Supporting Information:
For the paper entitled "Aminoacylation Reaction in the Histidyl-tRNA Synthetase: Fidelity Mechanism of the Activation Step" by Sindrila Dutta Banik and Nilashis Nandi

A. The variations in the mutual distances between residues (Glu-83, Arg-113, Arg-259 and Tyr-264) and the reactant (amino acid (His) moiety and ATP) which change during the reaction is measured from the crystal structures of the oligomeric complex of histidyl-tRNA synthetase (HisRS) from *Escherichia Coli* complexed with ATP and histidinol (an inhibitor) and histidyl-adenylate (PDB ID: 1KMM and 1KMN)[21]. For Glu-83, the distance between nitrogen atom of α-amino group of His and δC of Glu-83 changed from 3.79Å to 3.92 Å and chiral center of His and δC of Glu-83 changed from 4.87Å to 5.36Å in the $Model_{Reactant}$ and $Model_{Product}$, respectively. For Arg-113, the distance between αP atom of ATP and ξC of Arg-113 and chiral center of His and ξC of Arg-113 changed from 4.83 Å to 4.22 Å and 7.68 Å to 6.57 Å in the $Model_{Reactant}$ and $Model_{Product}$ respectively. For Arg 259, the distance between carbon atom of α carboxylic acid group of His and ξC of Arg-259 and chiral center of His and ξC of Arg-259 vary from 5.45 Å to 4.44 Å and 5.30 Å to 4.50 Å in the $Model_{Reactant}$ and $Model_{Product}$, respectively. For Tyr-264, the distance between δN of His and ηO of Tyr-264 and chiral center of His and ηO of Tyr-264 changed from 2.98Å to 2.52Å and 3.18Å to 3.38 Å in the $Model_{Reactant}$ and $Model_{Product}$, respectively.

B. The details of the variations of the hydrogen bonding pattern in the reactant, transition state and product as calculated in the present work are as follows. The hydrogen atom attached to the η_1N and η_2N of the guadinium side chain of Arg 113 is at 1.98 Å and 1.85 Å separation with the oxygen atom of the α-phosphate group, respectively. The two hydrogen atoms attached to the η_1N of the guadinium side chain of Arg 113 are at 3.36 Å and 3.51 Å separation, respectively with the oxygen atom attached to the carboxylic acid group of His. The hydrogen atom attached to the η_1N and η_2N the guadinium side chain of Arg 259 is at 1.60 Å and at 1.81 Å separation with the oxygen atom of the α-phosphate group and

with the oxygen atom attached to the carboxylic acid group of His respectively. The hydrogen bonding pattern in the transition state is similar to that in the reactant state. The hydrogen atom attached to the η_1N and η_2N of the guadinium side chain of Arg 113 is at 1.91 Å and 1.83 Å separation with the oxygen atom of the α-phosphate group. The hydrogen atoms attached to the η_1N of the guadinium side chain of Arg 113 are at 3.24 Å and 3.81 Å separation, respectively with the oxygen atom attached to the carboxylic acid group of His. The hydrogen atom attached to the η_1N and η_2N of the guadinium side chain of Arg 259 is at 1.69 Å and 2.16 Å separation with the oxygen atom of the α-phosphate group and with the oxygen atom attached to the carboxylic acid group of His (the later atom is attached with the phosphorous of the α-phosphate group in the transition state). This is shown in Fig. 9(a-c) and is schematically shown in Fig. 12

Table II(a). The Cartesian coordinates of the atoms of the $Model_{Reactant}$ and $Model_{Product}$ used in the theoretical calculation.

$Model_{Reactant}$			
C	0.192287	-2.80769	5.837793
C	1.473287	-2.42569	6.395793
O	2.141287	-3.30869	6.923793
O	1.793287	-1.22969	6.342793
C	-6.26771	-4.38269	2.659793
N	-5.31571	-3.35269	3.063793
C	-5.56471	-2.04369	2.950793
N	-6.76071	-1.58969	2.553793
N	-4.63671	-1.18069	3.301793
H	-4.45271	-3.63269	3.434793
C	0.111287	-5.10569	-1.98521
C	0.376287	-4.07169	-0.88521
O	1.165287	-4.32769	0.033793
N	-0.24871	-2.88969	-0.99621
C	9.479287	-1.70169	2.721793
C	8.294287	-0.80169	2.827793
O	8.483287	0.426307	2.959793
O	7.172287	-1.33169	2.754793
C	-1.27371	7.111307	-0.20321
N	-1.32571	5.659307	-0.07021
C	-0.35771	4.909307	0.449793
N	0.752287	5.443307	0.887793
N	-0.48471	3.599307	0.529793
H	-2.12871	5.203307	-0.38621
C	2.932287	8.506307	5.332793
C	2.590287	7.264307	4.570793
C	3.571287	6.513307	3.963793
C	1.283287	6.787307	4.541793
C	3.280287	5.305307	3.344793
C	0.969287	5.568307	3.923793
C	1.975287	4.824307	3.318793
O	1.649287	3.630307	2.648793
H	2.129098	2.850644	2.825486
C	8.686287	2.683307	0.329793
C	7.409287	2.887307	-0.42621
O	6.835287	3.989307	-0.45821
N	6.986287	1.818307	-1.07221
C	5.743287	1.807307	-1.80221
C	5.404287	0.323307	-2.05221
O	6.238287	-0.56869	-1.81821
C	5.836287	2.627307	-3.10021
C	6.622287	1.952307	-4.18721
C	6.094287	0.865307	-4.87421
C	7.934287	2.295307	-4.41621

C	6.872287	0.131307	-5.74521
C	8.704287	1.553307	-5.29221
C	8.174287	0.475307	-5.94821
H	7.530287	1.000307	-1.05821
N	4.150287	0.068307	-2.40521
C	3.680287	-1.27269	-2.67421
C	2.488104	-1.59314	-1.75355
H	3.505287	0.815307	-2.49521
N	2.417287	-0.52069	3.251793
C	1.691287	0.451307	2.464793
C	0.476287	-0.27369	1.922793
O	0.60682	-1.40129	1.37961
N	4.346287	2.625307	1.846793
C	4.981287	0.554307	2.140793
C	5.559287	2.656307	2.368793
N	5.964287	1.411307	2.564793
C	2.552287	0.933307	1.301793
C	3.942287	1.311307	1.704793
H	3.298782	-0.13624	3.525949
H	6.797287	1.156307	2.952793
P	-7.04871	1.833307	-2.61121
O	-7.87971	3.098307	-2.45821
O	-7.63271	0.678307	-1.80021
O	-6.81171	1.508307	-4.10221
P	-5.18771	1.789307	-0.34721
O	-5.41771	2.986307	0.485793
O	-5.75071	0.481307	0.068793
O	-5.65371	2.135307	-1.84921
P	-2.57171	0.730307	0.351793
O	-1.35471	1.456307	0.765793
O	-3.41671	0.075307	1.389793
O	-3.58271	1.717307	-0.40421
O	-2.17071	-0.33769	-0.77021
C	-1.22371	-0.03869	-1.80321
C	-1.75471	-0.47669	-3.15021
O	-2.11471	-1.86869	-3.02921
C	-3.00471	0.183307	-3.65221
O	-2.68771	1.369307	-4.34521
C	-3.58571	-0.87869	-4.57421
O	-3.00271	-0.97469	-5.85521
C	-3.24971	-2.15669	-3.82621
N	-4.29471	-2.72169	-2.95221
C	-4.54171	-2.38369	-1.64321
N	-5.52071	-3.06569	-1.08721
C	-5.95971	-3.90669	-2.09821
C	-6.97771	-4.89269	-2.13921
N	-7.76171	-5.17169	-1.10521
N	-7.15871	-5.57369	-3.29321
C	-6.36271	-5.27869	-4.33421
N	-5.36371	-4.37169	-4.42121

C	-5.20771	-3.71269	-3.25921
H	0.284725	-3.75441	5.347808
H	-0.53098	-2.88152	6.62286
H	-0.12313	-2.06932	5.130529
H	10.29332	-1.28665	3.278565
H	9.231887	-2.66509	3.116216
H	9.762603	-1.79887	1.694569
H	3.864323	8.895894	4.980046
H	2.163247	9.236207	5.188837
H	3.013785	8.274721	6.374247
H	1.634334	5.079012	0.58899
H	0.719302	6.216068	1.521631
H	0.329128	3.019299	0.565213
H	-1.39487	3.185814	0.555045
H	-0.3879	7.389243	-0.73518
H	-2.1341	7.451259	-0.74086
H	-1.261	7.55828	0.76888
H	-5.8381	-5.34905	2.822574
H	-7.16259	-4.28809	3.238717
H	-6.50034	-4.26602	1.621925
H	-3.67028	-1.41869	3.204997
H	-4.89743	-0.28641	3.665515
H	-6.81723	-0.83811	1.896575
H	-7.5971	-2.00233	2.914622
H	0.284688	-2.04754	-1.07529
H	-1.24795	-2.85086	-0.99985
H	0.910118	-5.81727	-2.00576
H	-0.81087	-5.61037	-1.78564
H	0.049623	-4.61126	-2.93211
H	5.06998	0.594166	-4.72528
H	6.453294	-0.70744	-6.26081
H	8.781502	-0.09586	-6.619
H	9.725741	1.824651	-5.45925
H	8.360319	3.139085	-3.91477
H	4.845228	2.810562	-3.45954
H	6.298583	3.566341	-2.87795
H	9.447034	3.315751	-0.07786
H	8.533652	2.927686	1.360269
H	8.990343	1.660765	0.246981
H	4.980209	2.232706	-1.18443
H	3.371048	-1.34398	-3.69606
H	4.470126	-1.97091	-2.49105
H	2.76502	-1.41331	-0.73577
H	1.658963	-0.96866	-2.01326
H	2.211992	-2.6201	-1.87194
H	1.886776	-0.75274	4.067093
H	2.56834	-1.34525	2.706556
H	1.391377	1.277147	3.075483
H	6.120066	3.539037	2.595097
H	5.0252	-0.51474	2.15164

O	-0.81878	0.323406	2.0285
H	-0.98264	-0.374	-3.88387
H	-0.30686	-0.55197	-1.60114
H	-1.04177	1.015572	-1.82114
H	-2.04628	-0.96852	-5.77278
H	-1.73384	1.462796	-4.39983
H	-3.67412	0.385788	-2.84239
H	-4.64651	-0.76353	-4.65389
H	-7.35826	-5.41006	-0.2218
H	-5.86754	-2.99383	-0.15203
H	-2.97658	-2.90172	-4.54401
Mg	-6.39702	3.537599	-0.81975
Mg	-6.79905	0.221611	-1.37119
O	-6.98197	6.737111	0.202108
H	-6.04389	6.927188	0.128141
H	-7.4836	7.546252	0.078592
O	3.767648	-3.17277	2.950732
H	3.936601	-3.57547	3.805652
H	4.588437	-3.11415	2.456294
H	2.608202	0.153271	0.571507
H	2.081335	1.785387	0.857875
H	-0.03988	5.212709	3.918052
H	0.504235	7.360767	4.999092
H	4.580583	6.868542	3.969192
H	4.064414	4.740856	2.884966
H	-6.54587	-5.84374	-5.22419

$Model_{Product}$			
C	-0.55823	-2.59528	5.740926
C	0.787771	-2.16328	6.189926
O	1.098771	-0.98028	6.021926
O	1.547771	-2.99028	6.702926
C	-7.03623	-3.87128	2.757926
N	-5.74023	-3.23728	2.999926
C	-5.36823	-2.05828	2.489926
N	-6.17423	-1.35228	1.703926
N	-4.17023	-1.58628	2.769926
H	-5.10423	-3.70528	3.575926
C	-0.28423	-4.82928	-2.19007
C	-0.24523	-3.95628	-0.94007
O	0.562771	-4.17428	-0.03107
N	-1.10923	-2.94828	-0.89707
C	9.045771	-1.87128	2.333926
C	7.808771	-0.99528	2.451926

O	7.929771	0.208719	2.729926
O	6.686771	-1.49828	2.266926
C	-0.14423	7.220719	0.356926
N	-0.98423	6.168719	-0.17707
C	-1.09023	4.954719	0.345926
N	-0.39523	4.612719	1.411926
N	-1.90623	4.077719	-0.20607
H	-1.51023	6.366719	-0.98007
C	2.421771	8.901719	5.329926
C	2.235771	7.632719	4.554926
C	3.334771	6.965719	3.983926
C	0.970771	7.084719	4.403926
C	3.166771	5.786719	3.285926
C	0.791771	5.911719	3.717926
C	1.887771	5.266719	3.162926
O	1.660771	4.088719	2.511926
H	2.476771	3.798719	2.207926
C	8.456771	2.914719	-0.10407
C	7.101771	3.077719	-0.73307
O	6.520771	4.170719	-0.70507
N	6.591771	1.996719	-1.30907
C	5.278771	1.995719	-1.93307
C	4.913771	0.542719	-2.15907
O	5.768771	-0.33228	-2.03807
C	5.308771	2.716719	-3.28407
C	6.113771	2.004719	-4.32807
C	5.572771	0.953719	-5.04407
C	7.441771	2.324719	-4.53507
C	6.344771	0.223719	-5.94107
C	8.197771	1.599719	-5.42507
C	7.646771	0.547719	-6.12507
H	7.112771	1.162719	-1.30207
N	3.650771	0.289719	-2.48107
C	3.189771	-1.05728	-2.76507
C	2.218771	-0.92428	-3.91207
H	3.010771	1.034719	-2.54407
N	0.844771	0.069719	2.960926
C	0.424771	0.999719	1.869926
C	-0.99423	0.613719	1.296926
O	-1.04523	-0.62728	1.161926
O	-3.35323	0.133719	-0.72107
C	-2.31323	0.260719	-1.69907
C	-2.72723	-0.34728	-3.02707
O	-3.06823	-1.73328	-2.83107
C	-3.91323	0.240719	-3.76807
O	-3.47723	1.290719	-4.62607
C	-4.35823	-0.91928	-4.64307
O	-3.54723	-1.02728	-5.79707
C	-4.09123	-2.10728	-3.73007
N	-5.22123	-2.56628	-2.93707

C	-5.55923	-2.16528	-1.67207
N	-6.57423	-2.81428	-1.16607
C	-6.95223	-3.69128	-2.18107
C	-7.97023	-4.68128	-2.26707
N	-8.83023	-4.94728	-1.28307
N	-8.06123	-5.39428	-3.41407
C	-7.20023	-5.12928	-4.39407
N	-6.20223	-4.22828	-4.43607
C	-6.13323	-3.53528	-3.28307
O	-4.35623	0.538719	1.529926
O	-1.95823	1.520719	1.112926
O	-4.00723	2.371719	-0.18607
P	-3.49823	1.160719	0.501926
C	1.539771	0.977719	0.779926
C	2.939771	1.286719	1.277926
C	3.986771	0.441719	1.485926
N	3.387771	2.582719	1.453926
C	4.671771	2.495719	1.763926
N	5.087771	1.234719	1.796926
H	0.922771	-0.88128	2.550926
H	0.112771	0.076719	3.688926
H	1.744771	0.391719	3.336926
H	5.995771	0.926719	1.986926
H	0.366903	1.989079	2.273308
H	4.005254	5.285344	2.849499
H	4.315952	7.378562	4.092296
H	0.124477	7.583567	4.827998
H	-0.18814	5.495507	3.610917
H	1.565577	9.52955	5.197033
H	2.537615	8.671666	6.368461
H	3.29493	9.41005	4.977659
H	0.604259	4.622486	1.381483
H	-0.86729	4.34341	2.251351
H	-1.53516	3.291827	-0.70073
H	-2.89596	4.198699	-0.12993
H	0.774327	7.256261	-0.1907
H	-0.64905	8.159949	0.268018
H	0.062639	7.023181	1.387985
H	9.843894	-1.43966	2.901025
H	8.828036	-2.84859	2.711238
H	9.335965	-1.94211	1.306467
H	-0.51489	-3.61234	5.411351
H	-1.24891	-2.51295	6.553998
H	-0.8819	-1.9722	4.933517
H	5.298826	3.339375	1.96379
H	3.967137	-0.62622	1.422555
H	-1.43589	-0.23833	-1.34393
H	-2.09238	1.2978	-1.84256
H	-2.51763	1.312079	-4.64353
H	-2.62219	-1.00336	-5.54148

H	-4.68675	0.558365	-3.10049
H	-5.39558	-0.84498	-4.89462
H	-1.88124	-0.30518	-3.68085
H	-3.74057	-2.92315	-4.32698
H	-6.9846	-2.70663	-0.26053
H	-8.49074	-5.19274	-0.37506
H	-7.3195	-5.71974	-5.2784
H	-3.35498	-2.08434	2.474466
H	-4.07634	-0.73003	3.277874
H	-5.78896	-0.73563	1.017404
H	-7.16604	-1.43765	1.798963
H	-6.94693	-4.92881	2.894162
H	-7.75747	-3.48265	3.446168
H	-7.3522	-3.66611	1.756444
H	7.883295	3.139807	-4.00067
H	9.225847	1.854839	-5.57631
H	8.246511	-0.01166	-6.81232
H	5.911933	-0.59061	-6.48368
H	4.543108	0.69757	-4.90593
H	4.304438	2.819344	-3.63859
H	5.722655	3.692982	-3.14086
H	2.657873	-1.32912	-4.79988
H	1.320563	-1.45865	-3.68279
H	1.989218	0.109252	-4.06704
H	9.156133	3.561919	-0.59082
H	8.40061	3.166693	0.934316
H	8.778372	1.899483	-0.20785
H	0.580016	-5.45976	-2.21189
H	-1.16672	-5.43418	-2.17526
H	-0.29335	-4.20637	-3.06001
H	-0.77667	-2.00606	-0.85688
H	-2.09224	-3.13165	-0.9049
H	4.01407	-1.67763	-3.04898
H	2.696026	-1.46694	-1.90875
H	1.550514	0.006462	0.331099
H	1.286274	1.694198	0.026734
O	-7.36709	6.191348	2.289056
O	-9.99468	6.082864	-1.86503
O	-8.9138	4.117797	2.312702
O	-9.56893	3.717833	-1.22563
O	-6.78299	4.287933	0.937139
O	-8.87025	5.630885	0.322704
O	-7.61758	5.295001	-1.78735
P	-8.02406	5.058915	1.565556
P	-9.00825	5.136545	-1.20252
Mg	-7.03226	5.93144	-0.62874
Mg	-9.75769	3.378745	0.219786
O	-6.16976	5.355508	-3.05034
H	-5.54552	4.823796	-3.54955
H	-6.70557	5.873329	-3.65562

O	2.608917	-1.76102	2.929415
H	2.153796	-2.36226	2.335298
H	3.557614	-1.86379	2.824482
H	4.563426	2.457702	-1.28519

Table II(b). The Cartesian coordinates of the atoms of the $Model^{Opt}_{Reactant\ (L)}$, $Model^{Unopt}_{Reactant\ (D)}$ and $Model^{Opt}_{Reactant\ (D)}$ at HF/6-31G**:PM3 level of theory. The model structures are used in the Fig. 3(a), 3(b) as well as Fig. 4(a), 4(b).

$Model^{Opt}_{Reactant\ (L)}$			
C	-6.79712	-2.55568	-0.68297
C	-6.00891	-1.26586	-0.72177
O	-4.71795	-1.29362	-0.75307
O	-6.55723	-0.1483	-0.71702
C	-5.55588	3.315376	-1.66551
N	-5.14245	2.226823	-0.76248
C	-3.8294	2.079394	-0.34663
N	-2.93063	3.174531	-0.35425
N	-3.49217	0.935878	0.319749
H	-5.71229	1.371258	-0.81685
C	0.774188	2.267357	-1.72358
C	-0.11955	2.427516	-2.9199
O	-1.09491	3.184294	-2.94612
N	0.212376	1.737107	-4.10268
C	-6.80493	2.826453	-5.2705
C	-6.21554	1.493616	-5.70127
O	-6.79501	0.773723	-6.558
O	-5.12801	1.081867	-5.20089
C	-0.32827	-5.43313	-0.37933
N	-1.31012	-4.62068	0.363567
C	-2.54242	-4.29132	-0.22586
N	-3.1523	-5.16184	-1.12797
N	-3.2514	-3.26157	0.332015
H	-0.89685	-3.84394	0.89149
C	-10.1971	-7.09937	-2.27086
C	-8.85437	-6.50748	-2.50202
C	-8.6833	-5.50687	-3.46012
C	-7.75148	-6.95607	-1.77356
C	-7.4317	-4.95591	-3.69682
C	-6.4913	-6.41901	-1.99377
C	-6.32859	-5.41367	-2.95966
O	-5.06645	-4.92263	-3.12119
H	-5.04167	-4.31528	-3.88826
N	-3.50869	-0.80215	-3.20789
C	-2.65843	-2.06031	-3.3244
C	-1.29886	-1.82607	-2.67243
O	-0.96247	-0.64811	-2.52586
C	-5.88424	-2.59845	-5.80496

C	-3.78692	-2.36498	-5.52682
H	-6.14205	-0.8104	-6.89641
H	-3.91501	-0.77918	-2.26448
C	-2.48872	-2.47316	-4.80246
N	-4.88061	-3.12057	-5.16242
N	-5.52506	-1.56098	-6.57388
C	-4.17445	-1.41187	-6.40576
C	4.731448	-0.95331	-0.61964
C	8.565424	1.292007	-1.31081
C	4.714111	-2.45571	-0.2008
C	3.271897	-2.64144	0.279205
C	6.720503	0.57674	-0.11383
C	2.528889	-1.61784	-0.57601
C	7.085538	1.385778	1.008503
C	1.137147	-1.24192	-0.15251
C	8.27369	2.177283	0.902823
C	5.21256	0.328625	1.570732
N	8.984244	2.086927	-0.30829
N	7.435998	0.505685	-1.26876
N	8.718213	2.974758	1.882641
N	6.135851	1.203616	2.015146
N	5.534841	-0.1042	0.261944
O	-1.09512	-2.19976	1.608948
O	-1.42161	-0.015	5.238651
O	2.127913	0.893013	7.510451
O	4.885808	-3.29478	-1.32115
O	-1.05943	0.377099	1.548201
O	0.522807	1.587416	4.238906
O	3.173606	0.199385	5.387387
O	2.811747	-3.94723	0.178052
O	-0.03716	-0.87851	3.480957
O	0.809288	-0.53559	5.731453
O	2.5297	-1.78064	7.272132
O	3.407499	-0.5024	-0.55938
O	1.067738	-0.97292	1.242229
P	-0.41928	-0.90965	1.828095
P	-0.08275	0.269927	4.573068
P	2.444559	-0.38082	6.712109
H	-7.87915	-2.37587	-0.70477
H	-6.5704	-3.12038	0.230259
H	-6.44323	3.796406	-1.23334
H	-4.77731	4.083334	-1.80229
H	-3.13709	3.835312	-1.07778
H	-1.96876	2.908829	-0.34845
H	-2.54523	0.807741	0.665585
H	-4.02446	0.088806	0.120691
H	0.739266	1.225404	-1.35281
H	1.818584	2.501211	-1.96767
H	0.69279	0.876784	-3.94576
H	-0.52918	1.645946	-4.76285

H	-7.90071	2.814621	-5.29651
H	-6.49311	3.090082	-4.24602
H	0.242858	-6.01684	0.353896
H	0.373415	-4.80446	-0.95155
H	-2.51317	-5.74664	-1.62505
H	-3.91922	-4.8204	-1.69161
H	-2.70965	-2.639	0.927091
H	-4.01063	-2.80917	-0.18236
H	-10.3089	-7.47044	-1.24349
H	-10.3657	-7.94771	-2.94836
H	-9.54761	-5.14987	-4.0318
H	-7.88146	-7.74121	-1.02046
H	-7.31873	-4.16843	-4.46093
H	-5.63108	-6.78083	-1.42054
H	-2.10224	-3.4819	-4.79639
H	-1.74041	-1.83606	-5.2748
H	-3.64216	-0.59605	-6.85074
H	-6.90063	-2.93763	-5.71149
H	-3.21921	-2.8232	-2.80922
H	-2.89324	0.018025	-3.27332
H	-4.23783	-0.78331	-3.90467
O	-0.69025	-2.86555	-2.4138
H	5.122369	-0.87337	-1.64841
H	9.164831	1.265808	-2.23137
H	3.192115	-2.3435	1.313778
H	2.439613	-1.98824	-1.60185
H	0.484618	-2.06629	-0.40287
H	0.812713	-0.36872	-0.71333
H	4.333621	-0.00312	2.137346
H	9.547555	3.480541	1.708169
H	3.092711	-4.29936	-0.65195
H	5.44739	-2.70577	0.564022
H	5.783229	-3.28636	-1.60667
H	-6.46474	3.626923	-5.93825
H	-6.54808	-3.19761	-1.5408
H	-10.999	-6.37067	-2.44886
H	-0.80932	-6.13359	-1.08043
H	-5.82397	2.930173	-2.66977
H	0.46956	2.921747	-0.89598
Mg	-0.70052	-1.65285	5.747861
Mg	2.011679	1.596758	5.296391
O	0.000848	-2.71618	7.106725
H	-0.12188	-3.65957	7.086675
H	0.955138	-2.5062	7.32318
O	-3.35449	1.800792	-3.40623
H	-2.63488	2.416029	-3.5622
H	-4.01058	1.856435	-4.12179
C	-2.07738	-3.97077	-11.0105
C	-0.81087	-4.08876	-10.2048
O	-0.58805	-4.98752	-9.40718

N	0.20921	-3.12135	-10.4715
C	1.288747	-2.89198	-9.47997
C	0.814194	-2.03145	-8.29717
O	-0.11712	-1.24244	-8.36457
C	2.515576	-2.26242	-10.1626
C	2.249706	-0.97708	-10.8796
C	2.374788	0.242714	-10.212
C	1.910647	-0.98498	-12.2344
C	2.151163	1.436732	-10.8881
C	1.688792	0.211112	-12.9073
C	1.80692	1.423015	-12.2355
H	-0.13335	-2.26813	-10.864
N	1.563066	-2.12737	-7.09196
C	1.007693	-1.53332	-5.84895
H	1.974966	-3.02501	-6.94865
H	-1.86743	-3.86727	-12.0835
H	-2.72017	-4.85164	-10.8814
H	-2.65562	-3.09141	-10.6945
H	-0.04966	-1.8575	-5.67777
H	0.967438	-0.43559	-6.00239
C	1.86672	-1.87527	-4.64955
H	1.940936	-2.95961	-4.48474
H	2.888722	-1.48437	-4.74081
H	1.426999	-1.44679	-3.73474
H	3.300929	-2.10149	-9.39589
H	2.941663	-2.99561	-10.8783
H	1.595341	-3.90071	-9.09871
H	2.641129	0.258978	-9.1487
H	2.242149	2.389083	-10.3556
H	1.628138	2.363891	-12.7657
H	1.420362	0.19737	-13.9686
H	1.82296	-1.93693	-12.7709

	$Model^{Unopt}_{Reactant\ (D)}$		
C	-6.79712	-2.55568	-0.68297
C	-6.00891	-1.26586	-0.72177
O	-4.71795	-1.29362	-0.75307
O	-6.55723	-0.1483	-0.71702
C	-5.55588	3.315376	-1.66551
N	-5.14245	2.226823	-0.76248
C	-3.8294	2.079394	-0.34663
N	-2.93063	3.174531	-0.35425
N	-3.49217	0.935878	0.319749
H	-5.71229	1.371258	-0.81685
C	0.774188	2.267357	-1.72358
C	-0.11955	2.427516	-2.9199
O	-1.09491	3.184294	-2.94612
N	0.212376	1.737107	-4.10268

C	-6.80493	2.826453	-5.2705
C	-6.21554	1.493616	-5.70127
O	-6.79501	0.773723	-6.558
O	-5.12801	1.081867	-5.20089
C	-0.32827	-5.43313	-0.37933
N	-1.31012	-4.62068	0.363567
C	-2.54242	-4.29132	-0.22586
N	-3.1523	-5.16184	-1.12797
N	-3.2514	-3.26157	0.332015
H	-0.89685	-3.84394	0.89149
C	-10.1971	-7.09937	-2.27086
C	-8.85437	-6.50748	-2.50202
C	-8.6833	-5.50687	-3.46012
C	-7.75148	-6.95607	-1.77356
C	-7.4317	-4.95591	-3.69682
C	-6.4913	-6.41901	-1.99377
C	-6.32859	-5.41367	-2.95966
O	-5.06645	-4.92263	-3.12119
H	-5.04167	-4.31528	-3.88826
N	-3.4543	-3.10827	-2.55767
C	-2.65843	-2.06031	-3.3244
C	-1.29886	-1.82607	-2.67243
O	-0.96247	-0.64811	-2.52586
C	-5.88424	-2.59845	-5.80496
C	-3.78692	-2.36498	-5.52682
H	-6.14205	-0.8104	-6.89641
H	-4.46319	-3.01283	-2.72698
C	-2.48872	-2.47316	-4.80246
N	-4.88061	-3.12057	-5.16242
N	-5.52506	-1.56098	-6.57388
C	-4.17445	-1.41187	-6.40576
C	4.731448	-0.95331	-0.61964
C	8.565424	1.292007	-1.31081
C	4.714111	-2.45571	-0.2008
C	3.271897	-2.64144	0.279205
C	6.720503	0.57674	-0.11383
C	2.528889	-1.61784	-0.57601
C	7.085538	1.385778	1.008503
C	1.137147	-1.24192	-0.15251
C	8.27369	2.177283	0.902823
C	5.21256	0.328625	1.570732
N	8.984244	2.086927	-0.30829
N	7.435998	0.505685	-1.26876
N	8.718213	2.974758	1.882641
N	6.135851	1.203616	2.015146
N	5.534841	-0.1042	0.261944
O	-1.09512	-2.19976	1.608948
O	-1.42161	-0.015	5.238651
O	2.127913	0.893013	7.510451
O	4.885808	-3.29478	-1.32115

O	-1.05943	0.377099	1.548201
O	0.522807	1.587416	4.238906
O	3.173606	0.199385	5.387387
O	2.811747	-3.94723	0.178052
O	-0.03716	-0.87851	3.480957
O	0.809288	-0.53559	5.731453
O	2.5297	-1.78064	7.272132
O	3.407499	-0.5024	-0.55938
O	1.067738	-0.97292	1.242229
P	-0.41928	-0.90965	1.828095
P	-0.08275	0.269927	4.573068
P	2.444559	-0.38082	6.712109
H	-7.87915	-2.37587	-0.70477
H	-6.5704	-3.12038	0.230259
H	-6.44323	3.796406	-1.23334
H	-4.77731	4.083334	-1.80229
H	-3.13709	3.835312	-1.07778
H	-1.96876	2.908829	-0.34845
H	-2.54523	0.807741	0.665585
H	-4.02446	0.088806	0.120691
H	0.739266	1.225404	-1.35281
H	1.818584	2.501211	-1.96767
H	0.69279	0.876784	-3.94576
H	-0.52918	1.645946	-4.76285
H	-7.90071	2.814621	-5.29651
H	-6.49311	3.090082	-4.24602
H	0.242858	-6.01684	0.353896
H	0.373415	-4.80446	-0.95155
H	-2.51317	-5.74664	-1.62505
H	-3.91922	-4.8204	-1.69161
H	-2.70965	-2.639	0.927091
H	-4.01063	-2.80917	-0.18236
H	-10.3089	-7.47044	-1.24349
H	-10.3657	-7.94771	-2.94836
H	-9.54761	-5.14987	-4.0318
H	-7.88146	-7.74121	-1.02046
H	-7.31873	-4.16843	-4.46093
H	-5.63108	-6.78083	-1.42054
H	-2.10224	-3.4819	-4.79639
H	-1.74041	-1.83606	-5.2748
H	-3.64216	-0.59605	-6.85074
H	-6.90063	-2.93763	-5.71149
H	-3.26933	-1.17371	-3.27311
H	-3.13058	-4.0408	-2.84283
H	-3.25115	-2.99771	-1.57582
O	-0.69025	-2.86555	-2.4138
H	5.122369	-0.87337	-1.64841
H	9.164831	1.265808	-2.23137
H	3.192115	-2.3435	1.313778
H	2.439613	-1.98824	-1.60185

H	0.484618	-2.06629	-0.40287
H	0.812713	-0.36872	-0.71333
H	4.333621	-0.00312	2.137346
H	9.547555	3.480541	1.708169
H	3.092711	-4.29936	-0.65195
H	5.44739	-2.70577	0.564022
H	5.783229	-3.28636	-1.60667
H	-6.46474	3.626923	-5.93825
H	-6.54808	-3.19761	-1.5408
H	-10.999	-6.37067	-2.44886
H	-0.80932	-6.13359	-1.08043
H	-5.82397	2.930173	-2.66977
H	0.46956	2.921747	-0.89598
Mg	-0.70052	-1.65285	5.747861
Mg	2.011679	1.596758	5.296391
O	0.000848	-2.71618	7.106725
H	-0.12188	-3.65957	7.086675
H	0.955138	-2.5062	7.32318
O	-3.35449	1.800792	-3.40623
H	-2.63488	2.416029	-3.5622
H	-4.01058	1.856435	-4.12179
C	-2.07738	-3.97077	-11.0105
C	-0.81087	-4.08876	-10.2048
O	-0.58805	-4.98752	-9.40718
N	0.20921	-3.12135	-10.4715
C	1.288747	-2.89198	-9.47997
C	0.814194	-2.03145	-8.29717
O	-0.11712	-1.24244	-8.36457
C	2.515576	-2.26242	-10.1626
C	2.249706	-0.97708	-10.8796
C	2.374788	0.242714	-10.212
C	1.910647	-0.98498	-12.2344
C	2.151163	1.436732	-10.8881
C	1.688792	0.211112	-12.9073
C	1.80692	1.423015	-12.2355
H	-0.13335	-2.26813	-10.864
N	1.563066	-2.12737	-7.09196
C	1.007693	-1.53332	-5.84895
H	1.974966	-3.02501	-6.94865
H	-1.86743	-3.86727	-12.0835
H	-2.72017	-4.85164	-10.8814
H	-2.65562	-3.09141	-10.6945
H	-0.04966	-1.8575	-5.67777
H	0.967438	-0.43559	-6.00239
C	1.86672	-1.87527	-4.64955
H	1.940936	-2.95961	-4.48474
H	2.888722	-1.48437	-4.74081
H	1.426999	-1.44679	-3.73474
H	3.300929	-2.10149	-9.39589
H	2.941663	-2.99561	-10.8783

H	1.595341	-3.90071	-9.09871
H	2.641129	0.258978	-9.1487
H	2.242149	2.389083	-10.3556
H	1.628138	2.363891	-12.7657
H	1.420362	0.19737	-13.9686
H	1.82296	-1.93693	-12.7709

$Model^{Opt}_{Reactant\ (D)}$			
C	-6.98224	-2.07812	-1.04071
C	-6.05906	-0.89265	-0.84183
O	-4.78719	-1.05083	-0.8473
O	-6.50078	0.262341	-0.65543
C	-5.37881	3.066717	-2.82229
N	-4.98879	2.370869	-1.58585
C	-3.67691	2.281979	-1.17295
N	-2.65422	3.060023	-1.75949
N	-3.42767	1.641469	0.022026
H	-5.62415	1.621696	-1.27104
C	1.15997	1.335942	-2.41208
C	0.360481	1.163439	-3.67296
O	-0.5505	1.927816	-4.00543
N	0.717845	0.134282	-4.55872
C	-5.66935	2.137564	-6.42932
C	-5.4441	0.634153	-6.43923
O	-5.68858	-0.05224	-7.47042
O	-5.00619	0.047838	-5.40831
C	-1.11182	-5.11797	1.310098
N	-1.98488	-4.01914	1.766037
C	-3.10097	-3.66048	0.990949
N	-3.78922	-4.61427	0.227459
N	-3.66313	-2.43525	1.211411
H	-1.47406	-3.20232	2.118197
C	-9.13624	-9.02153	-2.64133
C	-8.01824	-8.04786	-2.73502
C	-7.80887	-7.32904	-3.91315
C	-7.16115	-7.85371	-1.65023
C	-6.75888	-6.42795	-4.01776
C	-6.10513	-6.95828	-1.73358
C	-5.90044	-6.24135	-2.92336
O	-4.85214	-5.37648	-2.93702
H	-4.7745	-4.96601	-3.81921
N	-4.00861	-1.84901	-2.74148
C	-2.59435	-2.06466	-3.25273
C	-1.66734	-2.40795	-2.09623
O	-0.47192	-2.30863	-2.36058
C	-5.79749	-3.21884	-5.85119
C	-3.7631	-3.06231	-5.23641
H	-5.73222	-1.5744	-7.17335
H	-4.61875	-1.51134	-3.46782
C	-2.60799	-3.19798	-4.29995

N	-4.9555	-3.71258	-4.98917
N	-5.23891	-2.29939	-6.64615
C	-3.93008	-2.19528	-6.26102
C	4.475295	-1.80541	-0.15272
C	8.61413	-0.65587	-1.47942
C	4.244998	-3.07593	0.724831
C	2.791675	-2.89816	1.178976
C	6.724118	-0.58328	-0.14852
C	2.206969	-2.07802	0.031512
C	7.280216	0.464077	0.652337
C	0.894111	-1.38829	0.273042
C	8.586961	0.941315	0.31421
C	5.273179	0.016177	1.496465
N	9.214939	0.329819	-0.7864
N	7.363396	-1.15968	-1.20241
N	9.212326	1.917143	0.985181
N	6.35957	0.800015	1.645709
N	5.451076	-0.86809	0.406301
O	-1.39695	-1.3963	2.290222
O	-1.30529	2.056641	4.779134
O	2.417111	3.266533	6.584654
O	4.293155	-4.24869	-0.05601
O	-1.04	0.925288	1.229583
O	0.798569	2.861201	3.271739
O	3.278639	1.66947	4.914683
O	2.140903	-4.0964	1.444556
O	-0.11919	0.398515	3.51835
O	0.851589	1.460954	5.474954
O	2.444693	0.680556	7.407719
O	3.245225	-1.1445	-0.23445
O	0.889816	-0.69102	1.511782
P	-0.55732	-0.22205	2.00301
P	0.034373	1.872931	4.080281
P	2.529867	1.752711	6.348054
H	-7.50413	-1.9967	-2.00264
H	-7.74677	-2.12127	-0.25558
H	-6.47657	3.095595	-2.85563
H	-5.01489	4.10354	-2.83132
H	-2.78416	3.218316	-2.73701
H	-1.73244	2.736443	-1.55512
H	-2.47143	1.438684	0.301128
H	-4.10262	0.968587	0.317761
H	1.068949	0.447104	-1.76213
H	2.22574	1.479983	-2.63234
H	1.135291	-0.66218	-4.12981
H	0.043482	-0.0981	-5.25614
H	-6.71931	2.376347	-6.63477
H	-5.40782	2.578295	-5.45184
H	-0.61792	-5.54161	2.193665
H	-0.33718	-4.76421	0.610219

H	-3.2221	-5.3847	-0.06273
H	-4.35661	-4.24652	-0.50652
H	-3.05603	-1.761	1.669264
H	-4.29122	-2.04939	0.506344
H	-9.50339	-9.12372	-1.61153
H	-8.81024	-10.0161	-2.9756
H	-8.48179	-7.47661	-4.7654
H	-7.3246	-8.41419	-0.72312
H	-6.60623	-5.86866	-4.94945
H	-5.43518	-6.81206	-0.87954
H	-2.67429	-4.15133	-3.78927
H	-1.65354	-3.16088	-4.8156
H	-3.271	-1.47631	-6.70161
H	-6.83341	-3.48393	-5.92122
H	-2.31251	-1.12778	-3.71875
H	-4.35324	-2.72893	-2.38656
H	-4.01648	-1.22653	-1.92553
O	-2.23379	-2.77424	-1.05903
H	4.813161	-2.12356	-1.15416
H	9.15761	-1.09264	-2.32868
H	2.762301	-2.301	2.077577
H	2.055744	-2.70796	-0.8461
H	0.112821	-2.13697	0.265058
H	0.711733	-0.68667	-0.53784
H	4.376134	0.057349	2.126474
H	10.11162	2.173485	0.669499
H	2.385447	-4.72044	0.77916
H	4.937275	-3.16142	1.56079
H	5.177761	-4.43599	-0.31936
H	-5.06047	2.631848	-7.1952
H	-6.43911	-3.03292	-1.03575
H	-9.98776	-8.72572	-3.26838
H	-1.68152	-5.91894	0.81284
H	-5.03262	2.562556	-3.74854
H	0.818569	2.203567	-1.83138
Mg	-0.79403	0.658943	5.896262
Mg	2.313878	3.070784	4.269687
O	-0.19175	0.115751	7.572843
H	-0.44169	-0.73508	7.917918
H	0.789659	0.257882	7.70804
O	-3.01342	0.898712	-3.81973
H	-2.22631	1.233229	-4.25464
H	-3.70309	0.723526	-4.47879
C	-3.73465	-0.70153	-10.3166
C	-2.48569	-1.53638	-10.3593
O	-2.47474	-2.75592	-10.4526
N	-1.23805	-0.83338	-10.3613
C	0.016541	-1.54548	-10.0171
C	0.182374	-1.73368	-8.50066
O	-0.33425	-1.00481	-7.66486

C	1.229792	-0.81146	-10.6151
C	1.374787	0.616956	-10.1965
C	2.13285	0.949626	-9.07231
C	0.783133	1.633783	-10.9492
C	2.285777	2.280285	-8.69997
C	0.938996	2.963307	-10.5741
C	1.688632	3.288528	-9.44884
H	-1.2829	0.079712	-9.95677
N	1.045179	-2.77773	-8.06919
C	1.047475	-3.16867	-6.63577
H	1.075483	-3.55674	-8.69214
H	-3.63154	0.238806	-10.8743
H	-4.59332	-1.24252	-10.7363
H	-3.99243	-0.44563	-9.27517
H	0.008441	-3.31001	-6.24893
H	1.468324	-2.31608	-6.06361
C	1.868786	-4.42087	-6.4117
H	1.456207	-5.29065	-6.94195
H	2.910821	-4.30147	-6.73745
H	1.887986	-4.67225	-5.34283
H	2.148707	-1.37073	-10.3444
H	1.16524	-0.85959	-11.7219
H	-0.0408	-2.55332	-10.5053
H	2.601444	0.158619	-8.47538
H	2.872843	2.532643	-7.81102
H	1.806158	4.335483	-9.15183
H	0.468338	3.754859	-11.1661
H	0.195456	1.383649	-11.8403

Table II(c). The Cartesian coordinates of the atoms of the $Model_{Reactant\ (L)}$ and $Model_{Reactant\ (D)}$ used in the theoretical calculation. The model structures are used in the Fig. 5(a), 5(b); Fig. 6(a), 6(b), Fig. 7(a), 7(b) as well as Fig. 8(a), 8(b).

$Model_{Reactant\ (L)}$			
C	0.192287	-2.80769	5.837793
C	1.473287	-2.42569	6.395793
O	2.141287	-3.30869	6.923793
O	1.793287	-1.22969	6.342793
C	-6.26771	-4.38269	2.659793
N	-5.31571	-3.35269	3.063793
C	-5.56471	-2.04369	2.950793
N	-6.76071	-1.58969	2.553793
N	-4.63671	-1.18069	3.301793
H	-4.45271	-3.63269	3.434793
C	0.111287	-5.10569	-1.98521
C	0.376287	-4.07169	-0.88521
O	1.165287	-4.32769	0.033793
N	-0.24871	-2.88969	-0.99621
C	9.479287	-1.70169	2.721793

C	8.294287	-0.80169	2.827793
O	8.483287	0.426307	2.959793
O	7.172287	-1.33169	2.754793
C	-1.27371	7.111307	-0.20321
N	-1.32571	5.659307	-0.07021
C	-0.35771	4.909307	0.449793
N	0.752287	5.443307	0.887793
N	-0.48471	3.599307	0.529793
H	-2.12871	5.203307	-0.38621
C	2.932287	8.506307	5.332793
C	2.590287	7.264307	4.570793
C	3.571287	6.513307	3.963793
C	1.283287	6.787307	4.541793
C	3.280287	5.305307	3.344793
C	0.969287	5.568307	3.923793
C	1.975287	4.824307	3.318793
O	1.649287	3.630307	2.648793
H	2.129098	2.850644	2.825486
C	8.686287	2.683307	0.329793
C	7.409287	2.887307	-0.42621
O	6.835287	3.989307	-0.45821
N	6.986287	1.818307	-1.07221
C	5.743287	1.807307	-1.80221
C	5.404287	0.323307	-2.05221
O	6.238287	-0.56869	-1.81821
C	5.836287	2.627307	-3.10021
C	6.622287	1.952307	-4.18721
C	6.094287	0.865307	-4.87421
C	7.934287	2.295307	-4.41621
C	6.872287	0.131307	-5.74521
C	8.704287	1.553307	-5.29221
C	8.174287	0.475307	-5.94821
H	7.530287	1.000307	-1.05821
N	4.150287	0.068307	-2.40521
C	3.680287	-1.27269	-2.67421
C	2.488104	-1.59314	-1.75355
H	3.505287	0.815307	-2.49521
N	2.417287	-0.52069	3.251793
C	1.691287	0.451307	2.464793
C	0.476287	-0.27369	1.922793
O	0.60682	-1.40129	1.37961
N	4.346287	2.625307	1.846793
C	4.981287	0.554307	2.140793
C	5.559287	2.656307	2.368793
N	5.964287	1.411307	2.564793
C	2.552287	0.933307	1.301793
C	3.942287	1.311307	1.704793
H	3.298782	-0.13624	3.525949
H	6.797287	1.156307	2.952793
P	-7.04871	1.833307	-2.61121

O	-7.87971	3.098307	-2.45821
O	-7.63271	0.678307	-1.80021
O	-6.81171	1.508307	-4.10221
P	-5.18771	1.789307	-0.34721
O	-5.41771	2.986307	0.485793
O	-5.75071	0.481307	0.068793
O	-5.65371	2.135307	-1.84921
P	-2.57171	0.730307	0.351793
O	-1.35471	1.456307	0.765793
O	-3.41671	0.075307	1.389793
O	-3.58271	1.717307	-0.40421
O	-2.17071	-0.33769	-0.77021
C	-1.22371	-0.03869	-1.80321
C	-1.75471	-0.47669	-3.15021
O	-2.11471	-1.86869	-3.02921
C	-3.00471	0.183307	-3.65221
O	-2.68771	1.369307	-4.34521
C	-3.58571	-0.87869	-4.57421
O	-3.00271	-0.97469	-5.85521
C	-3.24971	-2.15669	-3.82621
N	-4.29471	-2.72169	-2.95221
C	-4.54171	-2.38369	-1.64321
N	-5.52071	-3.06569	-1.08721
C	-5.95971	-3.90669	-2.09821
C	-6.97771	-4.89269	-2.13921
N	-7.76171	-5.17169	-1.10521
N	-7.15871	-5.57369	-3.29321
C	-6.36271	-5.27869	-4.33421
N	-5.36371	-4.37169	-4.42121
C	-5.20771	-3.71269	-3.25921
H	0.284725	-3.75441	5.347808
H	-0.53098	-2.88152	6.62286
H	-0.12313	-2.06932	5.130529
H	10.29332	-1.28665	3.278565
H	9.231887	-2.66509	3.116216
H	9.762603	-1.79887	1.694569
H	3.864323	8.895894	4.980046
H	2.163247	9.236207	5.188837
H	3.013785	8.274721	6.374247
H	1.634334	5.079012	0.58899
H	0.719302	6.216068	1.521631
H	0.329128	3.019299	0.565213
H	-1.39487	3.185814	0.555045
H	-0.3879	7.389243	-0.73518
H	-2.1341	7.451259	-0.74086
H	-1.261	7.55828	0.76888
H	-5.8381	-5.34905	2.822574
H	-7.16259	-4.28809	3.238717
H	-6.50034	-4.26602	1.621925
H	-3.67028	-1.41869	3.204997

H	-4.89743	-0.28641	3.665515
H	-6.81723	-0.83811	1.896575
H	-7.5971	-2.00233	2.914622
H	0.284688	-2.04754	-1.07529
H	-1.24795	-2.85086	-0.99985
H	0.910118	-5.81727	-2.00576
H	-0.81087	-5.61037	-1.78564
H	0.049623	-4.61126	-2.93211
H	5.06998	0.594166	-4.72528
H	6.453294	-0.70744	-6.26081
H	8.781502	-0.09586	-6.619
H	9.725741	1.824651	-5.45925
H	8.360319	3.139085	-3.91477
H	4.845228	2.810562	-3.45954
H	6.298583	3.566341	-2.87795
H	9.447034	3.315751	-0.07786
H	8.533652	2.927686	1.360269
H	8.990343	1.660765	0.246981
H	4.980209	2.232706	-1.18443
H	3.371048	-1.34398	-3.69606
H	4.470126	-1.97091	-2.49105
H	2.76502	-1.41331	-0.73577
H	1.658963	-0.96866	-2.01326
H	2.211992	-2.6201	-1.87194
H	1.886776	-0.75274	4.067093
H	2.56834	-1.34525	2.706556
H	1.391377	1.277147	3.075483
H	6.120066	3.539037	2.595097
H	5.0252	-0.51474	2.15164
O	-0.81878	0.323406	2.0285
H	-0.98264	-0.374	-3.88387
H	-0.30686	-0.55197	-1.60114
H	-1.04177	1.015572	-1.82114
H	-2.04628	-0.96852	-5.77278
H	-1.73384	1.462796	-4.39983
H	-3.67412	0.385788	-2.84239
H	-4.64651	-0.76353	-4.65389
H	-7.35826	-5.41006	-0.2218
H	-5.86754	-2.99383	-0.15203
H	-2.97658	-2.90172	-4.54401
Mg	-6.39702	3.537599	-0.81975
Mg	-6.79905	0.221611	-1.37119
O	-6.98197	6.737111	0.202108
H	-6.04389	6.927188	0.128141
H	-7.4836	7.546252	0.078592
O	3.767648	-3.17277	2.950732
H	3.936601	-3.57547	3.805652
H	4.588437	-3.11415	2.456294
H	2.608202	0.153271	0.571507
H	2.081335	1.785387	0.857875

H	-0.03988	5.212709	3.918052
H	0.504235	7.360767	4.999092
H	4.580583	6.868542	3.969192
H	4.064414	4.740856	2.884966
H	-6.54587	-5.84374	-5.22419

$Model_{Reactant\ (D)}$			
C	0.192287	-2.80769	5.837793
C	1.473287	-2.42569	6.395793
O	2.141287	-3.30869	6.923793
O	1.793287	-1.22969	6.342793
C	-6.26771	-4.38269	2.659793
N	-5.31571	-3.35269	3.063793
C	-5.56471	-2.04369	2.950793
N	-6.76071	-1.58969	2.553793
N	-4.63671	-1.18069	3.301793
H	-4.45271	-3.63269	3.434793
C	0.111287	-5.10569	-1.98521
C	0.376287	-4.07169	-0.88521
O	1.165287	-4.32769	0.033793
N	-0.24871	-2.88969	-0.99621
C	9.479287	-1.70169	2.721793
C	8.294287	-0.80169	2.827793
O	8.483287	0.426307	2.959793
O	7.172287	-1.33169	2.754793
C	-1.27371	7.111307	-0.20321
N	-1.32571	5.659307	-0.07021
C	-0.35771	4.909307	0.449793
N	0.752287	5.443307	0.887793
N	-0.48471	3.599307	0.529793
H	-2.12871	5.203307	-0.38621
C	2.932287	8.506307	5.332793
C	2.590287	7.264307	4.570793
C	3.571287	6.513307	3.963793
C	1.283287	6.787307	4.541793
C	3.280287	5.305307	3.344793
C	0.969287	5.568307	3.923793
C	1.975287	4.824307	3.318793
O	1.649287	3.630307	2.648793
H	2.129098	2.850644	2.825486
C	8.686287	2.683307	0.329793
C	7.409287	2.887307	-0.42621
O	6.835287	3.989307	-0.45821
N	6.986287	1.818307	-1.07221
C	5.743287	1.807307	-1.80221
C	5.404287	0.323307	-2.05221
O	6.238287	-0.56869	-1.81821
C	5.836287	2.627307	-3.10021
C	6.622287	1.952307	-4.18721

C	6.094287	0.865307	-4.87421
C	7.934287	2.295307	-4.41621
C	6.872287	0.131307	-5.74521
C	8.704287	1.553307	-5.29221
C	8.174287	0.475307	-5.94821
H	7.530287	1.000307	-1.05821
N	4.150287	0.068307	-2.40521
C	3.680287	-1.27269	-2.67421
C	2.488104	-1.59314	-1.75355
H	3.505287	0.815307	-2.49521
N	1.578361	1.213006	3.68884
C	1.691287	0.451307	2.464793
C	0.476287	-0.27369	1.922793
O	0.60682	-1.40129	1.37961
N	4.346287	2.625307	1.846793
C	4.981287	0.554307	2.140793
C	5.559287	2.656307	2.368793
N	5.964287	1.411307	2.564793
C	2.552287	0.933307	1.301793
C	3.942287	1.311307	1.704793
H	0.974513	0.733312	4.325441
H	6.797287	1.156307	2.952793
P	-7.04871	1.833307	-2.61121
O	-7.87971	3.098307	-2.45821
O	-7.63271	0.678307	-1.80021
O	-6.81171	1.508307	-4.10221
P	-5.18771	1.789307	-0.34721
O	-5.41771	2.986307	0.485793
O	-5.75071	0.481307	0.068793
O	-5.65371	2.135307	-1.84921
P	-2.57171	0.730307	0.351793
O	-1.35471	1.456307	0.765793
O	-3.41671	0.075307	1.389793
O	-3.58271	1.717307	-0.40421
O	-2.17071	-0.33769	-0.77021
C	-1.22371	-0.03869	-1.80321
C	-1.75471	-0.47669	-3.15021
O	-2.11471	-1.86869	-3.02921
C	-3.00471	0.183307	-3.65221
O	-2.68771	1.369307	-4.34521
C	-3.58571	-0.87869	-4.57421
O	-3.00271	-0.97469	-5.85521
C	-3.24971	-2.15669	-3.82621
N	-4.29471	-2.72169	-2.95221
C	-4.54171	-2.38369	-1.64321
N	-5.52071	-3.06569	-1.08721
C	-5.95971	-3.90669	-2.09821
C	-6.97771	-4.89269	-2.13921
N	-7.76171	-5.17169	-1.10521
N	-7.15871	-5.57369	-3.29321

C	-6.36271	-5.27869	-4.33421
N	-5.36371	-4.37169	-4.42121
C	-5.20771	-3.71269	-3.25921
H	0.284725	-3.75441	5.347808
H	-0.53098	-2.88152	6.62286
H	-0.12313	-2.06932	5.130529
H	10.29332	-1.28665	3.278565
H	9.231887	-2.66509	3.116216
H	9.762603	-1.79887	1.694569
H	3.864323	8.895894	4.980046
H	2.163247	9.236207	5.188837
H	3.013785	8.274721	6.374247
H	1.634334	5.079012	0.58899
H	0.719302	6.216068	1.521631
H	0.329128	3.019299	0.565213
H	-1.39487	3.185814	0.555045
H	-0.3879	7.389243	-0.73518
H	-2.1341	7.451259	-0.74086
H	-1.261	7.55828	0.76888
H	-5.8381	-5.34905	2.822574
H	-7.16259	-4.28809	3.238717
H	-6.50034	-4.26602	1.621925
H	-3.67028	-1.41869	3.204997
H	-4.89743	-0.28641	3.665515
H	-6.81723	-0.83811	1.896575
H	-7.5971	-2.00233	2.914622
H	0.284688	-2.04754	-1.07529
H	-1.24795	-2.85086	-0.99985
H	0.910118	-5.81727	-2.00576
H	-0.81087	-5.61037	-1.78564
H	0.049623	-4.61126	-2.93211
H	5.06998	0.594166	-4.72528
H	6.453294	-0.70744	-6.26081
H	8.781502	-0.09586	-6.619
H	9.725741	1.824651	-5.45925
H	8.360319	3.139085	-3.91477
H	4.845228	2.810562	-3.45954
H	6.298583	3.566341	-2.87795
H	9.447034	3.315751	-0.07786
H	8.533652	2.927686	1.360269
H	8.990343	1.660765	0.246981
H	4.980209	2.232706	-1.18443
H	3.371048	-1.34398	-3.69606
H	4.470126	-1.97091	-2.49105
H	2.76502	-1.41331	-0.73577
H	1.658963	-0.96866	-2.01326
H	2.211992	-2.6201	-1.87194
H	2.483265	1.316623	4.10165
H	1.199215	2.115809	3.485871
H	2.230303	-0.45655	2.638437

H	6.120066	3.539037	2.595097
H	5.0252	-0.51474	2.15164
O	-0.81878	0.323406	2.0285
H	-0.98264	-0.374	-3.88387
H	-0.30686	-0.55197	-1.60114
H	-1.04177	1.015572	-1.82114
H	-2.04628	-0.96852	-5.77278
H	-1.73384	1.462796	-4.39983
H	-3.67412	0.385788	-2.84239
H	-4.64651	-0.76353	-4.65389
H	-7.35826	-5.41006	-0.2218
H	-5.86754	-2.99383	-0.15203
H	-2.97658	-2.90172	-4.54401
Mg	-6.39702	3.537599	-0.81975
Mg	-6.79905	0.221611	-1.37119
O	-6.98197	6.737111	0.202108
H	-6.04389	6.927188	0.128141
H	-7.4836	7.546252	0.078592
O	3.767648	-3.17277	2.950732
H	3.936601	-3.57547	3.805652
H	4.588437	-3.11415	2.456294
H	2.608202	0.153271	0.571507
H	2.081335	1.785387	0.857875
H	-0.03988	5.212709	3.918052
H	0.504235	7.360767	4.999092
H	4.580583	6.868542	3.969192
H	4.064414	4.740856	2.884966
H	-6.54587	-5.84374	-5.22419

Table II(d). The Cartesian coordinates of the optimized geometries of the reactant, transition state and product of the activation step of aminoacylation reaction using ONIOM (HF/3-21G*: PM3) level calculation. The details of the model are described in section II. The structures of the corresponding models are shown in the Fig. 9 (a), 9(b) and 9(c) respectively.

Reactant			
C	-7.01674	1.242065	2.475658
C	-5.90145	0.89987	1.514321
O	-5.69151	-0.31766	1.174084
O	-5.14646	1.76391	1.012169
C	-3.6122	3.48499	-0.78834
N	-2.17314	3.458819	-0.46161
C	-1.70866	2.856261	0.724332
N	-2.53976	2.484191	1.681094
N	-0.39687	2.888643	0.939433
H	-1.60676	3.248807	-1.25748
C	3.14424	1.200017	-1.95188
C	1.703302	1.52385	-1.66319

O	1.32404	2.620056	-1.2479
N	0.723147	0.559634	-1.96263
C	-6.4337	-2.2176	3.871946
N	-5.2156	-2.1889	4.703487
C	-3.94647	-1.88148	4.132711
N	-3.87513	-1.35052	2.939897
N	-2.88526	-2.09959	4.895026
H	-5.18285	-2.97175	5.324187
N	-4.30091	-0.80824	-1.10494
C	-3.03186	-1.48699	-0.64707
C	-2.09515	-0.40799	0.032803
O	-1.78077	0.561874	-0.69673
H	-4.77322	-0.40463	-0.27949
C	-2.27545	-2.16551	-1.78829
C	2.191481	-2.68879	-0.77148
C	3.560669	-2.21003	-0.23174
C	3.34114	-2.05382	1.306987
C	1.805245	-2.23017	1.479953
C	1.061778	-0.88128	1.615409
O	-0.63049	-0.88534	4.279367
O	1.471972	0.842599	7.529562
O	4.903923	3.373685	7.305446
O	4.597524	-3.12869	-0.47364
O	-0.41166	1.489171	3.348632
O	1.377686	3.323715	6.115477
O	4.406618	3.237036	4.900641
O	4.076045	-2.92871	2.115419
O	1.192597	0.658306	5.114086
O	3.330908	1.493068	6.311634
O	5.952286	1.200994	6.049106
O	1.326212	-2.92802	0.324886
O	1.37652	-0.26256	2.851561
P	0.219181	0.242588	3.853002
P	1.635842	1.814713	6.276873
P	5.038784	2.390001	6.135734
H	-6.78139	2.127365	3.07824
H	-7.22685	0.405002	3.16142
H	-3.7712	3.242675	-1.85128
H	-4.24357	2.791394	-0.18185
H	-3.53996	2.387507	1.514247
H	-2.10286	2.029363	2.475216
H	-0.0871	2.447831	1.800312
H	0.257416	2.997734	0.174508
H	3.464493	0.28343	-1.42517
H	3.301495	1.040872	-3.0272
H	1.058941	-0.38237	-1.92356
H	-0.19015	0.674447	-1.53627
H	-7.26296	-2.57853	4.4948
H	-6.35925	-2.86943	2.988502
H	-4.6976	-1.11928	2.372938

H	-2.97514	-1.12279	2.496876
H	-2.97354	-2.50919	5.803362
H	-1.96615	-1.69078	4.63441
H	-1.26578	-2.44223	-1.41905
H	-2.10324	-1.45291	-2.6249
H	-3.31209	-2.26452	0.110074
H	-4.07364	-0.07493	-1.77443
H	-4.90845	-1.47658	-1.54262
O	-1.78591	-0.64688	1.221484
H	2.226646	-3.64239	-1.32356
H	3.687985	-1.06275	1.673627
H	1.543185	-2.91158	2.318853
H	-0.04599	-1.0142	1.502743
H	1.406255	-0.17733	0.831643
H	3.954464	-3.81047	1.784451
H	3.830995	-1.21836	-0.68197
H	4.699321	-3.1764	-1.41462
H	-7.93842	1.454015	1.91933
H	-6.69537	-1.19658	3.531127
H	-3.97839	4.507264	-0.62196
H	3.81359	2.012088	-1.63837
Mg	2.779701	-0.22465	6.792797
Mg	3.100227	3.92327	5.960609
O	4.512868	-0.86015	7.034585
H	4.738699	-1.73686	6.738582
H	5.216326	-0.21836	6.735654
O	-3.54926	0.986056	-3.1404
H	-2.59773	0.906874	-3.12051
H	-3.77085	1.894491	-2.93476
H	1.718332	-1.92818	-1.42785
C	-4.59495	-4.67494	-3.07645
C	-2.94196	-3.38277	-2.3075
H	-3.30516	-6.32156	-3.45522
N	-4.31421	-3.45369	-2.57987
N	-3.40659	-5.39598	-3.12753
C	-2.36193	-4.59663	-2.64383
H	-1.32393	-4.92137	-2.57046
H	-5.58696	-5.01845	-3.38356

Transition state			
C	-4.97605	-4.45939	1.452202
C	-4.7208	-3.02513	1.056455
O	-4.72119	-2.66793	-0.16871
O	-4.49854	-2.11087	1.89531
C	-3.93575	-0.81823	4.460809
N	-2.49118	-0.53785	4.583407
C	-1.63455	-0.73165	3.475007
N	-1.92373	-1.66479	2.59279
N	-0.49513	-0.06307	3.418506
H	-2.3108	0.296611	5.102267

C	1.068481	4.449766	3.089285
C	-0.03197	3.42373	3.07162
O	-0.19368	2.582007	3.957913
N	-0.98787	3.476613	2.040675
C	-3.95995	-5.66093	-2.03529
N	-2.4933	-5.56408	-2.16298
C	-1.84567	-4.30466	-2.06657
N	-2.47586	-3.26735	-1.56564
N	-0.57364	-4.23456	-2.42792
H	-2.14788	-6.13057	-2.91013
N	-4.8848	0.077758	-0.23343
C	-3.73199	0.769235	-0.93859
C	-2.41925	0.558144	-0.1519
O	-2.16125	1.213704	0.832318
H	-4.76225	-0.94675	-0.26529
C	-4.01621	2.264286	-1.13603
C	0.75868	4.83196	-0.90055
C	2.260015	4.810932	-0.5375
C	2.823713	3.579562	-1.30908
C	1.548756	2.751354	-1.64573
C	1.419341	1.550685	-0.68241
O	0.052137	-1.79737	-1.56678
O	3.860324	-3.01376	-1.086
O	7.380129	-1.89681	1.072764
O	2.93829	5.975701	-0.93532
O	0.189831	-0.93805	0.892669
O	3.662546	-2.24474	1.656965
O	5.962347	0.05686	1.58709
O	3.580086	3.872503	-2.44896
O	2.707827	-0.84063	-0.65924
O	5.229602	-1.29046	-0.3569
O	7.431425	0.074307	-0.81482
O	0.418247	3.627387	-1.56437
O	0.315486	0.75718	-1.08171
P	0.010444	-0.7184	-0.56246
P	3.646574	-1.93321	0.118034
P	6.831857	-0.63597	0.379777
H	-4.36347	-4.75956	2.310998
H	-4.76828	-5.1548	0.622601
H	-4.52576	0.105414	4.328452
H	-4.19721	-1.50349	3.612536
H	-2.8354	-2.12115	2.554704
H	-1.26929	-1.7409	1.821886
H	0.05576	-0.21685	2.573018
H	-0.30697	0.762145	3.975727
H	1.575099	4.526679	2.108895
H	0.66817	5.44243	3.336685
H	-0.67384	3.954432	1.219653
H	-1.49056	2.629617	1.831804
H	-4.25264	-6.70097	-2.23241

H	-4.51308	-5.01103	-2.72986
H	-3.43363	-3.274	-1.2071
H	-1.93988	-2.41484	-1.46575
H	-0.07107	-5.01766	-2.79366
H	-0.0818	-3.35279	-2.21672
H	-3.14815	2.731329	-1.64372
H	-4.10638	2.779745	-0.15459
H	-3.62998	0.300229	-1.95443
H	-4.93394	0.39246	0.732273
H	-5.74601	0.348568	-0.71989
O	-1.69833	-0.42203	-0.67241
H	0.481156	5.652385	-1.5854
H	3.553847	3.004966	-0.69706
H	1.524901	2.405951	-2.70384
H	1.233679	1.904975	0.351076
H	2.343847	0.920839	-0.69149
H	3.108706	4.51792	-2.96157
H	2.384459	4.659255	0.569029
H	2.582896	6.683682	-0.41528
H	-6.02874	-4.58699	1.735228
H	-4.27633	-5.41799	-1.00263
H	-4.26195	-1.29335	5.395197
H	1.834247	4.209253	3.838792
Mg	4.54804	-1.61428	-2.06113
Mg	5.301531	-1.56504	2.078366
O	6.085958	-0.98159	-2.91608
H	5.977545	-0.38841	-3.65359
H	6.734778	-0.57715	-2.27142
O	-5.41135	1.346439	2.190511
H	-4.97741	2.175012	2.368591
H	-5.35235	0.800737	2.975355
H	0.106188	4.903051	-0.0078
C	-7.33789	2.162708	-2.64031
C	-5.24421	2.508305	-1.92999
H	-7.32871	3.876254	-3.89387
N	-6.37126	1.675668	-1.83465
N	-6.83997	3.306132	-3.25265
C	-5.52574	3.532132	-2.8184
H	-4.90387	4.364431	-3.15097
H	-8.33168	1.723358	-2.77233

Product			
C	-6.83811	0.112025	2.736624
C	-5.80933	-0.14723	1.671318
O	-4.69981	-0.74144	1.890498
O	-5.93781	0.193675	0.465741
C	1.170888	5.713018	-1.64238
N	1.276466	5.564988	-0.17682
C	0.912957	4.327106	0.418662

N	0.037398	3.547127	-0.1911
N	1.391105	4.034166	1.607857
H	2.142853	5.934323	0.161836
C	6.619333	4.479957	0.342953
C	5.321875	3.721091	0.367324
O	4.214548	4.254402	0.450017
N	5.354256	2.326046	0.195425
C	-5.22415	-2.12524	5.430574
N	-4.09846	-1.41833	6.072233
C	-2.95363	-1.09273	5.295601
N	-3.08147	-0.84334	4.007358
N	-1.79687	-0.97748	5.922398
H	-3.87694	-1.81689	6.963305
N	-3.77214	-0.70123	-0.72125
C	-2.36554	-1.20359	-0.47325
C	-1.48263	-0.08497	0.092544
O	-1.42267	1.003174	-0.42623
H	-4.30695	-0.51256	0.18089
C	-1.72717	-1.74393	-1.7618
C	4.679137	-3.4123	2.791076
C	5.280655	-2.41941	1.76912
C	4.488966	-1.0933	2.00259
C	3.421221	-1.47148	3.068614
C	2.006344	-1.64362	2.464216
O	-0.3901	-0.15481	3.600958
O	-2.27567	-2.44245	10.76609
O	0.662621	-0.28762	12.35828
O	6.655596	-2.1857	1.965413
O	0.21685	1.685499	1.900036
O	-1.86524	0.379316	10.43369
O	1.438037	0.208264	10.24545
O	5.264912	0.009039	2.384718
O	-1.76159	-1.66322	8.491667
O	-0.09224	-1.71432	10.41902
O	2.315374	-2.31259	11.29934
O	3.8318	-2.69806	3.67608
O	1.551768	-0.40187	1.95695
P	0.144814	0.266273	2.295551
P	-1.71063	-1.10899	10.01719
P	1.451723	-1.08435	11.20371
H	-6.87617	1.181375	2.978929
H	-6.6139	-0.43714	3.665158
H	1.977086	5.2052	-2.1927
H	0.206809	5.327959	-2.01267
H	-0.34767	3.784196	-1.08615
H	-0.24458	2.675812	0.246496
H	1.077355	3.145558	2.011545
H	2.090093	4.586722	2.061949
H	7.261813	4.191433	1.186049
H	7.176286	4.284283	-0.58372

H	6.204447	1.887141	0.465867
H	4.540779	1.821048	0.470674
H	-5.93756	-2.42318	6.210193
H	-4.92533	-3.02675	4.875524
H	-3.95013	-0.89353	3.474181
H	-2.22903	-0.56683	3.543213
H	-1.72135	-1.18824	6.959101
H	-1.00929	-0.66982	5.368068
H	-0.69646	-2.08217	-1.53017
H	-1.62246	-0.9385	-2.51853
H	-2.44376	-2.04608	0.269958
H	-3.74159	0.141742	-1.26453
H	-4.26942	-1.40072	-1.24198
O	-0.82466	-0.49328	1.182891
H	5.420497	-3.90118	3.444881
H	4.023463	-0.7211	1.062988
H	3.397954	-0.75513	3.919802
H	1.309039	-2.04528	3.223949
H	2.025993	-2.34559	1.609383
H	5.786954	-0.24357	3.136964
H	5.1273	-2.7819	0.72628
H	7.084582	-3.02718	1.88552
H	-7.83804	-0.1874	2.3997
H	-5.75758	-1.45204	4.734131
H	1.217237	6.785792	-1.87247
H	6.456828	5.564058	0.40757
Mg	-0.87891	-3.3533	10.00368
Mg	-0.15799	0.695611	11.03626
O	0.539479	-4.31265	10.75308
H	0.897644	-5.05282	10.27299
H	1.286518	-3.72751	11.05552
O	-5.92688	0.025849	-2.66159
H	-6.17493	0.776362	-3.19005
H	-6.48858	0.016394	-1.89018
H	4.082781	-4.19904	2.295991
C	-3.43829	-4.88707	-2.45789
C	-2.49179	-2.87048	-2.34528
H	-4.00311	-4.64956	-4.49688
N	-2.78553	-4.04242	-1.63789
N	-3.56199	-4.26759	-3.70061
C	-2.97411	-2.99983	-3.64094
H	-2.9316	-2.30268	-4.47837
H	-3.79978	-5.88215	-2.18284

Table II(e). The Cartesian coordinates of the optimized geometries of the reactant, transition state and product of the activation step of the aminoacylation reaction with modified Arg-259 (the -NH_2 groups of the guadinium side chains of the Arg 259 residue are replaced by -CH_3 group; details in the theoretical section) using ONIOM (HF/3-21G*: PM3) level of theory. The structures of the corresponding models are shown in the Fig. 13(a), 13(b) and 13(c) respectively.

Reactant with modified Arg 259			
C	-6.98875	0.905774	2.485519
C	-6.0624	1.074653	1.297747
O	-6.08745	0.234688	0.350821
O	-5.25432	2.040196	1.224575
C	-3.83574	3.326082	-0.96449
N	-2.41521	3.553685	-0.6416
C	-1.80007	2.91702	0.453903
N	-2.51246	2.453175	1.461307
N	-0.47391	3.031352	0.56402
H	-1.84951	3.54905	-1.46558
C	3.168469	1.714598	-2.2808
C	1.699228	1.915549	-2.0178
O	1.218931	3.002985	-1.68617
N	0.822423	0.846145	-2.24697
C	-6.20164	-2.8189	3.084347
N	-5.12732	-2.91337	4.086767
C	-3.76511	-2.62386	3.580744
H	-5.12629	-3.82671	4.491528
N	-4.24133	-0.4875	-1.32158
C	-3.12597	-1.12651	-0.53693
C	-1.88814	-0.16602	-0.34369
O	-1.77702	0.779584	-1.18933
H	-4.75257	0.179733	-0.71367
C	-2.64846	-2.42406	-1.19151
C	2.822233	-2.22644	-1.19355
C	4.146165	-1.6028	-0.6863
C	3.975554	-1.54192	0.867188
C	2.479678	-1.91425	1.080001
C	1.571956	-0.67013	1.223039
O	-0.31929	-0.91532	3.734718
O	0.967316	1.669015	7.03869
O	5.057259	2.422758	7.747972
O	5.286246	-2.35962	-1.0155
O	-0.18152	1.534529	2.916587
O	2.462936	3.280919	5.215992
O	5.284512	1.620065	5.438293
O	4.849047	-2.35802	1.594192
O	1.288166	0.716139	4.788177
O	3.132083	1.046857	6.565759
O	5.220774	-0.27992	7.513965
O	2.08293	-2.67172	-0.07008

O	1.745057	-0.0653	2.491063
P	0.453937	0.283226	3.406493
P	1.881002	1.952949	5.754577
P	5.002462	1.103761	6.955427
H	-6.76853	1.619511	3.288014
H	-6.89538	-0.11222	2.89955
H	-3.95259	2.758786	-1.90417
H	-4.42036	2.787978	-0.16611
H	-3.52323	2.326654	1.410617
H	-1.97839	1.994841	2.192552
H	-0.07431	2.551823	1.366258
H	0.099355	3.147762	-0.26233
H	3.573036	0.874785	-1.68871
H	3.348904	1.493413	-3.34116
H	1.242817	-0.05479	-2.13424
H	-0.11693	0.913707	-1.86092
H	-7.12987	-3.22616	3.504337
H	-5.98552	-3.35177	2.144034
H	-1.70726	-2.74276	-0.69685
H	-2.39135	-2.26121	-2.25873
H	-3.53468	-1.35602	0.496806
H	-3.87128	-0.00341	-2.14086
H	-4.87504	-1.20313	-1.62304
O	-1.16795	-0.43417	0.620681
H	2.944386	-3.11921	-1.82788
H	4.214867	-0.53483	1.27229
H	2.324676	-2.62254	1.922251
H	0.501216	-0.93675	1.042976
H	1.864738	0.095444	0.475326
H	4.769173	-3.24246	1.257813
H	4.272699	-0.56757	-1.0983
H	5.268192	-2.47191	-1.95668
H	-8.03315	1.048761	2.184185
H	-6.37825	-1.75525	2.841077
H	-4.29933	4.31063	-1.10936
H	3.752225	2.608854	-2.02675
Mg	1.695917	-0.01975	7.10127
Mg	4.217441	3.071277	5.680121
O	2.741675	-1.12313	8.182219
H	2.591648	-2.06353	8.146302
H	3.719301	-0.94365	8.085413
O	-3.1244	0.973317	-3.45078
H	-2.36756	0.831018	-2.86272
H	-3.4049	1.881141	-3.34534
H	2.211803	-1.48436	-1.75207
C	-5.13451	-5.05293	-1.65748
C	-3.65028	-3.5063	-1.04066
H	-5.50144	-5.68041	0.343343
N	-4.31391	-4.09234	-2.12441
N	-4.99975	-5.09302	-0.27062

C	-4.07348	-4.1229	0.129027
H	-3.78489	-3.91811	1.17035
H	-5.78387	-5.68207	-2.27065
C	-3.65715	-1.17739	3.008352
H	-4.25196	-1.06484	2.097145
H	-3.9949	-0.44721	3.740853
H	-2.6246	-0.9745	2.762353
C	-2.74246	-2.79725	4.748287
H	-3.06739	-2.23228	5.619482
H	-2.64007	-3.84139	5.037923
H	-1.78538	-2.40249	4.439147
H	-3.49359	-3.32152	2.765416

Transition state with modified Arg 259			
C	-5.47023	-2.77853	2.626153
C	-5.2001	-1.34619	2.230187
O	-5.98078	-0.71709	1.461641
O	-4.17015	-0.70977	2.611111
C	-3.0371	0.688138	4.856966
N	-1.57357	0.511783	4.812518
C	-0.96135	0.117156	3.590033
N	-1.52714	-0.81455	2.862967
N	0.234299	0.606678	3.29367
H	-1.10683	1.275721	5.257823
C	1.897244	4.925518	2.344894
C	0.74267	3.980286	2.544171
O	0.606959	3.279758	3.551081
N	-0.28581	3.963061	1.591061
C	-5.87711	-4.0099	-1.02469
N	-4.57753	-4.54099	-1.46842
C	-3.52408	-3.52014	-1.66659
H	-4.69325	-5.05297	-2.31813
N	-4.66101	1.432544	0.43982
C	-3.67906	0.780199	-0.51328
C	-2.18348	0.959862	-0.1244
O	-1.84701	1.821586	0.683494
H	-5.17943	0.69097	0.953556
C	-3.8973	1.265052	-1.95351
C	1.064545	4.79996	-1.80147
C	2.56818	4.908178	-1.45879
C	3.162299	3.527053	-1.87567
C	1.908468	2.664977	-2.21232
C	1.591495	1.670369	-1.06619
O	-0.10864	-1.80853	-1.38116
O	3.655807	-3.36695	-1.57319
O	6.643942	-3.1422	1.366708
O	3.230768	5.940509	-2.14818
O	0.393989	-0.39332	0.795111
O	3.04447	-3.30533	1.166845

O	5.831455	-1.094	2.017414
O	4.087842	3.562538	-2.9246
O	2.539399	-1.25705	-0.75033
O	4.97484	-1.98734	-0.17344
O	7.486153	-1.04074	-0.31192
O	0.829166	3.56893	-2.45934
O	0.784368	0.63232	-1.57474
P	0.225101	-0.57576	-0.67145
P	3.20464	-2.63529	-0.19166
P	6.526878	-1.67637	0.667904
H	-4.6639	-3.19789	3.23971
H	-5.56962	-3.40256	1.720727
H	-3.34188	1.721411	4.613817
H	-3.58429	0.003198	4.157125
H	-2.49281	-1.12726	2.990579
H	-1.04279	-1.02851	1.997543
H	0.595231	0.330321	2.375824
H	0.598965	1.445917	3.725344
H	2.214635	4.981309	1.288243
H	1.619712	5.939306	2.66425
H	-0.02175	4.283588	0.681339
H	-0.90201	3.160595	1.561304
H	-6.62432	-4.81311	-1.04233
H	-6.25484	-3.17475	-1.63731
H	-3.08043	0.872964	-2.59479
H	-3.82954	2.37062	-2.01985
H	-3.88861	-0.33913	-0.46985
H	-4.18228	2.03539	1.109481
H	-5.3143	1.987851	-0.08006
O	-1.44955	0.109575	-0.75736
H	0.696999	5.571972	-2.49814
H	3.771776	3.082995	-1.05751
H	2.002594	2.127588	-3.18316
H	1.064086	2.1857	-0.23761
H	2.536269	1.257188	-0.66159
H	3.692112	4.033503	-3.64806
H	2.708703	5.068211	-0.35673
H	2.742674	6.734269	-1.97393
H	-6.4053	-2.85908	3.192558
H	-5.78701	-3.65268	0.017561
H	-3.3676	0.469648	5.880005
H	2.770589	4.623266	2.937858
Mg	4.54199	-1.82246	-1.98587
Mg	5.080081	-2.75164	2.228386
O	6.22746	-1.37445	-2.66488
H	6.268776	-0.62353	-3.25132
H	6.890628	-1.24645	-1.93452
O	-3.49971	3.127699	2.347931
H	-2.69299	2.880342	1.874285
H	-3.4785	2.728357	3.216167

H	0.434298	4.837146	-0.88977
C	-7.30481	0.847878	-3.18525
C	-5.19096	0.771208	-2.48086
H	-7.38496	-1.24433	-3.56864
N	-6.29663	1.599962	-2.7021
N	-6.85065	-0.46645	-3.27991
C	-5.52555	-0.52808	-2.83697
H	-4.92092	-1.44521	-2.77776
H	-8.29785	1.218266	-3.4507
C	-3.17244	-2.80023	-0.32725
H	-3.95031	-2.08357	-0.04103
H	-3.04152	-3.52038	0.478334
H	-2.24878	-2.26575	-0.47754
C	-2.23483	-4.19607	-2.23152
H	-1.93061	-5.02351	-1.59476
H	-2.39125	-4.57805	-3.23802
H	-1.43589	-3.4668	-2.23536
H	-3.85504	-2.74538	-2.38394

Product with modified Arg 259			
C	-4.29326	3.743085	-0.21735
C	-3.64401	2.388923	-0.29199
O	-4.26472	1.30018	-0.29223
O	-2.37031	2.226737	-0.36149
C	-1.03453	5.739326	0.285491
N	-0.44452	5.505994	1.618248
C	-0.07209	4.18298	1.992264
N	-0.5416	3.143843	1.351931
N	0.708052	4.036792	3.0544
H	0.279384	6.169544	1.804621
C	4.854793	3.256319	0.119251
C	3.362135	3.181619	-0.04661
O	2.594391	4.104846	0.222113
N	2.812436	2.02132	-0.62976
C	-4.8975	-4.39387	5.108126
N	-4.71063	-2.97613	5.46616
C	-3.47473	-2.37957	4.909343
H	-4.72562	-2.87596	6.459805
N	-2.38259	-0.54059	-0.61894
C	-1.8352	-1.25397	0.602148
C	-0.5265	-0.6069	1.065072
O	0.157349	0.058248	0.32827
H	-2.67891	0.452823	-0.39199
C	-1.60983	-2.74667	0.320071
C	5.399074	-3.53664	1.868308
C	5.241282	-2.75494	0.542637
C	4.651155	-1.37383	0.973172
C	4.418737	-1.52406	2.504246

C	2.929233	-1.74136	2.864606
O	0.748269	-0.72555	4.646097
O	0.326948	-3.31285	9.824831
O	-0.04378	0.42932	11.19066
O	6.463818	-2.55939	-0.12929
O	0.695601	1.321412	3.057584
O	-1.93708	-2.24975	11.19517
O	-1.83911	0.733614	9.781075
O	5.435246	-0.25952	0.651442
O	-1.75656	-3.11797	8.472581
O	-0.31431	-1.15565	9.255498
O	0.705974	1.188159	8.563913
O	5.189068	-2.64336	2.948789
O	2.210725	-0.56323	2.552802
P	0.874039	-0.12042	3.320049
P	-1.14598	-2.60204	9.888904
P	-0.23335	0.627804	9.59318
H	-3.5559	4.541777	-0.0364
H	-5.03891	3.780427	0.586107
H	-0.42617	5.354573	-0.54727
H	-2.04	5.283361	0.223116
H	-1.2	3.154641	0.569201
H	-0.2246	2.243685	1.699579
H	0.902702	3.075173	3.340013
H	1.105125	4.805927	3.551302
H	5.231054	2.422888	0.72948
H	5.357919	3.207814	-0.85608
H	3.34139	1.191487	-0.47743
H	1.832219	1.892058	-0.50284
H	-5.86071	-4.73637	5.506636
H	-4.1109	-5.06703	5.483511
H	-1.20084	-3.22057	1.235808
H	-0.84	-2.88613	-0.46732
H	-2.59384	-1.15824	1.441237
H	-1.68379	-0.52171	-1.34018
H	-3.18221	-1.0475	-0.94882
O	-0.27049	-0.87143	2.354559
H	6.406421	-3.95161	2.037992
H	3.707069	-1.14238	0.431064
H	4.838959	-0.67231	3.083775
H	2.828643	-1.99487	3.937934
H	2.501663	-2.57481	2.274356
H	6.307921	-0.40093	0.998248
H	4.536718	-3.27739	-0.14499
H	6.801347	-3.4237	-0.32248
H	-4.80808	3.969433	-1.1594
H	-4.92685	-4.49005	4.013125
H	-1.15459	6.822251	0.150453
H	5.163153	4.191456	0.604261
Mg	0.546724	-2.44584	8.216858

Mg	-1.67208	-0.43259	11.20041
O	1.483829	-1.15987	7.228282
H	1.266894	-1.11799	6.275078
H	1.357442	-0.25164	7.59724
O	-0.97964	1.509976	-2.53967
H	-0.09228	1.551376	-2.19954
H	-1.55031	1.990253	-1.92695
H	4.668281	-4.36102	1.947094
C	-4.33402	-4.47274	-1.37538
C	-2.87228	-3.42796	-0.05301
H	-5.71277	-4.81872	0.209086
N	-3.1378	-3.85474	-1.35977
N	-4.84444	-4.4478	-0.0783
C	-3.93789	-3.79232	0.759632
H	-4.09742	-3.60803	1.832017
H	-4.80694	-4.91126	-2.25818
C	-3.83696	-1.60994	3.600071
H	-4.33276	-2.25888	2.871208
H	-4.4956	-0.77333	3.818735
H	-2.92047	-1.22496	3.153806
C	-2.7883	-1.42167	5.931446
H	-3.45465	-0.59058	6.17039
H	-2.49759	-1.93713	6.847084
H	-1.88881	-1.01854	5.469925
H	-2.75338	-3.16725	4.653088

Figure captions:

Fig. S.1. The model of the active site of HisRS with Mg^{2+} 2 and Mg^{2+} 3 ions located near the β-γ phosphate linkage as constructed from the model of active site of the crystal structure of the HisRS-Histidinol-ATP complex (PDB code:1KMN)[21] (as shown in Fig. 1 and described in section II). Water molecule in close proximity with the ions is also shown in the figure. The image is prepared using VMD[28].

Fig. S.2. Schematic description of the change in the orientation of the amino acid moiety relative to the ATP which occurs in a plane containing the α-phosphrous atom of ATP, carboxyl carbon of amino acid, chiral carbon and is nearly perpendicular to the plane containing the imidazole ring of the histidine moiety. The variation in the C5′ (ATP)-O5′ (ATP)---C(COO^- of His) mutual angle between ATP and His is indicated by the dotted line. The variation in the intramolecular N(His)—C^{α}—C($^{His}COO^-$)—O($^{His}COO^-$) dihedral angle of His in the $Model^{Opt}_{Reactant\ (L)}$, $Model^{Unopt}_{Reactant\ (D)}$ and $Model^{Opt}_{Reactant\ (D)}$ is shown by the bold line respectively.

Fig.S.3. (a) Superposition of the model of active site with D-His in the optimized state (denoted as $Model^{Opt}_{Reactant\ (D)}$) with the corresponding optimized L-structure (denoted as $Model^{Opt}_{Reactant\ (L)}$). The schematic position of the AH_3 is shown with which the Glu 83 is attached. (b) Superposition of the model of active site with D-His in the optimized state (denoted as $Model^{Opt}_{Reactant\ (D)}$) with the corresponding optimized L-structure (denoted as $Model^{Opt}_{Reactant\ (L)}$). The schematic position of the motif 2 is shown with which the Arg 113 is attached (c) superposition of the model of active site with D-His in the optimized state (denoted as $Model^{Opt}_{Reactant\ (D)}$) with the corresponding optimized L-structure (denoted as $Model^{Opt}_{Reactant\ (L)}$). The schematic position of the His A loop is shown with which the Arg 259 is attached. (d) superposition of the model of active site with D-His in the optimized state (denoted as $Model^{Opt}_{Reactant\ (D)}$) with the corresponding optimized L-structure (denoted as $Model^{Opt}_{Reactant\ (L)}$). The schematic position of the His A is shown with which the Tyr 264 is attached. In all cases, the position of the loop or motif to which a particular surrounding residue is attached is shown and the corresponding position in the $Model^{Opt}_{Reactant\ (D)}$ is also shown.

Fig.S.4. (a) Calculated electrostatic potential on the molecular surfaces (ESP) of (a) ATP with Mg^{2+} 2 and Mg^{2+} 3 ions in the geometry as present in the $Model_{Reactant}$ without any surrounding residues (b) ATP with Mg^{2+} 2 and Mg^{2+} 3 ions and His in the geometry as present in the $Model_{Reactant}$ without any surrounding residues using HF/6-31G** level of theory with isodensity value of 0.0004 a.u. The color variation ranges from red (electronegative) to blue (electropositive) with the ESP values ranging from –0.02 to +0.02 hartrees.

Fig.S.5. (a) Calculated electrostatic potential on the molecular surfaces of (a) ATP with Mg^{2+} 2 and Mg^{2+} 3 ions, His and Arg 259 in the geometry as present in the $Model_{Reactant}$ without surrounding residues (except Arg 259) (b) ATP with Mg^{2+} 2 and Mg^{2+} 3 ions, His, Arg 113 and Arg 259 in the geometry as present in the $Model_{Reactant}$ without surrounding residues (except Arg 113 and Arg 259) using HF/6-31G** level of theory with isodensity value of 0.0004 a.u. The ESP is mapped on an isosurface of the total electronic density at a value of 0.0004 a.u. The color variation ranges from red (electronegative) to blue (electropositive) with the mapped ESP values from –0.02 to +0.02 hartrees.

Fig.S.6. The numbering scheme of the atoms in the optimized geometry of the (a) reactant (b) transition state and (c) product calculated at the ONIOM (HF/3-21G*//PM3) level of theory

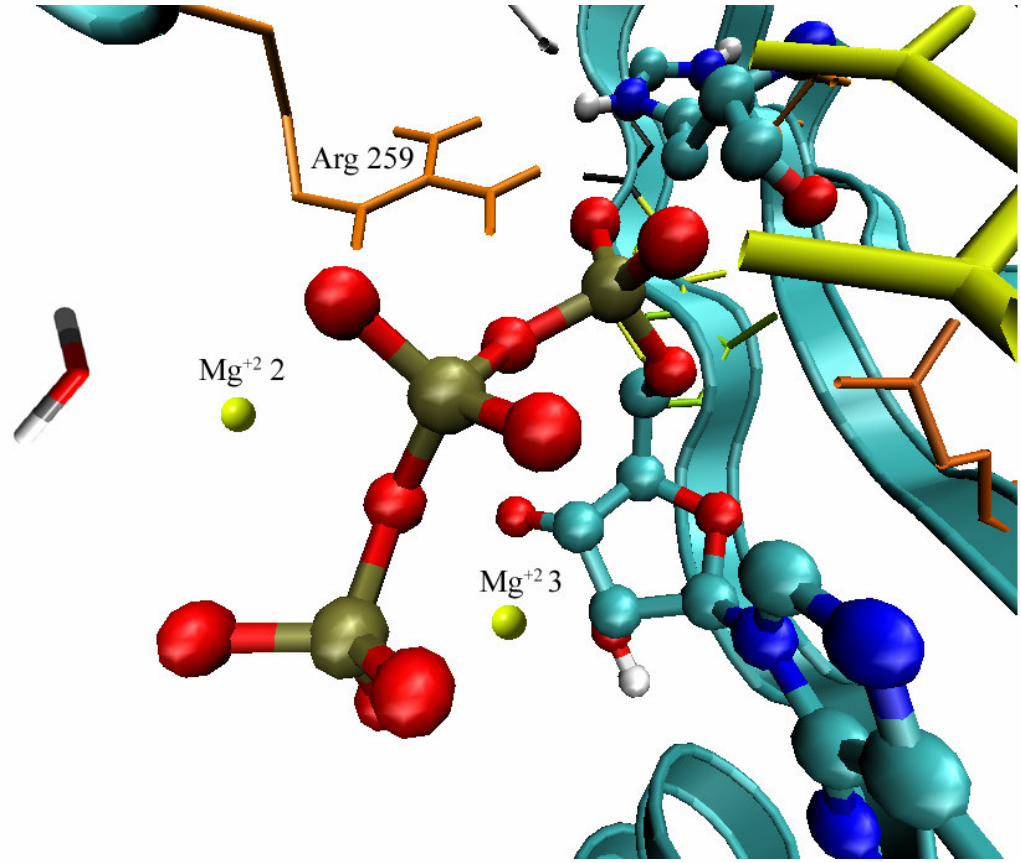

Fig. S.1

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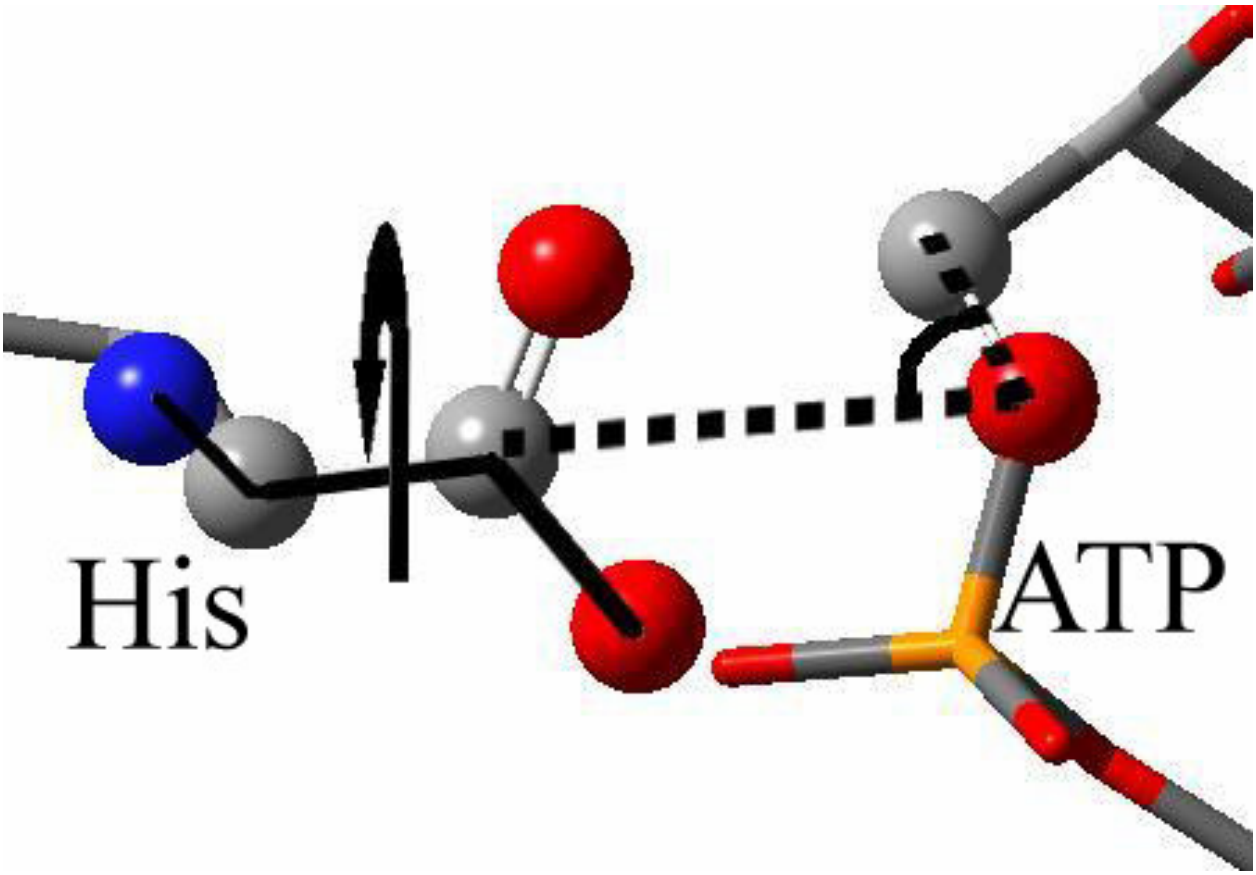

Fig. S.2

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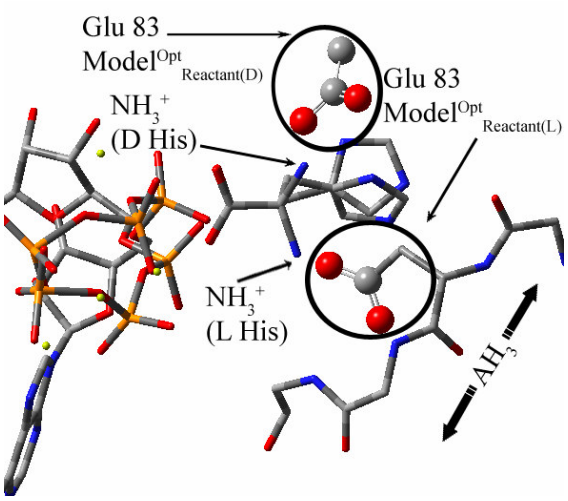
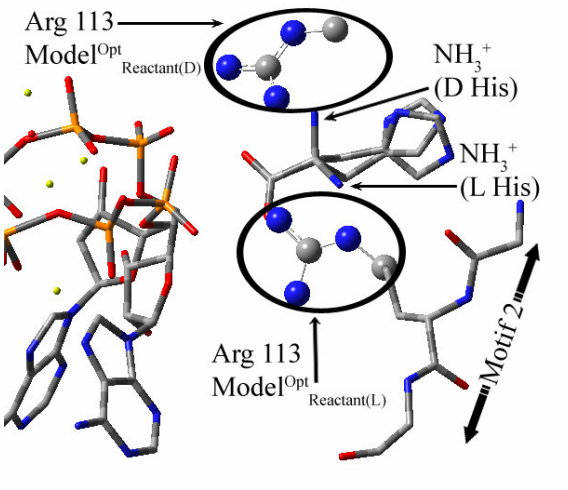
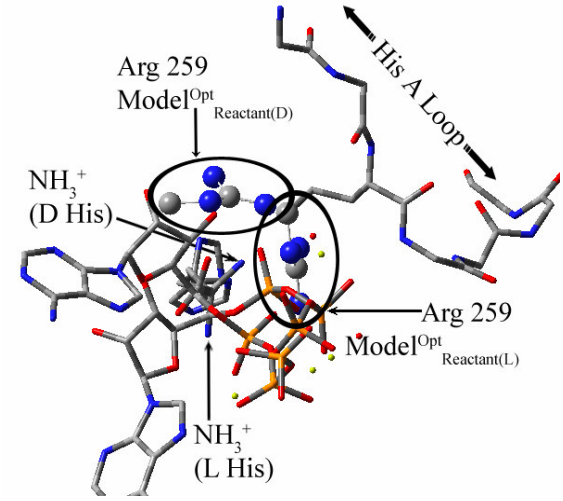

Glu 83
Model^Opt Reactant(D)
Glu 83
Model^Opt Reactant(L)
NH3+
(D His)
NH3+
(L His)
AH3

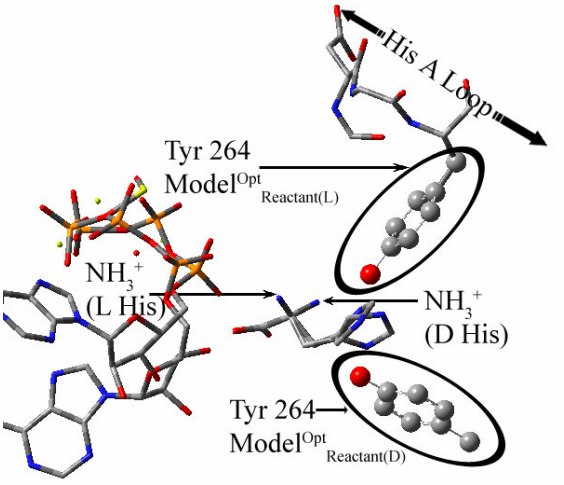
(a)


Arg 113
Model^Opt Reactant(D)
NH3+
(D His)
NH3+
(L His)
Arg 113
Model^Opt Reactant(L)
Motif 2

(b)



(c)



(d)

Fig. S.3

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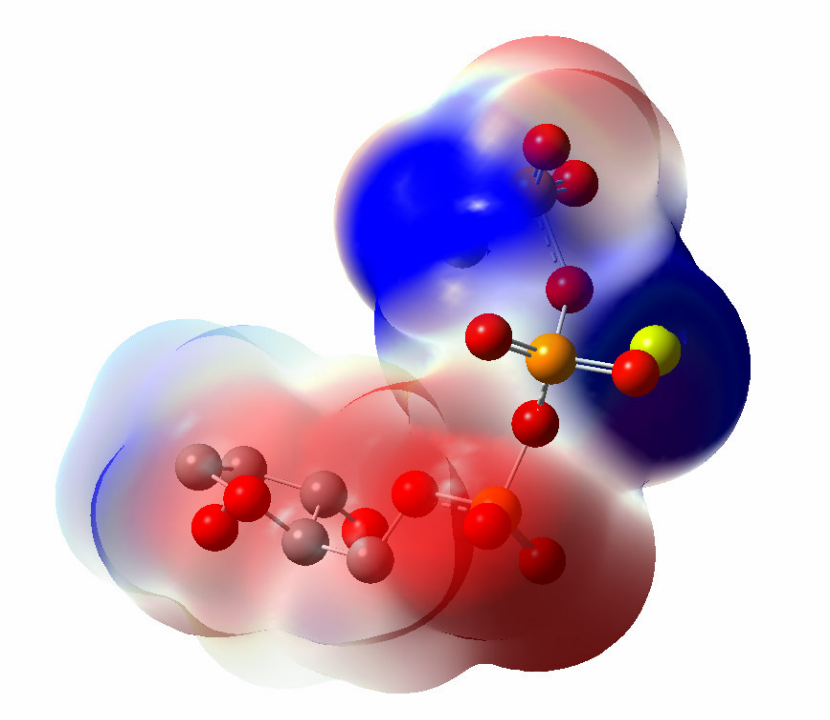
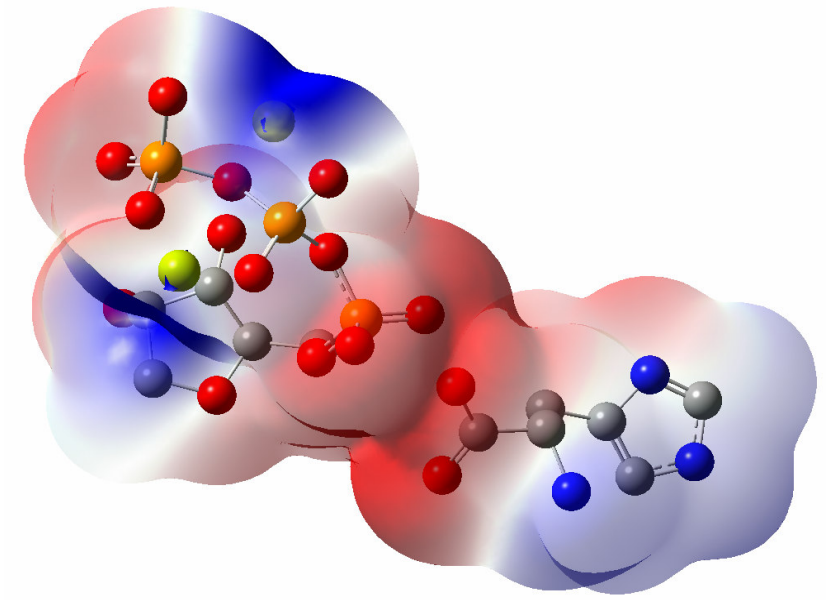


(a)



(b)

Fig. S.4.

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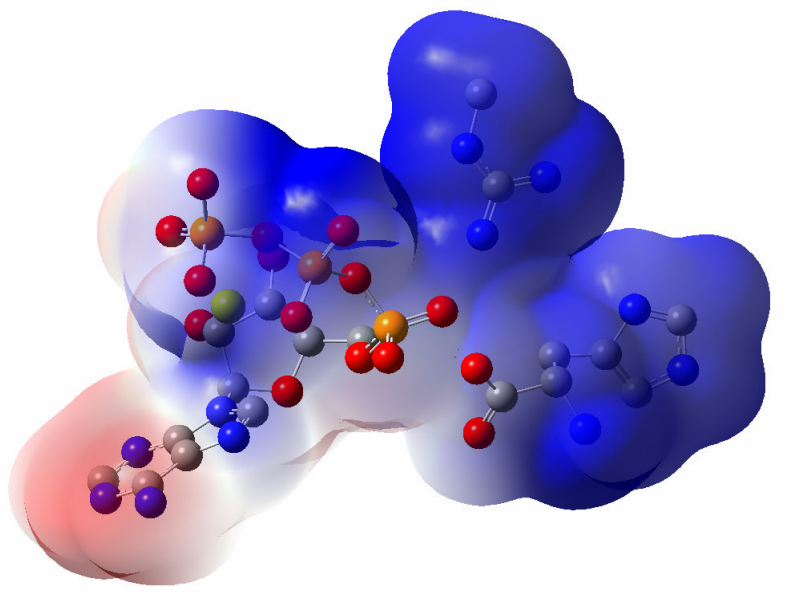
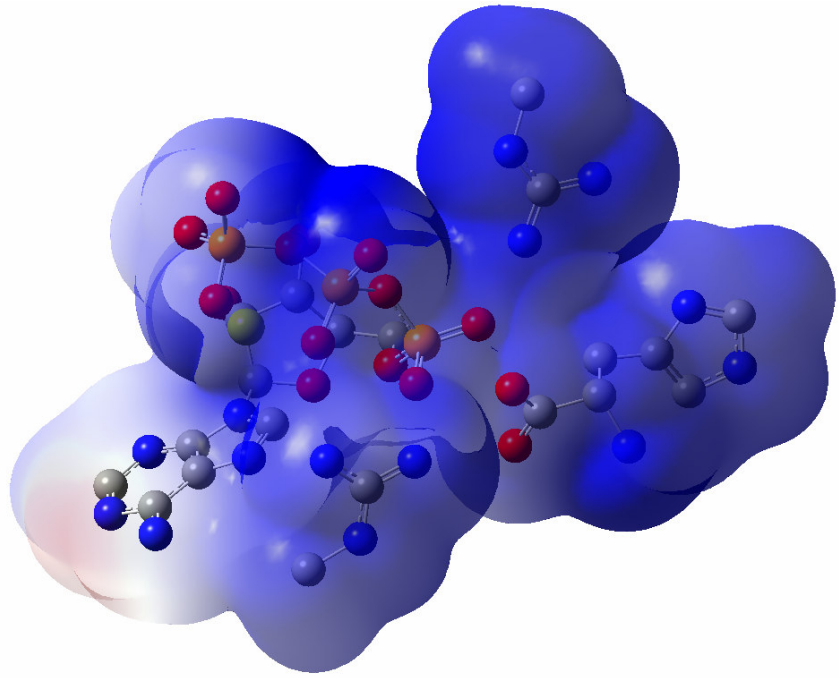


(a)



(b)

Fig. S.5.

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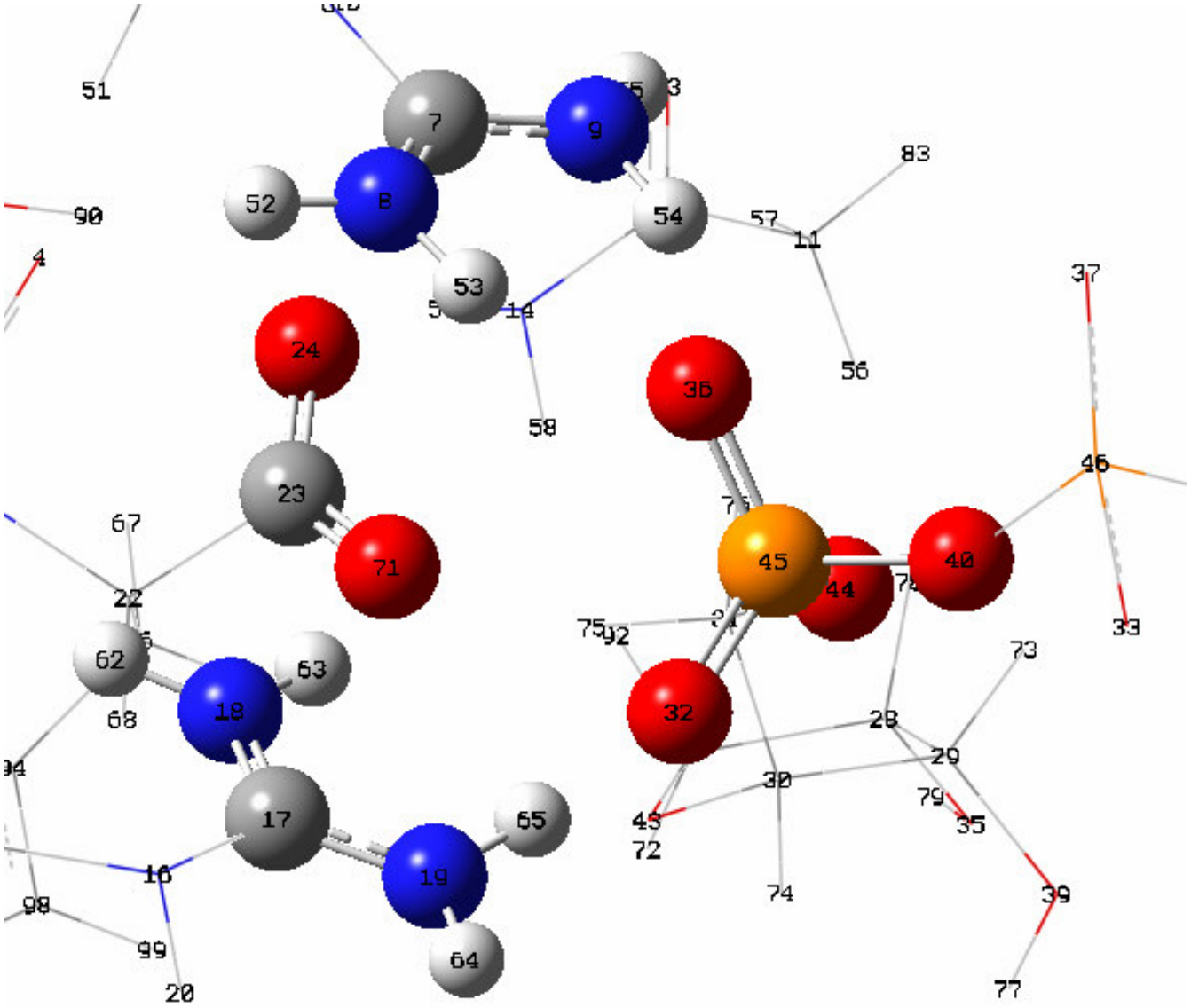
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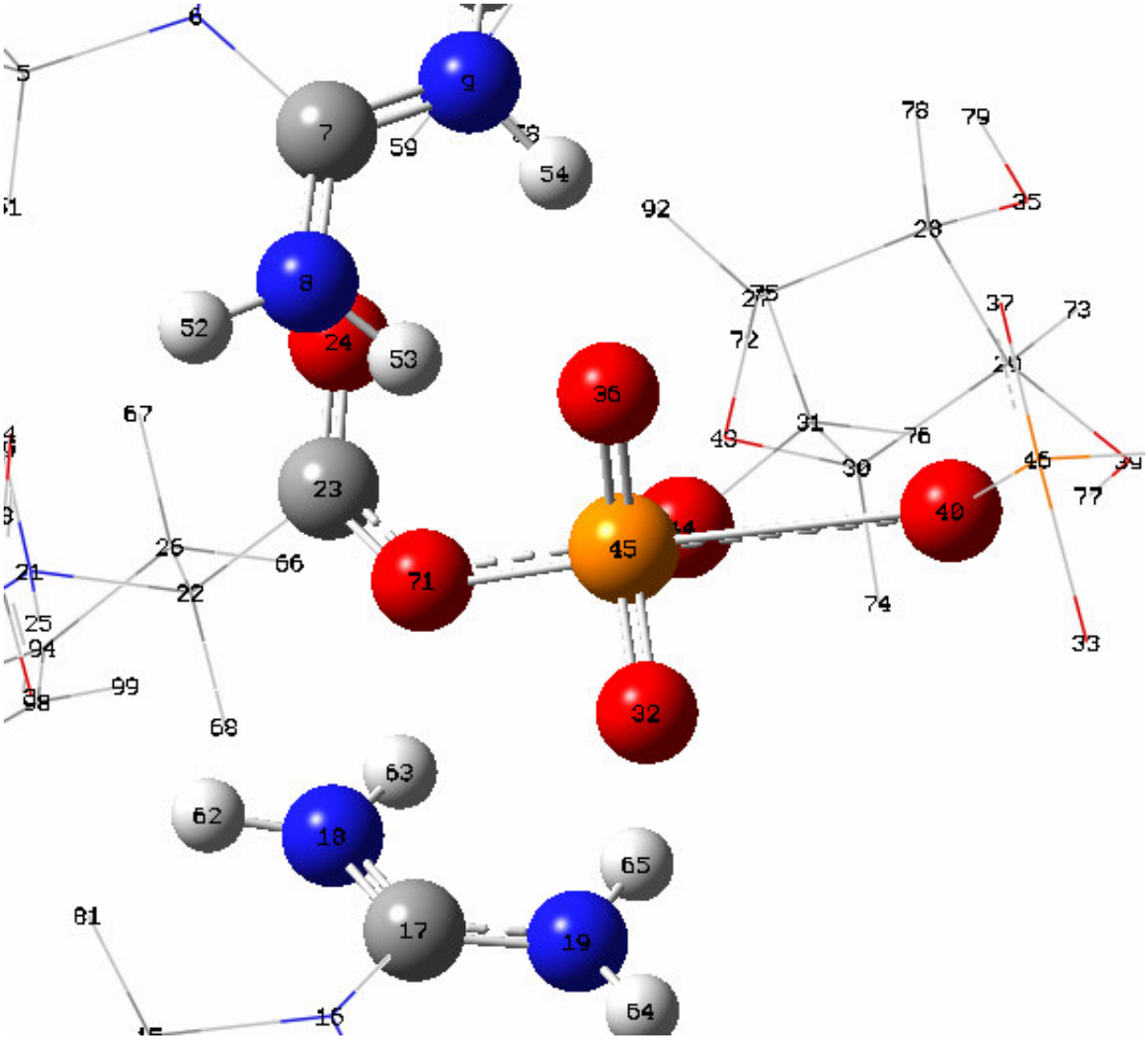
(a)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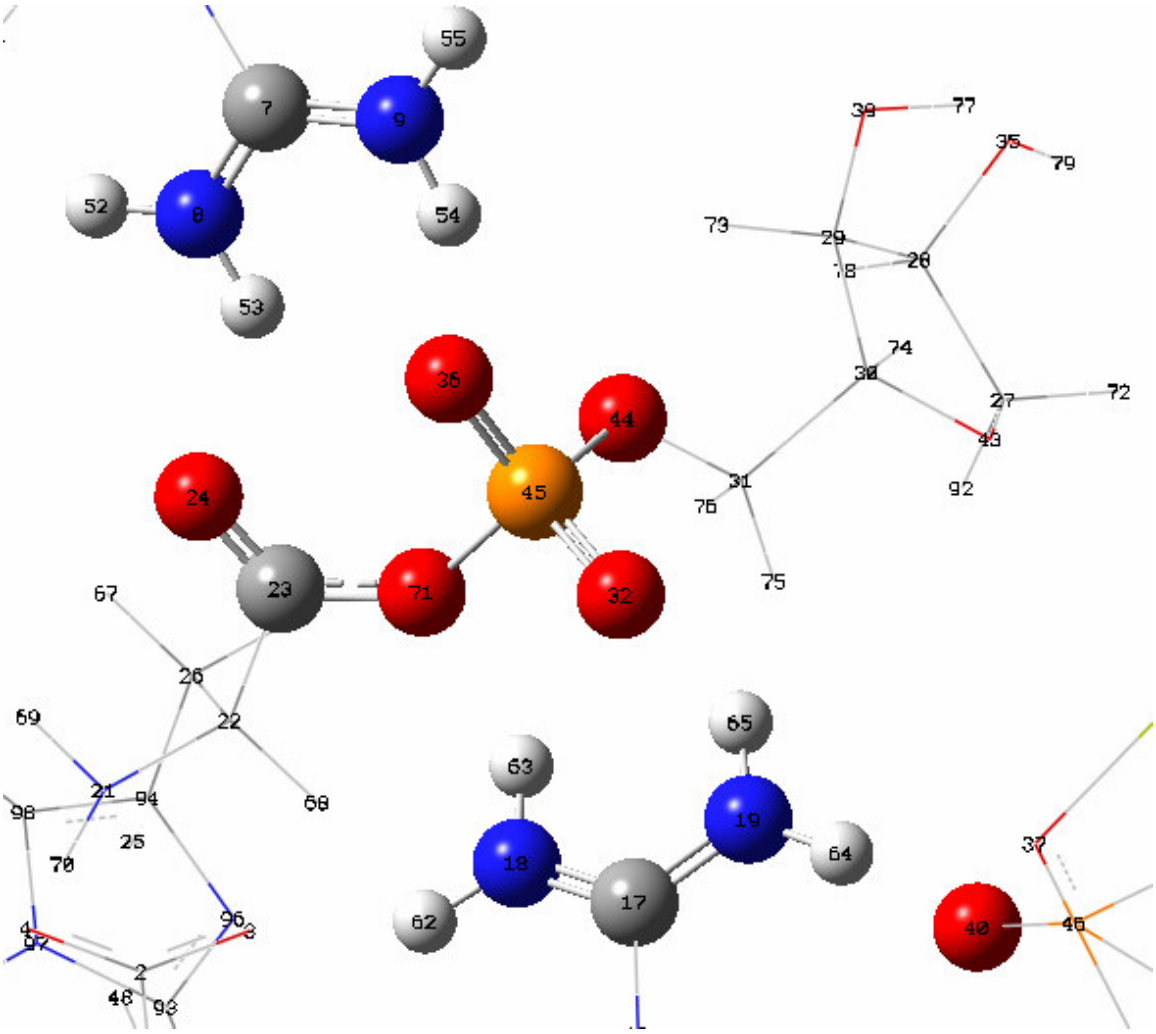
(b)



(c)

Fig. S.6.

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