25.499754	-0.576377
H75	10.530076	24.997732	-3.256876

Ibuprofen 3-2 Reactant Complex Quartet

C1	6.457553	21.159912	-2.316439
S2	6.328467	22.189479	-0.785045
H3	5.799086	20.290821	-2.169980
H4	6.071113	21.743292	-3.162352
O5	5.474609	26.317688	-1.439652
Fe6	5.680319	24.739593	-1.231268
N7	5.458091	24.232832	-3.180886
N8	3.695886	24.350911	-0.919037
N9	5.967414	24.849693	0.786209
N10	7.697124	24.766299	-1.490149
C11	6.419746	24.253892	-4.142775
C12	5.844025	24.005300	-5.439605
C13	4.513496	23.845948	-5.240695
C14	4.282140	23.982801	-3.825633
C15	2.760275	24.079440	-1.860152
C16	1.441482	24.031157	-1.266760
C17	1.602979	24.282076	0.057737

C18	3.023710	24.477943	0.250355
C19	4.978557	24.919325	1.712751
C20	5.527112	25.177514	3.009772
C21	6.872367	25.235735	2.874311
C22	7.136542	25.061392	1.461155
C23	8.620031	25.071868	-0.537019
C24	9.919513	25.221587	-1.135501
C25	9.772055	24.994373	-2.463991
C26	8.373324	24.725118	-2.679196
C27	7.786077	24.491696	-3.927123
H28	8.428504	24.512695	-4.800613
C29	3.019454	23.879096	-3.226194
H30	2.183291	23.628893	-3.869453
C31	3.607563	24.745531	1.493093
H32	2.964743	24.853415	2.357117
C33	8.379742	25.213848	0.832229
H34	9.231252	25.516360	1.427905
C35	8.104899	31.032829	-2.717842
C36	8.896990	31.133593	-1.571586
C37	9.400940	32.370434	-1.149821
C38	9.103354	33.540819	-1.854951
C39	8.284994	33.447071	-2.987612
C40	7.808714	32.211174	-3.414471
H41	7.198302	32.158557	-4.317939
H42	8.050767	34.347352	-3.555683
H43	10.034096	32.420398	-0.261613
H44	9.139335	30.235276	-1.000451
C45	9.657050	34.896009	-1.390165
C46	10.256114	35.635793	-2.639449
O47	11.442569	35.401740	-2.919996
O48	9.492426	36.344312	-3.265514
H49	10.472060	34.699310	-0.686241
C50	8.569149	35.747081	-0.705406
H51	8.985087	36.674136	-0.287753
H52	8.101686	35.186511	0.109468
H53	7.800612	36.010609	-1.432399
C54	7.597881	29.693540	-3.235589
C55	6.072418	29.636082	-3.473442
C56	5.308009	29.769185	-2.151666
C57	5.686600	28.339382	-4.200035
H58	5.941125	27.468202	-3.587370
H59	6.199860	28.257851	-5.166270
H60	4.606144	28.307635	-4.384885
H61	5.606577	30.675582	-1.612667
H62	5.502809	28.891330	-1.524184
H63	4.227562	29.815587	-2.333754
H64	5.803543	30.486782	-4.114273
H65	7.879229	28.891868	-2.541639
H66	8.099164	29.475791	-4.188707
H67	7.458620	20.767615	-2.625770
H68	6.402392	23.958274	-6.377565
H69	3.733712	23.703068	-5.988983
H70	0.525839	23.853052	-1.833860
H71	0.898892	24.342541	0.906480
H72	4.933595	25.264389	3.914032
H73	7.536781	25.351113	3.736419
H74	10.810434	25.499962	-0.566844
H75	10.532990	25.004714	-3.243908

Ibuprofen 3-2 Transition State Doublet

C1	6.452960	21.225842	-2.393626
S2	6.313170	22.277243	-0.889917
H3	5.793960	20.366388	-2.228795
H4	6.080044	21.780021	-3.257154
O5	5.512796	26.465213	-1.355828
Fe6	5.714715	24.691315	-1.302541
N7	5.481986	24.348654	-3.260374
N8	3.725590	24.373984	-1.008064
N9	5.975162	24.849499	0.708444
N10	7.698506	24.819180	-1.571570
C11	6.453905	24.335631	-4.225974
C12	5.879842	24.065609	-5.521912
C13	4.542043	23.905931	-5.323764
C14	4.305051	24.069274	-3.909422
C15	2.785143	24.105030	-1.958083
C16	1.463990	24.022214	-1.364548
C17	1.622557	24.256829	-0.028728
C18	3.042584	24.467687	0.168751
C19	4.982009	24.881230	1.636201
C20	5.521033	25.105253	2.948233
C21	6.872167	25.190689	2.820498
C22	7.144093	25.060034	1.394754
C23	8.618034	25.110827	-0.600464
C24	9.928175	25.247258	-1.186942
C25	9.791671	25.018837	-2.525029
C26	8.389826	24.770611	-2.757642
C27	7.807829	24.549628	-3.995564
H28	8.458111	24.551485	-4.861560
C29	3.058272	23.940401	-3.311476
H30	2.230608	23.679179	-3.958005
C31	3.626487	24.707390	1.400469
H32	2.984026	24.789214	2.264462
C33	8.367919	25.230964	0.759719
H34	9.218665	25.522411	1.356904
C35	8.138683	30.772658	-2.413345
C36	9.030135	30.979681	-1.354910
C37	9.531807	32.250694	-1.058819
C38	9.140470	33.369356	-1.803316
C39	8.237016	33.176072	-2.856559
C40	7.751789	31.897873	-3.158414
H41	7.055107	31.781855	-3.982572
H42	7.923370	34.030508	-3.448140
H43	10.221232	32.374344	-0.228837
H44	9.337149	30.135023	-0.747320
C45	9.653112	34.759785	-1.413078
C46	10.181878	35.516858	-2.648567
O47	11.401496	35.349653	-2.973343
O48	9.374509	36.235973	-3.267904
H49	10.493280	34.614394	-0.727398
C50	8.553607	35.578787	-0.707956
H51	8.941258	36.539972	-0.350191
H52	8.153439	35.033489	0.150268
H53	7.740621	35.775967	-1.406580
C54	7.678360	29.353638	-2.738040
C55	6.217493	29.181361	-3.206391
C56	5.215979	29.752829	-2.190984
C57	5.910262	27.729661	-3.528653
H58	5.764003	26.979584	-2.327658
H59	6.694940	27.171641	-4.038579

H60	4.919322	27.557920	-3.951254
H61	5.460141	30.786003	-1.933898
H62	5.236371	29.140369	-1.284323
H63	4.197500	29.720460	-2.590770
H64	6.101503	29.746366	-4.147411
H65	7.833923	28.722270	-1.856767
H66	8.328946	28.941620	-3.520489
H67	7.452457	20.813356	-2.676088
H68	6.444434	23.999529	-6.445412
H69	3.762238	23.732601	-6.057142
H70	0.559997	23.823603	-1.935542
H71	0.924491	24.297425	0.820257
H72	4.911847	25.131714	3.841277
H73	7.523928	25.288248	3.688910
H74	10.810397	25.515154	-0.610897
H75	10.547075	25.010397	-3.297600

Ibuprofen 3-2 Transition State Quartet

C1	6.465835	21.214586	-2.414978
S2	6.342474	22.263961	-0.897228
H3	5.794373	20.354958	-2.269796
H4	6.107555	21.785906	-3.280888
O5	5.441374	26.441716	-1.420792
Fe6	5.704908	24.680146	-1.271538
N7	5.475201	24.307851	-3.255614
N8	3.706498	24.343479	-0.976882
N9	5.967530	24.840451	0.736007
N10	7.702398	24.824207	-1.550959
C11	6.437523	24.311840	-4.212762
C12	5.867574	24.056871	-5.510060
C13	4.534070	23.900823	-5.311823
C14	4.304660	24.048891	-3.897000
C15	2.775230	24.085686	-1.927575
C16	1.453794	24.010248	-1.338177
C17	1.608993	24.240521	-0.009787
C18	3.029091	24.441089	0.188106
C19	4.979491	24.862856	1.663394
C20	5.522243	25.087268	2.971248
C21	6.865691	25.177668	2.839849
C22	7.133821	25.051413	1.416664
C23	8.616596	25.116754	-0.591757
C24	9.923556	25.254780	-1.179461
C25	9.784634	25.024437	-2.510038
C26	8.385112	24.772123	-2.735718
C27	7.807464	24.540619	-3.987160
H28	8.457797	24.553632	-4.855738
C29	3.039774	23.924067	-3.296629
H30	2.206630	23.678836	-3.945966
C31	3.612463	24.685265	1.438454
H32	2.968712	24.767761	2.304442
C33	8.371622	25.235805	0.785241
H34	9.221603	25.533409	1.384440
C35	8.144633	30.725251	-2.363037
C36	9.043747	30.936790	-1.313646
C37	9.543850	32.208931	-1.026262
C38	9.142780	33.323011	-1.772459
C39	8.232063	33.123059	-2.816421
C40	7.747443	31.844582	-3.107758
H41	7.036759	31.720970	-3.927032

H42	7.908792	33.979921	-3.411079
H43	10.242289	32.340014	-0.196829
H44	9.357040	30.088742	-0.703887
C45	9.647303	34.723229	-1.386608
C46	10.209118	35.484893	-2.642989
O47	11.405161	35.303218	-2.922907
O48	9.420222	36.182466	-3.249570
H49	10.480365	34.586497	-0.689547
C50	8.533757	35.548028	-0.711200
H51	8.914804	36.509564	-0.343235
H52	8.106681	35.003894	0.135721
H53	7.741708	35.747806	-1.433392
C54	7.680706	29.301973	-2.680614
C55	6.241614	29.140016	-3.214822
C56	5.202710	29.706197	-2.231797
C57	5.954937	27.691132	-3.565055
H58	5.735056	26.965488	-2.363911
H59	6.774952	27.134724	-4.020181
H60	4.993169	27.512222	-4.048416
H61	5.421711	30.750000	-1.982764
H62	5.211003	29.110172	-1.314266
H63	4.192534	29.652240	-2.653853
H64	6.164828	29.712815	-4.156800
H65	7.783302	28.684984	-1.781208
H66	8.365136	28.864247	-3.421861
H67	7.466094	20.798945	-2.692817
H68	6.431927	23.991715	-6.440328
H69	3.753840	23.733695	-6.052972
H70	0.544593	23.818433	-1.912748
H71	0.907065	24.287506	0.840467
H72	4.912660	25.124746	3.869573
H73	7.523407	25.279086	3.709248
H74	10.813353	25.519473	-0.604911
H75	10.544664	25.012123	-3.287342

Ibuprofen 3-3 Reactant Complex Doublet

C1	6.494962	21.153554	-2.247888
S2	6.397402	22.190949	-0.733297
H3	5.901565	20.253790	-2.049978
H4	6.038177	21.685893	-3.084090
O5	5.521122	26.250529	-1.486058
Fe6	5.726161	24.647985	-1.219165
N7	5.487093	24.169948	-3.157445
N8	3.754159	24.292512	-0.898152
N9	6.016120	24.815690	0.784297
N10	7.725909	24.751528	-1.493128
C11	6.448120	24.209262	-4.131350
C12	5.859921	23.992506	-5.429953
C13	4.523542	23.831443	-5.226021
C14	4.300451	23.944972	-3.804561
C15	2.800014	24.047009	-1.842490
C16	1.482396	23.999804	-1.240302
C17	1.655332	24.222726	0.094792
C18	3.081637	24.400101	0.282250
C19	5.032388	24.818391	1.728154
C20	5.583678	25.053010	3.033573
C21	6.928825	25.185294	2.886178
C22	7.189873	25.065302	1.458102
C23	8.648021	25.111368	-0.550014

C24	9.945573	25.268072	-1.163690
C25	9.801067	24.976998	-2.489768
C26	8.400868	24.685210	-2.689397
C27	7.801571	24.443734	-3.914628
H28	8.433173	24.471973	-4.792704
C29	3.053473	23.863893	-3.195884
H30	2.207981	23.644621	-3.833751
C31	3.677829	24.630014	1.511017
H32	3.043771	24.706291	2.382524
C33	8.402896	25.266338	0.809795
H34	9.243350	25.606372	1.396332
C35	8.069680	31.720712	-3.208104
C36	8.944871	31.583280	-2.121171
C37	9.398070	32.705032	-1.413681
C38	8.998977	34.001694	-1.768260
C39	8.156556	34.141068	-2.872574
C40	7.696301	33.023028	-3.568566
H41	7.017058	33.159511	-4.404096
H42	7.833408	35.129468	-3.170679
H43	10.043738	32.557226	-0.554265
H44	9.261679	30.601995	-1.795451
C45	9.384323	35.192201	-0.895781
C46	10.465614	36.134277	-1.452138
O47	11.466135	36.327835	-0.690067
O48	10.312338	36.698999	-2.563496
H49	9.804687	34.795947	0.031756
C50	8.159087	36.061324	-0.532982
H51	7.738423	36.518457	-1.431729
H52	8.447780	36.857383	0.159033
H53	7.379722	35.451569	-0.070050
C54	7.515025	30.544108	-4.001249
C55	6.995621	29.323343	-3.191749
C56	8.082911	28.265734	-2.940981
C57	5.819622	28.642582	-3.915689
H58	4.981563	29.332448	-4.057485
H59	5.479149	27.779286	-3.335890
H60	6.136211	28.287657	-4.905520
H61	7.662673	27.427683	-2.377693
H62	8.940023	28.658440	-2.391304
H63	8.450083	27.877686	-3.900474
H64	6.632401	29.689315	-2.225975
H65	8.278635	30.187209	-4.707146
H66	6.698455	30.929098	-4.621275
H67	7.495792	20.806172	-2.590167
H68	6.406708	23.960625	-6.368601
H69	3.744525	23.699036	-5.971031
H70	0.573184	23.849876	-1.818082
H71	0.966294	24.272676	0.949303
H72	4.982272	25.071322	3.938885
H73	7.587535	25.297446	3.749980
H74	10.823556	25.598332	-0.612345
H75	10.551405	24.965331	-3.281039

Ibuprofen 3-3 Reactant Complex Quartet

C1	6.520950	21.160958	-2.203165
S2	6.441801	22.201279	-0.667706
H3	5.904644	20.268608	-2.014214
H4	6.069452	21.720295	-3.032075
O5	5.484626	26.318001	-1.481907

Fe6	5.702504	24.747996	-1.220871
N7	5.470038	24.200853	-3.163273
N8	3.725970	24.346595	-0.896768
N9	5.997795	24.895757	0.795297
N10	7.717046	24.785757	-1.492267
C11	6.426513	24.221319	-4.130340
C12	5.843577	23.994210	-5.426299
C13	4.511308	23.842759	-5.223441
C14	4.289468	23.972804	-3.807103
C15	2.779907	24.091631	-1.834522
C16	1.465327	24.038354	-1.234360
C17	1.636245	24.266896	0.093131
C18	3.058470	24.458724	0.276834
C19	5.017760	24.907987	1.733457
C20	5.571241	25.140195	3.035130
C21	6.910830	25.251847	2.888312
C22	7.168304	25.129271	1.463995
C23	8.638998	25.135516	-0.554071
C24	9.935474	25.267336	-1.163888
C25	9.790366	24.974038	-2.483053
C26	8.391920	24.697922	-2.681858
C27	7.796450	24.446819	-3.921862
H28	8.430530	24.460450	-4.801561
C29	3.026602	23.894556	-3.202121
H30	2.180807	23.668229	-3.841448
C31	3.650860	24.708359	1.519807
H32	3.010500	24.791505	2.390131
C33	8.400808	25.308718	0.817582
H34	9.248327	25.642294	1.404069
C35	8.032153	31.662414	-3.252478
C36	8.939640	31.542554	-2.190335
C37	9.387347	32.670308	-1.493954
C38	8.951800	33.958658	-1.831803
C39	8.073178	34.080168	-2.908023
C40	7.617805	32.956266	-3.596938
H41	6.905588	33.080084	-4.413136
H42	7.712953	35.067338	-3.189768
H43	10.061989	32.533589	-0.645862
H44	9.284795	30.560943	-1.876502
C45	9.334520	35.157857	-0.958116
C46	10.437951	36.129734	-1.501481
O47	11.395903	36.304174	-0.728249
O48	10.281373	36.688996	-2.587186
H49	9.758663	34.762799	-0.031381
C50	8.108933	36.028040	-0.592790
H51	7.664308	36.459003	-1.493974
H52	8.401545	36.844989	0.074866
H53	7.345878	35.421873	-0.097252
C54	7.484612	30.464278	-4.027843
C55	7.013816	29.237359	-3.192642
C56	8.129248	28.198213	-2.986485
C57	5.814677	28.533204	-3.850907
H58	4.968386	29.218060	-3.988396
H59	5.493928	27.692604	-3.223136
H60	6.097775	28.137925	-4.836872
H61	7.757559	27.363629	-2.383504
H62	9.012541	28.614430	-2.494194
H63	8.445470	27.795585	-3.957429
H64	6.692212	29.604698	-2.210461
H65	8.243422	30.118426	-4.745703

H66	6.645081	30.823080	-4.634839
H67	7.515383	20.795760	-2.564172
H68	6.392630	23.959696	-6.368390
H69	3.731803	23.711507	-5.975860
H70	0.552313	23.870207	-1.810160
H71	0.943038	24.306593	0.950645
H72	4.974494	25.153572	3.949932
H73	7.579187	25.341785	3.754336
H74	10.821533	25.585655	-0.610204
H75	10.545931	24.962937	-3.275706

Ibuprofen 3-3 Transition State Doublet

C1	6.480371	21.229285	-2.238157
S2	6.418528	22.295216	-0.738659
H3	5.870453	20.347237	-2.014795
H4	6.022060	21.751944	-3.080227
O5	5.541342	26.429388	-1.389251
Fe6	5.769582	24.728263	-1.278243
N7	5.525061	24.303389	-3.220744
N8	3.790223	24.368015	-0.961615
N9	6.051472	24.880504	0.733427
N10	7.757564	24.830025	-1.556848
C11	6.489948	24.298723	-4.194157
C12	5.904619	24.039187	-5.487064
C13	4.568046	23.882356	-5.279636
C14	4.342028	24.045081	-3.864947
C15	2.836946	24.114690	-1.904771
C16	1.522818	24.026328	-1.297822
C17	1.697229	24.238649	0.039423
C18	3.120562	24.441955	0.223967
C19	5.073049	24.834174	1.676903
C20	5.625571	25.012520	2.990756
C21	6.969162	25.168903	2.845455
C22	7.225068	25.110292	1.409564
C23	8.678834	25.172851	-0.603363
C24	9.982500	25.306983	-1.208766
C25	9.843822	25.009081	-2.535226
C26	8.441954	24.742023	-2.745053
C27	7.846904	24.509017	-3.975111
H28	8.483989	24.517973	-4.848824
C29	3.092799	23.949124	-3.258858
H30	2.252906	23.717211	-3.899623
C31	3.717656	24.644807	1.454909
H32	3.083891	24.697308	2.329539
C33	8.435408	25.322000	0.757532
H34	9.278546	25.661488	1.342450
C35	7.933269	31.507213	-2.956442
C36	8.773497	31.435769	-1.839447
C37	9.298393	32.596283	-1.250949
C38	9.002276	33.872485	-1.747091
C39	8.206267	33.942052	-2.896100
C40	7.683462	32.786610	-3.480034
H41	7.032953	32.882848	-4.345036
H42	7.965706	34.910068	-3.317695
H43	9.911715	32.495414	-0.360144
H44	8.998836	30.483885	-1.377657
C45	9.393397	35.110865	-0.936869
C46	10.460556	36.074212	-1.496859
O47	11.445500	36.297532	-0.720471

O48	10.306328	36.643138	-2.605979
H49	9.812088	34.752177	0.006315
C50	8.152674	35.973028	-0.603698
H51	7.704604	36.361653	-1.521177
H52	8.434508	36.815900	0.034646
H53	7.398233	35.374339	-0.087966
C54	7.255357	30.295066	-3.609569
C55	7.098615	29.019752	-2.734430
C56	8.373658	28.172569	-2.742652
C57	5.916922	28.142392	-3.143966
H58	4.962628	28.677013	-3.135075
H59	5.775448	27.223367	-2.296188
H60	6.068030	27.654077	-4.112538
H61	8.281338	27.343423	-2.041700
H62	9.252512	28.759180	-2.476882
H63	8.537811	27.752893	-3.742439
H64	6.915091	29.369801	-1.716108
H65	7.807162	30.023713	-4.520286
H66	6.265834	30.622867	-3.945389
H67	7.473114	20.858141	-2.581476
H68	6.450614	23.979093	-6.423232
H69	3.790488	23.700051	-6.017117
H70	0.616081	23.843494	-1.868970
H71	1.010106	24.265276	0.897301
H72	5.025641	24.941887	3.892532
H73	7.627426	25.249725	3.710788
H74	10.854713	25.643007	-0.653752
H75	10.592876	24.982605	-3.323456

Ibuprofen 3-3 Transition State Quartet

C1	6.497558	21.250239	-2.307408
S2	6.428094	22.307482	-0.786535
H3	5.863287	20.370894	-2.118935
H4	6.073590	21.802303	-3.155910
O5	5.466365	26.471321	-1.399096
Fe6	5.756644	24.710281	-1.256574
N7	5.506417	24.319615	-3.237579
N8	3.764454	24.353499	-0.942123
N9	6.037203	24.871807	0.751518
N10	7.751180	24.863900	-1.559665
C11	6.462944	24.317701	-4.203327
C12	5.882278	24.052966	-5.493671
C13	4.551566	23.894760	-5.284903
C14	4.331965	24.059773	-3.870642
C15	2.820125	24.114818	-1.886111
C16	1.504384	24.032560	-1.283445
C17	1.676014	24.234282	0.045967
C18	3.099770	24.423372	0.231285
C19	5.067257	24.818974	1.695479
C20	5.623966	25.005417	3.004440
C21	6.958535	25.163342	2.854038
C22	7.207804	25.102447	1.420187
C23	8.666702	25.193750	-0.615251
C24	9.970447	25.321915	-1.216355
C25	9.830274	25.027778	-2.537392
C26	8.430132	24.769664	-2.744749
C27	7.836337	24.531158	-3.989191
H28	8.477114	24.531971	-4.864852
C29	3.069059	23.952905	-3.257213

H30	2.226350	23.716955	-3.896713
C31	3.700003	24.621696	1.481978
H32	3.065806	24.659607	2.359243
C33	8.430350	25.326919	0.765661
H34	9.279621	25.649583	1.352653
C35	7.904668	31.514782	-2.985172
C36	8.726514	31.425314	-1.856780
C37	9.260418	32.574791	-1.258143
C38	8.991750	33.853967	-1.754788
C39	8.219065	33.941013	-2.918317
C40	7.685918	32.797615	-3.511892
H41	7.049612	32.905534	-4.393177
H42	8.007526	34.918648	-3.346452
H43	9.864284	32.460232	-0.354387
H44	8.931266	30.461232	-1.395603
C45	9.371767	35.093418	-0.931764
C46	10.456342	36.086528	-1.484250
O47	11.405625	36.287048	-0.706435
O48	10.291989	36.641602	-2.570473
H49	9.793121	34.735290	0.011559
C50	8.115208	35.938659	-0.606001
H51	7.669520	36.321322	-1.528303
H52	8.369431	36.785779	0.040363
H53	7.366207	35.321673	-0.101698
C54	7.210038	30.314565	-3.652047
C55	7.060522	29.017251	-2.796965
C56	8.344192	28.179811	-2.806159
C57	5.901912	28.160392	-3.263473
H58	4.908892	28.607901	-3.189443
H59	5.734129	27.101664	-2.280947
H60	6.063962	27.611135	-4.194067
H61	8.275642	27.369885	-2.079118
H62	9.226582	28.780998	-2.578032
H63	8.487908	27.731239	-3.796829
H64	6.850952	29.343360	-1.772540
H65	7.745401	30.052642	-4.576546
H66	6.215939	30.653181	-3.967980
H67	7.492801	20.862267	-2.634949
H68	6.431690	23.986172	-6.433489
H69	3.773576	23.709330	-6.027160
H70	0.591531	23.863786	-1.860166
H71	0.984847	24.264337	0.906202
H72	5.024107	24.955370	3.914286
H73	7.625603	25.253859	3.718205
H74	10.851458	25.649899	-0.661164
H75	10.586082	24.992168	-3.326798

Ibuprofen 3-4 Reactant Complex Doublet

C1	6.636281	21.159441	-2.177718
S2	6.536324	22.278870	-0.725705
H3	6.007272	20.297767	-1.931022
H4	6.201359	21.670600	-3.038415
O5	5.480619	26.299896	-1.555244
Fe6	5.713165	24.704502	-1.304886
N7	5.490500	24.186503	-3.242223
N8	3.740616	24.329378	-0.997345
N9	5.997317	24.875312	0.696356
N10	7.704284	24.817906	-1.572060
C11	6.456584	24.200957	-4.214751

C12	5.879147	23.951757	-5.514154
C13	4.537895	23.825745	-5.315233
C14	4.305019	23.972081	-3.897315
C15	2.787845	24.108921	-1.950686
C16	1.465904	24.073752	-1.354087
C17	1.633853	24.280508	-0.015977
C18	3.061077	24.443384	0.180558
C19	5.006801	24.857179	1.633150
C20	5.546065	25.102099	2.938309
C21	6.890676	25.281923	2.797524
C22	7.161359	25.153655	1.373985
C23	8.625968	25.176165	-0.624120
C24	9.925583	25.316770	-1.230672
C25	9.780241	25.039864	-2.558944
C26	8.383356	24.750928	-2.766929
C27	7.799132	24.477696	-3.992982
H28	8.432723	24.518804	-4.868728
C29	3.050105	23.929852	-3.303313
H30	2.208487	23.737672	-3.955486
C31	3.652486	24.669335	1.409126
H32	3.012475	24.752875	2.276281
C33	8.377130	25.351171	0.729662
H34	9.217884	25.703172	1.307876
C35	8.166996	30.844267	-3.111024
C36	8.917911	31.054002	-1.949224
C37	9.238482	32.349934	-1.522251
C38	8.813712	33.473310	-2.240147
C39	8.109388	33.263224	-3.431537
C40	7.794417	31.971993	-3.856499
H41	7.226256	31.839580	-4.771635
H42	7.786065	34.112582	-4.021072
H43	9.791704	32.476677	-0.597240
H44	9.236614	30.209515	-1.350490
C45	9.001687	34.866587	-1.643336
C46	10.143548	35.709290	-2.243549
O47	11.117094	35.947689	-1.452916
O48	10.064808	36.187311	-3.399155
H49	9.274301	34.727070	-0.597035
C50	7.690894	35.677166	-1.687658
H51	7.402733	35.885712	-2.721510
H52	7.806924	36.623467	-1.149760
H53	6.889157	35.105521	-1.216815
C54	7.767920	29.448573	-3.557835
C55	6.264007	29.278323	-3.869601
C56	5.419532	29.456006	-2.602330
C57	6.001038	27.901109	-4.497550
H58	6.227996	27.107582	-3.780513
H59	6.608866	27.750344	-5.397071
H60	4.946499	27.802426	-4.773644
H61	4.356418	29.335039	-2.833878
H62	5.573947	30.444092	-2.155662
H63	5.680054	28.683228	-1.873859
H64	5.977346	30.049974	-4.594570
H65	8.050970	28.720421	-2.789908
H66	8.334713	29.184015	-4.460052
H67	7.613779	20.736104	-2.504829
H68	6.430692	23.911080	-6.457804
H69	3.750880	23.700055	-6.055562
H70	0.553721	23.917847	-1.925462
H71	0.937858	24.318180	0.838870

H72	4.949897	25.071661	3.842329
H73	7.534960	25.444107	3.665165
H74	10.811491	25.596480	-0.668955
H75	10.532530	25.009565	-3.338588

Ibuprofen 3-4 Reactant Complex Quartet

C1	6.634541	21.134545	-2.169488
S2	6.555035	22.272061	-0.716451
H3	6.010134	20.266805	-1.911822
H4	6.186648	21.641591	-3.033146
O5	5.445918	26.322949	-1.557608
Fe6	5.691792	24.760588	-1.303676
N7	5.476894	24.197052	-3.246241
N8	3.717277	24.347294	-0.988935
N9	5.982694	24.909452	0.715843
N10	7.701291	24.827881	-1.564090
C11	6.440297	24.201430	-4.208832
C12	5.868063	23.950728	-5.508376
C13	4.530325	23.829646	-5.310780
C14	4.298100	23.982719	-3.896558
C15	2.772613	24.124777	-1.936048
C16	1.453758	24.084335	-1.340721
C17	1.621159	24.288088	-0.009672
C18	3.045614	24.455491	0.184756
C19	4.998974	24.886780	1.650097
C20	5.541570	25.127972	2.951961
C21	6.878741	25.299584	2.810193
C22	7.143428	25.175086	1.389849
C23	8.620062	25.177803	-0.618716
C24	9.918338	25.306063	-1.221252
C25	9.775857	25.030125	-2.542779
C26	8.380312	24.748345	-2.751908
C27	7.799445	24.468185	-3.992718
H28	8.436865	24.496588	-4.868866
C29	3.026482	23.938299	-3.303931
H30	2.183220	23.740574	-3.953351
C31	3.634338	24.682588	1.431606
H32	2.992576	24.751843	2.300449
C33	8.376625	25.359351	0.746791
H34	9.223574	25.695882	1.330609
C35	8.168534	30.822048	-3.105610
C36	8.935122	31.032189	-1.956004
C37	9.250504	32.325536	-1.525955
C38	8.803949	33.448523	-2.229390
C39	8.080139	33.238196	-3.408044
C40	7.770784	31.951951	-3.835548
H41	7.176955	31.823492	-4.740933
H42	7.731172	34.092939	-3.987220
H43	9.819037	32.453481	-0.602553
H44	9.267465	30.179262	-1.365265
C45	8.989369	34.846362	-1.637091
C46	10.147435	35.708005	-2.252885
O47	11.088170	35.930023	-1.463785
O48	10.047153	36.168561	-3.382220
H49	9.276137	34.713449	-0.590610
C50	7.678359	35.656078	-1.673415
H51	7.365266	35.835463	-2.706174
H52	7.803873	36.620082	-1.166020
H53	6.891407	35.094842	-1.166804

C54	7.760336	29.422561	-3.549081
C55	6.254890	29.281359	-3.869212
C56	5.422036	29.474918	-2.594768
C57	5.941705	27.931910	-4.533859
H58	6.141817	27.101768	-3.848943
H59	6.535070	27.792186	-5.447662
H60	4.881928	27.884567	-4.808112
H61	4.352224	29.406480	-2.819268
H62	5.625455	30.452134	-2.139517
H63	5.649591	28.683527	-1.874843
H64	5.988102	30.071651	-4.583355
H65	8.024329	28.699927	-2.766161
H66	8.339286	29.142562	-4.440610
H67	7.615442	20.719732	-2.503887
H68	6.424538	23.909999	-6.454849
H69	3.742545	23.700256	-6.053593
H70	0.539447	23.922849	-1.914912
H71	0.924768	24.324453	0.847781
H72	4.944414	25.100758	3.859829
H73	7.533027	25.456208	3.679164
H74	10.808762	25.584847	-0.655744
H75	10.533037	25.003376	-3.326286

Ibuprofen 3-4 Transition State Doublet

C1	6.644589	21.204771	-2.226334
S2	6.551225	22.345354	-0.791267
H3	6.006292	20.355099	-1.966310
H4	6.223835	21.700259	-3.102920
O5	5.540723	26.416888	-1.618716
Fe6	5.758184	24.709241	-1.391797
N7	5.527547	24.246284	-3.329156
N8	3.775943	24.373177	-1.080745
N9	6.021180	24.935268	0.617345
N10	7.735723	24.855405	-1.661681
C11	6.496335	24.223141	-4.297558
C12	5.916004	23.967630	-5.594877
C13	4.572574	23.858401	-5.395819
C14	4.339599	24.026412	-3.980469
C15	2.821066	24.150327	-2.031264
C16	1.501660	24.093228	-1.430372
C17	1.672310	24.287927	-0.091993
C18	3.097251	24.461007	0.101542
C19	5.040437	24.873600	1.558790
C20	5.582662	25.083946	2.869495
C21	6.920530	25.284798	2.728619
C22	7.185173	25.199790	1.296885
C23	8.648456	25.227788	-0.708360
C24	9.951056	25.371408	-1.310821
C25	9.813501	25.078539	-2.636061
C26	8.421191	24.774050	-2.849476
C27	7.841797	24.481310	-4.074563
H28	8.479300	24.504699	-4.948701
C29	3.085015	23.980904	-3.386189
H30	2.243130	23.783070	-4.036110
C31	3.689223	24.666581	1.333346
H32	3.052324	24.714577	2.204496
C33	8.397688	25.402707	0.645343
H34	9.239374	25.751059	1.225663
C35	8.210408	30.693388	-2.909201

C36	8.996319	31.016346	-1.797281
C37	9.291671	32.344811	-1.475679
C38	8.808457	33.405603	-2.250311
C39	8.070963	33.085062	-3.398842
C40	7.781869	31.754778	-3.720657
H41	7.177613	31.544867	-4.598400
H42	7.684793	33.877191	-4.029127
H43	9.864403	32.552160	-0.575991
H44	9.354606	30.226906	-1.145546
C45	8.951416	34.840073	-1.727226
C46	10.123756	35.679729	-2.282890
O47	11.077590	35.905718	-1.460322
O48	10.079743	36.175389	-3.431016
H49	9.157099	34.752906	-0.659303
C50	7.643003	35.635319	-1.893364
H51	7.447538	35.832838	-2.949171
H52	7.706425	36.588627	-1.357197
H53	6.807123	35.064227	-1.485585
C54	7.839523	29.244169	-3.199816
C55	6.356132	28.986888	-3.556910
C56	5.397820	29.526142	-2.487211
C57	6.099935	27.498156	-3.788932
H58	5.891962	26.913546	-2.674596
H59	6.929986	26.971889	-4.263227
H60	5.165584	27.310250	-4.324300
H61	4.361378	29.359140	-2.794380
H62	5.551630	30.593424	-2.306758
H63	5.548217	28.971975	-1.556585
H64	6.147092	29.519368	-4.497234
H65	8.101004	28.630282	-2.330615
H66	8.448979	28.870092	-4.032570
H67	7.621156	20.765992	-2.535795
H68	6.470109	23.913987	-6.531420
H69	3.783342	23.719717	-6.128557
H70	0.591817	23.923136	-2.000551
H71	0.983044	24.314826	0.767679
H72	4.984693	25.001566	3.770163
H73	7.565321	25.426093	3.598127
H74	10.835945	25.655899	-0.747905
H75	10.561389	25.034321	-3.413935

Ibuprofen 3-4 Transition State Quartet

C1	6.644795	21.209832	-2.239247
S2	6.589988	22.375944	-0.809461
H3	5.996768	20.365600	-1.967274
H4	6.222979	21.703843	-3.124163
O5	5.449795	26.452148	-1.627345
Fe6	5.740279	24.716195	-1.367702
N7	5.511067	24.250076	-3.340788
N8	3.746225	24.372225	-1.065365
N9	6.001082	24.955145	0.634278
N10	7.726327	24.900312	-1.659264
C11	6.473399	24.224374	-4.298973
C12	5.900260	23.969446	-5.596998
C13	4.560508	23.866808	-5.398766
C14	4.332637	24.037683	-3.985031
C15	2.803034	24.158526	-2.018538
C16	1.482244	24.100757	-1.423373
C17	1.648075	24.290044	-0.090325

C18	3.072638	24.461190	0.104070
C19	5.026495	24.886555	1.572571
C20	5.571835	25.094101	2.880278
C21	6.902909	25.298111	2.735697
C22	7.161352	25.221844	1.305108
C23	8.634634	25.264842	-0.715608
C24	9.937729	25.390121	-1.314511
C25	9.800609	25.089652	-2.631321
C26	8.408759	24.797570	-2.840771
C27	7.835406	24.487664	-4.080097
H28	8.477838	24.503493	-4.952900
C29	3.059941	23.992669	-3.387769
H30	2.216087	23.800631	-4.040755
C31	3.662677	24.673614	1.354884
H32	3.023555	24.721937	2.226855
C33	8.387634	25.439770	0.655648
H34	9.230285	25.788532	1.237865
C35	8.202776	30.667071	-2.933762
C36	8.986892	30.984595	-1.821053
C37	9.279517	32.311626	-1.496592
C38	8.793990	33.371550	-2.268967
C39	8.057868	33.054592	-3.417599
C40	7.771621	31.727576	-3.743294
H41	7.163779	31.514845	-4.624264
H42	7.667775	33.854481	-4.047233
H43	9.852206	32.520774	-0.589845
H44	9.345723	30.188213	-1.168605
C45	8.926713	34.808421	-1.739218
C46	10.113481	35.677858	-2.299183
O47	11.029356	35.893623	-1.474796
O48	10.053752	36.156570	-3.423471
H49	9.140297	34.719242	-0.672296
C50	7.611728	35.595827	-1.899125
H51	7.415158	35.801117	-2.953570
H52	7.663479	36.545671	-1.353843
H53	6.781303	35.011018	-1.496795
C54	7.820550	29.218123	-3.227792
C55	6.330727	28.983269	-3.579600
C56	5.384180	29.523540	-2.493367
C57	6.071753	27.514591	-3.851835
H58	5.806040	26.882393	-2.600730
H59	6.911140	26.938157	-4.239419
H60	5.125839	27.284612	-4.343880
H61	4.341390	29.368196	-2.784710
H62	5.552215	30.592115	-2.318788
H63	5.540290	28.972601	-1.562518
H64	6.116124	29.534337	-4.510285
H65	8.077392	28.598477	-2.362486
H66	8.422146	28.838998	-4.066372
H67	7.620589	20.762882	-2.549069
H68	6.456314	23.909915	-6.539151
H69	3.771700	23.724020	-6.138893
H70	0.568721	23.929668	-1.996493
H71	0.955555	24.313069	0.770362
H72	4.976420	25.006706	3.786637
H73	7.555534	25.433867	3.605831
H74	10.829881	25.665098	-0.751075
H75	10.554884	25.036238	-3.411825

Ibuprofen 3-5 Reactant Complex Doublet

C1	6.657511	21.212061	-1.983737
S2	6.465002	22.322531	-0.553423
H3	6.039696	20.337964	-1.760531
H4	6.265202	21.695967	-2.880096
O5	5.677428	26.318263	-1.398457
Fe6	5.857967	24.701876	-1.206948
N7	5.624522	24.238894	-3.157958
N8	3.873175	24.382199	-0.914280
N9	6.142718	24.848493	0.789039
N10	7.860665	24.760644	-1.485709
C11	6.589759	24.242924	-4.129427
C12	6.008747	24.026100	-5.433142
C13	4.664621	23.917254	-5.234727
C14	4.437739	24.052654	-3.816569
C15	2.920898	24.179193	-1.870872
C16	1.600298	24.136867	-1.276442
C17	1.770094	24.314646	0.065088
C18	3.198534	24.472233	0.267190
C19	5.151711	24.876997	1.724672
C20	5.708043	25.105384	3.028869
C21	7.059209	25.175740	2.888013
C22	7.323026	25.047560	1.463671
C23	8.792100	25.069576	-0.532895
C24	10.096544	25.194326	-1.139947
C25	9.946162	24.943307	-2.473799
C26	8.537921	24.694958	-2.679671
C27	7.942629	24.467094	-3.908346
H28	8.576404	24.499347	-4.783728
C29	3.181726	24.017131	-3.226255
H30	2.340799	23.836875	-3.882988
C31	3.795307	24.691945	1.498146
H32	3.154796	24.772213	2.364982
C33	8.547159	25.210081	0.825355
H34	9.399210	25.505297	1.419550
C35	8.202416	31.006099	-2.450088
C36	9.160061	31.186109	-1.446281
C37	9.650528	32.456568	-1.125789
C38	9.178983	33.592770	-1.792874
C39	8.206123	33.421224	-2.781150
C40	7.729961	32.151231	-3.105908
H41	6.976660	32.062435	-3.879024
H42	7.825645	34.290537	-3.305146
H43	10.393875	32.562582	-0.340453
H44	9.527724	30.324874	-0.896213
C45	9.696412	34.984143	-1.439723
C46	10.362784	35.626517	-2.667710
O47	11.636575	35.637740	-2.700771
O48	9.637817	36.094641	-3.569193
H49	10.464311	34.874079	-0.669714
C50	8.565372	35.888077	-0.912176
H51	7.821518	36.038060	-1.695386
H52	8.952155	36.868981	-0.615082
H53	8.076114	35.426380	-0.050275
C54	7.748151	29.601429	-2.828265
C55	6.353772	29.483067	-3.467071
C56	5.273401	29.820348	-2.432228
C57	6.150555	28.074683	-4.048838
H58	5.144834	27.976725	-4.470742
H59	6.259889	27.316825	-3.268742

H60	6.876635	27.871870	-4.843270
H61	5.422781	30.822353	-2.016950
H62	5.315502	29.091782	-1.614917
H63	4.273618	29.770018	-2.875301
H64	6.285051	30.194334	-4.297883
H65	7.775485	28.963449	-1.937197
H66	8.480649	29.170838	-3.521834
H67	7.649093	20.799836	-2.239810
H68	6.569705	23.961150	-6.365722
H69	3.867610	23.789173	-5.961118
H70	0.691092	24.013901	-1.862438
H71	1.066259	24.340388	0.910456
H72	5.114730	25.179732	3.930443
H73	7.720690	25.251457	3.749388
H74	10.981724	25.471955	-0.577016
H75	10.700638	24.918921	-3.261547

Ibuprofen 3-5 Reactant Complex Quartet

C1	6.659880	21.216427	-1.979074
S2	6.488450	22.337390	-0.544777
H3	6.035781	20.340698	-1.752941
H4	6.264405	21.702463	-2.880576
O5	5.631218	26.338516	-1.376967
Fe6	5.842846	24.755003	-1.189322
N7	5.610929	24.257839	-3.154230
N8	3.849110	24.398950	-0.891593
N9	6.132527	24.879329	0.818863
N10	7.857963	24.787553	-1.470827
C11	6.570340	24.250809	-4.117319
C12	5.992171	24.030180	-5.418620
C13	4.655624	23.930848	-5.222018
C14	4.429073	24.073650	-3.806620
C15	2.906277	24.197729	-1.842683
C16	1.587628	24.150606	-1.252388
C17	1.754643	24.326250	0.083370
C18	3.181241	24.487506	0.283130
C19	5.148158	24.897210	1.751014
C20	5.707683	25.110498	3.053527
C21	7.051739	25.183669	2.908748
C22	7.308386	25.071631	1.486814
C23	8.786131	25.096641	-0.525264
C24	10.087175	25.211076	-1.132787
C25	9.936896	24.951944	-2.456576
C26	8.531784	24.707738	-2.659178
C27	7.939622	24.469071	-3.903124
H28	8.576833	24.492762	-4.779073
C29	3.159011	24.034250	-3.215835
H30	2.314618	23.852634	-3.871023
C31	3.777981	24.708625	1.530670
H32	3.134867	24.786167	2.399527
C33	8.546868	25.242238	0.847164
H34	9.400169	25.542133	1.442535
C35	8.222886	30.886041	-2.452256
C36	9.167100	31.083799	-1.439275
C37	9.644743	32.359074	-1.126012
C38	9.174363	33.485768	-1.811187
C39	8.215087	33.296903	-2.808302
C40	7.750382	32.021551	-3.125055
H41	7.001829	31.917559	-3.908218

H42	7.836006	34.163892	-3.350235
H43	10.381802	32.479642	-0.329114
H44	9.534272	30.225721	-0.874741
C45	9.672792	34.888544	-1.454658
C46	10.365606	35.559265	-2.690467
O47	11.608566	35.553747	-2.694924
O48	9.648662	36.031974	-3.559018
H49	10.437910	34.786203	-0.678526
C50	8.526257	35.778804	-0.937991
H51	7.793751	35.926855	-1.732670
H52	8.897098	36.762643	-0.626628
H53	8.027343	35.305023	-0.087234
C54	7.784824	29.467602	-2.821540
C55	6.437285	29.328622	-3.553225
C56	5.285094	29.632143	-2.583758
C57	6.302279	27.924382	-4.164022
H58	5.321207	27.798613	-4.636122
H59	6.400797	27.159547	-3.391802
H60	7.070950	27.749744	-4.926857
H61	5.384726	30.634183	-2.151365
H62	5.294368	28.892850	-1.774413
H63	4.313725	29.565809	-3.088554
H64	6.406789	30.047908	-4.381739
H65	7.742582	28.855482	-1.910864
H66	8.566759	29.012892	-3.443872
H67	7.651714	20.799773	-2.241697
H68	6.556684	23.960016	-6.355398
H69	3.858480	23.802718	-5.955714
H70	0.675592	24.023389	-1.840883
H71	1.045181	24.346418	0.929953
H72	5.117226	25.174871	3.963135
H73	7.720930	25.251540	3.770985
H74	10.980629	25.486681	-0.571039
H75	10.695375	24.923835	-3.248952

Ibuprofen 3-5 Transition State Doublet

C1	6.648862	21.280615	-1.980867
S2	6.471774	22.431749	-0.570864
H3	6.013720	20.424753	-1.737504
H4	6.262144	21.751851	-2.886453
O5	5.675161	26.539876	-1.340384
Fe6	5.867657	24.761825	-1.247904
N7	5.623191	24.372568	-3.205924
N8	3.870536	24.464796	-0.953224
N9	6.130145	24.965099	0.751768
N10	7.852922	24.859477	-1.539208
C11	6.590336	24.325078	-4.176796
C12	6.007988	24.060809	-5.471879
C13	4.664918	23.958283	-5.269100
C14	4.437634	24.144836	-3.855835
C15	2.917968	24.244182	-1.906408
C16	1.599195	24.168215	-1.307253
C17	1.770536	24.343535	0.035662
C18	3.195936	24.531112	0.230308
C19	5.144392	24.972345	1.687347
C20	5.698073	25.182063	2.997382
C21	7.049302	25.250827	2.857848
C22	7.309844	25.145060	1.427741
C23	8.781184	25.146236	-0.576332

C24	10.093685	25.231241	-1.169775
C25	9.951851	24.976203	-2.504334
C26	8.540597	24.763436	-2.724468
C27	7.947080	24.526463	-3.955020
H28	8.588035	24.513979	-4.826017
C29	3.182112	24.087891	-3.262212
H30	2.344455	23.877708	-3.915208
C31	3.792260	24.758070	1.460704
H32	3.151885	24.817823	2.329562
C33	8.534041	25.290334	0.784182
H34	9.392976	25.562336	1.380246
C35	8.189494	30.945470	-2.345466
C36	9.173060	31.175635	-1.377444
C37	9.652021	32.462373	-1.113446
C38	9.148800	33.571122	-1.801762
C39	8.160881	33.350942	-2.769444
C40	7.692944	32.059640	-3.037789
H41	6.921164	31.928149	-3.788640
H42	7.756437	34.196263	-3.314860
H43	10.410803	32.604039	-0.349185
H44	9.564585	30.340135	-0.807978
C45	9.655917	34.973965	-1.468901
C46	10.339096	35.615752	-2.687608
O47	11.612680	35.615687	-2.710737
O48	9.621414	36.102193	-3.584873
H49	10.416669	34.872457	-0.690264
C50	8.527370	35.890507	-0.958016
H51	7.794425	36.048260	-1.750004
H52	8.924863	36.868045	-0.663971
H53	8.024505	35.442636	-0.096951
C54	7.743549	29.512190	-2.624078
C55	6.312577	29.315061	-3.156919
C56	5.265530	29.879166	-2.185554
C57	6.042933	27.861266	-3.498152
H58	5.059666	27.670967	-3.927471
H59	5.912743	27.061179	-2.306587
H60	6.847616	27.330249	-4.008102
H61	5.469130	30.925116	-1.947580
H62	5.285469	29.294651	-1.259968
H63	4.258761	29.804030	-2.608067
H64	6.228699	29.874254	-4.105053
H65	7.849286	28.925922	-1.705124
H66	8.435872	29.060835	-3.344842
H67	7.634834	20.840697	-2.237156
H68	6.568226	23.970901	-6.400622
H69	3.864998	23.803184	-5.985953
H70	0.687982	24.021367	-1.881953
H71	1.069446	24.354915	0.884906
H72	5.103101	25.229618	3.898978
H73	7.705033	25.301318	3.723417
H74	10.977169	25.488806	-0.594144
H75	10.711331	24.934119	-3.283724

Ibuprofen 3-5 Transition State Quartet

C1	6.666957	21.298947	-2.003601
S2	6.500517	22.431585	-0.570875
H3	6.014930	20.442733	-1.788982
H4	6.301381	21.796677	-2.910916
O5	5.607843	26.519459	-1.446045

Fe6	5.856243	24.763082	-1.218645
N7	5.616095	24.334746	-3.200117
N8	3.848068	24.456331	-0.922641
N9	6.118259	24.982649	0.777119
N10	7.855096	24.875519	-1.518802
C11	6.573166	24.307406	-4.161956
C12	5.993562	24.069075	-5.459731
C13	4.655812	23.968788	-5.257102
C14	4.436423	24.132874	-3.842496
C15	2.907370	24.240835	-1.876177
C16	1.587689	24.171709	-1.283580
C17	1.753135	24.346726	0.052354
C18	3.178189	24.531080	0.247194
C19	5.137010	24.982954	1.712464
C20	5.694948	25.186272	3.019101
C21	7.038537	25.258389	2.875781
C22	7.295091	25.162158	1.448464
C23	8.776744	25.173209	-0.568083
C24	10.086300	25.260404	-1.162665
C25	9.943435	24.997312	-2.488697
C26	8.535426	24.772857	-2.701590
C27	7.946875	24.519427	-3.944680
H28	8.588874	24.516019	-4.818202
C29	3.163898	24.080490	-3.246465
H30	2.322119	23.880110	-3.900416
C31	3.772020	24.769580	1.496243
H32	3.129578	24.839294	2.364627
C33	8.533139	25.323406	0.807061
H34	9.390333	25.607668	1.405168
C35	8.217983	30.786702	-2.320952
C36	9.187939	31.031440	-1.345454
C37	9.653934	32.322700	-1.085780
C38	9.150378	33.421855	-1.791357
C39	8.170287	33.184636	-2.760090
C40	7.715147	31.890823	-3.021722
H41	6.943263	31.744069	-3.778058
H42	7.759441	34.029279	-3.316307
H43	10.404739	32.478468	-0.307839
H44	9.581109	30.197439	-0.765204
C45	9.633644	34.839555	-1.462392
C46	10.331247	35.520231	-2.692642
O47	11.574032	35.520914	-2.688498
O48	9.618426	36.007292	-3.558080
H49	10.396581	34.752946	-0.681772
C50	8.481770	35.727940	-0.955087
H51	7.747135	35.861941	-1.750753
H52	8.847155	36.718175	-0.658692
H53	7.987662	35.264552	-0.095940
C54	7.786086	29.344732	-2.605229
C55	6.397487	29.147278	-3.242265
C56	5.285139	29.672416	-2.318218
C57	6.175080	27.694336	-3.616082
H58	5.246784	27.487528	-4.151791
H59	5.916236	26.988907	-2.412010
H60	7.036009	27.163021	-4.023076
H61	5.439519	30.727788	-2.069778
H62	5.285459	29.087572	-1.393610
H63	4.299816	29.562066	-2.784741
H64	6.366544	29.720989	-4.185268
H65	7.815009	28.770586	-1.673191

H66	8.532695	28.877857	-3.262073
H67	7.651802	20.850869	-2.254824
H68	6.554054	23.981139	-6.393633
H69	3.854802	23.819460	-5.981415
H70	0.674093	24.025883	-1.864198
H71	1.047601	24.354433	0.902504
H72	5.101669	25.228153	3.928078
H73	7.702621	25.304723	3.743256
H74	10.978048	25.511266	-0.587487
H75	10.706173	24.950999	-3.272460

Ibuprofen 3-6 Reactant Complex Doublet

C1	6.354567	21.241307	-2.399460
S2	6.199995	22.198079	-0.835301
H3	5.714326	20.364148	-2.274488
H4	5.974589	21.823609	-3.237987
O5	5.488704	26.283790	-1.334237
Fe6	5.672861	24.659148	-1.193535
N7	5.443468	24.265906	-3.156581
N8	3.699975	24.308729	-0.898270
N9	5.963423	24.744036	0.823873
N10	7.667485	24.754598	-1.452898
C11	6.415650	24.276433	-4.121851
C12	5.843144	24.018154	-5.423741
C13	4.504534	23.864809	-5.226331
C14	4.265328	24.014128	-3.809424
C15	2.753863	24.072394	-1.850607
C16	1.435943	23.987459	-1.251082
C17	1.604489	24.172302	0.089557
C18	3.026779	24.367540	0.286823
C19	4.969452	24.767066	1.754428
C20	5.503865	25.047390	3.058262
C21	6.851271	25.180002	2.924921
C22	7.129179	25.008260	1.505488
C23	8.591072	25.064608	-0.493568
C24	9.894877	25.216694	-1.090883
C25	9.748431	24.980282	-2.423507
C26	8.348675	24.714851	-2.644064
C27	7.767139	24.495501	-3.883383
H28	8.419941	24.508118	-4.747799
C29	3.016158	23.914408	-3.208197
H30	2.176933	23.686615	-3.854397
C31	3.617122	24.571284	1.522444
H32	2.978462	24.636844	2.393054
C33	8.346724	25.194460	0.866208
H34	9.196188	25.511497	1.452985
C35	7.463660	31.388282	-1.985160
C36	8.611766	31.255210	-1.190396
C37	9.382261	32.372666	-0.840642
C38	9.031339	33.657017	-1.274146
C39	7.920959	33.786303	-2.113693
C40	7.155983	32.673211	-2.463867
H41	6.272168	32.804895	-3.079413
H42	7.625547	34.773268	-2.450165
H43	10.229963	32.246069	-0.175991
H44	8.885492	30.285736	-0.792300
C45	9.709043	34.892816	-0.691483
C46	10.339345	35.858421	-1.736905
O47	11.234401	35.382484	-2.489692

O48	9.970748	37.052807	-1.684559
H49	10.549264	34.530209	-0.083577
C50	8.717163	35.649926	0.221173
H51	8.248471	34.967669	0.930384
H52	7.927918	36.098832	-0.382715
H53	9.206389	36.451882	0.783651
C54	6.522128	30.232997	-2.274159
C55	6.949009	29.254066	-3.400063
C56	5.723874	28.487149	-3.925105
C57	7.998212	28.253865	-2.895325
H58	7.557941	27.624747	-2.114201
H59	8.875881	28.763492	-2.490800
H60	8.324121	27.592787	-3.705235
H61	6.013928	27.798649	-4.726092
H62	4.962370	29.169579	-4.317704
H63	5.282194	27.890055	-3.121404
H64	7.377614	29.845565	-4.220756
H65	5.545993	30.655203	-2.536643
H66	6.372132	29.639821	-1.364410
H67	7.355887	20.854049	-2.691837
H68	6.395259	23.967446	-6.366317
H69	3.725283	23.699196	-5.966508
H70	0.531657	23.836264	-1.836862
H71	0.916136	24.181510	0.947656
H72	4.882355	25.103781	3.946538
H73	7.502051	25.355452	3.786754
H74	10.779915	25.497668	-0.525079
H75	10.494225	24.967075	-3.204654

Ibuprofen 3-6 Reactant Complex Quartet

C1	6.350107	21.233518	-2.403355
S2	6.207200	22.200242	-0.830921
H3	5.706685	20.351810	-2.281006
H4	5.967658	21.821824	-3.243962
O5	5.512409	26.308129	-1.356106
Fe6	5.679508	24.711959	-1.198984
N7	5.450007	24.272209	-3.170737
N8	3.689412	24.342037	-0.901827
N9	5.966938	24.770147	0.832038
N10	7.683457	24.744228	-1.452678
C11	6.415701	24.276218	-4.128517
C12	5.845280	24.018932	-5.428682
C13	4.511944	23.869471	-5.230689
C14	4.276985	24.024978	-3.817156
C15	2.753172	24.100967	-1.848113
C16	1.437196	24.006364	-1.252785
C17	1.603605	24.189026	0.082650
C18	3.022938	24.392357	0.274866
C19	4.978229	24.784183	1.755341
C20	5.508658	25.047924	3.060530
C21	6.852512	25.180844	2.928752
C22	7.127545	25.018029	1.511414
C23	8.601728	25.050859	-0.498289
C24	9.902461	25.201830	-1.092139
C25	9.756493	24.968268	-2.419528
C26	8.360778	24.702508	-2.638326
C27	7.783449	24.488845	-3.895268
H28	8.439701	24.505995	-4.759794
C29	3.011095	23.928960	-3.220456

H30	2.173174	23.693737	-3.867700
C31	3.611940	24.587633	1.530805
H32	2.973769	24.644206	2.402885
C33	8.363049	25.194154	0.874934
H34	9.216927	25.512598	1.458686
C35	7.457367	31.388839	-1.980641
C36	8.599823	31.255867	-1.181918
C37	9.372719	32.369169	-0.833879
C38	9.029041	33.652105	-1.272851
C39	7.924791	33.782288	-2.117655
C40	7.157912	32.670942	-2.467052
H41	6.272688	32.802839	-3.091876
H42	7.634876	34.775720	-2.460581
H43	10.224259	32.241408	-0.161778
H44	8.868620	30.279317	-0.776940
C45	9.709377	34.894357	-0.690144
C46	10.349239	35.876908	-1.757445
O47	11.238732	35.398786	-2.467705
O48	9.955053	37.032422	-1.710732
H49	10.552493	34.529999	-0.083923
C50	8.719521	35.654658	0.223326
H51	8.250607	34.972341	0.933234
H52	7.930613	36.104645	-0.381334
H53	9.207662	36.457885	0.787874
C54	6.508736	30.231337	-2.271117
C55	6.939657	29.234713	-3.384401
C56	5.706698	28.499252	-3.937833
C57	7.941376	28.201594	-2.848676
H58	7.429843	27.554635	-2.121156
H59	8.800685	28.680668	-2.368987
H60	8.313272	27.559167	-3.656386
H61	5.991787	27.810239	-4.742335
H62	4.960985	29.199183	-4.333886
H63	5.245337	27.901519	-3.144504
H64	7.408289	29.814663	-4.194127
H65	5.538341	30.661281	-2.547832
H66	6.342373	29.648205	-1.356328
H67	7.353758	20.847559	-2.698160
H68	6.398486	23.966821	-6.373328
H69	3.728167	23.701233	-5.971529
H70	0.530593	23.842454	-1.838329
H71	0.912689	24.188457	0.944143
H72	4.883601	25.100513	3.950716
H73	7.505405	25.354941	3.792724
H74	10.788118	25.492243	-0.525128
H75	10.502414	24.961134	-3.205022

Ibuprofen 3-6 Transition State Doublet

C1	6.332149	21.278513	-2.408566
S2	6.148610	22.236474	-0.845559
H3	5.692258	20.399756	-2.292627
H4	5.958499	21.861657	-3.249317
O5	5.615286	26.461156	-1.363401
Fe6	5.740709	24.732410	-1.236946
N7	5.503950	24.335487	-3.186815
N8	3.729159	24.459630	-0.948047
N9	6.001284	24.791077	0.785029
N10	7.712746	24.777056	-1.482302
C11	6.476922	24.308916	-4.153875

C12	5.897482	24.047455	-5.450087
C13	4.556585	23.912771	-5.248348
C14	4.321376	24.092357	-3.836197
C15	2.787459	24.188711	-1.896527
C16	1.473276	24.036821	-1.295743
C17	1.640170	24.203942	0.046682
C18	3.056701	24.452277	0.236536
C19	5.003034	24.784000	1.711516
C20	5.527367	25.018109	3.026473
C21	6.876123	25.166716	2.904460
C22	7.162786	25.031500	1.482407
C23	8.631770	25.076429	-0.513604
C24	9.942127	25.201227	-1.098022
C25	9.805026	24.950257	-2.430492
C26	8.407108	24.698494	-2.661982
C27	7.831677	24.487228	-3.908041
H28	8.490105	24.475528	-4.767447
C29	3.064401	24.011767	-3.247207
H30	2.236412	23.760099	-3.897141
C31	3.650917	24.600064	1.478710
H32	3.016620	24.617994	2.352795
C33	8.384409	25.209266	0.845846
H34	9.239258	25.501987	1.435913
C35	7.427868	31.337747	-1.945162
C36	8.562876	31.203473	-1.133005
C37	9.351980	32.313692	-0.797795
C38	9.041352	33.596152	-1.268745
C39	7.955134	33.722384	-2.137110
C40	7.167686	32.615887	-2.468308
H41	6.301691	32.756083	-3.108130
H42	7.694160	34.704585	-2.517336
H43	10.184079	32.182840	-0.112816
H44	8.815556	30.239024	-0.706648
C45	9.729655	34.832634	-0.688969
C46	10.357258	35.812360	-1.726988
O47	11.249157	35.348500	-2.490970
O48	9.993934	37.009328	-1.658965
H49	10.571956	34.464493	-0.087298
C50	8.747895	35.588013	0.236871
H51	8.277680	34.904893	0.942942
H52	7.958382	36.049491	-0.357435
H53	9.247026	36.379939	0.805036
C54	6.434901	30.203656	-2.189237
C55	6.876788	29.021986	-3.107035
C56	5.688696	28.519555	-3.949661
C57	7.467570	27.831692	-2.350170
H58	6.522217	27.132981	-1.828796
H59	8.138393	28.096219	-1.531007
H60	7.964577	27.139275	-3.029514
H61	6.007240	27.715482	-4.622023
H62	5.251936	29.322638	-4.550129
H63	4.918058	28.108867	-3.289933
H64	7.644624	29.406671	-3.797019
H65	5.536901	30.655046	-2.623975
H66	6.125228	29.781507	-1.226673
H67	7.336792	20.890458	-2.695897
H68	6.442095	23.986285	-6.390829
H69	3.769663	23.732410	-5.977912
H70	0.571126	23.842407	-1.870838
H71	0.957259	24.166951	0.909125

H72	4.893364	25.035785	3.907923
H73	7.511074	25.335399	3.776882
H74	10.817122	25.486066	-0.523137
H75	10.541745	24.940174	-3.212169

Ibuprofen 3-6 Transition State Quartet

C1	6.333176	21.290038	-2.415518
S2	6.199369	22.289270	-0.854490
H3	5.682764	20.416589	-2.275368
H4	5.955352	21.867726	-3.264602
O5	5.576930	26.460114	-1.411511
Fe6	5.712595	24.687336	-1.215276
N7	5.490379	24.305795	-3.193553
N8	3.716114	24.446128	-0.939191
N9	5.990418	24.795097	0.800631
N10	7.729384	24.804216	-1.478414
C11	6.467092	24.289404	-4.148510
C12	5.893529	24.039729	-5.447730
C13	4.556886	23.912812	-5.252925
C14	4.320118	24.081890	-3.842356
C15	2.779042	24.188612	-1.891557
C16	1.464948	24.051831	-1.290074
C17	1.629542	24.215540	0.044618
C18	3.047043	24.450444	0.241197
C19	5.001658	24.788310	1.724313
C20	5.530951	25.022866	3.034504
C21	6.871756	25.169956	2.908822
C22	7.155970	25.035973	1.488903
C23	8.636475	25.095440	-0.519823
C24	9.948253	25.213620	-1.100529
C25	9.810112	24.956726	-2.425707
C26	8.410255	24.708052	-2.648849
C27	7.836259	24.475286	-3.910776
H28	8.494585	24.459795	-4.771923
C29	3.043514	24.011566	-3.252762
H30	2.209750	23.775871	-3.905603
C31	3.634799	24.603617	1.495019
H32	2.998206	24.630996	2.370993
C33	8.392252	25.221906	0.859406
H34	9.245781	25.515121	1.454167
C35	7.416070	31.340282	-1.947016
C36	8.550339	31.207525	-1.135523
C37	9.340811	32.316446	-0.808859
C38	9.029595	33.595129	-1.287754
C39	7.943888	33.718061	-2.157135
C40	7.156250	32.611754	-2.480159
H41	6.284228	32.745647	-3.124248
H42	7.683410	34.703800	-2.543312
H43	10.178045	32.189050	-0.120231
H44	8.800956	30.239038	-0.701722
C45	9.715129	34.839287	-0.708304
C46	10.358781	35.837844	-1.761333
O47	11.253827	35.370411	-2.473794
O48	9.969303	36.994475	-1.700600
H49	10.558533	34.472705	-0.104222
C50	8.728184	35.595580	0.211864
H51	8.257805	34.911604	0.918967
H52	7.940170	36.053478	-0.388091
H53	9.221625	36.392567	0.780310

C54	6.425820	30.199779	-2.186801
C55	6.869961	29.039098	-3.129144
C56	5.673246	28.521544	-3.957392
C57	7.534605	27.885713	-2.412199
H58	6.443670	27.036451	-1.809274
H59	8.144256	28.105736	-1.537286
H60	7.964396	27.124727	-3.060432
H61	5.985919	27.736417	-4.654914
H62	5.215290	29.331975	-4.532755
H63	4.919758	28.087507	-3.291663
H64	7.609479	29.455387	-3.839037
H65	5.515186	30.644804	-2.602006
H66	6.135097	29.759919	-1.225339
H67	7.336196	20.890697	-2.705892
H68	6.442225	23.978056	-6.393578
H69	3.769595	23.734400	-5.988105
H70	0.559986	23.854948	-1.867290
H71	0.942429	24.180287	0.908513
H72	4.897795	25.040694	3.922523
H73	7.513249	25.338315	3.784820
H74	10.830652	25.494159	-0.525119
H75	10.551937	24.938633	-3.211331

Warfarin 6-1 Reactant Complex Doublet

C1	-0.932689	2.052292	-4.812118
H2	-1.711416	1.537447	-5.382511
H3	-1.440856	2.637278	-4.048882
S4	0.084919	0.737285	-4.054998
O5	0.680219	1.075708	-0.011126
Fe6	0.330387	1.017352	-1.610376
N7	-1.092224	2.437615	-1.615545
N8	-1.091064	-0.379744	-1.296915
N9	1.729025	-0.417374	-1.896713
N10	1.718308	2.426808	-2.082268
C11	-0.908501	3.783343	-1.771188
C12	-2.147094	4.489869	-1.601931
C13	-3.105650	3.549693	-1.376156
C14	-2.435722	2.271154	-1.389485
C15	-2.421338	-0.179605	-1.087039
C16	-3.073138	-1.420902	-0.723113
C17	-2.100345	-2.374383	-0.687836
C18	-0.874234	-1.705994	-1.080260
C19	1.531868	-1.744178	-1.674377
C20	2.762503	-2.466878	-1.854052
C21	3.726035	-1.555351	-2.172233
C22	3.070926	-0.255160	-2.155507
C23	3.065840	2.230100	-2.168481
C24	3.749908	3.502012	-2.288280
C25	2.788599	4.467173	-2.318610
C26	1.527454	3.782593	-2.162964
C27	0.302597	4.409750	-2.036583
H28	0.287281	5.490226	-2.098330
C29	-3.061881	1.052033	-1.172162
H30	-4.133792	1.072436	-1.035735
C31	0.343942	-2.343163	-1.267825
H32	0.394658	-3.398599	-1.044491
C33	3.691766	0.988314	-2.210526
H34	4.770951	1.018160	-2.237628
C35	1.073011	2.437423	3.175122

H36	0.729240	1.651022	3.836488
C37	0.221936	2.895325	2.188283
H38	-0.751595	2.445664	2.060610
C39	0.655825	3.880928	1.290799
H40	-0.016973	4.222487	0.517390
C41	1.932285	4.410064	1.380107
H42	2.290035	5.160768	0.686363
C43	2.763054	3.991556	2.420429
O44	3.977751	4.596663	2.543518
C45	4.715604	4.578333	3.728852
O46	5.670774	5.318673	3.768591
C47	4.235388	3.679914	4.758072
C48	3.171095	2.842193	4.516942
O49	2.845539	1.945930	5.453040
H50	1.988712	1.545484	5.310402
C51	2.348901	3.017847	3.338331
H52	-0.462875	2.760079	-5.527962
H53	-2.240402	5.566185	-1.631807
H54	-4.164125	3.712680	-1.195807
H55	-4.138408	-1.503852	-0.529311
H56	-2.104836	-3.435923	-0.418599
H57	2.835368	-3.546732	-1.798672
H58	4.752615	-1.848478	-2.407659
H59	4.829082	3.617300	-2.306652
H60	2.868314	5.541648	-2.485799
H61	4.465888	3.924696	5.815414

Warfarin 6-1 Reactant Complex Quartet

C1	-0.927294	2.052237	-4.812614
H2	-1.703488	1.529775	-5.380588
H3	-1.437184	2.636257	-4.049914
S4	0.097314	0.744388	-4.056736
O5	0.645000	1.061244	-0.005917
Fe6	0.337950	1.011373	-1.608679
N7	-1.088868	2.433443	-1.614157
N8	-1.089121	-0.389725	-1.307114
N9	1.731264	-0.419966	-1.899402
N10	1.722624	2.419854	-2.074289
C11	-0.907307	3.776122	-1.768957
C12	-2.146731	4.482723	-1.599749
C13	-3.103622	3.542399	-1.371730
C14	-2.433344	2.263224	-1.384766
C15	-2.416145	-0.187987	-1.091721
C16	-3.067779	-1.429565	-0.724063
C17	-2.095230	-2.383379	-0.687812
C18	-0.867968	-1.716735	-1.084505
C19	1.534548	-1.747556	-1.680875
C20	2.765086	-2.469087	-1.864910
C21	3.728518	-1.557450	-2.179547
C22	3.075969	-0.256849	-2.156941
C23	3.068835	2.226293	-2.160840
C24	3.750043	3.499562	-2.285164
C25	2.787863	4.462718	-2.317906
C26	1.527718	3.777895	-2.159657
C27	0.304868	4.403974	-2.035988
H28	0.288413	5.484197	-2.103417
C29	-3.056876	1.044979	-1.170881
H30	-4.128881	1.065221	-1.030067
C31	0.347427	-2.348686	-1.269399

H32	0.405426	-3.403187	-1.038321
C33	3.697479	0.984190	-2.201488
H34	4.777068	1.014177	-2.221571
C35	1.072557	2.432633	3.170644
H36	0.729134	1.647942	3.833384
C37	0.217162	2.893321	2.189681
H38	-0.757499	2.444250	2.066117
C39	0.646658	3.879257	1.291126
H40	-0.028668	4.222568	0.521451
C41	1.923289	4.410532	1.377072
H42	2.276683	5.160649	0.681294
C43	2.756735	3.993444	2.415840
O44	3.967829	4.604920	2.539803
C45	4.709072	4.579739	3.722876
O46	5.666965	5.320329	3.762781
C47	4.233224	3.678323	4.750240
C48	3.172589	2.838286	4.507767
O49	2.849415	1.936270	5.441552
H50	1.995770	1.535676	5.301097
C51	2.347791	3.014623	3.330239
H52	-0.462999	2.757656	-5.533312
H53	-2.241097	5.559461	-1.629274
H54	-4.162343	3.705876	-1.192333
H55	-4.132708	-1.511284	-0.528343
H56	-2.099271	-3.443990	-0.416443
H57	2.839163	-3.548801	-1.809397
H58	4.754748	-1.848073	-2.416373
H59	4.828921	3.617338	-2.304572
H60	2.866423	5.538048	-2.484932
H61	4.463658	3.920103	5.808974

Warfarin 6-1 Transition State Doublet

C1	-0.903433	2.024337	-4.704474
H2	-1.653713	1.436845	-5.242071
H3	-1.438546	2.627094	-3.973410
S4	0.175803	0.795782	-3.863058
O5	0.818329	1.172519	0.296391
Fe6	0.363384	1.129524	-1.422241
N7	-1.063754	2.513584	-1.473976
N8	-1.048543	-0.303356	-1.094367
N9	1.767915	-0.339594	-1.670322
N10	1.720995	2.514381	-1.927700
C11	-0.913607	3.848398	-1.751293
C12	-2.165624	4.535518	-1.610583
C13	-3.104695	3.593056	-1.327233
C14	-2.412728	2.329082	-1.257873
C15	-2.387718	-0.118173	-0.926382
C16	-3.048442	-1.376616	-0.637558
C17	-2.074960	-2.329764	-0.613068
C18	-0.838477	-1.642412	-0.938336
C19	1.562766	-1.673801	-1.511094
C20	2.777662	-2.403474	-1.767780
C21	3.737110	-1.490460	-2.084844
C22	3.094818	-0.182737	-1.991402
C23	3.066860	2.305049	-2.032536
C24	3.746643	3.566139	-2.226284
C25	2.786340	4.530688	-2.298285
C26	1.523234	3.860905	-2.113559
C27	0.284422	4.476361	-2.072608

H28	0.246672	5.547280	-2.223154
C29	-3.030216	1.110604	-1.021199
H30	-4.105852	1.121181	-0.915666
C31	0.370268	-2.282815	-1.142094
H32	0.406791	-3.350402	-0.984679
C33	3.701938	1.065274	-2.074969
H34	4.777399	1.105463	-2.162437
C35	1.232476	2.099430	2.739435
H36	0.908357	1.289310	3.379728
C37	0.451284	2.393987	1.566034
H38	-0.594389	2.101931	1.592758
C39	0.758110	3.641782	0.928230
H40	0.055475	4.032764	0.218866
C41	1.920456	4.326831	1.176830
H42	2.187976	5.214239	0.617055
C43	2.744169	3.916878	2.228822
O44	3.868676	4.629198	2.449686
C45	4.606920	4.566283	3.641336
O46	5.549793	5.314668	3.710957
C47	4.114365	3.639453	4.636293
C48	3.094594	2.766430	4.342866
O49	2.738855	1.876610	5.270269
H50	1.905953	1.447425	5.083501
C51	2.360498	2.852713	3.078677
H52	-0.468163	2.721724	-5.465863
H53	-2.262797	5.607151	-1.649399
H54	-4.169794	3.739490	-1.170471
H55	-4.119944	-1.485411	-0.501398
H56	-2.086766	-3.404385	-0.385748
H57	2.838373	-3.488784	-1.777634
H58	4.744816	-1.798119	-2.377963
H59	4.826806	3.661224	-2.278603
H60	2.871359	5.596586	-2.485581
H61	4.364520	3.865480	5.701327

Warfarin 6-1 Transition State Quartet

C1	-0.918499	2.013559	-4.728641
H2	-1.653755	1.416281	-5.274864
H3	-1.470628	2.608282	-4.002479
S4	0.170496	0.806908	-3.875038
O5	0.673340	1.283681	0.271653
Fe6	0.384679	1.080036	-1.436756
N7	-1.067580	2.477906	-1.535179
N8	-1.031399	-0.333266	-1.119346
N9	1.765523	-0.348274	-1.688859
N10	1.747268	2.488944	-1.923174
C11	-0.902650	3.817720	-1.774174
C12	-2.152959	4.505369	-1.623251
C13	-3.096857	3.559690	-1.354086
C14	-2.408979	2.293889	-1.308377
C15	-2.377235	-0.140792	-0.953732
C16	-3.033580	-1.398351	-0.651080
C17	-2.060723	-2.350511	-0.621593
C18	-0.823552	-1.670463	-0.954946
C19	1.561915	-1.693518	-1.530491
C20	2.780441	-2.409172	-1.789906
C21	3.738307	-1.492434	-2.105554
C22	3.101417	-0.187261	-2.011876
C23	3.087856	2.288201	-2.034212

C24	3.761069	3.554671	-2.223259
C25	2.793907	4.513056	-2.285668
C26	1.534804	3.832266	-2.099065
C27	0.297970	4.448953	-2.064451
H28	0.264328	5.522819	-2.192411
C29	-3.025010	1.076392	-1.060790
H30	-4.099763	1.086600	-0.946787
C31	0.384754	-2.310872	-1.157531
H32	0.426339	-3.377817	-0.995590
C33	3.721079	1.050093	-2.089205
H34	4.796145	1.081648	-2.174514
C35	1.214964	2.122550	2.764701
H36	0.883085	1.320714	3.408407
C37	0.411835	2.442741	1.612695
H38	-0.628524	2.149207	1.657327
C39	0.721553	3.697890	0.982974
H40	0.008182	4.089717	0.279220
C41	1.890460	4.362391	1.216770
H42	2.156775	5.259157	0.669843
C43	2.736337	3.931980	2.252396
O44	3.862852	4.641958	2.464618
C45	4.612605	4.570326	3.649566
O46	5.558545	5.314596	3.716175
C47	4.124823	3.639743	4.643542
C48	3.101652	2.767364	4.350311
O49	2.754645	1.875812	5.280085
H50	1.914412	1.452935	5.109709
C51	2.360712	2.863024	3.090801
H52	-0.477016	2.713568	-5.484939
H53	-2.255240	5.578523	-1.648624
H54	-4.159983	3.712193	-1.180477
H55	-4.105120	-1.504978	-0.507014
H56	-2.069174	-3.421662	-0.387090
H57	2.844557	-3.494428	-1.799388
H58	4.749463	-1.798198	-2.392764
H59	4.839149	3.656612	-2.279330
H60	2.872423	5.581053	-2.472328
H61	4.376510	3.862147	5.710461

Warfarin 6-2 Reactant Complex Doublet

C1	-0.951599	1.818003	-4.863350
H2	-1.693113	1.232122	-5.419580
H3	-1.496151	2.388142	-4.112170
S4	0.169895	0.625516	-4.063650
O5	0.686263	1.100015	-0.023082
Fe6	0.367418	1.014528	-1.629224
N7	-1.065333	2.434358	-1.664944
N8	-1.053625	-0.382692	-1.320263
N9	1.778806	-0.410083	-1.885701
N10	1.752433	2.428098	-2.096119
C11	-0.883378	3.781999	-1.818140
C12	-2.123197	4.484951	-1.633186
C13	-3.077153	3.541962	-1.403698
C14	-2.404786	2.264972	-1.423720
C15	-2.384773	-0.184342	-1.108176
C16	-3.035568	-1.430011	-0.753270
C17	-2.060699	-2.382254	-0.731861
C18	-0.835677	-1.707983	-1.117885
C19	1.580101	-1.739535	-1.677952

C20	2.812109	-2.460184	-1.856482
C21	3.775290	-1.546118	-2.169672
C22	3.119028	-0.247338	-2.146662
C23	3.101523	2.236033	-2.178587
C24	3.784418	3.508538	-2.285232
C25	2.822237	4.471097	-2.298129
C26	1.559562	3.783352	-2.168737
C27	0.330023	4.408638	-2.073308
H28	0.313579	5.488963	-2.151704
C29	-3.026545	1.045193	-1.190572
H30	-4.097323	1.065851	-1.040957
C31	0.387187	-2.342798	-1.297698
H32	0.438683	-3.400825	-1.085184
C33	3.734254	0.998694	-2.213711
H34	4.813473	1.038926	-2.235980
C35	1.133865	2.554243	3.133579
H36	0.782196	1.781603	3.809951
C37	0.295329	2.992777	2.128349
H38	-0.676229	2.537765	1.991616
C39	0.739630	3.966808	1.223087
H40	0.080606	4.287144	0.430539
C41	2.001682	4.521735	1.336864
H42	2.360150	5.275677	0.643130
C43	2.815377	4.135897	2.401865
O44	3.998163	4.793500	2.569555
C45	4.696614	4.780713	3.775684
O46	5.597559	5.585174	3.876370
C47	4.261538	3.809472	4.753800
C48	3.233705	2.939712	4.469077
O49	2.948181	1.987256	5.358387
H50	2.135638	1.517270	5.163959
C51	2.404993	3.142445	3.301191
H52	-0.518823	2.534201	-5.587810
H53	-2.232053	5.559946	-1.645070
H54	-4.135397	3.707047	-1.220840
H55	-4.099720	-1.510333	-0.545617
H56	-2.058633	-3.444605	-0.474778
H57	2.885109	-3.539841	-1.802832
H58	4.800122	-1.836824	-2.411896
H59	4.863712	3.618136	-2.324017
H60	2.898319	5.546188	-2.435783
H61	4.485874	4.006992	5.820773

Warfarin 6-2 Reactant Complex Quartet

C1	-0.947454	1.820630	-4.861616
H2	-1.687477	1.228989	-5.414521
H3	-1.492010	2.390573	-4.110742
S4	0.179998	0.637386	-4.060535
O5	0.653176	1.086823	-0.016379
Fe6	0.371127	1.012278	-1.624775
N7	-1.064107	2.434448	-1.664214
N8	-1.056490	-0.386235	-1.326405
N9	1.776777	-0.410581	-1.883001
N10	1.753571	2.424896	-2.087559
C11	-0.883586	3.780214	-1.816542
C12	-2.123439	4.484219	-1.632282
C13	-3.077582	3.540537	-1.402957
C14	-2.405336	2.263641	-1.423254
C15	-2.385090	-0.185454	-1.111068

C16	-3.037032	-1.429098	-0.751181
C17	-2.063975	-2.383608	-0.729110
C18	-0.837128	-1.713190	-1.118883
C19	1.576688	-1.740029	-1.678823
C20	2.809157	-2.459056	-1.857127
C21	3.772336	-1.547102	-2.167224
C22	3.119221	-0.247004	-2.142331
C23	3.101628	2.234391	-2.172273
C24	3.783293	3.507341	-2.282669
C25	2.820904	4.469800	-2.296738
C26	1.558613	3.782275	-2.164836
C27	0.330944	4.407954	-2.072469
H28	0.314496	5.487078	-2.152988
C29	-3.026616	1.045472	-1.193349
H30	-4.096773	1.067845	-1.040609
C31	0.382549	-2.344926	-1.297659
H32	0.437373	-3.402191	-1.078551
C33	3.735450	0.996799	-2.206051
H34	4.814310	1.037670	-2.225218
C35	1.134951	2.551904	3.130951
H36	0.786823	1.774855	3.802842
C37	0.296290	2.993137	2.126520
H38	-0.674867	2.538272	1.989594
C39	0.740483	3.966551	1.221899
H40	0.083806	4.287934	0.428787
C41	2.006411	4.521363	1.333880
H42	2.362317	5.274150	0.642246
C43	2.816566	4.133765	2.400908
O44	3.998396	4.796421	2.571838
C45	4.697132	4.782069	3.778906
O46	5.596534	5.585020	3.880253
C47	4.259866	3.808910	4.752614
C48	3.235126	2.938928	4.466385
O49	2.948084	1.982111	5.354043
H50	2.136512	1.517534	5.162654
C51	2.407142	3.141232	3.298434
H52	-0.518925	2.534170	-5.589676
H53	-2.233362	5.559825	-1.644505
H54	-4.135673	3.705965	-1.218439
H55	-4.101147	-1.508937	-0.544290
H56	-2.066568	-3.445678	-0.470233
H57	2.883784	-3.538293	-1.808459
H58	4.796214	-1.838353	-2.409537
H59	4.862569	3.618840	-2.322940
H60	2.898108	5.546214	-2.435966
H61	4.481171	4.002949	5.819247

Warfarin 6-2 Transition State Doublet

C1	-0.920079	1.816264	-4.732316
H2	-1.647437	1.180862	-5.249742
H3	-1.475448	2.409141	-4.006492
S4	0.237439	0.686109	-3.869089
O5	0.856075	1.233128	0.283154
Fe6	0.406146	1.131433	-1.431605
N7	-1.031010	2.514127	-1.517516
N8	-1.008281	-0.298098	-1.099052
N9	1.817450	-0.332881	-1.655135
N10	1.754997	2.511461	-1.967995
C11	-0.884215	3.849273	-1.798269

C12	-2.135171	4.536256	-1.640518
C13	-3.071718	3.591116	-1.351822
C14	-2.376856	2.329861	-1.287318
C15	-2.349981	-0.114034	-0.935994
C16	-3.013729	-1.374594	-0.661925
C17	-2.041682	-2.328397	-0.652053
C18	-0.802534	-1.639586	-0.963845
C19	1.608837	-1.667715	-1.507824
C20	2.823560	-2.398045	-1.763089
C21	3.784745	-1.483983	-2.078475
C22	3.142041	-0.177683	-1.982893
C23	3.102488	2.307001	-2.060688
C24	3.782941	3.569198	-2.236190
C25	2.822352	4.532665	-2.296705
C26	1.556628	3.858892	-2.145953
C27	0.316342	4.474064	-2.124244
H28	0.281237	5.544161	-2.285160
C29	-2.992756	1.112638	-1.035508
H30	-4.067883	1.124446	-0.923386
C31	0.408081	-2.278946	-1.166890
H32	0.441475	-3.350066	-1.030549
C33	3.743836	1.071351	-2.089382
H34	4.819323	1.119927	-2.175283
C35	1.302299	2.221924	2.700396
H36	0.978025	1.413262	3.343466
C37	0.530488	2.501462	1.521834
H38	-0.517931	2.221892	1.549703
C39	0.853159	3.737764	0.870349
H40	0.161397	4.118480	0.144540
C41	2.006574	4.434709	1.132101
H42	2.275583	5.317807	0.564005
C43	2.808511	4.053272	2.210544
O44	3.907230	4.803040	2.469937
C45	4.601720	4.757749	3.684888
O46	5.493897	5.562163	3.810254
C47	4.143819	3.774102	4.639285
C48	3.152813	2.878008	4.310041
O49	2.823212	1.947640	5.206861
H50	2.015178	1.482098	4.995343
C51	2.425092	2.983543	3.048286
H52	-0.513924	2.514314	-5.502510
H53	-2.249259	5.605998	-1.661904
H54	-4.137028	3.737138	-1.195727
H55	-4.086210	-1.477125	-0.512946
H56	-2.052115	-3.404756	-0.440804
H57	2.885286	-3.482603	-1.772778
H58	4.791726	-1.790336	-2.374302
H59	4.862858	3.656649	-2.301303
H60	2.904639	5.600480	-2.448191
H61	4.386167	3.959999	5.712310

Warfarin 6-2 Transition State Quartet

C1	-0.928982	1.815915	-4.750771
H2	-1.646861	1.164679	-5.261251
H3	-1.491359	2.407585	-4.028900
S4	0.249299	0.723480	-3.875530
O5	0.713117	1.333697	0.254592
Fe6	0.421324	1.091057	-1.441308
N7	-1.035949	2.487863	-1.567541

N8	-0.999684	-0.319437	-1.119746
N9	1.808725	-0.337261	-1.668109
N10	1.777427	2.494502	-1.948021
C11	-0.874226	3.828051	-1.812328
C12	-2.122655	4.515750	-1.646652
C13	-3.064054	3.569202	-1.371276
C14	-2.375729	2.305726	-1.327374
C15	-2.346956	-0.127479	-0.958566
C16	-3.007990	-1.386886	-0.673017
C17	-2.037078	-2.342082	-0.659460
C18	-0.796036	-1.660804	-0.978704
C19	1.600240	-1.682648	-1.523414
C20	2.818294	-2.400098	-1.778005
C21	3.778247	-1.485564	-2.090483
C22	3.143628	-0.180163	-1.997401
C23	3.119862	2.294174	-2.051346
C24	3.795672	3.560593	-2.227316
C25	2.830932	4.519709	-2.278539
C26	1.567346	3.840161	-2.120858
C27	0.329767	4.456062	-2.109492
H28	0.297708	5.528455	-2.254532
C29	-2.992963	1.089367	-1.069253
H30	-4.067823	1.103009	-0.955264
C31	0.410939	-2.300806	-1.181207
H32	0.449444	-3.371220	-1.040684
C33	3.756727	1.059863	-2.096957
H34	4.831978	1.100698	-2.184762
C35	1.292724	2.243380	2.714062
H36	0.962812	1.435250	3.354327
C37	0.499758	2.550338	1.556725
H38	-0.545783	2.276656	1.597308
C39	0.829868	3.794774	0.914453
H40	0.136128	4.178298	0.191444
C41	1.990827	4.472274	1.170668
H42	2.262346	5.361308	0.613468
C43	2.808286	4.070527	2.235566
O44	3.909066	4.816301	2.491981
C45	4.612288	4.757374	3.701424
O46	5.504374	5.561977	3.831244
C47	4.160056	3.764177	4.646525
C48	3.163958	2.871927	4.313331
O49	2.835967	1.937650	5.207576
H50	2.023523	1.478097	5.001975
C51	2.429143	2.990508	3.056511
H52	-0.525695	2.510943	-5.523572
H53	-2.240058	5.587335	-1.659998
H54	-4.127892	3.721445	-1.203971
H55	-4.080346	-1.487095	-0.517755
H56	-2.047983	-3.416063	-0.441483
H57	2.887162	-3.484607	-1.782534
H58	4.789694	-1.792846	-2.378047
H59	4.874229	3.651231	-2.299449
H60	2.908613	5.589064	-2.435668
H61	4.400623	3.946029	5.720832

Warfarin 6-3Reactant Complex Doublet

C1	-1.025371	1.783309	-4.808321
H2	-1.618817	1.231172	-5.548813
H3	-1.722901	2.220361	-4.094228

S4	0.025333	0.540879	-3.992741
O5	0.704254	1.153062	0.001699
Fe6	0.328062	1.012570	-1.590987
N7	-1.114550	2.418871	-1.627277
N8	-1.072097	-0.389769	-1.243014
N9	1.736708	-0.410293	-1.873372
N10	1.694435	2.426651	-2.126515
C11	-0.935628	3.769140	-1.759169
C12	-2.178049	4.467888	-1.568580
C13	-3.130198	3.518571	-1.360012
C14	-2.452801	2.243766	-1.389999
C15	-2.407938	-0.200363	-1.051434
C16	-3.056137	-1.452211	-0.717022
C17	-2.080921	-2.403395	-0.706033
C18	-0.852929	-1.719414	-1.068910
C19	1.551902	-1.740255	-1.654145
C20	2.780777	-2.456632	-1.868257
C21	3.724184	-1.543294	-2.228993
C22	3.065271	-0.245976	-2.188462
C23	3.043345	2.235312	-2.233824
C24	3.721899	3.508349	-2.343974
C25	2.758376	4.473091	-2.332732
C26	1.500226	3.783129	-2.172384
C27	0.272033	4.401942	-2.011355
H28	0.249707	5.483820	-2.026255
C29	-3.064129	1.018055	-1.154608
H30	-4.138572	1.024226	-1.023991
C31	0.368190	-2.350442	-1.261060
H32	0.428043	-3.412714	-1.064744
C33	3.677341	0.998356	-2.280937
H34	4.755781	1.032489	-2.345458
C35	1.090889	2.517586	3.170060
H36	0.741889	1.761343	3.864744
C37	0.227626	2.977443	2.194712
H38	-0.757853	2.546727	2.093742
C39	0.651806	3.957328	1.286938
H40	-0.033764	4.304717	0.527968
C41	1.932816	4.481426	1.353585
H42	2.279896	5.235215	0.657479
C43	2.782594	4.052959	2.373727
O44	3.996117	4.664818	2.484766
C45	4.751273	4.633608	3.657316
O46	5.676645	5.413859	3.710638
C47	4.327151	3.680027	4.658051
C48	3.253844	2.849556	4.423623
O49	2.965777	1.912609	5.333835
H50	2.091281	1.541762	5.231424
C51	2.383598	3.069299	3.287917
H52	-0.543945	2.611911	-5.361045
H53	-2.286450	5.544950	-1.559632
H54	-4.189496	3.676940	-1.179760
H55	-4.119373	-1.520269	-0.509104
H56	-2.071654	-3.468542	-0.465766
H57	2.855652	-3.534746	-1.800353
H58	4.734453	-1.829334	-2.524271
H59	4.802839	3.615020	-2.373807
H60	2.848320	5.552737	-2.452107
H61	4.587842	3.883676	5.715771

Warfarin 6-3Reactant Complex Quartet

C1	-1.022706	1.783305	-4.806706
H2	-1.615252	1.230327	-5.547443
H3	-1.719715	2.218243	-4.090995
S4	0.027571	0.541245	-3.995087
O5	0.667542	1.130713	0.005053
Fe6	0.333013	1.009516	-1.591713
N7	-1.113502	2.418179	-1.628232
N8	-1.074058	-0.394335	-1.255935
N9	1.735434	-0.409921	-1.879887
N10	1.694500	2.422846	-2.121821
C11	-0.936078	3.767802	-1.760892
C12	-2.179201	4.466056	-1.571514
C13	-3.130502	3.516711	-1.361633
C14	-2.452756	2.241598	-1.390493
C15	-2.408077	-0.202770	-1.059696
C16	-3.056362	-1.453655	-0.720611
C17	-2.080979	-2.405114	-0.707130
C18	-0.853286	-1.722898	-1.073954
C19	1.549400	-1.740750	-1.661285
C20	2.778443	-2.455784	-1.873956
C21	3.722613	-1.542685	-2.230540
C22	3.066216	-0.245714	-2.188881
C23	3.043970	2.233221	-2.228603
C24	3.720281	3.507124	-2.342851
C25	2.755444	4.470892	-2.335147
C26	1.497626	3.781144	-2.172995
C27	0.271532	4.399694	-2.016397
H28	0.248379	5.481765	-2.041439
C29	-3.063376	1.016944	-1.158285
H30	-4.137264	1.024274	-1.023351
C31	0.368131	-2.351234	-1.262082
H32	0.433181	-3.411179	-1.054403
C33	3.679299	0.998414	-2.270863
H34	4.759171	1.032855	-2.322245
C35	1.098435	2.510449	3.157955
H36	0.755041	1.744494	3.844793
C37	0.232323	2.976984	2.189223
H38	-0.752110	2.542887	2.085639
C39	0.656710	3.955761	1.281071
H40	-0.028098	4.304829	0.522494
C41	1.938468	4.478474	1.345421
H42	2.284077	5.233326	0.648662
C43	2.786872	4.052294	2.367055
O44	3.995499	4.674837	2.485501
C45	4.751345	4.635238	3.657243
O46	5.678760	5.414087	3.714271
C47	4.327549	3.678592	4.654258
C48	3.256910	2.845680	4.413987
O49	2.968542	1.905932	5.323197
H50	2.089609	1.543712	5.225259
C51	2.391110	3.064971	3.276969
H52	-0.543349	2.611849	-5.361084
H53	-2.287752	5.543673	-1.561466
H54	-4.190063	3.675664	-1.180314
H55	-4.119783	-1.520323	-0.511577
H56	-2.071973	-3.469418	-0.464417
H57	2.851611	-3.533733	-1.803768
H58	4.734040	-1.827525	-2.524570
H59	4.800658	3.613551	-2.374876

H60	2.845077	5.550712	-2.454062
H61	4.585885	3.881586	5.713429

Warfarin 6-3 Transition State Doublet

C1	-0.979362	1.777666	-4.679895
H2	-1.561395	1.155738	-5.372126
H3	-1.684173	2.234434	-3.985555
S4	0.118454	0.609768	-3.794383
O5	0.880194	1.207240	0.266317
Fe6	0.362054	1.116049	-1.432342
N7	-1.078966	2.491670	-1.482418
N8	-1.033789	-0.315392	-1.065353
N9	1.779383	-0.339434	-1.670415
N10	1.699253	2.508442	-1.990663
C11	-0.936153	3.832531	-1.741787
C12	-2.191128	4.513302	-1.581676
C13	-3.125448	3.559985	-1.316625
C14	-2.425562	2.299871	-1.263426
C15	-2.376829	-0.141107	-0.910801
C16	-3.032824	-1.406432	-0.643810
C17	-2.055904	-2.356126	-0.643279
C18	-0.820463	-1.656582	-0.945492
C19	1.584120	-1.672918	-1.504197
C20	2.799353	-2.397673	-1.781313
C21	3.740477	-1.482923	-2.138981
C22	3.093290	-0.178579	-2.034882
C23	3.045094	2.304325	-2.109983
C24	3.721342	3.567171	-2.287936
C25	2.759281	4.533835	-2.323025
C26	1.497779	3.858700	-2.140481
C27	0.254949	4.468508	-2.061432
H28	0.205072	5.543519	-2.163790
C29	-3.033260	1.078012	-1.021193
H30	-4.111114	1.078797	-0.930459
C31	0.393605	-2.289604	-1.150021
H32	0.436576	-3.361388	-1.014286
C33	3.689228	1.070037	-2.153031
H34	4.762759	1.116978	-2.269675
C35	1.330104	2.127771	2.681215
H36	1.040791	1.299038	3.312236
C37	0.520996	2.433698	1.533969
H38	-0.523500	2.136703	1.572901
C39	0.805325	3.691077	0.908167
H40	0.085278	4.081616	0.213857
C41	1.962793	4.388423	1.148255
H42	2.206932	5.292009	0.600881
C43	2.808966	3.973458	2.180740
O44	3.921452	4.705985	2.409908
C45	4.680393	4.622116	3.585306
O46	5.593066	5.406441	3.673446
C47	4.236188	3.641383	4.552835
C48	3.209229	2.776133	4.256672
O49	2.862665	1.866246	5.172305
H50	1.974107	1.529804	5.052926
C51	2.456211	2.886515	3.009692
H52	-0.538396	2.590074	-5.299664
H53	-2.303558	5.585982	-1.580024
H54	-4.191220	3.701935	-1.161226
H55	-4.103543	-1.494093	-0.482942

H56	-2.053339	-3.432267	-0.438680
H57	2.858962	-3.481004	-1.769147
H58	4.733315	-1.781261	-2.479984
H59	4.802976	3.652883	-2.345453
H60	2.855426	5.606390	-2.455986
H61	4.502395	3.832219	5.618713

Warfarin 6-3 Transition State Quartet

C1	-0.996472	1.772530	-4.693944
H2	-1.566413	1.144403	-5.389360
H3	-1.711689	2.221987	-4.004668
S4	0.108601	0.623285	-3.801551
O5	0.710709	1.328237	0.248658
Fe6	0.383120	1.069191	-1.453042
N7	-1.084657	2.461766	-1.554714
N8	-1.018512	-0.344059	-1.092998
N9	1.773301	-0.345212	-1.686899
N10	1.726628	2.486337	-1.985940
C11	-0.925307	3.805014	-1.772963
C12	-2.177271	4.489019	-1.597777
C13	-3.116049	3.534679	-1.345505
C14	-2.422310	2.271281	-1.319695
C15	-2.367003	-0.158489	-0.941837
C16	-3.021109	-1.420573	-0.658102
C17	-2.048284	-2.372279	-0.650853
C18	-0.809334	-1.683262	-0.961352
C19	1.579372	-1.689834	-1.520204
C20	2.796584	-2.400328	-1.796935
C21	3.735262	-1.482410	-2.157465
C22	3.095668	-0.181315	-2.055436
C23	3.067536	2.290869	-2.109183
C24	3.737346	3.558931	-2.282225
C25	2.769588	4.518528	-2.310626
C26	1.511077	3.833808	-2.128040
C27	0.270587	4.444847	-2.060092
H28	0.226307	5.521735	-2.140410
C29	-3.028881	1.049584	-1.063749
H30	-4.105056	1.048558	-0.958810
C31	0.403842	-2.317705	-1.160161
H32	0.456718	-3.386882	-1.014109
C33	3.708421	1.057140	-2.165990
H34	4.781838	1.092864	-2.276143
C35	1.306187	2.159238	2.697785
H36	1.008987	1.333218	3.325566
C37	0.467447	2.498073	1.577152
H38	-0.571987	2.211004	1.644307
C39	0.761451	3.767242	0.958851
H40	0.034270	4.165163	0.275076
C41	1.933305	4.432420	1.180495
H42	2.185549	5.336949	0.639384
C43	2.799080	3.993406	2.194647
O44	3.917715	4.714653	2.414807
C45	4.682902	4.624463	3.587989
O46	5.599174	5.405434	3.673619
C47	4.238961	3.643800	4.553075
C48	3.208753	2.780881	4.255672
O49	2.862218	1.867798	5.169515
H50	1.976308	1.530901	5.051243
C51	2.449155	2.900887	3.014715

H52	-0.548829	2.586925	-5.306152
H53	-2.293005	5.563273	-1.583837
H54	-4.179858	3.681534	-1.173836
H55	-4.091159	-1.504202	-0.487991
H56	-2.047286	-3.446768	-0.439346
H57	2.863365	-3.483935	-1.781053
H58	4.731800	-1.778712	-2.493270
H59	4.817706	3.648362	-2.342928
H60	2.859621	5.593048	-2.445064
H61	4.506701	3.832136	5.620997

Warfarin 6-4 Reactant Complex Doublet

C1	-0.784448	1.969480	-4.895931
H2	-1.412567	1.385306	-5.580587
H3	-1.448922	2.487001	-4.204676
S4	0.200539	0.725503	-4.012876
O5	0.748643	1.095759	0.023335
Fe6	0.372778	1.032956	-1.570701
N7	-1.064444	2.452795	-1.607330
N8	-1.044465	-0.365846	-1.255417
N9	1.767024	-0.401072	-1.863366
N10	1.748879	2.436558	-2.063240
C11	-0.887219	3.800215	-1.778003
C12	-2.132668	4.502470	-1.611673
C13	-3.082914	3.557110	-1.373387
C14	-2.405609	2.282046	-1.371397
C15	-2.372502	-0.161858	-1.028309
C16	-3.025170	-1.402648	-0.664908
C17	-2.057218	-2.362908	-0.656221
C18	-0.831679	-1.694605	-1.052563
C19	1.571281	-1.728795	-1.636315
C20	2.799721	-2.452540	-1.822614
C21	3.755658	-1.543899	-2.166449
C22	3.103309	-0.243058	-2.144760
C23	3.098010	2.238659	-2.171443
C24	3.778587	3.510706	-2.290978
C25	2.816618	4.475300	-2.288922
C26	1.555523	3.792486	-2.133912
C27	0.327709	4.422377	-2.028165
H28	0.312274	5.501820	-2.104353
C29	-3.020013	1.062804	-1.120560
H30	-4.090895	1.074411	-0.971057
C31	0.386503	-2.332205	-1.237866
H32	0.448370	-3.386239	-1.005290
C33	3.725312	0.999007	-2.222867
H34	4.804447	1.028548	-2.268536
C35	1.042031	2.506754	3.135108
H36	0.748411	1.690735	3.783901
C37	0.157158	2.941521	2.167064
H38	-0.786950	2.433491	2.030250
C39	0.524842	3.971270	1.291549
H40	-0.169495	4.291342	0.528523
C41	1.765703	4.582995	1.396190
H42	2.067598	5.378169	0.726555
C43	2.618481	4.198741	2.430491
O44	3.768578	4.916240	2.603899
C45	4.482934	4.911966	3.801219
O46	5.336280	5.766183	3.911943
C47	4.116609	3.893586	4.753974

C48	3.138109	2.972474	4.455788
O49	2.915480	1.980822	5.323435
H50	2.125901	1.480505	5.134321
C51	2.284046	3.156617	3.302194
H52	-0.301052	2.730791	-5.544667
H53	-2.254599	5.580509	-1.629324
H54	-4.142063	3.722999	-1.189786
H55	-4.088946	-1.456253	-0.453053
H56	-2.057499	-3.431089	-0.412511
H57	2.864120	-3.532052	-1.768808
H58	4.765790	-1.839724	-2.442139
H59	4.857377	3.618256	-2.340228
H60	2.888814	5.549773	-2.433529
H61	4.342908	4.077615	5.821421

Warfarin 6-4 Reactant Complex Quartet

C1	-0.782825	1.968577	-4.900097
H2	-1.406129	1.379954	-5.585038
H3	-1.452299	2.484069	-4.211028
S4	0.206565	0.729925	-4.017358
O5	0.693888	1.088817	0.031028
Fe6	0.379389	1.025524	-1.569725
N7	-1.064680	2.445364	-1.616596
N8	-1.042311	-0.377980	-1.268855
N9	1.772067	-0.404707	-1.857328
N10	1.751103	2.428890	-2.057728
C11	-0.887655	3.792494	-1.777400
C12	-2.132791	4.493661	-1.606398
C13	-3.082371	3.547670	-1.371643
C14	-2.405408	2.271498	-1.377807
C15	-2.368980	-0.173157	-1.040424
C16	-3.020078	-1.413041	-0.672002
C17	-2.052927	-2.372717	-0.660038
C18	-0.827062	-1.705576	-1.058581
C19	1.575572	-1.734569	-1.638356
C20	2.804158	-2.456318	-1.833165
C21	3.758223	-1.547534	-2.173412
C22	3.108596	-0.246686	-2.142773
C23	3.100162	2.232643	-2.167945
C24	3.778590	3.505760	-2.290040
C25	2.815651	4.468971	-2.287109
C26	1.554451	3.786045	-2.129990
C27	0.329144	4.415123	-2.023677
H28	0.314785	5.495931	-2.095983
C29	-3.018129	1.052327	-1.131873
H30	-4.089406	1.061735	-0.981162
C31	0.391666	-2.340347	-1.242035
H32	0.454664	-3.395561	-1.013879
C33	3.729215	0.995799	-2.218411
H34	4.808744	1.026344	-2.267653
C35	1.037515	2.513098	3.143319
H36	0.741419	1.699154	3.794888
C37	0.152004	2.948410	2.177201
H38	-0.788224	2.437357	2.036678
C39	0.521009	3.977701	1.300109
H40	-0.174766	4.295435	0.536101
C41	1.760108	4.587100	1.402121
H42	2.063920	5.381417	0.730964
C43	2.616527	4.201307	2.432639

O44	3.766652	4.915966	2.602471
C45	4.482485	4.910642	3.797596
O46	5.338666	5.764985	3.907440
C47	4.117744	3.892910	4.752044
C48	3.137173	2.972167	4.457320
O49	2.915899	1.984435	5.326180
H50	2.125585	1.479724	5.136864
C51	2.281479	3.158133	3.305874
H52	-0.300009	2.730478	-5.548436
H53	-2.255026	5.572245	-1.622631
H54	-4.141192	3.712153	-1.186798
H55	-4.083105	-1.464110	-0.455104
H56	-2.051411	-3.439760	-0.413327
H57	2.868841	-3.536851	-1.780002
H58	4.771329	-1.840233	-2.451285
H59	4.857650	3.613114	-2.340108
H60	2.887903	5.543649	-2.431514
H61	4.345804	4.076412	5.818763

Warfarin 6-4 Transition State Doublet

C1	-0.750244	1.947879	-4.793163
H2	-1.359849	1.301841	-5.436383
H3	-1.432025	2.478683	-4.128153
S4	0.275906	0.772024	-3.840518
O5	0.858859	1.257286	0.296736
Fe6	0.395550	1.143504	-1.401353
N7	-1.045319	2.523222	-1.496982
N8	-1.008749	-0.288168	-1.066073
N9	1.807369	-0.324826	-1.636325
N10	1.745469	2.515790	-1.947843
C11	-0.897264	3.860261	-1.773503
C12	-2.151906	4.545841	-1.623591
C13	-3.086578	3.597870	-1.335149
C14	-2.390324	2.337071	-1.267259
C15	-2.348091	-0.103016	-0.889031
C16	-3.006782	-1.360036	-0.594659
C17	-2.036538	-2.317289	-0.590941
C18	-0.801490	-1.628800	-0.918300
C19	1.602282	-1.659655	-1.474335
C20	2.812574	-2.393555	-1.741476
C21	3.765522	-1.483482	-2.085141
C22	3.126486	-0.175617	-1.987679
C23	3.093430	2.305854	-2.063116
C24	3.772308	3.567363	-2.242838
C25	2.812952	4.533875	-2.276866
C26	1.547610	3.865195	-2.104709
C27	0.308319	4.484609	-2.073094
H28	0.276261	5.556892	-2.218460
C29	-2.998605	1.118757	-1.002200
H30	-4.074660	1.120675	-0.893774
C31	0.409565	-2.270014	-1.120918
H32	0.449881	-3.339295	-0.970588
C33	3.731468	1.070646	-2.106344
H34	4.805727	1.112204	-2.217608
C35	1.233000	2.190965	2.719833
H36	0.968053	1.354175	3.347482
C37	0.422828	2.462284	1.565558
H38	-0.599017	2.103251	1.586714
C39	0.646020	3.742793	0.958010

H40	-0.089448	4.109925	0.267964
C41	1.767167	4.493200	1.216102
H42	1.969310	5.413520	0.681579
C43	2.622189	4.115167	2.254593
O44	3.683001	4.919790	2.517696
C45	4.398562	4.881923	3.717674
O46	5.243969	5.738853	3.852615
C47	4.017976	3.848689	4.649090
C48	3.074792	2.904785	4.310364
O49	2.809049	1.940203	5.194031
H50	2.023345	1.436225	4.987375
C51	2.324763	2.999245	3.063771
H52	-0.297445	2.699860	-5.490586
H53	-2.275712	5.618021	-1.645536
H54	-4.150754	3.745147	-1.168913
H55	-4.076756	-1.439568	-0.430251
H56	-2.038590	-3.396579	-0.386133
H57	2.865312	-3.479209	-1.747962
H58	4.758812	-1.792982	-2.410505
H59	4.852417	3.650904	-2.317000
H60	2.891221	5.598968	-2.435885
H61	4.261592	4.023739	5.722059

Warfarin 6-4 Transition State Quartet

C1	-0.754609	1.944254	-4.825337
H2	-1.357968	1.295947	-5.471896
H3	-1.441687	2.473719	-4.164080
S4	0.270162	0.780521	-3.862763
O5	0.701350	1.337980	0.279738
Fe6	0.415943	1.101066	-1.407029
N7	-1.050645	2.491251	-1.555782
N8	-0.999582	-0.318572	-1.092896
N9	1.798301	-0.335478	-1.651236
N10	1.765594	2.490478	-1.933517
C11	-0.890599	3.832978	-1.791671
C12	-2.142382	4.519762	-1.631842
C13	-3.081222	3.570310	-1.356497
C14	-2.389868	2.306087	-1.313997
C15	-2.344031	-0.124474	-0.917373
C16	-3.001549	-1.379277	-0.608773
C17	-2.033451	-2.337510	-0.600357
C18	-0.796157	-1.657971	-0.935426
C19	1.594225	-1.681547	-1.491881
C20	2.807383	-2.402899	-1.760076
C21	3.758599	-1.490448	-2.101934
C22	3.125878	-0.184733	-2.004803
C23	3.107413	2.287844	-2.058977
C24	3.781527	3.552892	-2.237582
C25	2.817922	4.514501	-2.262220
C26	1.555888	3.839023	-2.084816
C27	0.319576	4.459853	-2.058771
H28	0.292628	5.534218	-2.181516
C29	-2.997803	1.087562	-1.040164
H30	-4.071662	1.090697	-0.922955
C31	0.412932	-2.299493	-1.135314
H32	0.458813	-3.367478	-0.980628
C33	3.742495	1.052165	-2.115885
H34	4.815755	1.086238	-2.226390
C35	1.214075	2.208726	2.747373

H36	0.932417	1.387535	3.387162
C37	0.386670	2.500910	1.616064
H38	-0.636542	2.147938	1.661340
C39	0.613554	3.782621	1.010384
H40	-0.129484	4.152716	0.326953
C41	1.743992	4.514588	1.254481
H42	1.944819	5.441647	0.727883
C43	2.617896	4.120982	2.276708
O44	3.681258	4.926248	2.534699
C45	4.406736	4.877973	3.727194
O46	5.256103	5.730664	3.860700
C47	4.029873	3.841212	4.655934
C48	3.083202	2.899146	4.317656
O49	2.820480	1.933498	5.204517
H50	2.028100	1.436025	5.008725
C51	2.326836	3.001005	3.076011
H52	-0.298907	2.696484	-5.519698
H53	-2.268994	5.594046	-1.644728
H54	-4.142823	3.723852	-1.175051
H55	-4.071410	-1.452928	-0.435146
H56	-2.038848	-3.415024	-0.387418
H57	2.866613	-3.488506	-1.761699
H58	4.757704	-1.795690	-2.420623
H59	4.860066	3.640382	-2.316369
H60	2.892156	5.581432	-2.422411
H61	4.273583	4.015138	5.729493

Warfarin 6-5 Reactant Complex Doublet

C1	-0.948323	2.080025	-4.925399
H2	-1.670769	1.571698	-5.575570
H3	-1.528128	2.622586	-4.179422
S4	0.024950	0.748849	-4.137106
O5	0.654334	1.147803	-0.072497
Fe6	0.306204	1.043490	-1.671840
N7	-1.113692	2.467776	-1.686040
N8	-1.113067	-0.352953	-1.349248
N9	1.698397	-0.399279	-1.956548
N10	1.695717	2.437608	-2.169979
C11	-0.923428	3.814890	-1.832896
C12	-2.159202	4.525462	-1.648860
C13	-3.117305	3.586086	-1.415010
C14	-2.452268	2.304928	-1.438795
C15	-2.443274	-0.146907	-1.134704
C16	-3.098276	-1.388640	-0.772970
C17	-2.126562	-2.344455	-0.735586
C18	-0.898767	-1.678885	-1.127740
C19	1.506475	-1.722885	-1.702747
C20	2.735506	-2.449592	-1.871884
C21	3.691882	-1.547500	-2.228001
C22	3.038071	-0.247043	-2.235530
C23	3.043578	2.234607	-2.276621
C24	3.733605	3.503212	-2.380398
C25	2.778607	4.473401	-2.362457
C26	1.513510	3.796089	-2.218553
C27	0.292497	4.433511	-2.090724
H28	0.287216	5.514909	-2.154543
C29	-3.077642	1.086178	-1.203422
H30	-4.144801	1.111668	-1.028088
C31	0.320780	-2.317787	-1.291324

H32	0.377911	-3.368646	-1.045307
C33	3.664762	0.991534	-2.322358
H34	4.744189	1.015608	-2.366923
C35	1.039180	2.487104	3.276995
H36	0.640845	1.761747	3.980495
C37	0.257807	2.881078	2.207397
H38	-0.709568	2.428443	2.041515
C39	0.741484	3.825460	1.290498
H40	0.121771	4.115969	0.454766
C41	1.999235	4.384847	1.446705
H42	2.389389	5.115563	0.746700
C43	2.765861	4.020016	2.553450
O44	3.956141	4.662435	2.739504
C45	4.585636	4.718468	3.980405
O46	5.483796	5.522421	4.079498
C47	4.088827	3.814813	4.996822
C48	3.076950	2.927961	4.699393
O49	2.732762	2.035752	5.629999
H50	1.962930	1.518312	5.398244
C51	2.310887	3.067966	3.476729
H52	-0.443195	2.831498	-5.576419
H53	-2.251748	5.603364	-1.665186
H54	-4.174212	3.748628	-1.226461
H55	-4.166035	-1.469206	-0.594605
H56	-2.128972	-3.403216	-0.457435
H57	2.808422	-3.527745	-1.783263
H58	4.708423	-1.846596	-2.482144
H59	4.812913	3.610257	-2.425618
H60	2.859895	5.550330	-2.473677
H61	4.200197	4.117116	6.062504

Warfarin 6-5 Reactant Complex Quartet

C1	-0.940828	2.079858	-4.919410
H2	-1.662708	1.563969	-5.565080
H3	-1.520424	2.620599	-4.172589
S4	0.041333	0.760028	-4.127718
O5	0.635634	1.101325	-0.064350
Fe6	0.315221	1.041374	-1.665405
N7	-1.109076	2.469741	-1.678325
N8	-1.112510	-0.354293	-1.353682
N9	1.702887	-0.395440	-1.953782
N10	1.697957	2.440497	-2.152289
C11	-0.923229	3.815406	-1.830975
C12	-2.160548	4.524917	-1.650651
C13	-3.117101	3.584886	-1.415799
C14	-2.449985	2.304081	-1.435059
C15	-2.439741	-0.147084	-1.131586
C16	-3.092947	-1.387225	-0.760695
C17	-2.121460	-2.342644	-0.723931
C18	-0.895082	-1.678848	-1.124504
C19	1.509265	-1.718873	-1.699113
C20	2.740450	-2.443204	-1.860986
C21	3.697022	-1.542706	-2.213198
C22	3.045255	-0.241248	-2.223418
C23	3.044820	2.239430	-2.261390
C24	3.733012	3.508599	-2.370257
C25	2.777252	4.478248	-2.356131
C26	1.512755	3.800361	-2.209740
C27	0.291877	4.436989	-2.090841

H28	0.283525	5.516995	-2.160278
C29	-3.074917	1.087603	-1.201343
H30	-4.140762	1.114571	-1.021435
C31	0.323808	-2.314847	-1.288297
H32	0.385244	-3.363228	-1.032480
C33	3.669621	0.997675	-2.306029
H34	4.748993	1.027600	-2.343614
C35	1.045871	2.471353	3.250749
H36	0.661368	1.725681	3.939813
C37	0.261428	2.872103	2.187206
H38	-0.697970	2.406050	2.009999
C39	0.742839	3.820781	1.273941
H40	0.126891	4.107533	0.433382
C41	1.996876	4.389943	1.434628
H42	2.383952	5.124304	0.740251
C43	2.760122	4.026858	2.544121
O44	3.949190	4.673241	2.734128
C45	4.583831	4.717219	3.972573
O46	5.481658	5.520180	4.076122
C47	4.088914	3.806094	4.981765
C48	3.074531	2.920814	4.680450
O49	2.732324	2.023682	5.606196
H50	1.950296	1.521842	5.381525
C51	2.310573	3.066486	3.459907
H52	-0.441294	2.830602	-5.575372
H53	-2.253646	5.603502	-1.665774
H54	-4.174742	3.746243	-1.225963
H55	-4.161481	-1.469004	-0.583922
H56	-2.121763	-3.402170	-0.448099
H57	2.810497	-3.522505	-1.781365
H58	4.711312	-1.843561	-2.472272
H59	4.812387	3.615147	-2.418938
H60	2.858590	5.555393	-2.471902
H61	4.201551	4.101420	6.047856

Warfarin 6-5 Transition State Doublet

C1	-0.906413	2.062874	-4.808980
H2	-1.606709	1.480752	-5.420084
H3	-1.507205	2.627010	-4.095499
S4	0.121073	0.815766	-3.927560
O5	0.801395	1.227102	0.289520
Fe6	0.357324	1.151562	-1.424381
N7	-1.070951	2.537835	-1.503192
N8	-1.057099	-0.278849	-1.112976
N9	1.752446	-0.323695	-1.698314
N10	1.709122	2.518973	-1.980663
C11	-0.918972	3.872629	-1.780807
C12	-2.171799	4.561013	-1.650826
C13	-3.111517	3.617765	-1.368452
C14	-2.419485	2.354962	-1.290082
C15	-2.397856	-0.091252	-0.948755
C16	-3.062885	-1.349552	-0.666597
C17	-2.090152	-2.305332	-0.643334
C18	-0.852187	-1.619885	-0.962487
C19	1.551212	-1.657072	-1.518303
C20	2.762382	-2.392324	-1.773232
C21	3.715686	-1.484028	-2.126814
C22	3.073998	-0.176444	-2.046252
C23	3.053914	2.305922	-2.115084

C24	3.737100	3.564149	-2.304990
C25	2.781033	4.534739	-2.330448
C26	1.517356	3.870316	-2.142288
C27	0.283899	4.494904	-2.094673
H28	0.254345	5.566369	-2.246150
C29	-3.037580	1.136977	-1.043696
H30	-4.112866	1.150270	-0.928187
C31	0.358119	-2.263749	-1.153606
H32	0.394512	-3.331298	-0.991986
C33	3.685169	1.065905	-2.164405
H34	4.758791	1.102479	-2.278932
C35	1.199567	2.173619	2.774159
H36	0.830737	1.391628	3.424143
C37	0.472188	2.459125	1.566931
H38	-0.579518	2.189382	1.562051
C39	0.826966	3.688385	0.923068
H40	0.160974	4.071010	0.173278
C41	1.977533	4.372712	1.221883
H42	2.265843	5.263227	0.673317
C43	2.744348	3.978303	2.322019
O44	3.845167	4.715444	2.606907
C45	4.484669	4.694370	3.847389
O46	5.383968	5.488188	3.986497
C47	3.964798	3.753837	4.818073
C48	2.984876	2.851873	4.463734
O49	2.599065	1.965954	5.384204
H50	1.799032	1.491521	5.161859
C51	2.323718	2.921968	3.158763
H52	-0.438078	2.800147	-5.517062
H53	-2.269075	5.634742	-1.676986
H54	-4.176124	3.760660	-1.207391
H55	-4.137669	-1.447476	-0.539405
H56	-2.098271	-3.377973	-0.411997
H57	2.822005	-3.476964	-1.757696
H58	4.713716	-1.793789	-2.441406
H59	4.815465	3.652500	-2.386490
H60	2.865158	5.603551	-2.469637
H61	4.119420	4.016940	5.898725

Warfarin 6-5 Transition State Quartet

C1	-0.921001	2.073839	-4.802320
H2	-1.616076	1.489158	-5.415654
H3	-1.527912	2.636059	-4.091914
S4	0.107867	0.835585	-3.915946
O5	0.688260	1.330635	0.245762
Fe6	0.372518	1.113659	-1.452531
N7	-1.076263	2.520048	-1.555016
N8	-1.049332	-0.295101	-1.131506
N9	1.742050	-0.324016	-1.712718
N10	1.732765	2.504436	-1.979220
C11	-0.910356	3.857171	-1.807158
C12	-2.159471	4.549778	-1.659075
C13	-3.102457	3.607584	-1.377677
C14	-2.416780	2.341090	-1.321373
C15	-2.394372	-0.096613	-0.965790
C16	-3.058513	-1.353681	-0.673350
C17	-2.090472	-2.310570	-0.646006
C18	-0.849056	-1.635019	-0.970393
C19	1.539611	-1.665920	-1.525091

C20	2.754288	-2.390797	-1.774608
C21	3.706224	-1.483626	-2.131201
C22	3.073404	-0.176068	-2.059431
C23	3.072120	2.297132	-2.114254
C24	3.750276	3.560784	-2.300090
C25	2.790127	4.524413	-2.324871
C26	1.527698	3.852222	-2.139744
C27	0.295291	4.478822	-2.107569
H28	0.271167	5.550550	-2.256043
C29	-3.036201	1.124540	-1.062263
H30	-4.108072	1.140305	-0.927856
C31	0.359656	-2.278964	-1.155827
H32	0.403627	-3.343922	-0.982111
C33	3.698031	1.055903	-2.173983
H34	4.772264	1.080806	-2.284832
C35	1.200391	2.189112	2.773665
H36	0.832380	1.402813	3.417969
C37	0.450166	2.500126	1.588035
H38	-0.597231	2.227998	1.597951
C39	0.811793	3.736399	0.948805
H40	0.143715	4.120195	0.200639
C41	1.972514	4.397790	1.235917
H42	2.270284	5.284329	0.687476
C43	2.752317	3.987720	2.325915
O44	3.860827	4.714900	2.606040
C45	4.499716	4.690869	3.848624
O46	5.399925	5.483422	3.988397
C47	3.975562	3.753681	4.817088
C48	2.989628	2.854434	4.459178
O49	2.592878	1.976693	5.380682
H50	1.789383	1.507296	5.152389
C51	2.332298	2.927569	3.154605
H52	-0.443985	2.809834	-5.507384
H53	-2.260974	5.624987	-1.679746
H54	-4.167201	3.755695	-1.210188
H55	-4.134191	-1.449535	-0.546571
H56	-2.099082	-3.383341	-0.412187
H57	2.816167	-3.475921	-1.754406
H58	4.703650	-1.797788	-2.440473
H59	4.827550	3.652546	-2.386019
H60	2.866959	5.595809	-2.463767
H61	4.124977	4.017793	5.899152

Warfarin 6-6 Reactant Complex Doublet

C1	-0.962989	2.044764	-4.822785
H2	-1.746223	1.545463	-5.404638
H3	-1.468042	2.634821	-4.060098
S4	0.029322	0.714761	-4.062691
O5	0.687144	1.067908	-0.013728
Fe6	0.328222	1.002249	-1.612336
N7	-1.090945	2.429762	-1.603809
N8	-1.094846	-0.394510	-1.313467
N9	1.715847	-0.435518	-1.928536
N10	1.718283	2.407172	-2.085565
C11	-0.903564	3.775131	-1.753707
C12	-2.140967	4.481484	-1.572245
C13	-3.100412	3.541448	-1.350578
C14	-2.431798	2.262892	-1.369122
C15	-2.423863	-0.190217	-1.096462

C16	-3.083708	-1.435604	-0.767863
C17	-2.117136	-2.397084	-0.760686
C18	-0.887986	-1.726619	-1.136370
C19	1.515879	-1.766437	-1.719047
C20	2.746033	-2.489448	-1.897974
C21	3.708293	-1.580410	-2.214096
C22	3.058045	-0.277390	-2.188721
C23	3.066653	2.207724	-2.165510
C24	3.754993	3.481010	-2.253867
C25	2.796546	4.447975	-2.270676
C26	1.532077	3.765019	-2.143301
C27	0.309727	4.397112	-2.020411
H28	0.301328	5.478189	-2.086255
C29	-3.057590	1.044701	-1.149818
H30	-4.125513	1.070256	-0.984331
C31	0.327493	-2.368221	-1.331590
H32	0.377419	-3.427892	-1.123949
C33	3.685697	0.962324	-2.226507
H34	4.765504	0.983605	-2.252341
C35	1.035188	2.433582	3.143000
H36	0.675957	1.653422	3.804561
C37	0.191685	2.912584	2.159389
H38	-0.787920	2.480685	2.028278
C39	0.631558	3.916713	1.286564
H40	-0.041418	4.288000	0.527662
C41	1.912662	4.432783	1.385831
H42	2.274430	5.199513	0.710267
C43	2.745712	3.976057	2.407153
O44	3.967282	4.560840	2.533382
C45	4.732994	4.480535	3.701133
O46	5.711541	5.185937	3.740709
C47	4.242321	3.569815	4.717678
C48	3.152245	2.769574	4.472228
O49	2.806195	1.867796	5.398443
H50	1.931788	1.508262	5.265065
C51	2.322273	2.987040	3.304791
H52	-0.470562	2.747277	-5.527843
H53	-2.242942	5.555959	-1.590697
H54	-4.162127	3.707554	-1.190211
H55	-4.151274	-1.511395	-0.589910
H56	-2.124330	-3.462593	-0.516674
H57	2.820631	-3.567998	-1.826156
H58	4.729457	-1.880666	-2.453672
H59	4.833166	3.605049	-2.266322
H60	2.880327	5.526275	-2.405741
H61	4.483653	3.792173	5.778287

Warfarin 6-6 Reactant Complex Quartet

C1	-0.955526	2.047253	-4.818034
H2	-1.736669	1.541173	-5.397801
H3	-1.462346	2.635062	-4.055402
S4	0.042520	0.725034	-4.056952
O5	0.655338	1.042495	-0.009333
Fe6	0.333763	1.000650	-1.608794
N7	-1.089310	2.431692	-1.602603
N8	-1.098167	-0.396477	-1.320525
N9	1.716691	-0.433740	-1.923554
N10	1.719048	2.405769	-2.073981
C11	-0.905004	3.775093	-1.753988

C12	-2.142159	4.481526	-1.574400
C13	-3.101234	3.541647	-1.352787
C14	-2.432121	2.263264	-1.369858
C15	-2.424245	-0.189914	-1.101013
C16	-3.084815	-1.434559	-0.767487
C17	-2.119727	-2.395929	-0.757174
C18	-0.889349	-1.728141	-1.135715
C19	1.515159	-1.763239	-1.715131
C20	2.744015	-2.487415	-1.892465
C21	3.707885	-1.580274	-2.205225
C22	3.061573	-0.276137	-2.178940
C23	3.066001	2.207880	-2.155764
C24	3.752845	3.480890	-2.250788
C25	2.794592	4.447235	-2.270500
C26	1.530122	3.765783	-2.139526
C27	0.309875	4.397847	-2.022981
H28	0.299096	5.478550	-2.095142
C29	-3.057831	1.046340	-1.154572
H30	-4.125630	1.072872	-0.988673
C31	0.324741	-2.366869	-1.326603
H32	0.379072	-3.424369	-1.111894
C33	3.688535	0.962923	-2.213311
H34	4.768529	0.987324	-2.236891
C35	1.043192	2.428389	3.138044
H36	0.689139	1.640230	3.792018
C37	0.199128	2.908071	2.155044
H38	-0.773360	2.465224	2.013532
C39	0.641967	3.907436	1.277922
H40	-0.027359	4.269124	0.510788
C41	1.920814	4.426279	1.378942
H42	2.282667	5.190928	0.702532
C43	2.751897	3.975915	2.406198
O44	3.970193	4.564287	2.536811
C45	4.736356	4.480996	3.704195
O46	5.717224	5.182562	3.744426
C47	4.241703	3.570069	4.720301
C48	3.155272	2.770505	4.472528
O49	2.806432	1.866275	5.396462
H50	1.929372	1.511612	5.261277
C51	2.327489	2.986315	3.303974
H52	-0.467541	2.749129	-5.526642
H53	-2.243692	5.556333	-1.591573
H54	-4.163047	3.706996	-1.190739
H55	-4.152799	-1.510085	-0.588142
H56	-2.128397	-3.462106	-0.511839
H57	2.816705	-3.567178	-1.824730
H58	4.727028	-1.883819	-2.446612
H59	4.831185	3.603209	-2.265671
H60	2.878900	5.525275	-2.406991
H61	4.481652	3.793577	5.781216

Warfarin 6-6 Transition State Doublet

C1	-0.932331	2.022873	-4.717774
H2	-1.695327	1.459208	-5.265472
H3	-1.457381	2.631657	-3.983742
S4	0.113196	0.766782	-3.879226
O5	0.826750	1.165649	0.273388
Fe6	0.357083	1.109963	-1.437276
N7	-1.064940	2.501432	-1.470674

N8	-1.055766	-0.319244	-1.115110
N9	1.756051	-0.361848	-1.701906
N10	1.717057	2.489425	-1.949599
C11	-0.911142	3.838140	-1.736890
C12	-2.160111	4.525813	-1.582802
C13	-3.102506	3.581876	-1.308883
C14	-2.412451	2.318285	-1.249354
C15	-2.393888	-0.131130	-0.940353
C16	-3.060490	-1.391507	-0.679205
C17	-2.091191	-2.350685	-0.680427
C18	-0.853410	-1.662067	-0.992751
C19	1.549526	-1.696718	-1.550180
C20	2.764277	-2.428869	-1.801238
C21	3.724044	-1.517075	-2.118834
C22	3.082401	-0.208865	-2.024138
C23	3.063741	2.277921	-2.046928
C24	3.749681	3.541298	-2.204332
C25	2.792500	4.509938	-2.257425
C26	1.525357	3.841029	-2.103329
C27	0.290258	4.462965	-2.056830
H28	0.260344	5.535798	-2.197526
C29	-3.031404	1.100216	-1.013531
H30	-4.105238	1.116954	-0.888991
C31	0.352815	-2.306538	-1.202848
H32	0.385612	-3.377174	-1.065512
C33	3.694460	1.036992	-2.101956
H34	4.769759	1.071342	-2.191963
C35	1.232150	2.073282	2.706778
H36	0.916391	1.254941	3.335969
C37	0.448596	2.387170	1.540525
H38	-0.595510	2.094214	1.558821
C39	0.748004	3.654200	0.936736
H40	0.036774	4.062212	0.243718
C41	1.906706	4.339293	1.199507
H42	2.163436	5.249365	0.670415
C43	2.743209	3.898938	2.229927
O44	3.873162	4.600198	2.460393
C45	4.640332	4.480288	3.632643
O46	5.597288	5.202759	3.703585
C47	4.143258	3.535876	4.613622
C48	3.099379	2.695558	4.313347
O49	2.718834	1.803472	5.232928
H50	1.850637	1.440135	5.067708
C51	2.364188	2.816135	3.054842
H52	-0.473264	2.713966	-5.468695
H53	-2.264969	5.595025	-1.607568
H54	-4.169450	3.731008	-1.167202
H55	-4.133782	-1.486326	-0.551130
H56	-2.099403	-3.427557	-0.476745
H57	2.826030	-3.513885	-1.795581
H58	4.727941	-1.830882	-2.409793
H59	4.829498	3.644574	-2.247729
H60	2.883698	5.579127	-2.409948
H61	4.398310	3.738982	5.682686

Warfarin 6-6 Transition State Quartet

C1	-0.952702	2.016462	-4.724095
H2	-1.705857	1.443092	-5.273583
H3	-1.488258	2.622282	-3.994630

S4	0.107099	0.781516	-3.876841
O5	0.685575	1.275442	0.250481
Fe6	0.380448	1.065764	-1.455903
N7	-1.068370	2.471324	-1.528659
N8	-1.038075	-0.346074	-1.139363
N9	1.753701	-0.365730	-1.719799
N10	1.744664	2.469619	-1.937932
C11	-0.900230	3.811716	-1.759234
C12	-2.146856	4.500948	-1.592699
C13	-3.093184	3.555916	-1.329690
C14	-2.408377	2.289568	-1.293589
C15	-2.382097	-0.147809	-0.964191
C16	-3.045294	-1.407038	-0.688773
C17	-2.080171	-2.366934	-0.685995
C18	-0.838122	-1.688797	-1.007871
C19	1.547350	-1.711999	-1.568069
C20	2.765343	-2.429593	-1.819547
C21	3.723120	-1.516333	-2.136876
C22	3.089809	-0.209619	-2.043454
C23	3.086415	2.265463	-2.042905
C24	3.764289	3.534812	-2.198677
C25	2.801347	4.496516	-2.244283
C26	1.537707	3.817433	-2.086616
C27	0.303797	4.439572	-2.050379
H28	0.276709	5.514354	-2.172162
C29	-3.025437	1.071231	-1.044621
H30	-4.096585	1.086662	-0.904119
C31	0.364980	-2.331497	-1.215007
H32	0.406910	-3.401332	-1.069450
C33	3.714343	1.026339	-2.113039
H34	4.789772	1.050921	-2.201710
C35	1.212129	2.099419	2.725607
H36	0.889278	1.282994	3.353746
C37	0.406916	2.438178	1.582232
H38	-0.634144	2.146777	1.619838
C39	0.709575	3.713908	0.983634
H40	-0.005701	4.123386	0.296269
C41	1.878768	4.375162	1.233337
H42	2.140356	5.286538	0.708486
C43	2.731467	3.916769	2.248953
O44	3.864106	4.612785	2.472581
C45	4.638712	4.484822	3.640253
O46	5.598330	5.203279	3.708824
C47	4.143969	3.537557	4.618963
C48	3.099105	2.697715	4.316926
O49	2.724375	1.800289	5.234591
H50	1.854311	1.436828	5.074590
C51	2.357044	2.827222	3.064105
H52	-0.487013	2.707809	-5.471748
H53	-2.254510	5.572311	-1.607087
H54	-4.158930	3.710751	-1.176148
H55	-4.119536	-1.497143	-0.554363
H56	-2.092179	-3.442269	-0.476473
H57	2.831104	-3.514851	-1.808098
H58	4.729037	-1.830610	-2.422579
H59	4.842425	3.642527	-2.249270
H60	2.886705	5.567826	-2.399706
H61	4.400807	3.737319	5.688315

Warfarin 6-7 Reactant Complex Doublet

C1	-0.857302	2.027099	-4.796507
H2	-1.587665	1.474683	-5.394570
H3	-1.414926	2.599924	-4.058684
S4	0.163651	0.752849	-3.987929
O5	0.667834	1.089308	0.060874
Fe6	0.336131	1.035744	-1.541013
N7	-1.098738	2.451134	-1.568739
N8	-1.081981	-0.367527	-1.251223
N9	1.741336	-0.392627	-1.826370
N10	1.719666	2.447560	-1.997220
C11	-0.921347	3.796387	-1.735276
C12	-2.164449	4.498904	-1.569986
C13	-3.116762	3.556402	-1.334348
C14	-2.440576	2.280755	-1.333035
C15	-2.409146	-0.167163	-1.027149
C16	-3.064011	-1.412131	-0.686866
C17	-2.094905	-2.369493	-0.671966
C18	-0.867725	-1.697751	-1.058391
C19	1.540044	-1.723520	-1.631608
C20	2.770305	-2.443851	-1.813673
C21	3.735846	-1.531968	-2.116260
C22	3.085043	-0.229126	-2.075951
C23	3.070104	2.255944	-2.072952
C24	3.746684	3.532605	-2.191728
C25	2.780418	4.490655	-2.230174
C26	1.520867	3.801787	-2.086356
C27	0.291343	4.423941	-1.988741
H28	0.270919	5.504285	-2.066038
C29	-3.054850	1.061770	-1.090183
H30	-4.122300	1.074608	-0.911991
C31	0.349389	-2.331313	-1.249686
H32	0.404967	-3.390319	-1.038008
C33	3.701594	1.017596	-2.113433
H34	4.781661	1.054416	-2.126633
C35	0.938039	2.481373	3.281022
H36	0.595209	1.710702	3.966670
C37	0.106821	2.889253	2.258133
H38	-0.839349	2.396605	2.097985
C39	0.535233	3.865255	1.348563
H40	-0.126999	4.168658	0.549481
C41	1.788437	4.439786	1.460382
H42	2.139796	5.192892	0.762884
C43	2.608024	4.061251	2.523381
O44	3.800875	4.706819	2.660995
C45	4.542538	4.678772	3.841118
O46	5.467909	5.458484	3.899556
C47	4.109182	3.730669	4.841608
C48	3.043383	2.890326	4.602361
O49	2.751675	1.962104	5.514827
H50	1.894876	1.555329	5.388439
C51	2.202514	3.084041	3.442975
H52	-0.394696	2.738453	-5.510690
H53	-2.267223	5.576315	-1.582487
H54	-4.179557	3.715662	-1.168543
H55	-4.137157	-1.473542	-0.534037
H56	-2.097042	-3.435704	-0.422756
H57	2.838923	-3.523130	-1.750126
H58	4.756311	-1.831182	-2.365125
H59	4.824357	3.660782	-2.214031

H60	2.853722	5.564681	-2.395786
H61	4.377369	3.921452	5.896249

Warfarin 6-7 Reactant Complex Quartet

C1	-0.854470	2.030912	-4.799709
H2	-1.585863	1.473589	-5.393820
H3	-1.411735	2.603256	-4.061096
S4	0.174993	0.763427	-3.993763
O5	0.625780	1.085858	0.068075
Fe6	0.344330	1.030205	-1.536927
N7	-1.096266	2.446198	-1.572767
N8	-1.080049	-0.375678	-1.262502
N9	1.745413	-0.396641	-1.824848
N10	1.724528	2.439877	-1.989950
C11	-0.920223	3.789806	-1.731926
C12	-2.162469	4.492814	-1.565814
C13	-3.115634	3.549415	-1.333801
C14	-2.439473	2.273262	-1.336419
C15	-2.405067	-0.174742	-1.036004
C16	-3.060009	-1.418831	-0.690837
C17	-2.091223	-2.376584	-0.673732
C18	-0.863971	-1.707058	-1.063292
C19	1.543929	-1.727429	-1.634275
C20	2.772666	-2.447822	-1.820192
C21	3.739593	-1.535680	-2.121477
C22	3.090262	-0.232867	-2.077006
C23	3.073082	2.250705	-2.069100
C24	3.747686	3.527886	-2.192097
C25	2.780478	4.485035	-2.229672
C26	1.522399	3.795696	-2.081658
C27	0.294856	4.419117	-1.983884
H28	0.275690	5.498497	-2.061471
C29	-3.053206	1.054921	-1.098569
H30	-4.120475	1.066034	-0.921341
C31	0.352722	-2.337435	-1.251829
H32	0.410842	-3.395654	-1.037836
C33	3.708001	1.011736	-2.110709
H34	4.786974	1.047658	-2.125093
C35	0.936649	2.485903	3.292607
H36	0.590399	1.719074	3.978393
C37	0.104463	2.893565	2.268970
H38	-0.843657	2.406513	2.113066
C39	0.533740	3.867860	1.356692
H40	-0.129996	4.172965	0.560254
C41	1.790479	4.438040	1.464360
H42	2.139533	5.187946	0.766066
C43	2.611396	4.057419	2.527397
O44	3.803785	4.702756	2.663513
C45	4.544470	4.677328	3.844876
O46	5.472576	5.458565	3.899606
C47	4.111214	3.732086	4.847854
C48	3.048772	2.893996	4.611976
O49	2.754463	1.967763	5.526813
H50	1.904487	1.551308	5.393572
C51	2.203853	3.083113	3.450286
H52	-0.393470	2.741401	-5.515852
H53	-2.265869	5.570294	-1.578052
H54	-4.178105	3.708394	-1.170142
H55	-4.133078	-1.478561	-0.535397

H56	-2.093898	-3.441292	-0.420892
H57	2.841908	-3.527780	-1.755957
H58	4.761429	-1.834125	-2.369650
H59	4.824939	3.656921	-2.216514
H60	2.853276	5.558934	-2.395577
H61	4.385300	3.925208	5.904241

Warfarin 6-7 Transition State Doublet

C1	-0.827811	2.005529	-4.687505
H2	-1.539903	1.394193	-5.248292
H3	-1.402735	2.592201	-3.973760
S4	0.244513	0.799363	-3.813043
O5	0.795799	1.207959	0.357051
Fe6	0.366200	1.142254	-1.367374
N7	-1.073941	2.518724	-1.447577
N8	-1.042243	-0.294933	-1.058727
N9	1.781758	-0.321749	-1.599425
N10	1.721567	2.526855	-1.865597
C11	-0.927279	3.854157	-1.726045
C12	-2.181938	4.538667	-1.584196
C13	-3.117863	3.592639	-1.297805
C14	-2.421504	2.332355	-1.222900
C15	-2.380022	-0.111017	-0.881417
C16	-3.043483	-1.370435	-0.609291
C17	-2.072515	-2.327214	-0.603643
C18	-0.835420	-1.637387	-0.922757
C19	1.572782	-1.657934	-1.464816
C20	2.787380	-2.385213	-1.724525
C21	3.748636	-1.472767	-2.031137
C22	3.109145	-0.163591	-1.917714
C23	3.070691	2.323443	-1.957806
C24	3.743988	3.589017	-2.146112
C25	2.777672	4.547578	-2.222686
C26	1.516508	3.871612	-2.053116
C27	0.274094	4.483185	-2.032625
H28	0.236596	5.554331	-2.184105
C29	-3.030086	1.114140	-0.962945
H30	-4.102690	1.114810	-0.822244
C31	0.374859	-2.274157	-1.127823
H32	0.413503	-3.345397	-0.991029
C33	3.712560	1.087456	-1.995671
H34	4.788591	1.132456	-2.075870
C35	1.155392	2.145804	2.797981
H36	0.853844	1.322629	3.431312
C37	0.383428	2.423881	1.617402
H38	-0.655128	2.108663	1.630521
C39	0.671717	3.679632	0.984955
H40	-0.030727	4.057067	0.268034
C41	1.817495	4.387652	1.248133
H42	2.075382	5.277405	0.687378
C43	2.631205	3.997630	2.315044
O44	3.734466	4.736347	2.561148
C45	4.469099	4.661573	3.753103
O46	5.383913	5.443669	3.845046
C47	4.007195	3.693598	4.723031
C48	2.983922	2.826105	4.422642
O49	2.626723	1.923341	5.335246
H50	1.760715	1.540786	5.183715
C51	2.258450	2.922775	3.156664

H52	-0.393285	2.710489	-5.441536
H53	-2.288200	5.610679	-1.602073
H54	-4.186140	3.733176	-1.156176
H55	-4.121101	-1.451557	-0.504158
H56	-2.079845	-3.404726	-0.393792
H57	2.845065	-3.471744	-1.723275
H58	4.751620	-1.785451	-2.336067
H59	4.822641	3.695905	-2.200820
H60	2.856726	5.611888	-2.404152
H61	4.284880	3.874892	5.788937

Warfarin 6-7 Transition State Quartet

C1	-0.849836	1.992298	-4.698712
H2	-1.549691	1.373304	-5.264109
H3	-1.434402	2.574077	-3.987552
S4	0.238821	0.813010	-3.816031
O5	0.664292	1.307846	0.315639
Fe6	0.392468	1.092714	-1.397501
N7	-1.072625	2.485578	-1.508004
N8	-1.024639	-0.325477	-1.087577
N9	1.777680	-0.330647	-1.626234
N10	1.752893	2.504053	-1.856650
C11	-0.912097	3.826223	-1.751475
C12	-2.164385	4.511295	-1.598617
C13	-3.104077	3.562614	-1.321505
C14	-2.412129	2.300661	-1.268019
C15	-2.367330	-0.131832	-0.907024
C16	-3.027538	-1.389425	-0.619586
C17	-2.059683	-2.346717	-0.610882
C18	-0.820846	-1.665990	-0.940735
C19	1.568637	-1.678005	-1.486432
C20	2.787066	-2.391780	-1.742753
C21	3.746736	-1.477229	-2.049412
C22	3.115800	-0.169498	-1.941425
C23	3.096326	2.306113	-1.957372
C24	3.762663	3.577994	-2.144739
C25	2.791393	4.529464	-2.211304
C26	1.533629	3.844525	-2.037971
C27	0.291928	4.457111	-2.030008
H28	0.257781	5.529636	-2.168302
C29	-3.021837	1.083942	-0.995863
H30	-4.091513	1.086315	-0.844188
C31	0.386992	-2.303035	-1.142059
H32	0.433882	-3.371772	-0.992807
C33	3.732545	1.070903	-2.010065
H34	4.809316	1.106125	-2.089463
C35	1.146618	2.164221	2.790624
H36	0.846449	1.331574	3.412681
C37	0.346015	2.471710	1.634843
H38	-0.687087	2.154994	1.664706
C39	0.631405	3.743434	1.018665
H40	-0.079499	4.125277	0.311729
C41	1.784477	4.431899	1.271396
H42	2.043558	5.324852	0.716248
C43	2.618770	4.019647	2.323302
O44	3.723734	4.755524	2.565658
C45	4.467590	4.664574	3.753221
O46	5.385880	5.442560	3.846387
C47	4.007564	3.690442	4.716809

C48	2.984406	2.823760	4.407175
O49	2.627505	1.911876	5.315258
H50	1.757179	1.542504	5.167190
C51	2.255686	2.932684	3.145423
H52	-0.410098	2.698557	-5.446872
H53	-2.277102	5.585172	-1.606396
H54	-4.171393	3.706624	-1.169870
H55	-4.105260	-1.466143	-0.506346
H56	-2.065727	-3.423284	-0.394864
H57	2.849631	-3.478303	-1.735284
H58	4.750752	-1.794752	-2.347559
H59	4.840092	3.689482	-2.205056
H60	2.863005	5.597289	-2.394063
H61	4.282634	3.868345	5.784507

Warfarin 6-8 Reactant Complex Doublet

C1	-0.850671	1.742477	-4.815863
H2	-1.514482	1.162375	-5.467361
H3	-1.473371	2.249371	-4.080818
S4	0.236939	0.533298	-4.005970
O5	0.686677	1.057025	0.016685
Fe6	0.358052	0.962905	-1.585965
N7	-1.083221	2.381341	-1.630468
N8	-1.067699	-0.430158	-1.275025
N9	1.763723	-0.456252	-1.839369
N10	1.740111	2.375297	-2.071821
C11	-0.898666	3.728783	-1.777056
C12	-2.136723	4.435221	-1.598800
C13	-3.093859	3.494507	-1.372217
C14	-2.423389	2.216713	-1.388863
C15	-2.398418	-0.227902	-1.058859
C16	-3.052405	-1.473625	-0.711726
C17	-2.085402	-2.431377	-0.706614
C18	-0.855840	-1.760170	-1.089884
C19	1.557059	-1.787005	-1.656073
C20	2.780008	-2.511107	-1.867091
C21	3.743733	-1.602302	-2.181747
C22	3.100934	-0.297221	-2.123663
C23	3.090416	2.185814	-2.161103
C24	3.763443	3.462668	-2.294065
C25	2.795436	4.420082	-2.320749
C26	1.539509	3.729666	-2.158286
C27	0.313680	4.354322	-2.035421
H28	0.297849	5.434865	-2.097200
C29	-3.043479	0.996605	-1.147239
H30	-4.114898	1.011856	-1.001176
C31	0.362356	-2.394216	-1.284956
H32	0.412775	-3.458377	-1.096876
C33	3.721152	0.946462	-2.192191
H34	4.800722	0.977424	-2.236955
C35	1.158317	2.389245	3.181081
H36	0.815858	1.603510	3.843183
C37	0.290784	2.879504	2.225026
H38	-0.695687	2.451386	2.123434
C39	0.720933	3.856943	1.318203
H40	0.037896	4.211700	0.557974
C41	2.010395	4.359415	1.378048
H42	2.366278	5.107582	0.679975
C43	2.858902	3.915069	2.393181

O44	4.081201	4.508488	2.500528
C45	4.819513	4.486962	3.681691
O46	5.756023	5.255108	3.727168
C47	4.364661	3.571546	4.706999
C48	3.298772	2.734948	4.467227
O49	2.981376	1.830622	5.400925
H50	2.119268	1.439392	5.276144
C51	2.453327	2.935376	3.308423
H52	-0.389718	2.507733	-5.461651
H53	-2.241768	5.511048	-1.623570
H54	-4.151982	3.665853	-1.191809
H55	-4.117545	-1.536518	-0.501525
H56	-2.089739	-3.496221	-0.457785
H57	2.838383	-3.589888	-1.830051
H58	4.758380	-1.900613	-2.455215
H59	4.841184	3.589982	-2.324032
H60	2.870552	5.496655	-2.472528
H61	4.568437	3.838347	5.768527

Warfarin 6-8 Reactant Complex Quartet

C1	-0.844532	1.746815	-4.816094
H2	-1.505864	1.162589	-5.467575
H3	-1.469129	2.250789	-4.080674
S4	0.245942	0.540608	-4.009205
O5	0.638594	1.053348	0.023198
Fe6	0.362527	0.961132	-1.583909
N7	-1.082102	2.380027	-1.636078
N8	-1.068797	-0.435249	-1.288298
N9	1.764358	-0.457274	-1.840333
N10	1.742063	2.371275	-2.064938
C11	-0.897723	3.725926	-1.777516
C12	-2.135045	4.432747	-1.599563
C13	-3.093384	3.491924	-1.375510
C14	-2.423378	2.213050	-1.394285
C15	-2.397488	-0.232300	-1.069371
C16	-3.051814	-1.476090	-0.715575
C17	-2.083679	-2.435417	-0.708132
C18	-0.855200	-1.765121	-1.095693
C19	1.556403	-1.787596	-1.660385
C20	2.778956	-2.512472	-1.870388
C21	3.744506	-1.602675	-2.183935
C22	3.102264	-0.298731	-2.123570
C23	3.090764	2.182406	-2.156327
C24	3.763440	3.458362	-2.294414
C25	2.795940	4.416238	-2.322776
C26	1.540372	3.726713	-2.155942
C27	0.315730	4.352890	-2.034541
H28	0.300039	5.432400	-2.098890
C29	-3.042887	0.993804	-1.156685
H30	-4.114247	1.007864	-1.008682
C31	0.363130	-2.397087	-1.287988
H32	0.417525	-3.459557	-1.094277
C33	3.724757	0.943168	-2.185687
H34	4.803419	0.973364	-2.225249
C35	1.160953	2.392972	3.188838
H36	0.815793	1.612414	3.855363
C37	0.291161	2.883945	2.233906
H38	-0.698870	2.464004	2.141968
C39	0.721973	3.857510	1.322692

H40	0.037527	4.214089	0.564327
C41	2.012591	4.357901	1.379924
H42	2.368589	5.102940	0.678656
C43	2.861102	3.916486	2.396342
O44	4.081561	4.513189	2.504345
C45	4.822780	4.489614	3.683952
O46	5.759537	5.256456	3.728218
C47	4.369305	3.574007	4.709676
C48	3.304177	2.736037	4.471720
O49	2.988207	1.831194	5.404563
H50	2.123947	1.443329	5.284793
C51	2.457101	2.936027	3.312094
H52	-0.386258	2.511732	-5.463207
H53	-2.238813	5.509261	-1.623952
H54	-4.151197	3.663263	-1.194187
H55	-4.114850	-1.537487	-0.499775
H56	-2.085305	-3.498969	-0.456112
H57	2.838664	-3.589748	-1.828438
H58	4.757840	-1.900158	-2.456590
H59	4.841438	3.582821	-2.325752
H60	2.871604	5.493330	-2.475740
H61	4.573979	3.841661	5.770572

Warfarin 6-8 Transition State Doublet

C1	-0.814901	1.742056	-4.681258
H2	-1.469773	1.101769	-5.282535
H3	-1.442247	2.275151	-3.968755
S4	0.316033	0.606132	-3.803957
O5	0.861688	1.127763	0.306049
Fe6	0.393041	1.073067	-1.405374
N7	-1.049976	2.459289	-1.474569
N8	-1.027648	-0.348763	-1.079006
N9	1.801373	-0.379572	-1.621516
N10	1.741560	2.465742	-1.920535
C11	-0.900517	3.796513	-1.747208
C12	-2.152204	4.484787	-1.602415
C13	-3.091325	3.541203	-1.321153
C14	-2.398680	2.278222	-1.252998
C15	-2.367936	-0.163298	-0.906621
C16	-3.032210	-1.422010	-0.630467
C17	-2.061829	-2.379477	-0.633239
C18	-0.823154	-1.691478	-0.949959
C19	1.586614	-1.714054	-1.491165
C20	2.796611	-2.442522	-1.769407
C21	3.754266	-1.533493	-2.086938
C22	3.123451	-0.222094	-1.960966
C23	3.089192	2.262227	-2.026628
C24	3.759789	3.526911	-2.232620
C25	2.793406	4.485678	-2.302921
C26	1.534743	3.810420	-2.111673
C27	0.296076	4.424359	-2.068955
H28	0.256718	5.495171	-2.220688
C29	-3.014661	1.060806	-1.005374
H30	-4.091159	1.067630	-0.901475
C31	0.387590	-2.327555	-1.158668
H32	0.423556	-3.401412	-1.035531
C33	3.728024	1.025548	-2.056465
H34	4.804032	1.066798	-2.158474
C35	1.327313	2.035814	2.735082

H36	1.009158	1.223025	3.377025
C37	0.523432	2.347303	1.585049
H38	-0.522400	2.062866	1.627937
C39	0.831849	3.590363	0.938632
H40	0.122405	3.983378	0.235847
C41	2.006776	4.261759	1.168855
H42	2.273239	5.147763	0.604533
C43	2.846680	3.837410	2.201012
O44	3.980662	4.542713	2.409313
C45	4.722357	4.477640	3.594253
O46	5.650695	5.247771	3.666504
C47	4.250972	3.539762	4.590273
C48	3.224707	2.669555	4.302521
O49	2.870609	1.783898	5.235034
H50	2.024982	1.369248	5.067055
C51	2.473311	2.770149	3.051205
H52	-0.387117	2.487785	-5.384196
H53	-2.259879	5.556066	-1.638212
H54	-4.157216	3.694397	-1.168256
H55	-4.104429	-1.509150	-0.472970
H56	-2.069305	-3.454778	-0.426167
H57	2.841502	-3.525724	-1.790272
H58	4.747893	-1.840819	-2.418846
H59	4.838338	3.629437	-2.296532
H60	2.874169	5.553457	-2.473462
H61	4.471231	3.789028	5.658956

Warfarin 6-8 Transition State Quartet

C1	-0.830969	1.735995	-4.701335
H2	-1.473733	1.085248	-5.302357
H3	-1.470730	2.263231	-3.992772
S4	0.315066	0.628831	-3.816269
O5	0.683219	1.239101	0.286372
Fe6	0.406138	1.029412	-1.418553
N7	-1.059298	2.431023	-1.544782
N8	-1.020264	-0.374357	-1.104215
N9	1.790244	-0.382765	-1.638674
N10	1.763909	2.447548	-1.906359
C11	-0.894536	3.772244	-1.774582
C12	-2.141782	4.463260	-1.618166
C13	-3.087212	3.517714	-1.351130
C14	-2.400384	2.251601	-1.308849
C15	-2.365544	-0.178887	-0.935332
C16	-3.027712	-1.436232	-0.645085
C17	-2.060390	-2.394575	-0.641891
C18	-0.818728	-1.715178	-0.966256
C19	1.576247	-1.728005	-1.509665
C20	2.788394	-2.444021	-1.787383
C21	3.745112	-1.530307	-2.106509
C22	3.120645	-0.223070	-1.982194
C23	3.105997	2.252203	-2.021309
C24	3.771389	3.520788	-2.225325
C25	2.798679	4.473472	-2.286535
C26	1.544735	3.789033	-2.091407
C27	0.307455	4.404037	-2.060191
H28	0.273098	5.477158	-2.189374
C29	-3.015685	1.035666	-1.047735
H30	-4.090326	1.044640	-0.931910
C31	0.390398	-2.351202	-1.172230

H32	0.433107	-3.423272	-1.039989
C33	3.741080	1.014579	-2.068187
H34	4.815951	1.044793	-2.168939
C35	1.314334	2.060275	2.751174
H36	0.993535	1.248392	3.388836
C37	0.483105	2.406278	1.629916
H38	-0.559130	2.126272	1.698138
C39	0.794908	3.658997	0.995316
H40	0.075665	4.059402	0.303051
C41	1.979166	4.307140	1.210620
H42	2.246260	5.202434	0.662148
C43	2.840676	3.857875	2.223676
O44	3.977196	4.561265	2.426936
C45	4.727046	4.484893	3.605851
O46	5.658049	5.251501	3.678644
C47	4.258954	3.540478	4.597179
C48	3.232250	2.670258	4.303352
O49	2.883044	1.777647	5.234457
H50	2.033736	1.368285	5.075255
C51	2.476045	2.781125	3.056562
H52	-0.397897	2.481622	-5.401019
H53	-2.252405	5.536221	-1.641547
H54	-4.149976	3.677682	-1.181752
H55	-4.100051	-1.518473	-0.480630
H56	-2.070254	-3.468062	-0.426372
H57	2.840063	-3.526344	-1.800350
H58	4.740737	-1.838739	-2.431770
H59	4.848128	3.628631	-2.295294
H60	2.873479	5.543260	-2.460083
H61	4.480195	3.784550	5.668007

Warfarin 6-9 Reactant Complex Doublet

C1	-0.839201	1.954054	-4.803050
H2	-1.621703	1.389701	-5.318923
H3	-1.330171	2.560038	-4.044636
S4	0.239764	0.708370	-4.030290
O5	0.718899	1.052432	0.019745
Fe6	0.370997	1.000481	-1.580555
N7	-1.061337	2.421651	-1.588926
N8	-1.057582	-0.397587	-1.294391
N9	1.765226	-0.426142	-1.875532
N10	1.750741	2.416218	-2.059998
C11	-0.878881	3.769531	-1.727313
C12	-2.122660	4.469663	-1.562969
C13	-3.081317	3.524176	-1.366604
C14	-2.407279	2.249118	-1.380734
C15	-2.389157	-0.197398	-1.087660
C16	-3.044776	-1.438817	-0.733866
C17	-2.074047	-2.394720	-0.707180
C18	-0.843378	-1.725607	-1.088515
C19	1.566123	-1.755195	-1.659502
C20	2.793390	-2.477196	-1.857119
C21	3.748331	-1.568343	-2.198906
C22	3.100649	-0.265077	-2.163184
C23	3.097382	2.219963	-2.185799
C24	3.773729	3.495566	-2.324931
C25	2.812143	4.459730	-2.317782
C26	1.555180	3.773391	-2.132310
C27	0.332071	4.398213	-1.992145

H28	0.313483	5.478568	-2.062528
C29	-3.032541	1.029444	-1.173493
H30	-4.106692	1.044681	-1.045981
C31	0.377651	-2.359205	-1.266282
H32	0.434185	-3.416169	-1.044772
C33	3.722477	0.979034	-2.235747
H34	4.801332	1.008890	-2.289507
C35	1.213227	2.447175	3.078200
H36	0.909485	1.618858	3.705095
C37	0.311978	2.951998	2.160203
H38	-0.663863	2.500795	2.054475
C39	0.697158	3.993929	1.303930
H40	-0.006449	4.366513	0.573784
C41	1.965584	4.548548	1.383233
H42	2.279302	5.351057	0.728255
C43	2.836953	4.093399	2.371399
O44	4.019473	4.756399	2.526645
C45	4.778899	4.673420	3.687083
O46	5.651792	5.508111	3.804271
C47	4.422897	3.626041	4.616351
C48	3.373112	2.779295	4.338462
O49	3.115591	1.787033	5.197152
H50	2.241677	1.411708	5.089779
C51	2.487587	3.036703	3.222454
H52	-0.415919	2.632701	-5.567390
H53	-2.236016	5.544050	-1.576640
H54	-4.145218	3.684930	-1.211631
H55	-4.111764	-1.502304	-0.531395
H56	-2.080040	-3.456843	-0.452632
H57	2.864977	-3.556068	-1.793234
H58	4.759407	-1.868420	-2.474442
H59	4.851418	3.610243	-2.387921
H60	2.887730	5.541398	-2.457485
H61	4.687981	3.778379	5.686713

Warfarin 6-9 Reactant Complex Quartet

C1	-0.834841	1.956606	-4.801791
H2	-1.614978	1.383287	-5.311579
H3	-1.327707	2.563255	-4.044916
S4	0.253055	0.721401	-4.028104
O5	0.673981	1.044189	0.029883
Fe6	0.377131	0.999524	-1.574110
N7	-1.060476	2.421246	-1.593197
N8	-1.056364	-0.402181	-1.301503
N9	1.769458	-0.424789	-1.866235
N10	1.752687	2.414118	-2.049148
C11	-0.878862	3.767693	-1.727631
C12	-2.123358	4.467891	-1.562319
C13	-3.081844	3.520986	-1.367381
C14	-2.407507	2.245810	-1.384524
C15	-2.386207	-0.201090	-1.093930
C16	-3.041886	-1.440962	-0.735425
C17	-2.070904	-2.397091	-0.704900
C18	-0.839790	-1.729546	-1.088373
C19	1.570041	-1.755172	-1.656906
C20	2.797403	-2.475102	-1.861570
C21	3.751969	-1.566029	-2.200844
C22	3.105353	-0.262552	-2.155989
C23	3.098712	2.220200	-2.175426

C24	3.773437	3.495187	-2.320047
C25	2.810296	4.459188	-2.315234
C26	1.554317	3.773140	-2.127366
C27	0.332270	4.397625	-1.990253
H28	0.314625	5.478175	-2.060328
C29	-3.031271	1.026901	-1.181442
H30	-4.105318	1.041026	-1.054361
C31	0.380951	-2.361145	-1.264870
H32	0.438129	-3.418954	-1.046939
C33	3.726030	0.980344	-2.223150
H34	4.805642	1.011225	-2.275617
C35	1.210378	2.449586	3.077928
H36	0.904392	1.621016	3.704531
C37	0.308679	2.960519	2.164390
H38	-0.669097	2.508060	2.057937
C39	0.693900	3.999434	1.307659
H40	-0.009865	4.372841	0.577500
C41	1.963163	4.550026	1.384532
H42	2.278837	5.353174	0.728132
C43	2.836101	4.090608	2.370217
O44	4.021494	4.750628	2.522738
C45	4.779552	4.665702	3.683882
O46	5.652458	5.500719	3.802511
C47	4.424776	3.618393	4.611907
C48	3.372348	2.772338	4.332115
O49	3.113883	1.777581	5.190546
H50	2.239646	1.406485	5.084583
C51	2.486151	3.034735	3.218592
H52	-0.415750	2.632627	-5.570524
H53	-2.236588	5.541951	-1.574894
H54	-4.145182	3.682095	-1.212335
H55	-4.108620	-1.504519	-0.532021
H56	-2.078547	-3.459179	-0.449039
H57	2.868740	-3.555184	-1.797443
H58	4.765455	-1.860281	-2.481450
H59	4.850633	3.608919	-2.387158
H60	2.886503	5.539741	-2.456430
H61	4.688525	3.768167	5.682247

Warfarin 6-9 Transition State Doublet

C1	-0.819416	1.929479	-4.708787
H2	-1.576115	1.312551	-5.202793
H3	-1.337790	2.547576	-3.978649
S4	0.297258	0.748533	-3.866258
O5	0.882959	1.194481	0.279703
Fe6	0.401329	1.114231	-1.415443
N7	-1.035702	2.499851	-1.466330
N8	-1.017459	-0.315404	-1.093441
N9	1.801159	-0.350061	-1.663080
N10	1.746941	2.500823	-1.952885
C11	-0.885375	3.839650	-1.718925
C12	-2.140762	4.520414	-1.576542
C13	-3.081466	3.570526	-1.327916
C14	-2.386054	2.310589	-1.266811
C15	-2.359820	-0.131963	-0.934611
C16	-3.024986	-1.388520	-0.654356
C17	-2.053397	-2.343507	-0.634968
C18	-0.812888	-1.656613	-0.948340
C19	1.594080	-1.684905	-1.504316

C20	2.804986	-2.415555	-1.775754
C21	3.757176	-1.505033	-2.117661
C22	3.120373	-0.195003	-2.011421
C23	3.092934	2.291657	-2.080049
C24	3.768239	3.555297	-2.277066
C25	2.808730	4.522050	-2.311069
C26	1.547564	3.851813	-2.111216
C27	0.312300	4.469104	-2.039584
H28	0.275871	5.542391	-2.175725
C29	-3.004702	1.091681	-1.042013
H30	-4.082739	1.098320	-0.958003
C31	0.399199	-2.295504	-1.148601
H32	0.434492	-3.366645	-1.005566
C33	3.726843	1.053021	-2.117215
H34	4.801302	1.093044	-2.224450
C35	1.406412	2.092794	2.667323
H36	1.137181	1.238447	3.272849
C37	0.561318	2.426375	1.555455
H38	-0.476560	2.118136	1.614061
C39	0.812997	3.709341	0.962331
H40	0.071757	4.112201	0.298665
C41	1.961625	4.422601	1.208341
H42	2.171590	5.354666	0.698276
C43	2.837621	3.986711	2.206865
O44	3.930270	4.753143	2.457248
C45	4.696872	4.644795	3.615788
O46	5.558482	5.485479	3.750606
C47	4.333236	3.584811	4.528104
C48	3.323743	2.704557	4.209918
O49	3.027455	1.741404	5.089879
H50	2.156108	1.365695	4.956658
C51	2.533355	2.855108	2.993301
H52	-0.416135	2.600625	-5.502397
H53	-2.256591	5.589749	-1.595540
H54	-4.151094	3.713439	-1.193215
H55	-4.099370	-1.475291	-0.504708
H56	-2.068188	-3.418494	-0.420853
H57	2.862406	-3.500698	-1.769474
H58	4.750429	-1.814861	-2.445669
H59	4.846502	3.647114	-2.364293
H60	2.891886	5.595222	-2.463736
H61	4.612028	3.731519	5.601242

Warfarin 6-9 Transition State Quartet

C1	-0.829169	1.916697	-4.736699
H2	-1.574563	1.293468	-5.238336
H3	-1.359277	2.526787	-4.006929
S4	0.296651	0.756955	-3.884857
O5	0.725652	1.300079	0.263677
Fe6	0.416600	1.078709	-1.421654
N7	-1.047855	2.470448	-1.535000
N8	-1.011717	-0.338637	-1.117157
N9	1.791449	-0.353332	-1.673961
N10	1.765743	2.480552	-1.942708
C11	-0.882493	3.814453	-1.742959
C12	-2.133023	4.499773	-1.584896
C13	-3.080286	3.547953	-1.350718
C14	-2.391461	2.284079	-1.320435
C15	-2.358622	-0.147540	-0.961928

C16	-3.021867	-1.401505	-0.665525
C17	-2.052164	-2.358221	-0.640911
C18	-0.809631	-1.678113	-0.961935
C19	1.584196	-1.697950	-1.516436
C20	2.797830	-2.418344	-1.788680
C21	3.750358	-1.504782	-2.130642
C22	3.119281	-0.197575	-2.024718
C23	3.106217	2.278918	-2.075663
C24	3.776747	3.546090	-2.270501
C25	2.811891	4.508514	-2.296464
C26	1.554207	3.829847	-2.094683
C27	0.320198	4.447003	-2.029400
H28	0.288401	5.522797	-2.140321
C29	-3.009469	1.065457	-1.082678
H30	-4.086009	1.070697	-0.984453
C31	0.401740	-2.316481	-1.158066
H32	0.444799	-3.386701	-1.009012
C33	3.738365	1.040518	-2.121920
H34	4.812988	1.071167	-2.222268
C35	1.385850	2.123253	2.702483
H36	1.097764	1.288413	3.327345
C37	0.525591	2.473160	1.612433
H38	-0.507859	2.168783	1.694611
C39	0.784819	3.756825	1.020473
H40	0.038291	4.167551	0.363687
C41	1.947314	4.449789	1.247544
H42	2.162609	5.377721	0.734333
C43	2.837091	4.000057	2.233146
O44	3.935337	4.759711	2.475164
C45	4.707297	4.645235	3.629567
O46	5.573926	5.483789	3.764206
C47	4.345887	3.583615	4.539077
C48	3.330494	2.707628	4.223041
O49	3.038416	1.741720	5.100508
H50	2.162960	1.372458	4.976314
C51	2.532420	2.869289	3.012954
H52	-0.424069	2.593342	-5.523975
H53	-2.251249	5.570141	-1.595213
H54	-4.147330	3.697360	-1.203285
H55	-4.095494	-1.485424	-0.508701
H56	-2.066194	-3.430560	-0.419116
H57	2.861251	-3.502803	-1.781060
H58	4.747833	-1.812392	-2.451088
H59	4.853221	3.642078	-2.361327
H60	2.891797	5.582687	-2.451004
H61	4.624838	3.725636	5.613667

Warfarin 6-10 Reactant Complex Doublet

C1	-0.897379	1.800702	-4.850402
H2	-1.628391	1.206120	-5.405012
H3	-1.439945	2.369170	-4.097902
S4	0.224363	0.604047	-4.064198
O5	0.700740	1.036270	-0.022365
Fe6	0.359383	0.957997	-1.622032
N7	-1.075603	2.381976	-1.634610
N8	-1.058196	-0.436711	-1.292821
N9	1.754185	-0.467413	-1.901000
N10	1.734785	2.372742	-2.111088
C11	-0.892804	3.730039	-1.776199

C12	-2.131833	4.434562	-1.592972
C13	-3.086412	3.491453	-1.363498
C14	-2.415349	2.214848	-1.386022
C15	-2.380311	-0.226906	-1.052833
C16	-3.030879	-1.459554	-0.667219
C17	-2.071518	-2.425202	-0.656657
C18	-0.844761	-1.763545	-1.072408
C19	1.554259	-1.796120	-1.685231
C20	2.778036	-2.519934	-1.894251
C21	3.736262	-1.612958	-2.231121
C22	3.089706	-0.308424	-2.191594
C23	3.081808	2.176169	-2.225911
C24	3.759918	3.450401	-2.358666
C25	2.799075	4.416419	-2.355535
C26	1.541241	3.730464	-2.178961
C27	0.318443	4.357732	-2.037131
H28	0.302863	5.438596	-2.098585
C29	-3.029715	0.996361	-1.138078
H30	-4.099084	1.004307	-0.969870
C31	0.371249	-2.397484	-1.269278
H32	0.429757	-3.453757	-1.044156
C33	3.709147	0.936211	-2.266500
H34	4.788558	0.968034	-2.314249
C35	1.155911	2.304136	3.303964
H36	0.796461	1.535388	3.977695
C37	0.335906	2.739037	2.281986
H38	-0.628505	2.278608	2.126510
C39	0.790006	3.706625	1.372631
H40	0.151250	4.008618	0.553908
C41	2.048515	4.271435	1.510004
H42	2.413284	5.022038	0.821098
C43	2.840393	3.888462	2.592299
O44	4.017149	4.555486	2.786188
C45	4.633621	4.612906	4.027881
O46	5.532284	5.427916	4.130398
C47	4.155381	3.696133	5.035836
C48	3.200170	2.751452	4.707803
O49	2.908919	1.820517	5.609957
H50	2.164221	1.268092	5.370188
C51	2.426741	2.897687	3.491395
H52	-0.478780	2.506966	-5.587077
H53	-2.237079	5.511099	-1.618849
H54	-4.142627	3.651127	-1.167287
H55	-4.088963	-1.478471	-0.437733
H56	-2.081043	-3.491885	-0.407443
H57	2.840637	-3.599761	-1.844611
H58	4.751112	-1.910339	-2.497889
H59	4.838074	3.557097	-2.415096
H60	2.874982	5.497695	-2.493182
H61	4.192361	4.008708	6.106235

Warfarin 6-10 Reactant Complex Quartet

C1	-0.894096	1.803671	-4.852562
H2	-1.624676	1.201583	-5.399405
H3	-1.434897	2.374384	-4.100431
S4	0.237721	0.617419	-4.067557
O5	0.654058	1.027055	-0.015384
Fe6	0.365346	0.956162	-1.618544
N7	-1.073812	2.380415	-1.638500

N8	-1.058209	-0.443093	-1.308204
N9	1.756789	-0.467906	-1.900927
N10	1.739617	2.368671	-2.099579
C11	-0.892279	3.727361	-1.776121
C12	-2.131483	4.431427	-1.590878
C13	-3.084917	3.488278	-1.361885
C14	-2.414444	2.210840	-1.388331
C15	-2.378116	-0.232283	-1.064444
C16	-3.028015	-1.464497	-0.674597
C17	-2.068767	-2.430365	-0.664989
C18	-0.842845	-1.770379	-1.084436
C19	1.556775	-1.796738	-1.692628
C20	2.780387	-2.520145	-1.902703
C21	3.739783	-1.610313	-2.235417
C22	3.093582	-0.307249	-2.190567
C23	3.086081	2.175896	-2.213388
C24	3.761204	3.450945	-2.347429
C25	2.798733	4.414914	-2.348491
C26	1.541359	3.728044	-2.172507
C27	0.321226	4.355110	-2.036371
H28	0.305923	5.435512	-2.101803
C29	-3.028015	0.992691	-1.146780
H30	-4.097123	1.000319	-0.978108
C31	0.372810	-2.402700	-1.279609
H32	0.433620	-3.458011	-1.053921
C33	3.715740	0.935013	-2.255381
H34	4.794753	0.966275	-2.297392
C35	1.156914	2.308910	3.297436
H36	0.794690	1.538227	3.971906
C37	0.330444	2.751482	2.282965
H38	-0.639223	2.301139	2.135638
C39	0.786270	3.719761	1.373625
H40	0.141958	4.030502	0.561899
C41	2.046522	4.275194	1.505396
H42	2.414318	5.025821	0.815109
C43	2.841894	3.889095	2.584773
O44	4.017588	4.557286	2.780425
C45	4.631170	4.615084	4.023209
O46	5.525762	5.434605	4.128511
C47	4.154842	3.692753	5.027878
C48	3.203375	2.748184	4.696434
O49	2.912863	1.811318	5.596362
H50	2.163890	1.265845	5.361106
C51	2.426760	2.894405	3.481491
H52	-0.479796	2.506838	-5.594224
H53	-2.237942	5.508128	-1.617725
H54	-4.141264	3.648769	-1.164731
H55	-4.084619	-1.485599	-0.440667
H56	-2.079987	-3.495649	-0.410665
H57	2.844867	-3.598441	-1.851038
H58	4.756707	-1.903080	-2.501021
H59	4.838701	3.561600	-2.405193
H60	2.873012	5.496711	-2.486677
H61	4.190091	4.000638	6.098635

Warfarin 6-10 Transition State Doublet

C1	-0.868807	1.778287	-4.736388
H2	-1.578059	1.119668	-5.244481
H3	-1.430982	2.368969	-4.014611

S4	0.306754	0.670913	-3.874259
O5	0.841186	1.118699	0.308907
Fe6	0.402381	1.066662	-1.398049
N7	-1.040394	2.454798	-1.470972
N8	-1.009839	-0.360591	-1.078811
N9	1.799466	-0.388954	-1.662252
N10	1.741995	2.459203	-1.935099
C11	-0.894092	3.792870	-1.734032
C12	-2.148104	4.477274	-1.593717
C13	-3.085012	3.528957	-1.315809
C14	-2.387736	2.269725	-1.250675
C15	-2.345314	-0.169570	-0.894080
C16	-3.007620	-1.420184	-0.592124
C17	-2.045306	-2.383910	-0.589972
C18	-0.806996	-1.702143	-0.928125
C19	1.591587	-1.725414	-1.516823
C20	2.800269	-2.452116	-1.805279
C21	3.753532	-1.539669	-2.134884
C22	3.119083	-0.231490	-2.012513
C23	3.087753	2.253383	-2.067109
C24	3.759028	3.516825	-2.275514
C25	2.796599	4.481890	-2.316040
C26	1.539694	3.808599	-2.107592
C27	0.303450	4.425104	-2.048552
H28	0.265217	5.496214	-2.195865
C29	-2.997613	1.051034	-1.000373
H30	-4.073461	1.051478	-0.891720
C31	0.401542	-2.338794	-1.146874
H32	0.438630	-3.410239	-1.005453
C33	3.723915	1.017087	-2.110356
H34	4.798061	1.059966	-2.221981
C35	1.283547	2.003952	2.800943
H36	0.932248	1.196481	3.431859
C37	0.528521	2.318929	1.618921
H38	-0.519058	2.040864	1.623270
C39	0.873021	3.557676	0.985200
H40	0.203994	3.946099	0.241684
C41	2.029634	4.237481	1.280068
H42	2.314023	5.130159	0.736500
C43	2.810724	3.825599	2.362780
O44	3.911951	4.568051	2.653364
C45	4.518712	4.566865	3.902484
O46	5.419536	5.373775	4.045097
C47	4.006680	3.625481	4.869364
C48	3.082368	2.669233	4.479914
O49	2.741613	1.745283	5.375135
H50	1.993749	1.207763	5.117503
C51	2.415191	2.747379	3.179545
H52	-0.479672	2.465838	-5.520726
H53	-2.259059	5.548589	-1.630515
H54	-4.147945	3.673145	-1.144796
H55	-4.074872	-1.476854	-0.420037
H56	-2.066095	-3.461220	-0.379271
H57	2.850522	-3.536143	-1.821511
H58	4.752579	-1.843556	-2.456130
H59	4.835508	3.605107	-2.367206
H60	2.876084	5.554080	-2.477887
H61	4.065883	3.913257	5.954799

Warfarin 6-10 Transition State Quartet

C1	-0.880562	1.776194	-4.747095
H2	-1.582078	1.111669	-5.256608
H3	-1.449155	2.363356	-4.026413
S4	0.301605	0.686387	-3.880957
O5	0.722746	1.208821	0.277177
Fe6	0.416536	1.033375	-1.407756
N7	-1.047624	2.434509	-1.524089
N8	-1.002418	-0.376502	-1.093946
N9	1.791661	-0.388906	-1.676555
N10	1.759211	2.444973	-1.932521
C11	-0.890659	3.775649	-1.757212
C12	-2.140877	4.462522	-1.603496
C13	-3.081129	3.513787	-1.332983
C14	-2.388676	2.252302	-1.288648
C15	-2.342624	-0.178504	-0.911527
C16	-3.001716	-1.429157	-0.599504
C17	-2.041600	-2.392361	-0.592751
C18	-0.801666	-1.716451	-0.935733
C19	1.585197	-1.733286	-1.530928
C20	2.794898	-2.451014	-1.817168
C21	3.748887	-1.536409	-2.145226
C22	3.120318	-0.229632	-2.026041
C23	3.100400	2.247887	-2.065163
C24	3.766999	3.514362	-2.270086
C25	2.800267	4.474013	-2.308283
C26	1.545285	3.793191	-2.101254
C27	0.310795	4.409998	-2.050881
H28	0.275959	5.482413	-2.183302
C29	-2.998207	1.033021	-1.026571
H30	-4.071613	1.034922	-0.905990
C31	0.405482	-2.354072	-1.154757
H32	0.448356	-3.422536	-1.008588
C33	3.736242	1.009953	-2.116042
H34	4.809525	1.045228	-2.223045
C35	1.274678	2.020453	2.811580
H36	0.919336	1.216469	3.443603
C37	0.505806	2.355262	1.651354
H38	-0.536997	2.071179	1.662006
C39	0.852898	3.597715	1.020739
H40	0.177931	3.989587	0.284138
C41	2.019086	4.260496	1.303629
H42	2.302873	5.156359	0.766480
C43	2.813105	3.834185	2.373768
O44	3.917639	4.574367	2.662187
C45	4.525656	4.568518	3.909184
O46	5.426884	5.374730	4.053715
C47	4.013775	3.623735	4.872567
C48	3.089538	2.668551	4.480848
O49	2.748398	1.743531	5.375637
H50	1.995404	1.209501	5.121253
C51	2.421036	2.751629	3.183149
H52	-0.487749	2.463739	-5.528117
H53	-2.253376	5.535824	-1.632538
H54	-4.143052	3.661226	-1.151977
H55	-4.070121	-1.483953	-0.426846
H56	-2.060389	-3.468291	-0.379555
H57	2.851858	-3.534815	-1.830004
H58	4.748697	-1.842319	-2.460804
H59	4.842583	3.606127	-2.364094

H60	2.874277	5.547818	-2.471668
H61	4.068823	3.910985	5.958916

Warfarin 7-1 Reactant Complex Doublet

C1	-0.969218	2.108680	-4.769114
H2	-1.759384	1.562735	-5.292464
H3	-1.459390	2.711251	-4.007544
S4	0.105627	0.846023	-4.009838
O5	0.566278	1.018441	0.071368
Fe6	0.299443	1.013783	-1.545643
N7	-1.115400	2.446408	-1.564064
N8	-1.124370	-0.388191	-1.311215
N9	1.705788	-0.419116	-1.832977
N10	1.692566	2.418147	-1.996619
C11	-0.933519	3.793642	-1.716211
C12	-2.179362	4.496212	-1.567073
C13	-3.135041	3.547049	-1.362148
C14	-2.460052	2.271138	-1.365902
C15	-2.455855	-0.186894	-1.103307
C16	-3.109110	-1.434563	-0.759600
C17	-2.138656	-2.389631	-0.740697
C18	-0.909512	-1.716714	-1.110048
C19	1.509788	-1.749691	-1.623891
C20	2.738351	-2.471869	-1.815562
C21	3.696220	-1.562771	-2.149780
C22	3.044395	-0.263356	-2.110789
C23	3.036765	2.213335	-2.130955
C24	3.722263	3.473225	-2.295179
C25	2.767473	4.444891	-2.300746
C26	1.505789	3.775595	-2.100215
C27	0.283899	4.413821	-1.980086
H28	0.276173	5.493968	-2.052580
C29	-3.090416	1.048041	-1.173320
H30	-4.164756	1.071612	-1.049422
C31	0.312899	-2.352219	-1.261189
H32	0.362988	-3.408766	-1.044140
C33	3.665558	0.975835	-2.188902
H34	4.743474	1.006469	-2.255687
C35	0.804302	2.672338	3.511437
H36	0.316976	2.092227	4.284779
C37	0.208513	2.877800	2.286510
H38	-0.755845	2.445288	2.056405
C39	0.880673	3.619557	1.302876
H40	0.408933	3.754317	0.346340
C41	2.138248	4.151988	1.531021
H42	2.661160	4.708850	0.764956
C43	2.724616	3.963542	2.780958
O44	3.947879	4.533085	3.007660
C45	4.539612	4.565217	4.259903
O46	5.565378	5.199310	4.356033
C47	3.865248	3.836874	5.326547
C48	2.703307	3.141203	5.069899
O49	2.009888	2.398243	5.940379
H50	2.413138	2.304484	6.795461
C51	2.073521	3.229699	3.776729
H52	-0.534948	2.797180	-5.521726
H53	-2.282626	5.575967	-1.596087
H54	-4.201257	3.681271	-1.212163
H55	-4.170445	-1.506461	-0.543337

H56	-2.129838	-3.455688	-0.489957
H57	2.830613	-3.547131	-1.771470
H58	4.708491	-1.863158	-2.429323
H59	4.800277	3.556576	-2.380067
H60	2.853070	5.511737	-2.474057
H61	4.278642	4.005603	6.342569

Warfarin 7-1 Reactant Complex Quartet

C1	-0.959763	2.114425	-4.766097
H2	-1.750321	1.564170	-5.283954
H3	-1.447695	2.716973	-4.002525
S4	0.117234	0.855913	-4.006373
O5	0.542993	1.034074	0.078646
Fe6	0.301857	1.014060	-1.537470
N7	-1.116094	2.446115	-1.566333
N8	-1.124208	-0.389294	-1.304442
N9	1.706705	-0.418513	-1.819756
N10	1.690368	2.415759	-2.000034
C11	-0.934194	3.792918	-1.716282
C12	-2.181597	4.494083	-1.569072
C13	-3.137318	3.544458	-1.368551
C14	-2.462016	2.268777	-1.371020
C15	-2.454638	-0.187055	-1.098134
C16	-3.108831	-1.433837	-0.752921
C17	-2.138662	-2.391052	-0.733286
C18	-0.908174	-1.718086	-1.102707
C19	1.508388	-1.750109	-1.616040
C20	2.737420	-2.472123	-1.809887
C21	3.695632	-1.562951	-2.140081
C22	3.046032	-0.262427	-2.098603
C23	3.034223	2.211363	-2.135671
C24	3.717958	3.472129	-2.303240
C25	2.763974	4.442194	-2.308639
C26	1.501783	3.774947	-2.106024
C27	0.282266	4.414001	-1.982100
H28	0.275764	5.493732	-2.055014
C29	-3.090991	1.047632	-1.176954
H30	-4.166072	1.071291	-1.057417
C31	0.311401	-2.354007	-1.257455
H32	0.360774	-3.411888	-1.045934
C33	3.665825	0.975651	-2.184483
H34	4.743543	1.009745	-2.253139
C35	0.818761	2.684366	3.512204
H36	0.331150	2.102849	4.283279
C37	0.227338	2.890574	2.284305
H38	-0.734781	2.454656	2.052027
C39	0.901036	3.631961	1.303471
H40	0.434465	3.765938	0.343778
C41	2.155848	4.169744	1.537084
H42	2.679771	4.729983	0.774746
C43	2.738892	3.979718	2.788580
O44	3.961794	4.549755	3.019398
C45	4.553014	4.575232	4.272717
O46	5.580012	5.204412	4.371333
C47	3.875398	3.843824	5.334886
C48	2.716753	3.148395	5.073714
O49	2.023560	2.397481	5.938248
H50	2.433231	2.293399	6.790772
C51	2.087699	3.242343	3.781410

H52	-0.530036	2.802129	-5.523000
H53	-2.284120	5.573347	-1.596147
H54	-4.203736	3.678408	-1.215046
H55	-4.171036	-1.506501	-0.540337
H56	-2.131247	-3.456887	-0.483793
H57	2.827317	-3.548421	-1.769808
H58	4.705332	-1.866298	-2.422558
H59	4.796865	3.553789	-2.384126
H60	2.849926	5.509056	-2.479333
H61	4.286591	4.009690	6.353821

Warfarin 7-1 Transition State Doublet

C1	-0.961739	2.079173	-4.679250
H2	-1.732719	1.503675	-5.198005
H3	-1.470219	2.689127	-3.935662
S4	0.119634	0.839102	-3.867022
O5	0.840141	1.303820	0.256301
Fe6	0.362811	1.150384	-1.446308
N7	-1.063654	2.544915	-1.465134
N8	-1.044695	-0.280676	-1.095667
N9	1.766484	-0.325381	-1.677712
N10	1.715629	2.521621	-1.956332
C11	-0.902217	3.897311	-1.664269
C12	-2.163799	4.575416	-1.543178
C13	-3.104442	3.613116	-1.324923
C14	-2.406072	2.353624	-1.275539
C15	-2.391152	-0.096654	-0.941931
C16	-3.054243	-1.359487	-0.672618
C17	-2.083412	-2.313407	-0.663265
C18	-0.844663	-1.619552	-0.961820
C19	1.563526	-1.661105	-1.497299
C20	2.777918	-2.393509	-1.745822
C21	3.730431	-1.489275	-2.091298
C22	3.088897	-0.181526	-2.014733
C23	3.060184	2.298954	-2.097232
C24	3.747493	3.551905	-2.278088
C25	2.799530	4.530021	-2.281488
C26	1.534769	3.874141	-2.067047
C27	0.308191	4.517175	-1.939510
H28	0.298330	5.595069	-2.036513
C29	-3.029199	1.128667	-1.049668
H30	-4.107264	1.145966	-0.958621
C31	0.369718	-2.263872	-1.146881
H32	0.402536	-3.331921	-0.987250
C33	3.693934	1.063709	-2.141764
H34	4.768980	1.102700	-2.246794
C35	0.613486	2.477215	3.482907
H36	0.088924	2.083332	4.343783
C37	0.034218	2.490815	2.249266
H38	-0.973065	2.126043	2.098708
C39	0.775793	2.898753	1.080215
H40	0.195880	3.349935	0.292238
C41	2.084164	3.478466	1.288352
H42	2.639363	3.884778	0.454003
C43	2.607280	3.546795	2.565050
O44	3.817695	4.174362	2.755954
C45	4.367228	4.407764	4.017991
O46	5.349841	5.105515	4.057236
C47	3.712229	3.778434	5.159196

C48	2.542610	3.069898	4.964475
O49	1.848463	2.412812	5.907417
H50	2.259932	2.397944	6.762289
C51	1.916971	3.014856	3.674902
H52	-0.536740	2.765604	-5.449335
H53	-2.284385	5.647084	-1.592200
H54	-4.177948	3.718933	-1.198155
H55	-4.125538	-1.458382	-0.521383
H56	-2.087259	-3.393596	-0.460723
H57	2.850529	-3.474495	-1.747442
H58	4.723865	-1.808845	-2.408554
H59	4.825507	3.612576	-2.366099
H60	2.883021	5.587954	-2.472624
H61	4.170898	3.979570	6.169759

Warfarin 7-1 Transition State Quartet

C1	-0.974832	2.078011	-4.670189
H2	-1.735856	1.487103	-5.183447
H3	-1.490888	2.686485	-3.930580
S4	0.138604	0.874994	-3.848021
O5	0.727046	1.369380	0.225209
Fe6	0.385435	1.110175	-1.467795
N7	-1.058243	2.521557	-1.506807
N8	-1.027450	-0.299969	-1.119349
N9	1.765001	-0.325474	-1.691892
N10	1.751355	2.509902	-1.922994
C11	-0.885086	3.876323	-1.682585
C12	-2.146187	4.554925	-1.552980
C13	-3.089877	3.592317	-1.340407
C14	-2.398027	2.330300	-1.307868
C15	-2.379125	-0.107263	-0.965483
C16	-3.039706	-1.368563	-0.684513
C17	-2.071012	-2.324584	-0.669873
C18	-0.828678	-1.639767	-0.975814
C19	1.560777	-1.670247	-1.509719
C20	2.778874	-2.390575	-1.757551
C21	3.731772	-1.482278	-2.104187
C22	3.097339	-0.175168	-2.026724
C23	3.087843	2.293275	-2.073607
C24	3.768431	3.550051	-2.258973
C25	2.813798	4.521506	-2.263035
C26	1.552541	3.857117	-2.042193
C27	0.325864	4.499692	-1.934869
H28	0.316009	5.576862	-2.027651
C29	-3.022092	1.109324	-1.076710
H30	-4.097930	1.126033	-0.975360
C31	0.381967	-2.283326	-1.156040
H32	0.423569	-3.348232	-0.984449
C33	3.717619	1.056299	-2.139244
H34	4.791871	1.086701	-2.243410
C35	0.615816	2.480168	3.487883
H36	0.095638	2.081178	4.347692
C37	0.025096	2.510178	2.264358
H38	-0.984032	2.151137	2.117610
C39	0.752364	2.933474	1.084472
H40	0.171598	3.405811	0.312510
C41	2.074592	3.491832	1.292412
H42	2.617623	3.913186	0.457232
C43	2.608744	3.544010	2.563124

O44	3.820868	4.163594	2.752826
C45	4.375432	4.401222	4.015330
O46	5.357040	5.098097	4.048522
C47	3.722763	3.774727	5.160158
C48	2.552725	3.062996	4.964925
O49	1.860257	2.405452	5.907976
H50	2.267440	2.394247	6.765304
C51	1.925070	3.009900	3.678226
H52	-0.547334	2.762080	-5.443079
H53	-2.271797	5.627808	-1.593713
H54	-4.162687	3.702037	-1.204852
H55	-4.110557	-1.465427	-0.529288
H56	-2.076280	-3.403295	-0.461594
H57	2.855454	-3.471127	-1.755322
H58	4.726385	-1.802070	-2.417763
H59	4.844889	3.615139	-2.354126
H60	2.889421	5.580963	-2.459478
H61	4.180246	3.979482	6.172851

Warfarin 7-2 Reactant Complex Doublet

C1	-0.949398	2.374224	-4.699381
H2	-1.924088	1.961798	-4.970601
H3	-1.137200	3.126385	-3.935011
S4	0.063891	1.005172	-4.028980
O5	0.578609	0.919393	0.075492
Fe6	0.298376	0.998027	-1.535384
N7	-1.112829	2.432787	-1.505897
N8	-1.127301	-0.404546	-1.348395
N9	1.698169	-0.427161	-1.862122
N10	1.695279	2.407452	-1.962152
C11	-0.929855	3.777318	-1.660657
C12	-2.172785	4.480470	-1.515810
C13	-3.131611	3.536782	-1.305480
C14	-2.463023	2.258260	-1.314063
C15	-2.456604	-0.204923	-1.145679
C16	-3.114917	-1.455804	-0.831494
C17	-2.142922	-2.411016	-0.796576
C18	-0.911345	-1.734823	-1.146451
C19	1.505715	-1.756136	-1.643231
C20	2.733969	-2.476941	-1.833049
C21	3.689077	-1.572959	-2.176757
C22	3.039909	-0.269930	-2.136048
C23	3.036986	2.205702	-2.117063
C24	3.717320	3.470561	-2.282630
C25	2.762577	4.440399	-2.275369
C26	1.504390	3.768354	-2.059857
C27	0.285901	4.401520	-1.934989
H28	0.274739	5.480023	-2.026794
C29	-3.093551	1.033146	-1.163523
H30	-4.167319	1.045752	-1.026218
C31	0.312759	-2.365431	-1.278042
H32	0.368846	-3.420738	-1.053883
C33	3.663471	0.967553	-2.200880
H34	4.740832	0.993927	-2.282157
C35	0.662904	2.559998	3.526427
H36	0.227394	1.974637	4.325088
C37	-0.003019	2.772249	2.339065
H38	-0.982700	2.344060	2.166905
C39	0.606783	3.527231	1.328490

H40	0.076542	3.675140	0.406063
C41	1.885228	4.038618	1.474722
H42	2.371897	4.588553	0.677593
C43	2.525527	3.875759	2.699101
O44	3.740248	4.477956	2.869330
C45	4.345939	4.603341	4.112823
O46	5.359148	5.260783	4.147210
C47	3.694742	3.929846	5.228416
C48	2.576675	3.155155	5.021464
O49	1.923224	2.430064	5.933521
H50	2.350020	2.375295	6.782146
C51	1.928359	3.151741	3.733191
H52	-0.569574	2.913410	-5.598467
H53	-2.267375	5.556418	-1.568063
H54	-4.195381	3.688291	-1.163057
H55	-4.186531	-1.521376	-0.682480
H56	-2.133887	-3.474321	-0.538352
H57	2.816520	-3.551723	-1.769010
H58	4.697779	-1.881595	-2.461834
H59	4.793065	3.557925	-2.383687
H60	2.839518	5.508197	-2.462616
H61	4.084316	4.193546	6.235541

Warfarin 7-2 Reactant Complex Quartet

C1	-0.934570	2.378069	-4.697257
H2	-1.906872	1.953855	-4.959727
H3	-1.123998	3.131834	-3.934640
S4	0.095840	1.025214	-4.023495
O5	0.555867	0.939516	0.084132
Fe6	0.305332	0.996226	-1.527357
N7	-1.111097	2.430248	-1.511800
N8	-1.122117	-0.408953	-1.344967
N9	1.705049	-0.428997	-1.846103
N10	1.697137	2.403886	-1.960803
C11	-0.928732	3.772994	-1.663977
C12	-2.173316	4.475154	-1.519842
C13	-3.131784	3.530571	-1.313218
C14	-2.461381	2.251770	-1.322246
C15	-2.451278	-0.209426	-1.143047
C16	-3.109372	-1.460387	-0.827656
C17	-2.138704	-2.416417	-0.793512
C18	-0.905858	-1.741107	-1.143823
C19	1.510949	-1.759323	-1.636008
C20	2.739280	-2.480006	-1.828889
C21	3.695219	-1.574600	-2.167836
C22	3.047351	-0.271542	-2.121620
C23	3.037322	2.202563	-2.116520
C24	3.716690	3.467771	-2.285439
C25	2.761438	4.437018	-2.278327
C26	1.503503	3.765871	-2.061355
C27	0.286782	4.399448	-1.936371
H28	0.275790	5.477826	-2.026438
C29	-3.090082	1.029124	-1.169891
H30	-4.164587	1.042683	-1.036288
C31	0.316256	-2.371171	-1.279606
H32	0.371557	-3.428765	-1.066127
C33	3.668396	0.966721	-2.192949
H34	4.744844	0.999882	-2.276710
C35	0.668052	2.574740	3.529239

H36	0.235521	1.983200	4.325151
C37	0.002414	2.789494	2.341825
H38	-0.973991	2.356951	2.167861
C39	0.612224	3.548671	1.334590
H40	0.083644	3.698237	0.410455
C41	1.888764	4.064841	1.484090
H42	2.374501	4.620737	0.692172
C43	2.528671	3.896738	2.709299
O44	3.744206	4.496317	2.880980
C45	4.353853	4.610370	4.122893
O46	5.372133	5.257071	4.159099
C47	3.698789	3.935764	5.237755
C48	2.580137	3.162217	5.026858
O49	1.929272	2.431127	5.937371
H50	2.358232	2.368231	6.783703
C51	1.932601	3.167136	3.740405
H52	-0.564281	2.916473	-5.600801
H53	-2.267257	5.550598	-1.567512
H54	-4.195284	3.681533	-1.166395
H55	-4.181517	-1.526943	-0.679281
H56	-2.128634	-3.480500	-0.535877
H57	2.821933	-3.556127	-1.773462
H58	4.702578	-1.882724	-2.457881
H59	4.793249	3.557263	-2.378541
H60	2.839368	5.504700	-2.462735
H61	4.087116	4.195837	6.244488

Warfarin 7-2 Transition State Doublet

C1	-0.960266	2.335495	-4.648805
H2	-1.915858	1.898003	-4.945539
H3	-1.185139	3.086872	-3.895626
S4	0.054690	0.977419	-3.929057
O5	0.785198	1.264656	0.250384
Fe6	0.345250	1.134874	-1.455671
N7	-1.076813	2.524670	-1.450412
N8	-1.055759	-0.305638	-1.138415
N9	1.751392	-0.337906	-1.704397
N10	1.707018	2.505465	-1.948114
C11	-0.910168	3.874738	-1.633878
C12	-2.166480	4.553771	-1.506326
C13	-3.112491	3.597535	-1.289692
C14	-2.422514	2.333442	-1.259125
C15	-2.399859	-0.123490	-0.990180
C16	-3.064994	-1.387358	-0.736479
C17	-2.092457	-2.341610	-0.709609
C18	-0.852735	-1.645373	-0.994789
C19	1.554567	-1.672290	-1.512938
C20	2.768199	-2.404997	-1.759912
C21	3.719087	-1.502655	-2.117124
C22	3.076523	-0.193578	-2.039877
C23	3.050263	2.286099	-2.097207
C24	3.734937	3.542454	-2.273192
C25	2.786588	4.519518	-2.267017
C26	1.523631	3.860246	-2.051216
C27	0.300743	4.498564	-1.914386
H28	0.288859	5.575528	-2.018339
C29	-3.042254	1.104133	-1.062836
H30	-4.119455	1.110145	-0.958840
C31	0.364973	-2.283873	-1.158431

H32	0.407026	-3.350059	-0.990238
C33	3.683929	1.050074	-2.157527
H34	4.757803	1.089008	-2.272575
C35	0.558129	2.385249	3.491470
H36	0.075749	1.961667	4.362286
C37	-0.051839	2.391782	2.273568
H38	-1.053353	2.003003	2.141956
C39	0.647004	2.844168	1.094942
H40	0.027823	3.277693	0.326763
C41	1.932941	3.471608	1.276961
H42	2.453889	3.909477	0.436255
C43	2.478939	3.554066	2.542506
O44	3.662052	4.232968	2.706038
C45	4.214231	4.510981	3.956363
O46	5.183895	5.227385	3.965408
C47	3.578449	3.899457	5.118196
C48	2.457945	3.108063	4.949541
O49	1.804451	2.439055	5.907261
H50	2.219066	2.451828	6.762821
C51	1.835058	2.988208	3.661907
H52	-0.576004	2.883582	-5.548456
H53	-2.273511	5.621641	-1.570091
H54	-4.181918	3.725357	-1.158212
H55	-4.142822	-1.475207	-0.644142
H56	-2.092366	-3.419406	-0.499356
H57	2.834515	-3.485586	-1.743384
H58	4.709047	-1.828232	-2.437475
H59	4.811454	3.609548	-2.372057
H60	2.865257	5.578862	-2.463728
H61	4.001144	4.181725	6.119814

Warfarin 7-2 Transition State Quartet

C1	-0.977078	2.334139	-4.640988
H2	-1.922669	1.882998	-4.941192
H3	-1.213032	3.088375	-3.894207
S4	0.063973	1.003083	-3.904615
O5	0.693369	1.334220	0.211708
Fe6	0.368168	1.098004	-1.481624
N7	-1.073633	2.501052	-1.482670
N8	-1.038025	-0.325486	-1.161126
N9	1.749533	-0.338784	-1.719880
N10	1.740105	2.494224	-1.920336
C11	-0.894951	3.854033	-1.644928
C12	-2.150934	4.532377	-1.510521
C13	-3.099914	3.575886	-1.299428
C14	-2.414578	2.309966	-1.283342
C15	-2.388877	-0.135720	-1.008899
C16	-3.049237	-1.400199	-0.745036
C17	-2.079373	-2.355458	-0.717091
C18	-0.836859	-1.666941	-1.011038
C19	1.552395	-1.684039	-1.528825
C20	2.770645	-2.403093	-1.772724
C21	3.720580	-1.498927	-2.125445
C22	3.086325	-0.190398	-2.050060
C23	3.075274	2.278973	-2.077747
C24	3.753429	3.539705	-2.257712
C25	2.798815	4.510496	-2.251256
C26	1.540014	3.841782	-2.029472
C27	0.314713	4.479463	-1.907002

H28	0.302224	5.555717	-2.008890
C29	-3.034617	1.080794	-1.080942
H30	-4.109628	1.085596	-0.964274
C31	0.376526	-2.304293	-1.174088
H32	0.425296	-3.369121	-1.001560
C33	3.705497	1.043251	-2.154693
H34	4.779199	1.072825	-2.267191
C35	0.565365	2.381082	3.502770
H36	0.081535	1.958133	4.375060
C37	-0.054797	2.400339	2.294052
H38	-1.057855	2.016125	2.167560
C39	0.624776	2.877836	1.109110
H40	0.000847	3.331115	0.358309
C41	1.917422	3.501190	1.293986
H42	2.416544	3.971184	0.458708
C43	2.472704	3.565231	2.553753
O44	3.647400	4.255325	2.718362
C45	4.211842	4.522732	3.969074
O46	5.181630	5.235109	3.974828
C47	3.581376	3.904806	5.130477
C48	2.466679	3.104949	4.959285
O49	1.817146	2.430127	5.916265
H50	2.231856	2.449781	6.773784
C51	1.843107	2.982783	3.674624
H52	-0.587026	2.880364	-5.542988
H53	-2.262639	5.601833	-1.568284
H54	-4.169276	3.705780	-1.163899
H55	-4.126513	-1.485887	-0.641591
H56	-2.077926	-3.432885	-0.502270
H57	2.843922	-3.484854	-1.754916
H58	4.715671	-1.823825	-2.440130
H59	4.828524	3.610335	-2.358514
H60	2.869929	5.571016	-2.450486
H61	4.004121	4.189663	6.133175

Warfarin 7-3 Reactant Complex Doublet

C1	-0.873903	2.261828	-4.740170
H2	-1.780796	1.774671	-5.112589
H3	-1.196445	2.952773	-3.965275
S4	0.196566	0.963444	-4.041822
O5	0.552815	0.980176	0.061879
Fe6	0.309647	1.026116	-1.555357
N7	-1.108890	2.455108	-1.566469
N8	-1.115365	-0.385171	-1.364055
N9	1.718739	-0.394496	-1.838550
N10	1.706213	2.444777	-1.959597
C11	-0.927219	3.801078	-1.711660
C12	-2.173915	4.499926	-1.574461
C13	-3.133868	3.553194	-1.391060
C14	-2.460406	2.276012	-1.390027
C15	-2.443604	-0.183604	-1.155787
C16	-3.097722	-1.427649	-0.807045
C17	-2.127173	-2.385042	-0.780207
C18	-0.895191	-1.712381	-1.146289
C19	1.527923	-1.725349	-1.629741
C20	2.762437	-2.440522	-1.814283
C21	3.716368	-1.526137	-2.146334
C22	3.059465	-0.228553	-2.098182
C23	3.051645	2.247311	-2.082352

C24	3.730861	3.514610	-2.243640
C25	2.773974	4.479223	-2.257484
C26	1.512959	3.803819	-2.066418
C27	0.288998	4.431277	-1.964726
H28	0.273939	5.511029	-2.045802
C29	-3.084060	1.051649	-1.216516
H30	-4.158360	1.063604	-1.089955
C31	0.332799	-2.339365	-1.273450
H32	0.391262	-3.395603	-1.049360
C33	3.681746	1.011531	-2.142842
H34	4.761267	1.042258	-2.191420
C35	0.673159	2.673602	3.491403
H36	0.216005	2.103296	4.289717
C37	0.033740	2.871697	2.287211
H38	-0.943372	2.444363	2.099099
C39	0.670385	3.603027	1.275865
H40	0.159451	3.738520	0.342709
C41	1.947432	4.112805	1.440178
H42	2.453322	4.649408	0.647240
C43	2.565416	3.959270	2.680341
O44	3.783654	4.546140	2.862886
C45	4.358437	4.696660	4.117904
O46	5.370681	5.354399	4.164434
C47	3.682153	4.041114	5.231583
C48	2.568299	3.258798	5.007750
O49	1.907317	2.540627	5.922488
H50	2.388456	2.401910	6.731958
C51	1.940381	3.251410	3.711482
H52	-0.475328	2.872996	-5.574849
H53	-2.278029	5.575253	-1.594448
H54	-4.198950	3.716612	-1.271595
H55	-4.162426	-1.491513	-0.599421
H56	-2.125679	-3.449659	-0.528793
H57	2.840305	-3.515771	-1.756438
H58	4.731329	-1.806696	-2.439402
H59	4.807603	3.603329	-2.341717
H60	2.850823	5.548584	-2.436113
H61	4.014344	4.346341	6.246288

Warfarin 7-3 Reactant Complex Quartet

C1	-0.860496	2.266718	-4.736471
H2	-1.764700	1.766753	-5.098490
H3	-1.184666	2.959520	-3.962975
S4	0.226560	0.986000	-4.035919
O5	0.526997	0.982993	0.068526
Fe6	0.315898	1.023521	-1.549233
N7	-1.106982	2.452773	-1.569093
N8	-1.112129	-0.388426	-1.369204
N9	1.723390	-0.395180	-1.829269
N10	1.712351	2.441107	-1.950265
C11	-0.924740	3.797281	-1.711201
C12	-2.172275	4.496536	-1.573838
C13	-3.132662	3.549161	-1.392808
C14	-2.459629	2.271888	-1.394245
C15	-2.439615	-0.187610	-1.161288
C16	-3.093266	-1.430832	-0.809181
C17	-2.123091	-2.387909	-0.781238
C18	-0.891493	-1.716938	-1.148834
C19	1.530877	-1.726954	-1.627426

C20	2.764590	-2.442303	-1.813431
C21	3.719612	-1.528127	-2.141545
C22	3.065563	-0.229246	-2.089369
C23	3.056049	2.245153	-2.073927
C24	3.733869	3.512675	-2.238830
C25	2.775654	4.477081	-2.253956
C26	1.515371	3.801441	-2.060827
C27	0.292331	4.429272	-1.961427
H28	0.277615	5.508401	-2.041875
C29	-3.082347	1.048167	-1.226084
H30	-4.157463	1.056651	-1.104839
C31	0.334829	-2.343126	-1.277543
H32	0.392765	-3.400454	-1.061002
C33	3.688721	1.008895	-2.133065
H34	4.767855	1.039272	-2.181781
C35	0.665255	2.671104	3.500202
H36	0.212659	2.098950	4.298746
C37	0.021005	2.870798	2.298291
H38	-0.955255	2.442269	2.113450
C39	0.653678	3.604539	1.286943
H40	0.138193	3.740129	0.354496
C41	1.931576	4.114165	1.446320
H42	2.433224	4.652282	0.652137
C43	2.552673	3.959121	2.683192
O44	3.773597	4.546850	2.862842
C45	4.352402	4.697129	4.116923
O46	5.362053	5.354761	4.160567
C47	3.678482	4.039091	5.230794
C48	2.565153	3.257166	5.011225
O49	1.906392	2.537398	5.926419
H50	2.387122	2.402048	6.737234
C51	1.933669	3.250950	3.716745
H52	-0.471375	2.875151	-5.576968
H53	-2.276448	5.571639	-1.592242
H54	-4.197662	3.713098	-1.271450
H55	-4.157413	-1.493317	-0.598000
H56	-2.118698	-3.452100	-0.528587
H57	2.842452	-3.518003	-1.757235
H58	4.733312	-1.810698	-2.434815
H59	4.810106	3.603614	-2.338654
H60	2.852555	5.546215	-2.433225
H61	4.012751	4.345830	6.244965

Warfarin 7-3 Transition State Doublet

C1	-0.887848	2.207359	-4.681121
H2	-1.767016	1.693636	-5.081536
H3	-1.251961	2.895568	-3.922730
S4	0.178296	0.921438	-3.923844
O5	0.782219	1.309901	0.254400
Fe6	0.366562	1.159237	-1.460379
N7	-1.062839	2.542796	-1.491427
N8	-1.037012	-0.286447	-1.140390
N9	1.778365	-0.307957	-1.668076
N10	1.726737	2.538048	-1.932746
C11	-0.900015	3.894984	-1.672939
C12	-2.161171	4.568132	-1.561569
C13	-3.105679	3.608329	-1.367989
C14	-2.409283	2.348024	-1.317084
C15	-2.381725	-0.102477	-0.989222

C16	-3.045238	-1.362453	-0.714824
C17	-2.073656	-2.318343	-0.696730
C18	-0.832252	-1.624816	-0.989234
C19	1.580695	-1.645233	-1.493246
C20	2.799445	-2.371877	-1.738292
C21	3.751383	-1.460093	-2.076701
C22	3.103543	-0.155837	-1.987028
C23	3.073916	2.323657	-2.055910
C24	3.755290	3.581910	-2.237108
C25	2.802641	4.554336	-2.248814
C26	1.539526	3.890008	-2.047220
C27	0.311136	4.523598	-1.932398
H28	0.293995	5.600719	-2.033195
C29	-3.024690	1.121622	-1.094133
H30	-4.100938	1.132118	-0.990907
C31	0.388783	-2.261490	-1.150217
H32	0.431543	-3.329316	-0.987404
C33	3.711327	1.091065	-2.087273
H34	4.788450	1.132083	-2.168279
C35	0.540164	2.477496	3.481667
H36	0.030250	2.089389	4.352901
C37	-0.053124	2.476314	2.256673
H38	-1.058949	2.103413	2.118835
C39	0.665332	2.900694	1.077989
H40	0.059096	3.340592	0.302496
C41	1.954963	3.516598	1.267554
H42	2.484482	3.950579	0.429875
C43	2.487679	3.609985	2.536854
O44	3.669911	4.287265	2.705656
C45	4.200838	4.591205	3.959550
O46	5.170809	5.306844	3.969510
C47	3.544594	3.998594	5.122127
C48	2.439445	3.192269	4.948845
O49	1.783386	2.523797	5.908458
H50	2.248231	2.470446	6.734765
C51	1.827921	3.058952	3.655633
H52	-0.487309	2.825853	-5.519294
H53	-2.281065	5.634534	-1.595386
H54	-4.177558	3.738390	-1.265099
H55	-4.117687	-1.457275	-0.571813
H56	-2.082812	-3.397776	-0.492394
H57	2.860336	-3.452968	-1.732854
H58	4.751336	-1.758191	-2.401952
H59	4.831437	3.652461	-2.337840
H60	2.878273	5.615138	-2.436700
H61	3.921349	4.332058	6.130369

Warfarin 7-3 Transition State Quartet

C1	-0.908590	2.203364	-4.668063
H2	-1.773557	1.671941	-5.071214
H3	-1.288350	2.891973	-3.917623
S4	0.194834	0.961586	-3.890305
O5	0.672620	1.386755	0.215850
Fe6	0.383337	1.127372	-1.489526
N7	-1.062681	2.527077	-1.534625
N8	-1.027513	-0.295482	-1.161568
N9	1.770520	-0.301373	-1.684455
N10	1.758721	2.534283	-1.895407
C11	-0.885623	3.882327	-1.692524

C12	-2.145551	4.556915	-1.569186
C13	-3.093687	3.597823	-1.379741
C14	-2.405234	2.334534	-1.347867
C15	-2.377368	-0.102930	-1.008772
C16	-3.037245	-1.361954	-0.721689
C17	-2.068406	-2.319584	-0.701157
C18	-0.824386	-1.634827	-1.002099
C19	1.570834	-1.646627	-1.507150
C20	2.792048	-2.362513	-1.747717
C21	3.744642	-1.450157	-2.085680
C22	3.107389	-0.145353	-1.998640
C23	3.096775	2.323374	-2.030868
C24	3.772760	3.584199	-2.220018
C25	2.814134	4.551274	-2.233009
C26	1.554388	3.879438	-2.022848
C27	0.325128	4.513858	-1.930689
H28	0.309294	5.590953	-2.026749
C29	-3.024871	1.111732	-1.118277
H30	-4.099201	1.123766	-1.004522
C31	0.391417	-2.272550	-1.162033
H32	0.440969	-3.337413	-0.992090
C33	3.730275	1.089317	-2.086327
H34	4.806262	1.121157	-2.171478
C35	0.532512	2.491451	3.475196
H36	0.035349	2.082205	4.342632
C37	-0.072833	2.506073	2.258775
H38	-1.077662	2.132879	2.123951
C39	0.635218	2.949239	1.071267
H40	0.030872	3.413277	0.311722
C41	1.947715	3.531959	1.262705
H42	2.477551	3.962269	0.421989
C43	2.484254	3.612372	2.525584
O44	3.676655	4.269045	2.694271
C45	4.202825	4.585994	3.950090
O46	5.166319	5.305152	3.958858
C47	3.545539	3.996982	5.113981
C48	2.436006	3.192729	4.940486
O49	1.780868	2.526267	5.900568
H50	2.246708	2.470474	6.727523
C51	1.823695	3.067806	3.649270
H52	-0.499710	2.822920	-5.504472
H53	-2.269552	5.625585	-1.597968
H54	-4.165233	3.732339	-1.270029
H55	-4.109967	-1.455380	-0.574516
H56	-2.080519	-3.397986	-0.494183
H57	2.855368	-3.443622	-1.734862
H58	4.743861	-1.753719	-2.408055
H59	4.847086	3.654499	-2.333404
H60	2.883120	5.613060	-2.429258
H61	3.920556	4.329126	6.123070

Warfarin 7-4 Reactant Complex Doublet

C1	-1.063421	2.105479	-4.644150
H2	-1.930381	1.601342	-5.081913
H3	-1.445843	2.754228	-3.860231
S4	0.031584	0.816298	-3.950660
O5	0.587888	1.019653	0.119754
Fe6	0.306021	1.010697	-1.496457
N7	-1.109480	2.430040	-1.480957

N8	-1.110857	-0.404629	-1.264070
N9	1.718437	-0.410214	-1.792940
N10	1.686066	2.429540	-1.948302
C11	-0.932812	3.781405	-1.601155
C12	-2.188339	4.470259	-1.486436
C13	-3.143048	3.512485	-1.337575
C14	-2.459851	2.243167	-1.332407
C15	-2.448779	-0.215216	-1.095767
C16	-3.103419	-1.470500	-0.785438
C17	-2.126149	-2.420548	-0.749335
C18	-0.891586	-1.732998	-1.077768
C19	1.536022	-1.739374	-1.570157
C20	2.771911	-2.451522	-1.755525
C21	3.718340	-1.538472	-2.115062
C22	3.054140	-0.243721	-2.081987
C23	3.026028	2.233696	-2.110564
C24	3.701608	3.497763	-2.288693
C25	2.746139	4.465004	-2.279117
C26	1.493761	3.788653	-2.035699
C27	0.276297	4.416447	-1.861322
H28	0.260365	5.497550	-1.928602
C29	-3.090258	1.016562	-1.174965
H30	-4.169386	1.036938	-1.085398
C31	0.340932	-2.355960	-1.218502
H32	0.398650	-3.414493	-1.010536
C33	3.662830	0.999779	-2.173037
H34	4.739697	1.043067	-2.256733
C35	0.931367	2.650085	3.795380
H36	0.464634	2.087615	4.597014
C37	0.284071	2.775875	2.582363
H38	-0.668914	2.292804	2.411927
C39	0.876038	3.519206	1.549092
H40	0.367888	3.594163	0.600080
C41	2.109146	4.123735	1.721425
H42	2.577127	4.691106	0.925107
C43	2.741278	4.025245	2.959327
O44	3.908314	4.714764	3.124150
C45	4.504494	4.899658	4.366100
O46	5.455324	5.637444	4.411209
C47	3.916472	4.159669	5.473191
C48	2.851754	3.324605	5.286364
O49	2.363465	2.607043	6.323116
H50	1.921188	1.818485	6.011070
C51	2.176960	3.281937	4.007259
H52	-0.644911	2.753037	-5.436734
H53	-2.288828	5.546405	-1.515999
H54	-4.216431	3.619414	-1.232550
H55	-4.171477	-1.541461	-0.603722
H56	-2.119098	-3.488504	-0.506589
H57	2.864646	-3.523920	-1.676445
H58	4.728969	-1.826857	-2.419409
H59	4.778740	3.582071	-2.373921
H60	2.829443	5.533656	-2.469561
H61	4.317970	4.380666	6.478925

Warfarin 7-4 Reactant Complex Quartet

C1	-1.050809	2.121428	-4.635904
H2	-1.924110	1.612532	-5.056363
H3	-1.422428	2.776606	-3.852378

S4	0.050443	0.839710	-3.944254
O5	0.563939	1.031161	0.126699
Fe6	0.309983	1.012972	-1.487708
N7	-1.108804	2.431798	-1.478356
N8	-1.108899	-0.404026	-1.261544
N9	1.721521	-0.407165	-1.781835
N10	1.688886	2.428232	-1.942495
C11	-0.933262	3.780910	-1.596941
C12	-2.188589	4.470156	-1.484943
C13	-3.144513	3.511266	-1.337741
C14	-2.460331	2.241558	-1.332223
C15	-2.444502	-0.216156	-1.095502
C16	-3.099958	-1.471259	-0.784301
C17	-2.121171	-2.422117	-0.745310
C18	-0.886300	-1.734423	-1.072838
C19	1.537758	-1.736119	-1.563788
C20	2.772929	-2.448798	-1.751759
C21	3.719544	-1.537477	-2.108736
C22	3.059274	-0.241391	-2.072710
C23	3.027565	2.233521	-2.105823
C24	3.701939	3.498050	-2.287627
C25	2.744671	4.465763	-2.277880
C26	1.493670	3.789373	-2.032246
C27	0.278165	4.417464	-1.856942
H28	0.262797	5.498107	-1.922930
C29	-3.089000	1.016016	-1.179297
H30	-4.169004	1.033863	-1.094953
C31	0.341752	-2.355701	-1.215866
H32	0.401233	-3.415125	-1.015477
C33	3.667889	1.000192	-2.165586
H34	4.744537	1.043383	-2.251771
C35	0.949371	2.654933	3.796018
H36	0.481377	2.093119	4.598731
C37	0.301811	2.783692	2.583546
H38	-0.652419	2.303939	2.414106
C39	0.894545	3.527928	1.552777
H40	0.385659	3.606814	0.603210
C41	2.127926	4.134076	1.725643
H42	2.594482	4.705847	0.934105
C43	2.760475	4.029444	2.964046
O44	3.928403	4.717200	3.131507
C45	4.519457	4.902771	4.375268
O46	5.473574	5.636608	4.422941
C47	3.924838	4.166954	5.482174
C48	2.864463	3.327928	5.290024
O49	2.375135	2.607033	6.325752
H50	1.930580	1.822540	6.012618
C51	2.195003	3.283773	4.010356
H52	-0.640512	2.761717	-5.438978
H53	-2.290175	5.546515	-1.514764
H54	-4.217264	3.618632	-1.233233
H55	-4.167731	-1.540432	-0.603323
H56	-2.111458	-3.490041	-0.503566
H57	2.864491	-3.521798	-1.675834
H58	4.728656	-1.829123	-2.416320
H59	4.778052	3.582728	-2.376049
H60	2.828013	5.534060	-2.469782
H61	4.324752	4.384846	6.489658

Warfarin 7-4 Transition State Doublet

C1	-1.065901	2.059583	-4.555869
H2	-1.905417	1.507324	-4.989756
H3	-1.484401	2.718640	-3.798544
S4	0.061447	0.824186	-3.792227
O5	0.848132	1.290922	0.346380
Fe6	0.383723	1.147612	-1.356242
N7	-1.044683	2.528046	-1.365704
N8	-1.022373	-0.300905	-1.036677
N9	1.790102	-0.317348	-1.620464
N10	1.725448	2.529779	-1.873701
C11	-0.892396	3.881271	-1.558798
C12	-2.161036	4.545908	-1.478215
C13	-3.099367	3.575808	-1.294222
C14	-2.392100	2.324963	-1.219916
C15	-2.372881	-0.127590	-0.919031
C16	-3.037797	-1.396419	-0.694190
C17	-2.060703	-2.347722	-0.673746
C18	-0.817744	-1.640903	-0.925676
C19	1.599348	-1.653945	-1.438951
C20	2.819898	-2.376242	-1.685804
C21	3.763498	-1.464929	-2.044368
C22	3.110354	-0.163222	-1.961951
C23	3.067657	2.317325	-2.032552
C24	3.744415	3.572939	-2.237582
C25	2.791431	4.545750	-2.243179
C26	1.537082	3.881732	-1.990558
C27	0.311104	4.514371	-1.838135
H28	0.287578	5.590490	-1.948783
C29	-3.015933	1.096355	-1.025803
H30	-4.097120	1.111603	-0.966868
C31	0.406311	-2.272059	-1.102535
H32	0.448463	-3.341498	-0.955144
C33	3.708716	1.086135	-2.081498
H34	4.782365	1.133052	-2.193067
C35	0.722971	2.412906	3.668802
H36	0.213206	2.022031	4.544786
C37	0.095713	2.392767	2.454884
H38	-0.907609	2.000770	2.355106
C39	0.760497	2.842621	1.252689
H40	0.120073	3.273892	0.495714
C41	2.036524	3.493104	1.424767
H42	2.531611	3.953974	0.576033
C43	2.601131	3.603544	2.683268
O44	3.746599	4.348530	2.826866
C45	4.289996	4.697990	4.070076
O46	5.213154	5.468768	4.062537
C47	3.705583	4.060011	5.242842
C48	2.651742	3.195449	5.097661
O49	2.162286	2.541377	6.184302
H50	1.777491	1.710216	5.918754
C51	1.998527	3.023568	3.825490
H52	-0.659258	2.699726	-5.371877
H53	-2.281877	5.612417	-1.531038
H54	-4.177464	3.655719	-1.217517
H55	-4.112490	-1.492368	-0.570976
H56	-2.065263	-3.429211	-0.481073
H57	2.895956	-3.456143	-1.659791
H58	4.762007	-1.765749	-2.378380
H59	4.819485	3.637659	-2.336963

H60	2.870483	5.604461	-2.453386
H61	4.136046	4.320349	6.251062

Warfarin 7-4 Transition State Quartet

C1	-1.073205	2.064792	-4.549672
H2	-1.905644	1.496901	-4.973575
H3	-1.495300	2.726887	-3.796927
S4	0.084446	0.865922	-3.778685
O5	0.756031	1.350461	0.312796
Fe6	0.399717	1.113208	-1.371025
N7	-1.044779	2.510116	-1.395847
N8	-1.012456	-0.313520	-1.055684
N9	1.784385	-0.316510	-1.631691
N10	1.748814	2.517748	-1.856401
C11	-0.881718	3.865207	-1.573483
C12	-2.149371	4.531200	-1.485127
C13	-3.090673	3.561979	-1.303319
C14	-2.389147	2.309153	-1.241169
C15	-2.370248	-0.132178	-0.934856
C16	-3.030737	-1.401766	-0.700562
C17	-2.055872	-2.353869	-0.679093
C18	-0.810170	-1.654741	-0.938526
C19	1.591706	-1.663522	-1.450167
C20	2.815416	-2.375399	-1.695494
C21	3.759750	-1.462240	-2.052275
C22	3.114655	-0.159876	-1.971290
C23	3.085262	2.309919	-2.021725
C24	3.756336	3.568274	-2.229006
C25	2.798495	4.536264	-2.234747
C26	1.546541	3.866023	-1.978187
C27	0.321207	4.499606	-1.838350
H28	0.299653	5.575448	-1.943588
C29	-3.014758	1.082083	-1.041452
H30	-4.095117	1.099006	-0.970704
C31	0.410844	-2.286099	-1.112936
H32	0.457870	-3.353810	-0.957206
C33	3.724268	1.078073	-2.082301
H34	4.797750	1.118811	-2.190606
C35	0.719758	2.417056	3.668049
H36	0.212576	2.018478	4.540662
C37	0.082669	2.411814	2.460990
H38	-0.922328	2.027993	2.364499
C39	0.737129	2.875495	1.253760
H40	0.098669	3.316427	0.506072
C41	2.024446	3.508189	1.426375
H42	2.509698	3.981324	0.581169
C43	2.597581	3.601398	2.681417
O44	3.746676	4.338725	2.824663
C45	4.291605	4.693409	4.069171
O46	5.212606	5.464522	4.056609
C47	3.708142	4.057478	5.242564
C48	2.652903	3.190683	5.096036
O49	2.167464	2.538569	6.182713
H50	1.776337	1.708583	5.915332
C51	1.999719	3.020170	3.826103
H52	-0.667102	2.700500	-5.369970
H53	-2.272825	5.599865	-1.532760
H54	-4.169087	3.646339	-1.221824
H55	-4.105860	-1.495494	-0.574137

H56	-2.060924	-3.434412	-0.482530
H57	2.895190	-3.454923	-1.665526
H58	4.759092	-1.766061	-2.379676
H59	4.830263	3.635873	-2.332457
H60	2.873320	5.596675	-2.446929
H61	4.135642	4.318221	6.253169

Warfarin 7-5 Reactant Complex Doublet

C1	-1.039507	1.882525	-4.774365
H2	-1.700496	1.312570	-5.438242
H3	-1.670516	2.358941	-4.026396
S4	0.071628	0.654401	-4.001486
O5	0.547189	1.048709	0.055744
Fe6	0.283956	0.981601	-1.563368
N7	-1.140661	2.400227	-1.604353
N8	-1.134560	-0.421175	-1.298426
N9	1.700928	-0.443033	-1.824684
N10	1.675998	2.394398	-2.027975
C11	-0.951502	3.751175	-1.721538
C12	-2.193273	4.456364	-1.563333
C13	-3.153914	3.508783	-1.384208
C14	-2.484188	2.228991	-1.398564
C15	-2.468059	-0.224617	-1.090051
C16	-3.117639	-1.479657	-0.760616
C17	-2.146667	-2.434207	-0.770417
C18	-0.919191	-1.750850	-1.126733
C19	1.504526	-1.775448	-1.630648
C20	2.737379	-2.494533	-1.809841
C21	3.696020	-1.580688	-2.120936
C22	3.039788	-0.281819	-2.093046
C23	3.022618	2.196775	-2.150509
C24	3.703793	3.463484	-2.293182
C25	2.747650	4.432266	-2.280251
C26	1.488086	3.752511	-2.096559
C27	0.263274	4.377858	-1.947093
H28	0.249221	5.460222	-1.948443
C29	-3.108775	1.006445	-1.174091
H30	-4.182040	1.030735	-1.032621
C31	0.306307	-2.384214	-1.289466
H32	0.355873	-3.446032	-1.099284
C33	3.655758	0.959001	-2.183381
H34	4.734607	0.992682	-2.240144
C35	0.865359	2.574215	3.492896
H36	0.408573	1.939026	4.239150
C37	0.254167	2.815913	2.282082
H38	-0.693244	2.354278	2.037715
C39	0.889641	3.624901	1.329867
H40	0.404277	3.791701	0.383757
C41	2.127246	4.196953	1.578565
H42	2.622478	4.816506	0.841163
C43	2.730389	3.972286	2.813121
O44	3.934337	4.579592	3.059854
C45	4.554519	4.540075	4.299059
O46	5.555348	5.209185	4.423789
C47	3.928160	3.710901	5.321629
C48	2.777346	3.008368	5.047279
O49	2.120520	2.191791	5.882064
H50	2.602995	1.956043	6.667827
C51	2.118204	3.163675	3.775364

H52	-0.594246	2.678081	-5.402954
H53	-2.282859	5.538507	-1.555559
H54	-4.218309	3.655190	-1.247719
H55	-4.177336	-1.557878	-0.534441
H56	-2.137992	-3.507491	-0.550213
H57	2.819014	-3.572986	-1.785840
H58	4.713037	-1.874107	-2.386999
H59	4.783615	3.556586	-2.367102
H60	2.838206	5.510013	-2.418392
H61	4.363266	3.807976	6.339324

Warfarin 7-5 Reactant Complex Quartet

C1	-1.032812	1.883624	-4.765447
H2	-1.691867	1.304828	-5.424127
H3	-1.663359	2.357824	-4.015900
S4	0.090909	0.668731	-3.996007
O5	0.536765	0.965058	0.052359
Fe6	0.297991	0.970126	-1.565465
N7	-1.126531	2.399455	-1.584814
N8	-1.126964	-0.427677	-1.321747
N9	1.712585	-0.441776	-1.846183
N10	1.690348	2.394442	-2.002629
C11	-0.940759	3.749353	-1.707351
C12	-2.184262	4.454122	-1.560682
C13	-3.143766	3.505019	-1.380656
C14	-2.471798	2.226675	-1.385966
C15	-2.456580	-0.228816	-1.101644
C16	-3.104756	-1.482493	-0.766365
C17	-2.132224	-2.437153	-0.775371
C18	-0.906036	-1.755671	-1.139783
C19	1.516874	-1.773130	-1.648469
C20	2.751016	-2.489458	-1.822487
C21	3.709878	-1.575015	-2.130315
C22	3.053982	-0.277154	-2.103559
C23	3.036013	2.199876	-2.134852
C24	3.713884	3.467475	-2.285889
C25	2.754727	4.435812	-2.272112
C26	1.498592	3.752985	-2.077310
C27	0.274161	4.379163	-1.934151
H28	0.256937	5.459779	-1.952271
C29	-3.096983	1.003785	-1.171519
H30	-4.168920	1.027821	-1.024838
C31	0.321001	-2.382542	-1.296096
H32	0.379609	-3.439904	-1.082578
C33	3.671460	0.964043	-2.177323
H34	4.750545	0.998352	-2.228902
C35	0.829996	2.531879	3.510119
H36	0.369802	1.913654	4.268522
C37	0.220573	2.753764	2.294756
H38	-0.727267	2.289972	2.057189
C39	0.861828	3.542424	1.328415
H40	0.380056	3.681690	0.375960
C41	2.105424	4.104196	1.558080
H42	2.612241	4.686636	0.799603
C43	2.701411	3.907875	2.801271
O44	3.904066	4.522507	3.036036
C45	4.519091	4.511253	4.277442
O46	5.518995	5.185874	4.390799
C47	3.893246	3.702306	5.315310

C48	2.741063	2.996837	5.054801
O49	2.083795	2.197135	5.908236
H50	2.562240	1.986792	6.702323
C51	2.084267	3.124468	3.780925
H52	-0.592415	2.675414	-5.400690
H53	-2.278207	5.536318	-1.557414
H54	-4.208900	3.651085	-1.247961
H55	-4.163570	-1.559995	-0.539515
H56	-2.122603	-3.507577	-0.551509
H57	2.832502	-3.566598	-1.795982
H58	4.726360	-1.866101	-2.393919
H59	4.792104	3.561995	-2.360483
H60	2.843395	5.513494	-2.413614
H61	4.339103	3.807694	6.326444

Warfarin 7-5 Transition State Doublet

C1	-1.018185	1.861675	-4.663666
H2	-1.669993	1.246987	-5.294750
H3	-1.654266	2.357537	-3.932161
S4	0.119785	0.679717	-3.836360
O5	0.850938	1.263774	0.247345
Fe6	0.365153	1.112195	-1.452177
N7	-1.067403	2.499359	-1.472295
N8	-1.042357	-0.317177	-1.091790
N9	1.776647	-0.349581	-1.674688
N10	1.718126	2.499720	-1.956797
C11	-0.903281	3.855570	-1.644766
C12	-2.161550	4.536375	-1.529758
C13	-3.106240	3.574397	-1.338173
C14	-2.411362	2.312304	-1.288173
C15	-2.390182	-0.135030	-0.933204
C16	-3.051000	-1.403706	-0.679519
C17	-2.079773	-2.357842	-0.700372
C18	-0.841370	-1.657173	-0.986280
C19	1.573807	-1.685706	-1.509159
C20	2.793457	-2.413869	-1.745041
C21	3.748113	-1.503129	-2.067119
C22	3.100039	-0.197346	-1.998096
C23	3.064237	2.285405	-2.094484
C24	3.746338	3.545907	-2.259209
C25	2.793964	4.522019	-2.241971
C26	1.534510	3.853191	-2.035607
C27	0.306637	4.485612	-1.881828
H28	0.287749	5.565993	-1.915196
C29	-3.032511	1.087742	-1.043830
H30	-4.109861	1.106982	-0.939051
C31	0.375912	-2.295626	-1.179634
H32	0.410393	-3.367017	-1.044449
C33	3.701945	1.050651	-2.126045
H34	4.778304	1.092010	-2.220519
C35	0.645751	2.308552	3.502468
H36	0.149920	1.860956	4.353630
C37	0.046119	2.351736	2.278254
H38	-0.947309	1.953031	2.125832
C39	0.752832	2.833786	1.116189
H40	0.144797	3.284551	0.347145
C41	2.042148	3.448516	1.327080
H42	2.571850	3.905626	0.500076
C43	2.583891	3.487553	2.598081

O44	3.771790	4.155569	2.795620
C45	4.343904	4.341494	4.055166
O46	5.302457	5.072494	4.110974
C47	3.735741	3.631985	5.177168
C48	2.584151	2.896673	4.975525
O49	1.935007	2.168938	5.898015
H50	2.400559	2.058051	6.718271
C51	1.931847	2.885592	3.695483
H52	-0.595388	2.642116	-5.335795
H53	-2.272347	5.610717	-1.548660
H54	-4.179004	3.689305	-1.232755
H55	-4.119676	-1.505972	-0.512255
H56	-2.086411	-3.441997	-0.524721
H57	2.859225	-3.496045	-1.762715
H58	4.747992	-1.812484	-2.370004
H59	4.823928	3.619167	-2.344257
H60	2.878449	5.590493	-2.401615
H61	4.224379	3.778485	6.182902

Warfarin 7-5 Transition State Quartet

C1	-1.030214	1.862554	-4.657132
H2	-1.674094	1.233788	-5.281307
H3	-1.669369	2.358501	-3.929105
S4	0.130330	0.713244	-3.820134
O5	0.734816	1.352321	0.219846
Fe6	0.391686	1.072503	-1.468395
N7	-1.062491	2.474264	-1.520026
N8	-1.020802	-0.336553	-1.108542
N9	1.778308	-0.349710	-1.687558
N10	1.752964	2.483374	-1.936512
C11	-0.888063	3.829842	-1.669219
C12	-2.144843	4.511417	-1.543536
C13	-3.092350	3.550550	-1.356496
C14	-2.403469	2.286091	-1.324079
C15	-2.374475	-0.147201	-0.954065
C16	-3.031811	-1.414491	-0.688965
C17	-2.062394	-2.370855	-0.704882
C18	-0.820626	-1.678500	-0.996852
C19	1.574945	-1.695891	-1.523256
C20	2.796274	-2.411192	-1.758460
C21	3.750338	-1.498888	-2.079754
C22	3.111911	-0.194043	-2.011769
C23	3.092762	2.277066	-2.080709
C24	3.766419	3.542034	-2.247059
C25	2.806557	4.511250	-2.229596
C26	1.550739	3.833817	-2.020416
C27	0.323089	4.464187	-1.885916
H28	0.302590	5.544017	-1.914173
C29	-3.023917	1.064159	-1.074260
H30	-4.100463	1.080541	-0.965189
C31	0.390377	-2.316505	-1.190171
H32	0.433670	-3.386038	-1.050830
C33	3.728506	1.042919	-2.130266
H34	4.803917	1.074494	-2.225614
C35	0.649792	2.310637	3.509214
H36	0.163992	1.844672	4.355779
C37	0.034340	2.378342	2.299548
H38	-0.958117	1.979909	2.150789
C39	0.722715	2.888175	1.128832

H40	0.111989	3.365529	0.381096
C41	2.027101	3.481072	1.340848
H42	2.542449	3.959024	0.516800
C43	2.581161	3.496687	2.603953
O44	3.770261	4.160120	2.801643
C45	4.342583	4.348599	4.064435
O46	5.294976	5.085464	4.119776
C47	3.739435	3.633954	5.184651
C48	2.591340	2.892464	4.980430
O49	1.944909	2.161246	5.902657
H50	2.405218	2.064132	6.726608
C51	1.938719	2.884373	3.702844
H52	-0.605918	2.638802	-5.333743
H53	-2.260088	5.587399	-1.552670
H54	-4.164297	3.670954	-1.241520
H55	-4.100685	-1.515128	-0.520324
H56	-2.068570	-3.453840	-0.525552
H57	2.867294	-3.493761	-1.772677
H58	4.751881	-1.809602	-2.377062
H59	4.842882	3.619872	-2.333884
H60	2.883914	5.581699	-2.391284
H61	4.227292	3.780518	6.192199

Warfarin 7-6 Reactant Complex Doublet

C1	-0.946032	1.780434	-4.699483
H2	-1.634834	1.248733	-5.369762
H3	-1.554336	2.271255	-3.943150
S4	0.123825	0.519775	-3.942522
O5	0.598435	0.974560	0.084407
Fe6	0.321824	0.940421	-1.534044
N7	-1.109147	2.374565	-1.568592
N8	-1.100057	-0.451022	-1.264461
N9	1.729611	-0.478614	-1.806661
N10	1.706348	2.356229	-2.010758
C11	-0.930097	3.717546	-1.764926
C12	-2.161000	4.430871	-1.565640
C13	-3.107153	3.497263	-1.271421
C14	-2.440052	2.217511	-1.279308
C15	-2.421316	-0.238978	-1.013318
C16	-3.086640	-1.491147	-0.721013
C17	-2.132953	-2.462756	-0.780707
C18	-0.902860	-1.788418	-1.146250
C19	1.517916	-1.814145	-1.665893
C20	2.744042	-2.537407	-1.867648
C21	3.715818	-1.623790	-2.134597
C22	3.072193	-0.318489	-2.062956
C23	3.055947	2.165766	-2.093078
C24	3.733164	3.437081	-2.245949
C25	2.766726	4.395278	-2.307184
C26	1.507696	3.709703	-2.139722
C27	0.279535	4.336215	-2.049668
H28	0.261389	5.414965	-2.136571
C29	-3.054081	0.996315	-1.026191
H30	-4.116553	1.015947	-0.819551
C31	0.314086	-2.428954	-1.347652
H32	0.356634	-3.501409	-1.214251
C33	3.689281	0.925317	-2.117671
H34	4.768428	0.960258	-2.153852
C35	0.658632	2.707282	3.506227

H36	0.218211	2.149505	4.322464
C37	-0.007685	2.888411	2.312852
H38	-0.990273	2.460880	2.157226
C39	0.604054	3.609968	1.278389
H40	0.073518	3.734868	0.351361
C41	1.885194	4.119565	1.410255
H42	2.375035	4.646053	0.600453
C43	2.530175	3.980503	2.637971
O44	3.750749	4.573148	2.787399
C45	4.354665	4.743339	4.027544
O46	5.365023	5.400963	4.040144
C47	3.698463	4.115098	5.168655
C48	2.571616	3.344171	4.986158
O49	1.899133	2.680695	5.932073
H50	2.325263	2.662044	6.782370
C51	1.929078	3.292172	3.695225
H52	-0.465702	2.563100	-5.310354
H53	-2.260404	5.509424	-1.606451
H54	-4.158835	3.674191	-1.069637
H55	-4.153345	-1.536121	-0.531498
H56	-2.134106	-3.534106	-0.571230
H57	2.794471	-3.617207	-1.849749
H58	4.736481	-1.921846	-2.381863
H59	4.813222	3.560520	-2.269402
H60	2.850397	5.471012	-2.467763
H61	4.062679	4.448564	6.167347

Warfarin 7-6 Reactant Complex Quartet

C1	-0.934771	1.788903	-4.693198
H2	-1.623869	1.249332	-5.357600
H3	-1.541163	2.280655	-3.936710
S4	0.142418	0.536720	-3.936331
O5	0.572106	0.974702	0.092026
Fe6	0.326914	0.934180	-1.525925
N7	-1.107928	2.370681	-1.566504
N8	-1.098312	-0.456733	-1.264585
N9	1.732410	-0.481511	-1.800607
N10	1.711542	2.350535	-2.002701
C11	-0.928983	3.712094	-1.761613
C12	-2.158841	4.426577	-1.561793
C13	-3.105641	3.493702	-1.265998
C14	-2.439901	2.212439	-1.274905
C15	-2.417646	-0.244056	-1.014041
C16	-3.083729	-1.494600	-0.719050
C17	-2.130414	-2.468374	-0.775658
C18	-0.899256	-1.795286	-1.142213
C19	1.519409	-1.816979	-1.662847
C20	2.746134	-2.539371	-1.868968
C21	3.718760	-1.625038	-2.136667
C22	3.075650	-0.319701	-2.060760
C23	3.060676	2.162012	-2.086152
C24	3.735509	3.435190	-2.241529
C25	2.767321	4.391215	-2.304914
C26	1.509629	3.704675	-2.135748
C27	0.282299	4.330603	-2.047934
H28	0.264994	5.409492	-2.134979
C29	-3.052785	0.992632	-1.025926
H30	-4.114747	1.009303	-0.816259
C31	0.317076	-2.433684	-1.342911

H32	0.360243	-3.506190	-1.207242
C33	3.694832	0.921315	-2.112642
H34	4.774015	0.953934	-2.148372
C35	0.660088	2.709899	3.512750
H36	0.220377	2.150651	4.328285
C37	-0.007419	2.891225	2.319539
H38	-0.990496	2.464928	2.163329
C39	0.605639	3.610907	1.284125
H40	0.074711	3.734013	0.357645
C41	1.888181	4.117973	1.416051
H42	2.379096	4.640134	0.602526
C43	2.532553	3.980418	2.643222
O44	3.755548	4.569999	2.792256
C45	4.359664	4.740839	4.032979
O46	5.369939	5.398455	4.044960
C47	3.702959	4.113841	5.173967
C48	2.572982	3.345793	4.992616
O49	1.899148	2.685238	5.938735
H50	2.325329	2.663879	6.786747
C51	1.930062	3.295040	3.700045
H52	-0.459792	2.569548	-5.310256
H53	-2.258481	5.505293	-1.604836
H54	-4.157844	3.671430	-1.067488
H55	-4.149782	-1.538121	-0.528689
H56	-2.132896	-3.538484	-0.564943
H57	2.797094	-3.618580	-1.850221
H58	4.740025	-1.922117	-2.383255
H59	4.814735	3.559977	-2.268165
H60	2.849933	5.467385	-2.467858
H61	4.066546	4.448491	6.173055

Warfarin 7-6 Transition State Doublet

C1	-0.922706	1.756310	-4.615943
H2	-1.592944	1.177889	-5.265557
H3	-1.547210	2.259819	-3.881258
S4	0.173887	0.547072	-3.795515
O5	0.780084	1.287071	0.265518
Fe6	0.368102	1.082477	-1.450944
N7	-1.071657	2.471112	-1.498358
N8	-1.030935	-0.344938	-1.080310
N9	1.789404	-0.376827	-1.633902
N10	1.724599	2.464479	-1.968353
C11	-0.908933	3.820593	-1.719023
C12	-2.154318	4.510015	-1.543304
C13	-3.090216	3.564855	-1.253453
C14	-2.402309	2.298262	-1.224404
C15	-2.370204	-0.151426	-0.887734
C16	-3.040257	-1.415595	-0.651117
C17	-2.080682	-2.380593	-0.705293
C18	-0.841009	-1.687494	-1.003570
C19	1.574540	-1.717110	-1.514574
C20	2.786846	-2.447277	-1.777126
C21	3.751473	-1.536387	-2.069897
C22	3.113007	-0.226660	-1.958271
C23	3.076525	2.258060	-2.059469
C24	3.753959	3.522414	-2.233719
C25	2.790919	4.485837	-2.289906
C26	1.530508	3.810647	-2.108998
C27	0.296133	4.440748	-2.008129

H28	0.274972	5.517533	-2.109336
C29	-3.010302	1.073945	-0.948074
H30	-4.079966	1.085485	-0.783039
C31	0.373194	-2.331024	-1.210141
H32	0.402393	-3.408123	-1.111201
C33	3.716332	1.023138	-2.069684
H34	4.793101	1.065283	-2.146981
C35	0.541476	2.505294	3.477891
H36	0.052859	2.118341	4.360748
C37	-0.065986	2.474323	2.257297
H38	-1.071138	2.091494	2.140233
C39	0.632413	2.887065	1.063844
H40	0.012065	3.300108	0.283928
C41	1.921322	3.514860	1.230145
H42	2.447191	3.921938	0.374451
C43	2.467681	3.632445	2.490628
O44	3.652786	4.313966	2.630946
C45	4.197728	4.647952	3.871428
O46	5.156536	5.376361	3.854375
C47	3.559795	4.078643	5.055409
C48	2.436028	3.290443	4.917247
O49	1.759117	2.690243	5.907147
H50	2.157707	2.762780	6.766149
C51	1.822966	3.108320	3.628583
H52	-0.465640	2.532739	-5.259489
H53	-2.268037	5.580615	-1.600132
H54	-4.150263	3.715480	-1.073755
H55	-4.114305	-1.486674	-0.516010
H56	-2.090196	-3.463786	-0.533506
H57	2.825486	-3.530269	-1.807070
H58	4.754803	-1.848450	-2.366982
H59	4.834344	3.623822	-2.271191
H60	2.872249	5.552903	-2.464315
H61	3.962887	4.430406	6.047624

Warfarin 7-6 Transition State Quartet

C1	-0.931861	1.765528	-4.619709
H2	-1.592956	1.170318	-5.260937
H3	-1.563007	2.271738	-3.891332
S4	0.184546	0.587805	-3.788867
O5	0.686651	1.385641	0.226110
Fe6	0.390776	1.036898	-1.462906
N7	-1.074188	2.439973	-1.544735
N8	-1.016323	-0.368728	-1.096306
N9	1.779489	-0.384218	-1.653623
N10	1.751291	2.443986	-1.955395
C11	-0.899045	3.789532	-1.741004
C12	-2.142166	4.482184	-1.556075
C13	-3.082743	3.537821	-1.270142
C14	-2.402838	2.267286	-1.256169
C15	-2.359875	-0.167197	-0.906763
C16	-3.029309	-1.428927	-0.662274
C17	-2.074282	-2.397809	-0.714288
C18	-0.829084	-1.716602	-1.018886
C19	1.564240	-1.733677	-1.536352
C20	2.780919	-2.449782	-1.793902
C21	3.745259	-1.535281	-2.084650
C22	3.114858	-0.227945	-1.976080
C23	3.096721	2.244546	-2.051709

C24	3.765697	3.513257	-2.228362
C25	2.796127	4.470165	-2.282527
C26	1.539234	3.786740	-2.098145
C27	0.305912	4.414776	-2.011615
H28	0.283336	5.491177	-2.104732
C29	-3.008843	1.049097	-0.972640
H30	-4.076080	1.056355	-0.798576
C31	0.375534	-2.360867	-1.229103
H32	0.413284	-3.436501	-1.131061
C33	3.733638	1.009102	-2.075871
H34	4.809498	1.041449	-2.150493
C35	0.555235	2.515465	3.488897
H36	0.063714	2.127748	4.370114
C37	-0.062366	2.503941	2.279422
H38	-1.067961	2.124340	2.163807
C39	0.617393	2.949398	1.076604
H40	-0.005903	3.395831	0.321124
C41	1.916108	3.568115	1.250030
H42	2.418219	4.012927	0.400898
C43	2.473338	3.659332	2.504990
O44	3.651005	4.345964	2.650077
C45	4.208698	4.660078	3.891746
O46	5.174113	5.379541	3.875142
C47	3.575331	4.085874	5.073736
C48	2.451583	3.289841	4.930589
O49	1.780849	2.684159	5.916693
H50	2.183962	2.754368	6.773607
C51	1.840259	3.113843	3.643837
H52	-0.472466	2.537152	-5.267755
H53	-2.257523	5.555644	-1.602534
H54	-4.140910	3.697824	-1.080890
H55	-4.103992	-1.494879	-0.520820
H56	-2.085164	-3.477689	-0.536482
H57	2.827184	-3.532764	-1.814500
H58	4.750153	-1.847085	-2.374564
H59	4.844538	3.621010	-2.269852
H60	2.872265	5.539456	-2.456504
H61	3.974285	4.438624	6.066928

Warfarin 7-7 Reactant Complex Doublet

C1	-0.905479	1.700784	-4.762753
H2	-1.488675	1.093088	-5.465079
H3	-1.601262	2.140854	-4.049752
S4	0.214694	0.538882	-3.927665
O5	0.609154	0.946563	0.111295
Fe6	0.350348	0.935342	-1.511543
N7	-1.083151	2.365518	-1.559995
N8	-1.074529	-0.457386	-1.260401
N9	1.762100	-0.482933	-1.778218
N10	1.739703	2.351163	-1.967826
C11	-0.896948	3.715885	-1.701978
C12	-2.136364	4.424656	-1.537471
C13	-3.092240	3.483537	-1.307028
C14	-2.424336	2.202482	-1.322516
C15	-2.406908	-0.254069	-1.060277
C16	-3.066903	-1.507958	-0.758277
C17	-2.098566	-2.464769	-0.743666
C18	-0.863293	-1.787375	-1.083511
C19	1.559665	-1.814193	-1.591752

C20	2.781345	-2.539672	-1.808292
C21	3.738854	-1.630784	-2.137395
C22	3.094590	-0.327300	-2.079667
C23	3.085363	2.154961	-2.114761
C24	3.758210	3.425162	-2.284411
C25	2.795681	4.388394	-2.278685
C26	1.544650	3.706364	-2.060338
C27	0.320404	4.336844	-1.930636
H28	0.310132	5.418441	-1.982722
C29	-3.045400	0.978518	-1.102186
H30	-4.113462	0.995561	-0.925506
C31	0.361445	-2.421401	-1.237281
H32	0.411891	-3.485562	-1.047913
C33	3.713921	0.915650	-2.170695
H34	4.791034	0.943816	-2.255832
C35	0.623766	2.524932	3.735187
H36	0.175502	1.971703	4.554032
C37	-0.084454	2.718020	2.564825
H38	-1.069740	2.287675	2.441499
C39	0.481703	3.465287	1.522930
H40	-0.077514	3.600732	0.609385
C41	1.762157	3.984477	1.627550
H42	2.220047	4.539230	0.816928
C43	2.447731	3.835121	2.830042
O44	3.647328	4.479566	2.953426
C45	4.255929	4.682065	4.186683
O46	5.235718	5.379651	4.202348
C47	3.654238	3.999852	5.323682
C48	2.598954	3.147959	5.159689
O49	2.116160	2.444595	6.210735
H50	1.746619	1.617126	5.909419
C51	1.901495	3.101926	3.893615
H52	-0.470501	2.515549	-5.364911
H53	-2.234834	5.507122	-1.567518
H54	-4.151803	3.648233	-1.133047
H55	-4.137584	-1.579936	-0.610951
H56	-2.099827	-3.531011	-0.512284
H57	2.841164	-3.618421	-1.792432
H58	4.748602	-1.927718	-2.419995
H59	4.834660	3.535063	-2.370281
H60	2.872164	5.464221	-2.442811
H61	4.011721	4.296688	6.325605

Warfarin 7-7 Reactant Complex Quartet

C1	-0.899165	1.708655	-4.754411
H2	-1.482727	1.096419	-5.452197
H3	-1.592184	2.149150	-4.038773
S4	0.224749	0.551464	-3.921379
O5	0.587757	0.962949	0.115472
Fe6	0.353521	0.933824	-1.504099
N7	-1.083485	2.365383	-1.564072
N8	-1.072588	-0.457424	-1.251950
N9	1.764889	-0.481912	-1.768124
N10	1.739489	2.349574	-1.969969
C11	-0.897663	3.714520	-1.704133
C12	-2.137153	4.423666	-1.540766
C13	-3.093684	3.482075	-1.311485
C14	-2.424899	2.200576	-1.326558
C15	-2.404536	-0.254295	-1.053765

C16	-3.064725	-1.507470	-0.752314
C17	-2.095834	-2.465100	-0.736767
C18	-0.860963	-1.787253	-1.075183
C19	1.560496	-1.814243	-1.585318
C20	2.782956	-2.538748	-1.806072
C21	3.739455	-1.629135	-2.134269
C22	3.097792	-0.324965	-2.072178
C23	3.084839	2.154925	-2.116036
C24	3.756769	3.425173	-2.287374
C25	2.793054	4.388092	-2.282924
C26	1.542386	3.705410	-2.063835
C27	0.320057	4.337242	-1.932874
H28	0.310435	5.418237	-1.984528
C29	-3.046031	0.979338	-1.103490
H30	-4.113409	0.997776	-0.929687
C31	0.363822	-2.422368	-1.233044
H32	0.411733	-3.486213	-1.049570
C33	3.715973	0.916292	-2.166003
H34	4.793195	0.948798	-2.252028
C35	0.628320	2.536485	3.737383
H36	0.177507	1.983461	4.554915
C37	-0.078690	2.733245	2.567541
H38	-1.063602	2.301152	2.441701
C39	0.487670	3.484080	1.527349
H40	-0.070487	3.622738	0.614721
C41	1.769607	3.998577	1.634282
H42	2.229038	4.554867	0.823785
C43	2.456111	3.844894	2.834599
O44	3.657323	4.483620	2.958836
C45	4.264968	4.684338	4.192734
O46	5.247926	5.379799	4.210120
C47	3.659931	4.002911	5.328363
C48	2.605755	3.155035	5.162653
O49	2.119947	2.450490	6.213615
H50	1.744148	1.626356	5.910692
C51	1.906679	3.109941	3.897018
H52	-0.467585	2.521474	-5.361976
H53	-2.235396	5.505602	-1.569479
H54	-4.152551	3.647484	-1.134022
H55	-4.136357	-1.579915	-0.608315
H56	-2.096542	-3.531652	-0.506515
H57	2.842721	-3.618108	-1.792820
H58	4.748344	-1.925641	-2.421923
H59	4.833350	3.537221	-2.369761
H60	2.870116	5.463459	-2.445540
H61	4.017264	4.300159	6.330379

Warfarin 7-7 Transition State Doublet

C1	-0.882257	1.677727	-4.667226
H2	-1.451959	1.022255	-5.335783
H3	-1.586908	2.132815	-3.972217
S4	0.263021	0.571531	-3.769248
O5	0.760266	1.250381	0.326072
Fe6	0.387926	1.078672	-1.395727
N7	-1.053365	2.462145	-1.474478
N8	-1.015719	-0.350548	-1.057190
N9	1.812087	-0.380715	-1.588084
N10	1.748209	2.460580	-1.901881
C11	-0.886632	3.815327	-1.663261

C12	-2.138315	4.503071	-1.521873
C13	-3.083064	3.551086	-1.278965
C14	-2.393754	2.283805	-1.246822
C15	-2.362256	-0.165699	-0.909875
C16	-3.026624	-1.432938	-0.671162
C17	-2.056140	-2.387413	-0.664615
C18	-0.814658	-1.689241	-0.936066
C19	1.603252	-1.718026	-1.442216
C20	2.809095	-2.451641	-1.721794
C21	3.763018	-1.542204	-2.055993
C22	3.128078	-0.233433	-1.947356
C23	3.095024	2.250254	-2.047530
C24	3.769306	3.511055	-2.247473
C25	2.809498	4.479688	-2.256984
C26	1.555706	3.808845	-2.028736
C27	0.324090	4.440480	-1.910833
H28	0.306059	5.518457	-1.995730
C29	-3.007638	1.057957	-0.996876
H30	-4.081350	1.067014	-0.862347
C31	0.405969	-2.328395	-1.111675
H32	0.439818	-3.400930	-0.978971
C33	3.731616	1.013952	-2.083083
H34	4.804847	1.052889	-2.206177
C35	0.537446	2.366219	3.611636
H36	0.028360	1.985182	4.492363
C37	-0.090880	2.354154	2.397693
H38	-1.095593	1.969638	2.294034
C39	0.581180	2.809639	1.201729
H40	-0.060710	3.222402	0.436009
C41	1.852024	3.465949	1.371745
H42	2.348034	3.923088	0.523178
C43	2.422430	3.555535	2.626285
O44	3.582268	4.278752	2.769215
C45	4.125912	4.611462	4.012783
O46	5.064215	5.363734	4.012732
C47	3.529072	3.974835	5.181323
C48	2.476717	3.111786	5.032326
O49	1.982387	2.449508	6.110698
H50	1.668153	1.587263	5.839767
C51	1.819358	2.963362	3.761664
H52	-0.470010	2.481967	-5.310684
H53	-2.247062	5.576941	-1.566429
H54	-4.148278	3.693607	-1.122196
H55	-4.102312	-1.527030	-0.576921
H56	-2.065897	-3.468884	-0.478821
H57	2.858766	-3.533030	-1.763385
H58	4.752901	-1.858714	-2.382115
H59	4.845653	3.599441	-2.341403
H60	2.886255	5.545050	-2.437660
H61	3.912492	4.273222	6.189274

Warfarin 7-7 Transition State Quartet

C1	-0.894140	1.684260	-4.668324
H2	-1.451895	1.016849	-5.333577
H3	-1.606642	2.137746	-3.979717
S4	0.264262	0.604050	-3.763094
O5	0.668021	1.343140	0.282446
Fe6	0.408305	1.042217	-1.409724
N7	-1.053626	2.438695	-1.521972

N8	-1.001242	-0.367380	-1.070667
N9	1.805186	-0.381108	-1.607245
N10	1.773480	2.445881	-1.892273
C11	-0.876334	3.792274	-1.689084
C12	-2.126710	4.481398	-1.538406
C13	-3.073953	3.530385	-1.298132
C14	-2.390857	2.261033	-1.279604
C15	-2.353724	-0.174968	-0.925354
C16	-3.016182	-1.440792	-0.678745
C17	-2.048228	-2.397368	-0.670167
C18	-0.801960	-1.708729	-0.947617
C19	1.596382	-1.729414	-1.461615
C20	2.806936	-2.448456	-1.738802
C21	3.758500	-1.538036	-2.072374
C22	3.131160	-0.230049	-1.965859
C23	3.115121	2.241918	-2.042283
C24	3.781298	3.507779	-2.242487
C25	2.815520	4.469872	-2.251784
C26	1.564847	3.791212	-2.021820
C27	0.333778	4.420654	-1.918569
H28	0.314197	5.498555	-1.997982
C29	-3.003363	1.038616	-1.019322
H30	-4.075369	1.046847	-0.873940
C31	0.411481	-2.347984	-1.126916
H32	0.452436	-3.420088	-0.992545
C33	3.748343	1.007060	-2.091306
H34	4.821879	1.036498	-2.209249
C35	0.544057	2.362889	3.619517
H36	0.034527	1.978133	4.498337
C37	-0.095930	2.374182	2.415450
H38	-1.102511	1.995639	2.314743
C39	0.555036	2.861908	1.214757
H40	-0.091829	3.298594	0.470299
C41	1.834177	3.508116	1.390526
H42	2.308408	3.999585	0.550002
C43	2.417304	3.567251	2.638353
O44	3.570755	4.297213	2.782861
C45	4.125509	4.617676	4.026976
O46	5.064488	5.366691	4.024745
C47	3.534056	3.974755	5.193253
C48	2.484165	3.105249	5.041541
O49	1.992135	2.443097	6.122622
H50	1.671321	1.584272	5.852648
C51	1.829991	2.955552	3.773866
H52	-0.477579	2.484358	-5.315357
H53	-2.237961	5.557465	-1.572259
H54	-4.138063	3.679469	-1.129412
H55	-4.092418	-1.531490	-0.578577
H56	-2.058256	-3.477158	-0.480872
H57	2.861629	-3.531581	-1.773231
H58	4.753930	-1.849965	-2.392963
H59	4.856093	3.601932	-2.336562
H60	2.885901	5.536976	-2.431970
H61	3.917681	4.275622	6.203002

Warfarin 7-8 Reactant Complex Doublet

C1	-1.035683	1.973297	-4.741800
H2	-1.720082	1.429521	-5.403353
H3	-1.647481	2.459294	-3.984413

S4	0.048190	0.705338	-3.997887
O5	0.615845	0.944895	0.048075
Fe6	0.317121	0.999723	-1.565351
N7	-1.106885	2.432483	-1.560456
N8	-1.098826	-0.403322	-1.308444
N9	1.724035	-0.415502	-1.877306
N10	1.697034	2.425483	-2.008147
C11	-0.930319	3.782680	-1.708358
C12	-2.174144	4.484370	-1.548015
C13	-3.126621	3.533969	-1.335844
C14	-2.450413	2.257796	-1.348616
C15	-2.428062	-0.203025	-1.095411
C16	-3.078787	-1.452616	-0.759650
C17	-2.106094	-2.408027	-0.747873
C18	-0.876785	-1.729852	-1.114176
C19	1.540952	-1.745928	-1.661928
C20	2.779494	-2.454349	-1.851609
C21	3.727873	-1.534496	-2.180599
C22	3.061448	-0.243104	-2.143833
C23	3.041458	2.234695	-2.145083
C24	3.717527	3.500073	-2.321908
C25	2.755185	4.462755	-2.335332
C26	1.502733	3.781166	-2.109695
C27	0.280256	4.410913	-1.966623
H28	0.263858	5.490767	-2.030947
C29	-3.070183	1.029430	-1.153222
H30	-4.143782	1.043600	-1.019690
C31	0.353255	-2.356384	-1.273884
H32	0.416168	-3.412167	-1.049096
C33	3.676951	0.999670	-2.196638
H34	4.755746	1.037489	-2.241477
C35	0.624273	2.590334	3.623426
H36	0.137477	2.057182	4.435412
C37	-0.026909	2.763304	2.417776
H38	-1.001837	2.327218	2.246976
C39	0.587188	3.503730	1.396713
H40	0.072098	3.618911	0.458954
C41	1.853590	4.039543	1.555879
H42	2.344368	4.590774	0.761084
C43	2.483653	3.904650	2.788844
O44	3.669570	4.559780	2.964610
C45	4.211827	4.780674	4.228584
O46	5.219502	5.433795	4.286408
C47	3.514013	4.157906	5.342550
C48	2.508325	3.264535	5.131825
O49	1.986943	2.562759	6.165953
H50	1.683760	1.710794	5.857632
C51	1.889662	3.174769	3.829515
H52	-0.578544	2.760075	-5.371930
H53	-2.277752	5.566517	-1.561348
H54	-4.187802	3.686782	-1.171176
H55	-4.140829	-1.525770	-0.551966
H56	-2.105150	-3.473645	-0.511515
H57	2.861167	-3.528618	-1.801155
H58	4.753656	-1.798104	-2.454903
H59	4.795617	3.594298	-2.398340
H60	2.833763	5.533445	-2.518152
H61	3.803615	4.455956	6.360126

Warfarin 7-8 Reactant Complex Quartet

C1	-1.025092	1.983433	-4.734508
H2	-1.712441	1.433250	-5.388185
H3	-1.632135	2.471938	-3.975129
S4	0.066211	0.723406	-3.992211
O5	0.587926	0.972539	0.054881
Fe6	0.316818	0.991557	-1.558727
N7	-1.111121	2.425236	-1.561732
N8	-1.099788	-0.411621	-1.303252
N9	1.721900	-0.421287	-1.866442
N10	1.695908	2.416222	-2.007461
C11	-0.933887	3.772872	-1.707800
C12	-2.177329	4.476003	-1.546229
C13	-3.130371	3.525901	-1.334840
C14	-2.455535	2.248706	-1.349161
C15	-2.428154	-0.210906	-1.093298
C16	-3.079105	-1.460593	-0.756602
C17	-2.107342	-2.415739	-0.743853
C18	-0.876783	-1.739554	-1.109148
C19	1.538391	-1.752599	-1.656851
C20	2.776575	-2.460105	-1.851480
C21	3.724429	-1.541254	-2.179397
C22	3.060570	-0.249012	-2.137531
C23	3.040010	2.226461	-2.142100
C24	3.714229	3.492666	-2.321478
C25	2.751295	4.454880	-2.337397
C26	1.498333	3.773670	-2.111878
C27	0.277504	4.402431	-1.969070
H28	0.259858	5.481215	-2.032098
C29	-3.073817	1.021287	-1.156793
H30	-4.147625	1.033181	-1.028037
C31	0.350072	-2.365723	-1.271847
H32	0.413942	-3.422851	-1.053803
C33	3.677088	0.992447	-2.190545
H34	4.755361	1.029670	-2.235405
C35	0.630615	2.602464	3.621504
H36	0.145251	2.062727	4.427983
C37	-0.019286	2.783460	2.416762
H38	-0.992604	2.345110	2.242612
C39	0.592043	3.531213	1.402098
H40	0.073568	3.658660	0.466838
C41	1.858721	4.067604	1.563429
H42	2.345176	4.626464	0.773164
C43	2.491351	3.923711	2.794502
O44	3.678840	4.573596	2.973560
C45	4.222410	4.786279	4.237891
O46	5.232074	5.438615	4.299244
C47	3.524158	4.158588	5.348830
C48	2.515977	3.270592	5.136234
O49	1.993295	2.564347	6.164365
H50	1.688486	1.715370	5.852079
C51	1.896508	3.188371	3.832913
H52	-0.573511	2.767593	-5.372218
H53	-2.278493	5.558627	-1.558670
H54	-4.191012	3.680479	-1.169738
H55	-4.141860	-1.532247	-0.550161
H56	-2.106910	-3.482441	-0.507271
H57	2.859008	-3.535456	-1.804060
H58	4.749443	-1.804870	-2.455016
H59	4.792535	3.588082	-2.396291

H60	2.830558	5.525755	-2.519152
H61	3.812460	4.457199	6.368363

Warfarin 7-8 Transition State Doublet

C1	-1.009925	1.947077	-4.650445
H2	-1.680444	1.359249	-5.287463
H3	-1.633058	2.447967	-3.912538
S4	0.095917	0.722696	-3.840921
O5	0.801358	1.288577	0.261763
Fe6	0.360953	1.137417	-1.455211
N7	-1.072929	2.522535	-1.482985
N8	-1.030231	-0.302676	-1.090741
N9	1.779257	-0.323313	-1.676534
N10	1.708826	2.524176	-1.960116
C11	-0.913868	3.877187	-1.672442
C12	-2.171483	4.555105	-1.533600
C13	-3.111147	3.593489	-1.312640
C14	-2.413867	2.331291	-1.280414
C15	-2.377084	-0.121592	-0.942227
C16	-3.036234	-1.386468	-0.678721
C17	-2.062367	-2.339254	-0.671372
C18	-0.822851	-1.639842	-0.959613
C19	1.588495	-1.661591	-1.504205
C20	2.809635	-2.381948	-1.762760
C21	3.754238	-1.464157	-2.101724
C22	3.098500	-0.164786	-2.011198
C23	3.055429	2.314814	-2.093651
C24	3.733838	3.570717	-2.294598
C25	2.776965	4.539901	-2.318563
C26	1.519416	3.873187	-2.085639
C27	0.290388	4.506012	-1.945503
H28	0.269012	5.584513	-2.029070
C29	-3.025109	1.099322	-1.052364
H30	-4.103008	1.103774	-0.961490
C31	0.399982	-2.275591	-1.145372
H32	0.441562	-3.345134	-0.992708
C33	3.698854	1.084532	-2.121227
H34	4.775009	1.133056	-2.207316
C35	0.524219	2.425114	3.532964
H36	-0.006336	2.058119	4.404865
C37	-0.065082	2.408934	2.301311
H38	-1.069819	2.029239	2.166834
C39	0.644225	2.853823	1.124677
H40	0.027222	3.286705	0.350825
C41	1.921301	3.499054	1.322437
H42	2.440665	3.950340	0.486749
C43	2.449602	3.602056	2.594370
O44	3.601195	4.328142	2.773020
C45	4.083332	4.697002	4.036309
O46	5.041172	5.416210	4.065315
C47	3.401910	4.120185	5.189396
C48	2.390264	3.214978	5.008439
O49	1.864545	2.560500	6.074282
H50	1.623586	1.674878	5.811214
C51	1.803154	3.024549	3.712583
H52	-0.573900	2.728270	-5.315347
H53	-2.285230	5.628871	-1.559444
H54	-4.178595	3.722621	-1.164757
H55	-4.107135	-1.486365	-0.529515

H56	-2.071372	-3.420205	-0.481095
H57	2.875129	-3.463450	-1.768808
H58	4.761041	-1.746075	-2.421889
H59	4.812305	3.640833	-2.378004
H60	2.856578	5.599846	-2.516142
H61	3.719566	4.425773	6.215209

Warfarin 7-8 Transition State Quartet

C1	-1.017248	1.948709	-4.651292
H2	-1.676111	1.342138	-5.280853
H3	-1.647905	2.449271	-3.918768
S4	0.111203	0.758086	-3.828522
O5	0.707244	1.377306	0.227696
Fe6	0.386557	1.092740	-1.468723
N7	-1.069971	2.493948	-1.523752
N8	-1.011911	-0.326045	-1.108988
N9	1.776040	-0.329566	-1.690276
N10	1.741789	2.503529	-1.942155
C11	-0.898636	3.848099	-1.689509
C12	-2.154726	4.528455	-1.543084
C13	-3.098843	3.567519	-1.328430
C14	-2.408556	2.302201	-1.311705
C15	-2.364385	-0.136373	-0.963320
C16	-3.021397	-1.399559	-0.690012
C17	-2.050998	-2.354624	-0.679229
C18	-0.806302	-1.666385	-0.973997
C19	1.584393	-1.677923	-1.519541
C20	2.810072	-2.384530	-1.774588
C21	3.754755	-1.463483	-2.107926
C22	3.107426	-0.165761	-2.019555
C23	3.081642	2.300856	-2.078776
C24	3.752312	3.562130	-2.280462
C25	2.788583	4.524661	-2.303138
C26	1.534295	3.849252	-2.069052
C27	0.306479	4.480435	-1.942761
H28	0.284606	5.558514	-2.019065
C29	-3.019108	1.074043	-1.078542
H30	-4.095564	1.075193	-0.979852
C31	0.408852	-2.302958	-1.159868
H32	0.458783	-3.371179	-1.005364
C33	3.722806	1.071592	-2.117989
H34	4.798709	1.110217	-2.196521
C35	0.535917	2.418750	3.547775
H36	0.005181	2.046519	4.419509
C37	-0.069166	2.424878	2.329722
H38	-1.074711	2.051525	2.199176
C39	0.618867	2.903907	1.143627
H40	-0.003872	3.360336	0.391738
C41	1.903347	3.540521	1.346799
H42	2.397575	4.029188	0.517344
C43	2.446233	3.615001	2.609926
O44	3.589307	4.349631	2.790219
C45	4.083666	4.703485	4.054469
O46	5.043385	5.421476	4.081372
C47	3.409108	4.116428	5.205748
C48	2.407490	3.204333	5.024949
O49	1.887501	2.544753	6.090090
H50	1.640837	1.661692	5.828013
C51	1.816896	3.012713	3.730856

H52	-0.582581	2.725351	-5.323541
H53	-2.272036	5.604514	-1.559544
H54	-4.165951	3.703111	-1.174678
H55	-4.092388	-1.498247	-0.536188
H56	-2.063312	-3.434283	-0.483290
H57	2.884154	-3.466069	-1.781796
H58	4.764741	-1.746210	-2.419975
H59	4.829177	3.637661	-2.362189
H60	2.862754	5.586809	-2.499837
H61	3.726480	4.425842	6.231821

Warfarin 7-9 Reactant Complex Doublet

C1	-0.751127	1.990302	-4.822178
H2	-1.499762	1.404504	-5.368884
H3	-1.285430	2.561871	-4.065403
S4	0.358537	0.785785	-4.035260
O5	0.618446	0.865693	0.050767
Fe6	0.370781	0.970939	-1.565163
N7	-1.052789	2.415809	-1.587440
N8	-1.065719	-0.421634	-1.364791
N9	1.775982	-0.438627	-1.863537
N10	1.763994	2.402229	-1.955750
C11	-0.868354	3.765746	-1.731125
C12	-2.110167	4.471970	-1.586416
C13	-3.068222	3.528091	-1.374671
C14	-2.399517	2.248303	-1.377842
C15	-2.386679	-0.208637	-1.109730
C16	-3.036514	-1.449945	-0.741066
C17	-2.072611	-2.413701	-0.753392
C18	-0.846349	-1.749310	-1.155127
C19	1.575303	-1.771828	-1.685907
C20	2.807659	-2.488077	-1.886435
C21	3.767270	-1.568692	-2.187581
C22	3.117160	-0.270129	-2.113834
C23	3.111108	2.206967	-2.070235
C24	3.788812	3.473687	-2.233543
C25	2.827833	4.438124	-2.269561
C26	1.570990	3.760178	-2.067084
C27	0.349614	4.392251	-1.957806
H28	0.336126	5.472063	-2.034549
C29	-3.022848	1.026754	-1.161875
H30	-4.092632	1.049825	-1.001902
C31	0.379693	-2.381049	-1.318012
H32	0.436645	-3.439891	-1.103692
C33	3.741749	0.971134	-2.130069
H34	4.821482	1.007542	-2.157624
C35	0.553625	2.495064	3.701269
H36	0.123138	1.946887	4.530956
C37	-0.162272	2.638724	2.526790
H38	-1.137879	2.181675	2.418582
C39	0.380294	3.374303	1.466798
H40	-0.181665	3.466113	0.551305
C41	1.653238	3.914221	1.546004
H42	2.103457	4.441026	0.713294
C43	2.333843	3.837439	2.759629
O44	3.503343	4.530537	2.862410
C45	4.082658	4.831939	4.093890
O46	5.050153	5.538492	4.077086
C47	3.459289	4.216621	5.262851

C48	2.466227	3.294788	5.127906
O49	2.002786	2.621902	6.208390
H50	1.648255	1.774897	5.942703
C51	1.803768	3.132601	3.849837
H52	-0.330555	2.701619	-5.557832
H53	-2.213348	5.554255	-1.599697
H54	-4.126756	3.696702	-1.212194
H55	-4.094652	-1.511797	-0.501081
H56	-2.079927	-3.481522	-0.517305
H57	2.875478	-3.564692	-1.863353
H58	4.785137	-1.839513	-2.472593
H59	4.866830	3.569361	-2.290272
H60	2.903390	5.510327	-2.459503
H61	3.787910	4.584360	6.253118

Warfarin 7-9 Reactant Complex Quartet

C1	-0.746445	2.001823	-4.822655
H2	-1.494424	1.410894	-5.364052
H3	-1.280895	2.575821	-4.067244
S4	0.369969	0.805064	-4.037062
O5	0.583964	0.910527	0.048073
Fe6	0.372799	0.970840	-1.570057
N7	-1.056016	2.413360	-1.605324
N8	-1.063275	-0.425366	-1.367279
N9	1.777080	-0.440653	-1.854030
N10	1.767439	2.397918	-1.964679
C11	-0.868596	3.762423	-1.739906
C12	-2.109898	4.469128	-1.585126
C13	-3.068138	3.525625	-1.373980
C14	-2.402000	2.244407	-1.388326
C15	-2.385019	-0.212222	-1.117700
C16	-3.035143	-1.453676	-0.748121
C17	-2.071937	-2.417638	-0.757237
C18	-0.844786	-1.754322	-1.156728
C19	1.575343	-1.774627	-1.682866
C20	2.805803	-2.491544	-1.890712
C21	3.765870	-1.572633	-2.192149
C22	3.118037	-0.273323	-2.113291
C23	3.114058	2.202918	-2.074024
C24	3.791336	3.470887	-2.232913
C25	2.829213	4.435084	-2.270020
C26	1.571177	3.756717	-2.073782
C27	0.351071	4.388251	-1.963895
H28	0.340226	5.469381	-2.029491
C29	-3.023524	1.022221	-1.175302
H30	-4.093909	1.040671	-1.017799
C31	0.378319	-2.387022	-1.322545
H32	0.432239	-3.449325	-1.128160
C33	3.744329	0.965607	-2.133056
H34	4.823764	0.998041	-2.167045
C35	0.554155	2.515709	3.705329
H36	0.126967	1.960693	4.532495
C37	-0.166403	2.669416	2.536048
H38	-1.142080	2.214312	2.426319
C39	0.372218	3.413873	1.478706
H40	-0.194688	3.514385	0.566654
C41	1.645699	3.951644	1.559569
H42	2.088628	4.492415	0.731183
C43	2.333615	3.859676	2.765900

O44	3.508789	4.545699	2.869101
C45	4.092631	4.834722	4.100341
O46	5.064815	5.537799	4.085160
C47	3.470468	4.217678	5.268148
C48	2.472587	3.297376	5.130268
O49	2.006105	2.625193	6.209581
H50	1.645559	1.780115	5.941878
C51	1.807429	3.146879	3.854043
H52	-0.328144	2.711752	-5.560606
H53	-2.211807	5.550980	-1.597696
H54	-4.126423	3.695421	-1.210585
H55	-4.092858	-1.513980	-0.504526
H56	-2.077726	-3.485054	-0.517615
H57	2.874430	-3.568861	-1.865198
H58	4.785976	-1.843945	-2.475852
H59	4.868956	3.568000	-2.290217
H60	2.903421	5.506255	-2.459467
H61	3.796185	4.586533	6.258732

Warfarin 7-9 Transition State Doublet

C1	-0.737883	1.959463	-4.748351
H2	-1.469148	1.344424	-5.285173
H3	-1.290890	2.540041	-4.012160
S4	0.380642	0.783710	-3.906221
O5	0.740500	1.257012	0.271693
Fe6	0.402572	1.112833	-1.451811
N7	-1.030943	2.502588	-1.530322
N8	-1.005678	-0.320162	-1.148945
N9	1.820501	-0.346551	-1.653584
N10	1.768129	2.498098	-1.919879
C11	-0.861291	3.855499	-1.708042
C12	-2.113689	4.540619	-1.574751
C13	-3.060508	3.587173	-1.353359
C14	-2.374681	2.320439	-1.320151
C15	-2.346120	-0.126783	-0.962354
C16	-3.006634	-1.383928	-0.666168
C17	-2.041033	-2.345393	-0.681387
C18	-0.802160	-1.659228	-1.002367
C19	1.613631	-1.686912	-1.521578
C20	2.828179	-2.413017	-1.794923
C21	3.783369	-1.497355	-2.106308
C22	3.144909	-0.192867	-1.978276
C23	3.117778	2.286348	-2.026407
C24	3.797548	3.543799	-2.216060
C25	2.841502	4.513567	-2.263792
C26	1.579937	3.849025	-2.057136
C27	0.352219	4.482641	-1.949792
H28	0.336266	5.561454	-2.038810
C29	-2.988974	1.096699	-1.067348
H30	-4.064452	1.110400	-0.945458
C31	0.415456	-2.299945	-1.185950
H32	0.451345	-3.372565	-1.050178
C33	3.755731	1.054344	-2.056861
H34	4.833069	1.097585	-2.131153
C35	0.494130	2.362157	3.578686
H36	-0.002586	1.966108	4.458565
C37	-0.130816	2.320562	2.365522
H38	-1.127289	1.911546	2.266186
C39	0.520432	2.797503	1.168483

H40	-0.135734	3.196039	0.407373
C41	1.772970	3.487874	1.333870
H42	2.254561	3.960686	0.487800
C43	2.334762	3.608721	2.589444
O44	3.464881	4.375326	2.717823
C45	3.979600	4.771801	3.956203
O46	4.913239	5.523949	3.937104
C47	3.358083	4.189670	5.141766
C48	2.360588	3.257987	5.012299
O49	1.876509	2.622529	6.110384
H50	1.578802	1.745747	5.870960
C51	1.748903	3.017332	3.732599
H52	-0.329702	2.669641	-5.504071
H53	-2.224019	5.614457	-1.598947
H54	-4.124613	3.731243	-1.204725
H55	-4.073749	-1.470255	-0.479254
H56	-2.055983	-3.426540	-0.491225
H57	2.878682	-3.495961	-1.823158
H58	4.784929	-1.785257	-2.436525
H59	4.875838	3.614797	-2.282306
H60	2.918732	5.574809	-2.465484
H61	3.708211	4.555505	6.139540

Warfarin 7-9 Transition State Quartet

C1	-0.757546	1.963544	-4.737684
H2	-1.479879	1.339773	-5.273189
H3	-1.317230	2.544192	-4.006162
S4	0.377634	0.815017	-3.884517
O5	0.649284	1.296960	0.234961
Fe6	0.422993	1.079319	-1.468847
N7	-1.026734	2.487514	-1.565577
N8	-0.993125	-0.334146	-1.162204
N9	1.815714	-0.343626	-1.669467
N10	1.795091	2.492540	-1.887992
C11	-0.848401	3.843454	-1.724265
C12	-2.099790	4.528466	-1.583668
C13	-3.049183	3.573982	-1.364425
C14	-2.367022	2.306002	-1.344026
C15	-2.338290	-0.132345	-0.974380
C16	-2.997095	-1.389188	-0.669020
C17	-2.035323	-2.352465	-0.681347
C18	-0.792377	-1.673781	-1.008677
C19	1.608439	-1.692604	-1.534079
C20	2.826369	-2.409086	-1.805245
C21	3.782100	-1.489349	-2.118660
C22	3.149615	-0.186796	-1.992010
C23	3.137033	2.284339	-2.006588
C24	3.812889	3.543475	-2.203326
C25	2.851921	4.509136	-2.251206
C26	1.593398	3.837480	-2.036158
C27	0.365171	4.471768	-1.947428
H28	0.349434	5.549798	-2.035878
C29	-2.981767	1.084425	-1.084063
H30	-4.055193	1.099854	-0.953543
C31	0.423789	-2.312262	-1.192475
H32	0.465496	-3.383137	-1.048270
C33	3.771718	1.050742	-2.056858
H34	4.847833	1.086247	-2.132758
C35	0.487431	2.363747	3.572280

H36	-0.010334	1.966509	4.449737
C37	-0.144654	2.334307	2.363457
H38	-1.140744	1.930852	2.262713
C39	0.500856	2.821518	1.161295
H40	-0.151130	3.225899	0.406355
C41	1.764664	3.490196	1.330185
H42	2.240935	3.972328	0.485336
C43	2.332333	3.598784	2.580698
O44	3.462891	4.359301	2.709196
C45	3.976588	4.763889	3.947428
O46	4.908389	5.521402	3.922277
C47	3.357240	4.184426	5.133122
C48	2.358237	3.253764	5.005487
O49	1.872106	2.621771	6.104743
H50	1.576473	1.745669	5.867186
C51	1.746446	3.009117	3.728140
H52	-0.342406	2.670858	-5.493230
H53	-2.214103	5.603369	-1.602063
H54	-4.113090	3.721607	-1.210184
H55	-4.065178	-1.472076	-0.481439
H56	-2.051125	-3.433870	-0.489092
H57	2.879038	-3.491565	-1.827235
H58	4.786509	-1.776724	-2.445607
H59	4.889208	3.616580	-2.279106
H60	2.923522	5.570717	-2.459076
H61	3.707934	4.551643	6.131230

Warfarin 7-10 Reactant Complex Doublet

C1	-0.946032	1.780434	-4.699483
H2	-1.634834	1.248733	-5.369762
H3	-1.554336	2.271255	-3.943150
S4	0.123825	0.519775	-3.942522
O5	0.598435	0.974560	0.084407
Fe6	0.321824	0.940421	-1.534044
N7	-1.109147	2.374565	-1.568592
N8	-1.100057	-0.451022	-1.264461
N9	1.729611	-0.478614	-1.806661
N10	1.706348	2.356229	-2.010758
C11	-0.930097	3.717546	-1.764926
C12	-2.161000	4.430871	-1.565640
C13	-3.107153	3.497263	-1.271421
C14	-2.440052	2.217511	-1.279308
C15	-2.421316	-0.238978	-1.013318
C16	-3.086640	-1.491147	-0.721013
C17	-2.132953	-2.462756	-0.780707
C18	-0.902860	-1.788418	-1.146250
C19	1.517916	-1.814145	-1.665893
C20	2.744042	-2.537407	-1.867648
C21	3.715818	-1.623790	-2.134597
C22	3.072193	-0.318489	-2.062956
C23	3.055947	2.165766	-2.093078
C24	3.733164	3.437081	-2.245949
C25	2.766726	4.395278	-2.307184
C26	1.507696	3.709703	-2.139722
C27	0.279535	4.336215	-2.049668
H28	0.261389	5.414965	-2.136571
C29	-3.054081	0.996315	-1.026191
H30	-4.116553	1.015947	-0.819551
C31	0.314086	-2.428954	-1.347652

H32	0.356634	-3.501409	-1.214251
C33	3.689281	0.925317	-2.117671
H34	4.768428	0.960258	-2.153852
C35	0.658632	2.707282	3.506227
H36	0.218211	2.149505	4.322464
C37	-0.007685	2.888411	2.312852
H38	-0.990273	2.460880	2.157226
C39	0.604054	3.609968	1.278389
H40	0.073518	3.734868	0.351361
C41	1.885194	4.119565	1.410255
H42	2.375035	4.646053	0.600453
C43	2.530175	3.980503	2.637971
O44	3.750749	4.573148	2.787399
C45	4.354665	4.743339	4.027544
O46	5.365023	5.400963	4.040144
C47	3.698463	4.115098	5.168655
C48	2.571616	3.344171	4.986158
O49	1.899133	2.680695	5.932073
H50	2.325263	2.662044	6.782370
C51	1.929078	3.292172	3.695225
H52	-0.465702	2.563100	-5.310354
H53	-2.260404	5.509424	-1.606451
H54	-4.158835	3.674191	-1.069637
H55	-4.153345	-1.536121	-0.531498
H56	-2.134106	-3.534106	-0.571230
H57	2.794471	-3.617207	-1.849749
H58	4.736481	-1.921846	-2.381863
H59	4.813222	3.560520	-2.269402
H60	2.850397	5.471012	-2.467763
H61	4.062679	4.448564	6.167347

Warfarin 7-10 Reactant Complex Quartet

C1	-0.934771	1.788903	-4.693198
H2	-1.623869	1.249332	-5.357600
H3	-1.541163	2.280655	-3.936710
S4	0.142418	0.536720	-3.936331
O5	0.572106	0.974702	0.092026
Fe6	0.326914	0.934180	-1.525925
N7	-1.107928	2.370681	-1.566504
N8	-1.098312	-0.456733	-1.264585
N9	1.732410	-0.481511	-1.800607
N10	1.711542	2.350535	-2.002701
C11	-0.928983	3.712094	-1.761613
C12	-2.158841	4.426577	-1.561793
C13	-3.105641	3.493702	-1.265998
C14	-2.439901	2.212439	-1.274905
C15	-2.417646	-0.244056	-1.014041
C16	-3.083729	-1.494600	-0.719050
C17	-2.130414	-2.468374	-0.775658
C18	-0.899256	-1.795286	-1.142213
C19	1.519409	-1.816979	-1.662847
C20	2.746134	-2.539371	-1.868968
C21	3.718760	-1.625038	-2.136667
C22	3.075650	-0.319701	-2.060760
C23	3.060676	2.162012	-2.086152
C24	3.735509	3.435190	-2.241529
C25	2.767321	4.391215	-2.304914
C26	1.509629	3.704675	-2.135748
C27	0.282299	4.330603	-2.047934

H28	0.264994	5.409492	-2.134979
C29	-3.052785	0.992632	-1.025926
H30	-4.114747	1.009303	-0.816259
C31	0.317076	-2.433684	-1.342911
H32	0.360243	-3.506190	-1.207242
C33	3.694832	0.921315	-2.112642
H34	4.774015	0.953934	-2.148372
C35	0.660088	2.709899	3.512750
H36	0.220377	2.150651	4.328285
C37	-0.007419	2.891225	2.319539
H38	-0.990496	2.464928	2.163329
C39	0.605639	3.610907	1.284125
H40	0.074711	3.734013	0.357645
C41	1.888181	4.117973	1.416051
H42	2.379096	4.640134	0.602526
C43	2.532553	3.980418	2.643222
O44	3.755548	4.569999	2.792256
C45	4.359664	4.740839	4.032979
O46	5.369939	5.398455	4.044960
C47	3.702959	4.113841	5.173967
C48	2.572982	3.345793	4.992616
O49	1.899148	2.685238	5.938735
H50	2.325329	2.663879	6.786747
C51	1.930062	3.295040	3.700045
H52	-0.459792	2.569548	-5.310256
H53	-2.258481	5.505293	-1.604836
H54	-4.157844	3.671430	-1.067488
H55	-4.149782	-1.538121	-0.528689
H56	-2.132896	-3.538484	-0.564943
H57	2.797094	-3.618580	-1.850221
H58	4.740025	-1.922117	-2.383255
H59	4.814735	3.559977	-2.268165
H60	2.849933	5.467385	-2.467858
H61	4.066546	4.448491	6.173055

Warfarin 7-10 Transition State Doublet

C1	-0.922706	1.756310	-4.615943
H2	-1.592944	1.177889	-5.265557
H3	-1.547210	2.259819	-3.881258
S4	0.173887	0.547072	-3.795515
O5	0.780084	1.287071	0.265518
Fe6	0.368102	1.082477	-1.450944
N7	-1.071657	2.471112	-1.498358
N8	-1.030935	-0.344938	-1.080310
N9	1.789404	-0.376827	-1.633902
N10	1.724599	2.464479	-1.968353
C11	-0.908933	3.820593	-1.719023
C12	-2.154318	4.510015	-1.543304
C13	-3.090216	3.564855	-1.253453
C14	-2.402309	2.298262	-1.224404
C15	-2.370204	-0.151426	-0.887734
C16	-3.040257	-1.415595	-0.651117
C17	-2.080682	-2.380593	-0.705293
C18	-0.841009	-1.687494	-1.003570
C19	1.574540	-1.717110	-1.514574
C20	2.786846	-2.447277	-1.777126
C21	3.751473	-1.536387	-2.069897
C22	3.113007	-0.226660	-1.958271
C23	3.076525	2.258060	-2.059469

C24	3.753959	3.522414	-2.233719
C25	2.790919	4.485837	-2.289906
C26	1.530508	3.810647	-2.108998
C27	0.296133	4.440748	-2.008129
H28	0.274972	5.517533	-2.109336
C29	-3.010302	1.073945	-0.948074
H30	-4.079966	1.085485	-0.783039
C31	0.373194	-2.331024	-1.210141
H32	0.402393	-3.408123	-1.111201
C33	3.716332	1.023138	-2.069684
H34	4.793101	1.065283	-2.146981
C35	0.541476	2.505294	3.477891
H36	0.052859	2.118341	4.360748
C37	-0.065986	2.474323	2.257297
H38	-1.071138	2.091494	2.140233
C39	0.632413	2.887065	1.063844
H40	0.012065	3.300108	0.283928
C41	1.921322	3.514860	1.230145
H42	2.447191	3.921938	0.374451
C43	2.467681	3.632445	2.490628
O44	3.652786	4.313966	2.630946
C45	4.197728	4.647952	3.871428
O46	5.156536	5.376361	3.854375
C47	3.559795	4.078643	5.055409
C48	2.436028	3.290443	4.917247
O49	1.759117	2.690243	5.907147
H50	2.157707	2.762780	6.766149
C51	1.822966	3.108320	3.628583
H52	-0.465640	2.532739	-5.259489
H53	-2.268037	5.580615	-1.600132
H54	-4.150263	3.715480	-1.073755
H55	-4.114305	-1.486674	-0.516010
H56	-2.090196	-3.463786	-0.533506
H57	2.825486	-3.530269	-1.807070
H58	4.754803	-1.848450	-2.366982
H59	4.834344	3.623822	-2.271191
H60	2.872249	5.552903	-2.464315
H61	3.962887	4.430406	6.047624

Warfarin 7-10 Transition State Quartet

C1	-0.931861	1.765528	-4.619709
H2	-1.592956	1.170318	-5.260937
H3	-1.563007	2.271738	-3.891332
S4	0.184546	0.587805	-3.788867
O5	0.686651	1.385641	0.226110
Fe6	0.390776	1.036898	-1.462906
N7	-1.074188	2.439973	-1.544735
N8	-1.016323	-0.368728	-1.096306
N9	1.779489	-0.384218	-1.653623
N10	1.751291	2.443986	-1.955395
C11	-0.899045	3.789532	-1.741004
C12	-2.142166	4.482184	-1.556075
C13	-3.082743	3.537821	-1.270142
C14	-2.402838	2.267286	-1.256169
C15	-2.359875	-0.167197	-0.906763
C16	-3.029309	-1.428927	-0.662274
C17	-2.074282	-2.397809	-0.714288
C18	-0.829084	-1.716602	-1.018886
C19	1.564240	-1.733677	-1.536352

C20	2.780919	-2.449782	-1.793902
C21	3.745259	-1.535281	-2.084650
C22	3.114858	-0.227945	-1.976080
C23	3.096721	2.244546	-2.051709
C24	3.765697	3.513257	-2.228362
C25	2.796127	4.470165	-2.282527
C26	1.539234	3.786740	-2.098145
C27	0.305912	4.414776	-2.011615
H28	0.283336	5.491177	-2.104732
C29	-3.008843	1.049097	-0.972640
H30	-4.076080	1.056355	-0.798576
C31	0.375534	-2.360867	-1.229103
H32	0.413284	-3.436501	-1.131061
C33	3.733638	1.009102	-2.075871
H34	4.809498	1.041449	-2.150493
C35	0.555235	2.515465	3.488897
H36	0.063714	2.127748	4.370114
C37	-0.062366	2.503941	2.279422
H38	-1.067961	2.124340	2.163807
C39	0.617393	2.949398	1.076604
H40	-0.005903	3.395831	0.321124
C41	1.916108	3.568115	1.250030
H42	2.418219	4.012927	0.400898
C43	2.473338	3.659332	2.504990
O44	3.651005	4.345964	2.650077
C45	4.208698	4.660078	3.891746
O46	5.174113	5.379541	3.875142
C47	3.575331	4.085874	5.073736
C48	2.451583	3.289841	4.930589
O49	1.780849	2.684159	5.916693
H50	2.183962	2.754368	6.773607
C51	1.840259	3.113843	3.643837
H52	-0.472466	2.537152	-5.267755
H53	-2.257523	5.555644	-1.602534
H54	-4.140910	3.697824	-1.080890
H55	-4.103992	-1.494879	-0.520820
H56	-2.085164	-3.477689	-0.536482
H57	2.827184	-3.532764	-1.814500
H58	4.750153	-1.847085	-2.374564
H59	4.844538	3.621010	-2.269852
H60	2.872265	5.539456	-2.456504
H61	3.974285	4.438624	6.066928

Diclofenac 4'-1 Reactant Complex Doublet

C1	-1.984816	0.077129	2.971950
S2	-1.291004	1.191700	1.707387
H3	-3.028195	0.375748	3.124001
H4	-1.978108	-0.948441	2.593088
O5	1.096838	-0.531957	-1.204658
Fe6	0.101145	0.010575	-0.020968
N7	-0.252331	-1.866502	0.682618
N8	-1.536604	-0.126609	-1.196050
N9	0.304159	1.977864	-0.502308
N10	1.593428	0.205548	1.332971
C11	0.562107	-2.589894	1.516506
C12	0.123259	-3.961573	1.591764
C13	-0.969627	-4.060505	0.783000
C14	-1.184856	-2.750262	0.209043
C15	-2.297192	-1.239925	-1.413917

C16	-3.288577	-0.977411	-2.438903
C17	-3.120887	0.319949	-2.826511
C18	-2.021039	0.833448	-2.028787
C19	-0.468501	2.659370	-1.396899
C20	-0.030690	4.031615	-1.489739
C21	1.012864	4.180378	-0.626546
C22	1.222780	2.876629	-0.019738
C23	2.376518	1.310986	1.519396
C24	3.430073	1.023579	2.463652
C25	3.293230	-0.281617	2.824191
C26	2.144997	-0.785026	2.106095
C27	1.677641	-2.088497	2.173839
H28	2.239503	-2.785762	2.782749
C29	-2.152144	-2.450235	-0.747762
H30	-2.841370	-3.243337	-1.002097
C31	-1.534311	2.135301	-2.114882
H32	-1.997689	2.802257	-2.829213
C33	2.218641	2.534476	0.884889
H34	2.988710	3.259483	1.097394
C35	5.012032	-3.195252	-3.435778
C36	4.849699	-2.701993	-2.124756
C37	3.607041	-2.609367	-1.510980
C38	2.467334	-3.003722	-2.209541
C39	2.583626	-3.480156	-3.510343
C40	3.837930	-3.576187	-4.100183
C141	6.262759	-2.121642	-1.263657
H42	3.522906	-2.191651	-0.515461
H43	1.494686	-2.895246	-1.746195
H44	1.716781	-3.775021	-4.085399
C145	3.921802	-4.190003	-5.752914
C46	9.164431	-6.078943	-2.824944
C47	9.555640	-4.851935	-3.369184
C48	8.621944	-3.873276	-3.725548
C49	7.253976	-4.190397	-3.590893
C50	6.856976	-5.413077	-3.031124
C51	7.808208	-6.348203	-2.629113
H52	9.912285	-6.814473	-2.548309
H53	10.605270	-4.624321	-3.510933
N54	6.282728	-3.250028	-4.025925
H55	5.798482	-5.630319	-2.930832
H56	7.488257	-7.289590	-2.194743
H57	6.308060	-3.025015	-5.007676
C58	9.013958	-2.476793	-4.202068
H59	8.255027	-1.777582	-3.847895
H60	9.013512	-2.438905	-5.299436
C61	10.401080	-2.012848	-3.732110
O62	11.385058	-2.626345	-4.221299
O63	10.459382	-1.070244	-2.905868
H64	-1.504115	0.053379	3.963486
H65	0.602905	-4.759681	2.161766
H66	-1.537338	-4.964394	0.572324
H67	-4.011334	-1.723326	-2.764901
H68	-3.626759	0.957605	-3.564958
H69	-0.510429	4.799053	-2.093803
H70	1.497394	5.149366	-0.459623
H71	4.172235	1.746710	2.786923
H72	3.892051	-0.865416	3.514699

Diclofenac 4'-1 Reactant Complex Quartet

C1	-1.957065	0.077094	2.962298
S2	-1.248478	1.186934	1.702396
H3	-2.999917	0.383961	3.105628
H4	-1.954512	-0.947696	2.582435
O5	1.116557	-0.557449	-1.235987
Fe6	0.141915	-0.002606	-0.046834
N7	-0.221453	-1.872701	0.662379
N8	-1.514362	-0.134053	-1.205994
N9	0.333753	1.968212	-0.518364
N10	1.626264	0.198001	1.306608
C11	0.589280	-2.595568	1.499910
C12	0.136042	-3.960584	1.592398
C13	-0.961826	-4.057271	0.790116
C14	-1.165138	-2.752138	0.202028
C15	-2.278989	-1.244256	-1.418334
C16	-3.276269	-0.981319	-2.437691
C17	-3.106186	0.315902	-2.827833
C18	-2.001377	0.825786	-2.036111
C19	-0.447292	2.648559	-1.407776
C20	-0.020023	4.021807	-1.497597
C21	1.024341	4.176162	-0.636506
C22	1.245746	2.871165	-0.034551
C23	2.404986	1.307503	1.499903
C24	3.449452	1.020905	2.454444
C25	3.309194	-0.284759	2.816912
C26	2.171134	-0.790578	2.086285
C27	1.706194	-2.094420	2.155471
H28	2.265082	-2.788363	2.771124
C29	-2.136223	-2.452904	-0.750728
H30	-2.830790	-3.243356	-1.000455
C31	-1.514220	2.127400	-2.123517
H32	-1.975725	2.794769	-2.838019
C33	2.246396	2.532279	0.869180
H34	3.014058	3.259547	1.081323
C35	4.984922	-3.105141	-3.362135
C36	4.817083	-2.607405	-2.053373
C37	3.570251	-2.483644	-1.451833
C38	2.428051	-2.858877	-2.155830
C39	2.553549	-3.358421	-3.449138
C40	3.810158	-3.472165	-4.032467
C141	6.236520	-2.060077	-1.182853
H42	3.484643	-2.057209	-0.460127
H43	1.453281	-2.747680	-1.701937
H44	1.690082	-3.658561	-4.024690
C145	3.900444	-4.087864	-5.685867
C46	9.113397	-6.055425	-2.813646
C47	9.514930	-4.829010	-3.351383
C48	8.590786	-3.836875	-3.694272
C49	7.219278	-4.127835	-3.531789
C50	6.813831	-5.350319	-2.976963
C51	7.755556	-6.306753	-2.605781
H52	9.853860	-6.805721	-2.560103
H53	10.565643	-4.615961	-3.504467
N54	6.257740	-3.169683	-3.950108
H55	5.753487	-5.552851	-2.859530
H56	7.427270	-7.253013	-2.188128
H57	6.276789	-2.953640	-4.934529
C58	9.009551	-2.464713	-4.215659
H59	8.257030	-1.738052	-3.906772
H60	9.030890	-2.479941	-5.313202

C61	10.397453	-2.007516	-3.737847
O62	11.381043	-2.626754	-4.223457
O63	10.457365	-1.068894	-2.908763
H64	-1.486518	0.051722	3.958752
H65	0.613549	-4.755877	2.166197
H66	-1.539299	-4.957072	0.584479
H67	-4.002326	-1.726332	-2.760288
H68	-3.610446	0.954219	-3.565251
H69	-0.509860	4.785984	-2.098204
H70	1.500622	5.146662	-0.469388
H71	4.188749	1.743360	2.781766
H72	3.899925	-0.869445	3.514021

Diclofenac 4'-1 Transition State Doublet

C1	-1.829916	0.042108	2.878601
S2	-1.112434	1.140487	1.600813
H3	-2.880373	0.330996	2.994478
H4	-1.801794	-0.989536	2.517864
O5	1.343950	-0.594358	-1.328778
Fe6	0.281209	-0.072607	-0.068984
N7	-0.093508	-1.910645	0.637998
N8	-1.374202	-0.202577	-1.257704
N9	0.485195	1.903473	-0.600040
N10	1.756804	0.138649	1.266323
C11	0.690584	-2.626966	1.516908
C12	0.216027	-3.980814	1.623460
C13	-0.882981	-4.073996	0.821299
C14	-1.062327	-2.783756	0.200051
C15	-2.167538	-1.298056	-1.439720
C16	-3.193716	-1.021761	-2.430559
C17	-3.017417	0.271643	-2.828111
C18	-1.880388	0.765601	-2.071745
C19	-0.326063	2.581880	-1.459972
C20	0.053744	3.969571	-1.523818
C21	1.104497	4.138816	-0.673176
C22	1.367819	2.823833	-0.095542
C23	2.518879	1.261130	1.455815
C24	3.551829	0.991567	2.428383
C25	3.407161	-0.307680	2.813929
C26	2.277051	-0.826684	2.083207
C27	1.802622	-2.128230	2.176156
H28	2.345476	-2.815609	2.811606
C29	-2.032966	-2.497009	-0.756047
H30	-2.740835	-3.281718	-0.983885
C31	-1.403544	2.064448	-2.159401
H32	-1.889938	2.741137	-2.845065
C33	2.349268	2.491851	0.833434
H34	3.092881	3.230526	1.084701
C35	4.744503	-2.533608	-2.942196
C36	4.753055	-2.141612	-1.579048
C37	3.608910	-2.001514	-0.822043
C38	2.325739	-2.236578	-1.397537
C39	2.309055	-2.670071	-2.751804
C40	3.463742	-2.766836	-3.495577
C141	6.301280	-1.768347	-0.864677
H42	3.687736	-1.691860	0.210230
H43	1.531014	-2.591114	-0.755502
H44	1.374304	-2.970842	-3.196276
C145	3.364817	-3.315538	-5.172495

C46	8.643990	-5.783096	-2.770155
C47	9.106395	-4.593221	-3.333618
C48	8.252433	-3.517918	-3.608657
C49	6.877964	-3.689734	-3.337663
C50	6.412168	-4.886464	-2.771624
C51	7.286878	-5.925924	-2.474052
H52	9.338097	-6.592408	-2.566877
H53	10.158844	-4.463545	-3.555762
N54	5.928192	-2.671975	-3.664930
H55	5.349348	-4.999332	-2.587093
H56	6.902459	-6.845060	-2.044935
H57	5.858524	-2.451684	-4.648005
C58	8.791428	-2.208239	-4.176754
H59	8.107940	-1.401327	-3.910015
H60	8.829032	-2.275237	-5.271432
C61	10.218909	-1.864743	-3.691498
O62	11.157535	-2.561247	-4.165286
O63	10.343368	-0.928960	-2.866007
H64	-1.385436	0.032753	3.892592
H65	0.699234	-4.769897	2.196204
H66	-1.505722	-4.949662	0.652323
H67	-3.944930	-1.755600	-2.717583
H68	-3.530560	0.923430	-3.553247
H69	-0.489554	4.719943	-2.098932
H70	1.539455	5.129058	-0.510313
H71	4.282346	1.723823	2.755950
H72	3.976529	-0.888362	3.528738

Diclofenac 4'-1 Transition State Quartet

C1	-1.840721	0.038490	2.896794
S2	-1.102161	1.122145	1.623832
H3	-2.888668	0.338807	3.007243
H4	-1.821657	-0.993923	2.536115
O5	1.325515	-0.748034	-1.299530
Fe6	0.287724	-0.056544	-0.132693
N7	-0.128055	-1.898364	0.630913
N8	-1.374818	-0.189434	-1.290047
N9	0.479098	1.898737	-0.626910
N10	1.757478	0.154411	1.228851
C11	0.669019	-2.612214	1.491595
C12	0.197338	-3.967424	1.603975
C13	-0.905432	-4.062906	0.805887
C14	-1.088298	-2.770657	0.187543
C15	-2.175085	-1.287496	-1.462485
C16	-3.202870	-1.009128	-2.449924
C17	-3.030692	0.283362	-2.846534
C18	-1.890703	0.780608	-2.096948
C19	-0.341018	2.588509	-1.482573
C20	0.043406	3.975016	-1.534020
C21	1.093251	4.139394	-0.682377
C22	1.361206	2.826076	-0.110374
C23	2.515165	1.271594	1.433932
C24	3.535427	0.999273	2.419852
C25	3.385860	-0.300008	2.797953
C26	2.265780	-0.817285	2.049914
C27	1.784372	-2.113159	2.147570
H28	2.323446	-2.798577	2.788590
C29	-2.055573	-2.480631	-0.771165
H30	-2.773542	-3.258046	-0.994660

C31	-1.418449	2.080574	-2.177502
H32	-1.912943	2.763971	-2.853204
C33	2.341861	2.503129	0.814720
H34	3.076294	3.249668	1.070618
C35	4.789073	-2.608873	-2.975050
C36	4.738272	-2.258780	-1.602088
C37	3.569103	-2.175081	-0.875229
C38	2.306242	-2.391496	-1.497101
C39	2.348254	-2.780306	-2.867565
C40	3.532810	-2.838978	-3.574479
C141	6.252976	-1.879300	-0.825021
H42	3.612225	-1.925469	0.175844
H43	1.485080	-2.758301	-0.904110
H44	1.445446	-3.101716	-3.359581
C145	3.495260	-3.337716	-5.268937
C46	8.734632	-5.822305	-2.775333
C47	9.188974	-4.629864	-3.346373
C48	8.327934	-3.562397	-3.622957
C49	6.952392	-3.734697	-3.349272
C50	6.495392	-4.937485	-2.780737
C51	7.378653	-5.968545	-2.480241
H52	9.433824	-6.625465	-2.566999
H53	10.240673	-4.496886	-3.568518
N54	6.006635	-2.716722	-3.656045
H55	5.434579	-5.056732	-2.596957
H56	6.998774	-6.887742	-2.044858
H57	6.010541	-2.378962	-4.605732
C58	8.858336	-2.249297	-4.194370
H59	8.172416	-1.446202	-3.922067
H60	8.893315	-2.314039	-5.289244
C61	10.282403	-1.891935	-3.708967
O62	11.230340	-2.571805	-4.179246
O63	10.389824	-0.954023	-2.880502
H64	-1.397733	0.029541	3.912163
H65	0.681435	-4.756242	2.177692
H66	-1.519901	-4.944308	0.632259
H67	-3.949504	-1.747561	-2.741032
H68	-3.544221	0.935261	-3.571293
H69	-0.489405	4.733299	-2.112190
H70	1.533051	5.130432	-0.517777
H71	4.263396	1.729171	2.756621
H72	3.954091	-0.882794	3.513958

Diclofenac 4'-2 Reactant Complex Doublet

C1	-1.930812	0.114312	3.121564
S2	-1.328084	1.231170	1.814260
H3	-2.957591	0.422689	3.354038
H4	-1.961112	-0.907994	2.736508
O5	1.106966	-0.432917	-1.073304
Fe6	0.092240	0.042189	0.121655
N7	-0.215370	-1.839177	0.835610
N8	-1.528544	-0.165922	-1.073537
N9	0.260120	1.992576	-0.397159
N10	1.571167	0.280011	1.474778
C11	0.610272	-2.545762	1.672211
C12	0.222052	-3.935531	1.729726
C13	-0.873882	-4.054240	0.926652
C14	-1.123525	-2.748290	0.365075
C15	-2.256082	-1.299156	-1.285795

C16	-3.209890	-1.098605	-2.355600
C17	-3.047440	0.185003	-2.786007
C18	-1.999851	0.751720	-1.959414
C19	-0.516724	2.625808	-1.317636
C20	-0.107632	3.997923	-1.456310
C21	0.943183	4.195283	-0.612039
C22	1.175755	2.915197	0.048764
C23	2.364346	1.385465	1.615801
C24	3.428897	1.113795	2.560595
C25	3.258804	-0.166405	2.993556
C26	2.113121	-0.684324	2.287010
C27	1.683560	-2.000473	2.360451
H28	2.255105	-2.674892	2.986072
C29	-2.090993	-2.492315	-0.596274
H30	-2.747449	-3.311688	-0.848406
C31	-1.546779	2.061286	-2.058144
H32	-2.011158	2.703606	-2.793638
C33	2.184789	2.598620	0.954637
H34	2.946577	3.336046	1.153833
C35	4.601801	-2.707257	-2.966656
C36	4.469947	-2.501125	-1.580112
C37	3.274981	-2.681674	-0.901930
C38	2.144565	-3.081376	-1.606679
C39	2.216954	-3.262802	-2.982922
C40	3.428927	-3.082586	-3.641611
C141	5.864734	-1.958990	-0.668987
H42	3.224477	-2.483551	0.161483
H43	1.205215	-3.210213	-1.083325
H44	1.341870	-3.568221	-3.544490
C145	3.490608	-3.359050	-5.388183
C46	8.813023	-5.413699	-2.722299
C47	9.146286	-4.060587	-2.769233
C48	8.189824	-3.080850	-3.053846
C49	6.872376	-3.497720	-3.307311
C50	6.536659	-4.856022	-3.260719
C51	7.498239	-5.817698	-2.965714
H52	9.573042	-6.154224	-2.500301
H53	10.163013	-3.737032	-2.576510
N54	5.844201	-2.530810	-3.598237
H55	5.509941	-5.145991	-3.459706
H56	7.227935	-6.867050	-2.944691
H57	5.765482	-2.304818	-4.577811
C58	8.550926	-1.601436	-3.017411
H59	8.499005	-1.265077	-1.977279
H60	7.808725	-1.042269	-3.581772
C61	9.952626	-1.306708	-3.553463
O62	10.069152	-0.947953	-4.746184
O63	10.914991	-1.469051	-2.744794
H64	-1.397859	0.066782	4.081426
H65	0.748796	-4.726719	2.270656
H66	-1.462149	-4.938506	0.693361
H67	-3.895941	-1.878456	-2.683663
H68	-3.502581	0.766357	-3.592712
H69	-0.626397	4.706474	-2.098941
H70	1.417676	5.175148	-0.506488
H71	4.225774	1.806784	2.807630
H72	3.824760	-0.750559	3.717227

Diclofenac 4'-2 Reactant Complex Quartet

C1	-1.957547	0.130544	3.120208
S2	-1.267331	1.213386	1.820993
H3	-2.985249	0.472422	3.291356
H4	-1.998439	-0.896135	2.747363
O5	1.083874	-0.564750	-1.148077
Fe6	0.105500	-0.000225	0.032450
N7	-0.249978	-1.864650	0.760125
N8	-1.541693	-0.148236	-1.138089
N9	0.287973	1.965414	-0.469439
N10	1.578126	0.213701	1.388440
C11	0.570305	-2.590993	1.585750
C12	0.154292	-3.972549	1.633877
C13	-0.935781	-4.070622	0.821820
C14	-1.167246	-2.755524	0.273582
C15	-2.289079	-1.270617	-1.355926
C16	-3.256719	-1.035193	-2.405045
C17	-3.081199	0.250913	-2.818636
C18	-2.010400	0.791440	-2.005104
C19	-0.487022	2.632877	-1.376205
C20	-0.072109	4.011075	-1.467638
C21	0.963574	4.178743	-0.594267
C22	1.189265	2.878513	0.017959
C23	2.358664	1.325098	1.564320
C24	3.410678	1.044824	2.514941
C25	3.261130	-0.250432	2.904037
C26	2.120866	-0.764983	2.184078
C27	1.670485	-2.074187	2.256875
H28	2.236308	-2.760759	2.873361
C29	-2.131132	-2.474948	-0.686420
H30	-2.791433	-3.286001	-0.950383
C31	-1.533676	2.093549	-2.107278
H32	-2.001359	2.745131	-2.834212
C33	2.187665	2.546691	0.929996
H34	2.943090	3.284457	1.151113
C35	4.790313	-2.845264	-3.026793
C36	4.600156	-2.550303	-1.662945
C37	3.357411	-2.579392	-1.045104
C38	2.231854	-2.931809	-1.782878
C39	2.374845	-3.268842	-3.124961
C40	3.630122	-3.214594	-3.726954
C141	5.986978	-2.063429	-0.709236
H42	3.268482	-2.294870	-0.004224
H43	1.258686	-2.961439	-1.311020
H44	1.523231	-3.585070	-3.712662
C145	3.746289	-3.625554	-5.443533
C46	9.161701	-5.444938	-2.824422
C47	9.410774	-4.073614	-2.786715
C48	8.399270	-3.137894	-3.024142
C49	7.110826	-3.616286	-3.319769
C50	6.856744	-4.993840	-3.344751
C51	7.872534	-5.910786	-3.096873
H52	9.967182	-6.150221	-2.654427
H53	10.407871	-3.701332	-2.579508
N54	6.047906	-2.695013	-3.638257
H55	5.852164	-5.332473	-3.578546
H56	7.669504	-6.975102	-3.140778
H57	5.976027	-2.517455	-4.626732
C58	8.696738	-1.647221	-2.914624
H59	8.726457	-1.380434	-1.853952
H60	7.886977	-1.087780	-3.379023

C61	10.043360	-1.287197	-3.547796
O62	10.079386	-0.981042	-4.756684
O63	11.059619	-1.363563	-2.788045
H64	-1.470668	0.084451	4.111043
H65	0.662419	-4.775240	2.170845
H66	-1.518719	-4.954679	0.571218
H67	-3.978967	-1.775086	-2.744004
H68	-3.553108	0.837947	-3.612674
H69	-0.554708	4.763607	-2.091878
H70	1.426227	5.156709	-0.434501
H71	4.171757	1.760676	2.806573
H72	3.840233	-0.830933	3.614084

Diclofenac 4'-2 Transition State Doublet

C1	-1.849302	0.081345	3.014957
S2	-1.169546	1.159529	1.695545
H3	-2.885013	0.398981	3.177051
H4	-1.862033	-0.950251	2.654966
O5	1.231184	-0.570439	-1.218788
Fe6	0.188045	-0.072753	0.085776
N7	-0.152600	-1.912464	0.799715
N8	-1.439570	-0.244910	-1.136621
N9	0.403818	1.880788	-0.513789
N10	1.681983	0.146976	1.393611
C11	0.645873	-2.627015	1.670344
C12	0.227999	-4.005910	1.719878
C13	-0.862348	-4.110219	0.905763
C14	-1.088770	-2.807584	0.330898
C15	-2.199276	-1.358683	-1.330426
C16	-3.174374	-1.133091	-2.379214
C17	-2.997144	0.149271	-2.807494
C18	-1.912080	0.689486	-2.011672
C19	-0.397239	2.530754	-1.404913
C20	-0.027052	3.920121	-1.488680
C21	1.014211	4.113893	-0.631071
C22	1.281605	2.811558	-0.022237
C23	2.446141	1.273308	1.550818
C24	3.481228	1.023743	2.528933
C25	3.315616	-0.255228	2.970054
C26	2.187724	-0.792347	2.249104
C27	1.728590	-2.101588	2.354917
H28	2.271425	-2.772715	3.007312
C29	-2.049237	-2.550135	-0.633163
H30	-2.722028	-3.359796	-0.872328
C31	-1.442948	1.985957	-2.127434
H32	-1.913301	2.634614	-2.852618
C33	2.266101	2.494342	0.910432
H34	3.006655	3.240531	1.152178
C35	4.515987	-2.559400	-2.773338
C36	4.499529	-2.214252	-1.395501
C37	3.344216	-2.062992	-0.667268
C38	2.071017	-2.271550	-1.275604
C39	2.067650	-2.713821	-2.633258
C40	3.235454	-2.806851	-3.348764
C141	6.018642	-1.879269	-0.607465
H42	3.401971	-1.756245	0.365442
H43	1.256346	-2.610665	-0.650472
H44	1.132744	-3.021714	-3.080505
C145	3.180026	-3.357758	-5.028744

C46	8.758896	-5.393111	-2.715870
C47	9.068969	-4.035060	-2.759237
C48	8.091945	-3.060954	-2.999476
C49	6.768450	-3.502203	-3.182565
C50	6.453141	-4.864435	-3.126879
C51	7.441710	-5.816659	-2.898764
H52	9.544647	-6.121906	-2.548074
H53	10.088676	-3.701817	-2.609215
N54	5.684635	-2.595081	-3.513045
H55	5.423244	-5.164111	-3.292421
H56	7.190884	-6.870979	-2.886205
H57	5.523098	-2.540965	-4.511397
C58	8.458230	-1.583731	-3.006612
H59	8.398807	-1.213368	-1.978796
H60	7.715531	-1.043416	-3.590408
C61	9.873452	-1.296107	-3.534121
O62	10.001011	-0.914436	-4.718005
O63	10.829294	-1.484327	-2.723521
H64	-1.370822	0.053165	4.014351
H65	0.745151	-4.799036	2.258123
H66	-1.468418	-4.981368	0.665478
H67	-3.898440	-1.879789	-2.696081
H68	-3.468431	0.748440	-3.596447
H69	-0.569106	4.651394	-2.090472
H70	1.441256	5.109783	-0.486405
H71	4.237731	1.750280	2.805205
H72	3.870418	-0.819202	3.710446

Diclofenac 4'-2 Transition State Quartet

C1	-1.878170	0.102875	3.066524
S2	-1.170688	1.165364	1.755365
H3	-2.910092	0.439677	3.215342
H4	-1.905901	-0.928629	2.704507
O5	1.217065	-0.773036	-1.178107
Fe6	0.200222	-0.051758	-0.011923
N7	-0.204154	-1.885179	0.779316
N8	-1.444356	-0.210862	-1.184173
N9	0.389478	1.890417	-0.543602
N10	1.665920	0.180249	1.348651
C11	0.609519	-2.600011	1.623379
C12	0.194997	-3.979533	1.677450
C13	-0.897419	-4.084319	0.865045
C14	-1.122840	-2.778571	0.297827
C15	-2.215465	-1.326896	-1.369489
C16	-3.198843	-1.092141	-2.406839
C17	-3.020586	0.190669	-2.833855
C18	-1.928231	0.727077	-2.047321
C19	-0.418563	2.560652	-1.426727
C20	-0.047916	3.949031	-1.489962
C21	0.991881	4.133168	-0.627433
C22	1.264091	2.829812	-0.034592
C23	2.431279	1.296542	1.525532
C24	3.455950	1.038718	2.512784
C25	3.287004	-0.245796	2.934859
C26	2.165273	-0.774565	2.197053
C27	1.700378	-2.076034	2.302415
H28	2.245345	-2.750199	2.949547
C29	-2.079037	-2.514768	-0.674215
H30	-2.754562	-3.319758	-0.916127

C31	-1.463963	2.026808	-2.153585
H32	-1.941622	2.683894	-2.865407
C33	2.253756	2.519724	0.888736
H34	2.988894	3.270756	1.128182
C35	4.588861	-2.630768	-2.837749
C36	4.508629	-2.332411	-1.454111
C37	3.331003	-2.270421	-0.746874
C38	2.080698	-2.475966	-1.394734
C39	2.144656	-2.879221	-2.759574
C40	3.340878	-2.909525	-3.447029
C141	5.997545	-1.987379	-0.609540
H42	3.351112	-2.031817	0.305264
H43	1.243329	-2.834673	-0.820319
H44	1.244765	-3.226521	-3.250352
C145	3.341840	-3.433694	-5.139429
C46	8.856687	-5.425471	-2.778260
C47	9.163799	-4.065832	-2.789437
C48	8.187225	-3.090973	-3.025924
C49	6.865608	-3.523453	-3.244995
C50	6.556637	-4.889473	-3.233092
C51	7.543897	-5.844399	-3.002871
H52	9.638687	-6.156461	-2.602020
H53	10.180389	-3.733572	-2.612091
N54	5.798246	-2.587790	-3.534389
H55	5.532577	-5.190042	-3.428758
H56	7.295862	-6.899478	-3.019121
H57	5.677744	-2.422295	-4.523873
C58	8.556723	-1.613243	-2.982993
H59	8.525659	-1.285686	-1.939339
H60	7.803700	-1.046495	-3.526988
C61	9.958202	-1.316923	-3.540363
O62	10.061184	-0.960755	-4.735399
O63	10.932799	-1.474969	-2.745311
H64	-1.406825	0.068770	4.069982
H65	0.713178	-4.773600	2.213297
H66	-1.496043	-4.958975	0.622315
H67	-3.928203	-1.833292	-2.726249
H68	-3.490660	0.786615	-3.621626
H69	-0.570732	4.691372	-2.097479
H70	1.427055	5.126909	-0.474304
H71	4.212992	1.759750	2.801366
H72	3.845357	-0.818794	3.666282

Diclofenac 4'-3 Reactant Complex Doublet

C1	-2.105625	0.200934	3.178028
S2	-1.362513	1.235220	1.857941
H3	-3.116627	0.586627	3.344800
H4	-2.192915	-0.829522	2.821398
O5	1.032836	-0.590560	-1.074902
Fe6	0.041224	0.020657	0.078024
N7	-0.323071	-1.835339	0.809092
N8	-1.601898	-0.121904	-1.102369
N9	0.234937	1.983420	-0.428138
N10	1.528176	0.242944	1.425120
C11	0.499310	-2.554734	1.637638
C12	0.098954	-3.940675	1.678993
C13	-0.980407	-4.049729	0.851870
C14	-1.221545	-2.734319	0.303737
C15	-2.342772	-1.245340	-1.331258

C16	-3.319118	-1.003928	-2.375062
C17	-3.157070	0.291508	-2.773658
C18	-2.077529	0.819985	-1.961106
C19	-0.541526	2.652201	-1.329864
C20	-0.120113	4.026417	-1.434866
C21	0.925698	4.191913	-0.576505
C22	1.151679	2.893379	0.041243
C23	2.336342	1.337403	1.570435
C24	3.402088	1.049112	2.503275
C25	3.228440	-0.235714	2.917014
C26	2.066216	-0.734640	2.222402
C27	1.600466	-2.038519	2.305148
H28	2.164867	-2.728196	2.919570
C29	-2.172529	-2.455602	-0.672079
H30	-2.820470	-3.268703	-0.957302
C31	-1.590325	2.119026	-2.061046
H32	-2.034640	2.769510	-2.800580
C33	2.168741	2.557576	0.925256
H34	2.939782	3.288460	1.118799
C35	4.872160	-2.846147	-3.467341
C36	4.659183	-2.684283	-2.083875
C37	3.401057	-2.750406	-1.497412
C38	2.291156	-3.027400	-2.291958
C39	2.463582	-3.262929	-3.652698
C40	3.728102	-3.149817	-4.224702
C141	6.032216	-2.306674	-1.056675
H42	3.287935	-2.548530	-0.440379
H43	1.303595	-3.047073	-1.850184
H44	1.626694	-3.530840	-4.285428
C145	3.875337	-3.388306	-5.964807
C46	9.095114	-5.646259	-3.496627
C47	9.398473	-4.308466	-3.248075
C48	8.438288	-3.296953	-3.381537
C49	7.150062	-3.662016	-3.804548
C50	6.836822	-5.008627	-4.034989
C51	7.797833	-6.005011	-3.879529
H52	9.863772	-6.408170	-3.397290
H53	10.404254	-4.021100	-2.956005
N54	6.147821	-2.655373	-4.027610
H55	5.830289	-5.256757	-4.354684
H56	7.541477	-7.041860	-4.067469
H57	6.127961	-2.345340	-4.991397
C58	8.800754	-1.864581	-3.026466
H59	9.081667	-1.828334	-1.970141
H60	7.922814	-1.234514	-3.170986
C61	9.957134	-1.332567	-3.881412
O62	9.727480	-1.001446	-5.045682
O63	11.110650	-1.270692	-3.315625
H64	-1.601528	0.150294	4.164058
H65	0.618891	-4.734535	2.221652
H66	-1.540831	-4.944136	0.588732
H67	-4.005173	-1.764438	-2.740219
H68	-3.644357	0.909238	-3.542023
H69	-0.600008	4.769782	-2.072939
H70	1.403619	5.164894	-0.430030
H71	4.194405	1.743587	2.763707
H72	3.808435	-0.822091	3.620946

Diclofenac 4'-3 Transition State Doublet

C1	-1.978502	0.188933	3.068911
S2	-1.206090	1.214518	1.753260
H3	-3.002567	0.557275	3.195532
H4	-2.029715	-0.843204	2.711579
O5	1.217314	-0.672814	-1.240444
Fe6	0.183434	-0.080292	-0.002508
N7	-0.199037	-1.899707	0.746582
N8	-1.483305	-0.212163	-1.168501
N9	0.373628	1.895615	-0.539230
N10	1.648656	0.163012	1.343992
C11	0.593856	-2.608316	1.618694
C12	0.168079	-3.982696	1.687441
C13	-0.911390	-4.094069	0.859868
C14	-1.126769	-2.794793	0.269444
C15	-2.246211	-1.325348	-1.374106
C16	-3.255516	-1.069812	-2.384701
C17	-3.102369	0.228269	-2.775587
C18	-1.991149	0.744861	-1.997417
C19	-0.452324	2.571128	-1.390248
C20	-0.081500	3.961362	-1.459902
C21	0.982302	4.135002	-0.625530
C22	1.260950	2.822397	-0.050482
C23	2.437044	1.274551	1.493482
C24	3.477030	1.011340	2.462337
C25	3.294248	-0.263571	2.906670
C26	2.155993	-0.786137	2.192023
C27	1.683849	-2.086293	2.298571
H28	2.226500	-2.763417	2.945014
C29	-2.083476	-2.527291	-0.700424
H30	-2.757882	-3.331485	-0.952045
C31	-1.525214	2.046558	-2.086563
H32	-2.015833	2.716556	-2.777583
C33	2.264962	2.495894	0.853771
H34	3.013768	3.239226	1.080575
C35	4.541463	-2.570233	-2.913638
C36	4.516218	-2.305765	-1.522651
C37	3.357109	-2.212746	-0.777999
C38	2.089346	-2.383806	-1.393226
C39	2.100285	-2.796208	-2.754093
C40	3.273173	-2.831992	-3.485401
C141	6.046755	-2.013720	-0.733895
H42	3.419530	-1.976322	0.275377
H43	1.257705	-2.712174	-0.788337
H44	1.182414	-3.131628	-3.214398
C145	3.208332	-3.310331	-5.187203
C46	8.766747	-5.426022	-3.442184
C47	9.089948	-4.083240	-3.256570
C48	8.118071	-3.073991	-3.284994
C49	6.783318	-3.455759	-3.512243
C50	6.455048	-4.807267	-3.682720
C51	7.434805	-5.795603	-3.649474
H52	9.549868	-6.177826	-3.436826
H53	10.123224	-3.786844	-3.100244
N54	5.722983	-2.480858	-3.657715
H55	5.418172	-5.064853	-3.874580
H56	7.164228	-6.835847	-3.805284
H57	5.558358	-2.246191	-4.628767
C58	8.548906	-1.636514	-3.028336
H59	8.765576	-1.528198	-1.961654
H60	7.723999	-0.968093	-3.273589

C61	9.798179	-1.247490	-3.842201
O62	9.652055	-0.901895	-5.013392
O63	10.931657	-1.320397	-3.236694
H64	-1.509031	0.152241	4.078363
H65	0.676597	-4.765945	2.249209
H66	-1.511075	-4.971135	0.631564
H67	-3.961601	-1.822323	-2.727481
H68	-3.611350	0.861317	-3.520276
H69	-0.614816	4.703126	-2.058110
H70	1.425645	5.123806	-0.473986
H71	4.256561	1.720237	2.725006
H72	3.846984	-0.829960	3.646172

Diclofenac 4'-4 Reactant Complex Doublet

C1	-2.048853	0.237620	3.077026
S2	-1.343649	1.270967	1.751854
H3	-3.058904	0.617564	3.273773
H4	-2.139289	-0.791253	2.717576
O5	1.098156	-0.565259	-1.105689
Fe6	0.077201	0.017791	0.036439
N7	-0.293359	-1.842954	0.756195
N8	-1.543209	-0.125245	-1.167634
N9	0.280690	1.981132	-0.461443
N10	1.536478	0.227815	1.421640
C11	0.520690	-2.570611	1.585408
C12	0.108360	-3.952867	1.624564
C13	-0.974872	-4.050300	0.802288
C14	-1.201218	-2.733157	0.253422
C15	-2.301213	-1.239120	-1.387162
C16	-3.280417	-0.986600	-2.425417
C17	-3.100303	0.303173	-2.831281
C18	-2.010388	0.822637	-2.026008
C19	-0.484892	2.656766	-1.367772
C20	-0.065835	4.034152	-1.448280
C21	0.968065	4.190733	-0.571819
C22	1.181273	2.888862	0.040243
C23	2.330478	1.328253	1.594605
C24	3.392631	1.034010	2.529532
C25	3.233584	-0.261738	2.917950
C26	2.078996	-0.758856	2.206982
C27	1.618352	-2.064621	2.267479
H28	2.175984	-2.761029	2.881091
C29	-2.151278	-2.448193	-0.721710
H30	-2.811488	-3.257862	-0.997526
C31	-1.525078	2.122364	-2.116523
H32	-1.976828	2.779944	-2.846986
C33	2.169086	2.552169	0.958641
H34	2.928781	3.284381	1.185182
C35	4.634611	-3.065847	-3.264740
C36	4.498143	-2.707231	-1.909289
C37	3.281893	-2.721622	-1.238936
C38	2.144297	-3.145559	-1.918589
C39	2.241176	-3.560287	-3.242745
C40	3.466999	-3.499120	-3.904027
C141	5.922046	-2.172358	-1.030132
H42	3.218095	-2.381830	-0.212633
H43	1.185520	-3.142855	-1.414184
H44	1.367160	-3.905854	-3.782088
C145	3.511407	-3.972858	-5.594897

C46	8.777863	-5.866818	-2.903868
C47	9.155887	-4.527504	-3.023653
C48	8.244108	-3.525950	-3.371051
C49	6.895991	-3.901157	-3.599323
C50	6.525797	-5.251656	-3.486188
C51	7.449518	-6.227031	-3.134608
H52	9.509512	-6.620695	-2.635020
H53	10.179212	-4.230000	-2.836176
N54	5.889481	-2.975630	-3.939288
H55	5.494375	-5.522604	-3.683783
H56	7.131455	-7.261224	-3.057393
H57	6.176069	-2.019646	-4.099423
C58	8.668953	-2.058165	-3.432762
H59	8.443331	-1.594391	-2.464547
H60	8.089228	-1.533402	-4.192865
C61	10.146341	-1.797852	-3.769317
O62	10.390856	-1.277236	-4.873854
O63	11.027837	-2.122421	-2.905345
H64	-1.526351	0.186472	4.048120
H65	0.619034	-4.748022	2.171382
H66	-1.559838	-4.930495	0.547882
H67	-3.994944	-1.733851	-2.762450
H68	-3.589358	0.922235	-3.594547
H69	-0.538598	4.790532	-2.076564
H70	1.452036	5.158382	-0.410109
H71	4.174094	1.736776	2.798581
H72	3.819719	-0.850229	3.619324

Diclofenac 4'-4 Transition State Doublet

C1	-1.934508	0.203121	2.982977
S2	-1.200538	1.228684	1.657392
H3	-2.957247	0.567482	3.136835
H4	-1.996525	-0.831104	2.632774
O5	1.281612	-0.746676	-1.301591
Fe6	0.214809	-0.095778	-0.031397
N7	-0.197003	-1.897161	0.719062
N8	-1.420250	-0.209431	-1.235295
N9	0.437530	1.890126	-0.574069
N10	1.646184	0.142644	1.353999
C11	0.578392	-2.617714	1.599252
C12	0.138864	-3.986235	1.657542
C13	-0.938099	-4.081826	0.826920
C14	-1.130951	-2.780007	0.239239
C15	-2.213065	-1.304490	-1.427030
C16	-3.218236	-1.033799	-2.436835
C17	-3.027665	0.252701	-2.845728
C18	-1.904387	0.749781	-2.073312
C19	-0.370161	2.575395	-1.434799
C20	-0.009506	3.971072	-1.470028
C21	1.028301	4.137131	-0.603715
C22	1.293609	2.818590	-0.036678
C23	2.421721	1.260246	1.537798
C24	3.449721	0.989557	2.516512
C25	3.274717	-0.295011	2.936708
C26	2.147061	-0.811374	2.201911
C27	1.666252	-2.110048	2.292418
H28	2.189947	-2.791571	2.949138
C29	-2.080916	-2.500460	-0.738677
H30	-2.770772	-3.296658	-0.979207

C31	-1.426282	2.049742	-2.160566
H32	-1.910485	2.722845	-2.853860
C33	2.260173	2.488226	0.908016
H34	2.990794	3.235487	1.178034
C35	4.497257	-2.736391	-2.883819
C36	4.504900	-2.328034	-1.528438
C37	3.372007	-2.155544	-0.762282
C38	2.072099	-2.368890	-1.332522
C39	2.065046	-2.931547	-2.659855
C40	3.221612	-3.060816	-3.400975
C141	6.060563	-1.983048	-0.806898
H42	3.453276	-1.825326	0.263794
H43	1.310414	-2.771135	-0.676298
H44	1.127564	-3.286060	-3.069105
C145	3.125962	-3.742263	-5.024115
C46	8.524454	-5.823771	-2.969696
C47	8.950656	-4.498915	-3.070954
C48	8.065531	-3.444223	-3.312147
C49	6.682200	-3.748584	-3.432793
C50	6.264084	-5.085408	-3.348447
C51	7.167036	-6.118698	-3.115687
H52	9.242392	-6.615791	-2.786653
H53	10.000070	-4.257468	-2.951032
N54	5.687966	-2.772256	-3.670194
H55	5.211935	-5.303527	-3.499894
H56	6.816493	-7.144243	-3.074593
H57	5.986905	-1.862413	-4.003142
C58	8.571269	-2.004497	-3.406829
H59	8.369623	-1.503870	-2.452481
H60	8.012703	-1.475433	-4.180411
C61	10.064596	-1.820233	-3.748238
O62	10.334389	-1.337948	-4.863402
O63	10.931647	-2.158919	-2.873256
H64	-1.452655	0.167469	3.980863
H65	0.651180	-4.769776	2.207512
H66	-1.548427	-4.943726	0.579484
H67	-3.953687	-1.768767	-2.752655
H68	-3.519470	0.888176	-3.594807
H69	-0.528902	4.724475	-2.067815
H70	1.472638	5.122460	-0.433757
H71	4.222459	1.701967	2.788481
H72	3.832858	-0.872664	3.665130

Diclofenac 4'-5 Reactant Complex Doublet

C1	-1.914183	0.204244	3.146755
S2	-1.353667	1.284105	1.793588
H3	-2.950167	0.491248	3.365654
H4	-1.914002	-0.833834	2.805120
O5	1.064217	-0.379009	-1.087573
Fe6	0.074509	0.103093	0.124316
N7	-0.255821	-1.765460	0.847396
N8	-1.559411	-0.075766	-1.056455
N9	0.275562	2.048564	-0.392649
N10	1.568148	0.318666	1.472224
C11	0.554151	-2.477005	1.693409
C12	0.140522	-3.855868	1.768930
C13	-0.955866	-3.965575	0.965975
C14	-1.181031	-2.662316	0.386863
C15	-2.309029	-1.196913	-1.258972

C16	-3.284437	-0.968077	-2.306109
C17	-3.111643	0.319023	-2.727656
C18	-2.027186	0.856133	-1.927680
C19	-0.470317	2.691290	-1.336323
C20	-0.012201	4.049031	-1.490449
C21	1.017373	4.228202	-0.616535
C22	1.210671	2.950120	0.051537
C23	2.389783	1.405527	1.599053
C24	3.465866	1.115707	2.523258
C25	3.277168	-0.158148	2.960431
C26	2.104751	-0.651756	2.280918
C27	1.642922	-1.953552	2.374147
H28	2.198330	-2.634484	3.006549
C29	-2.146903	-2.394185	-0.576218
H30	-2.805778	-3.210463	-0.828822
C31	-1.522874	2.146310	-2.055586
H32	-1.960103	2.781499	-2.813855
C33	2.227455	2.618114	0.941368
H34	3.019859	3.333041	1.109345
C35	4.595749	-2.622398	-2.943131
C36	4.478387	-2.377805	-1.561846
C37	3.289867	-2.555202	-0.866262
C38	2.166448	-3.013771	-1.546380
C39	2.227617	-3.245866	-2.917325
C40	3.428126	-3.046693	-3.594417
C141	5.877173	-1.791033	-0.689295
H42	3.238849	-2.310812	0.187046
H43	1.233745	-3.131221	-1.010874
H44	1.353958	-3.583055	-3.460132
C145	3.478681	-3.360503	-5.331711
C46	8.564185	-5.624429	-2.915675
C47	9.006601	-4.302249	-2.879539
C48	8.143561	-3.226327	-3.115248
C49	6.792735	-3.508995	-3.392923
C50	6.351119	-4.841388	-3.435133
C51	7.223882	-5.898097	-3.197863
H52	9.259762	-6.436403	-2.732869
H53	10.042369	-4.070445	-2.663906
N54	5.843631	-2.452706	-3.575655
H55	5.308410	-5.035847	-3.656539
H56	6.862142	-6.918331	-3.247883
H57	5.804659	-2.036771	-4.497811
C58	8.659042	-1.795375	-3.019915
H59	8.639499	-1.490302	-1.969892
H60	7.989889	-1.136983	-3.571251
C61	10.092119	-1.670189	-3.562600
O62	10.249896	-1.386570	-4.762162
O63	11.030766	-1.919917	-2.737872
H64	-1.373564	0.223142	4.108690
H65	0.676759	-4.639200	2.312896
H66	-1.560826	-4.840595	0.741331
H67	-3.980626	-1.731991	-2.648611
H68	-3.586832	0.924391	-3.507319
H69	-0.498463	4.782555	-2.128590
H70	1.494235	5.197761	-0.467860
H71	4.275709	1.799917	2.754108
H72	3.844562	-0.751405	3.671772

Diclofenac 4'-5 Transition State Doublet

C1	-1.839240	0.162970	3.073142
S2	-1.242128	1.222820	1.705652
H3	-2.888550	0.430841	3.243290
H4	-1.806400	-0.881648	2.754024
O5	1.186838	-0.564385	-1.187879
Fe6	0.159654	-0.008551	0.091777
N7	-0.206650	-1.831168	0.823918
N8	-1.482769	-0.150328	-1.113392
N9	0.389451	1.946414	-0.495793
N10	1.644222	0.213730	1.415668
C11	0.584209	-2.546582	1.694684
C12	0.157419	-3.919554	1.755680
C13	-0.931224	-4.021538	0.939424
C14	-1.142985	-2.720458	0.354558
C15	-2.257011	-1.256856	-1.301254
C16	-3.255134	-1.007252	-2.325004
C17	-3.078072	0.281453	-2.739279
C18	-1.963071	0.797396	-1.966383
C19	-0.383223	2.607282	-1.405774
C20	0.035218	3.982748	-1.515440
C21	1.059219	4.160778	-0.634059
C22	1.283830	2.862966	-0.010338
C23	2.442811	1.319462	1.551684
C24	3.497623	1.049714	2.502770
C25	3.314472	-0.223592	2.948330
C26	2.154950	-0.734128	2.258962
C27	1.678307	-2.032140	2.373112
H28	2.218712	-2.708953	3.021245
C29	-2.102292	-2.452222	-0.614943
H30	-2.773314	-3.261027	-0.859174
C31	-1.457882	2.081436	-2.101833
H32	-1.920028	2.733090	-2.828558
C33	2.279707	2.536708	0.907121
H34	3.047989	3.265616	1.113521
C35	4.517325	-2.444806	-2.782292
C36	4.506266	-2.093162	-1.410939
C37	3.356547	-1.996640	-0.660462
C38	2.087931	-2.248723	-1.252611
C39	2.083834	-2.699313	-2.603285
C40	3.248597	-2.746619	-3.339148
C141	6.030915	-1.700818	-0.658236
H42	3.418164	-1.699264	0.376619
H43	1.285926	-2.601604	-0.619936
H44	1.156734	-3.047037	-3.038661
C145	3.184171	-3.315492	-5.013581
C46	8.458476	-5.598342	-2.832330
C47	8.905568	-4.279564	-2.816589
C48	8.042794	-3.197235	-3.039904
C49	6.682795	-3.484988	-3.266061
C50	6.233589	-4.811253	-3.281105
C51	7.110323	-5.873701	-3.070792
H52	9.159487	-6.411220	-2.668210
H53	9.949958	-4.053621	-2.632227
N54	5.708695	-2.447392	-3.513689
H55	5.183388	-4.997775	-3.479755
H56	6.747617	-6.893871	-3.109794
H57	5.597848	-2.197834	-4.487067
C58	8.582457	-1.772906	-2.998502
H59	8.573663	-1.430899	-1.960194
H60	7.914520	-1.127156	-3.567601

C61	10.022046	-1.667112	-3.541819
O62	10.184891	-1.358557	-4.735826
O63	10.955798	-1.944524	-2.721694
H64	-1.341548	0.202282	4.063804
H65	0.686897	-4.701169	2.299717
H66	-1.548532	-4.886043	0.708701
H67	-3.973007	-1.751924	-2.662100
H68	-3.566667	0.900477	-3.504071
H69	-0.474603	4.730914	-2.121069
H70	1.503908	5.143401	-0.461305
H71	4.277333	1.759222	2.758519
H72	3.875500	-0.801432	3.671099

Diclofenac 5-1 Reactant Complex Doublet

C1	-2.032900	-0.385908	2.793425
S2	-1.484143	0.850878	1.577876
H3	-3.021889	-0.079302	3.156664
H4	-2.138506	-1.353647	2.294033
O5	1.241071	-0.592936	-1.179291
Fe6	0.136381	-0.163062	-0.040878
N7	-0.137634	-2.061558	0.610339
N8	-1.465402	-0.382343	-1.264816
N9	0.207086	1.820009	-0.452374
N10	1.564608	0.096380	1.377323
C11	0.690153	-2.749161	1.457236
C12	0.327428	-4.140845	1.510664
C13	-0.747958	-4.289836	0.688783
C14	-1.019874	-2.986643	0.125411
C15	-2.217905	-1.506661	-1.450358
C16	-3.270852	-1.259876	-2.415231
C17	-3.138757	0.036824	-2.816729
C18	-2.016907	0.570716	-2.061293
C19	-0.573293	2.462786	-1.366719
C20	-0.194438	3.848862	-1.457438
C21	0.825621	4.047951	-0.575840
C22	1.075000	2.759101	0.053500
C23	2.321725	1.219751	1.561350
C24	3.362921	0.963247	2.534479
C25	3.199039	-0.321249	2.962589
C26	2.107416	-0.863702	2.188761
C27	1.727465	-2.196982	2.187646
H28	2.310713	-2.881056	2.788609
C29	-2.021050	-2.717962	-0.802663
H30	-2.697578	-3.528874	-1.042480
C31	-1.599019	1.895826	-2.112343
H32	-2.097754	2.558047	-2.807157
C33	2.097223	2.446394	0.945876
H34	2.823976	3.209995	1.172289
C35	8.067858	-1.477570	-4.600244
C36	8.827782	-1.238981	-5.784266
C37	9.944016	-1.973567	-6.139357
C38	10.432611	-2.975558	-5.302653
C39	9.764058	-3.201434	-4.101728
C40	8.621289	-2.482420	-3.755423
C141	8.344515	0.038222	-6.901260
H42	10.400175	-1.771216	-7.098672
H43	11.290159	-3.572213	-5.586997
H44	10.105302	-3.968334	-3.418023
C145	7.920104	-2.920381	-2.204599

C46	3.932412	-1.345132	-1.450673
C47	3.800910	-1.906864	-2.716997
C48	4.765010	-1.713060	-3.715903
C49	5.906315	-0.969966	-3.379611
C50	6.027621	-0.356823	-2.129059
C51	5.044618	-0.547318	-1.161374
H52	3.175844	-1.515814	-0.699323
H53	2.933185	-2.514559	-2.948566
N54	6.936990	-0.736512	-4.363937
H55	6.891079	0.264742	-1.928371
H56	5.134190	-0.053570	-0.199337
H57	6.598930	-0.217996	-5.167328
C58	4.505806	-2.217188	-5.116796
H59	5.391781	-2.100163	-5.747480
H60	3.733944	-1.597011	-5.584278
C61	4.067728	-3.689517	-5.256914
O62	3.437128	-3.963691	-6.310674
O63	4.401429	-4.497487	-4.362244
H64	-1.392446	-0.565307	3.664793
H65	0.829471	-4.890383	2.116773
H66	-1.280794	-5.207904	0.460618
H67	-4.002353	-2.029530	-2.658359
H68	-3.672523	0.664839	-3.541288
H69	-0.708661	4.580183	-2.076298
H70	1.281341	5.033480	-0.439944
H71	4.157978	1.653937	2.799272
H72	3.702361	-0.850442	3.775851

Diclofenac 5-1 Transition State Doublet

C1	-1.881155	-0.454791	2.693562
S2	-1.345465	0.800021	1.489352
H3	-2.906148	-0.205811	2.995243
H4	-1.901203	-1.432813	2.202417
O5	1.384148	-0.396004	-1.374839
Fe6	0.251163	-0.167656	-0.073636
N7	0.039749	-2.085265	0.489600
N8	-1.354666	-0.380627	-1.325587
N9	0.277271	1.831539	-0.471227
N10	1.678512	0.062714	1.309757
C11	0.818683	-2.775955	1.392658
C12	0.405546	-4.151831	1.474407
C13	-0.654282	-4.287370	0.629353
C14	-0.876151	-2.996105	0.020533
C15	-2.100811	-1.506395	-1.519162
C16	-3.177550	-1.249648	-2.458308
C17	-3.062496	0.054837	-2.838949
C18	-1.931256	0.585653	-2.092875
C19	-0.510940	2.470706	-1.381489
C20	-0.156000	3.863184	-1.449501
C21	0.843723	4.073423	-0.549856
C22	1.112613	2.775079	0.068697
C23	2.388013	1.215007	1.536255
C24	3.417661	0.962846	2.522878
C25	3.274463	-0.333667	2.931822
C26	2.212192	-0.889802	2.132489
C27	1.836415	-2.225776	2.145134
H28	2.390838	-2.899373	2.782722
C29	-1.882575	-2.726134	-0.896912
H30	-2.559711	-3.535692	-1.134718

C31	-1.533914	1.911623	-2.128912
H32	-2.044663	2.579117	-2.808876
C33	2.129541	2.458116	0.970141
H34	2.825315	3.233474	1.249480
C35	7.330074	-1.541523	-4.130088
C36	8.128835	-1.336982	-5.298015
C37	9.321249	-2.003490	-5.538225
C38	9.811987	-2.931548	-4.623229
C39	9.044335	-3.202396	-3.490387
C40	7.839004	-2.542096	-3.262007
C141	7.612345	-0.245091	-6.575235
H42	9.823760	-1.824003	-6.481010
H43	10.728724	-3.475453	-4.820642
H44	9.346838	-3.968038	-2.790705
C145	6.956795	-3.063709	-1.844854
C46	2.856499	-1.604372	-1.366290
C47	2.928358	-2.103653	-2.702290
C48	3.980128	-1.809243	-3.561598
C49	5.067793	-1.075215	-3.049037
C50	5.034256	-0.560087	-1.736534
C51	3.970079	-0.830866	-0.900483
H52	2.283984	-2.180606	-0.648052
H53	2.131809	-2.751429	-3.053301
N54	6.193631	-0.778222	-3.910823
H55	5.868515	0.040761	-1.389822
H56	3.966753	-0.450765	0.113960
H57	5.912532	-0.221519	-4.712486
C58	3.961310	-2.309178	-4.987767
H59	4.882283	-2.031919	-5.508993
H60	3.149908	-1.841291	-5.549730
C61	3.832476	-3.835766	-5.138106
O62	3.256608	-4.228308	-6.183863
O63	4.336053	-4.558651	-4.252455
H64	-1.291231	-0.587997	3.608595
H65	0.867150	-4.905347	2.108416
H66	-1.236326	-5.184655	0.434728
H67	-3.920115	-2.010516	-2.691687
H68	-3.608731	0.688690	-3.551996
H69	-0.683512	4.575310	-2.080436
H70	1.271660	5.067171	-0.407480
H71	4.192411	1.670725	2.798285
H72	3.757068	-0.876211	3.748924

Diclofenac 5-2 Reactant Complex Doublet

C1	-1.962277	-0.533220	3.076824
S2	-1.364561	0.570791	1.754001
H3	-3.008006	-0.262256	3.270994
H4	-1.942094	-1.566238	2.718446
O5	0.869236	-1.026233	-1.334815
Fe6	-0.069307	-0.532072	-0.085555
N7	-0.364287	-2.395411	0.648083
N8	-1.778255	-0.702723	-1.159343
N9	0.098105	1.422053	-0.626088
N10	1.482783	-0.304757	1.174864
C11	0.498122	-3.104727	1.441701
C12	0.092712	-4.483284	1.539148
C13	-1.054307	-4.594843	0.812164
C14	-1.321169	-3.289766	0.251082
C15	-2.574408	-1.801219	-1.269562

C16	-3.655356	-1.557536	-2.201822
C17	-3.485834	-0.293753	-2.678952
C18	-2.313768	0.229905	-1.995538
C19	-0.732960	2.064898	-1.489511
C20	-0.282319	3.414829	-1.704587
C21	0.864162	3.581389	-0.985281
C22	1.087445	2.317350	-0.288382
C23	2.278476	0.798919	1.285587
C24	3.354091	0.542302	2.220215
C25	3.180686	-0.731074	2.682343
C26	2.031129	-1.257637	1.993583
C27	1.602648	-2.570857	2.081459
H28	2.195104	-3.252092	2.676245
C29	-2.369765	-3.005802	-0.609089
H30	-3.070101	-3.803837	-0.805876
C31	-1.838077	1.522296	-2.129927
H32	-2.338394	2.170249	-2.837455
C33	2.100505	2.002643	0.611492
H34	2.850082	2.744657	0.832881
C35	7.459000	-3.556934	-2.881559
C36	8.129338	-2.571195	-2.131222
C37	9.281386	-2.847743	-1.402201
C38	9.827885	-4.131004	-1.437564
C39	9.211150	-5.131029	-2.190484
C40	8.032858	-4.841686	-2.875846
C141	7.486216	-0.949079	-2.084601
H42	9.730652	-2.067779	-0.803555
H43	10.724436	-4.353112	-0.871334
H44	9.611843	-6.137474	-2.217920
C145	7.213032	-6.156607	-3.706656
C46	2.599731	-3.345447	-1.474560
C47	2.648141	-3.116347	-2.854233
C48	3.848791	-3.034411	-3.557525
C49	5.050473	-3.246321	-2.839152
C50	5.006644	-3.427682	-1.447899
C51	3.790397	-3.465989	-0.767252
H52	1.645520	-3.386988	-0.968777
H53	1.725402	-2.976084	-3.398909
N54	6.258377	-3.276872	-3.544298
H55	5.932895	-3.534119	-0.901758
H56	3.780036	-3.583001	0.312126
H57	6.173519	-3.589448	-4.520638
C58	3.834402	-2.629650	-5.025010
H59	4.512366	-1.779888	-5.156244
H60	2.827325	-2.309374	-5.283624
C61	4.269298	-3.698554	-6.048182
O62	5.509468	-3.970827	-6.095106
O63	3.387918	-4.204585	-6.763010
H64	-1.452730	-0.533589	4.056741
H65	0.622425	-5.256721	2.095618
H66	-1.654177	-5.480079	0.639086
H67	-4.409467	-2.309694	-2.408718
H68	-4.029369	0.310981	-3.414994
H69	-0.827227	4.137916	-2.311331
H70	1.407981	4.532796	-1.030506
H71	4.167532	1.235156	2.409173
H72	3.735786	-1.302401	3.423090

Diclofenac 5-2 Transition State Doublet

C1	-1.906490	-0.568940	2.970981
S2	-1.300869	0.523515	1.626779
H3	-2.961641	-0.318150	3.133021
H4	-1.853112	-1.608711	2.634722
O5	1.084370	-0.944788	-1.382439
Fe6	0.022700	-0.587822	-0.070961
N7	-0.263330	-2.449450	0.602196
N8	-1.675254	-0.773742	-1.215193
N9	0.183566	1.366492	-0.667503
N10	1.552996	-0.365569	1.177059
C11	0.561877	-3.151255	1.452793
C12	0.137673	-4.525528	1.544276
C13	-0.994862	-4.632476	0.794554
C14	-1.237806	-3.337981	0.206240
C15	-2.490074	-1.859112	-1.307665
C16	-3.590865	-1.598850	-2.215644
C17	-3.415864	-0.335469	-2.693311
C18	-2.221417	0.172347	-2.035600
C19	-0.656793	2.003238	-1.527779
C20	-0.229060	3.364569	-1.717409
C21	0.909787	3.540326	-0.989386
C22	1.152650	2.267184	-0.306935
C23	2.330724	0.752353	1.280302
C24	3.389260	0.511006	2.234486
C25	3.208648	-0.753863	2.720701
C26	2.063058	-1.293408	2.036220
C27	1.627880	-2.610427	2.142818
H28	2.191185	-3.281358	2.777827
C29	-2.291381	-3.063595	-0.647890
H30	-3.003010	-3.854694	-0.827414
C31	-1.756790	1.463929	-2.173124
H32	-2.261416	2.108452	-2.875308
C33	2.154013	1.959814	0.609694
H34	2.888797	2.711317	0.846462
C35	7.119821	-3.521778	-2.684523
C36	7.876694	-2.519626	-2.050138
C37	9.080561	-2.795675	-1.407531
C38	9.601067	-4.084458	-1.433540
C39	8.911735	-5.096932	-2.101768
C40	7.688572	-4.811742	-2.703848
C141	7.333665	-0.866002	-2.082873
H42	9.597365	-1.995472	-0.893533
H43	10.541117	-4.302226	-0.937974
H44	9.301204	-6.106577	-2.141746
C145	6.841427	-6.128860	-3.489875
C46	2.182546	-2.606184	-1.479974
C47	2.328106	-2.743879	-2.895915
C48	3.538413	-2.796039	-3.541683
C49	4.726208	-2.899653	-2.732299
C50	4.616267	-2.654632	-1.333019
C51	3.395181	-2.486405	-0.729070
H52	1.310735	-3.026138	-0.991595
H53	1.433264	-2.798757	-3.493650
N54	5.891732	-3.264101	-3.330805
H55	5.519012	-2.623642	-0.737725
H56	3.354376	-2.320212	0.336021
H57	5.812787	-3.582189	-4.327665
C58	3.579458	-2.611764	-5.053421
H59	4.193272	-1.725464	-5.254694
H60	2.568787	-2.391057	-5.387319

C61	4.131902	-3.727011	-5.960755
O62	5.367649	-4.017908	-5.837576
O63	3.350044	-4.232755	-6.775853
H64	-1.430568	-0.549330	3.977821
H65	0.652061	-5.302400	2.106204
H66	-1.625462	-5.502239	0.629475
H67	-4.380051	-2.319441	-2.404874
H68	-3.975601	0.281181	-3.412491
H69	-0.795079	4.097874	-2.292547
H70	1.428684	4.502240	-1.023246
H71	4.185870	1.222304	2.423710
H72	3.762539	-1.318763	3.461927

Diclofenac 5-3 Reactant Complex Doublet

C1	-1.990740	-0.456018	3.063474
S2	-1.444640	0.685512	1.748752
H3	-3.052457	-0.241437	3.237970
H4	-1.908220	-1.483967	2.701058
O5	0.950113	-0.846621	-1.252394
Fe6	-0.062636	-0.361225	-0.059272
N7	-0.328564	-2.230263	0.658367
N8	-1.740391	-0.572748	-1.170573
N9	0.067785	1.596887	-0.598730
N10	1.426287	-0.074824	1.261759
C11	0.538093	-2.910444	1.472206
C12	0.188432	-4.305107	1.539662
C13	-0.933103	-4.454738	0.782854
C14	-1.242146	-3.157316	0.231832
C15	-2.530436	-1.676915	-1.266001
C16	-3.627848	-1.442226	-2.179593
C17	-3.464251	-0.186545	-2.678545
C18	-2.292757	0.349823	-2.007246
C19	-0.753978	2.214182	-1.487824
C20	-0.337722	3.573944	-1.698619
C21	0.779210	3.780902	-0.946069
C22	1.017966	2.525543	-0.235788
C23	2.177695	1.056793	1.404169
C24	3.211655	0.840754	2.392036
C25	3.065103	-0.436709	2.849663
C26	1.969461	-1.006897	2.109264
C27	1.585515	-2.334276	2.170018
H28	2.163669	-2.993644	2.805640
C29	-2.302538	-2.888368	-0.624844
H30	-2.993991	-3.694678	-0.835101
C31	-1.835298	1.650548	-2.150314
H32	-2.332581	2.292685	-2.863846
C33	1.997296	2.249331	0.710580
H34	2.701954	3.022457	0.970774
C35	7.518740	-3.373633	-2.809273
C36	8.158573	-2.392860	-2.025726
C37	9.315557	-2.658546	-1.300843
C38	9.899923	-3.922539	-1.373322
C39	9.310369	-4.918492	-2.152385
C40	8.122914	-4.643196	-2.830041
C141	7.480720	-0.786595	-1.941993
H42	9.743523	-1.884177	-0.678474
H43	10.805109	-4.133405	-0.815367
H44	9.735620	-5.914810	-2.202714
C145	7.327569	-5.966065	-3.667801

C46	2.632983	-3.198584	-1.457841
C47	2.701037	-2.917373	-2.825218
C48	3.907819	-2.854481	-3.520654
C49	5.098920	-3.117304	-2.803889
C50	5.034112	-3.404656	-1.432810
C51	3.812633	-3.433688	-0.760643
H52	1.672448	-3.221930	-0.960659
H53	1.785755	-2.735503	-3.370627
N54	6.322519	-3.101992	-3.485461
H55	5.950590	-3.625983	-0.904297
H56	3.793245	-3.647170	0.303458
H57	6.262275	-3.396176	-4.468452
C58	3.914468	-2.442200	-4.986336
H59	4.600295	-1.597071	-5.102842
H60	2.912439	-2.117407	-5.262225
C61	4.354715	-3.530564	-5.989535
O62	5.601154	-3.772598	-6.056242
O63	3.475238	-4.091475	-6.665429
H64	-1.497234	-0.428838	4.057057
H65	0.743549	-5.061556	2.093522
H66	-1.488832	-5.361842	0.582092
H67	-4.420814	-2.170858	-2.287314
H68	-4.003521	0.401923	-3.430188
H69	-0.888303	4.249508	-2.350403
H70	1.299319	4.748278	-0.974193
H71	3.995304	1.562714	2.597158
H72	3.622338	-0.994852	3.600932

Diclofenac 5-3 Reactant Complex Quartet

C1	-2.040494	-0.463863	3.089597
S2	-1.420871	0.671609	1.798641
H3	-3.106274	-0.229241	3.219527
H4	-1.964757	-1.497525	2.729640
O5	0.961599	-0.832522	-1.282581
Fe6	-0.042046	-0.320490	-0.110780
N7	-0.302887	-2.175247	0.616938
N8	-1.730618	-0.540246	-1.206276
N9	0.050899	1.647361	-0.633349
N10	1.427951	-0.004619	1.215190
C11	0.582249	-2.853302	1.414463
C12	0.245962	-4.249322	1.482647
C13	-0.891545	-4.405002	0.747219
C14	-1.215028	-3.110761	0.198053
C15	-2.520625	-1.650952	-1.307410
C16	-3.616250	-1.417192	-2.226191
C17	-3.450456	-0.157836	-2.724331
C18	-2.288635	0.379750	-2.046008
C19	-0.785010	2.266293	-1.514060
C20	-0.401337	3.636192	-1.708692
C21	0.716799	3.855269	-0.956569
C22	0.983923	2.597040	-0.265233
C23	2.156434	1.142521	1.378225
C24	3.175073	0.944177	2.382775
C25	3.050047	-0.341194	2.830650
C26	1.982942	-0.929635	2.064833
C27	1.628656	-2.268252	2.108763
H28	2.225488	-2.923926	2.733063
C29	-2.281532	-2.855239	-0.656088
H30	-2.960753	-3.676239	-0.858139

C31	-1.856203	1.688691	-2.179183
H32	-2.373275	2.323854	-2.887864
C33	1.963523	2.336145	0.687108
H34	2.654791	3.124640	0.951175
C35	7.627246	-3.799713	-2.715260
C36	8.204653	-2.715704	-2.009391
C37	9.415770	-2.831212	-1.330986
C38	10.125605	-4.031683	-1.383433
C39	9.617650	-5.114478	-2.103521
C40	8.377470	-4.996299	-2.732307
C41	7.405949	-1.163009	-2.025863
H42	9.799325	-1.978920	-0.781557
H43	11.071925	-4.127517	-0.857730
H44	10.154940	-6.056788	-2.150075
C45	7.716227	-6.409558	-3.542544
C46	2.758790	-2.991573	-1.392797
C47	2.932460	-2.636712	-2.732698
C48	4.126328	-2.843045	-3.423713
C49	5.200515	-3.447733	-2.727345
C50	5.028091	-3.830497	-1.386575
C51	3.825211	-3.597121	-0.723226
H52	1.811802	-2.818554	-0.901043
H53	2.119305	-2.144857	-3.247946
N54	6.412985	-3.688122	-3.377754
H55	5.846789	-4.342652	-0.888428
H56	3.716657	-3.908313	0.313331
H57	6.396716	-3.748319	-4.412345
C58	4.281740	-2.324428	-4.840722
H59	5.089400	-1.583321	-4.832312
H60	3.354399	-1.824383	-5.133080
C61	4.632244	-3.373264	-5.925157
O62	5.879070	-3.645189	-6.062250
O63	3.702407	-3.877745	-6.583406
H64	-1.588811	-0.449025	4.109330
H65	0.805389	-5.002821	2.031434
H66	-1.443363	-5.319860	0.569054
H67	-4.428439	-2.118630	-2.379273
H68	-3.990291	0.423575	-3.482279
H69	-0.961958	4.327161	-2.337505
H70	1.203781	4.837245	-0.981781
H71	3.936885	1.684416	2.606447
H72	3.606637	-0.887968	3.590639

Diclofenac 5-3 Transition State Doublet

C1	-1.925955	-0.490328	2.969260
S2	-1.356181	0.641186	1.639306
H3	-2.995994	-0.299170	3.110787
H4	-1.807510	-1.523193	2.630413
O5	1.125369	-0.779116	-1.322953
Fe6	0.037688	-0.418083	-0.041215
N7	-0.217316	-2.278806	0.630665
N8	-1.639716	-0.635391	-1.200867
N9	0.164904	1.541162	-0.633788
N10	1.531330	-0.144623	1.243625
C11	0.621090	-2.955409	1.488174
C12	0.259276	-4.347411	1.545733
C13	-0.851368	-4.493988	0.768770
C14	-1.146272	-3.201935	0.201266
C15	-2.438713	-1.732502	-1.286887

C16	-3.553265	-1.483383	-2.180195
C17	-3.393035	-0.225718	-2.671412
C18	-2.205445	0.303512	-2.020293
C19	-0.672439	2.152484	-1.514731
C20	-0.277001	3.521952	-1.707294
C21	0.833498	3.738960	-0.949283
C22	1.097607	2.474623	-0.254841
C23	2.259824	1.001925	1.378101
C24	3.274433	0.807829	2.386779
C25	3.121531	-0.461342	2.872018
C26	2.036474	-1.048829	2.130422
C27	1.644104	-2.380941	2.217783
H28	2.205788	-3.033817	2.872314
C29	-2.208381	-2.944613	-0.651121
H30	-2.899101	-3.752078	-0.855888
C31	-1.758281	1.598362	-2.165674
H32	-2.268798	2.246235	-2.865340
C33	2.076132	2.200217	0.692204
H34	2.782333	2.971829	0.952987
C35	7.164659	-3.318548	-2.576593
C36	7.893095	-2.313422	-1.915746
C37	9.096120	-2.572012	-1.264036
C38	9.651026	-3.847134	-1.314903
C39	8.994858	-4.858195	-2.013733
C40	7.769242	-4.593319	-2.620489
C141	7.328247	-0.667930	-1.936564
H42	9.585902	-1.769989	-0.730608
H43	10.594167	-4.050235	-0.819002
H44	9.409750	-5.857623	-2.076964
C145	6.975259	-5.917641	-3.442281
C46	2.187792	-2.464504	-1.441922
C47	2.356017	-2.611150	-2.855458
C48	3.581033	-2.640724	-3.477728
C49	4.756449	-2.729592	-2.648744
C50	4.617878	-2.489732	-1.252771
C51	3.385508	-2.335330	-0.669826
H52	1.305864	-2.878796	-0.970692
H53	1.471731	-2.702035	-3.466262
N54	5.938185	-3.078656	-3.232377
H55	5.510972	-2.443189	-0.642021
H56	3.319095	-2.163124	0.394063
H57	5.882345	-3.388989	-4.230547
C58	3.653991	-2.451645	-4.987969
H59	4.275110	-1.566267	-5.171377
H60	2.650810	-2.229380	-5.341723
C61	4.227329	-3.571409	-5.878926
O62	5.469881	-3.823866	-5.764707
O63	3.448659	-4.123040	-6.669721
H64	-1.467693	-0.445705	3.985381
H65	0.797650	-5.105829	2.109884
H66	-1.432041	-5.391866	0.579680
H67	-4.370856	-2.186479	-2.280960
H68	-3.948863	0.371200	-3.408110
H69	-0.856980	4.198683	-2.333315
H70	1.320738	4.719064	-0.959670
H71	4.023575	1.559692	2.605907
H72	3.666433	-1.002296	3.638807

Diclofenac 5-3 Transition State Quartet

C1	-1.943098	-0.504869	2.981689
S2	-1.329603	0.614728	1.664592
H3	-3.012821	-0.299781	3.099030
H4	-1.829308	-1.539213	2.643709
O5	1.179185	-1.051355	-1.254919
Fe6	0.061175	-0.392031	-0.106848
N7	-0.254029	-2.247402	0.639118
N8	-1.623519	-0.613048	-1.250083
N9	0.187814	1.538115	-0.686061
N10	1.554665	-0.108212	1.192096
C11	0.602809	-2.919295	1.472063
C12	0.245568	-4.312834	1.536234
C13	-0.869859	-4.462091	0.766178
C14	-1.169250	-3.168117	0.202494
C15	-2.437769	-1.708083	-1.315814
C16	-3.554721	-1.455363	-2.206168
C17	-3.386951	-0.202074	-2.707760
C18	-2.191973	0.321008	-2.069247
C19	-0.662016	2.161972	-1.556039
C20	-0.286673	3.535962	-1.719763
C21	0.822601	3.755579	-0.958286
C22	1.104168	2.490720	-0.283883
C23	2.271321	1.035830	1.349254
C24	3.271544	0.843762	2.373484
C25	3.124423	-0.432051	2.842280
C26	2.052793	-1.021107	2.076927
C27	1.642834	-2.342690	2.180821
H28	2.202439	-2.993347	2.839448
C29	-2.225382	-2.911166	-0.663122
H30	-2.920943	-3.715525	-0.861769
C31	-1.746737	1.616939	-2.214775
H32	-2.259759	2.268338	-2.908074
C33	2.077944	2.236525	0.671438
H34	2.756137	3.025121	0.951421
C35	7.227014	-3.415213	-2.601691
C36	7.927804	-2.404818	-1.916468
C37	9.139986	-2.643506	-1.274210
C38	9.730391	-3.901697	-1.356347
C39	9.102232	-4.915533	-2.078119
C40	7.866966	-4.671073	-2.675564
C141	7.311371	-0.776115	-1.912624
H42	9.611958	-1.839736	-0.725335
H43	10.679057	-4.091455	-0.864519
H44	9.545697	-5.900827	-2.163422
C145	7.104328	-5.998592	-3.525115
C46	2.186132	-2.644543	-1.499074
C47	2.406998	-2.671068	-2.919577
C48	3.651198	-2.686164	-3.506611
C49	4.803013	-2.869373	-2.667629
C50	4.624795	-2.782649	-1.259109
C51	3.379653	-2.660645	-0.693069
H52	1.306711	-3.132964	-1.099934
H53	1.544589	-2.704275	-3.565173
N54	6.001124	-3.181955	-3.254827
H55	5.498292	-2.861799	-0.624809
H56	3.282417	-2.644017	0.383046
H57	5.963280	-3.449720	-4.262180
C58	3.782615	-2.414190	-4.998876
H59	4.469491	-1.568961	-5.112895
H60	2.808516	-2.107328	-5.372321

C61	4.308189	-3.533917	-5.918667
O62	5.550845	-3.806144	-5.842830
O63	3.496514	-4.070492	-6.682925
H64	-1.500518	-0.461883	4.006131
H65	0.792490	-5.070713	2.093556
H66	-1.442446	-5.362385	0.571169
H67	-4.384328	-2.144867	-2.313834
H68	-3.946425	0.392272	-3.444368
H69	-0.872688	4.222177	-2.330041
H70	1.298757	4.743005	-0.961578
H71	4.006244	1.604778	2.607770
H72	3.664733	-0.975650	3.613697

iv) Details of supplementary PDB files

The following PDB files are provided as supporting information:

dcl_c4_4-2_rc_qmmm.pdb

dcl_c4_4-2_ts_qmmm.pdb

dcl_c5_5-3_rc_qmmm.pdb

dcl_c5_5-3_ts_qmmm.pdb

ib_c2_2-3_rc_qmmm.pdb

ib_c2_2-3_ts_qmmm.pdb

ib_c3_3-1_rc_qmmm.pdb

ib_c3_3-1_ts_qmmm.pdb

war_c6_6-8_rc_qmmm.pdb

war_c6_6-8_ts_qmmm.pdb

war_c7_7-9_rc_qmmm.pdb

war_c7_7-9_ts_qmmm.pdb

These structures correspond to the reactant complexes (rc) and transition states (ts) of the pathways with the lowest energy barriers. Structures were optimized with the doublet spin state of Cpd I.

The atoms corresponding to QM atoms in the QM/MM calculations are as follows:

For diclofenac (dcl) calculations, the atoms with the following atom numbers were included in the QM region:

5190-5193, 5778-5807, 5852-5880.

For ibuprofen (ib) calculations, the atoms with the following atom numbers were included in the QM region:

5131-5134, 5702-5731, 5776-5807.

For warfarin (war) calculations, the atoms with the following atom numbers were included in the QM region.

5122-5125, 5683-5712, 5757-5773.