

Electronic Supplementary Information

Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase

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Section S2, Effect of dimerization of AGAO

XYZ atomic coordinates for all the QM/MM optimized states in the QM region. (0, 1, 2, 3, 4, 0⁻, 1⁻, 2⁻, 3⁻, 4⁻, 5⁻, 6⁻, 7⁻, 8⁻, 9⁻, 10⁻, 11⁻, 0²⁻, 1²⁻, 2²⁻, 3²⁻, 4²⁻, 5²⁻, 6²⁻, 7²⁻, 8²⁻, 0³⁻, 1³⁻, 2³⁻, 3³⁻, 4³⁻, 5³⁻, 6³⁻, 7³⁻, 8³⁻, 9³⁻, 10³⁻, imq(0²⁻), imq(0⁻), imq(keto⁻), imq(keto_{rot}⁻))

Table S1. Relative free energies (G) (relative energies (E))* and RMSD values to the neutron (ND) structure.

State	$G(E) / \text{kcal mol}^{-1}$	$RMSD / \text{\AA}$	Protonation state
Fully protonated (Full)			Asp298 protonated
0	0 (0)	0.251	TPQ382 O(2) protonated
1	0.69 (3.10)	0.167	TPQ382 keto form Asn381 side chain rotated
2	1.95 (4.54)	0.264	TPQ382 keto form
3	3.24 (4.44)	0.306	TPQ382 O(4) protonated
4	9.87 (9.25)	0.375	TPQ382 O(5) protonated
Deprotonated (-H⁺)			Asp298 protonated TPQ382 enolate form
0⁻	0 (0)	0.107	-
1⁻	7.84(7.77)	0.190	Asp298 rotated
2⁻	19.86 (20.59)	0.294	TPQ382 O(2) protonated His433 deprotonated Tyr384 OH rotated
3⁻	30.01 (31.50)	0.243	TPQ382 O(4) protonated His433 deprotonated Tyr384 OH rotated
4⁻	31.48 (34.21)	0.136	TPQ382 O(5) protonated His433 deprotonated
5⁻	33.96 (35.62)	0.225	TPQ382 keto (C(3) protonated) His433 deprotonated Tyr384 OH rotated
6⁻	34.84 (37.29)	0.241	TPQ382 O(5) protonated His433 deprotonated Tyr384 OH rotated
7⁻	36.82 (38.49)	0.253	W(ax) deprotonated (OH(ax)) TPQ382 keto form
8⁻	58.78(63.98)	0.167	TPQ382 keto (C(3) protonated) Asn381 rotated His431 deprotonated
9⁻	59.37(62.95)	0.122	Asp298 protonated W(ax) deprotonated (OH(ax)) TPQ382 O(4) protonated
10⁻	64.03(67.29)	0.117	Asp298 deprotonated TPQ382 keto form
11⁻	64.08(69.17)	0.193	Asp298 deprotonated TPQ382 keto form Asn281 side chain rotated
Doubly deprotonated (-2H⁺)			TPQ382 enolate form Asp298 protonated
0²⁻	0 (0)	0.238	His433 deprotonated Tyr384 OH rotated
1²⁻	3.00 (3.13)	0.302	Asp298 rotated His433 deprotonated Tyr384 OH rotated
2²⁻	4.16 (4.54)	0.132	His431 deprotonated
3²⁻	13.07(12.01)	0.158	His433 deprotonated
4²⁻	17.11(17.77)	0.317	Asp298 deprotonated
5²⁻	17.92(18.08)	0.182	W(ax) deprotonated (OH(ax))
6²⁻	24.79(17.70)	0.148	His592 deprotonated
7²⁻	37.02(39.35)	0.379	Asp298 deprotonated W(ax) deprotonated (OH(ax))

8²⁻	39.59(41.21)	0.392	TPQ382 keto form Asp298 deprotonated W(ax) deprotonated (OH(ax)) TPQ382 O(4) protonated
Triply deprotonated (-3H⁺)			
0³⁻	0 (0)	0.304	TPQ382 enolate form Asp298 protonated Asp298 rotated His433 deprotonated His431 deprotonated Tyr384 OH directs to His433
1³⁻	2.20 (1.95)	0.151	His433 deprotonated His431 deprotonated Tyr384 OH directs to His433
2³⁻	11.32(11.21)	0.329	Asp298 rotated His592 deprotonated His431 deprotonated Tyr384 OH directs to His433
3³⁻	13.19(13.23)	0.173	His433 deprotonated His431 deprotonated
4³⁻	20.72(21.07)	0.332	W(ax) deprotonated (OH(ax)) His433 is deprotonated Tyr384 OH directs to His433
5³⁻	28.10(27.79)	0.189	W(ax) deprotonated (OH(ax)) His431 deprotonated
6³⁻	33.51(34.95)	0.236	W(ax) deprotonated (OH(ax)) His433 is deprotonated
7³⁻	37.34(39.02)	0.299	W(ax) deprotonated (OH(ax)) His592 is deprotonated
8³⁻	48.08(48.55)	0.348	Asp298 deprotonated TPQ382 keto form W(ax) deprotonated (OH(ax)) His431 deprotonated
9³⁻	66.98(68.85)	0.224	W(ax) deprotonated (OH(ax)) His592 is deprotonated
10³⁻	69.58(75.55)	0.520	Asp298 deprotonated TPQ382 keto form W(ax) deprotonated (OH(ax)) His431 deprotonated Asn281 side chain rotated

* Free energies were calculated using $G(i) = E(i) + \delta H(i) - T S(i)$, where $E(i)$ is relative energy in state i , δH is the thermal energy correction to enthalpy, S is the total entropy, and T is temperature ($T = 298.15$ K). Zero energies are taken for the states in the most stable states (**0³⁻**).

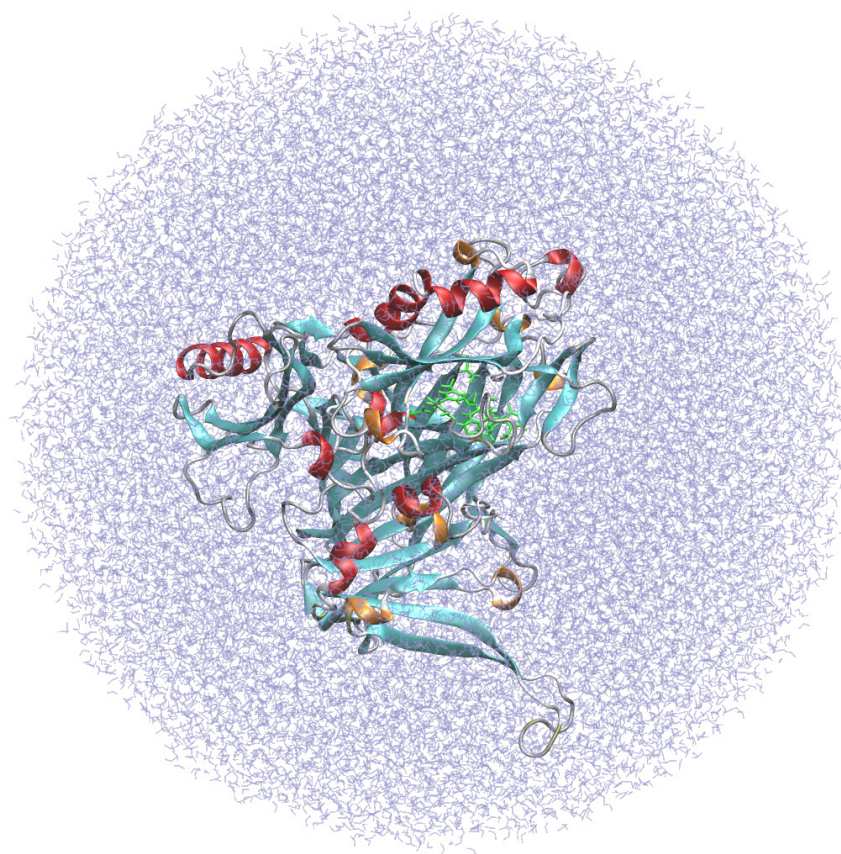


Figure S1. QM/MM whole system used in the present study. Solvent water molecules are colored blue, and CGAO is drawn in ribbon. The QM atoms in the active site are displayed in the green tube representation.

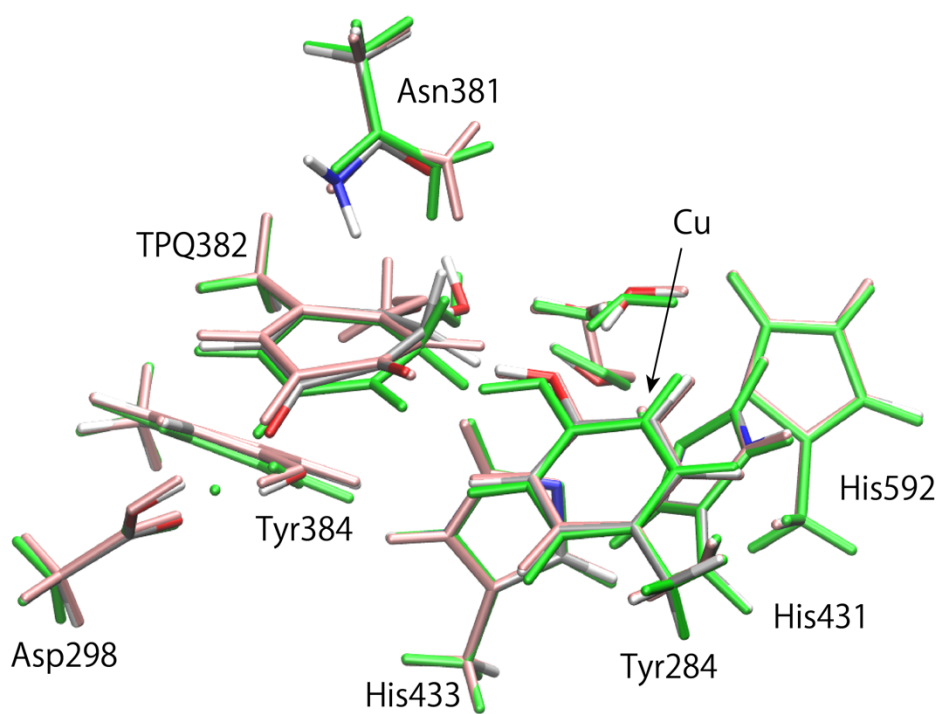


Figure S2. Superimposed view of the QM/MM optimized structures (**0** and **1**) in **Full** state compared to the ND structure. Only the atoms in the QM region are shown, and they are colored pink (**0**), by element (**1**), and green (ND).

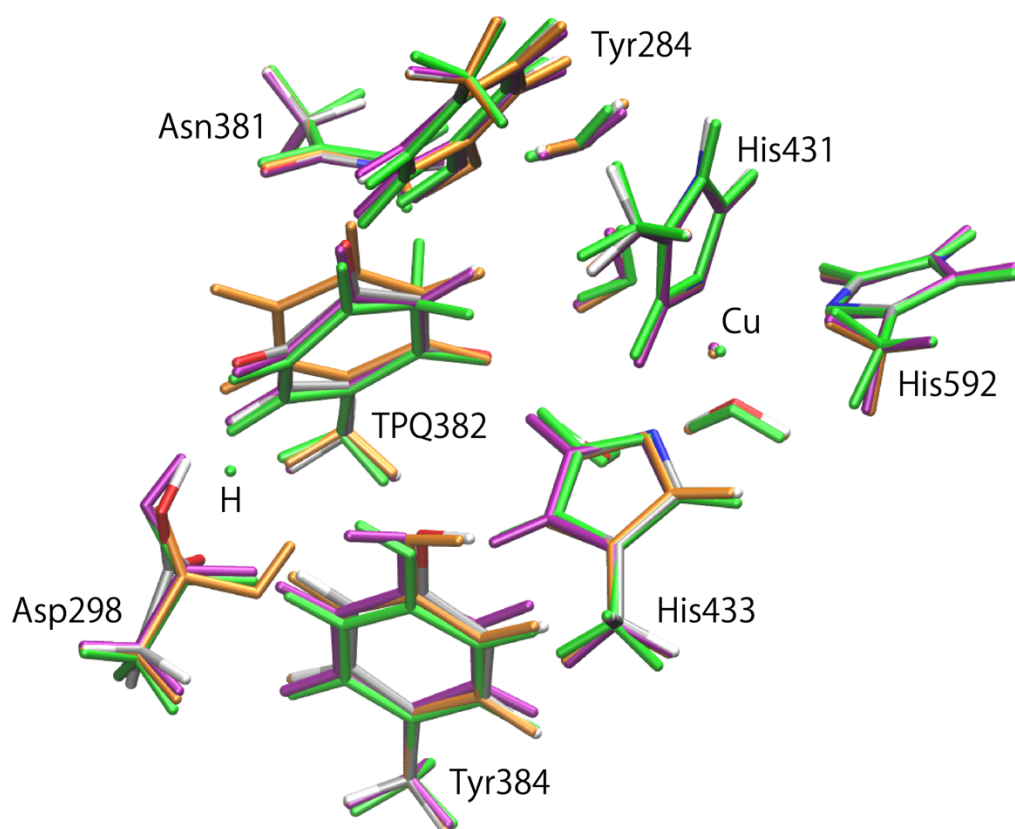


Figure S3. Superimposed view of the QM/MM optimized structures (0^{2-} , 1^{2-} , and 2^{2-}) in $-2H^+$ state compared to the ND structure. Only the atoms in the QM region are shown, and they are colored by element (0^{2-}), orange (1^{2-}), purple (2^{2-}) and green (ND).

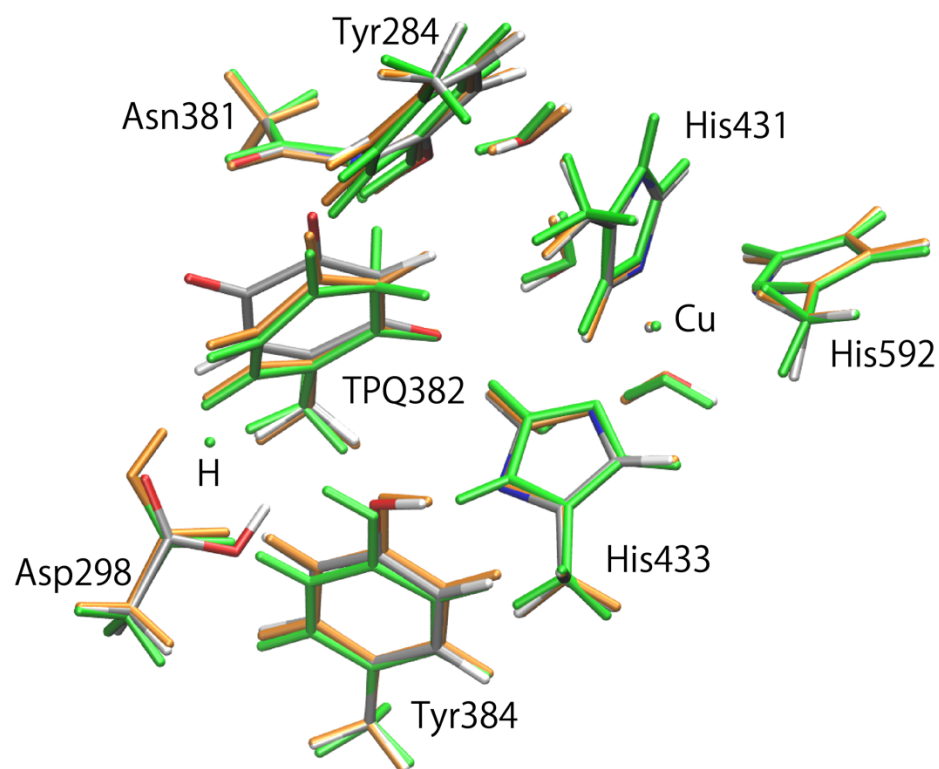


Figure S4. Superimposed view of the QM/MM optimized structures (0^{3-} , 1^{3-}) in $-3H^+$ state compared to the ND structure. Only the atoms in the QM region are shown, and they are colored by element (0^{3-}), orange (1^{3-}) and green (ND).

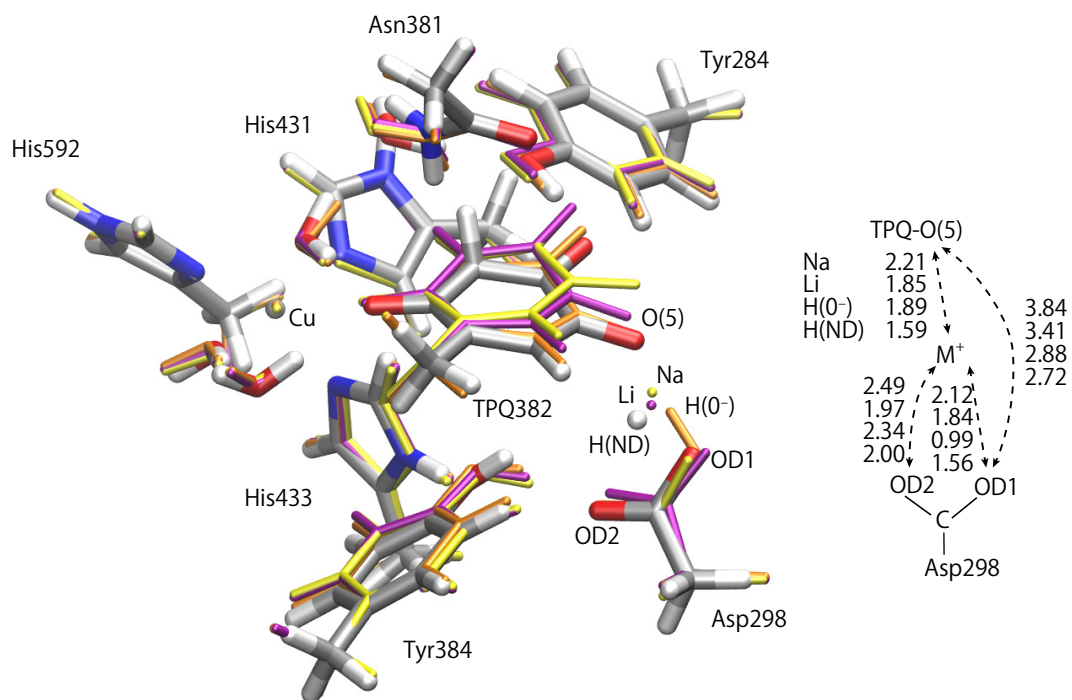


Figure S5. Superimposed view of the QM/MM optimized structures with H(0⁻), Li⁺ and Na⁺ compared to the ND structure. Only the atoms in the QM region are shown, and they are colored by element (ND), orange (H(0⁻)), purple (Li⁺) and yellow (Na⁺). Distances to the nearest oxygen atoms of Asp298 or TPQ are illustrated in the right panel.

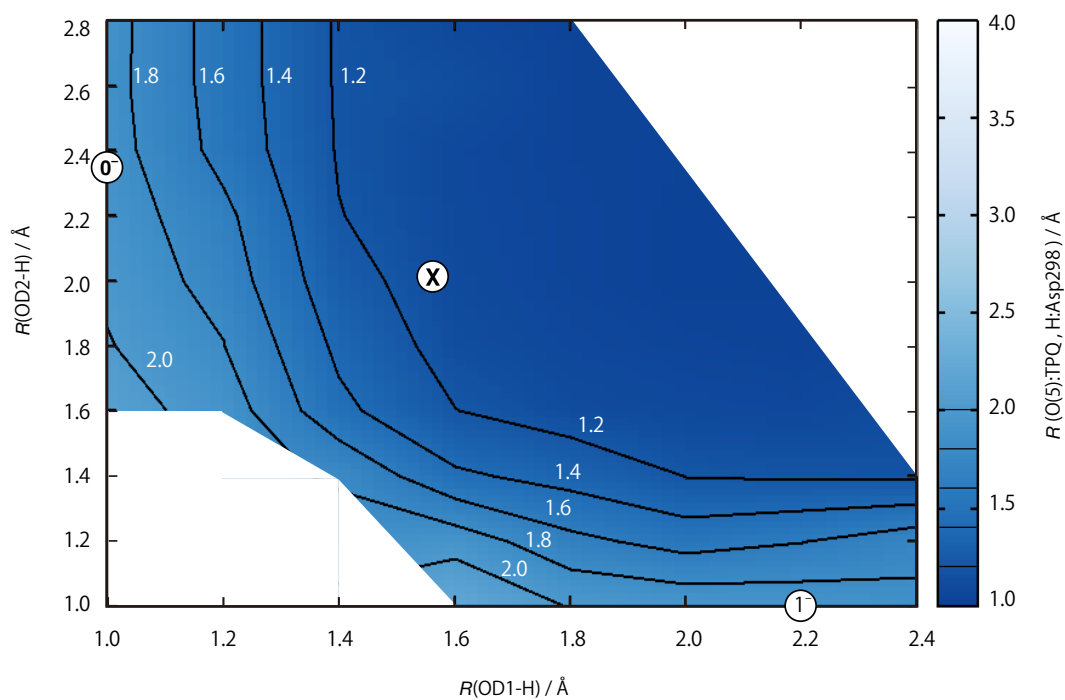


Figure S6. 2D-PES of the distance between the shared proton and O5 of TPQ ($R(\text{O}(5):\text{TPQ}, \text{H}:\text{Asp298})$) in $-\text{H}^+$ state at the QM/MM optimized structures along the $R(\text{OD}:\text{Asp298}, \text{H})$ variables .

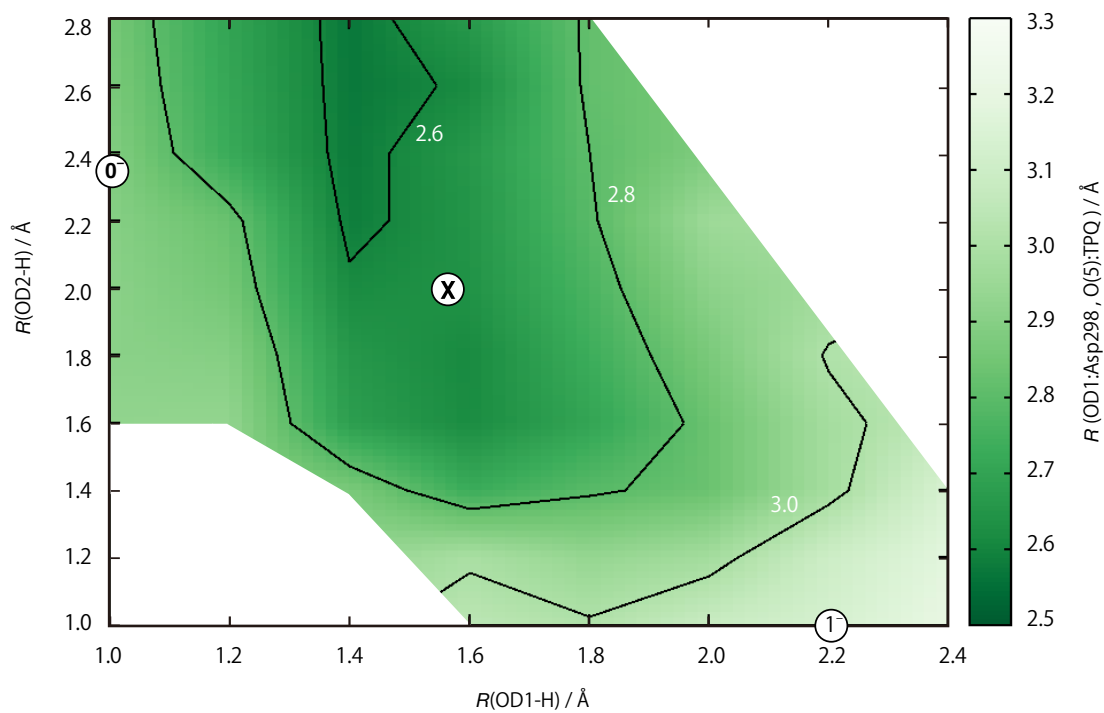


Figure S7. 2D-PES of the distance between the OD1 of Asp298 and O(5) of TPQ ($R(\text{OD1:Asp298}, \text{O}(5):\text{TPQ})$) in $-\text{H}^+$ at the QM/MM optimized structures along the $R(\text{OD:Asp298}, \text{H})$ variables.

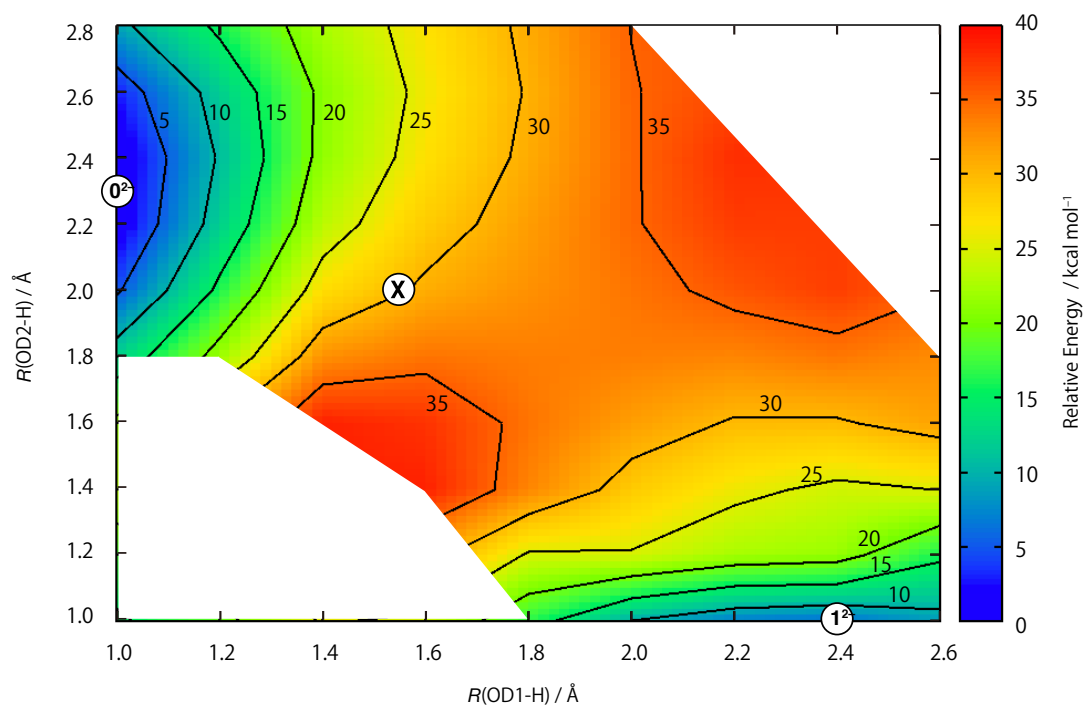


Figure S8. 2D-PES of the distal H atom along the distances between the OD atoms of Asp298 and the shared proton ($x=d(\text{OD1}, \text{H})$, $y=d(\text{OD2}, \text{H})$) in -2H^+ state.

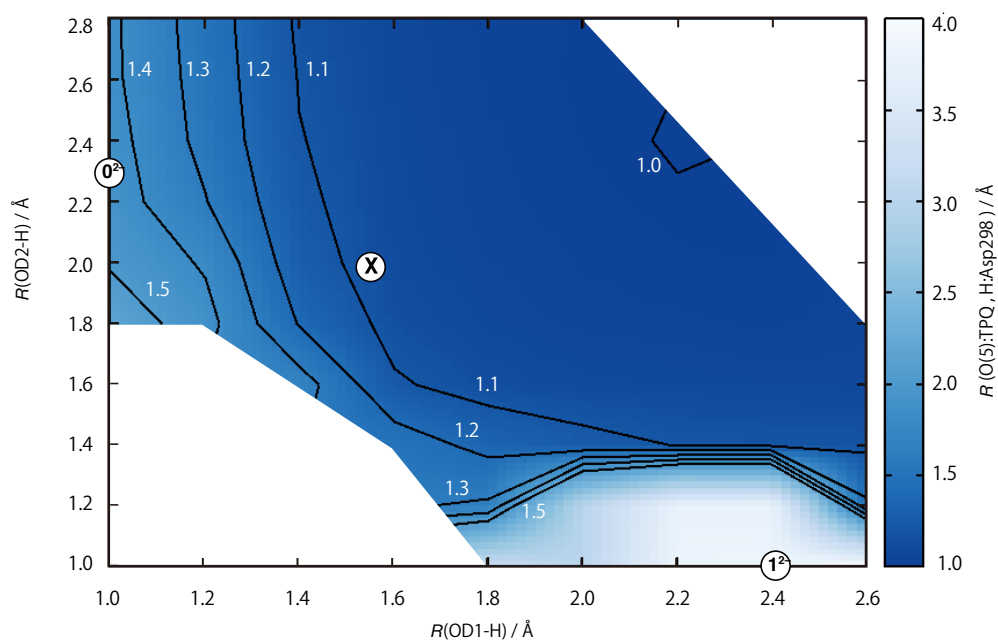


Figure S9. 2D-surface of the distance between the shared proton and O(5) of TPQ ($R(\text{O(5):TPQ, H:Asp298})$) in -2H^+ state at the QM/MM optimized structures along the $R(\text{OD:Asp298, H})$ variables.

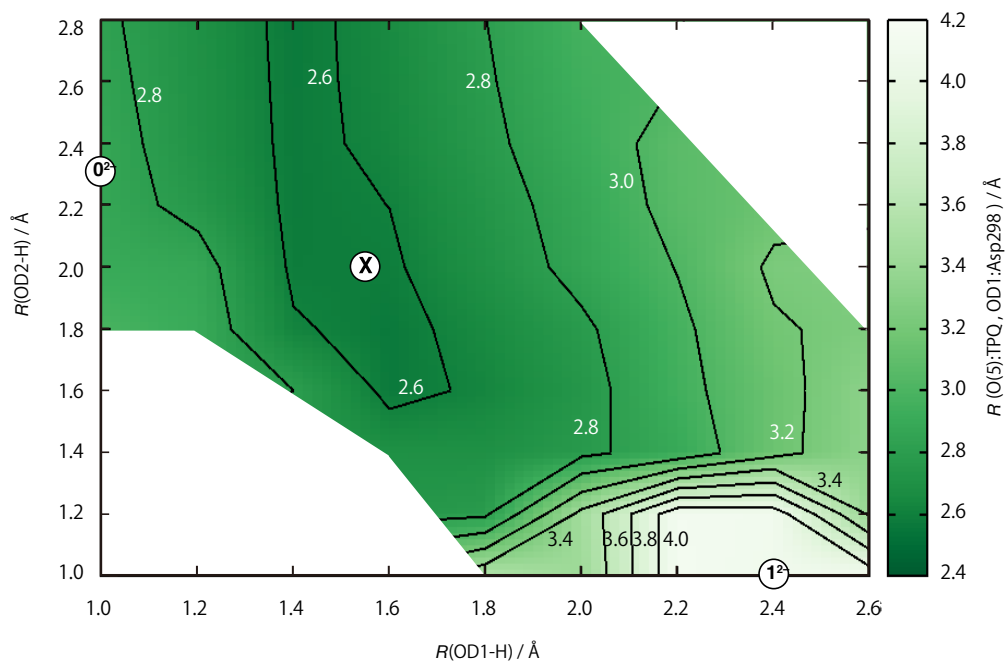


Figure S10. 2D-surface of the distance between the O(5) of TPQ and OD1 of Asp298 ($R(\text{O(5):TPQ, OD1:Asp298})$, OD1:Asp298,) in -2H^+ at the QM/MM optimized structures along the $R(\text{OD:Asp298, H})$ variables.

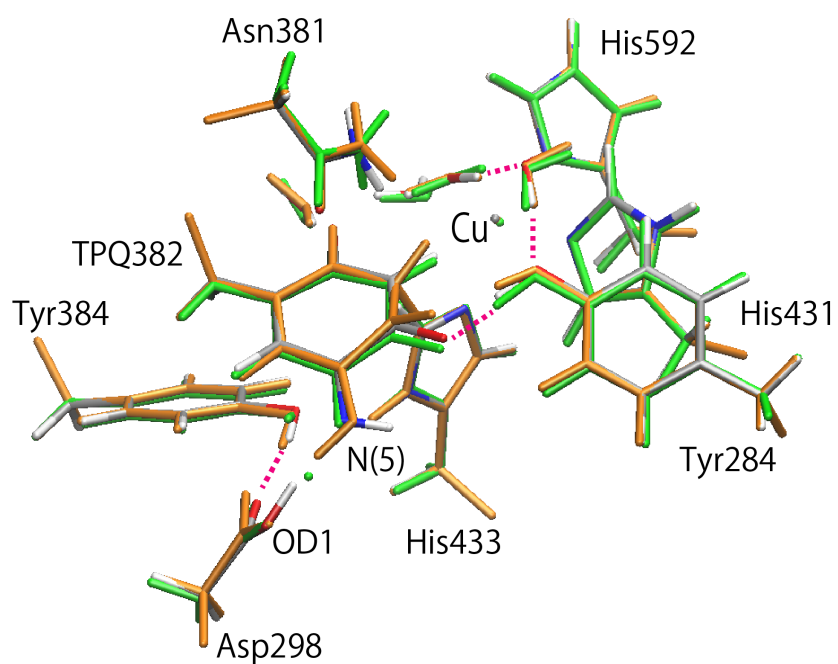


Figure S11. Superimposed view of the QM/MM optimized structures (*imq(0⁻)* and *imq(keto⁻)*) in *imq* state compared to the ND structure. Only the atoms in the QM region are shown, and they are colored by element (*imq(0⁻)*), orange (*imq(keto⁻)*) and green (ND).

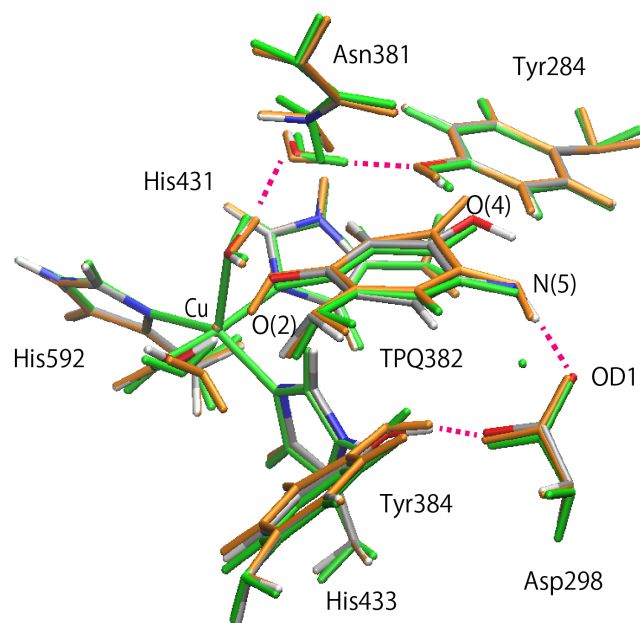


Figure S12. Superimposed view of the QM/MM optimized structures (**imq(O(2)H⁻**) and **imq(O(4)H⁻**) in **imq** state compared to the ND structure. Only the atoms in the QM region are shown, and they are colored by element (**imq(O(2)H⁻**), orange (**imq(O(4)H⁻**) and green (ND)).

Section S2, Effect of dimerization of AGAO

The TPQ active site is buried inside one monomer subunit of the AGAO dimer. In the dimer, a segment of beta strand-loop-beta strand from the other subunit wraps the TPQ active site domain (Figure S2.1(A)), although there are no direct H-bond interactions between the TPQ active site (QM region) and the amino acid residues in the segment from the other subunit. The shortest distances to the O4:A-TPQ382 atom are 10.8 Å and 11.2 Å for Cε:B-His355 and Cε2:B-Phe470 atoms, respectively. The distance between the active site in each subunit is $d(\text{O4:A-TPQ}, \text{O4:B-TPQ}) = 46 \text{ Å}$. Therefore, these rather long distances suggest that the electronic interactions from another subunit do not become a dominant factor. We also remark that the heavy atoms of proteins in the MM region are all fixed to the ND structure during the MD simulations, thus ensuring the protein structure in the MM region of the monomer subunit is not denatured. One theoretical difficulty for the dimer model is that the MM force field for the TPQ in another subunit should be refined, namely because the assumed protonation state of the active site is somehow arbitrary.

In order to actually evaluate the influence in the dimerization, we constructed new dimer and monomer models. Almost all the computational procedures are followed described in the main text, but only one difference is that the annealing of MDs were carried out for longer times (10ps) in rectangular simulation boxes. After extracting spherical regions from the center of the protein, new QM/MM models are constructed as shown in Figure S2.1(B) and (C). In the dimer model, we assumed a singly protonated state ($-\text{H}^+$) for TPQ in the MM region. Using these new QM/MM models, we performed QM/MM optimizations for the lowest states in four different protonation states.

Results summarized in Table S2.1 show that

1. the singly protonated state (0^-) is the closest one to the ND structure in either QM/MM model,
2. the conformational isomers in the singly protonated state (1^-) are in low energy states,
3. the trends of RMSD for other protonation states are qualitatively similar over the different QM/MM models and independent for the monomer/dimer models.

In conclusion, the monomer model used in the present QM/MM model is the one computationally less expensive and preferable to the scope of the present work. Moreover, the active site properties, structures and relative energies, are not dominantly influenced by the monomer/dimer model for AGAO.

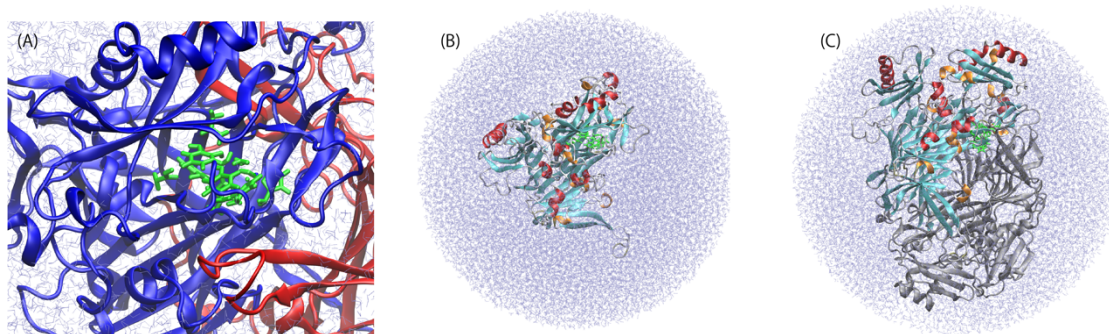


Figure S2.1 (A) Enlarged view of the active site in the dimer model, (B) newly constructed monomer model, (C) newly constructed dimer model. One monomer is colored according to the secondary structure,

and another monomer is colored gray to allow for a clearer visualization.

Table S2.1 RMSDs of the non-H atoms in the QM region from the neutron diffraction structure (PDBID: 6L9C) ($RMSD/\text{\AA}$) and the relative energies ($\Delta E/\text{kcal mol}^{-1}$).

States	Monomer in the main text	Monomer	Dimer
	$RMSD(\Delta E)$	$RMSD(\Delta E)$	$RMSD(\Delta E)$
Fully protonated (Full)			
0	0.251	0.247	0.244
Deprotonated (-H⁺)			
0⁻	0.107 (0)	0.1709 (0)	0.181 (0)
1⁻	0.190 (7.8)	0.302 (2.9)	0.283 (4.9)
Doubly deprotonated (-2H⁺)			
0²⁻	0.238	0.245	0.268
Triply deprotonated (-3H⁺)			
0³⁻	0.304	0.394	0.463

0, Full

C	14.51678455	-7.89663965	-1.97511077	C	2.82341080	-2.14765151	-4.50210360
H	14.95054944	-8.89893830	-1.99248162	H	3.52113087	-1.84015593	-5.27151586
H	15.22128250	-7.23217198	-2.47811879	C	1.51002196	-1.69237308	-4.50860219
C	13.16916918	-7.95333426	-2.65817522	H	1.18362383	-1.03377685	-5.30887984
C	12.53957396	-6.83131552	-3.21286031	C	10.51660545	-8.43711236	0.08129971
H	13.04458860	-5.86877090	-3.21477099	H	11.27880307	-8.84100360	-0.58458856
C	11.24827564	-6.92065038	-3.72912033	H	10.51502575	-7.35534913	-0.07708761
H	10.76125658	-6.04214065	-4.13707526	C	9.17177103	-8.98351581	-0.24852973
C	10.56739399	-8.14497183	-3.70578966	N	8.92287484	-10.30943796	-0.57269633
O	9.27972179	-8.25964430	-4.16350930	H	9.62458766	-11.03845152	-0.69863682
H	9.08455973	-7.50337347	-4.78206353	C	7.59178292	-10.47612063	-0.70405940
C	11.19080181	-9.28254506	-3.19469150	H	7.11169604	-11.40505616	-0.95946115
H	10.65390530	-10.22644664	-3.19286198	N	6.97152651	-9.32339297	-0.49235398
C	12.47599735	-9.16984236	-2.66961150	C	7.94346969	-8.38344960	-0.21654511
H	12.94431909	-10.02405469	-2.19237872	H	7.70009117	-7.35797406	0.00514974
C	5.95151276	1.22004777	-5.08269957	C	5.14835226	-3.80656628	1.42702136
H	5.01133716	1.34343916	-5.62667053	H	4.72022355	-2.93229206	0.92249813
H	5.75470650	1.42948151	-4.02744825	H	4.46220424	-4.07226522	2.23575519
C	6.34696359	-0.26494500	-5.19268695	C	5.23742228	-4.96399904	0.48544159
O	5.69762407	-1.11336147	-4.58938133	N	5.23736333	-4.85834563	-0.89522621
O	7.35490757	-0.58453345	-5.99828526	H	5.20402658	-4.01480076	-1.46773929
H	7.48598465	-1.56345503	-6.00713330	C	5.21902874	-6.10165498	-1.42473487
C	5.27294754	-8.66442537	-9.72775120	H	5.19150789	-6.29875934	-2.48264440
H	6.02712781	-8.81631651	-10.50121901	N	5.20976836	-7.00726895	-0.45798614
H	4.83725672	-9.63784314	-9.49952551	C	5.21987445	-6.31309128	0.73580230
C	5.97505627	-8.04087690	-8.50515150	H	5.21397262	-6.82032165	1.68978190
O	6.45743224	-6.90954165	-8.50028541	C	5.96151124	-10.23323421	2.56689617
N	6.05986832	-8.87240550	-7.43057876	H	6.81441986	-9.85995174	1.99443681
H	6.42100635	-8.46790625	-6.57723092	H	5.34083854	-9.36391854	2.82686734
H	5.38901035	-9.63277330	-7.34491844	C	5.12586123	-11.16282613	1.72228411
C	3.38551962	-4.80805982	-6.42210605	N	4.67665553	-10.78725650	0.45389193
H	3.36476446	-3.83803913	-6.92356603	C	3.90300444	-11.77137236	-0.00056380
H	2.80897497	-4.68917866	-5.50111940	H	3.38042344	-11.77438804	-0.94481307
C	4.81667371	-5.11650395	-6.10182211	N	3.83067510	-12.76135532	0.90138695
C	5.21209991	-6.23663048	-5.20362318	H	3.33324997	-13.65545263	0.76981168
O	4.29216604	-6.98123365	-4.57698128	C	4.58882714	-12.39797765	1.99467433
C	6.52291128	-6.56877339	-5.00507921	H	4.63738914	-13.01629617	2.87903274
H	6.77953177	-7.40772407	-4.36500618	Cu	4.99171201	-9.03944642	-0.54777138
H	3.38184362	-6.56819656	-4.41614066	O	7.38453780	-10.23015528	-3.77280809
C	7.57720792	-5.81181675	-5.62496669	H	7.89501154	-11.00640915	-3.42786904
O	8.76285555	-6.14825690	-5.63745414	H	8.06976673	-9.52694609	-3.86448391
C	7.17130170	-4.43843203	-6.18668619	O	2.96536212	-8.75608755	-0.72568975
O	7.97096325	-3.51290250	-6.20747104	H	2.61743857	-9.13820910	-1.55471104
C	5.77217676	-4.28075756	-6.55890084	H	2.37077138	-9.14357112	0.00818006
H	5.53083202	-3.41575124	-7.16305406	O	4.98301957	-9.31706456	-2.78467475
C	-0.76255178	-1.41254733	-3.45753259	H	4.75340712	-8.56572590	-3.36334702
H	-1.02399500	-1.15406853	-2.42290124	H	5.86580565	-9.64819965	-3.09725793
H	-0.74786877	-0.47490122	-4.02152957	O	1.96046133	-6.26291294	-3.72059354
C	0.60830813	-2.04106361	-3.49564590	H	1.23030766	-6.78192882	-4.14477114
C	1.05533560	-2.90679150	-2.49134899	H	1.64858725	-5.34470006	-3.63516260
H	0.37736341	-3.18770128	-1.68856294	C	14.38916956	-7.43765933	-0.51369988
C	2.37337397	-3.37128439	-2.46356736	C	6.99596014	2.23724852	-5.62156476
H	2.72188936	-4.00923215	-1.65632147	C	4.17201602	-7.73719604	-10.29445683
C	3.27130906	-2.95694618	-3.45307578	C	2.65670241	-5.83051907	-7.32726425
O	4.57762869	-3.37274895	-3.37861461	C	-1.88314104	-2.29830870	-4.02843756
H	5.13243123	-2.71523661	-3.85842417	C	10.94038660	-8.74438910	1.53758595
				C	6.50300572	-3.40368329	2.05654156
				C	6.47869923	-10.83959860	3.86963647

1, Full				C	2.82485594	-2.16771381	-4.44997868
C	14.53230681	-7.88811508	-1.97540369	H	3.53493771	-1.87196408	-5.21313706
H	14.95580477	-8.89393407	-1.99292344	C	1.51273232	-1.70828903	-4.48168833
H	15.24778128	-7.22689527	-2.46514167	H	1.19491579	-1.06506311	-5.29863478
C	13.19339304	-7.92911841	-2.67367548	C	10.51322422	-8.45012734	0.07713569
C	12.56291757	-6.79616171	-3.20485894	H	11.27491157	-8.86014425	-0.58610934
H	13.05849682	-5.82956327	-3.17888246	H	10.51418150	-7.36926337	-0.08695407
C	11.27436922	-6.88196759	-3.72879895	C	9.16591070	-8.99563963	-0.25057973
H	10.77968767	-5.99215685	-4.10228000	N	8.91170238	-10.32157910	-0.57473123
C	10.60316959	-8.10939767	-3.73702835	H	9.60995844	-11.05280059	-0.70340075
O	9.31034513	-8.22385520	-4.19195949	C	7.57803857	-10.48167838	-0.70202362
H	9.13501293	-7.52373800	-4.85926331	H	7.09305476	-11.40758618	-0.96014721
C	11.22943343	-9.25824954	-3.25628642	N	6.96014707	-9.32998295	-0.48769838
H	10.69991911	-10.20516506	-3.27971641	C	7.93831257	-8.39482699	-0.21268732
C	12.50854416	-9.14914592	-2.71910508	H	7.69925492	-7.36940658	0.01531789
H	12.98416458	-10.01112177	-2.26531270	C	5.14532964	-3.80719325	1.43514926
C	5.94384485	1.23742929	-5.07014676	H	4.71509011	-2.93394647	0.93148612
H	5.00786056	1.35360665	-5.62340431	H	4.46460685	-4.07632187	2.24643183
H	5.73662642	1.47152083	-4.02290514	C	5.23301733	-4.96394877	0.49248781
C	6.34389722	-0.24480899	-5.14012665	N	5.19628520	-4.85489887	-0.88660132
O	5.71716009	-1.08394313	-4.50347833	H	5.11197267	-4.01388597	-1.45902361
O	7.34071576	-0.58251885	-5.95706395	C	5.20087857	-6.10032343	-1.41278864
H	7.48697857	-1.55609584	-5.90219421	H	5.12076351	-6.31121158	-2.46426627
C	5.28687077	-8.68067242	-9.73919805	N	5.24691513	-7.00437831	-0.44904165
H	5.97216933	-8.91094563	-10.55608389	C	5.25993203	-6.31301725	0.74335172
H	4.81648872	-9.60310989	-9.40638798	H	5.28135618	-6.82507878	1.69480276
C	6.05913190	-8.10262555	-8.54321898	C	5.95842390	-10.23090504	2.57077548
O	5.88386350	-8.50635297	-7.39598033	H	6.81188267	-9.86335240	1.99458333
N	6.92941057	-7.07130386	-8.78406131	H	5.34141294	-9.36037213	2.83158157
H	7.53255530	-6.82079988	-8.01047945	C	5.11841881	-11.15769101	1.73001330
H	7.39395316	-6.90181465	-9.67699937	N	4.65483548	-10.77165248	0.47139066
C	3.35787336	-4.80918383	-6.40504852	C	3.87550922	-11.74907448	0.01548912
H	3.31835551	-3.83098927	-6.88792054	H	3.33944856	-11.72910239	-0.92031004
H	2.79157183	-4.72847122	-5.47028679	N	3.81560358	-12.74956318	0.90810503
C	4.77439909	-5.11571103	-6.07309075	H	3.32216860	-13.64408047	0.77305020
C	5.09636305	-6.26222677	-5.17297079	C	4.58738273	-12.39697886	1.99657921
O	4.22583107	-6.82417223	-4.51725700	H	4.64474143	-13.02140754	2.87646996
C	6.51380417	-6.75675828	-5.12805689	Cu	4.96959129	-9.03465302	-0.54329740
H	6.51562548	-7.60579949	-5.85064609	O	7.41259268	-10.21092231	-3.77797377
H	6.76932979	-7.17416372	-4.14706381	H	7.89448030	-10.99761838	-3.42300987
C	7.56091446	-5.78577234	-5.58813816	H	8.10615457	-9.52109695	-3.86021106
O	8.73152047	-6.10407550	-5.72760400	O	3.01841753	-8.65809381	-0.61257391
C	7.12666623	-4.36866448	-5.96820530	H	2.56974280	-8.36382237	-1.44493003
O	7.92417686	-3.44328250	-5.92964973	H	2.35981835	-9.12090604	0.00000276
C	5.74659333	-4.23216465	-6.40119848	O	5.03569958	-9.30446044	-2.74788427
H	5.51344441	-3.32752547	-6.95242183	H	4.62263732	-8.68142576	-3.36919016
C	-0.76631327	-1.40905089	-3.45568405	H	5.90519048	-9.58946296	-3.12381488
H	-1.03797270	-1.14045688	-2.42670333	O	1.99069017	-7.43320438	-2.86190810
H	-0.74594237	-0.47734556	-4.02915244	H	1.30003422	-7.66449383	-3.51921299
C	0.60494422	-2.03830770	-3.46990814	H	2.64256799	-6.94143853	-3.38531849
C	1.03854259	-2.88693569	-2.44513112	C	14.39138004	-7.43846988	-0.51422723
H	0.35049847	-3.14702156	-1.64458635	C	6.99605566	2.24089701	-5.61993446
C	2.34873278	-3.36156405	-2.39831725	C	4.19409459	-7.72356203	-10.28479744
H	2.67915039	-3.99671085	-1.58275713	C	2.64493678	-5.83562890	-7.31384381
C	3.25267249	-2.96498114	-3.38522709	C	-1.88148991	-2.29952553	-4.02726648
O	4.57200656	-3.36673945	-3.29446835	C	10.93959164	-8.74774919	1.53625382
H	5.11852372	-2.66027845	-3.70488943	C	6.50286417	-3.40225047	2.05769965
				C	6.47779061	-10.84029310	3.87065415

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C	14.52813382	-7.89796765	-1.97298936	C	2.84944948	-2.08126457	-4.51382587
H	14.93839008	-8.91072576	-1.98474984	H	3.56708247	-1.69426266	-5.22657121
H	15.25708906	-7.25196125	-2.46342232	C	1.54263706	-1.60365142	-4.49136874
C	13.19292148	-7.91928021	-2.68022392	H	1.24369707	-0.85182485	-5.21642232
C	12.61825712	-6.78130414	-3.26296609	C	10.51278288	-8.44389106	0.08116253
H	13.15260117	-5.83512290	-3.25484559	H	11.27332723	-8.85236133	-0.58406781
C	11.33895348	-6.83592314	-3.81465732	H	10.51438864	-7.36240513	-0.07999486
H	10.88494920	-5.94273512	-4.22789117	C	9.16464141	-8.98669141	-0.24764741
C	10.62465645	-8.03694107	-3.80245736	N	8.90502404	-10.31379641	-0.56199925
O	9.33679298	-8.11485989	-4.28896765	H	9.59964928	-11.05193126	-0.67089080
H	9.23423415	-7.52420620	-5.06937899	C	7.57110998	-10.46724364	-0.70146364
C	11.19035186	-9.18877849	-3.26080999	H	7.08191096	-11.39507562	-0.94504584
H	10.62216786	-10.11433422	-3.26153231	N	6.96013541	-9.30827552	-0.50483371
C	12.46177319	-9.11395181	-2.69853828	C	7.94016978	-8.37625190	-0.23006722
H	12.88923152	-9.98281547	-2.20916887	H	7.70463194	-7.34639017	-0.01950714
C	5.95957220	1.21376696	-5.08481977	C	5.15038113	-3.80575978	1.42143066
H	5.01958321	1.32842808	-5.63197088	H	4.71302641	-2.92491816	0.93753870
H	5.75460292	1.42406505	-4.03211525	H	4.46909158	-4.09593728	2.22585177
C	6.37656283	-0.26502861	-5.19000021	C	5.24326200	-4.93917389	0.44821689
O	5.77208789	-1.12528455	-4.56072061	N	5.13206016	-4.80625091	-0.92545465
O	7.36364169	-0.57128820	-6.03109236	H	5.03973443	-3.95540824	-1.47872598
H	7.50669257	-1.54592978	-6.03367268	C	5.12478911	-6.04066954	-1.48006324
C	5.27413403	-8.66170863	-9.72275545	H	4.98382731	-6.22201786	-2.53248583
H	6.04363790	-8.79469634	-10.48781109	N	5.23493278	-6.96356734	-0.53830890
H	4.83939997	-9.64252146	-9.52416321	C	5.30303982	-6.29397013	0.66536761
C	5.95790245	-8.08280076	-8.46820289	H	5.37506530	-6.82384010	1.60432422
O	6.36645144	-6.92548884	-8.35654633	C	5.96470796	-10.22561782	2.56568146
N	6.13979631	-9.00687657	-7.49071421	H	6.82147799	-9.85267528	1.99750686
H	6.58646340	-8.71107871	-6.63578583	H	5.34888294	-9.35413094	2.82891425
H	5.49581847	-9.79253508	-7.43166387	C	5.12474961	-11.14479548	1.71260155
C	3.39597803	-4.84183592	-6.39801321	N	4.65075700	-10.74395512	0.45960003
H	3.32144787	-3.84303404	-6.83323481	C	3.87217034	-11.71982061	-0.00219280
H	2.87701449	-4.81070125	-5.43268442	H	3.32699927	-11.69170026	-0.93322630
C	4.83927195	-5.14879465	-6.17144604	N	3.82514706	-12.73412661	0.87668034
C	5.21630246	-6.31686723	-5.34029333	H	3.32619242	-13.62724135	0.74553385
O	4.37993856	-7.05837311	-4.82593402	C	4.60255377	-12.39011928	1.96407941
C	6.68056329	-6.55288520	-5.01713685	H	4.67383839	-13.02766770	2.83281619
H	6.88305069	-7.62240065	-4.94190558	Cu	4.96899618	-9.01084071	-0.57721635
H	6.82586246	-6.15299680	-4.00097351	O	7.49824186	-10.14644559	-3.82345897
C	7.67044020	-5.83575529	-5.90636863	H	7.97801284	-10.93604338	-3.46733342
O	8.77644734	-6.26481210	-6.16897933	H	8.18499418	-9.44600605	-3.88513984
C	7.21671061	-4.43146136	-6.31199844	O	3.01071829	-8.63684562	-0.64895290
O	8.00719578	-3.49888527	-6.32077089	H	2.57598612	-8.33799682	-1.48418925
C	5.79225135	-4.27766154	-6.58060960	H	2.35516982	-9.10381417	-0.03984848
H	5.51937852	-3.37016154	-7.10541016	O	5.06296805	-9.37793879	-2.79228527
C	-0.75155887	-1.42207838	-3.46439181	H	4.72267399	-8.70807143	-3.40975566
H	-0.99397300	-1.18223663	-2.42021525	H	5.97258994	-9.61300532	-3.10135973
H	-0.74821193	-0.47451760	-4.01224102	O	2.11939492	-7.37867194	-3.01292285
C	0.61894033	-2.05249466	-3.54082961	H	1.34183405	-7.56547229	-3.58353728
C	1.03245634	-3.04221962	-2.64185198	H	2.80051805	-7.11696586	-3.65368935
H	0.33260597	-3.40663399	-1.89646356	C	14.39005387	-7.43896886	-0.51325171
C	2.33404694	-3.53941920	-2.65191323	C	6.99768072	2.23788628	-5.62189081
H	2.63787907	-4.30847066	-1.94901599	C	4.17740879	-7.72804396	-10.28758186
C	3.25689275	-3.01917495	-3.56156592	C	2.64850336	-5.83529958	-7.31617048
O	4.56679977	-3.46231555	-3.50637564	C	-1.88162062	-2.30039813	-4.02835805
H	5.12803976	-2.75935207	-3.90350800	C	10.94046249	-8.74743076	1.53701736
				C	6.50296685	-3.40308929	2.05665990
				C	6.47772241	-10.83919261	3.86696261

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C	14.53295530	-7.89010394	-1.97163565	C	2.83333135	-2.12419552	-4.51039474
H	14.96154545	-8.89427499	-1.98700840	H	3.53917508	-1.78037920	-5.25732198
H	15.24502716	-7.22778142	-2.46509997	C	1.52566731	-1.65029641	-4.49584857
C	13.19415461	-7.94107084	-2.66430996	H	1.21147480	-0.94091002	-5.25739710
C	12.57168887	-6.81141822	-3.21202791	C	10.51157614	-8.44436614	0.08114271
H	13.07341886	-5.84817726	-3.19178456	H	11.27475720	-8.84989626	-0.58283786
C	11.28311289	-6.90116647	-3.73389066	H	10.50700170	-7.36281471	-0.07925334
H	10.78214565	-6.01845024	-4.11643788	C	9.16582489	-8.99255537	-0.24893164
C	10.61395602	-8.12728120	-3.73200562	N	8.90920630	-10.32048597	-0.56258293
O	9.32768760	-8.23410065	-4.21802746	H	9.60444236	-11.05786456	-0.66994606
H	9.23903337	-7.64462819	-4.99070610	C	7.57536172	-10.47590413	-0.70294542
C	11.22250449	-9.26869638	-3.21934912	H	7.08817390	-11.40444609	-0.94714034
H	10.68169906	-10.20992030	-3.21844299	N	6.96186883	-9.31851362	-0.50741620
C	12.49968715	-9.15695749	-2.67805386	C	7.93998661	-8.38532068	-0.23159258
H	12.96654879	-10.01080512	-2.20005488	H	7.70081554	-7.35629398	-0.02042402
C	5.96965664	1.20299135	-5.09482479	C	5.14689218	-3.80449321	1.43071601
H	5.02495616	1.32687228	-5.63180861	H	4.70876407	-2.92603546	0.94262755
H	5.77666440	1.39480858	-4.03648026	H	4.46893204	-4.08869795	2.24006389
C	6.38253296	-0.27192375	-5.23338042	C	5.23929245	-4.94431691	0.47038410
O	5.78742902	-1.15371691	-4.63305867	N	5.19996677	-4.81781830	-0.90751634
O	7.37644672	-0.55428895	-6.08813322	H	5.12946708	-3.96992519	-1.46720086
H	7.49031488	-1.52388715	-6.12827084	C	5.20428126	-6.05432378	-1.45531751
C	5.26287260	-8.67997849	-9.74437168	H	5.14011454	-6.23997047	-2.51389125
H	5.99048760	-8.85311211	-10.53873981	N	5.24928173	-6.97187722	-0.50332090
H	4.81168440	-9.64054727	-9.49523521	C	5.26522977	-6.29683512	0.69948506
C	6.01710091	-8.07599974	-8.54985716	H	5.28281268	-6.82033390	1.64460493
O	6.58145646	-6.98028139	-8.58218775	C	5.96069621	-10.22934093	2.56442392
N	6.05767928	-8.89002071	-7.46453034	H	6.81563064	-9.85907461	1.99094954
H	6.47774100	-8.53145461	-6.62003657	H	5.34636188	-9.35666077	2.82487027
H	5.36526427	-9.63030972	-7.37268227	C	5.11857434	-11.14983362	1.71337944
C	3.38109677	-4.84974220	-6.36858585	N	4.65373176	-10.75187240	0.45654152
H	3.30110492	-3.84642648	-6.79261401	C	3.87320667	-11.72582904	-0.00601748
H	2.85296004	-4.83791404	-5.41023997	H	3.33413522	-11.69804142	-0.94051446
C	4.82661967	-5.14958952	-6.16524983	N	3.81687361	-12.73621774	0.87691598
C	5.24250474	-6.27271227	-5.25572885	H	3.31808752	-13.62874081	0.74264186
O	4.39959615	-6.89245434	-4.58792302	C	4.58896110	-12.39195417	1.96729088
C	6.64900240	-6.63223541	-5.17930057	H	4.64820480	-13.02658848	2.83917531
H	6.92666946	-7.46032448	-4.53526640	Cu	4.96842896	-9.00983740	-0.57423036
H	9.19780827	-5.79336976	-6.83157137	O	7.42897167	-10.22233367	-3.79771314
C	7.52955416	-6.00881218	-5.99190794	H	7.91772761	-11.00483880	-3.43463912
O	8.80437874	-6.38486017	-6.15153577	H	8.11998000	-9.53000269	-3.87139912
C	7.17492802	-4.72469898	-6.68161572	O	3.01445579	-8.62731972	-0.63061429
O	8.09098509	-4.03430755	-7.11962775	H	2.57379812	-8.31879915	-1.46116045
C	5.77159080	-4.36878324	-6.73034363	H	2.36032612	-9.09810569	-0.02387451
H	5.52496260	-3.48425880	-7.30178463	O	5.02334630	-9.30981954	-2.79902014
C	-0.75564724	-1.42141345	-3.45642600	H	4.73808380	-8.58109832	-3.38266461
H	-1.01086793	-1.17285700	-2.41762413	H	5.91181894	-9.60373921	-3.11601186
H	-0.74505373	-0.47706568	-4.01025545	O	2.06558555	-7.35087333	-2.92565974
C	0.61535973	-2.05160227	-3.51171062	H	1.34832893	-7.56814922	-3.55874016
C	1.04475619	-2.98720865	-2.56283837	H	2.76430050	-6.97822618	-3.49120584
H	0.35546333	-3.31307028	-1.78838752	C	14.38979167	-7.43664537	-0.51210421
C	2.34850088	-3.48154284	-2.56460659	C	7.00497616	2.23116252	-5.62702481
H	2.67041508	-4.20371036	-1.82048203	C	4.17083108	-7.73410526	-10.28944009
C	3.25504823	-3.01443775	-3.51855720	C	2.64747282	-5.83330415	-7.31200352
O	4.56091150	-3.46227388	-3.46959550	C	-1.88073856	-2.30144687	-4.02805857
H	5.11915256	-2.79431483	-3.91995990	C	10.93945479	-8.74639160	1.53735551
				C	6.50350393	-3.40266733	2.05583768
				C	6.47775895	-10.83883504	3.86644029

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C	14.53603413	-7.88951385	-1.97122361	C	2.84917266	-2.04338260	-4.59229363
H	14.96781231	-8.89193422	-1.98593484	H	3.55452534	-1.62433973	-5.30040638
H	15.24658604	-7.22444210	-2.46325029	C	1.54560787	-1.56170871	-4.52328826
C	13.19742482	-7.94642824	-2.66543886	H	1.23737640	-0.77277134	-5.20404022
C	12.55849763	-6.82132046	-3.20205038	C	10.51002695	-8.44209308	0.07993147
H	13.05254173	-5.85313387	-3.18413676	H	11.26984843	-8.85093464	-0.58649794
C	11.26826292	-6.92080428	-3.71737419	H	10.51133853	-7.36077513	-0.08117093
H	10.75611710	-6.04302577	-4.09518288	C	9.16173617	-8.98540489	-0.24995893
C	10.60354697	-8.15337241	-3.71373401	N	8.90795413	-10.31068521	-0.57567362
O	9.32058920	-8.26784101	-4.17648907	H	9.60608177	-11.04346508	-0.69614797
H	9.16377146	-7.58085745	-4.88069884	C	7.57548755	-10.46729488	-0.72278874
C	11.23716501	-9.29248316	-3.21906570	H	7.09167283	-11.39429828	-0.97970369
H	10.71122790	-10.24207293	-3.23072588	N	6.95900073	-9.31265877	-0.51874719
C	12.51895482	-9.17012420	-2.69194023	C	7.93481240	-8.37968946	-0.23148671
H	13.00243199	-10.02212946	-2.22702260	H	7.69354703	-7.35253961	-0.01419520
C	5.94579439	1.24135641	-5.07823975	C	5.14346812	-3.80431449	1.43451042
H	5.01347160	1.35171364	-5.63899709	H	4.70492304	-2.92467136	0.94875420
H	5.73316905	1.47331039	-4.03158821	H	4.46702132	-4.08719299	2.24555717
C	6.35732993	-0.23027508	-5.14792526	C	5.22795261	-4.94379977	0.47173913
O	5.77325818	-1.08437845	-4.50033123	N	5.17814542	-4.81381687	-0.90682879
O	7.34659088	-0.55609688	-5.99590187	H	5.12174627	-3.95912484	-1.45257635
H	7.48106667	-1.51938298	-5.92782914	C	5.17562490	-6.04969274	-1.45962073
C	5.27319463	-8.66947820	-9.73075712	H	5.10449268	-6.23397030	-2.51801754
H	6.01682999	-8.83028244	-10.51228565	N	5.22161213	-6.96869409	-0.50970319
H	4.82850329	-9.63657629	-9.49106691	C	5.24852192	-6.29741209	0.69512100
C	5.99111781	-8.05603151	-8.51661898	H	5.26980671	-6.82535640	1.63776381
O	6.55050221	-6.95261188	-8.55937489	C	5.96590126	-10.22759267	2.56343916
N	5.99681404	-8.83399551	-7.41350850	H	6.82279992	-9.85746891	1.99251186
H	6.38057832	-8.45046834	-6.56002266	H	5.34979748	-9.35545154	2.82266941
H	5.32345667	-9.59373797	-7.33515373	C	5.12711680	-11.14892624	1.71165930
C	3.42917103	-4.86973544	-6.37190866	N	4.65764523	-10.75228831	0.45593678
H	3.38811864	-3.86844591	-6.80564536	C	3.87834764	-11.72813899	-0.00358054
H	2.90133848	-4.84597939	-5.41271902	H	3.33421407	-11.70190929	-0.93517029
C	4.85475444	-5.23277569	-6.15001590	N	3.82698905	-12.73895796	0.87929857
C	5.22736133	-6.35835995	-5.18877805	H	3.32938058	-13.63223361	0.74634329
O	4.31326222	-6.90501097	-4.53158803	C	4.60174303	-12.39236630	1.96691939
C	6.59318643	-6.72758215	-5.04901614	H	4.66680112	-13.02636719	2.83876913
H	6.84786601	-7.47660502	-4.30906230	Cu	4.96842579	-9.01965533	-0.60143957
H	8.87605885	-5.11578123	-7.33185284	O	7.41973064	-10.21784142	-3.80760411
C	7.56999842	-6.16816136	-5.86219052	H	7.90356801	-11.00021420	-3.44177544
O	8.80989028	-6.41115966	-5.94395973	H	8.11968085	-9.52976064	-3.88447013
C	7.13950943	-5.05821670	-6.78363182	O	3.00880197	-8.69643221	-0.68526894
O	8.07600009	-4.53485968	-7.49215896	H	2.55161232	-8.33173535	-1.48386869
C	5.83497410	-4.53566409	-6.79447939	H	2.35649816	-9.13176271	-0.05205435
H	5.62650825	-3.68056911	-7.41854098	O	5.03655000	-9.26678206	-2.81844768
C	-0.73865235	-1.43364596	-3.46296181	H	4.74854178	-8.53207007	-3.39529239
H	-0.96134822	-1.22065860	-2.40906257	H	5.92007392	-9.56847715	-3.14359620
H	-0.74772554	-0.47229135	-3.98634230	O	2.01764858	-7.30527823	-2.89436019
C	0.63338313	-2.05710853	-3.58408681	H	1.31019442	-7.53806173	-3.53299679
C	1.05887936	-3.09405444	-2.74420894	H	2.74464036	-7.00129428	-3.46543583
H	0.36929108	-3.49892006	-2.01068398	C	14.39079694	-7.43716599	-0.51167017
C	2.35618000	-3.59918180	-2.80229506	C	6.99949357	2.24081862	-5.62487471
H	2.66822126	-4.40955478	-2.15138849	C	4.17702507	-7.73429798	-10.29144033
C	3.26838284	-3.03570972	-3.69901814	C	2.66042914	-5.83329889	-7.31429786
O	4.56702873	-3.50198772	-3.69784491	C	-1.87836925	-2.30022510	-4.02855930
H	5.13648024	-2.78849135	-4.05846178	C	10.93923541	-8.74603885	1.53632891
				C	6.50253255	-3.40327007	2.05693662
				C	6.47862789	-10.83813835	3.86633090

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C	14.54590454	-7.89719141	-1.96074398	H	3.48886917	-1.89965979	-5.18466429
H	14.96309270	-8.90622763	-1.96669180	C	1.46674506	-1.71065326	-4.46123621
H	15.27606301	-7.24465010	-2.44323998	H	1.14075901	-1.12244884	-5.31658153
C	13.22223127	-7.92852851	-2.68168738	C	10.51954390	-8.44397706	0.08163044
C	12.60530786	-6.78692661	-3.21101515	H	11.27880206	-8.85219270	-0.58786084
H	13.11226212	-5.82608956	-3.16912565	H	10.52037250	-7.36172494	-0.07789435
C	11.32163641	-6.85214599	-3.74725483	C	9.17012579	-8.98690022	-0.25037416
H	10.83896009	-5.95968945	-4.12850192	N	8.92078490	-10.30973374	-0.58701482
C	10.63439997	-8.07687727	-3.77778321	H	9.61960037	-11.04138883	-0.71318364
O	9.36523587	-8.17680562	-4.24819488	C	7.58879962	-10.46880336	-0.73980163
H	9.10601056	-7.32385671	-4.74062169	H	7.10712136	-11.39515223	-1.00495235
C	11.25747753	-9.23488425	-3.30555333	N	6.97022089	-9.31887031	-0.52817530
H	10.71989612	-10.17855022	-3.35481709	C	7.94056480	-8.38556733	-0.22899375
C	12.53188124	-9.14299739	-2.75487908	H	7.68944669	-7.36110341	-0.00904684
H	13.00243187	-10.01300342	-2.30982281	C	5.13997395	-3.80520235	1.42493939
C	5.93010339	1.23083211	-5.08907047	H	4.71511289	-2.93285695	0.91356001
H	4.98739815	1.34560297	-5.63218085	H	4.45263685	-4.06606586	2.23392657
H	5.73331643	1.46932288	-4.04114557	C	5.22782556	-4.96354189	0.48328270
C	6.31576688	-0.26250990	-5.15614591	N	5.20834658	-4.85013590	-0.89570459
O	5.67247163	-1.07366211	-4.50265536	H	5.12924950	-4.00819978	-1.47313733
O	7.29649860	-0.61312314	-5.98053120	C	5.20138963	-6.09059923	-1.43181640
H	7.41659690	-1.60044829	-5.96979579	H	5.15219721	-6.29142378	-2.48978385
C	5.27466743	-8.68817747	-9.77780099	N	5.22130754	-6.99908084	-0.47056301
H	5.96221941	-8.89543178	-10.59633626	C	5.23226904	-6.31523844	0.72582086
H	4.79943584	-9.62696673	-9.49101957	H	5.23107724	-6.83401410	1.67458568
C	6.08450827	-8.06868419	-8.63169740	C	5.98426826	-10.22909299	2.56578015
O	6.82539317	-7.09377752	-8.80681931	H	6.84799727	-9.86964819	1.99605680
N	5.94042518	-8.65636720	-7.42808188	H	5.38080572	-9.34419836	2.81559412
H	6.36764605	-8.20491521	-6.62559330	C	5.13638673	-11.14760346	1.72321590
H	5.21526432	-9.35673709	-7.27774543	N	4.67984767	-10.76788463	0.45928453
C	3.33386227	-4.84942873	-6.33635890	C	3.89900900	-11.74670691	0.01136247
H	3.27491394	-3.85470942	-6.78464666	H	3.35110213	-11.72717233	-0.91879047
H	2.75784556	-4.81859891	-5.40227944	N	3.83120622	-12.74037144	0.91311758
C	4.76662651	-5.12759727	-6.01367377	H	3.32972371	-13.63243949	0.78831691
C	5.14578157	-6.28432638	-5.11216772	C	4.59950697	-12.38145701	1.99985375
O	4.23520222	-6.97671048	-4.57177340	H	4.66034757	-13.00220289	2.88207654
C	6.51637107	-6.55212209	-4.91198803	Cu	4.98680407	-9.03301911	-0.63608386
H	6.78436347	-7.42014962	-4.31685370	O	7.47018988	-10.12760321	-3.82589172
C	7.53443695	-5.73580866	-5.43678056	H	7.95741136	-10.89169344	-3.43531587
O	8.76095608	-5.99352019	-5.42672388	H	8.15916180	-9.43073988	-3.93552123
C	7.09995041	-4.37567924	-5.99905975	O	3.02747376	-8.78107339	-0.74573413
O	7.88346479	-3.42993164	-6.04148063	H	2.57085408	-8.36369156	-1.52471776
C	5.70944748	-4.24895557	-6.41130942	H	2.37970595	-9.15851562	-0.08045326
H	5.46328885	-3.36703497	-6.99180379	O	5.06338587	-9.20255494	-2.83935874
C	-0.81558886	-1.36599248	-3.45978790	H	4.75191924	-8.47959580	-3.42899480
H	-1.11351567	-1.07599480	-2.44270144	H	5.95138063	-9.48398660	-3.16807705
H	-0.79063766	-0.44554800	-4.05202407	O	2.03791213	-7.35188178	-2.88433293
C	0.56048280	-1.97737838	-3.42884004	H	2.77553614	-7.05248840	-3.45154301
C	1.00354377	-2.74323420	-2.34491690	H	1.34863921	-7.60096136	-3.53425531
H	0.31756282	-2.95277007	-1.52641244	C	14.38464166	-7.43948936	-0.50429676
C	2.31738488	-3.20080795	-2.26965429	C	6.97689843	2.22951988	-5.65407088
H	2.66156144	-3.77303866	-1.41348874	C	4.19656690	-7.71048370	-10.29547294
C	3.21756206	-2.87558459	-3.28643922	C	2.64652384	-5.85308460	-7.29060564
O	4.52930942	-3.26784109	-3.15928993	C	-1.90832152	-2.27937098	-4.03596531
H	5.09013610	-2.64251889	-3.66493213	C	10.94782148	-8.75177533	1.53823020
C	2.78281703	-2.15516770	-4.40302073	C	6.49473238	-3.40011475	2.05288109
				C	6.48422815	-10.84176033	3.87216301

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C	14.53745031	-7.89770320	-1.95967269	H	3.54906097	-1.84606098	-5.18132855
H	14.96687384	-8.90244862	-1.96621133	C	1.50348726	-1.69524364	-4.49084484
H	15.25748429	-7.23898258	-2.44698502	H	1.18289463	-1.09931706	-5.34147847
C	13.20881926	-7.94957552	-2.67256958	C	10.51783209	-8.44245064	0.08267613
C	12.57752862	-6.82091627	-3.21407514	H	11.27869389	-8.84805035	-0.58624699
H	13.07557045	-5.85473486	-3.18789548	H	10.51905526	-7.36052629	-0.07544788
C	11.29130958	-6.90596532	-3.74171275	C	9.17008086	-8.98476328	-0.25133511
H	10.79584209	-6.02390651	-4.13122539	N	8.92127860	-10.30885772	-0.58541601
C	10.61494681	-8.13742840	-3.74592679	H	9.62109740	-11.03761137	-0.71598983
O	9.34498236	-8.26018378	-4.20440335	C	7.59059091	-10.46682368	-0.74468449
H	9.08767230	-7.43312811	-4.74293879	H	7.11096004	-11.39149725	-1.01706131
C	11.24852545	-9.28023455	-3.25309004	N	6.97067605	-9.31552244	-0.53639401
H	10.71498302	-10.22610117	-3.27706482	C	7.94167318	-8.38171389	-0.23697752
C	12.52593730	-9.17021666	-2.71387741	H	7.69549080	-7.35514655	-0.02149781
H	12.99979088	-10.02756374	-2.24876397	C	5.13874779	-3.81427173	1.42731872
C	6.05877462	1.09026167	-5.19859622	H	4.70510486	-2.94052440	0.92644860
H	5.09750283	1.17470152	-5.71401934	H	4.45607284	-4.08741575	2.23680594
H	5.87188809	1.18017237	-4.12325350	C	5.22868214	-4.96618486	0.47741568
C	6.69850926	-0.27110391	-5.52810153	N	5.20417079	-4.84266086	-0.90077625
O	6.14479245	-1.32507166	-4.85646600	H	5.13984856	-3.99182853	-1.46393805
O	7.59098606	-0.47614823	-6.31647890	C	5.19100140	-6.07999711	-1.44511906
H	6.70612080	-2.09063299	-5.16003925	H	5.13596006	-6.27623679	-2.50279449
C	5.30180148	-8.67421634	-9.77538065	N	5.21106478	-6.99530762	-0.48965225
H	5.99653359	-8.86482515	-10.59248933	C	5.23058232	-6.31860355	0.71184094
H	4.83638917	-9.62143705	-9.49897170	H	5.23699634	-6.84334974	1.65669038
C	6.09626594	-8.06008589	-8.61710854	C	5.98575644	-10.22805402	2.56260358
O	6.81580165	-7.06453012	-8.76372058	H	6.84787837	-9.86398556	1.99630609
N	5.96205012	-8.68459742	-7.43094235	H	5.37468210	-9.34954589	2.81425776
H	6.37025457	-8.23905912	-6.61580466	C	5.14695607	-11.14985777	1.71164304
H	5.23643668	-9.38768232	-7.29716237	N	4.67911714	-10.75735819	0.45637245
C	3.32566183	-4.92686179	-6.28445615	C	3.89913339	-11.73323783	0.00140871
H	3.27922331	-3.91333824	-6.69028395	H	3.35645489	-11.70636911	-0.93093276
H	2.74389124	-4.92987185	-5.35465688	N	3.84456573	-12.74046231	0.88936329
C	4.75533931	-5.23957132	-5.97213549	H	3.35148253	-13.63574947	0.75835155
C	5.12939025	-6.41511856	-5.09420388	C	4.61992508	-12.39133004	1.97524532
O	4.21474599	-7.10676207	-4.56076852	H	4.68678243	-13.02235431	2.84951026
C	6.50085328	-6.70705023	-4.90503334	Cu	4.98405409	-9.03648143	-0.65064442
H	6.75963303	-7.59309977	-4.33386180	O	7.45063392	-10.18583824	-3.81213061
C	7.52344969	-5.88494070	-5.41472918	H	7.93646705	-10.96304207	-3.43995695
O	8.75125359	-6.13622732	-5.44617736	H	8.14854326	-9.49449476	-3.90991772
C	7.06918226	-4.49874907	-5.84617312	O	3.01903684	-8.81551445	-0.77928300
O	7.77596594	-3.51667462	-5.63550339	H	2.55642700	-8.36103105	-1.53319040
C	5.70639601	-4.36674838	-6.35073030	H	2.37625218	-9.17244710	-0.09833371
H	5.47491444	-3.47172742	-6.91887124	O	5.05194220	-9.28983177	-2.84148824
C	-0.78772427	-1.37055134	-3.49022642	H	4.73721655	-8.57504838	-3.44050224
H	-1.06441239	-1.07158828	-2.47047389	H	5.94185925	-9.57110489	-3.16753640
H	-0.76523184	-0.45543978	-4.09006755	O	2.02000630	-7.31537606	-2.87327856
C	0.58666440	-1.99378360	-3.47639377	H	2.76939290	-7.07245869	-3.45450264
C	1.01915866	-2.78821377	-2.40802101	H	1.32242886	-7.56611402	-3.51410817
H	0.31952862	-3.04251826	-1.61437985	C	14.38122524	-7.43649096	-0.50360075
C	2.34043419	-3.21829783	-2.31334323	C	7.00166405	2.23388784	-5.66017432
H	2.67880848	-3.80524227	-1.46572878	C	4.21235578	-7.70793276	-10.28991032
C	3.25335771	-2.83641199	-3.29758429	C	2.63461809	-5.87992739	-7.28648390
O	4.57995770	-3.16863110	-3.13414117	C	-1.89822362	-2.27896791	-4.04129870
H	5.12311540	-2.48463358	-3.57368391	C	10.94590953	-8.75126156	1.53922501
C	2.82749320	-2.11835577	-4.41692998	C	6.49259773	-3.40475982	2.05603808
				C	6.48513393	-10.84181402	3.86939791

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C	14.53956436	-7.90680749	-1.95822673	H	3.59932484	-2.13436487	-4.96553815
H	14.96224524	-8.91464543	-1.96368839	C	1.55171889	-1.85142505	-4.33798830
H	15.26347964	-7.25306067	-2.44630209	H	1.31764224	-1.18928542	-5.16961886
C	13.20954483	-7.94876864	-2.67027049	C	10.54106992	-8.42909450	0.08657832
C	12.59414174	-6.81567311	-3.21832091	H	11.31154708	-8.82701964	-0.57410867
H	13.10257478	-5.85515792	-3.19830021	H	10.53756694	-7.34616413	-0.06189637
C	11.30837622	-6.88900994	-3.74862382	C	9.20173335	-8.97460766	-0.25725802
H	10.82631010	-5.99981745	-4.13834266	N	8.96144859	-10.30163218	-0.58668956
C	10.61760205	-8.10864331	-3.74193854	H	9.66502930	-11.02623713	-0.71767730
O	9.34018743	-8.21714358	-4.20771889	C	7.62822232	-10.47574853	-0.70349728
H	9.09988282	-7.40481434	-4.73604286	H	7.15060526	-11.40519025	-0.96256751
C	11.22922689	-9.25692435	-3.23650424	N	7.00546001	-9.33106768	-0.47445940
H	10.68094909	-10.19395906	-3.23870128	C	7.96856438	-8.38413563	-0.20515340
C	12.50813174	-9.15936607	-2.69820928	H	7.70630120	-7.36315890	0.02285048
H	12.96624557	-10.01913731	-2.22088474	C	5.12753674	-3.83001282	1.43654519
C	5.92575969	1.23685039	-5.07365412	H	4.72018903	-2.97451423	0.88661669
H	4.93403126	1.50056982	-5.44375236	H	4.42957775	-4.04827329	2.25227400
H	5.92184187	1.31366260	-3.97980803	C	5.19619780	-5.01881246	0.52066009
C	6.16714259	-0.22058958	-5.47958485	N	5.02486982	-4.92009617	-0.84506975
O	5.24877091	-0.95435054	-5.80472300	H	4.67158596	-4.02464334	-2.20684109
O	7.43247805	-0.63972485	-5.42105138	C	5.02589126	-6.17761858	-1.29515825
H	7.46996180	-1.58839107	-5.68606937	H	4.90161127	-6.44783985	-2.33369231
C	5.28284490	-8.68397876	-9.78012355	N	5.17762754	-7.09038886	-0.31789158
H	5.97266055	-8.88494525	-10.59849712	C	5.28500957	-6.35903146	0.84671187
H	4.81331282	-9.62711913	-9.49882796	H	5.40595674	-6.83917895	1.80959478
C	6.08655209	-8.07019049	-8.62656612	C	5.96528977	-10.24293624	2.57848434
O	6.81685791	-7.08215732	-8.77399771	H	6.81734163	-9.87365136	2.00071979
N	5.94711653	-8.68798624	-7.43740359	H	5.35259628	-9.36562374	2.82921983
H	6.38024459	-8.26633919	-6.62647648	C	5.13264939	-11.18334622	1.74614330
H	5.23526307	-9.40497722	-7.30393473	N	4.70518390	-10.82590630	0.46903138
C	3.32684670	-4.83713628	-6.34790583	C	3.92651090	-11.80392787	0.02097515
H	3.28382301	-3.85095528	-6.81480020	H	3.41232860	-11.80408737	-0.92752480
H	2.72771900	-4.76411975	-5.43498851	N	3.83286571	-12.77859325	0.93997718
C	4.75849924	-5.10727130	-6.00266744	H	3.33629864	-13.67135199	0.81355354
C	5.16324530	-6.26268102	-5.15249133	C	4.58374823	-12.40915785	2.03563187
O	4.25192888	-7.07510589	-4.61721388	H	4.62188935	-13.01670247	2.92854899
C	6.48222546	-6.57949898	-4.95474524	Cu	5.02279195	-9.04884090	-0.47380749
H	6.74458743	-7.44358332	-4.35124381	O	7.44883617	-10.18128483	-3.80674182
C	7.51818841	-5.75135850	-5.49376678	H	7.94137260	-10.95586794	-3.43597991
O	8.72094768	-6.04060680	-5.50839422	H	8.13233025	-9.47658140	-3.87553259
C	7.09386033	-4.36825526	-6.02278803	O	3.00959249	-8.83557544	-0.70901275
O	7.91314408	-3.46250619	-6.08830067	H	2.75493310	-7.90610051	-0.84927834
C	5.69286123	-4.20953196	-6.38380293	H	2.39007826	-9.20987836	0.00104708
H	5.43251257	-3.29663263	-6.90534890	O	5.03649625	-9.46972882	-2.70880538
C	-0.77518698	-1.41607450	-3.44664671	H	4.69747916	-8.73711095	-3.25250257
H	-1.08064037	-1.08306794	-2.44515715	H	5.94567670	-9.66377822	-3.04339648
H	-0.69521698	-0.51656608	-4.06431523	O	1.99267795	-6.38629498	-3.55993081
C	0.57108947	-2.10328475	-3.36694612	H	1.75259632	-5.45156351	-3.40408227
C	0.91844039	-2.94104195	-2.30077878	H	1.24212590	-6.82567731	-4.02987447
H	0.19023027	-3.12739768	-1.51356259	C	14.38408868	-7.44366391	-0.50244655
C	2.18888479	-3.52103919	-2.20284698	C	6.98356541	2.23048290	-5.63744792
H	2.45777807	-4.14212164	-1.35325981	C	4.19617692	-7.71432013	-10.29753987
C	3.16643664	-3.23671604	-3.17837248	C	2.64343804	-5.85133042	-7.29835232
O	4.41177688	-3.75273059	-3.15159927	C	-1.90326472	-2.29235502	-4.02214883
H	3.36222882	-6.66425810	-4.36075449	C	10.94890575	-8.74880029	1.54398413
C	2.82740695	-2.39442308	-4.25085752	C	6.48362744	-3.41484119	2.06348567
				C	6.48280396	-10.84596619	3.87960863

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C	14.55924674	-7.90942121	-1.95558383	H	3.58630951	-2.11185154	-4.99086997
H	14.97047817	-8.92147965	-1.95097830	C	1.54623800	-1.81636649	-4.35713275
H	15.29494944	-7.26505118	-2.43801803	H	1.31201076	-1.14737255	-5.18322497
C	13.23907629	-7.93780066	-2.67953028	C	10.52743150	-8.43784156	0.08466218
C	12.63348216	-6.78775186	-3.19848896	H	11.29039517	-8.84452682	-0.58064811
H	13.14333528	-5.82929570	-3.14792940	H	10.52902016	-7.35538985	-0.06897184
C	11.35048651	-6.84585096	-3.73205721	C	9.17931685	-8.97751190	-0.25066458
H	10.86951834	-5.93740913	-4.07318848	N	8.93006989	-10.30545902	-0.57529533
C	10.66027376	-8.06262928	-3.76330485	H	9.62599162	-11.04068496	-0.68399367
O	9.38579410	-8.15441671	-4.25185455	C	7.59448859	-10.46627490	-0.70471518
H	9.13399893	-7.28638088	-4.61981610	H	7.10845167	-11.39489993	-0.95171653
C	11.25646111	-9.22599862	-3.28129189	N	6.97854509	-9.31525967	-0.49411854
H	10.69829842	-10.15683474	-3.29970144	C	7.94931803	-8.37622497	-0.21962662
C	12.53262653	-9.14491212	-2.73638624	H	7.69019300	-7.35284287	0.00231966
H	12.98112388	-10.01490429	-2.27113090	C	5.14157125	-3.81190010	1.40565733
C	5.92820064	1.24786166	-5.09036659	H	4.74212317	-2.95224365	0.85578115
H	4.93812061	1.52147645	-5.44783527	H	4.43491382	-4.03374549	2.21239170
H	5.93979058	1.32303578	-3.99713274	C	5.21413474	-4.99670700	0.48062434
C	6.15922850	-0.20733244	-5.49974107	N	5.06578687	-4.89824347	-0.88838533
O	5.23029076	-0.94626581	-5.78130762	H	4.65660924	-4.03005952	-2.25494169
O	7.43266283	-0.62752027	-5.50324870	C	5.05560289	-6.15940276	-1.33265321
H	7.44140781	-1.57656162	-5.76107479	H	4.93071483	-6.43432621	-2.36878139
C	5.28267118	-8.68057783	-9.77344318	N	5.18081161	-7.07015084	-0.35387526
H	5.97622363	-8.88157808	-10.58860797	C	5.28108168	-6.33859619	0.80898303
H	4.81061426	-9.62159152	-9.49019719	H	5.37863314	-6.81547000	1.77592299
C	6.08405981	-8.06327889	-8.61963206	C	5.97556479	-10.24110470	2.57296196
O	6.84311199	-7.09851195	-8.77516650	H	6.83171028	-9.87710131	1.99839888
N	5.91047058	-8.64799004	-7.41696924	H	5.36448480	-9.36264235	2.82086403
H	6.37485721	-8.24354343	-6.61499874	C	5.13761291	-11.17629851	1.74121119
H	5.19407433	-9.35934611	-7.27476034	N	4.68812201	-10.80759011	0.47562789
C	3.24255096	-4.81159430	-6.33511255	C	3.89786502	-11.78076605	0.03670976
H	3.18016250	-3.82253554	-6.79377408	H	3.35598067	-11.76393353	-0.89643210
H	2.62772649	-4.77834357	-5.42496177	N	3.82158113	-12.76487687	0.94857157
C	4.64475491	-5.05921041	-5.95927558	H	3.32264299	-13.65699080	0.82630930
C	4.98934772	-6.25336506	-5.11164348	C	4.59437526	-12.40454987	2.03253145
O	4.10783013	-6.99498300	-4.66109448	H	4.64619165	-13.01718158	2.92104492
C	6.39678870	-6.52469119	-4.84418659	Cu	4.97571136	-9.02607017	-0.51843765
H	6.66082378	-7.40317020	-4.26383572	O	7.47531520	-10.14419163	-3.82685637
C	7.29818006	-5.62566425	-5.27627378	H	7.93857302	-10.92192913	-3.42843150
O	8.62423373	-5.72894468	-5.14677419	H	8.16264761	-9.44764968	-3.86518628
C	6.92701288	-4.31655876	-5.90427737	O	3.00547226	-8.95852486	-0.81513210
O	7.85251142	-3.49854717	-6.04060073	H	2.56752462	-8.34078632	-1.45121370
C	5.56943348	-4.13080605	-6.29111707	H	2.36855447	-9.22000125	-0.08373074
H	5.31468834	-3.21075875	-6.79776931	O	5.03337486	-9.35235675	-2.79360408
C	-0.77657182	-1.39625612	-3.46037983	H	4.64432503	-8.65021493	-3.34618706
H	-1.07996957	-1.06547882	-2.45725571	H	5.92921218	-9.55437525	-3.14437364
H	-0.70314710	-0.49469922	-4.07794686	O	1.94262206	-7.27288213	-2.78440074
C	0.57130946	-2.07760115	-3.38682638	H	2.62680229	-6.76323371	-3.24593998
C	0.91459596	-2.93440125	-2.33137717	H	1.33447598	-7.54488295	-3.50226910
H	0.17849853	-3.13939804	-1.55577018	C	14.38812652	-7.43728600	-0.50454367
C	2.17417100	-3.52350920	-2.24314380	C	6.98044345	2.23463198	-5.66173267
H	2.42382425	-4.18645299	-1.42200304	C	4.19839785	-7.71083467	-10.29585920
C	3.14691240	-3.23474996	-3.21887926	C	2.62849473	-5.85146736	-7.29936037
O	4.39503804	-3.76148309	-3.20118764	C	-1.90144936	-2.27878598	-4.03342126
H	8.90995551	-4.81026580	-5.38693343	C	10.95021395	-8.75065360	1.54204120
C	2.81702546	-2.37253989	-4.27670461	C	6.49160300	-3.40240112	2.05112077
				C	6.48579281	-10.84502970	3.87697272

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C	14.54233553	-7.90131422	-1.96062274	H	3.51026610	-2.01393481	-5.22140323
H	14.95287122	-8.91430922	-1.96582208	C	1.49770015	-1.77651480	-4.48855620
H	15.27799559	-7.25590099	-2.44245791	H	1.17804894	-1.19704295	-5.35229673
C	13.21786783	-7.92279735	-2.68329266	C	10.52612467	-8.43527483	0.08408718
C	12.61403455	-6.77462251	-3.21224364	H	11.28198888	-8.85211151	-0.58323418
H	13.12774544	-5.81791450	-3.16507961	H	10.54299966	-7.35349373	-0.07248311
C	11.33283482	-6.82761598	-3.75404968	C	9.16945908	-8.95449404	-0.25158155
H	10.85624756	-5.92703810	-4.12215401	N	8.90245018	-10.27745725	-0.57928287
C	10.63597389	-8.04411028	-3.78925266	H	9.59118657	-11.01766335	-0.69726751
O	9.37034227	-8.13729684	-4.28067326	C	7.56725332	-10.41720540	-0.72835212
H	9.11101445	-7.27727983	-4.72732797	H	7.07190094	-11.33786697	-0.98766164
C	11.23678740	-9.20679016	-3.30085496	N	6.96626179	-9.25638600	-0.52130294
H	10.68352204	-10.14084137	-3.32899256	C	7.94876125	-8.33368082	-0.23335583
C	12.50976640	-9.12800474	-2.74504968	H	7.70541289	-7.30447667	-0.02154578
H	12.95948560	-10.00099960	-2.28438333	C	5.14311300	-3.78276376	1.38124764
C	5.90938373	1.27013160	-5.08794667	H	4.73496456	-2.89266832	0.88677225
H	4.97949897	1.38841936	-5.65081325	H	4.44196695	-4.05684242	2.17626690
H	5.70207172	1.55934561	-4.05501101	C	5.22134427	-4.91254657	0.38920426
C	6.26793287	-0.22557994	-5.10203223	N	5.11448122	-4.76606459	-0.98595120
O	5.56984194	-0.82138694	-4.15113538	H	4.80354978	-3.73294245	-2.35416735
O	6.99866471	-0.81725728	-5.89655942	C	5.10236453	-6.01918076	-1.46367967
H	7.47304501	-2.42148556	-5.90813094	H	5.01866963	-6.26194072	-2.51130395
C	5.28332486	-8.68028436	-9.77193143	N	5.18136195	-6.96169541	-0.50749793
H	5.97679924	-8.88237127	-10.58690327	C	5.25276857	-6.26341267	0.67544765
H	4.81323865	-9.62228660	-9.48884199	H	5.30888529	-6.76884352	1.63090495
C	6.08152973	-8.05765567	-8.62002552	C	5.99003992	-10.22647850	2.56369348
O	6.81187066	-7.06933729	-8.77753131	H	6.85576866	-9.86004421	2.00410364
N	5.93282274	-8.65449982	-7.42242921	H	5.38003727	-9.34705186	2.81314075
H	6.37642534	-8.22928975	-6.61669067	C	5.15344208	-11.14170056	1.70323129
H	5.22316144	-9.37236174	-7.27888730	N	4.68364572	-10.73005303	0.45479669
C	3.32408081	-4.81974088	-6.36277228	C	3.90742312	-11.70126499	-0.01405200
H	3.26064528	-3.83541692	-6.83103350	H	3.35648253	-11.65334153	-0.94085548
H	2.74462194	-4.77505518	-5.42989580	N	3.85700143	-12.72559979	0.85733629
C	4.73634430	-5.08256598	-5.99939104	H	3.36177587	-13.61818661	0.72013570
C	5.10388459	-6.29404330	-5.14918041	C	4.63263587	-12.38968741	1.94829417
O	4.17461845	-7.00476835	-4.70083910	H	4.70256426	-13.03508331	2.81158075
C	6.47244637	-6.54660437	-4.92274922	Cu	4.97212770	-8.94589835	-0.59104689
H	6.74614082	-7.43421194	-4.36263654	O	7.49410813	-10.12520491	-3.84205269
C	7.47530566	-5.67451164	-5.36273203	H	7.96759396	-10.89447141	-3.44233304
O	8.71135261	-5.86746998	-5.35727668	H	8.18244015	-9.42780606	-3.92616452
C	6.99512966	-4.31425903	-5.82864625	O	2.99550695	-8.88157824	-0.82203249
O	7.84833706	-3.35823380	-5.76265463	H	2.54309359	-8.29357295	-1.47817708
C	5.67012069	-4.13261585	-6.28477650	H	2.36598839	-9.17251890	-0.09860366
H	5.41113893	-3.21205966	-6.79488768	O	5.04752811	-9.31342507	-2.84910574
C	-0.78217571	-1.38098411	-3.47169805	H	4.71494774	-8.59168241	-3.41575083
H	-1.06560895	-1.08264074	-2.45308377	H	5.95902459	-9.52375582	-3.15785722
H	-0.75081121	-0.46253500	-4.06827156	O	1.98878445	-7.25645449	-2.84813796
C	0.59166700	-2.01316255	-3.44811264	H	2.74866045	-6.96836607	-3.38400362
C	1.04137479	-2.76621379	-2.35589639	H	1.33338676	-7.53707098	-3.51976317
H	0.35803221	-2.96438478	-1.53221876	C	14.38421882	-7.43929180	-0.50436655
C	2.34704893	-3.24871171	-2.27770883	C	6.98475304	2.22156741	-5.67093815
H	2.68160301	-3.82015858	-1.41897713	C	4.19820846	-7.71290339	-10.29688928
C	3.25304421	-2.96290206	-3.30944232	C	2.64831526	-5.85152959	-7.29479021
O	4.56229075	-3.35532960	-3.27433154	C	-1.89804392	-2.28103920	-4.03481388
H	5.62783027	-1.80297313	-4.07190917	C	10.94855446	-8.75041226	1.54093725
C	2.80767173	-2.24283867	-4.42685834	C	6.49172004	-3.40022156	2.04803384
				C	6.48371343	-10.84411543	3.87248227

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C	14.53434662	-7.90623640	-1.96069993	H	3.56828983	-2.07938907	-5.05388183
H	14.95131233	-8.91667146	-1.96757511	C	1.52289280	-1.78786358	-4.42607225
H	15.26180458	-7.25629594	-2.44916774	H	1.25250011	-1.16222234	-5.27318780
C	13.20389826	-7.93698917	-2.67399666	C	10.51569069	-8.43924251	0.08549832
C	12.59988823	-6.79855362	-3.22428351	H	11.28038604	-8.83424500	-0.58461909
H	13.11642670	-5.84233664	-3.20122371	H	10.50669560	-7.35679150	-0.06850144
C	11.31651461	-6.85907452	-3.76159158	C	9.17221024	-8.99351811	-0.25130093
H	10.84476647	-5.96715646	-4.15713325	N	8.93491490	-10.32123604	-0.58023248
C	10.61355078	-8.07305147	-3.76396257	H	9.64007397	-11.04686497	-0.69931941
O	9.33980466	-8.16604162	-4.23451106	C	7.60560052	-10.49238026	-0.73794253
H	9.09537214	-7.33851782	-4.75724812	H	7.13462680	-11.42167935	-1.00956373
C	11.21463771	-9.22709216	-3.25376395	N	6.97533594	-9.34601302	-0.53522772
H	10.66078598	-10.16116920	-3.26026815	C	7.93769340	-8.40174553	-0.24093159
C	12.49262252	-9.14182409	-2.70874689	H	7.68128419	-7.37628340	-0.03183268
H	12.94231350	-10.00751321	-2.23294529	C	5.13515603	-3.82308666	1.44068599
C	5.92717011	1.23736434	-5.08572397	H	4.72726206	-2.96358157	0.89635808
H	4.93288443	1.51422151	-5.43928714	H	4.43587358	-4.04383361	2.25258886
H	5.92710813	1.30458513	-3.99244818	C	5.21024248	-5.01320163	0.53366033
C	6.14001319	-0.23254169	-5.50215707	N	5.03454410	-4.92800794	-0.83301009
O	5.16854968	-0.94896165	-5.70581012	H	4.89124360	-4.11290873	-1.44040530
O	7.39080020	-0.66229095	-5.58119038	C	4.99670669	-6.17519651	-1.34204590
H	7.42564236	-1.63787509	-5.81999865	H	4.80007486	-6.39296322	-2.37963971
C	5.27381561	-8.69319984	-9.78220581	N	5.15595580	-7.06779035	-0.37860670
H	5.95930799	-8.90050667	-10.60238484	C	5.28379914	-6.36075519	0.79907479
H	4.79531328	-9.63058426	-9.49650564	H	5.41365151	-6.85991225	1.74773023
C	6.09192617	-8.08283640	-8.63894707	C	5.98033391	-10.23939736	2.56926824
O	6.85087189	-7.12406607	-8.80543526	H	6.83999412	-9.87794224	1.99746997
N	5.93462030	-8.67152357	-7.43502393	H	5.36900369	-9.36045299	2.81760804
H	6.39535505	-8.25121505	-6.64192535	C	5.13944096	-11.17105261	1.73327255
H	5.19081982	-9.34932893	-7.27431338	N	4.68416613	-10.80462213	0.46762421
C	3.32292204	-4.86767950	-6.32044956	C	3.89515096	-11.78147414	0.03101939
H	3.31165525	-3.87552193	-6.77959151	H	3.35366349	-11.77039838	-0.90263596
H	2.70002276	-4.80875079	-5.41703522	N	3.82188860	-12.76317669	0.94454947
C	4.73593478	-5.19296351	-5.93122044	H	3.32566992	-13.65697306	0.82212598
C	5.06633560	-6.30647531	-5.11166070	C	4.59568301	-12.39908847	2.02537227
O	4.24468467	-7.13187564	-4.60531031	H	4.65101413	-13.01031404	2.91462518
C	6.52198538	-6.47380450	-4.72298872	Cu	4.98559927	-9.09315200	-0.63925905
H	6.57204258	-6.19284671	-3.66031303	O	7.48382840	-10.14885821	-3.82745011
C	7.55637109	-5.61217137	-5.41566757	H	7.96574777	-10.92654847	-3.45344971
O	8.73356166	-5.99576028	-5.50027404	H	8.16990362	-9.44560593	-3.89907409
C	7.09289843	-4.29273955	-5.89282311	O	3.01716253	-8.96659274	-0.85852055
O	7.89127955	-3.32559605	-6.05245426	H	2.57829042	-8.42205521	-1.56574092
C	5.70955575	-4.23893299	-6.22332247	H	2.37586900	-9.22739131	-0.13596771
H	5.40875531	-3.33169268	-6.73683163	O	5.09759254	-9.23528556	-2.84341399
C	-0.78763096	-1.36721537	-3.48757184	H	4.78372370	-8.53575128	-3.46342140
H	-1.08550092	-1.04215340	-2.48122482	H	5.99049201	-9.51756108	-3.15749689
H	-0.73399216	-0.47309089	-4.11407104	O	2.06192311	-7.31279166	-2.88984706
C	0.55872645	-2.03050183	-3.41994324	H	2.79627718	-7.11688223	-3.51127700
C	0.89985416	-2.85402521	-2.31789555	H	1.33715820	-7.56250109	-3.50076015
H	0.14727903	-3.03636731	-1.55445914	C	14.38387106	-7.44217849	-0.50394339
C	2.15562712	-3.39638901	-2.19755171	C	6.98045380	2.23113890	-5.64815653
H	2.42164458	-4.03429776	-1.36111104	C	4.19682617	-7.71090759	-10.29528927
C	3.17359469	-3.10956273	-3.18984640	C	2.64237896	-5.85586991	-7.29400190
O	4.36324576	-3.51744612	-3.06624523	C	-1.90125346	-2.27386030	-4.04403071
H	6.80185134	-7.53264134	-4.74134493	C	10.94647006	-8.75005087	1.54055139
C	2.79323147	-2.30549004	-4.33240364	C	6.48758897	-3.41067960	2.06598617
				C	6.48457500	-10.84471779	3.87620280

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C	14.54033163	-7.91057536	-1.95816669	H	3.57832303	-2.12133299	-5.00021661
H	14.94141009	-8.92773038	-1.95737516	C	1.53955438	-1.82316982	-4.36332915
H	15.28377850	-7.27540318	-2.44120804	H	1.30072655	-1.16125129	-5.19279451
C	13.21675152	-7.91861896	-2.68389644	C	10.52999071	-8.43714913	0.08454564
C	12.62602944	-6.75984459	-3.20647169	H	11.29335962	-8.84335730	-0.58121327
H	13.15210434	-5.80972294	-3.15729416	H	10.53253297	-7.35480516	-0.07030441
C	11.34561839	-6.79570477	-3.74998299	C	9.18239196	-8.97641297	-0.25404036
H	10.87613045	-5.88545564	-4.10281158	N	8.93254617	-10.30228338	-0.58337043
C	10.63045179	-8.00163833	-3.78836234	H	9.63002036	-11.03431078	-0.70270935
O	9.36363171	-8.07178124	-4.27926968	C	7.59829834	-10.46099889	-0.72163580
H	9.10735648	-7.18868401	-4.67734826	H	7.11369646	-11.38748110	-0.97975324
C	11.21493726	-9.17334536	-3.30160613	N	6.98199958	-9.31023067	-0.50734600
H	10.64931676	-10.09993044	-3.32919710	C	7.95377569	-8.37376539	-0.22560727
C	12.49032309	-9.11384343	-2.74812947	H	7.70048295	-7.34878897	-0.00871005
H	12.92479338	-9.99544513	-2.28953466	C	5.14144758	-3.80087640	1.39970453
C	5.92197570	1.25470581	-5.08145374	H	4.74088878	-2.93252152	0.86507857
H	4.92749327	1.52695253	-5.43308933	H	4.43611596	-4.03345775	2.20524372
H	5.93278524	1.32641613	-3.98714314	C	5.20961993	-4.97270473	0.46066424
C	6.14535304	-0.20281751	-5.49083517	N	5.03486201	-4.87520716	-0.90356620
O	5.21949106	-0.94262808	-5.77171654	H	4.66059158	-4.01879561	-2.21696873
O	7.41761653	-0.63150288	-5.49556925	C	5.03627225	-6.13817383	-1.35252253
H	7.41539096	-1.56887223	-5.77609876	H	4.91445348	-6.41025145	-2.38953532
C	5.28100735	-8.68050334	-9.77170376	N	5.18483246	-7.04849918	-0.37646061
H	5.97291945	-8.88471431	-10.58736674	C	5.29234335	-6.32216287	0.78112189
H	4.80929323	-9.62136614	-9.48713701	H	5.41213891	-6.79949905	1.74406896
C	6.08016746	-8.05557801	-8.61875422	C	5.97589196	-10.23731356	2.57226071
O	6.82849077	-7.08299743	-8.78482456	H	6.83252968	-9.87018459	2.00025249
N	5.91219949	-8.63593574	-7.41547225	H	5.36158669	-9.36088107	2.82315924
H	6.34155597	-8.19860655	-6.60780957	C	5.13886638	-11.16828368	1.73260373
H	5.19444059	-9.34569150	-7.27339557	N	4.68826822	-10.79191624	0.46735152
C	3.27385116	-4.84831540	-6.30570445	C	3.90115996	-11.76516834	0.02195903
H	3.21713600	-3.84998276	-6.74407503	H	3.36119134	-11.74572869	-0.91208473
H	2.66508410	-4.83728835	-5.38750284	N	3.82865505	-12.75694169	0.92595083
C	4.67619162	-5.12505016	-5.94721388	H	3.32872510	-13.64790960	0.80023544
C	5.06081147	-6.30501861	-5.08944108	C	4.59732616	-12.39974990	2.01361101
O	4.16007603	-7.04682618	-4.62422941	H	4.65160272	-13.01953313	2.89668979
C	6.44517402	-6.54239502	-4.85763974	Cu	4.98728214	-9.02592758	-0.56083919
H	6.72807337	-7.38606623	-4.23870959	O	7.51179567	-10.10496979	-3.84106005
C	7.40985532	-5.67538513	-5.35222166	H	7.99056263	-10.86950640	-3.44027421
O	8.68012269	-5.75997086	-5.27900539	H	8.18565877	-9.39379815	-3.91815686
C	6.93846283	-4.44298234	-6.03562285	O	3.01141179	-8.93309687	-0.82258782
O	7.87122311	-3.56635723	-6.33822242	H	2.57024364	-8.32943551	-1.47161089
C	5.61282421	-4.20901329	-6.35457035	H	2.37395823	-9.20414292	-0.09556768
H	5.34509352	-3.30793318	-6.88909910	O	5.07080457	-9.30903165	-2.82512110
C	-0.77915985	-1.40096609	-3.45502045	H	4.72495376	-8.59752361	-3.39969669
H	-1.08418888	-1.07753708	-2.45079145	H	5.97380418	-9.52991004	-3.15197286
H	-0.70576919	-0.50015615	-4.07122312	O	1.99198517	-7.24754856	-2.82394098
C	0.56963076	-2.07766244	-3.38230606	H	2.74149636	-6.98635505	-3.39046661
C	0.92039095	-2.92395827	-2.31529754	H	1.31663933	-7.52926008	-3.47404952
H	0.18563610	-3.12224581	-1.53850283	C	14.38422459	-7.43897269	-0.50443601
C	2.17841339	-3.50471431	-2.22083736	C	6.97568446	2.23623870	-5.65677603
H	2.43238116	-4.16716637	-1.40151579	C	4.19706542	-7.71014561	-10.29624230
C	3.15313385	-3.21133093	-3.20081990	C	2.63541138	-5.85481525	-7.29109835
O	4.40269838	-3.69044035	-3.16506979	C	-1.90204747	-2.28163345	-4.03369143
H	8.70322897	-4.00665662	-6.02577506	C	10.94939098	-8.75085929	1.54236610
C	2.80958943	-2.37186460	-4.28143331	C	6.49222861	-3.40167465	2.04951945
				C	6.48445742	-10.84480530	3.87642831

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C	14.53648362	-7.90105873	-1.96308028	H	3.53720118	-1.67838103	-5.22712404
H	14.94590020	-8.91511363	-1.96955725	C	1.51349582	-1.57341941	-4.48991826
H	15.27210975	-7.25769570	-2.44797698	H	1.21420141	-0.82282175	-5.21780218
C	13.21036583	-7.91975951	-2.68583978	C	10.50797368	-8.45214386	0.08275538
C	12.63178605	-6.77802504	-3.25668700	H	11.29257739	-8.81713892	-0.58195730
H	13.15775407	-5.82752188	-3.22881546	H	10.46151219	-7.36974354	-0.06718202
C	11.35649358	-6.83159733	-3.81752025	C	9.18992275	-9.05629932	-0.27725213
H	10.89821068	-5.93482100	-4.22037102	N	9.00048532	-10.40031866	-0.57074059
C	10.64254115	-8.03450984	-3.82059362	H	9.72200344	-11.11540112	-0.63563960
O	9.37120689	-8.12445457	-4.31561103	C	7.68368490	-10.60081503	-0.80525326
H	9.19103347	-7.40153340	-4.95956597	H	7.25412401	-11.55067395	-1.07551111
C	11.21214039	-9.18956416	-3.28344457	N	7.01815363	-9.46866967	-0.68911243
H	10.64048654	-10.11202124	-3.28470299	C	7.94251360	-8.49720304	-0.36446454
C	12.47946355	-9.11460467	-2.71568347	H	7.64590425	-7.47502170	-0.20534976
H	12.90611855	-9.98367928	-2.22501157	C	5.13812238	-3.77693448	1.43191901
C	5.94656545	1.21424344	-5.10145375	H	4.72582238	-2.89974879	0.91792045
H	4.99795649	1.33154049	-5.63160433	H	4.44460698	-4.02431654	2.24130762
H	5.76263396	1.42184009	-4.04331099	C	5.22830857	-4.93948850	0.50670935
C	6.36204311	-0.26466335	-5.21377747	N	5.04950450	-4.86906357	-0.86296179
O	5.75368508	-1.12148071	-4.58646798	H	4.91962975	-4.04193026	-1.43812302
O	7.34926306	-0.56668962	-6.05434973	C	5.10515489	-6.13603240	-1.35681320
H	7.49226254	-1.54600330	-6.06878959	H	4.90570985	-6.40395704	-2.38080553
C	5.28070099	-8.68989559	-9.78286153	N	5.31647415	-7.00271859	-0.38524232
H	5.96764826	-8.89109235	-10.60366701	C	5.38880515	-6.27649219	0.77443823
H	4.80334060	-9.62989524	-9.50774210	H	5.55447493	-6.75151727	1.73152469
C	6.10300489	-8.10452415	-8.62933629	C	5.98413826	-10.23527639	2.57192055
O	6.78481427	-7.07333016	-8.73943899	H	6.84455684	-9.89289621	1.98880298
N	6.07067389	-8.82891873	-7.49633269	H	5.39352926	-9.34420430	2.82023988
H	6.55788982	-8.48226221	-6.68207093	C	5.12267341	-11.15281537	1.74914571
H	5.33167550	-9.51457559	-7.34037780	N	4.63657314	-10.75042652	0.51132172
C	3.35411696	-4.85644433	-6.35493750	C	3.85298927	-11.72574942	0.06641135
H	3.23949478	-3.84593443	-6.75262676	H	3.29613602	-11.69949563	-0.85779202
H	2.83930875	-4.88682170	-5.38409703	N	3.81223327	-12.74254260	0.94622501
C	4.80190269	-5.11190049	-6.11580406	H	3.32403845	-13.63857565	0.81065143
C	5.21637830	-6.37928722	-5.42891465	C	4.60611056	-12.39814167	2.02036206
O	4.51946676	-7.36908087	-5.40393074	H	4.69094895	-13.03513128	2.88873031
C	6.58710911	-6.35639144	-4.74495003	Cu	4.97913592	-9.21537307	-0.87915338
H	6.88483229	-7.36208088	-4.44685076	O	7.43494022	-10.12692370	-3.87909385
C	7.58702510	-5.65618572	-5.61935995	H	7.89067405	-10.88712592	-3.45229211
O	8.67417632	-6.10325514	-5.94626333	H	8.11911843	-9.43087936	-3.91113807
C	7.13016405	-4.28078631	-6.11010883	O	3.02616370	-8.70362685	-0.69691624
O	7.93000509	-3.35352310	-6.18767311	H	2.58373360	-8.34923600	-1.50710295
C	5.72104197	-4.16766730	-6.43200988	H	2.38483951	-9.14522769	-0.07038133
H	5.42813618	-3.25335952	-6.93418192	O	4.92680668	-8.88726403	-2.76461426
C	-0.78293684	-1.39034335	-3.47014791	H	5.73215476	-9.23645691	-3.18733621
H	-1.03415192	-1.14651880	-2.42814525	H	6.45044115	-5.75381494	-3.83058434
H	-0.78251680	-0.44560118	-4.02223089	O	2.70284691	-7.45429271	-3.07213040
C	0.58951062	-2.01466482	-3.53757799	H	3.52075746	-8.01168444	-3.21402769
C	0.99842499	-3.00738699	-2.63837958	H	2.07308187	-7.69359056	-3.77324422
H	0.29258364	-3.37023501	-1.89711168	C	14.38297590	-7.43836230	-0.50579197
C	2.29465726	-3.51691024	-2.64793285	C	6.98154840	2.23364417	-5.65516096
H	2.59565483	-4.29768421	-1.95766086	C	4.20168359	-7.70906077	-10.29403578
C	3.21995918	-2.99937746	-3.55782385	C	2.64556986	-5.85379954	-7.29851792
O	4.52464414	-3.44305940	-3.49734809	C	-1.90286761	-2.27897455	-4.03754686
H	5.09122780	-2.74822677	-3.89123235	C	10.94466338	-8.75162324	1.53924497
C	2.81744191	-2.06084872	-4.51294047	C	6.49837246	-3.39376507	2.05824946
				C	6.48620977	-10.84621601	3.87643289

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C	14.56438953	-7.90987584	-1.94986567	H	3.48360481	-1.91695339	-5.22511591
H	14.97206648	-8.92349448	-1.94361878	C	1.46839078	-1.70869509	-4.48067610
H	15.30521364	-7.26817700	-2.42841974	H	1.13910526	-1.11339920	-5.32905643
C	13.25019520	-7.93425792	-2.68111012	C	10.51026384	-8.45005986	0.08528701
C	12.65069201	-6.78346128	-3.20477263	H	11.27174117	-8.85426990	-0.58360532
H	13.16364972	-5.82677270	-3.14978262	H	10.50778597	-7.36825088	-0.07341863
C	11.37282331	-6.84100994	-3.75104003	C	9.16098696	-8.99715686	-0.25308770
H	10.89350052	-5.93345089	-4.09989593	N	8.91652578	-10.31541863	-0.61743028
C	10.68130447	-8.05830223	-3.79049944	H	9.61355743	-11.04736645	-0.73390312
O	9.41773740	-8.15435515	-4.28770457	C	7.58653789	-10.46515841	-0.80945306
H	9.19060207	-7.31565571	-4.73593072	H	7.11491540	-11.37871827	-1.12545786
C	11.27339310	-9.22175045	-3.29833131	N	6.96452572	-9.32316989	-0.58310271
H	10.71334610	-10.15067610	-3.33088891	C	7.93059520	-8.39734192	-0.24677406
C	12.54430648	-9.14091752	-2.74216089	H	7.67943326	-7.37598546	-0.01566584
H	12.99330141	-10.00978716	-2.27426656	C	5.13296063	-3.78403951	1.43666782
C	5.94045395	1.21811074	-5.09790286	H	4.70828782	-2.90384019	0.93820495
H	4.99264273	1.33479719	-5.63138922	H	4.44937709	-4.04924140	2.24802026
H	5.75196565	1.43876491	-4.04375936	C	5.21609715	-4.93392301	0.49233921
C	6.33739911	-0.26998982	-5.18823570	N	5.18927533	-4.81840446	-0.88546568
O	5.69786398	-1.10331766	-4.56107532	H	5.11095280	-3.97739145	-1.45788479
O	7.33655967	-0.60278938	-6.00470115	C	5.20234326	-6.06460935	-1.41434952
H	7.46713616	-1.58668903	-6.00409887	H	5.14138180	-6.26812316	-2.47002530
C	5.27336481	-8.69326164	-9.78175120	N	5.24390587	-6.96952076	-0.45432803
H	5.95770458	-8.90342754	-10.60244413	C	5.24394501	-6.28352119	0.73708131
H	4.79307352	-9.62905407	-9.49525762	H	5.25730241	-6.79720846	1.68754159
C	6.09111268	-8.08435071	-8.63589461	C	5.97593821	-10.22538613	2.57278579
O	6.85091058	-7.12059524	-8.80638526	H	6.83501720	-9.86811919	1.99688499
N	5.94165394	-8.67952447	-7.43880006	H	5.37641564	-9.34150179	2.82964657
H	6.41012082	-8.27545926	-6.63858496	C	5.12620042	-11.14151646	1.72959757
H	5.22016764	-9.38285191	-7.28364154	N	4.65288579	-10.74210480	0.48225763
C	3.27661952	-4.83768503	-6.32367651	C	3.88599939	-11.72303242	0.02076104
H	3.20429384	-3.83987651	-6.76329256	H	3.35507997	-11.70592929	-0.91752611
H	2.68311169	-4.82581709	-5.39922408	N	3.83662312	-12.73710227	0.90270253
C	4.69622978	-5.09929171	-5.98855383	H	3.35197436	-13.63459194	0.76519143
C	5.07117084	-6.27893641	-5.16786260	C	4.61397184	-12.39014450	1.98788629
O	4.20502622	-7.03670368	-4.67197012	H	4.68804867	-13.02576432	2.85808697
C	6.48098888	-6.53147383	-4.95402136	Cu	4.95975896	-9.04623108	-0.70567308
H	6.76672218	-7.42764284	-4.41105787	O	7.46340260	-10.18001261	-3.84344915
C	7.38238259	-5.63203652	-5.42549157	H	7.95418326	-10.95102347	-3.47339382
O	8.71809041	-5.80202627	-5.34526767	H	8.12630184	-9.46798374	-3.84286148
C	7.00661974	-4.34231104	-6.02753194	O	3.00261835	-8.60027419	-0.61952449
O	7.92120989	-3.49584534	-6.22043273	H	2.54206277	-8.37961739	-1.46783324
C	5.62900683	-4.17333632	-6.35146911	H	2.37843967	-9.09470326	-0.00563588
H	5.35244160	-3.27832704	-6.89892819	O	4.80270296	-9.35410158	-2.72548844
C	-0.80796646	-1.37149235	-3.45978088	H	4.74779719	-8.58947192	-3.33193854
H	-1.09734439	-1.08947431	-2.43814019	H	9.08171129	-4.95858156	-5.71219876
H	-0.78780369	-0.44684349	-4.04569139	O	1.98424419	-7.35655845	-2.88651626
C	0.56828963	-1.98802113	-3.44660850	H	2.75429378	-7.13314056	-3.43965671
C	1.01227108	-2.77876650	-2.38075137	H	1.29820607	-7.57429678	-3.55242252
H	0.32833181	-3.00333655	-1.56517512	C	14.38677902	-7.43807369	-0.50115470
C	2.32186681	-3.25087600	-2.32227221	C	6.98009276	2.22973881	-5.65951424
H	2.66092504	-3.85206910	-1.48492577	C	4.19599332	-7.70992456	-10.29637784
C	3.21779388	-2.90967383	-3.33786695	C	2.63618395	-5.85552279	-7.29389791
O	4.52624681	-3.31928045	-3.23376013	C	-1.90785270	-2.28018725	-4.03525166
H	5.08163741	-2.70077403	-3.75421137	C	10.94731101	-8.75339611	1.54086709
C	2.78100293	-2.16515729	-4.43752087	C	6.49538191	-3.39503117	2.05850352
				C	6.48461265	-10.84285511	3.87394728

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C	14.52982654	-7.90676306	-1.95966234	H	3.49213413	-1.89316878	-5.23342912
H	14.95327794	-8.91456311	-1.96325419	C	1.47632370	-1.70267118	-4.49079670
H	15.25326618	-7.25357287	-2.44999127	H	1.14993646	-1.08928111	-5.32744003
C	13.19594246	-7.94772339	-2.66771258	C	10.48536652	-8.42901793	0.09117562
C	12.59419812	-6.81423959	-3.22844182	H	11.22379462	-8.87155474	-0.57722662
H	13.11437105	-5.85967643	-3.21957746	H	10.50239789	-7.34617428	-0.06870226
C	11.30327787	-6.87910539	-3.74887065	C	9.13791078	-8.97841748	-0.22938829
H	10.82711337	-5.98755610	-4.14138358	N	8.92559551	-10.26202523	-0.59659391
C	10.59676826	-8.08808547	-3.71509980	H	7.45191941	-1.63518204	-5.95875046
O	9.30625851	-8.18266453	-4.16619852	C	7.60208807	-10.36095421	-0.72789744
H	9.11070802	-7.42562889	-4.77206969	H	7.08046335	-11.26487370	-1.00630093
C	11.18970511	-9.23695254	-3.19067070	N	6.92307379	-9.19020157	-0.47967610
H	10.61943910	-10.15769118	-3.13450446	C	7.87957888	-8.29768231	-0.17010936
C	12.47513114	-9.14832490	-2.66668653	H	7.66234102	-7.26943272	0.08267704
H	12.91289847	-10.00832665	-2.17021067	C	5.12911744	-3.78831372	1.44360534
C	5.95630545	1.20336333	-5.09392635	H	4.70042224	-2.90555224	0.95444468
H	5.01251726	1.32791738	-5.62968927	H	4.45033341	-4.06214602	2.25596248
H	5.76739379	1.43376549	-4.04238733	C	5.19899155	-4.92987771	0.48543402
C	6.33575583	-0.29282938	-5.17455870	N	5.14475162	-4.79679237	-0.88954018
O	5.67834116	-1.10920786	-4.53854129	H	5.08741585	-3.94661993	-1.45207800
O	7.32169495	-0.64336569	-5.98629970	C	5.09845234	-6.03261224	-1.43758003
H	6.74268496	-6.96872745	-3.96990034	H	4.99579027	-6.22005034	-2.49241434
C	5.32501032	-8.64238835	-9.72322735	N	5.12927207	-6.95220271	-0.48911129
H	6.01573260	-8.86721361	-10.53673568	C	5.18836311	-6.28364784	0.71320295
H	4.86347508	-9.57133150	-9.39433417	H	5.21358584	-6.81390637	1.65462240
C	6.14128780	-8.11350450	-8.52857818	C	5.99944974	-10.23210439	2.55795903
O	6.44102216	-8.83615408	-7.59887332	H	6.86666131	-9.88079906	1.99175022
N	6.70308432	-6.82202055	-8.58944696	H	5.40078811	-9.34444499	2.80762398
H	7.15237924	-6.56761024	-7.71575838	C	5.15179427	-11.14492194	1.70884347
H	6.13729120	-6.05085767	-8.93720119	N	4.67140742	-10.73979194	0.46282879
C	3.31801744	-4.86344543	-6.32273213	C	3.90281328	-11.71941776	-0.00359521
H	3.28607842	-3.86869318	-6.77374316	H	3.35847859	-11.68803608	-0.93467264
H	2.71874935	-4.81376361	-5.40514779	N	3.86157183	-12.73793031	0.87251456
C	4.73626287	-5.17778270	-5.96895008	H	3.37379880	-13.63510157	0.73526952
C	5.07430250	-6.34937661	-5.16832988	C	4.63907219	-12.39543784	1.95854594
O	4.22081903	-7.05453026	-4.60346913	H	4.72107427	-13.03908866	2.82198346
C	6.53300619	-6.71243091	-5.01743597	Cu	4.95367802	-9.00106687	-0.61153060
H	6.68820633	-7.64867304	-5.57558783	O	7.42993506	-10.20615801	-3.76079535
C	7.55430815	-5.69929516	-5.48856614	H	7.93164849	-10.99214661	-3.41264710
O	8.74234741	-6.02223730	-5.59449218	H	8.10926225	-9.50119304	-3.82431913
C	7.09350124	-4.33012554	-5.87209741	O	2.98625726	-8.80214485	-0.76194818
O	7.89123349	-3.37146652	-5.95387547	H	2.51387675	-8.38282052	-1.52411825
C	5.70335439	-4.23591217	-6.22742554	H	2.34889867	-9.18098921	-0.08345968
H	5.41738092	-3.30830586	-6.71408397	O	5.06019018	-9.29234426	-2.80662800
C	-0.80004557	-1.37458356	-3.46546326	H	4.73641001	-8.62956227	-3.44584355
H	-1.08297599	-1.09430813	-2.44163593	H	5.93921022	-9.61523746	-3.13353405
H	-0.78096343	-0.44942978	-4.04999305	O	1.96439990	-7.33105925	-2.88493452
C	0.57499891	-1.99516265	-3.46122330	H	2.70288433	-7.06057987	-3.45915824
C	1.01617859	-2.81038327	-2.41182234	H	1.26946384	-7.58048877	-3.53077370
H	0.33136786	-3.05146221	-1.60132421	C	14.37725796	-7.44016817	-0.50431672
C	2.32752152	-3.27867669	-2.35668310	C	7.00290909	2.20758690	-5.65432173
H	2.66392148	-3.89198264	-1.52724593	C	4.22952617	-7.69221318	-10.26706795
C	3.22658648	-2.91576514	-3.36234975	C	2.63543284	-5.85957825	-7.28770005
O	4.53893693	-3.31595243	-3.25771452	C	-1.90416801	-2.28030914	-4.03635338
H	5.09445590	-2.66859549	-3.74576483	C	10.93559831	-8.74007034	1.54119813
C	2.78870005	-2.15988040	-4.45394301	C	6.49214983	-3.39989518	2.06278969
				C	6.49417198	-10.84815654	3.86463834

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C	14.53271841	-7.90375722	-1.96052990	H	3.49107671	-1.90567212	-5.23002397
H	14.94831178	-8.91478662	-1.96686060	C	1.47428012	-1.71747680	-4.48685383
H	15.26162742	-7.25554382	-2.44891206	H	1.14092819	-1.12310167	-5.33408998
C	13.20077086	-7.93147417	-2.67097282	C	10.52082926	-8.43875872	0.08521128
C	12.59127881	-6.78706501	-3.20419025	H	11.27870136	-8.84943188	-0.58337149
H	13.10395391	-5.82937033	-3.16988395	H	10.52982851	-7.35681677	-0.07317595
C	11.30368100	-6.84538173	-3.73145188	C	9.16855133	-8.97231071	-0.24909350
H	10.82346726	-5.95021199	-4.11038813	N	8.91410830	-10.29559779	-0.58336236
C	10.60876789	-8.06232443	-3.74533518	H	9.61035794	-11.02894963	-0.70619330
O	9.33241900	-8.15687556	-4.21657893	C	7.58182913	-10.44936633	-0.73654476
H	9.11262336	-7.35471823	-4.77664392	H	7.09901006	-11.37325971	-1.00685414
C	11.21341420	-9.21983930	-3.25409524	N	6.96567090	-9.29586647	-0.52712322
H	10.65848307	-10.15315497	-3.26810948	C	7.94127169	-8.36503018	-0.23131285
C	12.49278057	-9.13775528	-2.71418421	H	7.69878292	-7.33767102	-0.01331809
H	12.94628221	-10.00872309	-2.25337392	C	5.14385070	-3.79528325	1.41825680
C	5.92575310	1.22771547	-5.09034285	H	4.72170869	-2.91821257	0.91387943
H	4.97888541	1.34898872	-5.62300492	H	4.45365623	-4.06264515	2.22336989
H	5.75247371	1.44543245	-4.03201584	C	5.22652537	-4.94711522	0.46812233
C	6.29282017	-0.28861450	-5.17014976	N	5.12410870	-4.83102153	-0.90675806
O	5.60334322	-1.07341199	-4.49875603	H	5.05268759	-3.98734747	-1.48462461
O	7.22433111	-0.68332118	-5.95869916	C	5.07374772	-6.07137021	-1.43917277
H	6.64314883	-6.28940066	-3.71728494	H	4.91332461	-6.27077831	-2.48563167
C	5.26248703	-8.70478636	-9.79505080	N	5.15777922	-6.98488174	-0.48336602
H	5.93697662	-8.92041109	-10.62225627	C	5.24752936	-6.29969030	0.70971182
H	4.77441907	-9.63712875	-9.51014215	H	5.30576864	-6.81740276	1.65657212
C	6.10565478	-8.11432116	-8.66177134	C	5.97980458	-10.23054547	2.56794014
O	6.84378999	-7.13796417	-8.82001726	H	6.83924924	-9.86194080	2.00102769
N	6.01516222	-8.76029562	-7.48017979	H	5.36687491	-9.35329275	2.82133930
H	6.54574857	-8.39787167	-6.70242919	C	5.14105743	-11.15112826	1.71630914
H	5.27987180	-9.44449639	-7.30753053	N	4.67331743	-10.75408166	0.46197137
C	3.33243844	-4.86196579	-6.32514289	C	3.89373844	-11.72893103	0.00304924
H	3.31458984	-3.87031520	-6.78567900	H	3.34687395	-11.69563122	-0.92671748
H	2.72261778	-4.79584930	-5.41476397	N	3.83801015	-12.73835839	0.88779607
C	4.75026091	-5.18336921	-5.95079042	H	3.34329163	-13.63213078	0.75363742
C	5.08767080	-6.31209602	-5.14527964	C	4.61362749	-12.39301577	1.97583448
O	4.26500813	-7.12439014	-4.63383777	H	4.67995928	-13.02646777	2.84852818
C	6.55069099	-6.50740462	-4.79291756	Cu	4.96828952	-9.03035563	-0.64385480
H	6.81283572	-7.56626859	-4.88278048	O	7.48237130	-10.15658932	-3.82065506
C	7.58099631	-5.62929367	-5.46760691	H	7.96890637	-10.93599666	-3.45279254
O	8.75516109	-6.01030010	-5.56858026	H	8.16064497	-9.44571541	-3.87339151
C	7.11073570	-4.29520684	-5.90989212	O	3.00533925	-8.88535151	-0.83595976
O	7.91536248	-3.33022994	-6.04736435	H	2.55807437	-8.37606013	-1.56562085
C	5.72571610	-4.23086565	-6.23468840	H	2.36287383	-9.18498398	-0.12802206
H	5.43382566	-3.31754081	-6.74342136	O	5.07897094	-9.25419666	-2.84948724
C	-0.80051682	-1.37958819	-3.45982467	H	4.77278846	-8.55148485	-3.46514331
H	-1.08529255	-1.10079848	-2.43559779	H	5.96861497	-9.54401673	-3.16047287
H	-0.77796446	-0.45207230	-4.04027217	O	2.05467337	-7.33530523	-2.91601168
C	0.57448568	-2.00220497	-3.45370776	H	2.78240269	-7.11815259	-3.53339748
C	1.02090017	-2.79721329	-2.39373474	H	1.31850367	-7.55516670	-3.52493909
H	0.33818493	-3.04030091	-1.58213245	C	14.38329675	-7.43922769	-0.50427562
C	2.33607585	-3.25247602	-2.33425608	C	6.97929279	2.22609087	-5.65813281
H	2.67512407	-3.84990947	-1.49528800	C	4.19441683	-7.71017380	-10.29688133
C	3.23496214	-2.89700556	-3.34257396	C	2.64471044	-5.85540995	-7.29231982
O	4.54789796	-3.28303851	-3.22682178	C	-1.90682014	-2.28056117	-4.03650821
H	5.10299979	-2.64652761	-3.74159622	C	10.94771679	-8.75060758	1.54210330
C	2.79054674	-2.16129300	-4.44538278	C	6.49701193	-3.39866418	2.05468022
				C	6.48378899	-10.84326757	3.87373691

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C	14.54240486	-7.89834774	-1.96038080	H	3.47308721	-1.82035816	-5.26558834
H	14.97116016	-8.90306564	-1.96764359	C	1.45517600	-1.69446200	-4.51212478
H	15.26091190	-7.23860050	-2.44804577	H	1.10789921	-1.08187734	-5.34122185
C	13.21113279	-7.94900129	-2.66754513	C	10.52000562	-8.44033851	0.08607428
C	12.58063453	-6.81837041	-3.20267455	H	11.27634246	-8.85240086	-0.58277813
H	13.08005129	-5.85317592	-3.18309181	H	10.52833660	-7.35857483	-0.07226239
C	11.28758382	-6.90180589	-3.71374513	C	9.16706473	-8.97348045	-0.24330062
H	10.79585705	-6.01357044	-4.09420738	N	8.90757125	-10.29647852	-0.57432613
C	10.61095233	-8.12927760	-3.70661202	H	9.60146885	-11.03140042	-0.70118143
O	9.32072819	-8.24252685	-4.14310310	C	7.57445054	-10.44732109	-0.72022146
H	9.10068354	-7.46691290	-4.72104544	H	7.08686140	-11.37014791	-0.98454412
C	11.24100998	-9.27674305	-3.22436703	N	6.96266839	-9.29202248	-0.50800939
H	10.70434437	-10.22040310	-3.23474944	C	7.94194495	-8.36325592	-0.21904408
C	12.52537537	-9.16821110	-2.70066541	H	7.70270455	-7.33603918	0.00238575
H	13.00277889	-10.02497247	-2.23825960	C	5.14244608	-3.78581454	1.41067205
C	5.92480045	1.22616528	-5.09015729	H	4.72181207	-2.90240108	0.91632365
H	4.96908175	1.37121439	-5.60202685	H	4.45058630	-4.06323811	2.21086939
H	5.75837383	1.44263213	-4.03016184	C	5.23013740	-4.92607555	0.44737716
C	6.31021863	-0.28785634	-5.22026555	N	5.15967603	-4.80413646	-0.93025840
O	5.49531772	-1.08394670	-4.64828313	H	5.08991523	-3.95844081	-1.50806403
O	7.30575369	-0.66680524	-5.87242671	C	5.13628347	-6.04450887	-1.46564956
H	6.74215549	-6.95633823	-3.97290671	H	5.02071437	-6.23966102	-2.51711608
C	5.30457397	-8.65424999	-9.74489730	N	5.19880796	-6.96125299	-0.51170827
H	5.98311990	-8.89215903	-10.56636633	C	5.25202701	-6.27875234	0.68460539
H	4.84349476	-9.57663171	-9.40112226	H	5.28914253	-6.79872526	1.63145132
C	6.14713098	-8.11743451	-8.57486777	C	5.97896565	-10.22783607	2.57058417
O	6.51822015	-8.84707004	-7.67794233	H	6.83916123	-9.86046112	2.00418838
N	6.64908773	-6.79525040	-8.62048249	H	5.36843448	-9.35037633	2.82705334
H	7.15401950	-6.57656020	-7.76776235	C	5.13760137	-11.14572678	1.71792673
H	6.00691589	-6.03736179	-8.84959150	N	4.67184096	-10.74775311	0.46265554
C	3.33923540	-4.83781828	-6.34825297	C	3.89529976	-11.72422670	0.00077248
H	3.29739774	-3.84871018	-6.80891841	H	3.35575249	-11.69800791	-0.93314696
H	2.75730911	-4.77758811	-5.42146948	N	3.84035258	-12.73483573	0.88449598
C	4.76756687	-5.14317776	-6.02050301	H	3.34742613	-13.63028274	0.75014162
C	5.09089788	-6.30082684	-5.17735032	C	4.61193052	-12.38926902	1.97409481
O	4.22622669	-6.95228723	-4.57481690	H	4.67865293	-13.02475318	2.84534511
C	6.53545558	-6.71897803	-5.02482423	Cu	4.97276292	-9.01021521	-0.60585779
H	6.65359295	-7.66962090	-5.57316445	O	7.41319750	-10.20322076	-3.77948139
C	7.58761088	-5.76112923	-5.53447552	H	7.90778566	-10.98633691	-3.43051901
O	8.77169376	-6.09333093	-5.54460652	H	8.10003589	-9.50543397	-3.85658433
C	7.17431839	-4.43436046	-6.13948685	O	3.01110118	-8.76809408	-0.72339509
O	8.01781763	-3.62933645	-6.51162593	H	2.54458290	-8.36801854	-1.50201303
C	5.74500212	-4.25756982	-6.36972044	H	2.36620156	-9.15986115	-0.05941526
H	5.49411321	-3.32938652	-6.87306867	O	5.04303577	-9.26971646	-2.80729161
C	-0.80364057	-1.38200796	-3.45242631	H	4.69869411	-8.59412452	-3.42187334
H	-1.08436333	-1.11889054	-2.42343055	H	5.91581157	-9.57813520	-3.15704791
H	-0.78905345	-0.44675654	-4.02134093	O	1.97527792	-7.37051165	-2.86530343
C	0.57343574	-1.99661126	-3.46806449	H	2.67531094	-6.97759724	-3.41447804
C	1.04436350	-2.79947028	-2.42416081	H	1.28842257	-7.60899828	-3.52352047
H	0.37758935	-3.05101533	-1.60129729	C	14.38496204	-7.43883977	-0.50411401
C	2.36725930	-3.24259724	-2.38949997	C	6.97556108	2.22792426	-5.65592547
H	2.72309737	-3.83983657	-1.55546606	C	4.20997121	-7.70220784	-10.28343926
C	3.25199689	-2.86150892	-3.40368618	C	2.64456909	-5.85114352	-7.29096765
O	4.57606785	-3.21115846	-3.31657649	C	-1.90702317	-2.28079118	-4.03533539
H	5.10410469	-2.51500875	-3.81727755	C	10.94862233	-8.75145463	1.54162251
C	2.77482596	-2.12503639	-4.49625318	C	6.49484487	-3.39708668	2.05474617
				C	6.48342006	-10.84349008	3.87390738

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C	14.54214355	-7.89961878	-1.96469233	H	3.56216860	-2.16935612	-5.04340643
H	14.96403353	-8.90849842	-1.96795873	C	1.53353203	-1.84702446	-4.38314532
H	15.27017097	-7.24768028	-2.44999207	H	1.26803720	-1.26122061	-5.26034997
C	13.21672376	-7.94228595	-2.68657607	C	10.52412671	-8.42948984	0.08031475
C	12.60183155	-6.80779122	-3.23407590	H	11.28632947	-8.83372436	-0.58733938
H	13.10903780	-5.84649425	-3.20730437	H	10.53060734	-7.34664368	-0.07096942
C	11.31593420	-6.87501335	-3.76122837	C	9.17571325	-8.96269829	-0.25984017
H	10.83127301	-5.98702836	-4.14851546	N	8.93205966	-10.28793323	-0.59876225
C	10.61566654	-8.09530124	-3.76356978	H	9.63259124	-11.01263556	-0.73464979
O	9.35565091	-8.19821878	-4.23267815	C	7.59896658	-10.44728285	-0.75060191
H	9.07542961	-7.32162975	-4.70933864	H	7.12072452	-11.37246840	-1.02481022
C	11.23538453	-9.24549477	-3.25927404	N	6.97881979	-9.30062029	-0.53156768
H	10.68361993	-10.18122160	-3.25741159	C	7.94457963	-8.36330996	-0.23414998
C	12.51443274	-9.15176802	-2.72063132	H	7.68028125	-7.34092659	-0.01411448
H	12.96973854	-10.01348614	-2.24238395	C	5.10884552	-3.85870306	1.47257125
C	5.94606905	1.22149695	-5.08431853	H	4.66256666	-3.00087267	0.95740449
H	4.94593175	1.49827518	-5.42058940	H	4.44695882	-4.11635218	2.30782375
H	5.96527636	1.25950139	-3.98838143	C	5.17982421	-5.02166998	0.52441359
C	6.16779461	-0.23238760	-5.53515632	N	5.08484522	-4.87342052	-0.84171323
O	5.21932188	-0.95174286	-5.78294597	H	5.95938376	-9.53543993	-3.17863925
O	7.43472820	-0.65252276	-5.60627858	C	5.08101605	-6.11428281	-1.33386758
H	7.44410957	-1.61240075	-5.85387034	H	5.00155550	-6.34604243	-2.38494870
C	5.30161025	-8.67801277	-9.75534560	N	5.16246565	-7.06011109	-0.38026884
H	6.00117677	-8.87587594	-10.56688434	C	5.22240864	-6.37249549	0.81307281
H	4.83748660	-9.62333757	-9.47220717	H	5.29608403	-6.88557780	1.76328029
C	6.09032908	-8.04243062	-8.60356904	C	5.98917594	-10.24321944	2.55496603
O	6.83953405	-7.07536455	-8.78923846	H	6.85064051	-9.88574823	1.98423388
N	5.91182523	-8.60237897	-7.39314458	H	5.38211810	-9.35967049	2.79395529
H	6.29457614	-8.11437746	-6.58573622	C	5.14975635	-11.17622505	1.71581910
H	5.17360739	-9.28968031	-7.24863989	N	4.69589361	-10.80311813	0.45296467
C	3.33613489	-4.86636459	-6.32806525	C	3.91385181	-11.77949263	0.01248464
H	3.29118351	-3.86673956	-6.76447674	H	3.37182254	-11.76128234	-0.92058351
H	2.75296264	-4.83722835	-5.40054314	N	3.84253949	-12.77333435	0.91845466
C	4.76360618	-5.16121512	-5.99521221	H	3.35046422	-13.66711214	0.79308950
C	5.12820805	-6.33039528	-5.10915742	C	4.61581484	-12.41017266	2.00264489
O	4.21582285	-7.04734781	-4.61229183	H	4.67291009	-13.02433717	2.88988044
C	6.50291161	-6.60334067	-4.89791624	Cu	4.98048375	-9.00617549	-0.62017311
H	6.76101014	-7.46688978	-4.29211830	O	7.49956423	-10.18955666	-3.82737001
C	7.52307267	-5.78125664	-5.39476674	H	7.98793308	-10.94649091	-3.42821809
O	8.75793414	-6.03671179	-5.36185066	H	8.17271224	-9.47519981	-3.91654277
C	7.10122514	-4.42419918	-5.96886147	O	3.00448416	-8.97244494	-0.87678613
O	7.90657991	-3.49924213	-6.05272974	H	2.58451140	-8.35337329	-1.53267192
C	5.70882469	-4.27533468	-6.36522881	H	2.37657162	-9.18894161	-0.13150440
H	5.46097401	-3.36393680	-6.89606279	O	5.05459936	-9.30040385	-2.87102947
C	-0.77215298	-1.38032235	-3.46056697	H	4.75120720	-8.54977586	-3.42980199
H	-1.09211047	-1.04034878	-2.46529387	O	2.04233606	-7.27650329	-2.84030664
H	-0.71410388	-0.48641012	-4.08995782	H	2.80124425	-6.95367431	-3.36628166
C	0.58678179	-2.03225998	-3.36644707	H	1.39295424	-7.53591627	-3.52358978
C	0.97355205	-2.77750604	-2.24606514	C	14.38239426	-7.43585325	-0.50942973
H	0.26590950	-2.92158011	-1.43030314	C	6.98775268	2.23077102	-5.63543348
C	2.24745875	-3.33394752	-2.13905243	C	4.21276783	-7.71819458	-10.28644721
H	2.53115630	-3.91357875	-1.26778611	C	2.64557367	-5.85033668	-7.30101899
C	3.18913763	-3.12678127	-3.16323252	C	-1.88217146	-2.28295796	-4.03073151
O	4.44380305	-3.61884359	-3.12995156	C	10.94477249	-8.74869711	1.53665878
H	4.68918657	-3.91918332	-2.20017697	C	6.47720952	-3.41960615	2.06013344
C	2.81535123	-2.37260569	-4.28684478	C	6.48629716	-10.84428313	3.86571252

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C	14.55210106	-7.89745313	-1.96642387	H	3.51247987	-2.09034149	-5.18207017
H	14.99824464	-8.89451818	-1.96781179	C	1.50255894	-1.80298624	-4.46139844
H	15.25719655	-7.22640581	-2.45894380	H	1.19548279	-1.23785842	-5.34009832
C	13.22217979	-7.98487802	-2.67092440	C	10.51101402	-8.43785374	0.07944287
C	12.57210865	-6.87849389	-3.23491785	H	11.26128092	-8.85523443	-0.59232704
H	13.06473161	-5.90927922	-3.25742754	H	10.52722336	-7.35598732	-0.07996362
C	11.27457702	-6.98690523	-3.72331967	C	9.15448074	-8.95863314	-0.24808859
H	10.76721119	-6.12240669	-4.13430818	N	8.89277272	-10.28205419	-0.57879426
C	10.59213346	-8.21645485	-3.65444547	H	9.58550192	-11.01329941	-0.71896004
O	9.31202976	-8.33947092	-4.05844910	C	7.55837741	-10.42423934	-0.73306155
H	9.05145779	-7.51255113	-4.64291365	H	7.06735811	-11.34482612	-0.99835007
C	11.24885199	-9.34074401	-3.13972833	N	6.95337970	-9.26736045	-0.52215179
H	10.71198235	-10.28324985	-3.08653870	C	7.93141740	-8.34338858	-0.22704402
C	12.54239630	-9.20763483	-2.64563183	H	7.68034992	-7.31658668	-0.01100283
H	13.02792224	-10.04245033	-2.14827884	C	5.12747268	-3.79713443	1.42517682
C	5.91662858	1.28321036	-5.07819640	H	4.71030233	-2.91898414	0.91778923
H	4.98943818	1.39631609	-5.64810961	H	4.43850468	-4.05444901	2.23815865
H	5.69707158	1.56008376	-4.04376014	C	5.19244154	-4.94202818	0.45335526
C	6.33062441	-0.19466913	-5.12070447	N	5.05956947	-4.78808578	-0.91423834
O	5.52387787	-0.85989396	-4.27433921	H	5.90911743	-9.56610930	-3.18419044
O	7.17843632	-0.71851531	-5.80733849	C	5.04683954	-6.03211527	-1.40582949
H	5.72673105	-1.81719294	-4.23108815	H	4.93494373	-6.26360042	-2.45349657
C	5.27485967	-8.69904547	-9.77811739	N	5.15903816	-6.98040534	-0.45672528
H	5.96187346	-8.90259838	-10.59776706	C	5.24547043	-6.29303766	0.73402618
H	4.79663474	-9.63740740	-9.49697401	H	5.33225284	-6.80817366	1.68188599
C	6.08643431	-8.08535066	-8.63164967	C	5.98211808	-10.23534768	2.56577829
O	6.84074468	-7.12254793	-8.81708621	H	6.84246865	-9.86885053	1.99769075
N	5.92639961	-8.66350508	-7.42850253	H	5.37134271	-9.35547030	2.81155653
H	6.32776451	-8.20053026	-6.61538952	C	5.14464554	-11.15707519	1.71104304
H	5.18759510	-9.34971308	-7.28403407	N	4.66659564	-10.74839303	0.46711388
C	3.41957274	-4.87400993	-6.35903711	C	3.89793562	-11.72502200	0.00370258
H	3.40242456	-3.87841518	-6.80836912	H	3.34493729	-11.68458636	-0.92215155
H	2.87422053	-4.81756438	-5.41206799	N	3.85820330	-12.75361507	0.87364510
C	4.85127940	-5.25360226	-6.10373682	H	3.36923048	-13.64773062	0.73325649
C	5.17837403	-6.37190981	-5.14492351	C	4.63888274	-12.41120266	1.96013850
O	4.24213805	-6.98230723	-4.55597782	H	4.72708713	-13.05557279	2.82304638
C	6.54017396	-6.71218241	-4.93590337	Cu	4.96044724	-8.94627445	-0.62878434
H	6.75497219	-7.47161927	-4.19061266	O	7.42344867	-10.27156474	-3.80105330
C	7.59855557	-6.07248540	-5.59599653	H	7.90562915	-11.04081902	-3.41563908
O	8.82243523	-6.36584748	-5.48279489	H	8.11466058	-9.56830835	-3.85128449
C	7.26356922	-4.92965044	-6.56110606	O	2.98528543	-8.91176081	-0.87357493
O	8.14129612	-4.37284419	-7.20347006	H	2.55694731	-8.31362792	-1.54326990
C	5.84787316	-4.56106490	-6.69127711	H	2.35813000	-9.14594063	-0.13448172
H	5.65521035	-3.71080296	-7.33494533	O	5.02255927	-9.27568746	-2.86765351
C	-0.78249314	-1.37342486	-3.47140818	H	4.76007583	-8.50671348	-3.42148426
H	-1.08414403	-1.05736203	-2.46233631	O	2.02600881	-7.25208687	-2.85473939
H	-0.74532360	-0.46608956	-4.08403036	H	2.79344723	-6.94096919	-3.37537259
C	0.58898588	-2.00286264	-3.41770318	H	1.38206052	-7.51551954	-3.54230588
C	1.02443790	-2.73127465	-2.30402907	C	14.38654393	-7.43323465	-0.51104959
H	0.33498592	-2.89702452	-1.47637708	C	6.99254481	2.24038114	-5.64459952
C	2.32201683	-3.23300267	-2.21407393	C	4.19718955	-7.71646827	-10.29156186
H	2.65057031	-3.79262169	-1.34431308	C	2.65507820	-5.83876941	-7.29850785
C	3.23484505	-2.99276516	-3.25432484	C	-1.88798797	-2.28503370	-4.03555213
O	4.52457509	-3.40517178	-3.21493386	C	10.94376366	-8.75320808	1.53569201
H	4.75947434	-3.76310060	-2.29652078	C	6.48799180	-3.40188868	2.05813837
C	2.80178931	-2.28994365	-4.38955238	C	6.48341759	-10.84468559	3.87395305

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C	14.53676417	-7.91890986	-1.96005055	H	3.53458918	-1.81625482	-5.23483224
H	14.95151946	-8.93066918	-1.95358726	C	1.51423839	-1.65797286	-4.49316414
H	15.27009716	-7.27521350	-2.44978583	H	1.19844743	-0.98862911	-5.29076522
C	13.21338459	-7.95669207	-2.68558602	C	10.46017277	-8.43219389	0.09165581
C	12.63206945	-6.82536347	-3.26919281	H	11.19023892	-8.87627912	-0.58350855
H	13.16224729	-5.87556648	-3.26329786	H	10.49773606	-7.34983937	-0.07177272
C	11.34948280	-6.88168958	-3.80891810	C	9.09279204	-8.96220913	-0.22078960
H	10.88649068	-5.99261347	-4.21906800	N	8.88595638	-10.28140788	-0.56629976
C	10.62282764	-8.08118632	-3.76752280	H	5.97400039	-9.53251791	-3.16731250
O	9.35545091	-8.16791591	-4.24926506	C	7.57310295	-10.38748227	-0.71445007
H	9.10410606	-7.30942452	-4.70576597	H	7.05578192	-11.29799680	-0.98611900
C	11.19440697	-9.22700531	-3.20637828	N	6.90723303	-9.22263827	-0.50503660
H	10.59950245	-10.12930594	-3.11278646	C	7.88318161	-8.29984127	-0.18824766
C	12.47346137	-9.14615423	-2.66955818	H	7.64686097	-7.26983062	0.03106074
H	12.88614127	-9.99904489	-2.13936467	C	5.12368984	-3.79574767	1.45135656
C	5.95561650	1.20365991	-5.11708455	H	4.68939377	-2.90940614	0.97201498
H	5.01011841	1.31988402	-5.65395067	H	4.45095424	-4.07524376	2.26717796
H	5.76238330	1.44337528	-4.06776933	C	5.18494668	-4.93216335	0.48541133
C	6.34238360	-0.28771529	-5.17844146	N	5.19279206	-4.79008138	-0.89154234
O	5.70606479	-1.08726438	-4.50573627	H	5.18008263	-3.93721551	-1.44545284
O	7.31038576	-0.64611623	-6.01054006	C	5.14320991	-6.02405332	-1.44839641
H	7.44283854	-1.63697571	-5.97589551	H	5.11927346	-6.20102968	-2.51045208
C	5.29882201	-8.67349040	-9.75377806	N	5.10185956	-6.94674658	-0.50544314
H	5.99939349	-8.87308350	-10.56344774	C	5.12690089	-6.28582075	0.70053958
H	4.83078163	-9.61656716	-9.47132511	H	5.11424535	-6.82369140	1.63770220
C	6.08736284	-8.03993195	-8.59992275	C	6.00836803	-10.23275327	2.54914528
O	6.83162589	-7.06644756	-8.78035600	H	6.87867753	-9.90618536	1.97182422
N	5.90712141	-8.60272287	-7.39301581	H	5.42186605	-9.33219657	2.78034886
H	6.32836903	-8.15496306	-6.58463774	C	5.14751823	-11.14604673	1.71377867
H	5.19778801	-9.32030349	-7.24975666	N	4.64488188	-10.73172163	0.48398343
C	3.33095952	-4.83478571	-6.34711431	C	3.88773424	-11.71320724	0.01428471
H	3.26295406	-3.83763575	-6.78961231	H	3.33433516	-11.67196365	-0.91122093
H	2.75656674	-4.81570646	-5.41331355	N	3.86889085	-12.75064401	0.87381459
C	4.76277948	-5.10711779	-6.02274691	H	3.39843741	-13.65236954	0.72593437
C	5.13511264	-6.27098242	-5.12318466	C	4.65828711	-12.40812597	1.95524287
O	4.21412671	-6.98013028	-4.62906988	H	4.76873947	-13.06540746	2.80511914
C	6.50260741	-6.52222128	-4.89798553	Cu	4.99266651	-9.01613701	-0.67196698
H	6.77656716	-7.38395526	-4.29619432	O	7.46457641	-10.16154112	-3.83199551
C	7.51876588	-5.68621224	-5.40152431	H	7.90874592	-10.88008309	-3.32053055
O	8.74610431	-5.92350551	-5.38615443	H	8.13939918	-9.44819772	-3.85867134
C	7.07556734	-4.32722482	-5.95690842	O	2.98758198	-8.89889613	-0.86677239
O	7.85292117	-3.37224701	-5.96577674	H	2.52951170	-8.35700642	-1.55279674
C	5.69575544	-4.20962116	-6.39910019	H	2.36093169	-9.18885219	-0.14771130
H	5.43793759	-3.32193785	-6.96649882	O	5.05780361	-9.26235881	-2.89737223
C	-0.77160523	-1.39188584	-3.47618797	H	4.79233654	-8.51843250	-3.47545778
H	-1.04733037	-1.12150681	-2.44640696	O	1.99978909	-7.20709678	-2.90142572
H	-0.75709471	-0.45939522	-4.05005203	H	2.78369995	-6.99760633	-3.44751281
C	0.60193582	-2.01401919	-3.49466208	H	1.33667525	-7.47417185	-3.57101064
C	1.03025686	-2.89648467	-2.49631609	C	14.37791488	-7.44233245	-0.50731129
H	0.33527773	-3.19358760	-1.71343603	C	7.00040389	2.19990655	-5.68555017
C	2.33652521	-3.37739614	-2.46231973	C	4.21308238	-7.71131197	-10.28869285
H	2.66492485	-4.06209414	-1.68705427	C	2.64782075	-5.83905964	-7.30245683
C	3.24989402	-2.94964524	-3.43000230	C	-1.88084578	-2.29053548	-4.04808817
O	4.55054041	-3.36467882	-3.33012639	C	10.92764371	-8.74275448	1.53575532
H	5.11526273	-2.73331666	-3.82585481	C	6.49070026	-3.40810512	2.06581325
C	2.82545830	-2.12168411	-4.47461023	C	6.48657389	-10.83791188	3.86825242

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C	14.54766687	-7.89198243	-1.96904293	H	3.42160330	-1.83206983	-5.41939560
H	14.96443727	-8.90258374	-1.97514296	C	1.46038990	-1.62999022	-4.54739531
H	15.27994287	-7.24069904	-2.44883772	H	1.10670045	-0.95034178	-5.32070359
C	13.22472570	-7.92399532	-2.69436949	C	10.52758345	-8.43246401	0.07603912
C	12.59433488	-6.77874676	-3.20113393	H	11.28352982	-8.85112024	-0.59140021
H	13.09040515	-5.81289149	-3.14184430	H	10.54772989	-7.35030204	-0.07969864
C	11.31158121	-6.84509395	-3.73555337	C	9.17401273	-8.95166428	-0.26063768
H	10.81581866	-5.94944343	-4.09063728	N	8.92161724	-10.27490830	-0.60170096
C	10.62912855	-8.07469335	-3.78381402	H	9.61761889	-11.00471640	-0.73530723
O	9.37092848	-8.17899852	-4.25770379	C	7.58608368	-10.42405056	-0.75203749
H	9.08711052	-7.29813137	-4.71816373	H	7.09915425	-11.34628130	-1.02204793
C	11.25984995	-9.23225702	-3.31237394	N	6.97594453	-9.27209310	-0.53298442
H	10.72121764	-10.17508368	-3.35132627	C	7.94762930	-8.34280126	-0.23260689
C	12.53688187	-9.13976634	-2.76936875	H	7.68627274	-7.31968285	-0.01018968
H	13.00687990	-10.00981216	-2.32326713	C	5.11156285	-3.85924376	1.49278266
C	5.94605574	1.21636981	-5.08526724	H	4.65642095	-3.00156638	0.98379914
H	4.99391529	1.35380084	-5.60358946	H	4.46280983	-4.12468654	2.33349434
H	5.77216936	1.41652987	-4.02414765	C	5.18682170	-5.00755384	0.53365916
C	6.31615612	-0.27645854	-5.21320561	N	5.21231446	-4.80527823	-0.82507531
O	5.61005401	-1.10007657	-4.65688273	H	5.96186067	-9.51972123	-3.19571862
O	7.36028782	-0.61434792	-5.96961019	C	5.20322665	-6.02585001	-1.35373488
H	7.45961057	-1.60546518	-5.96258368	H	5.21221586	-6.22841166	-2.41415549
C	5.29095711	-8.68298635	-9.76038163	N	5.16686112	-7.01553564	-0.42413998
H	5.98661719	-8.88545212	-10.57366823	C	5.15018846	-6.36613554	0.79310319
H	4.82195244	-9.62445033	-9.47380469	H	5.10459231	-6.91596291	1.72586183
C	6.08628170	-8.04830665	-8.61209510	C	5.98455181	-10.24203266	2.55731834
O	6.84332585	-7.08841766	-8.80533534	H	6.84282598	-9.87602145	1.98660424
N	5.90616891	-8.60029832	-7.39948268	H	5.37352338	-9.36236316	2.79784569
H	6.30251920	-8.11728587	-6.59587994	C	5.15023129	-11.17086865	1.71059407
H	5.17042519	-9.28939600	-7.24930230	N	4.69185510	-10.77722995	0.45316688
C	3.35781062	-4.85032063	-6.35639229	C	3.91645172	-11.75090484	-0.00294436
H	3.29792517	-3.85162032	-6.79508050	H	3.37399330	-11.71789096	-0.93564847
H	2.79762864	-4.82403773	-5.41573248	N	3.85226844	-12.76307684	0.88543191
C	4.78860479	-5.15138724	-6.05016943	H	3.36144075	-13.65636590	0.74857575
C	5.14285570	-6.30904742	-5.13540593	C	4.62474309	-12.41258837	1.97645273
O	4.22312241	-7.01517247	-4.64577512	H	4.68548152	-13.04014146	2.85394035
C	6.51564357	-6.57617530	-4.91353100	Cu	4.97347470	-8.95567845	-0.62571834
H	6.77121237	-7.42765388	-4.29023804	O	7.51672779	-10.17618694	-3.84975260
C	7.53756013	-5.75384154	-5.40547767	H	7.99698145	-10.93011609	-3.43359415
O	8.77263020	-6.00393838	-5.36566970	H	8.18994510	-9.46255564	-3.93274252
C	7.11648011	-4.40666118	-5.99677728	O	2.99989253	-8.95596634	-0.88290155
O	7.89189006	-3.44952288	-6.00680538	H	2.58286080	-8.31090667	-1.51183533
C	5.74365389	-4.29193562	-6.45920758	H	2.38226271	-9.17283563	-0.13043375
H	5.50331641	-3.40983633	-7.04197846	O	5.05233667	-9.28991655	-2.89901261
C	-0.78061249	-1.38954548	-3.44330997	H	4.76150097	-8.52378272	-3.43956207
H	-1.04749872	-1.15570522	-2.40212822	O	2.06570025	-7.21732585	-2.81834844
H	-0.78512087	-0.43793023	-3.98701684	H	2.84987144	-6.89067986	-3.30019833
C	0.60071241	-1.99473695	-3.50633219	H	1.45782478	-7.49483858	-3.53177387
C	1.08053191	-2.88045297	-2.53082038	C	14.38503554	-7.43405117	-0.51174521
H	0.43045840	-3.16738767	-1.70619968	C	6.99015853	2.22900599	-5.63325633
C	2.37969896	-3.38182067	-2.57747448	C	4.20496885	-7.71829284	-10.29001208
H	2.78251288	-4.04354048	-1.81584137	C	2.64852273	-5.84121620	-7.30507334
C	3.23027163	-2.98517829	-3.61550668	C	-1.88897861	-2.28368500	-4.03179401
O	4.48844590	-3.49347645	-3.65575348	C	10.94571642	-8.75161905	1.53479100
H	5.07126976	-2.84201783	-4.09071189	C	6.48131444	-3.41788268	2.06647708
C	2.75714892	-2.12240030	-4.61403795	C	6.48683461	-10.84433864	3.86777589

4²⁻, -2H⁺

C	14.54916332	-7.89591296	-1.96373097	H	3.50186434	-1.74051546	-5.30704760
H	14.99436412	-8.89344862	-1.96644822	C	1.48243661	-1.64471976	-4.54796396
H	15.25463929	-7.22503527	-2.45559249	H	1.12989653	-1.01215760	-5.36013793
C	13.21728860	-7.97883324	-2.66467445	C	10.51460565	-8.43200261	0.08520252
C	12.56461568	-6.86658441	-3.21374495	H	11.27059288	-8.84173711	-0.58542490
H	13.05539858	-5.89589459	-3.22187807	H	10.52797805	-7.34961816	-0.06995821
C	11.26564857	-6.97117333	-3.69961208	C	9.16107889	-8.95681765	-0.25185055
H	10.75613023	-6.10268036	-4.10016523	N	8.90141553	-10.28138058	-0.57738558
C	10.58704339	-8.20419279	-3.64851538	H	9.59625847	-11.01332705	-0.70789610
O	9.30835653	-8.32590742	-4.05660426	C	7.56901246	-10.42132590	-0.75556621
H	9.06686724	-7.52163681	-4.68812175	H	7.08179776	-11.34245650	-1.02893432
C	11.24726776	-9.33250439	-3.14760024	N	6.95993035	-9.26310457	-0.56433687
H	10.71478462	-10.27848223	-3.11277512	C	7.93823988	-8.33964020	-0.25963622
C	12.54089561	-9.20299913	-2.65292988	H	7.69737182	-7.30649042	-0.06558320
H	13.02904176	-10.04338255	-2.16852137	C	5.13602006	-3.77828344	1.42297346
C	5.90914669	1.26526603	-5.05588890	H	4.70910863	-2.88297839	0.95546695
H	4.96444787	1.40920262	-5.59019009	H	4.45262604	-4.07686019	2.22347887
H	5.72904510	1.51607454	-4.00681535	C	5.21454495	-4.89137624	0.42809537
C	6.27891833	-0.26456312	-5.14037703	N	5.16977477	-4.73897794	-0.94858063
O	5.48921104	-0.97710886	-4.43648642	H	5.12799559	-3.88553759	-1.51664837
O	7.20143787	-0.67550284	-5.85945346	C	5.13455246	-5.96682030	-1.51290887
H	5.90608320	-9.56414912	-3.20441491	H	5.05233995	-6.13204962	-2.57516437
C	5.27589388	-8.69708843	-9.77911144	N	5.15901696	-6.90517841	-0.57599361
H	5.96345684	-8.89929936	-10.59865084	C	5.20402607	-6.24832862	0.63455059
H	4.79593275	-9.63583883	-9.50076277	H	5.21553779	-6.78941778	1.57076425
C	6.08734999	-8.08853611	-8.63090068	C	5.98571189	-10.23131430	2.56515039
O	6.83563994	-7.12072922	-8.81012136	H	6.84796779	-9.86727423	1.99633908
N	5.93677278	-8.67903889	-7.43153905	H	5.37918334	-9.34910950	2.81467577
H	6.33660406	-8.21567520	-6.61853755	C	5.14176831	-11.14291183	1.70666138
H	5.19688738	-9.36378933	-7.28813071	N	4.64969362	-10.71229077	0.47490285
C	3.43855106	-4.87198649	-6.36012223	C	3.88218052	-11.68466739	-0.00129412
H	3.42771306	-3.87842914	-6.81429821	H	3.32122719	-11.62434439	-0.92221794
H	2.89928751	-4.80082071	-5.40987223	N	3.85592618	-12.73141400	0.84874339
C	4.87344039	-5.26196401	-6.11672355	H	3.37044180	-13.62757760	0.70104911
C	5.21100847	-6.36967887	-5.15301087	C	4.64358333	-12.40394105	1.93575649
O	4.28567899	-6.95852262	-4.51507101	H	4.74102564	-13.06565240	2.78443546
C	6.57074291	-6.72606865	-4.96374463	Cu	4.95367998	-8.96882929	-0.71194277
H	6.78901506	-7.48867896	-4.22130517	O	7.42908068	-10.27546412	-3.78594820
C	7.62602228	-6.10563337	-5.64800395	H	7.92595950	-11.04738690	-3.41999851
O	8.84669743	-6.41915848	-5.55872377	H	8.11379802	-9.56562595	-3.83950645
C	7.28351719	-4.96473550	-6.61248979	O	2.96440668	-8.82975162	-0.85452853
O	8.15533218	-4.43260237	-7.27779684	H	2.50761254	-8.32638530	-1.58077433
C	5.87047965	-4.57665806	-6.71351637	H	2.33302966	-9.14310441	-0.14905452
H	5.68276671	-3.71458184	-7.34124407	O	5.02143084	-9.24995555	-2.90235486
C	-0.78121151	-1.38367893	-3.47350837	H	4.77345311	-8.47670955	-3.46355520
H	-1.04907322	-1.12686284	-2.43828281	O	2.00500458	-7.27331512	-2.91576246
H	-0.78421429	-0.44525194	-4.03766473	H	2.76466093	-6.97057152	-3.45513886
C	0.60181884	-1.98469088	-3.51345881	H	1.33945021	-7.52058790	-3.59108640
C	1.07623327	-2.82183711	-2.49990300	C	14.38503987	-7.43347353	-0.51078493
H	0.40848519	-3.10932368	-1.68875319	C	6.98122857	2.23222150	-5.63301299
C	2.39978870	-3.25781318	-2.48001218	C	4.20077809	-7.71208285	-10.29117445
H	2.75750257	-3.88559914	-1.67052261	C	2.66036274	-5.83725374	-7.28978142
C	3.29089492	-2.83499014	-3.47582076	C	-1.88703110	-2.28867320	-4.04202639
O	4.60574985	-3.16655636	-3.38631325	C	10.94403780	-8.74976707	1.53753457
H	5.13990963	-2.44090233	-3.87654354	C	6.49365302	-3.40270511	2.06351280
C	2.80397716	-2.06788492	-4.54712122	C	6.48593306	-10.84514818	3.87335053

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C	14.52244549	-7.89338422	-1.97650456	H	3.52239288	-1.89081871	-5.24417572
H	14.94239073	-8.90302898	-1.98718185	C	1.50932851	-1.69416030	-4.49010463
H	15.24769216	-7.24089785	-2.46707915	H	1.18682252	-1.05801560	-5.31154702
C	13.18621784	-7.92681061	-2.68928539	C	10.50914611	-8.44562470	0.07918506
C	12.55402042	-6.78592465	-3.20448555	H	11.29249339	-8.81476108	-0.58628675
H	13.05646228	-5.82197555	-3.16703210	H	10.46694299	-7.36266456	-0.07072455
C	11.26113855	-6.84856068	-3.71832793	C	9.18819823	-9.03850623	-0.28409513
H	10.77048723	-5.95195307	-4.07907004	N	9.00810183	-10.36417144	-0.64991095
C	10.55536143	-8.06879803	-3.72936098	H	9.73834024	-11.06226936	-0.76406234
O	9.28839598	-8.17852110	-4.16505496	C	7.68718140	-10.56358689	-0.87925842
H	8.99219181	-7.30981104	-4.60063278	H	7.26413526	-11.49017934	-1.23020761
C	11.19775819	-9.22610889	-3.26422290	N	7.01469426	-9.45021762	-0.67759134
H	10.64162331	-10.15932320	-3.26973467	C	7.93325778	-8.49020814	-0.31066515
C	12.48150958	-9.13700519	-2.73827377	H	7.63079438	-7.47714290	-0.09917900
H	12.94624968	-10.00768756	-2.28731195	C	5.11942365	-3.77165006	1.45676104
C	5.93604372	1.22540381	-5.08379006	H	4.71650441	-2.89650678	0.93081548
H	4.99536272	1.34351003	-5.63013111	H	4.42852326	-3.99400157	2.27612816
H	5.73446448	1.45505254	-4.03406169	C	5.17526889	-4.95459624	0.55741507
C	6.32546400	-0.26922586	-5.15081607	N	5.22482631	-4.89644398	-0.82471233
O	5.68387879	-1.06767038	-4.48252018	H	5.20813293	-4.07552814	-1.42459281
O	7.30081997	-0.62740545	-5.97526350	C	5.22392418	-6.17155286	-1.29476130
H	7.43805422	-1.62122172	-5.93167671	H	5.24755440	-6.44513418	-2.33770218
C	5.28849857	-8.67407783	-9.74621783	N	5.17582627	-7.03560233	-0.29618010
H	5.99007774	-8.88141100	-10.55365526	C	5.14384165	-6.29431028	0.85589787
H	4.81798142	-9.61342339	-9.45679542	H	5.10990433	-6.76253586	1.83091966
C	6.07032440	-8.02601180	-8.59325964	C	5.99234026	-10.23869323	2.56001530
O	6.84331188	-7.07914500	-8.79846377	H	6.85184896	-9.89581041	1.97777182
N	5.85128212	-8.54194055	-7.37372778	H	5.39610231	-9.34686056	2.79857937
H	6.24993059	-8.07263444	-6.56350140	C	5.13349620	-11.15534325	1.72526988
H	5.14300991	-9.25928682	-7.22596552	N	4.62431774	-10.73218047	0.50531569
C	3.32534969	-4.74099138	-6.44416236	C	3.86177684	-11.71285347	0.04112182
H	3.28579160	-3.78910675	-6.98146569	H	3.28837984	-11.66243725	-0.87411034
H	2.73772307	-4.62859143	-5.52660527	N	3.85133356	-12.75814203	0.89477189
C	4.73758418	-5.00485073	-6.06066456	H	3.37659388	-13.65636782	0.74872128
C	5.02458896	-6.12595016	-5.08463362	C	4.65013703	-12.42148284	1.97111665
O	4.03386843	-6.70043695	-4.57599960	H	4.76206479	-13.08105245	2.81886425
C	6.37886768	-6.46535852	-4.83259391	Cu	4.97281608	-9.20315074	-0.98115953
H	6.56118619	-7.33634425	-4.20426711	O	7.37389207	-10.40500801	-3.81120474
C	7.43593844	-5.67955155	-5.32211634	H	8.03804555	-11.05211201	-3.47247700
O	8.66529279	-5.95109343	-5.28328340	H	7.77357506	-9.53321299	-3.66134213
C	7.06065666	-4.31217928	-5.90617931	O	2.95209566	-8.99036331	-0.97185865
O	7.85855302	-3.37119630	-5.87859494	H	2.46969373	-8.41320215	-1.60741407
C	5.71211157	-4.15363013	-6.42918239	H	2.37679753	-9.22818285	-0.19803146
H	5.52399395	-3.28515354	-7.05080590	O	5.19363356	-8.80983623	-2.80974397
C	-0.77236133	-1.39024123	-3.46627890	H	4.43783136	-8.32781090	-3.18597255
H	-1.04730596	-1.11298990	-2.43837966	O	1.90091905	-7.19922783	-2.86157873
H	-0.75043897	-0.46000526	-4.04498689	H	2.67813937	-6.83679334	-3.33221904
C	0.60167964	-2.01957900	-3.47627804	H	1.30809046	-7.45594039	-3.59801040
C	1.03600129	-2.87511041	-2.45577580	C	14.38236071	-7.43376864	-0.51543332
H	0.34282375	-3.16206179	-1.66746724	C	6.98750044	2.22994649	-5.63659877
C	2.34455023	-3.35008101	-2.41171527	C	4.20345832	-7.70971586	-10.28864684
H	2.67875697	-4.00959617	-1.61637314	C	2.64757937	-5.82804424	-7.31136905
C	3.25405712	-2.95035586	-3.39558357	C	-1.88970153	-2.28464720	-4.03689841
O	4.55435471	-3.35558411	-3.29048764	C	10.94298587	-8.74988614	1.53685398
H	5.11315557	-2.74117132	-3.81180912	C	6.49295284	-3.39819112	2.06669728
C	2.81963253	-2.15807043	-4.46394316	C	6.48900648	-10.84384632	3.87285564

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C	14.54095669	-7.89639808	-1.96823229	H	3.50366284	-1.84883094	-5.26982662
H	14.95981506	-8.90594003	-1.97378408	C	1.49575102	-1.67098543	-4.50059838
H	15.26938340	-7.24441580	-2.45298410	H	1.16890179	-1.01796144	-5.30667433
C	13.21380870	-7.93153221	-2.68749464	C	10.52603856	-8.45859373	0.07107982
C	12.59173300	-6.78981119	-3.20947936	H	11.28940635	-8.87691326	-0.58668878
H	13.09460902	-5.82681640	-3.16305223	H	10.53735820	-7.37846653	-0.09779285
C	11.30779998	-6.85564772	-3.74278060	C	9.17681347	-8.99302823	-0.26405940
H	10.81934355	-5.96209767	-4.11238614	N	8.90003093	-10.32764688	-0.53520943
C	10.61619343	-8.07864468	-3.76717955	H	9.57902460	-11.07993731	-0.62683702
O	9.35145120	-8.18014840	-4.23939693	C	7.56116629	-10.46140510	-0.68093684
H	9.08503751	-7.32062606	-4.71053406	H	7.04519565	-11.38822126	-0.86613119
C	11.23752800	-9.23469402	-3.28293810	N	6.97264093	-9.28697320	-0.54269856
H	10.68901949	-10.17213264	-3.29673540	C	7.96246438	-8.36475501	-0.28771101
C	12.51591818	-9.14336025	-2.74251746	H	7.73585582	-7.32512445	-0.11938616
H	12.97480608	-10.01026946	-2.27873836	C	5.13242244	-3.79939679	1.44014832
C	5.94048532	1.22408450	-5.08675941	H	4.68352154	-2.91241642	0.97554406
H	4.99963428	1.34322909	-5.63112597	H	4.46461984	-4.10839262	2.24871161
H	5.74096177	1.45188772	-4.03684447	C	5.23108394	-4.91365663	0.45263040
C	6.32858560	-0.26724845	-5.16288557	N	5.22696846	-4.75290348	-0.92260080
O	5.68443476	-1.07616214	-4.50963253	H	5.17023001	-3.89611400	-1.46782403
O	7.30941560	-0.62004280	-5.98558322	C	5.24731422	-5.98128957	-1.49626531
H	7.43795502	-1.60953324	-5.95649557	H	5.21608249	-6.14417780	-2.55974564
C	5.28574423	-8.68544124	-9.76462152	N	5.26928876	-6.91776134	-0.56706379
H	5.97825825	-8.89069402	-10.57970825	C	5.25450240	-6.27052730	0.64746282
H	4.81316120	-9.62551875	-9.47890352	H	5.24652014	-6.82412033	1.57632723
C	6.08459642	-8.05582408	-8.61641283	C	6.04520695	-10.16088100	2.57094569
O	6.83853437	-7.09148053	-8.80304031	H	6.93903369	-9.82203688	2.03214073
N	5.91119031	-8.61783854	-7.40778067	H	5.49579740	-9.24363209	2.84471141
H	6.32642728	-8.15719575	-6.60320481	C	5.16011740	-11.01910705	1.71452426
H	5.19035768	-9.32271346	-7.25840306	N	4.68269112	-10.61714835	0.46705130
C	3.34586934	-4.81277338	-6.37720808	C	3.80099289	-11.59058134	0.08993728
H	3.28866097	-3.82716087	-6.84618660	H	3.25128154	-11.53371091	-0.84153460
H	2.77555921	-4.76361639	-5.44249711	N	3.66917900	-12.55610811	0.97796484
C	4.77352772	-5.09768263	-6.04990507	H	5.88699133	-9.49279844	-3.14862126
C	5.13186790	-6.26788064	-5.15526384	C	4.51913031	-12.21031900	1.99432650
O	4.20688567	-6.96621723	-4.66381698	H	4.59419098	-12.82028125	2.88957286
C	6.49957619	-6.53588283	-4.92350376	Cu	4.95790631	-8.99066296	-0.57834205
H	6.75147111	-7.40933580	-4.32947460	O	7.44886008	-10.18270244	-3.82327700
C	7.52637592	-5.71555348	-5.41651013	H	7.91047354	-10.93801507	-3.39424674
O	8.75549669	-5.96922300	-5.38506243	H	8.13259257	-9.47955616	-3.88488869
C	7.10027749	-4.34999588	-5.96883245	O	2.98467081	-8.50016326	-0.56124177
O	7.88063080	-3.39760732	-5.97076837	H	2.53803296	-8.28282581	-1.41242837
C	5.72493910	-4.22071367	-6.42719697	H	2.38096032	-9.06709784	0.01046395
H	5.48801609	-3.32780047	-6.99600390	O	5.00615178	-9.17181861	-2.85096200
C	-0.77903459	-1.39102741	-3.46134478	H	4.73086666	-8.46084768	-3.46439240
H	-1.05168150	-1.12714669	-2.42971289	O	1.99587826	-7.27028267	-2.91265696
H	-0.76615911	-0.45624318	-4.03138462	H	2.76069423	-7.03184465	-3.46929279
C	0.59677949	-2.01134418	-3.48423741	H	1.32225438	-7.53159543	-3.57290230
C	1.03778065	-2.88159678	-2.47971080	C	14.38315446	-7.43536821	-0.51167736
H	0.35283123	-3.17071977	-1.68561827	C	6.98961919	2.22925644	-5.63961040
C	2.34479950	-3.36296019	-2.45587946	C	4.20274224	-7.71427096	-10.28944195
H	2.68072913	-4.03641282	-1.67408376	C	2.64922252	-5.83444829	-7.30150423
C	3.24456929	-2.94873400	-3.44257778	C	-1.88847086	-2.28931604	-4.03516195
O	4.54769670	-3.36476181	-3.36070641	C	10.94289945	-8.75348079	1.53341153
H	5.10314899	-2.73493003	-3.86845043	C	6.49212264	-3.40216974	2.06501081
C	2.80589181	-2.13497223	-4.49162623	C	6.49568722	-10.83153403	3.86831489

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C	14.54901309	-7.88221151	-1.97127296	H	3.52099854	-1.55443743	-5.33994791
H	14.99876775	-8.87702818	-1.98410341	C	1.50712113	-1.55602383	-4.56539985
H	15.25052891	-7.20407245	-2.46007251	H	1.15509605	-0.82329209	-5.28811039
C	13.21696484	-7.96742156	-2.67544101	C	10.49138521	-8.44109381	0.08505173
C	12.55594971	-6.86410346	-3.23229830	H	11.26116723	-8.81928171	-0.58842086
H	13.03302436	-5.88711345	-3.24236749	H	10.46606883	-7.35787881	-0.06400375
C	11.25978852	-6.98909883	-3.72746279	C	9.15971303	-9.02184550	-0.27352736
H	10.74154115	-6.12481685	-4.12900652	N	8.98614802	-10.32079993	-0.72706979
C	10.60234048	-8.22725455	-3.67392739	H	9.71528039	-11.01196349	-0.88547012
O	9.31752858	-8.38299848	-4.06816052	C	7.67366915	-10.51300781	-0.98673456
H	9.03506106	-7.61358517	-4.62043047	H	7.26661951	-11.42606281	-1.38826958
C	11.26877952	-9.34945272	-3.17343088	N	6.98955418	-9.41610027	-0.71360035
H	10.74003684	-10.29637376	-3.14660331	C	7.90195741	-8.47555972	-0.27539204
C	12.55586713	-9.20160267	-2.67129469	H	7.59244461	-7.48203114	0.00377938
H	13.05384004	-10.03602879	-2.18673068	C	5.13093019	-3.75976075	1.42659764
C	5.91255218	1.25040677	-5.07215102	H	4.74504649	-2.88034649	0.89762332
H	4.96759130	1.40115701	-5.60560350	H	4.42574147	-3.97857490	2.23395512
H	5.73015692	1.49303735	-4.02162080	C	5.18372348	-4.94200328	0.51940079
C	6.28322719	-0.28824935	-5.17817868	N	5.15107787	-4.88939664	-0.86499019
O	5.52057662	-0.97626456	-4.40487033	H	5.11835309	-4.06678225	-1.46810366
O	7.14598993	-0.71315395	-5.95373392	C	5.11973869	-6.16754173	-1.32578346
H	6.60946827	-5.43720835	-3.81372033	H	5.05727858	-6.44555814	-2.36485362
C	5.28873436	-8.67131781	-9.74056803	N	5.13553114	-7.02983438	-0.32431345
H	6.00298993	-8.86246078	-10.54114853	C	5.16834044	-6.28099637	0.82571070
H	4.82174783	-9.61933024	-9.47498552	H	5.17383449	-6.74462703	1.80345525
C	6.07943875	-8.05855413	-8.56362304	C	5.98848872	-10.24061808	2.56751113
O	6.82802375	-7.08337304	-8.72828140	H	6.84790617	-9.89811169	1.98139264
N	5.91074678	-8.66673543	-7.37876073	H	5.39579325	-9.34728335	2.80855116
H	6.46324741	-8.46612505	-6.54655619	C	5.12797720	-11.16388623	1.74650458
H	5.23636572	-9.42392233	-7.28151439	N	4.63053046	-10.75853253	0.51570183
C	3.39590533	-4.73601795	-6.47521294	C	3.86186093	-11.74222693	0.06284884
H	3.34171368	-3.78722639	-7.01572738	H	3.30179569	-11.71184090	-0.85955605
H	2.85586701	-4.60401459	-5.53393268	N	3.83646367	-12.76721812	0.93567487
C	4.83605755	-5.03000410	-6.18758572	H	3.36005365	-13.66709166	0.79079780
C	5.11141096	-6.02023446	-5.12612960	C	4.63057200	-12.41925674	2.00963845
O	4.20496443	-6.62743443	-4.56681665	H	4.73329745	-13.06210312	2.87186739
C	6.53563053	-6.16917148	-4.63320039	Cu	4.95776260	-9.20624048	-0.87914737
H	6.68341788	-7.17086236	-4.22297356	O	6.77641693	-9.33736979	-4.62307160
C	7.59424472	-5.81098471	-5.63848777	H	7.62784888	-9.29989855	-4.15339748
O	8.69073979	-6.34902899	-5.67428160	H	6.07740792	-9.22385244	-3.89451029
C	7.26734410	-4.69833041	-6.63978167	O	2.95794476	-8.98444302	-0.89432051
O	8.14607944	-4.22178820	-7.33134626	H	2.48868808	-8.44047920	-1.56766558
C	5.85189426	-4.33089136	-6.75545527	H	2.35371792	-9.23311367	-0.14010052
H	5.66624990	-3.48587272	-7.40378693	O	5.02695110	-8.98274746	-2.78460904
C	-0.75653502	-1.41370145	-3.46490440	H	4.23767926	-8.55076232	-3.14100353
H	-0.99206322	-1.19933028	-2.41236559	O	1.97881514	-7.31928737	-2.91506525
H	-0.76990033	-0.45130557	-3.98779206	H	2.68195635	-6.82436488	-3.37064690
C	0.62745739	-2.01871660	-3.57745535	H	1.33784969	-7.51970416	-3.63008177
C	1.10866515	-2.98141969	-2.68399830	C	14.38652205	-7.43246723	-0.51145311
H	0.44723543	-3.37099703	-1.91277156	C	6.98098959	2.23179601	-5.63872288
C	2.43215169	-3.42507405	-2.72986174	C	4.20421615	-7.71289665	-10.28879190
H	2.78844418	-4.15902368	-2.01167270	C	2.65822250	-5.82087879	-7.30737324
C	3.32617345	-2.88017188	-3.66483759	C	-1.88646935	-2.28623654	-4.03858399
O	4.63906577	-3.22234652	-3.63819259	C	10.94142159	-8.74987912	1.53550808
H	5.17264270	-2.40633027	-4.03971926	C	6.49559675	-3.39564835	2.06027280
C	2.82715770	-1.98003226	-4.62606836	C	6.49056760	-10.84380673	3.87539011

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C	14.56530853	-7.87279713	-1.96736280	H	3.50831451	-1.55027107	-5.34859136
H	15.03210267	-8.85836375	-1.98009631	C	1.49739944	-1.54942824	-4.56252158
H	15.25377274	-7.17907031	-2.45064414	H	1.14244938	-0.81302632	-5.28113319
C	13.23846117	-7.99110768	-2.67072288	C	10.48814332	-8.44449215	0.08060765
C	12.53137519	-6.90797398	-3.20245485	H	11.25657990	-8.82730809	-0.59229088
H	12.97124458	-5.91442710	-3.20644149	H	10.46543334	-7.36132031	-0.06918647
C	11.23011162	-7.07553279	-3.67365742	C	9.15353451	-9.02008250	-0.27883923
H	10.66869958	-6.22201522	-4.03801074	N	8.97875022	-10.31278459	-0.74890037
C	10.61971388	-8.33710629	-3.62028298	H	9.70572927	-11.00512003	-0.90884628
O	9.33157654	-8.54702917	-3.97719234	C	7.66585844	-10.49995722	-1.01209911
H	9.01609397	-7.80788200	-4.53455928	H	7.25777817	-11.40825180	-1.42581487
C	11.33851190	-9.44043098	-3.15084790	N	6.98419164	-9.40394656	-0.73038529
H	10.84951807	-10.40792121	-3.12924107	C	7.89639440	-8.47135838	-0.27860729
C	12.62528593	-9.24845709	-2.67007480	H	7.58663833	-7.47904122	0.00631505
H	13.16756412	-10.06242319	-2.20186572	C	5.11948312	-3.75588370	1.44333383
C	5.91369278	1.25339143	-5.06622008	H	4.72629336	-2.87344549	0.92405335
H	4.96691538	1.40713329	-5.59690615	H	4.42315472	-3.98547404	2.25522824
H	5.73279102	1.49106760	-4.01379838	C	5.17213825	-4.92936996	0.53051688
C	6.28497197	-0.28346223	-5.18196466	N	5.20089476	-4.87103440	-0.85280957
O	5.51052223	-0.97812518	-4.43075984	H	5.19324670	-4.04930380	-1.45743593
O	7.16368023	-0.69738889	-5.94610092	C	5.18243199	-6.14520911	-1.31915516
H	9.11673579	-5.93733474	-6.28152632	H	5.16667508	-6.40835318	-2.36186194
C	5.28585748	-8.68034312	-9.74565870	N	5.14453039	-7.01239393	-0.32129104
H	5.99216976	-8.87627347	-10.55205964	C	5.13156624	-6.26847728	0.83178128
H	4.81291329	-9.62562426	-9.47761508	H	5.09162738	-6.73376229	1.80789084
C	6.09163745	-8.07788310	-8.57434744	C	5.98886893	-10.23460968	2.56842730
O	6.85064129	-7.11037990	-8.74189963	H	6.84886090	-9.89075725	1.98381154
N	5.93432311	-8.69357973	-7.39227521	H	5.39633028	-9.34309473	2.81371231
H	6.46453909	-8.44468460	-6.56168473	C	5.13164790	-11.15414960	1.74104919
H	5.25138745	-9.44085844	-7.28631632	N	4.63294556	-10.74085188	0.51253664
C	3.38551371	-4.72868444	-6.47029802	C	3.86765960	-11.72353682	0.05211242
H	3.35457422	-3.78672278	-7.02406457	H	3.30624467	-11.68668930	-0.86903121
H	2.82594836	-4.58256218	-5.54273835	N	3.84624773	-12.75642266	0.91602242
C	4.81029343	-5.04181196	-6.15867319	H	3.36928014	-13.65573763	0.76831294
C	5.05589413	-6.04197352	-5.06855294	C	4.63823258	-12.41360419	1.99376684
O	4.09942933	-6.49546974	-4.43339122	H	4.74156711	-13.06435326	2.85005813
C	6.42129419	-6.47774975	-4.78616121	Cu	4.94406026	-9.17914712	-0.87839842
H	6.55449822	-7.27490201	-4.06771770	O	6.80639804	-9.52016101	-4.48285014
C	7.40741423	-5.99970476	-5.56385227	H	7.61377050	-9.51735686	-3.94464485
O	8.68517214	-6.42905187	-5.53917379	H	6.06671976	-9.31413829	-3.82566953
C	7.19888603	-4.92253292	-6.58241003	O	2.94706922	-8.96827976	-0.88734350
O	8.18632519	-4.58164500	-7.23497208	H	2.46864798	-8.43584770	-1.56655913
C	5.84846863	-4.42383144	-6.76390381	H	2.34402430	-9.22399845	-0.13348521
H	5.73296804	-3.58791855	-7.43745020	O	5.01398543	-8.90528952	-2.77412293
C	-0.76232557	-1.41311470	-3.45919649	H	4.24796711	-8.42681852	-3.12891249
H	-1.00104876	-1.20103211	-2.40726761	O	1.90435789	-7.30153226	-2.85246855
H	-0.77750830	-0.45046123	-3.98127173	H	2.59849826	-6.75363974	-3.25871799
C	0.62115670	-2.01447683	-3.57267226	H	1.31032528	-7.51471876	-3.60288885
C	1.10426196	-2.97957876	-2.68256869	C	14.38695714	-7.43277474	-0.50985544
H	0.44634993	-3.37186936	-1.90909395	C	6.98261020	2.23364917	-5.63142286
C	2.42780196	-3.42151496	-2.73275410	C	4.20371415	-7.71276839	-10.28590531
H	2.79268533	-4.15413940	-2.01870377	C	2.65744508	-5.81671325	-7.30500829
C	3.31887594	-2.87463797	-3.67093902	C	-1.88898714	-2.28830255	-4.03625980
O	4.62697784	-3.21962718	-3.64566038	C	10.93798874	-8.75212084	1.53301937
H	5.16358993	-2.41763273	-4.05691376	C	6.48977117	-3.39630265	2.06575882
C	2.81673990	-1.97395188	-4.63111429	C	6.49113908	-10.84359094	3.87486933

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C	14.55856563	-7.91829706	-1.96276383	H	3.49556902	-2.14737734	-5.15835730
H	15.00315046	-8.91703776	-1.94458980	C	1.49046136	-1.83275356	-4.43425051
H	15.27705474	-7.25426566	-2.44677233	H	1.17634343	-1.29015078	-5.32540079
C	13.24468407	-8.00987456	-2.69625342	C	10.44079587	-8.43822926	0.08529185
C	12.64584207	-6.91613257	-3.33131709	H	11.17614024	-8.86607834	-0.59386674
H	13.16797294	-5.96272541	-3.38211476	H	10.46942327	-7.35293128	-0.06751816
C	11.35310600	-7.00773636	-3.83943983	C	9.07813368	-8.97151732	-0.22742968
H	10.87801637	-6.15015269	-4.30030695	N	8.86335024	-10.29235186	-0.56982253
C	10.62610715	-8.20340797	-3.70110867	C	7.54436994	-10.38166388	-0.70559583
O	9.35105653	-8.31339352	-4.12398156	H	7.01463546	-11.28703720	-0.97181406
H	9.10117667	-7.49704401	-4.68517696	N	6.89113625	-9.21232292	-0.48938774
C	11.22287068	-9.31499899	-3.09465123	C	7.87406176	-8.29990873	-0.18576238
H	10.62273711	-10.19877463	-2.90610965	H	7.64072923	-7.26771927	0.02725065
C	12.51449485	-9.20191065	-2.59994623	C	5.11776722	-3.74518263	1.40260979
H	12.94199263	-10.02284373	-2.03014436	H	4.73501626	-2.85528106	0.88718821
C	5.91339653	1.25507295	-5.03350689	H	4.41312025	-3.97208698	2.21170642
H	4.95946700	1.37491078	-5.55841598	C	5.15274532	-4.89753965	0.44251613
H	5.74122714	1.51911814	-3.98399867	N	5.03725588	-4.75780442	-0.92891379
C	6.32410817	-0.22891171	-5.11611525	H	4.76142209	-8.52260017	-3.40566836
O	5.51564021	-0.91258842	-4.29400755	C	5.00197822	-6.01398262	-1.39878854
O	7.17958273	-0.72616429	-5.81386492	H	4.91114047	-6.25909761	-2.44551578
H	5.71118133	-1.87348092	-4.25965339	N	5.07286632	-6.94719799	-0.43797281
C	5.28762608	-8.69694895	-9.77128328	C	5.16788132	-6.24675186	0.73813998
H	5.98135125	-8.89264655	-10.58766524	H	5.25339437	-6.75258856	1.69221316
H	4.81268659	-9.63953316	-9.49650755	C	6.01582255	-10.24427895	2.54632448
C	6.08931369	-8.08097284	-8.61693035	H	6.88688796	-9.92686554	1.96453421
O	6.82987682	-7.10765195	-8.80849803	H	5.43528265	-9.33778350	2.76724386
N	5.93660444	-8.66307827	-7.41860159	C	5.14754534	-11.15683893	1.71646919
H	6.33952224	-8.20231933	-6.60269326	N	4.63310732	-10.73060610	0.49717979
H	5.21215680	-9.36392050	-7.27244586	C	3.87853003	-11.70808722	0.02351024
C	3.39443684	-4.89841493	-6.33383649	H	3.31726321	-11.65381860	-0.89667136
H	3.35178001	-3.89395114	-6.76413883	N	3.86963892	-12.75885344	0.87161561
H	2.85252790	-4.87631567	-5.38272801	H	3.40176017	-13.65902162	0.71966394
C	4.83832443	-5.24493230	-6.09560018	C	4.66699775	-12.42392240	1.95129491
C	5.19096955	-6.37016229	-5.15191622	H	4.78763616	-13.09077626	2.79265186
O	4.25716058	-6.98640720	-4.56542195	Cu	4.97409977	-8.94733406	-0.62875062
C	6.55794028	-6.69523160	-4.96944401	O	7.38890954	-10.22145325	-3.80915877
H	6.79646526	-7.45665276	-4.23293623	H	7.82287198	-10.96021677	-3.31635788
C	7.60025981	-6.03133338	-5.64203749	H	8.07147610	-9.51469467	-3.77722839
O	8.82636393	-6.30469845	-5.55773219	O	2.96640679	-8.93089483	-0.88064153
C	7.23258232	-4.88132515	-6.58857950	H	2.53329283	-8.31022513	-1.51448880
O	8.08648264	-4.31141336	-7.25163443	H	2.35585339	-9.16588919	-0.13133549
C	5.81272715	-4.52327373	-6.68431067	O	4.98175400	-9.31340092	-2.86923402
H	5.59809592	-3.67060032	-7.31775565	H	5.89988526	-9.57911543	-3.12501059
C	-0.78887306	-1.37548849	-3.45549611	O	1.98811720	-7.17849993	-2.87095747
H	-1.10448535	-1.05554203	-2.45137488	H	2.79242430	-6.91188761	-3.35961957
H	-0.74242927	-0.46865022	-4.06889769	H	1.38798056	-7.47711161	-3.58200182
C	0.57998293	-2.00843882	-3.38427439	C	14.36520848	-7.43992243	-0.51587982
C	1.01881994	-2.71629859	-2.25810635	C	6.97161450	2.21533402	-5.63575241
H	0.33012685	-2.87054140	-1.42699399	C	4.20751218	-7.71822641	-10.28768381
C	2.31692482	-3.21501870	-2.16029377	C	2.64983078	-5.86016834	-7.29213358
H	2.64704582	-3.76258256	-1.28355476	C	-1.89066186	-2.28202509	-4.03332738
C	3.23111271	-2.99568932	-3.20712615	C	10.91224346	-8.76076488	1.52403262
O	4.51522060	-3.39928852	-3.16347677	C	6.48437816	-3.38969389	2.04489060
H	4.75642104	-3.78305899	-2.23728382	C	6.49069659	-10.84193047	3.86997764
C	2.78936870	-2.31711414	-4.35593963				

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C	14.54822083	-7.91469640	-1.96793496	H	3.56866086	-2.12271815	-5.02911122
H	14.97037110	-8.92378934	-1.95490277	C	1.53345917	-1.80164135	-4.37170402
H	15.28501027	-7.26570501	-2.44494908	H	1.28017497	-1.16544363	-5.21868614
C	13.23575723	-7.96304191	-2.71363576	C	10.44540665	-8.44294524	0.07911186
C	12.66081314	-6.84013748	-3.32120476	H	11.18108189	-8.87766649	-0.59689873
H	13.19547912	-5.89258085	-3.33160830	H	10.47886263	-7.35829846	-0.07746750
C	11.37774093	-6.89650525	-3.85951611	C	9.08237620	-8.97419872	-0.23750574
H	10.91832442	-6.01284676	-4.28528163	N	8.87192701	-10.29237436	-0.59273271
C	10.63512427	-8.08709890	-3.78538557	C	7.55211988	-10.38467709	-0.72610117
O	9.37199510	-8.17389335	-4.25415209	H	7.02371167	-11.29002290	-0.99671233
H	9.10064505	-7.30572665	-4.70591141	N	6.89683548	-9.21867714	-0.50185831
C	11.20289143	-9.22442068	-3.19832959	C	7.87631242	-8.30571929	-0.19016510
H	10.59230126	-10.11088835	-3.06286160	H	7.63943219	-7.27676320	0.03470547
C	12.48472566	-9.14574439	-2.67028656	C	5.10974732	-3.77349693	1.43717242
H	12.88783414	-9.99221739	-2.12093620	H	4.70886735	-2.89783258	0.91233798
C	5.93888483	1.21161250	-5.07804438	H	4.42096183	-4.00001827	2.26085081
H	4.97787813	1.36029611	-5.57880320	C	5.14644305	-4.93816311	0.49540415
H	5.79155329	1.40471146	-4.01256207	N	5.05536302	-4.79443226	-0.87214855
C	6.29521114	-0.28682123	-5.22802627	H	4.74348637	-8.53613856	-3.42579826
O	5.59262379	-1.11344918	-4.68809960	C	5.02862140	-6.04592278	-1.34907895
O	7.34705453	-0.61231012	-5.99803530	H	4.95978704	-6.28449889	-2.39986971
H	7.43388882	-1.60363616	-6.00365052	N	5.07948834	-6.98296127	-0.39132558
C	5.29177180	-8.68724207	-9.76071020	C	5.15256227	-6.28897226	0.79100507
H	5.98983955	-8.88401307	-10.57390902	H	5.22072670	-6.80236157	1.74218083
H	4.82189578	-9.62968809	-9.47906808	C	6.01577201	-10.24668963	2.54504936
C	6.08813356	-8.05429145	-8.60987323	H	6.88813472	-9.92765773	1.96567232
O	6.83571019	-7.08783112	-8.81081583	H	5.43509722	-9.34062941	2.76449245
N	5.91413848	-8.60304249	-7.39799971	C	5.15214616	-11.16083566	1.71154308
H	6.31464959	-8.12192494	-6.59326992	N	4.63830791	-10.73541205	0.49195688
H	5.19003540	-9.30270215	-7.24115144	C	3.88140678	-11.71016616	0.01846370
C	3.31420649	-4.86351559	-6.31791663	H	3.31238308	-11.64911807	-0.89653566
H	3.24144798	-3.85932327	-6.74419634	N	3.87348617	-12.76192469	0.86505255
H	2.73821560	-4.85897711	-5.38534749	H	3.40284682	-13.66122195	0.71491383
C	4.74738857	-5.12924458	-5.99461186	C	4.67226405	-12.42831474	1.94397115
C	5.12430699	-6.30506839	-5.12075712	H	4.79240973	-13.09594570	2.78452819
O	4.20616393	-7.02125103	-4.63640620	Cu	4.97544791	-8.95782695	-0.62771552
C	6.49923769	-6.56775390	-4.92039396	O	7.44289798	-10.14699289	-3.84409497
H	6.76949783	-7.42622885	-4.31261936	H	7.86550735	-10.86257203	-3.31257219
C	7.51186949	-5.72709658	-5.41239691	H	8.11116457	-9.42839511	-3.83533695
O	8.74571036	-5.96802823	-5.39459288	O	2.96419601	-8.93769630	-0.89645991
C	7.07660197	-4.37103808	-5.98870891	H	2.53540710	-8.29856019	-1.51578795
O	7.87763976	-3.44286253	-6.10003868	H	2.35615953	-9.15797998	-0.14038468
C	5.67948045	-4.23256509	-6.36881397	O	4.99656611	-9.31542271	-2.88794049
H	5.41816220	-3.33137116	-6.91160973	H	5.92433301	-9.53968073	-3.14508151
C	-0.78457476	-1.37720449	-3.46063658	O	1.98877752	-7.15548758	-2.87129662
H	-1.10499140	-1.03740750	-2.46397150	H	2.79056885	-6.89251174	-3.36464649
H	-0.72329396	-0.48272096	-4.09062895	H	1.37896540	-7.44386334	-3.57832192
C	0.57700839	-2.03136623	-3.37436587	C	14.36352409	-7.43984901	-0.51802542
C	0.94382890	-2.84567696	-2.29441115	C	6.97839104	2.21455940	-5.64123294
H	0.21013878	-3.04660314	-1.51334607	C	4.20746006	-7.71861571	-10.28740909
C	2.21619424	-3.40686129	-2.19420597	C	2.64216053	-5.85906778	-7.29403325
H	2.48989955	-4.04797975	-1.36031371	C	-1.89241883	-2.28214148	-4.03237263
C	3.17821442	-3.14125791	-3.18992149	C	10.91107400	-8.76077872	1.52202560
O	4.42393698	-3.62657693	-3.15477394	C	6.48388316	-3.39206540	2.04890071
H	4.68833778	-3.90173452	-2.20891940	C	6.48941272	-10.84362903	3.86996318
C	2.80845245	-2.34337033	-4.28970881				

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C	14.55484509	-7.90723391	-1.96312854	H	3.49189983	-2.12363439	-5.21109533
H	15.00090735	-8.90519579	-1.95255145	C	1.49196562	-1.81511198	-4.46911710
H	15.27261399	-7.24143219	-2.44540539	H	1.17042726	-1.27312332	-5.35757673
C	13.23752046	-7.99046420	-2.69109592	C	10.50801611	-8.43189073	0.06656520
C	12.59873763	-6.87944928	-3.25775262	H	11.27610548	-8.83268536	-0.59736245
H	13.09263357	-5.91021340	-3.26143250	H	10.51738585	-7.34734643	-0.07956975
C	11.30605855	-6.97973135	-3.75994666	C	9.15921621	-8.95079374	-0.28367184
H	10.80298596	-6.11212926	-4.16938517	N	8.86686634	-10.28716313	-0.53640201
C	10.61638504	-8.20698139	-3.70422924	C	7.52487952	-10.40368423	-0.68673038
O	9.34608736	-8.32664508	-4.12234586	H	6.99419541	-11.32542913	-0.85507866
H	9.08676693	-7.49825806	-4.70386715	N	6.95635936	-9.21963998	-0.56470408
C	11.26545726	-9.33619574	-3.18634354	C	7.95472296	-8.30605244	-0.32185402
H	10.72245821	-10.27515296	-3.14145719	H	7.73148446	-7.26201781	-0.17171804
C	12.55352430	-9.21066382	-2.67925601	C	5.12083969	-3.76716606	1.39830045
H	13.02761569	-10.04841992	-2.17602063	H	4.70386542	-2.86920509	0.92610127
C	5.91211842	1.26266655	-5.03176515	H	4.43390231	-4.05848885	2.20127714
H	4.96369051	1.38169027	-5.56520841	C	5.19940374	-4.87437295	0.38770016
H	5.73444093	1.53418389	-3.98746817	N	5.07761922	-4.69444245	-0.97826965
C	6.32007619	-0.21995768	-5.10303326	H	9.53809865	-11.04431962	-0.60859267
O	5.52716225	-0.88880170	-4.25738537	C	5.11335145	-5.93484988	-1.49053509
O	7.16015723	-0.72703027	-5.81286831	H	5.00673770	-6.14829807	-2.54148369
H	5.69441520	-1.85531944	-4.22434407	N	5.25212199	-6.89281249	-0.56442159
C	5.29964975	-8.68974593	-9.77203358	C	5.29755921	-6.22734222	0.63592579
H	5.99747129	-8.87916139	-10.58645916	H	5.36827247	-6.76148694	1.57530244
H	4.82550503	-9.63508126	-9.50435808	C	6.07357989	-10.15288967	2.56032551
C	6.09499549	-8.08105602	-8.61198557	H	6.97609931	-9.79966807	2.04169299
O	6.83142294	-7.10171317	-8.78735818	H	5.50242038	-9.24548473	2.81880747
N	5.94085356	-8.67670481	-7.41927496	C	5.22478730	-11.01528127	1.67029744
H	6.33480534	-8.21801067	-6.59824944	N	4.69792104	-10.56084516	0.46838076
H	5.21037098	-9.37318403	-7.28184193	C	3.91956733	-11.57948070	0.01495100
C	3.41892146	-4.88571898	-6.35467813	H	3.35582355	-11.49130087	-0.90457641
H	3.37992247	-3.88699574	-6.79779305	N	3.89255261	-12.63640405	0.81134893
H	2.88618250	-4.84475227	-5.39974596	H	4.68370762	-8.44251327	-3.38654570
C	4.85940413	-5.24740879	-6.12491676	C	4.71104922	-12.28744102	1.85181895
C	5.19398781	-6.37093287	-5.17706890	H	4.85291567	-12.95134384	2.69952506
O	4.25279209	-6.97158033	-4.59591750	Cu	4.94247585	-8.87544151	-0.53390912
C	6.55939519	-6.71453318	-4.97678043	O	7.35842438	-10.22375638	-3.80288937
H	6.77256989	-7.47423345	-4.23021204	H	7.81142325	-10.98514307	-3.37056680
C	7.60940659	-6.07650224	-5.64839917	H	8.05364381	-9.52879074	-3.82877012
O	8.83849442	-6.36082990	-5.54964393	O	2.95134764	-8.44567273	-0.51313731
C	7.26162442	-4.94243014	-6.61941218	H	2.52290486	-8.25567020	-1.37774194
O	8.12522208	-4.40782754	-7.29747521	H	2.35519561	-9.02752911	0.04816666
C	5.84915027	-4.55198920	-6.71818910	O	4.90278801	-9.21570645	-2.82435049
H	5.65498240	-3.69593773	-7.35358952	H	5.79203620	-9.52200612	-3.10907953
C	-0.78177432	-1.37143731	-3.46705326	O	1.96427456	-7.24041641	-2.90180794
H	-1.08502372	-1.05761905	-2.45773679	H	2.76314459	-6.92609748	-3.36211989
H	-0.74637233	-0.46184610	-4.07721381	H	1.36891187	-7.50097432	-3.63218343
C	0.59110259	-1.99735816	-3.41275706	C	14.36707668	-7.43472671	-0.51435293
C	1.03800099	-2.70975744	-2.29342061	C	6.97180396	2.21926652	-5.63393596
H	0.35450359	-2.87358553	-1.46071258	C	4.21952143	-7.71150937	-10.28792205
C	2.33714371	-3.20450082	-2.20647803	C	2.65845992	-5.85782101	-7.29023906
H	2.67003264	-3.75949172	-1.33584516	C	-1.88521448	-2.28292939	-4.03378857
C	3.24346237	-2.97321190	-3.25666812	C	10.92108678	-8.75919618	1.52400824
O	4.53307382	-3.36896798	-3.21897977	C	6.47979560	-3.39689507	2.04827953
H	4.77786637	-3.72814915	-2.28443637	C	6.49717587	-10.82952405	3.86732819
C	2.79284965	-2.29531568	-4.40094980				

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C	14.55476796	-7.91502040	-1.96624322	H	3.44562754	-1.71475717	-5.38159425
H	14.97632114	-8.92426060	-1.95192821	C	1.47250232	-1.55680446	-4.52522212
H	15.29250568	-7.26574087	-2.44170468	H	1.13201592	-0.83141500	-5.26236195
C	13.24464313	-7.96354036	-2.71342156	C	10.45466291	-8.43662620	0.07827026
C	12.66541584	-6.83806174	-3.31063201	H	11.19219762	-8.87244392	-0.59565097
H	13.19747473	-5.88895316	-3.31374452	H	10.49418664	-7.35166420	-0.07444076
C	11.38026092	-6.89378114	-3.84323635	C	9.08979053	-8.95787815	-0.24179086
H	10.91711754	-6.00782100	-4.25985612	N	8.87009020	-10.28001998	-0.57662155
C	10.64340199	-8.08849071	-3.77734281	C	7.54865859	-10.36146086	-0.70738390
O	9.38042489	-8.17877821	-4.24584018	H	7.01234823	-11.26756320	-0.96004341
H	9.11090597	-7.31304765	-4.69662441	N	6.90203812	-9.18724274	-0.50023117
C	11.21634716	-9.22868518	-3.20122711	C	7.88917164	-8.27872825	-0.20571905
H	10.60823947	-10.11763889	-3.07122914	H	7.65597717	-7.24433200	-0.00020618
C	12.49924716	-9.14952087	-2.67655805	C	5.10400679	-3.78371923	1.46313042
H	12.90701832	-9.99629255	-2.13141927	H	4.68160678	-2.90750792	0.95604027
C	5.94475606	1.19871901	-5.06786594	H	4.43715198	-4.03124123	2.29849110
H	4.98442250	1.32745142	-5.57564666	C	5.13849761	-4.92674374	0.49474620
H	5.78452095	1.40569230	-4.00711573	N	5.09422011	-4.71615849	-0.86133350
C	6.32311392	-0.29515159	-5.18682298	H	4.78607918	-8.56069487	-3.41891546
O	5.64995022	-1.10817257	-4.57996552	C	5.06686852	-5.94178266	-1.38763185
O	7.32775517	-0.63774898	-5.99107613	H	5.03623838	-6.14237894	-2.44920626
H	7.43782574	-1.63275317	-5.98038729	N	5.07107593	-6.93265305	-0.46402337
C	5.29132486	-8.68780407	-9.76148528	C	5.11765183	-6.28671854	0.74939599
H	5.98696940	-8.88752851	-10.57589986	H	5.15406749	-6.83760558	1.68159330
H	4.82028460	-9.62928816	-9.47875815	C	6.01462857	-10.24416235	2.54625169
C	6.09070717	-8.05685639	-8.61223561	H	6.88572049	-9.92120779	1.96861126
O	6.83502480	-7.08682040	-8.81210308	H	5.43045294	-9.34038325	2.76891752
N	5.92592458	-8.61444662	-7.40355859	C	5.15129535	-11.15430721	1.70631174
H	6.33625525	-8.14380009	-6.59770076	N	4.64075417	-10.71965305	0.48836375
H	5.20288599	-9.31549248	-7.24598374	C	3.88854911	-11.69478164	0.00690153
C	3.33682467	-4.87576279	-6.33322618	H	3.32920790	-11.63429087	-0.91460314
H	3.25375793	-3.86834504	-6.74909988	N	3.87820125	-12.75264391	0.84717236
H	2.78517680	-4.88369310	-5.38754564	H	3.40878318	-13.65120682	0.69237435
C	4.77525041	-5.15401532	-6.04752316	C	4.67263386	-12.42403537	1.93107400
C	5.14668636	-6.31905807	-5.15050379	H	4.79300241	-13.09695321	2.76760124
O	4.22352899	-7.02867851	-4.67417408	Cu	4.98206994	-8.90964606	-0.63642957
C	6.52069012	-6.57383622	-4.93395134	O	7.46246299	-10.16169241	-3.83737876
H	6.78752764	-7.42389156	-4.31336360	H	7.88385340	-10.88536001	-3.31212241
C	7.53282805	-5.73552441	-5.42882342	H	8.12726470	-9.44101274	-3.80349213
O	8.76742061	-5.96806973	-5.39972039	O	2.96663174	-8.92432939	-0.89788323
C	7.09124580	-4.38727206	-6.01134174	H	2.54527940	-8.26021998	-1.49221446
O	7.86249428	-3.42377011	-6.04036537	H	2.36895818	-9.14512736	-0.13629034
C	5.71436332	-4.28019027	-6.46119903	O	5.01088267	-9.35583430	-2.89670383
H	5.45703427	-3.38972000	-7.02459606	H	5.94705951	-9.57803779	-3.12639336
C	-0.78835822	-1.38174604	-3.44944568	O	2.01463818	-7.12345776	-2.85467960
H	-1.05163375	-1.14990261	-2.40643191	H	2.84846208	-6.89138598	-3.30661102
H	-0.80261771	-0.43042611	-3.99312031	H	1.44181774	-7.43032639	-3.58344649
C	0.59610938	-1.97718537	-3.52112167	C	14.36444314	-7.44017202	-0.51718661
C	1.05916037	-2.92242697	-2.59388865	C	6.97677208	2.20883748	-5.63922747
H	0.39568419	-3.25184680	-1.79585522	C	4.20798455	-7.71797182	-10.28734326
C	2.35377140	-3.42916524	-2.64986084	C	2.64245469	-5.86291777	-7.29611033
H	2.74391058	-4.13404785	-1.92261377	C	-1.89259735	-2.28299706	-4.03143021
C	3.22284291	-2.97709304	-3.65312041	C	10.91219685	-8.76104357	1.52141713
O	4.46918392	-3.50048505	-3.70010479	C	6.48432944	-3.39272244	2.05143609
H	5.07580502	-2.84365163	-4.08973538	C	6.48935286	-10.84349146	3.86985551
C	2.76857360	-2.05192710	-4.60475561				

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C	14.55981594	-7.89947623	-1.96765566	H	3.49938671	-2.12939382	-5.14457644
H	15.00405613	-8.89811921	-1.96080402	C	1.49424792	-1.82384562	-4.42465658
H	15.27844985	-7.23111307	-2.44491806	H	1.18215082	-1.28601947	-5.31987451
C	13.24425803	-7.98072935	-2.69940334	C	10.48584714	-8.44020210	0.07251709
C	12.59884409	-6.86833570	-3.25779550	H	11.24216749	-8.85093352	-0.59944426
H	13.09221984	-5.89850520	-3.26364532	H	10.50570154	-7.35715169	-0.07944785
C	11.30342601	-6.96709588	-3.75194738	C	9.13015136	-8.94670194	-0.27563898
H	10.79585559	-6.09858597	-4.15445714	N	8.83472619	-10.27701773	-0.56286197
C	10.61033588	-8.19541985	-3.69679663	C	7.50818807	-10.36023893	-0.84488252
O	9.34235466	-8.31413283	-4.09928131	H	6.97796098	-11.25337792	-1.13063652
H	9.05462450	-7.46015736	-4.65503561	N	6.95350279	-9.17033196	-0.75426156
C	11.27003550	-9.32590334	-3.18911613	C	7.94071044	-8.28239434	-0.40222163
H	10.72544659	-10.26405253	-3.13946221	H	7.71826098	-7.23657163	-0.26116351
C	12.55928034	-9.20074133	-2.68726381	C	5.11478635	-3.75646140	1.42660554
H	13.03995003	-10.04075431	-2.19391743	H	4.70588343	-2.86688944	0.93048310
C	5.91239150	1.25040359	-5.04157307	H	4.42934301	-4.01282938	2.24236703
H	4.97305181	1.36305594	-5.59128970	C	5.17308839	-4.88665157	0.44931949
H	5.71790695	1.51979416	-3.99988518	N	5.05021803	-4.71172695	-0.91376718
C	6.33460611	-0.23068729	-5.10773444	H	9.49927799	-11.04158397	-0.59302767
O	5.54000266	-0.90496498	-4.26497224	C	5.06077506	-5.95711627	-1.41471546
O	7.18309627	-0.72891851	-5.81435350	H	4.94481473	-6.18614936	-2.46419744
H	5.71529548	-1.86952107	-4.22467567	N	5.18154116	-6.91169109	-0.47920221
C	5.28760446	-8.69589239	-9.76752483	C	5.24851276	-6.24103143	0.71185433
H	5.98376786	-8.89258220	-10.58223829	H	5.33582689	-6.76632679	1.65516967
H	4.81179801	-9.63748045	-9.49177550	C	5.99433657	-10.23648476	2.57707156
C	6.08932404	-8.07831346	-8.61337422	H	6.85575690	-9.90796453	1.98420698
O	6.84103004	-7.11451939	-8.81197342	H	5.41677736	-9.33418813	2.81703994
N	5.91795817	-8.63927122	-7.40745500	C	5.12187420	-11.14695101	1.75753089
H	6.31309095	-8.16914114	-6.59285754	N	4.63315516	-10.68430775	0.55447948
H	5.18626298	-9.33216397	-7.25560091	C	3.91128721	-11.65923199	0.03630010
C	3.40024164	-4.85964972	-6.37656254	H	3.43012405	-11.60507324	-0.92879340
H	3.35729316	-3.86815701	-6.83752405	N	3.89188669	-12.74227659	0.85646489
H	2.86805801	-4.81281679	-5.42184856	H	3.41892660	-13.63497622	0.68358357
C	4.83927215	-5.20675826	-6.13070267	C	4.66396177	-12.43024602	1.96310309
C	5.14324706	-6.31647395	-5.15390960	H	4.77559060	-13.11825233	2.78968838
O	4.18637613	-6.87203383	-4.57979160	Cu	4.93226122	-8.81798437	-1.05251759
C	6.51020511	-6.68058924	-4.93564375	O	7.37217445	-10.27168238	-3.82883621
H	6.69712793	-7.45676415	-4.19710850	H	7.86766815	-11.02633442	-3.43353928
C	7.57187977	-6.04094635	-5.57384578	H	8.00638001	-9.52781460	-3.78690793
O	8.80588209	-6.32632126	-5.45439729	O	2.88380491	-8.47772309	-0.75169622
C	7.25323364	-4.89384844	-6.53734260	H	2.36136035	-8.26739286	-1.55910634
O	8.13948759	-4.32908186	-7.16319321	H	2.35959956	-9.05469518	-0.14055913
C	5.84259646	-4.51368955	-6.70093562	O	4.80684030	-10.10645874	-2.38365593
H	5.66772495	-3.66274231	-7.34931959	H	5.64218374	-10.06824584	-2.88253444
C	-0.79120249	-1.37172032	-3.45807696	O	1.87218541	-7.15504414	-2.94904298
H	-1.10518952	-1.05023978	-2.45327929	H	2.73814196	-6.98612995	-3.36802467
H	-0.74187582	-0.46583526	-4.07325738	H	1.30620583	-7.41939356	-3.70445730
C	0.57829620	-2.00643800	-3.38209984	C	14.36903089	-7.43562344	-0.51670862
C	1.00940823	-2.71844501	-2.25594881	C	6.97217681	2.21745058	-5.63490785
H	0.31340427	-2.89449809	-1.43515957	C	4.20952039	-7.71676201	-10.28680010
C	2.31025476	-3.20487674	-2.14950054	C	2.65063688	-5.85638236	-7.29643524
H	2.63592038	-3.75508981	-1.27328116	C	-1.89288097	-2.28119928	-4.03258089
C	3.23362625	-2.96923263	-3.18426381	C	10.92022888	-8.76042434	1.52287235
O	4.52454258	-3.34525907	-3.12143860	C	6.48372777	-3.39141115	2.05167829
H	4.75881825	-3.72891973	-2.19088986	C	6.49272631	-10.84490449	3.88055516
C	2.79485372	-2.30128276	-4.34038103				

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C	14.55252372	-7.91318784	-1.96817970	H	3.51162899	-1.77351173	-5.25022739
H	14.96543880	-8.92633119	-1.95575737	C	1.49935325	-1.61174704	-4.48834780
H	15.29841867	-7.27008618	-2.43979263	H	1.18312167	-0.91865685	-5.26624121
C	13.24476890	-7.94525444	-2.72174893	C	10.46238440	-8.44301016	0.07558737
C	12.67187501	-6.80830645	-3.30375981	H	11.21564097	-8.86585612	-0.59186593
H	13.21007461	-5.86189481	-3.29294166	H	10.48934745	-7.35700175	-0.07888079
C	11.38724059	-6.84876348	-3.84039983	C	9.11185256	-8.98529770	-0.27373529
H	10.93133245	-5.95336211	-4.24531792	N	8.89762437	-10.31849260	-0.55621233
C	10.64355657	-8.04169546	-3.80064946	C	7.58836888	-10.38570762	-0.80145083
O	9.38410628	-8.12351584	-4.27120219	H	7.05682661	-11.28764283	-1.07625738
H	9.10954293	-7.24932394	-4.69057007	N	6.94325980	-9.19928044	-0.71129605
C	11.21272154	-9.19469531	-3.24290683	C	7.91999567	-8.29402249	-0.37466733
H	10.60008826	-10.08496184	-3.14178655	H	7.70041575	-7.24716183	-0.22841407
C	12.49160614	-9.12791961	-2.70779168	C	5.11155422	-3.75890351	1.44538785
H	12.89712560	-9.98659515	-2.18062167	H	4.68259356	-2.86564784	0.97197228
C	5.93556745	1.21578657	-5.05693642	H	4.44146595	-4.03674662	2.26512488
H	4.98317894	1.33450742	-5.58094722	C	5.16701139	-4.89062566	0.48138336
H	5.76171144	1.45296187	-4.00508835	N	5.16872549	-4.74278060	-0.89426888
C	6.31427315	-0.27942663	-5.13108816	H	5.15276304	-3.89016511	-1.44300367
O	5.67569059	-1.07051516	-4.45285277	C	5.15909433	-5.98353837	-1.44681927
O	7.27157700	-0.64243356	-5.97311236	H	5.13360116	-6.16948386	-2.50882717
H	7.40165685	-1.64294020	-5.94236212	N	5.15095742	-6.90323494	-0.50451846
C	5.28902702	-8.68566392	-9.75603507	C	5.15101417	-6.24575510	0.69619312
H	5.98802961	-8.88619030	-10.56786796	H	5.14678500	-6.78685846	1.63180474
H	4.81765694	-9.62639525	-9.47231641	C	6.00086640	-10.23989004	2.56524097
C	6.08838870	-8.05355013	-8.60406042	H	6.86375294	-9.94125518	1.95923241
O	6.82901692	-7.07913071	-8.80597434	H	5.44211838	-9.32088109	2.79607475
N	5.92322885	-8.61169067	-7.39789534	C	5.10363553	-11.14257198	1.76361235
H	6.34923365	-8.16086728	-6.59123069	N	4.56553408	-10.67738080	0.58143581
H	5.21195941	-9.32449772	-7.23611722	C	3.85369084	-11.66366435	0.07152629
C	3.31246107	-4.82458507	-6.36132566	H	3.34048971	-11.61326675	-0.87810075
H	3.21284016	-3.82872754	-6.80401164	N	3.87775345	-12.75397624	0.87987570
H	2.75938918	-4.82902863	-5.41526966	H	3.42804606	-13.65716434	0.70223769
C	4.74908654	-5.06622688	-6.05512101	C	4.67344831	-12.43510853	1.96722701
C	5.10469183	-6.24983122	-5.17475673	H	4.82768336	-13.12851501	2.78253729
O	4.16293539	-6.93009968	-4.72498461	Cu	5.01263877	-8.94369521	-1.02996155
C	6.47975443	-6.50870847	-4.93160071	O	7.45603153	-10.18701039	-3.87241359
H	6.72846962	-7.39801339	-4.35730738	H	7.87908286	-10.91012308	-3.35224749
C	7.49413471	-5.65847089	-5.39203718	H	8.04037625	-9.42168063	-3.72256670
O	8.73279655	-5.87303320	-5.35570419	O	2.92989715	-8.51250878	-0.72576019
C	7.05377978	-4.29272970	-5.93204833	H	2.40671113	-8.33981198	-1.53524325
O	7.82845690	-3.32903642	-5.92136688	H	2.40511431	-9.08448599	-0.10986904
C	5.68230901	-4.15926701	-6.40173449	O	4.84911346	-9.96965534	-2.57642448
H	5.43840806	-3.25617932	-6.95104110	H	5.73742974	-9.99029275	-2.97955700
C	-0.78773762	-1.37742942	-3.46456578	O	1.94592145	-7.11537506	-2.98049054
H	-1.06024279	-1.11492145	-2.43172546	H	2.82382267	-7.14889447	-3.40692127
H	-0.78467462	-0.44137988	-4.03361175	H	1.34519085	-7.38138550	-3.70816521
C	0.59031683	-1.98965856	-3.49608562	C	14.36483457	-7.44078426	-0.51793372
C	1.01519497	-2.91250770	-2.53151719	C	6.97479518	2.20946791	-5.63819749
H	0.31845131	-3.23378378	-1.76058257	C	4.20581630	-7.71827132	-10.28763635
C	2.31317227	-3.41347393	-2.52227898	C	2.64233600	-5.85627250	-7.29791977
H	2.63367788	-4.14047618	-1.78394887	C	-1.89298583	-2.28356621	-4.03416045
C	3.22774058	-2.95875000	-3.47890126	C	10.91351453	-8.76185142	1.52339156
O	4.51861749	-3.38887204	-3.39784868	C	6.48644792	-3.38967646	2.05068870
H	5.08758130	-2.78012734	-3.91306603	C	6.49243902	-10.84210787	3.87682912
C	2.80418764	-2.09281842	-4.49334879				

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C	14.55720378	-7.89587271	-1.97099116	H	3.43452760	-1.73308350	-5.41087914
H	14.97240576	-8.90786079	-1.96840506	C	1.46913554	-1.56242432	-4.53902410
H	15.30243888	-7.24781724	-2.43561709	H	1.12120103	-0.84567327	-5.28147059
C	13.24845605	-7.92304613	-2.72221071	C	10.49077923	-8.43563146	0.07064055
C	12.63669758	-6.77602770	-3.24836346	H	11.24207560	-8.85940135	-0.60090118
H	13.14227320	-5.81443535	-3.19381365	H	10.52780753	-7.35353309	-0.08206601
C	11.35627546	-6.83023844	-3.78707627	C	9.12778447	-8.92056932	-0.27905165
H	10.86960284	-5.93393520	-4.15235919	N	8.82439215	-10.24243124	-0.59898367
C	10.64714320	-8.04791916	-3.81567516	C	7.49717626	-10.30943175	-0.88459494
O	9.39864408	-8.13923878	-4.28896436	H	6.95628096	-11.18738713	-1.19780687
H	9.09983293	-7.24258246	-4.72994589	N	6.95255614	-9.11798671	-0.76556855
C	11.26657352	-9.20981316	-3.32932641	C	7.94232417	-8.24420334	-0.38864041
H	10.70724809	-10.14103661	-3.34610112	H	7.71975526	-7.20205569	-0.21680426
C	12.54287062	-9.12974450	-2.78462492	C	5.09963909	-3.79212939	1.48513304
H	12.99541919	-10.00003583	-2.31904393	H	4.65822173	-2.91297378	1.00078025
C	5.94272634	1.19436197	-5.07240488	H	4.44946657	-4.06691063	2.32541614
H	4.98375656	1.32068887	-5.58353791	C	5.14698143	-4.90886612	0.49295029
H	5.77859267	1.39580504	-4.01033080	N	5.08737221	-4.65095372	-0.85335575
C	6.32658550	-0.29761284	-5.19470744	H	9.48105086	-11.01254381	-0.63214549
O	5.65122392	-1.11073604	-4.59124369	C	5.09465025	-5.86231589	-1.41356836
O	7.33924086	-0.63850656	-5.99163477	H	5.04097678	-6.03337213	-2.47986085
H	7.44968964	-1.63382237	-5.98229513	N	5.15088222	-6.88422870	-0.52480532
C	5.28826074	-8.69178379	-9.76235744	C	5.17908516	-6.27704731	0.70548156
H	5.98250555	-8.89510474	-10.57721764	H	5.20364975	-6.85615500	1.62176969
H	4.81241980	-9.63064637	-9.47821140	C	5.99694609	-10.23595562	2.57410768
C	6.09103358	-8.06311471	-8.61391585	H	6.85883621	-9.90006010	1.98695586
O	6.84605750	-7.10287193	-8.82255340	H	5.41789876	-9.33395270	2.81207625
N	5.92020495	-8.61067314	-7.40225680	C	5.12994472	-11.14508647	1.74640204
H	6.32658306	-8.13246553	-6.59867868	N	4.65045579	-10.67942514	0.54147444
H	5.18686260	-9.29948538	-7.23583512	C	3.92970027	-11.65132878	0.01862359
C	3.34254791	-4.84729829	-6.36550076	H	3.45002984	-11.59289527	-0.94702647
H	3.25513802	-3.84766160	-6.80080285	N	3.90132260	-12.73709002	0.83748941
H	2.80087509	-4.84207343	-5.41422627	H	3.42493692	-13.62739085	0.66560076
C	4.78217877	-5.11948094	-6.08138225	C	4.66841172	-12.42767546	1.94896660
C	5.12795271	-6.29533523	-5.18996340	H	4.77286628	-13.11458114	2.77741385
O	4.19710210	-6.98798303	-4.74296419	Cu	4.94304689	-8.76553526	-1.11669314
C	6.50979722	-6.56532626	-4.95357106	O	7.48804673	-10.17398427	-3.88977001
H	6.74702761	-7.43115369	-4.34122321	H	7.95704544	-10.91721441	-3.44757489
C	7.52802644	-5.73700302	-5.42444753	H	8.12267174	-9.43026853	-3.88284737
O	8.77395533	-5.97178926	-5.36899224	O	2.88511304	-8.53427765	-0.79284333
C	7.10877581	-4.38880206	-6.01683723	H	2.33916567	-8.29283179	-1.57106444
O	7.89254837	-3.43391525	-6.05109876	H	2.36693677	-9.08548945	-0.15377527
C	5.73629190	-4.25746906	-6.47922720	O	4.87585089	-10.10372043	-2.42060399
H	5.50031782	-3.35806739	-7.03830792	H	5.69051714	-10.00182682	-2.94122427
C	-0.78562811	-1.38067554	-3.45017409	O	1.90877934	-7.12589571	-2.97712479
H	-1.04761619	-1.15067548	-2.40619239	H	2.79704663	-7.02603994	-3.36966903
H	-0.80187376	-0.42829556	-3.99178990	H	1.35221157	-7.39255026	-3.73858101
C	0.60108469	-1.97432388	-3.52425011	C	14.36831284	-7.43701012	-0.51738639
C	1.07064619	-2.91193307	-2.59258789	C	6.97439481	2.21023515	-5.63698848
H	0.41194683	-3.23816945	-1.78981891	C	4.20890309	-7.71651263	-10.28807990
C	2.36500822	-3.41935921	-2.65303502	C	2.64314740	-5.85788793	-7.30108802
H	2.75740624	-4.12070114	-1.92337783	C	-1.89164540	-2.28066397	-4.03199240
C	3.22654169	-2.97432306	-3.66562882	C	10.91964436	-8.75953463	1.52194478
O	4.47384627	-3.49497902	-3.71776610	C	6.48343419	-3.39519181	2.05712559
H	5.07452942	-2.84366067	-4.12529855	C	6.49200574	-10.84504764	3.87924655
C	2.76443639	-2.05828347	-4.62291400				

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C	14.55466180	-7.91111347	-1.96479630	H	3.55853942	-1.62311873	-5.19031545
H	14.96402769	-8.92555600	-1.95289036	C	1.52988708	-1.52954842	-4.46791583
H	15.30423264	-7.27142481	-2.43397264	H	1.24257114	-0.75501727	-5.17624334
C	13.24676562	-7.93374978	-2.71573308	C	10.41246980	-8.48607513	0.07185557
C	12.66783362	-6.78613738	-3.27384649	H	11.16207023	-8.88629254	-0.61484814
H	13.19933862	-5.83760634	-3.24176798	H	10.39333871	-7.40620105	-0.10066545
C	11.38819048	-6.82061598	-3.81567318	C	9.05143742	-9.03808930	-0.24052192
H	10.92799596	-5.91919242	-4.20011796	N	8.72692643	-10.38977503	-0.32690848
C	10.64731665	-8.01932997	-3.81519966	C	7.41558180	-10.50067452	-0.64906798
O	9.39896797	-8.09103907	-4.29586677	H	6.87415419	-11.42990649	-0.72748610
H	9.12113382	-7.18144705	-4.71020042	N	6.88323105	-9.30746795	-0.80132798
C	11.23078446	-9.18351827	-3.28915717	C	7.88330582	-8.39134438	-0.55587633
H	10.64373452	-10.09730864	-3.27120870	H	7.68812818	-7.33451616	-0.60775553
C	12.50837455	-9.12325418	-2.74430982	C	5.10957357	-3.72223072	1.43919844
H	12.92973630	-9.99350921	-2.24867331	H	4.69550703	-2.81593587	0.97714218
C	5.93200158	1.20865409	-5.04970465	H	4.43031610	-4.00311383	2.25078573
H	4.98789755	1.31100372	-5.59140719	C	5.17962109	-4.83732576	0.46509659
H	5.73975574	1.44652256	-4.00048459	N	5.10876227	-4.70298885	-0.91050936
C	6.33516395	-0.28350498	-5.11215736	H	4.99597582	-3.86132173	-1.46429458
O	5.73042916	-1.07282240	-4.40314060	C	5.19334705	-5.94841982	-1.45220036
O	7.26628082	-0.64647386	-5.98329566	H	5.10750333	-6.16400503	-2.50478521
H	7.40299127	-1.64678831	-5.94292029	N	5.32260845	-6.85166019	-0.50280009
C	5.27697659	-8.70845479	-9.78018975	C	5.30778827	-6.18225057	0.68771669
H	5.95559271	-8.92229417	-10.60471648	H	5.38263245	-6.70998351	1.62970419
H	4.79205722	-9.64106635	-9.49069626	C	6.06352079	-10.12962260	2.57622155
C	6.10972557	-8.10212923	-8.64589313	H	6.95604036	-9.69639565	2.09917531
O	6.83583438	-7.11725076	-8.84568607	H	5.42496976	-9.27603523	2.85123926
N	6.02485151	-8.72307281	-7.46243276	C	5.31400037	-11.00010491	1.61486169
H	6.46509930	-8.27419609	-6.66372224	N	4.60821135	-10.47658305	0.54894064
H	5.26667579	-9.37888751	-7.27331355	C	4.12708286	-11.57205109	-0.11111231
C	3.33493416	-4.87635303	-6.33387220	H	3.49470678	-11.47594990	-0.98675868
H	3.21682977	-3.85702932	-6.71420428	N	4.46443706	-12.73577156	0.42770283
H	2.81163074	-4.93639842	-5.37148864	H	5.59562500	-13.12240462	2.20961497
C	4.78222530	-5.13373957	-6.08236284	C	5.19869110	-12.37554006	1.52703343
C	5.18715112	-6.43434914	-5.41902318	H	9.32002807	-11.17158406	-0.10275398
O	4.33409682	-7.31751416	-5.26540452	Cu	4.78614708	-9.02699150	-0.83634360
C	6.55977385	-6.59396034	-5.05747373	O	7.39764863	-10.11496552	-3.88518508
H	6.83110184	-7.51914090	-4.55818141	H	7.79004792	-10.85112667	-3.37256847
C	7.54545833	-5.67765769	-5.39902364	H	8.07237145	-9.41222906	-3.85745680
O	8.79645310	-5.85642463	-5.28337992	O	2.90027461	-8.29493511	-0.40135770
C	7.07957003	-4.31330074	-5.90969907	H	2.44679902	-8.02466711	-1.23450161
O	7.84355857	-3.33717028	-5.90438712	H	2.32507037	-8.93152807	0.12206769
C	5.69722492	-4.17840190	-6.33732922	O	4.46466823	-8.68974961	-2.69011509
H	5.42569490	-3.22546122	-6.78082766	H	5.24379552	-8.78985525	-3.25728465
C	-0.77879367	-1.38284177	-3.47396821	O	2.42949229	-7.06390827	-2.83541567
H	-1.03368996	-1.13348613	-2.43358602	H	3.27935833	-7.60644018	-2.95141945
H	-0.78585051	-0.44126041	-4.03307214	H	1.85794071	-7.36819847	-3.56084256
C	0.59726331	-1.99740635	-3.53957897	C	14.36681437	-7.43879367	-0.51533416
C	0.99215426	-3.02485372	-2.67296188	C	6.96780669	2.21536987	-5.62080973
H	0.27365018	-3.41510565	-1.95805493	C	4.20490405	-7.71921759	-10.28988692
C	2.28125813	-3.54462271	-2.68878514	C	2.63993671	-5.85901898	-7.30004946
H	2.56761133	-4.37824405	-2.05624801	C	-1.89161342	-2.28417013	-4.03445457
C	3.22268634	-2.99084189	-3.56408960	C	10.90915359	-8.76358836	1.51700924
O	4.51075125	-3.43143615	-3.47830791	C	6.48613583	-3.38528100	2.05519163
H	5.09472109	-2.79825521	-3.94356204	C	6.49785829	-10.82603523	3.86627922
C	2.83103128	-2.02197971	-4.49334732				

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C	14.55262132	-7.92250666	-1.96589625	H	3.50941437	-1.53762015	-5.32049177
H	14.97939177	-8.92930726	-1.94797571	C	1.49416605	-1.52212933	-4.54605712
H	15.28252186	-7.27112072	-2.45032061	H	1.15231918	-0.77052416	-5.25447426
C	13.23861699	-7.98134448	-2.70603310	C	10.42960758	-8.44725661	0.08481631
C	12.70449130	-6.88551505	-3.39064595	H	11.19291677	-8.83350101	-0.58888782
H	13.26255533	-5.95432761	-3.45126364	H	10.41105000	-7.36000607	-0.06019023
C	11.42606188	-6.94790623	-3.94211904	C	9.09608807	-9.04199878	-0.26637381
H	11.00492302	-6.08585074	-4.44561673	N	8.93680189	-10.38009747	-0.54597943
C	10.65492064	-8.10555221	-3.78701705	C	7.63535519	-10.50633543	-0.80424668
H	9.38241464	-8.18270104	-4.25738872	H	7.14904120	-11.44327327	-1.04601261
H	9.20216592	-7.46359365	-4.90743965	N	6.93952007	-9.34657924	-0.72911479
C	11.17285195	-9.21684524	-3.11793084	C	7.87800945	-8.39943805	-0.38817927
H	10.52945044	-10.06793499	-2.91838149	H	7.61771027	-7.36110620	-0.25885931
C	12.45739393	-9.14076726	-2.59349302	C	5.12818888	-3.72852869	1.39681954
H	12.83543360	-9.96761385	-1.99684924	H	4.73635667	-2.82820149	0.90562956
C	5.91030762	1.23545283	-5.04823059	H	4.42347967	-3.98938192	2.19288730
H	4.95065384	1.39327515	-5.55672161	C	5.20239468	-4.86524839	0.43605046
H	5.75215901	1.46682333	-3.99042037	N	5.08624331	-4.76631745	-0.94205443
C	6.28298076	-0.30044697	-5.18803908	H	5.02156205	-3.93091744	-1.52053321
O	5.52316551	-1.00673227	-4.43887456	C	5.09450606	-6.03243360	-1.44457278
O	7.15385989	-0.69562091	-5.97318933	H	4.93327474	-6.27811174	-2.48165793
H	6.58619880	-5.49205437	-4.04261191	N	5.21584116	-6.91662175	-0.47687144
C	5.28753915	-8.69742696	-9.77299688	C	5.27824082	-6.21057151	0.69206507
H	5.98122354	-8.89191083	-10.59008459	H	5.38346733	-6.70741664	1.64712289
H	4.81319520	-9.64242344	-9.50765660	C	6.02063977	-10.24606914	2.55048124
C	6.10476517	-8.11073058	-8.61344133	H	6.89404173	-9.95076961	1.95665752
O	6.80268669	-7.09530095	-8.75406834	H	5.45643363	-9.32886915	2.76818461
N	6.04392724	-8.80701621	-7.46751501	C	5.13422131	-11.15607148	1.74437197
H	6.51900175	-8.46453858	-6.64464527	N	4.61504065	-10.73278525	0.53010644
H	5.29768981	-9.48479644	-7.31140925	C	3.85723286	-11.71369874	0.06945806
C	3.39191126	-4.85276952	-6.36860776	H	3.30092772	-11.67956990	-0.85545043
H	3.26177178	-3.84066156	-6.76134907	N	3.84722141	-12.76099544	0.92464796
H	2.91035601	-4.88485065	-5.38417794	H	3.38566757	-13.66469745	0.77106596
C	4.85997101	-5.11187045	-6.20988337	C	4.65314280	-12.42030461	1.99601927
C	5.27412181	-6.33165702	-5.45677664	H	4.77778750	-13.07917549	2.84333106
O	4.56440107	-7.30829716	-5.32836883	Cu	4.97994612	-9.10985921	-0.87248138
C	6.66466516	-6.26492507	-4.82204101	O	7.23177829	-9.92946846	-3.97640841
H	6.92629078	-7.21462365	-4.35332438	H	7.37340103	-10.51792948	-3.20912040
C	7.66554537	-5.78717123	-5.83827618	H	8.01402450	-9.34689369	-3.93302160
O	8.75761024	-6.30387672	-6.02600554	O	3.00769109	-8.60707483	-0.61451242
C	7.23790180	-4.58465837	-6.70119313	H	2.58199251	-8.30600599	-1.45680073
O	8.06836429	-3.99666087	-7.36938898	H	2.37611738	-9.11313220	-0.03561546
C	5.80358755	-4.27643725	-6.70773137	O	4.71199857	-9.05074972	-2.79327256
H	5.54289512	-3.36943361	-7.23726475	H	5.55287327	-9.13764191	-3.27328877
C	-0.77397130	-1.39573061	-3.46133731	O	2.68205670	-7.44614665	-3.01689746
H	-1.01658996	-1.17509472	-2.41125588	H	3.50859161	-8.02956967	-3.13144545
H	-0.79359219	-0.43769653	-3.99261246	H	2.08083719	-7.68442497	-3.74129235
C	0.61003865	-1.99219858	-3.56827931	C	14.36640276	-7.43982409	-0.51816027
C	1.07559974	-2.97926874	-2.69311688	C	6.96796987	2.21648307	-5.63190309
H	0.40659666	-3.37560310	-1.93226866	C	4.20714405	-7.71862386	-10.28696204
C	2.38903859	-3.44286910	-2.74760012	C	2.65101044	-5.85088799	-7.29727800
H	2.72916290	-4.21794859	-2.06758257	C	-1.89191976	-2.28447341	-4.03361849
C	3.28799856	-2.89054150	-3.67316751	C	10.91080445	-8.76184370	1.52337823
O	4.59531793	-3.25568819	-3.64779623	C	6.48832476	-3.38684306	2.04964422
H	5.13642356	-2.47002186	-4.04810253	C	6.49250549	-10.84321566	3.87368328
C	2.80712720	-1.96772141	-4.61712783				

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C	14.53710151	-7.90225234	-1.97362329	H	3.47865545	-1.79981934	-5.27897280
H	14.93895355	-8.92039101	-1.97365510	C	1.46194174	-1.66525261	-4.51901552
H	15.28850266	-7.26632169	-2.44584769	H	1.10778444	-1.06759269	-5.35694116
C	13.22012268	-7.90447498	-2.71653079	C	10.46800155	-8.41914492	0.07754879
C	12.62834574	-6.74212501	-3.23422489	H	11.17956175	-8.87618000	-0.61670441
H	13.15723676	-5.79310637	-3.17724914	H	10.54550243	-7.33961151	-0.08405878
C	11.35347238	-6.76567974	-3.78863697	C	9.07791430	-8.86044328	-0.22645587
H	10.89096415	-5.85479335	-4.14942102	N	8.76477633	-10.15514230	-0.60511311
C	10.61845108	-7.96970146	-3.83877731	C	7.42937331	-10.24748465	-0.78532007
O	9.37846332	-8.03634710	-4.33121354	H	6.90015001	-11.13423723	-1.09200156
H	9.06886323	-7.10184184	-4.73529179	N	6.87168444	-9.08036956	-0.53592963
C	11.21446549	-9.14482306	-3.34809137	C	7.87865042	-8.20099689	-0.19901023
H	10.63893496	-10.06623844	-3.37827309	H	7.67622299	-7.16995075	0.04235079
C	12.48707376	-9.09513435	-2.78917967	C	5.11880417	-3.74006019	1.41049603
H	12.91242693	-9.98259337	-2.32996024	H	4.69016195	-2.82986650	0.97145590
C	5.92806942	1.20324307	-5.07349541	H	4.44298724	-4.05836086	2.20998166
H	4.96923460	1.35043561	-5.58286127	C	5.18630054	-4.82686458	0.39157348
H	5.76580709	1.41769366	-4.01344059	N	5.19550301	-4.64271719	-0.98033772
C	6.29953231	-0.32335664	-5.20537609	H	5.15865974	-3.77991222	-1.52748813
O	5.55324807	-1.04485507	-4.49000810	C	5.16413952	-5.86129797	-1.57269414
O	7.19959919	-0.72847237	-5.98921834	H	5.12891431	-6.01065614	-2.64054029
H	7.48488065	-2.36135921	-5.95169102	N	5.14363596	-6.81048135	-0.65490215
C	5.28531315	-8.69838119	-9.76609406	C	5.14840884	-6.18495329	0.56781634
H	5.97754698	-8.90236424	-10.58254423	H	5.10589703	-6.75019004	1.48860622
H	4.80804088	-9.63713900	-9.48154252	C	6.08212044	-10.15045472	2.56083410
C	6.09280332	-8.07185958	-8.62102081	H	6.99036642	-9.83594114	2.03331155
O	6.85553891	-7.11993844	-8.83291364	H	5.56043807	-9.21737333	2.82438964
N	5.91613969	-8.60877230	-7.40442395	C	5.17975401	-10.96552770	1.68587966
H	6.31368398	-8.11654370	-6.60517480	N	4.63374068	-10.50253973	0.50237316
H	5.17335382	-9.28646213	-7.23401759	C	3.79356035	-11.49647423	0.09560618
C	3.29952572	-4.85627924	-6.31468137	H	3.20506304	-11.40270037	-0.80684535
H	3.24524108	-3.85658324	-6.75748747	N	3.74438941	-12.54037234	0.91573066
H	2.69419481	-4.83004711	-5.39700535	H	4.77104395	-12.85925086	2.76711984
C	4.72272972	-5.12856692	-5.94697367	C	4.61050515	-12.21403924	1.90921990
C	5.10447160	-6.33004179	-5.17474832	H	9.42724773	-10.89916482	-0.72950351
O	4.21524342	-7.14235232	-4.74764196	Cu	4.86702549	-8.87351081	-0.65220923
C	6.48768842	-6.53642043	-4.94901843	O	7.51333923	-10.14053433	-3.87447125
H	6.78126757	-7.44117446	-4.41948213	H	7.99236926	-10.89228930	-3.46330528
C	7.47800578	-5.61038024	-5.33006491	H	8.15929757	-9.40843408	-3.92500406
O	8.73539069	-5.82758881	-5.24441438	O	2.90227589	-8.41138869	-0.55434112
C	7.00694511	-4.28850571	-5.81000595	H	2.48260705	-8.24371791	-1.43620474
O	7.88374985	-3.30772369	-5.87373696	H	2.32831835	-9.01057335	0.00738670
C	5.65774330	-4.14107693	-6.17825675	O	4.75265870	-9.26522343	-2.75146181
H	5.36278120	-3.19828733	-6.62679626	H	4.70777845	-8.53300848	-3.41108024
C	-0.80086676	-1.36786849	-3.46152402	O	2.03973798	-7.30289435	-2.97778257
H	-1.08450701	-1.09822255	-2.43326844	H	2.83444912	-7.16501780	-3.54018853
H	-0.79728712	-0.43574991	-4.03769993	H	1.35372929	-7.53003231	-3.63781086
C	0.58233215	-1.96633961	-3.47310615	C	14.37001032	-7.43762843	-0.51800856
C	1.05503475	-2.76274963	-2.42486445	C	6.97463669	2.20617545	-5.64165165
H	0.38360707	-3.03071726	-1.60951203	C	4.20629380	-7.71990254	-10.28746703
C	2.37823221	-3.19452413	-2.38393376	C	2.64018916	-5.86060592	-7.29152136
H	2.74168603	-3.79914304	-1.55998510	C	-1.89506906	-2.28432318	-4.03550031
C	3.26617183	-2.80901285	-3.39737549	C	10.92048194	-8.75666775	1.52172489
O	4.57755098	-3.14053312	-3.28750119	C	6.48536002	-3.38931113	2.04786047
H	5.11667073	-2.48414823	-3.82786336	C	6.49773592	-10.83024994	3.86431756
C	2.78546063	-2.08180829	-4.49690016				

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C	14.55295867	-7.91178127	-1.96617831	H	3.47625586	-1.53799611	-5.34123056
H	15.00121514	-8.90856734	-1.95383066	C	1.46709463	-1.51273677	-4.55320021
H	15.26602266	-7.24339763	-2.45160121	H	1.11824597	-0.77196966	-5.26959988
C	13.23321522	-8.00351228	-2.69209585	C	10.43651449	-8.44713365	0.08794402
C	12.64362513	-6.91659105	-3.34688215	H	11.19517715	-8.83982675	-0.58722926
H	13.16570316	-5.96388750	-3.40410813	H	10.42549067	-7.36028339	-0.06001542
C	11.35110310	-7.01690901	-3.86015778	C	9.09718327	-9.03164583	-0.24377546
H	10.87703180	-6.16247651	-4.33184390	N	8.91734990	-10.36898209	-0.53303694
C	10.62543516	-8.20467078	-3.69952917	C	7.60535299	-10.48377750	-0.72369875
O	9.33899780	-8.32548523	-4.11596175	H	7.10178017	-11.40687936	-0.97727620
H	9.14674037	-7.63896135	-4.79128909	N	6.92162523	-9.32230532	-0.59492669
C	11.20533833	-9.30749875	-3.06730257	C	7.88064728	-8.38265958	-0.29063060
H	10.59760690	-10.18310280	-2.86520403	H	7.63426271	-7.34610404	-0.12660806
C	12.49681854	-9.19165200	-2.57488592	C	5.12390038	-3.72955591	1.41341362
H	12.91663137	-10.00676342	-1.99187541	H	4.70469363	-2.81982894	0.96457514
C	5.91580312	1.23373044	-5.05897462	H	4.43863009	-4.03314901	2.21235831
H	4.95425715	1.40014008	-5.55870331	C	5.20377800	-4.82313117	0.40718425
H	5.76643522	1.45257047	-3.99679799	N	5.05902089	-4.65997524	-0.95986590
C	6.28182971	-0.30173041	-5.22587390	H	4.98314489	-3.80224343	-1.50197094
O	5.48809787	-1.01795151	-4.52303429	C	5.08478775	-5.89830692	-1.52515533
O	7.17705302	-0.69075764	-5.98682805	H	4.86934014	-6.07653126	-2.56569202
H	6.55156504	-6.39717603	-3.89451350	N	5.24793981	-6.82778326	-0.60601221
C	5.29209440	-8.70692436	-9.78676578	C	5.31749181	-6.17685474	0.59443728
H	5.94481090	-8.94607318	-10.62729391	H	5.44462933	-6.72176609	1.52027661
H	4.81036796	-9.62400885	-9.45585886	C	6.00548134	-10.24476824	2.55912854
C	6.18472734	-8.24120742	-8.63844538	H	6.86930368	-9.94025044	1.95862157
O	6.60784480	-9.03683976	-7.83451648	H	5.43802279	-9.33207722	2.78749356
N	6.69807353	-6.91701677	-8.63216206	C	5.11617994	-11.15364943	1.75405877
H	7.27626903	-6.80039525	-7.80383045	N	4.57591937	-10.70711170	0.56112247
H	6.02645256	-6.15352950	-8.68996578	C	3.83300377	-11.68784750	0.07700708
C	3.38451085	-4.92053551	-6.30454089	H	3.27742899	-11.64042167	-0.84789058
H	3.29478425	-3.88965940	-6.65517306	N	3.85062955	-12.75733127	0.90325902
H	2.87243665	-4.97953294	-5.33567608	H	3.39849143	-13.66260085	0.73479822
C	4.83488229	-5.24212273	-6.09665000	C	4.66169986	-12.43342901	1.97571540
C	5.19898841	-6.58619288	-5.52514669	H	4.80600394	-13.11632079	2.80037844
O	4.41875884	-7.51138922	-5.49278671	Cu	4.99422051	-9.06562372	-0.81347585
C	6.59910256	-6.75477425	-4.93663676	O	7.30442712	-10.26000370	-3.77438610
H	6.84155266	-7.81981540	-4.90156998	H	7.74038454	-11.02939340	-3.33451942
C	7.63585198	-5.96527059	-5.67742328	H	7.90096166	-9.52930911	-3.53859336
O	8.77935667	-6.36241608	-5.86648511	O	3.02418535	-8.47898801	-0.54320437
C	7.22373206	-4.62868448	-6.34202008	H	2.64501064	-8.20768852	-1.41747638
O	8.07445436	-3.95826190	-6.89856137	H	2.39058769	-9.03791032	-0.01987172
C	5.79488298	-4.32893676	-6.39306851	O	4.75651189	-9.19323082	-2.72998037
H	5.55852828	-3.33799346	-6.76890598	H	5.57949284	-9.47921902	-3.16130257
C	-0.79020858	-1.38048257	-3.45971173	O	2.85874212	-7.47478172	-3.04758110
H	-1.03965865	-1.16131114	-2.40994888	H	3.64209292	-8.12632159	-3.11844278
H	-0.81429976	-0.42246216	-3.99132173	H	2.24705954	-7.73176837	-3.75551512
C	0.59199295	-1.97003334	-3.56199411	C	14.36523610	-7.43882839	-0.51663600
C	1.05914165	-2.94817252	-2.67939892	C	6.96884318	2.21714976	-5.63612569
H	0.39229949	-3.34164239	-1.91458945	C	4.22123820	-7.70551199	-10.27559664
C	2.37070806	-3.41220316	-2.73534724	C	2.64233660	-5.85696233	-7.29066997
H	2.71809223	-4.17547604	-2.04851382	C	-1.89489188	-2.28135214	-4.03558920
C	3.26359412	-2.86585531	-3.66910363	C	10.91295670	-8.76123664	1.52554605
O	4.56947241	-3.22955850	-3.63404733	C	6.48897881	-3.38635872	2.05239531
H	5.11292444	-2.46509502	-4.05951084	C	6.49341228	-10.84348902	3.87347143
C	2.77939858	-1.95688799	-4.62750753				

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C	14.53432099	-7.89109390	-1.96754887	H	3.50763240	-1.78430326	-5.22408882
H	14.96277303	-8.89693104	-1.97832506	C	1.47277012	-1.69048662	-4.50290759
H	15.25542771	-7.23130959	-2.45276213	H	1.12572636	-1.09847779	-5.34742779
C	13.20368013	-7.93789727	-2.68187253	C	10.51737030	-8.43607890	0.07961362
C	12.56242248	-6.80509150	-3.20595764	H	11.27517659	-8.84477367	-0.59182148
H	13.05457402	-5.83584027	-3.17154008	H	10.52311118	-7.35448722	-0.07976384
C	11.27854539	-6.88793807	-3.73612770	C	9.16744405	-8.97059119	-0.25260776
H	10.77950987	-6.00363435	-4.11595567	N	8.91524010	-10.29360379	-0.58991642
C	10.59658661	-8.12151129	-3.75595621	H	9.61483366	-11.01864575	-0.73424796
O	9.33692325	-8.23512318	-4.21217658	C	7.58460741	-10.44529193	-0.75648663
H	9.05168594	-7.36738318	-4.76646219	H	7.10351708	-11.36781045	-1.03287793
C	11.24646040	-9.26809921	-3.27748547	N	6.96815272	-9.29311093	-0.54588395
H	10.72230357	-10.21883645	-3.31600128	C	7.94061316	-8.36355860	-0.24017224
C	12.52566371	-9.15970878	-2.73986928	H	7.69466240	-7.33561874	-0.02975794
H	13.00600025	-10.02167501	-2.28756354	C	5.14691277	-3.78706228	1.38299737
C	5.91634346	1.22835373	-5.08164277	H	4.73417716	-2.90059696	0.88675529
H	4.95719153	1.38941319	-5.58638224	H	4.44364194	-4.06766462	2.17265477
H	5.75954652	1.44787852	-4.02118369	C	5.24485763	-4.92369942	0.41242948
C	6.27743661	-0.29903680	-5.22655297	N	5.22004714	-4.80798440	-0.96932939
O	5.51723063	-1.03821387	-4.51454187	H	5.15957537	-3.96490792	-1.56046027
O	7.16946826	-0.68082938	-6.01093176	C	5.19706031	-6.04945148	-1.50086410
C	5.28009374	-8.69184353	-9.77972222	H	5.14409993	-6.25453093	-2.55806286
H	5.96584538	-8.89860353	-10.59977857	N	5.20761130	-6.96204840	-0.53662845
H	4.80191376	-9.62867505	-9.49220319	C	5.23415896	-6.27366541	0.65765965
C	6.09221929	-8.07280789	-8.63582562	H	5.23698285	-6.78658014	1.60900659
O	6.84779834	-7.11576988	-8.82965184	C	5.98715819	-10.22579745	2.56051934
N	5.93579872	-8.64498545	-7.42744320	H	6.85116899	-9.86743282	1.99319115
H	6.31589416	-8.14580674	-6.62505145	H	5.38502672	-9.34164918	2.81085101
H	5.18080329	-9.311117831	-7.27328280	C	5.14180601	-11.14006709	1.70903992
C	3.33530663	-4.90305662	-6.27847317	N	4.67860393	-10.74452806	0.45307765
H	3.29615392	-3.89188539	-6.69177295	C	3.90525111	-11.72274426	-0.00483786
H	2.73585227	-4.88624096	-5.35927322	H	3.36179603	-11.69848044	-0.93656387
C	4.76552609	-5.21240638	-5.94028672	N	3.84858465	-12.73439457	0.88116234
C	5.13888465	-6.39660726	-5.10818367	H	3.35659998	-13.62862370	0.74782106
O	4.23670628	-7.12923876	-4.57392793	C	4.62030857	-12.38521067	1.97008383
C	6.51047789	-6.68941696	-4.93812673	H	4.68747427	-13.01943947	2.84247348
H	6.77039257	-7.58070518	-4.37613452	Cu	4.98231452	-8.99950289	-0.69879603
C	7.53979201	-5.86479845	-5.43612673	O	7.46696931	-10.16534604	-3.81612395
O	8.76429004	-6.18463833	-5.44295854	H	7.96731022	-10.93127201	-3.44413887
C	7.13314455	-4.48565813	-5.89368880	H	8.14800935	-9.45411902	-3.92333827
N	8.00711443	-3.55260983	-5.85628995	O	3.01597163	-8.85518433	-0.85712677
C	5.72203337	-4.30841791	-6.24366330	H	2.56771671	-8.34551186	-1.59282837
H	5.46832249	-3.37276072	-6.73167077	H	2.38106647	-9.15083159	-0.14705896
H	7.61060701	-2.60911185	-6.05183659	O	5.05166246	-9.25274341	-2.87584032
C	-0.79895421	-1.38174507	-3.46080435	H	4.74735374	-8.52515331	-3.47876626
H	-1.08464444	-1.10903066	-2.43414643	H	5.94337542	-9.53502956	-3.19282736
H	-0.78469036	-0.45048209	-4.03690303	O	2.06150818	-7.34683455	-2.90457741
C	0.58241435	-1.98852301	-3.46323475	H	2.81356214	-7.08622426	-3.48370895
C	1.05535578	-2.76612329	-2.40209671	H	1.36109271	-7.57836290	-3.54919609
H	0.38238328	-3.01714890	-1.58276026	C	14.38123911	-7.43534646	-0.50811576
C	2.38603122	-3.17967023	-2.34271340	C	6.97423648	2.21800580	-5.65213497
H	2.74517028	-3.75557928	-1.49499103	C	4.20317617	-7.71084950	-10.29404600
C	3.28316061	-2.79617263	-3.34916533	C	2.64712440	-5.86233307	-7.28197004
O	4.60226436	-3.09611828	-3.22435340	C	-1.90136115	-2.28463640	-4.03793157
H	5.13522772	-2.41259497	-3.77202846	C	10.94467057	-8.74641909	1.53666692
C	2.79970371	-2.09295874	-4.46512564	C	6.49091239	-3.40017343	2.04986531
				C	6.48251763	-10.84390922	3.86715295

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C	14.54194968	-7.89678446	-1.96357258	C	2.79535915	-2.13592531	-4.46210239
H	14.95658234	-8.90822076	-1.96844712	H	3.50064277	-1.84978942	-5.23334074
H	15.27680232	-7.24892959	-2.44297417	C	1.48129481	-1.68281947	-4.49379118
C	13.21877451	-7.92271481	-2.69008727	H	1.15486099	-1.05494143	-5.31982784
C	12.59700347	-6.77548366	-3.20181423	C	10.51887950	-8.44408903	0.08116623
H	13.09942577	-5.81293557	-3.14945514	H	11.27911949	-8.85208549	-0.58773509
C	11.31499481	-6.83907781	-3.73852587	H	10.52068402	-7.36271666	-0.07778728
H	10.82591552	-5.94232230	-4.09838892	C	9.17094658	-8.98685492	-0.25192449
C	10.62863031	-8.06313691	-3.78565706	N	8.92200626	-10.31049194	-0.58688445
O	9.36212291	-8.15747489	-4.26108297	H	9.62067114	-11.04042426	-0.71593474
H	9.09270027	-7.28123694	-4.70081963	C	7.59066405	-10.46893626	-0.74226382
C	11.25431571	-9.22576900	-3.32618429	H	7.11113418	-11.39408717	-1.01265266
H	10.71993959	-10.16987982	-3.38166547	N	6.97100203	-9.31781184	-0.53188997
C	12.52910657	-9.13692034	-2.77503363	C	7.94222337	-8.38431055	-0.23315401
H	12.99966416	-10.01076784	-2.33905033	H	7.69571518	-7.35842831	-0.01558499
C	5.92890529	1.23536958	-5.08499444	C	5.13921394	-3.80333050	1.41800417
H	4.98747539	1.35517649	-5.62778362	H	4.71262917	-2.92758649	0.91510558
H	5.73489869	1.47679783	-4.03678452	H	4.45106107	-4.07360090	2.22365963
C	6.30883452	-0.25720741	-5.14919223	C	5.22969203	-4.95558982	0.46871327
O	5.66117133	-1.05660310	-4.48037996	N	5.20570318	-4.84159874	-0.91120296
O	7.28224045	-0.62038042	-5.96654814	H	5.13636113	-4.00008384	-1.48744448
H	8.71088230	-3.66862421	-5.56955968	C	5.19757684	-6.08270915	-1.44629003
C	5.29347693	-8.67680764	-9.77280584	H	5.14523135	-6.28384825	-2.50308142
H	5.98703085	-8.87431257	-10.58900017	N	5.21911295	-6.99186550	-0.48430262
H	4.82373757	-9.61997793	-9.49185223	C	5.23313088	-6.30635722	0.71223519
C	6.08764525	-8.05520149	-8.62035095	H	5.23752898	-6.82271566	1.66168037
O	6.82708002	-7.07716131	-8.78323310	C	5.98453284	-10.22908408	2.56329316
N	5.93096153	-8.64798911	-7.42088101	H	6.84771071	-9.87033537	1.99483532
H	6.34011876	-8.18818437	-6.61403049	H	5.37912073	-9.34677286	2.81382337
H	5.20111384	-9.34430369	-7.27883382	C	5.14079254	-11.14932381	1.71620223
C	3.28870515	-4.90192750	-6.29186500	N	4.67956577	-10.76435414	0.45585020
H	3.22222199	-3.89225413	-6.70367312	C	3.89827511	-11.74182532	0.00575373
H	2.70119545	-4.91017944	-5.36600910	H	3.35728951	-11.72372026	-0.92767879
C	4.71785165	-5.17448993	-5.97281655	N	3.83736040	-12.74198036	0.90103283
C	5.11333231	-6.35084548	-5.12333085	H	3.34414458	-13.63746721	0.77269400
O	4.22083097	-7.08818863	-4.61356990	C	4.60966786	-12.38757583	1.98667454
C	6.49261210	-6.59956592	-4.92095295	H	4.67290326	-13.01443741	2.86456116
H	6.77587047	-7.47805686	-4.35087287	Cu	4.98307801	-9.03263615	-0.64088512
C	7.48403067	-5.72603296	-5.37930126	O	7.47613488	-10.13439607	-3.83069409
O	8.73069160	-5.91420552	-5.31171818	H	7.96050982	-10.90389148	-3.44364073
C	7.02082589	-4.38829648	-5.91845367	H	8.16580517	-9.43847660	-3.93732240
N	7.79848168	-3.36702025	-5.92017830	O	3.02392179	-8.79036720	-0.76266013
C	5.64113581	-4.26226129	-6.32919855	H	2.56661789	-8.36526506	-1.53730036
H	5.37280769	-3.36461001	-6.87476615	H	2.37698237	-9.16322011	-0.09431402
H	7.40824620	-1.62503204	-5.94556331	O	5.05993378	-9.23137541	-2.84822337
C	-0.79656287	-1.37655329	-3.46909266	H	4.73837696	-8.52764302	-3.45650492
H	-1.07653936	-1.09965047	-2.44324046	H	5.95042286	-9.50636293	-3.17275751
H	-0.78082358	-0.44879354	-4.04972236	O	2.04226902	-7.35259075	-2.89656415
C	0.57757823	-1.99581067	-3.47329059	H	2.78419748	-7.10368898	-3.48496951
C	1.01831969	-2.82446374	-2.43559084	H	1.33649427	-7.59630141	-3.53272935
H	0.33056650	-3.08614690	-1.63428575	C	14.38025839	-7.43564384	-0.50616382
C	2.32861208	-3.29505296	-2.38931341	C	6.98037826	2.22827458	-5.65164973
H	2.66596481	-3.92101822	-1.56949564	C	4.20816905	-7.70845716	-10.29268720
C	3.23292526	-2.90930183	-3.38215164	C	2.62854268	-5.87614205	-7.28932292
O	4.54295894	-3.30593449	-3.27037786	C	-1.90172113	-2.28083696	-4.03837149
H	5.09896144	-2.67003985	-3.77522273	C	10.94597451	-8.75122461	1.53823764
				C	6.49218682	-3.40120092	2.05377243
				C	6.48350371	-10.84300485	3.86998314

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C	14.52450418	-7.89108563	-1.96905810	C	2.77530343	-2.08074142	-4.53209628
H	14.93719550	-8.90290461	-1.98604965	H	3.46645358	-1.74392494	-5.29374900
H	15.25460703	-7.24129654	-2.45362399	C	1.45135038	-1.66299944	-4.52851397
C	13.19236628	-7.90642663	-2.68277379	H	1.09207714	-1.03444118	-5.33993612
C	12.58821594	-6.75960038	-3.21985197	C	10.52109488	-8.44402731	0.08206662
H	13.09789348	-5.80097581	-3.17724614	H	11.28239260	-8.85161465	-0.58421195
C	11.30865925	-6.81938385	-3.77065932	H	10.52278905	-7.36236561	-0.07578943
H	10.83151215	-5.92198879	-4.14976683	C	9.17301963	-8.98657328	-0.25218258
C	10.62145059	-8.03699574	-3.80718489	N	8.92128256	-10.31004200	-0.58561278
O	9.34061771	-8.13189379	-4.28802935	H	9.61868508	-11.04368898	-0.70158155
H	9.17417452	-7.45852607	-4.99745880	C	7.58890102	-10.46762920	-0.73749018
C	11.21654464	-9.19603806	-3.31020691	H	7.10805728	-11.39394301	-1.00245413
H	10.67027143	-10.13387142	-3.35540566	N	6.97105253	-9.31458202	-0.52704169
C	12.48590482	-9.11403269	-2.74490202	C	7.94503837	-8.38201154	-0.23261680
H	12.93989547	-9.98929832	-2.29289948	H	7.70073658	-7.35643657	-0.01159418
C	5.93745762	1.19727377	-5.11056020	C	5.14345514	-3.78835953	1.40435426
H	4.97303415	1.35912169	-5.60170426	H	4.72258969	-2.90638778	0.90825059
H	5.78214116	1.38083256	-4.04346306	H	4.44983417	-4.06793571	2.20297644
C	6.32288967	-0.32219635	-5.29998892	C	5.23861399	-4.93029580	0.44386410
O	5.48457010	-1.11260801	-4.74870958	N	5.20302154	-4.81832397	-0.93733726
O	7.31880090	-0.67525376	-5.96721122	H	5.14712875	-3.97225868	-1.51463437
H	6.81758552	-7.61943501	-4.85879623	C	5.17905537	-6.06452539	-1.46005147
C	5.26979569	-8.69867040	-9.79022188	H	5.07733364	-6.27121900	-2.51249487
H	5.95070916	-8.90796962	-10.61369397	N	5.21235045	-6.97535547	-0.49859145
H	4.78626246	-9.63488691	-9.51104813	C	5.24177987	-6.28123913	0.69243541
C	6.10196196	-8.11065739	-8.64924302	H	5.24298212	-6.79182250	1.64479671
O	6.82099330	-7.11479420	-8.78202531	C	5.98263968	-10.22869071	2.56543345
N	6.02396343	-8.78843016	-7.48500590	H	6.84359252	-9.86444698	1.99878544
H	6.59774259	-8.49208741	-6.71000991	H	5.37247373	-9.35020244	2.81992088
H	5.31377855	-9.50385113	-7.33938467	C	5.14281162	-11.15109976	1.71725465
C	3.35205138	-4.84863118	-6.34771990	N	4.67192547	-10.76013383	0.46202975
H	3.30066747	-3.85577897	-6.79866081	C	3.89259086	-11.73913793	0.00874084
H	2.78050783	-4.79536407	-5.41445977	H	3.35221840	-11.72404852	-0.92519526
C	4.78919201	-5.14211188	-6.03435148	N	3.83878335	-12.74211198	0.90028253
C	5.14293109	-6.31156024	-5.23154386	H	3.33930875	-13.63523435	0.77455191
O	4.30805532	-7.08031214	-4.73120768	C	4.61155120	-12.38938056	1.98632833
C	6.60647998	-6.54770008	-4.88623763	H	4.67198108	-13.01515136	2.86509934
H	6.72826257	-6.19701316	-3.85071044	Cu	4.97881766	-9.02261367	-0.59625129
C	7.60775670	-5.76673700	-5.70755207	O	7.49091967	-10.12663462	-3.83625164
O	8.69755308	-6.22424387	-6.02149848	H	7.95144083	-10.91209816	-3.45296475
C	7.16917332	-4.35942363	-6.00265107	H	8.18868081	-9.43514555	-3.89769070
N	8.03845274	-3.43680522	-5.89028983	O	3.02291173	-8.77965084	-0.73738568
C	5.74303228	-4.20624061	-6.29436174	H	2.56883753	-8.37619001	-1.52086935
H	5.46195329	-3.25036863	-6.72679339	H	2.37033216	-9.15317652	-0.07341603
H	7.66320570	-2.45387694	-5.97250389	O	5.05850967	-9.26821883	-2.83589826
C	-0.80214002	-1.38942005	-3.44718266	H	4.72549138	-8.57635258	-3.43883369
H	-1.07518370	-1.14328977	-2.41134145	H	5.96228264	-9.50700047	-3.14862203
H	-0.79710571	-0.44452289	-4.00046688	O	2.05447818	-7.39256490	-2.94616479
C	0.57834052	-1.99685958	-3.48693866	H	2.76933933	-7.07768030	-3.52984286
C	1.06193636	-2.82084996	-2.46657944	H	1.33847405	-7.60792360	-3.58166181
H	0.40194748	-3.10187303	-1.64781519	C	14.38163313	-7.43858705	-0.50736502
C	2.38878560	-3.25388872	-2.45145541	C	6.97644297	2.22312035	-5.65706020
H	2.75404079	-3.86685659	-1.63310422	C	4.19816474	-7.70946392	-10.29574529
C	3.26696924	-2.83960505	-3.45901725	C	2.64862592	-5.85263715	-7.29306993
O	4.59228323	-3.17570124	-3.37794271	C	-1.90660978	-2.28384208	-4.03415925
H	5.11181385	-2.47042054	-3.88858275	C	10.94721643	-8.75075980	1.53966834
				C	6.49424423	-3.39741556	2.05228795
				C	6.48510123	-10.84217808	3.87082475

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C	14.52458184	-7.88848145	-1.97109690	C	2.78176534	-2.06656986	-4.51109076
H	14.94084081	-8.89890021	-1.98674551	H	3.48330947	-1.70237370	-5.25069837
H	15.25445349	-7.23597578	-2.45228147	C	1.45872996	-1.64714428	-4.51061011
C	13.19389052	-7.90793031	-2.68604864	H	1.10886500	-0.99787883	-5.31009609
C	12.58782808	-6.76197048	-3.22189579	C	10.51760883	-8.44191612	0.08202554
H	13.09765226	-5.80333656	-3.17928109	H	11.27917886	-8.84790544	-0.58477924
C	11.30654061	-6.82299054	-3.76874212	H	10.51813456	-7.35994160	-0.07405419
H	10.82652540	-5.92470272	-4.14283040	C	9.17051386	-8.98519196	-0.25176041
C	10.61729423	-8.04057053	-3.79272025	N	8.91897500	-10.30873603	-0.58488626
O	9.33314327	-8.14051959	-4.26261512	H	9.61596067	-11.04160327	-0.70712753
H	9.16270086	-7.46277706	-4.96193775	C	7.58659220	-10.46599702	-0.73403086
C	11.21735260	-9.19983701	-3.30339071	H	7.10598583	-11.39078058	-1.00419560
H	10.67084850	-10.13715320	-3.34870355	N	6.96905557	-9.31377236	-0.52080468
C	12.49074238	-9.11710732	-2.74787033	C	7.94302228	-8.38081623	-0.22931275
H	12.94539599	-9.99053444	-2.29312210	H	7.69969274	-7.35451213	-0.01006940
C	5.94400154	1.18140448	-5.11208837	C	5.14087586	-3.78751376	1.40316977
H	4.98017406	1.33827351	-5.60665734	H	4.71981341	-2.90447464	0.90886165
H	5.78716787	1.36440467	-4.04512419	H	4.44817272	-4.06880828	2.20181657
C	6.33549483	-0.33185267	-5.30275984	C	5.23435695	-4.92839329	0.44211995
O	5.50016708	-1.13259780	-4.76238940	N	5.20495169	-4.81421013	-0.93846468
O	7.34113978	-0.68067449	-5.95922140	H	5.14881299	-3.96849428	-1.51617020
H	6.68988269	-7.71604431	-5.61103667	C	5.18901070	-6.05881219	-1.46569653
C	5.32621720	-8.64778746	-9.73033750	H	5.11128062	-6.26208090	-2.51996526
H	6.00688418	-8.88421471	-10.55076819	N	5.21512207	-6.97034926	-0.50486230
H	4.86580299	-9.57391878	-9.39065592	C	5.23819936	-6.27931644	0.68808782
C	6.16084708	-8.11108252	-8.56583153	H	5.24172052	-6.79058337	1.64008066
O	6.53559940	-8.84430779	-7.67259056	C	5.98491518	-10.22855147	2.56244319
N	6.65334415	-6.78616047	-8.61431598	H	6.84766006	-9.86864886	1.99547617
H	7.20018875	-6.58917877	-7.78387931	H	5.37837670	-9.34782927	2.81570517
H	5.98603273	-6.03934023	-8.79573313	C	5.14158855	-11.14875595	1.71498278
C	3.33412919	-4.85560576	-6.32499939	N	4.67432593	-10.75808282	0.45851182
H	3.28671913	-3.85985311	-6.77134651	C	3.89800387	-11.73805128	0.00276836
H	2.75011782	-4.80672427	-5.39919604	H	3.35685615	-11.72216410	-0.93055258
C	4.76523870	-5.15095049	-5.99273122	N	3.84361426	-12.74216745	0.89285799
C	5.10963642	-6.35074117	-5.21485605	H	3.34803097	-13.63672619	0.76514021
O	4.25587321	-7.04478481	-4.65042208	C	4.61433625	-12.38986883	1.98029443
C	6.56427247	-6.75754420	-5.08728823	H	4.68204333	-13.02172199	2.85425763
H	6.79897907	-6.96265056	-4.03257821	Cu	4.97982803	-9.02229055	-0.60335719
C	7.57765848	-5.76968251	-5.62204900	O	7.47363113	-10.14741300	-3.81169237
O	8.71706728	-6.13828205	-5.89362431	H	7.95680961	-10.92972452	-3.44928340
C	7.13099169	-4.34994142	-5.84142118	H	8.15782605	-9.45160810	-3.91177380
N	8.01021712	-3.43250127	-5.75291121	O	3.02095222	-8.77889010	-0.73030360
C	5.71128356	-4.18952902	-6.16439654	H	2.55299274	-8.36570618	-1.50110744
H	5.43162231	-3.20679616	-6.53567297	H	2.37557591	-9.16194005	-0.06217234
H	7.64706125	-2.44593860	-5.86318685	O	5.07448015	-9.25398136	-2.82165432
C	-0.80203529	-1.39709795	-3.44709775	H	4.70957755	-8.59992067	-3.44795134
H	-1.07543254	-1.15635279	-2.41022735	H	5.95870017	-9.52630731	-3.16734707
H	-0.79498555	-0.44985698	-3.99554855	O	1.99877184	-7.37369392	-2.89389151
C	0.57510766	-2.00697241	-3.48784766	H	2.72187335	-7.03135279	-3.44539508
C	1.04604608	-2.85821063	-2.48409698	H	1.30973863	-7.60555930	-3.55092765
H	0.37394063	-3.16720016	-1.68588817	C	14.37532719	-7.43744876	-0.50955363
C	2.37245624	-3.29039978	-2.46308207	C	6.97894899	2.21116353	-5.65524653
H	2.72835255	-3.93025772	-1.66145722	C	4.23177602	-7.69557211	-10.26805736
C	3.26216131	-2.84494284	-3.44733340	C	2.64297428	-5.85719909	-7.28206378
O	4.58911455	-3.17025168	-3.35109217	C	-1.90562389	-2.28713123	-4.03955889
H	5.10824354	-2.46330078	-3.85487212	C	10.94478547	-8.75060747	1.53886506
				C	6.49237133	-3.39805176	2.05052121
				C	6.48451185	-10.84365249	3.86787462