
A two-metalloenzyme cascade constructs the azetidine-containing pharmacophore

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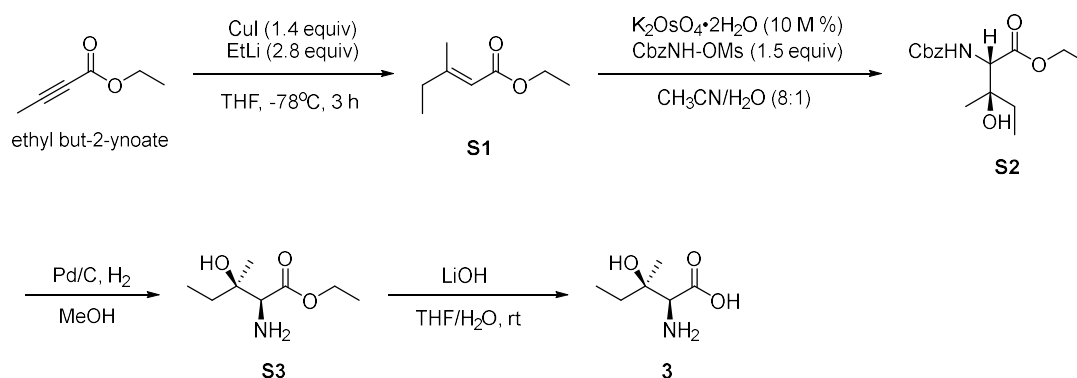
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Supplementary Methods

All chemicals for enzymatic reactions were purchased from Sigma-Aldrich, and all NMR spectra were collected on Bruker AVANCE III HD 400 (400 MHz, 100 MHz) or Bruker AVANCE NEO 600 (600 MHz, 150 MHz) NMR spectrometer unless otherwise noted. Chemical shifts (δ) are reported in parts per million (ppm) downfield from tetramethylsilane using the solvent resonance as internal standard for ^1H (D_2O = 4.79 ppm, CD_3OD = 4.89 ppm) and ^{13}C (CD_3OD = 49.86 ppm). Data are reported as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), integration and assignments. Some proton and carbon data were assigned using two-dimensional NMR spectroscopy techniques, including ^1H - ^1H COSY (Correlation Spectroscopy), ^1H - ^{13}C HSQC (Heteronuclear Singular Quantum Correlation), ^1H - ^{13}C HMBC (Heteronuclear Multiple Bond Correlation) and ^1H - ^1H (Nuclear Overhauser Effect), and all NMR solvents were obtained from J&K Scientific unless otherwise mentioned. NMR spectra were visualized using MestReNova.

1. Synthesis of (2*S*, 3*R*)-2-amino-3-hydroxy-3-methylpentanoic acid (3)



Synthesis of ethyl (*E*)-3-methylpent-2-enoate (S1): This compound was synthesized according to a published procedure¹. To a mixture of CuI (7.90 g, 42 mM, 1.4 equiv.) and THF (tetrahydrofuran, 100 ml) in a 500 ml round bottomed flask was added a solution of EtLi in hexane (1.6 M, 54 ml, 84 mM, 2.8 equiv.) at -78°C under nitrogen, and the resulting mixture was allowed to stir at -78°C for 1 h. Then a solution of ethyl 2-butynoate (3.5 ml, 30 mM) in

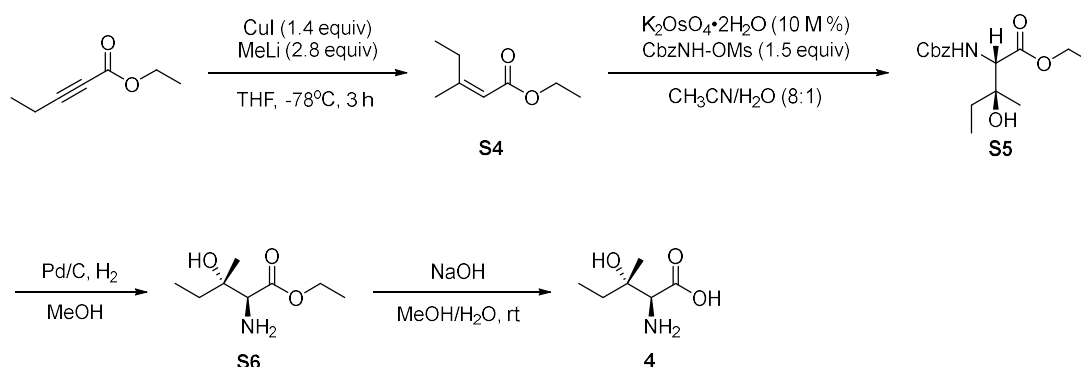
THF (20 ml) was added slowly and the resulting mixture was stirred for 2 h. After that, the reaction was quenched with saturated NH_4Cl solution and extracted with EtOAc. The combined organic layers were dried over Na_2SO_4 and concentrated. Purification by column chromatography gave **S1** as a colorless oil (3.82 g, 90% yield). ^1H NMR (400 MHz, CDCl_3): 5.62 (s, br, 1H), 4.10 (q, $J = 7.2$ Hz, 2H), 2.18–2.06 (m, 5H), 1.24 (t, $J = 7.2$ Hz, 3H), 1.03 (t, $J = 7.6$ Hz, 3H).

Synthesis of ethyl (2*S*, 3*R*)-2-(((benzyloxy)carbonyl)amino)-3-hydroxy-3-methylpentanoate (S2): This compound was synthesized according to a published procedure². To a 250 ml round bottomed flask was added benzyl ((methylsulfonyl)oxy) carbamate (6.21 g, 24 mM, 1.5 equiv.) and CH_3CN (60 ml), and $\text{K}_2\text{OsO}_4 \cdot 2\text{H}_2\text{O}$ (0.59 g, 1.6 mM, 10 M %) was then added. The resulting mixture was allowed to stir at room temperature for 10 min. After that, a solution of compound **S1** (2.29 g, 16 mM) in CH_3CN (20 ml) and H_2O (10 ml) was added, and the resulting mixture was stirred for 36 h at 45°C . Subsequently, the reaction was quenched with sat. aq. $\text{K}_2\text{S}_2\text{O}_5$ (50 ml) and stirred for an additional 10 min. It was then diluted with H_2O (20 ml) and extracted with EtOAc. The combined organic layers were washed with sat. aq. NaHCO_3 and brine, dried with Na_2SO_4 , and then concentrated *in vacuo*. Purification by column chromatography gave **S2** as a yellow oil (2.49 g, 50% yield). ^1H NMR (400 MHz, CDCl_3): 7.40–7.30 (m, 5H), 5.78 (d, $J = 8.8$ Hz, 1H), 5.10 (s, 2H), 4.35–4.15 (m, 3H), 2.58 (s, br, 1H), 1.60–1.50 (m, 2H), 1.28 (t, $J = 7.2$ Hz, 3H), 1.19 (s, 3H), 0.91 (t, $J = 7.6$ Hz, 3H).

Synthesis of ethyl (2*S*, 3*R*)-2-amino-3-hydroxy-3-methylpentanoate (S3): To a 100 ml round bottomed flask was added Pd/C (200 mg), **S2** (921.8 mg, 3 mM), and MeOH (20 ml) at -78°C under nitrogen. The flask was degassed and refilled with nitrogen for three times. The resulting mixture was allowed to stir at room temperature overnight, and the reaction mixture was filtrated through a pad of celite and concentrated *in vacuo*. Purification by column chromatography gave **S3** as a colorless oil (264.3 mg, 50% yield). ^1H NMR (400 MHz, CD_3OD): 4.25–4.15 (m, 2H), 3.36 (s, 1H), 1.70–1.50 (m, 2H), 1.28 (t, $J = 7.2$ Hz, 3H), 1.11 (s, 3H), 0.95 (t, $J = 7.6$ Hz, 3H).

Synthesis of 3: To a 25 ml round bottomed flask was added **S3** (131 mg, 0.75 mM), LiOH (1.0 M, 7.5 ml), and THF (10 ml). The resulting mixture was stirred at room temperature overnight, and then aqueous solution was acidified to pH 2.0. After that, the solvent was removed under reduced pressure. The residue was dissolved in THF, and the solution was filtered through a pad of celite and the filtrate was concentrated under reduced pressure to afford **3**. ¹H NMR (400 MHz, D₂O): 3.57 (s, 1H), 1.55–1.40 (m, 2H), 1.28 (s, 3H), 0.86 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, D₂O): 172.15, 72.04, 62.88, 29.04, 23.01, 6.89. The LC-HRMS analysis and NMR data of compound **3** were listed in **Supplementary Figure 42-44**.

2. Synthesis of (2*S*, 3*S*)-2-amino-3-hydroxy-3-methylpentanoic acid (**4**)



Synthesis of ethyl (Z)-3-methylpent-2-enoate (S4**):** This compound was synthesized according to a published procedure¹. To a mixture of CuI (6.67 g, 35 mM, 1.4 equiv.) and THF (80 ml) in a 250 ml round bottomed flask was added a solution of CH₃Li in hexane (1.6 M, 44 ml, 70 mM, 2.8 equiv.) at -78°C under nitrogen. The resulting mixture was allowed to stir at -78°C for 1 h. Then a solution of ethyl 2-pentynoate (3.3 ml, 25 mM) in THF (20 ml) were added slowly and the resulting mixture was stirred for 2 h. The reaction was quenched with saturated NH₄Cl solution and extracted with EtOAc. The combined organic layers were dried over Na₂SO₄ and concentrated. Purification by column chromatography gave **S4** as a colorless oil (1.67 g, 47% yield). ¹H NMR (400 MHz, CDCl₃): 5.60 (s, br, 1H), 4.10 (q, *J* = 7.2 Hz, 2H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.85 (s, 3H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.05 (t, *J* = 7.6 Hz, 3H).

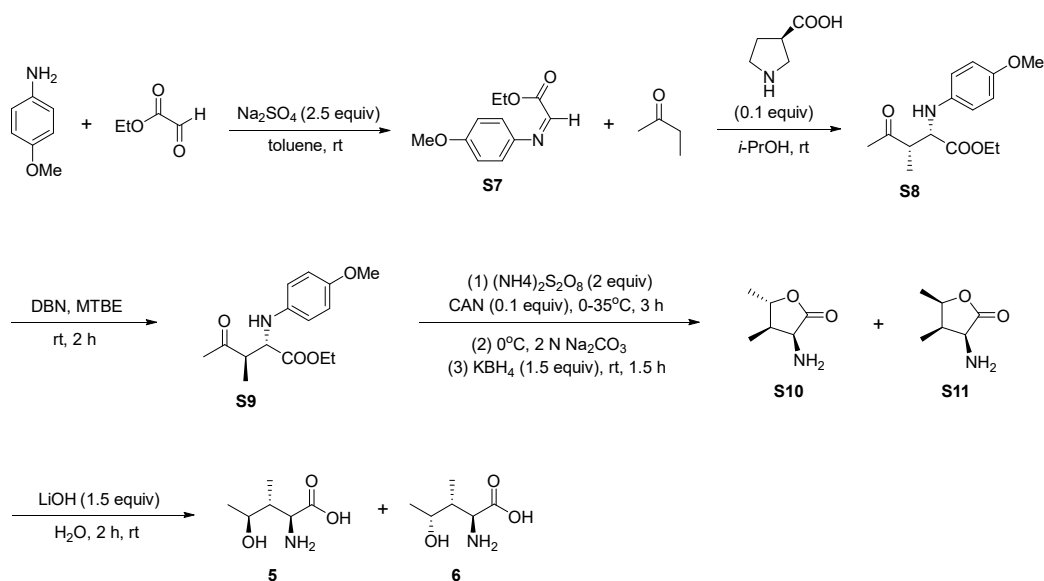
Synthesis of ethyl (2*S*, 3*S*)-2-(((benzyloxy)carbonyl)amino)-3-hydroxy-3-methylpentanoate (S5**):** This compound was synthesized according to a published procedure².

To a 250 ml round bottomed flask was added benzyl ((methylsulfonyl)oxy) carbamate (1.98 g, 7.5 mM, 1.5 equiv.) and CH₃CN (20 ml), and then K₂OsO₄·2H₂O (0.19 g, 0.5 mM, 10 M %) was then added. The resulting mixture was allowed to stir at room temperature for 10 min, subsequently, a solution of compound **S4** (0.72 g, 5 mM) in CH₃CN (12 ml) and H₂O (4 ml) was added. The resulting mixture was stirred for 36 h at 45°C. The reaction was quenched with sat. aq. K₂S₂O₅ (20 ml) and stirred for an additional 10 min. It was then diluted with H₂O (20 ml) and extracted with EtOAc. The combined organic layers were washed with sat. aq. NaHCO₃ and brine, dried with Na₂SO₄, and concentrated *in vacuo*. Purification by column chromatography gave **S5** as a yellow oil (618.9 mg, 40% yield). ¹H NMR (400 MHz, CDCl₃): 7.38–7.28 (m, 5H), 5.83 (d, *J* = 9.2 Hz, 1H), 5.10 (s, 2H), 4.30 (d, *J* = 9.2 Hz, 1H), 4.25–4.10 (m, 2H), 2.59 (s, br, 1H), 1.58–1.45 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.17 (s, 3H), 0.96 (t, *J* = 7.6 Hz, 3H).

Synthesis of ethyl (2*S*, 3*S*)-2-amino-3-hydroxy-3-methylpentanoate (S6**):** To a 50 ml round bottomed flask was added Pd/C (30 mg), **S5** (150 mg, 0.5 mM), and MeOH (10 ml) at -78°C under nitrogen. The flask was degassed and refilled with nitrogen for three times. The resulting mixture was allowed to stir at room temperature overnight. The reaction mixture was filtrated through a pad of celite and concentrated *in vacuo*. Purification by column chromatography gave **S6** as a colorless oil (72.1 mg, 82% yield). ¹H NMR (400 MHz, CD₃OD): 4.36–4.16 (m, 2H), 3.85 (s, br, 1H), 1.70–1.60 (m, 1H), 1.50–1.40 (m, 1H), 1.36 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 0.97 (t, *J* = 7.6 Hz, 3H).

Synthesis of 4: To a 25 ml round bottomed flask was added **S6** (70 mg, 0.4 mM), NaOH (2.0 M, 2.5 ml), and MeOH (10 ml). The resulting mixture was stirred at room temperature overnight. Then aqueous solution was acidified to pH 2.0. Then the solvent was then removed under reduced pressure. The residue was dissolved in THF. The solution was filtered through a pad of celite and the filtrate was concentrated under reduced pressure to afford **4**. ¹H NMR (400 MHz, D₂O): ¹H NMR (400 MHz, D₂O): 3.45 (s, 1H), 1.72–1.60 (m, 1H), 1.60–1.45 (m, 1H), 1.02 (s, 3H), 0.81 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, D₂O): 172.09, 72.13, 62.32, 31.83, 19.88, 6.63. The LC-HRMS and NMR data analysis of compound **4** were listed in **Supplementary Figure 45-47**.

3. Synthesis of (2*S*, 3*R*, 4*R*)-2-amino-4-hydroxy-3-methylpentanoic acid (**6**)³



Synthesis of ethyl (Z)-2-((4-methoxyphenyl)imino)acetate (S7**):** To a 500 ml round bottomed flask was added a solution of 4-methoxyaniline (5.00 g, 40.6 mM, 1.0 equiv.) in toluene (60 ml). Then sodium sulfate (14.42 g, 101.5 mM, 2.5 equiv.) and ethyl glyoxalate (8.46 g, 40 mM, 8.2 ml, 50%(w/w), 1.02 equiv.) were added. The reaction mixture was allowed to stir for 30 min. Then sodium sulfate was filtered off using celite, and toluene was removed under reduced pressure. Compound **S7** was used for the next step without further purification.

Synthesis of ethyl (2*S*, 3*S*)-2-((4-methoxyphenyl)amino)-3-methyl-4-oxopentanoate (S8**):** To a 250 ml round bottomed flask was added **S7** (8.3 g, 40 mM, 1.0 equiv.), 2-butanone (10.4 g, 13 ml, 144.8 M, 5.0 equiv.), and *i*-PrOH (80 ml). Then (S)-pyrrolidine-2-carboxylic acid (333 mg, 2.9 mM, 0.1 equiv.) was added. The resulting reaction mixture was stirred for 5 h at room temperature. The solvent was removed *in vacuo* and the residue was purified by flash column chromatography to give **S8** as a colorless solid (3.98 g, 35% yield). ¹H NMR (600 MHz, CDCl₃): 6.79–6.70 (m, 2H), 6.69–6.59 (m, 2H), 4.29–4.19 (m, 1H), 4.19–4.07 (m, 2H), 3.72 (s, 3H), 3.07–2.88 (m, 1H), 2.22 (s, 2H), 1.35–1.01 (m, 6H).

Configuration transformation from **S8 to its regioisomer **S9**:** DBN (35 mg, 0.05 ml, 0.3 mM, 0.04 equiv.) was added to a solution of a mixture of **S8** and its regioisomer **S9** (1.98 g, 7.1 mM, 1.0 equiv.) in MTBE (2 ml) at room temperature under nitrogen. After the reaction mixture was stirred for 2 h, the MTBE was evaporated slowly for 18 h at room temperature. The solvent

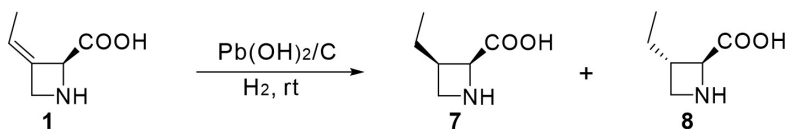
was removed *in vacuo* at room temperature and the mixture of **S9** and **S8** was used for the next step without further purification.

Synthesis of (2*S*, 3*S*, 4*R*)-amino-4,5-dimethyldihydrofuran-2(3*H*)-one (S10**) and its regioisomer (**S11**):** Compound **S8** and **S9** (1.98 g, 7.1 mM, 1.0 equiv.) was dissolved in acetonitrile (4 ml) at -10~0°C, and a solution of (NH₄)₂S₂O₈ (3.27 g, 14.32 mM, 2.0 equiv.) and CAN (0.39 g, 0.7 mM, 0.1 equiv.) in H₂O (10 ml) was added at -10~0°C. Then the reaction mixture was stirred at room temperature for 3 h. The reaction mixture was extracted with CH₂Cl₂ to purge the quinone, then the aqueous phase was neutralized to pH 8.0-8.5 at -10~0°C with 2N Na₂CO₃. Then KBH₄ (406 mg, 10.7 mM, 1.5 equiv.) was added into the aqueous phase and the reaction mixture was warmed up to room temperature and stirred for 1.5 h. Then the reaction mixture was basified to pH 9 at 0°C with 2N Na₂CO₃ and extracted with CH₂Cl₂. The combined organic phase was washed with H₂O, dried with Na₂SO₄, and evaporated under reduced pressure. Purification by column chromatography gave a mixture of **S10** and **S11** as a colorless oil (1:2 ratio, 100 mg, 5.4% yield). **Major isomer:** ¹H NMR (400 MHz, CDCl₃): 4.32–4.23 (m, 1H), 3.75 (d, *J* = 7.6 Hz, 1H), 2.30–2.20 (m, 1H), 1.55 (s, br, 2H), 1.36 (d, *J* = 6.4 Hz, 3H), 1.04 (d, *J* = 7.2 Hz, 1H). **Minor isomer:** ¹H NMR (400 MHz, CDCl₃): 4.55–4.45 (m, 1H), 3.82 (d, *J* = 6.8 Hz, 1H), 2.60–2.40 (m, 1H), 1.55 (s, br, 2H), 1.31 (d, *J* = 6.4 Hz, 3H), 0.87 (d, *J* = 7.2 Hz, 1H).

Synthesis of 6: A mixture of **S10** and **S11** (100 mg, 1.0 equiv.) was dissolved in H₂O (5 ml), and then LiOH (55 mg, 1.3 mM, 1.5 equiv.) was added. The reaction mixture was allowed to stir at room temperature for 2 h. Then the reaction mixture was acidified with AcOH to pH 5. H₂O was removed under reduced pressure to give a mixture of **5** and **6**, then **6** was separated by HPLC with C18 column. ¹H NMR (600 MHz, DMSO-*d*₆): 3.62 (d, *J* = 2.99 Hz, 1H), 3.56–3.35 (m, 1H), 1.72–1.66 (m, 1H), 1.11–1.09 (d, *J* = 6.34 Hz, 3H), 0.86-0.84 (d, *J* = 6.93 Hz, 3H); ¹³C NMR (150 MHz, DMSO-*d*₆): 169.29, 68.55, 54.03, 41.31, 22.35, 12.41. The LC-HRMS analysis and NMR data of compound **6** were listed in **Supplementary Figure 48-50**.

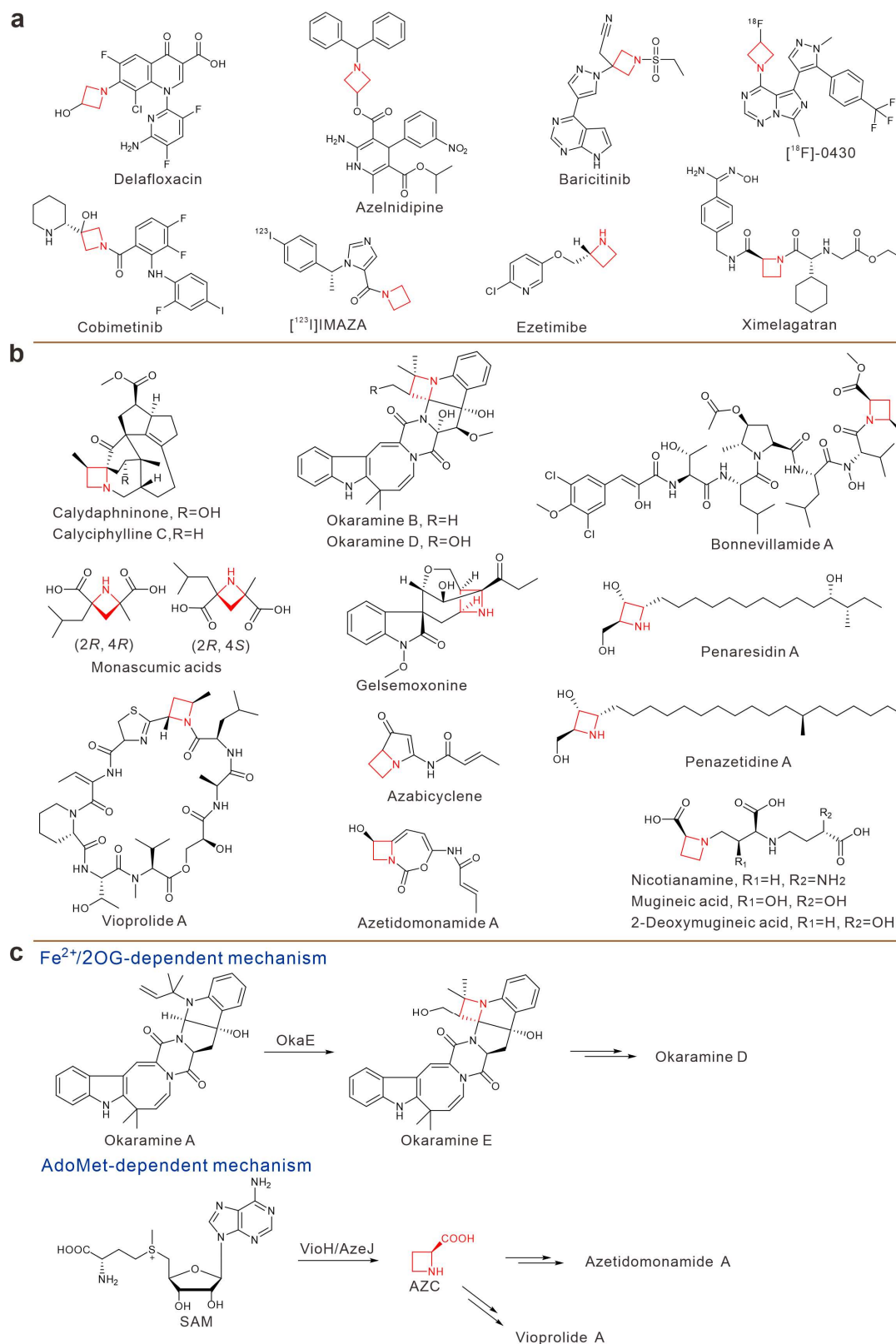
4. Synthesis of (2*S*, 3*R*)-3-ethylazetididine-2-carboxylic acid (**7**) and (2*S*, 3*S*)-3-

ethylazetidine-2-carboxylic acid (8)



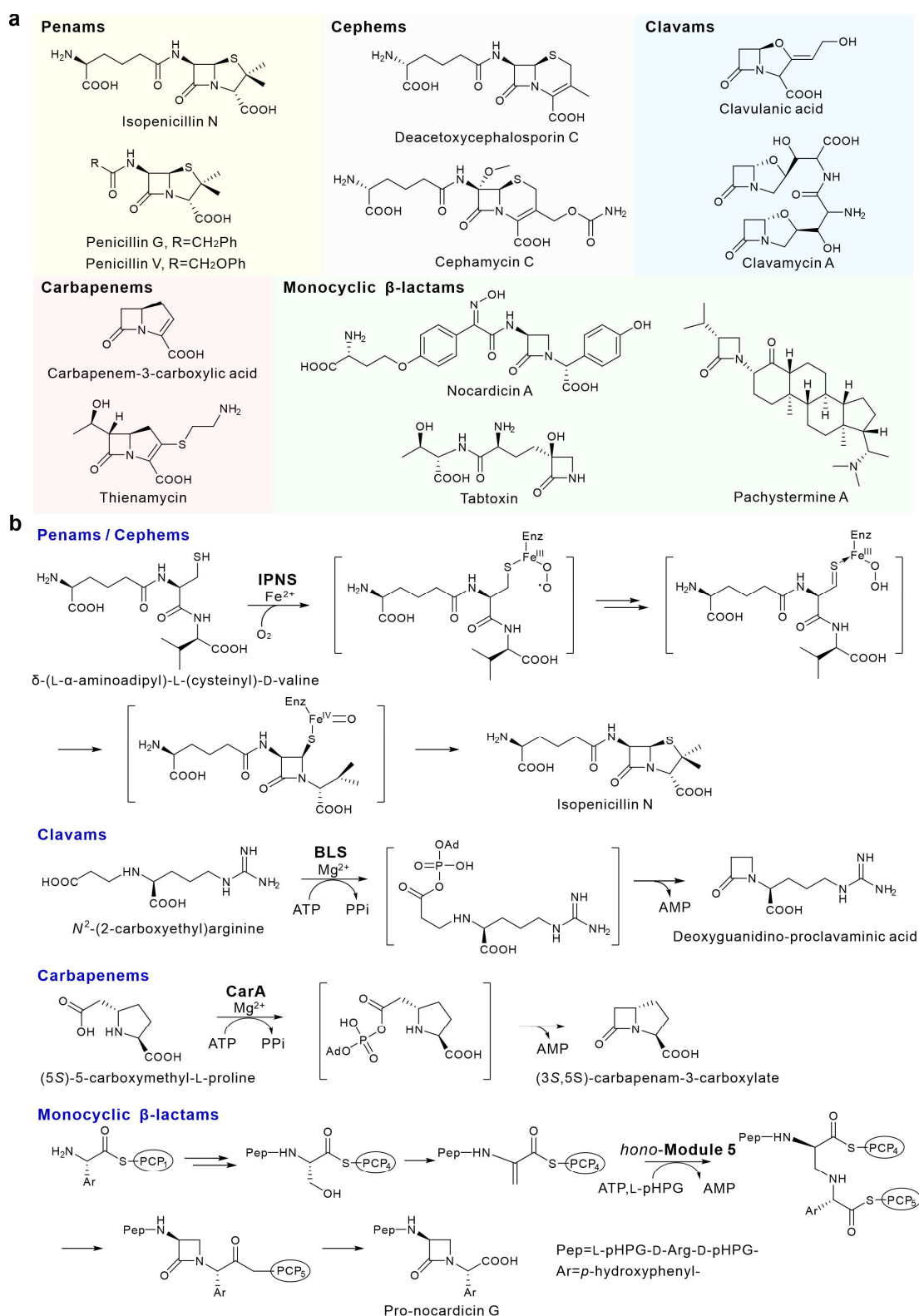
To a 50 ml round bottomed flask was added $\text{Pd}(\text{OH})_2/\text{C}$ (4 mg), compound **1** (12 mg), and MeOH (10 ml). Then the mixture was flash-frozen with liquid nitrogen. An atmosphere of hydrogen was introduced by briefly evacuating the flask, then flushing with pure hydrogen (1 atm, hydrogen balloon). The mixture was stirred at room temperature for 8 h under hydrogen atmosphere. The $\text{Pd}(\text{OH})_2/\text{C}$ was removed through 0.22 μm microporous membrane to give a mixture of **7** and **8**. Then **7** and **8** were separated by HPLC with C18 column. Compound **7**: ^1H NMR (600 MHz, CD_3OD): 4.71 (d, $J = 9.42$ Hz, 1H), 4.10 (dd, $J = 10.34, 8.51$ Hz, 1H), 3.58 (dd, $J = 10.31, 6.43$ Hz, 1H), 2.91 (ddt, $J = 15.37, 9.10, 4.65$ Hz, 1H), 1.65 (m, 2H), 0.89 (t, $J = 7.40$, 3H); ^{13}C NMR (150 MHz, CD_3OD): 171.44, 64.32, 49.64, 37.70, 24.14, 11.02. Compound **8**: ^1H NMR (600 MHz, CD_3OD): 4.55 (d, $J = 7.80$ Hz, 1H), 3.96 (t, $J = 9.56$ Hz, 1H), 3.71 (dd, $J = 10.33, 7.97$ Hz, 1H), 2.86 (h, $J = 7.88$ Hz, 1H), 1.77 (ddq, $J = 32.54, 14.01, 7.27$ Hz, 2H), 0.97 (t, $J = 7.39$, 3H); ^{13}C NMR (150 MHz, CD_3OD): 171.48, 64.90, 49.46, 40.75, 27.54, 11.01. The LC-HRMS analysis and NMR data of compound **7** and **8** were listed in **Supplementary Figure 113-125**.

Supplementary Figures

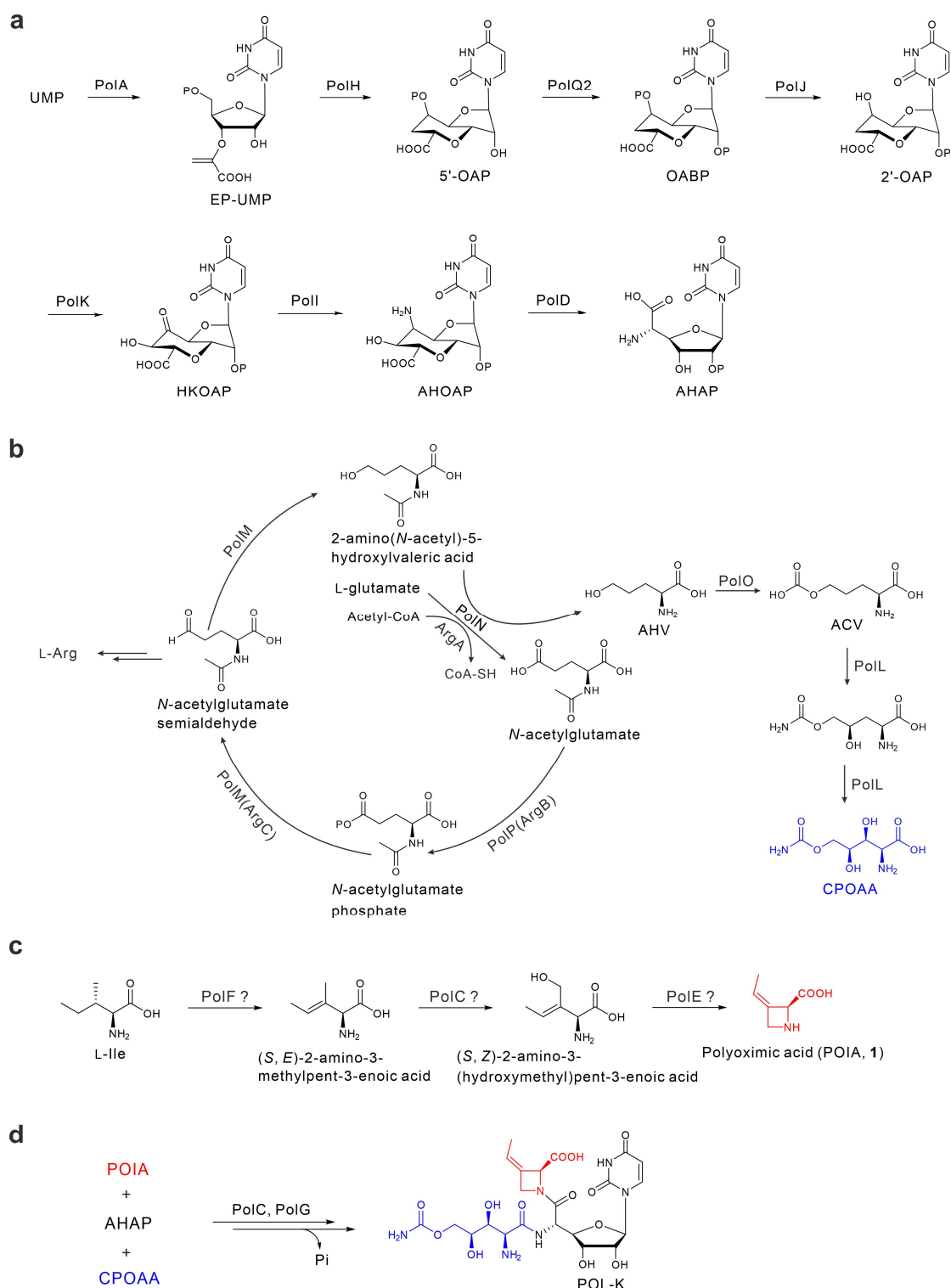


Supplementary Figure 1 | Representative azetidine-containing drugs and natural products, and related mechanisms reported so far for azetidine construction. a, Structures

of representative azetidine-containing drugs. **b**, Structures of representative azetidine-containing natural products. **c**, Two reported mechanisms for azetidine construction in related natural product biosynthesis. Currently, biosynthesis of the azetidine unit of few natural products, including okaramine, vioprolide, and azetidomonamide A, has merely been clarified so far. Top, Fe²⁺/2OG-dependent mechanism. The Fe²⁺/2OG-dependent enzyme OkaE was confirmed to govern the azetidine ring formation during the biosynthesis of okaramine D (produced by *Penicillium simplicissimum* ATCC 90288)⁴. Bottom, AdoMet-dependent mechanism. The AdoMet-dependent enzymes, VioH and AzeJ, were characterized to be capable of independently constructing the azetidine-2-carboxylic acid (AZC) moiety of vioprolide A (produced by *Cystobacter violaceus* Cb vi35) and azetidomonamide A (produced by *Pseudomonas aeruginosa*)⁵⁻⁷.

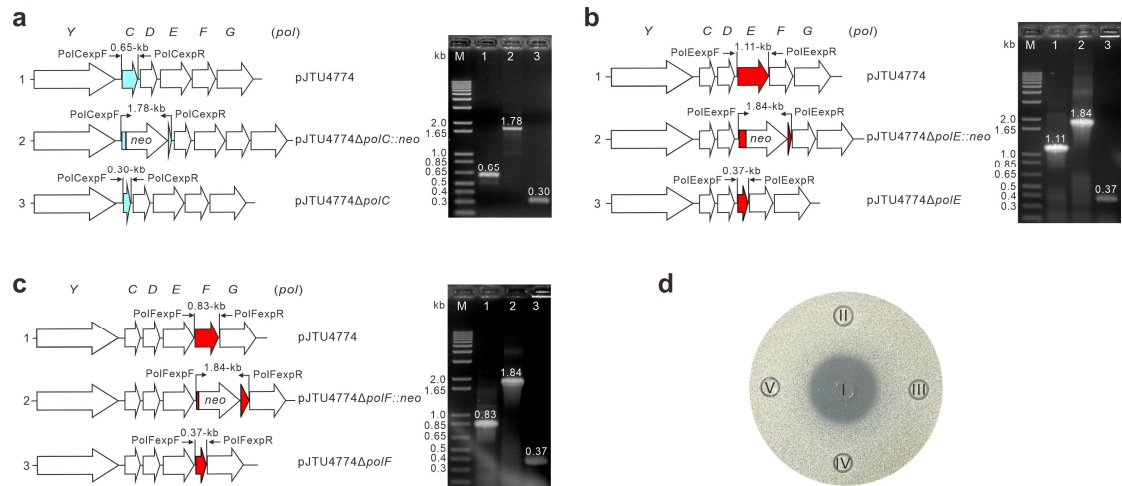


Supplementary Figure 2 | Representative β -lactam natural products and related mechanisms for β -lactam formation. **a**, Examples of the different types of naturally occurring β -lactam ring containing natural products. **b**, Related enzymes responsible for β -lactam formation during the biosynthesis of related natural products.

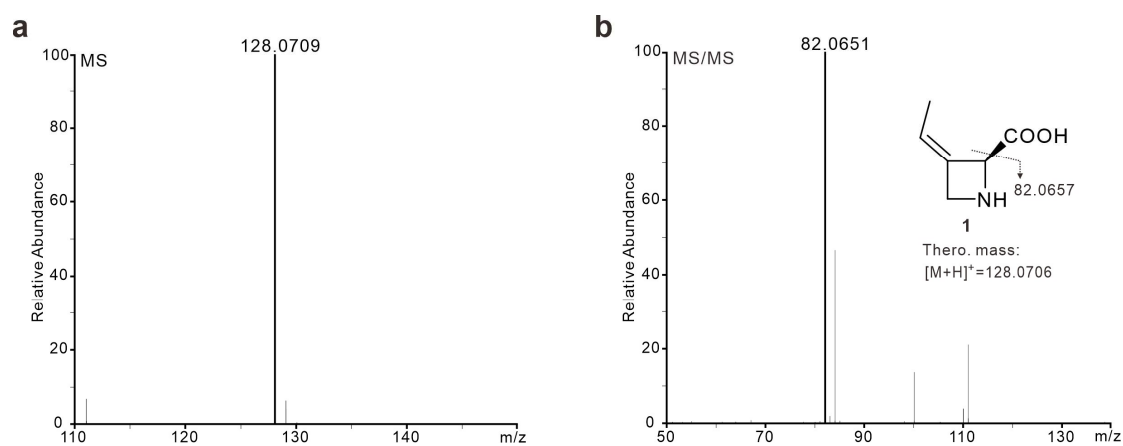


Supplementary Figure 3 | Overall biosynthetic pathway of polyoxin (POL). **a**, The confirmed biosynthetic pathway to AHAP⁸. The PolB enzyme was previously determined to catalyze UMP to 5-Me UMP⁹. Actually, this nucleotide (also including the C-5 modified intermediates derived from it) could also be correspondingly recognized by related enzyme described as above. UMP, uridine 5'-monophosphate; 5-Me UMP, 5-methyl UMP; EP-UMP,

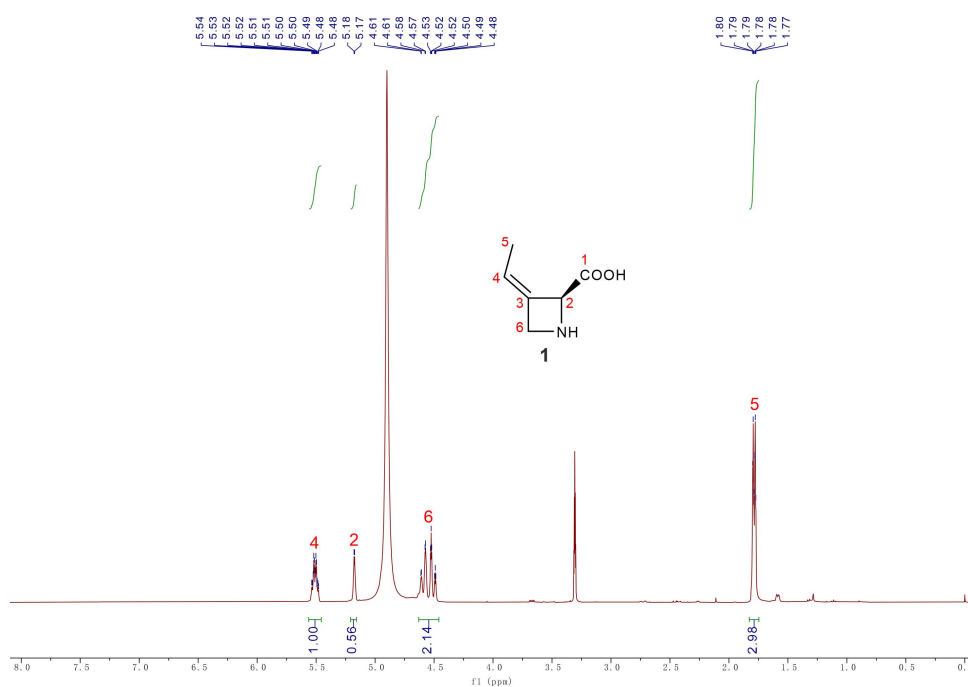
enolpyruvyl UMP; 5'-OAP, octosyl acid 5'-phosphate; OABP, octosyl acid 2',5'-bisphosphate; 2'-OAP, octosyl acid 2'-phosphate; HKOAP, 6'-hydroxy-5'-keto-octosyl acid 2'-phosphate; AHOAP, (4'*S*, 5'*S*, 6'*S*, 7'*R*)-5'-amino-6'-hydroxyoctosyl acid 2'-phosphate; AHAP, amino-hexuronic acid 2'-phosphate. **b**, The confirmed pathway for the peptidyl moiety CPOAA biosynthesis¹⁰. AHV, α -amino- δ -hydroxyvaleric acid; ACV, α -amino- δ -carbamoylhydroxyvaleric acid; CPOAA, carbamoylpolyoxamic acid. **c**, The previously proposed pathway for POIA (**1**) biosynthesis. The genes *polC*, *polE*, and *polF* were deduced to be responsible for the biosynthesis of **1**. **d**, Proposed logic for polyoxin assembly in this study. The genes *polC* and *polG* were responsible for the assembly of AHAP, CPOAA, and POIA. POIA, polyoximic acid; POL-K, polyoxin K.



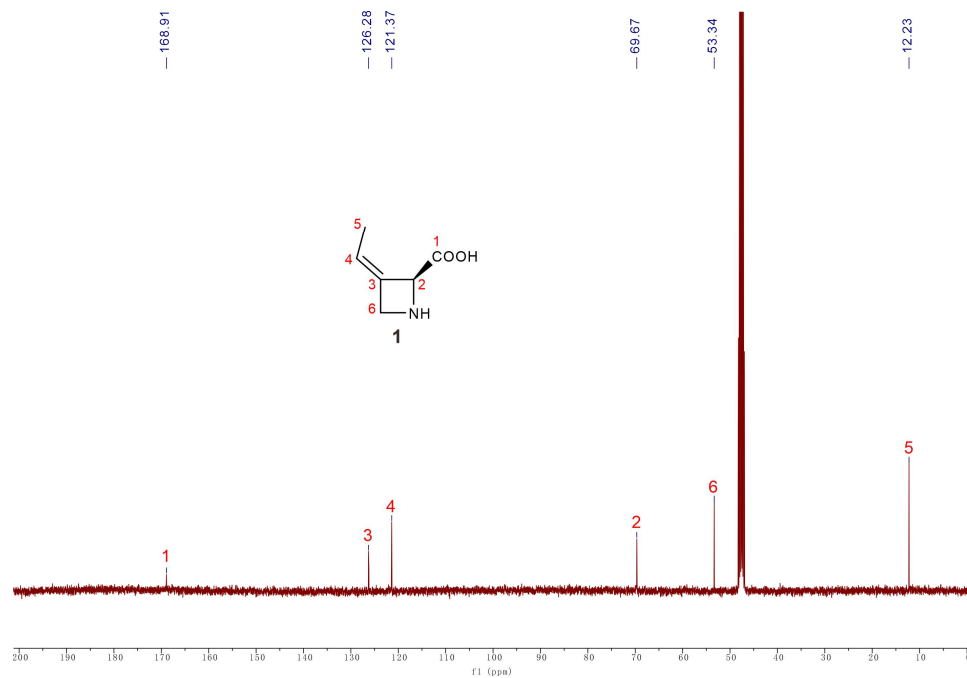
Supplementary Figure 4 | Genetic analysis of the target genes (*polC*, *E*, and *F*). **a**, In-frame deletion of *polC* in pJTU4774 by PCR-targeting technology. Left column, schematic illustration for the in-frame deletion of the target gene *polC*. Right column, PCR identification of pJTU4774Δ*polC*. M, 1 kb ladder; 1, PCR product using pJTU4774 as template; 2, PCR product using pJTU4774Δ*polC*::*neo* as template; 3, PCR product using pJTU4774Δ*polC* as template. **b**, In-frame deletion of *polE* in pJTU4774 by PCR-targeting technology. Left column, schematic illustration for the in-frame deletion of the target gene *polE*. Right column, PCR identification of pJTU4774Δ*polE*. M, 1 kb ladder; 1, PCR product using pJTU4774 as template; 2, PCR product using pJTU4774Δ*polE*::*neo* as template; 3, PCR product using pJTU4774Δ*polE* as template. **c**, In-frame deletion of *polF* in pJTU4774 by PCR-targeting technology. Left column, schematic illustration for the in-frame deletion of the target gene *polF*. Right column, PCR identification of pJTU4774Δ*polF*. M, 1 kb ladder; 1, PCR product using pJTU4774 as template; 2, PCR product using pJTU4774Δ*polF*::*neo* as template; 3, PCR product using pJTU4774Δ*polF* as template. Source data is provided as a Source Data file. **d**, Bioassay analysis of the metabolites produced by related strains using *Trichosporon cutaneum* as indicator strain. The Roman numerals I, II, III, IV, and V represent the target metabolites correspondingly produced by the recombinants CXR14::pJTU4774, CXR14::pJTU4774Δ*polC*, CXR14::pJTU4774Δ*polE*, CXR14::pJTU4774Δ*polF*, and CXR14::pJTU2463b.



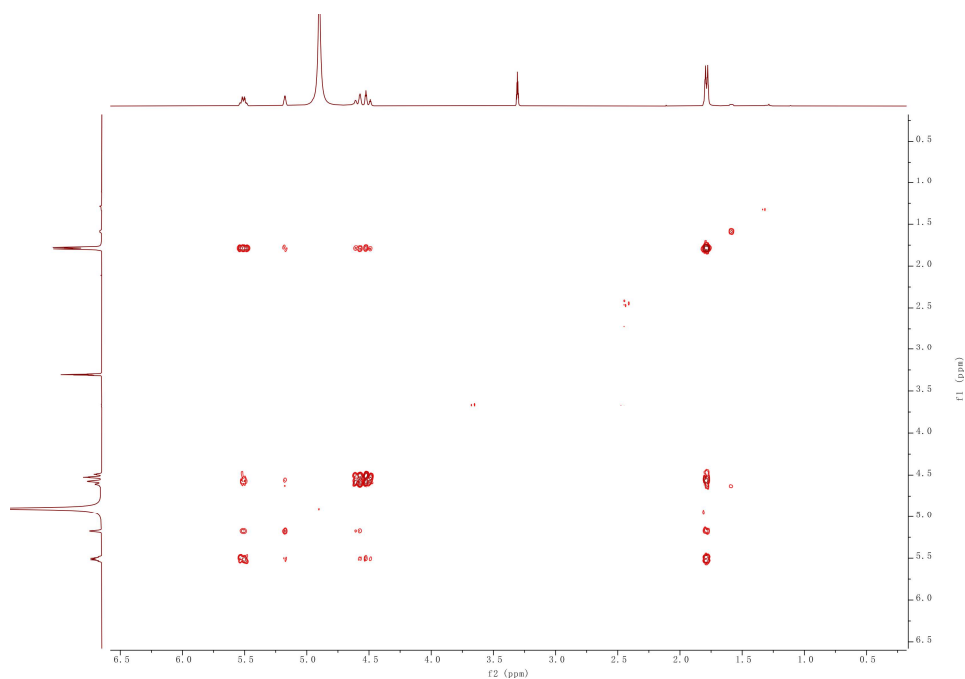
Supplementary Figure 5 | LC-HRMS analysis of the target metabolite 1 produced by the recombinant CXR14::pJTU4774 Δ polC. a, LC-HRMS analysis of the target metabolite **1** produced by CXR14::pJTU4774 Δ polC. **b**, LC-HRMS/MS analysis of the target metabolite **1** produced by CXR14::pJTU4774 Δ polC. The theoretical fragmentation pattern of **1** is included as a control.



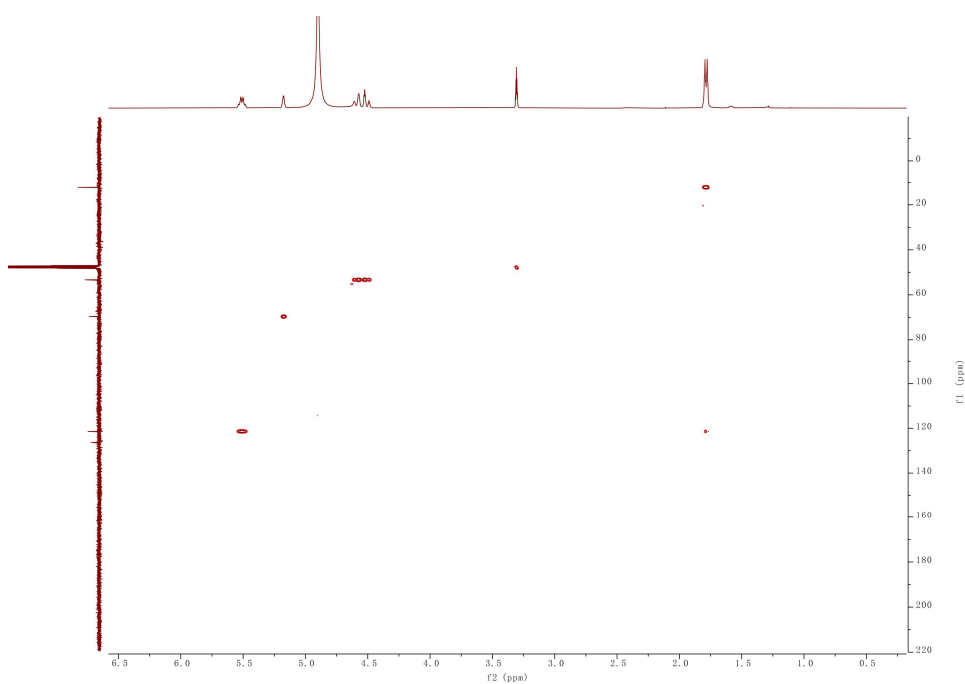
Supplementary Figure 6 | ¹H NMR spectrum of 1 produced by the recombinant CXR14::pJTU4774Δ*polC* (CD₃OD, 400 MHz).



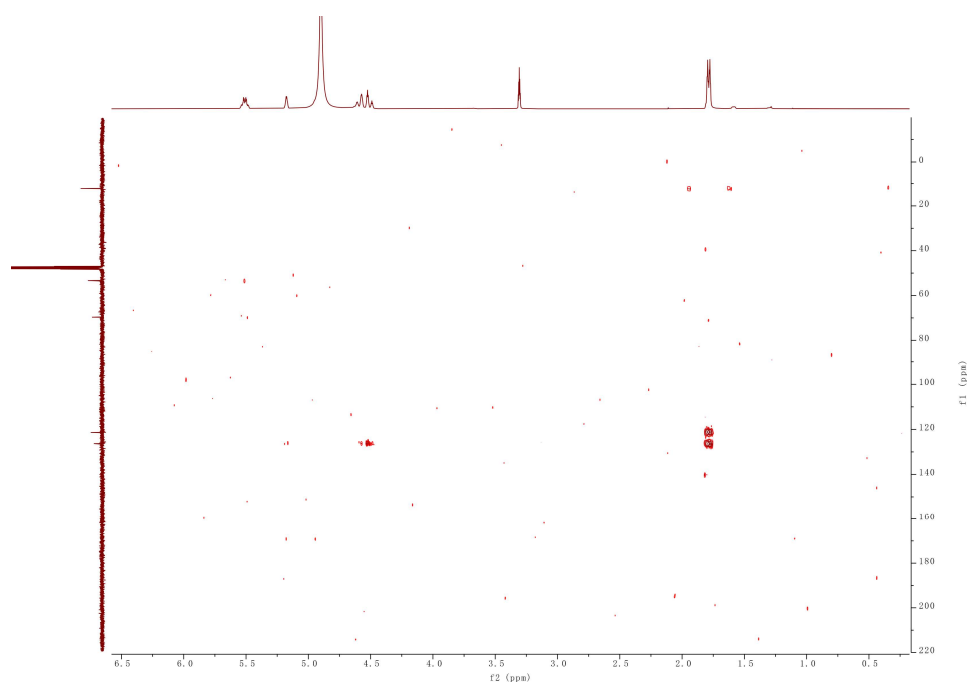
Supplementary Figure 7 | ¹³C NMR spectrum of 1 produced by the recombinant CXR14::pJTU4774Δ*polC* (CD₃OD, 100 MHz).



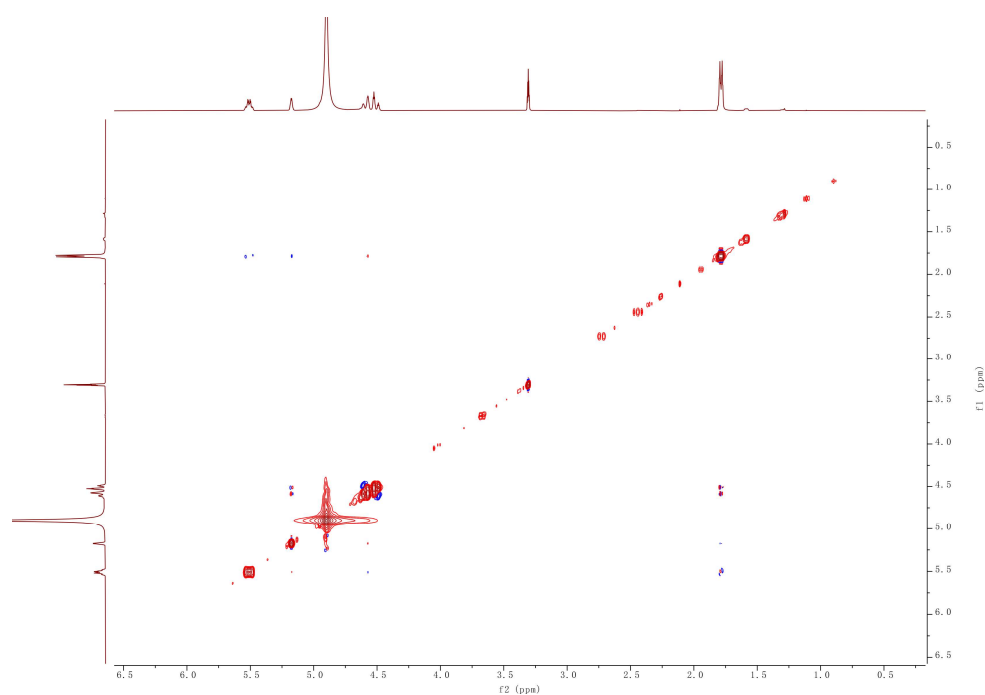
Supplementary Figure 8 | ^1H - ^1H COSY spectrum of 1 produced by the recombinant CXR14::pJTU4774 Δ *polC* (CD_3OD , 400 MHz).



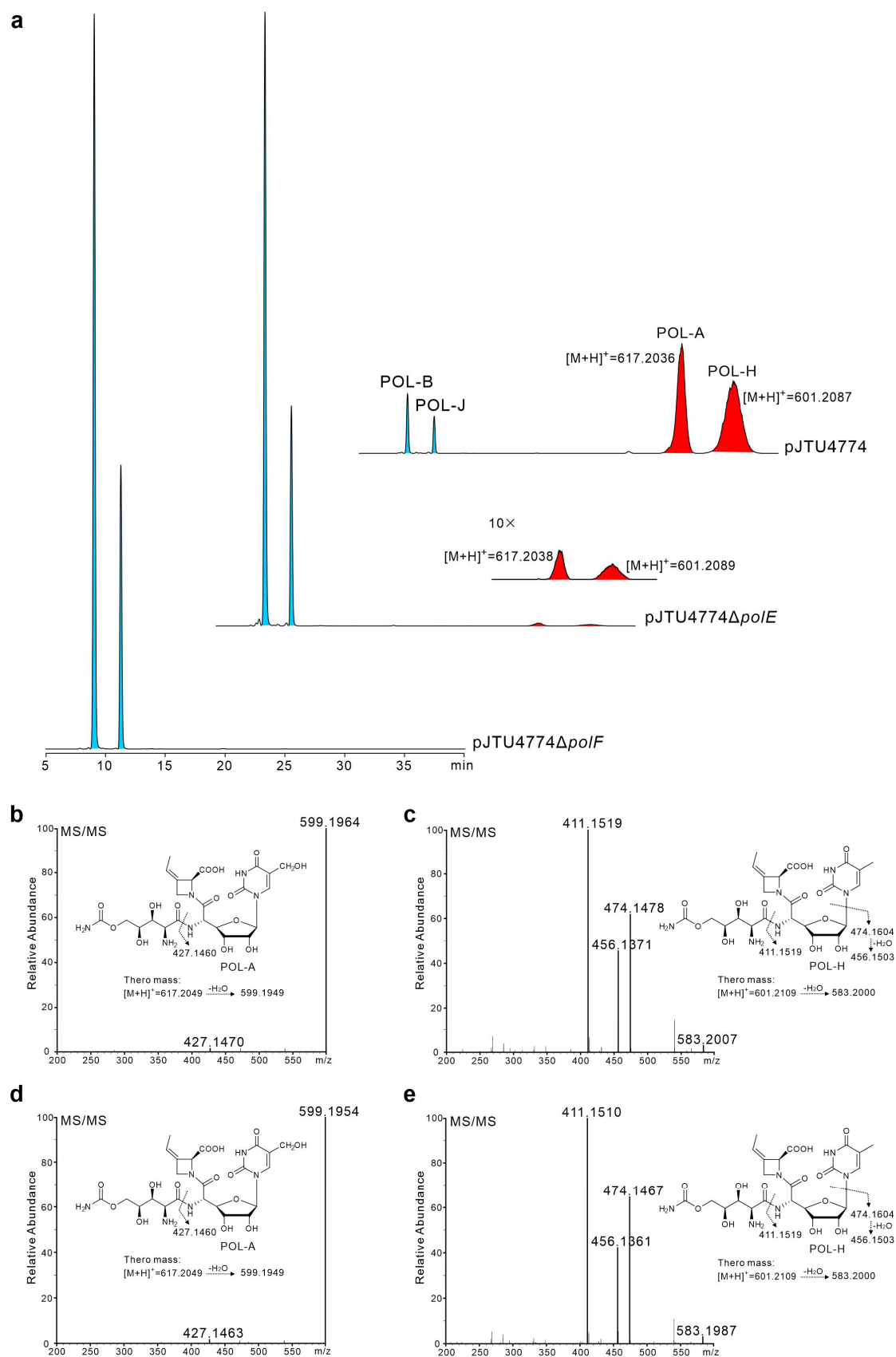
Supplementary Figure 9 | HSQC spectrum of 1 produced by the recombinant CXR14::pJTU4774 Δ *polC* (CD_3OD , 400 MHz).



Supplementary Figure 10 | HMBC spectrum of 1 produced by the recombinant CXR14::pJTU4774 Δ *polC* (CD₃OD, 400 MHz).

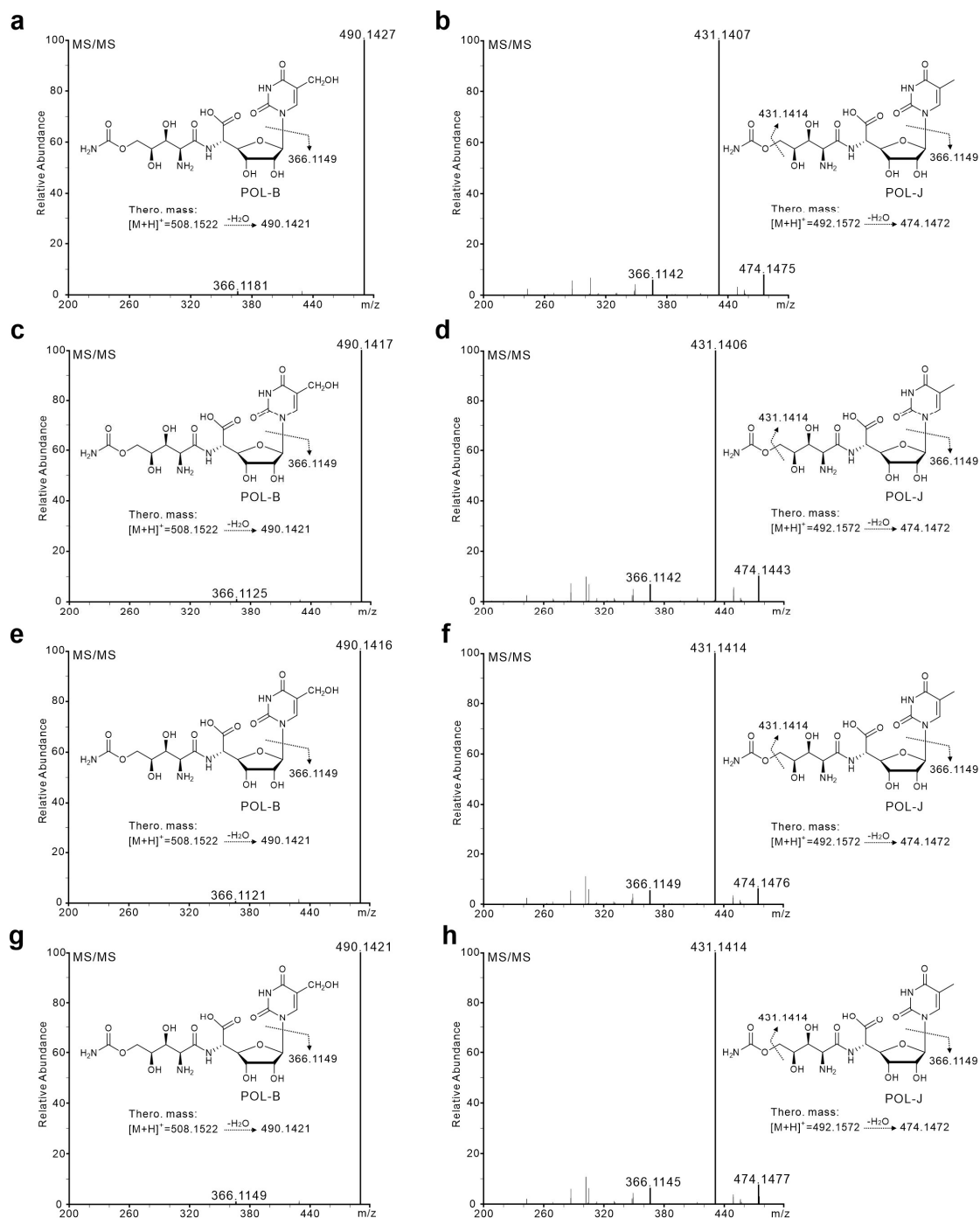


Supplementary Figure 11 | NOESY spectrum of 1 produced by the recombinant CXR14::pJTU4774 Δ *polC* (CD₃OD, 400 MHz).



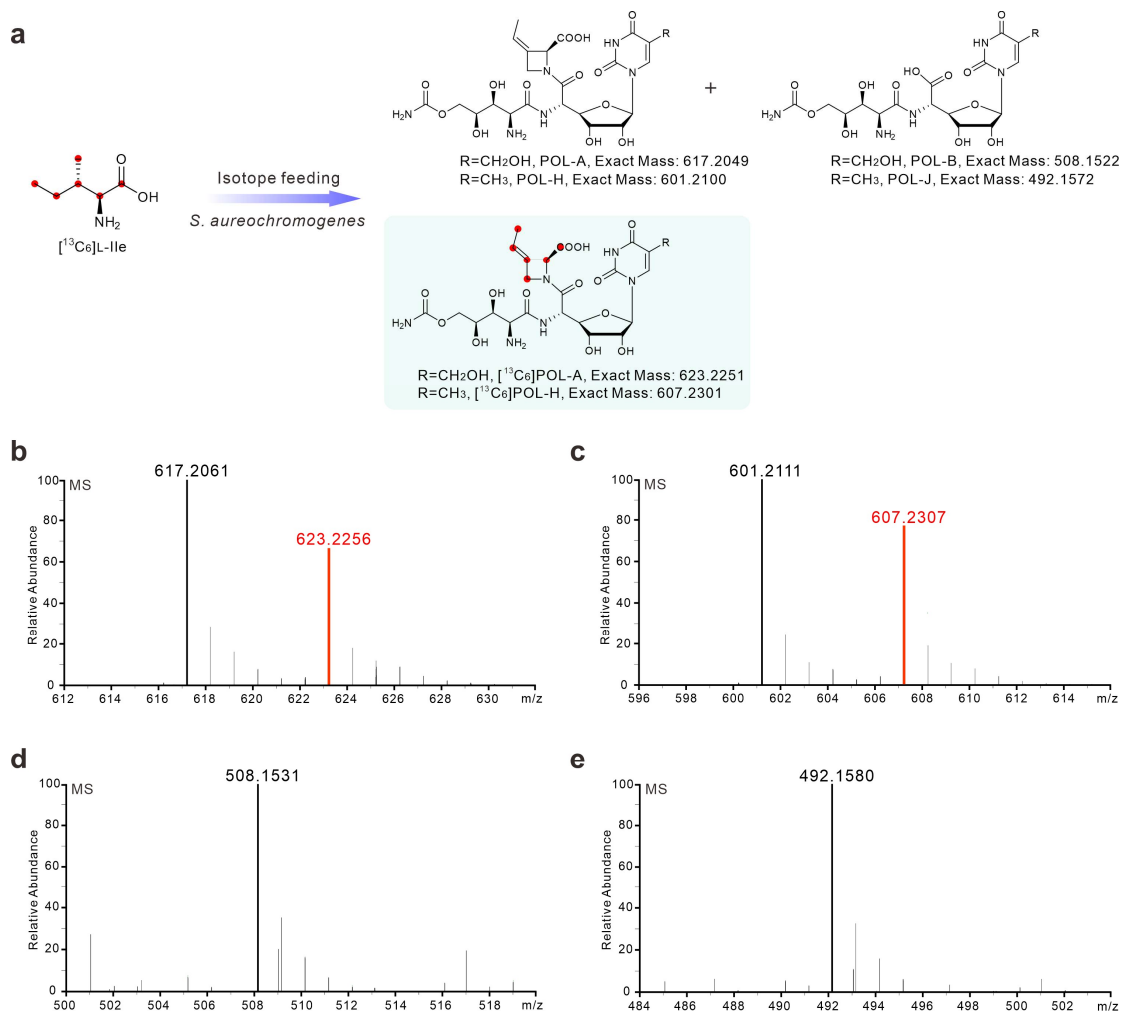
Supplementary Figure 12 | LC-HRMS analysis of the metabolites produced by related recombinants. a, LC-HRMS analysis of the metabolites produced by the recombinants of

CXR14::pJTU4774, CXR14::pJTU4774 Δ *polE* and CXR14::pJTU4774 Δ *polF*. As indicated, the recombinant CXR14::pJTU4774 Δ *polE* can produce a trace amount of POL-A and POL-H, while the recombinant CXR14::pJTU4774 Δ *polF* abolishes the capability of POL-A and POL-H production. **b**, LC-HRMS/MS analysis of the target metabolite POL-A produced by the recombinant CXR14::pJTU4774. **c**, LC-HRMS/MS analysis of the target metabolite POL-H produced by the recombinant CXR14::pJTU4774. **d**, LC-HRMS/MS analysis of the target metabolite POL-A produced by the recombinant CXR14::pJTU4774 Δ *polE*. **e**, LC-HRMS/MS analysis of the target metabolite POL-H produced by the recombinant CXR14::pJTU4774 Δ *polE*. For all LC-HRMS/MS analysis described in this figure, the theoretical fragmentation pattern of related metabolite is correspondingly included as a control.

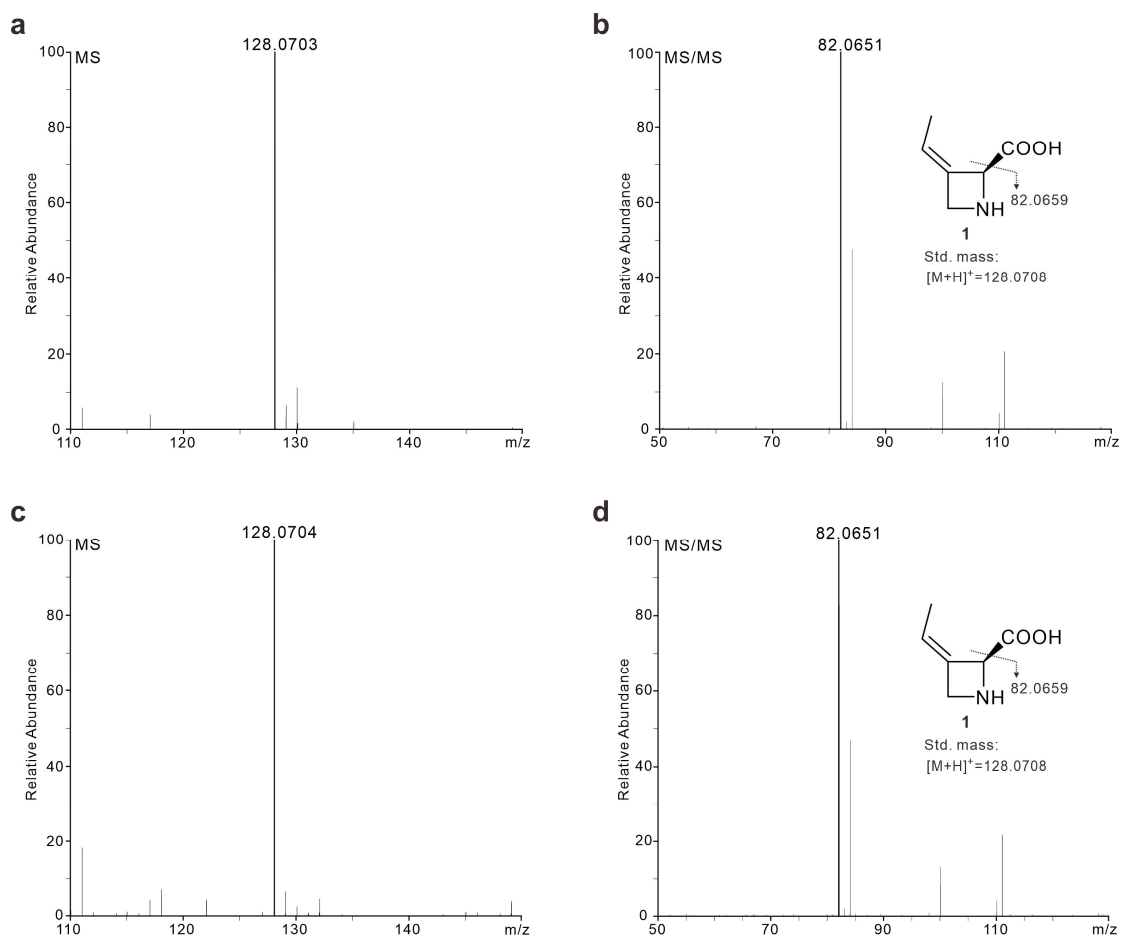


Supplementary Figure 13 | LC-HRMS/MS analysis of the target metabolites POL-B and POL-J produced by the related mutant strains. a, LC-HRMS/MS analysis of the target metabolite POL-B produced by the recombinant CXR14::pJTU4774. **b**, LC-HRMS/MS analysis of the target metabolite POL-J produced by the recombinant CXR14::pJTU4774. **c**, LC-HRMS/MS analysis of the target metabolite POL-B produced by the recombinant CXR14::pJTU4774Δ*polC*. **d**, LC-HRMS/MS analysis of the target metabolite POL-J produced by the recombinant CXR14::pJTU4774Δ*polC*. **e**, LC-HRMS/MS analysis of the target

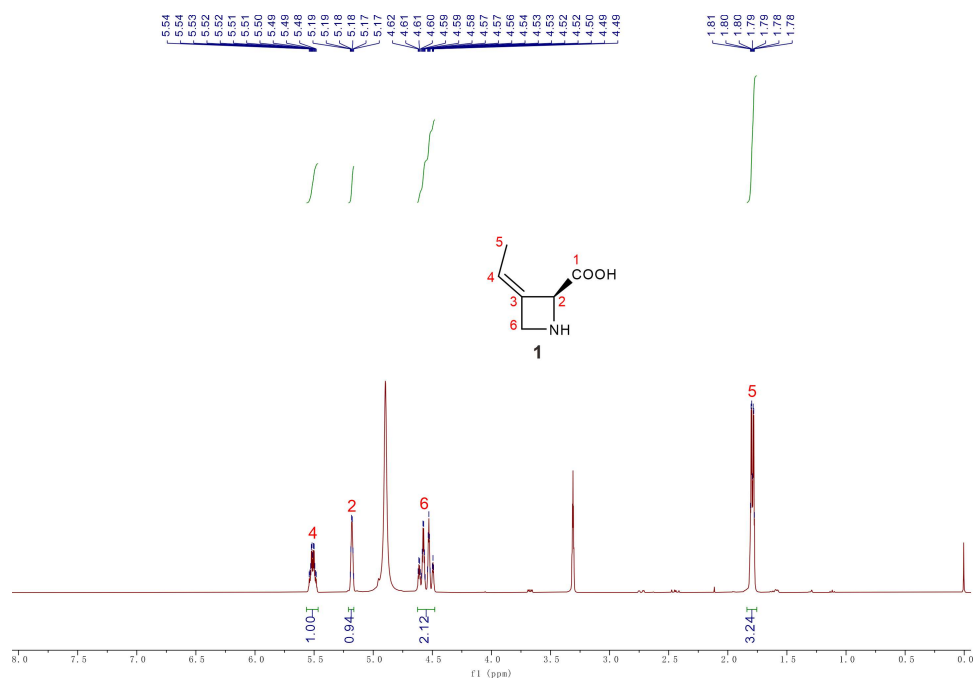
metabolite POL-B produced by the recombinant CXR14::pJTU4774 Δ *polE*. **f**, LC-HRMS/MS analysis of the target metabolite POL-J produced by the recombinant CXR14::pJTU4774 Δ *polE*. **g**, LC-HRMS/MS analysis of the target metabolite POL-B produced by the recombinant CXR14::pJTU4774 Δ *polF*. **h**, LC-HRMS/MS analysis of the target metabolite POL-J produced by the recombinant CXR14::pJTU4774 Δ *polF*. For all LC-HRMS/MS analysis described in this figure, the theoretical fragmentation pattern of related metabolite is correspondingly included as a control.



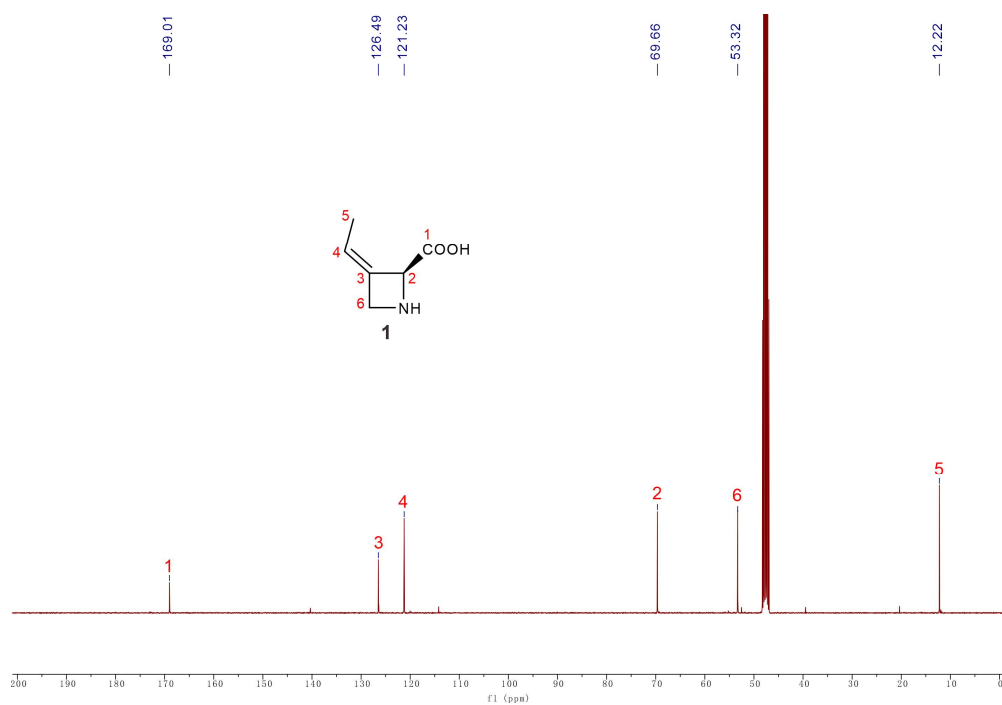
Supplementary Figure 14 | LC-HRMS analysis of POLs produced by *S. aureochromogenes* following $[^{13}\text{C}_6]\text{L}$ -isoleucine enrichment. *S. aureochromogenes* was fermented in 10 ml fermentation medium and $[^{13}\text{C}_6]\text{L}$ -isoleucine (4.0 mg) was pulse fed to the culture twice (at 12 h and 24 h). After fermentation for 3 d, the fermentation sample was subjected to LC-HRMS analysis. **a**, Diagrammatic sketch of feeding $[^{13}\text{C}_6]\text{L}$ -isoleucine to the POLs producing cultures of *S. aureochromogenes*. Theoretically, $[^{13}\text{C}_6]\text{POL-A}$ and $[^{13}\text{C}_6]\text{POL-H}$ could be detected if the labelled $[^{13}\text{C}_6]\text{L}$ -isoleucine can be consumed as a direct precursor. **b**, LC-HRMS spectra of POL-A following feeding with $[^{13}\text{C}_6]\text{L}$ -isoleucine. **c**, LC-HRMS spectra of POL-H following feeding with $[^{13}\text{C}_6]\text{L}$ -isoleucine. **d**, LC-HRMS spectra of POL-B followed feeding with $[^{13}\text{C}_6]\text{L}$ -isoleucine. **e**, LC-HRMS spectra of POL-J following feeding with $[^{13}\text{C}_6]\text{L}$ -isoleucine.



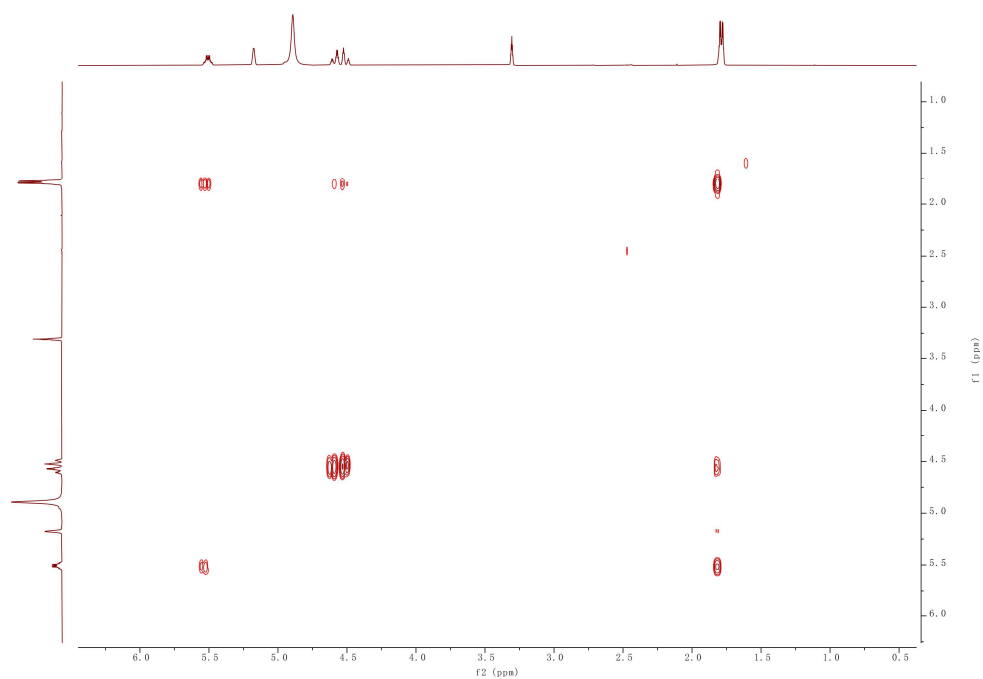
Supplementary Figure 15 | Metabolite analysis of the *E. coli* BL21(DE3) recombinant containing pRSFDuet-1/*polE*+*polF* or pRSFDuet-1/*polF*. a, LC-HRMS analysis of the target metabolite **1 produced by the recombinant of BL21(DE3)/*polE*+*polF*. b, LC-HRMS/MS analysis of the target metabolite **1** produced by the recombinant of BL21(DE3)/*polE*+*polF*. c, LC-HRMS analysis of the target metabolite **1** produced by the recombinant strain of BL21(DE3)/*polF*. d, LC-HRMS/MS analysis of the target metabolite **1** produced by the recombinant strain of BL21(DE3)/*polF*. The theoretical fragmentation pattern of **1** is included as a control.**



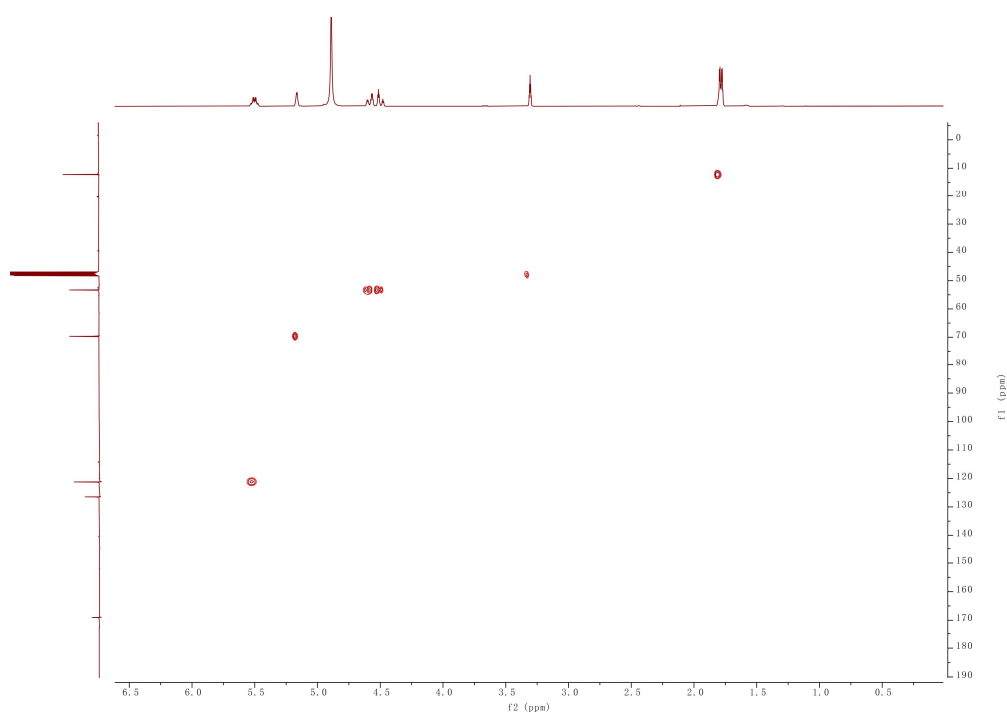
Supplementary Figure 16 | ¹H NMR spectrum of 1 produced by the recombinant BL21(DE3)/*polE+polF* (CD₃OD, 400 MHz).



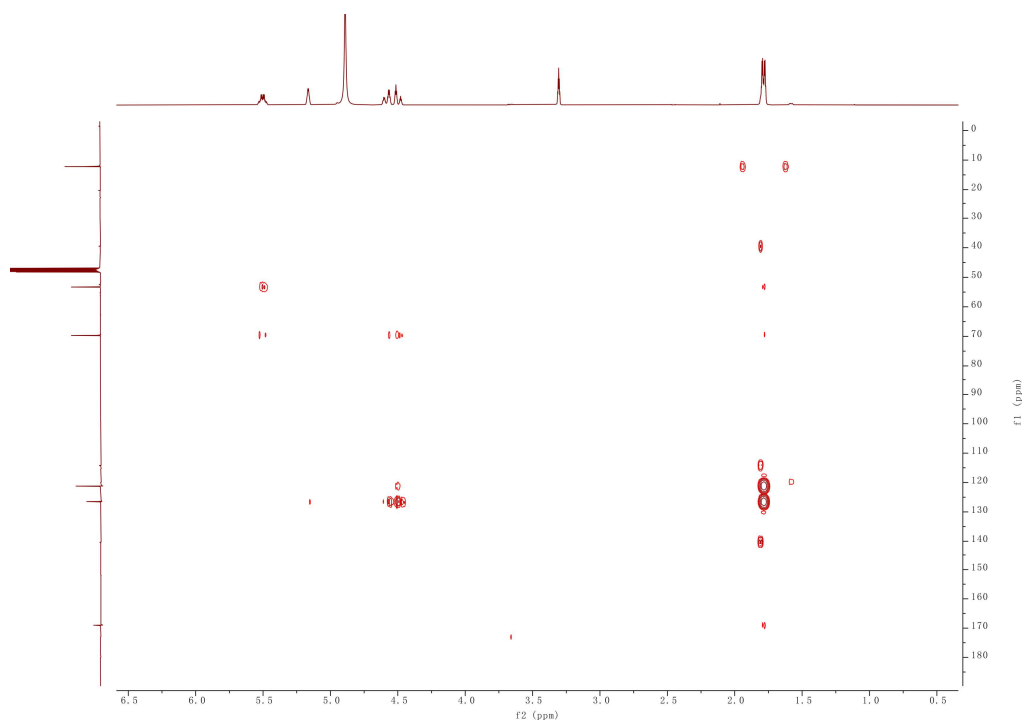
Supplementary Figure 17 | ¹³C NMR spectrum of 1 produced by the recombinant BL21(DE3)/*polE+polF* (CD₃OD, 100 MHz).



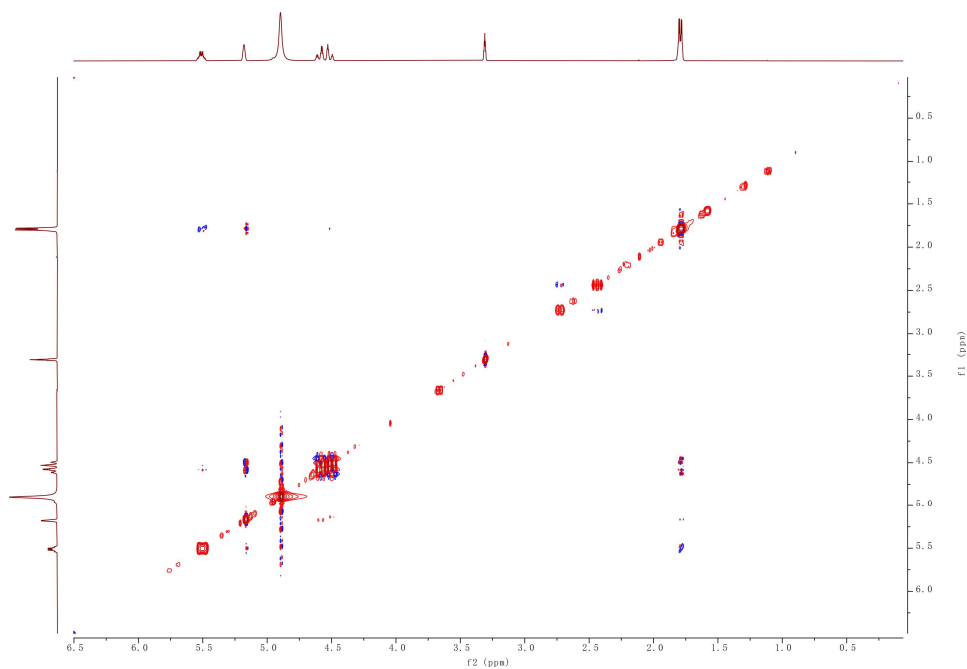
Supplementary Figure 18 | ^1H - ^1H COSY spectrum of **1 produced by the recombinant BL21(DE3)/*polE*+*polF* (CD_3OD , 400 MHz).**



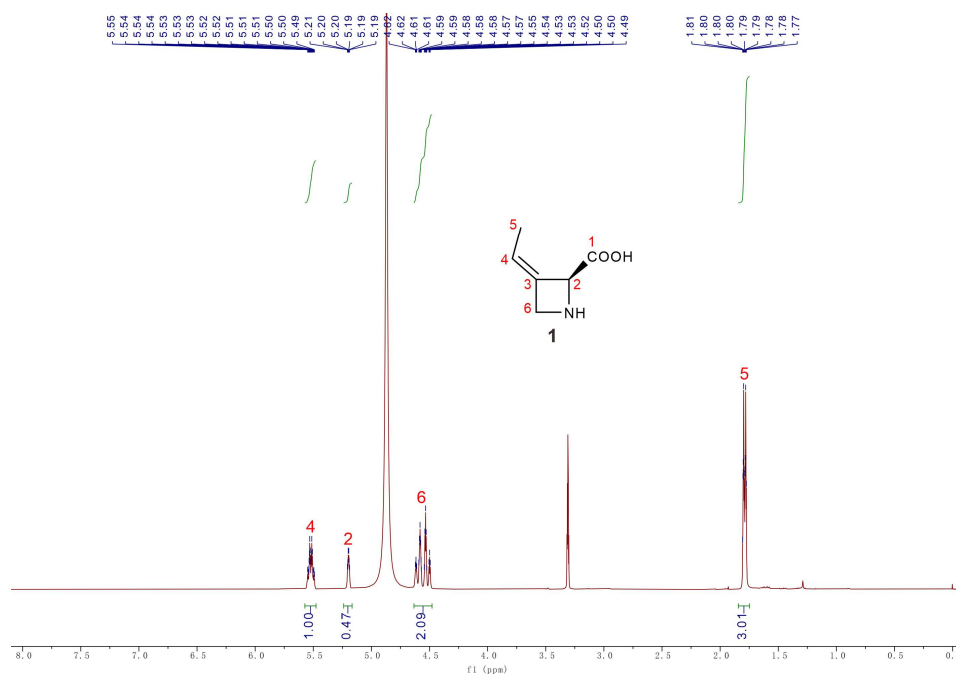
Supplementary Figure 19 | HSQC spectrum of **1 produced by the recombinant BL21(DE3)/*polE*+*polF* (CD_3OD , 400 MHz).**



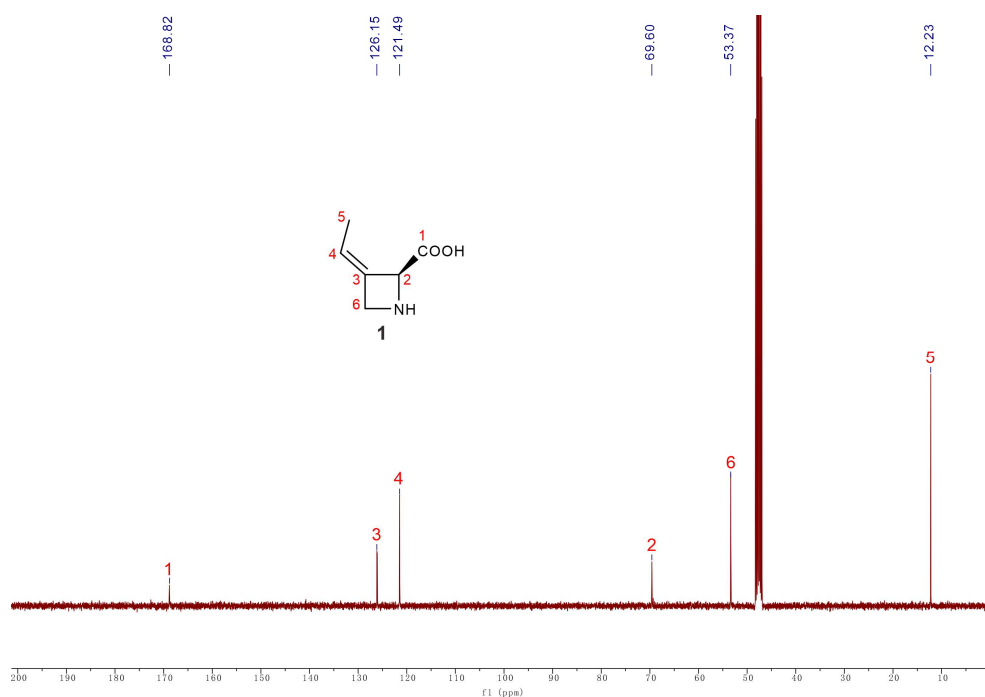
Supplementary Figure 20 | HMBC spectrum of 1 produced by the recombinant BL21(DE3)/*polE*+*polF* (CD₃OD, 400 MHz).



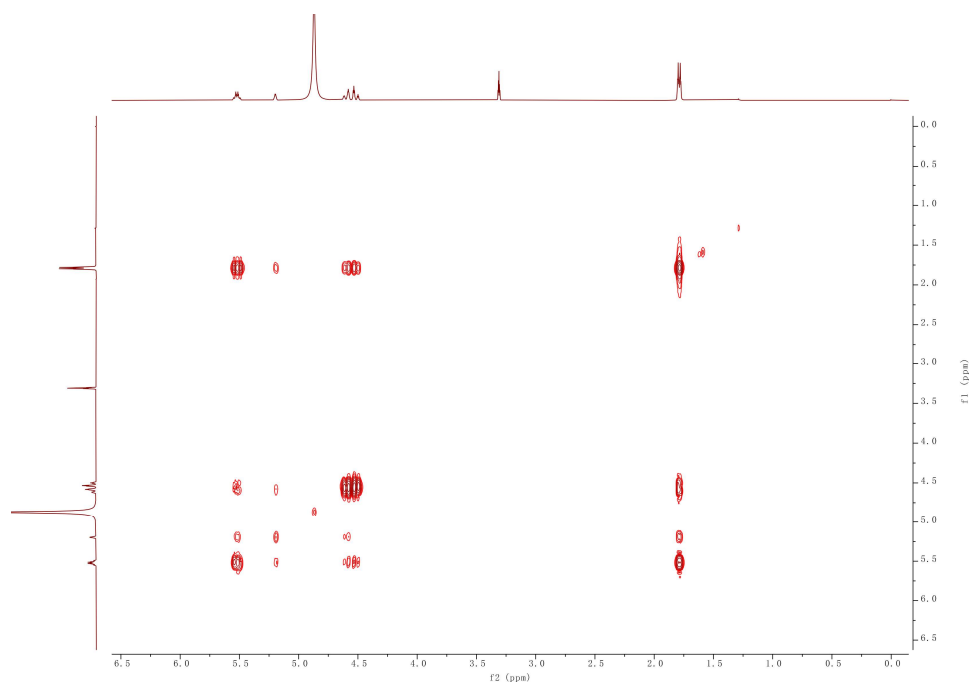
Supplementary Figure 21 | NOESY spectrum of 1 produced by the recombinant BL21(DE3)/*polE*+*polF* (CD₃OD, 400 MHz).



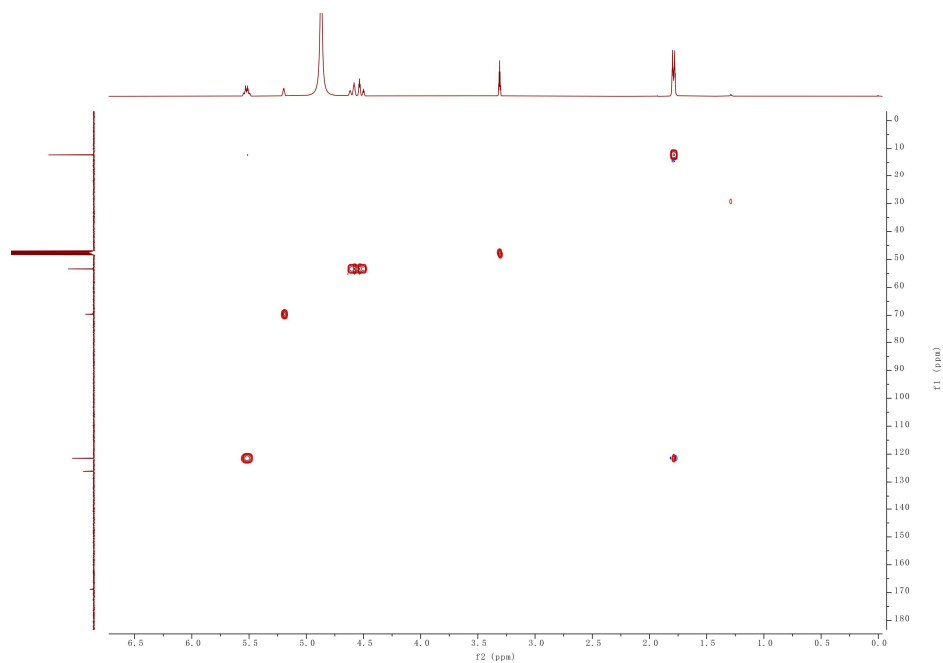
Supplementary Figure 22 | ^1H NMR spectrum of **1 produced by the recombinant BL21(DE3)/*polF* (CD_3OD , 400 MHz).**



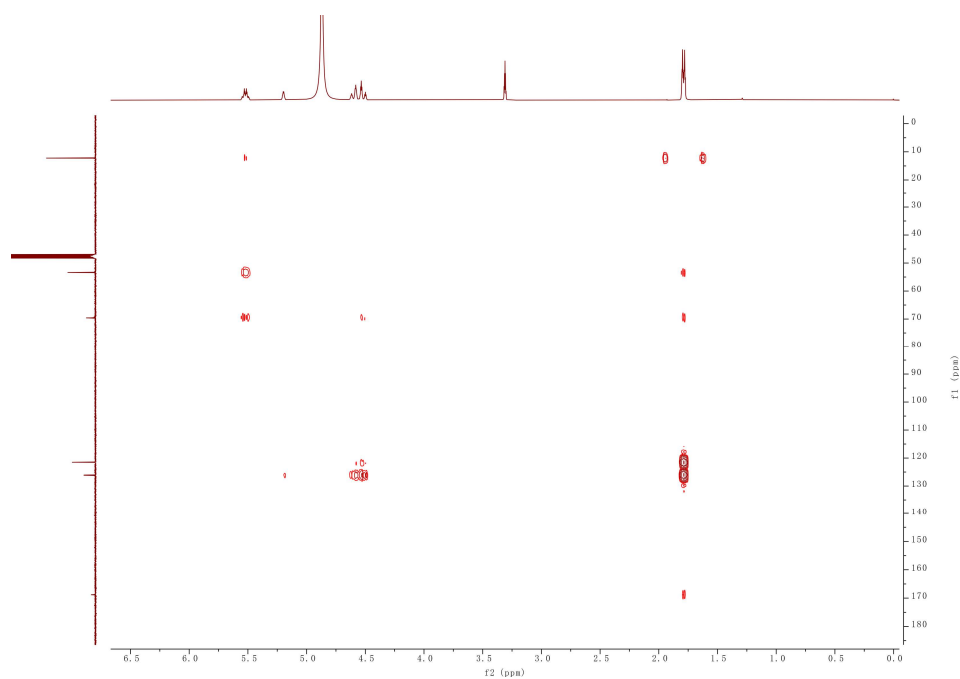
Supplementary Figure 23 | ^{13}C NMR spectrum of **1 produced by the recombinant BL21(DE3)/*polF* (CD_3OD , 100 MHz).**



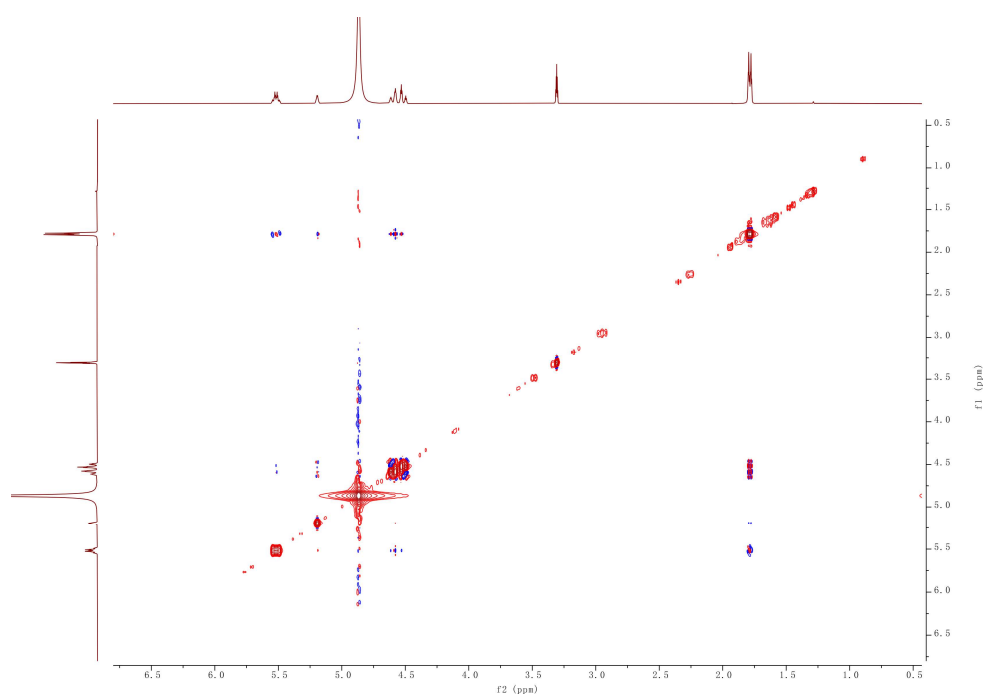
Supplementary Figure 24 | ^1H - ^1H COSY spectrum of 1 produced by the recombinant BL21(DE3)/*polF* (CD_3OD , 400 MHz).



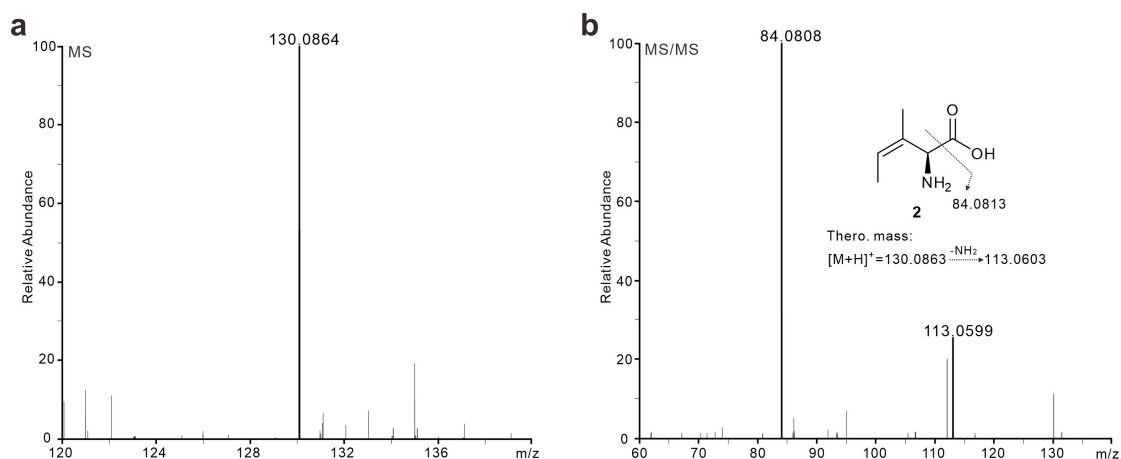
Supplementary Figure 25 | HSQC spectrum of 1 produced by the recombinant BL21(DE3)/*polF* (CD_3OD , 400 MHz).



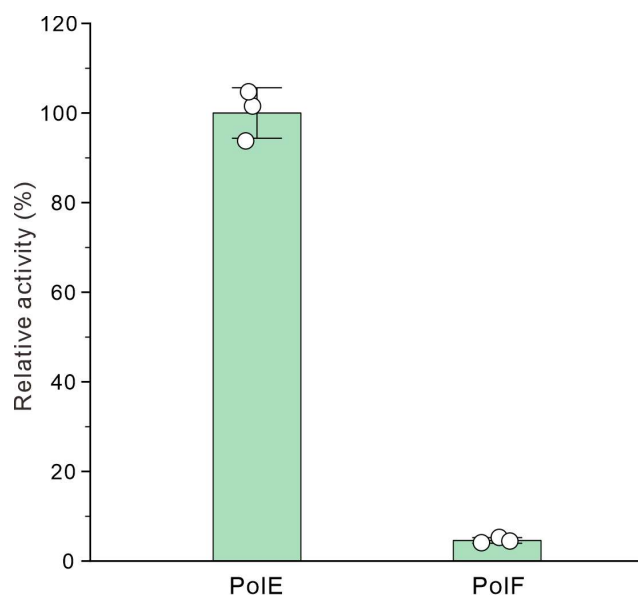
Supplementary Figure 26 | HMBC spectrum of 1 produced by the recombinant BL21(DE3)/*polF* (CD₃OD, 400 MHz).



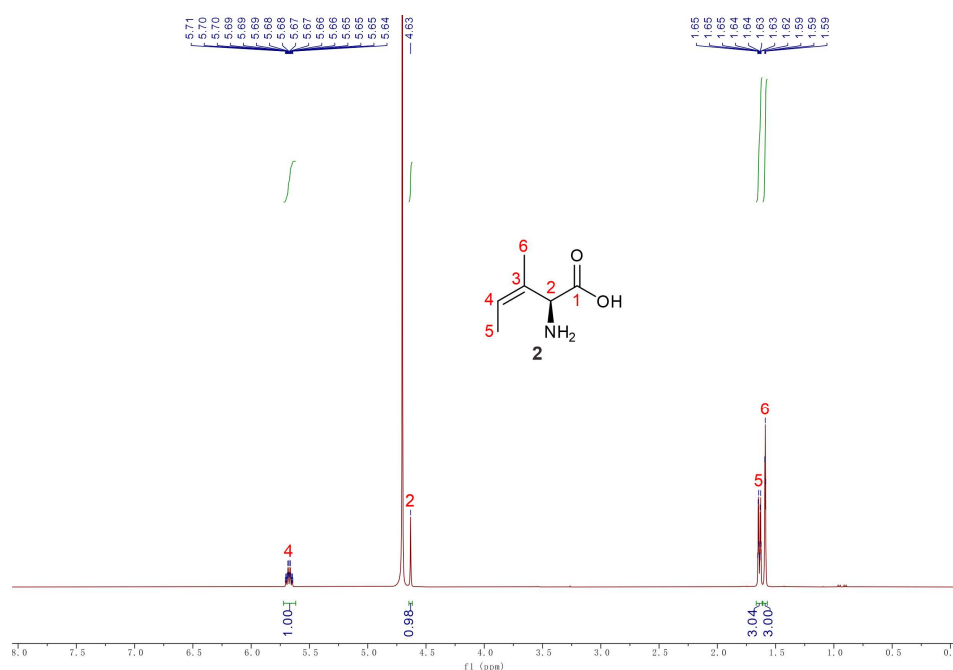
Supplementary Figure 27 | NOESY spectrum of 1 produced by the recombinant BL21(DE3)/*polF* (CD₃OD, 400 MHz).



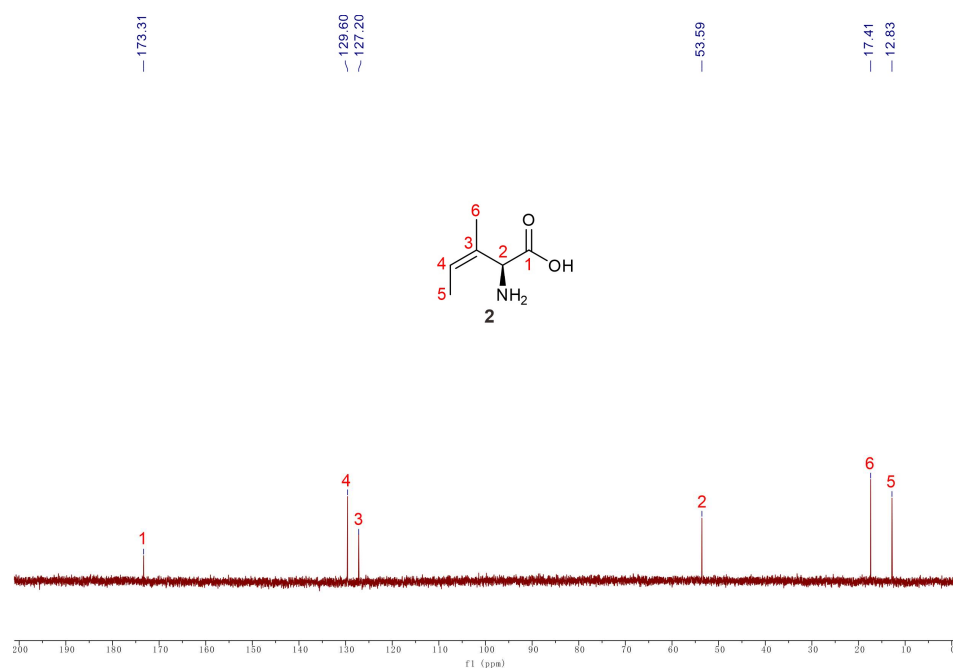
Supplementary Figure 28 | Metabolite analysis of the *E. coli* BL21(DE3) recombinant containing pRSFDuet-1/*polE*. **a**, LC-HRMS analysis of the target metabolite (**2**) produced by the recombinant of BL21(DE3)/*polE*. **b**, LC-HRMS/MS analysis of the target metabolite (**2**) produced by the recombinant of BL21(DE3)/*polE*. The theoretical fragmentation pattern of **2** is included as a control.



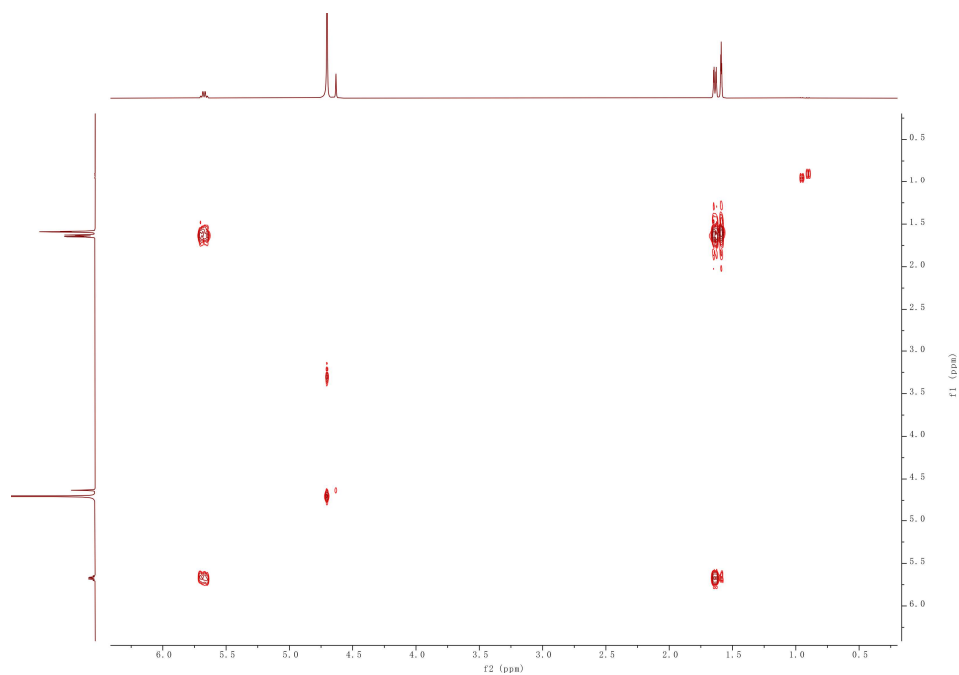
Supplementary Figure 29 | Relative activity analysis of PolE and PolF *in vivo* toward L-isoleucine. The yield ratio of the target product, corresponding to individual protein expression level, represents the relative activity. Source data is provided as a Source Data file.



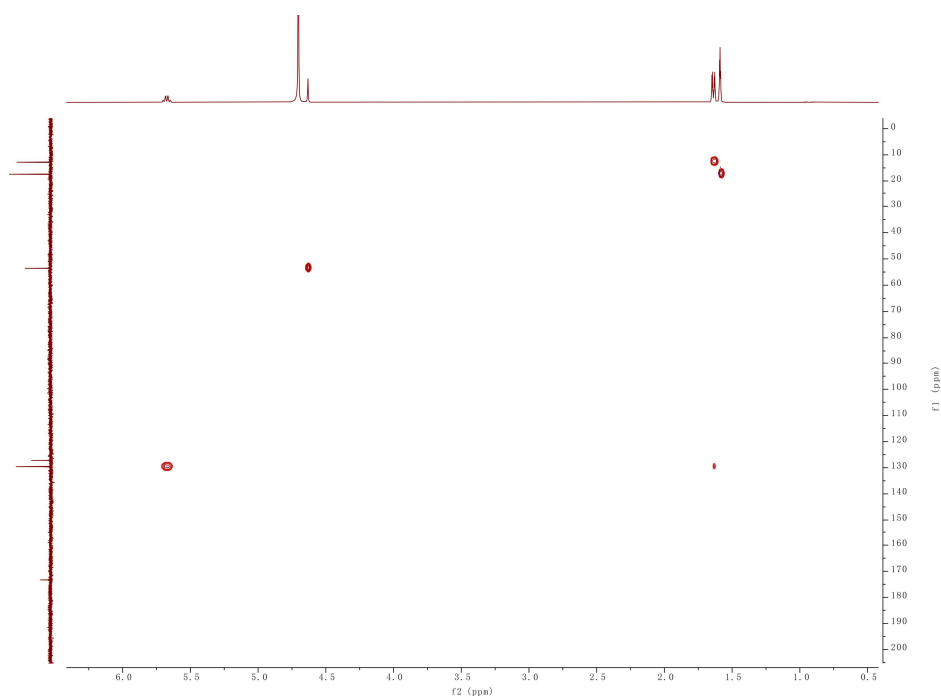
Supplementary Figure 30 | ¹H NMR spectrum of 2 produced by the recombinant BL21(DE3)/*polE* (D₂O, 400 MHz).



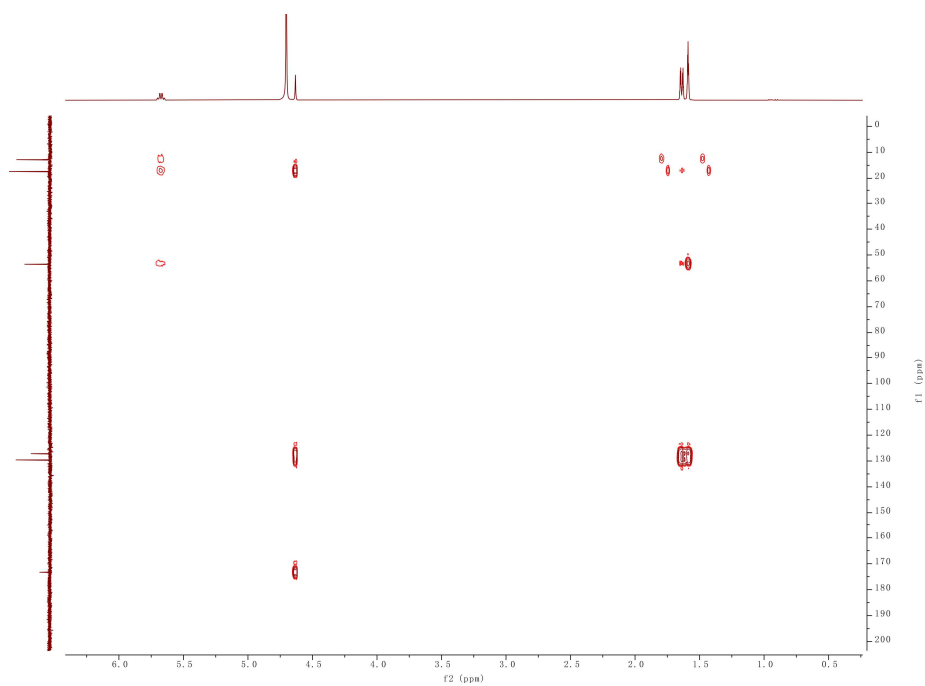
Supplementary Figure 31 | ¹³C NMR spectrum of 2 produced by the recombinant BL21(DE3)/*polE* (D₂O, 100 MHz).



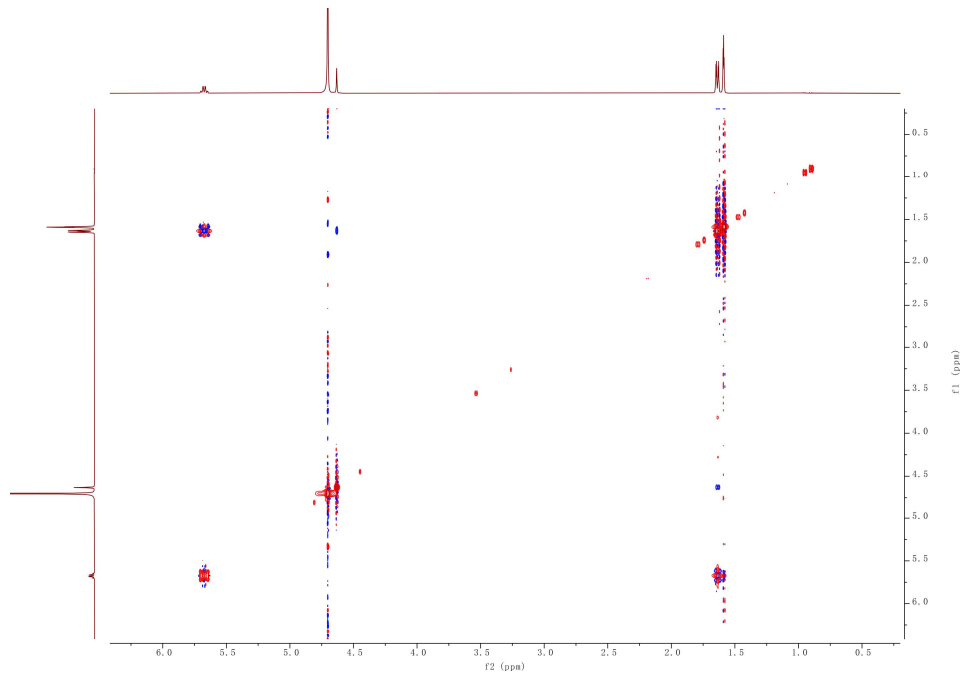
Supplementary Figure 32 | ^1H - ^1H COSY spectrum of **2 produced by the recombinant BL21(DE3)/*polE* (D_2O , 400 MHz).**



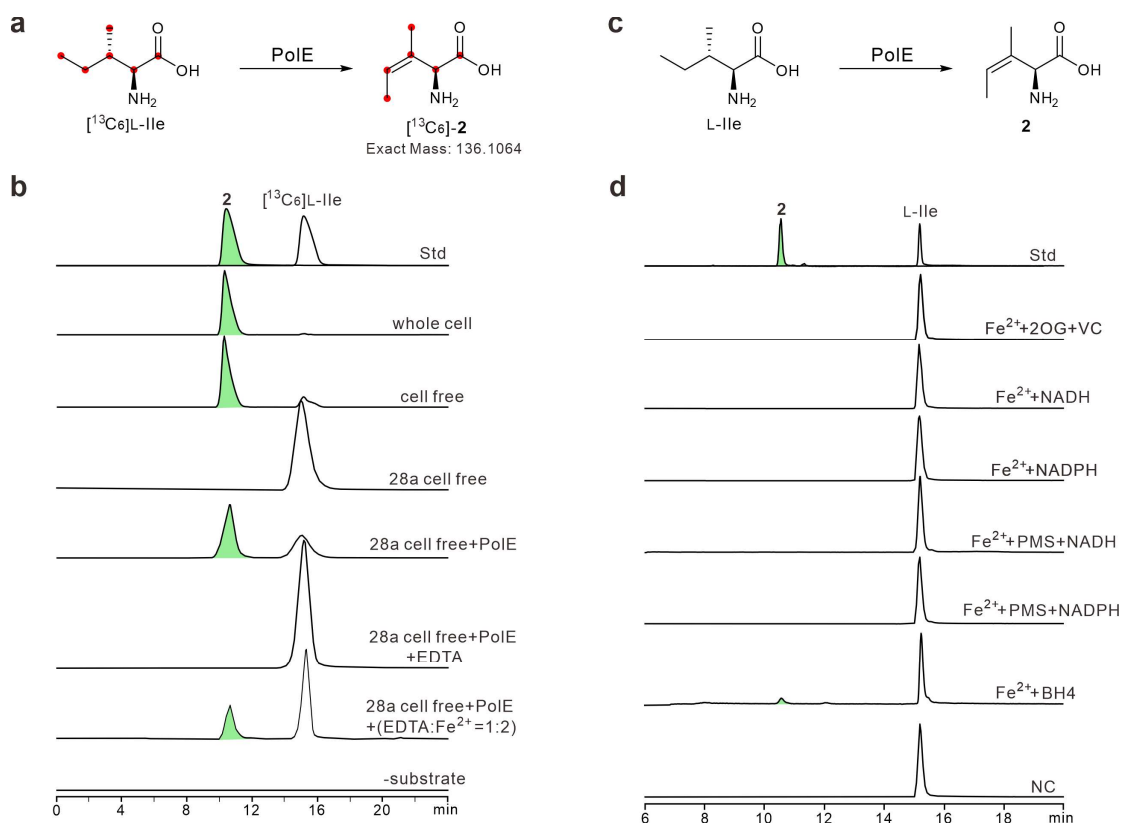
Supplementary Figure 33 | HSQC spectrum of **2 produced by the recombinant BL21(DE3)/*polE* (D_2O , 400 MHz).**



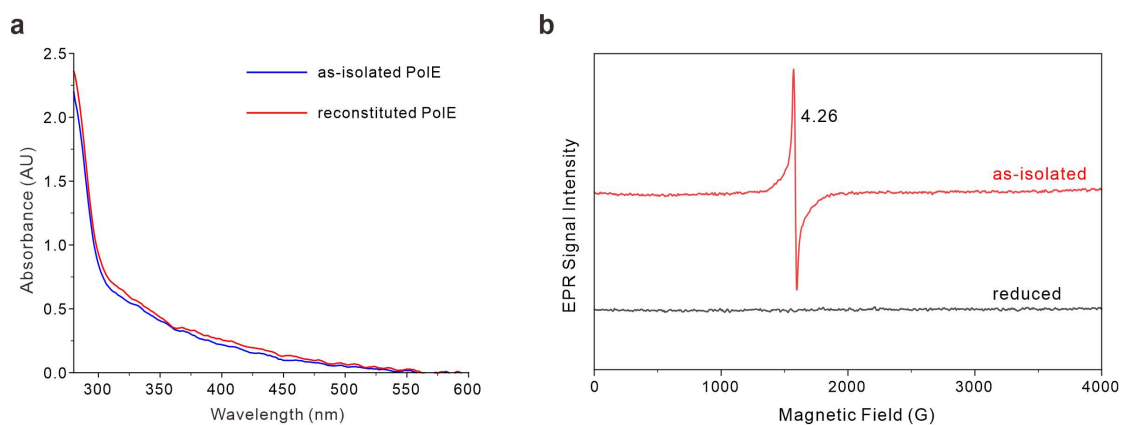
Supplementary Figure 34 | HMBC spectrum of 2 produced by the recombinant BL21(DE3)/*polE* (D₂O, 400 MHz).



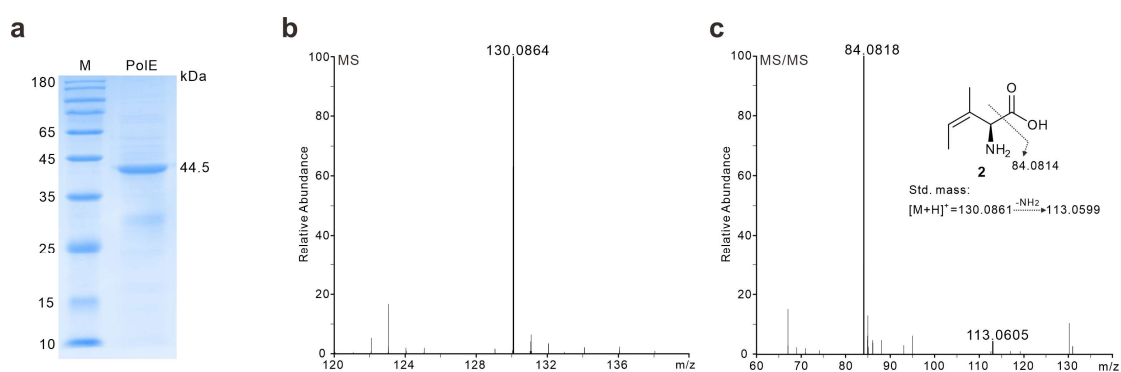
Supplementary Figure 35 | NOESY spectrum of 2 produced by the recombinant BL21(DE3)/*polE* (D₂O, 400 MHz).



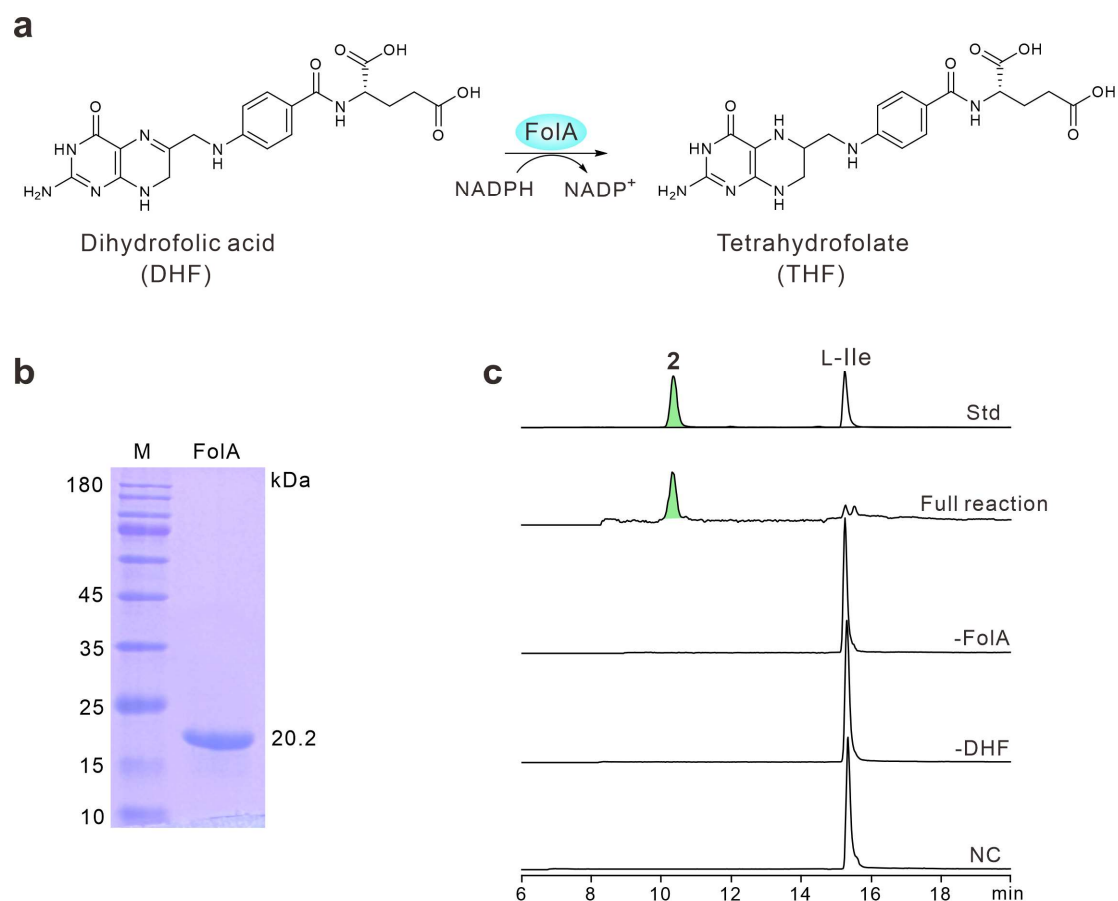
Supplementary Figure 36 | Reconstitution of PolE activity in a cell-free or cofactor-specific system. **a**, Schematic of the cell-free reaction catalyzed by PolE with $[^{13}\text{C}_6]$ L-isoleucine as substrate. **b**, LC-HRMS analysis of the PolE cell-free reactions. Std, the authentic $[^{13}\text{C}_6]$ L-isoleucine and compound 2 standards; whole cell, the reaction with adding the whole cell of BL21(DE3)/*polE*; cell free, the reaction with adding supernatant of BL21(DE3)/*polE*; 28a cell free, the reaction with adding supernatant of BL21(DE3)/pET28a as negative control; 28a cell free+PolE, the reaction with adding supernatant of BL21(DE3)/pET28a and the purified PolE; 28a cell free+PolE+EDTA, the reaction with adding supernatant of BL21(DE3)/pET28a, purified PolE, and EDTA (20 μM); 28a cell free+PolE+(EDTA:Fe²⁺=1:2), the reaction with adding supernatant of BL21(DE3)/pET28a, purified PolE, EDTA (20 μM), and Fe²⁺ (40 μM); -substrate, the reaction without $[^{13}\text{C}_6]$ L-isoleucine added as negative control (but with adding supernatant of BL21(DE3)/*polE*). For all reactions in this panel, 100 μl reaction containing 30 μM $[^{13}\text{C}_6]$ L-isoleucine, 20 μM Fe²⁺, and 20 μM purified PolE. **c**, Schematic of PolE reaction with L-isoleucine as substrate. **d**, LC-HRMS analysis of the PolE reaction against diverse cofactors. The results suggested that the cofactor BH₄ is essentially required for PolE activity.



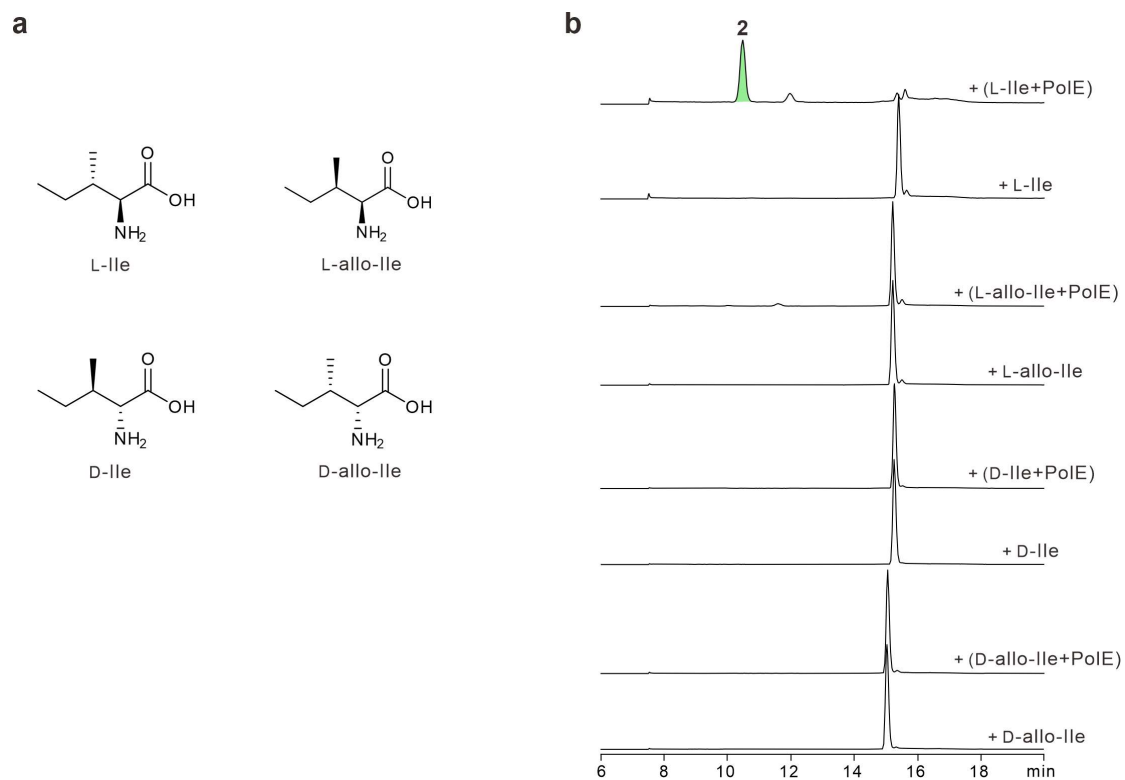
Supplementary Figure 37 | The UV-Visible absorbance spectrum and EPR spectrum of PoIE. a, The UV-Visible absorbance spectrum of as-isolated and reconstituted PoIE. **b,** EPR characterization of as-isolated and sodium dithionite reduced PoIE.



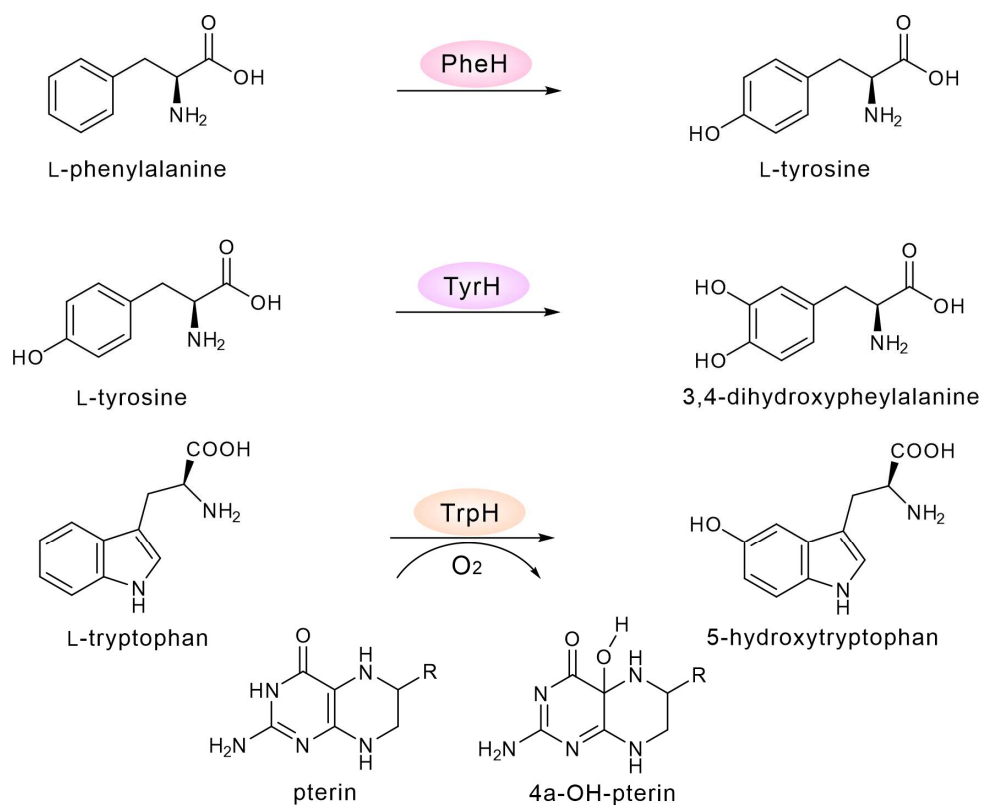
Supplementary Figure 38 | SDS-PAGE analysis of PoIE and LC-HRMS analysis of PoIE reaction. a, SDS-PAGE analysis of PoIE. Source data is provided as a Source Data file. **a,** LC-HRMS analysis of the PoIE reaction. **c,** LC-HRMS/MS analysis of the PoIE reaction. The fragmentation pattern of **2** standard is included as a control.



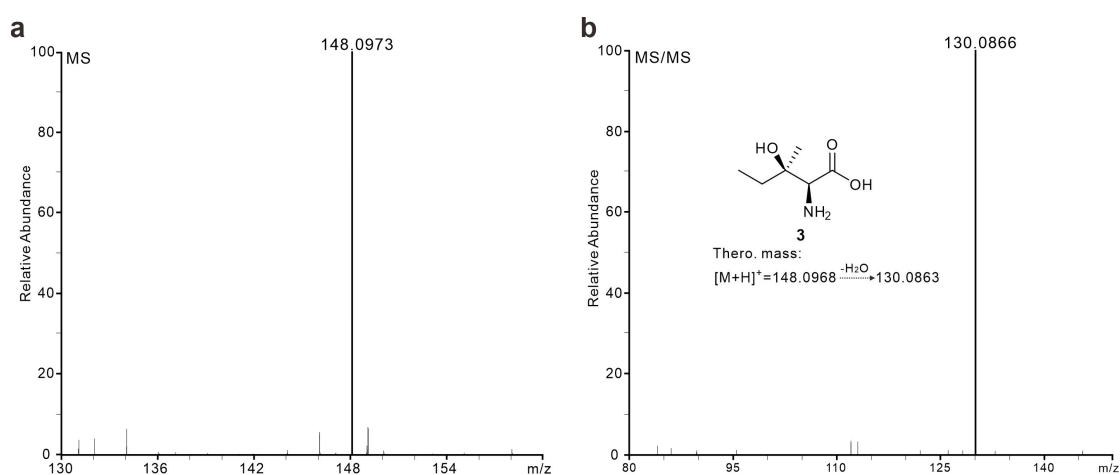
Supplementary Figure 39 | DHF reductase is capable of supporting PolE activity via regeneration of THF. **a**, Schematic of the reaction catalyzed by FolA. Dihydrofolate (DHF) reductase FolA (GenBank: CP001509.3) from *E. coli* BL21(DE3) catalyzes THF regeneration by reduction of dihydrofolate (DHF) with NADPH as cofactor. **b**, SDS-PAGE analysis of FolA (20.2 kDa). Source data is provided as a Source Data file. **c**, LC-HRMS analysis of the PolE reactions with addition of DHF and FolA. Std, the authentic L-isoleucine and **2** standards; Full reaction, the reaction with PolE, Fe^{2+} , DHF, NADPH, and FolA added; -FolA, the reaction without FolA added; -DHF, the reaction without DHF added; NC, the reaction without PolE added as negative control.



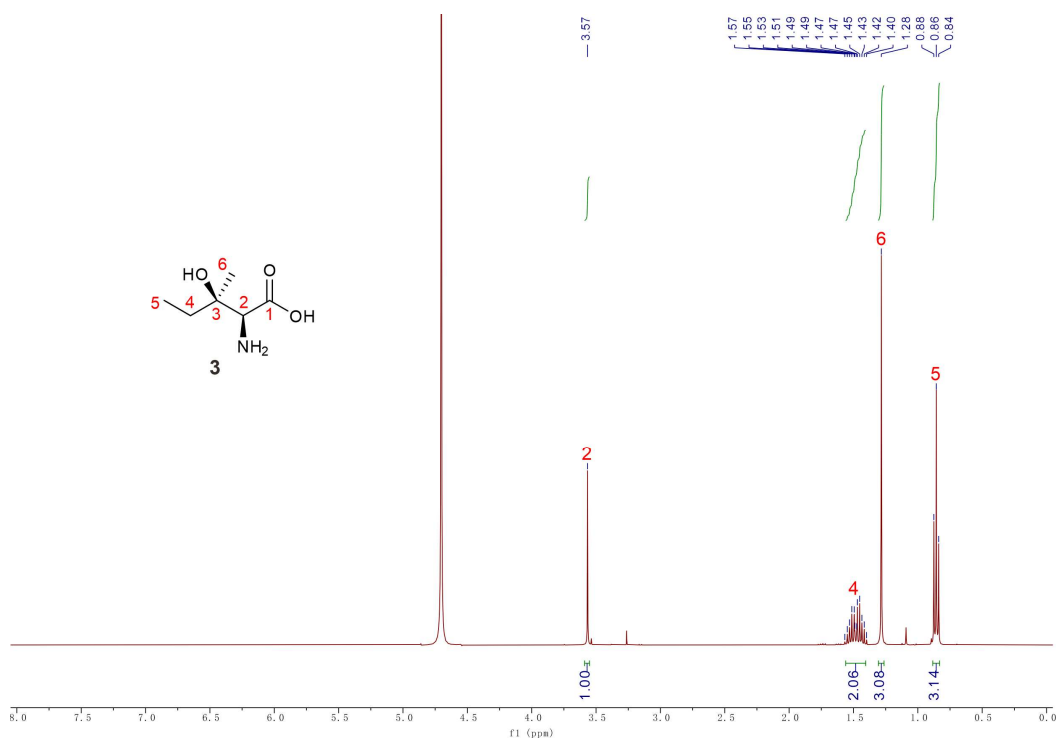
Supplementary Figure 40 | LC-HRMS analysis of the PolE reaction with different stereoisomers as substrate. a, Structure of related stereoisomers used as substrate. b, LC-HRMS analysis of the PolE activity using related isoleucine stereoisomers as substrate.



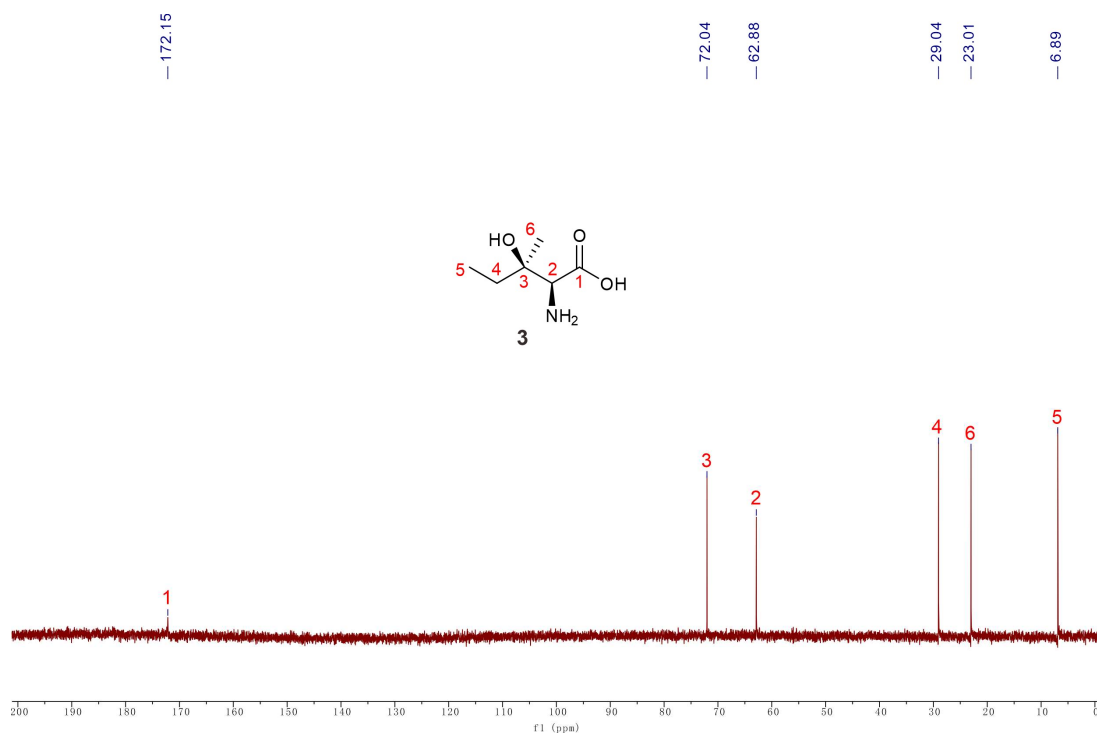
Supplementary Figure 41 | The reactions catalyzed by pterin-dependent aromatic amino acid hydroxylases.



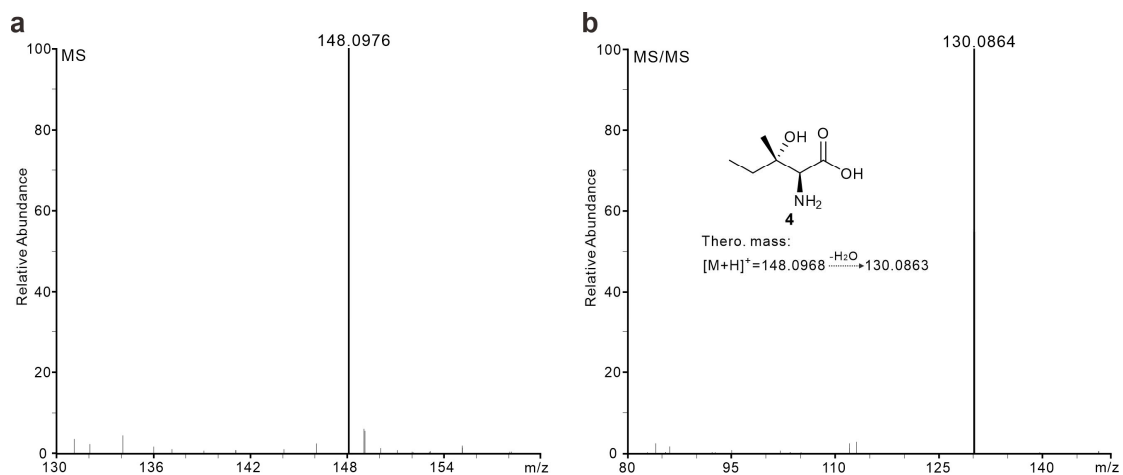
Supplementary Figure 42 | LC-HRMS analysis of the chemically-synthesized compound 3. a, LC-HRMS analysis of the compound 3. b, LC-HRMS/MS analysis of the compound 3. The theoretical fragmentation pattern of 3 is included as a control.



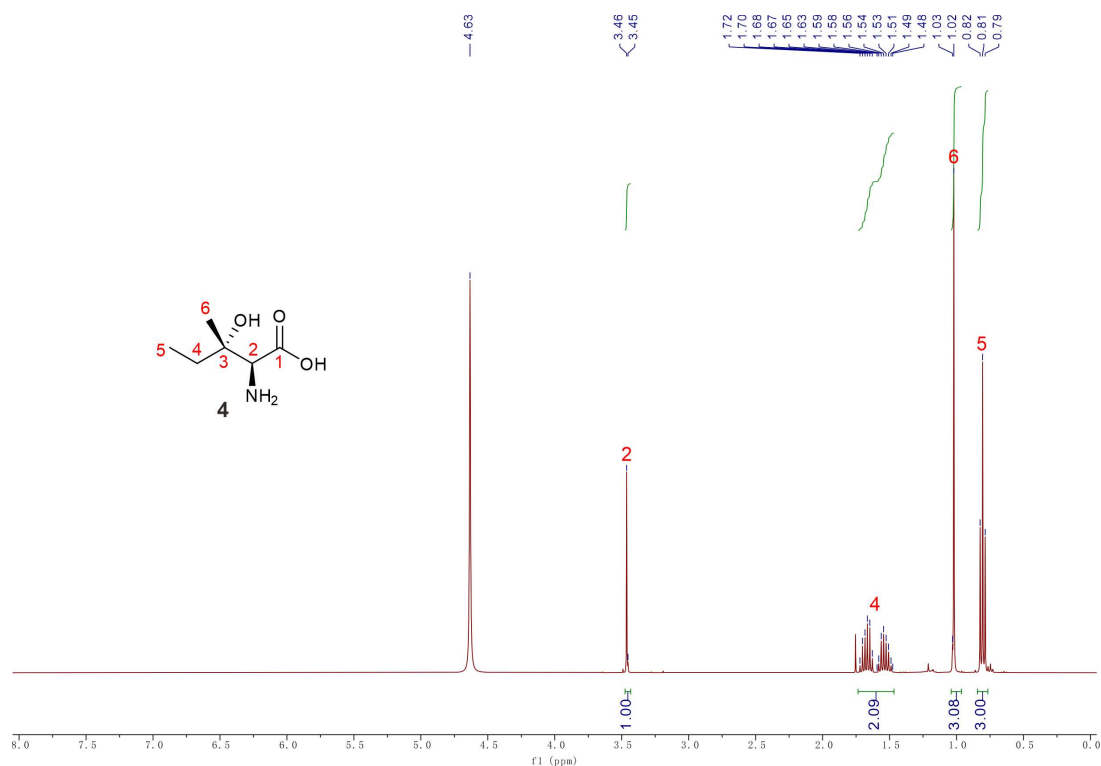
Supplementary Figure 43 | ¹H NMR spectrum of compound 3 (D₂O, 400 MHz).



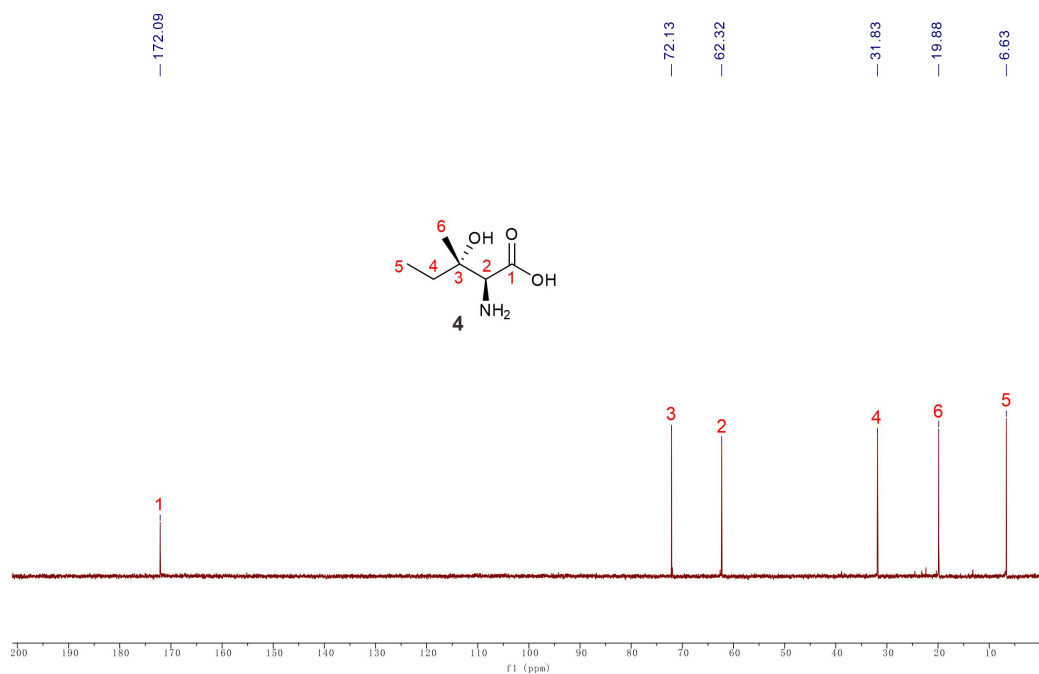
Supplementary Figure 44 | ¹³C NMR spectrum of compound 3 (D₂O, 100 MHz).



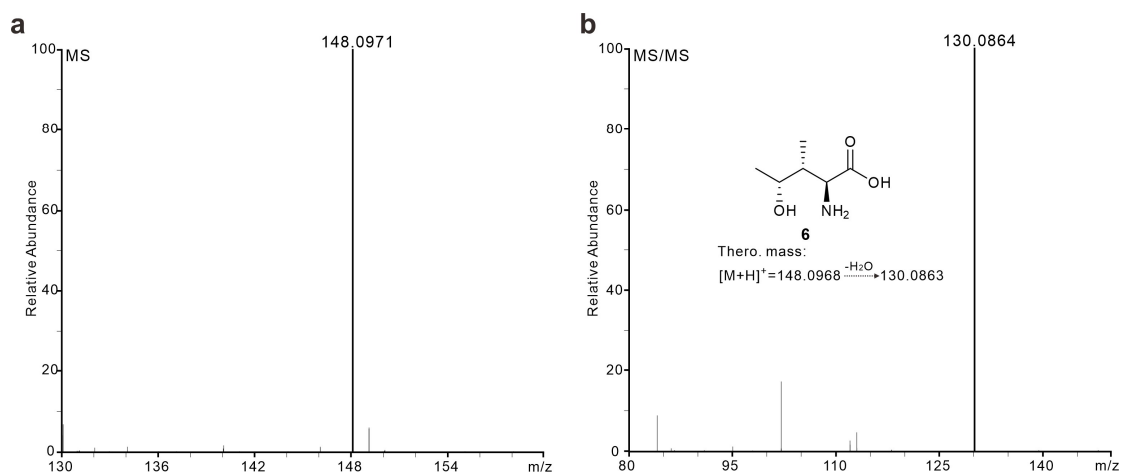
Supplementary Figure 45 | LC-HRMS analysis of the chemically-synthesized compound 4. **a**, LC-HRMS analysis of compound **4**. **b**, LC-HRMS/MS analysis of compound **4**. The theoretical fragmentation pattern of **4** is included as a control.



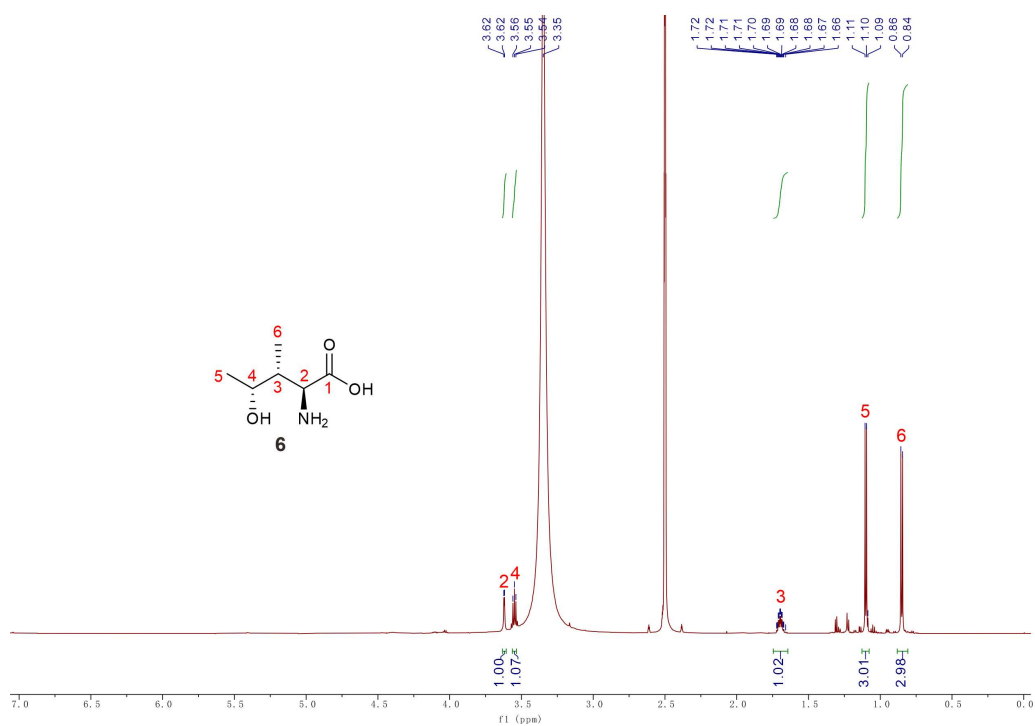
Supplementary Figure 46 | ¹H NMR spectrum of compound 4 (D₂O, 400 MHz).



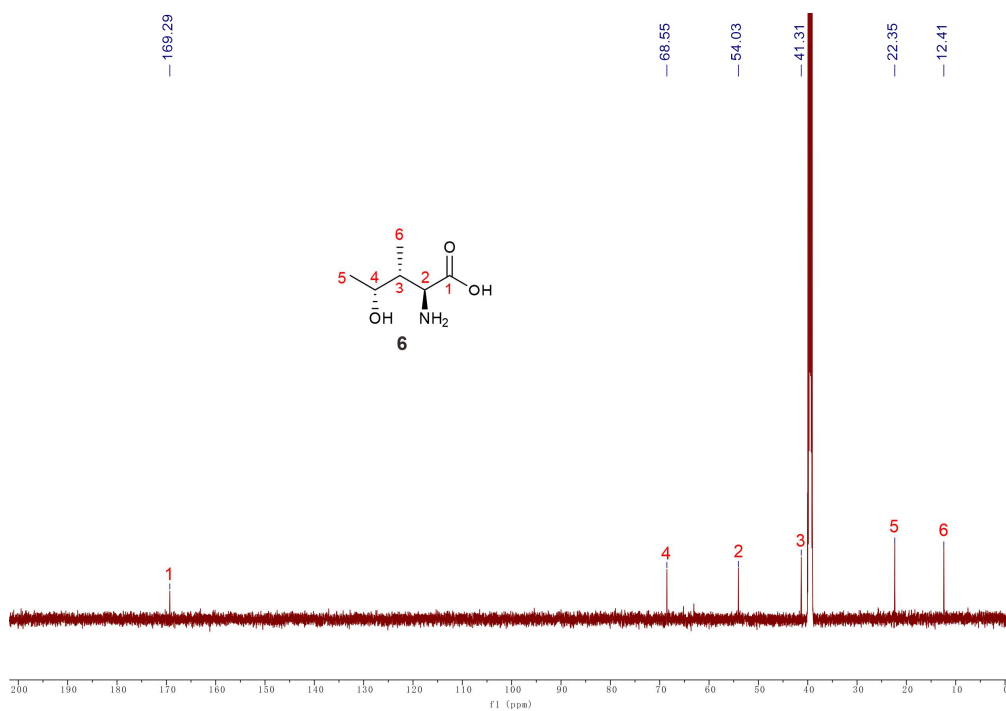
Supplementary Figure 47 | ¹³C NMR spectrum of compound 4 (D₂O, 100 MHz).



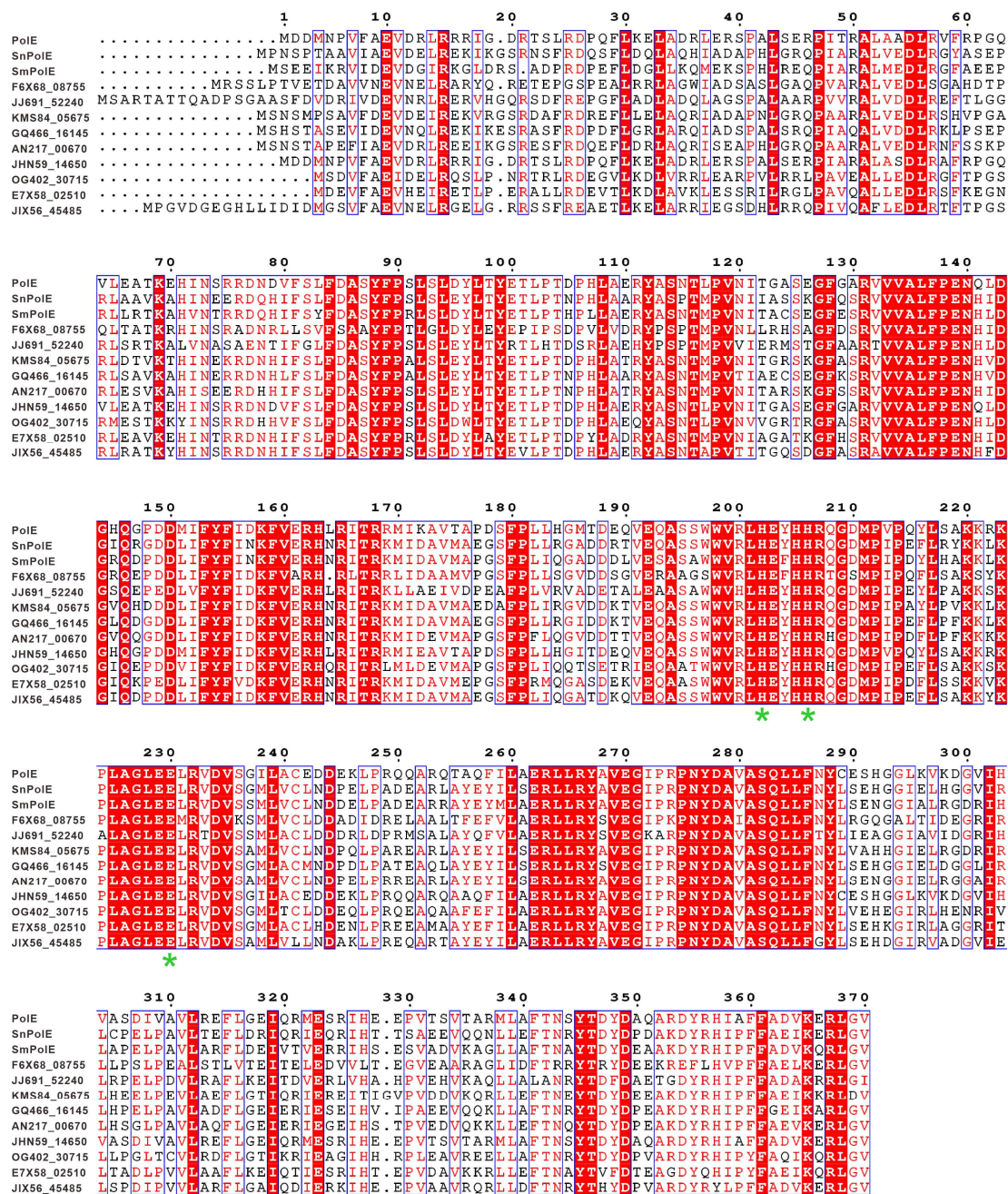
Supplementary Figure 48 | LC-HRMS analysis of the chemically-synthesized compound 6. a, LC-HRMS analysis of compound 6. b, LC-HRMS/MS analysis of compound 6. The theoretical fragmentation pattern of 6 is included as a control.



Supplementary Figure 49 | ¹H NMR spectrum of compound 6 (DMSO-d₆, 400 MHz).

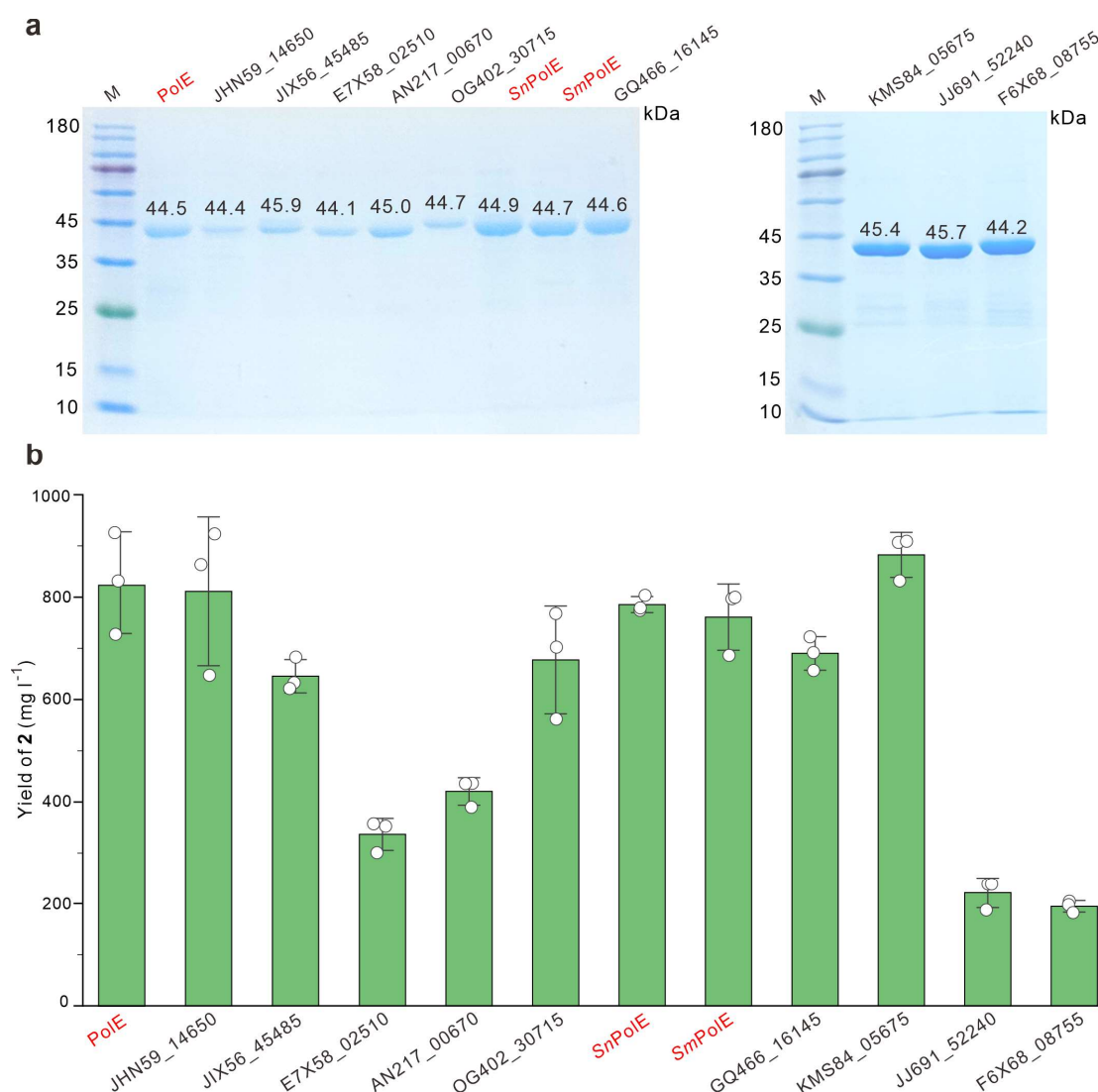


Supplementary Figure 50 | ¹³C NMR spectrum of compound 6 (DMSO-d₆, 100 MHz).

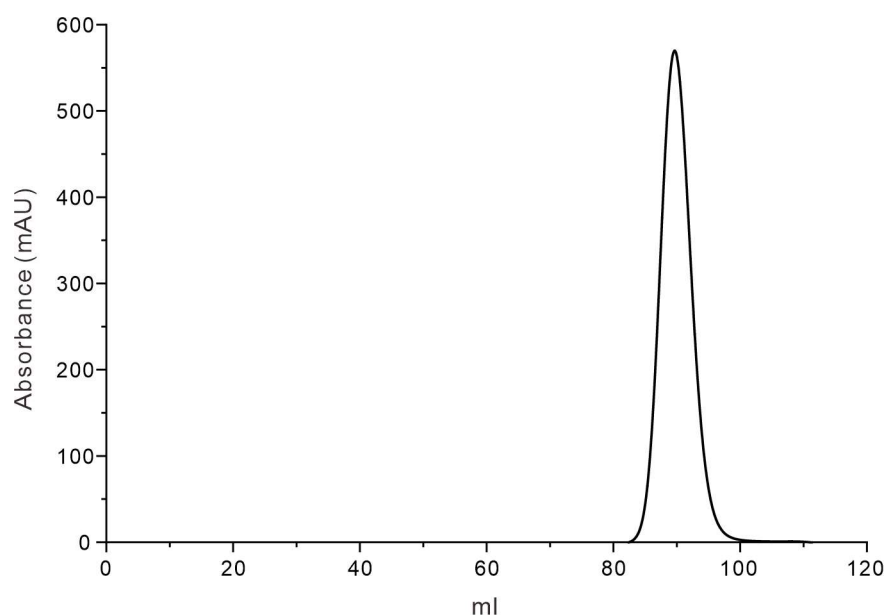


Supplementary Figure 51 | Sequence alignment of PoIE and its homologs. BlastP analysis indicates that PoIE belongs to DUF6421 (unknown function) family proteins. Sequence alignment of PoIE and its homologs was performed using ESPrpt 3.0. The following proteins are included: PoIE (GenBank: AFP55317.1) is from *Streptomyces aureochromogenes*, SnPoIE (C1197_07030, GenBank: PZH16170.1) is from *Streptomyces* sp. NTH33, SmPoIE (EAO71_13070, GenBank: TXS29575.1) is from *Streptomyces* sp. ms191, F6X68_08755 (GenBank: KAB1159241.1) is from *Micromonospora* sp. AMSO12t, JJ691_52240 (GenBank: QUQ67489.1) is from *Kutzneria* sp. CA-103260, KMS84_05675 (GenBank: MCQ9130297.1)

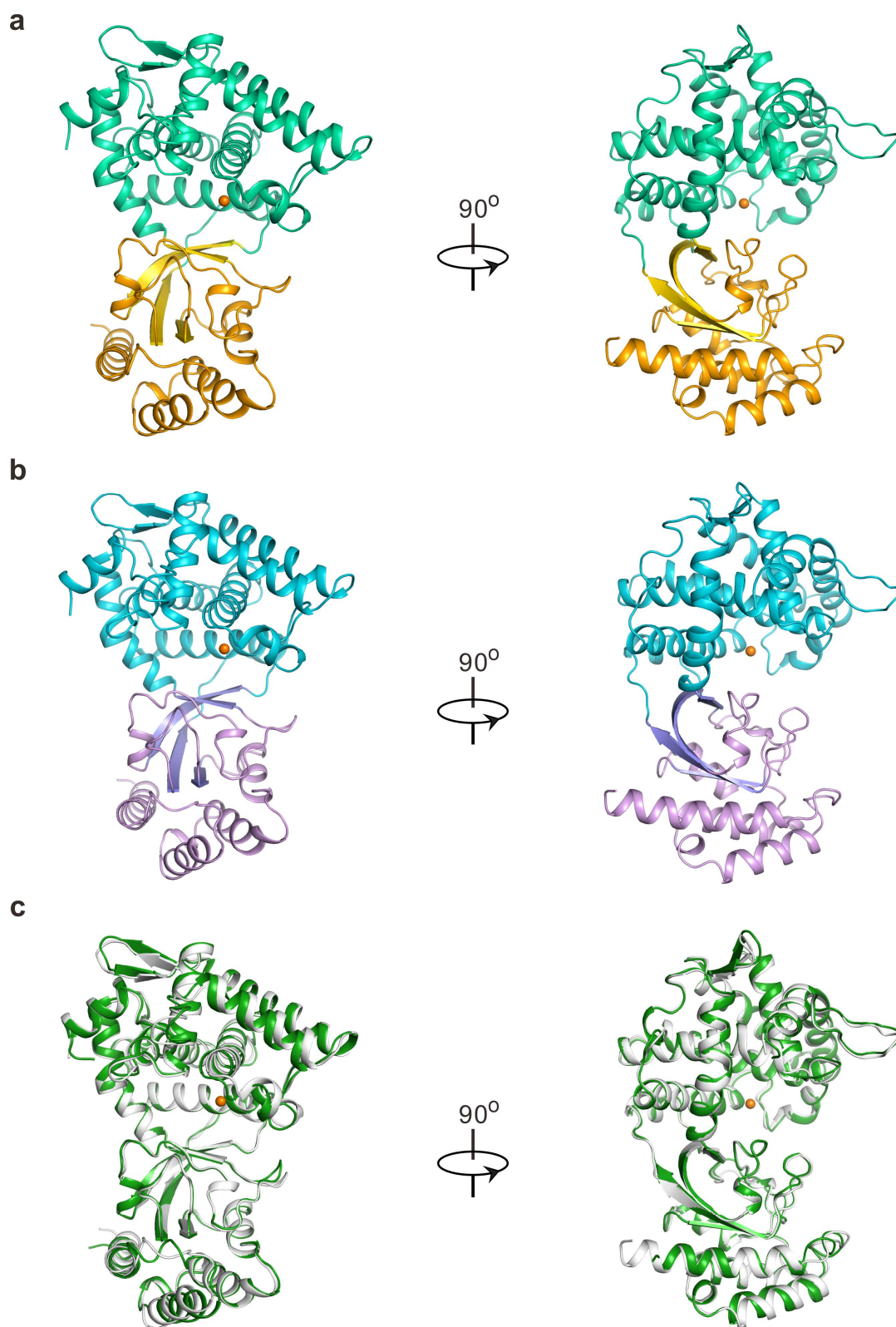
is from *Streptomyces hilarionis*, GQ466_16145 (GenBank: MXQ65560.1) is from *Actinomadura rayongensis*, AN217_00670 (GenBank: OEV01853.1) is from *Streptomyces qinglanensis*, JHN59_14650 (GenBank: MBK3626065.1) is from *Streptomyces* sp. MBT49, OG402_30715 (GenBank: MCX4604840.1) is from *Streptomyces anulatus*, E7X58_02510 (GenBank: THC55197.1) is from *Streptomyces* sp. A1499, and JIX56_45485 (GenBank: UUU36498.1) is from *Streptomyces* sp. CA-210063. The conserved iron binding sites are highlighted by green asterisk.



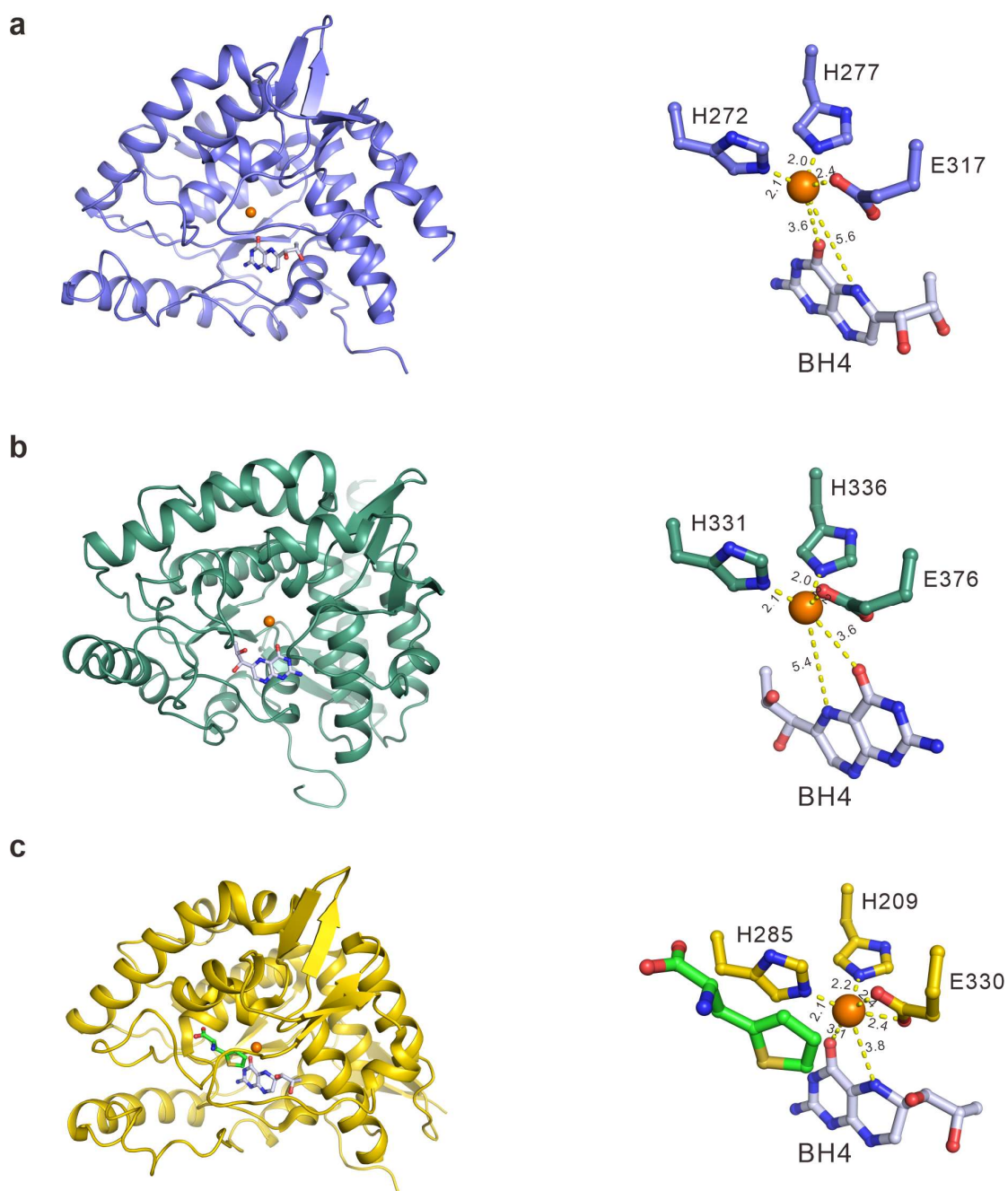
Supplementary Figure 52 | SDS-PAGE analysis of *polE*-related proteins and metabolite analysis of *polE*-related *E. coli* recombinants. **a**, Soluble protein-yield purified from *E. coli* BL21(DE3), including *polE*, JHN59_14650, JIX56_45485, E7X58_02510, AN217_00670, OG402_30715, *SnPolE*, *SmPolE*, GQ466_16145, KMS84_05675, JJ691_52240, and F6X68_08755, was about 4.0 mg l⁻¹, 2.0 mg l⁻¹, 1.4 mg l⁻¹, 4.8 mg l⁻¹, 1.9 mg l⁻¹, 0.6 mg l⁻¹, 13.6 mg l⁻¹, 7.0 mg l⁻¹, 1.7 mg l⁻¹, 6.8 mg l⁻¹, 11.2 mg l⁻¹, and 4.4 mg l⁻¹, respectively. Source data is provided as a Source Data file. **b**, Comparative analysis of *polE* and its homologous genes *in vivo*. For related recombinants of *E. coli* BL21(DE3) containing *polE* or its homologous genes, the yields of compound 2 indicate obvious difference. The error bars represent the $\pm$ s.d. from three different experiments. Source data is provided as a Source Data file.



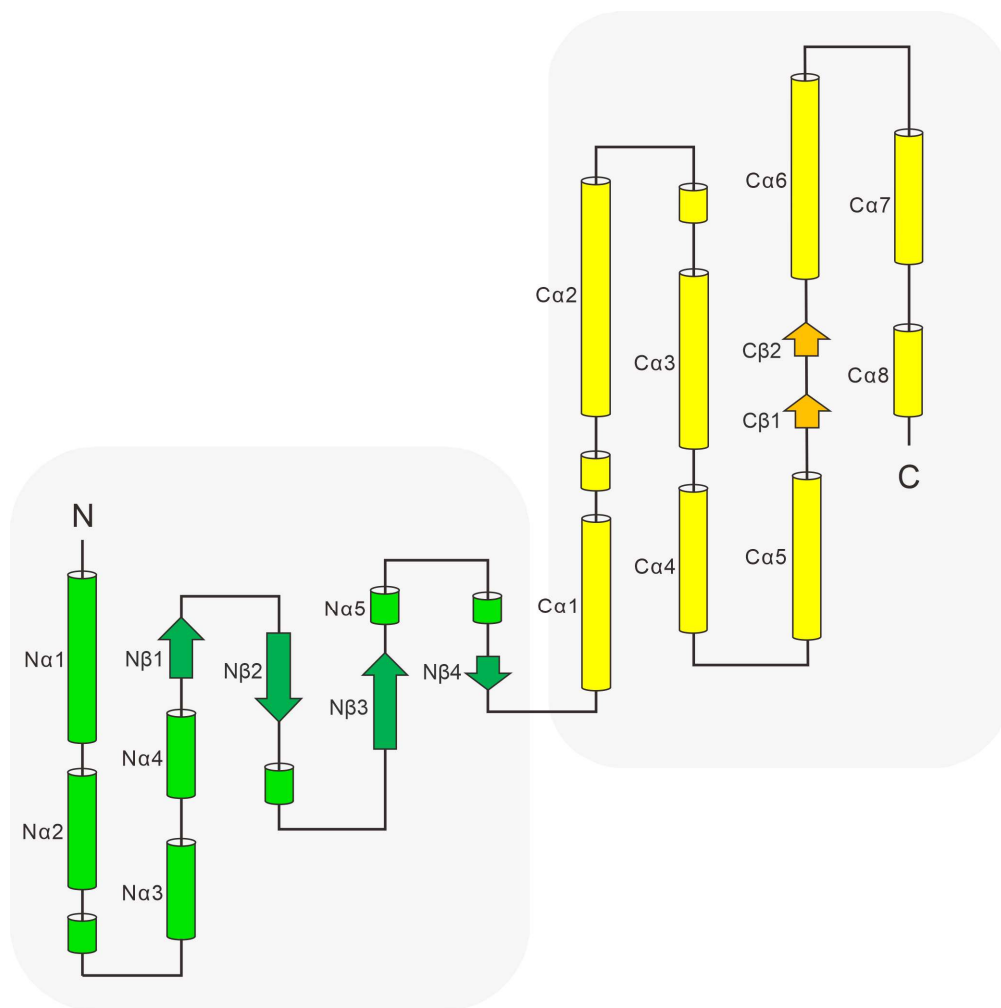
Supplementary Figure 53 | Size exclusion chromatography of *SnPolE* as a monomer in solution. Size exclusion chromatography of *SnPolE* indicates the protein is a monomer in solution (20 mM Tris-HCl, 300 mM NaCl, pH 8.0). *SnPolE* elutes at 89 ml on a HiLoad 16/600 Superdex™ 200 pg column (GE Healthcare), corresponding to an apparent molecular weight of 45 kDa. The value is consistent with the calculated MW (44.9 kDa) of the *SnPolE* monomer.



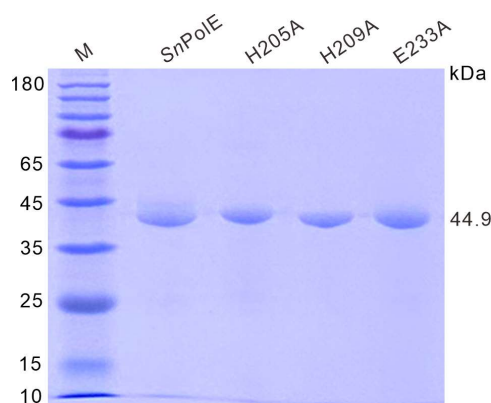
Supplementary Figure 54 | Structures comparison of *SnPolE* and *SmPolE*. **a**, The *apo* structure of *SnPolE*. **b**, The *apo* structure of *SmPolE*. **c**, Comparative views of the overall fold of *SnPolE* (green cartoon representation), and *SmPolE* (white cartoon representation).



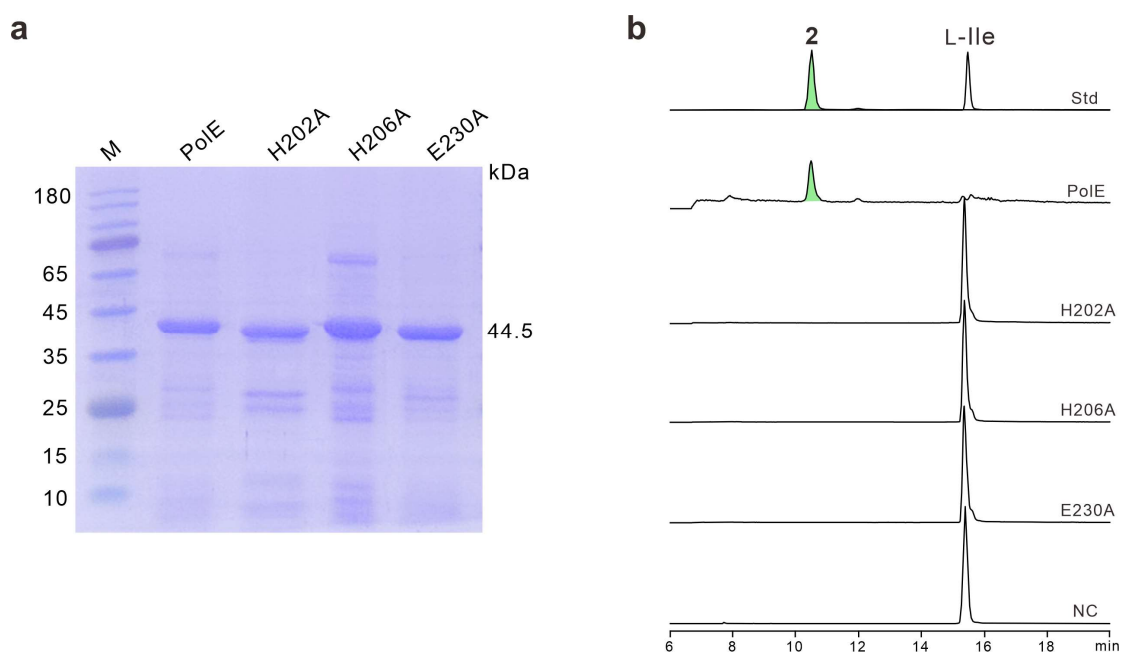
Supplementary Figure 55 | Structures of classical Fe^{2+} /pterin-dependent hydroxylases. **a**, Crystal structure of human tryptophan hydroxylase with bound BH4 and Fe (PDB: 1MLW)¹¹. **b**, Crystal structure of tyrosine hydroxylase with bound BH4 and Fe (PDB: 2TOH)¹². **c**, Crystal structure of human phenylalanine hydroxylase with bound BH4, thienylalanine (substrate analogues), and Fe (PDB: 1MMK)¹³. Up to date, several Fe^{2+} /pterin-dependent enzymes have been discovered to merely catalyze the hydroxylation of aromatic amino acids.



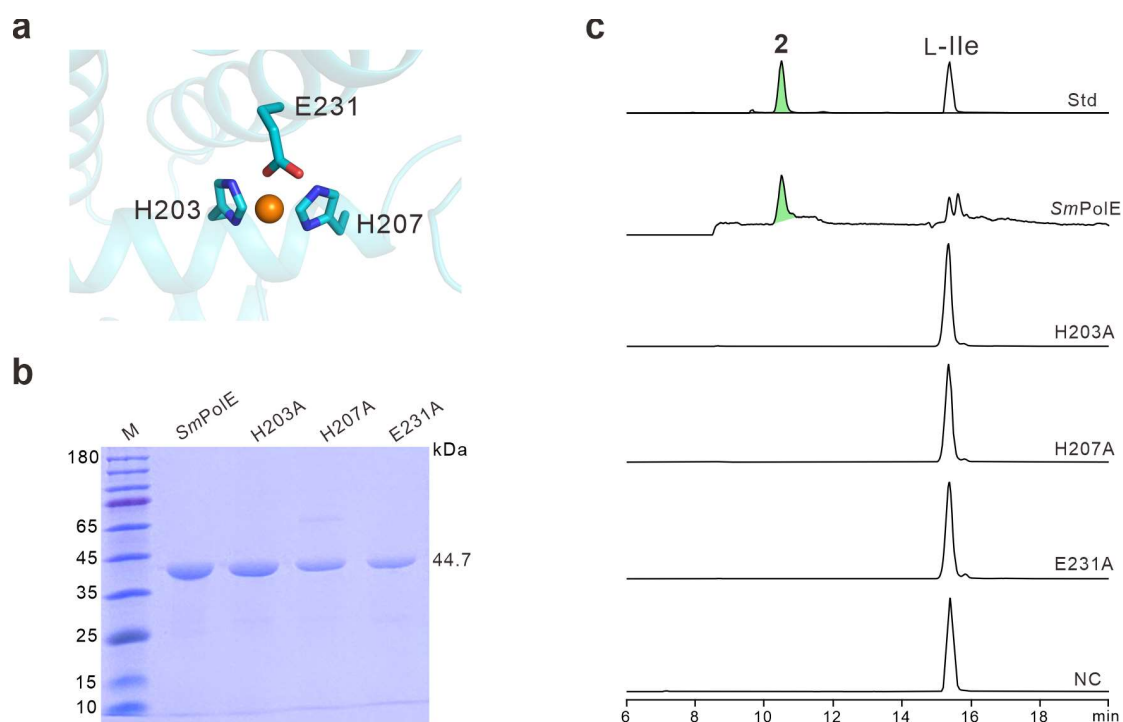
Supplementary Figure 56 | Secondary structure of *SnPolE*. A diagram of the secondary structure of *SnPolE* is indicated in this figure.



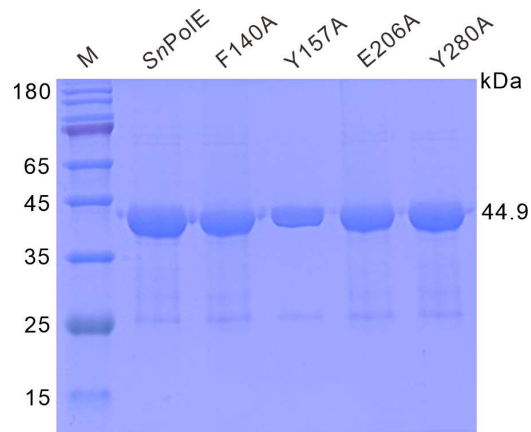
Supplementary Figure 57 | SDS-PAGE analysis of *SnPolE* variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file.



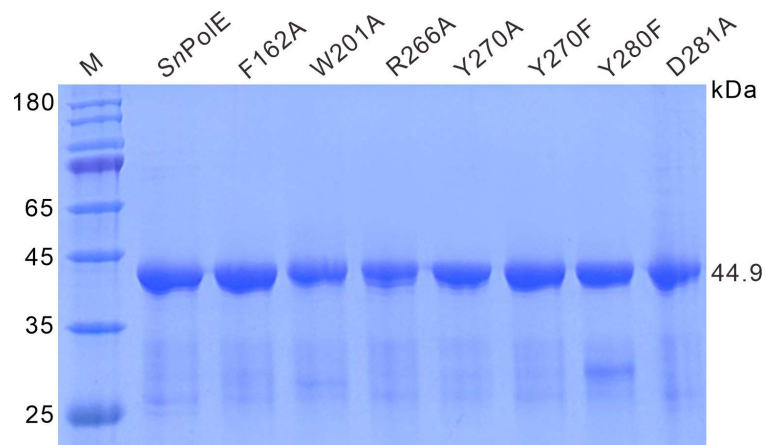
Supplementary Figure 58 | *In vitro* characterization of PolE variants correlating to Fe^{2+} binding sites. **a**, SDS-PAGE analysis of PolE variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file. **b**, *In vitro* characterization of PolE variants correlating to Fe^{2+} binding sites. Std, the authentic L-isoleucine and **2** standards; PolE, the PolE reaction; H202A, H206A, and E230A show the individual reactions of PolE variants; NC, the reaction without PolE added as negative control.



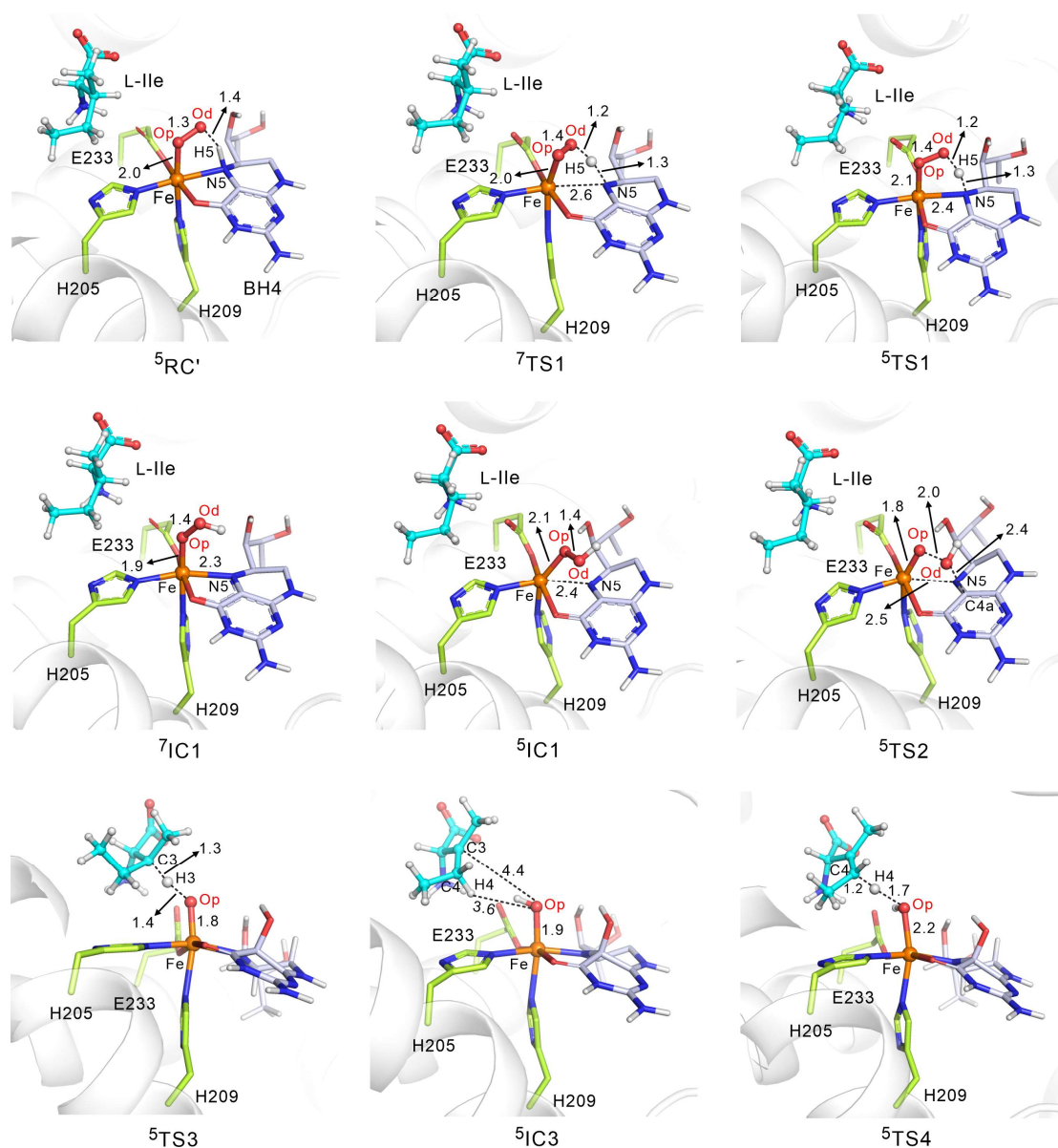
Supplementary Figure 59 | *In vitro* characterization of *SmPolE* variants correlating to Fe^{2+} binding sites. **a**, Fe coordination sites of *SmPolE*. Residues are shown in sticks and the Fe is illustrated as sphere. **b**, SDS-PAGE analysis of *SmPolE* variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file. **c**, *In vitro* characterization of *SmPolE* variants correlating to Fe^{2+} binding sites. Std, the authentic L-isoleucine and **2** standards; *SmPolE*, the *SmPolE* catalyzed reaction; H203A, H207A, and E231A show the individual reactions of *SmPolE* variants; NC, the reaction without *SmPolE* added as negative control.



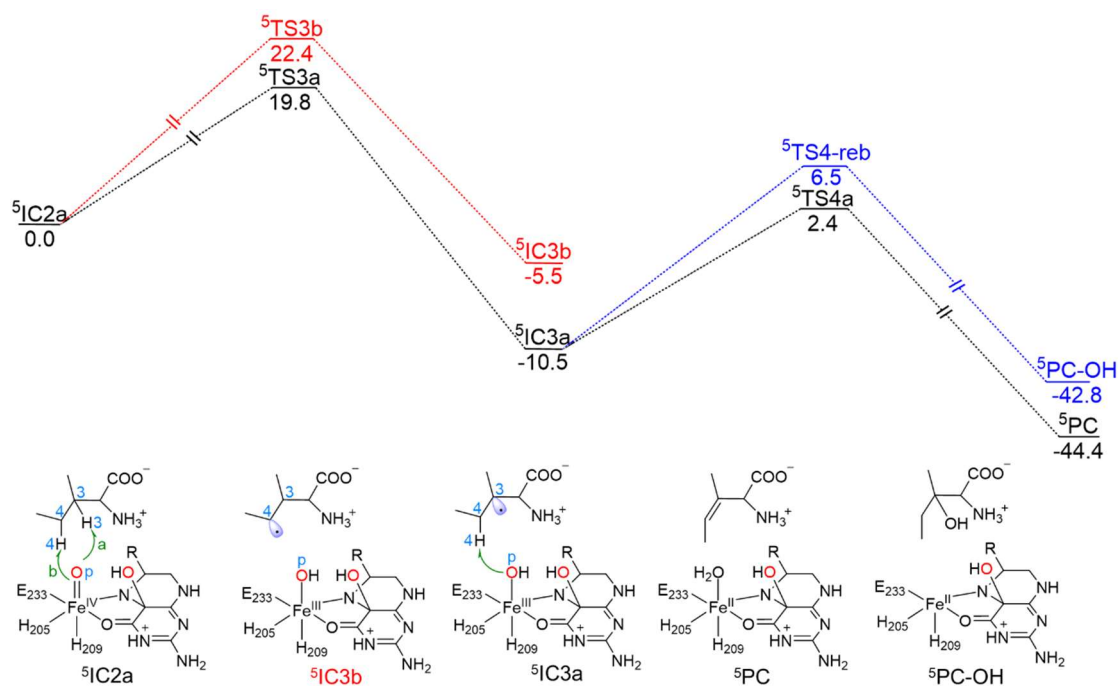
Supplementary Figure 60 | SDS-PAGE analysis of *SnPolE* variants correlating to BH4 binding sites. Source data is provided as a Source Data file.



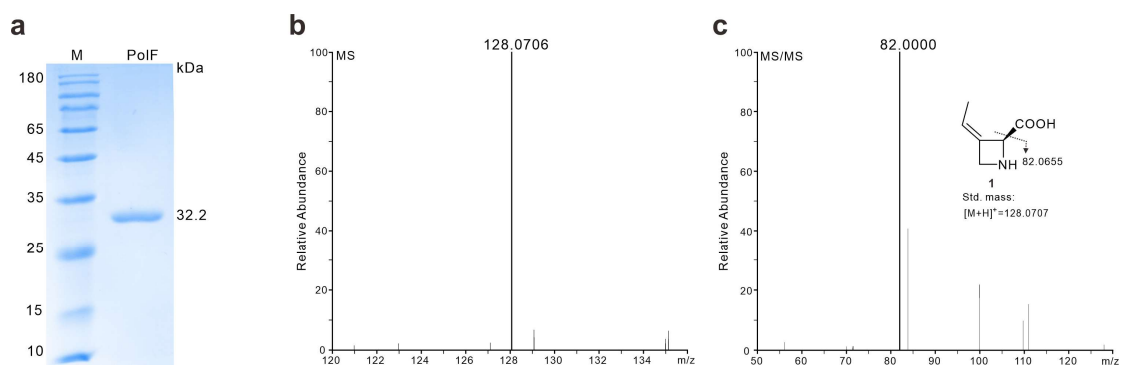
Supplementary Figure 61 | SDS-PAGE analysis of *SnPolE* variants correlating to L-isoleucine binding sites. Source data is provided as a Source Data file.



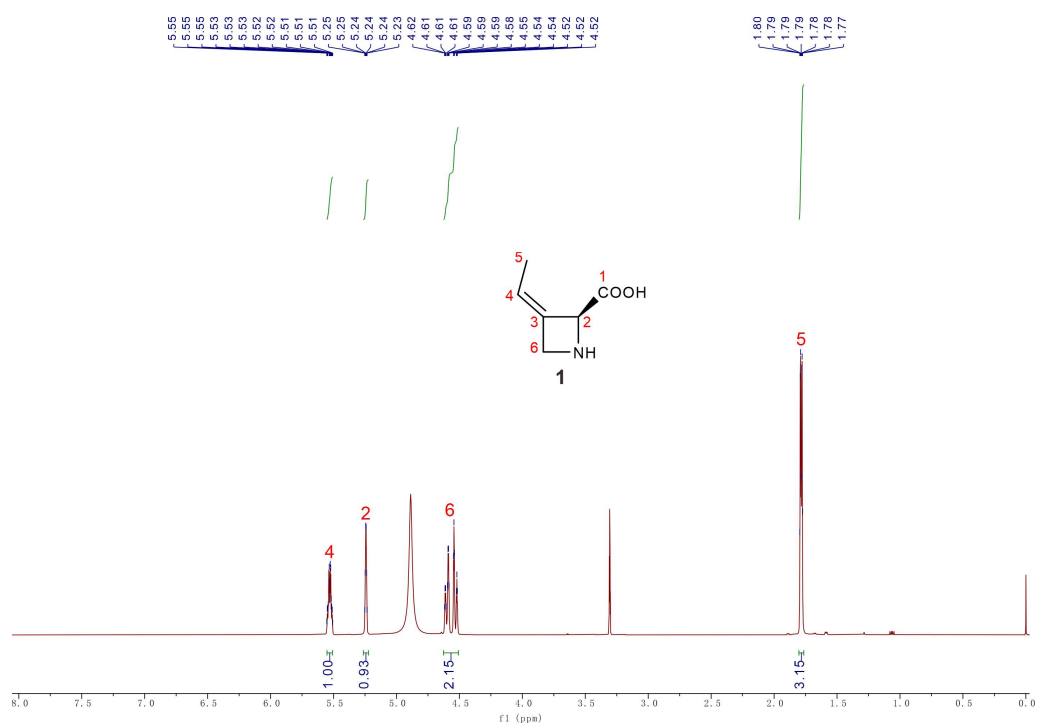
Supplementary Figure 62 | Structures of key intermediates and transition state involved in the formation of product 2 by *SnPolE*. QM(UB3LYP/B1)/MM optimized key intermediates and transition state structures (in Å) involved in the transformation of $^5\text{RC}'$ into ^5PC .



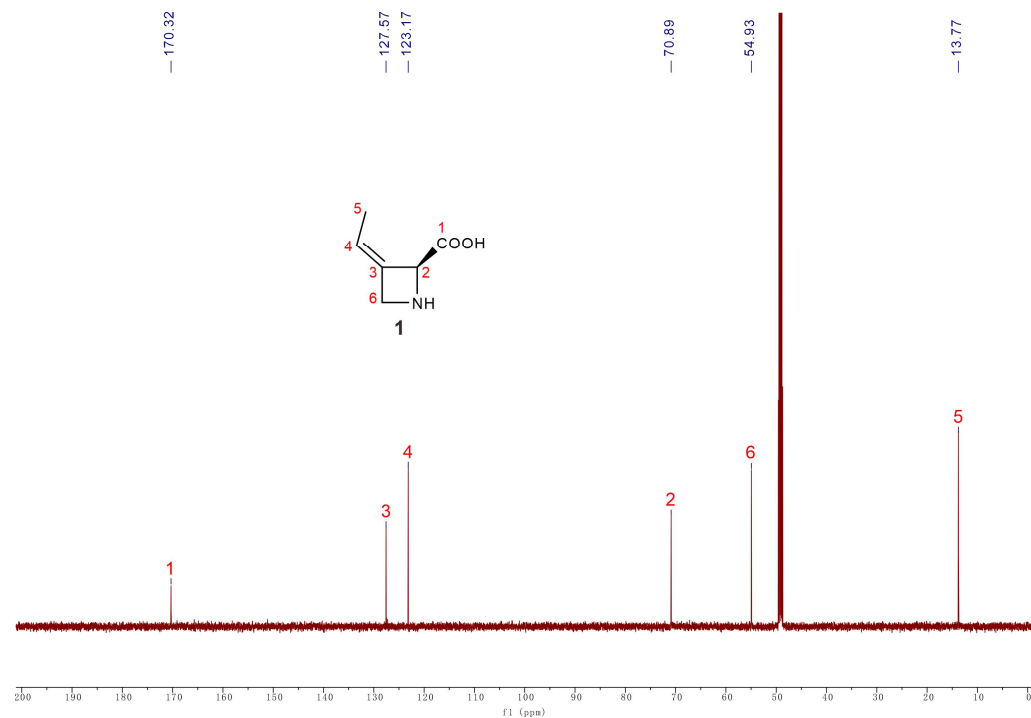
Supplementary Figure 63 | Competing pathways in *Sn*PolE-catalyzed desaturation of L-isoleucine to **2.** The potential energy surface (in kcal mol⁻¹) of *Sn*PolE-catalyzed desaturation of L-isoleucine to **2** obtained from QM/MM calculations using remodeled $^5\text{IC2a}$ as the starting reactant.



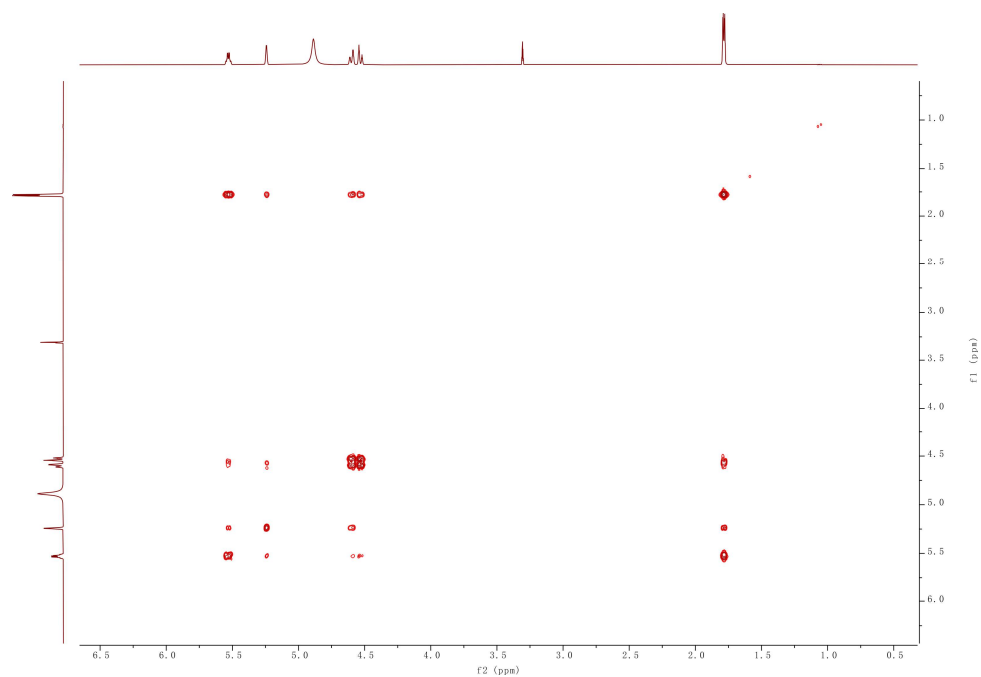
Supplementary Figure 64 | SDS-PAGE analysis of PolF and LC-HRMS analysis of the PolF reaction. a, SDS-PAGE analysis of PolF. Source data is provided as a Source Data file. **a**, LC-HRMS analysis of the PolF reaction. **c**, LC-HRMS/MS analysis of the PolF reaction. The fragmentation pattern of **1** standard is included as a control.



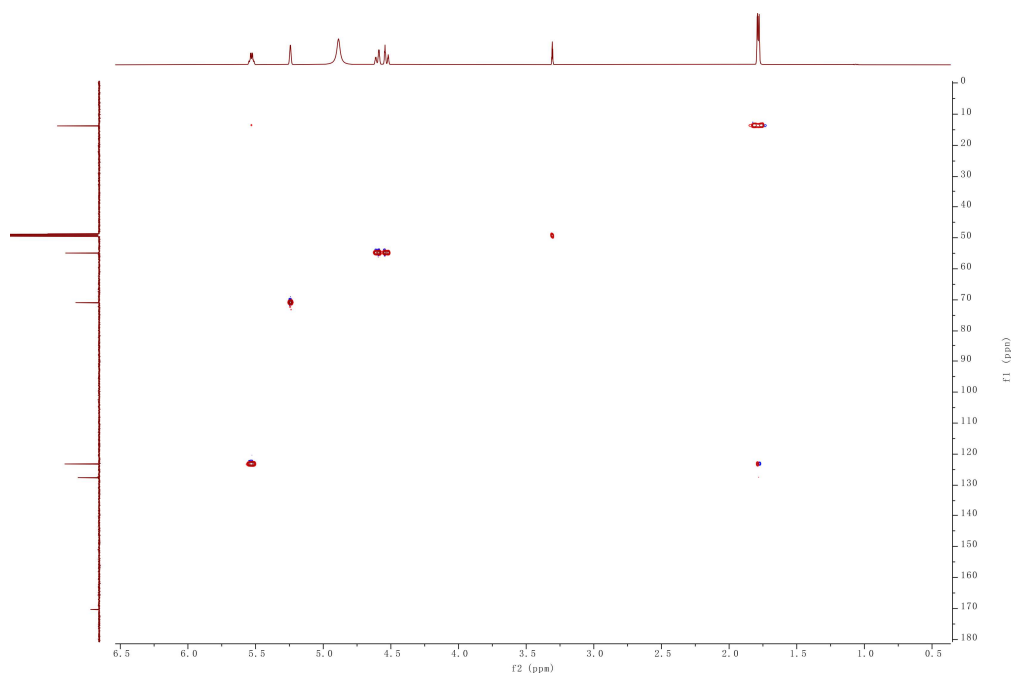
Supplementary Figure 65 | ^1H NMR spectrum of **1 purified from the PolF reaction using **2** as substrate (CD_3OD , 600 MHz).**



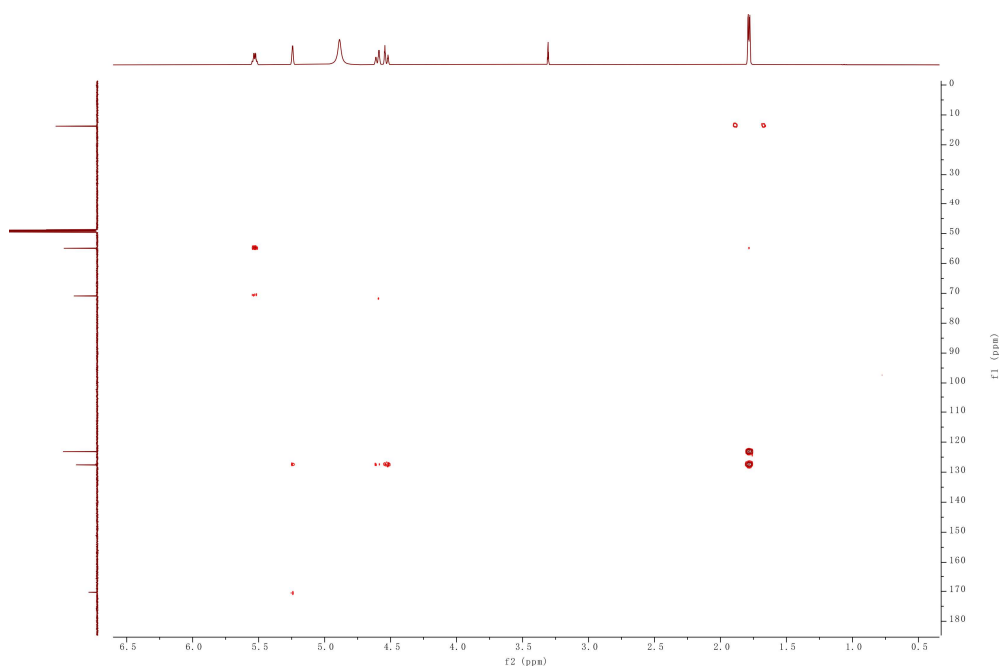
Supplementary Figure 66 | ^{13}C NMR spectrum of **1 purified from the PolF reaction using **2** as substrate (CD_3OD , 150 MHz).**



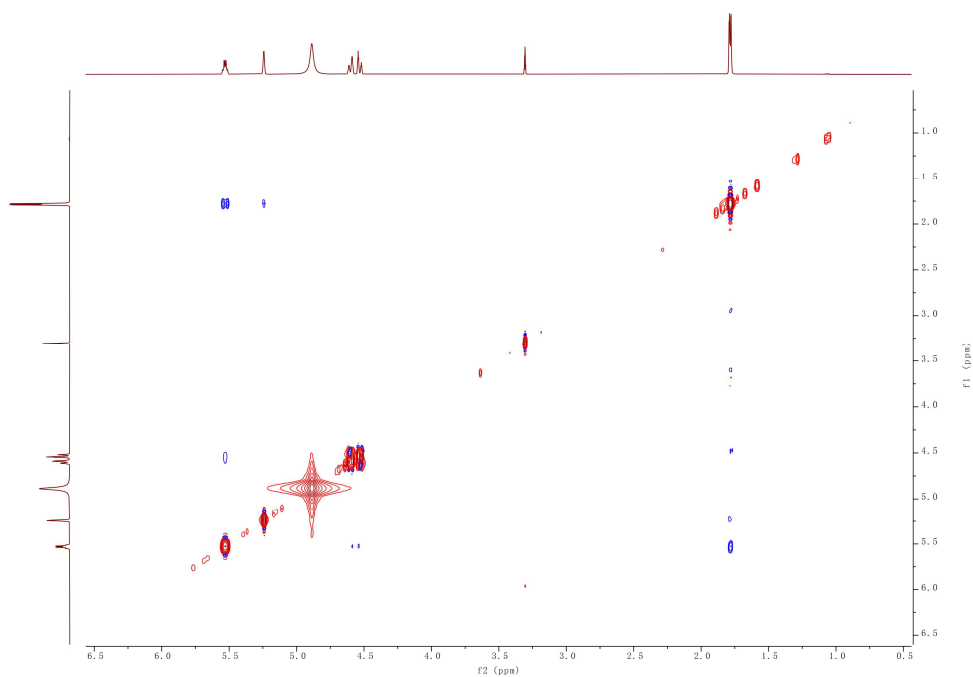
Supplementary Figure 67 | ^1H - ^1H COSY spectrum of **1 purified from the PolF reaction using **2** as substrate (CD_3OD , 600 MHz).**



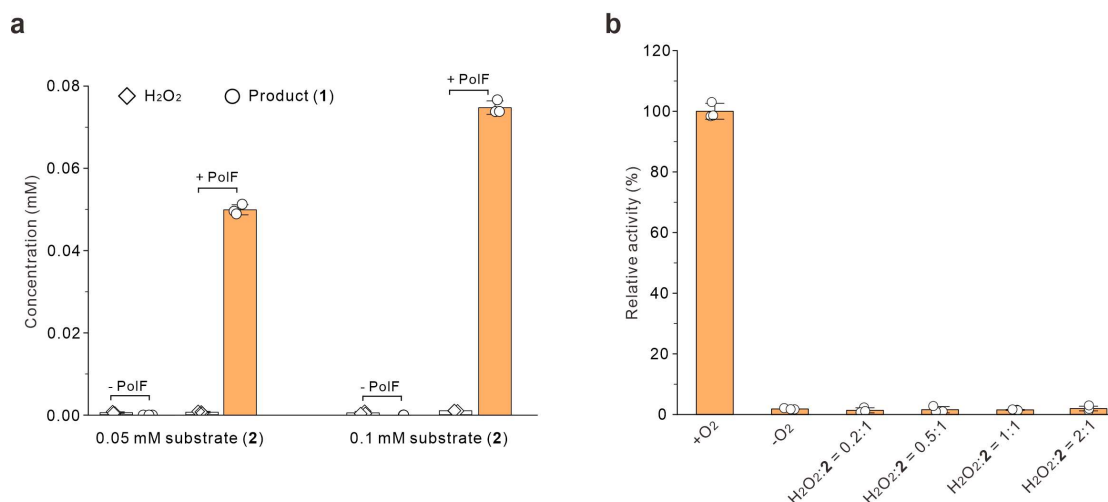
Supplementary Figure 68 | HSQC spectrum of **1 purified from the PolF reaction using **2** as substrate (CD_3OD , 600MHz).**



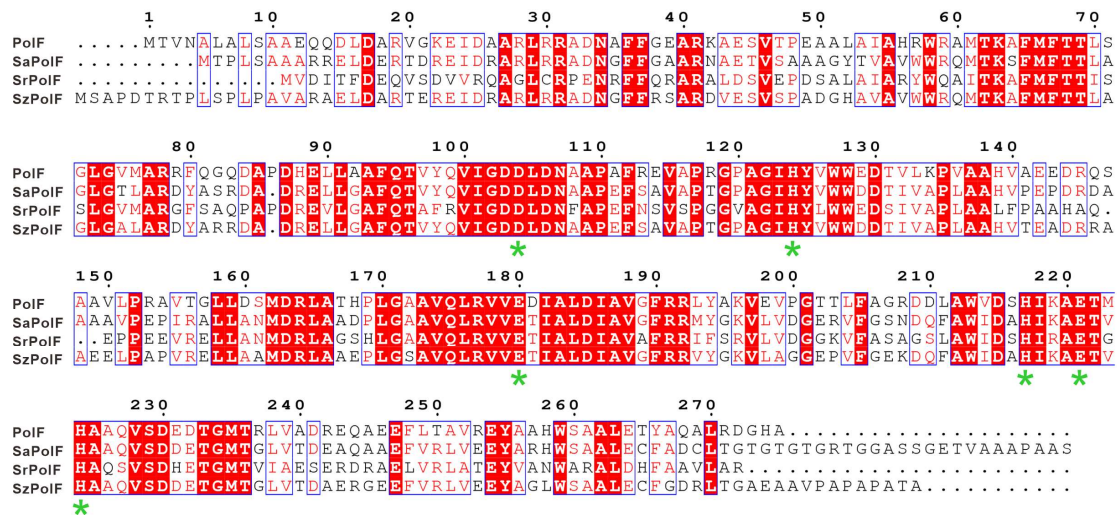
Supplementary Figure 69 | HMBC spectrum of 1 purified from the PolF reaction using 2 as substrate (CD₃OD, 600 MHz).



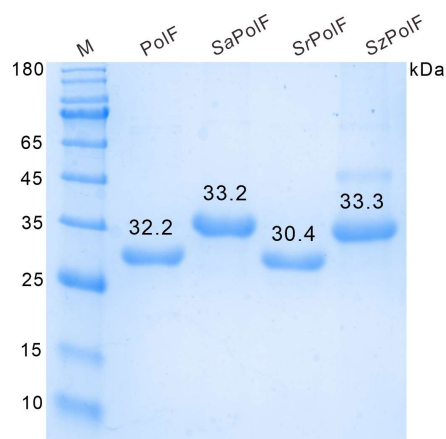
Supplementary Figure 70 | NOESY spectrum of 1 purified from the PolF reaction using 2 as substrate (CD₃OD, 600 MHz).



Supplementary Figure 71 | Determination of the PolF activity unrelated to H₂O₂. **a**, Determination of the potential H₂O₂ formation (with or without enzyme addition) in the PolF reaction. The product **1** formation under the same reaction condition was used as a control. H₂O₂ or **1** was detected when 0.05 mM or 0.1 mM **2** was incubated with 0.1 mM Fe²⁺ at 30 °C in solution (50 mM, pH 7.5) for 20 min. -PolF, without addition of PolF; +PolF, with addition of 20 μM PolF. Determination of H₂O₂ was carried out using the H₂O₂ Quantitative Assay Kit (Water-Compatible), and the standard curve for H₂O₂ determination was established within the concentration range of 0.01-0.1 mM. **b**, The PolF reactions with addition of H₂O₂. The varying concentration of H₂O₂ was added to the PolF reaction containing 0.1 mM **2**, 0.1 mM Fe²⁺ at 30 °C in buffer solution (50 mM, pH 7.5) for 20 min in the absence of O₂. The error bars represent the ± s.d. from three biological replicates. Source data is provided as a Source Data file.

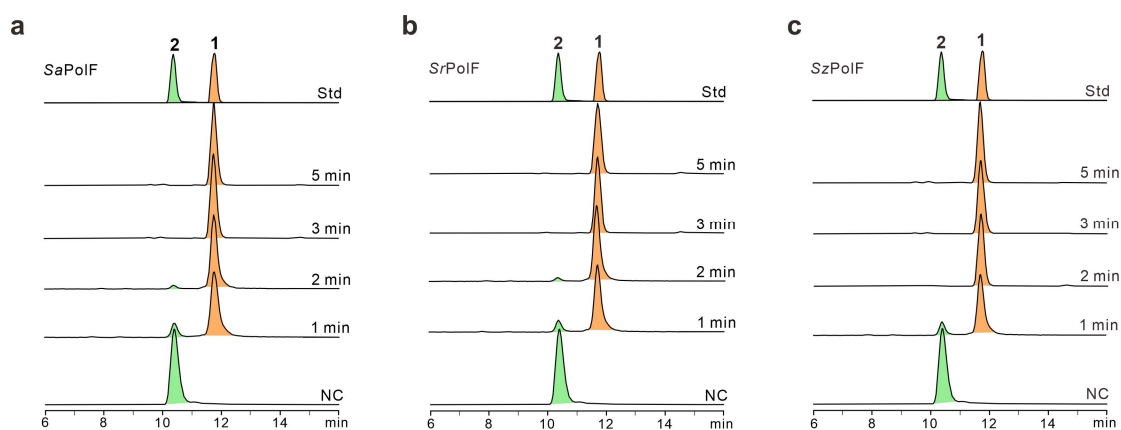


Supplementary Figure 72 | Sequence alignment of PolF and its homologs. BlastP analysis indicates that PolF belongs to DUF6202 (unknown function) family proteins. Sequence alignment of PolF with its homologs was performed using ESPrpt 3.0. The following proteins are included: PolF (GenBank: AFP55317.1) is from *Streptomyces aureochromogenes*, SaPolF (DVA86_03895, GenBank: AXK31912.1) is from *Streptomyces armeniacus*, SrPolF (Sros_3506, GenBank: ACZ86442.1) is from *Streptosporangium roseum* DSM 43021, and SzPolF (D7M15_25730, GenBank: RLL69652.1) is from *Streptomyces* sp. Z26, and the conserved iron binding sites are highlighted by green asterisk.



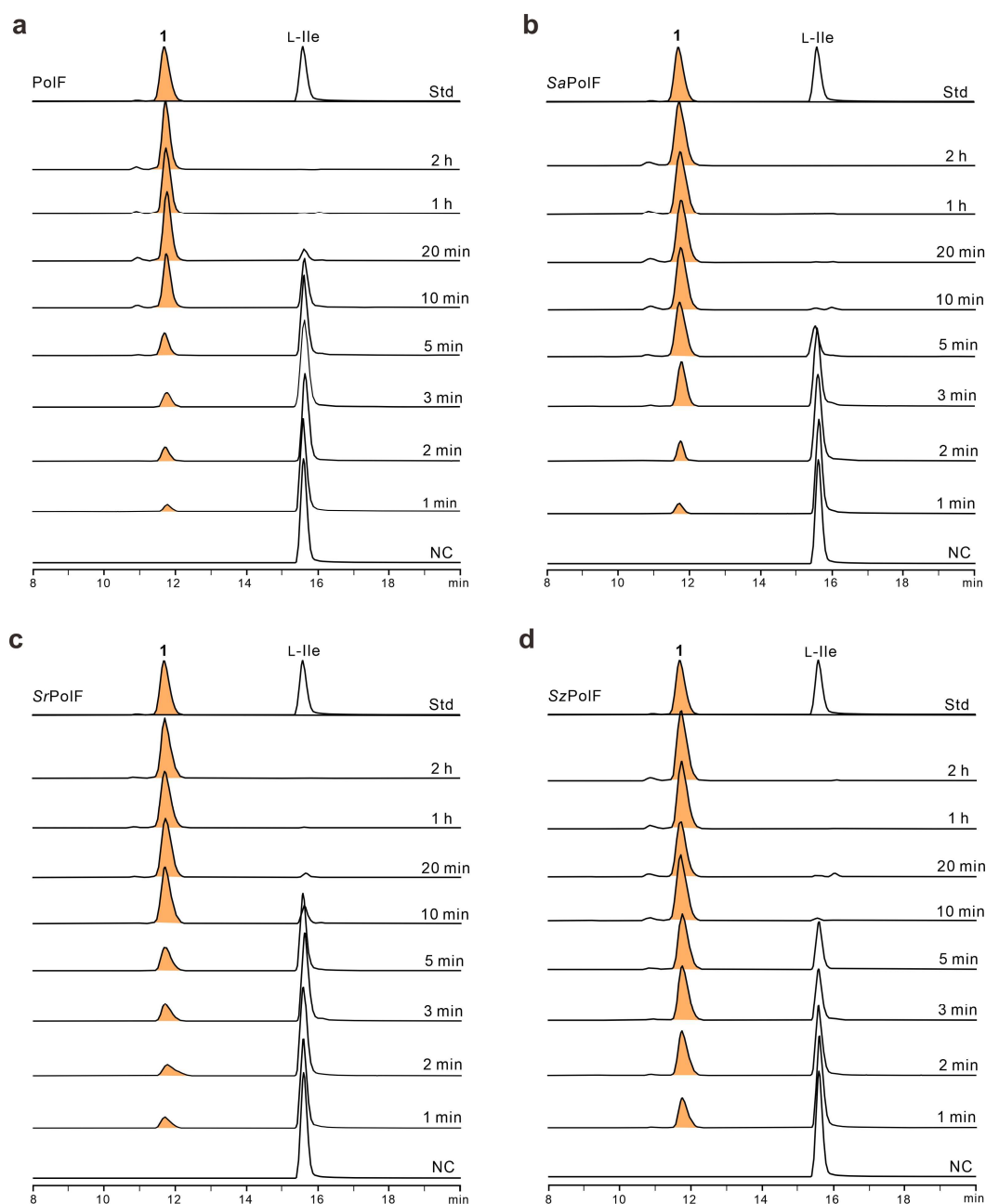
Supplementary Figure 73 | SDS-PAGE analysis of PolF, *Sa*PolF, *Sr*PolF, and *Sz*PolF.

Soluble protein-yield of PolF, *Sa*PolF, *Sr*PolF, and *Sz*PolF purified from *E. coli* BL21(DE3) was about 6 mg l⁻¹, 60 mg l⁻¹, 8 mg l⁻¹, and 51 mg l⁻¹, respectively. Source data is provided as a Source Data file.

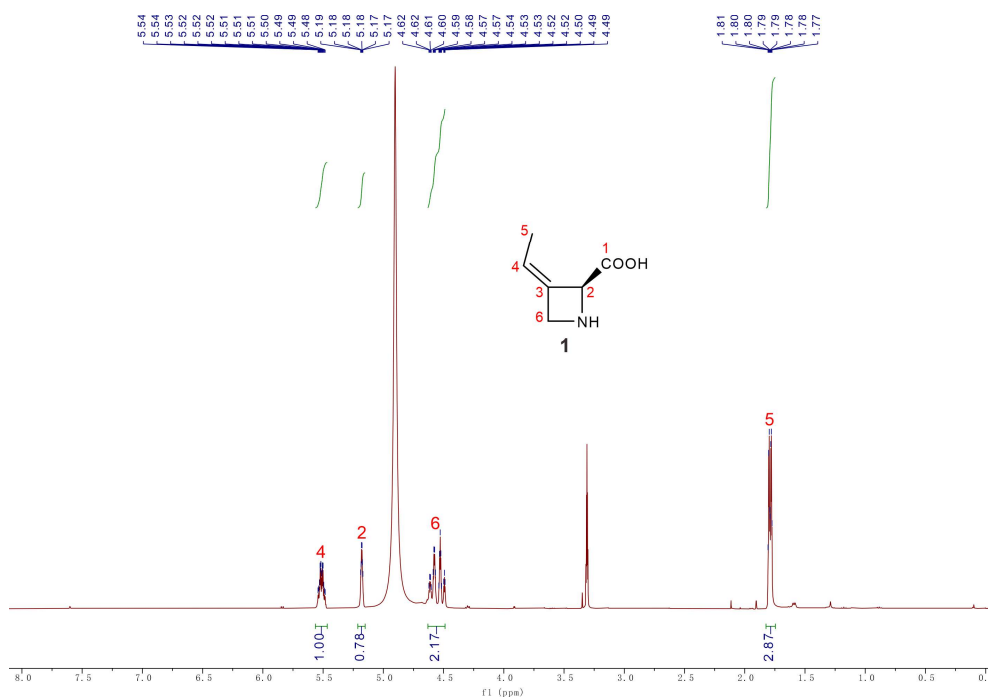


Supplementary Figure 74 | Time-course analysis of PolF homologs activity using 2 as substrate.

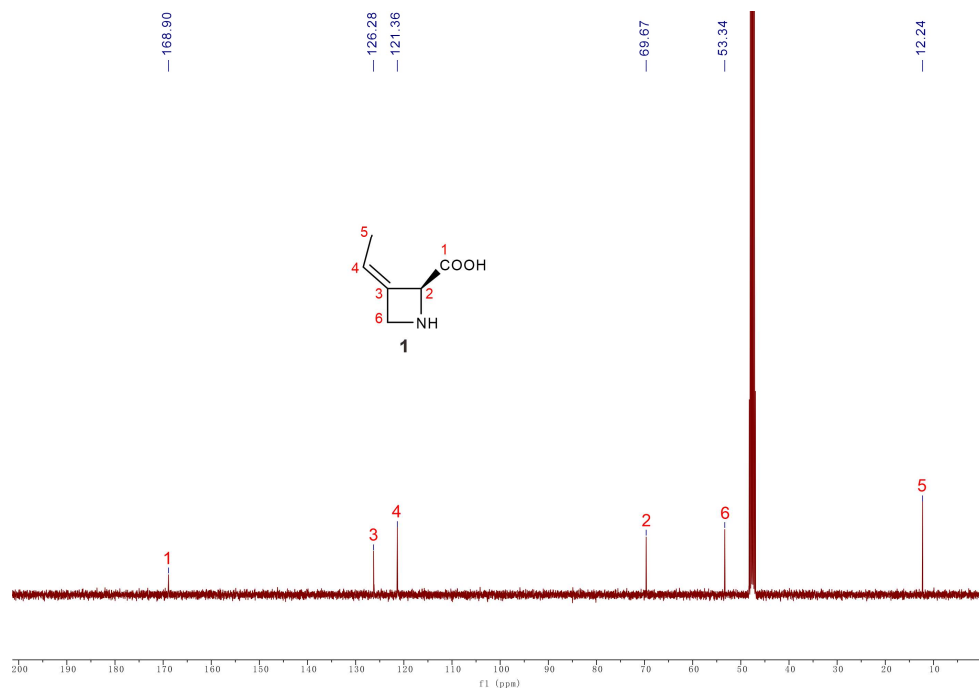
a, Time-course analysis of the *Sa*PolF reaction. Std, the authentic **1** and **2** standards; 1 min, 2 min, 3 min, and 5 min indicate that the *Sa*PolF reaction were individually incubated for the counterpart time; NC, the reaction without *Sa*PolF added as negative control. Similarly, the related annotations can also be correspondingly assigned for the reactions of PolF homologs mentioned in this figure. **b**, Time-course analysis of the *Sr*PolF reaction. **c**, Time-course analysis of the *Sz*PolF reaction.



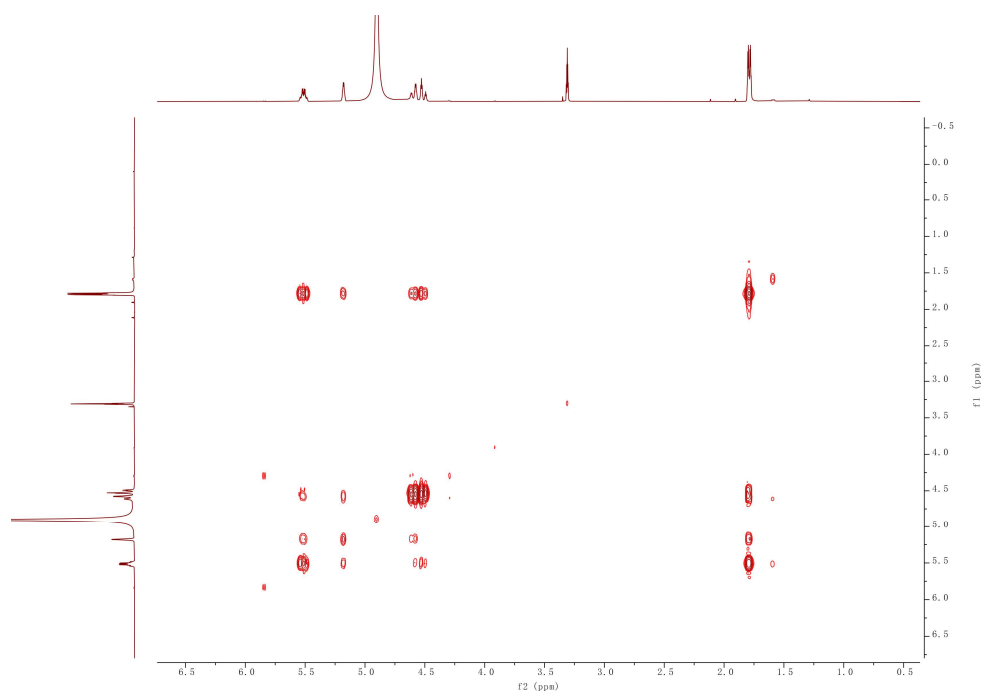
Supplementary Figure 75 | LC-HRMS analysis of the time-course reactions of PolF and its homologs. **a**, LC-HRMS analysis of the time-course reactions of PolF. Std, the authentic standards of L-isoleucine and **1**; 1 min, 2 min, 3 min, 5 min, 10 min, 20 min, 1 h, and 2 h means that the independent PolF reactions were incubated for the counterpart time; NC, the reaction without PolF added as negative control. Similarly, the related annotations can also be correspondingly assigned for the reactions of PolF homologs mentioned in this figure. **b**, LC-HRMS analysis of time-course reactions of SaPolF. **c**, LC-HRMS analysis of the time-course reactions of SrPolF. **d**, LC-HRMS analysis of the time-course reactions of SzPolF.



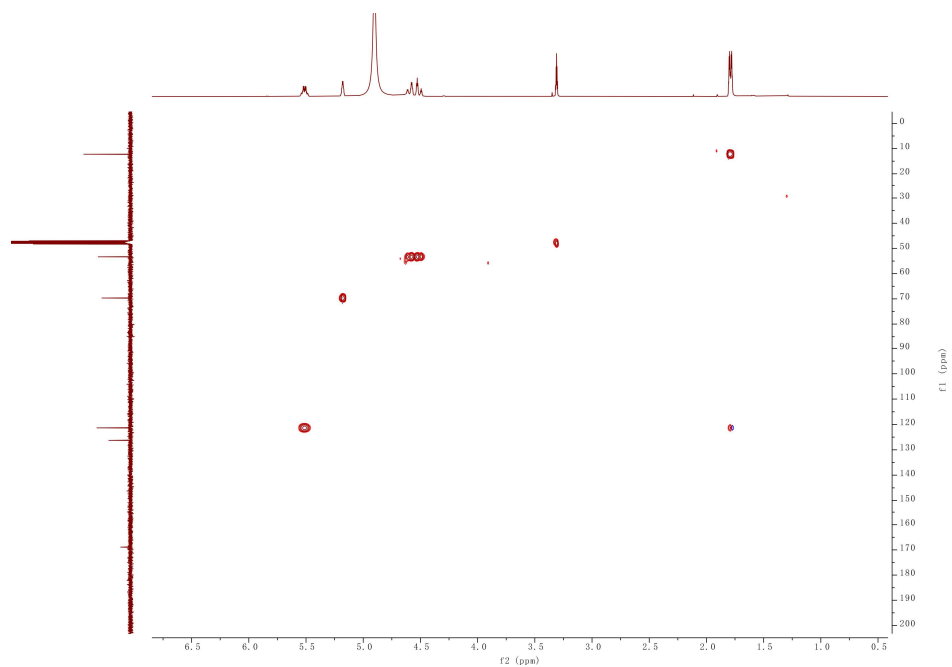
Supplementary Figure 76 | ¹H NMR spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD₃OD, 400 MHz).



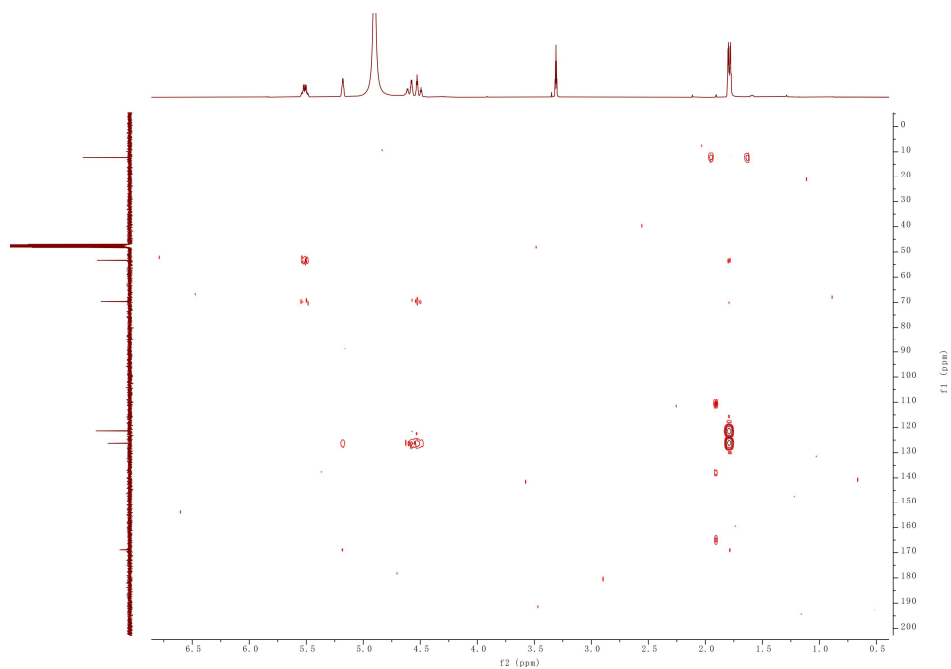
Supplementary Figure 77 | ¹³C NMR spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD₃OD, 100 MHz).



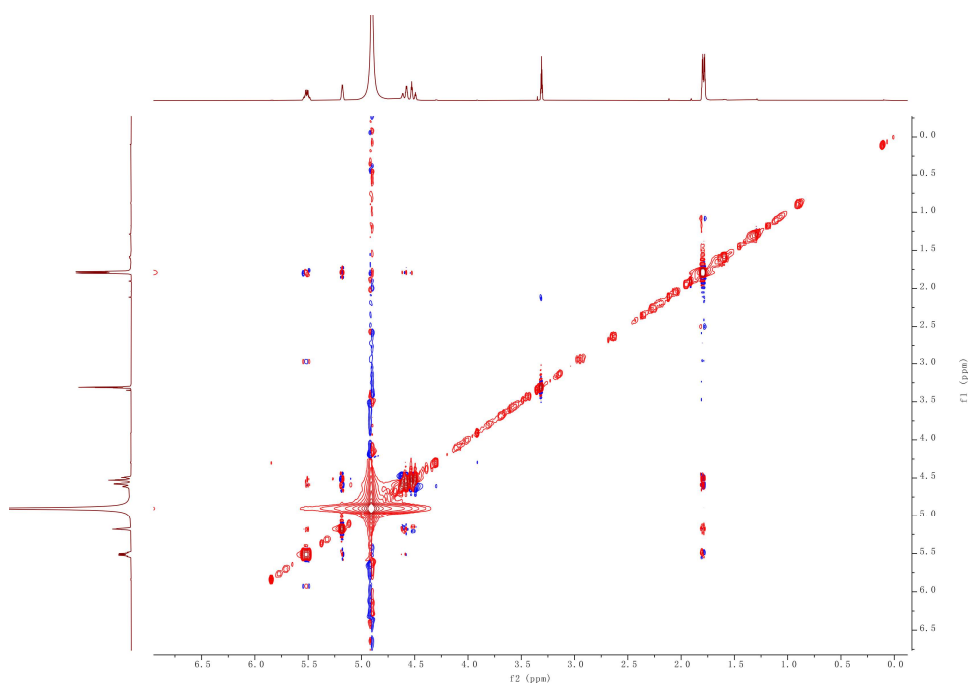
Supplementary Figure 78 | ^1H - ^1H COSY spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD_3OD , 400 MHz).



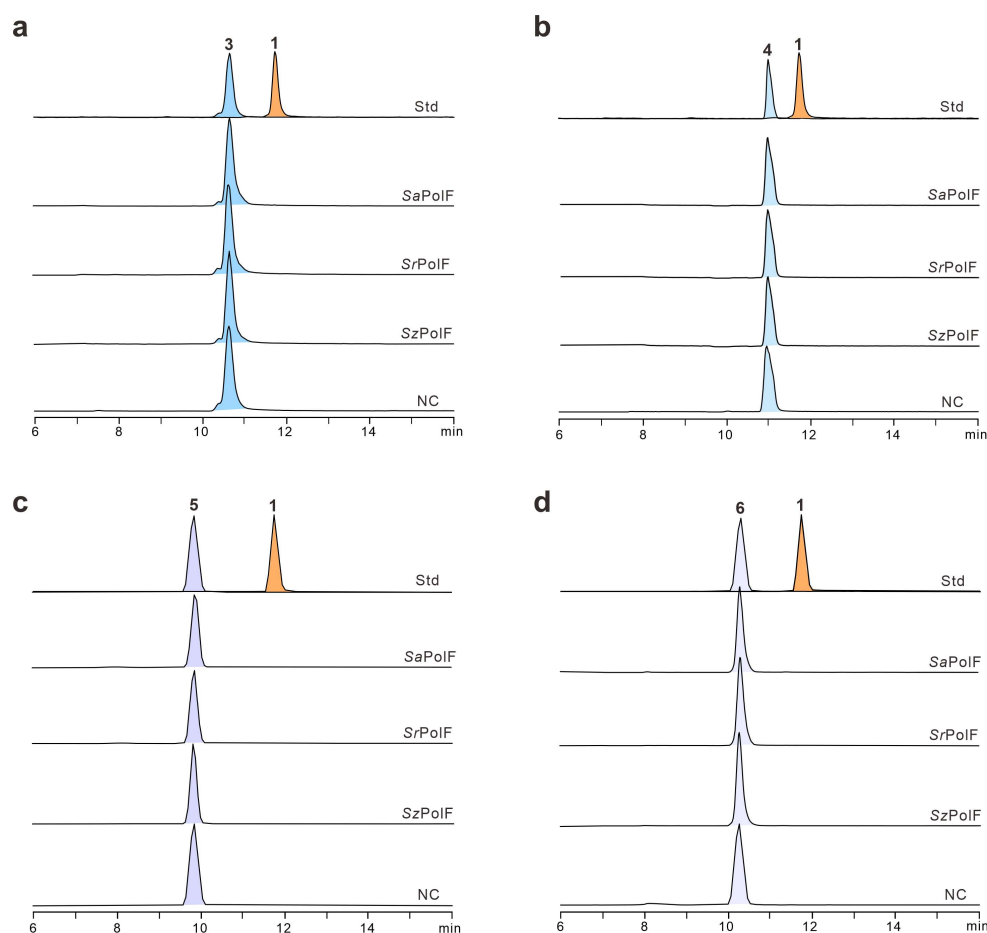
Supplementary Figure 79 | HSQC spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD_3OD , 400 MHz).



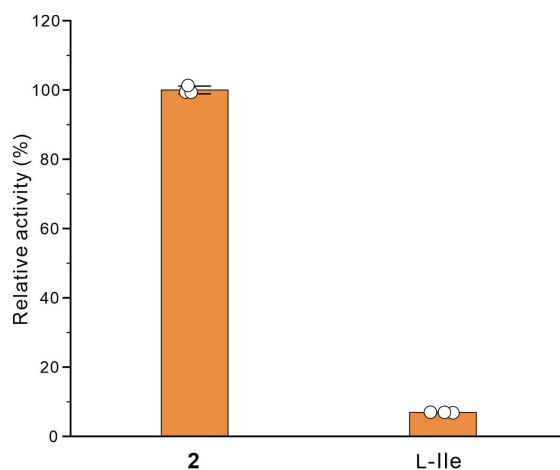
Supplementary Figure 80 | HMBC spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD₃OD, 400 MHz).



Supplementary Figure 81 | NOESY spectrum of 1 purified from the PolF reaction using L-isoleucine as substrate (CD₃OD, 400 MHz).

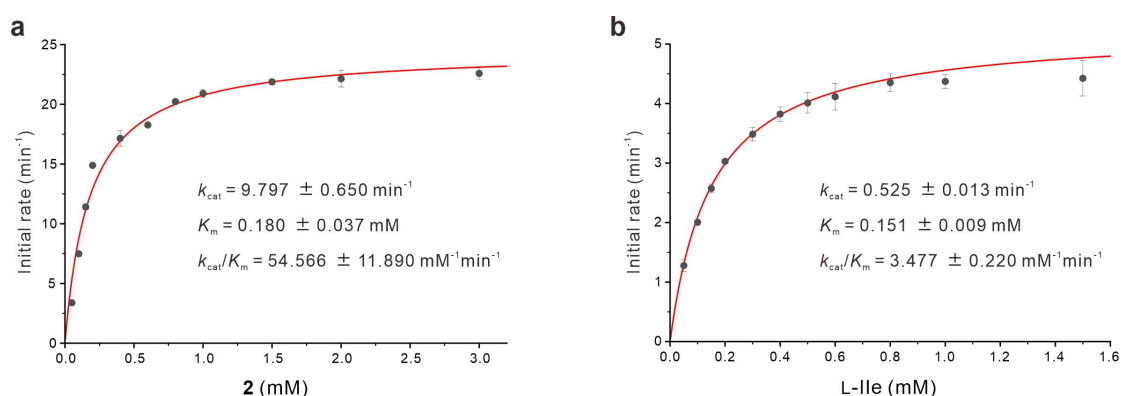


Supplementary Figure 82 | LC-HRMS analysis of the PolF-homolog catalyzed reactions using 3, 4, 5 or 6 as substrate. **a**, LC-HRMS analysis of the corresponding reaction of *SaPolF*, *SrPolF*, and *SzPolF* using **3** as substrate. Std, the authentic **1** and **3** standards; *SaPolF*, the *SaPolF* reaction; *SrPolF*, the *SrPolF* reaction; *SzPolF*, the *SzPolF* reaction. NC, the reaction without protein added as negative control. **b**, LC-HRMS analysis of the corresponding reaction of *SaPolF*, *SrPolF*, and *SzPolF* using **4** as substrate. Std, the authentic **1** and **4** standards; *SaPolF*, the *SaPolF* reaction; *SrPolF*, the *SrPolF* reaction; *SzPolF*, the *SzPolF* reaction. NC, the reaction without protein added as negative control. **c**, LC-HRMS analysis of the corresponding reaction of *SaPolF*, *SrPolF*, and *SzPolF* using **5** as substrate. Std, the authentic **1** and **5** standards; *SaPolF*, the *SaPolF* reaction; *SrPolF*, the *SrPolF* reaction; *SzPolF*, the *SzPolF* reaction. NC, the reaction without protein added as negative control. **d**, LC-HRMS analysis of corresponding reaction of the *SaPolF*, *SrPolF*, and *SzPolF* using **6** as substrate. Std, the authentic **1** and **6** standards; *SaPolF*, the *SaPolF* reaction; *SrPolF*, the *SrPolF* reaction; *SzPolF*, the *SzPolF* reaction. NC, the reaction without protein added as negative control.



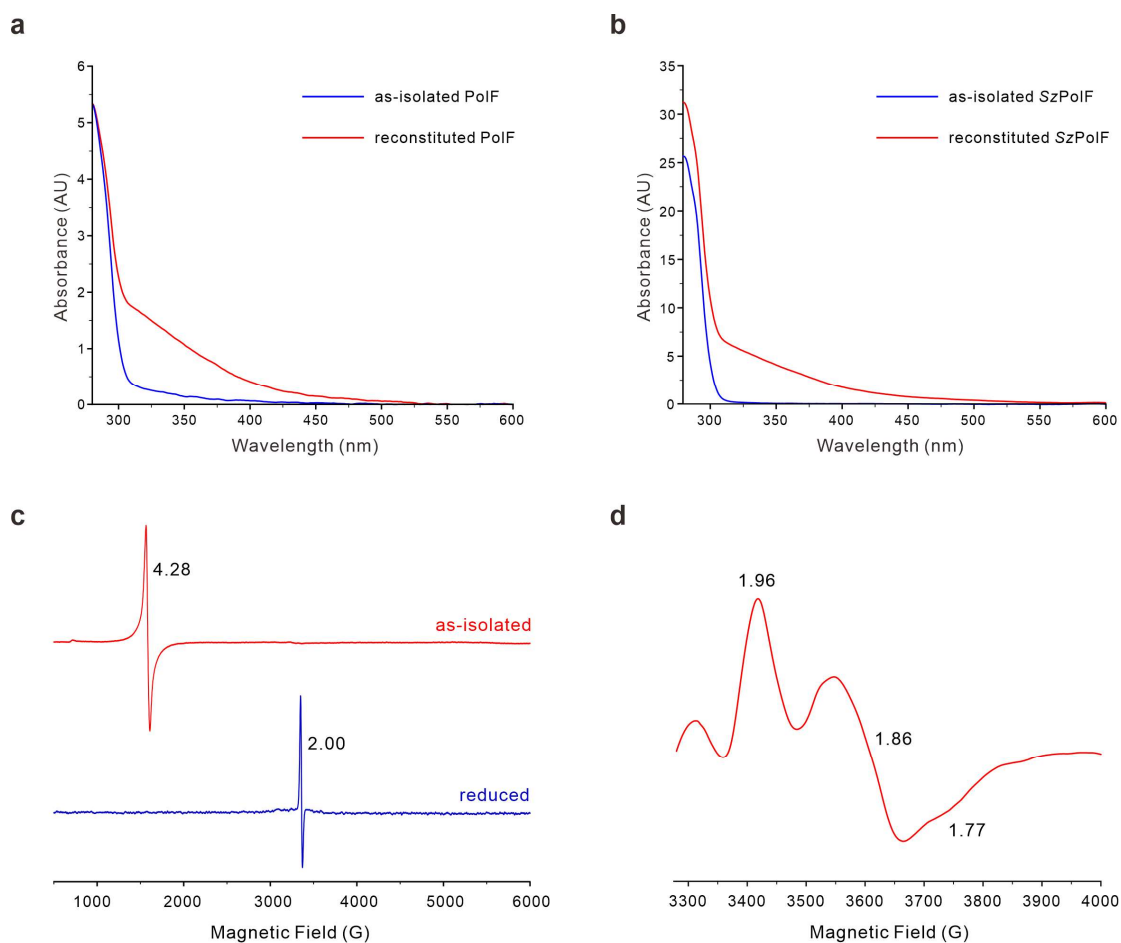
Supplementary Figure 83 | Relative-activity analysis of PolF against 2 and L-isoleucine.

Relative-activity analysis of PolF against 2 and L-isoleucine in the presence of O₂, Fe²⁺, and VC. The activity of PolF against 2 was set to 100%, and the error bars represent the $\pm$ s.d. from three biological replicates, respectively. The peak area represents the relative activity of PolF with different substrate. Source data is provided as a Source Data file.

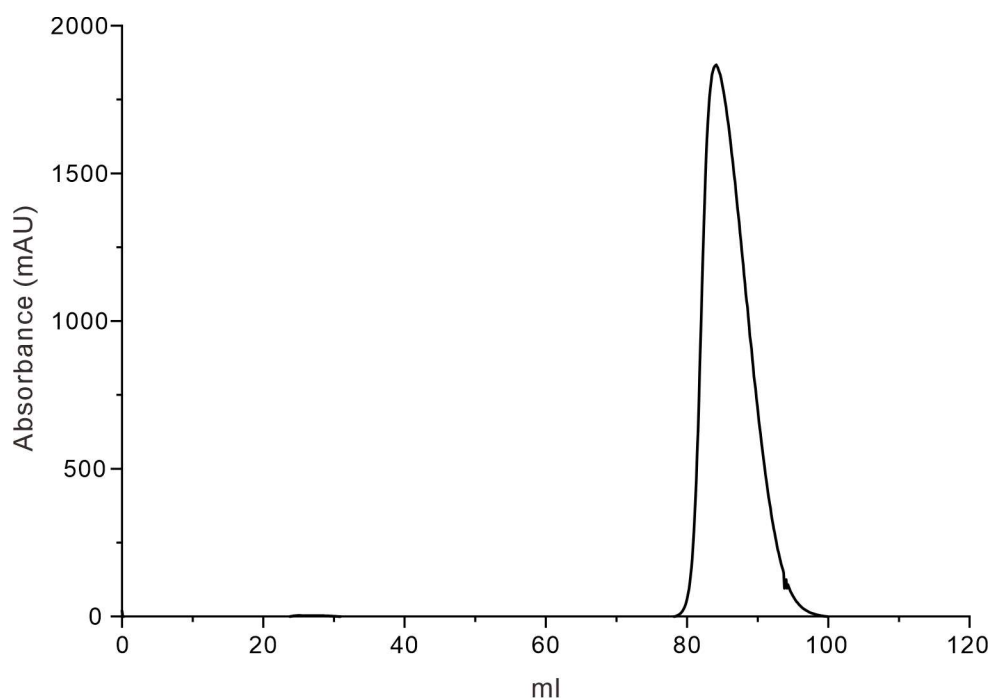


Supplementary Figure 84 | Steady-state kinetic analysis of PolF. a, Kinetic analysis of

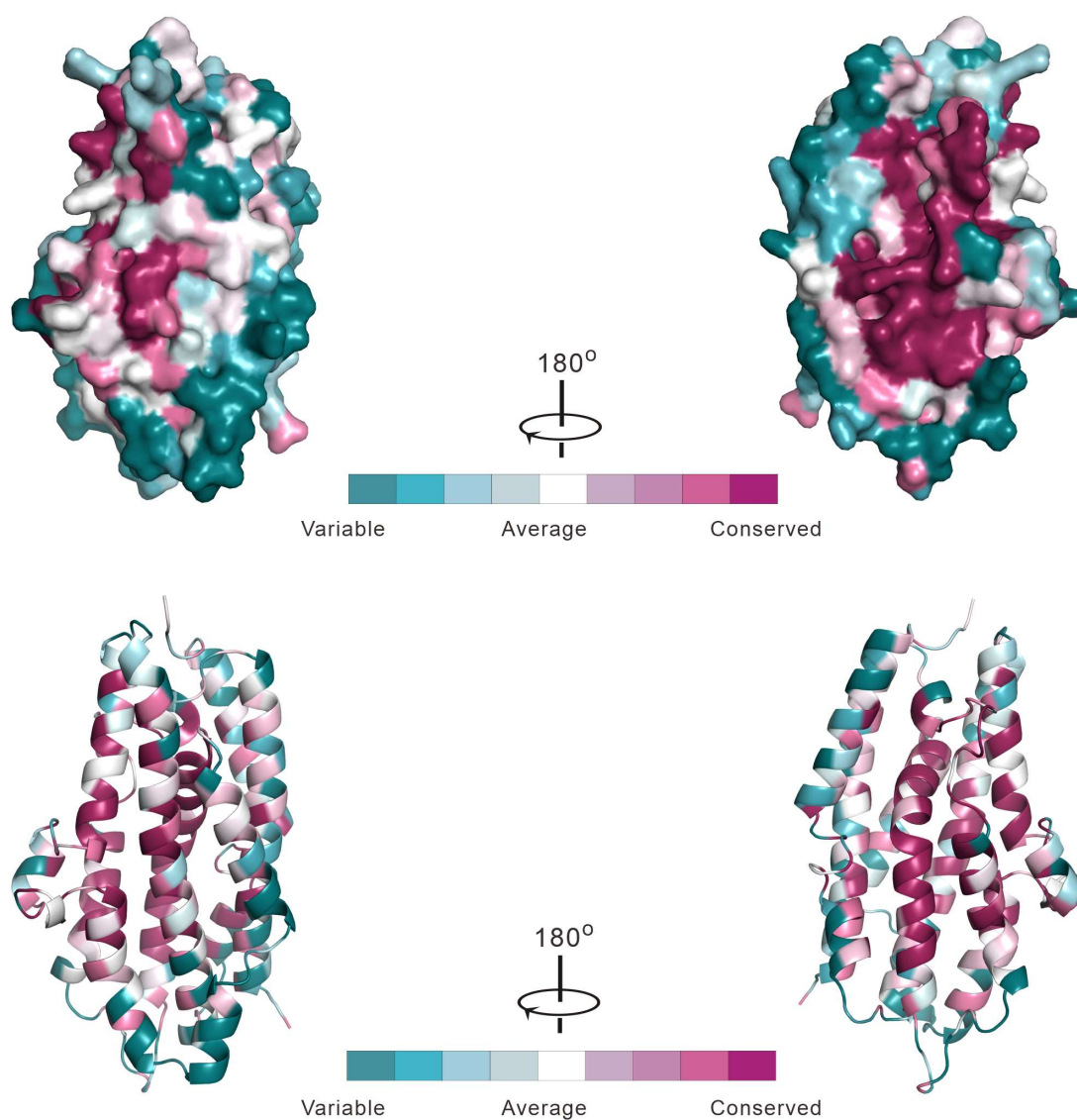
PolF with 2 in the presence of 0.1 mM Fe²⁺, 2 mM ascorbate, and 2.5 μ M protein. The kinetic parameters are $k_{cat} = 9.797 \pm 0.650 \text{ min}^{-1}$ and $K_m = 0.180 \pm 0.037 \text{ mM}$. **b**, Kinetic analysis of PolF with L-isoleucine in the presence of 0.1 mM Fe²⁺, 2 mM ascorbate, and 10 μ M protein. The kinetic parameters are $k_{cat} = 0.525 \pm 0.013 \text{ min}^{-1}$ and $K_m = 0.151 \pm 0.009 \text{ mM}$. Assays were run in triplicate and kinetic values are reported as mean $\pm$ s.d. of three replicates. Source data is provided as a Source Data file.



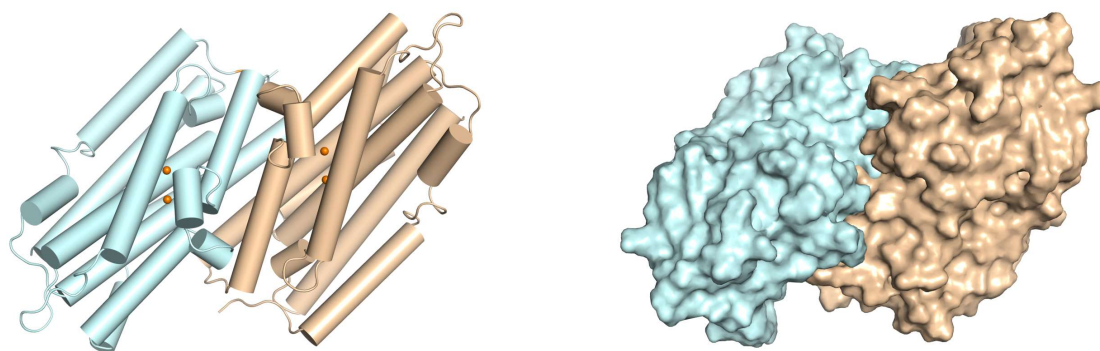
Supplementary Figure 85 | The UV-Visible absorbance spectrum and EPR spectrum of PolF. **a**, The UV-Visible absorbance spectrum of as-isolated and reconstituted PolF. **b**, The UV-Visible absorbance spectrum of as-isolated and reconstituted SzPolF. **c**, EPR characterization of as-isolated and sodium dithionite reduced SzPolF. **d**, EPR characterization of the partially reduced SzPolF by sodium dithionite. The partially reduced of iron-loaded SzPolF produces an EPR-active $S = 1/2$ species indicative of the mixed-valent Fe(II)/Fe(III) state.



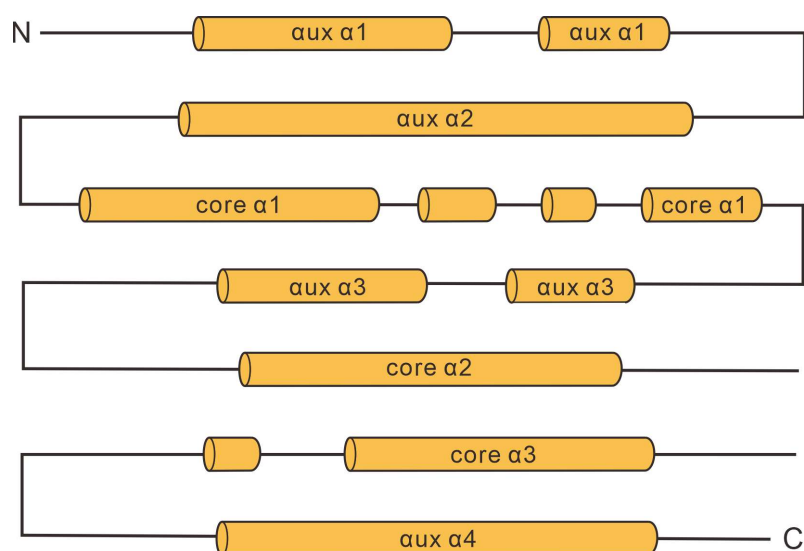
Supplementary Figure 86 | Size exclusion chromatography of PolF as a homodimer in solution. Size exclusion chromatography of PolF indicates the protein is in homodimer form in solution (20 mM Tris-HCl, 300 mM NaCl, pH 8.0). PolF elutes at 85 ml on a HiLoad 16/600 Superdex™ 200 pg column (GE Healthcare), corresponding to an approximate molecular weight of 32 kDa. The value is consistent with the calculated MW (32.2 kDa) of the PolF homodimer.



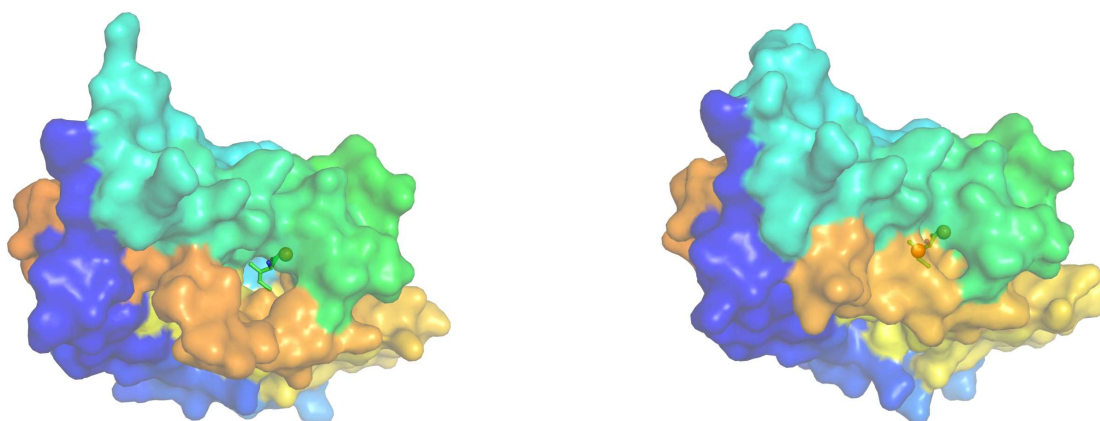
Supplementary Figure 87 | The conservation analysis of SzPolF structure by Consurf server. The analysis of evolutionary conservation patterns of SzPolF structure is generated using Consurf server online: the rate of evolution is not constant among acid sites, some positions evolve slowly and are commonly referred to as “conserved”, while others evolve rapidly and are referred to as “variable”.



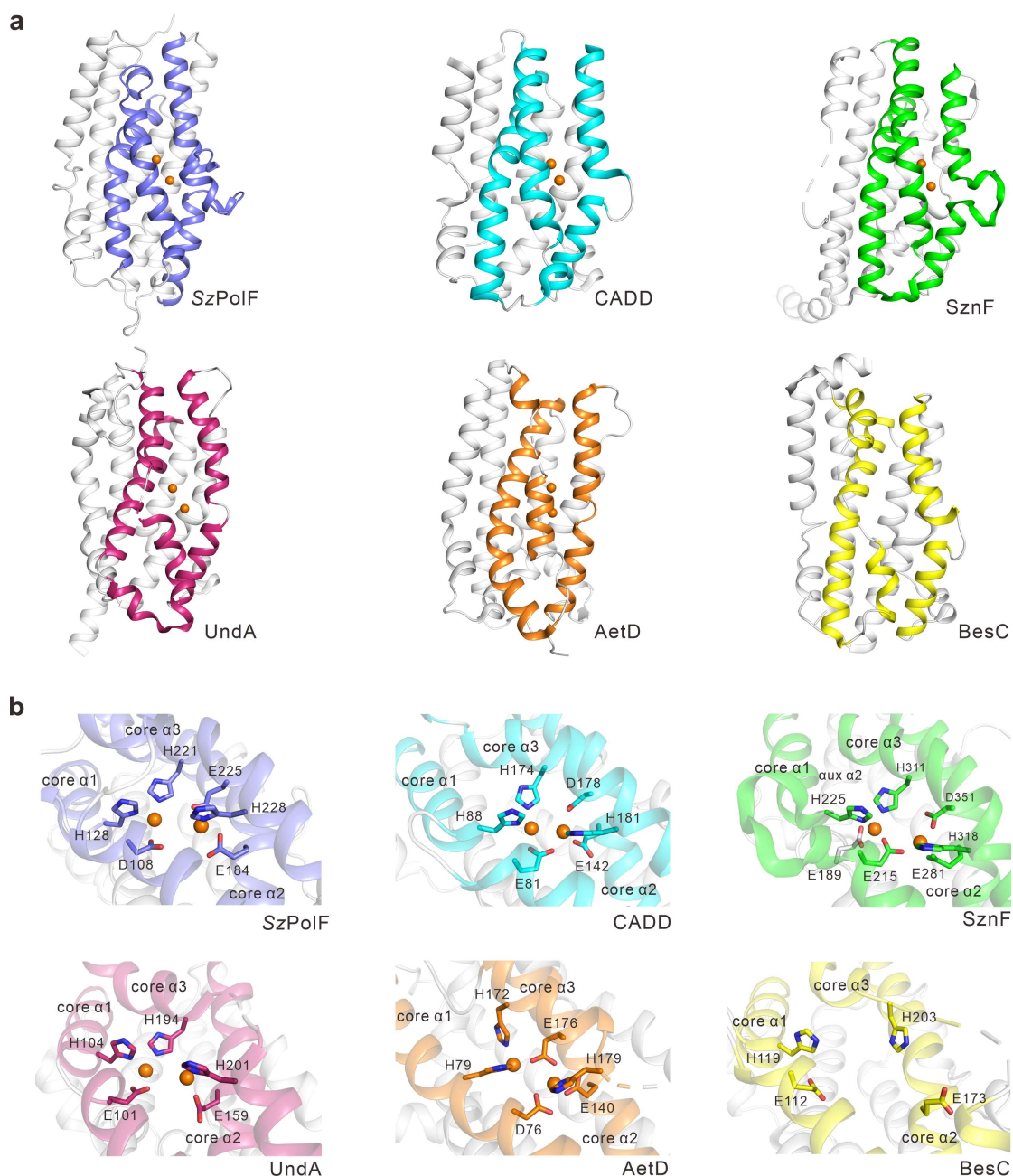
Supplementary Figure 88 | The overall structure of Fe₂(II/II)-SzPolF homodimer. SzPolF forms a homodimer in solution. Chain A is shown in pale cyan cylinder and surface while chain B is shown in wheat cylinder and surface.



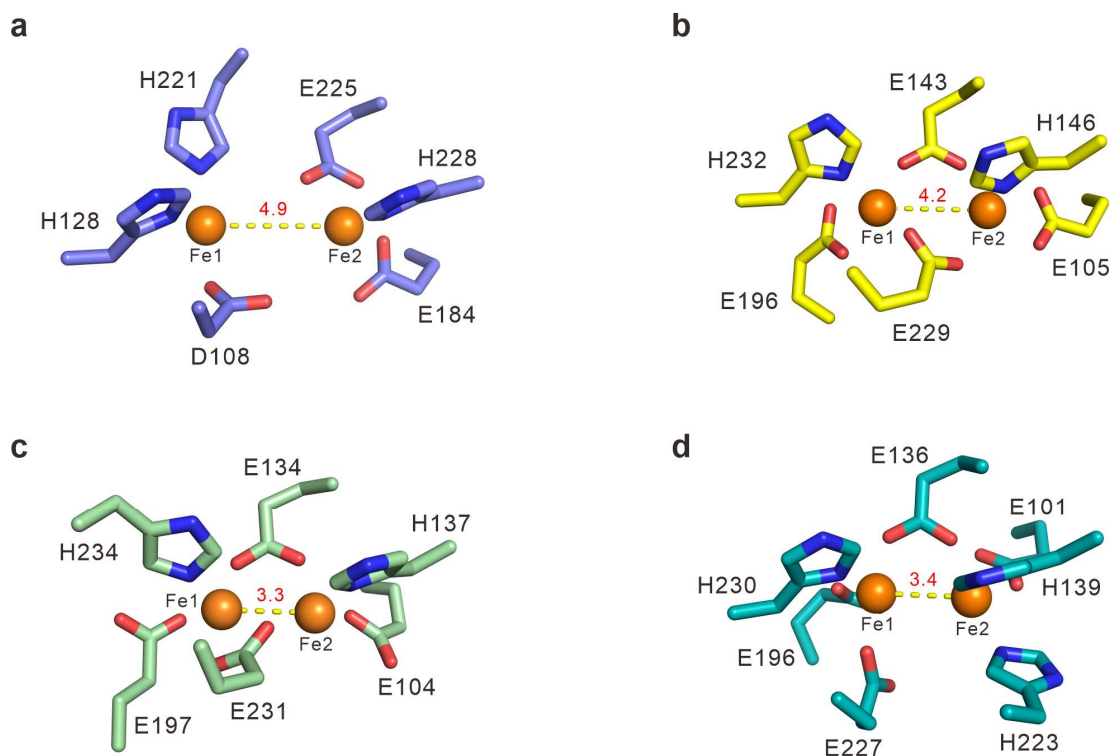
Supplementary Figure 89 | Secondary structure of SzPolF. A diagram of the secondary structure of SzPolF is indicated in this figure.



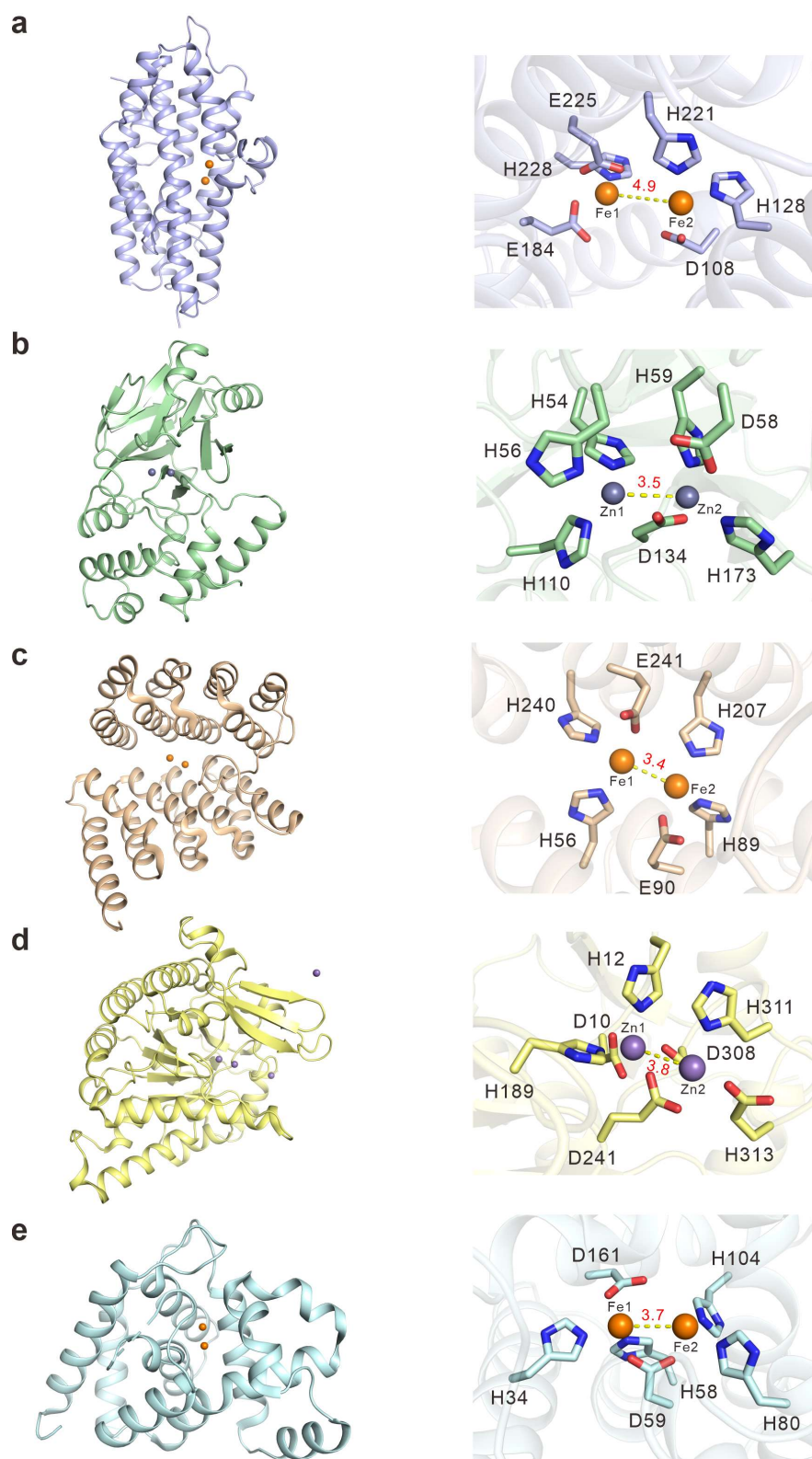
Supplementary Figure 90 | Surface representation of Fe(II)-*SzPolF* and Fe₂(II/II)-*SzPolF* with the cartoon diagram superimposed. Surface representation of Fe(II)-*SzPolF* (left) and Fe₂(II/II)-*SzPolF* (right) are shown as rainbow diagram. The substrate **2**, is shown in green stick format and diiron cofactors are shown as orange spheres.



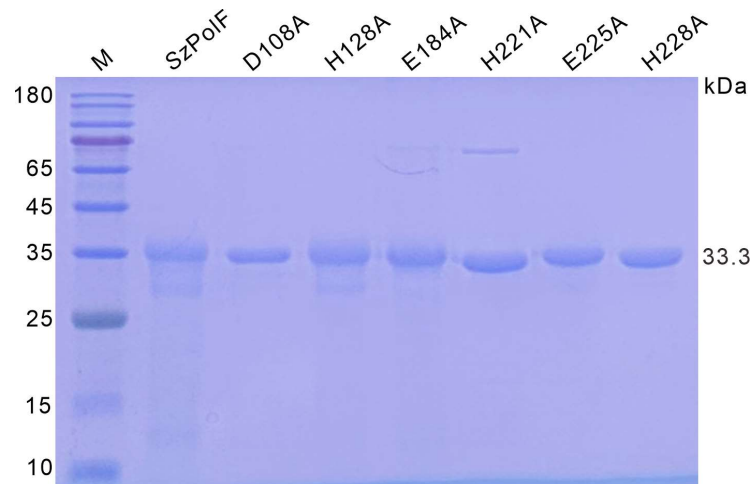
Supplementary Figure 91 | Structures comparison of *SzPolF* and other diverse HDO proteins. **a**, Overall structures of *SzPolF* and other reported HDO superfamily proteins. **b**, Zoomed-in views of the Fe coordination sites in all HDO superfamily proteins that have been structurally characterized by X-ray crystallography. CADD (PDB ID: 1RCW)¹⁴, SznF (PDB ID: 6VZY)¹⁵, UndA (PDB ID: 6P5Q)¹⁶, and AetD (PDB ID: 8JI7)¹⁷ contain full-occupancy diiron cofactors and ordered α -helical structure throughout core $\alpha 3$. BesC (PDB ID: 7TWA) lacks diiron cofactors and maintains disordered core helix $\alpha 3$ ¹⁸.



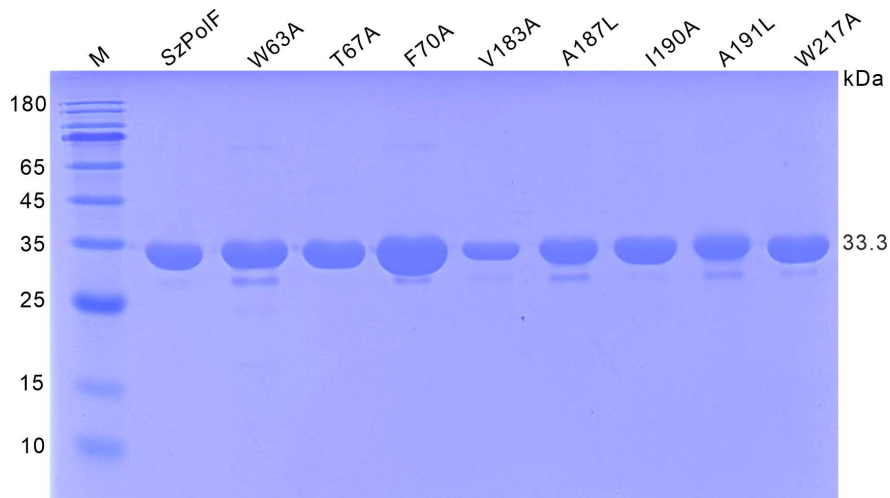
Supplementary Figure 92 | Comparison of the diiron-binding sites in the structure of *SzPolF* and representative structures of FDO. **a**, $\text{Fe}_2(\text{II/II})$ -*SzPolF*. $\text{Fe}_2(\text{II/II})$ -*SzPolF* belongs to HDO superfamily with the distance of 4.9 Å between two irons. **b**, Stearoyl acyl carrier Δ^9 desaturase (PDB ID: 1AFR). The stearyl acyl carrier Δ^9 desaturase belongs to FDO family, and the distance of 4.2 Å between two irons¹⁹. **c**, Toluene/o-xylene monooxygenase $\text{Fe}_2(\text{II/II})$ -TmoA (PDB ID: 5TDV). TmnA belongs to FDO family, and the distance of 3.3 Å between two irons²⁰. **d**, *p*-aminobenzoate *N*-oxygenase $\text{Fe}_2(\text{II/II})$ -AurF (PDB ID: 3CHT)²¹. AurF belongs to FDO family, and the distance of 3.4 Å between two irons. FDO, ferritin-like diiron oxidase and oxygenase.



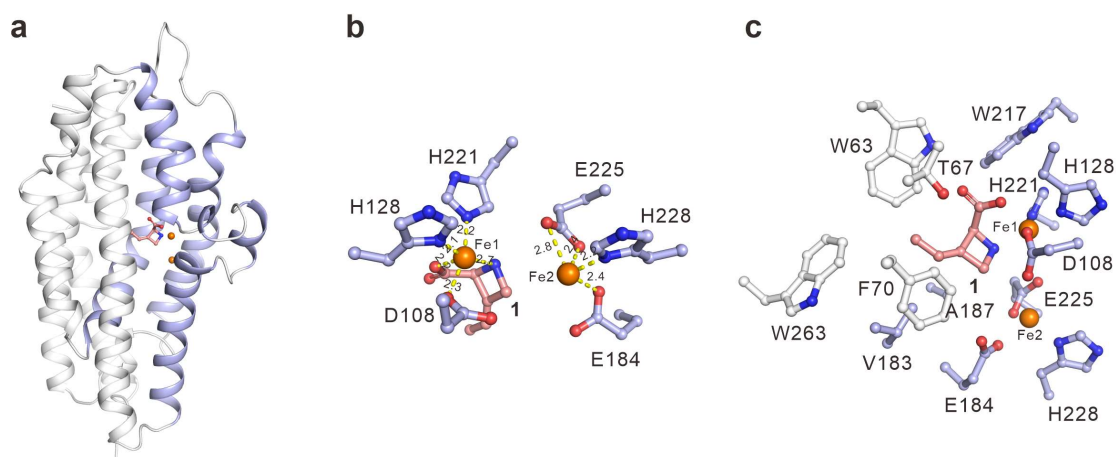
Supplementary Figure 93 | Protein architecture of O₂ reactivity with His/carboxylate coordinated to diiron cofactor. a, HDO central domain. **b**, Metallo- β -lactamase folds (PDB ID: 1QH5)²². **c**, HEAT repeat domain (PDB ID: 4D4Z)²³. **d**, TIM-barrels (PDB ID: 6OMP)²⁴. **e**, HD domain (PDB ID: 4N6W)²⁵.



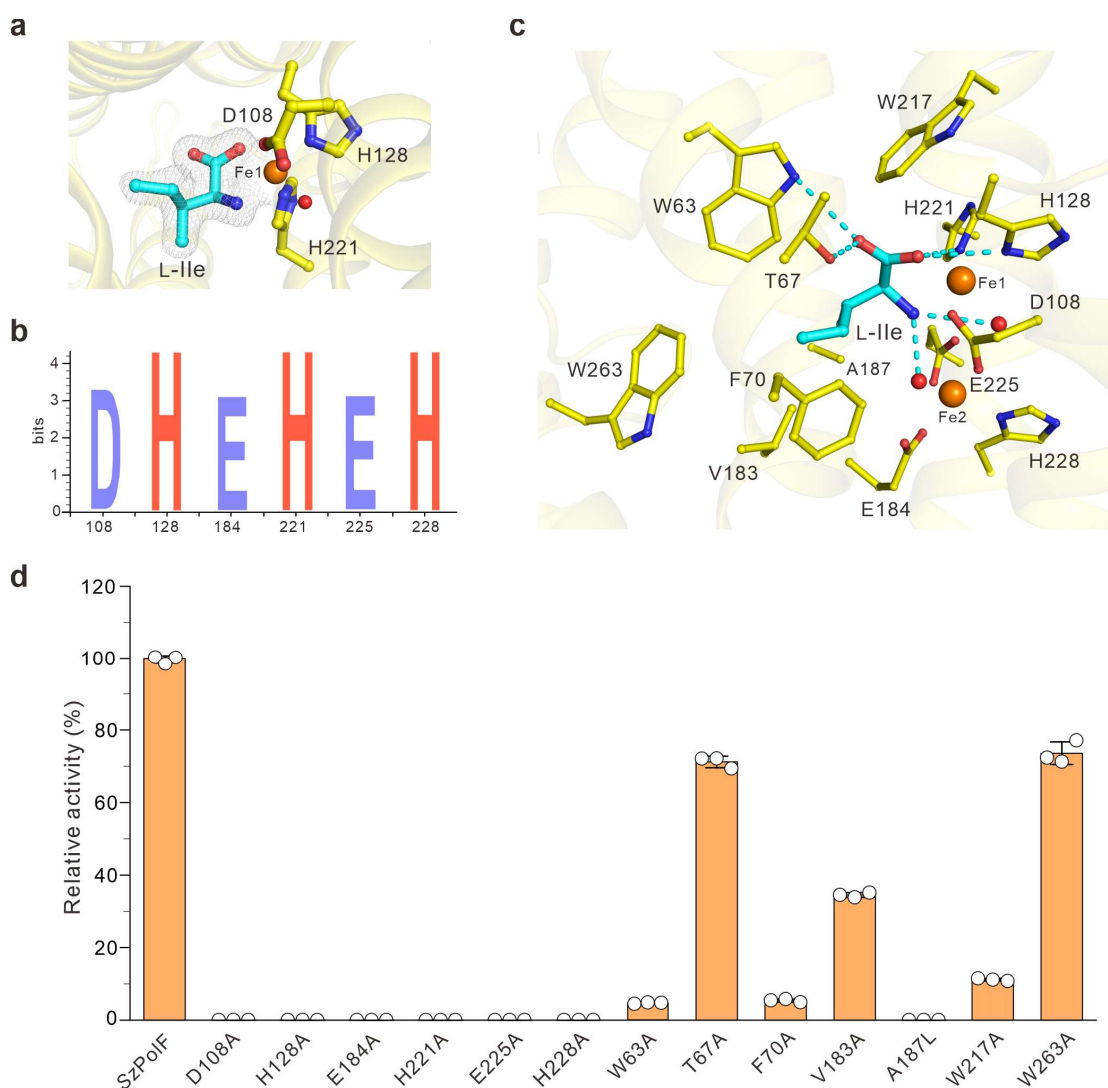
Supplementary Figure 94 | SDS-PAGE analysis of *SzPolF* variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file.



Supplementary Figure 95 | SDS-PAGE analysis of *SzPolF* variants correlating to substrate 2. Source data is provided as a Source Data file.



Supplementary Figure 96 | Crystal structure of $\text{Fe}_2(\text{II/II})$ -SzPolF-1 complex. **a**, Overall structure of $\text{Fe}_2(\text{II/II})$ -SzPolF-1 complex. **b**, Fe coordination sites. **c**, Product binding pocket of $\text{Fe}_2(\text{II/II})$ -SzPolF. The selected amino acid residues within 5 Å of **1**. The selected amino acid residues and **1** are shown in the stick and ball, and the Fe are illustrated as orange spheres.



Supplementary Figure 97 | Structural characterization of SzPolF-L-isoleucine and

functional analysis of its substrate-coordination sites. a, Overall structure of SzPolF bound

with the L-isoleucine. Selected amino acid residues and L-isoleucine (colored in blue) in the

active site of SzPolF are shown in the stick and ball, and Fe is illustrated as sphere. The $2F_o -$

F_c map is shown for L-isoleucine (grey mesh, contoured at 1.0σ). **b,** Amino acid occurrence of

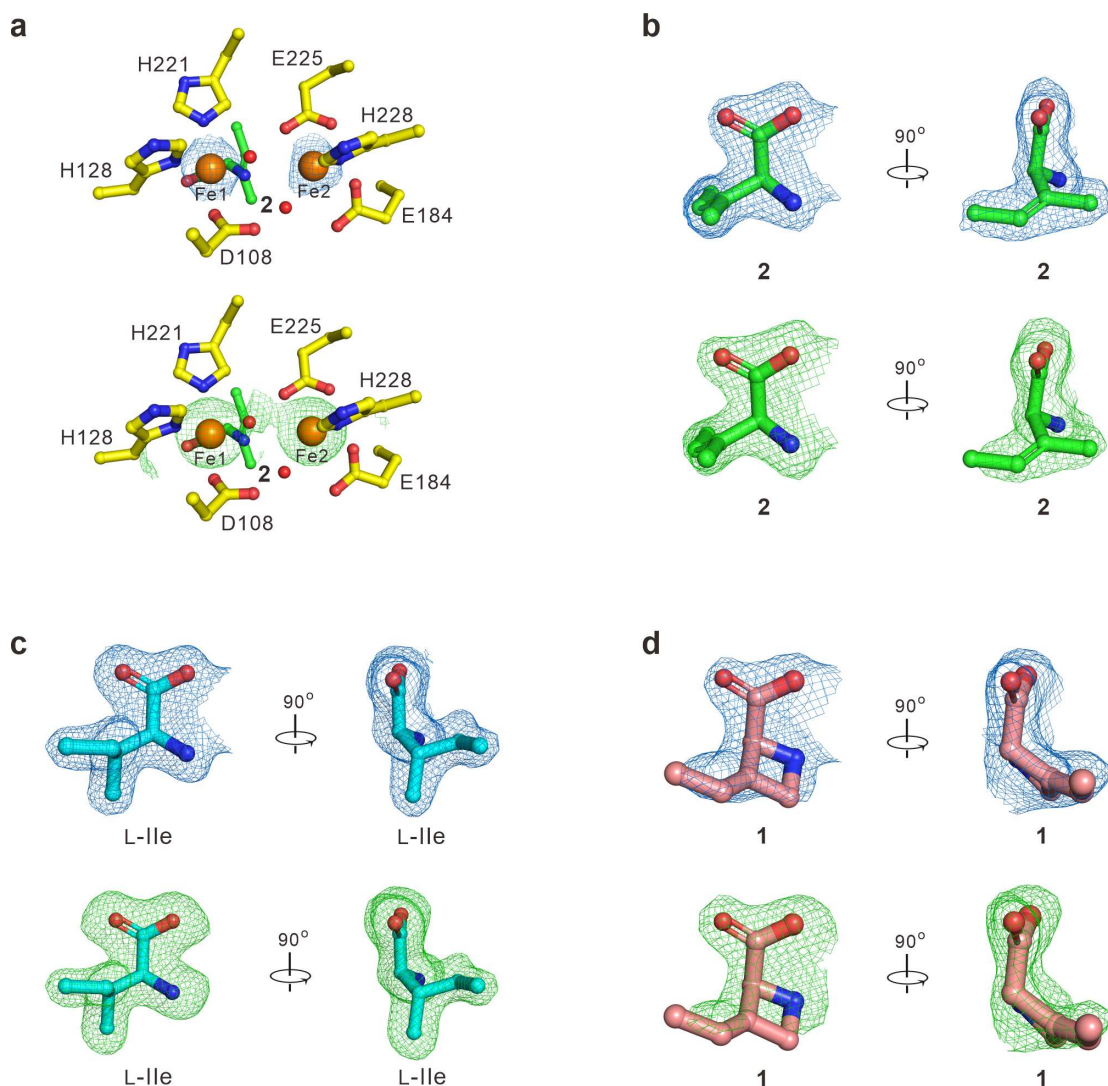
the conserved active sites in PolF and its homologs. The probability of amino acid occurrence,

within the diiron-cluster binding sites, was highlighted by sequence logo. **c,** Binding pocket of

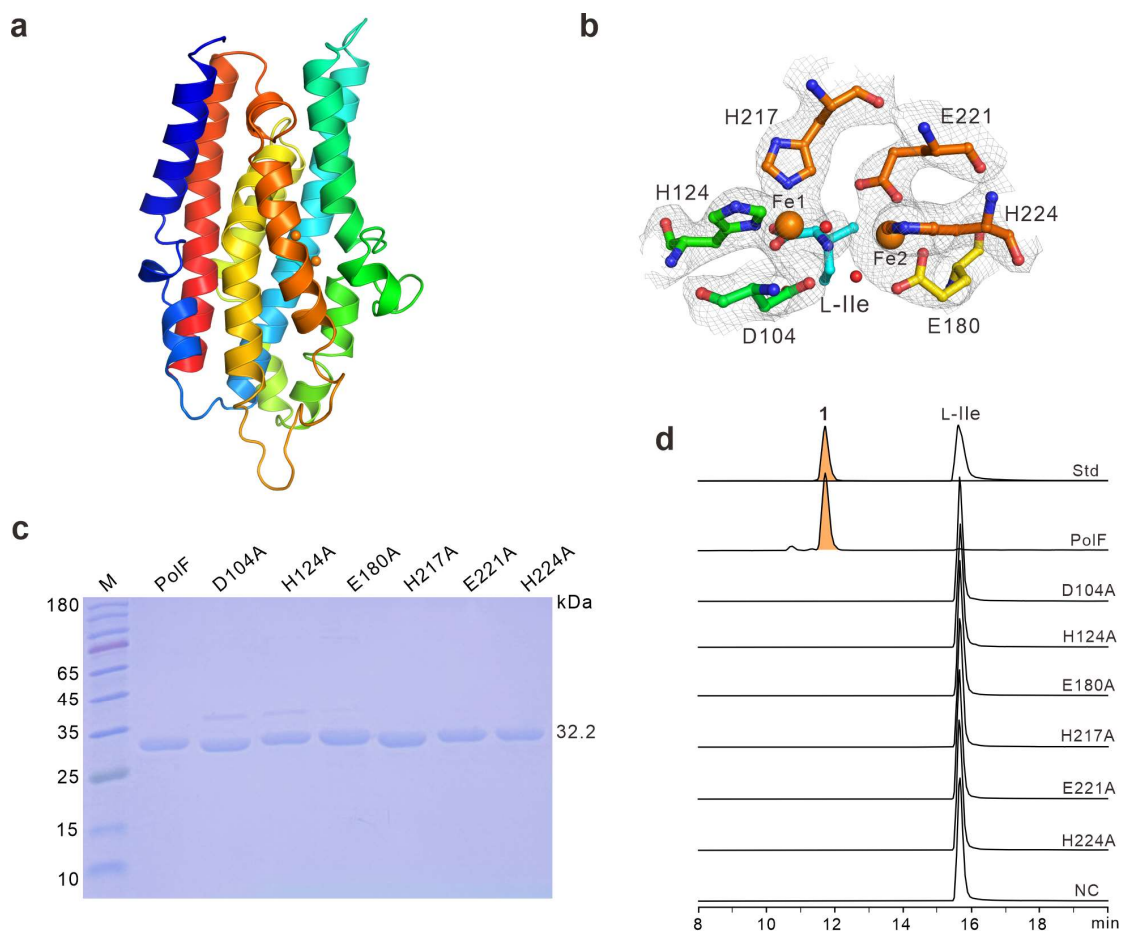
the L-isoleucine in SzPolF. Water molecule is shown as a red sphere, and the blue dashed lines

denote hydrogen bonds ($<5 \text{ \AA}$). **d,** The relative activity of SzPolF and its variants which binding

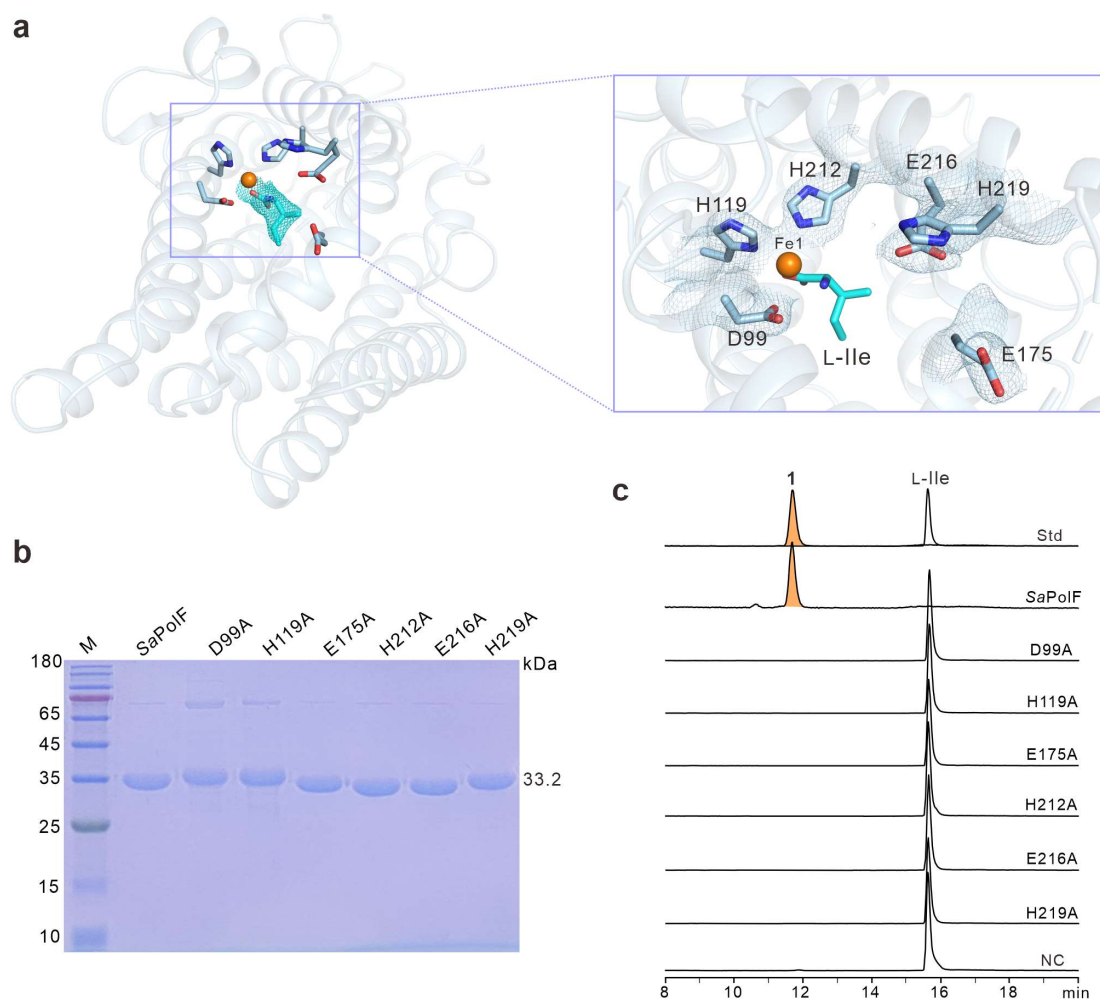
to diiron cofactors or form hydrogen bond interactions L-isoleucine. Wild-type activity was set to 100%, and the error bars represent the $\pm$ s.d. from three biological replicates, respectively. Source data is provided as a Source Data file.



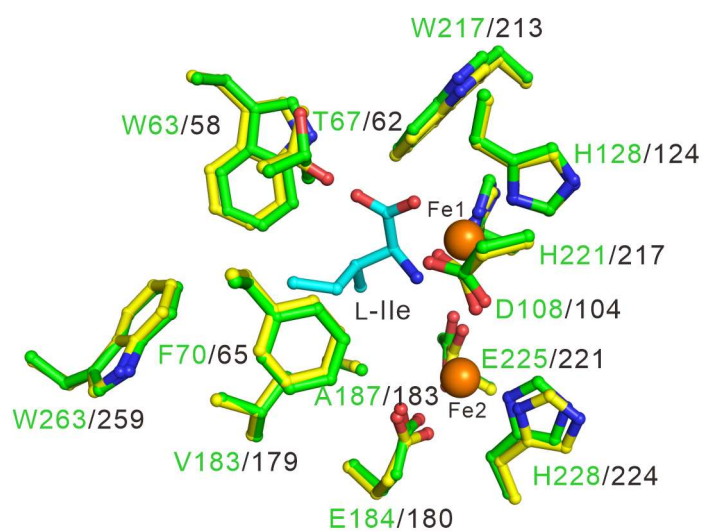
Supplementary Figure 98 | Electron maps of ligands bound in the *SzPolF*-2/*L*-isoleucine/1 complex structures. **a**, The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) and $F_o - F_c$ omit maps (shown as green mesh contoured to 2.5σ) of Fe ions (orange spheres), the Fe-coordinating water molecule (red sphere) and Fe-coordinating residues (yellow sticks). **b**, The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) and $F_o - F_c$ omit maps (shown as green mesh contoured to 2.5σ) of **2** (green stick). **c**, The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) and $F_o - F_c$ omit maps (shown as green mesh contoured to 2.5σ) of *L*-isoleucine (cyan stick). **d**, The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) and $F_o - F_c$ omit maps (shown as green mesh contoured to 2.5σ) of **1** (pink stick).



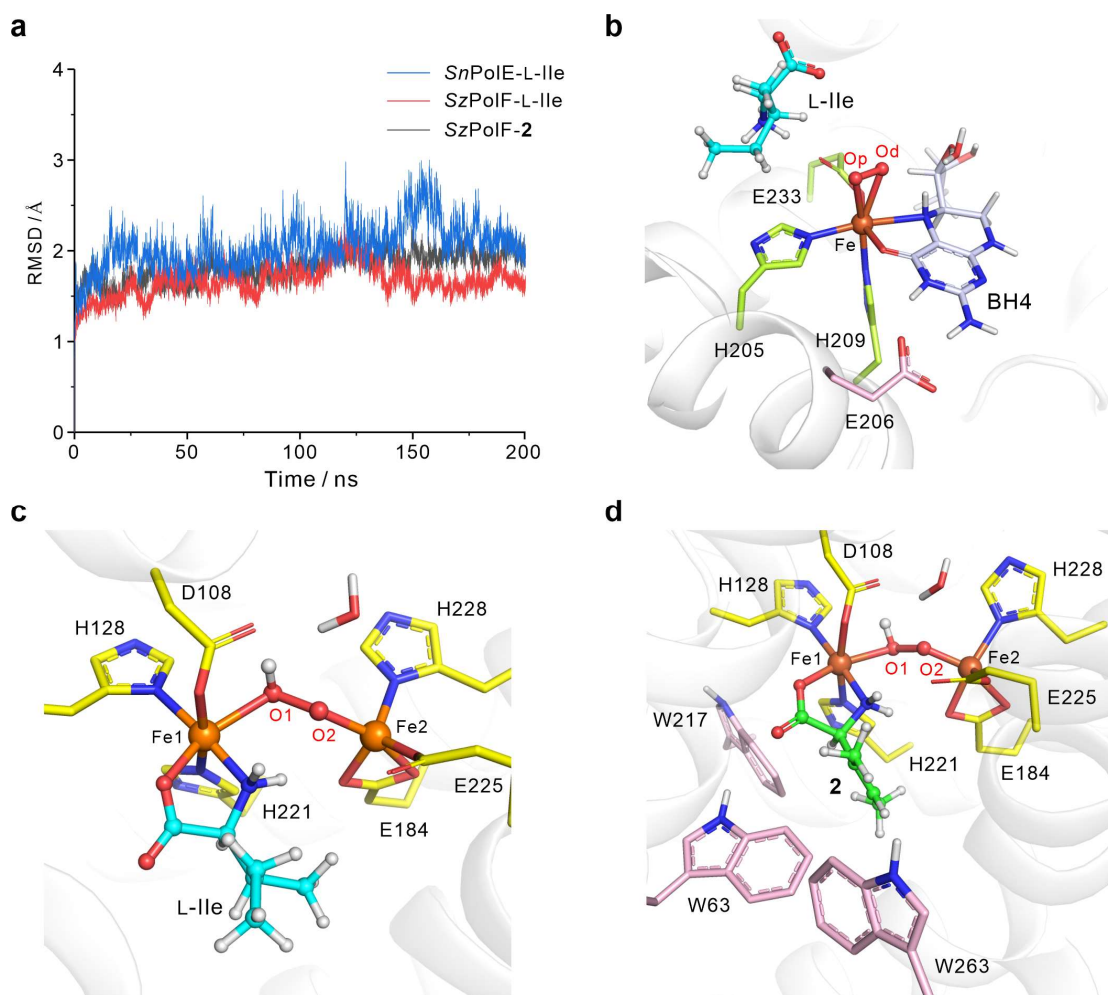
Supplementary Figure 99 | The Fe-coordination sites of PolF. **a**, Overall structure of $\text{Fe}_2(\text{II/II})$ -PolF-L-isoleucine complex. **b**, Fe coordination sites of PolF. The diiron cofactors (orange sphere) recruit L-isoleucine (blue stick) as a bidentate ligand. The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) of diiron cofactors, the Fe-coordinating water molecule (red sphere), Fe-coordinating residues and L-isoleucine (cyan stick). **c**, SDS-PAGE analysis of PolF variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file. **d**, *In vitro* characterization of PolF and the related variants correlating to Fe^{2+} binding sites. Std, the authentic standards of L-isoleucine and **1**; PolF, the PolF reaction; D104A, H124A, E180A, H217A, E221A, and H224A show the individual reactions of PolF variants; NC, the reaction without protein added as negative control.



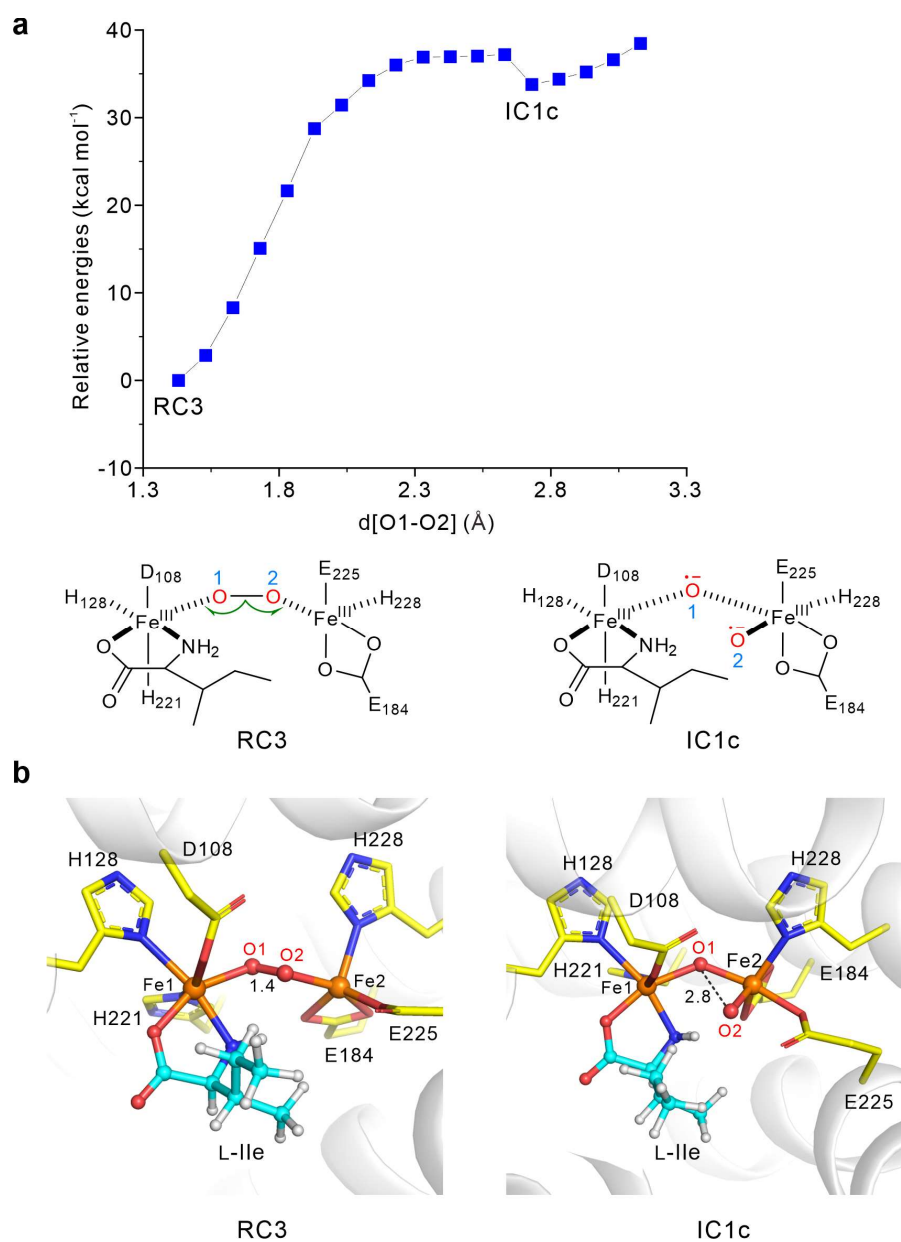
Supplementary Figure 100 | The Fe-coordination sites of SaPolF. **a**, Overall structure of Fe(II)-SaPolF-L-isoleucine complex with a zoom-in view of metal binding site. The $2F_o - F_c$ electron density maps (shown as blue mesh contoured to 1σ) of Fe ion (orange sphere), the Fe-coordinating water molecule (red sphere), Fe-coordinating residues and L-isoleucine (cyan stick). **b**, SDS-PAGE analysis of SaPolF variants correlating to Fe^{2+} binding sites. Source data is provided as a Source Data file. **c**, *In vitro* characterization of SaPolF and the related variants correlating to Fe^{2+} binding sites. Std, the authentic standards of L-isoleucine and **1**; SaPolF, the SaPolF reaction; D99A, H119A, E175A, H212A, E216A, and H219A show the individual reactions of SaPolF variants; NC, the reaction without protein added as negative control.



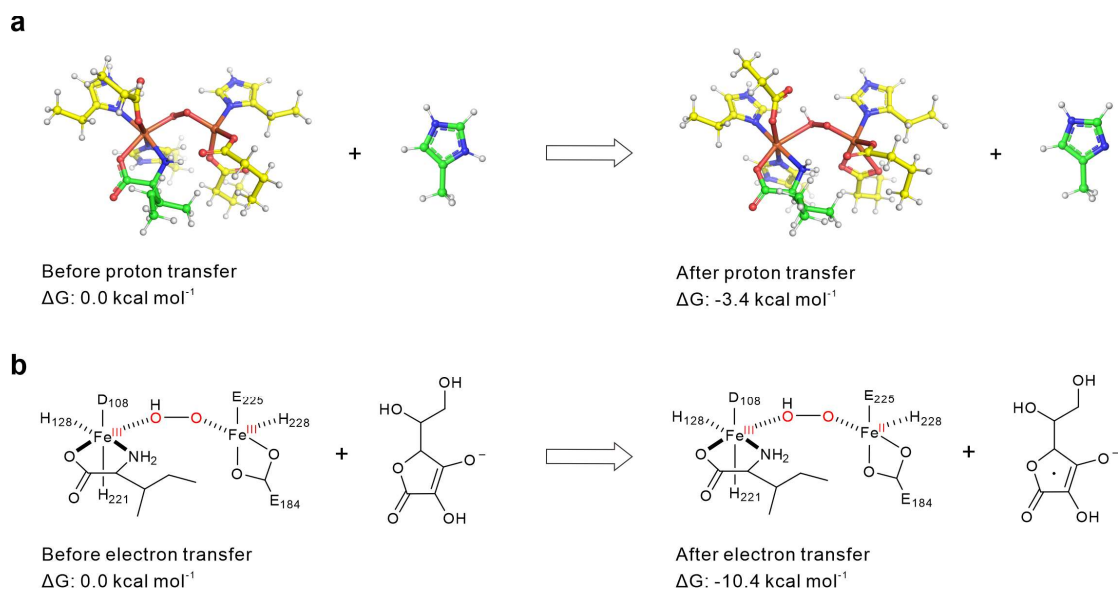
Supplementary Figure 101 | The substrate-binding pocket of Fe₂(II/II)-SzPolF and Fe₂(II/II)-PolF. The selected amino acid residues within 5 Å of the substrate in Fe₂(II/II)-SzPolF (blue stick) and Fe₂(II/II)-PolF (yellow stick) are shown in the stick and ball, and the Fe is illustrated as sphere.



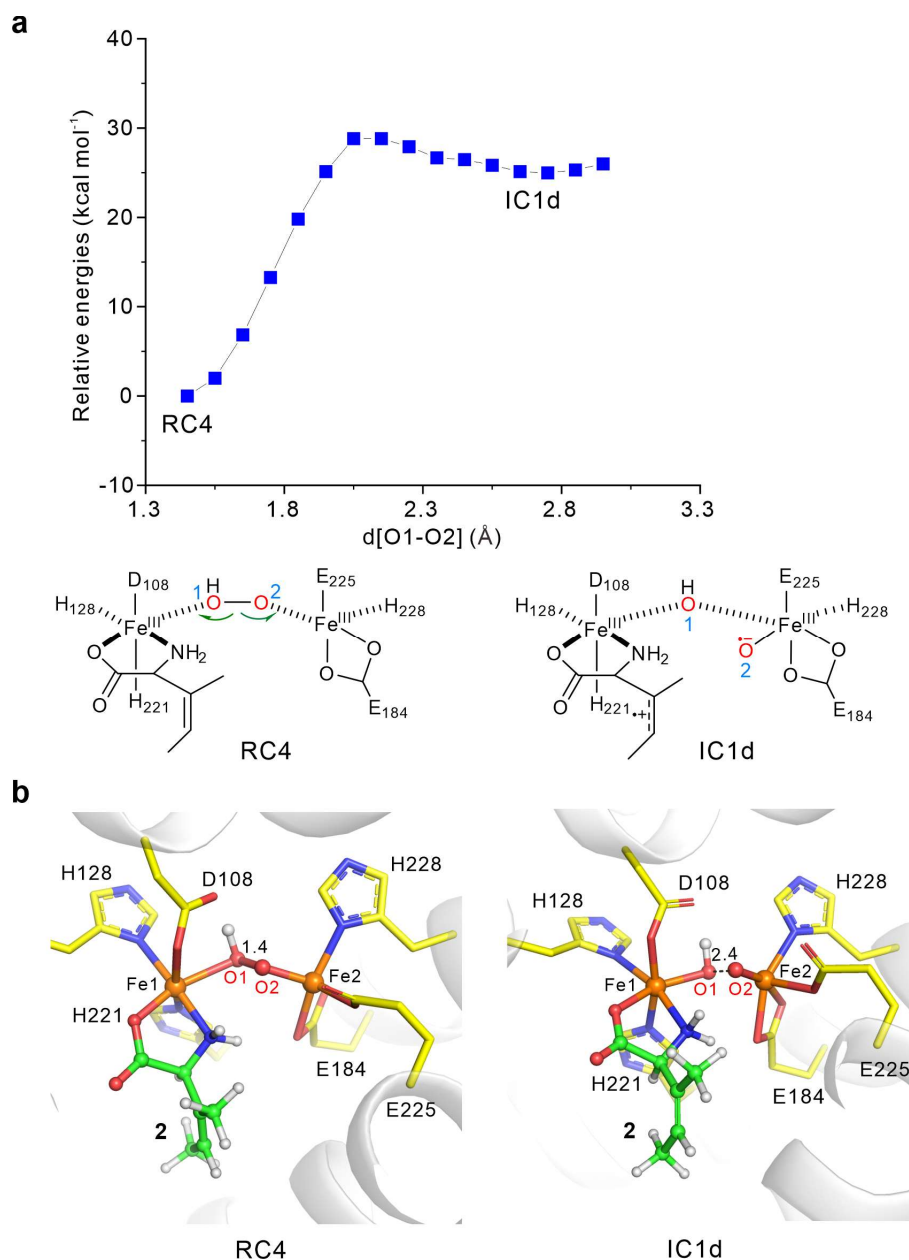
Supplementary Figure 102 | MD analysis results: RMSD profiles and most populated conformations of three substrate-binding proteins (*SnPolE*-L-Ile, *SzPolF*-L-Ile and *SzPolF*-2). **a**, Time-dependent root mean square deviations (RMSD) of the protein backbone and the substrates L-isoleucine or compound **2** during 200 ns molecular dynamics (MD) simulations. **b**, The most populated conformation of L-isoleucine bound to *SnPolE*. **c**, The most populated conformation of L-isoleucine bound to *SzPolF*. **d**, The most populated conformation of compound **2** bound to *SzPolF*. All most populated conformations were obtained from clustering analysis.



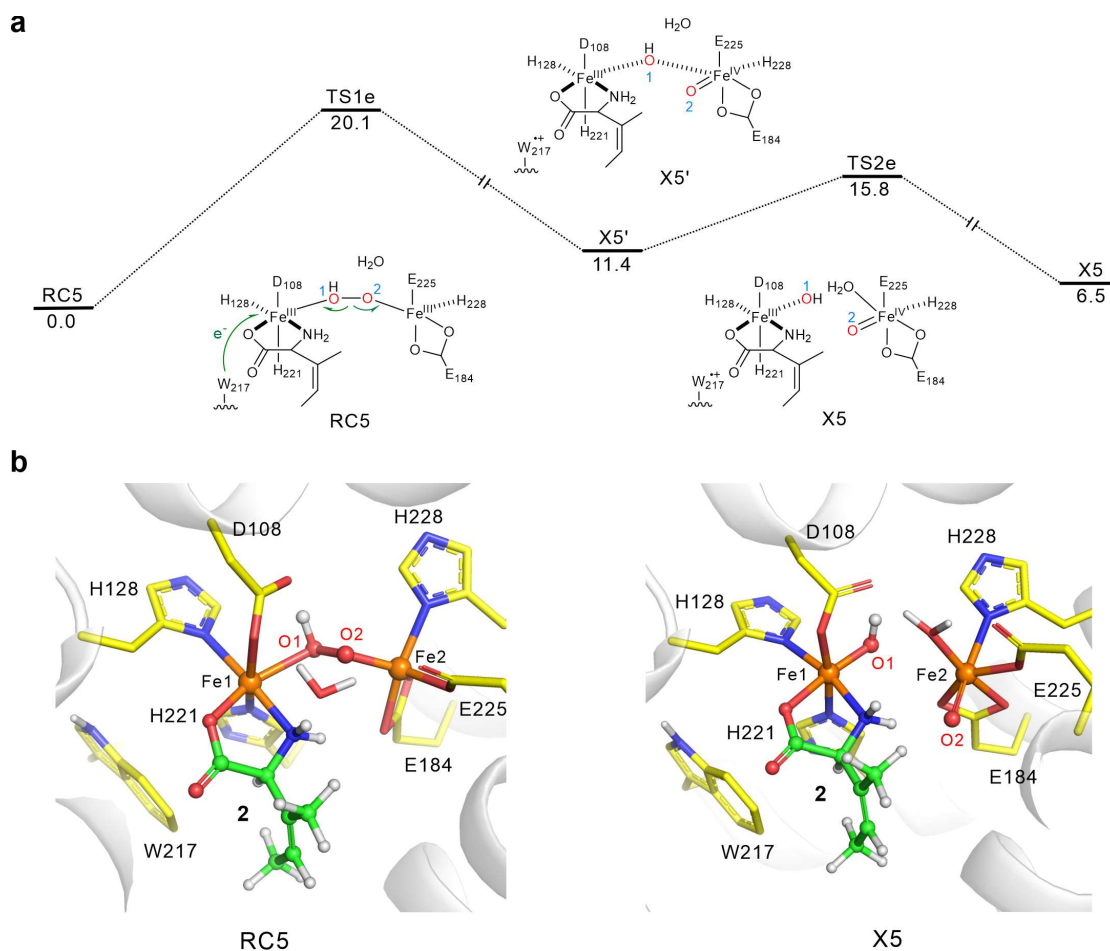
Supplementary Figure 103 | Reactivity analysis of Fe(III)Fe(III)-peroxo species. a, QM(UB3LYP-D3/B1)/MM scanned energy profile (in kcal mol⁻¹) for direct O-O cleavage of Fe(III)Fe(III)-peroxo species. **b,** QM(UB3LYP/B1)/MM optimized key intermediates structures (in Å).



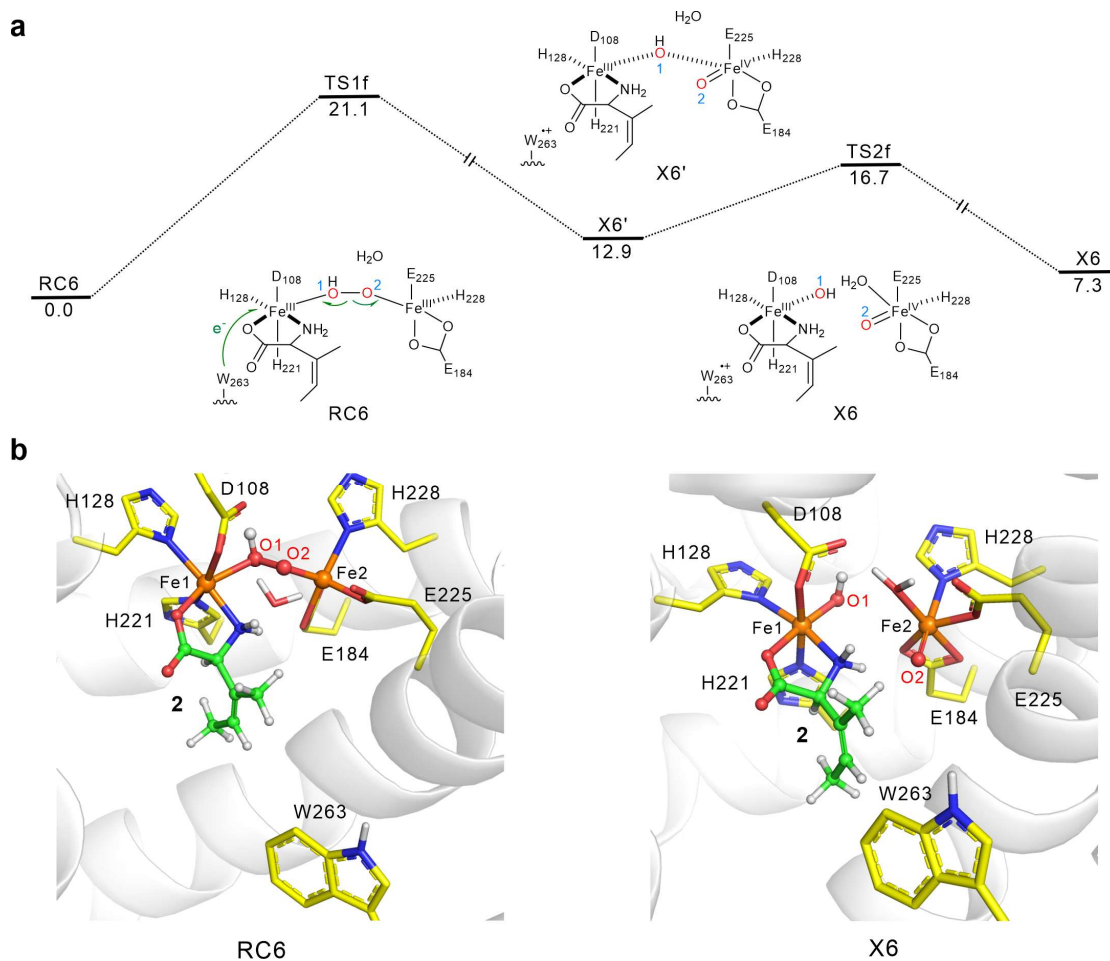
Supplementary Figure 104 | Transformation of Fe(III)Fe(III)-peroxo species. a, QM(B3LYP/def2-SVP) calculated free energy change (in kcal mol^{-1}) for the proton transfer from the histidine to unprotonated Fe(III)Fe(III)-peroxo species. **b,** QM(B3LYP/def2-SVP) calculated free energy change (in kcal mol^{-1}) for the electron transfer from the ascorbic acid anion to protonated Fe(III)Fe(III)-OOH species.



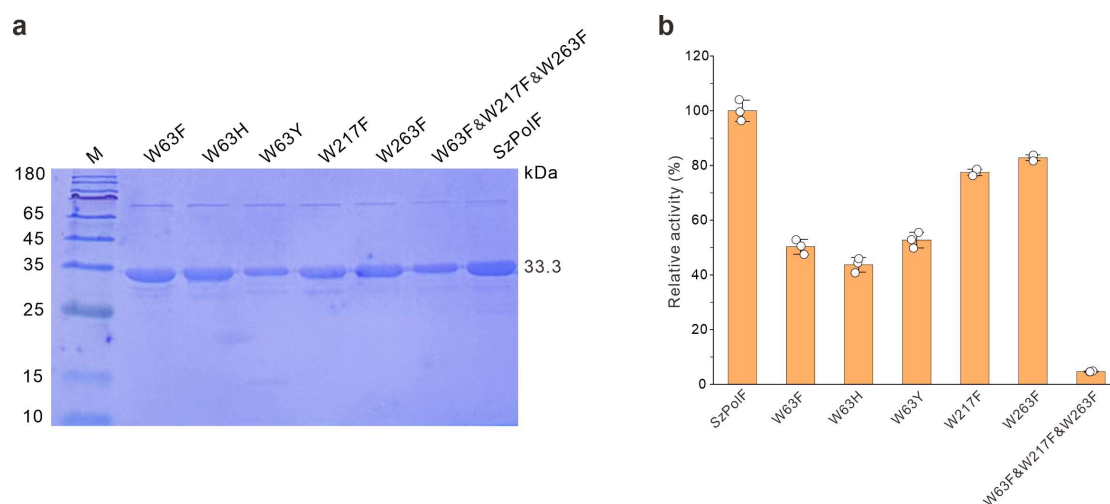
Supplementary Figure 105 | Reactivity analysis of Fe(III)Fe(III)-OOH species. a, QM(UB3LYP-D3/B1)/MM scanned energy profile (in kcal mol⁻¹) for the direct O-O cleavage of Fe(III)Fe(III)-OOH species. **b,** QM(UB3LYP/B1)/MM optimized key intermediates structures (in Å).



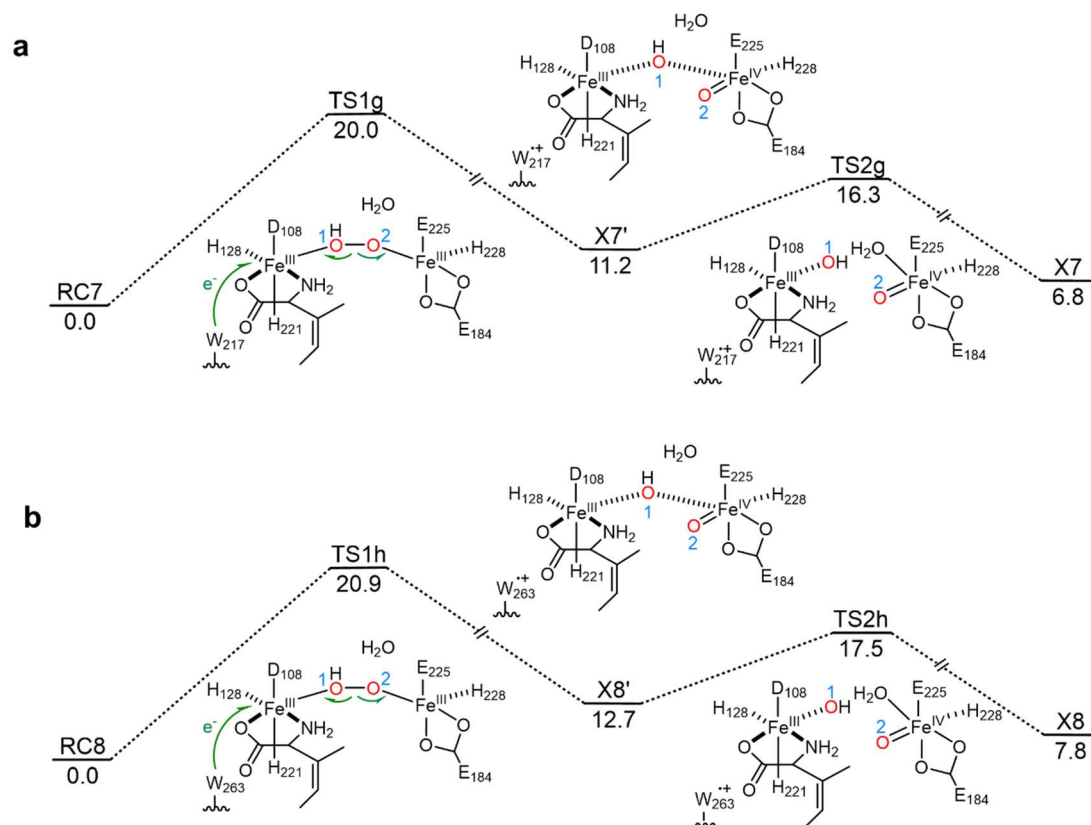
Supplementary Figure 106 | W217-mediated formation of the X5 species. **a**, The potential energy surface (in kcal mol⁻¹) for the formation of X5 was obtained from QM/MM calculations. **b**, QM(UB3LYP/B1)/MM optimized structures (in Å) involved in the transformation of RC5 into X5.



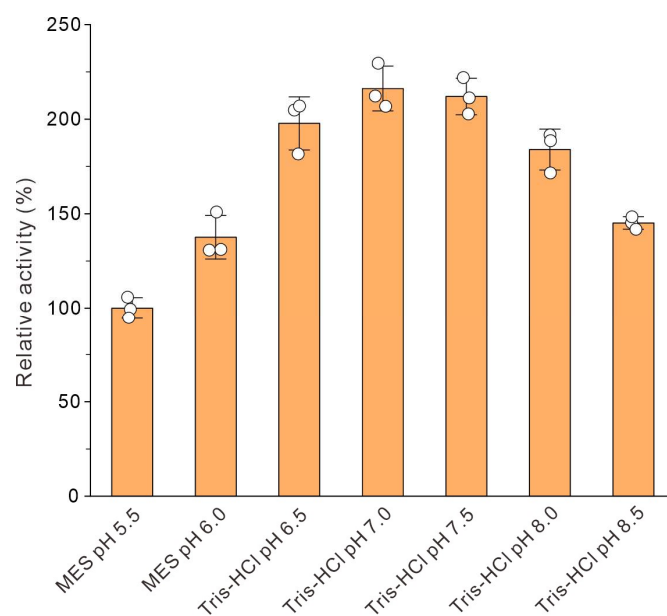
Supplementary Figure 107 | W263-mediated formation of the X6 species. **a**, The potential energy surface (in kcal mol⁻¹) for the formation of X6 was obtained from QM/MM calculations. **b**, QM(UB3LYP/B1)/MM optimized structures (in Å) involved in the transformation of RC6 into X6.



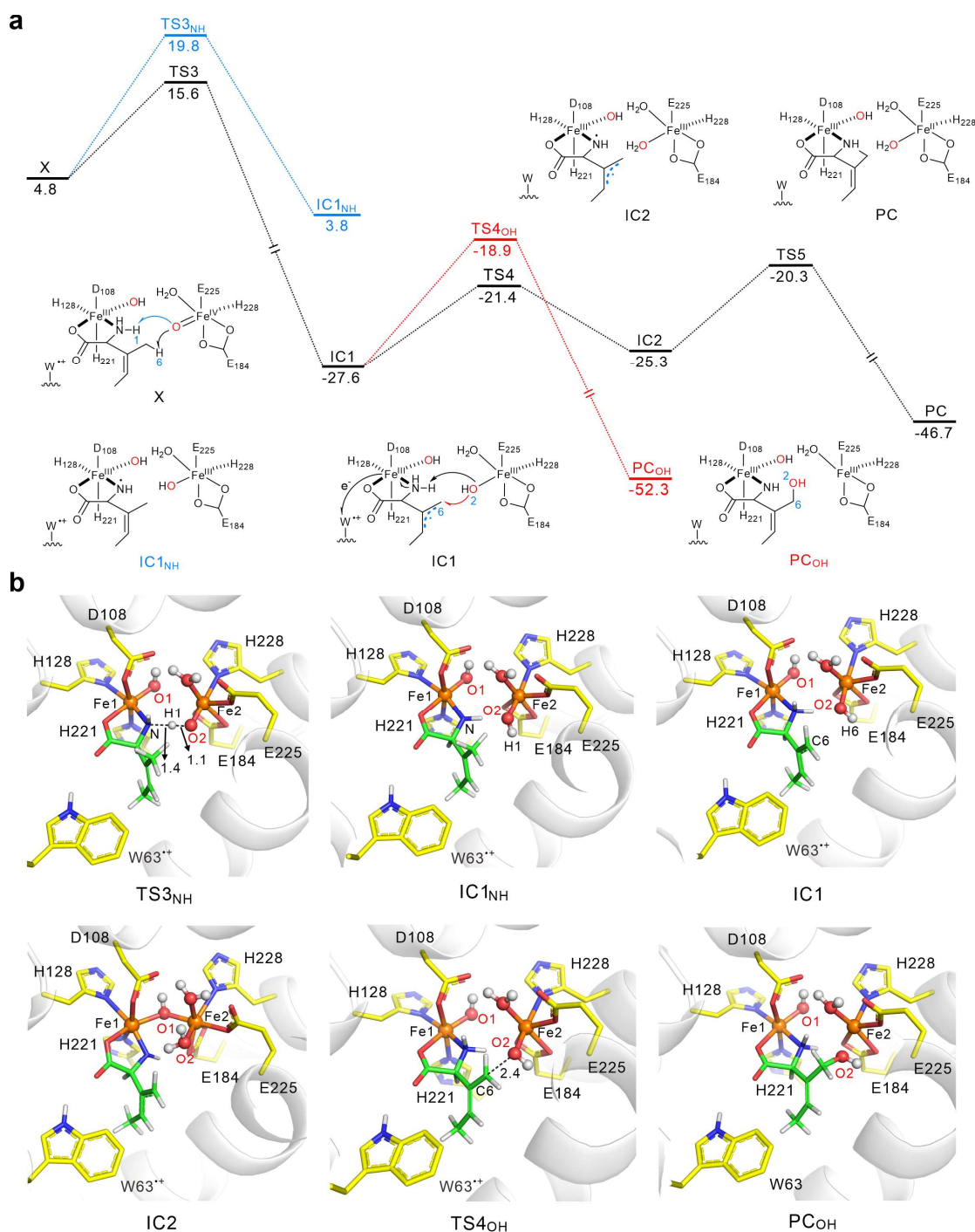
Supplementary Figure 108 | SDS-PAGE analysis and relative activity of W63 related variants. a, SDS-PAGE analysis of the W63 related variants of *SzPolF*. **b,** The relative activity of W63 related variants of *SzPolF*. Source data is provided as a Source Data file.



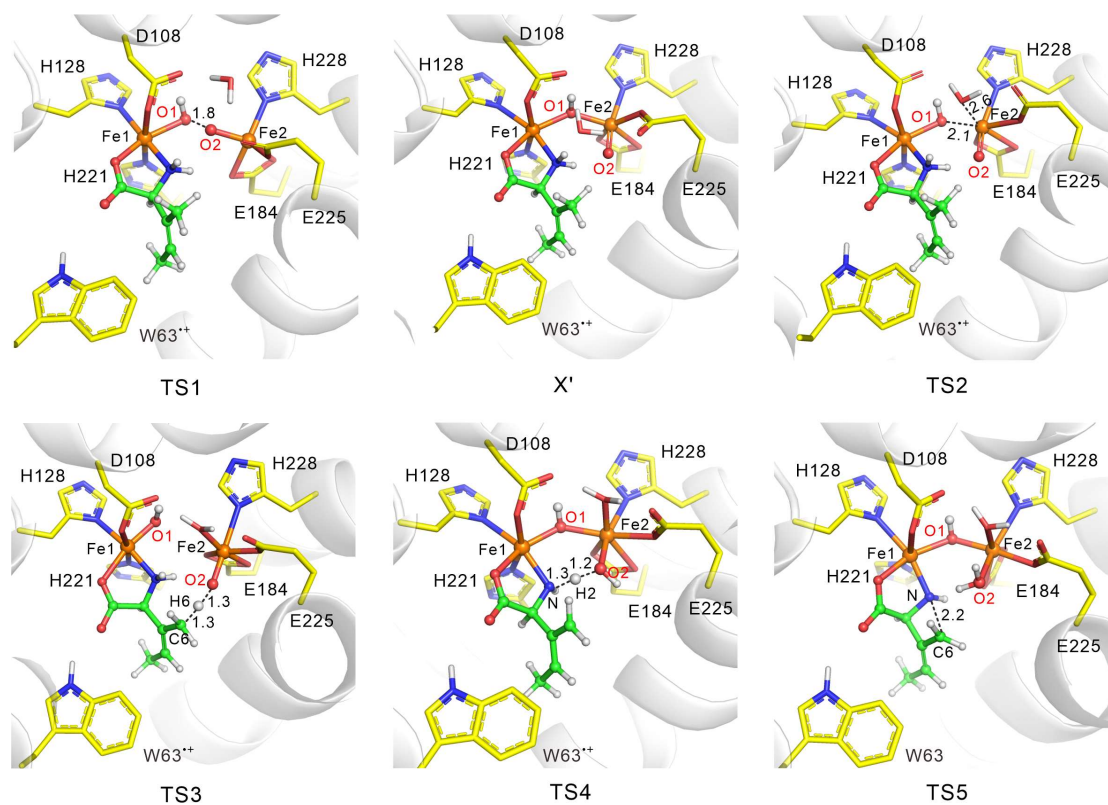
Supplementary Figure 109 | W263 and W217 mediate the formation of X7 and X8 in the W63F mutant. **a**, The potential energy surface (in kcal mol⁻¹) for the formation of X7 was obtained from QM/MM calculations. **b**, The potential energy surface (in kcal mol⁻¹) for the formation of X8 was obtained from QM/MM calculations.



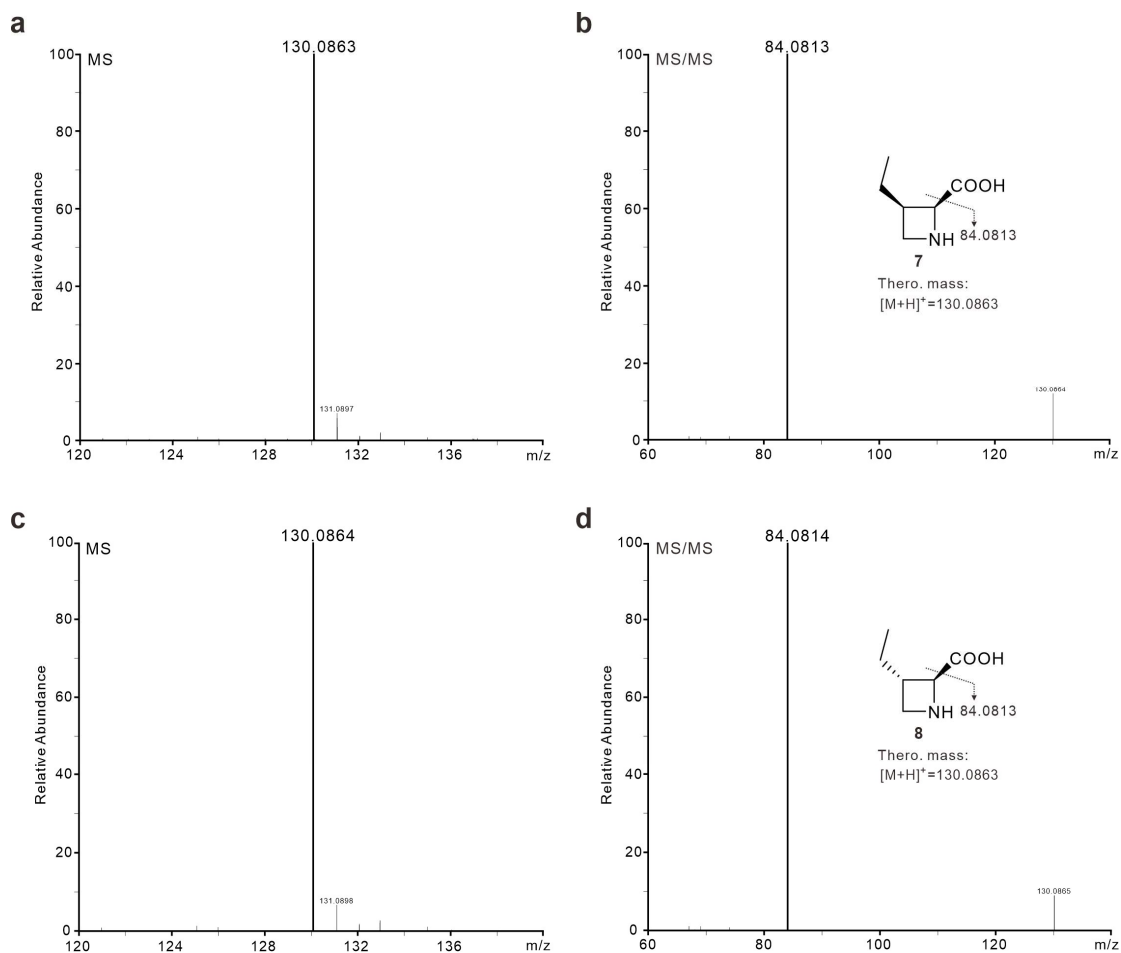
Supplementary Figure 110 | Related activity of SzPolF under different pH. Source data is provided as a Source Data file.



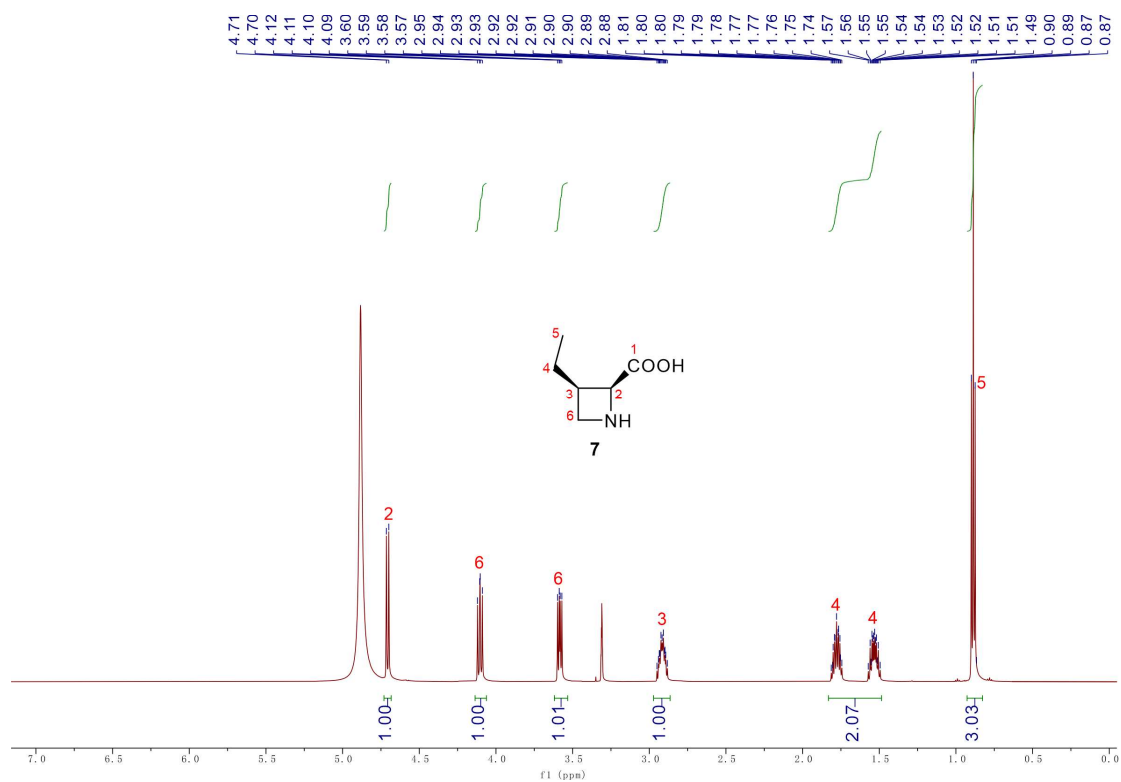
Supplementary Figure 111 | Competing pathways for the construction of azetidine by the *Sz*PolF enzyme. **a**, The potential energy surface (in kcal mol⁻¹) of *Sz*PolF-catalyzed intramolecular cyclization obtained from QM/MM calculations. **b**, The structures of key intermediates involved in *Sz*PolF-catalyzed intramolecular cyclization reaction.



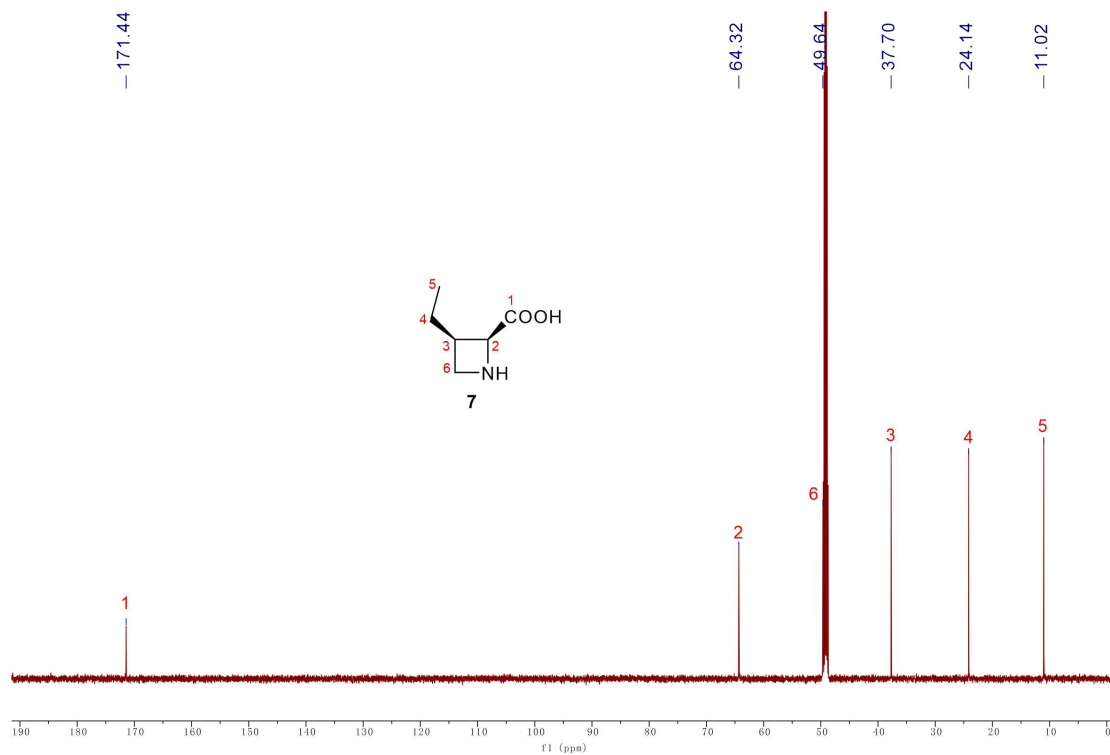
Supplementary Figure 112 | Structures of key intermediates and transition state involved in azetidine-construction by *S₂PolF*. QM(UB3LYP/B1)/MM optimized structures (in Å) involved in the transformation of RC into PC.



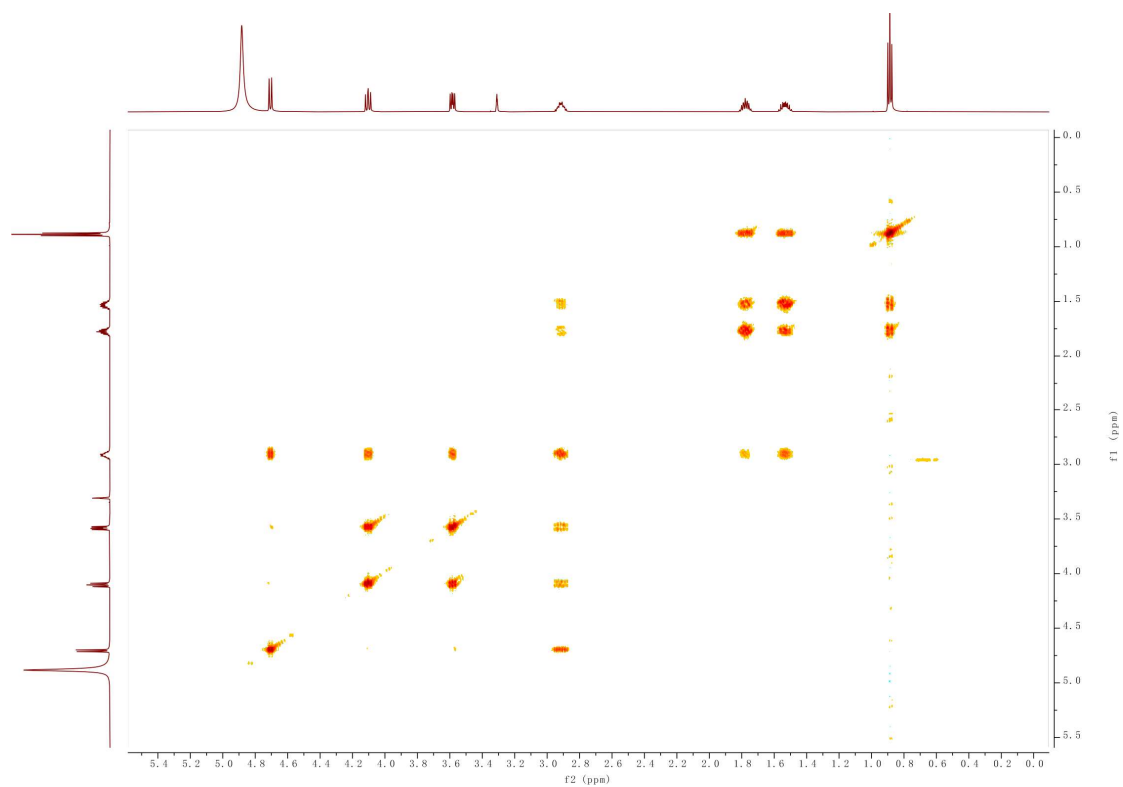
Supplementary Figure 113 | LC-HRMS analysis of the compound 7 and 8. a, LC-HRMS analysis of compound **7**. **b,** LC-HRMS/MS analysis of compound **7**. The theoretical fragmentation pattern of **7** is included as a control. **c,** LC-HRMS analysis of compound **8**. **d,** LC-HRMS/MS analysis of compound **8**. The theoretical fragmentation pattern of **8** is included as a control.



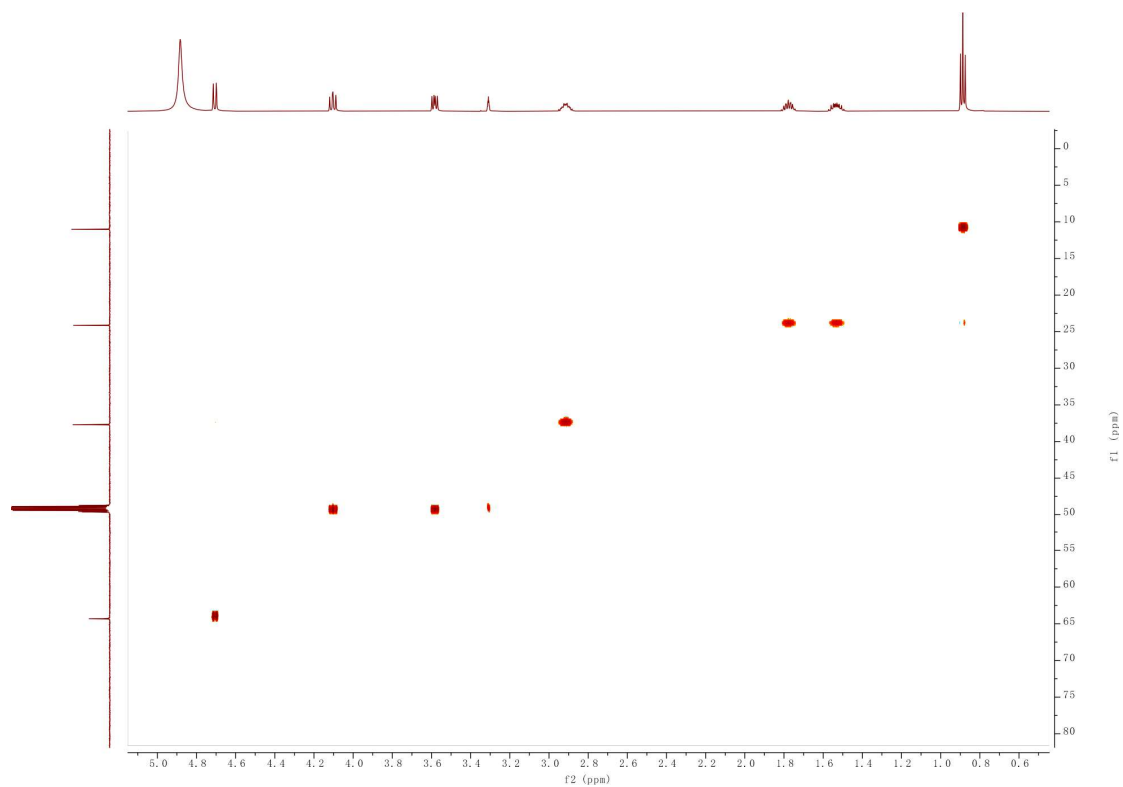
Supplementary Figure 114 | ¹H NMR spectrum of compound 7 (CD₃OD, 600 MHz).



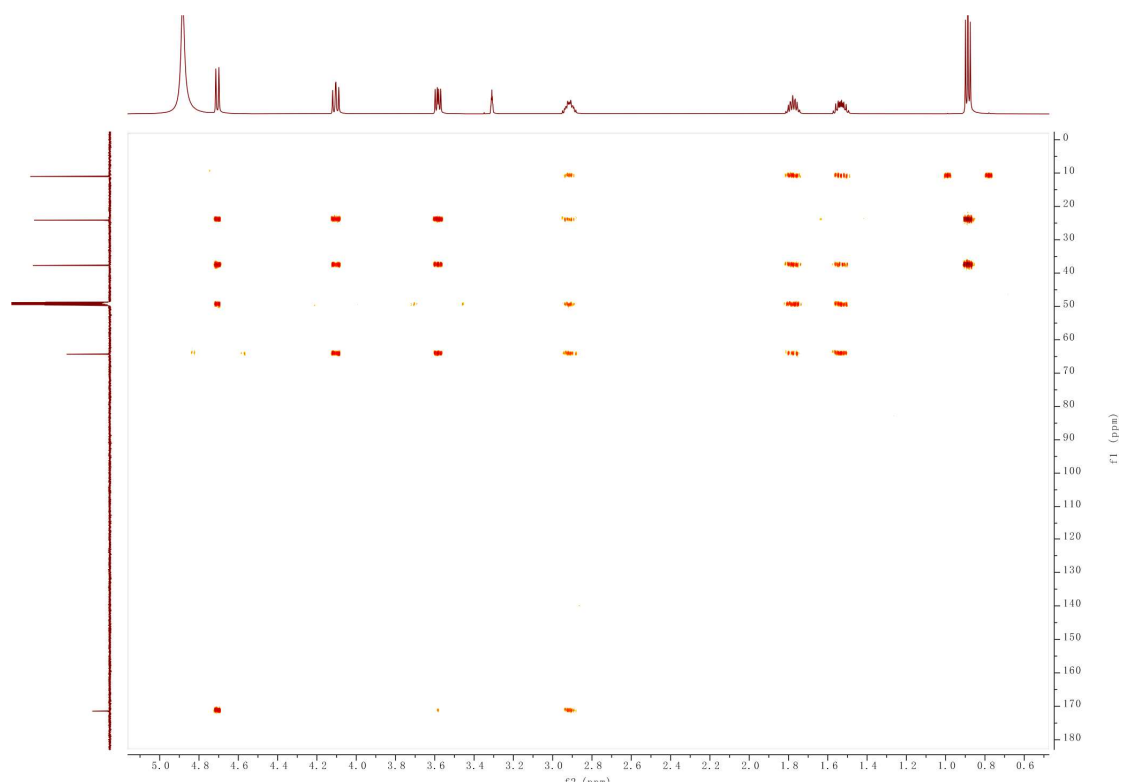
Supplementary Figure 115 | ¹³C NMR spectrum of compound 7 (CD₃OD, 150 MHz).



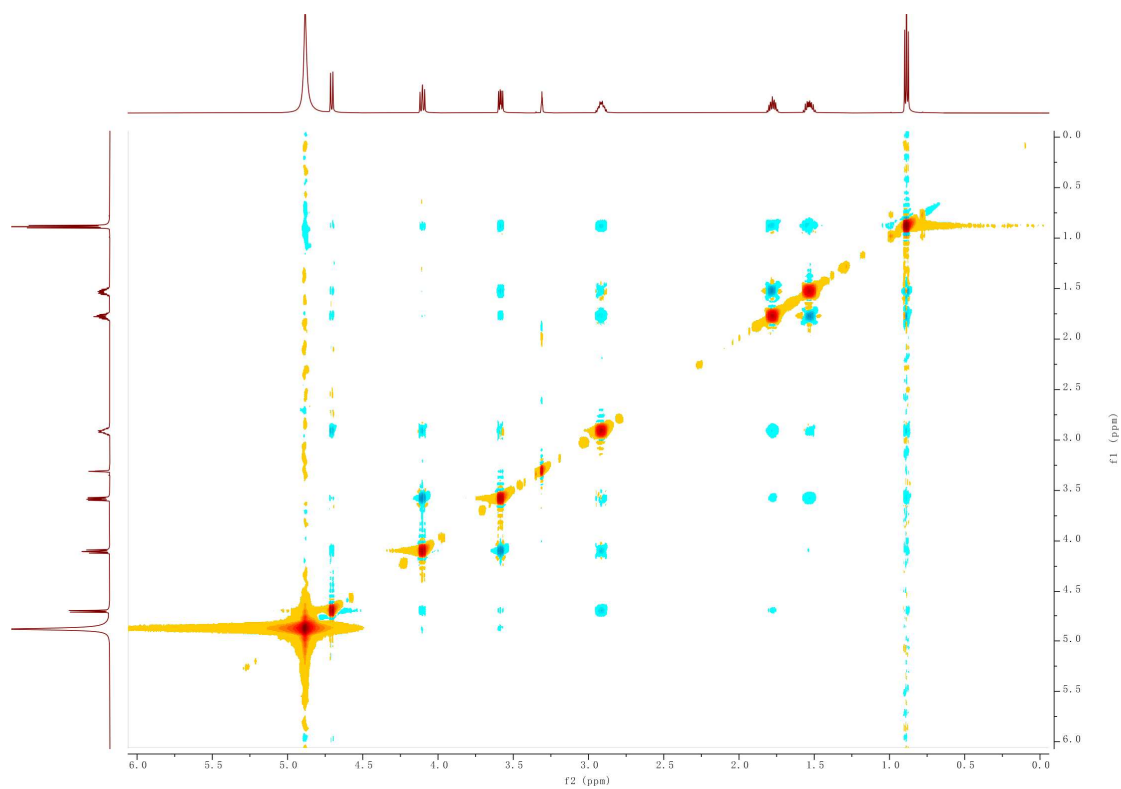
Supplementary Figure 116 | ^1H - ^1H COSY spectrum of compound 7 (CD_3OD , 600 MHz).



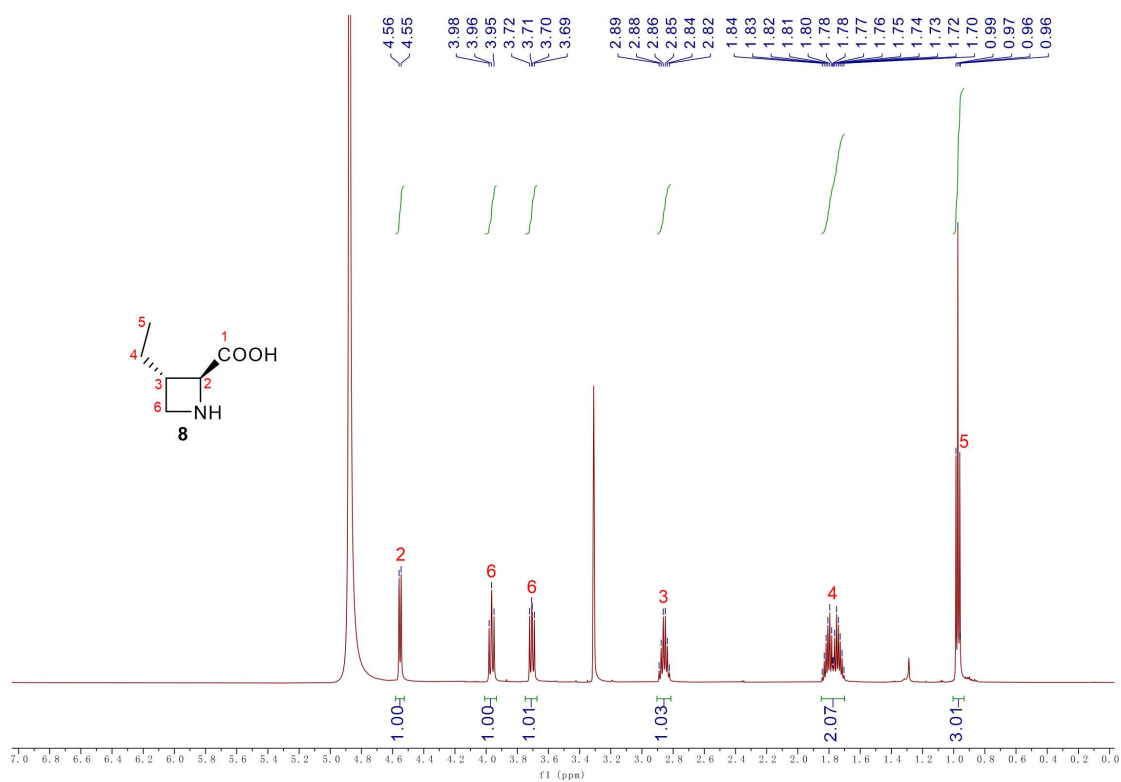
Supplementary Figure 117 | HSQC spectrum of compound 7 (CD_3OD , 600 MHz).



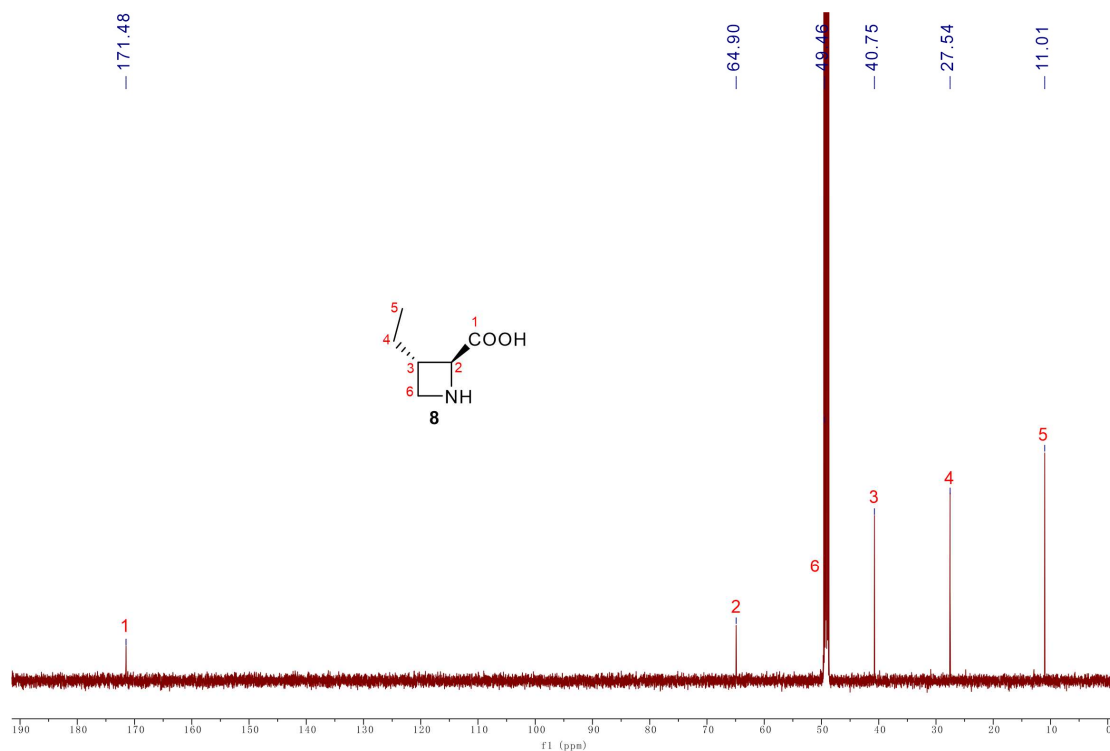
Supplementary Figure 118 | HMBC spectrum of compound 7 (CD₃OD, 600 MHz).



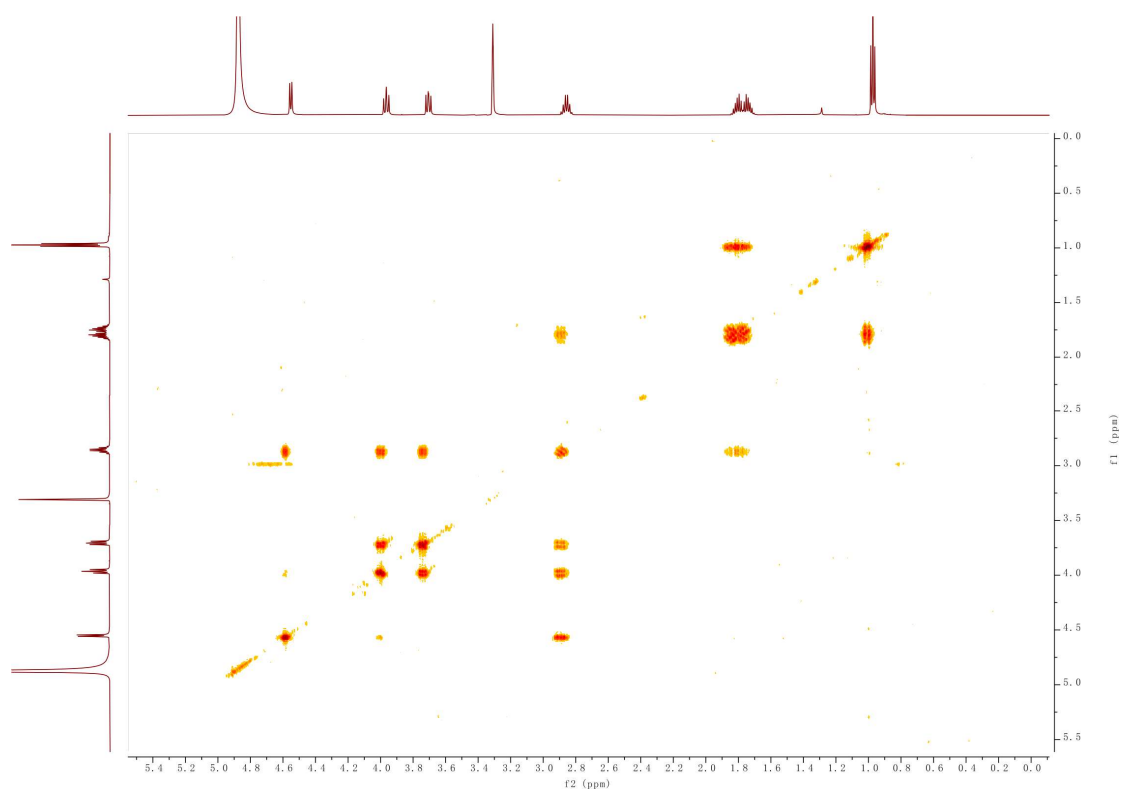
Supplementary Figure 119 | NOESY spectrum of compound 7 (CD₃OD, 600 MHz).



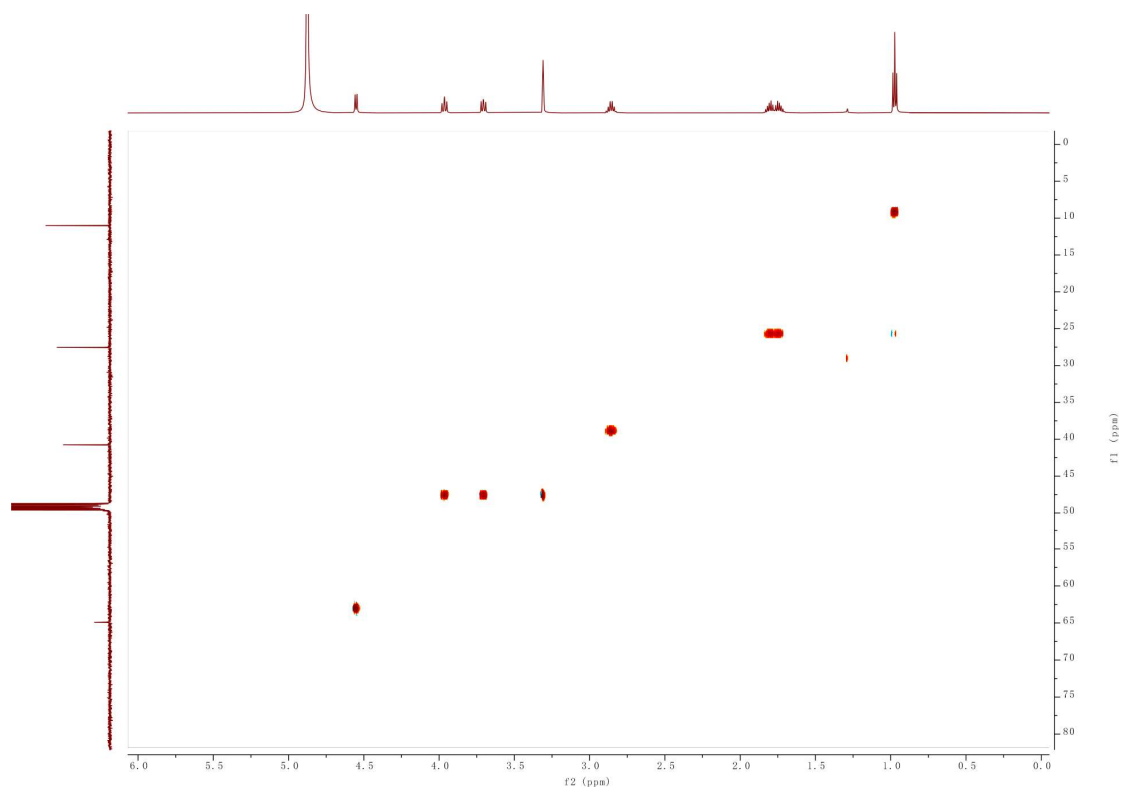
Supplementary Figure 120 | ¹H NMR spectrum of compound 8 (CD₃OD, 600 MHz).



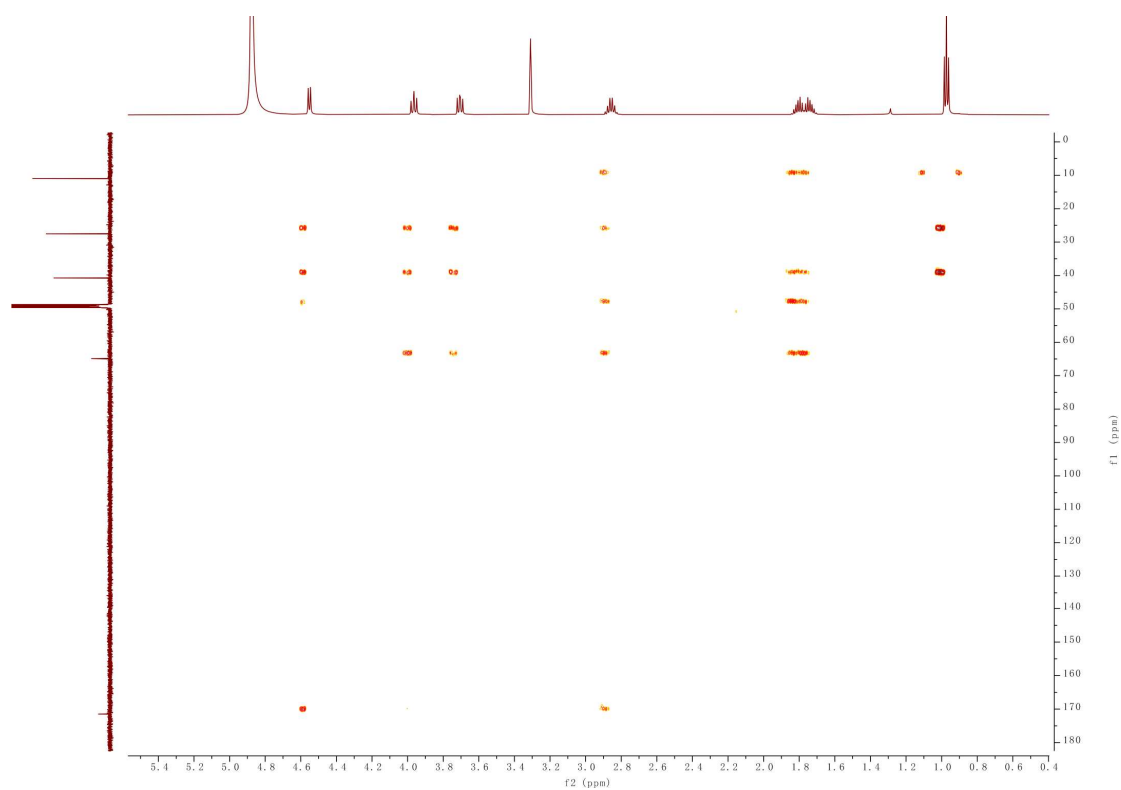
Supplementary Figure 121 | ¹³C NMR spectrum of compound 8 (CD₃OD, 150 MHz).



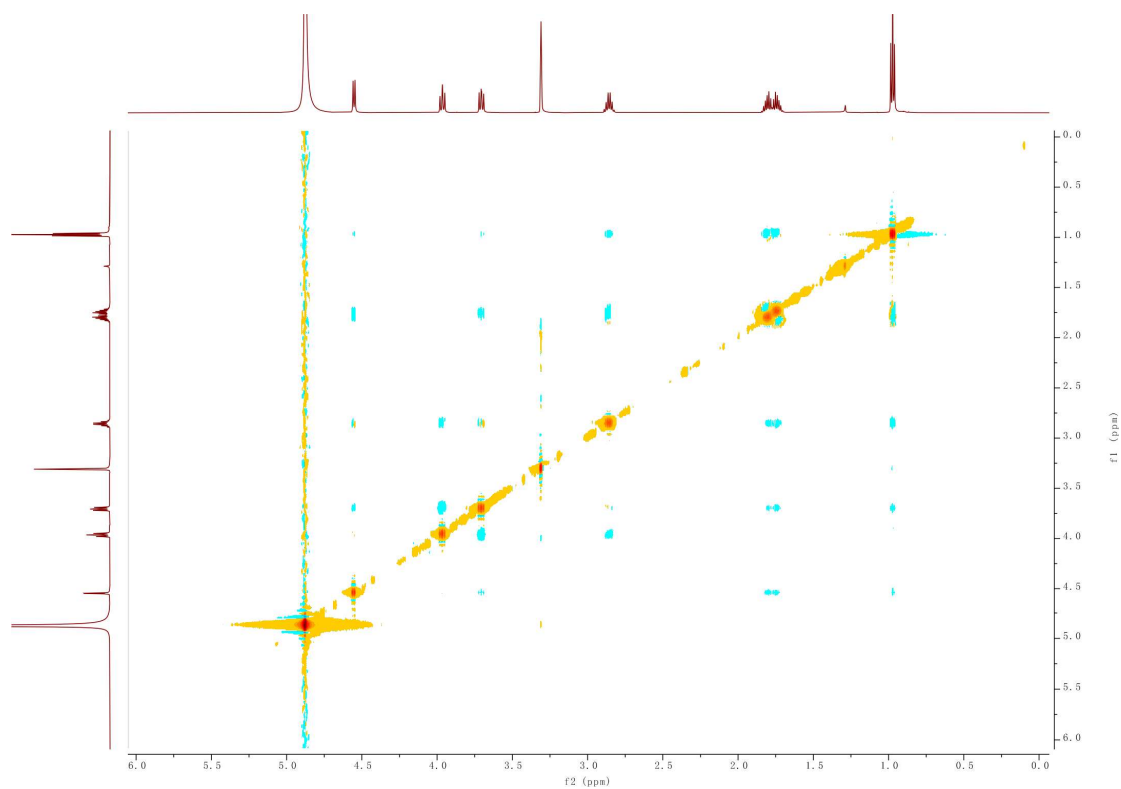
Supplementary Figure 122 | ^1H - ^1H COSY spectrum of compound 8 (CD_3OD , 600 MHz).



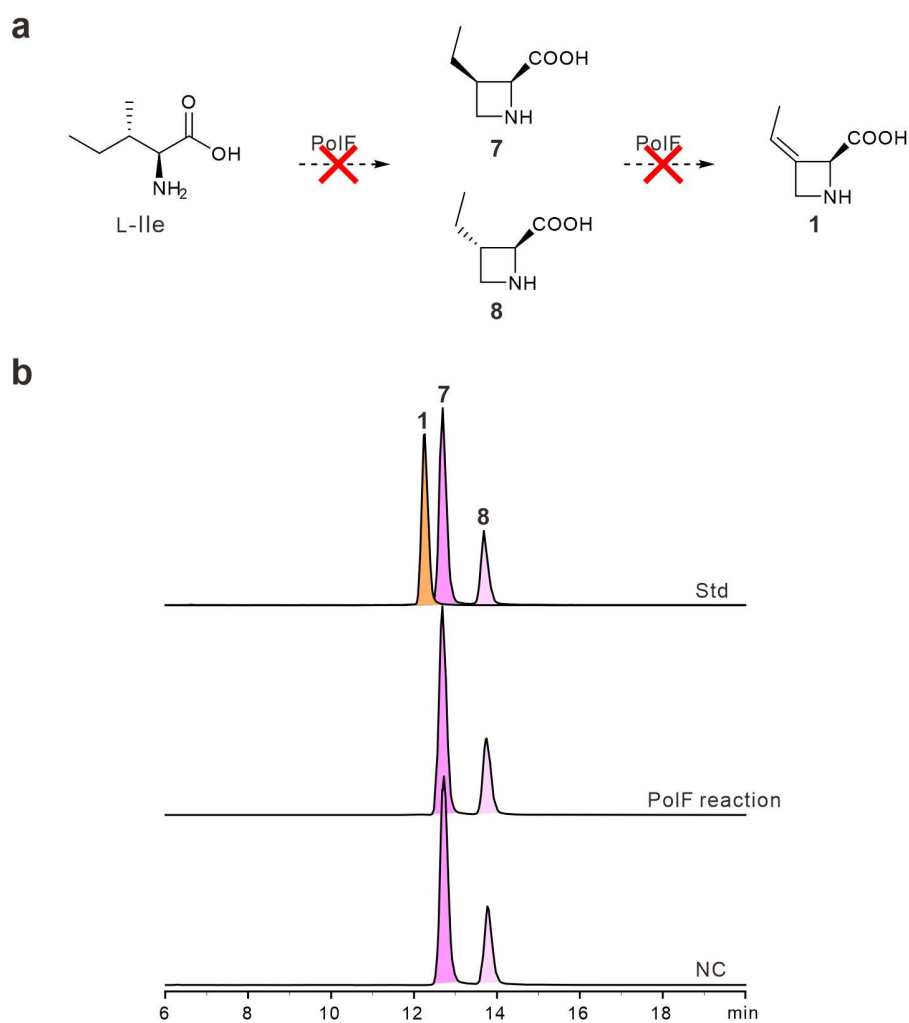
Supplementary Figure 123 | HSQC spectrum of compound 8 (CD_3OD , 600 MHz).



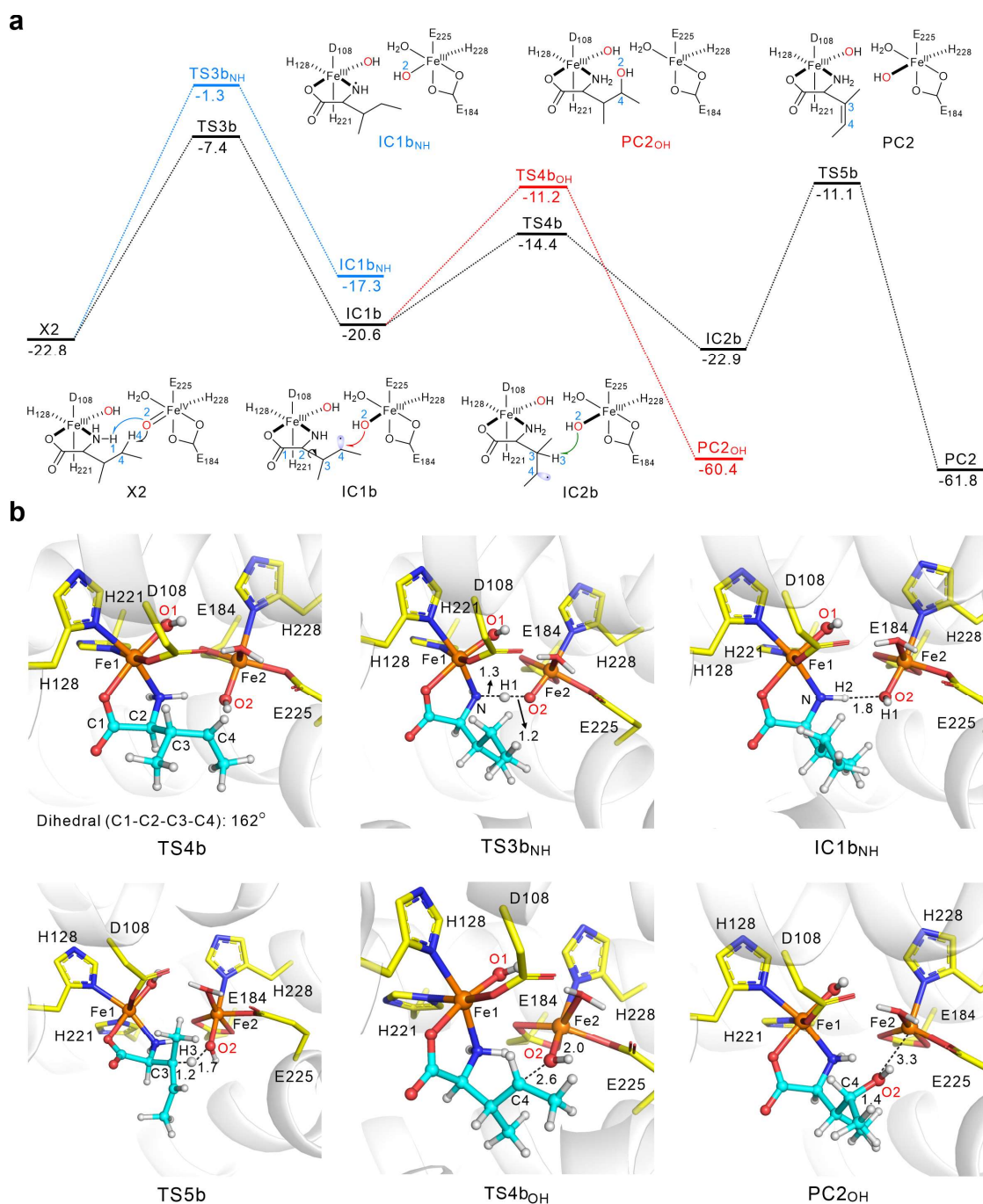
Supplementary Figure 124 | HMBC spectrum of compound 8 (CD₃OD, 600 MHz).



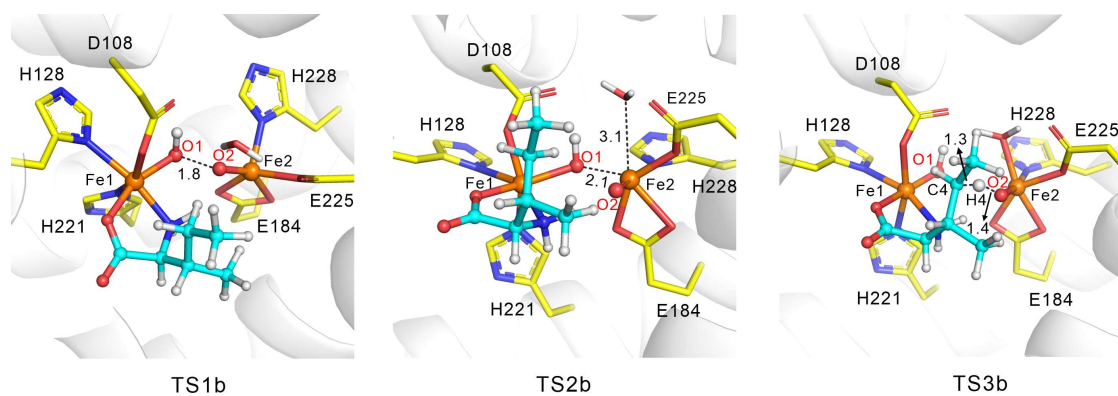
Supplementary Figure 125 | NOESY spectrum of compound 8 (CD₃OD, 600 MHz).



Supplementary Figure 126 | LC-HRMS analysis of the PolF reaction with 7 and 8 as substrates. a, Schematic of the proposed catalytic process by PolF. **b,** LC-HRMS analysis of the PolF reaction with 7 and 8 as substrates.



Supplementary Figure 127 | Competing pathways for the formation of product 2 by the SzPolF enzyme. **a**, The potential energy surface (in kcal mol⁻¹) of SzPolF-catalyzed desaturation reaction obtained from QM/MM calculations. **b**, The structures of key intermediates involved in SzPolF-catalyzed desaturation reaction.

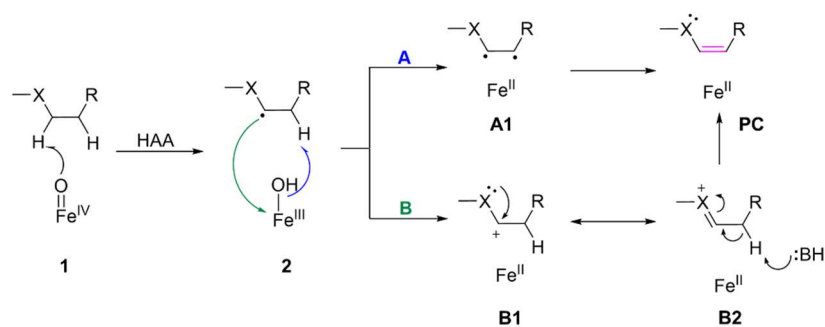


Supplementary Figure 128 | Structures of key transition state involved in **2 formation by **SzPolF**. QM(UB3LYP/B1)/MM optimized structures (in Å) involved in the transformation of RC2 into PC2.**



Supplementary Figure 129 | QM(UB3LYP/BS2) calculated bond dissociation energies (BDEs) for C4-H in L-Ile and C6-H in substrate **2 in Chlorobenzene phase.**

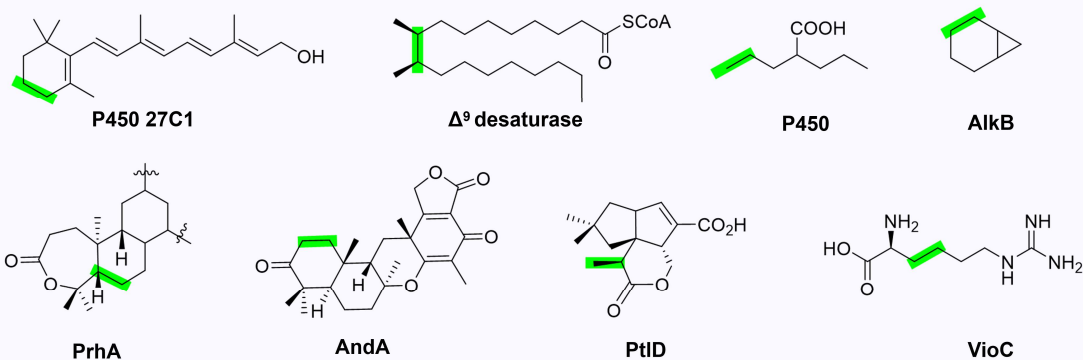
A: Sequential HAT pathway
B: Cation-dependent pathway



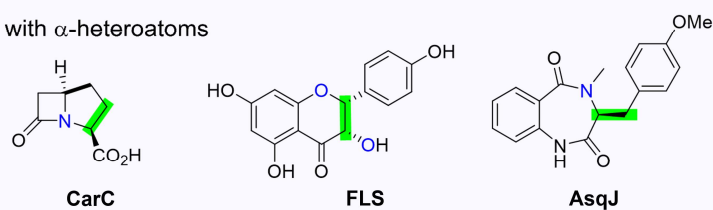
Supplementary Figure 130 | Proposed pathways for C-C desaturation reaction by Fe-dependent oxygenases, including P450s, Fe²⁺/2OG, and nonheme diiron enzymes.

(a) Pathway A: Sequential HAT pathway

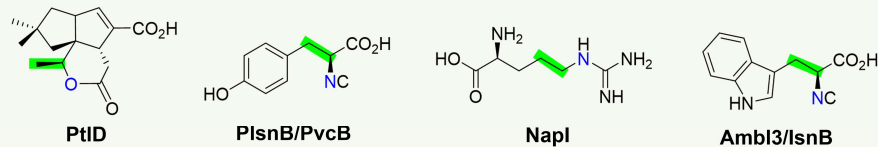
without α -heteroatoms



with α -heteroatoms



(b) Pathway B: Cation-dependent pathway



Supplementary Figure 131 | C-C desaturation catalyzed by Fe enzymes including P450s, nonheme diiron, and Fe²⁺/2OG enzymes through (a) sequential HAT mechanism and (b)

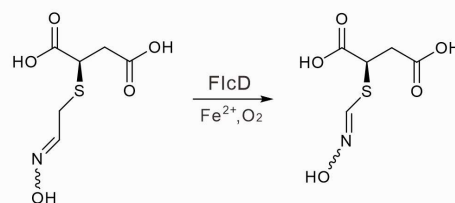
cation-dependent mechanism. The target region highlighted with green color indicate the C-C bond to be desaturated.

As shown in Supplementary Figure 130, for the desaturation reactions catalyzed by Fe enzymes (including P450s, Fe²⁺/2OG and nonheme diiron enzymes), two mechanisms have been widely proposed and confirmed by wet experiments and computational studies with mechanism A: sequential HAT pathway and B: cation-dependent pathway²⁶. Both the mechanisms begin with the hydrogen atom abstraction (HAA) by the Fe(IV)=O species (compound **1**) and generate the Fe(III)-OH species with substrate radical (compound **2**). This step aligns well with our studies on the desaturation catalyzed by *Sn*PolE shown in Extended Data Fig. 4 (⁵IC2) and the barrier for the HAA reaction is 21.1 kcal mol⁻¹ which is similar with previous computational results such as AsqJ²⁷ (19.3 kcal mol⁻¹), PrhA²⁸ (23.6 kcal mol⁻¹), ScoE²⁹ (17.6 kcal mol⁻¹), NapI³⁰ (17.2 kcal mol⁻¹). The first step HAA requires a barrier of ~20 kcal mol⁻¹. When compound **2** is formed, the reaction may proceed with two pathways. In pathway A, from **2**, a second HAA takes place and directly forms the desaturation product (**PC**). While in pathway B, the substrates with α -heteroatoms (O, N, S, P) adjacent to the target C-C may enable a carbocation intermediate-dependent pathway (see compound **B1**). After that, the second hydrogen could be removed as a proton by a basic amino acid in **B2** and finally form the desaturation product (**PC**). In our study, the C3-C4 in the substrate L-isoleucine have no α -heteroatoms, so pathway B is ruled out. As shown in Extended Data Fig. 4 from ⁵IC3 to ⁵TS4, the second HAA requires a 12 kcal mol⁻¹ barrier. As summarized in Supplementary Figure 131, many other desaturation reactions catalyzed by Fe enzymes have been demonstrated to proceed via one of two established mechanisms. Pathway A represents a widely proposed mechanistic model³¹, including P450³², P450 27C1³³, nonheme diiron enzymes: Δ^9 desaturase³⁴, AlkB³⁵ and Fe²⁺/2OG enzymes: AndA³⁶ and PtlD³⁷. Pathway A is supported by computational studies in PrhA^{28,38}, VioC³⁹⁻⁴¹, CarC⁴², FLS⁴³, and AsqJ^{43,44}. In addition to Pathway A, it was proposed that the substrates with α -heteroatoms adjacent to the target C-C may would prefer Pathway B, which has been suggested in NapI²⁶, PtlD³⁷, PlsB/PvcB⁴⁵, and Amb13/IsnB⁴⁶. So, the *Sn*PolE-catalyzed desaturation reaction in our study gives a reasonable reaction process.

NCCCC[C@@H](N)C(=O)O
 $\xrightarrow[\text{Fe}^{2+}, \text{O}_2]{\text{BesC}}$
C=C[C@@H](N)C(=O)O
 $\xrightarrow[\text{Fe}^{2+}, \text{O}_2]{\text{UndA}}$
C=C(CCCC)C(=O)O

Chemical reaction scheme showing the conversion of 2-(2-amino-3-carboxypropyl)-3,6-dibromo-L-tryptophan to 2-(2-cyanoethyl)-3,6-dibromo-L-tryptophan. The reaction is catalyzed by AetD in the presence of Fe^{2+} and O_2 .

Chemical reaction scheme showing the conversion of 5-bromo-L-tryptophan to 5-bromo-tryptophan by the enzyme SktA. The reaction uses Fe^{2+} and O_2 as cofactors.

Oc1ccc(cc1)C[C@H](N)C(=O)O>[CADD][Fe2+,O2]>Oc1ccc(cc1)C(=O)O

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Supplementary Tables

Supplementary Table 1 | Strains and plasmids used in this study.

Strains	Relevant characteristics	Reference or source
<i>Streptomyces</i>		
<i>S. aureochromogenes</i>	Industrial POLs producer	47
CXR14	<i>S. aureochromogenes</i> derivative with the entire POL gene cluster deleted	47
CXR14::pJTU4774	CXR14 strain containing pJTU4774	This study
CXR14::pJTU4774Δ <i>polC</i>	CXR14 strain containing pJTU4774Δ <i>polC</i>	This study
CXR14::pJTU4774Δ <i>polE</i>	CXR14 strain containing pJTU4774Δ <i>polE</i>	This study
CXR14::pJTU4774Δ <i>polF</i>	CXR14 strain containing pJTU4774Δ <i>polF</i>	This study
CXR14::pJTU2463b	CXR14 strain containing pJTU2463b	This study
<i>Escherichia coli</i>		
DH10B	F ⁻ , <i>mcrA</i> , Δ(<i>mrr</i> - <i>hsdRMS</i> - <i>mcrBC</i>), φ80d, <i>lacZ</i> ΔM15, Δ <i>lacX74</i> , <i>deoR</i> , <i>recA</i> , <i>lndA</i> , <i>lra</i> Δ139, D(<i>ara</i> , <i>leu</i>)7697, <i>galU</i> , <i>galK</i> , λ, <i>rpsL</i> , <i>nupG</i>	Gibco-BRL
BW25113/pIJ790	λRED(<i>gam</i> , <i>beta</i> , <i>exo</i>), <i>cat</i> , <i>araC</i> , <i>rep101</i>	48
ET12567/pUZ8002	ET12567 with plasmid pUZ8002(Kan ^r)	48
BL21(DE3)	F ⁻ , <i>ompT</i> , <i>hsdS_B</i> (<i>r_B⁻m_B⁻</i>), <i>gal dcm</i> λ(DE3)	Novagen
Plasmids	Relevant characteristics	Reference or source
pJTU2463b	<i>int</i> , <i>aac(3)IV</i> , <i>oriT</i> , RK2, <i>phiC31</i> , <i>attP</i>	47
pRSFDuet-1	<i>lacI</i> , RSF <i>ori</i> , T7 promoter, Kn ^R	Novagen
pET28a	<i>neo</i> , <i>rep^{MB1}</i> , T7 promoter	Novagen
pJTU4774	The cosmid containing the entire POL gene cluster with XbaI and SpeI sites infilled	This study
pJTU4774Δ <i>polC</i>	pJTU4774 derivative with <i>polC</i> in frame deleted <i>via</i> PCR-targeting technology	This study
pJTU4774Δ <i>polE</i>	pJTU4774 derivative with <i>polE</i> in frame deleted <i>via</i> PCR-targeting technology	This study

pJTU4774 Δ <i>polF</i>	pJTU4774 derivative with <i>polF</i> in frame deleted <i>via</i> PCR-targeting technology	This study
pRSFDuet-1/ <i>polE</i>	pRSFDuet-1 derivative carrying a EcoRI-HindIII fragment containing the optimized <i>polE</i>	This study
pRSFDuet-1/ <i>polF</i>	pRSFDuet-1 derivative carrying a NdeI-XhoI fragment containing <i>polF</i>	This study
pRSFDuet-1/ <i>polE+polF</i>	pRSFDuet-1 derivative carrying a EcoRI-HindIII fragment containing the optimized <i>polE</i> and a NdeI-XhoI fragment containing <i>polF</i>	This study
pET28a/ <i>polE</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing the optimized <i>polE</i> (with codon optimized)	This study
pET28a/ <i>JIX59_14650</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing the optimized <i>JIX59_14650</i> (with codon optimized)	This study
pET28a/ <i>JIX56_45485</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing the optimized <i>JIX56_45485</i> (with codon optimized)	This study
pET28a/ <i>E7X58_02510</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>E7X58_02510</i> (with codon optimized)	This study
pET28a/ <i>AN217_00670</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>AN217_00670</i> (with codon optimized)	This study
pET28a/ <i>OG402_30715</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>OG402_30715</i> (with codon optimized)	This study
pET28a/ <i>snpolE</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> (with codon optimized)	This study
pET28a/ <i>smpolE</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>smpolE</i> (with codon optimized)	This study
pET28a/ <i>GQ466_16145</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>GQ466_16145</i> (with codon optimized)	This study
pET28a/ <i>KMS84_05675</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>KMS84_05675</i> (with codon optimized)	This study

pET28a/ <i>JJ69I_52240</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>JJ69I_52240</i> (with codon optimized)	This study
pET28a/ <i>F6X68_08755</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>F6X68_08755</i> (with codon optimized)	This study
pET28a/ <i>folA</i>	pET28a derivative carrying a NdeI-XhoI fragment containing <i>folA</i>	This study
pET28a/ <i>polE_{H202A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polE_{H202A}</i>	This study
pET28a/ <i>polE_{H206A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polE_{H206A}</i>	This study
pET28a/ <i>polE_{E230A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polE_{E230A}</i>	This study
pET28a/ <i>smpolE_{H203A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>smpolE_{H203A}</i>	This study
pET28a/ <i>smpolE_{H207A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>smpolE_{H207A}</i>	This study
pET28a/ <i>smpolE_{E231A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>smpolE_{E231A}</i>	This study
pET28a/ <i>snpolE_{H205A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{H205A}</i>	This study
pET28a/ <i>snpolE_{H209A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{H209A}</i>	This study
pET28a/ <i>snpolE_{E233A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{E233A}</i>	This study
pET28a/ <i>snpolE_{F140A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{F140A}</i>	This study
pET28a/ <i>snpolE_{Y157A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{Y157A}</i>	This study
pET28a/ <i>snpolE_{E206A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{E206A}</i>	This study
pET28a/ <i>snpolE_{Y280A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{Y280A}</i>	This study
pET28a/ <i>snpolE_{F162A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{F162A}</i>	This study
pET28a/ <i>snpolE_{W201A}</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE_{W201A}</i>	This study

pET28a/ <i>snpolE</i> _{R266A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> _{R266A}	This study
pET28a/ <i>snpolE</i> _{Y270A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> _{Y270A}	This study
pET28a/ <i>snpolE</i> _{Y270F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> _{Y270F}	This study
pET28a/ <i>snpolE</i> _{Y280F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> _{Y280F}	This study
pET28a/ <i>snpolE</i> _{D281A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>snpolE</i> _{D281A}	This study
pET28a/ <i>polF</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i>	This study
pET28a/ <i>sapolF</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i>	This study
pET28a/ <i>srpolF</i>	pET28a derivative carrying a NdeI-HindIII fragment containing <i>srpolF</i>	This study
pET28a/ <i>szpolF</i>	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> (with codon optimized)	This study
pET28a/ <i>polF</i> _{D104A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{D104A}	This study
pET28a/ <i>polF</i> _{H124A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{H124A}	This study
pET28a/ <i>polF</i> _{E180A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{E180A}	This study
pET28a/ <i>polF</i> _{H217A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{H217A}	This study
pET28a/ <i>polF</i> _{E221A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{E221A}	This study
pET28a/ <i>polF</i> _{H224A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>polF</i> _{H224A}	This study
pET28a/ <i>sapolF</i> _{D99A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{D99A}	This study
pET28a/ <i>sapolF</i> _{H119A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{H119A}	This study
pET28a/ <i>sapolF</i> _{E175A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{E175A}	This study

pET28a/ <i>sapolF</i> _{H212A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{H212A}	This study
pET28a/ <i>sapolF</i> _{E216A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{E216A}	This study
pET28a/ <i>sapolF</i> _{H219A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>sapolF</i> _{H219A}	This study
pET28a/ <i>szpolF</i> _{D108A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{D108A}	This study
pET28a/ <i>szpolF</i> _{H128A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{H128A}	This study
pET28a/ <i>szpolF</i> _{E184A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{E184A}	This study
pET28a/ <i>szpolF</i> _{H221A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{H221A}	This study
pET28a/ <i>szpolF</i> _{E225A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{E225A}	This study
pET28a/ <i>szpolF</i> _{H228A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{H228A}	This study
pET28a/ <i>szpolF</i> _{W63A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W63A}	This study
pET28a/ <i>szpolF</i> _{T67A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{T67A}	This study
pET28a/ <i>szpolF</i> _{F70A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{F70A}	This study
pET28a/ <i>szpolF</i> _{V183A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{V183A}	This study
pET28a/ <i>szpolF</i> _{A187L}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{A187L}	This study
pET28a/ <i>szpolF</i> _{I190A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{I190A}	This study
pET28a/ <i>szpolF</i> _{A191L}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{A191L}	This study
pET28a/ <i>szpolF</i> _{W217A}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W217A}	This study
pET28a/ <i>szpolF</i> _{W36F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W36F}	This study
pET28a/ <i>szpolF</i> _{W36H}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W36H}	This study

pET28a/ <i>szpolF</i> _{W36Y}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W63Y}	This study
pET28a/ <i>szpolF</i> _{W217F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W217F}	This study
pET28a/ <i>szpolF</i> _{W263F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W263F}	This study
pET28a/ <i>szpolF</i> _{W36F & W217F & W263F}	pET28a derivative carrying a NdeI-EcoRI fragment containing <i>szpolF</i> _{W63F&W217F&W263F}	This study

Supplementary Table 2 | Primers used in this study.

Primers	Sequence (5'--3')
polCtgt-F	GTGCACCACACCGGACTCCACCTGATCGACGCCGAG GACTCTAGAGCTATTCCAGAAGT
polCtgt-R	CTCGCTCAGGACGAGGACGGCGTTCATCGCCCGGTC GGGACTAGTCTGGATGCCGACG
polEtgt-F	AGCCGACGGGACAACGACGTCTTCTCCCTCTTCGAC GCGTCTAGAGCTATTCCAGAAGT
polEtgt-R	GGTGTACGAGTTGGTGAAGGCGAGCATGCGGGCGGT CACACTAGTCTGGATGCCGACG
polFtgt-F	CAAGACCTCGACGCGCGCGTGGGGAAGGAGATCGA CGCCTCTAGAGCTATTCCAGAAGT
polFtgt-R	ACGACGGAAGCCGACGGCGATGTCCAGGGCGATGT CCTCACTAGTCTGGATGCCGACG
polF _{pRSFDuet-1} -F	GTCCATATGACCGTGAACGCTTTG
polF _{pRSFDuet-1} -R	CCGCTCGAGTCAGGCGTGGCCGTCGCG
polE _{pRSFDuet-1} -F	GGAATTCGATGGATGATATGAATCCG
polE _{pRSFDuet-1} -R	CCCAAGCTTTTACACACCCAGACGTTC
polE-F	GTCCATATGGATGATATGAATCCG
polE-R	GGAATTCTTACACACCCAGACGTTC
smpolE-F	GTCCATATGAGCGAAGAAATTAAG
smpolE-R	GGAATTCTTACACACCCAGACGCTG
snpolE-F	GTCCATATGCCGAATAGTCCGACC
snpolE-R	GGAATTCTTAAACGCCCAGGCGTTC
folA-F	GTCCATATGATCAGTCTGATTGCG
folA-R	CCGCTCGAGTTACCGCCGCTCCAGAAT
polE _{H202A} -F	TTCGTCTG <u>GCC</u> GAATATCAT
polE _{H202A} -R	ATGATATTCG <u>GCC</u> CAGACGAA
polE _{H206A} -F	TGAATATCATG <u>CCC</u> CGTCAGG
polE _{H206A} -R	CCTGACG <u>GGC</u> ATGATATTCA
polE _{E230A} -F	GCCTGGAAG <u>CC</u> CTGCGTGTT
polE _{E230A} -R	AACACGCAG <u>GG</u> CTTCCAGGC
smpolE _{H203A} -F	TTCGTCTG <u>GCA</u> GAATTCAT
smpolE _{H203A} -R	ATGAAATTCTG <u>CC</u> CAGACGAA

smpolE _{H207A} -F	GAATTTTCATGCACGTCAGGG
smpolE _{H207A} -R	CCCTGACGTGCATGAAATTC
smpolE _{E231A} -F	GCCTGGAAGCACTGCGTGTG
smpolE _{E231A} -R	CACACGCAGTGCTTCCAGGC
snpolE _{H205A} -F	CGCCTGGCCGAATATCATCATCGTCAGGGTGAT
snpolE _{H205A} -R	TGATATTTCGGCCAGGCGAACCCACCAGCTACTTGC
snpolE _{H209A} -F	TATCATGCCCGTCAGGGTGATATGCCGATTCCGGAA
snpolE _{H209A} -R	ACCCTGACGGGCATGATATTCATGCAGGCGAACCCA CCA
snpolE _{E233A} -F	CTGGAAGCCCTGCGTGTTGATGTTAGCGGTATGCT
snpolE _{E233A} -R	ACACGCAGGGCTTCCAGGCCGGCCAGCGGTTTCAGT
snpolE _{F140A} -F	GGCCCTGGCGCCGGAAAATCATATTGATGGTATT
snpolE _{F140A} -R	TTTCCGGCGCCAGGGCCACCACCACACGGCTCTGA
snpolE _{Y157A} -F	TCTGATTTTTGCGTTTATTAACAAGTTCGTGGAGCGT
snpolE _{Y157A} -R	AAACGCGAAAAATCAGATCATCACCGCGCTGA
snpolE _{E206A} -F	TCGCCTGCATGCGTATCATCATCGTCAGGGTGATAT G
snpolE _{E206A} -R	ATACGCGATGCAGGCGAACCCACCAGCTACT
snpolE _{Y280A} -F	GCGCCCGAATGCGGATGCAGTTGCCAGTCAGCTGCT
snpolE _{Y280A} -R	ATCCGCGATTCGGGCGCGGAATACCTTCCA
snpolE _{F162A} -F	TATTAACAAGGCCGTGGAGCGTCATAATCGCATTAC C
snpolE _{F162A} -R	CACGGCCTTGTTAATAAAATAAAAAATCAG
snpolE _{W201A} -F	GTAGCTGGGCCGTTTCGCCTGCATGAATATCATCAT
snpolE _{W201A} -R	GAACGGCCAGCTACTTGCCTGTTCCACGGTA
snpolE _{R266A} -F	CTGAGCGAAGCCCTGCTGCGCTATGCCGTGGAAGGT
snpolE _{R266A} -R	CAGGGCTTCGCTCAGAATATATTCGTATGCCA
snpolE _{Y270A} -F	TGCTGCGCGCCGCGCGTGGGAAGGTATTCCGCGCCCGA A
snpolE _{Y270A} -R	CGGCGGCGCGCAGCAGACGTTTCGCTCAGAAT
snpolE _{Y270F} -F	GCTGCGCTTTGCCGTGGAAGGTATTCCGCGCCCGAA
snpolE _{Y270F} -R	CCACGGCAAAAGCGCAGCAGACGTTTCGCTCAGAA
snpolE _{Y280F} -F	CCCGAATTTTGATGCAGTTGCCAGTCAGCTGCTG
snpolE _{Y280F} -R	TGCATCAAAATTCGGGCGCGGAATACCTTCCACG

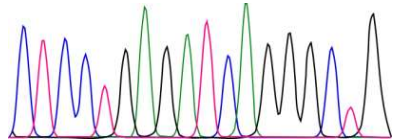
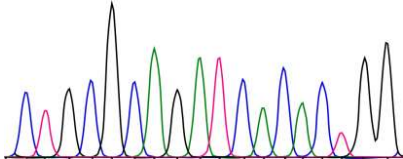
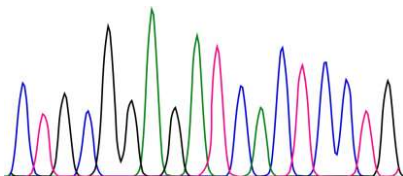
snpolE _{D281A} -F	CCGAATTATG <u>CCG</u> CAGTTGCCAGTCAGCTGCTGTTT
snpolE _{D281A} -R	CTGCGGCATAAATTCGGGCGCGGAATACCTTC
polF-F	GTCCATATGACCGTGAACGCTTTG
polF-R	GGAATTCTCAGGCGTGGCCGTCGCG
sapolF-F	GTCCATATGACCCCCCTCTCCGCC
sapolF-R	GGAATTCTCAGGAGGCGGCGGGAGC
srpolF-F	GTCCATATGGTTGATATCACTTTC
srpolF-R	CCCAAGCTTTCACCGGGCCAGCACGGC
szpolF-F	GTCCATATGAGTGCACCGGATACC
szpolF-R	GGAATTCTTAAGCTGTTGCAGGGG
polF _{D104A} -F	ATCGGCGACG <u>CC</u> CTGGACAAC
polF _{D104A} -R	GTTGTCCAGGGC <u>G</u> TCGCCGAT
polF _{H124A} -F	CGGCATCG <u>C</u> CTACGTCTG
polF _{H124A} -R	AGACGTAG <u>G</u> CGATGCCGG
polF _{E180A} -F	GCGTGGTG <u>G</u> CCGACATCGCC
polF _{E180A} -R	GGCGATGTG <u>G</u> CCACCACGC
polF _{H217A} -F	TGGACTCCG <u>C</u> CATCAAGG
polF _{H217A} -R	GCCTTGATG <u>G</u> CGGAGTCC
polF _{E221A} -F	ATCAAGGCCG <u>C</u> CACCATGCA
polF _{E221A} -R	TGCATGGTG <u>G</u> CGGCCTTGAT
polF _{H224A} -F	GAGACCATGG <u>C</u> CGCGGCC
polF _{H224A} -R	GGCCGCG <u>G</u> CCATGGTCTC
sapolF _{D99A} -F	ATCGGCGACG <u>CC</u> CTCGACAAC
sapolF _{D99A} -R	GTTGTTCGAGGGC <u>G</u> TCGCCGAT
sapolF _{H119A} -F	GCCGGCATCG <u>C</u> CTACGTCTGG
sapolF _{H119A} -R	CCAGACGTAG <u>G</u> CGATGCCGGC
sapolF _{E175A} -F	CGGGTCGTGG <u>C</u> CACCATCGCG
sapolF _{E175A} -R	CGCGATGGTG <u>G</u> CCACGACCCG
sapolF _{H212A} -F	ATCGACGCG <u>G</u> CCATCAAGGCC
sapolF _{H212A} -R	GGCCTTGATG <u>G</u> CCCGCGTCGAT
sapolF _{E216A} -F	ATCAAGGCCG <u>C</u> CACGGTGCA
sapolF _{E216A} -R	TGCACCGTG <u>G</u> CGGCCTTGAT
sapolF _{H219A} -F	GAGACGGTG <u>G</u> CCGCCGCGCAG

sapolF _{H219A} -R	CTGCGCGGCGGCCACCGTCTC
szpolF _{D108A} -F	ATTGGCGATGCCCTGGATAAT
szpolF _{D108A} -R	ATTATCCAGGGCATCGCCAAT
szpolF _{H128A} -F	CCGGTATCGCCTATGTGTGGT
szpolF _{H128A} -R	ACCACACATAGGCGATACCGG
szpolF _{E184A} -F	TGTTGTGGCCACCATTGC
szpolF _{E184A} -R	GCAATGGTGGCCACAACA
szpolF _{H221A} -F	ATTGATGCAGCCATTAAAGCA
szpolF _{H221A} -R	TGCTTTAATGGCTGCATCAAT
szpolF _{E225A} -F	ATTAAAGCAGCCACCGTTCA
szpolF _{E225A} -R	TGAACGGTGGCTGCTTTAAT
szpolF _{H228A} -F	AAACCGTTGCCGCAGCCC
szpolF _{H228A} -R	GGGCTGCGGCAACGGTTT
szpolF _{W63A} -F	TGGGCACGTCAGATGACCAAAGCATTTA
szpolF _{W63A} -R	CATCTGACGTGCCCAAAGTGCCACGGCATGACCA
szpolF _{T67A} -F	ATGGCGAAAGCATTTATGTTTACCACCC
szpolF _{T67A} -R	AAATGCTTTCGCCATCTGACGCCACCAAAGTGCC
szpolF _{F70A} -F	GCAGCAATGTTTACCACCCTGGCAGGCCT
szpolF _{F70A} -R	GGTAAACATTGCTGCTTTGGTCATCTGACGCCA
szpolF _{V183A} -F	GTTGCAGAAACCATTGCACTGGATATTG
szpolF _{V183A} -R	AATGGTTTCTGCAACACGCAGCTGAACTGCGCT
szpolF _{A187L} -F	ATTCTGCTGGATATTGCAGTGGGTTTTTCG
szpolF _{A187L} -R	AATATCCAGCAGAATGGTTTCCACAACACGCA
szpolF _{I190A} -F	TGCACTGGATGCCGCAGTGGGTTTTTCGTCGTGTTTAT
szpolF _{I190A} -R	TGCGGCATCCAGTGCAATGGTTTCCACAACA
szpolF _{A191L} -F	ACTGGATATTCTGGTGGGTTTTTCGTCGTGTTTATGGT
szpolF _{A191L} -R	CACCAGAATATCCAGTGCAATGGTTTCCACAA
szpolF _{W217A} -F	GCCGCGATTGATGCACATATTAAAGCAG
szpolF _{W217A} -R	TGCATCAATCGCGGCAAAGTATCTTTTTTCGCC
szpolF _{W63F} -F	GTTTGGTTTCGTCAGATGACCAAAGCATTAT
szpolF _{W63F} -R	CATCTGACGAAACCAAAGTGCCACGGCATGACCATC G
szpolF _{W63H} -F	TGGCATCGTCAGATGACCAAAGCATTTA

szpolF _{W63H} -R	CATCTGACGATGCCAAACTGCCACGGCATGACCA
szpolF _{W63Y} -F	GGCAGTTTGGTATCGTCAGATGACCAAAGCATTAT G
szpolF _{W63Y} -R	CGATACCAAAGTGCCACGGCATGACCATC
szpolF _{W217F} -F	GCCTTTATTGATGCACATATTAAAGCAG
szpolF _{W217F} -R	TGCATCAATAAAGGCCAAACTGATCTTTTTCGC
szpolF _{W263F} -F	GCAGGCCTGTTTAGTGCAGCCCTGGAATGTTTTGGT GAT
szpolF _{W263R} -F	GCACTAAACAGGCCTGCATATTCTTCCACCAGGCGA

Modified triplet codons in mutational primers are underlined.

Supplementary Table 3 | Validation of the mutant strains by sequencing analysis.

Plasmid	Determined sequence	Theoretical sequence
		
pJTU4774Δ <i>polC</i>	GAG GAC TCT AGT CCC GAC	GAG GAC TCT AGT CCC GAC
		
pJTU4774Δ <i>polE</i>	GAC GCG TCT AGT GTG ACC	GAC GCG TCT AGT GTG ACC
		
pJTU4774Δ <i>polF</i>	GAC GCC TCT AGT GAG GAC	GAC GCC TCT AGT GAG GAC

Supplementary Table 4 | ICP-MS analysis the quantification of metals bound to PolF.

Fe	Mg	Co	Cu	Zn
0.20	0.02	0.00	0.00	0.03

PolF was recombinantly expressed in LB media without exogenously added metals and the purified protein did not incubate additional metals, and the metals content was determined by inductively coupled plasma mass spectrometry (ICP-MS).

Supplement Table 5 | Data collection and refinement statistics.

	<i>apo SnPolE</i>	<i>SnPolE-BH4</i>	<i>SnPolE-BH4-L-isoleucine</i>
PDB ID	9J2E	9J2M	9J2P
Data collection			
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell			
a, b, c (Å)	82.805, 91.079, 112.593	82.675, 91.322, 113.123	82.918, 91.25, 113.002
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90
Resolution(Å)	23.92-2.0	18.12-1.65	23.97-1.75
No. reflections	58150 (5736)	101684 (9323)	86911 (8552)
Redundancy	13.0 (12.4)	9.7 (4.3)	12.9 (11.4)
Completeness (%)	99.87 (99.81)	97.99 (91.21)	99.37 (99.76)
Average I/σ (I)	14.72 (2.09)	15.07 (2.50)	10.82 (2.11)
R _{merge}	0.1418 (1.188)	0.08302 (0.5226)	0.1652 (0.9969)
R _{pim}	0.0408 (0.3499)	0.02722 (0.2839)	0.04809 (0.3036)
CC _{1/2}	0.998 (0.779)	0.992 (0.807)	0.995 (0.872)
Refinement			
R _{work}	0.1959	0.2059	0.1989
R _{free}	0.2412	0.2253	0.2284
r.m.s.d. bonds (Å)	0.007	0.007	0.007
r.m.s.d. angles (°)	0.88	0.90	0.93
Ramachandran favored (%)	98.64	98.64	98.37
Ramachandran outliers (%)	0	0	0
Rotamer outliers (%)	0.47	0	0.16
Average B-factor (Å²)			
Protein	31.38	22.02	27.04
Water	33.42	28.97	32.82
Ligand/ion	29.88	24.00	31.14

*Values in parentheses are for highest-resolution shell.

PDB ID	<i>SnPolE</i> _{Y157A} 9J2R	<i>SnPolE</i> _{Y280A} 9J30	<i>SnPolE</i> _{F140A} 9J33	<i>apo SmPolE</i> 9J3G
Data collection				
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell				
a, b, c (Å)	83.516, 91.674, 113.551	82.952, 91.523, 113.285	83.454, 90.969, 113.515	53.2505, 83.2926, 94.1891
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Resolution(Å)	23.79-1.92	23.98-2.0	23.98-2.3	31.2-1.87
No. reflections	67163 (6320)	58734 (5837)	39043 (3872)	35326 (3468)
Redundancy	13.0 (13.2)	5.0 (4.9)	13.0 (13.2)	12.6 (12.8)
Completeness (%)	98.74 (95.31)	99.59 (99.86)	99.79 (100.0)	99.90 (99.43)
Average I/σ (I)	13.60 (2.58)	10.70 (1.98)	11.60 (2.37)	15.26 (2.38)
R _{merge}	0.1294 (0.8627)	0.099 (0.7139)	0.1949 (1.049)	0.0944 (0.9082)
R _{pim}	0.0374 (0.2468)	0.049 (0.359)	0.0562 (0.2987)	0.0275 (0.2627)
CC _{1/2}	0.998 (0.912)	0.995 (0.818)	0.996 (0.85)	0.999 (0.611)
Refinement				
R _{work}	0.1994	0.1961	0.1945	0.2176
R _{free}	0.2321	0.2358	0.2459	0.2614
r.m.s.d. bonds (Å)	0.008	0.007	0.008	0.008
r.m.s.d. angles (°)	1.01	0.90	0.94	1.11
Ramachandran favored (%)	98.51	98.10	98.23	96.71
Ramachandran outliers (%)	0	0	0	0.55
Rotamer outliers (%)	0	0.63	0.31	1.26
Average B-factor (Å²)				
Protein	28.54	31.72	35.38	35.86
Water	31.61	34.15	34.33	37.11
Ligand/ion	30.89	35.93	32.79	32.27

*Values in parentheses are for highest-resolution shell.

	Fe(II)-SzPolF- L-isoleucine	Fe ₂ (II/II)-SzPolF- L-isoleucine	Fe(II)-SzPolF- 2	Fe ₂ (II/II)-SzPolF- 2
PDB ID	9J2C	9J2B	9J28	9J2A
Data collection				
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell				
a, b, c (Å)	38.436, 121.322, 134.191	38.844, 122.092, 139.29	38.507, 122.295, 136.19	38.586, 121.295, 133.423
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Resolution(Å)	24.54-1.8	32.56-2.3	24.97-2.2	24.71-2.1
No. reflections	59289 (5862)	29383 (2929)	33604 (2703)	37369 (3658)
Redundancy	12.9 (13.5)	7.7 (6.2)	12.5 (11.5)	12.9 (13.2)
Completeness	99.94 (100.0)	97.69 (99.97)	97.9 (81.12)	99.33 (98.57)
Average I/σ (I)	23.5 (2.5)	17.99 (4.52)	13.4 (2.2)	12.95 (3.62)
R _{merge}	0.06481 (1.171)	0.02513 (0.1765)	0.1342 (1.262)	0.3146 (0.9447)
R _{pim}	0.01883 (0.3305)	0.02513 (0.1765)	0.04007 (0.3868)	0.09079 (0.2688)
CC _{1/2}	1 (0.853)	0.999 (0.912)	0.998 (0.916)	0.993 (0.895)
Refinement				
R _{work}	0.2009	0.1953	0.2184	0.1914
R _{free}	0.2296	0.2359	0.2611	0.2299
r.m.s.d. bonds	0.007	0.008	0.008	0.008
r.m.s.d. angles	0.93	0.90	0.95	0.97
Ramachandran favored (%)	98.03	98.47	96.85	98.46
Ramachandran outliers (%)	0	0	0	0
Rotamer outliers (%)	0	1.26	0.26	0.26
Average B-factor (Å²)				
Protein	37.07	42.65	44.85	22.85
Water	36.67	46.08	42.32	26.57
Ligand/ion	32.61	45.84	36.78	22.92

*Values in parentheses are for highest-resolution shell.

	Fe ₂ (II/II)-SzPolF- 1	Fe ₂ (II/II)-PolF- L-isoleucine	Fe(II)-SaPolF- L-isoleucine
PDB ID	9J29	9J3V	9J28
Data collection			
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 1 2 ₁ 1	<i>P</i> 3 ₂ 2 1
Unit cell			
a, b, c (Å)	38.67, 121.78, 139.72	85.852, 120.876, 89.221	90.168, 90.168, 64.733
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 120
Resolution(Å)	26.73-2.13	24.74-2.6	21.81-2.2
No. reflections	36967 (3689)	55912 (5561)	15733 (1533)
Redundancy	12.5 (13.5)	6.8 (7.1)	13.0 (13.2)
Completeness (%)	96.44 (99.97)	99.82 (99.96)	99.42 (99.74)
Average I/σ (I)	18.57 (2.71)	13.23 (2.17)	27.49 (5.44)
R _{merge}	0.02476 (0.2237)	0.0408 (0.3707)	0.0137 (0.1773)
R _{pim}	0.02476 (0.2237)	0.0408 (0.3707)	0.0137 (0.1773)
CC _{1/2}	0.999 (0.891)	0.998 (0.749)	1 (0.923)
Refinement			
R _{work}	0.2070	0.2316	0.2226
R _{free}	0.2420	0.2507	0.2658
r.m.s.d. bonds (Å)	0.009	0.005	0.008
r.m.s.d. angles (°)	1.04	0.90	1.04
Ramachandran favored (%)	97.70	96.66	95.67
Ramachandran outliers (%)	0	0.32	0
Rotamer outliers (%)	0.5	0	1.14
Average B-factor (Å²)			
Protein	42.33	67.11	56.94
Water	37.72	75.31	49.95
Ligand/ion	44.41	64.76	50.96

*Values in parentheses are for highest-resolution shell.

Supplementary Table 6 | NMR data of 1 produced by the recombinant CXR14::pJTU4774Δ*polC* (CD₃OD, 400 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
2	5.18 (d, <i>J</i> = 1.84 Hz, 1H)	69.67
3		126.28
4	4.55 (m, 2H)	53.34
5	5.51 (dt, <i>J</i> = 9.00, 4.86, 1.99, 1H)	121.37
6	1.79 (dt, <i>J</i> = 7.01, 1.79 Hz, 3H)	12.23
7		168.91

[a] Carbon numbering as shown in **Supplementary Figure 6-11**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 7 | NMR data of 1 produced by the recombinant BL21(DE3)/*polE+polF* (CD₃OD, 400 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
2	5.18 (h, <i>J</i> = 2.15 Hz, 1H)	69.66
3		126.49
4	4.55 (m, 2H)	53.32
5	5.51 (dt, <i>J</i> = 7.07, 4.76, 2.36 Hz, 1H)	121.23
6	1.79(dq, <i>J</i> = 6.75, 2.13 Hz, 3H)	12.22
7		169.01

[a] Carbon numbering as shown in **Supplementary Figure 16-21**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 8 | NMR data of 1 produced by the recombinant BL21(DE3)/*polF* (CD₃OD, 400 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
2	5.20 (td, <i>J</i> = 2.76, 1.56 Hz, 1H)	69.60
3		126.15
4	4.56 (m, 1H)	53.37
5	5.52 (m, 1H)	121.49
6	1.79 (m, 3H)	12.23
7		168.82

[a] Carbon numbering as shown in **Supplementary Figure 22-27**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 9 | NMR data of 2 produced by the recombinant BL21(DE3)/*polE* (D₂O, 400 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
1		173.31
2	4.63 (s, 1H)	53.59
3		127.20
4	5.67 (qq, <i>J</i> = 6.88 Hz, 1.44, 1H)	129.60
5	1.64 (dq, <i>J</i> = 6.92 Hz, 1.58, 3H)	12.83
6	1.59 (t, <i>J</i> = 1.58, 3H)	17.41

[a] Carbon numbering as shown in **Supplementary Figure 30-35**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 10 | NMR data of 1 produced from the PolF reaction with 2 as substrate (CD₃OD, 600 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
2	5.24 (h, <i>J</i> = 2.16, 1H)	70.89
3		127.57
4	4.56 (m, 1H)	54.93
5	5.53 (qt, <i>J</i> = 4.72, 2.36 Hz, 1H)	123.17
6	1.79 (dq, <i>J</i> = 6.82, 2.08 Hz, 3H)	13.77
7		170.32

[a] Carbon numbering as shown in **Supplementary Figure 65-70**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 11 | NMR data of 1 produced from the PolF reaction with L-isoleucine as substrate (CD₃OD, 400 MHz).

Position ^[a]	¹ H (δ, mult, <i>J</i>) ^[b]	¹³ C (δ) ^[b]
2	5.20 (td, <i>J</i> = 2.76, 1.56 Hz, 1H)	69.67
3		126.28
4	4.56 (m, 2H)	53.34
5	5.52 (m, 1H)	121.36
6	1.79 (m, 3H)	12.24
7		168.90

[a] Carbon numbering as shown in **Supplementary Figure 76-81**. [b] Chemical shifts δ in ppm and coupling constants *J* are given in Hertz.

Supplementary Table 12 | Spin densities of all species in the construction of azetidine by the SzPolF.

Species	Fe1	Fe2	O1	O2	TRP	C6	N
RC	4.08	-3.97	0.06	-0.22	0.00	0.00	0.13
TS1	4.23	-3.86	0.44	-0.26	-0.81	0.00	0.12
X'	4.11	-3.11	0.09	-0.54	-0.89	0.00	0.15
TS2	4.21	-3.20	0.10	-0.42	-0.94	0.00	0.12
X	4.09	-3.12	0.37	-0.57	-0.88	0.00	0.10
TS3	4.21	-3.95	0.31	-0.15	-0.93	0.32	0.08
IC1	4.10	-4.17	0.36	-0.32	-0.51	0.26	0.10
TS3 _{NH}	4.10	-4.03	0.40	-0.22	-0.93	0.00	0.57
IC1 _{NH}	4.12	-4.15	0.17	-0.28	-0.88	0.00	0.93
TS4	4.10	-4.15	-0.03	-0.10	-0.30	0.27	-0.22
IC2	4.07	-4.16	-0.11	-0.09	-0.35	0.25	-0.30
TS5	4.07	-4.15	-0.10	-0.08	-0.11	0.03	-0.06
TS5 _{OH}	4.10	-4.17	0.36	-0.22	-0.67	-0.13	0.11
PC _{OH}	4.10	-3.98	0.32	-0.02	-0.57	0.00	0.12
PC	4.11	-4.03	0.00	-0.06	0.00	0.00	0.09
RC4	4.07	-4.03	0.00	-0.34	/	0.00	0.15
TS1d	4.10	-4.06	-0.78	0.44		0.00	0.14
IC1d	4.06	-4.06	-0.41	0.98		0.25	0.08
RC5	4.07	-4.02	-0.01	-0.34	0.01	0.00	0.15
TS1e	4.11	-3.96	0.43	-0.24	-0.63	0.00	0.13
X5'	4.10	-3.10	0.36	-0.58	-0.80	0.00	0.12
TS2e	4.10	-3.11	0.34	-0.60	-0.81	0.00	0.14
X5	4.08	-3.11	0.33	-0.59	-0.80	0.00	0.10
RC6	4.08	-3.98	0.05	-0.24	0.00	0.00	0.14
TS1f	4.09	-3.97	0.46	-0.23	-0.60	0.00	0.13
X6'	4.01	-3.09	0.30	-0.57	-0.59	0.00	0.12
TS2f	4.01	-3.10	0.31	-0.59	-0.57	0.00	0.10
X6	3.98	-3.10	0.29	-0.61	-0.56	0.00	0.08

Supplementary Table 13 | Spin densities of all species in the *Sn*PolE-catalyzed desaturation reaction.

Species	Fe1	O1	O2	BH4	C3	C4
⁷ RC1	3.90	0.86	0.81	0.18	0.00	0.00
⁵ RC1	4.00	-0.26	-0.21	0.21	0.00	0.00
⁵ RC1'	3.81	0.01	-0.25	0.20	0.00	0.00
⁷ TS1	3.94	0.44	0.33	1.01	0.00	0.00
⁵ TS1	4.01	-0.34	-0.19	0.22	0.00	0.00
⁷ IC1	3.94	0.49	0.19	1.13	0.00	0.00
⁵ IC1	3.71	0.10	0.02	0.02	0.00	0.00
⁵ TS2	3.94	0.34	0.00	0.12	0.00	0.00
⁵ IC2	3.18	0.62	0.00	0.11	0.00	0.00
⁵ TS3	3.98	-0.08	0.01	0.25	-0.44	0.00
⁵ IC3	4.07	0.27	0.02	0.36	-0.87	0.00
⁵ TS6	3.71	0.06	0.01	0.12	-0.03	0.00
⁵ PC	3.67	0.04	0.07	0.14	0.00	0.00

Supplementary Table 14 | Spin densities of all species in the *Sz*PolF-catalyzed desaturation reaction in the presence of reductants.

Species	Fe1	Fe2	O1	O2	C3	C4	N
RC2	4.08	-3.96	0.06	-0.22	0.00	0.00	0.16
TS1b	4.08	-3.82	0.14	-0.17	0.00	0.00	0.12
X1'	4.12	-3.15	0.10	-0.51	0.00	0.00	0.14
TS2b	4.10	-3.15	0.28	-0.54	0.00	0.00	0.13
X1	4.09	-3.14	0.36	-0.55	0.00	0.00	0.10
TS3b	4.15	-3.88	0.27	-0.06	0.18	0.01	0.10
IC1b	4.19	-4.11	0.27	-0.32	0.86	-0.02	0.10
TS3b_{NH}	4.12	-3.29	0.29	-0.37	0.00	0.00	0.16
IC1b_{NH}	4.17	4.06	0.26	-0.38	0.00	0.00	0.96
TS4b	4.16	-4.10	0.27	-0.29	0.83	-0.03	0.10
IC2b	4.19	-4.10	0.26	-0.32	0.82	-0.03	0.10
TS5b	4.15	-3.94	0.28	-0.21	0.53	-0.05	0.10
TS5b_{OH}	4.16	-3.98	0.27	-0.27	0.61	-0.13	0.11
PC2_{OH}	4.18	-3.72	0.26	0.00	0.00	0.00	0.10
PC2	4.11	-3.70	0.00	-0.06	0.00	0.00	0.10

Supplementary Table 15 | QM/MM energies (in Hartree) of all species.

	B1		B2	
	QM	MM	QM/MM	QM/MM
RC	-4958.855928	-110.923854	-5069.779782	-5072.868041
TS1	-4958.827502	-110.925411	-5069.752913	-5072.840506
X'	-4958.848364	-110.921672	-5069.770036	-5072.857005
TS2	-4958.840912	-110.918410	-5069.759322	-5072.846162
X	-4958.854277	-110.920913	-5069.775140	-5072.860350
TS3	-4958.838079	-110.917568	-5069.755647	-5072.843146
IC1	-4958.896764	-110.923107	-5069.819871	-5072.911962
TS3_{NH}	-4958.824887	-110.922002	-5069.746889	-5072.836476
IC1_{NH}	-4958.850135	-110.923107	-5069.773242	-5072.816201
TS4	-4958.892694	-110.921901	-5069.814595	-5072.902123
IC2	-4958.897745	-110.923850	-5069.821595	-5072.908401
TS4_{OH}	-4958.889187	-110.919805	-5069.808992	-5072.898236
PC_{OH}	-4958.944144	-110.920555	-5069.864699	-5072.279699
TS5	-4958.893745	-110.919498	-5096.813243	-5072.900420
PC	-4958.927624	-110.917667	-5069.845291	-5072.942527
⁷RC1	-3690.457075	-151.500206	-3841.957281	-3844.894364
⁵RC1	-3690.446317	-151.504474	-3841.950791	-3844.888447
⁵RC1'	-3690.445828	-151.500824	-3841.946679	-3844.885347
⁷TS1	-3690.410636	-151.506177	-3841.916813	-3844.854047
⁵TS1	-3690.415656	-151.511152	-3841.926808	-3844.863047
⁷IC1	-3690.447395	-151.505253	-3841.952648	-3844.889640
⁵IC1	-3690.449496	-151.504452	-3841.953949	-3844.890345
⁵TS2	-3690.410318	-151.515023	-3841.925341	-3844.866856
⁵IC2	-3690.464278	-151.508086	-3841.972364	-3844.916421
⁵TS3	-3690.426378	-151.510751	-3841.936250	-3844.882602
⁵IC3	-3690.468208	-151.514583	-3841.982791	-3844.920732
⁵TS6	-3690.438826	-151.512689	-3841.951515	-3844.901610
⁵PC	-3690.527651	-151.509428	-3842.037079	-3844.981201
RC2	-4557.657314	-111.962335	-4669.619649	-4672.272861
TS1b	-4557.644381	-111.963016	-4669.607397	-4672.262201
X2'	-4557.684779	-111.960444	-4669.645223	-4672.301236
TS2b	-4557.676771	-111.961345	-4669.638116	-4672.293135
X2	-4557.689826	-111.962536	-4669.652363	-4672.310737
TS3b	-4557.669067	-111.964225	-4669.633292	-4672.284698

IC1b	-4557.689236	-111.962436	-4669.651672	-4672.305740
TS3b_{NH}	-4457.661231	-111.960531	-4669.621762	-4672.274933
IC1b_{NH}	-4557.690715	-111.959901	-4669.650616	-4672.300430
TS4b	-4557.681046	-111.954271	-4669.641451	-4672.295809
IC2b	-4557.692324	-111.960039	-4669.656085	-4672.309354
TS4b_{OH}	-4557.670670	-111.964551	-4669.635221	-4672.290709
PC2_{OH}	-4557.755586	-111.963424	-4669.719010	-4672.36115
TS5b	-4557.677724	-111.959596	-4669.637320	-4672.290550
PC2	-4557.754444	-111.963617	-4669.718061	-4672.371345

Cartesian coordinates of QM region from QM/MM

calculations

RC

C	43.3879031	37.4243670	37.1246024
H	43.5196721	36.3421361	36.9811867
H	44.0366027	37.9353093	36.3995743
C	43.6786357	37.8415507	38.5390807
C	44.2377786	39.0418333	38.9851191
H	44.6777023	39.8517657	38.4084382
N	44.1394111	39.1292922	40.3446083
H	44.4502042	39.9028938	40.9257071
C	43.5091501	37.9975237	40.8331768
C	43.1374620	37.6688446	42.1332222
H	43.3370462	38.3561111	42.9521448
C	42.5019932	36.4349908	42.3267403
H	42.1993105	36.1390162	43.3345110
C	42.2461897	35.5684607	41.2471248
H	41.7778900	34.6017065	41.4329091
C	42.5891431	35.9208960	39.9415286
H	42.3675421	35.2450625	39.1113861
C	43.2268458	37.1562083	39.7196701
C	43.4657341	46.4369660	47.2209050
H	42.6302988	46.5165694	47.9358321
H	43.0698721	46.3427445	46.2025539
C	44.2855781	45.2029051	47.5483344
O	45.0352086	45.1621689	48.5521755
O	44.2069376	44.2319523	46.7084985
C	46.4603413	45.8887399	44.8240985
N	46.7060937	44.9403983	45.8023962
C	47.5315684	45.5186582	46.6755358
H	47.9192980	45.0681101	47.5857246
N	47.8185719	46.7755605	46.2895280
H	48.3777438	47.4885742	46.7870851
C	47.1600522	47.0379007	45.1176418
H	47.2532054	47.9978312	44.6153444
C	41.4410515	39.7263831	52.3602887
H	40.4406563	39.6322210	51.9265632
H	41.3650829	40.2431129	53.3293199
C	42.3863438	40.5064375	51.4170491
O	43.5812375	40.0830558	51.2497749
O	41.8605595	41.5095112	50.9672265
C	49.4193037	40.8186365	46.2994607
N	49.6043811	41.7337146	45.2771457
H	50.4374395	41.7876307	44.6790658
C	48.5373800	42.5435341	45.1809865

H	48.4333485	43.3323421	44.4408439
N	47.6402234	42.2168272	46.1121189
C	48.1780727	41.1418217	46.8107643
H	47.6386793	40.6900625	47.6377780
C	48.2687015	39.0767645	50.0382795
H	49.0702387	39.8089293	49.8579727
H	48.1942903	38.4139111	49.1641229
C	46.9889320	39.8551103	50.1436661
O	46.8153730	40.7148669	51.0774006
O	46.0583988	39.7409210	49.2905778
C	45.1362044	42.3237699	53.4666676
N	44.8614975	42.5982352	52.1475833
C	44.9266142	43.9259281	52.0465529
H	44.6836642	44.4976232	51.1498863
N	45.2350704	44.4643724	53.2430502
H	45.4446557	45.4596569	53.4359335
C	45.3651844	43.4767440	54.1758248
H	45.6022038	43.6807936	55.2188225
Fe	45.6960926	43.0012327	46.2508202
Fe	44.9835806	41.2665453	50.4694998
O	45.8477542	42.8689651	48.4630949
O	44.6080077	42.3203232	48.9587590
H	45.6183491	43.9126495	48.6078804
C	46.4301448	37.6195714	44.3761726
C	45.0272991	37.8003445	44.8702115
C	44.4079839	38.9281257	45.2646540
C	42.9568326	38.9402824	45.6692142
C	45.1119481	40.2595187	45.2958860
N	45.0081203	40.9709364	46.5855143
C	44.6842253	41.2668021	44.1979369
O	44.1812562	40.9095645	43.1430077
O	44.9774557	42.4994496	44.5069565
H	42.5011355	37.9474706	45.5517754
H	42.8251416	39.2310126	46.7265252
H	42.3793060	39.6562644	45.0584735
H	44.4200433	36.8872400	44.8577491
H	46.8960114	36.7381271	44.8427264
H	46.4218369	37.4311966	43.2867082
H	47.0816887	38.4864871	44.5608568
H	46.1880961	40.1150899	45.1170954
H	44.0377162	41.0691800	46.8937683
H	45.4889518	40.4762243	47.3458883
O	42.6437287	44.1419412	49.8964091
H	42.0806559	43.4866944	50.3350564
H	43.2447532	43.5736791	49.3853368
H	42.3506841	37.6412466	36.8692454
H	44.0733356	47.3355050	47.3282140

H	45.8317206	45.6959723	43.9547633	H	50.3453918	41.6548726	44.6375956
H	41.7307315	38.7183195	52.6568702	C	48.4267377	42.4136434	45.0569255
H	50.1460733	40.0590581	46.5874083	H	48.3144891	43.1260454	44.2437430
H	48.5335857	38.4879410	50.9164540	N	47.5378343	42.1757476	46.0167895
H	45.0252258	41.3141008	53.8620398	C	48.0925270	41.1906908	46.8261849
TS1				H	47.5800692	40.8664044	47.7297850
C	43.4337216	37.5145798	37.1887445	C	48.2893688	38.6196278	50.1094173
H	43.5875733	36.4343464	37.0510623	H	49.0996435	39.1983664	49.6556498
H	44.0847795	38.0433199	36.4804983	H	47.9766005	37.8112876	49.4303860
C	43.6818065	37.9305557	38.6116017	C	47.1383973	39.5569136	50.3166818
C	44.2260953	39.1618152	39.0865391	O	45.9345385	39.1572242	50.2283294
H	44.6931610	39.9633867	38.5172468	O	47.3369306	40.7860940	50.5760693
N	44.0661910	39.2526934	40.4176901	C	45.2182139	42.3265970	53.5335595
H	44.3342949	40.0284161	41.0357427	N	45.2503954	42.5115081	52.1775613
C	43.4204258	38.1071924	40.8899820	C	45.4627205	43.8116108	52.0128224
C	42.9785862	37.8102293	42.1649006	H	45.5379180	44.3125732	51.0494998
H	43.1196020	38.5174249	42.9783066	N	45.5508400	44.4274395	53.2089288
C	42.3459418	36.5599081	42.3443643	H	45.7833412	45.4214581	53.3782260
H	41.9958009	36.2806700	43.3407675	C	45.3980593	43.5108470	54.2070673
C	42.1591186	35.6732667	41.2742621	H	45.4430525	43.7735679	55.2629840
H	41.6908464	34.7054199	41.4536527	Fe	45.5998843	43.0823539	46.1611939
C	42.5668576	36.0092115	39.9784907	Fe	45.2467874	41.0865502	50.5668800
H	42.3970813	35.3195257	39.1481562	O	45.8473314	43.1666826	48.2204711
C	43.2037300	37.2504628	39.7759467	O	44.9589029	41.8276295	49.0134122
C	43.1276350	46.4349065	47.0053470	H	45.0930097	43.7684813	48.5048054
H	42.2794875	46.6992998	47.6536556	C	46.2816410	37.6957007	44.3584777
H	42.8175598	46.4310319	45.9521957	C	44.8686636	37.8979918	44.8184521
C	43.6877339	45.0693496	47.3777093	C	44.2489716	39.0431016	45.1702374
O	43.8016195	44.7281892	48.5664738	C	42.7943293	39.0750243	45.5521244
O	44.0674568	44.3333822	46.3875587	C	44.9657483	40.3691945	45.1928082
C	46.5077184	45.8813524	44.7472905	N	44.7972936	41.1284869	46.4360396
N	46.6736027	44.9495666	45.7507779	C	44.6319634	41.3437773	44.0327728
C	47.4761212	45.5092959	46.6539737	O	44.1662743	40.9401173	42.9601098
H	47.7910489	45.0504495	47.5892598	O	44.9557703	42.5601753	44.2995076
N	47.8299402	46.7461189	46.2542357	H	42.3263937	38.0867461	45.4401209
H	48.3764268	47.4539451	46.7701322	H	42.6578430	39.3979591	46.5965469
C	47.2363819	47.0097503	45.0493675	H	42.2399326	39.8014312	44.9326240
H	47.3843973	47.9555309	44.5355647	H	44.2607616	36.9850906	44.8347235
C	41.4449218	39.7335656	52.2938516	H	46.7343794	36.8180772	44.8453081
H	40.4068310	39.6411300	51.9645134	H	46.3072727	37.4940245	43.2708930
H	41.5062511	40.3249328	53.2206800	H	46.9317432	38.5614421	44.5482597
C	42.3607618	40.3125080	51.1704574	H	46.0467559	40.2008354	45.0753161
O	43.6033151	40.2848844	51.4295481	H	43.8109170	41.3018768	46.7297341
O	41.7598274	40.7609099	50.2081134	H	45.2408649	40.7078032	47.2555250
C	49.3381588	40.8246391	46.3449193	O	42.4098508	41.9790422	47.6886927
N	49.5079789	41.6307865	45.2302509	H	42.1503477	41.4608677	48.4730307
				H	42.9327642	42.6923364	48.0936519

H	42.3980931	37.7124089	36.9123309	C	49.3127964	40.8127901	46.3304401
H	43.8918496	47.1951286	47.1669193	N	49.4224560	41.7227631	45.2892070
H	45.8972202	45.6799344	43.8670690	H	50.2266123	41.7957838	44.6552976
H	41.7284808	38.7385642	52.6368293	C	48.3257054	42.5043113	45.2465426
H	50.0615064	40.0766421	46.6694741	H	48.1613834	43.2826399	44.5070862
H	48.6437543	38.1696366	51.0367716	N	47.4855848	42.1637997	46.2256342
H	45.0027301	41.3427767	53.9503708	C	48.0862802	41.1050321	46.8976468
X'				H	47.6261275	40.6903551	47.7909170
C	43.4465158	37.5216791	37.2309809	C	48.1822876	38.7890826	50.2361235
H	43.5846407	36.4352008	37.1295549	H	48.9789780	39.3906231	49.7863976
H	44.1025038	38.0195742	36.5047930	H	47.8717256	38.0355561	49.4888480
C	43.7067234	37.9821471	38.6385609	C	46.9889215	39.6915673	50.4292528
C	44.2574039	39.2387979	39.0594320	O	45.9783409	39.4137449	51.1160778
H	44.7170928	40.0168246	38.4531493	O	46.9767582	40.7790392	49.7484294
N	44.1048208	39.3855773	40.3803303	C	45.3944613	42.2079017	53.1394343
H	44.3871530	40.1808474	40.9661367	N	45.4766805	42.4266918	51.7819953
C	43.4586889	38.2628551	40.9072801	C	45.6419012	43.7385999	51.6613892
C	42.9955253	38.0491346	42.1879027	H	45.7294678	44.2569124	50.7089180
H	43.1122008	38.8154369	42.9504518	N	45.6552377	44.3350296	52.8727600
C	42.3509169	36.8097844	42.4296592	H	45.8505934	45.3260233	53.0922606
H	41.9839011	36.5915785	43.4347622	C	45.5053049	43.3867903	53.8381302
C	42.1695006	35.8674840	41.4101438	H	45.5131100	43.6301548	54.9013334
H	41.6864868	34.9173730	41.6388039	Fe	45.5169176	42.9666912	46.5441903
C	42.5929428	36.1293209	40.0997669	Fe	45.0156107	41.1895674	50.0310534
H	42.4238036	35.3966759	39.3065300	O	45.2644503	42.7216014	48.6249444
C	43.2416350	37.3538245	39.8348932	O	44.5028903	40.0845174	48.9793162
C	43.0148594	46.3854741	47.1393179	H	44.5075690	43.3449074	48.7859734
H	42.1673061	46.7176032	47.7538379	C	46.2819964	37.6808703	44.3487471
H	42.7278867	46.3602285	46.0787057	C	44.8591869	37.8835996	44.7712994
C	43.4739337	44.9887550	47.5493657	C	44.2397729	39.0309316	45.1347115
O	43.2739001	44.5465454	48.6919801	C	42.7902303	39.0513176	45.5338430
O	44.0714865	44.3212662	46.6231081	C	44.9604820	40.3522561	45.2148471
C	46.4318668	45.8015069	44.8873228	N	44.7850474	41.0043611	46.5081162
N	46.5993724	44.8952852	45.9208040	C	44.6015415	41.4185952	44.1465791
C	47.4145211	45.4819171	46.7921307	O	44.1442535	41.0860016	43.0390070
H	47.7539047	45.0518406	47.7320939	O	44.8850595	42.6031805	44.5334120
N	47.7751376	46.7070431	46.3564015	H	42.3086316	38.0782926	45.3640044
H	48.3300372	47.4263139	46.8455775	H	42.6786018	39.2917521	46.6030893
C	47.1704333	46.9359826	45.1523922	H	42.2328057	39.8302211	44.9853852
H	47.3178864	47.8691061	44.6129631	H	44.2468526	36.9730554	44.7780619
C	41.5385366	39.8476646	52.1698625	H	46.7120576	36.7955249	44.8427155
H	40.4627137	39.7291754	52.0048795	H	46.3396092	37.4858006	43.2606384
H	41.7435571	40.4491592	53.0665104	H	46.9311830	38.5408663	44.5677932
C	42.2462347	40.4140113	50.8889568	H	46.0415797	40.1941498	45.0786193
O	43.3494139	40.9970921	51.1374704	H	43.7915728	41.1952990	46.7728720
O	41.6223997	40.3059339	49.8439278	H	45.1482426	40.4544163	47.2920181
				O	42.3470207	41.8253105	47.6189310

H	42.0770691	41.2405717	48.3572727	O	43.4220126	40.2707406	51.1593987
H	42.5240940	42.6821342	48.0431207	O	41.5674223	41.5740179	51.2560760
H	42.4143129	37.7235054	36.9448158	C	49.3420334	40.8236353	46.2838415
H	43.8120546	47.1169527	47.2715525	N	49.4584275	41.7046426	45.2175430
H	45.8325864	45.6077719	43.9977179	H	50.2738716	41.7731020	44.5972993
H	41.8579030	38.8552518	52.4879650	C	48.3557839	42.4727956	45.1332681
H	50.0658086	40.0726481	46.6010499	H	48.1953708	43.2293951	44.3699018
H	48.5431307	38.2563141	51.1159059	N	47.5053436	42.1496721	46.1095373
H	45.2742115	41.2266303	53.5984699	C	48.1057547	41.1208134	46.8263586
TS2				H	47.6340538	40.7351727	47.7271381
C	43.4651959	37.5378648	37.2266756	C	48.2515862	38.8978751	50.1584331
H	43.6097978	36.4534016	37.1130008	H	49.0642053	39.5164777	49.7653954
H	44.1172310	38.0489013	36.5065391	H	47.9516166	38.1900947	49.3643866
C	43.7191898	37.9811987	38.6401425	C	47.0662264	39.8040151	50.3609933
C	44.2615969	39.2370803	39.0875502	O	46.0316103	39.4930338	50.9957362
H	44.7247288	40.0251536	38.4962553	O	47.0739254	40.9194422	49.7398993
N	44.0980332	39.3611261	40.4073219	C	45.2637156	42.1585636	53.1200121
H	44.3651527	40.1480641	41.0189195	N	45.2401107	42.4146499	51.7601795
C	43.4542473	38.2233319	40.9091944	C	45.4102001	43.7317522	51.6709314
C	42.9862787	37.9828617	42.1819939	H	45.4205845	44.2999841	50.7430359
H	43.0960544	38.7350776	42.9576310	N	45.5266994	44.2930019	52.8925503
C	42.3543143	36.7332504	42.4013904	H	45.7383748	45.2802009	53.1175768
H	41.9881507	36.4930980	43.4020236	C	45.4338640	43.3197124	53.8382244
C	42.1866915	35.8064656	41.3657204	H	45.5079975	43.5352069	54.9053587
H	41.7149304	34.8466036	41.5757094	Fe	45.5796379	42.9530104	46.4688882
C	42.6125650	36.0953182	40.0618494	Fe	45.0211872	41.1918310	49.9038857
H	42.4539057	35.3745236	39.2557994	O	45.5097312	42.6318596	48.5030755
C	43.2513966	37.3299071	39.8222413	O	44.6913566	40.0698973	48.7985421
C	43.2446006	46.4328581	47.0636999	H	44.9994886	43.4416719	48.7486457
H	42.3591922	46.7014564	47.6606914	C	46.3478043	37.7294049	44.3164944
H	42.9730057	46.3478423	46.0040519	C	44.9183840	37.8967589	44.7329114
C	43.8395642	45.1129218	47.5466185	C	44.2653263	39.0287194	45.0747863
O	44.0915848	44.9278345	48.7524996	C	42.8166385	39.0096772	45.4857570
O	44.0798051	44.2454643	46.6280325	C	44.9461320	40.3712993	45.1371197
C	46.4668957	45.8382080	44.8447539	N	44.6788116	41.0701833	46.3937464
N	46.6098097	44.9312051	45.8828557	C	44.6466701	41.4108998	44.0204681
C	47.4225688	45.5106534	46.7628724	O	44.1978319	41.0478485	42.9145612
H	47.7408243	45.0804575	47.7101927	O	44.9493530	42.5946656	44.3788503
N	47.8055541	46.7295454	46.3274182	H	42.3630418	38.0200876	45.3354602
H	48.3641662	47.4440419	46.8205137	H	42.7092249	39.2500206	46.5569891
C	47.2191010	46.9626253	45.1137686	H	42.2265065	39.7566862	44.9249562
H	47.3859040	47.8916079	44.5720841	H	44.3337326	36.9684255	44.7524016
C	41.4454130	39.7010635	52.4997755	H	46.8028004	36.8697423	44.8334839
H	40.4178078	39.5845694	52.1425788	H	46.4129176	37.5105820	43.2335834
H	41.4271587	40.1686619	53.4953557	H	46.9698626	38.6141949	44.5148424
C	42.2652758	40.5860693	51.5104442	H	46.0362677	40.2315428	45.0863770
				H	43.6835950	41.2743222	46.5274473

H	44.9435280	40.5344646	47.2395977	H	41.2207765	40.1963222	53.5121971
O	42.8535097	42.5337290	49.2084011	C	42.1567531	40.4973594	51.5575677
H	42.2535092	42.3313965	49.9637989	O	43.3872305	40.2230515	51.5380302
H	43.1045250	43.4699443	49.2963579	O	41.5281133	41.3742162	50.9667768
H	42.4313941	37.7361062	36.9437954	C	49.3671075	40.8548393	46.2522575
H	43.9609447	47.2422282	47.2045482	N	49.5469755	41.6864643	45.1602157
H	45.8738758	45.6493117	43.9499283	H	50.3868821	41.7210458	44.5731257
H	41.7816970	38.6912798	52.7349714	C	48.4663260	42.4761994	45.0002771
H	50.0911855	40.0879165	46.5763412	H	48.3591255	43.2115885	44.2071415
H	48.5673012	38.3232008	51.0291458	N	47.5722266	42.2136108	45.9463024
H	45.1144380	41.1860686	53.5890930	C	48.1174372	41.2109752	46.7350593
X				H	47.5991990	40.8709745	47.6304906
C	43.4525254	37.5360919	37.2585229	C	48.2250795	39.0301202	50.1775704
H	43.5930225	36.4503813	37.1515033	H	49.0045728	39.7238292	49.8413739
H	44.1122644	38.0392751	36.5394637	H	48.0077812	38.3459237	49.3364769
C	43.7057715	37.9852939	38.6719781	C	46.9584790	39.8137369	50.4011643
C	44.2635791	39.2339279	39.1127277	O	46.0061908	39.4098226	51.1154188
H	44.7257060	40.0182150	38.5156447	O	46.7918989	40.9158864	49.7670162
N	44.1197769	39.3591372	40.4366541	C	45.2726816	42.0884857	53.4077074
H	44.3930219	40.1459797	41.0457841	N	45.3787837	42.2389759	52.0484852
C	43.4755581	38.2266438	40.9468887	C	45.6640831	43.5257122	51.8749779
C	43.0435584	37.9810829	42.2332574	H	45.8246952	44.0004385	50.9100476
H	43.1974740	38.7233550	43.0136223	N	45.7107758	44.1707260	53.0576285
C	42.3990700	36.7404342	42.4586759	H	45.9718319	45.1589840	53.2232620
H	42.0560694	36.4968466	43.4667905	C	45.4615531	43.2834052	54.0624082
C	42.1911406	35.8235518	41.4200454	H	45.4610092	43.5684603	55.1147702
H	41.7085577	34.8702627	41.6357083	Fe	45.6975861	43.1922402	46.2816981
C	42.5931953	36.1119566	40.1090787	Fe	44.8246506	41.0354142	50.3197043
H	42.4087897	35.3963355	39.3037908	O	46.0413153	43.3970407	48.1047052
C	43.2417915	37.3396585	39.8599594	O	44.3623475	40.1884446	49.0319260
C	43.1448492	46.4593459	46.9220352	H	45.3611098	43.9626708	48.5104941
H	42.2708568	46.7808980	47.5081914	C	46.2971221	37.8027937	44.4262644
H	42.8994781	46.4419318	45.8520408	C	44.8840458	37.9995421	44.8850169
C	43.5950324	45.0666553	47.3553568	C	44.2653889	39.1499804	45.2307687
O	43.6022689	44.7853461	48.5733385	C	42.8190981	39.1700813	45.6460857
O	43.9652152	44.2748368	46.4229378	C	44.9765128	40.4780461	45.2322380
C	46.5405288	45.9562898	44.6870135	N	44.7663026	41.2599795	46.4609635
N	46.6609495	45.0580584	45.7243929	C	44.6707295	41.4327338	44.0342788
C	47.4714794	45.6231852	46.6181880	O	44.2041356	40.9637163	42.9725791
H	47.7472645	45.1800172	47.5727186	O	44.9884190	42.6369344	44.2663216
N	47.8738234	46.8303175	46.1776651	H	42.3472528	38.1857109	45.5173782
H	48.4308732	47.5373623	46.6819862	H	42.7154423	39.4425525	46.7103487
C	47.3004008	47.0722209	44.9582183	H	42.2467180	39.9108514	45.0593900
H	47.4756792	47.9987558	44.4197418	H	44.2796607	37.0842906	44.9237307
C	41.2602843	39.7005405	52.5317280	H	46.7483286	36.9251931	44.9154100
H	40.2524507	39.5939426	52.1268725	H	46.3253227	37.6017220	43.3382922
				H	46.9444483	38.6708716	44.6177116

H	46.0604023	40.3102666	45.1626872	C	41.2157945	39.6831830	52.5597742
H	43.7767662	41.4800071	46.5959168	H	40.1918314	39.5915474	52.1957651
H	45.0446953	40.7563316	47.3110417	H	41.2266263	40.1815994	53.5396793
O	43.6160656	42.6279099	49.9393824	C	42.0875402	40.4527541	51.5443600
H	42.6910075	42.3829718	50.1828485	O	43.3065884	40.1301288	51.4778692
H	43.6236404	43.4025859	49.2918541	O	41.4742795	41.3456196	50.9666721
H	42.4224155	37.7366308	36.9640318	C	49.4270976	40.9155230	46.2070486
H	43.9216447	47.2015400	47.1058933	N	49.6087105	41.7466737	45.1206020
H	45.9341836	45.7405422	43.8073172	H	50.4399807	41.7630067	44.5215087
H	41.5919742	38.6959634	52.7941662	C	48.5502237	42.5744537	44.9914413
H	50.0854689	40.1041597	46.5816575	H	48.4514570	43.3197282	44.2061999
H	48.5531609	38.4303175	51.0264912	N	47.6691811	42.3329103	45.9545352
H	45.0258746	41.1366184	53.8779224	C	48.1976093	41.3097099	46.7207662
TS3				H	47.6921971	40.9732768	47.6249176
C	43.4405749	37.5302174	37.3170491	C	48.1984896	39.0016844	50.0753561
H	43.5722674	36.4428451	37.2156619	H	48.9538945	39.7461547	49.7932511
H	44.1150929	38.0243047	36.6050231	H	48.0919437	38.3137860	49.2150700
C	43.6866930	37.9806341	38.7331414	C	46.8687941	39.7033567	50.2009986
C	44.2663822	39.2185089	39.1709397	O	45.9422795	39.3089223	50.9557951
H	44.7338757	39.9974965	38.5708006	O	46.6284317	40.7196025	49.4542496
N	44.1426895	39.3402775	40.4991863	C	45.2291962	42.0420962	53.3090745
H	44.4337953	40.1223605	41.1004846	N	45.3412913	42.1529691	51.9491614
C	43.4898704	38.2150642	41.0157070	C	45.6551015	43.4272935	51.7505375
C	43.0896040	37.9607330	42.3132243	H	45.8526106	43.8698489	50.7764436
H	43.2754777	38.6917486	43.1024122	N	45.7107590	44.1055866	52.9217799
C	42.4332890	36.7286707	42.5391051	H	45.9867016	45.0903408	53.0782044
H	42.1087565	36.4788560	43.5519549	C	45.4385507	43.2461915	53.9443045
C	42.1900341	35.8237468	41.4953969	H	45.4398075	43.5529452	54.9910687
H	41.6992456	34.8754808	41.7142283	Fe	45.7736216	43.2976676	46.3151589
C	42.5673157	36.1167794	40.1796304	Fe	44.6425609	40.7680147	50.1055184
H	42.3587675	35.4095649	39.3729029	O	46.1323298	43.5645141	48.1275320
C	43.2244651	37.3392893	39.9253121	O	44.0149292	39.8346118	48.7968414
C	43.1487760	46.4724098	46.9267993	H	45.4231044	44.0820215	48.5474982
H	42.2754067	46.7998538	47.5101214	C	46.1148770	37.8098813	44.3006796
H	42.9045238	46.4435913	45.8566832	C	44.8742674	38.0086925	45.1085153
C	43.6059218	45.0871120	47.3746056	C	44.3826288	39.1753727	45.6181774
O	43.5881383	44.8001316	48.5900352	C	43.1871059	39.1664965	46.4632646
O	44.0147711	44.3046577	46.4478470	C	45.0946887	40.4967355	45.4381514
C	46.5823056	46.0162786	44.6713313	N	45.0359052	41.3300480	46.6415676
N	46.7171447	45.1342818	45.7184127	C	44.7084054	41.3885285	44.2079667
C	47.5349759	45.7120283	46.5976091	O	44.2275254	40.8524278	43.1870826
H	47.8159617	45.2832074	47.5573838	O	45.0134820	42.6071788	44.3665445
N	47.9284780	46.9123245	46.1356937	H	42.6775589	38.1978318	46.5311032
H	48.4904778	47.6240668	46.6273030	H	43.5576357	39.4064196	47.6510927
C	47.3416183	47.1373460	44.9198952	H	42.4840158	40.0002278	46.3141548
H	47.5081625	48.0560910	44.3680102	H	44.2926729	37.1019479	45.3121237
				H	46.6430471	36.9005043	44.6325362

H	45.8744394	37.6617378	43.2311534
H	46.8113725	38.6578789	44.3673661
H	46.1629975	40.2983746	45.2630680
H	44.0777226	41.4711879	46.9664086
H	45.5156084	40.8881776	47.4290836
O	43.5478377	42.4464658	49.6303246
H	42.6438037	42.3114423	49.9945248
H	43.6141384	43.3551625	49.1960167
H	42.4178757	37.7388503	37.0030018
H	43.9284181	47.2134600	47.1030657
H	45.9603093	45.7849496	43.8066495
H	41.5455079	38.6741299	52.8070961
H	50.1237522	40.1436193	46.5340107
H	48.5119262	38.4169779	50.9401930
H	44.9821112	41.0996124	53.7976852

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C	43.3913580	37.4423913	37.2689777
H	43.4951879	36.3493919	37.2050120
H	44.0637907	37.8842612	36.5200236
C	43.6925200	37.9552502	38.6557391
C	44.2735380	39.1865325	38.9901239
H	44.7046100	39.9409779	38.3376191
N	44.2013193	39.3944344	40.3337216
H	44.5264481	40.2134260	40.8442013
C	43.5673842	38.3220248	40.9323436
C	43.1776287	38.1534009	42.2579348
H	43.3404841	38.9604960	42.9703879
C	42.5130193	36.9544149	42.5777066
H	42.1751721	36.7814106	43.6025600
C	42.2445317	35.9846435	41.5960698
H	41.7396420	35.0613411	41.8824250
C	42.5969447	36.1916089	40.2582453
H	42.3547848	35.4394142	39.5028435
C	43.2599900	37.3832295	39.9032034
C	43.1639579	46.4868310	47.0104421
H	42.2867850	46.8233039	47.5830738
H	42.9224442	46.4302783	45.9410152
C	43.6230760	45.1133627	47.4902830
O	43.6361930	44.8673688	48.7210778
O	43.9946593	44.2947744	46.5871578
C	46.5579791	46.0058986	44.7365730
N	46.6810404	45.1374095	45.7998974
C	47.5024949	45.7224509	46.6710816
H	47.7859263	45.3026668	47.6339883
N	47.9071578	46.9133825	46.1938041
H	48.4757259	47.6274347	46.6745001

C	47.3263221	47.1240730	44.9726862
H	47.5026083	48.0342141	44.4079012
C	41.1998447	39.7283774	52.5953849
H	40.1829749	39.6513855	52.2077132
H	41.1930290	40.2188360	53.5792062
C	42.1036001	40.5008723	51.6079133
O	43.3193793	40.1562283	51.5486604
O	41.5159618	41.4147864	51.0384201
C	49.4128214	40.9101631	46.2088455
N	49.5723114	41.7725984	45.1376063
H	50.3960778	41.8067721	44.5288217
C	48.5036555	42.5876026	45.0396659
H	48.3831173	43.3465479	44.2706949
N	47.6377747	42.3121181	46.0072892
C	48.1899860	41.2716240	46.7427037
H	47.6987587	40.9172069	47.6464180
C	48.1492336	39.0039750	50.0601953
H	48.9175642	39.7137014	49.7280932
H	47.9733856	38.3058142	49.2202684
C	46.8587794	39.7578638	50.2490418
O	45.9400779	39.3895479	51.0297389
O	46.6315133	40.8004711	49.5355292
C	45.1717300	42.1349964	53.3826808
N	45.2404319	42.2804600	52.0212751
C	45.5290926	43.5655400	51.8420289
H	45.6837263	44.0386528	50.8753875
N	45.6144518	44.2121371	53.0248807
H	45.8851327	45.1975669	53.1886424
C	45.3864229	43.3269845	54.0355906
H	45.4140471	43.6115316	55.0876680
Fe	45.7687784	43.2760407	46.4159751
Fe	44.6801738	40.9267663	50.2186160
O	46.1277464	43.5334378	48.2285841
O	43.9468807	39.8273775	48.8885299
H	45.4532455	44.1055430	48.6324934
C	46.2031845	37.8389688	44.3231502
C	44.8460259	38.0418403	44.8703217
C	44.2989350	39.2220210	45.4080897
C	43.0263931	39.1420405	45.9369729
C	45.0601456	40.5342723	45.4240280
N	44.9776311	41.2668260	46.6865634
C	44.6967273	41.5087502	44.2533901
O	44.1980556	41.0424615	43.2167823
O	45.0220028	42.7103801	44.4893189
H	42.4803347	38.1958679	45.9359797
H	43.7283214	38.9461117	49.2214075
H	42.5216019	39.9998350	46.3837780

H	44.2099588	37.1517876	44.9107141	N	47.8830396	46.8332930	46.1926234
H	46.6515739	36.9302788	44.7646839	H	48.4399410	47.5428474	46.6939765
H	46.1364397	37.6370589	43.2364932	C	47.3074510	47.0703711	44.9734610
H	46.8769541	38.6915726	44.4778111	H	47.4824815	47.9949603	44.4309533
H	46.1288177	40.3284471	45.2685414	C	41.3340458	39.6940724	52.5074067
H	44.0166612	41.3859243	47.0135669	H	40.3122154	39.5922435	52.1338989
H	45.4406496	40.7616099	47.4450337	H	41.3221755	40.1942486	53.4868091
O	43.5499304	42.4861001	49.5815609	C	42.2069635	40.4932628	51.5094497
H	42.6547660	42.3496890	49.9684529	O	43.4048069	40.1476165	51.3340792
H	43.6344591	43.4450456	49.2312156	O	41.5757873	41.4492205	51.0570721
H	42.3678026	37.6675484	36.9694683	C	49.3392969	40.8447445	46.2895067
H	43.9373350	47.2380453	47.1705419	N	49.5100487	41.6742320	45.1951523
H	45.9470036	45.7763557	43.8635975	H	50.3493201	41.7157578	44.6057937
H	41.5080311	38.7130572	52.8448107	C	48.4193222	42.4502502	45.0313941
H	50.1323552	40.1494862	46.5116805	H	48.3033120	43.1809558	44.2353950
H	48.4851117	38.4240835	50.9198341	N	47.5260876	42.1808353	45.9793561
H	44.9339648	41.1811241	53.8534912	C	48.0818086	41.1882828	46.7719454
TS3_{NH}				H	47.5604096	40.8394541	47.6619832
C	43.4451505	37.5075752	37.2358478	C	48.2601848	38.9788019	50.1595158
H	43.5744454	36.4211398	37.1229500	H	49.0655556	39.6301287	49.8039746
H	44.1064378	38.0073934	36.5156649	H	48.0019165	38.2731070	49.3489210
C	43.7075111	37.9497562	38.6480961	C	47.0393083	39.8290842	50.3763582
C	44.2731061	39.1918358	39.0826001	O	45.9919272	39.3856087	50.9371091
H	44.7359736	39.9742925	38.4843028	O	47.0004173	41.0094697	49.9030761
N	44.1339097	39.3200971	40.4085548	C	45.2599813	42.1220000	53.4191212
H	44.4250167	40.1063805	41.0015601	N	45.3635552	42.2979278	52.0682148
C	43.4845307	38.1942342	40.9249402	C	45.6350998	43.5881625	51.9243146
C	43.0540771	37.9483029	42.2132495	H	45.7953738	44.0885204	50.9727713
H	43.2091392	38.6832420	43.0008449	N	45.6776156	44.2128689	53.1218603
C	42.4042310	36.7117908	42.4394922	H	45.9343039	45.1994038	53.3002803
H	42.0628402	36.4696338	43.4485508	C	45.4384682	43.3026268	54.1069986
C	42.1881227	35.7967443	41.4005620	H	45.4335743	43.5657725	55.1644115
H	41.7021493	34.8455874	41.6173939	Fe	45.6823606	43.2170693	46.3288692
C	42.5874876	36.0840525	40.0891937	Fe	44.9023592	41.0134162	50.1710224
H	42.3968847	35.3700887	39.2839552	O	46.0112080	43.3854024	48.1467503
C	43.2420837	37.3080944	39.8385170	O	44.6634255	40.2688281	48.5521118
C	43.1389682	46.4991292	46.8972298	H	45.3226383	43.9407966	48.5570697
H	42.2653403	46.8163934	47.4858075	C	46.2552389	37.8822661	44.4747991
H	42.8955469	46.4884525	45.8264501	C	44.8320460	38.0377426	44.9169022
C	43.5939929	45.1105861	47.3302764	C	44.1847449	39.1637940	45.2916399
O	43.5896974	44.8211227	48.5417937	C	42.7425970	39.1485519	45.7089392
O	43.9888458	44.3264408	46.3941266	C	44.8828930	40.4900549	45.3381490
C	46.5471200	45.9538016	44.7066580	N	44.5558174	41.3637298	46.4153674
N	46.6714822	45.0579616	45.7482040	C	44.6818974	41.4513257	44.0296492
C	47.4827147	45.6282025	46.6386384	O	44.2118621	40.9376203	43.0039881
H	47.7624454	45.1927368	47.5959393	O	45.0692768	42.6257034	44.2314172
				H	42.2923847	38.1567385	45.5640727

H	42.6573242	39.3976857	46.7806386
H	42.1473563	39.8851723	45.1390531
H	44.2491832	37.1078874	44.9319743
H	46.7284091	37.0283016	44.9858940
H	46.3030760	37.6614999	43.3914693
H	46.8740837	38.7724963	44.6574844
H	45.9726503	40.3501766	45.3381729
H	43.5481142	41.4512674	46.5731849
H	44.8249078	40.8228106	47.6434274
O	43.6132187	42.6000134	49.8533582
H	42.7216291	42.4168564	50.2356934
H	43.5835874	43.4079466	49.2667699
H	42.4153265	37.7205122	36.9491641
H	43.9178499	47.2370702	47.0892027
H	45.9443201	45.7384806	43.8244243
H	41.6596075	38.6866797	52.7667071
H	50.0633300	40.0980981	46.6156392
H	48.5685314	38.3928263	51.0253230
H	45.0367635	41.1484754	53.8555738

IC1_{NH}

C	43.4415589	37.5054366	37.2241919
H	43.5762720	36.4204782	37.1043142
H	44.1001286	38.0140595	36.5080069
C	43.6979560	37.9381147	38.6399926
C	44.2492370	39.1864168	39.0914431
H	44.7076260	39.9781195	38.5013068
N	44.1026434	39.2985775	40.4152684
H	44.3731299	40.0829540	41.0251657
C	43.4634077	38.1580027	40.9160104
C	43.0295614	37.8964097	42.1980130
H	43.1667667	38.6289473	42.9886084
C	42.3954220	36.6476167	42.4112007
H	42.0525827	36.3936710	43.4168609
C	42.1973917	35.7388216	41.3642875
H	41.7240895	34.7786714	41.5695887
C	42.5975352	36.0442890	40.0563742
H	42.4182727	35.3363228	39.2432980
C	43.2375253	37.2791748	39.8212466
C	43.1233510	46.4880984	46.9448800
H	42.2415104	46.7819693	47.5343010
H	42.8742348	46.4554082	45.8763919
C	43.6401129	45.1263763	47.3949519
O	43.7286517	44.8832725	48.6161715
O	43.9976089	44.3166325	46.4680806
C	46.4422628	45.8612452	44.8464882
N	46.5741887	44.9601854	45.8874647

C	47.3943518	45.5289661	46.7670558
H	47.7062315	45.0934395	47.7140916
N	47.7922252	46.7393012	46.3247928
H	48.3525681	47.4511670	46.8193900
C	47.2085800	46.9768482	45.1106497
H	47.3848785	47.9028725	44.5675399
C	41.3785374	39.7053862	52.5868573
H	40.3252233	39.6007065	52.3209167
H	41.4719082	40.2168163	53.5566238
C	42.1581156	40.4725709	51.4788459
O	43.3813378	40.2666995	51.3355727
O	41.4067527	41.2901010	50.9282435
C	49.3669624	40.9062236	46.2523513
N	49.5120025	41.7865138	45.1935746
H	50.3333519	41.8367567	44.5804426
C	48.4290729	42.5872799	45.1091101
H	48.2981189	43.3561612	44.3522514
N	47.5676117	42.2828721	46.0763077
C	48.1348204	41.2389794	46.7926382
H	47.6448989	40.8637026	47.6883670
C	48.1550753	39.0067220	50.0816466
H	48.9803259	39.6272139	49.7149712
H	47.8850571	38.3006081	49.2748203
C	46.9526393	39.8973058	50.2752332
O	45.9211450	39.5518988	50.8996753
O	46.9394206	41.0334482	49.6860581
C	45.2714572	42.2043812	53.2984012
N	45.3710046	42.4211426	51.9501782
C	45.6195016	43.7194238	51.8432572
H	45.7472266	44.2542978	50.9048331
N	45.6585659	44.3122228	53.0565280
H	45.9034914	45.2955479	53.2622893
C	45.4367144	43.3706020	54.0143942
H	45.4362769	43.6041282	55.0790228
Fe	45.5628098	43.0203332	46.3923687
Fe	44.8953403	41.3408555	49.9339264
O	45.4757502	42.8198539	48.3358793
O	44.2554291	40.0268132	48.7360539
H	44.9447944	43.6113036	48.5854224
C	46.5005751	37.6342957	44.2296923
C	45.0926446	37.8207725	44.7073405
C	44.4737189	38.9632648	45.0706015
C	43.0470460	38.9839385	45.5510783
C	45.1655147	40.3033239	45.0717882
N	45.1587955	40.9504853	46.3280129
C	44.6686494	41.3739000	44.0223586
O	44.1797291	40.9838921	42.9481544

O	44.8843850	42.5676640	44.3908114	C	46.4196735	45.8687121	44.8627195
H	42.6025686	37.9782886	45.5355869	N	46.5592501	44.9781109	45.9125701
H	42.9929261	39.3602571	46.5870960	C	47.3943771	45.5553945	46.7714726
H	42.4258971	39.6561662	44.9316903	H	47.7244447	45.1289732	47.7163683
H	44.4923998	36.9038854	44.7632316	N	47.7929634	46.7609679	46.3120750
H	46.9626543	36.7663206	44.7243263	H	48.3645776	47.4744112	46.7909379
H	46.5236731	37.4264272	43.1431968	C	47.1942727	46.9855698	45.1032338
H	47.1423868	38.5080167	44.4174151	H	47.3676918	47.9036478	44.5457203
H	46.2294817	40.1921468	44.7740678	C	41.3470610	39.7441138	52.4996002
H	44.0795032	39.2396122	49.2687788	H	40.3100754	39.6277100	52.1780674
H	44.9031073	40.3902515	47.1771783	H	41.3773403	40.2358817	53.4835195
O	43.3425115	42.6936929	49.9948126	C	42.1539462	40.5690207	51.4577130
H	42.4560970	42.3089418	50.2328371	O	43.3791156	40.3666460	51.3085753
H	43.2807509	43.5191135	49.4610000	O	41.4117445	41.4260624	50.9579727
H	42.4105218	37.7148958	36.9393122	C	49.4618106	41.0004157	46.2742869
H	43.8777086	47.2533411	47.1276788	N	49.5095325	41.8286662	45.1658503
H	45.8415130	45.6651490	43.9583929	H	50.2829098	41.8572685	44.4926298
H	41.7182157	38.6989907	52.8315078	C	48.4252739	42.6324331	45.1475386
H	50.0943961	40.1478793	46.5418703	H	48.2208530	43.3623429	44.3685823
H	48.4563777	38.4205427	50.9497928	N	47.6572606	42.3779851	46.2023887
H	45.0419227	41.2323200	53.7348392	C	48.2932093	41.3675490	46.9099860
TS4				H	47.9006342	41.0451176	47.8715746
C	43.3905949	37.4310056	37.2447219	C	48.1059852	39.0095461	50.0529214
H	43.4941693	36.3385450	37.1731661	H	48.9332166	39.6355562	49.6995977
H	44.0605073	37.8779364	36.4967360	H	47.8693608	38.2739256	49.2624392
C	43.6899659	37.9362495	38.6335974	C	46.8854176	39.8850801	50.2051845
C	44.2616626	39.1693488	38.9756697	O	45.7724419	39.4839148	50.6328764
H	44.6982178	39.9261068	38.3296845	O	46.9466655	41.0915682	49.7893632
N	44.1676694	39.3774275	40.3179271	C	45.2559865	42.2132500	53.3436163
H	44.4794815	40.1982517	40.8334813	N	45.4168284	42.4409606	52.0019041
C	43.5262595	38.3048246	40.9058404	C	45.6742812	43.7409544	51.9137626
C	43.0994857	38.1439720	42.2201274	H	45.8358380	44.2811458	50.9836653
H	43.2296474	38.9605719	42.9255686	N	45.6612802	44.3206255	53.1289139
C	42.4314195	36.9434453	42.5316434	H	45.9023239	45.3039524	53.3435835
H	42.0576790	36.7808040	43.5454290	C	45.3987158	43.3738600	54.0716160
C	42.1997497	35.9634753	41.5513663	H	45.3604435	43.6012909	55.1374900
H	41.6956312	35.0378511	41.8311206	Fe	45.5921090	42.9508690	46.5019319
C	42.5813735	36.1667298	40.2208295	Fe	44.8967368	41.5141631	50.0281993
H	42.3599404	35.4097531	39.4638915	O	45.4867731	42.8417621	48.5338391
C	43.2435086	37.3618519	39.8741237	O	43.9896139	40.3930347	48.6150453
C	43.1849622	46.4786885	46.9883747	H	44.9616808	43.6619680	48.7049788
H	42.2882497	46.7764517	47.5534535	C	46.1049940	37.4888543	44.1042589
H	42.9509082	46.4035151	45.9187238	C	44.7872019	37.7989811	44.6973252
C	43.7064060	45.1378868	47.4963583	C	44.3465592	39.0353327	45.2093584
O	43.8389361	44.9648981	48.7319710	C	43.0814354	39.0848030	45.7600992
O	44.0111933	44.2671715	46.6173812	C	45.1979405	40.3011478	45.2124081
				N	45.3098289	40.8767227	46.5389251

C	44.6710522	41.3794545	44.2216714
O	44.1402759	41.0406521	43.1560478
O	44.9086640	42.5741977	44.6077137
H	42.4398047	38.1999455	45.7882920
H	44.0657253	39.4610669	48.8693288
H	42.6827309	40.0067771	46.1896120
H	44.1005363	36.9535732	44.8104495
H	46.5036850	36.5536170	44.5346708
H	45.9887496	37.2979324	43.0196558
H	46.8409761	38.2930796	44.2335436
H	46.2017088	40.0627699	44.8163500
H	44.4520366	40.5618411	47.6361243
H	46.1717968	40.5353467	46.9662556
O	43.3640870	42.8798706	50.1788891
H	42.4660338	42.4901113	50.3582011
H	43.3362559	43.7034062	49.6296386
H	42.3654566	37.6592234	36.9530452
H	43.9177320	47.2678567	47.1566875
H	45.8114460	45.6733057	43.9795758
H	41.6938315	38.7394590	52.7414392
H	50.1896009	40.2324385	46.5362019
H	48.4095767	38.4447959	50.9343728
H	45.0243594	41.2339744	53.7624666

IC2

C	43.3995969	37.4336709	37.1881757
H	43.5196102	36.3441495	37.1007257
H	44.0535543	37.8996885	36.4378434
C	43.7052644	37.9262820	38.5789759
C	44.2593477	39.1598585	38.9365652
H	44.6785405	39.9352575	38.3011947
N	44.1731288	39.3436343	40.2852617
H	44.4759157	40.1602369	40.8119635
C	43.5526542	38.2518685	40.8569900
C	43.1480124	38.0542303	42.1732679
H	43.2809064	38.8563986	42.8927536
C	42.5016266	36.8393572	42.4688714
H	42.1477879	36.6462226	43.4845750
C	42.2658618	35.8790401	41.4691229
H	41.7759053	34.9413138	41.7331488
C	42.6290659	36.1151168	40.1396548
H	42.4074855	35.3717617	39.3692836
C	43.2734302	37.3243887	39.8113716
C	43.3217470	46.3848828	47.1594400
H	42.4151212	46.6264498	47.7381526
H	43.0588860	46.2587436	46.1018574
C	43.9434920	45.0883900	47.6783761

O	44.3443993	45.0078261	48.8707040
O	44.0223529	44.1283244	46.8475403
C	46.3978343	45.8071828	44.8996566
N	46.5298708	44.9140724	45.9492808
C	47.3474703	45.4995784	46.8196568
H	47.6672795	45.0803359	47.7708061
N	47.7427440	46.7113210	46.3690625
H	48.3134542	47.4241764	46.8505790
C	47.1589811	46.9312375	45.1513500
H	47.3322673	47.8513331	44.5969766
C	41.5265981	39.6595748	52.5585365
H	40.4979071	39.5582890	52.2019789
H	41.5138505	40.0878858	53.5723623
C	42.3424917	40.5783844	51.6149032
O	43.5094177	40.2797802	51.2474563
O	41.6701086	41.5916287	51.4072856
C	49.4065894	40.8645037	46.2390172
N	49.5231564	41.8181065	45.2423760
H	50.3322411	41.9085183	44.6179668
C	48.4210613	42.5953650	45.2202643
H	48.2582745	43.4042913	44.5134797
N	47.5761828	42.2065124	46.1715328
C	48.1769356	41.1299695	46.8059223
H	47.6834201	40.6351836	47.6343784
C	48.1008679	39.1952504	49.9521681
H	48.8890521	39.9446057	49.7781292
H	48.0567376	38.5374422	49.0715347
C	46.7925087	39.9382405	50.0340082
O	45.9092875	39.8033224	49.1265055
O	46.5388597	40.7872521	50.9378535
C	45.1450304	42.3937038	53.3353735
N	44.9729229	42.7100354	52.0107607
C	45.1833656	44.0188579	51.9550064
H	45.1160653	44.6292873	51.0564902
N	45.4607220	44.5189824	53.1796351
H	45.7318706	45.4906434	53.4041896
C	45.4325388	43.5089727	54.0900062
H	45.6183919	43.6692470	55.1517228
Fe	45.5586268	42.8148345	46.5212465
Fe	44.7749469	41.4582176	49.9677342
O	45.6399681	42.6446278	48.6457858
O	43.3685980	40.7377188	48.4992001
H	45.3351104	43.5633909	48.8584090
C	46.1949121	37.5150782	44.1674205
C	44.8392458	37.7582913	44.7008375
C	44.3115366	38.9770354	45.1636878
C	43.0076595	38.9788158	45.6136927

C	45.1045033	40.2740179	45.2189117
N	45.0734572	40.8603458	46.5376306
C	44.6310983	41.3479849	44.2044126
O	44.1302821	41.0216736	43.1218180
O	44.8753908	42.5404859	44.6046014
H	42.4082793	38.0655200	45.6101848
H	43.9004219	40.7695859	47.6219862
H	42.5319359	39.8906237	45.9784750
H	44.1870303	36.8832281	44.7843044
H	46.5902162	36.5547985	44.5374373
H	46.1399547	37.4199851	43.0643091
H	46.9019519	38.3235611	44.3987745
H	46.1484371	40.0682509	44.9101497
H	42.8256318	41.5467299	48.4924572
H	45.6467966	40.3164312	47.1888665
O	43.1597038	42.9081515	49.8252852
H	42.5018677	42.7549854	50.5478876
H	43.4216829	43.8485409	49.6776626
H	42.3667583	37.6508413	36.9158730
H	43.9888652	47.2374057	47.2868181
H	45.7991923	45.6108954	44.0101814
H	41.8733465	38.6435045	52.7467749
H	50.1595158	40.1183777	46.4929163
H	48.3775213	38.6008871	50.8229506
H	44.9897558	41.3926354	53.7376408

TS4_{OH}

C	43.3959935	37.4607381	37.2985335
H	43.5143863	36.3702197	37.2139289
H	44.0730549	37.9234611	36.5661556
C	43.6706177	37.9523912	38.7018385
C	44.2437081	39.1664975	39.0752968
H	44.7117575	39.9257613	38.4533283
N	44.1213395	39.3572673	40.4275934
H	44.4287028	40.1658846	40.9639352
C	43.4557630	38.2820319	40.9811636
C	42.9941377	38.0871552	42.2857660
H	43.1163673	38.8769178	43.0267996
C	42.3432830	36.8785786	42.5608289
H	41.9631503	36.6857363	43.5678687
C	42.1435982	35.9130861	41.5530614
H	41.6567246	34.9713239	41.8072981
C	42.5387884	36.1489594	40.2363605
H	42.3414181	35.4052104	39.4597812
C	43.1935086	37.3572557	39.9251425
C	43.1379951	46.5124252	46.9921171
H	42.2725394	46.8419090	47.5852645

H	42.8793965	46.4786750	45.9258138
C	43.6033483	45.1282801	47.4269788
O	43.5894779	44.8288213	48.6490284
O	44.0093756	44.3555481	46.5018097
C	46.5810711	46.0336153	44.6943931
N	46.7165668	45.1624974	45.7523648
C	47.5335311	45.7492814	46.6272524
H	47.8196163	45.3274217	47.5886679
N	47.9240898	46.9445935	46.1547985
H	48.4904131	47.6581061	46.6384493
C	47.3388147	47.1563348	44.9357950
H	47.5064652	48.0685966	44.3743474
C	41.2182435	39.7401341	52.5117457
H	40.2157845	39.6436057	52.0913573
H	41.1629739	40.2287741	53.4949913
C	42.1284386	40.5367935	51.5532726
O	43.3388616	40.1788358	51.4599195
O	41.5494743	41.4806120	51.0224632
C	49.3715639	40.8722481	46.2514440
N	49.5409012	41.6936443	45.1490201
H	50.3691317	41.7102213	44.5445861
C	48.4808003	42.5129062	45.0165118
H	48.3665462	43.2418051	44.2180967
N	47.6110120	42.2814064	45.9930992
C	48.1497614	41.2625501	46.7681606
H	47.6416700	40.9373910	47.6737846
C	48.1848485	39.0802595	50.1371904
H	48.9585853	39.7944797	49.8328349
H	48.0237692	38.3899970	49.2883868
C	46.8860761	39.8165239	50.3085297
O	45.8921234	39.3401489	50.9282076
O	46.7123932	40.9484966	49.7324000
C	45.1850037	42.1449128	53.3902028
N	45.1950819	42.3183668	52.0281043
C	45.4463296	43.6142291	51.8644420
H	45.5406226	44.1154634	50.9046808
N	45.5696465	44.2380087	53.0549737
H	45.8264760	45.2271600	53.2238507
C	45.4041266	43.3291013	54.0561055
H	45.4697272	43.5955120	55.1119704
Fe	45.8079071	43.3372663	46.3568441
Fe	44.7106566	40.9874906	50.1956541
O	46.1404088	43.5801022	48.1805551
O	44.1450906	39.8118990	48.7426193
H	45.4718571	44.1571459	48.5844789
C	45.8593166	38.0165971	44.1870068
C	44.6488679	38.1641696	45.0205674

C	44.2173140	39.3262488	45.6686377
C	43.1687830	39.2296337	46.5804553
C	44.9524186	40.6386661	45.5126060
N	44.7554153	41.5191374	46.6552224
C	44.7139050	41.4943933	44.2244427
O	44.2563509	40.9575212	43.2061825
O	45.0810793	42.6994027	44.3864050
H	42.7033637	38.2590591	46.7759207
H	44.3867554	38.9366286	49.0778921
H	42.6969643	40.0932208	47.0354027
H	44.0567907	37.2564911	45.1830795
H	46.4076898	37.1121204	44.5096026
H	45.5781037	37.8346896	43.1330942
H	46.5227169	38.8893112	44.2244626
H	46.0307154	40.4107818	45.4821922
H	43.7996510	41.8802074	46.6969297
H	44.9115907	41.0048513	47.5264931
O	43.5460018	42.4695849	49.5129182
H	42.6710528	42.3675292	49.9624564
H	43.6287981	43.4331404	49.1283861
H	42.3740144	37.6796746	36.9891909
H	43.9213942	47.2534398	47.1510206
H	45.9704453	45.7949211	43.8236300
H	41.5384514	38.7304017	52.7686008
H	50.0866044	40.1140386	46.5706659
H	48.5046974	38.4822946	50.9905378
H	44.9889241	41.1780347	53.8536322

PCOH

C	43.3707293	37.4248233	37.2561200
H	43.4722560	36.3327008	37.1754253
H	44.0506481	37.8813573	36.5232710
C	43.6467043	37.9090484	38.6540966
C	44.2562497	39.1289573	39.0280133
H	44.7311461	39.8770312	38.3988324
N	44.1525062	39.3107920	40.3636613
H	44.5160867	40.0976517	40.8974777
C	43.4735695	38.2361259	40.9320261
C	43.0780475	38.0362054	42.2466625
H	43.2809835	38.7877611	43.0159073
C	42.4002524	36.8324237	42.5234944
H	42.0789424	36.6280283	43.5473799
C	42.1310844	35.8926074	41.5155584
H	41.6292533	34.9607056	41.7775456
C	42.4930729	36.1302203	40.1859817
H	42.2592604	35.3992859	39.4081007
C	43.1713140	37.3268329	39.8773099

C	43.1184222	46.5206046	47.0403792
H	42.2548057	46.8750323	47.6207833
H	42.8665655	46.4645043	45.9729717
C	43.5677170	45.1406135	47.5080082
O	43.4769091	44.8363430	48.7239679
O	44.0465785	44.3773070	46.6109823
C	46.6265413	46.1017986	44.7219685
N	46.7521255	45.2722926	45.8133738
C	47.5939506	45.8727241	46.6532324
H	47.8794572	45.4817684	47.6282094
N	48.0106013	47.0367793	46.1267624
H	48.5940560	47.7557173	46.5797949
C	47.4161755	47.2137609	44.9073400
H	47.5995971	48.0979193	44.3071826
C	41.1751315	39.7484993	52.4910720
H	40.1484668	39.6514689	52.1358618
H	41.1881440	40.2771995	53.4549811
C	42.0441974	40.4826661	51.4422644
O	43.2583430	40.1414067	51.3488033
O	41.4360038	41.3713791	50.8538385
C	49.4757441	41.0149061	46.2170200
N	49.6169123	41.8658332	45.1361168
H	50.4126308	41.8648825	44.4913177
C	48.5823418	42.7278975	45.0903002
H	48.4543181	43.4857133	44.3215464
N	47.7571022	42.4946269	46.1030999
C	48.3006427	41.4310820	46.8098770
H	47.8391937	41.0813122	47.7287351
C	48.1413738	38.9741818	49.9941726
H	48.8966315	39.7062526	49.6820975
H	48.0119913	38.2643140	49.1554183
C	46.8211917	39.6856226	50.1438135
O	45.8671613	39.2637199	50.8446911
O	46.6273219	40.7787077	49.4876097
C	45.1455711	42.1350933	53.3015017
N	45.2640778	42.2729559	51.9403646
C	45.6041534	43.5470423	51.7585706
H	45.8300803	43.9851086	50.7862615
N	45.6671130	44.1955798	52.9393981
H	45.9564794	45.1750578	53.1110539
C	45.3796870	43.3250089	53.9492481
H	45.3891642	43.6158299	55.0006497
Fe	45.8777239	43.4438509	46.4965531
Fe	44.7230924	41.0211036	50.2310663
O	46.1742760	43.8098995	48.3337176
O	43.8354344	39.6008914	48.5873657
H	45.4674896	44.3754204	48.6843215

C	45.6074993	37.8607989	44.6122020
C	44.5068490	38.2034300	45.5699235
C	44.2960445	39.3878310	46.1757019
C	43.2547121	39.5226139	47.2689443
C	45.1113333	40.6169710	45.8709574
N	45.1934281	41.5185492	47.0150937
C	44.7160566	41.4642661	44.6032085
O	44.1826857	40.9176988	43.6308863
O	45.0916311	42.6816944	44.6901583
H	42.5881953	38.6526228	47.2432089
H	43.6335082	38.7917290	49.0754272
H	42.6396879	40.4278218	47.1289477
H	43.8424495	37.3726668	45.8418543
H	46.1329685	36.9506773	44.9555181
H	45.2218072	37.6385341	43.6029882
H	46.3491376	38.6678086	44.5110310
H	46.1468878	40.3238450	45.6387718
H	44.2824959	41.7371888	47.4232141
H	45.7823943	41.1465212	47.7631289
O	43.4795912	42.3897529	49.3693523
H	42.5809577	42.2346495	49.7463287
H	43.5530926	43.3944837	49.1133087
H	42.3488126	37.6550227	36.9548533
H	43.9146685	47.2509694	47.1839976
H	45.9947394	45.8504087	43.8700903
H	41.4926157	38.7448370	52.7737960
H	50.1719131	40.2251572	46.4993541
H	48.4756464	38.4099217	50.8647698
H	44.9075288	41.1799293	53.7695452

TS5

C	43.3781930	37.4269329	37.1823526
H	43.5010413	36.3377282	37.0914642
H	44.0327164	37.8931151	36.4316930
C	43.6809852	37.9205408	38.5748396
C	44.2342987	39.1389068	38.9349766
H	44.6640941	39.9144396	38.3066449
N	44.1390340	39.3241782	40.2950523
H	44.4500381	40.1359675	40.8186727
C	43.5080876	38.2369913	40.8560260
C	43.1060529	38.0131454	42.1744897
H	43.2604435	38.7853907	42.9237744
C	42.4722355	36.8008493	42.4601762
H	42.1380815	36.5912865	43.4800224
C	42.2339049	35.8500327	41.4460461
H	41.7525982	34.9055413	41.7032755
C	42.5886801	36.1021445	40.1209693

H	42.3676825	35.3669940	39.3425143
C	43.2297473	37.3152583	39.8034425
C	43.3075511	46.3779514	47.1653662
H	42.4020754	46.6238076	47.7439014
H	43.0420571	46.2499996	46.1087147
C	43.9287590	45.0846211	47.6867886
O	44.3468139	45.0019141	48.8707403
O	43.9979958	44.1163334	46.8580278
C	46.3864047	45.7900292	44.9094694
N	46.5093594	44.9039649	45.9700137
C	47.3294323	45.4900642	46.8393121
H	47.6433076	45.0753650	47.7942178
N	47.7338903	46.6930559	46.3801449
H	48.3039668	47.4075494	46.8611130
C	47.1558111	46.9080817	45.1587498
H	47.3381813	47.8235040	44.5988020
C	41.5197134	39.6595824	52.5732876
H	40.4931148	39.5579609	52.2105766
H	41.4995660	40.0856975	53.5879285
C	42.3354528	40.5839919	51.6377617
O	43.5028140	40.2883181	51.2610113
O	41.6695447	41.6023557	51.4382096
C	49.3810622	40.8633512	46.2515409
N	49.4813865	41.8003819	45.2369407
H	50.2837230	41.8826310	44.6006785
C	48.3820272	42.5796569	45.2202554
H	48.2082798	43.3737965	44.4989030
N	47.5530764	42.2092367	46.1961931
C	48.1638193	41.1420276	46.8390874
H	47.6797612	40.6592788	47.6800193
C	48.0660817	39.1642029	49.9341195
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H	48.0034471	38.4936041	49.0644662
C	46.7696401	39.9244633	50.0210933
O	45.8756862	39.8145185	49.1202554
O	46.5359710	40.7755411	50.9312202
C	45.1525114	42.3906459	53.3357031
N	44.9989879	42.7069116	52.0072493
C	45.2135104	44.0160777	51.9521204
H	45.1598797	44.6246585	51.0516959
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C	45.4317618	43.5072827	54.0901756
H	45.6046758	43.6690462	55.1539785
Fe	45.5518027	42.8547587	46.5212838
Fe	44.7793289	41.4746389	50.0197166
O	45.5957143	42.6282387	48.6268697

O	43.3191079	40.7931021	48.5490847	H	41.7279500	34.6417551	41.4791075
H	45.2931860	43.5494454	48.8414720	C	42.5536013	35.9485580	39.9849713
C	46.1724894	37.4074579	44.0212921	H	42.3588082	35.2570028	39.1608671
C	44.9659072	37.7748176	44.8071155	C	43.1853674	37.1854708	39.7566900
C	44.5687238	39.0412438	45.1127533	C	43.3027601	46.4205145	47.1448806
C	43.4360971	39.3614161	45.9127795	H	42.3932471	46.6516170	47.7236912
C	45.3197434	40.3357254	45.0520367	H	43.0350542	46.2868433	46.0895202
N	45.0858192	40.7892377	46.4407949	C	43.9433206	45.1375311	47.6674260
C	44.7536475	41.4363220	44.1288540	O	44.4204440	45.0836235	48.8297146
O	44.2288730	41.1685059	43.0530567	O	43.9732349	44.1469249	46.8590631
O	44.9218109	42.6146651	44.6294085	C	46.3669138	45.8268959	44.9063849
H	42.9530365	38.6195637	46.5600859	N	46.4873740	44.9460944	45.9713598
H	43.7969220	40.8221067	47.6854940	C	47.3103276	45.5330099	46.8385175
H	42.8586970	40.2644027	45.7051906	H	47.6236496	45.1213087	47.7951332
H	44.3194365	36.9577445	45.1442108	N	47.7169602	46.7320386	46.3729659
H	46.6239258	36.4810764	44.4090735	H	48.2922810	47.4461839	46.8488185
H	45.8909704	37.2203717	42.9685562	C	47.1394558	46.9433494	45.1503173
H	46.9244986	38.2109036	44.0277214	H	47.3246826	47.8548698	44.5852301
H	46.3917128	40.2335973	44.8068479	C	41.5532578	39.6871343	52.5324736
H	42.7981987	41.6182819	48.5851147	H	40.5410005	39.5646315	52.1366182
H	45.6244988	40.2178147	47.1046255	H	41.4865290	40.1053961	53.5483836
O	43.1480998	42.9338866	49.8763053	C	42.3712845	40.6468735	51.6353288
H	42.4918555	42.7670414	50.6000133	O	43.5458720	40.3712367	51.2589771
H	43.3960277	43.8766290	49.7325184	O	41.7012999	41.6645950	51.4601240
H	42.3449680	37.6429926	36.9106330	C	49.3800282	40.9085924	46.2816929
H	43.9774056	47.2286570	47.2905146	N	49.4617311	41.8174146	45.2405926
H	45.7950723	45.5976791	44.0142629	H	50.2563090	41.8888286	44.5929155
H	41.8669818	38.6437855	52.7620424	C	48.3614169	42.5956423	45.2230733
H	50.1357152	40.1154446	46.4948548	H	48.1731226	43.3684083	44.4825036
H	48.3560537	38.5827049	50.8092444	N	47.5484756	42.2524205	46.2228621
H	44.9945771	41.3906017	53.7394796	C	48.1748269	41.2069636	46.8852283
PC				H	47.7122665	40.7493575	47.7513356
				C	48.0247540	39.1937369	49.9242369
	C	43.3877522	37.4239076	H	48.8334480	39.9134691	49.7205420
	H	43.5202507	36.3404989	H	47.9378076	38.5222963	49.0572214
	H	44.0431445	37.9282127	C	46.7489723	39.9873212	50.0253303
	C	43.6655190	37.8548277	O	45.8265406	39.8867076	49.1521241
	C	44.2196523	39.0530979	O	46.5671171	40.8640897	50.9243255
	H	44.6808719	39.8520039	C	45.1694784	42.4440873	53.3852018
	N	44.0877564	39.1634777	N	45.0630460	42.7688917	52.0549478
	H	44.3984584	39.9378049	C	45.3096718	44.0717640	52.0103903
	C	43.4382598	38.0456814	H	45.3010713	44.6796818	51.1085232
	C	43.0222527	37.7384123	N	45.5418316	44.5623214	53.2448017
	H	43.1859930	38.4400432	H	45.8244247	45.5301206	53.4752335
	C	42.3987270	36.5023055	C	45.4498752	43.5523652	54.1516870
	H	42.0710032	36.2216158	H	45.5962697	43.7062836	55.2206944
	C	42.1855655	35.6124702	Fe	45.5480663	42.9259272	46.4907250

Fe	44.8081891	41.6021600	50.0695678	O	44.4863395	42.9058648	47.7462016
O	45.5885775	42.6994770	48.6285770	O	43.4406024	44.7802715	47.1414258
O	43.2394830	41.1000228	48.5999925	C	46.3286120	44.8376636	42.2120488
H	45.2906179	43.6299730	48.8238115	N	47.0257769	45.5123651	41.2305460
C	46.0179058	37.2927669	43.8393160	H	47.6469203	45.0983334	40.5172541
C	44.9544765	37.7379839	44.7936266	C	46.7459748	46.8295428	41.3615916
C	44.7403278	38.9932401	45.1871968	H	47.1163704	47.6074507	40.6994037
C	43.9505211	39.6174845	46.3101676	N	45.9279873	47.0314560	42.3873824
C	45.4941289	40.2883535	45.0429620	C	45.6440546	45.7937043	42.9175112
N	45.0745962	40.6590669	46.4495798	H	44.9839934	45.6750159	43.7696310
C	44.8751599	41.3678565	44.1231199	C	46.4640984	51.3820472	39.8115810
O	44.3437385	41.0905716	43.0565714	H	47.4952835	51.0091597	39.8209846
O	44.9856050	42.5585918	44.6297844	H	46.4386605	52.4779689	39.8609915
H	43.7612492	39.0441294	47.2242232	C	45.5418860	50.8025660	40.9153594
H	43.6905790	41.2921995	47.7589222	O	44.4790686	51.3872527	41.1496548
H	43.0211608	40.1136494	45.9852179	O	45.9866597	49.7728285	41.5063146
H	44.2992575	36.9605325	45.2049032	N	42.4850124	52.5814690	39.5241018
H	46.5903857	36.4539184	44.2696294	H	43.2290858	52.1739727	40.1221078
H	45.5729350	36.9382321	42.8942419	H	41.9700533	51.8195578	39.0308760
H	46.7213772	38.1045436	43.6026067	H	43.0061475	53.1149583	38.7924184
H	46.5816283	40.2526261	44.8788563	C	41.5938320	53.4966857	40.3274579
H	42.7411401	41.9202144	48.7940549	H	40.6599073	53.6315066	39.7589462
H	45.7300833	40.2670645	47.1350221	C	41.3054760	52.8798618	41.7086710
O	43.1834294	43.1596699	50.0352449	H	42.2732157	52.8705618	42.2414810
H	42.5410634	42.9952818	50.7642995	C	40.3433925	53.7693092	42.5003894
H	43.4219157	44.0998500	49.8823124	H	40.7547234	54.7759958	42.6577249
H	42.3534741	37.6403772	36.8918048	H	39.3798287	53.8874052	41.9815685
H	43.9605526	47.2807161	47.2690961	H	40.1435110	53.3179433	43.4842850
H	45.7768595	45.6277944	44.0118114	C	40.8262006	51.4166328	41.6510275
H	41.9198282	38.6795300	52.7285017	H	41.6274826	50.7981120	41.2222512
H	50.1300570	40.1540482	46.5187308	H	40.7319849	51.0619776	42.6922624
H	48.3121212	38.6086510	50.7978282	C	39.5236371	51.1544502	40.8967028
H	44.9951632	41.4408018	53.7739173	H	38.6826182	51.7328313	41.3105228
				H	39.6066511	51.4075799	39.8288370
				H	39.2562687	50.0877837	40.9605276
⁷ RC				C	42.2894843	54.8829614	40.4828400
C	41.4455007	47.1893027	41.7655096	O	41.5570994	55.8839502	40.3662064
N	41.7406962	48.0039639	40.6934856	O	43.5192480	54.8570458	40.7494563
H	41.1948791	48.1561406	39.8305305	Fe	45.1181532	48.8819006	43.1859710
C	42.8737331	48.6768844	40.9722367	O	43.6950063	50.4251863	44.0624123
H	43.3153823	49.3977170	40.2936684	O	44.8427105	50.9319596	43.9927014
N	43.3307685	48.3375608	42.1706944	C	50.5338983	49.4716121	42.0037126
C	42.4462192	47.4106514	42.6839972	C	49.9769485	50.7336209	42.6379870
H	42.5932742	46.9817656	43.6723426	O	50.9053925	51.2366050	43.5857640
C	42.2163683	42.7144739	47.0169684	C	48.5952505	50.5899653	43.3152330
H	41.5645992	42.7622755	47.9040335	O	48.4010851	51.8227133	43.9944233
H	42.4632727	41.6542938	46.8726345	C	48.4393144	49.3654016	44.2285832
C	43.4752272	43.5385807	47.3074542				

C	49.3689510	49.4376595	45.4565453	O	44.4816739	42.9132815	47.7582855
N	49.0790714	48.3872587	46.4171939	O	43.4299746	44.7631858	47.0883618
C	47.8795167	47.7930617	46.4929699	C	46.3493835	44.8066966	42.1865058
N	47.7060216	46.8063999	47.4130792	N	47.0343218	45.4794428	41.1955697
C	46.5335309	46.1730774	47.4249876	H	47.6579142	45.0663925	40.4840341
N	46.3074222	45.2010650	48.3138642	C	46.7420134	46.7940775	41.3150620
N	45.5131094	46.4884184	46.5680449	H	47.1034597	47.5684852	40.6435607
C	45.6350538	47.5042158	45.6449085	N	45.9298211	46.9963145	42.3459468
O	44.6725309	47.7766191	44.8560990	C	45.6606220	45.7601154	42.8887599
C	46.8558968	48.1780910	45.6082017	H	45.0047185	45.6436904	43.7438862
N	47.0170852	49.2193919	44.6351185	C	46.4504059	51.3917552	39.8480834
H	51.5002282	49.6891543	41.5253792	H	47.4847750	51.0275126	39.8647159
H	50.7089031	48.6799973	42.7487392	H	46.4143826	52.4873475	39.9086359
H	49.8428858	49.0900900	41.2351774	C	45.5172407	50.7956045	40.9336098
H	49.8330890	51.4907989	41.8404290	O	44.4366807	51.3489756	41.1403877
H	50.3956301	51.8951083	44.0923557	O	45.9781793	49.7744266	41.5381718
H	47.8433820	50.4659848	42.5202520	N	42.4776346	52.5923306	39.5174472
H	47.8568289	51.7355767	44.8046810	H	43.2184384	52.1801830	40.1158624
H	48.6831236	48.4650380	43.6451459	H	41.9600897	51.8317565	39.0245016
H	49.2702421	50.4281986	45.9297250	H	43.0030254	53.1243104	38.7875133
H	50.4118602	49.3454539	45.1286646	C	41.5905134	53.5117708	40.3197524
H	47.0709031	44.9861111	48.9583700	H	40.6514581	53.6406802	39.7582633
H	49.8126093	48.0904295	47.0613088	C	41.3134576	52.9040610	41.7080071
H	44.6232316	45.9569160	46.6743700	H	42.2862099	52.8958790	42.2327235
H	45.5524186	44.5178768	48.1774912	C	40.3573755	53.7965147	42.5037306
H	46.7244478	50.1009170	45.0794954	H	40.7689445	54.8041181	42.6527910
O	46.8876698	51.5478289	46.3523485	H	39.3896829	53.9111944	41.9917979
H	47.2492037	51.1736515	47.1885586	H	40.1654695	53.3491453	43.4911960
H	46.5548207	52.4474627	46.6063751	C	40.8316479	51.4410721	41.6595980
H	40.6040436	46.4968094	41.7871935	H	41.6321761	50.8194658	41.2346162
H	46.4570926	43.7895015	42.4820784	H	40.7357911	51.0923617	42.7028517
H	41.6142808	43.0692671	46.1804999	C	39.5281590	51.1760366	40.9077313
H	46.0601375	51.1906976	38.8174643	H	38.6873253	51.7552658	41.3205781
				H	39.6095162	51.4255140	39.8390062
				H	39.2612511	50.1094734	40.9757749
				C	42.2864331	54.8987850	40.4580796
				O	41.5473513	55.8982290	40.3745727
				O	43.5248728	54.8738435	40.6785537
				Fe	45.1204532	48.8194720	43.1520467
				O	44.4093992	50.4367379	44.0360614
				O	44.9429678	51.5618343	44.1108832
				C	50.5295794	49.4651630	42.0523848
				C	49.9522647	50.7355680	42.6515545
				O	50.8625699	51.2656932	43.6019372
				C	48.5604033	50.5946488	43.3099872
				O	48.3427107	51.8358679	43.9663980
				C	48.3954849	49.3832166	44.2382649
⁵RC							
C	41.4109215	47.1646144	41.8092673				
N	41.7161366	47.9927290	40.7494407				
H	41.1843703	48.1478807	39.8777060				
C	42.8385084	48.6700569	41.0512197				
H	43.2867362	49.4011462	40.3886977				
N	43.2797274	48.3219920	42.2555563				
C	42.3953959	47.3815644	42.7453868				
H	42.5362481	46.9389814	43.7284444				
C	42.2171991	42.6899558	47.0176350				
H	41.5706126	42.7324764	47.9086821				
H	42.4739870	41.6316831	46.8757243				
C	43.4699557	43.5279085	47.2952329				

C	49.3140673	49.4788916	45.4718965	O	44.4898358	42.9106253	47.7426859
N	49.0090483	48.4553306	46.4552283	O	43.4438288	44.7853118	47.1397686
C	47.8216281	47.8352552	46.5107552	C	46.3238714	44.8512358	42.2158824
N	47.6631616	46.8503844	47.4355391	N	47.0232140	45.5266385	41.2362906
C	46.5100308	46.1836528	47.4328483	H	47.6434075	45.1121471	40.5221819
N	46.2961428	45.2106173	48.3248022	C	46.7482334	46.8444722	41.3707973
N	45.5000459	46.4608990	46.5546391	H	47.1209036	47.6227971	40.7105847
C	45.6044334	47.4694912	45.6202260	N	45.9311735	47.0467003	42.3977569
O	44.6478257	47.6765271	44.8072113	C	45.6433994	45.8079958	42.9245718
C	46.8017849	48.1910220	45.6049079	H	44.9830608	45.6876992	43.7760644
N	46.9652699	49.2320976	44.6263431	C	46.4676416	51.3729716	39.8137971
H	51.4959407	49.6829283	41.5738656	H	47.4984416	50.9990397	39.8255864
H	50.7094180	48.6949160	42.8184913	H	46.4429677	52.4685399	39.8707900
H	49.8489729	49.0547007	41.2893476	C	45.5373955	50.7876689	40.9070909
H	49.8147878	51.4742468	41.8355566	O	44.4700742	51.3646473	41.1319428
H	50.3404281	51.9309605	44.0865961	O	45.9800926	49.7559278	41.4998472
H	47.8240202	50.4551037	42.5043299	N	42.4815015	52.5771094	39.5225429
H	47.8257425	51.7460439	44.7941097	H	43.2271119	52.1665630	40.1163027
H	48.6509170	48.4755293	43.6711780	H	41.9638786	51.8172626	39.0289476
H	49.2231241	50.4802118	45.9212128	H	43.0006783	53.1123512	38.7908261
H	50.3580326	49.3681043	45.1525812	C	41.5953135	53.4903453	40.3335448
H	47.0554008	45.0172868	48.9810186	H	40.6608131	53.6321553	39.7676452
H	49.7390715	48.1633228	47.1059641	C	41.3084682	52.8668352	41.7121243
H	44.6204307	45.9079298	46.6519436	H	42.2765363	52.8525592	42.2437902
H	45.5598375	44.5080880	48.1823239	C	40.3491863	53.7548801	42.5090238
H	46.6656068	50.1165539	45.0626537	H	40.7617258	54.7610479	42.6670289
O	46.9288733	51.5411883	46.3936155	H	39.3839978	53.8749294	41.9935270
H	47.2973055	51.1811663	47.2321542	H	40.1523131	53.3018504	43.4927970
H	46.5726539	52.4325440	46.6416085	C	40.8269129	51.4046680	41.6491021
H	40.5728944	46.4676453	41.8126938	H	41.6262832	50.7873271	41.2149984
H	46.4807435	43.7603790	42.4622432	H	40.7364521	51.0454294	42.6889377
H	41.6085358	43.0360414	46.1822783	C	39.5216143	51.1477972	40.8977302
H	46.0596166	51.2038708	38.8480583	H	38.6825310	51.7250085	41.3170801
5RC'				H	39.6012722	51.4064397	39.8309178
C	41.4447513	47.1751106	41.7614495	H	39.2526590	50.0812235	40.9572607
N	41.7402342	47.9928770	40.6918714	C	42.2979045	54.8723255	40.4953654
H	41.1931717	48.1499479	39.8303586	O	41.5726700	55.8784157	40.3764742
C	42.8765178	48.6597756	40.9692970	O	43.5260441	54.8379620	40.7688048
H	43.3183895	49.3832464	40.2939746	Fe	45.0979793	48.9012568	43.1861771
N	43.3356279	48.3116742	42.1647466	O	43.6738185	50.4452061	44.0037715
C	42.4490270	47.3872680	42.6778870	O	44.8751922	50.8663772	43.9789685
H	42.5955722	46.9553980	43.6649501	C	50.5551892	49.4504066	41.9848803
C	42.2188917	42.7189752	47.0176540	C	49.9996960	50.7152899	42.6145413
H	41.5680654	42.7682346	47.9053495	O	50.9277048	51.2195420	43.5618993
H	42.4658121	41.6585600	46.8750197	C	48.6174034	50.5764763	43.2922952
C	43.4782867	43.5433851	47.3052985	O	48.4291398	51.8095141	43.9714299
				C	48.4590245	49.3523467	44.2060962

C	49.3883060	49.4224298	45.4345501	O	44.5052146	42.9357955	47.7669324
N	49.0949254	48.3716381	46.3941962	O	43.4761934	44.7768520	47.0441682
C	47.8921376	47.7859391	46.4740063	C	46.2853572	44.8070004	42.1391545
N	47.7112330	46.8046546	47.3974267	N	46.9948134	45.5019690	41.1803601
C	46.5336699	46.1808237	47.4140453	H	47.6540034	45.1024338	40.4939595
N	46.3026436	45.2129542	48.3057478	C	46.6430618	46.8035445	41.2733909
N	45.5128593	46.5036950	46.5594198	H	47.0118128	47.5913199	40.6215223
C	45.6432627	47.5153971	45.6336193	N	45.7650444	46.9781394	42.2563717
O	44.6783986	47.7960152	44.8463838	C	45.5164100	45.7339025	42.7909348
C	46.8696738	48.1753962	45.5879062	H	44.8236673	45.5911611	43.6121101
N	47.0375747	49.2108907	44.6122935	C	46.4167821	51.4188444	39.7813083
H	51.5223831	49.6649772	41.5070176	H	47.4658845	51.0988554	39.7998027
H	50.7283291	48.6607185	42.7324172	H	46.3228333	52.5101399	39.8464229
H	49.8641029	49.0677981	41.2170309	C	45.5053955	50.7517785	40.8408385
H	49.8575599	51.4702214	41.8146080	O	44.4392292	51.3071601	41.1231095
H	50.4167765	51.8789391	44.0664998	O	45.9439700	49.6653765	41.3264692
H	47.8635584	50.4543745	42.4984008	N	42.4777924	52.5826723	39.5348069
H	47.8815835	51.7270196	44.7802832	H	43.2118648	52.1646653	40.1397641
H	48.7010928	48.4512872	43.6229517	H	41.9592647	51.8268972	39.0371736
H	49.2906944	50.4124669	45.9088416	H	43.0093792	53.1122272	38.8075811
H	50.4313789	49.3281748	45.1079906	C	41.5884308	53.5079743	40.3294804
H	47.0664806	44.9935734	48.9484942	H	40.6585292	53.6458890	39.7551025
H	49.8259364	48.0761079	47.0420571	C	41.2869757	52.9022640	41.7130366
H	44.6206209	45.9770943	46.6669415	H	42.2505448	52.8867836	42.2528680
H	45.5438255	44.5336119	48.1717419	C	40.3267005	53.8027205	42.4943973
H	46.7414605	50.0952713	45.0492547	H	40.7473843	54.8046678	42.6559396
O	46.9260839	51.5432370	46.3313708	H	39.3691517	53.9304836	41.9665501
H	47.2765839	51.1639077	47.1697330	H	40.1136399	53.3534386	43.4763456
H	46.5775061	52.4349560	46.5899262	C	40.7956352	51.4433886	41.6604138
H	40.6007187	46.4857448	41.7826840	H	41.5979767	50.8183667	41.2452489
H	46.4494397	43.8024543	42.4848754	H	40.6897704	51.0961046	42.7028333
H	41.6154898	43.0719412	46.1813597	C	39.4990501	51.1835271	40.8952034
H	46.0673773	51.1879774	38.8169858	H	38.6574013	51.7694870	41.2969246
⁷TS1				H	39.5928426	51.4285406	39.8262524
C	41.3414647	47.2035739	41.7556302	H	39.2245663	50.1188109	40.9642096
N	41.6216983	47.9956794	40.6629082	C	42.2937247	54.8887360	40.4807054
H	41.0800803	48.1185068	39.7943232	O	41.5647657	55.8942103	40.3735433
C	42.7233549	48.7171657	40.9291528	O	43.5252580	54.8559841	40.7354674
H	43.1552289	49.4277649	40.2338329	Fe	44.9985724	48.8738889	43.0119090
N	43.1732349	48.4303372	42.1439049	O	44.3624986	50.1879322	44.3649608
C	42.3200591	47.4860136	42.6782245	O	45.5155840	50.7980808	43.8883961
H	42.4760405	47.0866350	43.6777944	C	50.5880828	49.5107413	42.0468111
C	42.2428449	42.7142499	47.0146725	C	49.9949895	50.7576760	42.6788042
H	41.6046508	42.7616507	47.9118534	O	50.9109166	51.2831299	43.6269474
H	42.4948260	41.6544240	46.8747958	C	48.6231959	50.5805298	43.3637368
C	43.5007289	43.5460739	47.2811516	O	48.3898463	51.8026570	44.0319321
				C	48.5265527	49.3635992	44.2958790

C	49.3624520	49.5179718	45.5705867	O	44.4302706	42.8847291	47.7768952
N	49.0735105	48.4336994	46.4968749	O	43.4213335	44.7577297	47.1129567
C	47.8982654	47.8034070	46.5294877	C	46.3659622	44.7991771	42.1418480
N	47.7118766	46.8360542	47.4563471	N	47.0505198	45.4593167	41.1428130
C	46.5515267	46.1743731	47.4414216	H	47.6859789	45.0421376	40.4445049
N	46.3313125	45.1956525	48.3169527	C	46.7386417	46.7704315	41.2280011
N	45.5478100	46.4578098	46.5596018	H	47.0963983	47.5377828	40.5465748
C	45.6477960	47.4303979	45.5912803	N	45.9113001	46.9805319	42.2444775
O	44.7382332	47.5686331	44.7550520	C	45.6547438	45.7553291	42.8148527
C	46.8893044	48.1766529	45.5730401	H	44.9907511	45.6471749	43.6646512
N	47.1163682	49.0693498	44.5864267	C	46.4696123	51.4249010	39.7528101
H	51.5371346	49.7587426	41.5496646	H	47.5106339	51.0809524	39.7657446
H	50.8091745	48.7357795	42.7976484	H	46.4029466	52.5189514	39.8070852
H	49.9004646	49.0918143	41.2948164	C	45.5563790	50.7988743	40.8335473
H	49.8278444	51.5089631	41.8807879	O	44.4849647	51.3538052	41.0806386
H	50.3864642	51.9316076	44.1321107	O	46.0143817	49.7446319	41.3814997
H	47.8742520	50.4099282	42.5693108	N	42.4714425	52.5985608	39.5273559
H	47.7891226	51.7050660	44.8078679	H	43.2168318	52.1889489	40.1214398
H	48.9044883	48.4866785	43.7407790	H	41.9556754	51.8385100	39.0329771
H	49.1564565	50.4892723	46.0462494	H	42.9928180	53.1332736	38.7965938
H	50.4276057	49.4930831	45.3118247	C	41.5847718	53.5146040	40.3350344
H	47.0803299	44.9991679	48.9849550	H	40.6534642	53.6607665	39.7648655
H	49.7936096	48.1553983	47.1672947	C	41.2875592	52.8915567	41.7117783
H	44.6735099	45.8845979	46.6428561	H	42.2519827	52.8750228	42.2505152
H	45.5772438	44.5057525	48.1844105	C	40.3228879	53.7793083	42.5023857
H	46.3455585	50.0944246	44.3807970	H	40.7321534	54.7867727	42.6591045
O	46.8876698	51.5478289	46.3523485	H	39.3592841	53.8947776	41.9828132
H	47.2492037	51.1736515	47.1885586	H	40.1235729	53.3281532	43.4864472
H	46.5548207	52.4474627	46.6063751	C	40.8042912	51.4301575	41.6439467
H	40.5249278	46.4822662	41.7880311	H	41.6097352	50.8126773	41.2220277
H	46.4540444	43.7697291	42.4284296	H	40.6980481	51.0723750	42.6829034
H	41.6284943	43.0585671	46.1827553	C	39.5092001	51.1710981	40.8758180
H	46.0376712	51.2110280	38.7807312	H	38.6647727	51.7491209	41.2829657
⁵TS1				H	39.6021218	51.4266527	39.8093615
C	41.3901906	47.2175209	41.7457008	H	39.2395815	50.1046010	40.9347108
N	41.6932217	48.0260622	40.6699026	C	42.2950710	54.8917941	40.5015892
H	41.1543461	48.1728265	39.8013708	O	41.5721784	55.9022119	40.4054525
C	42.8194153	48.7021843	40.9511840	O	43.5268538	54.8480241	40.7555635
H	43.2693287	49.4200667	40.2746972	Fe	45.1299849	48.8203860	42.9931662
N	43.2665797	48.3683167	42.1581401	O	44.5119131	50.6036896	43.8134061
C	42.3797959	47.4436456	42.6716459	O	45.4228178	51.2042023	44.5034295
H	42.5249082	47.0185581	43.6614843	C	50.5729887	49.4791895	42.0173012
C	42.1755793	42.7031278	47.0005663	C	49.9953192	50.7487242	42.6190708
H	41.5203850	42.7402621	47.8852805	O	50.8963016	51.2478269	43.5971236
H	42.4214333	41.6437843	46.8472410	C	48.5776823	50.6281216	43.2368346
C	43.4365380	43.5185860	47.3054963	O	48.3587434	51.8627838	43.8994417
				C	48.3718631	49.4105259	44.1472450

C	49.2595374	49.5186675	45.4049167	O	44.5074472	42.9468122	47.7729944
N	48.9671820	48.4726215	46.3625754	O	43.4575991	44.7937376	47.0952012
C	47.7735224	47.8737725	46.4110386	C	46.3127925	44.8315971	42.1953662
N	47.5941960	46.8972977	47.3325963	N	47.0184270	45.5050946	41.2190495
C	46.4299014	46.2559360	47.3481802	H	47.6511177	45.0916767	40.5161631
N	46.2049075	45.2996369	48.2545908	C	46.7160514	46.8195668	41.3304210
N	45.4211792	46.5466218	46.4703426	H	47.0900585	47.5968289	40.6691209
C	45.5520629	47.5337254	45.5182928	N	45.8767436	47.0214557	42.3381369
O	44.6299322	47.7271941	44.6657986	C	45.6006180	45.7858562	42.8759907
C	46.7590276	48.2531624	45.4847927	H	44.9203017	45.6643585	43.7116964
N	46.9321613	49.2024946	44.4625777	C	46.4487472	51.4395931	39.7488479
H	51.5524360	49.6944801	41.5642255	H	47.4953487	51.1127710	39.7558087
H	50.7296870	48.6995232	42.7792453	H	46.3655679	52.5329259	39.7943673
H	49.9076486	49.0820220	41.2342913	C	45.5504050	50.8124532	40.8454554
H	49.8916255	51.5005929	41.8105196	O	44.4691843	51.3566596	41.0835725
H	50.3788628	51.9222132	44.0742187	O	46.0237975	49.7793403	41.4103946
H	47.8678260	50.5064190	42.4027763	N	42.4742121	52.5885967	39.5318147
H	47.8610546	51.7577099	44.7404645	H	43.2230241	52.1730149	40.1203585
H	48.6877758	48.5153932	43.5858632	H	41.9487244	51.8318357	39.0425475
H	49.1317971	50.5079099	45.8684158	H	42.9907722	53.1204606	38.7960212
H	50.3104677	49.4414387	45.1003165	C	41.6013891	53.5095604	40.3476137
H	46.9471882	45.1186092	48.9329343	H	40.6689975	53.6681230	39.7826492
H	49.6797500	48.1910069	47.0389382	C	41.3040390	52.8845268	41.7234191
H	44.5434353	45.9999964	46.5625326	H	42.2713084	52.8498253	42.2553415
H	45.4450327	44.6214764	48.1378916	C	40.3597769	53.7846328	42.5248459
H	46.3223126	50.2543808	44.6418803	H	40.7865882	54.7846975	42.6837838
O	47.0163299	51.5784301	46.3442635	H	39.3944928	53.9184622	42.0126689
H	47.3690132	51.2043185	47.1815114	H	40.1603648	53.3321902	43.5083547
H	46.6415345	52.4566922	46.6140305	C	40.7969363	51.4316465	41.6530356
H	40.5572187	46.5147467	41.7639632	H	41.5875851	50.8031550	41.2205634
H	46.5046837	43.7587705	42.4357485	H	40.6961324	51.0702506	42.6911525
H	41.5796571	43.0693971	46.1646292	C	39.4909551	51.1967233	40.8960870
H	46.0727479	51.2174296	38.7590690	H	38.6596002	51.7887628	41.3102590
⁷¹ICl				H	39.5801114	51.4514052	39.8290852
C	41.4515581	47.2125001	41.7981724	H	39.2041760	50.1347997	40.9566588
N	41.7427655	48.0277298	40.7238228	C	42.3246640	54.8792707	40.5172323
H	41.2018719	48.1680624	39.8558703	O	41.6134176	55.8972629	40.4084986
C	42.8590835	48.7229125	41.0104671	O	43.5525842	54.8260126	40.7886147
H	43.2948366	49.4501382	40.3357479	Fe	45.1614194	48.9463938	43.1232366
N	43.3113243	48.4005026	42.2165967	O	44.4873603	50.5133598	43.9410487
C	42.4390741	47.4579304	42.7249014	O	44.5680629	51.1328619	45.1489994
H	42.5851511	47.0358402	43.7159486	C	50.5955991	49.6453223	42.0110288
C	42.2409476	42.7223381	47.0333243	C	49.9259824	50.8425321	42.6624568
H	41.5969116	42.7703838	47.9261275	O	50.7939235	51.3812105	43.6509905
H	42.4948368	41.6629224	46.8948044	C	48.5412652	50.5738770	43.2904428
C	43.4952182	43.5588302	47.3066129	O	48.2141890	51.7681571	43.9810771
				C	48.4679450	49.3288618	44.1863050

C	49.3213564	49.4857777	45.4579157	O	44.5198130	42.9423652	47.7520352
N	49.0765396	48.4053386	46.3981016	O	43.4301947	44.7858777	47.1369428
C	47.8958411	47.7883468	46.4679966	C	46.2781981	44.7275954	41.9975511
N	47.7025349	46.8531576	47.4260061	N	47.0231145	45.3995629	41.0488637
C	46.5337502	46.2093792	47.4414225	H	47.7309620	44.9933985	40.4202469
N	46.3200280	45.2327547	48.3245078	C	46.5924777	46.6818318	41.0284669
N	45.5050181	46.5187013	46.5928781	H	46.9697046	47.4472861	40.3544921
C	45.6084749	47.4876250	45.6245768	N	45.6347373	46.8643645	41.9243991
O	44.6595060	47.7315044	44.8503477	C	45.4060744	45.6460810	42.5163454
C	46.8884657	48.1391975	45.5036342	H	44.6461574	45.5128993	43.2779990
N	47.0754176	48.9631322	44.4611299	C	46.3907207	51.4997098	39.7284159
H	51.5592056	49.9450373	41.5741849	H	47.4488084	51.2111560	39.7347780
H	50.8062409	48.8465553	42.7394248	H	46.2625248	52.5894285	39.7456940
H	49.9608023	49.2363808	41.2090614	C	45.5366513	50.8419162	40.8450109
H	49.7496947	51.6120727	41.8839796	O	44.5396342	51.4652821	41.2443136
H	50.2348801	51.9985710	44.1561141	O	45.9288024	49.7078999	41.2250611
H	47.8303322	50.3917046	42.4697892	N	42.5137141	52.5928793	39.5853889
H	47.6623742	51.5918548	44.7674787	H	43.2497132	52.2014152	40.2098790
H	48.8814861	48.4877227	43.5984392	H	42.0044722	51.8243938	39.0994359
H	49.1095441	50.4547827	45.9365305	H	43.0409445	53.1124018	38.8478233
H	50.3821747	49.4875679	45.1823848	C	41.6094141	53.5286762	40.3501147
H	47.0862300	45.0204945	48.9679122	H	40.6922047	53.6631129	39.7549340
H	49.7968721	48.1650787	47.0829872	C	41.2746266	52.9352551	41.7313423
H	44.6229517	45.9664950	46.7014294	H	42.2294686	52.9114594	42.2867057
H	45.5682149	44.5417653	48.1904555	C	40.3120471	53.8506094	42.4924354
H	45.4579757	50.9298247	45.5361188	H	40.7431256	54.8468952	42.6609376
O	46.8440357	51.4844809	46.4459620	H	39.3665705	53.9902130	41.9463169
H	47.1881160	51.0529802	47.2641154	H	40.0735803	53.4053509	43.4704644
H	46.6007090	52.4089220	46.7327409	C	40.7647486	51.4824744	41.6758709
H	40.6150139	46.5139576	41.8154707	H	41.5669939	50.8423035	41.2846291
H	46.4492195	43.7863498	42.4726977	H	40.6265112	51.1438103	42.7175508
H	41.6306092	43.0658448	46.1981253	C	39.4837684	51.2327670	40.8811782
H	46.0528494	51.2249452	38.7562461	H	38.6412704	51.8370537	41.2529168
⁵¹Cr				H	39.6095201	51.4607898	39.8118413
C	41.3488340	47.2368833	41.7760808	H	39.1923626	50.1731282	40.9570650
N	41.6541258	48.0398269	40.6961842	C	42.3124550	54.9106308	40.5043120
H	41.1376301	48.1555923	39.8110278	O	41.5818676	55.9142467	40.3897895
C	42.7391481	48.7733310	41.0100216	O	43.5415508	54.8810188	40.7707215
H	43.1949685	49.4832713	40.3283761	Fe	45.1346421	48.7266203	42.9202719
N	43.1543172	48.4917714	42.2382390	O	45.6394871	50.2202242	44.2375120
C	42.2926160	47.5327270	42.7321750	O	45.3852242	49.9587193	45.5912331
H	42.4218966	47.1232333	43.7308634	C	50.9185519	49.3682827	42.0492300
C	42.2523156	42.6981790	47.0059511	C	49.9549761	50.4907899	42.3902078
H	41.6019455	42.7154726	47.8956137	O	50.5482530	51.3166989	43.3891936
H	42.5209384	41.6458734	46.8433840	C	48.5548595	50.0439486	42.8463973
C	43.4915524	43.5456801	47.3070192	O	47.8838113	51.2244002	43.2167007
				C	48.5564427	48.9889375	43.9748990

C	49.1009332	49.5294633	45.3045874	O	44.5261443	42.9382321	47.7626498
N	48.9238681	48.5369339	46.3655726	O	43.4369188	44.7749509	47.1323773
C	47.8381551	47.7857491	46.4097862	C	46.2668806	44.7465990	41.9762692
N	47.6569926	46.8967149	47.3978515	N	47.0137169	45.4254999	41.0344158
C	46.5285015	46.1723980	47.3879703	H	47.7203477	45.0216000	40.4027568
N	46.3515692	45.2191954	48.2949565	C	46.5883918	46.7097668	41.0273728
N	45.5080474	46.3720820	46.5000482	H	46.9694593	47.4788404	40.3605441
C	45.6099189	47.2271095	45.4314044	N	45.6326556	46.8892413	41.9272220
O	44.6837828	47.3933453	44.6428913	C	45.3987441	45.6634275	42.5039584
C	46.9188706	47.8793373	45.2711766	H	44.6380962	45.5200876	43.2618981
N	47.2323041	48.3803642	44.1140953	C	46.4194253	51.4386019	39.7559713
H	51.8665645	49.7809242	41.6748827	H	47.4675386	51.1163543	39.7697960
H	51.1565508	48.7480887	42.9285196	H	46.3283865	52.5308655	39.7949298
H	50.4918512	48.7199248	41.2687460	C	45.5252268	50.7953556	40.8461891
H	49.7818900	51.0974075	41.4789869	O	44.5404478	51.4356280	41.2327419
H	49.8314636	51.8973157	43.6983894	O	45.8767239	49.6379070	41.2180157
H	48.0575902	49.5589306	41.9875989	N	42.5119814	52.5883435	39.5800563
H	47.0322782	50.9845996	43.6673707	H	43.2471273	52.1971775	40.2025330
H	49.2062799	48.1724255	43.6160387	H	42.0029813	51.8193823	39.0935022
H	48.5697067	50.4542598	45.5813161	H	43.0398789	53.1087727	38.8434545
H	50.1658855	49.7609546	45.2093744	C	41.6088791	53.5221834	40.3489151
H	47.0856197	45.0957271	48.9975647	H	40.6907786	53.6583960	39.7554476
H	49.6304907	48.4193992	47.1001941	C	41.2777032	52.9255092	41.7295341
H	44.6216073	45.8299364	46.6661612	H	42.2331372	52.9032971	42.2837681
H	45.6138378	44.5050935	48.1850120	C	40.3144282	53.8377952	42.4933126
H	45.9870992	50.5986667	46.0640876	H	40.7417990	54.8364571	42.6568278
O	47.0470911	51.5707409	46.8532442	H	39.3654699	53.9714083	41.9517320
H	47.3729865	51.2890842	47.7386775	H	40.0835931	53.3941204	43.4737824
H	46.7365675	52.5075976	46.9729669	C	40.7714328	51.4715045	41.6734194
H	40.5363439	46.5103681	41.7862054	H	41.5735265	50.8343855	41.2762427
H	46.4636245	43.7073018	42.3332371	H	40.6397766	51.1302888	42.7150078
H	41.6409937	43.0546373	46.1769214	C	39.4871836	51.2209015	40.8843777
H	46.0013734	51.2366984	38.7449014	H	38.6453296	51.8223862	41.2619902
⁵TS2				H	39.6070746	51.4524007	39.8151212
C	41.3617342	47.2352028	41.8071445	H	39.1978651	50.1605779	40.9593200
N	41.6803635	48.0338921	40.7277261	C	42.3161395	54.9017223	40.5049246
H	41.1675561	48.1533950	39.8400769	O	41.5892218	55.9085360	40.3934584
C	42.7693925	48.7574567	41.0445619	O	43.5454298	54.8654262	40.7682577
H	43.2341369	49.4625973	40.3651505	Fe	45.1392964	48.7911548	42.9761518
N	43.1748638	48.4730180	42.2765629	O	45.4578243	50.1173257	44.0829514
C	42.3016204	47.5236932	42.7693919	O	45.4719095	49.6223300	46.0361494
H	42.4193576	47.1173813	43.7705059	C	50.9112877	49.4352391	42.0262859
C	42.2589967	42.6868005	47.0143203	C	49.8978723	50.5087660	42.3825340
H	41.6111065	42.7027935	47.9058582	O	50.4570869	51.3481708	43.3893529
H	42.5282720	41.6348286	46.8506919	C	48.5245481	49.9854044	42.8372323
C	43.4975780	43.5359517	47.3114910	O	47.7811752	51.1176255	43.2077583
				C	48.5933857	48.9284534	43.9643882

C	49.0969496	49.5122003	45.2911095	O	44.4965155	42.9042851	47.7561019
N	48.9038769	48.5509270	46.3808466	O	43.4074036	44.7416957	47.1288211
C	47.8258435	47.8009991	46.4318552	C	46.2879723	44.7926236	42.0635492
N	47.6273657	46.9283600	47.4259446	N	46.9921701	45.4667920	41.0879356
C	46.5024217	46.1983715	47.4004185	H	47.6506127	45.0571712	40.4074237
N	46.3223081	45.2457315	48.3030103	C	46.6438818	46.7719305	41.1572459
N	45.4908852	46.3833076	46.4953312	H	47.0007064	47.5412774	40.4785452
C	45.6035601	47.2168457	45.4187108	N	45.7770814	46.9658440	42.1438911
O	44.6999581	47.3437396	44.6017847	C	45.5256048	45.7344433	42.7018658
C	46.9310462	47.8592269	45.2564977	H	44.8249344	45.6043229	43.5172184
N	47.2922443	48.2707963	44.0974135	C	46.4758861	51.3912083	39.7568779
H	51.8405005	49.8921415	41.6568360	H	47.5090486	51.0252045	39.7745606
H	51.1778888	48.8171321	42.8984574	H	46.4335079	52.4852694	39.8105665
H	50.5137666	48.7760828	41.2394033	C	45.5341909	50.7783022	40.8237483
H	49.6932574	51.1166183	41.4786990	O	44.5450548	51.4374130	41.1510204
H	49.7212850	51.9000047	43.7062274	O	45.8609617	49.6183391	41.2268405
H	48.0622591	49.4677854	41.9768215	N	42.5056288	52.5943269	39.5609559
H	46.9082302	50.8363831	43.6084358	H	43.2512837	52.2023186	40.1685676
H	49.2847657	48.1484010	43.6057785	H	41.9958470	51.8242351	39.0761309
H	48.5445038	50.4344791	45.5340998	H	43.0239613	53.1208442	38.8222382
H	50.1615255	49.7523509	45.2201587	C	41.6072964	53.5167032	40.3472643
H	47.0523755	45.1243096	49.0111413	H	40.6841934	53.6570929	39.7626266
H	49.5987343	48.4597207	47.1316634	C	41.2893606	52.9052752	41.7243562
H	44.6054593	45.8374574	46.6592019	H	42.2474953	52.8868162	42.2736619
H	45.5873950	44.5284446	48.1894745	C	40.3217812	53.8058416	42.4973682
H	46.0673044	50.3946411	46.1937206	H	40.7438926	54.8058630	42.6676263
O	47.2160683	51.5991466	46.8034312	H	39.3717530	53.9393462	41.9575113
H	47.4889357	51.3432062	47.7122637	H	40.0933949	53.3545340	43.4750634
H	46.8196866	52.5009084	46.9066277	C	40.7958306	51.4469872	41.6604401
H	40.5451773	46.5131975	41.8103846	H	41.5994713	50.8189019	41.2503469
H	46.4524949	43.7269124	42.3136914	H	40.6764384	51.0967157	42.7005788
H	41.6455741	43.0431225	46.1867851	C	39.5048117	51.1948470	40.8829341
H	46.0291337	51.2064513	38.7650900	H	38.6636252	51.7879360	41.2751271
⁵¹IC2				H	39.6114672	51.4370696	39.8147108
C	41.4630913	47.2194172	41.8007326	H	39.2220656	50.1323448	40.9517149
N	41.7771942	48.0537523	40.7480842	C	42.3117653	54.8970521	40.5122078
H	41.2473126	48.2144939	39.8760735	O	41.5865578	55.9039012	40.3931333
C	42.9070203	48.7189107	41.0587086	O	43.5383886	54.8609907	40.7888211
H	43.3667152	49.4460521	40.4016904	Fe	45.2583559	48.8198356	43.0463016
N	43.3443148	48.3564934	42.2592410	O	44.8821871	50.2614728	43.6946144
C	42.4475447	47.4236821	42.7401894	O	46.0237834	49.3584902	46.4164272
H	42.5716541	46.9735802	43.7196045	C	50.7731656	49.3738518	42.0714153
C	42.2276297	42.6562073	47.0117863	C	49.8010298	50.4964070	42.3953412
H	41.5766732	42.6729026	47.9005963	O	50.3780360	51.3243817	43.4014097
H	42.4958379	41.6041082	46.8478052	C	48.3907714	50.0390962	42.8084207
C	43.4669421	43.5020572	47.3096168	O	47.6825201	51.2270192	43.1209564
				C	48.3064190	48.9934468	43.9389685

C	49.0527717	49.4469599	45.2031259	O	44.4012505	42.7221896	47.7264502
N	48.8935449	48.4318437	46.2436994	O	43.4779394	44.7112508	47.3808117
C	47.7535112	47.8032347	46.3975238	C	46.2647339	44.9893622	42.1039687
N	47.6469331	46.8106754	47.2863044	N	46.9956513	45.6221688	41.1193996
C	46.5005203	46.1277006	47.3367443	H	47.6469379	45.1790458	40.4525051
N	46.3413061	45.1733443	48.2417297	C	46.6742635	46.9409594	41.1550951
N	45.4505886	46.3340083	46.4758419	H	47.0638914	47.6792683	40.4591426
C	45.4355802	47.3400100	45.5610151	N	45.7986989	47.1893924	42.1183770
O	44.5298380	47.4610641	44.7461192	C	45.5207523	45.9772568	42.7076432
C	46.5762934	48.3516928	45.5851052	H	44.8030939	45.8810903	43.5158670
N	46.9172500	48.6368996	44.2424847	C	46.8727307	51.3618960	39.5532002
H	51.7321734	49.7916924	41.7314408	H	47.7770866	50.7466970	39.5863763
H	50.9788181	48.7382874	42.9465477	H	47.1223083	52.4269473	39.4927223
H	50.3710158	48.7384644	41.2680775	C	45.8849184	51.1061608	40.7069886
H	49.6508801	51.1025124	41.4791002	O	45.2268446	52.0797538	41.0715376
H	49.6656283	51.9120416	43.7040059	O	45.8245010	49.9044871	41.1173212
H	47.9463996	49.5565741	41.9218858	N	42.7833011	52.6832385	40.1183799
H	46.8301381	50.9895319	43.5341504	H	43.7251720	52.3540256	40.4198122
H	48.8368028	48.1019704	43.5483625	H	42.2885382	51.9408570	39.6047135
H	48.6553204	50.4100212	45.5590619	H	43.0180940	53.4388536	39.4282308
H	50.1223234	49.5669754	45.0064400	C	42.0403451	53.1821447	41.3232180
H	47.0966425	45.0375677	48.9201372	H	40.9824035	53.2689452	41.0295251
H	49.6672982	48.2068680	46.8803967	C	42.0801393	52.1588832	42.4951317
H	44.5920336	45.7387405	46.6317091	H	43.2104711	51.5923568	42.6889040
H	45.5813573	44.4778302	48.1663544	C	41.8396674	52.7976944	43.8519524
H	46.4662644	50.2399637	46.3095006	H	42.6681057	53.4605364	44.1383741
O	47.2758598	51.6665149	46.7073673	H	40.9336847	53.4224180	43.8216883
H	47.5701559	51.4214233	47.6145286	H	41.7361125	52.0149036	44.6186844
H	46.8282760	52.5431080	46.8182473	C	41.1633152	50.9641818	42.2118915
H	40.6223720	46.5257025	41.8049710	H	41.3803863	50.5674381	41.2094668
H	46.4467960	43.7586592	42.3697516	H	41.4133509	50.1567918	42.9147653
H	41.6203266	43.0172345	46.1817806	C	39.6610352	51.2690199	42.2935132
H	46.0760364	51.1887932	38.7632908	H	39.3544488	51.5459884	43.3142398
⁵TS3				H	39.3618392	52.0882008	41.6198990
C	41.4065062	47.2686861	41.6319092	H	39.0923648	50.3745331	41.9925935
N	41.7682860	47.9745719	40.5058695	C	42.4787213	54.6485309	41.6429452
H	41.2408901	48.0841349	39.6247911	O	41.6390478	55.3164387	42.2776513
C	42.8977213	48.6588398	40.7794524	O	43.6038303	54.9972364	41.2144860
H	43.4077689	49.2861323	40.0535146	Fe	45.0542802	49.2727805	42.9253054
N	43.2862400	48.4290223	42.0253288	O	44.2041250	50.8395013	43.3057556
C	42.3660295	47.5623969	42.5737519	O	46.1407390	49.7431195	46.4484631
H	42.4540236	47.2189828	43.5994589	C	50.6470296	49.3109062	42.0112976
C	42.1333957	42.7434697	46.9886078	C	49.8542270	50.5762951	42.2890610
H	41.4565587	42.7989518	47.8559307	O	50.5441984	51.3566498	43.2566685
H	42.3144279	41.6768747	46.8041571	C	48.3874967	50.3612978	42.7199618
C	43.4365130	43.4441005	47.3737354	O	47.8873100	51.6552772	43.0059726
				C	48.1503941	49.3483149	43.8464638

C	48.9710617	49.6643428	45.1069704	O	44.5123438	42.9404045	47.7333473
N	48.7992247	48.5663737	46.0484377	O	43.4670372	44.7806439	47.0377016
C	47.6243108	48.0068789	46.1896793	C	46.2851942	44.8394108	42.1148292
N	47.4626884	46.9761413	47.0145128	N	46.9961088	45.4964553	41.1325349
C	46.2529487	46.4301011	47.1270738	H	47.6471868	45.0749206	40.4519729
N	46.0000835	45.5050182	48.0248040	C	46.6614907	46.8077193	41.1941800
N	45.1917285	46.7795182	46.3003942	H	47.0332335	47.5644574	40.5081541
C	45.2384185	47.8241143	45.4353426	N	45.7979634	47.0242263	42.1767908
O	44.3255292	48.0585632	44.6483340	C	45.5370084	45.8002035	42.7471047
C	46.4658736	48.7262266	45.4820530	H	44.8376804	45.6839238	43.5678752
N	46.7208979	49.1952894	44.1659255	C	46.5084205	51.4362134	39.7460438
H	51.6450870	49.5670593	41.6247815	H	47.5377861	51.0591080	39.7669140
H	50.7874993	48.7035049	42.9188094	H	46.4793472	52.5325991	39.7616222
H	50.1304760	48.6950042	41.2592651	C	45.5838526	50.8810164	40.8548109
H	49.7910341	51.1577663	41.3465684	O	44.6250738	51.5907334	41.1965492
H	49.9128864	52.0475123	43.5237150	O	45.8754856	49.7343952	41.2980706
H	47.8708569	49.9343286	41.8467415	N	42.5386197	52.6433865	39.6468476
H	47.2084415	51.6444257	43.7165221	H	43.2995174	52.2421650	40.2260499
H	48.5417906	48.3849348	43.4580969	H	41.9916176	51.8867192	39.1870331
H	48.6390804	50.6085051	45.5666928	H	43.0433688	53.1520535	38.8850155
H	50.0340380	49.7611207	44.8733724	C	41.7102146	53.6184156	40.4667764
H	46.7341639	45.2469548	48.6933841	H	40.7432240	53.7248228	39.9381559
H	49.5603115	48.2625693	46.6670217	C	41.5150120	53.1274741	41.8787357
H	44.3118353	46.2546091	46.4112741	H	44.0129934	51.0818214	43.0918179
H	45.0610949	45.0455214	48.0008652	C	41.5860781	54.1326840	42.9863581
H	45.1678818	51.8032249	44.4690443	H	42.5841330	54.6000791	43.0305049
O	45.9578662	51.9416438	45.0550840	H	40.8874224	54.9751829	42.8372597
H	46.0308722	50.6014361	45.9342968	H	41.3846721	53.6769237	43.9665474
H	45.8643783	52.7781984	45.5691045	C	41.2313786	51.6802938	42.1730855
H	40.5685356	46.5731917	41.6783840	H	40.9783152	51.5896645	43.2416963
H	46.3965461	43.9550196	42.4215030	H	42.1580306	51.0694886	42.0581387
H	41.5775616	43.1728707	46.1551029	C	40.0978001	51.0392492	41.3534325
H	46.3444142	51.1714979	38.6190175	H	39.1722543	51.6301042	41.4434500
⁵¹IC3				H	40.3325832	50.9564553	40.2811395
C	41.4570513	47.2138490	41.7866623	H	39.8922799	50.0176028	41.7121743
N	41.7657124	48.0392123	40.7257481	C	42.4177021	55.0158162	40.4636777
H	41.2403733	48.1810181	39.8485144	O	41.6611667	55.9994387	40.3731057
C	42.8710560	48.7412300	41.0448704	O	43.6658993	55.0061548	40.6009356
H	43.3193609	49.4693061	40.3772210	Fe	45.2331652	48.9806917	43.1341889
N	43.2996739	48.4140271	42.2585082	O	44.5340777	50.6321937	43.7747564
C	42.4215013	47.4644098	42.7377966	O	46.2783341	49.4881065	46.5780445
H	42.5425140	47.0362629	43.7286382	C	50.7551754	49.2690296	42.0965507
C	42.2347820	42.7190265	47.0158904	C	49.8981208	50.4892698	42.3792017
H	41.5969838	42.7814904	47.9123500	O	50.5577196	51.3130078	43.3336350
H	42.4794515	41.6563107	46.8864255	C	48.4547089	50.2035577	42.8432705
C	43.4970071	43.5467975	47.2686856	O	47.8901760	51.4770314	43.0994602
				C	48.3085988	49.1890981	43.9912644

C	49.0992294	49.5606423	45.2559034	O	44.4856681	42.9048569	47.7389568
N	48.9802224	48.4588968	46.2077541	O	43.4212334	44.7597506	47.1167887
C	47.8403294	47.8324804	46.3580558	C	46.2613758	44.8606733	42.1462941
N	47.7282215	46.7955772	47.1875797	N	46.9708441	45.5121742	41.1579079
C	46.5548059	46.1644252	47.2611836	H	47.6265783	45.0881916	40.4849397
N	46.3880330	45.1816086	48.1288193	C	46.6269913	46.8247809	41.2111619
N	45.4741393	46.4607248	46.4553848	H	46.9979508	47.5791745	40.5213094
C	45.4714767	47.5058302	45.5931934	N	45.7603725	47.0466761	42.1859881
O	44.5533220	47.6942849	44.7973770	C	45.5098380	45.8286421	42.7697150
C	46.6537282	48.4706299	45.6383459	H	44.8136692	45.7237640	43.5966625
N	46.9007120	48.9128646	44.3089441	C	46.6065853	51.4986301	39.6047159
H	51.7305344	49.5765294	41.6905118	H	47.6055844	51.0502054	39.6400595
H	50.9451177	48.6768877	43.0053344	H	46.6533837	52.5942252	39.5763724
H	50.2600475	48.6213257	41.3567983	C	45.6569753	51.0227220	40.7261729
H	49.7850264	51.0606645	41.4352228	O	44.8028445	51.8750037	41.1002821
H	49.8936915	51.9756733	43.5933539	O	45.7919658	49.8619411	41.1416585
H	47.9366289	49.7383280	41.9887517	N	42.5685211	52.5724415	39.7375402
H	47.3171720	51.4940215	43.8995190	H	43.3852411	52.1511164	40.2476536
H	48.7745647	48.2606720	43.6036171	H	41.9940121	51.8450225	39.2598023
H	48.7116854	50.4877629	45.7065804	H	43.0368772	53.1177600	38.9714316
H	50.1582417	49.7123975	45.0302187	C	41.8228802	53.5287388	40.6268701
H	47.1500683	45.0015609	48.7902047	H	40.7840537	53.6135331	40.2476202
H	49.7561572	48.2108277	46.8333116	C	41.7212490	53.1075154	42.0792145
H	44.6167417	45.8590606	46.5843578	H	44.4017831	51.3498568	42.7222191
H	45.6002704	44.5166003	48.0656731	C	41.8135967	54.2115623	43.0649643
H	45.4520800	51.5074907	44.7397038	H	42.7989279	54.6926540	42.9698790
O	46.2609157	51.7485016	45.2976399	H	41.1017469	55.0130118	42.7971649
H	46.2576832	50.3723954	46.0928360	H	41.6510565	53.8786426	44.0964620
H	46.1057550	52.5738110	45.8162349	C	41.5258204	51.7839010	42.5463143
H	40.6209361	46.5145905	41.7906743	H	41.1353522	51.8067301	43.5777325
H	46.4293607	43.8022231	42.4173598	H	42.6149407	51.3928010	42.8877201
H	41.6227283	43.0597189	46.1807940	C	40.8119860	50.7406546	41.6943813
H	46.0974751	51.2108772	38.7619632	H	39.7722932	51.0603679	41.5169217
⁵TS4				H	41.2756537	50.5632091	40.7188719
C	41.3804909	47.1505978	41.7377422	H	40.7886810	49.7830182	42.2298434
N	41.7749620	47.8292294	40.6062564	C	42.4593181	54.9846934	40.5078728
H	41.2635021	47.9339972	39.7197143	O	41.6344676	55.8998623	40.3648562
C	42.8827405	48.5415555	40.9098999	O	43.7000169	55.0428950	40.6242364
H	43.4103435	49.1569523	40.1863500	Fe	45.0656546	49.0113117	43.1142351
N	43.2257507	48.3551748	42.1718584	O	44.0577711	50.8750002	43.5031875
C	42.3008806	47.4872401	42.7075349	O	46.1924650	49.6106738	46.6060221
H	42.3711099	47.1624288	43.7426564	C	50.6020551	49.4355327	42.0687458
C	42.2133233	42.6859608	47.0102127	C	49.7310055	50.6353572	42.3983344
H	41.5653684	42.7226963	47.9006431	O	50.4012386	51.4483346	43.3566085
H	42.4688662	41.6286419	46.8598110	C	48.3047651	50.3102644	42.8839481
C	43.4660044	43.5198107	47.2965648	O	47.7242609	51.5706758	43.1845044
				C	48.1893939	49.2804362	44.0188115

C	48.9902022	49.6561415	45.2749007	O	44.5165909	42.9291793	47.7314928
N	48.8753956	48.5501021	46.2206821	O	43.4699663	44.7815026	47.0675437
C	47.7329183	47.9243834	46.3694101	C	46.2981764	44.7708375	42.1333407
N	47.6455045	46.8657521	47.1753248	N	46.9734801	45.4197430	41.1203941
C	46.4782826	46.2231380	47.2485389	H	47.6338961	45.0015792	40.4481125
N	46.3339605	45.2255205	48.1077121	C	46.5914181	46.7178177	41.1419053
N	45.3942121	46.5274927	46.4616693	H	46.9297711	47.4670284	40.4296675
C	45.3477478	47.6177910	45.6363463	N	45.7313769	46.9327521	42.1266794
O	44.3812022	47.8214001	44.9106059	C	45.5242267	45.7236302	42.7450100
C	46.5443369	48.5700176	45.6528993	H	44.8463722	45.6190066	43.5865489
N	46.7890695	48.9997024	44.3336754	C	46.4171605	51.5622098	39.7016220
H	51.5722109	49.7693768	41.6706158	H	47.4712350	51.2580557	39.7052191
H	50.8019767	48.8148875	42.9558060	H	46.3042585	52.6544917	39.7017262
H	50.1132826	48.8058864	41.3091173	C	45.5887058	50.9326193	40.8426389
H	49.5936477	51.2283832	41.4696940	O	44.6713199	51.6539063	41.3232456
H	49.7208668	52.0677758	43.6745701	O	45.8746224	49.7705041	41.1827057
H	47.7778658	49.8485685	42.0326423	N	42.5136061	52.5604424	39.6072243
H	47.0608474	51.5102780	43.9096450	H	43.2483696	52.2084562	40.2472319
H	48.6744665	48.3643907	43.6168286	H	42.0359238	51.7748503	39.1139615
H	48.5946836	50.5781419	45.7293354	H	43.0381888	53.0999236	38.8788765
H	50.0491154	49.8127001	45.0513116	C	41.5593889	53.4694796	40.3515810
H	47.1035209	45.0448964	48.7588628	H	40.6748923	53.6041119	39.7104429
H	49.6588455	48.2795425	46.8254956	C	41.1384972	52.8401575	41.6764981
H	44.5443261	45.9340430	46.5936392	H	44.2126990	51.1721391	42.8324028
H	45.5452319	44.5657134	48.0555221	C	41.8013691	53.3585471	42.9291361
H	44.9955587	51.5948705	44.6569067	H	42.8874961	53.2009072	42.9053577
O	45.8253686	51.8035711	45.1912144	H	41.6469841	54.4446180	43.0410638
H	46.0176897	50.4346292	46.0668777	H	41.3994099	52.8574415	43.8224752
H	45.7276996	52.6225521	45.7258579	C	40.2154848	51.8627364	41.7461116
H	40.5464361	46.4492354	41.7603394	H	39.9821130	51.4832436	42.7500894
H	46.4116613	43.8232629	42.4450601	H	43.3156492	50.4189030	43.8675077
H	41.6062310	43.0408822	46.1774241	C	39.4459014	51.2132780	40.6407985
H	46.1626453	51.2516531	38.6403577	H	38.3620530	51.3579536	40.7913601
⁵ PC				H	39.7027252	51.5875531	39.6424443
				H	39.6203283	50.1243976	40.6482747
	C	41.4239150	47.2477477	C	42.2381172	54.8660104	40.5328446
	N	41.6680127	48.1450738	O	41.4720057	55.8450810	40.5048427
	H	41.1533398	48.2687805	O	43.4825914	54.8665078	40.7057662
	C	42.7433588	48.8850613	Fe	45.2865656	48.8222446	43.0559368
	H	43.1465436	49.6659646	O	44.2021979	50.7932628	43.7546815
	N	43.2134623	48.5197902	O	46.3126564	49.5218755	46.6013973
	C	42.3925462	47.4985576	C	50.7425946	49.2796930	42.0743886
	H	42.5601742	47.0232071	C	49.8770823	50.4921638	42.3695594
	C	42.2401510	42.7195008	O	50.5444614	51.3186421	43.3178593
	H	41.5977977	42.7740510	C	48.4455983	50.1852267	42.8537749
	H	42.4843349	41.6578066	O	47.8650276	51.4518405	43.1295871
	C	43.5021030	43.5450404	C	48.3242024	49.1729057	44.0041984

C	49.1272748	49.5515600	45.2570076
N	48.9987590	48.4557622	46.2140926
C	47.8532710	47.8371746	46.3681379
N	47.7546209	46.7883377	47.1850923
C	46.5823020	46.1543154	47.2605105
N	46.4255554	45.1629367	48.1233497
N	45.4999002	46.4591306	46.4696645
C	45.4673651	47.5347865	45.6318684
O	44.5104795	47.7382046	44.8917527
C	46.6681136	48.4828752	45.6483666
N	46.9201064	48.9085795	44.3275531
H	51.7104759	49.5966423	41.6576733
H	50.9481495	48.6885629	42.9801718
H	50.2449226	48.6270240	41.3409952
H	49.7495700	51.0644987	41.4278724
H	49.8759065	51.9665500	43.6004937
H	47.9176200	49.7183445	42.0045888
H	47.2639791	51.4246337	43.9035603
H	48.7984914	48.2490306	43.6125512
H	48.7496201	50.4847759	45.7047037
H	50.1879637	49.6901552	45.0301154
H	47.1906868	44.9827238	48.7800903
H	49.7785677	48.1907280	46.8264501
H	44.6415583	45.8684753	46.6039169
H	45.6346561	44.5033875	48.0662242
H	45.2642098	51.6967420	44.8735277
O	46.1307373	51.8461529	45.3095238
H	46.2360479	50.3741466	46.0941240
H	46.0770337	52.6688267	45.8583577
H	40.6028394	46.5308784	41.7854874
H	46.4670568	43.7374973	42.4362508
H	41.6321593	43.0688761	46.1753360
H	46.0098625	51.2803109	38.7306902

RC2

C	46.9682939	43.4694011	49.0721088
H	46.6463499	43.2624046	50.1030842
H	46.3092865	44.2186433	48.6171455
C	46.9380009	42.1949146	48.2383242
O	47.5511982	41.1716060	48.6055327
O	46.3022982	42.2770460	47.1263469
C	48.2496558	44.5040600	45.4995256
N	48.3205426	43.1257962	45.4881937
C	49.5766779	42.8195506	45.7980452
H	49.9794029	41.8159136	45.9015623
N	50.3025016	43.9402745	45.9916685
H	51.2767213	44.0255211	46.3176612

C	49.4884789	45.0250587	45.8086303
H	49.8629753	46.0405234	45.9229420
C	43.4347940	35.1437862	49.6472606
H	42.3876921	35.2449796	49.9532691
H	44.0782386	35.0985499	50.5396994
C	43.8883851	36.3290870	48.7277610
O	44.8724834	36.0772296	47.9735979
O	43.2492147	37.3552812	48.9027429
C	48.5688881	39.5961459	42.0079351
N	48.8299353	40.9293635	41.7487521
H	49.2847956	41.2826912	40.9023924
C	48.4072483	41.6806907	42.7832331
H	48.4607793	42.7653891	42.8124019
N	47.8965908	40.8941044	43.7295939
C	47.9938438	39.5914567	43.2598551
H	47.6669977	38.7397142	43.8581596
C	47.3840425	35.2582629	43.4636116
H	48.1931960	35.9217590	43.1368986
H	46.5863305	35.3596850	42.7057966
C	46.8548477	35.8315528	44.7671315
O	46.4482257	35.1227591	45.7162898
O	46.8339847	37.1079412	44.8801588
C	48.5418249	35.2952799	48.5927394
N	48.0636055	36.4616584	48.0473881
C	48.8828847	37.4160023	48.4660774
H	48.7887690	38.4721450	48.2266423
N	49.8569509	36.9001066	49.2455051
H	50.5996723	37.4229238	49.7398120
C	49.6602036	35.5520380	49.3552327
H	50.3052765	34.9204783	49.9612701
Fe	46.7050488	41.5282899	45.3408672
Fe	46.3069803	37.0197396	46.9367149
O	47.3507775	39.7488260	46.5647511
O	46.2035579	39.0013020	47.0869164
H	47.5474334	40.2885515	47.4210071
C	41.7016351	41.1486102	47.3484906
C	42.9873611	41.0775204	46.5282188
C	42.7991798	40.4091495	45.1543089
C	42.4436049	38.9247242	45.2738832
C	44.0352853	40.6089286	44.2555366
N	45.2541980	40.0357200	44.8368012
C	44.2511965	42.1072820	43.9667422
O	43.4050416	42.7529662	43.3687338
O	45.3772581	42.5939147	44.4159557
H	41.9765365	40.9282159	44.6341261
H	41.4992623	38.8030530	45.8199448
H	42.3339221	38.4568463	44.2821414

H	43.2131679	38.3670411	45.8341686
H	43.7565924	40.5352009	47.1058124
H	43.3894130	42.0945361	46.3854006
H	41.8605138	41.7239924	48.2731844
H	40.8852474	41.6268103	46.7812694
H	41.3491907	40.1521363	47.6534896
H	43.8492061	40.1259265	43.2829930
H	45.6721209	39.3165551	44.2436777
H	45.1530790	39.5900137	45.7691517
O	46.2766541	38.6167917	49.8804358
H	46.3628599	39.0254684	48.9965804
H	46.9824815	39.0002277	50.4330273
H	47.9917649	43.8375676	49.1430147
H	47.3415854	45.0545114	45.2536016
H	43.5214271	34.1407119	49.2296440
H	48.8221864	38.7650222	41.3498009
H	47.7242937	34.2229577	43.4845777
H	48.0050587	34.3490912	48.5243577

TS1b

C	48.9939319	40.7124363	45.3434440
H	48.7760555	41.4130415	46.1623572
H	48.4926316	41.0525887	44.4310278
C	48.5008861	39.3081035	45.6779634
O	48.8711364	38.7393131	46.7206385
O	47.7603305	38.7752926	44.7751581
C	50.0762571	38.0979562	42.4820165
N	49.6599691	37.2684816	43.4998059
C	50.7525876	36.9381782	44.1766880
H	50.7820256	36.2953262	45.0537690
N	51.8437851	37.5192687	43.6291049
H	52.8187197	37.4981252	43.9599093
C	51.4447282	38.2605365	42.5473699
H	52.1595428	38.8203579	41.9471849
C	43.1590729	38.1106609	51.2487961
H	42.3045322	38.7719979	51.0716305
H	43.8088949	38.5550879	52.0179953
C	43.9650460	37.8873500	49.9337752
O	44.5603506	36.7725404	49.8160613
O	43.9569383	38.8690737	49.2057275
C	47.9976273	32.5961109	43.9714755
N	48.5707051	33.0203560	42.7869578
H	48.9421260	32.4058541	42.0583884
C	48.6126545	34.3682710	42.7635981
H	48.9911980	34.9560906	41.9320387
N	48.1034281	34.8485481	43.8920503
C	47.7185843	33.7584134	44.6568341

H	47.2847768	33.8879499	45.6480224
C	45.5186420	31.9653547	48.0482095
H	46.3813058	31.7065447	47.4250561
H	44.6236526	31.7963578	47.4270570
C	45.6091536	33.4432985	48.3249854
O	45.0036232	34.0301084	49.2688393
O	46.3236398	34.1584779	47.5474053
C	47.6084200	35.6383373	51.3980732
N	47.4710342	36.0590252	50.0901179
C	48.5952474	36.7033607	49.7892104
H	48.8032846	37.2001251	48.8409315
N	49.4299707	36.6999229	50.8472365
H	50.3639620	37.1448244	50.8930326
C	48.8305106	36.0386938	51.8855344
H	49.3057468	35.9251014	52.8584027
Fe	47.5460933	36.8278559	44.3384754
Fe	45.9360647	35.9075633	48.6309495
O	47.8013626	36.4643176	46.2922432
O	46.3339445	36.9996709	47.3128835
H	48.2739439	37.3019557	46.5977527
C	43.4827626	40.0580224	45.1093107
C	44.3749038	38.9120413	44.6385608
C	43.6142636	37.6380464	44.2320519
C	42.7129294	37.1073525	45.3553643
C	44.5761453	36.5352041	43.7370032
N	45.5371473	36.1314123	44.7711965
C	45.3401403	36.9943554	42.4717013
O	44.7502453	37.1430112	41.4135513
O	46.6130749	37.2091353	42.6571081
H	42.9815013	37.8825029	43.3613251
H	42.2484636	36.1464066	45.0786614
H	43.2789369	36.9528767	46.2902896
H	41.9053712	37.8181586	45.5818532
H	45.0879065	38.6958198	45.4481310
H	44.9846249	39.2468540	43.7836105
H	42.6911523	40.2956189	44.3784115
H	42.9926507	39.8254970	46.0683176
H	44.0874904	40.9633444	45.2693151
H	43.9787309	35.6596991	43.4349148
H	45.5746716	35.1185655	44.8984859
H	45.4047686	36.5467600	45.7042688
O	46.0510110	39.7866786	47.5279645
H	46.4390385	38.9064556	47.3665899
H	45.2356090	39.5549001	48.0053757
H	50.0760638	40.6861110	45.2155195
H	49.3803303	38.4858449	41.7381781
H	42.7550185	37.2301361	51.7482790

H	47.7980481	31.5610076	44.2485972
H	45.4682147	31.3144518	48.9210495
H	46.7899262	35.1960013	51.9659410
X2'			
C	48.7985796	40.8425280	45.3935219
H	48.6693842	41.6738784	46.0992405
H	48.3973497	41.1118665	44.4051514
C	48.0748197	39.5815501	45.8772102
O	47.6603240	39.4841341	47.0418282
O	47.9570522	38.6755947	44.9835441
C	50.0999987	38.0317330	42.5424809
N	49.7341906	37.1995012	43.5756008
C	50.8556518	36.9102015	44.2147672
H	50.9437458	36.2606812	45.0835684
N	51.9178653	37.5239116	43.6372100
H	52.9014010	37.5236251	43.9379470
C	51.4655456	38.2452752	42.5679466
H	52.1448280	38.8332340	41.9536040
C	43.4319465	38.1631053	51.1095483
H	42.5797635	38.7809022	50.8021531
H	43.9638050	38.6740128	51.9270480
C	44.4155345	37.9448008	49.9138630
O	45.0923900	36.8669699	49.9224671
O	44.4635132	38.8951032	49.1515106
C	48.0806132	32.6238299	44.0741003
N	48.5452810	33.1973427	42.9031539
H	48.8664584	32.6759635	42.0841587
C	48.5531461	34.5388098	43.0298279
H	48.8431992	35.2305612	42.2466317
N	48.1248776	34.8751234	44.2474319
C	47.8243288	33.6900091	44.9036818
H	47.4181929	33.7029616	45.9121475
C	45.5976761	31.9811869	48.0202770
H	46.4710104	31.7129713	47.4157375
H	44.7164484	31.8123673	47.3805489
C	45.6818247	33.4628640	48.2928763
O	45.0843878	34.0586633	49.2216484
O	46.3903979	34.1646283	47.4952724
C	47.6195995	35.3614758	51.1540240
N	47.5445689	35.6124565	49.7926031
C	48.7585282	36.0127804	49.4376952
H	49.0173821	36.3249412	48.4296426
N	49.5945225	36.0173232	50.4945323
H	50.5474483	36.4149174	50.5436143
C	48.8911685	35.6254824	51.6010273
H	49.3471219	35.5708211	52.5872724

Fe	47.4051758	36.7501682	44.8193481
Fe	45.9463789	35.9546675	48.3794986
O	47.2406774	36.7400240	46.8836171
O	44.6395133	36.2343891	47.4678180
H	47.3728292	37.6916013	47.1123293
C	43.7165822	39.9067248	45.5445939
C	44.5149309	38.7035573	45.0455122
C	43.6761951	37.6246249	44.3330623
C	42.5359668	37.0913599	45.2116604
C	44.5668586	36.4814154	43.7856734
N	45.4080416	35.8671596	44.8251129
C	45.4735272	37.0252130	42.6648964
O	45.0222194	37.2766990	41.5587104
O	46.7066215	37.2314953	43.0343555
H	43.2307475	38.0803513	43.4310035
H	42.0220160	36.2435983	44.7304698
H	42.9049179	36.7547060	46.1925137
H	41.7854620	37.8758507	45.3876160
H	45.0353540	38.2562551	45.9086597
H	45.3024749	39.0501360	44.3561355
H	43.1177468	40.3622151	44.7371769
H	43.0312718	39.6322267	46.3597806
H	44.3930103	40.6762507	45.9486680
H	43.9195969	35.7148862	43.3313073
H	45.5078958	34.8591760	44.6663151
H	45.0226554	35.9726017	45.7788358
O	47.8710963	38.6586649	49.7291929
H	48.4997822	39.3601962	50.0056782
H	47.5026742	39.0402557	48.9190610
H	49.8676374	40.6539103	45.2955123
H	49.3811111	38.4023683	41.8117982
H	42.9997602	37.2971238	51.6109047
H	47.9063637	31.5635080	44.2569167
H	45.5274913	31.3364752	48.8963411
H	46.7857568	35.0979624	51.8046653

TS2b

C	48.8759229	40.9037996	45.3031913
H	48.7498749	41.7573831	45.9826300
H	48.4960189	41.1470873	44.2999789
C	48.1295974	39.6740900	45.8258153
O	47.7683418	39.6052995	47.0067059
O	47.9366958	38.7630182	44.9483653
C	50.1027224	38.0330744	42.5686637
N	49.7255721	37.2367259	43.6295770
C	50.8469298	36.9298583	44.2628875
H	50.9256043	36.3015353	45.1476548

N	51.9178397	37.4953102	43.6564165	H	42.0920949	36.2236739	44.7450751
H	52.9020110	37.4905345	43.9559688	H	42.9782858	36.7875723	46.1834125
C	51.4738091	38.2038577	42.5755055	H	41.8188885	37.8631158	45.3728637
H	52.1621278	38.7613279	41.9428730	H	45.0269384	38.3882546	45.8511557
C	43.3901296	38.1005989	51.2562301	H	45.2939654	39.1041250	44.2649535
H	42.5403977	38.7034740	50.9118594	H	43.0688413	40.3707513	44.5287430
H	43.8663237	38.6186240	52.1026073	H	42.9639916	39.7374228	46.1857021
C	44.4468972	37.9267193	50.1223154	H	44.3075470	40.7959094	45.7435601
O	45.0324003	36.8141605	50.0116188	H	44.0093004	35.7083303	43.3561872
O	44.6340672	38.9782826	49.5123998	H	45.5949875	34.9383563	44.7419961
C	48.0745424	32.6520579	44.0718681	H	45.1004514	36.0957509	45.8020671
N	48.5625656	33.2150371	42.9057069	O	47.4519123	38.5524962	49.4485906
H	48.8817104	32.6870420	42.0899862	H	47.9669363	39.1636168	48.8990603
C	48.5921785	34.5575212	43.0312294	H	46.5527423	38.9240514	49.4083032
H	48.9014745	35.2401163	42.2472002	H	49.9435428	40.6953864	45.2337744
N	48.1563276	34.9045510	44.2435297	H	49.3945904	38.4076275	41.8295249
C	47.8286205	33.7253772	44.8961555	H	42.9597171	37.2179989	51.7293363
H	47.4187790	33.7475170	45.9026977	H	47.8861009	31.5951306	44.2601804
C	45.6286429	32.0771241	48.0031486	H	45.5362910	31.4310975	48.8761824
H	46.5137732	31.8026160	47.4188121	H	46.8044921	35.1256642	51.8591028
H	44.7632352	31.9121107	47.3407032				
C	45.7144590	33.5593121	48.2763960	X2			
O	45.1195437	34.1556984	49.2031307	C	48.8478975	41.0007788	45.3071633
O	46.4293372	34.2623339	47.4819452	H	48.7601066	41.8036840	46.0512760
C	47.6480715	35.3818172	51.2181452	H	48.4915962	41.3443099	44.3250511
N	47.5922862	35.6294252	49.8562780	C	48.0485961	39.7589987	45.7158724
C	48.8150199	36.0132887	49.5161162	O	47.7721031	39.5858731	46.9220853
H	49.0927073	36.3166515	48.5095636	O	47.7579233	38.9731483	44.7628506
N	49.6359823	36.0229017	50.5851391	C	50.1402531	38.0707409	42.4735589
H	50.5940669	36.4103084	50.6344554	N	49.7285520	37.3257737	43.5555997
C	48.9162803	35.6383664	51.6832088	C	50.8254254	37.0229425	44.2382995
H	49.3560195	35.5872629	52.6772566	H	50.8404168	36.4527648	45.1642941
Fe	47.4816583	36.8186337	44.8133779	N	51.9130937	37.5416815	43.6297160
Fe	46.0355038	36.0570881	48.3932787	H	52.8892413	37.5347599	43.9544260
O	47.3150889	36.7915044	46.9072170	C	51.5100822	38.2178180	42.5096177
O	44.7372839	36.4052397	47.4980709	H	52.2208507	38.7476090	41.8788162
H	47.4395420	37.7373918	47.1606327	C	43.2389220	38.2043407	51.4146059
C	43.6638625	39.9827342	45.3732345	H	42.4165029	38.7548490	50.9414942
C	44.5040291	38.7752578	44.9598900	H	43.6056930	38.7955969	52.2648027
C	43.7029941	37.6383198	44.2959526	C	44.4052545	37.9670934	50.4248907
C	42.5881419	37.0957640	45.2009924	O	44.8829936	36.8037483	50.3244712
C	44.6313318	36.5074655	43.7897682	O	44.7686234	39.0059848	49.8631817
N	45.4808388	35.9499067	44.8534773	C	48.0397146	32.6389317	44.0064016
C	45.5282275	37.0434877	42.6579530	N	48.5540043	33.0812907	42.8018684
O	45.0671833	37.2844318	41.5536182	H	48.8913598	32.4786523	42.0475193
O	46.7626350	37.2545156	43.0166584	C	48.6000058	34.4310366	42.8003224
H	43.2383387	38.0438125	43.3798672	H	48.9374621	35.0333701	41.9616725

N	48.1509953	34.8932739	43.9585554	H	49.4339157	38.4187086	41.7198527
C	47.8013490	33.7925821	44.7219664	H	42.8034627	37.3195529	51.8789259
H	47.4204150	33.9156873	45.7349321	H	47.8346420	31.6014344	44.2702419
C	45.7452392	32.2012627	48.0301782	H	45.6139230	31.5305139	48.8792479
H	46.6554965	31.9501741	47.4738362	H	46.8320812	35.1094142	52.0845547
H	44.9037431	32.0624061	47.3302328				
C	45.8123885	33.6674600	48.3728392	TS3b			
O	45.1285110	34.2047370	49.2846446	C	48.8567193	40.9831922	45.2797443
O	46.5878345	34.4293594	47.6969850	H	48.7620890	41.7982007	46.0102826
C	47.6883295	35.3604514	51.4585465	H	48.5043388	41.3083887	44.2900680
N	47.5914342	35.6096872	50.1069498	C	48.0594108	39.7475027	45.7131089
C	48.8168758	35.9305667	49.7060131	O	47.8172230	39.5888874	46.9284368
H	49.0799936	36.1851458	48.6783012	O	47.7285879	38.9582726	44.7750859
N	49.6734909	35.9104085	50.7468746	C	50.1326646	38.0672607	42.4869055
H	50.6425160	36.2767008	50.7476782	N	49.7249476	37.3223783	43.5693959
C	48.9830689	35.5608204	51.8773194	C	50.8233450	37.0176162	44.2489423
H	49.4557316	35.4914195	52.8550544	H	50.8406198	36.4440583	45.1728016
Fe	47.7397620	36.9043539	44.5088127	N	51.9087681	37.5370678	43.6375446
Fe	46.0191192	36.1013966	48.7556650	H	52.8861280	37.5292093	43.9592432
O	48.4088522	36.6862205	46.2711774	C	51.5030375	38.2139396	42.5187278
O	44.9385087	36.5438034	47.6511928	H	52.2126053	38.7439888	41.8867584
H	48.5238938	37.5444662	46.7054049	C	43.2153960	38.2011462	51.4140250
C	43.5727145	40.0530170	45.3166638	H	42.3812261	38.7651257	50.9794324
C	44.4327669	38.8171883	45.0587156	H	43.6070617	38.7676395	52.2696897
C	43.7339557	37.7021105	44.2575308	C	44.3564864	37.9887236	50.3894290
C	42.5084368	37.1319262	44.9878370	O	44.7845617	36.8167475	50.2040520
C	44.7445375	36.6116053	43.8134750	O	44.7485065	39.0500172	49.8932957
N	45.6755857	36.1944888	44.8821786	C	48.1035403	32.6184173	43.9788357
C	45.5446204	37.0967621	42.5756024	N	48.6031812	33.0621943	42.7693918
O	44.9588293	37.2702484	41.5139772	H	48.9215616	32.4586128	42.0080866
O	46.8056223	37.3032534	42.7805960	C	48.6792176	34.4103415	42.7800881
H	43.3729957	38.1350180	43.3089979	H	49.0156185	35.0130549	41.9410858
H	42.0496265	36.3030841	44.4280042	N	48.2600626	34.8694519	43.9498594
H	42.7462199	36.7456598	45.9880205	C	47.9026455	33.7682920	44.7098251
H	41.7375080	37.9077226	45.1114912	H	47.5317883	33.8915789	45.7266875
H	44.7740732	38.4131280	46.0294103	C	45.7339981	32.2338267	47.9697750
H	45.3462807	39.1171164	44.5219913	H	46.6613466	31.9836351	47.4407626
H	43.1847030	40.4798893	44.3760742	H	44.9125696	32.0506956	47.2554406
H	42.7035187	39.8313590	45.9544830	C	45.7619442	33.7160767	48.2526492
H	44.1581085	40.8329956	45.8298663	O	45.0529501	34.2751512	49.1363396
H	44.1732381	35.7349620	43.4675756	O	46.5239158	34.4673913	47.5550776
H	45.7707651	35.1771618	44.8878228	C	47.6774527	35.3762560	51.3975446
H	45.3494614	36.4396551	45.8245083	N	47.5872719	35.5688615	50.0392372
O	46.9369123	37.9426802	48.7244731	C	48.8119391	35.8883743	49.6402359
H	47.1787195	38.4131425	47.8711777	H	49.0811929	36.1162654	48.6076382
H	46.2405492	38.5192385	49.1345081	N	49.6627317	35.9196531	50.6893635
H	49.9045849	40.7449785	45.2294133	H	50.6285369	36.2921287	50.6923441

C	48.9651978	35.6064817	51.8255776	C	50.8315985	37.0496905	44.2490330
H	49.4290904	35.5777351	52.8094083	H	50.8421280	36.4896452	45.1812774
Fe	47.7533692	36.8543763	44.5105907	N	51.9219253	37.5505884	43.6306969
Fe	45.9376591	36.1661930	48.6327902	H	52.8986663	37.5392547	43.9533649
O	48.4033678	36.6831204	46.2744340	C	51.5222332	38.2160747	42.5030744
O	44.9388774	36.8405974	47.3935886	H	52.2358055	38.7329624	41.8648259
H	48.4654509	37.5441094	46.7152342	C	43.2330757	38.1978219	51.4332203
C	43.6846063	39.6539492	45.8797820	H	42.4106181	38.7540786	50.9671741
C	44.4722174	38.4450750	45.4259204	H	43.6065142	38.7832124	52.2844067
C	43.7667506	37.4446220	44.5114531	C	44.3932993	37.9580114	50.4375918
C	42.6196545	36.7369342	45.2456447	O	44.8560813	36.7922334	50.3174298
C	44.7652023	36.4435523	43.8756474	O	44.7633582	38.9996002	49.8807699
N	45.7552351	35.9433773	44.8420625	C	48.0660554	32.6436685	43.9798212
C	45.4917502	37.0659275	42.6543778	N	48.5811191	33.0864769	42.7757714
O	44.8560205	37.2968080	41.6334175	H	48.9162405	32.4832753	42.0211164
O	46.7519993	37.3048173	42.8294733	C	48.6317530	34.4364006	42.7767908
H	43.3408608	38.0087393	43.6593381	H	48.9719838	35.0387841	41.9391696
H	42.1293925	35.9823555	44.6129071	N	48.1837555	34.8977862	43.9355528
H	43.0062458	36.2396772	46.1461154	C	47.8313756	33.7966772	44.6968377
H	41.8524759	37.4587201	45.5633906	H	47.4471882	33.9179547	45.7086600
H	44.7480993	37.8117478	46.4435864	C	45.7072057	32.1942072	48.0075363
H	45.4669672	38.7236903	45.0481102	H	46.6153456	31.9442673	47.4466421
H	43.3232300	40.2261882	45.0044212	H	44.8637083	32.0311457	47.3149594
H	42.7991763	39.3824313	46.4718089	C	45.7645815	33.6661901	48.3133373
H	44.3060043	40.3262049	46.4890378	O	45.1032093	34.2196995	49.2393763
H	44.1818186	35.6020835	43.4688466	O	46.5065083	34.4270362	47.6006887
H	45.8952149	34.9395118	44.7191376	C	47.7248264	35.3481028	51.4684100
H	45.4637857	36.0707673	45.8196864	N	47.6344717	35.5479999	50.1105057
O	46.9811973	37.9933188	48.8029413	C	48.8592251	35.8669973	49.7113961
H	47.2334128	38.4767541	47.9666118	H	49.1288850	36.0991966	48.6801085
H	46.2800684	38.5600931	49.2068308	N	49.7103656	35.8905562	50.7593973
H	49.9164287	40.7367428	45.2138201	H	50.6757748	36.2646218	50.7568515
H	49.4208499	38.4159167	41.7386902	C	49.0132766	35.5739476	51.8954437
H	42.7911958	37.3047023	51.8662524	H	49.4765329	35.5407216	52.8795368
H	47.8799185	31.5845577	44.2418850	Fe	47.7518787	36.9003539	44.5075661
H	45.5989976	31.5795817	48.8310563	Fe	45.9691291	36.0960216	48.7109716
H	46.8142624	35.1444694	52.0214392	O	48.4349959	36.6675358	46.2623782
IC1b				O	44.8127929	36.8320757	47.4594039
C	48.8421978	40.9868808	45.3082589	H	48.5357609	37.5153997	46.7193564
H	48.7582380	41.8065678	46.0346926	C	43.6045550	39.6339840	45.7811471
H	48.4793456	41.3068652	44.3208234	C	44.3315994	38.7272724	44.8484530
C	48.0451862	39.7555618	45.7556149	C	43.7095525	37.5186591	44.2094906
O	47.8205399	39.5969014	46.9757291	C	42.6248780	36.8555624	45.0757351
O	47.6992059	38.9690585	44.8228792	C	44.8011564	36.5102463	43.7642085
C	50.1510902	38.0808091	42.4722339	N	45.7210882	36.1615991	44.8625148
N	49.7353913	37.3544696	43.5654392	C	45.5812110	37.0695050	42.5490883
				O	44.9937494	37.2425145	41.4874785

O	46.8269786	37.3358780	42.7743214
H	43.2351850	37.8375118	43.2564104
H	42.2397650	35.9435828	44.5938590
H	43.0241416	36.5733736	46.0608252
H	41.7734127	37.5365078	45.2287343
H	44.7186278	37.7951827	47.4229763
H	45.3003207	39.0550471	44.4608582
H	42.7997941	40.2066199	45.2719413
H	43.0945291	39.0864959	46.5945274
H	44.2834556	40.3674682	46.2434528
H	44.2965584	35.5999944	43.4028306
H	45.8151543	35.1477353	44.9433774
H	45.3756496	36.4792868	45.7841758
O	47.0008181	37.9368163	48.7757303
H	47.2666882	38.4463917	47.9522580
H	46.3539042	38.5228958	49.2331392
H	49.9002268	40.7364162	45.2313877
H	49.4450870	38.4232990	41.7157107
H	42.7967764	37.3117091	51.8942130
H	47.8558287	31.6076714	44.2454937
H	45.5913306	31.5343334	48.8673076
H	46.8600499	35.1167700	52.0902731

TS3_{NH}

C	48.8464334	40.8935015	45.2806731
H	48.7172311	41.7183280	45.9948796
H	48.4859348	41.1845854	44.2836254
C	48.0943965	39.6408743	45.7370909
O	47.8319762	39.4860935	46.9468952
O	47.8049252	38.8141302	44.8161120
C	50.0626775	38.0293469	42.5177923
N	49.6477680	37.2395698	43.5678187
C	50.7469309	36.9263149	44.2387641
H	50.7896431	36.3041959	45.1301863
N	51.8388700	37.4816533	43.6615027
H	52.8133909	37.4779135	43.9917562
C	51.4329557	38.1897963	42.5639327
H	52.1428270	38.7411088	41.9502480
C	43.3486949	38.1149499	51.3300121
H	42.5090287	38.7035312	50.9395174
H	43.7811357	38.6586287	52.1819393
C	44.4538434	37.9096817	50.2557818
O	44.8950051	36.7637539	50.0120357
O	44.8079784	39.0075220	49.7917892
C	48.0294411	32.6230591	44.0071667
N	48.5461513	33.1258984	42.8260189
H	48.8972388	32.5588877	42.0502220

C	48.5629355	34.4732968	42.8786121
H	48.8920305	35.1166729	42.0683859
N	48.0902502	34.8785736	44.0554129
C	47.7523061	33.7379264	44.7643594
H	47.3560638	33.8102954	45.7743908
C	45.7368251	32.1672838	47.9830792
H	46.5886692	31.8188079	47.3902530
H	44.8444317	32.0768444	47.3423232
C	45.9593324	33.6305954	48.2633333
O	45.2377242	34.3156891	49.0363882
O	46.9017386	34.2409963	47.6588140
C	47.7825600	35.3601101	51.4142253
N	47.7723173	35.5455144	50.0529681
C	49.0158019	35.8659142	49.7287723
H	49.3460519	36.1125619	48.7211593
N	49.8071022	35.9020221	50.8212676
H	50.7695668	36.2793417	50.8613433
C	49.0456009	35.5933998	51.9144279
H	49.4519017	35.5707466	52.9237559
Fe	47.4275773	36.8082205	44.5301031
Fe	46.3223085	36.1237591	48.4220096
O	47.4392383	36.6978338	46.6605165
O	45.0963105	36.6333388	47.1201294
H	47.5031767	37.6663648	46.8038994
C	43.5590040	40.0647686	45.1231704
C	44.4217121	38.8777060	44.6994382
C	43.6354240	37.6820154	44.1304955
C	42.5811747	37.1506489	45.1115562
C	44.5855962	36.5515112	43.6601772
N	45.4625053	36.0665520	44.7237377
C	45.4311276	37.0534429	42.4681679
O	44.9328363	37.2497466	41.3708981
O	46.6826384	37.2802640	42.7676284
H	43.1170643	38.0224587	43.2162382
H	42.1148995	36.2251504	44.7366761
H	43.0225095	36.9235329	46.0960850
H	41.7785147	37.8867764	45.2685395
H	45.0120825	38.5429517	45.5670144
H	45.1549485	39.2085021	43.9453883
H	42.9091234	40.4124859	44.3023703
H	42.9059310	39.8151907	45.9730978
H	44.1885967	40.9097615	45.4454940
H	43.9687601	35.7235342	43.2733848
H	45.5383169	35.0467457	44.6748032
H	45.1780387	36.3521527	45.9504379
O	47.1035738	38.0255025	49.0437496
H	47.5713805	38.5828337	48.3852102

H	46.2979830	38.5555584	49.2945599	C	47.9447549	32.6119818	43.9545810
H	49.9144882	40.6836801	45.2232180	N	48.5478504	33.0077915	42.7869572
H	49.3674650	38.3980301	41.7635911	H	48.9526522	32.3795098	42.0845814
H	42.9183708	37.2268121	51.7927209	C	48.5630002	34.3610353	42.7234449
H	47.8485028	31.5745014	44.2435039	H	48.9714901	34.9309385	41.8932607
H	45.6012264	31.5301424	48.8569963	N	48.0035785	34.8691585	43.8178061
H	46.8928657	35.1371671	52.0031291	C	47.6144398	33.8108383	44.5971701
IC1_{NH}				H	47.1478119	33.9636095	45.5705568
C	40.2729116	36.2264585	36.7002008	C	45.7056982	32.1171624	48.0277053
H	39.4819924	35.4596517	36.6912597	H	46.5955512	31.8560974	47.4449686
H	40.9258079	36.0441521	35.8343352	H	44.8394434	31.9679303	47.3609625
C	41.0409155	36.1855062	37.9951676	C	45.7953013	33.5836966	48.3373922
C	42.4185230	36.4955584	38.2229464	O	45.1285666	34.1444709	49.2584031
H	43.1796228	36.7618048	37.4900695	O	46.5617094	34.3372047	47.6430702
N	42.7028668	36.4338484	39.5319796	C	47.7340511	35.2822203	51.5116737
H	43.5870863	36.6823486	40.0220836	N	47.6503465	35.5107086	50.1563441
C	41.5510764	36.0847319	40.2355163	C	48.8817044	35.8262068	49.7719966
C	41.3668270	35.9244787	41.5981878	H	49.1672773	36.0813304	48.7529795
H	42.1920265	36.0788431	42.2905625	N	49.7273263	35.8176662	50.8222163
C	40.0738839	35.5686469	42.0359358	H	50.6929700	36.1929361	50.8277616
H	39.8896862	35.4458643	43.1062838	C	49.0227104	35.4861141	51.9482193
C	39.0190690	35.3807237	41.1281913	H	49.4823189	35.4316846	52.9333986
H	38.0332424	35.0997870	41.5034351	Fe	47.7426796	36.9359703	44.3431071
C	39.2152142	35.5534245	39.7531656	Fe	45.9782010	35.9996344	48.7602323
H	38.3876998	35.4148382	39.0529186	O	48.4629341	36.6395682	46.0509683
C	40.4980056	35.9133675	39.2931156	O	44.8414438	36.6835336	47.4441181
C	48.7804948	40.9422665	45.2340727	H	48.5267155	37.4493140	46.5799977
H	48.6631740	41.7337604	45.9863727	C	43.2290198	40.0400408	44.8560051
H	48.4508992	41.3000920	44.2485441	C	44.2361798	38.9294558	44.5738790
C	47.9728242	39.6956722	45.6037654	C	43.6119843	37.6058119	44.0983767
O	47.7084490	39.4739707	46.7987558	C	42.5973129	37.0142752	45.0813312
O	47.6500007	38.9500737	44.6173238	C	44.7431163	36.5794249	43.7494880
C	50.1212573	38.0814080	42.3687700	N	45.6986579	36.4519389	44.7945839
N	49.7064068	37.3022394	43.4249781	C	45.4544520	36.9589396	42.4265878
C	50.8010597	37.0021830	44.1193032	O	44.7792035	37.0070389	41.3869769
H	50.8123087	36.4234077	45.0397633	O	46.7027539	37.2083644	42.5323978
N	51.8838565	37.5521297	43.5367033	H	43.1078863	37.8032250	43.1368768
H	52.8547518	37.5575196	43.8829532	H	42.1890705	36.0628182	44.7016169
C	51.4867535	38.2503510	42.4277597	H	43.0558496	36.8065381	46.0601046
H	52.1971377	38.8064245	41.8193595	H	41.7523827	37.7016198	45.2367128
C	43.2694845	38.1709071	51.4322656	H	44.8433895	38.7440688	45.4763644
H	42.4600090	38.7326230	50.9487701	H	44.9602592	39.2633736	43.8119063
H	43.6373725	38.7630505	52.2811634	H	42.5437598	40.1980286	44.0063268
C	44.4401420	37.9042438	50.4587801	H	42.6095093	39.8231012	45.7386845
O	44.8656217	36.7221505	50.3274411	H	43.7452788	40.9896963	45.0605377
O	44.8612914	38.9322132	49.9159823	H	44.2569123	35.5911181	43.5958617
				H	45.3117015	36.2803593	45.7461247

H	44.6969079	37.6418512	47.4711300	C	47.6983520	35.3544248	51.4780605
O	47.0422360	37.8327953	48.7178296	N	47.5922313	35.6012502	50.1304886
H	47.2216145	38.3238534	47.8694150	C	48.8041685	35.9662818	49.7348029
H	46.4639722	38.4370553	49.2398592	H	49.0661038	36.2258414	48.7085770
H	39.7594149	37.1751445	36.5440496	N	49.6631304	35.9750289	50.7781379
H	49.8440382	40.7088268	45.1845888	H	50.6245805	36.3583096	50.7771630
H	49.4091654	38.4313139	41.6214025	C	48.9834614	35.5989709	51.9063903
H	42.8151131	37.2958868	51.8969733	H	49.4542101	35.5453768	52.8859702
H	47.7635368	31.5811115	44.2587743	Fe	47.8445948	36.8610854	44.4745470
H	45.6010307	31.4597931	48.8908260	Fe	45.8872161	35.9620890	48.7016866
H	46.8650319	35.0498656	52.1272094	O	48.5601566	36.7051499	46.2115869
TS4b				O	44.6220350	36.2922543	47.4285229
C	48.8566152	40.9707542	45.2491984	H	48.6397619	37.5466297	46.6845570
H	48.7556103	41.7766459	45.9884623	C	42.2153709	37.2990095	45.5701503
H	48.5156448	41.3110750	44.2607061	C	43.4555430	38.1145165	45.7098675
C	48.0479198	39.7331667	45.6512524	C	44.5067008	38.2380307	44.6395569
O	47.7686187	39.5612246	46.8567853	C	44.0693993	39.2952988	43.6116753
O	47.7422538	38.9523393	44.6978891	C	44.8908080	36.8976815	43.9620802
C	50.1979502	38.0732501	42.4313822	N	45.7907207	36.1429338	44.8459928
N	49.7994187	37.3195408	43.5120698	C	45.6131532	37.1190765	42.6105027
C	50.9015416	37.0272367	44.1915605	O	44.9708409	37.2020956	41.5708877
H	50.9247983	36.4552396	45.1164697	O	46.8975263	37.2256684	42.7226535
N	51.9792600	37.5625525	43.5821297	H	45.4236479	38.6189532	45.1164207
H	52.9568825	37.5570393	43.9022955	H	44.9307750	39.5926059	42.9959386
C	51.5656390	38.2377704	42.4650900	H	43.2941938	38.9050666	42.9355210
H	52.2680189	38.7779835	41.8340108	H	43.6811208	40.1880567	44.1217819
C	43.2220022	38.2050924	51.3981575	H	44.2440598	37.1475477	47.1256197
H	42.4069513	38.7963560	50.9637965	H	43.4251243	38.9469500	46.4265975
H	43.6339958	38.7555319	52.2552517	H	41.4024072	37.8790327	45.0866416
C	44.3493463	37.9394771	50.3710897	H	42.3733532	36.3915780	44.9684032
O	44.8152198	36.7730765	50.2795451	H	41.8428359	36.9731822	46.5543798
O	44.6969199	38.9643457	49.7701978	H	43.9799087	36.3234752	43.7341528
C	48.0791289	32.6091332	44.0066320	H	45.8112322	35.1579224	44.5696209
N	48.6039527	33.0332515	42.8000278	H	45.4544734	36.1453819	45.8245993
H	48.9300930	32.4202093	42.0492851	O	46.7973335	37.8304465	48.5172219
C	48.6851802	34.3804778	42.7919484	H	47.1134702	38.3307885	47.7111648
H	49.0336979	34.9712966	41.9494983	H	46.1676870	38.4378800	48.9738518
N	48.2490445	34.8574553	43.9491292	H	49.9162948	40.7228495	45.1884571
C	47.8690457	33.7701223	44.7180443	H	49.4845924	38.4088635	41.6786860
H	47.4804296	33.9037366	45.7273098	H	42.7680176	37.3214938	51.8467315
C	45.7114124	32.0673296	48.0451988	H	47.8581016	31.5778032	44.2815366
H	46.5958807	31.7983220	47.4583564	H	45.5982493	31.4104246	48.9076007
H	44.8413774	31.9368228	47.3797768	H	46.8401647	35.0832024	52.0928941
C	45.8212030	33.5301568	48.3728421	IC2b			
O	45.1475675	34.0811983	49.2955113	C	48.9676602	40.9661217	45.3984857
O	46.5987852	34.2752332	47.6888314	H	48.8921262	41.7988398	46.1101939

H	48.5493923	41.2454115	44.4211681	C	44.0775147	38.3579373	44.9587947
C	48.2448434	39.7170414	45.9039735	C	44.8790871	39.2707891	45.8863187
O	48.0729657	39.5545842	47.1329148	C	44.9686980	37.3996656	44.1146100
O	47.9049259	38.9038785	44.9959311	N	45.7829666	36.4975274	44.9657994
C	50.2504246	38.0770301	42.5074336	C	45.9031244	38.0811003	43.0886724
N	49.8642910	37.3183005	43.5931929	O	45.5604292	39.0931119	42.4889065
C	50.9771192	37.0096133	44.2475655	O	47.0139414	37.4482268	42.9167932
H	51.0117222	36.4310361	45.1680368	H	43.4865349	37.6751540	45.6017356
N	52.0487166	37.5367648	43.6219525	H	45.5594184	38.7045432	46.5293975
H	53.0316494	37.5207349	43.9238975	H	45.4691389	39.9923072	45.3032338
C	51.6202247	38.2253200	42.5190731	H	44.1941159	39.8267287	46.5438598
H	52.3159187	38.7658850	41.8806743	H	43.8616509	35.8040497	47.4969068
C	43.2778696	38.2103921	51.4438222	H	43.3500108	40.1961154	43.9520338
H	42.4678465	38.7918167	50.9868074	H	42.3949318	38.2644274	42.2813048
H	43.6674355	38.7742797	52.3023710	H	41.6720525	37.5838956	43.7684661
C	44.4299287	37.9506160	50.4428278	H	41.1883870	39.1920006	43.1689312
O	44.8844911	36.7760305	50.3447310	H	44.2805656	36.7880833	43.5037557
O	44.8053292	38.9785625	49.8720443	H	45.7051107	35.5317713	44.6414055
C	48.0084688	32.6336742	44.0233837	H	45.4264721	36.4957027	45.9377861
N	48.5952404	33.0753789	42.8518416	O	46.8515036	37.8390135	48.5738703
H	48.9535301	32.4723620	42.1074473	H	47.3437262	38.3830384	47.8739857
C	48.6660453	34.4235794	42.8635860	H	46.1990506	38.4536544	48.9938207
H	49.0667189	35.0254545	42.0525984	H	50.0250799	40.7272442	45.2850476
N	48.1629019	34.8851321	44.0007448	H	49.5367117	38.4519329	41.7738609
C	47.7494678	33.7858608	44.7337246	H	42.8209147	37.3287432	51.8932159
H	47.3215744	33.9058362	45.7278201	H	47.8060202	31.5948840	44.2841453
C	45.6881277	32.1121570	48.0390762	H	45.5812849	31.4577362	48.9041688
H	46.5737386	31.8445058	47.4531984	H	46.8645370	35.0931227	52.1300019
H	44.8157292	31.9704226	47.3785788				
C	45.7900363	33.5779879	48.3596579				
O	45.0724292	34.1400794	49.2432092	TS4b_{OH}			
O	46.6044718	34.3136359	47.7126933	C	48.8849991	40.9728640	45.2547535
C	47.7269524	35.3302181	51.5070312	H	48.7693453	41.7399208	46.0326856
N	47.6223365	35.5175589	50.1497715	H	48.5457541	41.3548278	44.2809811
C	48.8412277	35.8412588	49.7345487	C	48.1044825	39.6970740	45.5896787
H	49.1026380	36.0493548	48.6948669	O	47.8580126	39.4323245	46.7867415
N	49.7006070	35.8827187	50.7763075	O	47.8055720	38.9748619	44.5869507
H	50.6649284	36.2599960	50.7628556	C	50.1290149	38.0738142	42.4211046
C	49.0168322	35.5694783	51.9214939	N	49.7040186	37.2756506	43.4566070
H	49.4880877	35.5479482	52.9019921	C	50.7876001	36.9614657	44.1555331
Fe	47.9300504	36.8857717	44.6260257	H	50.7988973	36.3439092	45.0508021
Fe	45.9470570	36.0165072	48.7529755	N	51.8799800	37.5275463	43.5996353
O	48.6762647	36.5853974	46.3426092	H	52.8486489	37.5244522	43.9481035
O	44.5972187	36.4304716	47.5316035	C	51.4941615	38.2427724	42.4970330
H	48.8289563	37.4213287	46.8083392	H	52.2114219	38.8067161	41.9043616
C	42.0479266	38.5142312	43.3060182	C	43.1992536	38.1824421	51.4108270
C	43.1204159	39.1423826	44.1210982	H	42.3660690	38.7432229	50.9702046
				H	43.5929796	38.7591920	52.2586551

C	44.3356929	37.9518878	50.3848804	H	44.5678993	40.3676417	46.1493882
O	44.7397659	36.7774248	50.1828587	H	43.9994961	35.7081924	43.2104548
O	44.7410868	39.0138572	49.8945959	H	45.7812448	34.8279715	44.2704963
C	48.0931977	32.6096258	43.9823241	H	45.3958094	35.8570641	45.5108538
N	48.5977302	32.9959473	42.7540566	O	47.0689555	37.9797344	48.9656564
H	48.9261720	32.3615185	42.0224013	H	47.3393689	38.4350523	48.1364840
C	48.6814838	34.3410212	42.7028968	H	46.3334153	38.5339986	49.3168009
H	49.0277361	34.9034600	41.8401573	H	49.9465693	40.7333255	45.1934576
N	48.2595694	34.8538126	43.8499031	H	49.4230927	38.4375213	41.6744734
C	47.8959513	33.7912722	44.6625101	H	42.7742868	37.2913099	51.8727291
H	47.5334982	33.9556137	45.6784030	H	47.8611366	31.5874405	44.2812420
C	45.6790237	32.1168799	48.0003378	H	45.5666286	31.4798851	48.8776474
H	46.5281686	31.7817603	47.3961352	H	46.8485505	35.0919825	52.1142707
H	44.7748632	32.0077972	47.3794793				
C	45.8776445	33.5869847	48.2806989	PC2 _{OH}			
O	45.0902014	34.2261489	49.0593812	C	48.9145821	40.9768046	45.3588820
O	46.8177986	34.2173272	47.7256987	H	48.8374888	41.8023173	46.0790005
C	47.7274592	35.3326818	51.5162318	H	48.5208040	41.2772438	44.3778488
N	47.6552590	35.5244848	50.1600085	C	48.1568588	39.7357698	45.8379690
C	48.8808737	35.8533338	49.7796787	O	48.0388730	39.5307617	47.0684992
H	49.1678444	36.0908374	48.7565362	O	47.7393923	38.9732838	44.9172294
N	49.7171992	35.8905527	50.8393094	C	50.2111493	38.0871551	42.4883145
H	50.6780811	36.2739350	50.8411216	N	49.8272686	37.3688016	43.5991082
C	49.0070513	35.5711573	51.9656078	C	50.9428899	37.0712396	44.2553655
H	49.4561162	35.5447915	52.9558012	H	50.9759519	36.5238778	45.1947895
Fe	47.6793683	36.8324470	44.2771876	N	52.0132375	37.5689693	43.6039972
Fe	46.0221201	36.0499496	48.7445834	H	52.9986146	37.5511391	43.8989182
O	48.0512667	36.6994306	46.1256497	C	51.5824826	38.2250256	42.4824085
O	45.4663005	36.7246136	47.0689144	H	52.2785499	38.7368772	41.8211226
H	48.2009254	37.5829837	46.5075241	C	43.1695234	38.2082591	51.3443442
C	44.0168774	39.4145572	46.1851676	H	42.3238242	38.7580830	50.9134710
C	44.6212435	38.4222015	45.2591224	H	43.5725733	38.7989652	52.1783828
C	43.8058568	37.4678138	44.4430469	C	44.2858417	37.9645288	50.2932966
C	42.7401224	36.7591410	45.3003106	O	44.6748224	36.7898576	50.0873763
C	44.6771578	36.4576400	43.6495306	O	44.6758525	39.0231906	49.7778500
N	45.6659664	35.8129703	44.5147546	C	48.0304126	32.6465155	44.0233567
C	45.4062719	37.1122374	42.4506890	N	48.6008138	33.1073179	42.8507925
O	44.7998143	37.3445985	41.4153381	H	48.9496247	32.5151845	42.0936097
O	46.6635330	37.3716433	42.6596778	C	48.6595665	34.4554604	42.8791762
H	43.2733843	38.0658361	43.6705488	H	49.0371766	35.0711822	42.067

O	45.1262885	34.0013287	49.3790752	C	49.0230718	40.9739609	45.3691261
O	46.1003651	34.3577888	47.4600892	H	48.9428496	41.8156432	46.0696062
C	47.8082624	35.3295380	51.4873662	H	48.6030852	41.2359948	44.3877990
N	47.7334348	35.5691203	50.1357946	C	48.3181960	39.7275436	45.8997909
C	48.9545952	35.9326447	49.7611265	O	48.1645129	39.5801516	47.1291951
H	49.2350238	36.1809300	48.7345710	O	47.9696832	38.9010469	45.0020108
N	49.7899560	35.9398048	50.8227236	C	50.2731706	38.0815793	42.5037506
H	50.7519752	36.3230407	50.8351702	N	49.9008161	37.3140613	43.5865017
C	49.0853947	35.5702806	51.9386835	C	51.0206540	37.0054294	44.2298122
H	49.5339917	35.5162909	52.9286641	H	51.0659956	36.4237885	45.1479599
Fe	47.9072879	36.9051759	44.6275516	N	52.0828481	37.5423784	43.5983277
Fe	46.0869640	35.9066607	48.8378251	H	53.0684364	37.5257739	43.8923604
O	48.7217070	36.7004344	46.3302259	C	51.6424069	38.2367186	42.5037985
O	44.5370428	38.8727495	46.1099121	H	52.3304993	38.7840432	41.8629571
H	48.7847226	37.5434431	46.8067516	C	43.2369483	38.2511997	51.4417693
C	42.8231084	39.8321952	44.6882457	H	42.4151616	38.8252320	50.9979262
C	44.0143888	38.8853601	44.7856631	H	43.6244399	38.8123111	52.3029253
C	43.6756817	37.4325362	44.3963336	C	44.3838322	38.0133623	50.4244420
C	42.7620526	36.7358324	45.4091931	O	44.8279623	36.8456548	50.2945994
C	44.9379713	36.5924318	44.1044238	O	44.7544715	39.0602832	49.8774255
N	45.8753872	36.5279313	45.2459923	C	48.0364178	32.6412708	44.0156138
C	45.6418312	37.0969468	42.8134319	N	48.6290656	33.0764467	42.8448538
O	44.9748917	37.2579817	41.7965170	H	48.9779512	32.4693518	42.0992538
O	46.9108682	37.3024938	42.9197963	C	48.7248768	34.4230277	42.8611367
H	43.1643371	37.5104668	43.4265085	H	49.1376861	35.0186814	42.0515066
H	42.4805726	35.7365436	45.0407682	N	48.2307948	34.8902072	44.0003017
H	43.2641477	36.6088185	46.3808212	C	47.7982750	33.7948037	44.7309631
H	41.8374403	37.3065856	45.5834472	H	47.3668591	33.9173645	45.7250529
H	44.8154629	39.7626983	46.3650507	C	45.6911515	32.1271515	47.9827927
H	44.7952380	39.2388024	44.0834906	H	46.6127811	31.8904992	47.4393035
H	42.3874981	39.8192856	43.6774804	H	44.8569888	31.9327603	47.2866982
H	42.0388357	39.5619923	45.4099589	C	45.7005798	33.6084326	48.2760135
H	43.1390252	40.8630907	44.9177439	O	44.9749945	34.1304107	49.1642384
H	44.6192657	35.5625049	43.8717275	O	46.4599697	34.3722571	47.5828570
H	45.8078079	35.6425319	45.7573961	C	47.6651087	35.3432874	51.4602716
H	45.6759200	37.2843665	45.9142069	N	47.5569123	35.5004124	50.1012762
O	46.4361072	37.8048797	48.1630495	C	48.7711443	35.8330547	49.6831574
H	47.1050534	38.3565895	47.6593837	H	49.0338056	36.0235710	48.6405832
H	45.8187844	38.4282493	48.6171243	N	49.6320600	35.9103330	50.7248756
H	49.9729802	40.7353885	45.2610106	H	50.5937400	36.2919145	50.7095036
H	49.4886251	38.4270269	41.7463489	C	48.9505308	35.6105982	51.8745824
H	42.7567616	37.3216123	51.8255429	H	49.4210590	35.6165193	52.8555591
H	47.8283594	31.6040673	44.2694124	Fe	48.0047492	36.8865475	44.6538677
H	45.5651896	31.3863959	48.8620925	Fe	45.8701293	36.0627405	48.6805332
H	46.9283577	35.0693011	52.0756786	O	48.7877741	36.6061824	46.3420732
				O	44.4091841	36.5696292	47.4682266
				H	48.8893502	37.4329546	46.8388124

TS5

C	42.1469709	38.1284637	43.6701035	H	42.4234568	38.7714822	50.9314293
C	43.0036493	38.7881435	44.6808122	H	43.6129430	38.7829884	52.2544024
C	44.2313804	38.2620123	45.2354458	C	44.4055139	37.9235339	50.4185377
C	45.0672932	39.3400314	45.9283131	O	44.8433690	36.7607494	50.3138758
C	45.0112222	37.3041600	44.3069998	O	44.8033854	38.9693387	49.8689679
N	45.8982444	36.3981956	45.0602707	C	48.0467477	32.6156177	43.9869304
C	45.8407566	38.0308919	43.2115277	N	48.5850940	32.9926153	42.7688946
O	45.3745978	39.0169381	42.6468902	H	48.9469605	32.3543759	42.0558376
O	46.9718239	37.4751700	42.9734036	C	48.6274327	34.3372892	42.6900734
H	43.9634216	37.5686130	46.1445786	H	48.9862233	34.8922719	41.8277390
H	45.8557481	38.8811617	46.5258840	N	48.1473899	34.8612542	43.8113326
H	45.5191740	40.0181133	45.1909294	C	47.7857674	33.8044842	44.6345325
H	44.4352634	39.9190335	46.6182873	H	47.3910246	33.9720588	45.6390585
H	43.7288393	35.8830730	47.4314997	C	45.7118103	32.0310667	48.0196997
H	42.6539997	39.7398601	45.0929847	H	46.5558598	31.6925725	47.4116675
H	42.6236397	38.1788325	42.6711908	H	44.8067219	31.9138197	47.4013733
H	41.9992643	37.0579014	43.9084491	C	45.9266376	33.5042698	48.2948933
H	41.1607660	38.6065008	43.5903484	O	45.2072749	34.1161219	49.1521395
H	44.2746072	36.7003936	43.7506993	O	46.8218274	34.1354190	47.6692136
H	45.8534254	35.4547321	44.6711971	C	47.8661231	35.2701650	51.6587260
H	45.5453782	36.3120462	46.0270889	N	47.8166646	35.4292640	50.3018363
O	46.8155192	37.9068406	48.5644804	C	49.0475131	35.7450475	49.9348551
H	47.3585202	38.4382830	47.9122343	H	49.3564741	35.9646651	48.9150965
H	46.1649481	38.5238205	48.9778503	N	49.8692069	35.8032662	51.0069249
H	50.0815278	40.7367749	45.2619777	H	50.8255722	36.1953858	51.0034498
H	49.5471544	38.4590054	41.7836693	C	49.1385218	35.5117642	52.1283578
H	42.7959360	37.3586824	51.8856027	H	49.5674562	35.5011045	53.1275796
H	47.8193235	31.6059003	44.2781880	Fe	47.5932575	36.8530805	44.1761987
H	45.5770764	31.4812029	48.8533123	Fe	46.2076299	35.9185745	48.9201898
H	46.8067209	35.1049394	52.0883066	O	47.7088509	36.7058515	46.0725195
PC2				O	45.3749419	36.7234470	47.1173807
C	48.9150549	40.9391324	45.2112315	H	47.9659061	37.5756405	46.4387537
H	48.7796983	41.6987466	45.9930291	C	42.0712225	36.4884924	45.1476796
H	48.5889939	41.3258457	44.2351261	C	42.8262684	37.7361831	44.8107088
C	48.1426221	39.6551959	45.5218590	C	43.9448957	37.8639044	44.0769039
O	47.9029955	39.3566650	46.7120739	C	44.6311601	39.1984489	43.9573643
O	47.8365557	38.9592893	44.5009716	C	44.6169079	36.6621095	43.4122067
C	50.1323046	38.0496361	42.4055365	N	45.5151366	35.9704261	44.3519228
N	49.6872724	37.2444954	43.4292834	C	45.4516150	37.1070360	42.1924567
C	50.7599273	36.9256238	44.1429004	O	44.9327035	37.2736127	41.1006589
H	50.7627108	36.2990419	45.0320590	O	46.7061025	37.3179277	42.4712450
N	51.8630819	37.4950667	43.6097794	H	45.0229964	37.6263366	47.0975187
H	52.8267284	37.4897223	43.9720888	H	45.5800343	39.2032194	44.5118050
C	51.4958618	38.2159240	42.5042061	H	44.8762738	39.4285929	42.9101446
H	52.2235061	38.7798660	41.9239585	H	43.9945475	39.9962959	44.3595420
C	43.2354755	38.2029116	51.4013297	H	46.2870172	36.7510913	46.6464766
				H	42.4238009	38.6550727	45.2564156

H	42.5166748	35.5726249	44.7321594	H	46.4290216	38.4758849	49.3479071
H	42.0352507	36.3727203	46.2433193	H	49.9800582	40.7109423	45.1692278
H	41.0216354	36.5546526	44.8110652	H	49.4416638	38.4105863	41.6434359
H	43.8503107	35.9679213	43.0405441	H	42.7841140	37.3234410	51.8605370
H	45.6042785	34.9796027	44.1083556	H	47.8408104	31.5912368	44.2972540
H	45.1568263	36.0035586	45.3123825	H	45.6009256	31.4061454	48.9058402
O	47.1699899	37.9228688	49.0026708	H	46.9626093	35.0566833	52.2298263
H	47.5522786	38.4306193	48.2603920				

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