Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Supporting Information

## Decoding Regioselective Reaction Mechanism of the Gentisic Acid Catalyzed by Gentisate 1,2-Dioxygenase Enzyme

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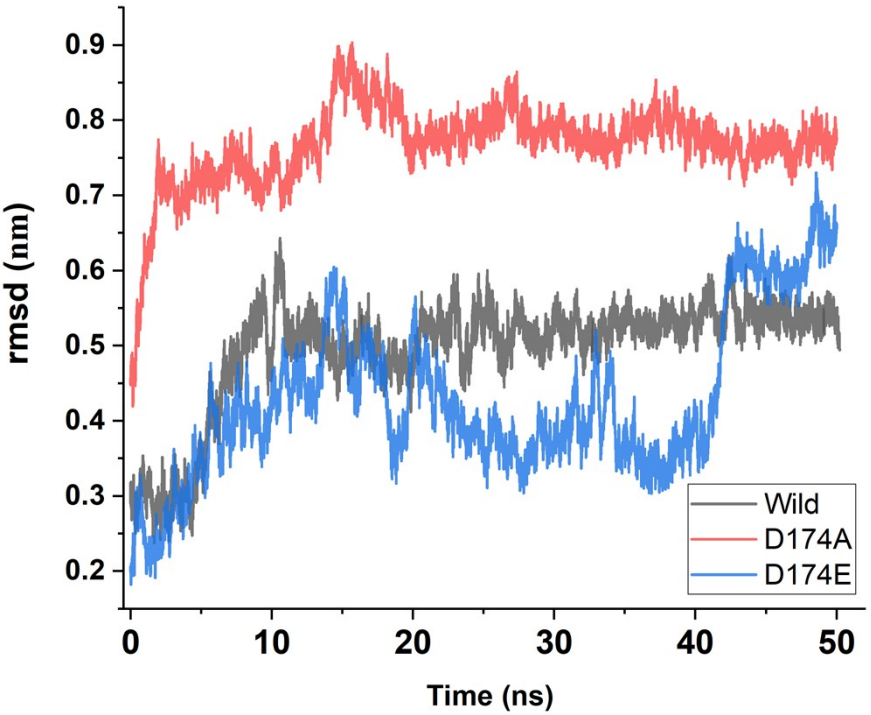



**Figure S1**. Time evolution of root means square deviation (RMSD) of the protein backbone of wild type GDO and its mutate enzymes (such as D174A, D174E) with respect to their corresponding crystal structure obtained from the classical MD simulations.

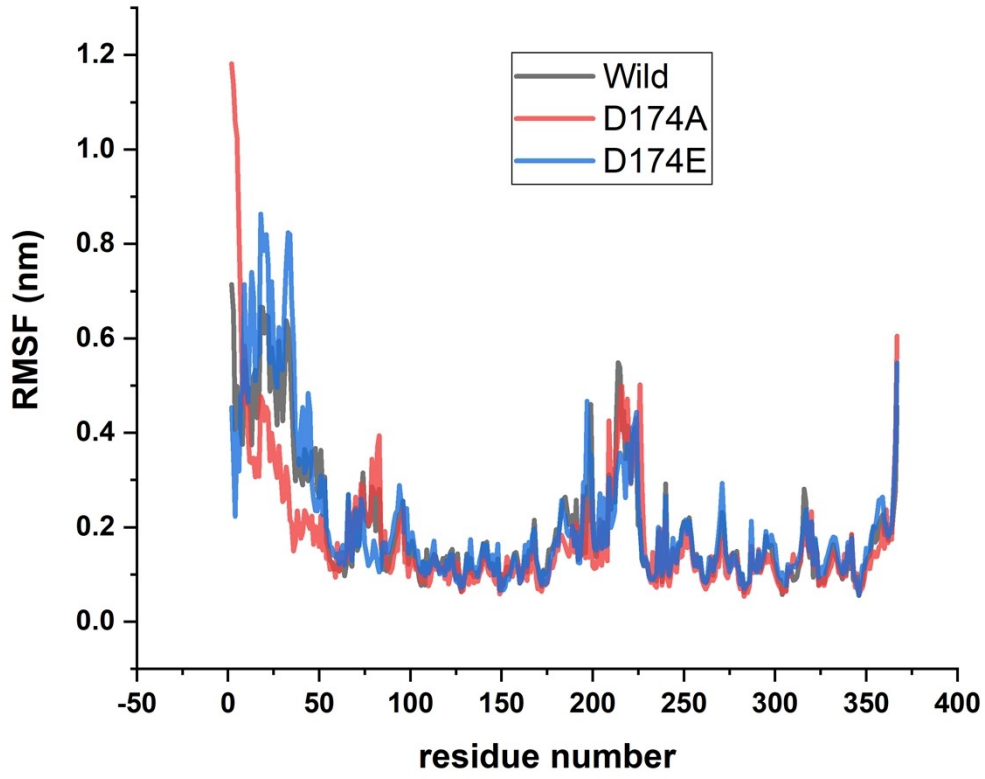



**Figure S2**. Time evolution of root means square fluctuation (RMSF) of the protein of wild type GDO and its mutate enzymes (such as D174A, D174E) with respect to their corresponding crystal structure obtained from the classical MD simulations.

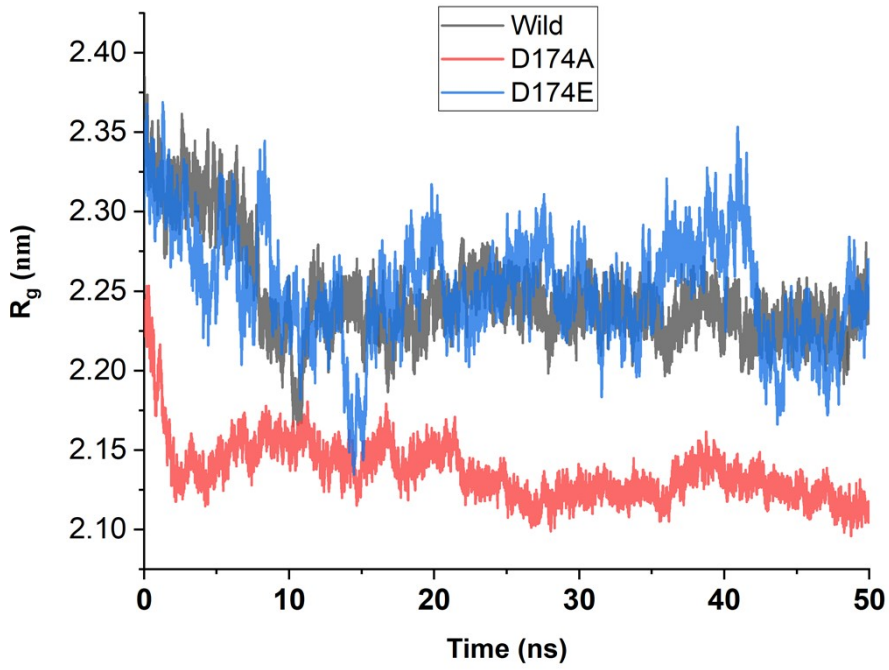



**Figure S3**. Radius of gyration (Rg) of the protein backbone of wild type GDO and its mutate enzymes (such as D174A, D174E) obtained from the classical MD simulations.

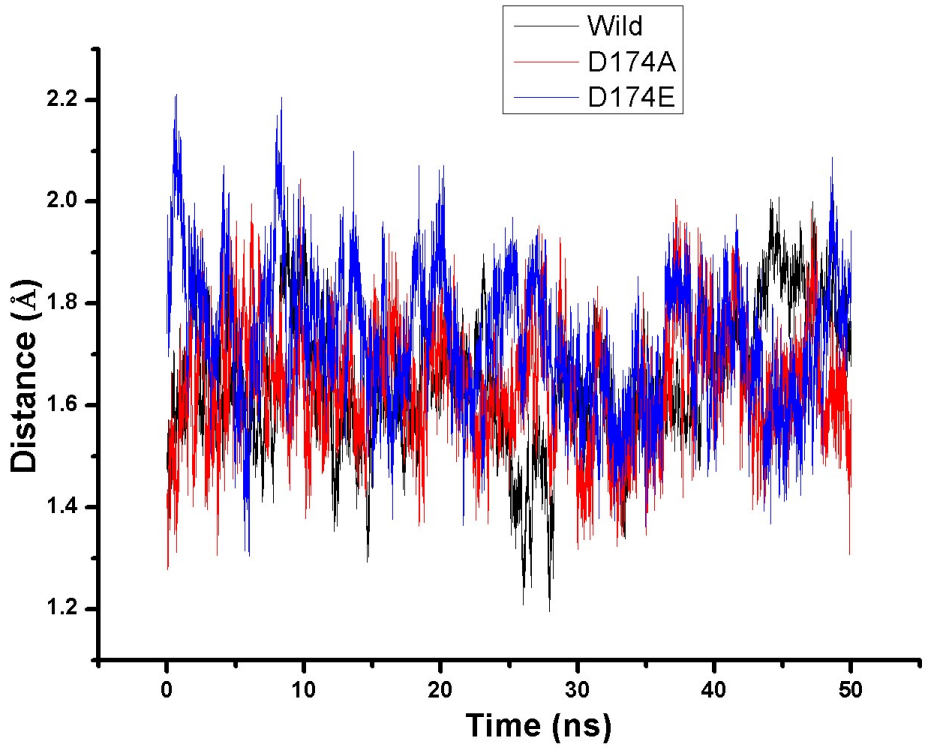
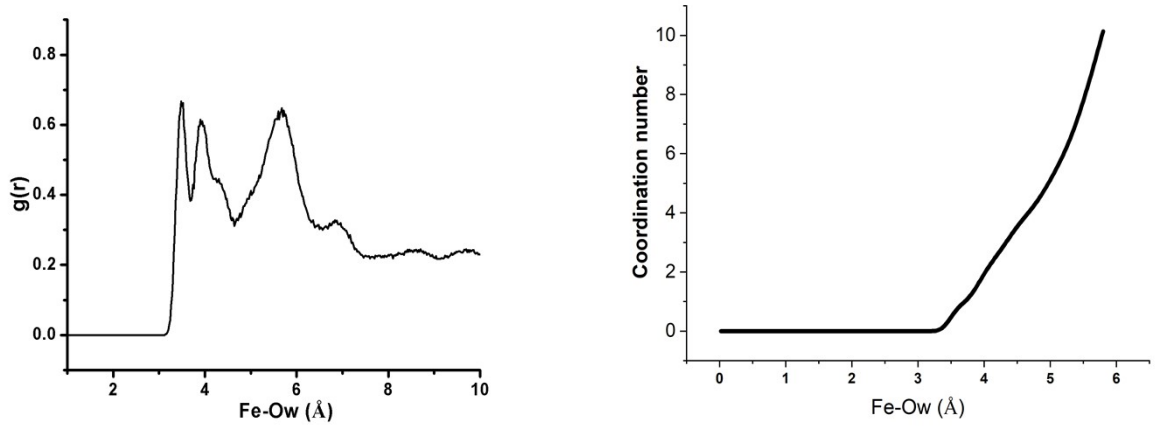



**Figure S4**. Time evolution of the distance between the $O_{w1}$ atom of the W2 water and the $H_d$ atom of the GTQ for the wild type GDO and its mutate enzymes (such as D174A, D174E) obtained from the classical MD simulations.

After the classical MD simulations, we witnessed that there were three water molecules present in the active site of the GDO enzyme. Classical MD simulations of the whole enzyme disclosed a sharp peak in the radial distribution function (g(r)) between iron and water at ~4.5Å distance (Figure S5a). Thus, it strongly suggests that the active center of the enzyme is hydrated. Additionally, the coordination number plot (Figure S5b) clearly displays that two water molecules are present in the close vicinity (~4.5Å) of the iron center. Furthermore, equilibrium MD simulations revealed that with the progression of the simulations, the interatomic distance of (GTQ)$H_d$-$O_{w1}$($H_2O$) is within the range of 2.2 Å (Figure S4). We strongly believe that these water molecules form hydrogen bonds with the GTQ moiety. We notice that these water molecules come from the bulk water region to the active site of the GTQ-GDO enzyme complex during the simulations. Thus, it is reasonable to believe that the presence of these water molecules in the active site of GTQ-GDO enzyme is not a mere artifact, rather stabilizing hydrogen bond interaction pulls the single water molecule from bulk to come in the close vicinity of the substrate GTQ. Recently, QM/MM studies on Glycoside Hydrolases enzymes showed that the presence of water in the active site of the enzyme can influence the barrier of a reaction. Such presence of water in the enzyme pocket was indicated by classical MD simulations.[1]




(a) (b)

**Figure S5**. (a) Radial distribution function ( g(r) ) and (b) Coordination number of waters around iron obtained from the classical MD simulations.

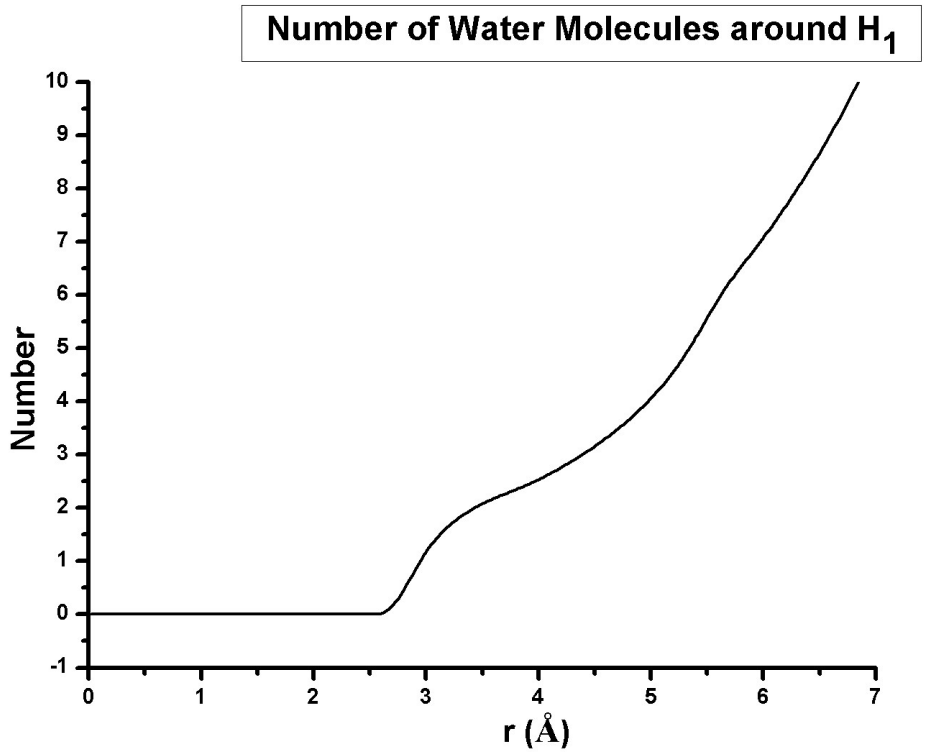



**Figure S6**. Coordination number of waters around the $H_1$ atom of GTQ substrate up to 7 Å radius obtained from the classical MD simulations.

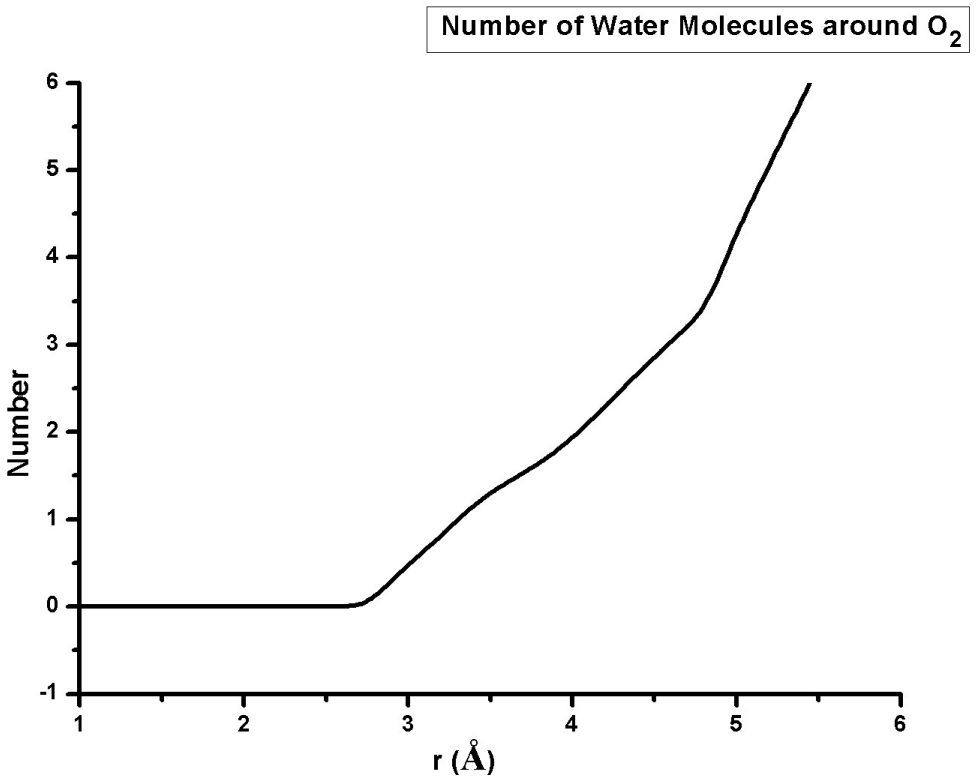



**Figure S7**. Coordination number of waters around molecular oxygen up to 6 Å radius obtained from the classical MD simulations.

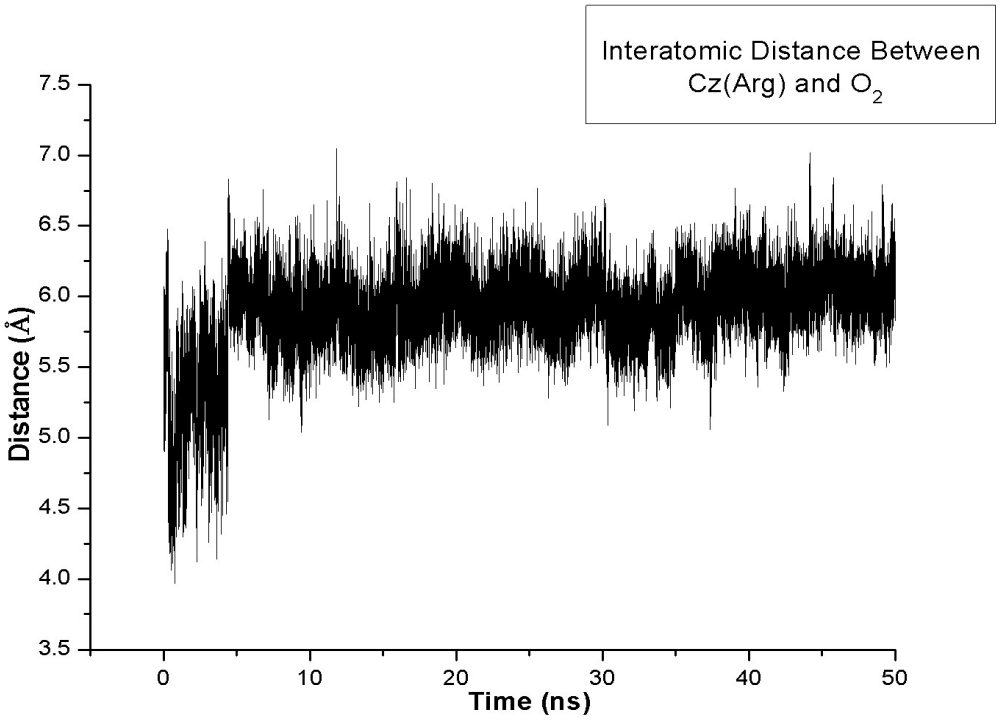


**Figure S8**. Interatomic distances between the Cz atom of Arg127 and dioxygen molecule in the active site of GDO enzyme obtained from the classical MD simulations.

**Discussion on Spin States of Dioxygen bound State**

In our starting substrate (1) we have found that molecular oxygen is non interacting with $Fe^{2+}$ in both triplet and septet spin states. We have predicted that one of the electrons of triplet molecular oxygen re orients it's spin due to high spin-orbit coupling and it is quite natural phenomena in presence of an atom like iron with high molecular weight. Then one of the unpaired electrons from $Fe^{2+}$ transfers to π*orbital of dioxygen resulting $Fe^{3+}..O^{2-}$ couple (Figure S9) and it is supported by orbital analysis using ORCA program.

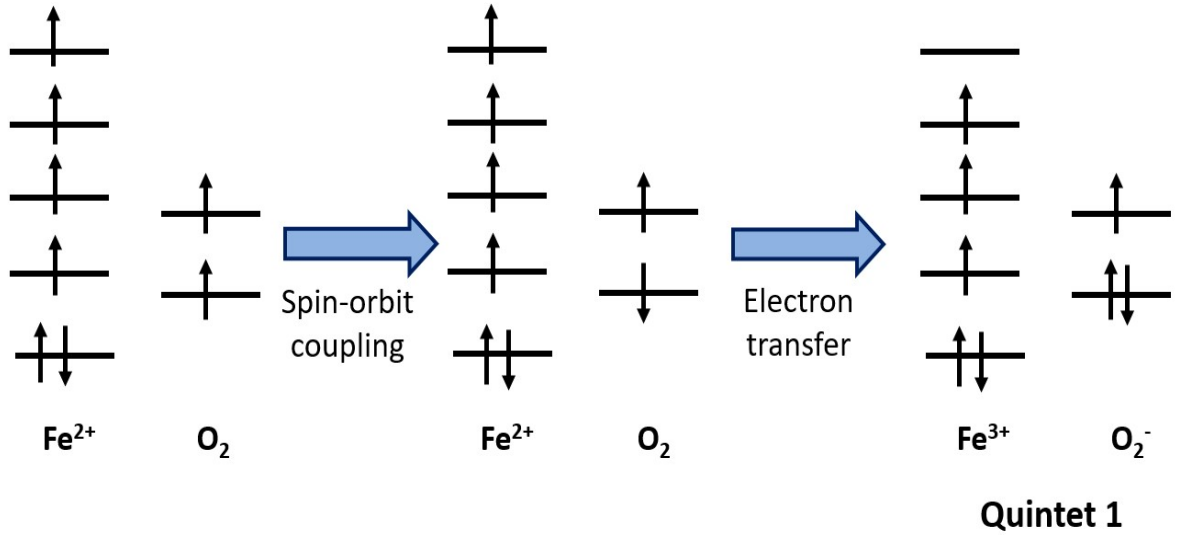



**Figure S9**. The change of valance electron configuration via spin-orbit coupling and transfer of one electron from $Fe^{2+}$ to $O_2$.

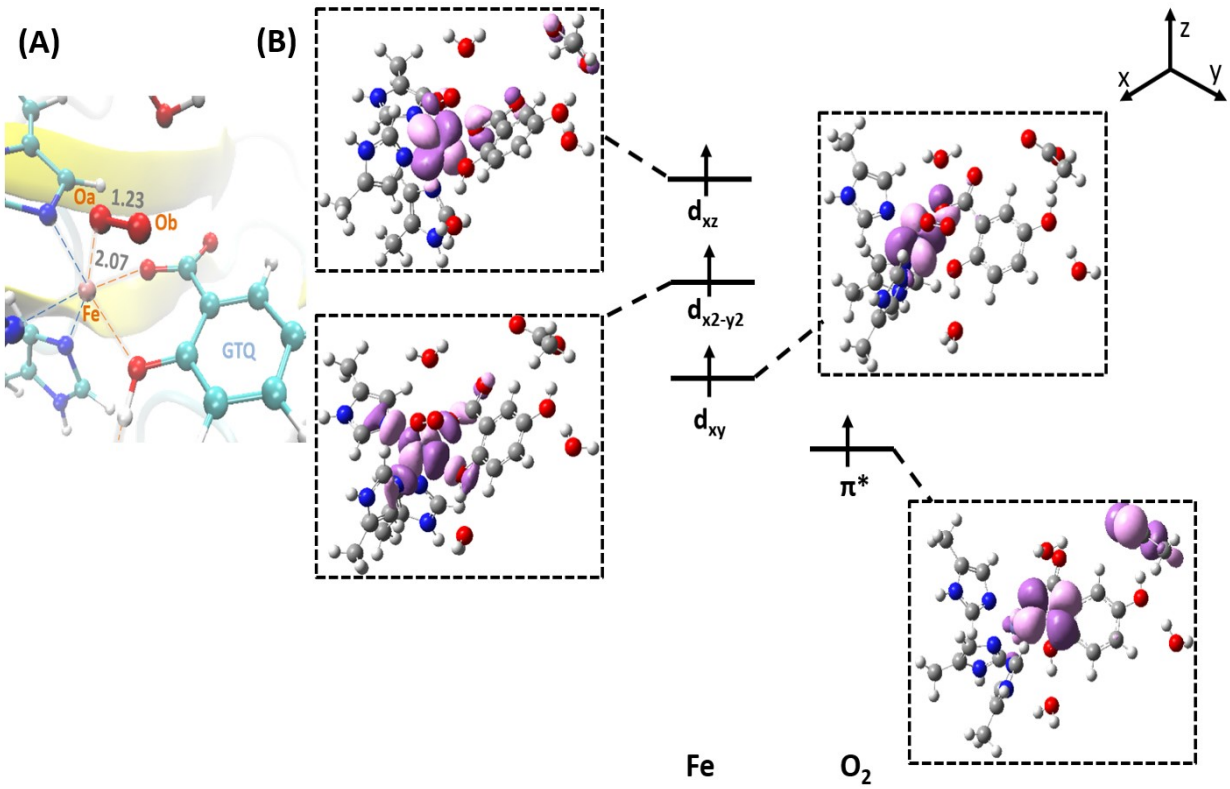



**Figure S10**. (A) Optimized geometry of 1 in quintet surface (distances are in Å). (B) Schematic MO diagram for the $O_2$ adduct (1) in quintet spin state (only unpaired electrons are shown).

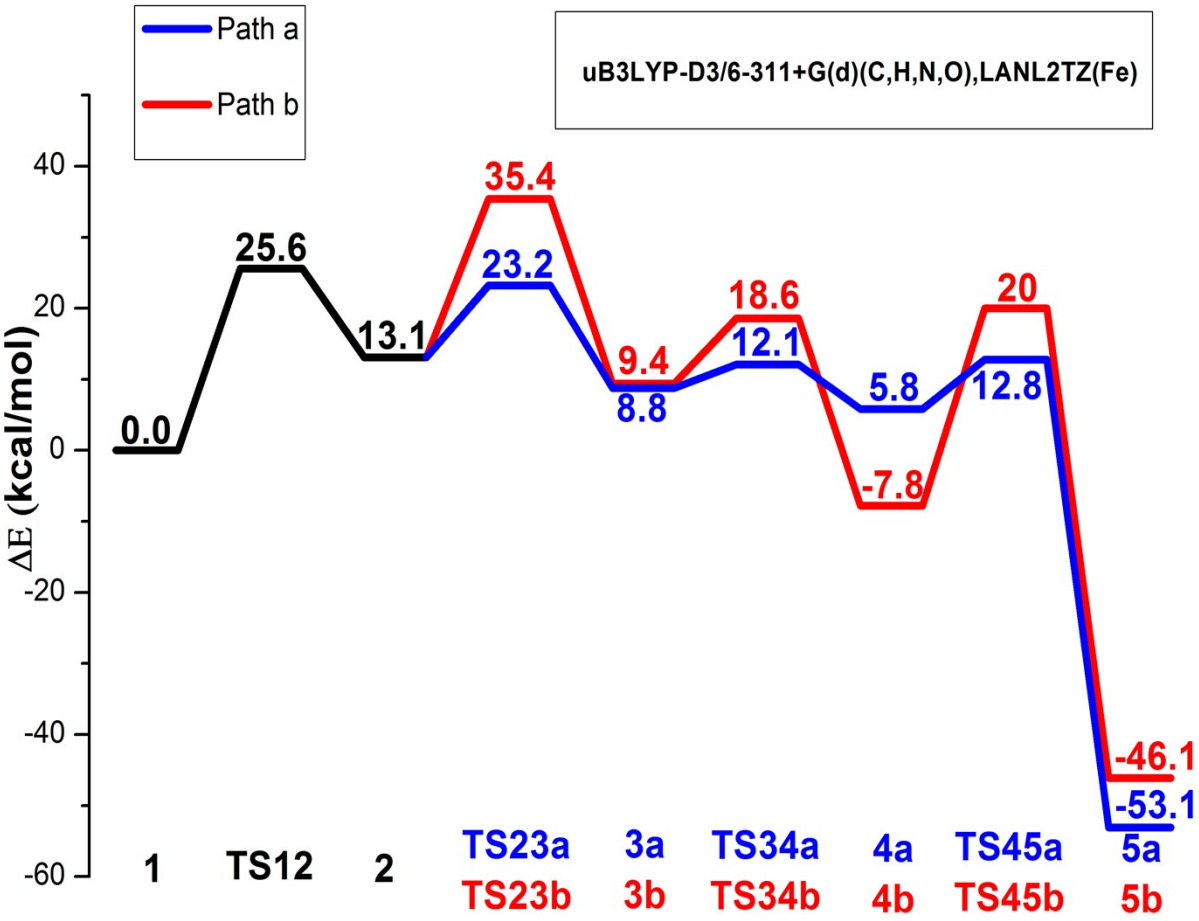



**Figure S11.** The potential energy profile for the oxidative cleavage of the C-C aromatic bond of the GTQ substrate in the active site of the GDO enzyme following pathway A and B at the uB3LYP-D3/6-311+G(d)(C,H,N,O), LANL2TZ(Fe)/OPLS level of theory.

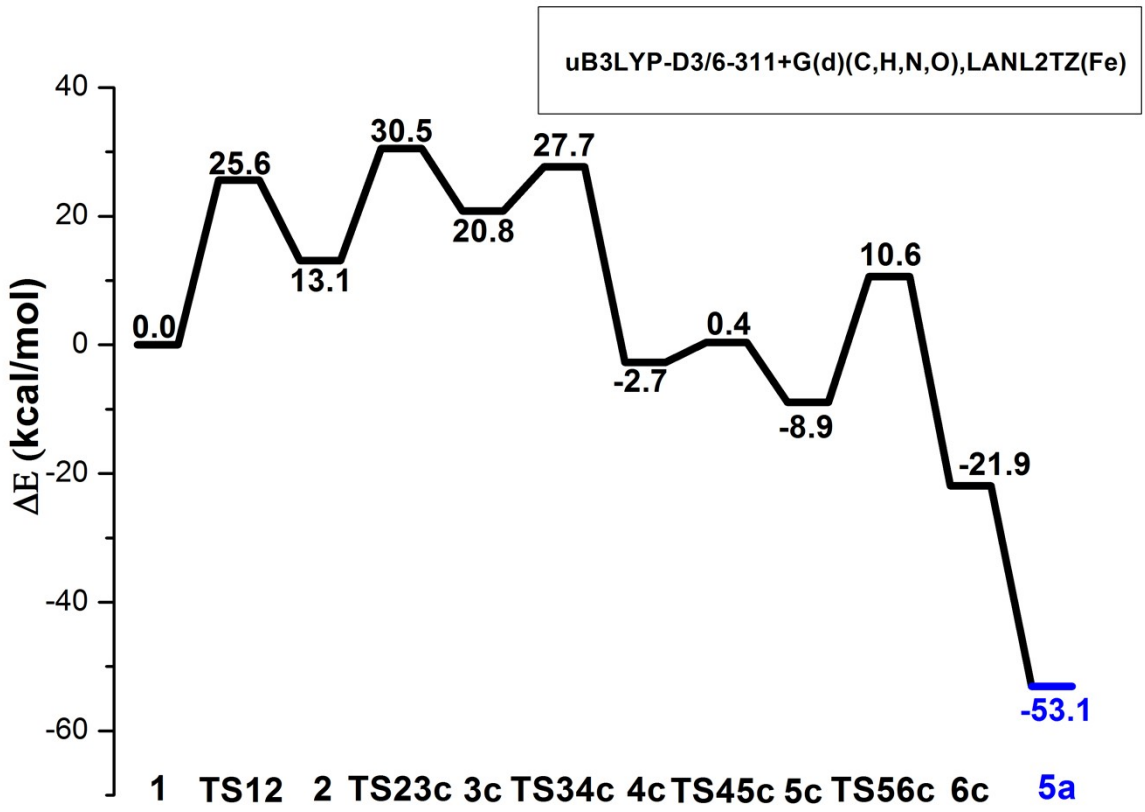



**Figure S12.** The potential energy profile for the oxidative cleavage of the C-C aromatic bond of the GTQ substrate in the active site of the GDO enzyme following pathway C at the uB3LYP-D3/6-311+G(d)(C,H,N,O), LANL2TZ(Fe)/OPLS level of theory.

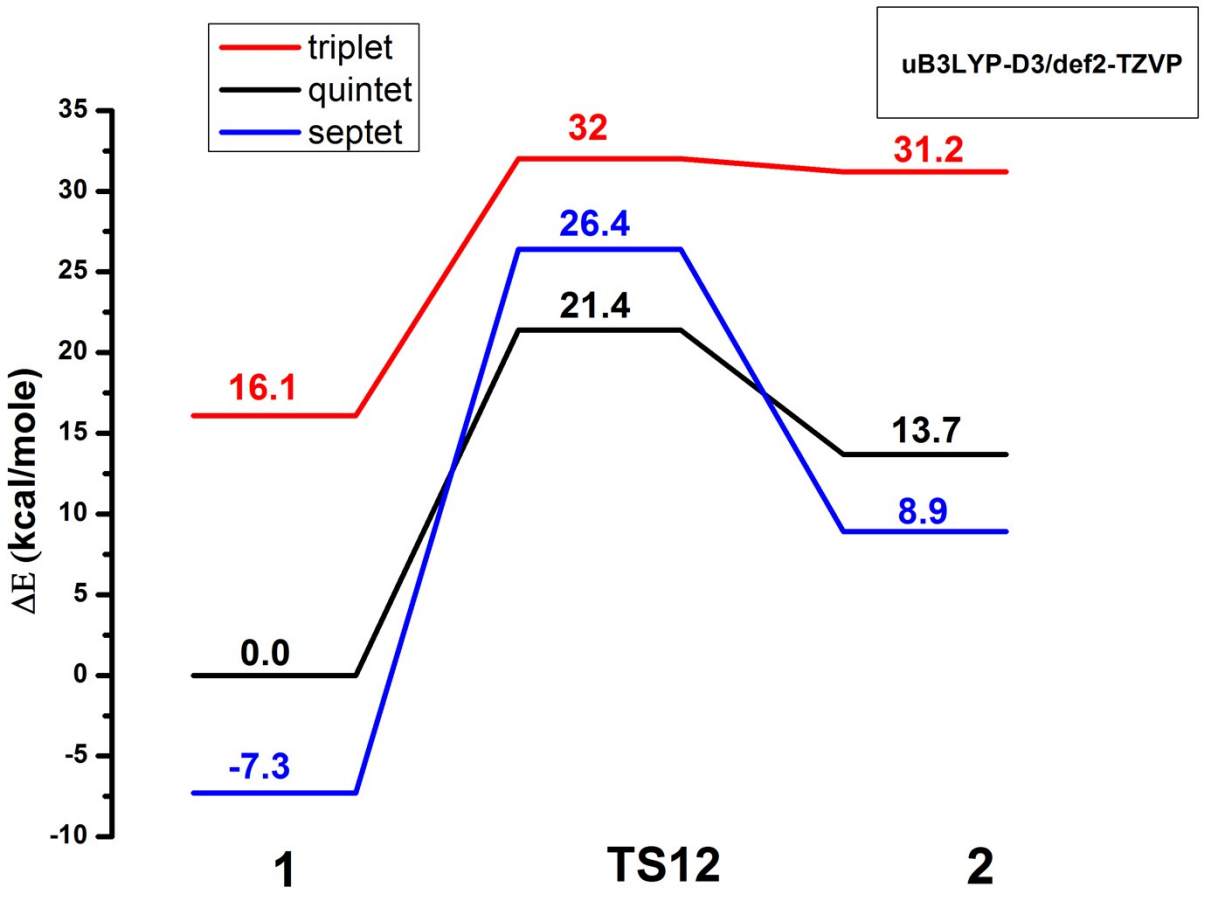



**Figure S13.** The potential energy profiles for the formation of alkylperoxo intermediate in the active site of the GDO enzyme on the quintet (black), triplet (red) and septet (blue) spin states at the uB3LYP-D3/def2-TZVP/OPLS level of theory.

**Table S1**. Calculated potential Energy (KJ/mol) for the all the stationary structures for the degradation of GTQ substrate catalyzed by GDO enzyme at the uB3LYP-D3/def2-TVZP/OPLS and uB3LYP-D3/6-311+G(d,p)(C, H, N, O),LANL2TZ(Fe)/OPLS level of theory on the quintet spin state respectively.

| **Structure** | **uB3LYP-D3/def2-TZVP/OPLS level of theory** | | **uB3LYP-D3/6-311+G(d,p)(C,H,N,O), LANL2TZ(Fe)/OPLS level of theorey** | |
|---|---|---|---|---|
| | **Potential Energy (kj/mol)** | **ΔE (kcal/mol)** | **Potential Energy (kj/mol)** | **ΔE (kcal/mol)** |
| **1** | -8507636.185 | 0.0 | -5513159.817 | 0.0 |
| **TS12** | -8507546.797 | 21.4 | -5513052.974 | 25.6 |

| | | | | |
|---|---|---|---|---|
| **2** | -8507578.981 | 13.7 | -5513105.02 | 13.1 |
| **TS23a** | -8507562.07 | 17.7 | -5513062.946 | 23.2 |
| **TS23b** | -8507481.087 | 37.1 | -5513011.838 | 35.4 |
| **TS23c** | -8507535.304 | 24.1 | -5513032.459 | 30.5 |
| **3a** | -8507626.688 | 2.3 | -5513123.054 | 8.8 |
| **3b** | -8507625.893 | 2.5 | -5513120.402 | 9.4 |
| **3c** | -8507581.647 | 13 | -5513073.082 | 20.8 |
| **TS34a** | -8507599.562 | 8.8 | -5513109.083 | 12.1 |
| **TS34b** | -8507568.819 | 16.1 | -5513081.985 | 18.6 |
| **TS34c** | -8507553.601 | 19.8 | -5513043.887 | 27.7 |
| **4a** | -8507632.072 | 0.9 | -5513135.464 | 5.8 |
| **4b** | -8507663.906 | -6.6 | -5513192.646 | -7.8 |
| **4c** | -8507686.038 | -11.9 | -5513171.03 | -2.7 |
| **TS45a** | -8507601.975 | 8.2 | -5513106.38 | 12.8 |
| **TS45b** | -8507565.748 | 16.9 | -5513076.34 | 20 |
| **TS45c** | -8507673.03 | -8.8 | -5513157.95 | 0.4 |
| **5a** | -8507888.084 | -60.3 | -5513381.757 | -53.1 |
| **5b** | -8507847.246 | -50.5 | -5513352.403 | -46.1 |
| **5c** | -8507713.649 | -18.5 | -5513196.895 | -8.9 |
| **TS56c** | -8507631.394 | 1.1 | -5513115.395 | 10.6 |
| **6c** | -8507752.259 | -27.8 | -5513251.314 | -21.9 |

**Table S2**. Imaginary frequencies for the transition state structures for the oxidative cleavage of aromatic C−C bond of GTQ substrate catalyzed by GDO enzyme at the B3LYP/6-31+G(d)/OPLS level of theory on the quintet respectively.

| **Structure** | **Frequency ($cm^{-1}$)** |
|---|---|
| TS12 | -329.4 |
| TS23a | -220.2 |
| TS23b | -390.9 |
| TS23c | -392.9 |
| TS34a | -683.6 |
| TS34b | -752.1 |
| TS34c | -183.6 |
| TS45a | -691.4 |
| TS45b | -858.7 |
| TS45c | -465.0 |
| TS56c | -467.1 |

**Snapshot Pictures of all Optimized Structures of all Stationary States**

All stationary and transition state structures for all three pathways (A, B C) were optimized in B3LYP/6-31+G(d)(C,H,N,O),LANL2DZ(Fe)/OPLS level of theorey and the optimized

structures of all stationary states in quintet surface are provided below with key inter atomic distances.

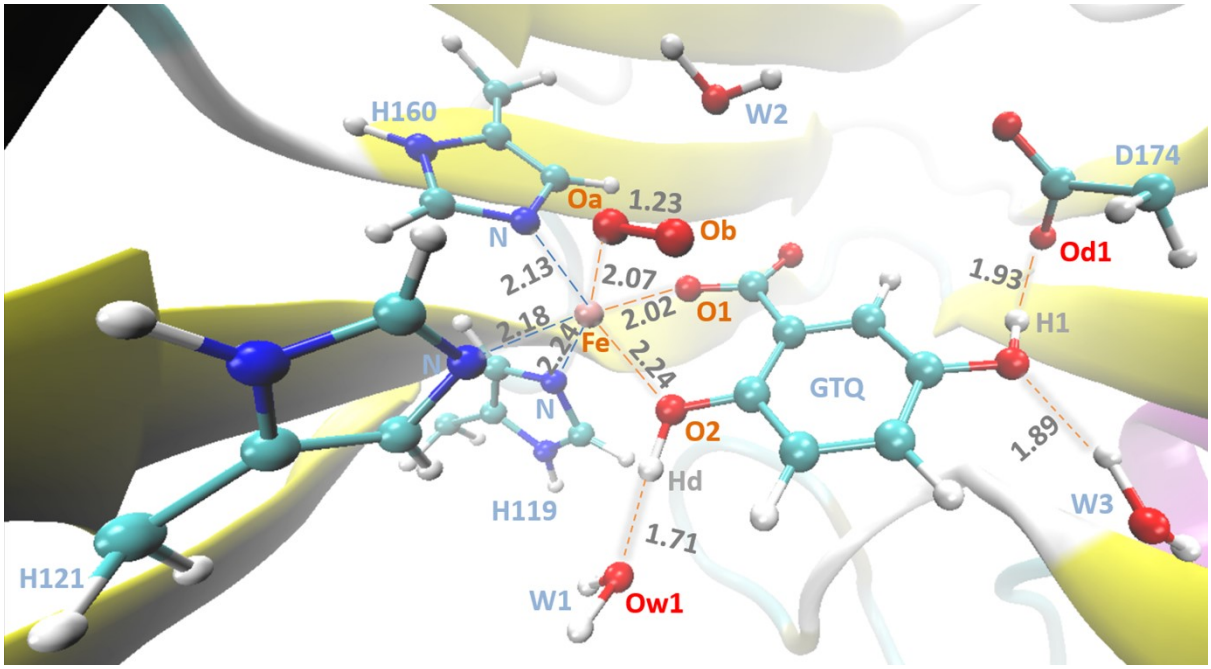



**Figure S14**. Optimized structure of 1 in quintet spin state with key inter atomic distances (Å).

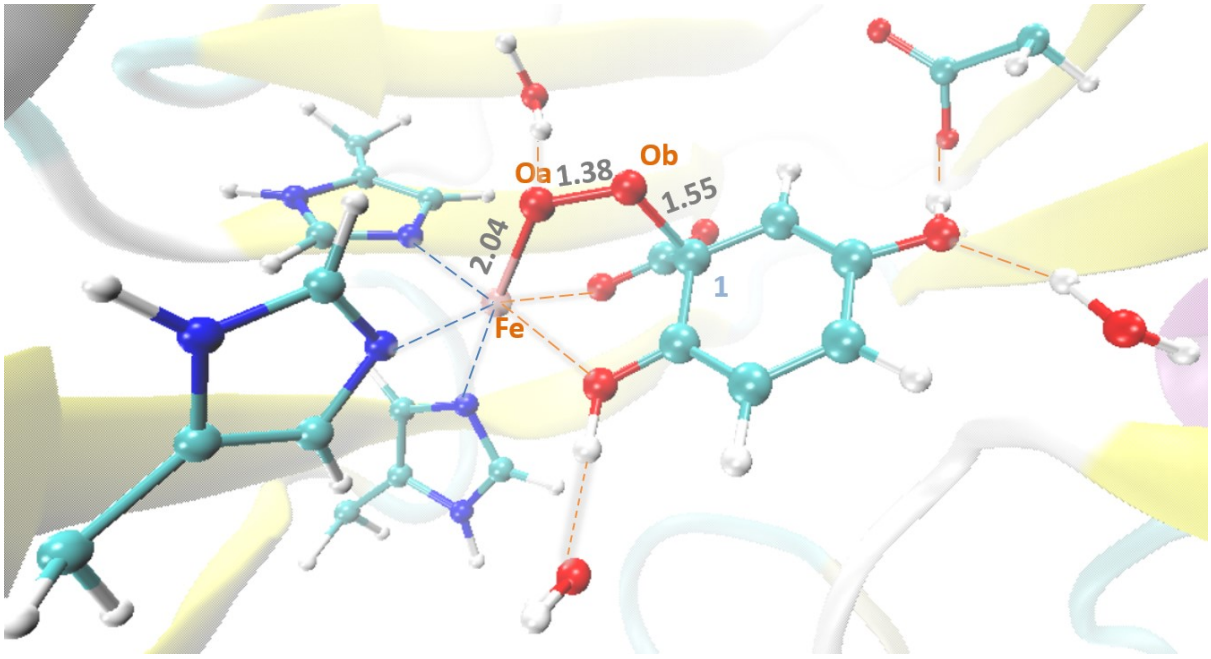



**Figure S15**. Optimized structure of 2 in quintet spin state with key interatomic distances (Å).

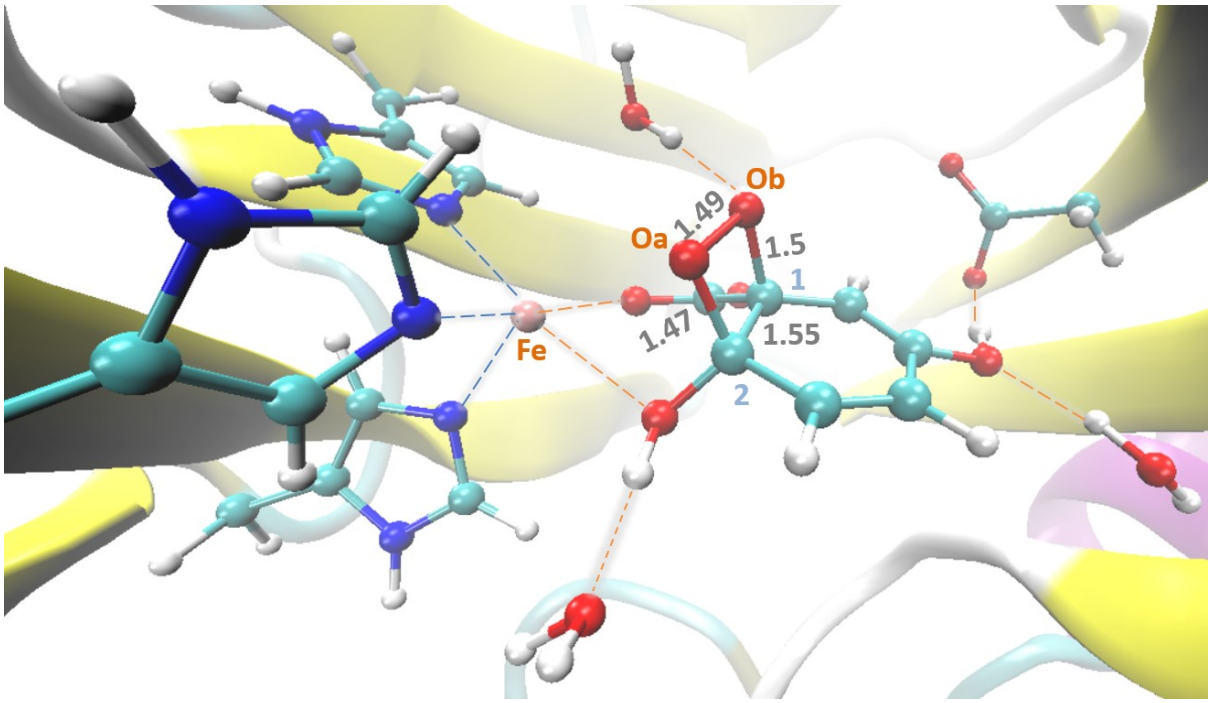



**Figure S16**. Optimized structure of 3a in quintet spin state with key interatomic distances (Å).

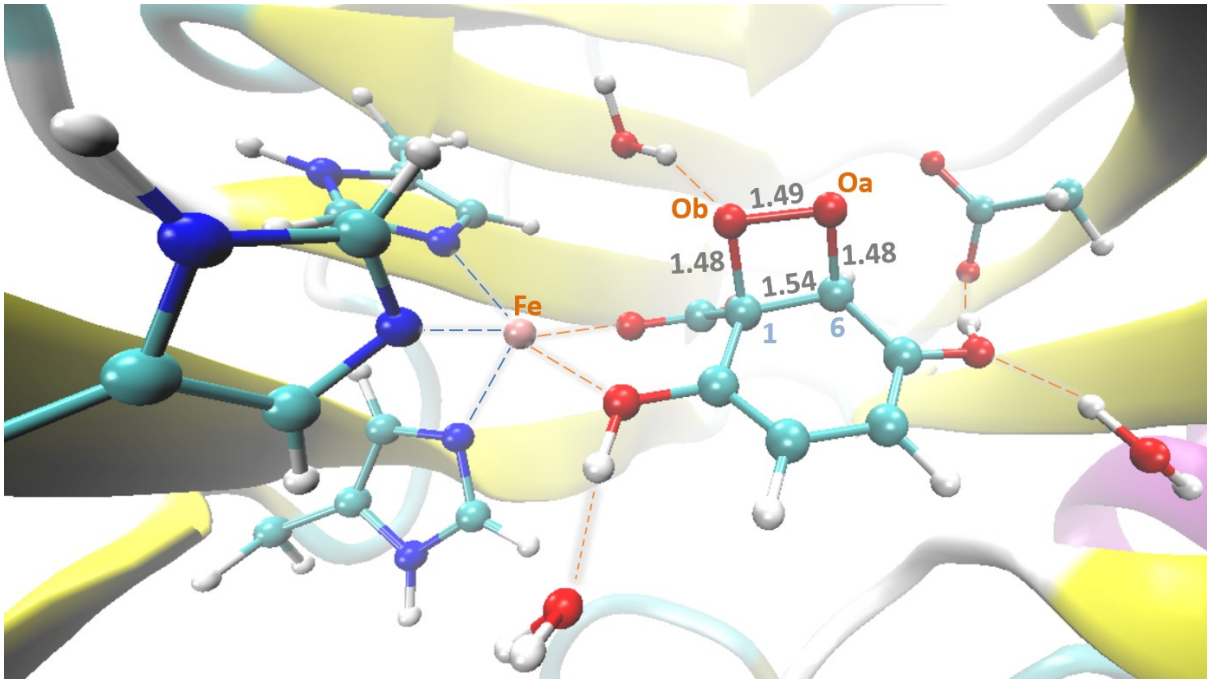



**Figure S17**. Optimized structure of 3b in quintet spin state with key interatomic distances (Å).

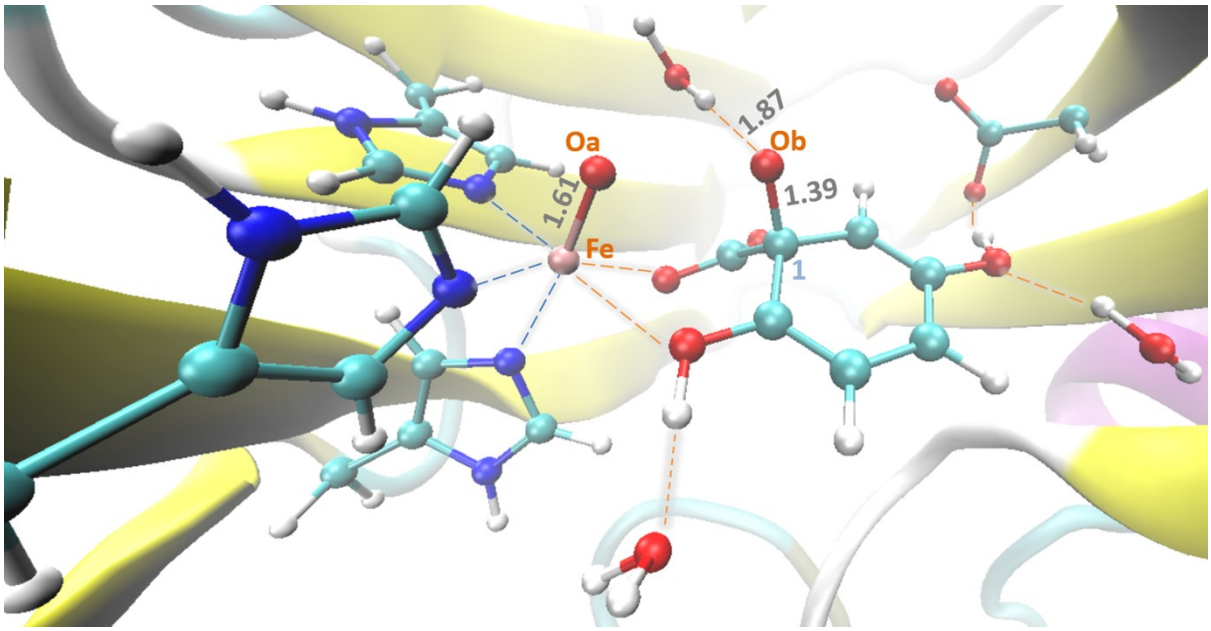



**Figure S18**. Optimized structure of 3c in quintet spin state with key interatomic distances (Å).

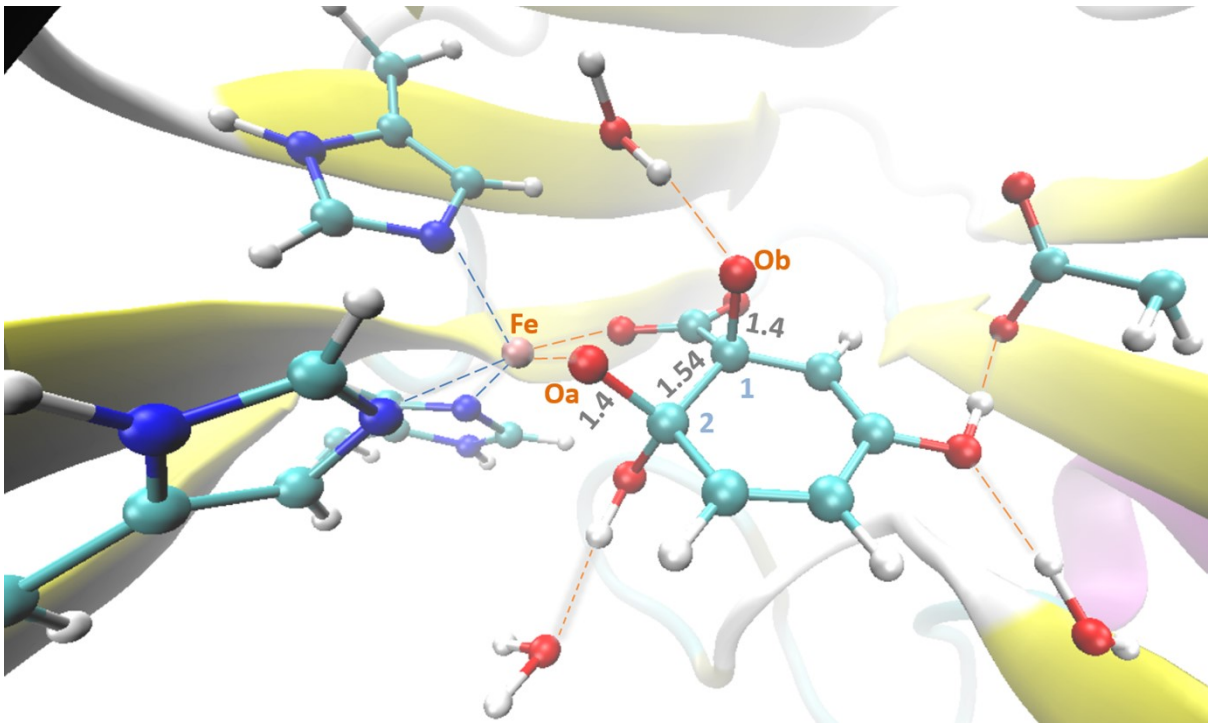



**Figure S19**. Optimized structure of 4a in quintet spin state with key interatomic distances (Å).

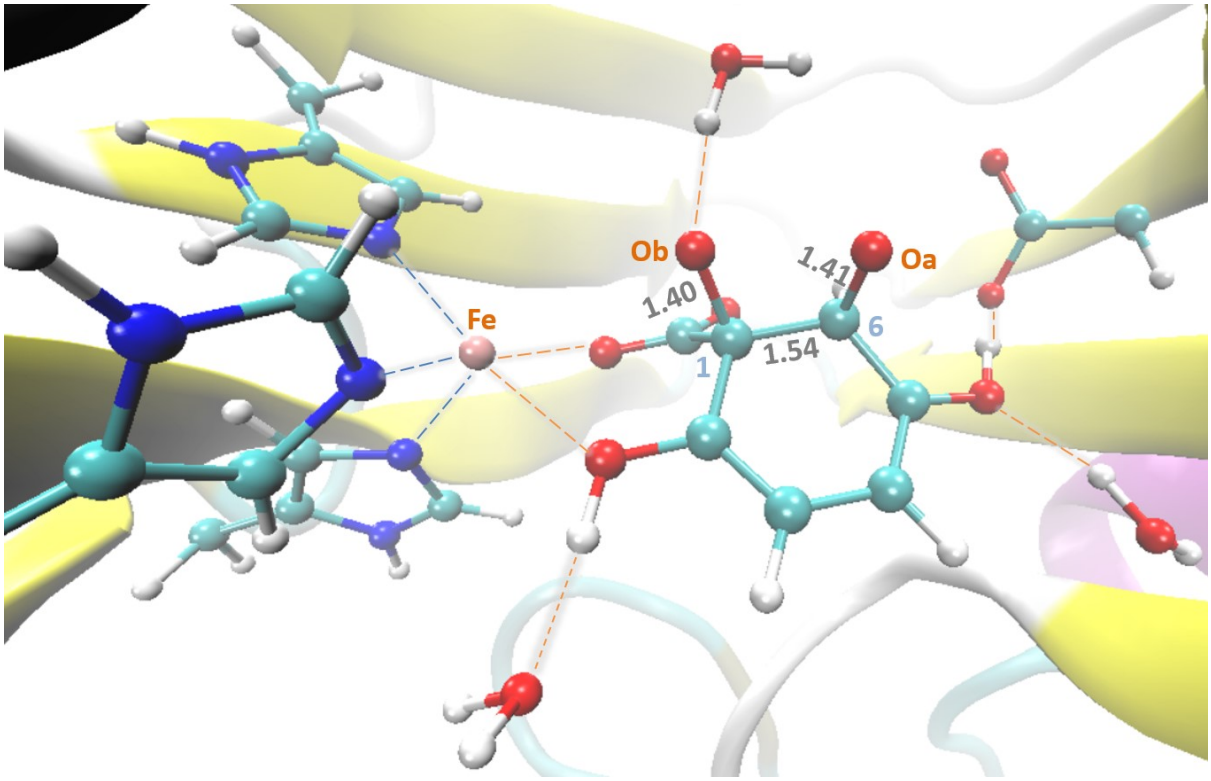



**Figure S20**. Optimized structure of 4b in quintet spin state with key interatomic distances (Å).

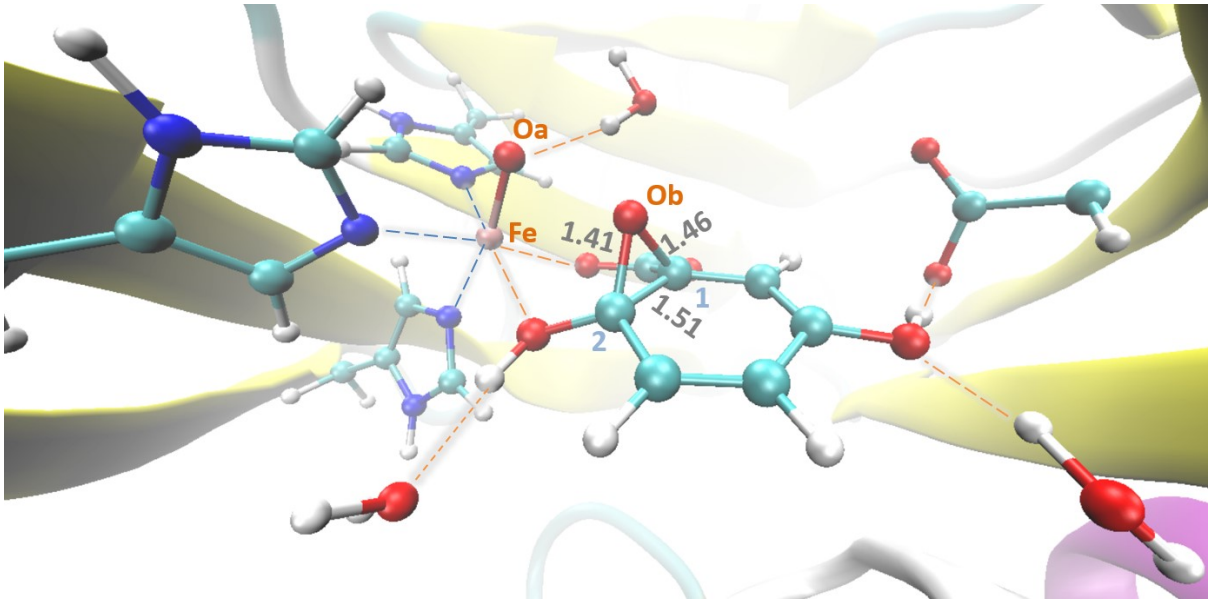



**Figure S21**. Optimized structure of 4c in quintet spin state with key interatomic distances (Å).

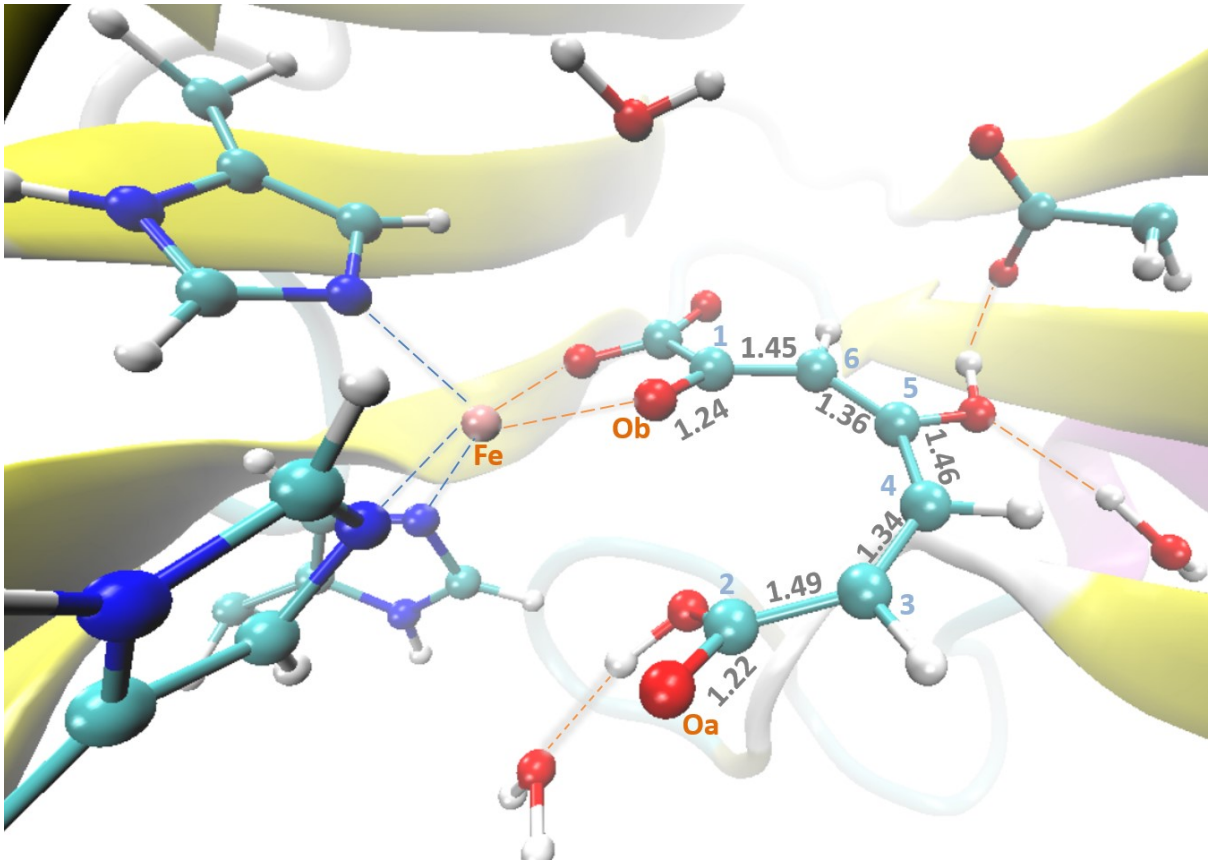



**Figure S22**. Optimized structure of 5a in quintet spin state with key interatomic distances (Å).

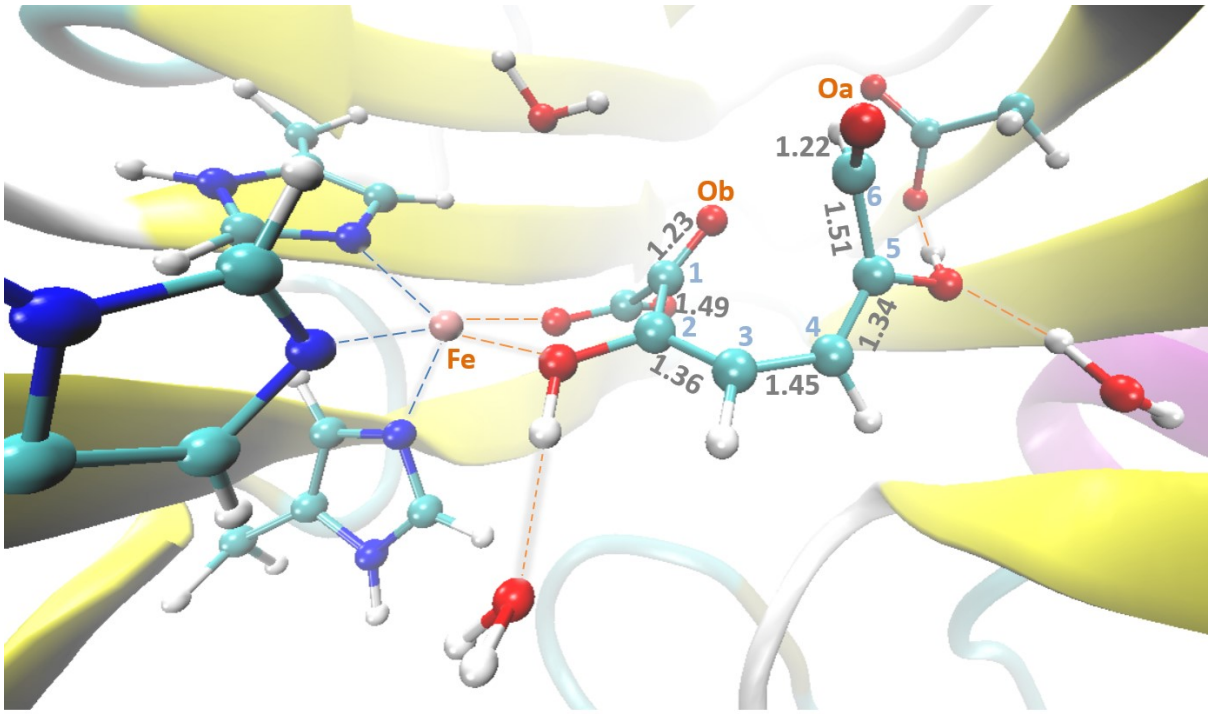


**Figure S23**. Optimized structure of 5b in quintet spin state with key interatomic distances (Å).

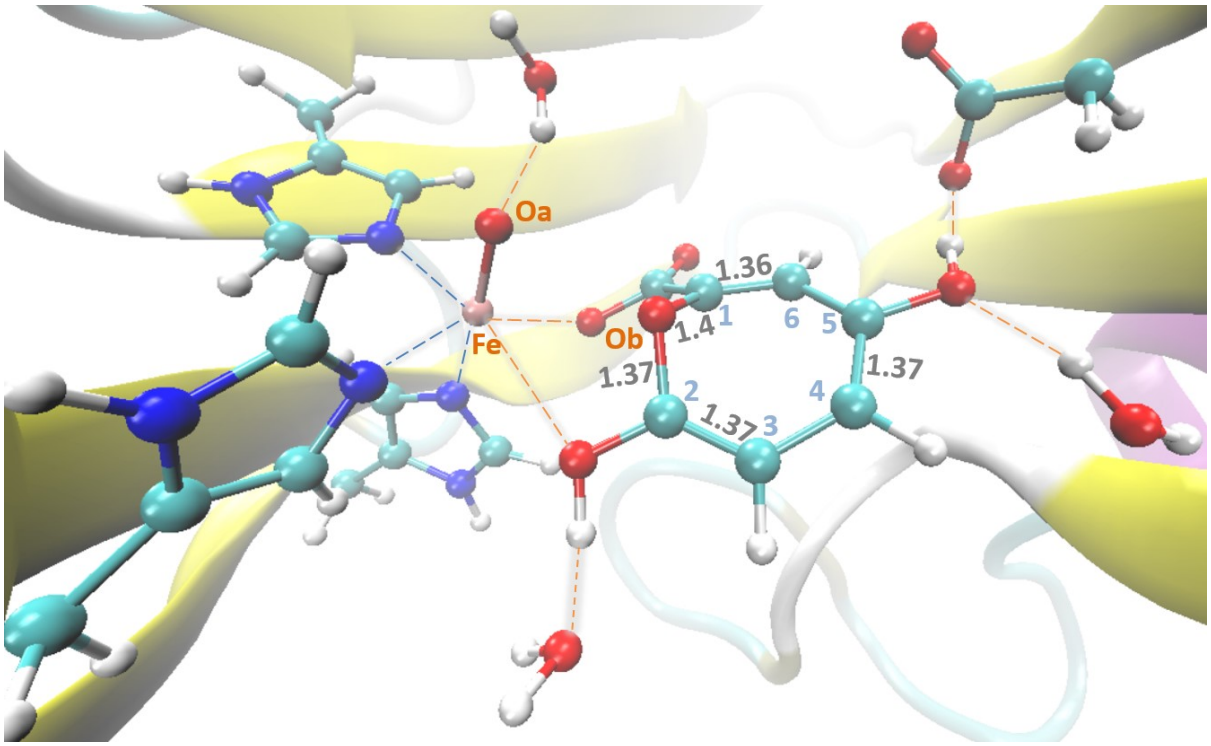



**Figure S24**. Optimized structure of 5c in quintet spin state with key interatomic distances (Å).

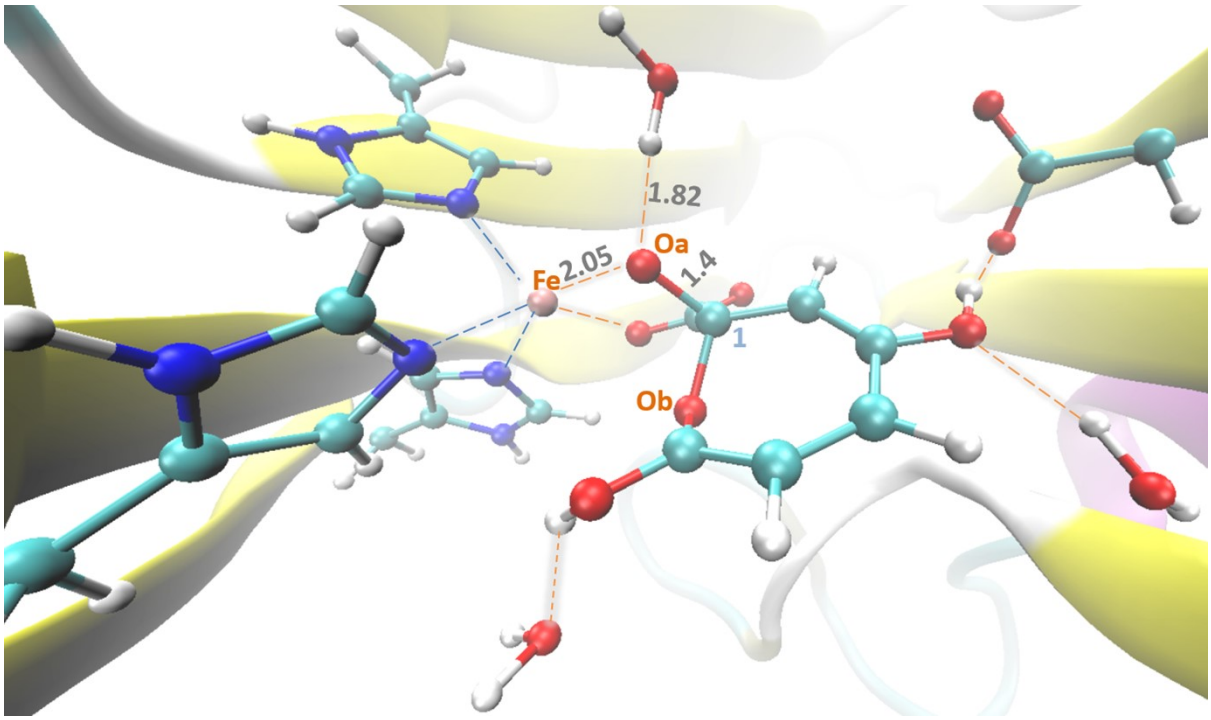


**Figure S25**. Optimized structure of 6c in quintet spin state with key interatomic distances (Å).

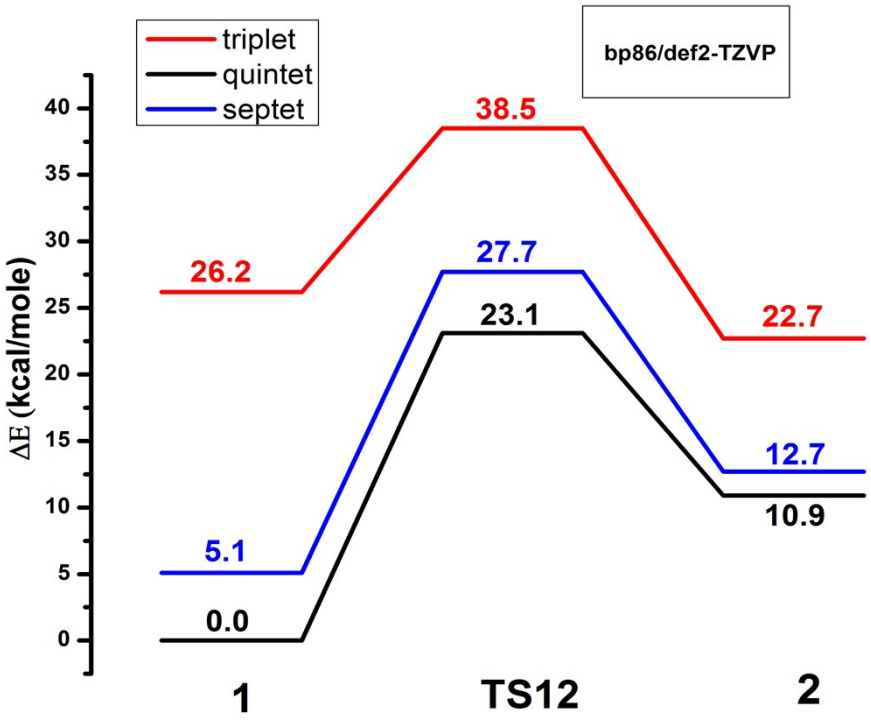



**Figure S26:** The potential energy profiles for the formation of alkylperoxo intermediate in the active site of the GDO enzyme on the quintet (black), triplet (red) and septet (blue) spin states at the BP86/def2-TZVP/OPLS level of theory.

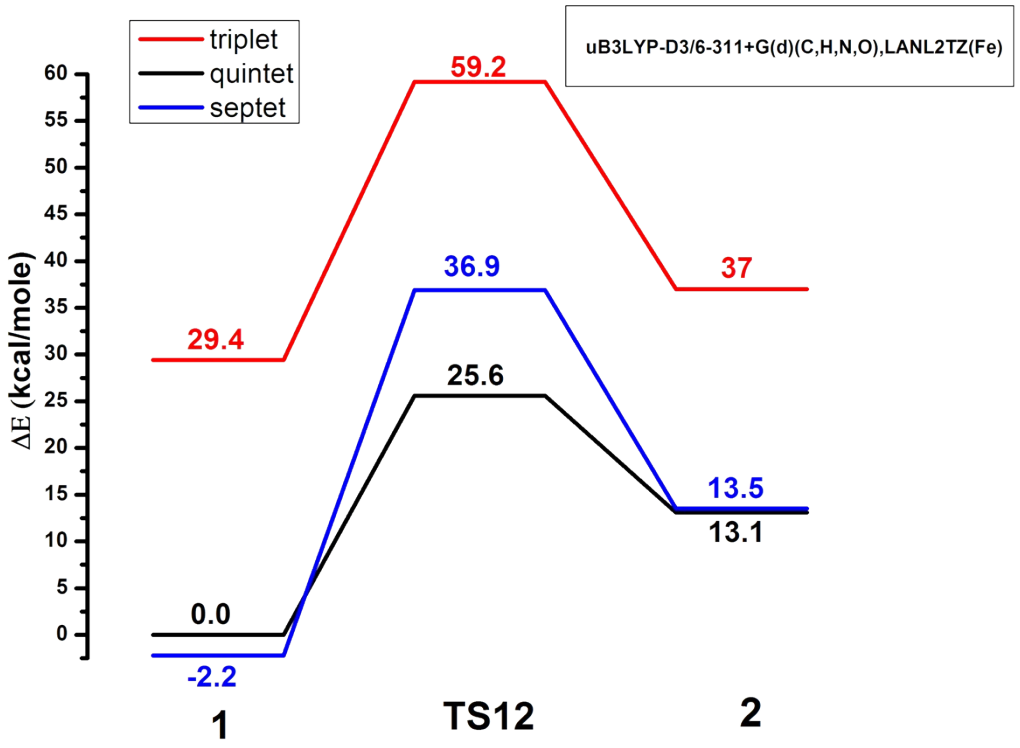



**Figure S27:** The potential energy profiles for the formation of alkylperoxo intermediate in the active site of the GDO enzyme on the quintet (black), triplet (red) and septet (blue) spin states at the uB3LYP-D3/6-311+G(d)(C,H,N,O)Lanl2TZ(Fe)/OPLS level of theory.

We have also performed single-point calculation in the ORCA programme using the QM part of intermediate 1 of our system in uB3LYP-D3/def2-TZVP level of theory. We used CPCM solvation model with ϵ = 4.0 to mimic the enzyme environment. The obtained results show similar trends of spin state (quintet, septet, triplet) ordering. The septet spin state is more stabilised (~ -1.7 kcal/mol) and the triplet spin state is 21.8 kcal/mol uphill in energy compared to the quintet spin state. If we use Gaussian 16 in place of ORCA without changing the rest of the conditions then also we will observe the same trend of stabilised septet spin state (~ -1.6 kcal/mol) and highly destabilised triplet spin state (~22.4 kcal/mol) over quintet spin state of intermediate 1.


(a) (b)

**Figure S28:** The potential energy diagram of the intermediate 1 considering three spin states at uB3LYP-D3/def2-TZVP level of theory using a) ORCA programme and b) Gaussian 16.

## Multiple Sequence Alignment (MSA) Analysis

Clustal Omega program was used for multiple sequence alignment (MSA) analysis of gentisate 1,2-dioxygenase (GDO) enzyme.[2] His119, His121, His160 and Asp174 residues are marked in rectangle boxes. MSA analysis indicated that these residues are highly conserved among the several bacteria species (Figure S31). GDO enzymes from different bacteria species ( for instance, *Pseudaminobacter sallicylatoxidans* (Ps), *Escherichia coli* (Ec), *Silicibacter pomeroyi* (Sp), and GDO (Ps) docked with Gentisate ) are taken for this for this MSA analysis study. Bacterial GDO enzyme sequences were obtained from the NCBI (www.ncbi.nlm.nih.gov) protein sequence database.

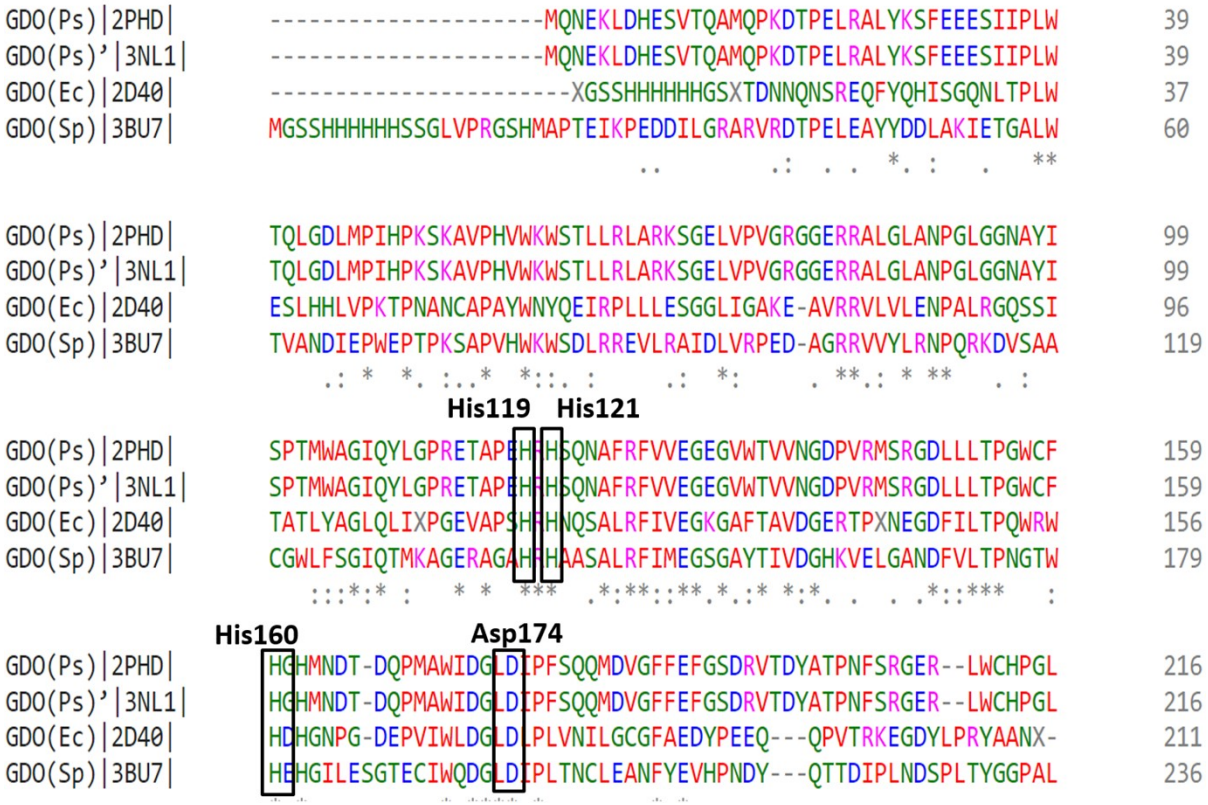



**Figure S29:** Multiple Sequence Alignment (MSA) analysis of gentisate-1,2-dioxygenase (GDO) enzyme from different bacterial sources.

We have computed the energies of one transition state and two stationary state structures on the quintet spin surface, for the substrate without having the hydroxyl group at the 5-position (i.e. salicylate). Those stationary states and transition state structures are common for all the three pathways. The obtained energy barrier for the salicylate substrate is significantly larger (38.0 kcal/mol) compared to the gentisate substrate (21.4 kcal/mol) at the uB3LYP-D3/def2-TZVP/OPLS level of theory (Figure S30). In the salicylate-GDO enzyme system, the strong hydrogen bonding interaction between the 5-OH group and Asp174 residue is absent in their corresponding stationary and saddle points. This interaction is very important for the substrate to facilitate the reaction in the active site of the GDO enzyme.

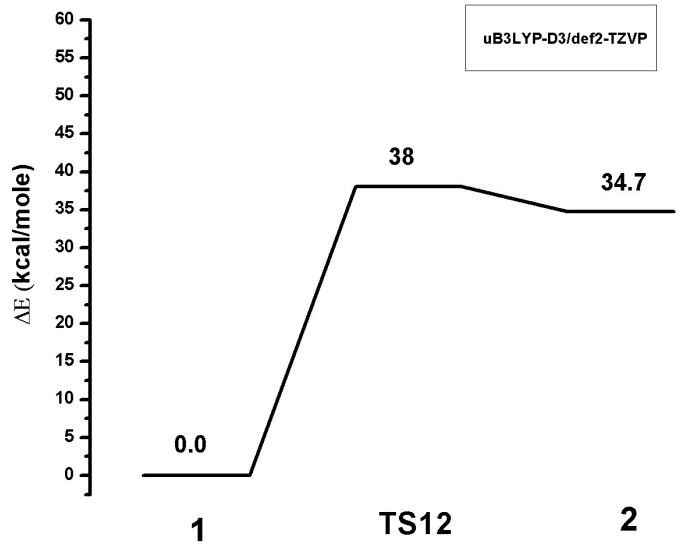
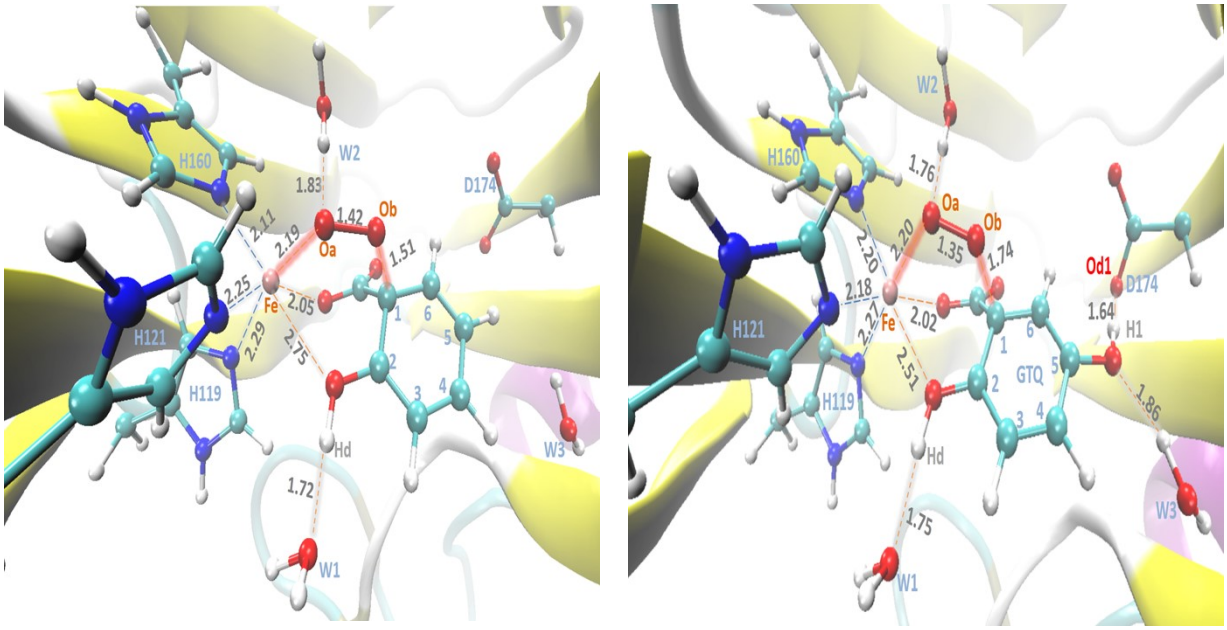



**Figure S30:** The potential energy profiles for the formation of alkylperoxo intermediate in the active site of the salicylate-GDO system on the quintet spin state at the uB3LYP-D3/def2-TZVP/OPLS level of theory.




(a) (b)

**Figure S31**. Optimized TS12 structures of the (a) Salicylate-GDO and (b) Gentisate-GDO systems, respectively. All the key distances are given in Å.

The QM/MM energy profile for the first three points (1, TS12, 2) of mutated GTQ-GDO(Asp174Ala) system has been carried out. The obtained barrier for the rate-determining step along the pathway A for GTQ-GDO (Asp174Ala) system is higher (32.1 kcal/mol) compared to the wild-type GTQ-GDO systems (21.4 kcal/mol) (Figure S32). In the mutated Asp174Ala system, the hydrogen bond between the para-hydroxyl group of the GTQ and the carboxylic group of ASP174 is absent.

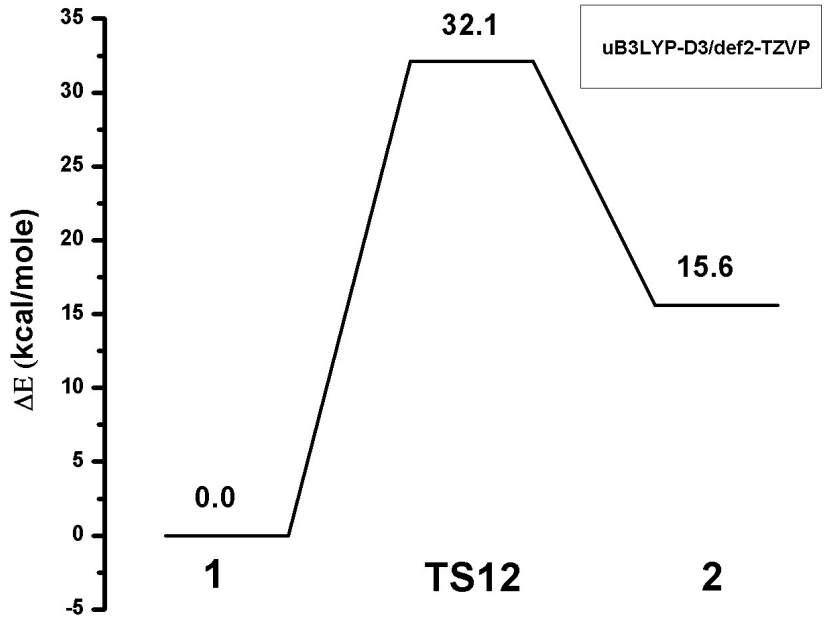
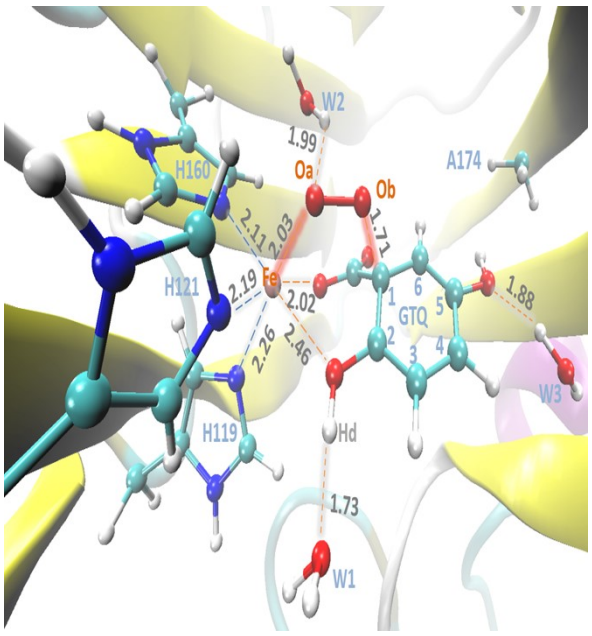



**Figure S32:** The potential energy profiles for the formation of alkylperoxo intermediate in the active site of the GDO (D174A) system on the quintet spin state at the uB3LYP-D3/def2-TZVP/OPLS level of theory.




(a) (b)

**Figure S33:** Optimized TS12 structures for the a) mutated GTQ-GDO (Asp174Ala) and b) wild-type GTQ-GDO system. All the key distances are given in Å

The QM/MM optimizations calculations of the GDO enzyme structure without having water molecules in the active sites have been performed. The calculations unearthed that the inter-atomic distance between the oxygen atom of the oxygen molecule and the catalytic iron center in this system is longer (3.13 Å) (Figure S34) compared to the system with the water model (2.07 Å) (Figure 1). This indicates that a system without water does not provide a proper oxygen-binding structure to initiate the reaction.

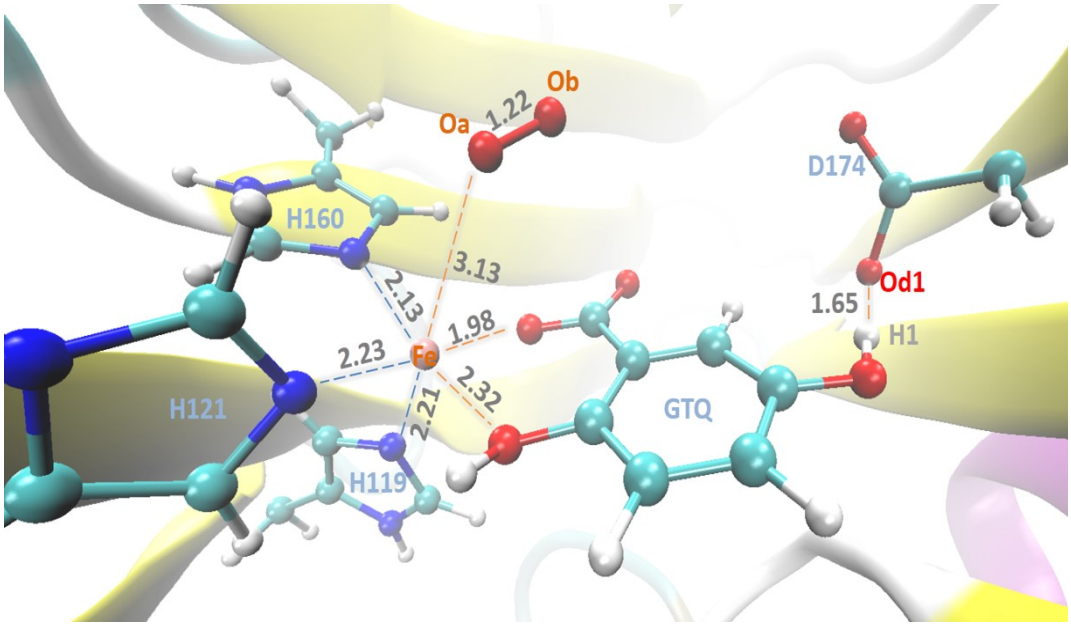



**Figure S34:** . Optimized structure of the enzyme-substrate complex of the GTQ-GDO system without having active site water molecules. All the key distances are given in Å.

**Cartesian Coordinates for all Stationary Structures**

Cartesian coordinates of QM region of all optimized stationary states for the degradation of 2,5-dihydroxybenzoate substrate catalyzed by GDO enzyme at the B3LYP/6-31+G(d)/OPLS level of theory on the quintet spin state are given below.

Structure of **1**

| | | | |
|---|---|---|---|
| C | 31.2772299166 | 62.7883537178 | 48.4100487636 |
| H | 30.6628664934 | 63.3403471641 | 47.6872006508 |
| H | 31.1263584663 | 61.7244216385 | 48.1723997084 |
| C | 32.7443559706 | 63.1123898231 | 48.1715993473 |
| N | 33.2397294744 | 63.2506319136 | 46.8766087854 |
| H | 32.7081252922 | 63.2034311328 | 46.0116206807 |
| C | 34.5840084432 | 63.4225363381 | 46.9362261559 |

| | | | |
|---|---|---|---|
| H | 35.2065741739 | 63.5578355377 | 46.0621995927 |
| N | 35.0051037886 | 63.3994034368 | 48.1938985662 |
| C | 33.8684469333 | 63.2138338416 | 48.9659194437 |
| H | 33.9457887426 | 63.1775842671 | 50.0431222142 |
| C | 35.5325617911 | 57.9435060712 | 49.5336098768 |
| H | 34.7075309510 | 58.1284646804 | 48.8407330535 |
| H | 36.1357877645 | 57.1366986229 | 49.0879456253 |
| C | 36.3335994733 | 59.2129506849 | 49.6078281161 |
| N | 37.4616201023 | 59.4237909327 | 50.3870666721 |
| H | 37.8190565514 | 58.8235831754 | 51.1315547923 |
| C | 37.8838289616 | 60.6897433311 | 50.1943175731 |
| H | 38.7292762901 | 61.1051765124 | 50.7173657534 |
| N | 37.1002219021 | 61.3210914761 | 49.3266499155 |
| C | 36.1367930723 | 60.4003028717 | 48.9510687791 |
| H | 35.3644109394 | 60.6470260337 | 48.2393728088 |
| C | 35.1222198862 | 66.1716374760 | 53.7012670672 |
| H | 35.2597824574 | 65.8109306482 | 54.7278122845 |
| H | 35.7162920573 | 67.0877232586 | 53.6034530148 |
| C | 35.6086243734 | 65.1565181871 | 52.7129631913 |
| N | 35.3968647808 | 63.7994488188 | 52.8837473326 |
| H | 34.9179356157 | 63.3416887011 | 53.6647322534 |
| C | 35.8591094996 | 63.1541004174 | 51.7962029564 |
| H | 35.8282705904 | 62.0839740046 | 51.6704093097 |
| N | 36.3635337424 | 64.0185102372 | 50.9256707131 |
| C | 36.2135555466 | 65.2749138932 | 51.4845014130 |
| H | 36.4947850770 | 66.1631510476 | 50.9356301733 |
| C | 45.0510992831 | 66.6628098507 | 46.5628350039 |
| H | 44.6947887706 | 65.6497322033 | 46.7994722915 |
| H | 45.1361444558 | 66.7276976240 | 45.4758614082 |
| C | 43.8764407421 | 67.5575240861 | 47.0074387372 |

| | | | |
|---|---|---|---|
| O | 43.4948322726 | 67.5868040345 | 48.2064466801 |
| O | 43.2442911900 | 68.1387309948 | 46.0614873197 |
| Fe | 37.0954765552 | 63.4785298079 | 48.9992892425 |
| O | 40.0104296845 | 63.2034262218 | 49.3443473420 |
| O | 38.9364980257 | 63.3298803526 | 49.9370566726 |
| H | 37.8254164093 | 62.2318701257 | 46.4845185367 |
| O | 38.0426998756 | 63.0481261916 | 47.0189979055 |
| C | 39.2220367658 | 63.6461928336 | 46.6228922589 |
| C | 40.1382852845 | 62.9254516439 | 45.8425357378 |
| C | 39.5049581970 | 64.9781621906 | 46.9897343087 |
| H | 39.9274217767 | 61.8884911207 | 45.6007784777 |
| C | 41.2973868766 | 63.5261532865 | 45.3537210991 |
| C | 38.6164304416 | 65.8726562346 | 47.8442150508 |
| C | 40.6924354904 | 65.5432631134 | 46.5139307653 |
| H | 41.9872397001 | 62.9742498115 | 44.7243792809 |
| C | 41.5538027852 | 64.8646549925 | 45.6632583430 |
| O | 38.9142314138 | 67.0878914537 | 47.9063403385 |
| O | 37.6068434121 | 65.3470457039 | 48.4239099581 |
| H | 40.9069035109 | 66.5706711150 | 46.7850735106 |
| O | 42.6409903080 | 65.4811763907 | 45.0852697969 |
| H | 42.7064583827 | 66.4315550187 | 45.3470239514 |
| O | 40.0288990157 | 65.7360550124 | 50.8908523670 |
| H | 40.9363614601 | 66.0426445850 | 50.7013444641 |
| H | 40.0935475029 | 65.2898220776 | 51.7689180509 |
| O | 37.2169764011 | 61.0532171208 | 45.4106117127 |
| H | 36.2365508790 | 61.0257749512 | 45.2740227794 |
| H | 37.4922122991 | 60.0928323238 | 45.4835704359 |
| O | 43.9462760184 | 63.7019805243 | 43.2882732782 |
| H | 43.6553084321 | 64.4059051053 | 43.9050670253 |
| H | 44.1630862728 | 64.1308594399 | 42.4343610539 |

| | | | |
|---|---|---|---|
| H | 45.9647762500 | 66.7899571335 | 46.9488764118 |
| H | 34.1523237312 | 66.3914837663 | 53.5965338008 |
| H | 35.1305977400 | 57.6419927661 | 50.3981991599 |
| H | 30.8814214954 | 62.9726059099 | 49.3097080454 |

Structure of **TS12**

| | | | |
|---|---|---|---|
| C | 31.1139142265 | 62.9711538554 | 48.4877546654 |
| H | 30.4937227546 | 63.5443572816 | 47.7853902706 |
| H | 30.9612786922 | 61.9131781525 | 48.2286034668 |
| C | 32.5776887322 | 63.2934738144 | 48.2467559530 |
| N | 33.1043271570 | 63.1835929993 | 46.9641568821 |
| H | 32.5903964668 | 62.9607385927 | 46.1189779536 |
| C | 34.4418993219 | 63.4029434308 | 47.0192289263 |
| H | 35.0852864556 | 63.3733992176 | 46.1510480558 |
| N | 34.8268227591 | 63.6483645406 | 48.2609522698 |
| C | 33.6719268905 | 63.5989901601 | 49.0288889398 |
| H | 33.7110426879 | 63.7900245584 | 50.0905466840 |
| C | 35.2933332757 | 58.1041015761 | 49.5319080474 |
| H | 34.4362436851 | 58.3127244928 | 48.8843266273 |
| H | 35.8618201061 | 57.2969450770 | 49.0482135378 |
| C | 36.1178742650 | 59.3636708029 | 49.5743618026 |
| N | 37.3466293268 | 59.5266863697 | 50.2015270463 |
| H | 37.7715096289 | 58.8928477132 | 50.8757179022 |
| C | 37.7746956733 | 60.7938285140 | 49.9939209019 |
| H | 38.6891353652 | 61.1999779744 | 50.4016139836 |
| N | 36.8992992129 | 61.4642383681 | 49.2550987678 |
| C | 35.8678601416 | 60.5783081501 | 48.9879860711 |
| H | 35.0123440116 | 60.8672444009 | 48.3961550714 |
| C | 34.8669452515 | 66.0248697580 | 53.8845993166 |
| H | 34.9672524001 | 65.5777579725 | 54.8819505578 |

| | | | |
|---|---|---|---|
| H | 35.4975677556 | 66.9225729661 | 53.8832191312 |
| C | 35.3970601444 | 65.0748623382 | 52.8396807973 |
| N | 35.1375320213 | 63.7165471035 | 52.8741631394 |
| H | 34.5914103462 | 63.2259521599 | 53.5893465086 |
| C | 35.6992895258 | 63.1414421476 | 51.7889134479 |
| H | 35.6560102626 | 62.0836024915 | 51.5827872955 |
| N | 36.3067380332 | 64.0511328133 | 51.0376106632 |
| C | 36.1327687157 | 65.2617532634 | 51.6908766275 |
| H | 36.5256949085 | 66.1788507078 | 51.2778218688 |
| C | 45.5241988489 | 67.6373952585 | 46.0676911116 |
| H | 45.5489772027 | 67.0903520920 | 45.1185416199 |
| H | 45.5976596474 | 68.6963081168 | 45.7746284670 |
| C | 44.1028425905 | 67.5322245774 | 46.6473266441 |
| O | 43.8641414305 | 67.4335504259 | 47.8700870764 |
| O | 43.1788484318 | 67.6423875388 | 45.7494016361 |
| Fe | 36.9784845312 | 63.6224771433 | 48.9873378465 |
| O | 40.1440121453 | 63.7177597302 | 48.6087842615 |
| O | 39.1231967157 | 63.4969557947 | 49.4636944525 |
| H | 37.8854774230 | 62.0237932304 | 46.4213644795 |
| O | 38.1053803236 | 62.8896281966 | 46.8691970816 |
| C | 39.2861273720 | 63.3794114461 | 46.5188194071 |
| C | 40.1113401040 | 62.7056626798 | 45.5839578486 |
| C | 39.7431840265 | 64.6078088550 | 47.1708388766 |
| H | 39.7800451871 | 61.7595178744 | 45.1691005007 |
| C | 41.2821438379 | 63.2814333522 | 45.1636060723 |
| C | 38.7239964094 | 65.6961122345 | 47.6225215926 |
| C | 40.9969630218 | 65.1561012703 | 46.6767725601 |
| H | 41.9012634579 | 62.8016360064 | 44.4110980412 |
| C | 41.7071230651 | 64.5535824901 | 45.6828397993 |
| O | 39.0794574981 | 66.8852775871 | 47.5111848546 |

| | | | |
|---|---|---|---|
| O | 37.6000583425 | 65.2972568516 | 48.0524173658 |
| H | 41.3200803441 | 66.1079188045 | 47.0779000578 |
| O | 42.7994616750 | 65.1018691048 | 45.0873705527 |
| H | 42.9162879389 | 66.0691489672 | 45.3466805880 |
| O | 39.4915456190 | 65.5873169869 | 51.1931144070 |
| H | 39.3173939907 | 64.8285788146 | 50.5967603910 |
| H | 39.8616528778 | 65.2107737332 | 52.0294283121 |
| O | 37.2417480962 | 60.7601023143 | 45.3923958805 |
| H | 36.2422712253 | 60.7026632535 | 45.4283488434 |
| H | 37.5489517482 | 59.8192519898 | 45.6063215573 |
| O | 43.9792528277 | 63.6182979953 | 43.0091151899 |
| H | 43.7105357432 | 64.2602908217 | 43.6990605392 |
| H | 44.2688567820 | 64.1185150440 | 42.2183913661 |
| H | 46.3267592158 | 67.4096867653 | 46.6190945026 |
| H | 33.9096440455 | 66.2928852270 | 53.7762383025 |
| H | 34.9256616567 | 57.7842355709 | 50.4051224078 |
| H | 30.7286321044 | 63.1334582302 | 49.3961681045 |

Structure of **2**

| | | | |
|---|---|---|---|
| C | 31.30831200 | 62.87233400 | 48.40879700 |
| H | 30.69819600 | 63.42682400 | 47.68394700 |
| H | 31.17702100 | 61.80941600 | 48.15724300 |
| C | 32.77334300 | 63.21852900 | 48.19458100 |
| N | 33.29532000 | 63.24496000 | 46.90571800 |
| H | 32.78246700 | 63.11531700 | 46.03928700 |
| C | 34.63313200 | 63.44738400 | 46.97595200 |
| H | 35.26954800 | 63.51454800 | 46.10575000 |
| N | 35.02649200 | 63.55416800 | 48.23480700 |
| C | 33.87398300 | 63.42846400 | 48.99901400 |
| H | 33.92122400 | 63.50669400 | 50.07353400 |

| | | | |
|---|---|---|---|
| C | 35.55553600 | 58.08446800 | 49.54973100 |
| H | 34.74160600 | 58.28829100 | 48.84769400 |
| H | 36.16814800 | 57.29626800 | 49.08395500 |
| C | 36.35887200 | 59.35538600 | 49.65705600 |
| N | 37.55756800 | 59.53916800 | 50.33612700 |
| H | 37.98645400 | 58.92161500 | 51.02694700 |
| C | 37.97914500 | 60.80743200 | 50.12894700 |
| H | 38.87987500 | 61.21736900 | 50.56115100 |
| N | 37.12336600 | 61.46502500 | 49.35501800 |
| C | 36.11655200 | 60.56334200 | 49.05421700 |
| H | 35.28454200 | 60.83386900 | 48.42279300 |
| C | 35.07111000 | 66.07432900 | 53.77106400 |
| H | 35.18585000 | 65.66844800 | 54.78405600 |
| H | 35.69753200 | 66.97356800 | 53.72389000 |
| C | 35.57033700 | 65.08977000 | 52.75560100 |
| N | 35.37758400 | 63.72335700 | 52.87374500 |
| H | 34.89298700 | 63.23880100 | 53.63559200 |
| C | 35.88667100 | 63.12104200 | 51.78369900 |
| H | 35.88300200 | 62.05600600 | 51.62304600 |
| N | 36.40410000 | 64.02443200 | 50.95756900 |
| C | 36.21093600 | 65.25770800 | 51.55553600 |
| H | 36.52995600 | 66.16918600 | 51.07684700 |
| C | 45.23592100 | 66.80171000 | 46.25864100 |
| H | 44.90338300 | 65.75390000 | 46.22679200 |
| H | 45.39839800 | 67.10015200 | 45.21883100 |
| C | 43.99551300 | 67.54409700 | 46.77803900 |
| O | 43.67579700 | 67.56164100 | 47.99052500 |
| O | 43.24805300 | 68.01831900 | 45.85140900 |
| Fe | 37.14844400 | 63.62130600 | 49.01401500 |
| O | 40.18896100 | 64.00423600 | 48.72122500 |

| | | | |
|---|---|---|---|
| O | 39.13379200 | 63.54051900 | 49.47845400 |
| H | 37.83800300 | 62.15735000 | 46.38857000 |
| O | 38.09923500 | 62.97948800 | 46.91326500 |
| C | 39.30003700 | 63.48894100 | 46.56553700 |
| C | 40.07521600 | 62.91410800 | 45.56115900 |
| C | 39.78728400 | 64.65132300 | 47.37122700 |
| H | 39.72720600 | 62.00842100 | 45.07398900 |
| C | 41.23588000 | 63.53827900 | 45.12304500 |
| C | 38.73081200 | 65.76451000 | 47.72189100 |
| C | 41.04027300 | 65.24706200 | 46.84309000 |
| H | 41.81759400 | 63.13421500 | 44.30168300 |
| C | 41.65809100 | 64.76204100 | 45.73171400 |
| O | 39.06506800 | 66.95329600 | 47.59369200 |
| O | 37.59279800 | 65.35871000 | 48.12902500 |
| H | 41.39769500 | 66.14516000 | 47.33309500 |
| O | 42.69662000 | 65.39383500 | 45.09652900 |
| H | 42.77156600 | 66.35236600 | 45.34652500 |
| O | 39.09599500 | 65.72960300 | 51.28811100 |
| H | 39.15305300 | 65.03062900 | 50.61388300 |
| H | 39.60929300 | 65.36493200 | 52.05218400 |
| O | 37.22119100 | 61.02971700 | 45.34646900 |
| H | 36.23019000 | 61.00166400 | 45.27873000 |
| H | 37.49480300 | 60.06731500 | 45.48091100 |
| O | 43.94921400 | 63.69685400 | 43.19239900 |
| H | 43.69710300 | 64.39424400 | 43.83233900 |
| H | 44.20964800 | 64.13986900 | 42.35670100 |
| H | 46.10192100 | 66.87680800 | 46.75301400 |
| H | 34.11026200 | 66.32769400 | 53.65891800 |
| H | 35.13512200 | 57.74681500 | 50.39189700 |
| H | 30.89118400 | 63.03890500 | 49.30225000 |

Structure of **TS23a**

| | | | |
|---|---|---|---|
| C | 31.2480067056 | 62.7974996808 | 48.4646624437 |
| H | 30.6107838650 | 63.3028452803 | 47.7293136973 |
| H | 31.1434607846 | 61.7243858872 | 48.2530946523 |
| C | 32.6943663064 | 63.1964440462 | 48.2358279032 |
| N | 33.0991525921 | 63.9989635264 | 47.1771980027 |
| H | 32.5115802513 | 64.4081570149 | 46.4579418916 |
| C | 34.4510457597 | 64.1339082905 | 47.2227117741 |
| H | 35.0173161601 | 64.7560697345 | 46.5453247329 |
| N | 34.9539451993 | 63.4609280732 | 48.2433324553 |
| C | 33.8710949064 | 62.8721252703 | 48.8702839465 |
| H | 34.0062350021 | 62.2648058047 | 49.7514918296 |
| C | 35.5067694183 | 57.9765462180 | 49.5657731365 |
| H | 34.6832057804 | 58.1709963590 | 48.8731300908 |
| H | 36.0945362580 | 57.1571826752 | 49.1248742074 |
| C | 36.3251839741 | 59.2380197844 | 49.6201557815 |
| N | 37.4665110490 | 59.4639245273 | 50.3786540897 |
| H | 37.8344706981 | 58.8747050382 | 51.1255592852 |
| C | 37.8928208143 | 60.7282861482 | 50.1438416087 |
| H | 38.7556872966 | 61.1727108655 | 50.6176164159 |
| N | 37.0991937011 | 61.3371770685 | 49.2732260142 |
| C | 36.1302433824 | 60.4096002842 | 48.9346424056 |
| H | 35.3525998229 | 60.6360745764 | 48.2211342922 |
| C | 34.9766468626 | 66.0373469367 | 53.7967124681 |
| H | 35.0881103459 | 65.6256316562 | 54.8074670579 |
| H | 35.6063445062 | 66.9335797150 | 53.7494156529 |
| C | 35.4596997038 | 65.0483674788 | 52.7729414106 |
| N | 35.2497180292 | 63.6842905320 | 52.8894974809 |

| | | | |
|---|---|---|---|
| H | 34.7445037281 | 63.2050953467 | 53.6415664998 |
| C | 35.7601074321 | 63.0774827864 | 51.8001621512 |
| H | 35.7567089002 | 62.0103976684 | 51.6459244620 |
| N | 36.2943678573 | 63.9718190371 | 50.9782572687 |
| C | 36.1081298468 | 65.2064936727 | 51.5741292243 |
| H | 36.4305031880 | 66.1146884604 | 51.0895930421 |
| C | 45.3548814164 | 67.2000745546 | 45.9949183152 |
| H | 45.1859309896 | 66.2664222351 | 45.4450585436 |
| H | 45.5278975783 | 67.9506766685 | 45.2135842551 |
| C | 43.9956812172 | 67.5881653060 | 46.5894715367 |
| O | 43.7581313326 | 67.6864360889 | 47.8122419679 |
| O | 43.0974511197 | 67.7927617963 | 45.6890816014 |
| Fe | 37.0677377375 | 63.5292843155 | 49.0538363929 |
| O | 40.0812260138 | 64.1511135531 | 48.6674828557 |
| O | 39.1156535334 | 63.0788838456 | 48.9321871294 |
| H | 37.9193759013 | 62.1154082199 | 46.0093516563 |
| O | 38.1306209970 | 63.0341667659 | 46.4516588509 |
| C | 39.3807484011 | 63.3483209967 | 46.5889759713 |
| C | 40.3993469151 | 62.6081852956 | 45.9254106420 |
| C | 39.7704498708 | 64.6351139459 | 47.3372921783 |
| H | 40.2034780545 | 61.5901958329 | 45.6061766866 |
| C | 41.5439118494 | 63.2584475945 | 45.5606733793 |
| C | 38.6118504635 | 65.7120533795 | 47.5112818528 |
| C | 41.0072775637 | 65.2752906369 | 46.7892752970 |
| H | 42.2954639830 | 62.7507254558 | 44.9611339832 |
| C | 41.7832040937 | 64.6490645568 | 45.8819237580 |
| O | 38.9153140509 | 66.9070068239 | 47.3067419539 |
| O | 37.5105184026 | 65.2606049487 | 47.9206035660 |
| H | 41.2425954578 | 66.2729070913 | 47.1347350186 |
| O | 42.8279867133 | 65.2157807848 | 45.2136583195 |

| | | | |
|---|---|---|---|
| H | 42.8448639002 | 66.2156240751 | 45.3358889144 |
| O | 39.0133796265 | 65.3488402528 | 50.9446489830 |
| H | 39.5015376615 | 64.8670824403 | 50.2509401122 |
| H | 39.4048935981 | 65.0361987243 | 51.7945495235 |
| O | 37.3302683080 | 60.9385633858 | 45.2494930783 |
| H | 36.3262425277 | 60.9323900505 | 45.2877380987 |
| H | 37.6028992183 | 59.9964941771 | 45.5275643993 |
| O | 43.9425507298 | 63.6910599870 | 43.1740275800 |
| H | 43.6869920674 | 64.3616531000 | 43.8419886161 |
| H | 44.2135430273 | 64.1564327908 | 42.3550241446 |
| H | 46.1697388063 | 67.1311243077 | 46.5704644017 |
| H | 34.0173816193 | 66.3006007470 | 53.6942057641 |
| H | 35.0959714665 | 57.6794749120 | 50.4277439491 |
| H | 30.8575949171 | 62.9942995639 | 49.3640224613 |

Structure of **TS23b**

| | | | |
|---|---|---|---|
| C | 31.22147100 | 62.78932200 | 48.39462000 |
| H | 30.57209700 | 63.32014000 | 47.68671500 |
| H | 31.09955300 | 61.72003700 | 48.17200800 |
| C | 32.66607100 | 63.15662600 | 48.12959900 |
| N | 33.15792500 | 63.16673000 | 46.83047300 |
| H | 32.62593500 | 63.01560300 | 45.97956500 |
| C | 34.49369900 | 63.38532200 | 46.86769600 |
| H | 35.11233600 | 63.43269700 | 45.98389000 |
| N | 34.90921200 | 63.52008300 | 48.11781700 |
| C | 33.77687400 | 63.39780200 | 48.90787900 |
| H | 33.84982400 | 63.50152100 | 49.97954200 |
| C | 35.60237700 | 58.04780000 | 49.56368200 |
| H | 34.78979300 | 58.23584500 | 48.85548100 |
| H | 36.23042600 | 57.26867100 | 49.10394400 |
| C | 36.37857600 | 59.33725200 | 49.67597000 |

| | | | |
|---|---|---|---|
| N | 37.54297800 | 59.56226200 | 50.39994200 |
| H | 37.96486200 | 58.95961500 | 51.10952900 |
| C | 37.94112900 | 60.83789000 | 50.18746800 |
| H | 38.81322800 | 61.26769200 | 50.65837600 |
| N | 37.10550800 | 61.46346400 | 49.36579600 |
| C | 36.13315300 | 60.52907000 | 49.04126600 |
| H | 35.31854100 | 60.76797200 | 48.37472000 |
| C | 35.12667800 | 66.12416800 | 53.73775400 |
| H | 35.24265500 | 65.75556700 | 54.76544200 |
| H | 35.74893100 | 67.02357200 | 53.65493600 |
| C | 35.61125400 | 65.10426700 | 52.75421100 |
| N | 35.34723200 | 63.75184500 | 52.88655900 |
| H | 34.85812800 | 63.28712800 | 53.65825400 |
| C | 35.80422300 | 63.11584000 | 51.79178200 |
| H | 35.73246600 | 62.05167200 | 51.63745600 |
| N | 36.35973000 | 63.98133500 | 50.95489300 |
| C | 36.25053200 | 65.22662700 | 51.54663000 |
| H | 36.60499400 | 66.11414100 | 51.04554200 |
| C | 45.08774500 | 66.68503900 | 46.44740200 |
| H | 44.72923300 | 65.65490300 | 46.59785700 |
| H | 45.21796500 | 66.82075200 | 45.37040000 |
| C | 43.90048800 | 67.53663600 | 46.90946400 |
| O | 43.55058500 | 67.59772500 | 48.11259100 |
| O | 43.22518700 | 68.05758100 | 45.95308200 |
| Fe | 36.92615400 | 63.60557700 | 48.96148300 |
| O | 40.38057200 | 64.10962300 | 48.57391600 |
| O | 41.76010100 | 63.95193400 | 48.36588600 |
| H | 37.86848400 | 62.18564600 | 46.48314500 |
| O | 38.16871400 | 62.99668500 | 47.02674800 |
| C | 39.32272000 | 63.53376200 | 46.62304100 |

| | | | |
|---|---|---|---|
| C | 40.10288900 | 62.95501000 | 45.62930300 |
| C | 39.83050800 | 64.74965700 | 47.35376700 |
| H | 39.82700600 | 61.99375800 | 45.20767400 |
| C | 41.20875500 | 63.64297200 | 45.12956400 |
| C | 38.76119900 | 65.78083300 | 47.83932200 |
| C | 40.99428000 | 65.43792500 | 46.70131400 |
| H | 41.79260700 | 63.19893800 | 44.32714000 |
| C | 41.58521200 | 64.93594700 | 45.58596300 |
| O | 39.04195400 | 66.98865500 | 47.74365400 |
| O | 37.69472800 | 65.31135700 | 48.34665900 |
| H | 41.31187200 | 66.36333300 | 47.15839800 |
| O | 42.59523500 | 65.55684200 | 44.89046900 |
| H | 42.75632100 | 66.48334900 | 45.21808900 |
| O | 39.35931500 | 65.52734300 | 50.99762900 |
| H | 39.98902400 | 65.19622800 | 50.33196100 |
| H | 39.72282100 | 65.20361500 | 51.85926100 |
| O | 37.20815800 | 61.17953600 | 45.47535600 |
| H | 36.22353200 | 61.16002600 | 45.35430500 |
| H | 37.45560600 | 60.20376700 | 45.54760800 |
| O | 43.88844400 | 63.63929800 | 43.19362800 |
| H | 43.66616100 | 64.37529100 | 43.80065700 |
| H | 44.15520900 | 64.04851200 | 42.34119700 |
| H | 45.97959500 | 66.80511100 | 46.88350500 |
| H | 34.16400400 | 66.36660700 | 53.61741000 |
| H | 35.17957000 | 57.70313900 | 50.40180000 |
| H | 30.84941000 | 62.97146200 | 49.30478200 |

Structure of **TS23c**

| | | | |
|---|---|---|---|
| C | 31.3822099271 | 62.9048060505 | 48.4338654706 |

| | | | |
|---|---|---|---|
| H | 30.8065266400 | 63.4789017951 | 47.6966809189 |
| H | 31.2506641170 | 61.8486425197 | 48.1552416937 |
| C | 32.8647431547 | 63.2388385300 | 48.2660558590 |
| N | 33.4099251035 | 63.3162105534 | 46.9858297780 |
| H | 32.9074338870 | 63.2260593698 | 46.1083979035 |
| C | 34.7473486726 | 63.5009425000 | 47.0792505663 |
| H | 35.4002343559 | 63.6047063857 | 46.2256537784 |
| N | 35.1233120320 | 63.5428300996 | 48.3494091869 |
| C | 33.9576713681 | 63.3949540664 | 49.0941439526 |
| H | 33.9923839221 | 63.4238317745 | 50.1706231803 |
| C | 35.5415674732 | 58.0933706875 | 49.5413623988 |
| H | 34.7239951295 | 58.2860667428 | 48.8404703672 |
| H | 36.1614565943 | 57.3110113097 | 49.0751089951 |
| C | 36.3335986162 | 59.3749860862 | 49.6340272088 |
| N | 37.5363852545 | 59.5796587272 | 50.3031234074 |
| H | 37.9806800469 | 58.9698090493 | 50.9913498717 |
| C | 37.9444962780 | 60.8486672889 | 50.0836499745 |
| H | 38.8412722403 | 61.2807178416 | 50.5015848860 |
| N | 37.0725794072 | 61.4880597276 | 49.3099437792 |
| C | 36.0730394498 | 60.5739029973 | 49.0202377340 |
| H | 35.2361066558 | 60.8275960351 | 48.3889662174 |
| C | 35.0678323152 | 66.1022469470 | 53.7668757846 |
| H | 35.1925446225 | 65.7011073120 | 54.7803591514 |
| H | 35.6809198874 | 67.0109059192 | 53.7162911964 |
| C | 35.5856907824 | 65.1212098183 | 52.7544285770 |
| N | 35.4208670561 | 63.7537912116 | 52.8884036486 |
| H | 34.9491794321 | 63.2701315710 | 53.6566784512 |
| C | 35.9358696850 | 63.1489522400 | 51.8001617923 |
| H | 35.9563144098 | 62.0825401147 | 51.6523157023 |
| N | 36.4244679846 | 64.0540601360 | 50.9625396467 |

| | | | |
|---|---|---|---|
| C | 36.2198460558 | 65.2890927298 | 51.5478930489 |
| H | 36.5276968766 | 66.1995202854 | 51.0591120035 |
| C | 45.2713234804 | 66.8403273030 | 46.2138087034 |
| H | 44.9516575729 | 65.7935544188 | 46.1091745361 |
| H | 45.4465895672 | 67.1999418649 | 45.1946556497 |
| C | 44.0109154728 | 67.5402996314 | 46.7449464802 |
| O | 43.7053432130 | 67.5714321939 | 47.9599476275 |
| O | 43.2356779300 | 67.9727493688 | 45.8186923441 |
| Fe | 37.1637328089 | 63.5888668365 | 49.0298348754 |
| O | 40.2362125064 | 64.0085145546 | 48.5530641323 |
| O | 38.7620597616 | 63.5551331854 | 49.6444768628 |
| H | 37.8490372294 | 62.0618686552 | 46.2810139940 |
| O | 38.1224383700 | 62.8550696654 | 46.8450853217 |
| C | 39.2904134177 | 63.3974985039 | 46.4848261727 |
| C | 40.0563723001 | 62.8865286529 | 45.4531517743 |
| C | 39.7624439729 | 64.5610119196 | 47.3393196272 |
| H | 39.7326261396 | 61.9929350567 | 44.9283817162 |
| C | 41.2225916825 | 63.5454717601 | 45.0468127911 |
| C | 38.6791754353 | 65.6596510180 | 47.6500921103 |
| C | 41.0202977176 | 65.1813756332 | 46.8182299831 |
| H | 41.8046770467 | 63.1675940959 | 44.2117847106 |
| C | 41.6663930837 | 64.7178572619 | 45.6977344253 |
| O | 38.9861535681 | 66.8543509280 | 47.5275519931 |
| O | 37.5245057780 | 65.2403802612 | 48.0400069122 |
| H | 41.3920081648 | 66.0360939587 | 47.3702405074 |
| O | 42.7434195203 | 65.3468151248 | 45.1225992205 |
| H | 42.7929017216 | 66.3141031784 | 45.3504312317 |
| O | 39.1646700099 | 65.7415392137 | 51.2448084096 |
| H | 39.1608415273 | 65.0267119356 | 50.5773449459 |
| H | 39.6667582679 | 65.3617340790 | 52.0070355953 |

| | | | |
|---|---|---|---|
| O | 37.2214322516 | 60.9692126772 | 45.2381379916 |
| H | 36.2267250782 | 60.9554087613 | 45.2108335317 |
| H | 37.4901893791 | 60.0087696768 | 45.4181145012 |
| O | 43.9396706555 | 63.6855789384 | 43.1560184243 |
| H | 43.7128423644 | 64.3823454226 | 43.8062445967 |
| H | 44.2165155636 | 64.1307832386 | 42.3259479261 |
| H | 46.1270732894 | 66.8959187336 | 46.7282033547 |
| H | 34.1028431207 | 66.3406744380 | 53.6575680262 |
| H | 35.1268656513 | 57.7522590986 | 50.3849649608 |
| H | 30.9275958507 | 63.0561470472 | 49.3116023015 |

Structure of **3a**

| | | | |
|---|---|---|---|
| C | 31.19751100 | 62.84270600 | 48.42446700 |
| H | 30.55579800 | 63.37867000 | 47.71346700 |
| H | 31.07830600 | 61.77435000 | 48.19163500 |
| C | 32.64725400 | 63.20872000 | 48.16901400 |
| N | 33.13877700 | 63.21486700 | 46.86869700 |
| H | 32.60731900 | 63.06212600 | 46.01786800 |
| C | 34.47408000 | 63.43042500 | 46.90276400 |
| H | 35.09220000 | 63.47432600 | 46.01803600 |
| N | 34.89193800 | 63.56888000 | 48.15148800 |
| C | 33.76036300 | 63.44835100 | 48.94571600 |
| H | 33.83597500 | 63.54879800 | 50.01733100 |
| C | 35.54656500 | 58.07530200 | 49.52610600 |
| H | 34.72494500 | 58.26084500 | 48.82795900 |
| H | 36.16172100 | 57.28539000 | 49.06584400 |

| | | | |
|---|---|---|---|
| C | 36.33953700 | 59.35775500 | 49.59849300 |
| N | 37.52458400 | 59.57899700 | 50.29043600 |
| H | 37.95109900 | 58.98332400 | 51.00150000 |
| C | 37.93899600 | 60.84253200 | 50.04247600 |
| H | 38.82904800 | 61.26919500 | 50.48032000 |
| N | 37.09503900 | 61.46372100 | 49.22520800 |
| C | 36.10017600 | 60.53959600 | 48.94305700 |
| H | 35.27815300 | 60.77723000 | 48.28531600 |
| C | 35.10190200 | 66.02732700 | 53.78342400 |
| H | 35.20654400 | 65.61045000 | 54.79353800 |
| H | 35.74155900 | 66.91749900 | 53.74777400 |
| C | 35.59213300 | 65.04099400 | 52.76163000 |
| N | 35.35817100 | 63.68064400 | 52.86286700 |
| H | 34.86896700 | 63.19949400 | 53.62395000 |
| C | 35.84184500 | 63.07893300 | 51.75640600 |
| H | 35.80233300 | 62.01514100 | 51.58503100 |
| N | 36.38178900 | 63.97336200 | 50.93971700 |
| C | 36.23705600 | 65.20151000 | 51.55942700 |
| H | 36.58181700 | 66.10656400 | 51.08413300 |
| C | 45.17116200 | 66.73672500 | 46.26149900 |
| H | 44.83153400 | 65.69039400 | 46.29038100 |
| H | 45.33469600 | 66.97179400 | 45.20554800 |
| C | 43.93719800 | 67.52151400 | 46.73899100 |
| O | 43.65047000 | 67.65436300 | 47.95332000 |
| O | 43.16897100 | 67.91931600 | 45.79203800 |
| Fe | 36.94333000 | 63.60812400 | 48.89647900 |
| O | 40.48101100 | 64.21615000 | 48.74339100 |
| O | 39.78384300 | 62.94055600 | 48.42427800 |
| H | 37.99060400 | 62.33862000 | 46.32109700 |
| O | 38.18573500 | 63.23529300 | 46.72413800 |

| | | | |
|---|---|---|---|
| C | 39.53305600 | 63.40612000 | 47.05513100 |
| C | 40.43680800 | 62.74152800 | 46.05578000 |
| C | 39.96064000 | 64.83583000 | 47.48312400 |
| H | 40.24539000 | 61.69385600 | 45.83984100 |
| C | 41.41476600 | 63.41797200 | 45.43500900 |
| C | 38.81207700 | 65.82921700 | 47.87232400 |
| C | 41.02302000 | 65.49470100 | 46.69796600 |
| H | 42.04347700 | 62.93873700 | 44.69056800 |
| C | 41.66936200 | 64.83536200 | 45.71838400 |
| O | 38.99568800 | 67.04059700 | 47.65429700 |
| O | 37.78727000 | 65.33085600 | 48.43404300 |
| H | 41.21706300 | 66.54268000 | 46.88374800 |
| O | 42.58796200 | 65.41592200 | 44.89403700 |
| H | 42.73837700 | 66.37793000 | 45.13193000 |
| O | 39.29631700 | 65.49133900 | 51.07035100 |
| H | 39.78873900 | 65.03267200 | 50.36559800 |
| H | 39.71746800 | 65.18965500 | 51.91411300 |
| O | 37.28501700 | 61.08141800 | 45.37896400 |
| H | 36.29743800 | 61.06229000 | 45.30057000 |
| H | 37.54937900 | 60.11732800 | 45.46479200 |
| O | 43.88412300 | 63.66370100 | 43.10220400 |
| H | 43.56789000 | 64.37061700 | 43.70184100 |
| H | 44.15489700 | 64.09409000 | 42.26185700 |
| H | 46.03936700 | 66.83173700 | 46.74852300 |
| H | 34.14534800 | 66.29636600 | 53.67107400 |
| H | 35.13521700 | 57.74460800 | 50.37547900 |
| H | 30.81168700 | 63.01525600 | 49.33075900 |

Structure of **3b**

| | | | |
|---|---|---|---|
| C | 31.17735600 | 62.80465200 | 48.39885100 |

| | | | |
|---|---|---|---|
| H | 30.52823000 | 63.33004300 | 47.68599800 |
| H | 31.05596300 | 61.73345600 | 48.18096600 |
| C | 32.62451900 | 63.16591600 | 48.12759900 |
| N | 33.13049100 | 63.11204900 | 46.83468800 |
| H | 32.61442400 | 62.91051900 | 45.98370600 |
| C | 34.46436900 | 63.34088100 | 46.87442000 |
| H | 35.09164900 | 63.34138200 | 45.99509600 |
| N | 34.86652900 | 63.54683300 | 48.11832600 |
| C | 33.72560400 | 63.45769300 | 48.90283600 |
| H | 33.78310900 | 63.61373600 | 49.96868800 |
| C | 35.58302800 | 58.06482700 | 49.55771000 |
| H | 34.77633400 | 58.24499400 | 48.84097500 |
| H | 36.21673800 | 57.28293000 | 49.10956400 |
| C | 36.35460800 | 59.35413900 | 49.66973900 |
| N | 37.52594800 | 59.57678900 | 50.38100300 |
| H | 37.96565300 | 58.96619000 | 51.07164800 |
| C | 37.90269900 | 60.86304700 | 50.19145500 |
| H | 38.77470800 | 61.29427300 | 50.66073900 |
| N | 37.04791600 | 61.49399400 | 49.39708600 |
| C | 36.08619800 | 60.55514200 | 49.06282500 |
| H | 35.26363500 | 60.79523600 | 48.40657800 |
| C | 35.08367400 | 66.08621200 | 53.77303400 |
| H | 35.19391600 | 65.69775100 | 54.79319700 |
| H | 35.71089400 | 66.98293700 | 53.70761200 |
| C | 35.56633000 | 65.08166100 | 52.77108500 |
| N | 35.29010600 | 63.72868900 | 52.87334400 |
| H | 34.79689100 | 63.25432000 | 53.63656200 |
| C | 35.75174500 | 63.11129200 | 51.77015400 |
| H | 35.67639900 | 62.05058100 | 51.59561600 |
| N | 36.31957900 | 63.98958000 | 50.95388400 |

| | | | |
|---|---|---|---|
| C | 36.21527500 | 65.22336700 | 51.57065100 |
| H | 36.57654700 | 66.11874000 | 51.08847400 |
| C | 45.16774600 | 66.70539600 | 46.35733400 |
| H | 44.81444600 | 65.66805800 | 46.45113200 |
| H | 45.30871500 | 66.89099400 | 45.28940000 |
| C | 43.96964100 | 67.53092400 | 46.83980900 |
| O | 43.64823900 | 67.59936700 | 48.05019000 |
| O | 43.25147400 | 68.01985600 | 45.89865300 |
| Fe | 36.89175300 | 63.63881000 | 48.95565800 |
| O | 40.57748600 | 64.27476000 | 48.69068200 |
| O | 41.90206400 | 64.56065700 | 48.06439400 |
| H | 37.91598400 | 62.14641300 | 46.64737400 |
| O | 38.24902100 | 62.89820200 | 47.21678200 |
| C | 39.37816900 | 63.47734300 | 46.70419800 |
| C | 40.03744600 | 63.00102800 | 45.62585000 |
| C | 39.88252100 | 64.68755200 | 47.45066800 |
| H | 39.67147400 | 62.10650500 | 45.12959900 |
| C | 41.17026500 | 63.69213000 | 45.02922100 |
| C | 38.80766200 | 65.75741200 | 47.81828700 |
| C | 41.22919500 | 65.23566600 | 46.93797200 |
| H | 41.53915900 | 63.34906700 | 44.06805600 |
| C | 41.70733700 | 64.78963800 | 45.59435300 |
| O | 39.10407200 | 66.95405700 | 47.64689000 |
| O | 37.71711900 | 65.32904600 | 48.30604500 |
| H | 41.31242400 | 66.31499400 | 47.07658700 |
| O | 42.69241500 | 65.49488900 | 44.95121100 |
| H | 42.78573100 | 66.43578200 | 45.26131000 |
| O | 39.34395600 | 65.49201200 | 50.98446600 |
| H | 39.98498000 | 65.16607100 | 50.32622300 |
| H | 39.70577900 | 65.19136900 | 51.85536000 |

| | | | |
|---|---|---|---|
| O | 37.22222500 | 61.11323600 | 45.48931600 |
| H | 36.24037300 | 61.07678200 | 45.35385700 |
| H | 37.49637300 | 60.14664800 | 45.52634800 |
| O | 43.93647000 | 63.67841700 | 43.14193200 |
| H | 43.67869900 | 64.38339700 | 43.77093700 |
| H | 44.20914900 | 64.12086200 | 42.30975200 |
| H | 46.04915700 | 66.81017700 | 46.81791600 |
| H | 34.12323200 | 66.33776900 | 53.65358000 |
| H | 35.15549600 | 57.73021600 | 50.39750200 |
| H | 30.80509500 | 62.99166100 | 49.30794400 |

Structure of **3c**

| | | | |
|---|---|---|---|
| C | 31.3201417106 | 62.8731969454 | 48.4294311554 |
| H | 30.7166750525 | 63.4196512966 | 47.6936601601 |
| H | 31.1941537029 | 61.8082196355 | 48.1828203305 |
| C | 32.7885724921 | 63.2258564497 | 48.2347872548 |
| N | 33.3210671061 | 63.3807822068 | 46.9575186458 |
| H | 32.8136758372 | 63.3316988257 | 46.0791315672 |
| C | 34.6593473489 | 63.5728966621 | 47.0543595975 |
| H | 35.3023248544 | 63.7371079600 | 46.2016603226 |
| N | 35.0433378413 | 63.5459459010 | 48.3231729646 |
| C | 33.8849004881 | 63.3428696073 | 49.0614207650 |
| H | 33.9253472755 | 63.3056375293 | 50.1376060455 |
| C | 35.4856467550 | 58.0636844047 | 49.5168475014 |
| H | 34.6536152783 | 58.2407561181 | 48.8300212276 |
| H | 36.1070023241 | 57.2803709193 | 49.0559706600 |
| C | 36.2579510542 | 59.3490187616 | 49.6030107636 |
| N | 37.4548222013 | 59.5531410069 | 50.2793585241 |
| H | 37.9005018547 | 58.9330467657 | 50.9566138581 |
| C | 37.8335649667 | 60.8340780334 | 50.1077494568 |

| | | | |
|---|---|---|---|
| H | 38.7203857225 | 61.2694371128 | 50.5402705366 |
| N | 36.9476459444 | 61.4803426491 | 49.3548169185 |
| C | 35.9669868759 | 60.5590187621 | 49.0291258955 |
| H | 35.1224968668 | 60.8173920944 | 48.4097388357 |
| C | 35.0280456665 | 66.1612124884 | 53.8064035634 |
| H | 35.1485540450 | 65.7813766650 | 54.8273959138 |
| H | 35.6199638449 | 67.0818207993 | 53.7389233668 |
| C | 35.5443642001 | 65.1715059728 | 52.8076889726 |
| N | 35.3263235717 | 63.8134409792 | 52.9369590634 |
| H | 34.8573833201 | 63.3364271896 | 53.7118977398 |
| C | 35.7768331551 | 63.1963607060 | 51.8294283204 |
| H | 35.7562831577 | 62.1305207946 | 51.6762766431 |
| N | 36.2682556842 | 64.0902856333 | 50.9834452496 |
| C | 36.1490991168 | 65.3269873453 | 51.5833398608 |
| H | 36.4579044025 | 66.2299120703 | 51.0776079257 |
| C | 45.3424375877 | 67.0110155929 | 46.1110092740 |
| H | 45.0596453536 | 66.0028417550 | 45.7900817713 |
| H | 45.5412042399 | 67.5558758090 | 45.1846470758 |
| C | 44.0395486035 | 67.5906579239 | 46.6833053064 |
| O | 43.7658526143 | 67.6281831412 | 47.9033743906 |
| O | 43.2110532383 | 67.9620987421 | 45.7729576735 |
| Fe | 37.0751598030 | 63.5613414930 | 49.1384143316 |
| O | 40.5972605529 | 64.0456669071 | 48.5106911621 |
| O | 38.5200598746 | 63.4362446503 | 49.8410640402 |
| H | 38.1315140771 | 61.8749643126 | 46.4020005151 |
| O | 38.4634451456 | 62.6051636635 | 47.0131401598 |
| C | 39.5021962027 | 63.2656993991 | 46.5527231907 |
| C | 40.1801317475 | 62.8543111077 | 45.4127384147 |
| C | 39.9459775050 | 64.4887655604 | 47.3616487598 |
| H | 39.8887022367 | 61.9420989367 | 44.9001168398 |

| | | | |
|---|---|---|---|
| C | 41.2360044474 | 63.6227353577 | 44.9211105732 |
| C | 38.7577938174 | 65.4981935717 | 47.6353343479 |
| C | 41.0772514903 | 65.2211033551 | 46.7013948347 |
| H | 41.7689581274 | 63.2884900815 | 44.0341753803 |
| C | 41.6808032847 | 64.8071921444 | 45.5401468803 |
| O | 38.9981620606 | 66.7098735806 | 47.5139668866 |
| O | 37.5941434312 | 65.0296496228 | 47.9609577765 |
| H | 41.4525915922 | 66.0683204477 | 47.2622347907 |
| O | 42.7328511816 | 65.4541861531 | 44.9281180303 |
| H | 42.8081613860 | 66.4124782794 | 45.2028911878 |
| O | 39.8243543159 | 65.5652120074 | 50.7875071947 |
| H | 40.1501023972 | 64.9878800165 | 50.0611547979 |
| H | 39.9926078783 | 65.1044343667 | 51.6408194681 |
| O | 37.3209459690 | 60.9044954416 | 45.2874540200 |
| H | 36.3292412145 | 60.9360608665 | 45.3039992232 |
| H | 37.5494456208 | 59.9263414198 | 45.4422236000 |
| O | 43.9491721509 | 63.7092726209 | 43.1027298931 |
| H | 43.7131929592 | 64.4270064740 | 43.7290157894 |
| H | 44.2375397515 | 64.1392768089 | 42.2678162353 |
| H | 46.1765563181 | 66.9927840894 | 46.6622928271 |
| H | 34.0586464395 | 66.3716184651 | 53.6799343433 |
| H | 35.0895177530 | 57.7392396195 | 50.3758104780 |
| H | 30.8940029647 | 63.0473385505 | 49.3171701208 |

Structure of **TS34a**

| | | | |
|---|---|---|---|
| C | 31.3022388941 | 62.8294557254 | 48.4677646393 |
| H | 30.6734004134 | 63.3400942906 | 47.7295552261 |
| H | 31.2078706142 | 61.7582700173 | 48.2399766409 |
| C | 32.7533760818 | 63.2331516389 | 48.2468727436 |

| | | | |
|---|---|---|---|
| N | 33.1559636782 | 64.0258646489 | 47.1782509335 |
| H | 32.5660863370 | 64.4447647075 | 46.4655333442 |
| C | 34.5060109631 | 64.1441316747 | 47.1978630881 |
| H | 35.0701447271 | 64.7490353558 | 46.5040249790 |
| N | 35.0167360207 | 63.4699476644 | 48.2160537908 |
| C | 33.9355711442 | 62.8994902729 | 48.8689153557 |
| H | 34.0784996081 | 62.2958174757 | 49.7510321404 |
| C | 35.5299272032 | 57.9747835111 | 49.5376525832 |
| H | 34.7129395384 | 58.1638052189 | 48.8356703265 |
| H | 36.1274923932 | 57.1614055415 | 49.0972088790 |
| C | 36.3506933504 | 59.2421756210 | 49.5770388193 |
| N | 37.5177216645 | 59.4718305788 | 50.2968692845 |
| H | 37.9226027004 | 58.8870353993 | 51.0289093185 |
| C | 37.9528977122 | 60.7231203714 | 50.0274218437 |
| H | 38.8364039210 | 61.1544253531 | 50.4748628937 |
| N | 37.1340307767 | 61.3316001966 | 49.1742312915 |
| C | 36.1438091392 | 60.4071827040 | 48.8808401962 |
| H | 35.3572307737 | 60.6271378668 | 48.1757346199 |
| C | 35.0808250179 | 66.0082650131 | 53.6463574477 |
| H | 35.2331723052 | 65.5870430434 | 54.6488039506 |
| H | 35.7227547145 | 66.8960916739 | 53.5866455544 |
| C | 35.5533123108 | 65.0189730971 | 52.6090422371 |
| N | 35.3577736140 | 63.6510849222 | 52.7373126875 |
| H | 34.8483214503 | 63.1801325903 | 53.4908962795 |
| C | 35.9159301688 | 63.0337469118 | 51.6790164807 |
| H | 35.9283496577 | 61.9645010205 | 51.5428609776 |
| N | 36.4735548380 | 63.9218758267 | 50.8612230585 |
| C | 36.2490261980 | 65.1666635366 | 51.4328857509 |
| H | 36.5885264342 | 66.0683113220 | 50.9481471969 |
| C | 45.2501887479 | 66.8133903635 | 46.1381514317 |

| | | | |
|---|---|---|---|
| H | 44.9409357800 | 65.7649692166 | 46.0231375664 |
| H | 45.4514045770 | 67.1620988117 | 45.1185910076 |
| C | 43.9471174191 | 67.5291802090 | 46.5880157694 |
| O | 43.7349620378 | 67.9249113546 | 47.7627827223 |
| O | 43.0654612383 | 67.6185512374 | 45.6584975219 |
| Fe | 37.1347763793 | 63.5113625625 | 48.8733493022 |
| O | 40.3713615341 | 64.5049257496 | 48.7032030987 |
| O | 39.2028121676 | 63.1515628799 | 48.5915689968 |
| H | 38.0063545807 | 62.2931990169 | 46.1751866566 |
| O | 38.1216382725 | 63.2138967200 | 46.5514519157 |
| C | 39.3686198156 | 63.4322238676 | 47.1643442721 |
| C | 40.4610858004 | 62.6266024079 | 46.5108202605 |
| C | 39.7837051579 | 64.8912933572 | 47.4190200064 |
| H | 40.3580535268 | 61.5447189575 | 46.5317050605 |
| C | 41.4916988008 | 63.2170147833 | 45.8811163611 |
| C | 38.6034696407 | 65.8699287208 | 47.7125528871 |
| C | 40.8304725387 | 65.4806426280 | 46.5597281084 |
| H | 42.2553390307 | 62.6295586718 | 45.3785181164 |
| C | 41.6414705987 | 64.6748949739 | 45.8394521609 |
| O | 38.8040739052 | 67.0872747800 | 47.5575229167 |
| O | 37.5162949144 | 65.3489166625 | 48.1516740312 |
| H | 40.9371572530 | 66.5563624675 | 46.5271888948 |
| O | 42.6257742550 | 65.1359600029 | 45.0285654896 |
| H | 42.7688048515 | 66.1348981838 | 45.1656251775 |
| O | 39.2193666743 | 65.5191936922 | 50.9928780371 |
| H | 39.7518586201 | 65.1472381575 | 50.2611199780 |
| H | 39.6517201122 | 65.2021856221 | 51.8241645481 |
| O | 37.3163417593 | 60.9612830958 | 45.2409856154 |
| H | 36.3228940730 | 60.9701513108 | 45.2586834877 |
| H | 37.5619178001 | 60.0067409382 | 45.4576427914 |

| | | | |
|---|---|---|---|
| O | 43.9101958593 | 63.6226864576 | 43.0686352399 |
| H | 43.5292317788 | 64.2411058069 | 43.7260431843 |
| H | 44.1852732074 | 64.1360235630 | 42.2803975269 |
| H | 46.0987541957 | 66.8681556374 | 46.6643998955 |
| H | 34.1231829939 | 66.2915776324 | 53.5948238320 |
| H | 35.1130421241 | 57.6765010942 | 50.3962761507 |
| H | 30.8911009146 | 63.0078662579 | 49.3617082862 |

Structure of **TS34b**

| | | | |
|---|---|---|---|
| C | 31.1333676559 | 62.9011782082 | 48.4324760102 |
| H | 30.4905781364 | 63.4476373329 | 47.7296321987 |
| H | 30.9931511374 | 61.8351161889 | 48.2020483513 |
| C | 32.5843156317 | 63.2402798737 | 48.1675829786 |
| N | 33.1058530223 | 63.1199001489 | 46.8863227373 |
| H | 32.5961224120 | 62.8766464376 | 46.0432301522 |
| C | 34.4386878850 | 63.3529962959 | 46.9303727474 |
| H | 35.0784873881 | 63.3079779259 | 46.0613192865 |
| N | 34.8240249708 | 63.6234236879 | 48.1672290073 |
| C | 33.6740939399 | 63.5731356914 | 48.9420843220 |
| H | 33.7158165439 | 63.7798607892 | 50.0006739460 |
| C | 35.5093462203 | 58.1775919589 | 49.5153080972 |
| H | 34.6893078205 | 58.3820743411 | 48.8199044153 |
| H | 36.1200778236 | 57.3937552316 | 49.0464939267 |
| C | 36.3004345025 | 59.4549100700 | 49.6309949174 |
| N | 37.4970591748 | 59.6519118495 | 50.3082780307 |
| H | 37.9432466451 | 59.0249803047 | 50.9785153988 |
| C | 37.8851389509 | 60.9366641647 | 50.1296772859 |
| H | 38.7746158600 | 61.3529665043 | 50.5800322568 |
| N | 37.0148465798 | 61.5904381986 | 49.3708738455 |
| C | 36.0301467278 | 60.6686617490 | 49.0519498080 |

| | | | |
|---|---|---|---|
| H | 35.1893852246 | 60.9294132767 | 48.4277126276 |
| C | 34.9835341622 | 66.0656655241 | 53.8544612745 |
| H | 35.0668222132 | 65.6454133601 | 54.8645882929 |
| H | 35.6076836393 | 66.9662293200 | 53.8346395295 |
| C | 35.5031078518 | 65.0938219284 | 52.8359840225 |
| N | 35.2079914336 | 63.7425707827 | 52.8794203379 |
| H | 34.6887801723 | 63.2526545089 | 53.6170474680 |
| C | 35.7021596449 | 63.1562792633 | 51.7734267560 |
| H | 35.6216869575 | 62.1020540185 | 51.5634898206 |
| N | 36.3078309921 | 64.0550254925 | 51.0068185509 |
| C | 36.1985405486 | 65.2679190655 | 51.6651715214 |
| H | 36.5924864226 | 66.1739574002 | 51.2311477863 |
| C | 45.4522186057 | 67.3684891816 | 46.0063256935 |
| H | 45.3392918974 | 66.5610689006 | 45.2734797867 |
| H | 45.5846033935 | 68.2755220320 | 45.3958119316 |
| C | 44.0870604708 | 67.5976937729 | 46.6664477880 |
| O | 43.9382539466 | 67.7177682139 | 47.9005289209 |
| O | 43.1101098903 | 67.7112338371 | 45.8295662735 |
| Fe | 36.8545595403 | 63.7280399054 | 48.9905081570 |
| O | 40.3288554475 | 64.0699976725 | 48.7346142417 |
| O | 41.9685196726 | 64.2445565348 | 47.9896271146 |
| H | 37.8865281361 | 62.0710937990 | 46.4431745749 |
| O | 38.1661838554 | 62.8501306341 | 47.0063158701 |
| C | 39.3653090727 | 63.3570026239 | 46.6500795760 |
| C | 40.1071060119 | 62.8276664007 | 45.6217211382 |
| C | 39.8650997985 | 64.5353372657 | 47.4581039885 |
| H | 39.7299251519 | 61.9495327461 | 45.1038444843 |
| C | 41.2848468223 | 63.4544208254 | 45.1162909446 |
| C | 38.8049799559 | 65.6623063525 | 47.6787080181 |
| C | 41.2629201014 | 65.0249353089 | 47.0161317325 |

| | | | |
|---|---|---|---|
| H | 41.7202824054 | 63.0951697350 | 44.1887340259 |
| C | 41.7836578100 | 64.6036393369 | 45.6856580983 |
| O | 39.1376323477 | 66.8296815981 | 47.4149593265 |
| O | 37.6758253479 | 65.3082375464 | 48.1576389529 |
| H | 41.3847358276 | 66.0971182719 | 47.1873281475 |
| O | 42.7188149931 | 65.3134854479 | 45.0353303665 |
| H | 42.8357809534 | 66.2720171292 | 45.3764582920 |
| O | 39.3257667786 | 65.4477785980 | 50.9342158303 |
| H | 39.8177356037 | 64.9699182357 | 50.2335899213 |
| H | 39.7287865004 | 65.1472437989 | 51.7855602290 |
| O | 37.2293324666 | 60.8803532334 | 45.3362207275 |
| H | 36.2358594097 | 60.8925957790 | 45.3036858595 |
| H | 37.4558771625 | 59.9280741151 | 45.5939302271 |
| O | 43.9930558210 | 63.7462903054 | 43.0970290675 |
| H | 43.6963184218 | 64.4135120189 | 43.7498977741 |
| H | 44.2834012255 | 64.2221897164 | 42.2904808064 |
| H | 46.2694945993 | 67.2371940301 | 46.5674152884 |
| H | 34.0258714508 | 66.3182537759 | 53.7163261729 |
| H | 35.0935757520 | 57.8291594529 | 50.3553852999 |
| H | 30.7682261422 | 63.0827387270 | 49.3455518302 |

Structure of **TS34c**

| | | | |
|---|---|---|---|
| C | 31.28180700 | 62.92019700 | 48.42971800 |
| H | 30.68775300 | 63.48740700 | 47.70113000 |
| H | 31.15920700 | 61.86251100 | 48.15345800 |
| C | 32.75239800 | 63.27615500 | 48.25959500 |
| N | 33.30776200 | 63.38799700 | 46.98841800 |
| H | 32.80961400 | 63.33901500 | 46.10604600 |
| C | 34.64498600 | 63.57636800 | 47.10212400 |
| H | 35.30538000 | 63.70319400 | 46.25720700 |

| | | | |
|---|---|---|---|
| N | 35.00654100 | 63.58853300 | 48.37616500 |
| C | 33.83383100 | 63.41944600 | 49.10106900 |
| H | 33.85389800 | 63.42613700 | 50.17778200 |
| C | 35.35875000 | 58.03628400 | 49.51570800 |
| H | 34.50683500 | 58.21327100 | 48.85331100 |
| H | 35.96339700 | 57.24882000 | 49.04079300 |
| C | 36.14066300 | 59.31999200 | 49.57300100 |
| N | 37.35115400 | 59.50157100 | 50.22987300 |
| H | 37.78728800 | 58.87156700 | 50.90283400 |
| C | 37.74668000 | 60.77718100 | 50.06481600 |
| H | 38.64623500 | 61.19160600 | 50.49087500 |
| N | 36.86145400 | 61.44558600 | 49.32940800 |
| C | 35.85976700 | 60.54033100 | 49.01227100 |
| H | 35.01036400 | 60.81820300 | 48.40734800 |
| C | 34.93696500 | 66.10970400 | 53.87074000 |
| H | 35.03998300 | 65.70857700 | 54.88624100 |
| H | 35.55235100 | 67.01638300 | 53.82851200 |
| C | 35.45213500 | 65.12375000 | 52.86343900 |
| N | 35.21094100 | 63.76612400 | 52.96614100 |
| H | 34.72833600 | 63.28052800 | 53.72840800 |
| C | 35.68550500 | 63.15741600 | 51.86374100 |
| H | 35.65295300 | 62.09445100 | 51.69210000 |
| N | 36.21425300 | 64.05529100 | 51.04543100 |
| C | 36.09355700 | 65.28564500 | 51.65856900 |
| H | 36.43616100 | 66.18788200 | 51.17573500 |
| C | 45.29041700 | 67.06896800 | 46.08379500 |
| H | 45.02829300 | 66.06727400 | 45.71409400 |
| H | 45.47598700 | 67.66617800 | 45.18364900 |
| C | 43.98796100 | 67.59831200 | 46.69275100 |
| O | 43.71601700 | 67.54966100 | 47.91190400 |

| | | | |
|---|---|---|---|
| O | 43.16129900 | 68.02663100 | 45.80640200 |
| Fe | 37.02581000 | 63.55335900 | 49.19881300 |
| O | 40.46641300 | 64.02029800 | 48.54621800 |
| O | 38.46589000 | 63.35518100 | 49.89951700 |
| H | 38.17294400 | 61.90217800 | 46.48868400 |
| O | 38.39098100 | 62.73223100 | 47.01936500 |
| C | 39.51212100 | 63.32902800 | 46.68126100 |
| C | 40.34757700 | 62.76249000 | 45.68837500 |
| C | 39.89438800 | 64.59556100 | 47.41050700 |
| H | 40.14454700 | 61.76146300 | 45.32113100 |
| C | 41.35053600 | 63.52594800 | 45.14261100 |
| C | 38.71439600 | 65.57512700 | 47.74314100 |
| C | 40.99993900 | 65.33753700 | 46.69582500 |
| H | 41.96845500 | 63.12011900 | 44.34540400 |
| C | 41.64991300 | 64.84445100 | 45.61258000 |
| O | 38.94019000 | 66.79384300 | 47.65219100 |
| O | 37.57320500 | 65.08521100 | 48.10786600 |
| H | 41.31597000 | 66.26593900 | 47.15722700 |
| O | 42.65291000 | 65.49268500 | 44.92456600 |
| H | 42.73322400 | 66.44843200 | 45.19512700 |
| O | 39.39342900 | 65.60876800 | 50.95495600 |
| H | 39.77690300 | 65.04268000 | 50.25390300 |
| H | 39.71370800 | 65.22495800 | 51.80571300 |
| O | 37.42108900 | 60.86182400 | 45.38210800 |
| H | 36.42820900 | 60.90283800 | 45.38677200 |
| H | 37.63401000 | 59.87961000 | 45.49857600 |
| O | 43.93361200 | 63.74735800 | 43.10953900 |
| H | 43.66813000 | 64.46880400 | 43.71846700 |
| H | 44.21507400 | 64.16653200 | 42.26790100 |
| H | 46.12250400 | 67.04120500 | 46.63774600 |

| | | | |
|---|---|---|---|
| H | 33.97471100 | 66.34706400 | 53.73759000 |
| H | 34.99464100 | 57.71964100 | 50.39158600 |
| H | 30.84411700 | 63.06973400 | 49.31632200 |

Structure of **4a**

| | | | |
|---|---|---|---|
| C | 31.3067166238 | 62.8377507322 | 48.4665474117 |
| H | 30.6845059247 | 63.3675315329 | 47.7352692797 |
| H | 31.1968511448 | 61.7718947896 | 48.2251255618 |
| C | 32.7645903048 | 63.2296380849 | 48.2478296065 |
| N | 33.1717343394 | 64.0197850513 | 47.1771639631 |
| H | 32.5822459649 | 64.4475390839 | 46.4684456967 |
| C | 34.5208211316 | 64.1343773341 | 47.1946062243 |
| H | 35.0855366322 | 64.7345854005 | 46.4972823476 |
| N | 35.0321852019 | 63.4580755985 | 48.2136189290 |
| C | 33.9461130957 | 62.8927567752 | 48.8696333313 |
| H | 34.0831363334 | 62.2913969751 | 49.7535227659 |
| C | 35.5200680667 | 57.9660836733 | 49.5317508105 |
| H | 34.6929565196 | 58.1649860877 | 48.8429587933 |
| H | 36.1003240479 | 57.1457894288 | 49.0835118749 |
| C | 36.3420862936 | 59.2283471699 | 49.5724743108 |
| N | 37.5146211267 | 59.4637705902 | 50.2808974234 |
| H | 37.9287193802 | 58.8768020907 | 51.0053454936 |
| C | 37.9293505713 | 60.7243443213 | 50.0208639865 |
| H | 38.8174393726 | 61.1631688847 | 50.4491706401 |
| N | 37.0829034085 | 61.3292266592 | 49.1925226943 |
| C | 36.1061159630 | 60.3983785912 | 48.8973666655 |
| H | 35.3055382572 | 60.6139653331 | 48.2060867762 |
| C | 35.0818500123 | 66.0055088947 | 53.6384261145 |
| H | 35.2386419332 | 65.5826152691 | 54.6392274988 |
| H | 35.7243640970 | 66.8931847362 | 53.5784216544 |
| C | 35.5558125920 | 65.0180693418 | 52.5968239192 |

| | | | |
|---|---|---|---|
| N | 35.3614016992 | 63.6482437219 | 52.7211294256 |
| H | 34.8493513673 | 63.1774850449 | 53.4736358719 |
| C | 35.9185472221 | 63.0312850653 | 51.6642431418 |
| H | 35.9262145109 | 61.9627584862 | 51.5247752441 |
| N | 36.4769980622 | 63.9237245789 | 50.8462038335 |
| C | 36.2532506557 | 65.1689696421 | 51.4216893846 |
| H | 36.5942420132 | 66.0706795805 | 50.9379302898 |
| C | 45.2465937737 | 66.8020603469 | 46.1449846791 |
| H | 44.9306342763 | 65.7507893776 | 46.0601794859 |
| H | 45.4464933302 | 67.1151860584 | 45.1139657114 |
| C | 43.9473830644 | 67.5315798692 | 46.5866615793 |
| O | 43.7378377023 | 67.9409615080 | 47.7560240850 |
| O | 43.0613781889 | 67.6108449433 | 45.6578009477 |
| Fe | 37.1727068388 | 63.5017503889 | 48.8735315162 |
| O | 40.5836655409 | 64.7934773880 | 48.6246374105 |
| O | 39.0372419978 | 63.0069805116 | 48.5575470418 |
| H | 37.9981426041 | 62.3449787478 | 46.1750760221 |
| O | 38.1347822992 | 63.2796101848 | 46.4918749666 |
| C | 39.3521806190 | 63.4184873168 | 47.2618106890 |
| C | 40.4505793935 | 62.6275016589 | 46.5760694298 |
| C | 39.7784821060 | 64.8873073432 | 47.4803136241 |
| H | 40.3526284510 | 61.5443086717 | 46.6053658878 |
| C | 41.4676022254 | 63.2052831177 | 45.9022322178 |
| C | 38.5924594469 | 65.8579629160 | 47.7362189359 |
| C | 40.8067757044 | 65.4705465783 | 46.5725227789 |
| H | 42.2065081350 | 62.6032544916 | 45.3799827278 |
| C | 41.6285057675 | 64.6532545668 | 45.8517776916 |
| O | 38.7639406576 | 67.0735146039 | 47.5593641226 |
| O | 37.4984102306 | 65.3336530459 | 48.1929808813 |
| H | 40.9383486665 | 66.5433325365 | 46.5630287983 |

| | | | |
|---|---|---|---|
| O | 42.6035515334 | 65.1274035845 | 45.0451045739 |
| H | 42.7509833708 | 66.1283100492 | 45.1864733657 |
| O | 39.2393022144 | 65.5036342610 | 50.9595950122 |
| H | 39.8357475647 | 65.2146547402 | 50.2348302310 |
| H | 39.6627056181 | 65.1781682784 | 51.7918348525 |
| O | 37.3075105221 | 60.9577854340 | 45.2351931181 |
| H | 36.3135976879 | 60.9664519695 | 45.2499972870 |
| H | 37.5496807840 | 60.0045038795 | 45.4569986067 |
| O | 43.9112428538 | 63.6189916436 | 43.0687267532 |
| H | 43.5131150080 | 64.2299783609 | 43.7204640527 |
| H | 44.1708541026 | 64.1277168941 | 42.2729273089 |
| H | 46.0972426338 | 66.8638094999 | 46.6670800334 |
| H | 34.1243691862 | 66.2902411089 | 53.5919714713 |
| H | 35.1089131609 | 57.6733819258 | 50.3950452739 |
| H | 30.8931454804 | 63.0109530378 | 49.3603929636 |

Structure of **4b**

| | | | |
|---|---|---|---|
| C | 31.0800025239 | 62.8551825973 | 48.5049352372 |
| H | 30.4437236083 | 63.3753081443 | 47.7797256863 |
| H | 30.9475794183 | 61.7865572377 | 48.2941472151 |
| C | 32.5302700255 | 63.2052364613 | 48.2412196931 |
| N | 32.9304485846 | 63.8782955377 | 47.0888525481 |
| H | 32.3294969344 | 64.1938070669 | 46.3381099528 |
| C | 34.2828513538 | 63.9920004433 | 47.0924336683 |
| H | 34.8454030361 | 64.5007919066 | 46.3263184503 |
| N | 34.7925239426 | 63.4323724382 | 48.1852576165 |
| C | 33.7103010394 | 62.9295536036 | 48.8961380319 |
| H | 33.8471651413 | 62.4236259076 | 49.8286188480 |
| C | 35.4337867668 | 58.0600613486 | 49.5432573408 |
| H | 34.6163254106 | 58.2750719642 | 48.8492490729 |
| H | 36.0062032670 | 57.2316435165 | 49.1013800313 |

| | | | |
|---|---|---|---|
| C | 36.2776537800 | 59.3060257349 | 49.6177950222 |
| N | 37.4349785405 | 59.5135930460 | 50.3596720309 |
| H | 37.8372838493 | 58.9048148950 | 51.0749624754 |
| C | 37.8519360744 | 60.7837598888 | 50.1654940298 |
| H | 38.7190415303 | 61.2044357357 | 50.6537676273 |
| N | 37.0355550862 | 61.4197621541 | 49.3317349366 |
| C | 36.0638210145 | 60.4969088184 | 48.9757134409 |
| H | 35.2753422061 | 60.7388714216 | 48.2801992303 |
| C | 34.8578367206 | 65.9195223036 | 53.8352854197 |
| H | 34.9453742223 | 65.4580875686 | 54.8262745257 |
| H | 35.5248812745 | 66.7894215306 | 53.8355019114 |
| C | 35.3401515057 | 64.9575336321 | 52.7793094477 |
| N | 35.0701129342 | 63.6017174125 | 52.8176502665 |
| H | 34.5432904514 | 63.1077111810 | 53.5473082728 |
| C | 35.6089016399 | 63.0209037832 | 51.7292575713 |
| H | 35.5790118338 | 61.9602344311 | 51.5366138625 |
| N | 36.2141051538 | 63.9261753484 | 50.9678519359 |
| C | 36.0552493077 | 65.1395884059 | 51.6187729539 |
| H | 36.4199772214 | 66.0586308695 | 51.1845171039 |
| C | 45.7381955902 | 67.5568823899 | 45.9065485017 |
| H | 45.7307210533 | 66.8734565979 | 45.0530633153 |
| H | 45.9051720558 | 68.5587794376 | 45.4772898634 |
| C | 44.3425705316 | 67.6807370107 | 46.4941705766 |
| O | 44.2328557269 | 68.1290271762 | 47.6573315807 |
| O | 43.3298947449 | 67.4250676602 | 45.7398785125 |
| Fe | 36.8694104625 | 63.5180113964 | 48.9838354586 |
| O | 40.3227961683 | 63.8757105879 | 48.7924238499 |
| O | 42.3096165412 | 64.0820914848 | 47.7601809426 |
| H | 38.0876714600 | 61.7710435626 | 46.5087456749 |
| O | 38.4346267256 | 62.5049164924 | 47.0867360148 |

| | | | |
|---|---|---|---|
| C | 39.5307427460 | 63.1064839098 | 46.6516850091 |
| C | 40.2026879415 | 62.6528141799 | 45.5148108027 |
| C | 40.0194993574 | 64.2848811844 | 47.4862776257 |
| H | 39.8218835835 | 61.7769642860 | 44.9952548472 |
| C | 41.3129758711 | 63.3167987078 | 44.9865336980 |
| C | 38.9150695523 | 65.3986968638 | 47.6802889841 |
| C | 41.3835444066 | 64.8145729085 | 46.9981540054 |
| H | 41.7566929111 | 62.9880158425 | 44.0511990563 |
| C | 41.8197751260 | 64.4704359353 | 45.5999063142 |
| O | 39.2640519546 | 66.5946188441 | 47.5839982805 |
| O | 37.7510897390 | 65.0161421090 | 48.0432533441 |
| H | 41.4332533637 | 65.8962212436 | 47.1675322192 |
| O | 42.7428476820 | 65.1563515605 | 44.9615709988 |
| H | 43.0112690601 | 66.0932174436 | 45.3643650637 |
| O | 41.4521083980 | 65.5340051554 | 50.8019292636 |
| H | 40.9596060546 | 64.9468995201 | 50.1885657073 |
| H | 42.3088822328 | 65.7050649562 | 50.3223824334 |
| O | 37.0882925600 | 60.6512321019 | 45.4417167370 |
| H | 36.0925239572 | 60.6916416165 | 45.4990060723 |
| H | 37.3060168716 | 59.6727143355 | 45.6176830370 |
| O | 44.0446922461 | 63.7267396878 | 42.9079836341 |
| H | 43.7451479509 | 64.3575401424 | 43.5923259860 |
| H | 44.3693666906 | 64.2451953418 | 42.1417022063 |
| H | 46.4814467088 | 67.3575478164 | 46.5451747636 |
| H | 33.9128978067 | 66.2311684663 | 53.7354499640 |
| H | 35.0167013524 | 57.7649928405 | 50.4028935037 |
| H | 30.7096433571 | 63.0643741805 | 49.4099617390 |

Structure of **4c**

| | | | |
|---|---|---|---|
| C | 31.2781844702 | 62.9765755312 | 48.4270178337 |
| H | 30.6977823945 | 63.5722861885 | 47.7094021129 |

| | | | |
|---|---|---|---|
| H | 31.1292912239 | 61.9288693549 | 48.1261401137 |
| C | 32.7623643693 | 63.2924897590 | 48.2438897703 |
| N | 33.3294237492 | 63.2989057562 | 46.9695952944 |
| H | 32.8385099331 | 63.1834339926 | 46.0886651611 |
| C | 34.6709263399 | 63.4664386275 | 47.0768748224 |
| H | 35.3439875559 | 63.5000846225 | 46.2317514625 |
| N | 35.0267192982 | 63.5693566098 | 48.3493743091 |
| C | 33.8426344267 | 63.4809040566 | 49.0777223986 |
| H | 33.8472147605 | 63.5688702353 | 50.1503418064 |
| C | 35.2743213801 | 58.0371055581 | 49.5010174821 |
| H | 34.4129117586 | 58.2333424828 | 48.8561026559 |
| H | 35.8479259126 | 57.2313698539 | 49.0206586482 |
| C | 36.0896316782 | 59.3001330161 | 49.5345825054 |
| N | 37.3157661638 | 59.4475267814 | 50.1696867139 |
| H | 37.7514973962 | 58.8009611551 | 50.8265762347 |
| C | 37.7326299258 | 60.7161335854 | 50.0232747263 |
| H | 38.6432830283 | 61.1030471050 | 50.4501553539 |
| N | 36.8496279060 | 61.4126599517 | 49.3118045848 |
| C | 35.8254134977 | 60.5328603101 | 48.9924804464 |
| H | 34.9757775838 | 60.8360703999 | 48.4008206304 |
| C | 34.8873141151 | 66.0718556459 | 53.8511568846 |
| H | 34.9996094517 | 65.6511189337 | 54.8577180272 |
| H | 35.5129123232 | 66.9719103763 | 53.8176276874 |
| C | 35.3915373541 | 65.0959243659 | 52.8240479361 |
| N | 35.1485033213 | 63.7377722854 | 52.9109437613 |
| H | 34.6528234674 | 63.2514228828 | 53.6653113852 |
| C | 35.6435646563 | 63.1354606044 | 51.8133354254 |
| H | 35.6122618486 | 62.0735983702 | 51.6334480708 |
| N | 36.1850136632 | 64.0374568220 | 51.0079496396 |
| C | 36.0525581695 | 65.2648004655 | 51.6286800154 |

| | | | |
|---|---|---|---|
| H | 36.3842118830 | 66.1740274498 | 51.1494743846 |
| C | 45.4462844830 | 67.3192409180 | 45.9157141155 |
| H | 45.3420690633 | 66.4620209576 | 45.2387011635 |
| H | 45.6054781429 | 68.1781423670 | 45.2474893064 |
| C | 44.0631950691 | 67.5832662515 | 46.5242915707 |
| O | 43.8362841885 | 67.5796646785 | 47.7539381707 |
| O | 43.1592953403 | 67.8380900524 | 45.6446200917 |
| Fe | 37.0796080933 | 63.4949180945 | 49.1704938466 |
| O | 40.1772128626 | 63.4966675157 | 47.9770324716 |
| O | 38.4537837037 | 63.2643055386 | 49.9801118138 |
| H | 38.0053333032 | 61.9939023212 | 46.4546065695 |
| O | 38.1715557566 | 62.8349396420 | 46.9422408832 |
| C | 39.4751400643 | 63.2905416514 | 46.7681859253 |
| C | 40.2400892289 | 62.7291089244 | 45.6318965824 |
| C | 39.8308237821 | 64.6925152192 | 47.2074788993 |
| H | 39.9231996034 | 61.7780878781 | 45.2138740264 |
| C | 41.2908610633 | 63.3955868627 | 45.1091476352 |
| C | 38.7493725490 | 65.6195896632 | 47.7781800872 |
| C | 40.9590697036 | 65.3594098130 | 46.5395479051 |
| H | 41.8673521566 | 62.9765030999 | 44.2895691838 |
| C | 41.6543185202 | 64.7260700400 | 45.5678648921 |
| O | 38.9260844203 | 66.8414756076 | 47.6309728558 |
| O | 37.6771718886 | 65.1296192679 | 48.3107764648 |
| H | 41.2146385641 | 66.3746663170 | 46.8150502635 |
| O | 42.6915177519 | 65.3038733191 | 44.8838662849 |
| H | 42.8081834250 | 66.2646009979 | 45.1369342258 |
| O | 40.1869641721 | 65.2511638423 | 50.4878461364 |
| H | 39.7951003387 | 64.4710960471 | 50.0575153583 |
| H | 40.1320710083 | 65.0189644262 | 51.4426844985 |
| O | 37.3366006685 | 60.7431394377 | 45.3348249429 |

| | | | |
|---|---|---|---|
| H | 36.3370316820 | 60.7207618182 | 45.3885196306 |
| H | 37.6252490629 | 59.7923430764 | 45.5378815926 |
| O | 44.0065438564 | 63.7119302476 | 43.0276498403 |
| H | 43.6669189091 | 64.3725826025 | 43.6687683381 |
| H | 44.2886087528 | 64.1886987262 | 42.2187827783 |
| H | 46.2463299980 | 67.2163624471 | 46.5067667310 |
| H | 33.9267898537 | 66.3267795651 | 53.7397704453 |
| H | 34.9230488192 | 57.7332479583 | 50.3866122805 |
| H | 30.8388337554 | 63.1134921485 | 49.3148380798 |

Structure of **TS45a**

| | | | |
|---|---|---|---|
| C | 31.2538319736 | 62.7917805428 | 48.4524871454 |
| H | 30.6174092755 | 63.3046597626 | 47.7220643030 |
| H | 31.1487951284 | 61.7207219988 | 48.2333484010 |
| C | 32.7015593168 | 63.1874436259 | 48.2228298452 |
| N | 33.1001847580 | 64.0562413999 | 47.2152931451 |
| H | 32.5072157847 | 64.5079166170 | 46.5270156261 |
| C | 34.4521508487 | 64.1670288167 | 47.2392580039 |
| H | 35.0146874854 | 64.8181770499 | 46.5870631169 |
| N | 34.9631200840 | 63.4174521205 | 48.2022053420 |
| C | 33.8836632546 | 62.8021570285 | 48.8112197628 |
| H | 34.0267062078 | 62.1303477786 | 49.6430854432 |
| C | 35.4955630131 | 57.9041938593 | 49.5112528159 |
| H | 34.6615357427 | 58.0981171468 | 48.8311074618 |
| H | 36.0649727219 | 57.0692198143 | 49.0726856788 |
| C | 36.3272849842 | 59.1562620930 | 49.5256574026 |
| N | 37.4703027752 | 59.3920547398 | 50.2776775407 |
| H | 37.8425924935 | 58.8157428835 | 51.0321071542 |
| C | 37.8924127270 | 60.6533379104 | 50.0272612430 |
| H | 38.7536311242 | 61.0971040503 | 50.5038292285 |
| N | 37.0945742263 | 61.2499665448 | 49.1517703256 |

| | | | |
|---|---|---|---|
| C | 36.1284299087 | 60.3173825330 | 48.8236710653 |
| H | 35.3570489793 | 60.5304698819 | 48.0988450031 |
| C | 35.0871491327 | 66.0151259812 | 53.6777334919 |
| H | 35.2212653310 | 65.6008418591 | 54.6859522648 |
| H | 35.7351394608 | 66.8981597401 | 53.6193747988 |
| C | 35.5539037086 | 65.0164241784 | 52.6524404358 |
| N | 35.3132716145 | 63.6560439926 | 52.7684683179 |
| H | 34.7980385645 | 63.1885756088 | 53.5211804044 |
| C | 35.8412759214 | 63.0333193168 | 51.6972768794 |
| H | 35.8162982286 | 61.9660239480 | 51.5447457203 |
| N | 36.4193092191 | 63.9099762719 | 50.8866121174 |
| C | 36.2444626501 | 65.1529306631 | 51.4724112177 |
| H | 36.6051969621 | 66.0477992068 | 50.9896515437 |
| C | 45.2064238428 | 66.7010253496 | 46.2120708925 |
| H | 44.8802946110 | 65.6499131521 | 46.2471283010 |
| H | 45.3977292519 | 66.9066751935 | 45.1537136965 |
| C | 43.9326411506 | 67.4776045820 | 46.6067886903 |
| O | 43.7175044425 | 67.9106774520 | 47.7623329790 |
| O | 43.0666236328 | 67.5675065838 | 45.6544380893 |
| Fe | 37.0572775540 | 63.4258855349 | 48.9196236292 |
| O | 40.7753889875 | 65.2352801836 | 48.4459355998 |
| O | 39.1944202501 | 63.0339459947 | 48.6029181762 |
| H | 38.0706887833 | 62.3723403422 | 46.2431606287 |
| O | 38.2531049832 | 63.3016040784 | 46.5561841535 |
| C | 39.4213509162 | 63.3736735643 | 47.3780618634 |
| C | 40.5993569124 | 62.6936840386 | 46.7016609371 |
| C | 39.8918218866 | 65.0921317575 | 47.4917539483 |
| H | 40.6509275397 | 61.6247226616 | 46.9012792533 |
| C | 41.5696967320 | 63.2709858139 | 45.9609230632 |
| C | 38.5306518148 | 65.9420131715 | 47.7580623358 |

| | | | |
|---|---|---|---|
| C | 40.7237346380 | 65.5454299974 | 46.3463318241 |
| H | 42.3611512481 | 62.6681482234 | 45.5240985624 |
| C | 41.6341788317 | 64.6997368041 | 45.7517927207 |
| O | 38.7209682445 | 67.1314096061 | 47.4391339285 |
| O | 37.5528234141 | 65.3796618488 | 48.2742987126 |
| H | 40.7417396774 | 66.6023907689 | 46.1070079895 |
| O | 42.5742063195 | 65.1750760955 | 44.9243376665 |
| H | 42.7574087299 | 66.1839463935 | 45.1034707301 |
| O | 39.3528318103 | 65.5366659438 | 50.9024211914 |
| H | 39.9729539179 | 65.2193627630 | 50.2182626948 |
| H | 39.7120889212 | 65.1999493004 | 51.7597832674 |
| O | 37.3092406615 | 61.0155695684 | 45.2492726636 |
| H | 36.3176322818 | 61.0268988645 | 45.2618995848 |
| H | 37.5506043785 | 60.0601432458 | 45.4502621805 |
| O | 43.8734499843 | 63.5805276915 | 43.0323613224 |
| H | 43.4944567055 | 64.2214922387 | 43.6651723915 |
| H | 44.1561570761 | 64.0728588589 | 42.2313998476 |
| H | 46.0620641283 | 66.8142859592 | 46.7170973632 |
| H | 34.1312819103 | 66.2995924374 | 53.6042713364 |
| H | 35.0999918203 | 57.6381308035 | 50.3903056481 |
| H | 30.8641678633 | 62.9814679013 | 49.3536977685 |

Structure of **TS45b**

| | | | |
|---|---|---|---|
| C | 31.1312457768 | 62.9267464080 | 48.4611735083 |
| H | 30.5001666510 | 63.4825428696 | 47.7550357588 |
| H | 30.9976335463 | 61.8643337155 | 48.2117547850 |
| C | 32.5888388726 | 63.2719264265 | 48.2144014652 |
| N | 33.1164847642 | 63.1581760310 | 46.9330173792 |
| H | 32.6110761732 | 62.9097548813 | 46.0887871268 |
| C | 34.4481075467 | 63.3980745252 | 46.9817916723 |

| | | | |
|---|---|---|---|
| H | 35.0909171117 | 63.3621313744 | 46.1140328964 |
| N | 34.8306984744 | 63.6654006387 | 48.2210802750 |
| C | 33.6773190427 | 63.6061893807 | 48.9929918303 |
| H | 33.7155017730 | 63.8091964270 | 50.0530198305 |
| C | 35.4731273019 | 58.2010672219 | 49.5053325222 |
| H | 34.6453198657 | 58.4176342010 | 48.8227731417 |
| H | 36.0696185273 | 57.4158791137 | 49.0209668682 |
| C | 36.2860017848 | 59.4723315231 | 49.6000301885 |
| N | 37.5016858615 | 59.6615611745 | 50.2500262713 |
| H | 37.9464746321 | 59.0433044873 | 50.9297171378 |
| C | 37.9218967846 | 60.9279418415 | 50.0259856674 |
| H | 38.8335979427 | 61.3375487828 | 50.4380626045 |
| N | 37.0523000465 | 61.5817431630 | 49.2621391458 |
| C | 36.0362369363 | 60.6760635214 | 48.9905922084 |
| H | 35.1923256310 | 60.9407095113 | 48.3722689992 |
| C | 34.9534241022 | 66.0713880733 | 53.8514080700 |
| H | 35.0514010980 | 65.6500998486 | 54.8594263046 |
| H | 35.5678665101 | 66.9796432123 | 53.8316628363 |
| C | 35.4920073742 | 65.1080444237 | 52.8303308087 |
| N | 35.2285073008 | 63.7514313038 | 52.8783643211 |
| H | 34.7117007618 | 63.2574634340 | 53.6128327497 |
| C | 35.7575397579 | 63.1695733309 | 51.7832979126 |
| H | 35.7073849826 | 62.1115034660 | 51.5810687688 |
| N | 36.3532565052 | 64.0748342844 | 51.0179779714 |
| C | 36.2011488179 | 65.2889334286 | 51.6660665008 |
| H | 36.5659159812 | 66.2049609160 | 51.2250866409 |
| C | 45.5545530186 | 67.5906230812 | 45.9617648518 |
| H | 45.5466319214 | 66.9415023015 | 45.0819733057 |
| H | 45.7017942958 | 68.6076627987 | 45.5614162843 |
| C | 44.1299262938 | 67.6831969101 | 46.5232429146 |

| | | | |
|---|---|---|---|
| O | 43.9100865338 | 68.1048287972 | 47.6849578782 |
| O | 43.1955528362 | 67.4372444884 | 45.6740445659 |
| Fe | 36.9137972169 | 63.7079645886 | 48.9840711585 |
| O | 39.8398572095 | 63.5781866112 | 48.5735045159 |
| O | 42.2920411761 | 64.8812028870 | 48.0215338377 |
| H | 37.7552919622 | 62.2037147374 | 46.2043500000 |
| O | 37.9723356706 | 63.0869251867 | 46.6385182000 |
| C | 39.2757532079 | 63.4181521126 | 46.5531180779 |
| C | 40.1300961151 | 62.7561709826 | 45.6713447849 |
| C | 39.7521750443 | 64.4268101907 | 47.5772136778 |
| H | 39.7351335906 | 61.9026591554 | 45.1247722141 |
| C | 41.3927254752 | 63.2477155400 | 45.3054281807 |
| C | 38.8359141892 | 65.6956279799 | 47.8310800860 |
| C | 41.4145729318 | 65.1042763196 | 47.0921424675 |
| H | 41.9188162104 | 62.7828087344 | 44.4779009922 |
| C | 41.9002580021 | 64.4351667952 | 45.8184527066 |
| O | 39.1902249842 | 66.8424398695 | 47.5170576095 |
| O | 37.7101862983 | 65.3964332816 | 48.3575912925 |
| H | 41.0620323114 | 66.1396839668 | 46.9542206031 |
| O | 42.9307299672 | 64.9883233791 | 45.1910506761 |
| H | 43.0742584641 | 65.9871354243 | 45.4353784476 |
| O | 40.8094643515 | 66.0016199224 | 50.3422272655 |
| H | 41.4317390691 | 65.5880485537 | 49.7102483261 |
| H | 41.3359425416 | 66.1769740713 | 51.1447346139 |
| O | 37.1865262394 | 60.8641109272 | 45.3370130146 |
| H | 36.1907214538 | 60.8638150375 | 45.2976049038 |
| H | 37.4255168908 | 59.9324664479 | 45.6478983567 |
| O | 43.9341092503 | 63.6384505969 | 42.9659148214 |
| H | 43.7014766691 | 64.2568557656 | 43.6874067466 |
| H | 44.2739004763 | 64.1575807497 | 42.2062720171 |

| | | | |
|---|---|---|---|
| H | 46.3304212619 | 67.3767828291 | 46.5553141890 |
| H | 33.9923566040 | 66.3157401070 | 53.7224067231 |
| H | 35.0660689771 | 57.8435687988 | 50.3458671126 |
| H | 30.7469357157 | 63.0927308840 | 49.3693336982 |

Structure of **TS45c**

| | | | |
|---|---|---|---|
| C | 31.3547424097 | 62.9405641556 | 48.4342015077 |
| H | 30.7765450795 | 63.5280476374 | 47.7091029271 |
| H | 31.2138472019 | 61.8888865446 | 48.1439666134 |
| C | 32.8371716889 | 63.2616943188 | 48.2723595619 |
| N | 33.4229880047 | 63.2347004116 | 47.0089967496 |
| H | 32.9474079608 | 63.0819945790 | 46.1250125353 |
| C | 34.7582822199 | 63.4229552000 | 47.1310150220 |
| H | 35.4419043173 | 63.4467506471 | 46.2956904697 |
| N | 35.0918544500 | 63.5682701681 | 48.4056102518 |
| C | 33.9005879577 | 63.4890407477 | 49.1194005858 |
| H | 33.8930017992 | 63.6143229798 | 50.1887137710 |
| C | 35.4661880352 | 58.0986511644 | 49.5195523904 |
| H | 34.6314084278 | 58.2930227098 | 48.8402279601 |
| H | 36.0808240215 | 57.3227079033 | 49.0389491953 |
| C | 36.2501842478 | 59.3778968838 | 49.6250263021 |
| N | 37.4483849764 | 59.5553763717 | 50.3071706310 |
| H | 37.8765688028 | 58.9187207945 | 50.9804992057 |
| C | 37.8488049368 | 60.8309698688 | 50.1559065632 |
| H | 38.7362211458 | 61.2456963984 | 50.6063990148 |
| N | 36.9773390676 | 61.5007084803 | 49.4064803281 |
| C | 35.9815143879 | 60.5996913279 | 49.0651333447 |
| H | 35.1446009071 | 60.8795865462 | 48.4456842088 |
| C | 34.9827088347 | 66.0708771744 | 53.8859818987 |
| H | 35.0560956156 | 65.6564863676 | 54.8986797704 |

| | | | |
|---|---|---|---|
| H | 35.6103813219 | 66.9693083951 | 53.8663342139 |
| C | 35.4924669192 | 65.0942586285 | 52.8755098313 |
| N | 35.2801408742 | 63.7331483123 | 52.9751309512 |
| H | 34.7968489654 | 63.2391138010 | 53.7332075665 |
| C | 35.7443517443 | 63.1396989853 | 51.8624493711 |
| H | 35.7248117352 | 62.0788221476 | 51.6813380029 |
| N | 36.2362996549 | 64.0573428176 | 51.0406756134 |
| C | 36.0974733171 | 65.2809462341 | 51.6594613193 |
| H | 36.4135732010 | 66.1961281115 | 51.1857637807 |
| C | 45.3340115882 | 66.9632496890 | 46.1484023437 |
| H | 45.0464941882 | 65.9329721202 | 45.8966707621 |
| H | 45.5201017531 | 67.4555674029 | 45.1880877236 |
| C | 44.0342316451 | 67.5681856430 | 46.7099957383 |
| O | 43.7599069228 | 67.6212832736 | 47.9305936538 |
| O | 43.2072868482 | 67.9261161529 | 45.7955661839 |
| Fe | 37.1131476009 | 63.5722718302 | 49.2236207633 |
| O | 39.9874053087 | 63.4478922963 | 47.7808316533 |
| O | 38.5389442046 | 63.4758779712 | 49.9834294965 |
| H | 37.8645855940 | 61.9148800952 | 46.1239240852 |
| O | 38.0992531813 | 62.6804532782 | 46.7226263380 |
| C | 39.3944181330 | 63.1058626099 | 46.5976178793 |
| C | 40.1997190984 | 62.7653299541 | 45.4819161608 |
| C | 39.8388227116 | 64.7545025838 | 47.2540401678 |
| H | 39.8116684210 | 62.0302118776 | 44.7805959504 |
| C | 41.3835828774 | 63.4093403825 | 45.1841168659 |
| C | 38.7303091625 | 65.6357215048 | 47.7684196955 |
| C | 40.9585655361 | 65.3490672673 | 46.6242939550 |
| H | 41.9780979474 | 63.0502345435 | 44.3500405002 |
| C | 41.7558268503 | 64.6598795508 | 45.7347512865 |
| O | 38.8902849652 | 66.8653304740 | 47.6880638595 |

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|---|---|---|---|
| O | 37.6176000696 | 65.0988066100 | 48.1875649613 |
| H | 41.1026483370 | 66.4183531259 | 46.7359066301 |
| O | 42.8372074834 | 65.2695593015 | 45.1338988959 |
| H | 42.8641138587 | 66.2436192918 | 45.3290261757 |
| O | 39.0246660452 | 65.7652479166 | 51.3898809512 |
| H | 38.9326623532 | 65.0251192616 | 50.7612487405 |
| H | 39.5751407726 | 65.3868686096 | 52.1210580219 |
| O | 37.1495948667 | 60.7592169556 | 45.0871782602 |
| H | 36.1592297814 | 60.7762827576 | 45.1276508800 |
| H | 37.4167089389 | 59.8097857783 | 45.3202581743 |
| O | 43.9914076435 | 63.6994404481 | 43.1545271727 |
| H | 43.7274163137 | 64.3668670652 | 43.8241949859 |
| H | 44.2568885299 | 64.1723042158 | 42.3384405299 |
| H | 46.1780539728 | 66.9704447068 | 46.6846305459 |
| H | 34.0272183610 | 66.3207898120 | 53.7291966052 |
| H | 35.0777847462 | 57.7562923874 | 50.3750834260 |
| H | 30.9111865385 | 63.0826235999 | 49.3191180594 |

Structure of **5a**

| | | | |
|---|---|---|---|
| C | 31.2210155769 | 62.8444319267 | 48.4316538995 |
| H | 30.5814739376 | 63.3785775804 | 47.7168551086 |
| H | 31.1090076135 | 61.7774864912 | 48.1917052402 |
| C | 32.6712283681 | 63.2283197934 | 48.1831680275 |
| N | 33.1395181551 | 63.3718240298 | 46.8823887849 |
| H | 32.5883802574 | 63.3193843406 | 46.0326909325 |
| C | 34.4764178890 | 63.5886571923 | 46.9143205385 |
| H | 35.0751422988 | 63.7351721708 | 46.0273962050 |
| N | 34.9196462112 | 63.5926660669 | 48.1616485545 |
| C | 33.8024591054 | 63.3801445776 | 48.9576310232 |
| H | 33.8979212433 | 63.3577294983 | 50.0318591428 |
| C | 35.5636076886 | 58.1442705738 | 49.5142073728 |

| | | | |
|---|---|---|---|
| H | 34.7408457583 | 58.3283940161 | 48.8150417843 |
| H | 36.1902158882 | 57.3727786105 | 49.0379809093 |
| C | 36.3390805329 | 59.4383515720 | 49.6040216968 |
| N | 37.5543006487 | 59.6413530909 | 50.2471116149 |
| H | 38.0109768881 | 59.0226750889 | 50.9154982552 |
| C | 37.9533623558 | 60.9149931451 | 50.0183651133 |
| H | 38.8639976037 | 61.3299973469 | 50.4251323970 |
| N | 37.0688448383 | 61.5619461827 | 49.2694036102 |
| C | 36.0662134716 | 60.6417231699 | 49.0025336583 |
| H | 35.2290050429 | 60.8886926662 | 48.3698254792 |
| C | 35.0723225963 | 66.1049793951 | 53.8162950032 |
| H | 35.1766902475 | 65.6822460329 | 54.8241402268 |
| H | 35.6792802213 | 67.0172343145 | 53.7966884680 |
| C | 35.6141798878 | 65.1424930716 | 52.7988141837 |
| N | 35.4323673675 | 63.7717425720 | 52.8919658458 |
| H | 34.9372871944 | 63.2720425315 | 53.6363702200 |
| C | 35.9771817266 | 63.1892407621 | 51.8062927661 |
| H | 35.9872816154 | 62.1251172145 | 51.6330450930 |
| N | 36.5080337650 | 64.1079688118 | 51.0054481840 |
| C | 36.2899413371 | 65.3309693971 | 51.6183029682 |
| H | 36.5681097193 | 66.2529133819 | 51.1294512479 |
| C | 45.1280577470 | 66.7467827378 | 46.3061049832 |
| H | 44.7956413481 | 65.6990642784 | 46.3311781974 |
| H | 45.2548126631 | 67.0056661923 | 45.2511062275 |
| C | 43.9062292885 | 67.5217968669 | 46.8391099877 |
| O | 43.6157568593 | 67.5427434684 | 48.0600237348 |
| O | 43.1533993138 | 68.0357324101 | 45.9349861359 |
| Fe | 36.9954017399 | 63.7381024104 | 48.9733853535 |
| O | 39.2473661016 | 63.8429745826 | 48.2223179169 |
| O | 39.4832040771 | 60.6938068772 | 46.8728383228 |

| | | | |
|---|---|---|---|
| H | 37.7202504615 | 61.9562319697 | 46.0555512672 |
| O | 38.5459171417 | 62.5412879686 | 46.0114228294 |
| C | 39.5979547740 | 61.7781956124 | 46.3306701376 |
| C | 40.9415380308 | 62.2178296049 | 45.8736147518 |
| C | 39.4984198450 | 64.9821556868 | 47.8011071444 |
| H | 41.5180790363 | 61.3317632782 | 45.6184533734 |
| C | 41.6398327442 | 63.3625897368 | 45.7815464876 |
| C | 38.4840613003 | 66.1234269193 | 48.1088550447 |
| C | 40.5861486029 | 65.4187851164 | 46.9504875485 |
| H | 42.6438896669 | 63.2326744846 | 45.3847645284 |
| C | 41.4024466989 | 64.7751031909 | 46.0706451423 |
| O | 38.8305205852 | 67.3055873996 | 47.8917645425 |
| O | 37.3532669149 | 65.7193504902 | 48.5100004419 |
| H | 40.6716265171 | 66.4992400112 | 46.9358716999 |
| O | 42.2512659864 | 65.5067288097 | 45.2875002787 |
| H | 42.3064379060 | 66.4696898801 | 45.5283453684 |
| O | 40.2161461213 | 65.6467553226 | 50.7597692708 |
| H | 41.1586259768 | 65.8787433972 | 50.6233568272 |
| H | 40.1787840457 | 65.2138989119 | 51.6451729663 |
| O | 36.5704983900 | 60.8889235972 | 45.7636356294 |
| H | 35.6897314128 | 60.9026914486 | 45.3125388726 |
| H | 36.9713752169 | 59.9887696182 | 45.6104936155 |
| O | 43.9116030675 | 63.9799777207 | 43.3156621909 |
| H | 43.4709099375 | 64.6585577223 | 43.8622946774 |
| H | 44.1081429423 | 64.3727610845 | 42.4398408757 |
| H | 46.0094420579 | 66.8385954580 | 46.7694969564 |
| H | 34.1080522216 | 66.3418230490 | 53.6976032675 |
| H | 35.1548232816 | 57.7907823884 | 50.3555999158 |
| H | 30.8279450633 | 63.0166302747 | 49.3348943438 |

Structure of **5b**

| | | | |
|---|---|---|---|
| C | 31.0659686437 | 62.8109866797 | 48.4340214572 |
| H | 30.4288821492 | 63.3505593948 | 47.7208695990 |
| H | 30.9204336273 | 61.7423722140 | 48.2173509058 |
| C | 32.5217706672 | 63.1295703666 | 48.1575806964 |
| N | 33.0478406205 | 63.0044630606 | 46.8767896599 |
| H | 32.5476647965 | 62.7513200055 | 46.0306465230 |
| C | 34.3841548883 | 63.2198200347 | 46.9277638356 |
| H | 35.0275338547 | 63.1735635849 | 46.0608569204 |
| N | 34.7654575470 | 63.4814141202 | 48.1671752330 |
| C | 33.6135823629 | 63.4454134847 | 48.9350506007 |
| H | 33.6565709186 | 63.6535830665 | 49.9927829755 |
| C | 35.5257686705 | 58.0772911646 | 49.5351511547 |
| H | 34.7210975530 | 58.2662530217 | 48.8187426388 |
| H | 36.1513363445 | 57.2890150088 | 49.0899486894 |
| C | 36.3090806368 | 59.3605923894 | 49.6490947814 |
| N | 37.4854761682 | 59.5759483878 | 50.3550306384 |
| H | 37.9249201286 | 58.9572892052 | 51.0380687277 |
| C | 37.8578508342 | 60.8664957178 | 50.1840791856 |
| H | 38.7291070031 | 61.2937586466 | 50.6591531423 |
| N | 36.9978449165 | 61.5070532556 | 49.4026129879 |
| C | 36.0374971997 | 60.5689849395 | 49.0597433796 |
| H | 35.2124731154 | 60.8152578451 | 48.4097483936 |
| C | 34.9513020402 | 65.9997561806 | 53.8874709040 |
| H | 35.0371001186 | 65.5724584466 | 54.8943457494 |
| H | 35.5963912262 | 66.8854990083 | 53.8653639912 |
| C | 35.4385721341 | 65.0196388697 | 52.8608221503 |
| N | 35.1557433231 | 63.6663467611 | 52.9202757653 |
| H | 34.6499145934 | 63.1756877567 | 53.6663847282 |
| C | 35.6338027120 | 63.0755575919 | 51.8086658481 |
| H | 35.5629864662 | 62.0190865207 | 51.6058096936 |

| | | | |
|---|---|---|---|
| N | 36.2162523677 | 63.9722846167 | 51.0240606875 |
| C | 36.1062117272 | 65.1891009318 | 51.6731378202 |
| H | 36.4523354143 | 66.1007636501 | 51.2098430255 |
| C | 45.3619412513 | 66.7832035133 | 46.2313686106 |
| H | 45.0155637658 | 65.7419109396 | 46.2621941430 |
| H | 45.5408605877 | 67.0102278533 | 45.1772696479 |
| C | 44.1549550830 | 67.5966569390 | 46.7172087938 |
| O | 43.9150348972 | 67.7288357769 | 47.9421530243 |
| O | 43.3502354167 | 67.9945037993 | 45.8042419523 |
| Fe | 36.7685821958 | 63.6672911115 | 49.0088336848 |
| O | 40.5304908529 | 65.7162357441 | 47.6876843339 |
| O | 42.9693336995 | 63.6649530189 | 47.6801646446 |
| H | 38.1021232484 | 62.2480909474 | 46.8273093644 |
| O | 38.3148922573 | 63.0343463486 | 47.3887959782 |
| C | 39.4016057285 | 63.7526805211 | 46.9477821712 |
| C | 40.2075376013 | 63.2744212246 | 45.9625195116 |
| C | 39.4614726854 | 65.1444715416 | 47.4575590125 |
| H | 39.9068715732 | 62.3202965520 | 45.5280182416 |
| C | 41.2259292864 | 63.9975944947 | 45.2335324439 |
| C | 38.1561957968 | 65.9580165918 | 47.5613462970 |
| C | 42.7466101461 | 64.7226937121 | 47.1214216909 |
| H | 41.1392587593 | 63.9499995127 | 44.1481378246 |
| C | 42.2083067413 | 64.7819652905 | 45.7141635353 |
| O | 38.1684667330 | 67.0536659854 | 46.9886816471 |
| O | 37.2125054117 | 65.4332394203 | 48.2387775809 |
| H | 43.0215890026 | 65.6741871648 | 47.5940051371 |
| O | 42.9384542977 | 65.5357647025 | 44.8186638018 |
| H | 43.0651473528 | 66.4837924675 | 45.1205928343 |
| O | 39.6700193164 | 65.1739503466 | 50.6791600643 |
| H | 40.5714838419 | 65.2520309897 | 50.3229756849 |

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|---|---|---|---|
| H | 39.8086267141 | 64.9626064128 | 51.6343973318 |
| O | 37.3190853075 | 61.0094384491 | 45.6439808401 |
| H | 36.3327413993 | 60.9022109676 | 45.5764487578 |
| H | 37.6506052127 | 60.0581621635 | 45.6854055035 |
| O | 44.0177000631 | 63.6929985598 | 43.0445247697 |
| H | 43.7718318149 | 64.3992311672 | 43.6775011040 |
| H | 44.3168553847 | 64.1414686001 | 42.2248328908 |
| H | 46.2228775817 | 66.8625169763 | 46.7338604112 |
| H | 33.9983188207 | 66.2759851622 | 53.7628894720 |
| H | 35.0956200015 | 57.7464588519 | 50.3751047864 |
| H | 30.7067002273 | 63.0094573372 | 49.3459071973 |

Structure of **5c**

| | | | |
|---|---|---|---|
| C | 31.3569786653 | 62.9727539228 | 48.4367700829 |
| H | 30.7717607015 | 63.5520292022 | 47.7104755945 |
| H | 31.2401902323 | 61.9208993557 | 48.1372038684 |
| C | 32.8308394788 | 63.3330203717 | 48.2806182507 |
| N | 33.3963989751 | 63.4782007135 | 47.0137873964 |
| H | 32.9082393635 | 63.4352758442 | 46.1243450409 |
| C | 34.7318081084 | 63.6683745568 | 47.1383983447 |
| H | 35.4045664949 | 63.8260259280 | 46.3075337278 |
| N | 35.0824527086 | 63.6486962712 | 48.4168922347 |
| C | 33.9065863044 | 63.4576485252 | 49.1319840610 |
| H | 33.9187522389 | 63.4363740618 | 50.2087605620 |
| C | 35.4804378759 | 58.2009196102 | 49.5288668008 |
| H | 34.6500432013 | 58.4092303148 | 48.8460277234 |
| H | 36.0953607656 | 57.4400447078 | 49.0261282670 |
| C | 36.2724249003 | 59.4871870422 | 49.6402507783 |
| N | 37.4977999534 | 59.6595051401 | 50.2783926727 |
| H | 37.9587324688 | 59.0127920200 | 50.9185777934 |
| C | 37.9019917227 | 60.9363488815 | 50.1136788010 |

| | | | |
|---|---|---|---|
| H | 38.8122428555 | 61.3427974030 | 50.5276272926 |
| N | 37.0101763451 | 61.6155117628 | 49.4004881215 |
| C | 35.9994931420 | 60.7158633792 | 49.0896916031 |
| H | 35.1526243402 | 61.0021411453 | 48.4867218889 |
| C | 34.9450910657 | 66.0572277734 | 53.9078698589 |
| H | 35.0094117284 | 65.6194000864 | 54.9113033349 |
| H | 35.5715355244 | 66.9563372696 | 53.9150130512 |
| C | 35.4808505706 | 65.1032263315 | 52.8853795337 |
| N | 35.2657023964 | 63.7396656529 | 52.9397681059 |
| H | 34.7729118528 | 63.2258491970 | 53.6788861407 |
| C | 35.7628284927 | 63.1756988039 | 51.8244186229 |
| H | 35.7555839117 | 62.1180524891 | 51.6204396889 |
| N | 36.2767069586 | 64.1162664779 | 51.0412165113 |
| C | 36.1268006882 | 65.3213165654 | 51.6944159684 |
| H | 36.4587752973 | 66.2500387310 | 51.2574944278 |
| C | 45.3989116837 | 67.0842053575 | 46.0727202192 |
| H | 45.1336543746 | 66.0823615317 | 45.7054839416 |
| H | 45.6006351388 | 67.6702608139 | 45.1660419006 |
| C | 44.0821851110 | 67.6409386360 | 46.6464509692 |
| O | 43.8700791509 | 67.8230206126 | 47.8673803984 |
| O | 43.1962713623 | 67.8742232648 | 45.7445409186 |
| Fe | 37.1075366308 | 63.7191933946 | 49.1857005695 |
| O | 39.9270417540 | 63.5137604862 | 47.5266454007 |
| O | 38.5672223040 | 63.7935333645 | 49.8823317269 |
| H | 37.9835914348 | 61.5607211537 | 46.0401194788 |
| O | 38.3869280508 | 62.0862249708 | 46.7910087170 |
| C | 39.5102172092 | 62.7318766726 | 46.4797968492 |
| C | 40.2747015981 | 62.6167604804 | 45.3551421241 |
| C | 39.8455524101 | 64.8545146778 | 47.1370272500 |
| H | 39.9782769629 | 61.8799438737 | 44.6129171537 |

| | | | |
|---|---|---|---|
| C | 41.4511990534 | 63.3922307578 | 45.0791364083 |
| C | 38.6417449313 | 65.6453023031 | 47.5298717945 |
| C | 40.8460439726 | 65.3905741499 | 46.3892688210 |
| H | 42.1114071036 | 63.0182193219 | 44.3005381497 |
| C | 41.7484095757 | 64.6368294752 | 45.5747980293 |
| O | 38.6858683533 | 66.8820102797 | 47.4788317164 |
| O | 37.5321261198 | 64.9819630102 | 47.8194799994 |
| H | 40.8734387450 | 66.4698251281 | 46.2734210668 |
| O | 42.8561089480 | 65.2849230840 | 45.0552062357 |
| H | 42.8776348019 | 66.2534639565 | 45.2875657437 |
| O | 39.2175064415 | 66.2406270178 | 51.2977292942 |
| H | 39.0552924764 | 65.5692166082 | 50.6117528492 |
| H | 39.6591533644 | 65.7339978172 | 52.0173653768 |
| O | 37.1011937145 | 60.6437927280 | 45.0233304462 |
| H | 36.1157424035 | 60.7401241960 | 45.0910492462 |
| H | 37.3105370373 | 59.6893945482 | 45.2977840726 |
| O | 44.0451552203 | 63.7546618235 | 43.0909183147 |
| H | 43.7547352613 | 64.4228841031 | 43.7510057840 |
| H | 44.3145556753 | 64.2258842028 | 42.2739338433 |
| H | 46.2285976030 | 67.0555673681 | 46.6302156369 |
| H | 33.9893476626 | 66.3075343753 | 53.7532698832 |
| H | 35.0795255958 | 57.8283317124 | 50.3657942780 |
| H | 30.9022459440 | 63.1045309419 | 49.3175952469 |

Structure of **TS56c**

| | | | |
|---|---|---|---|
| C | 31.2860362767 | 62.9454696730 | 48.4655044205 |
| H | 30.6724880003 | 63.4858120426 | 47.7348002993 |
| H | 31.1987743351 | 61.8833241325 | 48.1992166847 |
| C | 32.7347314504 | 63.3671013065 | 48.3058895900 |
| N | 33.1841988757 | 64.0006091349 | 47.1537658462 |
| H | 32.6207150725 | 64.3109168960 | 46.3685885412 |

| | | | |
|---|---|---|---|
| C | 34.5257898286 | 64.1675321945 | 47.2346459886 |
| H | 35.1207038305 | 64.6829020656 | 46.4962766464 |
| N | 34.9854893489 | 63.6725388165 | 48.3739632855 |
| C | 33.8809271174 | 63.1770056494 | 49.0455583884 |
| H | 33.9887493517 | 62.7297890036 | 50.0211188384 |
| C | 35.4909725641 | 58.2365806670 | 49.4903930821 |
| H | 34.6585395170 | 58.4509858183 | 48.8116618534 |
| H | 36.0924422557 | 57.4633173967 | 48.9926118914 |
| C | 36.2951866017 | 59.5176947323 | 49.5874561612 |
| N | 37.5167359924 | 59.7078714576 | 50.2260914919 |
| H | 37.9775071829 | 59.0789979118 | 50.8834305203 |
| C | 37.9254559659 | 60.9813988697 | 50.0121832761 |
| H | 38.8436770288 | 61.3904657362 | 50.4070480216 |
| N | 37.0413921832 | 61.6418687577 | 49.2750293649 |
| C | 36.0324634480 | 60.7301473729 | 48.9960564420 |
| H | 35.1884207571 | 60.9898891840 | 48.3771187511 |
| C | 34.9510712976 | 66.1030995343 | 53.8399649254 |
| H | 35.0623862744 | 65.6513220297 | 54.8340556355 |
| H | 35.5439874149 | 67.0262508921 | 53.8548935521 |
| C | 35.5365224491 | 65.1838192725 | 52.7954411607 |
| N | 35.3858656103 | 63.8079782101 | 52.8505523957 |
| H | 34.8902521075 | 63.2864135284 | 53.5778416828 |
| C | 35.9782622743 | 63.2635948696 | 51.7688379318 |
| H | 36.0273691840 | 62.2025599604 | 51.5869752303 |
| N | 36.5114829819 | 64.2105297459 | 51.0002461735 |
| C | 36.2488932882 | 65.4132164430 | 51.6405318932 |
| H | 36.5625738266 | 66.3523101793 | 51.2115694228 |
| C | 45.5237055333 | 67.5657207772 | 45.9852640301 |
| H | 45.4982065915 | 66.9148419250 | 45.1057418018 |
| H | 45.6880622831 | 68.5752476086 | 45.5718076838 |

| | | | |
|---|---|---|---|
| C | 44.0911993578 | 67.6814023141 | 46.5364431294 |
| O | 43.8468541699 | 67.8693656162 | 47.7544649629 |
| O | 43.1769852024 | 67.6928204467 | 45.6381201479 |
| Fe | 37.1071087978 | 63.8004459043 | 48.9382136762 |
| O | 38.7836661743 | 63.6790021816 | 46.2630222253 |
| O | 38.8832603917 | 63.8350616409 | 48.8500345408 |
| H | 37.7818064936 | 61.2857812568 | 46.2037057450 |
| O | 38.6201891441 | 61.4550512038 | 46.7581036998 |
| C | 39.3810737879 | 62.4288733371 | 46.3406292393 |
| C | 40.6507088040 | 62.1968110854 | 45.8818875736 |
| C | 39.3732825425 | 64.7195546803 | 47.0079053158 |
| H | 40.9308092980 | 61.1510910110 | 45.8136580006 |
| C | 41.5834753875 | 63.1618551489 | 45.4765927519 |
| C | 38.3732994755 | 65.8022968026 | 47.4202772611 |
| C | 40.6749677701 | 65.1258834955 | 46.7014540157 |
| H | 42.4441547499 | 62.8188705181 | 44.9091518556 |
| C | 41.5833874707 | 64.5140497817 | 45.8072771879 |
| O | 38.7394895920 | 66.9882344142 | 47.4045428631 |
| O | 37.1930444997 | 65.3792212694 | 47.7169539910 |
| H | 40.9645967777 | 66.0831919530 | 47.1229638404 |
| O | 42.6144611308 | 65.2100671864 | 45.2570212624 |
| H | 42.6631017794 | 66.1910854036 | 45.4707280500 |
| O | 39.4083477449 | 65.7046369907 | 50.9306217833 |
| H | 39.3435324616 | 65.0285226462 | 50.2212388931 |
| H | 39.7550327350 | 65.2551244334 | 51.7338004887 |
| O | 36.9099877165 | 60.5529925371 | 45.1327369293 |
| H | 35.9170556341 | 60.6640793978 | 45.1311206352 |
| H | 37.0928440569 | 59.5893324738 | 45.3885601099 |
| O | 43.9620646792 | 63.7883459588 | 43.1335865829 |
| H | 43.6376115925 | 64.4425603150 | 43.7857557090 |

| | | | |
|---|---|---|---|
| H | 44.2111155058 | 64.2628915426 | 42.3126143679 |
| H | 46.2967538591 | 67.3382700563 | 46.5774316209 |
| H | 33.9841644885 | 66.3316352702 | 53.7265513466 |
| H | 35.0898532766 | 57.8660848389 | 50.3281497046 |
| H | 30.8529594909 | 63.0981057150 | 49.3538437342 |

Structure of **6c**

| | | | |
|---|---|---|---|
| C | 31.2290527679 | 62.9405272133 | 48.4779527923 |
| H | 30.6016834865 | 63.4733863154 | 47.7524441380 |
| H | 31.1426581114 | 61.8763444432 | 48.2180478372 |
| C | 32.6704630165 | 63.3765941565 | 48.3018052226 |
| N | 33.1061848933 | 64.0183915230 | 47.1505608457 |
| H | 32.5364278538 | 64.3305160137 | 46.3715036673 |
| C | 34.4476743977 | 64.2071936627 | 47.2324303440 |
| H | 35.0367574769 | 64.7243674370 | 46.4915077169 |
| N | 34.9158779385 | 63.7210137182 | 48.3692465922 |
| C | 33.8222065639 | 63.2063128074 | 49.0380055314 |
| H | 33.9345319967 | 62.7622277214 | 50.0151618128 |
| C | 35.4335271246 | 58.2442993942 | 49.4573950443 |
| H | 34.5838188257 | 58.4602620866 | 48.8007670369 |
| H | 36.0199780794 | 57.4653165185 | 48.9498876779 |
| C | 36.2449279772 | 59.5192519338 | 49.5377687310 |
| N | 37.4789902158 | 59.6817216736 | 50.1556124033 |
| H | 37.9224097653 | 59.0308902116 | 50.8003594493 |
| C | 37.8973492267 | 60.9548930374 | 49.9611432247 |
| H | 38.8193013263 | 61.3442587604 | 50.3690063132 |
| N | 37.0169313317 | 61.6374053657 | 49.2433691122 |
| C | 35.9885581343 | 60.7436005238 | 48.9677721118 |
| H | 35.1322325512 | 61.0323681463 | 48.3782805616 |
| C | 34.9415367855 | 66.1213346793 | 53.8450960531 |
| H | 35.0484541101 | 65.6713509621 | 54.8396007605 |

| | | | |
|---|---|---|---|
| H | 35.5212227617 | 67.0524645385 | 53.8600897408 |
| C | 35.5356375319 | 65.2084233962 | 52.8054854282 |
| N | 35.4043031397 | 63.8336706374 | 52.8741704909 |
| H | 34.8948782041 | 63.3186528788 | 53.5977049758 |
| C | 35.9999009898 | 63.2862972376 | 51.7962949648 |
| H | 36.0573861833 | 62.2240285122 | 51.6209145719 |
| N | 36.5149821851 | 64.2317273078 | 51.0168530541 |
| C | 36.2363859613 | 65.4384699777 | 51.6436781622 |
| H | 36.5131267913 | 66.3819958526 | 51.1950243747 |
| C | 45.5402300896 | 67.8061330682 | 46.0280310155 |
| H | 45.5823012230 | 67.3055358314 | 45.0552118611 |
| H | 45.6638182810 | 68.8779274264 | 45.8048778211 |
| C | 44.0828258896 | 67.7379090307 | 46.5411110728 |
| O | 43.7948332304 | 67.9101731919 | 47.7539213391 |
| O | 43.1959966473 | 67.6267304052 | 45.6203257038 |
| Fe | 37.0987775802 | 63.8350495837 | 48.9834390812 |
| O | 38.7603855406 | 63.4714023809 | 46.3859310736 |
| O | 39.0978175931 | 64.1146564264 | 48.5991858854 |
| H | 37.7498328220 | 61.3011268873 | 46.4727617348 |
| O | 38.7209508487 | 61.2551878664 | 46.6870639311 |
| C | 39.3895978234 | 62.3332687619 | 46.3767701429 |
| C | 40.7272479959 | 62.1202031658 | 45.9504596836 |
| C | 39.2829409182 | 64.6020731763 | 47.2961530573 |
| H | 40.9938463531 | 61.0785380699 | 45.8112039872 |
| C | 41.6315320516 | 63.0901448303 | 45.6448929043 |
| C | 38.1922073073 | 65.7412909731 | 47.2017838000 |
| C | 40.6140433386 | 65.0864878463 | 46.7542807671 |
| H | 42.5638108981 | 62.7824768791 | 45.1774439388 |
| C | 41.5458502279 | 64.4963314736 | 45.9416082176 |
| O | 38.5180373203 | 66.9180020973 | 46.9896034082 |

| | | | |
|---|---|---|---|
| O | 37.0447703423 | 65.3032407229 | 47.5312126726 |
| H | 40.7874627163 | 66.1308612970 | 46.9944464300 |
| O | 42.5942758231 | 65.1564925840 | 45.3772942889 |
| H | 42.6661669260 | 66.1455725733 | 45.5673542007 |
| O | 40.2031844051 | 65.6006690975 | 50.6926261362 |
| H | 39.7939482753 | 65.0032614955 | 50.0230154177 |
| H | 40.2343636693 | 65.1379334896 | 51.5620377857 |
| O | 36.7599149982 | 60.5330811188 | 45.1500576489 |
| H | 35.7638179409 | 60.5995121977 | 45.1271331203 |
| H | 36.9598313719 | 59.5791095349 | 45.4128482668 |
| O | 44.0020613514 | 63.8087089477 | 43.1774908596 |
| H | 43.6676610763 | 64.4450832224 | 43.8408800633 |
| H | 44.2207164112 | 64.2926922206 | 42.3560447666 |
| H | 46.3152289054 | 67.5238828094 | 46.5934614948 |
| H | 33.9732086147 | 66.3402391786 | 53.7250070281 |
| H | 35.0513218262 | 57.8760137538 | 50.3049118860 |
| H | 30.8084667611 | 63.0947678764 | 49.3719982211 |

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