Supporting information

for

Insights into the Stereochemistry of the Abasic Product in Thymine DNA Glycosylase: A Displacement Reaction Pathway from Computational Simulations

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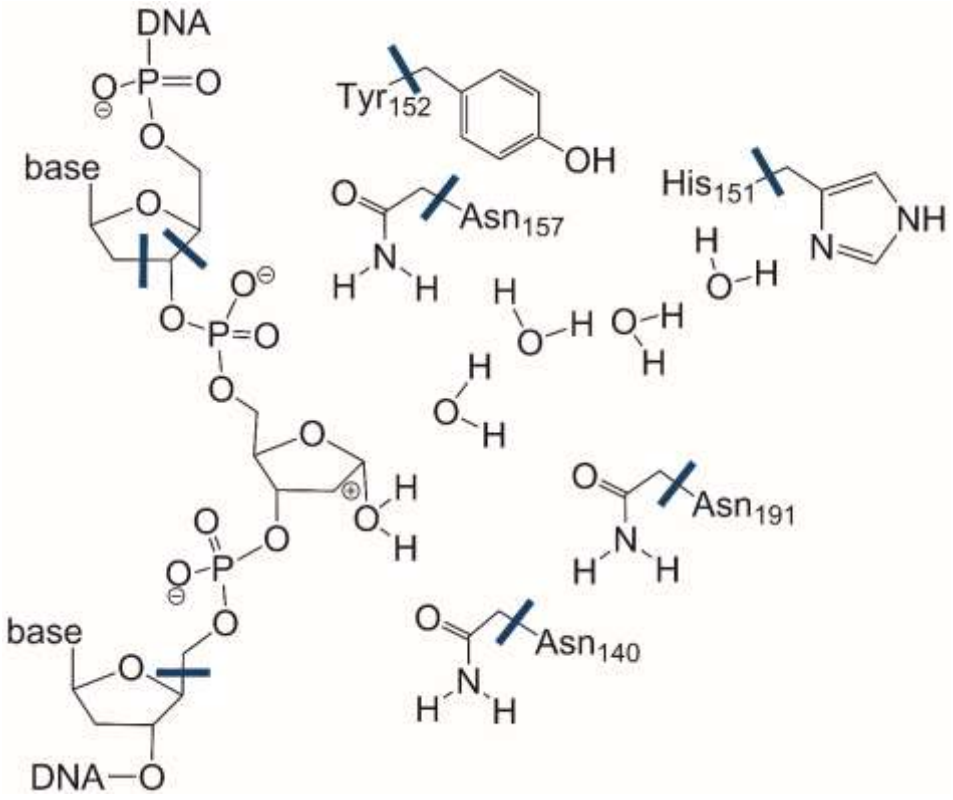


Figure S1. Illustration of the QM region used in the His151-mediated displacement reaction and the ring-opening reaction. The bold lines represent the cleavage bonds between the QM and MM regions.

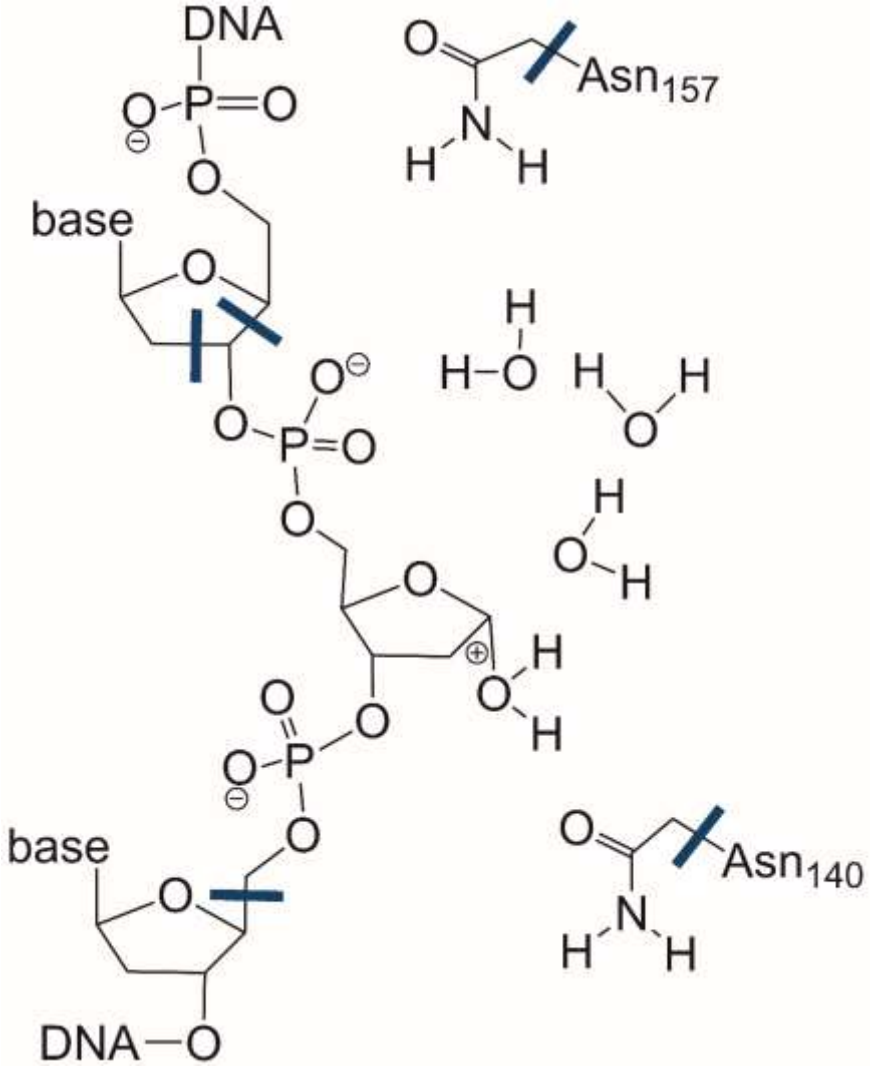


Figure S2. Illustration of the QM region used in the phosphate-mediated displacement reaction. The bold lines represent the cleavage bonds between the QM and MM regions.

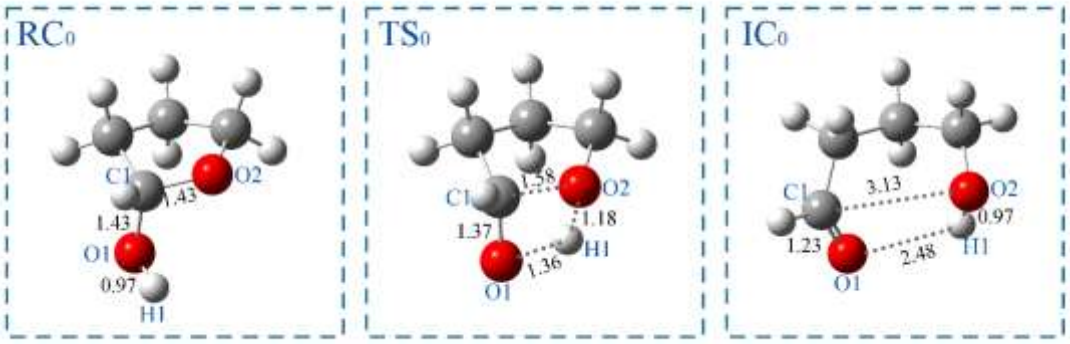


Figure S3. Density functional theory (B3LYP-D3/6-31+G*) optimized geometries of the ring-opening reaction with the assistance of 0 explicit water molecules. Distances are given in Å.

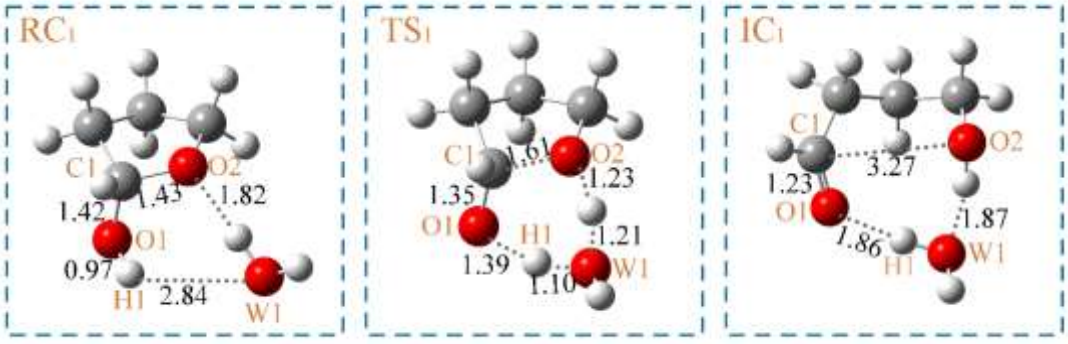


Figure S4. Density functional theory (B3LYP-D3/6-31+G*) optimized geometries of the ring-opening reaction with the assistance of 1 explicit water molecule. Distances are given in Å.

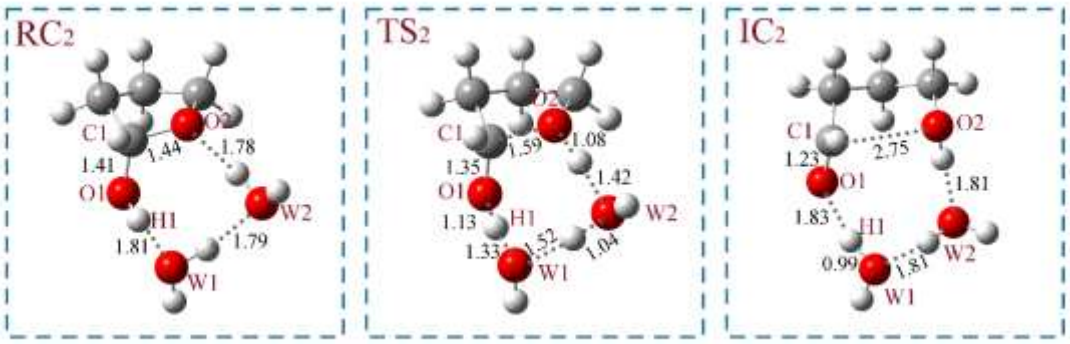


Figure S5. Density functional theory (B3LYP-D3/6-31+G*) optimized geometries of the ring-opening reaction with the assistance of 2 explicit water molecules. Distances are given in Å.

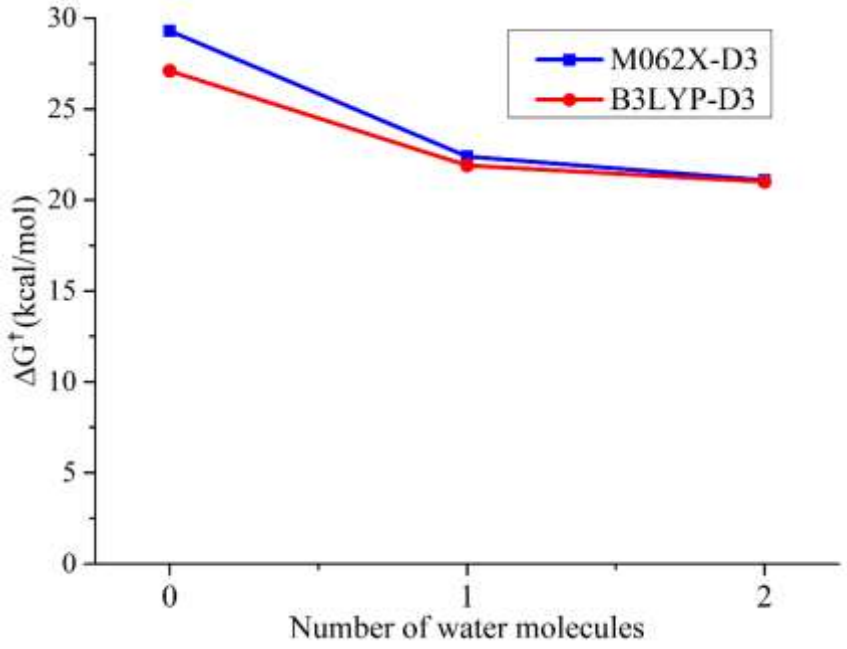


Figure S6. Functional-dependence test for the auxiliary effect of water molecules in aqueous solution, confirming that the aqueous aldehyde-mediated anomerization pathway strictly requires at least one auxiliary water molecule to achieve kinetically accessible reaction barriers, while additional water molecules offer negligible energetic benefit. Notably, the Gibbs free energy barrier (at 298.15 K) includes the quantum mechanical tunneling effect.

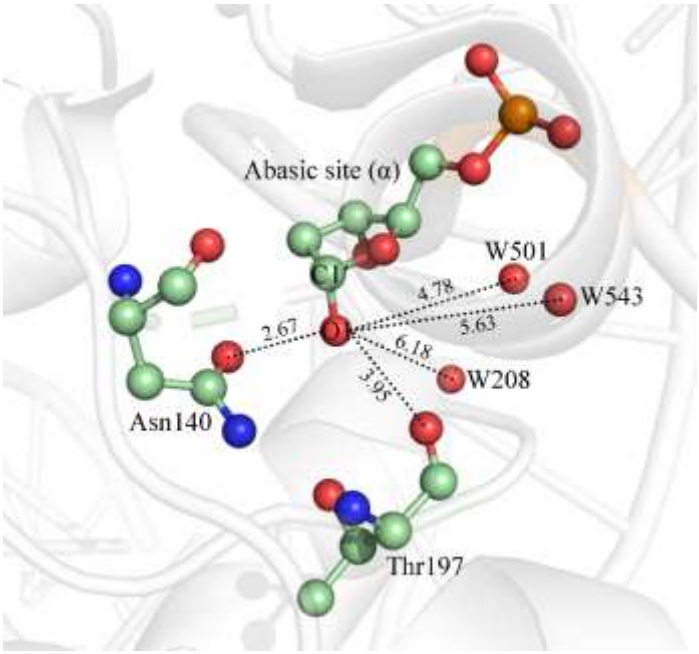


Figure S7. A high-resolution crystal structure (PDB ID: 4Z3A; resolution: 1.72 Å) of the α-anomeric abasic site, showing that there are no water molecules close to the atom O1 (the oxygen atom of the hydroxyl group of α anomer) to facilitate the ring-opening reaction to form the aldehyde intermediate.

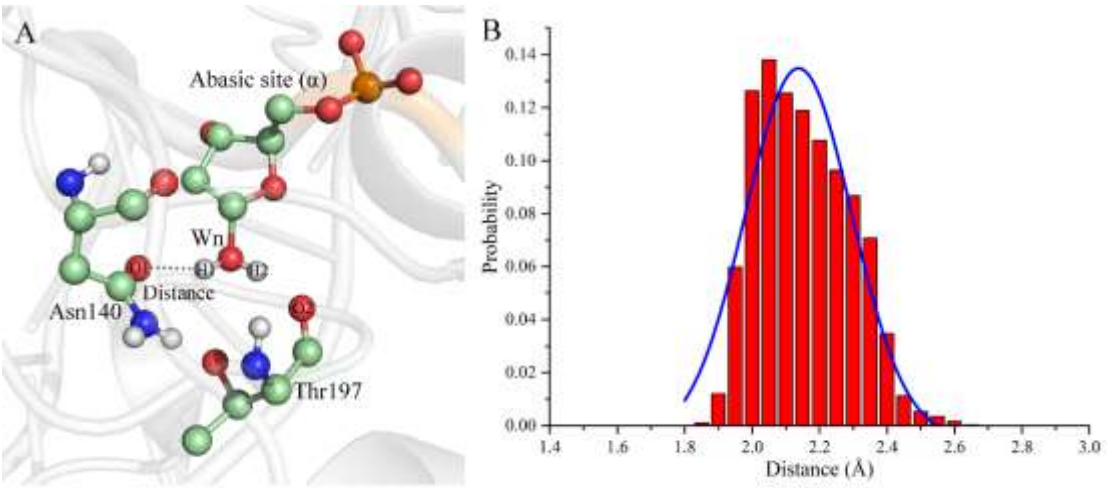


Figure S8. A stable H-bond formed between Wn and Asn140. (A) Illustration of the H-bond, shown along with the labels of key atoms. (B) Distribution of the distance between the O1 atom and the H1 atom along 1200 ns MD simulations.

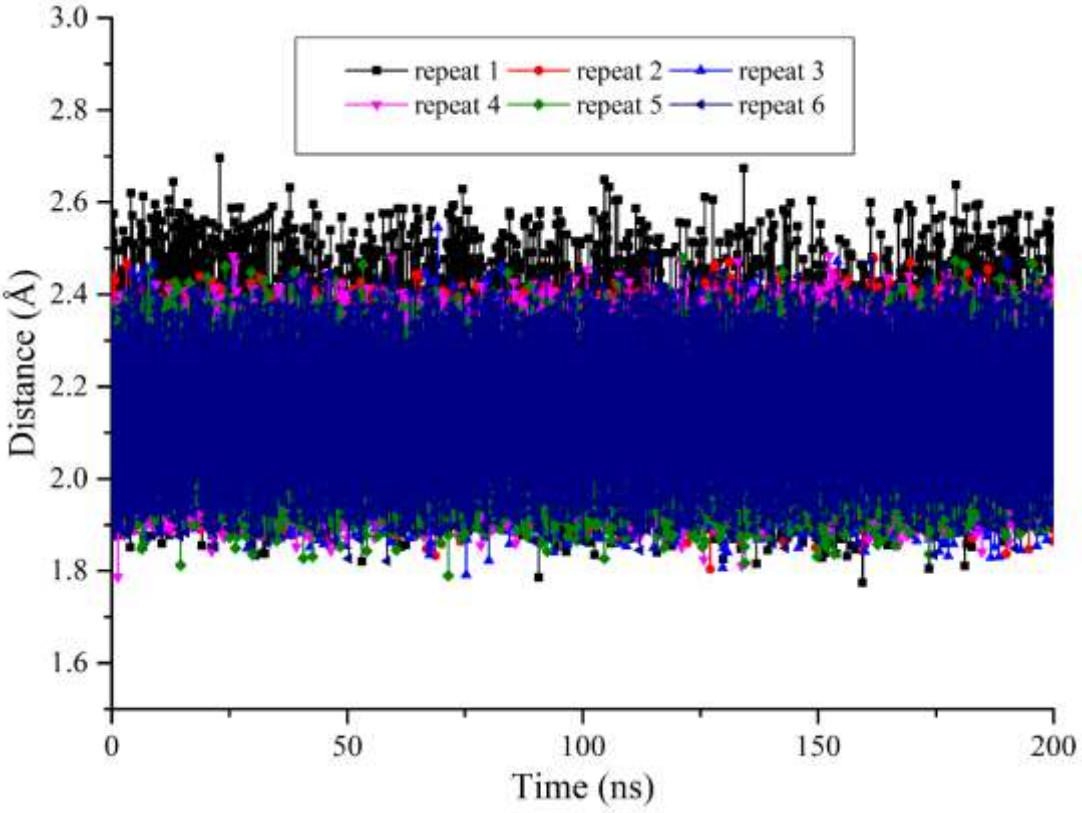


Figure S9. Time evolution of the H-bond distance between the water nucleophile Wn and the side chain of Asn140 in 6 independent 200 ns MD simulations, indicating a stable H-bond between them.

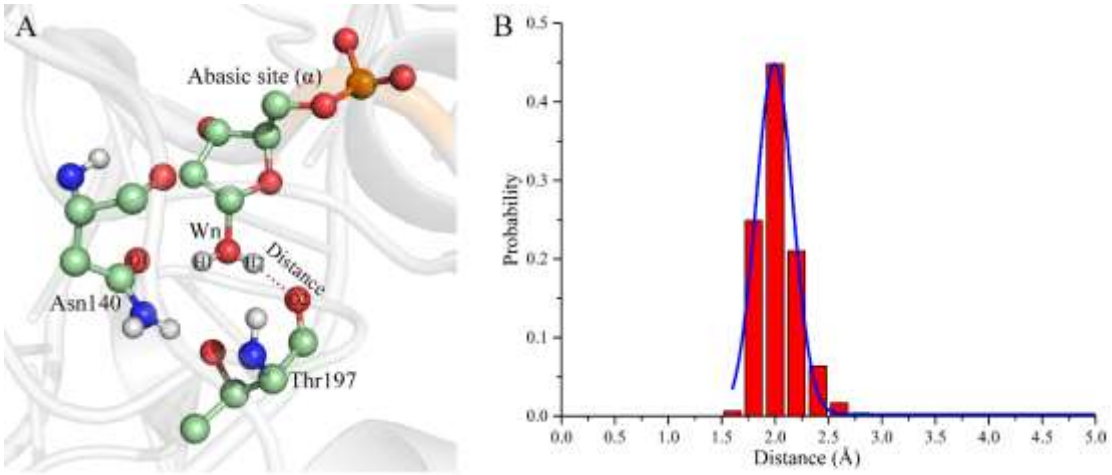


Figure S10. A stable H-bond formed between Wn and Thr197. (A) Illustration of the H-bond, shown along with the labels of key atoms. (B) Distribution of the distance between the O2 atom and the H2 atom along 1200 ns MD simulations.

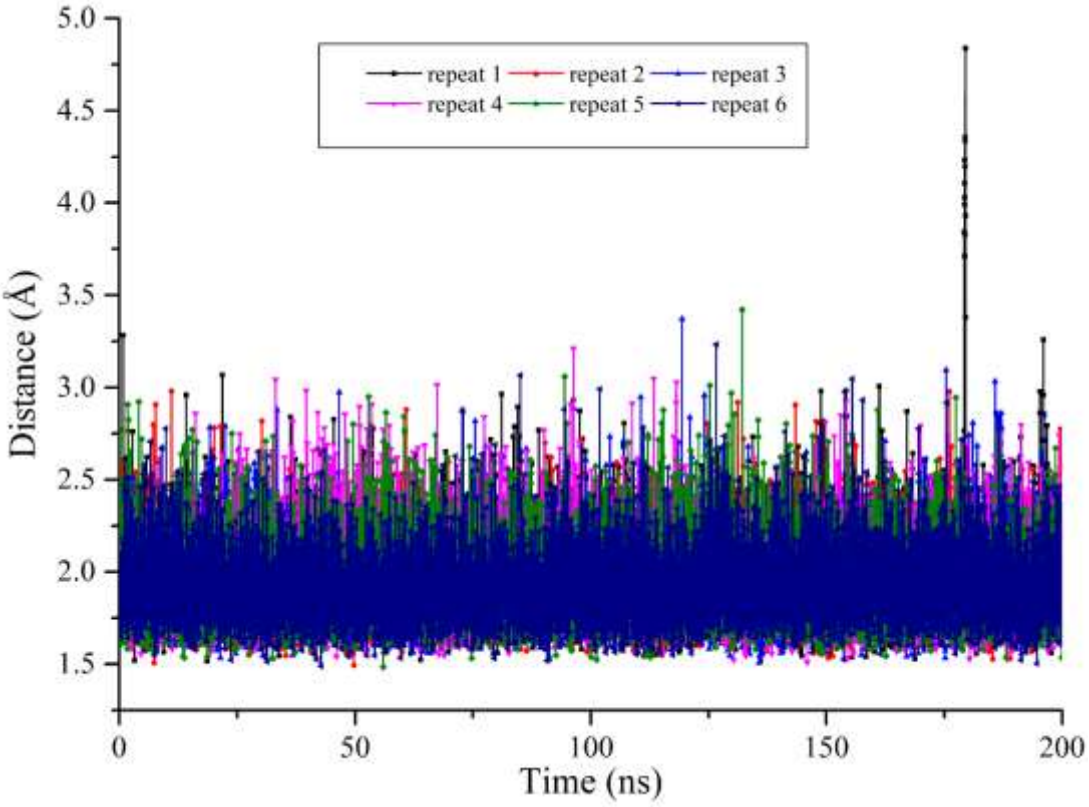


Figure S11. Time evolution of the H-bond distance between the water nucleophile Wn and the main chain carbonyl group of Thr197 in 6 independent 200 ns MD simulations, indicating a stable H-bond between them.

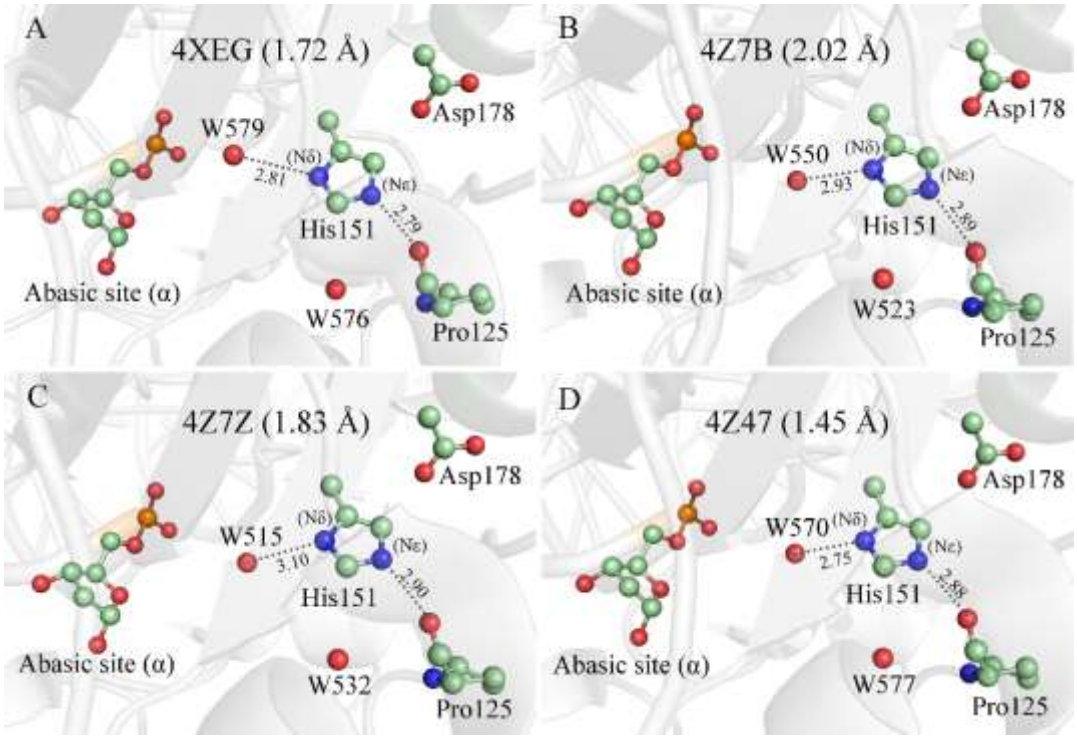


Figure S12. Four high-resolution crystal structures of the product complex of TDG, showing that His151 exclusively adopts conformation A when the abasic site solely contains the α anomer.

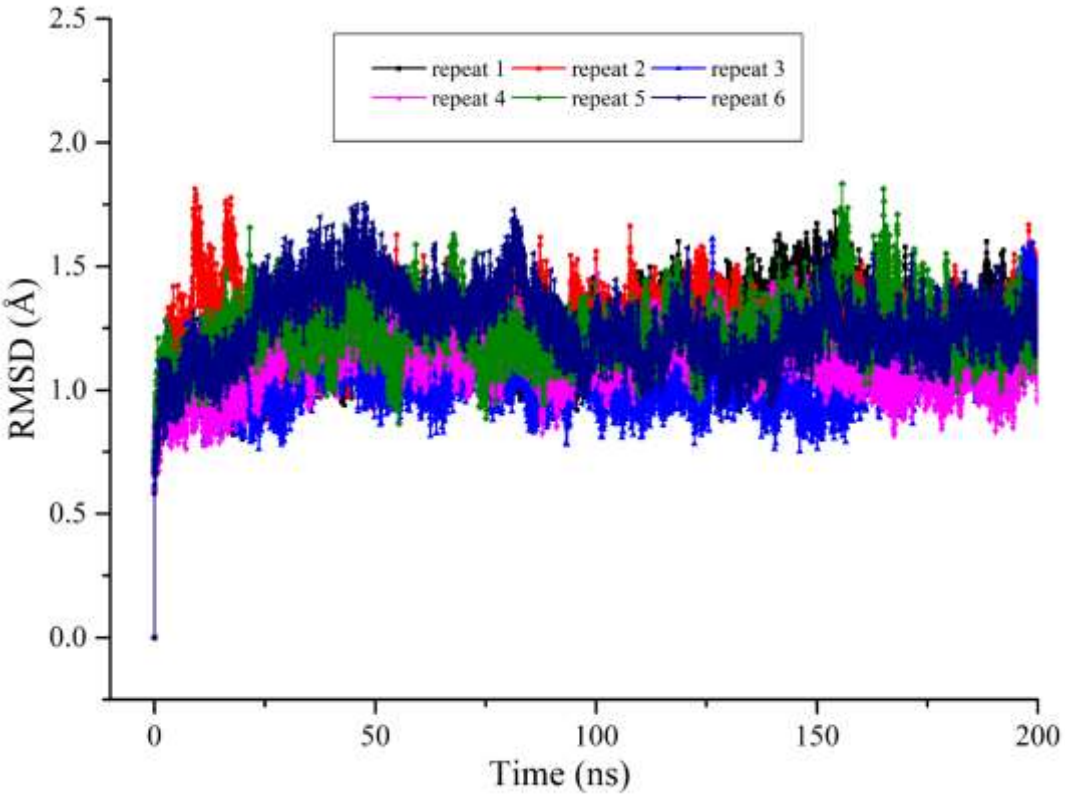


Figure S13. Root mean square deviation (RMSD) values of the protein backbone during the 6 independent 200 ns MD simulations. The small RMSD values indicate a stable protein scaffold, which facilitates the formation of a proton transfer channel.

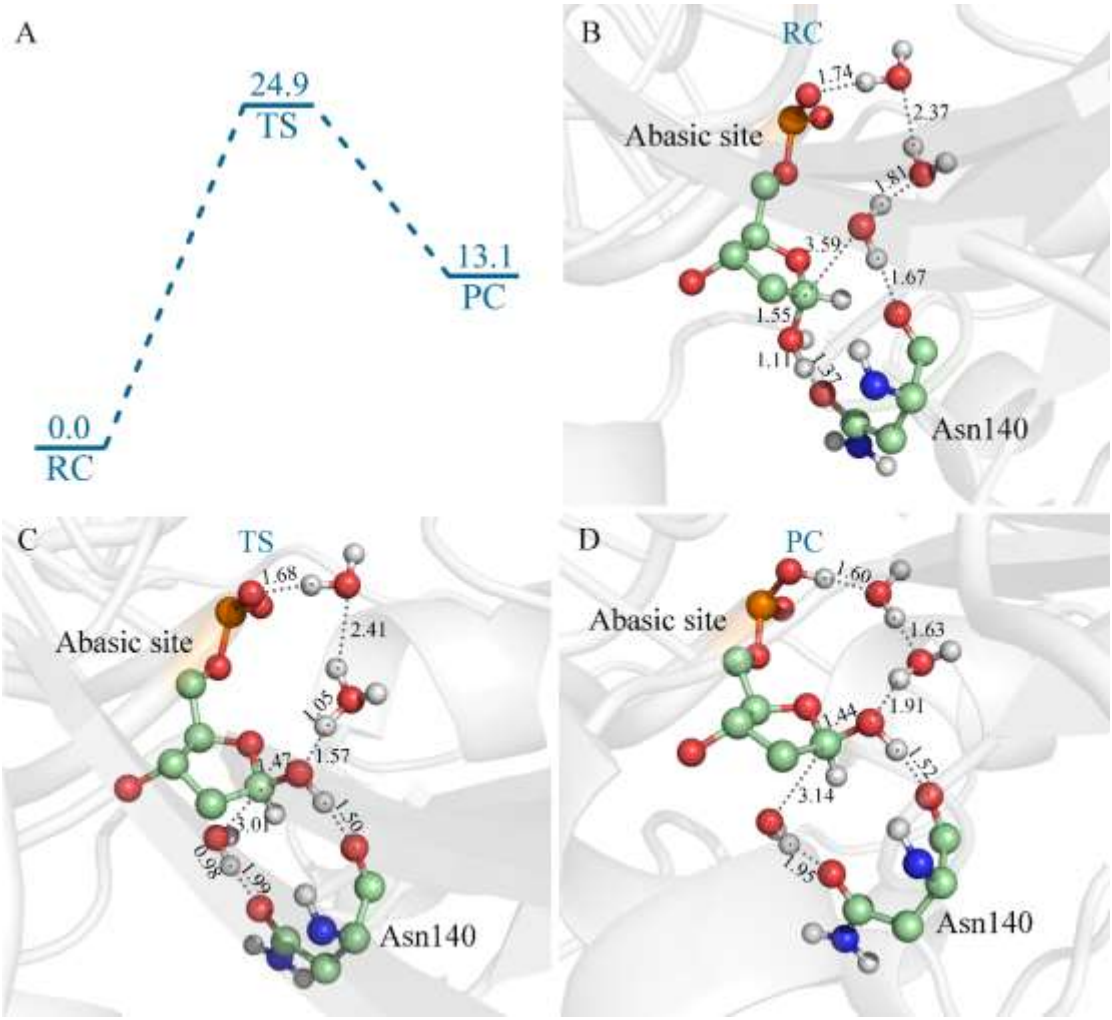


Figure S14. The phosphate-mediated displacement pathway is disfavored over the His151-mediated pathway. (A) QM/MM calculated energy profile of the phosphate-mediated displacement reaction. QM/MM optimized geometries of the reactant complex (RC), transition state (TS), and the β-anomeric product complex (PC) are shown in B, C, and D, respectively. Distances are given in Å.

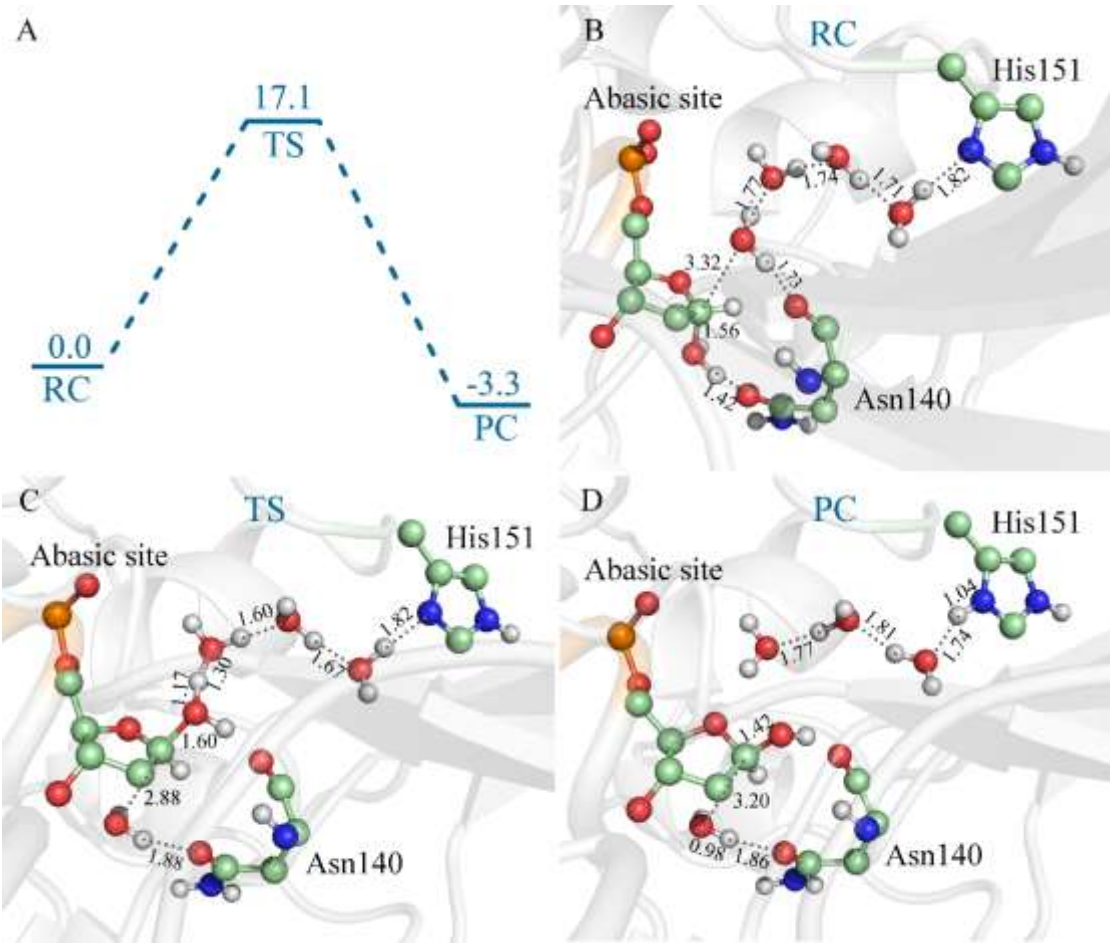


Figure S15. The His151-assisted displacement pathway is kinetically and thermodynamically feasible. (A) QM/MM calculated energy profile of the His151-mediated displacement reaction (snapshot 2). QM/MM optimized geometries of the reactant complex (RC), transition state (TS), and the β-anomeric product complex (PC) are shown in B, C, and D, respectively. Distances are given in Å.

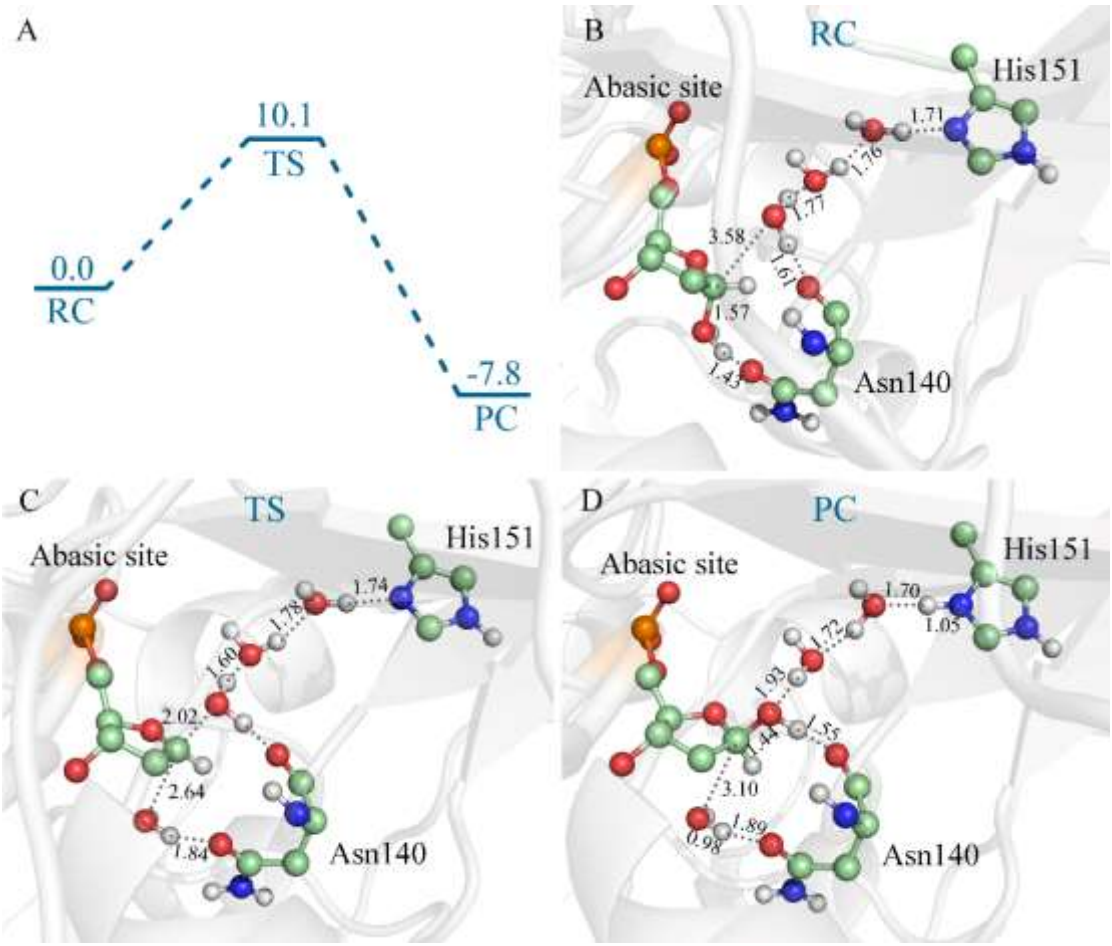


Figure S16. The His151-assisted displacement pathway is kinetically and thermodynamically feasible. (A) QM/MM calculated energy profile of the His151-mediated displacement reaction (snapshot 3). QM/MM optimized geometries of the reactant complex (RC), transition state (TS), and the β-anomeric product complex (PC) are shown in B, C, and D, respectively. Distances are given in Å.

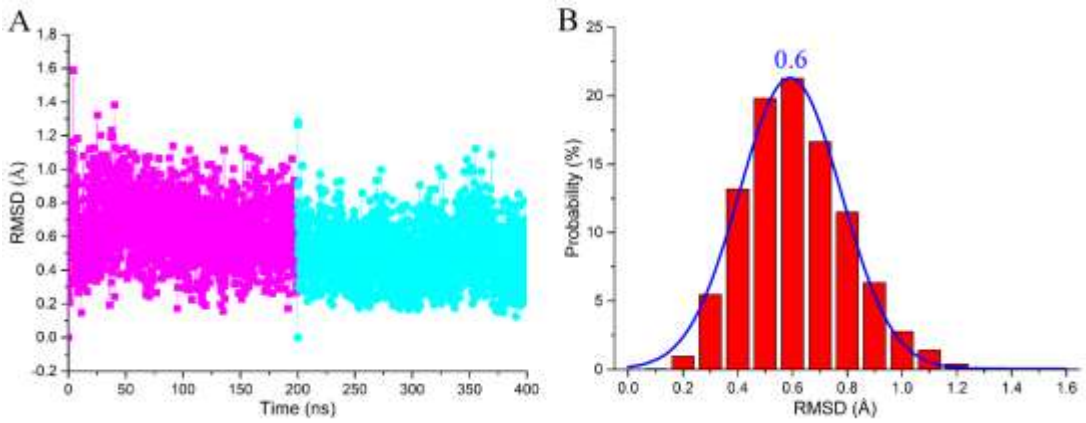


Figure S17. Acetate is stable in the active site. (A) Root mean square deviation (RMSD) values of the acetate ion along the 2 independent 200 ns MD simulations. (B) Distributions of the RMSD values.

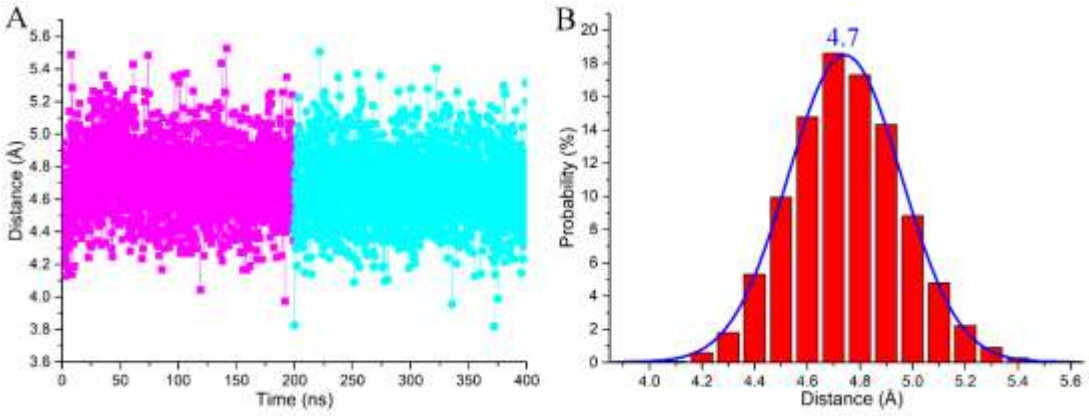


Figure S18. Acetate is stable in the active site. (A) Time evolution of the distance between C1′ anomeric carbon and acetate C1 atom along 2 independent 200 ns MD simulations. (B) Distributions of the distances.

Table S1. Energy data of the His151-mediated displacement reaction of snapshot 2.

Snapshot 2	Activation barrier (in kcal/mol)	Reaction energy (in kcal/mol)
Electronic energy	17.1	-3.3
Correction to Gibbs free energy	-2.6	-0.5
Gibbs free energy	14.5	-3.8

Table S2. H-bonding interaction energy (in kcal/mol) between the α-anomeric abasic site and the side chain of Asn140 and the main chain of Thr197, estimated with B3LYP-D3/def2-TZVPP and M062X-D3/def2-TZVPP methods.

H-bonding interaction	Abasic site---Asn140	Abasic site---Thr197
B3LYP-D3 (gas)	33.2	28.1
M062X-D3 (gas)	34.1	27.5
B3LYP-D3 (water)	27.4	14.7

Table S3. QM/MM calculated activation barriers (in kcal/mol) of the His151-mediated displacement reaction from three different snapshots.

	Snapshot 1	Snapshot 2	Snapshot 3
Activation barrier	15.0	17.1	10.1
Average value	**14.1**		
Deviation	0.9	3.0	4.0
Average deviation	**2.6**		

Table S4. QM/MM calculated reaction energies (in kcal/mol) of the His151-mediated displacement reaction from three different snapshots.

	Snapshot 1	Snapshot 2	Snapshot 3
Reaction energy	-3.3	-3.3	-7.8
Average value	**-4.8**		
Deviation	1.5	1.5	3.0
Average deviation	**2.0**		

Table S5. Gibbs free energy barrier ($\Delta G^{\dagger}$, in kcal/mol), reaction energy (ΔG, in kcal/mol), imaginary frequency (in cm^{-1}) of the transition state, transmission coefficient, and the estimated energy barrier reduction (in kcal/mol) by quantum mechanical tunneling for the water-assisted ring-opening reactions. Frequency analysis was performed at the B3LYP-D3/B1 level, and the electronic energies were further corrected at the B3LYP-D3/def2-TZVPP level.

Number of water molecules	$\Delta G^{\dagger}$ (kcal/mol)	ΔG (kcal/mol)	Imaginary frequency (cm^{-1})	Transmission coefficient	$\Delta G_{Tunneling}$ (kcal/mol)
0	37.5	3.6	-1665.3	1,242,335	8.4
1	23.9	4.6	-1224.0	13.9	1.6
2	21.3	5.0	-526.6	1.33	0.2

Table S6. Gibbs free energy barrier ($\Delta G^{\dagger}$, in kcal/mol), reaction energy (ΔG, in kcal/mol), imaginary frequency (in cm^{-1}) of the transition state, transmission coefficient, and the estimated energy barrier reduction (in kcal/mol) by quantum mechanical tunneling for the water-assisted ring-opening reactions. Frequency analysis was performed at the B3LYP-D3/B1 level, and the electronic energies were further corrected at the M062X-D3/def2-TZVPP level.

Number of water molecules	$\Delta G^{\dagger}$ (kcal/mol)	ΔG (kcal/mol)	Imaginary frequency (cm^{-1})	Transmission coefficient	$\Delta G_{Tunneling}$ (kcal/mol)
0	35.9	-1.2	-1665.3	4,109,027	9.1
1	23.4	-0.1	-1224.0	14.7	1.6
2	21.2	0.3	-526.6	1.33	0.2

Table S7. Atom types and charges for acetate ion.

Atom	Atom type	Atom Charge
C1	c	0.943441
O1	o	-0.859454
O2	o	-0.859454
C2	c3	-0.415428
H1	hc	0.063632
H2	hc	0.063632
H3	hc	0.063632

Table S8. Non-standard improper dihedral parameters for the acetate ion.

Improper Dihedral	Barrier (kcal/mol)	Phase(º)	Periodicity
c3-c-c-o	1.1	180.0	2.0

Table S9. Atom types[a] and charges for oxocarbenium ion.

Atom	Atom type	Atom charge	Atom	Atom type	Atom charge
P	P	1.1659	O4’	OS	-0.3691
OP1	O2	-0.7761	C1’	CT	0.5431
OP2	O2	-0.7761	H1’	H2	0.0838
O5’	OS	-0.4954	C3’	CT	0.3713
C5’	CT	0.0877	H3’	H1	0.0985
H5’	HC	0.0754	C2’	CT	-0.0854
H5’’	HC	0.0754	H2’	HC	0.0718
C4’	CT	0.3330	H2’’	HC	0.0718
H4’	H1	0.0476	O3’	OS	-0.5232

a: Amber ff14SB atom type was used.

Table S10. Non-standard bond parameters for oxocarbenium ion.

Bond	Force constant ((kcal/mol)/Å^2)	Equilibrium value (Å)
O2-P	479.50	1.487
OS-P	330.60	1.615
CT-OS	308.60	1.432
CT-HC	330.60	1.097
CT-CT	300.90	1.538
CT-H1	330.60	1.097
CT-H2	331.70	1.096

Table S11. Non-standard angle parameters for oxocarbenium ion.

Angle	Force constant ((kcal/mol)/rad^2)	Equilibrium value (º)
CT-OS-P	77.7	119.540
O2-P-O2	45.8	115.800
O2-P-OS	43.9	115.460
HC-CT-OS	51.0	108.700
CT-CT-OS	68.0	107.970
CT-CT-H1	46.4	109.560
CT-CT-CT	62.9	111.510
HC-CT-HC	39.4	107.580
CT-CT-HC	46.3	109.800
CT-OS-CT	62.7	112.480
H1-CT-OS	50.8	109.780
H2-CT-OS	50.9	109.580
CT-CT-H2	46.2	110.220

Table S12. Non-standard dihedral parameters for oxocarbenium ion

Dihedral	Divider	Barrier (kcal/mol)	Phase (º)	Periodicity
HC-CT-OS-P	3	1.150	0.000	3.000
CT-CT-OS-P	3	1.150	0.000	-3.000
CT-CT-OS-P	1	3.950	180.000	1.000
CT-OS-P -O2	1	0.800	0.000	-2.000
CT-OS-P -O2	1	0.550	0.000	3.000
H1-CT-CT-OS	1	0.000	0.000	-3.000
H1-CT-CT-OS	1	0.250	0.000	1.000
OS-CT-CT-OS	1	0.144	0.000	-3.000
OS-CT-CT-OS	1	1.175	0.000	2.000
CT-CT-CT-OS	9	1.400	0.000	3.000
CT-CT-OS-CT	1	0.383	0.000	-3.000
CT-CT-OS-CT	1	0.100	180.000	2.000
CT-CT-CT-H1	9	1.400	0.000	3.000
CT-CT-CT-CT	1	0.180	0.000	-3.000
CT-CT-CT-CT	1	0.250	180.000	-2.000
CT-CT-CT-CT	1	0.200	180.000	1.000
H1-CT-CT-HC	9	1.400	0.000	3.000
HC-CT-CT-OS	1	0.000	0.000	-3.000
HC-CT-CT-OS	1	0.250	0.000	1.000
CT-CT-CT-HC	1	0.160	0.000	3.000
H2-CT-OS-CT	3	1.150	0.000	3.000
H1-CT-OS-CT	3	1.150	0.000	3.000
CT-CT-CT-H2	9	1.400	0.000	3.000
H2-CT-CT-HC	9	1.400	0.000	3.000
H1-CT-CT-H1	9	1.400	0.000	3.000

Table S13. Missing bond parameter for the bond between oxocarbenium and the water nucleophile.

Bond	Force constant ((kcal/mol)/Å^2)	Equilibrium value (Å)
CT-OW	300.00	1.550

Table S14. Missing angle parameters for the bond between oxocarbenium and the water nucleophile.

Angle	Force constant ((kcal/mol)/rad^2)	Equilibrium value (º)
CT-CT-OW	60.0	109.380
OS-CT-OW	60.0	105.760
CT-OW-HW	20.0	110.000
H2-CT-OW	46.2	105.830

Table S15. Missing dihedral parameters for the bond between oxocarbenium and the water nucleophile.

Dihedral	Divider	Barrier (kcal/mol)	Phase (º)	Periodicity
X-CT-OW-X	3	0.000	0.000	3.000
CT-OW-HW-HW	1	0.000	0.000	3.000

Cartesian coordinates of the QM region for key species

His151-mediated pathway_snapshot 1-RC (RC_B of Figure 5 in the main text)				His151-mediated pathway_snapshot 2-RC (RC of Figure S13)			
C	36.9559091	30.9331763	44.1005644	C	50.4060727	30.6491987	39.3289476
H	37.3638476	30.0129597	44.5260249	H	50.4530535	29.5595838	39.2853590
H	36.2556638	31.3172080	44.8516954	H	50.2774764	30.9748203	38.2903936
C	36.1863415	30.6268804	42.8367988	C	51.7080037	31.2151541	39.8496209
O	35.8481024	31.5164381	41.9989717	O	51.8181499	32.3995823	40.2717052
N	35.8262051	29.3586502	42.6792443	N	52.7576800	30.3987896	39.7735430
H	35.1697339	29.1016083	41.9396107	H	53.7027058	30.7424478	39.9608846
H	36.1704615	28.6256206	43.3027463	H	52.6448398	29.4251828	39.4871557
C	47.4428128	35.6120092	40.9495154	C	42.3886561	30.1121334	47.2975404
H	48.4040362	36.0982971	40.7487886	H	41.5274171	29.9787356	47.9610034
H	46.6785039	36.3955984	40.9902809	H	42.4371143	31.1686210	47.0125704
C	47.4505809	34.8739316	42.2623962	C	42.2506618	29.2952629	46.0421156
N	46.3093490	34.7906515	43.0417210	N	42.8513188	29.6962188	44.8557080
C	46.6188617	34.0425869	44.0912839	C	42.5523688	28.7724815	43.9573884
H	45.9520075	33.7566405	44.8945099	H	42.8789497	28.7843381	42.9306895
N	47.9095649	33.6444190	44.0316053	N	41.7823697	27.7916816	44.4961093
H	48.3333104	33.0266320	44.7273884	H	41.4655969	26.9593679	44.0032729
C	48.4585044	34.1596001	42.8745478	C	41.5784488	28.1130740	45.8273703
H	49.4827141	33.9758210	42.5889514	H	41.0018217	27.4903221	46.4913852
C	44.7308677	37.7589240	37.4846907	C	44.5973021	34.1493917	48.8591396
H	45.7437788	38.1670499	37.5565999	H	43.6591139	34.0369582	49.4119861
H	44.2055265	38.2842017	36.6791000	H	45.0777946	35.0732861	49.2021252
C	43.9566464	37.9360722	38.7729106	C	44.3410187	34.2438789	47.3729850
C	42.5619012	37.7719764	38.7655541	C	45.3295956	34.7266260	46.4996638
H	42.0540162	37.5657908	37.8301734	H	46.2882065	35.0520870	46.8962193
C	41.8117091	37.8628562	39.9351087	C	45.1047147	34.7944254	45.1230425
H	40.7346843	37.7385370	39.9057031	H	45.8863651	35.1370882	44.4508304
C	42.4535896	38.1311495	41.1461787	C	43.8627072	34.4153033	44.6013754
O	41.6526338	38.2138974	42.2746719	O	43.6615691	34.5896276	43.2487745
H	42.1888008	38.0579946	43.0982208	H	42.9711108	33.9508630	42.9045936
C	43.8335201	38.3446928	41.1748092	C	42.8583686	33.9519694	45.4547417
H	44.3254162	38.5846236	42.1127648	H	41.8927794	33.6716168	45.0432653
C	44.5734969	38.2454394	39.9914106	C	43.1069562	33.8701430	46.8262529
H	45.6471434	38.4142782	40.0200177	H	42.3214908	33.5281535	47.4951285
C	41.5172139	37.6644192	34.0006099	C	48.2454261	36.8337657	50.1485968
H	41.2107007	36.6245820	33.8505259	H	49.0483701	36.1067131	50.2861484
H	42.6048639	37.7465205	33.9084849	H	47.3944989	36.5422451	50.7706658
C	41.0934622	38.1533122	35.3794150	C	47.8111967	36.8948617	48.6918122
O	41.6234772	39.1682234	35.8742696	O	46.7175375	37.4122619	48.3883932

N	40.1392500	37.4328479	35.9950211	N	48.6634556	36.3793018	47.7865369
H	39.7702105	37.6801085	36.9139245	H	48.4659447	36.4469216	46.7828494
H	39.8182388	36.5511220	35.5883717	H	49.5502684	35.9650266	48.0778415
C	40.8621182	33.1325940	46.5677799	C	45.3739192	29.7806900	39.0107995
H	41.5004887	32.3289225	46.9475622	H	45.3755726	28.7118780	38.7791333
H	39.8375648	32.7589995	46.4956653	H	46.2971396	30.2135971	38.6037713
C	41.2777942	33.6569349	45.1929623	C	45.3717394	30.0569562	40.5108372
O	40.4657020	34.2653635	44.4757626	O	45.2355119	31.2099504	40.9678786
N	42.5526507	33.4314174	44.8098751	N	45.6250853	29.0019651	41.3106104
H	42.8965028	33.9187212	43.9795395	H	45.5799096	29.1649833	42.3153646
H	43.2305218	32.9768237	45.4260943	H	45.6156165	28.0414692	40.9589585
C	36.8802359	33.7662307	32.6922773	C	54.6664745	36.2558365	48.8488872
H	36.4551047	33.0770871	33.4270365	H	55.1180922	35.5292308	48.1678140
O	38.0126465	34.4638612	33.2171436	O	53.2424229	36.1026833	48.9283272
P	39.0234713	33.7622313	34.2848585	P	52.5296358	34.6803725	48.6064008
O	39.8558457	34.8758545	34.8781544	O	53.2549033	33.5290031	49.2936288
O	39.7536794	32.5927631	33.6355582	O	51.0453020	34.8963583	48.8613347
O	38.0063227	33.1363360	35.4031474	O	52.8258630	34.4309831	47.0224357
C	37.4045155	34.0656727	36.3233894	C	52.1953432	35.2634885	46.0328126
H	36.8996909	34.8682831	35.7732903	H	52.3297107	36.3178893	46.2928609
H	38.1788632	34.5016668	36.9651069	H	51.1280811	35.0207321	45.9732141
C	36.3672846	33.3404731	37.1622508	C	52.8872745	34.9880043	44.7140487
H	35.6119907	32.8830508	36.5236720	H	53.9575380	35.1418859	44.8265758
O	37.0243981	32.2732522	37.8988390	O	52.6667318	33.5844379	44.3681922
C	36.7641241	32.3378999	39.2290727	C	52.1160408	33.4588970	43.1393433
H	37.6151272	31.9896039	39.8085498	H	51.4618877	32.5916769	43.0889973
C	35.7307714	34.2778099	38.2256726	C	52.3410298	35.8139181	43.5271664
H	36.0543748	35.3146708	38.0813217	H	51.6937551	36.6292641	43.8665919
C	36.2439924	33.7253178	39.5639324	C	51.5463649	34.7936007	42.7025765
H	37.0964554	34.3157409	39.9088542	H	50.4969993	34.8058032	43.0041006
H	35.4713354	33.7233542	40.3352523	H	51.6298274	34.9711498	41.6283296
O	34.2890517	34.2465041	38.2268273	O	53.3975747	36.3538236	42.7215929
P	33.4544848	35.0828456	37.0833300	P	54.1831129	37.7037575	43.2814656
O	31.9954387	34.7413770	37.3364609	O	55.3358405	37.9136215	42.3315954
O	34.1227314	34.8234035	35.7372636	O	54.3897957	37.5684668	44.7787394
O	33.7515556	36.6445268	37.3771043	O	53.0525831	38.8685450	43.1258634
C	33.0747807	37.3863920	38.3949947	C	52.6477326	39.3045041	41.8277216
H	33.8166179	37.7018349	39.1296621	H	51.8433508	38.6603398	41.4533191
H	32.2905904	36.7919505	38.8716291	H	53.4815134	39.2775104	41.1206212
O	39.3483093	34.6950072	40.1860821	O	53.2645428	33.1089838	42.1399396
H	40.0714142	34.3492042	39.6022909	H	52.7814086	32.7478090	41.2501539
H	39.2098849	33.9672244	40.8392457	H	53.8125585	32.3722205	42.5570598

O	41.3708145	33.4556887	38.7669804
H	41.5714123	33.6952858	37.8262447
H	42.1383631	33.8030892	39.2860008
O	35.6493430	31.3157520	39.5665393
H	35.8652735	30.4366627	39.1426426
H	35.6429689	31.2470427	40.6757013
O	43.3549582	34.8384047	40.0818830
H	43.4253905	34.9220886	41.0700291
H	43.0226438	35.7142605	39.8114008
O	43.6730926	35.2582489	42.7674891
H	44.6760018	35.1847505	42.8447726
H	43.4331695	36.1109225	43.1788664
H	37.7513968	31.6744102	44.0241517
H	40.8860901	33.9523240	47.2857878
H	41.0493820	38.2599912	33.2167129
H	47.2291222	34.9419822	40.1167686
H	44.8173842	36.7055618	37.2182135
H	37.1151171	33.2401265	31.7670139
H	36.1487929	34.5142748	32.3865184
H	32.6143873	38.2748223	37.9627948

His151-mediated pathway_snapshot 1-TS (TS_B in Figure 5 of the main text)

C	37.0377874	30.8882727	44.1020794
H	37.4272934	29.9451756	44.4926825
H	36.3394356	31.2479041	44.8674069
C	36.2658935	30.6703121	42.8075958
O	36.0385542	31.5665669	41.9674307
N	35.7791419	29.4252543	42.6740491
H	35.1588676	29.2022143	41.8938810
H	36.0930812	28.6654330	43.2784700
C	47.4116395	35.6015779	40.9481000
H	48.3751358	36.0840825	40.7494979
H	46.6511991	36.3893856	40.9841139
C	47.4112713	34.8666050	42.2618462
N	46.2596464	34.7711809	43.0253561
C	46.5659308	34.0312492	44.0827117
H	45.8935728	33.7412261	44.8799482
N	47.8623772	33.6500003	44.0408530
H	48.2872762	33.0386691	44.7424160
C	48.4199871	34.1675243	42.8890765
H	49.4499705	33.9949795	42.6153385
O	45.2150113	30.6974651	43.7713225
H	45.1170354	31.1831437	42.9239755
H	44.3111046	30.5235299	44.1527623
O	46.2821889	31.6998089	46.0360243
H	45.9900162	31.2880824	45.1784440
H	45.9679846	32.6204659	45.9655242
O	48.9377417	32.0554497	46.5135846
H	47.9752633	31.8359786	46.4333448
H	49.0972197	32.3299932	47.4533595
O	49.0206490	33.7102799	44.3140237
H	49.0421929	33.1893108	45.1548505
H	48.9758916	33.0433230	43.5940394
H	49.4976831	30.9533617	39.8489286
H	44.5198561	30.2350702	38.5086223
H	48.6242624	37.8031524	50.4723863
H	43.2807614	29.8574927	47.8697060
H	45.2322072	33.3060094	49.1305598
H	55.1117692	36.2121225	49.8428031
H	54.8837968	37.2777614	48.5382303
H	52.2845882	40.3265063	41.9359111

His151-mediated pathway_snapshot 2-TS (TS of Figure S13)

C	50.3554548	30.6076578	39.3849652
H	50.4400251	29.5201182	39.3486764
H	50.2498219	30.9219199	38.3401323
C	51.6192489	31.2418866	39.9508098
O	51.6581716	32.3939340	40.4279988
N	52.7148309	30.4735347	39.8249961
H	53.6399154	30.8433680	40.0555767
H	52.6453422	29.5064598	39.5099855
C	42.4102828	30.0947340	47.2690449
H	41.5473348	29.9429427	47.9260633
H	42.4433148	31.1543488	46.9950918
C	42.2950934	29.2899274	46.0039980
N	42.9280386	29.7006329	44.8372115
C	42.6397309	28.7917835	43.9195298
H	42.9856346	28.8149211	42.8989767
N	41.8489082	27.8116776	44.4284538
H	41.5300876	26.9899716	43.9177178
C	41.6181354	28.1162313	45.7592212
H	41.0246418	27.4862742	46.4024376

C	44.7033007	37.7548183	37.5014541	C	44.5939927	34.1408489	48.8474118
H	45.7195759	38.1544192	37.5725836	H	43.6582185	34.0085804	49.3996173
H	44.1817288	38.2857881	36.6972678	H	45.0618622	35.0672311	49.2000765
C	43.9326782	37.9404970	38.7902240	C	44.3365244	34.2474590	47.3636216
C	42.5348943	37.8004470	38.7830547	C	45.3015524	34.7966026	46.5034661
H	42.0241595	37.6032099	37.8474392	H	46.2320174	35.1813048	46.9138183
C	41.7866539	37.9091438	39.9530208	C	45.0802224	34.8676779	45.1259341
H	40.7065270	37.8085994	39.9280008	H	45.8393052	35.2754614	44.4636330
C	42.4343819	38.1718649	41.1616507	C	43.8650829	34.4259089	44.5898996
O	41.6333438	38.2750105	42.2916880	O	43.6686225	34.5989966	43.2401314
H	42.1675182	38.1102943	43.1194118	H	42.9836016	33.9542579	42.8918703
C	43.8168953	38.3639733	41.1907059	C	42.8805994	33.9036333	45.4332032
H	44.3119503	38.6037649	42.1270056	H	41.9331652	33.5792941	45.0129704
C	44.5545733	38.2463500	40.0074442	C	43.1250439	33.8204639	46.8045864
H	45.6300836	38.4026520	40.0342541	H	42.3537896	33.4353192	47.4660075
C	41.5657942	37.6957918	33.9932134	C	48.2420748	36.8339009	50.1546629
H	41.2724044	36.6523231	33.8459174	H	49.0394437	36.1054112	50.3153304
H	42.6513499	37.7941995	33.8971768	H	47.3801209	36.5511863	50.7651556
C	41.1373911	38.1819337	35.3708649	C	47.8295085	36.8757536	48.6912038
O	41.6720934	39.1868871	35.8804526	O	46.7295264	37.3628065	48.3646535
N	40.1691392	37.4673744	35.9739681	N	48.7048569	36.3650102	47.8022956
H	39.7876754	37.7239561	36.8842817	H	48.5171386	36.4138842	46.7969967
H	39.8372931	36.5977155	35.5491483	H	49.6051372	35.9916196	48.1106011
C	40.7574939	33.2993478	46.4900030	C	45.3636941	29.8032408	39.0297114
H	41.3114031	32.4217478	46.8370447	H	45.3852471	28.7378933	38.7836523
H	39.7046978	33.0294228	46.3841847	H	46.2835301	30.2529542	38.6344681
C	41.2526943	33.8371741	45.1476632	C	45.3487896	30.0508274	40.5344490
O	40.5129835	34.5218730	44.4142342	O	45.1665027	31.1837134	41.0258678
N	42.5151273	33.5214344	44.7939014	N	45.6525213	28.9883065	41.3082056
H	42.9007392	33.9675417	43.9592462	H	45.6305873	29.1245305	42.3152080
H	43.1460344	33.0106644	45.4173795	H	45.6679625	28.0329424	40.9412394
C	36.9010886	33.7590142	32.6571795	C	54.7065062	36.2624207	48.9208967
H	36.5098563	33.0718252	33.4118722	H	55.1475851	35.5265629	48.2433666
O	38.0421669	34.4809809	33.1339311	O	53.2843630	36.1085169	49.0321510
P	39.0479442	33.8230561	34.2300532	P	52.5692090	34.7086016	48.6455247
O	39.8944687	34.9544153	34.7735932	O	53.2509874	33.5169722	49.3050246
O	39.7706146	32.6172995	33.6432162	O	51.0794207	34.9404860	48.8768298
O	38.0286052	33.2646096	35.3748762	O	52.8874390	34.5131909	47.0644891
C	37.3393037	34.2401736	36.1791454	C	52.3796156	35.4680808	46.1162692
H	36.6268513	34.8023896	35.5694627	H	52.8819250	36.4264992	46.2481507
H	38.0633532	34.9349742	36.6222778	H	51.2974756	35.5891343	46.2563957
C	36.5949566	33.4998627	37.2708215	C	52.6720307	34.9275669	44.7354395

H	35.9050920	32.7587766	36.8608031	H	53.7359634	34.7235830	44.6121020
O	37.5798469	32.7478190	38.0376103	O	51.9814296	33.6533852	44.6019221
C	37.5006917	32.9933389	39.3420049	C	51.1700951	33.6221929	43.5280021
H	37.6595133	32.1173852	39.9642021	H	51.2530938	32.6886869	42.9745720
C	35.8742488	34.4246009	38.2919685	C	52.1654793	35.8338534	43.5860948
H	36.1693826	35.4694062	38.1371921	H	51.5612046	36.6573666	43.9837817
C	36.3388347	33.9008358	39.6621692	C	51.3036490	34.9002804	42.7146107
H	36.6227352	34.6969839	40.3516465	H	50.3288475	35.3308511	42.4676844
H	35.5483381	33.2991877	40.1139757	H	51.8352075	34.6774747	41.7896387
O	34.4411318	34.3362261	38.2605351	O	53.2208664	36.3745067	42.7907451
P	33.5540338	35.0935599	37.1115980	P	54.0872635	37.6732639	43.3314723
O	32.1181821	34.6797364	37.3753636	O	55.2386566	37.8340229	42.3714853
O	34.2160387	34.8479107	35.7590169	O	54.3144363	37.5455707	44.8278132
O	33.7639391	36.6782899	37.3762205	O	53.0182621	38.9009150	43.1792963
C	33.0547414	37.3839725	38.3978074	C	52.6254259	39.3235785	41.8732414
H	33.7634861	37.6686341	39.1792839	H	51.8200304	38.6810257	41.4970976
H	32.2487272	36.7777206	38.8191930	H	53.4633559	39.2817270	41.1715074
O	38.8670690	33.8872560	39.7497340	O	53.6961056	33.2139308	42.2047779
H	39.7203460	33.6720621	39.1804501	H	53.1601732	32.8671274	41.4612752
H	39.0801871	33.5496862	40.6732797	H	54.0274105	32.4112031	42.6736148
O	41.1586253	33.4386704	38.6708735	O	45.3058991	30.7988554	43.8514740
H	41.3908964	33.6829523	37.7333024	H	45.1866430	31.1824792	42.9528770
H	41.8541878	33.8842375	39.2294120	H	44.4070689	30.5601269	44.2140145
O	35.4876934	31.0195782	39.1871662	O	46.4895482	31.9229764	45.9614809
H	35.8009862	30.1585845	38.8314680	H	46.1225283	31.4813315	45.1361532
H	35.5549514	30.9502369	40.1620232	H	46.0339568	32.7876288	45.9880912
O	43.1299070	34.8269391	39.9804866	O	49.0668745	32.3695759	46.1436774
H	43.2730123	34.8983397	40.9635375	H	48.0650756	32.1976650	46.0781224
H	42.9034654	35.7404940	39.7224059	H	49.2630780	32.6466269	47.0849031
O	43.6332908	35.2342238	42.6467154	O	49.6687503	33.5503768	44.0827989
H	44.6356876	35.1495203	42.7532534	H	49.5053440	33.0485501	45.1279841
H	43.3939125	36.0857054	43.0566368	H	49.2206744	32.9261460	43.4387743
H	37.8398622	31.6255395	44.0677153	H	49.4190819	30.8877445	39.8674839
H	40.8289013	34.0666010	47.2609055	H	44.5110910	30.2503733	38.5186266
H	41.0843641	38.2819832	33.2104798	H	48.6185908	37.8048290	50.4765346
H	47.2001065	34.9295511	40.1164144	H	43.3021592	29.8457213	47.8440373
H	44.7819518	36.7015139	37.2323238	H	45.2406411	33.3031291	49.1084455
H	37.1208271	33.2284867	31.7307224	H	55.1618198	36.2312177	49.9107366
H	36.1498552	34.4928524	32.3652945	H	54.9149994	37.2804764	48.5920193
H	32.6128637	38.2846085	37.9715846	H	52.2690832	40.3491977	41.9691175
His151-mediated pathway_snapshot 1-PC				**His151-mediated pathway_snapshot 2-PC**			

(PC$_B$ in Figure 5 of the main text)				(PC of Figure S13)			
C	37.1584829	30.8461300	44.0558715	C	50.3416832	30.5577688	39.4184791
H	37.5063846	29.8871549	44.4467577	H	50.4449424	29.4727589	39.3619173
H	36.4438357	31.2138769	44.8024683	H	50.2338007	30.8899241	38.3792934
C	36.4276132	30.6761882	42.7279184	C	51.5911773	31.2093099	39.9978026
O	36.2619662	31.5970092	41.9043196	O	51.6090086	32.3691881	40.4489555
N	35.9113463	29.4468199	42.5551669	N	52.6943959	30.4446812	39.9112133
H	35.3153867	29.2532220	41.7484635	H	53.6108622	30.8286423	40.1523779
H	36.1744869	28.6710682	43.1627532	H	52.6419861	29.4761269	39.5991985
C	47.0759083	35.5073484	40.9661678	C	42.4586624	30.0811658	47.2276655
H	48.0105501	36.0644498	40.8445734	H	41.5809861	29.9549551	47.8682580
H	46.2595989	36.2377764	40.9533264	H	42.5054794	31.1336585	46.9268558
C	47.0629349	34.7776677	42.2771072	C	42.3480446	29.2339447	45.9946744
N	45.9058208	34.6087618	43.0301167	N	43.0306496	29.5599929	44.8284636
C	46.1838341	33.9156824	44.1376094	C	42.7923062	28.6516207	43.8874648
H	45.4772350	33.6121574	44.8975144	H	43.2298054	28.6716009	42.9031236
N	47.4916343	33.6412962	44.1315122	N	41.9524005	27.7403478	44.3966499
H	47.9472414	33.0715072	44.8552957	H	41.6162403	26.9230109	43.8818664
C	48.0656850	34.1641894	42.9866544	C	41.6598758	28.0802689	45.7127046
H	49.1187753	34.0608532	42.7681145	H	41.0203244	27.4754565	46.3357756
C	44.6531211	37.7181530	37.4339074	C	44.6033528	34.1353382	48.8419336
H	45.6702869	38.1177504	37.5006671	H	43.6760527	34.0119049	49.4109031
H	44.1240404	38.2609185	36.6422887	H	45.0755084	35.0666927	49.1758699
C	43.9008681	37.8783813	38.7371022	C	44.3186650	34.2240086	47.3619783
C	42.5043898	37.7310848	38.7559409	C	45.2726048	34.7514030	46.4751696
H	41.9723131	37.5616364	37.8267638	H	46.2195347	35.1222043	46.8586350
C	41.7832407	37.7889159	39.9460071	C	45.0232975	34.8160310	45.1031812
H	40.7033561	37.6846804	39.9360146	H	45.7774255	35.2013294	44.4231281
C	42.4513511	38.0040025	41.1560543	C	43.7891482	34.3911551	44.5980726
O	41.6763720	38.0462770	42.2931054	O	43.5609512	34.5632519	43.2525003
H	42.2440390	37.9744294	43.1163931	H	42.8939690	33.8995864	42.9165887
C	43.8355015	38.2030309	41.1586381	C	42.8145518	33.8913971	45.4659809
H	44.3457211	38.4140775	42.0938599	H	41.8438290	33.6081605	45.0680028
C	44.5447805	38.1448747	39.9525369	C	43.0885093	33.8109636	46.8342980
H	45.6180259	38.3254974	39.9577374	H	42.3207257	33.4579528	47.5192142
C	41.6410701	37.7366747	33.9348421	C	48.2408598	36.8131091	50.1199231
H	41.3819931	36.6856638	33.7815139	H	49.0491785	36.0917624	50.2562847
H	42.7222688	37.8732102	33.8418186	H	47.3921765	36.5149456	50.7423045
C	41.1847469	38.2046075	35.3106984	C	47.8030046	36.8607689	48.6629401
O	41.6922765	39.2166561	35.8373225	O	46.7036415	37.3695900	48.3585921
N	40.2172671	37.4708117	35.8841451	N	48.6481538	36.3291388	47.7617485
H	39.7878760	37.7263500	36.7773713	H	48.4338604	36.3559998	46.7588069

H	39.9136068	36.5998877	35.4400120	H	49.5406836	35.9259751	48.0565162
C	40.7748563	33.3132635	46.4840214	C	45.3545167	29.7890285	39.0135959
H	41.1420948	32.3743909	46.9077166	H	45.3646045	28.7239848	38.7650002
H	39.7131872	33.1855477	46.2570255	H	46.2789437	30.2268726	38.6150310
C	41.4823772	33.6879535	45.1883350	C	45.3614930	30.0319777	40.5164587
O	41.1018951	34.6236107	44.4616821	O	45.1217530	31.1454455	41.0233812
N	42.5051188	32.8799565	44.8142218	N	45.7528080	28.9834047	41.2760627
H	42.9737579	33.1161532	43.9437546	H	45.8122915	29.1283843	42.2791547
H	43.0278422	32.3251160	45.4936340	H	45.8283367	28.0325202	40.9044320
C	36.9315023	33.7202930	32.6235119	C	54.6774261	36.2351145	48.8613310
H	36.5696968	33.0198297	33.3813155	H	55.1250745	35.5008454	48.1856021
O	38.0597703	34.4696199	33.0822736	O	53.2533195	36.0920662	48.9462768
P	39.1083888	33.8448838	34.1612049	P	52.5130603	34.6921377	48.5868769
O	39.9944964	34.9961474	34.5887176	O	53.2132388	33.5077031	49.2463091
O	39.7961405	32.6120058	33.5824043	O	51.0370198	34.9379108	48.8901111
O	38.1616467	33.3393651	35.3826974	O	52.7571264	34.4691132	47.0002597
C	37.3749156	34.3366118	36.0796829	C	52.3812918	35.5160008	46.0700535
H	36.4484060	34.5124517	35.5297511	H	53.1676963	36.2720084	46.0556920
H	37.9378607	35.2741528	36.1498102	H	51.4348285	35.9696769	46.3859416
C	37.0568099	33.8410603	37.4727354	C	52.2296925	34.9208549	44.6906022
H	36.6619793	32.8175242	37.4648802	H	53.0826135	34.2833607	44.4376157
O	38.2734041	33.8919426	38.2520654	O	51.0061991	34.1544756	44.6450861
C	37.9026368	33.8063072	39.6314799	C	50.5815893	34.0441308	43.2806925
H	37.8113332	32.7560784	39.9231775	H	50.9451091	33.1032419	42.8620547
C	36.0914936	34.7539730	38.2834697	C	52.0542092	35.9736251	43.5663991
H	36.2136164	35.7980202	37.9731757	H	51.5538829	36.8638807	43.9587516
C	36.5668468	34.5542890	39.7319141	C	51.1523746	35.2644442	42.5499667
H	36.7312399	35.5099690	40.2390607	H	50.3302585	35.9046518	42.2208387
H	35.8334020	33.9670733	40.2903637	H	51.7436620	34.9583492	41.6850519
O	34.6936446	34.4043183	38.1930811	O	53.2750160	36.3679699	42.9316901
P	33.6932696	35.0984367	37.1077748	P	54.1145673	37.6904749	43.4142183
O	32.2934644	34.6030808	37.4308189	O	55.2631753	37.8268991	42.4430737
O	34.2720366	34.8990739	35.7092719	O	54.3630366	37.6384060	44.9122512
O	33.8105277	36.6984966	37.3581649	O	53.0367270	38.9081474	43.2236844
C	33.0911992	37.3727197	38.3917755	C	52.6405373	39.3008805	41.9106170
H	33.7925085	37.6594994	39.1806318	H	51.8328764	38.6515706	41.5488267
H	32.2957125	36.7454455	38.8025273	H	53.4769464	39.2458430	41.2076310
O	38.9378817	34.4256701	40.3764179	O	53.5166471	33.1433820	42.3870051
H	40.2539347	33.7720407	38.0317916	H	52.9623314	32.8298848	41.6420363
H	39.2850920	33.7503178	41.0162424	H	53.8868038	32.3276062	42.7974877
O	41.2200024	33.6046358	38.0440311	O	45.1879287	30.7646195	43.7881985
H	41.5587451	33.8117294	37.1399439	H	45.2167612	31.1843197	42.8962132

H	42.3291894	34.2234652	39.2421034	H	43.7448309	30.2976056	44.6407475
O	35.9537107	31.1198241	39.0346164	O	46.4875153	31.8616042	45.9500106
H	36.1400514	30.1975516	38.7594175	H	45.8197898	31.2150768	44.3993403
H	36.0125291	31.1281195	40.0127405	H	46.0916660	32.7539255	45.9489506
O	43.0155480	34.6877105	39.7951570	O	49.1446409	32.4422174	46.4205077
H	43.0034808	34.5907369	41.5617675	H	47.4600149	32.0333957	46.0557890
H	42.7935558	35.6312737	39.6761609	H	49.2654518	32.6177204	47.3904566
O	43.2340363	34.6471594	42.5245630	O	49.1615960	34.0519315	43.2688274
H	44.9213790	34.8599897	42.7748509	H	49.7138724	33.0809783	45.9405167
H	42.4238670	34.8982701	43.0263892	H	48.8683913	33.1276452	43.0863234
H	37.9809138	31.5614405	44.0535348	H	49.4012332	30.8174920	39.9044470
H	40.8463129	34.0865962	47.2488205	H	44.5041640	30.2471215	38.5085037
H	41.1356223	38.3086328	33.1567331	H	48.6138882	37.7825394	50.4502593
H	46.9703880	34.8404569	40.1104878	H	43.3397716	29.8370507	47.8210639
H	44.7260974	36.6684839	37.1494139	H	45.2573648	33.3040851	49.1052843
H	37.1493830	33.2030526	31.6891364	H	55.1212894	36.1966435	49.8561036
H	36.1598315	34.4372959	32.3433368	H	54.9017689	37.2542368	48.5464863
H	32.6326582	38.2695327	37.9752017	H	52.2851340	40.3283613	41.9883271
His151-mediated pathway_snapshot 3-RC (RC of Figure S14)				**Aldehyde-mediated pathway-RC (RC_A in Figure 3 of the main text)**			
C	48.3792457	41.3234462	47.0062486	C	36.9060105	30.9550088	44.1770126
H	48.7816388	42.3147195	46.7860534	H	37.3230107	30.0120086	44.5280127
H	47.4595008	41.4883878	47.5757011	H	36.2190103	31.2850089	44.9520128
C	49.3399470	40.5390774	47.8722450	C	36.1100103	30.6980088	42.9110122
O	49.2111876	39.3002060	48.0839198	O	35.7450102	31.5850090	42.1530120
N	50.2928519	41.2576504	48.4596067	N	35.8250102	29.4560084	42.6360122
H	50.8902938	40.8297476	49.1699547	H	35.2260101	29.2590084	41.8450119
H	50.4515596	42.2363917	48.2103531	H	36.1720103	28.7130082	43.2360123
C	49.5024403	37.5915706	36.2315217	C	47.5550136	35.6520102	40.9420117
H	49.4893603	37.6539411	35.1388461	H	48.5610139	36.0690103	40.8020116
H	48.9561336	36.6853807	36.5173170	H	46.8600134	36.5000104	40.9300117
C	48.7990498	38.7648194	36.8609198	C	47.4500135	34.9880100	42.2930121
N	48.4147888	38.7140954	38.1937724	N	46.2680132	34.8610100	43.0260123
C	47.7717908	39.8415128	38.4465435	C	46.5720133	34.0950097	44.0870126
H	47.3088156	40.1056431	39.3867133	H	45.8740131	33.7820096	44.8540128
N	47.7179896	40.6268971	37.3433800	N	47.8630137	33.7390096	44.0490126
H	47.3141488	41.5664684	37.3494313	H	48.3000138	33.1110095	44.7260128
C	48.3719946	39.9591611	36.3209008	C	48.4350138	34.2830098	42.9200123
H	48.4645683	40.3678046	35.3253143	H	49.4450141	34.1380097	42.5670121
C	49.9728763	33.2883898	38.1355449	C	44.6960128	37.6810108	37.5490107
H	49.8216610	33.2554443	37.0516452	H	45.6820130	38.1550109	37.6420107
H	50.0594402	32.2543872	38.4929400	H	44.1650126	38.2220109	36.7560105

C	48.7982206	33.9463423	38.8348002	C	43.9060125	37.8710108	38.8280111
C	48.6410769	33.8347844	40.2262783	C	42.5120121	37.6880108	38.8030111
H	49.3656095	33.2697754	40.8054204	H	42.0190120	37.4440107	37.8740108
C	47.5745218	34.4415796	40.8933618	C	41.7580119	37.8280108	39.9790114
H	47.4793586	34.3663387	41.9726069	H	40.6870116	37.7140108	39.9450114
C	46.6273742	35.1640159	40.1619288	C	42.4010121	38.1370109	41.1950118
O	45.5421333	35.7064136	40.8450632	O	41.6660119	38.2440109	42.3330121
H	45.3598727	36.6397892	40.5222399	H	42.2250121	38.0850109	43.1180123
C	46.7449251	35.2676322	38.7736194	C	43.8000125	38.3260109	41.2220118
H	45.9999802	35.8231274	38.2117143	H	44.2910126	38.5780110	42.1480120
C	47.8225014	34.6584050	38.1228985	C	44.5500127	38.2010109	40.0360114
H	47.8961278	34.7315037	37.0408380	H	45.6200130	38.3630109	40.0490114
C	51.7118827	30.1167498	41.2776791	C	41.5040118	37.5760107	33.9250097
H	52.6504450	30.6083468	41.5376129	H	41.2980118	36.5290104	33.7080096
H	51.6418490	30.0474114	40.1879254	H	42.5860122	37.7030108	33.9380097
C	50.5059213	30.8641438	41.8234724	C	40.9480117	37.8960108	35.2960101
O	49.3624366	30.5800904	41.4333267	O	41.2430118	38.9290111	35.8710102
N	50.7631268	31.8191090	42.7563043	N	40.1210115	37.0450106	35.8550102
H	49.9971357	32.1036150	43.3724588	H	39.6860113	37.2550106	36.7420105
H	51.7003206	31.8694942	43.1739553	H	39.9350114	36.1600103	35.3800101
C	45.8674698	42.1784714	42.7641283	C	40.8600117	33.2050095	46.5340133
H	46.1717707	43.2274315	42.7224951	H	41.4920118	32.3710092	46.8410134
H	45.8919853	41.8625796	43.8113710	H	39.8400114	32.8380094	46.4470133
C	46.7751582	41.2675203	41.9498962	C	41.2840118	33.7170096	45.1710129
O	46.5403989	40.0590098	41.7811216	O	40.5150116	34.3450098	44.4600127
N	47.8980290	41.8509301	41.4747874	N	42.5100121	33.4990096	44.7650128
H	48.5216364	41.2908437	40.9071462	H	42.7880122	33.9240097	43.8910125
H	48.0589108	42.8613135	41.5192128	H	43.1670123	32.9970094	45.3610129
C	54.3971932	31.2497697	47.1528961	C	36.7980105	33.7900096	32.7050093
H	54.2644373	32.1900472	47.6918558	H	36.2980104	33.1240095	33.4210095
O	53.8968945	31.3407167	45.8105293	O	37.9240108	34.4400098	33.3250095
P	54.0957142	32.7084467	44.9507152	P	38.9590111	33.6390096	34.2460098
O	55.5207747	33.2330840	45.0079483	O	40.0400114	34.4920098	34.7850099
O	53.4591119	32.3834320	43.6025044	O	39.7110113	32.5610093	33.5570096
O	53.2714661	33.8379716	45.7776993	O	38.0140109	33.1110095	35.4260101
C	51.8650263	33.7368504	46.0209221	C	37.5000107	34.0470097	36.3950104
H	51.5995836	32.7084704	46.2853868	H	37.0030106	34.8740100	35.8710102
H	51.3099758	34.0503141	45.1287446	H	38.3350109	34.4700098	36.9710106
C	51.5416595	34.6322950	47.2014756	C	36.5000104	33.3320095	37.3360107
H	52.1692478	34.3592354	48.0494494	H	35.7320102	32.8170094	36.7480105
O	51.8636458	36.0092544	46.8415288	O	37.2260106	32.3610092	38.1180109
C	50.8079934	36.8373860	47.0164680	C	36.6190105	32.1990092	39.3920112

H	50.7998240	37.6241986	46.2655350
C	50.0453207	34.6228851	47.5863855
H	49.4944206	33.8478847	47.0492554
C	49.5453432	36.0171786	47.1825159
H	49.0627766	35.9724317	46.2049778
H	48.8484852	36.4354139	47.9122206
O	49.8581007	34.4330960	48.9984959
P	49.9870443	32.9244463	49.6566571
O	49.8823682	33.1714068	51.1444779
O	51.1875931	32.1847573	49.0938044
O	48.6716219	32.1326962	49.0992222
C	47.3638166	32.5735402	49.5025264
H	46.9797953	33.2891060	48.7651730
H	47.3970618	33.0448187	50.4893928
O	51.0280366	37.6277444	48.3545017
H	50.3131045	38.4301077	48.3570929
H	51.9599858	38.0115019	48.3388414
O	51.0235826	36.9934204	42.2668344
H	50.6017472	37.2087588	41.3988526
H	51.3371358	36.0466375	42.1460722
O	48.9542226	36.4480010	43.9776540
H	49.6585720	36.5059918	43.2853353
H	48.9679045	37.3675686	44.3367350
O	49.7211953	37.0423703	39.8853666
H	49.1153875	36.3118322	40.0976053
H	49.1775227	37.6715631	39.3158363
H	48.0688511	40.8524780	46.0735582
H	44.8327212	42.1034235	42.4298677
H	51.7199733	29.1192281	41.7169422
H	50.5413538	37.4950849	36.5468252
H	50.9259937	33.7881326	38.3084361
H	55.4401577	30.9333756	47.1665718
H	53.8731431	30.4342866	47.6513195
H	46.7053035	31.7063950	49.5523952

His151-mediated pathway_snapshot 3-TS (TS of Figure S14)

C	48.3975072	41.3819389	46.9095751
H	48.8457089	42.3531139	46.6894608
H	47.4885237	41.5945881	47.4815609
C	49.3128139	40.5367748	47.7803503
O	49.1865682	39.3004821	47.9164679
H	37.2890106	31.7570091	40.1410115
C	35.8340102	34.2710098	38.3900110
H	36.2750104	35.2760101	38.3610109
C	36.1060103	33.5980096	39.7420113
H	36.8790105	34.1450097	40.2890115
H	35.2130101	33.5460096	40.3770115
O	34.4010098	34.3430098	38.2760109
P	33.6940096	34.9940100	37.0050106
O	32.3530092	34.3960098	36.8730105
O	34.3960098	34.6800099	35.7410102
O	33.6390096	36.5650104	37.2830106
C	32.6720093	37.1390106	38.1510109
H	33.0420094	37.0890106	39.1740112
H	31.7370091	36.5820104	38.0950109
O	39.4330113	34.7200099	40.1780115
H	40.1180115	34.3540098	39.5600113
H	39.3330112	33.9390097	40.7710116
O	41.3830118	33.7470096	38.5630110
H	41.7060119	33.8480097	37.6470107
H	42.1630120	34.0820097	39.0620111
O	35.4650101	31.2270089	39.1130112
H	35.8730102	30.4560087	38.6750110
H	35.2620101	30.8600088	39.9880114
O	43.3030124	34.9570100	40.0720114
H	43.3600124	34.9320100	41.0610117
H	43.1740123	35.9170103	39.9440114
O	43.5880124	35.3660101	42.7380122
H	44.5550127	35.1950100	42.8430122
H	43.4910124	36.1390103	43.3330124
H	37.7199480	31.6720659	44.0702319
H	40.8812911	33.9958938	47.2837574
H	41.0550251	38.2144911	33.1642069
H	47.3088864	34.9696635	40.1284445
H	44.8134105	36.6378684	37.2555164
H	37.0921494	33.2454648	31.8077800
H	36.1085131	34.5671188	32.3752187
H	32.4677715	38.1772195	37.8893312

Aldehyde-mediated pathway-TS (TS_A in Figure 3 of the main text)

C	36.9573339	30.9166812	44.1230933
H	37.3708205	29.9981444	44.5464158

N	50.2234171	41.2475081	48.4634051	H	36.2484210	31.2952622	44.8683433
H	50.8083998	40.7903448	49.1655645	C	36.2052215	30.6230030	42.8420461
H	50.4015125	42.2284647	48.2445265	O	35.8464354	31.5257236	42.0384659
C	49.5158311	37.6023573	36.2837977	N	35.8864696	29.3483312	42.6345070
H	49.4892109	37.6938691	35.1932392	H	35.3011688	29.1018300	41.8336894
H	48.9758109	36.6868656	36.5489409	H	36.2394745	28.6039785	43.2372189
C	48.8188914	38.7563560	36.9507152	C	47.4505669	35.6141902	40.9536689
N	48.4852722	38.6992319	38.2981425	H	48.4133377	36.0977169	40.7537510
C	47.8263740	39.8149439	38.5684370	H	46.6882427	36.3997659	40.9929936
H	47.3833932	40.0674513	39.5207739	C	47.4546797	34.8764190	42.2666735
N	47.7179123	40.5968283	37.4668979	N	46.3123552	34.7951629	43.0446556
H	47.2988254	41.5310300	37.4786143	C	46.6189714	34.0449508	44.0937289
C	48.3494071	39.9401589	36.4245780	H	45.9503491	33.7591780	44.8956175
H	48.4014060	40.3477151	35.4254706	N	47.9087022	33.6439619	44.0346945
C	49.9753072	33.2902437	38.0956218	H	48.3304245	33.0242580	44.7300830
H	49.8388418	33.2798592	37.0094743	C	48.4600781	34.1589782	42.8789723
H	50.0526537	32.2496181	38.4341703	H	49.4840045	33.9726527	42.5938019
C	48.7974655	33.9420312	38.7936907	C	44.7371054	37.7591765	37.4908479
C	48.6152638	33.7855531	40.1774163	H	45.7504439	38.1658392	37.5637869
H	49.3127236	33.1779321	40.7463168	H	44.2137361	38.2849851	36.6844507
C	47.5537527	34.3965530	40.8479421	C	43.9613773	37.9380050	38.7780747
H	47.4328847	34.2693313	41.9200248	C	42.5662212	37.7785383	38.7686365
C	46.6417446	35.1764406	40.1301943	H	42.0596100	37.5748284	37.8320039
O	45.5742373	35.7393818	40.8220870	C	41.8146759	37.8714663	39.9372413
H	45.3888270	36.6706699	40.4901831	H	40.7371297	37.7520689	39.9076024
C	46.7781952	35.3168785	38.7472138	C	42.4553409	38.1366500	41.1497125
H	46.0576966	35.9112328	38.1938273	O	41.6531731	38.2225901	42.2769092
C	47.8461230	34.6960655	38.0917098	H	42.1862165	38.0604656	43.1018522
H	47.9329791	34.7954107	37.0129850	C	43.8359685	38.3454729	41.1801506
C	51.7160400	30.0793974	41.2513277	H	44.3273629	38.5825218	42.1190632
H	52.6538171	30.5735856	41.5093458	C	44.5772609	38.2447574	39.9977839
H	51.6473013	30.0022545	40.1623142	H	45.6514035	38.4097662	40.0281945
C	50.5098668	30.8267032	41.7933410	C	41.5170407	37.6654693	33.9961955
O	49.3674370	30.5627797	41.3879998	H	41.2132094	36.6248029	33.8468083
N	50.7662681	31.7621693	42.7474247	H	42.6041332	37.7502634	33.9005447
H	49.9953731	32.0361461	43.3621837	C	41.0964917	38.1529600	35.3761436
H	51.6999377	31.7980318	43.1750634	O	41.6214472	39.1703833	35.8691858
C	45.8180098	42.1743784	42.7824782	N	40.1469842	37.4281371	35.9959673
H	46.1251820	43.2228535	42.7590778	H	39.7802438	37.6787653	36.9141763
H	45.8173255	41.8486322	43.8261430	H	39.8302924	36.5433360	35.5941754
C	46.7425478	41.2718792	41.9818951	C	40.8519144	33.1463912	46.5705352
O	46.5197003	40.0606742	41.8043722	H	41.4825193	32.3358519	46.9487154

N	47.8718398	41.8622252	41.5320617	H	39.8246006	32.7818698	46.4963268
H	48.5130633	41.3078243	40.9790132	C	41.2742051	33.6726723	45.1987406
H	48.0269912	42.8738983	41.5765291	O	40.4708411	34.2953099	44.4839258
C	54.4242855	31.2228344	47.1478027	N	42.5463081	33.4323345	44.8146102
H	54.2889289	32.1666582	47.6794459	H	42.8950414	33.9177364	43.9856348
O	53.9264971	31.3006612	45.8024045	H	43.2198635	32.9694915	45.4294477
P	54.0809975	32.6812749	44.9586815	C	36.8724569	33.7353448	32.7323085
O	55.4838753	33.2576585	45.0197414	H	36.4431948	33.0350253	33.4546586
O	53.4497058	32.3577473	43.6071641	O	37.9934551	34.4345560	33.2812200
O	53.2112535	33.7677437	45.8062137	P	39.0417123	33.7344356	34.3099945
C	51.8189153	33.5790693	46.0631484	O	39.8692091	34.8550702	34.8950544
H	51.6435651	32.6064581	46.5337125	O	39.7639738	32.5750179	33.6403743
H	51.2522180	33.6572760	45.1294491	O	38.0651191	33.0899055	35.4676780
C	51.3889850	34.6589286	47.0320246	C	37.5325671	34.0231864	36.4169299
H	52.0784900	34.7201315	47.8759182	H	37.1558759	34.9136379	35.8986301
O	51.5092591	35.9630101	46.3479342	H	38.3140600	34.3345713	37.1196203
C	50.4168954	36.6450303	46.4190271	C	36.3568584	33.4116518	37.1530951
H	50.5065546	37.7104395	46.2531250	H	35.6426395	32.9808109	36.4556879
C	49.9201031	34.5875825	47.5171065	O	36.8214935	32.2807061	38.0076596
H	49.3632713	33.8269953	46.9643820	C	36.6626829	32.6324269	39.4298480
C	49.3551222	35.9937298	47.2437123	H	37.5356418	32.3031147	39.9879531
H	48.3853466	35.9845724	46.7497219	C	35.7139402	34.4313212	38.1266240
H	49.2709653	36.5485261	48.1802260	H	35.9721389	35.4547644	37.8386388
O	49.8180612	34.3418517	48.9184568	C	36.3090097	34.0939546	39.4953746
P	50.0123283	32.8441442	49.5749017	H	37.2237677	34.6657373	39.6698985
O	49.9582580	33.0987963	51.0639888	H	35.5962175	34.2801713	40.3005100
O	51.2082366	32.1348593	48.9680872	O	34.2822773	34.3092688	38.1895819
O	48.6888264	32.0265071	49.0704534	P	33.4042524	35.0768037	37.0273787
C	47.3934885	32.4971021	49.4821734	O	31.9613472	34.6977086	37.3017061
H	47.0193481	33.2201469	48.7467319	O	34.0854112	34.7942736	35.6923172
H	47.4452731	32.9716978	50.4665795	O	33.6567051	36.6532410	37.2783725
O	51.2387928	37.6147203	48.7346679	C	33.0067166	37.3706846	38.3328395
H	50.5957841	38.3519277	48.6320542	H	33.7502077	37.6160007	39.0939433
H	52.1228048	38.0092024	48.5334267	H	32.1916103	36.7872751	38.7690208
O	50.9874274	36.7992659	42.4665224	O	39.3974678	34.7049338	40.2176490
H	50.4892148	37.0583530	41.6470735	H	40.1235359	34.3535721	39.6402385
H	51.3153404	35.8687510	42.2427365	H	39.2597649	33.9925357	40.8886167
O	49.5256552	36.4476975	44.6145862	O	41.3928083	33.4738913	38.7721359
H	50.1525056	36.4752018	43.7979870	H	41.6004969	33.7070438	37.8315602
H	49.1747881	37.3839303	44.5666856	H	42.1637802	33.8123474	39.2934015
O	49.7502946	36.9936194	40.0344518	O	35.5615977	31.7274902	39.5979944
H	49.1467907	36.2365162	40.1297359	H	35.9663610	31.4492734	38.4164441

H	49.2432688	37.6468242	39.4561225
H	48.0514788	40.9264897	45.9817295
H	44.7871859	42.1048736	42.4351480
H	51.7234278	29.0859127	41.6996588
H	50.5587835	37.5027002	36.5844401
H	50.9275684	33.7825382	38.2928827
H	55.4679467	30.9088164	47.1630110
H	53.9005493	30.4106475	47.6519058
H	46.7168271	31.6444468	49.5385237

His151-mediated pathway_snapshot 3-PC (PC of Figure S14)

C	48.4450270	41.4028483	46.8383831
H	48.8947233	42.3776245	46.6386242
H	47.5338139	41.6098775	47.4093892
C	49.3496813	40.5328257	47.6988303
O	49.2025825	39.3009644	47.8146707
N	50.2691113	41.2255319	48.3909821
H	50.8449841	40.7495873	49.0881384
H	50.4516302	42.2098493	48.1955050
C	49.4981349	37.6215402	36.3378593
H	49.4518254	37.7191735	35.2493241
H	48.9605056	36.7061129	36.6081400
C	48.8055010	38.7739738	37.0032969
N	48.4669923	38.7368497	38.3532270
C	47.7997090	39.8411776	38.6886793
H	47.3928044	40.0571663	39.6710340
N	47.6906840	40.5994359	37.5926133
H	47.2619714	41.5344134	37.6104377
C	48.3096266	39.9612831	36.5267576
H	48.3400030	40.3860228	35.5346291
C	49.9803424	33.3015024	38.1018029
H	49.8454309	33.2843097	37.0152779
H	50.0565750	32.2625994	38.4449495
C	48.7961606	33.9528999	38.7916111
C	48.6009703	33.8018435	40.1762710
H	49.3002120	33.2072598	40.7559512
C	47.5231800	34.3999751	40.8346823
H	47.3980604	34.2798814	41.9072136
C	46.6036574	35.1591147	40.1041312
O	45.5165894	35.7035853	40.7783655
H	45.3369550	36.6355486	40.4616167
H	35.5756220	31.3407018	40.5745226
O	43.3656911	34.8453897	40.0953945
H	43.4355545	34.9273743	41.0843480
H	43.0357219	35.7224837	39.8267364
O	43.6774934	35.2642764	42.7763524
H	44.6807400	35.1915434	42.8536478
H	43.4343707	36.1128967	43.1945147
H	37.7453648	31.6667360	44.0560676
H	40.8800600	33.9633043	47.2915954
H	41.0448319	38.2607189	33.2146817
H	47.2360982	34.9437178	40.1214808
H	44.8222852	36.7055498	37.2249862
H	37.1172320	33.2218606	31.8025309
H	36.1421390	34.4840537	32.4254894
H	32.5882165	38.2939822	37.9322818

Aldehyde-mediated pathway-IC (IC_A in Figure 3 of the main text)

C	36.8879289	30.8981671	44.3506350
H	37.3595165	29.9783675	44.7004381
H	36.2488658	31.2730661	45.1543622
C	36.0683985	30.6395287	43.1277881
O	35.3077527	31.6008573	42.7034022
N	36.1357342	29.4893386	42.5129858
H	35.5606585	29.2824101	41.6868308
H	36.6775714	28.7252982	42.9282784
C	47.4262774	35.6080416	40.9504217
H	48.3845586	36.1004505	40.7504165
H	46.6570820	36.3868928	40.9908811
C	47.4391385	34.8699121	42.2633379
N	46.3002356	34.7801576	43.0458902
C	46.6176610	34.0351846	44.0954113
H	45.9549675	33.7460233	44.9008294
N	47.9105609	33.6449956	44.0325646
H	48.3390201	33.0289966	44.7268717
C	48.4529660	34.1624584	42.8735683
H	49.4777257	33.9849588	42.5854555
C	44.7061131	37.7414423	37.4829622
H	45.7158822	38.1574141	37.5542619
H	44.1758048	38.2648115	36.6792657
C	43.9332147	37.9102417	38.7735912
C	42.5399805	37.7320082	38.7719429

C	46.7505214	35.2912042	38.7202630	H	42.0304949	37.5182786	37.8391400
H	46.0076021	35.8455988	38.1536821	C	41.7928411	37.8206567	39.9439156
C	47.8373715	34.6873628	38.0770531	H	40.7169267	37.6868570	39.9193659
H	47.9212765	34.7632076	36.9953347	C	42.4360343	38.1002816	41.1518041
C	51.7138373	30.1097750	41.2565726	O	41.6375377	38.1826397	42.2825266
H	52.6530614	30.5999087	41.5168002	H	42.1773765	38.0368446	43.1053547
H	51.6449918	30.0355790	40.1671500	C	43.8141918	38.3256532	41.1751397
C	50.5102654	30.8627033	41.7996884	H	44.3076308	38.5741021	42.1103592
O	49.3668954	30.5974824	41.3901454	C	44.5510524	38.2289997	39.9893747
N	50.7653434	31.8003816	42.7483208	H	45.6230407	38.4086833	40.0139957
H	49.9930331	32.0717574	43.3650154	C	41.5381443	37.6564873	33.9900487
H	51.7022970	31.8506431	43.1719276	H	41.2539173	36.6124781	33.8270884
C	45.8223721	42.2055384	42.7458985	H	42.6244503	37.7606543	33.9051798
H	46.1048797	43.2614256	42.7356105	C	41.0986330	38.1213492	35.3717760
H	45.8465422	41.8744081	43.7876673	O	41.6107465	39.1364372	35.8837026
C	46.7834679	41.3516203	41.9407576	N	40.1501584	37.3786378	35.9716010
O	46.5590097	40.1749135	41.5955149	H	39.7717359	37.6077318	36.8914008
N	47.9762102	41.9335524	41.6835443	H	39.8497135	36.4977338	35.5483917
H	48.6875055	41.3848192	41.2187008	C	40.8904031	33.0702963	46.6203309
H	48.1426485	42.9396760	41.7888799	H	41.5662795	32.3007090	47.0062194
C	54.4937959	31.2201440	47.1302826	H	39.8797936	32.6571622	46.5879205
H	54.3632068	32.1652222	47.6605218	C	41.2523280	33.5676813	45.2204049
O	54.0130140	31.2994206	45.7799363	O	40.3954321	34.1115166	44.5012459
P	54.0971974	32.7127397	44.9748051	N	42.5301080	33.3970866	44.8226979
O	55.4970889	33.3082266	44.9765968	H	42.8474657	33.8825801	43.9808929
O	53.4333805	32.3939542	43.6325508	H	43.2324452	32.9750495	45.4348934
O	53.2482923	33.7513701	45.8785019	C	36.9175405	33.7123191	32.6844376
C	51.8852826	33.4704418	46.2516495	H	36.5075642	33.0148012	33.4207774
H	51.8660137	32.6585542	46.9854749	O	38.0518524	34.4105197	33.2010203
H	51.3207398	33.1905342	45.3598025	P	39.1249830	33.7065738	34.2047126
C	51.2794377	34.7211930	46.8531037	O	39.9447448	34.8325614	34.7939156
H	51.9496400	35.1545687	47.6063693	O	39.8608052	32.5754919	33.4948853
O	51.0568712	35.6628132	45.7960598	O	38.1972665	33.0003200	35.3470655
C	49.9358231	36.4740290	46.0682390	C	37.7740361	33.7850085	36.4798119
H	50.2574237	37.4920372	46.2957243	H	37.8107088	34.8539742	36.2439511
C	49.8904158	34.4995706	47.4905978	H	38.4615746	33.5860906	37.3096925
H	49.3678000	33.6694282	47.0078149	C	36.3507149	33.3725699	36.8381756
C	49.1745541	35.8282843	47.2351904	H	35.7366398	33.4744203	35.9419566
H	48.1185252	35.6901489	46.9950619	O	36.3253875	32.0328067	37.3264616
H	49.2630981	36.4484778	48.1273128	C	36.0694205	32.5191283	39.7565103
O	49.9445664	34.2668948	48.9043210	H	36.9030297	31.8051804	39.6954751
P	50.0322371	32.8003034	49.6149448	C	35.7696525	34.2976679	37.9245762

O	49.9227243	33.1112933	51.0908376
O	51.2087380	31.9821853	49.1032794
O	48.6977355	32.0063693	49.0835287
C	47.4043843	32.4899795	49.4740972
H	47.0400898	33.2077196	48.7277070
H	47.4455065	32.9759219	50.4538042
O	51.3250251	37.5698950	48.6191497
H	50.6576744	38.2665953	48.4446798
H	52.1920130	37.9730587	48.3799471
O	50.7811410	36.8812033	42.4673298
H	50.0330723	37.0854736	40.9363409
H	51.1529876	35.9628986	42.2750327
O	49.1507380	36.5187527	44.8563698
H	50.2452044	36.7231088	43.2757498
H	49.0089879	37.4808383	44.6512652
O	49.6686429	36.9374656	40.0156516
H	49.1882078	36.0930176	40.0988121
H	48.7881069	38.0143286	39.0368397
H	48.1022513	40.9583318	45.9040508
H	44.7873883	42.1188431	42.4152029
H	51.7203952	29.1139051	41.6995932
H	50.5456472	37.5230972	36.6226299
H	50.9351831	33.7894946	38.2972767
H	55.5352428	30.8994209	47.1546152
H	53.9605263	30.4129479	47.6324032
H	46.7241123	31.6402558	49.5312522

Phosphate-mediated pathway_RC (RC of Figure S12)

C	36.9618542	30.9236663	44.0974469
H	37.3678618	30.0034208	44.5244640
H	36.2622729	31.3095157	44.8485921
C	36.1920184	30.6184039	42.8336848
O	35.8641082	31.5068526	41.9907191
N	35.8202013	29.3527605	42.6829614
H	35.1621521	29.0973252	41.9440828
H	36.1594353	28.6198992	43.3095872
C	41.4552887	37.6757867	33.9628139
H	41.1364390	36.6409950	33.8084053
H	42.5444041	37.7438253	33.8782256
C	41.0309841	38.1649319	35.3417030
O	41.5483454	39.1891114	35.8275311
H	36.0497912	35.3365555	37.7141434
C	36.3077406	33.9401632	39.3162231
H	37.3812849	34.1496925	39.3462127
H	35.8044427	34.5869375	40.0408951
O	34.3271666	34.2176694	37.9977472
P	33.4113597	35.0691321	36.9411325
O	31.9712773	34.7016025	37.2593707
O	34.0050635	34.8639633	35.5513383
O	33.6972176	36.6298455	37.2649511
C	33.0385196	37.3424310	38.3130962
H	33.7796398	37.5966822	39.0729516
H	32.2295325	36.7529380	38.7516805
O	39.3339212	34.6538511	40.2836779
H	40.0703075	34.2829948	39.7330955
H	39.0927306	33.9225776	40.8967780
O	41.3434451	33.4077822	38.8658482
H	41.5266573	33.6411393	37.9185565
H	42.1250744	33.7570187	39.3631037
O	35.0115298	32.1861856	40.2966920
H	35.9183755	31.4191286	36.6706789
H	35.0470644	31.5625576	41.7198162
O	43.3601739	34.8098031	40.0992062
H	43.4301176	34.9033486	41.0864977
H	43.0195543	35.6799716	39.8203033
O	43.6590817	35.2324746	42.7879988
H	44.6630347	35.1584826	42.8607556
H	43.4253099	36.0915406	43.1894059
H	37.6439400	31.6677182	44.1947331
H	40.9045078	33.9112652	47.3136126
H	41.0622400	38.2525056	33.2113674
H	47.2171775	34.9374072	40.1169987
H	44.8017735	36.6895948	37.2136429
H	37.1400096	33.1970001	31.7500817
H	36.1769903	34.4577159	32.3945476
H	32.6107192	38.2631154	37.9163668

N	40.0812680	37.4397137	35.9610471
H	39.7227289	37.6862354	36.8840832
H	39.7802678	36.5449394	35.5693555
C	36.8758609	33.7631963	32.6938944
H	36.4535658	33.0711744	33.4274562
O	38.0071169	34.4625421	33.2196917
P	39.0200838	33.7607962	34.2844671
O	39.8609942	34.8706295	34.8739741
O	39.7523983	32.5932173	33.6361790
O	38.0053361	33.1388646	35.4057059
C	37.3957670	34.0698889	36.3183944
H	36.8800670	34.8622479	35.7631554
H	38.1673249	34.5193504	36.9543833
C	36.3684634	33.3399623	37.1652854
H	35.6140945	32.8729030	36.5325994
O	37.0389300	32.2819064	37.9040093
C	36.7668613	32.3376170	39.2315003
H	37.6156700	31.9920221	39.8160694
C	35.7263795	34.2748594	38.2277663
H	36.0520108	35.3117458	38.0871896
C	36.2300001	33.7186329	39.5690252
H	37.0705151	34.3154116	39.9302337
H	35.4464768	33.7029321	40.3291156
O	34.2859617	34.2439242	38.2225035
P	33.4530059	35.0794420	37.0760688
O	31.9944168	34.7381220	37.3291300
O	34.1235289	34.8166685	35.7319746
O	33.7502203	36.6410423	37.3701660
C	33.0719099	37.3823764	38.3877216
H	33.8123940	37.6941314	39.1252822
H	32.2852312	36.7882715	38.8602720
O	39.3494160	34.6559570	40.1569083
H	40.0875914	34.3522833	39.5729746
H	39.2271648	33.9172570	40.8023229
O	41.5006278	33.5855876	38.7462304
H	41.6957148	33.7383187	37.8025419
H	42.2333330	34.0434648	39.2470579
O	35.6574903	31.3060387	39.5575048
H	35.8784440	30.4288721	39.1308010
H	35.6505713	31.2326675	40.6626937
O	42.4054914	34.2249893	35.5927378
H	42.9322046	34.3063379	34.7668042

H	41.4988993	34.5372111	35.3396357
H	37.7585787	31.6636313	44.0216246
H	40.9983501	38.2780425	33.1775991
H	37.1129831	33.2401355	31.7674778
H	36.1418689	34.5093288	32.3895769
H	32.6143778	38.2731015	37.9572099

Phosphate-mediated pathway_TS
(TS of Figure S12)

C	37.0495621	30.8465285	44.1147466
H	37.4106216	29.8951277	44.5119752
H	36.3368060	31.2175803	44.8611055
C	36.3149382	30.6518507	42.7937021
O	36.1361733	31.5566775	41.9512720
N	35.8058739	29.4180248	42.6409405
H	35.2102043	29.2100098	41.8378617
H	36.0903848	28.6489523	43.2480843
C	41.5301625	37.7304154	33.9306356
H	41.2282326	36.6898135	33.7823884
H	42.6163047	37.8197548	33.8347509
C	41.1018966	38.2188603	35.3079116
O	41.6228213	39.2319326	35.8116172
N	40.1357254	37.4997789	35.9093620
H	39.7388990	37.7677256	36.8132507
H	39.8045689	36.6309014	35.4861944
C	36.9398677	33.7291413	32.6339297
H	36.5506931	33.0342019	33.3820475
O	38.0978347	34.4301006	33.1072463
P	39.0639489	33.7885400	34.2465326
O	39.8733454	34.9346485	34.8280297
O	39.8582722	32.6072903	33.7032628
O	38.0197839	33.2106083	35.3473340
C	37.2164997	34.1740507	36.0666456
H	36.3592218	34.4725331	35.4612995
H	37.8223459	35.0588995	36.2968140
C	36.7514262	33.5350644	37.3562705
H	36.1883510	32.6114579	37.1842928
O	37.9457736	33.2243892	38.1058704
C	37.6951730	33.2745234	39.4783853
H	37.6671388	32.2772057	39.9198730
C	35.9410467	34.4769230	38.2896726
H	36.1894379	35.5247516	38.0780183

C	36.4073843	34.0656459	39.6959008
H	36.5921577	34.9287143	40.3381231
H	35.6539108	33.4305436	40.1643573
O	34.5150080	34.3140993	38.2242194
P	33.5892979	35.0976536	37.1255849
O	32.1610610	34.6743399	37.4148068
O	34.2015602	34.8859903	35.7440881
O	33.8071141	36.6769180	37.4210432
C	33.0789941	37.3811014	38.4311200
H	33.7797769	37.6881478	39.2112693
H	32.2836164	36.7644131	38.8570449
O	38.8795437	33.9570905	40.0301770
H	40.0560772	33.7827726	39.0041586
H	39.1128654	33.4423134	40.8660592
O	41.0023453	33.6526136	38.5631208
H	41.0355851	33.8628022	37.5985713
H	41.6892742	34.2259148	39.0867280
O	35.7106057	31.0441815	39.1074344
H	35.9470595	30.1474587	38.7833053
H	35.7525699	30.9943293	40.0854155
O	42.3458370	34.3359433	35.6274330
H	42.9270375	34.3648243	34.8350067
H	41.4584063	34.6314995	35.2804816
H	37.8656849	31.5689737	44.1055949
H	41.0498613	38.3197039	33.1495357
H	37.1461423	33.2076362	31.6992905
H	36.1899507	34.4705805	32.3583222
H	32.6214479	38.2684356	37.9936768
Phosphate-mediated pathway_PC (PC of Figure S12)			
C	37.0617721	30.8435000	44.1036907
H	37.4189166	29.8908682	44.5017824
H	36.3425374	31.2130322	44.8444742
C	36.3389164	30.6509544	42.7757824
O	36.1564112	31.5593513	41.9386084
N	35.8449433	29.4123020	42.6093011
H	35.2560700	29.2056806	41.8011804
H	36.1264291	28.6427867	43.2171527
C	41.5491374	37.7536232	33.9126962
H	41.2664683	36.7082248	33.7584872
H	42.6331913	37.8549064	33.8100347

C	41.1287679	38.2320615	35.2972664
O	41.6985576	39.1942460	35.8373673
N	40.1166273	37.5502578	35.8738305
H	39.7225260	37.8029253	36.7847015
H	39.6911885	36.7661404	35.3941727
C	36.8617663	33.7148319	32.6062784
H	36.4475778	33.0224692	33.3421772
O	38.0306169	34.3960503	33.1093942
P	38.9635478	33.6755613	34.1884139
O	39.8221188	34.9103656	34.6911663
O	39.7952710	32.5460153	33.6434653
O	38.0162396	33.1756163	35.3629821
C	37.1732903	34.1557412	36.0600961
H	36.2748762	34.3325703	35.4704491
H	37.7329637	35.0894452	36.1750851
C	36.8267647	33.5992226	37.4201416
H	36.3444438	32.6164664	37.3525997
O	38.0568483	33.5025476	38.1480716
C	37.7701207	33.4733602	39.5345301
H	37.7376209	32.4436077	39.8948778
C	35.9537508	34.5398412	38.2977345
H	36.1644781	35.5884268	38.0528873
C	36.4283437	34.1956053	39.7180714
H	36.5711656	35.0897733	40.3263152
H	35.7040336	33.5399966	40.2060009
O	34.5342955	34.3162400	38.2090597
P	33.5949110	35.0842948	37.1176460
O	32.1712545	34.6478123	37.4086397
O	34.1979812	34.8750193	35.7281294
O	33.7958264	36.6685642	37.3980778
C	33.0764476	37.3659425	38.4206180
H	33.7808678	37.6572530	39.2039964
H	32.2770535	36.7499742	38.8399580
O	38.8730772	34.1480374	40.1692489
H	40.4574578	33.8458993	39.1544008
H	39.1294660	33.5686713	40.9470408
O	41.3578653	33.6028771	38.8385677
H	41.5971987	33.9308483	37.2653524
H	42.0039808	34.1143085	39.4053665
O	35.8136879	31.0526784	39.0996522
H	36.0351225	30.1422577	38.8080618
H	35.8622858	31.0417825	40.0798141

O	41.7095808	34.0200415	36.2620316	
H	42.6353404	34.1982499	36.0415000	
H	40.5753874	34.6232002	35.3055413	
H	37.8789662	31.5647872	44.1012760	
H	41.0585012	38.3393057	33.1353164	
H	37.0872427	33.2019501	31.6713026	
H	36.1350669	34.4775294	32.3265147	
H	32.6246102	38.2604068	37.9918481	