



Supplementary material: The structure–activity relationship and computational studies of 1,3-thiazole derivatives as cholinesterase inhibitors with anti-inflammatory activity

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1. Molecular docking of AChE

Cartesian coordinates of AChE docked with molecule 3

N	-52.999000	39.125000	148.492000
C	-52.055000	38.338000	149.394000
C	-51.756000	36.970000	148.699000
O	-51.182000	36.981000	147.619000

C	-52.548000	38.292000	150.858000
O	-51.645000	37.729000	151.893000
N	-54.083000	44.654000	155.630000
C	-54.120000	44.053000	154.335000
C	-55.500000	43.515000	154.097000
O	-56.146000	43.097000	154.971000
C	-53.048000	43.021000	154.151000
C	-53.340000	41.752000	154.832000
N	-54.205000	40.824000	154.317000
C	-52.917000	41.265000	156.011000

* Corresponding authors.

C	-54.301000	39.812000	155.151000	N	-53.603000	32.992000	152.649000
N	-53.521000	40.051000	156.181000	C	-52.384000	32.305000	153.070000
N	-49.431000	46.211000	156.370000	C	-52.203000	30.886000	152.533000
C	-49.529000	44.840000	155.995000	D	-51.409000	30.116000	153.057000
C	-49.237000	43.838000	157.199000	N	-52.131000	35.821000	149.230000
D	-49.768000	42.731000	157.218000	C	-51.810000	34.580000	148.493000
C	-48.521000	44.557000	154.862000	C	-52.408000	34.561000	147.023000
C	-48.748000	45.262000	153.517000	D	-51.933000	33.802000	146.148000
C	-49.831000	44.610000	152.663000	C	-52.335000	33.409000	149.231000
D	-50.361000	43.563000	153.042000	N	-46.700000	34.724000	160.195000
D	-50.212000	45.167000	151.617000	C	-46.719000	34.886000	158.719000
N	-64.271000	36.916000	156.421000	C	-46.014000	33.715000	158.054000
C	-63.273000	36.130000	155.722000	D	-45.257000	33.855000	157.097000
C	-63.454000	34.614000	155.818000	C	-46.098000	36.212000	158.322000
D	-62.789000	33.871000	155.140000	C	-46.873000	36.965000	157.273000
C	-61.877000	36.477000	156.263000	C	-47.271000	36.342000	156.089000
C	-61.581000	37.892000	156.250000	C	-47.127000	38.306000	157.427000
C	-61.418000	38.737000	157.343000	C	-47.913000	37.070000	155.118000
C	-61.353000	38.689000	155.101000	C	-47.762000	39.006000	156.462000
N	-61.134000	40.006000	156.910000	C	-48.178000	38.387000	155.302000
C	-61.110000	40.006000	155.539000	N	-47.149000	29.671000	156.790000
C	-61.354000	38.424000	153.719000	C	-48.258000	28.770000	156.596000
C	-60.828000	41.045000	154.646000	C	-47.737000	27.411000	156.213000
C	-61.108000	39.486000	152.827000	D	-46.695000	27.253000	155.598000
C	-60.837000	40.749000	153.292000	C	-49.247000	29.360000	155.541000
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C	-54.861000	39.674000	146.961000	C	-50.031000	31.350000	156.881000
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D	-54.666000	37.592000	148.109000	C	-50.201000	32.735000	157.054000
C	-55.946000	40.479000	147.656000	C	-49.208000	33.108000	154.922000
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D	-60.099000	33.808000	163.913000	F	-58.585000	35.837000	159.975000
D	-59.985000	35.181000	162.351000	C	-54.187000	35.813000	159.834000
N	-54.136000	28.594000	153.017000	N	-53.494000	35.373000	158.741000
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C	-56.276000	27.976000	154.088000	D	-54.014000	36.922000	160.306000
D	-56.986000	27.244000	154.770000	C	-52.589000	36.137000	158.017000
C	-54.167000	27.802000	155.377000	N	-51.680000	36.832000	158.632000
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C	-55.472000	29.355000	156.892000	C	-51.236000	37.315000	156.411000
C	-53.400000	30.100000	156.013000	S	-52.587000	36.241000	156.280000
C	-55.678000	30.595000	157.553000	H	-53.190292	40.000209	148.936642
C	-53.554000	31.318000	156.659000	H	-53.162967	45.012680	155.788672
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D	-54.810000	32.788000	158.100000	H	-64.152665	37.907134	156.358237
N	-51.423000	23.133000	161.742000	H	-55.897372	39.640605	145.184297
C	-50.509000	24.157000	162.258000	H	-52.835903	43.224426	160.691585
C	-49.433000	23.559000	163.114000	H	-56.678647	34.803263	151.230635
D	-48.527000	24.251000	163.415000	H	-53.489454	33.878309	152.199719
C	-51.236000	25.200000	163.059000	H	-51.754156	35.832973	150.156356
C	-52.205000	25.906000	162.252000	H	-47.163874	35.494491	160.632555
C	-53.529000	25.651000	162.169000	H	-47.495231	30.574123	157.044523
C	-51.927000	26.946000	161.315000	H	-58.690946	24.882921	157.590229
N	-54.114000	26.484000	161.267000	H	-60.577708	30.616464	160.664305
C	-53.158000	27.309000	160.734000	H	-53.158143	28.401080	152.934131
C	-50.776000	27.659000	160.976000	H	-52.140738	23.531891	161.171012
C	-53.278000	28.347000	159.788000	H	-53.577983	38.962665	165.329889
C	-50.879000	28.715000	160.023000	H	-51.225957	38.850419	149.474020
C	-52.130000	29.038000	159.445000	H	-52.065407	37.775388	152.649832
N	-52.851000	38.437000	165.772000	H	-53.370064	37.750656	150.964100
C	-53.148000	37.058000	165.982000	H	-52.759620	39.190847	151.214918
C	-52.043000	36.259000	166.654000	H	-52.564097	39.279797	147.593670
D	-52.353000	35.381000	167.417000	H	-53.931216	44.752577	153.678311
C	-53.623000	36.362000	164.719000	H	-52.090491	43.407299	154.558493
C	-55.081000	36.603000	164.412000	H	-52.929495	42.801266	153.069439
C	-55.542000	37.868000	164.110000	H	-54.692331	40.914541	153.425535
C	-55.997000	35.556000	164.372000	H	-54.927898	38.919498	155.008036
C	-56.900000	38.106000	163.832000	H	-52.267683	41.722929	156.650601
C	-57.351000	35.780000	164.064000	H	-54.755489	45.406066	155.677486
C	-57.799000	37.065000	163.802000	H	-54.306741	43.964767	156.333561
D	-59.118000	37.338000	163.486000	H	-50.448532	44.677360	155.704660
C	-56.505000	34.910000	160.589000	H	-48.486148	43.598539	154.616566
C	-55.107000	34.822000	160.501000	H	-47.596472	44.815263	155.104174
C	-54.460000	33.749000	161.114000	H	-47.933904	45.274795	152.953809
C	-55.183000	32.753000	161.759000	H	-49.024825	46.206222	153.626148
C	-56.569000	32.832000	161.821000	H	-50.097891	46.414324	157.100764
C	-57.225000	33.917000	161.247000	H	-48.499610	46.407626	156.707567
C	-57.271000	36.075000	160.018000	H	-63.340263	36.375968	154.641687
F	-56.891000	36.344000	158.746000	H	-61.105865	35.972819	155.643926
F	-57.084000	37.194000	160.725000	H	-61.792857	36.131878	157.314623

H	-61.499871	38.452451	158.402400	H	-50.346587	30.654059	157.672246
H	-60.959062	40.856551	157.500305	H	-50.653842	33.116328	157.981105
H	-60.604414	42.067642	154.983954	H	-49.945845	34.704290	156.168665
H	-60.618616	41.561073	152.582884	H	-48.890880	33.812316	154.138818
H	-61.131512	39.309228	151.741551	H	-48.487435	31.363120	153.850310
H	-61.541818	37.412031	153.330872	H	-46.550035	29.323044	157.525029
H	-65.187773	36.714841	156.047955	H	-46.615519	29.745862	155.935662
H	-64.256982	36.689658	157.405212	H	-59.598905	25.574332	159.700572
H	-54.185122	40.300465	146.633862	H	-57.666541	27.602399	158.391170
H	-56.629166	39.904070	148.083597	H	-57.179676	26.021620	159.134531
H	-56.434227	41.073759	147.033107	H	-57.655373	25.642002	161.602882
H	-55.940231	42.189788	148.899449	H	-57.393509	26.778440	163.828493
H	-54.473113	41.693944	148.565674	H	-57.341842	28.769115	164.849575
H	-54.711459	38.536052	145.283152	H	-57.697531	30.637127	161.858115
H	-56.119665	38.324347	146.108554	H	-57.879368	29.533578	159.677465
H	-53.999185	41.551846	161.984422	H	-60.267041	25.283567	157.452919
H	-53.293240	39.753571	159.788984	H	-59.100238	26.301153	156.894136
H	-53.240638	41.451210	159.153580	H	-60.153359	31.274440	162.803348
H	-55.422899	39.691097	161.624145	H	-61.434198	33.362685	161.245246
H	-57.895329	39.741562	161.404989	H	-59.913506	32.957538	161.063434
H	-58.953062	40.762779	159.386906	H	-61.544898	29.793296	161.722639
H	-57.507740	41.765136	157.591362	H	-62.169616	31.029314	160.833180
H	-55.066347	41.791883	157.884547	H	-54.699409	26.651284	153.571580
H	-52.037671	42.806778	162.029544	H	-53.070084	27.649007	155.303046
H	-51.556495	42.251459	160.556709	H	-54.605566	27.029653	156.042762
H	-56.240221	33.873633	153.397004	H	-56.197316	28.537607	157.017635
H	-56.725533	32.689432	152.362489	H	-56.586099	30.793442	158.141198
H	-55.141624	34.928122	151.675644	H	-55.643334	32.790977	158.596432
H	-55.627047	33.744014	150.640557	H	-52.780743	32.094189	156.560996
H	-51.623172	32.816666	152.729960	H	-52.477145	29.922015	155.441458
H	-52.413428	32.218432	154.043616	H	-54.551160	28.498299	152.101258
H	-50.837113	34.529127	148.408199	H	-54.239818	29.548801	153.329534
H	-51.972609	33.403191	150.152270	H	-50.015328	24.642174	161.390248
H	-52.065990	32.574600	148.771098	H	-50.505506	25.935353	163.456158
H	-53.323187	33.453406	149.271171	H	-51.768085	24.712565	163.902441
H	-53.132788	35.923276	149.307844	H	-54.072325	24.884272	162.740774
H	-47.778953	34.886480	158.389454	H	-55.129439	26.513647	161.001471
H	-45.081130	36.035305	157.913522	H	-54.239842	28.614947	159.326411
H	-46.030810	36.869385	159.213869	H	-52.201836	29.851781	158.708386
H	-47.071910	35.271549	155.932479	H	-49.983106	29.283710	159.733271
H	-48.213018	36.573980	154.183145	H	-49.802486	27.419839	161.428850
H	-48.719675	38.961252	154.535956	H	-50.909682	22.466600	161.182969
H	-47.952088	40.081003	156.597037	H	-51.864534	22.649630	162.511092
H	-46.812279	38.823493	158.345233	H	-54.024752	36.997247	166.660023
H	-47.171809	33.868571	160.451393	H	-53.481625	35.266293	164.826416
H	-45.745412	34.686763	160.522833	H	-53.034709	36.729076	163.852242
H	-48.799613	28.682863	157.560968	H	-54.822393	38.699710	164.089377
H	-50.235771	28.866683	155.646214	H	-57.241540	39.133429	163.637732
H	-48.848658	29.179452	154.520791	H	-59.196647	38.291405	163.325583

H	-58.054619	34.935113	164.031038	C	-54.152000	38.693000	147.919000
H	-55.667114	34.528218	164.583753	O	-54.666000	37.592000	148.109000
H	-52.670501	38.886887	166.658071	C	-55.946000	40.479000	147.656000
H	-52.035026	38.525452	165.183389	C	-55.391000	41.378000	148.760000

Cartesian coordinates of AChE docked with molecule 7

N	-52.999000	39.125000	148.492000	C	-53.151000	41.290000	161.318000
C	-52.055000	38.338000	149.394000	C	-52.416000	40.126000	161.997000
C	-51.756000	36.970000	148.699000	O	-52.953000	39.410000	162.872000
O	-51.182000	36.981000	147.619000	C	-53.644000	40.794000	159.952000
C	-52.548000	38.292000	150.858000	C	-55.093000	40.785000	159.808000
O	-51.645000	37.729000	151.893000	C	-55.888000	40.181000	160.756000
N	-54.083000	44.654000	155.630000	C	-55.691000	41.338000	158.668000
C	-54.120000	44.053000	154.335000	C	-57.266000	40.188000	160.621000
C	-55.500000	43.515000	154.097000	C	-57.063000	41.329000	158.498000
O	-56.146000	43.097000	154.971000	C	-57.858000	40.761000	159.491000
C	-53.048000	43.021000	154.151000	N	-55.873000	34.262000	151.472000
C	-53.340000	41.752000	154.832000	C	-56.035000	33.338000	152.605000
N	-54.205000	40.824000	154.317000	C	-54.810000	32.515000	152.972000
C	-52.917000	41.265000	156.011000	O	-54.949000	31.430000	153.522000
C	-54.301000	39.812000	155.151000	N	-53.603000	32.992000	152.649000
N	-53.521000	40.051000	156.181000	C	-52.384000	32.305000	153.070000
N	-49.431000	46.211000	156.370000	C	-52.203000	30.886000	152.533000
C	-49.529000	44.840000	155.995000	O	-51.409000	30.116000	153.057000
C	-49.237000	43.838000	157.199000	N	-52.131000	35.821000	149.230000
O	-49.768000	42.731000	157.218000	C	-51.810000	34.580000	148.493000
C	-48.521000	44.557000	154.862000	C	-52.408000	34.561000	147.023000
C	-48.748000	45.262000	153.517000	O	-51.933000	33.802000	146.148000
C	-49.831000	44.610000	152.663000	C	-52.335000	33.409000	149.231000
O	-50.361000	43.563000	153.042000	N	-46.700000	34.724000	160.195000
O	-50.212000	45.167000	151.617000	C	-46.719000	34.886000	158.719000
N	-64.271000	36.916000	156.421000	C	-46.014000	33.715000	158.054000
C	-63.273000	36.130000	155.722000	O	-45.257000	33.855000	157.097000
C	-63.454000	34.614000	155.818000	C	-46.098000	36.212000	158.322000
O	-62.789000	33.871000	155.140000	C	-46.873000	36.965000	157.273000
C	-61.877000	36.477000	156.263000	C	-47.271000	36.342000	156.089000
C	-61.581000	37.892000	156.250000	C	-47.127000	38.306000	157.427000
C	-61.418000	38.737000	157.343000	C	-47.913000	37.070000	155.118000
C	-61.353000	38.689000	155.101000	C	-47.762000	39.006000	156.462000
N	-61.134000	40.006000	156.910000	C	-48.178000	38.387000	155.302000
C	-61.110000	40.006000	155.539000	N	-47.149000	29.671000	156.790000
C	-61.354000	38.424000	153.719000	C	-48.258000	28.770000	156.596000
C	-60.828000	41.045000	154.646000	C	-47.737000	27.411000	156.213000
C	-61.108000	39.486000	152.827000	O	-46.695000	27.253000	155.598000
C	-60.837000	40.749000	153.292000	C	-49.247000	29.360000	155.541000
N	-55.438000	39.005000	145.805000	C	-49.455000	30.833000	155.694000
C	-54.861000	39.674000	146.961000	C	-50.031000	31.350000	156.881000

C	-49.007000	31.727000	154.749000	C	-52.130000	29.038000	159.445000
C	-50.201000	32.735000	157.054000	N	-52.851000	38.437000	165.772000
C	-49.208000	33.108000	154.922000	C	-53.148000	37.058000	165.982000
C	-49.801000	33.619000	156.063000	C	-52.043000	36.259000	166.654000
N	-59.339000	25.644000	157.623000	D	-52.353000	35.381000	167.417000
C	-59.297000	26.313000	158.929000	C	-53.623000	36.362000	164.719000
C	-60.266000	27.451000	158.978000	C	-55.081000	36.603000	164.412000
D	-60.336000	28.231000	158.019000	C	-55.542000	37.868000	164.110000
C	-57.913000	26.854000	159.173000	C	-55.997000	35.556000	164.372000
C	-57.779000	27.516000	160.493000	C	-56.900000	38.106000	163.832000
C	-57.650000	26.740000	161.669000	C	-57.351000	35.780000	164.064000
C	-57.786000	28.922000	160.587000	C	-57.799000	37.065000	163.802000
C	-57.517000	27.360000	162.903000	D	-59.118000	37.338000	163.486000
C	-57.678000	29.539000	161.797000	N	-54.927000	33.232000	162.039000
C	-57.543000	28.774000	162.954000	C	-55.490000	33.882000	161.068000
D	-57.431000	29.433000	164.148000	S	-57.226000	33.792000	160.985000
N	-61.343000	30.690000	161.304000	C	-57.173000	32.792000	162.398000
C	-60.934000	31.648000	162.348000	C	-55.890000	32.608000	162.798000
C	-62.110000	31.761000	163.331000	N	-54.717000	34.603000	160.166000
D	-63.198000	32.148000	162.939000	C	-54.149000	35.829000	160.423000
C	-60.650000	32.994000	161.724000	D	-54.275000	36.396000	161.486000
C	-60.245000	34.060000	162.736000	H	-54.693000	34.200000	159.238000
D	-60.099000	33.808000	163.913000	C	-53.351000	36.397000	159.276000
D	-59.985000	35.181000	162.351000	N	-53.455000	35.766000	158.132000
N	-54.136000	28.594000	153.017000	C	-52.749000	36.277000	157.092000
C	-54.801000	27.685000	153.963000	C	-51.951000	37.445000	157.244000
C	-56.276000	27.976000	154.088000	C	-52.809000	35.630000	155.830000
D	-56.986000	27.244000	154.770000	N	-51.881000	38.096000	158.437000
C	-54.167000	27.802000	155.377000	C	-51.225000	37.945000	156.135000
C	-54.366000	29.129000	156.075000	C	-52.566000	37.578000	159.425000
C	-55.472000	29.355000	156.892000	C	-51.299000	37.300000	154.927000
C	-53.400000	30.100000	156.013000	C	-52.098000	36.136000	154.774000
C	-55.678000	30.595000	157.553000	H	-53.190292	40.000209	148.936642
C	-53.554000	31.318000	156.659000	H	-53.162967	45.012680	155.788672
C	-54.704000	31.562000	157.443000	H	-49.614284	46.839940	155.614268
D	-54.810000	32.788000	158.100000	H	-64.152665	37.907134	156.358237
N	-51.423000	23.133000	161.742000	H	-55.897372	39.640605	145.184297
C	-50.509000	24.157000	162.258000	H	-52.835903	43.224426	160.691585
C	-49.433000	23.559000	163.114000	H	-56.678647	34.803263	151.230635
D	-48.527000	24.251000	163.415000	H	-53.489454	33.878309	152.199719
C	-51.236000	25.200000	163.059000	H	-51.754156	35.832973	150.156356
C	-52.205000	25.906000	162.252000	H	-47.163874	35.494491	160.632555
C	-53.529000	25.651000	162.169000	H	-47.495231	30.574123	157.044523
C	-51.927000	26.946000	161.315000	H	-58.690946	24.882921	157.590229
N	-54.114000	26.484000	161.267000	H	-60.577708	30.616464	160.664305
C	-53.158000	27.309000	160.734000	H	-53.158143	28.401080	152.934131
C	-50.776000	27.659000	160.976000	H	-52.140738	23.531891	161.171012
C	-53.278000	28.347000	159.788000	H	-53.577983	38.962665	165.329889
C	-50.879000	28.715000	160.023000	H	-51.225957	38.850419	149.474020

H	-52.065407	37.775388	152.649832	H	-55.141624	34.928122	151.675644
H	-53.370064	37.750656	150.964100	H	-55.627047	33.744014	150.640557
H	-52.759620	39.190847	151.214918	H	-51.623172	32.816666	152.729960
H	-52.564097	39.279797	147.593670	H	-52.413428	32.218432	154.043616
H	-53.931216	44.752577	153.678311	H	-50.837113	34.529127	148.408199
H	-52.090491	43.407299	154.558493	H	-51.972609	33.403191	150.152270
H	-52.929495	42.801266	153.069439	H	-52.065990	32.574600	148.771098
H	-54.692331	40.914541	153.425535	H	-53.323187	33.453406	149.271171
H	-54.927898	38.919498	155.008036	H	-53.132788	35.923276	149.307844
H	-52.267683	41.722929	156.650601	H	-47.778953	34.886480	158.389454
H	-54.755489	45.406066	155.677486	H	-45.081130	36.035305	157.913522
H	-54.306741	43.964767	156.333561	H	-46.030810	36.869385	159.213869
H	-50.448532	44.677360	155.704660	H	-47.071910	35.271549	155.932479
H	-48.486148	43.598539	154.616566	H	-48.213018	36.573980	154.183145
H	-47.596472	44.815263	155.104174	H	-48.719675	38.961252	154.535956
H	-47.933904	45.274795	152.953809	H	-47.952088	40.081003	156.597037
H	-49.024825	46.206222	153.626148	H	-46.812279	38.823493	158.345233
H	-50.097891	46.414324	157.100764	H	-47.171809	33.868571	160.451393
H	-48.499610	46.407626	156.707567	H	-45.745412	34.686763	160.522833
H	-63.340263	36.375968	154.641687	H	-48.799613	28.682863	157.560968
H	-61.105865	35.972819	155.643926	H	-50.235771	28.866683	155.646214
H	-61.792857	36.131878	157.314623	H	-48.848658	29.179452	154.520791
H	-61.499871	38.452451	158.402400	H	-50.346587	30.654059	157.672246
H	-60.959062	40.856551	157.500305	H	-50.653842	33.116328	157.981105
H	-60.604414	42.067642	154.983954	H	-49.945845	34.704290	156.168665
H	-60.618616	41.561073	152.582884	H	-48.890880	33.812316	154.138818
H	-61.131512	39.309228	151.741551	H	-48.487435	31.363120	153.850310
H	-61.541818	37.412031	153.330872	H	-46.550035	29.323044	157.525029
H	-65.187773	36.714841	156.047955	H	-46.615519	29.745862	155.935662
H	-64.256982	36.689658	157.405212	H	-59.598905	25.574332	159.700572
H	-54.185122	40.300465	146.633862	H	-57.666541	27.602399	158.391170
H	-56.629166	39.904070	148.083597	H	-57.179676	26.021620	159.134531
H	-56.434227	41.073759	147.033107	H	-57.655373	25.642002	161.602882
H	-55.940231	42.189788	148.899449	H	-57.393509	26.778440	163.828493
H	-54.473113	41.693944	148.565674	H	-57.341842	28.769115	164.849575
H	-54.711459	38.536052	145.283152	H	-57.697531	30.637127	161.858115
H	-56.119665	38.324347	146.108554	H	-57.879368	29.533578	159.677465
H	-53.999185	41.551846	161.984422	H	-60.267041	25.283567	157.452919
H	-53.293240	39.753571	159.788984	H	-59.100238	26.301153	156.894136
H	-53.240638	41.451210	159.153580	H	-60.153359	31.274440	162.803348
H	-55.422899	39.691097	161.624145	H	-61.434198	33.362685	161.245246
H	-57.895329	39.741562	161.404989	H	-59.913506	32.957538	161.063434
H	-58.953062	40.762779	159.386906	H	-61.544898	29.793296	161.722639
H	-57.507740	41.765136	157.591362	H	-62.169616	31.029314	160.833180
H	-55.066347	41.791883	157.884547	H	-54.699409	26.651284	153.571580
H	-52.037671	42.806778	162.029544	H	-53.070084	27.649007	155.303046
H	-51.556495	42.251459	160.556709	H	-54.605566	27.029653	156.042762
H	-56.240221	33.873633	153.397004	H	-56.197316	28.537607	157.017635
H	-56.725533	32.689432	152.362489	H	-56.586099	30.793442	158.141198

H	-55.643334	32.790977	158.596432	O	-49.768000	42.731000	157.218000
H	-52.780743	32.094189	156.560996	C	-48.521000	44.557000	154.862000
H	-52.477145	29.922015	155.441458	C	-48.748000	45.262000	153.517000
H	-54.551160	28.498299	152.101258	C	-49.831000	44.610000	152.663000
H	-54.239818	29.548801	153.329534	O	-50.361000	43.563000	153.042000
H	-50.015328	24.642174	161.390248	O	-50.212000	45.167000	151.617000
H	-50.505506	25.935353	163.456158	N	-64.271000	36.916000	156.421000
H	-51.768085	24.712565	163.902441	C	-63.273000	36.130000	155.722000
H	-54.072325	24.884272	162.740774	C	-63.454000	34.614000	155.818000
H	-55.129439	26.513647	161.001471	O	-62.789000	33.871000	155.140000
H	-54.239842	28.614947	159.326411	C	-61.877000	36.477000	156.263000
H	-52.201836	29.851781	158.708386	C	-61.581000	37.892000	156.250000
H	-49.983106	29.283710	159.733271	C	-61.418000	38.737000	157.343000
H	-49.802486	27.419839	161.428850	C	-61.353000	38.689000	155.101000
H	-50.909682	22.466600	161.182969	N	-61.134000	40.006000	156.910000
H	-51.864534	22.649630	162.511092	C	-61.110000	40.006000	155.539000
H	-54.024752	36.997247	166.660023	C	-61.354000	38.424000	153.719000
H	-53.481625	35.266293	164.826416	C	-60.828000	41.045000	154.646000
H	-53.034709	36.729076	163.852242	C	-61.108000	39.486000	152.827000
H	-54.822393	38.699710	164.089377	C	-60.837000	40.749000	153.292000
H	-57.241540	39.133429	163.637732	N	-55.438000	39.005000	145.805000
H	-59.196647	38.291405	163.325583	C	-54.861000	39.674000	146.961000
H	-58.054619	34.935113	164.031038	C	-54.152000	38.693000	147.919000
H	-55.667114	34.528218	164.583753	O	-54.666000	37.592000	148.109000
H	-52.670501	38.886887	166.658071	C	-55.946000	40.479000	147.656000
H	-52.035026	38.525452	165.183389	C	-55.391000	41.378000	148.760000

Cartesian coordinates of AChE docked with molecule 8

N	-52.999000	39.125000	148.492000	O	-55.995000	39.620000	150.212000
C	-52.055000	38.338000	149.394000	O	-54.624000	41.180000	150.998000
C	-51.756000	36.970000	148.699000	N	-52.357000	42.466000	161.134000
O	-51.182000	36.981000	147.619000	C	-53.151000	41.290000	161.318000
C	-52.548000	38.292000	150.858000	C	-52.416000	40.126000	161.997000
O	-51.645000	37.729000	151.893000	O	-52.953000	39.410000	162.872000
N	-54.083000	44.654000	155.630000	C	-53.644000	40.794000	159.952000
C	-54.120000	44.053000	154.335000	C	-55.093000	40.785000	159.808000
C	-55.500000	43.515000	154.097000	C	-55.888000	40.181000	160.756000
O	-56.146000	43.097000	154.971000	C	-55.691000	41.338000	158.668000
C	-53.048000	43.021000	154.151000	C	-57.266000	40.188000	160.621000
C	-53.340000	41.752000	154.832000	C	-57.063000	41.329000	158.498000
N	-54.205000	40.824000	154.317000	C	-57.858000	40.761000	159.491000
C	-52.917000	41.265000	156.011000	N	-55.873000	34.262000	151.472000
C	-54.301000	39.812000	155.151000	C	-56.035000	33.338000	152.605000
N	-53.521000	40.051000	156.181000	C	-54.810000	32.515000	152.972000
N	-49.431000	46.211000	156.370000	O	-54.949000	31.430000	153.522000
C	-49.529000	44.840000	155.995000	N	-53.603000	32.992000	152.649000
C	-49.237000	43.838000	157.199000	C	-52.384000	32.305000	153.070000
				C	-52.203000	30.886000	152.533000
				O	-51.409000	30.116000	153.057000
				N	-52.131000	35.821000	149.230000

C	-51.810000	34.580000	148.493000	D	-56.986000	27.244000	154.770000
C	-52.408000	34.561000	147.023000	C	-54.167000	27.802000	155.377000
D	-51.933000	33.802000	146.148000	C	-54.366000	29.129000	156.075000
C	-52.335000	33.409000	149.231000	C	-55.472000	29.355000	156.892000
N	-46.700000	34.724000	160.195000	C	-53.400000	30.100000	156.013000
C	-46.719000	34.886000	158.719000	C	-55.678000	30.595000	157.553000
C	-46.014000	33.715000	158.054000	C	-53.554000	31.318000	156.659000
D	-45.257000	33.855000	157.097000	C	-54.704000	31.562000	157.443000
C	-46.098000	36.212000	158.322000	D	-54.810000	32.788000	158.100000
C	-46.873000	36.965000	157.273000	N	-51.423000	23.133000	161.742000
C	-47.271000	36.342000	156.089000	C	-50.509000	24.157000	162.258000
C	-47.127000	38.306000	157.427000	C	-49.433000	23.559000	163.114000
C	-47.913000	37.070000	155.118000	D	-48.527000	24.251000	163.415000
C	-47.762000	39.006000	156.462000	C	-51.236000	25.200000	163.059000
C	-48.178000	38.387000	155.302000	C	-52.205000	25.906000	162.252000
N	-47.149000	29.671000	156.790000	C	-53.529000	25.651000	162.169000
C	-48.258000	28.770000	156.596000	C	-51.927000	26.946000	161.315000
C	-47.737000	27.411000	156.213000	N	-54.114000	26.484000	161.267000
D	-46.695000	27.253000	155.598000	C	-53.158000	27.309000	160.734000
C	-49.247000	29.360000	155.541000	C	-50.776000	27.659000	160.976000
C	-49.455000	30.833000	155.694000	C	-53.278000	28.347000	159.788000
C	-50.031000	31.350000	156.881000	C	-50.879000	28.715000	160.023000
C	-49.007000	31.727000	154.749000	C	-52.130000	29.038000	159.445000
C	-50.201000	32.735000	157.054000	N	-52.851000	38.437000	165.772000
C	-49.208000	33.108000	154.922000	C	-53.148000	37.058000	165.982000
C	-49.801000	33.619000	156.063000	C	-52.043000	36.259000	166.654000
N	-59.339000	25.644000	157.623000	D	-52.353000	35.381000	167.417000
C	-59.297000	26.313000	158.929000	C	-53.623000	36.362000	164.719000
C	-60.266000	27.451000	158.978000	C	-55.081000	36.603000	164.412000
D	-60.336000	28.231000	158.019000	C	-55.542000	37.868000	164.110000
C	-57.913000	26.854000	159.173000	C	-55.997000	35.556000	164.372000
C	-57.779000	27.516000	160.493000	C	-56.900000	38.106000	163.832000
C	-57.650000	26.740000	161.669000	C	-57.351000	35.780000	164.064000
C	-57.786000	28.922000	160.587000	C	-57.799000	37.065000	163.802000
C	-57.517000	27.360000	162.903000	D	-59.118000	37.338000	163.486000
C	-57.678000	29.539000	161.797000	N	-52.999000	39.125000	148.492000
C	-57.543000	28.774000	162.954000	C	-52.055000	38.338000	149.394000
D	-57.431000	29.433000	164.148000	C	-51.756000	36.970000	148.699000
N	-61.343000	30.690000	161.304000	D	-51.182000	36.981000	147.619000
C	-60.934000	31.648000	162.348000	C	-52.548000	38.292000	150.858000
C	-62.110000	31.761000	163.331000	D	-51.645000	37.729000	151.893000
D	-63.198000	32.148000	162.939000	N	-54.083000	44.654000	155.630000
C	-60.650000	32.994000	161.724000	C	-54.120000	44.053000	154.335000
C	-60.245000	34.060000	162.736000	C	-55.500000	43.515000	154.097000
D	-60.099000	33.808000	163.913000	D	-56.146000	43.097000	154.971000
D	-59.985000	35.181000	162.351000	C	-53.048000	43.021000	154.151000
N	-54.136000	28.594000	153.017000	C	-53.340000	41.752000	154.832000
C	-54.801000	27.685000	153.963000	N	-54.205000	40.824000	154.317000
C	-56.276000	27.976000	154.088000	C	-52.917000	41.265000	156.011000

C	-54.301000	39.812000	155.151000	N	-53.603000	32.992000	152.649000
N	-53.521000	40.051000	156.181000	C	-52.384000	32.305000	153.070000
N	-49.431000	46.211000	156.370000	C	-52.203000	30.886000	152.533000
C	-49.529000	44.840000	155.995000	D	-51.409000	30.116000	153.057000
C	-49.237000	43.838000	157.199000	N	-52.131000	35.821000	149.230000
D	-49.768000	42.731000	157.218000	C	-51.810000	34.580000	148.493000
C	-48.521000	44.557000	154.862000	C	-52.408000	34.561000	147.023000
C	-48.748000	45.262000	153.517000	D	-51.933000	33.802000	146.148000
C	-49.831000	44.610000	152.663000	C	-52.335000	33.409000	149.231000
D	-50.361000	43.563000	153.042000	N	-46.700000	34.724000	160.195000
D	-50.212000	45.167000	151.617000	C	-46.719000	34.886000	158.719000
N	-64.271000	36.916000	156.421000	C	-46.014000	33.715000	158.054000
C	-63.273000	36.130000	155.722000	D	-45.257000	33.855000	157.097000
C	-63.454000	34.614000	155.818000	C	-46.098000	36.212000	158.322000
D	-62.789000	33.871000	155.140000	C	-46.873000	36.965000	157.273000
C	-61.877000	36.477000	156.263000	C	-47.271000	36.342000	156.089000
C	-61.581000	37.892000	156.250000	C	-47.127000	38.306000	157.427000
C	-61.418000	38.737000	157.343000	C	-47.913000	37.070000	155.118000
C	-61.353000	38.689000	155.101000	C	-47.762000	39.006000	156.462000
N	-61.134000	40.006000	156.910000	C	-48.178000	38.387000	155.302000
C	-61.110000	40.006000	155.539000	N	-47.149000	29.671000	156.790000
C	-61.354000	38.424000	153.719000	C	-48.258000	28.770000	156.596000
C	-60.828000	41.045000	154.646000	C	-47.737000	27.411000	156.213000
C	-61.108000	39.486000	152.827000	D	-46.695000	27.253000	155.598000
C	-60.837000	40.749000	153.292000	C	-49.247000	29.360000	155.541000
N	-55.438000	39.005000	145.805000	C	-49.455000	30.833000	155.694000
C	-54.861000	39.674000	146.961000	C	-50.031000	31.350000	156.881000
C	-54.152000	38.693000	147.919000	C	-49.007000	31.727000	154.749000
D	-54.666000	37.592000	148.109000	C	-50.201000	32.735000	157.054000
C	-55.946000	40.479000	147.656000	C	-49.208000	33.108000	154.922000
C	-55.391000	41.378000	148.760000	C	-49.801000	33.619000	156.063000
C	-55.332000	40.662000	150.083000	N	-59.339000	25.644000	157.623000
D	-55.995000	39.620000	150.212000	C	-59.297000	26.313000	158.929000
D	-54.624000	41.180000	150.998000	C	-60.266000	27.451000	158.978000
N	-52.357000	42.466000	161.134000	D	-60.336000	28.231000	158.019000
C	-53.151000	41.290000	161.318000	C	-57.913000	26.854000	159.173000
C	-52.416000	40.126000	161.997000	C	-57.779000	27.516000	160.493000
D	-52.953000	39.410000	162.872000	C	-57.650000	26.740000	161.669000
C	-53.644000	40.794000	159.952000	C	-57.786000	28.922000	160.587000
C	-55.093000	40.785000	159.808000	C	-57.517000	27.360000	162.903000
C	-55.888000	40.181000	160.756000	C	-57.678000	29.539000	161.797000
C	-55.691000	41.338000	158.668000	C	-57.543000	28.774000	162.954000
C	-57.266000	40.188000	160.621000	D	-57.431000	29.433000	164.148000
C	-57.063000	41.329000	158.498000	N	-61.343000	30.690000	161.304000
C	-57.858000	40.761000	159.491000	C	-60.934000	31.648000	162.348000
N	-55.873000	34.262000	151.472000	C	-62.110000	31.761000	163.331000
C	-56.035000	33.338000	152.605000	D	-63.198000	32.148000	162.939000
C	-54.810000	32.515000	152.972000	C	-60.650000	32.994000	161.724000
D	-54.949000	31.430000	153.522000	C	-60.245000	34.060000	162.736000

D	-60.099000	33.808000	163.913000	C	-57.453000	34.440000	160.329000
D	-59.985000	35.181000	162.351000	C	-58.353000	34.141000	159.303000
N	-54.136000	28.594000	153.017000	N	-59.002000	35.170000	158.626000
C	-54.801000	27.685000	153.963000	C	-58.755000	36.496000	158.972000
C	-56.276000	27.976000	154.088000	C	-57.848000	36.797000	159.986000
D	-56.986000	27.244000	154.770000	C	-57.193000	35.772000	160.659000
C	-54.167000	27.802000	155.377000	H	-53.190292	40.000209	148.936642
C	-54.366000	29.129000	156.075000	H	-53.162967	45.012680	155.788672
C	-55.472000	29.355000	156.892000	H	-49.614284	46.839940	155.614268
C	-53.400000	30.100000	156.013000	H	-64.152665	37.907134	156.358237
C	-55.678000	30.595000	157.553000	H	-55.897372	39.640605	145.184297
C	-53.554000	31.318000	156.659000	H	-52.835903	43.224426	160.691585
C	-54.704000	31.562000	157.443000	H	-56.678647	34.803263	151.230635
D	-54.810000	32.788000	158.100000	H	-53.489454	33.878309	152.199719
N	-51.423000	23.133000	161.742000	H	-51.754156	35.832973	150.156356
C	-50.509000	24.157000	162.258000	H	-47.163874	35.494491	160.632555
C	-49.433000	23.559000	163.114000	H	-47.495231	30.574123	157.044523
D	-48.527000	24.251000	163.415000	H	-58.690946	24.882921	157.590229
C	-51.236000	25.200000	163.059000	H	-60.577708	30.616464	160.664305
C	-52.205000	25.906000	162.252000	H	-53.158143	28.401080	152.934131
C	-53.529000	25.651000	162.169000	H	-52.140738	23.531891	161.171012
C	-51.927000	26.946000	161.315000	H	-53.577983	38.962665	165.329889
N	-54.114000	26.484000	161.267000	H	-53.190292	40.000209	148.936642
C	-53.158000	27.309000	160.734000	H	-53.162967	45.012680	155.788672
C	-50.776000	27.659000	160.976000	H	-49.614284	46.839940	155.614268
C	-53.278000	28.347000	159.788000	H	-64.152665	37.907134	156.358237
C	-50.879000	28.715000	160.023000	H	-55.897372	39.640605	145.184297
C	-52.130000	29.038000	159.445000	H	-52.835903	43.224426	160.691585
N	-52.851000	38.437000	165.772000	H	-56.678647	34.803263	151.230635
C	-53.148000	37.058000	165.982000	H	-53.489454	33.878309	152.199719
C	-52.043000	36.259000	166.654000	H	-51.754156	35.832973	150.156356
D	-52.353000	35.381000	167.417000	H	-47.163874	35.494491	160.632555
C	-53.623000	36.362000	164.719000	H	-47.495231	30.574123	157.044523
C	-55.081000	36.603000	164.412000	H	-58.690946	24.882921	157.590229
C	-55.542000	37.868000	164.110000	H	-60.577708	30.616464	160.664305
C	-55.997000	35.556000	164.372000	H	-53.158143	28.401080	152.934131
C	-56.900000	38.106000	163.832000	H	-52.140738	23.531891	161.171012
C	-57.351000	35.780000	164.064000	H	-53.577983	38.962665	165.329889
C	-57.799000	37.065000	163.802000	H	-51.225957	38.850419	149.474020
D	-59.118000	37.338000	163.486000	H	-52.065407	37.775388	152.649832
N	-54.988000	31.189000	161.830000	H	-53.370064	37.750656	150.964100
C	-54.532000	32.297000	161.332000	H	-52.759620	39.190847	151.214918
S	-52.812000	32.542000	161.451000	H	-52.564097	39.279797	147.593670
C	-52.715000	31.001000	162.237000	H	-53.931216	44.752577	153.678311
C	-53.950000	30.449000	162.348000	H	-52.090491	43.407299	154.558493
N	-55.395000	33.209000	160.745000	H	-52.929495	42.801266	153.069439
H	-55.005000	33.678000	159.937000	H	-54.692331	40.914541	153.425535
C	-56.710000	33.396000	161.100000	H	-54.927898	38.919498	155.008036
D	-57.231000	32.734000	161.980000	H	-52.267683	41.722929	156.650601

H	-54.755489	45.406066	155.677486	H	-45.081130	36.035305	157.913522
H	-54.306741	43.964767	156.333561	H	-46.030810	36.869385	159.213869
H	-50.448532	44.677360	155.704660	H	-47.071910	35.271549	155.932479
H	-48.486148	43.598539	154.616566	H	-48.213018	36.573980	154.183145
H	-47.596472	44.815263	155.104174	H	-48.719675	38.961252	154.535956
H	-47.933904	45.274795	152.953809	H	-47.952088	40.081003	156.597037
H	-49.024825	46.206222	153.626148	H	-46.812279	38.823493	158.345233
H	-50.097891	46.414324	157.100764	H	-47.171809	33.868571	160.451393
H	-48.499610	46.407626	156.707567	H	-45.745412	34.686763	160.522833
H	-63.340263	36.375968	154.641687	H	-48.799613	28.682863	157.560968
H	-61.105865	35.972819	155.643926	H	-50.235771	28.866683	155.646214
H	-61.792857	36.131878	157.314623	H	-48.848658	29.179452	154.520791
H	-61.499871	38.452451	158.402400	H	-50.346587	30.654059	157.672246
H	-60.959062	40.856551	157.500305	H	-50.653842	33.116328	157.981105
H	-60.604414	42.067642	154.983954	H	-49.945845	34.704290	156.168665
H	-60.618616	41.561073	152.582884	H	-48.890880	33.812316	154.138818
H	-61.131512	39.309228	151.741551	H	-48.487435	31.363120	153.850310
H	-61.541818	37.412031	153.330872	H	-46.550035	29.323044	157.525029
H	-65.187773	36.714841	156.047955	H	-46.615519	29.745862	155.935662
H	-64.256982	36.689658	157.405212	H	-59.598905	25.574332	159.700572
H	-54.185122	40.300465	146.633862	H	-57.666541	27.602399	158.391170
H	-56.629166	39.904070	148.083597	H	-57.179676	26.021620	159.134531
H	-56.434227	41.073759	147.033107	H	-57.655373	25.642002	161.602882
H	-55.940231	42.189788	148.899449	H	-57.393509	26.778440	163.828493
H	-54.473113	41.693944	148.565674	H	-57.341842	28.769115	164.849575
H	-54.711459	38.536052	145.283152	H	-57.697531	30.637127	161.858115
H	-56.119665	38.324347	146.108554	H	-57.879368	29.533578	159.677465
H	-53.999185	41.551846	161.984422	H	-60.267041	25.283567	157.452919
H	-53.293240	39.753571	159.788984	H	-59.100238	26.301153	156.894136
H	-53.240638	41.451210	159.153580	H	-60.153359	31.274440	162.803348
H	-55.422899	39.691097	161.624145	H	-61.434198	33.362685	161.245246
H	-57.895329	39.741562	161.404989	H	-59.913506	32.957538	161.063434
H	-58.953062	40.762779	159.386906	H	-61.544898	29.793296	161.722639
H	-57.507740	41.765136	157.591362	H	-62.169616	31.029314	160.833180
H	-55.066347	41.791883	157.884547	H	-54.699409	26.651284	153.571580
H	-52.037671	42.806778	162.029544	H	-53.070084	27.649007	155.303046
H	-51.556495	42.251459	160.556709	H	-54.605566	27.029653	156.042762
H	-56.240221	33.873633	153.397004	H	-56.197316	28.537607	157.017635
H	-56.725533	32.689432	152.362489	H	-56.586099	30.793442	158.141198
H	-55.141624	34.928122	151.675644	H	-55.643334	32.790977	158.596432
H	-55.627047	33.744014	150.640557	H	-52.780743	32.094189	156.560996
H	-51.623172	32.816666	152.729960	H	-52.477145	29.922015	155.441458
H	-52.413428	32.218432	154.043616	H	-54.551160	28.498299	152.101258
H	-50.837113	34.529127	148.408199	H	-54.239818	29.548801	153.329534
H	-51.972609	33.403191	150.152270	H	-50.015328	24.642174	161.390248
H	-52.065990	32.574600	148.771098	H	-50.505506	25.935353	163.456158
H	-53.323187	33.453406	149.271171	H	-51.768085	24.712565	163.902441
H	-53.132788	35.923276	149.307844	H	-54.072325	24.884272	162.740774
H	-47.778953	34.886480	158.389454	H	-55.129439	26.513647	161.001471

H	-54.239842	28.614947	159.326411	C	-61.581000	37.892000	156.250000
H	-52.201836	29.851781	158.708386	C	-61.418000	38.737000	157.343000
H	-49.983106	29.283710	159.733271	C	-61.353000	38.689000	155.101000
H	-49.802486	27.419839	161.428850	N	-61.134000	40.006000	156.910000
H	-50.909682	22.466600	161.182969	C	-61.110000	40.006000	155.539000
H	-51.864534	22.649630	162.511092	C	-61.354000	38.424000	153.719000
H	-54.024752	36.997247	166.660023	C	-60.828000	41.045000	154.646000
H	-53.481625	35.266293	164.826416	C	-61.108000	39.486000	152.827000
H	-53.034709	36.729076	163.852242	C	-60.837000	40.749000	153.292000
H	-54.822393	38.699710	164.089377	N	-55.438000	39.005000	145.805000
H	-57.241540	39.133429	163.637732	C	-54.861000	39.674000	146.961000
H	-59.196647	38.291405	163.325583	C	-54.152000	38.693000	147.919000
H	-58.054619	34.935113	164.031038	O	-54.666000	37.592000	148.109000
H	-55.667114	34.528218	164.583753	C	-55.946000	40.479000	147.656000
H	-52.670501	38.886887	166.658071	C	-55.391000	41.378000	148.760000
H	-52.035026	38.525452	165.183389	C	-55.332000	40.662000	150.083000

Cartesian coordinates of AChE docked with molecule 9

N	-52.999000	39.125000	148.492000	O	-54.624000	41.180000	150.998000
C	-52.055000	38.338000	149.394000	N	-52.357000	42.466000	161.134000
C	-51.756000	36.970000	148.699000	C	-53.151000	41.290000	161.318000
O	-51.182000	36.981000	147.619000	C	-52.416000	40.126000	161.997000
C	-52.548000	38.292000	150.858000	O	-52.953000	39.410000	162.872000
O	-51.645000	37.729000	151.893000	C	-53.644000	40.794000	159.952000
N	-54.083000	44.654000	155.630000	C	-55.093000	40.785000	159.808000
C	-54.120000	44.053000	154.335000	C	-55.888000	40.181000	160.756000
C	-55.500000	43.515000	154.097000	C	-55.691000	41.338000	158.668000
O	-56.146000	43.097000	154.971000	C	-57.266000	40.188000	160.621000
C	-53.048000	43.021000	154.151000	C	-57.063000	41.329000	158.498000
C	-53.340000	41.752000	154.832000	C	-57.858000	40.761000	159.491000
N	-54.205000	40.824000	154.317000	N	-55.873000	34.262000	151.472000
C	-52.917000	41.265000	156.011000	C	-56.035000	33.338000	152.605000
C	-54.301000	39.812000	155.151000	C	-54.810000	32.515000	152.972000
N	-53.521000	40.051000	156.181000	O	-54.949000	31.430000	153.522000
N	-49.431000	46.211000	156.370000	N	-53.603000	32.992000	152.649000
C	-49.529000	44.840000	155.995000	C	-52.384000	32.305000	153.070000
C	-49.237000	43.838000	157.199000	C	-52.203000	30.886000	152.533000
O	-49.768000	42.731000	157.218000	O	-51.409000	30.116000	153.057000
C	-48.521000	44.557000	154.862000	N	-52.131000	35.821000	149.230000
C	-48.748000	45.262000	153.517000	C	-51.810000	34.580000	148.493000
C	-49.831000	44.610000	152.663000	C	-52.408000	34.561000	147.023000
O	-50.361000	43.563000	153.042000	O	-51.933000	33.802000	146.148000
O	-50.212000	45.167000	151.617000	C	-52.335000	33.409000	149.231000
N	-64.271000	36.916000	156.421000	N	-46.700000	34.724000	160.195000
C	-63.273000	36.130000	155.722000	C	-46.719000	34.886000	158.719000
C	-63.454000	34.614000	155.818000	C	-46.014000	33.715000	158.054000
O	-62.789000	33.871000	155.140000	O	-45.257000	33.855000	157.097000
C	-61.877000	36.477000	156.263000	C	-46.098000	36.212000	158.322000
				C	-46.873000	36.965000	157.273000
				C	-47.271000	36.342000	156.089000
				C	-47.127000	38.306000	157.427000

C	-47.913000	37.070000	155.118000	O	-48.527000	24.251000	163.415000
C	-47.762000	39.006000	156.462000	C	-51.236000	25.200000	163.059000
C	-48.178000	38.387000	155.302000	C	-52.205000	25.906000	162.252000
N	-47.149000	29.671000	156.790000	C	-53.529000	25.651000	162.169000
C	-48.258000	28.770000	156.596000	C	-51.927000	26.946000	161.315000
C	-47.737000	27.411000	156.213000	N	-54.114000	26.484000	161.267000
O	-46.695000	27.253000	155.598000	C	-53.158000	27.309000	160.734000
C	-49.247000	29.360000	155.541000	C	-50.776000	27.659000	160.976000
C	-49.455000	30.833000	155.694000	C	-53.278000	28.347000	159.788000
C	-50.031000	31.350000	156.881000	C	-50.879000	28.715000	160.023000
C	-49.007000	31.727000	154.749000	C	-52.130000	29.038000	159.445000
C	-50.201000	32.735000	157.054000	N	-52.851000	38.437000	165.772000
C	-49.208000	33.108000	154.922000	C	-53.148000	37.058000	165.982000
C	-49.801000	33.619000	156.063000	C	-52.043000	36.259000	166.654000
N	-59.339000	25.644000	157.623000	O	-52.353000	35.381000	167.417000
C	-59.297000	26.313000	158.929000	C	-53.623000	36.362000	164.719000
C	-60.266000	27.451000	158.978000	C	-55.081000	36.603000	164.412000
O	-60.336000	28.231000	158.019000	C	-55.542000	37.868000	164.110000
C	-57.913000	26.854000	159.173000	C	-55.997000	35.556000	164.372000
C	-57.779000	27.516000	160.493000	C	-56.900000	38.106000	163.832000
C	-57.650000	26.740000	161.669000	C	-57.351000	35.780000	164.064000
C	-57.786000	28.922000	160.587000	C	-57.799000	37.065000	163.802000
C	-57.517000	27.360000	162.903000	O	-59.118000	37.338000	163.486000
C	-57.678000	29.539000	161.797000	N	-53.352000	35.296000	155.538000
C	-57.543000	28.774000	162.954000	C	-53.033000	35.836000	156.675000
O	-57.431000	29.433000	164.148000	S	-51.653000	36.898000	156.660000
N	-61.343000	30.690000	161.304000	C	-51.504000	36.571000	154.965000
C	-60.934000	31.648000	162.348000	C	-52.478000	35.716000	154.563000
C	-62.110000	31.761000	163.331000	N	-53.773000	35.565000	157.817000
O	-63.198000	32.148000	162.939000	H	-53.915000	34.578000	157.989000
C	-60.650000	32.994000	161.724000	C	-54.284000	36.506000	158.681000
C	-60.245000	34.060000	162.736000	O	-54.132000	37.697000	158.487000
O	-60.099000	33.808000	163.913000	C	-54.996000	35.930000	159.891000
O	-59.985000	35.181000	162.351000	C	-56.469000	35.642000	159.549000
N	-54.136000	28.594000	153.017000	C	-57.164000	34.980000	160.734000
C	-54.801000	27.685000	153.963000	N	-56.485000	33.753000	161.118000
C	-56.276000	27.976000	154.088000	C	-57.203000	33.078000	162.183000
O	-56.986000	27.244000	154.770000	C	-55.108000	34.022000	161.512000
C	-54.167000	27.802000	155.377000	C	-54.321000	34.644000	160.364000
C	-54.366000	29.129000	156.075000	H	-53.190292	40.000209	148.936642
C	-55.472000	29.355000	156.892000	H	-53.162967	45.012680	155.788672
C	-53.400000	30.100000	156.013000	H	-49.614284	46.839940	155.614268
C	-55.678000	30.595000	157.553000	H	-64.152665	37.907134	156.358237
C	-53.554000	31.318000	156.659000	H	-55.897372	39.640605	145.184297
C	-54.704000	31.562000	157.443000	H	-52.835903	43.224426	160.691585
O	-54.810000	32.788000	158.100000	H	-56.678647	34.803263	151.230635
N	-51.423000	23.133000	161.742000	H	-53.489454	33.878309	152.199719
C	-50.509000	24.157000	162.258000	H	-51.754156	35.832973	150.156356
C	-49.433000	23.559000	163.114000	H	-47.163874	35.494491	160.632555

H	-47.495231	30.574123	157.044523	H	-58.953062	40.762779	159.386906
H	-58.690946	24.882921	157.590229	H	-57.507740	41.765136	157.591362
H	-60.577708	30.616464	160.664305	H	-55.066347	41.791883	157.884547
H	-53.158143	28.401080	152.934131	H	-52.037671	42.806778	162.029544
H	-52.140738	23.531891	161.171012	H	-51.556495	42.251459	160.556709
H	-53.577983	38.962665	165.329889	H	-56.240221	33.873633	153.397004
H	-51.225957	38.850419	149.474020	H	-56.725533	32.689432	152.362489
H	-52.065407	37.775388	152.649832	H	-55.141624	34.928122	151.675644
H	-53.370064	37.750656	150.964100	H	-55.627047	33.744014	150.640557
H	-52.759620	39.190847	151.214918	H	-51.623172	32.816666	152.729960
H	-52.564097	39.279797	147.593670	H	-52.413428	32.218432	154.043616
H	-53.931216	44.752577	153.678311	H	-50.837113	34.529127	148.408199
H	-52.090491	43.407299	154.558493	H	-51.972609	33.403191	150.152270
H	-52.929495	42.801266	153.069439	H	-52.065990	32.574600	148.771098
H	-54.692331	40.914541	153.425535	H	-53.323187	33.453406	149.271171
H	-54.927898	38.919498	155.008036	H	-53.132788	35.923276	149.307844
H	-52.267683	41.722929	156.650601	H	-47.778953	34.886480	158.389454
H	-54.755489	45.406066	155.677486	H	-45.081130	36.035305	157.913522
H	-54.306741	43.964767	156.333561	H	-46.030810	36.869385	159.213869
H	-50.448532	44.677360	155.704660	H	-47.071910	35.271549	155.932479
H	-48.486148	43.598539	154.616566	H	-48.213018	36.573980	154.183145
H	-47.596472	44.815263	155.104174	H	-48.719675	38.961252	154.535956
H	-47.933904	45.274795	152.953809	H	-47.952088	40.081003	156.597037
H	-49.024825	46.206222	153.626148	H	-46.812279	38.823493	158.345233
H	-50.097891	46.414324	157.100764	H	-47.171809	33.868571	160.451393
H	-48.499610	46.407626	156.707567	H	-45.745412	34.686763	160.522833
H	-63.340263	36.375968	154.641687	H	-48.799613	28.682863	157.560968
H	-61.105865	35.972819	155.643926	H	-50.235771	28.866683	155.646214
H	-61.792857	36.131878	157.314623	H	-48.848658	29.179452	154.520791
H	-61.499871	38.452451	158.402400	H	-50.346587	30.654059	157.672246
H	-60.959062	40.856551	157.500305	H	-50.653842	33.116328	157.981105
H	-60.604414	42.067642	154.983954	H	-49.945845	34.704290	156.168665
H	-60.618616	41.561073	152.582884	H	-48.890880	33.812316	154.138818
H	-61.131512	39.309228	151.741551	H	-48.487435	31.363120	153.850310
H	-61.541818	37.412031	153.330872	H	-46.550035	29.323044	157.525029
H	-65.187773	36.714841	156.047955	H	-46.615519	29.745862	155.935662
H	-64.256982	36.689658	157.405212	H	-59.598905	25.574332	159.700572
H	-54.185122	40.300465	146.633862	H	-57.666541	27.602399	158.391170
H	-56.629166	39.904070	148.083597	H	-57.179676	26.021620	159.134531
H	-56.434227	41.073759	147.033107	H	-57.655373	25.642002	161.602882
H	-55.940231	42.189788	148.899449	H	-57.393509	26.778440	163.828493
H	-54.473113	41.693944	148.565674	H	-57.341842	28.769115	164.849575
H	-54.711459	38.536052	145.283152	H	-57.697531	30.637127	161.858115
H	-56.119665	38.324347	146.108554	H	-57.879368	29.533578	159.677465
H	-53.999185	41.551846	161.984422	H	-60.267041	25.283567	157.452919
H	-53.293240	39.753571	159.788984	H	-59.100238	26.301153	156.894136
H	-53.240638	41.451210	159.153580	H	-60.153359	31.274440	162.803348
H	-55.422899	39.691097	161.624145	H	-61.434198	33.362685	161.245246
H	-57.895329	39.741562	161.404989	H	-59.913506	32.957538	161.063434

H	-61.544898	29.793296	161.722639
H	-62.169616	31.029314	160.833180
H	-54.699409	26.651284	153.571580
H	-53.070084	27.649007	155.303046
H	-54.605566	27.029653	156.042762
H	-56.197316	28.537607	157.017635
H	-56.586099	30.793442	158.141198
H	-55.643334	32.790977	158.596432
H	-52.780743	32.094189	156.560996
H	-52.477145	29.922015	155.441458
H	-54.551160	28.498299	152.101258
H	-54.239818	29.548801	153.329534
H	-50.015328	24.642174	161.390248
H	-50.505506	25.935353	163.456158
H	-51.768085	24.712565	163.902441
H	-54.072325	24.884272	162.740774
H	-55.129439	26.513647	161.001471
H	-54.239842	28.614947	159.326411
H	-52.201836	29.851781	158.708386
H	-49.983106	29.283710	159.733271
H	-49.802486	27.419839	161.428850
H	-50.909682	22.466600	161.182969
H	-51.864534	22.649630	162.511092
H	-54.024752	36.997247	166.660023
H	-53.481625	35.266293	164.826416
H	-53.034709	36.729076	163.852242
H	-54.822393	38.699710	164.089377
H	-57.241540	39.133429	163.637732
H	-59.196647	38.291405	163.325583
H	-58.054619	34.935113	164.031038
H	-55.667114	34.528218	164.583753
H	-52.670501	38.886887	166.658071
H	-52.035026	38.525452	165.183389

2. Quantum mechanical cluster-continuum approach for geometry optimizations of complexes between compounds 7 and 3 and active site of AChE, and calculation of enthalpy of complex formation

The model system for QM cluster-continuum calculations is prepared by modifying residues of the active site: carboxyl and amino groups are removed from α carbons and substituted with hydrogen atoms, thus deriving methyl groups. The geometry optimization of complexes is then carried out; coordinates of α carbons were held frozen, so the architecture of the active site initially present in the enzyme is conserved during the optimization. The final energies are calculated at

CPCM/B3LYP+D3/6-311+G(2df,p)//CPCM/B3LYP/6-31G(d) level of theory, with Gaussian16 program suite [19]. The protein environment is described by implicit solvation, with dielectric constant $\epsilon = 4$ [17]. The inhibitory potential of candidates for cholinesterase inhibitors is linked to their ability to block the enzyme's active site sterically. Thus thermodynamical stability of the complex can be interpreted as an indicator of the inhibitor's ability. The stability of the examined complexes is assessed by calculating the enthalpy of the complex formation $\Delta_r H^{298}$:



where **N** stands for the examined molecule (here 7 and 3) $\Delta_r H^{298}$ is calculated as a difference between the enthalpy of complex and the sum of enthalpies of the active site (AS) and molecule **N**:

$$\Delta_r H^{298} = H_{[\text{N}-\text{AS}]} - (H_{\text{AS}} + H_{\text{N}}).$$

Enthalpy, H , is given as a sum of the calculated total energy of a system and thermal correction to H . ($H = E + \text{Thermal correction to enthalpy}$). The latter is obtained by vibrational analysis. All calculated geometries were localized as a minimum at the Potential Energy Surface, with no imaginary frequencies.

3. Cartesian coordinates of optimized structures of complexes [7-AS] and [3-AS]

3.1. [7-AS]

C	-8.691744	0.014060	-5.986018
C	-3.664530	-4.515206	-5.890062
C	-10.658538	-6.404162	0.840200
C	-7.224541	5.444465	-2.618774
C	8.921193	1.359080	5.560547
C	-3.995842	3.827693	6.783807
C	0.881673	-4.206136	-3.217821
C	1.174572	-1.156084	-5.354113
C	-0.187507	7.005469	-6.637550
C	5.569585	-5.198114	-4.995043
C	7.740523	-2.662040	-3.033295
C	9.718491	-0.769597	-5.876068
C	8.410072	3.795483	1.281210
C	-3.104097	-7.816687	0.228862
C	0.396865	-4.939447	5.180085
C	2.136440	4.296505	5.356915
H	2.170188	4.314692	6.452738
H	3.159077	4.419736	4.982747
H	1.550692	5.159593	5.020049
C	1.518371	2.980535	4.848473

H	2.104929	2.136546	5.232355	H	0.429218	6.801001	-7.521413
H	0.508487	2.876161	5.266190	N	8.775874	-1.969911	-3.863641
C	0.392116	3.497125	2.633500	H	9.557772	-1.574330	-3.359314
H	-0.402331	3.997591	3.183662	C	8.589873	-1.576303	-5.167274
C	1.450098	2.900435	3.336199	O	7.589820	-1.914598	-5.802983
C	0.344458	3.456382	1.238307	H	9.961506	-1.374167	-6.757274
H	-0.482718	3.927954	0.713523	H	10.622977	-0.723036	-5.255730
C	1.356105	2.812208	0.520533	C	9.303457	0.648685	-6.326689
H	1.319166	2.779898	-0.565325	H	8.251317	0.632800	-6.627719
C	2.415082	2.210457	1.204771	H	9.891830	0.889537	-7.222177
C	2.456522	2.257566	2.601065	C	0.226243	9.327103	-2.128191
H	3.284088	1.787127	3.128430	C	-0.747567	9.107847	-1.128374
H	6.175118	0.445958	1.639444	C	-1.609605	8.017800	-1.185843
C	6.347599	0.853633	0.651137	H	-2.351656	7.840452	-0.411826
C	7.369904	1.686313	0.250132	H	-0.820761	9.802584	-0.294823
N	7.131349	1.922525	-1.092520	H	9.485159	2.730418	-5.802274
C	6.014630	1.237454	-1.431458	H	10.526428	1.692204	-4.853823
N	5.497993	0.566553	-0.406054	C	0.354264	8.459107	-3.206908
H	5.662659	1.223552	-2.452533	H	1.113245	8.636422	-3.965856
H	7.792547	2.303400	-1.820707	H	0.887365	10.186797	-2.047943
H	3.206098	1.703384	0.656825	H	8.244508	-2.977919	-2.115619
C	8.517741	2.281065	1.010667	H	7.160931	-0.742091	-2.344971
H	8.593708	1.756118	1.969678	O	8.211725	-4.790398	-4.064046
H	9.458238	2.080993	0.478202	C	7.340830	-3.967294	-3.780969
H	8.459277	4.370209	0.348776	N	6.026512	-4.155249	-4.069443
H	7.457820	4.032016	1.770827	O	5.761140	-2.132407	-1.686337
H	9.224249	4.106977	1.944575	H	5.500120	-1.341540	-1.160065
C	10.771306	3.945682	5.047962	C	6.649978	-1.643258	-2.688692
O	10.747334	5.140054	5.443516	H	5.606558	-4.814825	-6.024835
C	10.898193	2.863918	6.169595	H	1.194818	-1.079869	-6.444738
H	10.354274	3.220940	7.055577	C	4.160395	-5.672339	-4.653640
H	11.959285	2.831070	6.464753	H	3.836053	-6.436466	-5.368724
C	10.434892	1.455846	5.781706	H	3.441555	-4.845899	-4.699029
H	8.368047	1.626127	6.471425	H	4.123751	-6.102415	-3.646935
H	8.615768	0.345127	5.271498	H	0.448330	-0.419842	-4.988609
H	10.736582	0.734061	6.556599	C	0.729194	-2.528805	-4.948567
H	10.949916	1.171308	4.856977	O	-0.145678	-3.164167	-5.540152
H	8.615934	2.046994	4.765641	N	1.352046	-3.001745	-3.843373
C	-1.677846	5.481858	-3.748560	H	2.001019	-2.407521	-3.349205
N	-2.181236	6.002407	-2.577659	H	1.500028	-4.425967	-2.345083
H	-2.955772	5.611762	-2.001092	H	-0.162442	-4.108644	-2.895960
C	-1.479823	7.145544	-2.275915	H	0.942464	-5.051331	-3.910554
C	-0.504699	7.346810	-3.299748	H	-2.641557	-4.794380	-5.615950
C	-0.651044	6.261118	-4.237625	H	-3.596473	-3.652299	-6.562505
C	0.142022	6.026868	-5.494258	H	-4.116683	-5.344311	-6.447122
H	-0.030713	5.000303	-5.842857	H	-8.561690	-0.459256	-6.966427
H	1.217358	6.094073	-5.274111	H	-9.638298	0.566817	-5.997914
H	-1.241044	6.922280	-6.929158	C	-3.895391	-3.082237	-3.780971
H	-0.008998	8.043236	-6.333981	C	-3.221596	-3.382835	-2.588277

H	-3.151445	-4.418528	-2.262462	H	-11.542311	-7.053281	0.818687
H	-6.747168	-0.228497	-3.086743	H	-11.309224	0.557325	-1.306090
H	-2.131792	-2.631499	-0.872768	H	-5.902531	-2.926277	4.540387
C	-2.734507	-1.051665	-2.197030	H	-0.553214	-5.460740	-0.126859
O	-2.146760	-0.106429	-1.391632	C	-9.189763	0.771708	-0.948558
H	-2.307390	0.780292	-1.754090	O	-9.286482	1.358662	0.283814
H	-3.479683	0.316763	-3.692936	H	-10.222689	1.460584	0.519045
C	-3.403832	-0.722527	-3.380343	C	-0.044729	-6.321577	0.302585
C	-3.974459	-1.733816	-4.156124	C	1.122359	-6.132405	1.046711
H	-4.491074	-1.461028	-5.073992	H	1.517806	-5.130144	1.187533
C	-8.682135	-1.038165	-4.861450	H	-7.883160	0.740992	-5.849092
H	-9.480343	-1.768174	-5.048549	H	-5.508882	-3.880417	-4.956894
H	-7.736653	-1.593975	-4.899352	H	6.290678	-6.015292	-4.926381
C	-8.858051	-0.436076	-3.482193	H	2.158940	-0.887185	-4.960694
C	-7.752115	-0.053828	-2.708240	C	1.726456	-1.836419	0.179471
C	-7.904465	0.544895	-1.457525	C	1.150369	-1.564557	1.446799
H	-7.043325	0.852587	-0.871418	C	1.887987	-1.857672	2.639577
C	1.785577	-7.230366	1.601079	C	3.181932	-2.426276	2.531826
H	2.692271	-7.084443	2.181816	H	3.723888	-2.650810	3.445098
H	1.785987	-9.376931	1.822121	C	3.719632	-2.673536	1.287464
C	1.274036	-8.515103	1.401015	H	4.717769	-3.091380	1.197074
C	0.108301	-8.697550	0.654442	H	3.462596	-2.557484	-0.855657
H	-0.280139	-9.702307	0.498901	H	-5.140810	5.940283	-3.018572
C	-0.570824	-7.604795	0.095926	H	-6.024470	7.165936	-2.106750
C	-1.858848	-7.804158	-0.676483	C	-5.357479	5.515988	-0.892987
H	-1.810731	-8.749099	-1.232729	O	-4.149165	5.121582	-0.850855
C	-10.133398	-0.203415	-2.949987	H	-7.631395	5.884166	-3.538052
H	-1.965623	-7.006629	-1.422536	H	-7.114227	4.365510	-2.785497
H	-4.015423	-7.963518	-0.362377	H	-1.986198	-0.071460	0.795232
H	-7.981371	-1.609219	0.163019	N	-2.525958	0.131923	1.636198
C	-7.988090	-2.867385	1.889008	C	-1.925571	-0.114544	2.842896
H	-3.201754	-6.871505	0.774621	C	4.668743	-6.785375	5.029312
C	-6.902658	-2.498338	2.694452	C	-5.364697	2.594474	1.002347
C	-6.733845	-3.187803	3.890986	C	3.317841	-6.763353	5.386784
C	-10.308159	0.391007	-1.698804	H	2.707683	-7.652332	5.240409
C	-7.620580	-4.215506	4.279127	H	-6.816318	1.375412	2.061995
H	-7.457047	-4.730697	5.222413	N	-4.860369	0.539143	1.998927
C	-8.696665	-4.575697	3.476020	C	-3.703410	0.877808	1.502170
H	-9.374784	-5.366724	3.787973	C	2.733063	-5.612985	5.934744
C	-8.898356	-3.901374	2.256724	C	1.259498	-5.576097	6.285597
C	-9.888576	-3.995832	1.208923	H	1.119673	-5.011293	7.216482
C	-9.546594	-3.044317	0.277302	H	0.905299	-6.595995	6.481461
H	-10.034330	-2.782065	-0.652184	H	0.710724	-3.909280	4.985100
N	-8.409268	-2.368851	0.674731	H	0.484657	-5.500572	4.242605
C	-11.053215	-4.945704	1.140274	H	-0.660014	-4.926582	5.471581
H	-11.754176	-4.599518	0.369797	C	-2.904176	3.804380	5.699081
H	-11.608055	-4.919393	2.089353	H	-1.919135	3.813349	6.183279
H	-9.971639	-6.793467	1.599904	H	-2.968643	2.858492	5.145575
H	-10.155810	-6.478964	-0.130815	H	3.109629	-3.579201	6.543982

C	3.543099	-4.482319	6.119743	3.2. [3-AS]			
H	-4.566770	4.086440	3.541108				
C	4.893807	-4.498377	5.765368	C	4.103679	5.429462	-5.093913
H	-0.272706	-0.822016	4.872099	C	-9.016964	3.918187	-5.074785
C	0.164970	-1.049844	3.904892	C	-8.505757	4.426169	-0.175911
H	-4.759097	5.978447	1.963970	C	1.939672	-7.709163	-3.660776
C	-0.569606	-0.760927	2.720996	C	-0.050831	3.453445	8.454848
H	6.513193	-5.665875	4.941779	C	9.605826	-6.894389	-3.588850
N	1.363864	-1.592082	3.872842	C	7.862817	-3.499961	5.192137
C	-3.228256	7.141677	2.949573	C	7.012150	2.927153	4.218892
C	-3.931849	4.958454	3.682146	C	2.485961	-7.131762	3.269507
C	-3.001092	4.969111	4.734320	C	-1.074078	-2.806917	-7.115512
C	-2.188880	6.101517	4.868728	C	-1.888827	-5.372623	0.887749
C	-2.295431	7.182792	3.989393	C	-2.026039	-3.387497	4.049067
H	-1.647334	8.049370	4.107390	C	-2.028665	5.883241	-3.660829
H	-1.453195	6.143566	5.669522	C	-8.578830	-3.235222	1.255096
H	-3.933011	4.742934	7.384509	C	-6.720810	-6.530281	2.082648
H	-3.897372	2.969160	7.458942	C	-10.523452	-2.426395	4.593194
H	-4.995348	3.791446	6.335154	C	-5.337354	-6.965428	1.610475
H	-2.091157	4.568845	-4.159188	H	-4.561258	-6.283114	1.976201
H	5.503611	-3.612274	5.922322	H	-5.284302	-6.987767	0.516569
C	-5.796774	1.516159	1.721036	H	-5.106832	-7.967361	1.989031
H	5.101518	-7.690003	4.609266	H	-7.498437	-7.193834	1.698078
N	-0.092378	-1.017483	1.519108	H	-6.779303	-6.560726	3.180160
S	-3.674209	2.419289	0.658958	N	-7.046237	-5.177731	1.613714
C	2.991397	-2.375084	0.105178	H	-6.320886	-4.474483	1.670751
O	-6.177071	5.474602	0.061834	C	-8.328833	-4.760425	1.448762
O	-3.374378	8.170961	2.049852	O	-9.283469	-5.537827	1.423059
C	-4.055303	6.023374	2.792641	C	-7.388531	-2.279545	1.346483
C	-5.887023	6.081928	-2.229261	H	-6.901872	-2.399485	2.323512
H	5.387912	-3.394646	-3.878398	H	-7.795162	-1.266734	1.330682
C	-4.499257	-4.176268	-4.640474	O	-6.472712	-2.478734	0.273395
C	5.461969	-5.651482	5.216749	H	-6.154098	-1.581940	0.031206
H	-11.013012	-0.492509	-3.521712	N	-9.587660	-2.817789	2.279483
H	-3.043998	-8.624241	0.967605	H	-10.276441	-2.144022	1.972559
H	-2.694489	8.841220	2.224800	C	-9.446970	-3.015190	3.632446
H	1.149186	-1.590431	-0.706591	O	-8.540725	-3.713297	4.090146
O	10.744599	3.524657	3.856359	H	-10.924142	-3.304045	5.113409
C	8.487153	1.843007	-4.136400	H	-11.353341	-1.974621	4.034418
O	8.877968	2.498000	-3.116211	C	-9.962668	-1.426949	5.629251
O	7.362422	1.316351	-4.310918	H	-10.581366	-1.511636	6.532761
C	-2.644657	-2.388169	-1.798569	H	-8.948948	-1.735563	5.903850
H	-5.886496	3.495713	0.688703	C	-9.950031	0.042618	5.187966
H	-7.951163	5.582485	-1.812970	H	-10.921311	0.328432	4.762659
H	-4.620483	-5.081750	-4.032906	H	-9.824124	0.677240	6.078152
C	9.520479	1.757644	-5.288796	C	-8.837318	0.466319	4.195708
H	6.113698	-1.359363	-3.604400	O	-7.843965	-0.284001	4.054838
H	-6.221891	-1.700555	2.404936	O	-9.028262	1.594315	3.632492
O	-2.401120	0.164889	3.938734	H	-9.063916	-3.124326	0.280963

C	-11.273047	4.577127	-2.957925	H	-2.110033	-6.395452	1.206762
O	-11.376653	5.521417	-2.129421	H	-0.818733	-5.316590	0.656065
O	-11.212584	3.338414	-2.718091	C	2.575496	4.851560	5.999683
C	-11.251667	4.993952	-4.463192	H	2.797295	4.938798	7.060973
H	-10.816980	6.000186	-4.538523	C	3.604440	4.868428	5.063930
H	-12.298200	5.089709	-4.794391	H	4.633213	4.968652	5.399515
C	-10.514949	4.015243	-5.383716	C	3.341261	4.752993	3.680840
H	-10.654954	4.309050	-6.435522	C	2.037649	4.625434	3.211030
H	-10.968367	3.024903	-5.261086	H	1.830860	4.527675	2.150147
H	-8.870709	3.576045	-4.045952	C	1.003852	4.618576	4.155929
H	-8.508259	3.213375	-5.745325	N	-0.360737	4.519337	3.983763
H	-8.524077	4.893964	-5.182824	C	-0.977415	4.582498	5.218920
H	3.930261	4.668187	-4.325701	H	-2.056131	4.536782	5.290987
H	4.893004	5.064854	-5.761617	H	-0.249839	3.572979	9.526716
H	3.181630	5.531714	-5.678675	C	-0.310464	4.770120	7.696982
C	4.498876	6.772813	-4.453389	H	0.305764	5.562809	8.144655
C	6.997530	7.170575	-4.222469	H	-1.353928	5.070923	7.856310
C	5.797039	6.705854	-3.674201	H	0.988981	3.127553	8.337565
H	6.997059	7.617076	-5.215081	H	1.445044	-7.126465	2.928383
H	4.585261	7.535559	-5.238042	H	2.811342	-8.173037	3.378589
H	9.124604	7.450696	-3.965611	C	3.397232	-6.374876	2.284533
C	8.202828	7.077576	-3.521761	H	3.423475	-6.920157	1.332510
C	8.221449	6.505451	-2.246485	H	4.424485	-6.378559	2.671057
O	9.374899	6.387343	-1.510945	C	3.426239	-3.880370	2.804999
H	10.115181	6.733731	-2.033952	C	2.962283	-4.945894	2.022826
C	5.844029	6.141924	-2.388149	C	2.064467	-4.644661	0.987762
C	7.034685	6.032717	-1.672635	H	1.690456	-5.447036	0.356524
H	7.050362	5.575343	-0.684273	C	3.020095	-2.564340	2.566777
H	4.926316	5.777036	-1.933475	H	3.400255	-1.753367	3.184116
H	3.686197	7.098970	-3.790947	C	2.127668	-2.295111	1.525961
C	-8.936509	2.946393	-0.089852	H	2.122523	-0.382549	1.829806
H	-9.364530	5.040572	-0.466543	H	1.134615	-8.332473	-4.066825
H	-8.107068	4.785956	0.780638	H	0.952848	-3.124958	-0.075771
H	-9.682013	2.837796	0.709206	C	1.473841	-6.952373	-2.404969
H	-9.451858	2.689632	-1.021780	H	2.311822	-6.364476	-2.011093
H	-7.724173	4.555985	-0.934466	H	1.209133	-7.681857	-1.628223
C	-7.816263	1.980256	0.167145	H	4.123366	-4.074478	3.617326
N	-7.411555	1.629068	1.442984	H	2.249311	-7.010583	-4.446637
H	-7.964409	1.748536	2.336087	H	1.468241	-4.238746	-2.798020
C	-6.384301	0.758984	1.320317	H	2.790519	-8.360874	-3.430595
H	-5.937048	0.289358	2.184068	C	0.292043	-6.039870	-2.666000
N	-6.075903	0.517313	0.049289	C	-1.008394	-6.560364	-2.750184
C	-6.972960	1.287079	-0.675517	C	-0.040007	4.698772	6.217853
H	-6.959181	1.297603	-1.758108	H	-1.167309	-7.626354	-2.598559
H	-2.722914	-3.579576	1.648688	H	4.167331	4.759159	2.973334
H	-1.165812	-2.706922	4.053362	H	1.186701	-0.169168	-0.497000
H	-2.907771	-2.819404	3.739205	N	0.785121	0.274160	-1.323823
H	-2.170844	-3.737194	5.074890	H	-0.839723	4.526253	3.093818
H	-2.453540	-5.159185	-0.021527	H	-0.466368	-2.756288	-3.255324

C	-0.620122	-3.824209	-3.122455	O	7.848100	2.537444	1.280587
C	0.467663	-4.661924	-2.858653	C	5.085690	0.118215	-1.233627
C	-3.024841	0.038145	-1.249956	C	3.740640	0.123252	-1.613621
S	-1.699710	0.283207	-0.153940	H	-0.303598	-3.207789	-7.784767
C	-1.908816	-4.358423	-3.204599	H	-4.030586	5.099132	-0.869464
H	-5.938904	-3.255517	-4.727160	C	1.245232	4.726433	5.556444
C	-5.331524	-2.572667	-5.315693	C	4.902654	-3.961895	-1.652157
C	-4.340227	-3.076404	-6.161350	C	5.197784	-4.569707	-2.891442
C	-5.547367	-1.194848	-5.231078	C	6.506581	-4.877303	-3.245100
H	-4.929451	0.744736	-5.946314	C	7.549687	-4.571699	-2.350955
C	-3.774517	-0.838495	-6.841984	C	7.228332	-3.950022	-1.108868
H	-3.171916	-0.156055	-7.438004	C	5.910604	-3.644653	-0.746017
C	-3.545103	-2.218740	-6.935296	H	5.680510	-3.179153	0.208306
C	-2.442685	-2.764690	-7.819864	H	3.871298	-3.739407	-1.394190
H	-2.360666	-2.149216	-8.724997	H	4.386668	-4.797670	-3.578224
C	-3.097068	5.457722	-0.441071	H	6.720501	-5.343716	-4.203773
H	-2.707733	-3.776596	-8.151642	H	8.556448	-7.155468	-3.764107
C	-2.541798	-0.117642	-2.516599	H	10.199285	-7.308811	-4.412776
H	-4.025309	6.089590	1.396780	H	10.854634	-5.145363	-3.329868
H	-3.158182	-0.279154	-3.393988	H	9.526059	-4.915911	-4.453975
N	-1.169624	-0.076065	-2.666193	C	8.983818	-4.734558	-2.390034
C	-0.591791	0.127167	-1.518374	C	9.456357	-4.216858	-1.207564
C	-1.920949	4.782425	-2.588440	C	7.390548	3.593209	1.802104
C	-1.911809	5.345149	-1.182184	O	6.607003	4.430407	1.264353
H	-1.184141	6.579030	-3.595502	H	8.514198	-3.299815	0.467696
H	-2.763605	4.089134	-2.699471	H	5.930223	3.075828	4.123976
H	-2.950820	6.462621	-3.536415	C	10.511239	-0.771925	1.773013
C	-0.718473	5.801567	-0.603348	O	11.358015	0.137296	1.196282
H	0.212427	5.702334	-1.155445	H	12.214283	-0.288653	1.031254
C	-0.710330	6.362560	0.675390	H	10.473934	-4.138732	-0.848459
H	0.225381	6.709329	1.106880	C	10.901790	-2.086867	2.050336
H	-0.763599	-1.803534	-6.802712	H	11.909438	-2.419203	1.806665
H	-1.896603	6.915687	2.394854	C	9.995994	-2.970701	2.642820
C	-3.095142	6.015029	0.839282	H	10.314691	-3.989014	2.856978
H	-1.111046	-3.437081	-6.220258	C	8.691082	-2.571287	2.965711
C	1.532992	1.255946	-1.954208	H	7.901537	-4.542282	3.298598
O	1.087428	2.015153	-2.801307	H	6.700643	-3.261379	3.383474
C	2.969452	1.284218	-1.498670	C	7.731348	-3.519036	3.657941
C	2.773725	3.721771	-0.797962	H	7.153128	-4.196053	5.654706
F	1.550318	3.490749	-0.252999	H	8.873772	-3.788701	5.502646
F	3.397298	4.600867	0.020879	H	8.860016	3.693350	3.397896
F	2.559167	4.384852	-1.964390	H	7.317732	-0.908321	2.897667
H	3.286849	-0.778903	-2.013679	H	7.569270	4.907020	3.525048
C	3.565872	2.451634	-0.976044	C	9.212763	-0.345156	2.079382
C	4.900117	2.434379	-0.567037	H	7.281040	3.097472	5.269462
C	5.661594	1.269954	-0.703945	C	7.781873	3.861312	3.274647
H	5.364234	3.302703	-0.099749	H	9.919487	-7.386302	-2.660929
H	6.687983	1.300959	-0.350168	H	7.664779	-2.498029	5.589673
H	5.665873	-0.794155	-1.339470	H	2.506892	-6.663223	4.260345

N	-2.260169	-4.437538	1.912591	O	135.857000	122.445000	48.749000
H	-6.320547	-0.800422	-4.577495	N	127.315000	114.527000	36.716000
C	-1.729484	-4.551947	3.152418	C	128.658000	114.946000	36.299000
O	-1.043247	-5.517099	3.496150	C	129.137000	114.263000	35.005000
C	-1.900698	6.473811	1.401651	O	130.169000	114.662000	34.419000
H	-4.050411	0.041286	-0.888112	C	129.685000	114.674000	37.435000
C	-2.098792	-5.731163	-3.020051	C	129.244000	115.295000	38.783000
N	8.412026	-3.749963	-0.433331	C	128.735000	114.639000	39.872000
H	-2.032800	5.448046	-4.666950	C	129.219000	116.697000	39.109000
H	-3.098183	-6.155073	-3.079314	N	128.389000	115.556000	40.866000
H	-4.181177	-4.151052	-6.223860	C	128.679000	116.816000	40.415000
H	7.229738	1.880203	3.979817	C	129.609000	117.859000	38.423000
H	-0.695213	2.652665	8.074850	C	128.511000	118.067000	41.044000
H	-1.008859	4.196281	-2.756783	C	129.449000	119.089000	39.042000
H	8.904290	0.677039	1.857080	C	128.903000	119.185000	40.355000
C	8.325768	-1.246761	2.666198	N	136.240000	125.194000	39.029000
C	9.791810	-5.368775	-3.487957	C	136.139000	124.430000	40.256000
H	-2.756222	-3.710220	-3.409319	C	136.953000	123.167000	40.167000
O	1.691561	-1.020755	1.237781	O	137.085000	122.568000	39.107000
C	1.643860	-3.339831	0.733831	C	134.660000	124.118000	40.566000
C	-4.764884	-0.328331	-5.999391	C	134.406000	123.354000	41.900000

4. Molecular docking of BChE

Cartesian coordinates of AChE docked with molecule 5

N	137.535000	122.777000	41.301000	O	134.453000	121.418000	40.532000
C	138.359000	121.574000	41.397000	O	134.198000	121.098000	42.687000
C	139.504000	121.632000	40.371000	N	134.496000	111.349000	48.107000
O	140.294000	122.580000	40.398000	C	135.416000	110.331000	47.653000
C	137.503000	120.311000	41.198000	C	135.390000	109.069000	48.477000
O	138.006000	119.308000	42.047000	O	135.845000	108.039000	48.023000
N	131.849000	118.411000	47.957000	C	136.860000	110.882000	47.569000
C	132.703000	118.950000	46.906000	C	136.976000	112.161000	46.761000
C	131.828000	119.049000	45.639000	C	136.736000	113.409000	47.357000
O	131.165000	118.065000	45.286000	C	137.215000	112.108000	45.391000
C	133.808000	117.936000	46.635000	C	136.730000	114.589000	46.578000
C	134.716000	118.304000	45.512000	C	137.205000	113.264000	44.618000
N	135.687000	119.269000	45.631000	C	136.956000	114.513000	45.215000
C	134.899000	117.737000	44.288000	N	137.086000	118.020000	37.172000
C	136.442000	119.280000	44.542000	C	136.907000	116.636000	36.817000
N	135.979000	118.356000	43.713000	C	138.238000	115.904000	36.844000
N	134.513000	118.891000	51.772000	O	138.447000	114.964000	36.066000
C	135.176000	118.503000	50.526000	N	139.141000	116.339000	37.738000
C	135.487000	117.007000	50.388000	C	140.436000	115.677000	37.886000
O	135.364000	116.449000	49.312000	C	141.359000	115.664000	36.668000
C	136.506000	119.252000	50.366000	O	142.295000	114.893000	36.643000
C	136.361000	120.762000	50.312000	N	139.637000	120.641000	39.486000
C	135.913000	121.224000	48.947000	C	140.744000	120.716000	38.532000
O	135.639000	120.362000	48.080000	C	140.579000	121.968000	37.697000
				O	141.565000	122.490000	37.123000
				C	140.816000	119.443000	37.628000
				N	141.169000	109.629000	44.148000
				C	141.531000	110.981000	43.741000

C	142.684000	110.988000	42.747000	C	129.493000	123.503000	34.269000
D	143.290000	112.029000	42.510000	C	129.590000	123.577000	35.678000
C	141.924000	111.815000	44.949000	C	130.191000	122.472000	33.616000
C	140.762000	112.453000	45.681000	C	130.356000	122.625000	36.410000
C	140.836000	112.056000	47.132000	C	130.951000	121.547000	34.307000
C	140.831000	113.968000	45.516000	C	131.025000	121.613000	35.707000
N	144.960000	111.195000	39.512000	D	131.685000	120.622000	36.365000
C	144.989000	112.005000	38.320000	N	135.209000	118.525000	39.093000
C	146.073000	111.303000	37.512000	C	135.062000	118.037000	40.287000
D	147.235000	111.686000	37.533000	S	133.465000	118.145000	40.970000
C	145.352000	113.457000	38.711000	C	132.961000	118.913000	39.500000
C	145.640000	114.290000	37.506000	C	134.009000	119.026000	38.645000
C	144.178000	114.059000	39.508000	N	136.140000	117.466000	40.947000
N	131.922000	107.849000	34.992000	H	136.372000	117.925000	41.819000
C	131.684000	107.324000	36.343000	C	136.777000	116.309000	40.569000
C	130.504000	106.333000	36.256000	D	136.413000	115.671000	39.597000
D	129.375000	106.758000	36.089000	C	137.925000	115.879000	41.434000
C	131.343000	108.500000	37.291000	C	138.194000	114.419000	41.219000
C	130.951000	108.049000	38.683000	C	139.342000	113.990000	42.084000
D	130.678000	108.920000	39.544000	C	140.564000	114.782000	41.722000
D	130.911000	106.821000	38.935000	F	140.838000	114.591000	40.570000
N	133.916000	105.822000	46.957000	F	141.483000	114.439000	42.414000
C	134.582000	105.275000	45.792000	C	140.295000	116.242000	41.937000
C	135.786000	104.400000	46.212000	C	139.146000	116.671000	41.072000
D	136.829000	104.378000	45.549000	H	136.790674	122.739296	41.967968
C	135.026000	106.394000	44.847000	H	132.416175	118.346828	48.778270
C	133.863000	107.070000	44.114000	H	134.310260	119.866240	51.861962
C	133.137000	108.100000	44.715000	H	127.003835	114.970686	37.556600
C	133.474000	106.650000	42.818000	H	135.699137	126.033202	39.088136
C	132.059000	108.713000	44.067000	H	134.513251	112.186317	47.560289
C	132.376000	107.258000	42.150000	H	136.209782	118.501887	37.154225
C	131.686000	108.286000	42.783000	H	138.972151	117.098419	38.366540
D	130.633000	108.907000	42.159000	H	139.746004	119.813888	40.037628
N	135.773000	123.963000	33.656000	H	140.411500	109.624401	44.801040
C	135.264000	122.868000	34.497000	H	144.248327	111.655880	40.042472
C	136.346000	122.002000	35.112000	H	132.686662	108.491186	35.048378
D	137.484000	121.921000	34.599000	H	133.137352	106.387878	46.685379
C	134.297000	121.948000	33.698000	H	135.059277	124.534242	33.250326
C	134.930000	121.297000	32.455000	H	127.004054	123.524086	35.389005
C	135.872000	120.258000	32.571000	H	138.748841	121.552803	42.293584
C	134.592000	121.742000	31.176000	H	137.516227	118.602938	41.925764
C	136.471000	119.675000	31.400000	H	137.527109	119.980076	40.265258
C	135.173000	121.182000	30.026000	H	136.548804	120.462079	41.414299
C	136.101000	120.166000	30.132000	H	138.099534	123.593970	41.485286
D	136.699000	119.698000	28.966000	H	132.990212	119.841846	47.186014
N	126.537000	124.115000	34.731000	H	133.354289	116.955885	46.378835
C	127.435000	125.135000	34.163000	H	134.439174	117.827373	47.541598
C	126.711000	126.051000	33.143000	H	135.796387	119.877140	46.442542
D	127.351000	126.784000	32.390000	H	137.302263	119.940548	44.358635
C	128.651000	124.491000	33.456000	H	134.333631	116.991352	43.882086

H 131.064337	119.028152	48.110383	H 142.401672	111.285536	45.635729
H 131.506132	117.500478	47.685908	H 139.908956	112.129810	45.328646
H 134.572032	118.721587	49.788619	H 140.083567	112.463427	47.629944
H 136.983544	119.002890	49.535340	H 141.690520	112.368649	47.522059
H 137.133255	119.073610	51.110868	H 140.783342	111.070743	47.213211
H 137.209821	121.231433	50.510080	H 140.073788	114.392046	45.992355
H 135.697192	121.102373	50.962850	H 140.782947	114.203266	44.555562
H 133.629296	118.408848	51.853840	H 141.681769	114.307802	45.891268
H 135.096630	118.648757	52.559905	H 140.888039	109.092131	43.339958
H 128.626478	116.036138	36.092349	H 141.960940	109.179691	44.585096
H 130.666412	115.112065	37.157457	H 144.109689	111.940942	37.896919
H 129.794516	113.578786	37.578570	H 146.155296	113.429738	39.288990
H 128.609245	113.550488	39.968576	H 143.992682	113.510510	40.296226
H 127.975411	115.350622	41.809008	H 143.376295	114.092268	38.948853
H 128.082235	118.164502	42.052293	H 144.400718	114.966140	39.797790
H 128.789919	120.169226	40.833029	H 146.394615	113.897431	36.999496
H 129.745250	120.010437	38.519325	H 145.878883	115.209809	37.783463
H 130.035528	117.804140	37.410545	H 144.840578	114.324097	36.923023
H 126.646625	114.751445	35.992813	H 144.726160	110.242080	39.272497
H 127.303088	113.530516	36.880247	H 145.865583	111.211447	39.958932
H 136.506517	124.978383	40.977454	H 132.491529	106.848537	36.622501
H 134.237454	123.555397	39.869557	H 130.586909	109.046588	36.959838
H 134.106721	124.936028	40.635371	H 132.103490	109.122291	37.411449
H 133.549093	123.608827	42.325293	H 132.147931	107.090147	34.364945
H 135.111352	123.523253	42.573745	H 131.093624	108.319880	34.657088
H 137.204095	125.442484	38.859071	H 133.856554	104.627160	45.257087
H 135.898360	124.643569	38.254140	H 135.708455	105.977313	44.077113
H 135.121551	110.039824	46.623138	H 135.555522	107.178211	45.427275
H 137.515929	110.125659	47.089619	H 133.431041	108.427396	45.723143
H 137.231318	111.100567	48.591962	H 131.504671	109.525835	44.558953
H 136.551526	113.463994	48.440026	H 130.293370	109.592657	42.755176
H 136.546596	115.564771	47.051534	H 132.083429	106.913847	41.147024
H 136.941523	115.424055	44.598745	H 134.024103	105.842023	42.313461
H 137.392240	113.203579	43.535738	H 133.581468	105.071151	47.543868
H 137.415545	111.141956	44.904646	H 134.562015	106.391808	47.484336
H 133.550642	110.994989	48.074227	H 134.706057	123.319282	35.343843
H 134.718321	111.612232	49.056411	H 133.427212	122.542427	33.348393
H 136.321365	116.231569	37.487639	H 133.944634	121.125021	34.354234
H 136.560036	116.606607	35.903194	H 136.149109	119.892101	33.570664
H 137.475572	118.087178	38.101420	H 137.205590	118.860292	31.481413
H 137.714279	118.462770	36.516775	H 137.356110	119.028915	29.213853
H 140.935754	116.155123	38.577327	H 134.889215	121.552972	29.030085
H 140.266453	114.734679	38.084929	H 133.855119	122.549137	31.051356
H 141.573665	120.780941	39.045544	H 136.359166	124.573565	34.207107
H 140.923710	118.636678	38.192219	H 136.314777	123.584384	32.892307
H 141.587168	119.512923	37.011145	H 127.787190	125.780580	34.994437
H 139.983466	119.360004	37.098756	H 129.355170	125.286899	33.135392
H 138.758602	120.605830	38.988727	H 128.303042	123.923276	32.567904
H 140.754659	111.373781	43.294562	H 129.063491	124.384119	36.208422
H 142.523027	112.566656	44.711767	H 130.428435	122.673163	37.506555

H	131.585735	120.776794	37.317410	O	137.085000	122.568000	39.107000
H	131.494869	120.763048	33.759619	C	134.660000	124.118000	40.566000
H	130.142494	122.382895	32.520688	C	134.406000	123.354000	41.900000
H	125.767911	124.563593	35.207830	C	134.356000	121.846000	41.695000
H	126.172876	123.530229	33.992382	O	134.453000	121.418000	40.532000

Cartesian coordinates of AChE docked with molecule 6

N	137.535000	122.777000	41.301000	C	135.390000	109.069000	48.477000
C	138.359000	121.574000	41.397000	O	135.845000	108.039000	48.023000
C	139.504000	121.632000	40.371000	C	136.860000	110.882000	47.569000
O	140.294000	122.580000	40.398000	C	136.976000	112.161000	46.761000
C	137.503000	120.311000	41.198000	C	136.736000	113.409000	47.357000
O	138.006000	119.308000	42.047000	C	137.215000	112.108000	45.391000
N	131.849000	118.411000	47.957000	C	136.730000	114.589000	46.578000
C	132.703000	118.950000	46.906000	C	137.205000	113.264000	44.618000
C	131.828000	119.049000	45.639000	C	136.956000	114.513000	45.215000
O	131.165000	118.065000	45.286000	N	137.086000	118.020000	37.172000
C	133.808000	117.936000	46.635000	C	136.907000	116.636000	36.817000
C	134.716000	118.304000	45.512000	C	138.238000	115.904000	36.844000
N	135.687000	119.269000	45.631000	O	138.447000	114.964000	36.066000
C	134.899000	117.737000	44.288000	N	139.141000	116.339000	37.738000
C	136.442000	119.280000	44.542000	C	140.436000	115.677000	37.886000
N	135.979000	118.356000	43.713000	C	141.359000	115.664000	36.668000
N	134.513000	118.891000	51.772000	O	142.295000	114.893000	36.643000
C	135.176000	118.503000	50.526000	N	139.637000	120.641000	39.486000
C	135.487000	117.007000	50.388000	C	140.744000	120.716000	38.532000
O	135.364000	116.449000	49.312000	C	140.579000	121.968000	37.697000
C	136.506000	119.252000	50.366000	O	141.565000	122.490000	37.123000
C	136.361000	120.762000	50.312000	C	140.816000	119.443000	37.628000
C	135.913000	121.224000	48.947000	N	141.169000	109.629000	44.148000
O	135.639000	120.362000	48.080000	C	141.531000	110.981000	43.741000
O	135.857000	122.445000	48.749000	C	142.684000	110.988000	42.747000
N	127.315000	114.527000	36.716000	O	143.290000	112.029000	42.510000
C	128.658000	114.946000	36.299000	C	141.924000	111.815000	44.949000
C	129.137000	114.263000	35.005000	C	140.762000	112.453000	45.681000
O	130.169000	114.662000	34.419000	C	140.836000	112.056000	47.132000
C	129.685000	114.674000	37.435000	C	140.831000	113.968000	45.516000
C	129.244000	115.295000	38.783000	N	144.960000	111.195000	39.512000
C	128.735000	114.639000	39.872000	C	144.989000	112.005000	38.320000
C	129.219000	116.697000	39.109000	C	146.073000	111.303000	37.512000
N	128.389000	115.556000	40.866000	O	147.235000	111.686000	37.533000
C	128.679000	116.816000	40.415000	C	145.352000	113.457000	38.711000
C	129.609000	117.859000	38.423000	C	145.640000	114.290000	37.506000
C	128.511000	118.067000	41.044000	C	144.178000	114.059000	39.508000
C	129.449000	119.089000	39.042000	N	131.922000	107.849000	34.992000
C	128.903000	119.185000	40.355000	C	131.684000	107.324000	36.343000
N	136.240000	125.194000	39.029000	C	130.504000	106.333000	36.256000
C	136.139000	124.430000	40.256000	O	129.375000	106.758000	36.089000
C	136.953000	123.167000	40.167000	C	131.343000	108.500000	37.291000
				C	130.951000	108.049000	38.683000

O	130.678000	108.920000	39.544000	C	132.687000	119.001000	39.895000
O	130.911000	106.821000	38.935000	C	133.604000	119.018000	38.894000
N	133.916000	105.822000	46.957000	N	134.831000	118.472000	39.191000
C	134.582000	105.275000	45.792000	H	136.790674	122.739296	41.967968
C	135.786000	104.400000	46.212000	H	132.416175	118.346828	48.778270
O	136.829000	104.378000	45.549000	H	134.310260	119.866240	51.861962
C	135.026000	106.394000	44.847000	H	127.003835	114.970686	37.556600
C	133.863000	107.070000	44.114000	H	135.699137	126.033202	39.088136
C	133.137000	108.100000	44.715000	H	134.513251	112.186317	47.560289
C	133.474000	106.650000	42.818000	H	136.209782	118.501887	37.154225
C	132.059000	108.713000	44.067000	H	138.972151	117.098419	38.366540
C	132.376000	107.258000	42.150000	H	139.746004	119.813888	40.037628
C	131.686000	108.286000	42.783000	H	140.411500	109.624401	44.801040
O	130.633000	108.907000	42.159000	H	144.248327	111.655880	40.042472
N	135.773000	123.963000	33.656000	H	132.686662	108.491186	35.048378
C	135.264000	122.868000	34.497000	H	133.137352	106.387878	46.685379
C	136.346000	122.002000	35.112000	H	135.059277	124.534242	33.250326
O	137.484000	121.921000	34.599000	H	127.004054	123.524086	35.389005
C	134.297000	121.948000	33.698000	H	138.748841	121.552803	42.293584
C	134.930000	121.297000	32.455000	H	137.516227	118.602938	41.925764
C	135.872000	120.258000	32.571000	H	137.527109	119.980076	40.265258
C	134.592000	121.742000	31.176000	H	136.548804	120.462079	41.414299
C	136.471000	119.675000	31.400000	H	138.099534	123.593970	41.485286
C	135.173000	121.182000	30.026000	H	132.990212	119.841846	47.186014
C	136.101000	120.166000	30.132000	H	133.354289	116.955885	46.378835
O	136.699000	119.698000	28.966000	H	134.439174	117.827373	47.541598
N	126.537000	124.115000	34.731000	H	135.796387	119.877140	46.442542
C	127.435000	125.135000	34.163000	H	137.302263	119.940548	44.358635
C	126.711000	126.051000	33.143000	H	134.333631	116.991352	43.882086
O	127.351000	126.784000	32.390000	H	131.064337	119.028152	48.110383
C	128.651000	124.491000	33.456000	H	131.506132	117.500478	47.685908
C	129.493000	123.503000	34.269000	H	134.572032	118.721587	49.788619
C	129.590000	123.577000	35.678000	H	136.983544	119.002890	49.535340
C	130.191000	122.472000	33.616000	H	137.133255	119.073610	51.110868
C	130.356000	122.625000	36.410000	H	137.209821	121.231433	50.510080
C	130.951000	121.547000	34.307000	H	135.697192	121.102373	50.962850
C	131.025000	121.613000	35.707000	H	133.629296	118.408848	51.853840
O	131.685000	120.622000	36.365000	H	135.096630	118.648757	52.559905
C	138.470000	114.766000	40.635000	H	128.626478	116.036138	36.092349
C	137.752000	115.813000	41.216000	H	130.666412	115.112065	37.157457
C	138.209000	116.394000	42.401000	H	129.794516	113.578786	37.578570
C	139.365000	115.917000	43.009000	H	128.609245	113.550488	39.968576
C	140.067000	114.858000	42.439000	H	127.975411	115.350622	41.809008
C	139.619000	114.285000	41.249000	H	128.082235	118.164502	42.052293
C	136.525000	116.272000	40.496000	H	128.789919	120.169226	40.833029
O	136.030000	115.646000	39.575000	H	129.745250	120.010437	38.519325
N	135.968000	117.445000	40.946000	H	130.035528	117.804140	37.410545
H	136.315000	117.896000	41.783000	H	126.646625	114.751445	35.992813
C	134.835000	118.044000	40.418000	H	127.303088	113.530516	36.880247
S	133.360000	118.272000	41.314000	H	136.506517	124.978383	40.977454

N	135.687000	119.269000	45.631000	O	138.447000	114.964000	36.066000
C	134.899000	117.737000	44.288000	N	139.141000	116.339000	37.738000
C	136.442000	119.280000	44.542000	C	140.436000	115.677000	37.886000
N	135.979000	118.356000	43.713000	C	141.359000	115.664000	36.668000
N	134.513000	118.891000	51.772000	O	142.295000	114.893000	36.643000
C	135.176000	118.503000	50.526000	N	139.637000	120.641000	39.486000
C	135.487000	117.007000	50.388000	C	140.744000	120.716000	38.532000
O	135.364000	116.449000	49.312000	C	140.579000	121.968000	37.697000
C	136.506000	119.252000	50.366000	O	141.565000	122.490000	37.123000
C	136.361000	120.762000	50.312000	C	140.816000	119.443000	37.628000
C	135.913000	121.224000	48.947000	N	141.169000	109.629000	44.148000
O	135.639000	120.362000	48.080000	C	141.531000	110.981000	43.741000
O	135.857000	122.445000	48.749000	C	142.684000	110.988000	42.747000
N	127.315000	114.527000	36.716000	O	143.290000	112.029000	42.510000
C	128.658000	114.946000	36.299000	C	141.924000	111.815000	44.949000
C	129.137000	114.263000	35.005000	C	140.762000	112.453000	45.681000
O	130.169000	114.662000	34.419000	C	140.836000	112.056000	47.132000
C	129.685000	114.674000	37.435000	C	140.831000	113.968000	45.516000
C	129.244000	115.295000	38.783000	N	144.960000	111.195000	39.512000
C	128.735000	114.639000	39.872000	C	144.989000	112.005000	38.320000
C	129.219000	116.697000	39.109000	C	146.073000	111.303000	37.512000
N	128.389000	115.556000	40.866000	O	147.235000	111.686000	37.533000
C	128.679000	116.816000	40.415000	C	145.352000	113.457000	38.711000
C	129.609000	117.859000	38.423000	C	145.640000	114.290000	37.506000
C	128.511000	118.067000	41.044000	C	144.178000	114.059000	39.508000
C	129.449000	119.089000	39.042000	N	131.922000	107.849000	34.992000
C	128.903000	119.185000	40.355000	C	131.684000	107.324000	36.343000
N	136.240000	125.194000	39.029000	C	130.504000	106.333000	36.256000
C	136.139000	124.430000	40.256000	O	129.375000	106.758000	36.089000
C	136.953000	123.167000	40.167000	C	131.343000	108.500000	37.291000
O	137.085000	122.568000	39.107000	C	130.951000	108.049000	38.683000
C	134.660000	124.118000	40.566000	O	130.678000	108.920000	39.544000
C	134.406000	123.354000	41.900000	O	130.911000	106.821000	38.935000
C	134.356000	121.846000	41.695000	N	133.916000	105.822000	46.957000
O	134.453000	121.418000	40.532000	C	134.582000	105.275000	45.792000
O	134.198000	121.098000	42.687000	C	135.786000	104.400000	46.212000
N	134.496000	111.349000	48.107000	O	136.829000	104.378000	45.549000
C	135.416000	110.331000	47.653000	C	135.026000	106.394000	44.847000
C	135.390000	109.069000	48.477000	C	133.863000	107.070000	44.114000
O	135.845000	108.039000	48.023000	C	133.137000	108.100000	44.715000
C	136.860000	110.882000	47.569000	C	133.474000	106.650000	42.818000
C	136.976000	112.161000	46.761000	C	132.059000	108.713000	44.067000
C	136.736000	113.409000	47.357000	C	132.376000	107.258000	42.150000
C	137.215000	112.108000	45.391000	C	131.686000	108.286000	42.783000
C	136.730000	114.589000	46.578000	O	130.633000	108.907000	42.159000
C	137.205000	113.264000	44.618000	N	135.773000	123.963000	33.656000
C	136.956000	114.513000	45.215000	C	135.264000	122.868000	34.497000
N	137.086000	118.020000	37.172000	C	136.346000	122.002000	35.112000
C	136.907000	116.636000	36.817000	O	137.484000	121.921000	34.599000
C	138.238000	115.904000	36.844000	C	134.297000	121.948000	33.698000

C	134.930000	121.297000	32.455000	H	135.059277	124.534242	33.250326
C	135.872000	120.258000	32.571000	H	127.004054	123.524086	35.389005
C	134.592000	121.742000	31.176000	H	138.748841	121.552803	42.293584
C	136.471000	119.675000	31.400000	H	137.516227	118.602938	41.925764
C	135.173000	121.182000	30.026000	H	137.527109	119.980076	40.265258
C	136.101000	120.166000	30.132000	H	136.548804	120.462079	41.414299
O	136.699000	119.698000	28.966000	H	138.099534	123.593970	41.485286
N	126.537000	124.115000	34.731000	H	132.990212	119.841846	47.186014
C	127.435000	125.135000	34.163000	H	133.354289	116.955885	46.378835
C	126.711000	126.051000	33.143000	H	134.439174	117.827373	47.541598
O	127.351000	126.784000	32.390000	H	135.796387	119.877140	46.442542
C	128.651000	124.491000	33.456000	H	137.302263	119.940548	44.358635
C	129.493000	123.503000	34.269000	H	134.333631	116.991352	43.882086
C	129.590000	123.577000	35.678000	H	131.064337	119.028152	48.110383
C	130.191000	122.472000	33.616000	H	131.506132	117.500478	47.685908
C	130.356000	122.625000	36.410000	H	134.572032	118.721587	49.788619
C	130.951000	121.547000	34.307000	H	136.983544	119.002890	49.535340
C	131.025000	121.613000	35.707000	H	137.133255	119.073610	51.110868
O	131.685000	120.622000	36.365000	H	137.209821	121.231433	50.510080
C	134.233000	116.584000	40.895000	H	135.697192	121.102373	50.962850
C	134.120000	117.928000	40.505000	H	133.629296	118.408848	51.853840
C	133.013000	118.648000	40.956000	H	135.096630	118.648757	52.559905
C	132.044000	118.051000	41.759000	H	128.626478	116.036138	36.092349
C	132.167000	116.718000	42.130000	H	130.666412	115.112065	37.157457
C	133.267000	115.985000	41.698000	H	129.794516	113.578786	37.578570
C	135.411000	115.763000	40.440000	H	128.609245	113.550488	39.968576
F	136.578000	116.338000	40.751000	H	127.975411	115.350622	41.809008
F	135.415000	114.541000	41.003000	H	128.082235	118.164502	42.052293
F	135.401000	115.575000	39.111000	H	128.789919	120.169226	40.833029
C	135.176000	118.609000	39.658000	H	129.745250	120.010437	38.519325
N	134.555000	119.485000	38.673000	H	130.035528	117.804140	37.410545
H	133.945000	120.190000	39.069000	H	126.646625	114.751445	35.992813
C	134.094000	118.905000	37.514000	H	127.303088	113.530516	36.880247
S	132.880000	117.637000	37.577000	H	136.506517	124.978383	40.977454
C	132.882000	117.621000	35.838000	H	134.237454	123.555397	39.869557
C	133.756000	118.545000	35.375000	H	134.106721	124.936028	40.635371
N	134.451000	119.269000	36.322000	H	133.549093	123.608827	42.325293
H	136.790674	122.739296	41.967968	H	135.111352	123.523253	42.573745
H	132.416175	118.346828	48.778270	H	137.204095	125.442484	38.859071
H	134.310260	119.866240	51.861962	H	135.898360	124.643569	38.254140
H	127.003835	114.970686	37.556600	H	135.121551	110.039824	46.623138
H	135.699137	126.033202	39.088136	H	137.515929	110.125659	47.089619
H	134.513251	112.186317	47.560289	H	137.231318	111.100567	48.591962
H	136.209782	118.501887	37.154225	H	136.551526	113.463994	48.440026
H	138.972151	117.098419	38.366540	H	136.546596	115.564771	47.051534
H	139.746004	119.813888	40.037628	H	136.941523	115.424055	44.598745
H	140.411500	109.624401	44.801040	H	137.392240	113.203579	43.535738
H	144.248327	111.655880	40.042472	H	137.415545	111.141956	44.904646
H	132.686662	108.491186	35.048378	H	133.550642	110.994989	48.074227
H	133.137352	106.387878	46.685379	H	134.718321	111.612232	49.056411

C	128.658000	114.946000	36.299000	D	143.290000	112.029000	42.510000
C	129.137000	114.263000	35.005000	C	141.924000	111.815000	44.949000
D	130.169000	114.662000	34.419000	C	140.762000	112.453000	45.681000
C	129.685000	114.674000	37.435000	C	140.836000	112.056000	47.132000
C	129.244000	115.295000	38.783000	C	140.831000	113.968000	45.516000
C	128.735000	114.639000	39.872000	N	144.960000	111.195000	39.512000
C	129.219000	116.697000	39.109000	C	144.989000	112.005000	38.320000
N	128.389000	115.556000	40.866000	C	146.073000	111.303000	37.512000
C	128.679000	116.816000	40.415000	D	147.235000	111.686000	37.533000
C	129.609000	117.859000	38.423000	C	145.352000	113.457000	38.711000
C	128.511000	118.067000	41.044000	C	145.640000	114.290000	37.506000
C	129.449000	119.089000	39.042000	C	144.178000	114.059000	39.508000
C	128.903000	119.185000	40.355000	N	131.922000	107.849000	34.992000
N	136.240000	125.194000	39.029000	C	131.684000	107.324000	36.343000
C	136.139000	124.430000	40.256000	C	130.504000	106.333000	36.256000
C	136.953000	123.167000	40.167000	D	129.375000	106.758000	36.089000
D	137.085000	122.568000	39.107000	C	131.343000	108.500000	37.291000
C	134.660000	124.118000	40.566000	C	130.951000	108.049000	38.683000
C	134.406000	123.354000	41.900000	D	130.678000	108.920000	39.544000
C	134.356000	121.846000	41.695000	D	130.911000	106.821000	38.935000
D	134.453000	121.418000	40.532000	N	133.916000	105.822000	46.957000
D	134.198000	121.098000	42.687000	C	134.582000	105.275000	45.792000
N	134.496000	111.349000	48.107000	C	135.786000	104.400000	46.212000
C	135.416000	110.331000	47.653000	D	136.829000	104.378000	45.549000
C	135.390000	109.069000	48.477000	C	135.026000	106.394000	44.847000
D	135.845000	108.039000	48.023000	C	133.863000	107.070000	44.114000
C	136.860000	110.882000	47.569000	C	133.137000	108.100000	44.715000
C	136.976000	112.161000	46.761000	C	133.474000	106.650000	42.818000
C	136.736000	113.409000	47.357000	C	132.059000	108.713000	44.067000
C	137.215000	112.108000	45.391000	C	132.376000	107.258000	42.150000
C	136.730000	114.589000	46.578000	C	131.686000	108.286000	42.783000
C	137.205000	113.264000	44.618000	D	130.633000	108.907000	42.159000
C	136.956000	114.513000	45.215000	N	135.773000	123.963000	33.656000
N	137.086000	118.020000	37.172000	C	135.264000	122.868000	34.497000
C	136.907000	116.636000	36.817000	C	136.346000	122.002000	35.112000
C	138.238000	115.904000	36.844000	D	137.484000	121.921000	34.599000
D	138.447000	114.964000	36.066000	C	134.297000	121.948000	33.698000
N	139.141000	116.339000	37.738000	C	134.930000	121.297000	32.455000
C	140.436000	115.677000	37.886000	C	135.872000	120.258000	32.571000
C	141.359000	115.664000	36.668000	C	134.592000	121.742000	31.176000
D	142.295000	114.893000	36.643000	C	136.471000	119.675000	31.400000
N	139.637000	120.641000	39.486000	C	135.173000	121.182000	30.026000
C	140.744000	120.716000	38.532000	C	136.101000	120.166000	30.132000
C	140.579000	121.968000	37.697000	D	136.699000	119.698000	28.966000
D	141.565000	122.490000	37.123000	N	126.537000	124.115000	34.731000
C	140.816000	119.443000	37.628000	C	127.435000	125.135000	34.163000
N	141.169000	109.629000	44.148000	C	126.711000	126.051000	33.143000
C	141.531000	110.981000	43.741000	D	127.351000	126.784000	32.390000
C	142.684000	110.988000	42.747000	C	128.651000	124.491000	33.456000

C	129.493000	123.503000	34.269000	H	134.333631	116.991352	43.882086
C	129.590000	123.577000	35.678000	H	131.064337	119.028152	48.110383
C	130.191000	122.472000	33.616000	H	131.506132	117.500478	47.685908
C	130.356000	122.625000	36.410000	H	134.572032	118.721587	49.788619
C	130.951000	121.547000	34.307000	H	136.983544	119.002890	49.535340
C	131.025000	121.613000	35.707000	H	137.133255	119.073610	51.110868
O	131.685000	120.622000	36.365000	H	137.209821	121.231433	50.510080
N	133.005000	115.192000	44.820000	H	135.697192	121.102373	50.962850
C	133.341000	114.608000	43.711000	H	133.629296	118.408848	51.853840
S	133.501000	112.876000	43.773000	H	135.096630	118.648757	52.559905
C	133.068000	112.963000	45.448000	H	128.626478	116.036138	36.092349
C	132.850000	114.252000	45.813000	H	130.666412	115.112065	37.157457
N	133.548000	115.355000	42.561000	H	129.794516	113.578786	37.578570
C	134.718000	114.939000	41.793000	H	128.609245	113.550488	39.968576
C	132.690000	116.311000	42.074000	H	127.975411	115.350622	41.809008
O	131.639000	116.568000	42.634000	H	128.082235	118.164502	42.052293
C	133.121000	116.996000	40.815000	H	128.789919	120.169226	40.833029
C	132.595000	116.690000	39.558000	H	129.745250	120.010437	38.519325
C	133.052000	117.367000	38.430000	H	130.035528	117.804140	37.410545
C	134.032000	118.347000	38.556000	H	126.646625	114.751445	35.992813
C	134.567000	118.644000	39.808000	H	127.303088	113.530516	36.880247
C	134.118000	117.965000	40.935000	H	136.506517	124.978383	40.977454
O	134.481000	119.018000	37.436000	H	134.237454	123.555397	39.869557
C	134.470000	120.396000	37.683000	H	134.106721	124.936028	40.635371
H	136.790674	122.739296	41.967968	H	133.549093	123.608827	42.325293
H	132.416175	118.346828	48.778270	H	135.111352	123.523253	42.573745
H	134.310260	119.866240	51.861962	H	137.204095	125.442484	38.859071
H	127.003835	114.970686	37.556600	H	135.898360	124.643569	38.254140
H	135.699137	126.033202	39.088136	H	135.121551	110.039824	46.623138
H	134.513251	112.186317	47.560289	H	137.515929	110.125659	47.089619
H	136.209782	118.501887	37.154225	H	137.231318	111.100567	48.591962
H	138.972151	117.098419	38.366540	H	136.551526	113.463994	48.440026
H	139.746004	119.813888	40.037628	H	136.546596	115.564771	47.051534
H	140.411500	109.624401	44.801040	H	136.941523	115.424055	44.598745
H	144.248327	111.655880	40.042472	H	137.392240	113.203579	43.535738
H	132.686662	108.491186	35.048378	H	137.415545	111.141956	44.904646
H	133.137352	106.387878	46.685379	H	133.550642	110.994989	48.074227
H	135.059277	124.534242	33.250326	H	134.718321	111.612232	49.056411
H	127.004054	123.524086	35.389005	H	136.321365	116.231569	37.487639
H	138.748841	121.552803	42.293584	H	136.560036	116.606607	35.903194
H	137.516227	118.602938	41.925764	H	137.475572	118.087178	38.101420
H	137.527109	119.980076	40.265258	H	137.714279	118.462770	36.516775
H	136.548804	120.462079	41.414299	H	140.935754	116.155123	38.577327
H	138.099534	123.593970	41.485286	H	140.266453	114.734679	38.084929
H	132.990212	119.841846	47.186014	H	141.573665	120.780941	39.045544
H	133.354289	116.955885	46.378835	H	140.923710	118.636678	38.192219
H	134.439174	117.827373	47.541598	H	141.587168	119.512923	37.011145
H	135.796387	119.877140	46.442542	H	139.983466	119.360004	37.098756
H	137.302263	119.940548	44.358635	H	138.758602	120.605830	38.988727

H 140.754659	111.373781	43.294562	H 135.555522	107.178211	45.427275
H 142.523027	112.566656	44.711767	H 133.431041	108.427396	45.723143
H 142.401672	111.285536	45.635729	H 131.504671	109.525835	44.558953
H 139.908956	112.129810	45.328646	H 130.293370	109.592657	42.755176
H 140.083567	112.463427	47.629944	H 132.083429	106.913847	41.147024
H 141.690520	112.368649	47.522059	H 134.024103	105.842023	42.313461
H 140.783342	111.070743	47.213211	H 133.581468	105.071151	47.543868
H 140.073788	114.392046	45.992355	H 134.562015	106.391808	47.484336
H 140.782947	114.203266	44.555562	H 134.706057	123.319282	35.343843
H 141.681769	114.307802	45.891268	H 133.427212	122.542427	33.348393
H 140.888039	109.092131	43.339958	H 133.944634	121.125021	34.354234
H 141.960940	109.179691	44.585096	H 136.149109	119.892101	33.570664
H 144.109689	111.940942	37.896919	H 137.205590	118.860292	31.481413
H 146.155296	113.429738	39.288990	H 137.356110	119.028915	29.213853
H 143.992682	113.510510	40.296226	H 134.889215	121.552972	29.030085
H 143.376295	114.092268	38.948853	H 133.855119	122.549137	31.051356
H 144.400718	114.966140	39.797790	H 136.359166	124.573565	34.207107
H 146.394615	113.897431	36.999496	H 136.314777	123.584384	32.892307
H 145.878883	115.209809	37.783463	H 127.787190	125.780580	34.994437
H 144.840578	114.324097	36.923023	H 129.355170	125.286899	33.135392
H 144.726160	110.242080	39.272497	H 128.303042	123.923276	32.567904
H 145.865583	111.211447	39.958932	H 129.063491	124.384119	36.208422
H 132.491529	106.848537	36.622501	H 130.428435	122.673163	37.506555
H 130.586909	109.046588	36.959838	H 131.585735	120.776794	37.317410
H 132.103490	109.122291	37.411449	H 131.494869	120.763048	33.759619
H 132.147931	107.090147	34.364945	H 130.142494	122.382895	32.520688
H 131.093624	108.319880	34.657088	H 125.767911	124.563593	35.207830
H 133.856554	104.627160	45.257087	H 126.172876	123.530229	33.992382
H 135.708455	105.977313	44.077113			