

Supporting Information

Structural and Mechanistic Insights into Oxidative Biaryl Coupling to form Arylomycin Core by an Engineered CYP450

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Table of Contents

Figure S1: Distance plots of WT enzymes.....	S2
Figure S2: Distance plots of Mutant enzyme.....	S2
Figure S3: RMSD plots of WT and Mutant enzymes.	S2
Figure S4: Active site residues of the mutant enzyme.....	S3
Table S1. Spin density and charges over all the geometries obtained during mechanism of Mutant enzyme.	SError! Bookmark not defined.
Table S2. Mulliken charges for the substrate and Fe-OH.....	S4
QM Coordinates of all the geometries obtained in Wild type 1 and Variant 2	S4-S38

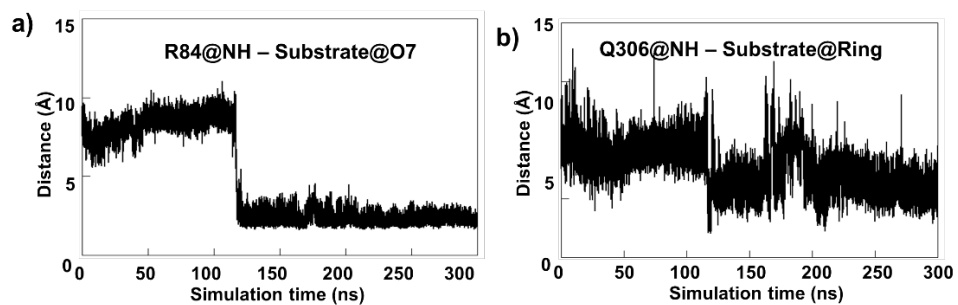


Figure S1: Distance plots of WT enzymes.

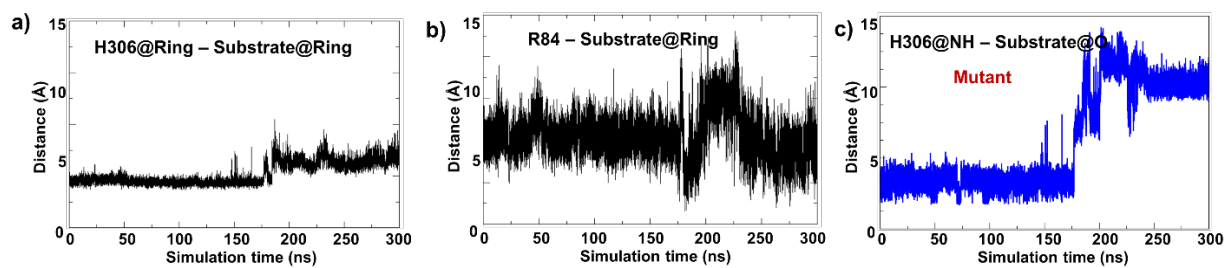


Figure S2: Distance plots of Mutant enzyme.

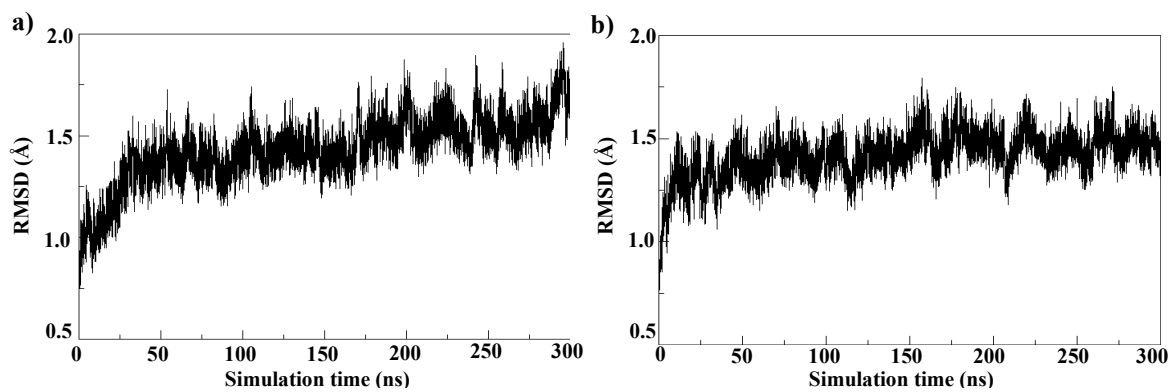


Figure S3: Root Mean Square Deviation (RMSD) plots for a) WT enzyme b) Mutant enzyme.

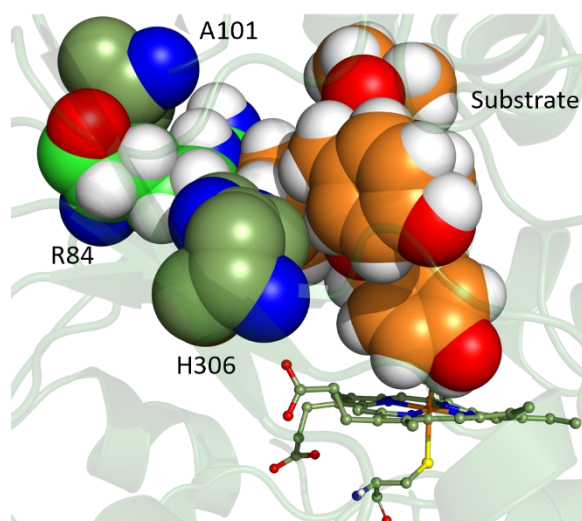


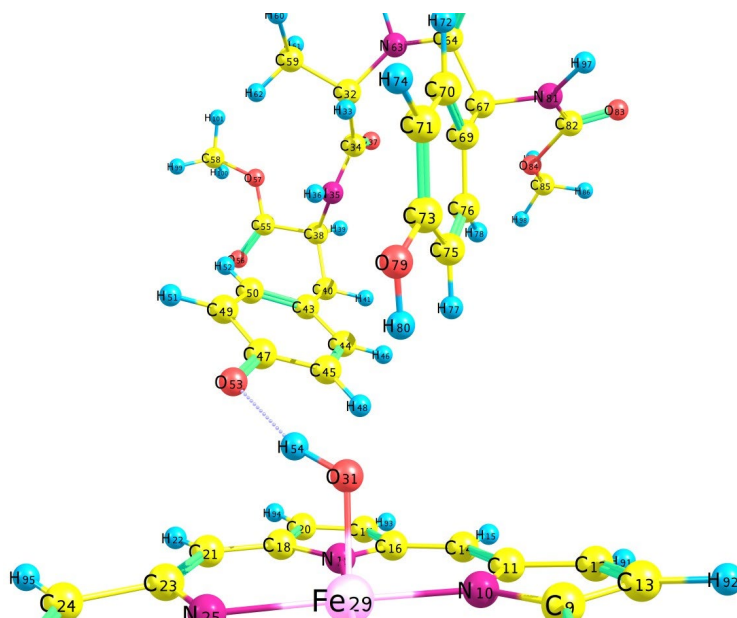
Figure S4: Active site residues as seen via their van der Waals' radii. As can be seen, A101 applies the steric kick to the substrate via the intermediary R84 residue.

Table S1. Spin density and charges over all the geometries obtained during mechanism of Mutant enzyme.

Spin density	Fe-O	SH	Por.	Subs.
RC	2.14	-0.11	-0.76	-0.28
IM1	2.19	-0.05	-0.18	-0.99
IM2	1.13	-0.03	-0.11	0.01
PC	1.12	-0.03	-0.11	0
PC'	1.32	-0.11	-0.26	0
Charge	Fe-O	SH	Por.	Subs.
RC	0.6	-0.51	0.11	0.24
IM1	0.51	-0.36	0.08	0.09
IM2	0.29	-0.37	0	0.13
PC	0.29	-0.37	-0.04	0.13
PC'	0.28	-0.33	-0.07	0.03

Table S2. Mulliken charges (elementary charge unit e) for the substrate and Fe-OH. Atoms involved in the hydroxylation reaction are shown in bold.

31o	-0.36992
32c	-0.02007
33h	0.02008
34c	0.13480
35n	-0.15490
36h	0.13059
37o	-0.31722
38c	0.01550
39h	0.03420
40c	0.20425
41h	0.02370
42h	0.04728
43c	-0.07816
44c	0.01180
45c	-0.03515
46h	0.02155
47c	0.18803
48h	0.00696
49c	-0.00808
50c	-0.00055
51h	-0.01444
52h	-0.00767



QM Coordinates of all the geometries obtained in Wild type 1 and Variant 2

	C	32.8139568	37.9956466	43.0911918
RC	C	32.4438950	38.6062346	44.3572405
S	C	32.7798859	39.9327307	44.2628860
N	C	32.7721089	36.6291391	42.8154604
C	H	32.4096376	35.9721887	43.6100379
C	C	33.1790517	36.0200039	41.6241719
C	C	33.1642391	34.5945621	41.3789590
C	C	34.1087946	35.7117700	39.6606906
C	N	33.7251114	36.6817563	40.5551084
H	C	33.7767392	34.3963274	40.1721786
C	C	34.6982395	35.9515145	38.4233624
N	H	34.9686399	35.0658835	37.8494392

C	34.9045685	37.1971123	37.8125044	C	40.7174311	31.2237632	42.2637375
C	35.3831474	37.3989052	36.4489166	O	40.1300410	30.7124592	41.3237114
N	34.6023987	38.3788821	38.4075328	O	41.9997964	31.2490289	42.5007011
C	34.8618686	39.3451942	37.4679069	C	43.0654191	30.4897700	41.7189434
C	34.7209757	40.7010930	37.7181933	C	43.6025458	34.1196935	43.7773281
H	34.9667433	41.3805483	36.9059335	H	44.2002608	35.0252026	43.5834081
Fe	34.0216199	38.6625339	40.3600822	H	44.2510247	33.3519315	44.2285942
C	35.3253463	38.7513126	36.2089101	H	43.2205784	33.7184820	42.8294180
O	35.5713157	38.5766439	40.9096351	N	42.9837366	34.9742567	45.9612457
C	42.4308702	34.4405012	44.7181267	C	42.4456544	35.9715844	46.7355411
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O	41.7792257	32.2752642	45.6614118	C	40.2540637	36.8671650	45.7913703
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C	38.4606340	32.2087166	43.0294828	H	41.9184712	38.2158582	45.4446482
H	37.8589571	32.2860085	43.9465295	C	38.9590051	38.3520112	43.7517212
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C	42.4492324	34.4590739	44.7136799	C	42.4295422	36.0027794	46.7185693
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N	40.6200108	33.1590624	43.8663844	C	40.8895794	36.0494402	46.8747736
H	40.5862695	33.9592519	43.2434138	H	40.5219792	35.0206422	46.7917733
O	41.7658025	32.3019020	45.6568512	C	40.2242458	36.8735660	45.7648772
C	39.9385917	31.9642134	43.3976432	C	40.8640590	37.9409444	45.1060547
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C	38.4659776	32.2276618	43.0273523	H	41.8892514	38.2106331	45.3749048

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C	38.2367627	37.3159034	44.4161803	C	33.8138339	41.6532777	41.0976534
C	38.9004494	36.5795334	45.3977095	C	34.4195744	42.7330792	39.2064642
H	37.2009626	37.0767535	44.1637459	C	33.9394217	42.9650409	40.4762899
H	38.3719624	35.7631920	45.8978255	C	33.5516371	41.3808611	42.4421408
O	38.3273286	39.0759586	42.7478973	H	33.4996386	42.2290080	43.1208781
H	37.4154004	38.7969849	42.5565464	C	33.3349212	40.1295975	43.0145189
N	40.5229309	36.4721223	48.2403032	N	33.4056853	38.9305830	42.3484216
C	39.9701343	35.6275770	49.1809734	C	32.9177148	37.9794448	43.2098040
O	39.8760716	35.8494527	50.3774708	C	32.4984772	38.5996135	44.4534614
O	39.4787175	34.5124137	48.6048232	C	32.8216529	39.9311296	44.3590496
C	38.9859675	33.4824774	49.4640174	C	32.8581049	36.6126517	42.9368743
H	38.4251375	33.9217926	50.3000719	H	32.4703298	35.9639630	43.7249983
H	39.8139431	32.8740189	49.8587834	C	33.2525164	36.0036791	41.7477382
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H	34.6392664	43.4984159	38.3812676	C	34.1485334	35.6849879	39.7588622
H	33.6702482	43.9841523	40.7658267	N	33.8163707	36.6540137	40.6737745
H	31.8859937	38.1141306	45.1621094	C	33.7778851	34.3789758	40.2635296
H	32.7162147	40.6915595	45.0496449	C	34.7316793	35.9096346	38.5137478
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H	34.0162101	33.4423461	39.7366779	C	34.9916386	37.1484081	37.9295112
H	35.7718049	36.5835582	35.8468331	C	35.4262375	37.3525838	36.5538659
H	35.5488020	39.3100355	35.3441301	N	34.7640788	38.3464955	38.5478986
H	40.7310303	37.4017016	48.5445224	C	34.9814201	39.3079177	37.5957370
H	38.3342310	32.8614954	48.8494542	C	34.8273496	40.6691879	37.8337762
H	43.0455011	30.7519543	40.6521542	H	35.0455068	41.3437528	37.0099879
H	42.9111199	29.4277975	41.8879688	Fe	34.1484504	38.6390761	40.4964491
H	44.0011551	30.8077334	42.1708379	C	35.3849643	38.7083972	36.3205482
				O	36.0193800	38.4611354	41.2145816
				C	42.3870402	34.5662976	44.6556404
				H	41.7586327	35.2902977	44.1073297
TS2							
S	31.7168167	38.9453718	39.4621049				

C	41.5638515	33.2653954	44.8291484	H	43.8796840	35.3061508	45.9207165
N	40.6340145	33.1433597	43.8443238	C	40.7137979	36.1713501	46.7483276
H	40.5715153	33.9094467	43.1820656	H	40.4028240	35.1225057	46.6780393
O	41.7843413	32.4247896	45.6898309	C	39.9763884	36.9421069	45.6405034
C	39.9805994	31.9091831	43.4413538	C	40.5257532	38.0549665	44.9641835
H	39.9793556	31.2610983	44.3276422	C	39.8086835	38.7317582	43.9821324
C	38.5151411	32.1392002	43.0215686	H	41.5356178	38.3946812	45.2131377
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C	42.4657945	34.4443055	44.6928644	C	42.3611435	36.1058953	46.6022373
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C	33.0239271	39.4383045	44.3040178	C	36.7572197	35.8028678	40.8698694
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C	34.9016614	36.8490511	37.7397903	C	40.3770923	31.7217540	42.3107034
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C	34.9129379	40.3717027	37.7723402	C	43.6768231	34.2792797	43.9069586
H	35.1603632	41.0652933	36.9734059	H	44.3784642	35.1169157	43.7610296
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Variant 2

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H	39.3877416	37.5555969	24.9965529	C	34.5902108	31.3189460	26.5256361
H	33.9456037	40.1322612	29.6354493	N	35.2192060	33.5220200	26.9231616
H	36.3053799	40.5516127	28.4793895	C	36.1176497	32.9249613	26.0717169
H	30.7676645	35.8770000	30.4440190	C	37.2314763	33.5704646	25.5460696
H	30.8814133	33.3092038	29.7093849	H	37.9156341	32.9663875	24.9563181
H	34.0242653	30.3524050	26.6835626	Fe	35.2034102	35.4867184	27.5029872
H	36.2453336	30.8590802	25.0870175	C	35.7230419	31.5408328	25.7783633
				O	36.2242461	35.2005257	28.8911489
				C	35.7771238	33.3752403	39.0693377
IM1				H	36.5763101	32.7456116	39.4825103
S	34.2431794	35.9315173	25.3638078	C	34.6369917	32.3528791	38.8520336
N	36.8718983	35.8547656	26.3716004	N	33.9374289	32.3480105	37.6919639
C	37.5908959	34.9096166	25.6952703	H	34.0181442	33.1437393	37.0613841
C	37.5317736	37.0517780	26.2378788	O	34.4011577	31.5825820	39.7701177
C	38.7520750	35.5276169	25.0898787	C	32.8640875	31.3847653	37.5408064
C	38.6945399	36.8743198	25.3779757	H	32.2365354	31.3925960	38.4458424
C	37.1903332	38.2073056	26.9437598	C	31.9333218	31.7323829	36.3569860
H	37.8972697	39.0320867	26.9037018	H	31.4580832	32.6984401	36.5865510
C	36.0893100	38.3956799	27.7734503	H	31.1343701	30.9757420	36.3752149
N	35.1376349	37.4437291	28.0496264	C	32.5595039	31.7831165	34.9793827
C	34.2331354	38.0321989	28.8976201	C	33.0126106	30.6050704	34.3503168
C	34.5853576	39.4208267	29.1162614				

C	33.5627407	30.6407836	33.0757266	O	34.6135713	34.9451998	36.7830764
H	32.9367641	29.6486980	34.8719658	H	37.4039152	34.1424627	37.9772201
C	33.6437467	31.8420614	32.3534343	C	36.7697088	35.6732328	36.0803808
H	33.9531347	29.7458923	32.5877234	H	36.2215306	36.6184878	35.9648456
C	33.1957562	33.0271054	32.9653485	C	36.8322650	35.0483262	34.6908414
C	32.6726430	32.9877187	34.2633829	C	36.6779492	33.6555466	34.4996448
H	33.2368129	33.9701094	32.4141226	C	36.5360417	33.1269565	33.2327162
H	32.3296835	33.9195697	34.7226481	H	36.6136331	32.9925400	35.3654780
O	34.1221277	31.7798232	31.0854598	C	36.5123158	33.9852431	32.0663731
H	34.7921994	32.4803510	30.9181894	H	36.3938661	32.0586515	33.0717703
C	33.4482872	29.9594854	37.4566574	C	36.7874790	35.3939607	32.2705749
O	34.5986971	29.7149718	37.1697682	C	36.9349463	35.8909517	33.5466870
O	32.4973133	29.0704315	37.7318302	H	36.8165450	36.0388286	31.3890354
C	32.7822573	27.6425925	38.0052328	H	37.0907964	36.9635770	33.6939856
C	33.2868627	26.9593319	36.7306364	O	36.2157676	33.5095380	30.9277077
H	32.5446499	27.0667987	35.9223703	H	36.1251726	34.4227618	29.5054617
H	33.4357280	25.8856056	36.9223750	N	38.0785480	35.9767777	36.6826939
H	34.2406843	27.3909645	36.4006964	C	38.1428655	36.9043729	37.7051113
C	31.4268212	27.0848075	38.4253033	O	39.1712900	37.2767565	38.2396941
H	31.5196785	26.0134359	38.6561579	O	36.9111968	37.3232780	38.0497585
H	30.6953695	27.2076607	37.6184600	C	36.8113306	38.3287154	39.0902271
H	31.0517819	27.6120077	39.3149481	H	37.2589445	39.2551392	38.7000002
C	33.7782170	27.5403788	39.1537771	H	37.4128807	38.0050882	39.9503101
H	34.7620696	27.9340986	38.8747491	C	35.3613944	38.5300113	39.4488820
H	33.4183397	28.1058419	40.0266554	C	34.5639312	39.4290897	38.7213634
H	33.8740641	26.4842063	39.4415431	H	35.0095236	39.9779177	37.8869789
C	35.3718125	34.3799471	40.1536078	C	33.2294113	39.6519073	39.0729563
H	34.5771411	35.0518770	39.7994559	C	32.6634614	38.9619649	40.1531788
H	35.0095027	33.8236314	41.0275564	H	32.6245112	40.3779469	38.5242516
H	36.2380635	34.9849407	40.4608403	H	31.6272256	39.1601036	40.4417680
N	36.3967264	34.0393011	37.9012251	C	33.4439176	38.0456971	40.8702469
C	35.8184112	34.8520995	36.9900540	C	34.7848223	37.8379023	40.5248543

H	33.0143528	37.5082727	41.7200937	N	35.0416573	37.3466797	28.6061713
H	35.3934945	37.1540251	41.1206409	C	34.0442804	37.9882532	29.2959194
C	39.3280143	35.4595147	36.1301744	C	34.3777014	39.3878422	29.4876743
H	39.5854848	35.9346864	35.1683167	C	35.6304522	39.5715229	28.9561749
H	39.2609094	34.3727929	35.9707245	C	32.8676617	37.3824720	29.7386432
H	40.1315076	35.6696225	36.8462781	H	32.1788432	38.0104929	30.3042953
O	41.1633116	40.4920114	41.0440115	C	32.4908300	36.0617238	29.5191297
H	41.2603116	40.6340114	40.1880113	C	31.2605133	35.4512161	29.9880010
H	41.6963117	41.0770115	41.4110116	C	32.5506830	33.9637860	28.8773909
O	40.0103112	37.9030107	41.0350115	N	33.2525542	35.1409721	28.8384121
H	40.6103114	38.5330108	40.9750115	C	31.3024131	34.1398239	29.5998147
H	39.9303112	37.6180106	40.2140113	C	32.9604592	32.7599617	28.3089941
H	32.8827924	36.0928154	25.5301726	H	32.2571529	31.9321192	28.4010410
H	39.4819951	35.0343691	24.4480138	C	34.1434161	32.5165081	27.6149091
H	39.3815327	37.5951266	24.9346411	C	34.4489540	31.2776572	26.9062388
H	33.9583757	40.1631390	29.6101575	N	35.1354222	33.4436508	27.4282067
H	36.3001155	40.5933273	28.4233265	C	36.0451014	32.8440617	26.5894350
H	30.7910530	35.9175169	30.4279855	C	37.1936334	33.4808372	26.1302255
H	30.9002350	33.3492993	29.6963897	H	37.8668308	32.8903394	25.5152949
H	34.0469158	30.3887575	26.6919097	Fe	35.0676708	35.4209461	27.9923120
H	36.2578147	30.8936580	25.0832014	C	35.6181715	31.4897504	26.2145081
				O	35.7941805	34.8413976	29.8734671
TS2'				C	35.8336686	33.4105517	38.3886400
S	34.3827358	35.8393807	25.7687777	H	36.6791920	32.8067625	38.7480193
N	36.8878658	35.7221445	27.0808448	C	34.7022585	32.3583619	38.2927638
C	37.5792957	34.8052557	26.3350870	N	33.8205794	32.4216277	37.2721810
C	37.5172795	36.9337136	26.9041591	H	33.8470124	33.2208289	36.6418664
C	38.7023620	35.4432549	25.6804497	O	34.6356899	31.5307495	39.1889103
C	38.6376534	36.7861749	25.9823477	C	32.7491467	31.4482715	37.1789604
C	37.1597181	38.0878864	27.6077072	H	32.1309957	31.4704497	38.0899638
H	37.8498259	38.9271847	27.5508968	C	31.8112595	31.7815928	35.9894761
C	36.0182001	38.2899131	28.3821679	H	31.2334331	32.6721328	36.2797179

H	31.0978278	30.9474726	35.9122681	H	36.3645853	35.0537840	39.7185978
C	32.4973284	32.0364846	34.6642883	N	36.3410727	34.0592657	37.1524819
C	33.0719983	30.9861447	33.9218768	C	35.6900354	34.8771063	36.2894816
C	33.7636893	31.2297720	32.7418050	O	34.4761177	34.9829549	36.1860146
H	32.9883115	29.9606233	34.2889928	H	37.3493380	34.1797552	37.1516399
C	33.9269797	32.5414814	32.2612030	C	36.5876251	35.7170387	35.3208122
H	34.2004055	30.4175154	32.1573083	H	35.9971767	36.6301603	35.1707164
C	33.3233803	33.5973568	32.9627690	C	36.7433061	35.0282667	33.9550213
C	32.6180765	33.3351388	34.1436131	C	37.1030085	33.6172385	33.9130234
H	33.4141545	34.6227387	32.5944455	C	37.4956586	33.0131828	32.7635423
H	32.1720803	34.1757263	34.6820149	H	37.0483784	33.0432334	34.8410015
O	34.6773810	32.6906062	31.1487280	C	37.5535915	33.7559725	31.5025934
H	34.7743701	33.6137933	30.8208319	H	37.7614707	31.9558425	32.7188742
C	33.3390523	30.0235421	37.1036922	C	37.0650534	35.1788885	31.5261106
O	34.4352499	29.7718610	36.6547685	C	36.6430389	35.7445793	32.7701439
O	32.4629239	29.1449341	37.5803860	H	37.5090172	35.8534062	30.7961848
C	32.8156671	27.7394734	37.8874152	H	36.3989796	36.8092064	32.8009406
C	33.2071329	26.9953692	36.6076238	O	37.9489105	33.2503625	30.4565789
H	32.3987974	27.0784226	35.8640670	H	36.4628465	34.1866904	29.5881420
H	33.3584905	25.9290088	36.8360276	N	37.8902413	36.0747713	35.9304749
H	34.1324605	27.3995426	36.1780434	C	37.9428943	36.9157025	37.0369288
C	31.5301359	27.1666785	38.4778744	O	38.9762792	37.2822210	37.5620293
H	31.7025231	26.1283069	38.7981195	O	36.7184405	37.2644350	37.4817568
H	30.7223257	27.1712834	37.7359101	C	36.7153016	38.1662861	38.6296670
H	31.2095579	27.7597030	39.3473578	H	37.2023675	39.0994510	38.3084802
C	33.9277615	27.7195547	38.9301082	H	37.3359564	37.7292327	39.4248918
H	34.8661117	28.1298478	38.5376665	C	35.3136840	38.4283898	39.1160216
H	33.6428150	28.3098482	39.8135550	C	34.5004563	39.3716946	38.4670907
H	34.0869068	26.6789633	39.2458138	H	34.8972113	39.8923992	37.5924344
C	35.4900117	34.4295299	39.4818705	C	33.2233416	39.6733210	38.9488836
H	34.6615561	35.0825826	39.1732521	C	32.7331090	39.0267846	40.0916212
H	35.1965126	33.8835931	40.3893162	H	32.6063235	40.4278673	38.4550627

H	31.7387543	39.2768719	40.4725828	C	37.1808912	37.9419879	27.1981540
C	33.5342226	38.0810474	40.7439433	H	37.8886581	38.7681918	27.1938769
C	34.8178920	37.7920146	40.2655747	C	36.0740282	38.1028314	28.0222911
H	33.1654510	37.5774301	41.6416409	N	35.0856639	37.1522444	28.2110361
H	35.4439764	37.0804028	40.8094323	C	34.1116485	37.7879415	28.9571702
C	39.1614715	35.7825292	35.2652915	C	34.4773259	39.1647487	29.2171260
H	39.2407784	36.2928252	34.2910366	C	35.7305784	39.3482320	28.6862399
H	39.2958730	34.7021892	35.1040163	C	32.9366013	37.1886694	29.4054705
H	39.9664464	36.1442756	35.9146972	H	32.2690235	37.8010683	30.0125561
O	41.1633116	40.4920114	41.0440115	C	32.5604840	35.8747504	29.1733325
H	41.2603116	40.6340114	40.1880113	C	31.3699124	35.2433910	29.7122995
H	41.6963117	41.0770115	41.4110116	C	32.6362935	33.7761968	28.5457943
O	40.0103112	37.9030107	41.0350115	N	33.3100289	34.9717464	28.4432298
H	40.6103114	38.5330108	40.9750115	C	31.4321954	33.9279503	29.3436232
H	39.9303112	37.6180106	40.2140113	C	33.0345110	32.5856151	27.9534853
H	33.0132514	36.0044082	25.8091000	H	32.3670770	31.7370242	28.1003997
H	39.3992766	34.9795669	24.9823303	C	34.1678332	32.3860746	27.1675688
H	39.2869355	37.5159458	25.4986802	C	34.4887583	31.1427112	26.4789459
H	33.6867152	40.1648234	29.8146385	N	35.1055597	33.3544885	26.9002735
H	36.1944304	40.5042222	28.9644064	C	36.0009959	32.7595182	26.0330068
H	30.4639407	35.9256188	30.5611337	C	37.1129127	33.4133596	25.5201445
H	30.5952768	33.3472342	29.8444100	H	37.7791678	32.8346345	24.8856099
H	33.8684404	30.3607392	27.0078879	Fe	34.9565368	35.3322846	27.3345411
H	36.1539789	30.8600896	25.5042231	C	35.6196977	31.3774145	25.7320857
PC'				O	36.4286689	35.8702689	31.2737659
S	34.2517092	35.8075288	25.2058884	C	35.8340068	33.3119828	38.9878978
N	36.8065930	35.6361157	26.5070563	H	36.6160233	32.6867295	39.4360680
C	37.4988362	34.7338663	25.7422366	C	34.7016336	32.2856165	38.7392581
C	37.4890603	36.8319579	26.4106920	N	33.9412840	32.3647020	37.6241877
C	38.6580581	35.3649100	25.1493128	H	34.0655897	33.1430444	36.9799752
C	38.6288881	36.6927916	25.5153783	O	34.5088622	31.4525144	39.6133069
				C	32.8796307	31.3967601	37.4317680

H	32.2828086	31.3267935	38.3534896	C	35.3860330	34.3242047	40.0496228
C	31.9034698	31.8150093	36.3022096	H	34.6097430	34.9977892	39.6598234
H	31.2425936	32.5851118	36.7240136	H	34.9851832	33.7747628	40.9115408
H	31.2711914	30.9379165	36.0981598	H	36.2410355	34.9279429	40.3897618
C	32.5293748	32.3502031	35.0307488	N	36.4997565	33.9697755	37.8403183
C	33.1456589	31.5103904	34.0860226	C	35.9544459	34.8258838	36.9437923
C	33.7353155	32.0230834	32.9304295	O	34.7561741	34.9483605	36.7258236
H	33.1789718	30.4325808	34.2680732	H	37.5019808	34.0781908	37.9629980
C	33.7370679	33.4059113	32.6916982	C	36.9442045	35.6782639	36.0995422
H	34.2231466	31.3708679	32.2020683	H	36.3844869	36.6117825	35.9610177
C	33.1278003	34.2580436	33.6190077	C	37.1665534	35.0929857	34.7111457
C	32.5263365	33.7282324	34.7638680	C	37.5440027	33.6834597	34.5357580
H	33.1231392	35.3388516	33.4524408	C	37.7487766	33.1106782	33.3224260
H	32.0494125	34.4147914	35.4681360	H	37.6114286	33.0615104	35.4332773
O	34.3332457	33.8545655	31.5485635	C	37.5340341	33.8782373	32.0938262
H	34.6042750	34.7840672	31.6321208	H	37.9628307	32.0450385	33.2164489
C	33.4717409	29.9857452	37.2391271	C	37.3330905	35.3943260	32.2468686
O	34.5967929	29.7616547	36.8504717	C	36.9987598	35.8733493	33.6212547
O	32.5570471	29.0762730	37.5712566	H	38.3563467	35.8071105	32.0511763
C	32.8792809	27.6573627	37.8274573	H	36.7012983	36.9214057	33.7141363
C	33.3690314	26.9853313	36.5417558	O	37.5103585	33.4054029	30.9693655
H	32.6360064	27.1439463	35.7351516	H	36.5610044	35.2786478	30.5088827
H	33.4798080	25.9029635	36.7081984	N	38.2074225	35.9928380	36.8010074
H	34.3351884	27.3960349	36.2240993	C	38.1893804	36.9338890	37.8088793
C	31.5490298	27.0667665	38.2846920	O	39.1835996	37.3825981	38.3521348
H	31.6778682	26.0046332	38.5408222	O	36.9312690	37.2898643	38.1263918
H	30.7973445	27.1491996	37.4912497	C	36.7866640	38.3149387	39.1422372
H	31.1760166	27.6039617	39.1691209	H	37.2162016	39.2438345	38.7380488
C	33.9047342	27.5739344	38.9512993	H	37.3889662	38.0233058	40.0121072
H	34.8683187	28.0074167	38.6578435	C	35.3320381	38.4965035	39.4901794
H	33.5480307	28.1136859	39.8411031	C	34.5370249	39.4113071	38.7800406
H	34.0426319	26.5171707	39.2200527	H	34.9839694	39.9730745	37.9549412

C	33.2046529	39.6362265	39.1395259	C	37.4612585	36.8525740	26.4883020
C	32.6392014	38.9333886	40.2113551	C	38.6630063	35.3734252	25.2640091
H	32.6018886	40.3753202	38.6059343	C	38.6194480	36.7063512	25.6117850
H	31.6054215	39.1336692	40.5071656	C	37.1039472	37.9945517	27.2107796
C	33.4165304	37.9996476	40.9098226	H	37.8182395	38.8145236	27.2094804
C	34.7542574	37.7884113	40.5556853	C	35.9623660	38.1895052	27.9863462
H	32.9865668	37.4518375	41.7526560	N	34.9842882	37.2481103	28.2028659
H	35.3609560	37.0912219	41.1381558	C	34.0293223	37.8561112	28.9817252
C	39.5116540	35.6206447	36.2562952	C	34.3938582	39.2378945	29.2341039
H	39.7178108	36.1254110	35.2972191	C	35.6078743	39.4492929	28.6300485
H	39.5798105	34.5348820	36.0973578	C	32.8658270	37.2445986	29.4501529
H	40.2789386	35.9203822	36.9791389	H	32.2012395	37.8529515	30.0648239
O	41.1633116	40.4920114	41.0440115	C	32.4827530	35.9291610	29.2068705
H	41.2603116	40.6340114	40.1880113	C	31.2788984	35.2977929	29.7230810
H	41.6963117	41.0770115	41.4110116	C	32.5521909	33.8343237	28.5531689
O	40.0103112	37.9030107	41.0350115	N	33.2249131	35.0258657	28.4843150
H	40.6103114	38.5330108	40.9750115	C	31.3328658	33.9864386	29.3328415
H	39.9303112	37.6180106	40.2140113	C	32.9634895	32.6403459	27.9645820
H	32.8981807	36.0034818	25.3900360	H	32.2876199	31.7961111	28.0978068
H	39.3694792	34.8925721	24.4719326	C	34.1142300	32.4220922	27.2039606
H	39.3203385	37.4280699	25.1038818	C	34.4399056	31.1695015	26.5253712
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H	30.5691746	35.7166559	30.2805481	C	37.1159623	33.4178269	25.6311872
H	30.7579494	33.1225073	29.6346921	H	37.7980945	32.8301464	25.0223249
H	33.9535871	30.2058251	26.6335531	Fe	35.0017094	35.3299215	27.5179439
H	36.1630095	30.7375117	25.0368133	C	35.5912201	31.3896994	25.8050872
IM2				O	35.8258304	34.8403216	29.3096587
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N	36.8003679	35.6512281	26.5963617	H	36.6073942	32.6686683	39.3870398
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C	32.8343709	31.4738941	37.3233298	H	34.1563604	26.6141872	39.1294177
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H	31.2449386	32.6965942	36.5495216	H	34.9152126	33.6983199	40.8332960
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H	33.3857969	30.5253542	34.2738756	H	37.5065445	34.0726421	37.9315376
C	33.8252823	33.4849646	32.5398746	C	36.9726627	35.6504418	36.0466391
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C	33.1102909	34.3428784	33.4664452	C	37.1956781	35.0265878	34.6736530
C	32.5025056	33.8254382	34.5893347	C	37.3863860	33.6287240	34.5018498
H	33.0761069	35.4101179	33.2401253	C	37.5560209	33.0854925	33.2466647
H	31.9489061	34.4938718	35.2542208	H	37.3750231	32.9745008	35.3774586
O	34.3755876	33.9362865	31.5040236	C	37.4985982	33.9160068	32.0534548
H	35.1751341	34.5966557	30.0050154	H	37.7011293	32.0134711	33.0976662
C	33.4050189	30.0517232	37.1306266	C	37.3209317	35.3457856	32.2587594
O	34.4756643	29.8222466	36.6099449	C	37.1882879	35.8648251	33.5285914
O	32.5400156	29.1588155	37.5911981	H	37.2674676	35.9800604	31.3717582
C	32.8789294	27.7360042	37.8322909	H	37.0514746	36.9414016	33.6625642
C	33.2687727	27.0469434	36.5222902	O	37.5742500	33.4110931	30.9066578
H	32.4803141	27.2061267	35.7705545	H	36.5971656	34.2605704	29.4875511
H	33.3733355	25.9647416	36.6950305	N	38.2298364	35.9710832	36.7515581
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C	31.5881856	27.1494602	38.3960845	O	39.2028160	37.3436423	38.3188964
H	31.7544534	26.1016747	38.6876799	O	36.9514462	37.2771839	38.0712521
H	30.7852082	27.1793589	37.6496994	C	36.8106846	38.3092306	39.0841175
H	31.2648503	27.7170499	39.2811288	H	37.2335215	39.2364126	38.6692460
C	33.9883027	27.6694198	38.8730239	H	37.4208094	38.0270112	39.9522063

C	35.3591724	38.4922897	39.4447330	S	34.2213912	35.8135263	25.3585219
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C	33.4564247	38.0076704	40.8862160	H	37.7839594	38.8567715	27.2198006
C	34.7880856	37.7862436	40.5156732	C	35.9219552	38.2176032	27.9723937
H	33.0316636	37.4608927	41.7324542	N	34.9496158	37.2679014	28.1743270
H	35.3959646	37.0828738	41.0898897	C	33.9667537	37.8731116	28.9198065
C	39.5359136	35.5668325	36.2298596	C	34.3038752	39.2646575	29.1578252
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O	41.1633116	40.4920114	41.0440115	C	32.4592410	35.9175759	29.1515048
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H	39.3101796	37.4368422	25.1906674	C	34.4943816	31.1827764	26.4823145
H	33.7564475	39.9932326	29.6937114	N	35.1143168	33.3790979	26.9384054
H	36.1617938	40.3879120	28.6453672	C	36.0296550	32.7966694	26.0973785
H	30.4839590	35.7631237	30.3058380	C	37.1596498	33.4567551	25.6229415
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H	33.8892459	30.2394633	26.6663322	Fe	35.0099709	35.3452388	27.4983251
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				O	35.8747274	34.9387494	29.2842101
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C	34.0413147	34.4574740	32.6952188	C	36.8375862	35.7240390	36.1316206
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C	33.2184254	35.0510212	33.7030541	C	36.8810201	34.9947314	34.7936860
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H	36.5460421	32.7082668	39.5011431	H	30.9304404	27.2745320	37.4139565
C	34.6801392	32.3113460	38.6704751	H	31.3247331	27.8164116	39.0652477
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C	32.5373145	34.2038705	34.7149486	C	36.3678395	33.7069876	34.6632315
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C	33.0027659	27.8599503	37.6913696	H	37.8453324	36.6449523	33.8001482
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C	36.8834402	38.3650727	39.1030841	H	36.1867340	30.7730590	25.0816128
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