

Supplementary Material

Phosphoryl transfer reaction catalyzed by membrane diacylglycerol kinase: a theoretical mechanism study

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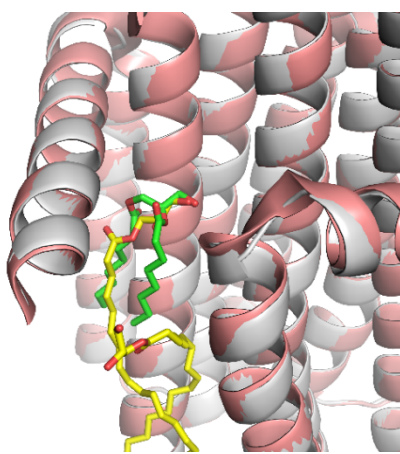


Figure S1. Alignment of the DAG-docked structure and crystal structure (PDB code: 4CK0). The DAG-docked structure is shown as grey cartoon while crystal structure is shown as brown cartoon. The substrate DAG in the docked structure is shown in green sticks and the ligand OLC in the crystal structure is shown in yellow sticks.

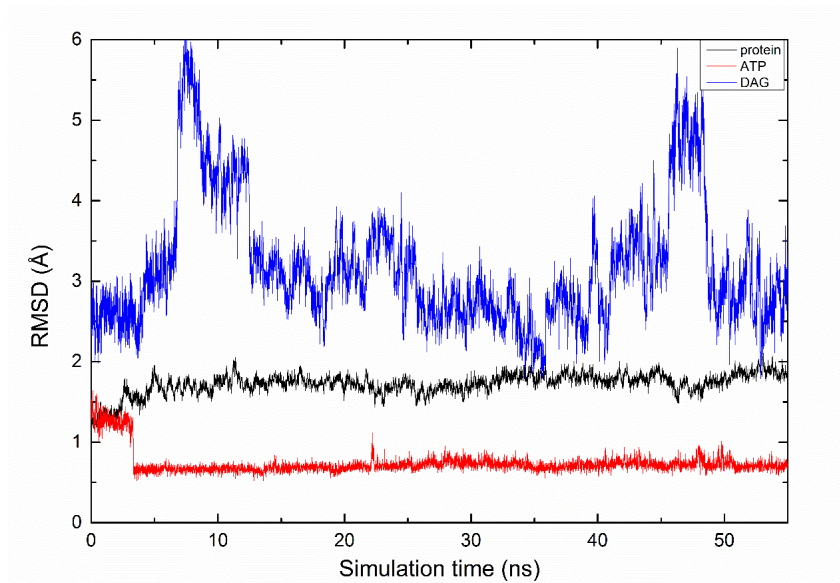
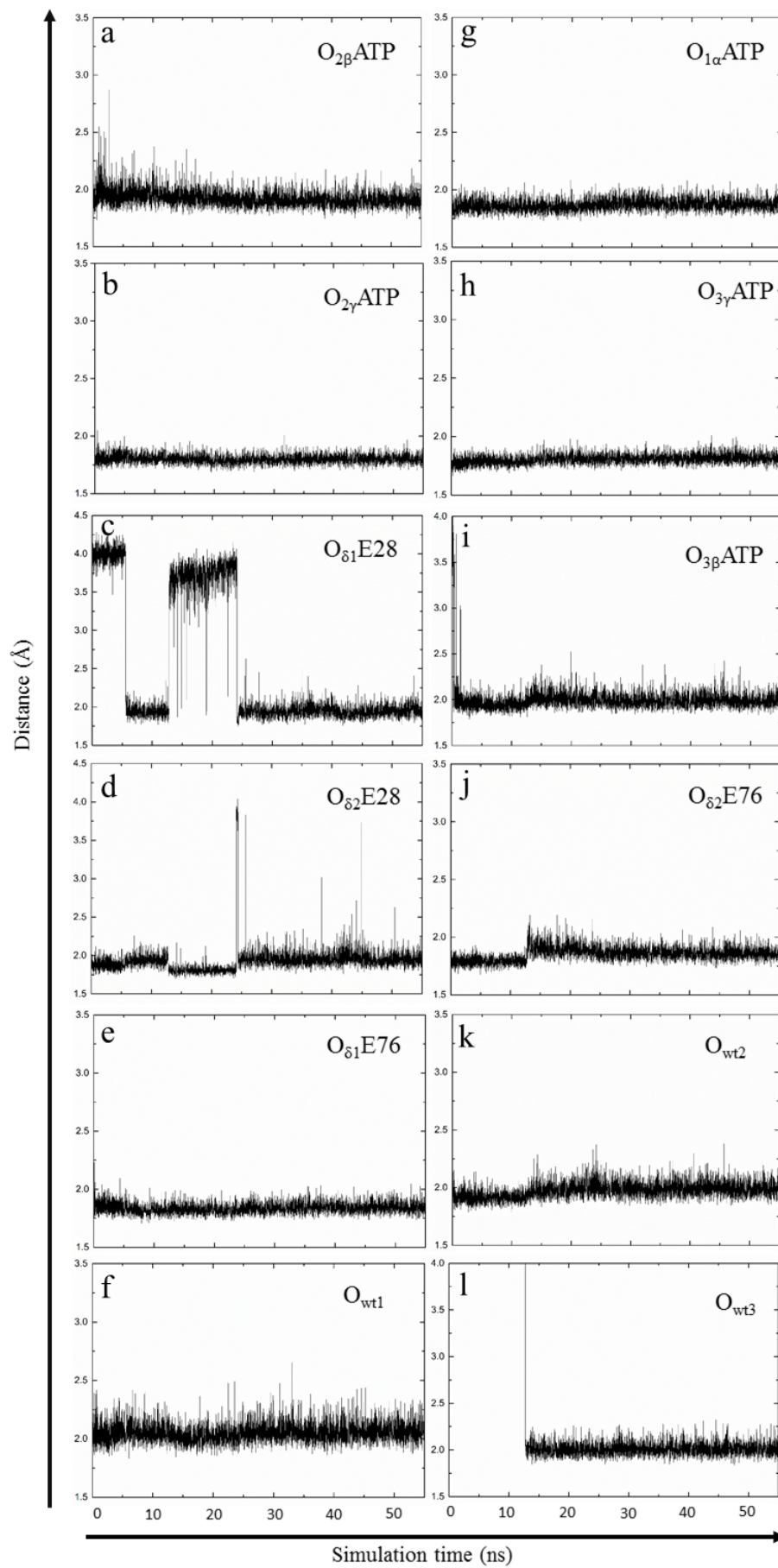


Figure S2. The RMSD values for backbone of protein, ATP and DAG in the 55ns MD runs relative to the initial structure.

Figure S3. Evolution of the coordination bond distances around Mg^{2+} ions. (a-f) hexa-coordination of Mg1. (g-l) hexa-coordination of Mg2.



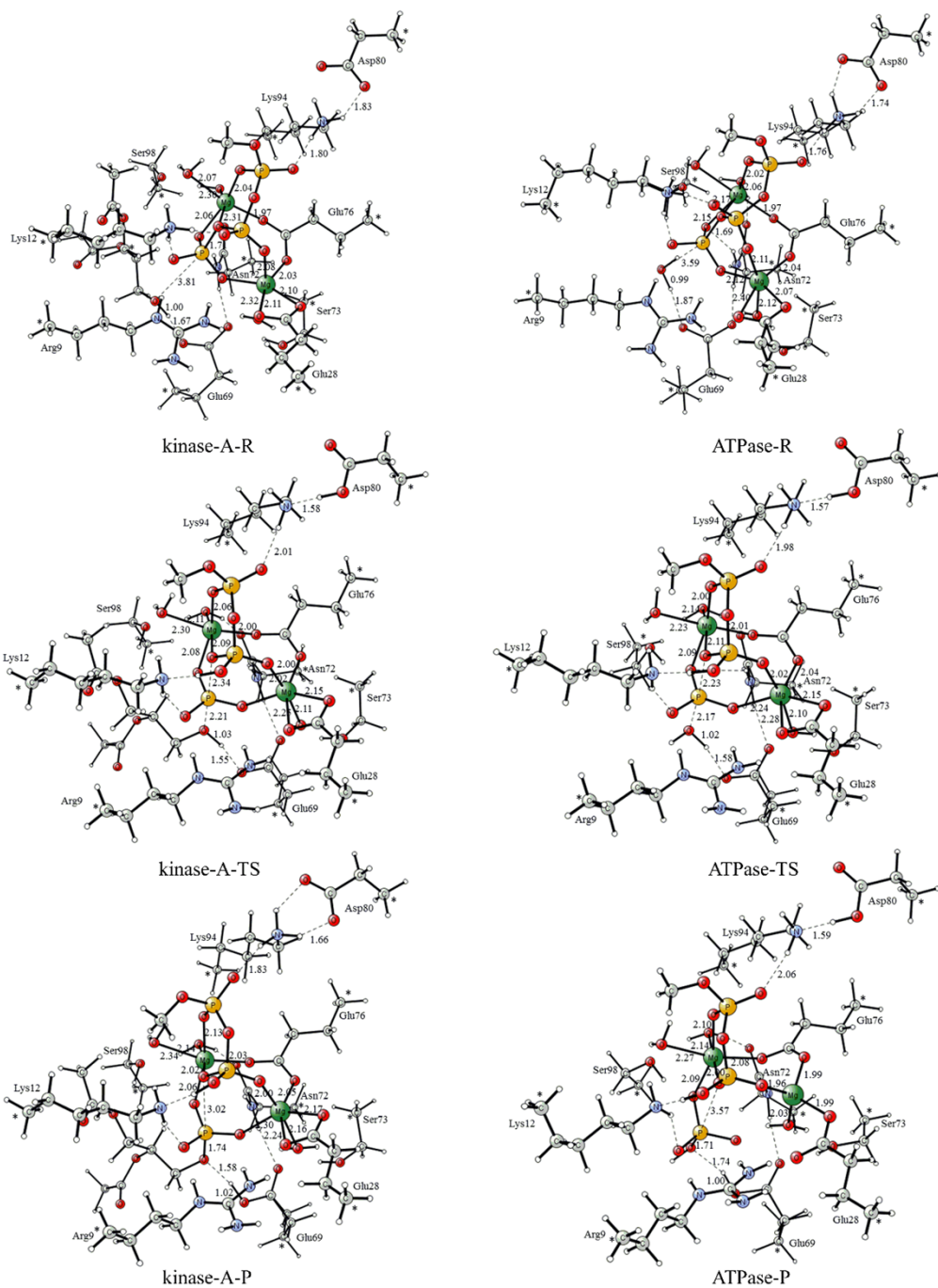


Figure S4. Optimized structures of reactants (R), transition states (TS) and products (P). The left column represents the stationary points along the dissociative reaction path of DgkA kinase reaction in which the proton transfers from the substrate to conserved residue Glu69. The right column represents the stationary points along the reaction path of DgkA ATPase reaction.

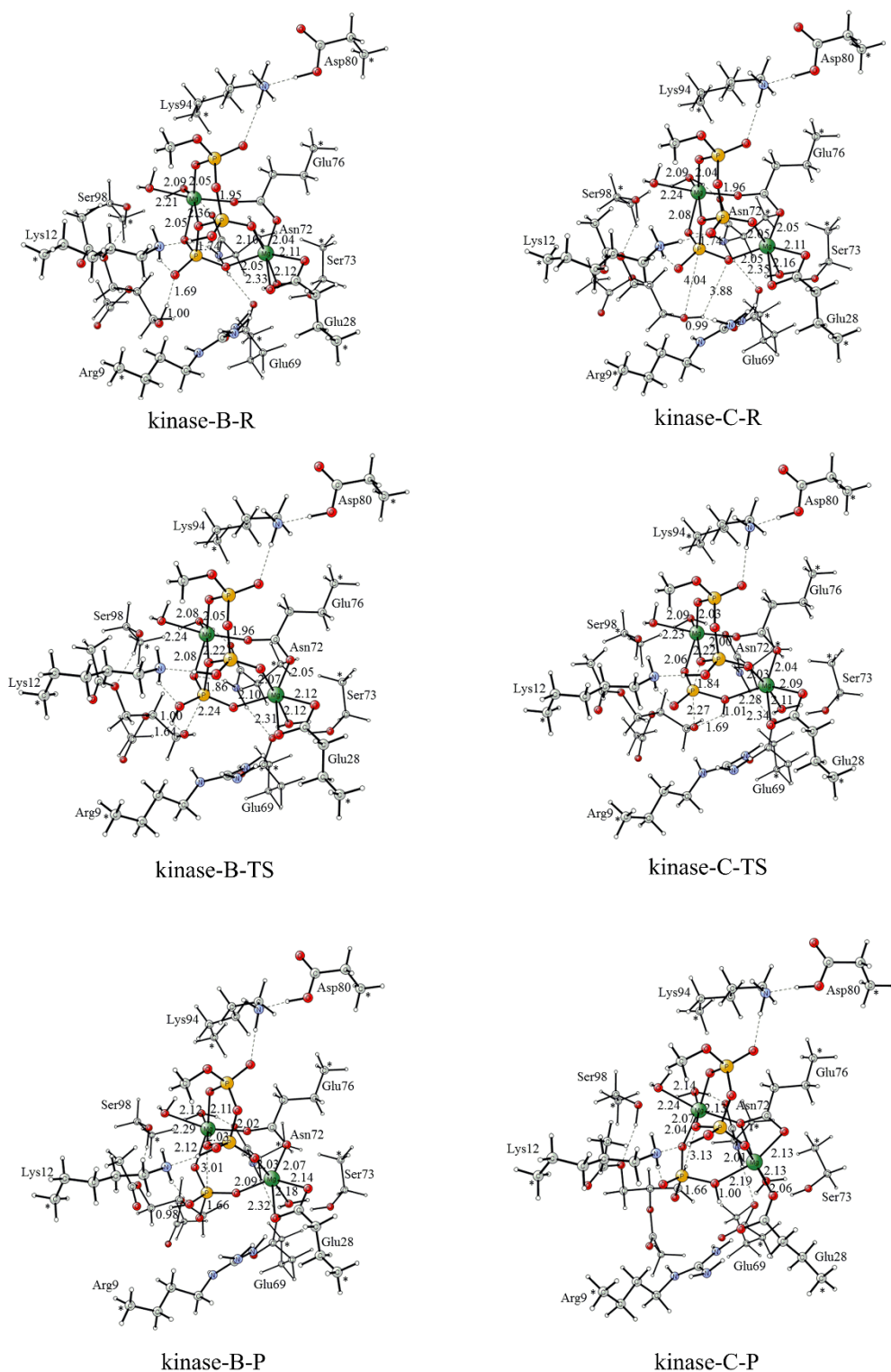


Figure S5. Optimized structures of reactants (R), transition states (TS) and products (P). The left column represents the stationary points along the reaction path of DgkA kinase reaction in which the proton of substrate DAG transfers to the non-coordinated oxygen O_{17} . The right column represents the stationary points along the reaction path of DgkA kinase reaction in which the proton of substrate DAG transfers to the coordinated oxygen O_{27} .

Cartesian coordinates of reactants, transition structures and products

Kinase reaction Path A

Kinase-A-R

C	-8.39767100	-3.04517400	-1.88095000
H	-8.59877900	-2.94617900	-2.95538000
C	-7.78371300	-1.76381000	-1.30977600
H	-7.62161700	-1.88549300	-0.23039200
H	-8.49877000	-0.93510300	-1.41840700
C	-6.45551200	-1.38009600	-1.97525200
H	-6.60297800	-1.25784900	-3.05985300
H	-5.73127100	-2.19698600	-1.85253600
C	-5.86370400	-0.09593500	-1.38337400
H	-5.69346200	-0.20299100	-0.30662500
H	-6.55322500	0.74425200	-1.51872300
N	-4.56868600	0.26483100	-1.96790500
H	-3.73049600	-0.19097000	-1.57433200
C	-4.32575100	1.38919700	-2.65556900
N	-5.35374400	2.01429100	-3.31251900
H	-5.11110000	2.82924800	-3.85796700
H	-6.07891100	1.43232100	-3.70620900
N	-3.11560100	1.90003800	-2.68238600
H	-2.40096500	1.59676600	-1.99592300
H	-2.78247900	2.65101800	-3.29008000
C	-5.25470900	-6.09112100	-3.13571400
H	-5.70908800	-7.07673100	-2.97952000
C	-4.55546600	-6.02525100	-4.49887800
H	-5.27419000	-6.28500900	-5.28808000
H	-3.76644800	-6.79011300	-4.54355100
C	-3.94076200	-4.65576600	-4.83264200
H	-4.73060700	-3.89023600	-4.82149600
H	-3.55317400	-4.68269800	-5.86163300
C	-2.81451900	-4.23208000	-3.87981600
H	-2.07081500	-5.04188500	-3.81873300
H	-3.19770500	-4.09045900	-2.86365400
C	-2.11480700	-2.95420300	-4.33840300
H	-2.82234400	-2.12516000	-4.43739800
H	-1.62608900	-3.09275900	-5.30875300
N	-1.08607000	-2.50781800	-3.36181500
H	-0.43570800	-1.73396300	-3.74887200
H	-0.49428900	-3.28218200	-3.05401500
H	-1.52361600	-2.06092100	-2.49678800
C	-1.77784900	6.34636400	-6.58535000
H	-0.90609400	6.26110500	-7.24641200

C	-1.71118800	5.32223200	-5.44810700
H	-1.72191600	4.30482100	-5.85663300
H	-2.60860200	5.40854100	-4.81997300
C	-0.46849800	5.48906500	-4.57154900
H	-0.43723300	6.48745400	-4.11670900
H	0.44135600	5.41602300	-5.18414600
C	-0.32521700	4.46518800	-3.44840800
O	-1.09354300	3.45578700	-3.40283900
O	0.58741300	4.64214800	-2.59086500
C	-6.46451100	4.21106700	4.08697600
H	-6.14138200	3.16643400	4.07865800
C	-6.00661200	4.91553500	2.80543000
H	-6.37230000	5.95237900	2.80755700
H	-6.45818700	4.41825900	1.93926700
C	-4.48542400	4.92859300	2.62656400
H	-3.99328700	5.31688500	3.52958500
H	-4.19309700	5.61770800	1.82288200
C	-3.84540500	3.56875200	2.29711200
O	-4.59575100	2.58238400	2.11516300
O	-2.56639500	3.56084100	2.22159600
C	0.35692600	2.68975300	5.97329500
H	0.96191000	1.86787900	6.36553700
C	-0.78822000	2.14084400	5.11857300
H	-1.38138200	2.94703800	4.67380400
H	-1.47244400	1.55972100	5.75350400
C	-0.29702700	1.19693300	4.02353500
O	0.61796200	0.38060000	4.27714600
N	-0.92570700	1.27965400	2.84889100
H	-1.59215200	2.03421700	2.64296900
H	-0.66522300	0.66254900	2.07482900
C	0.77351600	5.30207300	2.58693200
H	1.16344500	4.89532300	1.64853200
C	-0.27992900	6.37472900	2.32477800
H	0.16282600	7.21606000	1.77896800
H	-0.66050700	6.77483500	3.27988300
O	-1.36068300	5.91273600	1.52307900
H	-1.78420500	5.13117400	1.96454800
C	5.63832200	4.44096200	0.55915400
H	6.29488000	3.85231400	-0.09421200
C	4.16599900	4.07916300	0.33723600
H	3.87573000	4.30327000	-0.69497700
H	3.53081200	4.70996700	0.97122500
C	3.87608100	2.60473300	0.62454400
H	4.11367300	2.34854600	1.66698600

H	4.51039100	1.95710400	0.00310800
C	2.44524400	2.14866700	0.34983300
O	2.17994900	0.94042000	0.63112400
O	1.62800200	2.97157500	-0.13766800
C	12.68577800	-1.18409900	-1.39193400
H	12.80299600	-0.49948200	-0.54479100
C	11.57866700	-2.20243000	-1.12247400
H	11.80878700	-2.81787100	-0.24300100
H	11.49434200	-2.91086300	-1.95897500
C	10.17912200	-1.59052600	-0.90847600
O	10.03574600	-0.35492300	-1.13226400
O	9.27799000	-2.40501800	-0.53117700
C	5.06513400	-1.02526700	5.45989500
H	4.60816200	-0.02987100	5.51591800
C	5.23516200	-1.47064700	4.00326400
H	4.25048500	-1.52113400	3.52128600
H	5.65168100	-2.48868600	3.97809700
C	6.14591600	-0.53768100	3.19420000
H	7.12754700	-0.46752900	3.68815300
H	5.72158600	0.47694900	3.20612800
C	6.33624100	-0.99006700	1.74049400
H	5.36394200	-1.03268200	1.23446200
H	6.75641800	-2.00557400	1.72068800
C	7.26911100	-0.06197400	0.96420600
H	8.26745000	-0.03958500	1.41269000
H	6.87780600	0.96023400	0.94588900
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H	6.56269200	-0.42722300	-0.98165600
H	7.89020400	-1.48541400	-0.46369700
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H	-1.34820200	-2.82171400	5.08893200
C	0.25545400	-4.05285800	4.30335700
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H	1.31100400	-4.26166000	4.50149400
O	0.21817100	-3.60468400	2.93646400
H	-0.70621800	-3.48227200	2.63996400
C	-3.31954600	-1.79086400	2.55315700
C	-4.33446800	-0.63891100	2.49900100
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H	-5.35435100	-1.04805500	2.52839700
O	-4.11042900	0.10127200	1.32063300
H	-4.17396300	1.07055200	1.55773300

O	-3.45138300	-2.54206600	3.80480700
C	-4.53555900	-3.30349200	4.06047700
O	-5.48322800	-3.45514000	3.31876300
C	-4.40510700	-3.95660100	5.42155700
H	-3.51863200	-4.59901400	5.44993900
H	-5.29779400	-4.54969100	5.62423600
C	-3.38206500	-2.67278100	1.32181800
O	-2.37495100	-3.72385400	1.46365500
H	-3.13115300	-2.07303900	0.44542300
H	-4.35477000	-3.14710300	1.20158000
C	-2.34475800	-4.63392700	0.46496100
C	-1.21393600	-5.62011700	0.63147600
O	-3.12918200	-4.63307100	-0.46206600
H	-1.08053900	-5.90606700	1.67782900
H	-0.28582200	-5.14503500	0.29338300
Mg	0.15505300	2.88254700	-1.53248900
Mg	1.55065600	-0.92281200	0.52332500
C	3.63716100	-3.37616800	-3.08014000
H	4.28379400	-4.07609600	-3.61575500
H	3.15850000	-3.90123800	-2.24285500
O	4.46867100	-2.31818700	-2.62011700
P	3.83518800	-1.08575300	-1.77088900
O	4.90820500	-0.06536100	-1.58229900
O	3.11995200	-1.67056300	-0.54438600
O	2.68409900	-0.59648400	-2.83634500
P	1.19360200	0.05885100	-2.88088900
O	1.25702300	1.54647200	-2.68619400
O	0.49804300	-0.53392500	-4.08631800
O	0.52810900	-0.65459900	-1.52748900
P	-0.91279600	-0.21322700	-0.72170800
O	-2.04672800	-1.03551900	-1.35806800
O	-0.48820400	-0.64787900	0.69076300
O	-1.09030000	1.29361700	-0.93682100
O	1.76895400	-1.30213900	2.54144400
H	1.43573500	-0.55506000	3.12029700
H	1.18202400	-2.05170000	2.77680300
O	1.23974300	-3.19523500	0.35679100
H	2.16702200	-3.20379700	0.04160600
H	1.20869400	-3.58001200	1.25345800
O	-1.26868100	3.94112000	-0.38701600
H	-1.70261700	3.41229900	0.31019700
H	-1.07278800	4.79209900	0.06610400
H	-1.79526800	7.37286900	-6.19743100
H	-2.67574200	6.20862600	-7.20085500

H	12.44022600	-0.57039500	-2.26365300
H	13.65024000	-1.67875100	-1.56993800
H	-7.55725000	4.23148900	4.18642100
H	-6.04152800	4.69583000	4.97735200
H	-4.56439900	-5.90614200	-2.30646800
H	-6.05664700	-5.34443300	-3.07131900
H	-0.18293800	-3.38230600	6.30807700
H	0.25068100	-2.06666700	5.19110200
H	-9.34475500	-3.28854600	-1.38581600
H	-7.72322400	-3.89937700	-1.74629700
H	6.03111800	-0.97898000	5.97987400
H	-0.03059200	3.27753700	6.81318000
H	1.01472500	3.33674100	5.38242900
H	1.60958500	5.71500100	3.16659300
H	0.34600600	4.46866200	3.15635900
H	2.86634400	-2.99611500	-3.76096000
H	5.82579300	5.50092100	0.34820100
H	5.94766900	4.24949600	1.59561200
H	4.41918700	-1.71498300	6.01649100
H	-4.27929900	-3.19321400	6.19607800
H	-1.41469900	-6.50154200	0.02016300

Kinase-A-TS

C	7.83843900	-2.53847200	4.01128200
H	7.54524600	-2.40446300	5.05992200
C	7.62189800	-1.25590900	3.20545100
H	7.95599600	-1.41267500	2.17046600
H	8.25468800	-0.45339100	3.61180800
C	6.15919400	-0.79842600	3.19631700
H	5.81477000	-0.63050300	4.22818100
H	5.52067500	-1.59344500	2.78926600
C	5.95239100	0.47360600	2.36309300
H	6.31534300	0.30169800	1.34272300
H	6.53702500	1.30622700	2.77004800
N	4.56098400	0.89127000	2.26017000
H	3.93376200	0.36351500	1.62166500
C	3.97997200	1.84437500	2.99234900
N	4.60830100	2.32188300	4.11491900
H	4.08891600	3.01863100	4.63372900
H	5.08903100	1.64456400	4.69117000
N	2.84242100	2.39880300	2.61194700
H	2.39683400	2.07394200	1.74655200
H	2.12196400	2.67207200	3.30085000
C	5.22768800	-7.60375900	0.94776500

H	5.41769500	-8.54634700	0.42021200
C	4.20703700	-7.79754100	2.07377500
H	4.58070300	-8.56284600	2.76863500
H	3.27175000	-8.19773100	1.65627700
C	3.88989200	-6.52028100	2.86866500
H	4.82418100	-6.10614800	3.27822600
H	3.27445900	-6.79496000	3.73815500
C	3.15332500	-5.43324300	2.07092800
H	2.27786400	-5.88475600	1.57804800
H	3.78362400	-5.03256000	1.26819100
C	2.66071300	-4.28711400	2.96564500
H	3.51077600	-3.79001800	3.45072700
H	2.04980000	-4.70839300	3.77663300
N	1.86449900	-3.25407500	2.29084400
H	0.78668000	-2.32612700	3.14290900
H	1.23593700	-3.66195700	1.59920900
H	2.42265500	-2.56893500	1.77502800
C	1.09635000	4.70985900	7.44299800
H	0.62609600	4.06158800	8.19317300
C	1.03113900	4.08024200	6.05157500
H	1.57269000	3.12645800	6.04329100
H	1.53718500	4.73516900	5.32761800
C	-0.40177100	3.82290800	5.57642000
H	-0.98224700	4.75149200	5.53676700
H	-0.91819500	3.16591800	6.29149800
C	-0.48213000	3.14912900	4.21117000
O	0.48912800	2.41152300	3.83116000
O	-1.50289000	3.30757500	3.49466500
C	2.92851200	6.60062400	-3.16986500
H	2.53052600	5.60154600	-3.37308600
C	3.89390000	6.58609400	-1.98061100
H	4.30517600	7.59339000	-1.82845600
H	4.74413000	5.92775500	-2.20117900
C	3.23672200	6.11298600	-0.66964100
H	2.40710100	6.77471700	-0.39932100
H	3.97818300	6.13265800	0.13648600
C	2.71768200	4.68215200	-0.81662800
O	3.55832800	3.75360400	-0.70414600
O	1.47688300	4.52772900	-1.08694500
C	-1.19841500	4.71938600	-4.40455100
H	-2.20699600	4.35655800	-4.63030500
C	-0.16742700	3.58124500	-4.53842300
H	0.82712100	3.95596000	-4.26728200
H	-0.12923000	3.23093500	-5.57435100

C	-0.51737900	2.37154500	-3.67204800
O	-1.15950200	1.41836100	-4.15606300
N	-0.13242800	2.43539900	-2.39054800
H	0.48487600	3.16328700	-2.02704700
H	-0.38474900	1.67845400	-1.75860300
C	-2.43327800	6.03257000	-0.92648300
H	-2.87759700	5.82125500	0.05190200
C	-1.22582700	6.95503700	-0.77545700
H	-1.53126700	7.89294700	-0.29404300
H	-0.82310200	7.22145100	-1.76614000
O	-0.20177700	6.39456500	0.03783300
H	0.36185100	5.80426900	-0.51873200
C	-6.13256900	2.77268800	-1.13762800
H	-6.76041600	1.93230200	-0.81480300
C	-4.75919000	2.73326600	-0.46314200
H	-4.86519000	2.83089100	0.62291000
H	-4.16615100	3.59740800	-0.78606900
C	-3.99268100	1.44860400	-0.78076000
H	-3.94190800	1.27637800	-1.86401500
H	-4.50508200	0.57154800	-0.35878700
C	-2.56776900	1.40014000	-0.24825600
O	-1.81135600	0.49131800	-0.71564400
O	-2.20021500	2.25242400	0.60076500
C	-11.12851900	0.95074900	1.23792800
H	-10.97205400	1.01052800	0.15464200
C	-11.51812700	-0.47577300	1.65790000
H	-12.44579100	-0.79061500	1.17088200
H	-11.67145600	-0.50633600	2.74429300
C	-10.43189300	-1.48061300	1.29108000
O	-9.29925200	-1.23916200	1.93294700
O	-10.60316700	-2.37571700	0.47371900
C	-4.50768800	-1.59211900	-4.76482000
H	-4.23380900	-0.58237500	-4.43824700
C	-4.86202200	-2.47554600	-3.56892300
H	-3.99456800	-2.53425400	-2.89946900
H	-5.06879300	-3.50196400	-3.90883600
C	-6.06097900	-1.94764000	-2.77223400
H	-6.96432200	-1.95401400	-3.40215500
H	-5.87195700	-0.89446400	-2.51809700
C	-6.29895100	-2.72511000	-1.47395100
H	-5.35588000	-2.76907100	-0.92117200
H	-6.59366300	-3.76213700	-1.69974000
C	-7.34159100	-2.07549000	-0.55890900
H	-8.35763400	-2.18935900	-0.95339300

H	-7.13955800	-0.99979300	-0.48767800
N	-7.33801400	-2.59012400	0.82696600
H	-6.39674600	-2.44614300	1.21390300
H	-7.51195300	-3.59519400	0.81942900
H	-8.52200100	-1.84562000	1.55841100
C	1.59111500	-1.13874800	-6.05068000
H	2.55694000	-0.87211800	-5.60766900
C	1.11146300	-2.49611800	-5.54530700
H	1.83074700	-3.28653800	-5.80776300
H	0.15239200	-2.76010900	-6.00101700
O	0.87143200	-2.51461700	-4.13115300
H	1.71404900	-2.39572900	-3.64961200
C	3.81534200	-0.39411000	-2.62592800
C	4.15520100	0.82490100	-1.74308200
H	2.75186800	-0.32767200	-2.85493700
H	4.55708400	1.62604300	-2.37122200
H	4.92300600	0.56833200	-1.00163500
O	2.96972200	1.29591500	-1.11908600
H	3.08427200	2.29238500	-0.90639600
O	4.44551200	-0.33767400	-3.94598500
C	5.78822700	-0.25293000	-4.03244100
O	6.53778000	-0.19074800	-3.07977600
C	6.22812900	-0.23957200	-5.48016700
H	5.88956200	-1.14989300	-5.98574600
H	7.31545300	-0.16957700	-5.52837900
C	4.10709200	-1.71292900	-1.93166100
O	3.39431100	-2.77888500	-2.62530500
H	3.74220900	-1.66486700	-0.90402600
H	5.17304200	-1.94290400	-1.93045500
C	3.55483300	-4.01952800	-2.09497600
C	2.62344500	-5.02408900	-2.72499100
O	4.33877400	-4.25761700	-1.20092000
H	2.53162100	-4.86934700	-3.80301400
H	1.62960600	-4.89416100	-2.28020500
Mg	-0.67294500	2.07124300	1.93801900
Mg	-0.88864300	-1.27022900	-0.91081000
C	-2.18037500	-5.02056400	1.62536300
H	-2.55125900	-6.02183600	1.86331200
H	-1.60112700	-5.06721500	0.69370600
O	-3.31771400	-4.17862500	1.49061800
P	-3.12651400	-2.61020100	1.07892200
O	-4.45020300	-1.93791100	1.18633600
O	-2.35137000	-2.56191700	-0.24850700
O	-2.10000500	-2.14843200	2.28580700

P	-0.81977600	-1.13006300	2.32779300
O	-1.29003700	0.27024700	2.62095000
O	0.04943400	-1.71871800	3.51777600
O	-0.04986800	-1.33686500	1.00006200
P	1.60651900	0.04846500	0.09741600
O	2.76141000	-0.65154500	0.78872600
O	1.02844400	-0.51257200	-1.18707000
O	1.02399100	1.29251100	0.74807000
O	-1.24535600	-1.08920400	-2.98682900
H	-1.36981700	-0.14713900	-3.27558500
H	-0.46389900	-1.39903000	-3.48928100
O	-0.24504000	-3.37739100	-1.57414300
H	-1.15453600	-3.59040000	-1.26942400
H	-0.25843700	-3.35502400	-2.54793000
O	0.24212300	3.86094300	1.28857000
H	0.71475400	3.80938200	0.43016000
H	-0.28360200	4.68070000	1.21108600
H	0.57268100	5.67368900	7.46863900
H	2.13179300	4.88785800	7.76028200
H	-10.20062100	1.25362300	1.73065000
H	-11.91482000	1.66727600	1.50409700
H	3.42679500	6.95842900	-4.07941200
H	2.07282400	7.25902500	-2.97549200
H	4.88883500	-6.86802300	0.20970800
H	6.18670300	-7.24815900	1.34653100
H	1.70793800	-1.16165300	-7.14136500
H	0.86532600	-0.35830900	-5.79528000
H	8.89009400	-2.84667600	3.99637200
H	7.24298000	-3.36460900	3.60467100
H	-5.35166000	-1.50238400	-5.46240500
H	-0.96388500	5.53297700	-5.10060600
H	-1.20138000	5.12895500	-3.39148800
H	-3.20012000	6.48967100	-1.56551600
H	-2.14380900	5.07222800	-1.36536700
H	-1.53031300	-4.67230500	2.43671100
H	-6.67085800	3.69820600	-0.89794000
H	-6.04233700	2.71362900	-2.23026700
H	2.98637100	-6.03120200	-2.51424100
H	5.77610600	0.61051800	-6.00160800
H	-3.65316500	-1.99404500	-5.32234200
Kinase-A-P			
C	7.91793200	-2.17841100	3.98721800
H	7.59829500	-2.06597000	5.03060600

C	7.66707000	-0.89837700	3.18944800
H	8.02666000	-1.03019800	2.15947100
H	8.25745700	-0.07417900	3.61609300
C	6.18665600	-0.50723500	3.15933500
H	5.81703200	-0.37508800	4.18782600
H	5.59267200	-1.32336500	2.72805300
C	5.93133400	0.76696900	2.34428000
H	6.31210500	0.62614000	1.32563000
H	6.47580300	1.61801300	2.77041500
N	4.52392900	1.11693300	2.23075900
H	3.92501300	0.57577200	1.55474000
C	3.87930500	1.97738800	3.01806800
N	4.48322200	2.45613600	4.15697100
H	3.89857400	3.05394800	4.72775300
H	5.03344800	1.79403600	4.68725800
N	2.69623100	2.45897200	2.67425600
H	2.23889200	2.11167900	1.81545700
H	1.97936400	2.66842100	3.38710600
C	5.53447700	-7.35281400	0.92079300
H	5.63665600	-8.35387500	0.48460200
C	4.64957200	-7.38532100	2.17250600
H	5.09678300	-8.07375800	2.90369200
H	3.66929400	-7.81248100	1.91652300
C	4.43152700	-6.02204600	2.85387100
H	5.40874000	-5.55893600	3.06203600
H	3.96929100	-6.20302300	3.83558600
C	3.54471200	-5.03147600	2.07941700
H	2.63840900	-5.55842700	1.74193000
H	4.04526600	-4.66957400	1.17345200
C	3.10356800	-3.84322600	2.95119300
H	3.97814100	-3.26192600	3.27238400
H	2.65188800	-4.24297600	3.87121100
N	2.14202500	-2.92001400	2.33197300
H	0.82258500	-2.28703200	3.20520800
H	1.55441700	-3.39221400	1.64624300
H	2.56859200	-2.14567600	1.81475500
C	0.85899600	4.74493600	7.45267300
H	0.44458200	4.08488000	8.22499300
C	0.81885600	4.07713000	6.07589000
H	1.42885600	3.16507100	6.08342600
H	1.26824600	4.74876500	5.33017400
C	-0.59728400	3.70341100	5.62403600
H	-1.24852400	4.58392200	5.58743900
H	-1.04873500	3.01398100	6.35224100

C	-0.64884700	3.01533200	4.26251900
O	0.35488100	2.31919300	3.88570400
O	-1.67374000	3.12355700	3.54437100
C	2.57115300	6.73830500	-3.16145200
H	2.28432500	5.71733500	-3.43137800
C	3.50360800	6.76692800	-1.94634600
H	3.82183500	7.79790300	-1.74740000
H	4.41417900	6.19348600	-2.16133300
C	2.85587500	6.21364900	-0.65661300
H	1.98643700	6.81476200	-0.37426100
H	3.58124900	6.23154300	0.16214400
C	2.38504800	4.79574700	-0.87316900
O	3.31176300	3.88779800	-0.67080700
O	1.24060400	4.53377100	-1.26509200
C	-1.46827100	4.67120500	-4.38830800
H	-2.53160400	4.42078400	-4.31264200
C	-0.63324400	3.42640800	-4.74509100
H	0.43390000	3.68664600	-4.73516400
H	-0.88321200	3.07903100	-5.75114100
C	-0.87780400	2.24147800	-3.80844800
O	-1.52547700	1.25694100	-4.20362000
N	-0.38594500	2.34750100	-2.56287500
H	0.23201500	3.09667500	-2.27111700
H	-0.54054200	1.59054200	-1.89765000
C	-2.75220100	5.91946200	-0.90410600
H	-3.08626600	5.36495500	-0.02147300
C	-1.65337300	6.90542600	-0.52766500
H	-2.01948600	7.61565700	0.22164100
H	-1.34178400	7.49383900	-1.40620800
O	-0.52048600	6.26946600	0.06389100
H	-0.05711800	5.74276800	-0.61907900
C	-6.29792300	2.49294700	-1.11143400
H	-6.79837000	1.52170600	-1.01923500
C	-4.94772200	2.49736500	-0.37857200
H	-5.10180400	2.30674000	0.68989900
H	-4.49324100	3.49285900	-0.44262400
C	-3.97767300	1.45709900	-0.94117100
H	-3.78705500	1.63293800	-2.01017800
H	-4.42315800	0.45683500	-0.89568100
C	-2.61138300	1.34613800	-0.26678400
O	-1.85168800	0.42456000	-0.69687700
O	-2.28984300	2.17176800	0.62867400
C	-11.19767500	0.43817400	1.27450100
H	-10.81433300	0.64456200	0.26716800

C	-11.27248200	-1.07051800	1.53505000
H	-11.91256100	-1.57550500	0.80359300
H	-11.70975500	-1.24530500	2.52897900
C	-9.87818200	-1.72626300	1.51089500
O	-8.97352100	-1.11143500	2.16225500
O	-9.74032500	-2.79275900	0.84877600
C	-4.48419900	-1.78542600	-4.75206100
H	-3.51778700	-1.51718100	-4.31232200
C	-5.32666800	-2.59586700	-3.76205100
H	-4.78442900	-3.51027900	-3.48306600
H	-6.26239400	-2.92389900	-4.23891700
C	-5.64227900	-1.79358100	-2.49698100
H	-6.24057500	-0.91113400	-2.77286000
H	-4.69844500	-1.41613400	-2.08452900
C	-6.35928400	-2.58835500	-1.40092800
H	-5.69925400	-3.39004300	-1.05089200
H	-7.27669200	-3.05366400	-1.78945600
C	-6.70544500	-1.69390600	-0.21194600
H	-7.54632900	-1.03035900	-0.43308200
H	-5.84224600	-1.08820000	0.07159600
N	-7.07523500	-2.47871300	0.99463400
H	-6.22874900	-2.95927300	1.34062100
H	-7.90103200	-3.08582800	0.79910500
H	-7.55464500	-1.84069500	1.70480500
C	1.58345900	-1.04899600	-6.05420900
H	2.53308100	-0.77215500	-5.58521800
C	1.11903500	-2.42712900	-5.59106900
H	1.86238300	-3.19525400	-5.85299500
H	0.17941300	-2.69994800	-6.08108900
O	0.84209500	-2.48220400	-4.18729800
H	1.67426700	-2.39112900	-3.68203800
C	3.69320800	-0.32489500	-2.70183800
C	3.96168700	0.90188200	-1.79857200
H	2.63338700	-0.31094000	-2.95554600
H	4.36335200	1.71141200	-2.41371800
H	4.69989200	0.66215100	-1.02686200
O	2.76757900	1.41494000	-1.20582200
H	2.96708800	2.94279700	-0.84829400
O	4.35062500	-0.21678400	-4.00626400
C	5.68942100	-0.06714500	-4.06065600
O	6.40971000	0.04825300	-3.09044200
C	6.16683900	-0.06348300	-5.49641900
H	5.96324600	-1.03552500	-5.95846500
H	7.23833800	0.13844300	-5.52213100

C	4.03732800	-1.63918600	-2.01986500
O	3.35968500	-2.72164900	-2.71956200
H	3.68023300	-1.61023700	-0.98873100
H	5.11138400	-1.82846100	-2.02629900
C	3.58814400	-3.96647700	-2.21866900
C	2.66016200	-4.98992100	-2.82050300
O	4.42277100	-4.18824800	-1.36821200
H	2.53094900	-4.83519500	-3.89496600
H	1.67795300	-4.87991800	-2.34447400
Mg	-0.77073900	1.91836500	1.98648300
Mg	-0.80722600	-1.30958600	-0.82840400
C	-1.06015400	-4.94948400	1.66291100
H	-1.01432800	-6.01810600	1.89442400
H	-0.43614400	-4.75077000	0.78203500
O	-2.42848500	-4.64625200	1.41690300
P	-2.93101400	-3.13061700	1.07457000
O	-4.41420900	-3.13455900	1.22546600
O	-2.32027500	-2.69337000	-0.26554500
O	-2.26761800	-2.24131400	2.28707900
P	-0.89572800	-1.33319800	2.32746200
O	-1.30777400	0.09443200	2.61529500
O	-0.08288400	-1.96524600	3.55066100
O	-0.11597200	-1.59537700	1.04472400
P	1.81171800	0.39309000	-0.16719000
O	2.88526700	-0.35291100	0.63926700
O	1.01834800	-0.41989700	-1.19030300
O	1.03369100	1.46365600	0.62738700
O	-1.27711000	-1.19773100	-2.91174900
H	-1.52053400	-0.29029100	-3.21905500
H	-0.50782000	-1.45397600	-3.46214200
O	-0.17927400	-3.43630100	-1.57862100
H	-1.07803500	-3.60726500	-1.20423200
H	-0.28687900	-3.40000400	-2.54460600
O	0.09302100	3.79362100	1.34958300
H	0.47964000	3.50363800	0.50513900
H	-0.45947300	4.57251300	1.14037400
H	0.27089500	5.67115400	7.46304400
H	1.88438700	5.00039500	7.74861400
H	-10.51361200	0.90157200	1.99020900
H	-12.18261300	0.91661000	1.36050100
H	3.05771700	7.19102000	-4.03317600
H	1.64849100	7.29739700	-2.96520600
H	5.12692100	-6.68859200	0.14991800
H	6.54229600	-6.99152300	1.16352700

H	1.72399600	-1.04381100	-7.14263900
H	0.83288000	-0.29222700	-5.79965900
H	8.98079200	-2.44622700	3.99185100
H	7.36324300	-3.02312700	3.56163600
H	-4.99309500	-0.85524500	-5.03607800
H	-1.35427000	5.44270200	-5.15841200
H	-1.14894400	5.09949100	-3.43420300
H	-3.61463800	6.44347600	-1.33513900
H	-2.39832200	5.18741100	-1.63647900
H	-0.67943300	-4.38018200	2.51768600
H	-6.97497100	3.25199300	-0.70187100
H	-6.17151800	2.69881100	-2.18266600
H	3.05137600	-5.98923900	-2.62419500
H	5.62662000	0.69221900	-6.07526400
H	-4.29130300	-2.35045400	-5.67350100

Kinase reaction Path B

Kinase-B-R

C	-7.82030900	-2.62175000	-3.76544000
H	-6.98284900	-3.21443100	-4.15395800
C	-7.54689100	-1.11843100	-3.89748200
H	-8.42213600	-0.56189000	-3.53226700
H	-7.44766200	-0.85860000	-4.96174900
C	-6.30109400	-0.63500300	-3.13856000
H	-5.40381600	-1.14703600	-3.51572300
H	-6.37590000	-0.89407800	-2.07458100
C	-6.12474900	0.88869000	-3.26033100
H	-7.06612500	1.37459200	-2.96982100
H	-5.93598500	1.18023800	-4.29893700
N	-5.07202300	1.45729800	-2.42965800
H	-5.16019700	1.33231900	-1.41518900
C	-3.85746600	1.85441500	-2.86051900
N	-3.41811500	1.53414000	-4.10769100
H	-2.41330400	1.73585000	-4.25314400
H	-3.70478800	0.62383600	-4.44332900
N	-3.11146200	2.63441600	-2.09717600
H	-3.41668000	2.96885400	-1.17270100
H	-2.11671000	2.70438200	-2.30599700
C	-5.14611500	-7.61628700	-0.64108700
H	-5.29170300	-8.57482000	-0.12822700
C	-4.30890700	-7.79589700	-1.91152900
H	-4.80924300	-8.51594600	-2.57400900
H	-3.33944200	-8.24591100	-1.65184000

C	-4.05700900	-6.49614300	-2.69206200
H	-5.02002400	-6.04927300	-2.98061400
H	-3.54159300	-6.74568700	-3.63130000
C	-3.22075700	-5.46157600	-1.92540700
H	-2.33423400	-5.96416200	-1.50582000
H	-3.78012100	-5.05940100	-1.07264100
C	-2.73554800	-4.30943100	-2.81115800
H	-3.58471900	-3.75277300	-3.22507800
H	-2.18005600	-4.71744000	-3.66653300
N	-1.86404100	-3.34671600	-2.11455100
H	-0.88120800	-2.55441200	-2.91090100
H	-1.27713600	-3.82630400	-1.43077400
H	-2.37432000	-2.62689100	-1.58203800
C	-1.15475200	4.56858900	-7.45860200
H	-1.29004900	3.69876900	-8.11442600
C	-1.02045200	4.14175600	-5.99704500
H	-1.93571900	3.63313600	-5.67349900
H	-0.91984100	5.03056000	-5.35979200
C	0.18319300	3.21636500	-5.76625700
H	1.11733700	3.71925300	-6.03509900
H	0.08697600	2.32850600	-6.40734100
C	0.28349600	2.73843500	-4.32610500
O	-0.70867900	2.12018400	-3.80974600
O	1.33359700	2.95415400	-3.66443500
C	-2.81578000	6.67588500	3.14162000
H	-2.47848500	5.65494200	3.33766500
C	-3.82992300	6.71492900	1.99259900
H	-4.21942700	7.73704700	1.88591000
H	-4.69032500	6.07770900	2.23709700
C	-3.25674900	6.26769700	0.63333000
H	-2.40192800	6.89869000	0.36340600
H	-4.02985700	6.38462500	-0.13415500
C	-2.81455200	4.79695200	0.63735200
O	-3.66842900	3.91734000	0.39705100
O	-1.57409400	4.57518500	0.91192900
C	1.33585900	4.82998600	4.34642300
H	1.92300400	4.25193200	5.06715400
C	0.04685900	4.08325800	3.98090200
H	-0.52597900	4.65376900	3.24572500
H	-0.58171400	3.99301100	4.87850500
C	0.25044200	2.65879900	3.45732900
O	1.00026500	1.85802400	4.05849100
N	-0.47123300	2.34357400	2.37636800
H	-0.99122600	3.05920700	1.85843700

H	-0.42683600	1.40907100	1.96533500
C	2.50957000	6.07323700	0.82177700
H	2.97148500	5.90200500	-0.15644700
C	1.24210700	6.91505400	0.67328300
H	1.49473800	7.88269800	0.21897500
H	0.81419600	7.13072200	1.66474800
O	0.26485900	6.30646300	-0.16300400
H	-0.35926200	5.77560800	0.38996400
C	6.22023500	2.82674300	1.03916200
H	6.84989900	1.97240600	0.75914900
C	4.85806300	2.76445200	0.34465100
H	4.98148200	2.81240600	-0.74302300
H	4.26063500	3.64176300	0.61984900
C	4.09415100	1.49392500	0.71091700
H	4.01101700	1.38780800	1.80092600
H	4.63244800	0.60124600	0.36100800
C	2.69069500	1.37460800	0.13609900
O	1.97726800	0.42987600	0.58774500
O	2.30892800	2.18483800	-0.74815800
C	11.18087500	0.96692000	-1.38066000
H	11.08760200	0.97793800	-0.28858100
C	11.49025500	-0.45029400	-1.88997100
H	12.43160900	-0.82137900	-1.47410200
H	11.57753300	-0.43370400	-2.98367700
C	10.38830200	-1.42784500	-1.50176000
O	9.23666300	-1.13180800	-2.08664800
O	10.55994800	-2.34742600	-0.71226000
C	4.66696300	-1.46519300	4.78278900
H	4.23162000	-0.53776500	4.39526200
C	5.07822500	-2.39420100	3.63925200
H	4.19847200	-2.61168600	3.01885400
H	5.42394200	-3.35823500	4.04216500
C	6.16673500	-1.79117300	2.74303900
H	7.09949900	-1.67204400	3.31550500
H	5.85451000	-0.77874400	2.45008700
C	6.41322800	-2.60839400	1.47069000
H	5.45320600	-2.75528800	0.96692300
H	6.80060500	-3.60708500	1.72631000
C	7.35992200	-1.92092400	0.48063600
H	8.40038400	-1.96917500	0.82103200
H	7.09194300	-0.86089700	0.39812700
N	7.31145800	-2.46929400	-0.89041900
H	6.35331000	-2.36225500	-1.24310800
H	7.52306400	-3.46676900	-0.86964000

H	8.46496100	-1.72201900	-1.68833300
C	-1.41085800	-0.99877900	6.16008700
H	-2.28918300	-0.53964500	5.69438500
C	-1.16100700	-2.38107500	5.57740200
H	-2.00505100	-3.05540700	5.77906800
H	-0.26330500	-2.83346800	6.00961800
O	-0.91554200	-2.32775600	4.16340500
H	-1.74725300	-2.13433300	3.68757300
C	-4.06886400	-0.41857000	2.33706800
C	-4.78216200	0.63457200	1.45685000
H	-2.99485300	-0.37247900	2.13979300
H	-4.25592800	1.59246800	1.56313400
H	-5.81359600	0.76092900	1.79192200
O	-4.84507800	0.22932700	0.09490900
H	-3.94777500	-0.10017400	-0.19710800
O	-4.14956800	-0.03332100	3.74787700
C	-5.33927400	0.00969500	4.38693100
O	-6.40423800	-0.32782600	3.91307300
C	-5.16406800	0.53321000	5.79708200
H	-4.57144600	-0.17073300	6.39110800
H	-6.14529200	0.65949100	6.25654800
C	-4.53530300	-1.83733600	2.07119600
O	-3.58704100	-2.76203200	2.68921300
H	-4.53417600	-2.00849500	0.99629300
H	-5.52941500	-2.03632200	2.47035300
C	-3.64834500	-4.03683000	2.23149400
C	-2.57418000	-4.90783300	2.83629600
O	-4.46286400	-4.41214900	1.41418400
H	-2.47504100	-4.73076100	3.91039300
H	-1.61369300	-4.66668900	2.36719600
Mg	0.67406100	1.93179100	-1.94612100
Mg	1.07822400	-1.17768600	1.23258800
C	2.40210300	-5.17007000	-1.06920300
H	2.86688500	-6.14939200	-1.21276600
H	1.91991200	-5.14248100	-0.08413700
O	3.43943100	-4.20228900	-1.16820400
P	3.13906600	-2.62938800	-0.87413600
O	4.37364500	-1.85338000	-1.15498500
O	2.42550700	-2.52636800	0.47818800
O	1.97131600	-2.39907200	-2.05323600
P	0.82248400	-1.29529000	-2.28637800
O	1.34609000	0.06307000	-2.61721500
O	-0.12125000	-1.92912100	-3.35823300
O	0.02608600	-1.37488300	-0.87533900

P	-1.19174600	-0.27473000	-0.28477400
O	-2.53158200	-0.90782800	-0.65056300
O	-0.81838200	-0.38908200	1.21231300
O	-0.87824700	1.06262300	-0.93175400
O	1.28106600	-0.73270000	3.26149100
H	1.27170000	0.24784600	3.47296800
H	0.47708400	-1.08615500	3.69225400
O	0.34662200	-3.15754200	1.89297300
H	1.22845000	-3.55109700	1.75807500
H	0.13483900	-3.13855400	2.84803400
O	-0.23696800	3.73980000	-1.32695600
H	-0.73873600	3.74745100	-0.47828300
H	0.27266600	4.57329500	-1.29073200
H	-0.25944200	5.10208300	-7.80202500
H	-2.01473400	5.23345600	-7.60577400
H	10.24006700	1.32888700	-1.80447600
H	11.97895900	1.66614200	-1.65704400
H	-3.25390000	7.07059900	4.06710200
H	-1.92899400	7.27775300	2.90709800
H	-4.68339200	-6.92216000	0.06830800
H	-6.13945400	-7.21597000	-0.88108100
H	-1.58030200	-1.06230100	7.24202500
H	-0.55445800	-0.33956000	5.98089600
H	-8.71972800	-2.91086900	-4.32117400
H	-7.96676800	-2.90585500	-2.71665000
H	5.52752600	-1.19907400	5.41118400
H	1.10023300	5.80452300	4.78840700
H	1.96173600	4.99862100	3.46521900
H	3.24023600	6.57583100	1.46883700
H	2.27887200	5.09246500	1.24994000
H	1.64531900	-5.01209000	-1.84654500
H	6.76683400	3.74018300	0.77349000
H	6.11159600	2.81034200	2.13154700
H	-2.81816100	-5.95446300	2.64848000
H	-4.62578500	1.48575200	5.78538200
H	3.91389000	-1.93165700	5.42973600

Kinase-B-TS

C	-7.83760500	-2.84914900	-3.90868800
H	-7.08931800	-3.31031500	-4.56494500
C	-7.55586300	-1.35419000	-3.70587500
H	-8.35080300	-0.92165500	-3.08150600
H	-7.62304600	-0.84019700	-4.67585700
C	-6.19443300	-1.03118200	-3.06429700

H	-5.37819600	-1.42604500	-3.68578800
H	-6.11115300	-1.52943300	-2.08879800
C	-6.02942500	0.48787800	-2.88060900
H	-6.87998300	0.86040800	-2.29231900
H	-6.08826500	0.98306300	-3.85628600
N	-4.80857500	0.94692800	-2.23030100
H	-4.61097400	0.76593100	-1.22889600
C	-3.82866400	1.64354400	-2.84486800
N	-3.52998800	1.41637000	-4.15767600
H	-2.58776300	1.75901800	-4.39996500
H	-3.66857900	0.45302700	-4.43869000
N	-3.18693200	2.59026200	-2.18915200
H	-3.44555900	2.84076400	-1.22528900
H	-2.25001500	2.85183400	-2.49525900
C	-4.99711600	-7.78037200	-0.83087500
H	-5.48502900	-8.54737300	-0.21722800
C	-3.75309400	-8.34371700	-1.52634100
H	-4.03929200	-9.22641900	-2.11494400
H	-3.03817000	-8.70143000	-0.77089200
C	-3.04824300	-7.34048700	-2.45224900
H	-3.77020200	-6.97212700	-3.19688000
H	-2.26655500	-7.86537300	-3.02066300
C	-2.41558500	-6.14651300	-1.72486000
H	-1.68853700	-6.51791600	-0.98543500
H	-3.17215300	-5.58978400	-1.15757200
C	-1.70061800	-5.18622700	-2.68180100
H	-2.40954800	-4.80098500	-3.42518200
H	-0.92556800	-5.72489900	-3.24279700
N	-1.06915100	-4.02613900	-2.03823600
H	-0.31454900	-2.89206000	-2.91278000
H	-0.43012100	-4.31998200	-1.29917900
H	-1.75241900	-3.41253000	-1.58542800
C	-1.42596400	4.64384900	-7.44646700
H	-1.43226200	3.79029000	-8.13661500
C	-1.26948000	4.18115200	-5.99991900
H	-2.11832100	3.54488800	-5.72711100
H	-1.30611100	5.04766800	-5.32598600
C	0.03759500	3.41210800	-5.76473600
H	0.90769000	4.04761600	-5.95707700
H	0.09062900	2.56265300	-6.46124200
C	0.14024800	2.85371500	-4.35414500
O	-0.83489400	2.16625700	-3.89423600
O	1.16916400	3.06719000	-3.66089200
C	-3.25063800	6.53638000	3.16735400

H	-2.88068500	5.51870500	3.31765900
C	-4.19504200	6.61102900	1.96217000
H	-4.62459800	7.62067200	1.89853500
H	-5.03682700	5.92139300	2.10750900
C	-3.51919100	6.28104100	0.61756400
H	-2.67363000	6.95674100	0.44499000
H	-4.24596800	6.42821400	-0.18928100
C	-3.03197800	4.82622800	0.54296000
O	-3.85312900	3.93943500	0.24568400
O	-1.78248500	4.62417200	0.81299000
C	0.95960400	4.83504400	4.38156800
H	1.47353700	4.25514900	5.15480900
C	-0.30780700	4.10860200	3.91778400
H	-0.81429800	4.68496500	3.13952700
H	-1.00582400	4.02877200	4.76351100
C	-0.07920600	2.68238400	3.41360100
O	0.63183100	1.87975700	4.05501800
N	-0.73982200	2.36779800	2.29173900
H	-1.22607900	3.08598400	1.74439700
H	-0.65500900	1.43929600	1.88305200
C	2.11213000	6.17201200	0.88434300
H	2.65504600	5.84501000	-0.00860600
C	0.91860800	7.04323400	0.49319600
H	1.26757000	7.91526400	-0.07503000
H	0.42222300	7.43025200	1.39796000
O	-0.01949400	6.36727600	-0.33285300
H	-0.62682600	5.83573700	0.23873700
C	5.94363600	3.06814900	1.08830800
H	6.57444400	2.20603000	0.83697100
C	4.57844700	2.97784700	0.39529400
H	4.70454000	2.98638800	-0.69310900
H	3.98193800	3.86535500	0.63857100
C	3.81156800	1.71971100	0.80267800
H	3.70332000	1.66297700	1.89409800
H	4.36537200	0.81778300	0.50457600
C	2.42245200	1.55103500	0.20135100
O	1.70540800	0.62460300	0.69190100
O	2.04718600	2.29735300	-0.73957900
C	10.99135200	1.43502400	-1.31501400
H	10.86742700	1.46836600	-0.22645100
C	11.43347800	0.03565100	-1.77355300
H	12.39042000	-0.24301800	-1.32269600
H	11.54969500	0.02892400	-2.86472000
C	10.40536800	-1.01811300	-1.38351700

O	9.24710800	-0.82807700	-1.99911600
O	10.63140600	-1.90189400	-0.56751200
C	4.52791600	-1.33263700	4.75940900
H	3.96085200	-0.52203300	4.28933500
C	5.10018300	-2.28200700	3.70442100
H	4.27804400	-2.67302600	3.08987800
H	5.56999400	-3.14970600	4.19209900
C	6.11263200	-1.59528700	2.78096700
H	6.99327300	-1.28080200	3.36216900
H	5.65616900	-0.67546700	2.39026000
C	6.53819400	-2.45995300	1.58965700
H	5.63622000	-2.79832800	1.07047800
H	7.06298600	-3.36314100	1.93792000
C	7.41345400	-1.69944500	0.58283900
H	8.46001300	-1.67430100	0.90527400
H	7.06518600	-0.66357700	0.50808600
N	7.37910200	-2.23951200	-0.79224300
H	6.42112400	-2.13047500	-1.14193400
H	7.59482700	-3.23617500	-0.78021700
H	8.51071800	-1.45458200	-1.59318900
C	-1.57404400	-1.12013200	6.09178500
H	-2.51442700	-0.78975800	5.63725200
C	-1.17320400	-2.49308600	5.57120300
H	-1.92196100	-3.25267100	5.83690200
H	-0.21519400	-2.80874200	5.99522600
O	-0.97701000	-2.49140600	4.14733100
H	-1.84173100	-2.42496700	3.69310200
C	-3.76995800	-0.50525200	2.45014700
C	-4.00866900	0.57324500	1.36207300
H	-2.69057300	-0.60880900	2.54257600
H	-3.52746900	1.49767700	1.71249400
H	-5.08714800	0.78151600	1.29498900
O	-3.51895100	0.17512100	0.11568800
H	-3.22501400	-1.19057400	-0.73586700
O	-4.17017800	-0.03251000	3.77877000
C	-5.46615200	0.20716300	4.06269800
O	-6.40265100	-0.03388500	3.32861500
C	-5.59692200	0.81742600	5.44292100
H	-5.13067100	0.17135900	6.19404400
H	-6.65258800	0.96026000	5.67745600
C	-4.35507400	-1.86292000	2.10239400
O	-3.48939000	-2.91048800	2.65541600
H	-4.37063500	-1.98187200	1.02059300
H	-5.36160300	-2.00865300	2.49224400

C	-3.54272200	-4.11944700	2.04091200
C	-2.51674000	-5.07463000	2.60185600
O	-4.30864400	-4.37467100	1.13561600
H	-2.47083200	-5.01498300	3.69264900
H	-1.52995000	-4.80330900	2.20925700
Mg	0.46946100	1.94134700	-2.00611300
Mg	0.94734600	-1.11428800	1.19221500
C	2.89789000	-4.91552400	-0.95377200
H	3.47587500	-5.82597800	-1.13441700
H	2.39900400	-4.99587500	0.02037300
O	3.81648900	-3.83068100	-0.97784700
P	3.31209400	-2.30874100	-0.68439400
O	4.46926400	-1.39492200	-0.86496700
O	2.50082100	-2.32096500	0.61697600
O	2.20873000	-2.18149100	-1.92907900
P	0.92332900	-1.24571200	-2.21889500
O	1.27637100	0.14163900	-2.64781600
O	0.13598700	-2.05106300	-3.31808300
O	0.10231700	-1.34556900	-0.84935800
P	-1.39646300	-0.36711100	-0.35828800
O	-2.32959300	-1.50686100	-1.05130600
O	-1.04604200	-0.51818600	1.12569400
O	-1.13044300	0.90900900	-1.11490300
O	1.02686900	-0.69027000	3.23090800
H	0.96836400	0.28277100	3.46180800
H	0.25081900	-1.10728500	3.65514100
O	0.36794600	-3.17650000	1.83828800
H	1.30247200	-3.43951300	1.73300600
H	0.14527100	-3.16535000	2.79130000
O	-0.50465200	3.71660200	-1.39050700
H	-0.99834700	3.78300200	-0.53520300
H	0.02534100	4.53805600	-1.40054600
H	-0.60152300	5.30260200	-7.74768300
H	-2.36216300	5.19654300	-7.59221800
H	10.03526200	1.70263200	-1.77292000
H	11.73463300	2.19196100	-1.59216900
H	-3.75938800	6.84933800	4.08796400
H	-2.37915000	7.18814300	3.02757800
H	-4.76188800	-6.93332300	-0.17728600
H	-5.73166500	-7.43191200	-1.56833200
H	-1.70378900	-1.14849100	7.18075300
H	-0.80706500	-0.37422700	5.85550400
H	-8.82272200	-3.00569100	-4.36283200
H	-7.81785900	-3.38915500	-2.95442600

H	5.32553900	-0.88245800	5.36529500
H	0.70660400	5.81890900	4.79213100
H	1.66093200	4.98274900	3.55554600
H	2.80564500	6.72163600	1.53411700
H	1.77868700	5.27278900	1.41159300
H	2.14308500	-4.80618000	-1.74180500
H	6.48576900	3.97385400	0.78962000
H	5.83526300	3.08927200	2.18064500
H	-2.76494000	-6.09018100	2.29012100
H	-5.07622100	1.78023000	5.47240800
H	3.84578000	-1.85342700	5.44306100

Kinase-B-P

C	7.76408900	-4.33939000	2.91184900
H	6.86697800	-4.85432100	3.27595300
C	7.68213500	-2.82807000	3.17164600
H	8.61572900	-2.35478000	2.83431700
H	7.63161100	-2.65249200	4.25605300
C	6.49395200	-2.12041200	2.49571200
H	5.54764600	-2.57329300	2.82247300
H	6.53707200	-2.25746100	1.40710000
C	6.49298300	-0.61663400	2.82500400
H	7.44998700	-0.18079800	2.51063200
H	6.42461100	-0.47431100	3.90896600
N	5.43113100	0.17871300	2.21146000
H	5.58739700	0.57400800	1.29381600
C	4.33348600	0.63506500	2.86084200
N	3.90486100	-0.00689600	3.97720400
H	2.96869700	0.31083100	4.28946300
H	4.00375300	-1.01384600	3.94888800
N	3.73020700	1.73860500	2.46307400
H	4.03434200	2.26693000	1.62928500
H	2.77262400	1.89789200	2.78412000
C	4.25476100	-8.39488000	-0.70698000
H	4.51513400	-9.10203200	-1.50319400
C	2.94704000	-8.79947300	-0.01553500
H	3.05781800	-9.82196700	0.37148600
H	2.13870300	-8.84457400	-0.75947100
C	2.50759200	-7.88684900	1.14356600
H	3.33028400	-7.79857600	1.86906300
H	1.68882500	-8.38993100	1.67826100
C	2.02307100	-6.48245800	0.74307400
H	1.30050600	-6.57225500	-0.08274900
H	2.85201400	-5.86736900	0.36675200

C	1.33374800	-5.75601800	1.91369200
H	2.04120700	-5.63319400	2.74390200
H	0.52644600	-6.39680400	2.29418700
N	0.75775500	-4.44023900	1.62383200
H	-0.40497600	-3.58250600	2.61613100
H	0.18370900	-4.44783000	0.78129600
H	1.45833300	-3.71628700	1.45910800
C	2.39756400	3.12372700	7.93900700
H	2.43231400	2.19719800	8.52646100
C	2.13674300	2.83094300	6.45887700
H	2.95347400	2.22469600	6.04925800
H	2.13759700	3.77244700	5.89335300
C	0.80255700	2.10411800	6.22578400
H	-0.03271200	2.69577100	6.61320000
H	0.81106000	1.14661700	6.76530600
C	0.54293000	1.81059300	4.75486200
O	1.39524800	1.11006500	4.10130500
O	-0.48890600	2.25645100	4.19563200
C	3.95873600	6.47847700	-2.35043500
H	3.38997500	5.57580200	-2.59684200
C	4.92795100	6.22118700	-1.19036400
H	5.50292700	7.13730000	-0.99649100
H	5.65829000	5.45235400	-1.47572400
C	4.24699200	5.78642200	0.12316400
H	3.45488200	6.49444900	0.39172200
H	4.99566300	5.79493100	0.92308300
C	3.66190900	4.36482700	0.06675000
O	4.44095500	3.40945800	0.28893100
O	2.40947900	4.25937300	-0.20775500
C	-0.46527900	5.44067800	-3.55299000
H	-1.40674800	5.14973100	-4.03050400
C	0.55923100	4.29495500	-3.64601900
H	1.48643900	4.58415900	-3.14024500
H	0.78943400	4.08849700	-4.69650800
C	0.01273800	3.00654300	-3.04032300
O	-0.74895100	2.27707400	-3.70065800
N	0.37370800	2.75283200	-1.77055400
H	1.04617000	3.33432000	-1.27128200
H	-0.06759700	1.97779300	-1.26971500
C	-1.30615600	6.31760100	0.17129600
H	-1.85483600	6.00769700	1.06699200
C	0.04592800	6.91534700	0.55689800
H	-0.10691400	7.77361800	1.22429100
H	0.55972500	7.29768700	-0.34026900

O	0.88072500	5.99732400	1.25022400
H	1.39408000	5.47238800	0.58994600
C	-5.46805000	3.70273700	-0.27276300
H	-6.20145300	2.88986300	-0.20602400
C	-4.13075900	3.29805600	0.37093300
H	-4.27504300	3.09403500	1.43772400
H	-3.42980600	4.14067300	0.31713200
C	-3.50183900	2.06700800	-0.29194200
H	-3.39706000	2.21226100	-1.37541400
H	-4.15577400	1.19109400	-0.16733700
C	-2.13281000	1.64970000	0.23600000
O	-1.46306500	0.82655100	-0.48219900
O	-1.70029300	2.11761300	1.31805600
C	-10.55782100	2.24424400	2.15406600
H	-10.39684600	2.57056100	1.12005100
C	-11.35831800	0.93266600	2.19702700
H	-12.34183900	1.05313500	1.73305500
H	-11.50581400	0.63037300	3.24199100
C	-10.62704100	-0.18716000	1.46505000
O	-9.45847900	-0.45590300	2.02486000
O	-11.07608100	-0.73216500	0.46502600
C	-4.71848600	-0.18194000	-4.65404400
H	-4.08203300	0.38405000	-3.96561800
C	-5.48909200	-1.27441400	-3.90828300
H	-4.77271100	-1.93304100	-3.39953800
H	-6.04395400	-1.90083400	-4.62371600
C	-6.45014300	-0.69935100	-2.86346800
H	-7.21795200	-0.08801500	-3.36379600
H	-5.88564300	-0.02284000	-2.20886800
C	-7.11005000	-1.75841800	-1.97343000
H	-6.31669000	-2.35423600	-1.51048200
H	-7.71889900	-2.44726600	-2.57938700
C	-7.96094300	-1.13346100	-0.85134500
H	-9.01411100	-1.04277200	-1.13680700
H	-7.59413400	-0.12350300	-0.64064200
N	-7.90408800	-1.85149100	0.44010600
H	-6.92502400	-1.82059600	0.75088900
H	-8.15389600	-2.83157800	0.30852600
H	-8.88068100	-1.09895500	1.41989300
C	1.30458800	-0.39843100	-6.30632600
H	2.31054800	-0.27621900	-5.88976500
C	0.71783500	-1.76130800	-5.96012300
H	1.34333200	-2.57175800	-6.36292900
H	-0.28130600	-1.87139400	-6.39209300

O	0.54122300	-1.94366700	-4.54955600
H	1.41621000	-1.93924900	-4.11633300
C	3.35486700	0.19922100	-2.91511300
C	3.53278600	0.93900100	-1.57635200
H	2.29663800	-0.01975500	-3.04423300
H	2.80626200	1.75114600	-1.50981300
H	4.52912000	1.37588400	-1.50784100
O	3.41901800	0.04261100	-0.47215100
H	3.06755900	-2.30095900	0.24418800
O	3.63679900	1.12826500	-4.00309200
C	4.91035000	1.53265500	-4.20969200
O	5.87685200	1.07635800	-3.63434200
C	4.95707100	2.63031500	-5.24736000
H	4.32743200	2.38158700	-6.10633900
H	5.98925800	2.79018000	-5.56192900
C	4.13837200	-1.11980300	-3.03861500
O	3.20788900	-2.22910600	-3.24601800
H	4.72490100	-1.32972300	-2.14672200
H	4.78393100	-1.12213600	-3.91492700
C	3.11079000	-3.18732200	-2.29280800
C	2.08052700	-4.22366900	-2.64288600
O	3.78308600	-3.19734500	-1.27650500
H	1.97919800	-4.34355800	-3.72378200
H	1.10936200	-3.90399100	-2.24222500
Mg	-0.08479400	1.30345000	2.32775400
Mg	-0.97668500	-1.05660600	-1.03487200
C	-3.39872900	-4.57283500	0.69890100
H	-3.97111200	-5.50180300	0.78136300
H	-2.73239800	-4.64226700	-0.17148200
O	-4.34290000	-3.51849300	0.54620900
P	-3.83138000	-1.97284300	0.37938200
O	-5.04220700	-1.10388900	0.43371900
O	-2.89966400	-1.90818200	-0.84086000
O	-2.94057200	-1.74762600	1.74453700
P	-1.32703600	-1.71756000	2.04194100
O	-1.02143100	-0.43705300	2.78390600
O	-1.12981400	-2.99285900	2.99756000
O	-0.58685200	-1.97414700	0.73142300
P	1.94181000	-0.47784100	0.07242200
O	2.51955900	-1.78054200	0.86812800
O	1.12593500	-0.84841700	-1.16234000
O	1.37085000	0.50230400	1.05840800
O	-1.18512800	-0.36146300	-3.02313600
H	-1.16303600	0.62260000	-3.14160100

H	-0.52012800	-0.72147400	-3.64312300
O	-0.96266700	-3.05990100	-2.14354100
H	-1.90320800	-3.01157900	-1.84245900
H	-0.95824400	-2.83211100	-3.08873700
O	1.05430000	3.11715300	1.92355400
H	1.54691400	3.24863200	1.08113700
H	0.61473400	3.97560000	2.07232600
H	1.60607000	3.75314900	8.36448500
H	3.35158200	3.64578500	8.08205700
H	-9.57879500	2.10908600	2.62127400
H	-11.08879600	3.04645400	2.68063800
H	4.49439100	6.80083000	-3.25206200
H	3.23446300	7.26102500	-2.09264400
H	4.18632700	-7.39821400	-1.15867700
H	5.08772000	-8.37476700	0.00724400
H	1.37100600	-0.27773200	-7.39475400
H	0.67619900	0.40501600	-5.90574500
H	8.63112000	-4.77772400	3.41859800
H	7.85651600	-4.55395300	1.84042100
H	-5.40188900	0.52466900	-5.14422600
H	-0.08605900	6.33667800	-4.05752400
H	-0.67652600	5.70084500	-2.51327300
H	-1.91883900	7.04412300	-0.37819700
H	-1.17580300	5.42745000	-0.45275100
H	-2.79839300	-4.43444400	1.60477500
H	-5.89658600	4.58190200	0.22379500
H	-5.34110800	3.94665500	-1.33566300
H	2.35609200	-5.17142100	-2.17688500
H	4.56505500	3.55554000	-4.80988500
H	-4.06628800	-0.60410600	-5.42922700

Kinase reaction Path C

Kinase-C-R

C	-7.72887600	-2.89062300	-3.82767600
H	-6.88982800	-3.42846200	-4.28648000
C	-7.46787000	-1.37959100	-3.79266600
H	-8.34746600	-0.87313000	-3.36955300
H	-7.37366900	-1.00697500	-4.82312600
C	-6.22248500	-0.95893300	-2.99333500
H	-5.32830700	-1.45061400	-3.40248300
H	-6.30492600	-1.29185800	-1.95067900
C	-6.04556600	0.56904500	-3.03692300
H	-6.96490500	1.03851400	-2.66240400

H	-5.92753100	0.89386100	-4.07666900
N	-4.93774800	1.13014800	-2.27233500
H	-5.04927800	1.28790600	-1.26689900
C	-3.77284100	1.54072500	-2.81499300
N	-3.33585000	1.00332400	-3.98233100
H	-2.37116300	1.28446300	-4.22934000
H	-3.50235300	0.00910500	-4.07172400
N	-3.09230700	2.53737700	-2.27058600
H	-3.43716500	3.02593500	-1.44203100
H	-2.09807800	2.62343400	-2.48625600
C	-5.02838200	-7.75496600	-0.52561800
H	-5.20682200	-8.76086500	-0.12788100
C	-4.40359200	-7.82077700	-1.92339400
H	-5.05282500	-8.41576800	-2.58003500
H	-3.44741400	-8.36143900	-1.87116400
C	-4.16471400	-6.45130000	-2.58047000
H	-5.12440300	-5.92646500	-2.69448300
H	-3.77989700	-6.61509800	-3.59757200
C	-3.18607400	-5.55507100	-1.80818900
H	-2.28452200	-6.13857700	-1.56176200
H	-3.62968700	-5.22377500	-0.86279700
C	-2.76077100	-4.32754100	-2.61297000
H	-3.62361200	-3.70184400	-2.86171000
H	-2.28449200	-4.62850300	-3.55254100
N	-1.79448200	-3.47365300	-1.86858900
H	-1.05032700	-3.02184500	-2.51018700
H	-1.27289900	-4.01046500	-1.17271700
H	-2.21651300	-2.62862300	-1.35519300
C	-1.11484000	4.29062200	-7.62974000
H	-1.12453300	3.43791200	-8.32094600
C	-1.05143700	3.82256500	-6.17500800
H	-1.94046400	3.22881600	-5.93216300
H	-1.07210200	4.69487900	-5.50763400
C	0.20477100	2.99100500	-5.88106300
H	1.11087300	3.56024300	-6.11150300
H	0.20657900	2.09545900	-6.51882600
C	0.28038300	2.53087400	-4.43243000
O	-0.70767400	1.89684400	-3.92867600
O	1.31073500	2.78098700	-3.75344300
C	-2.95880000	6.67103900	2.88211200
H	-2.73927800	5.62112800	3.09468500
C	-3.86713300	6.81682300	1.65578400
H	-4.13941800	7.87295900	1.52497600
H	-4.80443300	6.27024200	1.82351400

C	-3.23066700	6.31178500	0.34501000
H	-2.31674400	6.87301600	0.12457300
H	-3.93792200	6.46200500	-0.47783100
C	-2.89818100	4.82061600	0.42725900
O	-3.83713100	4.00979300	0.19008100
O	-1.71090700	4.49719200	0.75942000
C	1.20115200	4.92152700	4.19688400
H	1.77525500	4.37322200	4.95018400
C	-0.06822400	4.14608400	3.82235000
H	-0.63331100	4.68406100	3.05666000
H	-0.71924200	4.07626500	4.70600200
C	0.17141400	2.70648500	3.35389700
O	0.97343600	1.96632000	3.95709100
N	-0.59084200	2.30964500	2.32289600
H	-1.12078200	2.99309600	1.77970000
H	-0.50070400	1.37286500	1.91969500
C	2.40754100	6.08210600	0.65515900
H	2.88982200	5.83038400	-0.29506400
C	1.13100900	6.88307900	0.40986300
H	1.37054500	7.80356500	-0.13817200
H	0.68413700	7.18939400	1.36877100
O	0.17396000	6.17801600	-0.37522300
H	-0.41703800	5.65632200	0.21551400
C	6.16108900	2.89829200	1.01662800
H	6.78224900	2.02791800	0.76967900
C	4.80426100	2.82897200	0.31021400
H	4.93882200	2.83912700	-0.77709800
H	4.21596900	3.72278800	0.55132700
C	4.02359300	1.57889900	0.71088700
H	3.92840900	1.51083900	1.80279200
H	4.55719400	0.67118800	0.39414300
C	2.62583900	1.44441100	0.12575500
O	1.88843400	0.54826800	0.63480000
O	2.26468700	2.19372400	-0.82032800
C	11.18236100	1.04460000	-1.27965200
H	11.08536400	1.07361500	-0.18818300
C	11.51953800	-0.37561700	-1.76207600
H	12.46601200	-0.72202600	-1.33647000
H	11.61029100	-0.37723900	-2.85567800
C	10.43246200	-1.36447100	-1.35883800
O	9.27845600	-1.09691900	-1.94989400
O	10.61927900	-2.26655500	-0.55218600
C	4.61583400	-1.30894600	4.85848500
H	4.07906700	-0.47494000	4.39432500

C	5.12842700	-2.28535200	3.79770000
H	4.28070700	-2.64086400	3.19713900
H	5.56715100	-3.17179100	4.28078300
C	6.15621600	-1.64857900	2.85537700
H	7.06235800	-1.37743300	3.41927300
H	5.73805300	-0.70756100	2.47197200
C	6.51288800	-2.53607500	1.65828200
H	5.58478500	-2.82344700	1.15563500
H	6.99388200	-3.46617100	1.99945500
C	7.41092900	-1.82844800	0.63482700
H	8.45691400	-1.82340500	0.96144500
H	7.09260200	-0.78505500	0.53159600
N	7.36517800	-2.40583500	-0.72441800
H	6.40695000	-2.29287000	-1.07711500
H	7.56644600	-3.40481900	-0.68335200
H	8.50739900	-1.68404100	-1.53373800
C	-1.48734400	-0.89391300	6.13661600
H	-2.24187400	-0.25442800	5.66602600
C	-1.41569200	-2.24263000	5.43436700
H	-2.38741900	-2.75452800	5.46363400
H	-0.68303800	-2.89432400	5.92142900
O	-0.97631400	-2.12548500	4.07405000
H	-1.70951500	-1.83103400	3.49716800
C	-4.16514200	0.08115600	2.51559000
C	-5.01916100	1.21656100	1.91596900
H	-3.11222200	0.36682800	2.46156200
H	-4.92613200	2.09560900	2.56725400
H	-6.07216700	0.91802400	1.89941300
O	-4.59199200	1.50798000	0.59971600
H	-4.12430300	2.38386400	0.58337200
O	-4.39318000	-0.04382600	3.95908400
C	-5.59369200	-0.42453700	4.43966700
O	-6.57737500	-0.66055500	3.76947000
C	-5.54901200	-0.52041000	5.95100700
H	-4.84274300	-1.29966900	6.25687700
H	-6.54457200	-0.75891400	6.32748600
C	-4.36301100	-1.22385600	1.76781500
O	-3.57087000	-2.26181900	2.42312700
H	-3.99168000	-1.10291100	0.74649500
H	-5.40571100	-1.54194600	1.77148600
C	-3.63985400	-3.47921300	1.84301400
C	-2.73900900	-4.48522100	2.51963000
O	-4.34278300	-3.72564400	0.88312300
H	-2.77424000	-4.38428400	3.60741700

H	-1.70441300	-4.31643000	2.20022900
Mg	0.66778300	1.74090800	-2.03131800
Mg	1.07504700	-1.13492800	1.21807900
C	2.85063900	-5.12207400	-0.80235600
H	3.41529600	-6.05614100	-0.87740900
H	2.30018700	-5.11425700	0.14762500
O	3.79294200	-4.06117700	-0.86609400
P	3.30898800	-2.51258100	-0.67202600
O	4.48296300	-1.63496300	-0.92797500
O	2.55287800	-2.42912700	0.66472800
O	2.17743800	-2.46051100	-1.87463400
P	0.93314300	-1.47659800	-2.26333500
O	1.40974600	-0.08945100	-2.59780400
O	0.08009500	-2.24758900	-3.24785100
O	0.14259100	-1.46271000	-0.80391300
P	-1.17286000	-0.42488600	-0.34255100
O	-2.44188200	-1.16248100	-0.76868000
O	-0.88162500	-0.44489800	1.18175700
O	-0.91531100	0.91402800	-1.01895500
O	1.27560900	-0.66215300	3.24524700
H	1.27740100	0.32155800	3.41889200
H	0.47395600	-0.99452900	3.69752000
O	0.38731700	-3.15204500	1.91091100
H	1.31429400	-3.44603500	1.80977600
H	0.16784700	-3.07051500	2.85949500
O	-0.32923200	3.57296100	-1.48948000
H	-0.79978400	3.54888400	-0.63056700
H	0.18465700	4.40361300	-1.44989400
H	-0.24622400	4.91027400	-7.88567700
H	-2.01626400	4.88557700	-7.82231600
H	10.23595600	1.38024100	-1.71241900
H	11.96775800	1.75413300	-1.56642500
H	-3.43076300	7.10299200	3.77335800
H	-2.00130500	7.18391000	2.72889400
H	-4.38509000	-7.22575500	0.18568600
H	-5.99037400	-7.22805800	-0.54729300
H	-1.75438200	-1.02616600	7.19260900
H	-0.52211400	-0.37922700	6.08540000
H	-8.62987500	-3.12220000	-4.40714200
H	-7.86656700	-3.29309000	-2.81685400
H	5.44192300	-0.89453900	5.45199200
H	0.94217000	5.90648900	4.60120900
H	1.84929800	5.06922900	3.32851400
H	3.11733700	6.65420400	1.26652500

H	2.18651000	5.13991000	1.16631200
H	2.13761600	-5.06208300	-1.63300900
H	6.72144900	3.79657600	0.72810900
H	6.04113800	2.91688500	2.10785100
H	-3.04944100	-5.49045300	2.22880200
H	-5.19974000	0.42306100	6.38205700
H	3.92053600	-1.79708600	5.55297600

Kinase-C-TS

C	7.90008400	-2.89276400	3.79859600
H	7.28893800	-3.15158300	4.67215300
C	7.63959600	-1.45019300	3.34243500
H	8.30733900	-1.21647600	2.50092300
H	7.92909500	-0.76455500	4.15281200
C	6.19137500	-1.13297400	2.92035400
H	5.49911200	-1.38132300	3.73779100
H	5.89082000	-1.74668800	2.06220200
C	6.07840600	0.36121600	2.56051400
H	6.83888300	0.58883900	1.80249000
H	6.33291600	0.96023000	3.44339900
N	4.81404500	0.86814600	2.03845200
H	4.49891600	0.71138100	1.05141100
C	3.89083200	1.51398000	2.77039100
N	3.67878200	1.20712200	4.08289300
H	2.77528900	1.55757100	4.42162700
H	3.81869300	0.22676300	4.29620100
N	3.19157200	2.49683000	2.22038100
H	3.46333000	2.91542700	1.31736600
H	2.30785400	2.77867500	2.64479000
C	5.05973000	-7.77329500	0.64089300
H	5.48466800	-8.56064100	0.00642600
C	3.88624800	-8.30834500	1.46772400
H	4.22892000	-9.16455900	2.06544800
H	3.10918000	-8.69977700	0.79480500
C	3.25724600	-7.26856200	2.40787400
H	4.03358200	-6.87354300	3.08038000
H	2.52194100	-7.77126900	3.05325400
C	2.56856200	-6.10364900	1.68444300
H	1.82453400	-6.50854800	0.97986600
H	3.28806000	-5.53659800	1.08075200
C	1.85887000	-5.14645500	2.64749500
H	2.58088700	-4.70607700	3.34544300
H	1.13153700	-5.70045100	3.25619100
N	1.15621100	-4.03647500	1.98848300

H	0.38947200	-3.03963800	2.81158100
H	0.53882600	-4.38323000	1.25323000
H	1.79997400	-3.36964400	1.53254700
C	1.48296800	4.51193900	7.50827800
H	1.47922600	3.67040200	8.21288600
C	1.36217000	4.02445900	6.06627400
H	2.22247000	3.39290900	5.81670000
H	1.40036700	4.88199600	5.38100500
C	0.06661400	3.23909600	5.82421100
H	-0.81049200	3.85585600	6.04320900
H	0.03484000	2.37062600	6.49770400
C	-0.04898600	2.72197400	4.40106600
O	0.91863900	2.04943100	3.90378200
O	-1.09114700	2.95779600	3.73134000
C	3.25160400	6.61143100	-3.07608500
H	2.89552100	5.58801400	-3.22706300
C	4.13177700	6.71252600	-1.82591300
H	4.54779500	7.72732700	-1.75691300
H	4.98639200	6.02948700	-1.91495900
C	3.38937000	6.40072500	-0.51298200
H	2.51548200	7.05398200	-0.41008500
H	4.06315600	6.59952300	0.32804400
C	2.94813600	4.93358700	-0.40273800
O	3.78895700	4.09316400	-0.03725900
O	1.71379800	4.67624200	-0.70064800
C	-0.95927800	4.92058300	-4.30268700
H	-1.68911400	4.39128800	-4.92364100
C	0.25928400	4.02506300	-4.03331600
H	0.98208000	4.55423300	-3.40653100
H	0.74793800	3.77730500	-4.98337500
C	-0.14275100	2.71275500	-3.37118300
O	-0.85071200	1.89044200	-3.98677400
N	0.29771100	2.53459400	-2.11802400
H	0.87698000	3.23466100	-1.64912700
H	-0.03498400	1.73679500	-1.57981100
C	-2.09916500	6.18726700	-0.77529900
H	-2.68972200	5.76471400	0.04437200
C	-0.97041600	7.05756700	-0.22501700
H	-1.38370700	7.84180400	0.42158300
H	-0.44990800	7.56705000	-1.05255600
O	-0.04242800	6.32559100	0.56347400
H	0.56367900	5.83670900	-0.04589100
C	-5.92235100	3.07609600	-1.02030000
H	-6.56586100	2.21124700	-0.81559200

C	-4.56017400	2.93403400	-0.32458600
H	-4.69504000	2.89042000	0.76176500
H	-3.95689200	3.82890800	-0.51960400
C	-3.78709500	1.69280900	-0.78165100
H	-3.67317200	1.67691600	-1.87345900
H	-4.33467700	0.77771100	-0.51346600
C	-2.39795800	1.51752900	-0.18218400
O	-1.62631900	0.66891100	-0.74047800
O	-2.05743800	2.19644100	0.82083800
C	-10.95367900	1.38207800	1.37517200
H	-10.81702700	1.46047800	0.29041900
C	-11.42109100	-0.02895800	1.76782800
H	-12.37571100	-0.27471000	1.29349000
H	-11.55142600	-0.08070400	2.85616700
C	-10.40119700	-1.07815600	1.34533000
O	-9.25024300	-0.93055800	1.98534700
O	-10.62657800	-1.92101100	0.48698200
C	-4.51091900	-1.24976700	-4.78102800
H	-3.99009600	-0.40943700	-4.31014500
C	-5.05130000	-2.21845400	-3.72703600
H	-4.21840000	-2.57465800	-3.10604300
H	-5.48309500	-3.10532700	-4.21529900
C	-6.09599800	-1.57288600	-2.80957200
H	-6.98558200	-1.29346300	-3.39493000
H	-5.67905400	-0.63534900	-2.41631600
C	-6.49199700	-2.45612500	-1.62145500
H	-5.57884700	-2.76806500	-1.10511500
H	-6.98462100	-3.37544700	-1.97466700
C	-7.39551500	-1.73251800	-0.61267100
H	-8.43905700	-1.72825700	-0.94571500
H	-7.07423100	-0.68929900	-0.51980400
N	-7.36099700	-2.29003000	0.75526100
H	-6.41333900	-2.14960700	1.12233900
H	-7.53836100	-3.29388500	0.72826100
H	-8.51210100	-1.54392900	1.56147600
C	1.58399600	-0.99324700	-6.13771200
H	2.48674200	-0.58427500	-5.67070500
C	1.25378500	-2.36864000	-5.56930000
H	2.06922600	-3.07978700	-5.76126800
H	0.34712400	-2.77206900	-6.03114000
O	0.97753300	-2.32776600	-4.15918700
H	1.81303000	-2.23473100	-3.65497000
C	3.66486700	-0.28040900	-2.47603400
C	3.75969000	0.89832400	-1.47301100

H	2.60779800	-0.41902800	-2.68972900
H	3.19103700	1.73009800	-1.92009000
H	4.80675700	1.23063300	-1.40872100
O	3.28962900	0.53702700	-0.20900600
H	2.00669600	1.20688700	0.65832700
O	4.20923200	0.08974600	-3.78997200
C	5.52813500	0.30189800	-3.96051200
O	6.38567600	0.14423500	-3.11608000
C	5.80434700	0.76409300	-5.37801200
H	5.41970400	0.03559000	-6.09944400
H	6.87914500	0.89115300	-5.51458700
C	4.20480900	-1.59724200	-1.94858900
O	3.48435300	-2.68183000	-2.63442500
H	3.98537100	-1.67049300	-0.88328500
H	5.27191200	-1.72630300	-2.12259900
C	3.63116800	-3.92094600	-2.10955800
C	2.68357500	-4.90904500	-2.75297700
O	4.41225900	-4.18964800	-1.22213000
H	2.66020800	-4.78868800	-3.83986700
H	1.67038500	-4.73112300	-2.37459400
Mg	-0.48151600	1.84085700	2.07089500
Mg	-0.99549900	-1.17412100	-1.20530900
C	-3.01479800	-4.87894500	0.92599700
H	-3.61309500	-5.78306700	1.06823600
H	-2.51670700	-4.92552700	-0.05004300
O	-3.91029900	-3.77508200	0.99706300
P	-3.37181200	-2.26003000	0.73116200
O	-4.50295100	-1.32103700	0.95473800
O	-2.59139400	-2.25761400	-0.58584200
O	-2.24852900	-2.18865400	1.96256900
P	-0.90372800	-1.34126500	2.24547400
O	-1.18156100	0.05315600	2.72373300
O	-0.11752100	-2.21190200	3.27549800
O	-0.15615600	-1.38615000	0.83489000
P	1.47434400	-0.73588100	0.27719300
O	2.39584700	-1.68838800	0.97545300
O	1.03612500	-0.81442300	-1.18525600
O	1.17466300	0.73252800	0.97216900
O	-1.14028700	-0.70319500	-3.23161500
H	-1.13567800	0.27821800	-3.42058400
H	-0.33985800	-1.05729300	-3.66993800
O	-0.52086400	-3.21520700	-1.96328200
H	-1.45199400	-3.48964600	-2.02014500
H	-0.16895000	-3.12663600	-2.87353000

O	0.50566900	3.59128900	1.41704800
H	1.00317500	3.77866400	0.57563000
H	-0.04814600	4.39140100	1.51723800
H	0.64679000	5.16928600	7.77765000
H	2.41145500	5.07401500	7.66597200
H	-9.99897300	1.61512500	1.85438800
H	-11.68888600	2.13759500	1.67675000
H	3.80465600	6.90952400	-3.97554100
H	2.37069700	7.26010900	-2.99274300
H	4.76746600	-6.94257900	-0.01078300
H	5.86255500	-7.40687100	1.29347200
H	1.75113600	-1.06122500	-7.21981000
H	0.76141200	-0.29215200	-5.95794600
H	8.95209400	-3.03235000	4.07279400
H	7.66167100	-3.61000400	3.00410700
H	-5.32122200	-0.84333300	-5.40097200
H	-0.65621500	5.83453300	-4.82611800
H	-1.45410600	5.21228100	-3.37375300
H	-2.76798400	6.76539600	-1.42600300
H	-1.69125100	5.34918800	-1.34829300
H	-2.25847000	-4.81852700	1.71756900
H	-6.45119500	3.97293700	-0.67581600
H	-5.80803600	3.15233400	-2.10943700
H	2.99280800	-5.92306700	-2.49533800
H	5.29183000	1.71319100	-5.56732900
H	-3.79452200	-1.74141600	-5.45062000

Kinase-C-P

C	-7.82031800	4.32811500	2.40541500
H	-6.94181400	4.47377800	3.04503500
C	-8.18499800	2.84119200	2.29821800
H	-9.09732200	2.72928600	1.69502500
H	-8.43800000	2.46237400	3.29986000
C	-7.07004800	1.96836700	1.69830500
H	-6.12757500	2.16049700	2.22934000
H	-6.87697700	2.24973500	0.65588600
C	-7.42474000	0.46906300	1.76644700
H	-8.29102400	0.26946300	1.12693500
H	-7.72275500	0.20020100	2.78772400
N	-6.37468800	-0.45550000	1.34628500
H	-6.30619800	-0.68238200	0.35335300
C	-5.35385600	-0.82882500	2.13355100
N	-5.22390500	-0.30442900	3.37865800
H	-4.29212000	-0.46724700	3.79916500

H	-5.57165900	0.63581600	3.50183200
N	-4.50081100	-1.78056900	1.76002000
H	-4.55901700	-2.30311300	0.87789700
H	-3.62787600	-1.83455500	2.28288200
C	-4.12329700	8.42056100	-0.97718700
H	-4.34409600	9.12292500	-1.78970800
C	-2.86763600	8.84633200	-0.20642800
H	-3.01706900	9.86749900	0.17202600
H	-2.01563100	8.90280900	-0.89928300
C	-2.48586000	7.93901700	0.97747800
H	-3.34801300	7.84262900	1.65464600
H	-1.70360400	8.44982200	1.55802500
C	-1.96818400	6.54000700	0.60207200
H	-1.19647500	6.63970200	-0.17714200
H	-2.76871500	5.92531800	0.17021400
C	-1.34973200	5.80596300	1.80675900
H	-2.11344100	5.64802600	2.57900000
H	-0.58807300	6.45799200	2.25785000
N	-0.72521200	4.50897900	1.52838600
H	0.45679500	3.81797400	2.55225600
H	-0.11031200	4.55824100	0.71596000
H	-1.40259600	3.77260600	1.29495600
C	-2.73902000	-3.27449300	7.51937200
H	-3.54737900	-2.64445700	7.91185900
C	-2.41817400	-2.92329000	6.05921500
H	-3.30093700	-3.10595900	5.43199800
H	-1.62725000	-3.58563800	5.68584800
C	-1.96480100	-1.46059700	5.87996700
H	-1.07524900	-1.27543900	6.49073000
H	-2.76074100	-0.78495300	6.21724100
C	-1.61745500	-1.13522400	4.42665000
O	-2.56920400	-0.76046200	3.65189800
O	-0.42628500	-1.27302100	4.06522500
C	-3.87104100	-6.42122200	-2.89131800
H	-3.55181000	-5.39266800	-3.09619400
C	-4.61626800	-6.51137700	-1.55320600
H	-4.96819200	-7.54223600	-1.40848700
H	-5.51017300	-5.87730800	-1.58031500
C	-3.76715500	-6.10740100	-0.33876800
H	-2.83428200	-6.68231300	-0.31955500
H	-4.31670900	-6.36309000	0.57841800
C	-3.43517000	-4.60435500	-0.23358500
O	-4.37006100	-3.78018200	-0.39899700
O	-2.22674500	-4.30937500	0.06033600

C	0.60967400	-5.39919700	-3.87810900
H	1.30406500	-4.89777900	-4.55800300
C	-0.36109000	-4.38145000	-3.27796200
H	-1.04948100	-4.85612900	-2.57137600
H	-0.97339300	-3.94521600	-4.07924200
C	0.37772000	-3.23143300	-2.60362300
O	1.31940100	-2.66311700	-3.18842900
N	-0.05948900	-2.88984800	-1.38553300
H	-0.83404000	-3.37971200	-0.94011900
H	0.38917600	-2.13570900	-0.86525700
C	1.27865700	-6.35332700	-0.13800500
H	1.83415700	-5.41047700	-0.14017400
C	0.59465200	-6.57412200	1.21089900
H	1.34590800	-6.64612300	2.00475400
H	0.04583800	-7.53085400	1.19855100
O	-0.27125500	-5.51670000	1.59713800
H	-0.98132700	-5.37496000	0.92820200
C	5.47633600	-3.76658300	-0.34847400
H	6.24131400	-2.99249700	-0.48530700
C	4.33814900	-3.27039200	0.55268700
H	4.72243300	-3.03847100	1.55182500
H	3.60636400	-4.07659100	0.69352600
C	3.62351800	-2.03044500	-0.00359000
H	3.30947000	-2.18362800	-1.04410200
H	4.30089500	-1.16395500	-0.00817000
C	2.40142500	-1.62203200	0.79468600
O	1.51576300	-0.83728800	0.25134300
O	2.21071500	-2.04053200	1.95945500
C	10.46533200	-2.39804900	2.32722600
H	10.22359900	-2.76053000	1.32135500
C	11.40888200	-1.18618200	2.26021900
H	12.34949800	-1.44358800	1.76420000
H	11.63693800	-0.84486600	3.27812200
C	10.76706800	-0.03796600	1.49018200
O	9.67986600	0.40896900	2.09766900
O	11.20413300	0.37402800	0.42344900
C	4.95099300	0.20626400	-4.68306400
H	4.19428900	-0.24545300	-4.03247500
C	5.77212900	1.25107700	-3.92199400
H	5.09328700	2.00551300	-3.50084500
H	6.43885400	1.78524900	-4.61576500
C	6.59392300	0.63843900	-2.78378100
H	7.35269400	-0.04006900	-3.20453100
H	5.92975600	0.02028300	-2.16494100

C	7.25750000	1.67268100	-1.86790100
H	6.47379100	2.29755300	-1.42583700
H	7.90787000	2.34247100	-2.45260900
C	8.06059000	1.01543100	-0.73378600
H	9.07724200	0.76428000	-1.05496000
H	7.56796400	0.08430600	-0.43702000
N	8.15759900	1.82126000	0.50135000
H	7.20635900	1.88312200	0.88566300
H	8.47183300	2.76679400	0.28377000
H	9.12878000	1.05846400	1.47407700
C	-0.99149400	0.50584000	-6.59397200
H	-1.98948000	0.19124600	-6.26575800
C	-0.47406900	1.67035900	-5.75127500
H	-1.14758800	2.53457100	-5.83261100
H	0.50882800	1.98616300	-6.11491500
O	-0.27982000	1.33978000	-4.36888400
H	-1.13333400	1.35654800	-3.89243800
C	-3.71632700	-0.49269500	-2.95220400
C	-2.95430300	-0.89912300	-1.66787100
H	-3.06265300	-0.66911900	-3.81173100
H	-1.89257100	-0.96147800	-1.90605000
H	-3.29935200	-1.88803600	-1.35062900
O	-3.14838700	0.01861500	-0.59416000
H	-1.99996700	-0.11767100	2.10222400
O	-4.80908200	-1.42464200	-3.24447800
C	-5.82556500	-1.55677300	-2.38047200
O	-6.05701300	-0.76828900	-1.47888000
C	-6.61357800	-2.81356100	-2.63078500
H	-6.54416200	-3.13575500	-3.67173800
H	-7.65527800	-2.66529500	-2.33795200
C	-4.20564800	0.95329400	-3.00471100
O	-3.03220500	1.79390200	-3.09064800
H	-4.76570200	1.21621100	-2.11224200
H	-4.83338700	1.10710300	-3.88919100
C	-3.24823800	3.11224500	-2.76740500
C	-1.95806400	3.84402300	-2.53198600
O	-4.36069900	3.57347200	-2.66142400
H	-1.16921900	3.53417100	-3.21936100
H	-1.62447400	3.59011500	-1.51900700
Mg	0.40584000	-0.94470800	2.21128500
Mg	1.28035700	0.97613200	-0.83416800
C	3.67849800	4.58228000	0.31185700
H	4.23808500	5.50255900	0.11911100
H	2.94426500	4.43320500	-0.48941100

O	4.63118800	3.52202000	0.35221600
P	4.12563500	1.97756100	0.54605900
O	5.32802600	1.14681200	0.84516600
O	3.24617200	1.60336300	-0.65531200
O	3.18727000	2.10999300	1.89473700
P	1.55921400	2.03311900	2.09708300
O	1.24052200	0.76175200	2.86415600
O	1.26044000	3.33884200	2.96520000
O	0.89015900	2.17771100	0.73609000
P	-1.85805400	0.85125600	0.02523300
O	-2.39599900	2.16499300	0.49937000
O	-0.73941900	0.71434800	-0.99728100
O	-1.40141300	-0.10800600	1.30320100
O	1.58285200	-0.01874600	-2.70211900
H	1.63007500	-1.00876500	-2.75919200
H	0.90980700	0.23323200	-3.36464400
O	1.39521200	2.72565900	-2.22470600
H	2.35932700	2.63846900	-2.06508900
H	1.21493300	2.37471900	-3.11369400
O	-0.50118600	-2.77678100	1.62062300
H	-1.32844100	-2.99161200	1.14463700
H	-0.09113700	-3.65260800	1.78833900
H	-1.86208300	-3.12712400	8.16140600
H	-3.05276700	-4.32068800	7.61519200
H	9.52930000	-2.12521400	2.82174100
H	10.92530200	-3.22543900	2.88101000
H	-4.50747800	-6.74456800	-3.72392100
H	-2.97531800	-7.05492700	-2.89002500
H	-4.01269200	7.42442400	-1.42075600
H	-4.99873100	8.38969500	-0.31596400
H	-1.05939400	0.80232600	-7.64755700
H	-0.31771100	-0.35366600	-6.51642200
H	-8.64712300	4.90673200	2.83270000
H	-7.58541100	4.75165100	1.42196700
H	5.59053900	-0.59811000	-5.07002600
H	0.06955000	-6.17355600	-4.43462800
H	1.20203400	-5.89131200	-3.10019500
H	1.97639300	-7.17144100	-0.35641000
H	0.53845500	-6.31567300	-0.94508000
H	3.15166700	4.66887000	1.26857100
H	5.96634400	-4.64681300	0.08480400
H	5.10534700	-4.04378400	-1.34348400
H	-2.13300000	4.91877000	-2.60339000
H	-6.16502800	-3.58105900	-1.98638200

H	4.42760200	0.65125600	-5.53966600
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ATPase reaction Path

ATPase-R

C	-8.25396100	4.91986600	-0.55032400
H	-8.71417900	4.82246700	0.44096000
C	-7.67652400	3.58118900	-1.02747800
H	-7.25326500	3.69761000	-2.03432800
H	-8.48849700	2.84614600	-1.12334000
C	-6.59944200	3.03069600	-0.08558200
H	-7.01383100	2.95923300	0.93301900
H	-5.76550000	3.74282100	-0.01566400
C	-6.04501100	1.66184600	-0.51216900
H	-5.56332700	1.70882300	-1.49441700
H	-6.84917400	0.92105800	-0.58568000
N	-5.02865700	1.15988900	0.40857200
H	-4.04703700	1.41442500	0.21439400
C	-5.23197500	0.26414800	1.37749100
N	-6.49953100	0.04590600	1.84270600
H	-6.60998000	-0.64842800	2.56727600
H	-7.14117700	0.82405400	1.87145400
N	-4.22624800	-0.44777300	1.84868600
H	-3.31702300	-0.41570800	1.36115700
H	-4.16386300	-0.86169800	2.78057200
C	-4.72712600	7.79518300	-0.39362900
H	-5.44477100	8.32133000	-1.03323800
C	-3.29081900	8.23882600	-0.69896100
H	-3.22216400	9.32641700	-0.56435300
H	-3.06128100	8.04886200	-1.75691700
C	-2.22001300	7.57264200	0.18222800
H	-2.51191000	7.67556300	1.23804500
H	-1.27524800	8.12338700	0.07367900
C	-1.95653100	6.09071800	-0.13108100
H	-1.56613100	5.99490600	-1.15398300
H	-2.88873400	5.51280100	-0.09711000
C	-0.96285500	5.48663600	0.86056300
H	-1.37727500	5.49413200	1.87338600
H	-0.03209800	6.06374900	0.88531800
N	-0.60960200	4.07508400	0.56105300
H	-0.10539500	3.62843500	1.38993900
H	-0.01634000	3.95512500	-0.27390700
H	-1.43893500	3.43508000	0.40361300
C	-3.23961800	-2.36539400	8.16388300

H	-2.53578300	-3.10454100	8.56623300
C	-2.72612300	-1.77345700	6.84384400
H	-1.77513600	-1.25455800	7.02207300
H	-3.42303900	-1.01447000	6.46868300
C	-2.51985700	-2.83546000	5.75143700
H	-3.48211500	-3.32247000	5.53564300
H	-1.82720800	-3.61037200	6.09507100
C	-1.98409600	-2.25328600	4.44372600
O	-2.63838200	-1.34472700	3.84822600
O	-0.88813000	-2.69813700	3.98605100
C	-7.26299900	-4.35086700	-2.80389100
H	-6.59606800	-3.80819900	-3.48231900
C	-7.08198000	-3.84735600	-1.36618100
H	-7.78941000	-4.37204800	-0.70773700
H	-7.32894800	-2.78053500	-1.32335400
C	-5.66091400	-4.03331300	-0.82080500
H	-5.31342600	-5.06410400	-0.96442700
H	-5.65305700	-3.87488200	0.26766300
C	-4.59966600	-3.07230800	-1.39506000
O	-4.97224900	-2.02534700	-1.95703600
O	-3.37525500	-3.43006200	-1.20173900
C	-0.24213600	-4.62267900	-4.54690600
H	0.64105900	-4.22114500	-5.05192400
C	-1.26514000	-3.51042500	-4.31082900
H	-2.14581800	-3.88637200	-3.78071100
H	-1.60087700	-3.10280700	-5.27273600
C	-0.61991900	-2.37754300	-3.53049300
O	0.39796200	-1.81450600	-3.99717800
N	-1.17680400	-2.07920700	-2.35881600
H	-2.02870600	-2.54736300	-2.01340500
H	-0.81786400	-1.29480800	-1.82021200
C	-0.31226400	-5.59891100	-0.36276100
H	0.04879900	-5.15165900	0.56939000
C	-1.62162400	-6.35328700	-0.13687500
H	-1.46822000	-7.16350700	0.58656200
H	-1.95408500	-6.82188900	-1.07773100
O	-2.65583400	-5.53630600	0.39846600
H	-2.95128400	-4.89170100	-0.29690100
C	4.56946300	-4.57598600	1.54560800
H	5.36119700	-3.86099100	1.80267300
C	3.18541200	-3.90387400	1.56456200
H	2.96567000	-3.53101900	2.57105600
H	2.41177400	-4.65075800	1.34565600
C	3.07609300	-2.74494800	0.56876300

H	3.27548100	-3.08638900	-0.45635500
H	3.83615200	-1.98104700	0.78506300
C	1.74691900	-1.98817900	0.54350800
O	1.62165700	-1.12184500	-0.38369100
O	0.87733400	-2.23961200	1.41374600
C	12.32142900	0.42578700	1.61130800
H	12.36393500	-0.45034300	0.95384100
C	11.42501400	1.51095500	1.01946300
H	11.78669800	1.84733600	0.04028400
H	11.43253700	2.40315800	1.66315800
C	9.95538000	1.07961800	0.86104300
O	9.57025200	0.08844500	1.55021100
O	9.25177300	1.77105700	0.06304700
C	4.95181800	-1.65179800	-5.20185800
H	4.31858800	-2.46363500	-4.82403600
C	5.22428500	-0.61618000	-4.10842200
H	4.27249300	-0.18640500	-3.77189500
H	5.81645600	0.21268400	-4.52388900
C	5.96534500	-1.20743200	-2.90347800
H	6.92689900	-1.62890100	-3.23593500
H	5.38245000	-2.04863000	-2.50084800
C	6.20862600	-0.18475500	-1.78845800
H	5.24796600	0.19501700	-1.41985100
H	6.76641200	0.67508800	-2.18636700
C	6.98982500	-0.77668200	-0.61792400
H	7.99465300	-1.08505300	-0.92435300
H	6.47345600	-1.65022600	-0.20717000
N	7.15605100	0.20966600	0.47820300
H	6.23585000	0.44023100	0.90219500
H	7.70616200	1.05521400	0.14526500
H	7.87930300	-0.11143200	1.17485500
C	-0.04693500	0.87789400	-6.32493700
H	0.25824500	-0.11407900	-5.97628900
C	-0.93541300	1.55736200	-5.27917500
H	-1.82018400	0.95106400	-5.05758600
H	-1.28269900	2.53211400	-5.64623400
O	-0.21833300	1.78592700	-4.03992100
H	-0.71235900	1.39004800	-3.28774600
O	-3.65192300	0.38186200	-2.71664100
H	-4.03955100	-0.50167300	-2.51440300
Mg	-0.86336100	-1.57008700	2.24709200
Mg	1.32987600	0.70934300	-1.05815000
C	3.33183500	4.05537900	1.68661800
H	4.02283000	4.82188100	2.04760100

H	3.06319300	4.27715900	0.64594900
O	4.02701400	2.81239300	1.77739600
P	3.45571800	1.44038400	1.13632300
O	4.51595700	0.40119800	1.28559500
O	2.86177100	1.75259300	-0.24586000
O	2.20265500	0.99565000	2.11471400
P	0.62565500	1.35472300	2.26739400
O	-0.05413500	0.22585200	2.98854200
O	0.44473700	2.79612100	2.69056200
O	0.15568500	1.30996000	0.66089400
P	-1.32036300	0.84275900	-0.02237500
O	-2.30326700	1.99907900	0.16514200
O	-0.77811300	0.65448200	-1.46642100
O	-1.73838300	-0.45725400	0.66565900
O	1.78179400	0.24085600	-3.01045300
H	1.40524800	-0.66228600	-3.23069300
H	1.24757800	0.81192000	-3.60732200
O	1.04217200	2.94582700	-1.80493100
H	2.00683200	3.07189700	-1.76964700
H	0.75742600	2.90051400	-2.74167300
O	-2.16382400	-2.99104400	1.35983700
H	-2.51313900	-2.79928600	0.46537000
H	-2.13416800	-3.97094300	1.38229100
H	-4.20406500	-2.87159500	8.02506100
H	-3.37710500	-1.58714900	8.92460500
H	11.92282900	0.08573100	2.57074500
H	13.34797900	0.78734500	1.76070200
H	-8.29290500	-4.20454200	-3.15278100
H	-7.03157100	-5.42131500	-2.88218000
H	-4.86743100	6.72057000	-0.55911800
H	-4.99071200	8.00789100	0.64980900
H	-0.60113100	0.76925500	-7.26484400
H	0.84881700	1.47786200	-6.52317500
H	-9.02115000	5.29251800	-1.23873300
H	-7.47159900	5.68535500	-0.47710600
H	5.88396900	-2.09996300	-5.57105100
H	-0.66459200	-5.42415200	-5.16429800
H	0.08263800	-5.06484100	-3.59842800
H	0.46333100	-6.27523900	-0.74573600
H	-0.44670000	-4.78684000	-1.08588100
H	2.43226300	4.03857200	2.30923700
H	4.61932900	-5.40082700	2.26652000
H	4.80253000	-4.98526800	0.55370900
H	4.43432300	-1.20415400	-6.05875100

H	-2.74839000	0.32394000	-2.36561600
ATPase-TS			
C	-8.61900300	3.83667700	1.33617900
H	-8.56329000	3.85607300	2.43150300
C	-8.32307400	2.43852500	0.79005000
H	-8.42152000	2.44374500	-0.30466900
H	-9.07973400	1.73130600	1.15964800
C	-6.92612200	1.93314200	1.16616300
H	-6.81587300	1.92834800	2.26108700
H	-6.16134700	2.62474600	0.78909900
C	-6.64522200	0.53279600	0.60466900
H	-6.77390400	0.55038000	-0.48434200
H	-7.36714600	-0.19240500	0.99712100
N	-5.30203700	0.03872900	0.87058800
H	-4.51988100	0.38364000	0.27467400
C	-4.96921200	-0.78250100	1.87213500
N	-5.84466800	-0.97466000	2.91197600
H	-5.50561900	-1.58159000	3.64784800
H	-6.34103800	-0.15871600	3.24379900
N	-3.84871200	-1.47806700	1.84118300
H	-3.21547700	-1.36705100	1.03759900
H	-3.30642400	-1.65051500	2.70434100
C	-5.14837300	7.97926900	-2.22077900
H	-5.18640400	8.88480600	-2.83775900
C	-4.67413000	8.29736400	-0.80031600
H	-5.31826100	9.07680500	-0.37032700
H	-3.66294600	8.72659000	-0.84254400
C	-4.66217900	7.08630300	0.14423500
H	-5.68685100	6.69907500	0.25469400
H	-4.35752300	7.42727100	1.14425300
C	-3.73043000	5.94645500	-0.29440500
H	-2.75554600	6.36704100	-0.58547100
H	-4.12555900	5.43986300	-1.18453000
C	-3.49657700	4.91763500	0.81878700
H	-4.44850200	4.46397000	1.12414400
H	-3.11205700	5.44343600	1.70435500
N	-2.56723700	3.83361200	0.49193300
H	-1.79227900	3.06835900	1.72038900
H	-1.77968300	4.16341900	-0.06508000
H	-2.97891300	3.05711000	-0.03521600
C	-3.12969500	-2.66683100	7.44703900
H	-2.72430800	-1.87530800	8.08990800
C	-2.81626800	-2.39458400	5.97369800

H	-3.28013200	-1.45229400	5.65780800
H	-3.26031700	-3.18557100	5.35210700
C	-1.31441400	-2.31302200	5.68381300
H	-0.80626200	-3.24786700	5.94614500
H	-0.85827600	-1.53030000	6.30758900
C	-0.97553500	-1.97581500	4.23458500
O	-1.82118300	-1.32310800	3.53589400
O	0.14010500	-2.31688600	3.76398700
C	-3.24413100	-6.85967800	-2.65106000
H	-2.72895500	-5.97391500	-3.03485200
C	-4.39641600	-6.47709200	-1.71827600
H	-4.91847900	-7.38474500	-1.38536700
H	-5.13081100	-5.87187300	-2.26545000
C	-3.93192400	-5.68450200	-0.48180200
H	-3.23149000	-6.28201400	0.11088700
H	-4.79856400	-5.43798900	0.14129100
C	-3.25642900	-4.38205900	-0.91390800
O	-4.00794800	-3.42086500	-1.21146000
O	-1.97768800	-4.37474600	-0.98989500
C	1.16273000	-5.45130600	-3.48238200
H	2.24105500	-5.27621500	-3.40244100
C	0.46096300	-4.24811600	-4.13694100
H	-0.62276500	-4.41883800	-4.14981500
H	0.80034100	-4.12981600	-5.17015800
C	0.76877800	-2.93536100	-3.41850900
O	1.65374300	-2.17561500	-3.85751600
N	0.06526700	-2.69446100	-2.30315200
H	-0.70223200	-3.28691700	-1.98164200
H	0.25670700	-1.84672000	-1.77248600
C	1.67876700	-5.97987700	0.36477500
H	1.91741000	-5.50336100	1.32133400
C	0.39004600	-6.79110400	0.47884200
H	0.50267200	-7.56362400	1.25014100
H	0.18312100	-7.31417400	-0.46885200
O	-0.73092200	-6.00178300	0.86053300
H	-1.09966900	-5.54715600	0.06440100
C	5.59257600	-2.98226700	0.13543600
H	6.21941800	-2.11529000	0.38038400
C	4.13155500	-2.74084000	0.52109800
H	4.04203500	-2.59070800	1.60275500
H	3.53705500	-3.63294500	0.29068600
C	3.53489100	-1.53688300	-0.20755200
H	3.67694600	-1.62414600	-1.29295900
H	4.04187000	-0.60781200	0.09046500

C	2.04968400	-1.30420300	0.02795700
O	1.47259300	-0.47682400	-0.74410300
O	1.46202300	-1.94483500	0.93776500
C	10.22720300	-0.83963600	2.93750800
H	10.27666600	-1.08998700	1.87143900
C	10.54065900	0.64759000	3.16704300
H	11.54603300	0.89725300	2.81514500
H	10.48671200	0.86934600	4.24070400
C	9.55165000	1.54793100	2.43454600
O	8.31538300	1.39154300	2.88018400
O	9.88445300	2.29649900	1.52436300
C	4.94744400	0.49540700	-4.59086300
H	4.49105300	-0.40386900	-4.16205600
C	5.11363500	1.58552200	-3.53201800
H	4.12849700	1.82983300	-3.11627100
H	5.49695100	2.50616700	-3.99808200
C	6.04314900	1.17056700	-2.38519200
H	7.06443000	1.01549300	-2.76726600
H	5.70950500	0.19610300	-1.99993000
C	6.04668700	2.17769000	-1.23074700
H	5.01379300	2.34719900	-0.91078300
H	6.44057900	3.14679200	-1.57624900
C	6.84674600	1.70297000	-0.01477600
H	7.92117600	1.66909300	-0.22967200
H	6.53691100	0.68396100	0.24898900
N	6.66001600	2.52592400	1.19836600
H	5.65621900	2.55342600	1.41968800
H	6.95371700	3.48382700	1.00697300
H	7.63237900	1.91798100	2.26626900
C	-0.85559500	-0.02960900	-6.84994900
H	-0.08919500	-0.75518700	-6.55684500
C	-1.71843100	0.34665400	-5.64938700
H	-2.20734700	-0.54476900	-5.23702100
H	-2.51105600	1.04519900	-5.95863500
O	-0.92131200	0.95701200	-4.62777800
H	-1.22197800	0.64074600	-3.73485200
O	-3.17922300	-1.13407300	-2.07989400
H	-3.37301000	-2.07274400	-1.72063100
Mg	-0.28678400	-1.43690600	1.85241700
Mg	0.76563300	1.22892200	-1.53108000
C	1.57812300	5.39619900	0.13979300
H	1.93350800	6.43102300	0.16054000
H	1.31648000	5.12210200	-0.88921400
O	2.63242500	4.58496900	0.64026700

P	2.48851700	2.95878700	0.58864900
O	3.69569500	2.36446300	1.22404100
O	2.08597400	2.56563900	-0.83447700
O	1.14919400	2.79805200	1.56020700
P	-0.09734600	1.74972900	1.54900700
O	0.28614400	0.45933100	2.22300600
O	-1.21608900	2.51965200	2.36852400
O	-0.55467600	1.64599600	0.06398300
P	-1.98421800	0.20091500	-0.84824200
O	-3.21163500	1.07781200	-0.65487900
O	-1.07025000	0.38485200	-2.05767500
O	-1.67562200	-0.87233100	0.18879600
O	1.55194100	0.53658000	-3.39857700
H	1.76101300	-0.43256700	-3.35954100
H	0.84086200	0.57669500	-4.07280700
O	0.13189000	2.91756100	-2.83333500
H	1.00853200	3.26471500	-3.06344100
H	-0.25029800	2.54148800	-3.65308800
O	-1.20845300	-3.27022100	1.40971700
H	-1.47486300	-3.38534400	0.47172600
H	-0.76059900	-4.11288900	1.62246300
H	-2.69045400	-3.61582700	7.77921700
H	-4.21075700	-2.72118800	7.62787300
H	9.22109200	-1.07717400	3.29383000
H	10.94443600	-1.47868500	3.46651100
H	-3.60569300	-7.44040500	-3.50891200
H	-2.49792700	-7.46819600	-2.12534100
H	-4.48239300	7.26810200	-2.72143600
H	-6.15496000	7.54100300	-2.21289700
H	-1.47384200	-0.46995400	-7.64135700
H	-0.35337500	0.85501900	-7.25770200
H	-9.62095400	4.17464400	1.04797100
H	-7.89767700	4.57070100	0.95679900
H	5.91432800	0.20700700	-5.02595800
H	1.00757800	-6.35862300	-4.07772500
H	0.76937700	-5.63433400	-2.47891800
H	2.52075100	-6.62230300	0.07548200
H	1.57973700	-5.18433800	-0.38048700
H	0.68640300	5.31013600	0.77382300
H	6.00894800	-3.84959000	0.66291000
H	5.69503900	-3.16693300	-0.94192300
H	4.29797400	0.82741900	-5.40969100
H	-4.03903600	-0.68669500	-2.09002400

ATPase-P

C	8.78548300	-2.94510900	2.49706700
H	8.34342300	-3.11522100	3.48637900
C	8.37372400	-1.58180500	1.93319700
H	8.86130800	-1.42671100	0.95991100
H	8.75144600	-0.78564100	2.59126200
C	6.85644600	-1.42373900	1.76626400
H	6.36228900	-1.59504700	2.73352400
H	6.46819000	-2.19528600	1.09053800
C	6.48529200	-0.03584000	1.21989300
H	6.97502100	0.10799600	0.24946700
H	6.87766100	0.73831400	1.89176600
N	5.06325700	0.20857900	1.01399800
H	4.64106300	0.08154100	0.07392400
C	4.26415000	0.78256200	1.92929300
N	4.61302400	0.80192300	3.25265800
H	3.84000300	1.09769900	3.85685700
H	5.08763200	-0.02762000	3.58375300
N	3.16414800	1.40714200	1.56111100
H	2.86325600	1.46315600	0.57301200
H	2.45148000	1.58954000	2.27352600
C	5.79322400	-7.59684700	-0.85939600
H	6.23309800	-8.55675000	-0.56228600
C	6.62706400	-6.42148400	-0.34529600
H	7.67104700	-6.55151300	-0.66352800
H	6.63698100	-6.43325100	0.75412200
C	6.11783700	-5.06029500	-0.83610100
H	6.16410800	-5.03580100	-1.93562600
H	6.80369700	-4.27327900	-0.48831500
C	4.69377900	-4.71961200	-0.38062900
H	4.63303800	-4.74367100	0.71658400
H	3.98774000	-5.47819500	-0.74415600
C	4.24189700	-3.34839800	-0.87249600
H	4.31242200	-3.30708100	-1.97196900
H	4.92650100	-2.57839600	-0.50128600
N	2.89942500	-2.99622400	-0.39772600
H	2.26946400	-3.04613000	1.18001600
H	2.18181400	-3.45790100	-0.96033200
H	2.76387000	-2.00083900	-0.59384200
C	2.55088700	3.74499600	7.60994800
H	2.09602600	3.21722100	8.45828200
C	2.44086200	2.93030800	6.32442100
H	2.98920600	1.98649500	6.43167400
H	2.92500500	3.46753500	5.49955400

C	0.99382100	2.62649900	5.93991500
H	0.40212400	3.54894900	5.87148300
H	0.50175300	2.01973600	6.71292400
C	0.85081900	1.89030200	4.61019600
O	1.88250500	1.46432500	4.03376400
O	-0.33835000	1.75900800	4.16273200
C	3.11878500	6.99876200	-2.81381300
H	2.82900400	6.14220300	-3.43013100
C	4.07431600	6.58417800	-1.69079600
H	4.44697500	7.47006000	-1.16164200
H	4.94592200	6.07801900	-2.12112200
C	3.40278200	5.64292300	-0.66827000
H	2.67713600	6.18432500	-0.05491800
H	4.15277500	5.19536000	-0.00756500
C	2.66257500	4.55394200	-1.40984400
O	3.47840600	3.74675200	-2.05918700
O	1.43498100	4.51551100	-1.47266200
C	-1.13875300	5.25685400	-3.78000900
H	-2.10913000	5.44219000	-3.30686000
C	-1.09466600	3.85831800	-4.41898300
H	-0.09807100	3.68202000	-4.84857400
H	-1.81301400	3.78246700	-5.24014200
C	-1.40316700	2.69101900	-3.47931500
O	-2.18374300	1.79096200	-3.83778800
N	-0.80079200	2.70019900	-2.27812700
H	0.01018400	3.28202400	-2.08761800
H	-0.93108200	1.88512100	-1.67700400
C	-1.94132100	6.10194300	-0.03989000
H	-2.45584900	5.18303500	-0.33821500
C	-0.99506400	5.83204900	1.12820700
H	-1.55898000	5.50321700	2.00681300
H	-0.47129000	6.76120200	1.40811600
O	-0.04930700	4.79878000	0.87013100
H	0.38953400	4.93249300	0.00452600
C	-5.66203800	2.86495800	-0.22649500
H	-6.41388800	2.06662100	-0.19039300
C	-4.35493100	2.42340700	0.43438900
H	-4.51717900	2.19157700	1.49219000
H	-3.63401000	3.25237200	0.40886900
C	-3.74444300	1.20174600	-0.26112500
H	-3.63828500	1.37204900	-1.33763200
H	-4.40869100	0.33594900	-0.13645400
C	-2.39220100	0.78458000	0.29275800
O	-1.50239400	0.41808400	-0.53473000

O	-2.22684700	0.84523600	1.54679700
C	-10.35198500	0.71079100	2.47276700
H	-10.46616500	0.76784500	1.38409700
C	-10.44787000	-0.74559700	2.95847800
H	-11.41805700	-1.17827400	2.69688000
H	-10.33874000	-0.77301800	4.04979300
C	-9.36556600	-1.62393400	2.33808200
O	-8.15481800	-1.30822100	2.77363100
O	-9.61316400	-2.49437300	1.51396600
C	-4.51125800	-0.98382500	-4.55212500
H	-4.17341300	-0.02361600	-4.14959300
C	-4.69384200	-2.02072800	-3.44230000
H	-3.73127200	-2.16468700	-2.93978400
H	-4.97409600	-2.99254600	-3.87667300
C	-5.73967500	-1.60673200	-2.39804600
H	-6.74853700	-1.62697100	-2.83928400
H	-5.55377700	-0.55960400	-2.11808900
C	-5.68689100	-2.46770700	-1.13006300
H	-4.65526900	-2.49007300	-0.76374500
H	-5.96009800	-3.50805400	-1.36533500
C	-6.58182600	-1.94290300	-0.00374200
H	-7.64472100	-2.05191400	-0.24800100
H	-6.39757500	-0.86955600	0.13598500
N	-6.36372100	-2.58253400	1.31126600
H	-5.36244700	-2.54580300	1.54325200
H	-6.60903300	-3.57073200	1.24952400
H	-7.42198000	-1.86797900	2.26443800
C	1.39395000	-0.31744600	-6.48576300
H	1.77166700	0.49008800	-5.84787400
C	1.47337500	-1.65268300	-5.75175300
H	2.51952200	-1.89462000	-5.51004400
H	1.09085700	-2.46115400	-6.38555800
O	0.68448100	-1.66725400	-4.56699100
H	1.08590200	-1.08870300	-3.85228400
O	2.83455300	1.39302900	-3.20263300
H	3.00993400	2.95818900	-2.46509400
Mg	-0.46588900	0.72911600	2.46108100
Mg	-0.45324000	-1.19430200	-1.31912800
C	-1.35201800	-5.65973100	0.12890400
H	-1.73379400	-6.68366600	0.18234700
H	-1.11615100	-5.42382600	-0.91672300
O	-2.37412800	-4.81242600	0.63946700
P	-2.15127500	-3.19702700	0.70563700
O	-3.30520500	-2.59594800	1.43027500

O	-1.78484600	-2.68890700	-0.69395900
O	-0.75330600	-3.18534100	1.60466000
P	0.42962700	-2.06196000	1.70293300
O	0.09361100	-1.10959600	2.84736700
O	1.72099100	-2.92639100	2.04226400
O	0.61842400	-1.36952900	0.36059100
P	2.35019700	0.50783700	-1.81737200
O	3.61951600	-0.23274300	-1.39356200
O	1.19002700	-0.37301400	-2.33429400
O	1.89240300	1.61999800	-0.86562600
O	-1.52765600	-0.83586000	-3.12905100
H	-1.85596200	0.09210400	-3.22608800
H	-0.96364300	-0.99228100	-3.91239400
O	0.24973800	-3.12405200	-2.27513100
H	-0.64936500	-3.44821400	-2.06723700
H	0.31321500	-2.93242900	-3.23450400
O	0.43792000	2.08802300	1.25777200
H	0.80758300	1.83542500	0.36446600
H	0.13536400	3.02216800	1.20223900
H	2.03843300	4.71118700	7.51547200
H	3.59683600	3.94968000	7.87046300
H	-9.37953700	1.13811600	2.73454900
H	-11.13627000	1.32766200	2.92724700
H	3.59081100	7.73506300	-3.47497800
H	2.20157800	7.44809300	-2.41477600
H	4.77037300	-7.57208000	-0.47029800
H	5.73152800	-7.58612000	-1.95540400
H	1.99192900	-0.34298800	-7.40584300
H	0.35661900	-0.08661700	-6.75113500
H	9.87413200	-3.02156000	2.60018200
H	8.45325900	-3.76074600	1.84358500
H	-5.45032900	-0.80759100	-5.09616300
H	-0.98488800	6.02680700	-4.54559700
H	-0.36070700	5.37926800	-3.02182500
H	-2.69249900	6.85041400	0.24045300
H	-1.39453900	6.48200800	-0.91076800
H	-0.43899700	-5.57909000	0.72931300
H	-6.08858100	3.74321300	0.27406500
H	-5.50683800	3.12279900	-1.28171100
H	-3.76179900	-1.31125700	-5.28284100
H	3.72907100	1.07664500	-3.40942100