nature chemical biology

SUPPLEMENTARY INFORMATION

https://doi.org/10.1038/s41589-018-0003-x

In the format provided by the authors and unedited.

Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis

Sean A. Newmister[1], Shasha Li[1,2], Marc Garcia-Borràs[3], Jacob N. Sanders[3], Song Yang[3], Andrew N. Lowell[1], Fengan Yu[1], Janet L. Smith[1,4], Robert M. Williams[5,6]*, K. N. Houk[3]* and David H. Sherman[1,2,7,8]*

[1]Life Sciences Institute, University of Michigan, Ann Arbor, MI, USA. [2]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI, USA. [3]Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA, USA. [4]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI, USA. [5]Department of Chemistry, Colorado State University, Fort Collins, CO, USA. [6]University of Colorado Cancer Center, Aurora, CO, USA. [7]Department of Chemistry, University of Michigan, Ann Arbor, MI, USA. [8]Department of Microbiology and Immunology, University of Michigan, Ann Arbor, MI, USA. *e-mail: robert.williams@colostate.edu; houk@chem.ucla.edu; davidhs@umich.edu

SUPPLEMENTARY MATERIALS

Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis

Sean A. Newmister[1], Shasha Li[1,2], Marc Garcia-Borràs[3], Jacob N. Sanders[3], Song Yang[3], Andrew N. Lowell[1], Fengan Yu[1], Janet L. Smith[1,4], Robert M. Williams[5,6], K. N. Houk[3]*, David H. Sherman[1,2,7,8]*

[1]Life Sciences Institute, University of Michigan, Ann Arbor, MI 48109, USA

[2]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI 48109, USA

[3]Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095, USA

[4]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI 48109, USA

[5]Department of Chemistry, Colorado State University, Fort Collins, CO 80523, USA

[6]University of Colorado Cancer Center, Aurora, CO 80045, United States

[7]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, USA

[8]Department of Microbiology & Immunology, University of Michigan, Ann Arbor, MI 48109, USA

*Corresponding authors. Email: davidhs@umich.edu (D.H.S.); houk@chem.ucla.edu (K.N.H.)

Contents

SUPPLEMENTARY TABLES

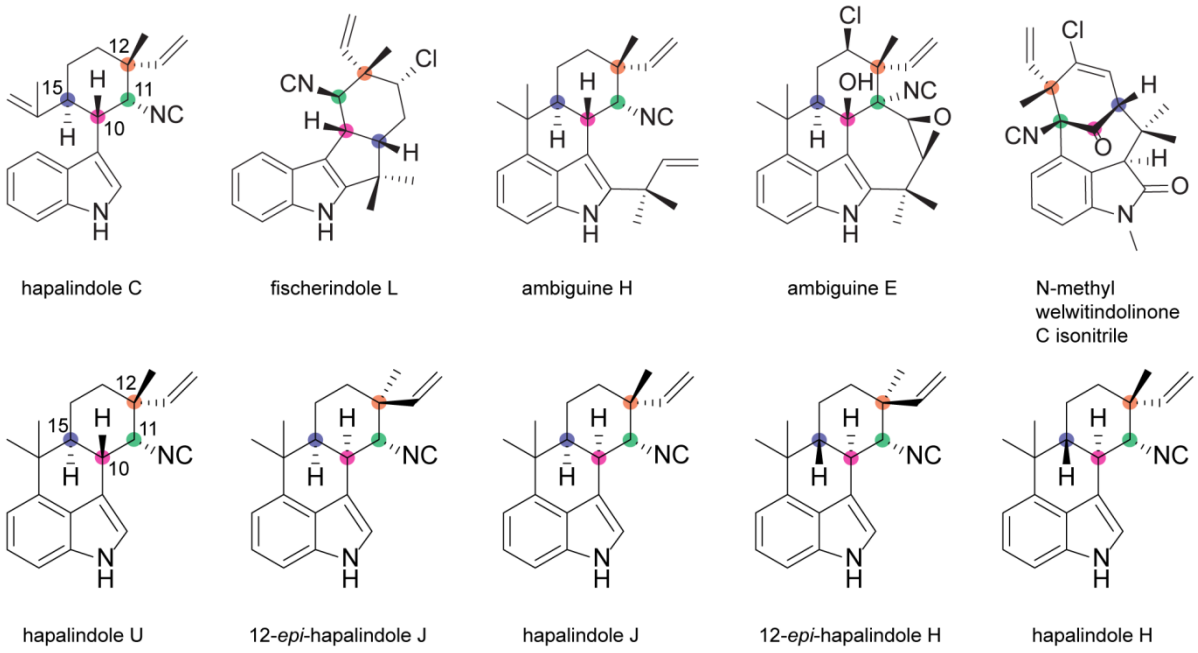
Supplementary Table 1. Data collection and refinement statistics.

	Form 1 HpiC1 SeMet	Form 2 HpiC1 native	Form 3 HpiC1 native	Form 3 HpiC1 Y101F	Form 3 HpiC1 Y101S	Form4 HpiC1 F138S	Form 4 HpiC1 Y101F/F138S
$CaCl_2$ (mM)	200	200	<150	<150	<150	20	20
Data collection*							
Space group	$P2_12_12_1$	$P4_2$	*C*2	*C2*	*C2*	$P2_1$	$P2_1$
Cell dimensions							
a, *b*, *c* (Å)	44.9, 81.1, 131.7	71.3, 71.3, 80.6	113.8, 49.5, 53.1	113.8, 49.8, 53.4	113.9, 49.6, 53.4	62.0, 47.9, 174.2	62.0, 48.0, 174.8
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 110.5, 90	90, 110.4, 90	90, 110.3, 90	90, 97.2, 90	90, 97.0, 90
Wavelength (Å)	0.979	1.033	1.033	1.033	1.033	1.033	1.033
Resolution (Å)**	39.3-1.7 (1.76-1.70)	42.76-2.09 (2.16-2.09)	45.11-1.49 (1.54-1.49)	36.28-1.39 (1.44-1.39)	45.21-1.39 (1.44-1.39)	46.2-1.69 (1.75-1.69)	46.22-1.64 (1.70-1.64)
R_{sym} or R_{merge}	0.069 (0.815)	0.104 (1.287)	0.050 (0.984)	0.050 (1.496)	0.055 (0.9158)	0.054 (1.653)	0.065 (1.020)
I / σI	16.87 (2.04)	18.94 (1.62)	19.41 (1.30)	20.44 (0.66)	18.24 (0.92)	16.37 (1.11)	13.42 (0.97)
Completeness (%)	99.5 (99.0)	99.8 (98.9)	99.7 (97.6)	90.5 (51.3)	93.6 (58.6)	97.8 (95.4)	97.7 (79.9)
Redundancy	6.7 (7.0)	13.5 (13.7)	6.6 (5.5)	6.6 (4.9)	6.3 (4.3)	6.9 (7.0)	6.6 (5.0)
Refinement							
Resolution (Å)	39.3-1.7	42.76-2.09	45.11-1.49	36.28-1.39	45.21-1.39	46.2-1.69	46.22-1.64
No. reflections	53,600	24,033	45,278	51,294	52,971	112,827	122,677
R_{work} / R_{free}	0.181/0.215	0.210/0.255	0.164/0.184	0.137/0.167	0.149/0.182	0.218/0.252	0.218/0.245
No. atoms							
Protein	3024	2953	1547	1556	1535	5957	6102
Ligand/ion	33	6	14	18	10	9	9
Water	426	107	233	318	316	404	507
B-factors							
Protein	28.0	46.4	23.9	23.1	21.2	53.6	50.9
Ligand/ion	42.2	39.5	33.9	33.2	36.3	58.1	60.8
Water	36.3	46.8	36.9	43.6	40.4	49.3	48.4
R.m.s. deviations							
Bond lengths (Å)	0.005	0.008	0.005	0.005	0.005	0.009	0.009
Bond angles (°)	0.81	0.99	0.83	0.82	0.80	0.99	0.93

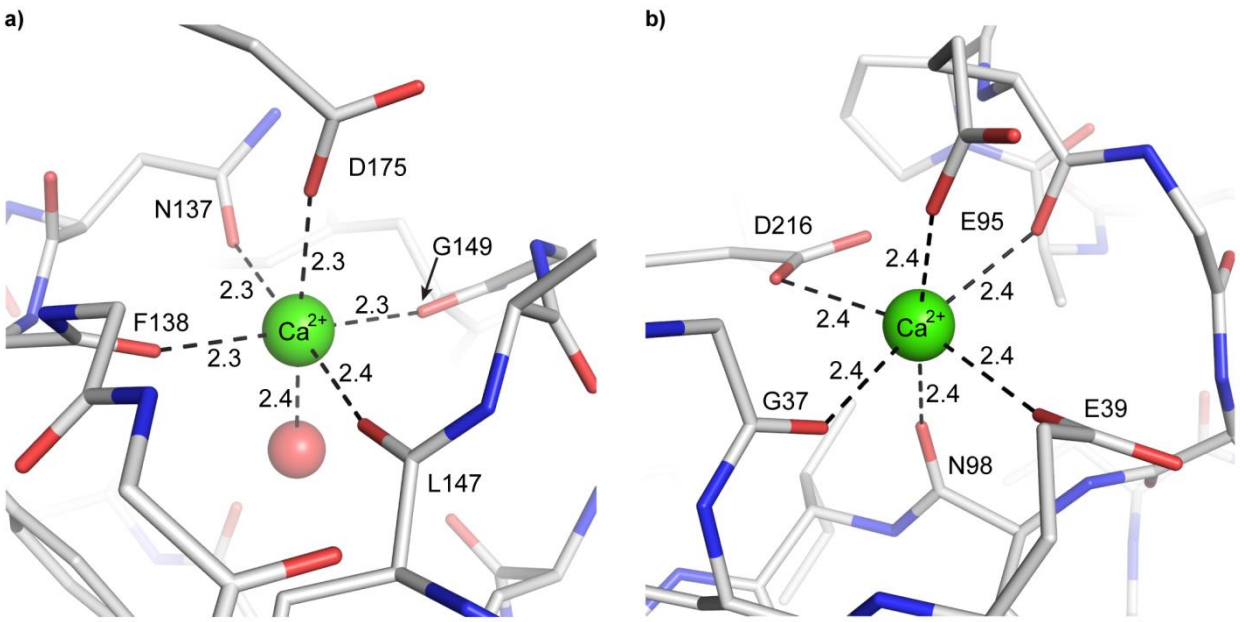
*Single crystal data collections. **Values in parentheses are for highest-resolution shell.

Supplementary Table 2. Mutagenic primer sequences (5'→3').	
SN_hpiC1_W73M	CTGGTTCCGGAGAAGCGTACCACCatgACCAGCAACAACGGTGTGGGCTAC
SN_hpiC1_K132M	GGAACCGGATACCAAGTACACCCTGatgGTGGACGTTGGTAACTTCGGTGGC
SN_hpiC1_Y101S	CGCCGGAAGGTCGTAACATCGGCtctATTTATCTGGCGCAGAAACCGGG
SN_hpiC1_Y101F	CGCCGGAAGGTCGTAACATCGGCttcATTTATCTGGCGCAGAAACCGGG
SN_hpiC1_F138S	CCCTGAAAGTGGACGTTGGTAACtctGGTGGCGAGTTTCAGAAAATTAGCC
SN_hpiC1_F210S	CTGATTAACCTGCTGCAAGGCACCtctAGCGGCCTGGACTTTGATAACGTG
SN_hpiC1_D214A	CAAGGCACCTTCAGCGGCCTGgcgTTTGATAACGTGCGTCTGACCGTTG
SN_hpiC1_D214N	CAAGGCACCTTCAGCGGCCTGaacTTTGATAACGTGCGTCTGACCGTTG
SN_hpiC1_D214E	CAAGGCACCTTCAGCGGCCTGgaaTTTGATAACGTGCGTCTGACCGTTG
SN_fimC5_F102Y	CCGGAAGGCCGTAACGTGGCGtatGTTTACCTGGCGCAGGAGATCGG
SN_fimC5_S139L	CAAATATACCCTGACCGTTGATATTGGTAACctgGGTGGCAGCTTCCAGGGCAAAAC

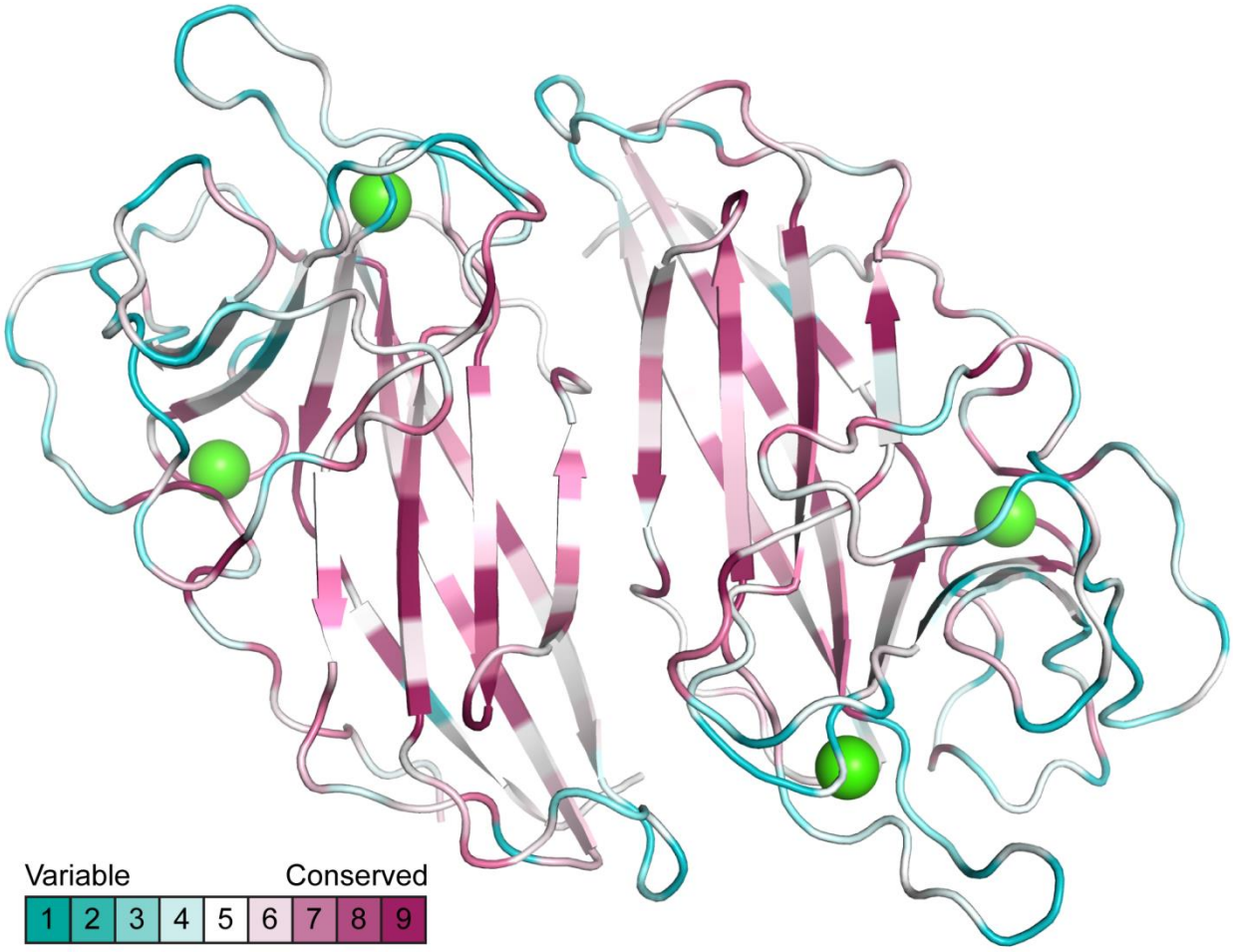
SUPPLEMENTARY FIGURES



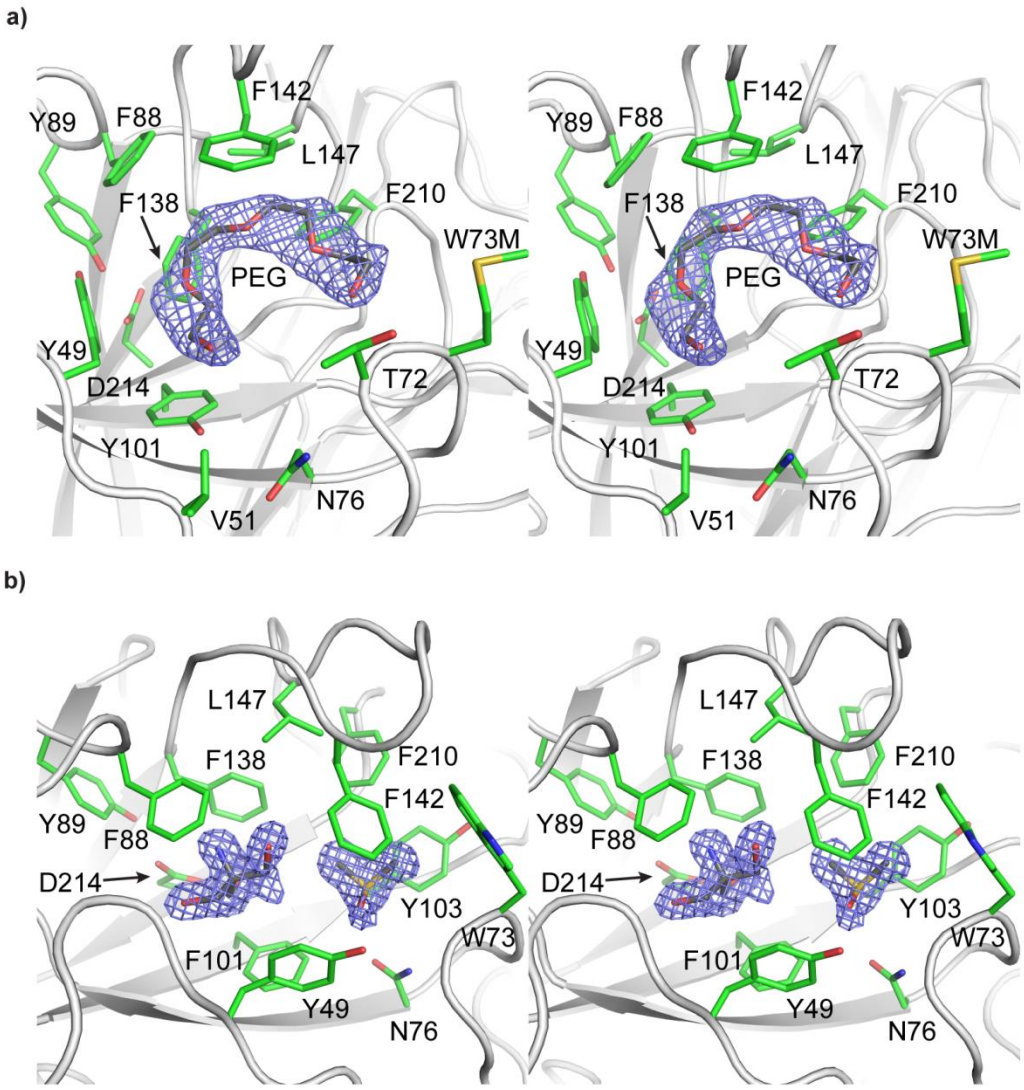
Supplementary Fig. 1. Representative hapalindole-type alkaloids. Tricyclic, tetracyclic, and pentacyclic species are shown. Stereochemical differences among the hapalindole U, J, and H series are highlighted.



Supplementary Fig. 2. Two hexacoordinate Ca^{2+} ions are present in each HpiC1 monomer. (**a**) The first site is closer to the active site, and is ligated by carbonyl oxygen atoms from F138, L147, G149, and aspartate/asparagine side chain atoms from N137 and D175. A water molecule is the sixth ligand. (**b**) A second Ca^{2+} is ligated by carbonyl oxygen atoms from G37, E95, N98, and carboxylate/amide side chain atoms from E39, E95, and D216.

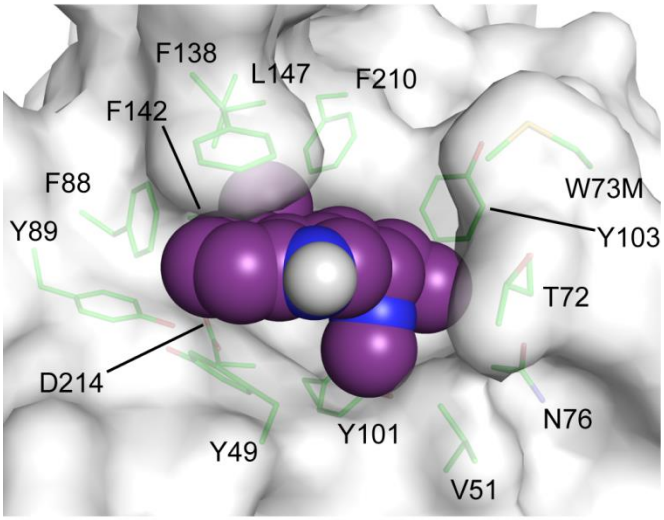


Supplementary Fig. 3. ConSurf Analysis of HpiC1[1]. ConSurf sequence conservation projected onto the HpiC1 structure. High conservation is most evident in the secondary structure elements including the dimer interface, while the active site region shows higher variability. Amino acid positions for which conservation could not be determined (20 out of 200 residues) are colored white. The Uniprot-90 database was used to generate the alignment.

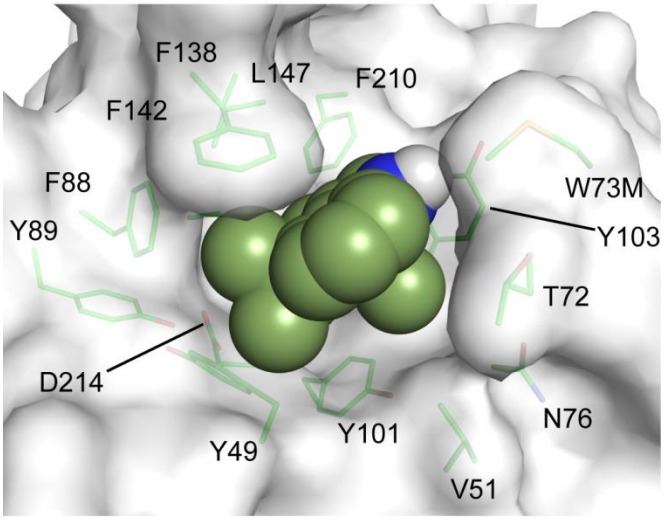


Supplementary Fig. 4. Stereo representation of HpiC1 active sites. Key residues are highlighted as green sticks. (**a**) Polyethylene glycol (4 units) modeled into difference density in the SeMet HpiC1 W73M/K132M active site. The 1.7 Å omit electron density (Fo-Fc, 3.0σ contour) was calculated from a model where polyethylene glycol was omitted from the phase calculation and refinement. (**b**) DMSO and Tris were modeled into difference density in the HpiC1 Y101F active site. The 1.4 Å omit electron density (Fo-Fc, 3.0σ contour) was calculated from a model where DMSO and Tris were omitted from the phase calculation and refinement.

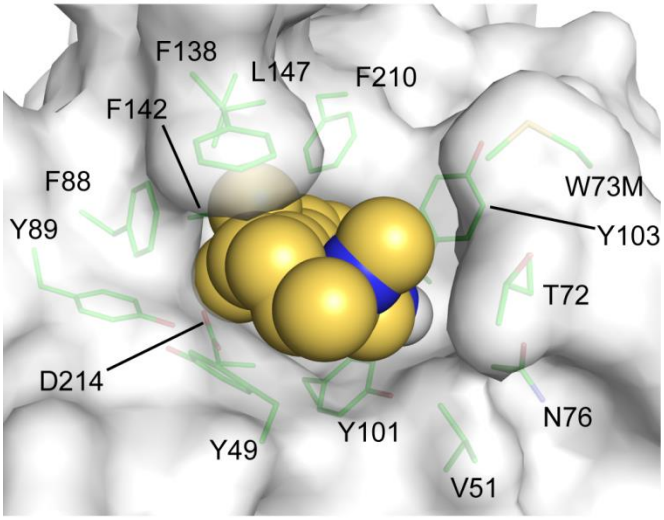
a)


F138
L147
F210
F142
F88
W73M
Y89
Y103
T72
D214
N76
Y49
Y101
V51

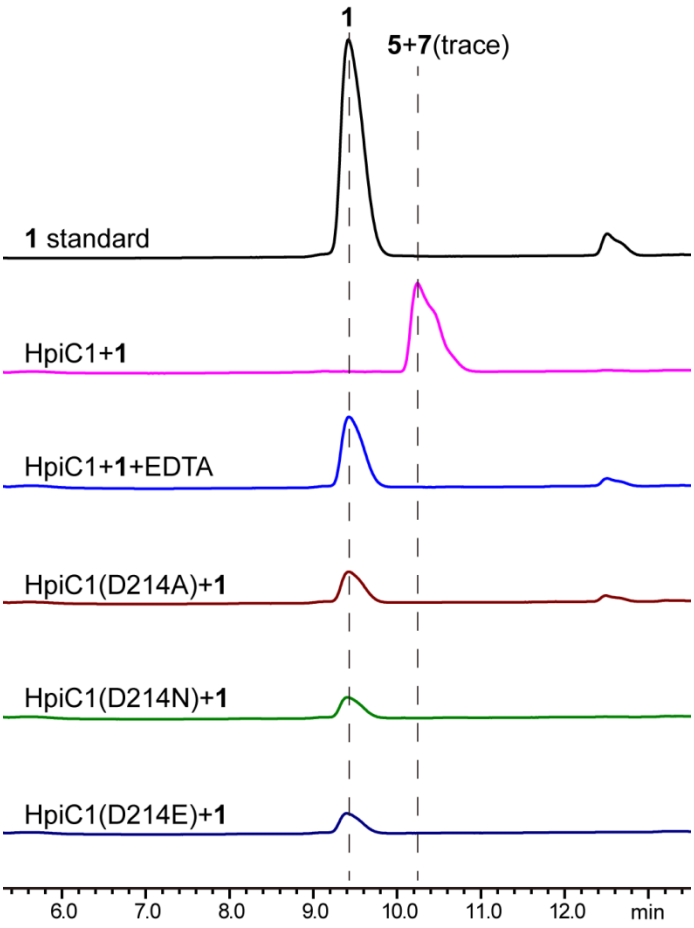
b)


F138
L147
F210
F142
F88
W73M
Y89
Y103
T72
D214
N76
Y49
Y101
V51

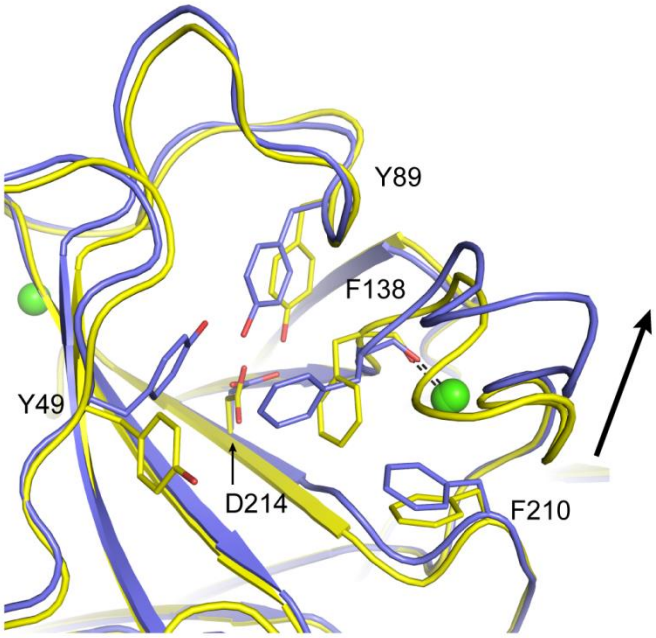
c)


F138
L147
F210
F142
F88
W73M
Y89
Y103
T72
D214
N76
Y49
Y101
V51

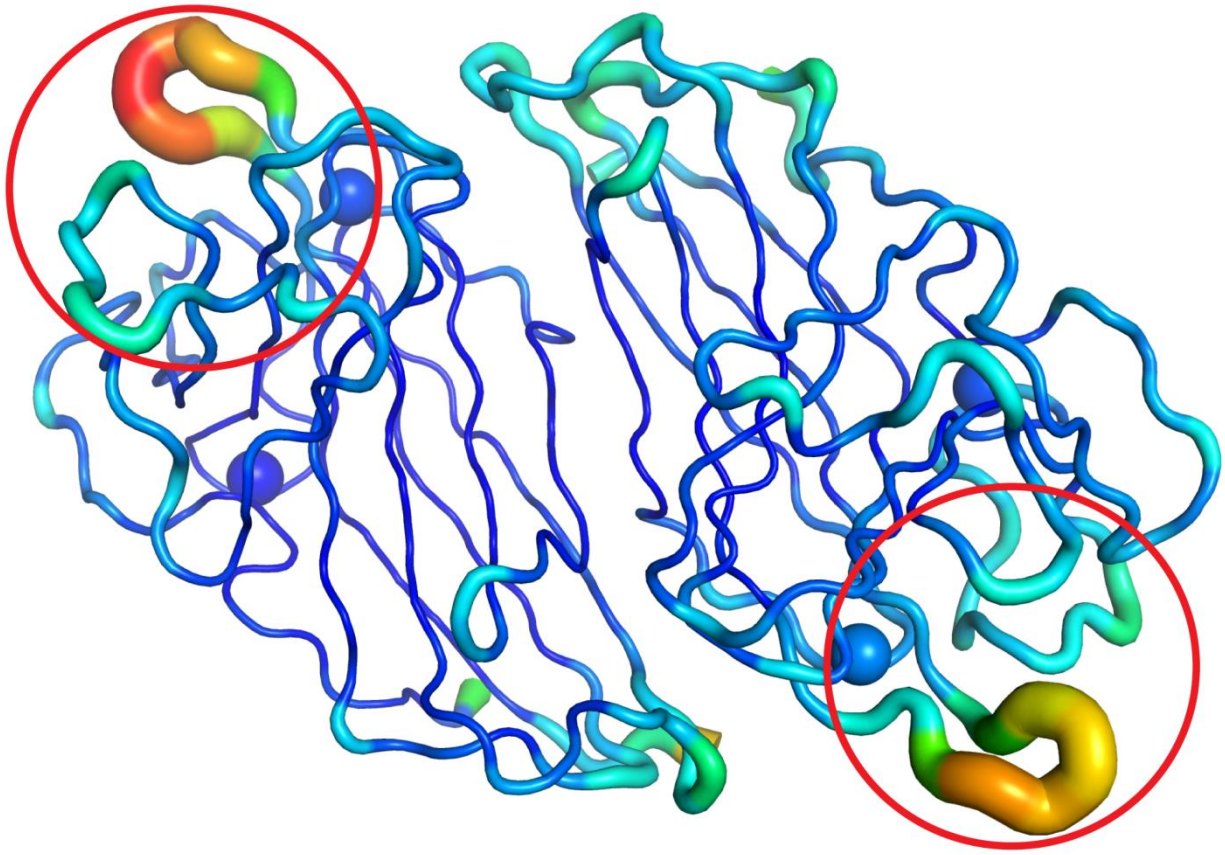
Supplementary Fig. 5. Autodock VINA[2] was used to examine if the binding pocket was appropriately sized for 12-epi-hapalindole U. Several docked structures of similar energy were generated (**a-c**): -9.7 kcal/mol, -9.4 kcal/mol, -9.2 kcal/mol.



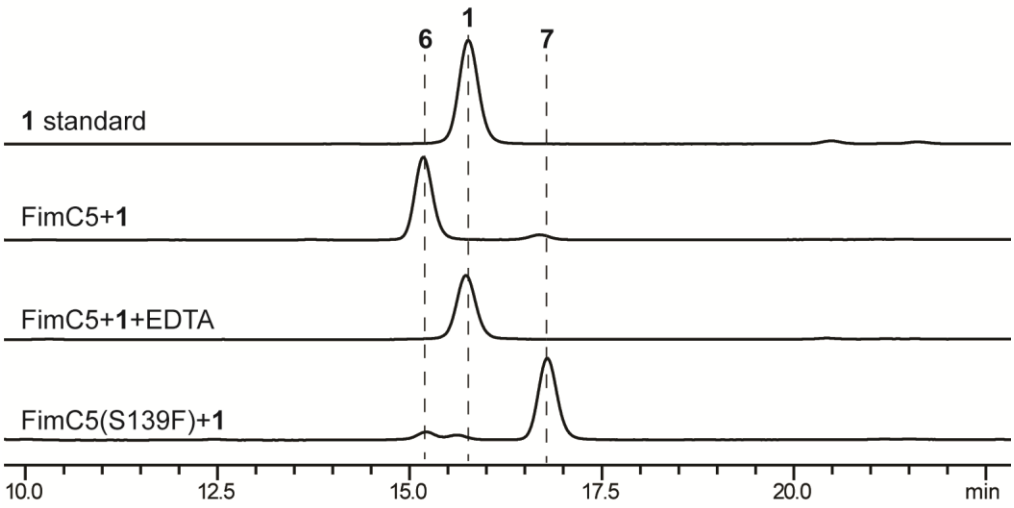
Supplementary Fig. 6. UV traces of HpiC1 in vitro reactions. HpiC1 is inactivated by 5 mM EDTA. The D214A, D214N, D214E variants had no activity with **1**. Identity of reaction products was confirmed by ^{1}H-NMR.



Supplementary Fig. 7. Comparison of SeMet HpiC1 W73M/K132M (*blue*, Form 1) and native HpiC1 (*yellow*, Forms 2 and 3) shows coupled side chain and main chain differences in the active site. D214 is shielded by F138 in SeMet HpiC1, whereas this residue is shifted in the native protein to expose D214 to the binding pocket. D214 is 100% conserved in known Stig cyclases. The loop containing F138 is also shifted ~3 Å from its position in the SeMet protein, although coordination of the structural calcium ion by the carbonyl oxygen of F138 is maintained.

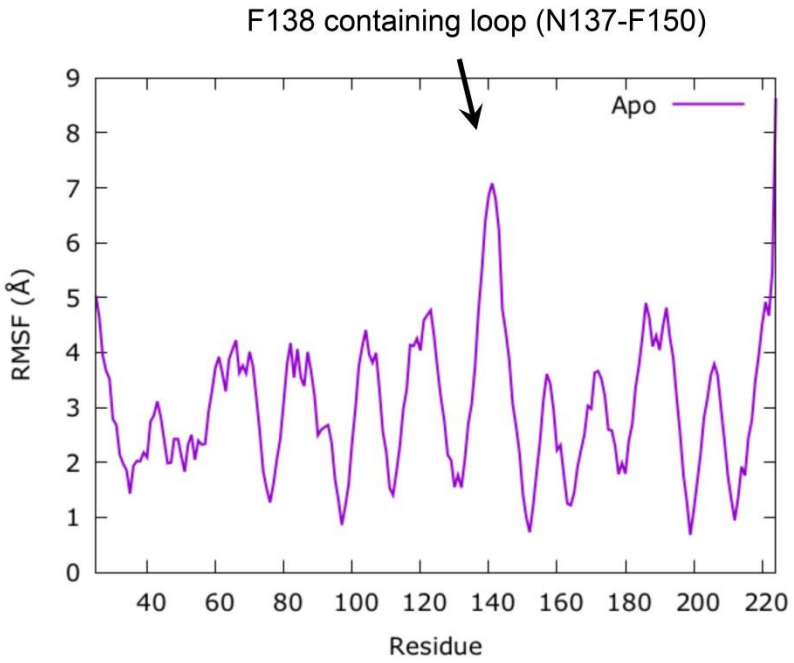


Supplementary Fig. 8. B-factor putty representation of HpiC1 in crystal form 1 suggests that the enzyme active site is a comparatively mobile region of the protein (PyMOL, Version 1.8 Schrödinger, LLC).

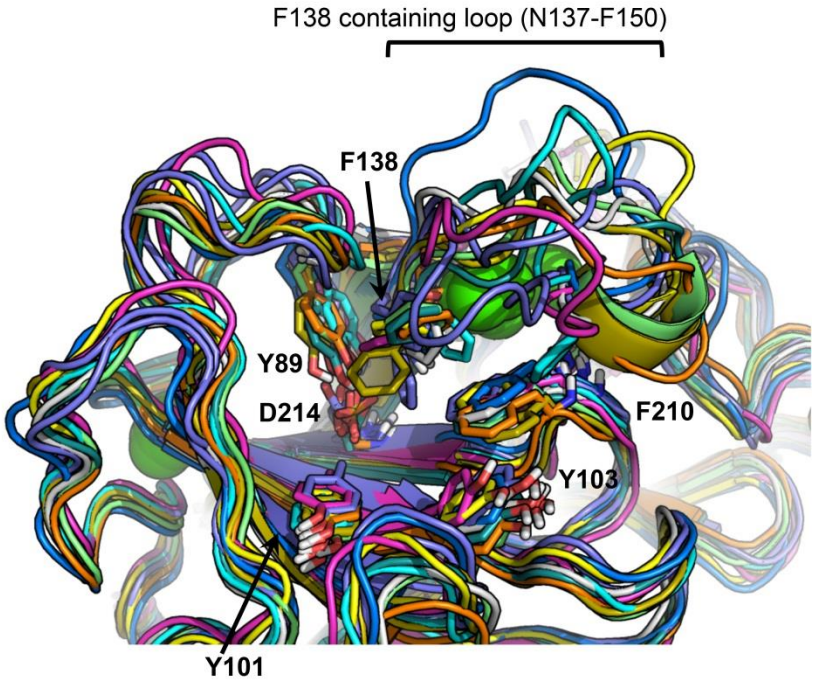


Supplementary Fig. 9. UV traces of FimC5 in vitro reactions. FimC5 is inactivated by 5 mM EDTA. The S139F variant produced predominantly the tricyclic 12-*epi*-hapalindole C. Identity of reaction products was confirmed by ^{1}H-NMR.

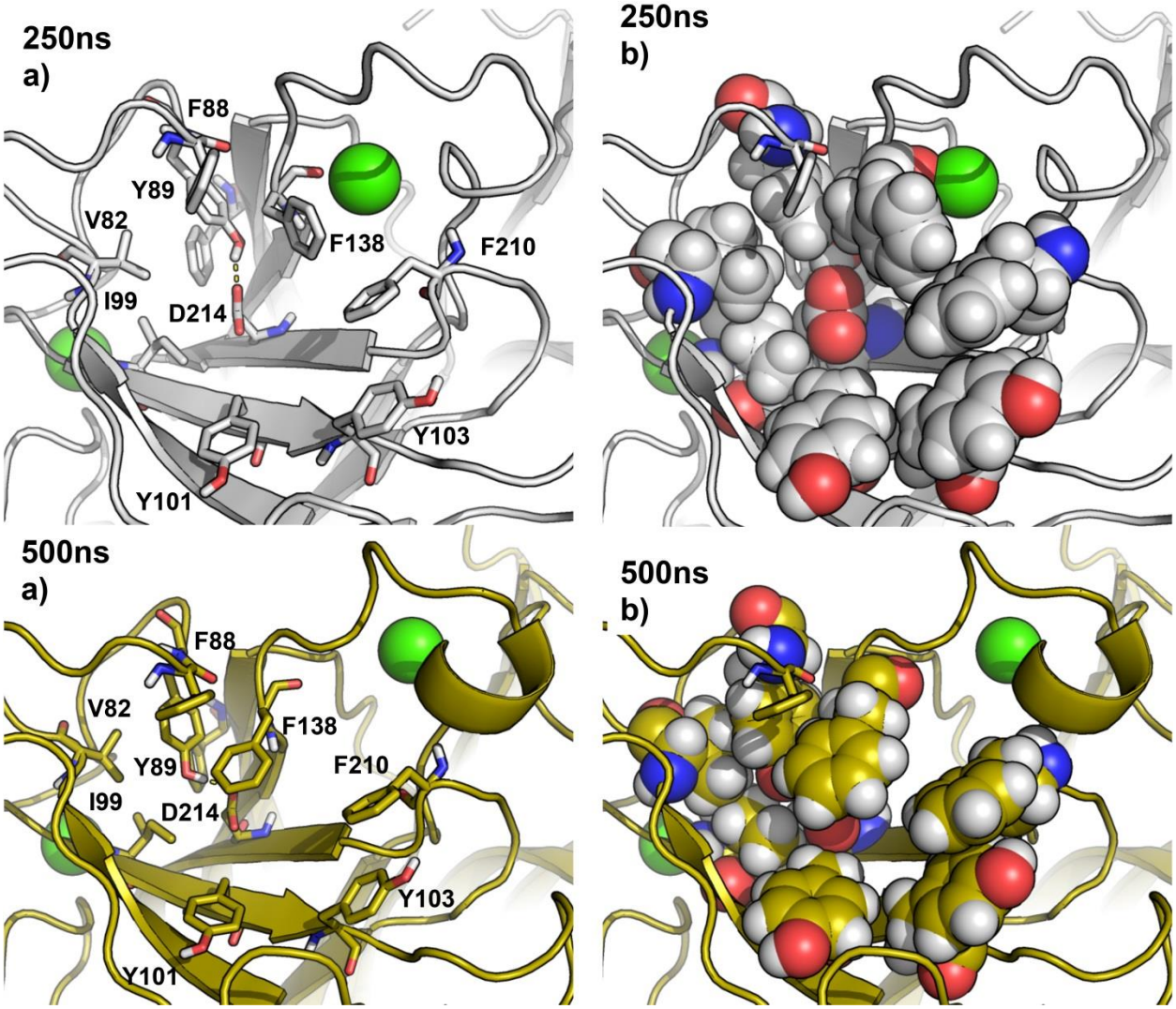
a)



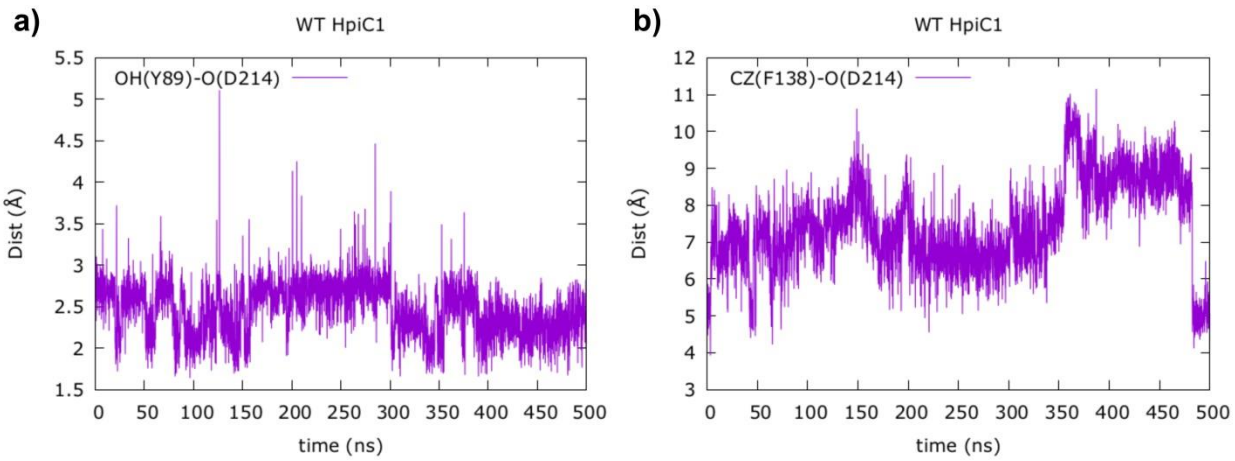
b)



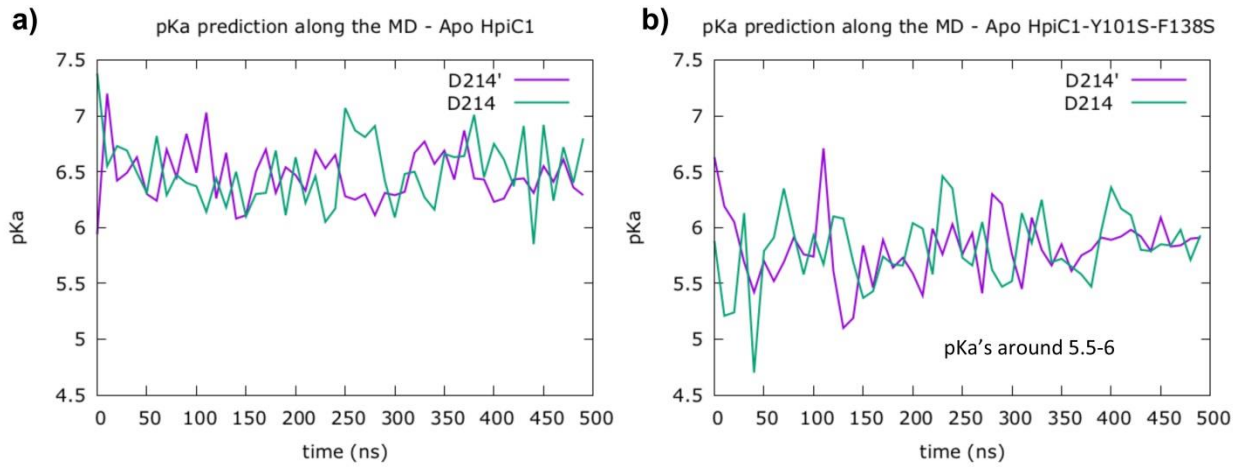
Supplementary Fig. 10. (**a**) RMSF measured over 500 ns MD simulation for the apo HpiC1 enzyme. (**b**) Overlay of representative snapshots obtained from this MD simulation for apo wild-type.



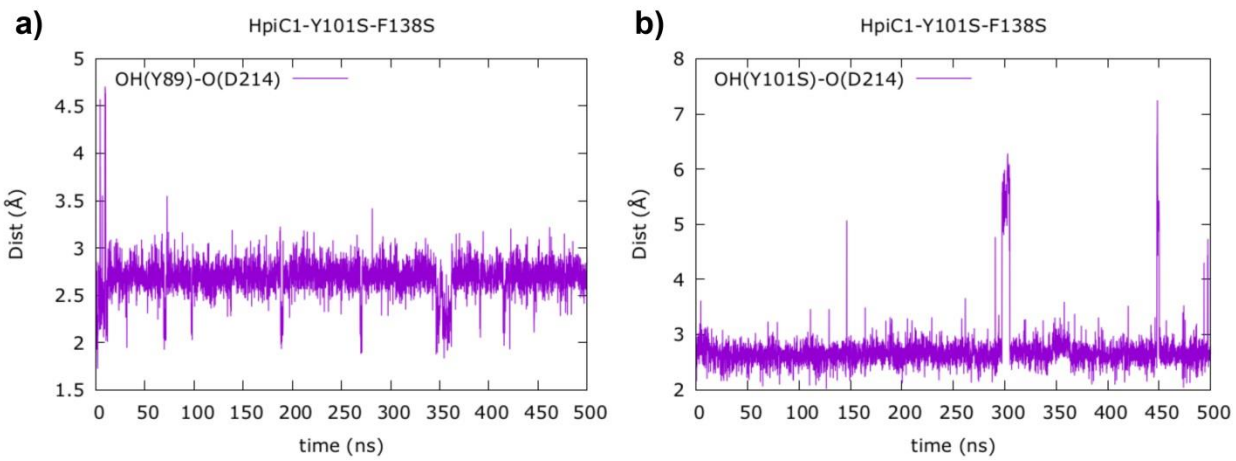
Supplementary Fig. 11. Representative snapshots (at 250 ns and 500 ns) of the active site arrangement and the two conformations of F138 side chain observed during the 500 ns of MD trajectory for the apo wild-type HpiC1 enzyme. The most important active site residues are represented (**a**) as sticks, and (**b**) in space-filling representation.



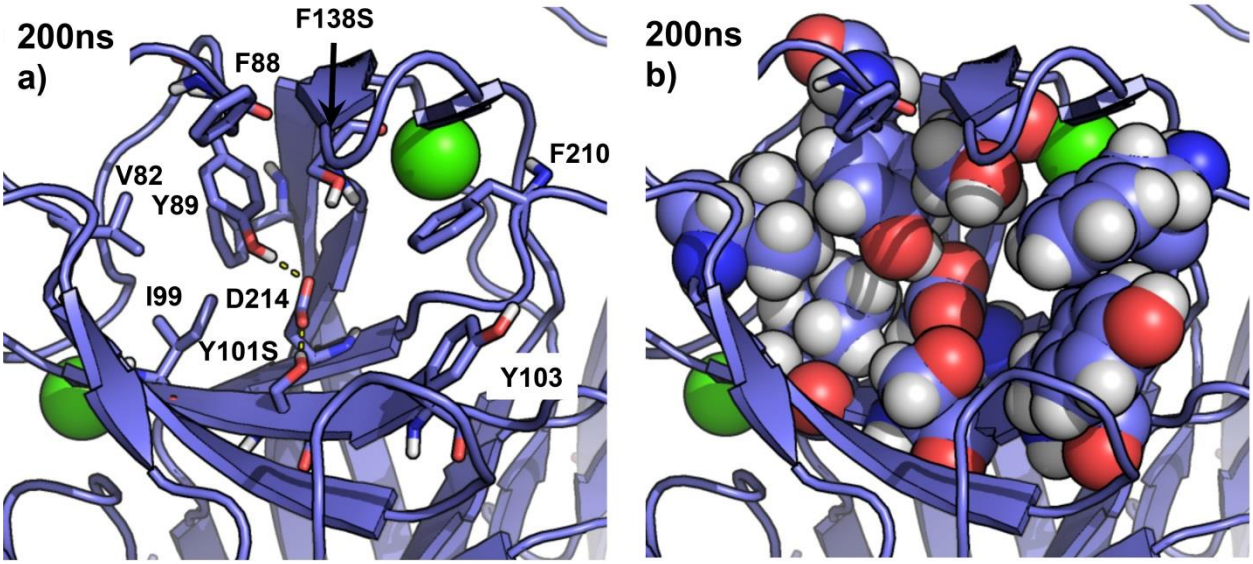
Supplementary Fig. 12. Distances measured along the 500 ns MD trajectory for the apo wild-type HpiC1 enzyme between (**a**) the center of mass of the two oxygen atoms of the D214 carboxylate group and the HO(Y89); and (**b**) Cz from the F138 side chain and the center of mass of the two oxygen atoms of the D214 carboxylate group.



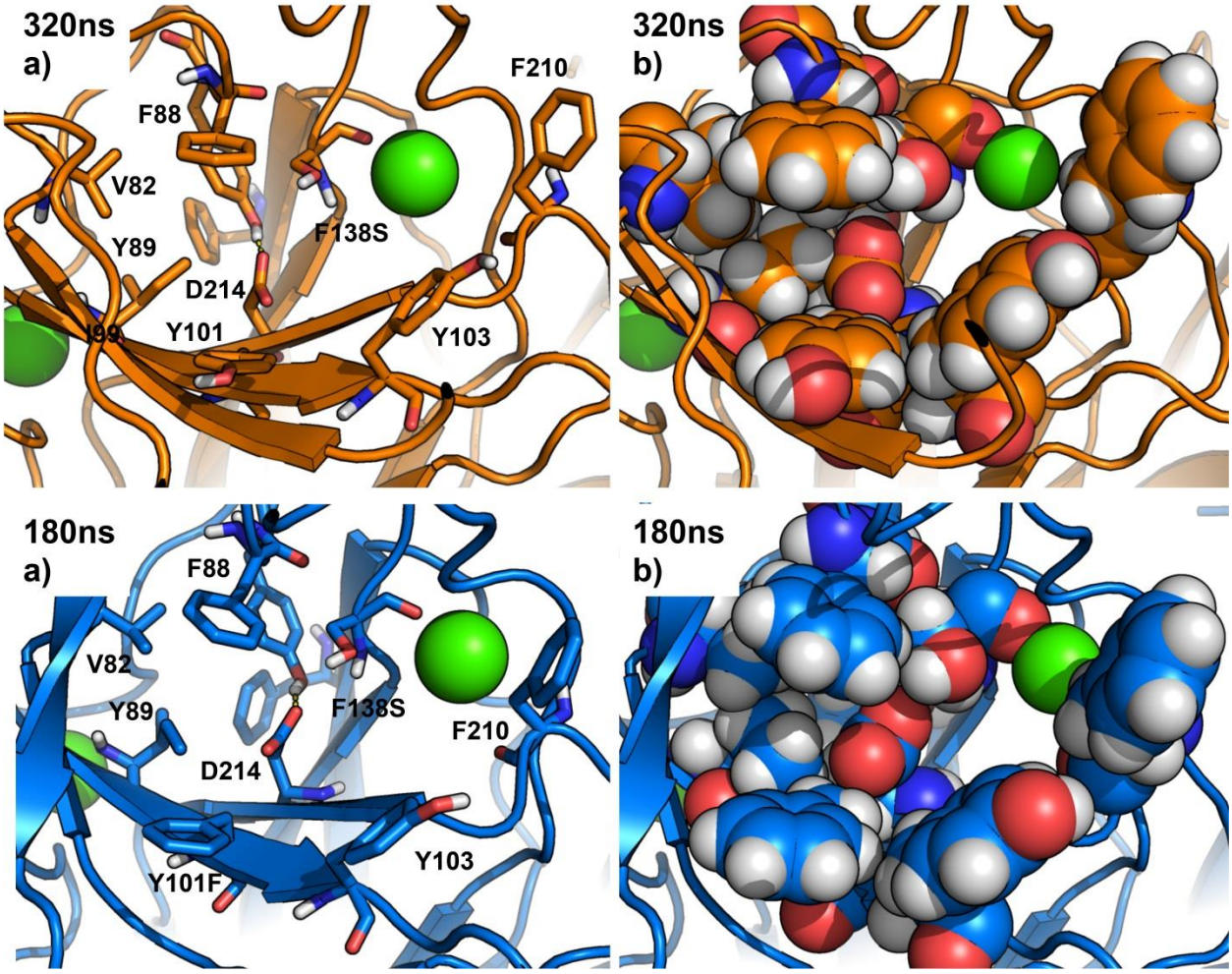
Supplementary Fig. 13. pK_a predictions for catalytic D214 and D214' in the apo state of the dimeric (**a**) wild-type HpiC1 enzyme and the (**b**) Y101S/F138S double mutant, for different snapshots obtained during the 500 ns MD trajectories. pKa estimations are obtained from the Propka3.1 program[3,4].



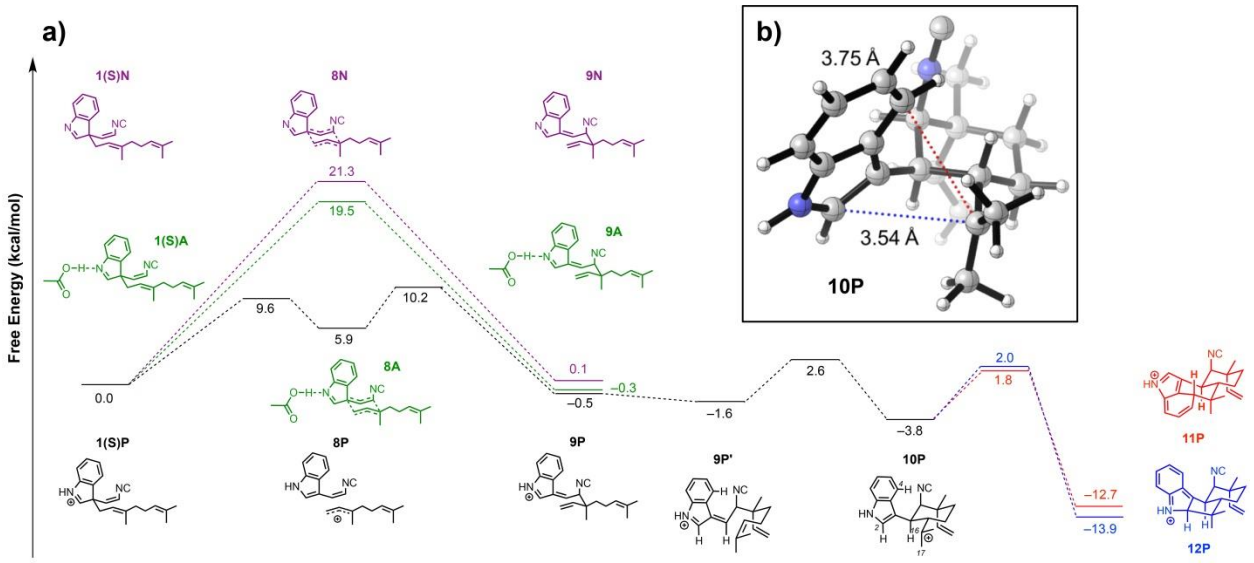
Supplementary Fig. 14. Distances measured along the 500 ns MD trajectory for the apo HpiC1 Y101S/F138S double mutant between the center of mass of the two oxygen atoms of the D214 carboxylate group and the (**a**) HO(Y89); and (**b**) HO(Y101S) side chains.



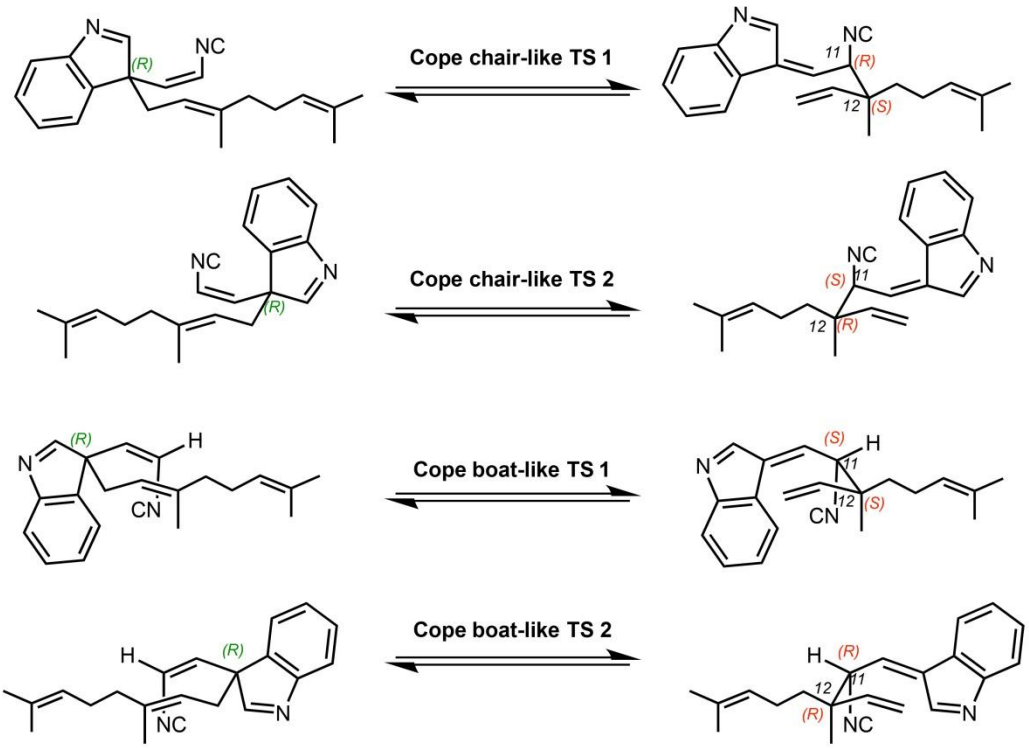
Supplementary Fig. 15. Representative snapshot (at 200 ns) of the active site arrangement in the MD trajectory of the apo HpiC1 F138S/Y101S double mutant. The most important active site residues are represented (**a**) as sticks, and (**b**) in space-filling representation.



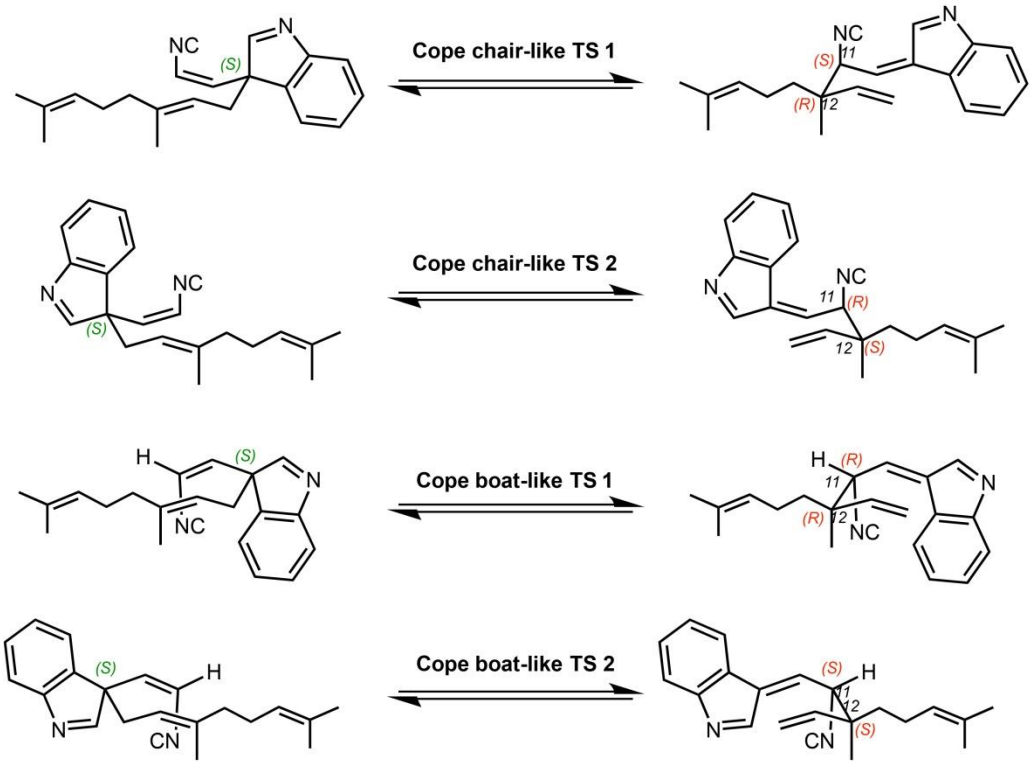
Supplementary Fig. 16. Representative snapshots of the active site arrangement observed during the 500 ns of MD trajectories for the HpiC1 F138S (top in orange, at 320 ns) and Y101F/F138S (bottom in blue, at 180 ns) mutants. The most important active site residues are represented (**a**) as sticks, and (**b**) in a space-filling representation.



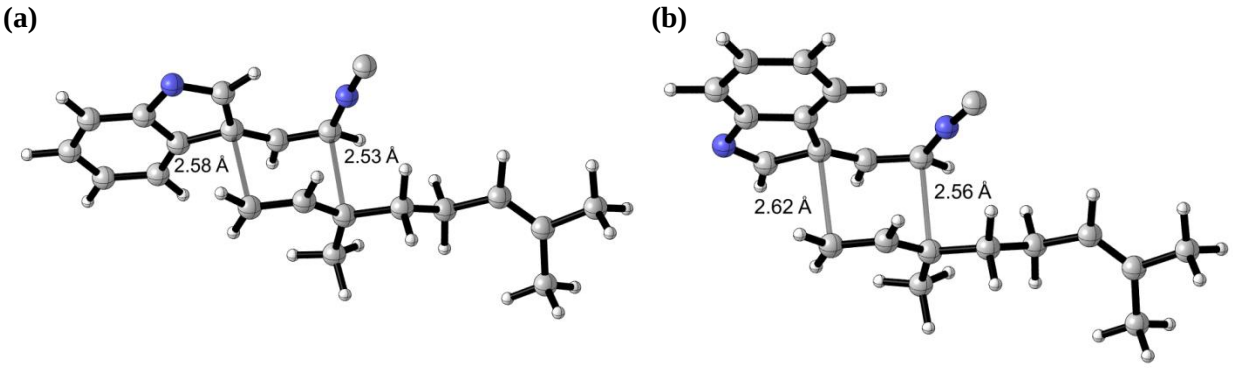
Supplementary Fig. 17. Cope rearrangement, cyclization, and electrophilic aromatic substitution cascade starting from the (*S*)-enantiomer of starting material. (**a**) **1**(*S*) in a near-attack conformation and leading to 12-*epi*-hapalindole U precursor 11P and 12-*epi*-fischerindole U precursor 12P. The energetics of the Cope rearrangement are computed with the neutral indole (pathway N), the *N*-protonated indole (pathway P), and the indole forming a hydrogen bond with acetic acid (pathway A). (**b**): Optimized geometry of key intermediate 10P which undergoes regioselective electrophilic aromatic substitution to form 12-*epi*-hapalindole U or 12-*epi*-fischerindole U.



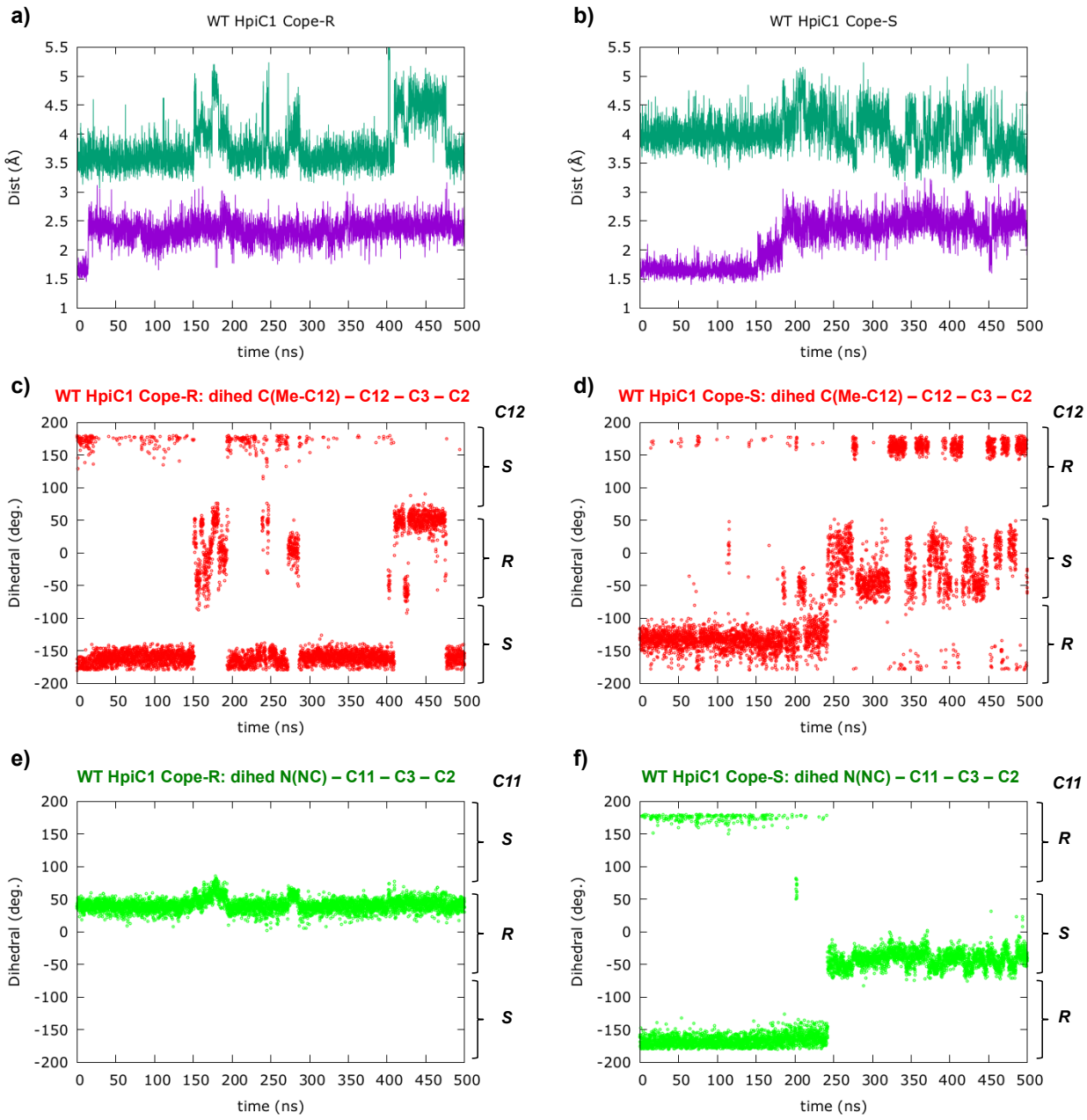
Supplementary Fig. 18. The four possible chair-like and boat-like transition states for the Cope rearrangement starting from the (*R*)-enantiomer of the starting material. Only chair-like TS 1 yields a product consistent with the known stereochemistry of 12-*epi*-hapalindole U and 12-*epi*-fischerindole U at positions 11 and 12, so only this possibility was investigated computationally (Fig. 5).



Supplementary Fig. 19. The four possible chair-like and boat-like transition states for the Cope rearrangement starting from the (*S*)-enantiomer of the starting material. Only chair-like TS 2 yields a product consistent with the known stereochemistry of 12-*epi*-hapalindole U and 12-*epi*-fischerindole U at positions 11 and 12, so only this possibility was investigated computationally (Supplementary Fig. 16).

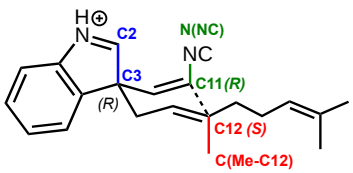


Supplementary Fig. 20. Optimized Cope rearrangement transition states (**a**) 2N coming from the 1(*R*)N starting material and (**b**) 8N coming from the 1(*S*)N starting material. Both transition states are chair-like with dissociative character, featuring breaking and forming partial single bonds with long lengths ranging from 2.53 Å to 2.62 Å.



MD simulations predict that (*R*) substrate 1(*R*)P is stabilized by the enzyme active site in a near attack conformation (NAC) that leads to the C11-(*R*) and C12-(*S*) configurations in the Cope rearrangement product, which corresponds to the stereochemistry of 12-*epi*-hapalindole U. On the other hand, (*S*) substrate 1(*S*)P does not explore any conformation that could lead to the C11-(*R*) and C12-(*S*) configurations during the entire 500 ns MD trajectory.

Dihedral angles explored:

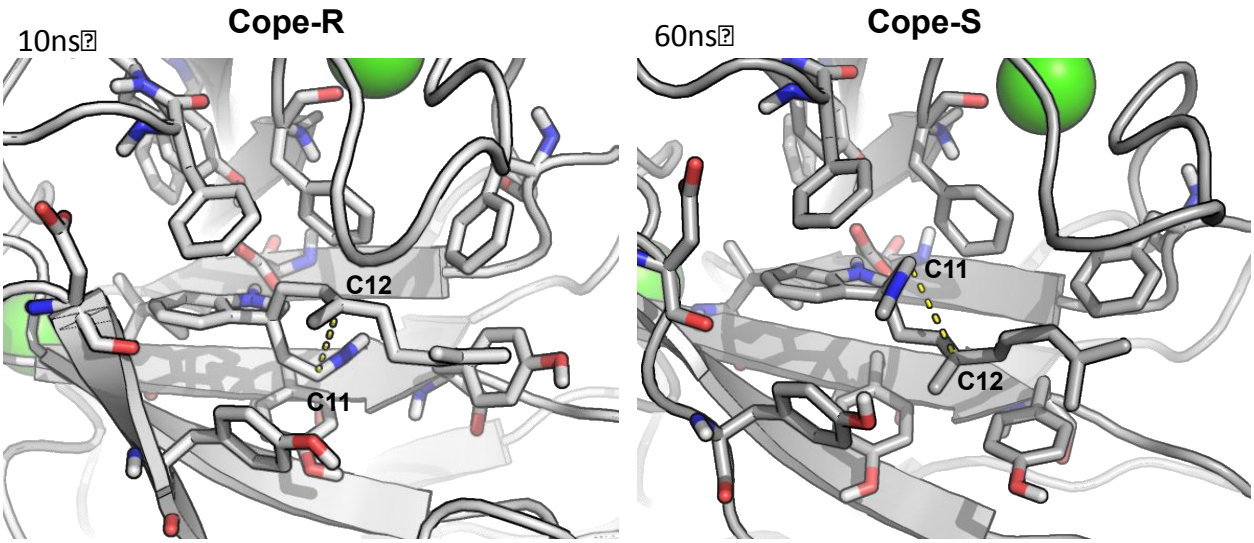


Supplementary Fig. 21. (**a**) and (**b**) show the distances between HN(indole) - O(D214) (*purple*), and C11-C12 (*green*) measured along the 500 ns MD trajectories for wild-type HpiC1 with (*R*) substrate 1(*R*)P (**a**, left) and (*S*) substrate 1(*S*)P (**b**, right) bound. During the simulations, the indole ring is protonated on nitrogen while D214 side chain is in the deprotonated carboxylate form. The 1(*R*)P

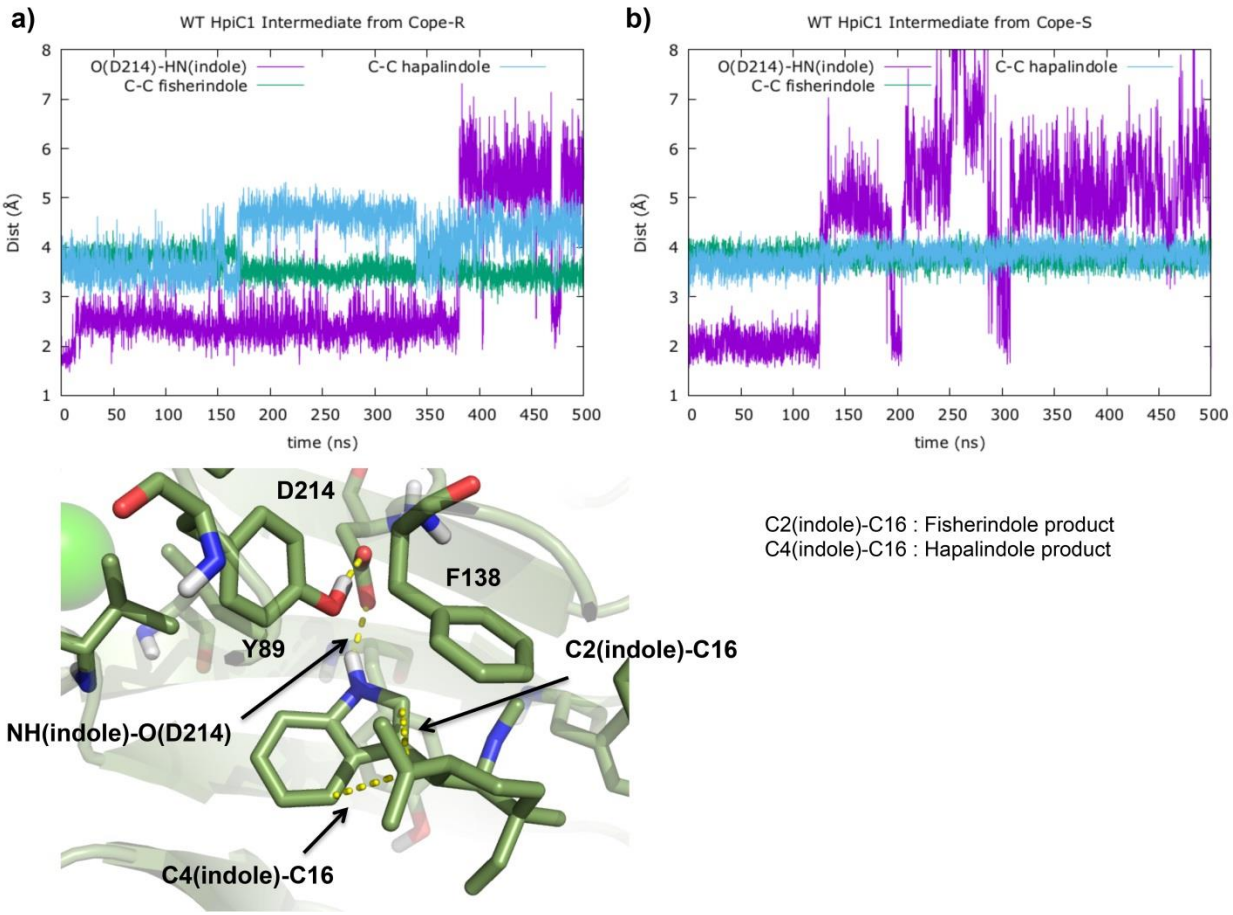
substrate mantains a shorter C11-C12 distance than 1(*S*)P, which is the new C-C bond formed during the Cope rearrangement.

(c) and (**d**) show the dihedral angle defined by C(Me-C12) – C12 – C3 – C2 explored during the 500 ns MD simulation for both substrate 1(*R*)P (**c**, left) and 1(*S*)P (**d**, right) bound complexes. This dihedral angle describes the relative orientation of the alkyl chain substituent with respect to the indole ring. On the right of each plot, the stereochemistry at C12 in the product of the Cope rearrangement that comes from this particular near attack conformation (NAC) is reported, as shown in Supplementary Figs. 20 and 21.

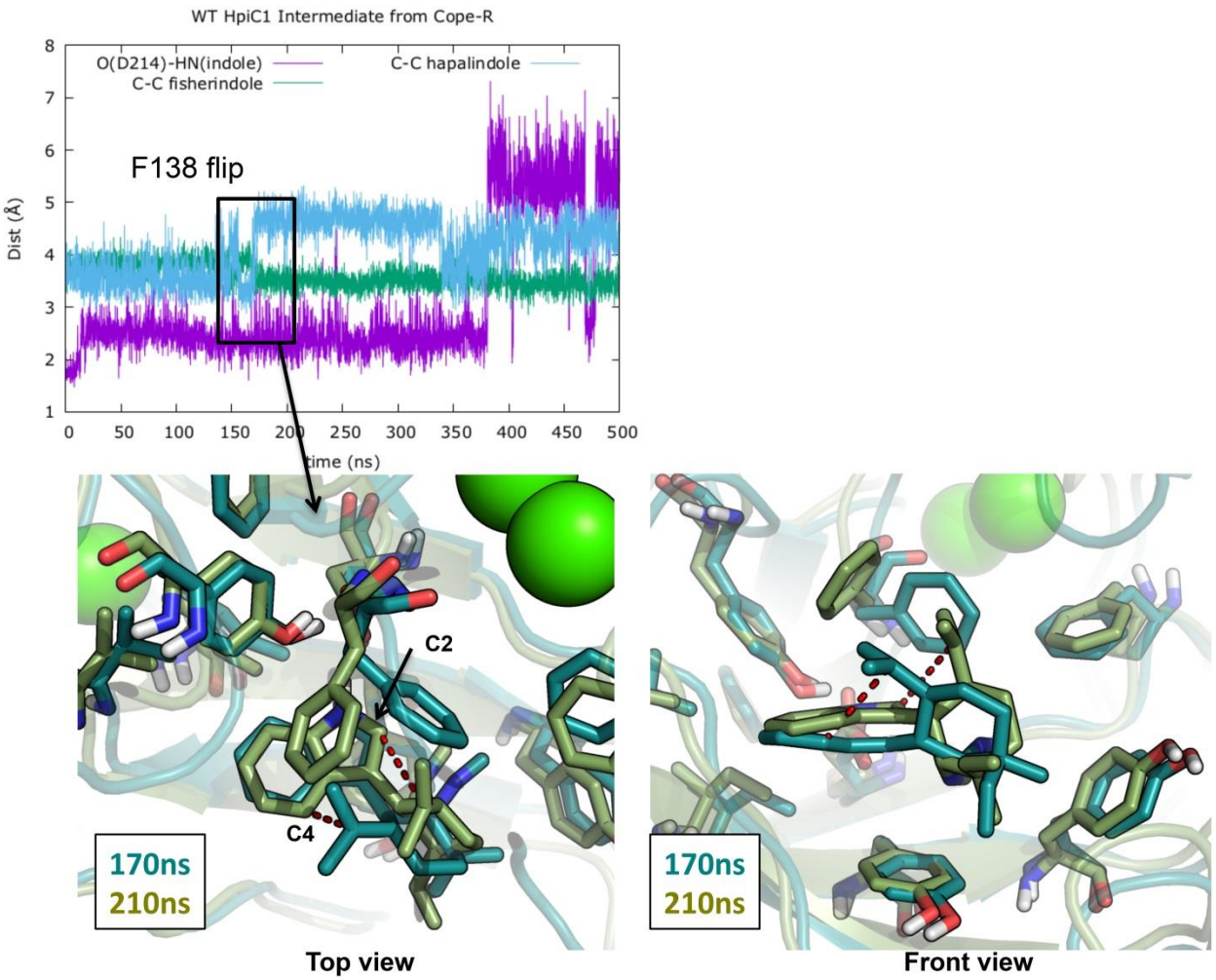
(e) and (**f**) show the dihedral angle defined by N(NC) – C11 – C3 – C2 explored during the 500 ns MD simulation for both substrate 1(*R*)P (**e**, left) and 1(*S*)P (**f**, right) bound complexes. This dihedral angle describes the relative orientation of the NC-containing substituent with respect to the indole ring. On the right of each plot, the stereochemistry at C11 in the product of the Cope rearrangement that comes from this particular near attack conformation (NAC) is reported, as shown in Supplementary Figs. 20 and 21.



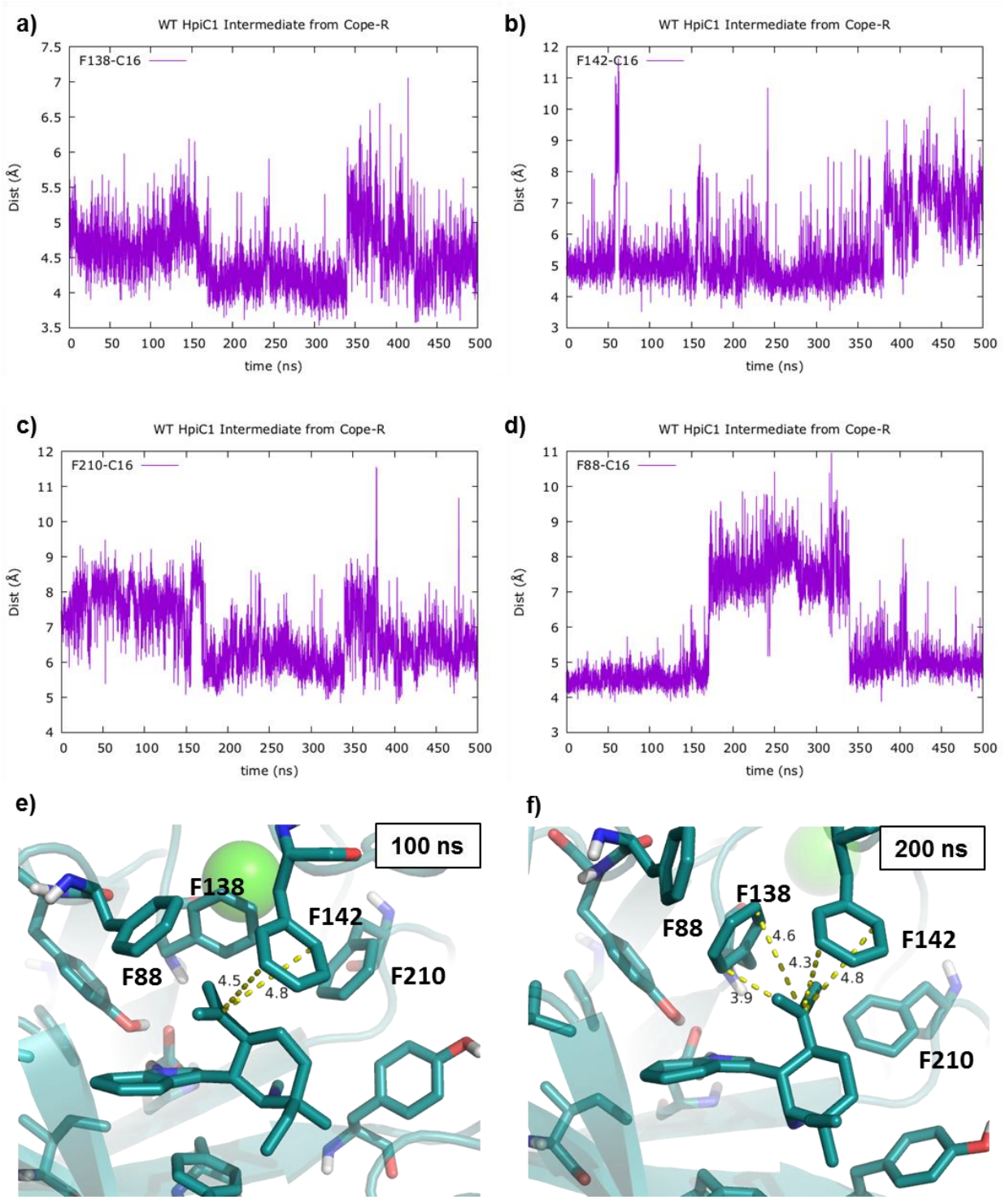
Supplementary Fig. 22. Representative snapshots of the active site arrangement observed during the 500 ns MD trajectories for substrate 1(*R*)P (Cope-R, left) and 1(*S*)P (Cope-S, right) bound into wild-type HpiC1 enzyme. MD simulations predict that substrate 1(*R*)P is stabilized by the enzyme active site in a near attack conformation that leads to the C11-*R* and C12-*S* configurations (left), as described in Figure S17. This observation highlights the importance of the active site shape and arrangement in controlling the stereochemistry of the Cope rearrangement.



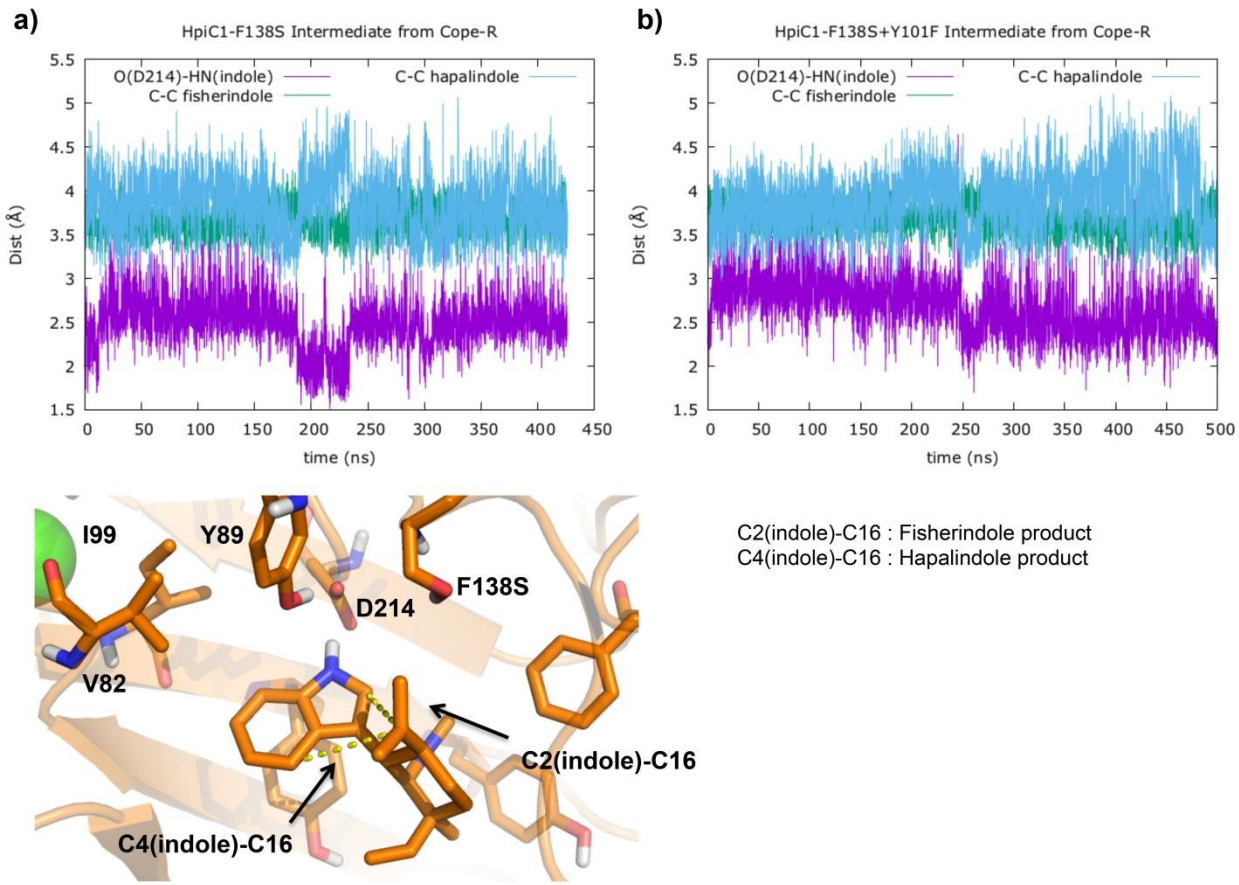
Supplementary Fig. 23. Key distances measured along the 500 ns MD trajectory for intermediate 4P bound into wild-type HpiC1 enzyme. Two possible intermediates are considered: (**a**) 4P coming from Cope-R pathway; and (**b**) 10P coming from Cope-S pathway. 10P rapidly dissociates from the active site, as illustrated by the disruption of the O(D214)-HN(indole) H-bond.



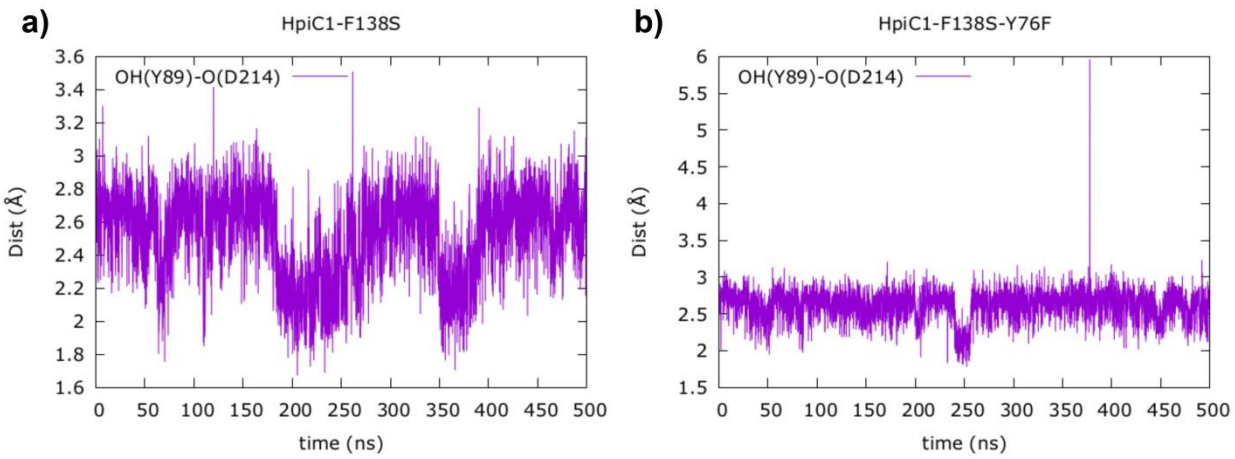
Supplementary Fig. 24. Representative snapshots of the active site arrangement observed during the 500 ns MD trajectories for intermediate 4P (from Cope-R pathway) bound into wild-type HpiC1 enzyme. Preference for C-C hapalindole formation is observed (snapshot at 170ns) for the preferred orientation of F138 side chain, and C-C fischerindole formation could be possible due to a flip of the F138 side chain after ~180ns of MD trajectory. This observation highlights the importance of F138 residue in dictating the regiochemistry of the process.



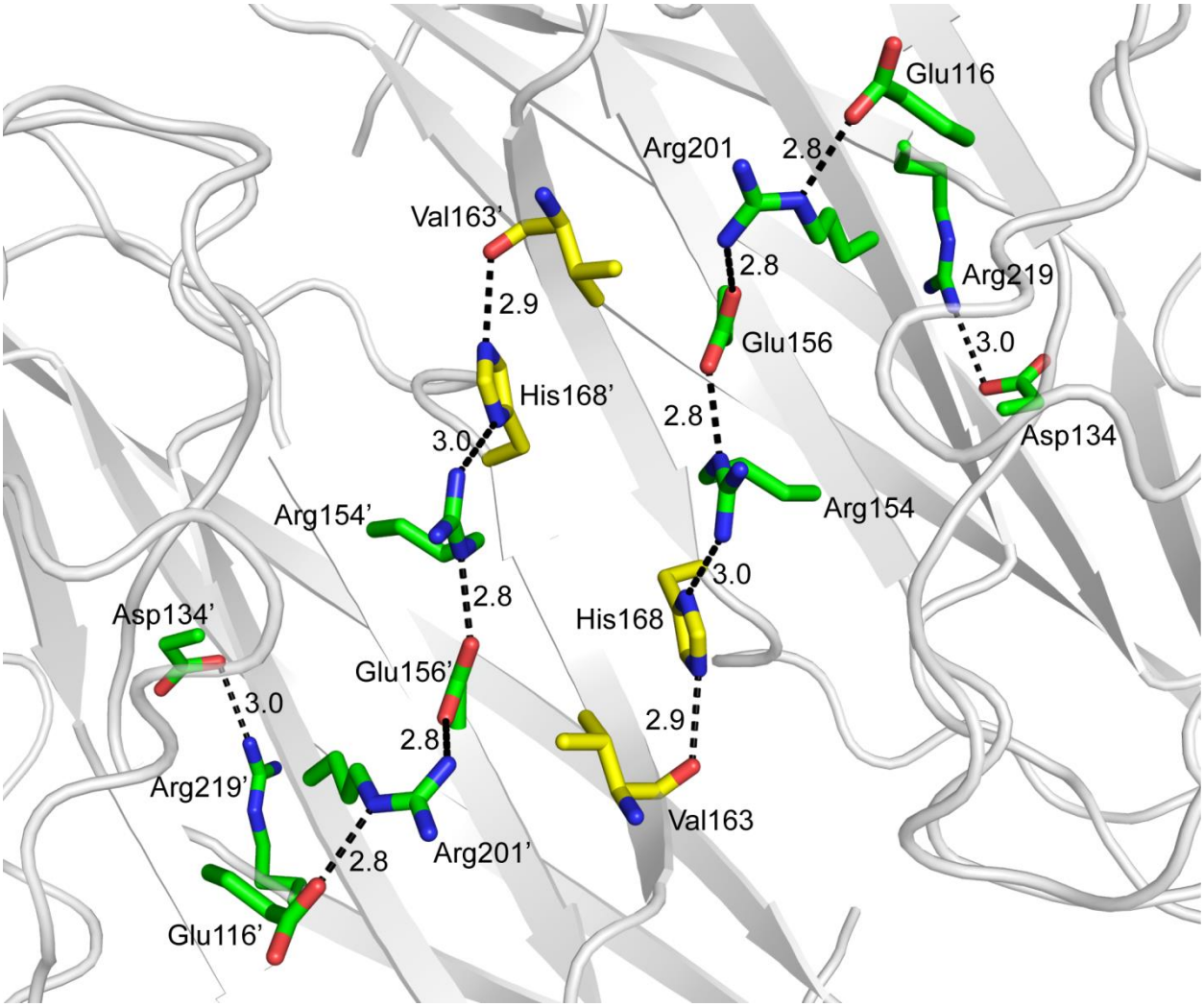
Supplementary Fig. 25. Cation–π interactions with intermediate 4P. (**a-d**) Key distances between C16 and Phe center measured along the 500 ns MD trajectory for intermediate 4P (from Cope-R pathway) bound into HpiC1. (**e**) 100 ns snapshot which shows F142 cation–π interaction with C16. (**f**) 200 ns snapshot which shows F138 and F142 cation–π interactions.



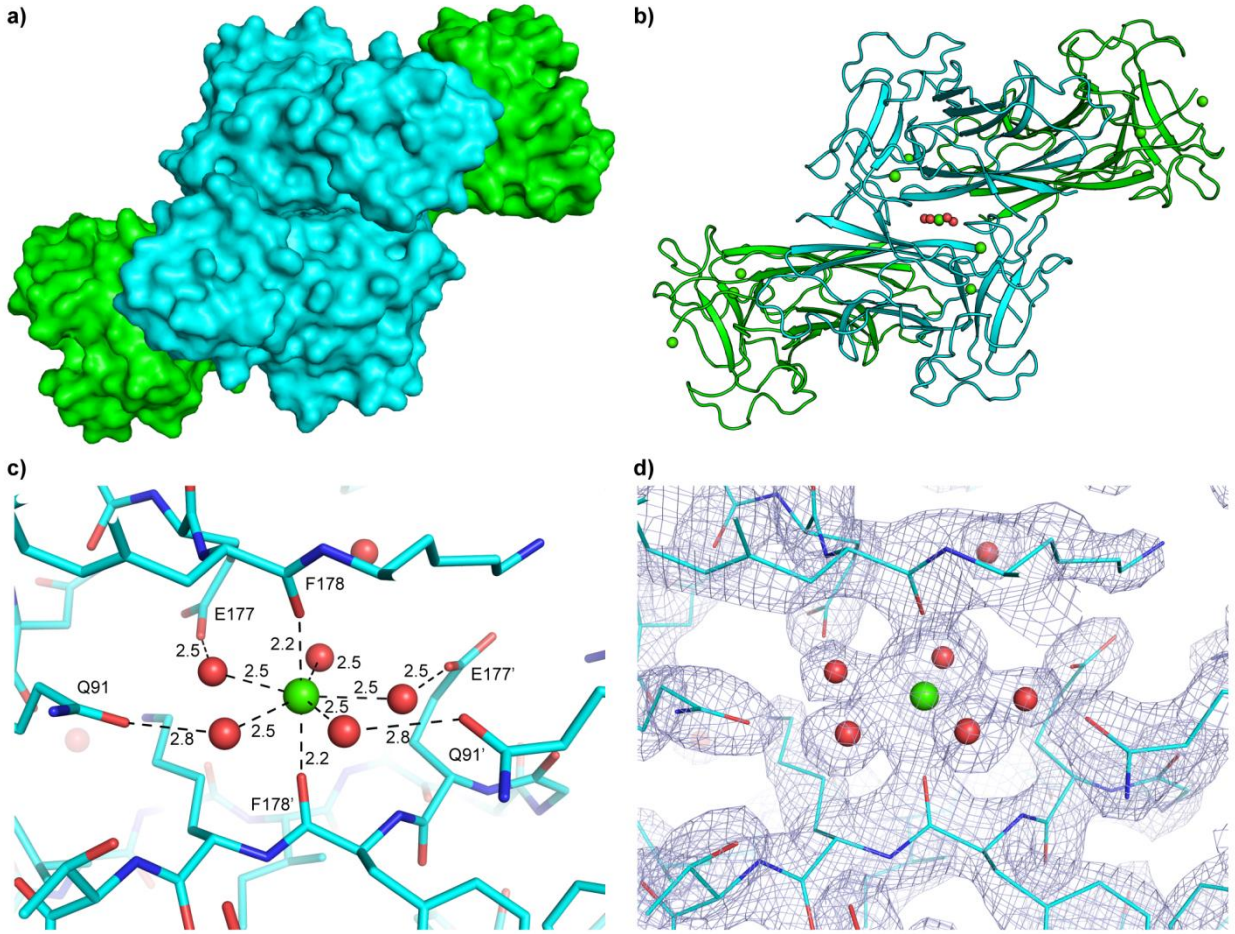
Supplementary Fig. 26. Key distances measured along the 500 ns MD trajectory for intermediate 4P (from Cope-R pathway) bound into (**a**) F138S mutant and (**b**) Y101F/F138S double mutant. Preference for C-C fischerindole formation (C2-C16 distance ~3.5Å) is observed over hapalindole (C4-C16 distance ~4.0Å).



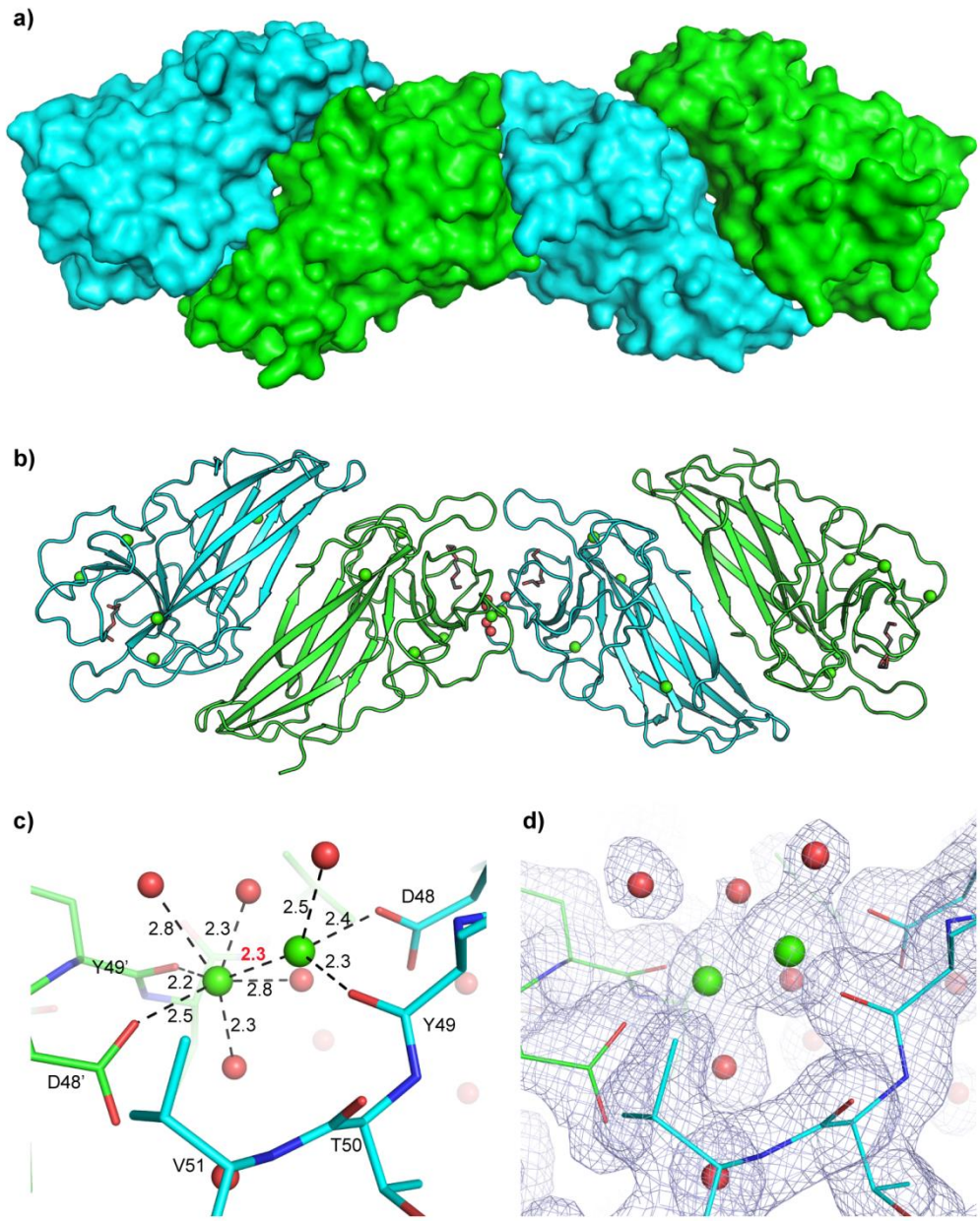
Supplementary Fig. 27. Distances measured along the 500 ns MD trajectory for the apo (**a**) F138S mutant and (**b**) Y101S/F138S double mutant between the center of mass of the two oxygen atoms of the D214 carboxylate group and the HO(Y89) side chain.



Supplementary Fig. 28. As with the CBMs[5], HpiC1 and other Stig cyclases are thermostable. This characteristic was highly beneficial for facile purification of an HpiC1 homolog, FamC1, from the *Fischerella ambigua* cell-free lysate[6]. As observed with other thermophilic proteins[7] an extended salt bridge array in HpiC1 is readily apparent, and spans the dimeric interface in coordination with hydrogen bonds. These residues are conserved in other Stig cyclases and we expect that many will share this thermostable property. Charged amino acids are shown as green sticks and hydrogen bonded amino acids are shown as yellow sticks.



Supplementary Fig. 29. Bridging calcium ion at crystal packing interface in HpiC1 crystal form 2. (**a**) Surface representation showing two dimers, each with green and cyan monomers. The total buried surface area for this assembly is 1700 $Å^2$ (PISA)[8]. (**b**) Cartoon representation: calcium ions are shown as green spheres; ligating waters are shown as red spheres. (**c**) Stick representation of the bridging calcium and ligating waters. (**d**) 2Fo-Fc electron density map at 2.1 Å resolution contoured at 1.5σ.



Supplementary Fig. 30. Second bridging calcium site. (**a**) Surface representation of HpiC1 in crystal form 1 showing adjacent dimers, each with green and cyan monomers. The total buried surface area for this assembly is 2160 Å^2 (PISA)[8] (**b**) cartoon representation of the HpiC1 packing interaction. PEG molecules bound in the active site are shown as sticks. All calcium ions are shown as green spheres, ligating waters at the bridging calcium ions are shown as red spheres. (**c**) Stick representation of the bridging calcium ions and ligating waters. Due to the close positioning between the two cations, each calcium ion was modeled at half occupancy. (**d**) 2Fo-Fc electron density map at 1.7 Å resolution contoured at 1.0σ.

SUPPLEMENTARY NOTES

Optimized quantum mechanical energies and geometries

Structure	**Single-Point Energy** (Hartree) B3LYP/6-31G++(d,p)_ IEFPCM diethyl ether solvent D3(BJ) dispersion correction	**Gibbs Free Energy Correction** (Hartree) B3LYP/6-31G(d)
1(*R*)N	−924.425824090	0.340862
2N	−924.393217694	0.341123
3N	−924.426853546	0.342661
1(*R*)A	−1153.62045448	0.393464
2A	−1153.59150325	0.393800
3A	−1153.62254503	0.396355
1(*R*)P	−924.850912128	0.353083
Transition State from 1(*R*)P to 2P	−924.839929132	0.352990
2P	−924.844007992	0.350001
Transition State from 2P to 3P	−924.841330396	0.354031
3P	−924.856552200	0.355725
3P'	−924.860987388	0.358801
Transition State from 3P' to 4P	−924.859836609	0.361036
4P	−924.869068910	0.362161
Transition State from 4P to 5P	−924.861768738	0.366601
5P	−924.879360164	0.369401
Transition State from 4P to 6P	−924.869011094	0.364728
6P	−924.890827959	0.367863

1(*S*)N	−924.423171624	0.341591
8N	−924.388956592	0.341246
9N	−924.425100306	0.343603
1(*S*)A	−1153.61832077	0.394940
8A	−1153.58652059	0.394254
9A	−1153.62074201	0.396923
1(*S*)P	−924.850798839	0.353838
Transition State from 1(*S*)P to 8P	−924.834447297	0.352745
8P	−924.836870979	0.349290
Transition State from 8P to 9P	−924.833948046	0.353167
9P	−924.854144460	0.356362
9P'	−924.859128498	0.359602
Transition State from 9P' to 10P	−924.853367472	0.360556
10P	−924.865986928	0.363015
Transition State from 10P to 11P	−924.860432474	0.366380
11P	−924.886299741	0.369146
Transition State from 10P to 12P	−924.860123783	0.366291
12P	−924.887673330	0.368484

1(*R*)N

C	0.527702	0.921932	1.999973
C	1.432854	0.099038	1.453807
C	1.215539	-1.054432	-0.791798
C	-0.219160	-0.718751	-1.092009
C	-1.331115	-1.275012	-0.582356
N	-0.117797	1.959500	1.361040
H	0.234243	0.800907	3.039019
H	1.769849	-1.170049	-1.732047
H	1.307553	-2.005406	-0.257467
C	-1.344171	-2.387141	0.439253
C	-2.695849	-0.799585	-1.042996
C	1.993110	0.037182	0.050636
C	2.052355	1.362582	-0.716313
N	3.225467	1.732253	-1.092926
C	-0.736804	2.849445	0.890941
C	4.136655	0.751591	-0.616013
C	3.482465	-0.279115	0.077341
C	4.204561	-1.334993	0.615131
C	5.597622	-1.343320	0.450470
C	6.243275	-0.313093	-0.240859
C	5.516922	0.751275	-0.786573
H	3.715368	-2.144900	1.152486
H	6.181141	-2.160990	0.864553
H	7.323432	-0.340460	-0.355633
H	6.003705	1.557645	-1.326267
H	1.175090	1.948389	-0.968963
C	-3.491474	-0.009862	0.029888
C	-4.804347	0.495923	-0.505031
C	-6.049737	0.158629	-0.135339
C	-6.392681	-0.832451	0.950581
C	-7.249695	0.782526	-0.808938
H	-1.915723	-3.246302	0.062571
H	-0.346005	-2.741023	0.707380
H	-1.838556	-2.066903	1.365287
H	-3.301247	-1.664227	-1.351963
H	-2.582473	-0.165309	-1.930664
H	-2.878399	0.845571	0.347005
H	-3.640147	-0.634681	0.916482
H	-4.705404	1.226773	-1.310206
H	-6.987960	-0.352486	1.740043
H	-7.012265	-1.646686	0.549237
H	-5.515374	-1.282142	1.421443
H	-7.888594	0.016184	-1.270698
H	-7.880217	1.314250	-0.082141
H	-6.957257	1.494317	-1.587236
H	-0.354192	0.070566	-1.832105
H	1.811590	-0.669508	2.124322

2N

C	0.180564	0.593310	-1.296793
C	-1.098949	0.057792	-1.235582
C	-1.128602	-0.488534	1.712179
C	0.170212	-0.067260	1.549385
C	1.131303	-0.643781	0.697035
N	0.505980	1.859750	-0.862353
H	0.887810	0.184860	-2.010913
H	-1.801623	0.048808	2.370872
H	-1.480761	-1.452158	1.365106
C	0.982075	-2.044520	0.162388
C	2.527733	-0.057287	0.747962
C	-2.184657	0.440380	-0.445583
C	-2.456708	1.717227	0.248107
N	-3.683705	1.839123	0.667062
C	0.861902	2.926976	-0.498066
C	-4.347856	0.653486	0.283195
C	-3.486816	-0.232659	-0.408370
C	-3.963459	-1.455781	-0.878565
C	-5.303788	-1.783362	-0.648020
C	-6.149785	-0.903987	0.041925
C	-5.680230	0.325789	0.515723
H	-3.318104	-2.147875	-1.416314
H	-5.694115	-2.731009	-1.009197
H	-7.186991	-1.182340	0.208805
H	-6.328812	1.015886	1.046973
H	-1.728985	2.505001	0.404831
C	3.497748	-0.413815	-0.397468
C	4.798426	0.335372	-0.269406
C	6.032400	-0.156159	-0.077769
C	6.374602	-1.621439	0.042857
C	7.220394	0.770829	0.030699
H	1.500885	-2.746805	0.833013
H	-0.059050	-2.364042	0.094500
H	1.437964	-2.158100	-0.825324
H	2.987469	-0.391742	1.693130
H	2.449972	1.033979	0.835525
H	3.031195	-0.148594	-1.357630
H	3.666298	-1.494574	-0.424649
H	4.695700	1.419991	-0.334973
H	7.081536	-1.919502	-0.743809
H	6.875507	-1.822669	0.999884
H	5.505592	-2.280401	-0.023633
H	7.734053	0.643905	0.994043
H	7.964341	0.552515	-0.748350
H	6.929496	1.821573	-0.063094
H	0.445074	0.880786	2.009367
H	-1.209427	-0.875066	-1.786142

3N

C	0.307370	0.210312	-0.633889
C	-1.105353	-0.319159	-0.688706
C	0.005185	-0.254034	2.965620
C	0.475379	0.371467	1.886194
C	1.104790	-0.260388	0.658564
N	0.390056	1.629551	-0.788271
H	0.835024	-0.218764	-1.494660
H	-0.400360	0.308952	3.801615
H	0.001041	-1.335162	3.070242
C	1.075979	-1.797712	0.708961
C	2.576431	0.253334	0.590245
C	-2.275103	0.270577	-0.376051
C	-2.577138	1.634314	0.132135
N	-3.836017	1.836038	0.359334
C	0.532105	2.790910	-0.925181
C	-4.508008	0.632450	0.014101
C	-3.610722	-0.354835	-0.442937
C	-4.077147	-1.604650	-0.832200
C	-5.454220	-1.855140	-0.757298
C	-6.338369	-0.871030	-0.302411
C	-5.873146	0.390939	0.090553
H	-3.400938	-2.377893	-1.190556
H	-5.838910	-2.825764	-1.057842
H	-7.401802	-1.089059	-0.253950
H	-6.549337	1.162915	0.444575
H	-1.844080	2.410927	0.310210
C	3.430772	-0.186988	-0.618582
C	4.813468	0.409403	-0.553027
C	5.991700	-0.218648	-0.417951
C	6.171397	-1.713765	-0.312825
C	7.280579	0.567815	-0.363633
H	1.731271	-2.159146	1.508129
H	0.070069	-2.180300	0.904339
H	1.426955	-2.236667	-0.231145
H	3.071539	-0.082964	1.509390
H	2.569551	1.348825	0.634085
H	2.955638	0.153839	-1.550423
H	3.476806	-1.278930	-0.673149
H	4.831514	1.499130	-0.612818
H	6.804130	-2.086316	-1.130436
H	6.688472	-1.975158	0.620862
H	5.231057	-2.269409	-0.339604
H	7.819715	0.379299	0.575500
H	7.959558	0.271262	-1.175573
H	7.106221	1.645199	-0.444332
H	0.450861	1.461022	1.865863
H	-1.147981	-1.355991	-1.017854

1(*R*)A

C	0.019798	-1.334161	2.209873
C	0.810047	-1.819042	1.243653
C	0.705661	-1.437583	-1.255560
C	-0.645093	-0.780919	-1.334555
C	-1.856376	-1.350698	-1.218728
N	-0.357529	-0.019199	2.374959
C	-2.095499	-2.824001	-0.989615
C	-3.105417	-0.497053	-1.323473
C	1.497054	-1.135554	0.084452
C	1.724616	0.366984	0.206967
N	2.960188	0.727429	0.139704
C	-0.765333	1.065811	2.609839
C	3.750293	-0.446015	0.012018
C	2.945716	-1.594836	-0.026315
C	3.523834	-2.849641	-0.159114
C	4.920535	-2.934910	-0.252308
C	5.713901	-1.783678	-0.212960
C	5.135511	-0.516439	-0.081268
C	-3.846695	-0.297347	0.025410
C	-5.031605	0.619982	-0.115683
C	-6.335080	0.340271	0.039654
C	-6.892458	-1.011179	0.416560
C	-7.382130	1.411978	-0.155310
O	1.084970	3.379835	-0.402267
C	2.110367	4.032899	-0.309753
O	3.314543	3.509132	-0.053312
C	2.173085	5.535868	-0.468341
H	-0.394175	-2.002848	2.959698
H	1.338676	-1.082145	-2.078347
H	0.641961	-2.525766	-1.356848
H	2.919722	-3.753548	-0.193783
H	5.391581	-3.908224	-0.357327
H	6.793973	-1.874598	-0.286378
H	5.740051	0.384823	-0.050694
H	0.946271	1.119019	0.266384
H	-2.736333	-3.234915	-1.781531
H	-1.176110	-3.413834	-0.964021
H	-2.622863	-2.996142	-0.042615
H	-3.806687	-0.952434	-2.037668
H	-2.843130	0.488484	-1.726515
H	-3.136284	0.138887	0.742026
H	-4.144776	-1.268993	0.432662
H	-4.771696	1.643295	-0.393652
H	-7.462284	-0.948142	1.354285
H	-7.596791	-1.366079	-0.348916
H	-6.124595	-1.777862	0.544070
H	-8.094206	1.132171	-0.944871
H	-7.975100	1.557618	0.758880
H	-6.936320	2.374200	-0.425915
H	-0.614859	0.294731	-1.509427
H	0.973256	-2.893972	1.283686
H	3.226874	2.515582	0.035332
H	1.180519	5.924803	-0.697918
H	2.545957	5.991240	0.455376
H	2.874251	5.800893	-1.266640

2A

C	-0.992439	-1.102050	1.466678
C	0.170858	-1.713630	1.027395
C	0.615554	0.237596	-1.386466
C	-0.640309	0.584998	-0.951339
C	-1.762921	-0.260833	-0.863046
N	-1.032981	0.129290	2.079457
C	-1.815592	-1.592243	-1.561058
C	-3.072136	0.383677	-0.461825
C	1.433793	-1.168575	0.780541
C	1.983844	0.142987	1.122501
N	3.266115	0.244689	0.872520
C	-1.143500	1.183470	2.604702
C	3.678264	-0.993269	0.348547
C	2.592890	-1.900536	0.275504
C	2.793205	-3.194536	-0.211256
C	4.075456	-3.561927	-0.624638
C	5.143109	-2.653252	-0.554677
C	4.956938	-1.357470	-0.067034
C	-4.233934	-0.541638	-0.046287
C	-5.422155	0.250314	0.433719
C	-6.655729	0.309539	-0.091448
C	-7.116940	-0.446580	-1.313786
C	-7.718559	1.177449	0.540542
O	2.468501	2.912904	-0.940396
C	3.487956	3.381065	-0.456171
O	4.288592	2.740969	0.393465
C	3.988161	4.778258	-0.757693
H	-1.873028	-1.709232	1.647413
H	1.408644	0.980036	-1.381999
H	0.825776	-0.710315	-1.868177
H	1.975402	-3.909890	-0.270186
H	4.249765	-4.564678	-1.005068
H	6.130748	-2.964515	-0.884062
H	5.779079	-0.650410	-0.007082
H	1.427324	0.976000	1.531921
H	-2.291483	-1.463657	-2.545675
H	-0.826939	-2.022666	-1.726957
H	-2.420667	-2.319472	-1.012597
H	-3.410763	0.983836	-1.323354
H	-2.876116	1.114299	0.333643
H	-3.894523	-1.199540	0.767592
H	-4.507366	-1.197641	-0.878156
H	-5.225850	0.855079	1.320845
H	-7.959146	-1.106868	-1.064714
H	-7.486368	0.248785	-2.080041
H	-6.336329	-1.060587	-1.769290
H	-8.092653	1.925589	-0.172314
H	-8.587793	0.578149	0.845826
H	-7.344346	1.706240	1.422458
H	-0.754564	1.585343	-0.537350
H	0.034732	-2.753603	0.735756
H	3.928651	1.813421	0.583694
H	3.312971	5.271678	-1.457848
H	4.054499	5.358544	0.168742
H	4.996767	4.730355	-1.181848

3A

C	0.991288	-0.937675	-0.759851
C	-0.296183	-1.695022	-0.516934
C	0.133981	0.909362	2.235078
C	0.746150	0.814844	1.053814
C	1.628225	-0.314901	0.558870
N	0.860796	0.053180	-1.783448
C	1.776836	-1.444556	1.591705
C	3.016953	0.311286	0.223101
C	-1.560036	-1.229522	-0.484115
C	-2.047998	0.160030	-0.622956
N	-3.328851	0.262354	-0.445598
C	0.813808	0.855796	-2.645257
C	-3.832265	-1.044032	-0.203372
C	-2.791845	-1.995845	-0.217514
C	-3.070127	-3.340659	-0.001922
C	-4.399541	-3.717845	0.230189
C	-5.424058	-2.765344	0.243521
C	-5.151708	-1.408330	0.025502
C	4.106642	-0.621582	-0.348894
C	5.370740	0.141493	-0.651869
C	6.581738	0.015118	-0.087586
C	6.933431	-0.969206	1.001530
C	7.731001	0.890921	-0.529035
O	-1.919688	3.210480	0.128550
C	-3.059266	3.647309	0.138837
O	-4.151045	2.912700	-0.090623
C	-3.404079	5.095478	0.409955
H	1.715345	-1.668466	-1.137031
H	-0.467913	1.783373	2.465909
H	0.194847	0.142120	3.002022
H	-2.283313	-4.091357	-0.013583
H	-4.637019	-4.764131	0.400346
H	-6.447166	-3.082743	0.424758
H	-5.940546	-0.662435	0.033069
H	-1.448622	1.042064	-0.800014
H	2.317024	-1.079698	2.471410
H	0.804326	-1.816979	1.927620
H	2.338556	-2.291755	1.183606
H	3.394118	0.758696	1.150846
H	2.865456	1.144313	-0.473693
H	3.751410	-1.077728	-1.285032
H	4.302879	-1.445574	0.343892
H	5.257041	0.901653	-1.426869
H	7.736129	-1.642939	0.670669
H	7.317399	-0.443495	1.886781
H	6.090379	-1.586589	1.320610
H	8.126431	1.478224	0.311738
H	8.568052	0.285787	-0.905121
H	7.434417	1.587424	-1.319337
H	0.631256	1.642525	0.354874
H	-0.146849	-2.754476	-0.316288
H	-3.890284	1.956290	-0.247665
H	-2.493634	5.661950	0.608724
H	-3.925239	5.520942	-0.454311
H	-4.084343	5.166099	1.265194

1(*R*)P

C	1.385869	1.813943	1.637534
C	1.002214	0.655969	1.082671
C	0.797102	-1.277869	-0.572068
C	-0.625573	-0.945362	-0.906570
C	-1.739081	-1.344682	-0.260716
N	2.437542	2.561226	1.158810
H	0.877129	2.230299	2.501804
H	1.311228	-1.728465	-1.429237
H	0.874331	-1.992892	0.250942
C	-1.758533	-2.221391	0.967271
C	-3.098651	-0.924217	-0.779184
C	1.673814	-0.016431	-0.106115
C	1.821077	0.894005	-1.285453
N	3.047695	0.899609	-1.722313
C	3.337032	3.212505	0.748029
C	3.907644	0.103128	-0.917725
C	3.121188	-0.444062	0.102964
C	3.722778	-1.263031	1.049240
C	5.098705	-1.502211	0.938180
C	5.860396	-0.941510	-0.096576
C	5.271502	-0.116994	-1.057561
H	3.152246	-1.699252	1.863339
H	5.587878	-2.133396	1.673336
H	6.924419	-1.146261	-0.151472
H	5.852895	0.326590	-1.859610
H	1.038973	1.467027	-1.768626
C	-3.810472	0.132060	0.110828
C	-5.101448	0.601173	-0.505675
C	-6.353424	0.428001	-0.052816
C	-6.724985	-0.290394	1.221228
C	-7.530895	0.973816	-0.825109
H	-2.287883	-3.157281	0.746932
H	-0.768034	-2.485679	1.346061
H	-2.311904	-1.740773	1.782772
H	-3.749630	-1.805111	-0.855623
H	-2.999087	-0.519779	-1.793581
H	-3.130449	0.988850	0.232984
H	-3.977254	-0.277152	1.111842
H	-4.979378	1.138653	-1.447880
H	-7.270205	0.382060	1.897036
H	-7.403482	-1.126644	1.005676
H	-5.867454	-0.689419	1.768562
H	-8.225310	0.169487	-1.103590
H	-8.106610	1.682832	-0.214759
H	-7.220383	1.487323	-1.740098
H	-0.763497	-0.345350	-1.807433
H	0.142127	0.148657	1.504926
H	3.365112	1.441154	-2.524037

Transition State from 1(*R*)P to 2P

C	0.138099	0.976362	1.909397
C	1.207259	0.240996	1.552793
C	1.141344	-0.774548	-1.100077
C	-0.237041	-0.470085	-1.296459
C	-1.294934	-1.155650	-0.755390
N	-0.313672	2.069153	1.207782
H	-0.420363	0.752439	2.812590
H	1.834213	-0.517337	-1.896379
H	1.404445	-1.694512	-0.588715
C	-1.162275	-2.321541	0.181387
C	-2.698562	-0.781704	-1.143069
C	2.083060	0.401872	0.389876
C	2.169480	1.564007	-0.451462
N	3.375419	1.628518	-1.011619
C	-0.731953	3.007034	0.620056
C	4.203240	0.585620	-0.557976
C	3.442419	-0.177755	0.347834
C	4.036838	-1.277965	0.971888
C	5.365476	-1.574990	0.669052
C	6.099594	-0.799700	-0.245073
C	5.527661	0.301061	-0.879697
H	3.489528	-1.889375	1.683537
H	5.845222	-2.420786	1.151254
H	7.131503	-1.059349	-0.457983
H	6.092064	0.906439	-1.582177
H	1.408182	2.298336	-0.670388
C	-3.439518	0.055102	-0.047411
C	-4.822360	0.439323	-0.498364
C	-5.999297	-0.021873	-0.044022
C	-6.165793	-1.050791	1.046859
C	-7.296712	0.493403	-0.618907
H	-1.462715	-3.241070	-0.339532
H	-0.156677	-2.469502	0.578656
H	-1.851142	-2.212182	1.026447
H	-3.283059	-1.692109	-1.323170
H	-2.693592	-0.206388	-2.075084
H	-2.852874	0.962641	0.144114
H	-3.466438	-0.512237	0.888067
H	-4.845059	1.180571	-1.298131
H	-6.747749	-0.636311	1.880694
H	-6.733392	-1.914053	0.674696
H	-5.221067	-1.422653	1.451730
H	-7.891776	-0.327301	-1.041811
H	-7.915303	0.954842	0.162530
H	-7.132251	1.236189	-1.404991
H	-0.468023	0.344394	-1.980662
H	1.456400	-0.584087	2.213365
H	3.651532	2.330638	-1.689213

2P

C	0.173433	1.195734	-1.716007
C	-0.863897	0.344597	-1.521192
C	-0.971073	0.812838	1.920906
C	0.401550	0.820735	1.770692
C	1.188878	-0.307401	1.509297
N	0.242700	2.450785	-1.166328
H	1.005006	0.931038	-2.360320
H	-1.474871	1.701751	2.281328
H	-1.560343	-0.095822	1.892877
C	0.625682	-1.666813	1.253243
C	2.670445	-0.179294	1.518117
C	-2.063175	0.537863	-0.752234
C	-2.532151	1.706688	-0.112700
N	-3.775194	1.477640	0.386441
C	0.314035	3.526413	-0.676724
C	-4.167974	0.168247	0.123839
C	-3.112776	-0.450054	-0.591313
C	-3.256087	-1.789819	-0.994505
C	-4.429465	-2.460031	-0.675418
C	-5.462421	-1.821691	0.041047
C	-5.348614	-0.497859	0.453846
H	-2.473204	-2.293914	-1.554330
H	-4.559086	-3.492198	-0.985121
H	-6.368178	-2.373377	0.272550
H	-6.147665	-0.006763	1.000822
H	-2.098397	2.694521	-0.089908
C	3.250372	0.128454	0.075570
C	4.743815	0.257301	0.115986
C	5.657599	-0.618492	-0.340661
C	5.340855	-1.941825	-0.990355
C	7.130207	-0.308126	-0.235499
H	0.740715	-2.273606	2.164439
H	-0.427637	-1.671406	0.969799
H	1.206900	-2.179608	0.478494
H	3.129444	-1.111444	1.862621
H	2.986457	0.630624	2.183432
H	2.802241	1.068974	-0.264779
H	2.923297	-0.658697	-0.610107
H	5.106902	1.174495	0.579900
H	5.759976	-1.981030	-2.004278
H	5.811059	-2.761894	-0.431903
H	4.271481	-2.156822	-1.061828
H	7.651622	-1.082769	0.342639
H	7.597811	-0.294685	-1.228896
H	7.315280	0.658299	0.241762
H	0.920830	1.765236	1.916624
H	-0.778756	-0.611195	-2.030958
H	-4.348870	2.176525	0.838732

Transition State from 2P to 3P

C	0.251313	0.615394	-1.107665
C	-0.979713	-0.038221	-1.078145
C	-0.765766	0.281903	2.333892
C	0.411396	0.606352	1.751208
C	1.179098	-0.229364	0.856319
N	0.362466	1.972222	-0.890004
H	1.042322	0.199791	-1.722897
H	-1.250229	0.974595	3.015607
H	-1.246034	-0.682864	2.210018
C	0.896986	-1.702176	0.747913
C	2.604670	0.222454	0.623971
C	-2.202599	0.382742	-0.542308
C	-2.534558	1.649568	0.015212
N	-3.826062	1.650411	0.368432
C	0.489770	3.131680	-0.691107
C	-4.426730	0.414293	0.086832
C	-3.434141	-0.406684	-0.487332
C	-3.773286	-1.708111	-0.874706
C	-5.081603	-2.143004	-0.674085
C	-6.050536	-1.303897	-0.096533
C	-5.738120	-0.003767	0.295901
H	-3.042318	-2.370876	-1.329370
H	-5.360830	-3.148594	-0.972214
H	-7.061305	-1.673166	0.044112
H	-6.484882	0.648271	0.738435
H	-1.923342	2.531964	0.125052
C	3.475170	-0.547596	-0.388941
C	4.822390	0.108378	-0.554653
C	6.030932	-0.393696	-0.255087
C	6.286385	-1.764277	0.321815
C	7.278064	0.422195	-0.497457
H	1.463801	-2.210679	1.542079
H	-0.155641	-1.955813	0.880463
H	1.247050	-2.116973	-0.200330
H	3.088418	0.142501	1.613478
H	2.613936	1.297582	0.403481
H	2.969220	-0.573408	-1.366981
H	3.580881	-1.589066	-0.072611
H	4.782944	1.116490	-0.970029
H	6.923680	-2.350371	-0.353275
H	6.834217	-1.683967	1.269952
H	5.379019	-2.344430	0.508294
H	7.839029	0.567041	0.435491
H	7.955118	-0.095700	-1.189776
H	7.051550	1.407089	-0.916239
H	0.824298	1.594165	1.943738
H	-0.953865	-1.053573	-1.465664
H	-4.306600	2.446552	0.769926

3P

C	0.322906	0.278959	-0.418787
C	-1.079854	-0.210310	-0.537229
C	0.151367	-1.419028	2.808551
C	0.562696	-0.442813	1.998297
C	1.179685	-0.600121	0.620388
N	0.413981	1.667607	-0.126276
H	0.792319	0.118317	-1.400677
H	-0.235084	-1.192775	3.798149
H	0.198498	-2.471420	2.544283
C	1.199832	-2.058780	0.131571
C	2.629198	-0.029121	0.677629
C	-2.280720	0.387863	-0.290735
C	-2.541517	1.733646	0.174334
N	-3.844136	1.900240	0.287111
C	0.537909	2.812252	0.126552
C	-4.562346	0.737706	-0.077101
C	-3.612618	-0.230337	-0.445911
C	-4.055832	-1.486654	-0.854987
C	-5.432485	-1.728534	-0.880365
C	-6.357047	-0.742299	-0.506299
C	-5.934286	0.522882	-0.093151
H	-3.360237	-2.266569	-1.150154
H	-5.794057	-2.701504	-1.197145
H	-7.418733	-0.963822	-0.537883
H	-6.643841	1.291130	0.197531
H	-1.846572	2.526896	0.406095
C	3.438259	-0.004107	-0.636449
C	4.789533	0.633246	-0.430190
C	6.001235	0.065517	-0.535657
C	6.258384	-1.374775	-0.905341
C	7.250453	0.875928	-0.283733
H	1.925386	-2.628871	0.719117
H	0.232546	-2.557930	0.244919
H	1.502169	-2.130754	-0.918055
H	3.166081	-0.641543	1.411888
H	2.598256	0.982244	1.098665
H	2.896096	0.581138	-1.396796
H	3.540697	-1.016759	-1.037269
H	4.749029	1.687661	-0.152804
H	6.866185	-1.434484	-1.818026
H	6.836590	-1.875129	-0.117094
H	5.348946	-1.957338	-1.072658
H	7.844447	0.439325	0.530585
H	7.898283	0.883940	-1.170725
H	7.021890	1.912996	-0.020594
H	0.510896	0.586764	2.353709
H	-1.129920	-1.239438	-0.884282
H	-4.277292	2.766268	0.595044

3P'

C	3.678862	-2.364598	-0.860084
C	4.648229	-1.487290	-0.352617
C	4.292578	-0.418889	0.473954
H	3.988198	-3.185623	-1.498870
H	5.692865	-1.640055	-0.603344
H	5.038793	0.261274	0.872623
C	0.978810	0.498803	1.583501
C	0.655405	-0.672818	0.798977
C	1.947250	-1.144441	0.263616
C	2.940031	-0.280375	0.756210
N	2.286627	0.687651	1.554121
H	0.329073	1.135384	2.162466
C	0.447957	2.612290	-1.014503
C	-0.735901	2.092294	-0.629876
C	-0.565897	-1.231339	0.563298
C	-1.517908	1.015840	-1.347510
C	-2.887520	0.686470	-0.705105
C	-3.048160	-0.687030	-0.011284
C	-1.927423	-0.921312	1.104772
C	1.088247	3.740270	-0.245948
C	1.199245	2.159297	-2.240586
N	-1.940372	0.117801	2.075913
C	-2.003876	0.988347	2.867668
C	-2.999574	-1.878295	-0.953223
C	-2.952365	-1.860975	-2.286048
C	-4.419956	-0.721332	0.705928
H	-1.211835	2.520004	0.252669
H	-0.581060	-2.096574	-0.095575
H	-0.916878	0.095389	-1.430605
H	-1.675194	1.323531	-2.389912
H	-3.674637	0.736267	-1.464732
H	-3.143336	1.462347	0.024731
H	-2.236301	-1.845695	1.620268
H	2.101008	3.470447	0.090074
H	1.212119	4.624880	-0.884353
H	0.497499	4.037175	0.626292
H	2.230334	1.877217	-1.988384
H	0.729937	1.311575	-2.745066
H	1.276265	2.981450	-2.964810
H	-3.079836	-2.846966	-0.453836
H	-2.990180	-2.785062	-2.855500
H	-2.897984	-0.944166	-2.865456
H	-4.492525	0.055784	1.472954
H	-5.215288	-0.554401	-0.026036
H	-4.603165	-1.692455	1.179265
C	2.323552	-2.205906	-0.558210
H	1.590649	-2.900000	-0.958890
H	2.758172	1.446043	2.036212

Transition State from 3P' to 4P

C	3.801953	1.235561	-1.550887
C	4.819038	0.322328	-1.215925
C	4.533998	-0.852655	-0.526532
H	4.059016	2.136923	-2.098604
H	5.843001	0.533575	-1.507015
H	5.314543	-1.565302	-0.277920
C	1.285527	-1.969538	0.610562
C	0.919705	-0.755076	0.004047
C	2.161609	-0.168618	-0.495170
C	3.201379	-1.073619	-0.179155
N	2.617472	-2.147596	0.492863
H	0.671574	-2.700967	1.114696
C	0.019709	1.728180	1.705309
C	-1.118138	0.987896	1.400331
C	-0.384902	-0.206484	-0.168686
C	-2.366931	1.599743	0.790812
C	-3.404874	0.553818	0.362646
C	-2.939996	-0.425010	-0.732798
C	-1.605067	-1.133220	-0.308973
C	1.062015	1.156826	2.600464
C	0.274220	3.093011	1.149750
N	-1.775801	-1.959674	0.841908
C	-1.942763	-2.636461	1.793481
C	-2.684482	0.223269	-2.087221
C	-3.089095	1.422070	-2.510038
C	-4.023994	-1.509697	-0.944780
H	-1.297050	0.137679	2.057586
H	-0.429978	0.599872	-0.897342
H	-2.109781	2.250402	-0.050438
H	-2.823942	2.248863	1.550569
H	-4.310234	1.064766	0.019025
H	-3.707685	-0.029540	1.240862
H	-1.336339	-1.804445	-1.138137
H	1.888327	0.774285	1.977276
H	1.497256	1.931549	3.242376
H	0.692345	0.336040	3.218413
H	1.344669	3.299942	1.060912
H	-0.215118	3.267393	0.188121
H	-0.136169	3.836881	1.851510
H	-2.172830	-0.424236	-2.802991
H	-2.909869	1.740192	-3.532882
H	-3.634370	2.121670	-1.882611
H	-4.219116	-2.067633	-0.023906
H	-4.955840	-1.036083	-1.266047
H	-3.728919	-2.223285	-1.722631
C	2.474796	1.001526	-1.201199
H	1.703596	1.713100	-1.483683
H	3.118985	-2.953846	0.843236

4P

C	-3.514752	2.323036	-0.919023
C	-4.631133	1.713579	-0.311448
C	-4.504197	0.564819	0.467282
H	-3.659192	3.217824	-1.515951
H	-5.615288	2.149323	-0.453066
H	-5.369711	0.100061	0.929423
C	-1.433591	-1.197740	1.195781
C	-0.942157	-0.160015	0.385836
C	-2.078233	0.643549	0.027683
C	-3.219971	0.049236	0.626963
N	-2.780798	-1.070067	1.329387
H	-0.891712	-1.936683	1.767641
C	-0.084588	-2.100048	-1.004059
C	1.037414	-1.371321	-0.317839
C	0.494153	0.034567	-0.023712
C	2.393314	-1.287859	-1.059636
C	3.369572	-0.470167	-0.183700
C	2.866841	0.923831	0.273527
C	1.444972	0.790383	0.938180
C	-0.344288	-3.528584	-0.674624
C	-0.655823	-1.607631	-2.286482
N	1.493421	0.103507	2.189513
C	1.488677	-0.525809	3.186743
C	2.731266	1.933572	-0.858078
C	3.225260	1.855084	-2.094727
C	3.862648	1.514792	1.298492
H	1.221820	-1.878256	0.636685
H	0.509261	0.614199	-0.953091
H	2.250639	-0.814869	-2.036832
H	2.808478	-2.287334	-1.231248
H	4.316783	-0.350099	-0.720164
H	3.604272	-1.056112	0.713288
H	1.051521	1.795054	1.133462
H	-1.382066	-3.820765	-0.862422
H	0.272295	-4.131116	-1.366555
H	-0.047052	-3.802094	0.339572
H	-1.711347	-1.879690	-2.389199
H	-0.534561	-0.537050	-2.451251
H	-0.124839	-2.133115	-3.099733
H	2.221494	2.855383	-0.568868
H	3.119614	2.682902	-2.789872
H	3.775381	0.993315	-2.462571
H	3.962809	0.868124	2.175394
H	4.847142	1.629519	0.835593
H	3.537775	2.503971	1.640214
C	-2.239207	1.797936	-0.762509
H	-1.384477	2.279525	-1.229412
H	-3.364462	-1.667346	1.898760

Transition State from 4P to 5P

C	-3.497926	-1.417648	-0.871284
C	-4.537352	-0.518690	-0.654609
C	-4.303382	0.863331	-0.466489
H	-3.729712	-2.459322	-1.072533
H	-5.562340	-0.875281	-0.657043
H	-5.136515	1.541698	-0.306173
C	-1.046114	2.397105	-0.185033
C	-0.700614	1.080820	-0.471471
C	-1.916076	0.397641	-0.684607
C	-2.989734	1.302462	-0.475862
N	-2.408805	2.535596	-0.216978
H	-0.420239	3.243097	0.061572
C	-0.858496	-1.536921	1.001761
C	0.451268	-0.784217	0.814919
C	0.551985	0.283472	-0.376954
C	1.690113	-1.708135	0.724982
C	3.001977	-0.907186	0.783177
C	3.133760	0.193381	-0.289551
C	1.858171	1.099572	-0.230848
C	-1.756621	-1.011268	2.079257
C	-0.907431	-3.020408	0.782549
N	1.811358	1.875834	0.971755
C	1.749900	2.490689	1.976393
C	3.242404	-0.334335	-1.714129
C	3.560782	-1.568183	-2.108064
C	4.395733	1.044405	-0.019309
H	0.541760	-0.164624	1.717397
H	0.668719	-0.303333	-1.296678
H	1.649026	-2.294359	-0.198699
H	1.683955	-2.420411	1.557619
H	3.848263	-1.598259	0.706124
H	3.088735	-0.436036	1.770139
H	1.903812	1.809354	-1.066313
H	-2.763513	-1.431778	2.037182
H	-1.310057	-1.315066	3.041246
H	-1.801331	0.080759	2.088587
H	-1.931385	-3.398467	0.800394
H	-0.407150	-3.346812	-0.131641
H	-0.374037	-3.495752	1.621849
H	3.109829	0.429987	-2.483100
H	3.680530	-1.802804	-3.161732
H	3.742572	-2.385107	-1.414882
H	4.361517	1.508398	0.970998
H	5.285414	0.410518	-0.075482
H	4.506309	1.839403	-0.765620
C	-2.147595	-0.981751	-0.884714
H	-1.397534	-1.599707	-1.367308
H	-2.903022	3.399073	-0.040020

5P

C	3.540333	1.337070	-0.254846
C	4.532774	0.403160	-0.156895
C	4.265518	-1.008142	-0.222102
H	3.800615	2.391056	-0.222185
H	5.562577	0.718123	-0.024331
H	5.087058	-1.712359	-0.117865
C	1.014722	-2.506372	-0.502058
C	0.700799	-1.132706	-0.552073
C	1.913340	-0.476196	-0.493308
C	2.968201	-1.421243	-0.397567
N	2.359611	-2.673677	-0.427149
H	0.359488	-3.366955	-0.491658
C	0.977074	1.732813	0.371196
C	-0.330513	0.835930	0.538516
C	-0.557347	-0.313418	-0.506214
C	-1.611024	1.687772	0.659288
C	-2.862705	0.844606	0.949314
C	-3.113848	-0.281277	-0.074965
C	-1.819371	-1.152284	-0.172001
C	1.521277	2.007885	1.788932
C	0.714174	3.071815	-0.344948
N	-1.588546	-1.896238	1.032064
C	-1.356232	-2.498592	2.018944
C	-3.432575	0.207394	-1.481821
C	-3.857847	1.416269	-1.850825
C	-4.301566	-1.159737	0.381859
H	-0.196953	0.308635	1.492157
H	-0.741890	0.130266	-1.494974
H	-1.762027	2.255959	-0.262726
H	-1.489411	2.420075	1.465945
H	-3.741010	1.497751	0.996128
H	-2.773853	0.387843	1.942931
H	-1.965559	-1.890778	-0.971881
H	2.349054	2.724737	1.774645
H	0.733382	2.435241	2.417922
H	1.868994	1.088755	2.273664
H	1.655225	3.611616	-0.504257
H	0.242809	2.931257	-1.324637
H	0.070821	3.725326	0.248996
H	-3.371740	-0.569153	-2.248091
H	-4.128715	1.621015	-2.882555
H	-3.978947	2.240363	-1.153229
H	-4.121038	-1.594438	1.369620
H	-5.209014	-0.551038	0.431135
H	-4.488151	-1.977976	-0.323524
C	2.110587	0.974910	-0.489108
H	1.919563	1.314490	-1.527713
H	2.826637	-3.568340	-0.353829

Transition State from 4P to 6P

C	2.225726	-1.887033	-0.679098
C	3.500951	-2.400374	-0.848392
C	4.629799	-1.731302	-0.325125
C	4.515084	-0.534300	0.375567
H	1.361741	-2.409164	-1.080319
H	3.641377	-3.330404	-1.389645
H	5.615136	-2.161421	-0.476138
H	5.390254	-0.025180	0.767163
N	2.800950	1.135216	1.181209
C	3.228308	-0.026459	0.552428
C	2.073596	-0.684287	0.043401
C	0.942421	0.115792	0.393141
C	0.095351	2.154689	-0.878075
C	0.710377	1.724332	-2.165537
C	0.260017	3.595719	-0.528749
C	-1.023093	1.371221	-0.242724
C	-2.377222	1.336258	-0.990717
C	-3.362195	0.480343	-0.161696
C	-2.870082	-0.937711	0.227396
C	-1.448112	-0.848303	0.899887
C	-0.491444	-0.053309	-0.024546
H	-2.234746	0.915920	-1.991809
H	-2.786183	2.345894	-1.109679
H	-4.307717	0.392805	-0.707305
H	-3.597321	1.021795	0.762712
C	-3.871362	-1.570783	1.221549
C	-2.739973	-1.892143	-0.951710
N	-1.491858	-0.223048	2.183028
H	-1.064301	-1.864844	1.046114
H	-1.214349	1.819760	0.739714
H	-0.510927	-0.586741	-0.981813
C	-3.226572	-1.747934	-2.185363
C	-1.486897	0.356452	3.210198
H	0.624550	0.657200	-2.369921
H	0.191020	2.266047	-2.974606
H	1.761589	2.025416	-2.227137
H	1.277436	3.957155	-0.705920
H	-0.392734	4.166747	-1.213040
H	-0.057027	3.834979	0.488645
H	-3.554458	-2.578090	1.514309
H	-3.967300	-0.967314	2.129140
H	-4.856248	-1.654931	0.752979
H	-2.241761	-2.832672	-0.705640
H	-3.125822	-2.541771	-2.919753
H	-3.765333	-0.863209	-2.513293
C	1.440601	1.230232	1.094656
H	0.906405	1.958814	1.685901
H	3.391388	1.761421	1.710727

6P

C	2.315459	-2.174391	-0.368852
C	3.607146	-2.586507	-0.547989
C	4.701422	-1.676347	-0.371737
C	4.531633	-0.352854	-0.028639
H	1.482053	-2.858421	-0.490617
H	3.823106	-3.613266	-0.823202
H	5.709569	-2.051819	-0.522450
H	5.377817	0.315976	0.088689
N	2.758418	1.339002	0.425423
C	3.206584	0.097693	0.152253
C	2.081220	-0.815438	0.012012
C	0.942180	-0.076838	0.256024
C	0.288479	2.215211	-0.162126
C	0.629111	2.304407	-1.657574
C	0.188012	3.618441	0.446919
C	-0.970004	1.334416	0.147959
C	-2.309306	1.562037	-0.548066
C	-3.333733	0.552154	0.024862
C	-2.911811	-0.942666	0.002971
C	-1.473401	-1.124482	0.626832
C	-0.512264	-0.131752	-0.070319
H	-2.202497	1.441988	-1.631770
H	-2.678548	2.578689	-0.370369
H	-4.289428	0.651358	-0.500220
H	-3.536233	0.824925	1.068131
C	-3.928183	-1.773853	0.819787
C	-2.850979	-1.546685	-1.393005
N	-1.443904	-0.910761	2.037519
H	-1.150121	-2.157446	0.450481
H	-1.147909	1.450811	1.227213
H	-0.583042	-0.380072	-1.140925
C	-3.308684	-1.030294	-2.535110
C	-1.392461	-0.695620	3.196458
H	0.716600	1.324796	-2.139699
H	-0.150116	2.864260	-2.183794
H	1.573565	2.836298	-1.811875
H	1.118887	4.181676	0.312911
H	-0.606019	4.189412	-0.045529
H	-0.040583	3.581381	1.518353
H	-3.665342	-2.837950	0.819224
H	-3.975575	-1.435137	1.858978
H	-4.923748	-1.676811	0.377201
H	-2.436414	-2.557301	-1.420354
H	-3.264601	-1.598900	-3.459510
H	-3.765807	-0.047395	-2.601859
C	1.323430	1.312279	0.623650
H	1.112943	1.463218	1.697238
H	3.356744	2.098579	0.725303

1(*S*)N

C	0.833537	-0.816360	2.291109
C	1.556025	-1.480143	1.378419
C	1.365832	-1.613979	-1.133478
C	0.045809	-0.917140	-1.312918
C	-1.184345	-1.373308	-1.021765
N	0.483212	0.515041	2.280995
H	0.443574	-1.353156	3.152090
H	1.978325	-1.477190	-2.033707
H	1.234671	-2.693327	-1.000884
C	-1.482534	-2.738173	-0.448225
C	-2.395251	-0.496498	-1.275837
C	2.228372	-1.081728	0.083430
C	0.087377	1.624347	2.374849
N	4.611596	-1.053447	-0.151293
C	3.586088	-1.796723	0.045766
C	-3.090582	0.010957	0.015502
C	-4.225812	0.950969	-0.289653
C	-5.538034	0.787868	-0.059631
C	-6.159176	-0.423419	0.592994
C	-6.528624	1.859432	-0.451113
H	-2.210829	-3.266715	-1.078150
H	-0.597219	-3.371840	-0.357145
H	-1.933070	-2.658992	0.549404
H	-3.136660	-1.051382	-1.869089
H	-2.099598	0.371077	-1.878582
H	-2.340143	0.535681	0.624460
H	-3.432801	-0.841350	0.611137
H	-3.917826	1.879819	-0.774216
H	-6.695871	-0.138173	1.508678
H	-6.905181	-0.880732	-0.071989
H	-5.432462	-1.194516	0.859130
H	-7.276933	1.469531	-1.155827
H	-7.086691	2.221692	0.423978
H	-6.037834	2.718844	-0.918548
C	2.719928	0.347248	-0.122240
C	4.120510	0.275525	-0.268317
C	4.897577	1.400009	-0.522203
C	4.247597	2.631637	-0.642325
C	2.858292	2.715387	-0.518411
C	2.082651	1.575173	-0.264293
H	5.973879	1.306427	-0.627894
H	4.826252	3.530264	-0.838122
H	2.366161	3.678967	-0.615852
H	1.008503	1.670969	-0.164797
H	3.677490	-2.875330	0.172949
H	1.659569	-2.541242	1.602849
H	0.119608	0.083024	-1.737763

8N

C	-0.037776	-0.356098	1.566572
C	1.151102	-1.061627	1.435118
C	1.230049	-1.506239	-1.515903
C	0.087999	-0.758144	-1.374079
C	-1.062954	-1.124827	-0.647294
N	-0.203263	0.996359	1.376768
H	-0.822272	-0.795001	2.175017
H	2.078541	-1.118808	-2.068001
H	1.278260	-2.554644	-1.246599
C	-1.326470	-2.554065	-0.250105
C	-2.246249	-0.183849	-0.719944
C	2.346094	-0.817163	0.753604
C	-0.484277	2.136427	1.238301
N	4.519090	-1.492105	0.215071
C	3.375114	-1.869900	0.698612
C	-3.373872	-0.366550	0.316967
C	-4.397215	0.734126	0.212983
C	-5.692900	0.643064	-0.124271
C	-6.411738	-0.637971	-0.472168
C	-6.561695	1.877936	-0.176200
H	-1.912654	-3.050208	-1.038976
H	-0.411059	-3.131733	-0.110131
H	-1.915213	-2.621839	0.668785
H	-2.689441	-0.294332	-1.723990
H	-1.880005	0.849904	-0.680173
H	-2.937845	-0.346357	1.326325
H	-3.837613	-1.350699	0.199605
H	-4.004242	1.727116	0.437653
H	-7.250353	-0.810500	0.216627
H	-6.847767	-0.574207	-1.478743
H	-5.769551	-1.521533	-0.442542
H	-6.990664	2.017688	-1.178465
H	-7.411601	1.792520	0.515506
H	-6.002839	2.782253	0.083228
C	3.061527	0.360805	0.231514
C	4.363641	-0.120175	-0.081661
C	5.341878	0.710836	-0.616819
C	5.021449	2.053312	-0.839507
C	3.746919	2.540648	-0.529553
C	2.758914	1.705657	0.005268
H	6.325954	0.312322	-0.844539
H	5.768768	2.724826	-1.253940
H	3.514996	3.587971	-0.703277
H	1.784277	2.115997	0.236382
H	3.205871	-2.893294	1.030308
H	1.060443	-2.081309	1.809726
H	0.117993	0.266875	-1.741274

9N

C	0.213775	-0.407471	-0.840583
C	-1.050430	-1.225496	-0.958684
C	-0.316036	-0.708900	2.743085
C	0.124739	-0.055240	1.667993
C	0.974078	-0.608763	0.539377
N	0.034000	0.978663	-1.137981
H	0.890997	-0.787314	-1.615241
H	-0.900717	-0.198123	3.502943
H	-0.122658	-1.763378	2.916945
C	1.263091	-2.110632	0.707665
C	2.305410	0.204398	0.535349
C	-2.354050	-0.964876	-0.722415
C	-0.022598	2.121667	-1.417320
N	-4.577207	-1.695851	-0.704545
C	-3.358410	-2.035763	-0.955821
C	3.333100	-0.112612	-0.572943
C	4.549044	0.770325	-0.455692
C	5.816231	0.420209	-0.186263
C	6.294960	-0.991633	0.050946
C	6.902186	1.467295	-0.102605
H	1.893563	-2.275138	1.587454
H	0.344370	-2.688999	0.841599
H	1.792479	-2.516831	-0.160752
H	2.779857	0.038885	1.510400
H	2.064599	1.273338	0.493839
H	2.877935	0.062187	-1.559009
H	3.612061	-1.170200	-0.540726
H	4.343682	1.832442	-0.601152
H	7.060944	-1.269979	-0.686226
H	6.771288	-1.076496	1.037549
H	5.497807	-1.737106	0.000786
H	7.384897	1.458694	0.884873
H	7.696340	1.273210	-0.837350
H	6.513888	2.474693	-0.281689
C	-3.188238	0.161753	-0.256781
C	-4.513359	-0.345390	-0.266578
C	-5.598323	0.425412	0.125374
C	-5.356731	1.740343	0.540887
C	-4.057272	2.252684	0.559793
C	-2.962878	1.470453	0.166842
H	-6.599359	0.005995	0.106124
H	-6.187592	2.367822	0.852119
H	-3.886435	3.275786	0.882758
H	-1.969946	1.899021	0.184742
H	-3.100102	-3.030626	-1.314083
H	-0.839392	-2.240004	-1.294289
H	-0.105790	1.005864	1.576320

1(S)A

C	-0.242662	-0.283965	2.296176
C	0.630578	-0.745324	1.390856
C	0.483200	-0.911024	-1.125075
C	-0.966131	-0.555552	-1.304767
C	-2.047300	-1.302167	-1.021739
N	-0.913931	0.917861	2.281690
C	-2.002898	-2.702033	-0.456965
C	-3.435562	-0.748595	-1.278452
C	1.187420	-0.187555	0.098358
C	-1.573898	1.893807	2.371620
N	3.473209	0.423250	-0.132464
C	2.669001	-0.559475	0.062640
C	-4.240384	-0.436958	0.011339
C	-5.570568	0.196967	-0.295880
C	-6.803250	-0.286674	-0.076715
C	-7.110041	-1.619155	0.562992
C	-8.025258	0.510784	-0.468523
C	1.312239	1.320179	-0.102576
C	2.685088	1.599736	-0.248475
C	3.165403	2.879491	-0.498743
C	2.231601	3.912842	-0.615768
C	0.864522	3.651051	-0.492731
C	0.392965	2.354713	-0.242320
O	5.240769	-2.354862	0.164724
C	6.221934	-1.649964	-0.007492
O	6.174422	-0.329261	-0.203687
C	7.641836	-2.170923	-0.023990
H	-0.492905	-0.902539	3.154126
H	1.045887	-0.625712	-2.022954
H	0.620731	-1.989239	-0.994641
H	-2.576742	-3.388662	-1.093847
H	-0.989848	-3.100246	-0.364394
H	-2.463479	-2.742298	0.538368
H	-4.014339	-1.465202	-1.879131
H	-3.360169	0.169064	-1.874796
H	-3.645150	0.252065	0.628004
H	-4.365146	-1.351458	0.599846
H	-5.498446	1.177071	-0.771912
H	-7.706217	-1.482750	1.476114
H	-7.715890	-2.240880	-0.110956
H	-6.217155	-2.189243	0.829936
H	-8.650143	-0.045744	-1.181514
H	-8.660453	0.716799	0.404686
H	-7.758961	1.468586	-0.926407
H	4.231154	3.057335	-0.604486
H	2.571429	4.926528	-0.808676
H	0.150520	4.464048	-0.588286
H	-0.671439	2.182490	-0.143764
H	3.056906	-1.568881	0.183609
H	0.997920	-1.745513	1.615706
H	-1.138610	0.434011	-1.725753
H	5.219852	-0.023670	-0.184297
H	7.642473	-3.249486	0.136986
H	8.114755	-1.936049	-0.983416
H	8.229970	-1.676443	0.756350

8A

C	-1.074243	0.115390	1.545635
C	0.263456	-0.225621	1.400744
C	0.446457	-0.597133	-1.595197
C	-0.854910	-0.208894	-1.412780
C	-1.837871	-0.908016	-0.678191
N	-1.617422	1.366181	1.367691
C	-1.662804	-2.354550	-0.299373
C	-3.244443	-0.353329	-0.723453
C	1.343859	0.363170	0.737593
C	-2.212661	2.379342	1.235840
N	3.580945	0.313154	0.125489
C	2.597896	-0.383400	0.622754
C	-4.262605	-0.885451	0.305777
C	-5.566021	-0.134248	0.225031
C	-6.779162	-0.598361	-0.112235
C	-7.089626	-2.027826	-0.484942
C	-7.974644	0.324928	-0.137409
C	1.701741	1.704475	0.246976
C	3.073779	1.606045	-0.114496
C	3.780051	2.685765	-0.633467
C	3.105356	3.899532	-0.789221
C	1.757505	4.015956	-0.429851
C	1.046051	2.928809	0.088527
O	4.618464	-2.808677	0.483051
C	5.691680	-2.376584	0.092055
O	5.922762	-1.104203	-0.231134
C	6.926879	-3.235116	-0.081679
H	-1.701581	-0.536892	2.144784
H	1.137057	0.031302	-2.146185
H	0.805140	-1.587443	-1.340811
H	-2.088117	-2.990249	-1.091216
H	-0.616724	-2.640024	-0.176771
H	-2.195332	-2.602982	0.622554
H	-3.640324	-0.563791	-1.731454
H	-3.197031	0.741309	-0.658893
H	-3.847324	-0.761695	1.316583
H	-4.415129	-1.959533	0.163488
H	-5.482800	0.926012	0.469645
H	-7.833633	-2.453739	0.202357
H	-7.533802	-2.076508	-1.488733
H	-6.214835	-2.682489	-0.475448
H	-8.433410	0.350240	-1.135831
H	-8.755673	-0.021523	0.553910
H	-7.706526	1.349056	0.139464
H	4.827246	2.577863	-0.900109
H	3.632741	4.761201	-1.189401
H	1.249741	4.968779	-0.551836
H	0.005719	3.054212	0.359428
H	2.748378	-1.424607	0.894547
H	0.463468	-1.239091	1.747183
H	-1.131860	0.785695	-1.759573
H	5.081898	-0.558917	-0.105315
H	7.733675	-2.860380	0.557283
H	6.699246	-4.269863	0.177315
H	7.281000	-3.177553	-1.116386

9A

C	1.185337	-0.124322	-0.678908
C	-0.262459	-0.536369	-0.571827
C	0.899717	0.554392	2.877861
C	1.420609	0.789440	1.673327
C	1.974528	-0.230742	0.696446
N	1.379051	1.150318	-1.294107
C	1.836367	-1.673030	1.214474
C	3.476468	0.125736	0.472249
C	-1.414812	0.145586	-0.388182
C	1.625495	2.166401	-1.836978
N	-3.727253	0.130271	-0.165454
C	-2.684328	-0.614655	-0.339616
C	4.269157	-0.725532	-0.543452
C	5.692064	-0.242998	-0.663885
C	6.824711	-0.885341	-0.339157
C	6.898639	-2.283763	0.224410
C	8.167693	-0.220013	-0.529840
C	-1.853866	1.544333	-0.203227
C	-3.263382	1.468534	-0.072846
C	-4.051136	2.592085	0.129914
C	-3.411243	3.834509	0.207491
C	-2.022568	3.928293	0.086754
C	-1.232171	2.789201	-0.114325
O	-4.709699	-3.022470	-0.347094
C	-5.838479	-2.581339	-0.203464
O	-6.129660	-1.285737	-0.063806
C	-7.080479	-3.444778	-0.162986
H	1.655002	-0.850770	-1.353150
H	0.555454	1.372957	3.503637
H	0.791700	-0.443255	3.293176
H	2.470752	-1.816640	2.095050
H	0.807418	-1.906804	1.502689
H	2.147215	-2.402207	0.458920
H	3.967474	0.051065	1.450268
H	3.548117	1.179545	0.177681
H	3.798225	-0.651030	-1.534861
H	4.236185	-1.782052	-0.260780
H	5.786912	0.770205	-1.058633
H	7.483850	-2.937486	-0.437194
H	7.417082	-2.281836	1.193234
H	5.920499	-2.747895	0.371026
H	8.712739	-0.149267	0.422032
H	8.805099	-0.803336	-1.209232
H	8.069653	0.789603	-0.940643
H	-5.128489	2.498603	0.225734
H	-4.000640	4.733649	0.364375
H	-1.541723	4.900382	0.148071
H	-0.160375	2.896006	-0.211051
H	-2.785235	-1.692109	-0.438339
H	-0.379082	-1.616096	-0.648222
H	1.503040	1.822729	1.336896
H	-5.283401	-0.745531	-0.096554
H	-6.805968	-4.494239	-0.275316
H	-7.608554	-3.295964	0.784820
H	-7.765836	-3.150462	-0.964917

1(*S*)P

C	1.939606	-2.163036	1.682993
C	1.321235	-1.393087	0.778711
C	1.013442	-0.683009	-1.656117
C	-0.342093	-0.080042	-1.440587
C	-1.520301	-0.729945	-1.348680
N	3.301632	-2.373063	1.704411
H	1.386009	-2.673640	2.465118
H	1.535204	-0.146889	-2.457271
H	0.952616	-1.735578	-1.943602
C	-1.689136	-2.227566	-1.418144
C	-2.801570	0.062753	-1.192710
C	1.962175	-0.608854	-0.346309
C	4.466976	-2.576694	1.763140
N	4.168898	-0.164789	-0.852253
C	3.287555	-1.123027	-0.806000
C	-3.422605	-0.022972	0.229313
C	-4.638664	0.854552	0.360788
C	-5.913317	0.487226	0.568451
C	-6.392834	-0.934531	0.729288
C	-7.004757	1.526482	0.665292
H	-2.266014	-2.496042	-2.312690
H	-0.748681	-2.783093	-1.448291
H	-2.264438	-2.595567	-0.560574
H	-3.544876	-0.299151	-1.915128
H	-2.617424	1.116447	-1.433358
H	-2.659166	0.299068	0.954599
H	-3.659071	-1.063965	0.469811
H	-4.435054	1.921969	0.257869
H	-6.879204	-1.068306	1.704830
H	-7.152115	-1.170671	-0.028208
H	-5.597928	-1.679985	0.648208
H	-7.773784	1.361291	-0.101503
H	-7.516934	1.469178	1.635361
H	-6.617149	2.542638	0.545114
C	2.317077	0.832434	0.004872
C	3.653749	1.061061	-0.347358
C	4.308396	2.275065	-0.189574
C	3.555898	3.310178	0.369735
C	2.221095	3.108668	0.745806
C	1.587381	1.871708	0.570483
H	5.346555	2.416098	-0.473533
H	4.016304	4.280897	0.521103
H	1.665602	3.929958	1.187475
H	0.555932	1.733521	0.876035
H	3.513593	-2.121733	-1.158859
H	0.244697	-1.277359	0.855793
H	-0.358329	1.008041	-1.411192
H	5.124089	-0.286340	-1.182571

Transition State from 1(*S*)P to 8P

C	0.409528	-0.787711	2.325585
C	1.331269	-1.416688	1.574079
C	1.335802	-1.555215	-1.257315
C	0.111866	-0.835873	-1.354360
C	-1.142055	-1.341785	-1.114021
N	0.127077	0.554042	2.351689
H	-0.185655	-1.371635	3.021930
H	2.156287	-1.225889	-1.887657
H	1.297429	-2.627455	-1.094854
C	-1.420272	-2.745741	-0.661849
C	-2.347569	-0.480142	-1.362723
C	2.290875	-0.958216	0.561427
C	-0.226735	1.677102	2.471524
N	4.430940	-1.107697	-0.188794
C	3.433410	-1.799114	0.351704
C	-2.985894	0.083262	-0.048042
C	-4.151441	0.983437	-0.353926
C	-5.456610	0.749451	-0.138562
C	-6.023785	-0.507057	0.474334
C	-6.490530	1.786736	-0.504811
H	-1.894236	-3.304039	-1.480883
H	-0.537538	-3.300109	-0.338644
H	-2.142735	-2.743892	0.162008
H	-3.115209	-1.065463	-1.883423
H	-2.083107	0.362920	-2.009920
H	-2.217841	0.650652	0.492977
H	-3.281229	-0.748713	0.598445
H	-3.877738	1.935089	-0.811143
H	-6.582175	-0.269698	1.389508
H	-6.741745	-0.976428	-0.211299
H	-5.268324	-1.254694	0.729168
H	-7.216769	1.380515	-1.221791
H	-7.065425	2.095108	0.378683
H	-6.038919	2.680449	-0.945301
C	2.760381	0.395250	0.163967
C	4.077592	0.244616	-0.327419
C	4.838428	1.283380	-0.856536
C	4.241390	2.540163	-0.890820
C	2.930451	2.723377	-0.423325
C	2.179438	1.667398	0.093592
H	5.848177	1.123084	-1.222035
H	4.795635	3.385437	-1.285706
H	2.487441	3.713603	-0.460714
H	1.174392	1.848916	0.447386
H	3.529782	-2.855243	0.569472
H	1.374283	-2.489271	1.752799
H	0.182205	0.193411	-1.698698
H	5.323649	-1.500839	-0.465585

8P

C	0.123958	0.450916	1.988067
C	1.165555	-0.412209	1.955851
C	1.143611	-1.827247	-1.111497
C	-0.012226	-1.080639	-1.185631
C	-1.297321	-1.521160	-0.836491
N	-0.121460	1.477609	1.108615
H	-0.623431	0.356487	2.770154
H	2.069063	-1.436140	-1.516822
H	1.148507	-2.866982	-0.802988
C	-1.588698	-2.880992	-0.294073
C	-2.447875	-0.595562	-1.022118
C	2.324106	-0.513778	1.095949
C	-0.473566	2.337406	0.375472
N	4.184294	-1.537013	0.308199
C	3.073969	-1.705910	1.059797
C	-3.332792	-0.386860	0.263829
C	-4.276595	0.765185	0.079492
C	-5.606585	0.715562	-0.116806
C	-6.422935	-0.549712	-0.195585
C	-6.403088	1.987895	-0.267182
H	-2.430652	-3.329997	-0.835464
H	-0.743904	-3.569406	-0.328847
H	-1.916266	-2.793615	0.751230
H	-3.109008	-1.017444	-1.793907
H	-2.102393	0.376072	-1.386400
H	-2.660105	-0.176556	1.105016
H	-3.859201	-1.316144	0.496201
H	-3.799647	1.745160	0.103555
H	-7.193817	-0.558193	0.586120
H	-6.956781	-0.599141	-1.153780
H	-5.834218	-1.464991	-0.093332
H	-6.930094	2.006698	-1.230595
H	-7.175411	2.058915	0.510211
H	-5.772253	2.879087	-0.204447
C	3.086417	0.453079	0.312339
C	4.237438	-0.226976	-0.167166
C	5.219925	0.381696	-0.947118
C	5.047597	1.730471	-1.241254
C	3.930944	2.438583	-0.761727
C	2.953877	1.820907	0.011461
H	6.088786	-0.167724	-1.297167
H	5.791903	2.244893	-1.840937
H	3.830879	3.493682	-0.996138
H	2.112152	2.395548	0.372993
H	2.878598	-2.639158	1.571196
H	1.102343	-1.190543	2.714107
H	0.074055	-0.060058	-1.549109
H	4.896762	-2.238539	0.157793

Transition State from 8P to 9P

C	0.118103	-0.052848	-1.301828
C	-1.011467	-0.867131	-1.338188
C	-0.797552	-1.438198	2.103844
C	0.120256	-0.602802	1.575149
C	1.142053	-0.965402	0.612331
N	0.111015	1.291088	-1.012654
H	0.961154	-0.354849	-1.915312
H	-1.501254	-1.082656	2.850041
H	-0.850027	-2.493818	1.857169
C	1.325590	-2.396948	0.194404
C	2.363457	-0.078798	0.613687
C	-2.329373	-0.741761	-0.865489
C	0.254032	2.442907	-0.781172
N	-4.398117	-1.583416	-0.528921
C	-3.176325	-1.875008	-0.978682
C	3.463013	-0.307551	-0.442376
C	4.554293	0.725248	-0.317747
C	5.845634	0.532292	-0.005439
C	6.480923	-0.804546	0.287698
C	6.796385	1.703012	0.067382
H	1.980017	-2.884357	0.932453
H	0.392466	-2.961032	0.156682
H	1.830873	-2.478667	-0.770845
H	2.811699	-0.240657	1.610762
H	2.053479	0.973357	0.627470
H	3.024543	-0.238952	-1.449964
H	3.866395	-1.319803	-0.349673
H	4.227066	1.748049	-0.509572
H	7.290015	-1.008068	-0.426009
H	6.943260	-0.798162	1.283580
H	5.784389	-1.645979	0.248044
H	7.251783	1.776676	1.064030
H	7.623866	1.578994	-0.643862
H	6.298763	2.652179	-0.151880
C	-3.170572	0.318590	-0.288124
C	-4.452043	-0.252982	-0.092681
C	-5.539981	0.434641	0.436985
C	-5.333269	1.766846	0.783360
C	-4.078636	2.368159	0.596768
C	-2.998313	1.664225	0.067766
H	-6.505962	-0.043359	0.569062
H	-6.152491	2.345902	1.197338
H	-3.943821	3.410772	0.867102
H	-2.051394	2.167443	-0.066940
H	-2.938481	-2.852510	-1.377524
H	-0.789350	-1.845974	-1.759012
H	0.126496	0.435915	1.899429
H	-5.181033	-2.225817	-0.517426

9P

C	0.235139	-0.347396	-0.792539
C	-0.996578	-1.179331	-0.910082
C	-0.241929	-0.872653	2.771767
C	0.207575	-0.153396	1.742113
C	1.035108	-0.649951	0.572178
N	0.014331	1.041644	-0.987256
H	0.902673	-0.677788	-1.598660
H	-0.787123	-0.398949	3.583097
H	-0.071181	-1.940581	2.871710
C	1.326418	-2.158789	0.639806
C	2.363209	0.166397	0.553319
C	-2.325681	-0.932077	-0.691787
C	-0.059801	2.199868	-1.200488
N	-4.481970	-1.604316	-0.779297
C	-3.247632	-2.004805	-0.990828
C	3.365475	-0.115982	-0.585513
C	4.567325	0.790043	-0.484594
C	5.843619	0.453767	-0.240600
C	6.346490	-0.951933	-0.020402
C	6.915421	1.515676	-0.173905
H	2.002529	-2.363803	1.474986
H	0.421648	-2.754221	0.799841
H	1.814062	-2.517829	-0.272174
H	2.854741	-0.036367	1.512789
H	2.122116	1.235708	0.560210
H	2.884108	0.062467	-1.560307
H	3.666832	-1.167515	-0.573568
H	4.342224	1.848468	-0.623648
H	7.101072	-1.212579	-0.774513
H	6.845297	-1.031997	0.954707
H	5.562584	-1.712619	-0.057435
H	7.417725	1.506306	0.802936
H	7.695238	1.333613	-0.925736
H	6.511368	2.518779	-0.339733
C	-3.176535	0.187897	-0.236933
C	-4.510604	-0.270846	-0.310806
C	-5.621443	0.481292	0.042649
C	-5.374433	1.775601	0.504052
C	-4.064619	2.260102	0.604184
C	-2.959755	1.480536	0.246984
H	-6.630126	0.086887	-0.031337
H	-6.207775	2.408211	0.791601
H	-3.897197	3.268289	0.969232
H	-1.964641	1.889767	0.339030
H	-3.019321	-2.998623	-1.355056
H	-0.768897	-2.196389	-1.222706
H	0.023376	0.920857	1.738002
H	-5.308468	-2.175517	-0.928846

9P'

C	-2.576079	-1.524183	-0.549176
C	-3.914752	-1.860135	-0.767090
C	-4.962882	-1.091475	-0.242428
C	-4.701767	0.044379	0.524479
H	-1.794372	-2.131417	-0.985214
H	-4.146129	-2.737712	-1.362221
H	-5.990967	-1.381411	-0.433348
H	-5.504683	0.645334	0.940157
N	-2.825181	1.430568	1.472260
C	-3.365152	0.361178	0.729567
C	-2.284374	-0.387302	0.211970
C	-1.054722	0.274112	0.682772
C	1.138407	2.535987	-0.953982
C	1.454620	3.482279	0.173838
C	-0.078612	2.893590	-1.762229
C	1.876483	1.444904	-1.268185
C	3.151209	0.968079	-0.622854
C	3.328550	-0.565153	-0.632056
C	2.447476	-1.448157	0.287507
C	0.901671	-1.278260	0.030512
C	0.290880	-0.009151	0.597339
H	3.261240	1.367295	0.389946
H	3.994805	1.381221	-1.196254
H	4.369953	-0.791214	-0.378169
H	3.196881	-0.921349	-1.660867
C	2.792409	-2.930300	-0.013368
C	2.665167	-1.232331	1.777379
N	0.563939	-1.469257	-1.342008
H	0.413748	-2.097429	0.585848
H	1.574598	0.888587	-2.154091
H	0.963675	0.604580	1.185257
C	3.660082	-0.572088	2.373476
C	0.337337	-1.639862	-2.487197
H	2.249696	3.131946	0.836076
H	1.768304	4.454985	-0.228606
H	0.559080	3.689297	0.778422
H	-0.008568	3.918450	-2.149494
H	-0.232057	2.215876	-2.606178
H	-0.983296	2.867668	-1.133098
H	2.239580	-3.611482	0.644097
H	2.560342	-3.189933	-1.051352
H	3.859025	-3.102742	0.153965
H	1.948687	-1.756234	2.415248
H	3.745920	-0.555742	3.456146
H	4.439333	-0.051480	1.825053
C	-1.501628	1.397862	1.454349
H	-0.902900	2.127940	1.982561
H	-3.379144	2.121950	1.966618

Transition State from 9P' to 10P

C	-2.480944	-1.283929	-0.823169
C	-3.803005	-1.687300	-0.984396
C	-4.834382	-1.184994	-0.171941
C	-4.563990	-0.252853	0.823002
H	-1.718698	-1.690999	-1.472676
H	-4.041525	-2.409187	-1.759282
H	-5.853713	-1.524977	-0.324824
H	-5.351630	0.149378	1.453189
N	-2.705225	1.069842	1.871664
C	-3.236168	0.144788	0.974777
C	-2.167955	-0.352423	0.182570
C	-0.954028	0.316793	0.660443
C	0.558581	2.344256	-1.182583
C	1.038549	3.578586	-0.494531
C	-0.807217	2.401232	-1.755483
C	1.276280	1.147225	-1.202121
C	2.767645	1.082400	-0.897831
C	3.314107	-0.346218	-0.756722
C	2.664665	-1.197512	0.353302
C	1.103911	-1.199970	0.165186
C	0.454857	0.184788	0.396745
H	3.000329	1.663001	-0.000305
H	3.297301	1.571731	-1.726092
H	4.394238	-0.297948	-0.584187
H	3.188656	-0.872883	-1.709872
C	3.181497	-2.653101	0.254975
C	2.952390	-0.720410	1.769689
N	0.750912	-1.792088	-1.080516
H	0.677161	-1.837145	0.953323
H	0.927518	0.431924	-1.946033
H	1.046590	0.730348	1.129435
C	3.900176	0.128757	2.170719
C	0.556888	-2.301184	-2.126255
H	1.865004	3.408668	0.197449
H	1.392572	4.289546	-1.257532
H	0.215649	4.082721	0.027150
H	-1.034711	3.389236	-2.169866
H	-1.000425	1.626135	-2.500310
H	-1.517238	2.240552	-0.921133
H	2.739433	-3.286726	1.032373
H	2.954004	-3.096235	-0.719008
H	4.266166	-2.665103	0.394653
H	2.343778	-1.206944	2.535469
H	4.057537	0.329300	3.226510
H	4.575442	0.632736	1.484740
C	-1.377079	1.186023	1.681504
H	-0.777521	1.835810	2.305779
H	-3.234391	1.553076	2.585765

10P

C	-2.332887	-1.027775	-0.959879
C	-3.655837	-1.366555	-1.241809
C	-4.699663	-1.052575	-0.354325
C	-4.442671	-0.390174	0.841862
H	-1.546701	-1.349728	-1.633361
H	-3.879989	-1.904296	-2.157848
H	-5.717439	-1.338646	-0.599624
H	-5.242906	-0.149320	1.535653
N	-2.593155	0.621743	2.209288
C	-3.117309	-0.047528	1.115147
C	-2.037324	-0.347066	0.239300
C	-0.839380	0.205690	0.848904
C	-0.136870	2.006645	-1.063386
C	0.154696	3.214604	-0.263185
C	-1.207716	2.058023	-2.064888
C	0.745629	0.803648	-1.014846
C	2.236297	1.101570	-1.349522
C	3.079422	-0.174325	-1.157586
C	2.940118	-0.855714	0.224824
C	1.414078	-1.112414	0.511673
C	0.615326	0.213246	0.410141
H	2.603481	1.902258	-0.700206
H	2.326441	1.448549	-2.385175
H	4.131649	0.070118	-1.339293
H	2.801143	-0.903679	-1.927269
C	3.707368	-2.198101	0.218766
C	3.486691	-0.033100	1.383386
N	0.884988	-2.095446	-0.377368
H	1.302252	-1.499410	1.532460
H	0.369302	0.070654	-1.736175
H	1.141668	0.891782	1.091317
C	4.321869	1.006013	1.331075
C	0.496610	-2.894438	-1.152237
H	0.836485	3.052311	0.571875
H	0.635007	3.931552	-0.955663
H	-0.764787	3.706651	0.070847
H	-1.761118	2.998453	-2.085541
H	-0.783362	1.841262	-3.058573
H	-1.902057	1.211723	-1.886858
H	3.619018	-2.707758	1.184838
H	3.330664	-2.871175	-0.556848
H	4.770221	-2.015361	0.035286
H	3.200970	-0.410480	2.367820
H	4.702478	1.461485	2.240692
H	4.689386	1.427320	0.399110
C	-1.249034	0.764579	2.055322
H	-0.654227	1.254618	2.815076
H	-3.126881	0.951519	3.001601

Transition State from 10P to 11P

C	2.254920	0.603772	0.900655
C	3.614110	0.958311	1.051866
C	4.632673	0.168393	0.521816
C	4.346744	-1.025171	-0.164766
H	1.548317	1.017733	1.606504
H	3.872286	1.826908	1.650448
H	5.668818	0.453142	0.672848
H	5.151493	-1.645459	-0.549210
N	2.433967	-2.396639	-1.067853
C	3.013868	-1.367967	-0.349662
C	1.948316	-0.566244	0.154496
C	0.729964	-1.092193	-0.356318
C	0.669965	1.905367	-0.437624
C	1.133249	1.737454	-1.842101
C	0.942472	3.229484	0.202238
C	-0.492825	1.109589	0.078457
C	-1.842293	1.812718	-0.309950
C	-3.003038	1.128851	0.438388
C	-3.106508	-0.402171	0.249979
C	-1.705469	-1.054636	0.524288
C	-0.599740	-0.384765	-0.343780
H	-1.982773	1.761478	-1.394405
H	-1.814048	2.869735	-0.026546
H	-3.945667	1.598248	0.135869
H	-2.893002	1.335303	1.509855
C	-4.154670	-0.973571	1.232144
C	-3.526334	-0.821345	-1.152257
N	-1.338730	-0.994071	1.903709
H	-1.760988	-2.115657	0.254059
H	-0.456854	1.159522	1.171506
H	-1.002434	-0.420722	-1.364137
C	-4.057571	-0.064512	-2.113685
C	-1.000074	-0.898415	3.029434
H	1.180146	0.692914	-2.156687
H	0.378535	2.228693	-2.481516
H	2.087571	2.235193	-2.028250
H	0.319227	3.979410	-0.313087
H	0.680436	3.257147	1.262613
H	1.979511	3.543629	0.063338
H	-4.255755	-2.058534	1.115957
H	-3.881608	-0.767178	2.271282
H	-5.132572	-0.525346	1.032549
H	-3.431481	-1.893272	-1.339728
H	-4.381932	-0.503603	-3.052608
H	-4.220364	1.004697	-2.008693
C	1.077197	-2.214100	-1.095019
H	0.447691	-2.887927	-1.661377
H	2.929052	-3.144178	-1.533169

11P

C	-2.116509	0.788189	-0.538207
C	-3.553539	1.193617	-0.482200
C	-4.553665	0.316312	-0.168160
C	-4.281313	-1.035340	0.230882
H	-1.958082	0.702521	-1.636971
H	-3.813186	2.196194	-0.808392
H	-5.589681	0.635569	-0.211438
H	-5.107291	-1.689181	0.499746
N	-2.385416	-2.607987	0.806047
C	-2.973905	-1.450971	0.305370
C	-1.904490	-0.560375	0.012206
C	-0.706471	-1.137320	0.395417
C	-0.958923	1.759123	-0.061014
C	-1.125552	2.076765	1.437059
C	-1.036949	3.061969	-0.876535
C	0.385483	0.996863	-0.384051
C	1.665461	1.833729	-0.195146
C	2.912055	1.072557	-0.686280
C	3.116155	-0.324091	-0.059669
C	1.785508	-1.139959	-0.194864
C	0.577342	-0.351439	0.379631
H	1.778889	2.108386	0.859561
H	1.596293	2.766821	-0.761821
H	3.807461	1.679676	-0.514437
H	2.839452	0.946450	-1.773961
C	4.260546	-1.065766	-0.787703
C	3.469910	-0.295323	1.421172
N	1.506643	-1.516388	-1.546542
H	1.904608	-2.072864	0.372560
H	0.325775	0.743120	-1.452880
H	0.851776	-0.125193	1.419281
C	3.891368	0.742522	2.144936
C	1.225044	-1.801315	-2.655608
H	-1.140788	1.176110	2.059798
H	-0.306022	2.711159	1.788008
H	-2.058616	2.622251	1.617590
H	-0.300920	3.788776	-0.524116
H	-0.854090	2.887049	-1.943595
H	-2.017005	3.539782	-0.773217
H	4.423942	-2.063145	-0.362952
H	4.045991	-1.180750	-1.854411
H	5.191793	-0.502055	-0.679178
H	3.432883	-1.274287	1.905397
H	4.183235	0.615721	3.183464
H	3.988106	1.746649	1.741930
C	-1.043850	-2.419914	0.873796
H	-0.405660	-3.200281	1.268406
H	-2.869689	-3.446852	1.098886

Transition State from 10P to 12P

C	2.281791	-1.808072	0.179132
C	3.588867	-2.233835	0.335448
C	4.679630	-1.417554	-0.036350
C	4.486547	-0.150102	-0.570364
H	1.465708	-2.452444	0.474028
H	3.781130	-3.216633	0.753424
H	5.691208	-1.787877	0.099308
H	5.324949	0.479591	-0.851881
N	2.697532	1.478290	-1.230693
C	3.167904	0.274654	-0.735998
C	2.038087	-0.527949	-0.378770
C	0.868946	0.234359	-0.710504
C	0.229626	1.966527	0.908098
C	-0.244490	3.302516	0.430917
C	1.371115	1.954612	1.858866
C	-0.767209	0.800848	0.959725
C	-2.239722	1.147078	1.255552
C	-3.125928	-0.105053	1.073237
C	-2.956478	-0.852295	-0.274795
C	-1.426383	-1.188972	-0.479254
C	-0.624490	0.126445	-0.412367
H	-2.577786	1.939124	0.580496
H	-2.351681	1.522348	2.279563
H	-4.176235	0.178791	1.197301
H	-2.910026	-0.814427	1.880527
C	-3.779556	-2.160878	-0.246235
C	-3.417723	-0.065406	-1.493354
N	-0.999284	-2.125807	0.510298
H	-1.290036	-1.659301	-1.460688
H	-0.402885	0.097738	1.719733
H	-1.118627	0.766388	-1.154421
C	-4.212174	1.006045	-1.523501
C	-0.732236	-2.891760	1.365624
H	-0.944558	3.251454	-0.406424
H	-0.797769	3.752460	1.273590
H	0.579319	3.979821	0.193733
H	2.103935	2.739679	1.656947
H	0.951227	2.141550	2.863307
H	1.863220	0.978387	1.910253
H	-3.670614	-2.718070	-1.183685
H	-3.471704	-2.812644	0.576448
H	-4.840260	-1.924496	-0.121972
H	-3.106648	-0.499466	-2.446408
H	-4.536363	1.432919	-2.468186
H	-4.599246	1.483310	-0.627267
C	1.331262	1.463905	-1.222184
H	0.771755	2.221363	-1.750813
H	3.269916	2.202383	-1.641690

12P

C	2.268896	-2.047509	-0.412091
C	3.555584	-2.474036	-0.242034
C	4.633994	-1.536150	-0.119379
C	4.453422	-0.171030	-0.158976
H	1.450658	-2.751603	-0.499914
H	3.779378	-3.534161	-0.194194
H	5.638776	-1.925992	0.017431
H	5.286483	0.515808	-0.052954
N	2.677056	1.558880	-0.342911
C	3.132661	0.295407	-0.325825
C	2.019924	-0.636513	-0.481823
C	0.888169	0.126982	-0.658580
C	0.183825	2.280634	0.284257
C	-0.476778	3.435243	-0.488054
C	0.810029	2.806536	1.583325
C	-0.812779	1.089786	0.594780
C	-2.307005	1.373546	0.756283
C	-3.074405	0.057724	1.012324
C	-2.830913	-1.068390	-0.024456
C	-1.282643	-1.315326	-0.182796
C	-0.588929	0.015939	-0.521318
H	-2.693994	1.871193	-0.138328
H	-2.474524	2.053000	1.600871
H	-4.148840	0.262039	1.066999
H	-2.792157	-0.328985	1.999379
C	-3.511890	-2.370601	0.455264
C	-3.369800	-0.764479	-1.415777
N	-0.709491	-1.886202	0.996366
H	-1.133397	-2.036515	-0.996307
H	-0.457519	0.630088	1.526985
H	-1.057209	0.380527	-1.447947
C	-4.239196	0.183445	-1.769922
C	-0.234791	-2.335403	1.978363
H	0.266182	4.194778	-0.757873
H	-0.958632	3.095658	-1.412608
H	-1.238722	3.925625	0.124750
H	1.490866	3.644468	1.395615
H	0.020821	3.173183	2.248654
H	1.362047	2.026915	2.118479
H	-3.353654	-3.188939	-0.256726
H	-3.128625	-2.686642	1.430111
H	-4.590369	-2.210601	0.542327
H	-3.043754	-1.470953	-2.182888
H	-4.605321	0.249471	-2.790373
H	-4.643392	0.909626	-1.070463
C	1.254035	1.577445	-0.657484
H	1.145808	1.982756	-1.675752
H	3.277686	2.371018	-0.405935

SUPPLEMENTARY REFERENCES

1. Landau, M. *et al.* ConSurf 2005: the projection of evolutionary conservation scores of residues on protein structures. *Nucleic Acids Res.* **33**, W299-302 (2005).
2. Trott, O. & Olson, A. J. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J. Comput. Chem.* **31**, 455-461 (2010).
3. Olsson, M. H., Sondergaard, C. R., Rostkowski, M. & Jensen, J. H. PROPKA3: consistent treatment of internal and surface residues in empirical pKa predictions. *J. Chem. Theory Comput.* **7**, 525-537 (2011).
4. Sondergaard, C. R., Olsson, M. H., Rostkowski, M. & Jensen, J. H. Improved treatment of ligands and coupling effects in empirical calculation and rationalization of pKa Values. *J. Chem. Theory Comput.* **7**, 2284-2295 (2011).
5. Abou-Hachem, M. *et al.* Calcium binding and thermostability of carbohydrate binding module CBM4-2 of Xyn10A from *Rhodothermus marinus*. *Biochemistry* **41**, 5720-5729 (2002).
6. Li, S. *et al.* Hapalindole/Ambiguine biogenesis is mediated by a Cope rearrangement, C-C bond-forming cascade. *J. Am. Chem. Soc.* **137**, 15366-15369 (2015).
7. Kumar, S., Tsai, C. J. & Nussinov, R. Factors enhancing protein thermostability. *Protein Eng.* **13**, 179-191 (2000).
8. Krissinel, E. & Henrick, K. Inference of macromolecular assemblies from crystalline state. *J. Mol. Biol.* **372**, 774-797 (2007).