

Electronic Supplementary Information

Computational Study of the Reaction Mechanism and Stereospecificity of Dihydropyrimidinase

Wijitra Meelua,^{ab} Tanchanok Wanjai,^b Natechanok Thinkumrob,^b Julianna Oláh,^c
James R. Ketudat Cairns,^d Supa Hannongbua,^e Ulf Ryde^f and Jitrayut Jitonnom*^b

^a *Demonstration School, University of Phayao, Phayao 56000, Thailand;* ^b *Unit of Excellence in Computational Molecular Science and Catalysis, and Division of Chemistry, School of Science, University of Phayao, Phayao 56000, Thailand;* ^c *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Műgyetem rakpart 3, Budapest H-1111, Hungary;* ^d *Center for Biomolecular Structure, Function and Application and School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand;* ^e *Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900 Thailand;* ^f *Department of Theoretical Chemistry, Lund University, Chemical Centre, P.O. Box 124, Lund SE-221 00, Sweden*

*Correspondence to Jitrayut Jitonnom, E-mail: jitrayut.018@gmail.com, jitrayut.ji@up.ac.th,
Tel.: +66 54 466 666; fax: +66 54 466 664.

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1. Results of Model I

For comparison purposes, we first designed a small model (hereafter Model I) of the (*S. kluyveri*) dihydropyrimidinase (*SkDHPase*) active site, containing only substrate (dihydropyrimidines DHU/DHT, hydantoid HYD or dihydroorotate DHO; see Scheme 2), the two zinc ions, and their ligands (namely, His62, His64, His199, His255, the carboxylated lysine Kcx167, and the catalytic residue Asp358). Asp358 was deprotonated and the four histidines were singly protonated on the N atom not coordinated to Zn. The resulting models consist of 81–83 atoms and have a total charge of +1, except for DHO which has zero net charge, owing to the negative charge of the COO⁻ group. This model lacks the important substrate-binding residues of the SGLs and, therefore, it is not expected to rationalize the enzyme substrate specificity and stereospecificity. Nevertheless, it still provides important information on the intrinsic reaction energetics, mechanism, and the transition states of the active site, which will be used for comparison when discussing the impact of SGLs by Model II within the main text.

We first examined how the results of Model I for DHU hydrolysis change if the continuum-solvation (CPCM) model is included or not, as shown in Figure S1. The results show that the solvation significantly affects the shape of the energy profile: The dielectric constant increases the activation energies and reaction energies, especially for the ring-opening step (INT1 → EP, Figure S1) involving the protonation of the cyclic amide ring of the substrate, assisted by Asp358 (see mechanistic detail in Scheme 1B). In particular, the activation barrier for the DHU hydrolysis is 21.9 kcal mol⁻¹ with the CPCM solvation ($\epsilon=4$), which is high compared to the experimental value (17.9 kcal mol⁻¹, estimated from $k_{\text{cat}} = 2 \text{ s}^{-1}$ in *SmDHPase* (1) and transition state theory). Similar results were also found for the hydrolysis of other substrates of cyclic amidohydrolases, shown in Scheme 2, using Model I and the CPCM($\epsilon=4$) model, as summarized in Figure S2. The results of Model I show relatively high energy profiles for most substrates with the activation barriers of 17.5–22.3 kcal mol⁻¹. These data suggest us that this model is too small to rationalize the stereospecificity of DHPase. Similar results have also been reported that a small model might not account well enough for the different electronic properties and flexibility of the surrounding environment (2). Therefore, a more realistic representation of the active site is required, so we generated Model II and used it for further discussion in the main text.

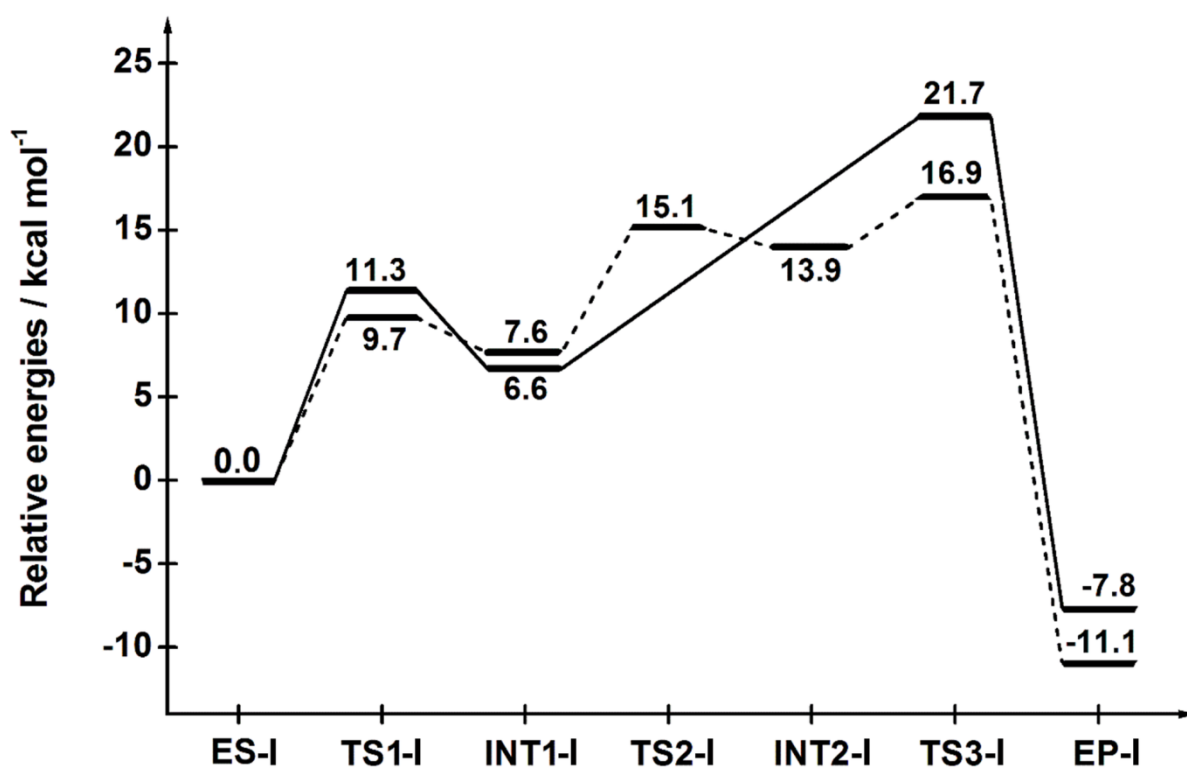


Figure S1. Calculated energy profiles for hydrolysis of DHU by *SkDHPase* in Model I. cluster + CPCM ($\epsilon=4$) (—) and cluster (-----).

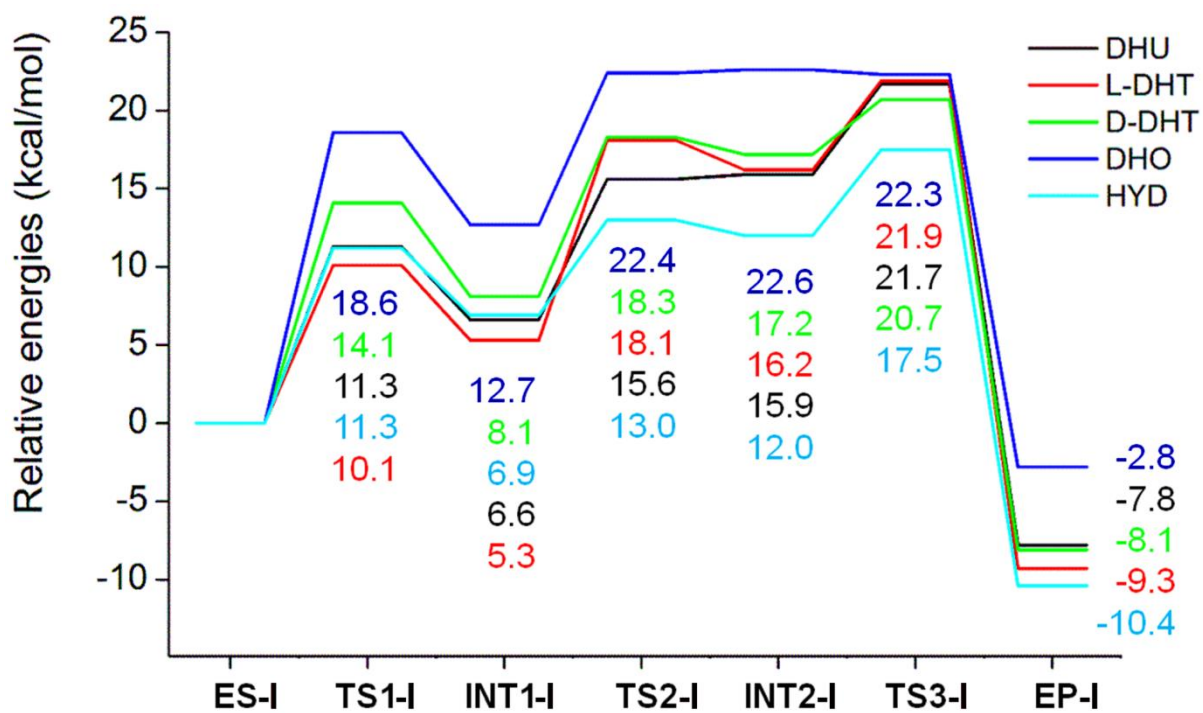


Figure S2. Calculated energy profiles for *SkDHPase*-catalyzed hydrolysis of the substrates of cyclic amidohydrolases (DHU, *L*-DHT, *D*-DHT, DHO, HYD; see Figure 1) in Model I. Reported energies are corrected for ZPE and solvation (CPCM and $\epsilon=4$).

2. Effects of dielectric constant and dispersion: results of Model II

In order to test the sensitivity of the large model (Model II) with the solvent dielectric, the energy profile of DHU hydrolysis was computed using the CPCM calculations with different dielectric constants ($\epsilon = 1.0, 4.0$ and 78.4 mimicking gas-phase, protein and water, respectively). The results of the Model II calculations (Figure S3 and Table S1) yielded almost identical computed energy profiles at $\epsilon = 4.0$ and $\epsilon = 78.4$, which shows that the size of Model II is large enough for further investigations. Thus, we chose Model II to describe the catalytic mechanism and the stereospecificity of DHPase in the main text.

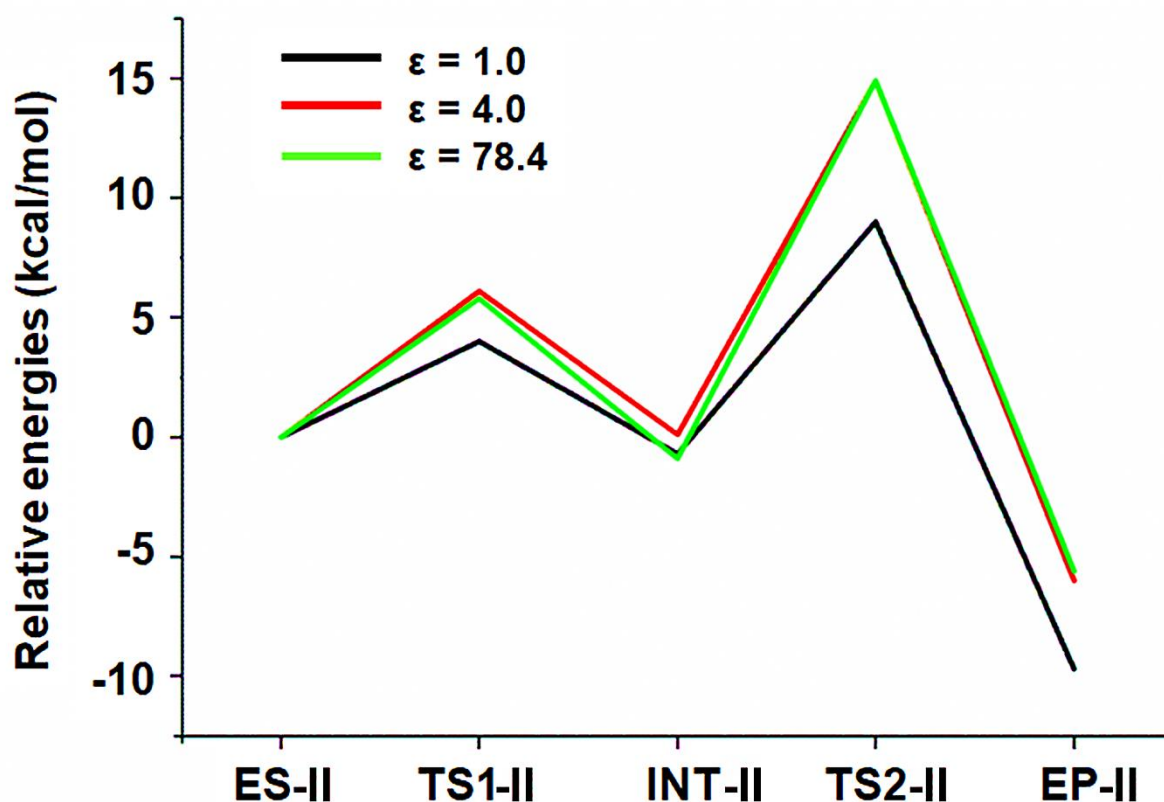


Figure S3. Effects of different dielectric constants (ϵ) on the relative energies of the DHU hydrolysis in **Model II** obtained at the B3LYP/6-311+G(2d,2p) level with CPCM ($\epsilon=1.0, 4.0, 78.4$).

Table S1. Effect of the solvation energy (dielectric constant) and the inclusion of dispersion energy (E_{disp}) for the various states in the DHU hydrolysis in Model II (also shown in Figure S3).

Structure	$\epsilon = 1.0$	$\epsilon = 4.0$	$\epsilon = 78.4$	Solvation ($\epsilon = 4$) + E_{disp}
ES-II	0.0	0.0	0.0	0.0
TS1-II	6.5	6.0	5.7	6.1
INT-II	2.0	-0.5	-1.6	0.1
TS2-II	17.3	17.4	17.4	14.9
EP-II	-7.7	-7.0	-6.6	-6.0

3. Results of Model II: DHU, L-DHT, D-DHT, HYD, DHO, 5FU, 5FUH2

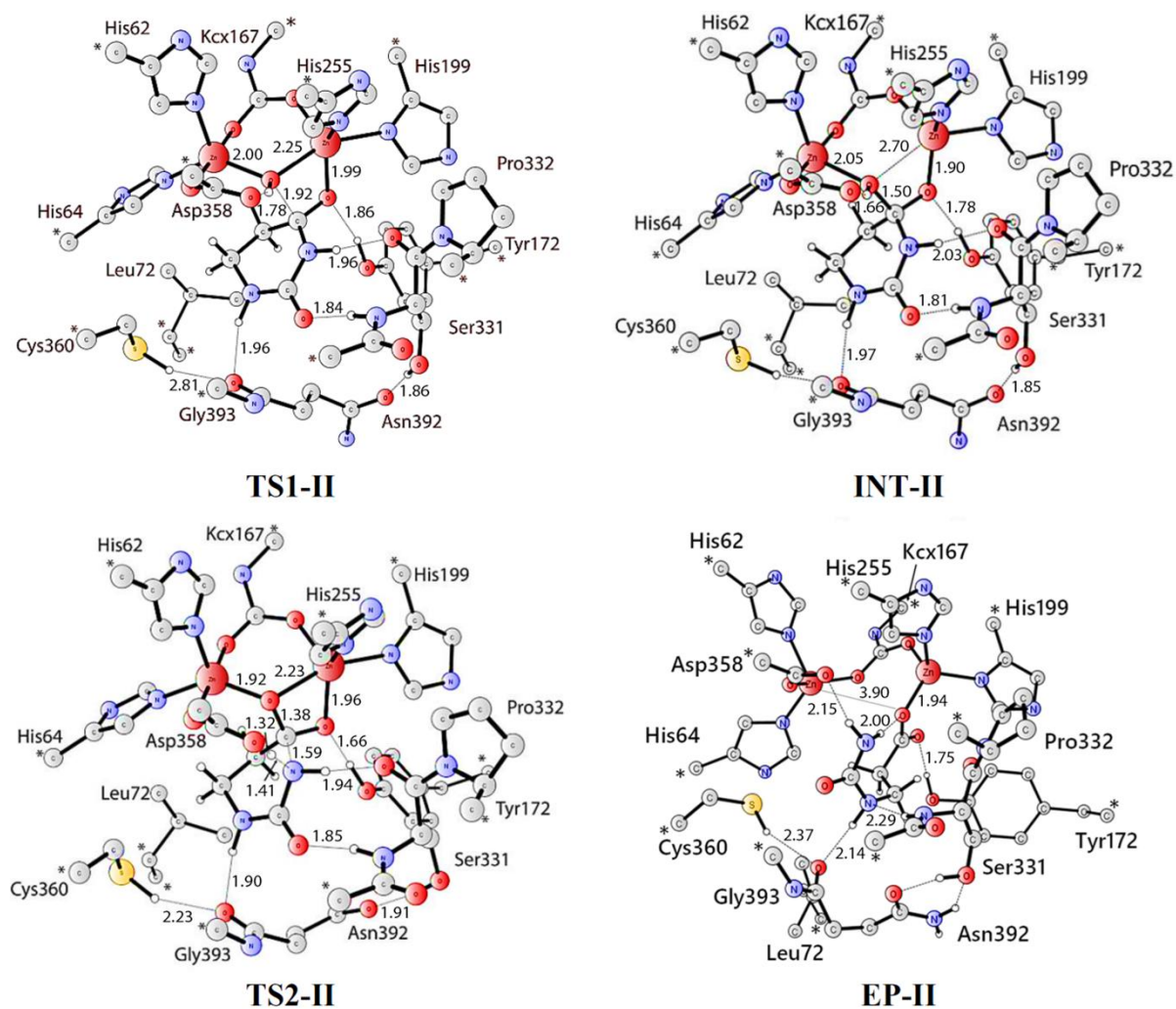


Figure S4. Optimized stationary points (TS1-II, INT-II, TS2-II, and EP-II) for the hydrolysis of DHU in Model II. Distances are in Å. Fixed atoms are shown by an asterisk. For clarity, only selected hydrogen atoms are shown.

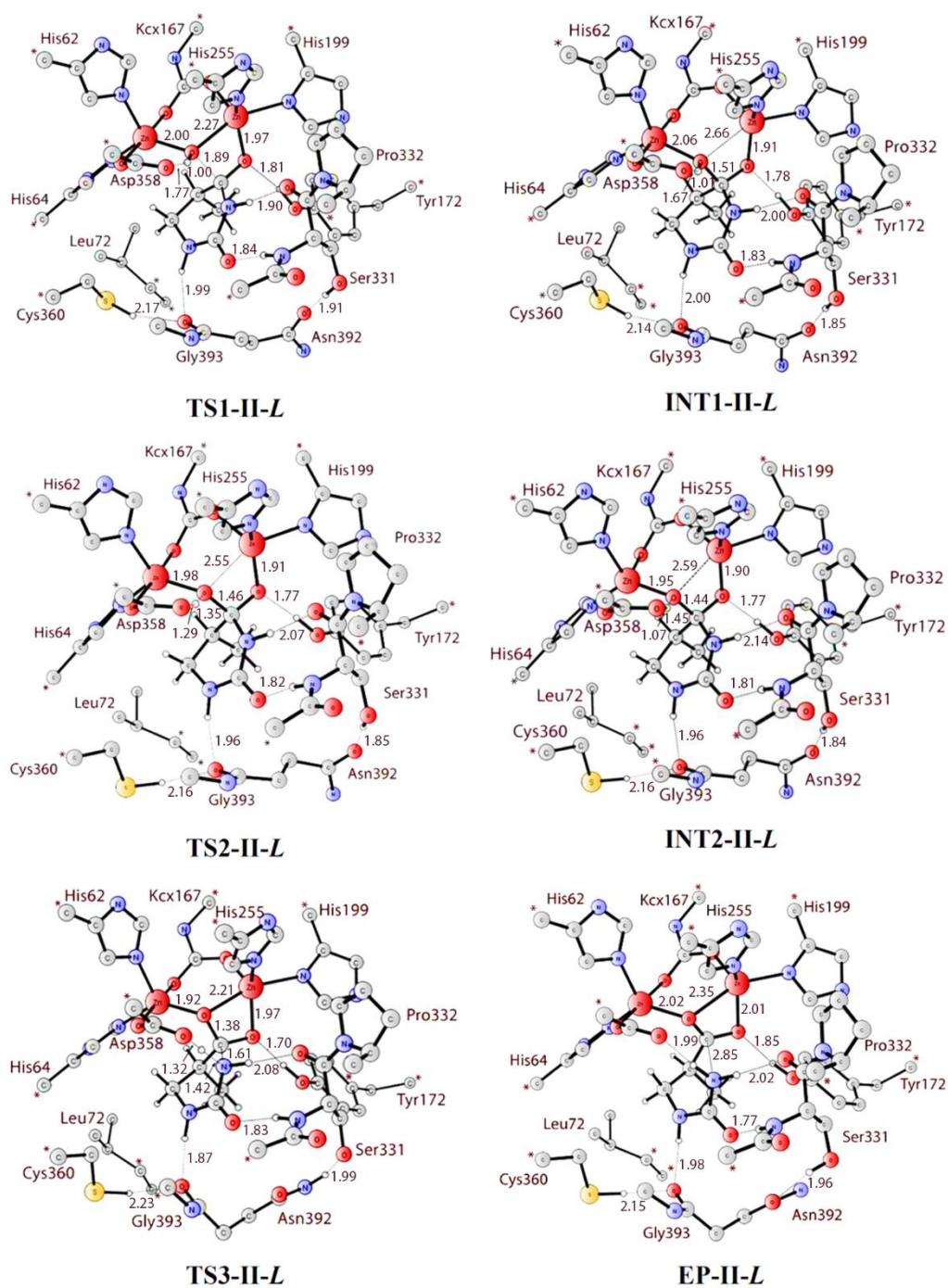
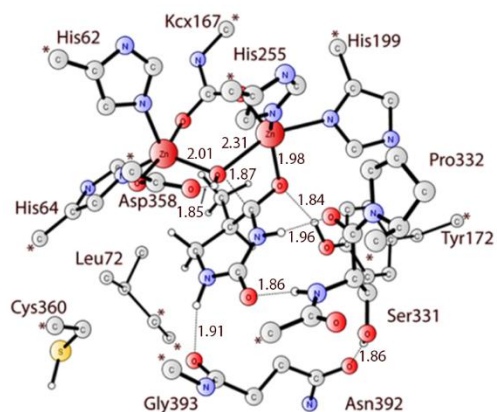
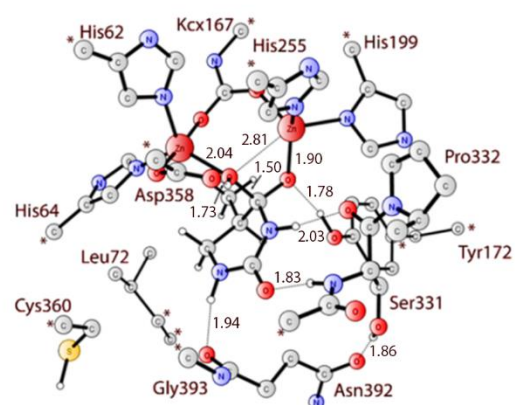


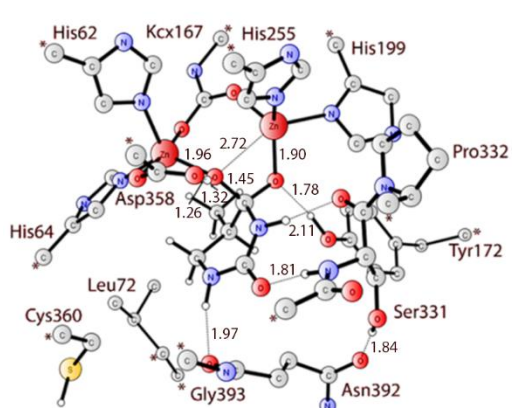
Figure S5. Optimized stationary points for the hydrolysis of *L*-DHT in Model II. Distances are in Å. Fixed atoms are shown by an asterisk.



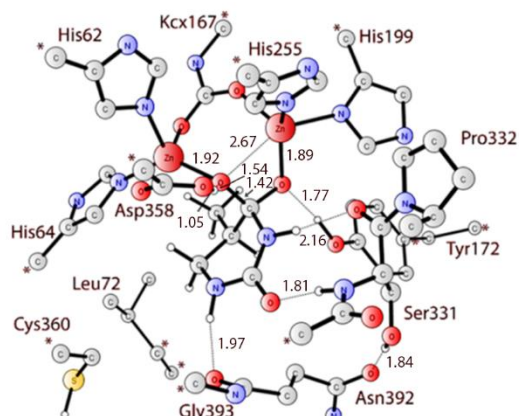
TS1-II-D



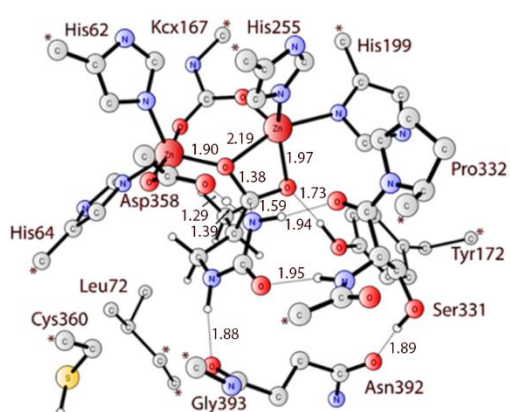
INT1-II-D



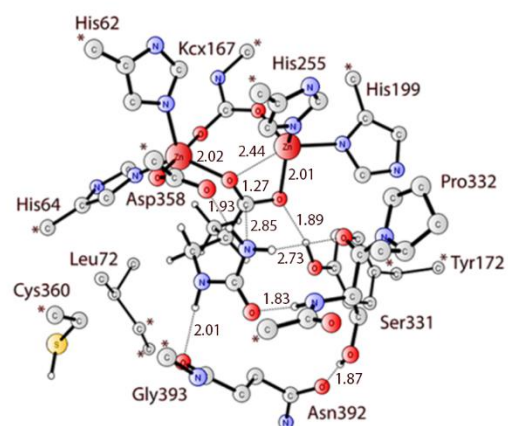
TS2-II-D



INT2-II-D



TS3-II-D



EP-II-D

Figure S6. Optimized stationary points for hydrolysis of *D*-DHT by *SkDHPase* in Model II. Distances are in Å. Fixed atoms are shown by an asterisk.

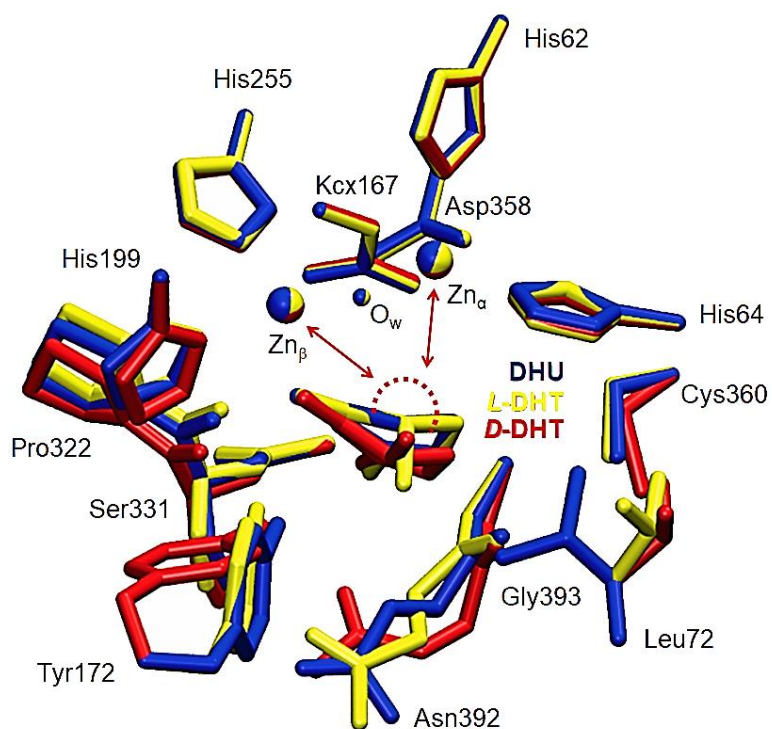


Figure S7. Overlay of the optimized structures of the ES-II with DHU (blue), *L*-DHT (yellow) and *D*-DHT (red) as substrates. The repulsion between the R group of the substrate and the zinc metals is also indicated with red dotted semicircle and the two-headed arrows.

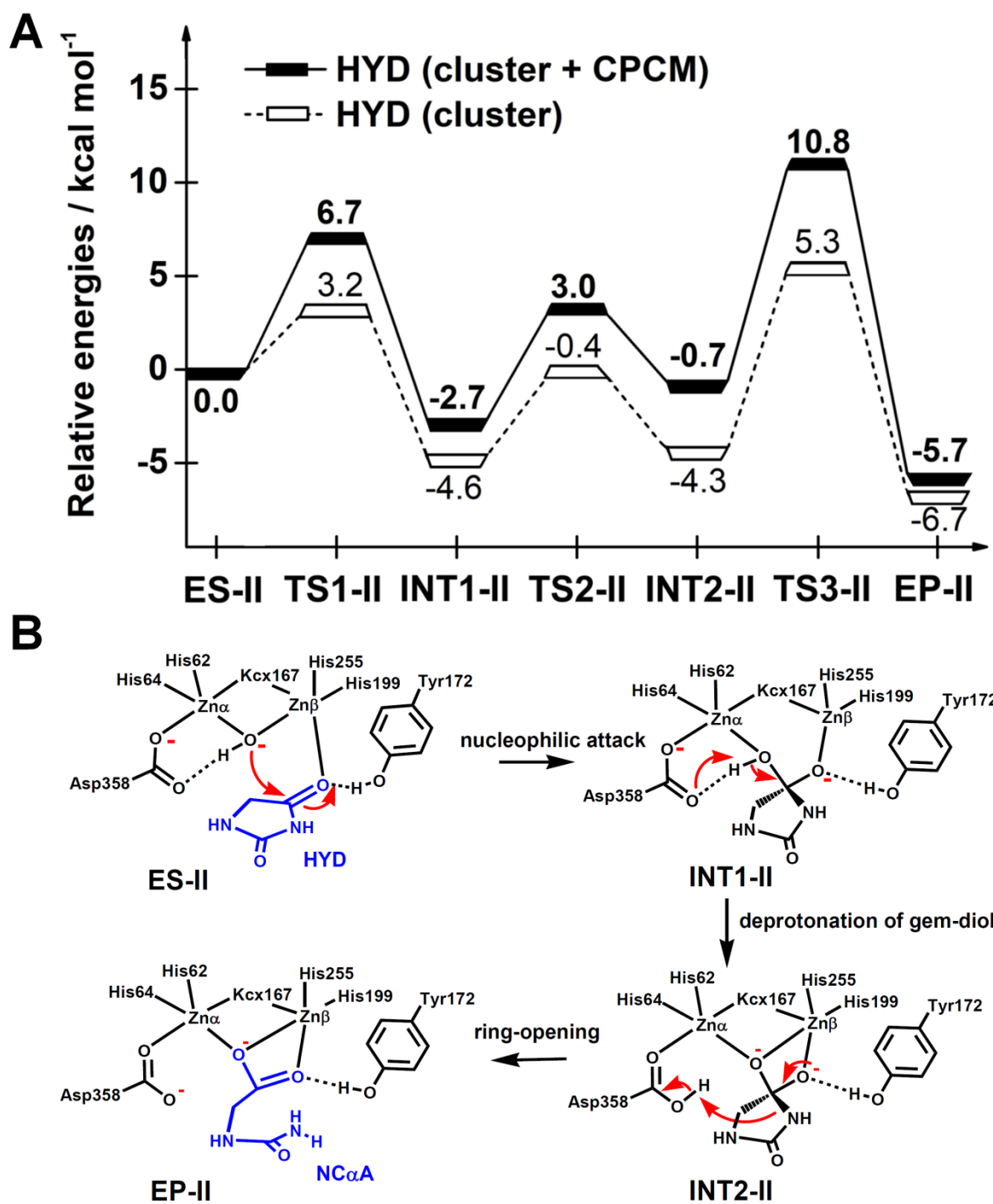


Figure S8. (A) Calculated energy profile for the hydrolysis of hydantoin (HYD) into *N*-carbamyl- α -amino acid (NC α A) by *Sk*DHPase in Model II; cluster + CPCM (—) and cluster (····). Energies were obtained at the B3LYP-D3/6-311+G(2d,2p)(CPCM, $\epsilon=4$)/B3LYP/6-31G(d,p) level of theory. (B) Suggested mechanism for the HYD hydrolysis in *Sk*DHPase.

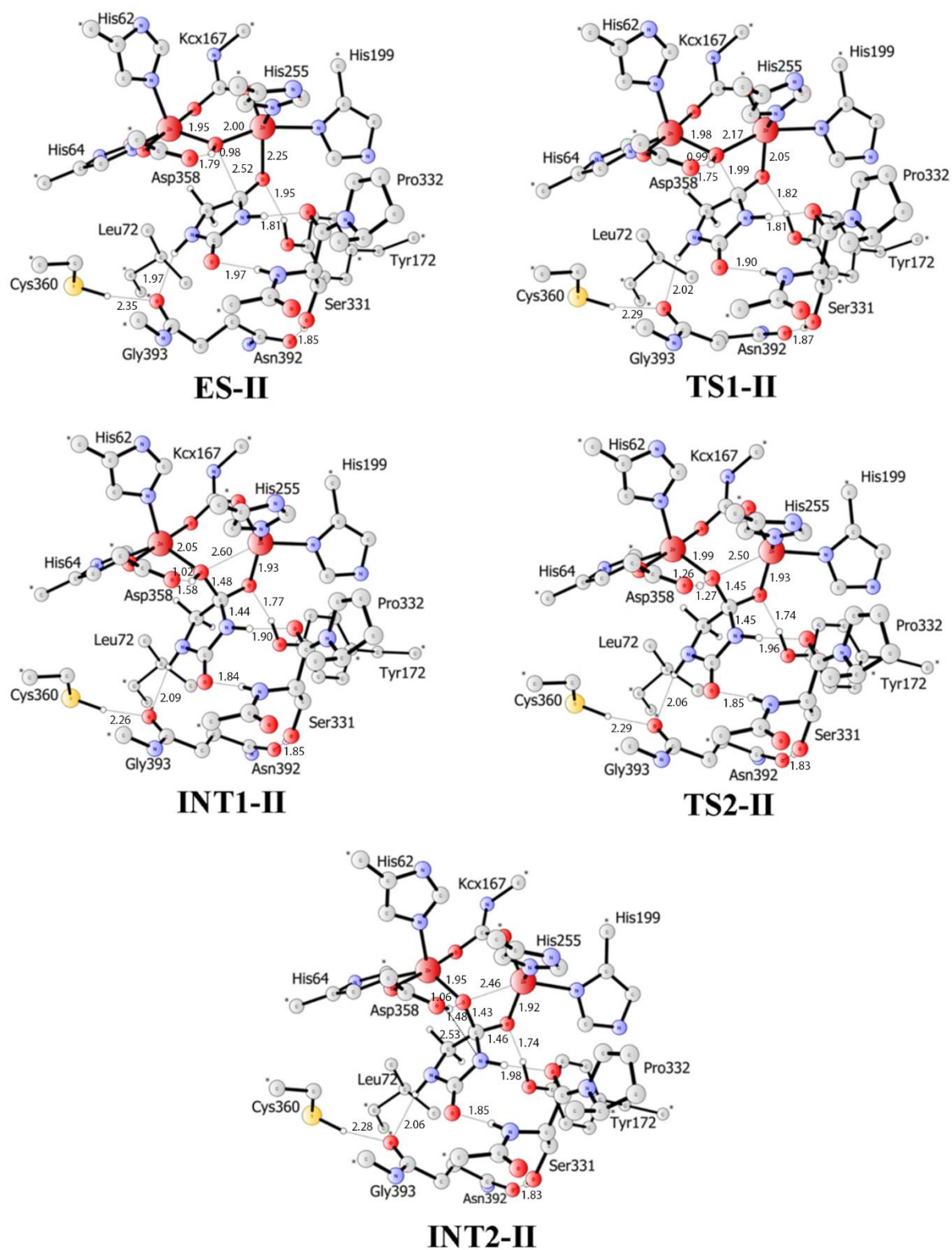
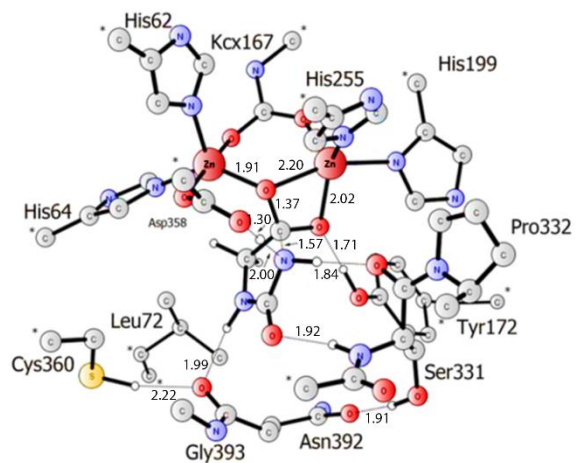
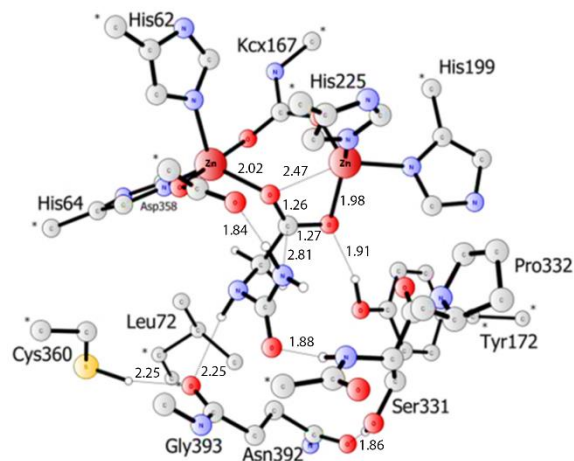


Figure S9. Optimized stationary points for the hydrolysis of HYD by *SkDHPase* in Model II. Distances are in Å. Fixed atoms are shown by an asterisk.



TS3-II



EP-II

Figure S9. Continued.

Reaction mechanism of DHO hydrolysis by *SkDHPase*. Starting from the ES, the hydroxide performs a nucleophilic attack on the C4 atom of the substrate and a tetrahedral intermediate (INT) is formed with a C4–O_w bond length of 1.51 Å. The barrier of this step is 12.0 kcal mol⁻¹ at TS1. During this step, the coordination number of Zn β changes from 5 to 4, due to the elongation of Zn β –O_w distance (1.98 Å at ES to 2.64 Å at INT). The shortening of the two distances between the substrate carbonyl oxygen (O4) to Zn β and Tyr172 from ES to INT (O4–Zn β = 1.94 Å at ES to 1.89 Å at INT and O4...HO@Tyr172 = 1.85 Å at ES to 1.75 Å at INT, Figure S11) indicates that these groups play roles in the stabilization of the transition state. The next step is the opening of the DHO ring and Asp358 plays a dual role by shuttling the proton from the hydroxide ion in INT to the nitrogen leaving group. This step was found to occur simultaneously through TS2. The scissile C–N bond is 1.59 Å and the transferring proton is in between the carboxylate group of Asp and the ring nitrogen (1.26 Å and 1.40 Å). After TS2, the C4–N3 bond is fully broken with a distance of 2.73 Å, and the product carbamoyl aspartate is formed.

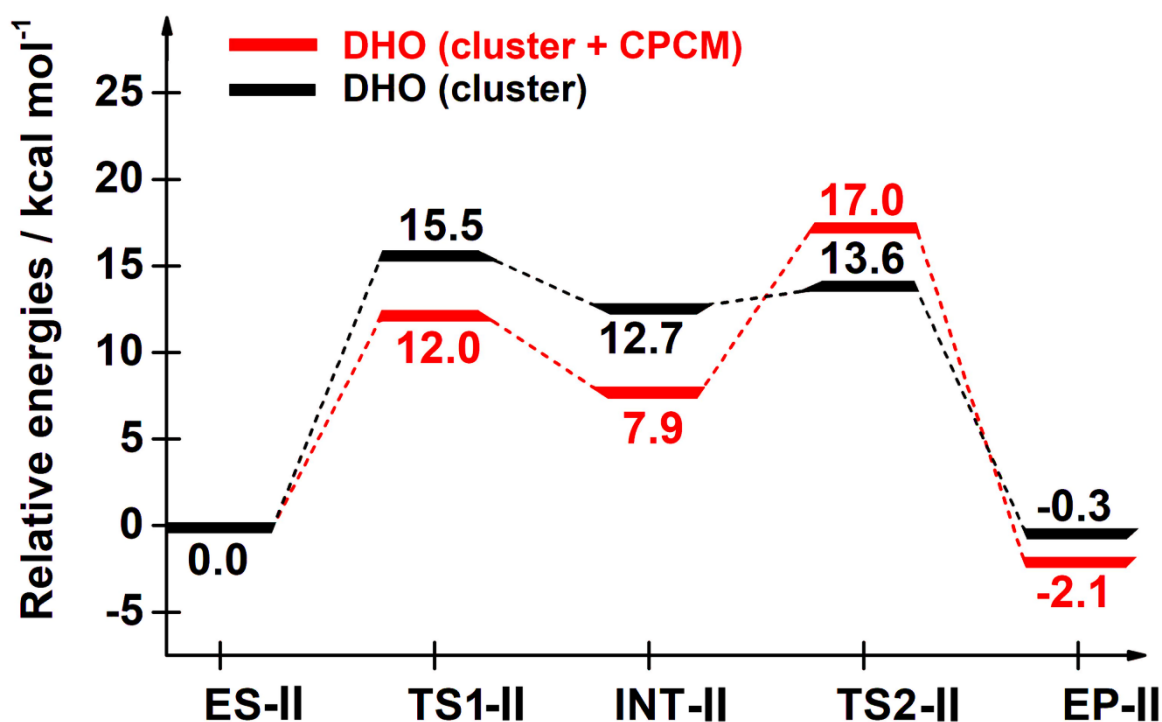


Figure S10. Calculated energy profile for the hydrolysis of DHO by *SkDHPase* in Model II; cluster + CPCM (black) and cluster (red). Energies were obtained at the B3LYP-D3/6-311+G(2d,2p)(CPCM, $\epsilon=4$)/B3LYP/6-31G(d,p) level of theory.

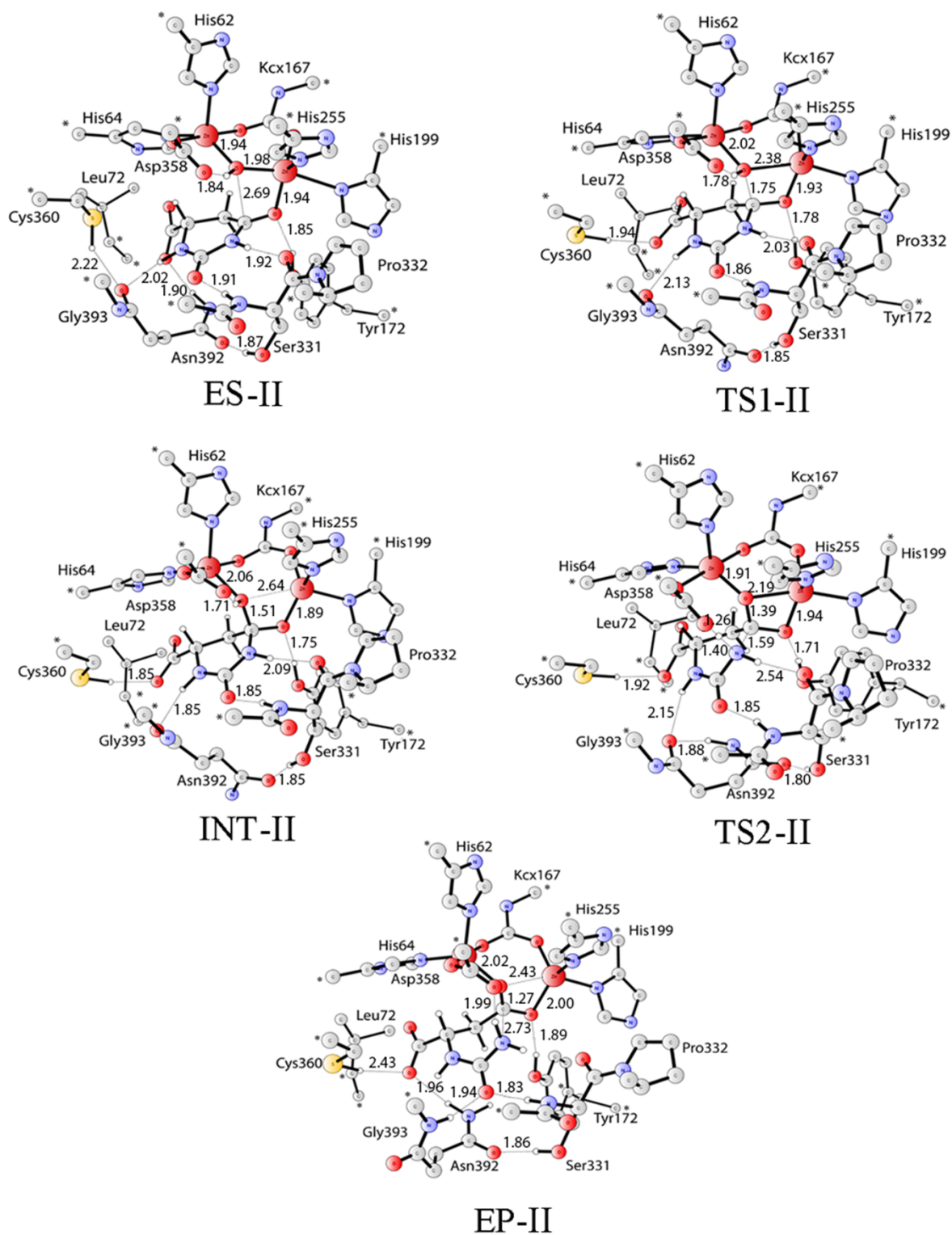


Figure S11. Optimized stationary points for the hydrolysis of DHO by *SkDHPase* in Model II. Distances are in Å. Fixed atoms are indicated by asterisks.

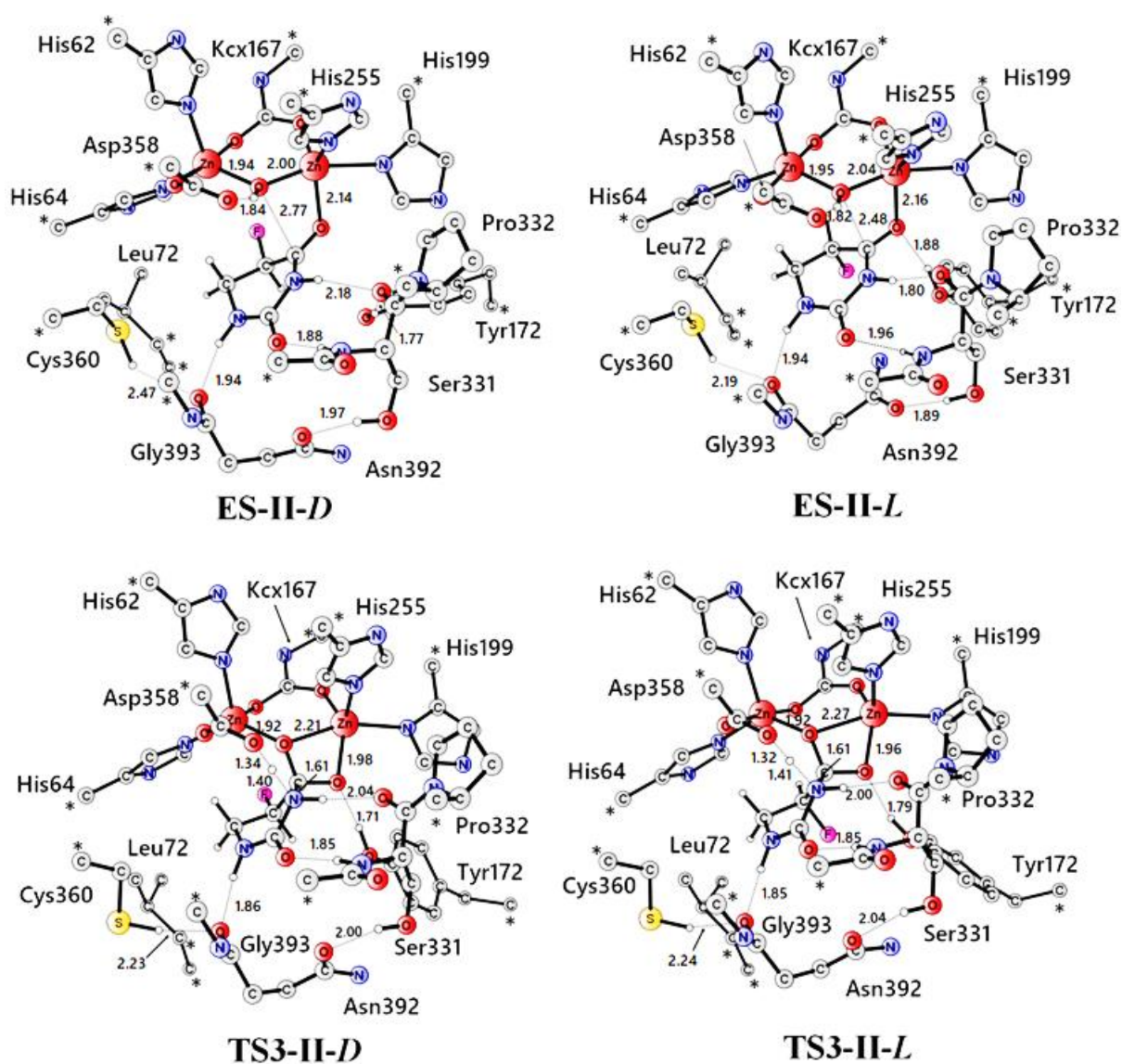


Figure S12. Optimized structures of the *SkDHPase-5FUH2* complexes at **ES-II** and **TS3-II** in *L*- and *D*-configurations in Model II. Distances are given in Å. Fixed atoms are indicated by asterisks.

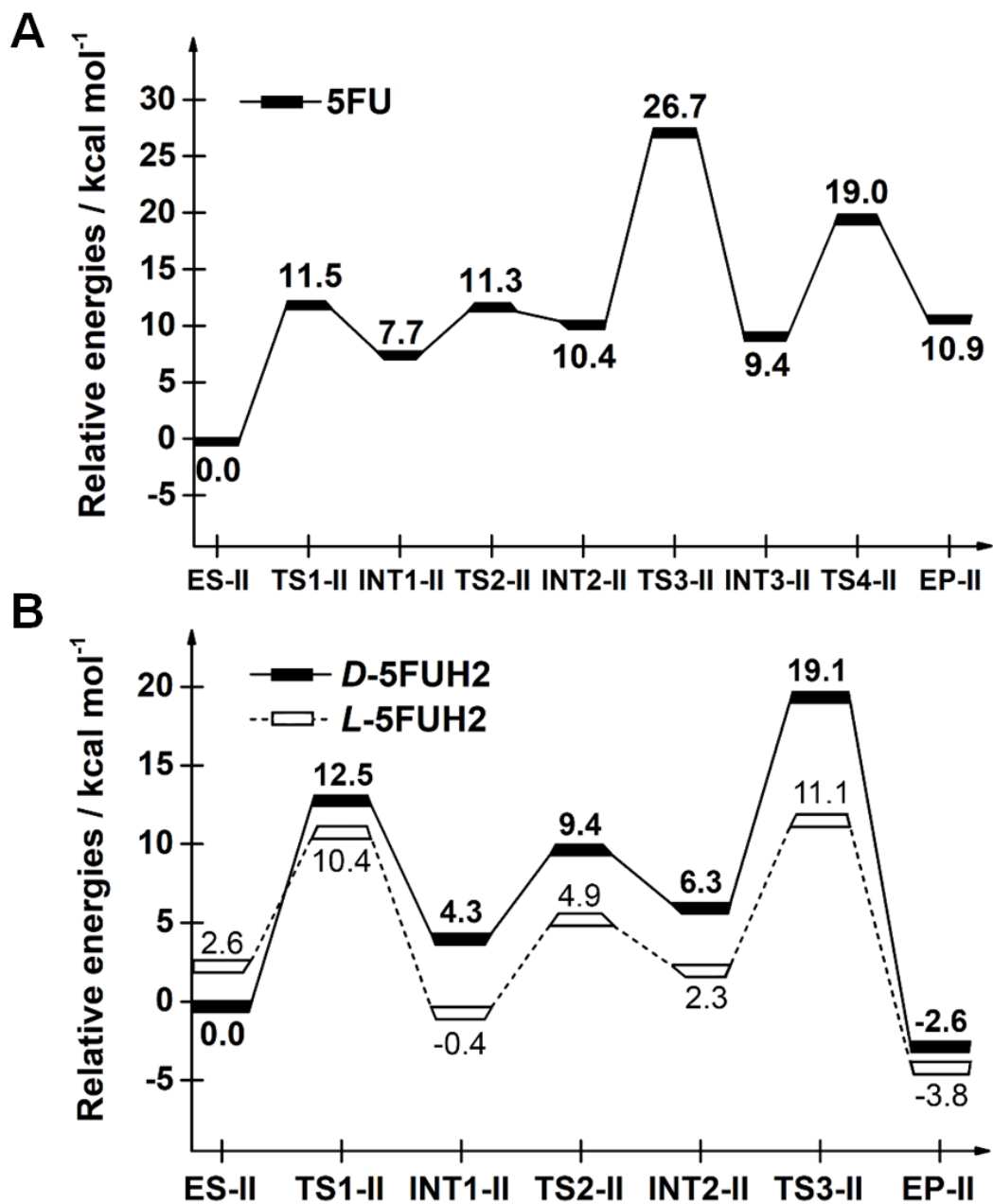


Figure S13. Calculated energy profiles for the hydrolysis of 5-fluorouracil (5FU) and dihydro-5-fluorouracil in either *L*- or *D*-configurations (*L*-5FUH2 and *D*-5FUH2) in Model II. Relative energies were obtained at the B3LYP-D3/6-311+G(2d,2p)(CPCM, $\epsilon=4$)/B3LYP/6-31G(d,p) level of theory.

4. Binding interaction energies in *Sk*DHPase and *Sm*DHPase

Table S2. Binding energies (BE, kcal mol⁻¹) for different substrates in the active site pocket of *Sk*DHPase and *Sm*DHPase, obtained using the B3LYP and B3LYP-D3 methods

Substrate	B3LYP			B3LYP-D3		
	<i>Sk</i> DHPase	<i>Sm</i> DHPase	Δ	<i>Sk</i> DHPase	<i>Sm</i> DHPase	Δ
HYD	-6.0	-11.3	5.4	-30.2	-39.1	8.9
(5 <i>R</i>)-MeHYD	+10.9	-7.8	18.7	-16.4	-37.4	21.0
(5 <i>S</i>)-MeDHU	+8.5	-6.2	14.7	-22.4	-40.8	18.4
(5 <i>S</i> ,6 <i>S</i>)-Me ₂ DHU	-11.1	-7.3	3.8	-39.6	-43.9	4.3
(5 <i>S</i> ,6 <i>R</i>)-Me ₂ DHU	-13.1	-8.5	4.6	-46.5	-45.2	1.3

5. *In silico* point mutation of stereo-gate-loop (SGL) residues in *SkDHPase*: Y172F, L72F

Table S3. Effects of Tyr172Phe and Leu72Phe *SkDHPase* mutants on the binding energies (BE, kcal mol⁻¹) and activation energies E_a (Model II). The energies were obtained at the B3LYP/6-311+G(2d,2p) + CPCM($\epsilon=4$) level of theory

Substrate	BE			E_a -II		
	WT	Tyr172Phe	Leu72Phe	WT	Tyr172Phe	Leu72Phe
DHU	-10.8	-11.9	-11.0	14.9	25.1	19.1
<i>L</i> -DHT	-15.0	-13.6	-11.8	15.7	33.1	27.2
<i>D</i> -DHT	-5.8	-11.9	-9.8	25.8	34.4	33.1
HYD	-6.0	-10.8	-11.5	10.8	25.5	16.2
<i>L</i> -HYD	-6.8	-9.2	-6.7	16.9	26.7	21.8
<i>D</i> -HYD	-11.1	-11.0	-8.9	14.4	23.3	17.2

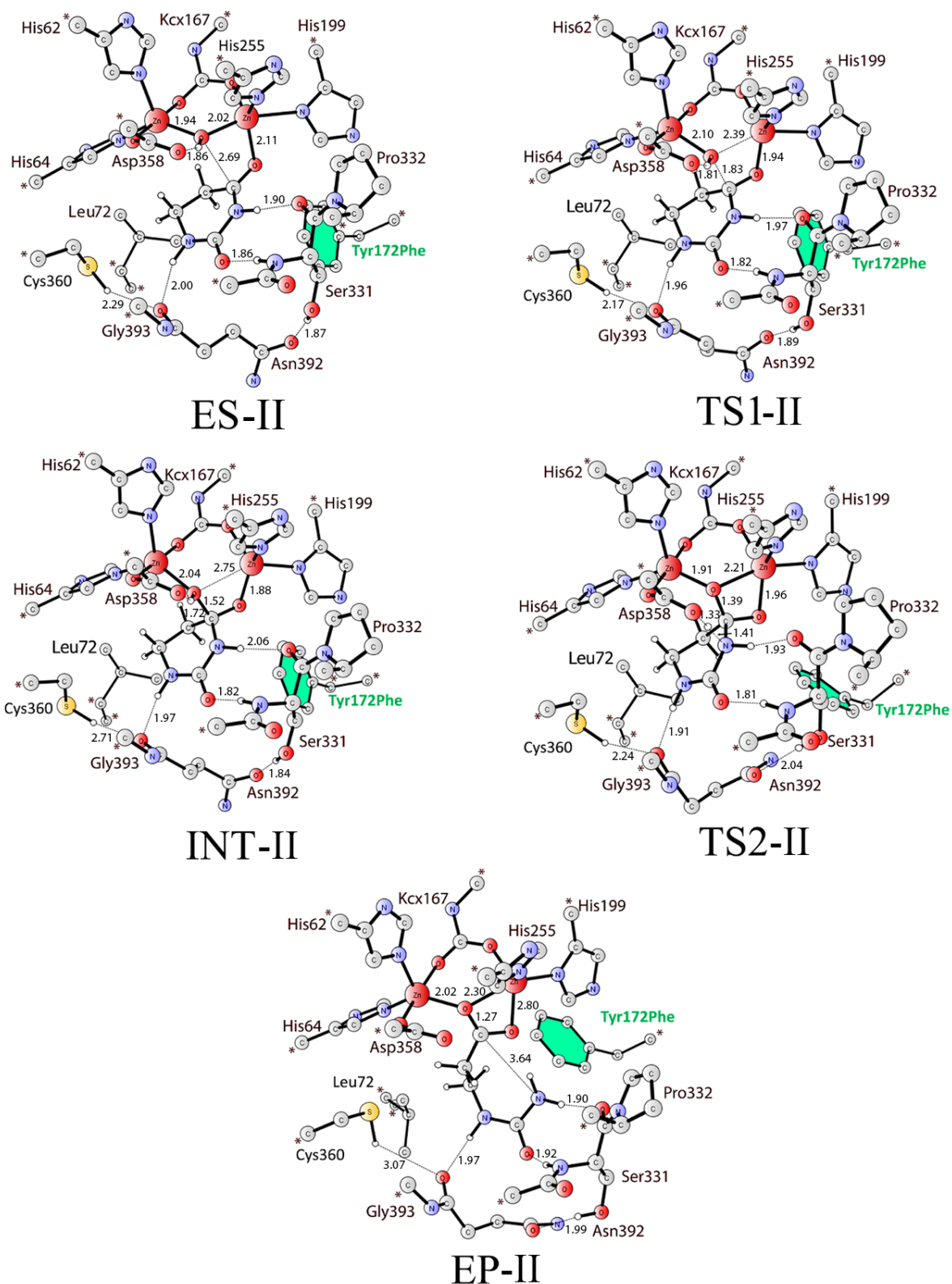


Figure S14. Optimized stationary points for the hydrolysis of DHU by the Y172F *SkDHPase* mutant in Model II. Distances are in Å. Fixed atoms are indicated by asterisks.

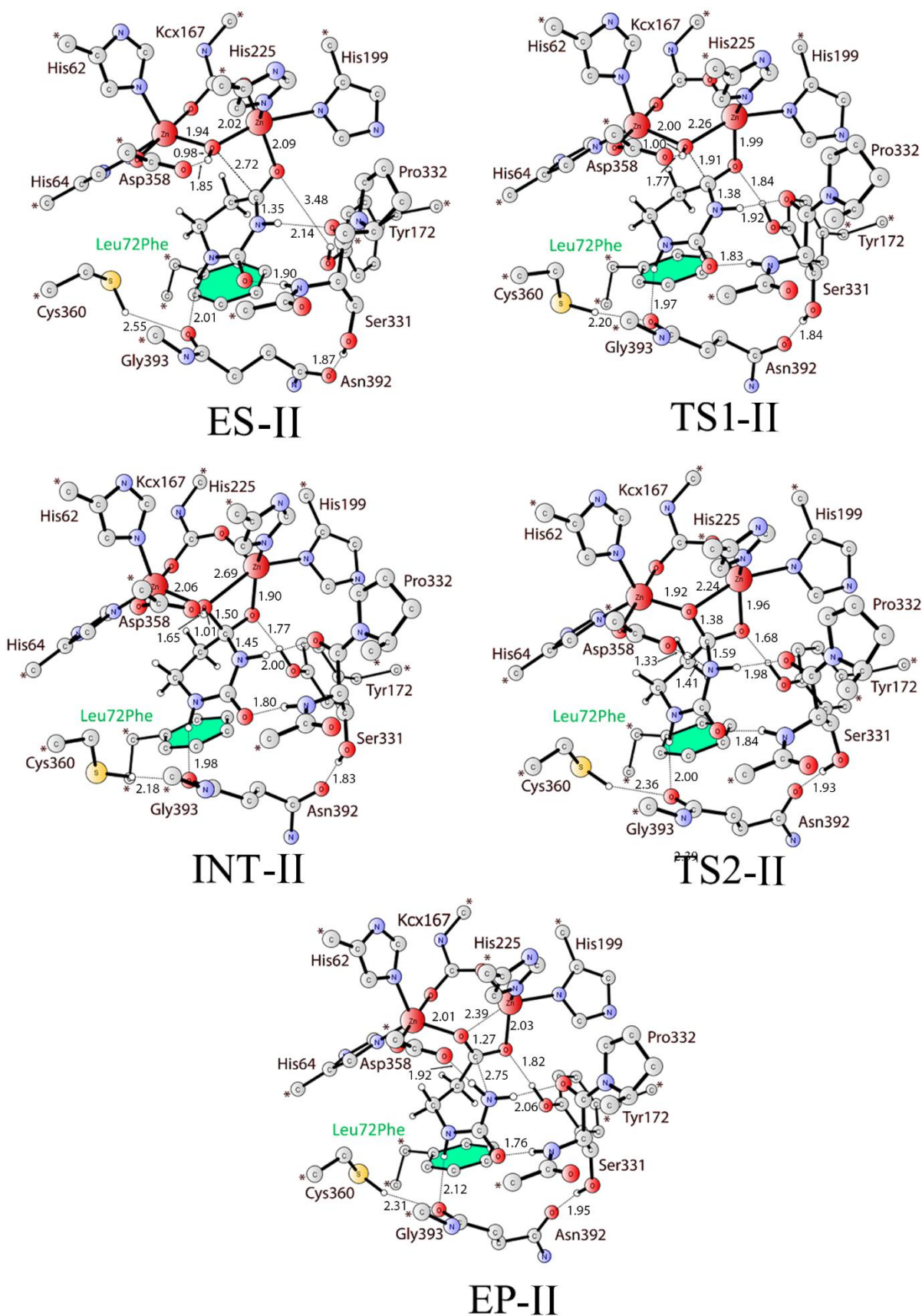


Figure S15. Optimized stationary points for the hydrolysis of DHU by the L72F *SkDHPase* mutant in Model II. Distances are in Å. Fixed atoms are marked by asterisks.

6. References

- 1) Martínez-Rodríguez, S., Martínez-Gómez, A. I., Clemente-Jiménez, J. M., Rodríguez-Vico, F., García-Ruíz, J. M., Las Heras-Vázquez, F. J., and Gavira, J. A. (2010) Structure of dihydropyrimidinase from *Sinorhizobium meliloti* CECT4114: New features in an amidohydrolase family member. *J. Struct. Biol.* **169**, 200-208
- 2) Jafari, S., Ryde, U., and Irani, M. (2016) Catalytic mechanism of human glyoxalase I studied by quantum-mechanical cluster calculations. *J. Mol. Catal. B: Enzym.* **131**, 18-30

7. XYZ coordinates for all optimized structures in Model II

*S*kDHPase.DHU-ES-II

C	-8.43178100	-2.04663400	-1.93631500	H	-5.55176400	-2.68526600	1.65449800
C	-7.28193400	-1.91423000	-1.00573100	H	-5.74627200	5.03349800	-1.26421000
N	-7.10021700	-2.66161700	0.14917400	H	-4.81290700	5.86475200	-0.01186000
C	-6.18675200	-1.10415900	-1.07247500	H	-4.63111900	2.38252400	-1.43999700
C	-5.92818400	-2.28745700	0.72290500	H	-4.97654700	4.08859500	2.38621200
N	-5.34649000	-1.34775400	-0.00326600	H	-4.07326600	1.70780200	2.65091400
C	-5.54413200	5.06698400	-0.19071700	H	-1.21980100	-4.52482300	4.37606500
C	-5.03480800	3.73965000	0.27591200	H	2.38713100	-5.70281000	4.22551900
N	-4.83382000	3.44862700	1.61725700	H	3.68589600	-4.22825700	2.58227600
C	-4.63647300	2.60406300	-0.38396000	H	2.13839100	-2.86321500	1.10846100
C	-4.32458600	2.19909800	1.72402600	H	-3.11001100	-4.42456100	-3.69158000
N	-4.19075400	1.65962200	0.52441500	H	-2.22508300	-5.93991200	-3.90222700
C	-4.12449500	-3.30869200	4.37224900	H	-2.17324700	-2.88842400	-1.72023600
N	-4.24837100	-2.08597900	3.60580300	H	-1.55991900	-7.00298900	-1.20706300
C	-3.22273600	-1.64864400	2.79450800	H	-0.52684300	-5.82187600	0.79970900
O	-2.26932500	-2.48543600	2.62856800	H	-3.86757300	-4.13657800	3.70874700
O	-3.33694800	-0.50143300	2.27301600	H	-3.61492100	-1.41011900	-4.85072200
C	-0.57368300	-5.30709800	3.96598200	H	-4.87362000	-1.84580200	-3.67299100
C	0.61986700	-4.71181600	3.27832000	H	-1.61463200	1.89691100	-0.31513400
N	0.56516400	-3.75334600	2.26251200	H	-0.97148000	3.22299200	0.65792200
C	1.93308600	-5.02644600	3.51767400	H	-1.13815500	0.89731700	1.86179200
C	1.82077300	-3.52249200	1.90397600	H	0.43825200	1.71044500	1.96001100
N	2.67792700	-4.26910800	2.63717500	H	-6.47784800	5.34395600	0.31345300
C	-2.84934600	-5.36731100	-3.20461000	H	-1.18781200	-5.90000000	3.27610000
C	-2.14545300	-5.06785500	-1.92981000	H	-0.25211500	-5.96305500	4.77960000
N	-1.57891200	-6.00135900	-1.07238000	H	-5.08428900	-3.52571200	4.85088300
C	-1.91760100	-3.86179500	-1.33518200	H	-3.35373000	-3.24786900	5.15266000
C	-1.04137600	-5.33935300	-0.01674300	H	-8.31791900	-1.33523400	-2.75799300
N	-1.23456400	-4.03641600	-0.14874100	H	-4.82763700	-0.20185200	-4.32425100
C	-4.20390600	-1.04325600	-4.00715000	H	-3.77462400	-5.93682900	-3.04742700
C	-3.28884400	-0.65345700	-2.83907500	H	-4.85673200	-1.35672600	3.95098000
O	-3.78312600	0.14091100	-1.95696500	H	1.57371000	-0.54443100	-0.87476100
O	-2.15330400	-1.17297200	-2.78031000	H	0.48661700	3.36530500	-1.21731900
Zn	-3.57704600	-0.26760800	0.11470200	O	-1.82401900	-1.08290600	-0.03344400
Zn	-0.96885600	-2.46857400	1.16661100	H	-1.66825700	-1.10638700	-1.00512200
N	0.98135300	0.22772600	-0.53734200	C	0.09056100	7.86937000	4.28033000
C	1.10809100	1.45975000	-1.21726000	C	-0.65039600	7.08726500	3.18827000
O	1.89193800	1.55184100	-2.16477200	C	-0.94368600	5.62814900	3.59514200
N	0.36412100	2.47120300	-0.74139000	C	-2.10030100	5.04845200	2.77362100
C	-0.72424100	2.26076600	0.20837300	C	0.30516100	4.73970900	3.48907000
C	-0.29058700	1.25562100	1.27392500	C	-3.50488000	5.92229300	-3.73369700
C	0.39837000	0.06245900	0.67223300	C	-2.75613600	4.97549800	-2.79877900
O	0.57042900	-1.00808100	1.29990100	S	-1.84944600	5.83262400	-1.43061400
H	-8.49748200	-3.05120100	-2.37358200	C	3.80414500	4.65860200	-2.54284500
H	-9.39193400	-1.83750700	-1.44746600	C	2.33211000	4.59571900	-2.94877500
H	-5.91938600	-0.37400900	-1.81735300	O	1.43368800	4.84404900	-2.13215000
H	-7.73155200	-3.36386500	0.50928300	C	4.09929800	3.70148900	-1.37057000

C	5.46845300	3.83620200	-0.71550700	H	4.64231000	0.74758800	7.41975200
O	6.16070300	2.85503900	-0.43695700	H	3.10954900	-0.58775100	5.85023000
N	5.88981300	5.09363300	-0.41554600	H	6.32357900	1.83965800	4.36472800
N	2.06862900	4.30106900	-4.23975400	H	2.17437400	-0.75413500	3.55950000
C	0.70626500	4.14473300	-4.73585600	H	5.39592400	1.65750600	2.05870400
H	-1.59811100	7.59936500	2.97194000	H	2.66040500	-0.41336700	1.33457500
H	-0.07667900	7.09811000	2.25085400	H	5.49771300	-1.55616400	6.83591300
H	-1.26052400	5.63641800	4.64957000	H	6.97166800	-0.83600500	6.17332700
H	-3.02029700	5.62514500	2.94056100	H	6.62478300	-0.70557600	7.90847900
H	-2.29548000	4.00409600	3.04736400	C	2.86377200	0.66751800	-5.18872300
H	-1.88533800	5.08278000	1.69818700	C	3.77498300	-0.37331400	-4.56719400
H	0.10153500	3.72267500	3.84646700	O	4.53529500	-1.05874400	-5.24869200
H	0.64557200	4.67014400	2.44706400	N	3.63506200	-0.50075300	-3.22048900
H	1.13753700	5.13268600	4.08259300	C	4.49828300	-1.35206900	-2.42794300
H	1.05432000	7.41060000	4.52972200	C	3.62722700	-2.42528600	-1.76024200
H	-3.44830600	4.28985200	-2.30485100	O	2.77405500	-2.08258200	-0.90846600
H	-2.03875100	4.35636800	-3.34340200	C	5.25432600	-0.53910100	-1.35695700
H	-0.61908600	5.81558700	-1.98706800	O	5.96433900	0.48861500	-2.00810000
H	-4.22243300	6.53810300	-3.18174100	N	3.77574600	-3.72145400	-2.09375300
H	4.01411300	2.66743600	-1.70512700	C	4.69388700	-4.32799400	-3.10000200
H	3.33805600	3.85485700	-0.59503300	C	4.14956400	-4.21393200	-4.53044500
H	5.29139500	5.90119100	-0.49947500	C	4.77872200	-5.78267700	-2.59915200
H	6.75524400	5.19226000	0.09791400	C	3.36035300	-6.06887500	-2.07975000
H	4.46523000	4.43890600	-3.38855700	C	2.94252000	-4.74182800	-1.42776400
H	0.12763800	5.04999200	-4.53317500	H	1.88081500	-4.50456100	-1.54630400
H	0.21296600	3.28979400	-4.26059000	H	3.15630400	-4.73367000	-0.35264000
H	2.83151000	4.01180300	-4.83485000	H	2.69190100	-6.31543700	-2.91160300
H	3.98820100	5.70163400	-2.25672900	H	3.32551700	-6.90247900	-1.37192500
H	0.74358600	3.98258200	-5.81455000	H	5.09676400	-6.46899500	-3.38872700
H	-2.81750300	6.60048400	-4.24982700	H	5.50309600	-5.85433500	-1.77855600
H	-4.05523900	5.35084200	-4.49229500	H	5.67037700	-3.84079600	-3.03892900
H	-0.50385100	7.91228300	5.20089400	H	3.14724100	-4.65026800	-4.60766300
H	0.29065400	8.90014600	3.96667700	H	4.11623800	-3.17373900	-4.86342200
C	6.17241800	-0.69555000	6.90971400	H	4.81143000	-4.75945500	-5.21343900
C	5.41648400	0.61834500	6.65182400	H	5.21902000	-1.78065100	-3.12419100
C	4.79296700	0.62850300	5.27522800	H	6.07686800	1.23530800	-1.38521800
C	3.61960200	-0.09353200	5.02547400	H	5.92939600	-1.22940800	-0.81822400
C	5.41300900	1.26921600	4.19420900	H	4.53993800	-0.14764600	-0.62361900
C	3.09301300	-0.20044700	3.74047000	H	3.05242600	0.17828700	-2.73502300
C	4.90494700	1.17556700	2.89975300	H	2.10954500	0.15639800	-5.79802300
C	3.75070500	0.42314200	2.67507400	H	2.35924200	1.29614100	-4.45364400
O	3.28443100	0.32968700	1.38681400	H	3.46045500	1.28163500	-5.87159600
H	6.10593100	1.46472500	6.75817600				

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C	-8.17514900	-2.93961500	-1.41326500	N	-4.94421800	-2.01143300	0.15839800
C	-6.91218100	-2.75425400	-0.65008100	C	-5.94944200	4.49602000	-0.09162700
N	-6.40706600	-3.64470600	0.28820200	C	-5.33579400	3.22336200	0.39333900
C	-5.98975700	-1.75050100	-0.70672300	N	-5.07341800	2.98112000	1.73368900
C	-5.22675500	-3.15864900	0.75020700	C	-4.87593700	2.10564100	-0.25454400

C	-4.47108700	1.77519200	1.85130500	H	0.20652500	-5.75893400	0.99814200
N	-4.33415400	1.21819600	0.65950700	H	-3.24056300	-4.35355300	4.02972700
C	-3.43020200	-3.49648000	4.67925800	H	-3.60791300	-1.98211100	-4.59871600
N	-3.73122000	-2.32648600	3.88327700	H	-4.78058500	-2.42091500	-3.33161800
C	-2.89845000	-1.91143400	2.88080100	H	-2.06584900	1.66964900	-0.53932100
O	-1.97779500	-2.74122700	2.55852100	H	-1.51696500	3.10081400	0.33659400
O	-3.13640000	-0.78851600	2.34099900	H	-1.43431200	0.92424000	1.75519200
C	0.28144000	-5.14025300	4.14197700	H	0.11473000	1.77783200	1.61901100
C	1.36595000	-4.36589100	3.45162700	H	-6.88763900	4.72107100	0.42980700
N	1.15656200	-3.47889800	2.39352600	H	-0.20362600	-5.85678400	3.46681900
C	2.70811800	-4.40677800	3.72768000	H	0.69590100	-5.70119900	4.98405300
C	2.35290200	-3.01644500	2.04742900	H	-4.29017300	-3.72230900	5.31636600
N	3.31426400	-3.55384700	2.82766600	H	-2.55094200	-3.35614100	5.32245700
C	-2.35494900	-5.72778700	-2.87969700	H	-8.32118800	-2.08932000	-2.08382700
C	-1.59827000	-5.28657300	-1.67775200	H	-4.89325400	-0.83687300	-4.10455800
N	-0.92354600	-6.12397400	-0.79993100	H	-3.21523200	-6.35825200	-2.62013800
C	-1.42367800	-4.03087600	-1.17081100	H	-4.36358400	-1.62867200	4.24648400
C	-0.38190700	-5.36462500	0.18402600	H	1.42690200	-0.47768700	-0.92730000
N	-0.67415800	-4.08861900	-0.01298900	H	-0.04132300	3.26281100	-1.49713700
C	-4.19014600	-1.60009200	-3.75750800	O	-1.50239700	-1.03849900	-0.01980600
C	-3.26833000	-1.04839800	-2.66770100	H	-1.46344900	-1.11347000	-1.01150100
O	-3.79956600	-0.26895400	-1.79483800	C	-0.40428700	8.03740800	3.94610400
O	-2.07598100	-1.43027100	-2.64779100	C	-1.11759500	7.13970300	2.92696700
Zn	-3.43141800	-0.59186100	0.25372400	C	-1.24018000	5.67164200	3.38542900
Zn	-0.49076800	-2.54767300	1.30563100	C	-2.36595900	4.95575800	2.62847100
N	0.70410500	0.21362600	-0.68924700	C	0.08697100	4.91152400	3.24164400
C	0.73543800	1.41282400	-1.40285800	C	-4.20140200	5.40575400	-3.77395500
O	1.57070400	1.58375400	-2.30224400	C	-3.23893200	4.71292800	-2.81221000
N	-0.14882300	2.36083100	-1.03669300	S	-2.43831700	5.88551200	-1.61837100
C	-1.19966900	2.13289700	-0.05639500	C	3.14398100	4.29736100	-2.64317900
C	-0.66004300	1.24000600	1.05553200	C	1.69370300	4.40698500	-3.11512300
C	0.02455600	0.01268800	0.49844600	O	0.78704200	4.81381000	-2.37253200
O	0.54662600	-0.84708600	1.31537600	C	3.24267700	4.34708000	-1.10981000
H	-8.15740200	-3.84860200	-2.02775300	C	4.68840900	4.38354700	-0.63743200
H	-9.05339300	-3.00091600	-0.75823900	O	5.42333100	3.39390700	-0.64096000
H	-5.97673200	-0.87529200	-1.33405000	N	5.14452900	5.59233900	-0.21821000
H	-6.84174600	-4.50837900	0.58267200	N	1.46281300	4.08580700	-4.40776500
H	-4.62120500	-3.65148000	1.49547600	C	0.11147700	4.02364600	-4.95150500
H	-6.17406300	4.41912900	-1.15835000	H	-2.12317300	7.54543300	2.74892400
H	-5.27117500	5.34674100	0.04726600	H	-0.60061400	7.17557200	1.95758500
H	-4.87720600	1.86873600	-1.30724800	H	-1.51067500	5.67824900	4.45285500
H	-5.24188800	3.62714200	2.49258000	H	-3.33384800	5.43576600	2.82782600
H	-4.14779200	1.33155300	2.77966900	H	-2.43735800	3.90206800	2.92707500
H	-0.50148300	-4.47359400	4.51655600	H	-2.20252000	4.99300200	1.54390700
H	3.26731900	-4.95334200	4.47134100	H	0.00623000	3.88912400	3.63070100
H	4.29480300	-3.31145600	2.79439100	H	0.38504000	4.84653700	2.18660100
H	2.55164300	-2.32576500	1.23995200	H	0.89998900	5.40384200	3.78610300
H	-2.72779000	-4.84635600	-3.40690300	H	0.61618100	7.69368500	4.15157300
H	-1.73056500	-6.29491500	-3.58142600	H	-3.75954300	3.95818600	-2.21678800
H	-1.75997000	-3.10045500	-1.60233900	H	-2.44259400	4.19722100	-3.35344300
H	-0.83327600	-7.12742900	-0.88252000	H	-1.16941000	5.73375700	-2.05597700

H	-4.99179200	5.93718700	-3.23273500	C	2.58967100	0.76694800	-5.40252100
H	2.78913200	3.44511800	-0.69119200	C	3.58413100	-0.17156800	-4.74336600
H	2.67888400	5.20789100	-0.73813400	O	4.44110800	-0.76567700	-5.39565600
H	4.55119800	6.40543900	-0.15824700	N	3.41363000	-0.30198900	-3.40251800
H	6.10216500	5.66528200	0.09788400	C	4.35978300	-1.00883400	-2.56339100
H	3.59184800	3.36773900	-3.01026200	C	3.62169800	-2.17449100	-1.89189200
H	-0.41816100	4.95077400	-4.72263500	O	2.72951000	-1.93549700	-1.04856200
H	-0.44920500	3.17823800	-4.53393700	C	4.95520000	-0.06482000	-1.49943300
H	2.19371800	3.60072100	-4.90977100	O	5.57098600	1.01063600	-2.16816500
H	3.70867800	5.12847600	-3.08873700	N	3.92659600	-3.44703600	-2.21960700
H	0.17346400	3.90948200	-6.03575600	C	4.93038200	-3.94675200	-3.20108200
H	-3.67946100	6.13884700	-4.39682300	C	4.40650100	-3.92774000	-4.64477700
H	-4.67760400	4.66851700	-4.43317400	C	5.19449400	-5.36878500	-2.66912800
H	-0.94600500	8.05360100	4.89956700	C	3.81843600	-5.82679600	-2.15870700
H	-0.33574100	9.07011600	3.58608900	C	3.21850100	-4.55159100	-1.54463000
C	6.66196800	0.24862900	6.52746900	H	2.13813500	-4.45718900	-1.69136300
C	5.68411400	1.42044900	6.34028700	H	3.40262400	-4.48876600	-0.46505500
C	4.89041100	1.28900100	5.06018400	H	3.20123900	-6.17845400	-2.99250000
C	3.71477900	0.53088900	5.01771600	H	3.88395500	-6.64214800	-1.43181000
C	5.34871100	1.85184600	3.86016200	H	5.60945200	-6.02437700	-3.43976500
C	3.02535600	0.32280700	3.82339100	H	5.91032900	-5.32989400	-1.83890900
C	4.67732500	1.65718900	2.65612800	H	5.83473800	-3.33658100	-3.13475700
C	3.51385900	0.88048800	2.63552100	H	3.47204300	-4.49369100	-4.73484400
O	2.88753200	0.69791800	1.43542300	H	4.24548700	-2.90594200	-4.99620300
H	6.24532300	2.36334000	6.33731300	H	5.14963500	-4.39176200	-5.30408700
H	5.00430800	1.46573400	7.20102100	H	5.15883300	-1.34949300	-3.22189300
H	3.32786600	0.09241300	5.93594700	H	5.51384100	1.80327200	-1.59891000
H	6.25744300	2.45057800	3.86681400	H	5.67940000	-0.64105200	-0.89444100
H	2.10496900	-0.25706700	3.80805100	H	4.16084800	0.26729300	-0.81964100
H	5.03908900	2.09284900	1.72887700	H	2.74990700	0.31863200	-2.93830100
H	2.15013700	0.06055600	1.53993000	H	2.06775800	0.22695400	-6.19923200
H	6.12440000	-0.70604900	6.56706900	H	1.86017900	1.17937800	-4.70291000
H	7.37173200	0.19580900	5.69412100	H	3.15095900	1.57539600	-5.88719000
H	7.23571700	0.35270700	7.45604100				

***S*kDHPase.DHU-INT1-II**

C	-7.16175200	-4.86267300	-1.45501300	C	-2.25720100	-2.66924200	2.76896100
C	-5.95629500	-4.39116800	-0.72315200	O	-1.20784300	-3.29447500	2.38267200
N	-5.16661800	-5.17166200	0.11136000	O	-2.75672300	-1.62574300	2.24314600
C	-5.35459900	-3.16719300	-0.72337200	C	1.61863700	-4.93743700	4.03284700
C	-4.14163200	-4.40953500	0.57113800	C	2.50731900	-3.88968300	3.43511700
N	-4.22673700	-3.18778300	0.07474900	N	2.11649400	-3.08517200	2.36859500
C	-6.89430000	2.86884400	0.00830600	C	3.78845900	-3.55040200	3.78302200
C	-5.98724300	1.78276300	0.47623600	C	3.14304200	-2.29001900	2.08186300
N	-5.65716000	1.59625600	1.81016100	N	4.17184600	-2.54752100	2.91314200
C	-5.27964700	0.82011600	-0.19383600	C	-0.83457600	-6.04728600	-2.99208200
C	-4.77797200	0.57294400	1.90429200	C	-0.19795400	-5.47419700	-1.77468500
N	-4.52842000	0.08105100	0.70228800	N	0.69519100	-6.15194900	-0.95672700
C	-2.38513200	-4.30444000	4.61258500	C	-0.33887700	-4.24275400	-1.19780300
N	-2.93070700	-3.22419900	3.81919900	C	1.05269900	-5.33159400	0.06039800

N	0.43504700	-4.16672000	-0.05655200	H	-0.78428300	3.23524500	-1.39754000
C	-3.66769100	-2.50826500	-3.78274800	O	-1.21408300	-1.14253200	-0.18379300
C	-2.92340600	-1.76838000	-2.67658400	H	-1.17801400	-1.22198400	-1.19257500
O	-3.63339900	-1.16308600	-1.79591100	C	-2.40396800	7.63130700	4.10089400
O	-1.67049600	-1.83993600	-2.64991400	C	-2.87273300	6.60048700	3.06601000
Zn	-3.20529200	-1.39320900	0.23763600	C	-2.65994900	5.13954400	3.51270800
Zn	0.36171200	-2.70685900	1.34569300	C	-3.58115500	4.19365500	2.73147100
N	0.52223000	0.33409900	-0.81393300	C	-1.19166400	4.70695100	3.38462800
C	0.35495100	1.57614000	-1.38080800	C	-5.46398800	4.26229600	-3.65984100
O	1.15296200	2.01465700	-2.23281200	C	-4.32515600	3.89828000	-2.71031700
N	-0.71298800	2.30989400	-0.98235400	S	-3.88785100	5.29126700	-1.56613200
C	-1.66667800	1.87398100	0.02134200	C	1.92737900	5.02533000	-2.55791300
C	-0.95669900	0.97788000	1.02814300	C	0.49362500	4.78686700	-3.03309600
C	-0.20827300	-0.16280700	0.33304500	O	-0.48444800	4.96296400	-2.29066800
O	0.61960000	-0.82985800	1.17492500	C	2.00853200	5.05370100	-1.02276900
H	-6.93015600	-5.67932800	-2.15034100	C	3.39591600	5.43644900	-0.53131400
H	-7.94842300	-5.21864500	-0.77793400	O	4.34908000	4.65474700	-0.51978900
H	-5.62675600	-2.28192400	-1.27262800	N	3.54094200	6.72011900	-0.10947100
H	-5.32483900	-6.14303800	0.34188300	N	0.34672400	4.42784500	-4.32865700
H	-3.37235900	-4.76651600	1.23925700	C	-0.95042200	4.04742000	-4.87611500
H	-7.09660300	2.75052100	-1.05906500	H	-3.94184900	6.76446600	2.87177500
H	-6.44389200	3.85818100	0.15493900	H	-2.36290400	6.76384500	2.10607100
H	-5.23488200	0.60821500	-1.25083300	H	-2.93997700	5.07195500	4.57561500
H	-5.96131900	2.17866400	2.57843600	H	-4.63605600	4.43027400	2.92809200
H	-4.33786900	0.21636000	2.82224100	H	-3.40403500	3.14729100	3.01131500
H	0.63133600	-4.52575000	4.26265500	H	-3.42421500	4.28812300	1.64930800
H	4.44310700	-3.92468900	4.55469900	H	-1.03979600	3.68847200	3.76207100
H	5.03756100	-2.02624400	2.94147500	H	-0.87038700	4.72590700	2.33472100
H	3.16594200	-1.55251800	1.29009500	H	-0.52265900	5.36680300	3.94756500
H	-1.43640700	-5.27489400	-3.47696300	H	-1.33529400	7.53137900	4.32386100
H	-0.09367200	-6.39676300	-3.72169600	H	-4.59280700	3.03338100	-2.09644300
H	-0.91018300	-3.40549500	-1.56972300	H	-3.42246900	3.63198600	-3.26395800
H	1.04173800	-7.09035700	-1.10252700	H	-2.57634100	5.35842700	-1.88423500
H	1.74810800	-5.60337100	0.83991400	H	-6.36476200	4.55680300	-3.10959600
H	-2.01470300	-5.09701900	3.95919200	H	1.79126800	4.05364600	-0.64044600
H	-3.00112000	-2.72778700	-4.61918800	H	1.24713500	5.73624800	-0.63328300
H	-4.05145700	-3.45121800	-3.37391300	H	2.76893200	7.36720500	-0.06484900
H	-2.50530000	1.34703100	-0.45068800	H	4.44910700	7.02328700	0.21519800
H	-2.07634000	2.75835700	0.51602200	H	2.58959800	4.24411100	-2.94513400
H	-1.64927400	0.54704800	1.75350400	H	-1.68635600	4.81900400	-4.64066100
H	-0.20788700	1.56238000	1.57210300	H	-1.29224900	3.08918300	-4.46568600
H	-7.85712800	2.85266300	0.53321000	H	1.17214400	4.12200700	-4.82541300
H	1.46613800	-5.78238300	3.34880300	H	2.26757200	5.98272500	-2.97751200
H	2.05624300	-5.33204700	4.95401500	H	-0.86226800	3.96031800	-5.96116200
H	-3.17656300	-4.71352100	5.24678200	H	-5.18584000	5.09991400	-4.30674600
H	-1.55896000	-3.97893100	5.25935200	H	-5.72084400	3.40435800	-4.29447800
H	-7.57644600	-4.03768400	-2.03925600	H	-2.95089600	7.51524200	5.04444600
H	-4.52829000	-1.92957300	-4.13122100	H	-2.57013700	8.65426400	3.74495500
H	-1.49172200	-6.89411600	-2.75608600	C	6.43331800	1.85476200	6.50804800
H	-3.69573300	-2.67816000	4.18668600	C	5.03533000	2.48949600	6.40379600
H	1.42340900	-0.12003100	-0.98565800	C	4.32125800	2.14044900	5.11486800

C	3.36819000	1.11805000	5.05916500	N	4.70163500	-2.28323900	-2.29625400
C	4.62059100	2.81339800	3.91916100	C	5.77920900	-2.45734900	-3.30815200
C	2.73906500	0.76633000	3.86193500	C	5.23125900	-2.55060000	-4.73900100
C	4.00903100	2.47867000	2.71566000	C	6.44706900	-3.75877600	-2.82329200
C	3.06280100	1.44405300	2.67908100	C	5.27061500	-4.59628900	-2.29543300
O	2.49919100	1.14915700	1.47593300	C	4.35340100	-3.55381500	-1.63546600
H	5.13284200	3.57983900	6.48907500	H	3.28650200	-3.76663500	-1.75662200
H	4.42835900	2.16744300	7.25955400	H	4.54139000	-3.46263500	-0.55796500
H	3.10163600	0.58682800	5.97138100	H	4.75395000	-5.09073900	-3.12539000
H	5.34963000	3.62150000	3.93185800	H	5.58333100	-5.37471000	-1.59259400
H	1.98415400	-0.01651100	3.84403500	H	7.00685900	-4.25512800	-3.62097900
H	4.24119800	3.01162800	1.79757200	H	7.14706100	-3.53746700	-2.00829000
H	1.86519800	0.39237500	1.53543600	H	6.47784600	-1.61938500	-3.24157400
H	6.37031500	0.76078100	6.46885100	H	4.48540200	-3.34942800	-4.82564300
H	7.07548800	2.17971800	5.68152400	H	4.78817800	-1.60407800	-5.05672600
H	6.92489500	2.13263400	7.44767900	H	6.05357400	-2.77746900	-5.42813500
C	2.27233500	1.53903400	-5.39839800	H	5.28461000	0.09544700	-3.24442800
C	3.46287200	0.85147300	-4.75051700	H	4.80046200	3.17990600	-1.54298600
O	4.44838800	0.52041200	-5.40907300	H	5.56899800	0.85682000	-0.88807600
N	3.31620400	0.62361000	-3.41958400	H	3.86073900	1.32490500	-0.83027700
C	4.41946600	0.18388500	-2.58707200	H	2.52226200	1.05890200	-2.94191200
C	4.04710500	-1.15640800	-1.93732400	H	1.90383800	0.91451600	-6.21877600
O	3.14230700	-1.20110300	-1.07867500	H	1.46063700	1.73681400	-4.69504600
C	4.72588600	1.23103500	-1.49822100	H	2.62324400	2.47563100	-5.84898800
O	5.04241500	2.44416000	-2.13994700				

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C	-6.20200200	-5.73139500	-1.81796500	C	0.29696700	-5.77988100	-3.06701200
C	-5.19666800	-5.04982800	-0.95747300	C	0.68161100	-5.20270900	-1.75040300
N	-4.53197500	-5.65662100	0.09868200	N	1.56971300	-5.80838500	-0.87261000
C	-4.70280300	-3.77616900	-0.98998100	C	0.29203100	-4.05299200	-1.11803700
C	-3.68473200	-4.75526300	0.65311800	C	1.68437600	-5.02673100	0.22844500
N	-3.76055200	-3.60364500	0.00674500	N	0.91538900	-3.95912000	0.10986500
C	-7.27997400	1.83882400	0.05791900	C	-3.04227200	-2.70581600	-3.82594800
C	-6.20623100	0.90943800	0.51101100	C	-2.44978300	-1.78417000	-2.76091300
N	-5.88373200	0.73125300	1.84772600	O	-3.18561600	-1.37569400	-1.82722600
C	-5.31886100	0.11600100	-0.16712100	O	-1.20015600	-1.53264200	-2.90002300
C	-4.83965500	-0.12313700	1.93638100	Zn	-2.90220700	-1.76382800	0.35690400
N	-4.47087400	-0.51264600	0.72663900	Zn	0.56464700	-2.45772500	1.45278000
C	-1.86279400	-4.77280700	4.52205400	H	-5.77462100	-6.59047800	-2.35010900
N	-2.62661400	-3.82748600	3.74146400	H	-7.06197600	-6.09341400	-1.24088500
C	-1.98189800	-2.90444400	2.94986300	H	-4.94449100	-2.97026000	-1.66223300
O	-0.73379200	-3.10455900	2.78913600	H	-4.66263700	-6.60828300	0.41352100
O	-2.69964600	-1.99081600	2.43964800	H	-3.07485300	-4.95401500	1.52170600
C	2.21264300	-4.71230600	4.12952600	H	-7.45790000	1.71293700	-1.01298200
C	2.90670000	-3.50640600	3.56442600	H	-7.00423700	2.88662100	0.22932100
N	2.37759200	-2.69830000	2.55839400	H	-5.20792600	-0.03667200	-1.22934500
C	4.13325900	-3.00731400	3.92055100	H	-6.32242800	1.20165400	2.62736300
C	3.27397100	-1.74843200	2.32220700	H	-4.37395400	-0.44384100	2.85470100
N	4.34919600	-1.90195900	3.12183000	H	1.20147600	-4.45778400	4.46137200

H	4.85081200	-3.33457600	4.65710700	H	0.18060000	5.42442500	-0.53363300
H	5.13412500	-1.26698500	3.16928400	H	1.16240200	6.84084100	-0.85931100
H	3.16631800	-0.95477000	1.59719600	H	1.30721500	5.80449000	1.63903000
H	-0.35206900	-5.07708900	-3.59543100	H	2.79697300	4.96106500	1.88064700
H	1.16852900	-5.96707900	-3.70637700	H	1.88295300	4.40315600	-2.44441600
H	-0.35848300	-3.26910700	-1.47254900	H	-2.14734200	4.57779100	-4.75496600
H	2.06465900	-6.67507300	-1.03280300	H	-1.32351300	3.00046200	-4.68329300
H	2.32939300	-5.25197500	1.06368700	H	0.79097900	4.69536300	-4.81116100
H	-1.21496900	-5.36181500	3.86923700	H	1.72641400	6.05041400	-3.02827400
H	-2.42173400	-2.71576000	-4.72399800	H	-1.06629300	4.08521000	-6.07589100
H	-3.09651200	-3.72285200	-3.42036000	H	-5.28937100	4.34708500	-4.55146500
H	-8.22882100	1.64995800	0.57445900	H	-5.96098900	2.70631200	-4.63623800
H	2.11753300	-5.51814000	3.39037400	H	-3.95467100	6.84724200	4.94382700
H	2.77334300	-5.10734200	4.98114600	H	-4.00979600	8.11507900	3.71023200
H	-2.55273600	-5.45178800	5.03231300	C	5.96292600	2.71988500	6.64526400
H	-1.23016600	-4.28919300	5.27859900	C	4.62221100	3.37777400	6.27029000
H	-6.57842300	-5.03093500	-2.56751000	C	4.02922500	2.86549200	4.97218900
H	-4.05932200	-2.39204100	-4.07622300	C	2.96564900	1.95554500	4.95808100
H	-0.24552400	-6.72818100	-2.96104300	C	4.53887500	3.28009400	3.73019100
H	-3.53704200	-3.54330600	4.07495700	C	2.41716100	1.47783100	3.76402900
C	-3.54668200	7.15779800	3.97448300	C	4.01341400	2.81376500	2.52670300
C	-3.81403400	6.09303000	2.90297800	C	2.93485200	1.91048500	2.53509500
C	-3.15735300	4.73378400	3.22785400	O	2.44902700	1.50493000	1.33532900
C	-3.90520200	3.58437400	2.54229900	H	4.77036400	4.46379200	6.20113800
C	-1.66440500	4.72006200	2.86291700	H	3.90422300	3.21877600	7.08471900
C	-5.76129200	3.55191200	-3.96504300	H	2.54355300	1.61614500	5.90232400
C	-4.86841600	3.11259400	-2.80767600	H	5.36934800	3.98345000	3.70253800
S	-4.52169000	4.45011100	-1.57762600	H	1.58049300	0.78331200	3.77810500
C	1.24428300	5.29385800	-2.39892100	H	4.41951000	3.13279600	1.57000100
C	-0.09925400	4.90438300	-2.99893500	H	1.78428300	0.75919400	1.39385800
O	-1.12757000	4.75415000	-2.31935800	H	6.35253000	3.13112300	7.58341300
C	1.14537300	5.74728500	-0.94248900	H	5.84705000	1.63693700	6.77124800
C	2.27169900	5.17831800	-0.07880000	H	6.71567600	2.88551100	5.86604400
O	3.21873100	4.55176500	-0.54659900	N	0.12985400	0.08018400	-1.14829700
N	2.16749800	5.44553600	1.25049300	C	-0.04113200	1.41670200	-1.65038700
N	-0.10003700	4.69099800	-4.33317600	O	0.73982300	1.88780400	-2.48190400
C	-1.22366900	4.04681700	-4.99597900	N	-1.13191500	2.06146000	-1.21221600
H	-4.90037900	5.95689300	2.81131500	C	-1.99361000	1.53062100	-0.16385000
H	-3.46869100	6.44173300	1.91978200	C	-1.12508500	0.85733300	0.89200000
H	-3.23614100	4.57785000	4.31485800	C	-0.30670700	-0.31548900	0.32364800
H	-4.94329400	3.53595300	2.89749300	O	0.81169900	-0.55191500	1.06830300
H	-3.43094100	2.61673400	2.74934200	H	-2.71169700	0.82943800	-0.59677200
H	-3.93805300	3.72529400	1.45473700	H	-2.55894700	2.36470900	0.25384100
H	-1.18359500	3.78280300	3.16759100	H	-1.72000600	0.46436800	1.72159200
H	-1.53271300	4.82855700	1.77741300	H	-0.42959800	1.60047100	1.29564900
H	-1.12617600	5.54072000	3.35221800	H	1.11701200	-0.19909400	-1.28508400
H	-2.47414000	7.34080900	4.11105100	H	-1.24768000	3.01695800	-1.55219600
H	-5.34451600	2.30918500	-2.23890300	O	-1.00570100	-1.49807400	0.18601300
H	-3.90917800	2.72384200	-3.16094100	H	-0.60841000	-0.75771900	-2.00377100
H	-3.34443800	4.85888700	-2.09946600	C	2.35268400	2.02418200	-5.40172400
H	-6.71999400	3.93474600	-3.60086300	C	3.59249100	1.55260700	-4.65577700

O	4.65784200	1.37830100	-5.24620800	H	7.44238800	-3.43773000	-3.51440900
N	3.41136300	1.32622100	-3.32549100	H	7.22173400	-2.99248300	-1.81536500
C	4.42461600	0.69478500	-2.50068600	H	6.69823000	-0.91351300	-2.81488800
C	3.97658300	-0.73473400	-2.15936800	H	5.24279500	-2.40075000	-5.08202700
O	2.88919100	-0.92743900	-1.58387800	H	5.40368000	-0.63250800	-4.94397100
C	4.66767100	1.44276600	-1.16844200	H	6.83612100	-1.63226800	-5.20604500
O	5.23838300	2.71570400	-1.35946100	H	5.34531800	0.71603900	-3.08121300
N	4.79874900	-1.77100900	-2.43572500	H	4.53072000	3.37799700	-1.27620200
C	6.08378300	-1.74089500	-3.18192100	H	5.37668400	0.83790500	-0.58142000
C	5.86815300	-1.58867300	-4.69185900	H	3.73444900	1.48953800	-0.59904700
C	6.70948800	-3.09146000	-2.78024600	H	2.47310200	1.42013900	-2.93760000
C	5.50008700	-4.03107200	-2.64008700	H	2.07576100	1.25410400	-6.13016200
C	4.41418600	-3.13235500	-2.02796200	H	1.50139100	2.21678200	-4.74577000
H	3.40229400	-3.36154100	-2.37537900	H	2.60963800	2.92274300	-5.97335000
H	4.39748300	-3.19073500	-0.93125100				
H	5.18518400	-4.39406600	-3.62471300				
H	5.71247500	-4.90705200	-2.01909500				

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C	-7.81664600	-3.77222600	-2.12380200	O	-3.67623500	-0.89010600	-1.69133500
C	-6.85220500	-3.43678900	-1.06288600	O	-2.06094600	-1.77207100	-2.99429300
N	-6.54436300	-4.22882200	0.03089100	Zn	-3.67263600	-1.18321700	0.21978200
C	-6.02624000	-2.36155800	-0.96804500	Zn	0.22526900	-3.31499800	0.69686600
C	-5.55307500	-3.62398300	0.72952900	H	-7.54436100	-4.69446700	-2.65325500
N	-5.21543400	-2.49031600	0.13835700	H	-8.83795900	-3.90517500	-1.74386600
C	-6.78384100	3.39303300	0.97161100	H	-5.91237400	-1.53516800	-1.64933300
C	-5.71275100	2.35654600	1.11656600	H	-6.97666400	-5.11140500	0.26787800
N	-4.58811400	2.51960300	1.90996500	H	-5.09018800	-4.02986700	1.61698900
C	-5.54734500	1.12531000	0.54007600	H	-7.54715500	3.04148100	0.27296200
C	-3.78905500	1.44072900	1.76860000	H	-6.37071200	4.33023400	0.58263400
N	-4.34819300	0.56370000	0.94908400	H	-6.20610200	0.61320800	-0.14439200
C	-2.90481900	-4.99163600	3.73541900	H	-4.31453200	3.37284900	2.38101200
N	-3.18138000	-3.74840600	3.01012600	H	-2.83385500	1.32694900	2.25931200
C	-2.32678600	-3.22186900	2.06349300	H	0.05887300	-5.35261000	3.11190500
O	-1.34195000	-3.94676400	1.71863100	H	3.84510000	-5.24173900	3.91258700
O	-2.59950300	-2.06946200	1.59013900	H	4.79375600	-3.17129300	2.74779400
C	1.00922000	-5.83879000	2.88127500	H	3.20358300	-2.23398000	0.99944600
C	2.07636400	-4.82095800	2.60862400	H	-2.06904500	-4.15518600	-4.29159200
N	1.90154800	-3.81289600	1.66913700	H	-1.05215100	-5.42688800	-4.99094800
C	3.32450800	-4.67674100	3.15516600	H	-1.11016200	-3.10987100	-1.99536400
C	3.01090300	-3.08353100	1.64519600	H	0.02636700	-7.06938300	-2.80133000
N	3.89685300	-3.58313500	2.52924000	H	1.11932600	-6.40246300	-0.60562700
C	-1.65962400	-5.15363200	-4.11925900	H	-2.63425400	-5.77111900	3.02145900
C	-0.85729600	-5.11542500	-2.86325200	H	-3.58496000	-1.27010400	-4.94662200
N	-0.10016300	-6.16716000	-2.36333600	H	-4.76452700	-2.19931000	-3.99875200
C	-0.69883500	-4.10892200	-1.95110900	H	-7.27633100	3.60903700	1.92732700
C	0.47124100	-5.77435200	-1.19847600	H	0.84097000	-6.48545500	2.01085400
N	0.12055200	-4.52778500	-0.92293100	H	1.29637300	-6.47899200	3.72030500
C	-4.15347400	-1.28759100	-4.01531200	H	-3.81120400	-5.29223100	4.26719200
C	-3.19585800	-1.31625400	-2.82035800	H	-2.08948300	-4.88224100	4.46140100

H	-7.84363200	-2.96610600	-2.86112500	C	3.58837100	-1.23274800	5.50185500
H	-4.82795100	-0.42727600	-3.97307200	C	4.15160300	1.04832400	5.96036200
H	-2.49150600	-5.86696900	-4.05660500	C	2.49422800	-0.82241900	4.73990600
H	-3.76237800	-3.05910900	3.46937500	C	3.06317800	1.47890800	5.20633400
C	-1.78773900	6.71728000	5.82771500	C	2.22351100	0.54588900	4.58279100
C	-2.37091600	5.98531800	4.61220800	O	1.16597400	1.00806300	3.86685800
C	-1.47376900	6.02605200	3.35822000	H	5.89653400	-0.02699700	7.67774200
C	-1.98001000	5.04682000	2.29080000	H	5.41607700	-1.69999500	7.44853300
C	-1.35064900	7.44052100	2.77181000	H	3.76974100	-2.29962400	5.62940800
C	-5.28981000	5.42391200	-2.35798500	H	4.78949200	1.78956200	6.43814000
C	-4.54780000	4.09089200	-2.45036600	H	1.83594400	-1.55306900	4.27799900
S	-3.44702800	3.72377000	-1.01716600	H	2.84399800	2.53641700	5.09112100
C	1.51983900	6.70941100	-1.23038100	H	0.75696200	0.26401300	3.35887300
C	0.50187000	5.71538500	-1.78843300	H	6.70051700	-1.78354500	5.27930200
O	-0.04357400	4.86607300	-1.06739800	H	7.16847800	-0.09179900	5.49123700
C	2.35712500	6.12658700	-0.09213900	H	7.75410000	-1.32243100	6.62915000
C	3.41364900	5.14490900	-0.58584900	C	3.08414700	3.02428100	-4.99767100
O	3.32277100	4.60169500	-1.69520200	C	4.07032700	1.99143200	-4.46186300
N	4.43308100	4.88790100	0.26364600	O	5.07352300	1.65118300	-5.08243100
N	0.17808500	5.87891100	-3.08645000	N	3.77923900	1.48579500	-3.21187900
C	-0.83925000	5.07696400	-3.76152400	C	4.79552300	0.79462900	-2.42587100
H	-2.54257000	4.93395700	4.88639400	C	4.41877700	-0.64381800	-2.00448000
H	-3.35741000	6.40505100	4.36281100	O	3.84992500	-0.84370100	-0.91599700
H	-0.46859700	5.69500100	3.66174500	C	5.12984400	1.60136900	-1.15334600
H	-2.00052700	4.02086600	2.68470000	O	5.58268300	2.90938100	-1.46626700
H	-1.34423500	5.04338500	1.39805500	N	4.79776200	-1.69152000	-2.77740300
H	-2.99328100	5.31762100	1.96061000	C	5.49519100	-1.71172400	-4.08551900
H	-0.70252400	7.44179500	1.88727100	C	4.51501000	-1.85427900	-5.25734500
H	-2.33286400	7.82166900	2.46213500	C	6.40429500	-2.94291900	-3.92157300
H	-0.92974800	8.14987400	3.49195300	C	5.51519700	-3.94207500	-3.15592100
H	-1.66500300	7.78958700	5.64094100	C	4.65131700	-3.05442000	-2.23424400
H	-5.25639300	3.25659300	-2.46989800	O	-0.13838700	1.93004000	-3.59314000
H	-3.95779100	4.02260800	-3.36874900	C	0.32067200	1.28303300	-2.64431100
H	-2.35588900	4.42875500	-1.38438600	N	0.31739100	-0.08389700	-2.61786600
H	-5.89682100	5.48041100	-1.44877900	C	1.30604600	1.27637500	-0.32949100
H	1.69076500	5.58985800	0.59455400	C	0.10430200	0.83516300	0.56827600
H	2.83449300	6.93089400	0.47963100	C	0.19844100	-0.62026800	1.00593100
H	4.51495700	5.35340500	1.15465300	O	0.25498600	-0.94910400	2.20633200
H	5.14372500	4.21566400	-0.03161500	O	0.20916500	-1.49176500	0.04408900
H	2.16609600	7.09025100	-2.02807700	H	0.37945700	-0.58300000	-1.73446000
H	-0.74990400	5.24893900	-4.83677000	H	1.91759200	1.98803300	0.23143200
H	-1.84495100	5.38304300	-3.44774400	H	1.95199100	0.42139900	-0.54436900
H	0.68686800	6.56579600	-3.62354400	H	0.03624600	1.47081300	1.45424600
H	-0.68920800	4.01205100	-3.56409800	H	-0.82248400	0.95010400	-0.00664200
H	-4.59232400	6.26834400	-2.34467400	H	3.59786200	-3.35700700	-2.21236100
H	-5.95564900	5.55033200	-3.22141500	H	5.00531300	-3.05379100	-1.19776000
H	-0.80530500	6.31010100	6.09590900	H	4.88418000	-4.50349300	-3.85248500
H	-2.44001200	6.61112900	6.70182100	H	6.09772400	-4.67295900	-2.58711100
C	6.89299000	-1.00586800	6.02913100	H	6.75629200	-3.33198400	-4.88151300
C	5.65287700	-0.77245100	6.91042800	H	7.28313800	-2.67713900	-3.32236600
C	4.44263500	-0.31373800	6.12406000	H	6.06331500	-0.79051700	-4.22095000

H 3.91501100 -2.76778200 -5.17860000
H 3.83681600 -0.99790100 -5.29474600
H 5.06979400 -1.88590200 -6.20151400
H 5.68351000 0.78500800 -3.05942200
H 4.82899800 3.38974000 -1.87602800
H 5.94227800 1.10645700 -0.61186700
H 4.25741200 1.62335900 -0.48844600
H 2.93872800 1.80535000 -2.73248000

H 3.24515000 3.13620300 -6.07087600
H 2.04505700 2.74063500 -4.79468100
H 3.26955800 3.98327800 -4.49965600
N 0.96208400 1.92640700 -1.58827700
H 0.70362200 2.90916000 -1.52570800
H -0.34304500 -0.50407600 -3.26071900
H 0.94677500 7.56240600 -0.84259300

SkDHPase.DHT-ES-II-L

C -2.73099300 -0.10103300 -4.80017700
C -3.70403400 -0.13088400 -5.92124900
N -4.02038600 0.94828500 -6.73390900
C -4.44728400 -1.16455200 -6.40948100
C -4.91976300 0.53663400 -7.66367100
N -5.19111400 -0.74695200 -7.49602100
C -9.56332500 -3.95540600 -4.12769300
C -9.07345900 -3.27689800 -5.36646100
N -9.86204500 -2.41425400 -6.11503300
C -7.87802900 -3.31906500 -6.03777300
C -9.14620600 -1.97928500 -7.17895000
N -7.93752000 -2.51512600 -7.16164500
C -6.95819100 2.60919600 -10.69330100
N -7.29763000 1.54459800 -9.77188500
C -7.26231300 0.22486000 -10.17077000
O -6.73614900 0.02106900 -11.31887600
O -7.70719200 -0.64294600 -9.36500100
C -5.99742500 1.45357700 -14.50229300
C -6.20842400 0.04709900 -14.98721600
N -6.19282400 -1.09507100 -14.18078400
C -6.41589300 -0.33588000 -16.28822000
C -6.37007800 -2.12499300 -14.99650500
N -6.51120600 -1.71169500 -16.27663200
C -0.67058800 -2.26303000 -10.70606800
C -1.89466200 -1.90752700 -11.47071200
N -1.94438800 -1.07009000 -12.57683300
C -3.18900800 -2.28029700 -11.25310000
C -3.23695700 -0.96895800 -12.97618800
N -4.01703200 -1.69114400 -12.18777200
C -2.92952000 -4.25382000 -7.22607700
C -4.19168100 -4.13774000 -8.09083700
O -5.23910300 -3.65356000 -7.52402300
O -4.11266700 -4.45886800 -9.29661300
Zn -6.39020100 -2.13498300 -8.46467300
Zn -6.06961100 -1.69958000 -11.97087400
N -7.33904600 -5.20442900 -11.80156100
C -7.77689200 -6.37436800 -11.14089100
O -7.36847900 -7.47241700 -11.52358800
N -8.65361200 -6.18149500 -10.14220500
C -8.85791700 -4.86163300 -9.55160200

C -8.99736400 -3.80691500 -10.65591400
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O -7.60235400 -3.08350000 -12.51015000
H -1.71853000 0.15670100 -5.13669500
H -3.01157100 0.61951000 -4.02123400
H -4.49669700 -2.18810000 -6.07950300
H -3.65116100 1.88531100 -6.64998800
H -5.36377300 1.18129300 -8.40903000
H -8.73765600 -4.48239700 -3.64260100
H -10.34763300 -4.68850800 -4.34916300
H -6.97602000 -3.86572900 -5.80977500
H -10.82957500 -2.19032200 -5.92579800
H -9.50119900 -1.28220700 -7.92208900
H -6.68617800 1.69440100 -13.68677900
H -6.50510600 0.24123200 -17.19580200
H -6.71363700 -2.30840900 -17.06655100
H -6.36269600 -3.16661900 -14.70834400
H -0.93729500 -2.98243800 -9.92804600
H 0.09871200 -2.72591700 -11.33720000
H -3.55285900 -2.95754800 -10.49647000
H -1.15704800 -0.61465300 -13.01770500
H -3.56172300 -0.38615900 -13.82395400
H -5.96782900 2.43021000 -11.11608200
H -2.23125300 -4.97293000 -7.66019100
H -2.44108300 -3.27189300 -7.18789200
H -8.01877600 -4.61371100 -8.89276200
H -9.76090200 -4.90471400 -8.93936800
H -8.84709800 -2.81198000 -10.22816800
H -9.96779000 -3.23712600 -3.40424100
H -4.98074600 1.60450800 -14.11735900
H -6.15588100 2.16129800 -15.32055700
H -6.94229400 3.55796900 -10.14831600
H -7.67080900 2.69879200 -11.52456700
H -2.68313300 -1.08844800 -4.33439300
H -3.17366900 -4.54315400 -6.19930800
H -0.21588800 -1.39022100 -10.21965400
H -7.93774000 1.74236900 -9.01529300
H -6.66829600 -5.34676800 -12.57507800
H -8.99128100 -7.02671500 -9.68258800
O -6.06972300 -2.76638200 -10.26656900

H	-5.43909600	-3.51141400	-10.13965700	C	-10.14207300	-2.97954600	-15.03018100
C	-15.72460400	-5.23248300	-8.59995300	C	-10.65745600	-5.24869300	-15.71720500
C	-14.28163800	-5.20646500	-8.07990300	C	-9.81993500	-4.34124600	-15.06321600
C	-14.08880500	-4.24382400	-6.88838700	O	-8.69094600	-4.82975700	-14.47108400
C	-12.77374800	-4.52409800	-6.15225500	H	-13.96873000	-3.66321600	-17.45152600
C	-14.16583000	-2.76935100	-7.31407900	H	-13.75983000	-2.06543100	-16.74113200
C	-8.21561900	-7.89747600	-4.42193300	H	-11.52273400	-1.46895400	-15.67346100
C	-8.24000400	-7.19428000	-5.77701800	H	-12.42789100	-5.47881600	-16.90658000
S	-9.90125200	-7.18277200	-6.59175000	H	-9.49904800	-2.28364300	-14.49622100
C	-9.17502300	-10.10152300	-11.70699100	H	-10.40343300	-6.30488700	-15.70239200
C	-8.85183600	-9.75585200	-10.25908800	H	-8.22275200	-4.10198200	-14.02171400
O	-9.52504900	-8.96514700	-9.58448100	H	-11.92780600	-1.55760400	-18.40129800
C	-10.57619300	-9.66739000	-12.13395100	H	-12.13125400	-3.16332800	-19.11476100
C	-10.65743600	-9.43585300	-13.64035000	H	-13.43792300	-1.96929300	-19.23437100
O	-9.72919400	-8.94913300	-14.28475900	C	-10.37304600	-3.86059200	-11.35520200
N	-11.83890300	-9.76008800	-14.22433000	H	-11.16000900	-3.65122300	-10.62231300
N	-7.74399000	-10.35383900	-9.75902500	H	-10.44223500	-3.11848200	-12.15405900
C	-7.14861800	-9.92147600	-8.50393300	H	-10.56410100	-4.84727100	-11.78815400
H	-13.99748700	-6.21997500	-7.76684200	C	-4.78800700	-9.59698500	-11.86439800
H	-13.59043200	-4.92927700	-8.88973800	C	-4.67042500	-9.13565800	-13.30650800
H	-14.90946900	-4.43159400	-6.17930300	O	-3.83653600	-9.62610000	-14.06584400
H	-12.72710600	-5.55478000	-5.78424300	N	-5.52531600	-8.13640200	-13.65681500
H	-12.66122300	-3.85718700	-5.28574200	C	-5.48591300	-7.49849600	-14.95814700
H	-11.91076100	-4.38007000	-6.81512700	C	-4.95334200	-6.06682300	-14.79605500
H	-14.06894200	-2.10190000	-6.44805000	O	-5.56415200	-5.25426300	-14.06463800
H	-13.35945800	-2.52622400	-8.02080100	C	-6.88036900	-7.45949900	-15.62826900
H	-15.11490000	-2.52808000	-7.80354400	O	-7.34728400	-8.76170700	-15.89128800
H	-16.04535400	-4.25396300	-8.97420800	N	-3.84964700	-5.68021300	-15.46402300
H	-7.96722200	-6.14114200	-5.67291500	C	-2.96559800	-6.50079000	-16.33791900
H	-7.52103600	-7.63584700	-6.47207900	C	-2.02126900	-7.39225700	-15.52492800
H	-9.74180600	-8.27223400	-7.37376700	C	-2.22896800	-5.41240300	-17.14218500
H	-8.93183200	-7.44483700	-3.72857200	C	-2.04649500	-4.27371700	-16.12548500
H	-10.80587100	-8.71429100	-11.64183300	C	-3.35811900	-4.29502600	-15.32694800
H	-11.33803400	-10.38137400	-11.80143800	H	-3.24039200	-4.03612300	-14.27074000
H	-12.60743700	-10.16264500	-13.71001200	H	-4.09847200	-3.60524000	-15.74876700
H	-11.95307500	-9.59092400	-15.21440200	H	-1.19459700	-4.48196300	-15.46959700
H	-8.44979000	-9.56272700	-12.32709600	H	-1.86896600	-3.30331900	-16.59890100
H	-7.87549200	-10.01435000	-7.69279600	H	-1.28558100	-5.77900900	-17.55602900
H	-6.80954300	-8.88012300	-8.56113000	H	-2.85486200	-5.07523200	-17.97764100
H	-7.16618700	-10.88466700	-10.39617800	H	-3.58063000	-7.11843700	-16.99831100
H	-9.02037000	-11.17320600	-11.88245500	H	-1.40854700	-6.79578200	-14.83878300
H	-6.29352800	-10.56300000	-8.28138000	H	-2.56585900	-8.14447500	-14.94968700
H	-8.47256700	-8.95760300	-4.51699400	H	-1.34498000	-7.92151900	-16.20715000
H	-7.21497800	-7.82826600	-3.97593300	H	-4.82829900	-8.11156800	-15.57287000
H	-16.42025400	-5.52974300	-7.80612500	H	-8.09090500	-8.93939100	-15.28991400
H	-15.83656300	-5.94782700	-9.42267300	H	-6.77932200	-6.91496800	-16.58050200
C	-12.65108500	-2.36154800	-18.57849700	H	-7.57245400	-6.88714500	-15.00280500
C	-13.22835700	-2.87877400	-17.25230300	H	-6.19050400	-7.79452400	-12.96499400
C	-12.11515200	-3.41330800	-16.38630300	H	-3.85478300	-9.34955300	-11.34661500
C	-11.28431000	-2.53077900	-15.68743000	H	-5.62181500	-9.13863100	-11.32950500
C	-11.78975800	-4.77585900	-16.37491500	H	-4.87718400	-10.68891800	-11.85336800

SkDHPase.DHT-TS1-II-L

C	-2.73099100	-0.10103300	-4.80017600	H	-0.92218100	-2.96331000	-9.90590100
C	-3.56411000	-0.18860600	-6.02902300	H	0.09973800	-2.73410400	-11.32944200
N	-3.56387900	0.73659000	-7.06466700	H	-3.56248100	-2.99952700	-10.49893200
C	-4.44539800	-1.15163600	-6.42524700	H	-1.16531600	-0.68214700	-13.04712100
C	-4.42239000	0.30717800	-8.02470700	H	-3.56883100	-0.47318100	-13.86323900
N	-4.96830700	-0.84158900	-7.66621200	H	-5.92987300	2.49278500	-11.04166000
C	-9.56332900	-3.95540700	-4.12770900	H	-2.21097600	-4.93052600	-7.69331400
C	-9.03331000	-3.21961400	-5.31205100	H	-2.47975600	-3.25632200	-7.14610600
N	-9.77623300	-2.27909100	-6.01081400	H	-9.94023900	-3.27136200	-3.35764500
C	-7.83643100	-3.27798600	-5.97707900	H	-4.95471500	1.54876200	-14.17354900
C	-9.03540600	-1.81793100	-7.04473500	H	-6.16204100	2.17422000	-15.30791500
N	-7.85211600	-2.40929800	-7.05349000	H	-7.04831200	3.57072600	-10.17971200
C	-6.95819100	2.60919900	-10.69330100	H	-7.61561500	2.62469400	-11.57324200
N	-7.29151200	1.54965600	-9.76672100	H	-2.93012900	-0.96787600	-4.16543100
C	-7.09745700	0.23376700	-10.08309400	H	-3.15748100	-4.59245000	-6.21086800
O	-6.40397400	0.02044800	-11.13889300	H	-0.22447900	-1.37060500	-10.24844100
O	-7.56797900	-0.63940000	-9.29322200	H	-7.94778000	1.72980000	-9.02131000
C	-5.99742500	1.45357800	-14.50229300	C	-15.72461200	-5.23246300	-8.59997700
C	-6.31090100	0.06475600	-14.97952900	C	-14.28162700	-5.20649100	-8.07986800
N	-6.28365800	-1.07925700	-14.17781000	C	-14.05131000	-4.11429800	-7.01264300
C	-6.65248200	-0.30487100	-16.25487900	C	-12.74244800	-4.34566500	-6.24866600
C	-6.59093600	-2.10041500	-14.97009600	C	-14.08444100	-2.69910900	-7.61051800
N	-6.81949100	-1.67424500	-16.23001100	C	-8.21561800	-7.89747700	-4.42193400
C	-0.67058800	-2.26303000	-10.70606800	C	-8.41101500	-7.25320600	-5.79195400
C	-1.90316900	-1.94243400	-11.47489200	S	-10.15243600	-7.38494300	-6.41483900
N	-1.95375900	-1.12596600	-12.59632900	C	-9.22881100	-9.83381000	-11.67990300
C	-3.19732700	-2.32227000	-11.25690000	C	-8.86456600	-9.58827600	-10.22256200
C	-3.24342900	-1.03892300	-13.00401600	O	-9.49530800	-8.80400400	-9.49822500
N	-4.02249900	-1.75171300	-12.20583700	C	-10.65411300	-9.40351800	-12.01881000
C	-2.92952000	-4.25382000	-7.22607700	C	-10.81868700	-9.08006100	-13.50079500
C	-4.20129700	-4.14706800	-8.07149000	O	-9.90814400	-8.62387000	-14.19067400
O	-5.24613100	-3.67057700	-7.49482900	N	-12.06013800	-9.28843400	-14.00950700
O	-4.14137900	-4.46654000	-9.28095200	N	-7.77946200	-10.25894300	-9.77165300
Zn	-6.36660000	-2.16202400	-8.45074800	C	-7.14862000	-9.92147200	-8.50393000
Zn	-6.05362900	-1.65762800	-12.08052000	H	-14.04114400	-6.18508900	-7.64369400
H	-1.65750200	-0.09495600	-5.02772200	H	-13.57861900	-5.05888100	-8.91284300
H	-2.94878500	0.79899200	-4.21139300	H	-14.87438900	-4.19071800	-6.28570600
H	-4.71520200	-2.06863300	-5.92955100	H	-12.72286200	-5.33140300	-5.77143000
H	-3.02068800	1.58815000	-7.10141900	H	-12.61491200	-3.59117500	-5.45873100
H	-4.61848600	0.84077800	-8.94221800	H	-11.87558400	-4.29557600	-6.92012700
H	-8.76814700	-4.55454700	-3.67679700	H	-13.96496500	-1.93682500	-6.82970100
H	-10.37900500	-4.63310700	-4.40513700	H	-13.27290100	-2.56528300	-8.33954100
H	-6.96763300	-3.88690500	-5.78049200	H	-15.02750100	-2.48929700	-8.12523200
H	-10.73572500	-2.02690500	-5.81588300	H	-15.99967400	-4.29721600	-9.09994300
H	-9.36003400	-1.07658500	-7.75778400	H	-8.16886600	-6.18747800	-5.75936600
H	-6.62716700	1.73060100	-13.65107700	H	-7.75306000	-7.70401100	-6.53855600
H	-6.79010900	0.27699500	-17.15320100	H	-9.91128200	-8.21567200	-7.45321300
H	-7.13090500	-2.25775700	-16.99423300	H	-8.88350700	-7.45446400	-3.67528400
H	-6.63864500	-3.13880100	-14.67401500	H	-10.88027100	-8.48983700	-11.45468000

H	-11.38713000	-10.15391100	-11.7008340	H	-8.72670800	-2.73868200	-9.84322300
H	-12.82490700	-9.63444300	-13.45026900	H	-6.53257500	-5.17690400	-12.39335600
H	-12.23990600	-9.02800700	-14.96941000	H	-8.75521200	-6.95906000	-9.50949200
H	-8.53628200	-9.22919600	-12.27668600	O	-6.20672100	-3.00117100	-10.26108000
H	-7.88668100	-9.96905900	-7.69986600	H	-5.53129100	-3.71216500	-10.08478300
H	-6.71181000	-8.91567900	-8.53081800	C	-10.08960400	-3.86319500	-11.07162100
H	-7.22812700	-10.76734300	-10.44952400	H	-10.92245300	-3.79988200	-10.36185300
H	-9.05596800	-10.88352600	-11.94605700	H	-10.20716100	-3.06230300	-11.80495100
H	-6.35958500	-10.64799400	-8.29897000	H	-10.16318200	-4.81933700	-11.59718700
H	-8.42580900	-8.97109800	-4.45524800	C	-4.82810800	-9.59760900	-11.88554500
H	-7.18210200	-7.75878200	-4.07886700	C	-4.72146400	-9.07768400	-13.31107900
H	-16.43276000	-5.39183900	-7.77796600	O	-3.95437300	-9.59525600	-14.12228600
H	-15.87068100	-6.04266600	-9.32347400	N	-5.51040500	-8.00449300	-13.58307300
C	-12.65108600	-2.36154800	-18.57849800	C	-5.51331100	-7.33667500	-14.86964500
C	-13.20937100	-2.81426100	-17.22029700	C	-4.90697000	-5.93500800	-14.70821600
C	-12.10252300	-3.29410500	-16.31157800	O	-5.45579600	-5.10221500	-13.95449300
C	-11.36760100	-2.38880800	-15.53878600	C	-6.94154700	-7.20837000	-15.44979900
C	-11.71116500	-4.64050000	-16.29342300	O	-7.48430600	-8.47917600	-15.72106100
C	-10.26504900	-2.79933400	-14.79042000	N	-3.80273900	-5.59512400	-15.40388000
C	-10.61898300	-5.07459800	-15.54839900	C	-2.98728000	-6.44386800	-16.31508800
C	-9.88270700	-4.14680300	-14.80219300	C	-2.06137000	-7.39288100	-15.54607700
O	-8.80206400	-4.60508100	-14.11084800	C	-2.22919800	-5.37966200	-17.13257500
H	-13.94365600	-3.61462900	-17.37625300	C	-1.96861600	-4.25720600	-16.11480900
H	-13.74957500	-1.98106500	-16.75249300	C	-3.25178500	-4.23379900	-15.27029900
H	-11.65572300	-1.33912500	-15.52683900	H	-3.08358400	-3.99457700	-14.21620000
H	-12.27296300	-5.36390800	-16.88143200	H	-3.98198300	-3.50906500	-15.65233600
H	-9.70244900	-2.08373500	-14.19518400	H	-1.10399800	-4.50486400	-15.48960300
H	-10.32695000	-6.12073000	-15.52168800	H	-1.76772500	-3.29112000	-16.58811000
H	-8.41922000	-3.89288700	-13.55258300	H	-1.31463300	-5.78089100	-17.57802700
H	-11.93669400	-1.53976000	-18.45197000	H	-2.86560100	-5.00952400	-17.94577500
H	-12.12589600	-3.18370600	-19.07774600	H	-3.65194400	-7.02281900	-16.96227100
H	-13.45023400	-2.01529000	-19.24492900	H	-1.40187700	-6.83745400	-14.86861700
N	-7.11292900	-5.05981300	-11.55220400	H	-2.62506100	-8.12970200	-14.96885300
C	-7.54571200	-6.23539900	-10.94163700	H	-1.43086700	-7.94083200	-16.25684200
O	-7.21405500	-7.33707000	-11.40121000	H	-4.92528100	-7.96341400	-15.53897600
N	-8.35236900	-6.09722100	-9.87148000	H	-8.23681000	-8.62217200	-15.12159100
C	-8.59669200	-4.80983600	-9.23861300	H	-6.87129400	-6.63549300	-16.38911900
C	-8.75788800	-3.72462400	-10.30917800	H	-7.56437000	-6.62513200	-14.76365100
C	-7.58368500	-3.78425800	-11.28332000	H	-6.12403300	-7.64777300	-12.84914900
O	-7.54614400	-2.94859400	-12.28339000	H	-3.84615200	-9.50460300	-11.40927300
H	-7.77067800	-4.56679500	-8.56225700	H	-5.57010300	-9.06528600	-11.28771800
H	-9.50416900	-4.89524100	-8.63503100	H	-5.06031000	-10.66822800	-11.92358900

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C	-2.73099300	-0.10103300	-4.80017700	C	-9.56332600	-3.95540800	-4.12769600
C	-3.53622200	-0.20013100	-6.04571300	C	-9.03256400	-3.20358600	-5.29915500
N	-3.47698400	0.68311900	-7.11580200	N	-9.78047300	-2.27450700	-6.00746900
C	-4.44391500	-1.14396300	-6.42585000	C	-7.82560100	-3.24243800	-5.94503600
C	-4.32909400	0.24930000	-8.07950300	C	-9.03327800	-1.80141000	-7.03043900
N	-4.92606100	-0.86354700	-7.68996400	N	-7.84042200	-2.37330900	-7.02033200

C	-6.95819100	2.60919600	-10.69330100	H	-3.15749600	-4.61071300	-6.21728900
N	-7.27189500	1.51228700	-9.80364300	H	-0.21238700	-1.37081500	-10.26051400
C	-7.00949200	0.21010400	-10.12071300	H	-7.93857500	1.65443000	-9.05929300
O	-6.27028900	0.01945300	-11.14909900	C	-15.72460900	-5.23248200	-8.59995500
O	-7.47270600	-0.68162600	-9.34334100	C	-14.28163200	-5.20646700	-8.07990100
C	-5.99742500	1.45357800	-14.50229300	C	-14.03978000	-4.07930100	-7.05175900
C	-6.34141100	0.09831100	-15.04227700	C	-12.74811900	-4.31136400	-6.25912300
N	-6.29463100	-1.06861300	-14.28094900	C	-14.02994900	-2.68888500	-7.70593500
C	-6.72747300	-0.23270500	-16.31448400	C	-8.21561800	-7.89747700	-4.42193300
C	-6.63612500	-2.07055700	-15.08628600	C	-8.44270700	-7.25567100	-5.78810700
N	-6.90072000	-1.60293900	-16.32197000	S	-10.19768300	-7.39752900	-6.36787800
C	-0.67058800	-2.26303000	-10.70606800	C	-9.29632700	-9.76265500	-11.66073800
C	-1.89428000	-1.93270000	-11.48894500	C	-8.86218300	-9.52042700	-10.21551700
N	-1.90767200	-1.13524700	-12.62476900	O	-9.52656500	-8.81790900	-9.43949900
C	-3.20170100	-2.28241400	-11.28943200	C	-10.28010000	-8.68109300	-12.13435000
C	-3.18601200	-1.02935700	-13.05982500	C	-10.78796100	-8.94937800	-13.54249100
N	-3.99612800	-1.71087900	-12.26505000	O	-10.11115900	-8.74995300	-14.55226700
C	-2.92951900	-4.25382000	-7.22607700	N	-12.04963600	-9.44676100	-13.63304500
C	-4.19975400	-4.13885100	-8.06491500	N	-7.74141100	-10.16246500	-9.81381300
O	-5.24110300	-3.65978100	-7.48706100	C	-7.14862100	-9.92147200	-8.50393100
O	-4.14721800	-4.45687400	-9.27753600	H	-14.05440000	-6.17209800	-7.60911400
Zn	-6.37009500	-2.16152900	-8.41308600	H	-13.57595200	-5.09701500	-8.91618400
Zn	-6.02373200	-1.57515500	-12.28221000	H	-14.87464500	-4.10743700	-6.33496300
H	-1.65285200	-0.14432900	-4.99981500	H	-12.76034500	-5.27682900	-5.74189600
H	-2.92731300	0.82699800	-4.24856400	H	-12.61456900	-3.52890200	-5.49733400
H	-4.75676500	-2.02901700	-5.89872100	H	-11.87056600	-4.31102300	-6.91827800
H	-2.90040400	1.51144600	-7.17204900	H	-13.90563700	-1.89818100	-6.95448800
H	-4.48133300	0.74968500	-9.02386100	H	-13.20415200	-2.60377700	-8.42611400
H	-8.76395800	-4.54638200	-3.67358400	H	-14.95949100	-2.47911300	-8.24474000
H	-10.36520200	-4.64306000	-4.42045800	H	-15.98986600	-4.30875700	-9.12614600
H	-6.95357300	-3.84290700	-5.73757500	H	-8.19877700	-6.18989900	-5.76197400
H	-10.74941000	-2.04500100	-5.83102200	H	-7.80298400	-7.70861400	-6.54888700
H	-9.36398800	-1.07199900	-7.75323300	H	-9.96526100	-8.18304800	-7.44288000
H	-6.55376900	1.66231700	-13.58344100	H	-8.86739700	-7.45489000	-3.66070300
H	-6.89086800	0.37376100	-17.19179100	H	-9.75548700	-7.72318300	-12.15411800
H	-7.24936900	-2.16128800	-17.08919600	H	-11.10405300	-8.60188100	-11.41907600
H	-6.68942500	-3.11575600	-14.81050300	H	-12.64071200	-9.57751200	-12.82670000
H	-0.93694200	-2.94742700	-9.89699300	H	-12.42589400	-9.64762700	-14.54965200
H	0.09321400	-2.75637700	-11.31976300	H	-8.42304100	-9.77911500	-12.32072300
H	-3.59667700	-2.94410600	-10.53260400	H	-7.91034700	-10.03733100	-7.72995000
H	-1.10068800	-0.71950400	-13.06959000	H	-6.72153600	-8.91306000	-8.43781900
H	-3.48132800	-0.47196400	-13.93559600	H	-7.15068000	-10.56560500	-10.52785500
H	-5.93005300	2.51746700	-11.04920300	H	-9.76412100	-10.75604200	-11.71205300
H	-2.20825100	-4.91965700	-7.70416900	H	-6.35794000	-10.65565700	-8.33536200
H	-2.48547900	-3.25555300	-7.12759300	H	-8.42525600	-8.97129200	-4.44966700
H	-9.95944600	-3.28407600	-3.35611800	H	-7.17505100	-7.75693100	-4.10139700
H	-4.93033700	1.53865000	-14.25954700	H	-16.43463400	-5.36141400	-7.77428300
H	-6.23380200	2.22774400	-15.23740400	H	-15.87883400	-6.06103300	-9.30059000
H	-7.05781600	3.55048300	-10.14553300	C	-12.65108500	-2.36154800	-18.57849700
H	-7.62140000	2.64786600	-11.56838100	C	-13.09939600	-2.60187000	-17.12722500
H	-2.97967300	-0.93639500	-4.14121200	C	-11.96237200	-3.07639400	-16.25015100

C	-11.22000500	-2.18406100	-15.47027300	H	-9.94559600	-4.75168200	-11.67700800
C	-11.57720900	-4.42614200	-16.24045000	C	-4.82810800	-9.59760800	-11.88554600
C	-10.12198600	-2.60875500	-14.71858000	C	-4.67662300	-9.04282100	-13.29184300
C	-10.49015800	-4.87174700	-15.49665400	O	-3.93975100	-9.58392500	-14.11572900
C	-9.74738900	-3.95894800	-14.73434300	N	-5.38748800	-7.90945200	-13.52184400
O	-8.67567800	-4.44021900	-14.04762700	C	-5.48711200	-7.30515200	-14.83566300
H	-13.91033300	-3.34181100	-17.12008900	C	-4.90441000	-5.88658000	-14.77241400
H	-13.52243800	-1.67486300	-16.71970100	O	-5.45062000	-5.01695700	-14.06322600
H	-11.50202000	-1.13283200	-15.44690700	C	-6.95440100	-7.26097900	-15.30740200
H	-12.14549500	-5.14577400	-16.82676400	O	-7.42289700	-8.58380700	-15.41720700
H	-9.56115700	-1.90090600	-14.11285600	N	-3.80269800	-5.58454000	-15.49417400
H	-10.21345500	-5.92215000	-15.47733900	C	-2.98785500	-6.48057800	-16.35952700
H	-8.30678700	-3.77743900	-13.41186700	C	-2.06137000	-7.39288100	-15.54607600
H	-11.86436900	-1.59921900	-18.62298900	C	-2.22986700	-5.46130400	-17.23301200
H	-12.24882000	-3.27956000	-19.02170700	C	-1.97279700	-4.28364500	-16.27917300
H	-13.48681900	-2.02285900	-19.20219100	C	-3.25751500	-4.21699700	-15.43930500
N	-6.97705200	-5.06073600	-11.46281500	H	-3.09170800	-3.91621800	-14.40037200
C	-7.52202600	-6.22079400	-10.96567900	H	-3.98922300	-3.51686800	-15.86372100
O	-7.30547600	-7.32436700	-11.50525400	H	-1.10872200	-4.49517700	-15.63991100
N	-8.31035100	-6.11359000	-9.86911500	H	-1.77254500	-3.34475400	-16.80479200
C	-8.56474500	-4.84982500	-9.19972100	H	-1.31381800	-5.88458600	-17.65442400
C	-8.64918100	-3.72187400	-10.23590300	H	-2.86541300	-5.13754900	-18.06645900
C	-7.35056500	-3.71727800	-11.07741400	H	-3.65303400	-7.09150100	-16.97605800
O	-7.39096700	-2.90457700	-12.16175900	H	-1.40845900	-6.80697700	-14.88792500
H	-7.77616100	-4.64813500	-8.46460800	H	-2.62489000	-8.11049100	-14.94531400
H	-9.50585500	-4.93897000	-8.64897400	H	-1.42429200	-7.96572600	-16.23095200
H	-8.67210100	-2.76098700	-9.71782700	H	-4.92663000	-7.94850700	-15.51357500
H	-6.47879100	-5.14432000	-12.35377400	H	-8.33830500	-8.61862200	-15.07929300
H	-8.76723700	-6.97009800	-9.56797600	H	-6.98842600	-6.73992300	-16.28184700
O	-6.25126400	-3.19689700	-10.18674600	H	-7.54288100	-6.66249900	-14.60274100
H	-5.55236400	-3.90216500	-9.99759700	H	-6.05900500	-7.60423900	-12.81278800
C	-9.91940600	-3.83148800	-11.08793600	H	-3.84104500	-9.63453600	-11.41269900
H	-10.80029800	-3.82462600	-10.43469100	H	-5.50714200	-9.00813700	-11.26598700
H	-10.00418500	-2.98753200	-11.77541200	H	-5.17956900	-10.63388900	-11.96107600

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C	-2.73099300	-0.10103300	-4.80017800	O	-6.77596600	0.03682600	-11.22753500
C	-3.63148500	-0.17344400	-5.98105800	O	-7.72962400	-0.54682400	-9.23245000
N	-3.81519400	0.85211000	-6.89731200	C	-5.99742500	1.45357400	-14.50229300
C	-4.42666200	-1.18744100	-6.43185100	C	-6.28728000	0.05776300	-14.97353900
C	-4.69155100	0.43490700	-7.84394600	N	-6.27907700	-1.07193100	-14.15301000
N	-5.07492100	-0.80592300	-7.59140500	C	-6.58885100	-0.33687600	-16.25118300
C	-9.56332500	-3.95541200	-4.12770300	C	-6.56041000	-2.10942000	-14.93197800
C	-9.04933600	-3.18629800	-5.28940800	N	-6.75126400	-1.70702100	-16.20577400
N	-9.80218000	-2.23959700	-5.96715100	C	-0.67058700	-2.26303000	-10.70606800
C	-7.85258500	-3.22086800	-5.95146300	C	-1.93412700	-1.88487200	-11.39999300
C	-9.06691300	-1.75196200	-6.99139800	N	-1.97343100	-1.05702600	-12.51312100
N	-7.87804700	-2.33350200	-7.00973100	C	-3.24453100	-2.20021800	-11.15291800
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H	-4.57537600	-2.16976300	-6.01694000	H	-15.41541400	-2.67883200	-7.43536200
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H	-6.62656700	-3.13915600	-14.60930400	H	-7.64324800	-9.76752100	-7.54148400
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H -10.15109100 -3.72565100 -11.60412000
H -9.35244400 -5.29703700 -11.77856900

SkDHPase.DHT-ES-II-D

C -6.01387700 -5.71069600 -3.33604700
C -5.16760400 -5.15751300 -2.24627000
N -4.67430700 -5.89561500 -1.18004600
C -4.67546400 -3.89868600 -2.05427600
C -3.91831400 -5.07818100 -0.40389300
N -3.89270900 -3.85889800 -0.91589800
C -7.39988300 1.32996500 -0.09609700
C -6.22010600 0.48074800 0.24268600
N -5.93199900 0.07453100 1.53894600
C -5.23226000 -0.08278800 -0.52310100
C -4.82129500 -0.69980100 1.51635600
N -4.37198700 -0.81199100 0.27813500
C -1.92331300 -5.87393200 3.23541400
N -2.66336900 -4.77392800 2.65512000
C -2.01205900 -3.72530200 2.03752300
O -0.75907800 -3.90119900 1.85033100
O -2.71332700 -2.73299700 1.68903200
C 2.15887500 -5.63537900 3.02146000
C 2.76700300 -4.28537100 2.77239100
N 2.29133700 -3.33557300 1.86022900
C 3.88806400 -3.78591700 3.38446500
C 3.13544300 -2.31385300 1.93275400
N 4.11270000 -2.54276300 2.83306200
C 0.52147500 -5.35315300 -4.31604300
C 0.93252500 -4.95998300 -2.93811900
N 1.90074300 -5.59275400 -2.16786800
C 0.46297100 -3.95147500 -2.14727200
C 1.97645100 -4.95865700 -0.97011600
N 1.11194200 -3.95724200 -0.92712600
C -2.88865400 -2.27687000 -4.60563700
C -2.36424500 -1.69078900 -3.28831900

O -3.23886300 -1.45863000 -2.37581400
O -1.13036400 -1.53614000 -3.15897100
Zn -2.90722100 -2.08921100 -0.38835500
Zn 0.39084600 -2.84301600 0.66761000
N 0.72285300 0.73661000 -0.19511900
C 0.34827000 2.00254000 -0.70236100
O 0.96372700 2.48898300 -1.64887900
N -0.69146300 2.58583500 -0.07990900
C -1.46932700 1.90783200 0.94917000
C -0.53466900 1.09938200 1.85998700
C 0.36584300 0.21899100 1.01065000
O 0.80526300 -0.87113200 1.39823300
H -5.50153100 -6.50467800 -3.89442800
H -6.95747900 -6.12778300 -2.96149400
H -4.80388000 -3.01367200 -2.65385300
H -4.84772900 -6.87556900 -1.00433000
H -3.43662300 -5.38913400 0.51245300
H -7.47684400 1.43894200 -1.18102400
H -7.32221900 2.33382900 0.33591200
H -5.07357500 -0.03701300 -1.58962400
H -6.45222300 0.33398500 2.36584400
H -4.38023600 -1.17641600 2.37755100
H 1.08719500 -5.54782100 3.22393000
H 4.52781900 -4.20430400 4.14636100
H 4.77706800 -1.84124100 3.14305900
H 3.06667800 -1.39944100 1.36753100
H -0.20627400 -4.62728500 -4.68658000
H 1.36637400 -5.36474900 -5.01610500
H -0.27279100 -3.20756300 -2.40637100
H 2.45818900 -6.38912200 -2.44495700
H 2.65141600 -5.24088400 -0.17662100

H	-1.26926400	-6.31823000	2.48248600	H	3.56377200	6.52978400	1.08438300
H	-2.17100200	-2.11269100	-5.41278400	H	4.50635800	5.54159000	-0.01863600
H	-3.02763600	-3.35758900	-4.47577800	H	1.07562600	7.43051000	-2.32741100
H	-2.22617700	1.24862500	0.50126900	H	-2.49482800	4.97759500	-3.61165700
H	-1.99196500	2.66795100	1.53616100	H	-1.23598400	3.72956000	-3.37406700
H	-8.33630200	0.88220000	0.25919200	H	0.05913700	6.21997400	-3.85833200
H	2.27136900	-6.30352300	2.15721100	H	-0.20686600	7.89103800	-1.20358800
H	2.64327100	-6.11375000	3.87724100	H	-1.28819000	4.67159400	-4.88272600
H	-2.63065400	-6.63540000	3.57803000	H	-5.79179700	4.54976700	-3.93149700
H	-1.30150100	-5.56931000	4.08833400	H	-6.14486300	2.84230000	-3.59601000
H	-6.26238800	-4.91624800	-4.04421400	H	-4.92922000	6.49458300	5.51914600
H	-3.85854500	-1.84793600	-4.87553200	H	-3.24174000	5.97459800	5.61672900
H	0.05592700	-6.34681600	-4.34338800	C	5.32470200	1.04664600	7.57886100
H	-3.56826400	-4.54093900	3.03976500	C	5.38428200	-0.09434100	6.55214700
H	1.46756400	0.27159400	-0.70658200	C	4.76382500	0.29936400	5.22988200
H	-0.95108400	3.50868300	-0.43577700	C	5.50990100	0.37348000	4.04746500
O	-0.98784500	-1.88542100	-0.41009400	C	3.41017000	0.66486500	5.16759300
H	-0.80188000	-1.59461200	-1.33005100	C	4.93236400	0.79025100	2.84099600
C	-4.27212700	5.61650600	5.51068900	C	2.82584000	1.09414900	3.98457500
C	-4.44611000	4.81357800	4.21519300	C	3.58076700	1.15717100	2.80569600
C	-5.89584800	4.36267300	3.94839200	O	2.95402300	1.58570900	1.67572300
C	-6.03139100	3.76098400	2.54390200	H	4.86843800	-0.97367500	6.96348100
C	-6.41007500	3.37704800	5.00913900	H	6.42786700	-0.39398000	6.39585200
C	-5.99743900	3.82703800	-3.13592700	H	6.57036100	0.12731400	4.06837500
C	-4.84976500	3.77326300	-2.13012700	H	2.80114900	0.61431300	6.06705800
S	-4.63628800	5.42151700	-1.31467100	H	5.53008500	0.85069300	1.93589500
C	0.46823500	7.07474700	-1.49003000	H	1.77801400	1.37450500	3.95372300
C	-0.43738900	5.92321500	-1.91344200	H	3.41532500	1.24367400	0.87144800
O	-1.08954600	5.28099100	-1.07390700	H	5.85392200	1.93207200	7.21015800
C	1.35855200	6.73470200	-0.29031900	H	4.29121600	1.34121000	7.78916500
C	2.63314500	5.99705100	-0.68965000	H	5.78456900	0.74578700	8.52709300
O	2.73511500	5.40698400	-1.77166500	C	-1.27020200	0.30139500	2.93672600
N	3.63838200	6.02253300	0.21591600	H	-1.92317700	0.96483700	3.51522300
N	-0.55880200	5.71698800	-3.23846700	H	-1.86896300	-0.49998100	2.49507700
C	-1.45128700	4.71225200	-3.80427600	H	-0.55692700	-0.16162000	3.62352300
H	-4.10946600	5.42541600	3.36739900	H	0.15352400	1.81691100	2.33162100
H	-3.79129000	3.92825400	4.23543400	C	2.24035400	2.97381100	-4.45191700
H	-6.53122600	5.26054500	3.98795300	C	3.61495600	2.54544200	-3.98459100
H	-5.71362500	4.46286000	1.76405600	O	4.58864100	2.46260600	-4.72927600
H	-7.07362800	3.48347000	2.33994800	N	3.67034900	2.25659100	-2.64691500
H	-5.41460300	2.85618200	2.44612000	C	4.90896500	1.91129600	-1.97908300
H	-7.44222700	3.07302700	4.79569900	C	4.78306100	0.49459200	-1.40826700
H	-5.78969300	2.46952000	5.03187700	O	3.97657800	0.27830200	-0.46794900
H	-6.39977100	3.80783600	6.01528700	C	5.21562500	2.93111000	-0.85875700
H	-4.50270600	5.01940900	6.39937800	O	5.31237000	4.24657200	-1.36687900
H	-5.03725200	3.01418300	-1.36460500	N	5.50563000	-0.51604300	-1.91520900
H	-3.91521300	3.51180100	-2.63254800	C	6.52373900	-0.48605800	-3.00526600
H	-3.31997300	5.29995100	-1.02910600	C	5.89279800	-0.57192500	-4.40133800
H	-6.93839100	4.11835200	-2.65535000	C	7.38725100	-1.71168500	-2.64845300
H	0.78994800	6.10279600	0.40372500	C	6.37054200	-2.72944900	-2.10611600
H	1.62219000	7.64869500	0.25432300	C	5.37271500	-1.86403600	-1.32114800

H	4.33806400	-2.21287800	-1.39462400	H	6.68741500	-0.63906100	-5.15324400
H	5.61814400	-1.80701300	-0.25446100	H	5.68694900	1.98246400	-2.73911400
H	5.86591100	-3.24106800	-2.93260100	H	4.45121600	4.47449900	-1.78789800
H	6.83074400	-3.49594700	-1.47609100	H	6.18333500	2.69650900	-0.39972900
H	7.94845500	-2.07997100	-3.51150900	H	4.44704800	2.86286400	-0.07643800
H	8.10863500	-1.44498500	-1.86665700	H	2.80590300	2.32494300	-2.10857100
H	7.10796600	0.43427800	-2.92559200	H	1.50870100	2.17771400	-4.28142100
H	5.25710000	-1.45946500	-4.49669100	H	1.90552300	3.84716200	-3.88391800
H	5.30048800	0.31895600	-4.62420600	H	2.29089100	3.20771000	-5.51677800

SkDHPase.DHT-TS1-II-D

C	3.99702300	7.60046100	-1.60936400	H	7.30650500	0.60729300	-1.39453400
C	3.15118500	6.62676400	-0.87413200	H	7.44839500	-0.47048200	-0.00356200
N	2.14481600	6.95617700	0.02350200	H	4.66683600	1.61996200	-1.48011100
C	3.14194100	5.26387700	-0.92241900	H	6.37441900	1.04680300	2.31884000
C	1.57958600	5.80633500	0.47339300	H	4.03733400	2.04625200	2.63729700
N	2.16056500	4.76279400	-0.09026200	H	-2.63024700	3.67049000	4.57097600
C	7.29761000	0.57284100	-0.30242500	H	-5.82993700	1.64018300	4.48175200
C	6.01990600	1.12904500	0.21048100	H	-5.56701600	-0.26835300	2.79223800
N	5.75535400	1.30010400	1.56110900	H	-3.59069600	0.09708300	1.24661400
C	4.89014700	1.56703100	-0.42577600	H	-1.38758300	5.42157500	-3.46398200
C	4.51198500	1.81390300	1.69793700	H	-3.11394500	5.78468000	-3.57009900
N	3.96062500	1.98282000	0.50807100	H	-0.85421100	3.46296200	-1.64658200
C	0.22937300	4.92703100	4.60360700	H	-4.20846900	5.85016300	-0.82583200
N	1.22565600	4.38300400	3.71580200	H	-3.99519900	4.15948300	1.06544100
C	0.89667500	3.47158000	2.75143800	H	-0.58609200	5.37042200	4.02786900
O	-0.35485700	3.33619300	2.51610100	H	1.12157100	3.82433800	-4.67561400
O	1.85574500	2.89151400	2.16489700	H	1.75532700	4.93749200	-3.43692900
C	-3.65021200	3.68972100	4.17366000	H	8.16369400	1.14692900	0.05070400
C	-3.98509800	2.40510200	3.47656600	H	-3.71443800	4.55186700	3.49758500
N	-3.25154700	1.86214400	2.41950700	H	-4.34298500	3.86133900	5.00199400
C	-5.04690400	1.57991800	3.74171200	H	0.68690700	5.70938100	5.21613400
C	-3.87788500	0.74589600	2.06213700	H	-0.20158800	4.17110600	5.27473000
N	-4.96484900	0.54212000	2.83564100	H	4.69969100	7.06011800	-2.24841400
C	-2.24162400	5.81192200	-2.90530800	H	2.86383200	3.83414300	-4.25893800
C	-2.44015300	4.98644100	-1.68094600	H	-2.03992300	6.86409100	-2.66683400
N	-3.46662900	5.16628400	-0.76346900	H	2.19237200	4.37217500	4.00594900
C	-1.70861800	3.94135600	-1.18879100	C	5.59938000	-5.71727100	3.83809300
C	-3.32404600	4.25156200	0.22574000	C	5.51223300	-4.58198700	2.81003400
N	-2.26097800	3.49570300	-0.00300800	C	6.32310800	-3.32945100	3.19955700
C	1.84739100	3.93254100	-3.86668100	C	6.36166400	-2.32351200	2.04238700
C	1.58199100	2.90574000	-2.75899700	C	5.79732900	-2.65916400	4.47805200
O	2.54571900	2.67513700	-1.94081300	C	6.50283900	-1.30217800	-3.94866800
O	0.44114600	2.39947700	-2.66422200	C	6.01867000	-2.13350700	-2.76196700
Zn	2.09145100	2.68831100	0.09766800	S	7.35491200	-3.08792300	-1.92094100
Zn	-1.39889800	2.19862900	1.31284600	C	0.70815900	-5.68598900	-2.66016100
H	3.40416000	8.26223800	-2.25364300	C	1.64841900	-4.58679600	-3.15174500
H	4.58410900	8.23719800	-0.93528000	O	2.47712800	-4.07029500	-2.39024100
H	3.74439400	4.60156700	-1.52106400	C	-0.17446700	-5.17615600	-1.50259200
H	1.87679500	7.89056900	0.30018300	C	-0.93897500	-6.24223600	-0.72765100
H	0.77638400	5.77116900	1.19343300	O	-2.13747000	-6.13286800	-0.45918700

N	-0.22954500	-7.32446600	-0.31054500	C	0.24104300	-1.45983300	-1.53654300
N	1.55458100	-4.24224300	-4.45422000	O	-0.24127500	-2.02946300	-2.52555800
C	2.33136500	-3.14016900	-5.00624400	N	1.53213900	-1.62100700	-1.17105000
H	5.87571300	-4.94658600	1.84008900	C	2.11225800	-1.07972100	0.05052900
H	4.46003900	-4.29760900	2.65748200	C	1.01987100	-0.85404700	1.09208700
H	7.35721500	-3.65526800	3.39018200	C	-0.16700000	-0.10728700	0.48325900
H	6.75633000	-2.78026100	1.12770000	O	-1.13763000	0.23889800	1.27902400
H	7.00091600	-1.46617700	2.29346500	H	2.65292100	-0.15084300	-0.15627200
H	5.35634900	-1.93975100	1.81932400	H	2.83797700	-1.80634700	0.43119400
H	6.39073400	-1.77103400	4.72984700	H	-1.53905800	-0.53389500	-0.99973000
H	4.75375800	-2.33936700	4.35025200	H	2.02474900	-2.35321000	-1.68433000
H	5.83489400	-3.32979700	5.34215200	O	0.40580100	1.60253700	-0.00608500
H	5.15628300	-5.43740200	4.79984900	H	0.27077500	1.63239800	-0.99099400
H	5.61889500	-1.48651000	-1.97397200	H	0.56752700	-1.83782700	1.29150200
H	5.21316100	-2.81973700	-3.04019800	C	1.52472700	-0.30645400	2.42275300
H	7.70898400	-3.84667200	-2.98067700	H	1.91138400	0.70734000	2.33009300
H	7.29732800	-0.60996000	-3.65165900	H	0.71462100	-0.29178700	3.15702000
H	-0.91271300	-4.46632600	-1.87877300	H	2.31517500	-0.95921900	2.81159300
H	0.46503000	-4.63859200	-0.79084000	C	-1.71080900	-2.30640800	-5.31853800
H	0.77480300	-7.37611200	-0.38898700	C	-3.06469000	-2.25341700	-4.63750300
H	-0.69754100	-7.99841100	0.28016300	O	-4.11493000	-2.39328700	-5.26325700
H	0.08343600	-6.08028900	-3.46940500	N	-2.99876600	-2.02121700	-3.30001800
H	3.39065800	-3.28793400	-4.78290700	C	-4.16149200	-2.08862300	-2.44003000
H	2.00881200	-2.18243000	-4.58291900	C	-4.35046300	-0.71360400	-1.78618200
H	0.77341200	-4.59224200	-4.99022600	O	-3.48292300	-0.28453700	-0.99396500
H	1.35545500	-6.50670000	-2.32856400	C	-3.99441000	-3.17125800	-1.35560100
H	2.19405900	-3.12152900	-6.08926400	O	-3.76001100	-4.39974500	-2.00312600
H	6.90050100	-1.94037200	-4.74566400	N	-5.44104400	0.02672800	-2.06883100
H	5.67290600	-0.72021500	-4.36946700	C	-6.55029500	-0.27644000	-3.01477100
H	6.64255400	-6.00264700	4.02122800	C	-6.16517400	0.00827100	-4.47238100
H	5.07114200	-6.60968500	3.48370600	C	-7.66463200	0.64752200	-2.48660500
C	-4.78843300	-4.55252200	6.66596000	C	-6.90711700	1.90381100	-2.02656100
C	-3.27675800	-4.73909600	6.45899700	C	-5.61013100	1.34187300	-1.42255500
C	-2.82911300	-4.13666900	5.14798500	H	-4.73148400	1.96889200	-1.60216300
C	-2.48752100	-2.78297600	5.05840900	H	-5.68971700	1.20212800	-0.33733300
C	-2.84509700	-4.88863100	3.96444700	H	-6.68317000	2.54757900	-2.88389800
C	-2.19317200	-2.18743300	3.83221900	H	-7.47245600	2.50164900	-1.30512600
C	-2.55442000	-4.31620900	2.72977100	H	-8.42108300	0.85405600	-3.24877000
C	-2.23969700	-2.95474900	2.66223200	H	-8.16700800	0.17676900	-1.63262200
O	-1.98197300	-2.42101200	1.43159400	H	-6.83836800	-1.32581200	-2.91041700
H	-3.03549100	-5.80919900	6.48441900	H	-5.82427300	1.04271600	-4.59728700
H	-2.73462800	-4.27626300	7.29370800	H	-5.38459400	-0.67232200	-4.82105800
H	-2.45619200	-2.17825100	5.96302600	H	-7.04203500	-0.13933800	-5.11417000
H	-3.10208800	-5.94516400	4.00935800	H	-4.99816300	-2.36010500	-3.08364900
H	-1.92348400	-1.13508300	3.77684600	H	-3.27577700	-4.99121700	-1.39104700
H	-2.57150700	-4.90277700	1.81547000	H	-4.91954800	-3.19367300	-0.74961400
H	-1.82512400	-1.45611200	1.51092600	H	-3.17561700	-2.89197500	-0.68164600
H	-5.11950200	-4.99096300	7.61503300	H	-2.07306900	-2.00208300	-2.87205800
H	-5.05201800	-3.48847300	6.67437600	H	-1.72266500	-1.62120600	-6.17244900
H	-5.35422800	-5.02822500	5.85699700	H	-0.88107000	-2.06257600	-4.65618100
N	-0.54992800	-0.63485900	-0.74374000	H	-1.57415000	-3.31511600	-5.72788700

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C	3.79074600	7.65758800	-1.70683100	H	-1.49217500	5.28264300	-3.54466300
C	2.95156000	6.68170900	-0.96836600	H	-3.22415400	5.58432200	-3.72101100
N	1.88629700	6.99752500	-0.13584300	H	-0.96691700	3.38208100	-1.63719000
C	3.00772900	5.32012400	-0.96013000	H	-4.43133100	5.68057000	-1.04688600
C	1.35152000	5.84059900	0.33318100	H	-4.25409300	4.05550200	0.90399100
N	2.00860700	4.80538200	-0.15806500	H	-0.74527800	5.42587000	3.92318900
C	7.29287100	0.75701800	-0.25547500	H	1.04002100	3.74636300	-4.71635800
C	6.02280300	1.32888700	0.25271200	H	1.67891800	4.90587700	-3.52159800
N	5.76579000	1.54739500	1.59778200	H	8.16355100	1.34469700	0.06224600
C	4.88634400	1.73124700	-0.39260800	H	-3.96879100	4.42891300	3.36911900
C	4.51702200	2.05025300	1.72392700	H	-4.40774200	3.78156400	4.95649200
N	3.95902300	2.16926400	0.53143300	H	0.52786600	5.75227700	5.11537000
C	0.05040700	4.97106900	4.51698800	H	-0.40768300	4.24449000	5.20289300
N	1.03492800	4.37632000	3.64735900	H	4.54736800	7.12034700	-2.28378000
C	0.69739100	3.51774600	2.63993700	H	2.78730300	3.78893400	-4.32363300
O	-0.54524500	3.46171600	2.33324400	H	-2.22031000	6.72072500	-2.80637700
O	1.65049500	2.90296500	2.07694100	H	1.99359200	4.31916100	3.95748700
C	-3.78542600	3.60821500	4.07431400	C	5.75040400	-5.51410200	3.97383200
C	-4.09721000	2.27332300	3.46921700	C	5.63789900	-4.39896800	2.92645400
N	-3.38253400	1.72880300	2.40416300	C	6.33618600	-3.08691300	3.33727200
C	-5.09124600	1.39565600	3.81364600	C	6.36381000	-2.09546800	2.16705500
C	-3.94532000	0.55853000	2.11581200	C	5.69826000	-2.44004000	4.57613400
N	-4.98183200	0.32711100	2.94489300	C	6.58900300	-1.20070000	-3.87689700
C	-2.37821000	5.65719100	-3.02646900	C	6.11342000	-2.02877200	-2.68419900
C	-2.59672700	4.85493000	-1.78981200	S	7.47095300	-2.89830700	-1.78687100
N	-3.67035700	5.02600800	-0.92683400	C	0.83896100	-5.71977400	-2.60003900
C	-1.85544700	3.84793800	-1.23385800	C	1.79386300	-4.63163500	-3.08978800
C	-3.54643100	4.14489500	0.09399500	O	2.63615300	-4.13297700	-2.33224000
N	-2.44994300	3.41945100	-0.06202200	C	0.04090500	-5.23413900	-1.37316900
C	1.77497200	3.88903600	-3.92148900	C	-0.72694500	-6.30944900	-0.61674100
C	1.54032700	2.89634500	-2.78108200	O	-1.92292300	-6.20204800	-0.33580200
O	2.50632000	2.71919700	-1.95421100	N	-0.01981700	-7.40637000	-0.23271600
O	0.41376900	2.35740500	-2.66890500	N	1.70087000	-4.28261500	-4.39280800
Zn	2.07460200	2.74313400	0.08290500	C	2.48551300	-3.18306100	-4.93963700
Zn	-1.66511600	2.18008500	1.34013000	H	6.07662600	-4.74780000	1.98215900
H	3.20384800	8.26161900	-2.41051400	H	4.57777900	-4.19305000	2.71480000
H	4.31496900	8.35082500	-1.03673500	H	7.37954500	-3.33515300	3.58618600
H	3.66965000	4.66835300	-1.50481800	H	6.83683100	-2.53532300	1.28167400
H	1.56124300	7.92812600	0.08766400	H	6.92670900	-1.19125500	2.43658400
H	0.51007400	5.79226800	1.00773400	H	5.34729000	-1.78715900	1.88642300
H	7.28523300	0.74853200	-1.34791400	H	6.21542800	-1.51024100	4.84532800
H	7.44931700	-0.27374800	0.08156200	H	4.64368300	-2.19407300	4.38952600
H	4.65600000	1.73861500	-1.44671700	H	5.73592500	-3.09696900	5.45073700
H	6.39125900	1.32505400	2.36010600	H	5.23966300	-5.25582200	4.90770800
H	4.04202700	2.30032800	2.65897500	H	5.66099000	-1.38591500	-1.92167700
H	-2.73406600	3.66890300	4.37233500	H	5.34986100	-2.75943700	-2.96713600
H	-5.84630400	1.43768100	4.58322600	H	7.88875900	-3.66369100	-2.81818100
H	-5.52540900	-0.52489800	2.96847100	H	7.34108600	-0.46399900	-3.57610600
H	-3.64108800	-0.10820800	1.31932000	H	-0.67905900	-4.47435800	-1.67899300

H	0.74234900	-4.76079100	-0.67440400	H	-1.46724900	-0.61132500	-0.99812000
H	0.98391200	-7.45858000	-0.31972500	H	2.09470700	-2.39573300	-1.67024300
H	-0.48629100	-8.09408500	0.34299600	O	0.56140400	1.39759700	-0.18662300
H	0.15659000	-6.04823600	-3.39187200	H	0.39443600	1.47520700	-1.17571400
H	3.54187000	-3.33603200	-4.70711500	H	0.54109200	-1.68931200	1.23341800
H	2.16433100	-2.22297400	-4.51970300	C	1.61712500	-0.23984400	2.35662100
H	0.89302700	-4.59345200	-4.91359600	H	2.21424500	0.66362400	2.24522200
H	1.46717600	-6.58194500	-2.34372000	H	0.79082700	-0.01263700	3.03536200
H	2.35743000	-3.16512800	-6.02397200	H	2.23642500	-1.01276100	2.82773200
H	7.03825900	-1.83608900	-4.64827300	C	-1.57727800	-2.47919200	-5.30038000
H	5.74344200	-0.66967100	-4.33247900	C	-2.93575000	-2.44347900	-4.62155600
H	6.79984400	-5.72453700	4.21397500	O	-3.97819900	-2.63234800	-5.24883100
H	5.30398900	-6.44462200	3.60531500	N	-2.88340500	-2.16178700	-3.29308800
C	-4.69344500	-4.62347200	6.69283200	C	-4.04435900	-2.25928300	-2.43170500
C	-3.16664100	-4.52680500	6.53395900	C	-4.30745600	-0.88426600	-1.80168400
C	-2.76745200	-3.89512800	5.21873800	O	-3.48285000	-0.40355100	-0.99673300
C	-2.43336800	-2.54023500	5.12896900	C	-3.82786400	-3.30488300	-1.32038600
C	-2.78035600	-4.64296400	4.03061000	O	-3.56279800	-4.54313600	-1.93580400
C	-2.13860600	-1.93965300	3.90253000	N	-5.43022700	-0.20225300	-2.11589500
C	-2.49144500	-4.06629000	2.79897900	C	-6.50500600	-0.57182400	-3.07637100
C	-2.17764900	-2.70174100	2.72807700	C	-6.10790000	-0.28911000	-4.53086600
O	-1.92734700	-2.17892200	1.49594100	C	-7.67401700	0.30123500	-2.58037100
H	-2.73406300	-5.53291500	6.61209700	C	-6.98907400	1.59768100	-2.11795800
H	-2.75077400	-3.94579800	7.36689300	C	-5.67812900	1.10561000	-1.48369600
H	-2.40016800	-1.93721800	6.03474600	H	-4.82888500	1.77560000	-1.65040800
H	-3.02372100	-5.70297700	4.07174600	H	-5.77209800	0.97019900	-0.39840400
H	-1.86773900	-0.88745800	3.85345700	H	-6.77972300	2.24369600	-2.97753700
H	-2.49313800	-4.65557600	1.88614400	H	-7.59786400	2.17361600	-1.41407400
H	-1.66537700	-1.22648100	1.54025000	H	-8.42428200	0.46323300	-3.35933200
H	-5.15348200	-3.62889300	6.65690800	H	-8.16986000	-0.18563400	-1.73160700
H	-5.13466900	-5.22204000	5.88787300	H	-6.74337800	-1.63271100	-2.96322700
H	-4.96510000	-5.08848700	7.64784500	H	-5.81227500	0.75830400	-4.66391900
N	-0.45661900	-0.60571500	-0.84026000	H	-5.29175800	-0.93897400	-4.85586700
C	0.30675500	-1.50627000	-1.54153900	H	-6.96525900	-0.48517900	-5.18606100
O	-0.17426400	-2.18348300	-2.46977000	H	-4.86767600	-2.58651000	-3.06681600
N	1.61908600	-1.62523700	-1.20188000	H	-3.06466000	-5.10596100	-1.30809200
C	2.19036000	-1.10127500	0.03099000	H	-4.74341500	-3.33893500	-0.70006000
C	1.08344700	-0.75926100	1.02443900	H	-3.00985200	-2.97693500	-0.66713900
C	0.00244500	0.11015700	0.33192600	H	-1.95772600	-2.12418100	-2.86001800
O	-1.03296300	0.39339800	1.15884100	H	-1.57683800	-1.75344200	-6.12086200
H	2.81091500	-0.21980500	-0.17336500	H	-0.74936400	-2.27307500	-4.62225800
H	2.84600300	-1.86848600	0.45927300	H	-1.45324600	-3.46846100	-5.75754200

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C	3.74936900	7.64262400	-1.62158700	C	6.01273200	1.32753800	0.22659600
C	2.91708900	6.63251700	-0.91223600	N	5.80364700	1.58032200	1.57263200
N	1.78795900	6.91569800	-0.15377300	C	4.86471500	1.72996500	-0.39360100
C	3.03254300	5.27349000	-0.86448500	C	4.56583200	2.09991200	1.72591400
C	1.27551700	5.74762500	0.31054900	N	3.97245000	2.19752000	0.54760300
N	2.00665300	4.73121200	-0.11313000	C	0.04822400	4.86486400	4.58558100
C	7.24244200	0.70959900	-0.30980000	N	1.09394500	4.26707800	3.80431200

C	0.82104500	3.46772100	2.73759700	H	2.01740500	4.16953300	4.19902200
O	-0.38604900	3.46751700	2.30824100	C	5.71377700	-5.62566200	3.82793700
O	1.80477700	2.84527500	2.23799300	C	5.59662500	-4.49321800	2.79978900
C	-3.79473500	3.52000400	4.14971100	C	6.24753600	-3.17076600	3.25285500
C	-4.04440900	2.19611500	3.49450900	C	6.27919400	-2.15686800	2.10179900
N	-3.27334400	1.68924000	2.44882500	C	5.55995100	-2.56435400	4.48562800
C	-5.03058100	1.29008800	3.78389700	C	6.50572800	-1.18661600	-3.95733900
C	-3.79865500	0.51180800	2.12031800	C	6.04214300	-2.02818100	-2.76920400
N	-4.86132100	0.24043400	2.90263700	S	7.40990500	-2.90070200	-1.89051300
C	-2.43506700	5.68110500	-2.92705500	C	0.77314900	-5.62670600	-2.61169000
C	-2.61437100	4.85750400	-1.69863500	C	1.73251600	-4.56419800	-3.14429300
N	-3.72495800	4.91584100	-0.86868600	O	2.60508400	-4.07104600	-2.41796500
C	-1.80149000	3.91860200	-1.12601500	C	0.01302300	-5.10425900	-1.37502400
C	-3.55049800	4.03422500	0.14590500	C	-0.72185200	-6.16860800	-0.57203400
N	-2.38732700	3.41735900	0.01834500	O	-1.92758500	-6.10790500	-0.32079700
C	1.70616400	3.91641500	-3.88226800	N	0.03074000	-7.20769100	-0.11855600
C	1.57717400	2.88637600	-2.77280900	N	1.60694900	-4.22757500	-4.44811800
O	2.52541200	2.70755300	-1.97362700	C	2.38868000	-3.13999700	-5.02127700
O	0.43311500	2.30037200	-2.66283500	H	6.06846100	-4.81125800	1.86052100
Zn	2.04997300	2.68701800	0.23728100	H	4.53694900	-4.31237100	2.56467100
Zn	-1.53352400	2.15320600	1.36836200	H	7.29039400	-3.39551200	3.52551300
H	3.17398200	8.19789500	-2.37294600	H	6.78814400	-2.56752500	1.22219000
H	4.18947500	8.37585300	-0.93425300	H	6.80742300	-1.24202400	2.40344900
H	3.76235100	4.64373700	-1.34453900	H	5.26257000	-1.87133300	1.79889400
H	1.41258000	7.83561400	0.03228300	H	6.04754100	-1.62877700	4.78776400
H	0.39692500	5.67163100	0.93407100	H	4.50581000	-2.33788900	4.27423600
H	7.19820200	0.67873100	-1.40091800	H	5.58848700	-3.23851900	5.34744300
H	7.37815400	-0.31894700	0.04333700	H	5.17230200	-5.40059400	4.75305300
H	4.60581700	1.70995100	-1.44031900	H	5.59307500	-1.39474700	-1.99688900
H	6.45161800	1.37038500	2.31947300	H	5.27867300	-2.75858700	-3.05273400
H	4.11757700	2.37020800	2.66796300	H	7.81500600	-3.66352500	-2.92877300
H	-2.79618600	3.56113900	4.59795100	H	7.25699100	-0.44944500	-3.65534800
H	-5.81527500	1.30122900	4.52441800	H	-0.71965900	-4.35649300	-1.68033300
H	-5.38187000	-0.62601200	2.89035300	H	0.73527600	-4.61124500	-0.71240900
H	-3.45022200	-0.13396800	1.32618100	H	1.03789700	-7.20836400	-0.18036300
H	-1.49744000	5.40368100	-3.41473600	H	-0.41130100	-7.88549400	0.48736900
H	-3.24292000	5.52155300	-3.65167400	H	0.06595700	-5.95877500	-3.37975900
H	-0.86592500	3.54018500	-1.50197100	H	3.44882300	-3.30347000	-4.81501500
H	-4.54021400	5.49773800	-1.00566400	H	2.08784900	-2.17443500	-4.59864800
H	-4.27199200	3.86314500	0.92997600	H	0.77117300	-4.51755700	-4.93604100
H	-0.67605800	5.35166200	3.92957300	H	1.39129500	-6.49456500	-2.35104700
H	0.98244800	3.73555400	-4.67962200	H	2.23331100	-3.12681700	-6.10222700
H	1.51815200	4.90502600	-3.44616700	H	6.95220100	-1.81272200	-4.73784700
H	8.14325500	1.27318000	-0.03458800	H	5.65456000	-0.65521400	-4.40210100
H	-3.86029000	4.34914900	3.43417900	H	6.76224800	-5.81181300	4.09128500
H	-4.53083300	3.69771000	4.93851200	H	5.30347800	-6.56068300	3.42990200
H	0.48024600	5.62106100	5.24771800	C	-4.70671800	-4.75091600	6.64006400
H	-0.49159800	4.13570900	5.20669600	C	-3.18192200	-4.60425600	6.49440100
H	4.57006300	7.13866700	-2.13779600	C	-2.77367900	-3.95480300	5.18892200
H	2.72168700	3.91924300	-4.28568000	C	-2.38965500	-2.61160000	5.12409100
H	-2.39739500	6.75510100	-2.70427500	C	-2.80203700	-4.67959900	3.98637500

C	-2.05529800	-2.00163000	3.91162500	C	-1.67466800	-2.41912200	-5.33968500
C	-2.47597800	-4.09321300	2.76860200	C	-3.01608300	-2.37750900	-4.62859800
C	-2.10380900	-2.74135500	2.72286700	O	-4.07287700	-2.57921400	-5.22788300
O	-1.80964700	-2.21351700	1.50323500	N	-2.93262600	-2.08002700	-3.30551700
H	-2.72056500	-5.59768300	6.57439100	C	-4.07302800	-2.17819900	-2.41693500
H	-2.79288200	-4.01639600	7.33543900	C	-4.33444000	-0.79943000	-1.79551500
H	-2.34357900	-2.02506200	6.04010800	O	-3.50133900	-0.30496500	-1.00967600
H	-3.08427800	-5.73068200	4.00472400	C	-3.82466700	-3.21201200	-1.30193700
H	-1.74323100	-0.96017100	3.88573500	O	-3.57175800	-4.45416800	-1.91462800
H	-2.48969600	-4.66742500	1.84644400	N	-5.46793600	-0.12764100	-2.09913100
H	-1.52613100	-1.26423100	1.55484800	C	-6.55694800	-0.51244000	-3.03684900
H	-5.19866100	-3.77160200	6.60766700	C	-6.19305900	-0.22947400	-4.50023600
H	-5.12333900	-5.35802900	5.82840100	C	-7.72606600	0.34743800	-2.51877000
H	-4.96900700	-5.23132500	7.58993100	C	-7.04768300	1.65408600	-2.07551000
N	-0.42038500	-0.50855500	-0.89866800	C	-5.71633500	1.18066400	-1.46945400
C	0.31423800	-1.37953700	-1.65352700	H	-4.87947900	1.85985800	-1.66086900
O	-0.19660100	-2.04489000	-2.57764400	H	-5.78143300	1.05087500	-0.38134200
N	1.64690700	-1.49149500	-1.38082500	H	-6.86649300	2.29982200	-2.94176500
C	2.25070300	-1.02516500	-0.13925500	H	-7.64833700	2.22422400	-1.35990600
C	1.17453000	-0.74462200	0.90487300	H	-8.49553300	0.49739400	-3.28126300
C	0.07650100	0.17210900	0.29455500	H	-8.19643400	-0.14243100	-1.65741600
O	-0.95236500	0.35350300	1.18081300	H	-6.78028200	-1.57577500	-2.91681600
H	2.85411400	-0.12680400	-0.31871000	H	-5.90990500	0.82030700	-4.64225500
H	2.93039700	-1.80447100	0.22543000	H	-5.37761900	-0.87328900	-4.83888500
H	-1.43363100	-0.51160500	-1.02557500	H	-7.06155700	-0.43561300	-5.13740500
H	2.08831800	-2.27817500	-1.85404700	H	-4.90698700	-2.51889200	-3.03072500
O	0.55110000	1.47556600	-0.13095200	H	-3.07155500	-5.01838400	-1.28937900
H	0.43462100	1.74032500	-1.46987500	H	-4.72448900	-3.24370700	-0.65864300
H	0.63961600	-1.68641600	1.07636500	H	-2.99121700	-2.87684900	-0.67188000
C	1.74942200	-0.30745600	2.24931200	H	-1.99627400	-2.02215100	-2.89625400
H	2.38866800	0.57021300	2.16912600	H	-1.71006400	-1.73539400	-6.19465100
H	0.94352800	-0.07092200	2.94884400	H	-0.83493300	-2.16636000	-4.69273100
H	2.34078800	-1.12550800	2.67854900	H	-1.54166600	-3.42720000	-5.75176700

SkDHPase.DHT-INT2-II-D

C	4.10460800	7.45876200	-1.60107100	O	2.02972800	2.74240500	2.28321900
C	3.23877500	6.46028100	-0.91101600	C	-3.56646600	3.67138100	4.23226600
N	2.12751600	6.77737300	-0.13974600	C	-3.86465500	2.36394200	3.56425900
C	3.29623900	5.09516900	-0.88588900	N	-3.11650700	1.84086000	2.50921900
C	1.56843200	5.62609700	0.30959300	C	-4.88244800	1.49162900	3.84760600
N	2.25182900	4.58458000	-0.13568100	C	-3.68744800	0.68772800	2.16933300
C	7.25523700	0.34451800	-0.39675600	N	-4.75656600	0.44718600	2.95276400
C	6.08461200	1.04954600	0.15972800	C	-2.18803000	5.82753300	-2.84238000
N	5.93370200	1.35934000	1.50118000	C	-2.39364600	4.98320700	-1.63234400
C	4.93789900	1.48452400	-0.43833600	N	-3.59135000	4.89052000	-0.93794600
C	4.72672100	1.94154900	1.67397800	C	-1.54374400	4.14307500	-0.96797800
N	4.09864300	2.02550200	0.51192500	C	-3.42951100	4.01839700	0.08683400
C	0.34540500	4.81439200	4.62943100	N	-2.19321100	3.54991400	0.09370200
N	1.37089200	4.16113500	3.87021900	C	1.84517800	3.86319800	-3.86755200
C	1.07512600	3.41535700	2.77428100	C	1.73654800	2.82973800	-2.76879900
O	-0.11434400	3.50975700	2.30598300	O	2.70708500	2.52408100	-2.06738300

O	0.52639600	2.36435600	-2.56568600	H	5.86591300	-5.11504400	1.75329900
Zn	2.17192700	2.55016300	0.28800400	H	4.33449400	-4.58869800	2.43674800
Zn	-1.36081100	2.24398300	1.41403300	H	7.09228000	-3.74324600	3.44882100
H	3.54441500	8.05392600	-2.33291700	H	6.63440600	-2.87448900	1.15159800
H	4.57399100	8.15615400	-0.89628500	H	6.65769500	-1.56276800	2.34980300
H	4.00002900	4.44126800	-1.37359000	H	5.11304800	-2.16120800	1.71745900
H	1.79461600	7.70943300	0.06634100	H	5.86857100	-1.96903600	4.71992100
H	0.69256900	5.57680500	0.93995500	H	4.32013200	-2.64104700	4.17896600
H	7.16873700	0.28085900	-1.48381900	H	5.37202300	-3.57727700	5.25255900
H	7.34302800	-0.67884600	-0.01429100	H	4.90234000	-5.71792200	4.62136300
H	4.64885000	1.43845000	-1.47562800	H	5.43462300	-1.66075600	-2.10131400
H	6.59681600	1.14817200	2.23423800	H	5.06182400	-2.99421300	-3.17721500
H	4.32111300	2.26123900	2.61969900	H	7.54088900	-4.03526900	-3.03718900
H	-2.56844900	3.67100000	4.68391600	H	7.16192400	-0.78307600	-3.73355000
H	-5.66280900	1.52309900	4.59213700	H	-0.25887200	-4.14600400	-0.76638400
H	-5.30679800	-0.40059600	2.93358300	H	1.08918400	-5.28751700	-0.66575100
H	-3.37005300	0.03855900	1.36526400	H	0.66404500	-7.42701000	0.08212300
H	-1.16752800	5.69417800	-3.20961000	H	-0.93818900	-7.98018700	0.46632200
H	-2.86903900	5.54905500	-3.65585200	H	-0.84252400	-4.89978100	-3.00061900
H	-0.52911900	3.88930400	-1.21824200	H	3.15446100	-3.62241100	-4.95253200
H	-4.44966200	5.37347900	-1.16625300	H	2.12151900	-2.21112600	-4.62038400
H	-4.20872600	3.74979400	0.78329700	H	0.25157700	-4.12904000	-4.88656600
H	-0.32809300	5.35267200	3.96005600	H	0.23569800	-6.29612400	-2.89563600
H	1.05206400	3.74631400	-4.60900300	H	1.93394900	-3.12133300	-6.14476300
H	1.75895300	4.85492700	-3.40756500	H	6.79729900	-2.11634400	-4.83471600
H	8.19769800	0.86093600	-0.17297300	H	5.55803500	-0.89731500	-4.49705800
H	-3.59966300	4.50670700	3.52188000	H	6.49627000	-6.15530600	3.98667200
H	-4.29717500	3.86977700	5.02114600	H	5.03584800	-6.86494600	3.28688400
H	0.80441400	5.53468000	5.31326900	C	-4.86817900	-4.56560900	6.66112300
H	-0.25645700	4.11429300	5.22658200	C	-3.34173800	-4.47598300	6.48222700
H	4.90404300	6.94028100	-2.13596500	C	-2.92036900	-3.82909800	5.17800500
H	2.82501100	3.80063300	-4.34581300	C	-2.44380700	-2.51486500	5.12883500
H	-2.33675200	6.89490400	-2.63525600	C	-3.00659300	-4.53040300	3.96394500
H	2.27252200	3.98930000	4.28933500	C	-2.07071400	-1.91204600	3.92366300
C	5.45751300	-5.94362700	3.70454700	C	-2.64367500	-3.95029800	2.75310800
C	5.38531800	-4.79694000	2.68809900	C	-2.17239200	-2.62880700	2.72404100
C	6.05730000	-3.49431500	3.16706800	O	-1.83839400	-2.10833400	1.51116900
C	6.12097300	-2.46622900	2.02981500	H	-2.91955400	-5.48813000	6.54338600
C	5.36685700	-2.89100600	4.39983000	H	-2.91318900	-3.91518500	7.32255800
C	6.37641600	-1.47688500	-4.05087200	H	-2.35053700	-1.94662800	6.05277000
C	5.85845400	-2.30720400	-2.87718600	H	-3.36095200	-5.55959100	3.96745700
S	7.17108200	-3.25856000	-1.99606400	H	-1.68428700	-0.89558000	3.91247600
C	0.10924100	-5.24879500	-2.58674800	H	-2.70095000	-4.50869500	1.82287200
C	1.27862900	-4.45041800	-3.16624200	H	-1.50046500	-1.17632700	1.57041600
O	2.29039200	-4.18346600	-2.50493100	H	-5.32307100	-3.56804200	6.65295000
C	0.07498000	-5.14706400	-1.05144000	H	-5.32712000	-5.14583100	5.85253200
C	-0.89186200	-6.14436400	-0.43522700	H	-5.12544200	-5.04841000	7.61099400
O	-2.11253900	-5.97031700	-0.39332400	N	-0.44031800	-0.43539900	-0.90856100
N	-0.33324300	-7.27944700	0.06018200	C	0.22064700	-1.35426300	-1.66865700
N	1.17244800	-4.09982500	-4.47103600	O	-0.35557800	-2.02849100	-2.54944500
C	2.15176700	-3.20768200	-5.07782000	N	1.56359300	-1.50851900	-1.45864300

C	2.22497500	-1.08274600	-0.23029300	N	-5.55655700	0.05802100	-2.05458700
C	1.19469300	-0.75981100	0.84593600	C	-6.62767000	-0.25070800	-3.03951800
C	0.13832700	0.23269200	0.27328100	C	-6.23371600	0.14078800	-4.47075600
O	-0.86739300	0.42888600	1.19597900	C	-7.80403200	0.57165400	-2.47948600
H	2.86222200	-0.21125100	-0.42170300	C	-7.13164400	1.84323500	-1.93558800
H	2.87924200	-1.89591000	0.10634100	C	-5.80171800	1.33083800	-1.35658600
H	-1.45804500	-0.42652600	-0.97617500	H	-4.96375900	2.01860100	-1.51176900
H	1.94021900	-2.33392700	-1.91960100	H	-5.86486700	1.14275300	-0.27699100
O	0.64264600	1.48783500	-0.17269700	H	-6.94763300	2.55173000	-2.75091100
H	0.61340000	-1.67291400	1.01975800	H	-7.73895200	2.35751300	-1.18421500
C	1.82964700	-0.38176000	2.18164700	H	-8.56268500	0.77684800	-3.23998900
H	2.55594900	0.42484000	2.09347600	H	-8.28654300	0.02180000	-1.66234600
H	1.06176800	-0.06473500	2.89176900	H	-6.85599200	-1.31889600	-3.00718800
H	2.34312100	-1.25436700	2.60364400	H	-5.92963100	1.19278700	-4.52457900
H	0.50893900	1.82101200	-1.66927400	H	-5.42454100	-0.49234000	-4.84194500
C	-1.84411900	-2.26826000	-5.38894400	H	-7.09322500	0.00050500	-5.13712200
C	-3.17489900	-2.16474700	-4.66372200	H	-5.03929400	-2.31409000	-3.04721600
O	-4.24521600	-2.30797500	-5.25543600	H	-3.16127100	-4.86953000	-1.42565000
N	-3.06337800	-1.88703400	-3.33873000	H	-4.81973700	-3.13981200	-0.71435900
C	-4.19215300	-2.00145500	-2.43647800	H	-3.08900200	-2.76280200	-0.73206800
C	-4.43617100	-0.64445700	-1.76275900	H	-2.12310500	-1.89630900	-2.93164300
O	-3.60901500	-0.19615400	-0.94547100	H	-1.85568500	-1.59228400	-6.25047500
C	-3.92785900	-3.07746400	-1.36591000	H	-0.98999100	-2.04280700	-4.74901700
O	-3.67546700	-4.29422900	-2.02856400	H	-1.75956000	-3.28495900	-5.79360700

SkDHPase.DHT-TS3-II-D

C	3.68277500	7.61017000	-1.60971700	N	-3.60511700	5.02030100	-0.65451600
C	2.87441300	6.59409600	-0.89068300	C	-1.81368800	3.83983800	-1.06539300
N	1.87652000	6.87978900	0.03044100	C	-3.39825300	4.16557400	0.37659800
C	2.90405700	5.23168700	-0.95986800	N	-2.31487200	3.44165400	0.15774500
C	1.35561200	5.70938300	0.47661400	C	1.64737800	3.86465300	-3.84540600
N	1.95603500	4.69189300	-0.11438400	C	1.45704800	2.72940300	-2.82553200
C	7.23483100	0.70468200	-0.31110100	O	2.35039000	2.52317300	-1.96894000
C	5.97647400	1.28819500	0.20445000	O	0.34423500	2.08715600	-2.89550400
N	5.72773900	1.47966100	1.55391000	Zn	1.99001100	2.66662900	0.22541700
C	4.84133700	1.71303800	-0.42754100	Zn	-1.43512100	2.06028700	1.39930900
C	4.48394200	1.98645900	1.69729900	H	3.06409900	8.27042000	-2.23075700
N	3.91929900	2.13419700	0.50949200	H	4.25643500	8.24585700	-0.92348400
C	0.05177100	4.82075300	4.63355200	H	3.52786400	4.59673600	-1.56678700
N	1.11267900	4.39972500	3.76291000	H	1.59113400	7.80189700	0.33042900
C	0.87067500	3.39937300	2.85985600	H	0.57688300	5.63963800	1.22045600
O	-0.35908300	3.10934500	2.68369900	H	7.23010900	0.70926700	-1.40372800
O	1.88816600	2.91286900	2.28258200	H	7.37507700	-0.33231600	0.01411000
C	-3.78510000	3.44811800	4.23199700	H	4.60865000	1.73362600	-1.48081500
C	-4.03617400	2.14846000	3.52356400	H	6.35603900	1.24008400	2.30852000
N	-3.23863900	1.64035500	2.49702600	H	4.01159800	2.22309500	2.63651300
C	-5.06383800	1.26958300	3.75048100	H	-2.78281300	3.47009600	4.67233900
C	-3.79158600	0.49271600	2.12066800	H	-5.87714400	1.29056300	4.45943700
N	-4.89567100	0.23582500	2.85155300	H	-5.44363500	-0.61184500	2.79862800
C	-2.49819400	5.60256300	-2.86039000	H	-3.42041700	-0.14756400	1.33325400
C	-2.60082400	4.82878500	-1.59259200	H	-1.65946200	5.22509700	-3.45062900

H	-3.40194300	5.50883600	-3.47509100	H	0.18682200	-6.01481200	-3.17186600
H	-0.95141000	3.36064200	-1.50212700	H	3.42757600	-3.22513000	-4.70474900
H	-4.37535000	5.67018100	-0.73394100	H	1.94791300	-2.23049600	-4.65541500
H	-4.04696800	4.08815400	1.23520200	H	0.90571600	-4.73076200	-4.84485300
H	-0.79133600	5.20007400	4.05135500	H	1.49183600	-6.41851200	-2.05359400
H	0.99758400	3.72709100	-4.71191500	H	2.27488700	-3.28436800	-6.05808600
H	1.40046000	4.81441400	-3.35782500	H	6.90264400	-1.83692800	-4.73818500
H	8.11569300	1.27316300	0.01394300	H	5.61991500	-0.67225100	-4.37056200
H	-3.85706400	4.30896400	3.55520400	H	6.83797500	-5.83661000	4.07857400
H	-4.51796300	3.58947000	5.03108100	H	5.34203400	-6.56084600	3.47592500
H	0.41509900	5.62844200	5.27680100	C	-4.61888800	-4.82329700	6.74800700
H	-0.32177400	4.01084400	5.27510000	C	-3.12192200	-4.58828600	6.46817700
H	4.39619000	7.10931100	-2.26880700	C	-2.81399100	-3.97080100	5.11551600
H	2.69287100	3.91071200	-4.15998900	C	-2.34851000	-2.65656500	4.99585800
H	-2.33035900	6.67207400	-2.67967800	C	-2.96155200	-4.70856900	3.92857500
H	2.06985000	4.48144800	4.07382200	C	-2.03055900	-2.09396600	3.75505900
C	5.78426600	-5.63167400	3.85300000	C	-2.65400500	-4.16882100	2.68334200
C	5.65081000	-4.50239800	2.82333000	C	-2.17420500	-2.85262600	2.58568900
C	6.34379000	-3.19064400	3.24350600	O	-1.87111800	-2.38561000	1.34244300
C	6.34181100	-2.18113800	2.08840200	H	-2.59690500	-5.54978500	6.55385700
C	5.72109400	-2.56918400	4.50287900	H	-2.70783300	-3.94722900	7.25674500
C	6.48177600	-1.20489200	-3.94827500	H	-2.21518500	-2.05517200	5.89343800
C	6.05090700	-2.03760400	-2.74212100	H	-3.31903400	-5.73544700	3.98025500
S	7.43978700	-2.91203100	-1.89988500	H	-1.65830200	-1.07430400	3.69414700
C	0.86704900	-5.59637300	-2.42172900	H	-2.76792500	-4.75275600	1.77409200
C	1.79556400	-4.54750900	-3.02124300	H	-1.58627500	-1.43077000	1.33039000
O	2.62279200	-3.95244800	-2.31598800	H	-5.17597800	-3.87932400	6.72918800
C	0.06410900	-4.97015200	-1.26034800	H	-5.06432800	-5.48606200	5.99737900
C	-0.83585300	-5.96774200	-0.54479600	H	-4.76299000	-5.28394900	7.73184800
O	-2.06298500	-5.93437600	-0.61304700	N	-0.21531000	-0.00412000	-1.32779700
N	-0.19486700	-6.93751900	0.16513600	C	0.45075300	-1.11380500	-1.94576900
N	1.66721300	-4.29771900	-4.34195600	O	-0.10374000	-1.76642900	-2.83507900
C	2.36997400	-3.18939100	-4.97430300	N	1.71972900	-1.33098600	-1.55058000
H	6.08028600	-4.83441700	1.86868200	C	2.23675000	-0.82224100	-0.28256100
H	4.58656800	-4.30118200	2.62803600	C	1.09158000	-0.68647100	0.71731000
H	7.39358300	-3.43272300	3.47040100	C	0.03332400	0.32637400	0.21147200
H	6.80351100	-2.60293400	1.18824000	O	-1.13483200	0.17923700	0.89631400
H	6.90036100	-1.27567700	2.36224900	H	2.74937400	0.12960900	-0.43857600
H	5.31735600	-1.87862800	1.83083000	H	2.97955900	-1.54130500	0.07742500
H	6.23367100	-1.63844300	4.77716400	H	-1.23529400	-0.12430400	-1.44759600
H	4.66115400	-2.33094500	4.33862600	H	2.14015300	-2.18206800	-1.92996400
H	5.78093200	-3.23886800	5.36650000	O	0.37373500	1.65853800	0.22554400
H	5.28184600	-5.39121200	4.79604600	H	0.57605700	-1.65539500	0.72956000
H	5.62846800	-1.39702700	-1.96077700	C	1.55777000	-0.39743100	2.14513700
H	5.27569300	-2.76573500	-2.99855500	H	2.02760400	0.58208500	2.23910500
H	7.81001100	-3.68199100	-2.94589200	H	0.70536000	-0.42065800	2.82953900
H	7.24420600	-0.46903100	-3.67262100	H	2.26834900	-1.16608600	2.47249500
H	-0.57150300	-4.16670800	-1.63765300	H	0.13468500	1.11289900	-2.07787400
H	0.77227500	-4.53097400	-0.54846900	C	-1.67206600	-2.48716800	-5.31373400
H	0.79278900	-6.88745400	0.36661800	C	-3.00753300	-2.54884500	-4.59461800
H	-0.75859200	-7.57571200	0.71044500	O	-4.06563400	-2.70060100	-5.20186100

N	-2.92305000	-2.39356800	-3.24044800	H	-7.22248500	2.57523300	-1.51005300
C	-4.10237400	-2.18601300	-2.42192600	H	-8.34050300	0.74790900	-3.18695300
C	-4.15742100	-0.72188400	-1.97038900	H	-7.99485000	0.25503500	-1.52224900
O	-3.17714200	-0.20857100	-1.39937700	H	-6.79157700	-1.42772500	-2.67751300
C	-4.13150900	-3.09962900	-1.17293900	H	-5.86428000	0.67931700	-4.72051400
O	-4.29537500	-4.44673200	-1.53757500	H	-5.44100300	-1.04976700	-4.75437300
N	-5.30140700	-0.02146700	-2.13515300	H	-7.11376800	-0.54591600	-5.00632400
C	-6.48792300	-0.41012500	-2.93973900	H	-4.95075400	-2.45911900	-3.04652400
C	-6.19868800	-0.32720500	-4.44230100	H	-3.45804400	-4.91879500	-1.37282600
C	-7.53939200	0.60691800	-2.45595800	H	-4.99490100	-2.79119500	-0.55995800
C	-6.72271100	1.88427800	-2.19617400	H	-3.23271400	-2.92911400	-0.56899300
C	-5.39477800	1.35789100	-1.62730200	H	-2.01714600	-2.11742000	-2.86637100
H	-4.52080300	1.93776800	-1.93879700	H	-1.34152000	-1.44536700	-5.39152200
H	-5.39386100	1.34035600	-0.52939200	H	-0.89103400	-3.02608600	-4.77485400
H	-6.54904000	2.42139900	-3.13515500	H	-1.80190500	-2.89337200	-6.31904400

SkDHPase.DHT-EP-II-D

C	4.17402800	7.46919000	-1.87606400	Zn	-1.52637300	2.39251500	1.37321000
C	3.32318600	6.54623700	-1.08050000	H	3.57838700	8.15016400	-2.49704800
N	2.38540900	6.93913500	-0.13518000	H	4.82595000	8.08447600	-1.24319900
C	3.24621600	5.18425500	-1.09988100	H	3.78445300	4.48147100	-1.71357400
C	1.79270000	5.82782000	0.37060700	H	2.17754800	7.89050400	0.13582100
N	2.29082400	4.74638100	-0.20256700	H	1.03116700	5.84591600	1.13502600
C	7.32392800	0.42509700	-0.31143400	H	7.33052600	0.39553400	-1.40355800
C	6.05726600	1.03845400	0.17220100	H	7.45068800	-0.60208500	0.04759500
N	5.80555300	1.29002500	1.51309200	H	4.69868200	1.46181000	-1.53314600
C	4.93035000	1.46583300	-0.47912000	H	6.42286200	1.05974300	2.27975800
C	4.57474800	1.83653200	1.63084500	H	4.10994400	2.12544300	2.55979100
N	4.01661500	1.95253700	0.43708000	H	-2.48023300	3.92966900	4.37809800
C	0.37501300	5.12057100	4.44809000	H	-5.76894700	1.95877800	4.57615100
N	1.33525300	4.45768400	3.59983800	H	-5.61593300	-0.01392400	2.94955800
C	0.94552100	3.53045600	2.67280600	H	-3.70766700	0.24182300	1.30322800
O	-0.31784500	3.48355500	2.44836100	H	-1.28263200	5.32242500	-3.63811700
O	1.85772900	2.85776900	2.11108100	H	-2.98760000	5.77622600	-3.73620800
C	-3.53281900	3.95442200	4.07946700	H	-0.83888000	3.37263000	-1.68915600
C	-3.95070400	2.64721600	3.47254700	H	-4.08075100	5.97782800	-1.06010400
N	-3.27997300	2.04396600	2.40938900	H	-3.98352800	4.38428200	0.92125700
C	-5.01659000	1.85523000	3.80974000	H	-0.39277400	5.60665300	3.84187400
C	-3.93813600	0.92575300	2.11343200	H	1.25066100	3.66829100	-4.82934900
N	-4.99299800	0.78226000	2.93968500	H	1.85580200	4.78212800	-3.57700700
C	-2.10820600	5.77169400	-3.08068000	H	8.20167700	1.00086500	0.00783500
C	-2.34335500	4.98933700	-1.83352700	H	-3.65000100	4.78693100	3.37393700
N	-3.37289800	5.26534800	-0.94416500	H	-4.14073300	4.17632400	4.96068600
C	-1.67043200	3.93213200	-1.27912900	H	0.88932300	5.88632200	5.03596700
C	-3.29455600	4.39904700	0.09067500	H	-0.12555000	4.43201200	5.14257900
N	-2.26574700	3.58177600	-0.07989600	H	4.81417300	6.88743300	-2.54368400
C	1.93403100	3.76620300	-3.98327700	H	2.96622200	3.62894500	-4.32054800
C	1.57540400	2.76162300	-2.88553100	H	-1.84632400	6.81550500	-2.86614400
O	2.48433400	2.54871700	-1.99026200	H	2.29675100	4.39250300	3.90005400
O	0.44032800	2.25361600	-2.89320800	C	5.50483100	-5.66223000	4.07360700
Zn	2.16205800	2.68913000	0.01841500	C	5.43836500	-4.56557500	3.00302000

C	6.27807900	-3.31721700	3.34240900	O	-1.85037500	-2.25101000	1.49098800
C	6.32217300	-2.34993300	2.15275000	H	-2.98283100	-5.24987600	6.74788300
C	5.78099500	-2.59519200	4.60423000	H	-2.81381300	-3.64211700	7.43308300
C	6.47211200	-1.57022800	-3.88017200	H	-2.51364800	-1.67564100	5.97753700
C	5.96194500	-2.34743700	-2.66758700	H	-3.18907500	-5.54780200	4.25386300
S	7.27605100	-3.28717800	-1.77593000	H	-1.87395200	-0.79567000	3.75400700
C	0.39764900	-5.63084100	-2.41429000	H	-2.55625200	-4.66642700	2.02092700
C	1.49453800	-4.71156700	-2.95432100	H	-1.65696700	-1.29019200	1.48704300
O	2.45206600	-4.34702000	-2.26140300	H	-5.21303800	-3.12826900	6.83677100
C	0.24575000	-5.47126200	-0.89173800	H	-5.38274700	-4.74541500	6.13897000
C	-0.79629200	-6.41888500	-0.32088200	H	-5.09519800	-4.55901900	7.87926200
O	-2.00609100	-6.18026700	-0.33253200	N	-0.45572500	-0.36307500	-1.95300900
N	-0.31935300	-7.58112900	0.19932500	C	0.18416100	-1.56431100	-1.98327700
N	1.37825200	-4.35568100	-4.25807300	O	-0.38804700	-2.62644600	-2.30093200
C	2.25645900	-3.35403000	-4.85183700	N	1.50669300	-1.57690100	-1.60511300
H	5.78945600	-4.97412100	2.04624500	C	2.00431500	-0.71154300	-0.53988800
H	4.39198400	-4.26436800	2.84335200	C	1.07006100	-0.65950100	0.69842700
H	7.30789200	-3.65708600	3.53191000	C	0.13851400	0.53891900	0.68944700
H	6.69654500	-2.84363500	1.24884200	O	-0.96651600	0.45971300	1.33037600
H	6.98090600	-1.49760800	2.36926100	H	2.18135600	0.29242700	-0.93009800
H	5.32177600	-1.95433500	1.92890700	H	2.97873000	-1.11280700	-0.24799000
H	6.39320600	-1.70973000	4.81799500	H	-1.43692000	-0.39104100	-2.20356400
H	4.74164800	-2.26160500	4.47909600	H	1.89109700	-2.52013400	-1.62788600
H	5.81908400	-3.23702900	5.48988900	O	0.44017300	1.64230300	0.13919200
H	5.06867800	-5.33726700	5.02429700	H	0.43118500	-1.54760600	0.68884800
H	5.56497400	-1.66382500	-1.90948300	C	1.83644700	-0.68081900	2.04083400
H	5.14811000	-3.03153800	-2.92560100	H	2.46571300	0.20343500	2.16246800
H	7.60143300	-4.12018200	-2.78784000	H	1.13722400	-0.72026800	2.88163400
H	7.27459200	-0.87919500	-3.60192600	H	2.47003700	-1.57307400	2.08487400
H	-0.08816200	-4.45230900	-0.68422600	H	0.02596800	0.52006000	-2.14947900
H	1.22121600	-5.61874400	-0.41769100	C	-1.73820000	-2.43613500	-5.23469700
H	0.66650900	-7.78617800	0.25255900	C	-3.09504900	-2.32801500	-4.55443400
H	-0.97732800	-8.25426900	0.56776600	O	-4.13912400	-2.35175000	-5.20278100
H	-0.55805500	-5.41251000	-2.90163200	N	-3.03974400	-2.15077700	-3.20037500
H	3.29734100	-3.67967100	-4.77640700	C	-4.23047200	-2.26405200	-2.36844500
H	2.15728400	-2.38513800	-4.34959000	C	-4.52765200	-0.92040700	-1.67586600
H	0.48952200	-4.52216200	-4.70875000	O	-3.76517900	-0.49996200	-0.78714700
H	0.66632800	-6.66629400	-2.66673300	C	-4.01650900	-3.34780000	-1.29241400
H	1.99693300	-3.24462800	-5.90699900	O	-3.71498100	-4.56235700	-1.94029900
H	6.86803700	-2.24521600	-4.64705600	N	-5.63424100	-0.21501200	-2.01725500
H	5.65550500	-0.99337900	-4.33296300	C	-6.62782000	-0.47601600	-3.09228400
H	6.54241200	-5.96131600	4.26677400	C	-6.13655800	0.00794800	-4.46265200
H	4.95842700	-6.55671300	3.75371800	C	-7.85144100	0.30198700	-2.57242400
C	-4.84236500	-4.15879500	6.89062700	C	-7.23403200	1.55098100	-1.92149300
C	-3.32332100	-4.21143100	6.64490700	C	-5.94020400	1.02224700	-1.27903600
C	-2.91076100	-3.67662700	5.28829400	H	-5.10260100	1.72554100	-1.34060200
C	-2.53735100	-2.33932400	5.11475800	H	-6.07715800	0.78261300	-0.21663800
C	-2.91074600	-4.50066600	4.15125200	H	-7.00378400	2.30194200	-2.68483000
C	-2.17980300	-1.83372300	3.86228600	H	-7.89608100	2.02136500	-1.18804300
C	-2.55913900	-4.01900500	2.89361500	H	-8.56036900	0.53728500	-3.37130100
C	-2.19017800	-2.67565700	2.74259800	H	-8.37883600	-0.29446700	-1.81809700

H -6.84131200 -1.54652900 -3.14128100
H -5.86094300 1.06896500 -4.43430900
H -5.28347800 -0.58226700 -4.80134200
H -6.93619400 -0.11546300 -5.20302900
H -5.04366000 -2.56806100 -3.02868300
H -3.11590000 -5.07913900 -1.36551200

H -4.94144300 -3.42359500 -0.69211000
H -3.21575800 -3.02317000 -0.61656400
H -2.14885600 -2.39745500 -2.75874400
H -1.56449700 -1.52715000 -5.82226700
H -0.91844700 -2.56817300 -4.52821700
H -1.77820500 -3.27030300 -5.94301600

SkDHPase.HYD-ES-II

C -2.73099200 -0.10103300 -4.80017600
C -3.72409400 -0.13985100 -5.90461100
N -4.04598700 0.93726400 -6.71780600
C -4.47850000 -1.17270900 -6.38041800
C -4.95718300 0.52625300 -7.63580400
N -5.23258500 -0.75561900 -7.46062600
C -9.56332300 -3.95540400 -4.12769400
C -9.07161400 -3.30567200 -5.38367300
N -9.82246500 -2.36665200 -6.07811000
C -7.91776900 -3.42985500 -6.11699000
C -9.12698900 -1.96522600 -7.16770700
N -7.96480800 -2.59481100 -7.22142700
C -6.95819100 2.60919700 -10.69330100
N -7.30193100 1.57106000 -9.74360400
C -7.29667200 0.25253100 -10.14850700
O -6.82306800 0.07371900 -11.32408400
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C -5.99742500 1.45357600 -14.50229100
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Zn -6.39652400 -2.14947100 -8.48693200
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H -8.75847200 -4.53730300 -3.67143200
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H -7.19517000 -2.25270500 -16.96405300
H -6.73933900 -3.13169100 -14.63411700
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H -0.06752500 -3.02471200 -11.21519100
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H -1.06420200 -1.40597600 -13.43216200
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H -2.44858200 -3.28203300 -7.05617300
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H -2.67545800 -1.08364300 -4.32507000
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H -0.01617200 -1.40774700 -10.49386600
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C -15.72461000 -5.23247600 -8.59993100
C -14.28162800 -5.20647700 -8.07993500
C -13.26141500 -4.66223000 -9.10123300
C -11.98337100 -4.18772100 -8.39835000
C -12.93261400 -5.69074200 -10.19673100
C -8.21561700 -7.89748400 -4.42193200
C -8.72403500 -7.37559500 -5.76272000
S -10.56179500 -7.56901300 -5.89686200
C -9.94099500 -9.39236900 -11.07404800
C -9.07328600 -9.15093200 -9.84084500
O -9.24580800 -8.15044700 -9.12736600
C -9.70946800 -8.28304000 -12.12280200
C -10.69342000 -8.29606400 -13.28550800
O -10.33616500 -8.42688900 -14.45869500
N -12.00558100 -8.15067600 -12.96200300
N -8.12458700 -10.07215500 -9.57983500
C -7.14862200 -9.92147100 -8.50393000
H -14.24900600 -4.57871500 -7.17874900

H	-13.97483000	-6.21168900	-7.75747800	N	-6.85954900	-5.07648000	-11.80439100
H	-13.71722500	-3.78837600	-9.59141300	C	-7.13032000	-6.11050400	-10.88146000
H	-12.21380400	-3.39962400	-7.67089500	O	-6.61507300	-7.21943500	-10.90951100
H	-11.25985600	-3.77722500	-9.11297700	N	-8.08059300	-5.63994800	-10.03060100
H	-11.49860400	-5.00770800	-7.85289100	C	-8.58913800	-4.34946300	-10.46357700
H	-12.30205700	-5.24936800	-10.97904100	C	-7.66176400	-4.01419500	-11.61757900
H	-12.39297000	-6.54706000	-9.76703900	O	-7.72894400	-3.01942600	-12.36629500
H	-13.84228300	-6.06618000	-10.68014900	H	-8.54096300	-3.57799300	-9.69351200
H	-15.83184800	-5.86823400	-9.48675300	H	-9.61559600	-4.41127100	-10.84809200
H	-8.47177300	-6.31925900	-5.89134100	H	-6.21331200	-5.15267900	-12.60757300
H	-8.28333100	-7.92474200	-6.59602000	H	-8.60123900	-6.32110900	-9.47896000
H	-10.58331500	-7.73813900	-7.23596900	O	-5.98187900	-2.64987800	-10.32455700
H	-8.68597200	-7.37583200	-3.58021200	H	-5.27776800	-3.33287400	-10.20930200
H	-8.70858300	-8.37017700	-12.55019000	C	-4.79935200	-9.57942100	-11.88501100
H	-9.78365400	-7.30826400	-11.62724300	C	-4.65778900	-9.05013300	-13.29664900
H	-12.29607900	-7.85487800	-12.04082000	O	-4.03366100	-9.63396500	-14.17748500
H	-12.66777300	-8.04300200	-13.71887100	N	-5.28235200	-7.84746700	-13.48157500
H	-9.75235900	-10.37513400	-11.52042800	C	-5.53302400	-7.31959800	-14.80804300
H	-7.63216100	-9.99817400	-7.52504300	C	-4.93237000	-5.91239500	-14.89648600
H	-6.65317200	-8.95080400	-8.59041700	O	-5.44789000	-4.98055400	-14.23445200
H	-8.02946000	-10.85639200	-10.20863400	C	-7.04228600	-7.27516900	-15.12346000
H	-10.98174300	-9.38753200	-10.73145500	O	-7.55972200	-8.56603000	-14.90094300
H	-6.40629900	-10.71609900	-8.59595400	N	-3.86524800	-5.67330900	-15.67760700
H	-8.42397100	-8.96591300	-4.30780700	C	-3.03572600	-6.64195900	-16.44698200
H	-7.13210000	-7.74608800	-4.34494300	C	-2.03261400	-7.37469300	-15.54554100
H	-16.06083900	-4.22485900	-8.87261600	C	-2.37116700	-5.71722400	-17.48356000
H	-16.41173300	-5.61786800	-7.83863900	C	-2.11166300	-4.41912900	-16.70054800
C	-12.65108400	-2.36154900	-18.57849600	C	-3.33369300	-4.29896000	-15.77414700
C	-13.44761900	-2.81482800	-17.34402200	H	-3.09410900	-3.91453000	-14.77811100
C	-12.51245200	-3.35631800	-16.29005700	H	-4.10985400	-3.64689700	-16.19251200
C	-11.83662800	-2.48673300	-15.42626100	H	-1.19214700	-4.50856900	-16.11237300
C	-12.18956300	-4.71864300	-16.23876300	H	-2.00168900	-3.54635000	-17.35090000
C	-10.84751800	-2.95044700	-14.56229300	H	-1.46175900	-6.15682400	-17.90212300
C	-11.20128900	-5.20432900	-15.38511100	H	-3.06498700	-5.52757200	-18.31137800
C	-10.51776400	-4.30955400	-14.55920100	H	-3.68620000	-7.37022800	-16.93754400
O	-9.51644800	-4.79630200	-13.75427500	H	-1.42082200	-6.66793700	-14.97391700
H	-14.17593600	-3.58074200	-17.63725000	H	-2.54389800	-8.05028800	-14.85634400
H	-14.02227900	-1.96794900	-16.94776800	H	-1.36307600	-7.98322000	-16.16439200
H	-12.07675900	-1.42538000	-15.43884300	H	-5.05257500	-8.01458100	-15.49679400
H	-12.70359900	-5.41235900	-16.90112700	H	-8.53953300	-8.51518400	-14.87805300
H	-10.32689700	-2.26594200	-13.89541500	H	-7.16524100	-6.95244600	-16.17310800
H	-10.93360800	-6.25662900	-15.36948900	H	-7.53314000	-6.51862700	-14.49566300
H	-8.98231500	-4.03695500	-13.45564200	H	-5.85635700	-7.52671400	-12.70536700
H	-11.93497700	-1.57572200	-18.31209000	H	-4.54697200	-8.81487700	-11.14535500
H	-12.08527400	-3.19774800	-19.00443700	H	-5.83831400	-9.87370100	-11.70100500
H	-13.31206500	-1.96637600	-19.35915400	H	-4.14951000	-10.44825400	-11.76571000

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C	-2.73099200	-0.10103200	-4.80017500	C	-4.49522400	-1.13795800	-6.38964400
C	-3.59536300	-0.18451200	-6.00902500	C	-4.48062800	0.31900100	-7.99128200
N	-3.60243700	0.73976000	-7.04569500	N	-5.03431300	-0.82302300	-7.62296700

C	-9.56332400	-3.95540600	-4.12769400	H	-9.87548300	-3.24668600	-3.35118700
C	-9.04475900	-3.25410800	-5.34024400	H	-4.94297000	1.50439500	-14.20280900
N	-9.75256600	-2.24858600	-5.98408700	H	-6.15188200	2.17125300	-15.31254700
C	-7.89648600	-3.39242800	-6.07691800	H	-7.10673600	3.57786000	-10.20710400
C	-9.03949500	-1.82500000	-7.05302400	H	-7.55542800	2.59015500	-11.61477200
N	-7.90607400	-2.50254300	-7.13711400	H	-2.92469300	-0.96180700	-4.15551100
C	-6.95819200	2.60919200	-10.69330100	H	-3.17517300	-4.61007400	-6.22106700
N	-7.32927700	1.55958200	-9.76835100	H	-0.19363100	-1.36333200	-10.29628400
C	-7.10804000	0.24479900	-10.07370400	H	-8.02284700	1.74173300	-9.05821000
O	-6.36106600	0.05597700	-11.10012200	C	-15.72463400	-5.23247500	-8.59994100
O	-7.59968100	-0.64219200	-9.31677800	C	-14.28160300	-5.20647800	-8.07992100
C	-5.99742600	1.45356800	-14.50229100	C	-13.30999700	-4.39507500	-8.95956300
C	-6.38664700	0.07603200	-14.95156100	C	-12.00290500	-4.11253200	-8.20732300
N	-6.37501100	-1.06248300	-14.14095400	C	-13.02649400	-5.09050400	-10.30010800
C	-6.80643400	-0.28433700	-16.20560200	C	-8.21562000	-7.89747100	-4.42193300
C	-6.77238500	-2.07109900	-14.90820700	C	-8.68667800	-7.39053200	-5.78261500
N	-7.03972400	-1.64372900	-16.15973300	S	-10.51068800	-7.63790600	-5.99117000
C	-0.67059200	-2.26302900	-10.70606900	C	-9.43289500	-9.12096100	-11.43967600
C	-1.88722800	-1.94308700	-11.50309200	C	-8.87632200	-9.04645300	-10.01944900
N	-1.91619500	-1.21445500	-12.68499300	O	-9.20534300	-8.16242000	-9.21296900
C	-3.19163100	-2.25946600	-11.25563700	C	-10.74696200	-8.35948800	-11.58696900
C	-3.20574000	-1.11702900	-13.09580900	C	-11.01484600	-7.86120900	-13.00400400
N	-4.00441300	-1.74029300	-12.24362700	O	-10.22059800	-7.98503500	-13.93623400
C	-2.92951200	-4.25382200	-7.22607000	N	-12.22160400	-7.25841400	-13.17619100
C	-4.18485200	-4.11933700	-8.08609800	N	-7.97254200	-9.99854600	-9.70405100
O	-5.23077600	-3.64642600	-7.51441500	C	-7.14861700	-9.92148000	-8.50393500
O	-4.10352100	-4.41164000	-9.30280600	H	-14.28219900	-4.77640400	-7.06889900
Zn	-6.38058800	-2.16941800	-8.47043700	H	-13.90035700	-6.23193300	-7.97073300
Zn	-6.03757800	-1.60851600	-12.04761700	H	-13.78756000	-3.42759400	-9.17964300
H	-1.66373200	-0.10981500	-5.05512000	H	-12.19955800	-3.54623700	-7.28845500
H	-2.92300900	0.80494100	-4.21157200	H	-11.30544300	-3.52734400	-8.81978400
H	-4.76439200	-2.05381500	-5.89114600	H	-11.50158500	-5.04308500	-7.91198000
H	-3.04971700	1.58460800	-7.09254900	H	-12.36300700	-4.48822300	-10.93257900
H	-4.68128400	0.85141500	-8.90847900	H	-12.53942700	-6.05981600	-10.12503300
H	-8.78115700	-4.58971600	-3.70308500	H	-13.94874100	-5.26772500	-10.86590900
H	-10.41796700	-4.59935100	-4.36885300	H	-15.80196500	-5.71146400	-9.58267500
H	-7.05907400	-4.05754300	-5.93337400	H	-8.46023500	-6.32704300	-5.90256500
H	-10.66524300	-1.90737400	-5.71566100	H	-8.19542000	-7.92497200	-6.59719600
H	-9.34269300	-1.04526200	-7.73369700	H	-10.46720000	-7.85963100	-7.32226700
H	-6.58956400	1.77000600	-13.63795200	H	-8.73586100	-7.39127700	-3.60024000
H	-6.95951000	0.29813700	-17.10100000	H	-10.72257900	-7.49017100	-10.91843700
H	-7.40496100	-2.21850700	-16.90626700	H	-11.59786900	-8.96792500	-11.25576100
H	-6.85651600	-3.10288600	-14.60321200	H	-12.79738100	-7.01463500	-12.38274600
H	-0.95602500	-2.90692900	-9.87082000	H	-12.37222100	-6.74351600	-14.03482000
H	0.08503900	-2.79793800	-11.29484700	H	-8.67806500	-8.68484200	-12.10515100
H	-3.56873900	-2.86905900	-10.45027100	H	-7.76861400	-10.01106600	-7.60734500
H	-1.11680300	-0.82926900	-13.16923000	H	-6.60520900	-8.97156200	-8.47174600
H	-3.51694800	-0.60645200	-13.99437000	H	-7.68570200	-10.63396500	-10.43540100
H	-5.90631100	2.51384000	-10.97012000	H	-9.54529700	-10.16613200	-11.74999000
H	-2.20812600	-4.92644900	-7.69489200	H	-6.43403500	-10.74660900	-8.51914000
H	-2.47331900	-3.26148700	-7.11898400	H	-8.39648000	-8.97160100	-4.31612900

H	-7.14091900	-7.71399200	-4.30132200	H	-5.42505200	-3.61201600	-10.10054800
H	-16.12726400	-4.21643900	-8.69357900	C	-4.81184500	-9.56723600	-11.86295200
H	-16.37810400	-5.78631500	-7.91699200	C	-4.65051300	-8.99879800	-13.25844700
C	-12.65108500	-2.36154900	-18.57849700	O	-4.03365800	-9.58158200	-14.14638100
C	-13.33857500	-2.76522000	-17.26452400	N	-5.25956400	-7.78808100	-13.42350100
C	-12.31976000	-3.23282200	-16.25305500	C	-5.52558000	-7.24835200	-14.74277500
C	-11.71573800	-2.33443200	-15.36738000	C	-4.91383200	-5.84513100	-14.83412600
C	-11.85937200	-4.55785300	-16.25965700	O	-5.41868000	-4.90571400	-14.17640400
C	-10.67304200	-2.72879100	-14.52852000	C	-7.04208600	-7.18642500	-15.01961000
C	-10.81819900	-4.97300700	-15.43382400	O	-7.57377500	-8.47729900	-14.82445200
C	-10.21377600	-4.04982600	-14.57061500	N	-3.84252500	-5.61822600	-15.61525000
O	-9.18111500	-4.48765300	-13.79567200	C	-3.03848800	-6.59222600	-16.40376100
H	-14.06889600	-3.55950200	-17.46439600	C	-2.04509800	-7.36252300	-15.52347900
H	-13.90292600	-1.91179900	-16.86829000	C	-2.36054000	-5.66641500	-17.43134800
H	-12.05837600	-1.30190300	-15.33746700	C	-2.07486900	-4.38320000	-16.63322400
H	-12.31122200	-5.27432400	-16.94348800	C	-3.29507700	-4.25009400	-15.70713900
H	-10.21453000	-2.01919300	-13.84297500	H	-3.05189200	-3.87158700	-14.70970700
H	-10.45796000	-5.99749700	-15.44160900	H	-4.06280500	-3.58695700	-16.12409300
H	-8.75949800	-3.73189400	-13.33241200	H	-1.15824900	-4.49815500	-16.04483100
H	-11.93790800	-1.54635600	-18.40996800	H	-1.94631200	-3.50482500	-17.27266700
H	-12.09749500	-3.20581000	-19.00462000	H	-1.46087700	-6.11750200	-17.85887500
H	-13.38052000	-2.02440000	-19.32451700	H	-3.05361100	-5.45329100	-18.25421100
N	-6.83850000	-4.96746400	-11.72845600	H	-3.70790500	-7.29834700	-16.90150800
C	-7.16334400	-6.02998100	-10.88718100	H	-1.40999200	-6.67825200	-14.94961200
O	-6.74553100	-7.17828000	-11.00393800	H	-2.56477000	-8.03600700	-14.83879700
N	-8.04207000	-5.55786300	-9.95435200	H	-1.39690600	-7.97748800	-16.15873300
C	-8.50828900	-4.22876500	-10.31918900	H	-5.06595800	-7.94111500	-15.44813000
C	-7.47876200	-3.81124700	-11.36782300	H	-8.51058700	-8.38237300	-14.56809400
O	-7.65154600	-2.84949600	-12.20106000	H	-7.18894100	-6.83374400	-16.05684100
H	-8.55891700	-3.53714600	-9.48028700	H	-7.51077200	-6.44578900	-14.36035700
H	-9.48773900	-4.25925600	-10.81896800	H	-5.84497200	-7.47699500	-12.64882500
H	-6.23731900	-5.04317000	-12.56263400	H	-3.95587000	-10.20757400	-11.63756000
H	-8.60482800	-6.25178200	-9.46478500	H	-4.92344600	-8.79240600	-11.10270800
O	-6.11594300	-2.91894800	-10.29156100	H	-5.71354000	-10.19163900	-11.84787200

SkDHPase.HYD-INT1-II

C	-2.73099200	-0.10103300	-4.80017600	O	-6.18394700	0.04321100	-11.06150600
C	-3.55496200	-0.19998600	-6.03525000	O	-7.51320600	-0.68457200	-9.35802100
N	-3.46160000	0.65261000	-7.12799600	C	-5.99742500	1.45357600	-14.50229100
C	-4.50459200	-1.11341800	-6.39000600	C	-6.42910300	0.11329000	-15.01118200
C	-4.33281400	0.23155600	-8.07961900	N	-6.39029000	-1.04258500	-14.23558400
N	-4.97649400	-0.84428100	-7.66098500	C	-6.91064900	-0.21529300	-16.25092300
C	-9.56332500	-3.95540700	-4.12769100	C	-6.83402000	-2.03757600	-14.99803400
C	-9.04396900	-3.23312000	-5.32374200	N	-7.15220800	-1.57559400	-16.22280600
N	-9.76824800	-2.25300600	-5.98717800	C	-0.67058900	-2.26303000	-10.70606800
C	-7.87411500	-3.33618300	-6.02893900	C	-1.88264900	-1.94484400	-11.51551900
C	-9.04453800	-1.80963400	-7.03984900	N	-1.87083400	-1.33130000	-12.76099100
N	-7.88774000	-2.45005100	-7.09104800	C	-3.20539300	-2.16109000	-11.24745500
C	-6.95819100	2.60919700	-10.69330200	C	-3.15048100	-1.20414800	-13.19038900
N	-7.33261900	1.51562400	-9.82140600	N	-3.98527000	-1.69677100	-12.28833500
C	-7.01472100	0.21780100	-10.09822000	C	-2.92952000	-4.25382000	-7.22607700

C	-4.18328300	-4.10266500	-8.07294100	N	-7.90558700	-9.95280100	-9.75031300
O	-5.22684200	-3.63110100	-7.50201100	C	-7.14861800	-9.92147700	-8.50393300
O	-4.10411400	-4.38167400	-9.29695700	H	-14.27472300	-4.72367500	-7.09277600
Zn	-6.38900300	-2.15337000	-8.42893400	H	-13.91935300	-6.23159800	-7.91702300
Zn	-6.01243200	-1.50504500	-12.25229200	H	-13.76213500	-3.50117600	-9.27949400
H	-1.65909800	-0.20459000	-5.01058200	H	-12.17981600	-3.52295900	-7.38462000
H	-2.87486700	0.85309100	-4.27782700	H	-11.28056000	-3.61490100	-8.91176300
H	-4.85127800	-1.97238400	-5.84080800	H	-11.49972400	-5.06631700	-7.91080600
H	-2.85024300	1.45378000	-7.20581700	H	-12.35281100	-4.67594500	-10.96681000
H	-4.46200500	0.70840200	-9.03968500	H	-12.53530000	-6.19497500	-10.06956600
H	-8.77092700	-4.56984600	-3.69306900	H	-13.94226500	-5.44150000	-10.85397200
H	-10.39363100	-4.62245100	-4.39005500	H	-15.80856300	-5.75712500	-9.55845600
H	-7.02494400	-3.98159000	-5.86666900	H	-8.41420300	-6.32385300	-5.90625800
H	-10.70215200	-1.94898700	-5.74807300	H	-8.19133700	-7.92860600	-6.59824900
H	-9.36279800	-1.05057800	-7.73698000	H	-10.45253000	-7.82722000	-7.32677500
H	-6.54870000	1.72775100	-13.59733000	H	-8.72533400	-7.37721300	-3.60232200
H	-7.10026400	0.38569100	-17.12670400	H	-9.92033800	-7.01502500	-11.61809500
H	-7.57248200	-2.12718800	-16.95830400	H	-11.21468000	-8.01070500	-10.96927800
H	-6.91455300	-3.07373500	-14.70027500	H	-12.89781100	-7.54166100	-12.39589200
H	-0.97309000	-2.82427300	-9.81877900	H	-12.76547100	-7.68825600	-14.11953700
H	0.04466200	-2.88205200	-11.26118700	H	-8.59638000	-9.03958500	-12.18927000
H	-3.62322800	-2.67730100	-10.39962600	H	-7.82454100	-10.02377900	-7.65087800
H	-1.04950600	-1.04403700	-13.27568900	H	-6.58957200	-8.98386300	-8.40555000
H	-3.42993400	-0.76838500	-14.13780200	H	-7.51418300	-10.47648000	-10.52100900
H	-5.90907400	2.51401900	-10.97835500	H	-9.89100500	-10.08401200	-11.60165500
H	-2.21173300	-4.91982700	-7.70897000	H	-6.44982000	-10.76041400	-8.50035600
H	-2.47216300	-3.26386500	-7.10319000	H	-8.42451500	-8.96640400	-4.31529700
H	-9.91112800	-3.26235600	-3.35213400	H	-7.13677600	-7.74197800	-4.29775200
H	-4.93061300	1.46643100	-14.24586900	H	-16.10888800	-4.21523300	-8.74425700
H	-6.16970900	2.22369200	-15.25918400	H	-16.38901400	-5.74069800	-7.89231600
H	-7.09440200	3.55331300	-10.15824600	C	-12.65108400	-2.36154900	-18.57849600
H	-7.56186100	2.64374400	-11.61067600	C	-13.13235100	-2.40885100	-17.11766500
H	-3.01231200	-0.90115500	-4.11125000	C	-12.07129700	-2.90114100	-16.15518100
H	-3.17268600	-4.62565900	-6.22635200	C	-11.35956200	-2.02149500	-15.33270300
H	-0.14242100	-1.35911500	-10.37681200	C	-11.74685800	-4.26533700	-16.07713500
H	-8.05134400	1.65693800	-9.12715300	C	-10.36015700	-2.47258200	-14.46554400
C	-15.72461300	-5.23247400	-8.59993300	C	-10.75395600	-4.73663500	-15.22441000
C	-14.28162700	-5.20647900	-8.07993100	C	-10.05039100	-3.83754600	-14.40906700
C	-13.29693900	-4.46035400	-9.00300900	O	-9.08659600	-4.34846200	-13.59296900
C	-11.98771600	-4.14953300	-8.26520100	H	-14.01606100	-3.05811200	-17.05683000
C	-13.01900900	-5.23598400	-10.29984100	H	-13.46603400	-1.40850400	-16.81450400
C	-8.21561900	-7.89747300	-4.42193400	H	-11.59349900	-0.95871600	-15.35987800
C	-8.66953500	-7.38084100	-5.78488200	H	-12.28544000	-4.97621600	-16.70148300
S	-10.49837800	-7.58069200	-6.00001000	H	-9.83340800	-1.77342500	-13.81992200
C	-9.41487400	-9.10360200	-11.46500800	H	-10.51245300	-5.79447400	-15.17045700
C	-8.84955800	-9.02823700	-10.04515500	H	-8.58490200	-3.63986900	-13.11618700
O	-9.25262700	-8.21130900	-9.20470100	H	-11.79486100	-1.68529900	-18.68703600
C	-10.42377800	-7.98287900	-11.72419800	H	-12.33636600	-3.35327000	-18.92273900
C	-11.01002700	-8.00840600	-13.12743400	H	-13.44722200	-2.01017700	-19.24485400
O	-10.33625600	-8.18628600	-14.14460400	N	-6.63796300	-4.95770000	-11.59237600
N	-12.34879600	-7.79293600	-13.20424500	C	-7.18917900	-6.03274000	-10.94705300

O	-6.95616800	-7.22288700	-11.18209500	C	-2.04510100	-7.36252100	-15.52347900
N	-8.04817200	-5.56025400	-9.98346100	C	-2.41084000	-5.75120600	-17.49462500
C	-8.38355000	-4.17051500	-10.26354800	C	-2.14505000	-4.43422700	-16.74636200
C	-7.16484600	-3.70608100	-11.10728100	C	-3.35787500	-4.29475300	-15.81067300
O	-7.42755900	-2.79854200	-12.06950300	H	-3.10748000	-3.88281100	-14.82773000
H	-8.50515400	-3.57417500	-9.35958800	H	-4.13993300	-3.65397500	-16.23647100
H	-9.28891300	-4.07899300	-10.87710000	H	-1.21923900	-4.50860800	-16.16589800
H	-6.17666600	-5.02659900	-12.50409700	H	-2.04290300	-3.57672600	-17.41832700
H	-8.69440800	-6.23453300	-9.58024800	H	-1.50558500	-6.19900700	-17.91388300
O	-6.12915200	-3.11763900	-10.21843900	H	-3.11541200	-5.58236500	-18.31796900
H	-5.40859000	-3.80818300	-9.98539900	H	-3.71495500	-7.39322200	-16.89184500
C	-4.81183800	-9.56725100	-11.86294900	H	-1.42906900	-6.64245500	-14.97268200
C	-4.66637000	-8.99320100	-13.26148100	H	-2.54889000	-8.02600500	-14.81730800
O	-4.01243700	-9.56097400	-14.13448300	H	-1.38027500	-7.98115400	-16.13778700
N	-5.31258800	-7.80688600	-13.44361200	H	-5.11328600	-7.98214800	-15.47026500
C	-5.57069100	-7.28101100	-14.77140400	H	-8.56691800	-8.42241200	-14.63242000
C	-4.96349000	-5.87567200	-14.89242800	H	-7.23919700	-6.86226000	-16.07774400
O	-5.47926700	-4.91960800	-14.27297600	H	-7.54908800	-6.47866400	-14.37648100
C	-7.08813100	-7.21943700	-15.04246100	H	-5.93808100	-7.51370100	-12.68983100
O	-7.61742800	-8.51104400	-14.85034700	H	-3.82527600	-9.86894700	-11.49808800
N	-3.88394600	-5.66589300	-15.67368600	H	-5.27840600	-8.87587600	-11.16022100
C	-3.06133800	-6.65109700	-16.42706000	H	-5.41558500	-10.48055300	-11.93578600

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C	-2.73099400	-0.10103300	-4.80017700	C	-3.19846400	-1.50827300	-13.24935000
C	-3.56376600	-0.20852600	-6.03167900	N	-4.01151800	-1.64273700	-12.21528400
N	-3.43539900	0.60663700	-7.14962000	C	-2.92952100	-4.25382000	-7.22607700
C	-4.54987200	-1.09363800	-6.36294500	C	-4.19821000	-4.05916700	-8.02612900
C	-4.31964700	0.19300200	-8.09167800	O	-5.23202500	-3.63244600	-7.45209100
N	-5.00622700	-0.84552800	-7.64491000	O	-4.11067100	-4.26840900	-9.28993500
C	-9.56332700	-3.95540900	-4.12768800	Zn	-6.45758900	-2.09055200	-8.45449900
C	-9.04567300	-3.21403000	-5.30840100	Zn	-6.04436800	-1.47997700	-12.13732200
N	-9.76909500	-2.22269200	-5.95351500	H	-1.66547400	-0.25656600	-5.01028800
C	-7.87888200	-3.31182500	-6.01762500	H	-2.83363400	0.87645300	-4.31284300
C	-9.04865700	-1.76726400	-7.00220400	H	-4.93746600	-1.91519500	-5.78442200
N	-7.89389200	-2.41162000	-7.06675700	H	-2.79581900	1.38332300	-7.24773100
C	-6.95819000	2.60919700	-10.69330100	H	-4.43075800	0.64371300	-9.06699600
N	-7.42405200	1.55839700	-9.81979900	H	-8.76800800	-4.56835900	-3.69606300
C	-7.08176300	0.25754500	-10.02059400	H	-10.38524000	-4.62764100	-4.40348500
O	-6.17651600	0.04832400	-10.90763600	H	-7.03423900	-3.96483700	-5.86457400
O	-7.63134400	-0.61984400	-9.28648900	H	-10.70155000	-1.92018100	-5.70714900
C	-5.99742500	1.45357600	-14.50229200	H	-9.36537100	-0.99825100	-7.68842900
C	-6.43581900	0.09792000	-14.96136000	H	-6.61325000	1.81026900	-13.66999800
N	-6.42125800	-1.02960600	-14.14296600	H	-7.07984300	0.30397200	-17.09246400
C	-6.90783600	-0.26836900	-16.19411400	H	-7.59194400	-2.19533900	-16.83809700
C	-6.86986300	-2.04418800	-14.87627300	H	-6.96891400	-3.06656800	-14.54242400
N	-7.16740000	-1.62360900	-16.12076500	H	-0.95543600	-2.51669800	-9.68226200
C	-0.67059000	-2.26303000	-10.70606800	H	-0.12330700	-3.12023100	-11.11639500
C	-1.89812200	-1.96098500	-11.49760600	H	-3.63000900	-2.11913800	-10.15635100
N	-1.91269800	-1.68982700	-12.85904100	H	-1.10546900	-1.65364300	-13.46649600
C	-3.21223300	-1.91663300	-11.12524800	H	-3.49888200	-1.29279800	-14.26325700

H	-5.88543300	2.50591200	-10.86481200	H	-9.90878600	-9.93304000	-11.60826800
H	-2.22448200	-4.90131700	-7.75080500	H	-6.46583200	-10.77354900	-8.51425400
H	-2.46711700	-3.27011500	-7.07657000	H	-8.45777100	-8.95878500	-4.30991300
H	-9.92256800	-3.27699800	-3.34432100	H	-7.13077700	-7.77701300	-4.31172700
H	-4.95725900	1.44494800	-14.15458600	H	-16.13718300	-4.21813700	-8.66424400
H	-6.07554900	2.17664000	-15.31889900	H	-16.37294300	-5.81260600	-7.93392000
H	-7.14768500	3.57684700	-10.21977800	C	-12.65108400	-2.36154900	-18.57849600
H	-7.46286600	2.60120200	-11.66891000	C	-12.98653300	-2.17727300	-17.07110900
H	-3.04302900	-0.86334400	-4.08219400	C	-11.94682300	-2.73112400	-16.11526000
H	-3.15552200	-4.66325400	-6.23800100	C	-11.27969700	-1.91060800	-15.19989400
H	0.02180300	-1.41253200	-10.66730200	C	-11.62500300	-4.09932200	-16.10738300
H	-8.18672300	1.73161300	-9.18229500	C	-10.32917200	-2.41945900	-14.30913000
C	-15.72468000	-5.23247300	-8.59994800	C	-10.67936500	-4.62687300	-15.23374700
C	-14.28154600	-5.20648100	-8.07991900	C	-10.02063500	-3.78569900	-14.32281600
C	-13.32036000	-4.36847300	-8.94757800	O	-9.10029400	-4.34832300	-13.49114300
C	-12.02523800	-4.05711800	-8.18525900	H	-13.95328000	-2.65337500	-16.86028200
C	-13.00873800	-5.05053900	-10.28874600	H	-13.13134500	-1.11323100	-16.85204100
C	-8.21562200	-7.89747300	-4.42193400	H	-11.50912500	-0.84691400	-15.17251400
C	-8.66942400	-7.36958400	-5.78070400	H	-12.12560600	-4.76855600	-16.80486900
S	-10.50602100	-7.51054600	-5.97260500	H	-9.83458800	-1.76400100	-13.59623000
C	-9.38494100	-8.98038400	-11.45118300	H	-10.44055000	-5.68675400	-15.23656300
C	-8.82623900	-8.96373900	-10.02667500	H	-8.58440000	-3.66415000	-12.98645200
O	-9.22386900	-8.17136900	-9.16005300	H	-11.68730300	-2.86299000	-18.71342300
C	-10.33729000	-7.80666500	-11.69172800	H	-13.40707400	-2.96224400	-19.09408500
C	-10.95823600	-7.79993600	-13.08006000	H	-12.59447100	-1.39852800	-19.09694000
O	-10.32987700	-8.05408800	-14.11020100	N	-6.54479000	-4.92259200	-11.48670300
N	-12.27434500	-7.46814500	-13.12860400	C	-7.05359000	-6.00528600	-10.83058800
N	-7.89846000	-9.91154300	-9.75529000	O	-6.79675300	-7.19373600	-11.06084600
C	-7.14862000	-9.92147600	-8.50393700	N	-7.91410200	-5.55379500	-9.85316600
H	-14.28467300	-4.79681000	-7.06038700	C	-8.30540800	-4.18287500	-10.15663600
H	-13.89159600	-6.23067400	-7.99247600	C	-7.10149400	-3.67130800	-10.99967000
H	-13.81881300	-3.41136000	-9.16701400	O	-7.43248100	-2.80778700	-11.99813700
H	-12.24241400	-3.48987700	-7.27085200	H	-8.46510300	-3.58353800	-9.26059400
H	-11.33347300	-3.46376500	-8.79639500	H	-9.21138800	-4.14022200	-10.77515100
H	-11.50795800	-4.97591900	-7.88144800	H	-6.07626400	-4.98488800	-12.39280400
H	-12.36307400	-4.42559500	-10.91687400	H	-8.56075000	-6.24537700	-9.47961300
H	-12.48725300	-6.00139200	-10.11307500	O	-6.10041400	-3.02796000	-10.17127400
H	-13.92238900	-5.25846000	-10.85811100	H	-5.14098200	-3.77569900	-9.81860500
H	-15.79666700	-5.68289200	-9.59652600	C	-4.81770800	-9.58761800	-11.88278000
H	-8.38155600	-6.32164500	-5.90838300	C	-4.67283700	-8.98939500	-13.26992800
H	-8.22023100	-7.93449700	-6.59871400	O	-4.05321800	-9.56037700	-14.16576400
H	-10.48525600	-7.74752900	-7.30147300	N	-5.28324000	-7.77956700	-13.41777600
H	-8.69724600	-7.35905900	-3.59702600	C	-5.56043900	-7.23475300	-14.73377400
H	-9.78308800	-6.86495800	-11.60148300	C	-4.92168500	-5.84541200	-14.86284300
H	-11.11042400	-7.79179200	-10.91832400	O	-5.38852700	-4.88013900	-14.22208800
H	-12.77266600	-7.14270200	-12.31354300	C	-7.08078400	-7.13908000	-14.97069600
H	-12.69376500	-7.31795600	-14.03635100	O	-7.62619100	-8.42525300	-14.78761700
H	-8.56165400	-8.94598400	-12.17221700	N	-3.86510600	-5.66269900	-15.68467400
H	-7.83217800	-10.02905200	-7.65788800	C	-3.07428100	-6.67174200	-16.43944600
H	-6.57336600	-8.99623700	-8.38355200	C	-2.05097000	-7.38289000	-15.54331400
H	-7.49703500	-10.40282600	-10.54208200	C	-2.43369800	-5.79911900	-17.53475800

C	-2.12811400	-4.47599900	-16.81266500	H	-2.55221100	-8.02992800	-14.82039400
C	-3.30902300	-4.30715300	-15.84046300	H	-1.40401900	-8.01903500	-16.15877700
H	-3.01536500	-3.90339800	-14.86597700	H	-5.13747100	-7.94190900	-15.44802900
H	-4.08811300	-3.64566300	-16.23971300	H	-8.57817800	-8.32672200	-14.58184400
H	-1.18517500	-4.55599200	-16.26094500	H	-7.24685700	-6.76298900	-15.99711400
H	-2.03512800	-3.62920700	-17.49940600	H	-7.51515400	-6.40123400	-14.28372300
H	-1.54589000	-6.26781400	-17.96821600	H	-5.87373500	-7.47428900	-12.64031800
H	-3.15442500	-5.63040900	-18.34390300	H	-5.21794400	-8.88552800	-11.15083600
H	-3.74715000	-7.41200500	-16.87863300	H	-5.48540700	-10.45509000	-11.96138300
H	-1.41689900	-6.66317900	-15.01266700	H	-3.84513300	-9.96704400	-11.55496200

SkDHPase.HYD-INT2-II

C	-2.73099300	-0.10103300	-4.80017600	H	-4.45394300	0.58517600	-9.06832000
C	-3.57015200	-0.23823900	-6.02816100	H	-8.77023500	-4.57774300	-3.70547400
N	-3.45159900	0.56831900	-7.15350100	H	-10.39320600	-4.61942100	-4.40033500
C	-4.55189600	-1.13393800	-6.35155400	H	-7.05163200	-3.97991600	-5.87632900
C	-4.33470600	0.14196700	-8.09022100	H	-10.69436400	-1.89729600	-5.68363300
N	-5.01352200	-0.89921400	-7.63556500	H	-9.36209800	-0.97646900	-7.66752100
C	-9.56332700	-3.95540800	-4.12768700	H	-6.62841100	1.83833300	-13.69396200
C	-9.04895800	-3.21061600	-5.30577800	H	-7.07045500	0.26233500	-17.07118700
N	-9.76713100	-2.20843100	-5.93880600	H	-7.59644600	-2.23068700	-16.77545500
C	-7.88806300	-3.31550500	-6.02259400	H	-6.98857000	-3.06343000	-14.46388000
C	-9.04896200	-1.75329000	-6.98878500	H	-0.92748100	-2.41262300	-9.65459900
N	-7.90061600	-2.40869800	-7.06565400	H	-0.17748500	-3.17753800	-11.05727100
C	-6.95819000	2.60919700	-10.69330100	H	-3.61871400	-1.98967800	-10.09695300
N	-7.46180000	1.57990600	-9.81872400	H	-1.15555500	-1.80357600	-13.48211600
C	-7.11052100	0.27840500	-9.98183600	H	-3.55733600	-1.42755500	-14.24783300
O	-6.17814200	0.04933400	-10.83519700	H	-5.87823900	2.50678700	-10.81283300
O	-7.67989200	-0.58402400	-9.24488900	H	-2.23179300	-4.89998300	-7.76225100
C	-5.99742500	1.45357600	-14.50229200	H	-2.47194300	-3.26453500	-7.10180400
C	-6.43651500	0.08921800	-14.93414800	H	-9.91211900	-3.28020700	-3.33680000
N	-6.43054400	-1.02370100	-14.09504900	H	-4.96509100	1.44726700	-14.13219800
C	-6.90487500	-0.29578700	-16.16269300	H	-6.05307600	2.15456400	-15.33977000
C	-6.88071500	-2.04786600	-14.81412000	H	-7.17185200	3.58761100	-10.25324100
N	-7.17128900	-1.64810500	-16.06727900	H	-7.41653700	2.57605200	-11.69071700
C	-0.67058900	-2.26303000	-10.70606800	H	-3.02832100	-0.85606200	-4.06837400
C	-1.91061000	-1.97162100	-11.48206900	H	-3.12863200	-4.65444400	-6.22942900
N	-1.94934600	-1.78144500	-12.85657900	H	0.06020500	-1.44647300	-10.76361600
C	-3.21479500	-1.86968000	-11.08579400	H	-8.24185500	1.76771000	-9.20704600
C	-3.23871800	-1.58960300	-13.22974400	C	-15.72468000	-5.23246900	-8.59994400
N	-4.03112400	-1.64083900	-12.17341300	C	-14.28154700	-5.20648600	-8.07992400
C	-2.92952200	-4.25382000	-7.22607800	C	-13.31452000	-4.37662800	-8.94812700
C	-4.21762700	-4.07824800	-7.98694900	C	-12.00816300	-4.09655200	-8.19273300
O	-5.25657900	-3.70992200	-7.41829700	C	-13.02522700	-5.05035300	-10.29852800
O	-4.11763500	-4.25399200	-9.27688700	C	-8.21562100	-7.89747500	-4.42193600
Zn	-6.50353400	-2.07973800	-8.49113600	C	-8.70812100	-7.36563100	-5.76581400
Zn	-6.06624700	-1.48583700	-12.07040500	S	-10.53157800	-7.62628600	-5.95943300
H	-1.66484100	-0.24445100	-5.01488600	C	-9.38758500	-8.98460200	-11.44911700
H	-2.84615200	0.88268100	-4.32882700	C	-8.82996000	-8.97015400	-10.02467400
H	-4.93965500	-1.94874100	-5.76306400	O	-9.23370500	-8.18399600	-9.15520800
H	-2.81977200	1.35057300	-7.25844000	C	-10.34767300	-7.81630500	-11.68419400

C	-10.96812800	-7.80742000	-13.07248100	H	-11.77252900	-1.72863600	-18.75056500
O	-10.34031000	-8.06430800	-14.10241500	H	-12.39552800	-3.37798600	-18.89867500
N	-12.28293600	-7.47034300	-13.12169300	H	-13.46107000	-2.00034600	-19.22219100
N	-7.89655900	-9.91357100	-9.75603000	N	-6.55558800	-4.91086200	-11.46530400
C	-7.14862100	-9.92147400	-8.50393300	C	-7.06147000	-5.99916700	-10.82239700
H	-14.28415700	-4.79205500	-7.06224400	O	-6.80318900	-7.18748800	-11.06176900
H	-13.89479500	-6.23144700	-7.98679100	N	-7.92048000	-5.56069200	-9.83625900
H	-13.79817200	-3.40891200	-9.15413900	C	-8.32049100	-4.18957400	-10.12945600
H	-12.20768200	-3.54010500	-7.26776800	C	-7.11429700	-3.65495800	-10.95902300
H	-11.31226700	-3.50544200	-8.80112600	O	-7.46680700	-2.80014100	-11.96805900
H	-11.50357200	-5.02851700	-7.90799800	H	-8.49253600	-3.60379300	-9.22646000
H	-12.36600200	-4.43448400	-10.92147600	H	-9.22418200	-4.14958000	-10.75173400
H	-12.52720500	-6.01606100	-10.13576500	H	-6.09300300	-4.96619900	-12.37401300
H	-13.94558300	-5.22853900	-10.86697900	H	-8.56670800	-6.25823800	-9.47345900
H	-15.79883400	-5.69529800	-9.59058200	O	-6.11892500	-3.02625300	-10.14985700
H	-8.49586500	-6.29667500	-5.86415500	H	-5.00061200	-3.89929800	-9.74050300
H	-8.22322900	-7.87482700	-6.60024400	C	-4.81770800	-9.58761800	-11.88278100
H	-10.49497600	-7.85100200	-7.29022400	C	-4.67529900	-8.98437700	-13.26798000
H	-8.73163500	-7.41574800	-3.58290400	O	-4.05647700	-9.55299700	-14.16615100
H	-9.79942600	-6.87149300	-11.58879900	N	-5.28563400	-7.77440100	-13.41119600
H	-11.12119400	-7.80994300	-10.91102700	C	-5.56594600	-7.22845800	-14.72620900
H	-12.77699800	-7.13602400	-12.30753500	C	-4.92073700	-5.84278000	-14.86122000
H	-12.69841000	-7.31099200	-14.02974800	O	-5.37675300	-4.87352100	-14.22003000
H	-8.56413600	-8.94104800	-12.16941000	C	-7.08687200	-7.12718000	-14.95561700
H	-7.83644800	-10.00862100	-7.65923200	O	-7.63298900	-8.41375500	-14.77660700
H	-6.55954800	-9.00367500	-8.39154600	N	-3.86876900	-5.66827500	-15.69232500
H	-7.48729300	-10.39457700	-10.54521100	C	-3.08109400	-6.68371900	-16.44129200
H	-9.90472600	-9.94013400	-11.61084300	C	-2.05097000	-7.38289000	-15.54331400
H	-6.47915100	-10.78418600	-8.50285600	C	-2.44939200	-5.82181200	-17.54988300
H	-8.38452800	-8.97545400	-4.33847100	C	-2.13908600	-4.49117300	-16.84353100
H	-7.14113000	-7.70632100	-4.30850000	C	-3.30825100	-4.31618100	-15.85760300
H	-16.13322800	-4.21734600	-8.67702100	H	-2.99954900	-3.91290200	-14.88744600
H	-16.37500100	-5.80143600	-7.92635200	H	-4.08947200	-3.65133400	-16.24685000
C	-12.65108400	-2.36154900	-18.57849600	H	-1.18882900	-4.56324000	-16.30331900
C	-13.07136800	-2.33149500	-17.09750100	H	-2.05711200	-3.65055100	-17.53914600
C	-12.00905900	-2.83457800	-16.13832600	H	-1.56452400	-6.29391000	-17.98571500
C	-11.34914200	-1.97577700	-15.25242500	H	-3.17653700	-5.66171100	-18.35496300
C	-11.65523700	-4.19375700	-16.09895400	H	-3.75446400	-7.43052600	-16.86805000
C	-10.37975400	-2.44040600	-14.35724200	H	-1.41557000	-6.65625100	-15.02366000
C	-10.69053700	-4.67769000	-15.22072600	H	-2.54782300	-8.02309200	-14.81140900
C	-10.04434000	-3.80079800	-14.33416400	H	-1.40579200	-8.02444500	-16.15502300
O	-9.11539900	-4.32879200	-13.49016200	H	-5.15060700	-7.93837200	-15.44210700
H	-13.98315200	-2.93348400	-16.98049300	H	-8.58539600	-8.31714800	-14.57173600
H	-13.34872600	-1.30598700	-16.82306200	H	-7.25704000	-6.74567100	-15.97928800
H	-11.60349300	-0.91733700	-15.24816800	H	-7.51631900	-6.39193900	-14.26271700
H	-12.14954400	-4.89259700	-16.77173400	H	-5.87539500	-7.46936500	-12.63220700
H	-9.89647400	-1.75573700	-13.66414200	H	-5.22905400	-8.89180200	-11.15078200
H	-10.43146700	-5.73239900	-15.19762200	H	-5.47452400	-10.46292200	-11.96605300
H	-8.62069600	-3.63547000	-12.97412100	H	-3.84202800	-9.95656000	-11.55195700

SkDHPase.HYD-TS3-II

C	-2.73099300	-0.10103300	-4.80017700	H	-3.66780300	-2.75898700	-10.39641100
C	-3.66170900	-0.18741200	-5.95579900	H	-1.12417600	-0.71691900	-13.04479100
N	-3.92064700	0.85880100	-6.82884700	H	-3.51970700	-0.36348500	-13.83357800
C	-4.41930200	-1.22384100	-6.42207500	H	-5.96575700	2.44141200	-11.11651700
C	-4.80108700	0.43369100	-7.76705200	H	-2.20467200	-4.99513700	-7.56757600
N	-5.11552700	-0.83335700	-7.54989500	H	-2.48129200	-3.25641300	-7.30503000
C	-9.56332600	-3.95540700	-4.12768600	H	-9.88868800	-3.25747100	-3.34660400
C	-9.04710400	-3.24274700	-5.32678900	H	-4.93580100	1.51821700	-14.23147700
N	-9.77227200	-2.26192100	-5.98620200	H	-6.18510900	2.18686900	-15.29139300
C	-7.88139400	-3.35098100	-6.03721400	H	-6.96884500	3.59236100	-10.21221800
C	-9.05273200	-1.82072600	-7.04160300	H	-7.68054100	2.62090900	-11.52034800
N	-7.89825500	-2.46611400	-7.09916500	H	-2.70973000	-1.05791300	-4.27275300
C	-6.95819000	2.60920000	-10.69330200	H	-3.17668100	-4.42814900	-6.17541700
N	-7.25319900	1.59999200	-9.70472000	H	-0.15271900	-1.39487600	-10.27891900
C	-7.25828200	0.27514900	-10.08517100	H	-7.87674600	1.83046800	-8.94336100
O	-6.77726500	0.05345500	-11.24359800	C	-15.72469300	-5.23245900	-8.59994400
O	-7.69325300	-0.56135300	-9.23916900	C	-14.28152900	-5.20650000	-8.07992600
C	-5.99742700	1.45357800	-14.50229200	C	-13.26492900	-4.57630900	-9.05222100
C	-6.37706900	0.07786200	-14.97014200	C	-11.91740100	-4.34872900	-8.35363600
N	-6.35689700	-1.05774400	-14.16038100	C	-13.07933700	-5.41743300	-10.32542500
C	-6.79160200	-0.29306300	-16.22328100	C	-8.21562000	-7.89747800	-4.42194100
C	-6.74437100	-2.07598500	-14.91899700	C	-8.67140200	-7.39938500	-5.79124700
N	-7.01176300	-1.65542300	-16.17226600	S	-10.44741800	-7.82574500	-6.09321400
C	-0.67058800	-2.26303000	-10.70606800	C	-9.34316400	-9.21926800	-11.52109600
C	-1.91919800	-1.87372900	-11.42424200	C	-8.84824500	-9.10462100	-10.08514300
N	-1.93503200	-1.08875700	-12.56918600	O	-9.19085600	-8.18717000	-9.32263400
C	-3.23797500	-2.14474900	-11.17093000	C	-10.63997100	-8.45616600	-11.77660900
C	-3.22261200	-0.91865000	-12.95713500	C	-10.70027800	-7.85561900	-13.18083200
N	-4.03680500	-1.54384200	-12.12483300	O	-9.80563100	-7.99838300	-14.01051600
C	-2.92952300	-4.25382200	-7.22607800	N	-11.83523500	-7.15813900	-13.45668100
C	-4.19726600	-4.29263800	-8.08270700	N	-7.96048000	-10.05072000	-9.70742600
O	-5.25524100	-3.78550400	-7.63567500	C	-7.14862200	-9.92146800	-8.50392600
O	-4.04890800	-4.82787300	-9.24055900	H	-14.25811900	-4.64201500	-7.13712400
Zn	-6.45188700	-2.08028000	-8.46612300	H	-13.95487900	-6.22596300	-7.82906000
Zn	-6.10014200	-1.57156400	-12.11581500	H	-13.65837900	-3.59353600	-9.35589600
H	-1.70472300	0.12869700	-5.11327900	H	-12.03676700	-3.69622100	-7.47937800
H	-3.03656000	0.66765400	-4.07937200	H	-11.19144200	-3.87670500	-9.02757500
H	-4.51462000	-2.22565800	-6.03897500	H	-11.48846800	-5.29406700	-7.99751600
H	-3.52902500	1.78903200	-6.77248700	H	-12.35558800	-4.94882500	-11.00411500
H	-5.21049200	1.06280100	-8.54450100	H	-12.70733200	-6.41897400	-10.06920000
H	-8.77867200	-4.58588900	-3.70187600	H	-14.02133700	-5.53640400	-10.87268900
H	-10.41098600	-4.60596400	-4.37664100	H	-15.82949100	-5.85521100	-9.49531800
H	-7.03534600	-4.00021600	-5.87412800	H	-8.54929700	-6.31479400	-5.87213000
H	-10.69967700	-1.94719400	-5.73594200	H	-8.08638200	-7.85587600	-6.59185500
H	-9.36572800	-1.05639000	-7.73488700	H	-10.32235200	-7.99655400	-7.42731200
H	-6.57429900	1.73573800	-13.61618900	H	-8.82676800	-7.47460700	-3.61596900
H	-6.94687200	0.28197800	-17.12310600	H	-10.72324300	-7.64214100	-11.04672500
H	-7.39049900	-2.23270800	-16.91043800	H	-11.51963100	-9.09360900	-11.62373700
H	-6.83648700	-3.10050100	-14.58740100	H	-12.47441500	-6.90297400	-12.71695700
H	-0.91952100	-2.94422900	-9.88859000	H	-11.84019400	-6.58259200	-14.29053700
H	0.03733300	-2.78191700	-11.36388100	H	-8.55646100	-8.79407700	-12.15634100

H	-7.77974400	-9.95097800	-7.61124500	H	-5.65137300	-5.04426000	-11.94292100
H	-6.58840500	-8.98095000	-8.51999600	H	-8.73579300	-6.32427300	-9.83703600
H	-7.67174700	-10.72573300	-10.40166600	O	-6.17125400	-2.73118700	-10.24370600
H	-9.43435600	-10.27211300	-11.81098300	H	-5.06480000	-4.87267900	-10.04918500
H	-6.44888900	-10.75852700	-8.46531600	C	-4.81771100	-9.58762000	-11.88278000
H	-8.28756100	-8.98730400	-4.35418700	C	-4.73687300	-9.05535300	-13.30504100
H	-7.17305700	-7.60849600	-4.23949000	O	-4.02751100	-9.58614200	-14.15760200
H	-16.07101300	-4.22304500	-8.85449300	N	-5.48216000	-7.93452500	-13.53099000
H	-16.40621600	-5.63552900	-7.84277500	C	-5.42610100	-7.19719500	-14.77814800
C	-12.65108300	-2.36154900	-18.57849500	C	-4.71057600	-5.85443100	-14.56835800
C	-12.98800900	-2.52354300	-17.08405200	O	-5.13507200	-5.05137600	-13.71343500
C	-11.85028000	-3.04338900	-16.22269500	C	-6.83275700	-6.89616800	-15.35254100
C	-11.27099700	-2.25902500	-15.21834800	O	-7.51533900	-8.07362900	-15.70885700
C	-11.35242500	-4.34847100	-16.38210400	N	-3.67930500	-5.51188000	-15.36703000
C	-10.25115700	-2.74340500	-14.39158900	C	-2.93161800	-6.38815600	-16.30412900
C	-10.33340600	-4.85066400	-15.57568700	C	-2.05097000	-7.38288900	-15.54331400
C	-9.77884000	-4.05226400	-14.55779400	C	-2.13579800	-5.35769100	-17.12772300
O	-8.80811400	-4.60800400	-13.78938100	C	-1.79973700	-4.25527000	-16.10951700
H	-13.84895100	-3.20085500	-16.99359400	C	-3.05357800	-4.18498300	-15.22264800
H	-13.32303100	-1.55738000	-16.68636100	H	-2.83877300	-3.98039500	-14.16967300
H	-11.63153000	-1.24373300	-15.06330700	H	-3.75881100	-3.41530400	-15.56230100
H	-11.77211100	-4.98986100	-17.15510400	H	-0.92667600	-4.54254500	-15.51340400
H	-9.83201400	-2.11609700	-13.60830900	H	-1.57341200	-3.29489600	-16.58285800
H	-9.95571400	-5.86137600	-15.70638100	H	-1.25075600	-5.80033800	-17.59315800
H	-8.36099400	-3.97375300	-13.16249200	H	-2.76844200	-4.95202600	-17.92655000
H	-11.83009400	-1.64953100	-18.72258100	H	-3.63521200	-6.92849100	-16.94377300
H	-12.34652900	-3.31475800	-19.02523800	H	-1.37012300	-6.86082000	-14.86066300
H	-13.52104400	-1.99439500	-19.13420500	H	-2.64615000	-8.09968400	-14.97268200
N	-6.07416500	-4.96337300	-11.00057300	H	-1.44203600	-7.95585500	-16.25337200
C	-6.91790800	-6.08698900	-10.72166100	H	-4.90003600	-7.84060100	-15.48148500
O	-6.59786700	-7.25357900	-10.93626100	H	-8.22143700	-8.21951400	-15.05602900
N	-8.06369900	-5.64043900	-10.18422500	H	-6.69083600	-6.28442000	-16.25832500
C	-8.19954200	-4.19676200	-10.14053900	H	-7.39682200	-6.28946200	-14.63660600
C	-6.93911500	-3.65707400	-10.90510500	H	-5.96044600	-7.52607200	-12.73172700
O	-7.23657100	-3.19193900	-12.14650000	H	-4.14809200	-9.00854400	-11.23633200
H	-8.23588600	-3.84218700	-9.10873600	H	-5.82056400	-9.50147900	-11.46237700
H	-9.10290200	-3.86329200	-10.66001200	H	-4.48501600	-10.62779400	-11.88629500

SkDHPase.HYD-EP-II

C	-2.73099300	-0.10103300	-4.80017600	C	-6.95819000	2.60919900	-10.69330200
C	-3.67303300	-0.19271100	-5.94750800	N	-7.22454600	1.51460100	-9.78484100
N	-3.95184900	0.84969100	-6.81943200	C	-7.11669200	0.20316400	-10.18815100
C	-4.41707500	-1.23963100	-6.41116300	O	-6.57242600	0.04103100	-11.33852300
C	-4.82959500	0.40895000	-7.75437600	O	-7.51853200	-0.68465400	-9.38459200
N	-5.12446000	-0.86298300	-7.53862700	C	-5.99742500	1.45357800	-14.50229300
C	-9.56332800	-3.95541100	-4.12768300	C	-6.27377900	0.10910400	-15.10665900
C	-9.06898700	-3.29963800	-5.37393800	N	-6.22678400	-1.07551800	-14.37475100
N	-9.80309700	-2.34498200	-6.06433200	C	-6.58656000	-0.20281900	-16.40334800
C	-7.91629300	-3.44048100	-6.10164800	C	-6.49517200	-2.07174100	-15.21528400
C	-9.09983800	-1.95035800	-7.15034800	N	-6.71645900	-1.57798000	-16.44963200
N	-7.94825800	-2.59958000	-7.19992100	C	-0.67059000	-2.26303000	-10.70606900

C	-1.87959700	-1.90431100	-11.50536200	C	-8.91637600	-9.07267600	-9.99997600
N	-1.84621400	-1.15189900	-12.67220300	O	-9.26205100	-8.20710300	-9.18484000
C	-3.20510700	-2.18564300	-11.30724300	C	-10.33022400	-7.97499600	-11.79331900
C	-3.11047300	-1.00566800	-13.13052700	C	-11.06955700	-8.15533300	-13.10788700
N	-3.95990100	-1.61892300	-12.31806700	O	-10.50896400	-8.48436100	-14.15707200
C	-2.92952000	-4.25382000	-7.22607500	N	-12.40825200	-7.93018400	-13.07269300
C	-4.11432700	-4.13346500	-8.17144800	N	-7.95543900	-9.98493800	-9.71537600
O	-5.21085500	-3.70403900	-7.64954300	C	-7.14862200	-9.92146500	-8.50392800
O	-3.92544400	-4.40266300	-9.37258800	H	-14.25066900	-4.62408200	-7.14846900
Zn	-6.37656400	-2.26695400	-8.43911700	H	-13.95983800	-6.22316400	-7.81227600
Zn	-5.97324400	-1.48294300	-12.38117800	H	-13.64715800	-3.60702800	-9.36539200
H	-1.71010900	0.13838600	-5.12357400	H	-11.98434600	-3.77256900	-7.51805800
H	-3.03506000	0.66223100	-4.07288800	H	-11.18900900	-3.93574100	-9.09584900
H	-4.49007600	-2.24437200	-6.03171100	H	-11.47594500	-5.36653200	-8.08459500
H	-3.57149400	1.78478900	-6.76761100	H	-12.39909500	-5.01023500	-11.03771800
H	-5.24207100	1.03174700	-8.53434100	H	-12.80975800	-6.45921500	-10.09657000
H	-8.76587600	-4.55659700	-3.68404300	H	-14.08819700	-5.51352400	-10.89160600
H	-10.40805800	-4.62436500	-4.33269300	H	-15.83645900	-5.88316600	-9.47411000
H	-7.06441000	-4.07970500	-5.92787100	H	-8.52987400	-6.33895400	-5.90226900
H	-10.72765900	-2.02125800	-5.81495100	H	-8.20942200	-7.92482100	-6.59830300
H	-9.42348100	-1.20678000	-7.86186800	H	-10.48143300	-7.93069000	-7.31142900
H	-6.62260400	1.62030700	-13.61993400	H	-8.74977200	-7.41140400	-3.59686800
H	-6.72814400	0.41886400	-17.27372400	H	-9.59893000	-7.17547000	-11.94687300
H	-6.98147900	-2.13064200	-17.25343100	H	-11.00465500	-7.66230500	-10.99210000
H	-6.49366800	-3.13234500	-14.98338900	H	-12.87208000	-7.57551200	-12.25010600
H	-0.96517700	-2.95167500	-9.91037700	H	-12.92734200	-7.97670300	-13.93906200
H	0.09142200	-2.76358400	-11.31561100	H	-8.82876700	-9.48996000	-12.12465300
H	-3.64977400	-2.80321300	-10.53898600	H	-7.78370200	-10.01220500	-7.61822200
H	-1.01587200	-0.78956600	-13.12100700	H	-6.59484400	-8.97740800	-8.44545000
H	-3.36869800	-0.47412300	-14.03378900	H	-7.62889200	-10.57192700	-10.46976900
H	-5.95766600	2.50650300	-11.11855600	H	-10.27276000	-10.09169400	-11.3040210
H	-2.19587400	-4.96217000	-7.61742900	H	-6.44003800	-10.75216100	-8.51330500
H	-2.44690200	-3.27237400	-7.13559700	H	-8.35467100	-8.97768600	-4.31440000
H	-9.88179400	-3.21900500	-3.38010400	H	-7.14767500	-7.67382200	-4.30756300
H	-4.95206300	1.54660700	-14.18116400	H	-16.05850100	-4.22785800	-8.88819900
H	-6.19531700	2.24691700	-15.22819800	H	-16.41239100	-5.60182600	-7.83113400
H	-7.00663000	3.54984400	-10.13707100	C	-12.65108400	-2.36154900	-18.57849600
H	-7.67770100	2.66011900	-11.52165300	C	-13.08749600	-2.42602900	-17.10405700
H	-2.69622600	-1.06021800	-4.27777400	C	-12.03162500	-3.01633100	-16.19202500
H	-3.24400200	-4.56086900	-6.22387600	C	-11.17167500	-2.20347500	-15.44545100
H	-0.20529000	-1.38287200	-10.24473100	C	-11.86116200	-4.40605500	-16.08868400
H	-7.84763500	1.66891600	-9.00463300	C	-10.18048700	-2.74504500	-14.62301000
C	-15.72468300	-5.23247100	-8.59994700	C	-10.87803500	-4.96766400	-15.27953200
C	-14.28154500	-5.20648400	-8.07992000	C	-10.03135400	-4.13422200	-14.53729100
C	-13.27080200	-4.59999900	-9.07287800	O	-9.09485800	-4.73114100	-13.74071800
C	-11.90156600	-4.40864000	-8.40815700	H	-14.00864300	-3.01912000	-17.03224300
C	-13.13759500	-5.44165000	-10.35170800	H	-13.34533900	-1.41610700	-16.76051400
C	-8.21562100	-7.89747600	-4.42194500	H	-11.28260100	-1.12170100	-15.49569100
C	-8.71477200	-7.41021100	-5.77970700	H	-12.51418900	-5.06516300	-16.65785100
S	-10.52787500	-7.72906800	-5.97670700	H	-9.53769400	-2.09558200	-14.03312000
C	-9.57942200	-9.24098900	-11.36794400	H	-10.74854200	-6.04399000	-15.21188700

H	-8.46230800	-4.06994900	-13.39086600	O	-7.77162800	-8.85854400	-14.79641400
H	-11.75501000	-1.74065100	-18.69484300	N	-4.09684600	-6.01587000	-16.01891400
H	-12.41472000	-3.36008900	-18.96330900	C	-3.15856900	-7.03832300	-16.54791000
H	-13.44302700	-1.93592000	-19.20546800	C	-2.05097300	-7.38288800	-15.54331300
N	-5.65941800	-5.66883900	-11.22004400	C	-2.62877400	-6.33741900	-17.81260100
C	-6.82173300	-6.27521600	-10.89213000	C	-2.50651900	-4.86530100	-17.38128400
O	-7.17275800	-7.37816500	-11.33888300	C	-3.70254500	-4.65806600	-16.43308200
N	-7.64035600	-5.55849000	-9.99741100	H	-3.46125300	-4.03785300	-15.56186200
C	-8.24399700	-4.32128800	-10.51649000	H	-4.55356900	-4.18170800	-16.93511100
C	-7.22460100	-3.34487000	-11.08072500	H	-1.56248900	-4.70149000	-16.85103200
O	-7.34357700	-2.96952500	-12.29341900	H	-2.52870300	-4.17156100	-18.22708300
H	-8.74343300	-3.81488900	-9.68267500	H	-1.68261600	-6.76408800	-18.15764700
H	-8.98830200	-4.52186900	-11.29552500	H	-3.35922600	-6.43530600	-18.62459000
H	-5.08378900	-6.16132100	-11.89262600	H	-3.70586100	-7.94893700	-16.79821100
H	-8.36827500	-6.19496200	-9.66828200	H	-1.50820100	-6.48680100	-15.22048400
O	-6.29496300	-2.87262900	-10.36631700	H	-2.46904800	-7.88943900	-14.67219100
H	-5.18026300	-5.06302200	-10.54250800	H	-1.33320700	-8.06864400	-16.00827300
C	-4.81770400	-9.58762800	-11.88278200	H	-5.29425100	-8.32616100	-15.59020800
C	-4.69766100	-9.05917600	-13.30695600	H	-8.72779800	-8.76499800	-14.60565600
O	-3.94691500	-9.57830100	-14.12748600	H	-7.47918100	-7.37450000	-16.24161500
N	-5.46092400	-7.94952400	-13.57528800	H	-7.73844600	-6.77817800	-14.59329100
C	-5.76018900	-7.57061200	-14.95600400	H	-6.21111700	-7.77618800	-12.90313900
C	-5.22686800	-6.16004900	-15.27988400	H	-3.83488800	-9.53948000	-11.40136400
O	-5.85054100	-5.15719400	-14.89496900	H	-5.54998600	-9.04562600	-11.28342700
C	-7.28434500	-7.58863700	-15.17593400	H	-5.08934900	-10.64740400	-11.94193600

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C	3.55821900	7.90015000	-1.60236800	C	-2.65667400	5.88202500	-2.65181300
C	3.00992100	6.85447900	-0.70132300	C	-2.77146300	5.02939800	-1.44122800
N	2.50050000	7.07376300	0.57123800	N	-3.70671700	5.19255700	-0.42747000
C	2.86103400	5.51567900	-0.90998900	C	-2.00481700	3.97109000	-1.04902500
C	2.07223700	5.88362300	1.07050600	C	-3.47418800	4.24863400	0.51947000
N	2.27074100	4.92142400	0.18733700	N	-2.44492600	3.49671300	0.17001800
C	7.21001600	0.98675500	-0.67579100	C	1.45478200	4.21004500	-3.86703900
C	5.85499300	1.26203600	-0.11427500	C	1.25529500	3.15037400	-2.77785500
N	5.33317000	0.60512000	0.98972400	O	2.23124000	2.98540200	-1.96677000
C	4.88136100	2.15084400	-0.48669100	O	0.14704800	2.57145200	-2.71603100
C	4.10183900	1.09238600	1.23483800	Zn	1.96405300	2.84739100	0.13928800
N	3.79230600	2.03591000	0.36040600	Zn	-1.30252600	2.19461200	1.27600400
C	0.21707900	4.88635400	4.69821300	H	2.81222500	8.66472900	-1.85692700
N	1.16912200	4.25886200	3.80790300	H	4.42335900	8.41822200	-1.16779900
C	0.76362400	3.27873100	2.91569100	H	3.11813600	4.92213900	-1.77062600
O	-0.50722800	3.14847000	2.79329400	H	2.46152500	7.95989100	1.05454200
O	1.66180200	2.65294500	2.29697100	H	1.65368700	5.75032700	2.05911800
C	-3.62393400	3.49549200	4.41702900	H	7.37974900	1.61072700	-1.55804200
C	-4.00855700	2.26045800	3.65807100	H	7.31946200	-0.06242700	-0.97418900
N	-3.35886500	1.83207200	2.50289900	H	4.87521200	2.84417800	-1.31320700
C	-5.04658500	1.40472400	3.93126000	H	5.64033300	-0.27570300	1.39001800
C	-4.01170100	0.75730600	2.09025900	H	3.47245200	0.71309600	2.01980800
N	-5.03908700	0.46181800	2.92311400	H	-2.53810200	3.54405000	4.53859000

H	-5.76766700	1.38475900	4.73412600	C	-2.82928200	-5.07302200	6.28399400
H	-5.62792200	-0.35643200	2.85764400	C	-2.58168400	-4.36650400	4.97582800
H	-3.79371400	0.19286800	1.19483900	C	-2.26700500	-3.00360000	4.95477500
H	-1.86093200	5.48578600	-3.28751000	C	-2.83215200	-5.00833300	3.75616000
H	-3.57991500	5.89712400	-3.24588800	C	-2.26073300	-2.28041400	3.76481200
H	-1.18335100	3.51935900	-1.58632500	C	-2.82892900	-4.30796800	2.55383900
H	-4.43967100	5.88706400	-0.39611700	C	-2.57972900	-2.93070400	2.56694400
H	-4.05859500	4.13594900	1.41871900	O	-2.67636100	-2.26346700	1.38247000
H	-0.60385100	5.31171400	4.11752900	H	-2.62555400	-6.14692700	6.18910900
H	0.76250000	4.04821700	-4.69718600	H	-2.16050300	-4.69046600	7.06561600
H	1.25401300	5.19917400	-3.43524100	H	-2.04616200	-2.49087900	5.88909500
H	8.00342700	1.20841900	0.04939200	H	-3.05382700	-6.07353200	3.74867100
H	-3.93214400	4.40999400	3.89194700	H	-2.02291600	-1.21950400	3.75819700
H	-4.09691900	3.50536800	5.40365100	H	-3.01533400	-4.80207000	1.60455700
H	0.71747000	5.69422500	5.24234200	H	-2.37036600	-1.34225100	1.49289800
H	-0.21351700	4.19035200	5.43232000	H	-4.50725300	-3.78950100	6.82351700
H	3.88687000	7.43582800	-2.53558600	H	-4.97481800	-5.24847700	5.93982000
H	2.48495900	4.21158500	-4.23694700	H	-4.52072900	-5.35886800	7.65191500
H	-2.40609400	6.92274000	-2.40640700	C	-1.89030900	-2.17497700	-5.38914800
H	2.12183500	4.14566500	4.12811600	C	-3.20511200	-2.24436100	-4.64198500
O	0.20612500	2.05050800	-0.00490100	O	-4.28071300	-2.28858000	-5.24254200
H	0.04308600	2.00030900	-0.97394000	N	-3.08636900	-2.21600400	-3.29117300
C	6.31508100	-0.81385000	-4.33635500	C	-4.24070900	-2.26384500	-2.41734600
C	5.10517600	-0.61137900	-3.42678000	C	-4.40264900	-0.89490800	-1.73814000
S	5.04042600	-1.77373400	-1.99780800	O	-3.49137800	-0.45219900	-1.00812400
C	0.63689200	-5.48158400	-3.01597100	C	-4.08934800	-3.36968200	-1.34474800
C	1.60182700	-4.39125400	-3.48256200	O	-3.94159600	-4.63253300	-1.94759400
O	2.54697400	-3.99068100	-2.79686300	N	-5.53794400	-0.18167700	-1.90767800
C	0.83723200	-5.86476100	-1.54183800	C	-6.68791500	-0.46688700	-2.80365700
C	-0.22146400	-5.28442400	-0.60325900	C	-6.39021900	-0.08073300	-4.25773900
O	-1.43080700	-5.36155500	-0.86413600	C	-7.79526600	0.39226200	-2.16415700
N	0.24951700	-4.78372600	0.55619600	C	-7.04723400	1.65306800	-1.69991300
N	1.40563700	-3.92696000	-4.74399600	C	-5.69265200	1.11159000	-1.21348800
C	2.17687600	-2.79889700	-5.24881800	H	-4.84775800	1.76980600	-1.43708200
H	5.11679600	0.38612800	-2.97791100	H	-5.68977500	0.94258300	-0.13104800
H	4.16706700	-0.69122200	-3.98364100	H	-6.90723700	2.34296700	-2.53890100
H	4.40638800	-2.79242900	-2.61585600	H	-7.57760600	2.19790700	-0.91270200
H	7.24975800	-0.72094200	-3.77368600	H	-8.60747600	0.60400000	-2.86572500
H	1.84215200	-5.58275300	-1.21732400	H	-8.22301100	-0.13229700	-1.30069400
H	0.74910200	-6.95263400	-1.43450400	H	-6.94072400	-1.52897900	-2.74855600
H	1.22652500	-4.47737800	0.67273500	H	-6.09457000	0.97216800	-4.33340100
H	-0.43947800	-4.41935900	1.20370300	H	-5.60107300	-0.70641900	-4.68161900
H	-0.39778600	-5.16032700	-3.18125300	H	-7.29206300	-0.22398600	-4.86606800
H	3.24460300	-3.02183300	-5.18233600	H	-5.09063500	-2.50552800	-3.05496800
H	1.97254700	-1.88594800	-4.67665400	H	-3.05274300	-4.96206400	-1.71205500
H	0.52646900	-4.14063500	-5.19391800	H	-4.99783700	-3.35590500	-0.71960400
H	0.80075000	-6.35246200	-3.66392800	H	-3.24801800	-3.12937900	-0.69085400
H	1.91406500	-2.63425100	-6.29650700	H	-2.15367400	-2.23986900	-2.87537600
H	6.30451800	-1.80838300	-4.79594500	H	-1.86066000	-1.23927100	-5.95842400
H	6.32299800	-0.06723700	-5.14236700	H	-1.01891500	-2.21680900	-4.73177600
C	-4.29235500	-4.85740300	6.70266900	H	-1.85724800	-2.99242500	-6.11804000

C	5.97725100	-5.48411300	3.40366300	C	2.99672900	-2.33754700	1.07006600
C	6.31655400	-4.53946000	2.24864900	O	3.78617100	-1.72478900	1.82993800
C	7.22403600	-3.35650200	2.63921900	O	2.88431700	-3.57161400	0.86622000
C	7.59005800	-2.54689900	1.38633600	H	1.28055400	-0.09765400	1.92557000
C	6.57026300	-2.45260200	3.69751800	H	5.39592600	-6.34214600	3.04622800
N	-0.65048900	-0.92818800	-0.55670500	H	6.88284300	-5.87458200	3.88881500
C	0.15573600	-1.83127000	-1.30751700	H	5.37636000	-4.98460500	4.17138500
O	-0.32889000	-2.33907700	-2.32678600	H	5.38417800	-4.15188900	1.81834000
N	1.36665200	-2.07939200	-0.81215800	H	6.81685000	-5.11325200	1.45441600
C	1.98657600	-1.39725500	0.32159900	H	6.67980000	-2.18688700	0.89022100
C	0.91507000	-0.92121700	1.31032300	H	8.22475500	-1.68450800	1.63266400
C	-0.37243900	-0.49169700	0.67702000	H	5.58303600	-2.12386200	3.35136700
O	-1.25674800	0.12682400	1.34049200	H	6.43614600	-2.97659600	4.65089000
H	2.54330200	-0.53500000	-0.05618300	H	7.19227200	-1.56928900	3.89920600
H	-1.60268000	-0.76207800	-0.91216300	H	8.13000300	-3.15996800	0.65414300
H	1.92666300	-2.77354900	-1.30778600	H	8.15775500	-3.76390300	3.06165100
H	0.63738900	-1.73380800	1.99928500				

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C	3.28246300	7.97180600	-1.58003900	O	2.10677600	3.01305400	-1.98880000
C	2.58421000	6.91608500	-0.79533300	O	0.00393100	2.59589200	-2.66531200
N	1.64421300	7.14931800	0.20140600	Zn	1.83162000	2.85315000	0.08320400
C	2.66559500	5.55652200	-0.88163000	Zn	-1.62457700	2.12506300	1.42611100
C	1.20599200	5.94863800	0.66484000	H	2.58178400	8.59857000	-2.14688700
N	1.80302700	4.96384900	0.02021200	H	3.88230700	8.63693800	-0.94549000
C	7.12402800	1.15229000	-0.72813000	H	3.25444300	4.95421300	-1.55228900
C	5.82689400	1.56012200	-0.12058500	H	1.34042000	8.05328600	0.53449200
N	5.50469800	1.29928500	1.20265100	H	0.47497200	5.83637400	1.45117800
C	4.72423700	2.18402300	-0.63602900	H	7.22981900	1.60543000	-1.71833300
C	4.24184200	1.71057700	1.42775100	H	7.18618700	0.06374000	-0.85585200
N	3.73997200	2.27352500	0.34012500	H	4.54574900	2.54669700	-1.63602200
C	0.06240400	4.82235400	4.71723200	H	5.97579700	0.62098400	1.78912700
N	1.02096300	4.26703800	3.79103900	H	3.71577200	1.56925400	2.35549500
C	0.63330900	3.41058600	2.79151400	H	-2.66875000	3.52723300	4.53248700
O	-0.63130100	3.36556500	2.56992500	H	-5.51834900	0.95056200	5.04166000
O	1.54132800	2.80151300	2.16351000	H	-5.19175000	-0.89756400	3.29394300
C	-3.74159100	3.33094000	4.44843400	H	-3.54835700	-0.21885300	1.48710100
C	-3.98617000	2.00240700	3.79597600	H	-2.03634200	5.46635200	-3.21592500
N	-3.34451800	1.58423500	2.63172200	H	-3.77944500	5.75930000	-3.23901100
C	-4.85415600	1.01865700	4.19392800	H	-1.31778900	3.48720500	-1.50504300
C	-3.83154300	0.38380500	2.33919500	H	-4.77460700	5.63072900	-0.46134400
N	-4.74859000	0.00985000	3.25634100	H	-4.37801900	3.88534200	1.35415000
C	-2.88244100	5.79533300	-2.60764800	H	-0.74212800	5.31945300	4.17049300
C	-2.99257800	4.90997200	-1.41622900	H	0.50685300	4.11862900	-4.63699500
N	-3.99075200	4.99331300	-0.45406900	H	1.14846300	5.23444900	-3.40323100
C	-2.18152500	3.89316200	-0.99671300	H	7.97609700	1.47789600	-0.11822600
C	-3.75161800	4.05058300	0.49108400	H	-4.17775100	4.15712600	3.87091500
N	-2.65691200	3.37242100	0.19017700	H	-4.18582600	3.35450800	5.44773000
C	1.26478400	4.24354000	-3.86018200	H	0.56477000	5.56300900	5.34727900
C	1.10676700	3.18293300	-2.76952300	H	-0.39068500	4.06427200	5.37200600

H	3.95903000	7.49957200	-2.29653700	C	-1.91720700	-2.21749900	-5.41093900
H	2.26434700	4.20305800	-4.30375700	C	-3.20730400	-2.27159700	-4.61829100
H	-2.71422900	6.84449000	-2.33097900	O	-4.30038400	-2.39554100	-5.17425400
H	1.98467300	4.17290000	4.07823800	N	-3.03090500	-2.14942500	-3.27974700
C	6.25508000	-0.64431400	-4.39691300	C	-4.12619700	-2.32084500	-2.34603700
C	5.44304100	-1.21644900	-3.23313800	C	-4.40336300	-0.98181300	-1.64931200
S	6.48188200	-2.31525400	-2.17074000	O	-3.56413000	-0.50417700	-0.86242400
C	0.48131500	-5.18391700	-2.90478000	C	-3.79710800	-3.41659600	-1.31257500
C	1.53480900	-4.23292200	-3.48185300	O	-3.65369100	-4.63768200	-1.99850300
O	2.56163800	-3.94420600	-2.87088700	N	-5.56310400	-0.32078900	-1.88608200
C	0.58294800	-5.21648000	-1.37244900	C	-6.69351900	-0.68633100	-2.78010200
C	-0.35664600	-6.21919400	-0.73261400	C	-6.46458300	-0.25341900	-4.23667000
O	-1.58725100	-6.15219700	-0.81120800	C	-7.86526700	0.05316100	-2.10496000
N	0.23958600	-7.23225300	-0.04731500	C	-7.22776400	1.36295600	-1.61183900
N	1.30645800	-3.77307400	-4.74533200	C	-5.82390700	0.93204700	-1.15413500
C	2.16604200	-2.73295000	-5.29971600	H	-5.04585100	1.67155800	-1.36862700
H	5.04638600	-0.40732100	-2.61181100	H	-5.78470600	0.73261500	-0.07622100
H	4.59511900	-1.80500100	-3.59299100	H	-7.15983400	2.08474700	-2.43326200
H	5.51036600	-2.53659700	-1.23551700	H	-7.79640600	1.83679500	-0.80533000
H	7.10016400	-0.04601700	-4.03730100	H	-8.70294600	0.21124600	-2.79069700
H	0.30419700	-4.23152200	-0.99005900	H	-8.23231600	-0.53098400	-1.25195800
H	1.62336500	-5.39226200	-1.08656600	H	-6.84839200	-1.76760300	-2.74590200
H	1.23102900	-7.23097600	0.13907700	H	-6.26031000	0.82176000	-4.30251800
H	-0.34865600	-7.86942900	0.47218900	H	-5.63737000	-0.80908400	-4.68377400
H	-0.52626200	-4.88162100	-3.20745200	H	-7.36676000	-0.46520200	-4.82382300
H	3.20685800	-3.05950900	-5.25448100	H	-4.97920500	-2.65210400	-2.93929100
H	2.07325000	-1.79165800	-4.74402700	H	-2.89041200	-5.12443800	-1.62689400
H	0.36208300	-3.83352400	-5.09873600	H	-4.62657500	-3.46138000	-0.58290600
H	0.66202800	-6.18486700	-3.32199500	H	-2.89660000	-3.13573800	-0.75599700
H	1.88787400	-2.56639000	-6.34383100	H	-2.06690800	-2.18081600	-2.93213400
H	6.65741300	-1.44279100	-5.03067000	H	-1.99470700	-1.42464100	-6.16216200
H	5.62379000	-0.00078300	-5.02230100	H	-1.03932900	-2.03812000	-4.78590100
C	-4.17158600	-5.05373900	6.67420800	H	-1.80446100	-3.16102200	-5.95891900
C	-2.67264500	-5.09706500	6.33509800	C	6.09052700	-5.37965300	3.30912000
C	-2.36716200	-4.37921400	5.04018600	C	6.40786700	-4.11098700	2.50890900
C	-2.02440300	-3.02295900	5.02551400	C	6.78368200	-2.88714100	3.36926600
C	-2.49058500	-5.03479400	3.80590100	C	7.23607300	-1.73524300	2.45769100
C	-1.82962400	-2.33205600	3.82903000	C	5.62442600	-2.42020500	4.26405100
C	-2.30044200	-4.36726300	2.60080700	H	5.90710100	-6.22822700	2.63907800
C	-1.97838000	-3.00264500	2.60732000	H	6.92371600	-5.65411100	3.97022700
O	-1.82737900	-2.38566200	1.40748700	H	5.19807900	-5.25904400	3.93369700
H	-2.34863000	-6.14398000	6.26965500	H	5.55889900	-3.84393500	1.86473600
H	-2.10190900	-4.64648500	7.15737500	H	7.24735100	-4.32679300	1.83205800
H	-1.90227200	-2.49226600	5.96839400	H	6.40423200	-1.46514800	1.79560700
H	-2.74276300	-6.09377700	3.78886100	H	7.53262700	-0.85593400	3.04930700
H	-1.54062900	-1.28387800	3.83391900	H	4.78148400	-2.09615500	3.64272000
H	-2.38267100	-4.88376900	1.64848500	H	5.28198500	-3.21285400	4.93931300
H	-1.61189200	-1.42861800	1.51694000	H	5.93443600	-1.57199300	4.88996100
H	-4.51786400	-4.01822800	6.77503200	H	8.09232100	-2.02065300	1.83421000
H	-4.76478100	-5.52522800	5.88221100	H	7.63078500	-3.17328700	4.01482600
H	-4.38594500	-5.57601100	7.61496500	N	-0.52877800	-0.57656900	-0.75782800

C	0.23427300	-1.52483400	-1.44170100	H	2.09888700	-2.36675800	-1.51982700
O	-0.32083300	-2.23728600	-2.30267400	O	0.15454600	1.73770500	-0.10021600
N	1.52824300	-1.62796300	-1.10320900	H	-0.00062400	1.77432600	-1.08551500
C	2.18746400	-0.79899500	-0.10007700	H	0.92506700	-1.29809700	1.56526400
C	1.18191100	-0.40955000	0.97391600	C	3.43778500	-1.54000800	0.49243000
C	-0.13199400	0.08794300	0.40839500	O	3.87410500	-1.05097400	1.56511000
O	-1.11544200	0.26756800	1.28604700	O	3.87470800	-2.49995900	-0.18639300
H	2.57152700	0.10746600	-0.58905500	H	1.59380400	0.32666700	1.66031700
H	-1.53603600	-0.61484400	-0.92976100				

SkDHPase.DHO-INT1-II

C	3.13878100	7.99783300	-1.66533000	H	0.36012000	5.85479800	1.38571500
C	2.46108200	6.94345900	-0.86339400	H	7.22278400	1.73487600	-1.67048300
N	1.50610400	7.17197900	0.11965700	H	7.18976100	0.18805800	-0.81546200
C	2.57983600	5.58577300	-0.92083700	H	4.55014300	2.66873600	-1.59420000
C	1.09561200	5.96996400	0.60413300	H	5.94915700	0.69319900	1.81403500
N	1.72478200	4.98858700	-0.01503600	H	3.67405900	1.60751000	2.36819900
C	7.11822200	1.27561600	-0.68296400	H	-2.76684900	3.52456400	4.40436000
C	5.81693000	1.66747700	-0.07868700	H	-5.53955400	0.87205300	5.07895500
N	5.48104100	1.38065300	1.23541100	H	-5.17043200	-1.02155500	3.39035300
C	4.71807400	2.29336800	-0.59702700	H	-3.57738300	-0.34804000	1.53302300
C	4.21260800	1.77680600	1.45218600	H	-2.12094400	5.33002100	-3.30866200
N	3.72234400	2.35812200	0.36861200	H	-3.86380600	5.62248900	-3.34512400
C	-0.06662100	4.87032400	4.65032800	H	-1.41132600	3.39119300	-1.53054600
N	0.87429100	4.30037900	3.71396800	H	-4.87595300	5.56751200	-0.58390700
C	0.47484500	3.43802200	2.72453600	H	-4.50257900	3.87482300	1.28363200
O	-0.78995300	3.38828500	2.51129400	H	-0.88192500	5.35811000	4.11105500
O	1.37903100	2.82377400	2.09394000	H	0.46503400	4.04678300	-4.68203000
C	-3.83534600	3.29356400	4.37195900	H	1.10186500	5.19637400	-3.47586200
C	-4.06184700	1.93459700	3.77805600	H	7.96604900	1.60489000	-0.06902100
N	-3.42877300	1.49781300	2.61770600	H	-4.32172900	4.08285700	3.78308500
C	-4.89016900	0.93573600	4.21959100	H	-4.24032500	3.34172100	5.38694200
C	-3.87560700	0.27164900	2.36884000	H	0.44750300	5.62128300	5.25798300
N	-4.76546500	-0.09886100	3.31177500	H	-0.50563300	4.12255400	5.32610300
C	-2.96907000	5.67447800	-2.71186000	H	3.83365100	7.52709700	-2.36513900
C	-3.08530400	4.81894900	-1.49865400	H	2.22137700	4.14535900	-4.34830400
N	-4.09249600	4.93047600	-0.54926100	H	-2.80144100	6.72989500	-2.46012600
C	-2.28038000	3.81159200	-1.04324200	H	1.84289000	4.21007200	3.98576800
C	-3.86589600	4.01340500	0.42315700	C	6.31929900	-0.59171700	-4.33229300
N	-2.76954900	3.32505800	0.15301800	C	5.49434600	-1.18379700	-3.18721800
C	1.22099100	4.19463500	-3.90760900	S	6.54482500	-2.21848900	-2.07338400
C	1.06740000	3.16259600	-2.79283600	C	0.62393900	-5.22501000	-2.82214800
O	2.05774600	3.03046800	-1.99383500	C	1.67360900	-4.27990800	-3.41607200
O	-0.02486900	2.55399500	-2.68834700	O	2.71097700	-3.99964700	-2.81965800
Zn	1.82192200	2.88351700	0.07200600	C	0.64722400	-5.14375300	-1.28612900
Zn	-1.79839100	2.08319900	1.44098100	C	-0.21410600	-6.20121000	-0.62658300
H	2.42811100	8.59392900	-2.25243400	O	-1.44863100	-6.20564900	-0.67226600
H	3.71613200	8.69233900	-1.04143200	N	0.45856000	-7.18845100	0.02539700
H	3.19163100	4.98871000	-1.57514300	N	1.43017800	-3.82247500	-4.67830200
H	1.17552800	8.07428200	0.43115700	C	2.28381300	-2.78073200	-5.23825100

H	5.03972300	-0.38497200	-2.59285400	H	-5.86681400	0.55649200	-0.11330000
H	4.68723600	-1.81594500	-3.56582800	H	-7.21222100	1.86405100	-2.51218500
H	5.55397700	-2.47906100	-1.16820700	H	-7.88652400	1.60681000	-0.90087700
H	7.12392200	0.04961200	-3.95447400	H	-8.69834000	-0.04700400	-2.90504400
H	0.24741300	-4.17154400	-0.99022700	H	-8.25621400	-0.77103800	-1.34953200
H	1.68563000	-5.19248200	-0.94639100	H	-6.80126300	-1.98357500	-2.79177200
H	1.45247400	-7.12962500	0.18806400	H	-6.21718700	0.60501900	-4.34962000
H	-0.07690200	-7.87117500	0.54396100	H	-5.55831500	-1.01854100	-4.70191000
H	-0.37805100	-4.99055100	-3.19508800	H	-7.28700700	-0.70280500	-4.89537600
H	3.32498100	-3.10692300	-5.20099300	H	-4.89800200	-2.81665900	-2.94965100
H	2.19387800	-1.84013100	-4.68065600	H	-2.75110700	-5.20103400	-1.51909800
H	0.47260700	-3.85306500	-4.99847800	H	-4.56732500	-3.57976300	-0.57916800
H	0.86878500	-6.24417900	-3.15376100	H	-2.84741100	-3.18722800	-0.71356100
H	1.99805000	-2.61366800	-6.28037400	H	-2.00896800	-2.21005000	-2.87480900
H	6.77825400	-1.38003400	-4.93964200	H	-1.91605800	-1.60458000	-6.18034100
H	5.68100500	0.01328600	-4.98826900	H	-0.94779600	-2.10771900	-4.76476200
C	-4.10450000	-5.06565900	6.71562000	H	-1.65086700	-3.31909800	-5.88956200
C	-2.60353300	-4.88056300	6.43211600	C	6.19056600	-5.21852600	3.44006300
C	-2.33340200	-4.17918400	5.11796200	C	6.47771800	-3.96408200	2.60728500
C	-1.99964000	-2.82192700	5.06471900	C	6.81710200	-2.70899500	3.43690800
C	-2.44124700	-4.86880400	3.89940300	C	7.24851600	-1.57218400	2.49710200
C	-1.79341400	-2.16385700	3.84964200	C	5.63865400	-2.24629100	4.30854700
C	-2.24239700	-4.23469100	2.67847500	H	6.03184800	-6.08929100	2.79260600
C	-1.92268800	-2.86790000	2.64405100	H	7.02806200	-5.45330000	4.11094500
O	-1.76153300	-2.29416800	1.42624400	H	5.29279500	-5.10456700	4.05823100
H	-2.11811700	-5.86590300	6.43447500	H	5.62453100	-3.73615000	1.95360300
H	-2.14819800	-4.31245700	7.25343600	H	7.32539700	-4.17540900	1.93932200
H	-1.88643400	-2.26328900	5.99252000	H	6.41482600	-1.34275700	1.82203700
H	-2.68171300	-5.93066600	3.90795800	H	7.51923400	-0.66982200	3.06627200
H	-1.50669300	-1.11534900	3.82980000	H	4.79143900	-1.96746200	3.67116200
H	-2.30796600	-4.78117800	1.74172800	H	5.31391900	-3.02588900	5.00731500
H	-1.52505500	-1.33158400	1.48202300	H	5.91992700	-1.36950900	4.90823900
H	-4.61542300	-4.09645900	6.76356800	H	8.11598900	-1.85273000	1.88720300
H	-4.58402700	-5.65325600	5.92434100	H	7.66540700	-2.95659200	4.09661000
H	-4.26917400	-5.58357200	7.66841800	N	-0.47867200	-0.52659600	-0.88517200
C	-1.80844800	-2.35505900	-5.39049600	C	0.29088300	-1.49764100	-1.50548000
C	-3.10318900	-2.43000500	-4.60386400	O	-0.23381100	-2.24962100	-2.35931200
O	-4.18462700	-2.61205000	-5.16872900	N	1.58714400	-1.58278800	-1.15134000
N	-2.95721000	-2.26326400	-3.26632400	C	2.21814500	-0.75586100	-0.13046800
C	-4.06453600	-2.45209100	-2.34880600	C	1.17645400	-0.35681700	0.90501900
C	-4.39027800	-1.11532100	-1.66709100	C	-0.08009700	0.23428400	0.27168600
O	-3.57426100	-0.60286000	-0.87966400	O	-1.11271400	0.33948400	1.15934000
C	-3.72020900	-3.51751300	-1.28788400	H	2.62421700	0.14841800	-0.60830100
O	-3.50810500	-4.74577900	-1.94163700	H	-1.48668400	-0.61528200	-1.01464300
N	-5.57403000	-0.49946200	-1.91181900	H	2.15877000	-2.34146700	-1.52574700
C	-6.67022700	-0.89916900	-2.83060900	O	0.20976500	1.63226100	-0.21855300
C	-6.40672400	-0.47281200	-4.28227600	H	0.04605400	1.69467900	-1.20895700
C	-7.87750200	-0.18264300	-2.19448500	H	0.85810200	-1.24935000	1.45463800
C	-7.28495700	1.14383000	-1.68967800	C	3.45154600	-1.49040900	0.50259100
C	-5.88344400	0.74900500	-1.19347500	O	3.87706600	-0.97374800	1.56811800
H	-5.11850800	1.50657400	-1.39210400	O	3.89793500	-2.46994300	-0.14143400

H 1.58849000 0.34503400 1.62772800

SkDHPase.DHO-TS2-II

C	2.84069800	7.90212300	-2.05673300	H	-3.25706900	-0.34572200	1.58586900
C	2.19439100	6.80824300	-1.26408600	H	-2.30019500	5.17645600	-3.42817200
N	1.07988000	6.98607200	-0.45090600	H	-4.06092600	5.12263900	-3.53292800
C	2.48087800	5.47360800	-1.16060700	H	-1.34469600	3.41987400	-1.51626700
C	0.74502800	5.78807900	0.09450700	H	-5.14630600	5.05250200	-0.79832600
N	1.57305300	4.84771100	-0.32430200	H	-4.56980700	3.50886600	1.15395800
C	7.01370600	1.34087700	-0.82170900	H	-0.90206700	5.46677700	3.79623200
C	5.75469000	1.78786300	-0.18562800	H	0.26258600	3.66775200	-4.84433600
N	5.50437700	1.64776000	1.16728600	H	0.65726400	4.87739000	-3.59874200
C	4.61421900	2.32047400	-0.71186000	H	7.89797300	1.72662600	-0.29837800
C	4.23117600	2.01218500	1.40211900	H	-4.19542100	4.10824500	3.62447300
N	3.66616600	2.45759200	0.28999000	H	-4.54658400	3.40355100	5.21185500
C	-0.16934400	5.00930300	4.46359700	H	0.25706900	5.79002800	5.10167800
N	0.88167400	4.40037200	3.69538400	H	-0.69940500	4.29334600	5.10841500
C	0.58949800	3.53906000	2.67867600	H	3.69493000	7.49738700	-2.60507400
O	-0.63225600	3.52236900	2.28847000	H	1.96652200	4.12235500	-4.51910300
O	1.55263400	2.88562500	2.18512100	H	-3.26931900	6.45301200	-2.67470400
C	-3.89921100	3.32461900	4.33369100	H	1.80432400	4.30459100	4.09397000
C	-4.00526700	1.95389300	3.73092900	C	6.20072200	-0.72433000	-4.35961500
N	-3.26870400	1.52705700	2.62627200	C	5.47080100	-1.24327800	-3.12121100
C	-4.81668700	0.92611900	4.13733700	S	6.58110600	-2.28497400	-2.07640000
C	-3.64454300	0.27680400	2.38032200	C	0.71511500	-5.96394000	-3.11672500
N	-4.58194100	-0.11892600	3.26578500	C	1.60864200	-4.77558800	-3.44665300
C	-3.22077800	5.37408700	-2.87318600	O	2.39207500	-4.29549600	-2.62216300
C	-3.22658700	4.56992200	-1.62354400	C	-0.50763800	-5.61114200	-2.24180900
N	-4.27131600	4.55506000	-0.70995300	C	-0.30919900	-5.37829100	-0.74500200
C	-2.28852100	3.72607100	-1.09719100	O	-1.28929100	-5.49366500	0.01046800
C	-3.93465400	3.72341000	0.30842700	N	0.92015600	-5.06970400	-0.29533600
N	-2.73597400	3.21382400	0.09978100	N	1.51638600	-4.28320100	-4.70752700
C	0.98545300	3.94488300	-4.07375000	C	2.20945800	-3.05817000	-5.08127200
C	1.09257200	2.88435900	-3.00014900	H	5.10459600	-0.40740900	-2.51685800
O	2.08372900	2.78535300	-2.28249300	H	4.60503800	-1.84952400	-3.39954000
Zn	1.72157300	2.80417800	0.15707600	H	5.61726400	-2.54666800	-1.13587200
Zn	-1.59778400	2.07126500	1.34882400	H	7.06640200	-0.11042400	-4.08420700
H	2.15102000	8.34232500	-2.78788800	H	-1.23737400	-6.42298300	-2.31484900
H	3.21024200	8.71231400	-1.41591100	H	-1.00813000	-4.71526900	-2.62339800
H	3.26740800	4.91507400	-1.64072000	H	1.66672200	-4.78661000	-0.93524700
H	0.60729600	7.86160500	-0.27521800	H	0.99237400	-4.78319200	0.67277700
H	-0.08050000	5.63448300	0.77488000	H	0.35030200	-6.42668400	-4.04154900
H	7.05888300	1.69497400	-1.85595200	H	3.28186500	-3.17335800	-4.90512900
H	7.08336700	0.24506500	-0.84632100	H	1.84749600	-2.20922500	-4.49123100
H	4.38984400	2.57304300	-1.73539700	H	0.76067400	-4.60524200	-5.29405400
H	6.02428800	1.03138000	1.78079000	H	1.33894300	-6.70926100	-2.61129100
H	3.73988300	1.93318300	2.35664600	H	2.03897300	-2.86888700	-6.14390000
H	-2.87151700	3.54384600	4.64066000	H	6.56405800	-1.55025100	-4.98151400
H	-5.52065600	0.85041300	4.95175700	H	5.52887800	-0.10864000	-4.97127900
H	-4.93519400	-1.06259300	3.34505300	C	-3.90534900	-4.91276200	7.08820100

C	-2.44614600	-4.46171400	6.88891900	H	-2.86694100	-5.16004000	-0.78578300
C	-2.16354400	-3.85763200	5.52671300	H	-4.59979500	-3.33028300	-0.13494500
C	-1.91571800	-2.49069700	5.36395900	H	-2.86284700	-3.07267300	-0.35628500
C	-2.12701800	-4.66008100	4.37303300	H	-2.03945500	-2.33551500	-2.67957200
C	-1.65180600	-1.93282300	4.10834800	H	-2.00827400	-1.95970900	-5.93239800
C	-1.87210000	-4.12870100	3.11410200	H	-0.99990700	-2.55425300	-4.58111800
C	-1.63732200	-2.75015800	2.96843600	H	-1.79887100	-3.69401000	-5.71788300
O	-1.41365100	-2.28886800	1.71339900	C	6.33111600	-4.96328700	3.63085700
H	-1.78845300	-5.32736500	7.05011800	C	6.52638100	-3.68706800	2.80644400
H	-2.18622000	-3.73436800	7.66901400	C	6.86962000	-2.42815700	3.62906100
H	-1.91232100	-1.84152400	6.23857900	C	7.04549400	-1.23627300	2.67328000
H	-2.29157000	-5.73260400	4.46469000	C	5.78902700	-2.09538800	4.67022300
H	-1.43177400	-0.87238200	4.01261900	H	6.18279500	-5.83040700	2.97669400
H	-1.81893200	-4.75603600	2.22836300	H	7.20586000	-5.17038500	4.26233300
H	-1.22811500	-1.30940700	1.66709200	H	5.45635400	-4.89884700	4.28768400
H	-4.59497500	-4.06599600	6.98725700	H	5.62848000	-3.48461800	2.20636300
H	-4.19208300	-5.66256700	6.34211900	H	7.33731500	-3.85398300	2.08323800
H	-4.05037700	-5.35318400	8.08215100	H	6.08021300	-1.08467300	2.17158700
C	-1.89469100	-2.74558300	-5.17710900	H	7.33903400	-0.32885100	3.22392600
C	-3.16516700	-2.79959100	-4.34056000	H	4.82595200	-1.92275900	4.17331500
O	-4.25395100	-3.06492100	-4.85853600	H	5.65599600	-2.89865500	5.40345500
N	-2.99317000	-2.51213600	-3.02594600	H	6.04806500	-1.18439900	5.22600400
C	-4.08659100	-2.54958100	-2.07206200	H	7.81010400	-1.43411100	1.91220300
C	-4.37440500	-1.12859400	-1.56333500	H	7.81699400	-2.61349300	4.16129900
O	-3.51036600	-0.51051800	-0.91932200	O	0.00289900	2.14728000	-2.86653300
C	-3.76606600	-3.44335300	-0.85472200	N	-0.39821000	-0.40065900	-1.00539600
O	-3.63540700	-4.78083200	-1.26919600	C	0.30037000	-1.44118200	-1.59147600
N	-5.58963400	-0.56538900	-1.78220400	O	-0.27667000	-2.24903700	-2.35947600
C	-6.73110100	-1.09665300	-2.56661000	N	1.62707800	-1.50847300	-1.35053000
C	-6.52114300	-0.92938700	-4.07596100	C	2.29824600	-0.67844300	-0.36126400
C	-7.90292100	-0.26178800	-2.01268500	C	1.30815600	-0.31419500	0.73705400
C	-7.27244600	1.11419700	-1.74209600	C	0.04108700	0.36173800	0.20240800
C	-5.86578900	0.76900800	-1.22679400	O	-0.98104500	0.29030400	1.14010200
H	-5.09523800	1.48015100	-1.54071100	O	0.18631300	1.71367600	-0.20875800
H	-5.82723000	0.72120100	-0.13043700	H	0.05120300	1.61154700	-2.00798000
H	-7.20892600	1.69055500	-2.67197100	C	3.56188400	-1.39747800	0.21291800
H	-7.84312800	1.71073500	-1.02283400	O	4.12401000	-0.78085100	1.15190700
H	-8.74614200	-0.22280400	-2.70872000	O	3.89068900	-2.47923800	-0.33833200
H	-8.26100800	-0.70057100	-1.07313500	H	2.66320900	0.23772700	-0.84737400
H	-6.87343300	-2.15579400	-2.33430000	H	0.99444400	-1.23347300	1.24235400
H	-6.33112800	0.11996100	-4.33281500	H	1.78298700	0.32362600	1.48388800
H	-5.68935600	-1.54266700	-4.43218800	H	2.13187500	-2.34261100	-1.64871900
H	-7.42358900	-1.25126600	-4.61110500	H	-1.41112900	-0.51584300	-1.04814000
H	-4.93886800	-2.97608500	-2.60119700				

***S*kDHPase.DHO-INT2-II**

C	2.94614000	7.74089100	-2.28737800	C	1.36608200	5.86119500	0.42951300
C	2.40231100	6.72445500	-1.34439400	N	1.77422200	4.83110100	-0.29172600
N	1.71958600	7.02447100	-0.17381700	C	7.03023500	1.16851200	-0.83369900
C	2.42621200	5.35924600	-1.39019600	C	5.77168000	1.62311500	-0.20130900

N	5.49910200	1.43987700	1.14281800	H	0.25744200	5.96687200	4.84818200
C	4.65245900	2.20630500	-0.72050500	H	-0.51059900	4.37549200	5.04604200
C	4.23609000	1.83612600	1.37902600	H	3.44360200	7.23686100	-3.11978300
N	3.69822800	2.33451200	0.27588700	H	2.04103300	3.89165300	-4.61518300
C	-0.12153800	5.09165600	4.30916600	H	-3.06849500	6.35698400	-2.94408500
N	0.93235100	4.54787400	3.49503100	H	1.88169500	4.58306400	3.84166900
C	0.64631200	3.43802100	2.72675000	C	6.20185000	-0.99549800	-4.30841400
O	-0.59325700	3.17032200	2.61292500	C	5.43923000	-1.44394800	-3.06260800
O	1.63030400	2.85127300	2.19599900	S	6.49801300	-2.49702700	-1.97707700
C	-3.87240000	3.45160400	4.21854200	C	0.51051000	-6.01902300	-2.88801600
C	-4.02100500	2.07311100	3.63595200	C	1.45546000	-4.88393500	-3.25696200
N	-3.31036500	1.61473100	2.52724300	O	2.21171600	-4.36619600	-2.42910000
C	-4.85825600	1.07242400	4.05912000	C	-0.69925100	-5.56942500	-2.03783400
C	-3.72511200	0.37619500	2.29545000	C	-0.50275900	-5.33724000	-0.53973000
N	-4.66631500	0.01420300	3.19292600	O	-1.48354100	-5.44600500	0.21506700
C	-3.14483700	5.26638200	-3.04622900	N	0.72594000	-5.02484800	-0.09235200
C	-3.10322900	4.57425200	-1.73093600	N	1.43622800	-4.47627000	-4.54969400
N	-4.06557900	4.74943900	-0.74601700	C	2.18310800	-3.29945300	-4.97120300
C	-2.20737700	3.68918900	-1.19407800	H	5.10145100	-0.57526700	-2.48878600
C	-3.72820300	3.98346400	0.32093400	H	4.55185800	-2.02231100	-3.33163400
N	-2.60471100	3.33686200	0.07793400	H	5.51145300	-2.71589700	-1.05184500
C	1.04637500	3.74671100	-4.18671200	H	7.08962900	-0.40950200	-4.04305900
C	1.10995500	2.65779100	-3.10963300	H	-1.48598400	-6.32512200	-2.11268500
O	2.05608500	2.61157700	-2.31877200	H	-1.12820500	-4.64555400	-2.44210900
Zn	1.78202700	2.79665500	0.13844100	H	1.48078000	-4.77047800	-0.73492200
Zn	-1.56019600	2.06546900	1.29920300	H	0.80192700	-4.73841200	0.87544400
H	2.15895700	8.38046600	-2.70705800	H	0.13166300	-6.50400000	-3.79540300
H	3.68489300	8.39610600	-1.80855600	H	3.23578000	-3.41907100	-4.70415300
H	2.86032800	4.71137100	-2.13275200	H	1.79709600	-2.39700800	-4.48554200
H	1.53310800	7.95001700	0.18582700	H	0.70556600	-4.82380700	-5.15294200
H	0.86814700	5.80250500	1.38692900	H	1.09530400	-6.76990700	-2.34527500
H	7.08355000	1.53025100	-1.86492900	H	2.09757800	-3.19955900	-6.05601900
H	7.09309900	0.07247700	-0.86488200	H	6.53601300	-1.85520700	-4.90001800
H	4.44696500	2.50498900	-1.73574000	H	5.56234100	-0.37190200	-4.94600600
H	6.00074300	0.79999900	1.74693500	C	-3.99350000	-4.69507700	7.22831300
H	3.73318600	1.73866800	2.32540600	C	-2.58846800	-4.09673500	7.02156800
H	-2.81504100	3.70167300	4.34577200	C	-2.31078800	-3.58191500	5.62005300
H	-5.55619400	1.02355400	4.88083700	C	-2.03571300	-2.23255700	5.37262500
H	-5.04150100	-0.91919800	3.29010500	C	-2.27723700	-4.45422400	4.51797500
H	-3.35475800	-0.26266400	1.50524400	C	-1.74209500	-1.75902600	4.08841800
H	-2.30804100	4.92930200	-3.66335200	C	-1.99577800	-4.00675000	3.23227500
H	-4.06784900	5.04969800	-3.59896600	C	-1.72597200	-2.64571600	3.00201500
H	-1.32821400	3.24713800	-1.63647700	O	-1.46729600	-2.27517200	1.72265500
H	-4.89016100	5.32872800	-0.81834700	H	-1.84491900	-4.86394100	7.28167500
H	-4.31498600	3.90950300	1.22317200	H	-2.43917100	-3.27939700	7.73908500
H	-0.95656000	5.40945600	3.68104200	H	-2.03129700	-1.52852500	6.20365800
H	0.33221000	3.49098700	-4.97221400	H	-2.46481600	-5.51581000	4.67083800
H	0.74057300	4.68620300	-3.71253600	H	-1.50306600	-0.70999200	3.93238900
H	7.91506000	1.54356800	-0.30340600	H	-1.95170600	-4.68833200	2.38744300
H	-4.31649100	4.22329700	3.57505100	H	-1.29429700	-1.29979900	1.59279800
H	-4.36873100	3.50901300	5.19167900	H	-4.77219900	-3.94750500	7.03517000

H	-4.17053700	-5.53814400	6.55110100	C	6.50720300	-3.79546000	2.87725000
H	-4.11697700	-5.05814700	8.25563900	C	6.75275800	-2.45564600	3.60046400
C	-1.91634400	-2.93751600	-5.09133200	C	7.21957000	-1.39748500	2.58854200
C	-3.18209900	-2.94637000	-4.25131900	C	5.50123300	-1.95597300	4.33997400
O	-4.27061600	-3.25976800	-4.73970500	H	6.14531600	-5.91411400	3.23950900
N	-3.00374000	-2.56953400	-2.95969700	H	7.08276300	-5.12178700	4.51612100
C	-4.10292500	-2.46110500	-2.02081400	H	5.33599200	-4.85659200	4.39787600
C	-4.31540800	-0.98225300	-1.66823400	H	5.66566100	-3.67065200	2.18191000
O	-3.38647500	-0.32013300	-1.18014100	H	7.38596300	-4.02160500	2.25610200
C	-3.84663300	-3.25265400	-0.72019300	H	6.43284800	-1.25712600	1.83678800
O	-3.83382700	-4.63057700	-1.00108700	H	7.42526600	-0.43884800	3.08992600
N	-5.53793200	-0.42251200	-1.84897600	H	4.69565100	-1.76299400	3.62166600
C	-6.71272900	-1.00319200	-2.54266000	H	5.14449600	-2.68071000	5.08070000
C	-6.52243400	-1.02880000	-4.06376800	H	5.71285800	-1.02087500	4.87675600
C	-7.84402600	-0.06470100	-2.07769600	H	8.13818800	-1.70314500	2.07284100
C	-7.16067400	1.30917500	-1.97447900	H	7.55819200	-2.61020200	4.33747700
C	-5.75631600	0.97577100	-1.44532800	O	0.07882200	1.84539100	-3.08625300
H	-4.96851400	1.61742100	-1.85190000	N	-0.25919100	-0.09353200	-1.31469700
H	-5.69749200	1.05241500	-0.35150400	C	0.36559100	-1.28944800	-1.76570500
H	-7.09516200	1.77483900	-2.96440700	O	-0.23872200	-2.05426800	-2.54270900
H	-7.69709000	2.00339100	-1.31951200	N	1.63336100	-1.47978200	-1.37962700
H	-8.69519900	-0.07427100	-2.76503400	C	2.28415900	-0.68307100	-0.34569800
H	-8.20505100	-0.37903600	-1.09058800	C	1.23588000	-0.28062300	0.68409100
H	-6.88871300	-2.02016400	-2.17973200	C	0.01469600	0.44365600	0.09327500
H	-6.31088200	-0.02341200	-4.44770000	O	-1.09009400	0.24301000	0.89812600
H	-5.71286300	-1.70074400	-4.35972000	O	0.15617900	1.83838000	-0.07081900
H	-7.44144700	-1.38761600	-4.54460100	H	0.08786000	1.13559300	-2.32051500
H	-4.96911200	-2.89790200	-2.51658600	C	3.46343600	-1.49217600	0.29486700
H	-3.06390600	-5.02354800	-0.53261400	O	3.98894300	-0.95062300	1.29797400
H	-4.66404200	-3.00253100	-0.01647600	O	3.76980000	-2.56829900	-0.28027600
H	-2.91328400	-2.91164800	-0.25735300	H	2.72935500	0.20593900	-0.80898100
H	-2.06506100	-2.28645400	-2.66184500	H	0.87116700	-1.19705700	1.15893300
H	-2.06815800	-2.25335800	-5.93384700	H	1.67132300	0.33973800	1.46782900
H	-1.02809700	-2.64132300	-4.53331900	H	2.09377300	-2.36158700	-1.61445900
H	-1.78098600	-3.93744800	-5.52055700	H	-1.27597900	-0.20371300	-1.40602700
C	6.25232400	-4.98442600	3.81066000				

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C	3.11098100	7.69216700	-2.27182900	C	-0.02110900	5.09777400	4.31623900
C	2.54370400	6.69906900	-1.32345500	N	1.00744400	4.54585100	3.47384500
N	1.91550700	7.01209600	-0.12638600	C	0.69812400	3.43836800	2.70520600
C	2.49641200	5.33755400	-1.39528200	O	-0.54826400	3.17507900	2.63139200
C	1.52297900	5.85586800	0.46774700	O	1.66203200	2.85464800	2.14227400
N	1.85457700	4.82231600	-0.28663600	C	-3.80138600	3.52730600	4.21589700
C	7.06946100	1.04498000	-0.81081200	C	-3.98475600	2.14827400	3.64553900
C	5.80426900	1.52152500	-0.20315900	N	-3.29161300	1.66838100	2.53534200
N	5.51736900	1.37100400	1.14264300	C	-4.83971900	1.16787700	4.08048600
C	4.69383100	2.10437000	-0.74372300	C	-3.73343700	0.43745700	2.31344600
C	4.25676600	1.78814300	1.35978800	N	-4.67574400	0.10065400	3.21946200
N	3.73304500	2.26592300	0.24189700	C	-3.02279600	5.33083200	-3.04639000

C	-3.00442600	4.63805600	-1.73082000	N	1.38183800	-4.49507800	-4.54331600
N	-3.94300000	4.86999500	-0.73472400	C	2.15071000	-3.33128400	-4.96177400
C	-2.15072800	3.70723400	-1.20190400	H	5.12266800	-0.65578400	-2.46691500
C	-3.63383400	4.09231400	0.33188600	H	4.53408600	-2.08604700	-3.31221100
N	-2.55049700	3.38378800	0.07797900	H	5.47592900	-2.80729300	-1.03547700
C	1.14239200	3.73440000	-4.17730100	H	7.11288900	-0.54032800	-4.02292400
C	1.11692200	2.64472100	-3.08330600	H	-1.56802500	-6.36778900	-2.13635200
O	2.03951400	2.61993300	-2.23997600	H	-1.23564600	-4.68553400	-2.47238200
Zn	1.82356700	2.77625700	0.04149300	H	1.36889600	-4.79467500	-0.72961900
Zn	-1.54295100	2.10187700	1.31791000	H	0.66781600	-4.75611500	0.87213400
H	2.34882300	8.38055400	-2.65993600	H	0.06276200	-6.52075300	-3.80946100
H	3.90178000	8.30052300	-1.81418800	H	3.19696100	-3.46007400	-4.67421100
H	2.87353900	4.68175800	-2.16102000	H	1.76752900	-2.41883400	-4.49316600
H	1.78694500	7.93878300	0.25478400	H	0.67590100	-4.85768200	-5.16655200
H	1.05516900	5.80157300	1.44093200	H	1.00982600	-6.78829000	-2.34922400
H	7.14281300	1.39325800	-1.84540300	H	2.08589300	-3.24039300	-6.04867200
H	7.12110800	-0.05181100	-0.82763700	H	6.52044700	-1.96946300	-4.88169200
H	4.49721000	2.38703200	-1.76567100	H	5.58639100	-0.46072300	-4.92417200
H	6.01018500	0.74445800	1.76734000	C	-4.08022400	-4.61677900	7.22220700
H	3.74546700	1.72093000	2.30436600	C	-2.64803100	-4.09304500	7.00095200
H	-2.73725900	3.76621000	4.30009900	C	-2.36680200	-3.57843000	5.60046700
H	-5.53298200	1.13844600	4.90704300	C	-2.06510600	-2.23418900	5.35650200
H	-5.07147200	-0.82344300	3.32376000	C	-2.36243200	-4.44684900	4.49498400
H	-3.38181500	-0.21415000	1.52531000	C	-1.77315600	-1.76196700	4.07163000
H	-2.21586900	4.94352800	-3.67369400	C	-2.08267100	-4.00042800	3.20841400
H	-3.96477800	5.17009000	-3.58611800	C	-1.78535600	-2.64486300	2.98236400
H	-1.30180400	3.21893500	-1.65665000	O	-1.52704600	-2.27282200	1.70241600
H	-4.73352300	5.49583500	-0.79868600	H	-1.94312500	-4.90212900	7.24012900
H	-4.21129600	4.05654200	1.24252300	H	-2.44410900	-3.29320600	7.72464200
H	-0.86535500	5.43143100	3.70882300	H	-2.03784000	-1.53409300	6.19033000
H	0.45978700	3.48899400	-4.99358500	H	-2.57215900	-5.50456400	4.64600000
H	0.84146600	4.68820600	-3.72909300	H	-1.51227200	-0.71792800	3.91714000
H	7.94898500	1.41840500	-0.27081400	H	-2.06134300	-4.67949300	2.36060300
H	-4.26415700	4.30038200	3.58727000	H	-1.33880600	-1.30006600	1.58230100
H	-4.25883200	3.59391700	5.20737100	H	-4.81958000	-3.82554400	7.04943900
H	0.38193400	5.96440400	4.85173700	H	-4.31237900	-5.44041000	6.53766000
H	-0.40325300	4.38203900	5.05719200	H	-4.20878500	-4.98520000	8.24700400
H	3.55039500	7.16965300	-3.12525800	C	-1.94105500	-2.89365700	-5.09168700
H	2.16013100	3.84727900	-4.56047000	C	-3.21630100	-2.90160700	-4.26615500
H	-2.87929200	6.41474000	-2.94580300	O	-4.30544700	-3.18032200	-4.77251100
H	1.96429700	4.56989200	3.80039500	N	-3.04451600	-2.55936600	-2.96347300
C	6.20969400	-1.10216800	-4.28836200	C	-4.15048500	-2.42320400	-2.03697600
C	5.43669200	-1.53192900	-3.04270600	C	-4.31434000	-0.94045600	-1.67526400
S	6.46763700	-2.61473400	-1.95958700	O	-3.36292700	-0.31329100	-1.18209300
C	0.42881300	-6.03728600	-2.89603200	C	-3.93460700	-3.23365100	-0.74023600
C	1.37635000	-4.89916600	-3.24994100	O	-3.94965500	-4.60890100	-1.03315500
O	2.11471600	-4.37669000	-2.40862700	N	-5.51593900	-0.33934400	-1.85361100
C	-0.79390300	-5.59917300	-2.05859200	C	-6.70720100	-0.87803800	-2.55368900
C	-0.61785100	-5.35623200	-0.55936000	C	-6.51359200	-0.90055100	-4.07454200
O	-1.60985300	-5.45724800	0.18156400	C	-7.80876100	0.09377900	-2.08605100
N	0.60506000	-5.04479600	-0.09598500	C	-7.08187900	1.44439600	-1.97247100

C	-5.69021500	1.06330600	-1.44191800	H	7.31922200	-4.10946900	2.30263700
H	-4.88121600	1.68163800	-1.84260300	H	6.37136300	-1.33993800	1.90262900
H	-5.63193900	1.13104200	-0.34759700	H	7.34150100	-0.53798900	3.18230000
H	-6.99880300	1.91429800	-2.95900900	H	4.60579300	-1.86615100	3.65094300
H	-7.59738800	2.15111100	-1.31421200	H	5.02753100	-2.80691300	5.10336400
H	-8.65764900	0.11575000	-2.77589500	H	5.60037800	-1.14451500	4.93474200
H	-8.18274700	-0.21483600	-1.10197700	H	8.07350700	-1.78953200	2.16225300
H	-6.91634500	-1.89091000	-2.19690100	H	7.45545200	-2.72347400	4.40526600
H	-6.27067800	0.10016100	-4.45182900	O	0.10323600	1.84967900	-3.10363100
H	-5.72376000	-1.59429900	-4.37354400	N	-0.27925500	-0.07945400	-1.33045200
H	-7.44194400	-1.22830700	-4.55948900	C	0.34351200	-1.30645300	-1.77218900
H	-5.02490800	-2.82636200	-2.54630700	O	-0.27778200	-2.07183300	-2.52633600
H	-3.18432100	-5.01925300	-0.57272600	N	1.60140600	-1.49476600	-1.37404100
H	-4.75707400	-2.97086200	-0.04759900	C	2.25455200	-0.70290300	-0.33512300
H	-3.00091400	-2.91916600	-0.25949100	C	1.21244200	-0.30340000	0.70149600
H	-2.10767900	-2.28891800	-2.65497800	C	0.00478100	0.45939900	0.13662300
H	-1.04456800	-2.69333400	-4.50578300	O	-1.10667400	0.25381600	0.91152400
H	-1.85713600	-3.85830300	-5.60540200	O	0.16362800	1.83008400	-0.03135600
H	-2.04228100	-2.13066000	-5.87225900	H	0.01148700	0.96026700	-2.22159000
C	6.16677800	-5.09413100	3.82926300	C	3.42741100	-1.53108200	0.29760100
C	6.43133800	-3.89291000	2.91410600	O	3.95570400	-1.00699800	1.30679700
C	6.66262600	-2.56095900	3.65640800	O	3.71892400	-2.60378700	-0.29137900
C	7.14570800	-1.49029200	2.66521200	H	2.70464400	0.18369500	-0.79542400
C	5.39823300	-2.07129600	4.38041500	H	0.83463400	-1.22171200	1.16211600
H	6.07101900	-6.01707900	3.24532200	H	1.66223200	0.29797500	1.49231300
H	6.98757900	-5.23746300	4.54469100	H	2.06411600	-2.37950400	-1.60223900
H	5.24184600	-4.97642700	4.40492200	H	-1.29971600	-0.20853600	-1.38916800
H	5.59924800	-3.76224500	2.20855400				

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C	2.46166900	7.92992500	-2.72486800	C	-5.39395000	1.21155800	3.73005900
C	1.90880500	6.96128000	-1.74332100	C	-4.17568900	0.35615900	2.09030900
N	1.14998600	7.29928000	-0.63158100	N	-5.15432400	0.07847300	2.97578600
C	1.99241900	5.60047500	-1.70583200	C	-3.34099300	4.88055600	-3.63564600
C	0.81400500	6.15688000	0.02152200	C	-3.41872000	4.21217000	-2.30564800
N	1.30348000	5.10675100	-0.61450600	N	-4.47604800	4.39249500	-1.42360900
C	6.96123000	1.87812200	-0.46238800	C	-2.55632000	3.36638100	-1.65885500
C	5.58901300	2.21392800	0.00119400	C	-4.22933700	3.67661100	-0.30300200
N	5.21335500	2.15867400	1.33342300	N	-3.06847300	3.04970100	-0.41349400
C	4.45783500	2.58384600	-0.67093300	C	1.02816000	3.64457700	-4.38345100
C	3.89759000	2.43100300	1.42092200	C	0.85104700	2.73481700	-3.16266900
N	3.40972900	2.71906500	0.22612600	O	1.76769700	2.82331200	-2.26042400
C	-0.81998100	5.56686800	3.87742100	Zn	1.50026000	3.05059200	-0.25775700
N	0.24513100	4.99776700	3.08993500	Zn	-2.10325500	2.17382200	1.12662000
C	0.02886100	3.87423100	2.32112700	H	1.67510300	8.50789700	-3.22737900
O	-1.20744900	3.56318400	2.16045000	H	3.15186800	8.64639400	-2.26091600
O	1.04349000	3.31414600	1.83398000	H	2.48701400	4.92721900	-2.38460400
C	-4.40937200	3.60417600	3.70118400	H	0.89915700	8.23453000	-0.34333000
C	-4.53894000	2.17406300	3.26023000	H	0.26046200	6.13422100	0.94839700
N	-3.77672400	1.61592900	2.23560500	H	7.07659700	2.15186700	-1.51511900

H	7.15807300	0.80157600	-0.37755800	H	7.16821700	-1.40781900	-4.23305100
H	4.30597500	2.73860100	-1.72773200	H	5.91931800	-0.19501900	-4.56817300
H	5.74422200	1.69328200	2.05912400	C	-4.06815800	-4.25115200	7.39160400
H	3.32735000	2.40403300	2.33436300	C	-2.59201100	-3.87407600	7.17155300
H	-3.35873400	3.86636700	3.85599500	C	-2.27332800	-3.45960000	5.74883900
H	-6.13191900	1.23346900	4.51691400	C	-2.18002000	-2.11267100	5.38191600
H	-5.57545100	-0.83118500	3.10476800	C	-2.06632400	-4.41993600	4.74546900
H	-3.81144900	-0.34685500	1.34797800	C	-1.88707000	-1.72608900	4.07123800
H	-2.45337300	4.52413200	-4.16428500	C	-1.77838600	-4.05811100	3.43353700
H	-4.21320500	4.65653200	-4.26237900	C	-1.68255400	-2.70338400	3.09032700
H	-1.63342800	2.93081000	-2.02463900	O	-1.37335400	-2.40322100	1.79345600
H	-5.30398200	4.94545700	-1.59635400	H	-1.96344100	-4.72949500	7.45211200
H	-4.89677200	3.62740300	0.54361800	H	-2.32379200	-3.05978900	7.85699300
H	-1.66935800	5.81249700	3.23607400	H	-2.31922600	-1.34259300	6.13893700
H	0.42663600	3.28187500	-5.22007300	H	-2.12202800	-5.47686100	4.99861900
H	0.69639300	4.65819100	-4.12495700	H	-1.78384400	-0.67503400	3.81439800
H	7.72736600	2.41654200	0.10944900	H	-1.61233400	-4.80777600	2.66541200
H	-4.81130200	4.29905400	2.95205800	H	-1.41219500	-1.43408300	1.62985400
H	-4.95717200	3.76773700	4.63348800	H	-4.72717500	-3.40471800	7.16405300
H	-0.46244800	6.48856700	4.34745400	H	-4.36278500	-5.08358000	6.74238300
H	-1.17750900	4.89387500	4.66977500	H	-4.24783400	-4.55209200	8.43056800
H	3.01682800	7.38842400	-3.49481000	C	-1.30991400	-3.32371100	-4.88476300
H	2.07946400	3.70650300	-4.68180900	C	-2.64685000	-3.40797200	-4.16340100
H	-3.26638600	5.97168000	-3.54291200	O	-3.68606600	-3.71092600	-4.75088900
H	1.19709000	5.09983700	3.41380600	N	-2.59842600	-3.09648700	-2.83271400
C	6.55037900	-0.62439000	-3.78073900	C	-3.73544000	-3.31878000	-1.95166700
C	5.68003000	-1.18617200	-2.65767700	C	-4.31567700	-1.98060200	-1.45681200
S	6.72239300	-1.92591900	-1.32271200	O	-3.68142100	-1.29520200	-0.63563900
C	2.19706200	-6.37811900	-2.27109000	C	-3.32584500	-4.15583700	-0.71361300
C	2.77794700	-5.51038200	-3.39064800	O	-2.86645200	-5.43053500	-1.08258200
O	3.62853500	-5.94515700	-4.16445000	N	-5.54325600	-1.57015900	-1.87337800
C	2.32299200	-5.79295100	-0.84758900	C	-6.45863600	-2.17325600	-2.87475300
C	1.02831700	-5.17756900	-0.30895700	C	-6.11573200	-1.74677000	-4.30812700
O	-0.07653100	-5.63332700	-0.61745400	C	-7.82415500	-1.64517500	-2.39507100
N	1.19645300	-4.18247500	0.59469400	C	-7.50752600	-0.21757900	-1.91777100
N	2.30783800	-4.23217500	-3.46493000	C	-6.11288600	-0.34872300	-1.28063500
C	2.78776000	-3.31599500	-4.48477800	H	-5.46499600	0.51438100	-1.46947400
H	5.06107100	-0.39665100	-2.22075200	H	-6.16832800	-0.47017100	-0.19127900
H	5.01448200	-1.96199000	-3.04295400	H	-7.47705500	0.46908200	-2.77066900
H	5.68068700	-2.25843700	-0.51495900	H	-8.24812400	0.17087100	-1.21141500
H	7.22030400	0.16219500	-3.41461200	H	-8.58151000	-1.67886100	-3.18395300
H	3.14627900	-5.07409100	-0.77568400	H	-8.18390400	-2.25232400	-1.55515700
H	2.56543600	-6.60665600	-0.15091500	H	-6.41386000	-3.26241700	-2.80371000
H	2.08044300	-3.67699500	0.64175100	H	-6.09784300	-0.65449500	-4.40530900
H	0.36225200	-3.69699300	0.90986700	H	-5.15093100	-2.15762100	-4.61021100
H	1.13647100	-6.58293300	-2.46337700	H	-6.87293800	-2.13792300	-4.99888000
H	3.84856000	-3.50656900	-4.66337100	H	-4.46680500	-3.88391700	-2.53070600
H	2.64881600	-2.28842500	-4.13743400	H	-1.89700500	-5.46116500	-0.95460600
H	1.51523900	-3.92966300	-2.90064600	H	-4.21978600	-4.26513900	-0.07816700
H	2.73259900	-7.32699400	-2.34142800	H	-2.58579600	-3.59399500	-0.13254100
H	2.25929700	-3.44049900	-5.44068700	H	-1.66088700	-3.04483300	-2.42087200

H	-1.48787700	-3.45640100	-5.95334200	O	-0.16456200	2.01939700	-3.10117300
H	-0.81859900	-2.36400400	-4.70232500	N	-0.42425100	-0.60527400	-1.76798600
H	-0.62928600	-4.10432500	-4.53039800	C	0.46135700	-1.65067900	-1.75942000
C	6.37536600	-3.92238800	4.64101900	O	0.13450500	-2.79244500	-2.15562700
C	6.55539300	-2.81313700	3.59810400	N	1.71092200	-1.41947300	-1.27707500
C	6.56637100	-1.38484900	4.17977700	C	2.11858300	-0.49856900	-0.22338400
C	7.01988200	-0.38401400	3.10568900	C	1.07879400	-0.25148700	0.88317000
C	5.19364400	-0.97281900	4.73504000	C	-0.09303300	0.65592500	0.63606300
H	6.42949500	-4.91184600	4.17252800	O	-1.19054500	0.40262200	1.25614000
H	7.15830300	-3.87534800	5.40936700	O	-0.01862500	1.73125500	-0.03645400
H	5.40675500	-3.85609400	5.14931200	H	-0.11727700	0.33306300	-2.03746800
H	5.76618300	-2.87736000	2.83605300	C	3.36884600	-1.14737800	0.50855800
H	7.50455800	-2.98205900	3.06990700	O	3.89240300	-0.43504700	1.38948100
H	6.31425900	-0.40843600	2.26604400	O	3.68230300	-2.31872300	0.14688000
H	7.06432300	0.63652500	3.51839300	H	2.44220600	0.45545500	-0.64806200
H	4.45483700	-0.94535900	3.92497400	H	0.70629200	-1.20278200	1.26744400
H	4.83770700	-1.66409500	5.50723000	H	1.63934500	0.21988200	1.70248200
H	5.23949100	0.02640800	5.18964600	H	2.30574700	-2.24839500	-1.24300500
H	8.01848500	-0.62427900	2.72126200	H	-1.34182100	-0.84981300	-2.12056600
H	7.29802700	-1.36154800	5.00386200				

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C	5.24174600	6.76225800	-1.77819200	N	-1.58043000	3.87367300	0.09109900
C	4.44895300	5.92101900	-0.84860100	C	2.41936400	3.51250500	-3.93302700
N	3.91780300	6.34075300	0.36194000	C	1.99368700	2.58696900	-2.78381100
C	4.05428200	4.62268200	-0.97285500	O	2.90482900	2.23255500	-1.94889000
C	3.23407800	5.30557300	0.91269200	O	0.78379800	2.28221400	-2.68897400
N	3.29221900	4.25002700	0.11746300	Zn	2.56858100	2.31836200	0.16101400
C	7.31410900	-0.72527700	-0.50096200	Zn	-0.81119400	2.39735400	1.29953200
C	6.11406600	-0.03511400	0.06067500	N	-0.70522100	-0.76490300	-0.67933800
N	5.75811800	-0.11602800	1.39871400	C	-0.02664300	-1.68731300	-1.52092900
C	5.14000900	0.74503800	-0.50855000	O	-0.60731800	-2.13706500	-2.50538100
C	4.61840100	0.58727300	1.59264600	N	1.21200100	-2.03545000	-1.13565000
N	4.21467500	1.11857600	0.45006200	C	1.94512400	-1.35928600	-0.07890600
C	1.26463000	4.81180900	4.57174900	C	1.01664500	-0.94449600	1.04231400
N	2.08983500	3.94734500	3.75267800	C	-0.29744000	-0.37062400	0.53478400
C	1.52121600	3.02587000	2.90228900	O	-1.06499100	0.25855500	1.30846200
O	0.25327300	3.12442400	2.76685300	H	4.67339200	7.62683600	-2.14115100
O	2.29167500	2.20887000	2.31704600	H	6.16033500	7.14340600	-1.31661700
C	-2.78220700	4.26437700	4.27112300	H	4.23923400	3.92499200	-1.77105500
C	-3.35046400	3.07719100	3.54277800	H	4.02256400	7.25691000	0.77262800
N	-2.73940500	2.39978000	2.48080800	H	2.74328000	5.34167500	1.87421000
C	-4.56181400	2.48641800	3.79805400	H	7.45196600	-0.43716000	-1.54500000
C	-3.58382400	1.44271000	2.11802800	H	7.20874000	-1.81429600	-0.46117200
N	-4.69411500	1.45946300	2.88756500	H	5.01967700	1.06218700	-1.53236800
C	-1.24996800	6.07723400	-2.86788800	H	6.23756500	-0.66166700	2.10041200
C	-1.56243100	5.34155400	-1.61435500	H	4.11793700	0.71034500	2.54007100
N	-2.50149700	5.72006400	-0.66517100	H	-1.78432800	4.04299400	4.65917300
C	-1.00846200	4.19491700	-1.12367800	H	-5.31609500	2.70386000	4.53757300
C	-2.48110700	4.81088200	0.34138600	H	-5.45445000	0.79817500	2.83211600

H	-3.43348700	0.74786400	1.30510100	H	4.45708300	-6.22821100	4.75378900
H	-0.52131500	5.50115400	-3.44104800	H	5.14833500	-1.17887300	-2.62002000
H	-2.13423900	6.21849900	-3.50013400	H	4.00528800	-2.08054900	-3.59456800
H	-0.26449000	3.57707400	-1.60080500	H	3.89445400	-4.15013800	-2.27451900
H	-3.10502400	6.52812200	-0.71106500	H	7.06465700	-2.50849700	-3.60489700
H	-3.12343100	4.85462500	1.20643600	H	0.53315500	-5.88075200	-0.70550000
H	0.54104200	5.33394100	3.94444400	H	-0.81571100	-6.99759500	-0.95399000
H	1.69412200	3.46925600	-4.74690600	H	-0.38737300	-4.31152300	0.66049900
H	2.46045900	4.53993000	-3.55300200	H	-1.88532600	-3.50455900	0.37520100
H	2.45381300	-0.47296900	-0.46789000	H	-0.95891200	-6.12538300	-3.35802900
H	2.70741900	-2.03853800	0.30743000	H	2.69094300	-3.78087400	-4.87155700
H	1.48026900	-0.22589700	1.71938600	H	1.40671000	-2.59427400	-4.51826900
H	8.22706500	-0.45376200	0.04063400	H	0.02139300	-4.93963900	-5.03764500
H	-2.68496000	5.13821800	3.61621900	H	0.47056600	-7.09352500	-2.97216700
H	-3.43363300	4.53749600	5.10395700	H	1.43987200	-3.43999500	-6.08432300
H	1.90242000	5.55094100	5.06388500	H	5.92328600	-3.40765200	-4.60537500
H	0.70975700	4.26552700	5.34540600	H	6.14603200	-1.66859000	-4.86941500
H	5.53053000	6.16736100	-2.64664600	H	5.63181600	-7.14952300	3.80680500
H	3.41523200	3.25532000	-4.30322200	H	3.90217300	-7.33015700	3.49509600
H	-0.82288400	7.06807300	-2.67203100	C	-5.25258300	-3.64378700	6.87880300
H	3.02226900	3.72072200	4.06580300	C	-4.11001500	-4.51209200	6.33098400
H	-1.65414200	-0.46627500	-0.98080500	C	-3.62500800	-3.94537400	5.02058000
H	1.63192300	-2.80824400	-1.65302500	C	-2.65645900	-2.93610700	4.99432700
O	0.68289300	1.85088300	0.02840500	C	-4.23780800	-4.31014200	3.81456800
H	0.52444000	1.85346500	-0.94299700	C	-2.32884200	-2.27943900	3.81012900
C	4.68240700	-6.60615500	3.75142700	C	-3.93149800	-3.66328600	2.62170800
C	4.76108200	-5.47776100	2.71517600	C	-2.99256600	-2.63053400	2.63380700
C	5.87258000	-4.45671800	3.04666300	O	-2.73607300	-1.99413500	1.44222400
C	6.25660600	-3.62085800	1.82149700	H	-4.46048200	-5.54168200	6.19551700
C	5.49018300	-3.54809000	4.22505800	H	-3.29153400	-4.54936400	7.05935700
C	6.09249000	-2.45085300	-4.10274500	H	-2.15684200	-2.64968600	5.91669100
C	4.98036500	-2.14215400	-3.10629800	H	-4.98310100	-5.10159100	3.81257400
S	4.85093800	-3.36987700	-1.72902000	H	-1.56242500	-1.50956600	3.78841100
C	-0.03560300	-6.14131900	-2.77183000	H	-4.41269500	-3.93857400	1.68788600
C	0.91114500	-5.03087600	-3.21087000	H	-2.20734200	-1.18990500	1.59649900
O	1.77501900	-4.57243800	-2.44568100	H	-4.91453500	-2.61531800	7.04240400
C	-0.37947700	-6.04766400	-1.28305200	H	-6.08835900	-3.61037600	6.17260100
C	-1.42331200	-4.96708000	-1.00300500	H	-5.63059500	-4.03092900	7.83137400
O	-2.39093500	-4.81795800	-1.75396500	C	-2.18481900	-2.01690600	-5.25382900
N	-1.23413500	-4.24010000	0.11929700	C	-3.51006800	-1.78537400	-4.55795300
N	0.80201800	-4.61394800	-4.48760500	O	-4.54535300	-1.57536700	-5.18788700
C	1.63455900	-3.54210600	-5.01587800	N	-3.43866700	-1.77939200	-3.19616300
H	4.95828600	-5.91325000	1.72756600	C	-4.56280600	-1.38913900	-2.37040500
H	3.79566000	-4.95862300	2.63785300	C	-4.31233700	0.01180400	-1.79358400
H	6.76261000	-5.03135900	3.34252600	O	-3.28593300	0.22892300	-1.10744400
H	6.59441500	-4.25070300	0.99279900	C	-4.79208500	-2.36142500	-1.18496300
H	7.07573200	-2.92910200	2.06192200	O	-5.00040000	-3.68741200	-1.58704300
H	5.40393000	-3.03796700	1.45427800	N	-5.21905700	0.98744000	-1.97578500
H	6.31521600	-2.87702100	4.49249500	C	-6.45608300	0.93896100	-2.80274200
H	4.61887300	-2.92966200	3.97203300	C	-6.14198100	1.03936900	-4.29716800
H	5.23634600	-4.12008400	5.12203900	C	-7.24060200	2.14739500	-2.25735800

C	-6.14497200	3.17660900	-1.93395600	H	-7.07873900	1.05431800	-4.86543200
C	-4.99903100	2.31872900	-1.37847400	H	-5.43418300	-1.41509900	-3.02248800
H	-4.00243100	2.68841300	-1.63339400	H	-4.12468900	-4.09057600	-1.73864200
H	-5.04308900	2.23700400	-0.28596500	H	-5.69421600	-2.02680900	-0.65379500
H	-5.82800000	3.69290200	-2.84541000	H	-3.95587400	-2.26010100	-0.48548500
H	-6.47321300	3.93781000	-1.22096800	H	-2.53357900	-1.96148600	-2.76984700
H	-7.97828600	2.51211500	-2.97600400	H	-1.65311500	-1.06261800	-5.33630000
H	-7.77362400	1.86538200	-1.34204900	H	-1.54268200	-2.70438600	-4.70121500
H	-6.99270900	0.00845100	-2.59796400	H	-2.38134500	-2.39058300	-6.25990500
H	-5.59922800	1.96397700	-4.52183200	F	0.63406800	-2.08180400	1.78378300
H	-5.55414000	0.19068000	-4.65079900				

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C	-5.69499600	-6.35911900	-1.98267600	H	-4.67101800	-3.52720500	-1.79469000
C	-4.74994900	-5.62206700	-1.10247200	H	-4.06338700	-7.14750300	0.23833700
N	-4.02309200	-6.18478700	-0.06267500	H	-2.59590700	-5.38098200	1.33621300
C	-4.36973900	-4.31193100	-1.12261000	H	-7.44080900	0.99005900	-1.49346500
C	-3.24813400	-5.21862500	0.49252900	H	-7.11546000	2.26269600	-0.30866000
N	-3.43127200	-4.07022100	-0.13633000	H	-5.10465300	-0.65225300	-1.56437100
C	-7.30126600	1.19049700	-0.42940500	H	-6.29494400	0.84247300	2.17604400
C	-6.16484100	0.37613800	0.09513500	H	-4.26833900	-0.68253600	2.53765800
N	-5.83511800	0.32471100	1.44101500	H	1.43933000	-4.36879500	4.44242500
C	-5.22819500	-0.41432700	-0.51981000	H	4.99123400	-3.04820200	4.67763800
C	-4.74364700	-0.45942500	1.59571500	H	5.24283700	-1.06119300	3.07487600
N	-4.34774000	-0.92044600	0.42026900	H	3.34956600	-0.93970900	1.40920900
C	-1.60604200	-4.89061700	4.42571500	H	0.13188200	-5.40918000	-3.62121200
N	-2.36718200	-3.96275100	3.61505700	H	1.69571800	-6.22580100	-3.70118300
C	-1.75705300	-3.13141900	2.71357800	H	0.04468900	-3.47219800	-1.74378800
O	-0.52325200	-3.38409100	2.48701200	H	2.64777100	-6.65997700	-0.93340300
O	-2.46590100	-2.23572400	2.16173500	H	2.79856800	-5.03861100	1.02446300
C	2.46692300	-4.58336100	4.13674600	H	-0.94958300	-5.48777400	3.79096400
C	3.10713700	-3.37453000	3.52176700	H	-1.93531500	-3.22969000	-4.82351900
N	2.57897500	-2.65436600	2.44766500	H	-2.82282200	-4.23400400	-3.65210000
C	4.29397200	-2.79840700	3.89387500	H	-8.24115500	0.94995900	0.07963700
C	3.44580400	-1.68219900	2.18708600	H	2.42397400	-5.42576100	3.43595200
N	4.49244700	-1.73511800	3.03717400	H	3.03427100	-4.90575800	5.01258900
C	0.82680500	-6.03672300	-3.06029400	H	-2.29718800	-5.55956600	4.94472900
C	1.19585400	-5.34026000	-1.79953300	H	-0.98442200	-4.38717400	5.17739900
N	2.10580400	-5.81104500	-0.86363400	H	-6.12549800	-5.66789600	-2.70948300
C	0.73575200	-4.16219600	-1.28345400	H	-3.63797600	-2.86374800	-4.40986400
C	2.16084000	-4.92679900	0.16208800	H	0.33907800	-7.00065700	-2.87231500
N	1.33513600	-3.91703700	-0.06407300	H	-3.28262600	-3.67206800	3.92272600
C	-2.67699800	-3.21332500	-4.02369300	C	-4.31215300	6.73881600	4.02873400
C	-2.19788500	-2.33926900	-2.86086000	C	-4.46023000	5.65590800	2.95216400
O	-3.08805100	-1.94889800	-2.02015700	C	-5.60123400	4.67166600	3.28749000
O	-0.97244500	-2.10453000	-2.75617100	C	-5.97153600	3.80647600	2.07804500
Zn	-2.72310500	-2.12367800	0.05051600	C	-5.27345800	3.79446600	4.52684300
Zn	0.72466800	-2.50861500	1.27035000	C	-5.97488500	2.96754700	-3.96855800
H	-5.19847900	-7.16218100	-2.53973800	C	-4.87530800	2.57923800	-2.98575100
H	-6.52185600	-6.80883400	-1.42081300	S	-4.66809600	3.77640200	-1.59010400

C	0.28432700	6.37567300	-2.61885400	H	4.92374300	2.92835000	1.87937200
C	-0.64621200	5.24319000	-3.03150200	H	2.07439300	0.85460500	1.70552900
O	-1.46175100	4.75705400	-2.23198200	H	4.97390100	2.07531600	7.21483800
C	0.97343400	6.12493000	-1.27533500	H	6.27248700	2.91023300	6.35384200
C	2.26864800	5.32450500	-1.40806900	H	5.80344800	3.44453900	7.97572000
O	2.64841500	4.86140900	-2.48903000	N	0.65639800	0.61923300	-0.58243600
N	2.98455800	5.18396700	-0.26926100	C	0.13325500	1.69968100	-1.31192400
N	-0.60009900	4.86617100	-4.32476000	O	0.80151300	2.21086400	-2.21370400
C	-1.45793700	3.81419100	-4.85068400	N	-1.08076300	2.14820400	-0.93938200
H	-4.66498900	6.13167800	1.98494000	C	-1.93642900	1.47021200	0.01888300
H	-3.51947500	5.10061800	2.83468700	C	-1.11261800	0.78708500	1.09376300
H	-6.48260500	5.28303800	3.52540100	C	0.11044300	0.06904300	0.53954300
H	-6.24569500	4.41644900	1.21176800	O	0.90401800	-0.51874700	1.36453500
H	-6.82975700	3.16194900	2.31354800	H	-2.56913100	0.72935100	-0.47902500
H	-5.13152200	3.17037900	1.77510300	H	-2.59491600	2.20640100	0.48496300
H	-5.30863600	2.72587200	4.28284000	H	-1.70022700	0.08778600	1.68809900
H	-4.27008200	3.99456400	4.91564300	H	1.60781200	0.31147300	-0.83566100
H	-5.97612000	3.95817600	5.34901200	H	-1.39344100	2.99452200	-1.41505100
H	-4.09489600	6.30812600	5.01170100	O	-0.80649100	-1.57820600	-0.08433300
H	-5.09450600	1.61622500	-2.51989300	H	-0.67992100	-1.59698100	-1.06769800
H	-3.90817300	2.47412500	-3.48191600	C	2.27049400	2.09626500	-5.12000100
H	-3.59141900	4.43339600	-2.07258300	C	3.56864500	1.71474100	-4.44510200
H	-6.93873600	3.07380100	-3.46218500	O	4.61967100	1.54844000	-5.06157000
H	0.28493000	5.59345200	-0.60821400	N	3.44503700	1.55147600	-3.09765800
H	1.21004400	7.07860100	-0.79006100	C	4.54751000	1.15419700	-2.24946700
H	2.65103400	5.52208600	0.61875500	C	4.28541100	-0.25430400	-1.69637600
H	3.86118300	4.67008200	-0.32110800	O	3.26662300	-0.47292000	-1.00717500
H	1.03199200	6.57486000	-3.39052800	C	4.69450200	2.14692900	-1.07945400
H	-2.50915100	4.07240400	-4.69821900	O	4.97238200	3.46134900	-1.52773300
H	-1.24789300	2.85917500	-4.35885700	N	5.17051900	-1.24107000	-1.93431300
H	0.16609700	5.19765600	-4.89105500	C	6.38482400	-1.19656700	-2.79359800
H	-0.35282300	7.26352900	-2.53080000	C	6.03124500	-1.23121800	-4.28350300
H	-1.27350100	3.71333100	-5.92102000	C	7.14902000	-2.44564900	-2.31363900
H	-5.75419700	3.92111600	-4.45691800	C	6.03431000	-3.45526800	-1.99504900
H	-6.08013800	2.20180600	-4.74659100	C	4.92674500	-2.58660300	-1.38098100
H	-5.23389900	7.32382200	4.12025600	H	3.91473400	-2.91869200	-1.62727900
H	-3.50094500	7.43415000	3.79003100	H	4.99482600	-2.54601000	-0.28698900
C	5.42045800	3.05694500	7.02536700	H	5.67976000	-3.93123900	-2.91466800
C	4.39063700	4.01216300	6.40117400	H	6.36016800	-4.24897700	-1.31731200
C	3.87962500	3.45251000	5.09581200	H	7.85642700	-2.80479800	-3.06487300
C	2.68399700	2.72918800	5.02766200	H	7.71425200	-2.21097900	-1.40438700
C	4.66536400	3.53481300	3.93808600	H	6.95525100	-0.29061600	-2.57026600
C	2.29508600	2.07218300	3.86069100	H	5.43868100	-2.12009100	-4.52551100
C	4.30173200	2.87874200	2.76748000	H	5.48043000	-0.34199400	-4.59500100
C	3.12461400	2.12119700	2.73575400	H	6.95286900	-1.27086900	-4.87476800
O	2.84327500	1.44566800	1.58716200	H	5.44330400	1.19485500	-2.86799900
H	4.85346000	4.99373800	6.24173700	H	4.24911100	3.74960200	-2.12453700
H	3.55926400	4.16664900	7.09847000	H	5.53933100	1.84244600	-0.44992900
H	2.04745600	2.66724200	5.90728200	H	3.79148400	2.10399100	-0.46001200
H	5.59097200	4.10566500	3.96074800	H	2.53427000	1.74137200	-2.67496700
H	1.35407000	1.53225900	3.80806100	H	1.57451300	1.25117600	-5.09785700

H	1.79477500	2.92884900	-4.59588000	F	-0.58734800	1.76465200	1.95528200
H	2.47829900	2.36353800	-6.15657300				

SkDHPase.5FUH2-INT1-II- L

C	4.79878700	7.01404200	-2.04117100	H	-2.02646600	4.27412300	4.14120300
C	3.89965700	6.18317500	-1.19733200	H	-5.25745000	2.26978500	4.88720200
N	2.94596600	6.67133200	-0.31409300	H	-5.20013800	0.17628600	3.40354200
C	3.77799000	4.82699700	-1.12355000	H	-3.43612200	0.33107700	1.59895500
C	2.29695900	5.61812800	0.24479400	H	-0.81483400	5.26236800	-3.69500500
N	2.77697800	4.48348600	-0.23428200	H	-2.47603100	5.84336200	-3.83599400
C	7.39225900	-0.22413500	-0.34650100	H	-0.53717800	3.37951300	-1.72400100
C	6.16915000	0.45068000	0.16845600	H	-3.56535300	6.22575300	-1.14145200
N	5.81622800	0.46556200	1.50899500	H	-3.58387200	4.67297700	0.87424300
C	5.16112300	1.12764400	-0.46482500	H	0.19560600	5.65630200	3.70417200
C	4.64165300	1.12145000	1.64458900	H	1.50209700	3.37023000	-4.83848900
N	4.21771700	1.53365600	0.46086600	H	2.28605300	4.49378800	-3.69809800
C	0.87670200	5.10706300	4.35602700	H	8.29640700	0.12582400	0.16381500
N	1.71188600	4.22670600	3.56451900	H	-3.39371300	5.04261900	3.33493400
C	1.21900100	3.42096800	2.57869300	H	-3.56485300	4.48891400	5.00297000
O	-0.00010800	3.62094900	2.24194100	H	1.51209900	5.82264700	4.88340000
O	2.02277600	2.58831800	2.04991900	H	0.27720800	4.56652700	5.09995100
C	-3.11421300	4.24793400	4.03752400	H	5.43561400	6.36112500	-2.64069400
C	-3.56886600	2.90146800	3.56741600	H	3.24401300	3.22125800	-4.45466400
N	-2.98995400	2.23733200	2.48895200	H	-1.26853600	6.82440700	-2.99330600
C	-4.58014100	2.12073400	4.06166000	H	2.64033900	4.00234200	3.88709200
C	-3.64757200	1.09097600	2.33925800	C	5.13134600	-6.05496600	4.17932600
N	-4.61516800	0.98865500	3.27030000	C	5.14348200	-4.97900300	3.08594900
C	-1.60790100	5.79677600	-3.16884800	C	6.14195200	-3.84121400	3.39361800
C	-1.91553800	5.08534600	-1.89714700	C	6.40875600	-2.97764100	2.15668500
N	-2.91702600	5.46230900	-1.01417700	C	5.68613600	-2.96703000	4.57210100
C	-1.32745800	3.99368300	-1.31841700	C	6.35589900	-2.21923200	-3.86620900
C	-2.90062200	4.61405200	0.04151800	C	5.21336800	-2.12123100	-2.85987900
N	-1.94164000	3.71507600	-0.11217900	S	5.27616000	-3.44913700	-1.56911900
C	2.25497600	3.45785800	-4.05428300	C	0.56476700	-6.40977600	-2.52085700
C	1.91721000	2.55323200	-2.87476700	C	1.36174000	-5.18274100	-2.94088200
O	2.84912400	2.32020700	-2.02684400	O	2.12341000	-4.60791600	-2.14651200
O	0.73737400	2.13370000	-2.76092300	C	-0.13959900	-6.23400500	-1.17351100
Zn	2.46274000	2.45549800	0.03512100	C	-1.53351400	-5.62090900	-1.30434300
Zn	-1.29791800	2.44375900	1.33034200	O	-2.00474300	-5.28402900	-2.39506100
H	4.23905300	7.65782900	-2.72949700	N	-2.23250600	-5.51998200	-0.14994900
H	5.45267300	7.65920200	-1.44309500	N	1.26694000	-4.81668200	-4.23463200
H	4.30621500	4.07273000	-1.68010900	C	2.00424700	-3.68199000	-4.77241500
H	2.76225700	7.64399800	-0.11560400	H	5.41625200	-5.44186100	2.12948000
H	1.50148200	5.71118400	0.96784200	H	4.13730400	-4.55874300	2.95115000
H	7.50941000	-0.01384400	-1.41131100	H	7.09434800	-4.31409200	3.67584700
H	7.33176800	-1.31028900	-0.22166600	H	6.77325600	-3.57543700	1.31619100
H	5.02670700	1.33737400	-1.51401600	H	7.16928500	-2.21431600	2.37405200
H	6.31548600	-0.00479700	2.25060700	H	5.49432800	-2.47521600	1.81964600
H	4.12433200	1.28086300	2.57741300	H	6.42779800	-2.19163000	4.79912300

H	4.73577400	-2.46823400	4.34127300	C	1.24443300	-0.56756100	0.99156400
H	5.53879700	-3.54859800	5.48622800	C	0.10718700	0.21615700	0.30499000
H	4.80381700	-5.65725400	5.14491500	O	-0.83416300	0.60682400	1.19095600
H	5.23820400	-1.16243000	-2.33596100	H	2.79756200	-0.52195000	-0.48864500
H	4.24149300	-2.18733000	-3.35207200	H	2.80569800	-1.96200600	0.53006600
H	4.12543200	-4.07338400	-1.90462300	H	1.79468200	0.11535800	1.64148600
H	7.32967400	-2.17237200	-3.36871900	H	-1.47582500	-0.44607400	-0.89853200
H	0.47561300	-5.60559400	-0.51953400	H	1.71538300	-2.87976300	-1.35842300
H	-0.24377900	-7.20366300	-0.67349100	O	0.73016400	1.41381500	-0.30502300
H	-1.80967100	-5.70147100	0.74586100	H	0.61118200	1.45608100	-1.31495300
H	-3.16038500	-5.10553700	-0.19838300	C	-1.91877400	-2.48790500	-5.10264900
H	-0.16318900	-6.69070500	-3.28578800	C	-3.25308500	-2.26136400	-4.42117700
H	3.07861500	-3.83277700	-4.63858000	O	-4.31655300	-2.26060400	-5.04169800
H	1.70751600	-2.75336400	-4.27475400	N	-3.15226700	-2.01973400	-3.08513700
H	0.52896300	-5.22331200	-4.78948500	C	-4.30490900	-1.77275000	-2.24420600
H	1.29757900	-7.22108300	-2.43807300	C	-4.28079100	-0.32825100	-1.71985700
H	1.79155000	-3.59973400	-5.83910400	O	-3.33116400	0.06505500	-1.01552600
H	6.31618400	-3.16167400	-4.41929300	C	-4.29287500	-2.73522600	-1.03990300
H	6.30371700	-1.39408500	-4.58681300	O	-4.41504100	-4.09018100	-1.43195100
H	6.13059000	-6.48253000	4.31669900	N	-5.31738500	0.49491600	-1.98829400
H	4.45438500	-6.87570500	3.92113800	C	-6.48504800	0.24357600	-2.87361100
C	-5.04072400	-3.67519800	7.02990600	C	-6.10288600	0.31372200	-4.35483300
C	-3.72490600	-4.25035500	6.48087600	C	-7.45454300	1.35778600	-2.43286800
C	-3.30471200	-3.59211800	5.18512300	C	-6.52765100	2.53726100	-2.09753800
C	-2.21321500	-2.71941300	5.11503500	C	-5.31212400	1.86369100	-1.44360100
C	-4.04056500	-3.80883500	4.01057700	H	-4.36080000	2.35509400	-1.66504600
C	-1.86661000	-2.06832500	3.92894900	H	-5.40409200	1.82064000	-0.35057500
C	-3.71927000	-3.16392600	2.82169000	H	-6.22869700	3.05601200	-3.01395400
C	-2.63044500	-2.28010300	2.77533300	H	-6.99693900	3.27393200	-1.43952400
O	-2.38859000	-1.65726100	1.59242000	H	-8.18854500	1.59092300	-3.20801400
H	-3.84381800	-5.33090800	6.32885900	H	-8.00084800	1.04367300	-1.53607900
H	-2.93282100	-4.13055000	7.22878100	H	-6.90861300	-0.73942600	-2.64919000
H	-1.61535800	-2.54327900	6.00644300	H	-5.64815200	1.28049300	-4.59743900
H	-4.88474400	-4.49460000	4.02719400	H	-5.41459700	-0.48523800	-4.63690500
H	-0.99860300	-1.41787600	3.88113000	H	-7.00323500	0.20218600	-4.96950300
H	-4.29584200	-3.33561100	1.91830800	H	-5.18524800	-1.97495300	-2.85359000
H	-1.65673700	-1.00372800	1.64433200	H	-3.66955700	-4.32062700	-2.02757200
H	-4.94477200	-2.60272300	7.23035300	H	-5.15447600	-2.51643600	-0.39694300
H	-5.85896900	-3.80763100	6.31481400	H	-3.38595500	-2.55343800	-0.45086000
H	-5.33017000	-4.16905400	7.96344400	H	-2.22756700	-2.09825700	-2.64659100
N	-0.47152600	-0.57828300	-0.74757500	H	-1.51431800	-1.52294800	-5.42885800
C	0.08768900	-1.70477700	-1.30755500	H	-1.19509900	-2.95450800	-4.43226700
O	-0.55169400	-2.42169500	-2.09546500	H	-2.08221200	-3.10336400	-5.98915400
N	1.37053200	-2.00156900	-0.97626300	F	0.64403800	-1.53957300	1.80041000
C	2.15326200	-1.26526100	-0.00404900				

SkDHPase.5FUH2-TS2-II- L

C	3.37271700	7.78301900	-1.94590300	C	2.83375800	5.42364200	-1.00270300
C	2.62939500	6.76690000	-1.14436700	C	1.06788100	5.86832800	0.17298300
N	1.49741300	7.02953600	-0.38215800	N	1.85666100	4.87169200	-0.19266800

C	7.23112300	1.12032800	-0.29949900	H	8.06857800	1.63916800	0.18043500
C	5.92160300	1.57868000	0.22679700	H	-4.15301900	4.30942300	3.27196100
N	5.59849200	1.57819500	1.57406600	H	-4.62565600	3.72577600	4.87360000
C	4.79906700	2.04048500	-0.40417300	H	0.27295900	5.96876400	4.92371100
C	4.32843500	2.01744300	1.71728100	H	-0.72527900	4.51852300	5.13522600
N	3.81636600	2.30440400	0.53060300	H	4.21659900	7.30361700	-2.44524600
C	-0.17806900	5.12242100	4.39890700	H	2.55452300	3.89128700	-4.39837300
N	0.85148000	4.37488600	3.71946800	H	-2.72299800	6.51357900	-2.96721000
C	0.59564100	3.56310300	2.65979600	H	1.76720100	4.28968800	4.13189100
O	-0.58897400	3.60499200	2.17128300	C	6.04136100	-5.07469100	4.15018100
O	1.56866800	2.87818800	2.20883600	C	5.86435100	-4.00245300	3.06738400
C	-3.94327200	3.55396800	4.03815000	C	6.75921300	-2.76372700	3.27534800
C	-4.10565300	2.16460700	3.50852000	C	6.64073500	-1.79829500	2.09025800
N	-3.34959300	1.65301200	2.45651500	C	6.46126000	-2.03237400	4.59318700
C	-4.97504200	1.19356200	3.92993100	C	6.59911700	-0.99106600	-3.84708800
C	-3.76702800	0.40655100	2.25194200	C	5.68269900	-1.52855700	-2.75135100
N	-4.74734400	0.09649200	3.12181400	S	6.42263900	-3.01358200	-1.92982900
C	-2.69708600	5.43117500	-3.13979000	C	1.94111300	-6.02316600	-2.30456700
C	-2.85698800	4.65720500	-1.87770100	C	2.42289300	-4.69052900	-2.85869700
N	-3.98988900	4.68496900	-1.07764400	O	3.09452300	-3.90960700	-2.16207900
C	-2.00249100	3.79958900	-1.24177300	C	1.17148100	-5.88129000	-0.98759900
C	-3.78757400	3.86516100	-0.01714300	C	-0.32120100	-5.62186000	-1.19414100
N	-2.58609800	3.31740800	-0.08873800	O	-0.80900600	-5.43857300	-2.31361000
C	1.53322800	3.84534600	-4.01497500	N	-1.07412200	-5.65036100	-0.06981600
C	1.44061800	2.87349500	-2.85832800	N	2.15714500	-4.44087100	-4.15499400
O	2.37076100	2.80995800	-2.01920700	C	2.59315800	-3.21222700	-4.80442200
O	0.33900300	2.21192400	-2.75960100	H	6.09328200	-4.43687000	2.08627300
Zn	1.89984600	2.83848900	0.18897700	H	4.81221100	-3.68564700	3.02581000
Zn	-1.67872300	2.17853000	1.32983600	H	7.80064500	-3.11638100	3.31465400
H	2.74086400	8.23732000	-2.71750800	H	6.85408900	-2.29023600	1.13569100
H	3.76975100	8.59170800	-1.32205300	H	7.34532800	-0.96297800	2.20121000
H	3.59183200	4.80983600	-1.45736500	H	5.62553600	-1.38430100	2.02695400
H	1.06604800	7.93318700	-0.25296400	H	7.10467000	-1.15178400	4.70784400
H	0.20192000	5.77834300	0.81152900	H	5.41761900	-1.69268500	4.62335500
H	7.28838000	1.32051700	-1.37132800	H	6.62669000	-2.66831600	5.46691300
H	7.37410100	0.04447800	-0.15307400	H	5.71646400	-4.72308000	5.13400700
H	4.61460000	2.18158700	-1.45694800	H	5.49329700	-0.76173400	-1.99420300
H	6.19086200	1.23949900	2.31875100	H	4.71779500	-1.83688800	-3.15569000
H	3.80427700	2.11243900	2.65456200	H	5.25026100	-3.64546300	-1.70538000
H	-2.92136200	3.72655400	4.38849500	H	7.58380800	-0.72013700	-3.45127100
H	-5.71279400	1.18984900	4.71622100	H	1.60168100	-5.06297600	-0.39829100
H	-5.17117200	-0.81609700	3.20743000	H	1.28063900	-6.79179900	-0.38773000
H	-3.37939500	-0.27703200	1.50948700	H	-0.65964500	-5.68703900	0.84746000
H	-1.73679500	5.18321900	-3.59561600	H	-2.06710300	-5.45056900	-0.16611000
H	-3.47925500	5.19321800	-3.86934600	H	1.33169000	-6.56034800	-3.03487600
H	-1.03503900	3.46624900	-1.57406300	H	3.68021600	-3.12274200	-4.74328100
H	-4.83414500	5.20782100	-1.26025300	H	2.13208100	-2.33704600	-4.33606200
H	-4.51623400	3.68589500	0.75794100	H	1.45968000	-5.01119200	-4.60979100
H	-0.89462600	5.50118900	3.66999200	H	2.84867400	-6.61081400	-2.12527200
H	0.84006600	3.57951500	-4.81398000	H	2.30253600	-3.25057500	-5.85532200
H	1.27784700	4.84170200	-3.63670700	H	6.75341300	-1.73586900	-4.63243100

H	6.16275500	-0.09470300	-4.30284500	H	0.33231900	1.75215500	-1.54905700
H	7.09061400	-5.37955700	4.23446000	C	-1.47954800	-2.74947200	-5.15642100
H	5.45648400	-5.96993700	3.91613000	C	-2.82001800	-2.77522200	-4.45324200
C	-4.41267100	-4.62025000	6.93705500	O	-3.87374100	-2.99638900	-5.05118700
C	-2.96646100	-4.84147100	6.46314200	N	-2.74657400	-2.49393100	-3.12344300
C	-2.65329300	-4.11372900	5.17306800	C	-3.91404500	-2.48472100	-2.26719400
C	-1.76432500	-3.03386000	5.12505600	C	-4.18670700	-1.06082700	-1.75802700
C	-3.27991300	-4.49116800	3.97583500	O	-3.34311400	-0.48008200	-1.04885500
C	-1.51032400	-2.33999200	3.93942700	C	-3.68126000	-3.40843700	-1.05536400
C	-3.05001500	-3.80804100	2.78694600	O	-3.48669600	-4.75936300	-1.43616300
C	-2.16440600	-2.71903200	2.76092700	N	-5.36249200	-0.46029100	-2.04898200
O	-2.00505000	-2.07755400	1.57574500	C	-6.45487900	-0.94182300	-2.93496300
H	-2.79634000	-5.91816900	6.33239000	C	-6.10915900	-0.76572900	-4.41708600
H	-2.27192700	-4.51509500	7.24562300	C	-7.63654900	-0.06924900	-2.46958100
H	-1.25237300	-2.72653700	6.03424200	C	-6.98230400	1.28037300	-2.13273000
H	-3.96382800	-5.33696300	3.97305300	C	-5.63547500	0.88234200	-1.50861300
H	-0.79510600	-1.52338200	3.91172000	H	-4.81648900	1.56391800	-1.75571500
H	-3.54318700	-4.10641300	1.86722200	H	-5.68714900	0.82799900	-0.41366400
H	-1.42317100	-1.28478800	1.63587100	H	-6.82309400	1.86194900	-3.04638000
H	-4.60578600	-3.55797600	7.12088800	H	-7.58841700	1.88938700	-1.45612600
H	-5.13262200	-4.96368400	6.18733200	H	-8.41567000	0.00629300	-3.23198300
H	-4.61196300	-5.16591500	7.86521700	H	-8.08755300	-0.50221900	-1.56940500
N	-0.36279800	-0.56411800	-0.76873900	H	-6.65510900	-1.99649300	-2.72810000
C	0.40044500	-1.51629000	-1.39305400	H	-5.86652400	0.27828700	-4.64364200
O	-0.08562600	-2.30321900	-2.22546200	H	-5.27189200	-1.40140400	-4.71214300
N	1.72357700	-1.56807500	-1.08114800	H	-6.97093500	-1.05232700	-5.03010200
C	2.34944600	-0.77755500	-0.04140300	H	-4.73857800	-2.87387600	-2.86414500
C	1.32256700	-0.31515700	0.97590900	H	-2.70006700	-4.81848500	-2.01830500
C	0.06902500	0.29658100	0.31475900	H	-4.57112400	-3.39023100	-0.41407700
O	-0.93483900	0.43583000	1.22558700	H	-2.84171600	-3.01977500	-0.46768000
H	2.86300500	0.09534900	-0.45975800	H	-1.81760900	-2.36228600	-2.70495400
H	3.10105000	-1.38829600	0.46963800	H	-1.30004100	-1.74166000	-5.54806200
H	1.73911900	0.41225300	1.67558500	H	-0.66058200	-3.00768700	-4.48360500
H	-1.37224100	-0.61680700	-0.91861200	H	-1.51949000	-3.43580500	-6.00446000
H	2.23126300	-2.34815300	-1.49450800	F	0.90984800	-1.42968100	1.71698800
O	0.41737300	1.59497400	-0.21903900				

SkDHPase.5FUH2-INT2-II- L

C	3.81838500	7.68538800	-1.55671100	C	0.15265600	4.86435200	4.65196400
C	3.02287900	6.66311400	-0.81670300	N	1.13400100	4.07131300	3.95629200
N	1.89747700	6.93715200	-0.04908800	C	0.85084800	3.37878100	2.82426200
C	3.16494200	5.30623100	-0.74553100	O	-0.30561300	3.56294100	2.30005900
C	1.40954900	5.77013900	0.44043000	O	1.77922300	2.65215200	2.34488600
N	2.15560700	4.75866800	0.02681100	C	-3.70027700	3.54273500	4.23341800
C	7.28715600	0.72264800	-0.34134300	C	-3.91559600	2.18811600	3.63441500
C	6.02055700	1.23302300	0.23655900	N	-3.17529900	1.69813000	2.56067900
N	5.70699300	1.16094600	1.58434000	C	-4.82423900	1.23206900	4.00414900
C	4.92999200	1.81340500	-0.34892000	C	-3.63912600	0.47909500	2.29423500
C	4.47097900	1.67618400	1.77012200	N	-4.63595100	0.16795500	3.14369800
N	3.97242900	2.07831100	0.61120900	C	-2.38587000	5.76724100	-2.83224600

C	-2.59031700	4.92621400	-1.62057600	C	1.55286000	-4.34202300	-3.13217200
N	-3.78976000	4.82251500	-0.93132000	O	2.54260600	-4.01975500	-2.45417300
C	-1.73229900	4.09975700	-0.95005100	C	0.43726700	-5.16665200	-1.02119100
C	-3.62170000	3.95663700	0.09798800	C	-0.58462100	-6.11530200	-0.41686800
N	-2.37982000	3.50373600	0.11116400	O	-1.80014100	-5.98871300	-0.57621900
C	1.73883900	3.99183800	-3.83777000	N	-0.08208300	-7.13900300	0.31949600
C	1.64379800	2.98790600	-2.71239900	N	1.44060900	-3.98786500	-4.43092900
O	2.61357200	2.77737100	-1.96026300	C	2.37718800	-3.05617700	-5.05184700
O	0.47450000	2.44756400	-2.54439900	H	5.71090700	-4.91472500	1.71510100
Zn	2.07508300	2.72178600	0.32996600	H	4.64401300	-4.04267500	2.80446000
Zn	-1.51622400	2.24104100	1.44213500	H	7.69628500	-3.90025400	2.83496500
H	3.21425300	8.21082200	-2.30499100	H	6.72145400	-2.88975300	0.75722100
H	4.24755900	8.43899000	-0.88687400	H	7.44527100	-1.66159100	1.81039900
H	3.90038600	4.68347500	-1.22485400	H	5.67907700	-1.86397500	1.75067400
H	1.50737900	7.85187700	0.12582200	H	7.39660500	-1.91042100	4.32383100
H	0.53532300	5.68377300	1.06852500	H	5.64560800	-2.19630700	4.35496000
H	7.33588800	0.97561600	-1.40237600	H	6.75368600	-3.36425700	5.08393700
H	7.36534500	-0.36587300	-0.25403800	H	5.59702700	-5.30360500	4.77218800
H	4.75051600	2.03536000	-1.38820300	H	5.44745800	-1.07489900	-2.11199600
H	6.28226800	0.74059800	2.30029400	H	4.50107100	-1.72939400	-3.44707400
H	3.95946400	1.74001300	2.71695400	H	4.68301300	-3.87159500	-2.37373200
H	-2.67726700	3.65365700	4.60515900	H	7.52510100	-1.13424200	-3.58500600
H	-5.56537000	1.21824200	4.78715100	H	0.17514800	-4.15842000	-0.68876600
H	-5.09547100	-0.73031700	3.18434300	H	1.44634600	-5.38133900	-0.66056500
H	-3.28066800	-0.17787700	1.51372300	H	0.90190100	-7.23459300	0.50791700
H	-1.36680000	5.63134000	-3.19884100	H	-0.73059100	-7.77230000	0.76351100
H	-3.06731400	5.48670100	-3.64313700	H	-0.54042400	-4.86088600	-2.93052700
H	-0.71496300	3.85690800	-1.19836200	H	3.40010000	-3.39710100	-4.88324600
H	-4.65247400	5.29194300	-1.16563100	H	2.26316400	-2.04635000	-4.64110800
H	-4.40108000	3.67946400	0.79047800	H	0.54233900	-4.11489100	-4.87370100
H	-0.51562900	5.33082600	3.92855100	H	0.57602400	-6.22955600	-2.91578800
H	0.95730000	3.83291700	-4.58161700	H	2.18548500	-3.02875700	-6.12573200
H	1.62488400	4.99289200	-3.40657600	H	6.53338900	-1.72346900	-4.92163500
H	8.16617100	1.16083900	0.14501200	H	6.25643400	-0.09971300	-4.26133800
H	-3.86721100	4.34108300	3.50116200	H	6.75164200	-6.10964100	3.70213600
H	-4.38621500	3.70332400	5.06816500	H	5.02145900	-6.42851800	3.54395600
H	0.65506700	5.64770800	5.22595200	C	-4.63370500	-4.74792800	6.64908500
H	-0.45548800	4.27147800	5.34838200	C	-3.12655200	-4.80059800	6.34157500
H	4.64316200	7.19574900	-2.07759800	C	-2.74756600	-4.08288000	5.06246400
H	2.72419000	3.94559900	-4.30534400	C	-2.13800400	-2.82366100	5.07699700
H	-2.53459700	6.83391300	-2.62730500	C	-3.01481900	-4.65745500	3.80930200
H	2.02713600	3.88194900	4.38326000	C	-1.81842600	-2.14795800	3.89605700
C	5.75974600	-5.64579300	3.74563500	C	-2.70514100	-4.00345500	2.62169000
C	5.64009700	-4.50261800	2.72967500	C	-2.10910900	-2.73358500	2.65712200
C	6.71383100	-3.40799100	2.88776000	O	-1.86711700	-2.12085900	1.46826500
C	6.63725000	-2.40059200	1.73344700	H	-2.81522900	-5.85112300	6.27888500
C	6.62306100	-2.68299700	4.23884300	H	-2.57097600	-4.36710900	7.18154400
C	6.51219600	-1.13364400	-4.00145600	H	-1.90069000	-2.35789600	6.03116800
C	5.50013400	-1.69915500	-3.00913700	H	-3.46987700	-5.64449000	3.76222800
S	5.95029100	-3.42593500	-2.51672200	H	-1.32814300	-1.17859700	3.92833900
C	0.42943700	-5.20167100	-2.55712500	H	-2.89110000	-4.47007400	1.65935700

H	-1.34798000	-1.29270600	1.56809100	O	-3.65025300	-4.43334300	-1.98677700
H	-4.97388000	-3.71304000	6.76361300	N	-5.45328700	-0.08920600	-2.03547900
H	-5.21679700	-5.20077600	5.84058700	C	-6.53648800	-0.45227400	-2.98830200
H	-4.86707300	-5.28532600	7.57417500	C	-6.16377900	-0.13287900	-4.44200000
N	-0.38820700	-0.41406200	-0.87028900	C	-7.71042300	0.39036500	-2.45390300
C	0.30471700	-1.37264300	-1.54935300	C	-7.03866200	1.68495800	-1.96782400
O	-0.25375200	-2.14664700	-2.35517500	C	-5.70786800	1.19875100	-1.37115600
N	1.64959300	-1.45777600	-1.34174800	H	-4.87362600	1.88543800	-1.54303600
C	2.34419400	-0.77618100	-0.26523800	H	-5.77348900	1.04035000	-0.28701800
C	1.36913000	-0.36345300	0.82016400	H	-6.85618100	2.35627800	-2.81347400
C	0.13890800	0.37187000	0.24431100	H	-7.64476400	2.23077200	-1.23915200
O	-0.83134900	0.49648200	1.19576300	H	-8.47468700	0.56068500	-3.21613100
H	2.87363500	0.10491600	-0.63873500	H	-8.18487200	-0.12496800	-1.61109200
H	3.08805100	-1.45523100	0.16395500	H	-6.75999300	-1.51804200	-2.89673300
H	1.83652100	0.27436400	1.57297800	H	-5.88766200	0.92119600	-4.55580000
H	-1.40680200	-0.45760700	-0.93593700	H	-5.34362000	-0.76328600	-4.79068300
H	2.07307200	-2.29455100	-1.73505000	H	-7.02560700	-0.32832000	-5.08964700
O	0.55034400	1.64933900	-0.24905500	H	-4.89681100	-2.43379800	-3.04077400
H	0.45502400	1.92554200	-1.57278000	H	-2.98347700	-4.95089300	-1.49923900
C	-1.66313000	-2.33621200	-5.33901100	H	-4.70483900	-3.20801900	-0.66882900
C	-3.00181200	-2.28152800	-4.62608400	H	-2.96168700	-2.91193300	-0.72727500
O	-4.05945900	-2.44093100	-5.23631900	H	-1.98306900	-2.01203100	-2.86900800
N	-2.91294000	-2.02161900	-3.29745000	H	-1.67009000	-1.61149200	-6.15855800
C	-4.05948000	-2.12117000	-2.41723700	H	-0.81958600	-2.13796900	-4.67659600
C	-4.30868000	-0.75777700	-1.76100900	H	-1.56543100	-3.32593900	-5.79960700
O	-3.47062600	-0.27498600	-0.97502900	F	0.92459300	-1.52304000	1.46244700
C	-3.82553900	-3.19721100	-1.33912000				

SkDHPase.5FUH2-TS3-II- L

C	3.25419700	7.72956800	-2.09721300	C	-3.62708800	0.36969200	2.33490000
C	2.55483800	6.70882200	-1.26532700	N	-4.57607600	0.03236200	3.22997900
N	1.50492400	6.98895300	-0.40082900	C	-2.80961700	5.30587000	-3.17187700
C	2.73594400	5.35755300	-1.16049100	C	-2.89433100	4.57127300	-1.88027000
C	1.09868900	5.83339800	0.17956300	N	-3.96464300	4.68021100	-1.00432200
N	1.82628800	4.82331200	-0.26662400	C	-2.03161700	3.69942200	-1.27190800
C	7.18915700	1.13062600	-0.37690600	C	-3.72047500	3.89393800	0.07250600
C	5.89520800	1.60796600	0.16673300	N	-2.55252800	3.29268100	-0.06113300
N	5.59479700	1.61855000	1.51873500	Zn	1.86298800	2.85273500	0.26358000
C	4.76554400	2.07089500	-0.44922800	Zn	-1.57386700	2.11715600	1.28810300
C	4.32940900	2.06254600	1.67964900	H	2.57214900	8.22561200	-2.79697300
N	3.79765100	2.34250500	0.49868700	H	3.72484000	8.50596900	-1.48373600
C	-0.19538600	5.15736400	4.33921200	H	3.43967800	4.72866600	-1.67939600
N	0.90089500	4.50353000	3.67619200	H	1.11291600	7.90216800	-0.22191300
C	0.65465600	3.54103700	2.74507700	H	0.29688900	5.76038500	0.89854600
O	-0.56253900	3.42516900	2.38171200	H	7.23076900	1.31826500	-1.45177300
O	1.66047600	2.89966500	2.29848800	H	7.32356500	0.05505300	-0.22068200
C	-3.95126400	3.55138200	4.05433600	H	4.56546100	2.19640900	-1.50079100
C	-4.02541300	2.13917300	3.55370700	H	6.19787800	1.28359300	2.25649300
N	-3.26186600	1.63726600	2.49849900	H	3.81959400	2.16692600	2.62373600
C	-4.83878000	1.13707400	4.01515100	H	-2.92039200	3.83124300	4.28716800

H	-5.56170800	1.11913400	4.81507200	H	-2.07880600	-5.35915700	0.00578000
H	-4.94413000	-0.90025500	3.35172000	H	1.22888900	-6.63551600	-2.92757100
H	-3.22122200	-0.31103200	1.60023100	H	3.61083900	-3.18729800	-4.62791400
H	-1.89424100	5.02177300	-3.69456100	H	2.00834100	-2.45937500	-4.32358200
H	-3.65139200	5.07270500	-3.83368800	H	1.47100100	-5.16518200	-4.56334500
H	-1.09662900	3.30242800	-1.63165100	H	2.76459200	-6.69451200	-2.05032600
H	-4.79721200	5.23222800	-1.15087200	H	2.30115800	-3.40180800	-5.80640900
H	-4.39864500	3.77512800	0.90278800	H	6.63462200	-1.80413200	-4.66278900
H	-0.88961800	5.57326000	3.60674900	H	6.13893500	-0.13275600	-4.32881800
H	8.04101500	1.64483700	0.08239100	H	7.15509500	-5.30576500	4.25900000
H	-4.32266000	4.27025700	3.31388700	H	5.50557300	-5.88402500	4.00399300
H	-4.55525700	3.66437500	4.95741900	C	-4.31532900	-4.57146700	7.10860300
H	0.19236700	5.97480700	4.95296300	C	-2.83867400	-4.55782000	6.67601200
H	-0.76101600	4.47996500	4.99154300	C	-2.58098400	-3.90020700	5.33276100
H	4.03985900	7.24768400	-2.68198300	C	-1.67744900	-2.83950100	5.19104900
H	-2.79329900	6.39268200	-3.02763200	C	-3.22413300	-4.35474800	4.17075100
H	1.82231200	4.51237600	4.08453600	C	-1.41444200	-2.24824000	3.95185800
C	6.10707400	-4.99075100	4.20038000	C	-2.98584400	-3.77363200	2.92943800
C	5.90760300	-3.94018300	3.10034100	C	-2.07245900	-2.71270800	2.80578300
C	6.81809900	-2.70497300	3.25313600	O	-1.89470300	-2.19236100	1.56727600
C	6.67219300	-1.76651600	2.04928700	H	-2.47264400	-5.59345700	6.64985900
C	6.56404400	-1.94013500	4.56106800	H	-2.24270600	-4.04952400	7.44294000
C	6.53149500	-1.05113100	-3.87692400	H	-1.15517600	-2.46731300	6.06961000
C	5.60234400	-1.53707000	-2.76795400	H	-3.92363300	-5.18485300	4.23331000
S	6.27597000	-3.05649300	-1.95258700	H	-0.68952100	-1.44460300	3.86003400
C	1.85622400	-6.10170800	-2.20983200	H	-3.49120500	-4.13585200	2.03930000
C	2.32648800	-4.76818500	-2.77165300	H	-1.32692900	-1.38306400	1.53332300
O	2.94697400	-3.95762300	-2.06116100	H	-4.71319100	-3.55385300	7.18298500
C	1.11919900	-5.95414400	-0.87619000	H	-4.93917200	-5.12069800	6.39652200
C	-0.35917500	-5.60564900	-1.05055400	H	-4.42928900	-5.05169100	8.08560100
O	-0.84961500	-5.36686900	-2.15931600	C	-1.55518700	-2.89022800	-5.06274300
N	-1.09649300	-5.61532500	0.08277600	C	-2.89563800	-2.89603900	-4.36159600
N	2.11212800	-4.55186800	-4.08298300	O	-3.94989000	-3.16895000	-4.93543800
C	2.53309000	-3.32271100	-4.74324200	N	-2.81156700	-2.55874900	-3.04517300
H	6.10260700	-4.39793500	2.12248000	C	-3.96662400	-2.47707700	-2.17957500
H	4.85746100	-3.61477500	3.08337400	C	-4.19002700	-1.01755100	-1.75455400
H	7.85756200	-3.06511200	3.27086000	O	-3.28683700	-0.39737900	-1.16704800
H	6.85383500	-2.28281100	1.10099600	C	-3.73985800	-3.33385400	-0.91978800
H	7.38529700	-0.93414700	2.12014500	O	-3.52797300	-4.70139300	-1.23206100
H	5.65817500	-1.34709600	2.00578900	N	-5.38923900	-0.43730400	-1.98901500
H	7.21867800	-1.06363600	4.63723700	C	-6.51274700	-0.96672000	-2.80466500
H	5.52486600	-1.58941600	4.61214800	C	-6.19205700	-0.93157100	-4.30230900
H	6.74770900	-2.55734300	5.44454900	C	-7.66344000	-0.02664200	-2.39564500
H	5.81672500	-4.61447200	5.18590700	C	-6.96981700	1.32759300	-2.17542900
H	5.46349500	-0.75975500	-2.01071500	C	-5.62490600	0.94445200	-1.53880100
H	4.61666700	-1.79018400	-3.16117200	H	-4.79328500	1.58742400	-1.84065700
H	5.07773900	-3.63438300	-1.71655600	H	-5.66602200	0.96741300	-0.44203300
H	7.53445500	-0.83405000	-3.49421500	H	-6.80802900	1.83034500	-3.13455000
H	1.60600800	-5.17549300	-0.27735200	H	-7.55074200	2.00446000	-1.54260400
H	1.18854300	-6.88520200	-0.30259000	H	-8.45167400	0.00914200	-3.15160300
H	-0.67219500	-5.69735700	0.99253800	H	-8.11233300	-0.37441200	-1.45825000

H	-6.73548400	-1.99342100	-2.50024300	O	-0.07901300	-2.09680300	-2.48337500
H	-5.93089900	0.08347100	-4.62089800	N	1.75836500	-1.41162900	-1.35270700
H	-5.37554400	-1.60745100	-4.56310300	C	2.36523700	-0.57379700	-0.33658500
H	-7.07244700	-1.24707700	-4.87355800	C	1.35226100	-0.23754600	0.74574400
H	-4.80565600	-2.88172700	-2.74405000	C	0.09894100	0.47814400	0.19688500
H	-2.76180900	-4.76877200	-1.83945900	O	-0.96424000	0.29515700	1.01401700
H	-4.63613400	-3.29269000	-0.28836700	H	0.78442200	3.48285000	-4.87049300
H	-2.90897500	-2.91016300	-0.34626300	H	1.11947600	4.65895800	-3.57534900
H	-1.88416400	-2.33624300	-2.67349400	H	2.75290800	0.35046000	-0.77347400
H	-1.12603300	-1.88416800	-5.05784600	H	3.20611300	-1.11843200	0.10113000
H	-0.85154400	-3.54004000	-4.53664900	H	1.78032300	0.39669400	1.52750800
H	-1.69540000	-3.22740000	-6.09033200	H	2.46760100	3.85130500	-4.38185600
C	1.44220100	3.71792100	-4.03305900	H	-1.22092300	-0.27112400	-1.33338800
C	1.40179500	2.63121600	-2.97050600	H	2.19420500	-2.29921900	-1.60299800
O	2.29571100	2.52797000	-2.12443100	O	0.29312700	1.82802200	-0.03108500
O	0.32701800	1.87703500	-3.02078000	H	0.24446500	1.17793400	-2.27646000
N	-0.20537500	-0.14040000	-1.25754600	F	0.96451500	-1.44036400	1.34517300
C	0.45895000	-1.28583000	-1.71693300				

SkDHPase.5FUH2-EP-II- L

C	-5.43060200	-6.47405600	-2.50927500	Zn	0.99447200	-2.74762000	1.24698200
C	-4.58686500	-5.76082300	-1.51994900	H	-4.89476500	-7.30129300	-2.98930600
N	-4.02431600	-6.33555500	-0.39031900	H	-6.34003600	-6.88813500	-2.05850100
C	-4.17253600	-4.46238100	-1.49473300	H	-4.37392100	-3.66583600	-2.18950700
C	-3.30686700	-5.38914300	0.26389300	H	-4.13217900	-7.29501300	-0.09518200
N	-3.37069800	-4.24079700	-0.39119900	H	-2.79363700	-5.55695200	1.19859700
C	-7.38996100	0.81725500	-0.27612300	H	-7.46868700	0.73825700	-1.36217300
C	-6.20189900	0.05853300	0.19651500	H	-7.32265000	1.87979800	-0.02237700
N	-5.90194100	-0.12877800	1.53771500	H	-5.03945700	-0.68741900	-1.54098400
C	-5.20096700	-0.58602200	-0.47936400	H	-6.42182600	0.25469100	2.31414600
C	-4.76735700	-0.85934500	1.63293600	H	-4.30092800	-1.16795500	2.55510300
N	-4.31863000	-1.14982900	0.42232000	H	1.54168800	-4.87313000	3.84523400
C	-1.42127200	-5.41420400	4.02872400	H	4.81478400	-3.10088000	4.91296400
N	-2.21953900	-4.46312100	3.28799200	H	4.90957700	-0.86833200	3.63874900
C	-1.63395900	-3.51171400	2.48710700	H	3.23912700	-0.77137400	1.75530700
O	-0.38217300	-3.67828800	2.27427700	H	0.34935700	-5.12056800	-4.04240300
O	-2.38857500	-2.61228500	2.01487200	H	1.95384500	-5.84881100	-4.15796400
C	2.63314100	-4.89254400	3.79090700	H	0.20027200	-3.29367200	-1.90673700
C	3.16784500	-3.52904700	3.46579000	H	2.91330300	-6.48302100	-1.50865900
N	2.67141000	-2.73729400	2.43079500	H	3.05078400	-5.09282000	0.61539100
C	4.18460400	-2.84329600	4.07688600	H	-0.75509700	-5.95076300	3.35094000
C	3.38127200	-1.61179400	2.42373600	H	-8.31868500	0.42617100	0.15434400
N	4.30462500	-1.64298700	3.40240600	H	2.91363900	-5.63378500	3.03259500
C	1.07004100	-5.75074500	-3.51798400	H	3.02765900	-5.23787300	4.74906300
C	1.40192400	-5.13193500	-2.19989400	H	-2.08471700	-6.13813100	4.50871700
N	2.34323300	-5.66850800	-1.33218600	H	-0.80735100	-4.94253200	4.80669300
C	0.91167800	-4.02763300	-1.55047800	H	-5.73683400	-5.77898000	-3.29315600
C	2.39229800	-4.90520600	-0.21822400	H	0.62892900	-6.74694500	-3.39872300
N	1.52943400	-3.90463400	-0.31591500	H	-3.13556500	-4.21978100	3.63447400
Zn	-2.73810400	-2.31170300	-0.09171400	C	-4.66822000	6.06382900	4.68968800

C	-4.76432900	5.07907200	3.51731200	C	2.97936700	1.88086800	2.82981100
C	-6.14776300	4.41835800	3.36132900	O	2.65413500	1.35005500	1.61935700
C	-6.21269300	3.59209100	2.07076100	H	4.82641300	4.48056200	6.44666600
C	-6.52942000	3.55404200	4.57278800	H	3.42862400	3.77955700	7.24040500
C	-6.14462700	2.97284300	-3.62951900	H	1.74807100	2.83932900	5.84421600
C	-5.00541600	3.12726900	-2.62547500	H	5.78685200	2.97769400	4.39945100
S	-4.98141200	4.83773900	-1.92034600	H	0.99980700	1.89782000	3.67271400
C	0.23362600	6.49442200	-2.10672000	H	5.03921800	2.02460500	2.23496700
C	-0.74181200	5.40044100	-2.52179300	H	1.71490700	1.10141400	1.56735100
O	-1.52794800	4.89018900	-1.70787300	H	4.71301800	1.63535000	7.61169700
C	0.94485900	6.19795900	-0.78290000	H	6.12028900	2.34037900	6.80575400
C	2.32193900	5.56329300	-0.97022500	H	5.54839500	3.02116100	8.33290500
O	2.77616900	5.27857900	-2.08258400	C	2.13833800	2.58473600	-4.82316500
N	3.03390400	5.38297100	0.16802300	C	3.48544500	2.20714900	-4.23993700
N	-0.74911100	5.07900900	-3.83239100	O	4.47993100	2.03865300	-4.94600200
C	-1.67135700	4.10634800	-4.40595900	N	3.46775000	2.02627400	-2.89132800
H	-4.52355700	5.60597800	2.58567300	C	4.62323400	1.59469500	-2.13543400
H	-4.00194100	4.29416800	3.62944600	C	4.44893900	0.14039100	-1.65789100
H	-6.89079000	5.22511800	3.27730300	O	3.43141700	-0.19491900	-1.02726600
H	-5.98327300	4.19414500	1.18536800	C	4.79304900	2.49543600	-0.89347100
H	-7.21286400	3.16214600	1.93549600	O	5.07564000	3.83912800	-1.23530900
H	-5.48786600	2.76717000	2.10314400	N	5.45330600	-0.74172900	-1.86674400
H	-7.51400400	3.09289900	4.43327400	C	6.57017500	-0.60567500	-2.83661600
H	-5.79795500	2.74817600	4.72233900	C	6.04983300	-0.62721300	-4.27660000
H	-6.57253400	4.13360400	5.49888000	C	7.44956000	-1.81656300	-2.47252900
H	-4.80012100	5.56775700	5.65614900	C	6.43480500	-2.90084700	-2.07325100
H	-5.10944900	2.40527000	-1.80967000	C	5.32598100	-2.11677700	-1.35331100
H	-4.04216200	2.94563100	-3.10548400	H	4.31995600	-2.49949600	-1.54675700
H	-3.64704700	4.90322500	-1.70461700	H	5.46478700	-2.11288400	-0.26425400
H	-7.11561800	3.18617500	-3.17021500	H	6.03435000	-3.39133800	-2.96628800
H	0.32273800	5.53046000	-0.17657700	H	6.87115200	-3.67774200	-1.43932900
H	1.07655500	7.12010900	-0.20582700	H	8.09707500	-2.11503100	-3.30055900
H	2.61519500	5.50551600	1.07566300	H	8.08953600	-1.56767100	-1.61833400
H	3.93666900	4.92158800	0.08664300	H	7.11197500	0.32606300	-2.65019800
H	0.97570800	6.67738200	-2.88772700	H	5.46901400	-1.53688800	-4.46539300
H	-2.69678800	4.48929100	-4.39596900	H	5.43417300	0.24332400	-4.50751500
H	-1.63463100	3.17013600	-3.84327300	H	6.89532800	-0.62018500	-4.97435200
H	-0.03917200	5.48258200	-4.42417900	H	5.49283000	1.71363100	-2.78082200
H	-0.37266100	7.40136700	-1.99769700	H	4.34620400	4.18848300	-1.79272800
H	-1.37671800	3.91343800	-5.43833500	H	5.64500500	2.13627700	-0.30319500
H	-6.02090300	3.65649600	-4.47360200	H	3.89076600	2.40348100	-0.27525200
H	-6.17435600	1.94869100	-4.01911100	H	2.61110300	2.26791900	-2.37574100
H	-5.43124700	6.84624700	4.61033300	H	1.54907300	1.67506000	-4.98538000
H	-3.69138200	6.55742900	4.70767100	H	1.57787400	3.23803000	-4.15052300
C	5.22303000	2.57788500	7.38631600	H	2.29751500	3.06905300	-5.78783800
C	4.29687400	3.53438900	6.61844500	C	-2.57378700	-2.99342500	-4.19686600
C	3.82428200	2.96888700	5.29582700	C	-2.08441000	-2.15392300	-3.01223200
C	2.48041100	2.65619500	5.06158000	O	-2.96171200	-1.93552600	-2.08211500
C	4.73804900	2.72703100	4.25848600	O	-0.90303600	-1.77485700	-2.99582800
C	2.04916800	2.12009600	3.84554600	N	0.62629600	0.43727800	-1.65164300
C	4.33206300	2.18629600	3.04277600	C	0.27085500	1.74614600	-1.54574100

O	1.07634900	2.68981600	-1.61017100	H	-2.80527800	1.63967600	-0.29691600
N	-1.06787100	1.99479700	-1.32646900	H	-2.04032000	0.33357100	1.47333500
C	-1.89404600	1.09313900	-0.54995000	H	-3.58957500	-2.71027900	-4.48636100
C	-1.24225600	0.59678100	0.76633000	H	1.62535000	0.24073600	-1.66011900
C	-0.39220400	-0.66068100	0.65460500	H	-1.24983000	2.99097500	-1.22055500
O	0.68486200	-0.74775800	1.31278400	O	-0.84498400	-1.65794900	0.01430500
H	-1.90026200	-2.87966000	-5.04748700	H	-0.00636000	-0.26629400	-2.03639800
H	-2.59699300	-4.04890300	-3.90270700	F	-0.48854500	1.61344800	1.34688900
H	-2.19596900	0.21633100	-1.13057600				

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C	-6.72181000	-4.79848500	-3.36269900	C	-1.35883900	1.96003900	0.61221700
C	-5.80964600	-4.36405800	-2.27396800	C	-0.60451000	1.06272000	1.58717700
N	-5.44396700	-5.15022600	-1.19193700	C	0.41139700	0.19686600	0.85122700
C	-5.13493700	-3.19093600	-2.09564700	O	0.76063200	-0.91272700	1.25813100
C	-4.58147000	-4.44294300	-0.41841700	H	-6.33304600	-5.66931700	-3.90393100
N	-4.36673900	-3.25061300	-0.94900000	H	-7.71949000	-5.06046800	-2.99079500
C	-7.15124600	2.37032300	-0.13578000	H	-5.12665000	-2.30630500	-2.70807600
C	-6.08433800	1.38285500	0.20855400	H	-5.76569400	-6.08783500	-1.00234500
N	-5.68735100	1.11773500	1.51223100	H	-4.16383100	-4.80801600	0.50890000
C	-5.28860800	0.57725800	-0.56411100	H	-7.36115500	2.32715300	-1.20659000
C	-4.69597700	0.19496500	1.48808300	H	-6.85198000	3.39521000	0.10874800
N	-4.43188900	-0.15001500	0.24055800	H	-5.25636300	0.46110800	-1.63593400
C	-2.74437500	-5.51406000	3.24119500	H	-6.04184100	1.57633200	2.33885300
N	-3.32666700	-4.33388000	2.64322100	H	-4.19916800	-0.20608100	2.35725200
C	-2.54398800	-3.38423000	2.01796900	H	0.28254300	-5.60919200	3.25397600
O	-1.31643800	-3.71221800	1.85403300	H	3.85350500	-4.75266100	4.22343900
O	-3.11864000	-2.32732400	1.64089100	H	4.43468800	-2.43657900	3.24579500
C	1.33336100	-5.83975200	3.05971600	H	2.81732200	-1.75103300	1.45953800
C	2.11879600	-4.58234600	2.82695500	H	-0.80341400	-4.52604500	-4.67386600
N	1.78631600	-3.57002000	1.91855000	H	0.65585900	-5.47596800	-4.97313000
C	3.28859900	-4.24426000	3.45816400	H	-0.71511600	-3.10521300	-2.39314300
C	2.75991600	-2.67231600	2.01334200	H	1.54805100	-6.63426700	-2.38893700
N	3.68496400	-3.03770800	2.92388900	H	1.86413700	-5.52008000	-0.11805200
C	-0.19193100	-5.34490300	-4.29067800	H	-2.12376200	-6.03144000	2.50787800
C	0.24405100	-5.00941500	-2.90562200	H	-2.41125600	-1.75398000	-5.41383100
N	1.10282900	-5.76877400	-2.12099400	H	-3.41012800	-2.88426900	-4.47709300
C	-0.09473200	-3.94412800	-2.12199000	H	-2.01143700	1.34814000	-0.02066900
C	1.24660500	-5.15008200	-0.92138500	H	-1.98196600	2.67408100	1.15192100
N	0.52817600	-4.03915900	-0.89200300	H	-8.08704600	2.15850900	0.39364700
C	-3.14394000	-1.82906300	-4.60826100	H	1.36218400	-6.51010400	2.19171100
C	-2.55518200	-1.31031900	-3.29200800	H	1.74119600	-6.38404200	3.91448200
O	-3.39370700	-0.95299000	-2.38922800	H	-3.54635300	-6.18726400	3.55647700
O	-1.31082100	-1.32673800	-3.15632400	H	-2.11890700	-5.29062000	4.11575900
Zn	-3.16592000	-1.63112700	-0.38088600	H	-6.84071300	-3.98717300	-4.08350300
Zn	-0.04064900	-2.81614900	0.67840600	H	-4.05465000	-1.28841600	-4.87934100
N	0.97777300	0.78760500	-0.23176700	H	-0.79024100	-6.26314000	-4.32602100
C	0.72950600	2.11030100	-0.67466900	H	-4.19949800	-3.98123900	3.00751000
O	1.50535400	2.64943400	-1.45970200	H	1.81273100	0.34641500	-0.61682100
N	-0.37433700	2.69437300	-0.16977200	H	-0.55208200	3.64683200	-0.49468600

O	-1.23015300	-1.64136500	-0.41367000	C	3.38878100	0.25522200	5.19752300
H	-1.00830900	-1.41398400	-1.34161300	C	4.98443800	0.16502300	2.91887400
C	-3.50756000	6.19336100	5.49460700	C	2.91163400	0.77280100	4.00170200
C	-3.78018500	5.42024200	4.19798100	C	3.70550400	0.73149500	2.84769500
C	-5.21635300	4.86034500	4.11755200	O	3.18814700	1.25832200	1.70511800
C	-5.58431600	4.48542400	2.67791100	H	4.49495100	-1.54279900	7.04765200
C	-5.42593200	3.66592400	5.06058500	H	6.14528100	-1.30771000	6.49315300
C	-5.39470300	4.64653400	-3.16500400	H	6.46443700	-0.74607900	4.18645500
C	-4.35339300	3.85897700	-2.37275400	H	2.75188600	0.28918000	6.07769100
S	-3.81193700	4.68046700	-0.80420800	H	5.61250500	0.14209300	2.03310600
C	1.47896400	6.96797200	-1.50727700	H	1.91773600	1.20330800	3.93883600
C	0.39967400	5.97903600	-1.92915400	H	3.61016500	0.85659800	0.91187900
O	-0.36970000	5.47206800	-1.09886100	H	6.06106100	1.09612800	7.26872900
C	2.30728000	6.48835700	-0.31103500	H	4.40175300	0.85811600	7.82517600
C	3.49991800	5.62743900	-0.71855100	H	5.72403900	-0.02296100	8.60065400
O	3.58426000	5.10747900	-1.83688500	C	2.63008100	2.66060500	-4.46348500
N	4.45729300	5.46997800	0.22461200	C	3.93996900	2.06126600	-4.00167700
N	0.26794800	5.76590300	-3.25405500	O	4.85672600	1.77054300	-4.76647200
C	-0.76488000	4.89689500	-3.79733900	N	3.99757300	1.85890000	-2.65089100
H	-3.61164500	6.08907800	3.34442900	C	5.16599700	1.30885300	-1.99595000
H	-3.06147600	4.59554200	4.08871300	C	4.79548500	-0.06204700	-1.41884900
H	-5.89960800	5.66188300	4.43462800	O	3.94495700	-0.12861000	-0.49169400
H	-5.52373300	5.34775300	2.00703200	C	5.64325400	2.26450500	-0.87983400
H	-6.60856700	4.09471000	2.62298200	O	5.95231300	3.54646000	-1.38672100
H	-4.90032600	3.72548700	2.28163900	N	5.34189900	-1.18432800	-1.90511400
H	-6.46219200	3.30983200	5.02452900	C	6.37126200	-1.33961400	-2.97527200
H	-4.76976400	2.83048000	4.78082700	C	5.75937500	-1.35388900	-4.38285200
H	-5.20702600	3.91719500	6.10237600	C	7.01993600	-2.67909000	-2.57690000
H	-3.62430200	5.56251100	6.38163600	C	5.84178600	-3.51168700	-2.04569400
H	-4.75074600	2.89123400	-2.06034300	C	4.97490800	-2.48485300	-1.30101400
H	-3.46419500	3.65078300	-2.97195900	H	3.90057400	-2.66276300	-1.40207000
H	-2.69187900	5.27645300	-1.26469700	H	5.19535400	-2.45048500	-0.22873400
H	-6.28469300	4.84391500	-2.56072800	H	5.28284600	-3.95348600	-2.87634000
H	1.66296500	5.90429100	0.35710100	H	6.15918200	-4.32785600	-1.39195000
H	2.66750100	7.34631300	0.26689800	H	7.53512100	-3.14810400	-3.41839900
H	4.39508400	5.91494800	1.12562400	H	7.75531400	-2.51491700	-1.78123600
H	5.27083600	4.90640600	-0.01154300	H	7.09266900	-0.52257100	-2.89929100
H	2.13400000	7.22045700	-2.34495000	H	5.00021100	-2.13700500	-4.47732200
H	-1.75928500	5.31268800	-3.60885800	H	5.31242000	-0.38900800	-4.63066400
H	-0.70454400	3.90003300	-3.35174800	H	6.54828800	-1.55489700	-5.11499800
H	0.98235300	6.12032600	-3.87124600	H	5.93869800	1.23981700	-2.76154700
H	0.94193700	7.87947400	-1.21991400	H	5.15099400	3.90841900	-1.82318500
H	-0.62133200	4.81293500	-4.87525000	H	6.55928500	1.87087600	-0.42441300
H	-5.00035700	5.61156300	-3.49676900	H	4.87587400	2.31901200	-0.09494500
H	-5.70203000	4.08087700	-4.05265400	H	3.18623400	2.12026800	-2.08987600
H	-4.19615200	7.03915100	5.59612200	H	1.82106500	1.93239900	-4.34579200
H	-2.48855500	6.59336700	5.51199400	H	2.37564400	3.53664200	-3.86175800
C	5.35262000	0.34931700	7.64041500	H	2.72122300	2.92940900	-5.51626500
C	5.18533000	-0.79703500	6.63155700	F	-1.47795800	0.26792500	2.29655600
C	4.67027000	-0.30926100	5.29578000	H	-0.03268200	1.67630500	2.29825500
C	5.45531500	-0.34184900	4.13692000				

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C	-6.15308600	-6.03379300	-1.74335800	H	3.26136000	-1.22716000	1.34017300
C	-5.09068600	-5.34602000	-0.96634900	H	-0.29554500	-5.61000400	-3.42602900
N	-4.30838100	-5.94239400	0.01209400	H	1.22238000	-6.51117600	-3.48065900
C	-4.64032900	-4.05970300	-1.03580400	H	-0.25098400	-3.58846900	-1.63439100
C	-3.43643500	-5.01634300	0.48691900	H	2.16376000	-6.88866300	-0.70003400
N	-3.61026900	-3.86513500	-0.13697000	H	2.42691200	-5.19713500	1.18435500
C	-7.17692600	1.67303500	-0.49995500	H	-1.27452600	-5.27615400	4.02555700
C	-6.09189000	0.80799200	0.03968700	H	-2.18594900	-3.33139600	-4.71948700
N	-5.75034200	0.77191800	1.38372100	H	-3.13053900	-4.19433700	-3.48251200
C	-5.22563200	-0.06552000	-0.56261000	H	-8.13302200	1.48968100	0.00343400
C	-4.71938700	-0.08820800	1.54892100	H	1.95575300	-5.47852300	3.61544600
N	-4.37746500	-0.61022300	0.38356500	H	2.74239100	-4.99644200	5.12558800
C	-1.93480600	-4.61773700	4.59260300	H	-2.62885600	-5.23488400	5.16925100
N	-2.68450700	-3.77604400	3.69508200	H	-1.31640600	-4.04730300	5.29870100
C	-2.06012800	-3.02280500	2.73973900	H	-6.60255600	-5.32873500	-2.44512600
O	-0.82193800	-3.29732900	2.54348800	H	-3.85273500	-2.81637000	-4.31689700
O	-2.76557500	-2.17914600	2.12241900	H	-0.16738500	-7.17866000	-2.61398300
C	2.14833000	-4.63178600	4.28477900	H	-3.60320100	-3.45674100	3.96123700
C	2.87168800	-3.51955300	3.58552200	C	-3.75618800	7.15714000	3.72103700
N	2.36179200	-2.78350900	2.51290400	C	-3.99066800	6.04531700	2.69026100
C	4.13400400	-3.06576500	3.86833400	C	-5.29090300	5.25367600	2.94117400
C	3.31277000	-1.92376100	2.16501400	C	-5.60469800	4.31978800	1.76762100
N	4.39645100	-2.06238900	2.95863700	C	-5.25499900	4.46532800	4.25943200
C	0.36929800	-6.25044400	-2.84365900	C	-5.73666000	3.19809300	-4.11141300
C	0.78472400	-5.52388700	-1.61409500	C	-4.59870900	3.02270800	-3.11112000
N	1.67350100	-6.00681300	-0.66412800	S	-4.32061700	4.54389000	-2.08683400
C	0.39988900	-4.29917700	-1.14694900	C	1.45215200	5.18890800	-2.71035500
C	1.79044700	-5.08364200	0.32132500	C	0.09428000	4.68197200	-3.19492700
N	1.02417700	-4.03670600	0.05678200	O	-0.90532900	4.68679400	-2.45843800
C	-2.91560300	-3.21175500	-3.91703600	C	1.51526800	5.24177600	-1.17486500
C	-2.36095400	-2.30685100	-2.81172100	C	2.79749100	5.89114500	-0.67729200
O	-3.21145300	-1.77952900	-2.00859800	O	3.86443800	5.28179200	-0.57823800
O	-1.11784300	-2.18035800	-2.70954900	N	2.71070300	7.20785600	-0.35895600
Zn	-2.84870300	-1.93025200	0.06894600	N	0.02899800	4.27690600	-4.48032900
Zn	0.49687900	-2.53391600	1.33596300	C	-1.17284400	3.66351700	-5.03482600
H	-5.76075900	-6.87669100	-2.32444300	H	-4.03637500	6.48668700	1.68680000
H	-6.95399700	-6.41981600	-1.10187500	H	-3.13777600	5.35155900	2.68407200
H	-4.95656500	-3.26289800	-1.68690900	H	-6.10917600	5.98602200	3.00971600
H	-4.37586700	-6.89950300	0.32550400	H	-5.65470100	4.86052900	0.81795400
H	-2.71985400	-5.21122700	1.26920900	H	-6.56944700	3.81777800	1.91936100
H	-7.31879700	1.46758900	-1.56295400	H	-4.82929000	3.55102600	1.65969600
H	-6.93869300	2.73633700	-0.39164500	H	-6.19150500	3.91683800	4.41509500
H	-5.13498300	-0.34004600	-1.60157500	H	-4.43469500	3.73565200	4.25475800
H	-6.16293800	1.33969600	2.10949600	H	-5.11375100	5.11472000	5.12763400
H	-4.24038400	-0.31053800	2.48820800	H	-3.60994800	6.75894200	4.72958300
H	1.17807000	-4.29575600	4.66127900	H	-4.80648200	2.19736700	-2.42597600
H	4.84393200	-3.36235800	4.62395100	H	-3.66223400	2.78877200	-3.62060200
H	5.22384000	-1.48575500	2.92075900	H	-3.01754000	4.72579500	-2.39132200

H	-6.67309000	3.45865000	-3.60794400	H	-2.40242100	0.75095200	-0.52358400
H	1.49783400	4.22482900	-0.77857400	H	-2.42424800	2.33882400	0.26108500
H	0.63244500	5.76593300	-0.79860900	H	1.70109200	0.13978900	-0.88036300
H	1.83897800	7.71136900	-0.37407400	H	-1.11782800	2.97690700	-1.59576200
H	3.54251200	7.67896900	-0.03467100	O	-0.89122600	-1.50914800	-0.06031900
H	2.25355200	4.54869800	-3.09260300	H	-0.76268400	-1.58974200	-1.04068300
H	-2.03911200	4.29009100	-4.81641500	C	2.41379200	1.65869400	-5.23900900
H	-1.33864900	2.66354600	-4.61803900	C	3.68577100	1.21389900	-4.54146700
H	0.89650100	4.15313700	-4.98128000	O	4.71514100	0.96786100	-5.16809600
H	1.60735700	6.19048500	-3.13350000	N	3.56122200	1.09281300	-3.19515500
H	-1.05968100	3.58269500	-6.11693100	C	4.68174100	0.79796300	-2.32780400
H	-5.51585500	3.99504500	-4.82659300	C	4.41035100	-0.54429700	-1.63664900
H	-5.90107500	2.26849700	-4.66917300	O	3.44486200	-0.64475700	-0.84534600
H	-4.60772600	7.84584600	3.75481100	C	4.86805300	1.90930300	-1.27393500
H	-2.86669100	7.74539800	3.47302200	O	5.07347100	3.12611200	-1.94784700
C	5.68433600	2.87491700	6.85145600	N	5.20406800	-1.60436100	-1.88108500
C	4.38739800	3.63620000	6.53278200	C	6.35984800	-1.70579500	-2.81689800
C	3.79568900	3.20356100	5.21080800	C	5.91621600	-1.90686400	-4.27206900
C	3.03089200	2.03446500	5.12052700	C	7.11617000	-2.91704600	-2.23828700
C	4.06033600	3.90600000	4.02715900	C	5.99349300	-3.84793900	-1.75257900
C	2.55908700	1.56779300	3.89533900	C	4.94218200	-2.88063100	-1.18781800
C	3.59976600	3.45779700	2.79110900	H	3.91020800	-3.20081200	-1.35667900
C	2.85473300	2.27755100	2.72602700	H	5.06060600	-2.73403700	-0.10790500
O	2.42322600	1.85364900	1.49695400	H	5.58013000	-4.41525900	-2.59236300
H	4.59184500	4.71293400	6.51485300	H	6.33239900	-4.56930300	-1.00415500
H	3.66283400	3.47071900	7.33963600	H	7.77205400	-3.38095800	-2.97879700
H	2.79897100	1.47616400	6.02488900	H	7.73603100	-2.60055600	-1.39155900
H	4.64926700	4.81911700	4.07138700	H	6.96753700	-0.80071100	-2.74119000
H	1.95506800	0.66540100	3.84003200	H	5.27080900	-2.78604600	-4.36969700
H	3.81535800	3.99999300	1.87522700	H	5.39134400	-1.02990600	-4.65593500
H	2.07980200	0.94488100	1.57572600	H	6.79985300	-2.06402800	-4.90001200
H	5.50145500	1.79648300	6.90501100	H	5.56405800	0.76336500	-2.96683500
H	6.43689700	3.04532200	6.07475200	H	4.65639100	3.84215800	-1.43515000
H	6.10810700	3.19323900	7.80993500	H	5.73310700	1.63894900	-0.64147100
N	0.75466100	0.49312100	-0.67921400	H	3.98906100	1.93464000	-0.61783300
C	0.31637400	1.58606100	-1.43045000	H	2.69458700	1.41198700	-2.76569000
O	1.04226500	2.06845400	-2.30776300	H	2.14518400	0.90601600	-5.98620700
N	-0.89329400	2.10007200	-1.12689400	H	1.57781100	1.81060400	-4.55731600
C	-1.77363800	1.54541100	-0.11351100	H	2.63289700	2.57991900	-5.79071000
C	-0.90594000	1.00044000	1.00885800	F	-1.67354300	0.38733900	1.97506200
C	0.17488700	0.05759600	0.48999900	H	-0.34926000	1.81927000	1.48605600
O	0.91979000	-0.56303200	1.33007200				

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C	-5.26965900	-6.75155100	-1.77209900	C	-7.33956400	0.72404600	-0.42297300
C	-4.27347200	-5.94844600	-1.01975800	C	-6.17262900	-0.02021800	0.11519900
N	-3.32917100	-6.45704900	-0.13906800	N	-5.79485800	0.01092200	1.44924700
C	-4.04597300	-4.60424000	-1.03513100	C	-5.24091300	-0.81439400	-0.49441500
C	-2.58427000	-5.42523500	0.33458100	C	-4.67673900	-0.73279200	1.60233300
N	-2.99311800	-4.28819500	-0.19959700	N	-4.31684800	-1.24446100	0.43788500

C	-1.21777000	-4.83285300	4.54013100	H	-3.45381200	-3.20981900	-4.35504400
N	-2.03267100	-4.04776100	3.64786200	H	0.85446100	-7.06081300	-2.71122400
C	-1.49682700	-3.30568800	2.63580800	H	-2.96188300	-3.77799300	3.93145800
O	-0.26453000	-3.53245600	2.35660500	C	-4.66605000	6.58350700	3.83290000
O	-2.27608500	-2.51092000	2.03941600	C	-4.75551000	5.46137700	2.79071900
C	2.82404100	-4.27596200	4.19287700	C	-5.87785600	4.44742800	3.09937900
C	3.39159600	-3.01982400	3.60443400	C	-6.15897500	3.54343800	1.89423800
N	2.82325400	-2.35428800	2.52012000	C	-5.57709300	3.60322900	4.34729000
C	4.51694500	-2.33696800	3.98483200	C	-6.16574500	2.47411400	-4.02883100
C	3.59815800	-1.30558600	2.25627900	C	-5.00897600	2.31323700	-3.04691200
N	4.63168600	-1.26648800	3.11942200	S	-4.85918700	3.72838000	-1.85872700
C	1.20682200	-6.04759800	-2.93773300	C	0.68827000	5.41331700	-2.65573900
C	1.56176400	-5.29033800	-1.70605600	C	-0.60019900	4.76206500	-3.15740800
N	2.58149900	-5.64632400	-0.83550600	O	-1.61035500	4.68001100	-2.44135100
C	1.01191700	-4.16182200	-1.16247600	C	0.73917600	5.42053800	-1.11839400
C	2.61299600	-4.74944100	0.17902900	C	1.91039500	6.22518300	-0.57842100
N	1.66710500	-3.83903900	0.01008600	O	3.04381500	5.76020500	-0.43934800
C	-2.48003900	-3.48325500	-3.94150100	N	1.64382600	7.51931500	-0.26385300
C	-2.07906700	-2.52948400	-2.81927800	N	-0.59983400	4.33060700	-4.43758200
O	-2.99624400	-2.15168900	-2.01124400	C	-1.72144100	3.57937100	-4.99024400
O	-0.86561800	-2.21436700	-2.70431300	H	-4.94022500	5.90274400	1.80331600
Zn	-2.61807600	-2.25852700	0.06083200	H	-3.79483100	4.93257200	2.71772000
Zn	1.08703200	-2.48079800	1.40503200	H	-6.79254800	5.02582700	3.29772400
H	-4.79512400	-7.48315500	-2.43657800	H	-6.41580000	4.12453200	1.00341100
H	-5.94849000	-7.30054500	-1.10905200	H	-7.00040700	2.86862300	2.10344100
H	-4.53894800	-3.84322000	-1.61482400	H	-5.28050500	2.93774200	1.64081200
H	-3.21397400	-7.42755200	0.11378500	H	-6.40280900	2.91585200	4.56692900
H	-1.77747800	-5.53641600	1.04238300	H	-4.66874700	3.00409200	4.20209800
H	-7.48801900	0.46814000	-1.47400200	H	-5.42619700	4.21967400	5.23775300
H	-7.19233800	1.80740700	-0.35817000	H	-4.41186300	6.20295800	4.82698400
H	-5.14777300	-1.09211000	-1.53209100	H	-5.13228400	1.41083000	-2.44328900
H	-6.23774500	0.56072500	2.17137500	H	-4.05497200	2.21508800	-3.56839300
H	-4.14229200	-0.86706200	2.52825900	H	-3.70201400	4.24185000	-2.33011900
H	1.76943100	-4.14550700	4.44996600	H	-7.11963400	2.58480500	-3.50416100
H	5.22508900	-2.51627400	4.77789700	H	0.85965100	4.39466300	-0.76681600
H	5.31992200	-0.52908700	3.16374500	H	-0.21073200	5.80295100	-0.73431800
H	3.44653900	-0.59635900	1.45269600	H	0.71575100	7.90661100	-0.31177500
H	0.40931600	-5.52047900	-3.46448800	H	2.39687600	8.09306000	0.08609400
H	2.05548700	-6.13753200	-3.62521400	H	1.56207100	4.88729300	-3.05221300
H	0.22598500	-3.54798600	-1.57617300	H	-2.65238900	4.11395200	-4.79433300
H	3.20986300	-6.42907800	-0.94431200	H	-1.78548800	2.57694700	-4.55113300
H	3.31871800	-4.78316400	0.99429600	H	0.29104300	4.25635700	-4.90643100
H	-0.51206800	-5.43477400	3.96549600	H	0.71762400	6.43972800	-3.04584000
H	-1.72614300	-3.49381000	-4.72988700	H	-1.58690800	3.48747200	-6.06917700
H	-2.57297300	-4.49036200	-3.52010100	H	-6.03238800	3.35899800	-4.65727200
H	-8.26462500	0.47922400	0.11130200	H	-6.23724300	1.59604600	-4.68207500
H	2.88399600	-5.11644300	3.49144200	H	-5.61918000	7.11762000	3.91428800
H	3.37209500	-4.55438300	5.09564600	H	-3.89952500	7.31657900	3.56134000
H	-1.85923200	-5.50490800	5.11598700	C	5.31222500	3.62059200	6.81874800
H	-0.64438100	-4.21927300	5.24852200	C	3.80431300	3.84226600	6.60963500
H	-5.87663100	-6.08740600	-2.39012300	C	3.30157300	3.29540700	5.29043200

C	2.68821900	2.04114700	5.20481000	N	3.30072400	1.58138200	-3.21965300
C	3.46661200	4.01965300	4.09905300	C	4.45017600	1.46722600	-2.34497800
C	2.25883200	1.51734300	3.98299900	C	4.42501500	0.08833100	-1.67145200
C	3.04956500	3.51654600	2.87118800	O	3.51747200	-0.18985300	-0.86006300
C	2.44372700	2.25399000	2.80617600	C	4.42700800	2.57316200	-1.27110500
O	2.05581600	1.80377000	1.58055400	O	4.43194000	3.81791700	-1.92572300
H	3.59072000	4.91675900	6.66761200	N	5.38774400	-0.81560200	-1.95470900
H	3.25285400	3.37479900	7.43409600	C	6.51816300	-0.70315000	-2.91715900
H	2.53166700	1.46102200	6.11182500	C	6.08049800	-0.95987700	-4.36521300
H	3.93068500	5.00278800	4.13435900	C	7.49036900	-1.76779000	-2.37338400
H	1.76270600	0.55108100	3.94066100	C	6.56232200	-2.88465500	-1.86889300
H	3.17436100	4.08849600	1.95634700	C	5.37137200	-2.12043500	-1.26974000
H	1.67436200	0.89554600	1.61618900	H	4.40829000	-2.61729700	-1.41922700
H	5.55596100	2.55273100	6.80771600	H	5.48579400	-1.96271500	-0.19002300
H	5.89378100	4.10096500	6.02513900	H	6.23352400	-3.51094700	-2.70449000
H	5.64376000	4.03339600	7.77731500	H	7.04280900	-3.53954900	-1.13677400
N	0.55343900	0.51178300	-0.84434000	H	8.19707000	-2.10490700	-3.13558500
C	0.05909800	1.63069600	-1.47089400	H	8.06810000	-1.35348700	-1.53918800
O	0.75001400	2.28568200	-2.27399100	H	6.96061400	0.29329000	-2.84255600
N	-1.21787800	2.00585200	-1.19420800	H	5.59005600	-1.93438200	-4.46163100
C	-2.02645100	1.40660600	-0.15067500	H	5.40792200	-0.17802200	-4.72290300
C	-1.09740100	0.80786500	0.88911000	H	6.96199700	-0.95833300	-5.01566100
C	-0.09167800	-0.17832900	0.25693600	H	5.33087800	1.60255400	-2.97302200
O	0.82355900	-0.60893600	1.15774600	H	3.95907900	4.46378800	-1.36874500
H	-2.68890900	0.63019300	-0.54955200	H	5.31464600	2.44217700	-0.62514000
H	-2.65459200	2.17730100	0.30291500	H	3.54453100	2.43449100	-0.63364500
H	1.56049600	0.34967400	-0.92763000	H	2.39650300	1.78396600	-2.78705300
H	-1.50052400	2.89346700	-1.60158000	H	1.95740100	1.36284200	-6.05319100
O	-0.81020700	-1.33578700	-0.29213500	H	1.25091800	2.08255900	-4.57833200
H	-0.68610400	-1.45207500	-1.29641500	H	2.19999700	3.07269000	-5.74008600
C	2.10628500	2.09479000	-5.25390700	F	-1.85589700	0.17300100	1.86489200
C	3.42107300	1.79270400	-4.55488500	H	-0.50464900	1.58841400	1.37525900
O	4.48063300	1.72891200	-5.17794800				

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C	3.69874800	7.69386300	-1.82907100	O	-0.40984300	3.62474700	2.23444000
C	2.89435900	6.68153800	-1.08839700	O	1.77865800	3.00097300	2.15389400
N	1.79959900	6.97185600	-0.28484500	C	-3.77872500	3.67101200	4.09726900
C	3.00475200	5.32077200	-1.04071700	C	-4.01614800	2.31836400	3.50009200
C	1.30148300	5.80859400	0.20546700	N	-3.25189000	1.78672000	2.46277200
N	2.00896300	4.78594600	-0.24377800	C	-4.97971700	1.40500300	3.83848500
C	7.27388700	0.84467100	-0.31366800	C	-3.75739800	0.58715800	2.18619800
C	5.98124000	1.33592500	0.21010100	N	-4.80229200	0.32588200	2.99506800
N	5.63875700	1.31309300	1.55299700	C	-2.46773500	5.62371500	-3.04891600
C	4.89344400	1.86387300	-0.42483200	C	-2.65004200	4.82683400	-1.80398700
C	4.38893000	1.80833000	1.68843100	N	-3.80094500	4.83264000	-1.02984800
N	3.91284100	2.14884200	0.50273600	C	-1.80649700	3.95997900	-1.16623900
C	0.05037300	5.07150500	4.47617000	C	-3.61994600	3.99081900	0.01703600
N	1.08562900	4.44603800	3.70385900	N	-2.41445000	3.44914500	-0.03831700
C	0.80348300	3.62948800	2.65441400	C	1.68972900	3.87600400	-3.96398100

C	1.54957600	2.86403800	-2.84461200	N	1.49950100	-4.14497900	-4.29234600
O	2.49364700	2.68853200	-2.03813900	C	2.44747900	-3.20467900	-4.88363300
O	0.40028100	2.29048300	-2.73603200	H	5.58736500	-4.74332800	1.97702700
Zn	2.02744600	2.74341700	0.17904000	H	4.77331200	-3.70472700	3.13655900
Zn	-1.53741100	2.26247000	1.36772000	H	7.79934900	-3.89900500	2.76149700
H	3.09309500	8.25017100	-2.55367900	H	6.67660800	-2.89219100	0.76608200
H	4.16496400	8.42320800	-1.15691700	H	7.63126500	-1.68802400	1.64703500
H	3.71073500	4.68518500	-1.54695900	H	5.86241800	-1.72142700	1.81406000
H	1.43611900	7.89283500	-0.08748700	H	7.90769900	-1.81433400	4.14555700
H	0.44803200	5.74047200	0.86308200	H	6.15889900	-1.91076800	4.42733100
H	7.34088000	1.05110600	-1.38392600	H	7.23667800	-3.15236300	5.07523700
H	7.38945900	-0.23528700	-0.17593300	H	5.84316100	-4.96483700	5.04124900
H	4.73308200	2.04037800	-1.47609200	H	5.48070100	-1.14113700	-2.00739500
H	6.21016800	0.94612000	2.30030200	H	4.51674700	-1.71764700	-3.36703100
H	3.84973700	1.89228500	2.61706200	H	4.64193400	-3.89233000	-2.28381700
H	-2.77606200	3.74390500	4.52918000	H	7.55708100	-1.21805800	-3.47900400
H	-5.75241900	1.43017400	4.59009800	H	-0.02255700	-4.34743600	-0.63031500
H	-5.30764400	-0.54777100	3.02067100	H	1.36491700	-5.43920700	-0.52214000
H	-3.40889200	-0.07952200	1.40923100	H	0.99133600	-7.69152400	-0.01951400
H	-1.49695400	5.38815800	-3.48873700	H	-0.59432500	-8.27662600	0.38361400
H	-3.23345600	5.39384300	-3.79822600	H	-0.52429200	-5.07663200	-2.89576900
H	-0.83013100	3.63887000	-1.48275600	H	3.46675400	-3.51976300	-4.65485800
H	-4.64249600	5.35722800	-1.21981400	H	2.28939200	-2.18943100	-4.50192800
H	-4.36442900	3.79484200	0.77273600	H	0.62326200	-4.29113700	-4.77175100
H	-0.70008100	5.50126100	3.81147900	H	0.63208800	-6.40968400	-2.80193400
H	0.97222100	3.68571400	-4.76333800	H	2.31160900	-3.20365900	-5.96631600
H	1.49903400	4.86916600	-3.54242100	H	6.55045600	-1.73412700	-4.83547600
H	8.12701900	1.33420900	0.17053300	H	6.32289200	-0.12442000	-4.12481200
H	-3.86557900	4.46571400	3.34760000	H	6.75409200	-5.94745400	3.88716400
H	-4.50691600	3.87050200	4.88651700	H	4.99384400	-6.07760600	3.97052000
H	0.48148100	5.87526400	5.07903900	C	-4.58925700	-4.52723200	6.84929600
H	-0.45828700	4.37440600	5.15672300	C	-3.06572000	-4.40092900	6.67292500
H	4.49717100	7.19158200	-2.37834400	C	-2.65876400	-3.78246400	5.35117100
H	2.70740400	3.87444600	-4.35930400	C	-2.29338500	-2.43560100	5.25367100
H	-2.50278200	6.70280400	-2.85841200	C	-2.65193400	-4.54154400	4.16980200
H	2.01735000	4.36626100	4.08011200	C	-1.93655200	-1.85795400	4.03227500
C	5.83067900	-5.37410000	4.02657400	C	-2.30395600	-3.98665800	2.94254800
C	5.69727400	-4.27577800	2.96376300	C	-1.94315100	-2.63356300	2.86566200
C	6.88873500	-3.30002500	2.91048200	O	-1.60870700	-2.13866300	1.64169400
C	6.75856900	-2.34912200	1.71371700	H	-2.61466600	-5.39693300	6.76468000
C	7.05821600	-2.50373100	4.21332500	H	-2.65631400	-3.80309600	7.49592900
C	6.54597900	-1.17322200	-3.89711300	H	-2.27392500	-1.82229100	6.15215400
C	5.51441500	-1.73688200	-2.92440300	H	-2.92095300	-5.59467800	4.21258800
S	5.91551300	-3.49161500	-2.49299500	H	-1.63119900	-0.81595500	3.98350500
C	0.43435400	-5.38271700	-2.46595200	H	-2.29366500	-4.58662000	2.03727700
C	1.56513000	-4.49834100	-2.99152900	H	-1.41348800	-1.17000300	1.66189700
O	2.51923900	-4.16466300	-2.26940000	H	-5.07120400	-3.54445700	6.80782100
C	0.35659700	-5.32593900	-0.93022300	H	-5.02741200	-5.14425600	6.05801600
C	-0.58233200	-6.37443700	-0.35670300	H	-4.83825500	-4.98612100	7.81181400
O	-1.79793500	-6.20340100	-0.23732400	N	-0.42819600	-0.52043500	-0.83442400
N	-0.00464100	-7.54738500	0.01054800	C	0.28744500	-1.49653700	-1.47412200

O	-0.24867300	-2.28936400	-2.27302700	C	-7.73433500	0.09148700	-2.46944400
N	1.62435400	-1.58194300	-1.22349100	C	-7.09985300	1.40358200	-1.98010500
C	2.28353900	-0.85738300	-0.15507100	C	-5.76799200	0.95171100	-1.35955200
C	1.24957200	-0.48660000	0.89236900	H	-4.94636900	1.65570500	-1.52251000
C	0.06311700	0.28951000	0.27714400	H	-5.84821900	0.79970000	-0.27594600
O	-0.93082800	0.46368500	1.19728800	H	-6.91959000	2.07528400	-2.82573300
H	2.77211600	0.04892500	-0.52776600	H	-7.72875200	1.93913600	-1.26351400
H	3.05303700	-1.49371200	0.29213000	H	-8.49008100	0.24044400	-3.24449100
H	-1.44514700	-0.57628500	-0.91685900	H	-8.21027400	-0.43122800	-1.63196900
H	2.06523900	-2.41702700	-1.60235600	H	-6.73292100	-1.79662500	-2.89318400
O	0.47454700	1.57260100	-0.22200000	H	-5.88272100	0.65984100	-4.53739900
H	0.38191300	1.78251400	-1.53087300	H	-5.30554400	-1.01503100	-4.76264300
C	-1.60257100	-2.56324400	-5.21626100	H	-6.98973400	-0.60944300	-5.09023400
C	-2.95528700	-2.52242600	-4.52545200	H	-4.86191400	-2.70921100	-2.94590100
O	-4.00066100	-2.72079100	-5.14468200	H	-2.91596500	-5.14972500	-1.23367000
N	-2.89090500	-2.22986200	-3.20164600	H	-4.66596200	-3.45897000	-0.58145800
C	-4.03806300	-2.35583000	-2.32567100	H	-2.94739900	-3.03299200	-0.58221800
C	-4.33368100	-0.98910000	-1.69383800	H	-1.96495600	-2.20235500	-2.76707100
O	-3.52376900	-0.48729900	-0.88813300	H	-1.61606000	-1.86470200	-6.05811600
C	-3.76518400	-3.39373100	-1.21944900	H	-0.77465700	-2.32447100	-4.54887100
O	-3.46776500	-4.62042500	-1.84011800	H	-1.47525800	-3.56404400	-5.64498200
N	-5.47538900	-0.33765600	-2.00906000	F	1.86481000	0.27281700	1.88309400
C	-6.53303800	-0.72601200	-2.98145600	H	0.83607900	-1.38291600	1.36367100
C	-6.14233500	-0.39863400	-4.42875900				

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C	3.73224200	7.66064900	-1.83881000	N	-3.83016500	4.71280300	-1.11731100
C	2.93156700	6.62965900	-1.11456500	C	-1.75051900	4.05708200	-1.10140900
N	1.82209200	6.90869200	-0.32710300	C	-3.63931300	3.89154000	-0.05603300
C	3.05404000	5.26836700	-1.06350000	N	-2.38352400	3.47960400	-0.02134400
C	1.32735700	5.74210000	0.15675600	C	1.69069600	3.85741700	-3.96896700
N	2.05041000	4.72407500	-0.28076300	C	1.61374800	2.85072000	-2.84652800
C	7.26052100	0.78564000	-0.33061400	O	2.59185300	2.60667100	-2.12698200
C	5.98756500	1.30486100	0.20637600	O	0.42635800	2.34115400	-2.64546000
N	5.66161300	1.30403700	1.55282600	Zn	2.03037100	2.69484500	0.22738100
C	4.90064200	1.83683600	-0.42417100	Zn	-1.49201200	2.29355600	1.37047900
C	4.41900000	1.81454000	1.69433600	H	3.12715800	8.21215500	-2.56735200
N	3.93313500	2.14395900	0.50911200	H	4.17677600	8.39137200	-1.15382100
C	0.07858700	5.06552000	4.47463300	H	3.77710300	4.63915500	-1.55416500
N	1.12362100	4.41803500	3.73953100	H	1.44861600	7.82652700	-0.13336800
C	0.85935300	3.63227800	2.66561200	H	0.46589900	5.66459400	0.80342700
O	-0.33406800	3.66833000	2.19128600	H	7.31385200	0.97773400	-1.40435700
O	1.83641300	2.98619100	2.19199200	H	7.35997500	-0.29457100	-0.18196500
C	-3.76147000	3.69303500	4.10423400	H	4.73372100	1.99887800	-1.47620200
C	-3.97923800	2.33710900	3.50684100	H	6.23704000	0.94102600	2.29888300
N	-3.20364800	1.81159100	2.47410300	H	3.89070000	1.91538800	2.62727400
C	-4.93616900	1.41507300	3.84033300	H	-2.76138800	3.77987800	4.53979900
C	-3.69775500	0.60746600	2.19542500	H	-5.71309100	1.43383700	4.58778900
N	-4.74493100	0.33748800	2.99799800	H	-5.23940800	-0.54240300	3.02321500
C	-2.45186600	5.63555300	-3.04498000	H	-3.34003500	-0.05720800	1.42134600
C	-2.63142700	4.83075600	-1.80502200	H	-1.42603100	5.52715600	-3.40175800

H	-3.11709100	5.30038200	-3.84860900	H	-0.57808500	-5.07236200	-2.87846700
H	-0.72339600	3.84134900	-1.33382600	H	3.41256500	-3.55298100	-4.66781100
H	-4.70529000	5.14851100	-1.36994800	H	2.24907400	-2.21159800	-4.50773300
H	-4.41159900	3.61811100	0.64559600	H	0.55917600	-4.29399900	-4.76014500
H	-0.64624700	5.49687600	3.78358600	H	0.57024800	-6.41194400	-2.77361500
H	0.92128800	3.67741200	-4.72122000	H	2.25084600	-3.22776000	-5.97133100
H	1.53849500	4.85282300	-3.53737200	H	6.49790200	-1.77922800	-4.85581700
H	8.13114900	1.26465300	0.13291400	H	6.29162600	-0.17462900	-4.12701300
H	-3.85771900	4.48546800	3.35335300	H	6.69897000	-6.00388100	3.87042700
H	-4.49445200	3.88268000	4.89147700	H	4.93793200	-6.11799200	3.96093300
H	0.50208900	5.87079100	5.08121300	C	-4.62590600	-4.49885300	6.85878300
H	-0.45880800	4.38368300	5.14886600	C	-3.10399600	-4.33804300	6.69172400
H	4.54631400	7.17523300	-2.38025000	C	-2.69131100	-3.71545900	5.37254200
H	2.68152500	3.84000700	-4.42569500	C	-2.29713500	-2.37603600	5.28390500
H	-2.64257000	6.70220000	-2.87839500	C	-2.69285500	-4.46705800	4.18598500
H	2.03880800	4.30926900	4.14767100	C	-1.91882300	-1.79901500	4.06804700
C	5.78136100	-5.42208600	4.01333100	C	-2.32431500	-3.91262300	2.96452100
C	5.65365700	-4.32296200	2.95080300	C	-1.93203900	-2.56719900	2.89646900
C	6.85403400	-3.35843000	2.89223500	O	-1.57796800	-2.07613500	1.67678700
C	6.72840200	-2.40653000	1.69567200	H	-2.63248900	-5.32394500	6.79141900
C	7.03644800	-2.56346200	4.19415400	H	-2.71435000	-3.72962300	7.51652300
C	6.51003100	-1.22717600	-3.91225200	H	-2.26997200	-1.76795500	6.18573200
C	5.48743600	-1.79260200	-2.93113700	H	-2.98295600	-5.51491900	4.21999200
S	5.88092900	-3.55425200	-2.52149400	H	-1.59133400	-0.76333200	4.02853600
C	0.38027700	-5.37981600	-2.44911700	H	-2.31957200	-4.50875000	2.05666000
C	1.51535500	-4.50960700	-2.98852400	H	-1.35670800	-1.11188900	1.69322000
O	2.47929200	-4.18341900	-2.27632300	H	-5.13031700	-3.52759100	6.81344200
C	0.30950700	-5.30387000	-0.91363800	H	-5.04575100	-5.12708300	6.06638200
C	-0.62465100	-6.34612200	-0.32179100	H	-4.86892500	-4.96220400	7.82058900
O	-1.83971400	-6.17489700	-0.19541200	N	-0.41917100	-0.49135800	-0.85059100
N	-0.04371300	-7.51465400	0.05424500	C	0.27402400	-1.47446100	-1.49771900
N	1.44228500	-4.15932800	-4.29004600	O	-0.28202300	-2.27555600	-2.27699200
C	2.39463900	-3.22868600	-4.88962300	N	1.61908800	-1.56198400	-1.28338000
H	5.53542500	-4.78977700	1.96467100	C	2.30235100	-0.84943200	-0.22117700
H	4.73576800	-3.74331600	3.12707500	C	1.28889900	-0.46539400	0.84076100
H	7.75827900	-3.96616600	2.73976100	C	0.11166000	0.33936500	0.24160400
H	6.63571200	-2.94949000	0.74892000	O	-0.87094000	0.51020100	1.18617500
H	7.60848700	-1.75582700	1.62423100	H	2.79551300	0.05208900	-0.59889800
H	5.84048500	-1.76793700	1.80028600	H	3.07046200	-1.49675800	0.21269200
H	7.89206300	-1.88206700	4.12249300	H	-1.43687300	-0.54649600	-0.90426600
H	6.14367900	-1.96199800	4.41164400	H	2.03975800	-2.41158900	-1.65186400
H	7.21254000	-3.21357300	5.05546700	O	0.51990400	1.58660300	-0.28989400
H	5.80163800	-5.01269100	5.02783800	H	0.41475100	1.84312500	-1.70395900
H	5.47079800	-1.20546200	-2.00816700	C	-1.65133100	-2.55767800	-5.21345200
H	4.48384500	-1.76194800	-3.35960600	C	-2.99884700	-2.50276900	-4.51302600
H	4.60691700	-3.94655000	-2.29977100	O	-4.04968900	-2.69967800	-5.12376400
H	7.52624300	-1.28329900	-3.50812000	N	-2.92401700	-2.20066200	-3.19183900
H	-0.06845200	-4.32150500	-0.62487100	C	-4.06491300	-2.32776300	-2.30738400
H	1.32003400	-5.41132200	-0.50947200	C	-4.36748900	-0.96118700	-1.67867200
H	0.95223900	-7.65800400	0.01949500	O	-3.56230800	-0.45244600	-0.87375800
H	-0.63021900	-8.23971600	0.44023700	C	-3.77848000	-3.35856900	-1.19827800

O	-3.47869400	-4.58601500	-1.81615200	H	-5.91930900	0.70132200	-4.51091500
N	-5.51510500	-0.31849800	-1.99492700	H	-5.33242700	-0.96821000	-4.75417600
C	-6.56538600	-0.70835900	-2.97414500	H	-7.01731100	-0.56739700	-5.08318100
C	-6.17341200	-0.35986900	-4.41623300	H	-4.89067400	-2.68955100	-2.92017900
C	-7.77738400	0.08875400	-2.45571700	H	-2.93885500	-5.11930900	-1.20195200
C	-7.16003200	1.40447000	-1.95402100	H	-4.67434300	-3.42582000	-0.55359200
C	-5.81937900	0.96568100	-1.34193700	H	-2.95789800	-2.99010900	-0.56876800
H	-5.00745200	1.68017100	-1.50907500	H	-1.99457700	-2.17728500	-2.76285000
H	-5.89014500	0.81091300	-0.25803400	H	-1.66548700	-1.86538300	-6.06049100
H	-6.99249700	2.08733400	-2.79337700	H	-0.81736900	-2.32073600	-4.55275300
H	-7.79470400	1.92330500	-1.23022700	H	-1.53446900	-3.56252600	-5.63558200
H	-8.53489100	0.23542800	-3.22949000	F	1.93501500	0.28381100	1.82306400
H	-8.24654300	-0.44793200	-1.62335500	H	0.86988900	-1.35417400	1.32070400
H	-6.75294600	-1.78211400	-2.89948400				

SkDHPase.5FUH2-TS3-II- D

C	2.86946000	7.78530000	-2.39673700	H	0.85403600	7.95930600	-0.38867200
C	2.20388400	6.76452900	-1.54602400	H	0.09716100	5.81658900	0.75744500
N	1.21862700	7.04443300	-0.61042800	H	7.19123500	1.62556500	-1.42349700
C	2.37034000	5.41034800	-1.47941000	H	7.35681400	0.44091100	-0.12419300
C	0.83553700	5.88213900	-0.02606300	H	4.48080800	2.32868000	-1.60328900
N	1.51452800	4.87139300	-0.53931100	H	6.01575200	1.63760500	2.24424300
C	7.12693400	1.48922000	-0.34184900	H	3.56850600	2.36146800	2.48497800
C	5.77792500	1.87270000	0.13276400	H	-3.18140600	3.69602500	4.29041600
N	5.42163600	1.90184200	1.47179900	H	-6.01044700	1.17332200	4.37062400
C	4.64723000	2.24009100	-0.54170700	H	-5.36451100	-0.84327600	2.92999700
C	4.12468700	2.26788400	1.56719800	H	-3.40707600	-0.32346800	1.39167000
N	3.62941700	2.47846800	0.35919500	H	-2.16265500	4.65459300	-3.95815700
C	-0.51311200	5.32585600	4.11884400	H	-3.92352900	4.74716800	-4.02097800
N	0.60268100	4.88600900	3.33105500	H	-1.28834300	3.08454700	-1.82026500
C	0.45507100	3.78941400	2.52553000	H	-4.95416000	5.07511600	-1.32277900
O	-0.75178700	3.40483600	2.35163800	H	-4.49773400	3.74570300	0.80083300
O	1.51211000	3.32166600	2.01660100	H	-1.36331500	5.56269000	3.47628900
C	-4.17558500	3.51117300	3.87356100	H	7.91219300	2.10317900	0.11450400
C	-4.27837000	2.11940700	3.32243700	H	-4.34697400	4.27250800	3.10361000
N	-3.42838300	1.59084900	2.35047100	H	-4.91671400	3.65988700	4.66195800
C	-5.20025900	1.16228900	3.65902900	H	-0.23388400	6.23129200	4.66524200
C	-3.84593900	0.35274700	2.11189500	H	-0.84554300	4.57560800	4.84858600
N	-4.91576600	0.05923000	2.87948700	H	3.60445200	7.30012900	-3.04177500
C	-3.04544100	4.99655100	-3.41452100	H	-2.99427100	6.08916800	-3.33874100
C	-3.08692100	4.34524700	-2.07690100	H	1.54246500	5.06598400	3.65008700
N	-4.12387000	4.52075200	-1.17253600	C	6.31680500	-4.46859400	4.49982000
C	-2.20714600	3.50701000	-1.44468500	C	6.07483500	-3.48078500	3.35128200
C	-3.84634800	3.80384500	-0.05665400	C	6.98765700	-2.23943000	3.39046100
N	-2.68773800	3.18330800	-0.19119200	C	6.80772700	-1.39351100	2.12388700
Zn	1.69296500	2.89614500	0.01854400	C	6.76355700	-1.38121600	4.64449700
Zn	-1.67459800	2.09225300	1.22461500	C	6.62530200	-0.87990500	-3.74454300
H	2.15752000	8.31324100	-3.04181500	C	5.67656900	-1.37723300	-2.65730400
H	3.39745800	8.53843600	-1.80053700	S	6.30262100	-2.95481100	-1.91882700
H	3.03082900	4.77910300	-2.04926900	C	2.20486700	-6.25107600	-2.06018300

C	2.52979300	-4.85467000	-2.57451100	H	-1.35738100	-1.33326400	1.60494700
O	2.96130600	-3.97551400	-1.80776900	H	-4.88824100	-3.70001200	7.06899000
C	1.44645300	-6.23468400	-0.73133300	H	-4.34936900	-5.32588800	6.63516500
C	-0.03352800	-5.90868300	-0.90864700	H	-4.29824500	-4.80337900	8.32425200
O	-0.46006000	-5.38828700	-1.94551100	C	-1.33907300	-3.19807700	-4.91829800
N	-0.83986700	-6.22075200	0.13123400	C	-2.68808000	-3.28961400	-4.23419900
N	2.41954800	-4.66168600	-3.90145800	O	-3.71327600	-3.65119500	-4.80919700
C	2.76239900	-3.39766200	-4.54248300	N	-2.64677100	-2.92143900	-2.92160500
H	6.22954700	-3.99662000	2.39502200	C	-3.80743600	-2.89132800	-2.05919500
H	5.02452800	-3.15490500	3.35767900	C	-4.10624000	-1.43380600	-1.68098100
H	8.02813800	-2.59656400	3.40790200	O	-3.24077300	-0.76823000	-1.07993300
H	6.98871900	-1.97513200	1.21372000	C	-3.52709600	-3.71433100	-0.78176800
H	7.50304600	-0.54426800	2.12312900	O	-3.18638200	-5.05257200	-1.10206300
H	5.78464200	-0.99900200	2.06430100	N	-5.30704700	-0.89375200	-1.97852400
H	7.42436600	-0.50628600	4.64534300	C	-6.40410100	-1.48254700	-2.79171100
H	5.72745400	-1.02086200	4.69037400	C	-6.08115500	-1.45655500	-4.28989500
H	6.96077800	-1.93541300	5.56612600	C	-7.59262300	-0.58214600	-2.40365400
H	6.07763300	-4.03291300	5.47461700	C	-6.95465000	0.80484900	-2.22168300
H	5.56766800	-0.63048700	-1.86568400	C	-5.59436100	0.49583000	-1.57732800
H	4.68347600	-1.56849900	-3.06822900	H	-4.78916100	1.15965100	-1.90432000
H	5.09423300	-3.45945700	-1.58612600	H	-5.63334500	0.55516300	-0.48256200
H	7.63450200	-0.71782100	-3.35176200	H	-6.81526800	1.28832600	-3.19380800
H	1.89402100	-5.47610700	-0.07816700	H	-7.56131900	1.47415600	-1.60559400
H	1.55189900	-7.19945400	-0.22335700	H	-8.38267200	-0.59903400	-3.15825900
H	-0.48008800	-6.63484300	0.97551900	H	-8.02521400	-0.92407200	-1.45641400
H	-1.82523100	-5.96939900	0.05933700	H	-6.58372100	-2.51272100	-2.47167600
H	1.65319600	-6.82611400	-2.80878100	H	-5.86107400	-0.43781300	-4.62619500
H	3.80968600	-3.15179900	-4.35184700	H	-5.23523300	-2.10237200	-4.53438800
H	2.12012200	-2.59249500	-4.17500300	H	-6.94576600	-1.81932700	-4.85664400
H	1.95705800	-5.37138400	-4.44880500	H	-4.61907000	-3.35771700	-2.61671600
H	3.17059000	-6.74856500	-1.90885000	H	-2.39847200	-5.02768000	-1.68511500
H	2.61803200	-3.50481800	-5.61840200	H	-4.43280400	-3.75533300	-0.16541700
H	6.70005700	-1.60059900	-4.56326900	H	-2.74339800	-3.21824200	-0.19486000
H	6.26816500	0.07129900	-4.15518600	H	-1.75129300	-2.59398000	-2.56307800
H	7.36347000	-4.79212800	4.52714300	H	-0.98030200	-2.16598600	-4.92163300
H	5.69823100	-5.36434100	4.38399300	H	-0.59966600	-3.79528900	-4.38029800
C	-4.14578700	-4.47367900	7.29160900	H	-1.44693100	-3.55619900	-5.94294800
C	-2.71455000	-3.94134800	7.09198200	C	1.29376100	3.59981700	-4.16395100
C	-2.40031000	-3.48011100	5.68057500	C	1.19832500	2.55033600	-3.05054300
C	-2.13411600	-2.13809500	5.38554400	O	2.08407300	2.52430800	-2.15989900
C	-2.34005100	-4.39403200	4.61579900	O	0.16635100	1.78804600	-3.09657600
C	-1.81824600	-1.71095900	4.09189500	N	-0.24131300	-0.18675100	-1.25362200
C	-2.03424700	-3.98819900	3.32136600	C	0.51111100	-1.32199600	-1.72790800
C	-1.76698900	-2.63862500	3.04269500	O	0.02255100	-2.09466800	-2.54837700
O	-1.47099700	-2.31067500	1.75762900	N	1.77154100	-1.42907600	-1.27573300
H	-2.00575800	-4.72883600	7.38089700	C	2.30706300	-0.56949200	-0.23572100
H	-2.54028900	-3.11072600	7.78588100	C	1.21200300	-0.32659300	0.79121400
H	-2.15912400	-1.40334900	6.18744600	C	-0.01180200	0.42757500	0.21625300
H	-2.53031900	-5.44813600	4.80567400	O	-1.11394800	0.21308400	0.97615600
H	-1.59424400	-0.66602100	3.89722400	H	0.70162400	3.30457400	-5.03112700
H	-1.98373700	-4.70157300	2.50482600	H	0.91374500	4.55151700	-3.77860600

H	2.66162500	0.37462500	-0.65540600	O	0.14356100	1.76533100	0.00948800
H	3.15323000	-1.07537100	0.23477500	H	0.00701400	0.84524300	-2.14251700
H	2.33662900	3.74824400	-4.45141700	F	1.73125600	0.41159100	1.85183000
H	-1.24635500	-0.41249200	-1.32135500	H	0.86223400	-1.28495100	1.18720200
H	2.25403900	-2.29299000	-1.54195900				

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C	4.54709600	6.98622800	-2.73424900	H	-5.37467700	0.54015000	3.26140100
C	3.76720400	6.19784200	-1.74935900	H	-3.53940900	0.52120200	1.51301300
N	3.08470300	6.73308900	-0.66781100	H	-1.05462400	4.90004700	-4.18304600
C	3.53355000	4.85589100	-1.68023400	H	-2.72823300	5.45469300	-4.28281700
C	2.47871600	5.72170000	0.00235800	H	-0.66951100	3.16246000	-2.01384900
N	2.72599200	4.56847500	-0.59671700	H	-3.69739600	6.05645500	-1.62829400
C	7.38173600	0.03903400	-0.34875900	H	-3.64714800	4.71304200	0.52927000
C	6.11300900	0.66440800	0.10484700	H	-0.01791000	6.04618900	3.21074100
N	5.75949300	0.78828500	1.44097400	H	8.25715300	0.52095500	0.10150400
C	5.07275400	1.22323300	-0.58565300	H	-3.46326400	5.35179900	2.91330900
C	4.55509000	1.39670400	1.51771000	H	-3.71281400	4.92117200	4.60807000
N	4.11535900	1.67345800	0.30265600	H	1.30736900	6.43417700	4.32150100
C	0.74100900	5.61690000	3.86742100	H	0.22647700	5.07126800	4.66918000
N	1.64111500	4.78457200	3.10851300	H	4.97800200	6.31416500	-3.47865100
C	1.16939100	3.74974700	2.34200600	H	-1.49019700	6.50570700	-3.57558200
O	-0.10470900	3.73187500	2.18225100	H	2.59816700	4.68629400	3.41273200
O	2.02419100	2.96453700	1.84967900	C	5.34398600	-5.37069500	4.76750000
C	-3.22335700	4.60852300	3.68322500	C	5.31296900	-4.41085100	3.57117600
C	-3.67806000	3.23190500	3.29189300	C	6.59534300	-3.57426500	3.39869400
N	-3.06779600	2.47001700	2.29547500	C	6.55657500	-2.79105600	2.08051000
C	-4.72781400	2.51001400	3.79651500	C	6.84348100	-2.62527000	4.58113800
C	-3.74437800	1.32822900	2.20565000	C	6.37928700	-2.33237300	-3.63725600
N	-4.75526800	1.32020100	3.09578500	C	5.29468900	-2.61123400	-2.60012200
C	-1.82725700	5.46615300	-3.65946200	S	5.49234500	-4.30990900	-1.89270100
C	-2.06697900	4.85293500	-2.32083400	C	0.60063000	-6.64234300	-1.98852800
N	-3.04239800	5.30990900	-1.44588500	C	1.36719800	-5.40117100	-2.42861500
C	-1.44958000	3.82369100	-1.65759000	O	2.05666900	-4.75106200	-1.62639400
C	-2.98867100	4.57437900	-0.31377200	C	-0.15693300	-6.44556200	-0.67329200
N	-2.02684300	3.66760900	-0.40785300	C	-1.59236500	-5.96458600	-0.87367800
Zn	2.38242900	2.56894100	-0.19368500	O	-2.04322500	-5.66611100	-1.98345600
Zn	-1.33932500	2.62318800	1.17651700	N	-2.35058800	-5.92380600	0.24885800
H	3.92464800	7.71547800	-3.26596400	N	1.31599300	-5.10751100	-3.74357200
H	5.37205400	7.53599800	-2.26627500	C	2.06847000	-4.01143600	-4.34113000
H	3.87083100	4.06981000	-2.33307000	H	5.14907200	-4.98894700	2.65307200
H	3.04974100	7.70888400	-0.41135500	H	4.45199600	-3.73275500	3.66253200
H	1.91186000	5.85631200	0.91043800	H	7.44245000	-4.27410600	3.34588100
H	7.47274500	0.13500600	-1.43263900	H	6.42992300	-3.45027200	1.21526200
H	7.42333700	-1.02694200	-0.10319400	H	7.48499900	-2.22431000	1.93741500
H	4.92940300	1.32647900	-1.64955400	H	5.71724900	-2.08262400	2.07720000
H	6.28770600	0.42973700	2.22341400	H	7.75922800	-2.04129300	4.43265700
H	4.02417600	1.60893400	2.43110900	H	6.00871700	-1.92068900	4.69656100
H	-2.14071400	4.62865700	3.83120500	H	6.95260700	-3.16190200	5.52757300
H	-5.43726400	2.73565700	4.57647400	H	5.40824000	-4.83780700	5.72118200

H	5.33753600	-1.87796900	-1.78921300	C	-6.64392800	-0.31862400	-2.79401100
H	4.30311700	-2.54510300	-3.05192600	C	-6.16293100	-0.23320200	-4.24571700
H	4.18465500	-4.52363900	-1.62116100	C	-7.67558900	0.76274500	-2.41969100
H	7.38087400	-2.42845200	-3.20510100	C	-6.81155700	1.97597400	-2.03843800
H	0.37958100	-5.71755600	-0.05417500	C	-5.60752600	1.35012200	-1.31831400
H	-0.18691900	-7.38340800	-0.10717600	H	-4.66277200	1.86955600	-1.50260100
H	-1.95727400	-6.10502000	1.15791100	H	-5.75166300	1.32256500	-0.23028800
H	-3.29976800	-5.56700600	0.16173600	H	-6.48337300	2.50575700	-2.93845800
H	-0.08829600	-6.97749000	-2.76775700	H	-7.34191400	2.69529900	-1.40838500
H	3.14333400	-4.21159300	-4.29408000	H	-8.36894000	0.96657300	-3.23916800
H	1.85819500	-3.07136200	-3.82527600	H	-8.26402900	0.43379800	-1.55548400
H	0.67227000	-5.62645300	-4.32087700	H	-7.04858200	-1.31513900	-2.59680800
H	1.35943600	-7.42199800	-1.85266800	H	-5.72272200	0.74818100	-4.45336600
H	1.77355600	-3.91686400	-5.38704100	H	-5.43425100	-1.01092700	-4.47980900
H	6.31192300	-3.03078400	-4.47569400	H	-7.01439300	-0.36937700	-4.92206200
H	6.27883400	-1.31395500	-4.02980200	H	-5.29425600	-2.51014800	-2.64260800
H	6.20273300	-6.04868200	4.70656300	H	-3.74399600	-4.77368700	-1.68407700
H	4.43953200	-5.98649100	4.79927100	H	-5.31635400	-2.95222600	-0.15909400
C	-4.87378300	-3.02660100	7.48095800	H	-3.54309800	-2.93741200	-0.17199500
C	-3.37140000	-3.19375800	7.19567800	H	-2.35290000	-2.64713000	-2.31634000
C	-2.98709400	-2.81650500	5.78043000	H	-1.39306400	-2.00270200	-4.87773800
C	-2.35053800	-1.60567500	5.48845500	H	-1.27879700	-3.59461600	-4.11204900
C	-3.28413300	-3.66757500	4.70415600	H	-2.02329800	-3.42296700	-5.73868400
C	-2.02046500	-1.24402800	4.17956100	C	2.11556900	3.14829100	-4.30970100
C	-2.96775000	-3.32444000	3.39460200	C	1.71713000	2.28823000	-3.10486800
C	-2.33143000	-2.10597400	3.12071700	O	2.61413200	2.17595700	-2.17897000
O	-2.05109900	-1.82611500	1.81772900	O	0.57623800	1.79579300	-3.07035100
H	-3.08690600	-4.23595200	7.38780200	N	-0.59702400	-0.58320600	-1.64633000
H	-2.79792600	-2.58467200	7.90406600	C	-0.06141000	-1.84107700	-1.59730300
H	-2.09572800	-0.92899800	6.30113000	O	-0.73005100	-2.88086900	-1.69890500
H	-3.77155900	-4.62052100	4.89755400	N	1.29559200	-1.90441500	-1.37035500
H	-1.50587900	-0.30793600	3.98045700	C	1.95366200	-0.91398700	-0.53174700
H	-3.19680600	-3.98665300	2.56583500	C	1.15409900	-0.56650400	0.73661200
H	-1.64106300	-0.94366700	1.71878400	C	0.22374700	0.64510100	0.62435900
H	-5.18578200	-1.98594100	7.34168000	O	-0.85728700	0.65586900	1.30241100
H	-5.47477500	-3.64565000	6.80694400	H	1.45955700	2.94450400	-5.15739100
H	-5.11468200	-3.31744600	8.50860900	H	2.02457600	4.20592900	-4.03800100
C	-1.89896300	-2.96701400	-4.75561400	H	2.18421300	-0.00459800	-1.09315500
C	-3.27281900	-2.74309200	-4.14929800	H	2.90061100	-1.34156800	-0.19418300
O	-4.29826400	-2.73181600	-4.82963300	H	3.15627300	2.96903000	-4.59285400
N	-3.24778800	-2.51342000	-2.80584000	H	-1.61178000	-0.53482400	-1.66798400
C	-4.43670600	-2.26051000	-2.01783400	H	1.61921400	-2.86905100	-1.29719100
C	-4.47124400	-0.79588800	-1.54279900	O	0.56614600	1.67638400	-0.01940000
O	-3.54078100	-0.34730100	-0.84519200	H	-0.08131800	0.19544900	-2.06533900
C	-4.43364100	-3.17199500	-0.77107900	H	0.58467600	-1.43035000	1.08983400
O	-4.50847400	-4.54362800	-1.11246000	F	2.06198000	-0.21177600	1.75220900
N	-5.54335600	-0.02743500	-1.83689800				

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C	-2.73099300	-0.10103300	-4.80017700	C	-3.72556600	-0.17136400	-5.90158000
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N	-4.08472600	0.89721100	-6.70988300	H	-6.41829400	1.70945900	-13.52529500
C	-4.45107900	-1.22534400	-6.37659900	H	-7.24250000	0.41643400	-17.00807500
C	-4.98981900	0.46071700	-7.62261500	H	-7.77265000	-2.10288100	-16.83736000
N	-5.22481500	-0.82929000	-7.45013200	H	-6.97953300	-3.07245900	-14.66544100
C	-9.56332600	-3.95540900	-4.12769400	H	-0.94190400	-2.91582000	-9.87295200
C	-9.10249900	-3.34650600	-5.41226700	H	0.08579600	-2.78464900	-11.30599500
N	-9.92987200	-2.59713900	-6.23867700	H	-3.57342500	-2.88938400	-10.42946700
C	-7.89496300	-3.36419900	-6.06089200	H	-1.15683800	-0.80144600	-13.14677500
C	-9.22070300	-2.20197000	-7.32371700	H	-3.56606200	-0.60943600	-13.95900400
N	-7.98326500	-2.65578800	-7.24365800	H	-5.96624500	2.45088900	-11.12150100
C	-6.95819100	2.60919600	-10.69330100	H	-2.21934900	-4.97114400	-7.64450000
N	-7.26179200	1.54896400	-9.75724200	H	-2.45489700	-3.26455600	-7.20997500
C	-7.20737600	0.21948400	-10.13342400	H	-9.93042100	-5.22830000	-9.27897700
O	-6.69509100	0.00028800	-11.28615400	H	-10.02057600	-3.21041000	-3.46498700
O	-7.62294000	-0.62838500	-9.29766200	H	-4.90456700	1.50967900	-14.40869900
C	-5.99742500	1.45357700	-14.50229300	H	-6.30752200	2.20821000	-15.23053300
C	-6.45810500	0.09364800	-14.94023700	H	-6.96003400	3.56479800	-10.15981500
N	-6.38222000	-1.07683400	-14.17557300	H	-7.67880200	2.67260100	-11.52047800
C	-7.01070000	-0.20799500	-16.15879900	H	-2.63981900	-1.08222000	-4.32741300
C	-6.86916100	-2.03974100	-14.94910700	H	-3.16730200	-4.52426800	-6.19258900
N	-7.25435300	-1.56440000	-16.15099000	H	-0.20098100	-1.36093100	-10.29317400
C	-0.67058800	-2.26303000	-10.70606800	H	-7.90483200	1.74031800	-9.00129700
C	-1.90050600	-1.95048700	-11.49103400	H	-6.76847300	-5.54190900	-12.87390700
N	-1.94657500	-1.21155000	-12.66745700	H	-9.01596000	-7.32539800	-9.99012400
C	-3.20051100	-2.28267000	-11.23860900	O	-6.04920100	-2.80923200	-10.27449800
C	-3.24087800	-1.12666100	-13.06914900	H	-5.42768700	-3.56139500	-10.15298000
N	-4.02750900	-1.76615200	-12.21884000	C	-15.72460200	-5.23248300	-8.59995200
C	-2.92951900	-4.25382000	-7.22607700	C	-14.28163900	-5.20646500	-8.07990200
C	-4.19271800	-4.17456500	-8.09062900	C	-14.11380000	-4.34335600	-6.81059800
O	-5.24610200	-3.71165600	-7.52372900	C	-12.81536600	-4.68869700	-6.07321800
O	-4.10231200	-4.50132800	-9.29548900	C	-14.17913700	-2.83990800	-7.12093200
Zn	-6.41701100	-2.20928500	-8.47931000	C	-8.21561900	-7.89747400	-4.42193400
Zn	-6.09229500	-1.73785700	-11.95589600	C	-8.14590800	-7.17745500	-5.76742700
N	-7.39180000	-5.43943300	-12.06915200	S	-9.76260500	-7.05719800	-6.65521200
C	-7.79022200	-6.62013100	-11.45938800	C	-9.83081500	-11.09874300	-10.95631700
O	-7.36104700	-7.72042600	-11.79137700	C	-9.07715300	-10.17376700	-10.00775900
N	-8.70416100	-6.45649200	-10.44477500	O	-9.54835800	-9.07791800	-9.66661400
C	-9.23081100	-5.23904600	-10.10559600	C	-10.34949300	-10.39374200	-12.2148300
C	-8.86604800	-4.12082400	-10.77431800	C	-9.32217200	-10.35331400	-13.34395500
C	-7.88751500	-4.17404500	-11.83397300	O	-8.11743500	-10.54644000	-13.14608500
O	-7.51301600	-3.21172100	-12.52623400	N	-9.81871100	-10.09267700	-14.57588200
H	-1.73481400	0.18750000	-5.15977800	N	-7.93243100	-10.65877000	-9.48459500
H	-3.01963800	0.61623800	-4.02102800	C	-7.14861800	-9.92147600	-8.50393300
H	-4.47066100	-2.24866100	-6.04338200	H	-13.96787600	-6.23493400	-7.85536100
H	-3.73847700	1.84350200	-6.63397500	H	-13.60155200	-4.84032900	-8.86329200
H	-5.45917200	1.09607400	-8.36101600	H	-14.94967300	-4.58348300	-6.13624100
H	-8.71030500	-4.38719900	-3.59730100	H	-12.79056600	-5.73989000	-5.76640000
H	-10.29657000	-4.75376300	-4.29248900	H	-12.70119800	-4.07699000	-5.16774000
H	-6.96421800	-3.83129100	-5.77796400	H	-11.94080900	-4.52358600	-6.71554800
H	-10.91151400	-2.41597900	-6.07970500	H	-14.10636200	-2.24237300	-6.20328700
H	-9.60569900	-1.59501500	-8.12810500	H	-13.35496600	-2.54395600	-7.78607600

H	-15.11438300	-2.55953000	-7.61643400	H	-13.27030200	-2.44380300	-17.67868800
H	-16.08135400	-4.23265500	-8.87160400	H	-13.14226100	-1.65802800	-19.26046900
H	-7.83521000	-6.13766900	-5.64072000	C	-4.78800700	-9.59698500	-11.86439800
H	-7.41575700	-7.64029300	-6.43685100	C	-4.58460300	-9.33998100	-13.34169700
H	-9.76894200	-8.28824400	-7.20835300	O	-3.64347700	-9.79555400	-13.98606300
H	-8.93552600	-7.41623700	-3.75267100	N	-5.54760600	-8.53521400	-13.88459900
H	-10.63257500	-9.36528100	-11.95754300	C	-5.54755200	-8.14134600	-15.27767100
H	-11.25810400	-10.89004000	-12.57495200	C	-5.29470300	-6.63042500	-15.34649900
H	-10.80280700	-9.94023600	-14.73591400	O	-6.14698200	-5.84481900	-14.85289000
H	-9.16537700	-10.04531200	-15.35688000	C	-6.90237200	-8.50699800	-15.92451400
H	-9.22323700	-11.96601200	-11.22999600	O	-7.18201400	-9.88736100	-15.80163100
H	-7.73118400	-9.76133500	-7.59146900	N	-4.17489500	-6.14296400	-15.89515000
H	-6.83799200	-8.95068700	-8.90303500	C	-3.05111700	-6.88162300	-16.54254400
H	-7.54586100	-11.50409300	-9.87894100	C	-2.02126900	-7.39225700	-15.52492800
H	-10.69044800	-11.46700200	-10.38249800	C	-2.49074300	-5.80619600	-17.49322500
H	-6.26069800	-10.50572400	-8.25594000	C	-2.64626900	-4.49861600	-16.69916400
H	-8.51998100	-8.94295500	-4.54109700	C	-3.98158100	-4.67660700	-15.95960000
H	-7.23132900	-7.88558500	-3.93681100	H	-3.98657600	-4.24750400	-14.95320800
H	-16.40569300	-5.63327800	-7.83992800	H	-4.82358900	-4.23368100	-16.50320000
H	-15.81466700	-5.86394300	-9.49119400	H	-1.82460300	-4.38669700	-15.98386300
C	-12.65108500	-2.36154800	-18.57849700	H	-2.64944300	-3.61143100	-17.33865800
C	-11.22879700	-1.89409400	-18.23366300	H	-1.45701700	-6.01595000	-17.78105700
C	-10.53357600	-2.85061500	-17.29076300	H	-3.09371300	-5.76654800	-18.40839800
C	-9.47010100	-3.66152500	-17.70581500	H	-3.45642100	-7.72499900	-17.10751400
C	-10.99058000	-2.99989700	-15.97123800	H	-1.62952700	-6.57269000	-14.91192400
C	-8.87728000	-4.58956300	-16.84033100	H	-2.45173600	-8.15387000	-14.87010900
C	-10.42219500	-3.92267500	-15.10380300	H	-1.18107100	-7.84771600	-16.06156100
C	-9.35820200	-4.72774800	-15.53258500	H	-4.75612000	-8.71806500	-15.75604700
O	-8.84551800	-5.62329100	-14.64484300	H	-7.16325100	-10.12028000	-14.84497300
H	-11.27902300	-0.89308400	-17.78329000	H	-6.87515500	-8.28279900	-16.99707200
H	-10.64357900	-1.79076100	-19.15594400	H	-7.69928400	-7.89871200	-15.47352300
H	-9.11185900	-3.59085900	-18.73177100	H	-6.27864500	-8.18162000	-13.26698800
H	-11.81003300	-2.37823000	-15.61751900	H	-4.61594100	-8.67743400	-11.29374600
H	-8.06072500	-5.21946200	-17.18370700	H	-5.81352500	-9.92183600	-11.66699700
H	-10.77653700	-4.02753700	-14.08304600	H	-4.07608900	-10.35824900	-11.54004600
H	-7.91325700	-5.83905900	-14.87675800	F	-9.38378900	-2.92392100	-10.46160300
H	-12.63299100	-3.34554400	-19.05976700				

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C	-2.73099300	-0.10103300	-4.80017700	N	-7.90638700	-2.53090700	-7.13945400
C	-3.56615500	-0.21808200	-6.02457100	C	-6.95819100	2.60919300	-10.69330100
N	-3.56276300	0.68549100	-7.07869500	N	-7.24851600	1.56305100	-9.74076300
C	-4.45035300	-1.18699300	-6.40167600	C	-7.03438700	0.24625700	-10.04254700
C	-4.42280100	0.23942000	-8.02950900	O	-6.34199200	0.03454500	-11.10286300
N	-4.97203200	-0.90006800	-7.64805600	O	-7.48086200	-0.61952200	-9.23930100
C	-9.56332600	-3.95540700	-4.12770200	C	-5.99742500	1.45357700	-14.50229300
C	-9.06303000	-3.28065200	-5.35883500	C	-6.37820200	0.07844100	-14.96768500
N	-9.81837000	-2.36972500	-6.08472100	N	-6.33934400	-1.06680800	-14.16983000
C	-7.87508000	-3.36232800	-6.03562100	C	-6.80709200	-0.27805400	-16.22004100
C	-9.09074900	-1.94369100	-7.14265900	C	-6.72752900	-2.07661900	-14.94105700

N	-7.01640900	-1.64161900	-16.18457400	S	-10.25305100	-7.67949100	-6.34824900
C	-0.67058700	-2.26303000	-10.70606800	C	-9.18535900	-9.78917400	-11.70511400
C	-1.89979800	-1.93378600	-11.47888800	C	-8.83498000	-9.55054600	-10.24456100
N	-1.94313100	-1.10857600	-12.59451100	O	-9.44803000	-8.73183400	-9.53859500
C	-3.19678600	-2.31016600	-11.26907400	C	-10.61628100	-9.38541000	-12.05364500
C	-3.23130100	-1.01325300	-13.00590400	C	-10.75742700	-9.00130800	-13.52386800
N	-4.01646400	-1.72890600	-12.21670600	O	-9.82759900	-8.53533700	-14.18007900
C	-2.92952000	-4.25382000	-7.22607700	N	-11.99354400	-9.17087600	-14.05688100
C	-4.19939600	-4.15422100	-8.07367500	N	-7.78557400	-10.25388900	-9.77111800
O	-5.24826900	-3.69975300	-7.49428200	C	-7.14862000	-9.92147300	-8.50393000
O	-4.13455100	-4.45842500	-9.28932100	H	-14.00795000	-6.21171100	-7.73269200
Zn	-6.38632200	-2.20659600	-8.44882100	H	-13.58854800	-4.96258300	-8.89876700
Zn	-6.04932200	-1.61574000	-12.09847700	H	-14.87259600	-4.39592500	-6.18358500
H	-1.65786700	-0.10122200	-5.02984800	H	-12.64605100	-5.46879000	-5.84391900
H	-2.94699200	0.81351600	-4.23339700	H	-12.62188200	-3.76401700	-5.35968800
H	-4.72423300	-2.09260200	-5.88738900	H	-11.89421800	-4.27625400	-6.90249000
H	-3.01778500	1.53496100	-7.13177300	H	-14.07597100	-2.05691800	-6.53391700
H	-4.61544600	0.75466500	-8.95804000	H	-13.42386700	-2.50745400	-8.12347200
H	-8.76621600	-4.55992500	-3.68729800	H	-15.16907200	-2.53316300	-7.83399000
H	-10.40874200	-4.61930600	-4.34212400	H	-16.02744800	-4.26856000	-9.02317400
H	-6.99893900	-3.95522400	-5.82361300	H	-8.35947100	-6.25691900	-5.83854700
H	-10.77590800	-2.11217600	-5.88803800	H	-7.83958400	-7.77392000	-6.55723900
H	-9.42660200	-1.23419700	-7.88138200	H	-9.96008400	-8.29615500	-7.51440400
H	-6.54899500	1.73009100	-13.59849700	H	-8.90258500	-7.48679000	-3.67363000
H	-6.97934100	0.30898700	-17.10891800	H	-10.88184800	-8.50455000	-11.45542900
H	-7.39512300	-2.21316200	-16.92723900	H	-11.33279800	-10.17076600	-11.78680600
H	-6.80712100	-3.10919000	-14.63443600	H	-12.77564800	-9.50669000	-13.51536200
H	-0.92757600	-2.97073000	-9.91419700	H	-12.16035400	-8.85341000	-15.00195400
H	0.10277400	-2.72833500	-11.32993700	H	-8.49959300	-9.16515600	-12.29137900
H	-3.56701800	-2.98919500	-10.51512300	H	-7.88713300	-9.94693600	-7.69942100
H	-1.15167600	-0.66247400	-13.03767200	H	-6.69130200	-8.92598200	-8.54463000
H	-3.55068300	-0.43869600	-13.86171300	H	-7.25917800	-10.81120700	-10.43013800
H	-5.93003600	2.51786700	-11.04980600	H	-8.98641900	-10.83054700	-11.98431500
H	-2.20155100	-4.92047100	-7.69361000	H	-6.37584800	-10.66363400	-8.29437900
H	-2.49048900	-3.25231800	-7.13872600	H	-8.32015700	-8.98664400	-4.40210000
H	-9.88795600	-3.23202300	-3.36948600	H	-7.19249800	-7.64196600	-4.11749600
H	-4.92906400	1.52511000	-14.26119100	H	-16.42632400	-5.47806800	-7.79374100
H	-6.21303500	2.18877600	-15.28233500	H	-15.84849500	-5.98578500	-9.38638400
H	-7.07194800	3.57950000	-10.20097300	C	-12.65108500	-2.36154800	-18.57849700
H	-7.62463800	2.58617400	-11.56668000	C	-13.22832700	-2.90086900	-17.25935100
H	-2.92875600	-0.95134500	-4.14290100	C	-12.13670000	-3.35483000	-16.31722700
H	-3.15887200	-4.60053700	-6.21406600	C	-11.52597700	-2.45644200	-15.43503800
H	-0.22690900	-1.37518400	-10.23743600	C	-11.64463900	-4.66769100	-16.35755800
H	-7.90801900	1.73735600	-8.99670300	C	-10.44870900	-2.83861800	-14.63561700
C	-15.72461500	-5.23247800	-8.59996200	C	-10.57330400	-5.07295900	-15.56675700
C	-14.28162300	-5.20647100	-8.07988900	C	-9.96222400	-4.14966400	-14.70931700
C	-14.07671000	-4.20833200	-6.92061400	O	-8.89503700	-4.57475700	-13.97589700
C	-12.73553800	-4.44301900	-6.21671600	H	-13.90790200	-3.73491300	-17.47601000
C	-14.19645100	-2.74662700	-7.37930900	H	-13.83519200	-2.12030200	-16.78286900
C	-8.21561800	-7.89747800	-4.42193300	H	-11.89592500	-1.43470100	-15.37166500
C	-8.50976500	-7.33956300	-5.81214100	H	-12.10836300	-5.38737200	-17.02986800

H	-9.99055600	-2.13186300	-13.94712400	O	-7.49674400	-8.28142300	-15.80180200
H	-10.20340200	-6.09421600	-15.59052600	N	-3.75191500	-5.55822600	-15.29588100
H	-8.54352000	-3.84693100	-13.41658300	C	-2.97854200	-6.39148600	-16.25746800
H	-11.99405500	-1.50345800	-18.39455500	C	-2.06136800	-7.39288300	-15.54607700
H	-12.05923700	-3.13001100	-19.08878900	C	-2.21201000	-5.31586700	-17.05167600
H	-13.44703700	-2.03843500	-19.25991900	C	-1.90485800	-4.23587600	-16.00142000
N	-7.09513900	-5.04346800	-11.50703300	C	-3.16773000	-4.21451400	-15.12659400
C	-7.48424300	-6.20012100	-10.87851300	H	-2.96984200	-4.01775800	-14.06907200
O	-7.02158200	-7.30638600	-11.17532100	H	-3.89185500	-3.46216400	-15.46413900
N	-8.45537000	-6.06117400	-9.91602600	H	-1.03185800	-4.52257800	-15.40507000
C	-9.11250500	-4.86481000	-9.70301400	H	-1.69373300	-3.25840500	-16.44591300
C	-8.69550900	-3.74684900	-10.31416500	H	-1.31603800	-5.72163100	-17.52957500
C	-7.54469600	-3.74204200	-11.23354400	H	-2.85553800	-4.90328900	-17.83832200
O	-7.54351900	-2.90932800	-12.24188700	H	-3.67194700	-6.92838700	-16.91063600
H	-9.96641100	-4.88867100	-9.03705900	H	-1.37214200	-6.87967600	-14.86518200
H	-6.45467200	-5.14520100	-12.30995400	H	-2.63180400	-8.13422500	-14.98135200
H	-8.85444400	-6.94271400	-9.58254300	H	-1.46279600	-7.93118900	-16.29081300
O	-6.18706000	-3.01481500	-10.27777600	H	-4.93331600	-7.89073400	-15.49981100
H	-5.52096300	-3.73564300	-10.07956600	H	-8.20349000	-8.49177600	-15.16775500
C	-4.82811300	-9.59760100	-11.88554600	H	-6.79835400	-6.43069600	-16.32050300
C	-4.75514400	-9.06937400	-13.30963100	H	-7.54111500	-6.49654700	-14.71912000
O	-4.01731500	-9.58752200	-14.14591900	H	-6.08152600	-7.59928200	-12.78218200
N	-5.54462900	-7.98709000	-13.55693500	H	-3.83572500	-9.49829100	-11.43228200
C	-5.50702600	-7.26706600	-14.81594000	H	-5.55756500	-9.07623300	-11.26537000
C	-4.85371400	-5.89568600	-14.59752000	H	-5.04922800	-10.67042500	-11.92497900
O	-5.37007500	-5.07970700	-13.80272500	F	-9.34587300	-2.58014000	-10.15006200
C	-6.91545900	-7.05744100	-15.42205500				

SkDHPase.5FU-INT1-II

C	-2.73099300	-0.10103300	-4.80017700	C	-6.83720400	-2.03674600	-15.01190200
C	-3.54694800	-0.21593900	-6.03564200	N	-7.19620500	-1.56165300	-16.22034500
N	-3.51138100	0.66844200	-7.10510100	C	-0.67058700	-2.26303000	-10.70606800
C	-4.44395500	-1.17362600	-6.40701400	C	-1.88879600	-1.92519600	-11.49545800
C	-4.36722800	0.22256700	-8.05975500	N	-1.89788700	-1.11899900	-12.62544500
N	-4.94292400	-0.89940000	-7.66494800	C	-3.19729300	-2.27366200	-11.30233100
C	-9.56332600	-3.95540800	-4.12769800	C	-3.17561500	-1.00692100	-13.06210000
C	-9.06259500	-3.26067000	-5.34624300	N	-3.98897500	-1.69304100	-12.27498000
N	-9.84844600	-2.41959600	-6.12142100	C	-2.92952000	-4.25382000	-7.22607800
C	-7.84772000	-3.27817200	-5.97617700	C	-4.19968700	-4.14175400	-8.06601600
C	-9.11339400	-1.97343700	-7.16492500	O	-5.24356000	-3.68151300	-7.48568600
N	-7.89385700	-2.48024800	-7.10294400	O	-4.14360700	-4.44416600	-9.28523600
C	-6.95819100	2.60919600	-10.69330100	Zn	-6.38790100	-2.19058800	-8.41269500
N	-7.23304800	1.52931800	-9.77487600	Zn	-6.01755500	-1.54257400	-12.26449600
C	-6.96776500	0.22678400	-10.09105700	H	-1.65425200	-0.12780300	-5.01062600
O	-6.24195100	0.04343200	-11.13403800	H	-2.93577000	0.82530700	-4.24859100
O	-7.40844500	-0.66015500	-9.30590300	H	-4.74015800	-2.06281700	-5.87717300
C	-5.99742500	1.45357800	-14.50229300	H	-2.94916000	1.50619300	-7.16560400
C	-6.44607400	0.11620500	-15.00865300	H	-4.53638600	0.72268700	-9.00116000
N	-6.37707800	-1.04956300	-14.24953500	H	-8.74102300	-4.48269300	-3.63736600
C	-6.96470600	-0.19981300	-16.23705400	H	-10.33850900	-4.69173300	-4.37018400

H	-6.94785000	-3.81611500	-5.72222700	H	-8.02531300	-6.10771700	-5.63763800
H	-10.83074600	-2.23220000	-5.97185700	H	-7.64959000	-7.58291400	-6.50520900
H	-9.47393800	-1.31913800	-7.94207200	H	-9.87400200	-8.13171900	-7.34447700
H	-6.40735300	1.64935000	-13.50716300	H	-8.88606900	-7.46199600	-3.67379100
H	-7.18450000	0.41106600	-17.09884000	H	-9.79091100	-7.59646800	-12.15616000
H	-7.64667500	-2.10415500	-16.94479000	H	-11.07138000	-8.51788800	-11.36174900
H	-6.91615800	-3.07360400	-14.71612200	H	-12.61076500	-9.61118300	-12.68686100
H	-0.94409500	-2.95569200	-9.90649200	H	-12.48867300	-9.65034600	-14.41943900
H	0.09889000	-2.74938600	-11.31826000	H	-8.37386700	-9.58628600	-12.33949500
H	-3.59401900	-2.93614700	-10.54755800	H	-7.91685900	-10.01966700	-7.73419100
H	-1.08971500	-0.69846200	-13.06350900	H	-6.69277600	-8.92634800	-8.43144200
H	-3.46767400	-0.44037000	-13.93314700	H	-7.15492300	-10.54239800	-10.53436500
H	-5.92308000	2.55489100	-11.03769800	H	-9.67652400	-10.64241100	-11.78467100
H	-2.20392500	-4.91573300	-7.70347400	H	-6.38132900	-10.68037200	-8.33726700
H	-2.48990700	-3.25387900	-7.12599100	H	-8.48621900	-8.95257300	-4.53268200
H	-9.98548500	-3.25163600	-3.39977900	H	-7.18987700	-7.84698000	-4.03381300
H	-4.90419500	1.51585300	-14.42201700	H	-16.42841700	-5.43958500	-7.78505600
H	-6.32368900	2.24823900	-15.17892900	H	-15.86036200	-6.01041600	-9.36003200
H	-7.10306000	3.56161500	-10.17529900	C	-12.65108500	-2.36154800	-18.57849700
H	-7.61323600	2.59477500	-11.57540800	C	-13.15236700	-2.54348000	-17.13487000
H	-2.95901700	-0.93798700	-4.13565500	C	-12.07584000	-3.04141100	-16.19352900
H	-3.15858800	-4.61330700	-6.21861500	C	-11.35041100	-2.16321700	-15.38106300
H	-0.21709300	-1.37512400	-10.24734600	C	-11.74524600	-4.40456800	-16.13142100
H	-7.90485200	1.66706300	-9.03411700	C	-10.32503600	-2.61429500	-14.54586600
C	-15.72460800	-5.23248100	-8.59995500	C	-10.72763600	-4.87621800	-15.30834100
C	-14.28163100	-5.20646800	-8.07989900	C	-10.00379500	-3.97760100	-14.51162400
C	-14.06995500	-4.13491100	-6.98703200	O	-9.00512100	-4.48421600	-13.73665600
C	-12.80099600	-4.40572300	-6.17131700	H	-13.99554700	-3.24666200	-17.13723100
C	-14.04730400	-2.71235300	-7.56790800	H	-13.54945400	-1.58839000	-16.76812700
C	-8.21561800	-7.89747700	-4.42193300	H	-11.59389400	-1.10216400	-15.39130300
C	-8.31633300	-7.15480400	-5.75244400	H	-12.30074000	-5.11504400	-16.74081200
S	-10.02592600	-7.12142700	-6.46157000	H	-9.78909800	-1.91882000	-13.90397000
C	-9.24974700	-9.63461600	-11.68370200	H	-10.48953600	-5.93512900	-15.25809600
C	-8.83083000	-9.44440300	-10.22449400	H	-8.54557600	-3.77797100	-13.22246600
O	-9.48203900	-8.73673500	-9.44055500	H	-11.83326700	-1.63224500	-18.61970300
C	-10.27785900	-8.57390000	-12.11292400	H	-12.27405700	-3.30662000	-18.98581200
C	-10.84742200	-8.85394000	-13.49577200	H	-13.45448700	-2.00695200	-19.23464400
O	-10.24762800	-8.59088000	-14.53996000	N	-6.97732500	-5.03938100	-11.44065400
N	-12.07239100	-9.44050800	-13.52225700	C	-7.46776600	-6.18903800	-10.89253200
N	-7.74236200	-10.13577500	-9.81923400	O	-7.10279100	-7.31834000	-11.25662100
C	-7.14862100	-9.92147200	-8.50393100	N	-8.41948600	-6.03627400	-9.91283200
H	-14.03364400	-6.19297100	-7.66602000	C	-9.07261900	-4.82644700	-9.71873300
H	-13.57925800	-5.03185900	-8.90780200	C	-8.59656800	-3.71148100	-10.27613700
H	-14.92399200	-4.20137300	-6.29591000	C	-7.32859800	-3.68102800	-11.08379500
H	-12.82883600	-5.39211100	-5.69559200	O	-7.39125200	-2.88263700	-12.16571300
H	-12.68323700	-3.65851500	-5.37269500	H	-9.97145200	-4.85330400	-9.11582100
H	-11.90702000	-4.38170900	-6.80729800	H	-6.41388900	-5.12889600	-12.29464100
H	-13.96229700	-1.96072400	-6.77230500	H	-8.84628900	-6.90044600	-9.57773500
H	-13.19475800	-2.58342800	-8.24935700	O	-6.20304700	-3.15025300	-10.22393600
H	-14.95627800	-2.48254200	-8.13325400	H	-5.51995500	-3.86932200	-10.00104900
H	-16.01434700	-4.27920900	-9.05588300	C	-4.82810800	-9.59760800	-11.88554600

C	-4.69241900	-9.02856300	-13.28563400	H	-1.76582200	-3.33155500	-16.74832400
O	-4.01049000	-9.58299700	-14.14593600	H	-1.36614600	-5.86049100	-17.65575000
N	-5.36258200	-7.86180300	-13.46913500	H	-2.92127500	-5.08827400	-18.00403200
C	-5.51563400	-7.25038500	-14.77389100	H	-3.69314300	-7.05634800	-16.92237100
C	-4.90575900	-5.84414900	-14.71395600	H	-1.38684400	-6.82429100	-14.89501700
O	-5.43732800	-4.96901300	-13.99829500	H	-2.61614500	-8.11637000	-14.94396700
C	-7.00177900	-7.18322400	-15.17394900	H	-1.44874000	-7.95688900	-16.25957600
O	-7.50434000	-8.49853600	-15.17446700	H	-4.99301900	-7.89822500	-15.47757800
N	-3.78974400	-5.56523000	-15.42017200	H	-8.46158300	-8.46807900	-14.97725600
C	-3.00524500	-6.45926100	-16.31763600	H	-7.06932900	-6.71591000	-16.17401000
C	-2.06137100	-7.39288100	-15.54607600	H	-7.54028200	-6.52838300	-14.47716200
C	-2.26297800	-5.43416500	-17.19768500	H	-5.98868400	-7.55449100	-12.72360000
C	-1.96116200	-4.27667600	-16.23231800	H	-3.82756600	-9.74013300	-11.46392800
C	-3.21835700	-4.20772100	-15.35153100	H	-5.41958800	-8.96691000	-11.22038700
H	-3.01530100	-3.93413800	-14.31174700	H	-5.27669700	-10.59595400	-11.96553100
H	-3.95258600	-3.48799200	-15.73550900	F	-9.26568600	-2.54245900	-10.16374100
H	-1.07995900	-4.50920800	-15.62459400				

SkDHPase.5FU-TS2-II

C	-2.73099300	-0.10103300	-4.80017700	O	-5.25809800	-3.71963300	-7.43512800
C	-3.54068100	-0.25173500	-6.04165400	O	-4.16026200	-4.41044400	-9.26494900
N	-3.43495400	0.56275600	-7.16180900	Zn	-6.46740000	-2.13753000	-8.44778000
C	-4.48862000	-1.17610800	-6.37714400	Zn	-6.05253900	-1.52176700	-12.14105200
C	-4.29771400	0.11254800	-8.10737500	H	-1.65642400	-0.21025400	-4.99317600
N	-4.94699700	-0.94962400	-7.66170900	H	-2.88389300	0.87377700	-4.32062500
C	-9.56332600	-3.95540800	-4.12769800	H	-4.85257700	-2.00659100	-5.79620500
C	-9.06943100	-3.25269400	-5.33886200	H	-2.82616000	1.36393500	-7.25814800
N	-9.85175600	-2.39061200	-6.09215300	H	-4.42201400	0.56152300	-9.08173500
C	-7.86150000	-3.27862500	-5.97895300	H	-8.74340100	-4.50184100	-3.65447600
C	-9.12121500	-1.93854300	-7.13482700	H	-10.35198600	-4.67771600	-4.36950000
N	-7.90793900	-2.46381200	-7.09196700	H	-6.96868300	-3.83308100	-5.73753400
C	-6.95819100	2.60919600	-10.69330100	H	-10.82996100	-2.19267700	-5.93012000
N	-7.30464100	1.58815400	-9.74017700	H	-9.47670300	-1.26280800	-7.89501300
C	-7.02367100	0.27688900	-9.97523000	H	-6.57824100	1.78091100	-13.63380400
O	-6.22874800	0.03634800	-10.95392500	H	-7.09914100	0.31447400	-17.08549500
O	-7.51900600	-0.56837800	-9.17544000	H	-7.59267300	-2.18997700	-16.84543400
C	-5.99742500	1.45357800	-14.50229300	H	-6.93721000	-3.07513900	-14.56216000
C	-6.42974500	0.09554600	-14.96329600	H	-0.95893500	-2.72286900	-9.75777800
N	-6.39551500	-1.03909600	-14.15488800	H	-0.03124800	-2.97826300	-11.23779000
C	-6.91216300	-0.26433200	-16.19428800	H	-3.63742400	-2.48702100	-10.26323100
C	-6.84252300	-2.05090000	-14.89317700	H	-1.09131400	-1.17985700	-13.32372900
N	-7.15887400	-1.62200600	-16.13048800	H	-3.48970100	-0.86090600	-14.12509500
C	-0.67058700	-2.26303000	-10.70606800	H	-5.91072700	2.51044900	-10.98472700
C	-1.89845300	-1.92831900	-11.48241400	H	-2.22548100	-4.92824200	-7.71786900
N	-1.90530300	-1.39805100	-12.76533700	H	-2.48247700	-3.25391600	-7.16766700
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C	-3.19377100	-1.24327400	-13.16004600	H	-4.94096100	1.46546500	-14.20640500
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C	-15.72460900	-5.23248100	-8.59995500	C	-10.70411300	-4.82988700	-15.29170300
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H	-10.52607200	-5.84964600	-15.17224500	H	-5.38096700	-8.95947600	-11.19465400
H	-8.59971700	-3.73866100	-13.06364700	H	-5.31984200	-10.57443400	-11.97753800
H	-11.79013600	-1.69409200	-18.70340800	F	-9.25586300	-2.54097000	-10.04397500
H	-12.35661900	-3.35374000	-18.93920000				
H	-13.46035300	-1.99540500	-19.22069600				
N	-6.90516800	-4.98956600	-11.31742400				

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C	-2.73099300	-0.10103300	-4.80017800	H	-9.87584800	-3.21317100	-3.38242400
C	-3.64855500	-0.24007000	-5.96317200	H	-4.90691100	1.53769800	-14.40472300
N	-3.87146900	0.76384700	-6.89358200	H	-6.32066200	2.21133400	-15.22143900
C	-4.42033900	-1.28442300	-6.39135800	H	-6.97931400	3.59999700	-10.22847800
C	-4.74535900	0.30782900	-7.82330900	H	-7.70805100	2.58819600	-11.49558700
N	-5.09044200	-0.93975500	-7.54994700	H	-2.73177000	-1.02500200	-4.21646700
C	-9.56332500	-3.95541300	-4.12770100	H	-0.19236100	-1.41000200	-10.20818700
C	-9.08760900	-3.31287200	-5.38136700	H	-7.77217500	1.84136100	-8.88850400
N	-9.85895200	-2.42789500	-6.12132900	C	-15.72463000	-5.23248300	-8.59996200
C	-7.90405200	-3.39735600	-6.06324100	C	-14.28161000	-5.20646400	-8.07989100
C	-9.14270600	-2.01560700	-7.19170500	C	-14.13542100	-4.60303500	-6.66912700
N	-7.95111700	-2.58847500	-7.18123700	C	-12.70526300	-4.78628300	-6.14700900
C	-6.95819100	2.60919700	-10.69330100	C	-14.54207000	-3.12212500	-6.61589400
N	-7.18974200	1.61132900	-9.68160300	C	-8.21562100	-7.89747300	-4.42192900
C	-7.18537900	0.27984500	-10.03323200	C	-8.72690800	-7.43782500	-5.78276300
O	-6.74746100	0.03651500	-11.20723200	S	-10.28585500	-8.32514100	-6.24868000
O	-7.56540900	-0.53461500	-9.14519600	C	-9.82537500	-10.43412600	-11.19565600
C	-5.99742500	1.45357700	-14.50229300	C	-9.07117500	-9.78035200	-10.04279900
C	-6.42181300	0.08759000	-14.95848100	O	-9.47159600	-8.71659300	-9.53498100
N	-6.38809300	-1.05276200	-14.15560600	C	-10.66549000	-9.41241600	-11.96369100
C	-6.88780100	-0.26858300	-16.19780900	C	-9.77474400	-8.35842000	-12.61972300
C	-6.81615600	-2.05903200	-14.90786000	O	-8.64553200	-8.65670100	-13.02537700
N	-7.12359600	-1.62795000	-16.14802700	N	-10.29305900	-7.11898600	-12.73208900
C	-0.67058600	-2.26303000	-10.70606800	N	-7.98660100	-10.43199000	-9.58646500
C	-1.93032500	-1.86890100	-11.40440100	C	-7.14861700	-9.92147600	-8.50393200
N	-1.96571700	-0.98492100	-12.47440700	H	-13.88763200	-6.23157700	-8.06246800
C	-3.24057900	-2.21423100	-11.19524800	H	-13.64527900	-4.64305100	-8.77982600
C	-3.25478800	-0.83058100	-12.86297600	H	-14.80847400	-5.16110700	-6.00058400
N	-4.05277500	-1.55938200	-12.10263000	H	-12.40413300	-5.83999500	-6.13296400
Zn	-6.46648400	-2.17644400	-8.48188700	H	-12.61052200	-4.39518000	-5.12537100
Zn	-6.12105500	-1.59850700	-12.10469300	H	-11.98868100	-4.25020800	-6.78566000
H	-1.69726400	0.09352700	-5.11260300	H	-14.42198500	-2.71741000	-5.60321500
H	-3.03354800	0.71374100	-4.13053100	H	-13.91994800	-2.52180300	-7.29524000
H	-4.54228200	-2.26235200	-5.95744100	H	-15.58647200	-2.96776000	-6.90442300
H	-3.46491500	1.68909600	-6.87626900	H	-16.13230900	-4.22463400	-8.73194200
H	-5.12690700	0.91066100	-8.63379900	H	-8.91875900	-6.36095400	-5.78521300
H	-8.75693700	-4.54631400	-3.68552600	H	-7.98330200	-7.63585900	-6.55919000
H	-10.41064800	-4.62720800	-4.30521800	H	-9.96291400	-8.48005900	-7.55219000
H	-7.02455800	-3.98149900	-5.84224100	H	-8.96464300	-7.73786700	-3.63791400
H	-10.81410600	-2.16762300	-5.91681300	H	-11.39416700	-8.94433000	-11.29585800
H	-9.48772500	-1.32106700	-7.94037400	H	-11.22195100	-9.92741100	-12.75678900
H	-6.43313200	1.68602100	-13.52617500	H	-11.20725600	-6.90072400	-12.36521000
H	-7.06792400	0.31495000	-17.08746700	H	-9.73836300	-6.35533000	-13.12139900
H	-7.53873100	-2.19466000	-16.87472100	H	-9.11882100	-10.91631000	-11.87778700
H	-6.91623100	-3.08127100	-14.57537200	H	-7.73913900	-9.80391500	-7.59126700
H	-0.89676900	-3.01465600	-9.94565200	H	-6.70513400	-8.96314500	-8.78894800
H	0.06235000	-2.70003500	-11.39522600	H	-7.68056300	-11.25548800	-10.08532800
H	-3.64908200	-2.91292300	-10.48162800	H	-10.47669000	-11.21527800	-10.78268900
H	-1.16533100	-0.54076700	-12.90326900	H	-6.35163200	-10.64347300	-8.31719700
H	-3.56367100	-0.20757300	-13.68812700	H	-7.96990300	-8.96383000	-4.43197900
H	-5.97559200	2.46437600	-11.14830500	H	-7.31316600	-7.33843700	-4.14313700

H	-16.38275900	-5.77071900	-7.90704000	H	-1.41819200	-3.23510000	-16.21375000
H	-15.78418400	-5.73759100	-9.57073900	H	-1.21333400	-5.65279100	-17.44305400
C	-12.65108500	-2.36154800	-18.57849600	H	-2.69980600	-4.71954900	-17.67367300
C	-13.01556300	-2.47957000	-17.08866100	H	-3.63898100	-6.73140000	-16.84950300
C	-11.90218600	-3.02026500	-16.21098000	H	-1.30543000	-6.96840700	-14.85674400
C	-11.34934800	-2.25776400	-15.17530000	H	-2.65462400	-8.12044500	-15.00734500
C	-11.40437700	-4.32098200	-16.39380900	H	-1.50202000	-7.93167800	-16.33185000
C	-10.35662900	-2.76682100	-14.33195000	H	-4.88736800	-7.74353600	-15.43632900
C	-10.40789900	-4.84461100	-15.57560000	H	-7.89362000	-8.23781800	-14.69000900
C	-9.88921700	-4.07037600	-14.52760500	H	-6.65725100	-6.18402200	-16.17431500
O	-8.95616600	-4.65799400	-13.71671900	H	-7.28297700	-6.07235700	-14.52386100
H	-13.89859100	-3.12717300	-16.99431200	H	-5.99684200	-7.57311000	-12.69748500
H	-13.32220900	-1.49539400	-16.71335100	H	-4.31469000	-8.92112400	-11.18230400
H	-11.71409200	-1.24666900	-15.00550400	H	-5.85286900	-9.68623200	-11.56413400
H	-11.80943000	-4.94310000	-17.18909900	H	-4.31945900	-10.57069400	-11.86432600
H	-9.96313300	-2.17129800	-13.51192900	C	-2.97579800	-4.24489600	-7.22765000
H	-10.02165500	-5.84913500	-15.72934200	C	-4.23618800	-4.31081100	-8.08612200
H	-8.45243500	-4.01220200	-13.13484500	O	-5.30835900	-3.83295700	-7.63529600
H	-11.80390000	-1.68116800	-18.72423200	O	-4.07510000	-4.83059000	-9.24410400
H	-12.37325100	-3.33326100	-19.00177200	N	-6.43892500	-5.00221200	-10.95940600
H	-13.49838600	-1.97645400	-19.15671600	C	-7.04609100	-6.24995300	-10.56190900
C	-4.81204300	-9.59659800	-11.88594600	O	-6.46325500	-7.30533200	-10.77728400
C	-4.71910400	-9.04084400	-13.29348900	N	-8.22281200	-6.15833600	-9.90392200
O	-3.99891700	-9.54135000	-14.15530500	C	-8.95731800	-4.96939500	-9.80923100
N	-5.48115300	-7.92798200	-13.49637100	C	-8.46015700	-3.82327900	-10.26836300
C	-5.39749300	-7.12620600	-14.69886700	C	-7.12050500	-3.65870200	-10.95416500
C	-4.64293800	-5.82479500	-14.39197400	O	-7.29440000	-3.21314100	-12.23587700
O	-5.05079200	-5.07426200	-13.48181500	H	-2.23594500	-4.97422800	-7.56345500
C	-6.79760400	-6.74541800	-15.24034800	H	-2.54524900	-3.24033700	-7.30933200
O	-7.59740100	-7.85943700	-15.54332500	H	-9.93976400	-5.05041900	-9.36144600
N	-3.58649800	-5.46890400	-15.14869600	H	-3.22146700	-4.41990900	-6.17677500
C	-2.89657200	-6.28695500	-16.18003000	H	-5.96478700	-5.12677100	-11.87955200
C	-2.04530500	-7.39187100	-15.54647600	H	-8.66848400	-7.05420500	-9.68014900
C	-2.07275200	-5.21853200	-16.92470600	O	-6.25755500	-2.79151900	-10.30585600
C	-1.67616700	-4.22342100	-15.82094000	H	-5.29267800	-4.87372000	-10.07289700
C	-2.91176800	-4.18097200	-14.90731800	F	-9.20415200	-2.69682100	-10.21435600
H	-2.67235400	-4.07165600	-13.84557700				
H	-3.59442100	-3.36221200	-15.16907900				
H	-0.80608900	-4.59531500	-15.26901500				

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C	-2.73099300	-0.10103300	-4.80017700	C	-9.15351400	-1.92413700	-7.12482800
C	-3.57547400	-0.27726800	-6.01667400	N	-7.95393600	-2.48281000	-7.11606600
N	-3.52835300	0.55981200	-7.12354900	C	-6.95819100	2.60919600	-10.69330100
C	-4.50849900	-1.22368400	-6.34159800	N	-7.29050000	1.66096400	-9.66809400
C	-4.40768000	0.10560100	-8.04964400	C	-7.17188100	0.32856000	-9.93615400
N	-5.01409400	-0.98203500	-7.60530500	O	-6.54064800	0.04246100	-11.00836100
C	-9.56332200	-3.95541400	-4.12769600	O	-7.65149900	-0.46849300	-9.07508200
C	-9.09740200	-3.26933700	-5.35425700	C	-5.99742500	1.45357700	-14.50229300
N	-9.87421400	-2.37509300	-6.07485400	C	-6.48289800	0.08900000	-14.89503700
C	-7.90737800	-3.32191400	-6.02261100	N	-6.46137000	-1.03048900	-14.06106500

C	-7.00646100	-0.28128000	-16.10693700	C	-9.83971600	-8.21503400	-12.49590000
C	-6.95328700	-2.03752800	-14.77312300	O	-8.74749800	-8.56971800	-12.95343000
N	-7.29081500	-1.62823700	-16.01187700	N	-10.30487800	-6.95280200	-12.58223800
C	-0.67058700	-2.26303000	-10.70606800	N	-8.03553000	-10.38288700	-9.56619500
C	-1.92707700	-1.87526400	-11.40876000	C	-7.14861700	-9.92147600	-8.50393200
N	-1.95999200	-1.05975000	-12.53178700	H	-13.89624900	-6.23446800	-8.04424600
C	-3.23971100	-2.17566700	-11.15901200	H	-13.64067500	-4.66145600	-8.78996600
C	-3.25284800	-0.90206700	-12.90966400	H	-14.81977100	-5.10644900	-6.00489700
N	-4.05124700	-1.56257000	-12.09169400	H	-12.43782500	-5.84877800	-6.09516600
Zn	-6.54986800	-2.05128800	-8.46476500	H	-12.60741600	-4.37051800	-5.13319900
Zn	-6.10841700	-1.60498800	-12.01512200	H	-11.97175800	-4.28991000	-6.79303400
H	-1.66026500	-0.16637800	-5.03002400	H	-14.38391500	-2.66654300	-5.65398900
H	-2.90820600	0.86552500	-4.31276700	H	-13.85262800	-2.51655400	-7.34233800
H	-4.84086500	-2.07094600	-5.76436300	H	-15.53507900	-2.91339800	-6.96765100
H	-2.94816400	1.38202700	-7.21996400	H	-16.12826700	-4.22453200	-8.74372500
H	-4.57917100	0.57614200	-9.00622300	H	-9.06103000	-6.47138600	-5.82375300
H	-8.74819900	-4.54675500	-3.70224100	H	-8.18909800	-7.79905800	-6.58964700
H	-10.39854200	-4.63674800	-4.32602600	H	-10.38717300	-8.52547700	-7.34227400
H	-7.02951500	-3.90954800	-5.80862800	H	-8.89001800	-7.67900000	-3.58594500
H	-10.83510100	-2.13392300	-5.87348100	H	-11.42736500	-8.71428400	-11.10249400
H	-9.49979100	-1.21572700	-7.85927300	H	-11.37990400	-9.69679000	-12.57354100
H	-6.46681400	1.78595800	-13.57120200	H	-11.18653500	-6.69589400	-12.16466000
H	-7.19626600	0.28623500	-17.00490900	H	-9.73926000	-6.20817600	-12.99205400
H	-7.75809800	-2.19927800	-16.70308200	H	-9.29313100	-10.80509800	-11.78164200
H	-7.08044500	-3.04653400	-14.41310700	H	-7.70765800	-9.81422200	-7.57062300
H	-0.90660700	-2.94450800	-9.88491600	H	-6.69041700	-8.96723800	-8.77999400
H	0.03066100	-2.78147800	-11.37147500	H	-7.74391900	-11.16489000	-10.13514800
H	-3.65809100	-2.81728500	-10.40079500	H	-10.63455900	-11.04700500	-10.65251600
H	-1.15728200	-0.66692400	-13.00419600	H	-6.36519200	-10.66847800	-8.36069200
H	-3.56391600	-0.32537400	-13.76711600	H	-7.96017900	-8.96049000	-4.37382500
H	-5.91933800	2.48465900	-11.00841300	H	-7.29711100	-7.31582900	-4.27396500
H	-9.89061100	-3.24398800	-3.35879000	H	-16.38500200	-5.75990600	-7.90095700
H	-4.91147400	1.47760500	-14.34392900	H	-15.78571600	-5.74852000	-9.56480400
H	-6.23222800	2.17746400	-15.28750500	C	-12.65108500	-2.36154800	-18.57849700
H	-7.07766400	3.62227800	-10.29657200	C	-13.00476000	-2.40821100	-17.08236000
H	-7.59371300	2.51234500	-11.58387700	C	-11.89830000	-2.92118800	-16.17771400
H	-2.96396700	-0.88437800	-4.07472000	C	-11.43899600	-2.16922600	-15.08942600
H	-0.14697000	-1.39503700	-10.28524300	C	-11.32634900	-4.18936600	-16.37447600
H	-7.93682700	1.91240300	-8.93473400	C	-10.47139800	-2.66049200	-14.20660600
C	-15.72461900	-5.23249300	-8.59995400	C	-10.35133400	-4.69308400	-15.51859100
C	-14.28162300	-5.20645100	-8.07990200	C	-9.93257600	-3.93396400	-14.41578100
C	-14.12914500	-4.57908500	-6.68029800	O	-9.02632700	-4.51538900	-13.57302100
C	-12.70718700	-4.78728700	-6.14423100	H	-13.89592900	-3.03942000	-16.95445000
C	-14.49909300	-3.08778200	-6.66059000	H	-13.29948800	-1.40473400	-16.75085600
C	-8.21562100	-7.89747300	-4.42192900	H	-11.86096500	-1.18248500	-14.90909800
C	-8.85572000	-7.54468500	-5.76245100	H	-11.65516600	-4.80355800	-17.20978800
S	-10.43585400	-8.48035600	-5.99218300	H	-10.15350500	-2.07538000	-13.34695800
C	-9.95337600	-10.29597400	-11.07317300	H	-9.90323600	-5.67077500	-15.67865200
C	-9.13678400	-9.70193500	-9.93100100	H	-8.52113000	-3.88676500	-12.97434900
O	-9.49544300	-8.66391100	-9.34611100	H	-11.79377100	-1.70316600	-18.76147100
C	-10.75883100	-9.22165500	-11.80390700	H	-12.39619600	-3.35439500	-18.96514900

H	-13.49741300	-1.98589800	-19.16409900	H	-7.11977000	-5.77348100	-14.12397800
C	-4.81204300	-9.59659800	-11.88594500	H	-5.83791100	-7.43616200	-12.49526600
C	-4.73412200	-8.96265400	-13.26060500	H	-4.24903900	-8.99789400	-11.16240700
O	-4.10551700	-9.46765000	-14.18971100	H	-5.84513700	-9.63618500	-11.53091400
N	-5.40116700	-7.77763200	-13.34949600	H	-4.38524800	-10.60011300	-11.93947100
C	-5.32375900	-6.91783200	-14.51092000	C	-2.97579800	-4.24489600	-7.22765000
C	-4.44739600	-5.69723100	-14.19328200	C	-4.30275100	-4.31065400	-7.95588100
O	-4.72922900	-4.96969600	-13.22209100	O	-5.34458100	-3.88733900	-7.45337400
C	-6.71974400	-6.39867700	-14.93019200	O	-4.22086500	-4.80461300	-9.17582300
O	-7.61013700	-7.42122800	-15.29695500	N	-6.39278400	-5.01504600	-10.81931800
N	-3.41852000	-5.38106800	-15.00862300	C	-6.94309300	-6.22698200	-10.41505700
C	-2.83923500	-6.20514900	-16.10039800	O	-6.37731100	-7.30218700	-10.63930800
C	-2.04530500	-7.39187100	-15.54647600	N	-8.09949000	-6.16137400	-9.68558300
C	-1.96978900	-5.17176100	-16.84267500	C	-8.86533000	-4.99838500	-9.62635800
C	-1.44501700	-4.26118300	-15.71975900	C	-8.40778000	-3.85043700	-10.12527000
C	-2.63289200	-4.16246200	-14.74957800	C	-7.08391300	-3.67499600	-10.82735600
H	-2.34180200	-4.11699900	-13.69603900	O	-7.27222800	-3.19854900	-12.10166100
H	-3.25800400	-3.28210800	-14.94868800	H	-2.26450900	-4.97108200	-7.62624700
H	-0.58477900	-4.72530100	-15.22524300	H	-2.56282700	-3.23721000	-7.35240900
H	-1.12437800	-3.28010700	-16.08413100	H	-9.84289600	-5.08770800	-9.16782500
H	-1.17281600	-5.64701600	-17.42130600	H	-3.13141400	-4.41391600	-6.16013700
H	-2.59040600	-4.59227800	-17.53709400	H	-5.78641400	-5.11190200	-11.64966100
H	-3.64052900	-6.56749300	-16.75122600	H	-8.54026800	-7.06109300	-9.47783900
H	-1.25650400	-7.05032100	-14.86559500	O	-6.20273100	-2.79526900	-10.18282600
H	-2.68617800	-8.10161100	-15.01828800	H	-5.10266700	-4.76941800	-9.67011000
H	-1.56597900	-7.93208700	-16.37230000	F	-9.19186500	-2.74222400	-10.09895100
H	-4.91647000	-7.52826800	-15.31522400				
H	-7.90940200	-7.86939300	-14.47695800				
H	-6.59137100	-5.75311900	-15.81047000				

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C	-2.73099300	-0.10103300	-4.80017700	N	-6.38263800	-1.05018100	-14.15450900
C	-3.67101200	-0.20813500	-5.94519200	C	-6.88193500	-0.27301900	-16.19879200
N	-3.94024000	0.82473700	-6.83016900	C	-6.80668200	-2.06006400	-14.90402300
C	-4.42693200	-1.25415100	-6.39242200	N	-7.11383500	-1.63296800	-16.14554600
C	-4.82566600	0.38213200	-7.75583800	C	-0.67058700	-2.26303000	-10.70606800
N	-5.13243400	-0.88333200	-7.52054600	C	-1.92506200	-1.84789300	-11.39932500
C	-9.56332200	-3.95541300	-4.12769700	N	-1.95021800	-0.95894700	-12.46533300
C	-9.09935900	-3.30960700	-5.38251700	C	-3.23865700	-2.17773000	-11.18886400
N	-9.87940100	-2.43135300	-6.12152800	C	-3.23733600	-0.78655000	-12.85153700
C	-7.91489000	-3.38195900	-6.06291500	N	-4.04304700	-1.50858400	-12.09262500
C	-9.16587400	-2.00999100	-7.19040300	Zn	-6.47141400	-2.14256400	-8.45228600
N	-7.96908600	-2.57144500	-7.17882600	Zn	-6.10350200	-1.56218500	-12.10643100
C	-6.95819100	2.60919700	-10.69330100	H	-1.70804200	0.12694900	-5.12567900
N	-7.21056000	1.61698200	-9.68203300	H	-3.03190200	0.67767500	-4.08802300
C	-7.22456500	0.28548600	-10.03864300	H	-4.51637100	-2.24979300	-5.99302100
O	-6.80071500	0.04520000	-11.21897800	H	-3.55465200	1.75808700	-6.78785900
O	-7.60750800	-0.52737400	-9.15217200	H	-5.24355300	1.00247800	-8.53561400
C	-5.99742400	1.45357700	-14.50229300	H	-8.75050200	-4.54219400	-3.69175900
C	-6.41851000	0.08761700	-14.95983700	H	-10.40787500	-4.63246100	-4.29899200

H	-7.02932900	-3.95679900	-5.84185500	H	-8.90284800	-7.68116100	-3.59595700
H	-10.83627400	-2.17844600	-5.91585100	H	-11.43830900	-8.72310300	-11.11726500
H	-9.51627000	-1.31764700	-7.93863100	H	-11.38026100	-9.71939700	-12.57755000
H	-6.42471900	1.67851400	-13.52071300	H	-11.23054800	-6.73146000	-12.28560300
H	-7.06280100	0.30749800	-17.09024600	H	-9.74659000	-6.24575500	-13.05283100
H	-7.52634200	-2.20273000	-16.87138600	H	-9.31385900	-10.83653000	-11.76493800
H	-6.90426300	-3.08171500	-14.56923900	H	-7.70025600	-9.81510900	-7.56605900
H	-0.90602900	-3.01451900	-9.94833900	H	-6.69729900	-8.96529200	-8.78225200
H	0.05448800	-2.70772800	-11.39866200	H	-7.77846800	-11.20708200	-10.09105500
H	-3.65558300	-2.87351200	-10.47683200	H	-10.64895500	-11.03939000	-10.6212080
H	-1.14475700	-0.52205300	-12.89214000	H	-6.35924100	-10.66306700	-8.36711900
H	-3.53885100	-0.15632600	-13.67389000	H	-7.95671000	-8.95951100	-4.37002300
H	-5.97240700	2.45304200	-11.13759300	H	-7.30158700	-7.31262300	-4.26094800
H	-9.87509900	-3.21604100	-3.37917000	H	-16.37985700	-5.78141800	-7.91284900
H	-4.90642000	1.54403100	-14.41657400	H	-15.78268600	-5.72641800	-9.57656900
H	-6.33259600	2.21321200	-15.21400400	C	-12.65108500	-2.36154800	-18.57849700
H	-6.97322400	3.60159200	-10.23130000	C	-13.00528800	-2.44094500	-17.08367700
H	-7.69960300	2.59457700	-11.50343000	C	-11.89170500	-2.97230500	-16.20031300
H	-2.70142100	-1.04946100	-4.25793100	C	-11.34116800	-2.19996900	-15.17072200
H	-0.17862300	-1.41951100	-10.20533600	C	-11.39370600	-4.27488200	-16.36961100
H	-7.80092400	1.85466900	-8.89688600	C	-10.35136900	-2.70156400	-14.31907400
C	-15.72462000	-5.23249100	-8.59995600	C	-10.39982900	-4.79090900	-15.54371100
C	-14.28162200	-5.20645200	-8.07990000	C	-9.88465900	-4.00695900	-14.50121000
C	-14.13626600	-4.61074800	-6.66562500	O	-8.95708100	-4.59256800	-13.68238000
C	-12.71603700	-4.82609200	-6.12815800	H	-13.89395400	-3.07737400	-16.96796100
C	-14.51244300	-3.12177800	-6.61383900	H	-13.29987900	-1.44540300	-16.72928400
C	-8.21562100	-7.89747300	-4.42192900	H	-11.70577900	-1.18709500	-15.01184200
C	-8.83703900	-7.54672500	-5.77150800	H	-11.79661900	-4.90453600	-17.15995500
S	-10.40781500	-8.49241600	-6.02331700	H	-9.96126600	-2.09797200	-13.50321900
C	-9.96290300	-10.30498700	-11.06276000	H	-10.01199200	-5.79655600	-15.68598400
C	-9.12879900	-9.69788400	-9.94027500	H	-8.44466300	-3.95492300	-13.10222900
O	-9.46107700	-8.63603500	-9.38059900	H	-11.79826300	-1.69351700	-18.74663300
C	-10.76398700	-9.23719800	-11.80834500	H	-12.38686300	-3.34547700	-18.98171000
C	-9.83926300	-8.23525800	-12.49904700	H	-13.49903400	-1.98110300	-19.15877000
O	-8.72315100	-8.58000900	-12.90410100	C	-4.81204300	-9.59659800	-11.88594500
N	-10.31755000	-6.98185600	-12.63459900	C	-4.73337900	-9.02832600	-13.28849700
N	-8.03996000	-10.38803200	-9.56078800	O	-4.04370900	-9.53314800	-14.17215700
C	-7.14861700	-9.92147600	-8.50393200	N	-5.47565000	-7.89672200	-13.46206400
H	-13.88781100	-6.23188600	-8.06787400	C	-5.39889900	-7.08305100	-14.65662000
H	-13.64503700	-4.63942400	-8.77661800	C	-4.60965000	-5.80159700	-14.35003300
H	-14.82782700	-5.15591500	-6.00550900	O	-4.98496600	-5.05534200	-13.42323500
H	-12.44339900	-5.88749000	-6.09989000	C	-6.80419400	-6.66485600	-15.15526400
H	-12.62150600	-4.43025400	-5.10843000	O	-7.64607800	-7.75558300	-15.43014700
H	-11.97912400	-4.31324000	-6.76279300	N	-3.56069800	-5.45568600	-15.12220700
H	-14.40263800	-2.72302100	-5.59768400	C	-2.89381300	-6.27660400	-16.16571800
H	-13.86561400	-2.53266700	-7.27992500	C	-2.04530500	-7.39187100	-15.54647600
H	-15.54787200	-2.94465300	-6.92122300	C	-2.06827100	-5.21390700	-16.91634100
H	-16.13673900	-4.22490500	-8.71995400	C	-1.64074700	-4.23278500	-15.81144900
H	-9.04779400	-6.47476900	-5.83590400	C	-2.85990300	-4.18235400	-14.87608000
H	-8.15645700	-7.79778500	-6.58839700	H	-2.60080800	-4.09063800	-13.81726700
H	-10.36067400	-8.49976500	-7.37394200	H	-3.53360400	-3.34940200	-15.11520200

H	-0.76584600	-4.61977000	-15.27797900	N	-6.32193400	-4.99455900	-10.86380000
H	-1.37720100	-3.24456900	-16.20076600	C	-6.94834500	-6.24404300	-10.49334400
H	-1.22307900	-5.65541800	-17.45166800	O	-6.36646100	-7.30147400	-10.70043700
H	-2.70086100	-4.70118200	-17.65122800	N	-8.14369400	-6.15181500	-9.86959900
H	-3.64932800	-6.71134200	-16.82680400	C	-8.89073700	-4.96968700	-9.80083800
H	-1.29467200	-6.97894700	-14.86214700	C	-8.41065900	-3.81372600	-10.25200700
H	-2.65728500	-8.11671000	-15.00497700	C	-7.07052400	-3.60729400	-10.91992400
H	-1.51546000	-7.93367900	-16.33956000	O	-7.23058900	-3.21641300	-12.21018200
H	-4.91917200	-7.70307000	-15.41226200	H	-2.25160600	-4.97939500	-7.58565100
H	-7.93131500	-8.12629500	-14.56966100	H	-2.53198300	-3.24508100	-7.29817400
H	-6.67912600	-6.10857300	-16.09442700	H	-9.88183300	-5.06236200	-9.37475500
H	-7.24741400	-5.97853400	-14.42471200	H	-3.21131200	-4.43389800	-6.17677400
H	-5.95109100	-7.53226700	-12.64302100	H	-5.85489400	-5.11696500	-11.78767200
H	-4.28810800	-8.93948700	-11.18444900	H	-8.61759100	-7.04527800	-9.69368400
H	-5.84856000	-9.66754200	-11.54599300	O	-6.23222800	-2.72859500	-10.28191100
H	-4.34044600	-10.58128800	-11.88294700	H	-5.29937900	-4.85047100	-10.03540000
C	-2.97579900	-4.24489700	-7.22765200	F	-9.18841800	-2.70780700	-10.21591600
C	-4.25141100	-4.27859000	-8.07370000				
O	-5.30527200	-3.77719600	-7.59573900				
O	-4.13686700	-4.78905400	-9.23719000				

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C	-2.73099400	-0.10103300	-4.80017800	N	-4.00096000	-1.73784100	-12.28155600
C	-3.57395500	-0.22175200	-6.01980100	Zn	-6.37509000	-2.24418400	-8.40963600
N	-3.60132900	0.70011100	-7.05755200	Zn	-6.00488900	-1.48079100	-12.25319000
C	-4.43881600	-1.20440200	-6.40768700	H	-1.66062300	-0.06905300	-5.03969200
C	-4.45936100	0.25286600	-8.00891800	H	-2.96700300	0.79898700	-4.21855100
N	-4.97912400	-0.90608400	-7.64418300	H	-4.68982700	-2.12469600	-5.90755500
C	-9.56332600	-3.95541700	-4.12769600	H	-3.07614500	1.56269400	-7.09940700
C	-9.08385100	-3.29842700	-5.37544800	H	-4.67113700	0.78143100	-8.92547000
N	-9.85622000	-2.41799100	-6.12181700	H	-8.75128600	-4.53600000	-3.68239500
C	-7.89013100	-3.36280400	-6.04162700	H	-10.39796700	-4.63954600	-4.31721900
C	-9.12980000	-1.98815700	-7.17915700	H	-7.00639400	-3.94039600	-5.81908100
N	-7.93094200	-2.54453700	-7.15474300	H	-10.82009100	-2.17754100	-5.93396300
C	-6.95819100	2.60919600	-10.69330100	H	-9.48075500	-1.30329100	-7.93423000
N	-7.26412800	1.55470800	-9.75552400	H	-6.41563700	1.64824500	-13.51029800
C	-7.03306300	0.24469500	-10.06687600	H	-7.16271800	0.39413300	-17.10187800
O	-6.31820500	0.06479000	-11.12403500	H	-7.59488300	-2.12778700	-16.94826000
O	-7.48224600	-0.63749300	-9.28466300	H	-6.88490400	-3.08736500	-14.71964200
C	-5.99742500	1.45357600	-14.50229300	H	-0.91574800	-2.95682200	-9.89820700
C	-6.43052400	0.11048000	-15.00857700	H	0.10423000	-2.73260000	-11.32430800
N	-6.35376200	-1.05471000	-14.24755700	H	-3.63144900	-2.98743200	-10.55594000
C	-6.94106200	-0.21322600	-16.23814000	H	-1.10269800	-0.73361100	-13.05152800
C	-6.80139500	-2.04815300	-15.00999900	H	-3.47435600	-0.48331300	-13.93833800
N	-7.16182300	-1.57689200	-16.21925500	H	-5.90959400	2.55726300	-10.99546700
C	-0.67058800	-2.26303000	-10.70606800	H	-9.89399500	-3.22141500	-3.38227400
C	-1.90579600	-1.96052200	-11.48748100	H	-4.90528700	1.52593100	-14.41634000
N	-1.91324800	-1.15618900	-12.61963800	H	-6.32746000	2.24322600	-15.18271800
C	-3.21558200	-2.31867600	-11.29981300	H	-7.13225000	3.57476400	-10.20960800
C	-3.18528700	-1.04848100	-13.06535500	H	-7.57747500	2.56265900	-11.59922200

H	-2.89982100	-0.96595700	-4.15407800	C	-11.65052400	-2.64309500	-15.18701600
H	-0.23893600	-1.35872200	-10.25899800	C	-11.17948400	-4.47268200	-16.66203000
H	-7.93213600	1.71936700	-9.01688600	C	-10.56622100	-2.99800100	-14.38030000
C	-15.72463100	-5.23250100	-8.59995100	C	-10.09095200	-4.83924400	-15.87722900
C	-14.28160600	-5.20644000	-8.07990400	C	-9.77638700	-4.09963400	-14.72820400
C	-14.12736300	-4.55993400	-6.68921400	O	-8.69106900	-4.49819200	-14.00478400
C	-12.70920800	-4.77369700	-6.14564500	H	-13.76339300	-3.82690700	-17.44603000
C	-14.48266300	-3.06488700	-6.69311200	H	-13.75829400	-2.22691600	-16.72234300
C	-8.21562100	-7.89747300	-4.42192900	H	-12.25682200	-1.78470200	-14.90501600
C	-8.87107200	-7.55188700	-5.75690500	H	-11.41367600	-5.06226800	-17.54627900
S	-10.47137400	-8.46107500	-5.94846600	H	-10.33821300	-2.43653000	-13.47723300
C	-10.07728500	-10.26204200	-10.93455400	H	-9.47616500	-5.69588500	-16.13717600
C	-9.16989900	-9.64671500	-9.87779600	H	-8.51163500	-3.87919400	-13.26494900
O	-9.48492300	-8.60066000	-9.28427200	H	-12.04619100	-1.46205600	-18.41431200
C	-10.56270600	-9.25344400	-11.98057700	H	-12.03774200	-3.07868700	-19.13580600
C	-9.63310000	-9.14283700	-13.18932300	H	-13.50272200	-2.08634300	-19.21096900
O	-8.55778100	-9.74565800	-13.25824000	C	-4.81204300	-9.59659900	-11.88594600
N	-10.09577000	-8.37190200	-14.20365500	C	-4.66680700	-9.10571000	-13.31206400
N	-8.06079900	-10.34241300	-9.55903100	O	-3.84317800	-9.57881100	-14.09274600
C	-7.14861700	-9.92147600	-8.50393200	N	-5.49523900	-8.06675900	-13.61804200
H	-13.90186700	-6.23581200	-8.02983100	C	-5.48307500	-7.39338900	-14.90052400
H	-13.63718500	-4.67596600	-8.79735900	C	-4.86616300	-5.98837400	-14.76389200
H	-14.82527100	-5.07000800	-6.00795500	O	-5.37538600	-5.16760900	-13.97683700
H	-12.45116400	-5.83687400	-6.07752200	C	-6.92919200	-7.23652400	-15.41397200
H	-12.60729000	-4.34060800	-5.14163500	O	-7.56283800	-8.48208700	-15.64445600
H	-11.96708600	-4.29649900	-6.80161600	N	-3.81996000	-5.63768400	-15.54202600
H	-14.36791500	-2.62964500	-5.69238100	C	-2.97439200	-6.51525400	-16.39307300
H	-13.82732500	-2.51043300	-7.38029600	C	-2.04530500	-7.39187100	-15.54647600
H	-15.51545500	-2.88477100	-7.00781300	C	-2.22887100	-5.48190800	-17.25919100
H	-16.12409000	-4.22458900	-8.75625400	C	-2.00485500	-4.29773900	-16.30379600
H	-9.05708900	-6.47579100	-5.82980300	C	-3.28690200	-4.26592100	-15.45602500
H	-8.22426500	-7.83075100	-6.59162700	H	-3.11873400	-3.98992400	-14.41086300
H	-10.46456900	-8.48427700	-7.29989000	H	-4.03027000	-3.56458400	-15.85756000
H	-8.87067400	-7.65138200	-3.57821200	H	-1.13193800	-4.48275900	-15.66867100
H	-10.66626100	-8.26633700	-11.51421600	H	-1.83409900	-3.35384700	-16.83056800
H	-11.55834900	-9.53727800	-12.34209900	H	-1.29984200	-5.88672900	-17.67007700
H	-10.90812000	-7.78277900	-14.09734100	H	-2.86218900	-5.17318900	-18.09988400
H	-9.48120900	-8.23263400	-15.00415900	H	-3.61286500	-7.14758100	-17.01667500
H	-9.59221900	-11.10678100	-11.43105600	H	-1.41789000	-6.77858000	-14.88856200
H	-7.67646800	-9.86926000	-7.54759900	H	-2.60359300	-8.10926200	-14.94166800
H	-6.71228500	-8.94216700	-8.72532200	H	-1.38143000	-7.96464100	-16.20571800
H	-7.79709400	-11.11750500	-10.15017700	H	-4.92189800	-8.02778700	-15.58631100
H	-10.94413700	-10.65043700	-10.38551800	H	-7.58291700	-8.99372200	-14.80324000
H	-6.34545900	-10.65658100	-8.42510800	H	-6.91560400	-6.71357000	-16.37801900
H	-7.98175800	-8.96489100	-4.36084500	H	-7.48627400	-6.61336900	-14.70224500
H	-7.28269000	-7.33346100	-4.29998000	H	-6.20207100	-7.80081400	-12.92595800
H	-16.38769200	-5.74827300	-7.89474300	H	-4.20891500	-8.96458500	-11.22247900
H	-15.78723700	-5.76019600	-9.55836300	H	-5.84990100	-9.55289900	-11.54615600
C	-12.65108500	-2.36154800	-18.57849700	H	-4.43099700	-10.61832700	-11.82538300
C	-13.12517400	-2.95676600	-17.24141600	C	-2.97579700	-4.24489600	-7.22764900
C	-11.97812100	-3.36421900	-16.34081300	C	-4.21728900	-4.19759600	-8.11863300

O	-5.27937500	-3.71542400	-7.56628100	H	-2.21813900	-4.90632000	-7.65385900
O	-4.12482100	-4.57234600	-9.30178800	H	-2.55930000	-3.23369600	-7.14274000
N	-6.17838500	-5.57148200	-11.16075400	H	-9.67815700	-5.20510500	-9.19454400
C	-7.13030400	-6.47886400	-10.87709600	H	-3.23205000	-4.57708600	-6.21676800
O	-7.36993300	-7.49558100	-11.53654800	H	-5.71783500	-5.65007300	-12.06747400
N	-7.93777500	-6.19057500	-9.74853500	H	-8.46641200	-7.02944700	-9.48777900
C	-8.73007100	-5.04972900	-9.70332100	O	-6.36612400	-2.87874300	-10.34001400
C	-8.57525700	-3.83100300	-10.24532400	H	-5.66728600	-5.08228700	-10.41779900
C	-7.45261500	-3.14880900	-10.94073200	F	-9.65379800	-2.98090100	-10.15411700
O	-7.63379700	-2.71408800	-12.12484300				

SkDHPase.PTA-ES-II

C	-6.20441700	-5.40411000	-3.67679100	H	-5.13893900	-6.71117700	-1.37430700
C	-5.36115600	-4.92840000	-2.54463500	H	-3.70411500	-5.35229000	0.23840800
N	-4.92263500	-5.73226000	-1.50153100	H	-7.36026700	1.78207000	-1.26385200
C	-4.82277300	-3.69999700	-2.28334500	H	-7.28871700	2.51289000	0.34422300
C	-4.15277300	-4.98162800	-0.67267500	H	-5.04179500	0.16675700	-1.68267900
N	-4.06544200	-3.74256500	-1.12677600	H	-6.54687500	0.39039500	2.23740000
C	-7.36226500	1.56112600	-0.19339500	H	-4.53780000	-1.20566800	2.23739500
C	-6.22847900	0.64390200	0.13519100	H	0.71540800	-5.80332900	2.99700600
N	-6.00390400	0.15792700	1.41726700	H	4.16658200	-4.70069800	4.20709200
C	-5.24119400	0.07200000	-0.62629800	H	4.58890200	-2.30863900	3.33653300
C	-4.93002600	-0.66762500	1.38869700	H	3.00494300	-1.69658100	1.49740400
N	-4.44456600	-0.73871300	0.16215900	H	-0.32590800	-4.52388000	-4.80954200
C	-2.29938200	-6.00697500	2.98134400	H	1.22262900	-5.29959100	-5.16407400
N	-2.95217300	-4.83661100	2.43149900	H	-0.42318100	-3.29416100	-2.44416700
C	-2.22237400	-3.79354000	1.89597200	H	2.25101000	-6.51534800	-2.65188000
O	-0.97079700	-4.02765100	1.75536800	H	2.43181100	-5.51884700	-0.31092800
O	-2.85075300	-2.74734700	1.57194100	H	-1.64494000	-6.45379500	2.23009300
C	1.79357700	-5.94527700	2.87734300	H	-2.15375300	-1.91584100	-5.51631800
C	2.48804400	-4.62480300	2.73266100	H	-3.11555200	-3.14189700	-4.66139700
N	2.11188300	-3.61269600	1.84364800	H	-8.33207400	1.10977900	0.05093400
C	3.59471400	-4.21486400	3.43137400	H	1.94092500	-6.58717100	1.99828700
C	3.00041800	-2.64070600	2.01419600	H	2.17979900	-6.48250400	3.74817900
N	3.91173100	-2.96103800	2.95488300	H	-3.06296000	-6.73943000	3.26049100
C	0.36387300	-5.30494200	-4.48102300	H	-1.69325900	-5.78164000	3.86929400
C	0.75936200	-5.02774400	-3.07203900	H	-6.40565700	-4.57239700	-4.35659200
N	1.70369100	-5.72830200	-2.33136300	H	-3.82919800	-1.55802800	-4.99519200
C	0.29479600	-4.06615500	-2.22380700	H	-0.13934400	-6.27429600	-4.59111800
C	1.77280200	-5.17472400	-1.09345900	H	-3.86027800	-4.57536200	2.78941200
N	0.92569900	-4.16234500	-0.99931800	C	-4.19649900	5.48111200	5.65510200
C	-2.89798600	-2.06858000	-4.73121300	C	-4.37163600	4.73770800	4.32470900
C	-2.36139900	-1.59068400	-3.37698500	C	-5.84823400	4.49637400	3.94619300
O	-3.23613800	-1.33183900	-2.47293500	C	-5.98772900	4.03950400	2.48768300
O	-1.12163900	-1.54417200	-3.21812700	C	-6.53723700	3.50022200	4.89185700
Zn	-2.99581200	-2.03558700	-0.49946300	C	-5.77120700	4.10817800	-3.09579700
Zn	0.24229300	-3.03535700	0.58713200	C	-4.58413100	4.03449700	-2.13683700
H	-5.70934400	-6.19430200	-4.25553100	S	-4.31327900	5.67378500	-1.31728500
H	-7.17137900	-5.79826400	-3.33911900	C	1.12729100	7.26375500	-1.79976900
H	-4.90067000	-2.78466300	-2.84511000	C	0.03327300	6.21837700	-2.00264100

O	-0.70565600	5.87418100	-1.07419400	H	5.84922700	1.15344300	7.42213400
C	1.96095500	7.01756500	-0.53755800	H	4.17216000	0.91189700	7.92716300
C	3.15045500	6.09287500	-0.77470200	H	5.47433100	0.03477900	8.74710300
O	3.24871700	5.38838600	-1.78778300	N	1.24260200	0.66015900	-0.24914500
N	4.09451500	6.08882500	0.19511700	C	0.81096700	1.98893200	-0.38873200
N	-0.12624400	5.75931800	-3.26459200	O	1.33513200	2.82163300	-1.10649400
C	-1.17433500	4.81200100	-3.61648100	C	-0.50961100	0.92061000	1.20813000
H	-3.89589600	5.32637900	3.52855900	C	0.56253700	0.00663900	0.75599800
H	-3.84003900	3.77540000	4.36359900	O	0.86896700	-1.10081300	1.19832700
H	-6.36899800	5.46142300	4.03901000	H	2.16411000	0.35251300	-0.56445300
H	-7.04518200	3.92366500	2.21751200	O	-1.06345300	-1.96888300	-0.48561500
H	-5.49241100	3.07128600	2.32719900	H	-0.83993300	-1.67118600	-1.39590400
H	-5.54401700	4.75731600	1.78782500	C	2.43907400	2.91782500	-4.26697800
H	-7.59068300	3.36219700	4.61965100	C	3.80092400	2.42110000	-3.83600200
H	-6.04711700	2.51671700	4.84599600	O	4.72551400	2.21800400	-4.61774200
H	-6.50982700	3.83207500	5.93463500	N	3.89863900	2.19670500	-2.48825900
H	-4.58679900	4.90725200	6.50249700	C	5.14000500	1.78907000	-1.85913200
H	-4.74746600	3.27191100	-1.36917500	C	4.97453500	0.37345000	-1.29486800
H	-3.67620000	3.76484600	-2.68114500	O	4.15376100	0.17955200	-0.35813800
H	-2.97417300	5.57855700	-1.15080200	C	5.51524100	2.78340500	-0.73661200
H	-6.68828800	4.40961300	-2.57668300	O	5.69744400	4.08917300	-1.24058800
H	1.31490300	6.57492200	0.23112700	N	5.67930700	-0.65440800	-1.78065500
H	2.32814200	7.96824700	-0.13301300	C	6.64435200	-0.67464800	-2.91670000
H	4.03830600	6.69830600	0.99685100	C	5.92844100	-0.78885300	-4.26832700
H	4.92398600	5.51439500	0.05633000	C	7.49990400	-1.90615000	-2.56533500
H	1.77654000	7.34031700	-2.67673600	C	6.48850500	-2.89323600	-1.95794200
H	-2.15963100	5.28706700	-3.57201500	C	5.52179700	-1.99380500	-1.17000500
H	-1.15613300	3.95979700	-2.93084900	H	4.47815200	-2.31726700	-1.22762200
H	0.54622100	6.02872600	-3.96709000	H	5.78013100	-1.92798100	-0.10735700
H	0.60362400	8.22158000	-1.69188800	H	5.95360900	-3.42732000	-2.75024200
H	-0.99702900	4.45497300	-4.63303700	H	6.96075400	-3.64327100	-1.31741200
H	-5.58802800	4.83241100	-3.89537800	H	8.01899500	-2.30513600	-3.44091800
H	-5.94943100	3.12727100	-3.55356300	H	8.25639500	-1.63338800	-1.81997400
H	-4.71961000	6.44461200	5.63557600	H	7.24720600	0.23646400	-2.89501700
H	-3.13869200	5.68320900	5.85808800	H	5.27406600	-1.66734500	-4.29850800
C	5.13099800	0.40489300	7.77415500	H	5.34054800	0.10677900	-4.48090100
C	4.99610000	-0.74265800	6.76173900	H	6.67358200	-0.89267800	-5.06551800
C	4.52326100	-0.24126100	5.41647200	H	5.90112800	1.83355000	-2.63793200
C	5.37871700	-0.16424500	4.31077700	H	4.85701100	4.37814800	-1.66949200
C	3.21548200	0.24741600	5.26579900	H	6.46473500	2.48235400	-0.27898100
C	4.95188700	0.38197000	3.09408900	H	4.74343100	2.75816100	0.04663000
C	2.77862600	0.80219300	4.07068800	H	3.09927000	2.44516000	-1.90620200
C	3.64734000	0.87627800	2.97368400	H	1.68238500	2.14088300	-4.10859200
O	3.17272100	1.43881000	1.82899700	H	2.14565800	3.79309000	-3.67909300
H	4.29287600	-1.48972600	7.15475200	H	2.47802400	3.16834500	-5.32853100
H	5.96220600	-1.25100200	6.65226900	C	-1.19332700	3.21144800	0.74257000
H	6.40796500	-0.50732100	4.40524700	C	-0.35733400	2.12895400	0.51916600
H	2.52735900	0.19449100	6.10661400	C	-1.51057300	0.74064300	2.14952500
H	5.63291700	0.44769400	2.24959600	C	-2.36102000	1.82946200	2.38615000
H	1.76517900	1.17504400	3.95877200	C	-2.20643500	3.03856300	1.69685400
H	3.69051500	1.12009200	1.05471800	H	-1.06163200	4.14658000	0.20523200

H -1.63615700 -0.20954200 2.65843300
H -3.15698000 1.73628600 3.11921700

H -2.88384300 3.85973400 1.90499500

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C -2.73099300 -0.10103300 -4.80017800
C -3.63548100 -0.17636100 -5.98023900
N -3.77399000 0.82566500 -6.93086700
C -4.46165600 -1.17624800 -6.40875200
C -4.65349400 0.40490700 -7.87481100
N -5.08305800 -0.81248600 -7.58972900
C -9.56333600 -3.95541400 -4.12770500
C -9.02872300 -3.24539100 -5.33344600
N -9.66624000 -2.14800700 -5.89383600
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C -8.95056000 -1.72088600 -6.95979400
N -7.88350000 -2.48517100 -7.12174000
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O -6.58077000 0.07058300 -11.25156300
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C -0.67059100 -2.26303000 -10.70606900
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Zn -6.01350300 -1.57638600 -12.09137300
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H -4.96352600 1.00457800 -8.71695100
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H -7.63431000 2.62114100 -11.55850200
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H -3.20843500 -4.61808700 -6.23292200
H -0.12808700 -1.37972500 -10.34499500
H -7.91319900 1.75191400 -8.99066100
C -15.72463300 -5.23248500 -8.59993500
C -14.28159700 -5.20646000 -8.07991900
C -14.20250500 -4.78461800 -6.59354700
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C -8.21562000 -7.89747300 -4.42193200
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C -9.38678200 -9.69131200 -11.58260700
C -9.01944800 -9.96729300 -10.12339500
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H -14.93321500 -5.40108600 -6.04826000
H -12.53410400 -6.11682800 -6.09454700
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H -12.04707400 -4.44595600 -6.44070700
H -14.55329600 -3.04291200 -5.32120400
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H -15.59783000 -3.09118600 -6.74344500
H -16.18695800 -4.23997800 -8.58185900
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H	-9.26166400	-9.79972400	-4.41489300	C	-4.81183900	-9.56725400	-11.86294900
H	-10.06457800	-9.58488900	-7.19656300	C	-4.64523200	-9.02643000	-13.26880700
H	-7.74029800	-7.21483900	-5.13422000	O	-4.02882400	-9.62116900	-14.14709800
H	-10.72875100	-8.03462300	-11.20356100	N	-5.24612800	-7.81141200	-13.45411700
H	-11.51172400	-9.61076000	-11.19952600	C	-5.53339500	-7.30086300	-14.78114200
H	-13.12466100	-9.20728300	-12.77398900	C	-4.93664300	-5.89299300	-14.89562200
H	-12.76709800	-8.68791300	-14.39311400	O	-5.44453800	-4.95190600	-14.24130200
H	-8.62039500	-9.10204400	-12.09375700	C	-7.05529300	-7.26121900	-15.04141500
H	-7.67041400	-10.76670200	-8.05097500	O	-7.57217400	-8.54640100	-14.78114700
H	-7.23072000	-9.05557900	-7.83424000	N	-3.87557300	-5.66317200	-15.68884000
H	-7.24747700	-9.00641000	-10.40511900	C	-3.04381100	-6.64322800	-16.44044800
H	-9.41774900	-10.66553400	-12.08784300	C	-2.04510400	-7.36252000	-15.52347800
H	-6.09071600	-10.17405100	-8.62246100	C	-2.37450400	-5.73439100	-17.48798400
H	-8.97641300	-7.33897000	-3.86433400	C	-2.11770000	-4.42485100	-16.72337200
H	-7.45798800	-8.23148400	-3.70353800	C	-3.34368200	-4.29043300	-15.80435500
H	-16.34563400	-5.90145500	-7.99233300	H	-3.10848200	-3.88993500	-14.81345100
H	-15.76748100	-5.59073600	-9.63497200	H	-4.11744900	-3.64457700	-16.23660500
C	-12.65108500	-2.36154900	-18.57849700	H	-1.20094000	-4.50560100	-16.12976900
C	-13.33098900	-2.76983800	-17.26181500	H	-2.00448600	-3.56167900	-17.38590600
C	-12.30797300	-3.27187700	-16.27137800	H	-1.46360100	-6.18067000	-17.89617900
C	-11.54529000	-2.36952700	-15.52161400	H	-3.06494200	-5.55689400	-18.32132200
C	-12.00590800	-4.63631200	-16.16323600	H	-3.69246100	-7.37875900	-16.92256300
C	-10.49130800	-2.80327800	-14.72094500	H	-1.43809500	-6.64716700	-14.95732600
C	-10.96048500	-5.09380700	-15.36513900	H	-2.55953500	-8.03025400	-14.82923300
C	-10.18618500	-4.16802800	-14.65945400	H	-1.37059700	-7.97817600	-16.12986100
O	-9.13180000	-4.63405500	-13.92728600	H	-5.07131400	-8.00033100	-15.47809400
H	-14.08004200	-3.54613500	-17.46116000	H	-8.51881300	-8.46342400	-14.55314100
H	-13.87285900	-1.90914400	-16.84880800	H	-7.21637700	-6.95570600	-16.09121300
H	-11.76980100	-1.30573800	-15.57446000	H	-7.52158300	-6.49429400	-14.41170600
H	-12.59394300	-5.35605100	-16.72960800	H	-5.84134600	-7.49730200	-12.69269600
H	-9.90600600	-2.09221600	-14.14138000	H	-4.00098400	-10.26860200	-11.65410500
H	-10.73078900	-6.15184200	-15.27643500	H	-4.81816700	-8.77193500	-11.11372300
H	-8.66793300	-3.87484900	-13.52576000	H	-5.75777100	-10.11662800	-11.79867700
H	-11.91929900	-1.56347900	-18.40796200	C	-9.13849400	-6.13513300	-9.19962300
H	-12.11920200	-3.21151600	-19.02075500	C	-8.52062700	-4.15723900	-10.47082700
H	-13.38147000	-1.99923500	-19.31197200	C	-9.57688100	-3.42271200	-9.96067500
N	-6.80496400	-4.97614100	-11.76381900	C	-10.42750000	-4.07110100	-9.05457000
C	-7.22130300	-6.02430400	-10.96627400	C	-10.20386300	-5.39698000	-8.66747500
O	-6.78356900	-7.16717600	-11.03561800	H	-8.97990700	-7.16794300	-8.90837400
C	-7.51338400	-3.81094100	-11.50772300	H	-9.72959100	-2.38913700	-10.25134600
O	-7.59906300	-2.88493500	-12.36449200	H	-11.27883600	-3.53543600	-8.64501800
H	-6.19807100	-5.06793400	-12.59465000	H	-10.86619500	-5.87204400	-7.95281900
O	-6.08479900	-2.82423700	-10.35278900	C	-8.31864300	-5.49480000	-10.11579800
H	-5.38448100	-3.50926600	-10.19063600				

SkDHPase.PTA-INT1-II

C	1.14314300	8.50765300	-1.80309900	N	0.39067900	5.28156000	-0.12409600
C	0.67622900	7.32953000	-1.02214800	C	6.60589600	3.09278000	-0.12182600
N	-0.45272000	7.30689200	-0.21300900	C	5.19333400	3.17101500	0.34280200
C	1.18206600	6.06402500	-0.94430100	N	4.84154200	3.27118900	1.68192300
C	-0.58538100	6.06076900	0.30819400	C	4.00129800	3.16940600	-0.33045600

C	3.49354300	3.32183000	1.77528900	H	-2.05876200	4.08991400	5.08421200
N	2.95610700	3.26091200	0.56898600	H	2.05069500	8.24341100	-2.35126600
C	-1.70664700	4.89290000	4.42231300	H	1.48616600	4.43510500	-4.32162900
N	-0.53913900	4.51273000	3.65853300	H	-4.36208600	5.67508600	-2.99675600
C	-0.60258800	3.61521200	2.63316700	H	0.38004700	4.68925800	4.03555700
O	-1.78322300	3.29843300	2.24502700	C	7.01830400	-3.26581500	4.23609400
O	0.49491400	3.22156400	2.13006700	C	6.58497100	-2.26263200	3.15947200
C	-4.90592500	2.38130100	3.94964100	C	7.57699100	-1.08699100	3.00928800
C	-4.72787900	0.98511600	3.44169100	C	7.33247300	-0.28611700	1.72331000
N	-3.87134400	0.67359800	2.39038700	C	7.56492400	-0.15516000	4.23149100
C	-5.32238400	-0.17210000	3.87067200	C	6.64098600	0.94679100	-3.70458900
C	-3.95549700	-0.63893800	2.19331700	C	6.74668900	-0.56016700	-3.94282800
N	-4.82755100	-1.18061600	3.06534000	S	6.39491400	-1.49111500	-2.38236500
C	-4.04797500	4.63881000	-3.17547100	C	2.23408300	-4.98959800	-2.40361700
C	-4.08245000	3.81505200	-1.93366200	C	3.22922100	-4.13818200	-3.19655300
N	-5.23193000	3.47239700	-1.23472000	O	4.43490200	-4.39773200	-3.22792400
C	-3.06362100	3.23228100	-1.23412800	C	2.74390500	-5.31733300	-0.99573700
C	-4.87811200	2.71135400	-0.17024200	C	1.74484300	-6.14799000	-0.19842600
N	-3.56415400	2.55130000	-0.14290600	O	0.53340600	-5.92259100	-0.19022200
C	0.47080300	4.25551600	-3.95654800	N	2.28000200	-7.14429900	0.55315300
C	0.47521100	3.27422500	-2.79180800	N	2.65404600	-3.12679500	-3.90118800
O	1.41120000	3.38697500	-1.92660000	C	3.39768700	-2.24843500	-4.78609400
O	-0.47504100	2.45340600	-2.70611500	H	6.50712100	-2.78613800	2.19694800
Zn	0.98492400	3.30248200	0.12347300	H	5.58081700	-1.87550900	3.38666100
Zn	-2.44257100	1.70044800	1.31640500	H	8.58409400	-1.52430100	2.93306300
H	0.39633500	8.83883800	-2.53554200	H	7.36934300	-0.92185200	0.83129100
H	1.38025900	9.36538800	-1.16130200	H	8.09493500	0.49478900	1.60447600
H	2.03594400	5.64630100	-1.45091500	H	6.34968900	0.20460300	1.74075100
H	-1.07331400	8.08528700	-0.03767100	H	8.29989200	0.65138000	4.11953000
H	-1.38454500	5.76133600	0.96971700	H	6.57552600	0.30766200	4.35815000
H	6.63172100	3.02608400	-1.21202600	H	7.80090900	-0.68567900	5.15935300
H	7.11622000	2.20912500	0.27668300	H	7.04818300	-2.81309600	5.23297000
H	3.80965800	3.10346600	-1.39004900	H	6.02602700	-0.87409900	-4.70196300
H	5.48647100	3.28075600	2.46028400	H	7.74734500	-0.82422800	-4.29649400
H	2.93854900	3.38373300	2.69759200	H	5.95948900	-2.64690100	-2.93694700
H	-3.94103200	2.83138400	4.20264400	H	5.62893200	1.22524700	-3.39176700
H	-6.03346400	-0.36157800	4.65968300	H	2.89080300	-4.38628000	-0.43202700
H	-5.00545500	-2.17087600	3.16459400	H	3.71996000	-5.80817700	-1.05941100
H	-3.41352400	-1.20045600	1.44485200	H	3.26226300	-7.37119700	0.52942700
H	-3.02675100	4.65271300	-3.56367400	H	1.66125900	-7.71817600	1.10963400
H	-4.69393400	4.22662200	-3.96010800	H	1.25273100	-4.51335100	-2.34193900
H	-2.01913200	3.21461700	-1.49468200	H	4.26403000	-2.79272800	-5.16724900
H	-6.17826600	3.72614000	-1.48405900	H	3.74751500	-1.34445400	-4.27094200
H	-5.57975300	2.29653900	0.53764900	H	1.74858900	-2.80592900	-3.57550300
H	-2.52236700	5.16176200	3.74849400	H	2.10075400	-5.92207100	-2.96812800
H	-0.16109800	3.89136200	-4.76897200	H	2.76101600	-1.95320900	-5.62572300
H	0.07684200	5.21527700	-3.59945100	H	7.34355200	1.27427700	-2.92942800
H	7.18280100	3.97836900	0.17331400	H	6.88294200	1.49111900	-4.62492300
H	-5.37795700	3.02888000	3.19973900	H	8.01731100	-3.66268200	4.01956800
H	-5.53771300	2.38842000	4.84212500	H	6.32815000	-4.11572800	4.28651000
H	-1.46019300	5.76161800	5.03930800	C	-3.23554400	-5.66671900	6.75695600

C	-1.79140600	-5.15472600	6.60955500	N	-5.18198900	-1.98883600	-2.14587000
C	-1.55468500	-4.41659900	5.30866700	C	-5.97643700	-2.69485100	-3.18671600
C	-1.63947600	-3.02219600	5.23388200	C	-5.64814600	-2.18218000	-4.59500700
C	-1.27546400	-5.11290800	4.12159300	C	-7.41578900	-2.38457800	-2.73535600
C	-1.47298000	-2.34183400	4.02491100	C	-7.32696700	-0.94628700	-2.19780800
C	-1.10450100	-4.45671000	2.90679900	C	-5.94551500	-0.89196200	-1.52304100
C	-1.21368600	-3.05957800	2.84949100	H	-5.42620100	0.06120800	-1.66502900
O	-1.07416200	-2.46473200	1.63392800	H	-6.00410000	-1.06696500	-0.44139600
H	-1.10282900	-6.00674200	6.68169600	H	-7.37774000	-0.22954200	-3.02452800
H	-1.55524100	-4.49612500	7.45513600	H	-8.13542800	-0.70229600	-1.50197100
H	-1.83415700	-2.44984000	6.13937800	H	-8.13535300	-2.49578300	-3.55119900
H	-1.18574600	-6.19734100	4.15130500	H	-7.70914800	-3.07086500	-1.93182100
H	-1.52379100	-1.25571000	3.99249800	H	-5.77821300	-3.76822800	-3.13405700
H	-0.86620600	-5.00270200	1.99811900	H	-5.75542700	-1.09299500	-4.65574100
H	-1.11989800	-1.48050500	1.69471400	H	-4.63565000	-2.46530500	-4.88968600
H	-3.95013500	-4.83539300	6.73080000	H	-6.33695400	-2.63317000	-5.31920700
H	-3.49426600	-6.35266700	5.94223000	H	-3.71230400	-3.98556600	-3.01082800
H	-3.37128200	-6.20036500	7.70484500	H	-0.93800800	-5.40318800	-1.25907200
N	-0.57723700	-0.48967800	-0.90601500	H	-3.27027700	-4.57581900	-0.64310100
C	0.49793900	-1.21014300	-1.32483700	H	-1.85711200	-3.51067400	-0.61821400
O	0.50090300	-2.02157800	-2.25698700	H	-1.19200000	-2.50395300	-2.84876700
C	-0.29124500	0.35447300	0.25379200	H	-0.78441800	-2.74505700	-6.31207500
O	-1.18825700	0.24778700	1.24820600	H	-0.21746000	-1.92228400	-4.82706100
H	-1.54609200	-0.76948900	-1.10297100	H	0.07006900	-3.65946100	-5.05999900
O	-0.32378400	1.75442100	-0.24125200	C	2.92112400	-1.38564300	-0.38696800
H	-0.39002400	1.78818900	-1.26411100	C	1.14143400	-0.04476400	0.58870000
C	-0.64129000	-2.84435000	-5.23381500	C	1.91827800	0.26739900	1.69352600
C	-1.97170100	-3.19276400	-4.59039600	C	3.21535100	-0.26038900	1.74676400
O	-2.87235900	-3.76221400	-5.20165100	C	3.71982300	-1.05594700	0.71159800
N	-2.06389800	-2.80565500	-3.28381300	H	3.30072300	-2.01102400	-1.18742500
C	-3.08785800	-3.33244500	-2.40064400	H	1.52543300	0.88995800	2.49004300
C	-3.88828200	-2.16415700	-1.80689300	H	3.84176500	-0.05324000	2.61059700
O	-3.34381600	-1.38381800	-0.99572800	H	4.73468000	-1.43369400	0.76631500
C	-2.45379500	-4.16507800	-1.26503600	C	1.62546800	-0.88540200	-0.41254000
O	-1.68163600	-5.18593700	-1.85367200				

SkDHPase.PTA-TS2-II

C	1.14735700	8.28655300	-2.12791800	C	-0.31856100	3.51663000	2.73667500
C	0.80704900	7.14333700	-1.23911300	O	-1.44106500	2.91711700	2.65759500
N	-0.01047500	7.24160800	-0.12264700	O	0.77527400	3.21500500	2.17375000
C	1.16223800	5.82491600	-1.29291800	C	-4.72660700	2.46168400	4.09983300
C	-0.11829100	6.01546300	0.44503100	C	-4.55037600	1.06735300	3.57358100
N	0.57780000	5.13097500	-0.25008500	N	-3.70965500	0.74071500	2.51098800
C	6.59474400	2.83566700	-0.51452800	C	-5.15860500	-0.08034400	4.01251500
C	5.20456500	2.92441400	0.00473900	C	-3.82397800	-0.56780100	2.32104000
N	4.91594300	3.03647800	1.35623400	N	-4.69317300	-1.09914300	3.20470000
C	3.98307700	2.92446900	-0.61414900	C	-4.16276200	4.46578900	-3.12964400
C	3.57515400	3.09792200	1.51117000	C	-4.06419900	3.78018200	-1.80909800
N	2.98135800	3.03042300	0.33110700	N	-5.10059800	3.73381300	-0.88662300
C	-1.46919300	4.93116500	4.34035100	C	-3.03613600	3.09966800	-1.21244600
N	-0.32529800	4.65705800	3.50711200	C	-4.67693500	3.04718800	0.20234100

N	-3.42611200	2.65465800	0.03605500	O	0.21575900	-5.00229500	-1.67362200
C	0.30841100	3.97763000	-4.10261400	N	1.09635700	-4.35343400	0.32108100
C	0.41751700	2.89003600	-3.02914000	N	2.78393900	-3.92597100	-4.32495700
O	1.28787000	2.99836600	-2.13198500	C	3.08958500	-2.60055200	-4.84321800
O	-0.44610300	1.94182300	-3.11879300	H	6.68201300	-2.91497600	1.97106900
Zn	0.98363600	3.13560300	0.06634000	H	5.58025800	-2.16719700	3.11905400
Zn	-2.19073700	1.65472100	1.34338700	H	6.95994200	-0.52174000	2.00348100
H	0.25678900	8.72352200	-2.59688000	H	6.26334400	-0.04165500	4.36894100
H	1.66506800	9.08953000	-1.58853000	H	7.79340900	0.75802700	3.95109000
H	1.78732600	5.31684100	-2.00785600	H	7.80063800	-0.69277800	4.95379500
H	-0.44523000	8.08683100	0.22145900	H	9.40871700	-0.34872200	2.27414300
H	-0.66088300	5.81767500	1.35772000	H	9.44741400	-1.82949200	3.23502500
H	6.58578400	2.83291000	-1.60734800	H	8.98260500	-1.89523900	1.52517900
H	7.09600500	1.91619800	-0.18746100	H	7.04020200	-2.93837000	5.03408400
H	3.74687900	2.85318300	-1.66428600	H	5.33774700	0.42695400	-2.14533400
H	5.59530500	3.04636000	2.10465900	H	4.85356600	-0.76188700	-3.34885500
H	3.06107800	3.18133400	2.45482400	H	5.94828500	-2.52449400	-2.22687400
H	-3.75448900	2.93854500	4.25600600	H	7.31816500	1.07758100	-3.62408000
H	-5.86363200	-0.25502300	4.81054000	H	3.29805700	-5.28026900	-0.61625500
H	-4.88855200	-2.08554300	3.30725300	H	2.33647000	-6.75021600	-0.82169200
H	-3.29190600	-1.13311000	1.57022000	H	1.91568100	-4.27422300	0.90484700
H	-3.24517400	4.29272400	-3.69743100	H	0.27859400	-3.80712200	0.59054300
H	-4.99854700	4.08547400	-3.72965000	H	1.92068700	-6.06270000	-3.23260400
H	-2.05919300	2.86618900	-1.60446100	H	4.17083100	-2.44414100	-4.83466000
H	-6.02210200	4.13104400	-1.00905800	H	2.60223700	-1.82410600	-4.24451600
H	-5.29389500	2.84573900	1.06455600	H	2.02887300	-4.44556800	-4.74888700
H	-2.36770700	5.03122600	3.72733900	H	3.61054000	-6.43448900	-2.85123100
H	-0.24045600	3.61458400	-4.97354300	H	2.73232500	-2.53609400	-5.87353500
H	-0.22260000	4.83756500	-3.67835500	H	6.75889700	-0.07718200	-4.83765200
H	7.20694700	3.68626600	-0.18987300	H	5.76120100	1.33765200	-4.43364900
H	-5.29618500	3.09590900	3.40780300	H	8.14251500	-3.70049000	3.87831100
H	-5.26752800	2.44481200	5.05008400	H	6.48360200	-4.28238800	4.03364900
H	-1.30623100	5.87516800	4.86983700	C	-3.05711400	-5.51662700	7.10002300
H	-1.65382900	4.14488400	5.08423300	C	-1.69727500	-4.86769700	6.78185400
H	1.80960700	7.94609100	-2.92776000	C	-1.58298200	-4.24326200	5.40155200
H	1.30553100	4.31265100	-4.40009800	C	-1.33842200	-2.87461600	5.23640700
H	-4.29655700	5.54983000	-3.02307300	C	-1.67207700	-5.02516800	4.23738600
H	0.58471500	4.98010000	3.80480100	C	-1.16011700	-2.30079600	3.97289000
C	7.10643200	-3.38088000	4.03379100	C	-1.50920600	-4.47423000	2.96924000
C	6.63979400	-2.40652400	2.94441000	C	-1.23329000	-3.10554900	2.83097300
C	7.42795900	-1.08144400	2.82889600	O	-1.02525900	-2.63118400	1.56403900
C	7.31222300	-0.21780000	4.09518500	H	-0.91381900	-5.63018400	6.89513700
C	8.89846900	-1.30442600	2.44456100	H	-1.48101600	-4.10160000	7.53688700
C	6.42998400	0.57149100	-4.02012300	H	-1.26211800	-2.23795000	6.11574400
C	5.71284400	-0.23067900	-2.93568900	H	-1.86215700	-6.09300900	4.32224200
S	6.82411200	-1.49809800	-2.16431700	H	-0.94202300	-1.24056300	3.87229800
C	2.79395300	-5.72575100	-2.66704500	H	-1.58681800	-5.08858400	2.07583600
C	3.26886100	-4.35401600	-3.13738200	H	-1.02627900	-1.63183600	1.48767300
O	4.07626700	-3.68975800	-2.47621100	H	-3.86708900	-4.77914800	7.05571600
C	2.46297200	-5.71778400	-1.17160500	H	-3.29640600	-6.31618100	6.38992300
C	1.15812900	-4.97919100	-0.87276700	H	-3.05060300	-5.95365800	8.10457800

N	-0.45669200	-0.07418600	-1.34304400	H	-7.90693200	0.20126400	-1.51824300
C	0.61610100	-0.98349700	-1.63372200	H	-8.33648900	-2.01734900	-3.03350300
O	0.61330600	-1.74827900	-2.58264600	H	-7.85605000	-2.23664300	-1.34392400
C	-0.28396700	0.48762400	0.11237400	H	-6.15226900	-3.50276600	-2.39851800
O	-1.21988300	-0.03062100	0.95481900	H	-5.95967700	-1.35917400	-4.59848700
H	-1.39775900	-0.49717900	-1.45954900	H	-4.98620700	-2.84907200	-4.51515300
O	-0.44726300	1.85156800	0.02992200	H	-6.72749000	-2.94651900	-4.78092200
H	-0.39864800	0.99860200	-2.22653900	H	-4.06731700	-3.90915400	-2.66802800
C	-0.98208900	-3.16798200	-5.08966500	H	-1.58677500	-5.21726600	-1.28455900
C	-2.24409300	-3.50047000	-4.32352700	H	-3.91696400	-4.05153000	-0.19616300
O	-3.23280800	-3.98442600	-4.86988600	H	-2.29942600	-3.34040400	-0.23753600
N	-2.20019800	-3.16737500	-3.00116400	H	-1.32890100	-2.80185800	-2.63358400
C	-3.35263400	-3.28825800	-2.13046700	H	-1.00006400	-2.11159100	-5.38262000
C	-3.91070600	-1.89552900	-1.80559800	H	-0.08630800	-3.32655700	-4.48448300
O	-3.16329500	-1.03273700	-1.30411600	H	-0.95162200	-3.77764400	-5.99525300
C	-2.99635600	-3.98064400	-0.79158600	C	2.88135400	-1.44025700	-0.48627700
O	-2.50749200	-5.28595600	-0.95451400	C	1.63198100	-0.82095900	-0.58236800
N	-5.22257500	-1.64176800	-1.98601300	C	1.12254300	-0.01313400	0.43367200
C	-6.20483900	-2.46435100	-2.73845600	C	1.84338200	0.16631700	1.61159200
C	-5.94287800	-2.39733300	-4.24594400	C	3.09330200	-0.44844300	1.72042000
C	-7.53943000	-1.82492000	-2.30998500	C	3.61662200	-1.23166000	0.67895500
C	-7.20113600	-0.33187000	-2.16256000	H	3.25658700	-2.07741700	-1.28112100
C	-5.77604000	-0.33549800	-1.58561900	H	1.44372700	0.77822600	2.41272100
H	-5.14479300	0.47439100	-1.96286500	H	3.67198400	-0.32592900	2.63302500
H	-5.77127600	-0.26353300	-0.49019600	H	4.59487300	-1.69065000	0.78583400
H	-7.21448900	0.15883900	-3.14190300				

***S*kDHPase.PTA-EP-II**

C	1.73123500	8.28910700	-2.29181700	C	-3.77668000	4.76859000	-3.32519700
C	1.30325300	7.18480100	-1.38942300	C	-3.83922600	4.04816500	-2.02050500
N	0.47326400	7.35083300	-0.28987700	N	-4.93640200	4.07083700	-1.16946000
C	1.57059600	5.84519100	-1.42017000	C	-2.91288300	3.26910700	-1.38072000
C	0.27393000	6.14081700	0.28889000	C	-4.65095400	3.32994400	-0.07451500
N	0.92146400	5.20186100	-0.38126200	N	-3.42496100	2.83457800	-0.17209700
C	6.81061700	2.56185200	-0.45126900	C	0.67571100	3.99504100	-4.19363800
C	5.39917400	2.65292800	0.02683400	C	0.54057300	3.04000800	-3.01792100
N	5.05754800	2.62840700	1.37235000	O	1.49788200	3.04770400	-2.15294300
C	4.20258800	2.77802100	-0.62990700	O	-0.49334300	2.35103200	-2.94322200
C	3.71448100	2.73751400	1.48499600	Zn	1.20781200	3.14275000	-0.15490400
N	3.16614800	2.82994800	0.28565600	Zn	-2.38758600	1.91456700	1.28488500
C	-1.20810300	5.23789400	4.18844800	H	0.87760400	8.77425800	-2.78151900
N	-0.13743000	4.76817600	3.33534400	H	2.29286100	9.06598200	-1.75816600
C	-0.28337700	3.67924000	2.51114600	H	2.16709400	5.28636500	-2.12120500
O	-1.48422900	3.24345300	2.39140900	H	0.08550200	8.22652100	0.03362700
O	0.75839100	3.24727700	1.93766600	H	-0.30723200	5.99223600	1.18623800
C	-4.60173800	2.96107900	3.93096300	H	6.84353700	2.69556000	-1.53535300
C	-4.67607400	1.54816600	3.43554700	H	7.25415800	1.58473400	-0.22401200
N	-3.90869700	1.08535500	2.37037100	H	4.00128600	2.83200700	-1.68867300
C	-5.45837400	0.51428400	3.87781700	H	5.70390800	2.51267300	2.14120600
C	-4.22872300	-0.19050500	2.17346900	H	3.17198800	2.75044900	2.41680800
N	-5.16528800	-0.56655200	3.06694700	H	-3.56328400	3.25391300	4.11112000

H	-6.17772900	0.45367800	4.67964900	H	3.28957600	-5.26975400	-0.46014100
H	-5.53847300	-1.50177300	3.15672800	H	2.55322500	-6.86265000	-0.66100200
H	-3.83704900	-0.82971400	1.38801000	H	1.71981500	-4.27049600	0.82069300
H	-2.84751700	4.49805200	-3.83279000	H	0.07508400	-4.06398800	0.40290100
H	-4.60931200	4.49807900	-3.98584100	H	2.19570200	-6.29413400	-3.12424400
H	-1.93962100	2.95757700	-1.73591800	H	4.14985600	-2.58543100	-4.82480900
H	-5.81339700	4.54265800	-1.34424200	H	2.63925800	-1.96590000	-4.10969600
H	-5.33785000	3.16841800	0.74223600	H	2.02951800	-4.59429900	-4.52962200
H	-2.10376500	5.43111100	3.59382700	H	3.88348500	-6.48667400	-2.62343900
H	0.07397800	3.64938500	-5.03699300	H	2.62778900	-2.69703900	-5.73455500
H	0.31057400	4.98449300	-3.89103400	H	7.03475100	-0.48097500	-4.60338300
H	7.44257100	3.33630800	0.00017200	H	5.90294800	0.88516000	-4.48010400
H	-5.01844500	3.66907500	3.20291800	H	7.92784300	-3.81776600	4.21228400
H	-5.16587000	3.07212500	4.86103900	H	6.30767000	-4.51249800	4.12933400
H	-0.89669400	6.17225300	4.66382700	C	-3.47101700	-5.03414800	7.13090300
H	-1.46975700	4.51933700	4.97681700	C	-2.09820900	-4.35862300	6.96628400
H	2.38030400	7.89087000	-3.07551700	C	-1.82522000	-3.88848000	5.55208200
H	1.71923500	4.10843000	-4.50292800	C	-1.88076200	-2.53547300	5.20227200
H	-3.79314000	5.85811200	-3.19572700	C	-1.52180900	-4.80753700	4.53496600
H	0.81688600	4.98471800	3.58582800	C	-1.64555000	-2.10344500	3.89355500
C	6.86042700	-3.57244200	4.23514200	C	-1.29081600	-4.40068300	3.22535100
C	6.47439300	-2.59636800	3.11616200	C	-1.35153800	-3.04033100	2.89741900
C	7.16398300	-1.21298300	3.13993000	O	-1.10626300	-2.69047500	1.59637200
C	6.78651200	-0.38919000	4.38153800	H	-1.31660000	-5.06531300	7.27576900
C	8.68913300	-1.31446000	2.98688400	H	-2.02947000	-3.50612300	7.65371500
C	6.58022100	0.23478600	-3.91169000	H	-2.10096400	-1.79511000	5.96924500
C	5.81509700	-0.48283300	-2.80066300	H	-1.46238400	-5.86744700	4.77335300
S	6.92126800	-1.55505800	-1.76792500	H	-1.66941300	-1.04471600	3.64952100
C	2.99351700	-5.85471000	-2.51909400	H	-1.05561200	-5.12342100	2.45011700
C	3.38160400	-4.46570900	-3.01691200	H	-1.25286600	-1.73192300	1.45753000
O	4.19109500	-3.75868400	-2.40434100	H	-4.28218700	-4.34291000	6.87373600
C	2.56089800	-5.83608200	-1.04852200	H	-3.56215500	-5.90925600	6.47782400
C	1.14631700	-5.28057000	-0.86837700	H	-3.62323900	-5.36734700	8.16381300
O	0.26599800	-5.51289600	-1.69963800	N	-0.28096000	-0.32979000	-2.21259500
N	0.93055400	-4.59840600	0.28256100	C	0.54299500	-1.27273600	-1.72067300
N	2.82400400	-4.07322200	-4.18654900	O	0.55936000	-2.43200100	-2.16534000
C	3.07332600	-2.75109600	-4.73862200	C	-0.26392200	0.63087400	0.54874400
H	6.68872300	-3.06631500	2.14638100	O	-1.27295400	0.22119900	1.20847200
H	5.38553600	-2.44285500	3.14585500	H	-0.89733800	-0.62662200	-2.95873600
H	6.78509100	-0.67336000	2.25741100	O	-0.30267800	1.75216600	-0.04141200
H	5.69749900	-0.29232200	4.48624900	H	-0.19867800	0.68346400	-2.09632300
H	7.21368600	0.62111600	4.32957500	C	-1.01930400	-3.08154700	-5.05872000
H	7.16468700	-0.84775200	5.30237100	C	-2.32063200	-3.36633800	-4.32819100
H	9.14290200	-0.31966400	2.90008500	O	-3.32511700	-3.72179000	-4.93998100
H	9.14973600	-1.80742700	3.85097300	N	-2.30099900	-3.14246100	-2.97719800
H	8.96061300	-1.88343400	2.09024100	C	-3.44670500	-3.49043100	-2.14204500
H	6.63202800	-3.16952900	5.22850200	C	-4.08395000	-2.23911100	-1.51299400
H	5.31962300	0.23606800	-2.14067700	O	-3.48176200	-1.61858300	-0.61900900
H	5.04370400	-1.13722800	-3.20946100	C	-3.04379300	-4.46372900	-1.00756200
H	6.14132000	-2.65584500	-1.81590700	O	-2.55288600	-5.68141800	-1.50020000
H	7.38558000	0.85908800	-3.50737500	N	-5.32703000	-1.85271700	-1.90089200

C	-6.23843200	-2.46681000	-2.90567100	H	-3.94475500	-4.67916900	-0.41626900
C	-5.94092400	-1.99989700	-4.33563500	H	-2.33776700	-3.95400400	-0.33811900
C	-7.61755300	-2.00765100	-2.39289200	H	-1.39162300	-3.01542100	-2.53465500
C	-7.34869700	-0.59363200	-1.85406300	H	-1.15058500	-2.18224700	-5.67208500
C	-5.96130700	-0.71974600	-1.20577600	H	-0.17272500	-2.93938100	-4.38328700
H	-5.34801800	0.18294100	-1.29944000	H	-0.82534400	-3.91071200	-5.74590700
H	-6.03346300	-0.94743600	-0.13416100	C	2.65056800	-1.61842000	-0.45090700
H	-7.32390400	0.12847600	-2.67741600	C	1.42258700	-0.94829600	-0.54000500
H	-8.10772300	-0.25508700	-1.14205900	C	0.99377300	-0.17619300	0.55326400
H	-8.37816300	-2.03449100	-3.17828900	C	1.75923800	-0.13153200	1.72648600
H	-7.95051400	-2.66314700	-1.57887100	C	2.98245200	-0.79340000	1.79444000
H	-6.15329900	-3.55525200	-2.85689800	C	3.44043600	-1.51860700	0.69226800
H	-5.97829100	-0.90662800	-4.41225900	H	2.98202800	-2.23390500	-1.27967400
H	-4.96357000	-2.35408000	-4.66796900	H	1.39185100	0.43694900	2.57538600
H	-6.69214000	-2.41438500	-5.01852700	H	3.57247200	-0.74857500	2.70591700
H	-4.14168400	-4.00525200	-2.80470900	H	4.40125200	-2.02358300	0.72451800
H	-1.58642100	-5.59522500	-1.63197300				

SkDHPase.ALN-ES-II

C	-8.72690900	-1.57363000	-1.91652700	O	-3.92944300	0.31348500	-1.94396000
C	-7.56260000	-1.47215200	-0.98978300	O	-2.44262800	-1.14536400	-2.79478300
N	-7.41374400	-2.21604600	0.17306700	Zn	-3.69610700	-0.09572000	0.10114200
C	-6.42670800	-0.71632000	-1.06212500	Zn	-1.27894400	-2.58474600	1.09596400
C	-6.22427300	-1.89562000	0.74263000	H	-8.83150400	-2.58228900	-2.33568000
N	-5.59448400	-0.99155900	0.00962200	H	-9.67385800	-1.31958600	-1.42390600
C	-5.38841100	5.30259200	-0.02942500	H	-6.12531500	-0.00726700	-1.81396000
C	-4.80504900	3.98812300	0.38385300	H	-8.07798000	-2.88329300	0.54067200
N	-4.44546900	3.71153000	1.69666500	H	-5.86495400	-2.31152600	1.67353500
C	-4.52237300	2.83272500	-0.29895000	H	-5.59404800	5.29725300	-1.10273400
C	-3.98086300	2.44354900	1.76703200	H	-4.70425300	6.13511900	0.17462700
N	-4.01322800	1.87970300	0.57042900	H	-4.64187500	2.60407500	-1.34676000
C	-4.43669400	-3.25908300	4.30414700	H	-4.49101400	4.36020300	2.47060600
N	-4.45327400	-1.99550700	3.58924200	H	-3.62135900	1.97454200	2.66767300
C	-3.39668900	-1.62917700	2.78524500	H	-1.63912600	-4.65052200	4.20218700
O	-2.53091000	-2.55107400	2.58606400	H	1.91505900	-5.97226700	4.15896800
O	-3.38585700	-0.45660600	2.30487100	H	3.32170200	-4.50797200	2.59500800
C	-1.02013300	-5.45988300	3.80361900	H	1.88653200	-3.06361900	1.10507900
C	0.21791000	-4.91462500	3.15715200	H	-3.62093100	-4.21644600	-3.75336500
N	0.23100100	-3.94357600	2.15254200	H	-2.78159000	-5.73544500	-4.08719900
C	1.51007300	-5.27450800	3.44222200	H	-2.63271900	-2.83834100	-1.70711600
C	1.50694800	-3.74563000	1.84994300	H	-2.02317000	-6.97787900	-1.49981600
N	2.31165000	-4.52994400	2.60148200	H	-0.89955400	-5.93870300	0.53769600
C	-3.37341500	-5.19588100	-3.33725000	H	-4.28497200	-4.08007300	3.60112400
C	-2.62696300	-4.99638900	-2.06600000	H	-3.91948000	-1.17674200	-4.87025600
N	-2.02943600	-5.98728600	-1.29805700	H	-5.21068600	-1.52151100	-3.69808800
C	-2.36967700	-3.83556200	-1.39916600	H	-6.33231800	5.50778000	0.49053800
C	-1.44337900	-5.40089200	-0.22363700	H	-1.64147600	-6.01698200	3.09069000
N	-1.63452900	-4.09063300	-0.25954600	H	-0.75354100	-6.13741600	4.61938700
C	-4.46822000	-0.77779400	-4.01420800	H	-5.40100600	-3.39470100	4.80272200
C	-3.51829000	-0.50922100	-2.84184800	H	-3.64331700	-3.30743700	5.06154000

H	-8.59054600	-0.88001100	-2.74986000	C	5.15608900	0.00544000	4.78557900
H	-5.00845500	0.12783100	-4.30598000	C	3.88231800	-0.53380700	4.55285200
H	-4.30816500	-5.75270100	-3.19185000	C	5.85614700	0.52492500	3.68928900
H	-4.98819000	-1.22711200	3.97003500	C	3.31994600	-0.54434600	3.27762100
C	0.45644900	7.63875500	4.43971400	C	5.30744400	0.52555600	2.40441000
C	-0.34307300	6.93187100	3.33774500	C	4.03524400	-0.00868200	2.20234500
C	0.43929300	5.91737000	2.48270500	O	3.44344500	0.08607200	0.94280300
C	-0.50640900	5.25711600	1.46868600	H	6.66342700	0.63096000	6.17544300
C	1.63395300	6.55712400	1.75795500	H	5.04480900	0.57369000	6.85073700
C	-3.33926300	6.12256200	-3.57506000	H	3.30566100	-0.92665500	5.38748400
C	-2.24050300	5.64300900	-2.63037100	H	6.84573900	0.94985000	3.84263400
S	-0.99579600	6.98559400	-2.37768300	H	2.31736000	-0.92873400	3.11358500
C	3.61191000	4.41046300	-2.14419300	H	5.84789700	0.94722700	1.56129000
C	2.17911000	4.29726200	-2.66563300	H	3.43863600	-0.78207500	0.48898300
O	1.21456200	4.25572400	-1.88805300	H	5.11751700	-1.95393300	6.83457100
C	4.01484100	3.16151800	-1.33255000	H	6.75495400	-1.89284200	6.16450800
C	5.35447200	3.26721700	-0.61375000	H	6.43622600	-1.26076000	7.79078500
O	6.25075100	2.43149600	-0.75501100	N	0.98350700	-0.33871300	-0.69732700
N	5.51443900	4.33306200	0.21336700	C	1.08429700	0.94188700	-1.29389800
N	2.03575700	4.26003000	-4.00749500	O	1.63646000	1.16458500	-2.35946200
C	0.74340100	4.11707300	-4.67394800	N	0.47687700	1.81646600	-0.45674300
H	-1.19172600	6.40695600	3.80024500	C	0.02930100	1.19816500	0.77975900
H	-0.78205200	7.68839600	2.66942600	C	0.42597800	-0.27127400	0.52605500
H	0.82223600	5.13034900	3.14935300	O	0.31953500	-1.19675900	1.33784500
H	-1.32535700	4.72923000	1.97357500	H	-1.05494800	1.25621300	0.89396500
H	0.02958600	4.53073500	0.84930300	H	1.55140700	-1.13051900	-1.01192900
H	-0.94426100	6.00591100	0.79558100	H	0.48193200	2.81038700	-0.68244200
H	2.12534000	5.82300000	1.10501200	O	-2.04067300	-1.10810500	-0.06035100
H	1.30843400	7.39240400	1.12375100	H	-1.91501600	-1.14002100	-1.03697900
H	2.38302300	6.94078000	2.45904400	C	2.64055100	0.48652900	-5.21037700
H	1.25009700	8.27159700	4.02780700	C	3.55185600	-0.62646800	-4.73203600
H	-2.65937100	5.35505000	-1.66131700	O	4.21917200	-1.32199600	-5.49160500
H	-1.72568000	4.77157400	-3.04237000	N	3.53836000	-0.79481700	-3.37322100
H	-0.03584400	6.19027500	-1.85786100	C	4.53356300	-1.60085000	-2.69368600
H	-3.84811100	7.00931000	-3.18049000	C	3.78601600	-2.64431300	-1.85362600
H	4.07634500	2.28927400	-1.98502000	O	3.14792900	-2.27474800	-0.82910100
H	3.24155000	2.95841000	-0.58261900	C	5.46224800	-0.74298200	-1.80869800
H	4.74851800	4.94168300	0.46290000	O	5.99835500	0.29314200	-2.59578900
H	6.35726300	4.37959000	0.77017600	N	3.76774900	-3.93272200	-2.22819400
H	4.32712600	4.57243500	-2.95872100	C	4.44469600	-4.58588700	-3.39094300
H	0.15618400	5.03739500	-4.59007600	C	3.63087000	-4.47979600	-4.69073300
H	0.19119400	3.29050500	-4.21973600	C	4.58788400	-6.03284800	-2.88216400
H	2.86388900	4.33166600	-4.58043100	C	3.29346800	-6.26762300	-2.08699600
H	3.63676500	5.30636200	-1.51343600	C	3.04157400	-4.91709300	-1.39852400
H	0.91926900	3.89556600	-5.72817500	H	1.98185100	-4.65168600	-1.32928100
H	-2.93270000	6.37995000	-4.55839100	H	3.44863700	-4.89008600	-0.38123200
H	-4.09018600	5.33528100	-3.71352300	H	2.46867500	-6.51145400	-2.76491800
H	0.92476400	6.91394500	5.11715300	H	3.37878500	-7.08488200	-1.36511300
H	-0.19509300	8.28279700	5.04102100	H	4.72431600	-6.74215700	-3.70281300
C	6.02852700	-1.34719200	6.77750000	H	5.45849100	-6.11186400	-2.22006300
C	5.73853100	0.04203500	6.18517300	H	5.42500100	-4.12683000	-3.53738700

H	2.61884500	-4.87994400	-4.56259900	H	3.01642300	1.45627200	-4.86774300
H	3.56992500	-3.44440900	-5.03378300	H	2.61398000	0.47199600	-6.30136700
H	4.13139300	-5.05959200	-5.47436500	C	0.13107900	1.83437900	3.22959400
H	5.12537000	-2.06313000	-3.48381200	O	0.78465300	2.31796700	4.14183200
H	6.20108800	1.04164100	-1.99544000	N	0.65945500	1.75735200	1.94407200
H	6.24852100	-1.40175600	-1.39759000	N	-1.18216900	1.41534300	3.39067500
H	4.89528800	-0.34295700	-0.96125000	H	-1.42523500	1.38941000	4.37331300
H	3.02163300	-0.10091100	-2.83913700	H	-1.55135300	0.62430900	2.86760500
H	1.63064200	0.37359500	-4.80741000	H	1.67066700	1.82108200	1.92704000

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C	-2.73098600	-0.10103200	-4.80017200	H	-8.85185200	-4.72035200	-3.80704200
C	-3.68153500	-0.14860600	-5.94506500	H	-10.52888800	-4.44865700	-4.29340900
N	-3.90668800	0.89500300	-6.83224700	H	-7.10001400	-4.10739700	-5.98964400
C	-4.47771800	-1.16240800	-6.39429100	H	-10.67305000	-1.90840700	-5.70697900
C	-4.80426500	0.48425600	-7.76295600	H	-9.37557400	-1.05109100	-7.72790400
N	-5.16444100	-0.76735300	-7.52924700	H	-6.59323500	1.73971200	-13.63028500
C	-9.56332400	-3.95542200	-4.12769700	H	-6.95128000	0.33345200	-17.11780100
C	-9.06437800	-3.28038400	-5.36273200	H	-7.33925300	-2.19510900	-16.98076200
N	-9.76631200	-2.25716500	-5.98626000	H	-6.77027100	-3.11836000	-14.69465900
C	-7.92953500	-3.42911200	-6.11658400	H	-0.97531700	-2.86216800	-9.84479300
C	-9.06126400	-1.83140000	-7.05647700	H	0.05000800	-2.85500600	-11.28372600
N	-7.93992400	-2.52573700	-7.16823400	H	-3.58564400	-2.70443500	-10.37682900
C	-6.95819100	2.60919800	-10.69330200	H	-1.09035700	-0.94477700	-13.24331100
N	-7.32155900	1.53886600	-9.78360900	H	-3.48976600	-0.68625400	-14.06125100
C	-7.22579500	0.22970600	-10.18342700	H	-5.93562800	2.46712400	-11.04771100
O	-6.61350900	0.05816700	-11.29127000	H	-2.21853700	-4.94817600	-7.67887300
O	-7.70540200	-0.67137700	-9.42693100	H	-2.44805500	-3.27256600	-7.12762300
C	-5.99742600	1.45357300	-14.50229100	H	-9.68656200	-3.24650500	-3.29958800
C	-6.36451700	0.07654000	-14.97618800	H	-4.94281400	1.51576100	-14.20521800
N	-6.33233200	-1.07963600	-14.18962400	H	-6.16698600	2.18259900	-15.29917900
C	-6.78366100	-0.26520200	-16.23576600	H	-7.01715500	3.56154800	-10.15830800
C	-6.71132000	-2.07843300	-14.97830800	H	-7.61870900	2.66087400	-11.56848000
N	-6.98323100	-1.63062000	-16.22186800	H	-2.75290200	-1.05587000	-4.26932100
C	-0.67059000	-2.26303000	-10.70606800	H	-3.19653900	-4.59393900	-6.22117200
C	-1.88217100	-1.91881200	-11.50134900	H	-0.14628300	-1.37252600	-10.33623000
N	-1.89799600	-1.26714500	-12.72766700	H	-7.97736500	1.72554900	-9.03836700
C	-3.19485000	-2.16122900	-11.21992500	C	-15.72465400	-5.23249600	-8.59992500
C	-3.18727300	-1.14581500	-13.13272000	C	-14.28156700	-5.20645700	-8.07995400
N	-3.99924500	-1.68003800	-12.23292000	C	-13.24703700	-5.99752200	-8.90220100
C	-2.92952400	-4.25381900	-7.22607700	C	-11.87003500	-5.90095300	-8.22793600
C	-4.16878600	-4.09848600	-8.10865100	C	-13.64625900	-7.46859300	-9.09456000
O	-5.22772600	-3.63924100	-7.54380200	C	-8.21561000	-7.89748000	-4.42193700
O	-4.06484800	-4.35721100	-9.32895500	C	-9.03252500	-7.73228300	-5.70087600
Z	-6.39385200	-2.17158100	-8.46678200	S	-10.21428300	-9.14165400	-5.87673000
Z	-6.03828000	-1.61878300	-12.08089400	C	-9.86216000	-9.44247900	-11.16166600
H	-1.69882100	0.07384700	-5.12895400	C	-9.02278700	-9.17093700	-9.91424300
H	-2.98635000	0.68589400	-4.07941400	O	-9.22213900	-8.16729000	-9.21319600
H	-4.59314500	-2.16056300	-6.00749800	C	-9.76489800	-8.25301900	-12.13743600
H	-3.48042700	1.81073300	-6.79364800	C	-10.69934100	-8.34830700	-13.33573000
H	-5.18195000	1.11210300	-8.55613800	O	-10.28432800	-8.45408700	-14.49351100

N	-12.02825800	-8.31751300	-13.06170900	C	-7.13033400	-6.05903300	-10.89410700
N	-8.07314100	-10.08076300	-9.62237000	O	-6.69312600	-7.19836100	-10.97678300
C	-7.14864100	-9.92145600	-8.50391900	N	-8.04850800	-5.57386300	-10.00785100
H	-13.94269000	-4.16225600	-8.02420700	C	-8.50755800	-4.24178700	-10.36908200
H	-14.26975300	-5.58665800	-7.04661700	C	-7.47551200	-3.87336400	-11.46840400
H	-13.17159000	-5.52450300	-9.89268700	O	-7.63001500	-2.93221600	-12.30594200
H	-11.53455100	-4.85854700	-8.16339400	H	-8.45083200	-3.54850300	-9.53345400
H	-11.11263600	-6.47035600	-8.77677100	H	-6.20221700	-5.10873700	-12.60104400
H	-11.91068900	-6.30947000	-7.20857000	H	-8.59861200	-6.24475200	-9.47245500
H	-12.86194900	-8.01726000	-9.63513900	O	-6.09945500	-2.83698500	-10.31184500
H	-13.78086700	-7.97339900	-8.12873300	H	-5.39340800	-3.51498500	-10.14328700
H	-14.57992300	-7.57460400	-9.65755500	C	-4.79935300	-9.57942300	-11.88501000
H	-16.15530100	-6.23910500	-8.56168600	C	-4.64593900	-9.04105800	-13.29329100
H	-9.59886700	-6.79582800	-5.68059900	O	-4.00768100	-9.61981800	-14.16755300
H	-8.39047500	-7.71784500	-6.58485700	N	-5.26971300	-7.83831600	-13.48139900
H	-10.53363000	-8.89212800	-7.16369400	C	-5.50337200	-7.30427600	-14.80910800
H	-8.85922000	-7.92912000	-3.53570600	C	-4.91259900	-5.89216800	-14.88335700
H	-8.74768600	-8.17775300	-12.52568200	O	-5.43767400	-4.96538100	-14.22098600
H	-9.98748300	-7.33612200	-11.58019800	C	-7.00819500	-7.27156700	-15.15009800
H	-12.38201300	-8.07213400	-12.14777900	O	-7.51128800	-8.57572900	-14.98788600
H	-12.67361400	-8.29061800	-13.83990700	N	-3.84081800	-5.64311200	-15.65523400
H	-9.55634900	-10.36706700	-11.66376400	C	-3.01521800	-6.60492700	-16.43816100
H	-7.68386900	-9.97921200	-7.55073400	C	-2.03261900	-7.37469100	-15.54554100
H	-6.64117900	-8.95595500	-8.58114300	C	-2.32620100	-5.66631600	-17.44652500
H	-7.95681100	-10.87270200	-10.23752600	C	-2.06940000	-4.38487900	-16.63621200
H	-10.89760600	-9.58184700	-10.82906500	C	-3.31185500	-4.26723300	-15.73849800
H	-6.40928800	-10.72292100	-8.54963500	H	-3.09746200	-3.88274700	-14.73685800
H	-7.62715800	-8.82057300	-4.44229300	H	-4.07900400	-3.61661600	-16.17611300
H	-7.51970300	-7.05748000	-4.30502500	H	-1.16615700	-4.49590900	-16.02663200
H	-15.78045400	-4.88352800	-9.63859800	H	-1.93316500	-3.50215500	-17.26797300
H	-16.36620800	-4.58008600	-7.99686900	H	-1.41385700	-6.10623600	-17.85840500
C	-12.65108300	-2.36155000	-18.57849300	H	-3.00461000	-5.45527000	-18.28195000
C	-13.33490800	-2.88464700	-17.30656100	H	-3.67063800	-7.31120100	-16.95384300
C	-12.31001700	-3.38531700	-16.31772500	H	-1.40927900	-6.68982400	-14.95966800
C	-11.63543800	-2.49081500	-15.47909100	H	-2.55867800	-8.05328100	-14.87064200
C	-11.92939000	-4.73273600	-16.28581500	H	-1.37221500	-7.98457500	-16.17295300
C	-10.60513600	-2.91783400	-14.64532100	H	-5.00717800	-7.99127400	-15.49449400
C	-10.90176600	-5.18246900	-15.45962300	H	-8.47581400	-8.52942000	-14.81517900
C	-10.23664400	-4.26602800	-14.64373200	H	-7.11763100	-6.91202500	-16.18972100
O	-9.22384900	-4.73137400	-13.83521200	H	-7.51791900	-6.54328700	-14.50586500
H	-14.03191000	-3.68982100	-17.56919900	H	-5.86104500	-7.52278200	-12.71544100
H	-13.93552000	-2.08311300	-16.85791900	H	-4.51803200	-8.82819800	-11.14112100
H	-11.92109100	-1.44081700	-15.47544800	H	-5.84557400	-9.84107600	-11.69454600
H	-12.44047100	-5.44576800	-16.92953900	H	-4.17423600	-10.46725600	-11.77557400
H	-10.10261900	-2.21753800	-13.98201500	C	-10.78446600	-3.20515900	-10.78422800
H	-10.61197100	-6.22854100	-15.43915700	O	-11.90776500	-3.33148000	-11.25033700
H	-8.75276100	-3.96333900	-13.45480000	N	-9.86148100	-4.24366900	-10.86629100
H	-11.97177800	-1.53384000	-18.34349600	N	-10.38462500	-2.07298200	-10.08958400
H	-12.06022800	-3.15139500	-19.05624600	H	-11.07197100	-1.33620300	-10.18967600
H	-13.38484500	-1.99899800	-19.30830000	H	-9.42302600	-1.74537200	-10.15370400
N	-6.78824400	-5.00629300	-11.75551200	H	-10.07038500	-4.88434000	-11.62423700

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C	2.15262800	8.45420500	-1.27696600	H	-3.55582000	-0.97158200	1.13068400
C	1.65322900	7.29428300	-0.48886900	H	-2.30058300	4.99796900	-3.51404300
N	0.68225900	7.36230400	0.50105300	H	-4.03251900	4.92309500	-3.85651600
C	1.97269900	5.97010500	-0.56856100	H	-1.52795000	3.23826100	-1.59771900
C	0.45378900	6.10990000	0.96871200	H	-5.48308900	4.59433700	-1.31436100
N	1.21754600	5.23735700	0.33097000	H	-5.09942900	2.96867600	0.60469500
C	7.03297400	2.48328400	0.31033700	H	-2.08934300	5.11127500	3.94399000
C	5.59999200	2.50641600	0.71927000	H	0.62225400	4.11138400	-4.57265300
N	5.16613900	2.15903600	1.99145700	H	0.82609300	5.35931500	-3.31786600
C	4.45771600	2.84004000	0.04300800	H	7.64197800	3.16262500	0.91949900
C	3.82193000	2.28736700	2.04759400	H	-4.99401600	3.37306300	3.15095700
N	3.36206400	2.70263200	0.87733700	H	-5.36090000	2.61692300	4.70927400
C	-1.28732800	4.78322400	4.60810800	H	-0.96774400	5.63015100	5.22143600
N	-0.15646700	4.31852300	3.82541100	H	-1.68839200	4.00618300	5.27238300
C	-0.29399500	3.38972500	2.82751700	H	2.91449600	8.11333400	-1.98211200
O	-1.49487300	3.12809500	2.47869300	H	2.25224200	4.55553900	-3.98105000
O	0.76934800	2.90921900	2.31926500	H	-3.39327000	6.21465500	-2.82675900
C	-4.67096000	2.60144500	3.86125000	H	0.77492600	4.41053100	4.20534600
C	-4.64935300	1.24012500	3.23265700	C	6.68214000	-4.11178500	4.30725000
N	-3.78126500	0.87775200	2.20237100	C	6.38885400	-3.01692700	3.27353100
C	-5.43700700	0.15913300	3.52908300	C	4.97346300	-2.99557000	2.68474500
C	-4.05282000	-0.38615100	1.89249600	C	4.88289500	-1.87477300	1.63939400
N	-5.04937300	-0.85127000	2.67039000	C	4.56158800	-4.34031600	2.07544300
C	-3.29167000	5.15195600	-3.08080200	C	7.04232300	0.53890300	-3.38588500
C	-3.44017200	4.27127200	-1.88513100	C	6.12458000	-0.28353700	-2.48535900
N	-4.60006700	4.13611200	-1.13426900	S	6.90637100	-1.91247100	-2.09593200
C	-2.53360500	3.44990200	-1.27474500	C	3.02886400	-5.26280400	-2.45401000
C	-4.36097300	3.26367000	-0.12527400	C	3.30810800	-3.81594600	-2.86221200
N	-3.10979900	2.83159300	-0.18158400	O	3.57180900	-2.93609300	-2.03004800
C	1.20658400	4.40272400	-3.69782200	C	2.44936700	-5.36084000	-1.04510800
C	1.08317400	3.36418400	-2.59715100	C	1.05044800	-4.76252800	-0.96957300
O	1.95152700	3.38802500	-1.65779600	O	0.32850900	-4.68470700	-1.96371300
O	0.09642600	2.58474700	-2.63377600	N	0.66347300	-4.30204400	0.25322800
Zn	1.46379400	3.16724400	0.36446900	N	3.30428200	-3.58875000	-4.19293700
Zn	-2.15873100	1.74376700	1.25347900	C	3.58239000	-2.28590100	-4.78128400
H	1.35304900	8.93338700	-1.85569600	H	6.58623100	-2.03624800	3.73254100
H	2.60835900	9.22389600	-0.64170300	H	7.11286300	-3.10909200	2.44938400
H	2.66267900	5.48137100	-1.23417800	H	4.25980300	-2.77397500	3.48953500
H	0.22316900	8.20190600	0.82699600	H	5.08383000	-0.89552000	2.09489600
H	-0.24219100	5.88052400	1.76081000	H	3.89114400	-1.83268100	1.18126500
H	7.12513300	2.79741900	-0.73221200	H	5.61827500	-2.02481600	0.83872900
H	7.46417600	1.47842000	0.39395700	H	3.52784800	-4.27830900	1.72082100
H	4.33196800	3.14983300	-0.98268700	H	5.20414400	-4.61071700	1.22653200
H	5.75096800	1.81324300	2.74036900	H	4.60626900	-5.15428700	2.80625200
H	3.21685600	2.03910000	2.90552100	H	6.64362800	-5.11275300	3.86487400
H	-3.67457300	2.88563600	4.21199800	H	5.91725400	0.24854300	-1.55139600
H	-6.21874300	0.02500400	4.26055600	H	5.16730400	-0.47678800	-2.97453500
H	-5.38813700	-1.80376100	2.67004300	H	5.75565000	-2.54183200	-1.77012200

H	8.01719700	0.71169200	-2.91534400	H	0.04351400	1.90883400	-1.23714100
H	3.11042200	-4.86038800	-0.33451500	C	-0.46870300	-2.48783300	-5.42693900
H	2.38256600	-6.41558800	-0.74706900	C	-1.85101600	-2.78076800	-4.86573900
H	1.17588500	-4.52675700	1.09771500	O	-2.78220500	-3.15610200	-5.57666400
H	-0.28659800	-3.96418300	0.37442100	N	-1.97310900	-2.56786500	-3.51954800
H	2.34818200	-5.73315700	-3.16994200	C	-3.20020600	-2.84816600	-2.79963000
H	4.64164100	-2.02666400	-4.67817800	C	-3.82804300	-1.57171500	-2.21686000
H	2.96703900	-1.52661500	-4.29160800	O	-3.19024700	-0.87036100	-1.40258100
H	3.04921700	-4.34977900	-4.80524600	C	-2.97685100	-3.81624600	-1.60916900
H	3.97968100	-5.81035000	-2.49220300	O	-2.47321000	-5.06687200	-1.99799100
H	3.32809500	-2.32207700	-5.84246500	N	-5.11099600	-1.27207100	-2.50114600
H	7.21856000	0.03143700	-4.33956300	C	-5.94382100	-1.84859600	-3.58743700
H	6.59195800	1.51658700	-3.59774100	C	-5.42146500	-1.40933000	-4.95564700
H	5.96139800	-4.08635000	5.13462900	C	-7.33953600	-1.29623600	-3.24287400
H	7.68283000	-3.98309200	4.73517700	C	-7.05080400	0.09776600	-2.66158100
C	-3.84832200	-5.70433500	6.26522200	C	-5.74868000	-0.10270500	-1.87000100
C	-2.36413700	-5.41291500	6.00373600	H	-5.07366000	0.75722600	-1.90351600
C	-2.16259500	-4.59858300	4.74676300	H	-5.94090400	-0.32211400	-0.81106800
C	-1.83047200	-3.24158100	4.79423000	H	-6.89688200	0.82120000	-3.46980300
C	-2.35301000	-5.18251300	3.48575200	H	-7.86379500	0.47354700	-2.03293300
C	-1.67469000	-2.48567400	3.63113800	H	-7.99591600	-1.27175800	-4.11700500
C	-2.20705600	-4.44741200	2.31483100	H	-7.81462500	-1.93005500	-2.48420200
C	-1.84878000	-3.09450900	2.38568700	H	-5.93713600	-2.94011500	-3.51873400
O	-1.67397500	-2.43590000	1.19831400	H	-5.35965900	-0.31630800	-5.01818800
H	-1.81887200	-6.36263500	5.92459200	H	-4.44209600	-1.83911100	-5.17504900
H	-1.93619500	-4.88193100	6.86279900	H	-6.10570700	-1.75291500	-5.74142900
H	-1.67391900	-2.76456800	5.75940300	H	-3.85777400	-3.33359800	-3.51902900
H	-2.61312500	-6.23676500	3.41763700	H	-1.51217200	-4.95757900	-2.14377800
H	-1.38252500	-1.44051600	3.68523500	H	-3.95051300	-3.99096600	-1.13052000
H	-2.35027400	-4.91255300	1.34274900	H	-2.33949500	-3.31647900	-0.87084100
H	-1.34201800	-1.50779700	1.31501000	H	-1.12453000	-2.29341900	-3.02588600
H	-4.41479300	-4.77317000	6.38407300	H	-0.22657300	-1.42684500	-5.31309100
H	-4.29457800	-6.25991600	5.43271600	H	0.29926600	-3.04716900	-4.88517400
H	-3.98248600	-6.30021200	7.17555200	H	-0.46520200	-2.75883800	-6.48410800
N	-0.44271200	-0.34705000	-1.09351800	C	1.35898400	-0.22816800	0.37974300
C	0.64436300	-0.89231100	-1.72668100	C	1.51543000	-1.40706000	2.61595900
O	0.64339900	-1.52291200	-2.77852600	O	1.67972700	-2.45980000	3.22680500
N	1.76761100	-0.60578800	-0.95923900	N	1.35694900	-1.38028600	1.25296200
C	-0.08316600	0.34552900	0.10772500	N	1.52647400	-0.16041400	3.24379100
O	-0.96465200	0.22887800	1.12453600	H	1.99848700	0.54200600	0.81100200
H	-1.41749800	-0.53748700	-1.35112000	H	1.28023600	-2.29238100	0.81363100
H	2.56908000	-1.21441800	-1.12005100	H	0.89027300	0.54120500	2.87407000
O	0.04068200	1.78628900	-0.21664300	H	1.46944400	-0.26811800	4.24948300

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C	3.92196100	7.78608700	-1.03625000	N	2.36359800	4.70338000	0.37274200
C	3.21381300	6.67580400	-0.33217400	C	7.40625200	0.80745200	0.03499200
N	2.34595700	6.87015700	0.73300800	C	6.04927900	1.18231400	0.51269100
C	3.21130500	5.32154400	-0.53177300	N	5.65972300	1.05311800	1.83712800
C	1.86251500	5.66846900	1.12855200	C	4.95114100	1.69166200	-0.12538300

C	4.38286800	1.46955300	1.96067800	H	-0.51685700	3.86926800	5.44895600
N	3.92159400	1.86612700	0.78325500	H	4.55072400	7.37803900	-1.83141400
C	-0.04140400	4.63231800	4.81942700	H	3.08503200	4.24899300	-3.81762500
N	1.02894600	4.09912000	4.01027000	H	-2.14545200	6.94169200	-2.50573700
C	0.73222700	3.11294000	3.10431400	H	1.96429600	4.06934800	4.39249000
O	-0.50573800	2.93138500	2.88689200	C	5.73810500	-5.76581400	3.72333800
O	1.71794300	2.51130900	2.56499600	C	5.65963700	-4.57605900	2.75786200
C	-3.84889500	3.29438700	4.12668600	C	4.28566200	-3.93265300	2.53760400
C	-4.13362900	2.03616100	3.36483000	C	4.43981900	-2.76850800	1.54649300
N	-3.35157800	1.59401700	2.30052100	C	3.23095800	-4.93035700	2.04249900
C	-5.15287900	1.14029100	3.55593500	C	6.85544700	-0.87748100	-3.74660000
C	-3.89714200	0.46416000	1.86489500	C	5.79910800	-1.50136500	-2.83752100
N	-4.98965100	0.16072300	2.59545000	S	6.16171100	-3.29341800	-2.56748500
C	-2.17893400	5.87047600	-2.74170200	C	0.73803800	-4.74024700	-2.58909600
C	-2.40122900	5.03271200	-1.52878300	C	1.89628600	-3.89926500	-3.11782000
N	-3.55991600	5.07029400	-0.76568900	O	2.71186300	-3.33505200	-2.37172700
C	-1.61418500	4.09575800	-0.91550300	C	1.00054800	-5.28465400	-1.18618800
C	-3.43921300	4.17763300	0.24710000	C	-0.27212500	-5.48021300	-0.36490700
N	-2.26548300	3.57284600	0.18250300	O	-1.40479200	-5.32537400	-0.82323400
C	2.01641500	4.18661400	-3.60194000	N	-0.07013700	-5.86043800	0.92288100
C	1.74610000	3.02446100	-2.67033800	N	1.95882400	-3.77800700	-4.46219000
O	2.53419000	2.70187400	-1.77926500	C	2.80833800	-2.78786200	-5.11370100
O	0.57731100	2.44936700	-2.87833500	H	6.34939800	-3.79506800	3.11200000
Zn	2.08803800	2.65516200	0.50592600	H	6.05404700	-4.89244000	1.78005900
Zn	-1.50982400	2.11038000	1.40448900	H	3.92496600	-3.52798400	3.49438300
H	3.21959000	8.49308000	-1.49451100	H	5.12935500	-2.00844500	1.93765500
H	4.57100300	8.35305800	-0.35793300	H	3.48200400	-2.28415600	1.34298300
H	3.75410800	4.74531000	-1.26229900	H	4.84877800	-3.12354500	0.59135700
H	2.11877200	7.75969700	1.15668400	H	2.26532700	-4.41852900	1.97278000
H	1.19760400	5.53389900	1.96889400	H	3.50418700	-5.33511800	1.05826500
H	7.50352300	1.03202600	-1.03007300	H	3.11640800	-5.77195000	2.73521800
H	7.60162900	-0.26395900	0.16530600	H	5.17313600	-6.63015200	3.35763400
H	4.81871300	1.93161200	-1.16839500	H	5.76891800	-0.99171400	-1.86894700
H	6.22026100	0.66042300	2.58131300	H	4.80343300	-1.42471400	-3.28020400
H	3.81781700	1.45521800	2.87685700	H	4.88813600	-3.64628600	-2.28482200
H	-2.83032600	3.28455500	4.52723600	H	7.86124600	-0.98144900	-3.32325800
H	-5.95595300	1.11316900	4.27612500	H	1.66080700	-4.58980600	-0.65481300
H	-5.53005200	-0.68869900	2.50535200	H	1.54055600	-6.23917600	-1.22573100
H	-3.53431200	-0.12748600	1.03593100	H	0.84721100	-5.79443300	1.34192300
H	-1.22751900	5.59680100	-3.20439300	H	-0.86216600	-5.81901800	1.55311600
H	-2.96397500	5.72011700	-3.49271100	H	-0.14026000	-4.08407100	-2.56691400
H	-0.64611600	3.72457100	-1.20354700	H	3.86079600	-2.99216200	-4.89945100
H	-4.36944500	5.64918800	-0.94406700	H	2.55740200	-1.77953900	-4.76648400
H	-4.20822600	3.98651100	0.97975400	H	1.20803800	-4.18388900	-5.00278000
H	-0.81202000	5.07128500	4.18285800	H	0.49709100	-5.54651200	-3.29089200
H	1.44906700	4.09228600	-4.52982100	H	2.64998400	-2.84980600	-6.19221400
H	1.71697400	5.11247600	-3.09695700	H	6.85943200	-1.35377900	-4.73200100
H	8.19196200	1.35957900	0.56539500	H	6.65797300	0.19319800	-3.88561100
H	-3.93828300	4.18580000	3.49241100	H	5.34302000	-5.50708600	4.71415200
H	-4.55008200	3.40475000	4.95851800	H	6.77750500	-6.08679600	3.85403700
H	0.36043100	5.41569400	5.46919800	C	-4.80875300	-5.11210500	6.08916300

C	-3.29985500	-4.98387200	5.82885000	C	-3.65896900	-3.01598300	-1.78228300
C	-2.97052700	-4.21382300	4.56743900	O	-3.43250000	-4.23775700	-2.44463800
C	-2.50224500	-2.89706800	4.61422600	N	-5.28677500	0.05616900	-2.39299200
C	-3.13322600	-4.79868000	3.30140300	C	-6.29931800	-0.28692900	-3.42614900
C	-2.17768200	-2.18962200	3.45482800	C	-5.79121500	0.03240500	-4.83591400
C	-2.81706200	-4.11127200	2.13201900	C	-7.49777300	0.57673200	-2.98838200
C	-2.31091000	-2.80452600	2.20573200	C	-6.84693600	1.85157100	-2.42705100
O	-1.95880100	-2.20044200	1.03325700	C	-5.58848600	1.32952100	-1.71610800
H	-2.86318300	-5.98985700	5.76937100	H	-4.72980000	2.00431300	-1.78320900
H	-2.82415300	-4.49509900	6.68820800	H	-5.76720500	1.14091900	-0.64923500
H	-2.36226700	-2.41591400	5.58025200	H	-6.57100200	2.52714900	-3.24424000
H	-3.50898300	-5.81803400	3.22890900	H	-7.50629500	2.40381800	-1.75041900
H	-1.77604300	-1.18217900	3.51988500	H	-8.18556300	0.77143400	-3.81579600
H	-2.92204100	-4.57715700	1.15624200	H	-8.05918000	0.06254300	-2.19885500
H	-1.61782900	-1.27052700	1.15159000	H	-6.54896900	-1.34943300	-3.35563200
H	-5.27366400	-4.12519000	6.19891900	H	-5.47401000	1.07943700	-4.91201000
H	-5.31096300	-5.62422900	5.26039600	H	-4.96268800	-0.61574600	-5.12903400
H	-5.00447900	-5.68255000	7.00453000	H	-6.59826300	-0.12825300	-5.56123300
N	-0.35268200	0.22225300	-1.34386500	H	-4.60362800	-2.20040400	-3.52758900
C	0.41971100	-0.82078000	-1.84158900	H	-2.72122300	-4.70559500	-1.97054000
O	0.20105000	-1.43330700	-2.88873700	H	-4.59008800	-3.05186900	-1.18743700
N	1.48172600	-1.01846600	-1.00585800	H	-2.84929500	-2.75773500	-1.09229400
C	0.03056700	0.53084700	0.06962200	H	-1.71525100	-1.66192200	-3.19037300
O	-1.00583300	0.30867000	0.92771400	H	-1.28551300	-1.75131300	-6.62793700
H	-1.36681200	0.12029400	-1.48473400	H	-0.49973300	-1.47992100	-5.03437400
H	2.08317500	-1.82207500	-1.18877600	H	-0.87300300	-3.12096500	-5.59396200
O	0.38686400	1.88279900	0.12639700	C	1.25071900	-0.47528500	0.31776600
H	0.36234100	1.71939700	-2.21670200	C	1.27029900	-1.57253600	2.60681000
C	-1.22107000	-2.08037900	-5.58763600	O	1.08143100	-2.58112400	3.27885600
C	-2.60877200	-2.04581400	-4.98115000	N	1.00115900	-1.54936000	1.25199200
O	-3.62115600	-2.25217500	-5.64718600	N	1.84429600	-0.42419700	3.14187200
N	-2.61878100	-1.76616600	-3.64769600	H	2.11848400	0.07267400	0.68616800
C	-3.81314900	-1.90401600	-2.83953400	H	0.33111900	-2.25663800	0.96924000
C	-4.11392000	-0.56685400	-2.15325200	H	1.51650800	0.48328100	2.81864500
O	-3.28761500	-0.07372300	-1.35906000	H	1.89088200	-0.49780300	4.15117000

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C	3.98050000	7.73084100	-1.08300000	N	1.05292300	4.10511200	3.97934800
C	3.27310100	6.64583600	-0.34854500	C	0.75940400	3.09562500	3.09375900
N	2.48051300	6.85552500	0.77054800	O	-0.48190100	2.88136100	2.91337800
C	3.20770400	5.29851500	-0.56999800	O	1.74484400	2.51198600	2.54052900
C	1.97838200	5.66498700	1.17799000	C	-3.82548800	3.33309200	4.10774000
N	2.39706400	4.69816100	0.37654400	C	-4.13183900	2.08148200	3.34321800
C	7.41381400	0.73532800	0.04142800	N	-3.34833800	1.62086800	2.28858500
C	6.05860100	1.13878800	0.50207400	C	-5.17481000	1.21031000	3.52093100
N	5.68523000	1.10148900	1.83718800	C	-3.91917600	0.50887500	1.84057800
C	4.95218700	1.60424900	-0.15622500	N	-5.02980400	0.23341200	2.55496200
C	4.41013100	1.52780000	1.94714900	C	-2.13305000	5.84677500	-2.77824300
N	3.93419100	1.84173000	0.75160300	C	-2.35256900	5.04468000	-1.54078600
C	-0.00885800	4.64861000	4.79307900	N	-3.45790400	5.18603500	-0.71326500

C	-1.60486700	4.05770400	-0.95629300	C	0.93937200	-5.36925700	-1.18298300
C	-3.34589900	4.30528600	0.31034000	C	-0.33248700	-5.51164500	-0.34813000
N	-2.22767900	3.60943100	0.19213100	O	-1.46306900	-5.32456900	-0.79860100
C	2.05056000	4.12651300	-3.62351100	N	-0.12661800	-5.88105700	0.94160200
C	1.69101400	2.98305800	-2.67546000	N	1.94219400	-3.86064600	-4.44067200
O	2.48880600	2.68053400	-1.75330900	C	2.79309100	-2.86436100	-5.08373700
O	0.54488700	2.44298500	-2.88498200	H	6.31325000	-3.83026800	3.15336600
Zn	2.11872000	2.66287000	0.41134500	H	6.02525900	-4.93994500	1.82910100
Zn	-1.50375400	2.12432100	1.41116500	H	3.89522900	-3.55047900	3.52196000
H	3.28326900	8.47424000	-1.48904800	H	5.03946500	-2.03827800	1.93800400
H	4.69687600	8.26188100	-0.44409200	H	3.41976500	-2.39907700	1.31001600
H	3.67595700	4.71273800	-1.34291900	H	4.83804900	-3.20315300	0.61919800
H	2.31118700	7.74605400	1.21817200	H	2.22603400	-4.46949300	2.02832800
H	1.36261900	5.53565700	2.05635800	H	3.45655100	-5.42140600	1.13825800
H	7.50424900	0.88828400	-1.03684900	H	3.07057500	-5.80475000	2.82874900
H	7.61387400	-0.32431500	0.24201000	H	5.13646800	-6.66561400	3.40957400
H	4.80480500	1.78207800	-1.21003400	H	5.71195900	-1.04866400	-1.88064400
H	6.25837400	0.76823900	2.60039700	H	4.77974900	-1.47528400	-3.31708200
H	3.85970300	1.59167500	2.86975700	H	4.80864600	-3.67698700	-2.22948800
H	-2.79441300	3.31995000	4.47426500	H	7.84397200	-1.08966000	-3.27411700
H	-5.98603700	1.20112900	4.23236000	H	1.62847500	-4.69607600	-0.66033400
H	-5.59526800	-0.59807600	2.45244000	H	1.44144500	-6.34410400	-1.22221300
H	-3.56229600	-0.08647100	1.01179200	H	0.80116700	-5.85400900	1.34137200
H	-1.25121500	5.46912900	-3.30160700	H	-0.90673000	-5.81386300	1.58419000
H	-2.98194700	5.77557300	-3.46906300	H	-0.20284700	-4.17977800	-2.57185800
H	-0.68892500	3.60877900	-1.30325600	H	3.84548700	-3.06113000	-4.86132700
H	-4.22732100	5.82638500	-0.85510400	H	2.52892500	-1.86041900	-4.73604300
H	-4.08413300	4.18816400	1.08865800	H	1.25050700	-4.33235600	-5.00582700
H	-0.79026400	5.07184600	4.15863600	H	0.46145000	-5.62791800	-3.29587100
H	1.48591300	4.05387600	-4.55491200	H	2.64259700	-2.92504000	-6.16329400
H	1.80877100	5.07843300	-3.13634800	H	6.87711000	-1.46074800	-4.70774100
H	8.20101000	1.32425900	0.52827700	H	6.67811200	0.09863100	-3.88513800
H	-3.93802200	4.23203300	3.48779000	H	5.28957300	-5.53405400	4.76122200
H	-4.49972600	3.43366500	4.96279900	H	6.73428500	-6.11787500	3.92169900
H	0.39809800	5.44666200	5.42155600	C	-4.84700900	-5.05169200	6.13102300
H	-0.47200400	3.89622100	5.44441000	C	-3.33898700	-4.88620900	5.88520300
H	4.53756600	7.30558700	-1.92143000	C	-3.01013000	-4.14598700	4.60517100
H	3.12329500	4.11913300	-3.83345300	C	-2.53321200	-2.83158900	4.62097200
H	-1.97061400	6.90989000	-2.55974500	C	-3.17537800	-4.75959800	3.35294300
H	1.99467000	4.09633600	4.34648600	C	-2.20235900	-2.15353000	3.44545300
C	5.69623100	-5.79860400	3.77668000	C	-2.85391000	-4.10176000	2.16800600
C	5.62689100	-4.61540300	2.80248700	C	-2.34028500	-2.79694700	2.21211200
C	4.25004800	-3.97751100	2.57281200	O	-1.98110800	-2.22426000	1.02354900
C	4.39149300	-2.83646000	1.55291900	H	-2.87238000	-5.88032400	5.86322100
C	3.18900600	-4.98527100	2.11099300	H	-2.88952800	-4.35776900	6.73505300
C	6.85306800	-0.97321500	-3.72809000	H	-2.39054200	-2.32858000	5.57524900
C	5.75991300	-1.56750400	-2.84347500	H	-3.55785400	-5.77771500	3.30357100
S	6.08352100	-3.36271000	-2.54769000	H	-1.79453100	-1.14741000	3.48777300
C	0.68632300	-4.82269300	-2.58771600	H	-2.96483200	-4.58755600	1.20261100
C	1.84057300	-3.96560500	-3.09881700	H	-1.66854800	-1.28365000	1.11230400
O	2.61520600	-3.36378600	-2.33729300	H	-5.34234000	-4.07647700	6.20630900

H	-5.32404900	-5.60299400	5.31263300	H	-4.57239500	2.06871300	-1.88454700
H	-5.03641900	-5.60071400	7.06058000	H	-5.61646300	1.29086600	-0.69575800
N	-0.29453300	0.33956200	-1.43976000	H	-6.42586800	2.60617100	-3.32537000
C	0.43358500	-0.80322900	-1.89778300	H	-7.32874400	2.58018900	-1.80729500
O	0.21855300	-1.36752800	-2.96421700	H	-8.12269700	0.89564700	-3.78830200
N	1.38724100	-1.09826800	-0.99109500	H	-7.98472000	0.24710100	-2.14708200
C	0.02592300	0.56377000	0.08035400	H	-6.55979300	-1.27027100	-3.27726300
O	-1.06119100	0.30140200	0.83677300	H	-5.43388900	1.05029200	-4.95845300
H	-1.31466900	0.22831800	-1.57923200	H	-4.98700200	-0.66703500	-5.11910500
H	1.97909600	-1.91364900	-1.16746000	H	-6.61587200	-0.14019800	-5.53125900
O	0.38061500	1.88120900	0.21048800	H	-4.63235800	-2.18504600	-3.50574300
H	0.18319500	1.42848400	-2.15833200	H	-2.83563000	-4.70961100	-1.89993400
C	-1.23084200	-2.13137500	-5.56536800	H	-4.66221200	-2.97024400	-1.14346700
C	-2.62233500	-2.11244800	-4.96643400	H	-2.91026200	-2.75233900	-1.04986000
O	-3.63480000	-2.32162700	-5.62998000	H	-1.73419100	-1.69366000	-3.18018800
N	-2.63205000	-1.83656800	-3.63176000	H	-1.31710800	-2.07705600	-6.65239800
C	-3.83084400	-1.90519700	-2.82394000	H	-0.61072600	-1.31790700	-5.18567500
C	-4.06493900	-0.53505100	-2.17838700	H	-0.73262000	-3.07039100	-5.29979900
O	-3.19738700	-0.04947400	-1.42282000	C	1.20909300	-0.48851500	0.31558900
C	-3.72886300	-2.99334500	-1.73514600	C	1.28637200	-1.52585800	2.63179700
O	-3.55976500	-4.24520900	-2.35656900	O	1.08729900	-2.51476900	3.32900500
N	-5.21929100	0.12205700	-2.40598400	N	0.95140200	-1.51927200	1.28883100
C	-6.27098900	-0.22233300	-3.39906800	N	1.92413200	-0.39186700	3.11334800
C	-5.78608100	0.01969800	-4.83199300	H	2.11164600	0.03751700	0.63107200
C	-7.42309100	0.70648400	-2.96958800	H	0.24295800	-2.20640300	1.05203700
C	-6.70857800	1.97517300	-2.47570200	H	1.62945500	0.52695000	2.78626000
C	-5.45493700	1.43203100	-1.77250100	H	2.02801200	-0.44869100	4.11923200

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C	-5.95657800	-6.49363600	-1.33397500	N	4.86066300	-1.84588600	2.65501300
C	-5.01922400	-5.66085000	-0.53042800	C	0.45567600	-6.22765200	-2.94992800
N	-4.37242400	-6.08852300	0.62074400	C	0.95347000	-5.53308400	-1.72870400
C	-4.57403100	-4.38438400	-0.72203000	N	1.97996400	-6.01342500	-0.92694400
C	-3.57935100	-5.08547400	1.07164500	C	0.55741700	-4.36523200	-1.13417700
N	-3.67296700	-4.03618100	0.26980200	C	2.17054000	-5.15059300	0.09621400
C	-7.44820600	1.11891600	0.01261300	N	1.31567300	-4.14162800	0.00061500
C	-6.21858000	0.40144100	0.45736800	C	-3.12086400	-3.44434900	-3.74865000
N	-5.80086300	0.38041300	1.78118100	C	-2.44658400	-2.57526300	-2.69594500
C	-5.28511600	-0.34523600	-0.21134700	O	-3.22525400	-2.08767600	-1.78883700
C	-4.66992100	-0.35119000	1.87391600	O	-1.21136500	-2.43956400	-2.75274800
N	-4.32901500	-0.80803900	0.67881000	Zn	-2.87290600	-2.12728900	0.18688000
C	-1.36481400	-4.75154800	4.65136400	Zn	1.02638100	-2.70692500	1.37608200
N	-2.13795900	-3.84388800	3.82699600	H	-5.47074600	-7.39477200	-1.72851400
C	-1.53451400	-3.00732000	2.91860800	H	-6.82894400	-6.81516300	-0.75158800
O	-0.29153200	-3.23935400	2.71154700	H	-4.81647700	-3.68875500	-1.50700800
O	-2.25976600	-2.12467400	2.36630100	H	-4.47565100	-6.99432100	1.05768500
C	2.67063600	-4.46280300	4.01993400	H	-2.98610500	-5.13953600	1.97282800
C	3.40157200	-3.34787600	3.33366500	H	-7.60314400	0.96318900	-1.05774700
N	2.86870400	-2.65726600	2.24819400	H	-7.37167700	2.19965200	0.18251100
C	4.64538300	-2.83667200	3.59436400	H	-5.21669800	-0.58457600	-1.26132900
C	3.77471200	-1.76224500	1.86142400	H	-6.24172400	0.87399200	2.54557000

H	-4.12111500	-0.51938700	2.78520700	H	-3.77074500	4.76666200	-2.09086400
H	1.66309400	-4.14813500	4.30726000	H	-7.35604000	3.08381000	-3.24957900
H	5.37594300	-3.08274100	4.34920100	H	-0.30224600	4.61104400	-0.46047100
H	5.66752400	-1.23949800	2.59602900	H	-0.29154100	6.32779700	-0.78036900
H	3.69815300	-1.09485600	1.00746600	H	0.62894000	6.12706300	1.49367700
H	-0.27350100	-5.58564000	-3.45027000	H	2.32845400	5.90371900	1.65158500
H	1.26255500	-6.43419200	-3.66343100	H	1.24010100	4.39818300	-2.57925700
H	-0.18116400	-3.65451300	-1.47966800	H	-2.96533900	3.99557000	-4.79508000
H	2.51458600	-6.85612300	-1.08946200	H	-2.01081800	2.50171400	-4.62589800
H	2.92229600	-5.27487900	0.86063100	H	-0.15364800	4.62096400	-4.85447000
H	-0.74999500	-5.39699400	4.02069900	H	0.60481300	5.98127400	-3.01666500
H	-2.50187100	-3.51075500	-4.64598600	H	-1.79040700	3.54664800	-6.05219500
H	-3.25400100	-4.45549600	-3.34338100	H	-6.29359200	3.25617800	-4.65268000
H	-8.34115500	0.75646200	0.53647900	H	-6.51678200	1.66404800	-3.90149500
H	2.56515100	-5.33995500	3.36852800	H	-3.75231500	6.46429800	4.92518700
H	3.20949300	-4.77908000	4.91722500	H	-5.05256900	7.39309800	4.16359700
H	-2.05238200	-5.37701700	5.22755600	C	5.83188100	3.29261000	6.32251700
H	-0.70274600	-4.22690900	5.35266000	C	4.42565300	3.80013900	5.97002900
H	-6.32178300	-5.91374400	-2.18501100	C	3.90696600	3.22996600	4.66844000
H	-4.11182800	-3.05994000	-4.00891000	C	3.23231900	2.00490500	4.63415000
H	-0.03232100	-7.18123500	-2.71201700	C	4.11527100	3.89347900	3.45036500
H	-3.03456600	-3.52425400	4.16646300	C	2.75574700	1.46694500	3.43856000
C	-4.11970000	6.85307900	3.96671800	C	3.64664300	3.37590700	2.24515800
C	-4.35207600	5.72420000	2.95406200	C	2.94420400	2.16598900	2.24324600
C	-3.16150500	4.80278100	2.65459100	O	2.44244300	1.73241800	1.04321700
C	-3.59181000	3.75552800	1.61617400	H	4.44257600	4.89565100	5.91107700
C	-1.92039900	5.56640000	2.17286100	H	3.73545400	3.54633600	6.78489900
C	-6.41694500	2.73750900	-3.69676400	H	3.05288300	1.46806100	5.56377200
C	-5.22913300	2.99504900	-2.77284300	H	4.65424000	4.83941600	3.44661300
S	-5.08775700	4.79854600	-2.39354300	H	2.19522200	0.53509700	3.43846200
C	0.39727200	5.07975500	-2.42721700	H	3.79443600	3.89933700	1.30472900
C	-0.85948800	4.39088600	-2.95823300	H	2.06880000	0.83264500	1.12018400
O	-1.75013500	3.93738000	-2.22541700	H	5.84142600	2.20061000	6.42185700
C	0.27878800	5.40567200	-0.94297100	H	6.55335400	3.56070300	5.54217400
C	1.61300400	5.50383700	-0.21190200	H	6.18245600	3.72068600	7.26891800
O	2.69196900	5.14430500	-0.68486900	N	0.48123400	-0.23208200	-2.07850400
N	1.52833800	6.02227500	1.04394900	C	0.09616900	1.03914000	-1.81700600
N	-0.93614200	4.29211000	-4.30673800	O	0.67515600	2.04305900	-2.25112100
C	-1.98825400	3.53853900	-4.97842900	N	-1.04553700	1.16451400	-1.00566600
H	-5.18663400	5.10092700	3.30876000	C	-0.31053400	-0.67307600	0.48939500
H	-4.69660900	6.16621100	2.00688900	O	0.82687800	-0.72990700	1.05272600
H	-2.87999100	4.27885700	3.57971700	H	1.33831900	-0.32811100	-2.61001800
H	-4.42915300	3.15165000	1.99081100	H	-1.39936600	2.12141500	-1.07007700
H	-2.77249400	3.07775900	1.36355600	O	-0.89713600	-1.72811500	0.11377500
H	-3.92368100	4.23980800	0.68884400	H	-0.20768500	-0.98891700	-2.15694200
H	-1.09218900	4.86275400	2.03679200	C	1.70790800	1.79082600	-5.47358100
H	-2.11969500	6.07833000	1.22161200	C	3.06377300	1.40452400	-4.89767200
H	-1.60418400	6.31902800	2.90444800	O	4.04409800	1.24586600	-5.61888800
H	-3.38943200	7.58478500	3.60471400	N	3.07731800	1.20193300	-3.53939700
H	-5.33665000	2.43956500	-1.83573200	C	4.33774300	1.20355500	-2.80064500
H	-4.29322800	2.67654400	-3.23718900	C	4.50341300	-0.09644900	-1.98968700

O	3.79713300	-0.30276600	-0.98774300	H	6.21640900	-1.60519500	-5.65011200
C	4.37052000	2.40266400	-1.83115000	H	5.12779500	1.31621500	-3.54379100
O	4.14412700	3.58536900	-2.56809500	H	3.66631000	4.20577300	-1.98526700
N	5.45157100	-0.99471700	-2.35490300	H	5.35692700	2.41570300	-1.33423700
C	6.30518700	-1.01299700	-3.57064600	H	3.61251200	2.25023000	-1.05579400
C	5.53136900	-1.50198000	-4.79999100	H	2.28213300	1.60336200	-3.03622200
C	7.43783300	-1.96360500	-3.13956300	H	1.33056500	0.96319200	-6.08489700
C	6.72172000	-3.00993100	-2.26965900	H	0.97056600	2.04106200	-4.70840400
C	5.65607500	-2.19111300	-1.52208900	H	1.85820400	2.64206500	-6.14493600
H	4.71224900	-2.72928400	-1.38127100	C	-1.03643400	0.68431800	0.37165400
H	5.99960700	-1.88239600	-0.52566500	C	-0.81173900	1.78827600	2.63078600
H	6.24654800	-3.76801200	-2.90194600	O	-0.37278900	2.70319000	3.31540300
H	7.39767900	-3.53098800	-1.58497100	N	-0.52399200	1.69043700	1.27853500
H	7.95796500	-2.39906000	-3.99733800	N	-1.69183500	0.83902300	3.14577000
H	8.17571900	-1.41592200	-2.54098800	H	-2.07123300	0.49096900	0.67058300
H	6.69506900	-0.01032400	-3.76251600	H	0.33177300	2.16796500	1.00746300
H	5.06988800	-2.47922100	-4.61456600	H	-1.65120200	-0.12548500	2.82425300
H	4.76337400	-0.78314900	-5.08988200	H	-1.75076900	0.92674400	4.15301600

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C	-8.94325400	-0.22292400	-1.99904900	C	-3.60711100	0.03814600	-2.85225200
C	-7.79232600	-0.30015700	-1.05821800	O	-3.92054000	0.92811300	-1.97962200
N	-7.78151400	-1.02889100	0.12305500	O	-2.61450900	-0.71902800	-2.78249200
C	-6.54757700	0.25540200	-1.13305200	Zn	-3.79552600	0.50790000	0.09547300
C	-6.56112300	-0.89353000	0.70201900	Zn	-1.76402900	-2.21502300	1.17101100
N	-5.78488500	-0.12488800	-0.04404600	N	0.99558600	-0.12361000	-0.42751700
C	-4.62359000	6.11668400	-0.22729300	C	1.37019200	1.05358900	-1.11470600
C	-4.30894700	4.73242100	0.24833300	O	2.15455300	0.97315200	-2.06220400
N	-3.98709900	4.44347900	1.56796600	N	0.83495400	2.19486500	-0.65854400
C	-4.24301900	3.52069200	-0.39174600	C	-0.25389100	2.24187500	0.31354200
C	-3.74853600	3.11462600	1.68000100	C	-0.08071600	1.13624400	1.35566900
N	-3.89151900	2.52732000	0.50450400	C	0.30305300	-0.17939800	0.73516500
C	-5.06823900	-2.35627600	4.35520600	O	0.10373800	-1.28023300	1.28339500
N	-4.90012600	-1.14052600	3.58396000	H	-9.21498600	-1.20750400	-2.40052100
C	-3.79416000	-0.94030000	2.78272200	H	-9.83959100	0.20010700	-1.52790400
O	-3.03851900	-1.96324000	2.63258500	H	-6.12542400	0.88693200	-1.89572800
O	-3.65559800	0.20040500	2.25447600	H	-8.55028000	-1.56856900	0.49608900
C	-2.02104100	-5.06668200	3.98747000	H	-6.28496600	-1.33474700	1.64955800
C	-0.71278700	-4.79754300	3.30850200	H	-4.94463700	6.08541100	-1.27157300
N	-0.53291000	-3.86426200	2.28719300	H	-3.74870000	6.77498000	-0.16528300
C	0.48675200	-5.40986400	3.57018100	H	-4.41561400	3.27649800	-1.42850200
C	0.74656100	-3.93388000	1.94847200	H	-3.92572000	5.11549000	2.32040900
N	1.39880300	-4.85408700	2.69659000	H	-3.49937400	2.60597100	2.59859000
C	-4.18431400	-4.66063600	-3.20662700	H	-2.46531800	-4.13682700	4.35529200
C	-3.44664800	-4.51330300	-1.92393300	H	0.76158200	-6.16658700	4.28891700
N	-3.09627100	-5.54539200	-1.06384000	H	2.39115000	-5.04033700	2.66219700
C	-2.97531600	-3.38232400	-1.32455400	H	1.23251900	-3.34311500	1.18689600
C	-2.43975700	-5.01269300	-0.00275800	H	-4.23663300	-3.68496500	-3.69571600
N	-2.35335800	-3.69813900	-0.13329500	H	-3.68589000	-5.35226600	-3.89758000
C	-4.57786400	-0.14950500	-4.02587600	H	-3.01717500	-2.37584400	-1.70783500

H	-3.28799700	-6.52842700	-1.20044400	C	4.74322800	-0.74019800	6.55343000
H	-2.04534800	-5.59263000	0.81703500	C	4.51838700	-0.66953400	5.05637000
H	-4.97660200	-3.22386800	3.69917500	C	3.43397600	-1.32129400	4.45454700
H	-4.07332800	-0.62719900	-4.86881400	C	5.39711500	0.03158300	4.21736000
H	-5.39976300	-0.79873300	-3.69849800	C	3.22449300	-1.27762200	3.07547800
H	-1.21607400	2.13590500	-0.19782800	C	5.20821300	0.08019800	2.83653500
H	-0.23001500	3.22207100	0.79198300	C	4.11634700	-0.57516100	2.25651400
H	-0.99749800	0.98609200	1.92870900	O	3.93986300	-0.44984400	0.90353000
H	0.72865900	1.39565900	2.05301900	H	5.28500100	0.15513300	6.88336900
H	-5.43432100	6.57153600	0.35485100	H	3.77450400	-0.72137000	7.06990200
H	-2.75037900	-5.52074000	3.30413300	H	2.72250500	-1.86051600	5.07758900
H	-1.87925400	-5.74984800	4.82958300	H	6.25126600	0.54708300	4.65185200
H	-6.06664600	-2.35641500	4.80292500	H	2.34655500	-1.74549400	2.64046300
H	-4.32710700	-2.45889300	5.15969000	H	5.90135800	0.61336200	2.19234700
H	-8.67997000	0.41814200	-2.84401600	H	3.49279200	-1.23159600	0.51457300
H	-5.01302100	0.80346300	-4.34211800	H	4.99079900	-2.90693600	6.71792500
H	-5.20985200	-5.02373300	-3.05975600	H	6.51232600	-2.02457800	6.53003300
H	-5.33590700	-0.29184200	3.91752700	H	5.66120800	-1.99917700	8.08649000
H	1.41449100	-0.99070500	-0.77084500	C	2.70367200	0.01230500	-5.13402300
H	1.11537500	3.03574100	-1.16240300	C	3.45430100	-1.19857000	-4.61688000
O	-2.26329000	-0.67645300	-0.03146900	O	3.91633700	-2.04535600	-5.37889600
H	-2.11279300	-0.74142700	-1.00162200	N	3.54473800	-1.27233000	-3.25920300
C	-2.41302700	6.50775700	-3.74911500	C	4.33626300	-2.29309100	-2.60217500
C	-1.99078000	5.27145100	-2.95927800	C	3.39675400	-3.11401400	-1.71030500
S	-0.96773300	5.62608600	-1.46109700	O	2.84537800	-2.58036700	-0.71129100
C	4.61140000	3.69855400	-2.72865000	C	5.51139300	-1.68373300	-1.80627100
C	3.13174000	3.92585300	-3.03021400	O	6.31033300	-0.94835800	-2.70210200
O	2.34373800	4.29040600	-2.14534600	N	3.13255800	-4.39574700	-2.02271600
C	4.82930600	2.46938200	-1.81531800	C	3.68044400	-5.22267200	-3.14185500
C	6.20782500	2.40024600	-1.16952500	C	2.91269500	-5.02916100	-4.45943300
O	6.99126000	1.47163800	-1.36340600	C	3.54206200	-6.64446800	-2.56446200
N	6.53328200	3.43774000	-0.34725700	C	2.22500000	-6.58789100	-1.77467700
N	2.72884200	3.73737700	-4.30600800	C	2.24070600	-5.18438500	-1.15009100
C	1.33241900	3.87071400	-4.70589400	H	1.25117800	-4.72061000	-1.09196400
H	-2.86372200	4.74148300	-2.57043000	H	2.65582300	-5.19183700	-0.13524200
H	-1.44745300	4.55851900	-3.58529500	H	1.37000700	-6.69607500	-2.45047800
H	0.23213000	5.72141000	-2.07232100	H	2.14673300	-7.37272500	-1.01670000
H	-2.97047800	7.20857300	-3.11970900	H	3.54231800	-7.40539900	-3.34957400
H	4.69833800	1.54631800	-2.38025100	H	4.37944300	-6.85684100	-1.88881600
H	4.07348600	2.47439700	-1.02321800	H	4.73212800	-4.96870400	-3.29258400
H	5.84100300	4.09731700	-0.02180700	H	1.84316300	-5.23068800	-4.33012000
H	7.40217700	3.37511700	0.16638500	H	3.04428700	-4.01692400	-4.84934600
H	5.19933400	3.59002200	-3.64706800	H	3.30393400	-5.72820000	-5.20747600
H	0.97899700	4.89010100	-4.52255900	H	4.75401100	-2.89652500	-3.40741700
H	0.70243800	3.17041100	-4.14806400	H	6.61067300	-0.13175600	-2.25323900
H	3.39290400	3.38368200	-4.97924300	H	6.07803600	-2.51304800	-1.34551800
H	4.96098800	4.60960500	-2.23082900	H	5.13107600	-1.05905200	-0.99160500
H	1.25268300	3.65415200	-5.77256900	H	3.14277000	-0.52251300	-2.69941000
H	-1.54541500	7.04187200	-4.15107600	H	1.83066600	-0.33117700	-5.69964100
H	-3.05229600	6.21788400	-4.59283600	H	2.37882800	0.69359200	-4.34659100
C	5.52272500	-1.99063700	6.99933200	H	3.35381700	0.53687300	-5.84312700

C	1.42284500	7.64667800	4.31818500	C	2.61949300	4.43719000	1.35665800
H	2.28920100	7.47899100	4.96740300	C	2.96005800	3.31347900	3.46965500
C	0.67469200	6.32990100	4.04988000	H	1.94842600	4.17379300	5.16550100
H	0.29615800	5.92882600	4.99849500	H	2.77868800	4.50822100	0.28351000
H	-0.20424600	6.54083400	3.42527600	C	3.20217300	3.40330800	2.09698800
C	1.54120500	5.29085800	3.36913700	H	3.40999100	2.51004600	4.04680400
C	1.79729000	5.36933200	1.99233600	H	3.82992600	2.66054100	1.61130300
C	2.13534900	4.25099200	4.09625800	H	0.76836800	8.37793900	4.80620200
H	1.34355700	6.16941100	1.40997900	H	1.78823600	8.08863000	3.38469200

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C	-8.76666800	1.34644900	-1.22411100	C	-0.14195500	2.43017200	-0.11525200
C	-7.54608600	0.92295600	-0.48523800	C	-0.08308700	1.38998200	0.99949300
N	-7.50574800	-0.07518300	0.47936700	C	-0.10516800	-0.02017800	0.45925000
C	-6.25525800	1.35410800	-0.59053500	O	-0.04005500	-1.01761700	1.28852500
C	-6.22529000	-0.20579100	0.91031200	H	-9.20423500	0.52411500	-1.80408100
N	-5.44069800	0.64595400	0.27329900	H	-9.54666100	1.73076800	-0.55482600
C	-3.21330200	6.80460900	-0.05886400	H	-5.83926200	2.09693200	-1.24990200
C	-3.21608200	5.39507500	0.43506000	H	-8.29419700	-0.61378100	0.81083200
N	-3.00647500	5.06061000	1.76599600	H	-5.91338800	-0.90741100	1.66873200
C	-3.38542900	4.19165900	-0.19956200	H	-3.48057800	6.82637400	-1.11828800
C	-3.05105100	3.71327800	1.89037800	H	-2.22458800	7.26827200	0.04479400
N	-3.27560000	3.15588700	0.71222500	H	-3.56480200	3.98287000	-1.24299200
C	-4.72902900	-1.39341600	4.78705200	H	-2.83085700	5.71328200	2.51774700
N	-4.44553300	-0.23316800	3.96935100	H	-2.92273100	3.17218800	2.81477000
C	-3.53089200	-0.27770600	2.95217000	H	-2.60985700	-3.65107000	4.58907900
O	-3.12007100	-1.44914500	2.63842900	H	0.41530300	-5.94975400	4.43936200
O	-3.21649200	0.81639400	2.39278400	H	2.06371100	-5.03868600	2.70241100
C	-2.27650900	-4.62061700	4.20630300	H	0.99097500	-3.31569400	1.18570800
C	-0.97524200	-4.49162900	3.46941300	H	-4.93768800	-2.95769300	-3.29658100
N	-0.75232100	-3.61889700	2.40243000	H	-4.78672300	-4.71166200	-3.45192000
C	0.17666100	-5.19705800	3.70385200	H	-3.20373500	-1.89100400	-1.53924900
C	0.50176900	-3.81491400	2.01061100	H	-4.36305600	-5.84325300	-0.74615100
N	1.09477500	-4.75969000	2.77073500	H	-2.74798000	-5.14048300	1.09412300
C	-5.03679400	-3.90165900	-2.75527300	H	-4.97760500	-2.24689500	4.15284900
C	-4.13765000	-3.87508100	-1.57145100	H	-4.38009300	-0.02015700	-4.51089100
N	-3.94585300	-4.92460100	-0.68360600	H	-5.58488900	0.15984100	-3.21165600
C	-3.35788900	-2.86160000	-1.09291600	H	-1.14333300	2.47992000	-0.55301200
C	-3.08173100	-4.51773800	0.27850100	H	0.10851400	3.41827500	0.27882600
N	-2.71175100	-3.26591000	0.05792700	H	-0.89406100	1.50405900	1.71900200
C	-4.68477400	0.59607500	-3.66237300	H	0.86756400	1.48947100	1.53924300
C	-3.58234000	0.63861900	-2.60201800	H	-3.93759100	7.42726300	0.48031400
O	-3.64601500	1.58252000	-1.73186500	H	-3.07719300	-5.00242200	3.56005600
O	-2.72374100	-0.27270700	-2.60135600	H	-2.16709900	-5.31062400	5.04740800
Zn	-3.41569600	1.13522100	0.31106500	H	-5.58551600	-1.17231900	5.43042900
Zn	-1.76462200	-2.00274000	1.34416500	H	-3.88180500	-1.67913600	5.42510500
N	0.56168000	-0.19221000	-0.74137800	H	-8.50818600	2.14473500	-1.92405700
C	1.15657000	0.83014900	-1.47880300	H	-4.94416300	1.60249900	-4.00459800
O	1.96836600	0.56345900	-2.37748000	H	-6.09069500	-4.02305900	-2.47328700
N	0.82972500	2.09355400	-1.14647300	H	-4.66095200	0.68709600	4.32382700

H	0.85886900	-1.14938100	-0.97304400	C	2.35772200	-0.59254800	-5.46938700
H	1.36944400	2.81321600	-1.62244900	C	2.79047700	-1.91058200	-4.84886400
O	-1.95211300	-0.19606700	0.00065300	O	3.21632800	-2.83579500	-5.53816700
H	-1.98563600	-0.28524300	-0.99025300	N	2.62927500	-1.96691000	-3.50123600
C	-1.33098500	6.74578700	-3.78662800	C	3.10263700	-3.07622700	-2.69868500
C	-0.60110700	5.75621300	-2.88218800	C	1.90287200	-3.69388600	-1.96944900
S	0.86471800	6.54462900	-2.06376700	O	1.27338400	-3.02106900	-1.12424400
C	4.72775300	2.14985400	-3.00156700	C	4.16596100	-2.61004300	-1.68489800
C	3.46243100	2.94794300	-3.32175100	O	5.25673200	-2.09274600	-2.40729300
O	2.91291400	3.68632500	-2.48898700	N	1.53409400	-4.96119700	-2.24410300
C	4.96352400	2.04560700	-1.48706900	C	2.13091800	-5.90232700	-3.23278700
C	6.27083400	1.34403300	-1.14816700	C	1.71449200	-5.57928600	-4.67323200
O	6.38037100	0.11904500	-1.07354800	C	1.59540700	-7.25855900	-2.73190800
N	7.34168300	2.15678700	-0.94935700	C	0.19293200	-6.92378200	-2.19925100
N	3.00859500	2.84191000	-4.58971200	C	0.38040700	-5.54979400	-1.53965400
C	1.75919800	3.45629500	-5.02266500	H	-0.49075600	-4.89370200	-1.62609000
H	-1.27001500	5.37163100	-2.10615700	H	0.61386600	-5.63725600	-0.47066400
H	-0.24476500	4.90017400	-3.45889900	H	-0.52134300	-6.85587600	-3.02697100
H	1.72330100	5.51473300	-2.23281000	H	-0.18611700	-7.67167700	-1.49603100
H	-1.66188100	7.62958000	-3.22908300	H	1.58880000	-8.01236700	-3.52400800
H	4.15493500	1.45911700	-1.04556800	H	2.22746000	-7.63247800	-1.91703800
H	4.93603300	3.04564500	-1.04578100	H	3.22096100	-5.86847400	-3.15069200
H	7.25470000	3.16001800	-0.89001900	H	0.62276500	-5.56787700	-4.77555900
H	8.22632100	1.73425200	-0.70166800	H	2.11422700	-4.61947600	-5.00867500
H	4.65260200	1.14511500	-3.43228200	H	2.10847300	-6.35186400	-5.34456800
H	1.75923400	4.51600000	-4.75811000	H	3.57039900	-3.77701900	-3.38953500
H	0.89387900	2.96855700	-4.55773200	H	5.62571200	-1.33483200	-1.91365600
H	3.40266700	2.11635900	-5.17225200	H	4.46108000	-3.47999600	-1.06940000
H	5.57674700	2.64818800	-3.48983800	H	3.72169800	-1.87268600	-1.00506800
H	1.68058700	3.36260400	-6.10765000	H	2.35910400	-1.11318900	-3.01208000
H	-0.68299000	7.09117400	-4.59775000	H	1.56593600	-0.79123500	-6.19951900
H	-2.21816700	6.27469800	-4.22820400	H	2.00189800	0.13182800	-4.73496200
C	5.96242700	-2.94862900	6.38944800	H	3.20677400	-0.18409200	-6.03091400
C	5.67585500	-1.46169500	6.12571000	C	3.44830100	7.26327400	3.85576900
C	4.88589200	-1.26866000	4.85199400	H	4.33174900	6.83931800	4.34565300
C	3.48759700	-1.33212700	4.85546100	C	2.26498700	6.28471400	3.92190400
C	5.53099200	-1.11117500	3.61646900	H	1.99627000	6.10423500	4.97021800
C	2.75201800	-1.25873000	3.67245500	H	1.38963400	6.74807600	3.44640600
C	4.81764400	-1.03600800	2.42353600	C	2.59140500	4.97523700	3.23985100
C	3.42040900	-1.11940100	2.44973700	C	2.60700900	4.89625400	1.84019400
O	2.75686800	-1.04898600	1.25993000	C	2.95964500	3.84272500	3.97651700
H	6.62477000	-0.91396700	6.06593200	H	2.32216900	5.76580600	1.25030300
H	5.12598700	-1.04104500	6.97747900	C	2.99357500	3.72321300	1.19289800
H	2.96006300	-1.44320600	5.80116700	C	3.34129900	2.66159900	3.33634200
H	6.61701500	-1.05065800	3.58714200	H	2.95416500	3.88938600	5.06382900
H	1.66511800	-1.29162900	3.69174400	H	3.00657100	3.68934000	0.10745000
H	5.32272200	-0.90809200	1.46990200	C	3.36276100	2.60049300	1.94146500
H	1.78954800	-1.12813300	1.40756900	H	3.62346600	1.79050300	3.92100100
H	5.02873100	-3.51524700	6.48453000	H	3.65661500	1.67964900	1.44650000
H	6.53502800	-3.38817000	5.56488800	H	3.20677100	8.21117700	4.35075500
H	6.53746100	-3.08645300	7.31283400	H	3.71770500	7.48301100	2.81700600

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C	-8.68212400	1.68279000	-1.22991900	H	-5.87637300	-0.86685500	1.46166800
C	-7.47610500	1.17739000	-0.51997700	H	-3.23108200	6.97206000	-0.99972800
N	-7.45414900	0.09540000	0.35051900	H	-1.94192800	7.34386600	0.15073200
C	-6.18070400	1.60222400	-0.57527900	H	-3.45573500	4.15729200	-1.16245200
C	-6.17866600	-0.08958100	0.77629400	H	-2.56347600	5.77911400	2.61166600
N	-5.38057200	0.80810500	0.22467800	H	-2.76846000	3.24125500	2.86812700
C	-2.95223300	6.92722900	0.05592500	H	-2.79778900	-3.60410000	4.33396000
C	-3.01351200	5.51670200	0.53428300	H	0.28225800	-5.94746600	4.52309300
N	-2.79241200	5.14951100	1.85443400	H	2.00663200	-5.06964200	2.84506300
C	-3.25298100	4.33645600	-0.11790000	H	1.00220100	-3.38362900	1.23375600
C	-2.89881400	3.80448300	1.95714400	H	-4.98893100	-2.70076900	-3.36049600
N	-3.17586400	3.28222700	0.77417000	H	-4.89463300	-4.45250300	-3.57143400
C	-4.75992000	-1.30632700	4.73874400	H	-3.21448200	-1.76478500	-1.52208600
N	-4.39289300	-0.16916000	3.92094900	H	-4.55106600	-5.69815600	-0.93188800
C	-3.53966000	-0.26945800	2.85822600	H	-2.93392800	-5.15323100	0.95732400
O	-3.24694100	-1.45923800	2.48557300	H	-5.07579500	-2.13635400	4.10333000
O	-3.16254500	0.81343500	2.31047100	H	-4.33111200	0.21846700	-4.51928100
C	-2.41543400	-4.60269100	4.10288000	H	-5.54385800	0.44512800	-3.23323100
C	-1.06688300	-4.51971900	3.45404100	H	-0.97396200	2.71399300	-0.51067600
N	-0.79259400	-3.68038900	2.37746300	H	0.39131600	3.40144300	0.38155700
C	0.07413100	-5.21425500	3.75938900	H	-0.84239200	1.57643800	1.70361800
C	0.47958800	-3.87599400	2.04376700	H	0.88256200	1.27143900	1.45817000
N	1.03252200	-4.79957100	2.85457400	H	-3.63960000	7.57780900	0.61033900
C	-5.12575300	-3.65783600	-2.85133200	H	-3.15316800	-5.08953400	3.45175400
C	-4.23786700	-3.70428400	-1.65755500	H	-2.36009800	-5.18047000	5.02963500
N	-4.09996300	-4.80065300	-0.81807300	H	-5.59418300	-1.02238600	5.38622600
C	-3.42101400	-2.74675200	-1.12356500	H	-3.93393100	-1.65538400	5.37324600
C	-3.23105800	-4.47760400	0.16976700	H	-8.40450200	2.53591200	-1.85365100
N	-2.80684100	-3.23341100	0.01385200	H	-4.82926900	1.86111300	-4.00883000
C	-4.61936200	0.84201500	-3.67063700	H	-6.18564000	-3.75267800	-2.58247100
C	-3.53429900	0.83333800	-2.59981800	H	-4.53440700	0.76340900	4.28012100
O	-3.57481800	1.76207800	-1.71517300	H	0.74406400	-1.13533700	-1.03606300
O	-2.70282800	-0.10683400	-2.60367600	H	1.56068600	2.77390200	-1.55930400
Zn	-3.36522400	1.30556200	0.31352900	O	-1.81666400	0.04207300	-0.16489000
Zn	-1.76943400	-2.15313300	1.38079800	H	-1.88302700	-0.03344700	-1.17266500
N	0.43383000	-0.17273400	-0.87522800	C	-1.06002700	6.87636800	-3.66694600
C	1.18066100	0.80774400	-1.48455900	C	-0.34285800	5.85240000	-2.79059200
O	2.04944700	0.52953300	-2.33546400	S	1.16937300	6.58568200	-2.00900000
N	0.93180800	2.09476900	-1.13917000	C	4.81271900	2.01754900	-2.94544900
C	0.01089100	2.48828000	-0.08501200	C	3.59872300	2.89398000	-3.26164900
C	-0.08059500	1.37169200	0.94923300	O	3.10462000	3.66817400	-2.42686100
C	-0.39220100	0.02366300	0.29757000	C	5.03223500	1.88953100	-1.42983500
O	-0.25713800	-1.01933600	1.15552300	C	6.31868800	1.15737400	-1.07832500
H	-9.12495900	0.92180600	-1.88471600	O	6.38841900	-0.06490600	-0.93531200
H	-9.46394800	2.01811900	-0.53693400	N	7.42275000	1.94000600	-0.94575100
H	-5.75587600	2.39709100	-1.16432100	N	3.13400700	2.81910500	-4.52894600
H	-8.25093700	-0.46269200	0.62516000	C	1.92193500	3.50880600	-4.95737300

H	-1.00517200	5.48354500	-2.00094500	O	5.11913700	-2.08375100	-2.41495900
H	-0.03213800	4.99011700	-3.38403400	N	1.41598300	-4.99186700	-2.33343800
H	1.96903400	5.50408900	-2.14639500	C	1.99952000	-5.90027600	-3.35802500
H	-1.34498200	7.76595800	-3.09326200	C	1.57184900	-5.52516200	-4.78216000
H	4.20193500	1.32171300	-1.00524400	C	1.46486600	-7.27145700	-2.89843000
H	5.02807700	2.88644600	-0.98015800	C	0.07054700	-6.95149300	-2.33620700
H	7.37159900	2.94744000	-0.93506800	C	0.27025400	-5.59959300	-1.63517800
H	8.29594700	1.49919100	-0.68987100	H	-0.60058300	-4.93929100	-1.69027100
H	4.67969600	1.02164500	-3.38203700	H	0.51470900	-5.72130200	-0.57141700
H	1.98148000	4.56251800	-4.67661700	H	-0.65448900	-6.85510900	-3.15191300
H	1.02859900	3.06423700	-4.50179900	H	-0.30119100	-7.72146100	-1.65301700
H	3.46583000	2.05680000	-5.10331700	H	1.44534700	-7.99735900	-3.71606600
H	5.69101100	2.47015500	-3.42659600	H	2.10569600	-7.67585500	-2.10523600
H	1.84311300	3.43549200	-6.04404900	H	3.09050600	-5.87353300	-3.28624100
H	-0.42036500	7.20633500	-4.49097100	H	0.47916900	-5.49922900	-4.87200600
H	-1.97424900	6.44187100	-4.09068500	H	1.98028400	-4.55922700	-5.08804200
C	5.86748900	-3.25164900	6.34109600	H	1.95095400	-6.27773400	-5.48426300
C	5.35553500	-1.80854400	6.19165000	H	3.46766100	-3.78953300	-3.42797900
C	4.56823200	-1.59280600	4.91665500	H	5.54554800	-1.40691200	-1.85259400
C	3.16905600	-1.58346300	4.91055700	H	4.33597100	-3.50654600	-1.10154700
C	5.22348100	-1.43206300	3.68481000	H	3.57003600	-1.91010300	-1.02109900
C	2.44130700	-1.42831600	3.72742600	H	2.29338600	-1.11589000	-3.03361400
C	4.51976400	-1.27984100	2.49474400	H	1.63221200	-0.70021900	-6.26072000
C	3.11664400	-1.28030600	2.50859200	H	2.01256900	0.16529300	-4.74355800
O	2.47763500	-1.12938300	1.31768900	H	3.27956600	-0.15435800	-5.97865900
H	6.21240000	-1.12244600	6.21853300	C	3.70739800	7.08589300	3.99747500
H	4.73098200	-1.55498000	7.05762800	H	4.56186100	6.61332900	4.49424400
H	2.63083800	-1.69233000	5.85059600	C	2.47802600	6.16428100	4.03210600
H	6.31137800	-1.42221800	3.65764900	H	2.18431300	5.98383600	5.07381200
H	1.35447300	-1.39869400	3.74666200	H	1.63361900	6.67604700	3.54996700
H	5.03710200	-1.14395000	1.54869000	C	2.75024000	4.84880300	3.33748000
H	1.49231500	-1.12083300	1.41766000	C	2.79331300	4.78888200	1.93748100
H	5.03341600	-3.96310400	6.36014600	C	3.03880000	3.68710900	4.06417000
H	6.51910600	-3.52673400	5.50398000	H	2.57033100	5.68097100	1.35452200
H	6.43906600	-3.37439900	7.26842300	C	3.12791300	3.60504300	1.28098000
C	2.38536000	-0.54862100	-5.48030000	C	3.36760000	2.49553300	3.41391200
C	2.74211400	-1.89678100	-4.87285500	H	3.01185200	3.71850700	5.15180400
O	3.16449600	-2.81983600	-5.56825700	H	3.16097500	3.58523500	0.19573300
N	2.52093300	-1.97897300	-3.53490000	C	3.41592500	2.45256700	2.01930300
C	2.98752300	-3.09659000	-2.73729000	H	3.58662000	1.60145500	3.99103900
C	1.78840700	-3.73166900	-2.02021300	H	3.66608100	1.52360800	1.51571600
O	1.16713500	-3.08829600	-1.15007200	H	3.50392100	8.03767500	4.50219000
C	4.03343700	-2.63111900	-1.70641700	H	4.00314600	7.30630100	2.96607700

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C	-8.63489000	0.26576900	-1.75350800	N	-5.39266300	0.12964700	0.06204800
C	-7.43861400	0.08426600	-0.88595200	C	-4.03009600	6.40709100	-0.00158500
N	-7.40422000	-0.73266400	0.23484900	C	-3.85080900	5.00655500	0.47423400
C	-6.18020000	0.61079000	-0.96747800	N	-3.58620600	4.68705800	1.79783700
C	-6.16337300	-0.67386700	0.77733200	C	-3.86442900	3.80148000	-0.17648500

C	-3.45046200	3.34565400	1.90481300	H	-4.03078100	-2.13962900	5.33339500
N	-3.61001100	2.78007700	0.71957200	H	-8.39966100	0.96168600	-2.56257700
C	-4.82019800	-2.04347600	4.57571100	H	-4.79901700	1.08675200	-4.06957400
N	-4.69560500	-0.84198100	3.78298800	H	-5.13616300	-4.66528300	-2.88424500
C	-3.58865700	-0.65174100	2.98380500	H	-5.12866600	0.00781000	4.11736700
O	-2.84133000	-1.67338700	2.83965600	C	-1.80325500	6.49505000	-4.06185700
O	-3.46235600	0.49279600	2.45250300	C	-1.44491600	5.53290700	-2.93144200
C	-1.91324000	-4.88647800	4.17535600	S	-0.16668200	6.18430400	-1.76178700
C	-0.57859200	-4.56907900	3.56423100	C	4.49107500	2.46211200	-2.74764200
N	-0.38788800	-3.62989600	2.55158100	C	3.29321000	3.26560800	-3.22494400
C	0.63675700	-5.12267700	3.87535500	O	2.59398800	3.94764200	-2.45826200
C	0.90807800	-3.63340900	2.26611400	C	5.29807000	3.14677000	-1.64487400
N	1.56038800	-4.52442300	3.04102900	C	6.06331600	2.13305500	-0.79777500
C	-4.08301200	-4.37560300	-2.99333100	O	5.66906000	0.97906300	-0.62866000
C	-3.40244700	-4.22476000	-1.68007800	N	7.19567500	2.59447000	-0.21050100
N	-3.19159100	-5.27209900	-0.79467100	N	3.00587000	3.15604900	-4.54137900
C	-2.87060500	-3.12710000	-1.05986200	C	1.74676300	3.62659300	-5.09487800
C	-2.55605200	-4.78635900	0.29926600	H	-2.32163000	5.32272500	-2.31238200
N	-2.35474100	-3.48749900	0.16798100	H	-1.09433000	4.57035600	-3.31442200
C	-4.29829100	0.14784600	-3.81818700	H	0.91399400	5.60518500	-2.33011800
C	-3.21524400	0.38790000	-2.76473200	H	-2.15790100	7.45256800	-3.66738300
O	-3.42923300	1.21197100	-1.84078300	H	4.61339000	3.67630100	-0.97150400
O	-2.16149900	-0.33023900	-2.90488200	H	5.98047300	3.89966000	-2.05669100
Zn	-3.45909100	0.78022800	0.36612700	H	7.47772100	3.56145300	-0.27047200
Zn	-1.50611300	-2.16479900	1.47526300	H	7.68087500	1.99081500	0.43932200
H	-8.95978500	-0.67764400	-2.20992600	H	4.08196800	1.52582900	-2.34931100
H	-9.48808900	0.67707100	-1.19982700	H	1.58453300	4.66814200	-4.80794100
H	-5.77542900	1.29494200	-1.69353600	H	0.90318500	3.02364400	-4.73689800
H	-8.17628800	-1.27489300	0.59774600	H	3.53354100	2.48526500	-5.08206000
H	-5.87620900	-1.18086700	1.68727300	H	5.13856400	2.19109900	-3.58957400
H	-4.33506200	6.40850700	-1.05108400	H	1.79439200	3.56453700	-6.18409800
H	-3.09997200	6.98361900	0.07644500	H	-0.93698200	6.70057900	-4.69914700
H	-4.01458300	3.58979000	-1.22366200	H	-2.59520500	6.06726400	-4.69046900
H	-3.48753900	5.34791300	2.55641200	C	6.01768400	-2.24619000	6.57542900
H	-3.24814300	2.81314300	2.82089800	C	5.31607500	-0.89895400	6.32490900
H	-2.40440900	-3.97470500	4.52861400	C	4.58178500	-0.83206900	5.00058200
H	0.91640100	-5.86973500	4.60214100	C	3.18778900	-0.93117700	4.92576500
H	2.56214600	-4.65707700	3.05745000	C	5.28305300	-0.67941300	3.79264700
H	1.38480400	-3.01209300	1.52142200	C	2.51010700	-0.88411200	3.70377000
H	-4.04887400	-3.42449500	-3.53062900	C	4.63071100	-0.63401500	2.56448100
H	-3.59718500	-5.12837300	-3.62651300	C	3.23114000	-0.73743500	2.51022700
H	-2.78574300	-2.11509200	-1.42299200	O	2.64445200	-0.68546900	1.28606700
H	-3.45022500	-6.23766900	-0.94465800	H	6.06598400	-0.09751800	6.37046400
H	-2.24900200	-5.39241800	1.13748000	H	4.61075900	-0.70348000	7.14258500
H	-4.77568400	-2.92324200	3.93036700	H	2.61104800	-1.03680200	5.84308200
H	-3.87447800	-0.30271000	-4.71769000	H	6.36776300	-0.58926900	3.81589300
H	-5.04999700	-0.53276900	-3.40172200	H	1.42483000	-0.93646200	3.67190000
H	-4.80354900	6.93683300	0.56782700	H	5.18095900	-0.49938500	1.63741600
H	-2.59342700	-5.36239100	3.45736700	H	1.65075600	-0.78504900	1.32048600
H	-1.79016400	-5.56973100	5.02022600	H	5.29374800	-3.06955000	6.58508200
H	-5.78842700	-2.03372400	5.08559300	H	6.75287800	-2.46038200	5.79133100

H	6.54202600	-2.24382000	7.53804200	H	0.40200400	-6.88089100	-3.47947000
N	-0.05233400	-0.11248600	-1.18941900	H	0.50512900	-7.60316100	-1.87103700
C	0.76878000	0.94085200	-1.71903800	H	2.68705900	-7.77800000	-3.48192900
O	1.62753900	0.70125700	-2.57414700	H	2.93068100	-7.28863000	-1.79813200
N	0.48420200	2.17648400	-1.28617400	H	3.95653500	-5.44790600	-2.87558700
C	-0.45489300	2.44268600	-0.20048000	H	1.75068200	-5.50346000	-5.02041100
C	-0.32564700	1.34407100	0.84825800	H	3.12079800	-4.36566800	-4.97167300
C	-0.61077500	-0.06190300	0.29445500	H	3.41183300	-6.08806300	-5.23341000
O	0.01834600	-1.02556500	1.02690700	H	4.12081200	-3.33883600	-3.14173200
H	-1.46870500	2.50338200	-0.60421500	H	5.49414800	-0.77595400	-1.40104200
H	-0.20159200	3.41664700	0.22282500	H	4.39320300	-3.16566200	-0.66111500
H	-1.00787700	1.50518300	1.68781100	H	3.63074000	-1.57238500	-0.69324800
H	0.69518000	1.36451800	1.24020000	H	2.52160000	-0.85133200	-3.00473800
H	0.44927100	-1.00833700	-1.31286600	H	2.15573200	-0.69746000	-6.23468500
H	1.09935900	2.90979800	-1.63716700	H	2.32027000	0.36362800	-4.81106600
O	-1.94866100	-0.39127200	0.18628000	H	3.66658900	0.16493800	-5.98790900
H	-1.18076700	-0.19153400	-2.02468100	C	2.40554000	7.60467600	3.80527700
C	2.84456900	-0.33636500	-5.46332500	H	3.38456500	7.38930500	4.24731000
C	3.40987600	-1.54090900	-4.72366700	C	1.48253500	6.37837600	3.89675300
O	4.05483300	-2.40531100	-5.31621200	H	1.31219100	6.12823600	4.95133700
N	3.12399400	-1.57528600	-3.39516500	H	0.50166900	6.64045200	3.47552300
C	3.46970600	-2.69970800	-2.54725100	C	2.04277300	5.17273500	3.17167400
C	2.17770900	-3.41156000	-2.12025000	C	2.05002600	5.13024300	1.77048000
O	1.29905300	-2.78658300	-1.49776900	C	2.59924500	4.09415500	3.87103500
C	4.24202600	-2.26569400	-1.27975500	H	1.62070900	5.95622400	1.20615200
O	5.50047400	-1.72531000	-1.61284700	C	2.59728200	4.04347200	1.08759100
N	2.02395800	-4.72765000	-2.38990800	C	3.14558700	3.00047900	3.19496500
C	2.91932300	-5.61165800	-3.18205500	H	2.60295200	4.11056900	4.95932200
C	2.78762400	-5.36776200	-4.69069700	H	2.59003000	4.03413900	0.00111200
C	2.44456000	-7.01067400	-2.74132500	C	3.14595800	2.97081000	1.79866300
C	0.93279000	-6.83421300	-2.52202900	H	3.56443600	2.16867500	3.75403300
C	0.81857800	-5.42745600	-1.91435000	H	3.55680400	2.11414800	1.27109800
H	-0.08164300	-4.88546800	-2.21969200	H	1.97516800	8.46334900	4.33380900
H	0.82215600	-5.44913000	-0.81629900	H	2.56965500	7.89721900	2.76236800

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C	-8.68569000	0.29656900	-1.98766600	C	-3.77724900	-0.80803000	2.79871100
C	-7.55254300	0.08886400	-1.05223500	O	-3.10062200	-1.87869300	2.60451000
N	-7.59003500	-0.70509200	0.08451700	O	-3.58968300	0.33422500	2.29182800
C	-6.28097000	0.57836000	-1.09326800	C	-2.13550200	-5.00119500	4.00451700
C	-6.37021800	-0.66840700	0.67632000	C	-0.75992200	-4.70273700	3.47774000
N	-5.54889000	0.09725400	-0.02427100	N	-0.49995500	-3.76182800	2.48138900
C	-4.14213300	6.39369100	0.05448400	C	0.43123400	-5.27143300	3.84721700
C	-3.93783100	4.98513100	0.49645700	C	0.81061200	-3.77775300	2.26074300
N	-3.71900100	4.63082700	1.82008700	N	1.40496600	-4.67983400	3.06590500
C	-3.90093400	3.80051000	-0.18982300	C	-4.09352700	-4.30966300	-3.20983700
C	-3.56374700	3.28907900	1.89366400	C	-3.37038200	-4.20607400	-1.90967900
N	-3.66685000	2.75794200	0.68663100	N	-3.15911900	-5.28435300	-1.06088300
C	-5.05650000	-2.17066700	4.39082700	C	-2.80843300	-3.13489800	-1.26657700
N	-4.86400400	-0.95737000	3.62880200	C	-2.50005900	-4.84836300	0.03645000

N	-2.27904900	-3.54552900	-0.05610600	H	-1.12798300	4.60766200	-3.29482700
C	-4.28995000	0.23314900	-3.92578700	H	0.84597100	5.58189800	-2.16202300
C	-3.30482100	0.31857700	-2.76016000	H	-2.16581400	7.51507200	-3.48936000
O	-3.60171700	1.16408200	-1.82715500	H	4.58820300	3.91538900	-0.78774300
O	-2.32630100	-0.44685900	-2.76385900	H	6.00157900	4.34633600	-1.74146200
Zn	-3.61532600	0.79043400	0.18580200	H	7.44715900	3.98889800	0.04429900
Zn	-1.61878700	-2.36588600	1.44139800	H	7.72546900	2.40197800	0.68979600
H	-9.01961000	-0.64144900	-2.44926800	H	4.38519100	1.84077200	-2.37006000
H	-9.55589700	0.74886400	-1.49522900	H	1.58755500	4.80544500	-4.75021400
H	-5.82413500	1.23107200	-1.81661800	H	0.98971800	3.15213600	-4.47060200
H	-8.39020900	-1.22126700	0.42371400	H	3.66633300	2.75806100	-4.95332600
H	-6.13245100	-1.16963500	1.60303600	H	5.39420300	2.76253000	-3.49117100
H	-4.40860600	6.41590000	-1.00510200	H	1.78407900	3.57071300	-6.01260100
H	-3.23351800	6.99503100	0.18188800	H	-0.90233100	6.83049300	-4.51717200
H	-4.01199900	3.61233800	-1.24651700	H	-2.56076100	6.20786400	-4.62660100
H	-3.65952500	5.27154600	2.59980800	C	5.71793400	-2.41882700	6.70377100
H	-3.39432100	2.73350400	2.80291700	C	5.25787500	-0.98051900	6.40963000
H	-2.64084100	-4.08166100	4.31418900	C	4.52851600	-0.85945400	5.08893600
H	0.66428900	-6.02539900	4.58304200	C	3.13780700	-0.99530700	5.01126000
H	2.40189300	-4.83731300	3.12460100	C	5.22823200	-0.65302300	3.88939800
H	1.34060800	-3.17241500	1.53662300	C	2.46358800	-0.94169100	3.78957400
H	-4.04726500	-3.34579100	-3.72269100	C	4.57741000	-0.59480400	2.66017000
H	-3.64505900	-5.06021100	-3.87208000	C	3.18487300	-0.74649900	2.60393200
H	-2.70669400	-2.11635600	-1.61830300	O	2.59501600	-0.69685400	1.37708200
H	-3.43288800	-6.24114200	-1.23862900	H	6.13254400	-0.31745100	6.41199300
H	-2.19534900	-5.48631900	0.85177500	H	4.60762300	-0.63687000	7.22434000
H	-5.07021400	-3.03397000	3.72226500	H	2.56363200	-1.13917300	5.92499300
H	-3.80937000	-0.21482500	-4.79810000	H	6.30935000	-0.53102500	3.91963300
H	-5.13761600	-0.39861200	-3.63161600	H	1.38019500	-1.02418400	3.75385400
H	-4.95172500	6.88243400	0.61002800	H	5.12440400	-0.40948300	1.73999700
H	-2.76811000	-5.48021300	3.24640100	H	1.61822400	-0.76468000	1.45093300
H	-2.07414700	-5.67592700	4.86255600	H	4.86171300	-3.10254000	6.74588200
H	-6.01865700	-2.11496300	4.90856700	H	6.39471300	-2.78166200	5.92172200
H	-4.27027000	-2.33261900	5.14060600	H	6.24575200	-2.47785500	7.66279600
H	-8.37514800	0.96823000	-2.79171000	N	0.39072400	-0.26058700	-1.68968400
H	-4.68823000	1.21898400	-4.18585600	C	1.15859200	0.85579400	-1.83796100
H	-5.14980200	-4.57337200	-3.07237200	O	2.35366900	0.82557000	-2.19087900
H	-5.25609400	-0.09363600	3.97685500	N	0.55916100	2.05287900	-1.54010300
C	-1.79661800	6.58569500	-3.93476000	C	-0.52587900	2.17822700	-0.57380800
C	-1.49130000	5.54342200	-2.86108300	C	-0.30238100	1.39979000	0.74595800
S	-0.26541700	6.09938500	-1.59106100	C	-0.81999300	-0.01748500	0.76382800
C	4.69310400	2.85344700	-2.65302600	O	-0.19267200	-0.92733900	1.40802200
C	3.41353100	3.54694100	-3.09837400	H	-1.47294200	1.87653000	-1.02766200
O	2.67926800	4.17772800	-2.32337900	H	-0.60394100	3.24413700	-0.34798600
C	5.36434000	3.50482100	-1.44500900	H	-0.85324000	1.91227100	1.54741500
C	6.15744000	2.49693600	-0.61568400	H	0.75059100	1.41476800	1.03479800
O	5.84143700	1.31127600	-0.51473600	H	0.87195700	-1.15231200	-1.79253600
N	7.22948500	3.00377200	0.04675200	H	1.21065900	2.83085000	-1.60247200
N	3.09417600	3.38542900	-4.40567600	O	-1.94272100	-0.32060900	0.24486600
C	1.78584900	3.74607700	-4.93491800	H	-0.60091500	-0.24026500	-1.94467600
H	-2.39608400	5.29713800	-2.29804500	C	2.89891800	-0.20572800	-5.37112700

C 3.44730900 -1.46773600 -4.71734000
 O 3.99693600 -2.34523700 -5.38380900
 N 3.22869300 -1.54095900 -3.37932500
 C 3.75063400 -2.60647500 -2.54536900
 C 2.58618100 -3.44754700 -1.99006200
 O 1.75324700 -2.92464400 -1.22549000
 C 4.54428900 -2.02128400 -1.35420000
 O 5.64831100 -1.28412000 -1.83132200
 N 2.49461100 -4.76161200 -2.29949300
 C 3.28088100 -5.53898400 -3.29144000
 C 2.82539700 -5.25513300 -4.72827400
 C 3.01099300 -6.98480400 -2.83260900
 C 1.55039500 -6.94838700 -2.35155700
 C 1.41645500 -5.56339400 -1.69582200
 H 0.44520600 -5.08824400 -1.86770200
 H 1.56351800 -5.60342600 -0.60838400
 H 0.86802700 -7.03481300 -3.20427200
 H 1.31109700 -7.75959600 -1.65695100
 H 3.18312200 -7.70922500 -3.63372000
 H 3.67625800 -7.24077500 -1.99888000
 H 4.34190500 -5.29591500 -3.18980700
 H 1.75102400 -5.44132000 -4.84403400
 H 3.04976800 -4.22707600 -5.02112300
 H 3.35987700 -5.91779800 -5.42004300
 H 4.42375600 -3.19604300 -3.16846900
 H 5.63260500 -0.39925000 -1.42564900
 H 4.88716300 -2.86308500 -0.72813600
 H 3.86933100 -1.41330000 -0.74246500
 H 2.89239300 -0.69756200 -2.90145200
 H 2.04055700 -0.47681700 -5.99632800
 H 2.58752000 0.54767700 -4.64489200
 H 3.66663400 0.19816300 -6.03974300
 C 2.17695000 7.49740600 4.07876500
 H 3.14772900 7.27956600 4.53747200
 C 1.27729900 6.24946000 4.08399600
 H 1.08300800 5.94647000 5.12065700
 H 0.30374200 6.51206200 3.64686400
 C 1.88348700 5.09119500 3.31934800
 C 1.87495800 5.08431100 1.91771800
 C 2.50454100 4.02574500 3.98443000
 H 1.39490200 5.89969000 1.37959500
 C 2.47360600 4.04788600 1.20031900
 C 3.10176900 2.98185200 3.27398300
 H 2.52077900 4.01450100 5.07278000
 H 2.46329700 4.07007000 0.11411500
 C 3.08968800 2.98982600 1.87706300
 H 3.57343700 2.16150800 3.80748900
 H 3.54774300 2.17684600 1.31963800
 H 1.71413100 8.32037300 4.63597000
 H 2.36329700 7.84292000 3.05598700

Y172F SkDHPase.DHU-ES-II

C -8.43307500 -1.85652700 -2.09086100
 C -7.28706300 -1.75554200 -1.14960500
 N -7.13195200 -2.52057300 -0.00226600
 C -6.17448200 -0.96679900 -1.19422900
 C -5.95887300 -2.17701800 0.58827400
 N -5.34996500 -1.24041900 -0.11943500
 C -5.43296700 5.17743100 -0.21683500
 C -4.95523000 3.83444300 0.24004000
 N -4.80235900 3.51572000 1.58154900
 C -4.54852800 2.70613900 -0.42758100
 C -4.31148400 2.25804000 1.68092800
 N -4.14407500 1.73953400 0.47646400
 C -4.27255000 -3.27181800 4.28334200
 N -4.36400700 -2.04255600 3.52303800
 C -3.32419100 -1.63072400 2.71605700
 O -2.40223300 -2.49905300 2.53922800
 O -3.39939600 -0.47443800 2.20779900
 C -0.75662100 -5.33940100 3.92238200
 C 0.46600300 -4.73986900 3.29268500
 N 0.45370400 -3.77560800 2.28130600
 C 1.76765500 -5.04196000 3.60036600
 C 1.72435400 -3.52452200 1.99545700
 N 2.54945700 -4.26857100 2.76641500
 C -2.89728300 -5.27952600 -3.28966600
 C -2.19546500 -4.99427700 -2.00875400
 N -1.65686800 -5.94314000 -1.14954900
 C -1.94643100 -3.79546500 -1.40647900
 C -1.11562400 -5.29739600 -0.08570000
 N -1.27912900 -3.99019600 -0.21354700
 C -4.14709300 -0.92032000 -4.07174900
 C -3.23554600 -0.55196600 -2.89411300
 O -3.72825500 0.24379500 -2.01239200
 O -2.10807400 -1.08686900 -2.82856400
 Zn -3.55336200 -0.19455300 0.04958800
 Zn -1.03354500 -2.45124300 1.14121300
 N 1.19214200 0.22977900 -0.26605400
 C 1.32987300 1.44167700 -0.97400100
 O 2.12778800 1.51194600 -1.91310800
 N 0.58513200 2.47256800 -0.53607800
 C -0.55949700 2.28764100 0.35246600
 C -0.21198400 1.27211900 1.43947500
 C 0.47726700 0.05680100 0.87592600
 O 0.49513700 -1.03954000 1.46265900
 H -8.51389800 -2.85519900 -2.53889300
 H -9.39249900 -1.63443400 -1.60637300
 H -5.88483200 -0.23170200 -1.92573200
 H -7.78067900 -3.21456700 0.34254000
 H -5.60350000 -2.59356100 1.51988400
 H -5.60234700 5.16659000 -1.29647300

H	-4.69756400	5.96215100	-0.00085500	H	0.05134800	7.02357900	2.36357400
H	-4.51421200	2.50201900	-1.48653500	H	-1.33477200	5.67539700	4.72131500
H	-4.96460700	4.14242400	2.35745000	H	-2.99196700	5.71925600	2.91486400
H	-4.09829100	1.74558500	2.60591600	H	-2.35715800	4.06602400	3.08460300
H	-1.41864700	-4.55905400	4.31025800	H	-1.81831300	5.10085200	1.74736500
H	2.19099000	-5.71829500	4.32703700	H	-0.03671700	3.67392100	4.02604400
H	3.55763800	-4.20537800	2.77253600	H	0.64917500	4.57189500	2.65618700
H	2.07901900	-2.83383600	1.24454700	H	1.05720500	5.02926100	4.31548300
H	-3.13905600	-4.33187500	-3.77689600	H	1.09865100	7.30988400	4.68359300
H	-2.27863200	-5.86195000	-3.98412900	H	-3.30887200	4.35691700	-2.32456800
H	-2.17555900	-2.81395000	-1.78853500	H	-1.89322500	4.40788100	-3.35499700
H	-1.65811900	-6.94434900	-1.28834400	H	-0.43767700	5.79156400	-1.94990100
H	-0.62037600	-5.79332900	0.73471900	H	-4.01243000	6.64844500	-3.14803600
H	-4.03783000	-4.10288100	3.61569000	H	4.18821600	2.65026400	-1.65714900
H	-3.55736300	-1.29017700	-4.91362300	H	3.57599900	3.84624400	-0.52460300
H	-4.83129000	-1.71496600	-3.74847200	H	5.70797300	5.84853900	-0.67216600
H	-1.42884000	1.94419600	-0.21882600	H	7.10956000	5.06783800	-0.01464900
H	-0.80875700	3.25537900	0.78884000	H	4.65376100	4.44095700	-3.33589100
H	-1.10445300	0.93463800	1.97013200	H	0.32435400	5.09571300	-4.47603700
H	0.48036000	1.71104200	2.17207600	H	0.36821500	3.34309200	-4.15472100
H	-6.37821000	5.45746000	0.26365600	H	3.00848300	4.05161900	-4.77939000
H	-1.34205200	-5.92611100	3.20269800	H	4.17974000	5.69008800	-2.18474200
H	-0.47186200	-6.00219500	4.74424700	H	0.91323900	3.97787800	-5.72754600
H	-5.23767700	-3.46570700	4.76129100	H	-2.60034100	6.69671700	-4.20739300
H	-3.50009700	-3.23552000	5.06369100	H	-3.87246900	5.49009600	-4.48734900
H	-8.29989100	-1.13897100	-2.90426900	H	-0.45665100	7.90481400	5.28146300
H	-4.75583300	-0.06757000	-4.38780100	H	0.44231900	8.83050400	4.07128400
H	-3.83308900	-5.83307700	-3.13813400	C	6.02627400	-0.89923000	7.03991500
H	-4.94989500	-1.29777900	3.87377500	C	5.42639900	0.45425000	6.61930000
H	1.76033100	-0.56648700	-0.59454100	C	4.85786700	0.43016900	5.21567900
H	0.70058900	3.33903600	-1.06198000	C	3.62604900	-0.18903900	4.95904400
O	-1.80099600	-1.01971800	-0.06421900	C	5.55766600	0.98786800	4.13738100
H	-1.62492300	-1.04105900	-1.03148000	C	3.11387000	-0.26298700	3.66370400
C	0.17285700	7.81653800	4.38786300	C	5.05087600	0.92518700	2.83715200
C	-0.56330800	7.06113000	3.27398600	C	3.82934900	0.29255000	2.59892600
C	-0.95814600	5.62858300	3.68771900	H	6.19799700	1.23032900	6.69054400
C	-2.09446300	5.09487600	2.80921300	H	4.63863400	0.73266400	7.33185600
C	0.24510600	4.67351600	3.67257800	H	3.06190700	-0.61637800	5.78626200
C	-3.31001500	6.02605500	-3.71193400	H	6.51141200	1.47895400	4.31932100
C	-2.59438200	5.03414900	-2.79757400	H	2.15657200	-0.74393600	3.48131000
S	-1.67131800	5.82672500	-1.40167700	H	5.60357100	1.37291600	2.01441400
C	4.00178300	4.64804900	-2.48001100	H	5.26980000	-1.69171300	7.00796300
C	2.52438100	4.58208000	-2.87071600	H	6.84290600	-1.19103700	6.37002100
O	1.63279100	4.81118800	-2.04249400	H	6.42355800	-0.85220800	8.06020500
C	4.31187400	3.68037500	-1.32205900	C	2.97537100	0.65502300	-5.10313100
C	5.69820400	3.76470200	-0.69601200	C	3.86711700	-0.40704800	-4.48622600
O	6.31025200	2.75318800	-0.34264200	O	4.63218200	-1.08818600	-5.16619600
N	6.22504600	5.00027400	-0.49984800	N	3.70100400	-0.55668800	-3.14491700
N	2.24920200	4.30427400	-4.16363900	C	4.55017000	-1.41387500	-2.34373500
C	0.88178700	4.17157400	-4.65400000	C	3.66385500	-2.47619000	-1.67881200
H	-1.46938400	7.62274400	3.00804700	O	2.83149600	-2.12277000	-0.81344600

C	5.29301100	-0.59762500	-1.26712800	H	5.66917600	-3.92727400	-2.97285300
O	6.02986100	0.41093200	-1.91282100	H	3.13532200	-4.66946900	-4.55696300
N	3.77589500	-3.77104900	-2.03116000	H	4.14150700	-3.21614700	-4.80045500
C	4.68193100	-4.39201200	-3.03925500	H	4.79993300	-4.81671600	-5.15433800
C	4.14768000	-4.25853600	-4.47243200	H	5.27930600	-1.84864800	-3.02760900
C	4.73398900	-5.85102200	-2.54541100	H	6.18427800	1.14509900	-1.28348300
C	3.31056200	-6.10785400	-2.02440000	H	5.93951600	-1.28399600	-0.69136000
C	2.92424200	-4.77574300	-1.36386400	H	4.55461500	-0.18562600	-0.56512300
H	1.86739000	-4.51549200	-1.47692700	H	3.12153400	0.12025000	-2.65198000
H	3.14289000	-4.77419800	-0.28951900	H	2.20164500	0.16356300	-5.70402900
H	2.63490100	-6.33399100	-2.85635200	H	2.49367000	1.29646200	-4.36210800
H	3.25851500	-6.94470000	-1.32154300	H	3.58076100	1.25571600	-5.78965200
H	5.03549400	-6.54072600	-3.33855100	H	3.43594900	0.22923400	1.58821400
H	5.45750300	-5.94249100	-1.72610900				

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C	-8.13717600	-2.94574000	-1.59292000	Zn	-0.47229800	-2.63611300	1.30651400
C	-6.86202600	-2.77167000	-0.84130100	N	0.80932700	0.21529800	-0.52343000
N	-6.32047800	-3.70737700	0.03129700	C	0.86470500	1.42100400	-1.20781200
C	-5.96086600	-1.74532100	-0.84762100	O	1.69635900	1.59664400	-2.11380800
C	-5.14312200	-3.22452700	0.50492100	N	0.01049600	2.39045700	-0.81665800
N	-4.89499900	-2.03609400	-0.01630000	C	-1.07066700	2.17767700	0.13331700
C	-5.96837400	4.46890700	-0.07354200	C	-0.62323300	1.18489100	1.20054200
C	-5.34923500	3.19048900	0.38736800	C	0.01754100	-0.05304100	0.60136000
N	-5.14062500	2.89804200	1.72718000	O	0.48215300	-0.95295800	1.40549800
C	-4.84206700	2.10808700	-0.28443000	H	-8.10691500	-3.81621600	-2.26025300
C	-4.52301700	1.69754900	1.82213100	H	-8.99975400	-3.06924000	-0.92606800
N	-4.32583100	1.19258200	0.61609600	H	-5.97667500	-0.83250500	-1.41907400
C	-3.49870700	-3.61352700	4.57004500	H	-6.73038700	-4.59812300	0.27632000
N	-3.77557200	-2.42738400	3.78855100	H	-4.50984500	-3.75131400	1.20284200
C	-2.96501100	-2.02784400	2.76257300	H	-6.14613600	4.42927900	-1.15112000
O	-2.08803200	-2.88482200	2.38718900	H	-5.31442300	5.32675000	0.12550100
O	-3.18272700	-0.88953200	2.24808100	H	-4.79733700	1.91228100	-1.34460500
C	0.22916200	-5.23031900	4.06415800	H	-5.35477500	3.50925000	2.50312500
C	1.33494900	-4.42961400	3.45033600	H	-4.23196600	1.22082500	2.74472900
N	1.14719200	-3.54268900	2.39269000	H	-0.59818500	-4.58393500	4.37320200
C	2.66050800	-4.42339000	3.79752400	H	3.20187700	-4.95607400	4.56401200
C	2.33860900	-3.02530100	2.11420200	H	4.24583900	-3.24732400	2.96251100
N	3.27797900	-3.53661700	2.93667100	H	2.54233800	-2.30188200	1.33841700
C	-2.27951300	-5.67820000	-3.01437000	H	-2.66198700	-4.79146900	-3.52564100
C	-1.53753100	-5.25312200	-1.79667600	H	-1.64116900	-6.22048700	-3.72310600
N	-0.86247900	-6.11059800	-0.93855300	H	-1.71116700	-3.06610500	-1.65709600
C	-1.37551300	-4.00998200	-1.25278800	H	-0.76431700	-7.11039700	-1.05057400
C	-0.33331100	-5.37706500	0.07065800	H	0.25082500	-5.79018800	0.87866700
N	-0.63368900	-4.09816800	-0.09143200	H	-3.31629900	-4.46208600	3.90784500
C	-4.11717300	-1.54016500	-3.83657700	H	-3.52876200	-1.91648300	-4.67625200
C	-3.20454100	-0.99574200	-2.73546800	H	-4.71213200	-2.36302600	-3.42135800
O	-3.74869100	-0.22336700	-1.86415400	H	-1.96414900	1.81251300	-0.38534900
O	-2.01165600	-1.37381700	-2.70552900	H	-1.32304700	3.13956600	0.58559600
Zn	-3.39520000	-0.59036600	0.16700300	H	-1.44758800	0.87541400	1.84391300

H	0.14828900	1.64141600	1.83436500	H	-0.32404400	3.24359700	-4.41956300
H	-6.93203900	4.65530800	0.41577700	H	2.29112000	3.87182000	-4.86673600
H	-0.18379200	-5.96572500	3.36148700	H	3.90874000	4.67552300	-3.35900100
H	0.59228200	-5.77483300	4.94029900	H	0.22703400	4.03252500	-5.92039100
H	-4.36739400	-3.83675900	5.19612900	H	-3.67508600	6.19348300	-4.36066200
H	-2.62339800	-3.49578600	5.22360300	H	-4.63616600	4.69774300	-4.32792200
H	-8.31854000	-2.06168900	-2.20903900	H	-1.09895600	7.98467600	5.06249400
H	-4.81678500	-0.77370700	-4.18347800	H	-0.39163500	8.97360900	3.77703700
H	-3.13190000	-6.32687100	-2.77450200	C	6.54230300	0.13219500	6.67748100
H	-4.38558900	-1.71771200	4.16638500	C	5.53546700	1.26305400	6.39844200
H	1.52383500	-0.48007700	-0.76362300	C	4.81575400	1.11144200	5.07324800
H	0.11179500	3.27734600	-1.30607400	C	3.62870500	0.37108000	4.97901000
O	-1.43517200	-0.94324600	-0.07431400	C	5.32919700	1.69024600	3.90364300
H	-1.36474400	-0.98645400	-1.06542900	C	2.97502800	0.21107200	3.75518800
C	-0.51159100	7.94563000	4.13709700	C	4.68224700	1.53770800	2.67552300
C	-1.20266800	7.06700800	3.08644700	C	3.50210300	0.79373700	2.59979600
C	-1.40047900	5.60569400	3.53805200	H	6.06400500	2.22442300	6.41928200
C	-2.50583100	4.92924700	2.71708100	H	4.80034300	1.29616100	7.21275300
C	-0.09389900	4.80086400	3.47046800	H	3.20658100	-0.07362100	5.87871600
C	-4.15929600	5.46432400	-3.70386100	H	6.24502100	2.27589200	3.96027700
C	-3.15039900	4.82258800	-2.75437300	H	2.04605300	-0.34984100	3.69463200
S	-2.35859600	6.06421400	-1.62583800	H	5.08513000	2.00994600	1.78277900
C	3.22505100	4.36277100	-2.56061900	H	6.04144500	-0.84274100	6.70079900
C	1.77699700	4.51329100	-3.01011100	H	7.31371600	0.09183500	5.90008000
O	0.86716600	4.82981100	-2.22844600	H	7.03993700	0.28036500	7.64251600
C	3.51231900	5.11623000	-1.26188300	C	2.68018300	0.88908500	-5.30951600
C	4.73489900	4.57459200	-0.53042000	C	3.69251000	-0.04276200	-4.66212800
O	5.01674800	3.37533300	-0.49420600	O	4.56138000	-0.61005100	-5.32313800
N	5.47919400	5.49653600	0.12976900	N	3.52544100	-0.20219500	-3.32318700
N	1.53546300	4.25404300	-4.31472800	C	4.47663300	-0.91755200	-2.49684000
C	0.17991000	4.12528100	-4.83346300	C	3.75895300	-2.09973200	-1.83029800
H	-2.18308200	7.50658900	2.85623000	O	2.89094800	-1.87902600	-0.95873600
H	-0.63648200	7.08173800	2.14441700	C	5.06211300	0.00805200	-1.41038200
H	-1.73086000	5.62337900	4.58841400	O	5.73561800	1.07691400	-2.03166800
H	-3.46883200	5.43469100	2.87111100	N	4.06681600	-3.36558500	-2.18143400
H	-2.62207400	3.87512900	2.99909700	C	5.05560900	-3.84469600	-3.18713300
H	-2.28685300	4.97214900	1.64238200	C	4.50413400	-3.81331100	-4.61973200
H	-0.23195500	3.78197800	3.85239400	C	5.34445600	-5.27013200	-2.67687300
H	0.26355800	4.72526800	2.43469700	C	3.98555600	-5.74591700	-2.13757300
H	0.70223500	5.26603900	4.06180500	C	3.39056000	-4.48287600	-1.49503300
H	0.48574000	7.57004700	4.39413400	H	2.30541500	-4.39895300	-1.60904800
H	-3.63089000	4.06328100	-2.13120800	H	3.60553000	-4.42638500	-0.42070300
H	-2.35340800	4.32471800	-3.31051100	H	3.35056300	-6.09366900	-2.95977800
H	-1.07501300	5.75395600	-1.91268200	H	4.07604900	-6.56844500	-1.42158000
H	-4.94801100	5.98983600	-3.15367800	H	5.74621300	-5.91385600	-3.46437100
H	2.65060400	4.98703500	-0.59525100	H	6.08024000	-5.23342200	-1.86419500
H	3.60861700	6.19339300	-1.44034100	H	5.95565900	-3.22688200	-3.13205900
H	5.25470300	6.47986000	0.12486600	H	3.56994000	-4.38133400	-4.69687500
H	6.27143100	5.18267200	0.67358400	H	4.33290100	-2.78810600	-4.95685100
H	3.38860900	3.29223400	-2.39124900	H	5.23567600	-4.26697600	-5.29885100
H	-0.39669100	5.01770100	-4.58001100	H	5.28028400	-1.23976000	-3.15926700

H	5.53815000	1.88911200	-1.53093100	H	2.11471200	0.33009800	-6.06257000
H	5.74564600	-0.58570100	-0.77784600	H	1.98764500	1.33433000	-4.59204500
H	4.24488700	0.35703900	-0.76714100	H	3.22992300	1.67270100	-5.84387700
H	2.83033000	0.37308500	-2.84374300	H	2.98636500	0.67321700	1.65118000

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C	-7.83712400	-3.66646500	-1.60200400	H	-8.66618300	-3.91176300	-0.92643100
C	-6.57155900	-3.39084000	-0.86658600	H	-5.91594800	-1.34719800	-1.37810800
N	-5.91259100	-4.29785300	-0.04615400	H	-6.21905100	-5.23707100	0.16732000
C	-5.78610400	-2.27434200	-0.84567100	H	-4.07799300	-4.19487800	1.08577700
C	-4.78272800	-3.71133500	0.42585800	H	-6.54967300	3.84949300	-1.11306600
N	-4.67613800	-2.48258300	-0.04835200	H	-5.78847900	4.82029500	0.15333300
C	-6.36789200	3.90859700	-0.03708600	H	-5.00278200	1.46520900	-1.31755800
C	-5.63783300	2.69190400	0.42164700	H	-5.63351300	3.01971400	2.53566900
N	-5.38591600	2.42252500	1.75861400	H	-4.31889100	0.83558000	2.76582400
C	-5.05146100	1.65574300	-0.25664000	H	-0.21656700	-4.65382500	4.21447600
C	-4.66740800	1.27965000	1.84670400	H	3.63263400	-4.55637600	4.68988700
N	-4.44811300	0.79043700	0.63812700	H	4.52103900	-2.73309000	3.12181400
C	-3.14544700	-3.93704200	4.55091500	H	2.78405800	-2.01888000	1.40638600
N	-3.49153300	-2.77361600	3.76149800	H	-2.21233500	-4.96555500	-3.53228900
C	-2.74079000	-2.34702000	2.70306800	H	-1.06743700	-6.28968100	-3.77182600
O	-1.82847000	-3.15268300	2.30038400	H	-1.41875800	-3.22457300	-1.58634000
O	-3.04684000	-1.22901800	2.18342100	H	-0.10332400	-7.18780600	-1.15338000
C	0.71626600	-5.19514500	4.03005300	H	0.80423000	-5.86233000	0.82379000
C	1.76509600	-4.27579600	3.49007900	H	-2.90810400	-4.77491200	3.89253100
N	1.52170000	-3.42547200	2.41886700	H	-3.34615700	-2.20715500	-4.67460800
C	3.06169500	-4.10028100	3.89608200	H	-4.50882500	-2.74140900	-3.43369100
C	2.64632300	-2.75786900	2.18362700	H	-2.13617800	1.77860200	-0.35925900
N	3.60079300	-3.14548900	3.05295400	H	-1.49457400	3.04944700	0.68304900
C	-1.75234700	-5.83048700	-3.04821900	H	-1.54020200	0.74510900	1.82036900
C	-1.05030100	-5.38147000	-1.81603400	H	0.06778600	1.48236700	1.75966600
N	-0.29316400	-6.20728200	-0.99721500	H	-7.34011100	4.01362900	0.45949700
C	-0.99752900	-4.15074900	-1.22269000	H	0.48553800	-6.00837800	3.32944500
C	0.17704400	-5.47020600	0.03760200	H	1.04590700	-5.65161400	4.96769500
N	-0.24031400	-4.21908100	-0.06994500	H	-4.00157700	-4.21094500	5.17388200
C	-3.97010300	-1.87714500	-3.84131800	H	-2.28286800	-3.76135300	5.20835000
C	-3.11739300	-1.26896800	-2.73155200	H	-8.12570500	-2.78016200	-2.17225600
O	-3.72982500	-0.55261700	-1.85916000	H	-4.71972200	-1.16295300	-4.19495500
O	-1.89486800	-1.54419600	-2.69438600	H	-2.54283000	-6.56058600	-2.83169600
Zn	-3.36616500	-0.87335500	0.16425100	H	-4.14536900	-2.10113100	4.13388400
Zn	-0.13137500	-2.79281200	1.36110900	H	1.50568400	-0.34216200	-0.81544000
N	0.68847000	0.25235900	-0.65982800	H	-0.12009500	3.32980800	-1.23516600
C	0.75073700	1.51548500	-1.19765200	O	-1.35470000	-0.88548400	-0.20007800
O	1.63414800	1.83016100	-2.02212100	H	-1.28173200	-0.95870800	-1.19893400
N	-0.17505000	2.41820100	-0.78788400	C	-1.25224900	7.85318200	4.18948100
C	-1.23415400	2.12424000	0.16205500	C	-1.86012800	6.92055500	3.13401500
C	-0.74369600	1.07209000	1.14909500	C	-1.93044800	5.44714100	3.58441900
C	-0.17841700	-0.15790400	0.43154100	C	-2.97071400	4.67647600	2.76151400
O	0.45149800	-1.00670100	1.24812100	C	-0.55820700	4.75990800	3.51989900
H	-7.73007200	-4.49772100	-2.31017100	C	-4.66629300	5.09177200	-3.66302900

C	-3.59055400	4.56805300	-2.71448800	C	4.51987000	1.79450300	2.61574500
S	-2.94670600	5.89443500	-1.58940700	C	3.38412800	0.98062100	2.59446500
C	2.77067500	4.69864100	-2.48983500	H	5.90104100	2.75854900	6.29717400
C	1.31651700	4.67265800	-2.96022700	H	4.70080500	1.80464100	7.15561800
O	0.37345100	4.96370700	-2.20954500	H	3.17896600	0.27156800	5.91961600
C	2.85455600	4.89140100	-0.96925000	H	6.05118200	2.68946800	3.83535800
C	4.29119200	4.92350900	-0.47013400	H	2.00983700	-0.18281300	3.77103000
O	5.04367700	3.94789500	-0.51885800	H	4.88553900	2.24714900	1.69713200
N	4.71355500	6.10485400	0.04883700	H	6.06468100	-0.28324600	6.75487600
N	1.11635400	4.35504300	-4.25957500	H	7.27375300	0.67832700	5.89004500
C	-0.22299300	4.17129000	-4.80652000	H	6.99833700	0.95085500	7.62091000
H	-2.87426200	7.27331400	2.90054200	C	2.56786200	1.18599500	-5.30659700
H	-1.29364800	6.98596100	2.19440200	C	3.64865400	0.32655800	-4.67326800
H	-2.26350700	5.43556500	4.63406000	O	4.56313800	-0.15210200	-5.34284100
H	-3.97493800	5.09423500	2.91641000	N	3.48925000	0.12648100	-3.33870900
H	-2.99109600	3.61571500	3.04198300	C	4.53831900	-0.45151300	-2.52039400
H	-2.75624400	4.73959000	1.68708500	C	3.99060700	-1.70194200	-1.81884900
H	-0.60770900	3.73151700	3.89780700	O	3.14595500	-1.58065800	-0.90819500
H	-0.19097900	4.71903600	2.48578600	C	5.02264300	0.57106300	-1.47496100
H	0.19135200	5.29146200	4.11618000	O	5.51452100	1.69987500	-2.15663000
H	-0.22744800	7.56439800	4.45048900	N	4.42164000	-2.92719700	-2.19372800
H	-3.98047600	3.75716300	-2.09244800	C	5.42212900	-3.29336100	-3.23508400
H	-2.74124600	4.16732700	-3.27131500	C	4.82446400	-3.32967000	-4.64958300
H	-1.63366300	5.69364000	-1.83753900	C	5.89130100	-4.67429500	-2.73595600
H	-5.50928300	5.52478800	-3.11253900	C	4.61710600	-5.30028800	-2.14603500
H	2.36172500	4.04364600	-0.48494000	C	3.90821000	-4.11057900	-1.47966900
H	2.31002800	5.79503200	-0.67991100	H	2.81650800	-4.15372400	-1.54795700
H	4.11330400	6.91155300	0.12397900	H	4.15922400	-4.02494700	-0.41482600
H	5.66211500	6.17078000	0.39265500	H	3.99489800	-5.71947400	-2.94446900
H	3.26502000	3.76225800	-2.76785200	H	4.82726500	-6.10556300	-1.43547000
H	-0.83749300	5.04279400	-4.57069700	H	6.33518600	-5.27143800	-3.53747800
H	-0.70312800	3.27407400	-4.39718600	H	6.64710900	-4.54968900	-1.95087200
H	1.89520000	3.97204300	-4.77747700	H	6.24700800	-2.57653900	-3.21132700
H	3.29115300	5.51363300	-3.01183600	H	3.95594200	-3.99684000	-4.69553100
H	-0.14860400	4.07278200	-5.89154700	H	4.53234400	-2.33058700	-4.98110200
H	-4.26765200	5.87111600	-4.31961500	H	5.57928900	-3.70343500	-5.35153800
H	-5.05408100	4.27668700	-4.28739300	H	5.36240900	-0.68494700	-3.19500300
H	-1.84500900	7.83920200	5.11215000	H	5.36325000	2.48301900	-1.59241400
H	-1.21975100	8.88861300	3.83222400	H	5.80110400	0.09506800	-0.85143700
C	6.50542300	0.71713500	6.67057800	H	4.18281000	0.82324000	-0.81448400
C	5.43044400	1.76817900	6.33650500	H	2.77414800	0.67029000	-2.84731000
C	4.70857400	1.50168800	5.03021000	H	2.07855100	0.61652300	-6.10357400
C	3.56494100	0.69085400	4.99185500	H	1.81869100	1.52668500	-4.58827200
C	5.17216300	2.04786300	3.82452200	H	3.05369100	2.04522500	-5.78452500
C	2.90674200	0.43125200	3.78756800	H	2.86352800	0.77719600	1.66253100

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C	4.68981000	6.91514600	-1.95354900	C	3.68234300	4.69062300	-1.05090100
C	3.78289000	6.05103300	-1.14475100	C	2.15148300	5.47809200	0.26423400
N	2.79432100	6.53296300	-0.29622000	N	2.66653400	4.34543300	-0.18007500

C	7.39615500	-0.15514100	0.20883500	H	8.28010300	0.28634000	0.68497900
C	6.14323300	0.54457900	0.60534200	H	-4.01485800	4.77494800	3.27524400
N	5.79377900	0.76141600	1.92912400	H	-3.69292600	4.56243600	4.99641700
C	5.09889500	1.05786600	-0.11723100	H	1.11173400	5.96086200	5.04852900
C	4.58499500	1.36562400	1.96961500	H	-0.07913100	4.63996700	5.02167300
N	4.13495700	1.55677900	0.73998900	H	5.37290600	6.28797200	-2.53164700
C	0.59573600	5.24487700	4.40193700	H	3.37124800	3.12713100	-4.08225500
N	1.57947100	4.44788700	3.70844800	H	-1.25322700	6.49857400	-3.14639800
C	1.19389500	3.48680400	2.80989400	H	2.49587100	4.32808400	4.11381000
O	-0.03374600	3.52036700	2.46537100	C	4.88802000	-6.02642400	4.30832000
O	2.09887400	2.70384200	2.38258700	C	4.92551600	-4.96787200	3.19863700
C	-3.35999400	4.26758200	3.99695300	C	4.12694100	-3.69245800	3.53972700
C	-3.40815600	2.77716100	3.84249900	C	4.63647600	-2.49609800	2.72590500
N	-2.73862700	2.07891600	2.84004500	C	2.61705300	-3.89436900	3.34096400
C	-4.10219500	1.87940900	4.61258600	C	6.34287300	-2.30519300	-3.75262500
C	-3.03620800	0.79697600	3.01113900	C	5.33923000	-2.28710700	-2.60122500
N	-3.85757700	0.63363800	4.06772000	S	5.67418600	-3.59517100	-1.32919200
C	-1.64297200	5.47566600	-3.22745200	C	0.96502200	-6.40972700	-2.17729100
C	-1.91906700	4.87221400	-1.89236700	C	1.63362800	-5.17518500	-2.76891800
N	-2.86211300	5.36802100	-1.00166000	O	2.35781700	-4.43984600	-2.07645800
C	-1.35798500	3.80152600	-1.24874100	C	0.29869200	-6.12336200	-0.83110100
C	-2.83654400	4.60307700	0.11809500	C	-1.02053700	-5.36428700	-0.97442100
N	-1.93100000	3.64947400	-0.00105400	O	-1.46164700	-5.01301700	-2.07308100
C	2.30326200	3.19407700	-3.85829300	N	-1.67390300	-5.10950100	0.18277300
C	1.92062100	2.19053100	-2.78040300	N	1.46231300	-4.97541500	-4.08962800
O	2.72444100	1.94686900	-1.84742400	C	2.04034600	-3.83115700	-4.78097600
O	0.74364500	1.69850300	-2.91417800	H	5.97366800	-4.69616800	3.01251900
Zn	2.31613700	2.37681100	0.32079400	H	4.55106300	-5.38933200	2.25505900
Zn	-1.18703300	2.31145200	1.36272300	H	4.29771200	-3.46672300	4.60394500
H	4.13598200	7.54470600	-2.66113500	H	5.68273800	-2.27599900	2.97639900
H	5.29821500	7.57735000	-1.32512000	H	4.04193800	-1.59518900	2.92319800
H	4.25125800	3.93145000	-1.56214800	H	4.60026300	-2.70178200	1.64862600
H	2.59100600	7.50649300	-0.11602700	H	2.05056100	-3.00843000	3.65293800
H	1.33929100	5.56626800	0.97020600	H	2.38811500	-4.08154200	2.28302900
H	7.53558500	-0.08741800	-0.87320800	H	2.24175500	-4.74655100	3.91869200
H	7.36278900	-1.21954800	0.47139300	H	3.86427900	-6.34872500	4.53290500
H	4.95417700	1.09201800	-1.18596300	H	5.35721300	-1.32127100	-2.08773100
H	6.32997000	0.46955600	2.73449000	H	4.31838900	-2.44467600	-2.95647000
H	4.06041000	1.65413200	2.86639100	H	4.51581900	-4.26941000	-1.49494500
H	-2.34172900	4.63768500	3.84409800	H	7.36817100	-2.17277400	-3.39007800
H	-4.73475900	2.01808200	5.47587400	H	0.98410500	-5.53988500	-0.20456400
H	-4.17510100	-0.26022900	4.41773300	H	0.10548000	-7.06440000	-0.30130300
H	-2.64474900	-0.00457800	2.40512300	H	-1.32199300	-5.40252400	1.08144300
H	-0.89774400	4.87040200	-3.74973000	H	-2.57294900	-4.63452300	0.12854600
H	-2.53954500	5.51240000	-3.85867000	H	0.23834200	-6.83656900	-2.87402200
H	-0.60005000	3.11936200	-1.60229200	H	3.12074000	-3.80470900	-4.61654500
H	-3.47777500	6.15297700	-1.16397600	H	1.59647600	-2.89640000	-4.42211100
H	-3.47382900	4.76904600	0.97336000	H	0.74052700	-5.50560100	-4.55674000
H	-0.01512400	5.80431500	3.68805100	H	1.75981600	-7.15145500	-2.02815900
H	1.71816200	3.03582400	-4.76636900	H	1.84871000	-3.93617500	-5.85075200
H	2.10543700	4.20541800	-3.48349900	H	6.30538800	-3.25511800	-4.29509700

H	6.12616500	-1.49357800	-4.45917000	H	0.34498300	0.82451300	-1.99855100
H	5.32249100	-5.63528300	5.23627200	C	-1.89021600	-2.66834200	-5.27544400
H	5.45730000	-6.91897300	4.02563100	C	-3.19027200	-2.41697400	-4.53593800
C	-5.39971500	-3.71669400	6.77578700	O	-4.29732600	-2.58021500	-5.04497600
C	-4.28614400	-4.59805900	6.18518600	N	-2.99709400	-1.97739100	-3.26024100
C	-3.63741700	-3.96577300	4.97305300	C	-4.07188400	-1.58265200	-2.37610300
C	-2.47337800	-3.19359200	5.09464500	C	-4.02992800	-0.05868500	-2.17563100
C	-4.21612900	-4.09888600	3.70257100	O	-3.01474200	0.45751700	-1.67747000
C	-1.90260100	-2.57402100	3.98027400	C	-3.88442200	-2.26244000	-1.00474100
C	-3.65414500	-3.47905000	2.58565000	O	-3.86898500	-3.67576400	-1.10131500
C	-2.49027100	-2.71432800	2.71950200	N	-5.09433600	0.69997300	-2.51431800
H	-4.70736900	-5.57334700	5.91130300	C	-6.34213000	0.28866400	-3.20809300
H	-3.52791100	-4.78953900	6.95423000	C	-6.12709900	0.09739800	-4.71449700
H	-2.00517900	-3.08591700	6.07105500	C	-7.28490400	1.45917400	-2.86654200
H	-5.11646400	-4.69895500	3.58764800	C	-6.35684600	2.68574600	-2.86188600
H	-0.99619200	-1.98410100	4.09166400	C	-5.05122500	2.15051400	-2.25281700
H	-4.12256800	-3.59870600	1.61235500	H	-4.14805000	2.58798600	-2.68857000
H	-5.00317000	-2.74612400	7.09687700	H	-4.99717800	2.31725200	-1.16953200
H	-6.18688200	-3.53002900	6.03643200	H	-6.18688000	3.03720100	-3.88536000
H	-5.86091800	-4.19643100	7.64614800	H	-6.76596500	3.52472400	-2.29065500
N	-0.18116700	-0.15224800	-1.13707000	H	-8.10881400	1.54344200	-3.58071800
C	0.31551300	-1.39844600	-1.64074000	H	-7.71641400	1.31060400	-1.86923500
O	-0.26969400	-1.99093600	-2.55263700	H	-6.71421800	-0.64226100	-2.76998100
N	1.47238200	-1.82126900	-1.10955100	H	-5.72471300	1.00846100	-5.17259900
C	2.15852000	-1.11275500	-0.03637600	H	-5.45034500	-0.73463500	-4.92320700
C	1.12986000	-0.59922800	0.96482000	H	-7.08647100	-0.12770700	-5.19612800
C	0.09966200	0.36135900	0.33983400	H	-4.99980400	-1.92774100	-2.83165500
O	-1.05989900	0.38242300	1.02682800	H	-3.16769600	-3.94219400	-1.73847700
H	2.74934300	-0.29156900	-0.45236800	H	-4.72169400	-2.00075300	-0.34778600
H	2.85141500	-1.81281100	0.43507200	H	-2.96561200	-1.87270900	-0.54350800
H	1.60946300	-0.06814300	1.79316700	H	-2.03299000	-1.84447900	-2.94442300
H	0.58716700	-1.45413800	1.38146500	H	-1.37866700	-1.71911600	-5.47170800
H	-1.19766100	-0.07917800	-1.31089200	H	-1.21744300	-3.28580400	-4.67301300
H	1.83736000	-2.70112000	-1.47727700	H	-2.11217600	-3.15930700	-6.22478100
O	0.55397200	1.66163100	0.17244500	H	-2.04320600	-2.22700700	1.85688900

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C	-8.42324300	-0.66453600	-3.47860600	N	-5.35376900	-2.02482900	2.56098800
C	-7.43862000	-0.76494100	-2.37211300	C	-4.17371500	-1.63290600	1.96009000
N	-7.56584900	-1.60693200	-1.27731400	O	-3.30048300	-2.56320000	1.85016900
C	-6.24750100	-0.12692000	-2.18330700	O	-4.09659600	-0.43620800	1.56420600
C	-6.47598600	-1.45330900	-0.48506700	C	-2.14241200	-5.69373700	3.03873400
N	-5.65151700	-0.56531000	-1.01679500	C	-0.94589200	-4.80258600	3.19711900
C	-5.19143100	5.70805400	-0.17183900	N	-0.62025200	-3.79276600	2.29431900
C	-4.75653100	4.31860200	0.16345600	C	0.00379200	-4.81607100	4.18550600
N	-4.50418300	3.89847800	1.46183500	C	0.49661200	-3.22598400	2.73669100
C	-4.50627800	3.21484800	-0.60916100	N	0.90511700	-3.81709400	3.87378500
C	-4.12563500	2.59890500	1.43623500	C	-3.07114300	-4.46422100	-4.32505400
N	-4.11573500	2.15638200	0.19099100	C	-2.66478400	-4.50567300	-2.89107000
C	-5.48553100	-3.33291600	3.16918100	N	-2.61696500	-5.66175900	-2.12349400

C	-2.29581100	-3.49979700	-2.04012500	C	5.45683900	4.20834800	-0.48240000
C	-2.23471800	-5.33235200	-0.86839600	C	6.37198600	3.03541200	-0.82776100
N	-2.03642200	-4.02492600	-0.78428000	O	6.45479400	2.56300300	-1.96573700
C	-3.80958000	0.06698500	-4.64008800	N	7.12419700	2.56245800	0.19816400
C	-3.03907300	0.06188800	-3.31862900	N	3.03774300	4.70860500	-3.27628600
O	-3.52809900	0.82402600	-2.38632600	C	1.65384600	4.63358800	-3.71641800
O	-2.05347900	-0.67895400	-3.21158100	H	-1.62779800	5.89665400	4.48746500
Zn	-3.83350800	0.25351700	-0.47216300	H	-1.27631500	7.42494300	3.68895000
Zn	-1.67341600	-2.83997400	0.80628400	H	0.73031300	5.13313900	3.93716300
H	-8.55126600	-1.61856400	-4.00578600	H	-1.22439400	4.37014800	2.61176300
H	-9.41338900	-0.34637200	-3.12817300	H	0.17814900	4.60460000	1.55089000
H	-5.75963700	0.60763500	-2.80047700	H	-1.11784400	5.80775100	1.58127700
H	-8.34150100	-2.22818900	-1.09291300	H	1.93653900	6.30230300	2.07902900
H	-6.32930400	-1.97057700	0.45263700	H	0.74677700	7.61277600	2.12669600
H	-5.41350500	5.77903600	-1.23962400	H	1.82189500	7.34049400	3.50758600
H	-4.40739200	6.44000500	0.05568300	H	0.56753200	7.86911500	5.37285900
H	-4.56386500	3.09767000	-1.68022300	H	-2.90411400	4.64993700	-3.09143700
H	-4.55681500	4.47706900	2.28900800	H	-1.30948900	5.02541100	-3.72178500
H	-3.89421000	2.00663000	2.30810400	H	-0.24015500	5.61874800	-1.38459100
H	-3.02805500	-5.10451600	2.78301300	H	-3.22382500	7.06770800	-2.41473300
H	0.11448600	-5.43843400	5.05987200	H	4.62986700	3.81133700	0.11638000
H	1.69337400	-3.50903800	4.42897100	H	6.00947600	4.90843600	0.15414200
H	1.00521000	-2.39653700	2.27200500	H	6.90495400	2.81957100	1.14964700
H	-2.96303800	-3.43932500	-4.68916000	H	7.61018700	1.68068900	0.03811000
H	-2.44482200	-5.11121300	-4.95138000	H	5.48427800	4.64948800	-2.59896200
H	-2.18898800	-2.44502100	-2.26491500	H	1.22817000	5.63249800	-3.88327200
H	-2.81434800	-6.59867800	-2.44795600	H	1.07367400	4.12510700	-2.94566800
H	-2.11388900	-6.04824000	-0.06966000	H	3.75504800	4.85696300	-3.97191900
H	-5.32560000	-4.11385700	2.42144900	H	1.59282700	4.06546900	-4.64905200
H	-3.15213600	-0.22125300	-5.46382400	H	-1.61176500	7.45488100	-3.03030900
H	-4.62282000	-0.66740200	-4.57988100	H	-2.88030800	6.93751600	-4.15329900
H	-6.09696200	5.99507700	0.37646500	H	0.24906800	6.29990800	6.12574400
H	-1.98754600	-6.44362300	2.25167200	H	-0.97217300	7.57988100	6.18629100
H	-2.34138100	-6.23598800	3.96740000	C	4.39052200	-2.43906200	7.74720100
H	-6.50033800	-3.43620900	3.56450700	C	4.05798600	-0.94713300	7.57691200
H	-4.77378500	-3.49464700	3.98893700	C	3.00136300	-0.69205400	6.52234200
H	-8.07913500	0.07228000	-4.20865800	C	1.65274100	-0.53702500	6.87255500
H	-4.25694100	1.04428300	-4.84730100	C	3.34644800	-0.62038600	5.16405100
H	-4.11520700	-4.77095600	-4.46607100	C	0.67877600	-0.30593200	5.89926900
H	-5.92696500	-1.26664500	2.90450500	C	2.37990600	-0.38407600	4.18339200
C	-0.20741000	7.11623200	5.55267100	C	1.04038100	-0.22428700	4.55302800
C	-0.81330700	6.59501900	4.24325500	H	4.97457500	-0.40427100	7.31419400
C	0.19516100	5.87564700	3.32498500	H	3.72054000	-0.54050200	8.53792200
C	-0.53325600	5.12094900	2.20613300	H	1.36618400	-0.58309900	7.92119900
C	1.23612200	6.83723200	2.73108600	H	4.38949700	-0.72627300	4.87246100
C	-2.46591200	6.77929500	-3.14955200	H	-0.35940500	-0.17658800	6.19505500
C	-2.04852300	5.32215500	-2.97174600	H	2.67246000	-0.30354400	3.13838500
S	-1.39530800	4.92524800	-1.29491200	H	3.50268900	-3.00845200	8.04670900
C	4.89579200	4.92450800	-1.71817400	H	4.76587900	-2.86893100	6.81108800
C	3.41101700	4.66465300	-1.97059500	H	5.15868500	-2.58389300	8.51473900
O	2.59509500	4.49144200	-1.05829600	C	4.59447400	1.13784200	-4.23319900

C	5.15504900	-0.21118100	-3.81563300	H	0.31464300	0.38501400	-1.56764800
O	5.64576200	-0.99935100	-4.62217400	H	3.11679600	-4.71805500	-1.04000700
N	5.10437900	-0.46021100	-2.47125700	H	4.64846600	-5.01345400	-0.22710600
C	5.89498300	-1.52300800	-1.86341600	H	3.49681700	-6.42885700	-2.63353300
C	5.01859100	-2.63279700	-1.25382200	H	4.75198300	-7.01533400	-1.54621300
O	4.54189600	-2.49110200	-0.11286700	H	5.43641000	-6.22052000	-4.08342800
C	6.77452900	-0.91379600	-0.75028200	H	6.48693000	-5.79312100	-2.72331800
O	7.69401800	0.04073700	-1.25888500	H	6.03354800	-3.60675000	-3.65221800
N	4.82060800	-3.79364500	-1.92294200	H	3.08771200	-4.43288800	-3.95598700
C	5.16779500	-4.17555900	-3.31092000	H	3.79786800	-2.84722800	-4.35010100
C	4.00036700	-3.91787700	-4.27677100	H	4.26380300	-4.27509900	-5.27869000
C	5.47919200	-5.67259500	-3.13739300	H	6.53994200	-1.91673800	-2.65007200
C	4.42093200	-6.14451600	-2.11957600	H	7.19746600	0.73309900	-1.74845600
C	4.18118600	-4.91718400	-1.21181000	H	7.37093500	-1.70133000	-0.27844600
O	4.02831600	1.26504800	-0.36426200	H	6.12062500	-0.47729700	0.01446400
C	2.88848400	0.90179400	-0.01688700	H	4.72575000	0.24666400	-1.83494500
N	2.64443900	-0.36090100	0.46618600	H	4.28181800	1.08514500	-5.27818200
C	0.47384400	1.47425200	0.31839100	H	3.75672100	1.45072800	-3.60177600
C	-0.34597200	0.67327200	-0.74274900	H	5.38228500	1.88957200	-4.12341000
C	-0.93066300	-0.60316800	-0.19957900	N	1.83617900	1.77228100	-0.06639900
O	-2.17138600	-0.86758800	-0.27071800	H	2.06495600	2.70006800	-0.41816500
O	-0.17928200	-1.46545700	0.36628800	H	3.40903800	-1.02346700	0.31674600
H	1.71448200	-0.76232000	0.38050200	H	4.98844800	6.01089900	-1.59004600
H	-0.02653300	2.42885100	0.49467600	H	0.28565300	-0.02393200	3.79605900
H	0.48145400	0.93544500	1.27351900				
H	-1.14223300	1.27699900	-1.18008300				

(5R)-MeHYD-ES-II (SkDHPase)

C	4.43043300	7.44188000	-1.61543500	N	-4.76624200	0.82247100	2.89804900
C	3.76398500	6.45838100	-0.72508800	C	-1.91028700	5.99596500	-2.84167000
N	3.16918900	6.76390000	0.48998200	C	-2.17819000	5.20837200	-1.60801300
C	3.55501500	5.12028200	-0.88943700	N	-3.19441900	5.44422100	-0.69180600
C	2.63167900	5.62827200	1.00320300	C	-1.49879700	4.13566000	-1.10983000
N	2.84270300	4.61404300	0.18077300	C	-3.09188200	4.52612400	0.30334300
C	7.36528000	0.24160200	-0.37772200	N	-2.06766200	3.71879300	0.07738100
C	6.03861500	0.68876600	0.14427500	C	2.06023900	3.90494500	-3.86094600
N	5.68850400	0.60076000	1.48505700	C	1.71301700	2.91088100	-2.74955000
C	4.94497100	1.25326600	-0.46122200	O	2.64687800	2.63576800	-1.91172200
C	4.44091700	1.10160100	1.64514600	O	0.53899300	2.48251100	-2.68567600
N	3.96204600	1.50496000	0.48001100	Zn	2.25930100	2.61766500	0.16645300
C	0.60029600	4.94474700	4.63259400	Zn	-1.08410100	2.36583100	1.30224900
N	1.55712200	4.22453200	3.81898200	H	3.74196500	8.22606700	-1.95213600
C	1.12367900	3.27112800	2.92185100	H	5.28029600	7.93634600	-1.13016600
O	-0.14623700	3.23431700	2.76407900	H	3.83978400	4.47790500	-1.70444700
O	1.99405200	2.57410800	2.33009400	H	3.14143500	7.67338200	0.92679000
C	-3.34492100	3.91891900	4.24545600	H	2.13101200	5.57135600	1.95895400
C	-3.70539400	2.64599000	3.53033700	H	7.45047100	0.50164300	-1.43474200
N	-2.99203400	2.06544700	2.47344800	H	7.49710600	-0.84138600	-0.28731900
C	-4.80201200	1.86704100	3.79733900	H	4.78343800	1.50931600	-1.49654400
C	-3.66880100	0.97902100	2.12582200	H	6.25700800	0.19676100	2.21504900

H	3.92025200	1.18327700	2.58620300	H	4.38715700	-4.08415700	-2.21996800
H	-2.32068400	3.87697400	4.62540700	H	7.44177000	-1.68487500	-3.62560000
H	-5.58037600	1.96706000	4.53707800	H	-1.16834300	-4.38133800	-1.95580200
H	-5.40663600	0.04399100	2.85280000	H	0.11622800	-4.46359500	-0.74972900
H	-3.42356500	0.31382500	1.31215600	H	0.39002100	-7.31418200	-0.38255700
H	-1.09707600	5.51818800	-3.39093600	H	-1.11693600	-7.85128000	0.28728800
H	-2.78088600	6.03986600	-3.50640200	H	0.00077900	-6.09603600	-3.34262400
H	-0.66077200	3.63300100	-1.56350400	H	3.22463900	-3.38006700	-4.98924400
H	-3.89400300	6.16985200	-0.74833600	H	1.93690200	-2.22646900	-4.54232900
H	-3.76379200	4.47165400	1.14534300	H	0.75451500	-4.78934800	-4.94811200
H	-0.14819800	5.41528900	3.99391000	H	1.21916800	-6.33512700	-2.09242900
H	1.36184800	3.81036100	-4.69407800	H	1.84420600	-3.11854400	-6.07978000
H	1.98387300	4.91978600	-3.45335900	H	6.36974600	-2.13628000	-4.95583600
H	8.19174500	0.72804300	0.15249700	H	6.27353800	-0.51110900	-4.25259500
H	-3.40573000	4.79131600	3.58423200	H	6.29015500	-6.56994400	3.63768100
H	-4.02730200	4.08148500	5.08238800	H	4.52463000	-6.63694600	3.63498600
H	1.12428300	5.72431100	5.19256800	C	-4.89294400	-4.26222900	6.71815800
H	0.07620400	4.29895300	5.34897000	C	-3.50043200	-4.84126000	6.42492700
H	4.80845100	6.93028300	-2.50262800	C	-2.97313100	-4.25885500	5.13791400
H	3.08546200	3.76592000	-4.21394600	C	-2.43353900	-2.96799500	5.12231700
H	-1.61224400	7.02765600	-2.61946100	C	-3.15184100	-4.91650900	3.91437400
H	2.49665400	4.09446300	4.16421600	C	-2.12472300	-2.33032700	3.92473900
C	5.38262600	-5.96800400	3.75786000	C	-2.84523600	-4.30024100	2.70367100
C	5.34398000	-4.82489900	2.73554300	C	-2.35753500	-2.99222500	2.71484600
C	6.57387400	-3.89815300	2.79206800	O	-2.11325300	-2.38159500	1.51271800
C	6.58365700	-2.93210400	1.60138900	H	-3.55944400	-5.93334200	6.35531200
C	6.66555200	-3.12376800	4.11563900	H	-2.82415900	-4.61320200	7.25775600
C	6.42717900	-1.57103500	-4.02151100	H	-2.27283100	-2.44380900	6.06165800
C	5.37959000	-2.04990100	-3.02094400	H	-3.56060100	-5.92414800	3.90694600
S	5.66042500	-3.82771800	-2.58928600	H	-1.71376700	-1.32361100	3.92089400
C	0.54243300	-5.59449700	-2.53403400	H	-2.98742900	-4.80907000	1.75526800
C	1.44592800	-4.48057400	-3.06278500	H	-1.86738800	-1.45723500	1.68623400
O	2.19326300	-3.85281100	-2.29828200	H	-4.84790800	-3.17276800	6.81641000
C	-0.44619300	-5.05128100	-1.48508500	H	-5.58783100	-4.49385500	5.90462700
C	-1.25823200	-6.08779900	-0.71696500	H	-5.31115500	-4.66739300	7.64631700
O	-2.45568800	-5.92414200	-0.46891900	N	-0.81182000	-0.60451400	-0.68170400
N	-0.60315200	-7.19048500	-0.27675000	C	0.04893100	-1.36085000	-1.50458900
N	1.39546300	-4.24773400	-4.38897900	O	-0.25221000	-1.79067800	-2.61113300
C	2.15074900	-3.17808500	-5.03503000	N	1.20388800	-1.52870300	-0.81656400
H	5.27317100	-5.24942200	1.72594000	C	1.12409900	-0.99206000	0.53931300
H	4.43350700	-4.22467100	2.88156800	C	-0.26628100	-0.36132300	0.51991800
H	7.46786600	-4.53418100	2.71221000	O	-0.86432700	0.16877900	1.48123000
H	6.56793400	-3.46149000	0.64294600	H	1.85156200	-0.18938400	0.68931700
H	7.48064700	-2.30087700	1.61990700	H	-1.79695600	-0.37996600	-0.91639800
H	5.70426900	-2.27516800	1.62698800	H	1.85952000	-2.23302700	-1.14660800
H	7.55128600	-2.47834200	4.13304400	O	0.41059700	2.05014300	0.01183900
H	5.78170600	-2.48702300	4.25664600	H	0.26509500	2.02758300	-0.95945100
H	6.73248200	-3.78814900	4.98154000	C	-1.83371800	-2.12082000	-5.30705000
H	5.36154700	-5.60020000	4.78818200	C	-3.18445700	-1.98955200	-4.63521400
H	5.41248900	-1.45144300	-2.10642600	O	-4.24741100	-2.11671700	-5.23711300
H	4.37422700	-1.96317500	-3.43699200	N	-3.09410100	-1.69869800	-3.30487200

C	-4.24190700	-1.76481700	-2.42384600	H	-6.90624300	-0.90097100	-2.86736900
C	-4.39461500	-0.40555500	-1.73241600	H	-5.74518300	1.43863100	-4.49449000
O	-3.51335300	-0.02001600	-0.92596400	H	-5.40362500	-0.29217300	-4.74935400
C	-4.08829800	-2.88155700	-1.37256600	H	-7.01995700	0.34116900	-5.05298200
O	-3.84688500	-4.08602200	-2.05986200	H	-5.09377600	-1.99982500	-3.06187900
N	-5.45777800	0.37267000	-1.98729900	H	-3.46735500	-4.73470500	-1.43484300
C	-6.56948700	0.13550200	-2.95136900	H	-5.01866400	-2.91990000	-0.77731600
C	-6.14710800	0.42496900	-4.39667900	H	-3.27764200	-2.62762700	-0.67849600
C	-7.64624600	1.10108900	-2.42081200	H	-2.15920900	-1.72806500	-2.90491400
C	-6.83899000	2.31070000	-1.92261000	H	-1.18427500	-1.27759100	-5.06055300
C	-5.58336500	1.67718800	-1.30536600	H	-1.32908400	-3.02616700	-4.95637900
H	-4.67346000	2.26629800	-1.44648800	H	-1.98160000	-2.18135100	-6.38566500
H	-5.69430800	1.50869300	-0.22769900	C	1.27493900	-2.04731100	1.64026800
H	-6.56656200	2.95804900	-2.76211900	H	2.26861000	-2.50165600	1.58996400
H	-7.38838400	2.92120000	-1.20122900	H	1.15969900	-1.57484300	2.61903600
H	-8.37855000	1.35720400	-3.18991200	H	0.51832900	-2.82852800	1.54068200
H	-8.18348100	0.63743000	-1.58568800				

(5R)-MeHYD-TS1-II (SkDHPase)

C	1.11654800	8.62024800	-1.24607900	O	-0.28981300	2.53028300	-2.59162700
C	0.70641400	7.40332600	-0.49471800	Zn	0.94316300	3.27866100	0.36440300
N	-0.32351500	7.35605500	0.43467600	Zn	-2.15329000	1.64368200	1.25206400
C	1.17816900	6.12355300	-0.55491200	H	0.30086100	9.01825600	-1.86087000
C	-0.43641400	6.08181800	0.88778400	H	1.45363400	9.42496300	-0.58239100
N	0.45903400	5.30793000	0.29920500	H	1.95318200	5.71290200	-1.17913800
C	6.60907300	3.20181800	0.32316300	H	-0.89502700	8.13457600	0.72826200
C	5.17498100	3.13227000	0.72892800	H	-1.15900700	5.76704500	1.62407200
N	4.77137600	3.02155000	2.05290000	H	6.68130100	3.29791600	-0.76180000
C	4.00721700	3.16582300	0.01232900	H	7.16005800	2.30044600	0.61411600
C	3.41921900	2.99890700	2.09687700	H	3.85136500	3.24695500	-1.05188100
N	2.92611600	3.08339900	0.87187400	H	5.38419900	2.96513000	2.85321200
C	-1.88073600	4.62409800	4.66920300	H	2.82574600	2.92760700	2.99429600
N	-0.64813500	4.35428500	3.95836600	H	-4.11403800	2.49052300	4.41708400
C	-0.61114900	3.46009200	2.92271900	H	-6.18316300	-0.65609300	4.18953100
O	-1.76152400	3.07967000	2.50289200	H	-5.04765200	-2.30780100	2.59116500
O	0.51638400	3.13476800	2.44777000	H	-3.29721600	-1.18766900	1.15725300
C	-5.01994200	2.09553100	3.94901400	H	-2.97235600	4.71175100	-3.46956600
C	-4.74879500	0.78631000	3.26611600	H	-4.69475800	4.45537700	-3.76286600
N	-3.78726000	0.58083700	2.27170200	H	-1.94332200	3.06748300	-1.61771600
C	-5.39606600	-0.39960700	3.49843600	H	-6.01305100	3.95394900	-1.15459700
C	-3.87867600	-0.69739700	1.92310700	H	-5.35634000	2.38562600	0.74146000
N	-4.83671800	-1.32194000	2.63859100	H	-2.67549300	4.86194400	3.96110300
C	-3.96013700	4.75710600	-3.00745800	H	0.04039000	4.13953700	-4.52993500
C	-3.97427800	3.86360000	-1.81705500	H	0.09041600	5.37491600	-3.25014700
N	-5.07810600	3.59822800	-1.01832100	H	7.11643900	4.06472200	0.76949300
C	-2.95373600	3.15443200	-1.25200000	H	-5.37443300	2.85763600	3.24537800
C	-4.69348100	2.76149200	-0.02198700	H	-5.78333200	1.96567300	4.71912600
N	-3.40571000	2.47713100	-0.13706500	H	-1.73016700	5.48147600	5.33034300
C	0.58816000	4.48458600	-3.65173000	H	-2.21319900	3.77416100	5.27929700
C	0.60172400	3.41137800	-2.56581700	H	1.94413600	8.37227800	-1.91326200
O	1.49300400	3.52496200	-1.64997000	H	1.60349600	4.77551700	-3.93290600

H	-4.16666400	5.80136500	-2.74427500	C	-1.28364100	-5.59296800	3.80444400
H	0.23577200	4.55606400	4.39947500	C	-1.41928500	-2.81572300	3.90786600
C	6.98039600	-3.38182700	4.33699700	C	-1.14984600	-4.85935900	2.63046200
C	6.56686500	-2.32692500	3.30264700	C	-1.23779700	-3.46432400	2.68140000
C	7.58799000	-2.05910600	2.18172000	O	-1.13866600	-2.77791700	1.50467000
C	6.98668500	-1.11646500	1.12971600	H	-1.25294000	-6.73136600	6.24936200
C	8.91519700	-1.50052300	2.71475900	H	-1.47531400	-5.25176300	7.17392700
C	6.80065600	1.25857500	-3.36871400	H	-1.70204500	-3.06303800	6.02140200
C	6.21321800	0.13795700	-2.51703600	H	-1.23091500	-6.67835700	3.75836400
S	7.10343600	-1.44746100	-2.84863100	H	-1.45667100	-1.72989500	3.94481900
C	2.93531000	-4.68704900	-2.18586300	H	-0.97410500	-5.34646800	1.67648600
C	3.38148100	-3.32625100	-2.72405100	H	-1.16734300	-1.81375600	1.67222800
O	3.81741000	-2.44964900	-1.96263000	H	-3.88088600	-5.13644700	6.41846500
C	1.77674500	-4.54200400	-1.18142500	H	-3.65719100	-6.62084000	5.48564000
C	1.40284300	-5.80807800	-0.42126200	H	-3.55437600	-6.66450900	7.25382300
O	0.23659700	-6.19783600	-0.32022600	N	-0.43920200	-0.68884800	-0.67972200
N	2.41460200	-6.48733000	0.17601300	C	0.70624000	-1.04509300	-1.38657800
N	3.30870900	-3.16847900	-4.06055600	O	0.71454200	-1.66416200	-2.44749200
C	3.64939700	-1.91934100	-4.73549200	N	1.78008000	-0.61529400	-0.66714500
H	5.61945400	-2.63832300	2.84110600	C	1.38356600	-0.15484900	0.66436100
H	6.35260000	-1.37817200	3.81745800	C	-0.14551700	-0.04274700	0.49055600
H	7.80108900	-3.01867700	1.68712500	O	-0.98519300	-0.02228500	1.46446100
H	6.06143900	-1.52453100	0.70694900	H	1.80656400	0.82362300	0.88508900
H	7.68041000	-0.94847000	0.29989900	H	-1.39806200	-0.93711600	-0.96896300
H	6.74564100	-0.14245600	1.57795200	H	2.68340000	-1.02432600	-0.89378200
H	9.61662300	-1.30825100	1.89625100	O	-0.37600900	1.83596800	-0.00133100
H	8.75498700	-0.55281800	3.24529100	H	-0.41144900	1.87034100	-0.99488700
H	9.40234900	-2.19045400	3.40969800	C	-0.38214000	-2.56376100	-5.36733300
H	7.86705100	-3.07783700	4.90157500	C	-1.69646100	-3.00669600	-4.75662900
H	6.30251300	0.37318300	-1.45278400	O	-2.58038100	-3.54015200	-5.42484300
H	5.15600000	-0.01948800	-2.74002600	N	-1.82034800	-2.71720300	-3.43088200
H	6.17469600	-2.23693300	-2.27059700	C	-2.92346700	-3.22492700	-2.63953800
H	7.86364200	1.41008800	-3.15507400	C	-3.69068400	-2.04401300	-2.03274900
H	0.87591200	-4.20495100	-1.69539100	O	-3.13660000	-1.32246600	-1.17060500
H	2.04857100	-3.77452200	-0.44706800	C	-2.42639700	-4.15533600	-1.51533100
H	3.36124000	-6.14525800	0.19551500	O	-1.67309100	-5.18433500	-2.10931800
H	2.17815200	-7.29256700	0.73659200	N	-4.95445500	-1.78497000	-2.41244200
H	2.64889000	-5.36741000	-2.99450700	C	-5.77695800	-2.47106500	-3.44786600
H	4.71548700	-1.70172400	-4.62684900	C	-5.41802400	-2.01215600	-4.86658900
H	3.06412100	-1.09640000	-4.31619900	C	-7.20217400	-2.07490300	-3.01817600
H	2.89413900	-3.90830700	-4.60582600	C	-7.03930800	-0.63665400	-2.50034500
H	3.81989700	-5.11952800	-1.70423600	C	-5.67999100	-0.66236800	-1.78515900
H	3.41254700	-2.02338900	-5.79495900	H	-5.10742700	0.26332100	-1.88880100
H	6.70111800	1.04151300	-4.43610200	H	-5.78216700	-0.85913900	-0.71125100
H	6.27825100	2.20085900	-3.16807500	H	-7.01782000	0.06771600	-3.33784000
H	7.20762500	-4.34008300	3.85581200	H	-7.84952700	-0.33017000	-1.83338700
H	6.17709100	-3.55723600	5.05978300	H	-7.91529000	-2.15951000	-3.84150600
C	-3.31114300	-6.07018900	6.36620800	H	-7.54355100	-2.73035300	-2.20883500
C	-1.80464600	-5.78418600	6.27372800	H	-5.63559800	-3.55163400	-3.36612300
C	-1.49909500	-4.96911000	5.04122600	H	-5.48710000	-0.92337300	-4.95981400
C	-1.54853000	-3.57180600	5.07225000	H	-4.41350600	-2.33602800	-5.14622500

H	-6.11798300	-2.45941100	-5.58052100	H	-0.04993000	-3.34307800	-6.05811900
H	-3.54042200	-3.80352200	-3.32731300	H	-0.55558900	-1.66073900	-5.96273300
H	-1.09186900	-5.58121600	-1.43139300	C	1.75982500	-1.13431800	1.78224600
H	-3.31161300	-4.54275600	-0.97821100	H	2.84825700	-1.23469300	1.83532600
H	-1.84358800	-3.57510700	-0.78923100	H	1.40024700	-0.75743700	2.74323900
H	-0.99066300	-2.36566900	-2.95661600	H	1.31890000	-2.11854400	1.60949600
H	0.38809200	-2.35074000	-4.62725200				

(5R)-MeHYD-INT1-II (SkDHPase)

C	3.49431700	7.85677800	-1.44009500	H	4.65572800	2.13363400	-1.41185500
C	2.75161500	6.80668500	-0.69243400	H	6.21696500	0.97760000	2.31312300
N	1.69203000	7.04014200	0.17435000	H	3.81048400	1.77808400	2.67598000
C	2.89425400	5.44979100	-0.70724800	H	-2.81010900	3.35229100	4.58845700
C	1.24127700	5.84608000	0.63638800	H	-5.78098400	0.97332600	4.65156900
N	1.94951400	4.86093000	0.11212400	H	-5.33955400	-0.91782300	2.97820000
C	7.30564900	1.06456800	-0.28737800	H	-3.47263000	-0.35424600	1.36831400
C	5.96554900	1.44316300	0.24181900	H	-1.66237500	5.37209800	-3.28543100
N	5.62555000	1.34854800	1.58348200	H	-3.40556300	5.52807600	-3.51521300
C	4.83700400	1.92027000	-0.37054000	H	-1.01922700	3.46400800	-1.45282100
C	4.34515800	1.75359000	1.73984400	H	-4.71901700	5.35057000	-0.88942700
N	3.83965700	2.10710800	0.56895400	H	-4.44078700	3.64667000	0.98024600
C	-0.06515800	4.77150000	4.70438900	H	-0.81134000	5.23829900	4.06084500
N	0.93296800	4.10828000	3.89119400	H	0.90894800	3.93686700	-4.59431100
C	0.61353600	3.35355500	2.80052300	H	1.45688900	5.08319600	-3.34505900
O	-0.60758200	3.42182300	2.41039900	H	8.11197400	1.59090800	0.23562200
O	1.54780300	2.70221000	2.23917400	H	-4.02545900	4.09535300	3.55325200
C	-3.84261500	3.26082200	4.24005100	H	-4.50944000	3.37870600	5.09699200
C	-4.07416200	1.93662800	3.57980400	H	0.41809800	5.54599100	5.30530900
N	-3.32276200	1.46727300	2.50291000	H	-0.58244500	4.08286400	5.38564400
C	-5.02105500	0.99564200	3.88699600	H	4.26957500	7.38733600	-2.04832900
C	-3.81923900	0.27776500	2.17452300	H	2.64318500	4.07493000	-4.17192100
N	-4.84687100	-0.03667400	2.98628100	H	-2.54186200	6.70177400	-2.51150800
C	-2.59499400	5.64178000	-2.78662200	H	1.86931000	3.99341000	4.24667200
C	-2.78261200	4.76222700	-1.59790500	C	6.07738100	-5.42642600	3.70658400
N	-3.89939600	4.77236800	-0.77425800	C	5.90644600	-4.27765700	2.70439000
C	-1.96076300	3.81066600	-1.06064200	C	6.83726900	-3.07769700	2.96941100
C	-3.71895700	3.85325900	0.20554500	C	6.73266700	-2.04875600	1.83751400
N	-2.54655700	3.25568500	0.06023400	C	6.57086300	-2.41198500	4.32796300
C	1.62179900	4.09223000	-3.78357900	C	6.65164500	-0.78072600	-3.97655900
C	1.43723600	3.05126600	-2.69147500	C	5.66848800	-1.35241900	-2.95880600
O	2.38497300	2.90834600	-1.84608500	S	6.24709200	-2.99653600	-2.33565600
O	0.33648900	2.44094000	-2.63639000	C	1.27989900	-5.36377500	-2.48351400
Zn	1.95799100	2.79132500	0.21369700	C	2.08767100	-4.19965000	-3.05866400
Zn	-1.63654300	2.05951200	1.43693800	O	2.83516500	-3.52040100	-2.34107900
H	2.83994000	8.42324900	-2.11271400	C	0.39090900	-4.90613600	-1.31194800
H	3.98420000	8.57489300	-0.77241600	C	-0.28433200	-6.02838000	-0.53653700
H	3.57713600	4.85058400	-1.28420900	O	-1.50429100	-6.07466000	-0.35805600
H	1.31531400	7.94338500	0.42202300	N	0.52851500	-6.98795000	-0.02251000
H	0.41616500	5.73157000	1.32260600	N	1.97369700	-4.00157200	-4.38876900
H	7.37031300	1.32547300	-1.34556800	C	2.62751300	-2.89758200	-5.08243700
H	7.48958100	-0.01091900	-0.19645500	H	6.10049800	-4.65072200	1.69087100

H	4.86228800	-3.93171000	2.70989200	O	0.00418800	-1.96441900	-2.53332100
H	7.86901500	-3.45958400	2.97855600	N	1.50325200	-1.15274200	-0.95738800
H	6.93637500	-2.49374600	0.85798100	C	1.39366400	-0.51635800	0.35603600
H	7.45034900	-1.23194100	1.99015600	C	0.03009600	0.25546000	0.20520600
H	5.72428200	-1.61655000	1.79619200	O	-0.75080100	0.35187000	1.30463000
H	7.24170100	-1.55913900	4.48533500	H	2.19309900	0.21282900	0.49289700
H	5.53838000	-2.04314100	4.38574500	H	-1.60659800	-0.45313200	-1.02223300
H	6.72269900	-3.10010800	5.16393200	H	2.17763400	-1.87949100	-1.18014500
H	5.79192100	-5.13334300	4.72134500	O	0.32067700	1.64608400	-0.23724500
H	5.54774700	-0.67325000	-2.11023000	H	0.26333900	1.74829300	-1.25901700
H	4.68251900	-1.50218300	-3.40098700	C	-1.45535700	-2.34967200	-5.39508800
H	5.01392400	-3.48477600	-2.08112000	C	-2.79793800	-2.36962700	-4.68702400
H	7.65274300	-0.66500700	-3.54752800	O	-3.84330200	-2.61324100	-5.28905500
H	-0.39562700	-4.25016900	-1.68285700	N	-2.73605400	-2.08064500	-3.35727900
H	1.00793800	-4.32588600	-0.61606600	C	-3.87114800	-2.29738700	-2.47991300
H	1.53258200	-6.91727600	-0.05226400	C	-4.26443000	-0.97643500	-1.80238200
H	0.11022600	-7.70859900	0.54688000	O	-3.49343400	-0.44468000	-0.97413800
H	0.66843700	-5.84741900	-3.25229300	C	-3.54739600	-3.34504600	-1.39646600
H	3.71442400	-2.99202200	-5.01256800	O	-3.14384700	-4.52807700	-2.04313100
H	2.32123600	-1.94110200	-4.64842000	N	-5.45248500	-0.40214300	-2.07974800
H	1.27364300	-4.52822200	-4.88791100	C	-6.47082200	-0.80875900	-3.08557200
H	2.01540100	-6.10579200	-2.15038500	C	-6.06869300	-0.39052300	-4.50401500
H	2.33778100	-2.92590000	-6.13344000	C	-7.72602300	-0.08575500	-2.56142300
H	6.73994700	-1.43257300	-4.84996000	C	-7.17732700	1.23917900	-2.00767300
H	6.31609300	0.20562200	-4.31659100	C	-5.83203500	0.84026100	-1.38143400
H	7.11780300	-5.76885800	3.73848800	H	-5.05011100	1.59594400	-1.49934900
H	5.45707000	-6.28536700	3.43067100	H	-5.92084000	0.63591000	-0.30727100
C	-4.36808100	-5.09756600	6.54288700	H	-7.02264100	1.95434300	-2.82168200
C	-2.85166400	-4.92059100	6.35964000	H	-7.84752300	1.70757100	-1.28175100
C	-2.50559900	-4.17579100	5.08904400	H	-8.47689200	0.05090500	-3.34330800
C	-2.15191500	-2.82307100	5.10284500	H	-8.18299800	-0.67055800	-1.75500500
C	-2.57711200	-4.81709900	3.84226800	H	-6.60835500	-1.89214300	-3.04888200
C	-1.89289600	-2.12198400	3.92213800	H	-5.85699700	0.68269700	-4.55469000
C	-2.32347400	-4.13975400	2.65527100	H	-5.19701200	-0.94989500	-4.84833300
C	-1.98846900	-2.77851100	2.68885400	H	-6.89010800	-0.60758000	-5.19555200
O	-1.77932200	-2.15518000	1.49602600	H	-4.67070800	-2.68060200	-3.11439700
H	-2.37502800	-5.90894200	6.35176300	H	-2.65645000	-5.08359400	-1.40376600
H	-2.43988600	-4.38687300	7.22426500	H	-4.45722400	-3.49332900	-0.78581500
H	-2.07444700	-2.30199800	6.05470300	H	-2.77517600	-2.94765400	-0.72581100
H	-2.83416300	-5.87327400	3.80084500	H	-1.80270000	-2.02286700	-2.94505900
H	-1.60805600	-1.07365700	3.95367300	H	-0.63418900	-2.03378300	-4.75257900
H	-2.36007500	-4.65131800	1.69837400	H	-1.26085900	-3.35801600	-5.77618400
H	-1.41018400	-1.24246600	1.59610400	H	-1.52925100	-1.69145900	-6.26533400
H	-4.87123900	-4.12606300	6.59416800	C	1.43631200	-1.51631300	1.51024300
H	-4.80280100	-5.65139800	5.70458600	H	2.41374400	-2.01060400	1.53477000
H	-4.59587500	-5.64578500	7.46315700	H	1.28528000	-1.00262800	2.46323400
N	-0.59108100	-0.42505800	-0.89829000	H	0.66236500	-2.27862700	1.40109100
C	0.27571900	-1.25081100	-1.55945400				

(5R)-MeHYD-TS2-II (SkDHPase)

C	3.27200100	7.87075300	-1.52203600	H	-1.03037700	3.50415900	-1.35899700
C	2.56562900	6.74891600	-0.83266200	H	-4.84521600	5.16215800	-0.79788000
N	1.45726300	6.91949400	-0.01331800	H	-4.41629300	3.52007500	1.10260200
C	2.78482700	5.39725300	-0.83481500	H	-0.73150200	5.30938200	3.99638100
C	1.05563000	5.70603200	0.43763900	H	0.76383700	3.90516100	-4.67762000
N	1.84109600	4.75933300	-0.04925800	H	1.07409900	4.95957400	-3.28188600
C	7.21771200	1.14601100	-0.42725900	H	8.04165500	1.68522900	0.05383600
C	5.90157000	1.53395300	0.13621700	H	-3.93388700	4.00983500	3.61037800
N	5.61624600	1.48303000	1.49036700	H	-4.67970800	3.27852400	5.04168200
C	4.74778200	1.97655900	-0.45088800	H	0.28805100	5.43355700	5.44286200
C	4.33954000	1.87760400	1.68153600	H	-0.76632300	4.02715900	5.21477900
N	3.78383500	2.18383900	0.51816900	H	4.11024700	7.47598600	-2.09911200
C	-0.11586300	4.74338300	4.69772800	H	2.44121000	4.25000100	-4.14967700
N	0.97199100	4.10319500	4.00898600	H	-2.85109100	6.61831700	-2.49748600
C	0.74240200	3.35579300	2.90162700	H	1.88325700	4.03232400	4.43255800
O	-0.45002700	3.38634400	2.43852100	C	6.17547200	-5.35363500	3.60529300
O	1.73607400	2.74235300	2.39562200	C	5.96602500	-4.21057900	2.60383700
C	-3.87587400	3.16883200	4.31039500	C	6.85539800	-2.98003800	2.87378400
C	-3.99231300	1.84750400	3.60810700	C	6.70693900	-1.94333800	1.75378200
N	-3.15735600	1.42140500	2.57218000	C	6.57571300	-2.33682800	4.24058700
C	-4.90890300	0.86000500	3.85933900	C	6.52327200	-0.71989400	-4.09863900
C	-3.57992700	0.21189400	2.21809400	C	5.58298800	-1.30050700	-3.04601300
N	-4.63609500	-0.15824000	2.96842900	S	6.24509900	-2.89479400	-2.37997500
C	-2.80444400	5.55113500	-2.74483800	C	1.36269200	-5.34481300	-2.40053400
C	-2.88813600	4.68888300	-1.53264700	C	2.09393600	-4.16836200	-3.04688300
N	-3.98612900	4.64375000	-0.68544500	O	2.83092800	-3.42388500	-2.38354100
C	-1.99441700	3.80632400	-0.98957300	C	0.32309000	-4.88524900	-1.35808800
C	-3.72448400	3.76053000	0.31058300	C	-0.28185600	-5.98911800	-0.50177900
N	-2.52029800	3.24110300	0.15326900	O	-1.49554100	-6.07752200	-0.30009300
C	1.41751500	4.06923400	-3.81973500	N	0.57946400	-6.87609200	0.06352800
C	1.38039400	2.90167100	-2.86622000	N	1.93317100	-4.02041800	-4.37897100
O	2.30335600	2.64081000	-2.09866700	C	2.51435400	-2.90638100	-5.12115100
O	0.23366800	2.24347800	-2.90613500	H	6.17548200	-4.57476700	1.59010900
Zn	1.84866100	2.74381300	0.36763500	H	4.91078900	-3.90096700	2.60807000
Zn	-1.45409300	2.01235900	1.41050000	H	7.90004600	-3.32541200	2.87186400
H	2.61151700	8.40619500	-2.21325300	H	6.90991000	-2.37258500	0.76706300
H	3.67246200	8.60012800	-0.80926400	H	7.40406000	-1.10869800	1.90621800
H	3.54155200	4.83714400	-1.35910300	H	5.68710000	-1.53735300	1.73133300
H	1.02497500	7.80177600	0.21964000	H	7.21525000	-1.46057100	4.40001200
H	0.21528200	5.54168300	1.09619100	H	5.53084500	-2.00751100	4.31007200
H	7.24814600	1.37961300	-1.49344400	H	6.76092700	-3.02597600	5.06889900
H	7.40779300	0.07326300	-0.31630200	H	5.87287100	-5.07310400	4.61855400
H	4.53379500	2.14388800	-1.49367100	H	5.44576100	-0.59931900	-2.21779300
H	6.23896100	1.14349200	2.20909500	H	4.59810800	-1.51212600	-3.46438700
H	3.84015400	1.93116900	2.63470800	H	5.03955300	-3.41945800	-2.07309000
H	-2.92035900	3.25612800	4.83665200	H	7.52444100	-0.54381000	-3.69087200
H	-5.70701500	0.79755800	4.58186700	H	-0.50498800	-4.37654300	-1.85059900
H	-5.07909700	-1.06456800	2.93376500	H	0.78351900	-4.15753200	-0.68004800
H	-3.15948600	-0.39189800	1.42720900	H	1.57683700	-6.73819000	0.04844500
H	-1.85962800	5.36441900	-3.25877900	H	0.19785400	-7.54621600	0.71490300
H	-3.61182800	5.34054000	-3.45523500	H	0.88225200	-5.97748000	-3.15444300

H	3.60618900	-2.95319000	-5.09003000	C	-6.20963300	-0.54274800	-4.38006900
H	2.18356700	-1.95425900	-4.69601800	C	-7.77878600	-0.11692300	-2.38573500
H	1.25314200	-4.60148800	-4.84450600	C	-7.20293200	1.23111600	-1.92290600
H	2.14674700	-5.95121300	-1.93278100	C	-5.83506400	0.85621800	-1.33147800
H	2.18733500	-2.97090000	-6.15955800	H	-5.05684200	1.60268900	-1.51530100
H	6.62836200	-1.39672100	-4.95094600	H	-5.88089500	0.70311200	-0.24597100
H	6.13816500	0.23808400	-4.46652100	H	-7.07827700	1.90233800	-2.77865400
H	7.22809500	-5.65599700	3.64289000	H	-7.84221100	1.74006700	-1.19624000
H	5.59022400	-6.23534800	3.32466800	H	-8.56073100	-0.01560600	-3.14223600
C	-4.21714300	-5.19086100	6.64296900	H	-8.20493000	-0.65652500	-1.53229100
C	-2.77951800	-4.60932900	6.52720400	H	-6.68939500	-1.95327600	-2.81670600
C	-2.43227000	-3.98775800	5.18615200	H	-6.00348600	0.52595300	-4.50324100
C	-1.97856200	-2.66835100	5.08675700	H	-5.35218300	-1.12040100	-4.73023700
C	-2.51504400	-4.72888600	3.99478000	H	-7.06033700	-0.79950600	-5.02098200
C	-1.62132200	-2.09931900	3.86018200	H	-4.74522800	-2.72568700	-2.97956600
C	-2.16930700	-4.18241500	2.76300200	H	-2.69583700	-5.09409400	-1.28661900
C	-1.71884600	-2.85452100	2.68339900	H	-4.44951300	-3.45643300	-0.62788300
O	-1.39774800	-2.36846000	1.45489100	H	-2.75615000	-2.93936500	-0.66347000
H	-2.05657100	-5.40682800	6.74166900	H	-1.87652600	-2.04145700	-2.91632800
H	-2.62173600	-3.85787500	7.30826100	H	-0.78155300	-1.96926800	-4.77604500
H	-1.89161900	-2.06665200	5.98914500	H	-1.30748500	-3.46106600	-5.59362500
H	-2.85302400	-5.76220800	4.03112200	H	-1.71702000	-1.90554000	-6.30680100
H	-1.25722100	-1.07680500	3.81237100	C	1.83230200	-0.88679900	1.55257100
H	-2.22363000	-4.77258700	1.85305000	H	2.82303900	-1.35549500	1.53643600
H	-1.14248900	-1.40540100	1.46598500	H	1.84332600	-0.07240300	2.28156000
H	-4.78116500	-5.04344500	5.71744400	H	1.10230700	-1.63160300	1.87217900
H	-4.20754200	-6.26416000	6.85209600	N	-0.47229700	-0.13322600	-1.17748800
H	-4.77999300	-4.70940600	7.44823600	C	0.22865500	-1.25225900	-1.59947700
C	-1.58237400	-2.42730500	-5.35582000	O	-0.08965800	-1.98705000	-2.54502000
C	-2.91057800	-2.44972800	-4.62186900	N	1.33301500	-1.40148700	-0.82799200
O	-3.96442700	-2.72303100	-5.19613400	C	1.47967500	-0.35372400	0.16985100
N	-2.81827300	-2.13397400	-3.30244000	C	0.09528200	0.41068800	0.08209500
C	-3.92434300	-2.32492200	-2.38473100	O	-0.74628300	0.21364900	1.15152700
C	-4.28263000	-0.97761600	-1.74162900	H	2.25529200	0.34408600	-0.16277400
O	-3.46880300	-0.41058000	-0.98467500	H	-1.49460600	-0.20901300	-1.20520200
C	-3.56668800	-3.34217200	-1.28407700	H	2.06516600	-2.03417000	-1.13974500
O	-3.21525300	-4.55163800	-1.91254900	O	0.25690800	1.79941900	-0.09295700
N	-5.48703000	-0.41735700	-1.98651600	H	0.16470300	1.58629900	-2.16114700
C	-6.54914500	-0.87451700	-2.92224900				

(5R)-MeHYD-INT2-II (SkDHPase)

C	3.26741300	7.87011300	-1.47698600	C	4.74799000	1.97062600	-0.44844800
C	2.56494200	6.74528800	-0.79134700	C	4.35343500	1.87571200	1.68734100
N	1.46155100	6.91174100	0.03513400	N	3.79046600	2.17940300	0.52669100
C	2.78518400	5.39404400	-0.80185000	C	-0.09886400	4.70474200	4.73526900
C	1.06366300	5.69598700	0.48286500	N	0.99734600	4.08509900	4.04286100
N	1.84762300	4.75325400	-0.01299400	C	0.76254400	3.31726500	2.95037500
C	7.22035100	1.14141400	-0.43383800	O	-0.44121900	3.31454800	2.52099700
C	5.90585000	1.53001200	0.13280300	O	1.76049100	2.72140100	2.43048900
N	5.62879800	1.48154900	1.48869500	C	-3.85921100	3.13029400	4.35077400

C	-3.98486800	1.81892000	3.63035300	C	6.71614900	-1.96048800	1.73009100
N	-3.14429300	1.39317900	2.59902000	C	6.59923400	-2.36957700	4.21506800
C	-4.91670400	0.84034900	3.86055000	C	6.51525700	-0.70355400	-4.11375800
C	-3.57806000	0.19352600	2.22655600	C	5.56879100	-1.28210800	-3.06554700
N	-4.64659600	-0.17196900	2.96202900	S	6.21238600	-2.89028800	-2.41512700
C	-2.81160200	5.55412300	-2.69388500	C	1.32227500	-5.31243500	-2.41839800
C	-2.88477100	4.69797000	-1.47713700	C	2.06352200	-4.14226400	-3.06309700
N	-3.95055600	4.70770500	-0.58872200	O	2.79308100	-3.39511700	-2.39395300
C	-2.00969000	3.78035200	-0.96098500	C	0.27195600	-4.84259900	-1.39076800
C	-3.68978000	3.82132200	0.40460100	C	-0.31861300	-5.93938000	-0.51516300
N	-2.51623200	3.24890600	0.20713200	O	-1.53288100	-6.06151000	-0.33660500
C	1.40773900	4.08092700	-3.79080000	N	0.55825900	-6.78190900	0.09277500
C	1.35525800	2.86703300	-2.88677300	N	1.91769800	-3.99939500	-4.39684800
O	2.25852900	2.58942100	-2.10105100	C	2.50432300	-2.88638500	-5.13617900
O	0.22570400	2.18985700	-3.00381600	H	6.18646600	-4.59198400	1.55346100
Zn	1.85938300	2.74676300	0.39928100	H	4.92611000	-3.92372300	2.58047800
Zn	-1.44564900	1.98704300	1.43581100	H	7.91635500	-3.34894300	2.83278500
H	2.60427700	8.40918300	-2.16288100	H	6.91290700	-2.38384000	0.73955300
H	3.67053900	8.59595000	-0.76205600	H	7.41408600	-1.12678700	1.88345900
H	3.53979900	4.83665500	-1.33235300	H	5.69628100	-1.55415400	1.71662900
H	1.03045900	7.79289000	0.27444800	H	7.23936600	-1.49414100	4.37647000
H	0.22749900	5.52779100	1.14562400	H	5.55469700	-2.04094000	4.29233000
H	7.24909300	1.37490800	-1.50010200	H	6.78918400	-3.06386800	5.03799100
H	7.41003400	0.06858000	-0.32325900	H	5.89582200	-5.10740900	4.58019100
H	4.52515900	2.13408100	-1.49025400	H	5.44091300	-0.58712400	-2.23068400
H	6.25674800	1.14491800	2.20421800	H	4.58097700	-1.47698100	-3.48523800
H	3.85957900	1.93159300	2.64327000	H	5.00155500	-3.40040700	-2.10439500
H	-2.92283000	3.18593300	4.91464300	H	7.51892800	-0.54391500	-3.70540500
H	-5.72371700	0.78026300	4.57335500	H	-0.56229600	-4.35711000	-1.89685200
H	-5.10336600	-1.07061000	2.91049800	H	0.71948200	-4.09627500	-0.72468400
H	-3.15646900	-0.40286000	1.43046100	H	1.54990800	-6.60638900	0.10054100
H	-1.90029200	5.32155200	-3.24815200	H	0.18405700	-7.44166800	0.75891700
H	-3.65832300	5.38338700	-3.36829800	H	0.84810200	-5.94915000	-3.17282400
H	-1.07199400	3.43194700	-1.35960200	H	3.59597100	-2.93341700	-5.09870200
H	-4.78979100	5.26247000	-0.67408900	H	2.17032800	-1.93478300	-4.71281900
H	-4.36190400	3.61800400	1.22359700	H	1.25097200	-4.58950300	-4.87012500
H	-0.71234300	5.28648200	4.04415600	H	2.09782800	-5.91844600	-1.93671500
H	0.79307200	3.94042900	-4.68106100	H	2.18322400	-2.95112400	-6.17639800
H	1.02580800	4.94247000	-3.23279400	H	6.61097600	-1.37364400	-4.97246300
H	8.04540900	1.68032400	0.04564500	H	6.14180400	0.26250400	-4.47232100
H	-3.86575300	3.97907500	3.65812900	H	7.24735400	-5.68464200	3.59613100
H	-4.68737000	3.25530600	5.05185400	H	5.60842800	-6.26230900	3.28069900
H	0.29566500	5.37803000	5.50070100	C	-4.18837200	-5.24299100	6.63584900
H	-0.75077000	3.97339200	5.22787000	C	-2.73122800	-4.77250200	6.46877400
H	4.10357400	7.47910200	-2.05964100	C	-2.41145300	-4.11769300	5.13608000
H	2.44089200	4.29080800	-4.06983500	C	-1.99047100	-2.78569000	5.05381100
H	-2.79545900	6.62238500	-2.44714600	C	-2.48390600	-4.84025900	3.93296800
H	1.91620000	4.04267000	4.45323800	C	-1.64780500	-2.19025600	3.83483200
C	6.19459600	-5.38212900	3.56420800	C	-2.15399200	-4.26749800	2.70879200
C	5.98132500	-4.23341200	2.57008400	C	-1.72670200	-2.93063200	2.64718400
C	6.87157300	-3.00413600	2.84276100	O	-1.40455800	-2.42994300	1.42400100

H	-2.06926800	-5.63749800	6.61142000	H	-8.19736000	-0.53855200	-1.49310000
H	-2.48615900	-4.07236800	7.27622400	H	-6.71364300	-1.89367800	-2.75148600
H	-1.91091100	-2.19623300	5.96496300	H	-5.99655400	0.52975800	-4.50480800
H	-2.79669500	-5.88195200	3.95369400	H	-5.37330100	-1.13044600	-4.69837000
H	-1.30266400	-1.16046200	3.80380600	H	-7.07845100	-0.79029000	-4.98169300
H	-2.20145300	-4.84492900	1.79049500	H	-4.76210800	-2.67231200	-2.97887500
H	-1.15949900	-1.46534500	1.42955900	H	-2.73279000	-5.06947000	-1.31057600
H	-4.88556000	-4.40188600	6.55874800	H	-4.46273400	-3.41581600	-0.63403400
H	-4.46342100	-5.97178000	5.86664200	H	-2.76475500	-2.91369100	-0.67429200
H	-4.33421700	-5.71658400	7.61194100	H	-1.89175400	-1.98724200	-2.93140500
C	-1.59340200	-2.40832100	-5.35502000	H	-0.83536800	-1.82186200	-4.83685500
C	-2.92428100	-2.42608500	-4.62759100	H	-1.23521600	-3.44051800	-5.44172700
O	-3.97643900	-2.71122400	-5.19823100	H	-1.75306800	-2.03194200	-6.36789000
N	-2.83273000	-2.09664100	-3.31119200	C	1.81831200	-0.86028200	1.51995700
C	-3.93444200	-2.28061000	-2.38776100	H	2.80772300	-1.33170900	1.50336500
C	-4.26970200	-0.92805900	-1.74431300	H	1.83298200	-0.04739100	2.25054100
O	-3.43396900	-0.36269700	-1.01118500	H	1.08563000	-1.60313700	1.83792600
C	-3.58179600	-3.30550800	-1.29339500	N	-0.42909200	-0.01618200	-1.27098100
O	-3.24478300	-4.51440800	-1.93152000	C	0.24113700	-1.17679000	-1.66645700
N	-5.47471600	-0.36138300	-1.96965100	O	-0.07959300	-1.89637000	-2.62022200
C	-6.55297500	-0.82067700	-2.88565800	N	1.30898200	-1.36831200	-0.85885700
C	-6.21857800	-0.53213100	-4.35361900	C	1.46686100	-0.32262900	0.13947700
C	-7.76381000	-0.02610000	-2.35951900	C	0.09013200	0.44949200	0.05536300
C	-7.15792800	1.31880200	-1.92699300	O	-0.79069700	0.17164300	1.07215300
C	-5.79798000	0.92625800	-1.32985100	H	2.24585100	0.36980600	-0.19719900
H	-5.00482700	1.65439600	-1.52239000	H	-1.45277100	-0.09331200	-1.30363400
H	-5.84831900	0.78795200	-0.24243500	H	2.02642800	-2.02883900	-1.14869200
H	-7.01949100	1.96837100	-2.79729700	O	0.24373600	1.83935000	-0.01348500
H	-7.78455500	1.85747400	-1.21079600	H	0.13424400	1.44598900	-2.33423500
H	-8.54706600	0.07572100	-3.11459600				

(5R)-MeHYD-TS3-II (SkDHPase)

C	3.46632300	7.76563200	-1.69067500	N	-3.23069800	1.52328500	2.52627300
C	2.82578900	6.70239800	-0.87215500	C	-4.90745200	1.05207300	3.93880200
N	2.08430100	6.94689300	0.27375600	C	-3.70350500	0.31599200	2.23860500
C	2.79200500	5.34457700	-1.02355000	N	-4.71982300	-0.00089900	3.06557900
C	1.64043000	5.76461900	0.76476800	C	-2.65158400	5.53763000	-2.87653300
N	2.04852700	4.77208000	-0.00914500	C	-2.74329600	4.73705300	-1.61937200
C	7.27341100	0.99314800	-0.41440700	N	-3.76963200	4.87642200	-0.69527800
C	5.93475900	1.38576300	0.10647500	C	-1.92765700	3.77165500	-1.08894400
N	5.61669200	1.34675900	1.45528500	C	-3.54683800	4.01761000	0.32967900
C	4.79308100	1.83107200	-0.50726500	N	-2.43312100	3.33715100	0.12206100
C	4.33784700	1.75237100	1.61576800	C	1.54311400	3.94547000	-3.89922400
N	3.80905300	2.05231100	0.43951300	C	1.32631800	2.78675000	-2.93054100
C	-0.00217600	4.86310600	4.59329800	O	2.15881400	2.58794000	-2.01042400
N	1.04433100	4.33482200	3.75146200	O	0.24905900	2.12408800	-3.14124700
C	0.75561800	3.30530500	2.88634500	Zn	1.90428400	2.73812300	0.19679900
O	-0.48577200	3.05365400	2.74992100	Zn	-1.49337300	2.01873900	1.41547700
O	1.73698900	2.75985600	2.29646300	H	2.73143800	8.47042200	-2.09648000
C	-3.79174600	3.35456300	4.23218700	H	4.19749000	8.34417000	-1.11449500
C	-3.98439700	2.00626400	3.59767000	H	3.24054000	4.73260100	-1.78705400

H	1.91022800	7.85248300	0.68474900	H	7.56354000	-1.57899600	4.29712000
H	1.07521400	5.66476800	1.67920100	H	5.83507800	-1.96674800	4.38315100
H	7.33597800	1.21591100	-1.48151400	H	7.03236000	-3.06983600	5.07218300
H	7.46243500	-0.07739300	-0.28520200	H	5.90814800	-5.03502200	4.79741600
H	4.59889700	1.99977800	-1.55456700	H	5.49882000	-0.80862700	-2.14778500
H	6.22394300	1.01679300	2.19149100	H	4.56176300	-1.57327000	-3.43019400
H	3.82075300	1.82517100	2.55875000	H	4.83334800	-3.55975900	-2.06411300
H	-2.74333800	3.50924100	4.50028200	H	7.56682500	-0.88929300	-3.63113700
H	-5.66066700	1.03434000	4.71030100	H	-0.70554000	-4.42743500	-1.80557000
H	-5.18568000	-0.89586700	3.09386600	H	0.56856200	-4.17247800	-0.61995900
H	-3.33975700	-0.32317400	1.44649000	H	1.34283900	-6.69265300	0.24076200
H	-1.80492600	5.18552200	-3.46889500	H	-0.04689200	-7.48846500	0.89794000
H	-3.55164600	5.43606100	-3.49306900	H	0.69218500	-6.05073100	-3.04800900
H	-1.03787100	3.33129400	-1.50741200	H	3.59246100	-3.13895900	-4.93570100
H	-4.55941000	5.50015300	-0.77616900	H	2.16183200	-2.11377500	-4.64472700
H	-4.20365600	3.90586900	1.17786500	H	1.26200300	-4.79646600	-4.76917600
H	-0.82792800	5.23015100	3.98149200	H	1.92407800	-6.03977900	-1.79364900
H	0.94657500	3.81438700	-4.80252600	H	2.22596800	-3.17638400	-6.07219600
H	1.24384500	4.87665500	-3.40681600	H	6.58984300	-1.59573400	-4.92201900
H	8.07889600	1.54129100	0.08703300	H	6.26108000	0.05546200	-4.36463000
H	-4.07870000	4.17102100	3.55853800	H	7.10544000	-5.78961800	3.73683400
H	-4.40259700	3.43761000	5.13377300	H	5.39592100	-6.20718400	3.58543300
H	0.39581500	5.69887400	5.17542000	C	-4.30720200	-4.93563700	6.77161200
H	-0.40534800	4.11843100	5.29120600	C	-2.86404000	-4.38085200	6.60572100
H	3.99270300	7.31358300	-2.53346900	C	-2.52586600	-3.83913700	5.22813000
H	2.60088400	4.03098400	-4.15918700	C	-2.05766000	-2.53285300	5.05118100
H	-2.50480100	6.60486600	-2.67344400	C	-2.63158600	-4.64314200	4.08023100
H	2.00084300	4.37481800	4.07115000	C	-1.70387000	-2.03783200	3.79208200
C	6.08920000	-5.38142900	3.77552600	C	-2.28993900	-4.17058200	2.81677200
C	5.90568100	-4.25986300	2.74511400	C	-1.81995600	-2.85672300	2.66072200
C	6.92527600	-3.11153000	2.87818500	O	-1.49160500	-2.44406300	1.40571900
C	6.76338300	-2.10695300	1.73087500	H	-2.14832000	-5.17463200	6.85519000
C	6.83484900	-2.39572500	4.23443400	H	-2.68637000	-3.58936800	7.34161500
C	6.55287200	-0.94990400	-4.04046000	H	-1.95447500	-1.88278800	5.91753600
C	5.56351200	-1.48165400	-3.00732500	H	-2.98588500	-5.66712800	4.17651900
S	6.07353800	-3.16010900	-2.41930100	H	-1.32787600	-1.02444800	3.68448900
C	1.16994500	-5.41955600	-2.29136100	H	-2.36789600	-4.80714500	1.94038900
C	1.94619500	-4.26899900	-2.93062700	H	-1.26183700	-1.47704000	1.36512100
O	2.63871000	-3.50236100	-2.24339100	H	-4.88087200	-4.83367100	5.84590100
C	0.11579200	-4.91822300	-1.28296600	H	-4.30860700	-5.99520800	7.04184200
C	-0.50604100	-5.99100700	-0.39773200	H	-4.85378900	-4.40148900	7.55451600
O	-1.72390800	-6.08288000	-0.22816500	C	-1.58147500	-2.52644900	-5.28310800
N	0.34727200	-6.84384400	0.22844900	C	-2.93474400	-2.51320400	-4.59623400
N	1.87024600	-4.16333800	-4.27315100	O	-3.97697800	-2.80614400	-5.17795500
C	2.50412600	-3.08101500	-5.02214100	N	-2.86898500	-2.13123000	-3.29040600
H	5.98751000	-4.68134600	1.73510700	C	-3.98207000	-2.26996600	-2.37383500
H	4.88902700	-3.84739000	2.82438200	C	-4.26437100	-0.89478500	-1.75421800
H	7.92995200	-3.55232100	2.79656000	O	-3.40043100	-0.34832100	-1.03634600
H	6.84791700	-2.58643300	0.74987500	C	-3.67640200	-3.29372600	-1.26440900
H	7.53196300	-1.32583900	1.79037000	O	-3.34863400	-4.51375200	-1.88672600
H	5.77898000	-1.62237500	1.77600700	N	-5.44322500	-0.28523100	-1.98941100

C	-6.53762300	-0.72722800	-2.89583400	H	-0.98916400	-1.64686300	-5.02418200
C	-6.17303400	-0.52624400	-4.37102000	H	-1.01376500	-3.40365700	-4.95747700
C	-7.70779500	0.15657000	-2.42269400	H	-1.73634200	-2.58037000	-6.36135800
C	-7.03280400	1.48163200	-2.03309900	C	1.69995000	-0.91384100	1.57927800
C	-5.71004600	1.03651700	-1.39292200	H	2.67471200	-1.41445600	1.57828600
H	-4.87396700	1.71381700	-1.58743600	H	1.73078500	-0.09618700	2.30380300
H	-5.79298300	0.93263500	-0.30377900	H	0.93945500	-1.63100900	1.89005100
H	-6.84021800	2.08557600	-2.92577400	N	-0.46470900	0.00024300	-1.33071600
H	-7.63968400	2.08459700	-1.35218400	C	0.20889600	-1.21414900	-1.67218900
H	-8.47208500	0.27135600	-3.19505500	O	-0.10369900	-1.93582600	-2.61758500
H	-8.18357100	-0.29445700	-1.54437000	N	1.21846800	-1.40619600	-0.80953100
H	-6.75836600	-1.78252500	-2.71302600	C	1.38635400	-0.36289500	0.19488900
H	-5.89076400	0.51357500	-4.56743800	C	0.04629700	0.46045700	0.11232500
H	-5.35876500	-1.18286400	-4.68253100	O	-0.89320300	0.14968700	1.03397200
H	-7.04024100	-0.76450000	-4.99675900	H	2.19738800	0.29513100	-0.12963200
H	-4.81912700	-2.63801600	-2.96637200	H	-1.49377500	-0.10311900	-1.33794800
H	-2.87787900	-5.08004300	-1.24352700	H	1.89490200	-2.13813500	-1.02427300
H	-4.57473300	-3.38153900	-0.62583100	O	0.21443500	1.82079700	0.06045100
H	-2.86605300	-2.91572500	-0.62824300	H	-0.06060600	1.08574300	-2.24680000
H	-1.93451800	-2.02428000	-2.90201200				

(5R)-MeHYD-EP-II (SkDHPase)

C	4.52929700	7.28048200	-1.66789400	C	2.15235200	3.71876100	-3.86660400
C	3.78104200	6.32422700	-0.81235400	C	1.64273200	2.80599600	-2.76358800
N	3.13440800	6.66423000	0.36630500	O	2.51569100	2.43688000	-1.88297000
C	3.54453800	4.98857400	-0.96601700	O	0.42980900	2.54198500	-2.75338100
C	2.54549600	5.55285000	0.87282200	Zn	2.33590700	2.49778500	0.11185300
N	2.77041100	4.51910700	0.07836600	Zn	-1.37138000	2.31767500	1.46434300
C	7.43564600	0.08926700	-0.31555400	H	3.88874700	8.08881500	-2.03944400
C	6.11816900	0.59203600	0.17815400	H	5.36971700	7.74202400	-1.13656600
N	5.75090800	0.54029400	1.51536300	H	3.85677200	4.32624400	-1.75471900
C	5.04642300	1.17267800	-0.45134800	H	3.10731800	7.58279700	0.78426500
C	4.51516200	1.07157300	1.65318500	H	2.00318000	5.52650600	1.80595300
N	4.05943300	1.46482100	0.47469000	H	7.54729000	0.32685800	-1.37523300
C	0.67461500	4.89005400	4.60671900	H	7.52192100	-0.99617700	-0.20499300
N	1.57477500	4.16499800	3.73699800	H	4.90186500	1.39944900	-1.49608300
C	1.11849900	3.20893600	2.85999300	H	6.29524800	0.12074300	2.25532000
O	-0.15746800	3.13788600	2.75145500	H	3.98408500	1.17264400	2.58624800
O	1.98943400	2.53529900	2.23865800	H	-2.19728200	3.86483500	4.41650000
C	-3.27319600	3.87231600	4.22472200	H	-5.48979300	1.89025300	4.80973500
C	-3.71373400	2.56357200	3.63426700	H	-5.40504100	-0.09593800	3.19519200
N	-3.08661400	1.94943700	2.54922200	H	-3.55327300	0.14615800	1.47716100
C	-4.76889000	1.77720700	4.01591500	H	-1.03608000	5.30508000	-3.43932400
C	-3.76045400	0.83337300	2.28745400	H	-2.69876600	5.90102200	-3.53097000
N	-4.78391900	0.69893500	3.15269300	H	-0.64223500	3.43600000	-1.46174300
C	-1.81335400	5.83854500	-2.88881800	H	-3.79320500	6.14798000	-0.85018900
C	-2.09219200	5.09422300	-1.62159400	H	-3.77325400	4.54984400	1.12359600
N	-3.11656900	5.40706800	-0.73683100	H	-0.11346800	5.36278700	4.01790600
C	-1.46054700	4.01740700	-1.05695500	H	1.53283500	3.61660600	-4.75913900
C	-3.07557200	4.53882700	0.30096600	H	2.08324400	4.75670500	-3.52000300
N	-2.07532000	3.68376600	0.13656200	H	8.27014600	0.55357000	0.22142700

H	-3.48064700	4.71360300	3.55260800	H	6.35964400	-6.61287900	3.84822800
H	-3.79913200	4.06042600	5.16321700	H	4.60273500	-6.76036300	3.74399200
H	1.23539400	5.67028000	5.12760400	C	-4.85625000	-4.26565000	6.81495000
H	0.19862300	4.24813700	5.35895800	C	-3.33972300	-4.27362600	6.55941200
H	4.93419900	6.75437400	-2.53437900	C	-2.95637000	-3.75378600	5.18930500
H	3.19765600	3.51794300	-4.11602200	C	-2.38891200	-2.48765500	5.01551000
H	-1.46423500	6.85978300	-2.69764500	C	-3.17521700	-4.52879000	4.03865000
H	2.54323600	4.06827100	4.00375900	C	-2.04391200	-2.00494500	3.74945000
C	5.42070200	-6.05110200	3.90689100	C	-2.84358800	-4.06866600	2.76903500
C	5.38866300	-4.92322500	2.86757400	C	-2.27052000	-2.79788200	2.61849600
C	6.57575500	-3.94624800	2.97198600	O	-1.94515800	-2.40431200	1.35252400
C	6.57644800	-2.96623400	1.79268800	H	-2.96614400	-5.29853600	6.67964600
C	6.59667100	-3.18342000	4.30525500	H	-2.83936000	-3.67429900	7.32910500
C	6.50038200	-1.77417400	-3.93436000	H	-2.19774600	-1.86473500	5.88668200
C	5.33130400	-2.05155600	-2.99410900	H	-3.61191500	-5.51991800	4.14009700
S	5.40823600	-3.78892600	-2.36176600	H	-1.58287600	-1.02688900	3.64050200
C	0.27999300	-5.55970300	-2.43172600	H	-3.01018300	-4.67963100	1.88693200
C	1.27349600	-4.52221200	-2.95166100	H	-1.61368500	-1.48550900	1.32729500
O	1.96692600	-3.87335500	-2.15347400	H	-5.25919600	-3.24919800	6.75045900
C	-0.74293000	-4.91058200	-1.47342900	H	-5.38439400	-4.87818800	6.07717000
C	-1.38452900	-5.84887900	-0.46098500	H	-5.09044200	-4.66036900	7.80899400
O	-2.60480600	-5.91290900	-0.28936500	C	-1.75912300	-2.31428400	-5.23287900
N	-0.53719700	-6.60843100	0.28274400	C	-3.11846600	-2.21868500	-4.55165600
N	1.34984100	-4.36566800	-4.28802200	O	-4.16090100	-2.49959300	-5.13674900
C	2.22089800	-3.38124500	-4.93486800	N	-3.07750200	-1.82789500	-3.24150100
H	5.38587300	-5.36072000	1.86128400	C	-4.23992800	-1.87316500	-2.36987800
H	4.44902100	-4.35888100	2.95928500	C	-4.39866400	-0.52162400	-1.65781300
H	7.49821200	-4.54258400	2.91157200	O	-3.55613600	-0.15776000	-0.81232600
H	6.59132900	-3.48365900	0.82787800	C	-4.12849700	-2.98736100	-1.31348000
H	7.45336900	-2.30760400	1.83513600	O	-4.03638500	-4.22016800	-1.98770900
H	5.67493800	-2.33987800	1.80928300	N	-5.46327500	0.25878300	-1.94282400
H	7.44813900	-2.49436600	4.35063200	C	-6.54269500	0.01668900	-2.93696900
H	5.67873300	-2.59367800	4.43127400	C	-6.06581300	0.25978700	-4.37163700
H	6.67730000	-3.85352800	5.16544500	C	-7.62625800	1.00908400	-2.47068000
H	5.32268900	-5.67254200	4.92883900	C	-6.82276200	2.20636600	-1.93907600
H	5.34403000	-1.36513400	-2.14294600	C	-5.62066100	1.54816200	-1.24764000
H	4.37727700	-1.92064600	-3.50782300	H	-4.69747000	2.13064500	-1.31532800
H	4.08616400	-3.90823700	-2.10279500	H	-5.80974600	1.36816100	-0.18131500
H	7.46317300	-1.93422500	-3.43726200	H	-6.48616900	2.83617000	-2.76911000
H	-1.55680000	-4.44900600	-2.03606000	H	-7.39812500	2.83833800	-1.25714900
H	-0.24702700	-4.11750300	-0.90192500	H	-8.31402800	1.27290000	-3.27759900
H	0.45678200	-6.44385900	0.28658900	H	-8.21442300	0.56315200	-1.66066700
H	-0.93476300	-7.15347400	1.03350400	H	-6.90142300	-1.01177800	-2.84123200
H	-0.23868900	-6.07941000	-3.24386400	H	-5.63708900	1.26138600	-4.48084200
H	3.26406600	-3.71371200	-4.91886600	H	-5.32533500	-0.48062300	-4.68160800
H	2.12102900	-2.42665800	-4.41710700	H	-6.91410400	0.17645400	-5.05951900
H	0.77893400	-4.95983500	-4.86970400	H	-5.08465000	-2.10573000	-3.01799600
H	0.88080700	-6.31243300	-1.90981200	H	-3.65788500	-4.87637500	-1.36883000
H	1.89906100	-3.26686500	-5.97106900	H	-5.02861700	-2.93643500	-0.67249400
H	6.46665300	-2.42800700	-4.81011300	H	-3.26333500	-2.79166500	-0.66947400
H	6.46994300	-0.73557300	-4.28266700	H	-2.21050000	-1.46613400	-2.86082300

H	-0.99887700	-1.66699900	-4.78695500	N	0.59395500	-1.44678500	-1.03312200
H	-1.40995000	-3.34974500	-5.15932200	C	1.10956400	-0.63468700	0.08643900
H	-1.88245000	-2.07692800	-6.29094000	C	0.14856700	0.49351700	0.47336100
C	1.41440800	-1.54234300	1.28162800	O	-0.94240600	0.27476400	1.08977800
H	2.18208100	-2.26867500	0.99811400	H	2.03740600	-0.13522700	-0.21997300
H	1.79282900	-0.95746400	2.12528000	H	-1.42421800	0.01053200	-1.37360000
H	0.52157100	-2.08636400	1.59169000	H	1.26502700	-2.18526200	-1.25619700
N	-0.83293900	0.00037200	-2.19725700	O	0.45607700	1.69672000	0.20446200
C	0.30307400	-0.76504900	-2.23692500	H	-0.77913500	0.85528800	-2.74133000
O	0.96278900	-0.90685400	-3.26101400				

(5S)-MeDHU-ES-II (SkDHPase)

C	-6.86514800	-5.20562900	-2.00334000	N	-0.50084200	2.40291800	-0.90017600
C	-5.90039500	-4.59561100	-1.05452200	C	-1.49630600	1.79432700	-0.02238600
N	-5.51325800	-5.14823800	0.15738000	C	-0.80333300	1.11335000	1.16310700
C	-5.18761300	-3.43753700	-1.15404200	C	0.34329200	0.26117200	0.66772600
C	-4.59974500	-4.32502600	0.73247100	O	0.86640100	-0.64037600	1.37315300
N	-4.37581100	-3.28056700	-0.04742100	H	-6.52775400	-6.18453700	-2.36412200
C	-6.96439300	2.53704100	-0.57842000	H	-7.85791700	-5.34330100	-1.55873600
C	-5.96463800	1.57158300	-0.02723000	H	-5.17531900	-2.70678700	-1.94400200
N	-5.60624700	1.54317500	1.31288000	H	-5.85226700	-6.01283400	0.55274000
C	-5.20488900	0.58750300	-0.60739300	H	-4.14948900	-4.49574300	1.69953600
C	-4.67303500	0.57922500	1.49604900	H	-7.18166300	2.29018000	-1.61961100
N	-4.40512800	-0.01649000	0.34630600	H	-6.59280000	3.56674900	-0.54569000
C	-2.62940100	-4.46710500	4.43533100	H	-5.15990100	0.26492900	-1.63564800
N	-3.18598800	-3.41003000	3.61664900	H	-5.94674900	2.17330900	2.02462800
C	-2.38181300	-2.65636900	2.78894300	H	-4.22568500	0.32082500	2.44282800
O	-1.18068700	-3.08059100	2.66805300	H	0.50411300	-4.49196100	4.52823500
O	-2.90627000	-1.66078500	2.21011400	H	4.29848100	-4.18194400	4.51248400
C	1.42667600	-4.97409300	4.19419800	H	4.98442900	-2.39794000	2.80644800
C	2.31897400	-3.99243500	3.49105200	H	3.08597800	-1.80882100	1.23858000
N	1.93372500	-3.17726600	2.42284700	H	-0.94367500	-5.43745500	-3.56877100
C	3.64427800	-3.76501100	3.76326700	H	0.42425100	-6.55289200	-3.63199200
C	3.01660500	-2.49968000	2.06679000	H	-0.70700800	-3.54336900	-1.69550400
N	4.07020100	-2.82286400	2.85090000	H	1.24712500	-7.15185500	-0.84024500
C	-0.39788200	-6.19381900	-3.00183800	H	1.68300200	-5.57024200	1.10709700
C	0.08427900	-5.58586000	-1.73440300	H	-2.04959900	-5.14872500	3.81171900
N	0.87936000	-6.21333000	-0.78552700	H	-2.55440700	-2.87882300	-4.86764700
C	-0.15264800	-4.34123600	-1.22844600	H	-3.55801400	-3.74165600	-3.68278300
C	1.08839500	-5.34528900	0.23611900	H	-2.09201800	1.06614200	-0.58217200
N	0.47016800	-4.19995900	-0.00442900	H	-2.16938400	2.58247600	0.31891500
C	-3.26575100	-2.75103200	-4.05012500	H	-1.49931500	0.42115600	1.64358100
C	-2.62308200	-1.97665800	-2.89276300	H	-7.90925100	2.50107500	-0.02501700
O	-3.42172900	-1.40807700	-2.06068900	H	1.13499000	-5.80228600	3.53731100
O	-1.37698200	-1.99648400	-2.79074400	H	1.94067900	-5.39676100	5.06027800
Zn	-3.14318600	-1.61547300	0.03848200	H	-3.44625000	-5.02478500	4.90142800
Zn	0.05493600	-2.60003600	1.22958800	H	-1.97075400	-4.09235800	5.22969000
N	0.90984500	0.58798400	-0.51193800	H	-6.97930600	-4.55414200	-2.87175700
C	0.60921700	1.74397300	-1.26538800	H	-4.16816000	-2.25166600	-4.41250300
O	1.37214500	2.09143100	-2.16951000	H	-1.07242500	-7.04050600	-2.82629200

H	-4.03054800	-2.94904700	3.92179000	C	4.63640800	2.90118000	6.62257400
H	1.76276700	0.07392800	-0.78759900	C	4.10971600	2.51496600	5.26301800
H	-0.69300500	3.26208100	-1.41212400	C	3.27468600	1.40125400	5.12413200
O	-1.20994300	-1.70707100	-0.05719900	C	4.55179900	3.15807100	4.09962700
H	-1.02583200	-1.69945200	-1.02148500	C	2.92009400	0.91500100	3.86892700
C	-2.98230700	7.45945700	3.83816300	C	4.20365200	2.69447100	2.83406300
C	-3.33071400	6.40947900	2.77541200	C	3.40443800	1.55384100	2.72152300
C	-4.73083900	5.79131800	2.97814300	O	3.12208200	1.09551400	1.46785500
C	-5.22333700	5.09305300	1.70558300	H	4.97311300	3.94420200	6.61890500
C	-4.77205200	4.82930200	4.17512400	H	3.84359000	2.82867500	7.37717300
C	-5.27883100	3.95897300	-4.12522100	H	2.91014600	0.89212000	6.01353400
C	-4.24201000	3.35312300	-3.18324300	H	5.19553900	4.03018600	4.18754400
S	-3.64043300	4.51725200	-1.87479800	H	2.27587600	0.04483800	3.77260400
C	2.16926300	5.12710200	-2.77853000	H	4.54087500	3.19137400	1.92943400
C	0.73500100	4.84402900	-3.20204500	H	2.54471900	0.31656700	1.53193600
O	-0.22739400	4.93341400	-2.42639700	H	5.47788700	0.93503700	7.04582900
C	2.26936300	5.90561300	-1.46906700	H	6.61302200	2.05115400	6.27939400
C	3.57730900	5.61934500	-0.73716900	H	6.20976300	2.23917400	7.99482800
O	4.12829600	4.51947900	-0.77063700	C	-0.28010000	2.12434100	2.20564800
N	4.07627000	6.64459900	-0.00251300	H	-1.12385900	2.68140100	2.62435400
N	0.57937200	4.44571000	-4.48582500	H	0.23743200	1.61988100	3.02366200
C	-0.67526000	3.88334500	-4.96140300	H	0.41142800	2.84103300	1.75480700
H	-3.29017200	6.87979700	1.78488800	C	2.62711200	1.43130200	-5.19014900
H	-2.57567800	5.61058700	2.76679400	C	3.84718500	0.85554500	-4.49480000
H	-5.42522900	6.61801000	3.18884100	O	4.80791400	0.43114500	-5.13546500
H	-5.26591400	5.78342300	0.85750000	N	3.76110200	0.82118700	-3.13847100
H	-6.23233100	4.68418800	1.84927700	C	4.80116300	0.25202800	-2.30602200
H	-4.55420900	4.27298200	1.41828800	C	4.27835200	-1.04317600	-1.66783800
H	-5.78522100	4.44343200	4.33916400	O	3.27440300	-1.00699800	-0.91952400
H	-4.10617800	3.97215500	4.00698200	C	5.24730600	1.23091300	-1.19441500
H	-4.45597000	5.31138500	5.10454000	O	5.80937600	2.39284100	-1.75673600
H	-2.97093300	7.03539400	4.84736400	N	4.91888400	-2.20710400	-1.88774300
H	-4.66046300	2.50357400	-2.63940800	C	6.07549900	-2.46826500	-2.78960300
H	-3.37321000	2.97793000	-3.72845300	C	5.64857400	-2.55837400	-4.25827100
H	-2.49896600	4.91762200	-2.47480600	C	6.60971900	-3.79985400	-2.22905800
H	-6.14692300	4.32885600	-3.57206300	C	5.33723000	-4.55008600	-1.80357300
H	1.44995300	5.58204300	-0.81582100	C	4.44102000	-3.44088200	-1.23338100
H	2.13540700	6.98095900	-1.62667800	H	3.37460500	-3.58608600	-1.42621000
H	3.63716500	7.55006900	0.03055500	H	4.56223400	-3.34351000	-0.14871300
H	4.91919900	6.48958100	0.53021100	H	4.86316700	-5.01897900	-2.67144600
H	2.64381400	4.15105800	-2.62875100	H	5.53202100	-5.33762000	-1.07061500
H	-1.48987900	4.59186600	-4.79549400	H	7.20607600	-4.34251000	-2.96630100
H	-0.91151100	2.94387400	-4.44900800	H	7.24486300	-3.61038800	-1.35610000
H	1.41122900	4.27447900	-5.03139800	H	6.81719900	-1.67460900	-2.66846600
H	2.71032200	5.63229900	-3.58661500	H	4.88554100	-3.33106300	-4.39955500
H	-0.59266000	3.69226900	-6.03234900	H	5.26286800	-1.60553700	-4.62584700
H	-4.86393200	4.80008800	-4.68808600	H	6.51565100	-2.82381600	-4.87301900
H	-5.62541600	3.20610500	-4.84317700	H	5.64810000	0.06869800	-2.96604800
H	-3.70993900	8.27822700	3.83021800	H	5.23763800	3.14271300	-1.53021300
H	-1.99386500	7.89427000	3.65788000	H	6.00194300	0.71624200	-0.57812000
C	5.80219000	1.98007000	7.01134400	H	4.39795600	1.45108600	-0.54045800

H 2.93818600 1.21932000 -2.69006600
H 2.14482800 0.62980600 -5.75856800

H 1.90117300 1.86367500 -4.50079100
H 2.96293600 2.17745600 -5.91694200

(5S)-MeDHU-TS1-II (S&DHPase)

C 4.49692300 7.35309800 -1.74485100
C 3.66781200 6.43607200 -0.91953300
N 2.82093300 6.83381700 0.10533000
C 3.52514500 5.08046900 -0.98171000
C 2.21110400 5.73220600 0.61149800
N 2.61402100 4.65139700 -0.03446800
C 7.37428200 0.16231800 -0.32967500
C 6.10152600 0.74555200 0.18570100
N 5.77299700 0.77154200 1.53375700
C 5.03379500 1.33274500 -0.44205600
C 4.55802400 1.35125400 1.67587200
N 4.08126100 1.69973900 0.49226000
C 0.61627800 5.02388700 4.53677600
N 1.54572300 4.27228200 3.72125100
C 1.11018600 3.39987000 2.76081700
O -0.13822500 3.46711800 2.48714900
O 1.97447000 2.65539500 2.20579800
C -3.33398300 4.01700600 4.15132600
C -3.74959000 2.73684300 3.48828000
N -3.07218300 2.13991300 2.42303400
C -4.84155200 1.96724400 3.79652900
C -3.75936200 1.04867900 2.10337600
N -4.83320900 0.91097200 2.90885700
C -1.84727700 5.92397600 -2.97277600
C -2.12039700 5.13766300 -1.74073300
N -3.12657000 5.41232600 -0.82568100
C -1.47227300 4.04630400 -1.23622200
C -3.05235900 4.50386100 0.17732400
N -2.05286700 3.66390500 -0.04321700
C 2.11372000 3.78304200 -3.92317800
C 1.77286300 2.79889700 -2.80169100
O 2.70189900 2.53726200 -1.95211400
O 0.60343700 2.35687800 -2.73199100
Zn 2.27025600 2.60350800 0.10831800
Zn -1.22375900 2.36883900 1.28874100
H 3.88640600 8.07919200 -2.29422400
H 5.21802000 7.91705900 -1.14180800
H 3.98225700 4.37865500 -1.65782200
H 2.68045400 7.78030500 0.42707000
H 1.51080000 5.75629700 1.43144500
H 7.45563500 0.34745100 -1.40260500
H 7.41958200 -0.91980200 -0.17178200
H 4.86582500 1.51269400 -1.49214300
H 6.33101000 0.38603100 2.28187300
H 4.05062500 1.50795000 2.61436300
H -2.29308300 3.96632400 4.48194200
H -5.60000100 2.07937100 4.55485300

H -5.47159300 0.12914900 2.89700400
H -3.52424900 0.36647900 1.29826300
H -1.03950500 5.44345200 -3.52771000
H -2.71952300 5.97667700 -3.63444300
H -0.65590000 3.50354300 -1.68761300
H -3.81021700 6.15193300 -0.89548200
H -3.72375300 4.47781700 1.02086000
H -0.11484800 5.52528300 3.90111000
H 1.41217800 3.67869100 -4.75216300
H 2.03954000 4.80039600 -3.52234100
H 8.25011100 0.61071800 0.15262000
H -3.41310800 4.87379500 3.47165900
H -3.96855400 4.21676500 5.01751100
H 1.16766500 5.77968600 5.10194200
H 0.06969400 4.39298900 5.24984000
H 5.06041200 6.77193700 -2.47711200
H 3.13797700 3.64134400 -4.27704600
H -1.54073400 6.95230900 -2.74711400
H 2.48700300 4.12343100 4.05102000
C 5.32599000 -5.93873000 3.93356400
C 5.30085600 -4.81864900 2.88563900
C 6.49755300 -3.85202800 2.97537200
C 6.50223200 -2.87915900 1.78942700
C 6.53544200 -3.08061700 4.30320900
C 6.44268100 -1.72533500 -3.93684900
C 5.36144000 -2.18070300 -2.96122800
S 5.61365600 -3.95167900 -2.48433900
C -0.00020300 -5.40461300 -2.57291900
C 1.18799600 -4.58174700 -3.06486000
O 2.14659300 -4.30217100 -2.32713300
C -0.04017800 -5.47467000 -1.04022500
C -1.21416300 -6.30394900 -0.54317200
O -2.38348800 -5.93003500 -0.64135300
N -0.90439000 -7.50148600 0.01563000
N 1.15504200 -4.21071200 -4.36219300
C 2.16042600 -3.32508600 -4.93726300
H 5.28782800 -5.26426800 1.88296500
H 4.36678900 -4.24487200 2.97786700
H 7.41378700 -4.45762900 2.91204700
H 6.49978600 -3.40550100 0.82890400
H 7.39057900 -2.23596700 1.81886600
H 5.61408100 -2.23319700 1.81374800
H 7.39353300 -2.39927300 4.33771900
H 5.62422800 -2.48129800 4.43201000
H 6.61618600 -3.74614900 5.16689000
H 5.23610200 -5.55137700 4.95292300
H 5.36881700 -1.56289800 -2.05833300

H	4.37239600	-2.09135100	-3.41460600	H	2.52378000	-0.02552600	-0.69190000
H	4.30857900	-4.24802400	-2.29866800	H	3.06069300	-1.44081100	0.21714000
H	7.44383600	-1.84470100	-3.50942500	H	1.74909500	0.32381000	1.58220900
H	-0.17575000	-4.46408900	-0.64825600	H	-1.52616300	-0.50494400	-0.82759900
H	0.91363800	-5.85379900	-0.66411200	H	1.88747700	-2.58404600	-1.49450300
H	0.04512500	-7.81489800	0.13118600	O	0.46813400	1.74888000	-0.09449700
H	-1.65760400	-8.08282000	0.35283700	H	0.36265500	1.75955100	-1.08217900
H	-0.93275600	-4.96876000	-2.94397700	C	1.05946500	-1.66782600	2.01410800
H	3.15820400	-3.70884900	-4.71720000	H	2.02420100	-2.01151400	2.40109300
H	2.07022200	-2.30804200	-4.53887500	H	0.44620200	-1.35518900	2.86064900
H	0.29118200	-4.33780100	-4.86861900	H	0.56540500	-2.51480000	1.53252500
H	0.08076600	-6.41249000	-3.00159900	C	-1.80610400	-2.27897800	-5.24917900
H	2.02465000	-3.29492700	-6.01942100	C	-3.15547000	-2.14083900	-4.56775600
H	6.40690800	-2.30510800	-4.86300400	O	-4.20418000	-2.17089100	-5.21072200
H	6.30819400	-0.66704000	-4.18810100	N	-3.08472200	-1.95332200	-3.22515400
H	6.25891200	-6.51055800	3.87527900	C	-4.26113400	-1.86945100	-2.38487400
H	4.49972700	-6.64010100	3.77916200	C	-4.31672100	-0.47408600	-1.75028900
C	-4.95277100	-4.09546300	6.79881000	O	-3.40948400	-0.10539700	-0.97192500
C	-3.50229900	-4.47058400	6.45894800	C	-4.23826200	-2.95165900	-1.28432000
C	-3.07368300	-3.85530200	5.14818000	O	-4.26284400	-4.21944500	-1.89248900
C	-2.59995800	-2.54026000	5.09578800	N	-5.35370700	0.34340600	-2.02343200
C	-3.23188600	-4.54384300	3.93725300	C	-6.49670400	0.11046800	-2.95116900
C	-2.31100100	-1.91935800	3.88146600	C	-6.10616500	0.31652900	-4.41974700
C	-2.94383900	-3.94642300	2.71401900	C	-7.52299400	1.14010200	-2.44014500
C	-2.49065900	-2.62273400	2.68357300	C	-6.65725300	2.33316800	-2.00476700
O	-2.23958600	-2.06516400	1.46592300	C	-5.42034200	1.66943900	-1.38185100
H	-3.40888000	-5.56176300	6.40993300	H	-4.49015600	2.21938600	-1.54857900
H	-2.84033100	-4.13643500	7.26716300	H	-5.52849000	1.54159000	-0.29772300
H	-2.46000000	-1.98555300	6.02118800	H	-6.37179900	2.93268400	-2.87499600
H	-3.59322000	-5.56954000	3.95259500	H	-7.16802500	2.99621900	-1.30113300
H	-1.94446400	-0.89643600	3.85646400	H	-8.25934000	1.39639800	-3.20548300
H	-3.05764800	-4.48793800	1.77978700	H	-8.06216100	0.73264200	-1.57731300
H	-1.87056100	-1.16444500	1.56936200	H	-6.87388800	-0.90609200	-2.81243000
H	-5.06484800	-3.00926200	6.88178300	H	-5.69170000	1.31772500	-4.57965800
H	-5.63757900	-4.44023700	6.01730500	H	-5.38149700	-0.42887000	-4.75316900
H	-5.27027700	-4.54102500	7.74784900	H	-6.99724800	0.21496000	-5.04892000
N	-0.52368500	-0.60837000	-0.62378700	H	-5.11455100	-2.05805400	-3.03547500
C	0.14486000	-1.60050000	-1.33599900	H	-3.57449500	-4.77370000	-1.48659700
O	-0.46023900	-2.28774900	-2.17219500	H	-5.12413600	-2.80290100	-0.64161800
N	1.44397200	-1.79024400	-1.03608900	H	-3.35740000	-2.80320500	-0.65018600
C	2.17768900	-0.90664700	-0.14348300	H	-2.17415400	-2.01674400	-2.77025600
C	1.28791300	-0.49993900	1.03652500	H	-1.69409500	-1.46290300	-5.96943300
C	-0.04718600	0.02256400	0.51448200	H	-0.96850100	-2.26197200	-4.55062300
O	-0.95637700	0.40431400	1.36213100	H	-1.80716800	-3.20937100	-5.82718000

(5S)-MeDHU-INT-II (SkDHPase)

C	3.78166100	7.70225100	-1.76397800	N	2.08402100	4.84888600	-0.11292300
C	2.98098200	6.72212300	-0.98428200	C	7.33625500	0.83858500	-0.26591900
N	1.93665900	7.03908900	-0.12599600	C	6.02668100	1.32762000	0.24479400
C	3.05417800	5.36058200	-0.95345200	N	5.68353100	1.32420000	1.58899000
C	1.42749400	5.88572500	0.37740200	C	4.92733700	1.83494700	-0.39445800

C	4.42732000	1.80934800	1.71894600	H	-0.40712200	4.39930200	5.23465600
N	3.94116900	2.12551500	0.53001700	H	4.51856000	7.16835200	-2.36667900
C	0.09151400	5.05082200	4.50468900	H	2.79775300	3.82390500	-4.32023100
N	1.06307400	4.34619300	3.69746100	H	-2.21319100	6.71077900	-2.81336100
C	0.71195600	3.52229400	2.66839000	H	2.00875100	4.24711200	4.03234700
O	-0.51706300	3.55838200	2.30754100	C	5.85686000	-5.40194100	4.03066800
O	1.63943200	2.84064400	2.12921900	C	5.73160500	-4.29752400	2.97335600
C	-3.73761100	3.65902600	4.09523200	C	6.82628500	-3.21605600	3.05705500
C	-4.05004200	2.32556200	3.48849300	C	6.72167600	-2.24630700	1.87317300
N	-3.33395300	1.77799900	2.42577000	C	6.79628300	-2.44629300	4.38601600
C	-5.04705700	1.45086100	3.83178500	C	6.62624800	-1.15795600	-3.86488000
C	-3.89918800	0.60856900	2.13793000	C	5.57243800	-1.68472900	-2.89516500
N	-4.93756400	0.38085200	2.96543000	S	5.97524300	-3.41141100	-2.36242300
C	-2.38093200	5.64952500	-3.03197200	C	0.51881900	-5.42114000	-2.53388800
C	-2.59844400	4.85092600	-1.79504300	C	1.64538200	-4.51257100	-3.02302100
N	-3.66501100	5.02514300	-0.92523600	O	2.58831900	-4.18405500	-2.28589000
C	-1.85300600	3.84597900	-1.24298100	C	0.43681400	-5.42614900	-0.99924600
C	-3.53249100	4.14618200	0.09693800	C	-0.59972200	-6.41053500	-0.48282100
N	-2.43740600	3.42061800	-0.06612700	O	-1.80928500	-6.17516100	-0.47830600
C	1.77895600	3.89986300	-3.93217400	N	-0.11758600	-7.59705400	-0.03029900
C	1.55188400	2.90372500	-2.79873400	N	1.58451000	-4.13015400	-4.31698500
O	2.50066500	2.75440500	-1.94871200	C	2.53027800	-3.17683700	-4.88707900
O	0.43500400	2.33376900	-2.71744200	H	5.76681500	-4.75051200	1.97455600
Zn	2.06196300	2.79111800	0.10722700	H	4.74545500	-3.81707400	3.05592900
Zn	-1.61423400	2.22511700	1.35277200	H	7.79868600	-3.72548700	2.98505600
H	3.15924700	8.29375700	-2.44535400	H	6.76382200	-2.76876500	0.91145100
H	4.32379600	8.40341200	-1.11899100	H	7.54090500	-1.51669100	1.89695800
H	3.70601400	4.70853500	-1.50873100	H	5.77217700	-1.69478300	1.90677800
H	1.60650500	7.96830100	0.09024200	H	7.58028000	-1.68047600	4.41507100
H	0.60055200	5.83783500	1.06912300	H	5.82924600	-1.94441500	4.52368700
H	7.40702500	1.02942400	-1.33859400	H	6.95239500	-3.10143900	5.24726400
H	7.45845800	-0.23771200	-0.10874300	H	5.72404100	-5.01701900	5.04633000
H	4.75736700	1.99729000	-1.44693100	H	5.50455600	-1.04437600	-2.01060100
H	6.25813900	0.97178500	2.34105700	H	4.58848300	-1.69961900	-3.36717000
H	3.89542300	1.91308300	2.65126100	H	4.69846900	-3.83217100	-2.22323200
H	-2.68867100	3.71531700	4.39863900	H	7.62541300	-1.17087300	-3.41669300
H	-5.80260800	1.49725800	4.59961100	H	0.13439100	-4.43122200	-0.66764100
H	-5.48096200	-0.46977400	2.98861400	H	1.42732700	-5.63630900	-0.58670700
H	-3.59340600	-0.06642500	1.34867100	H	0.86779000	-7.79764900	0.01535900
H	-1.50181400	5.26716700	-3.55381200	H	-0.77462000	-8.28417800	0.30864500
H	-3.23038800	5.58356800	-3.72125300	H	-0.43794900	-5.09523200	-2.95285300
H	-0.96767200	3.38393400	-1.65233500	H	3.54966900	-3.48728500	-4.65195900
H	-4.42639300	5.67806700	-1.04072600	H	2.36264000	-2.16660600	-4.49602200
H	-4.23242300	4.05691500	0.91284900	H	0.72168600	-4.29213200	-4.81509500
H	-0.67290800	5.48810600	3.86131300	H	0.71513500	-6.43359000	-2.91205100
H	1.05805100	3.74338700	-4.73557000	H	2.40577600	-3.16323400	-5.97106100
H	1.65629900	4.91194500	-3.53028300	H	6.66367200	-1.76506200	-4.77322000
H	8.17771700	1.34684800	0.21840500	H	6.39927600	-0.12439500	-4.15094400
H	-3.91285800	4.47924600	3.38916400	H	6.83997200	-5.88372600	3.98263200
H	-4.36412700	3.83390800	4.97262100	H	5.10146000	-6.17913800	3.87680500
H	0.59282000	5.85343500	5.05145200	C	-4.57821900	-4.55312200	6.79630900

C	-3.06394000	-4.51970500	6.53266000	H	0.53899100	-1.14238300	2.77377500
C	-2.72415800	-3.84988400	5.21994000	H	0.64793000	-2.31920100	1.46189900
C	-2.36108700	-2.50098500	5.15989100	C	-1.51664500	-2.52662000	-5.24010200
C	-2.82024400	-4.55270700	4.00867200	C	-2.87550300	-2.47870000	-4.56277300
C	-2.11503500	-1.86320100	3.94186200	O	-3.91363700	-2.64824700	-5.20220600
C	-2.57680100	-3.93882400	2.78528900	N	-2.82657500	-2.20443300	-3.23432900
C	-2.22842100	-2.58112000	2.74371900	C	-3.99942500	-2.27243300	-2.38522100
O	-2.02699500	-2.02184700	1.52084400	C	-4.24120600	-0.89389200	-1.75561900
H	-2.67637900	-5.54592500	6.53671800	O	-3.40691700	-0.41230000	-0.96157400
H	-2.56285000	-3.99678600	7.35594800	C	-3.81454100	-3.33398100	-1.28231900
H	-2.26710000	-1.93247100	6.08278500	O	-3.64692300	-4.58590900	-1.90100200
H	-3.08834900	-5.60677900	4.02532700	N	-5.36701400	-0.21066100	-2.05810200
H	-1.82676000	-0.81569400	3.91638600	C	-6.45395500	-0.58685900	-3.00415000
H	-2.63342300	-4.49642400	1.85530800	C	-6.05736800	-0.35869700	-4.46738900
H	-1.62892800	-1.12014300	1.57550600	C	-7.60306300	0.32547200	-2.53254600
H	-4.99024400	-3.53903200	6.83552000	C	-6.88855700	1.61504300	-2.09800200
H	-5.10242500	-5.09261600	6.00081600	C	-5.60341400	1.10238300	-1.43294200
H	-4.80607700	-5.04776200	7.74657100	H	-4.73725500	1.75395000	-1.57924900
N	-0.38878500	-0.57774600	-0.73466000	H	-5.72845900	0.97268200	-0.35021600
C	0.31848400	-1.58103000	-1.34941200	H	-6.64773700	2.22769400	-2.97288600
O	-0.23548300	-2.38652600	-2.12457900	H	-7.48907800	2.22861600	-1.42060800
N	1.64216400	-1.66767600	-1.07525900	H	-8.34647000	0.48613600	-3.31705700
C	2.32870100	-0.74163500	-0.19270100	H	-8.11260400	-0.12841700	-1.67475600
C	1.39704900	-0.32185400	0.95062900	H	-6.71545600	-1.63811500	-2.85672900
C	0.09261200	0.25305100	0.34714600	H	-5.74914000	0.67912800	-4.63420900
O	-0.89148900	0.46100600	1.25796100	H	-5.25135000	-1.02694900	-4.77632900
H	2.67355800	0.13325600	-0.75585100	H	-6.91880000	-0.56322900	-5.11281100
H	3.21563800	-1.24176000	0.20786700	H	-4.82575200	-2.57990000	-3.02579500
H	1.85427600	0.50158800	1.50182300	H	-2.99208600	-5.09962900	-1.39473500
H	-1.40368300	-0.60048300	-0.86313300	H	-4.71054200	-3.31648400	-0.63490600
H	2.12010600	-2.46979600	-1.47665400	H	-2.96154600	-3.05347000	-0.65374600
O	0.43505800	1.59035000	-0.24409100	H	-1.91309800	-2.20097600	-2.77334600
H	0.34098200	1.61481700	-1.25228100	H	-1.48258500	-1.75479900	-6.01492900
C	1.15079700	-1.47224000	1.93315300	H	-0.68901400	-2.38185700	-4.54401700
H	2.10829600	-1.82646400	2.33029900	H	-1.42621300	-3.49053000	-5.75278700

(5S)-MeDHU-TS2-II (SkDHPase)

C	3.36749800	7.59130700	-2.44839400	C	0.65052800	3.62399200	2.61090800
C	2.72151600	6.64931400	-1.49692200	O	-0.58345200	3.33908700	2.46895400
N	1.94389400	7.03302800	-0.41440800	O	1.65598900	3.01645600	2.13292500
C	2.71907900	5.28449600	-1.45950500	C	-3.93019800	3.79903900	3.84285200
C	1.51003200	5.91837000	0.22409800	C	-4.14267300	2.41473800	3.30305300
N	1.95926500	4.83842900	-0.39448300	N	-3.36132500	1.82837300	2.30591200
C	7.22536300	1.05476100	-0.35564800	C	-5.11754000	1.52373700	3.66995900
C	5.91310000	1.54475700	0.13771600	C	-3.87137500	0.62260700	2.08321200
N	5.58625700	1.61426600	1.48292500	N	-4.93412100	0.40363500	2.88483600
C	4.79219200	1.97637000	-0.51787200	C	-2.70911100	5.16962700	-3.45304700
C	4.31637400	2.06313500	1.59908800	C	-2.78368100	4.53070500	-2.10871300
N	3.80610000	2.28720500	0.39848000	N	-3.79126800	4.79959800	-1.19364300
C	-0.16209000	5.38406300	4.07951000	C	-1.97141000	3.62427500	-1.47890000
N	0.90670500	4.76292000	3.33759300	C	-3.56307400	4.06949400	-0.07545100

N	-2.46330100	3.35087300	-0.21721100	H	6.83730500	-2.38634200	1.20673500
Zn	1.87984300	2.83371300	0.05141500	H	7.48016700	-0.99750600	2.09916700
Zn	-1.55139300	2.17622300	1.20404500	H	5.73110200	-1.31983600	2.08131900
H	2.63368600	8.20676400	-2.98168400	H	7.45042000	-0.94627800	4.62455700
H	4.06636200	8.27016200	-1.94634300	H	5.72337200	-1.34223100	4.70954400
H	3.19790600	4.58464800	-2.12202600	H	6.91049200	-2.33878000	5.55911900
H	1.74113600	7.98199000	-0.13575900	H	5.84460300	-4.35544400	5.49260500
H	0.92125200	5.92926900	1.12901200	H	5.55456600	-0.98709300	-1.85699300
H	7.28773200	1.19063000	-1.43730800	H	4.62137700	-1.90994200	-3.03280100
H	7.36937200	-0.00967300	-0.14342500	H	4.96791700	-3.80857800	-1.58155000
H	4.60931200	2.06172000	-1.57697800	H	7.59789200	-1.16857800	-3.36822600
H	6.17890500	1.32402300	2.24730900	H	1.48684800	-5.38824800	-0.04243400
H	3.78954000	2.21073200	2.52812800	H	1.07691600	-7.10041800	-0.08666600
H	-2.88179300	3.95118700	4.11248800	H	-0.88849500	-6.14554900	1.10403300
H	-5.90354000	1.59154400	4.40514800	H	-2.22816100	-5.65473900	0.07838300
H	-5.43785400	-0.46822200	2.95348700	H	1.22753000	-6.86300800	-2.70109900
H	-3.50101000	-0.09516900	1.36465300	H	3.63511000	-3.42225200	-4.36523400
H	-1.86330800	4.75673600	-4.00615700	H	2.01122200	-2.70394700	-4.17132100
H	-3.61245000	4.98575200	-4.04554200	H	1.55014400	-5.44399200	-4.35849800
H	-1.09363200	3.12253200	-1.85421100	H	2.72844200	-6.86997900	-1.76712300
H	-4.57337700	5.42111200	-1.33941300	H	2.39052800	-3.69293200	-5.60063800
H	-4.20559000	4.07362400	0.79047800	H	6.61526700	-2.03046600	-4.55587300
H	-0.98258600	5.64568800	3.40925700	H	6.24988100	-0.33910000	-4.16218600
H	8.06141300	1.60177900	0.09488200	H	7.06765900	-5.20940100	4.54247000
H	-4.19305600	4.57295700	3.11113200	H	5.36553500	-5.66419200	4.41346600
H	-4.54920300	3.95858800	4.72853800	C	-4.39691800	-4.15256200	7.30637900
H	0.21064500	6.30066700	4.54516000	C	-2.91605400	-3.90936100	6.96685500
H	-0.56689300	4.73803700	4.86917600	C	-2.68470000	-3.38654000	5.56272100
H	3.93201100	7.02741900	-3.19329900	C	-2.16746000	-2.10863200	5.32491700
H	-2.57132000	6.25511200	-3.38461400	C	-2.98517900	-4.17785200	4.44225500
H	1.85386900	4.85128500	3.67504600	C	-1.95054600	-1.62660700	4.03021900
C	6.04610800	-4.81343600	4.51951800	C	-2.77857700	-3.71689300	3.14741500
C	5.86609200	-3.81908800	3.36529100	C	-2.25201900	-2.43389200	2.92462900
C	6.86634900	-2.64657700	3.38411400	O	-2.08483900	-2.04568900	1.63612600
C	6.72236700	-1.79139800	2.11908800	H	-2.36519500	-4.84977700	7.10192100
C	6.73089000	-1.77344100	4.64073800	H	-2.49012000	-3.20323700	7.68905200
C	6.57790800	-1.29805200	-3.74501100	H	-1.92194200	-1.46949000	6.17023300
C	5.62659000	-1.74806700	-2.63946400	H	-3.38465600	-5.17919400	4.58701100
S	6.19817000	-3.33779800	-1.88309300	H	-1.54641900	-0.63055900	3.87390000
C	1.81017200	-6.30416200	-1.96460000	H	-3.01367400	-4.33728800	2.28833500
C	2.26343100	-4.96328800	-2.52519400	H	-1.61052900	-1.17594200	1.51730400
O	2.81101600	-4.11765100	-1.79592200	H	-4.97422800	-3.22507500	7.23098500
C	1.02357800	-6.16767900	-0.65894200	H	-4.84798800	-4.87947400	6.62341100
C	-0.44404700	-5.81186700	-0.88971100	H	-4.50707200	-4.53883000	8.32481500
O	-0.86603800	-5.46858800	-1.99890600	C	-1.51496500	-3.12364600	-4.90928600
N	-1.24860600	-5.91246400	0.19298700	C	-2.87458200	-3.10937200	-4.24412000
N	2.12398000	-4.78693900	-3.85199300	O	-3.91514000	-3.39560700	-4.83469900
C	2.56614100	-3.57549300	-4.53039800	N	-2.82235200	-2.74219400	-2.93308400
H	5.97297600	-4.35153000	2.41187200	C	-3.99257400	-2.62685800	-2.09249800
H	4.84204400	-3.41788700	3.37878100	C	-4.18048100	-1.15274800	-1.70261800
H	7.87854400	-3.07758700	3.38134500	O	-3.26693300	-0.54752300	-1.11143500

C	-3.80503300	-3.48279000	-0.82331800	C	1.53502400	3.50176100	-4.19246400
O	-3.58433100	-4.84823400	-1.14403500	C	1.39343500	2.48587600	-3.05376800
N	-5.34862100	-0.53668400	-1.98665300	O	2.25656900	2.48007800	-2.13968400
C	-6.47919100	-1.05821300	-2.79920100	O	0.35802600	1.73070200	-3.10956400
C	-6.13976700	-1.08732400	-4.29304700	N	-0.18970200	-0.16290100	-1.21832900
C	-7.60246700	-0.06658000	-2.43947500	C	0.46122600	-1.37251900	-1.64555600
C	-6.86670200	1.27179000	-2.26282100	O	-0.11927600	-2.19587400	-2.35329000
C	-5.54232300	0.87087300	-1.59494800	N	1.74397500	-1.48670600	-1.27070800
H	-4.68647900	1.47335800	-1.91191600	C	2.35467700	-0.53457500	-0.35302500
H	-5.59543500	0.93997000	-0.50119100	C	1.38796400	-0.20704300	0.79310100
H	-6.67792300	1.73158300	-3.23815100	C	0.10439900	0.47201200	0.23113800
H	-7.43133700	1.99139300	-1.66362000	O	-0.99568100	0.29473700	1.00891100
H	-8.38046900	-0.03432000	-3.20592700	H	0.91925900	3.22076300	-5.04755000
H	-8.07282200	-0.36391000	-1.49523400	H	1.21540300	4.48296000	-3.82612400
H	-6.73845500	-2.06562100	-2.46085700	H	2.63485200	0.36769400	-0.90096100
H	-5.84334300	-0.09340500	-4.64526500	H	3.27162200	-0.98564200	0.03447800
H	-5.34105400	-1.79626600	-4.51944900	H	1.84605500	0.55466500	1.43003900
H	-7.02298400	-1.39647800	-4.86321400	H	2.58192200	3.58187900	-4.49343600
H	-4.82821400	-3.01912500	-2.67046100	H	-1.20844100	-0.30796800	-1.27654800
H	-2.80819300	-4.89937300	-1.73994100	H	2.18967900	-2.38071900	-1.48839700
H	-4.71712000	-3.44545200	-0.21580100	O	0.24954600	1.82160900	-0.03110000
H	-2.98862400	-3.06312700	-0.22580100	H	0.14252900	0.84262500	-2.14695300
H	-1.91152500	-2.48606900	-2.55054300	C	1.12444800	-1.44324000	1.66166000
H	-1.07915800	-2.12060900	-4.91071800	H	2.07745300	-1.88127600	1.97974400
H	-0.83129000	-3.77202300	-4.35570200	H	0.56308500	-1.17691100	2.55761700
H	-1.63101200	-3.47682800	-5.93456600	H	0.56057600	-2.21621400	1.13434100

(5S)-MeDHU-EP-II (SkDHPase)

C	4.83828700	6.86109800	-2.57605400	C	-1.58709400	5.60426000	-3.54242800
C	4.02956700	6.08991700	-1.59880300	C	-1.84046300	4.95784300	-2.22039600
N	3.35828700	6.63514400	-0.51447600	N	-2.79826900	5.41753200	-1.32724400
C	3.75193200	4.75578500	-1.54543600	C	-1.25271000	3.89084500	-1.58985100
C	2.71504200	5.63699600	0.14097400	C	-2.76211600	4.64670000	-0.21755900
N	2.92824100	4.48248000	-0.46933600	N	-1.82880000	3.71439500	-0.34222900
C	7.40234300	-0.23835000	-0.33714100	Zn	2.48852900	2.49311900	-0.13144800
C	6.16955500	0.44856500	0.13236400	Zn	-1.16757800	2.59637100	1.21416700
N	5.87634400	0.64802600	1.47319900	H	4.23887900	7.60755100	-3.11024900
C	5.11275600	0.99941200	-0.54219100	H	5.67344000	7.38797500	-2.10002700
C	4.69066400	1.29173900	1.56914700	H	4.06432400	3.96687100	-2.20718700
N	4.20267600	1.51670600	0.35985900	H	3.35096000	7.60899800	-0.24835900
C	0.96873900	5.49555800	3.98941100	H	2.14501000	5.77974700	1.04596300
N	1.84837500	4.63081300	3.23793000	H	7.46254400	-0.18381000	-1.42595700
C	1.34837400	3.61617300	2.46082700	H	7.41220900	-1.29586300	-0.05473100
O	0.07925600	3.64725100	2.28288100	H	4.92741700	1.06033400	-1.60289000
O	2.17940700	2.79599600	1.97488600	H	6.43372600	0.32309200	2.25017800
C	-3.03059700	4.64254200	3.77816500	H	4.21261000	1.58156600	2.49123500
C	-3.53382500	3.30391300	3.31919200	H	-1.96512300	4.59522100	4.01752800
N	-2.93002400	2.53525200	2.32115200	H	-5.36131700	2.87542800	4.52911600
C	-4.63870500	2.62912500	3.76766900	H	-5.37272200	0.71203200	3.15571500
C	-3.66744700	1.43737700	2.17811000	H	-3.48488700	0.62944000	1.48065200
N	-4.70677000	1.46122400	3.03466900	H	-0.83776700	5.02829100	-4.08862800

H	-2.49164000	5.64350200	-4.15944400	H	0.47033700	-5.53796100	-4.39746600
H	-0.49545200	3.21599800	-1.96801800	H	1.05961300	-7.37810600	-1.95069000
H	-3.43180300	6.18797600	-1.48405500	H	1.63506400	-3.86781600	-5.46001200
H	-3.41362500	4.77823600	0.63182100	H	6.22891200	-3.20522900	-4.50689900
H	0.22711100	5.94325000	3.32570200	H	6.24726800	-1.48261400	-4.08241600
H	8.30683100	0.22771000	0.06977600	H	6.02407100	-6.33560900	4.62481900
H	-3.15785200	5.41348700	3.00872700	H	4.25788600	-6.30957400	4.63253800
H	-3.57798000	4.96588700	4.66605300	C	-4.97750600	-3.00434400	7.40810600
H	1.55803600	6.29651200	4.44327600	C	-3.57047300	-3.44290500	6.97128500
H	0.43306400	4.96842500	4.78956100	C	-3.22017500	-2.94947200	5.58519800
H	5.25714200	6.17952000	-3.31868000	C	-2.36309900	-1.86304900	5.38419100
H	-1.21364100	6.62851600	-3.42898800	C	-3.79854000	-3.54112800	4.45162600
H	2.79776600	4.50007600	3.55342400	C	-2.08994800	-1.37093200	4.10552900
C	5.14990200	-5.67561000	4.65849800	C	-3.54013500	-3.06688200	3.17099500
C	5.15788700	-4.68978000	3.48310500	C	-2.68145200	-1.97391500	2.98913200
C	6.43371400	-3.83027600	3.39095600	O	-2.48477800	-1.54198900	1.71285200
C	6.43856600	-3.00089200	2.10068500	H	-3.51086000	-4.53808300	7.00202600
C	6.62273500	-2.92120200	4.61487100	H	-2.83192100	-3.07371400	7.69212000
C	6.31783700	-2.49874800	-3.67737200	H	-1.89707500	-1.38622000	6.24350600
C	5.22629600	-2.73314300	-2.63652000	H	-4.46451200	-4.39210500	4.57588100
S	5.36911500	-4.42687000	-1.90370900	H	-1.42134100	-0.52532600	3.96975900
C	0.35222200	-6.54831900	-2.06547900	H	-3.99025300	-3.52890000	2.29826300
C	1.19058500	-5.35606000	-2.50882400	H	-1.78081500	-0.86365700	1.66050800
O	1.92645000	-4.75106800	-1.71306200	H	-5.05920500	-1.91233300	7.42422900
C	-0.37081400	-6.31336500	-0.73686400	H	-5.73975000	-3.38382000	6.71998800
C	-1.79245000	-5.78304800	-0.91379900	H	-5.21518900	-3.37642800	8.41012800
O	-2.27572200	-5.53516000	-2.02232600	C	-1.97608100	-2.79459100	-4.82031300
N	-2.50767000	-5.65557200	0.23024900	C	-3.33702800	-2.51967300	-4.20806500
N	1.14276800	-5.05373800	-3.82268600	O	-4.35973500	-2.44935100	-4.88999800
C	1.94799800	-3.99749000	-4.42310500	N	-3.30302200	-2.31289100	-2.86255300
H	5.04647300	-5.24848400	2.54542800	C	-4.47777900	-1.99430200	-2.07842900
H	4.28231900	-4.02706100	3.54936000	C	-4.44661800	-0.52550900	-1.61415500
H	7.29126900	-4.51790900	3.34787800	O	-3.47538000	-0.09886600	-0.96172200
H	6.33243400	-3.62814000	1.20922700	C	-4.51274200	-2.88839400	-0.82023400
H	7.37533800	-2.43736300	2.00697300	O	-4.66633600	-4.25992300	-1.13665100
H	5.60679200	-2.28351100	2.09771400	N	-5.51431800	0.26764400	-1.85549400
H	7.53322500	-2.31787800	4.52041600	C	-6.62649600	0.01860500	-2.80974900
H	5.77303400	-2.23394500	4.72492200	C	-6.13443700	0.08746600	-4.25731700
H	6.70716700	-3.49064500	5.54445400	C	-7.61551900	1.13758100	-2.43399300
H	5.15690500	-5.16358400	5.62563800	C	-6.70583700	2.31890200	-2.05819700
H	5.29191800	-1.99108500	-1.83505800	C	-5.51808800	1.65090400	-1.34762100
H	4.23636500	-2.64406700	-3.08764000	H	-4.55592300	2.13026200	-1.54880900
H	4.04852800	-4.61154900	-1.67532600	H	-5.64904000	1.63793200	-0.25768400
H	7.31675500	-2.61995000	-3.24508800	H	-6.36655300	2.83754300	-2.96041400
H	0.20510200	-5.60493900	-0.13106400	H	-7.20593500	3.05592100	-1.42382000
H	-0.42919200	-7.24633200	-0.16492200	H	-8.30413400	1.36632300	-3.25095000
H	-2.07420400	-5.74288000	1.13512900	H	-8.21274700	0.83182400	-1.56727200
H	-3.44217300	-5.26118400	0.15183800	H	-7.06858700	-0.96228500	-2.61401400
H	-0.37287600	-6.82813900	-2.83366500	H	-5.65174700	1.04986500	-4.45986000
H	3.01002400	-4.26210300	-4.40519200	H	-5.43762200	-0.71891200	-4.49101600
H	1.80604500	-3.05559400	-3.88698400	H	-6.98595400	-0.01037600	-4.94052900

H	-5.34833600	-2.21142200	-2.69688600	C	1.36712800	-0.53644200	0.75967700
H	-3.92296400	-4.54353600	-1.71219100	C	0.36686100	0.60702700	0.69286900
H	-5.37574200	-2.61078000	-0.20316200	O	-0.71573900	0.59970600	1.36944300
H	-3.60487500	-2.69340400	-0.23534800	H	1.59694400	2.98322800	-5.08168100
H	-2.41774700	-2.48561100	-2.36467900	H	2.21348000	4.20923300	-3.94960300
H	-1.44999100	-1.84556900	-4.97336800	H	2.13891800	0.00684600	-1.21324400
H	-1.36387700	-3.42026900	-4.16666800	H	2.96373000	-1.34192900	-0.45495800
H	-2.11960800	-3.27324900	-5.78997200	H	2.19355100	-0.07918800	1.32286600
C	2.26642500	3.15296000	-4.23719500	H	3.29841600	2.94478600	-4.53273800
C	1.85073400	2.29241500	-3.04326400	H	-1.62645000	-0.38563400	-1.68720300
O	2.74768500	2.14546400	-2.12036300	H	1.50287300	-2.85663900	-1.31091700
O	0.69763200	1.83315100	-3.01022500	O	0.65476900	1.67072600	0.04731300
N	-0.61586700	-0.49399900	-1.70314200	H	-0.04928300	0.27744700	-2.05847700
C	-0.13326500	-1.75857100	-1.59460300	C	0.88397300	-1.76242500	1.53908600
O	-0.85172200	-2.77577000	-1.63284600	H	1.69134000	-2.49909500	1.59902400
N	1.22480500	-1.88092500	-1.39827500	H	0.59671800	-1.49560900	2.55882100
C	1.97840900	-0.90263300	-0.63017500	H	0.02986900	-2.24415100	1.05870800

(5S,6S)-Me₂DHU-ES-II (SkDHPase)

C	-2.73099200	-0.10103300	-4.80017600	O	-5.23584500	-3.65267900	-7.51344000
C	-3.70755800	-0.14197800	-5.92036500	O	-4.13407800	-4.49207900	-9.28626600
N	-4.00406900	0.92469500	-6.75672700	Zn	-6.40400300	-2.15658800	-8.46989400
C	-4.46963800	-1.17284100	-6.38771200	Zn	-6.06839600	-1.78038200	-11.97971000
C	-4.90932500	0.50923100	-7.67941500	N	-7.54624300	-5.61256800	-12.72281000
N	-5.20430600	-0.76533700	-7.48549900	C	-8.22782100	-6.76785700	-12.26927600
C	-9.56332900	-3.95540600	-4.12769800	O	-7.97977200	-7.85804700	-12.77917500
C	-9.08793600	-3.29929100	-5.38235400	N	-9.13371200	-6.56986800	-11.28896500
N	-9.87175400	-2.42603700	-6.12469500	C	-9.08519700	-5.38192500	-10.42419000
C	-7.90032600	-3.36192700	-6.06450700	C	-8.86237100	-4.12561500	-11.29062500
C	-9.15828800	-2.00113300	-7.19505900	C	-7.75532100	-4.34165900	-12.29797600
N	-7.95758800	-2.55362300	-7.18614700	O	-7.09985600	-3.41076000	-12.80086900
C	-6.95819100	2.60919700	-10.69330100	H	-1.71721500	0.13394300	-5.14537000
N	-7.27605700	1.49917200	-9.81640500	H	-3.00031900	0.64079600	-4.03911400
C	-7.27299000	0.18006800	-10.22943500	H	-4.53332300	-2.18929500	-6.03984600
O	-6.79741400	-0.04485600	-11.39798000	H	-3.61850000	1.85532000	-6.69330000
O	-7.70552400	-0.67570800	-9.40484800	H	-5.33770300	1.14338200	-8.44223600
C	-5.99742500	1.45357700	-14.50229300	H	-8.74654100	-4.52424500	-3.67878200
C	-6.15703000	0.07428300	-15.06318900	H	-10.39024900	-4.64708500	-4.31736700
N	-6.20193100	-1.09295400	-14.29896800	H	-7.00698000	-3.92512600	-5.84477400
C	-6.29043500	-0.25050400	-16.38932400	H	-10.82731300	-2.17382500	-5.91793500
C	-6.35823300	-2.08469600	-15.16383700	H	-9.50885600	-1.30373700	-7.93968600
N	-6.41350900	-1.62347900	-16.43552700	H	-6.74361500	1.64342300	-13.72608100
C	-0.67058800	-2.26303000	-10.70606800	H	-6.31649100	0.36401900	-17.27529400
C	-1.89926400	-1.91533900	-11.46966200	H	-6.56719700	-2.18620900	-17.25824300
N	-1.94505400	-1.10640900	-12.59687800	H	-6.45337600	-3.12700100	-14.90769200
C	-3.19648700	-2.27306600	-11.24081000	H	-0.93669300	-2.95873700	-9.90823000
C	-3.23662700	-1.00669500	-12.99970500	H	0.08583500	-2.74902500	-11.33327700
N	-4.02063100	-1.70189700	-12.19175000	H	-3.56688700	-2.92969400	-10.46919700
C	-2.92951900	-4.25382000	-7.22607700	H	-1.15624200	-0.66806500	-13.04933500
C	-4.19798800	-4.14920200	-8.08398600	H	-3.55955800	-0.44481400	-13.86160700

H	-6.04460200	2.38461400	-11.24509600	H	-10.40326700	-10.44941600	-15.00273600
H	-2.21886200	-4.95167500	-7.67184700	H	-8.76406800	-10.73736500	-15.53486600
H	-2.46436900	-3.26278000	-7.17152100	H	-9.07619500	-12.06937400	-11.23805900
H	-10.07655200	-5.29521400	-9.96643100	H	-7.68359600	-9.95292100	-7.54970800
H	-8.52813900	-3.30492900	-10.65196300	H	-7.03713800	-8.88101900	-8.81596600
H	-9.90170000	-3.21996700	-3.38908000	H	-7.51757300	-11.57816400	-9.79793400
H	-5.01366700	1.59712400	-14.03920400	H	-10.58652100	-11.46483300	-10.55319200
H	-6.10919600	2.19964900	-15.29242600	H	-6.15818300	-10.36023000	-8.37365000
H	-6.79524500	3.50670400	-10.09053200	H	-7.96785400	-8.95548500	-4.30062000
H	-7.75074700	2.82331300	-11.42303900	H	-7.34029400	-7.30585800	-4.13234300
H	-2.69743400	-1.07745500	-4.31323900	H	-16.37134700	-5.81458100	-7.93411000
H	-3.16756100	-4.56317400	-6.20483800	H	-15.77627600	-5.69047500	-9.59289000
H	-0.20404200	-1.38259900	-10.24815900	C	-12.65108500	-2.36154800	-18.57849700
H	-7.87214400	1.67411100	-9.02060500	C	-12.12867700	-2.14244700	-17.14895600
H	-6.90607700	-5.76699700	-13.50619800	C	-11.28625300	-3.29791000	-16.65514800
H	-9.42919800	-7.44643800	-10.85095800	C	-9.89707200	-3.31048800	-16.82072300
O	-6.08233800	-2.78782700	-10.26661800	C	-11.87903000	-4.42430700	-16.06576300
H	-5.47051400	-3.54384800	-10.14599800	C	-9.12151900	-4.39906500	-16.42038700
C	-15.72459800	-5.23247200	-8.59995700	C	-11.12256300	-5.51754000	-15.65577300
C	-14.28164200	-5.20647800	-8.07989500	C	-9.73212400	-5.51272800	-15.83046400
C	-14.13915700	-4.65976300	-6.64617900	O	-9.03576200	-6.59791900	-15.40385300
C	-12.71573900	-4.88046500	-6.11924200	H	-12.97986200	-1.99228600	-16.47374600
C	-14.53070900	-3.17808300	-6.54070100	H	-11.54135300	-1.21664800	-17.11534600
C	-8.21561400	-7.89748400	-4.42195300	H	-9.41075600	-2.44756500	-17.27139800
C	-8.60886700	-7.58320000	-5.86305200	H	-12.95702600	-4.44405100	-15.92268300
S	-10.11639700	-8.54641900	-6.33861600	H	-8.04406900	-4.40592800	-16.56160500
C	-9.67448300	-11.16761000	-11.08380600	H	-11.58781500	-6.38402100	-15.19667000
C	-8.97037200	-10.20101000	-10.13956700	H	-8.07033600	-6.44750800	-15.47492900
O	-9.43656900	-9.07876900	-9.88397900	H	-11.82233600	-2.48161700	-19.28388100
C	-10.06789100	-10.56024200	-12.43719200	H	-13.26593400	-3.26529000	-18.63656500
C	-9.00533600	-10.75328100	-13.51344800	H	-13.26085500	-1.51503800	-18.91157700
O	-7.81530700	-10.94927100	-13.23990600	C	-10.13433200	-3.69771600	-12.05733300
N	-9.45525100	-10.71393200	-14.78912600	H	-10.92141700	-3.44284400	-11.34139800
N	-7.86330400	-10.66980900	-9.52908600	H	-9.93783800	-2.81908000	-12.67641700
C	-7.14862300	-9.92146700	-8.50391200	H	-10.50271200	-4.49857900	-12.70369300
H	-13.87509200	-6.22550000	-8.10599900	C	-4.78800700	-9.59698500	-11.86439900
H	-13.65290200	-4.60894000	-8.75664800	C	-4.50397700	-9.37102900	-13.33308700
H	-14.82383100	-5.23444300	-6.00508100	O	-3.47646900	-9.76804200	-13.87836200
H	-12.43197200	-5.93802100	-6.13562600	N	-5.47420000	-8.66513500	-13.99085900
H	-12.62307200	-4.52445400	-5.08612700	C	-5.41644800	-8.44712600	-15.42351900
H	-11.98577400	-4.33690400	-6.73391300	C	-5.31388000	-6.94288400	-15.70673600
H	-14.42579700	-2.81484400	-5.51210300	O	-6.25794100	-6.17148200	-15.39024500
H	-13.89029500	-2.55914900	-7.18387500	C	-6.65994000	-9.05518600	-16.10981000
H	-15.56652400	-3.00109400	-6.84294700	O	-6.74929600	-10.44920200	-15.88174800
H	-16.15069800	-4.22798800	-8.68264700	N	-4.21421100	-6.44659000	-16.29333300
H	-8.80995500	-6.51593000	-5.98858000	C	-2.97313600	-7.16627600	-16.70583800
H	-7.79644100	-7.85110000	-6.54198600	C	-2.02126900	-7.39225700	-15.52492800
H	-9.93704300	-8.50754700	-7.67788000	C	-2.41109500	-6.21620300	-17.77994200
H	-9.02619400	-7.66225200	-3.72453500	C	-2.76228000	-4.81636700	-17.25158600
H	-10.23273800	-9.48325300	-12.32352900	C	-4.14598200	-5.00581600	-16.61204400
H	-11.01216400	-10.99439900	-12.78155400	H	-4.29442200	-4.40754600	-15.70912600

H -4.95966200 -4.76107900 -17.30529900
H -2.03510700 -4.49901500 -16.49795600
H -2.77454000 -4.05573400 -18.03619100
H -1.33939200 -6.36318800 -17.93249000
H -2.91470400 -6.39617900 -18.73624400
H -3.24364500 -8.12766400 -17.14833300
H -1.77036200 -6.44643500 -15.03350300
H -2.45088500 -8.07785100 -14.79240900
H -1.09211200 -7.84148500 -15.89115400
H -4.53329800 -8.98203500 -15.77093700
H -6.80848300 -10.60649800 -14.91532100

H -6.58228700 -8.91519200 -17.19397200
H -7.56337400 -8.53612500 -15.76788400
H -6.33987500 -8.41912300 -13.50905500
H -4.69546000 -8.65396000 -11.31399700
H -5.80348200 -9.97825300 -11.72238500
H -4.05850300 -10.30674500 -11.4742020
C -8.04542000 -5.56088700 -9.31176900
H -8.11269800 -4.74892700 -8.58577400
H -8.22999700 -6.50545600 -8.79241500
H -7.02326300 -5.57316400 -9.70112200

(5S,6S)-Me₂DHU-TS1-II (SkDHPase)

C -2.73098900 -0.10103100 -4.80017200
C -3.54697400 -0.18993700 -6.04184400
N -3.50019200 0.70725400 -7.10085900
C -4.45133100 -1.13497900 -6.42939900
C -4.35484600 0.27824200 -8.06562900
N -4.94277100 -0.84327100 -7.68815800
C -9.56332600 -3.95540600 -4.12769900
C -9.02407700 -3.17460700 -5.27750900
N -9.78604200 -2.27426200 -6.00913000
C -7.80427800 -3.18229300 -5.90116600
C -9.03132600 -1.78915600 -7.02350300
N -7.82509700 -2.33046600 -6.99104800
C -6.95819100 2.60919000 -10.69329900
N -7.32560600 1.54310900 -9.78559700
C -7.07309400 0.23067500 -10.06329500
O -6.30468500 0.01463500 -11.06798600
O -7.56595600 -0.64696900 -9.29198500
C -5.99742500 1.45357400 -14.50229200
C -6.27448400 0.05636900 -14.97238700
N -6.24723700 -1.07740500 -14.15724300
C -6.57332100 -0.33236000 -16.25278500
C -6.51122400 -2.11269800 -14.94706900
N -6.71493300 -1.70402400 -16.21701900
C -0.67059400 -2.26302900 -10.70607000
C -1.91384300 -1.97154800 -11.46552200
N -1.97792500 -1.16358700 -12.59135800
C -3.20229300 -2.36623500 -11.23785900
C -3.26935900 -1.09206300 -12.99351400
N -4.03616300 -1.80882500 -12.18703100
C -2.92951700 -4.25381900 -7.22607400
C -4.21485600 -4.14987300 -8.05035800
O -5.23794000 -3.63930000 -7.46514300
O -4.18985500 -4.50694700 -9.25099400
Zn -6.37047500 -2.16998400 -8.44857100
Zn -6.05398500 -1.66331600 -12.04000800
H -1.65565100 -0.13492000 -5.01036500
H -2.92897100 0.81806900 -4.23650000

H -4.75194000 -2.03109600 -5.91538000
H -2.93096800 1.53935900 -7.15082700
H -4.51603900 0.78959400 -9.00206200
H -8.75939500 -4.53081800 -3.66428700
H -10.33890900 -4.65892200 -4.44642100
H -6.92497600 -3.76630000 -5.67985400
H -10.75126300 -2.03786800 -5.82939800
H -9.36440500 -1.07281300 -7.75752300
H -6.67787400 1.74348500 -13.69650300
H -6.69721600 0.23858700 -17.15919300
H -6.98824900 -2.30248500 -16.98258700
H -6.53899500 -3.15059400 -14.64710700
H -0.90247800 -2.94996200 -9.89007400
H 0.09718300 -2.73568800 -11.32954400
H -3.55984000 -3.04440300 -10.47632300
H -1.19705300 -0.71508200 -13.04774200
H -3.60671100 -0.53488800 -13.85277200
H -5.93522100 2.46220600 -11.04143000
H -2.21822500 -4.93000500 -7.70234900
H -2.48356500 -3.25542900 -7.15239000
H -9.99507300 -3.30688400 -3.35702400
H -4.97809100 1.55892000 -14.11311200
H -6.11704600 2.15856300 -15.32788200
H -7.01782700 3.56468900 -10.16603100
H -7.61276400 2.66157000 -11.57338000
H -2.96941300 -0.94592300 -4.15157400
H -3.14342100 -4.59034900 -6.20820500
H -0.23140100 -1.35692900 -10.27188800
H -8.00731400 1.71606100 -9.06338300
C -15.72462800 -5.23248900 -8.59995600
C -14.28161200 -5.20645800 -8.07989900
C -14.13572000 -4.64946000 -6.65048500
C -12.71194600 -4.86863800 -6.12218300
C -14.52420000 -3.16642700 -6.55440200
C -8.21561900 -7.89747500 -4.42193800
C -8.79908000 -7.72906000 -5.81831000
S -10.18082800 -8.92160700 -6.11416100

C	-9.10608600	-10.05858700	-11.76640400	H	-10.19747600	-6.09449500	-15.57655500
C	-8.80047200	-9.70541700	-10.31891100	H	-8.39674400	-3.77510300	-13.61640400
O	-9.46018500	-8.87339500	-9.67401800	H	-12.00621400	-1.49841700	-18.38337500
C	-10.56059900	-9.80886500	-12.15774300	H	-12.04703000	-3.11671800	-19.09167700
C	-10.71155000	-9.55263900	-13.65561200	H	-13.44515700	-2.04133600	-19.26218100
O	-9.83456700	-9.02397500	-14.33471500	N	-7.23710200	-5.03489500	-11.68876800
N	-11.90783600	-9.90844800	-14.19021900	C	-7.92574500	-6.22485200	-11.45734500
N	-7.71901700	-10.31596300	-9.78643100	O	-7.57029300	-7.27392800	-12.00461800
C	-7.14862100	-9.92147200	-8.50393200	N	-9.00999600	-6.15528900	-10.64988500
H	-13.87827400	-6.22696900	-8.09851000	C	-9.07525500	-5.09077500	-9.64808700
H	-13.65168900	-4.61643000	-8.76209300	C	-8.88614200	-3.73913600	-10.36967100
H	-14.81956400	-5.21869600	-6.00374000	C	-7.68284700	-3.76898200	-11.32284700
H	-12.43070500	-5.92715500	-6.13809400	O	-7.60069200	-2.86206400	-12.25719800
H	-12.62081000	-4.51369000	-5.08870800	H	-10.09384100	-5.10457200	-9.24516200
H	-11.98171000	-4.32238900	-6.73529700	H	-8.69015100	-2.95611600	-9.63776700
H	-14.41661800	-2.79609600	-5.52857200	H	-6.60487900	-5.06505800	-12.49937800
H	-13.88429500	-2.55339000	-7.20353100	H	-9.34301800	-7.07775900	-10.36305700
H	-15.56042900	-2.99047300	-6.85559700	O	-6.27707200	-3.07664900	-10.24952500
H	-16.14809000	-4.22753000	-8.68979400	H	-5.60597800	-3.78635700	-10.07308100
H	-9.17192500	-6.71153700	-5.95853600	C	-10.15923600	-3.35814500	-11.14827900
H	-8.02720400	-7.90998800	-6.56795700	H	-10.99796700	-3.26251700	-10.45109900
H	-10.13838400	-8.86671500	-7.46444800	H	-10.02868400	-2.40589600	-11.66311200
H	-8.97229000	-7.73831500	-3.64654300	H	-10.41877100	-4.12041200	-11.88655200
H	-10.91024900	-8.90887900	-11.63785300	C	-4.82810800	-9.59760700	-11.88554700
H	-11.21291200	-10.62797800	-11.83582600	C	-4.67096900	-9.08758800	-13.31169200
H	-12.63636200	-10.34208500	-13.64722800	O	-3.87266700	-9.61149800	-14.08846500
H	-12.07212400	-9.71722700	-15.16723800	N	-5.44133500	-8.01174900	-13.61236100
H	-8.47838500	-9.39913700	-12.37573600	C	-5.44302500	-7.36154400	-14.90715300
H	-7.88273200	-10.04866300	-7.70498000	C	-4.87390900	-5.94343700	-14.75264400
H	-6.81897900	-8.87756200	-8.52445900	O	-5.43420700	-5.12014500	-13.99795200
H	-7.18333000	-10.93264600	-10.37855800	C	-6.87097600	-7.27096500	-15.49968800
H	-8.80821100	-11.09088200	-11.98080900	O	-7.38015400	-8.55409200	-15.77136200
H	-6.28837600	-10.55919100	-8.29581700	N	-3.78523900	-5.58302100	-15.46168700
H	-7.80193600	-8.90009900	-4.28218600	C	-2.94969200	-6.43795800	-16.34752400
H	-7.41043800	-7.17198300	-4.26106400	C	-2.06137000	-7.39288100	-15.54607600
H	-16.37310400	-5.80868900	-7.93060600	C	-2.15707100	-5.38168800	-17.14213400
H	-15.77615100	-5.69651100	-9.58998200	C	-1.93109900	-4.25281300	-16.12355300
C	-12.65108500	-2.36154800	-18.57849700	C	-3.24650000	-4.21726200	-15.33253300
C	-13.22478500	-2.92119000	-17.26872600	H	-3.12337500	-3.95774000	-14.27773200
C	-12.10837500	-3.35801000	-16.35268600	H	-3.96006300	-3.50154300	-15.75977200
C	-11.41110600	-2.41588800	-15.58880700	H	-1.09525900	-4.50121700	-15.46184000
C	-11.65646500	-4.68404300	-16.33616700	H	-1.70530100	-3.29215400	-16.59465000
C	-10.28226000	-2.77110600	-14.85518400	H	-1.22886900	-5.78940200	-17.54961000
C	-10.53661300	-5.06338800	-15.60203200	H	-2.76003600	-5.01512800	-17.98086400
C	-9.83596200	-4.09821300	-14.87123400	H	-3.59807600	-7.01056200	-17.01654400
O	-8.72110000	-4.49474800	-14.19584000	H	-1.41952900	-6.84051600	-14.85098300
H	-13.88820800	-3.76582700	-17.48769600	H	-2.64394200	-8.12532400	-14.98426200
H	-13.84107200	-2.15544900	-16.78185900	H	-1.41206500	-7.94763200	-16.23277900
H	-11.74797400	-1.38151900	-15.57857400	H	-4.83618300	-7.97851000	-15.56839800
H	-12.18886600	-5.43387500	-16.91673300	H	-8.11826200	-8.73396200	-15.16842900
H	-9.74529700	-2.02936100	-14.26991900	H	-6.80585500	-6.69956500	-16.43970200

H -7.50781800 -6.69892900 -14.81768000
H -6.12499600 -7.67290000 -12.93520500
H -3.91184400 -9.37177400 -11.33099700
H -5.67767000 -9.15386300 -11.36277300
H -4.92510000 -10.68666900 -11.91746100

C -8.09765200 -5.39996900 -8.51221300
H -7.05593900 -5.28691900 -8.81913800
H -8.27036900 -4.75816800 -7.65061900
H -8.25023800 -6.43486700 -8.20074800

(5S,6S)-Me₂DHU-INT1-II (SkDHPase)

C -2.73099300 -0.10103300 -4.80017700
C -3.52663000 -0.19653400 -6.05323700
N -3.42617800 0.66050700 -7.14132900
C -4.46002900 -1.11851300 -6.42470300
C -4.27997500 0.23177900 -8.10692200
N -4.91728800 -0.85248700 -7.70154700
C -9.56332400 -3.95540700 -4.12769400
C -9.02680700 -3.16068100 -5.26685800
N -9.79321600 -2.26915700 -6.00430100
C -7.80086800 -3.15148700 -5.87648900
C -9.03547700 -1.77227400 -7.00957500
N -7.82211500 -2.29682100 -6.96287300
C -6.95819100 2.60919600 -10.69330100
N -7.30217400 1.50317800 -9.82435700
C -6.99737100 0.20539300 -10.11443100
O -6.20640700 0.01672400 -11.10584700
O -7.47553400 -0.69213000 -9.35233400
C -5.99742500 1.45357800 -14.50229300
C -6.29506400 0.09053800 -15.04601400
N -6.26447600 -1.06887700 -14.27351600
C -6.62408600 -0.25539400 -16.33005000
C -6.55984000 -2.08224100 -15.08332000
N -6.78147700 -1.62741600 -16.33185100
C -0.67058800 -2.26303000 -10.70606800
C -1.89944600 -1.94714800 -11.48310900
N -1.91374800 -1.16968400 -12.63162100
C -3.20712300 -2.28996000 -11.27115600
C -3.19277300 -1.06590700 -13.06359000
N -4.00121200 -1.73101300 -12.25378800
C -2.92951900 -4.25382000 -7.22607700
C -4.21111900 -4.13214300 -8.04958900
O -5.23135100 -3.62081400 -7.46208200
O -4.19141500 -4.47893500 -9.25561300
Zn -6.38021500 -2.16239900 -8.40794400
Zn -6.02045000 -1.56148700 -12.27075500
H -1.65456600 -0.18959100 -4.98755700
H -2.89755200 0.84471200 -4.27157600
H -4.80143900 -1.98249100 -5.88224000
H -2.82400100 1.46789800 -7.20888200
H -4.40383000 0.71356100 -9.06464300
H -8.75743600 -4.53289200 -3.67043000
H -10.33557600 -4.65857500 -4.45499800
H -6.91894100 -3.72898200 -5.64897500

H -10.76562700 -2.05209300 -5.83851400
H -9.37500700 -1.06650600 -7.75108100
H -6.65429700 1.69456900 -13.66168400
H -6.75921200 0.34289700 -17.21680400
H -7.08530600 -2.19715000 -17.10801800
H -6.61495600 -3.12567900 -14.80147800
H -0.92916400 -2.92613300 -9.87848200
H 0.08388100 -2.77285300 -11.31593200
H -3.60389300 -2.93917200 -10.50400300
H -1.10769200 -0.76519900 -13.08545500
H -3.49034000 -0.52364400 -13.94730300
H -5.94167000 2.47971200 -11.06625800
H -2.21449300 -4.91517600 -7.71691200
H -2.48866800 -3.25609500 -7.12153600
H -9.99883300 -3.31806200 -3.34979300
H -4.96695900 1.53063800 -14.13663800
H -6.13569500 2.21026000 -15.27771900
H -7.01028700 3.54160900 -10.12565400
H -7.63139600 2.69549100 -11.55661300
H -3.01885500 -0.91158300 -4.12827200
H -3.14932200 -4.61907500 -6.21961000
H -0.20564800 -1.36236900 -10.28801100
H -7.98446600 1.63886800 -9.09472700
C -15.72461100 -5.23248300 -8.59995600
C -14.28163200 -5.20646700 -8.07990100
C -14.13047400 -4.62043400 -6.66274800
C -12.71021500 -4.84794200 -6.12832100
C -14.49756500 -3.13017800 -6.60026100
C -8.21561800 -7.89747700 -4.42193300
C -8.85723600 -7.78442200 -5.79781900
S -10.14957300 -9.08182500 -6.04946500
C -9.12985900 -9.98047800 -11.75607800
C -8.81567500 -9.66258300 -10.30205100
O -9.47241900 -8.84613100 -9.63556900
C -10.59515000 -9.75288800 -12.11944800
C -10.78274800 -9.48226400 -13.61037900
O -9.93070800 -8.93811400 -14.30806200
N -11.98929300 -9.84578700 -14.11875000
N -7.73039400 -10.28642800 -9.79020300
C -7.14862100 -9.92147200 -8.50393100
H -13.88684900 -6.23045200 -8.07680200
H -13.64670900 -4.63689000 -8.77440400
H -14.82278100 -5.16535000 -6.00421700

H	-12.44665900	-5.91103000	-6.11801100	C	-7.42433800	-3.72458500	-11.08689100
H	-12.61359800	-4.46938800	-5.10360700	O	-7.40313100	-2.85691100	-12.13618900
H	-11.97142200	-4.33011900	-6.75554200	H	-10.10497600	-5.04885700	-9.29452500
H	-14.38913400	-2.73890300	-5.58219800	H	-8.64444300	-2.95802700	-9.51466900
H	-13.84647500	-2.54106900	-7.26035900	H	-6.43157600	-5.08876800	-12.33131100
H	-15.52991500	-2.94601000	-6.90977500	H	-9.34458200	-7.02075500	-10.40968500
H	-16.14122700	-4.22648100	-8.70903100	O	-6.34193800	-3.28741400	-10.14595500
H	-9.31436900	-6.80048800	-5.92868300	H	-5.63622900	-3.98389000	-9.97955700
H	-8.09935800	-7.90843400	-6.57227300	C	-9.96232500	-3.28288800	-11.16175900
H	-10.16868500	-9.00159200	-7.39905700	H	-10.85552900	-3.19088600	-10.53382500
H	-8.95494600	-7.79221300	-3.62100600	H	-9.77625600	-2.31920400	-11.63541200
H	-10.95167900	-8.86641900	-11.58118100	H	-10.17620300	-4.01884000	-11.93889900
H	-11.22637400	-10.58794600	-11.79567600	C	-4.82810800	-9.59760800	-11.88554600
H	-12.69916800	-10.29273900	-13.5621800	C	-4.65892700	-9.04783400	-13.29578800
H	-12.17955300	-9.64646200	-15.08930800	O	-3.88983500	-9.58338600	-14.09474900
H	-8.52382900	-9.28604100	-12.34852500	N	-5.37745800	-7.92605700	-13.55277400
H	-7.87164200	-10.07486400	-7.69939900	C	-5.42092200	-7.29047300	-14.85524500
H	-6.82650300	-8.87493400	-8.50073000	C	-4.83060500	-5.87564600	-14.75043000
H	-7.19524200	-10.88248500	-10.40346500	O	-5.35965900	-5.02227600	-14.00956400
H	-8.81160400	-10.99852600	-12.00632200	C	-6.87116000	-7.19614000	-15.38782300
H	-6.28150900	-10.55824200	-8.32261900	O	-7.39268500	-8.48588900	-15.60310400
H	-7.72036500	-8.86391200	-4.29233900	N	-3.75273100	-5.55179500	-15.49793100
H	-7.46364600	-7.11103500	-4.29217100	C	-2.94140600	-6.44587900	-16.36626200
H	-16.37744800	-5.79159100	-7.92040900	C	-2.06137000	-7.39288100	-15.54607600
H	-15.77838300	-5.71460200	-9.58110400	C	-2.14022000	-5.42723000	-17.20091800
C	-12.65108500	-2.36154800	-18.57849700	C	-1.88825300	-4.26984500	-16.22159300
C	-13.10460300	-2.68013400	-17.14529500	C	-3.19507400	-4.19133100	-15.41922400
C	-11.94787900	-3.10923300	-16.27260700	H	-3.05762500	-3.89952400	-14.37451700
C	-11.22937000	-2.18167100	-15.51165500	H	-3.90346500	-3.47856900	-15.86161500
C	-11.51355700	-4.44305000	-16.25690300	H	-1.04940300	-4.50969900	-15.56037800
C	-10.10840400	-2.55842100	-14.77087800	H	-1.65316100	-3.32794600	-16.72521300
C	-10.40308600	-4.84131700	-15.52089100	H	-1.22189000	-5.86135600	-17.60354600
C	-9.68666100	-3.89457900	-14.77588000	H	-2.74543100	-5.07837300	-18.04561100
O	-8.59232900	-4.32791300	-14.09478400	H	-3.60550400	-7.02702700	-17.01211700
H	-13.86411500	-3.47080400	-17.17361100	H	-1.41013100	-6.83233400	-14.86621000
H	-13.59122300	-1.79775500	-16.71267200	H	-2.65121700	-8.10585700	-14.96723700
H	-11.54907900	-1.14178200	-15.49678400	H	-1.42159100	-7.97188600	-16.22178100
H	-12.06158900	-5.18700200	-16.83088300	H	-4.84847400	-7.92328500	-15.53238500
H	-9.56684000	-1.82565600	-14.17918300	H	-8.17096500	-8.61298300	-15.03797900
H	-10.08778800	-5.87982500	-15.49200100	H	-6.84247800	-6.64189000	-16.34102600
H	-8.26544600	-3.67094400	-13.43283900	H	-7.47206600	-6.60792000	-14.68816400
H	-11.91385800	-1.55160900	-18.58289700	H	-6.08254400	-7.61406300	-12.87969400
H	-12.18451100	-3.23580500	-19.04402000	H	-3.89941300	-9.43304100	-11.33004100
H	-13.49465200	-2.05431800	-19.20612300	H	-5.65487900	-9.13391900	-11.34356200
N	-7.07189100	-5.05950200	-11.53188000	H	-4.97481500	-10.67940300	-11.95466300
C	-7.85701100	-6.18406400	-11.42578100	C	-8.18679300	-5.45644400	-8.43452900
O	-7.55380300	-7.23803900	-12.01072000	H	-7.12058600	-5.40159000	-8.66439300
N	-8.97777900	-6.10284900	-10.65960200	H	-8.38357800	-4.82222800	-7.57014900
C	-9.06173600	-5.07083100	-9.63104500	H	-8.42087300	-6.48642700	-8.16202100
C	-8.77017900	-3.70909800	-10.29544900				

(5S,6S)-Me₂DHU-TS2-II (SkDHPase)

C	-2.73099400	-0.10103200	-4.80017700	H	-0.92173300	-2.85285900	-9.82257000
C	-3.53069400	-0.22031000	-6.05471600	H	0.03075100	-2.85279300	-11.30711900
N	-3.31019100	0.51187400	-7.21557500	H	-3.61519200	-2.80165700	-10.35816800
C	-4.56874600	-1.05084800	-6.36655600	H	-1.14832200	-0.89033800	-13.15758900
C	-4.19470700	0.10252300	-8.16107200	H	-3.55615000	-0.62411400	-13.94535100
N	-4.96822500	-0.85376900	-7.67629400	H	-5.92067300	2.42127500	-10.96953700
C	-9.56332700	-3.95540800	-4.12769200	H	-2.27652300	-4.98247400	-7.70799000
C	-9.02656400	-3.11664300	-5.22983900	H	-2.44669600	-3.27031000	-7.24699900
N	-9.80016700	-2.22414700	-5.95533600	H	-10.10894100	-3.36453400	-3.38431600
C	-7.79873800	-3.08557000	-5.83257700	H	-4.99329300	1.52523600	-14.06890500
C	-9.04722700	-1.70755900	-6.95182400	H	-6.05637700	2.15895400	-15.33414100
N	-7.82722700	-2.21995900	-6.90866300	H	-7.01424200	3.56126100	-10.15886000
C	-6.95819100	2.60919800	-10.69330100	H	-7.54669100	2.70253300	-11.61604100
N	-7.42876500	1.54953400	-9.83650100	H	-3.12182000	-0.79637900	-4.05516100
C	-7.08865100	0.24759700	-10.02205500	H	-3.08845400	-4.51936400	-6.17910700
O	-6.19208700	0.00260500	-10.90756000	H	-0.14324500	-1.36109800	-10.37338400
O	-7.64439300	-0.61045300	-9.26723300	H	-8.17086400	1.72495000	-9.17751000
C	-5.99742500	1.45357700	-14.50229300	C	-15.72462900	-5.23248500	-8.59995900
C	-6.30357400	0.06617700	-14.97602200	C	-14.28161300	-5.20646500	-8.07989900
N	-6.29873000	-1.05733400	-14.14971200	C	-14.04585400	-4.06027800	-7.07110000
C	-6.62391600	-0.33220500	-16.24718500	C	-12.78702900	-4.28098000	-6.22244500
C	-6.60012400	-2.10014900	-14.91906400	C	-13.99501900	-2.68670200	-7.75761300
N	-6.80156700	-1.70000000	-16.18956500	C	-8.21561800	-7.89747700	-4.42193200
C	-0.67058800	-2.26303000	-10.70606900	C	-8.91910100	-7.90889800	-5.77307500
C	-1.91488500	-1.94051200	-11.45426400	S	-10.08646200	-9.33256100	-5.91955500
N	-1.94855500	-1.23638700	-12.64841300	C	-9.17132400	-9.91109000	-11.72635800
C	-3.22423500	-2.21910700	-11.17485400	C	-8.84476700	-9.64098100	-10.26528500
C	-3.24064200	-1.11674000	-13.03929800	O	-9.50252100	-8.85831300	-9.56104300
N	-4.03775900	-1.69985400	-12.16007900	C	-10.63316900	-9.64494100	-12.07574200
C	-2.92951600	-4.25382200	-7.22607700	C	-10.82216900	-9.31740800	-13.55477600
C	-4.25607900	-4.13342800	-7.95017600	O	-9.95976000	-8.77265400	-14.23918200
O	-5.23206600	-3.60335400	-7.37035400	N	-12.04064500	-9.63166400	-14.06771000
O	-4.27979200	-4.52450700	-9.17971500	N	-7.74403600	-10.26654200	-9.78894600
Zn	-6.48336900	-2.06972000	-8.43220100	C	-7.14862200	-9.92147200	-8.50393200
Zn	-6.06598500	-1.56058500	-12.11837200	H	-14.06112700	-6.16445400	-7.59238000
H	-1.67475300	-0.34394600	-4.96352400	H	-13.57466400	-5.11373700	-8.91585700
H	-2.77827100	0.90683800	-4.37237200	H	-14.90237400	-4.05858000	-6.38084400
H	-5.03000200	-1.80005600	-5.74761200	H	-12.82309800	-5.23726500	-5.68991400
H	-2.61718100	1.23558000	-7.33815800	H	-12.68320600	-3.48908000	-5.46841300
H	-4.25086500	0.50168000	-9.16280300	H	-11.88497900	-4.28384600	-6.84827100
H	-8.74383500	-4.46154100	-3.61298700	H	-13.89438100	-1.87871300	-7.02296700
H	-10.24341000	-4.72679200	-4.50777400	H	-13.14122000	-2.62733300	-8.44523500
H	-6.91413000	-3.65877500	-5.60598500	H	-14.89867700	-2.48327500	-8.33863000
H	-10.78024400	-2.03485500	-5.80101100	H	-15.98651500	-4.31274400	-9.13244800
H	-9.39131900	-0.99814200	-7.68717200	H	-9.47506900	-6.98014600	-5.92594800
H	-6.70360100	1.77517500	-13.73066100	H	-8.18346000	-7.99575300	-6.57308400
H	-6.74111600	0.22839500	-17.16078500	H	-10.23524900	-9.23995400	-7.25961900
H	-7.10864300	-2.30036600	-16.94095500	H	-8.92911600	-7.82547100	-3.59450400
H	-6.67150300	-3.12956300	-14.59525800	H	-10.97151500	-8.77243200	-11.50381000

H	-11.27864100	-10.47950000	-11.77993500	O	-6.34754500	-3.19403700	-10.06935200
H	-12.76279300	-10.06846200	-13.51891100	H	-5.34908000	-4.01455500	-9.69540800
H	-12.23407800	-9.38526300	-15.02673400	C	-9.97529400	-3.30815300	-11.00382400
H	-8.55284700	-9.21284400	-12.30168100	H	-10.86790400	-3.24824700	-10.37003900
H	-7.85690100	-10.10338000	-7.69253600	H	-9.81782900	-2.33443200	-11.46723800
H	-6.84096200	-8.87064200	-8.48244100	H	-10.17258500	-4.04111700	-11.78807300
H	-7.20086100	-10.82261200	-10.43212100	C	-4.82810800	-9.59760700	-11.88554700
H	-8.87339700	-10.92772900	-12.00603400	C	-4.67374500	-9.02627100	-13.28884800
H	-6.27019500	-10.54992800	-8.34891700	O	-3.92239600	-9.55834400	-14.10751100
H	-7.62445100	-8.80578500	-4.27431700	N	-5.38421200	-7.89423300	-13.51720800
H	-7.53822400	-7.03846300	-4.35995700	C	-5.42495600	-7.22802700	-14.80412100
H	-16.43393300	-5.35302200	-7.77399000	C	-4.79437500	-5.83317400	-14.67331700
H	-15.88127200	-6.06442300	-9.29388800	O	-5.28973100	-4.98477800	-13.90562100
C	-12.65108600	-2.36154800	-18.57849800	C	-6.87736300	-7.07702400	-15.31730400
C	-13.08961400	-2.64247100	-17.13168000	O	-7.44160500	-8.34209300	-15.56804600
C	-11.94035000	-3.07153900	-16.24608000	N	-3.71680700	-5.52149500	-15.42872900
C	-11.24940900	-2.15250200	-15.44972200	C	-2.94115000	-6.41469000	-16.32973400
C	-11.50158300	-4.40461200	-16.22911000	C	-2.06136900	-7.39288100	-15.54607600
C	-10.15512100	-2.53562000	-14.67155900	C	-2.14021400	-5.39539600	-17.16371700
C	-10.41756600	-4.80936600	-15.45772100	C	-1.84245400	-4.26250800	-16.16869400
C	-9.73040100	-3.87121500	-14.67328200	C	-3.12713600	-4.17650100	-15.33119700
O	-8.66495200	-4.31391600	-13.95488000	H	-2.95550200	-3.91440700	-14.28342500
H	-13.86259800	-3.42087300	-17.13663300	H	-3.83161700	-3.43783100	-15.73580100
H	-13.56015000	-1.74370700	-16.71531100	H	-0.99128600	-4.53045400	-15.53433100
H	-11.57215100	-1.11354700	-15.43228500	H	-1.60269500	-3.31525800	-16.66014800
H	-12.02775800	-5.14453900	-16.82845500	H	-1.24030200	-5.83832400	-17.59724600
H	-9.63837000	-1.80836900	-14.05154900	H	-2.75890100	-5.01822100	-17.98613200
H	-10.10328200	-5.84831900	-15.42779300	H	-3.62933800	-6.97215300	-16.97104700
H	-8.33915400	-3.65908200	-13.28545800	H	-1.38594200	-6.85621700	-14.87051400
H	-11.90455800	-1.56080200	-18.61178500	H	-2.65374700	-8.10415400	-14.96755000
H	-12.20185000	-3.25134100	-19.03156800	H	-1.44685900	-7.97132400	-16.24526400
H	-13.50059900	-2.05847300	-19.19984500	H	-4.87860000	-7.86055800	-15.50276100
N	-7.03847500	-5.02360000	-11.38528800	H	-8.20451200	-8.47116900	-14.98274200
C	-7.80706200	-6.15528000	-11.30080100	H	-6.84096000	-6.49638100	-16.25447800
O	-7.49106000	-7.20498400	-11.89168100	H	-7.45461300	-6.49157600	-14.59562600
N	-8.93324200	-6.09873200	-10.53548800	H	-6.06792000	-7.57639100	-12.82322800
C	-9.01854200	-5.08266500	-9.49305900	H	-3.88344500	-9.46898900	-11.34778800
C	-8.76607000	-3.71036100	-10.14980300	H	-5.63084700	-9.12142500	-11.31874800
C	-7.41317800	-3.68085800	-10.93982600	H	-5.00495800	-10.67392400	-11.97059500
O	-7.45967600	-2.84223000	-12.03005000	C	-8.10414700	-5.45752700	-8.32211700
H	-10.05475800	-5.08728400	-9.13364000	H	-7.04935500	-5.38101400	-8.59207200
H	-8.66446200	-2.96391200	-9.36177500	H	-8.28286900	-4.82815800	-7.45014900
H	-6.38192600	-5.04152900	-12.16895100	H	-8.30857300	-6.49215100	-8.04305200
H	-9.29301200	-7.02225800	-10.29917500				

(5S,6S)-Me₂DHU-INT2-II (SkDHPase)

C	-2.73099300	-0.10103300	-4.80017700	C	-4.19621100	0.03046800	-8.16487900
C	-3.53345600	-0.25238400	-6.05156100	N	-4.97479900	-0.91267500	-7.66080200
N	-3.31026700	0.45404600	-7.22789000	C	-9.56333000	-3.95540900	-4.12770000
C	-4.57615000	-1.08503400	-6.34645300	C	-9.03843700	-3.10475700	-5.22327000

N	-9.81171000	-2.20117700	-5.93515100	H	-6.04312500	2.14652200	-15.34534900
C	-7.81316400	-3.07176800	-5.82832900	H	-7.01256900	3.56302300	-10.16152500
C	-9.05882000	-1.67673500	-6.92826700	H	-7.52449200	2.71023300	-11.62907900
N	-7.84082800	-2.19554500	-6.89518300	H	-3.12040800	-0.77654500	-4.03637400
C	-6.95819100	2.60919700	-10.69330100	H	-3.04074300	-4.56029200	-6.18470400
N	-7.46155700	1.55701800	-9.84824500	H	-0.10640700	-1.36576300	-10.42515100
C	-7.10122300	0.25748800	-9.99880100	H	-8.22476300	1.73697200	-9.21509800
O	-6.16979600	0.00238200	-10.84560800	C	-15.72461100	-5.23247900	-8.59995800
O	-7.67624000	-0.59279200	-9.24981500	C	-14.28162700	-5.20646900	-8.07989400
C	-5.99742500	1.45357800	-14.50229300	C	-14.09119700	-4.38074100	-6.79229900
C	-6.30767400	0.06104400	-14.95810700	C	-12.69331100	-4.60727800	-6.20165000
N	-6.30920000	-1.05240000	-14.11760400	C	-14.34475100	-2.88200600	-7.01189600
C	-6.62400600	-0.35265000	-16.22531000	C	-8.21561800	-7.89747700	-4.42193300
C	-6.60992700	-2.10402000	-14.87538500	C	-8.96802500	-7.95755400	-5.74575700
N	-6.80528800	-1.71917400	-16.15132500	S	-10.07878200	-9.43081900	-5.83037100
C	-0.67058800	-2.26303000	-10.70606800	C	-9.18656000	-9.89082100	-11.71497000
C	-1.91423300	-1.93386100	-11.45152700	C	-8.85534900	-9.63892600	-10.25173900
N	-1.94350500	-1.28721900	-12.67788400	O	-9.51531000	-8.87195800	-9.53317600
C	-3.22694500	-2.16128500	-11.14443200	C	-10.65004400	-9.62250600	-12.05442500
C	-3.23671800	-1.15108100	-13.06009000	C	-10.84831400	-9.27247300	-13.52704800
N	-4.03748900	-1.66948500	-12.14486000	O	-9.98378300	-8.73794900	-14.21673500
C	-2.92951900	-4.25382000	-7.22607700	N	-12.07966100	-9.55506100	-14.02829800
C	-4.28691400	-4.12694900	-7.88049100	N	-7.74662800	-10.26152700	-9.78870300
O	-5.26256900	-3.69116200	-7.25238800	C	-7.14862100	-9.92147200	-8.50393100
O	-4.32707800	-4.42341800	-9.15244100	H	-13.95624700	-6.23655700	-7.88540200
Zn	-6.52317800	-2.06138000	-8.44436200	H	-13.61145100	-4.81713700	-8.85996500
Zn	-6.06266400	-1.54492200	-12.08705100	H	-14.82416600	-4.74252200	-6.05612600
H	-1.67520400	-0.34781500	-4.95951200	H	-12.51009900	-5.66775300	-5.99775700
H	-2.77828700	0.91796600	-4.39998200	H	-12.57519500	-4.06169800	-5.25706900
H	-5.04390500	-1.81721900	-5.71182600	H	-11.91549800	-4.26409000	-6.89684900
H	-2.61559500	1.17372400	-7.36460600	H	-14.21718000	-2.31895000	-6.07964400
H	-4.25518200	0.41140900	-9.17379500	H	-13.64514300	-2.47332500	-7.75306700
H	-8.74711300	-4.52764200	-3.68211400	H	-15.35767000	-2.68343500	-7.37234500
H	-10.30993200	-4.66825600	-4.49283800	H	-16.07628900	-4.23766700	-8.89040900
H	-6.93227600	-3.65242200	-5.60880700	H	-9.56820100	-7.05506600	-5.88968300
H	-10.78792400	-2.00162600	-5.77011700	H	-8.26120000	-8.02709100	-6.57242700
H	-9.40321400	-0.96014500	-7.65637000	H	-10.28101500	-9.36304800	-7.16440700
H	-6.70969300	1.79236000	-13.74350200	H	-8.90018400	-7.83674800	-3.56955600
H	-6.73659300	0.19691700	-17.14616600	H	-10.98851100	-8.76084200	-11.46623600
H	-7.11242300	-2.32810500	-16.89576800	H	-11.29253200	-10.46341000	-11.7700130
H	-6.68366500	-3.12958900	-14.54008200	H	-12.80505400	-9.97988200	-13.47439200
H	-0.92744900	-2.80013900	-9.79112600	H	-12.28042700	-9.29101600	-14.98105000
H	0.00008000	-2.90598300	-11.28727000	H	-8.57073200	-9.18261100	-12.28113300
H	-3.62896100	-2.68812100	-10.29669400	H	-7.85607900	-10.10611900	-7.69253400
H	-1.14060000	-0.98756200	-13.21168100	H	-6.84035100	-8.87075400	-8.47755600
H	-3.55030000	-0.69483100	-13.98567900	H	-7.19747200	-10.79813700	-10.44324500
H	-5.91775100	2.40570500	-10.94567400	H	-8.88713700	-10.90255500	-12.01028600
H	-2.28855200	-4.95393800	-7.76353300	H	-6.27083700	-10.55161600	-8.35171200
H	-2.46071100	-3.26336600	-7.23311800	H	-7.58597000	-8.78090000	-4.28213700
H	-10.02933000	-3.36633700	-3.32942300	H	-7.56861300	-7.01341000	-4.39999400
H	-4.99736500	1.52449700	-14.05954900	H	-16.41038800	-5.61903800	-7.83775400

H	-15.81158200	-5.87734300	-9.48001200	C	-4.67745900	-9.01612700	-13.28497100
C	-12.65108500	-2.36154800	-18.57849700	O	-3.93351600	-9.54715500	-14.11125000
C	-13.05695800	-2.54851300	-17.10657300	N	-5.38155800	-7.87788900	-13.50131000
C	-11.90843000	-2.98395200	-16.22123200	C	-5.42945300	-7.20853400	-14.78669100
C	-11.21978400	-2.07412300	-15.41254700	C	-4.78754200	-5.81861500	-14.66003400
C	-11.47914100	-4.32066500	-16.20304000	O	-5.27280000	-4.96562200	-13.89161800
C	-10.13958300	-2.46895400	-14.61933100	C	-6.88606300	-7.04729700	-15.28421000
C	-10.40907000	-4.73650000	-15.41841800	O	-7.45803800	-8.30925300	-15.53227800
C	-9.72539800	-3.80772400	-14.61885600	N	-3.71008400	-5.51605500	-15.42055300
O	-8.67491000	-4.26519800	-13.88771400	C	-2.94440500	-6.41395600	-16.32525400
H	-13.86413800	-3.28987700	-17.05194100	C	-2.06137000	-7.39288100	-15.54607600
H	-13.47695200	-1.60999100	-16.72562800	C	-2.14714500	-5.39928500	-17.16817200
H	-11.53452700	-1.03275900	-15.39447000	C	-1.83584000	-4.26626800	-16.17750000
H	-12.00336300	-5.05534200	-16.81053700	C	-3.11226300	-4.17463600	-15.32771800
H	-9.62666200	-1.74750400	-13.98938400	H	-2.92907600	-3.91416500	-14.28140900
H	-10.10356600	-5.77809800	-15.38847800	H	-3.81687200	-3.43178700	-15.72457000
H	-8.34451500	-3.62030200	-13.21001700	H	-0.97945100	-4.53661200	-15.55118500
H	-11.87421400	-1.59567100	-18.67603800	H	-1.59734300	-3.32057100	-16.67263100
H	-12.25305100	-3.29143500	-18.99767800	H	-1.25295000	-5.84614300	-17.60944500
H	-13.50701000	-2.05557600	-19.18934600	H	-2.77200400	-5.02078900	-17.98528700
N	-7.02908700	-5.02366500	-11.33722700	H	-3.63911000	-6.97115300	-16.95963300
C	-7.79712600	-6.15262000	-11.26516100	H	-1.37992200	-6.85689200	-14.87602900
O	-7.48621400	-7.19831200	-11.86974700	H	-2.65282300	-8.10107800	-14.96274400
N	-8.92171700	-6.10474200	-10.49534300	H	-1.45338400	-7.97452600	-16.24831300
C	-9.00782500	-5.09940500	-9.44281600	H	-4.89454600	-7.84367000	-15.49196500
C	-8.74940700	-3.72049100	-10.08257000	H	-8.22224200	-8.43384300	-14.94757600
C	-7.38242600	-3.67915700	-10.85298900	H	-6.85635000	-6.46357100	-16.21989200
O	-7.43514900	-2.82956100	-11.94428900	H	-7.45254200	-6.46158700	-14.55415700
H	-8.66152700	-2.98482400	-9.28287800	H	-6.06424100	-7.56257100	-12.80398200
H	-6.37067600	-5.03172400	-12.11800900	H	-3.87661700	-9.48994200	-11.35530600
H	-9.28336200	-7.02876700	-10.26594400	H	-5.61842100	-9.11374300	-11.30779000
O	-6.32104500	-3.25111100	-9.97979100	H	-5.02329400	-10.67012100	-11.97886100
H	-5.24923500	-4.08384800	-9.57682100	C	-8.09925000	-5.48984900	-8.27256500
C	-9.95357800	-3.31130800	-10.94047100	H	-7.04450600	-5.41819200	-8.54245600
H	-10.85059200	-3.25916700	-10.31207500	H	-8.27267400	-4.86388200	-7.39693100
H	-9.79447200	-2.33237800	-11.39241100	H	-8.31486800	-6.52433900	-8.00155100
H	-10.14478400	-4.03671900	-11.73297000	H	-10.04526200	-5.10562300	-9.08653800
C	-4.82810800	-9.59760800	-11.88554600				

(5S,6S)-Me₂DHU-TS3-II (SkDHPase)

C	-2.73099300	-0.10103300	-4.80017700	C	-9.05321700	-1.53579000	-6.79723500
C	-3.54579400	-0.22846000	-6.03992100	N	-7.84888000	-2.09049600	-6.82001800
N	-3.37773500	0.54459100	-7.18166100	C	-6.95819100	2.60919700	-10.69330100
C	-4.56946800	-1.07945700	-6.34596700	N	-7.73140400	1.63493600	-9.97160100
C	-4.27902900	0.14459800	-8.11315000	C	-7.32697800	0.33874600	-9.97452900
N	-5.01350000	-0.84379000	-7.63220300	O	-6.40898300	0.03604900	-10.81286400
C	-9.56332300	-3.95541300	-4.12769900	O	-7.86865600	-0.44534600	-9.13088600
C	-9.02986500	-3.04699900	-5.16783800	C	-5.99742500	1.45357700	-14.50229300
N	-9.79453400	-2.08864500	-5.81273500	C	-6.27940300	0.02439300	-14.87453400
C	-7.81894300	-3.01826200	-5.79944300	N	-6.35171800	-1.04329400	-13.97461800

C	-6.51990200	-0.45502500	-16.13660300	C	-10.54105100	-9.24035800	-13.72231500
C	-6.62011200	-2.12628400	-14.69698400	O	-9.68084500	-8.59344100	-14.31546100
N	-6.72905500	-1.81179300	-16.00341000	N	-11.70162100	-9.60367900	-14.32565800
C	-0.67058800	-2.26303000	-10.70606800	N	-7.66906800	-10.26725200	-9.81937100
C	-1.95100300	-1.92317600	-11.38058100	C	-7.14861700	-9.92147600	-8.50393200
N	-2.02147200	-1.16575700	-12.53994500	H	-13.96886800	-6.23267800	-7.84710600
C	-3.25304400	-2.21521200	-11.07239000	H	-13.60619400	-4.85359600	-8.87253600
C	-3.32484200	-1.02827800	-12.88426200	H	-14.81694900	-4.66967400	-6.07281100
N	-4.09282000	-1.64891100	-12.00816400	H	-12.50083400	-5.59712600	-5.99442300
Zn	-6.59981500	-1.85515700	-8.39638300	H	-12.56821700	-3.97094700	-5.29888100
Zn	-6.13241500	-1.62898300	-11.88274700	H	-11.90868900	-4.21762200	-6.93132400
H	-1.66658600	-0.28454500	-4.98609100	H	-14.19979600	-2.25001900	-6.18327600
H	-2.82227100	0.89286800	-4.34759300	H	-13.63893700	-2.46461600	-7.85296300
H	-4.99671300	-1.86177600	-5.74232200	H	-15.35015100	-2.65643100	-7.45467500
H	-2.70581300	1.28891800	-7.29957400	H	-16.06009500	-4.24568800	-8.93319700
H	-4.37957400	0.57117700	-9.10034200	H	-10.30183900	-8.38859600	-4.74918300
H	-8.74895900	-4.53737000	-3.69125500	H	-9.28877000	-8.53998200	-6.19846300
H	-10.29230000	-4.65930000	-4.54322600	H	-10.16065400	-10.93706600	-5.44281300
H	-6.95474900	-3.64085800	-5.63808700	H	-8.25689100	-8.02467500	-3.33604200
H	-10.75838800	-1.86651000	-5.60935700	H	-10.83151600	-8.83632700	-11.65293600
H	-9.39396800	-0.77750400	-7.48322600	H	-10.99723600	-10.54147800	-12.0473520
H	-6.83958900	1.89698500	-13.96028600	H	-12.42188000	-10.11915900	-13.8469830
H	-6.56493700	0.04592000	-17.09060600	H	-11.85970700	-9.30884200	-15.27762000
H	-6.99431800	-2.45730300	-16.73284400	H	-8.34231100	-9.06621600	-12.35783000
H	-6.72336600	-3.13047300	-14.31069600	H	-7.88935300	-10.12630000	-7.72715100
H	-0.86927800	-2.88497000	-9.83096500	H	-6.87185700	-8.86310400	-8.46047600
H	0.00355700	-2.82586100	-11.36172600	H	-7.07381800	-10.79416200	-10.44047900
H	-3.64724300	-2.82205000	-10.27282700	H	-8.56172700	-10.80456000	-12.16181100
H	-1.23571800	-0.79867000	-13.05675800	H	-6.26572700	-10.53131200	-8.30657600
H	-3.66776300	-0.49981900	-13.75939900	H	-7.22426400	-8.21069100	-4.76348600
H	-5.95498100	2.75782200	-10.26937600	H	-8.32702600	-6.83231300	-4.64865600
H	-10.05428600	-3.41379800	-3.31094200	H	-16.41686700	-5.57507200	-7.82266800
H	-5.11521200	1.54335700	-13.85966300	H	-15.82151800	-5.91286000	-9.45176000
H	-5.82755400	2.04921300	-15.40210000	C	-12.65108500	-2.36154800	-18.57849700
H	-7.48045600	3.56933200	-10.67577300	C	-12.97806300	-2.52953800	-17.08256900
H	-6.83899500	2.29975400	-11.73074600	C	-11.82682600	-3.02759700	-16.22772800
H	-3.07159500	-0.83232600	-4.06490400	C	-11.15432100	-2.18291400	-15.33793600
H	-0.13274400	-1.36903900	-10.36861400	C	-11.40935400	-4.36847100	-16.27758100
H	-8.30955500	1.92326700	-9.19759100	C	-10.11497600	-2.64297800	-14.52325500
C	-15.72461500	-5.23248200	-8.59995800	C	-10.37888400	-4.84891600	-15.47561200
C	-14.28162600	-5.20646600	-8.07989600	C	-9.72219500	-3.98757600	-14.58072000
C	-14.08474800	-4.33573700	-6.82297500	O	-8.72911700	-4.51752200	-13.81965500
C	-12.68598500	-4.54294900	-6.22761300	H	-13.82378600	-3.22306200	-16.98623000
C	-14.33537000	-2.84495700	-7.09430400	H	-13.32868300	-1.56982300	-16.68452400
C	-8.21562100	-7.89747300	-4.42192900	H	-11.45462800	-1.13959000	-15.26529900
C	-9.31858700	-8.69439200	-5.11653200	H	-11.91463100	-5.05772500	-16.95106600
S	-9.08324300	-10.49372700	-4.76392200	H	-9.62088600	-1.96784500	-13.83069000
C	-8.94452300	-9.82759800	-11.84723600	H	-10.08170800	-5.89320200	-15.50452400
C	-8.71763800	-9.60680300	-10.35974000	H	-8.35392200	-3.90373700	-13.13353600
O	-9.41370200	-8.83180500	-9.68781300	H	-11.84559900	-1.63426800	-18.72588300
C	-10.40379800	-9.64489400	-12.25857700	H	-12.32636600	-3.30864600	-19.02183900

H -13.52856800 -2.01369100 -19.13326400
C -4.81204300 -9.59659900 -11.88594600
C -4.70410100 -9.03825600 -13.29970900
O -3.99351500 -9.58321300 -14.14534200
N -5.42735400 -7.90953200 -13.51824800
C -5.35625300 -7.14684300 -14.74803800
C -4.65944200 -5.80712200 -14.46803900
O -5.10053900 -5.03899400 -13.59503400
C -6.75339300 -6.85723100 -15.34665400
O -7.35417800 -8.02770500 -15.84564900
N -3.59494700 -5.45620500 -15.22842200
C -2.87766000 -6.29761900 -16.22100100
C -2.04530500 -7.39187100 -15.54647600
C -2.03098500 -5.24790300 -16.96773700
C -1.67710700 -4.21925900 -15.88118200
C -2.95070800 -4.14992400 -15.02507800
H -2.76095400 -3.98262200 -13.96104300
H -3.62651000 -3.35163400 -15.36008900
H -0.83369600 -4.57671800 -15.28121400
H -1.39873100 -3.24475000 -16.29273600
H -1.15381200 -5.69241800 -17.44430900
H -2.63309300 -4.77289000 -17.75085300
H -3.60031800 -6.75483900 -16.90305900
H -1.32670500 -6.95604000 -14.84342300
H -2.66496800 -8.11611900 -15.01409400
H -1.47881600 -7.94196300 -16.30655400
H -4.80912200 -7.75983100 -15.46176800
H -8.04711000 -8.30737200 -15.22742000
H -6.61259300 -6.15570100 -16.18482900
H -7.37233500 -6.34612500 -14.60186600
H -5.92549900 -7.49217200 -12.73050600
H -3.81791300 -9.56179200 -11.42902300

H -5.51807700 -9.05224300 -11.26036100
H -5.08615800 -10.65454300 -11.95647600
C -2.97579700 -4.24489600 -7.22764800
C -4.37389300 -4.30714000 -7.83855600
O -5.34489300 -3.81414200 -7.26318800
O -4.43427200 -4.88048300 -9.02550300
N -6.59043400 -4.98154000 -10.69980200
C -7.35567900 -6.15533100 -10.80749200
O -6.87020200 -7.19661000 -11.27239900
N -8.62537700 -6.11029900 -10.35577000
C -9.07024000 -5.08945100 -9.42162600
C -8.65954700 -3.68615100 -9.93075000
C -7.25926400 -3.61907800 -10.67248600
O -7.37710100 -3.12408500 -11.95407400
H -2.30539400 -4.97576300 -7.68141600
H -2.57675100 -3.23825500 -7.39032100
H -10.16527000 -5.13126400 -9.43107100
H -8.56325200 -3.05515200 -9.04824300
H -3.04580000 -4.40769300 -6.15114800
H -5.92709300 -4.98481200 -11.48327200
H -9.05240700 -7.03270600 -10.26042800
O -6.32037700 -2.80669900 -10.00927500
H -5.34890300 -4.84431500 -9.45809000
C -9.79480900 -3.08642500 -10.76996100
H -10.69633800 -2.99563000 -10.15217700
H -9.53495800 -2.09507000 -11.14133200
H -10.03637400 -3.72296300 -11.62387100
C -8.61352100 -5.43212600 -7.99648600
H -7.53574300 -5.29487300 -7.86996400
H -9.12189700 -4.79896100 -7.26560000
H -8.86029000 -6.47567600 -7.77757200

(5S,6S)-Me₂DHU-EP-II (SkDHPase)

C -2.73099400 -0.10103300 -4.80017800
C -3.54275400 -0.17826300 -6.04328300
N -3.51174600 0.73864400 -7.08535100
C -4.43169300 -1.13043500 -6.44609400
C -4.36146700 0.31412400 -8.05634000
N -4.93009200 -0.82359800 -7.69842200
C -9.56332600 -3.95541700 -4.12769600
C -9.03977400 -3.18971400 -5.28911500
N -9.78029200 -2.23610500 -5.97141100
C -7.84048600 -3.23730700 -5.94705700
C -9.03297200 -1.75444400 -6.99218100
N -7.85164400 -2.34936100 -7.00539200
C -6.95819100 2.60919600 -10.69330100
N -7.29924200 1.55231500 -9.77053900
C -7.04983600 0.24086300 -10.04926200
O -6.29354600 0.02844200 -11.06868800

O -7.53180200 -0.62944400 -9.26775200
C -5.99742500 1.45357600 -14.50229300
C -6.30071200 0.07113400 -15.00435800
N -6.27612200 -1.07896600 -14.21144000
C -6.62889500 -0.29810100 -16.28233200
C -6.57243000 -2.10446500 -15.00700200
N -6.79174500 -1.66876400 -16.26223900
C -0.67058800 -2.26303000 -10.70606800
C -1.93064200 -2.00716500 -11.46699500
N -1.97070700 -1.24672500 -12.62796500
C -3.23257300 -2.37439600 -11.24046800
C -3.25137700 -1.17102400 -13.05318500
N -4.04477800 -1.83922100 -12.22739600
Zn -6.35785700 -2.17669200 -8.39398700
Zn -6.05128800 -1.54422900 -12.19030600
H -1.65482200 -0.11085300 -5.00870400

H	-2.94620400	0.80191300	-4.21697300	H	-13.94139100	-2.51831700	-7.30023300
H	-4.71658400	-2.04178000	-5.94989000	H	-15.59651900	-2.98200800	-6.88968000
H	-2.95349800	1.57890400	-7.12187800	H	-16.13156000	-4.22577300	-8.73507500
H	-4.53153200	0.84076500	-8.98235700	H	-8.85878700	-6.51322700	-5.96227600
H	-8.76408000	-4.56097700	-3.69555100	H	-7.89424600	-7.86456500	-6.55485400
H	-10.37475200	-4.63039200	-4.41772500	H	-10.03597400	-8.52898100	-7.60362000
H	-6.97484200	-3.85221900	-5.75743200	H	-8.98823000	-7.64917200	-3.68658600
H	-10.73226100	-1.97121700	-5.76272700	H	-10.50899400	-9.01639400	-12.00302300
H	-9.35260000	-1.00211200	-7.69529300	H	-11.22804500	-10.47028600	-12.6845400
H	-6.66791800	1.73430200	-13.68506600	H	-10.76036200	-8.96290100	-14.63866400
H	-6.76014100	0.28593400	-17.17915700	H	-9.23138700	-9.25521500	-15.43510600
H	-7.08762200	-2.25307400	-17.03065200	H	-9.05963000	-11.63140300	-11.55809400
H	-6.62734200	-3.14952600	-14.72631600	H	-7.75066400	-9.91017100	-7.59088800
H	-0.88652200	-2.91733800	-9.85946900	H	-6.87041800	-8.89642100	-8.76199200
H	0.08841000	-2.75646800	-11.32332200	H	-7.52682800	-11.39792800	-9.99885800
H	-3.62721000	-3.03026600	-10.47366500	H	-10.54433300	-11.33867300	-10.6417760
H	-1.17509300	-0.83460800	-13.09339500	H	-6.23998500	-10.49709100	-8.32188900
H	-3.56478000	-0.64379400	-13.94045600	H	-7.97872200	-8.95879500	-4.30785100
H	-5.93184300	2.48432300	-11.04102700	H	-7.31833300	-7.31876600	-4.17525500
H	-9.94221900	-3.29508800	-3.33937400	H	-16.38332700	-5.76786700	-7.90692300
H	-4.97300200	1.53204600	-14.12078600	H	-15.78259600	-5.73983300	-9.56809500
H	-6.11296700	2.17950700	-15.30984900	C	-12.65108500	-2.36154800	-18.57849700
H	-7.03997400	3.57173600	-10.18207800	C	-13.13566200	-2.90478600	-17.22587900
H	-7.61483100	2.63370100	-11.57326900	C	-11.97874900	-3.31271400	-16.34406800
H	-2.95457400	-0.96400100	-4.17042300	C	-11.43274300	-2.43135600	-15.40560300
H	-0.23555900	-1.33501100	-10.31751500	C	-11.36573900	-4.56475700	-16.49966200
H	-7.97047300	1.72489700	-9.03849900	C	-10.31146200	-2.77336700	-14.64873400
C	-15.72463100	-5.23250100	-8.59995100	C	-10.25021200	-4.92604700	-15.75285400
C	-14.28160600	-5.20644000	-8.07990400	C	-9.71468800	-4.02828100	-14.82084000
C	-14.12623200	-4.60035900	-6.67182200	O	-8.61526300	-4.43033100	-14.12580800
C	-12.68824500	-4.76760300	-6.16399700	H	-13.79719400	-3.76281600	-17.39596100
C	-14.54815800	-3.12431700	-6.61388500	H	-13.73958100	-2.14204600	-16.72048500
C	-8.21562100	-7.89747300	-4.42192900	H	-11.89041400	-1.45506600	-15.26194500
C	-8.67099600	-7.58356300	-5.84228400	H	-11.77408200	-5.27096900	-17.21925000
S	-10.21028000	-8.51961100	-6.26198200	H	-9.90226900	-2.07937900	-13.92009000
C	-9.71909500	-10.84951600	-11.17312500	H	-9.78455200	-5.90016900	-15.86320400
C	-9.00767000	-10.00810000	-10.12026300	H	-8.40680200	-3.81027300	-13.39950100
O	-9.47277300	-8.93375100	-9.71050000	H	-12.01275600	-1.48251900	-18.43944700
C	-10.28414300	-10.03435800	-12.3393420	H	-12.06504800	-3.11495100	-19.11492400
C	-9.33167600	-9.94981900	-13.52966700	H	-13.49202100	-2.07106300	-19.21733900
O	-8.17104100	-10.36917200	-13.48056900	C	-4.81204300	-9.59659900	-11.88594600
N	-9.86765500	-9.42932500	-14.65996800	C	-4.58143100	-9.17443800	-13.32620600
N	-7.88255700	-10.54384600	-9.59783200	O	-3.64725700	-9.62395200	-13.98969400
C	-7.14861700	-9.92147600	-8.50393200	N	-5.45588900	-8.23591300	-13.79116000
H	-13.88850100	-6.23069100	-8.06266200	C	-5.41565300	-7.74147900	-15.15534900
H	-13.64614300	-4.64735000	-8.78296700	C	-4.97433600	-6.26625400	-15.21556400
H	-14.78515000	-5.16487000	-5.99561000	O	-5.58967000	-5.39640900	-14.57289500
H	-12.37430800	-5.81688300	-6.16176600	C	-6.82445000	-7.83921500	-15.78317900
H	-12.59143300	-4.38553900	-5.14047200	O	-7.25806300	-9.18094200	-15.90962100
H	-11.98505000	-4.21437900	-6.80178000	N	-3.97206600	-5.91682300	-16.05377300
H	-14.42061200	-2.71768500	-5.60404300	C	-2.94719700	-6.81798300	-16.64117500

C	-2.04530500	-7.39187100	-15.54647600	N	-6.67806400	-5.64547300	-11.89169200
C	-2.22550700	-5.87487600	-17.62102900	C	-7.72401400	-6.52405000	-11.79502800
C	-2.24241500	-4.51553200	-16.90269100	O	-7.88715500	-7.45753500	-12.60127100
C	-3.60359100	-4.49667800	-16.18905900	N	-8.65257000	-6.31821000	-10.81285700
H	-3.57755500	-4.01740500	-15.20614700	C	-8.62201100	-5.33248200	-9.73933300
H	-4.36901400	-3.97745200	-16.78058200	C	-8.81212600	-3.85332000	-10.23050000
H	-1.42984600	-4.46414500	-16.17114900	C	-7.61906600	-3.17854200	-10.89946400
H	-2.12235200	-3.67110200	-17.58671400	O	-7.70299000	-2.71289800	-12.08850200
H	-1.21802200	-6.22506400	-17.85825300	H	-2.24201800	-4.91797300	-7.67395000
H	-2.78885000	-5.81257700	-18.55893700	H	-2.53696300	-3.24458600	-7.13595100
H	-3.43484700	-7.63074000	-17.18650000	H	-9.55372900	-5.52248500	-9.19463700
H	-1.59360600	-6.58901100	-14.95346900	H	-8.91829800	-3.28000500	-9.30111500
H	-2.58763500	-8.06813000	-14.88488000	H	-3.22119100	-4.58140700	-6.21620000
H	-1.23270600	-7.97021400	-16.00131700	H	-6.14635300	-5.70156300	-12.75853200
H	-4.73742400	-8.38945600	-15.70965800	H	-9.19311300	-7.15632100	-10.61784400
H	-7.26362100	-9.60440500	-15.02385200	O	-6.54222800	-2.98336500	-10.25149400
H	-6.79767000	-7.42130400	-16.79607900	H	-6.20146000	-5.29238400	-11.07379000
H	-7.51130900	-7.23474300	-15.17655900	C	-10.10948600	-3.71007000	-11.03241500
H	-6.29878000	-8.00607400	-13.24915600	H	-10.95646000	-4.04885700	-10.42710500
H	-4.45984000	-8.80939600	-11.21007200	H	-10.28859300	-2.67067300	-11.31637400
H	-5.87530500	-9.76546600	-11.69109000	H	-10.08609000	-4.31937700	-11.93622400
H	-4.24308300	-10.50697000	-11.69603200	C	-7.48525100	-5.58103300	-8.74214400
C	-2.97579700	-4.24489600	-7.22764900	H	-6.49086700	-5.34077100	-9.11715900
C	-4.22726000	-4.15682900	-8.09581500	H	-7.63081600	-4.99564000	-7.83394300
O	-5.25272200	-3.60839500	-7.52110400	H	-7.50997800	-6.63865900	-8.46914300
O	-4.18575900	-4.55625600	-9.26864100				

(5S,6R)-Me₂DHU-ES-II (SkDHPase)

C	5.63384000	-2.00726400	6.51293800	N	2.67292800	2.82150600	-4.28026900
C	4.95552000	-1.07200000	5.57905900	C	6.25237700	-2.97655300	-0.00449600
N	5.48869300	0.12819700	5.13226700	C	5.61323500	-1.70827400	-0.43894300
C	3.74701100	-1.17108000	4.95324300	N	6.19487400	-0.74815500	-1.25459900
C	4.60694300	0.69667700	4.27107600	C	4.37931900	-1.21269400	-0.13423800
N	3.54186000	-0.07576000	4.13582200	C	5.31198300	0.26994900	-1.40995600
C	-2.09696200	-0.62150500	7.06389900	N	4.20051500	0.01592600	-0.73764700
C	-1.19061200	-0.06449400	6.01572900	C	2.98567000	-4.05280500	3.05273500
N	-1.03131500	1.29853200	5.80606100	C	2.16591600	-2.90381500	2.45363500
C	-0.36202300	-0.65423400	5.09516800	O	1.63028000	-2.08160600	3.28522600
C	-0.14061200	1.48497100	4.80193200	O	2.11889400	-2.79658300	1.20898600
N	0.28113900	0.31681200	4.34825300	Zn	1.80506200	0.00699200	2.99346600
C	4.62161700	4.44346200	2.35277000	Zn	2.61839300	1.23538100	-0.23568800
N	3.61137900	3.60709900	2.96684400	N	-0.60012800	-0.47843400	-0.95748700
C	2.81433400	2.77809600	2.20662500	C	-1.75601200	-1.21347600	-0.62877000
O	3.16183000	2.66846200	0.97977600	O	-2.10833600	-2.14703000	-1.35246300
O	1.85973300	2.18729400	2.78991400	N	-2.41866900	-0.80196500	0.46309600
C	4.89511600	4.22007600	-1.72672100	C	-1.81322100	0.09246200	1.45480900
C	3.89217100	3.49993300	-2.57878400	C	-1.09580900	1.24708100	0.72502100
N	3.11188100	2.42221400	-2.15400200	C	-0.26210800	0.71015900	-0.41908800
C	3.61220200	3.75577300	-3.89739200	O	0.63814400	1.39796200	-0.96561800
C	2.40366600	2.04151400	-3.20809800	H	6.58438400	-2.37591000	6.10958200

H	5.84511100	-1.54588200	7.48484000	N	-4.39731800	-4.51424900	-0.38878300
H	3.01039400	-1.95427800	5.00441000	C	-3.78255900	-4.98756800	0.84517500
H	6.37948900	0.51977600	5.40056000	H	-6.44159700	1.80424100	3.13460800
H	4.75442700	1.65521200	3.79536700	H	-5.21782600	3.06064600	3.27832000
H	-2.03728500	-1.71163600	7.06137700	H	-7.05246700	2.15045800	5.54627900
H	-3.14060800	-0.34182300	6.88911700	H	-5.51853900	0.29321100	4.85816300
H	-0.16514300	-1.69910600	4.91303100	H	-5.13097900	0.90832300	6.47069100
H	-1.50939100	2.03070900	6.31085000	H	-4.12870800	1.36705300	5.08144300
H	0.18845700	2.44254500	4.43054200	H	-5.44512200	3.33839400	7.05194700
H	4.44704500	4.53637200	-0.78104600	H	-4.53720900	3.90502300	5.63952900
H	3.99078200	4.50610300	-4.57326400	H	-6.19099600	4.46309000	5.91719800
H	2.21588000	2.76015200	-5.17790400	H	-7.00898800	4.75482500	3.82909400
H	1.73076400	1.19640900	-3.24617800	H	-3.14072200	-2.29432400	4.46051400
H	5.53034400	-3.55408100	0.57566400	H	-3.18801800	-3.68915300	3.37963000
H	6.56918900	-3.59590100	-0.85185900	H	-5.22993600	-2.59828300	2.50813600
H	3.61286700	-1.68943400	0.45567400	H	-4.09810200	-3.73904800	6.32211600
H	7.11405100	-0.79412800	-1.66943000	H	-5.63857700	-0.87998600	-1.26416000
H	5.50186000	1.14790500	-2.00624900	H	-7.04298600	-1.74355600	-1.87133700
H	5.26841500	3.83455900	1.71983700	H	-7.73967400	-0.15906600	-3.39439800
H	3.08982700	-4.86611100	2.33271400	H	-6.74670500	0.36326500	-4.72081100
H	3.98391900	-3.67280500	3.29887400	H	-4.20901800	-2.66691200	-2.49539300
H	-1.04823200	-0.46738800	2.00801300	H	-4.45647000	-4.82025700	1.68759300
H	-0.38052900	1.70625700	1.41381200	H	-2.83295100	-4.47521100	1.03494200
H	-1.81769000	-0.27512700	8.06555500	H	-4.30045700	-5.08507500	-1.21559000
H	5.75066100	3.58080200	-1.47757800	H	-5.66225600	-3.66947300	-2.48392900
H	5.27502100	5.09937200	-2.25169000	H	-3.59456400	-6.05814900	0.75322000
H	5.22867700	4.90369500	3.13706500	H	-4.07614500	-5.12661100	5.22853600
H	4.19697000	5.24320700	1.73192300	H	-2.55311500	-4.36328800	5.72093600
H	4.99165700	-2.87210100	6.68986500	H	-8.23106600	3.47743300	3.79741200
H	2.53510400	-4.42492900	3.97654800	H	-7.39102300	3.94109300	2.31379500
H	7.13393300	-2.80386200	0.62468000	C	-2.31308000	7.01875400	-5.68287000
H	3.20580200	3.89795800	3.84406300	C	-3.14974200	6.58674600	-4.47043600
H	-0.10562900	-0.77143500	-1.81650200	C	-2.69875400	5.22509200	-4.00662300
H	-3.26584600	-1.33273800	0.67014400	C	-1.50428700	5.09334000	-3.29042400
O	1.78111300	-0.05905900	1.05791100	C	-3.36509300	4.05874500	-4.40235600
H	1.77058700	-1.02136200	0.86588100	C	-0.96513900	3.84216800	-3.00865900
C	-7.26178300	3.78527500	3.38989700	C	-2.85047600	2.79596000	-4.12114600
C	-6.18840000	2.72649800	3.67293800	C	-1.63469700	2.69159100	-3.44099100
C	-6.04697600	2.39860100	5.17520500	O	-1.13491400	1.44153900	-3.21845000
C	-5.15863700	1.17005700	5.40614800	H	-4.21216000	6.56702300	-4.73852000
C	-5.53087100	3.59449000	5.99014100	H	-3.04055100	7.32471600	-3.66610400
C	-3.59670900	-4.16903700	5.44878800	H	-0.97479000	5.98602200	-2.96522600
C	-3.66486200	-3.23069300	4.24822100	H	-4.29794500	4.14208700	-4.95497800
S	-5.42700900	-2.86058100	3.82019300	H	-0.03321100	3.75116800	-2.45700100
C	-5.15783400	-2.84000900	-1.97568100	H	-3.36693000	1.88850100	-4.41897200
C	-4.79664300	-3.23502100	-0.55079700	H	-0.33514000	1.50668500	-2.67159800
O	-4.82679800	-2.43056900	0.39511800	H	-1.25038900	7.06800400	-5.42501300
C	-5.98031200	-1.55575700	-2.05737700	H	-2.42147700	6.30258000	-6.50359800
C	-5.77466800	-0.83629400	-3.38711700	H	-2.61598500	8.00501800	-6.05197300
O	-4.69402200	-0.83335600	-3.97623400	C	-2.04006200	2.33696300	0.17447500
N	-6.84724400	-0.15492000	-3.86065200	H	-2.54265800	2.85101400	0.99696000

H	-1.47841300	3.08105200	-0.39166500	H	5.08772800	-1.06262900	-5.87786100
H	-2.80220500	1.91292800	-0.48509600	H	4.00212900	-2.96580700	-7.48474900
C	-1.52387500	-5.19165400	-2.59389500	H	3.28047800	-1.35077700	-7.50742900
C	-1.00771200	-4.50504300	-3.84603100	H	1.35646700	-2.64062500	-6.97729200
O	-0.64325300	-5.15222400	-4.82668000	H	3.08642500	-4.36843300	-5.10832900
N	-0.95467600	-3.14910600	-3.76465100	H	1.34503400	-4.58902200	-5.40451300
C	-0.45304500	-2.31860600	-4.83934800	H	2.50226300	-4.85369900	-6.70842700
C	0.86013700	-1.65898200	-4.39325100	H	-0.30698200	-2.98167400	-5.69088700
O	0.87657400	-0.91611400	-3.38445400	H	-3.37524200	-1.58644700	-5.15299600
C	-1.47102900	-1.22560900	-5.24288500	H	-1.00269400	-0.60002100	-6.01974700
O	-2.64564900	-1.81299600	-5.75043500	H	-1.66558100	-0.57536800	-4.38501200
N	1.98309700	-1.85477600	-5.10935400	H	-1.30551800	-2.69566700	-2.92335800
C	2.18277900	-2.76409800	-6.27230300	H	-0.70452800	-5.77044000	-2.15602800
C	2.28051000	-4.22849700	-5.83644500	H	-1.90744500	-4.49691800	-1.84616300
C	3.49259100	-2.21839300	-6.87211500	H	-2.29670400	-5.90878900	-2.88752000
C	4.30264100	-1.78534000	-5.63996700	C	-2.88494600	0.54397100	2.44050900
C	3.23885200	-1.19363200	-4.70461700	H	-3.28695700	-0.31290800	2.98773400
H	3.43290800	-1.36383300	-3.64229700	H	-2.45929200	1.23822600	3.16889200
H	3.13951800	-0.11151500	-4.84597600	H	-3.71825800	1.03826900	1.93540600
H	4.78274100	-2.65224700	-5.17549900				

(5S,6R)-Me₂DHU-TS1-II (SkDHPase)

C	-2.73099000	-0.10103100	-4.80017200	C	-2.92951700	-4.25382000	-7.22607300
C	-3.57095000	-0.20349100	-6.02494300	C	-4.19850400	-4.14760500	-8.07700600
N	-3.58134800	0.72109500	-7.06065900	O	-5.25059000	-3.68866700	-7.49867300
C	-4.44709000	-1.17391100	-6.41859600	O	-4.13148600	-4.45026000	-9.29018600
C	-4.43951400	0.28554800	-8.01815100	Zn	-6.37202000	-2.19366300	-8.46569300
N	-4.97624800	-0.86740400	-7.65880300	Zn	-6.03675400	-1.64772400	-12.09691600
C	-9.56332400	-3.95540500	-4.12770500	H	-1.66049000	-0.08590500	-5.03552500
C	-9.02941900	-3.22147700	-5.31024300	H	-2.95480100	0.79989900	-4.21723600
N	-9.70566800	-2.17241500	-5.91662200	H	-4.70987800	-2.09311700	-5.92359800
C	-7.88220500	-3.36578500	-6.04578400	H	-3.04448500	1.57504000	-7.10004300
C	-8.97367300	-1.73083500	-6.96719600	H	-4.64213500	0.81889900	-8.93377900
N	-7.86200600	-2.43925500	-7.07259100	H	-8.84416000	-4.71143100	-3.80669000
C	-6.95819100	2.60919300	-10.69329900	H	-10.50452300	-4.46407400	-4.35858000
N	-7.28680000	1.54757900	-9.76720700	H	-7.06862700	-4.06340000	-5.92435800
C	-7.09786800	0.23143100	-10.08652400	H	-10.60380300	-1.80895300	-5.63228800
O	-6.41771600	0.01904800	-11.15134500	H	-9.25378200	-0.92478400	-7.62612300
O	-7.55958500	-0.64160800	-9.29147300	H	-6.65717700	1.69476700	-13.66429200
C	-5.99742500	1.45357300	-14.50229200	H	-6.65296700	0.27194300	-17.19356200
C	-6.25054000	0.06411700	-15.00477900	H	-6.91148800	-2.27420000	-17.05556100
N	-6.21576500	-1.07982100	-14.20671500	H	-6.47601200	-3.14899800	-14.72075200
C	-6.53009200	-0.30979300	-16.29391800	H	-0.92683000	-2.96735400	-9.91252800
C	-6.45659600	-2.10820500	-15.01232900	H	0.09810400	-2.73220300	-11.33105900
N	-6.65170100	-1.68409000	-16.27891200	H	-3.56109300	-2.98910200	-10.50292100
C	-0.67059400	-2.26302900	-10.70607000	H	-1.15287800	-0.66940600	-13.03726400
C	-1.89837000	-1.93287600	-11.47340400	H	-3.55330400	-0.44907100	-13.85795800
N	-1.94280700	-1.11187300	-12.59065200	H	-5.94538200	2.47099100	-11.07450200
C	-3.19332400	-2.30970900	-11.25772700	H	-2.20681400	-4.92339400	-7.69463400
C	-3.23094400	-1.01802200	-13.00057100	H	-2.48684100	-3.25508300	-7.13926000
N	-4.01284700	-1.73190400	-12.20600600	H	-9.74166400	-3.28460200	-3.27941000

H	-4.96821500	1.57763000	-14.14518100	H	-16.31785500	-5.98585400	-8.06976300
H	-6.16508800	2.18050000	-15.30009100	H	-15.75715300	-5.47866900	-9.66645900
H	-7.00883300	3.56746900	-10.17008800	C	-12.65108600	-2.36154800	-18.57849800
H	-7.64071300	2.65050600	-11.55229200	C	-13.17165300	-2.82950800	-17.21179100
H	-2.91806100	-0.96526000	-4.16021100	C	-12.03384200	-3.30150100	-16.33977300
H	-3.16117200	-4.59882000	-6.21513900	C	-11.24987600	-2.38236200	-15.63458300
H	-0.22212800	-1.37647300	-10.24187400	C	-11.66049700	-4.65164200	-16.29829500
H	-7.93206200	1.72736100	-9.01380000	C	-10.11763200	-2.78499500	-14.92973400
C	-15.72463100	-5.23248700	-8.59995900	C	-10.53969600	-5.07806500	-15.59217800
C	-14.28160800	-5.20645900	-8.07989700	C	-9.75591400	-4.13821500	-14.91345900
C	-14.20000900	-4.98042400	-6.55462600	O	-8.65101000	-4.58787700	-14.25732700
C	-12.76996600	-5.16070200	-6.03169700	H	-13.89914900	-3.63737600	-17.35269200
C	-14.75519400	-3.61081000	-6.13345300	H	-13.70835700	-2.00660800	-16.72386400
C	-8.21561700	-7.89747900	-4.42193200	H	-11.52253600	-1.32921100	-15.64446800
C	-8.66146200	-7.58482900	-5.84416800	H	-12.25998900	-5.38409500	-16.83425400
S	-10.17596100	-8.55277500	-6.28569900	H	-9.51575100	-2.05972600	-14.38873600
C	-9.12447900	-9.90592900	-11.75638000	H	-10.26331900	-6.12702700	-15.54337300
C	-8.81192600	-9.62798800	-10.29381900	H	-8.27564400	-3.88621600	-13.68595200
O	-9.48267000	-8.83374100	-9.61400600	H	-11.94305900	-1.53417800	-18.46332900
C	-10.56835100	-9.57696600	-12.12882800	H	-12.12931300	-3.17378300	-19.09481800
C	-10.71750600	-9.24284000	-13.60913100	H	-13.46732400	-2.01911600	-19.22415000
O	-9.82987100	-8.69106600	-14.25873500	N	-7.12043000	-5.05817000	-11.62238200
N	-11.91772300	-9.54900500	-14.16195700	C	-7.59335200	-6.22910200	-11.04063500
N	-7.73523500	-10.27031300	-9.79249400	O	-7.22339400	-7.33208800	-11.46676800
C	-7.14862100	-9.92147200	-8.50393100	N	-8.48371800	-6.09108900	-10.03991400
H	-13.79160200	-6.15835300	-8.32076100	C	-8.77007100	-4.81318100	-9.39095100
H	-13.70974100	-4.42210300	-8.59678300	C	-8.81540200	-3.70025900	-10.45823900
H	-14.82322200	-5.75359200	-6.08110900	C	-7.59101900	-3.78441000	-11.36817100
H	-12.35381700	-6.13754300	-6.29839700	O	-7.49639100	-2.94593800	-12.36058600
H	-12.74402900	-5.07486900	-4.93868400	H	-7.94956600	-4.58207400	-8.70009100
H	-12.10678000	-4.39026600	-6.44595200	H	-8.76285700	-2.73059500	-9.95912600
H	-14.68422500	-3.47584100	-5.04842300	H	-6.50453400	-5.17598200	-12.43797700
H	-14.18942600	-2.79821200	-6.60892900	H	-8.86521100	-6.96564700	-9.68363200
H	-15.80573400	-3.48547500	-6.40919900	O	-6.22967600	-3.01818200	-10.28176900
H	-16.22470300	-4.26739100	-8.47576400	H	-5.55247900	-3.72317500	-10.11245400
H	-8.87146600	-6.51692200	-5.95433300	C	-10.08974700	-3.73375300	-11.32337000
H	-7.87396200	-7.84045500	-6.55605300	H	-10.97187900	-3.55746000	-10.70346200
H	-9.90104400	-8.66321300	-7.60618100	H	-10.05489900	-2.94959100	-12.07966600
H	-9.00561600	-7.67560000	-3.69672500	H	-10.21375600	-4.69317300	-11.83198600
H	-10.87119000	-8.68870000	-11.56115800	C	-4.82811000	-9.59760700	-11.88554700
H	-11.25339100	-10.38114400	-11.8395510	C	-4.69951400	-9.08000000	-13.30937100
H	-12.65484800	-9.99585300	-13.64155700	O	-3.92373300	-9.60251200	-14.10940600
H	-12.07937300	-9.30232300	-15.12698600	N	-5.47735400	-8.00220300	-13.59190800
H	-8.46387800	-9.25207300	-12.33665800	C	-5.47065700	-7.34590400	-14.88377400
H	-7.89748200	-10.00963300	-7.71457200	C	-4.88122300	-5.93657600	-14.73071800
H	-6.75195500	-8.90017000	-8.51470300	O	-5.43113100	-5.10561300	-13.97513400
H	-7.17491000	-10.81273300	-10.43331000	C	-6.89218900	-7.24195300	-15.48371200
H	-8.87042200	-10.94008800	-12.01413900	O	-7.40237500	-8.52378500	-15.76326500
H	-6.33379900	-10.61536000	-8.29251700	N	-3.78991200	-5.58751400	-15.44068400
H	-7.95434400	-8.95347700	-4.31274700	C	-2.96654000	-6.44423200	-16.33670700
H	-7.33687700	-7.29860200	-4.15553600	C	-2.06137100	-7.39288000	-15.54607400

C	-2.18896100	-5.38869700	-17.14648100	H	-4.86783500	-7.97168400	-15.54049900
C	-1.94015100	-4.26244600	-16.13045300	H	-8.17593600	-8.67085300	-15.19707200
C	-3.23943200	-4.22542800	-15.31286800	H	-6.82059400	-6.66077000	-16.41776100
H	-3.09373600	-3.97310000	-14.25908200	H	-7.53325300	-6.67313300	-14.80315400
H	-3.95695600	-3.50330400	-15.72112700	H	-6.10600200	-7.64829900	-12.86976300
H	-1.09117400	-4.51327500	-15.48675900	H	-3.85917800	-9.48454900	-11.38957100
H	-1.72249100	-3.30115700	-16.60400300	H	-5.59196500	-9.07809900	-11.30632100
H	-1.27012600	-5.79729400	-17.57382800	H	-5.03710800	-10.67151400	-11.92827900
H	-2.80878000	-5.01982800	-17.97182600	C	-10.05689000	-4.93999900	-8.58091600
H	-3.62411400	-7.02151900	-16.99224900	H	-9.94223900	-5.67692800	-7.78244900
H	-1.41069000	-6.83668400	-14.86254700	H	-10.31170000	-3.98135700	-8.12263000
H	-2.63572000	-8.12379900	-14.97357600	H	-10.89479100	-5.25788800	-9.20561800
H	-1.42191300	-7.94868100	-16.24093600				

(5S,6R)-Me₂DHU-INT1-II (SkDHPase)

C	-2.73099300	-0.10103300	-4.80017700	H	-2.92492700	0.83651200	-4.26639900
C	-3.53559200	-0.21780300	-6.04573600	H	-4.76625400	-2.04062000	-5.88376400
N	-3.46853000	0.65222000	-7.12574800	H	-2.88736500	1.47517200	-7.19027400
C	-4.44723300	-1.16232800	-6.41817900	H	-4.46414000	0.70090400	-9.03855700
C	-4.31908900	0.21168300	-8.08773500	H	-8.83804600	-4.70685000	-3.80978900
N	-4.92342600	-0.89344600	-7.68771000	H	-10.49584600	-4.47272100	-4.37415100
C	-9.56332600	-3.95540800	-4.12769600	H	-7.05167700	-4.02043000	-5.88360500
C	-9.02751700	-3.20138000	-5.29357600	H	-10.61865500	-1.81225500	-5.63452300
N	-9.70896800	-2.15822300	-5.90404600	H	-9.25516900	-0.90330200	-7.60639700
C	-7.86821400	-3.32751500	-6.01091000	H	-6.61004800	1.64405500	-13.61683600
C	-8.96857300	-1.70265700	-6.94194800	H	-6.75644800	0.36931700	-17.23774400
N	-7.84615800	-2.39598400	-7.03181000	H	-7.04721500	-2.17552500	-17.15527200
C	-6.95819100	2.60919600	-10.69330100	H	-6.55385600	-3.12312100	-14.85704300
N	-7.27562500	1.51204600	-9.80597200	H	-0.95158000	-2.93776800	-9.89540200
C	-6.99974400	0.21095000	-10.11362400	H	0.08643100	-2.77189300	-11.31359100
O	-6.25310500	0.02051100	-11.13722300	H	-3.60218700	-2.89116800	-10.52870600
O	-7.45863600	-0.67965800	-9.33234300	H	-1.06530200	-0.73939300	-13.08576600
C	-5.99742500	1.45357800	-14.50229300	H	-3.43863300	-0.46555500	-13.96358200
C	-6.28460300	0.09942700	-15.07018200	H	-5.94312100	2.49317800	-11.07541900
N	-6.23691600	-1.06654200	-14.31122100	H	-2.20318500	-4.90620900	-7.71250500
C	-6.61121000	-0.23620400	-16.35754100	H	-2.49539600	-3.25418400	-7.11214200
C	-6.51897000	-2.07611600	-15.13009500	H	-9.75871800	-3.29862600	-3.27215700
N	-6.74826300	-1.61063800	-16.37369500	H	-4.94936400	1.55320400	-14.19595900
C	-0.67058800	-2.26303000	-10.70606800	H	-6.20360100	2.23037900	-15.24201800
C	-1.88338500	-1.91857100	-11.49413200	H	-7.01965400	3.54848900	-10.13808100
N	-1.87932200	-1.13592800	-12.63914100	H	-7.64071200	2.67332400	-11.55118200
C	-3.19589700	-2.24477800	-11.29235500	H	-2.98359500	-0.92338600	-4.12838600
C	-3.15428800	-1.01452100	-13.07962500	H	-3.15905200	-4.62670600	-6.22479900
N	-3.97608600	-1.67288400	-12.27762200	H	-0.19969400	-1.37670300	-10.26451100
C	-2.92951900	-4.25382000	-7.22607700	H	-7.93987500	1.65321600	-9.06102900
C	-4.19917700	-4.13460600	-8.06680800	C	-15.72461000	-5.23248800	-8.59995500
O	-5.24710800	-3.68013100	-7.48152600	C	-14.28163200	-5.20645900	-8.07990100
O	-4.14204600	-4.42461900	-9.28682200	C	-14.20126000	-4.95693300	-6.55804200
Zn	-6.37415000	-2.18941300	-8.42166800	C	-12.78065200	-5.17010500	-6.02158000
Zn	-5.99534000	-1.54302600	-12.30912500	C	-14.71924700	-3.56468900	-6.16465000
H	-1.65424500	-0.15178700	-4.99913800	C	-8.21561700	-7.89747900	-4.42193200

C	-8.75824200	-7.64241400	-5.82297400	H	-12.11839000	-5.15742700	-16.78773000
S	-10.26601600	-8.66811100	-6.13253500	H	-9.43183500	-1.84683600	-14.26275000
C	-9.25390200	-9.76534600	-11.69087500	H	-10.14175200	-5.90201700	-15.48514800
C	-8.83949300	-9.52159700	-10.24154700	H	-8.19965700	-3.73565400	-13.49594100
O	-9.49966400	-8.79348800	-9.48319400	H	-11.88025800	-1.58511900	-18.62861100
C	-10.38218400	-8.81421300	-12.11051600	H	-12.23711300	-3.26812300	-19.03167400
C	-10.79661100	-9.01560100	-13.55996000	H	-13.49957500	-2.03547300	-19.18972800
O	-10.05047500	-8.77918600	-14.51064100	N	-6.99231200	-5.05319100	-11.51280000
N	-12.05902400	-9.47448800	-13.75919900	C	-7.59611800	-6.20283200	-11.07120500
N	-7.73363900	-10.17114500	-9.81762400	O	-7.34791000	-7.30985000	-11.58977000
C	-7.14862000	-9.92147200	-8.50393100	N	-8.48662900	-6.08526200	-10.05722300
H	-13.79803700	-6.16537400	-8.30523400	C	-8.73303800	-4.84186600	-9.34024300
H	-13.70373400	-4.43479400	-8.60871400	C	-8.69073000	-3.67231600	-10.34406400
H	-14.84940700	-5.70315800	-6.07494400	C	-7.34847700	-3.70796900	-11.12243100
H	-12.39528300	-6.16651100	-6.26103400	O	-7.33027100	-2.89023600	-12.20580800
H	-12.75872100	-5.05916000	-4.93067000	H	-7.93071400	-4.68672600	-8.60424400
H	-12.08999200	-4.43251700	-6.45024600	H	-8.67718100	-2.73638100	-9.78095000
H	-14.65775200	-3.41465500	-5.08098800	H	-6.45554000	-5.13353400	-12.38081800
H	-14.12321300	-2.77746900	-6.64590400	H	-8.88824600	-6.96025300	-9.72832500
H	-15.76194000	-3.41183200	-6.45599500	O	-6.27595800	-3.22962600	-10.18472800
H	-16.22220200	-4.26506200	-8.48345500	H	-5.56366600	-3.92126700	-10.01166600
H	-9.00840900	-6.58513500	-5.95058100	C	-9.90264600	-3.63842700	-11.28188100
H	-8.01203900	-7.89906200	-6.57724900	H	-10.82462700	-3.50679000	-10.70978700
H	-10.12736900	-8.73889100	-7.47593000	H	-9.82190500	-2.79832900	-11.97099500
H	-8.96392800	-7.67147300	-3.65495400	H	-9.99584100	-4.55358600	-11.87094800
H	-10.01849100	-7.78758100	-12.02052000	C	-4.82810800	-9.59760900	-11.88554500
H	-11.23103700	-8.92256400	-11.43012900	C	-4.66453100	-9.03632500	-13.28699600
H	-12.69459700	-9.65740500	-13.00052000	O	-3.92409400	-9.57758600	-14.10802100
H	-12.37173700	-9.61982100	-14.70785400	N	-5.36656400	-7.89765600	-13.51642800
H	-8.39120800	-9.61953500	-12.34720800	C	-5.46086100	-7.29770800	-14.83257900
H	-7.91227100	-10.03168200	-7.73223000	C	-4.87865200	-5.87906500	-14.77932500
H	-6.71891800	-8.91493700	-8.44457000	O	-5.41519200	-5.00562800	-14.06710800
H	-7.15803000	-10.62263500	-10.51311300	C	-6.92747000	-7.25666900	-15.30846000
H	-9.57166300	-10.81178900	-11.79022700	O	-7.39277300	-8.57962900	-15.42130700
H	-6.35985500	-10.65439800	-8.32705600	N	-3.78965800	-5.57800200	-15.52004100
H	-7.91982700	-8.94268700	-4.29749900	C	-2.97621800	-6.48485400	-16.37480200
H	-7.33776200	-7.26915100	-4.23152200	C	-2.06137000	-7.39288100	-15.54607600
H	-16.31988900	-5.97992300	-8.06376600	C	-2.20817900	-5.47713300	-17.25220100
H	-15.75789400	-5.48676200	-9.66452500	C	-1.94968800	-4.29369400	-16.30644000
C	-12.65108500	-2.36154800	-18.57849700	C	-3.23920200	-4.21224900	-15.47625400
C	-13.07419200	-2.61924800	-17.12387100	H	-3.08016700	-3.90063800	-14.44004700
C	-11.91227300	-3.07547700	-16.27198900	H	-3.96271800	-3.51297200	-15.91450300
C	-11.14026900	-2.16309900	-15.54617500	H	-1.09231200	-4.50613300	-15.65990400
C	-11.52886300	-4.42468300	-16.24115000	H	-1.73942000	-3.36095500	-16.83723300
C	-10.01664400	-2.56977100	-14.82485500	H	-1.29334000	-5.90884400	-17.66525100
C	-10.41712000	-4.85244900	-15.52393300	H	-2.83705200	-5.15674600	-18.09087800
C	-9.64697900	-3.92146300	-14.81309600	H	-3.64085300	-7.09719500	-16.99005500
O	-8.55549400	-4.38559400	-14.14838200	H	-1.41070300	-6.80367700	-14.89050200
H	-13.86825300	-3.37562700	-17.10731800	H	-2.63115700	-8.10199200	-14.94271300
H	-13.50863400	-1.70437900	-16.70334500	H	-1.42246500	-7.97566700	-16.21905200
H	-11.41894100	-1.11136200	-15.54374200	H	-4.89954600	-7.94395200	-15.50697500

H -8.29428100 -8.62598400 -15.05828700
H -6.95933800 -6.73438800 -16.28168300
H -7.51734800 -6.65851300 -14.60554700
H -6.05020500 -7.59809900 -12.81602300
H -3.85054700 -9.60726600 -11.39417400
H -5.53473800 -9.02869700 -11.27924200

H -5.14740700 -10.64188700 -11.97165800
C -10.05121000 -4.95790900 -8.57787700
H -10.00080700 -5.75985600 -7.83673000
H -10.27154400 -4.02491000 -8.05277700
H -10.88327300 -5.18172000 -9.24932500

(5S,6R)-Me₂DHU-TS2-II (SkDHPase)

C -2.73099200 -0.10103300 -4.80017500
C -3.53692200 -0.24260200 -6.04830800
N -3.38485500 0.54428800 -7.18339000
C -4.52130600 -1.13164300 -6.37690100
C -4.25460300 0.11240500 -8.13129400
N -4.95526100 -0.91101300 -7.67244400
C -9.56333400 -3.95541100 -4.12770600
C -9.01978900 -3.16142500 -5.25784100
N -9.70669900 -2.11294100 -5.85064300
C -7.85978300 -3.27082600 -5.97364900
C -8.96979900 -1.63964900 -6.88187900
N -7.84382400 -2.32741700 -6.98236200
C -6.95819100 2.60919600 -10.69330100
N -7.40437600 1.55644600 -9.81737400
C -7.08099100 0.25233000 -10.02000200
O -6.21870600 0.00717400 -10.93666600
O -7.61643100 -0.60043900 -9.24389600
C -5.99742500 1.45357700 -14.50229300
C -6.29045400 0.07590900 -15.00606600
N -6.26961400 -1.05762500 -14.19635000
C -6.60375800 -0.30833000 -16.28312300
C -6.55410800 -2.09523600 -14.97898000
N -6.76001800 -1.67990600 -16.24428900
C -0.67058800 -2.26302900 -10.70606900
C -1.89666000 -1.92494300 -11.47600600
N -1.90298400 -1.32673100 -12.72701000
C -3.21554700 -2.11161600 -11.17162400
C -3.19026400 -1.18039600 -13.12612000
N -4.00892200 -1.64625900 -12.19782300
C -2.92951400 -4.25382000 -7.22607300
C -4.23647400 -4.14164900 -7.98623900
O -5.25607600 -3.69369200 -7.41028700
O -4.19782700 -4.44347200 -9.23949100
Zn -6.47091900 -2.10025000 -8.45843900
Zn -6.03696500 -1.53721800 -12.16488900
H -1.66181600 -0.25717000 -4.98329500
H -2.84921600 0.88748700 -4.34221900
H -4.92350500 -1.93626100 -5.78560900
H -2.74082600 1.31461800 -7.28905400
H -4.34942600 0.54316400 -9.11683600
H -8.84519900 -4.72345400 -3.83454100
H -10.49661700 -4.45710300 -4.40354900
H -7.04717100 -3.96965200 -5.85788900

H -10.61647200 -1.77276700 -5.57432500
H -9.26025800 -0.83513700 -7.53777000
H -6.69961600 1.74664100 -13.71582800
H -6.72922500 0.26290200 -17.18897700
H -7.05760000 -2.27408600 -17.00433000
H -6.59827800 -3.13120300 -14.67018000
H -0.95358900 -2.77476800 -9.78440600
H -0.00711600 -2.93353800 -11.26383600
H -3.62906200 -2.59895700 -10.30717800
H -1.09007100 -1.06373900 -13.26502400
H -3.48728400 -0.75326200 -14.07098100
H -5.92569200 2.42528900 -10.99066600
H -2.23556900 -4.93108700 -7.72548300
H -2.48345400 -3.25409000 -7.17885900
H -9.76444800 -3.33493600 -3.24661500
H -4.98963900 1.52402400 -14.07721800
H -6.07209700 2.18004200 -15.31461400
H -7.00826900 3.56610400 -10.16693100
H -7.56606700 2.69106200 -11.60452200
H -3.05692300 -0.84581300 -4.07185600
H -3.10994000 -4.58308500 -6.20089200
H -0.09035500 -1.37252900 -10.43654900
H -8.13068300 1.73540900 -9.14212300
C -15.72460500 -5.23249200 -8.59995500
C -14.28163400 -5.20645300 -8.07989200
C -14.19338300 -5.09085800 -6.54265800
C -12.77879700 -5.40091100 -6.03541600
C -14.65766000 -3.71765600 -6.03454600
C -8.21561800 -7.89747800 -4.42193400
C -9.09632400 -7.77438900 -5.66147100
S -10.15081700 -9.27519000 -5.90013800
C -9.35140600 -9.66407600 -11.61365400
C -8.88616500 -9.45752100 -10.17304900
O -9.52346900 -8.75614300 -9.37004900
C -10.23553200 -8.49926800 -12.08628300
C -10.80863800 -8.74403800 -13.47233700
O -10.14694000 -8.62441000 -14.50486500
N -12.11094300 -9.12732200 -13.51749500
N -7.76941000 -10.12212200 -9.80856600
C -7.14862000 -9.92147200 -8.50393100
H -13.77312300 -6.12727200 -8.39355000
H -13.72796600 -4.37593300 -8.54087900
H -14.86731100 -5.85021100 -6.11951800

H	-12.45030500	-6.40131200	-6.33625000	C	-7.31034600	-3.67236500	-10.99871100
H	-12.73568700	-5.35350600	-4.94079000	O	-7.38442400	-2.87506100	-12.11132300
H	-12.05644800	-4.67861400	-6.43618600	H	-7.75381500	-4.58582800	-8.46273200
H	-14.61300300	-3.66577200	-4.94113300	H	-8.71914300	-2.76727900	-9.68622900
H	-14.01806900	-2.91938300	-6.43472700	H	-6.42014900	-5.08166500	-12.30048500
H	-15.68629400	-3.49347400	-6.33032000	H	-8.66051200	-6.96768000	-9.53495700
H	-16.26151100	-4.30615300	-8.37302800	O	-6.26379100	-3.13241500	-10.13433100
H	-9.74716800	-6.89938400	-5.58250300	H	-5.25412500	-3.94292000	-9.75985100
H	-8.48178500	-7.66166800	-6.55764600	C	-9.87764700	-3.84370900	-11.11979600
H	-10.22264200	-9.17631700	-7.24607300	H	-10.79694600	-3.79825900	-10.52913100
H	-8.81433900	-8.03632100	-3.51590300	H	-9.90370900	-3.01690200	-11.82940600
H	-9.61777700	-7.60096400	-12.14363700	H	-9.88473800	-4.77644300	-11.68823800
H	-11.02457000	-8.32621700	-11.34951000	C	-4.82810800	-9.59760900	-11.88554500
H	-12.68154200	-9.19796600	-12.69134300	C	-4.67411200	-9.03093900	-13.28631200
H	-12.52611500	-9.31213700	-14.41868000	O	-3.94484500	-9.57322700	-14.11760300
H	-8.49186300	-9.76788300	-12.28223100	N	-5.37583100	-7.89110600	-13.50716400
H	-7.88313500	-10.07534900	-7.71160500	C	-5.48687300	-7.29496900	-14.82299000
H	-6.73233700	-8.91123800	-8.41491100	C	-4.88805100	-5.88272100	-14.78852100
H	-7.20351700	-10.52378000	-10.54144700	O	-5.40405100	-4.99883600	-14.07585500
H	-9.91143800	-10.60838500	-11.65048400	C	-6.96102300	-7.22989000	-15.27151100
H	-6.34348700	-10.64841900	-8.38497400	O	-7.45717000	-8.54344700	-15.35444700
H	-7.53281400	-8.74750000	-4.50390600	N	-3.80868200	-5.59844600	-15.55214600
H	-7.61464500	-6.98971800	-4.29161000	C	-3.00048900	-6.52399900	-16.39045700
H	-16.28597000	-6.06002900	-8.15237600	C	-2.06137000	-7.39288100	-15.54607600
H	-15.75167100	-5.36411600	-9.68655400	C	-2.26113200	-5.53753000	-17.31447900
C	-12.65108500	-2.36154800	-18.57849700	C	-1.99128700	-4.32406200	-16.41034100
C	-13.04779400	-2.52643600	-17.10209900	C	-3.25698100	-4.23336300	-15.54343800
C	-11.89792400	-2.99789900	-16.23931400	H	-3.06538100	-3.90800400	-14.51674900
C	-11.15406000	-2.10788400	-15.45860500	H	-3.99486300	-3.54002400	-15.96684200
C	-11.51228800	-4.34769700	-16.23164000	H	-1.11175400	-4.50696500	-15.78456400
C	-10.05755400	-2.53452400	-14.70547800	H	-1.80883800	-3.40485000	-16.97413500
C	-10.42700600	-4.79487800	-15.48676300	H	-1.35181200	-5.97320600	-17.73556500
C	-9.68421000	-3.88539900	-14.71912100	H	-2.91183500	-5.24769200	-18.14747100
O	-8.61882000	-4.36989900	-14.02852700	H	-3.66743100	-7.16520500	-16.97237800
H	-13.87912900	-3.23927100	-17.03301500	H	-1.41207800	-6.77436800	-14.91667100
H	-13.42838200	-1.57187100	-16.71963300	H	-2.61703600	-8.09083400	-14.91685900
H	-11.43478500	-1.05697100	-15.43423800	H	-1.42207500	-7.98763600	-16.20807800
H	-12.08056000	-5.06650200	-16.81798900	H	-4.94671400	-7.95130700	-15.50501200
H	-9.49705900	-1.82794400	-14.09944900	H	-8.37398700	-8.55124900	-15.02577400
H	-10.15320100	-5.84535600	-15.46763500	H	-6.99889200	-6.71902800	-16.25116700
H	-8.26120200	-3.72613800	-13.36642400	H	-7.52305500	-6.60738900	-14.56620900
H	-11.84746600	-1.62540100	-18.68738800	H	-6.03615700	-7.57832200	-12.78918200
H	-12.29156700	-3.30751400	-18.99627000	H	-3.83874700	-9.66858800	-11.42408100
H	-13.50082400	-2.02723400	-19.18326700	H	-5.48715200	-8.99899600	-11.25501500
N	-6.91299600	-5.01492500	-11.40827500	H	-5.20627300	-10.62232400	-11.97365300
C	-7.42996200	-6.18094000	-10.92034300	C	-9.82890300	-5.06487500	-8.33851500
O	-7.20081300	-7.28657600	-11.45736000	H	-9.62271500	-5.82757600	-7.58500700
N	-8.21874000	-6.09809100	-9.82089800	H	-10.13277000	-4.14549200	-7.83298800
C	-8.56106600	-4.84589100	-9.16040800	H	-10.65690500	-5.41601500	-8.95824300
C	-8.65023100	-3.72384200	-10.21047300				

(5S,6R)-Me₂DHU-INT2-II (SkDHPase)

C	-2.73099200	-0.10103300	-4.80017700	H	-0.95157600	-2.62745000	-9.71628800
C	-3.54193900	-0.26663600	-6.04407000	H	-0.08323600	-3.05073300	-11.19136200
N	-3.39090700	0.50482800	-7.18980700	H	-3.64021800	-2.35558300	-10.20331900
C	-4.52895800	-1.15915600	-6.36032900	H	-1.09187300	-1.33268900	-13.36906800
C	-4.26187500	0.06272400	-8.13099600	H	-3.48931500	-0.98161400	-14.15967100
N	-4.96401800	-0.95462600	-7.65908000	H	-5.92032300	2.41880600	-10.96679500
C	-9.56333100	-3.95540800	-4.12770100	H	-2.23683400	-4.88658300	-7.78242200
C	-9.02912100	-3.15350300	-5.25389200	H	-2.50225700	-3.24904600	-7.13533700
N	-9.70740700	-2.08942400	-5.82746200	H	-9.70676100	-3.35100200	-3.22318700
C	-7.87417400	-3.26576600	-5.97563000	H	-4.98405600	1.52489500	-14.09091800
C	-8.97040100	-1.61084500	-6.85612900	H	-6.08150600	2.17470000	-15.31854800
N	-7.85198700	-2.30918900	-6.97124000	H	-7.01548700	3.57140300	-10.17717300
C	-6.95819100	2.60919700	-10.69330100	H	-7.54603500	2.68553200	-11.61796400
N	-7.42612800	1.56674500	-9.81883900	H	-3.05201800	-0.83341900	-4.05709400
C	-7.09118500	0.26340100	-9.99783300	H	-3.07657700	-4.64419200	-6.21774600
O	-6.20209300	0.00803200	-10.88610800	H	-0.01458700	-1.39443400	-10.57418100
O	-7.64431000	-0.58188400	-9.22613300	H	-8.17203300	1.75019000	-9.16651900
C	-5.99742500	1.45357800	-14.50229300	C	-15.72461000	-5.23247300	-8.59996000
C	-6.29788600	0.07317200	-14.99293600	C	-14.28162800	-5.20647800	-8.07989000
N	-6.27611300	-1.05393400	-14.17411600	C	-14.18877400	-5.18346100	-6.53914500
C	-6.61745300	-0.32051500	-16.26545700	C	-12.76632300	-5.49608400	-6.05418200
C	-6.56552200	-2.09737600	-14.94760900	C	-14.67661600	-3.85232800	-5.94774700
N	-6.77513400	-1.69167800	-16.21532200	C	-8.21561800	-7.89747500	-4.42193400
C	-0.67058800	-2.26303000	-10.70606800	C	-9.02302100	-7.81134000	-5.71349000
C	-1.89768300	-1.93232300	-11.47631600	S	-10.10740600	-9.29351900	-5.92367300
N	-1.90403700	-1.48547000	-12.78898500	C	-9.34683900	-9.65219900	-11.61776100
C	-3.21622000	-2.00308100	-11.12577800	C	-8.88624900	-9.45643700	-10.17371200
C	-3.19109700	-1.31335100	-13.17777900	O	-9.53068500	-8.76660200	-9.36656900
N	-4.00841900	-1.62022100	-12.18531300	C	-10.23883000	-8.48833400	-12.07927500
C	-2.92951800	-4.25382000	-7.22607600	C	-10.83772400	-8.73547900	-13.45374600
C	-4.25960700	-4.12832300	-7.93597800	O	-10.20610500	-8.58801100	-14.50178100
O	-5.27972900	-3.77078000	-7.32547100	N	-12.12936100	-9.15559700	-13.47094800
O	-4.22848900	-4.33083100	-9.22432400	N	-7.76820700	-10.11972200	-9.81031600
Zn	-6.50823200	-2.09284900	-8.47235700	C	-7.14862100	-9.92147200	-8.50393100
Zn	-6.03114900	-1.52223500	-12.14068200	H	-13.75282800	-6.09432100	-8.45125500
H	-1.66221100	-0.25775200	-4.98538400	H	-13.74802300	-4.33687700	-8.49069100
H	-2.85069800	0.89522200	-4.36055700	H	-14.84673000	-5.97982400	-6.16106100
H	-4.93598500	-1.95271700	-5.75698800	H	-12.41788300	-6.46946900	-6.41515300
H	-2.74723000	1.27408100	-7.30573000	H	-12.72196200	-5.51461000	-4.95920500
H	-4.35965500	0.48184000	-9.12155100	H	-12.05880900	-4.73724100	-6.41057800
H	-8.86552200	-4.75741700	-3.88068900	H	-14.62880100	-3.86546800	-4.85328900
H	-10.52770900	-4.41279700	-4.37292000	H	-14.05307400	-3.01966000	-6.30047500
H	-7.06981700	-3.97483800	-5.86974600	H	-15.71028700	-3.62954000	-6.22665000
H	-10.61179700	-1.74268000	-5.54197300	H	-16.28280600	-4.33693600	-8.31069200
H	-9.25701100	-0.79670700	-7.50159800	H	-9.65286600	-6.91719400	-5.71056100
H	-6.68965600	1.75310900	-13.70944500	H	-8.36153600	-7.75499400	-6.58102800
H	-6.74564700	0.24394900	-17.17516200	H	-10.19568100	-9.20601600	-7.26986800
H	-7.08100900	-2.29102000	-16.96797800	H	-8.86808100	-7.97108800	-3.54554400
H	-6.61225000	-3.13093500	-14.63117200	H	-9.62266400	-7.58979900	-12.14699400

H	-11.01591400	-8.31550400	-11.32971500	O	-6.23429300	-3.17345500	-10.06502000
H	-12.67776500	-9.24777300	-12.63194700	H	-5.14424800	-3.99640200	-9.66629300
H	-12.56080600	-9.34569000	-14.36332900	C	-9.85050100	-3.80294100	-11.09533800
H	-8.48575600	-9.74310900	-12.28631400	H	-10.77852800	-3.75014800	-10.51927100
H	-7.87602200	-10.10248000	-7.71088600	H	-9.85319500	-2.96755600	-11.79505600
H	-6.75526600	-8.90311000	-8.40498200	H	-9.86258100	-4.72899400	-11.67443500
H	-7.19812400	-10.51144800	-10.54531500	C	-4.82810800	-9.59760800	-11.88554600
H	-9.90050200	-10.59990300	-11.66402900	C	-4.68481200	-9.01937900	-13.28147800
H	-6.32658800	-10.63116300	-8.39736700	O	-3.96378100	-9.55584300	-14.12385800
H	-7.55823100	-8.77091800	-4.42256600	N	-5.38672600	-7.87683200	-13.48693000
H	-7.59209400	-7.00350300	-4.30291600	C	-5.51588400	-7.28564800	-14.80365400
H	-16.26477200	-6.10159300	-8.20714200	C	-4.89998000	-5.88073600	-14.79180100
H	-15.75127800	-5.29278200	-9.69266500	O	-5.39541700	-4.98311200	-14.08307900
C	-12.65108500	-2.36154800	-18.57849700	C	-6.99716600	-7.21005100	-15.22291600
C	-13.02136100	-2.47181800	-17.08978600	O	-7.50204200	-8.52194800	-15.27938400
C	-11.87062300	-2.94404900	-16.22718300	N	-3.82684400	-5.61844400	-15.57375900
C	-11.12675300	-2.05638400	-15.44376800	C	-3.02779700	-6.56257200	-16.39910300
C	-11.49248300	-4.29617700	-16.21120400	C	-2.06137000	-7.39288100	-15.54607600
C	-10.03873100	-2.48693100	-14.67977900	C	-2.32050500	-5.59874300	-17.37018300
C	-10.41583100	-4.74691200	-15.45609700	C	-2.03289900	-4.35951900	-16.50670300
C	-9.67309700	-3.83994700	-14.68467200	C	-3.26962600	-4.25629600	-15.59875300
O	-8.61572100	-4.33070200	-13.98608200	H	-3.04074300	-3.92024700	-14.58291900
H	-13.86845400	-3.16152900	-16.98417300	H	-4.02005200	-3.56490500	-16.00258100
H	-13.37298800	-1.49733200	-16.73060700	H	-1.13041800	-4.51808100	-15.90731700
H	-11.40137800	-1.00376600	-15.42431300	H	-1.87832200	-3.45394200	-17.10012500
H	-12.06097600	-5.01468700	-16.79769400	H	-1.42027100	-6.03997100	-17.80487100
H	-9.47955400	-1.78083100	-14.07197500	H	-2.99651000	-5.33575700	-18.19173200
H	-10.15035900	-5.79937400	-15.43025600	H	-3.69916200	-7.23032000	-16.94439100
H	-8.25788200	-3.69634000	-13.31400600	H	-1.40952600	-6.74682300	-14.94793500
H	-11.83464500	-1.64671100	-18.72685600	H	-2.59966000	-8.07724600	-14.88784700
H	-12.32079300	-3.32740900	-18.97430800	H	-1.42617000	-8.00033100	-16.20049300
H	-13.50636700	-2.02760100	-19.17557900	H	-4.99590000	-7.95257200	-15.49110400
N	-6.90853700	-5.01804800	-11.35535100	H	-8.43194600	-8.51157300	-14.98768800
C	-7.44283900	-6.17847600	-10.87991300	H	-7.05031800	-6.70835100	-16.20679100
O	-7.21835900	-7.28518300	-11.42053500	H	-7.53963900	-6.57607100	-14.51229200
N	-8.24344300	-6.09530700	-9.78622400	H	-6.04643100	-7.57353400	-12.76371900
C	-8.58574000	-4.84312900	-9.12477400	H	-3.83545400	-9.67667500	-11.43260300
C	-8.63471800	-3.71096000	-10.16702500	H	-5.47995600	-9.00192500	-11.24452400
C	-7.27781000	-3.66412700	-10.92873700	H	-5.21115500	-10.61992800	-11.97935400
O	-7.35097800	-2.87020100	-12.05250100	C	-9.88741900	-5.02236600	-8.34709500
H	-7.79375500	-4.59958000	-8.40459000	H	-9.74635200	-5.72882700	-7.52625900
H	-8.70525800	-2.76057800	-9.63206700	H	-10.21305300	-4.06778700	-7.92316300
H	-6.41074700	-5.08344800	-12.24332600	H	-10.68737500	-5.40435200	-8.98580500
H	-8.69889600	-6.96197300	-9.51318500				

(5S,6R)-Me₂DHU-TS3-II (SkDHPase)

C	-2.73099300	-0.10103300	-4.80017800	C	-4.68202500	0.41380300	-7.85317400
C	-3.62974000	-0.18361500	-5.98236800	N	-5.06978200	-0.82410900	-7.59344300
N	-3.80754000	0.83534700	-6.90653700	C	-9.56333000	-3.95541300	-4.12770500
C	-4.42687200	-1.19909300	-6.42828300	C	-9.03603100	-3.17371900	-5.27439800

N	-9.74317400	-2.14996800	-5.88586400	C	-15.72463000	-5.23247500	-8.59996600
C	-7.86942800	-3.26574400	-5.98269600	C	-14.28160700	-5.20647300	-8.07988100
C	-9.01110900	-1.67372100	-6.91954500	C	-14.18292200	-5.09241800	-6.54415500
N	-7.86942100	-2.33708400	-7.00478900	C	-12.76443400	-5.40883900	-6.05162700
C	-6.95819100	2.60919500	-10.69330000	C	-14.63741900	-3.71787900	-6.03141300
N	-7.24890400	1.60357300	-9.70311200	C	-8.21562200	-7.89747200	-4.42193100
C	-7.27520000	0.28028100	-10.07628200	C	-9.10446400	-7.80343300	-5.65708300
O	-6.80804000	0.03748800	-11.23693800	S	-10.15485200	-9.31337400	-5.83559700
O	-7.71774200	-0.54225000	-9.21880200	C	-10.11700000	-10.30197100	-10.8794700
C	-5.99742500	1.45357400	-14.50229300	C	-9.19160200	-9.67550000	-9.84473200
C	-6.23035600	0.05716300	-14.99435600	O	-9.49529500	-8.61166500	-9.27472700
N	-6.22178400	-1.07148400	-14.17539100	C	-10.60021800	-9.29970200	-11.92981000
C	-6.46923600	-0.34234600	-16.28347700	C	-9.58407700	-9.08644300	-13.05107900
C	-6.44021000	-2.11638800	-14.96479400	O	-8.44069900	-9.55040400	-12.99395700
N	-6.59322700	-1.71668200	-16.24451600	N	-10.02425300	-8.37387700	-14.11312400
C	-0.67058700	-2.26303000	-10.70606800	N	-8.09073800	-10.37652700	-9.51911200
C	-1.92882500	-1.86265200	-11.39257700	C	-7.14861700	-9.92147700	-8.50393100
N	-1.96002500	-1.01795200	-12.49216300	H	-13.77415200	-6.12666800	-8.39734100
C	-3.24100200	-2.17304200	-11.15031500	H	-13.72869900	-4.37603600	-8.54225300
C	-3.25021600	-0.85070700	-12.86917200	H	-14.85565000	-5.84971600	-6.11548900
N	-4.04980600	-1.53483400	-12.06997100	H	-12.44545800	-6.41146500	-6.35554900
Zn	-6.47527700	-2.05998300	-8.45625400	H	-12.70866100	-5.36159700	-4.95755900
Zn	-6.10045200	-1.58760700	-12.09828400	H	-12.04078100	-4.69144700	-6.45980400
H	-1.68523200	0.05689000	-5.08825200	H	-14.58717900	-3.66757100	-4.93818800
H	-3.01432500	0.71256300	-4.12261100	H	-13.99609600	-2.92216800	-6.43400800
H	-4.58052100	-2.17763800	-6.00719400	H	-15.66637700	-3.48841700	-6.32203500
H	-3.37094300	1.74520300	-6.87816200	H	-16.26360200	-4.30846200	-8.36795800
H	-5.03348500	1.02822700	-8.66822000	H	-9.75995600	-6.93097600	-5.58974900
H	-8.84390800	-4.72497300	-3.84134600	H	-8.50274600	-7.70906100	-6.56370400
H	-10.50583200	-4.45410500	-4.37584700	H	-10.39405800	-9.14855400	-7.15417400
H	-7.04100700	-3.94369000	-5.85323200	H	-8.80800800	-8.01117200	-3.50839000
H	-10.66111700	-1.82536400	-5.61833800	H	-10.80531800	-8.33920800	-11.44242800
H	-9.31287400	-0.88227800	-7.58644000	H	-11.54388000	-9.63993600	-12.37086000
H	-6.68130000	1.69717100	-13.68441900	H	-10.94734500	-7.97270100	-14.14133300
H	-6.56243900	0.22094700	-17.19827300	H	-9.36997900	-8.21579300	-14.87851100
H	-6.84129100	-2.32021200	-17.01436600	H	-9.64383700	-11.15799200	-11.36659100
H	-6.48912200	-3.14785000	-14.64507300	H	-7.66653300	-9.78046800	-7.55261000
H	-0.89974000	-2.97449500	-9.91037400	H	-6.67142600	-8.98581100	-8.81015500
H	0.03369800	-2.74959100	-11.39036700	H	-7.83151600	-11.15253600	-10.10912100
H	-3.65601400	-2.83995400	-10.41109200	H	-10.98318700	-10.67309800	-10.3190230
H	-1.15746700	-0.60852500	-12.94774000	H	-6.38142700	-10.68659400	-8.37628000
H	-3.55969200	-0.25851500	-13.71548700	H	-7.53399100	-8.75029100	-4.48652600
H	-5.98762200	2.41493900	-11.15270900	H	-7.61108400	-6.98884100	-4.32025800
H	-9.74167100	-3.32584600	-3.24787300	H	-16.28450900	-6.06364100	-8.15735300
H	-4.97842700	1.59152000	-14.12116400	H	-15.75047300	-5.35854500	-9.68716400
H	-6.14986200	2.17094500	-15.31179700	C	-12.65108500	-2.36154800	-18.57849700
H	-6.92270000	3.58930000	-10.20937300	C	-12.92412300	-2.48495100	-17.07018100
H	-7.70601600	2.64943900	-11.49585500	C	-11.73396300	-2.99050800	-16.28109500
H	-2.78279300	-1.03430800	-4.23638200	C	-11.04854500	-2.17657600	-15.37357000
H	-0.15695200	-1.40560100	-10.25537700	C	-11.26744800	-4.30382400	-16.44987700
H	-7.84356400	1.84094400	-8.92296500	C	-9.94341000	-2.64020600	-14.65381800

C	-10.17046500	-4.78343900	-15.74437600	H	-4.83105000	-7.89887500	-15.50774900
C	-9.49718200	-3.95711500	-14.83029600	H	-7.42959700	-8.84479100	-14.62177300
O	-8.43049800	-4.48703500	-14.18134400	H	-6.82999800	-6.63760500	-16.30940700
H	-13.77832800	-3.15829200	-16.91936300	H	-7.38480600	-6.45818400	-14.63923700
H	-13.23273700	-1.50982700	-16.67586200	H	-5.91431600	-7.56441900	-12.76448700
H	-11.38395100	-1.15338200	-15.21898800	H	-4.44560300	-8.85521600	-11.17058100
H	-11.77790900	-4.96670100	-17.14507400	H	-5.86708700	-9.76822000	-11.65904700
H	-9.42845100	-1.98698000	-13.95551800	H	-4.24323000	-10.52146800	-11.78396800
H	-9.81834500	-5.80086000	-15.88167200	C	-2.97579400	-4.24489600	-7.22764600
H	-8.08844400	-3.94050300	-13.42057600	C	-4.27623400	-4.27792600	-8.04334700
H	-11.83193300	-1.66121000	-18.77249900	O	-5.30850100	-3.74869100	-7.55815400
H	-12.37043600	-3.32680900	-19.01193000	O	-4.19410400	-4.82281900	-9.20169500
H	-13.53793500	-2.00199000	-19.11053900	N	-6.32947000	-5.02148000	-10.89380000
C	-4.81204700	-9.59659100	-11.88594700	C	-7.00692300	-6.25004900	-10.58253500
C	-4.65952000	-9.08661200	-13.30237900	O	-6.66902600	-7.31267200	-11.10598800
O	-3.94486000	-9.63231000	-14.14189500	N	-7.96769400	-6.15173100	-9.65314900
N	-5.38984200	-7.96167600	-13.54436200	C	-8.40462600	-4.87142100	-9.09572000
C	-5.38748800	-7.27038700	-14.81390900	C	-8.50455900	-3.82550000	-10.22321700
C	-4.75139500	-5.88468800	-14.62735000	C	-7.11827500	-3.61855700	-10.90669200
O	-5.22457900	-5.09397500	-13.79053300	O	-7.21521700	-3.19744900	-12.19574800
C	-6.83498500	-7.11422700	-15.32196500	H	-2.25759200	-4.97266600	-7.60685500
O	-7.47151400	-8.37351100	-15.47966400	H	-2.54444000	-3.24120800	-7.30056300
N	-3.70090100	-5.52925600	-15.39918600	H	-7.64186800	-4.53526800	-8.38553000
C	-2.91715700	-6.39624300	-16.31726300	H	-8.72268600	-2.85669600	-9.76177400
C	-2.04530400	-7.39187200	-15.54647600	H	-3.19099700	-4.44147400	-6.17509700
C	-2.10691200	-5.35434400	-17.11225400	H	-5.89521600	-5.11925700	-11.82345000
C	-1.81167000	-4.25532400	-16.07836800	H	-8.48182500	-7.01414100	-9.45587800
C	-3.09781100	-4.19388000	-15.24018000	O	-6.26883700	-2.76640100	-10.22638700
H	-2.92702000	-3.97904100	-14.18160900	H	-5.26931300	-4.86917900	-9.97689100
H	-3.79423600	-3.43283000	-15.61375600	C	-9.63801400	-4.13439500	-11.20831700
H	-0.96153000	-4.54325100	-15.45167000	H	-10.59013100	-4.23179400	-10.67968300
H	-1.57064100	-3.29275800	-16.53779300	H	-9.74833800	-3.32225300	-11.92534700
H	-1.20564100	-5.78654400	-17.55365500	H	-9.46751800	-5.05604900	-11.77044900
H	-2.71871100	-4.94931000	-17.92651000	C	-9.71156400	-5.08510700	-8.33505200
H	-3.59786700	-6.93713900	-16.98099700	H	-9.54188000	-5.67984900	-7.43636600
H	-1.38093100	-6.87032000	-14.84918800	H	-10.13597400	-4.12420900	-8.03384300
H	-2.64066400	-8.11913400	-14.99119800	H	-10.44935900	-5.60911500	-8.94722000
H	-1.41972000	-7.95241700	-16.25023300				

(5S,6R)-Me₂DHU-EP-II (SkDHPase)

C	-2.73099400	-0.10103300	-4.80017800	C	-9.01340100	-1.75359500	-6.98785900
C	-3.58209200	-0.18387200	-6.01646900	N	-7.85491000	-2.39080900	-7.03206300
N	-3.67712000	0.80114600	-6.98927900	C	-6.95819100	2.60919600	-10.69330100
C	-4.40112100	-1.18372300	-6.45437300	N	-7.23077500	1.54814300	-9.75338100
C	-4.52919500	0.37300700	-7.95468900	C	-7.12181500	0.23128500	-10.11390700
N	-4.97936300	-0.83499800	-7.66119900	O	-6.54431300	0.02289900	-11.24061100
C	-9.56332600	-3.95541700	-4.12769600	O	-7.55726100	-0.62938800	-9.29516600
C	-9.02752500	-3.19535300	-5.28887100	C	-5.99742500	1.45357600	-14.50229300
N	-9.75063200	-2.21313900	-5.94963600	C	-6.27024800	0.08701400	-15.05515200
C	-7.84768500	-3.28358300	-5.97802700	N	-6.23353100	-1.07980500	-14.29129700

C	-6.57288000	-0.25519200	-16.34663600	C	-9.50216000	-9.41323200	-13.32756900
C	-6.49777100	-2.09097200	-15.11383600	O	-8.40245600	-9.97011600	-13.38572900
N	-6.70815600	-1.62939500	-16.36203800	N	-9.98764100	-8.66631800	-14.34941000
C	-0.67058800	-2.26303000	-10.70606800	N	-7.97116400	-10.42255700	-9.59771800
C	-1.91917000	-1.94378700	-11.45641500	C	-7.14861700	-9.92147600	-8.50393200
N	-1.94180100	-1.10914600	-12.56484400	H	-13.87015700	-6.22297500	-8.12104100
C	-3.22498800	-2.31590900	-11.26552000	H	-13.65418600	-4.59391200	-8.74364900
C	-3.21723000	-0.99881900	-12.99792000	H	-14.86361000	-5.25390300	-6.01662100
N	-4.02159200	-1.71429600	-12.22529200	H	-12.48764800	-5.99617700	-6.10907000
Zn	-6.37486600	-2.17660400	-8.41458100	H	-12.68099100	-4.60412700	-5.03235400
Zn	-6.03471700	-1.54967300	-12.27637500	H	-11.99534300	-4.38723100	-6.65719900
H	-1.66761500	-0.00167900	-5.04706500	H	-14.44427200	-2.85107100	-5.47872500
H	-3.00297900	0.74667400	-4.16069800	H	-13.85471300	-2.57839500	-7.12955800
H	-4.60115900	-2.14368400	-6.01032200	H	-15.54804200	-2.99651300	-6.84559300
H	-3.19959400	1.69060200	-6.98242100	H	-16.15878100	-4.22989300	-8.66084700
H	-4.80201200	0.95841300	-8.81850500	H	-9.79170100	-7.12135600	-5.68559700
H	-8.78612900	-4.60510900	-3.72045900	H	-8.46829000	-7.89084100	-6.57443400
H	-10.41061500	-4.58643100	-4.41383800	H	-10.31002000	-9.43842300	-7.08577800
H	-7.00396200	-3.93660700	-5.81967500	H	-8.81832600	-7.97261500	-3.51106100
H	-10.68293500	-1.90772700	-5.70999500	H	-10.59756000	-8.57692800	-11.67483000
H	-9.32139300	-0.98491700	-7.67840400	H	-11.41285100	-9.89658500	-12.50407900
H	-6.62021100	1.65065200	-13.62555200	H	-10.83273000	-8.12694400	-14.25437600
H	-6.70313300	0.34786000	-17.23089200	H	-9.37228500	-8.51004800	-15.14427000
H	-6.98211200	-2.19827600	-17.14983500	H	-9.31458400	-11.31064700	-11.54818600
H	-6.53633200	-3.13977300	-14.84742300	H	-7.63527400	-10.09672200	-7.53938500
H	-0.89879800	-2.97714800	-9.91262800	H	-6.96736900	-8.85016600	-8.62362400
H	0.09142100	-2.71485200	-11.35091000	H	-7.61795700	-11.17435000	-10.16953600
H	-3.62981600	-3.01000800	-10.53935800	H	-10.76339700	-11.01913600	-10.57433600
H	-1.13848600	-0.67224200	-12.99299200	H	-6.19253500	-10.44688000	-8.51858700
H	-3.51634600	-0.41824500	-13.85628300	H	-7.48483600	-8.71106500	-4.40789900
H	-5.96602200	2.47958300	-11.12924200	H	-7.66660300	-6.94966600	-4.38688200
H	-9.89663600	-3.29157700	-3.32194700	H	-16.36563800	-5.83406400	-7.94614100
H	-4.95261900	1.56598400	-14.18899300	H	-15.77394200	-5.66918200	-9.60250300
H	-6.20243500	2.21570500	-15.25716100	C	-12.65108500	-2.36154800	-18.57849700
H	-6.98442700	3.56727300	-10.16787900	C	-13.06643400	-2.86783500	-17.18855000
H	-7.68578300	2.64924300	-11.51458900	C	-11.87234400	-3.30950800	-16.37457500
H	-2.85100600	-1.01238600	-4.21165700	C	-11.30618500	-2.48791100	-15.39530900
H	-0.23274300	-1.37004800	-10.24516700	C	-11.24804100	-4.53832100	-16.63698900
H	-7.83218300	1.72910900	-8.96424500	C	-10.15408200	-2.86362200	-14.70114600
C	-15.72463000	-5.23250100	-8.59995100	C	-10.10236300	-4.93183800	-15.95583300
C	-14.28160600	-5.20643900	-8.07990400	C	-9.54626800	-4.09341700	-14.98054700
C	-14.15611900	-4.68220200	-6.63505300	O	-8.41196400	-4.52418400	-14.36183400
C	-12.74990300	-4.93340300	-6.07598000	H	-13.76977600	-3.70181400	-17.30352000
C	-14.52478200	-3.19567100	-6.51591700	H	-13.60764400	-2.07682900	-16.65661800
C	-8.21562100	-7.89747300	-4.42192900	H	-11.76987800	-1.53025000	-15.16983200
C	-9.08318900	-7.95405300	-5.67469700	H	-11.66913400	-5.19964200	-17.39093700
S	-10.03669800	-9.53421900	-5.76651300	H	-9.72581000	-2.21061500	-13.94599800
C	-9.91404000	-10.53332600	-11.06823400	H	-9.62408000	-5.88389600	-16.16178500
C	-9.13594300	-9.84341700	-9.95377500	H	-8.19447100	-3.97789700	-13.57904900
O	-9.58823400	-8.84850400	-9.36436000	H	-11.97282000	-1.50577800	-18.49528800
C	-10.43908700	-9.56132600	-12.12935300	H	-12.13080300	-3.14310700	-19.14152100

H -13.52139600 -2.04795600 -19.16462100
 C -4.81204300 -9.59659900 -11.88594600
 C -4.62542300 -9.11658900 -13.31138600
 O -3.76785800 -9.59196000 -14.05583200
 N -5.45160700 -8.09094400 -13.65816600
 C -5.42922800 -7.46873800 -14.96536700
 C -4.86176500 -6.03889500 -14.88257700
 O -5.37909900 -5.20409000 -14.11727000
 C -6.86813900 -7.38658300 -15.51819900
 O -7.43144900 -8.66608600 -15.74512700
 N -3.84695700 -5.68404900 -15.70347700
 C -2.95484300 -6.58644400 -16.47760200
 C -2.04530500 -7.39187100 -15.54647600
 C -2.19744900 -5.58594700 -17.37045600
 C -2.03111300 -4.34902500 -16.47257800
 C -3.34525800 -4.29889800 -15.67761900
 H -3.22495400 -3.95928400 -14.64503700
 H -4.08154300 -3.63595100 -16.15031200
 H -1.18181300 -4.48396400 -15.79533600
 H -1.85597800 -3.43106300 -17.04038400
 H -1.24758700 -5.99305900 -17.72526200
 H -2.80441300 -5.33555200 -18.24814100
 H -3.55567400 -7.26469000 -17.08979600
 H -1.46567500 -6.72633100 -14.89746200
 H -2.60878400 -8.09366200 -14.92973100
 H -1.33702500 -7.97980800 -16.14153600
 H -4.83232500 -8.10886700 -15.61469700
 H -7.44302800 -9.16782800 -14.90160700
 H -6.85609100 -6.87347000 -16.48716800
 H -7.46907500 -6.78318700 -14.82686300
 H -6.20677200 -7.83194100 -13.00755700
 H -4.20182000 -8.97975500 -11.21656700

H -5.85409700 -9.52079200 -11.56721200
 H -4.46082100 -10.62736200 -11.81560700
 C -2.97579700 -4.24489600 -7.22764900
 C -4.21862600 -4.19346700 -8.12216400
 O -5.27664200 -3.67326300 -7.58553600
 O -4.13144400 -4.60164700 -9.29202700
 N -6.14071800 -5.68613700 -11.23769800
 C -7.15931000 -6.55982100 -11.02617300
 O -7.46271400 -7.46542400 -11.82722900
 N -7.89677800 -6.38677600 -9.87770200
 C -8.20759900 -5.08191100 -9.29420400
 C -8.62887100 -3.99609400 -10.34102600
 C -7.45528600 -3.28223600 -10.99514400
 O -7.50420900 -2.93722700 -12.22727600
 H -2.24106800 -4.94052000 -7.63556400
 H -2.53155400 -3.24434900 -7.17934000
 H -7.32991000 -4.70501000 -8.75941200
 H -9.06507300 -3.18244200 -9.74097300
 H -3.23818500 -4.53606800 -6.20688600
 H -5.70141900 -5.71692800 -12.15330700
 H -8.61164900 -7.10620500 -9.78127600
 O -6.46539600 -2.88342700 -10.30184200
 H -5.61582500 -5.26223700 -10.47129000
 C -9.69704800 -4.48261900 -11.32461200
 H -10.54762500 -4.89705400 -10.77727000
 H -10.07179700 -3.66054900 -11.93698900
 H -9.31737900 -5.25981300 -11.99063600
 C -9.33402300 -5.30464800 -8.28138800
 H -8.98702400 -5.94191800 -7.46911200
 H -9.67031600 -4.35765500 -7.85685000
 H -10.19345600 -5.79863200 -8.74436400

(5R)-MeHYD-ES-II (*SmDHPase*)

C -0.08296900 8.83167900 -2.33962000
 C -0.03911500 7.68543100 -1.38618000
 N 0.01665000 7.85002600 -0.00998600
 C -0.02193300 6.32836300 -1.57186500
 C 0.07289000 6.62821000 0.57299000
 N 0.04741900 5.68166800 -0.35072100
 C 5.61649200 3.13334200 -2.13658500
 C 4.42855200 3.15745200 -1.23299000
 N 4.51716100 3.01255500 0.14267300
 C 3.09173300 3.32605400 -1.48665500
 C 3.27182000 3.10270100 0.66272100
 N 2.38162500 3.29018400 -0.29994100
 C 10.19409900 0.81403900 -0.67422800
 C 8.86267300 1.03312000 0.05629400
 C 8.96022700 2.15107600 1.09718500
 S 7.42292000 2.51799000 2.04156800

C 7.23291000 0.99620800 3.03726100
 C 7.70057500 -4.37793300 1.13764400
 C 6.60355200 -3.50957500 1.77177500
 C 5.22208600 -4.08735900 1.55911000
 C 4.57144000 -4.80563000 2.57048500
 C 4.58165600 -3.95208400 0.32081000
 C 3.31315600 -5.36804400 2.35510200
 C 3.32355200 -4.51225900 0.09820900
 C 2.68274500 -5.21991500 1.11849200
 C -0.81275700 5.34072700 4.91242300
 N 0.09416000 5.17182700 3.79422800
 C -0.19986100 4.23195000 2.83160400
 O -1.39123900 3.76896900 2.89998700
 O 0.68500000 3.95873200 1.97534500
 C -3.33407900 2.47964200 5.17066200
 C -2.90020700 1.16545100 4.58956400

N	-2.54170200	0.98659400	3.25086500	H	3.03773400	3.04527400	1.71400200
C	-2.80543900	-0.04669100	5.22130600	H	8.55706800	0.09898300	0.54186600
C	-2.25386300	-0.30132300	3.10015600	H	8.07521900	1.27952500	-0.66558700
N	-2.40108600	-0.95731200	4.26450700	H	9.74875600	1.94038100	1.82808200
C	-5.74653600	4.75182100	-1.67327000	H	9.21621800	3.10265200	0.61942300
C	-5.17201300	4.13842500	-0.44893200	H	6.38458000	1.15915800	3.70507200
N	-5.76808800	4.20351500	0.80185300	H	8.12708400	0.82858500	3.64225600
C	-4.01295500	3.43905400	-0.25628500	H	7.03295200	0.12106000	2.41629000
C	-4.97070300	3.56300400	1.68969100	H	10.51488700	1.72023900	-1.19932400
N	-3.90033600	3.08803300	1.07674000	H	6.64941300	-2.50080900	1.33992800
C	-2.88660300	-3.64653100	-4.63793300	H	6.79698600	-3.40111700	2.84535900
C	-3.93437100	-3.70566500	-3.53875600	H	5.05521300	-4.92071700	3.53765200
O	-5.02278500	-4.24523200	-3.70918100	H	5.06921400	-3.39619100	-0.47682700
N	-3.54425200	-3.14707900	-2.34934100	H	2.81481400	-5.90757200	3.15455000
C	-4.45497300	-3.06487700	-1.21275800	H	2.84780600	-4.36467500	-0.86754000
C	-4.68228400	-1.59642100	-0.85529200	H	1.69336600	-5.63948500	0.96635300
O	-3.72868500	-0.90955700	-0.42770600	H	7.69771100	-5.38441100	1.56746700
C	-3.91620600	-3.79758000	0.03906200	H	-6.74311100	4.35824800	-1.90444100
O	-3.92758900	-5.19633200	-0.09406800	H	-5.09851300	4.53581600	-2.52468700
N	-5.91390500	-1.06167700	-0.96954000	H	-3.26842100	3.15438900	-0.98872800
C	-7.17776400	-1.72678600	-1.39811800	H	-5.19417500	3.47150800	2.74135800
C	-7.30712900	-1.83858900	-2.92321600	H	-2.45647600	-4.64893000	-4.74870900
C	-8.24098000	-0.80617400	-0.76597900	H	-4.58101900	-3.55542600	0.87926200
C	-7.61253500	0.59319200	-0.85812300	H	-2.92343700	-3.40287300	0.28372900
C	-6.12987400	0.33840000	-0.55708400	H	-3.17663700	-5.48742700	-0.64294000
C	-0.65468600	2.69727500	-4.32910100	H	-5.36824400	-3.56673200	-1.52948800
C	-0.77832100	2.76594300	-2.81246600	H	-2.73830700	-2.52680600	-2.37369000
O	0.16786500	3.37757700	-2.19889900	H	-8.39421900	-1.08038600	0.28394700
O	-1.76078100	2.20788000	-2.26669200	H	-9.20357500	-0.88400800	-1.27709300
C	4.34067300	1.25928000	-5.73769800	H	-8.05858600	1.30694900	-0.15998400
C	3.77195300	0.47400800	-4.56009700	H	-7.73382700	0.99829500	-1.86805700
S	4.76911500	-1.06138800	-4.27625800	H	-5.90248500	0.43792900	0.51122700
C	0.88536000	-5.10401800	-3.18229000	H	-5.44716100	1.00154800	-1.09288400
C	1.25475400	-3.73193900	-3.72567100	H	-7.22661400	-2.72584700	-0.95697900
O	1.97196600	-2.95837900	-3.06925600	H	-1.60184800	2.40139900	-4.78159300
C	-0.03516200	-4.96224900	-1.95210400	H	-0.31737200	3.65333600	-4.73838500
C	-0.48741600	-6.28504700	-1.34648000	H	2.73762300	0.18792900	-4.76244300
O	-1.66789000	-6.52214600	-1.10322500	H	3.77600000	1.07782700	-3.64878600
N	0.48325600	-7.20586900	-1.09267700	H	3.79805100	-1.79826200	-3.69344500
N	0.75016300	-3.40594600	-4.93069500	H	5.38772500	1.53198500	-5.56925800
C	0.89930600	-2.07250800	-5.49904400	H	0.46377100	-4.37150300	-1.17602600
Zn	-2.14246500	2.35741200	1.79191000	H	-0.94776000	-4.42661300	-2.22052700
Zn	0.35476600	3.62682000	-0.13156900	H	0.20547400	-8.04946900	-0.61203800
O	-0.99922100	2.26379300	0.28418600	H	1.46469800	-6.97870900	-1.12346800
H	-0.96270400	9.46570600	-2.17948500	H	0.39948400	-5.71877600	-3.94738200
H	0.80616000	9.46702300	-2.25470400	H	0.26924400	-1.35299600	-4.96949100
H	-0.03648000	5.75844700	-2.48684300	H	1.94765400	-1.77393000	-5.44991800
H	0.13410800	6.47543400	1.63975700	H	0.09642300	-4.04028200	-5.36361700
H	6.11797700	2.15882600	-2.12919000	H	-0.88136200	4.44782900	5.54568900
H	5.30361500	3.33825300	-3.16257500	H	-1.81115600	5.58109200	4.54601600
H	2.57737300	3.46779500	-2.42386400	H	-3.22176600	2.46989500	6.25762700

H	-2.73922100	3.29360800	4.75604400	C	1.28875700	-0.06915400	-0.90539500
H	-2.99335500	-0.33050900	6.24431900	C	0.09590100	-0.40940800	-0.02110700
H	-1.89710300	-0.76232600	2.19521700	O	0.09823900	-0.49750500	1.20671100
H	-2.16516900	-1.93147300	4.40426800	H	1.44162400	1.01282100	-0.83957900
H	0.60122000	-2.10659800	-6.54853000	H	-1.92535000	-0.88375000	-0.58840300
H	1.82409100	-5.60080300	-2.91705400	H	1.38444100	-0.98655800	-2.83601400
H	-7.23038800	-0.85632500	-3.40073000	C	2.56188200	-0.80022300	-0.49042600
H	-6.54494600	-2.49812300	-3.34366100	H	3.40118900	-0.50300900	-1.12521500
H	-8.28463200	-2.26412000	-3.17319200	H	2.79862900	-0.54439700	0.54495200
H	-0.12598100	8.45756300	-3.36442900	H	2.44234000	-1.88219400	-0.56470500
H	6.35482900	3.89252800	-1.85533000	H	-1.40950500	2.09080600	-0.59866300
H	5.37572400	2.84613500	0.67108500	C	-0.98530700	-5.37581300	7.06970500
H	0.02582100	8.73238400	0.48003500	C	-0.15319900	-6.06652200	5.98160000
H	-5.83260700	5.84118700	-1.58506600	C	-0.26190500	-5.32744100	4.66948200
H	-6.64420700	4.65565100	1.01934600	C	0.35441000	-4.07922300	4.51494200
H	10.99024200	0.53490300	0.02417300	C	-1.04753700	-5.80895500	3.61399300
H	10.10478600	0.01381600	-1.41463300	C	0.19675300	-3.33290700	3.34944800
H	8.69299400	-3.94377800	1.29899500	C	-1.22006000	-5.08249400	2.43700000
H	7.54712800	-4.47874000	0.05869900	C	-0.58810600	-3.84179000	2.30573200
H	-3.38833900	-3.40663400	-5.57826200	O	-0.75133700	-3.14805300	1.14068300
H	-2.09710300	-2.92342600	-4.43718600	H	-0.49211100	-7.10091000	5.85780200
H	4.29296800	0.67605100	-6.66111700	H	0.89457300	-6.11751200	6.30394500
H	3.77286300	2.18443000	-5.88490500	H	0.97614600	-3.68529100	5.31581900
H	-4.39199000	2.68087700	4.95728600	H	-1.54644100	-6.76937300	3.71706000
H	1.07847800	5.34751000	3.93454600	H	0.70551400	-2.38057700	3.22473500
H	-0.46231800	6.17256400	5.52971700	H	-1.84987600	-5.45270600	1.63324300
H	0.10205900	1.94649700	-4.58125700	H	-0.34846300	-2.26413400	1.24431300
N	-0.94223500	-0.70817400	-0.85105500	H	-0.64587100	-4.34713500	7.23051300
C	-0.50929300	-0.85026300	-2.17146600	H	-2.04238500	-5.33831000	6.78627100
O	-1.17963000	-1.34649400	-3.06857700	H	-0.91225200	-5.90389800	8.02651300
N	0.78935800	-0.41111600	-2.24418600				

(5R)-MeHYD-TS1-II (*SmDHPase*)

C	0.85117200	8.74409700	-2.10532300	C	7.32394800	-5.23379000	1.03959500
C	0.69580000	7.58248400	-1.19185900	C	6.56296300	-4.03239800	1.61877500
N	0.51189000	7.69342000	0.17818800	C	5.06727200	-4.20151300	1.48481400
C	0.71682900	6.23785500	-1.43339800	C	4.29328100	-4.67766200	2.55109700
C	0.44009000	6.44843700	0.70830500	C	4.43402700	-3.94096000	0.26297100
N	0.55829900	5.54323500	-0.24924400	C	2.92205300	-4.88502200	2.40397500
C	5.99728400	2.53887200	-2.01145000	C	3.06322300	-4.14741400	0.10665500
C	4.82170400	2.69090900	-1.11350000	C	2.30256800	-4.61863400	1.18117600
N	4.86913100	2.51250200	0.25951400	C	-0.32209300	5.10604200	5.01502900
C	3.52151900	3.01310900	-1.38945700	N	0.46351200	4.84204400	3.81757100
C	3.63266100	2.73140200	0.75994000	C	0.13493500	3.88512100	2.87690900
N	2.78947100	3.03303900	-0.21757300	O	-1.03078100	3.36841500	2.96612900
C	10.31592100	-0.23987300	-0.56227700	O	1.00118100	3.64037500	1.98597800
C	9.00244700	0.07863400	0.16501600	C	-3.10026000	2.48396300	5.14169300
C	9.18803800	1.16729300	1.22494700	C	-3.41384600	1.22114900	4.40433300
S	7.68050800	1.66142100	2.16001000	N	-3.02623600	0.98734500	3.08823600
C	7.32079600	0.14145500	3.11075900	C	-4.08632800	0.11826800	4.86310700

C	-3.46282500	-0.22502400	2.76971000	H	8.24293800	0.40106900	-0.55666400
N	-4.10855100	-0.78129400	3.81524200	H	9.94518200	0.87414700	1.96048200
C	-5.17470800	5.18708400	-1.65625100	H	9.53566200	2.09864400	0.76543400
C	-4.65714300	4.36068000	-0.52934800	H	6.48729500	0.37524200	3.77623200
N	-5.33063400	4.16413800	0.66804800	H	8.18563600	-0.13571800	3.71816800
C	-3.49023200	3.65806700	-0.39575300	H	7.03586200	-0.69012300	2.46404200
C	-4.56948200	3.37218800	1.46237500	H	10.71372700	0.64435200	-1.07187600
N	-3.44530500	3.04847400	0.84556600	H	6.88023700	-3.12012200	1.09638300
C	-3.04959300	-3.34110000	-4.85853800	H	6.83034700	-3.90327500	2.67417100
C	-4.15132500	-3.28604500	-3.80746300	H	4.77116600	-4.88438500	3.50588400
O	-5.28030200	-3.70547700	-4.04732700	H	5.01837400	-3.56598900	-0.57449400
N	-3.78321600	-2.77048300	-2.59235700	H	2.32892200	-5.23758300	3.24201600
C	-4.71213700	-2.74476000	-1.47040400	H	2.60018700	-3.90127500	-0.84537400
C	-4.93080500	-1.32195800	-0.94850100	H	1.23050800	-4.75901100	1.08723700
O	-3.99021600	-0.69830300	-0.40694900	H	7.04541000	-6.15695300	1.55731500
C	-4.23429100	-3.61495300	-0.27849400	H	-6.14641900	4.83084700	-2.01698200
O	-4.31573600	-4.98685700	-0.55360100	H	-4.47241500	5.13737000	-2.49037300
N	-6.15810000	-0.77368000	-0.98223400	H	-2.70910200	3.53134300	-1.13102500
C	-7.38416700	-1.31407500	-1.62569900	H	-4.86109400	3.04989600	2.44979500
C	-7.31377700	-1.18721400	-3.14756800	H	-2.74933400	-4.38827700	-4.97701600
C	-8.48536900	-0.45068800	-0.98022700	H	-4.90604200	-3.40675600	0.56846400
C	-7.81442200	0.91899700	-0.78985700	H	-3.23088900	-3.29098600	0.02172300
C	-6.37526900	0.56186000	-0.39289200	H	-3.46337800	-5.31030200	-0.89681900
C	-0.09583700	3.13104400	-4.48981400	H	-5.63368700	-3.18577800	-1.84766600
C	-0.24429900	3.05797100	-2.97659900	H	-2.87722700	-2.30914200	-2.51193200
O	0.75906100	3.41622300	-2.26946800	H	-8.76458700	-0.87099000	-0.00748100
O	-1.34737000	2.66333500	-2.51762300	H	-9.38568600	-0.40991000	-1.59777200
C	4.61666400	0.90692000	-5.69091400	H	-8.31100900	1.53388800	-0.03422600
C	3.96871300	0.16504500	-4.52548900	H	-7.82236500	1.48027400	-1.72973900
S	4.85513000	-1.42795500	-4.20209900	H	-6.25226500	0.49846600	0.69551000
C	0.68281200	-4.96848300	-3.10300000	H	-5.62438800	1.26452500	-0.76248400
C	1.12729300	-3.64808400	-3.71662200	H	-7.51078300	-2.36432100	-1.34960100
O	1.87567700	-2.87765200	-3.09323000	H	-0.74577400	3.92266100	-4.87790400
C	-0.24108800	-4.71919400	-1.89332900	H	0.93397100	3.33698200	-4.78525400
C	-0.68154300	-5.98948000	-1.17876500	H	2.92532400	-0.06516900	-4.74968400
O	-1.86677900	-6.25758900	-0.98716100	H	3.98473400	0.77288000	-3.61672000
N	0.30751400	-6.83159700	-0.77268900	H	3.80476100	-2.08381400	-3.66096700
N	0.66294000	-3.37827200	-4.95127000	H	5.67297500	1.11827700	-5.49380400
C	0.87948300	-2.09776600	-5.61263400	H	0.26673900	-4.06456100	-1.17687800
Zn	-1.82311100	2.06607800	1.70739000	H	-1.14855700	-4.20294600	-2.20906700
Zn	0.81556300	3.50935500	-0.13873900	H	0.02927600	-7.62102300	-0.20714400
O	-0.67601100	2.18205600	-0.04755700	H	1.26725400	-6.52604100	-0.70679100
H	-0.02457700	9.40347900	-2.08997200	H	0.17543700	-5.60316300	-3.83735700
H	1.72778200	9.35145400	-1.85153600	H	0.43797700	-1.28995500	-5.02200200
H	0.84962600	5.70859600	-2.36241800	H	1.94900200	-1.91694400	-5.74465700
H	0.31961200	6.24794800	1.76263800	H	0.00153900	-4.02045200	-5.35973800
H	6.35074100	1.50204800	-2.05382900	H	-0.19478100	4.33774800	5.78896600
H	5.72480000	2.83674500	-3.02604600	H	-1.37766600	5.15257400	4.74716500
H	3.04615200	3.22484600	-2.33309300	H	-3.52525900	2.44751800	6.14787400
H	3.37076700	2.67562400	1.80461100	H	-2.02189600	2.63479700	5.21478700
H	8.61718500	-0.83427300	0.63420400	H	-4.52979000	-0.09962500	5.82147600

H	-3.34466600	-0.71204000	1.81332200	C	-0.46284600	0.29769000	0.13258900
H	-4.48608300	-1.71717700	3.83323300	O	-0.80183600	0.26105100	1.37589900
H	0.40532700	-2.12883800	-6.59436200	H	1.52033300	0.97463100	-0.46467000
H	1.59142900	-5.49525200	-2.79540000	H	-2.30113000	-0.39686800	-0.70314200
H	-7.11847700	-0.15300300	-3.44922600	H	1.38117900	-1.13987500	-2.18104900
H	-6.54325000	-1.83535700	-3.56884100	C	1.73594400	-0.90492200	0.55643100
H	-8.26875300	-1.49453100	-3.58750000	H	2.72624500	-1.12747700	0.15125600
H	0.98003000	8.38932100	-3.12970700	H	1.85793100	-0.43257800	1.53443500
H	6.83748100	3.16668900	-1.69427600	H	1.20316900	-1.84731500	0.69416600
H	5.69480800	2.23981400	0.79717300	H	-1.07119600	2.31200900	-0.96419700
H	0.45065300	8.55547600	0.69977200	C	-1.51803400	-5.61183900	6.81074200
H	-5.29039700	6.24035200	-1.37487800	C	-0.33614500	-5.76235600	5.84189100
H	-6.23320000	4.54482100	0.91210900	C	-0.52450500	-4.89431900	4.62038500
H	11.08190700	-0.59446100	0.13558600	C	-0.14504300	-3.54654400	4.63278900
H	10.16469500	-1.01869400	-1.31529500	C	-1.18694400	-5.37857400	3.48393700
H	8.40687600	-5.10382800	1.13814500	C	-0.42017800	-2.70384000	3.55824800
H	7.09493800	-5.36753300	-0.02217800	C	-1.47436600	-4.55431100	2.39845900
H	-3.46737000	-3.01296800	-5.81287100	C	-1.09180700	-3.20772200	2.43775400
H	-2.18126300	-2.73446900	-4.59663200	O	-1.38695400	-2.42764600	1.35854000
H	4.56157000	0.32036200	-6.61192500	H	-0.23798600	-6.81333100	5.54574800
H	4.10988700	1.86339100	-5.86107800	H	0.59419600	-5.49385600	6.35702900
H	-3.50557100	3.36312000	4.62982500	H	0.37150600	-3.14533000	5.50192600
H	1.44998500	5.05675800	3.84449100	H	-1.49843000	-6.42008900	3.45220900
H	-0.02108100	6.07011400	5.43227800	H	-0.11427500	-1.66142200	3.57705900
H	-0.43593900	2.19292600	-4.93571900	H	-1.99932400	-4.93938800	1.52950700
N	-1.29391900	-0.23191100	-0.83108600	H	-1.14366200	-1.49054300	1.53054500
C	-0.59966300	-0.78885400	-1.89426500	H	-1.62092900	-4.57288100	7.14105200
O	-1.11234700	-1.43255700	-2.81165300	H	-2.45669800	-5.90078700	6.32696900
N	0.72461900	-0.52281200	-1.70834600	H	-1.38942600	-6.23801800	7.70024200
C	0.97634400	0.03644400	-0.37608000				

(5R)-MeHYD-INT1-II (SmDHPase)

C	0.65985100	8.67036500	-2.17075400	C	5.36130300	-3.74944200	1.45043800
C	0.48448500	7.49732900	-1.27541500	C	4.53735700	-4.01520700	2.55220100
N	0.23887000	7.59792400	0.08540800	C	4.75804300	-3.47900100	0.21464700
C	0.54440900	6.15395000	-1.52039100	C	3.14752700	-4.01346400	2.42596500
C	0.17141900	6.35147000	0.60910900	C	3.36947100	-3.47837300	0.07792800
N	0.35058200	5.45189300	-0.34532300	C	2.56077600	-3.74607500	1.18762200
C	5.94049400	2.58004900	-2.03278100	C	-0.47706600	5.02081800	4.94961800
C	4.75888600	2.75617200	-1.14761000	N	0.28847200	4.74804300	3.73828400
N	4.80526300	2.62409500	0.22981300	C	-0.05647300	3.80005500	2.79631200
C	3.45422500	3.04688800	-1.43752300	O	-1.22588400	3.29899100	2.88118300
C	3.56502300	2.83445100	0.72064000	O	0.81018200	3.55263800	1.90002900
N	2.71807300	3.08842600	-0.26764800	C	-3.19763600	2.33849800	5.06455400
C	10.31016100	-0.10026200	-0.55154100	C	-3.51940500	1.02756000	4.42867300
C	8.96997700	0.20613700	0.13215800	N	-3.20725500	0.77815500	3.10102200
C	9.12201900	1.25180800	1.23950500	C	-4.09617400	-0.09691600	4.95739100
S	7.58370500	1.73546000	2.13010400	C	-3.58327300	-0.46716300	2.83287200
C	7.13099600	0.17547600	2.97109500	N	-4.13087000	-1.02440300	3.93166100
C	7.41889200	-5.15576400	1.04205600	C	-5.28900700	4.98248000	-1.75143200
C	6.86772000	-3.81996000	1.56336800	C	-4.81361200	4.16597000	-0.59636800

N	-5.59969500	3.78883000	0.48368100	H	6.81862600	-0.59682800	2.26646700
C	-3.59015900	3.60844600	-0.34659300	H	10.73717000	0.79720000	-1.01198100
C	-4.84796900	3.03156500	1.31952700	H	7.32137300	-2.99954000	0.99166200
N	-3.62044000	2.90094100	0.84093600	H	7.17013500	-3.68259100	2.60820800
C	-2.95714200	-3.50291600	-4.92338900	H	4.99147500	-4.22716400	3.51755700
C	-4.10716100	-3.40840100	-3.93243300	H	5.38240400	-3.26262100	-0.64961500
O	-5.20713800	-3.89739300	-4.17705400	H	2.51837400	-4.21030700	3.28901300
N	-3.81052600	-2.75602700	-2.76856500	H	2.92608400	-3.25476100	-0.88915200
C	-4.61862500	-2.97106000	-1.57915500	H	1.47972300	-3.72776900	1.09962600
C	-4.96057900	-1.63121900	-0.91887900	H	7.00614400	-5.99549200	1.60991000
O	-4.08800200	-0.99597200	-0.28911900	H	-6.14558000	4.51951100	-2.25401400
C	-3.88039100	-3.88444300	-0.57913800	H	-4.48284000	5.06884100	-2.48205200
O	-3.63204400	-5.10748500	-1.22868700	H	-2.72093100	3.64066800	-0.98106100
N	-6.21625300	-1.14500100	-0.99850100	H	-5.21782600	2.59143200	2.23260000
C	-7.38231800	-1.69825800	-1.73706400	H	-2.56871400	-4.52677100	-4.87635500
C	-7.27814300	-1.44014100	-3.24294000	H	-4.52385000	-4.01443000	0.31095000
C	-8.55509500	-0.95925800	-1.06429300	H	-2.96366300	-3.38415500	-0.24407200
C	-7.97974100	0.43222800	-0.75539200	H	-2.81942200	-5.51387700	-0.87038800
C	-6.53002500	0.13748500	-0.34319900	H	-5.51421800	-3.49135600	-1.91970800
C	-0.32407500	2.81887200	-4.48869600	H	-2.85948400	-2.40359200	-2.63947800
C	-0.40198000	2.96529500	-2.98809300	H	-8.82959100	-1.46727400	-0.13289500
O	0.65394500	3.25633300	-2.33706100	H	-9.44072800	-0.92944500	-1.70341100
O	-1.52675300	2.73812500	-2.45553100	H	-8.53475800	0.95709000	0.02740300
C	4.61883600	0.91117900	-5.71732900	H	-8.00120800	1.05896900	-1.65278100
C	4.00020700	0.19472500	-4.52035300	H	-6.42532900	0.02198200	0.74308600
S	5.05962100	-1.22572000	-3.98355400	H	-5.81642400	0.90502400	-0.65459600
C	0.92933500	-4.91035000	-2.98311000	H	-7.45205500	-2.77404900	-1.55673100
C	1.29010200	-3.60682800	-3.68697700	H	-0.34628200	1.75096500	-4.73104200
O	2.04195800	-2.77474500	-3.15270300	H	-1.20242800	3.27054200	-4.95528700
C	0.00813300	-4.67144400	-1.76714200	H	3.01664600	-0.20513200	-4.77236900
C	-0.11396800	-5.84722600	-0.80684900	H	3.87205200	0.87996600	-3.67784100
O	-1.20595500	-6.25208000	-0.39918500	H	4.04940600	-1.98912200	-3.51417200
N	1.04424800	-6.43262800	-0.39841500	H	5.62177400	1.28566700	-5.48636200
N	0.77814800	-3.42185900	-4.92009100	H	0.37553700	-3.81099600	-1.19675000
C	0.94822200	-2.17485500	-5.65588400	H	-1.00195300	-4.42082300	-2.09131800
Zn	-2.08233100	1.89366400	1.77796800	H	0.96077000	-7.10975300	0.34708400
Zn	0.73568400	3.45057700	-0.18617100	H	1.92352600	-5.94014400	-0.46805600
H	-0.22650800	9.31510200	-2.18584500	H	0.46169100	-5.62114100	-3.67259800
H	1.51498300	9.28768400	-1.87238900	H	0.51762500	-1.34001800	-5.09447600
H	0.72867200	5.63483000	-2.44651100	H	2.00890200	-1.98258400	-5.83411300
H	0.01744500	6.14625200	1.65801600	H	0.09710400	-4.08514100	-5.25707400
H	6.26912500	1.53494300	-2.06907100	H	-0.32679400	4.26219600	5.72837500
H	5.68619500	2.88176800	-3.05100000	H	-1.53781900	5.05602000	4.70107400
H	2.98049200	3.21316500	-2.39089500	H	-3.55706100	2.36207700	6.09673200
H	3.30117300	2.79716400	1.76535400	H	-2.12179700	2.51919200	5.06047700
H	8.55698600	-0.71896300	0.55119900	H	-4.46640100	-0.31588700	5.94598200
H	8.24416700	0.56282800	-0.60770100	H	-3.47840300	-0.96705800	1.87932800
H	9.84195900	0.91969800	1.99552400	H	-4.44136300	-1.98232500	4.00089800
H	9.50148100	2.19480600	0.83171600	H	0.43986600	-2.26412700	-6.61668200
H	6.29638600	0.40683100	3.63604100	H	1.87959600	-5.35230700	-2.66863800
H	7.96858000	-0.18227200	3.57457200	H	-7.12283700	-0.37701000	-3.45360500

H	-6.46719900	-2.01934900	-3.68728400	H	-2.12542600	-4.89458000	7.01204300
H	-8.20618100	-1.75317100	-3.73333700	H	-1.97048000	-6.37116900	6.05425600
H	0.83829800	8.32935300	-3.19232800	H	-1.25915700	-6.29219200	7.67255400
H	6.78899600	3.19079500	-1.70568700	C	-0.37554500	-4.39734700	4.88475000
H	5.63447000	2.37228000	0.77416400	C	-0.24754600	-3.00507400	4.83951200
H	0.13507400	8.45686500	0.60576600	C	-0.79321200	-5.04916900	3.71347200
H	-5.58549700	5.99391200	-1.45010700	C	-0.52718800	-2.27957600	3.67854300
H	-6.57108500	4.02519600	0.62429700	C	-1.08389000	-4.34743600	2.54972800
H	11.04296400	-0.48821400	0.16399800	C	-0.95324700	-2.95012600	2.52365600
H	10.18245300	-0.84981600	-1.33784600	O	-1.24422000	-2.31360300	1.36010400
H	8.51009300	-5.19435500	1.12508800	H	0.07807400	-2.47087900	5.72963500
H	7.15461900	-5.30438400	-0.00952600	H	-0.89922700	-6.13181200	3.71349400
H	-3.34067700	-3.34140900	-5.93317300	H	-0.40827300	-1.20005500	3.65862600
H	-2.15106000	-2.80090000	-4.70064400	H	-1.40470800	-4.86725700	1.65301100
H	4.70561500	0.24078100	-6.57658900	H	-1.13603800	-1.32692300	1.42892300
H	4.00127100	1.76822700	-6.00870700	N	-1.40612600	-0.08341500	-1.04874600
H	-3.66059900	3.17044700	4.52375700	C	-0.65542400	-0.99161100	-1.76631100
H	1.27446000	4.96642400	3.74714700	O	-1.09037600	-1.78096700	-2.61578000
H	-0.17494800	5.99198600	5.34865100	N	0.64450300	-0.87356300	-1.38554100
H	0.59015000	3.25504100	-4.89461400	C	0.85686400	0.18905200	-0.41457100
C	1.70495000	-0.22125200	0.78102600	C	-0.62049800	0.58865100	-0.03689800
H	2.72121600	-0.46989900	0.46178600	O	-1.02058500	0.33937800	1.22929700
H	1.75351100	0.59807900	1.50259800	H	1.31588200	1.04736200	-0.91520200
H	1.27953700	-1.09320300	1.27757800	H	-2.37503500	-0.33442800	-0.83802300
C	-1.44809500	-5.71737400	6.75964000	H	1.36567300	-1.34440900	-1.92229300
C	-0.14007500	-5.18380500	6.15531300	O	-0.79309600	2.05762600	-0.19674900
H	0.53005400	-6.02966000	5.95367200	H	-1.19618500	2.27211100	-1.14439700
H	0.37331900	-4.55318000	6.89054900				

(5R)-MeHYD-TS2-II (*SmDHPase*)

C	0.99868700	8.60074800	-2.35754300	C	4.54862800	-3.73296000	0.24744700
C	0.79969400	7.41520400	-1.46454200	C	2.92663800	-4.18694600	2.46874100
N	0.62167400	7.53597600	-0.09456100	C	3.16030900	-3.70428200	0.11050600
C	0.76669800	6.06227300	-1.69237900	C	2.34582500	-3.92946400	1.22539600
C	0.50244200	6.30082400	0.44559400	C	-0.24277300	5.15431900	4.84609200
N	0.58339800	5.37723300	-0.50048200	N	0.55539800	4.88405000	3.66736800
C	6.01581000	2.29448000	-2.12154000	C	0.22257500	3.89709500	2.76552500
C	4.83530000	2.53743800	-1.24738000	O	-0.93995900	3.39222800	2.86725200
N	4.89163400	2.46057400	0.13298500	O	1.10713200	3.63531300	1.88903200
C	3.53310800	2.85065100	-1.53487700	C	-3.07431600	2.59380500	5.03499400
C	3.66303400	2.72423400	0.62657200	C	-3.43999900	1.29239900	4.40709200
N	2.81015800	2.96139400	-0.36131800	N	-3.11629800	1.01591500	3.08809100
C	10.27755300	-0.53833900	-0.60999600	C	-4.06756100	0.19893500	4.94302800
C	9.02979800	-0.11330800	0.17736100	C	-3.53483700	-0.21807200	2.83285100
C	9.26571400	1.18114100	0.95900200	N	-4.12197800	-0.74013700	3.92906300
S	7.83237700	1.84009400	1.90909200	C	-5.09885200	5.18028000	-1.82310400
C	7.57815500	0.53127200	3.16132100	C	-4.59461100	4.36957900	-0.66841800
C	7.18469800	-5.43080800	1.10902500	N	-5.35843600	4.09969900	0.45903300
C	6.65014100	-4.07911400	1.60700000	C	-3.39937500	3.73839800	-0.42908500
C	5.14539600	-3.98936200	1.48904500	C	-4.62442500	3.33832100	1.30803100
C	4.31590700	-4.21694700	2.59504300	N	-3.42871900	3.10085100	0.79848500

C	-3.15304600	-3.46214700	-4.82695900	H	2.72287200	-3.48738700	-0.86088800
C	-4.28560700	-3.29071300	-3.82681500	H	1.26549800	-3.88200400	1.13991700
O	-5.41022900	-3.72850900	-4.05654500	H	6.75883400	-6.25558900	1.68891200
N	-3.94896000	-2.63313200	-2.67780800	H	-5.99455500	4.73620600	-2.27128700
C	-4.77432500	-2.76161800	-1.48723400	H	-4.33091600	5.23104000	-2.59723800
C	-5.02742100	-1.38369700	-0.86831200	H	-2.53404100	3.67222900	-1.06723800
O	-4.11237500	-0.77909000	-0.27250700	H	-4.98792000	2.96907700	2.25457900
C	-4.10791300	-3.69891000	-0.45958700	H	-2.83613300	-4.51047400	-4.78696300
O	-3.96043400	-4.95779200	-1.07108100	H	-4.75944200	-3.75159600	0.43244600
N	-6.25573800	-0.83001700	-0.95156600	H	-3.15448900	-3.26363700	-0.13705200
C	-7.46257100	-1.35276500	-1.64546500	H	-3.15561700	-5.39843200	-0.73699000
C	-7.37031600	-1.18147800	-3.16468400	H	-5.70046500	-3.22998500	-1.82025000
C	-8.58235200	-0.51544900	-0.99683700	H	-2.98873500	-2.30631800	-2.55685400
C	-7.92292900	0.85169000	-0.75539500	H	-8.87609800	-0.96410100	-0.04116800
C	-6.49115900	0.48865100	-0.33696800	H	-9.47170500	-0.46190900	-1.62927800
C	-0.24995900	2.74904400	-4.54371400	H	-8.43956300	1.44470900	0.00465000
C	4.59842000	0.60622700	-5.76139800	H	-7.91329900	1.43624700	-1.68122200
C	3.96772400	-0.10719500	-4.56875400	H	-6.38919300	0.40310400	0.75234500
S	4.85493500	-1.69045600	-4.20515000	H	-5.73565100	1.20333900	-0.67439900
C	0.59608100	-5.00818500	-2.89919100	H	-7.59043600	-2.41199800	-1.40701200
C	1.03085100	-3.73353300	-3.61289300	H	-0.06659800	1.75008800	-4.95488600
O	1.82108600	-2.93488400	-3.08272300	H	-1.19534500	3.09349200	-4.96981400
C	-0.30166500	-4.71546300	-1.67750700	H	2.92267900	-0.35069300	-4.77045300
C	-0.47745900	-5.88721100	-0.71950900	H	3.99235100	0.52493800	-3.67639300
O	-1.58717200	-6.24967000	-0.32151200	H	3.77387700	-2.35894800	-3.74584700
N	0.65417200	-6.52154200	-0.30828300	H	5.65814900	0.81981500	-5.58508900
N	0.54483100	-3.53823100	-4.85546900	H	0.11329200	-3.87554000	-1.10957600
C	0.80013800	-2.31805100	-5.61153100	H	-1.30033500	-4.41489500	-1.99496600
Zn	-1.87321700	2.02008300	1.74874600	H	0.53720200	-7.19448700	0.43667100
Zn	0.82039300	3.32669700	-0.11976800	H	1.55215800	-6.06169300	-0.36480400
H	0.14605200	9.28776200	-2.31828900	H	0.08380700	-5.69366200	-3.58265700
H	1.89803700	9.16384600	-2.08476700	H	0.43744100	-1.44755600	-5.05596100
H	0.87560400	5.53064400	-2.62400000	H	1.87003400	-2.20506100	-5.80372800
H	0.38398700	6.12153300	1.50397400	H	-0.15505700	-4.17723700	-5.20027600
H	6.33981600	1.24822000	-2.08553600	H	-0.14704700	4.37817200	5.61676800
H	5.76475100	2.52748700	-3.15850200	H	-1.29281200	5.22548800	4.56217800
H	3.06142600	2.99230300	-2.49347300	H	-3.41248400	2.62861800	6.07407300
H	3.40912700	2.74014900	1.67423400	H	-1.99443300	2.74685600	5.00789900
H	8.74560000	-0.91575800	0.86823300	H	-4.45835500	0.00765900	5.92947000
H	8.18293200	0.02304200	-0.50568600	H	-3.42708400	-0.74087400	1.89344500
H	10.09740600	1.06836800	1.66315200	H	-4.46400800	-1.68654100	4.00594900
H	9.53298600	1.99842700	0.28059100	H	0.27491900	-2.38214400	-6.56523700
H	6.79716800	0.88762100	3.83600900	H	1.52029900	-5.50464900	-2.58813700
H	8.49381300	0.37783800	3.73728200	H	-7.16614900	-0.13994900	-3.43402900
H	7.25626000	-0.40890100	2.71042600	H	-6.59787000	-1.82376300	-3.59070200
H	10.56911600	0.22678300	-1.33745700	H	-8.32164100	-1.47156100	-3.62381100
H	7.11550400	-3.27276900	1.02495100	H	1.11359600	8.27121700	-3.39197400
H	6.95072900	-3.93004000	2.65087000	H	6.86740400	2.92146000	-1.83567700
H	4.76542600	-4.41783300	3.56491100	H	5.72399100	2.21923600	0.67612300
H	5.17713400	-3.54703200	-0.62088900	H	0.59620700	8.40269200	0.42267700
H	2.29309900	-4.35017600	3.33543900	H	-5.34533900	6.20570100	-1.52508300

H	-6.30608200	4.40853000	0.61990300	C	-1.03148300	-5.01764700	3.78636900
H	11.13065500	-0.70791100	0.05550700	C	-0.58866100	-2.27277300	3.66470300
H	10.09294600	-1.46651200	-1.15851300	C	-1.30711200	-4.33046600	2.60999800
H	8.27510100	-5.48304400	1.19614100	C	-1.08594100	-2.94542400	2.53782900
H	6.92164900	-5.59311100	0.05911200	O	-1.35918100	-2.31913100	1.36763400
H	-3.53276900	-3.27127300	-5.83320800	H	0.05693300	-2.44712200	5.70435900
H	-2.29830800	-2.81733300	-4.61109800	H	-1.20860100	-6.09059100	3.82223000
H	4.53096500	-0.00332500	-6.66655000	H	-0.40463900	-1.20414000	3.60838200
H	4.09254800	1.56027800	-5.94917800	H	-1.68501000	-4.85337100	1.73769100
H	-3.52702700	3.43875100	4.50408400	H	-1.16560700	-1.33184700	1.41405100
H	1.54390600	5.08752500	3.70386900	C	-0.34708400	2.63366900	-3.06566500
H	0.06934300	6.10834500	5.27851700	O	0.57874900	2.98275400	-2.32646900
H	0.56575900	3.40852400	-4.84122300	O	-1.48966500	2.09884300	-2.70302500
C	1.75483500	-0.34519500	0.86261600	N	-1.37893600	0.06358400	-0.98279000
H	2.74132800	-0.67355900	0.52147100	C	-0.69330400	-0.94222800	-1.66830200
H	1.88617100	0.47152300	1.57750000	O	-1.18704600	-1.70383300	-2.50944800
H	1.27533800	-1.17587500	1.37989700	N	0.60318700	-0.91908400	-1.27876500
C	-1.65785100	-5.49191600	6.89134400	C	0.90689900	0.12649200	-0.30922000
C	-0.32826900	-5.12472300	6.21516100	C	-0.52405600	0.64264600	0.10465800
H	0.23898000	-6.04403500	6.02006300	O	-0.96928000	0.25897100	1.33007100
H	0.28058900	-4.52694400	6.90367400	H	1.41672700	0.94678100	-0.82324500
H	-2.23250900	-4.59184200	7.13437100	H	-2.33172200	-0.20365600	-0.70886600
H	-2.27575900	-6.11080800	6.23306600	H	1.28069700	-1.48935400	-1.77494300
H	-1.49345400	-6.04961600	7.81974900	O	-0.63991500	2.05279000	0.03864000
C	-0.53978300	-4.36285900	4.92629000	H	-1.44295600	1.58811600	-1.83416200
C	-0.32514700	-2.98303300	4.83781700				

(5R)-MeHYD-INT2-II (*SmDHPase*)

C	0.73647300	8.65419100	-2.34214000	C	3.08818600	-4.05336100	2.46865600
C	0.57337000	7.45635700	-1.45874900	C	3.29343500	-3.60325600	0.10155300
N	0.39403100	7.56453700	-0.08795200	C	2.49280100	-3.84196200	1.22342500
C	0.57987000	6.10408700	-1.69402600	C	-0.40812900	5.16204600	4.85551600
C	0.31252000	6.32389300	0.44599200	N	0.39201100	4.92537700	3.67047600
N	0.41941300	5.40838700	-0.50528900	C	0.10015300	3.91938400	2.77346200
C	5.96339300	2.52108100	-2.09613200	O	-1.03488500	3.35712100	2.89087500
C	4.76694100	2.71533700	-1.23083200	O	0.98821400	3.70052700	1.88960400
N	4.81786700	2.64300700	0.15019300	C	-3.15194600	2.50705600	5.03453200
C	3.45552100	2.98030600	-1.52634300	C	-3.49030300	1.19868900	4.40651500
C	3.57731000	2.86181800	0.63600500	N	-3.14627500	0.92580400	3.09257300
N	2.72236300	3.06670200	-0.35708300	C	-4.10729200	0.09615100	4.93626500
C	10.31422900	-0.16713100	-0.57434700	C	-3.54251700	-0.31436700	2.83286100
C	8.97844600	0.18309400	0.09690700	N	-4.13467700	-0.84458100	3.92274200
C	9.14738100	1.25217600	1.17937700	C	-5.24334400	5.02897300	-1.82754600
S	7.61604500	1.78758500	2.05217200	C	-4.71215100	4.23998900	-0.66927600
C	7.14540800	0.26446300	2.94929800	N	-5.44101900	4.02610300	0.49284700
C	7.38380000	-5.16278900	1.13241200	C	-3.52097700	3.59225000	-0.44979000
C	6.80154100	-3.81621500	1.58842700	C	-4.69228800	3.28142000	1.34336200
C	5.29379900	-3.78455600	1.47567300	N	-3.51958100	3.00240700	0.80246500
C	4.47794700	-4.02481200	2.58946600	C	-2.99772800	-3.54030300	-4.83180400
C	4.68247400	-3.57380700	0.23255600	C	-4.14372600	-3.41398100	-3.84027000

O	-5.25121800	-3.88774000	-4.08009100	H	6.99089600	-5.98298300	1.74136300
N	-3.83672900	-2.75166200	-2.68590600	H	-6.17231800	4.60049200	-2.21964100
C	-4.66597300	-2.90246400	-1.50108100	H	-4.51066700	5.02966100	-2.63673800
C	-4.94767500	-1.52873400	-0.88539200	H	-2.68024400	3.47789900	-1.11507900
O	-4.04271700	-0.90410100	-0.29396900	H	-5.03003100	2.95494700	2.31483300
C	-3.98535200	-3.82714400	-0.47135200	H	-2.64026900	-4.57549700	-4.79044600
O	-3.80263600	-5.07925700	-1.08740200	H	-4.64291200	-3.89945100	0.41485100
N	-6.18596900	-1.00019100	-0.97144300	H	-3.04538000	-3.37033100	-0.13934700
C	-7.38255600	-1.55593600	-1.65831300	H	-2.99501300	-5.50633500	-0.74306600
C	-7.29445000	-1.40492600	-3.18003800	H	-5.57991100	-3.38981100	-1.84026200
C	-8.51882900	-0.73216700	-1.02077700	H	-2.89043300	-2.39163500	-2.55882800
C	-7.88577200	0.64954400	-0.79245500	H	-8.80643500	-1.17590400	-0.06093000
C	-6.44923700	0.31774300	-0.36534700	H	-9.40760800	-0.70210200	-1.65555800
C	-0.30726300	2.76532000	-4.53593000	H	-8.41544100	1.24133400	-0.04058800
C	4.61427600	0.78871700	-5.74120600	H	-7.88356800	1.22419900	-1.72450800
C	3.96947600	0.04121000	-4.57769800	H	-6.35124200	0.24030000	0.72487000
S	4.85099600	-1.55565800	-4.27285400	H	-5.70612700	1.04516100	-0.70318100
C	0.72954400	-4.98043200	-2.91429000	H	-7.48944300	-2.61404100	-1.40448800
C	1.13973900	-3.68583100	-3.60706300	H	-0.08260400	1.79321600	-4.98885500
O	1.89271500	-2.86994800	-3.04955100	H	-1.25826700	3.09424800	-4.96225100
C	-0.17180000	-4.72551000	-1.68694600	H	2.92422300	-0.18622100	-4.79779600
C	-0.30022900	-5.90398300	-0.72968400	H	3.99320100	0.64254500	-3.66428700
O	-1.39382900	-6.30540000	-0.32505100	H	3.81433700	-2.18239200	-3.67294200
N	0.85585900	-6.49634400	-0.32392900	H	5.67203600	0.99518400	-5.54706400
N	0.67694800	-3.49315100	-4.85832500	H	0.21489900	-3.87360600	-1.11693800
C	0.91669600	-2.26250200	-5.60425200	H	-1.18276900	-4.46183300	-1.99830300
Zn	-1.93602600	1.96862300	1.76102700	H	0.76832100	-7.17486300	0.41992800
Zn	0.71904500	3.36980700	-0.13098800	H	1.73787100	-6.00798500	-0.38987700
H	-0.13528100	9.31631200	-2.29521900	H	0.23056500	-5.66556400	-3.60775300
H	1.62010700	9.24033500	-2.06640700	H	0.52456600	-1.40413200	-5.05022300
H	0.70110500	5.57994500	-2.62860400	H	1.98692200	-2.12441500	-5.77760200
H	0.20066500	6.13555400	1.50339800	H	0.01073500	-4.15425300	-5.22718900
H	6.33540700	1.49125400	-2.05039000	H	-0.27685500	4.38904200	5.62416400
H	5.70905400	2.73496600	-3.13637000	H	-1.46229900	5.19268500	4.57945100
H	2.98344300	3.10274200	-2.48755500	H	-3.49602200	2.53690900	6.07183700
H	3.31687800	2.87110000	1.68221700	H	-2.07505700	2.68031800	5.01219100
H	8.54435000	-0.72307400	0.53548100	H	-4.50691700	-0.10039800	5.91812100
H	8.26345400	0.53801200	-0.65441000	H	-3.41555100	-0.83489800	1.89445300
H	9.85792300	0.92435800	1.94605300	H	-4.46551300	-1.79519200	3.99634000
H	9.54721400	2.17704400	0.75016400	H	0.40813000	-2.33389700	-6.56636100
H	6.30807200	0.52744600	3.59885500	H	1.66405400	-5.46356100	-2.61246800
H	7.97616800	-0.07611500	3.57178600	H	-7.11189900	-0.36331100	-3.46425400
H	6.83184500	-0.53192100	2.27251000	H	-6.50960400	-2.03670500	-3.59916800
H	10.76162400	0.71032500	-1.05361700	H	-8.24033700	-1.72046500	-3.63350800
H	7.23550900	-3.01389300	0.97697700	H	0.85823800	8.33727000	-3.37974100
H	7.10141900	-3.62168800	2.62495500	H	6.78338800	3.18806400	-1.80868800
H	4.93866400	-4.19103100	3.56062500	H	5.65043100	2.41505700	0.69933900
H	5.30001900	-3.38017300	-0.64198500	H	0.34375300	8.42751200	0.43364100
H	2.46495000	-4.22744300	3.34069400	H	-5.44326400	6.07095700	-1.55297800
H	2.84372000	-3.42196900	-0.87153300	H	-6.37542100	4.36203000	0.67538600
H	1.41114400	-3.84177600	1.14143200	H	11.03611300	-0.55344000	0.15304000

H	10.17391700	-0.93221800	-1.34337900	C	-0.52964900	-2.28588000	3.64347600
H	8.47564800	-5.17169200	1.21596500	C	-1.14394900	-4.38173600	2.59854800
H	7.12308500	-5.36935200	0.08975600	C	-0.98640200	-2.98853100	2.51768100
H	-3.37736400	-3.36332100	-5.84059000	O	-1.27632700	-2.38305500	1.34010900
H	-2.17034200	-2.86302100	-4.60977300	H	0.10789800	-2.41582000	5.68889100
H	4.55408600	0.20763700	-6.66539600	H	-0.97314300	-6.12696200	3.82434700
H	4.11100100	1.74825400	-5.90583600	H	-0.39582700	-1.21018000	3.58114000
H	-3.61705600	3.34361900	4.50105800	H	-1.49455100	-4.92726200	1.72871500
H	1.37070100	5.17283600	3.70028500	H	-1.15038700	-1.38511600	1.39070900
H	-0.13046500	6.12693500	5.28729500	C	-0.42594000	2.58008900	-3.06336700
H	0.48762100	3.46653100	-4.79275700	O	0.47648900	2.95773900	-2.30215500
C	1.75281100	-0.27419200	0.90171500	O	-1.53433100	1.97004600	-2.74048300
H	2.75180800	-0.57626900	0.57277700	N	-1.36792400	0.08230800	-1.02050600
H	1.85391900	0.55164700	1.61094200	C	-0.64558700	-0.94435200	-1.66785000
H	1.29115400	-1.11413800	1.42012400	O	-1.11456100	-1.71729800	-2.50836600
C	-1.46800600	-5.52758000	6.88932500	N	0.63303400	-0.89920400	-1.24087100
C	-0.15338000	-5.10498100	6.21605400	C	0.90406800	0.16624500	-0.28116100
H	0.45612300	-5.99888600	6.03055800	C	-0.54044100	0.65309700	0.11585500
H	0.42417600	-4.47509400	6.90292100	O	-1.01024400	0.21047600	1.30926400
H	-2.08430900	-4.65298500	7.12310600	H	1.39876600	0.99039000	-0.80339200
H	-2.05402800	-6.17885500	6.23310200	H	-2.30928000	-0.22685400	-0.74038300
H	-1.28241700	-6.07036300	7.82252700	H	1.32676700	-1.47953000	-1.70366300
C	-0.39215400	-4.36281700	4.92033000	O	-0.68211800	2.04890900	0.09701700
C	-0.24200000	-2.97506500	4.82349100	H	-1.48107000	1.31496600	-1.91973000
C	-0.84493700	-5.04731700	3.78173800				

(5R)-MeHYD-TS3-II (SmDHPase)

C	0.54926300	8.67531400	-2.30145000	C	3.38410800	-3.54165000	0.09028400
C	0.40370800	7.48098500	-1.41550900	C	2.58881200	-3.80197000	1.21114100
N	0.22971400	7.58613600	-0.04382400	C	-0.52413200	5.13120200	4.88176400
C	0.42770600	6.13083100	-1.65425100	N	0.26952400	4.92314700	3.68561600
C	0.16891200	6.34320100	0.48833900	C	0.00734000	3.90549900	2.78924500
N	0.28405800	5.43297700	-0.46623700	O	-1.10181200	3.29470000	2.92978300
C	5.91983800	2.66709500	-2.06804300	O	0.88580200	3.72400300	1.89043300
C	4.70841600	2.82625600	-1.21398500	C	-3.20446500	2.41123700	5.04656000
N	4.74895600	2.74630400	0.16739900	C	-3.51670300	1.09902900	4.41234100
C	3.39339400	3.06541300	-1.51838800	N	-3.14770000	0.82947100	3.10468500
C	3.49960000	2.93681900	0.64422800	C	-4.13019900	-0.01054600	4.93163500
N	2.64884900	3.12981200	-0.35436600	C	-3.52697800	-0.41400000	2.83778400
C	10.33070100	0.07742000	-0.54818800	N	-4.13101200	-0.95132200	3.91779100
C	8.95886200	0.41864700	0.05039700	C	-5.34369100	4.90742400	-1.81018200
C	9.07388200	1.33494900	1.27097500	C	-4.79100000	4.14845400	-0.64189600
S	7.48760000	1.79043400	2.09334900	N	-5.47814300	4.01051100	0.55666900
C	6.98176100	0.20080600	2.86942800	C	-3.61313300	3.46937000	-0.44404000
C	7.51681000	-4.99244500	1.13571300	C	-4.72032000	3.27692400	1.40828600
C	6.89500200	-3.66017400	1.58115000	N	-3.58094000	2.93353400	0.83328600
C	5.38721800	-3.67037600	1.46624600	C	-2.89034800	-3.59533400	-4.84087300
C	4.57671400	-3.93283200	2.57913400	C	-4.04304400	-3.50988600	-3.85298200
C	4.77179100	-3.47529200	0.22259600	O	-5.13654100	-4.01167500	-4.09680400
C	3.18834300	-3.99832300	2.45690800	N	-3.75437900	-2.84744800	-2.69430400

C	-4.58922600	-2.99513000	-1.51419800	H	-4.64902500	4.84170500	-2.64962800
C	-4.87321400	-1.61407700	-0.91723600	H	-2.80607000	3.29571300	-1.14030200
O	-3.96250200	-0.97626400	-0.34581400	H	-5.02929800	3.00886400	2.40689100
C	-3.91331200	-3.91063500	-0.47303600	H	-2.49468700	-4.61658500	-4.79943400
O	-3.72803900	-5.16847000	-1.07545600	H	-4.57527700	-3.97507700	0.41048300
N	-6.11267700	-1.09316700	-1.00183400	H	-2.97517900	-3.45086100	-0.14012100
C	-7.31295700	-1.67448100	-1.66252700	H	-2.90421700	-5.57760200	-0.74900900
C	-7.23928100	-1.56843400	-3.18906800	H	-5.49942200	-3.48789600	-1.85502700
C	-8.44807900	-0.83774300	-1.03965200	H	-2.82453800	-2.45155500	-2.57139800
C	-7.81907700	0.55172200	-0.85057800	H	-8.72907300	-1.25755100	-0.06714100
C	-6.37948200	0.23700000	-0.42238200	H	-9.34036700	-0.82741700	-1.67008000
C	-0.35077800	2.77123900	-4.51792600	H	-8.34668800	1.16081200	-0.11136900
C	4.61828400	0.91629600	-5.72159400	H	-7.82378400	1.10250100	-1.79686600
C	3.97708900	0.14994400	-4.56860100	H	-6.27645100	0.18296700	0.66859900
S	4.86783900	-1.44652300	-4.28816800	H	-5.64169600	0.96037100	-0.77936100
C	0.83191500	-4.95382600	-2.92263700	H	-7.41197700	-2.72496900	-1.37568900
C	1.21627900	-3.64543600	-3.60328400	H	-0.16369000	1.77591700	-4.93618100
O	1.93162600	-2.80864400	-3.02590000	H	-1.27877200	3.12861000	-4.97165900
C	-0.08336200	-4.72629100	-1.70037300	H	2.93271900	-0.07811400	-4.79242200
C	-0.19117400	-5.91298100	-0.75005000	H	3.99897500	0.73814100	-3.64676300
O	-1.27791900	-6.34130100	-0.35564200	H	3.84656700	-2.07934700	-3.66908800
N	0.97550600	-6.48037200	-0.34009900	H	5.67451500	1.12695400	-5.52383500
N	0.77164800	-3.45984300	-4.86093700	H	0.27924000	-3.86989000	-1.12091100
C	0.99393100	-2.22226200	-5.60193200	H	-1.09876800	-4.48613500	-2.01743300
Zn	-1.98120700	1.91471200	1.77790800	H	0.89974400	-7.16805300	0.39658200
Zn	0.62747600	3.40354900	-0.16499100	H	1.84810600	-5.97483700	-0.40070600
H	-0.32819500	9.33002200	-2.25281000	H	0.35343500	-5.64589900	-3.62347300
H	1.42856600	9.27208900	-2.03408700	H	0.57799000	-1.37390200	-5.05060100
H	0.55053100	5.60713800	-2.58875000	H	2.06271200	-2.06121400	-5.76417700
H	0.06339500	6.14929700	1.54534600	H	0.14563600	-4.14687600	-5.25213000
H	6.32328600	1.64961500	-2.01557600	H	-0.36224000	4.35887300	5.64533700
H	5.66895000	2.87109200	-3.11110600	H	-1.58201400	5.13334100	4.61809900
H	2.92392700	3.18635000	-2.48129300	H	-3.55970700	2.43291200	6.08028600
H	3.23062500	2.93685500	1.68843900	H	-2.13035300	2.60116000	5.03452200
H	8.44216800	-0.50762000	0.32970100	H	-4.54377400	-0.21169600	5.90676400
H	8.33106900	0.90462400	-0.70518300	H	-3.37806200	-0.93068900	1.90069900
H	9.72312300	0.89736300	2.03641300	H	-4.45488500	-1.90471000	3.98573000
H	9.51619100	2.29740600	0.99322500	H	0.49619600	-2.30207300	-6.56893100
H	7.00429400	0.30185700	3.95555100	H	1.77486400	-5.41759000	-2.61667000
H	7.67074200	-0.59012500	2.56984600	H	-7.06807300	-0.53421800	-3.50535600
H	5.97720400	-0.07574800	2.54591000	H	-6.45338500	-2.20487800	-3.59913000
H	10.86184300	0.98005800	-0.86879100	H	-8.18715800	-1.90411200	-3.62338600
H	7.30614200	-2.84969400	0.96509200	H	0.66790300	8.35579300	-3.33865000
H	7.18699200	-3.45059400	2.61717500	H	6.71540500	3.36032300	-1.77402900
H	5.04051000	-4.08739600	3.55071800	H	5.58024600	2.52593900	0.72096800
H	5.38493600	-3.26488600	-0.65110800	H	0.16928900	8.44777100	0.47871900
H	2.56920400	-4.18956800	3.32825700	H	-5.48950800	5.96784600	-1.57478800
H	2.93071600	-3.37202100	-0.88323800	H	-6.39086500	4.38963300	0.76257100
H	1.50758700	-3.83060600	1.12827800	H	10.96516000	-0.44108100	0.17856800
H	7.14679000	-5.81960600	1.74950100	H	10.22225700	-0.57355100	-1.42048400
H	-6.30608100	4.50112600	-2.14057800	H	8.60820700	-4.96878600	1.22149700

H	7.26468200	-5.21373100	0.09395400	C	-1.02875400	-4.44616300	2.58161500
H	-3.27450700	-3.43289000	-5.85035800	C	-0.90772600	-3.05055700	2.48551800
H	-2.08888500	-2.88782600	-4.61960900	O	-1.19789200	-2.46617900	1.29562800
H	4.56203100	0.34732900	-6.65355600	H	0.14152500	-2.41068000	5.65862300
H	4.10853100	1.87429600	-5.87360100	H	-0.81888200	-6.17185000	3.82872800
H	-3.67622400	3.24265800	4.51104500	H	-0.37967500	-1.24388300	3.53389000
H	1.23851500	5.20724900	3.70434500	H	-1.36069300	-5.01075300	1.71663100
H	-0.26884700	6.10179700	5.31454200	H	-1.12024300	-1.46380400	1.34423000
H	0.47833800	3.42832800	-4.78569200	C	-0.51315600	2.63922800	-3.03490000
C	1.73968600	-0.24895100	0.90023800	O	0.40446000	3.04492900	-2.28263400
H	2.74770300	-0.52406300	0.57541300	O	-1.61289600	2.06940300	-2.68780800
H	1.81634700	0.57265300	1.61703400	N	-1.36918200	0.11195000	-1.05732800
H	1.29281700	-1.10433000	1.40597800	C	-0.61486000	-0.92334800	-1.71615100
C	-1.33342200	-5.58778600	6.87579500	O	-1.07843800	-1.67680400	-2.56866900
C	-0.03571400	-5.10171500	6.21247000	N	0.64215300	-0.87385600	-1.25421400
H	0.62076700	-5.96442200	6.03950800	C	0.89098900	0.18883600	-0.28234400
H	0.50161300	-4.43911000	6.90108800	C	-0.56327300	0.64741800	0.11128100
H	-1.99611700	-4.74507600	7.09952300	O	-1.05188200	0.13980600	1.26663300
H	-1.87931900	-6.27190000	6.21842800	H	1.37499300	1.02231900	-0.79883100
H	-1.12835800	-6.11552300	7.81343700	H	-2.30052500	-0.24104500	-0.77503900
C	-0.29506800	-4.38008600	4.90868600	H	1.34444200	-1.46702600	-1.69126900
C	-0.18504300	-2.98969700	4.79720100	O	-0.71608000	2.02777100	0.14768700
C	-0.72028600	-5.08964400	3.77476100	H	-1.51863500	1.14479500	-1.84970200
C	-0.48224700	-2.32232200	3.60690300				

(5R)-MeHYD-EP-II (*SmDHPase*)

C	1.91235300	8.47573100	-2.49470000	C	2.12255600	-3.83200300	1.27035900
C	1.53619200	7.41036100	-1.53798100	C	0.31389600	5.33814600	4.77935900
N	1.32938500	7.61565000	-0.18301900	N	1.05732300	4.99094300	3.57928900
C	1.36462700	6.06954300	-1.72104000	C	0.64367600	4.01055700	2.70191800
C	1.06274100	6.42274900	0.39975100	O	-0.54550700	3.56792100	2.88493900
N	1.07527300	5.46581000	-0.51393400	O	1.45152200	3.67591000	1.78976300
C	6.27272200	1.70665300	-2.09094200	C	-2.76009800	3.07857500	5.01271600
C	5.12994000	2.12895900	-1.23705600	C	-3.28733900	1.85404300	4.32713100
N	5.17675600	2.14243700	0.14607600	N	-2.88162100	1.48098900	3.04892300
C	3.86994100	2.55737500	-1.55787000	C	-4.19026100	0.92404700	4.77343800
C	3.98153800	2.56777600	0.61044600	C	-3.52836200	0.36168900	2.73519900
N	3.16171600	2.82350600	-0.40088000	N	-4.32743200	-0.00053400	3.75457400
C	10.22577500	-1.50230300	-0.49467500	C	-4.49816200	5.69522500	-1.91219600
C	8.94198300	-0.93455000	0.12794800	C	-4.11228900	4.88768400	-0.71855400
C	9.24181700	0.06938400	1.24388700	N	-4.91516700	4.73066700	0.40320900
S	7.78412200	0.82857300	2.07678300	C	-2.98688800	4.15480400	-0.45238800
C	7.02296100	-0.62009000	2.89477800	C	-4.27555300	3.92889600	1.28511100
C	6.65455200	-6.02001900	1.32016200	N	-3.09998500	3.56348300	0.79360600
C	6.35653200	-4.56741800	1.71958800	C	-3.41914700	-3.16555400	-4.70918800
C	4.88560500	-4.24933800	1.57956600	C	-4.60270300	-3.02579500	-3.75393400
C	4.02912600	-4.27052600	2.68845300	O	-5.73602500	-3.38065200	-4.05841100
C	4.33624200	-4.00765800	0.31315100	N	-4.29217900	-2.48924300	-2.52245100
C	2.65722300	-4.06254400	2.53950700	C	-5.08458600	-2.86776200	-1.35285600
C	2.96569800	-3.80338400	0.15399700	C	-5.51498500	-1.65899300	-0.50216200

O	-4.83982200	-1.29054100	0.47270800	H	-4.68489500	3.63257100	2.23861600
C	-4.30392100	-3.86185500	-0.47880300	H	-2.95644100	-4.13871100	-4.50927700
O	-3.98172600	-4.96889300	-1.29536300	H	-4.93989200	-4.14930300	0.37481400
N	-6.68184000	-1.02651200	-0.79607400	H	-3.41462200	-3.36664600	-0.06762900
C	-7.65662700	-1.29821000	-1.87905300	H	-3.32379400	-5.52440300	-0.83200800
C	-7.39130300	-0.43690000	-3.11971800	H	-5.96206500	-3.38285200	-1.74831600
C	-8.98705500	-0.95547300	-1.18504100	H	-3.29727500	-2.33362800	-2.36175300
C	-8.63245900	0.26383400	-0.31368200	H	-9.30091200	-1.79438200	-0.55439000
C	-7.18429800	-0.00718900	0.14044900	H	-9.78996100	-0.75285100	-1.89862500
C	0.09008300	2.72918800	-4.55321600	H	-9.31024500	0.38841900	0.53496000
C	4.70283400	0.08484900	-5.69829200	H	-8.68403500	1.18236100	-0.90693100
C	3.94089100	-0.41901800	-4.47654200	H	-7.12977600	-0.40959000	1.15806700
S	4.64489600	-2.02453100	-3.88220500	H	-6.55543100	0.89047400	0.12233500
C	0.30771400	-5.11333500	-2.78077900	H	-7.60608500	-2.34731400	-2.17294800
C	0.75600300	-3.83632000	-3.47873900	H	-0.16804600	1.67464400	-4.70151000
O	1.49071000	-3.01527200	-2.90075400	H	-0.64903700	3.32043100	-5.09836800
C	-0.57973100	-4.81370000	-1.55454200	H	2.88887300	-0.58419000	-4.71701900
C	-0.72626300	-5.97240000	-0.57740900	H	3.98287100	0.30883000	-3.66177000
O	-1.82671000	-6.37424500	-0.18849700	H	3.49178100	-2.51096800	-3.37073300
N	0.42397800	-6.54899100	-0.13355000	H	5.76727900	0.22036200	-5.47917700
N	0.35384800	-3.66144800	-4.75160200	H	-0.16918700	-3.96290500	-1.00116800
C	0.63066000	-2.44082500	-5.50038300	H	-1.58419500	-4.52908600	-1.86760000
Zn	-1.68212900	2.45858800	1.74869800	H	0.32582900	-7.22041900	0.61515500
Zn	1.23247300	3.45641000	-0.36885200	H	1.30522900	-6.05821800	-0.19344000
H	1.16389300	9.27533700	-2.54465500	H	-0.21671700	-5.78542500	-3.46817000
H	2.87237900	8.93792100	-2.23661300	H	0.22970900	-1.57267300	-4.96995200
H	1.45110400	5.48522700	-2.62210700	H	1.70717500	-2.31661900	-5.64099700
H	0.89373200	6.29274300	1.45821300	H	-0.31515100	-4.31344800	-5.13182100
H	6.46286600	0.63022300	-2.01224800	H	0.35967600	4.55900900	5.55112500
H	6.05284300	1.92714100	-3.13757300	H	-0.73247100	5.50556300	4.52358700
H	3.40999400	2.69000300	-2.52338600	H	-3.19445100	3.16698000	6.01159600
H	3.72854300	2.68489200	1.65209700	H	-1.67310700	3.03984200	5.09913500
H	8.33675600	-1.75773400	0.52489500	H	-4.72370100	0.83890700	5.70653800
H	8.33458600	-0.44718500	-0.64339000	H	-3.46880200	-0.19433500	1.80955500
H	9.85831800	-0.38642600	2.02661000	H	-4.90483700	-0.82894800	3.75156200
H	9.80307800	0.92546400	0.85490400	H	0.15435400	-2.51723500	-6.47851000
H	6.22976400	-0.23625800	3.53963000	H	1.22621600	-5.62652200	-2.47755600
H	7.76167100	-1.12943300	3.51814500	H	-7.43911200	0.63242900	-2.88792500
H	6.58925100	-1.31998800	2.17871600	H	-6.40592700	-0.66224300	-3.53190000
H	10.84267900	-0.70868200	-0.92988400	H	-8.13572200	-0.65572400	-3.89142300
H	6.94718800	-3.89357100	1.08523200	H	2.00877600	8.05170200	-3.49603900
H	6.68089000	-4.39626000	2.75266700	H	7.19511800	2.23392700	-1.82484800
H	4.44284300	-4.45844600	3.67669100	H	5.96779400	1.82422600	0.71081900
H	4.98864300	-3.97778700	-0.55681200	H	1.37727000	8.50321300	0.29567300
H	2.00304100	-4.07696000	3.40619300	H	-4.61769900	6.75767600	-1.67033700
H	2.55897400	-3.60506000	-0.83460200	H	-5.83115700	5.13328200	0.53847000
H	1.05847000	-3.65650900	1.15658400	H	10.83333900	-2.02457400	0.25195100
H	6.09895700	-6.71926100	1.95286000	H	9.98891400	-2.21491700	-1.28993800
H	-5.43702700	5.34532600	-2.35595500	H	7.72099500	-6.24893300	1.41756800
H	-3.71762300	5.60549200	-2.66990000	H	6.36222900	-6.20747500	0.28239400
H	-2.13861700	3.96437500	-1.09671600	H	-3.79318300	-3.16439900	-5.73444400

H	-2.66675400	-2.39343900	-4.55444500	C	-1.18760500	-2.93378900	2.48582400
H	4.62360100	-0.61933600	-6.53080600	O	-1.26916700	-2.49259300	1.19685000
H	4.30317400	1.05145400	-6.02507600	H	-0.42259300	-1.99903000	5.66312000
H	-3.00361400	3.98859400	4.45415500	H	-1.51062800	-5.86899100	4.16021700
H	2.05426800	5.15159800	3.57394800	H	-0.61870400	-1.05686100	3.38224700
H	0.72536800	6.26080500	5.19563600	H	-1.74154800	-4.92551600	1.88806900
H	1.08882200	2.90506300	-4.95690700	H	-1.15297000	-1.52251800	1.14289700
C	1.85478200	-0.37444200	0.12827400	C	0.00399000	3.04332200	-3.06534400
H	2.59853600	-0.83389700	-0.52773600	O	1.11241400	3.16476500	-2.42000800
H	2.35072700	0.39801300	0.71774200	O	-1.13150700	3.12225100	-2.55671400
H	1.46606200	-1.14046700	0.80045000	N	-1.87172400	0.31957300	-2.10092000
C	-2.16448500	-5.06315100	7.05937700	C	-1.10853600	-0.81584100	-2.13054000
C	-0.82015700	-4.59702000	6.47930500	O	-1.49206100	-1.84562200	-2.71374800
H	-0.12907800	-5.45008800	6.45771800	N	0.07412900	-0.84468800	-1.44689300
H	-0.36972300	-3.85691700	7.15107100	C	0.71524900	0.22316500	-0.71070700
H	-2.86813000	-4.22766600	7.13692100	C	-0.26113300	0.93168600	0.22558600
H	-2.62721200	-5.82601600	6.42556200	O	-0.99439600	0.33771500	1.04289800
H	-2.03565200	-5.49211300	8.05859400	H	1.12073000	0.98871600	-1.38257500
C	-0.94254500	-4.00671900	5.09033300	H	-2.72641500	0.22982100	-2.63107300
C	-0.71032000	-2.65042800	4.84068600	H	0.64128100	-1.65101300	-1.69936200
C	-1.31677600	-4.81070800	4.00135000	O	-0.28854600	2.22274500	0.19146600
C	-0.82457900	-2.10893400	3.55673200	H	-1.49227600	1.26477100	-2.06744300
C	-1.44593900	-4.29229600	2.71827400				

(5S)-MeDHU-ES-II (*Sm*DHPase)

C	1.32515300	8.66622900	-2.41399200	C	-0.16554200	5.40860300	4.83012000
C	1.13730500	7.56851200	-1.42836300	N	0.66866100	5.05365700	3.69472300
N	0.99882400	7.76864100	-0.06248600	C	0.35066900	4.01157500	2.84184300
C	1.07626700	6.21254200	-1.58965900	O	-0.82043000	3.51546900	2.97840400
C	0.87028100	6.56114800	0.54160000	O	1.22691100	3.67485200	1.99532400
N	0.91216700	5.59868000	-0.36341800	C	-1.92150300	-5.07256400	7.10283900
C	6.12203600	2.20259800	-1.95841100	C	-0.74326800	-5.41119700	6.17837700
C	4.94859100	2.47141800	-1.08438400	C	-0.90801700	-4.68787100	4.86530800
N	4.96840200	2.31136100	0.29144000	C	-1.43729100	-5.32411700	3.73550200
C	3.67638100	2.88303600	-1.37583100	C	-0.68424200	-3.30728100	4.80180500
C	3.74323200	2.62382300	0.77656700	C	-1.76007400	-4.61074500	2.58223600
N	2.93402500	2.96770600	-0.21352800	C	-1.00860700	-2.57386900	3.66656300
C	10.25717500	-0.73943500	-0.31001800	C	-1.55982400	-3.22798900	2.55837400
C	10.20715600	0.77922600	-0.11975100	O	-1.91962600	-2.54503000	1.43327000
C	9.75258300	1.26213800	1.26251200	C	-3.08464100	2.94800900	5.01420400
S	7.99427500	0.94483600	1.72637200	C	-3.54370200	1.74469300	4.25444500
C	8.06643500	-0.69070300	2.53984700	N	-3.10454300	1.42568500	2.97218800
C	6.97000300	-5.49075400	1.44398600	C	-4.43711600	0.78682300	4.65928000
C	6.06850900	-4.34057400	1.91908400	C	-3.73172900	0.31058500	2.61807700
C	4.60681900	-4.60541900	1.63415900	N	-4.54553600	-0.10542100	3.61123400
C	3.73426400	-5.03277900	2.64322200	C	-4.89289300	5.46191300	-1.93077300
C	4.10554700	-4.46986000	0.33279700	C	-4.44468300	4.72472600	-0.72022300
C	2.39859200	-5.32158900	2.36130700	N	-5.14402700	4.69967700	0.47751900
C	2.77345400	-4.76185400	0.04022500	C	-3.33325800	3.95856700	-0.49787100
C	1.91632000	-5.19150100	1.05793700	C	-4.45039500	3.93695600	1.35885300

N	-3.34838100	3.47315600	0.79608700	H	6.37773300	-3.41279300	1.42046100
C	-3.18326800	-3.29913000	-4.72758700	H	6.21258200	-4.18290400	2.99443700
C	-4.32443100	-3.18034200	-3.73428200	H	4.10528900	-5.13692800	3.66016100
O	-5.48083300	-3.44254600	-4.05488400	H	4.76509200	-4.12747600	-0.46154900
N	-3.95570800	-2.78498300	-2.48069400	H	1.72837000	-5.63296900	3.15681800
C	-4.93715300	-2.61471100	-1.42189900	H	2.41515200	-4.61786500	-0.97560300
C	-4.94186000	-1.15406100	-0.96775100	H	0.87279300	-5.40933600	0.85252800
O	-3.91181700	-0.65370600	-0.46102100	H	6.70482100	-6.42655800	1.94576500
C	-4.65715500	-3.53924500	-0.21111700	H	-0.69669200	-6.49391700	6.01576200
O	-4.81350600	-4.89410500	-0.54313800	H	0.19807600	-5.12357700	6.66311600
N	-6.06720100	-0.42325000	-1.07660500	H	-1.62641400	-6.39454100	3.76640500
C	-7.37673000	-0.83088900	-1.65970400	H	-0.27126200	-2.79267300	5.66652900
C	-7.35167400	-0.84646900	-3.19173700	H	-2.18758600	-5.10285600	1.71353600
C	-8.32301300	0.23678200	-1.07520200	H	-0.84828800	-1.49982700	3.63212700
C	-7.45412600	1.50326000	-1.01721400	H	-1.78514100	-1.59131400	1.58221200
C	-6.07773100	0.97217300	-0.59595700	H	-2.87035200	-5.36813600	6.64391100
C	0.07859600	2.96491800	-4.48116300	H	-5.87896400	5.12972300	-2.27589800
C	-0.10502400	2.92707600	-2.96674900	H	-4.18283200	5.28943500	-2.74173100
O	0.90746600	3.30596500	-2.27266000	H	-2.54965200	3.70317600	-1.19647100
O	-1.20777800	2.55264700	-2.50661300	H	-4.77756400	3.73908300	2.36793500
C	4.71672500	0.48953600	-5.59136000	H	-3.00545900	-4.36413000	-4.91706600
C	3.92274200	0.14518900	-4.33325900	H	-5.39659800	-3.29954600	0.56795900
S	4.65129500	-1.24658600	-3.34620600	H	-3.66790000	-3.30863300	0.19650600
C	0.28993000	-5.38524000	-3.27522900	H	-3.96019500	-5.24966700	-0.84619000
C	0.92411800	-4.10570300	-3.80582700	H	-5.88971200	-2.91546900	-1.85462900
O	1.83696300	-3.53910200	-3.18422900	H	-3.00123000	-2.46480700	-2.32679300
C	-0.55484300	-5.07504900	-2.02044400	H	-8.63325500	-0.05225000	-0.06446400
C	-1.17608400	-6.27649600	-1.32007300	H	-9.22468400	0.35651300	-1.68036300
O	-2.35053200	-6.28371700	-0.95623500	H	-7.83799500	2.25249300	-0.31936600
N	-0.36176500	-7.34411800	-1.09626000	H	-7.39667100	1.97057700	-2.00549600
N	0.43781000	-3.61933700	-4.96578900	H	-5.95469000	0.98116900	0.49410200
C	0.82009600	-2.30317400	-5.45787600	H	-5.23696300	1.52688400	-1.01945800
Zn	-1.76933600	2.38434500	1.66142100	H	-7.64464900	-1.82391700	-1.28864400
Zn	0.96932200	3.55551700	-0.15431200	H	-0.73133000	2.43388600	-4.98279300
O	-0.61551700	2.47875500	0.11084500	H	0.08222200	4.00625800	-4.82279300
H	0.48410400	9.36950600	-2.41556800	H	2.88958100	-0.11751300	-4.57141000
H	2.23780900	9.24152300	-2.21936300	H	3.87984200	0.99912200	-3.65345000
H	1.14767900	5.62187200	-2.48860100	H	3.75915700	-2.20391400	-3.67607300
H	0.75495500	6.42243700	1.60731800	H	5.75105800	0.74924900	-5.34762400
H	6.40851900	1.14522700	-1.93927300	H	0.06931100	-4.54328300	-1.29380400
H	5.88324300	2.47047800	-2.98973900	H	-1.37488900	-4.40365000	-2.27193200
H	3.22288700	3.11159300	-2.32668400	H	-0.73373100	-8.09916900	-0.53805100
H	3.46796600	2.60652800	1.81926300	H	0.63900400	-7.28158600	-1.19890700
H	9.56169100	1.22699200	-0.88482400	H	-0.32714400	-5.87367500	-4.03673300
H	11.21040900	1.19625600	-0.28332300	H	0.43589000	-1.51628400	-4.80151400
H	10.37362800	0.83579200	2.05788400	H	1.90819400	-2.23159900	-5.51527000
H	9.85507500	2.34942100	1.32873000	H	-0.37968100	-4.05681600	-5.36335800
H	7.06366700	-0.89520200	2.92070300	H	-0.13940500	4.66137000	5.63437700
H	8.76243500	-0.66393100	3.38151000	H	-1.19890600	5.51731200	4.50022200
H	8.35087400	-1.48090100	1.84429300	H	-3.53384000	2.95537000	6.01045600
H	10.87497400	-1.21840100	0.45791600	H	-1.99775600	2.95982200	5.10804800

H	-4.98136200	0.66473400	5.58200800	H	4.26193900	1.34575400	-6.10352200
H	-3.64652500	-0.19105800	1.66420900	H	-3.36430400	3.87779000	4.50707600
H	-5.09169200	-0.95400100	3.59856900	H	1.66009800	5.23486200	3.76115700
H	0.40817400	-2.16874500	-6.45917900	H	0.17565100	6.36409300	5.23683500
H	1.11448600	-6.06550200	-3.03957700	H	1.04403300	2.53292300	-4.75907500
H	-7.04878700	0.12750300	-3.59033100	N	-1.02170300	-0.55829300	-0.69709200
H	-6.67962400	-1.61406400	-3.57999100	C	-0.39598400	-1.23940300	-1.75806000
H	-8.35563300	-1.06962100	-3.56860500	O	-1.07592900	-1.92217800	-2.53160400
H	1.40694400	8.24583700	-3.41822200	N	0.93961800	-1.10402200	-1.81856300
H	6.99754100	2.78895800	-1.65745100	C	1.65092100	-0.13190900	-0.99065000
H	5.76653000	1.98490600	0.82777500	C	1.11784600	-0.15650700	0.44641600
H	0.99942100	8.66154500	0.40811400	C	-0.39538700	-0.13713000	0.43328200
H	-4.94992300	6.54328100	-1.75841000	O	-1.07052400	0.14052500	1.44664800
H	-6.01521700	5.17305700	0.66716400	H	2.71262400	-0.38351600	-1.02011900
H	9.25667100	-1.18125600	-0.26917700	H	1.41619700	0.76350400	0.95446600
H	10.68558900	-0.99183100	-1.28445700	H	-2.04900600	-0.62055300	-0.68089400
H	8.02434300	-5.28101100	1.65349300	H	1.43276500	-1.77094400	-2.40876000
H	6.86540400	-5.65196300	0.36654000	C	1.62035500	-1.36639200	1.25667400
H	-1.83803600	-5.58521900	8.06771100	H	2.71201200	-1.33967100	1.31765700
H	-1.96822600	-3.99636400	7.29690200	H	1.21896800	-1.35597300	2.27141100
H	-3.50218100	-2.85254400	-5.67247000	H	1.34008700	-2.31265300	0.78962000
H	-2.26558600	-2.82535400	-4.37709900	H	1.52949400	0.86962300	-1.41484400
H	4.74339200	-0.35250500	-6.28866700	H	-0.99202900	2.38983500	-0.79627400

(5S)-MeDHU-TS1-II (*SmDHPase*)

C	0.70009800	8.72432500	-2.33689500	C	-0.51003100	5.26996500	4.86827000
C	0.52009700	7.57990900	-1.40315600	N	0.28614600	4.97728000	3.68280800
N	0.31339200	7.72391700	-0.03917300	C	-0.00749900	3.97679300	2.77579100
C	0.54338100	6.22859300	-1.61020700	O	-1.15733600	3.42984700	2.87091600
C	0.23122500	6.49314400	0.52087000	O	0.87821300	3.72691500	1.90187900
N	0.36602400	5.56319700	-0.41089600	C	-3.22613400	2.58532100	5.02651400
C	5.99152100	2.65281700	-1.97107300	C	-3.62518200	1.32398300	4.33557700
C	4.79716900	2.87243400	-1.11193300	N	-3.25934200	1.05699300	3.02429800
N	4.82008800	2.76432500	0.26850500	C	-4.35076500	0.26317500	4.81237400
C	3.50137300	3.18199300	-1.42628600	C	-3.75592800	-0.13505000	2.71682700
C	3.57426800	3.00275700	0.73489700	N	-4.42409300	-0.64500200	3.77312300
N	2.74718000	3.25306900	-0.27053500	C	-5.24543900	5.03516200	-1.88310400
C	10.34965500	0.02489500	-0.36707400	C	-4.72666500	4.27974800	-0.70994900
C	8.97755100	0.36465100	0.23154300	N	-5.40854000	4.14691600	0.49066200
C	9.09192700	1.30831300	1.43090500	C	-3.55925200	3.58840200	-0.53076600
S	7.50710100	1.77671500	2.24841200	C	-4.65464400	3.39809600	1.33098000
C	7.00518200	0.20206300	3.05658200	N	-3.52517400	3.04401900	0.73993200
C	7.45101600	-4.99162000	1.33279700	C	-2.85999500	-3.52892900	-4.79289400
C	6.61063500	-3.79798400	1.81072900	C	-3.99197800	-3.47465700	-3.77640700
C	5.12974400	-4.04046600	1.62531100	O	-5.11763700	-3.87779200	-4.06093800
C	4.32304000	-4.45672000	2.69237100	N	-3.65390900	-2.97481300	-2.55088400
C	4.54548700	-3.90754500	0.35876700	C	-4.62046100	-2.91929700	-1.46497000
C	2.96936400	-4.73463600	2.50109900	C	-4.81169800	-1.47544100	-0.99142000
C	3.19376300	-4.18686200	0.15758000	O	-3.86231000	-0.84957100	-0.47249200
C	2.40164200	-4.60229400	1.23249900	C	-4.19742900	-3.79011800	-0.25536100

O	-4.25460200	-5.16093600	-0.55145500	H	-2.77231300	3.41609300	-1.25051100
N	-6.03038300	-0.90487900	-1.07544300	H	-4.95569600	3.12671900	2.33056600
C	-7.26395800	-1.46467000	-1.68999500	H	-2.56571200	-4.57744000	-4.91704100
C	-7.20410200	-1.43092900	-3.21900300	H	-4.91211200	-3.59419300	0.55891500
C	-8.35325100	-0.55035500	-1.09567200	H	-3.21348000	-3.46208800	0.09575200
C	-7.66253200	0.81796900	-0.98441800	H	-3.37825800	-5.47105900	-0.83939900
C	-6.23110700	0.46234900	-0.56018700	H	-5.53872100	-3.34343100	-1.86785800
C	-0.24522800	2.80874600	-4.50326700	H	-2.73956900	-2.53873300	-2.42093100
C	-0.35725600	2.87578000	-2.99185800	H	-8.63796100	-0.90900400	-0.09992600
O	0.64380100	3.33973400	-2.34067900	H	-9.25345400	-0.53266200	-1.71464300
O	-1.41281600	2.43241800	-2.47177200	H	-8.15227500	1.48496300	-0.26933600
C	4.71529300	0.87972800	-5.62281200	H	-7.65830800	1.32168300	-1.95647300
C	4.06356100	0.11224900	-4.47613700	H	-6.11710700	0.45878500	0.53124800
S	4.96438200	-1.47651900	-4.17175900	H	-5.46870700	1.13458600	-0.96166600
C	0.71030500	-5.17717100	-3.13717400	H	-7.40526000	-2.49481200	-1.35183400
C	1.23463500	-3.87488300	-3.72401600	H	-1.22561100	2.95020300	-4.96154800
O	2.06495800	-3.18813500	-3.10440200	H	0.46865200	3.53928300	-4.88924600
C	-0.09123300	-4.89626200	-1.84789800	H	3.02393900	-0.12084400	-4.71570200
C	-0.53804200	-6.14684000	-1.10463800	H	4.06673500	0.70746100	-3.55858400
O	-1.72079900	-6.38744900	-0.86912100	H	3.92264100	-2.16601300	-3.65620800
N	0.44928200	-7.00273400	-0.71860300	H	5.76798500	1.09606200	-5.41231000
N	0.75465600	-3.51176000	-4.92825100	H	0.52107200	-4.28333000	-1.17883000
C	1.05065900	-2.21222500	-5.51762200	H	-0.98681900	-4.31931300	-2.07571400
Zn	-1.96774800	2.06114700	1.68173900	H	0.17712800	-7.78222500	-0.13666700
Zn	0.73280000	3.54884300	-0.21567500	H	1.41506400	-6.71163700	-0.68829400
H	-0.17016000	9.39079100	-2.34718400	H	0.09040900	-5.72256700	-3.85643200
H	1.57797900	9.32770400	-2.07869400	H	0.61232900	-1.40921200	-4.91650900
H	0.69057700	5.67743700	-2.52450800	H	2.13147700	-2.07365700	-5.58582100
H	0.09569100	6.31932600	1.57828300	H	0.00497400	-4.05684500	-5.32591600
H	6.33923800	1.61428500	-1.92901600	H	-0.36279300	4.53859700	5.67352600
H	5.74512200	2.87821600	-3.01074300	H	-1.56601000	5.27546900	4.59766200
H	3.04279500	3.33532900	-2.38993400	H	-3.62252400	2.60344600	6.04509800
H	3.29095800	2.98988900	1.77552200	H	-2.13975800	2.68109200	5.06599100
H	8.47231500	-0.56078400	0.53390400	H	-4.79966200	0.07715200	5.77489000
H	8.34042300	0.82770700	-0.53070800	H	-3.65600300	-0.63550000	1.76308100
H	9.74559300	0.89098100	2.20381500	H	-4.84738200	-1.56072600	3.80555300
H	9.52897700	2.26635900	1.13034300	H	0.62831200	-2.18004400	-6.52291000
H	7.00501000	0.33326200	4.13969500	H	1.58240000	-5.80309100	-2.92242700
H	7.71025000	-0.58770700	2.79317100	H	-7.00791300	-0.41703000	-3.58341500
H	6.01010200	-0.09526100	2.72227800	H	-6.43921500	-2.10498400	-3.60874400
H	10.86781400	0.92539300	-0.71378300	H	-8.16515200	-1.75869300	-3.63026300
H	6.91080300	-2.90124300	1.25248800	H	0.84241600	8.34996000	-3.35247000
H	6.82440200	-3.59931200	2.86770400	H	6.82815200	3.29767100	-1.67988400
H	4.76064900	-4.56192600	3.68245500	H	5.63609600	2.50907500	0.83005900
H	5.15444400	-3.57804500	-0.48031200	H	0.24294100	8.59881200	0.45951400
H	2.34978600	-5.03936200	3.33910100	H	-5.38163000	6.09996100	-1.66034700
H	2.77012300	-4.04380200	-0.83313900	H	-6.31473600	4.53624700	0.70591000
H	1.34228100	-4.80051100	1.10248000	H	10.99471700	-0.46756900	0.36838500
H	7.19265300	-5.89730900	1.89025000	H	10.24370900	-0.64923500	-1.22190800
H	-6.20757400	4.64338800	-2.23253900	H	8.52147200	-4.80402800	1.46829900
H	-4.53514000	4.95361600	-2.70791900	H	7.27500400	-5.19437200	0.27188500

H	-3.24362100	-3.18264800	-5.75527800	H	-1.11926100	-6.31619900	3.62822800
H	-1.99646300	-2.93316300	-4.49175200	H	-0.65106600	-1.38230500	3.73654600
H	4.67365300	0.30825400	-6.55386900	H	-1.78441500	-4.96694700	1.65458400
H	4.20198400	1.83461100	-5.78148400	H	-1.45543300	-1.43278000	1.58359600
H	-3.59941800	3.46969500	4.49955800	O	-0.65204000	2.09281400	-0.03372700
H	1.26562600	5.22255300	3.70436000	N	-1.01480700	-0.33552300	-0.77168200
H	-0.23651900	6.25887400	5.24391000	C	-0.36104600	-0.99914500	-1.79883600
H	0.10619600	1.80851400	-4.78045800	O	-0.97293400	-1.78559500	-2.53868400
C	-1.47917000	-5.41647900	6.96315300	N	0.96416300	-0.75645100	-1.92782400
C	-0.23590100	-5.42546400	6.06266700	C	1.66589700	0.20756800	-1.08803700
H	0.02695700	-6.45892200	5.80830300	C	1.11266500	0.19383200	0.34189700
H	0.61758000	-5.00975500	6.61217500	C	-0.40876000	0.32377800	0.30404000
H	-1.74469200	-4.39327300	7.24846800	O	-1.07165500	0.26572800	1.42805700
H	-2.33921600	-5.84844600	6.44151300	H	2.72680100	-0.05469600	-1.08497000
H	-1.31647200	-5.99178300	7.88135300	H	1.48767200	1.06426700	0.88320000
C	-0.49280600	-4.62670800	4.80835200	H	-2.01593600	-0.54401900	-0.69282200
C	-0.36599900	-3.23278300	4.81435700	H	1.47384500	-1.45368000	-2.46563800
C	-1.00116100	-5.23525900	3.65266900	C	1.51983400	-1.07203000	1.10932700
C	-0.74453400	-2.46439700	3.71685400	H	2.60951300	-1.16601900	1.12468400
C	-1.37977400	-4.48736900	2.54082000	H	1.16394000	-1.03707200	2.13942300
C	-1.25551900	-3.09246100	2.57292100	H	1.11934600	-1.97519500	0.64594400
O	-1.64686000	-2.39307100	1.47583700	H	1.57290900	1.20637600	-1.52122400
H	0.02205900	-2.73640800	5.70130600	H	-1.06516900	2.14182900	-0.95487400

(5S)-MeDHU-INT1-II (*Sm*DHPase)

C	0.64303100	8.64075800	-2.57891700	N	0.18336900	5.04370600	3.52452500
C	0.44615700	7.52000600	-1.62084300	C	-0.13498700	4.04143900	2.62768200
N	0.20427100	7.69612000	-0.26659800	O	-1.30023900	3.53008300	2.71161000
C	0.48600900	6.16456200	-1.79314700	O	0.75406000	3.75885500	1.76410200
C	0.12075100	6.47955000	0.32258200	C	-3.29113400	2.68122900	4.92633400
N	0.28572600	5.52719600	-0.58196800	C	-3.67595900	1.36743600	4.33564300
C	5.97887400	2.62478500	-2.00184800	N	-3.36005400	1.05572400	3.02311700
C	4.78398500	2.87878000	-1.15502800	C	-4.32394200	0.29734000	4.89428000
N	4.79912700	2.82193800	0.22836800	C	-3.80488200	-0.17386400	2.79111800
C	3.49064200	3.17457900	-1.48900800	N	-4.39774200	-0.66154900	3.90024600
C	3.55087100	3.07457600	0.67823100	C	-5.27673500	4.91822300	-2.06475900
N	2.72981000	3.28635900	-0.34133100	C	-4.77531200	4.17946200	-0.87192400
C	10.34507300	0.07844000	-0.29171300	N	-5.49330100	4.04196200	0.30676500
C	8.98723100	0.40076700	0.34783100	C	-3.60035900	3.51299700	-0.64778500
C	9.10067500	1.50866500	1.39792200	C	-4.75356100	3.31722700	1.17870900
S	7.53652400	2.01179500	2.23033200	N	-3.59727400	2.98163600	0.62914100
C	7.11511500	0.50209400	3.17302000	C	-2.80217200	-3.70532600	-4.71274200
C	7.47289900	-4.91110600	1.52821500	C	-3.94794500	-3.57743000	-3.71961300
C	6.64179200	-3.66109100	1.85949900	O	-5.05834600	-4.04379100	-3.96851200
C	5.15890000	-3.90142800	1.68151700	N	-3.63857000	-2.92401200	-2.56504600
C	4.34635500	-4.24847700	2.76843500	C	-4.52972300	-2.96660000	-1.41843800
C	4.57830800	-3.84140300	0.40746700	C	-4.81729100	-1.54526300	-0.92251500
C	2.99285800	-4.53717600	2.58803200	O	-3.92024800	-0.87689700	-0.36847000
C	3.22727100	-4.13263200	0.21834600	C	-3.92322200	-3.80665100	-0.27675900
C	2.43166900	-4.48623400	1.31122400	O	-3.77060700	-5.12872300	-0.73702700
C	-0.59500300	5.38207400	4.71215400	N	-6.05657600	-1.02736300	-1.06230400

C	-7.25088700	-1.64159000	-1.70197100	H	-2.50158300	-4.75891700	-4.74177000
C	-7.17446100	-1.59862700	-3.23122000	H	-4.61270500	-3.75983500	0.58659200
C	-8.39206500	-0.78454200	-1.11924800	H	-2.97881000	-3.35459900	0.04284000
C	-7.77128100	0.61611300	-0.99747200	H	-2.93096600	-5.48913000	-0.40002200
C	-6.32928400	0.33025100	-0.55630400	H	-5.43405000	-3.46666200	-1.76459200
C	-0.23938500	2.65882800	-4.58360800	H	-2.69267100	-2.55853900	-2.42607600
C	-0.35176900	2.77701500	-3.08089000	H	-8.66969200	-1.15888100	-0.12726700
O	0.63401400	3.27200300	-2.43589600	H	-9.28481000	-0.81000400	-1.74874000
O	-1.40570800	2.33232500	-2.54905400	H	-8.30236500	1.25656600	-0.28747700
C	4.74448700	0.73885300	-5.61119100	H	-7.78091900	1.12137200	-1.96874000
C	4.09448700	-0.03212000	-4.46556000	H	-6.22583700	0.33686600	0.53623800
S	4.96580300	-1.64382600	-4.20498500	H	-5.59527600	1.03707000	-0.95238400
C	0.79766300	-5.35570700	-3.06318200	H	-7.34699300	-2.67960300	-1.37237000
C	1.28124000	-4.02903100	-3.63902100	H	-1.21646600	2.80337200	-5.04812400
O	2.09634200	-3.33100600	-3.01580400	H	0.48906500	3.36116200	-4.99331700
C	-0.09583700	-5.14313900	-1.82739900	H	3.04572800	-0.23810600	-4.69007500
C	-0.43631600	-6.36246700	-0.98054700	H	4.12740900	0.54751100	-3.53857300
O	-1.28446700	-6.28862500	-0.08717800	H	3.93439300	-2.30249400	-3.63089000
N	0.22670900	-7.52048000	-1.21325800	H	5.80475500	0.92949700	-5.41460800
N	0.80563900	-3.67583700	-4.84869500	H	0.37992200	-4.42298600	-1.15435900
C	1.10347600	-2.37825400	-5.44551900	H	-1.05028600	-4.68869900	-2.10535300
Zn	-2.11470700	2.03365500	1.68169600	H	0.01279400	-8.30886700	-0.62039500
Zn	0.72013300	3.53517000	-0.32119700	H	0.95667900	-7.61338100	-1.89889500
H	-0.23024000	9.30145200	-2.62799900	H	0.27843900	-5.95346200	-3.82046100
H	1.51088800	9.25574000	-2.31442700	H	0.70191700	-1.57098500	-4.82518000
H	0.66082800	5.59413000	-2.69031900	H	2.18358700	-2.25663400	-5.55286300
H	-0.03538900	6.33264100	1.38105800	H	0.06641600	-4.23029500	-5.25280400
H	6.33451900	1.59255000	-1.90606900	H	-0.43194000	4.68251800	5.54200000
H	5.73035800	2.79386200	-3.05160100	H	-1.65482400	5.37484300	4.45704700
H	3.03940600	3.28902100	-2.46130000	H	-3.64443200	2.75636700	5.95826600
H	3.26041500	3.08966300	1.71684100	H	-2.20796900	2.81207700	4.91381600
H	8.57875600	-0.50659000	0.80780200	H	-4.71937400	0.13431300	5.88392000
H	8.27225900	0.70647800	-0.42505200	H	-3.70650200	-0.71532600	1.85933400
H	9.81064600	1.23202200	2.18502400	H	-4.76078600	-1.59827300	3.99821300
H	9.47276900	2.43395500	0.94536500	H	0.64363800	-2.33647800	-6.43379500
H	6.23981800	0.74232100	3.77984200	H	1.71416900	-5.88835800	-2.78361500
H	7.93879000	0.23370500	3.83864400	H	-7.00815100	-0.57748900	-3.59008400
H	6.87371700	-0.33692300	2.51852000	H	-6.38221300	-2.24699400	-3.60979100
H	10.76889600	0.95612300	-0.79156700	H	-8.11874000	-1.95838300	-3.65432400
H	6.96389700	-2.83580500	1.21009900	H	0.81282800	8.24130000	-3.58058600
H	6.84677400	-3.35138100	2.89152600	H	6.81149700	3.28929700	-1.74534800
H	4.77937600	-4.29347900	3.76537400	H	5.61227300	2.58861200	0.80420900
H	5.19179400	-3.56450400	-0.44756100	H	0.11321200	8.58252300	0.20801100
H	2.36992600	-4.79026300	3.44076000	H	-5.44143700	5.98067700	-1.85072000
H	2.80419800	-4.05809700	-0.77945200	H	-6.41560100	4.41081100	0.48681100
H	1.37591300	-4.70551900	1.18322500	H	11.06830400	-0.25929900	0.45813900
H	7.19249500	-5.74646100	2.17731900	H	10.24437900	-0.71467600	-1.03818900
H	-6.21996200	4.50338500	-2.43787100	H	8.54412800	-4.72366200	1.65895900
H	-4.54253600	4.84793600	-2.86942300	H	7.30737500	-5.22610600	0.49329400
H	-2.78889100	3.34677100	-1.34029300	H	-3.16761800	-3.44388300	-5.70885400
H	-5.08271200	3.04669400	2.16959300	H	-1.94566600	-3.08321000	-4.44555900

H	4.67551700	0.18259700	-6.54986700	H	-0.86454100	-1.01379200	3.91017400
H	4.24918900	1.70659300	-5.74828600	H	-1.39213000	-4.75491700	1.86327600
H	-3.71597600	3.51741900	4.36112400	H	-1.40290700	-1.22100600	1.64115200
H	1.16745900	5.27070500	3.53328300	O	-0.62046000	1.96967900	-0.20707200
H	-0.31795000	6.38545400	5.04412300	N	-1.01304700	-0.30999400	-0.80844800
H	0.08948700	1.64170200	-4.82378200	C	-0.34260200	-1.09420500	-1.71457200
C	-1.49641900	-5.24825300	7.10202000	O	-0.92312500	-1.97296700	-2.38076500
C	-0.17410300	-4.93821300	6.38640300	N	0.98856500	-0.85947900	-1.86351100
H	0.35844300	-5.87504700	6.18228800	C	1.69635900	0.14785100	-1.08511300
H	0.47214300	-4.34738800	7.04667000	C	1.10138700	0.27095200	0.32377600
H	-2.03420200	-4.32432800	7.33962600	C	-0.41652000	0.52615300	0.21364100
H	-2.14877400	-5.85636400	6.46724300	O	-1.09226100	0.41915000	1.37981600
H	-1.33141000	-5.79384700	8.03792800	H	2.74793200	-0.14535900	-1.02308100
C	-0.43141400	-4.19099000	5.10073600	H	1.51946700	1.15755100	0.80703600
C	-0.46502700	-2.79319500	5.06970500	H	-1.99720000	-0.55191400	-0.67520300
C	-0.77184000	-4.88174000	3.92848900	H	1.49500600	-1.60461900	-2.33375000
C	-0.84313400	-2.09981800	3.92051800	C	1.42969900	-0.94631300	1.19271100
C	-1.14615300	-4.21050800	2.76942200	H	2.51259000	-1.09817700	1.22952200
C	-1.19317700	-2.80956600	2.76335800	H	1.06825000	-0.80618400	2.21183100
O	-1.58969200	-2.19539000	1.62018100	H	0.98259700	-1.86217100	0.80329300
H	-0.20200300	-2.23353000	5.96506700	H	1.65455300	1.11162900	-1.60176700
H	-0.75134000	-5.96940000	3.92517100	H	-1.03595000	2.01281400	-1.15457600

(5S)-MeDHU-TS2-II (*SmDHPase*)

C	0.99654800	8.66223600	-2.40178300	C	0.20165300	4.01724200	2.75095600
C	0.77676300	7.49296800	-1.49602500	O	-0.94750200	3.47991700	2.86963200
N	0.60805100	7.62923500	-0.12613100	O	1.08319400	3.77485800	1.86996100
C	0.72155700	6.14004500	-1.71300600	C	-3.08827100	2.70908900	5.02766100
C	0.47449900	6.39991700	0.42489700	C	-3.53348800	1.44723700	4.37022300
N	0.53666300	5.46886400	-0.51461400	N	-3.20279300	1.17037700	3.05419700
C	6.06408600	2.40191100	-2.04877600	C	-4.25837200	0.39739300	4.87099200
C	4.88263000	2.69450700	-1.19378900	C	-3.71504800	-0.01871400	2.76345300
N	4.91529200	2.62468400	0.18777400	N	-4.36510800	-0.51502900	3.83741400
C	3.59178700	3.03163900	-1.50445200	C	-5.07645200	5.19684500	-1.87743300
C	3.68128300	2.90929900	0.65831100	C	-4.53194500	4.44373300	-0.70767700
N	2.85010700	3.15316800	-0.34555300	N	-5.17086900	4.41570700	0.52341400
C	10.33647900	-0.37660700	-0.46808700	C	-3.40823600	3.67378400	-0.53473900
C	9.00823400	0.02377200	0.18976600	C	-4.43969800	3.65445700	1.37185800
C	9.20261700	1.10924000	1.25162100	N	-3.36302800	3.19082400	0.76146000
S	7.68374400	1.69321000	2.11481500	C	-3.03313900	-3.46380300	-4.76168200
C	7.20072000	0.20450500	3.06130400	C	-4.15290900	-3.36385500	-3.73333600
C	7.27027200	-5.27435900	1.28332100	O	-5.29347900	-3.72997000	-4.00768800
C	6.47721400	-4.05581800	1.77963300	N	-3.78795600	-2.86570300	-2.51612200
C	4.98657500	-4.23897100	1.60298500	C	-4.73998000	-2.75171300	-1.42129800
C	4.16685300	-4.60989600	2.67669800	C	-4.85734100	-1.29005100	-0.97628400
C	4.40260700	-4.08988800	0.33814200	O	-3.87034000	-0.69485700	-0.49791300
C	2.80058200	-4.82564100	2.49388700	C	-4.33351300	-3.61554900	-0.20148200
C	3.03845700	-4.30733000	0.14538400	O	-4.44566800	-4.98972500	-0.46793800
C	2.23293900	-4.67615800	1.22724600	N	-6.05457500	-0.67085100	-1.04939800
C	-0.27675600	5.29106600	4.83183900	C	-7.32020100	-1.19109800	-1.63132900
N	0.51298800	5.02285000	3.64525200	C	-7.28321400	-1.19937200	-3.16193100

C	-8.35971900	-0.21526500	-1.04538900	H	-2.85866800	-2.46561200	-2.38808800
C	-7.60805400	1.12338900	-0.97586100	H	-8.64578800	-0.53739900	-0.03764600
C	-6.18764300	0.71428100	-0.56207500	H	-9.26711200	-0.17227200	-1.65261900
C	-0.18461100	2.77466500	-4.52833900	H	-8.05782900	1.82830100	-0.27102600
C	4.69162300	0.65868500	-5.67993000	H	-7.59515400	1.60297600	-1.96012900
C	3.92587600	0.06991000	-4.49953100	H	-6.05746000	0.73096600	0.52746400
S	4.78796600	-1.42475400	-3.82107900	H	-5.40304400	1.34422900	-0.98856500
C	0.45956300	-5.23844100	-3.13251300	H	-7.50200000	-2.20505700	-1.26454000
C	1.03901300	-3.96396400	-3.72710300	H	0.03213500	1.77765900	-4.92755000
O	1.91477500	-3.32152900	-3.12278200	H	-1.13053600	3.09091900	-4.97499300
C	-0.28995400	-4.92428100	-1.81911500	H	2.92186600	-0.23050100	-4.80526500
C	-0.79757000	-6.15971800	-1.08974500	H	3.81879100	0.80512100	-3.69737700
O	-1.99395700	-6.36660000	-0.89776300	H	3.68106800	-2.15871400	-3.57321600
N	0.15366100	-7.04364200	-0.67485700	H	5.71413100	0.93070500	-5.39799800
N	0.55839300	-3.57294000	-4.92364500	H	0.37557400	-4.36131000	-1.15776100
C	0.91681000	-2.29566100	-5.52686500	H	-1.15241200	-4.29002000	-2.01776300
Zn	-1.86635500	2.10561800	1.73644000	H	-0.15941400	-7.81336600	-0.10028900
Zn	0.83085600	3.42742000	-0.18242100	H	1.12235400	-6.77008500	-0.59871900
H	0.16094000	9.37032200	-2.36602200	H	-0.20896000	-5.74376400	-3.83736000
H	1.91052300	9.20801700	-2.14196000	H	0.54755700	-1.46271600	-4.91992200
H	0.81482700	5.59637400	-2.63916800	H	2.00212000	-2.22041700	-5.62347700
H	0.35946600	6.22986500	1.48498900	H	-0.21514400	-4.08668900	-5.31737000
H	6.34968000	1.34521900	-1.99421200	H	-0.15878000	4.52511200	5.60983600
H	5.83338200	2.62929300	-3.09177400	H	-1.33141100	5.34060300	4.56002400
H	3.13570100	3.17634600	-2.47064900	H	-3.40857300	2.73249700	6.07269000
H	3.40702800	2.93198200	1.70111700	H	-2.00239900	2.80569100	4.98531600
H	8.54732300	-0.86137600	0.64356600	H	-4.68630800	0.21977300	5.84453500
H	8.30641000	0.38360700	-0.57158100	H	-3.62218600	-0.53211500	1.81628800
H	9.90665600	0.78072500	2.02401800	H	-4.78741300	-1.43037200	3.88755600
H	9.62222900	2.01670900	0.80464400	H	0.47057700	-2.24060300	-6.52060500
H	6.35574700	0.49062300	3.69086400	H	1.30106600	-5.91281800	-2.94360200
H	8.02373100	-0.11441900	3.70514600	H	-7.05127300	-0.20373700	-3.55501400
H	6.89570100	-0.61595800	2.40958600	H	-6.55305400	-1.91384100	-3.54612700
H	10.81163600	0.47900300	-0.96004500	H	-8.26334000	-1.49668300	-3.55079600
H	6.80746600	-3.16525400	1.22787700	H	1.09675400	8.31843600	-3.43314200
H	6.70609400	-3.87549400	2.83652500	H	6.93435900	3.00207800	-1.76165800
H	4.60358800	-4.72672700	3.66583900	H	5.73032900	2.36163600	0.74676700
H	5.02216900	-3.79484300	-0.50595800	H	0.59816200	8.50055600	0.38359400
H	2.17126000	-5.09331400	3.33728700	H	-5.12984400	6.27377000	-1.68036000
H	2.61819500	-4.15643400	-0.84550600	H	-6.03796100	4.88005100	0.75055000
H	1.16410400	-4.82215500	1.10535700	H	11.04328200	-0.77085500	0.26977000
H	6.98209400	-6.17571000	1.83316800	H	10.17789500	-1.15070800	-1.22445100
H	-6.08183200	4.85613900	-2.14933000	H	8.34766000	-5.12745400	1.41389800
H	-4.42997500	5.04708300	-2.74425200	H	7.08058500	-5.45964100	0.22153500
H	-2.65520900	3.39856900	-1.25902400	H	-3.39935800	-3.06572100	-5.71096600
H	-4.72280800	3.45252000	2.39296600	H	-2.13018100	-2.93333100	-4.45316700
H	-2.80927100	-4.52508300	-4.91724100	H	4.75611100	-0.05622900	-6.50431700
H	-5.03024800	-3.37970600	0.61719600	H	4.19341200	1.56433300	-6.04441400
H	-3.33417400	-3.31530000	0.13073000	H	-3.50170600	3.59384500	4.53034300
H	-3.59645000	-5.33430400	-0.79487800	H	1.49677600	5.24963900	3.67084000
H	-5.68038600	-3.14424600	-1.80420600	H	0.02328300	6.25530300	5.24989200

H	0.61821300	3.45384900	-4.81975900	O	0.60034500	3.10377200	-2.30719600
C	-1.61991500	-5.34177300	6.99205000	O	-1.40550000	2.08711000	-2.65810300
C	-0.41679700	-5.35324200	6.03823100	H	-1.23579800	1.13515300	-1.76267600
H	-0.18051400	-6.38767600	5.76175800	N	-1.02412500	-0.00584400	-0.94471100
H	0.46446400	-4.96112900	6.56100300	C	-0.39606100	-0.99098800	-1.76322400
H	-1.85944000	-4.31990700	7.30446500	O	-1.05783100	-1.82374100	-2.39390000
H	-2.50802400	-5.75472600	6.50273800	N	0.94171700	-0.89155100	-1.84369600
H	-1.42415700	-5.93329500	7.89323400	C	1.71208500	0.06793500	-1.05640600
C	-0.68964700	-4.53612000	4.79704200	C	1.16013000	0.17336100	0.37087900
C	-0.52043300	-3.14611500	4.80251700	C	-0.31844800	0.64419700	0.34759800
C	-1.21672700	-5.12405600	3.63891300	O	-1.05377300	0.27823300	1.41738700
C	-0.85919300	-2.36524800	3.70027600	H	1.69769300	1.04312000	-1.54974100
C	-1.55520200	-4.36363300	2.52186800	H	2.74825000	-0.27872200	-1.04137700
C	-1.37084900	-2.97314700	2.54314300	H	1.69806000	0.97822600	0.87975500
O	-1.70191600	-2.26499200	1.43572400	H	-1.97265800	-0.33004700	-0.70153200
H	-0.12005700	-2.66188100	5.69100800	H	1.40243700	-1.65590900	-2.33557500
H	-1.37322200	-6.20026400	3.61231800	O	-0.46276000	2.01348300	0.17092500
H	-0.72421100	-1.28811700	3.71909800	C	1.39150200	-1.11908500	1.15567200
H	-1.97088600	-4.83231300	1.63482200	H	2.45216700	-1.38767500	1.13533200
H	-1.42545100	-1.30401800	1.50992400	H	1.08753500	-0.99913900	2.19502400
C	-0.32086000	2.66656100	-3.03734300	H	0.83117000	-1.96079600	0.74498800

(5S)-MeDHU-EP-II (*SmDHPase*)

C	1.52511000	8.60560000	-2.38611000	O	-0.73556600	3.58170200	2.88205500
C	1.19149100	7.51812100	-1.43675000	O	1.29226700	3.74755100	1.85250900
N	0.98626500	7.69805300	-0.07760400	C	-2.88106800	2.91504600	5.06543600
C	1.06877200	6.17444200	-1.63553200	C	-3.34223700	1.65136800	4.41243000
C	0.76879100	6.48771900	0.49075500	N	-3.03315800	1.35201000	3.09168500
N	0.81055200	5.54254600	-0.43459100	C	-4.08551000	0.62023800	4.92443500
C	6.21771300	2.05942300	-2.03498900	C	-3.57977400	0.17301400	2.81335000
C	5.06409200	2.43832400	-1.17906800	N	-4.22538000	-0.29717600	3.89957700
N	5.09431400	2.39604500	0.20377800	C	-4.73919700	5.50329900	-1.83894200
C	3.79972700	2.85202400	-1.49951700	C	-4.29456100	4.67791400	-0.67534100
C	3.88312900	2.77388800	0.66884100	N	-5.04888400	4.50525600	0.47804000
N	3.07125300	3.05144200	-0.34302700	C	-3.15362600	3.94967200	-0.46121500
C	10.32418700	-0.96220200	-0.46058400	C	-4.36631900	3.70191600	1.32585600
C	9.02367200	-0.46449100	0.18644800	N	-3.20998800	3.34643600	0.78372700
C	9.28818300	0.59762400	1.25677400	C	-3.21542800	-3.26722100	-4.71243000
S	7.80815400	1.27305300	2.12176900	C	-4.37176000	-3.12783700	-3.72647000
C	7.23410800	-0.18690800	3.06214300	O	-5.52966400	-3.36656200	-4.06610400
C	6.98090100	-5.66866100	1.30823700	N	-4.01321700	-2.73924800	-2.46958000
C	6.20968400	-4.43951900	1.81266300	C	-4.97565300	-2.63747000	-1.38582600
C	4.71699800	-4.58351500	1.61675600	C	-5.05721100	-1.19637300	-0.86418200
C	3.87446600	-4.93777000	2.67803600	O	-4.05011200	-0.65881400	-0.35843300
C	4.15192600	-4.40949500	0.34639700	C	-4.59171100	-3.55237600	-0.19313200
C	2.50434800	-5.11221600	2.47794500	O	-4.70839700	-4.91490100	-0.50763700
C	2.78414100	-4.58539900	0.13646200	N	-6.23706900	-0.54091500	-0.87929200
C	1.95560900	-4.93741000	1.20651000	C	-7.48194100	-0.92257500	-1.59298700
C	0.07648500	5.32732200	4.85721700	C	-7.32088800	-0.75465600	-3.10551300
N	0.82828600	5.01921200	3.65208600	C	-8.50962300	0.03800800	-0.96559400
C	0.45241800	4.04710300	2.74662500	C	-7.70544100	1.32525200	-0.71945100

C	-6.31861300	0.81250900	-0.30077700	H	-9.37802700	0.18733500	-1.61161900
C	-0.00526700	2.79381000	-4.49844100	H	-8.15676800	1.96758500	0.04208900
C	4.73523300	0.39348300	-5.65916800	H	-7.63254300	1.90962500	-1.64232700
C	3.87014700	-0.08841700	-4.49905800	H	-6.21704900	0.74577500	0.79010800
S	4.63145400	-1.55246100	-3.65336200	H	-5.49230500	1.43014200	-0.66291200
C	0.22101700	-5.32595000	-3.17145300	H	-7.73724300	-1.96010400	-1.36184900
C	0.83779500	-4.04370800	-3.71798800	H	-0.96571300	2.97951700	-4.98072500
O	1.72063200	-3.44211200	-3.08511500	H	0.78038200	3.39521900	-4.96223700
C	-0.55407300	-5.04067300	-1.86793600	H	2.88017600	-0.38118200	-4.85226800
C	-1.09694500	-6.26656500	-1.15141500	H	3.73214200	0.70622000	-3.76095700
O	-2.28460800	-6.37646500	-0.84955400	H	3.49618000	-2.26147400	-3.46365300
N	-0.19691600	-7.24491000	-0.85000700	H	5.74425200	0.65629500	-5.32449300
N	0.38368200	-3.60929900	-4.91172700	H	0.09874900	-4.49155100	-1.18190600
C	0.79408500	-2.33409500	-5.49041700	H	-1.39996900	-4.38833000	-2.06863500
Zn	-1.75998300	2.31634100	1.78848000	H	-0.52420500	-8.00672400	-0.27318300
Zn	1.09928000	3.53367000	-0.32736200	H	0.79584700	-7.06689100	-0.87089100
H	0.75063400	9.38081500	-2.42279300	H	-0.43694900	-5.80054500	-3.90712100
H	2.47153500	9.09659700	-2.13086100	H	0.51948000	-1.50152300	-4.83679900
H	1.17288800	5.60484300	-2.54378400	H	1.87576600	-2.32496300	-5.64707000
H	0.61187700	6.33968400	1.54863500	H	-0.40284800	-4.08761300	-5.32365300
H	6.42446500	0.98436400	-1.98254600	H	0.16963300	4.55350400	5.63062500
H	6.00005000	2.30326500	-3.07700700	H	-0.97886500	5.43694800	4.60688200
H	3.34753800	3.00929200	-2.46543600	H	-3.21277700	2.94766600	6.10625900
H	3.61310800	2.84276500	1.71060200	H	-1.79363000	2.99530900	5.03471700
H	8.49132400	-1.31389100	0.63017900	H	-4.50933000	0.46075200	5.90285900
H	8.35937700	-0.04806600	-0.57961900	H	-3.53533200	-0.34620600	1.86344600
H	9.96629100	0.21720400	2.02868800	H	-4.67706700	-1.19823100	3.95827300
H	9.76823900	1.47873400	0.81820400	H	0.29922700	-2.21539100	-6.45515100
H	6.40638100	0.14731500	3.69095000	H	1.05135100	-6.01681700	-2.99043300
H	8.03497400	-0.55672700	3.70670700	H	-6.98555800	0.25738800	-3.35585500
H	6.88227400	-0.98589600	2.40723900	H	-6.61573000	-1.48011800	-3.51569600
H	10.87039300	-0.14259300	-0.93995600	H	-8.28297400	-0.92469000	-3.60162900
H	6.56683300	-3.54893300	1.27790500	H	1.62730200	8.19364700	-3.39189300
H	6.43019600	-4.27935300	2.87461100	H	7.13048200	2.59441600	-1.75108000
H	4.29603500	-5.07416300	3.67132100	H	5.89070000	2.08704600	0.76578800
H	4.78923600	-4.12727600	-0.48881700	H	1.00373000	8.57996800	0.41336800
H	1.85939300	-5.36881500	3.31296900	H	-4.85537100	6.56014000	-1.57228400
H	2.37758200	-4.41243700	-0.85652300	H	-5.95915800	4.90351300	0.65696500
H	0.88568800	-5.05635400	1.06638200	H	10.98953000	-1.41650300	0.28125000
H	6.66562200	-6.57094600	1.84143400	H	10.11373000	-1.71530000	-1.22538100
H	-5.69413700	5.15389200	-2.24730000	H	8.05967200	-5.54826900	1.45383600
H	-3.99254500	5.43482500	-2.63212500	H	6.80031200	-5.83455300	0.24167600
H	-2.32476300	3.77261000	-1.13412700	H	-3.50677100	-2.79355000	-5.65322300
H	-4.73319900	3.39397300	2.29233100	H	-2.28914400	-2.83286100	-4.33479600
H	-3.07277900	-4.33461800	-4.91660600	H	4.83323300	-0.37904500	-6.42639700
H	-5.29198900	-3.33815100	0.62853100	H	4.29279500	1.28466600	-6.11866300
H	-3.59069100	-3.26904500	0.15180500	H	-3.28002500	3.79912200	4.55586800
H	-3.84945400	-5.26702400	-0.80044500	H	1.82142900	5.20212800	3.65598400
H	-5.92577000	-2.98512800	-1.78948600	H	0.43880900	6.27200000	5.27001800
H	-3.03759700	-2.48109000	-2.29242100	H	0.25236700	1.73883600	-4.64902300
H	-8.86572800	-0.37038400	-0.01303700	C	-1.88195600	-5.20470600	7.04095900

C	-0.70665000	-5.36467700	6.06419600	O	-1.21754600	2.91939300	-2.45861700
H	-0.59476600	-6.42320600	5.80144300	N	-1.51643700	0.05846500	-1.63487000
H	0.22331800	-5.06770500	6.56436900	C	-0.76791700	-0.98572000	-2.06753000
H	-1.99820400	-4.15853200	7.34329100	O	-1.25801100	-2.09742800	-2.34701200
H	-2.82092300	-5.52188700	6.57577400	N	0.59233800	-0.80412400	-2.17938600
H	-1.73348300	-5.80349200	7.94598500	C	1.37334400	0.16510100	-1.42371300
C	-0.90523500	-4.54161300	4.81179100	C	1.22188500	0.12252800	0.12388700
C	-0.54264900	-3.19003600	4.77400000	C	0.01281200	0.89074100	0.62599100
C	-1.54044600	-5.07848300	3.68268300	O	-0.76917500	0.43533500	1.50844200
C	-0.81010200	-2.39359000	3.66156600	H	1.18579400	1.17800400	-1.77835800
C	-1.81241700	-4.30349900	2.55789100	H	2.41920900	-0.05365900	-1.65327600
C	-1.44991500	-2.95011800	2.54627100	H	2.06127100	0.72752500	0.49351300
O	-1.75055200	-2.22239400	1.43369800	H	-2.48943200	-0.14704600	-1.42484000
H	-0.04509700	-2.74696900	5.63407900	H	1.05782300	-1.68288800	-2.39499100
H	-1.83484700	-6.12543800	3.68441500	O	-0.19991700	2.09401600	0.22010600
H	-0.52203800	-1.34638200	3.64771700	H	-1.26574600	1.02854000	-1.80750700
H	-2.30229600	-4.73422700	1.68991300	C	1.35708400	-1.28612200	0.69819100
H	-1.36364400	-1.32584500	1.49033500	H	2.29811200	-1.73353000	0.36879800
C	-0.10715200	3.05268400	-3.00390200	H	1.35488100	-1.27424000	1.79006200
O	0.98921300	3.34264000	-2.38729500	H	0.54581100	-1.93733300	0.36953500

(5S,6S)-Me₂DHU-ES-II (*Sm*DHPase)

C	1.91702400	8.39404000	-3.11270200	O	1.50304900	3.87239000	1.72237600
C	1.65007900	7.41535900	-2.02551900	C	-2.22360800	-4.23028800	7.53374200
N	1.50439900	7.75148500	-0.68719200	C	-1.22037600	-4.81977200	6.53033200
C	1.51153900	6.05687400	-2.06068500	C	-1.45835000	-4.13440500	5.21183000
C	1.29675300	6.61450100	0.02373600	C	-2.41363800	-4.62747000	4.31445700
N	1.29402000	5.56993800	-0.78629900	C	-0.93756300	-2.85469100	4.99227200
C	6.35964200	1.76629000	-1.95844900	C	-2.88639600	-3.84736000	3.26463800
C	5.17300900	2.14707100	-1.14573700	C	-1.40424200	-2.05591100	3.95452800
N	5.11934200	2.01555400	0.23208400	C	-2.40771100	-2.54279100	3.11123700
C	3.95714500	2.66454300	-1.50362400	O	-2.96716300	-1.76631000	2.14114100
C	3.90603200	2.44472900	0.65307400	C	-2.92573300	3.61258800	4.69805100
N	3.17595000	2.84060000	-0.37818900	C	-3.53958600	2.47295800	3.95889600
C	10.30322800	-1.21624300	0.04772200	N	-3.08844100	2.04089300	2.71609000
C	9.97373900	0.27743800	0.14525700	C	-4.61822500	1.70937700	4.32281000
C	9.42952000	0.72772500	1.50747600	C	-3.89390100	1.05847900	2.33776000
S	7.70636100	0.13151900	1.80754000	N	-4.83000100	0.82715000	3.28211300
C	7.55992000	0.48312100	3.59596500	C	-4.46820300	5.56505900	-2.48740900
C	6.73933600	-5.61448000	2.14802100	C	-4.02685600	4.97331400	-1.20190300
C	5.89651000	-4.38905500	2.53517400	N	-4.66249200	5.20421300	0.00792800
C	4.43571000	-4.54308600	2.16854400	C	-2.98840900	4.13313100	-0.90659700
C	3.44699700	-4.68773500	3.14916100	C	-4.00757600	4.50977700	0.96962900
C	4.04440200	-4.57045700	0.82151200	N	-2.98969000	3.85099200	0.44492300
C	2.10301100	-4.84454300	2.79999800	C	-3.16672200	-3.49100800	-4.43538300
C	2.70775000	-4.73349300	0.46289800	C	-4.38037500	-3.19000000	-3.58885800
C	1.73149900	-4.86338000	1.45550100	O	-5.53139200	-3.33895400	-3.99377100
C	0.12108300	5.89563900	4.36018300	N	-4.06707500	-2.76499000	-2.33268400
N	0.96518600	5.41135300	3.28339600	C	-5.05285400	-2.60173700	-1.28536000
C	0.63102800	4.30212300	2.52770500	C	-5.06148600	-1.13040700	-0.84429200
O	-0.55107000	3.84313300	2.70460300	O	-4.03151300	-0.63148600	-0.34226100

C	-4.67634100	-3.51388700	-0.09655400	H	-1.36390200	-5.90288600	6.44542600
O	-4.63425100	-4.88204800	-0.46000900	H	-0.19574000	-4.65653400	6.88475500
N	-6.17672800	-0.38836600	-0.98770700	H	-2.82683400	-5.62158400	4.46870900
C	-7.42842300	-0.74403600	-1.71006200	H	-0.19374100	-2.45606000	5.67844200
C	-7.22940100	-0.70064700	-3.22769800	H	-3.64836400	-4.21779100	2.58709800
C	-8.39994600	0.33220800	-1.19199400	H	-1.02885800	-1.04715700	3.81545200
C	-7.51511500	1.58276100	-1.06497500	H	-2.43371200	-0.95522700	2.03154100
C	-6.17509100	1.02588200	-0.56060200	H	-3.25032800	-4.39212000	7.19164100
C	0.31886800	2.79188600	-4.68765000	H	-5.50161800	5.29460100	-2.73463600
C	0.16946600	2.77987800	-3.16905200	H	-3.82974500	5.20006000	-3.29422900
O	1.17745500	3.21288600	-2.50611500	H	-2.26572800	3.69524000	-1.58167900
O	-0.90646800	2.36326700	-2.67645200	H	-4.30479500	4.49541900	2.00649100
C	4.93561700	-0.20062100	-5.45289300	H	-2.94586200	-4.55685600	-4.33092500
C	4.18153400	-0.96922500	-4.37405000	H	-5.42860200	-3.41769200	0.69499100
S	4.75575400	-2.72590100	-4.30894300	H	-3.72212900	-3.16832400	0.31443300
C	0.07986500	-6.07653600	-3.41656500	H	-4.06896100	-4.99215700	-1.25257100
C	0.71092400	-4.70257200	-3.63185800	H	-6.00969800	-2.91703500	-1.70117700
O	1.58076900	-4.24499500	-2.87114200	H	-3.08442900	-2.74540000	-2.05930400
C	-0.21754000	-6.42434900	-1.95469500	H	-8.78895700	0.04301200	-0.20892900
C	-1.61774200	-6.01877000	-1.49058800	H	-9.25101700	0.47005200	-1.86287800
O	-2.51858400	-5.72182200	-2.27939100	H	-7.93006600	2.33158200	-0.38506100
N	-1.82652600	-6.06432800	-0.15371300	H	-7.38743600	2.05911400	-2.04177200
N	0.33648800	-4.05574700	-4.75495800	H	-6.10777100	1.07413400	0.53217300
C	0.89637400	-2.76937200	-5.15833800	H	-5.30016800	1.54457600	-0.96215600
Zn	-1.54793600	2.69738700	1.44464300	H	-7.75748500	-1.74113000	-1.40552500
Zn	1.24907800	3.54292800	-0.40865500	H	-0.51195900	2.27046600	-5.16436600
O	-0.34761100	2.50608100	-0.04699600	H	0.34232500	3.82702700	-5.04640500
H	1.12037100	9.14195000	-3.20291500	H	3.11184800	-0.95974100	-4.59310400
H	2.85998800	8.93215500	-2.96035000	H	4.33032600	-0.50599700	-3.39539100
H	1.55959800	5.38019000	-2.89779000	H	3.72980100	-3.21280000	-3.57642800
H	1.15844200	6.58358400	1.09508500	H	6.01469100	-0.20247000	-5.26785000
H	6.61103100	0.70586900	-1.84321700	H	-0.14559600	-7.51052800	-1.82039800
H	6.15682700	1.94845600	-3.01594900	H	0.53919600	-5.98142900	-1.30110400
H	3.56847000	2.90281700	-2.48081200	H	-2.75286700	-5.83066600	0.19040600
H	3.58190700	2.47309300	1.68143200	H	-1.09887900	-6.31746600	0.49477300
H	9.26652000	0.56135700	-0.64465300	H	-0.83494300	-6.18284900	-4.00528300
H	10.88268700	0.86224300	-0.04346600	H	0.68200600	-1.99886100	-4.41167900
H	10.05386400	0.32973500	2.31469300	H	1.97728200	-2.85211500	-5.29340700
H	9.43262800	1.81935600	1.58292600	H	-0.42725000	-4.43782800	-5.29136500
H	6.56017400	0.17247600	3.90631200	H	0.08428300	5.21340300	5.21974700
H	7.68640200	1.54803400	3.80578000	H	-0.89642900	6.03238000	3.99268300
H	8.29692500	-0.09374500	4.15936200	H	-3.38350900	3.71262700	5.68554500
H	11.05387000	-1.50054300	0.79303100	H	-1.84947400	3.47426000	4.81335500
H	6.30845000	-3.50037200	2.03866100	H	-5.23077700	1.71807100	5.21002800
H	5.98570800	-4.21059300	3.61302100	H	-3.85205600	0.51907100	1.40154200
H	3.73205300	-4.67402400	4.19852100	H	-5.48936500	0.06368200	3.26067500
H	4.79698500	-4.46247000	0.04378300	H	0.44167700	-2.47696000	-6.10568200
H	1.34705500	-4.93735800	3.57460500	H	0.80907700	-6.79470000	-3.81085200
H	2.43193900	-4.75074300	-0.58731200	H	-6.83643600	0.27072200	-3.54485500
H	0.68388200	-4.95099900	1.18127100	H	-6.55725400	-1.48920600	-3.56988000
H	6.37743500	-6.51435600	2.65515500	H	-8.19222500	-0.85464400	-3.72740100

H	1.98683500	7.86815000	-4.06685400	C	-0.58643600	-2.16931900	-0.98750000
H	7.24713100	2.34878600	-1.68514300	O	-1.30660100	-2.95898800	-1.60148800
H	5.86178500	1.61747400	0.80826700	N	0.75618400	-2.24648000	-0.93119400
H	1.55035000	8.68295400	-0.30126300	C	1.55450100	-1.05814100	-0.61068300
H	-4.40650200	6.65997100	-2.48219000	C	1.00309800	-0.39759600	0.67031900
H	-5.47215900	5.78977500	0.15107900	C	-0.51194600	-0.35613400	0.66749000
H	9.41746700	-1.83656500	0.21215400	O	-1.16459800	0.31615800	1.48987200
H	10.70581000	-1.45912400	-0.93991000	H	2.56593800	-1.41738900	-0.39793100
H	7.78985300	-5.47012900	2.42075200	H	1.30013000	0.65435000	0.67716400
H	6.69543000	-5.80182700	1.07073800	H	-2.19647500	-1.07380400	-0.27092100
H	-2.12208100	-4.68469100	8.52622000	H	1.15053300	-2.93664400	-1.57377000
H	-2.07546500	-3.15130200	7.63943900	C	1.51691200	-1.06255800	1.96164800
H	-3.39989300	-3.27096400	-5.47944100	H	2.60966400	-1.01486000	1.98536100
H	-2.28747500	-2.93157700	-4.11123000	H	1.13130500	-0.54229100	2.84073300
H	4.76509300	-0.63447000	-6.44211300	H	1.22972600	-2.11439700	2.02074800
H	4.59927900	0.84157600	-5.47546300	H	-0.71331900	2.33080400	-0.94544300
H	-3.06128900	4.56014600	4.16500700	C	1.58871100	-0.10940700	-1.81139900
H	1.95922600	5.57833200	3.34513700	H	2.26627000	0.72564100	-1.63567600
H	0.50179500	6.86130300	4.70273500	H	1.93322700	-0.65062500	-2.69545500
H	1.26771600	2.33179600	-4.97825900	H	0.59766800	0.30080300	-2.02226200
N	-1.16758200	-1.12741800	-0.23895400				

(5S,6S)-Me₂DHU-TS1-II (*Sm*DHPase)

C	0.40223300	8.53661400	-2.91220800	O	-1.61898600	3.66462400	2.56045000
C	0.18261100	7.50707100	-1.86389500	O	0.49101900	3.94595200	1.77298000
N	-0.16258400	7.77524400	-0.54743300	C	-1.82613500	-4.74935900	7.49848600
C	0.29527600	6.14894200	-1.92459200	C	-0.51152200	-4.84075300	6.71136400
C	-0.23371700	6.60091400	0.12801300	C	-0.67955600	-4.14503600	5.38522800
N	0.03697600	5.59303100	-0.68554300	C	-1.21537800	-4.82582600	4.28380100
C	5.90625600	2.78979800	-1.61764500	C	-0.48436200	-2.76384000	5.27457500
C	4.67545200	3.09725100	-0.84434600	C	-1.56490900	-4.15325100	3.11801500
N	4.58180100	2.96178400	0.53075300	C	-0.83101000	-2.07207300	4.11730400
C	3.42258700	3.46117300	-1.25536500	C	-1.38234900	-2.76728700	3.03376000
C	3.30703100	3.22721300	0.89787500	O	-1.76680900	-2.14861100	1.88989300
N	2.57513000	3.52120400	-0.16739200	C	-3.80463800	2.87765600	4.67731500
C	10.23878800	0.53112300	0.52705800	C	-4.06379000	1.55667600	4.03088600
C	9.73216000	1.87419300	1.06497000	N	-3.55064600	1.21052000	2.78554800
C	8.86229100	1.77348800	2.32530800	C	-4.80327300	0.50631300	4.50831100
S	7.19232200	1.07045700	1.96497700	C	-3.98115200	-0.01706700	2.52158400
C	6.63290300	0.67546500	3.66029100	N	-4.74275000	-0.47472800	3.53775700
C	7.43740200	-4.45502100	2.46294900	C	-5.39679300	4.61134900	-2.55328000
C	6.51020300	-3.26784600	2.76882700	C	-4.87010500	3.96257800	-1.32034500
C	5.07154300	-3.53885600	2.38325100	N	-5.57549800	3.93129700	-0.12675000
C	4.09320000	-3.80381200	3.34964700	C	-3.69334300	3.31228700	-1.05252700
C	4.69640800	-3.56942200	1.03216800	C	-4.82866300	3.28434300	0.79721600
C	2.77512500	-4.08553000	2.98159200	N	-3.67995700	2.89661500	0.26795300
C	3.38535200	-3.85541900	0.65389200	C	-2.43202100	-4.04557300	-4.49458100
C	2.41899600	-4.10945100	1.63257200	C	-3.66545800	-3.92908000	-3.62092200
C	-1.20207000	5.66939100	4.47133000	O	-4.74683400	-4.42790400	-3.93014100
N	-0.29919600	5.31737900	3.38182100	N	-3.45386100	-3.25242400	-2.45522700
C	-0.47852700	4.24013700	2.53494300	C	-4.40757400	-3.24861200	-1.36320400

C	-4.75118300	-1.79569700	-1.00228200	H	1.38908800	-4.29845600	1.34418000
O	-3.88874700	-1.06429500	-0.47132600	H	7.11988000	-5.34925200	3.00826800
C	-3.78185800	-3.94742900	-0.13461600	H	-0.23971900	-5.89265400	6.56460900
O	-3.41885000	-5.29078900	-0.40911600	H	0.29935400	-4.38105400	7.28880400
N	-5.98794900	-1.31471000	-1.24504400	H	-1.38489800	-5.89819200	4.35196200
C	-7.13430900	-1.98918600	-1.91122200	H	-0.07528400	-2.21417100	6.11953900
C	-6.96909900	-2.03576600	-3.43363400	H	-2.00161100	-4.67526300	2.27340400
C	-8.31739700	-1.11677600	-1.44840400	H	-0.68815500	-0.99833000	4.04804400
C	-7.72639700	0.30143000	-1.40014200	H	-1.52744500	-1.19174900	1.89859100
C	-6.30131400	0.07835000	-0.87340300	H	-2.64361900	-5.21954900	6.94274000
C	0.03880800	2.91295400	-4.67696700	H	-6.34924000	4.17307300	-2.87249600
C	-0.19580800	2.80741300	-3.17698300	H	-4.68302500	4.48199900	-3.36905500
O	0.67688800	3.37198700	-2.42614600	H	-2.87796300	3.09133600	-1.72813200
O	-1.20372000	2.18271100	-2.76488400	H	-5.14611900	3.10639800	1.81205900
C	4.98823100	0.64338000	-5.17544600	H	-1.94158000	-4.99195600	-4.25305200
C	5.50400600	-0.79105100	-5.07942600	H	-4.51543100	-3.98086000	0.68063200
S	5.20119100	-1.65708000	-6.68437600	H	-2.92901800	-3.35324500	0.20725200
C	1.43963000	-5.95324700	-3.20718800	H	-2.83740300	-5.30774600	-1.19785000
C	1.67893800	-4.46413600	-3.44734600	H	-5.27704400	-3.81065900	-1.70480100
O	2.30400400	-3.75875200	-2.64246600	H	-2.52212400	-2.88533200	-2.24988100
C	1.15179300	-6.30586900	-1.74781000	H	-8.63764000	-1.42417400	-0.44616800
C	-0.29190600	-6.02923800	-1.33268100	H	-9.17716800	-1.20570400	-2.11675100
O	-1.17685600	-5.78201000	-2.15656900	H	-8.30047700	0.98031400	-0.76335700
N	-0.55548000	-6.12645200	-0.00899400	H	-7.69918000	0.73538900	-2.40471700
N	1.25045300	-3.98613500	-4.63486900	H	-6.24715900	0.18135700	0.21743800
C	1.46224700	-2.60521100	-5.05326800	H	-5.56008500	0.76100400	-1.29732500
Zn	-2.15696500	2.12615700	1.43055500	H	-7.23367600	-3.00675800	-1.52381500
Zn	0.54015000	3.62006300	-0.33583900	H	-0.71544300	2.35062800	-5.22762900
O	-0.69122700	2.01439500	-0.19433600	H	0.00832500	3.96285500	-4.98759100
H	-0.49199800	9.14444500	-3.09374700	H	4.99033000	-1.33330900	-4.28075400
H	1.21903000	9.22013700	-2.65248700	H	6.57690100	-0.79953900	-4.87116400
H	0.56475700	5.52221900	-2.75719800	H	5.77022900	-2.83258300	-6.34874300
H	-0.45983600	6.52474300	1.18160100	H	5.51025500	1.20203100	-5.95787500
H	6.19805700	1.73921800	-1.50861800	H	1.33533100	-7.37563800	-1.58917000
H	5.73377100	2.98509000	-2.67806100	H	1.84003500	-5.76868000	-1.08836100
H	3.04874500	3.63255500	-2.25184600	H	-1.51296100	-5.96565400	0.29198700
H	2.93493300	3.19228600	1.90967700	H	0.17022000	-6.28141300	0.67203600
H	9.18259300	2.41341500	0.28235600	H	0.62860300	-6.32276300	-3.84002100
H	10.58954500	2.50985600	1.31863700	H	1.04273000	-1.91231000	-4.31875300
H	9.33719000	1.11633400	3.06178500	H	2.52747700	-2.39403300	-5.18398300
H	8.73013400	2.75791000	2.78403700	H	0.66993700	-4.57917400	-5.20739500
H	5.63467000	0.24064700	3.57757200	H	-1.07814200	5.02747000	5.35329200
H	6.58725700	1.57084000	4.28490000	H	-2.23111500	5.58077800	4.12334500
H	7.29717900	-0.06164900	4.11670100	H	-4.30364800	2.92819300	5.64840700
H	10.84316100	0.01187400	1.27859700	H	-2.73449200	3.04042700	4.81889300
H	6.87454000	-2.38195300	2.23186100	H	-5.34665200	0.37538100	5.43036500
H	6.56423900	-3.03143100	3.83833800	H	-3.77866500	-0.58275300	1.62265800
H	4.36644400	-3.78836300	4.40237100	H	-5.13835000	-1.40120800	3.59467300
H	5.44328800	-3.36908700	0.26690600	H	0.96136900	-2.45317700	-6.01021000
H	2.02580800	-4.27405200	3.74498100	H	2.35953800	-6.46320700	-3.51870000
H	3.11985000	-3.87584700	-0.39893400	H	-6.79606100	-1.03522300	-3.84336000

H	-6.14659600	-2.69159400	-3.72579300	N	-0.90369700	-0.54043400	-0.55827500
H	-7.88200300	-2.43604700	-3.88800100	C	-0.23687500	-1.61456200	-1.15637700
H	0.66610100	8.04716600	-3.85158300	O	-0.85389600	-2.45853800	-1.81066300
H	6.75885700	3.40225300	-1.30242300	N	1.09537000	-1.69917100	-0.93538900
H	5.33932900	2.64298100	1.13564700	C	1.85729200	-0.49911200	-0.60780500
H	-0.32677800	8.68861200	-0.15020000	C	1.16599000	0.23176800	0.57126300
H	-5.55508800	5.68702900	-2.41310800	C	-0.36879600	0.29672600	0.42635400
H	-6.49327200	4.32155100	0.02927900	O	-1.09418500	0.42400600	1.50729200
H	9.41251200	-0.12970700	0.24900200	H	2.82974300	-0.84176900	-0.23922000
H	10.86467800	0.68062800	-0.35757200	H	1.52443600	1.25943100	0.59555800
H	8.47109900	-4.23240200	2.74794700	H	-1.92019900	-0.66490900	-0.55401000
H	7.42759100	-4.69811200	1.39587800	H	1.55032900	-2.40598900	-1.51598300
H	-1.75118200	-5.24526400	8.47291600	C	1.53996500	-0.42181000	1.91237200
H	-2.10180100	-3.70408100	7.67168500	H	2.62662300	-0.39562000	2.04165200
H	-2.73924000	-4.05308000	-5.54241600	H	1.07629200	0.11226500	2.74252100
H	-1.71765300	-3.24097400	-4.30779600	H	1.23125200	-1.46784600	1.95385800
H	3.91664300	0.66718400	-5.39659500	H	-0.98983900	1.95044500	-1.15164800
H	5.14539900	1.15914800	-4.22298100	C	2.08279400	0.32913500	-1.87693500
H	-4.16816600	3.70809800	4.06277000	H	2.71315800	1.19730400	-1.68736800
H	0.66602100	5.60331500	3.46279400	H	2.57749600	-0.29745600	-2.62660600
H	-1.01671000	6.70483800	4.76735200	H	1.13441100	0.67345400	-2.29362300
H	1.03586900	2.53556900	-4.92273900				

(5S,6S)-Me₂DHU-INT1-II (*Sm*DHPase)

C	0.25855000	8.49265200	-2.97417100	N	-0.45903700	5.27167600	3.30756200
C	0.02320200	7.46625000	-1.92899200	C	-0.65854700	4.20176400	2.45550600
N	-0.39403400	7.72267400	-0.63153800	O	-1.80379900	3.63912400	2.48041600
C	0.18939400	6.11466400	-1.98162700	O	0.30539000	3.90315800	1.68411400
C	-0.45251700	6.54710000	0.04272000	C	-1.77979500	-4.76949700	7.50560600
N	-0.10629500	5.54956400	-0.75552200	C	-0.43219900	-4.52686800	6.81158000
C	5.86277900	2.85953700	-1.61150600	C	-0.63711800	-3.84310700	5.48212200
C	4.62820700	3.17333200	-0.84777000	C	-1.05276600	-4.57912000	4.36280000
N	4.52620300	3.05036600	0.52770600	C	-0.54737400	-2.45312000	5.35382700
C	3.37814000	3.53207900	-1.27013100	C	-1.37513200	-3.95453400	3.16407700
C	3.24960900	3.31514800	0.88504600	C	-0.86684500	-1.80811700	4.15956600
N	2.52377700	3.60011600	-0.18771400	C	-1.28491500	-2.55937600	3.05285300
C	10.22441500	0.69678700	0.57269500	O	-1.62362900	-2.00451400	1.86583300
C	9.68332900	2.02829300	1.10591000	C	-3.88569600	2.80115700	4.62546700
C	8.79016800	1.90682500	2.34829700	C	-4.12191900	1.43864100	4.06271300
S	7.13914800	1.17915000	1.95039000	N	-3.64245600	1.06518500	2.81367200
C	6.55855600	0.74358400	3.62858500	C	-4.78333600	0.37160300	4.61027000
C	7.50657600	-4.32981400	2.52300500	C	-4.00906100	-0.19590400	2.61302800
C	6.58475700	-3.14119500	2.83721800	N	-4.70264000	-0.64633600	3.67787600
C	5.14976800	-3.39127200	2.42437400	C	-5.46699000	4.46009700	-2.62502400
C	4.14145100	-3.60664500	3.37193600	C	-4.94801000	3.80781000	-1.38783200
C	4.80791400	-3.44890600	1.06541500	N	-5.68719900	3.74658800	-0.21632300
C	2.82610400	-3.86567200	2.97743400	C	-3.76192700	3.18519900	-1.08882700
C	3.50035200	-3.71282600	0.66134900	C	-4.95339000	3.11254200	0.72503600
C	2.50338300	-3.91655100	1.62100000	N	-3.77777200	2.76056800	0.22945700
C	-1.33538900	5.64056200	4.41746800	C	-2.32685300	-4.15057400	-4.49496200

C	-3.55723300	-4.02809500	-3.61373500	H	4.38874200	-3.57060000	4.43061600
O	-4.62956300	-4.55787100	-3.90472900	H	5.57818200	-3.28664300	0.31450500
N	-3.35732800	-3.31226100	-2.46889700	H	2.05338000	-4.01602000	3.72592100
C	-4.29959700	-3.32881100	-1.36461100	H	3.26045300	-3.75520400	-0.39690000
C	-4.71868400	-1.89262800	-1.01212500	H	1.47664400	-4.08491200	1.30955600
O	-3.90847600	-1.11757100	-0.46422900	H	7.17357000	-5.23127300	3.04678700
C	-3.63327000	-3.97810200	-0.13037200	H	0.08375300	-5.48476700	6.67207000
O	-3.25034400	-5.32159700	-0.37602200	H	0.21065400	-3.91603800	7.45624500
N	-5.97851200	-1.47823500	-1.27117700	H	-1.13688800	-5.66119700	4.43863900
C	-7.07987300	-2.20904200	-1.95142700	H	-0.23138500	-1.85903500	6.20871800
C	-6.90754600	-2.22096400	-3.47328500	H	-1.70517500	-4.52265200	2.30099300
C	-8.31388700	-1.41739200	-1.47739400	H	-0.79218100	-0.72830200	4.07593300
C	-7.81083100	0.03352300	-1.41137600	H	-1.40319100	-1.03558600	1.81080000
C	-6.37144500	-0.10850100	-0.89276000	H	-2.42979300	-5.39648400	6.88698800
C	0.01879400	2.99755300	-4.75268100	H	-6.40066500	4.00005500	-2.96735700
C	-0.18723200	2.80369700	-3.26014100	H	-4.73496000	4.36106000	-3.42874600
O	0.64863400	3.38100400	-2.48254100	H	-2.92232100	2.98659800	-1.74062400
O	-1.15320600	2.09577300	-2.87065700	H	-5.29856800	2.91642900	1.72769700
C	5.00701900	0.67437500	-5.16122800	H	-1.81654500	-5.07888500	-4.22483400
C	5.44712700	-0.74011200	-4.78909700	H	-4.35116400	-4.00485100	0.69911100
S	5.49657500	-1.78343400	-6.31437800	H	-2.78562000	-3.35794300	0.17817200
C	1.61561500	-5.94458600	-3.12435300	H	-2.67246700	-5.34934600	-1.16736400
C	1.81699600	-4.45661500	-3.40052200	H	-5.14528500	-3.93777700	-1.68555700
O	2.43254400	-3.71696400	-2.62005100	H	-2.42608600	-2.93664100	-2.26176200
C	1.32425300	-6.26480800	-1.65853900	H	-8.61275400	-1.75667500	-0.47888000
C	-0.13107300	-6.01871500	-1.26563000	H	-9.16788700	-1.54973900	-2.14602300
O	-1.01605100	-5.83324600	-2.10577600	H	-8.42334200	0.66717600	-0.76365500
N	-0.40268200	-6.08100100	0.05872400	H	-7.81485200	0.48168600	-2.41011100
N	1.36551800	-4.01620700	-4.59455100	H	-6.31558300	-0.00564300	0.19831100
C	1.54268500	-2.63985700	-5.03963900	H	-5.67442000	0.61903700	-1.31813100
Zn	-2.35221800	2.00401900	1.48944300	H	-7.11873100	-3.23733700	-1.58249600
Zn	0.49913500	3.61666700	-0.38431400	H	-0.67530800	2.37962900	-5.32222800
O	-0.61211900	1.86678400	-0.41149000	H	-0.13548500	4.04996300	-5.01505000
H	-0.64543900	9.06770000	-3.20711600	H	4.74997000	-1.18905000	-4.07620900
H	1.03720200	9.20698400	-2.68216100	H	6.44294100	-0.72607100	-4.33847000
H	0.52138100	5.50085400	-2.80047900	H	5.91179000	-2.92146000	-5.72210200
H	-0.72062700	6.46439100	1.08564000	H	5.71235700	1.14046400	-5.85555800
H	6.15451900	1.81059400	-1.48952100	H	1.53617600	-7.32401500	-1.46770000
H	5.69570300	3.04291800	-2.67483000	H	1.99053100	-5.68976000	-1.00848200
H	3.01239400	3.69467700	-2.27090900	H	-1.36575500	-5.92486800	0.34622500
H	2.87052900	3.27547800	1.89412000	H	0.32671400	-6.15848000	0.74904700
H	9.14007700	2.56116300	0.31453500	H	0.81994300	-6.35263100	-3.75293800
H	10.52399100	2.67806000	1.37914800	H	1.11047500	-1.94226700	-4.31693300
H	9.26042000	1.25265200	3.09036100	H	2.60338200	-2.40853200	-5.17513600
H	8.63413900	2.88633700	2.81003100	H	0.78860300	-4.63231100	-5.14583100
H	5.57405700	0.28389100	3.51964100	H	-1.17863200	5.01818200	5.30780200
H	6.47861000	1.62711300	4.26649100	H	-2.37285300	5.53581400	4.10010000
H	7.23301900	0.01603000	4.08523400	H	-4.35465100	2.89276700	5.60859300
H	10.82525600	0.18639400	1.33306900	H	-2.81762000	3.00302000	4.72270200
H	6.96524300	-2.24886600	2.32204100	H	-5.28432300	0.24901100	5.55702600
H	6.62424800	-2.92475200	3.91157500	H	-3.78879200	-0.78653700	1.73350700

H -5.04085300 -1.59040200 3.79137000
H 1.03641000 -2.51768000 -5.99819800
H 2.55174700 -6.43698900 -3.41496900
H -6.79024700 -1.20577900 -3.86670500
H -6.04797200 -2.82541100 -3.76868400
H -7.79353700 -2.66616200 -3.93905000
H 0.58594400 8.00400000 -3.89371200
H 6.71295000 3.47625100 -1.29820000
H 5.28060500 2.73274200 1.13824200
H -0.61108200 8.62944600 -0.24444100
H -5.65609900 5.52880200 -2.47187600
H -6.62175800 4.10594900 -0.08769300
H 9.41551300 0.02172300 0.27833000
H 10.86258700 0.86093800 -0.30046900
H 8.53771200 -4.12145800 2.82757900
H 7.51167900 -4.55345200 1.45174600
H -1.65128600 -5.26886000 8.47234500
H -2.30230600 -3.82316500 7.68076000
H -2.64178700 -4.19880500 -5.53922600
H -1.62686100 -3.32639200 -4.33957600
H 4.01850200 0.67222400 -5.63080800
H 4.94939200 1.29565000 -4.26188100
H -4.29557600 3.58365900 3.97848400
H 0.50775700 5.55826400 3.36386100

H -1.15033700 6.68359900 4.68506400
H 1.04884300 2.74677000 -5.02118500
N -0.88755700 -0.46930600 -0.71581300
C -0.21822900 -1.59618400 -1.15525100
O -0.80629900 -2.52237500 -1.73158800
N 1.12070800 -1.65200300 -0.92865600
C 1.86748300 -0.42873000 -0.67325500
C 1.15578100 0.34738400 0.46162700
C -0.37708800 0.52506500 0.21314700
O -1.11840300 0.54852100 1.35798800
H 2.84296400 -0.73527500 -0.27957600
H 1.57164200 1.35420400 0.49140800
H -1.89905800 -0.60867200 -0.68923200
H 1.58267100 -2.38440300 -1.46682200
C 1.45130000 -0.30900200 1.81588600
H 2.53279600 -0.32824000 1.98764100
H 0.97865000 0.24653500 2.62608100
H 1.10002300 -1.34081400 1.84949900
H -0.88741600 1.79710400 -1.40004200
C 2.10035500 0.33084900 -1.98595300
H 2.69613300 1.23166300 -1.83409600
H 2.63694700 -0.32280500 -2.68173100
H 1.15386400 0.61176200 -2.45203500

(5S,6S)-Me₂DHU-TS2-II (*Sm*DHPase)

C 0.81839500 8.35631100 -3.25173900
C 0.56522700 7.32659600 -2.20142100
N 0.26380400 7.63591600 -0.88342700
C 0.59125200 5.95848900 -2.23529200
C 0.13352100 6.48401300 -0.18286800
N 0.32372700 5.44202100 -0.97780400
C 6.03945500 2.38924000 -1.79199200
C 4.82955600 2.82600700 -1.04883300
N 4.76544300 2.88466800 0.33223500
C 3.57122600 3.14742400 -1.48098200
C 3.50580800 3.21729300 0.68524500
N 2.75104600 3.37194400 -0.39517600
C 10.27264700 -0.00726800 0.40092100
C 8.88713700 0.39685900 0.92431300
C 8.96182600 1.59446300 1.87463000
S 7.36129000 2.19898500 2.55606600
C 6.85237900 0.79684500 3.61457500
C 7.24283200 -4.77452900 2.53410500
C 6.40086900 -3.53194500 2.85938300
C 4.94344500 -3.70057600 2.48743300
C 3.94496900 -3.79810400 3.46384700
C 4.56792000 -3.79496500 1.13984200
C 2.60521300 -3.97347700 3.10763900
C 3.23528600 -3.97616700 0.77460600
C 2.24779400 -4.05801900 1.76176700

C -0.86095300 5.83645000 4.24102600
N 0.02182600 5.42443000 3.16406000
C -0.21618200 4.33451500 2.35330700
O -1.38116700 3.82163300 2.38292000
O 0.75255400 3.98388700 1.60790000
C -3.59796200 3.18823000 4.56549200
C -3.94283500 1.84146600 4.02549600
N -3.51410900 1.42715600 2.77214900
C -4.66681900 0.82939500 4.59798000
C -3.97081000 0.19331100 2.59262900
N -4.67505700 -0.19951800 3.67426900
C -5.16627400 4.74295000 -2.71086400
C -4.65899600 4.10902300 -1.45560800
N -5.39264500 4.09988900 -0.27907500
C -3.49569200 3.45118800 -1.14034900
C -4.67649100 3.45917300 0.67387500
N -3.51709100 3.05317900 0.18475900
C -2.65584600 -4.11543000 -4.36243500
C -3.85992600 -3.85518800 -3.47590800
O -4.96792800 -4.32849600 -3.73053500
N -3.60379000 -3.09030300 -2.37496700
C -4.53678300 -3.00174600 -1.26416800
C -4.84656100 -1.52925400 -0.95101200
O -3.97481500 -0.79107900 -0.45420300
C -3.91171500 -3.66331300 -0.01595600

O	-3.63267000	-5.03946700	-0.22711000	H	-4.62369900	-3.61445400	0.81757400
N	-6.08717700	-1.04356300	-1.18911000	H	-3.01819400	-3.10149200	0.26943200
C	-7.24489600	-1.72462400	-1.82442200	H	-3.06062300	-5.12884000	-1.01752200
C	-7.07698400	-1.84361800	-3.34146400	H	-5.42704700	-3.55586100	-1.56224100
C	-8.41355200	-0.81232000	-1.40237700	H	-2.65254200	-2.75814500	-2.18498800
C	-7.79546000	0.59495800	-1.40092600	H	-8.74570100	-1.07612400	-0.39166500
C	-6.37907400	0.36143100	-0.85601500	H	-9.27119400	-0.90880100	-2.07250600
C	-0.02568300	2.21293800	-4.71029600	H	-8.36131000	1.30798000	-0.79444400
C	4.98326700	0.16720900	-5.26404000	H	-7.75202800	0.99055900	-2.42103000
C	5.38718600	-1.30537500	-5.28499800	H	-6.33152800	0.49466900	0.23256000
S	4.94140800	-2.03524300	-6.92387700	H	-5.62244900	1.01998800	-1.29144800
C	1.17222500	-6.11172400	-2.94493800	H	-7.36520100	-2.72208400	-1.39265000
C	1.46238400	-4.64912600	-3.27557900	H	0.55466300	1.31935500	-4.96571300
O	2.10842000	-3.91228700	-2.51901200	H	-1.01440200	2.09149300	-5.15715000
C	0.85842600	-6.36340700	-1.47087900	H	4.86968300	-1.85751100	-4.49582000
C	-0.57675000	-6.00155800	-1.09349700	H	6.46459900	-1.40928000	-5.13362800
O	-1.43881400	-5.77004700	-1.94619200	H	5.41682900	-3.27501700	-6.68911600
N	-0.86150700	-6.01464300	0.22863400	H	5.50673400	0.73446900	-6.03942400
N	1.04978300	-4.23709500	-4.49569100	H	0.99544300	-7.42806600	-1.24542100
C	1.30043400	-2.89349800	-5.00030400	H	1.56147600	-5.81657100	-0.83582100
Zn	-2.08209900	2.20099000	1.43700900	H	-1.80770100	-5.76105800	0.50285600
Zn	0.72379000	3.48442200	-0.39083900	H	-0.14258700	-6.10831000	0.92798800
H	-0.04769300	9.01042000	-3.40384000	H	0.35351700	-6.49199200	-3.56120500
H	1.67594400	8.99039200	-2.99992500	H	0.95958800	-2.14784500	-4.27656900
H	0.79556400	5.30510500	-3.06667600	H	2.36470600	-2.73807700	-5.20195600
H	-0.07133800	6.44877000	0.87703400	H	0.45143100	-4.84852000	-5.02897100
H	6.27692800	1.33825100	-1.59032500	H	-0.77199900	5.20328000	5.13353200
H	5.87411200	2.49498500	-2.86621000	H	-1.89293500	5.79456500	3.89263200
H	3.18766800	3.18998500	-2.48767400	H	-4.01122500	3.31662200	5.56931400
H	3.15587000	3.32516300	1.69960000	H	-2.51569400	3.32395600	4.60819700
H	8.43069600	-0.45697500	1.43844000	H	-5.15557100	0.75043100	5.55575300
H	8.22618300	0.64382100	0.08481200	H	-3.80507000	-0.42272700	1.71935400
H	9.61598600	1.37944700	2.72674700	H	-5.06869900	-1.11941900	3.80526000
H	9.38218000	2.46742100	1.36410300	H	0.75052100	-2.76467500	-5.93364800
H	5.94939800	1.11099600	4.14183700	H	2.07715300	-6.66988100	-3.21530600
H	7.63008500	0.58151500	4.35094100	H	-6.88059500	-0.86582300	-3.79391900
H	6.62912400	-0.09884000	3.03261000	H	-6.26968400	-2.53105900	-3.60071700
H	10.74672500	0.81315000	-0.14859500	H	-7.99686000	-2.24326200	-3.78263900
H	6.82052600	-2.66937500	2.32165000	H	1.03569300	7.86619700	-4.20271400
H	6.48456600	-3.30244100	3.92797700	H	6.92249400	2.98393600	-1.53282600
H	4.21865300	-3.73226300	4.51446400	H	5.53578600	2.67455300	0.97221600
H	5.32983900	-3.72568100	0.36619700	H	0.16789100	8.56521500	-0.50072000
H	1.84044900	-4.03020100	3.87677100	H	-5.34021000	5.81717900	-2.58124300
H	2.97056400	-4.04137300	-0.27677800	H	-6.31285000	4.49563000	-0.15343700
H	1.20376900	-4.15441000	1.48011900	H	10.94154700	-0.28889700	1.22087100
H	6.87294600	-5.64787400	3.08006000	H	10.19846700	-0.86350400	-0.27587800
H	-6.10564000	4.28832300	-3.04443600	H	8.29294800	-4.62431500	2.80654400
H	-4.43482700	4.61712300	-3.51146100	H	7.20287500	-5.01212400	1.46665200
H	-2.66637700	3.20784300	-1.78505400	H	-2.98046900	-4.13161600	-5.40512100
H	-5.02493500	3.29422300	1.68085800	H	-1.86462900	-3.37656500	-4.21531200
H	-2.25407300	-5.09569000	-4.09428900	H	3.90681500	0.28536300	-5.42247000

H	5.23045300	0.60535700	-4.29202700	O	0.63111200	3.04077400	-2.56588400
H	-3.99126200	3.99190100	3.93295800	O	-1.02886200	1.50705900	-2.72712000
H	1.00164100	5.65550000	3.24512600	H	-0.89812400	1.41569300	-1.64410000
H	-0.62616700	6.86581300	4.52327600	N	-0.83184800	-0.31705600	-0.62314900
H	0.48018500	3.08525000	-5.12542100	C	-0.34153100	-1.55125900	-0.98641700
C	-2.02436200	-4.50203300	7.60109600	O	-1.02755600	-2.39514000	-1.58478000
C	-0.70538900	-4.52745600	6.81722000	N	0.95867300	-1.81311800	-0.67472800
H	-0.38498300	-5.56624500	6.67200700	C	1.86307500	-0.70546100	-0.42319900
H	0.08088900	-4.03430800	7.40115800	C	1.24516200	0.24405100	0.63325200
H	-2.35007400	-3.47158300	7.77764300	C	-0.25206400	0.67100100	0.39039400
H	-2.81795700	-5.00827200	7.04225600	O	-1.05917700	0.54278100	1.49343800
H	-1.92780000	-4.99764200	8.57378200	H	2.75678000	-1.13352800	0.04410900
C	-0.88135000	-3.83917300	5.48693400	H	1.82701200	1.16963600	0.58694300
C	-0.65170300	-2.46587400	5.34660900	H	-1.85224900	-0.35072500	-0.58852500
C	-1.42872000	-4.52734500	4.39507100	H	1.33098700	-2.60097300	-1.20115700
C	-0.95764800	-1.79195000	4.16621900	O	-0.47852800	1.93292900	-0.20329600
C	-1.73771500	-3.87334400	3.20805900	C	1.45684800	-0.33167300	2.03936600
C	-1.50085500	-2.49605900	3.08124500	H	2.52722700	-0.47313500	2.22416400
O	-1.82540500	-1.90648000	1.91053000	H	1.05575800	0.33993400	2.79926600
H	-0.23777600	-1.90754600	6.18387100	H	0.97547000	-1.30328400	2.15294400
H	-1.62996700	-5.59295400	4.48440600	C	2.30241000	-0.06701900	-1.74881200
H	-0.77816700	-0.72615900	4.07158800	H	1.45234400	0.36921600	-2.27802100
H	-2.17550300	-4.40372700	2.36956400	H	3.05381400	0.70961200	-1.59578000
H	-1.48749000	-0.96465500	1.83715600	H	2.73177700	-0.84493400	-2.38884400
C	-0.12336500	2.30110000	-3.22216000				

(5S,6S)-Me₂DHU-INT2-II (SmDHPase)

C	0.29556400	-8.84682900	-2.15073400	C	-3.15272900	6.14624800	2.24894500
C	0.54059100	-7.54135800	-1.45661300	C	1.18590500	-5.13518500	4.97263900
N	1.43747800	-7.40675300	-0.40568500	N	0.39587900	-5.12522000	3.76252800
C	0.00800400	-6.28545400	-1.60953700	C	0.55487000	-4.19194100	2.77524500
C	1.40817000	-6.12613200	0.03397700	O	1.58901600	-3.44622000	2.83997700
N	0.54994700	-5.41523900	-0.67717700	O	-0.33535200	-4.19562600	1.86361100
C	-5.58383400	-3.33767700	-1.87104900	C	3.61572900	-2.18583700	5.05551800
C	-4.36090900	-3.52886900	-1.04986500	C	3.77496400	-0.87707600	4.35740600
N	-4.38780200	-3.77862800	0.31118600	N	3.37480200	-0.70624800	3.04109000
C	-3.03518800	-3.50403700	-1.38401100	C	4.27011000	0.31300300	4.82277500
C	-3.11399100	-3.89139300	0.74877300	C	3.62058700	0.55776400	2.71936300
N	-2.26582100	-3.72433300	-0.25671600	N	4.16778400	1.20359300	3.76972200
C	-10.17813100	-1.13245800	-0.28943100	C	5.83743900	-4.56414800	-1.81687200
C	-8.92864900	-1.58172800	0.48337300	C	5.19652400	-3.82966300	-0.68086800
C	-9.03977900	-3.03516000	0.95168700	N	5.86040300	-3.57231000	0.50981200
S	-7.59950300	-3.71654100	1.87762400	C	3.95180300	-3.27408300	-0.50581300
C	-7.62312600	-2.70007800	3.39733500	C	5.02416300	-2.89340100	1.33332600
C	-7.79575400	4.18744800	1.28533700	N	3.85589000	-2.69923900	0.74921200
C	-6.69762600	4.60122200	0.28760900	C	2.57829800	3.64967000	-4.88477700
C	-5.45056700	5.14582600	0.95517600	C	3.67077300	3.69539000	-3.82733000
C	-4.46903100	4.27815900	1.45731200	O	4.76110300	4.21234900	-4.06636400
C	-5.25521900	6.52478700	1.10943200	N	3.34427200	3.14600100	-2.62228200
C	-3.32943100	4.76707900	2.09760300	C	4.26823000	3.18171500	-1.49836700
C	-4.11900700	7.02355400	1.74975400	C	4.65294300	1.75779700	-1.07877800

O	3.79924100	1.00033900	-0.57515900	H	5.29670200	-2.55255600	2.31994400
C	3.65369200	3.89890200	-0.27284100	H	2.19951300	4.66824900	-5.02280000
O	3.49722500	5.28485200	-0.45830100	H	4.34769500	3.77608800	0.57068000
N	5.93455000	1.34535300	-1.20254400	H	2.72091100	3.39477100	0.00252600
C	7.10006000	2.07636500	-1.76832700	H	2.74208000	5.45981000	-1.04898900
C	7.12141200	2.03758500	-3.30007800	H	5.12832200	3.75641300	-1.83924200
C	8.28092100	1.32720900	-1.12028400	H	2.45479500	2.65867400	-2.50342700
C	7.79450100	-0.12886600	-1.04967000	H	8.45686600	1.71294500	-0.10963900
C	6.30385900	0.00734200	-0.70557700	H	9.20489200	1.44808100	-1.69090600
C	0.62308600	-2.91318800	-4.44541200	H	8.33746000	-0.72245700	-0.30849200
C	-4.51367000	-1.52212300	-5.56784300	H	7.92071200	-0.61933200	-2.02045100
C	-3.98222100	-0.55565800	-4.51283100	H	6.12383300	-0.03603000	0.37565600
S	-5.00018400	0.98596700	-4.48937600	H	5.67265200	-0.75858700	-1.16417100
C	-1.10311300	4.93575800	-3.22104100	H	7.07696300	3.11607300	-1.43216000
C	-1.56851000	3.61376100	-3.80859800	H	0.20713200	-2.08819600	-5.03440500
O	-2.41996000	2.91090700	-3.24147000	H	1.65396000	-3.05058700	-4.78008900
C	-0.90570800	4.83037900	-1.69963000	H	-2.94744600	-0.28225800	-4.73044400
C	-0.00110200	5.94303800	-1.19229400	H	-4.00029600	-1.01338200	-3.51918800
O	1.09351800	6.15853200	-1.71879200	H	-4.06973100	1.77763800	-3.90704000
N	-0.45462100	6.66178500	-0.13934800	H	-5.56108000	-1.78185700	-5.38106500
N	-1.00338300	3.25479600	-4.98085900	H	-1.86625200	4.80124300	-1.17969200
C	-1.18194300	1.92753800	-5.55338000	H	-0.37409200	3.89893400	-1.47872800
Zn	2.18174200	-1.85223200	1.75823600	H	0.16423100	7.35102200	0.26243700
Zn	-0.24068900	-3.56536400	-0.08719300	H	-1.31391200	6.43763700	0.34209500
H	1.21036100	-9.24612500	-2.60246800	H	-0.16083200	5.25648100	-3.67348100
H	-0.09755700	-9.60147400	-1.46070100	H	-0.76938900	1.16567800	-4.88303200
H	-0.73560000	-5.95263100	-2.31667900	H	-2.24232300	1.72885900	-5.72255600
H	2.00100900	-5.75962900	0.85802100	H	-0.23861300	3.81693800	-5.32136700
H	-6.15482600	-2.45814900	-1.55376400	H	0.91434600	-4.33042500	5.66894900
H	-5.30900500	-3.19443900	-2.91794600	H	2.24234800	-5.02676200	4.72335600
H	-2.57821700	-3.32742200	-2.34298100	H	3.90342000	-2.10022200	6.10648900
H	-2.82420200	-4.07676400	1.77026600	H	2.58171300	-2.52973200	4.99622000
H	-8.78217200	-0.92379400	1.34793500	H	4.66428600	0.59892300	5.78470200
H	-8.03783200	-1.47012000	-0.14618700	H	3.40355300	1.01761700	1.76599900
H	-9.92411400	-3.17595100	1.58288000	H	4.38983400	2.18799600	3.79282100
H	-9.15035700	-3.70957500	0.09594000	H	-0.65991100	1.88721200	-6.51075000
H	-6.86127000	-3.10922200	4.06394400	H	-1.85676300	5.69858700	-3.45243300
H	-8.59569500	-2.77880500	3.88883700	H	7.08660700	1.00714600	-3.66916300
H	-7.39208000	-1.65331900	3.19251800	H	6.28609200	2.59986500	-3.72209300
H	-10.33792500	-1.74796600	-1.18119000	H	8.04509600	2.49925300	-3.66544600
H	-7.10121300	5.35558100	-0.39738700	H	-0.43768500	-8.70988700	-2.94776100
H	-6.42966100	3.73554900	-0.33027700	H	-6.25218500	-4.20444100	-1.81638200
H	-4.60247400	3.20521300	1.34497100	H	-5.23587900	-3.80655500	0.87660500
H	-6.00067900	7.21535300	0.72279000	H	2.00672400	-8.14504000	-0.01818000
H	-2.58184100	4.08095300	2.48560800	H	6.13626000	-5.57863900	-1.52919800
H	-3.99234700	8.09660200	1.86357500	H	6.81213700	-3.83203600	0.72447600
H	-2.27727100	6.52392100	2.76994900	H	-11.07739600	-1.20479900	0.33140200
H	-7.43600300	3.41038700	1.96792900	H	-10.08008900	-0.09296000	-0.61518700
H	6.72923400	-4.04464300	-2.18458800	H	-8.67331200	3.79889400	0.75854800
H	5.13478000	-4.64457200	-2.64855100	H	-8.11466000	5.03941700	1.89398000
H	3.13625100	-3.21276300	-1.20921400	H	3.02164500	3.33133300	-5.83096700

H	1.75844900	2.98390200	-4.60715200	C	0.57868600	-2.53538000	-3.00596300
H	-4.45493700	-1.08471600	-6.56823800	O	-0.28781100	-2.97402800	-2.24520600
H	-3.93201600	-2.45128200	-5.56623200	O	1.52709400	-1.68433700	-2.69300500
H	4.23639100	-2.96745900	4.60139800	H	1.31110200	-1.13781600	-1.86532400
H	-0.48930400	-5.60786100	3.75105700	N	0.90314100	0.15067100	-0.76814800
H	1.04548500	-6.09113800	5.48346200	C	0.17811900	1.08010800	-1.51207800
H	0.03672700	-3.81241700	-4.63442600	O	0.72473700	1.75342400	-2.40307400
C	1.07432100	5.63650400	6.83975800	N	-1.15299100	1.14186600	-1.26871100
C	-0.16121800	5.56092800	5.92890900	C	-1.71342100	0.79669100	0.03853500
H	-0.45376200	6.57558500	5.63211100	C	-1.16755100	-0.57533500	0.45729400
H	-1.00545900	5.14717100	6.49320600	C	0.38694300	-0.64030800	0.40276300
H	1.37013200	4.63762700	7.17745100	O	1.00887400	-0.20164100	1.53867800
H	1.92578700	6.07152600	6.30633300	H	-1.39554800	1.54494700	0.78074800
H	0.88155500	6.25035800	7.72639500	H	-1.53463200	-1.28038000	-0.29606500
C	0.10262300	4.71772300	4.70270500	H	1.87149900	0.46399600	-0.63458800
C	-0.14958600	3.34085600	4.70053400	H	-1.65388700	1.81280900	-1.84982200
C	0.70671200	5.26984400	3.56342200	O	0.83391300	-1.98015800	0.20289500
C	0.18965900	2.53728400	3.61200200	C	-1.67196300	-0.98231300	1.84600000
C	1.05333400	4.48824900	2.46490900	H	-2.75240000	-1.15269700	1.83427200
C	0.79811700	3.10770600	2.48243600	H	-1.18986600	-1.89983500	2.18561900
O	1.15262200	2.37636900	1.39964000	H	-1.45472200	-0.20107400	2.57833500
H	-0.61407100	2.88318800	5.57160400	C	-3.23862300	0.83118900	-0.07302800
H	0.92748200	6.33548700	3.54391000	H	-3.59855800	0.03500500	-0.73385000
H	0.00284900	1.46762100	3.62984400	H	-3.70768300	0.71167300	0.90635800
H	1.53930800	4.92736200	1.59885200	H	-3.56802200	1.78864800	-0.48807400
H	1.05616200	1.38121600	1.55280500				

(5S,6S)-Me₂DHU-TS3-II (*Sm*DHPase)

C	0.22874700	-8.85651200	-2.21125200	C	-4.12600800	7.11324200	1.69852000
C	0.37406600	-7.61632400	-1.39019300	C	-3.17124300	6.24669700	2.23726500
N	0.77899900	-7.65257300	-0.06495600	C	1.09749600	-5.18273000	4.93438100
C	0.14671500	-6.28653200	-1.64076800	N	0.33671500	-5.13746000	3.70447200
C	0.76922000	-6.39418800	0.43167600	C	0.47239200	-4.11103200	2.79427600
N	0.39027600	-5.53526300	-0.50172900	O	1.48871800	-3.35490400	2.92643700
C	-5.60581200	-3.29892900	-1.95136900	O	-0.41553000	-4.06972900	1.88666500
C	-4.38545400	-3.45841600	-1.11696800	C	3.55146800	-2.25447000	5.04787400
N	-4.42844700	-3.63359900	0.25524600	C	3.76482800	-0.94458500	4.36616700
C	-3.05457100	-3.47011000	-1.43763800	N	3.36743900	-0.73937600	3.05461700
C	-3.16080600	-3.74182900	0.71143600	C	4.30685900	0.21921500	4.84593200
N	-2.30048800	-3.64083800	-0.29175300	C	3.65905700	0.51827100	2.74872500
C	-10.19292900	-1.06154900	-0.39428300	N	4.23411300	1.12822100	3.80610900
C	-8.94807300	-1.49257100	0.39589000	C	5.80397600	-4.62243300	-1.81805900
C	-9.05701900	-2.93907600	0.88547000	C	5.15579400	-3.90121000	-0.67458100
S	-7.62073400	-3.59919500	1.83204700	N	5.79139300	-3.73021600	0.54725500
C	-7.66660800	-2.56659000	3.34034500	C	3.93473000	-3.28890100	-0.51506400
C	-7.77745200	4.23125400	1.22087600	C	4.96469500	-3.04495700	1.37377400
C	-6.67399300	4.65876900	0.23506800	N	3.82775400	-2.76334000	0.76240500
C	-5.44148600	5.21888600	0.91661400	C	2.63721700	3.63163600	-4.87466400
C	-4.47133300	4.36220800	1.45889100	C	3.72999500	3.69253200	-3.81747800
C	-5.24848000	6.60066500	1.04416400	O	4.81832600	4.21122100	-4.05734800
C	-3.34524700	4.86451000	2.11167200	N	3.40027100	3.15264700	-2.60848100

C	4.32522600	3.17547200	-1.48505000	H	5.14047600	-4.61118400	-2.68484600
C	4.66949600	1.74350600	-1.05889500	H	3.14615100	-3.15038300	-1.23958100
O	3.78983100	1.01368000	-0.55671800	H	5.22380800	-2.76119200	2.38185800
C	3.73175400	3.91606500	-0.26245700	H	2.25266100	4.64675800	-5.02344800
O	3.58932700	5.30050500	-0.46601900	H	4.43385200	3.79340000	0.57459000
N	5.93723100	1.29358200	-1.17717200	H	2.79576300	3.42690000	0.02779400
C	7.12660800	1.99585200	-1.73118200	H	2.79787100	5.47651400	-1.00508800
C	7.15465500	1.97439300	-3.26337300	H	5.19881400	3.72558100	-1.83208400
C	8.28232200	1.20444700	-1.08762000	H	2.52357800	2.64376700	-2.50509700
C	7.75087000	-0.23636300	-1.03078200	H	8.46816300	1.57562700	-0.07328000
C	6.26620700	-0.05708300	-0.68330800	H	9.21059100	1.30212900	-1.65565700
C	0.62341800	-2.91621000	-4.47794700	H	8.27516300	-0.85415400	-0.29619800
C	-4.49292500	-1.47689200	-5.63232000	H	7.86016300	-0.72095100	-2.00648700
C	-3.84325700	-0.63271700	-4.54010500	H	6.08807600	-0.09745800	0.39831800
S	-4.87466500	0.85843000	-4.17159300	H	5.61064900	-0.80155200	-1.14220900
C	-0.91227300	4.93962300	-3.23829200	H	7.13251100	3.03186700	-1.38259400
C	-1.42680100	3.63130400	-3.81683500	H	0.22542300	-2.02623800	-4.97771700
O	-2.28177700	2.94563000	-3.23250800	H	1.62795300	-3.07610200	-4.87710300
C	-0.96733500	4.95716100	-1.70545500	H	-2.85472200	-0.29479200	-4.85735200
C	-0.03207100	6.01897500	-1.14159800	H	-3.71433700	-1.21253600	-3.62141700
O	1.10881700	6.16315600	-1.58551600	H	-3.86002600	1.67462300	-3.80420400
N	-0.51779500	6.77085400	-0.12679500	H	-5.50314000	-1.79095800	-5.34854000
N	-0.90576200	3.26516900	-5.00646600	H	-1.99211300	5.07267200	-1.34456000
C	-1.13237000	1.94430000	-5.57842200	H	-0.59277000	4.00336300	-1.31805600
Zn	2.17961700	-1.86360900	1.76441200	H	0.11537500	7.41386100	0.32611800
Zn	-0.26101600	-3.57366800	-0.14018900	H	-1.41394500	6.58839400	0.30285700
H	1.17485600	-9.40259700	-2.29859100	H	0.12124800	5.11602100	-3.54940800
H	-0.51443300	-9.53801400	-1.78240200	H	-0.71812300	1.16923000	-4.92494800
H	-0.18815700	-5.81500900	-2.55104000	H	-2.20166800	1.77190900	-5.71697400
H	1.00390700	-6.16486800	1.45897200	H	-0.13687300	3.80937800	-5.36683300
H	-6.14523200	-2.37527400	-1.71360600	H	0.79606800	-4.41166700	5.65608600
H	-5.33099000	-3.25814100	-3.00733200	H	2.15633100	-5.04551200	4.71323100
H	-2.58189900	-3.36226500	-2.40008700	H	3.88044200	-2.20349600	6.08908300
H	-2.88515300	-3.87976300	1.74418900	H	2.49796500	-2.53640600	5.01900000
H	-8.81200100	-0.82087500	1.25153000	H	4.71525400	0.47638500	5.81004000
H	-8.05234300	-1.38688900	-0.22760500	H	3.45772200	0.99676400	1.80086500
H	-9.94583200	-3.07455100	1.51156900	H	4.49890600	2.10153200	3.84153100
H	-9.15771200	-3.62674000	0.03908200	H	-0.64095700	1.89642300	-6.55137100
H	-6.90629200	-2.96112300	4.01743700	H	-1.51650500	5.75942400	-3.64764300
H	-8.64242900	-2.64957000	3.82465200	H	7.09501600	0.94978600	-3.64499200
H	-7.44414000	-1.51979500	3.12629400	H	6.33649500	2.56214500	-3.68460700
H	-10.34186800	-1.69177800	-1.27759800	H	8.09202700	2.41620500	-3.61808600
H	-7.07915600	5.40798600	-0.45453100	H	-0.10027900	-8.59946300	-3.22004900
H	-6.38869000	3.79608300	-0.37938300	H	-6.30062700	-4.13578000	-1.81926200
H	-4.60336000	3.28720600	1.36734800	H	-5.28236100	-3.63099400	0.81316700
H	-5.98517600	7.28272900	0.62691400	H	1.02552500	-8.48265600	0.45393100
H	-2.60519100	4.18674800	2.52782600	H	6.01602700	-5.66866900	-1.57016700
H	-4.00228300	8.18851300	1.79326100	H	6.71809700	-4.05479700	0.78182000
H	-2.30634100	6.63559000	2.76746400	H	-11.09728900	-1.12868800	0.21971700
H	-7.41552000	3.45890200	1.90759600	H	-10.09718300	-0.02680900	-0.73557200
H	6.74677000	-4.14881300	-2.11326100	H	-8.64392300	3.83123700	0.68448800

H -8.11394900 5.07925200 1.82552000
H 3.08417800 3.30926100 -5.81789900
H 1.82349100 2.96039700 -4.59405800
H -4.57288200 -0.91641600 -6.56748700
H -3.90228900 -2.38067300 -5.82146700
H 4.10830000 -3.06263000 4.55969100
H -0.57681600 -5.56739900 3.69599700
H 0.96387100 -6.16166500 5.40184000
H -0.01788600 -3.76769300 -4.71033500
C 1.06305900 5.58152100 6.84686200
C -0.14584200 5.55912600 5.89783900
H -0.39939500 6.58685600 5.61077300
H -1.01831700 5.16157700 6.43020300
H 1.32009300 4.56853900 7.17396600
H 1.94242800 6.00165000 6.34782100
H 0.86020800 6.18401900 7.73893800
C 0.12665400 4.72999700 4.66355300
C -0.11110000 3.35021200 4.65321500
C 0.71944900 5.29557300 3.52526300
C 0.22981500 2.55804200 3.55742200
C 1.06669200 4.52497700 2.41841900
H 1.91970700 0.43277800 -0.64645500
H -1.53291400 1.88669000 -1.87932300
O 0.80933500 -1.98980500 0.24905700
C -1.65763300 -0.89568300 1.81842700
H -2.74365900 -1.02372000 1.80231800
H -1.21117100 -1.83220800 2.15255200
H -1.41349400 -0.12370000 2.55214800

C 0.82382100 3.14279900 2.42750800
O 1.17331200 2.41925300 1.33572500
H -0.56577400 2.88153300 5.52362100
H 0.93070300 6.36316800 3.51240000
H 0.05576400 1.48625700 3.56963400
H 1.54720800 4.97410700 1.55436100
H 1.09650100 1.42259200 1.49342900
C 0.68148200 -2.64336900 -3.00643000
O -0.16788500 -3.15664000 -2.24598200
O 1.63619000 -1.84036100 -2.67901600
H 1.32614700 -1.02020700 -1.76706100
N 0.97314200 0.07126600 -0.84389900
C 0.25974900 1.05355900 -1.59898200
O 0.81966500 1.63084500 -2.53766700
N -1.03170500 1.23143500 -1.27764000
C -1.60978800 0.89074400 0.02510600
C -1.13230100 -0.50778100 0.43173500
C 0.41537500 -0.64675900 0.38926500
O 1.05731600 -0.15629700 1.48529800
H -1.25493800 1.61722100 0.76921400
H -1.53276600 -1.19393900 -0.32301700
C -3.13084700 1.00327200 -0.09158300
H -3.52907400 0.24828000 -0.77764900
H -3.60633100 0.87738800 0.88359700
H -3.41151700 1.98804100 -0.47679300

(5S,6S)-Me2DHU-EP-II (SmDHPase)

C 2.59463400 8.22468100 -2.96527900
C 2.16480300 7.26360400 -1.92532200
N 2.01363400 7.56189600 -0.57966300
C 1.87858600 5.93586900 -2.02564600
C 1.66400600 6.42807900 0.07591300
N 1.57201900 5.42548600 -0.78175800
C 6.45259700 1.19713500 -2.11326000
C 5.36342900 1.77695100 -1.28572300
N 5.39359500 1.84106500 0.09703900
C 4.16152000 2.32110800 -1.64550500
C 4.24025100 2.40486100 0.52222400
N 3.46692400 2.70154900 -0.51323500
C 10.16208700 -2.18175600 -0.29807500
C 8.93574600 -1.49817200 0.32325400
C 9.33352500 -0.38720300 1.29826100
S 7.95286100 0.52095400 2.11261800
C 7.22540700 -0.78409100 3.16691100
C 6.27214000 -6.30516700 1.78106900
C 5.76002200 -4.89186200 2.10399500
C 4.27610200 -4.74058900 1.84673000
C 3.35045000 -4.72391900 2.89791300

C 3.79251300 -4.66133400 0.53340100
C 1.97932300 -4.63061600 2.64808000
C 2.42507500 -4.57614700 0.27419000
C 1.51358200 -4.55782700 1.33449800
C 0.77066100 5.67826700 4.48457300
N 1.44218500 5.13152800 3.31091300
C 0.88418500 4.20360600 2.45251600
O -0.38230400 4.01516500 2.57537500
O 1.64448100 3.66424700 1.60300400
C -2.45914700 3.66633800 4.84517100
C -3.12169900 2.44071800 4.30453800
N -2.89337500 1.99888400 3.00671700
C -4.00114900 1.57912000 4.90438700
C -3.62189000 0.90046500 2.82699600
N -4.30459800 0.62009400 3.95510100
C -4.00079000 5.95773000 -2.23967100
C -3.69970300 5.08785800 -1.06457700
N -4.56555300 4.93465600 0.00947900
C -2.61420800 4.30770600 -0.75944700
C -4.00136900 4.09752300 0.90697800
N -2.81355100 3.69845100 0.46905200

C	-3.56623400	-3.11728800	-4.46587700	H	2.07816400	-4.52442400	-0.75408800
C	-4.74955100	-2.78543500	-3.57372400	H	0.44856900	-4.46189100	1.14183100
O	-5.90626900	-2.76663000	-3.99195300	H	5.76017100	-7.05345700	2.39395400
N	-4.41970500	-2.52591600	-2.27233100	H	-4.93723500	5.67087200	-2.73114700
C	-5.42866400	-2.43973700	-1.22880700	H	-3.19441900	5.85775900	-2.96887200
C	-5.47375800	-1.03724400	-0.59608600	H	-1.72980200	4.13374200	-1.36143200
O	-4.51048700	-0.63351000	0.08777600	H	-4.46125400	3.80749500	1.83816300
C	-5.08985800	-3.45863900	-0.11578400	H	-3.21765800	-4.12427900	-4.21938400
O	-5.09077500	-4.79222100	-0.59076300	H	-5.84890200	-3.40434100	0.67306000
N	-6.58039000	-0.27390900	-0.71578400	H	-4.12337200	-3.17324400	0.31731300
C	-7.72214100	-0.43588000	-1.65213600	H	-4.50316800	-4.86013800	-1.37260600
C	-7.33056800	-0.01319800	-3.07148500	H	-6.38054600	-2.70408500	-1.69027500
C	-8.78023000	0.47433100	-1.00397000	H	-3.44977200	-2.66066600	-1.96025300
C	-7.95866200	1.65854500	-0.46632300	H	-9.26763000	-0.05377400	-0.17688600
C	-6.64183600	1.01390300	0.00122800	H	-9.55464400	0.77444500	-1.71391800
C	0.36112900	2.50614700	-4.66549300	H	-8.46497100	2.19295300	0.34205000
C	4.77035500	-0.53219500	-5.61857900	H	-7.76571700	2.37964800	-1.26674800
C	3.90188200	-0.96561500	-4.44253500	H	-6.63428400	0.82052800	1.08084400
S	4.32784500	-2.69009300	-3.92064600	H	-5.75731300	1.61867600	-0.22143600
C	-0.28883500	-5.91019900	-3.31348300	H	-8.05389800	-1.47655500	-1.65827700
C	0.29190300	-4.52497200	-3.59063800	H	-0.27478900	3.06496600	-5.35469800
O	1.08136900	-3.96184600	-2.81857400	H	1.36386300	2.38897400	-5.08230000
C	-0.64354800	-6.18079700	-1.84969000	H	2.84842400	-0.93783700	-4.72604700
C	-2.10096400	-5.88175100	-1.50097800	H	4.03369400	-0.29254200	-3.59145000
O	-2.93139200	-5.53634300	-2.34719200	H	3.14383400	-3.00433800	-3.34878400
N	-2.44349100	-6.09983600	-0.20884400	H	5.83621200	-0.57882500	-5.37126800
N	-0.03065500	-3.99395800	-4.79217900	H	-0.46489900	-7.23639200	-1.61464100
C	0.52571400	-2.73903300	-5.28143500	H	0.01127900	-5.60363700	-1.19063900
Zn	-1.50608500	2.71801300	1.65785800	H	-3.38532900	-5.83705800	0.07084600
Zn	1.56054500	3.41324200	-0.64153000	H	-1.73979000	-6.24392200	0.49781800
H	1.91411800	9.08011600	-3.05197400	H	-1.16686900	-6.09420800	-3.93838300
H	3.59847500	8.62103200	-2.77155100	H	0.13802500	-1.88260600	-4.72117000
H	1.88878500	5.30266300	-2.89537200	H	1.61397500	-2.76002300	-5.20211900
H	1.50701800	6.37196000	1.14253900	H	-0.73751000	-4.45567600	-5.34353200
H	6.55941600	0.11847200	-1.95083000	H	0.74614800	4.97607800	5.32813300
H	6.23216700	1.35257000	-3.17135400	H	-0.25449200	5.93852100	4.22111200
H	3.72803600	2.45605500	-2.62319600	H	-2.77530900	3.84483700	5.87602800
H	3.98096600	2.57880400	1.55450400	H	-1.37285500	3.56855600	4.81937200
H	8.32818000	-2.24859600	0.84249100	H	-4.42210800	1.56209300	5.89676000
H	8.30154000	-1.07653100	-0.46523700	H	-3.68848600	0.30056800	1.92740500
H	9.97775300	-0.77588300	2.09456700	H	-4.89011800	-0.19152200	4.08687000
H	9.90182700	0.39452300	0.78321200	H	0.25173000	-2.62353200	-6.33144000
H	6.44295400	-0.31009000	3.76300200	H	0.49071900	-6.61461200	-3.62871600
H	7.98338300	-1.18696600	3.84282700	H	-6.91878900	1.00126700	-3.08436500
H	6.78373300	-1.58947500	2.57754700	H	-6.60537200	-0.70818500	-3.49619400
H	10.77989200	-1.46659100	-0.85179900	H	-8.21353100	-0.03003000	-3.71967500
H	6.31479400	-4.16534000	1.49423800	H	2.61798300	7.72384400	-3.93493300
H	5.97883000	-4.65481500	3.15189300	H	7.42105000	1.66423400	-1.90253800
H	3.70803300	-4.78472300	3.92342000	H	6.14465600	1.47929100	0.68869300
H	4.49530700	-4.66900500	-0.29700500	H	2.14262700	8.46789600	-0.15380100
H	1.27571400	-4.60730400	3.47519500	H	-4.07850200	7.01387200	-1.95694300

H -5.46970500 5.37285700 0.10786000
H 10.79282700 -2.64237200 0.46955600
H 9.85675000 -2.96810500 -0.99437700
H 7.34751200 -6.38915900 1.97012700
H 6.09278000 -6.55814000 0.73164400
H -3.88822900 -3.07083500 -5.50659400
H -2.73677200 -2.42445300 -4.29478900
H 4.60328300 -1.17114900 -6.48987300
H 4.53611100 0.50029700 -5.89993500
H -2.71271700 4.55139200 4.25271200
H 2.45183300 5.11314200 3.31621100
H 1.29337400 6.58325800 4.80335400
H -0.07383100 1.50835200 -4.54507700
C -2.45606200 -4.35102900 7.40507500
C -1.23590800 -4.70314000 6.54125500
H -1.24022500 -5.77617200 6.31702600
H -0.31644300 -4.50239300 7.10406100
H -2.45706300 -3.28614000 7.65978500
H -3.38618600 -4.56490100 6.86875700
H -2.46641500 -4.92204300 8.34004800
C -1.25924800 -3.89917100 5.26525600
C -0.74102100 -2.59960800 5.23036400
C -1.93281200 -4.37002400 4.12934800
C -0.91394100 -1.77822000 4.11871800
C -2.10893800 -3.56778300 3.00647100
C -1.61505400 -2.25797500 3.00560800
O -1.85818400 -1.49524900 1.90834000
H -0.20957800 -2.21443200 6.09784700
H -2.33902000 -5.37913400 4.13322000

H -0.51468000 -0.76802800 4.10892200
H -2.62171500 -3.92826200 2.12074400
H -1.32282200 -0.67731600 1.92364400
C 0.39734800 3.19642400 -3.30433100
O 1.48448500 3.02055300 -2.61840600
O -0.58040800 3.85573000 -2.92709400
N -1.82688700 -0.62319700 -1.10062300
C -1.20246400 -1.83508100 -1.00688800
O -1.84358500 -2.89646800 -1.11168800
N 0.15480000 -1.89646500 -0.81219300
C 1.16070300 -0.84430100 -0.94291000
C 1.34044800 0.05549700 0.33238400
C 0.23433500 1.06250300 0.59743100
O -0.56985800 0.90862500 1.57431500
H 2.10338500 -1.40046500 -0.96868200
H 2.20659200 0.67625200 0.08701400
H -2.80088800 -0.62459000 -0.80071700
H 0.49226500 -2.81800200 -1.06351400
O 0.08784700 2.09218600 -0.14107900
H -1.32450500 0.23819400 -0.96902600
C 1.67204200 -0.78937000 1.56578500
H 2.58782300 -1.36078400 1.39034000
H 1.82213400 -0.15941700 2.44677700
H 0.88006200 -1.50586200 1.78118300
C 1.06498600 -0.08805900 -2.26949400
H 0.12973600 0.45860700 -2.38521100
H 1.87140600 0.63610600 -2.37992900
H 1.12771200 -0.82138100 -3.07551300

(5S,6R)-Me₂DHU-ES-II (*Sm*DHPase)

C 1.10234900 8.66194000 -2.62608900
C 0.91388200 7.57274000 -1.63028000
N 0.73752500 7.79539000 -0.27237500
C 0.88858200 6.21201700 -1.76589800
C 0.62358100 6.59756400 0.35272300
N 0.71021300 5.61860200 -0.53125000
C 6.09521100 2.37981700 -1.84992800
C 4.88286400 2.64709700 -1.02781500
N 4.89433700 2.69609500 0.35763600
C 3.58162900 2.88788300 -1.37906200
C 3.63698300 2.95630600 0.78890700
N 2.81674600 3.07486700 -0.24298200
C 10.28219500 -0.36928400 -0.01043200
C 10.27086300 1.15140600 0.15703400
C 9.63933500 1.65931600 1.45817400
S 7.84030100 1.29713200 1.66114100
C 7.84066900 -0.22296700 2.67605200
C 7.10964700 -5.17082900 1.81636300
C 6.12553600 -4.04700400 2.17783900

C 4.68995100 -4.41444300 1.87161100
C 3.80147500 -4.79001700 2.88715400
C 4.22957700 -4.42385100 0.54742600
C 2.49120100 -5.16915800 2.59098200
C 2.92225100 -4.80354600 0.24187400
C 2.04935100 -5.18045900 1.26696200
C -0.46013900 5.58411100 4.68124000
N 0.40163400 5.23207300 3.56515100
C 0.14049000 4.15382500 2.73674700
O -1.00924300 3.60929700 2.87617400
O 1.03861200 3.83645300 1.90696300
C -1.92830000 -4.87384000 7.24625100
C -0.71697200 -5.12387900 6.33780000
C -0.94376400 -4.41468100 5.02799700
C -1.43312300 -5.08752700 3.90211900
C -0.85393200 -3.01872200 4.97940800
C -1.84730600 -4.39564400 2.76551600
C -1.27827700 -2.30763000 3.86428600
C -1.78693700 -2.99967700 2.75878500

O	-2.24464100	-2.34121300	1.65655200	H	6.56472100	1.42726000	-1.58299900
C	-3.30090200	3.03417100	4.87471200	H	5.82229600	2.34195700	-2.90659000
C	-3.76295600	1.82804600	4.12451600	H	3.12418200	2.94197500	-2.35387000
N	-3.29633500	1.49215400	2.85838200	H	3.34514800	3.06331900	1.82157600
C	-4.68639100	0.89140400	4.51250000	H	9.75429800	1.61262700	-0.69322000
C	-3.93715300	0.38905700	2.49314200	H	11.30141100	1.53095200	0.13181500
N	-4.78556100	-0.00483400	3.46689900	H	10.14935600	1.25173600	2.33740300
C	-5.01768300	5.26801800	-2.18820300	H	9.72035900	2.74843500	1.51762100
C	-4.56268900	4.60110800	-0.94232500	H	6.79520300	-0.47406900	2.86689700
N	-5.26936200	4.62574300	0.25057200	H	8.34192400	-0.04868700	3.63081700
C	-3.44147000	3.86355900	-0.67691200	H	8.31331000	-1.05355000	2.14972900
C	-4.57085800	3.91761800	1.17213800	H	10.80419500	-0.85865400	0.81981400
N	-3.45924100	3.44291100	0.63871400	H	6.39866000	-3.14051300	1.62197700
C	-2.95376100	-3.51399400	-4.66153400	H	6.22350300	-3.80405300	3.24239200
C	-4.13068900	-3.39427400	-3.71166200	H	4.13959800	-4.78369800	3.92066800
O	-5.26638100	-3.70681000	-4.05985900	H	4.90248400	-4.13031400	-0.25527800
N	-3.81756600	-2.93453900	-2.46557700	H	1.80944200	-5.44148200	3.39102300
C	-4.83716000	-2.75992900	-1.44491200	H	2.59326400	-4.77085600	-0.79310300
C	-4.89023900	-1.28737500	-1.03237900	H	1.02720100	-5.47336100	1.04622300
O	-3.88320500	-0.73665600	-0.53302600	H	6.88399000	-6.08278300	2.37775000
C	-4.58017300	-3.65273600	-0.20624000	H	-0.58393300	-6.19972500	6.17766400
O	-4.71558900	-5.01608700	-0.51332700	H	0.19457300	-4.75963400	6.82786600
N	-6.03976900	-0.60077900	-1.17310000	H	-1.51838700	-6.17141300	3.92383300
C	-7.31722500	-1.07206700	-1.77729800	H	-0.47642400	-2.47713000	5.84384800
C	-7.23690700	-1.15540800	-3.30443100	H	-2.23524500	-4.91867900	1.89649500
C	-8.31165900	-0.00594300	-1.27615600	H	-1.22792100	-1.22272800	3.84298900
C	-7.47950800	1.28585800	-1.24728300	H	-2.04052900	-1.39136700	1.74079000
C	-6.10544000	0.81327500	-0.75479300	H	-2.84596100	-5.23843100	6.77407300
C	0.05798600	2.74368200	-4.55221900	H	-5.99639000	4.90175200	-2.51987500
C	-0.15613000	2.78634700	-3.04187700	H	-4.30172400	5.06869300	-2.98780500
O	0.82413200	3.25019500	-2.35352500	H	-2.64841600	3.58460700	-1.35602300
O	-1.25100000	2.39009100	-2.58125000	H	-4.90220800	3.76427000	2.18744200
C	4.83713000	0.50805900	-5.45846700	H	-2.75345400	-4.57926400	-4.82448000
C	4.06016400	-0.30520300	-4.43129200	H	-5.33857500	-3.40233700	0.55062800
S	4.85103600	-1.96285400	-4.21291300	H	-3.60500900	-3.40202100	0.21971500
C	0.39643000	-5.48605200	-3.15280100	H	-3.84833900	-5.37229000	-0.77232400
C	1.05623200	-4.20865000	-3.65925600	H	-5.76773500	-3.09398400	-1.89970200
O	1.95293500	-3.65586400	-3.00009800	H	-2.87725400	-2.58618300	-2.28764300
C	-0.40776300	-5.18824400	-1.86938400	H	-8.65063400	-0.25717500	-0.26452300
C	-1.04741000	-6.38794000	-1.18337900	H	-9.19373500	0.06055400	-1.91735400
O	-2.21688300	-6.37547200	-0.80439900	H	-7.90768700	2.05485000	-0.59847300
N	-0.25360800	-7.47496700	-0.98360600	H	-7.39902500	1.70941300	-2.25350700
N	0.61299000	-3.71413900	-4.83026300	H	-6.02421100	0.87495100	0.33745900
C	1.03177200	-2.40793900	-5.32811600	H	-5.26495900	1.37255700	-1.17265800
Zn	-1.88862400	2.40683700	1.57466900	H	-7.57117500	-2.05398700	-1.36847700
Zn	0.83115800	3.58348900	-0.26157700	H	-0.73696300	2.17858900	-5.04027700
O	-0.70162700	2.45126500	0.04483800	H	0.06446400	3.76445400	-4.95051400
H	0.24620400	9.34599600	-2.65747300	H	3.02949100	-0.44722600	-4.76263300
H	1.99702000	9.25942700	-2.41562200	H	4.03476300	0.21714700	-3.47096500
H	0.99576200	5.60521100	-2.65075400	H	3.79080500	-2.59277700	-3.65919000
H	0.48723900	6.47891900	1.41817400	H	5.88101200	0.64230900	-5.15608500

H	0.25191000	-4.69320000	-1.14811200	H	-2.05722100	-3.80422400	7.43819000
H	-1.21374200	-4.48781800	-2.08388700	H	-3.24543300	-3.08971700	-5.62551600
H	-0.63719100	-8.24124600	-0.44954200	H	-2.05625100	-3.01879400	-4.28879700
H	0.74243400	-7.44843200	-1.13241600	H	4.83433200	0.01834300	-6.43610600
H	-0.25115400	-5.93533600	-3.91292200	H	4.38976900	1.50153400	-5.57281800
H	0.72986200	-1.61936100	-4.63257500	H	-3.56752300	3.95994300	4.35353800
H	2.11477400	-2.38887700	-5.46411000	H	1.38301200	5.45951100	3.63680600
H	-0.17917800	-4.15995300	-5.26713300	H	-0.15709700	6.55992900	5.06934900
H	-0.41989700	4.85684200	5.50297200	H	1.03167500	2.30366000	-4.78643700
H	-1.49216200	5.65001700	4.33584900	N	-0.97900700	-0.64281600	-0.55967600
H	-3.75885700	3.05867300	5.86680100	C	-0.29747300	-1.39351300	-1.53359200
H	-2.21483400	3.03875300	4.97857800	O	-0.94157200	-2.05556300	-2.35423400
H	-5.25810600	0.78682200	5.42065000	N	1.04364700	-1.35276400	-1.45845300
H	-3.83795800	-0.11979300	1.54381800	C	1.76344200	-0.35372400	-0.65830500
H	-5.34148100	-0.84693200	3.44727700	C	1.08345100	-0.20869400	0.72013000
H	0.55305200	-2.23487300	-6.29279800	C	-0.42342000	-0.15544700	0.57696800
H	1.20700900	-6.19606100	-2.95710500	O	-1.16004300	0.21703600	1.51555300
H	-6.94571400	-0.19153800	-3.73499600	H	1.36377600	0.76215800	1.13937600
H	-6.53307100	-1.91969500	-3.63844100	H	-2.00598000	-0.68347300	-0.61909900
H	-8.22106000	-1.42092100	-3.70567600	H	1.53702400	-1.99662800	-2.07556300
H	1.21886800	8.23169300	-3.62271500	C	1.44771900	-1.31180600	1.73476400
H	6.85070200	3.16505300	-1.72922000	H	2.51096000	-1.26809700	1.97901900
H	5.70657600	2.52513800	0.94159200	H	0.88469900	-1.17892400	2.65862200
H	0.70465200	8.69720300	0.17968400	H	1.23460600	-2.31059000	1.34581100
H	-5.09475600	6.35559400	-2.07092200	H	1.68090400	0.61592000	-1.16589400
H	-6.14830500	5.09553800	0.41096400	H	-1.06008300	2.30405900	-0.86200200
H	9.26504400	-0.77045300	-0.05962400	C	3.23768100	-0.73841900	-0.57254500
H	10.79307000	-0.65361400	-0.93495900	H	3.69065800	-0.76524800	-1.56632700
H	8.14116000	-4.88052100	2.04214300	H	3.78383700	-0.00276700	0.02355400
H	7.05385600	-5.41525300	0.75109000	H	3.36772000	-1.72391200	-0.11988600
H	-1.82165800	-5.37859200	8.21328300				

(5S,6R)-Me₂DHU-TS1-II (*Sm*DHPase)

C	0.89108000	8.66446300	-2.49732500	C	6.44403400	-3.92799900	1.92426600
C	0.67872400	7.53150500	-1.55305400	C	4.96615800	-4.17725600	1.71950000
N	0.46939700	7.69989800	-0.19208600	C	4.12430100	-4.49035600	2.79429200
C	0.66841000	6.17587500	-1.73926600	C	4.41680700	-4.14356100	0.43063900
C	0.35506600	6.48011400	0.38589700	C	2.77087400	-4.76310200	2.59001200
N	0.46967000	5.53224500	-0.53052600	C	3.06531500	-4.41640900	0.21676400
C	6.03867500	2.48172600	-1.97557200	C	2.23806600	-4.72809100	1.30032800
C	4.85233600	2.76950400	-1.12698300	C	-0.44390300	5.38310800	4.76642000
N	4.88170100	2.75634100	0.25735600	N	0.35028700	5.05093300	3.59002000
C	3.55362700	3.04747600	-1.45668600	C	0.03988000	4.03829800	2.70160800
C	3.63387200	3.01346400	0.71164700	O	-1.12135600	3.51695100	2.80485400
N	2.80313300	3.18952700	-0.30576600	O	0.92231800	3.75433300	1.83567100
C	10.32482600	-0.21292600	-0.29038300	C	-3.22213600	2.76513600	4.95934200
C	8.99459600	0.19645300	0.35749100	C	-3.69412100	1.52242700	4.28390700
C	9.18049700	1.31903500	1.38157400	N	-3.34437100	1.22973400	2.97505300
S	7.65722100	1.91416400	2.22903100	C	-4.47883000	0.50749000	4.76704000
C	7.19239500	0.45037800	3.22227300	C	-3.90719400	0.06637800	2.67313700
C	7.30059600	-5.12677000	1.48873900	N	-4.60370400	-0.39984200	3.73190300

C	-5.14069400	5.12237800	-2.01093200	H	6.34433100	0.74591100	3.84328800
C	-4.63254600	4.39338800	-0.81941900	H	8.01934400	0.16164200	3.87525900
N	-5.29747800	4.35031300	0.39652500	H	6.89761600	-0.39406600	2.59682200
C	-3.49770800	3.65220300	-0.62984900	H	10.78897600	0.62954900	-0.81438600
C	-4.56656100	3.60418400	1.25778200	H	6.75116100	-3.04240800	1.35133700
N	-3.46820400	3.16673400	0.66414600	H	6.63788400	-3.70336500	2.97963300
C	-2.93501900	-3.55047400	-4.73444500	H	4.53356500	-4.51838700	3.80149400
C	-4.07372000	-3.43969400	-3.73229700	H	5.05268700	-3.89572800	-0.41637800
O	-5.20686100	-3.81852500	-4.02037600	H	2.12515200	-4.98788700	3.43356200
N	-3.73523100	-2.91580000	-2.51757700	H	2.66987200	-4.34748600	-0.79327100
C	-4.71293200	-2.81189200	-1.44539700	H	1.18020600	-4.92502100	1.15646900
C	-4.86615300	-1.35438700	-1.00183400	H	7.03850700	-6.02103700	2.06261300
O	-3.90076200	-0.73847300	-0.50201300	H	-6.12762100	4.76264100	-2.32403400
C	-4.33665100	-3.68160200	-0.22019200	H	-4.45438900	4.97506000	-2.84690600
O	-4.43442600	-5.05194900	-0.50909900	H	-2.73113400	3.40706900	-1.35148800
N	-6.07252000	-0.75892500	-1.09496100	H	-4.86259300	3.39386200	2.27321000
C	-7.31564500	-1.30385000	-1.70348100	H	-2.68662700	-4.61163700	-4.85009600
C	-7.23945400	-1.32245700	-3.23185800	H	-5.05621200	-3.45352600	0.58150400
C	-8.38411300	-0.33927200	-1.15242300	H	-3.34858400	-3.38273100	0.14266000
C	-7.65490800	1.01136200	-1.07731700	H	-3.55823300	-5.39756100	-0.75320800
C	-6.24036800	0.62787200	-0.62196900	H	-5.63808700	-3.21390500	-1.85437800
C	-0.17668700	2.73009400	-4.55257100	H	-2.80515700	-2.51714300	-2.37996000
C	-0.28617900	2.79158200	-3.03832800	H	-8.69061400	-0.65639700	-0.14903800
O	0.72206200	3.24410600	-2.39008500	H	-9.27644500	-0.31607800	-1.78254500
O	-1.34534800	2.36180300	-2.51524200	H	-8.13357400	1.71642300	-0.39193500
C	4.74501000	0.66590600	-5.60007600	H	-7.62265800	1.48115600	-2.06568700
C	3.99700600	-0.15893800	-4.56259100	H	-6.14247500	0.65458900	0.47081800
S	4.85147200	-1.77859700	-4.30888800	H	-5.45301800	1.26536800	-1.03175100
C	0.51137900	-5.30023400	-3.09784900	H	-7.49034500	-2.31753100	-1.33244000
C	1.11265100	-4.02956400	-3.68259000	H	-1.15857700	2.86977900	-5.00807800
O	1.99491200	-3.40635500	-3.06853700	H	0.53345300	3.46561300	-4.93604500
C	-0.24968700	-4.97836900	-1.79383600	H	2.97431900	-0.34920800	-4.89349200
C	-0.74348500	-6.19793100	-1.02947100	H	3.94537600	0.38013700	-3.61289300
O	-1.92719400	-6.35979600	-0.73753300	H	3.80976600	-2.43323800	-3.74753800
N	0.20183900	-7.11456200	-0.67975700	H	5.78070200	0.84919600	-5.29506600
N	0.64268500	-3.62490000	-4.87788400	H	0.40527000	-4.39312700	-1.14005300
C	1.00946200	-2.33849600	-5.45856600	H	-1.11850800	-4.35681000	-2.00595500
Zn	-1.96912800	2.15102600	1.64048700	H	-0.09370100	-7.87486800	-0.08415200
Zn	0.79456400	3.50663700	-0.28376200	H	1.18566300	-6.89299100	-0.70449300
H	0.03688700	9.35106600	-2.51648500	H	-0.15318000	-5.79888600	-3.81106800
H	1.78223400	9.24803400	-2.23934300	H	0.69181100	-1.52137500	-4.80347300
H	0.80523500	5.60702700	-2.64444500	H	2.08939700	-2.29074300	-5.61282200
H	0.21159800	6.32723500	1.44541400	H	-0.14060400	-4.12142500	-5.27401700
H	6.37054700	1.44223000	-1.87213900	H	-0.31816100	4.66248700	5.58491300
H	5.79038300	2.64694300	-3.02611700	H	-1.49832200	5.40938400	4.49095500
H	3.09021100	3.13595600	-2.42614600	H	-3.60365600	2.81278700	5.98276300
H	3.35279900	3.06728300	1.75144500	H	-2.13189500	2.80588400	4.98466200
H	8.54358800	-0.67740900	0.84220300	H	-4.93808400	0.35224000	5.73011400
H	8.28746600	0.52397800	-0.41357300	H	-3.83119600	-0.44539900	1.72307300
H	9.89042000	1.02455000	2.16226200	H	-5.07664200	-1.29072900	3.76947200
H	9.58842600	2.21560000	0.90300200	H	0.51149600	-2.23829200	-6.42388000

H	1.34541200	-5.98239500	-2.90330300	C	-1.05631800	-2.32432500	3.82721200
H	-7.01220100	-0.32636600	-3.62634100	C	-1.56029800	-4.36814300	2.62402000
H	-6.49050500	-2.02884200	-3.59372200	C	-1.50856500	-2.96955500	2.66802900
H	-8.20548800	-1.63627700	-3.64249600	O	-1.91058700	-2.28086000	1.56879300
H	1.02886200	8.27847000	-3.50917000	H	-0.30634800	-2.57100900	5.82057900
H	6.88702700	3.12936300	-1.72809300	H	-1.22676100	-6.18950400	3.70585900
H	5.70024600	2.53775400	0.82961400	H	-1.02556000	-1.23912800	3.85822500
H	0.41881300	8.58353200	0.29341600	H	-1.92266800	-4.86082000	1.72682500
H	-5.22284100	6.20064100	-1.83013700	H	-1.68235000	-1.32552900	1.64883700
H	-6.17876500	4.79510900	0.60753600	O	-0.59839200	2.06528900	-0.05357300
H	11.03825800	-0.57279900	0.45858600	N	-1.01379200	-0.37224400	-0.70299100
H	10.17229100	-1.01526200	-1.01799200	C	-0.33917500	-1.12345900	-1.65186600
H	8.36691200	-4.92774600	1.63895600	O	-0.96019300	-1.86911200	-2.42718700
H	7.14587500	-5.35580400	0.42985800	N	1.00752400	-1.01562000	-1.65482200
H	-3.29127000	-3.19250800	-5.70323600	C	1.74868400	-0.04802700	-0.84256600
H	-2.04945800	-2.99128300	-4.42657400	C	1.06943700	0.10783100	0.53438600
H	4.76922000	0.15849100	-6.56841100	C	-0.44006300	0.30653700	0.37389200
H	4.25819400	1.63789700	-5.73638100	O	-1.17345700	0.32527900	1.45750200
H	-3.55613600	3.66408300	4.43046900	H	1.44937200	1.01689500	1.00690800
H	1.33427100	5.27726900	3.61062800	H	-2.02814800	-0.51936600	-0.67859400
H	-0.14822900	6.37153100	5.12623100	H	1.49422700	-1.69536300	-2.23456300
H	0.17928500	1.73324800	-4.83623400	C	1.33130200	-1.07221500	1.48381100
C	-1.67242400	-5.23441000	7.06574200	H	2.39747100	-1.16294100	1.70052400
C	-0.43330300	-5.26367500	6.16180900	H	0.81047100	-0.91923700	2.42763300
H	-0.17670000	-6.30092900	5.91741300	H	0.99665900	-2.02152200	1.06038800
H	0.42520200	-4.84463200	6.70121700	H	1.70922600	0.92558800	-1.34563700
H	-1.92959800	-4.20613900	7.33975300	H	-1.00076000	2.08521100	-0.97900200
H	-2.53716700	-5.66565100	6.55140800	C	3.20890800	-0.48693200	-0.74499100
H	-1.51246700	-5.79972300	7.99081500	H	3.68019400	-0.49936800	-1.73005800
C	-0.70274600	-4.47809100	4.90313900	H	3.77102500	0.20426600	-0.11198700
C	-0.65153100	-3.07950000	4.92284900	H	3.29526700	-1.49061900	-0.32411700
C	-1.16267100	-5.10423400	3.73749400				

(5S,6R)-Me₂DHU-INT-II (*SmDHPase*)

C	0.66103800	8.62272800	-2.67564500	C	7.43568900	-4.88710900	1.65529500
C	0.45824400	7.50477400	-1.71271800	C	6.55968000	-3.66141700	1.96037900
N	0.20835900	7.69255100	-0.36133300	C	5.08574800	-3.94606900	1.77023000
C	0.49692500	6.14675400	-1.87196800	C	4.24982800	-4.21337100	2.86161400
C	0.11924500	6.48146200	0.23821900	C	4.53527100	-3.99636900	0.48221100
N	0.28811200	5.51995700	-0.65593600	C	2.90245800	-4.52722400	2.67384000
C	5.98256900	2.60661600	-1.98003500	C	3.19066300	-4.31293000	0.28607400
C	4.78773100	2.89079200	-1.14415900	C	2.37015200	-4.58211300	1.38494100
N	4.80479300	2.89843700	0.24024800	C	-0.64217300	5.45646300	4.64472800
C	3.48877000	3.14314500	-1.49024000	N	0.14193900	5.10230100	3.46556500
C	3.54946400	3.14031700	0.67951600	C	-0.17268300	4.08779300	2.58061500
N	2.72579500	3.28866900	-0.34838900	O	-1.33953300	3.57977200	2.66707000
C	10.33054300	0.07531600	-0.20246100	O	0.71986500	3.79281700	1.72572200
C	8.97230100	0.44443900	0.41060700	C	-3.34418000	2.76240500	4.87003300
C	9.10215100	1.55292900	1.45823900	C	-3.77975600	1.46286700	4.28589700
S	7.54097700	2.10590700	2.26448700	N	-3.46573000	1.13738100	2.97733000
C	7.06959100	0.61713100	3.21706300	C	-4.47626000	0.42157900	4.84052800

C	-3.95850900	-0.07274000	2.74160400	H	9.79094000	1.25872100	2.25773800
N	-4.58072600	-0.53444800	3.84623100	H	9.50869000	2.46475000	1.00805700
C	-5.26855400	4.91546500	-2.16440100	H	6.19588800	0.88668200	3.81384500
C	-4.77157600	4.20440400	-0.95577800	H	7.87957600	0.33243300	3.89264400
N	-5.47847100	4.13662400	0.23504300	H	6.81132100	-0.22123600	2.56801400
C	-3.61527700	3.50926300	-0.72142000	H	10.79226500	0.93672500	-0.69703000
C	-4.75155700	3.42333700	1.12578400	H	6.86317200	-2.83422700	1.30414200
N	-3.61410800	3.03007000	0.57549800	H	6.74218500	-3.33094700	2.99001300
C	-2.78565700	-3.74383000	-4.68485700	H	4.65898300	-4.17435300	3.86876000
C	-3.93916500	-3.59042700	-3.70632800	H	5.16626300	-3.78307300	-0.37806900
O	-5.04999800	-4.05364400	-3.95921500	H	2.26191400	-4.71661600	3.52994300
N	-3.63771300	-2.91788900	-2.56069400	H	2.79121800	-4.31831300	-0.72398300
C	-4.54255800	-2.94343400	-1.42405300	H	1.31936200	-4.82017000	1.24898100
C	-4.83424900	-1.51564900	-0.94952300	H	7.17707100	-5.72278700	2.31295100
O	-3.93986300	-0.83481000	-0.40718500	H	-6.22885200	4.51619800	-2.51020500
C	-3.95200900	-3.77286100	-0.26690700	H	-4.54952800	4.79814200	-2.97728600
O	-3.79740600	-5.09995800	-0.71394200	H	-2.81537600	3.29003500	-1.41395200
N	-6.07681700	-1.00653900	-1.09409200	H	-5.07663400	3.20201800	2.13000800
C	-7.26333600	-1.63152000	-1.73738300	H	-2.49741400	-4.80112800	-4.69799400
C	-7.16673500	-1.61257500	-3.26573600	H	-4.65078100	-3.71622500	0.58813100
C	-8.41165300	-0.76545200	-1.18284500	H	-3.01079700	-3.32024400	0.05926300
C	-7.79250100	0.63709000	-1.07507000	H	-2.96936300	-5.46384300	-0.35321800
C	-6.35632600	0.35813400	-0.61117300	H	-5.44361200	-3.44553800	-1.77531300
C	-0.21411900	2.61770100	-4.61334400	H	-2.68740500	-2.56777900	-2.41108500
C	-0.32930800	2.72347000	-3.10717200	H	-8.70206900	-1.12414500	-0.18870800
O	0.65048900	3.22843200	-2.46017400	H	-9.29634700	-0.80106700	-1.82313400
O	-1.37798900	2.26596700	-2.57729900	H	-8.33230000	1.28868100	-0.38206700
C	4.77506700	0.67789300	-5.57583600	H	-7.78956600	1.12701100	-2.05418100
C	4.03502400	-0.15304700	-4.53692700	H	-6.26842600	0.38119400	0.48257300
S	4.90885600	-1.76120500	-4.27891800	H	-5.61701200	1.05918000	-1.00755400
C	0.71786600	-5.42125600	-3.04886500	H	-7.36371100	-2.66409300	-1.39209900
C	1.25399400	-4.10901600	-3.61293100	H	-1.18678100	2.79119100	-5.07783300
O	2.09837000	-3.45160200	-2.98564600	H	0.53091300	3.30794600	-5.01329200
C	-0.13471300	-5.18469100	-1.78910600	H	3.01459400	-0.35564800	-4.86796300
C	-0.50991500	-6.39479200	-0.94452300	H	3.97696400	0.38642600	-3.58796400
O	-1.32794500	-6.28843200	-0.02636200	H	3.88815100	-2.41516800	-3.67918400
N	0.09030100	-7.58084100	-1.20534100	H	5.80768200	0.87500700	-5.26905100
N	0.78837300	-3.72531200	-4.81791400	H	0.38914900	-4.49278000	-1.12225400
C	1.12796400	-2.43162400	-5.40169100	H	-1.07367000	-4.68498000	-2.03986300
Zn	-2.16842200	2.07931500	1.65743000	H	-0.15043300	-8.36631100	-0.61893700
Zn	0.71735500	3.52303200	-0.35856400	H	0.78620200	-7.70458100	-1.92090000
H	-0.21232400	9.28262600	-2.73191500	H	0.15161900	-5.97855100	-3.80325600
H	1.52733900	9.23842600	-2.40797400	H	0.80815800	-1.62151600	-4.73925900
H	0.67560600	5.56718300	-2.76264400	H	2.20504300	-2.36623600	-5.57059700
H	-0.04377700	6.34561300	1.29709200	H	0.03150900	-4.25087200	-5.22753000
H	6.33206200	1.57589300	-1.85154200	H	-0.48763700	4.76487800	5.48286500
H	5.73666500	2.74395000	-3.03510600	H	-1.70050900	5.45141800	4.38345700
H	3.03497700	3.20626600	-2.46601900	H	-3.69541800	2.85823900	5.90103200
H	3.25814800	3.19621900	1.71641800	H	-2.25659700	2.85056100	4.85922800
H	8.52600600	-0.44730400	0.86601900	H	-4.88699500	0.27602700	5.82664300
H	8.28227000	0.77033200	-0.37654200	H	-3.87002400	-0.61932200	1.81171000

H	-4.98282000	-1.45528300	3.94204500	C	-0.84666600	-4.80422400	3.96212000
H	0.61369400	-2.33774700	-6.35906700	C	-1.06423700	-2.03013100	3.98907200
H	1.61245200	-6.00484800	-2.80118000	C	-1.25094200	-4.13857900	2.80941600
H	-6.99566900	-0.59692100	-3.63785400	C	-1.36909800	-2.74251500	2.82063100
H	-6.37022000	-2.26653900	-3.62475000	O	-1.78736500	-2.13212700	1.68338500
H	-8.10558200	-1.97846400	-3.69576300	H	-0.42106500	-2.15496600	6.03314500
H	0.83676900	8.21946600	-3.67477000	H	-0.77291300	-5.88944600	3.94746900
H	6.81825700	3.27437400	-1.74302200	H	-1.14568200	-0.94698100	3.99285900
H	5.62060100	2.69634000	0.82366700	H	-1.46470200	-4.68400400	1.89577800
H	0.11633500	8.58323500	0.10496800	H	-1.57403900	-1.16281100	1.68448600
H	-5.39996100	5.98881800	-1.98414000	O	-0.59255600	1.93743400	-0.21708300
H	-6.38588000	4.54275300	0.41029700	N	-1.00319600	-0.34742500	-0.75566600
H	11.02817900	-0.28321600	0.56187100	C	-0.30720000	-1.17597500	-1.59906000
H	10.21775800	-0.71687700	-0.94821900	O	-0.88472300	-2.02740800	-2.30439800
H	8.49816700	-4.66082000	1.79516500	N	1.04065200	-1.02124800	-1.63207600
H	7.29426100	-5.22242000	0.62319000	C	1.76516700	-0.00924000	-0.86452200
H	-3.13687200	-3.48965600	-5.68801100	C	1.06139300	0.22082300	0.49029700
H	-1.92482700	-3.12866000	-4.41533600	C	-0.44229400	0.50736900	0.26587200
H	4.80767800	0.16803600	-6.54272200	O	-1.18634300	0.45118700	1.39569100
H	4.27628600	1.64319800	-5.71677100	H	1.46907400	1.13398300	0.93442300
H	-3.73408000	3.61199700	4.29977800	H	-2.00131500	-0.55151600	-0.67586300
H	1.12641300	5.32737100	3.47747300	H	1.54009700	-1.74415300	-2.14254800
H	-0.36255800	6.46200800	4.96786400	C	1.27821100	-0.92541300	1.48329900
H	0.08869000	1.59550000	-4.86554000	H	2.33828200	-1.03530300	1.72186600
C	-1.57982000	-5.14210600	7.15849500	H	0.74817000	-0.72416100	2.41276400
C	-0.26418200	-4.85253000	6.42434900	H	0.92635200	-1.88203900	1.09233100
H	0.25529200	-5.79537400	6.21549100	H	1.73657300	0.93633000	-1.42219500
H	0.39789700	-4.26446500	7.07149500	H	-1.00307600	1.95330500	-1.16310300
H	-2.10333700	-4.21036300	7.39703000	C	3.22646400	-0.43499200	-0.72121200
H	-2.24714400	-5.74546300	6.53484400	H	3.71067800	-0.50492300	-1.69816300
H	-1.41089400	-5.68430700	8.09586700	H	3.77870700	0.29472700	-0.12316400
C	-0.54311500	-4.11017300	5.14166500	H	3.31180200	-1.41170600	-0.24100500
C	-0.65066400	-2.71566800	5.12927100				

(5S,6R)-Me₂DHU-TS2-II (*SmDHPase*)

C	0.94226800	8.64370800	-2.54285900	S	7.67690500	1.91188000	2.17699900
C	0.71460100	7.47800400	-1.63135300	C	7.17789800	0.46293900	3.17574100
N	0.50775800	7.63087800	-0.26839000	C	7.26481300	-5.17116700	1.49979500
C	0.68275200	6.12029700	-1.82899000	C	6.42574900	-3.95872400	1.93121100
C	0.37559400	6.40814500	0.29707000	C	4.94298500	-4.19178000	1.74261200
N	0.47374200	5.46343700	-0.62572900	C	4.10508400	-4.47375200	2.82913400
C	6.04849100	2.42857500	-1.99982800	C	4.38372500	-4.17153700	0.45785700
C	4.85841400	2.74254300	-1.16637000	C	2.74554600	-4.72677200	2.64059400
N	4.89052900	2.77255700	0.21687000	C	3.02598700	-4.42499900	0.26016600
C	3.55729700	3.00692300	-1.50096100	C	2.20200600	-4.70329300	1.35508600
C	3.64325700	3.03995300	0.66560700	C	-0.40171300	5.40744000	4.73943100
N	2.80859600	3.18195100	-0.35411200	N	0.39858200	5.12796600	3.56234600
C	10.31924200	-0.28696000	-0.30907700	C	0.10689400	4.10254700	2.68341800
C	8.99191400	0.16201400	0.31871200	O	-1.03639900	3.55286500	2.80464700
C	9.19389000	1.28182900	1.34291000	O	0.99802200	3.85635300	1.81347600

C	-3.19739100	2.80950400	4.95031600	H	8.30583600	0.50772600	-0.46334400
C	-3.65744800	1.54547800	4.30949700	H	9.88976500	0.97235000	2.13045300
N	-3.32638700	1.25429700	2.99768600	H	9.62639300	2.16822600	0.86706500
C	-4.39650000	0.50900300	4.81768200	H	6.33492300	0.77946700	3.79329500
C	-3.85141600	0.06909700	2.71503800	H	7.99695800	0.15959700	3.83200200
N	-4.51101600	-0.41064800	3.79122500	H	6.86634500	-0.37788400	2.55351500
C	-5.11263700	5.14537700	-2.02805400	H	10.81661100	0.54124700	-0.82533200
C	-4.57160400	4.42692600	-0.83745900	H	6.73784800	-3.08243000	1.34671300
N	-5.21123600	4.44493500	0.39301300	H	6.63193000	-3.72555400	2.98235100
C	-3.45311600	3.65553200	-0.63933500	H	4.52217200	-4.49134300	3.83334800
C	-4.48620600	3.70755500	1.26656700	H	5.01638700	-3.94848200	-0.39845700
N	-3.41334500	3.21626800	0.67183200	H	2.10296300	-4.92638900	3.49278900
C	-2.97123500	-3.55568000	-4.71261100	H	2.62370400	-4.36696800	-0.74776700
C	-4.10485900	-3.43689300	-3.70368500	H	1.13894400	-4.88068400	1.22473300
O	-5.24047500	-3.81046800	-3.98812100	H	6.99817700	-6.05683100	2.08484000
N	-3.75931000	-2.91247000	-2.49180200	H	-6.12014900	4.80193400	-2.28859700
C	-4.73230100	-2.77668200	-1.41821300	H	-4.46843900	4.96660500	-2.89110600
C	-4.85676200	-1.30649300	-1.00609000	H	-2.70041400	3.35070200	-1.35243200
O	-3.87568100	-0.69562500	-0.53568300	H	-4.77063800	3.54077800	2.29349600
C	-4.35664500	-3.62354100	-0.17719900	H	-2.74030500	-4.61910700	-4.84102600
O	-4.46827700	-5.00007800	-0.43195900	H	-5.07101700	-3.37335700	0.62202800
N	-6.05695900	-0.69580000	-1.10156100	H	-3.36436700	-3.32279200	0.17372200
C	-7.31377100	-1.23698500	-1.68409700	H	-3.60641900	-5.35509400	-0.71097500
C	-7.25758800	-1.29090600	-3.21329400	H	-5.66495100	-3.17432800	-1.81393300
C	-8.36349500	-0.24686200	-1.14186400	H	-2.83161000	-2.51281800	-2.35366200
C	-7.61561300	1.09505800	-1.10029700	H	-8.66383300	-0.54002300	-0.12942300
C	-6.20122700	0.70134400	-0.65302500	H	-9.26194500	-0.22377800	-1.76334000
C	-0.16976300	2.70670900	-4.56680300	H	-8.07738200	1.81941700	-0.42349800
C	4.73579200	0.60378500	-5.61296100	H	-7.58822800	1.54545100	-2.09795600
C	3.95107500	-0.20793000	-4.59233000	H	-6.08922500	0.74782500	0.43771900
S	4.77250200	-1.84023600	-4.31295600	H	-5.41107100	1.32159300	-1.08328000
C	0.43778200	-5.30399400	-3.05201800	H	-7.49795700	-2.23988800	-1.28899900
C	1.05177400	-4.04309300	-3.64331100	H	0.07064300	1.72284400	-4.98442000
O	1.93859700	-3.42227900	-3.03208300	H	-1.12411500	3.00765400	-5.00605700
C	-0.29526300	-4.97786000	-1.73275500	H	2.93471700	-0.38398200	-4.94977100
C	-0.80499300	-6.20107700	-0.98477500	H	3.88253600	0.33248500	-3.64407600
O	-1.99803000	-6.37960700	-0.74756500	H	3.69235400	-2.48376000	-3.81384600
N	0.13883400	-7.10487000	-0.59752100	H	5.76744100	0.76950600	-5.28507100
N	0.59050900	-3.64297400	-4.84400500	H	0.38115700	-4.41519100	-1.08186300
C	0.98009000	-2.37428200	-5.44984100	H	-1.15406100	-4.33726700	-1.92582900
Zn	-1.94278500	2.15386400	1.69057900	H	-0.17064600	-7.86803100	-0.01254400
Zn	0.78344500	3.42255500	-0.23367100	H	1.11784300	-6.86187900	-0.56982900
H	0.09547500	9.33915200	-2.53516100	H	-0.24817500	-5.78721100	-3.75551500
H	1.84095600	9.20446700	-2.26269300	H	0.72223600	-1.54206200	-4.78796500
H	0.80764700	5.56396500	-2.74407500	H	2.05348300	-2.36235900	-5.65149600
H	0.23679000	6.25402400	1.35650500	H	-0.18071800	-4.14968200	-5.25065200
H	6.37957500	1.39323900	-1.86008400	H	-0.28182100	4.65518200	5.53041400
H	5.80715000	2.55918600	-3.05694600	H	-1.45506000	5.44257500	4.46019700
H	3.09815300	3.06430400	-2.47469800	H	-3.50286400	2.84420900	5.99954900
H	3.36341700	3.12455400	1.70368200	H	-2.11196400	2.90110700	4.89159100
H	8.50877300	-0.69723000	0.79851200	H	-4.82979400	0.34466900	5.79118400

H	-3.75774600	-0.45414500	1.77323200	C	-1.06520900	-2.27952400	3.78977700
H	-4.94343000	-1.32084000	3.84839100	C	-1.59021300	-4.30927700	2.57751900
H	0.44319700	-2.26117600	-6.39245100	C	-1.49247900	-2.91093500	2.61096300
H	1.26185600	-6.00265200	-2.87358200	O	-1.81930200	-2.21595800	1.49430100
H	-7.02469700	-0.30616100	-3.63238500	H	-0.37271900	-2.54173200	5.80107500
H	-6.52046400	-2.01294200	-3.56863900	H	-1.33314900	-6.13825900	3.66737100
H	-8.23217200	-1.60287500	-3.60462500	H	-1.00216000	-1.19623100	3.82017100
H	1.07532800	8.29304900	-3.56817400	H	-1.94472500	-4.79700000	1.67449800
H	6.89505300	3.08425700	-1.76826000	H	-1.55415600	-1.25121900	1.56404600
H	5.71027700	2.56548800	0.79145500	C	-0.30136100	2.57161500	-3.07531900
H	0.47340100	8.50913400	0.22817400	O	0.60943800	3.02688400	-2.34014500
H	-5.16045200	6.22813000	-1.86409200	O	-1.36513900	1.95618900	-2.70368600
H	-6.07498400	4.92320400	0.60333600	H	-1.18622200	1.03703300	-1.74912400
H	11.00985300	-0.66818400	0.45062200	N	-0.99782200	-0.04597100	-0.88215000
H	10.15386500	-1.08435100	-1.03932300	C	-0.34307500	-1.07563700	-1.62810100
H	8.33462400	-4.98264400	1.63826500	O	-0.99513700	-1.88625500	-2.29590800
H	7.09784900	-5.40897500	0.44469000	N	0.99707000	-1.04025800	-1.59111400
H	-3.32521300	-3.18061500	-5.67580800	C	1.77164600	-0.05554900	-0.82475000
H	-2.07482000	-3.01455200	-4.40335100	C	1.11422900	0.16751500	0.55246400
H	4.77338000	0.09512900	-6.58017600	C	-0.36249100	0.64010500	0.39836200
H	4.26972400	1.58438500	-5.76094500	O	-1.16034300	0.32098400	1.44420000
H	-3.61445200	3.69233000	4.45212500	H	1.74817200	0.89469700	-1.37051500
H	1.37866400	5.36986100	3.58915500	H	1.62018100	1.01885700	1.01890200
H	-0.11358000	6.38106700	5.14384900	H	-1.95923200	-0.35635000	-0.67049600
H	0.61522900	3.41077600	-4.84755700	H	1.46460300	-1.79432900	-2.09346500
C	-1.69845100	-5.18995800	7.09346100	O	-0.49002400	2.00560000	0.16676100
C	-0.50714600	-5.24071600	6.12796100	C	1.26960200	-1.03674300	1.48351800
H	-0.28940000	-6.28298700	5.86715000	H	2.32358100	-1.25910700	1.66516000
H	0.38623000	-4.85187400	6.63293800	H	0.80290200	-0.82541000	2.44336400
H	-1.91818500	-4.15858000	7.38826300	H	0.80477400	-1.93753700	1.07832400
H	-2.59828500	-5.59746500	6.62140500	C	3.22228000	-0.52877100	-0.73956600
H	-1.50372500	-5.76628800	8.00479700	H	3.67949200	-0.58666100	-1.73028400
C	-0.78946100	-4.44214400	4.87786000	H	3.80838900	0.16908800	-0.13666200
C	-0.71111400	-3.04408000	4.89703700	H	3.29289000	-1.51860900	-0.28439200
C	-1.24293400	-5.05478800	3.70242900				

(5S,6R)-Me₂DHU-EP-II (*Sm*DHPase)

C	1.40364700	8.55127800	-2.67053100	C	8.92404000	-0.26199000	0.66226700
C	1.03714400	7.49436900	-1.69725700	C	9.10990700	0.83924700	1.70927900
N	0.77792600	7.72770500	-0.35559500	S	7.57414800	1.50875500	2.47542700
C	0.93216900	6.14156000	-1.84412700	C	6.98095300	0.06741600	3.43240700
C	0.54884000	6.54011700	0.25417500	C	6.92771500	-5.42707100	1.94020300
N	0.63392200	5.55713400	-0.62783400	C	6.09837400	-4.16899900	2.24555700
C	6.18560700	2.11931500	-1.79934800	C	4.62487800	-4.36256100	1.95937100
C	5.01351500	2.57544900	-1.01016800	C	3.71892900	-4.65911800	2.98529800
N	4.96957000	2.55749300	0.37329300	C	4.14185400	-4.29345500	0.64509700
C	3.76903000	2.98537900	-1.40442800	C	2.36880900	-4.88294900	2.70810000
C	3.73404200	2.94057800	0.76577600	C	2.79517000	-4.51982400	0.35810200
N	2.97830400	3.19788500	-0.29365000	C	1.90488300	-4.81718200	1.39383000
C	10.26736200	-0.74625400	0.09798900	C	-0.31464500	5.59030700	4.65009400

N	0.48815000	5.24191600	3.48892600	H	6.05807700	2.39869000	-2.84748300
C	0.17186000	4.22163700	2.61273100	H	3.36421300	3.10402500	-2.39644800
O	-1.01127300	3.73568900	2.71282200	H	3.40826000	3.02903200	1.78996300
O	1.05798900	3.90296400	1.77181400	H	8.39104700	-1.11051800	1.10699500
C	-3.23738400	3.13466500	4.84235800	H	8.28990500	0.11288100	-0.14930200
C	-3.65438800	1.83850400	4.22379300	H	9.75549500	0.49931000	2.52659200
N	-3.27812700	1.48173100	2.93471400	H	9.59301600	1.71655100	1.26639200
C	-4.41649900	0.82605700	4.74533900	H	6.11887700	0.40509800	4.01121000
C	-3.80462600	0.28718400	2.68461700	H	7.75670700	-0.26767100	4.12488500
N	-4.50088400	-0.13784100	3.75809300	H	6.67415700	-0.75757600	2.78722300
C	-4.82563400	5.35953100	-2.25338600	H	10.81687100	0.07146000	-0.38069800
C	-4.39939800	4.59222400	-1.04318700	H	6.48301900	-3.33384800	1.64426300
N	-5.17063900	4.49734000	0.10784500	H	6.23676300	-3.88955000	3.29687700
C	-3.27073000	3.86261400	-0.77109700	H	4.07452800	-4.71247200	4.01188800
C	-4.51007600	3.73792700	1.01098500	H	4.82962700	-4.05842300	-0.16480400
N	-3.35123700	3.33643800	0.50808000	H	1.67488600	-5.09558800	3.51590900
C	-3.02576600	-3.50584500	-4.63381400	H	2.44744000	-4.43433000	-0.66776700
C	-4.23029600	-3.33484500	-3.71135000	H	0.85118900	-4.98073000	1.18790800
O	-5.36736300	-3.59515000	-4.10381800	H	6.58910800	-6.27268100	2.54685800
N	-3.94051900	-2.88455500	-2.45947300	H	-5.77289800	4.98816800	-2.66033800
C	-4.95184200	-2.77523100	-1.42199500	H	-4.06636100	5.25751700	-3.03080600
C	-5.09887000	-1.32076600	-0.95201300	H	-2.43278700	3.63296600	-1.41706000
O	-4.13717100	-0.73942300	-0.40823700	H	-4.89452900	3.49254000	1.98842100
C	-4.59076000	-3.64255900	-0.18808900	H	-2.90943700	-4.57449400	-4.84541200
O	-4.63772900	-5.01234000	-0.49224500	H	-5.33579900	-3.43236600	0.59585300
N	-6.29198200	-0.69764300	-1.05514800	H	-3.61695300	-3.31615600	0.19328200
C	-7.48343000	-1.13243400	-1.82689100	H	-3.73357100	-5.36061200	-0.58526100
C	-7.24141700	-0.99904700	-3.33219300	H	-5.87450300	-3.16243600	-1.85284500
C	-8.56975700	-0.18507800	-1.28476800	H	-2.96704300	-2.66421800	-2.21865700
C	-7.81603600	1.13156500	-1.03484200	H	-8.96577000	-0.57633700	-0.34077500
C	-6.43906400	0.67238400	-0.52991200	H	-9.40559200	-0.07926700	-1.98054300
C	0.06857000	2.61851700	-4.56811100	H	-8.32444500	1.78110500	-0.31668800
C	4.89649700	0.25687600	-5.40175100	H	-7.71142100	1.69245800	-1.96908600
C	5.09604500	-1.20479600	-5.00526700	H	-6.39055900	0.64591800	0.56619200
S	6.54069100	-1.34467700	-3.85754600	H	-5.61217600	1.30042400	-0.87260600
C	0.47111700	-5.58644700	-3.02555800	H	-7.72361800	-2.17048600	-1.58255800
C	1.04694000	-4.26613700	-3.53388200	H	-0.84428600	2.90887100	-5.09151900
O	1.86581600	-3.62284400	-2.86676600	H	0.93197800	3.14096000	-4.98541100
C	-0.59496900	-5.33284900	-1.94288900	H	5.29494300	-1.81651000	-5.88878300
C	-1.14781700	-6.52208200	-1.17285100	H	4.21118300	-1.59906400	-4.49857000
O	-2.15968200	-6.40182600	-0.47972500	H	6.44965700	-2.67122500	-3.63529300
N	-0.48981400	-7.70598900	-1.24894000	H	4.67086700	0.87756400	-4.52937000
N	0.61195000	-3.83417000	-4.73985400	H	-0.20590300	-4.62840500	-1.20165000
C	0.99842100	-2.53423000	-5.27731900	H	-1.45977900	-4.82311600	-2.36945600
Zn	-1.93983400	2.37756600	1.63913400	H	-0.83822900	-8.47211400	-0.69182000
Zn	0.98680100	3.56339700	-0.39953400	H	0.37833700	-7.82179300	-1.74371400
H	0.62737500	9.31975400	-2.76512000	H	0.05626700	-6.18342300	-3.84585500
H	2.33648700	9.05612300	-2.39342900	H	0.80616400	-1.74334000	-4.54837800
H	1.07562100	5.53531200	-2.72323800	H	2.06245000	-2.52214800	-5.53363300
H	0.35317600	6.43616100	1.31082300	H	-0.10465000	-4.35988800	-5.21599700
H	6.30285900	1.03029600	-1.76383000	H	-0.22956100	4.85979900	5.46550600

H	-1.36267500	5.65742600	4.35737000	C	-0.86565500	-2.86275500	4.98427300
H	-3.61264700	3.20448500	5.86644400	C	-1.58636400	-4.88071200	3.90622400
H	-2.15066800	3.22948000	4.85288500	C	-1.10743400	-2.14144800	3.81644000
H	-4.88727000	0.70827700	5.70809200	C	-1.82673300	-4.18173400	2.72564100
H	-3.71346700	-0.27454100	1.76240700	C	-1.59333500	-2.80154900	2.67984200
H	-4.94799500	-1.03968400	3.83615200	O	-1.86185500	-2.14971200	1.51280100
H	0.41699900	-2.34416400	-6.18055400	H	-0.48647900	-2.34009100	5.86001600
H	1.32599500	-6.13148900	-2.61051700	H	-1.77889900	-5.95072600	3.93270900
H	-6.91161900	0.01282400	-3.59042200	H	-0.91445100	-1.07342900	3.77504300
H	-6.50088100	-1.72055400	-3.68241600	H	-2.18398000	-4.69338400	1.83703800
H	-8.17101400	-1.20118500	-3.87604900	H	-1.51548900	-1.23579400	1.54173200
H	1.54912800	8.10626100	-3.65675500	C	-0.08667200	2.86846400	-3.07569600
H	7.11911700	2.57210600	-1.44783000	O	0.96823800	3.24135400	-2.43351600
H	5.73499400	2.26405000	0.98444600	O	-1.20215700	2.66131900	-2.56378800
H	0.77036200	8.62928400	0.09847900	N	-1.51223800	-0.12876800	-1.55317600
H	-4.94859000	6.42723000	-2.03820900	C	-0.74137000	-1.20623900	-1.84145600
H	-6.07773200	4.91701300	0.24993900	O	-1.21240000	-2.34512400	-2.03624000
H	10.90521300	-1.15957000	0.88660800	N	0.61944800	-1.03142500	-1.90689400
H	10.11485400	-1.52803900	-0.65168700	C	1.42010300	-0.01072900	-1.23333700
H	7.99016800	-5.26283800	2.14945400	C	1.16773300	0.12211900	0.30869600
H	6.82980800	-5.71489600	0.88872200	C	-0.07651200	0.92450000	0.65946000
H	-3.24633200	-3.01099800	-5.58337200	O	-0.91811900	0.52836400	1.52019400
H	-2.10528400	-3.10743500	-4.20410200	H	1.22149800	0.96787700	-1.67802000
H	5.78745500	0.66130900	-5.89142300	H	1.97497300	0.78448500	0.65253200
H	4.05974700	0.34339700	-6.10218300	H	-2.49414500	-0.32083500	-1.37228500
H	-3.62585200	3.99191700	4.28140900	H	1.09370000	-1.91320300	-2.08939800
H	1.47688800	5.44464500	3.52374100	O	-0.26403300	2.09272400	0.16018100
H	0.00767600	6.56459400	5.02557900	H	-1.25476100	0.82080300	-1.81250300
H	0.21015600	1.54341300	-4.72725600	C	1.27242100	-1.19935600	1.06965100
C	-2.19130800	-4.86271900	7.24628800	H	2.25530200	-1.65160000	0.92641700
C	-0.94119000	-4.98572000	6.36155700	H	1.13111500	-1.04615900	2.14130200
H	-0.73877000	-6.04479700	6.16351100	H	0.52462100	-1.91894700	0.73422200
H	-0.07185200	-4.59895500	6.90757000	C	2.88503800	-0.37112300	-1.51312800
H	-2.39991300	-3.81402100	7.48321900	H	3.08043600	-0.32925700	-2.58791400
H	-3.07090000	-5.26841300	6.73598500	H	3.56240500	0.32341900	-1.01694400
H	-2.06799000	-5.40418000	8.19049900	H	3.11611300	-1.38462500	-1.17389900
C	-1.10581800	-4.23987300	5.05732600				