Multifunctional Cytochrome P450 Orchestrates Radical Cleavage and Non-radical Cyclization in 5-Oxaindolizidine Biosynthesis

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Experimental Procedures

General experimental procedures.

Specific rotations were obtained on a JASCO P-1020 digital polarimeter. UV spectra were recorded from 200 to 600 nm on a Hitachi 5430. NMR spectra were recorded on Agilent 500 MHz DD2 spectrometers (Agilent, Beijing, China) using tetramethylsilane as an internal standard, and the chemical shifts were recorded in δ values. Semipreparative HPLC was performed using an ODS column [HPLC (YMC-Pack ODS-A, 10 × 250 mm, 5 μm, 3 mL/min)]. Chiral Colum (Chiralpak AD-H) (Particle size 5 μm, 4.6 × 250 mm). High performance liquid chromatography-mass spectrometry (LC-MS) was performed on a Waters SQ Detector Liquid mass spectrometer (USA) using Waters ACQUITY UPLC Shield RP18 (1.7 μm, 21 × 50 mm, 0.5 mL/min, MeCN 5%-99%-10 min + 99%-3 min + 5%-3 min). Column chromatography (CC) was performed with silica gel (100−200 mesh, 200−300 mesh, Qingdao Marine Chemical Inc.) and Sephadex LH-20 (Amersham Biosciences), respectively. UV spectrum of DNA was recorded on a NP80 NanoPhotometer (Implen) with an 8.5 mm cuvette. All chemicals used in the study were of analytical grade except the preparative HPLC and LC-MS with chromatographic grade.

General DNA manipulation techniques.

All the DNA manipulations in this study were conducted according to the manufacturer's protocol. PCR reactions were performed using the Phusion® high-fidelity DNA polymerase, Q5® High-Fidelity DNA Polymerases (New England Biolabs), Hieff Canace® Gold High Fidelity DNA Polymerase (Yeasen) and KOD One™ PCR Master Mix (Toyobo) according to the manufacturer's instructions. cDNA was synthesized by using the PrimeScript RT-PCR Kit (TaKaRa). Custom oligonucleotides were synthesized by Shanghai Sangon DNA Technologies. Fragments were respectively amplified by the condition： step 1: 95 ℃ for 3 min; step 2: 95 ℃ for 15 s; step 3: Tm for 15 s; step 4: 72 ℃ by 30s/kb (KOD for 5s/kb); step 5: step 2 to step 4 for 35 cycles; step 6: 72 ℃ 10 min, then the productions were purified by gel. *Escherichia coli* strain DH10B, BL21 and XL-1 was used for routine cloning. *Saccharomyces cerevisiae* RC01, Y31 and BJ5464-NpgA were used for in vivo yeast DNA recombination cloning and cultured on yeast extract peptone dextrose (YPD) medium at 28 °C for microsomal in vitro assays. *Penicillium citrinum* HDN11-186 was cultured at 28 °C on PDA plates and spores were collected after 7 days of growth by flooding the plates with sterile 0.1% Tween 80. And HDN11-186 was allowed to grow in Elenmeyer flasks containing 150 mL of liquid culture medium, composed of glucose (1%), maltose (2%), mannitol (2%), monosodium glutamate (1%), KH2PO4 (0.05%), MgSO4·7H2O (0.03%), and yeast extract (0.3%) after adjusting its pH to 6.5 before the RNA isolation or in PDA medium for isolation of genomic DNA. *Penicillium brocae* (HDN12-143) was cultured at 28 °C on PDA plates and spores were collected after 7 days of growth by flooding the plates with sterile 0.1% Tween 80. *Aspergillus nidulans* A1145 was grown at 28 °C in CD (0.1% Glucose, 0.5 v/v% 20×Nitrate salts, 0.01 v/v% Trace elements, and 2% agar for solid media) media for sporulation or in CD-ST (2% starch, 2% Casamino acids, 5 v/v% 20×Nitrate salts, 0.1 v/v% Trace elements) media for heterologous expression.

Heterologous expression of gene cluster pnlt in *Aspergillus nidulans*.

All genes in *pnlt* gene cluster were amplified from genomic DNA extract from *Penicillium citrinum* HDN11-186. The primers used in this study are listed in Table S2. Plasmids pYTU, pYTP, pYTR with auxotrophic markers for uracil (pyrG), pyridoxine (pyroA), and riboflavin (riboB), respectively, were digested with PacI and SwaI and used as vectors to insert genes. The corresponding heterologous expression plasmids were obtained by yeast homologous recombination. The correct colonies checked by PCR were combined, and subjected to yeast miniprep to get small number of plasmids. The plasmids obtained from yeast miniprep using Zyppy Plasmid Miniprep Kit (Zymo Research, USA) was introduced into *Escherichia coli* DH10B and XL-1 by electroporation. After plasmid extraction from *E. coli* to obtain transformants with

single plasmid, plasmids were sequenced to confirm identities by sequencing.

The resulting recombinant plasmids listed in Table S2. For *A. nidulans* transformation, necessary plasmids were added to 50 μL *A. nidulans* A1145 protoplast suspension prepared above and the mixture was incubated on ice for 60 min. After incubating on ice, 500 μL of PEG solution (60% PEG, 50 mM calcium chloride and 50 mM Tris-HCl, pH 7.5) was added to the protoplast mixture, followed by additional incubation at room temperature for 20 min. The mixture was spread on the regeneration medium (CD solid medium with 1.2 M sorbitol and appropriate supplements including 0.5 μg/mL pyridoxine HCl) and incubated at 37 °C for 2-3 days until single colonies appear. Isolated transformants were grown in CD-ST media (1 L: 20 g starch, 20 g tryptone, 50 mL 20 × nitrate salts, 1 mL trace elements, pH 6.5) for the production of heterologously expressed metabolites.

Construction of *Saccharomyces cerevisiae* strains.

The intron free ORFs of *pnltC* was amplified by PCR using cDNA from *Penicillium citrinum* HDN11-186 as a template, which was culturing under condition of target metabolites produced. Gene of *pnltC* was inserted into PYET vector. The plasmid was introduced into *Saccharomyces cerevisiae* RC01 with Frozen E-Z Yeast Transformation Kit (Zymo) selected by dropout media, tryptophan-dropout for PYET vector selection. *Saccharomyces cerevisiae* RC01 was transformed with corresponding plasmid combinations and was grown on select nutrient dropout media plates at 28 °C for 3 days. Single colony was picked up and grown in 2 mL dropout media with selective nutrients dropped out for 1 day. 0.5 mL of dropout media was then transferred to 25 mL YPD (2% dextrose) in Elenmeyer flasks. The culture was shaken at 250 rpm at 28 °C for 2-3 days, in vivo feeding assays and in vitro microsomal assays could be carried on.

Construction of *Escherichia coli* BL21 strains.

The intron free ORFs of *pnltA-A* was amplified by PCR using cDNA from *Penicillium citrinum* HDN11-186 as a template, which was culturing under condition of target metabolites produced. Gene was ligated to modified pET28(a) vectors resulting in constructs harbouring either an N-terminal His6-tag, a C-terminal His6-tag, an N-terminal MBP-tag. The plasmid was introduced into *Escherichia coli* BL21 (DE3) competent cells by electroporation. Starter cultures were grown overnight in LB media containing Ampicillin (100 μg/mL). 2 mL of this culture was added to 200 mL LB media (1 L flasks) with ampicillin (100 μg/mL) and grown at 37 °C with shaking (180 rpm) till OD_{600}~0.6. The flasks were then incubated at 4 °C for ~2 h without shaking, induced with 500 μM IPTG followed by incubation at 15 °C for ~20 h with shaking at 180 rpm. The cells were harvested by centrifugation at 5,000 rpm for 20 min and stored in liquid nitrogen until further use. Typical yields were 9-10 g of cell pellet (wet weight) from 3 L cell culture. For purification, the cell pellets were thawed and resuspended in 40-50 mL of lysis buffer (100 mM KPi, 150 mM NaCl, pH 7.5) at room temperature and was stirred for ~1.5 h on an ice bath and sonicated to lyse the cells. Cell debris and the lysate were separated by centrifugation at 15,000 rpm for 30 min. Then two fractions of cell debris and lysate were added loading for 15 min at 90 °C.

Compound identification, isolation, and characterization.

Aspergillus nidulans A1145 transformants were selected for on CD sorbitol agar (2% glucose as carbon source) appropriately supplemented with riboflavin, uracil, and/or pyridoxine for the set of plasmids introduced. The CD-ST solid plate (5 mL in diameter 3 cm Petri dish) was inoculated with spores and incubated at 28 °C for 3 days. For small-scale the fermentation system was collected and extracted with Ethyl Acetate for 30 min with sonication. After centrifugation, the supernatant (200 μL) was dried down by Speedvac and then resuspended in methanol (100 μL).

For small scale and feeding assays metabolite analysis:

Aspergillus nidulans A1145 transformants were selected for on CD sorbitol agar (2% glucose as carbon source) appropriately supplemented with riboflavin, uracil, and/or pyridoxine for the set of plasmids introduced. The CD-ST solid

plate (5mL in diameter 3cm Petri dish) was inoculated with spores and incubated at 28 °C for 3 days. For small-scale the fermentation system was collected and extracted with Ethyl Acetate for 30 min with sonication. After centrifugation, the supernatant (200 μL) was dried down by Speedvac and then resuspended in methanol (100 μL). For feeding assays analysis of yeast expressing the *pnltC* was inoculated in 3 mL of dropout media for 2 days. 500 μL of starter culture was used to inoculate 25 mL of YPD. For the feeding experiments in A1145, we employed two equivalent experimental methods: one is liquid feeding, and the other is solid plate feeding. The description is as follows: for liquid feeding assays analysis,100 μL spores of A1145 expressing the *pnltC* were used to inoculate 25 mL of CD-ST. The cells were grown at 28 °C, 250 rpm for 2-3 days for protein expression. Briefly, the cells were harvested by centrifugation (4000 rpm at 4 °C for 10 min) and the cell pellet was washed and resuspended with 3 mL of culture medium for substrates adding. For solid plate feeding assays analysis, adding substrates to 25 mL CD-ST solid plate individually, then inoculating with spores of A1145 expressing the *pnltC* at 28 °C for 3 days. The above feeding system was collected and extracted with Ethyl Acetate for 30 min with sonication. After centrifugation, the supernatant (200 μL) was dried down by Speedvac and then resuspended in methanol (100 μL).

For large-scale compound purification:

Compound 1: The *Aspergillus nidulans* A1145 expression host co-transformed with plasmids PYTU-*pnltB*, PYTR-*pnltC* and PYTP-*pnltA* was selected on CD sorbitol agar. The harvested spores were used to inoculate CD-ST broth. The cultures were inoculated in 50 150 mm Petri dishes containing 5 L CD-ST media at 28 °C with aeration for 4 days. All system was extracted with ethyl acetate (3 ×). Using water/methanol as solvent system, the residue after solvent evaporation in vacuum was separated by reverse column chromatography (ODS-C18). Fractions determined by LC-MS to contain **1** were pooled and after solvent evaporation, the residue was further separated by Dextran gel column chromatography and then semi-preparative RP HPLC using an ODS column (YMC-Pack ODS-A, 10 mm × 250 mm, 5 μm, 3 mL/min, YMC Co., Ltd.), flow rate of 3 mL/min of solvents A (0.1% formic acid in water) and B (acetonitrile), with an isocratic concentration of 50% acetonitrile (MeCN)-50% water, to afford 6 mg **1** (t_R 27 min).

Compound 2: The *Aspergillus nidulans* A1145 expression host co-transformed with plasmids PYTP-*pnltA* and PYTU-*pnltB* was selected on CD sorbitol agar. The harvested spores were used to inoculate CD-ST broth. The cultures were inoculated in 50 150 mm Petri dishes containing 5 L CD-ST media at 28 °C with aeration for 4 days. All system was extracted with ethyl acetate (3 ×). Using water/methanol as solvent system, the residue after solvent evaporation in vacuum was separated by reverse column chromatography (ODS-C18). Fractions determined by LC-MS to contain **2** were pooled and after solvent evaporation, the residue was further separated by Dextran gel column chromatography and then semi-preparative RP HPLC using an ODS column (YMC-Pack ODS-A, 10 mm × 250 mm, 5 μm, 3 mL/min, YMC Co., Ltd.), flow rate of 3 mL/min of solvents A (0.1% formic acid in water) and B (acetonitrile), with an isocratic concentration of 35% acetonitrile (MeCN)-65% water, to afford 15 mg **2** (t_R 26 min).

In vitro assays with microsomals of *S. cerevisiae* and *Aspergillus nidulans*.

To verify the function of enzyme of PnltC in vitro assays, *S. cerevisiae* RC01, *Aspergillus nidulans* A1145 strains transformed with individual plasmids were used in vitro assays. For the *S. cerevisiae* RC01, the transformant yeast strain was selected on solid selective drop-out media for 2-3 days, then single colonies were inoculated into 3 mL selective drop-out media and grown for 24 h to be used as inoculums for YPD media. 500 μL of starter culture was used to inoculate 25 mL of YPD. For the *Aspergillus nidulans* A1145, spores of A1145 expressing the *pnltC* was used to inoculate 25 mL of CD-ST. The cells were grown at 28 °C, 250 rpm for 2-3 days for protein expression. Briefly, the cells were harvested by centrifugation (4000 rpm at 4 °C for 10 min) and the cell pellet was washed with 100 mL of TES buffer (50 mM Tris-HCl, pH 7.5, 1 mM EDTA, 0.6 M sorbitol). The cells were centrifuged as above, resuspended in 100 mL of TES-M (TES supplemented with 10 mM 2-mercaptoethanol), and allowed to incubate at room temperature for 10 min. The yeast cells

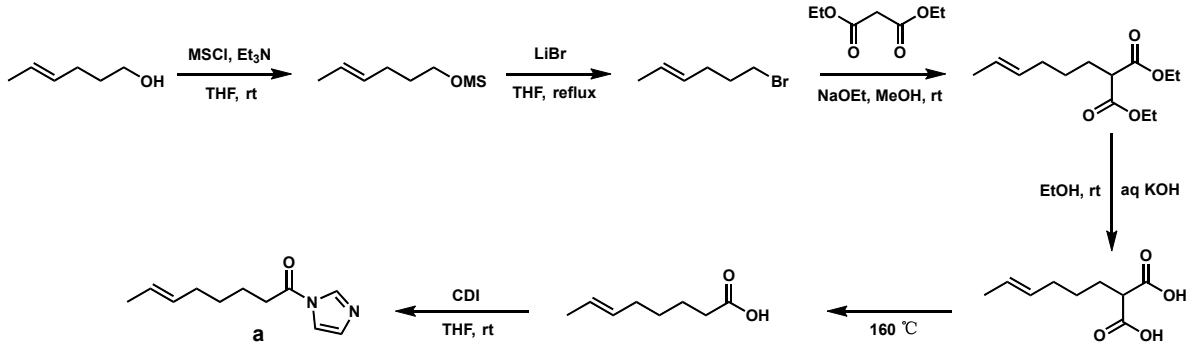
were centrifuged again at 4000 rpm for 10 min, and the pellet was resuspended in 2.5 mL of extraction buffer (1% bovine serum albumin, fraction V, 2 mM 2-mercaptoethanol, 1 mM phenylmethylsulfonyl fluoride, all dissolved in TES). Zirconia/silica beads (0.5 mm in diameter, Biospec Products) were added until skimming the surface of the cell suspension. Cell walls were disrupted manually by hand shaking in a cold room for 10 min at 30 s intervals separated by 30 s intervals on ice. Cell extracts were transferred to a 50 mL centrifuge tube, the Zirconia/silica beads were washed three times with 5 mL of extraction buffer, and the washes were pooled with the original cell extracts. Finally, microsomes were obtained by differential centrifugation at 10000g for 10 min at 4 °C to remove cellular debris followed by centrifugation at 100,000g for 30 min at 4 °C. The microsomes or crude enzymes were then extracted and co-incubated with substrates. The products of different reaction systems were analyzed and detected by LC-MS to judge the reaction situation.

In vitro assay of PnltC in *S. cerevisiae* and *Aspergillus nidulans*: The 100 μL PnltC microsomal fractions containing 0.2 mM compound **2** and 2 mM NADPH were incubated overnight at 28 ℃ and extracted twice with 200 μL ethyl acetate. The organic phase was dried and dissolved in 50 μL MeOH for LC-MS analysis.

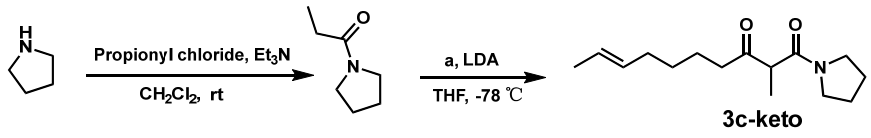
In vitro assay of PnltA-A in *Aspergillus nidulans*: The 100 μL PnltA-A crude enzyme fractions containing 10 mM *D*/*L* proline, 10 mM Mg^{2+} and overdose ATP were incubated overnight at 28 ℃ and added an equal amount of the control before quenched with 200 μL acetonitrile. Then samples were detected by LC-MS after filtering the membrane. The LC-MS method for detection: Solvent: A, MeCN; Solvent B, H_2O (0.1% formic acid). The elution gradient was 0-15 min 5-70% A, 15-16 min 70-5% A, 16-20 min 5% A. The flow rate was 0.5 mL/min.

Synthesis of compound 3 and 3c-keto.

The synthesis of the common intermediate **a**: the chemical synthesis of the key intermediate **a** was carried out according to the experimental procedures described in the literature, with the specific steps following those outlined in the reference[1,2].



Synthesis of compound **3**:

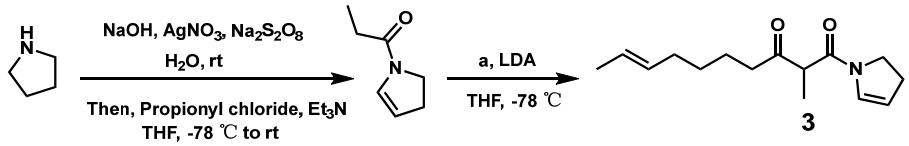


Sodium persulfate (0.15 mol, 1.0 eq.) was dissolved in water (125 mL), and slowly add it to a reaction solution containing sodium hydroxide (0.3 mol, 2.0 eq.), silver nitrate (0.0015 mol, 0.01 eq.), tetrahydropyrrole (0.15 mol, 1.0 eq.), and water (125 mL). After stirring the reaction mixture overnight, extract with dichloromethane (3 × 200 mL). Combine the organic phase, dry with anhydrous $MgSO_4$, and concentrate to obtain the intermediate with a yield of 60%. Dissolve the intermediate in THF and, under nitrogen protection, distill it into a pre-cooled flask at -78°C. Add triethylamine (0.15 mol, 1.0 eq.), stir well, then slowly add propionyl chloride (0.15 mol, 1.0 eq.). After raising the temperature to room temperature, filter off the white precipitate of triethylamine hydrochloride, and concentrate the filtrate. Separate by column chromatography (PE: EtOAC = 5:1) to obtain the intermediate with a yield of 65%.

Dissolve the intermediate (0.487 mmol, 1.2 eq.) in THF (2 mL), add it to the solution of LDA (0.527 mmol, 1.3 eq.) at -

78°C, and stir for 1 h. Then add compound **a** (0.406 mmol, 1.0 eq.) in THF (2 mL) to the reaction mixture, stir at -78°C for 4 h, and continue stirring at room temperature for 12 h. Quench the reaction with a saturated NH_4Cl solution, and extract with diethyl ether (3 × 10 mL). Wash the combined organic phase with saturated NaCl, dry over anhydrous $MgSO_4$, under vacuum, filter, and then concentrate. Separate by column chromatography (PE: EtOAC = 10:1) to obtain compound **3** as a light yellow oily substance with a yield of 20%.

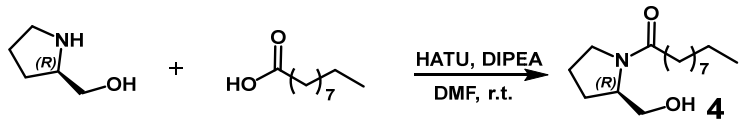
Synthesis of compound **3c-keto**:



Pyrrolidine (2.8 mmol, 1.0 eq.) and triethylamine (5.62 mmol, 2.0 eq.) were dissolved in CH_2Cl_2 (28 mL). Under an ice bath, propionyl chloride (3.37 mmol, 1.2 eq.) was slowly added. After the addition, the mixture was allowed to return to room temperature and stirred for 8 h. Water was added to quench the reaction, and the mixture was transferred to a separatory funnel. The mixture was extracted with CH_2Cl_2 (3 × 10 mL). The organic phase was combined, washed with saturated NaCl solution, and then dried with anhydrous Na_2SO_4. After filtration and concentration, the intermediate was obtained with a yield of 90%.

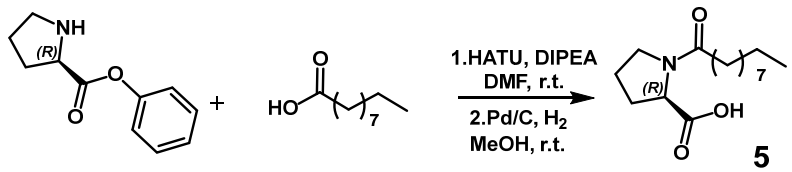
The intermediate (0.474 mmol, 1.2 eq.) was dissolved in THF (2 mL) and added dropwise at -78°C to a solution of LDA (0.514 mmol, 1.3 eq.) with stirring for 1 h. Then add compound **a** (0.514 mmol, 1.0 eq.) in THF (2 mL) was added. The reaction mixture was stirred at -78°C for 4 h, then allowed to stir at room temperature for 12 h. Saturated NaCl solution was added to quench the reaction, followed by extraction with ethyl acetate (3 × 10 mL). The combined organic phase was dried over anhydrous $MgSO_4$, filtered under vacuum, and concentrated. Column chromatography separation (PE: EtOAC = 9:1) yielded compound **3c-keto**, a colorless oily substance, with a yield of 45%.

Synthesis of compound 4.



D-Prolinol (1.2 mmol, 1.2 eq.), neo-Decanoic acid (1 mmol, 1.0 eq.), HATU (1.2 mmol, 1.2 eq.) and DIPEA (155 mg, 1.2 mmol, 1.2 eq.) were dissolved in DMF (10 mL). The reaction mixture was stirred for 3 h in room temperature. The solvent was quenched by water, and extracted three times with ethyl acetate, the combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvents under reduced pressure, the residue was purified by silica gel column chromatography with PE: EtOAC = 2:1) as eluent to afford the final product **4** (60% yield).

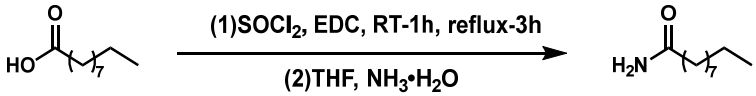
Synthesis of compound 5.



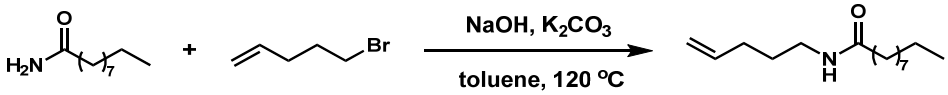
N-Benzyloxycarbonyl-*D*-proline (1.2 mmol, 1.2 eq.), neo-Decanoic acid (1 mmol, 1.0 eq.), HATU (1.2 mmol, 1.2 eq.) and DIPEA (1.2 mmol, 1.2 eq.) were dissolved in DMF (10 mL). The reaction mixture was stirred for 3 h in room temperature. The solvent was quenched by water, and extracted three times with ethyl acetate, the combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvents under reduced pressure, the residue was purified by silica gel column

chromatography with PE: EtOAC = 4:1) as eluent to afford a pale-yellow oil intermediate, then the Pd/C (0.1 mmol, 0.1 eq.) reduces the intermediate in a methanol solvent (10 mL) in the presence of hydrogen. The reaction mixture was stirred for 6 h in room temperature. The solvent was then fitered by diatomite to afford final product **5** (50% yield for two steps).

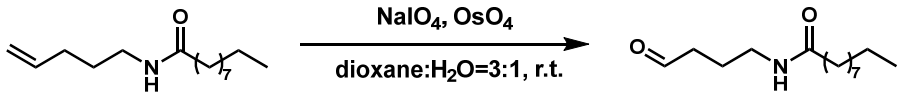
Synthesis of compound 7.



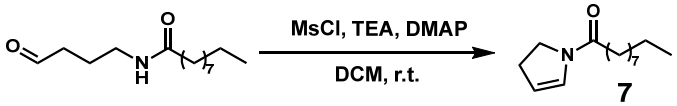
To a solution of decanoic acid (8 mmol, 1.0 eq.) in ethylene dichloride in room temperature, thionyl chloride (24 mmol, 3.0 eq.) was added slowly and the reaction mixture was stirred for 1 h in room temperature and then refluxed for 3 h. Excess thionyl chloride was distilled off. Without further purification the crude product was taken to next step. To a cold (5 ºC) aq. ammonia solution, the prepared acid chloride in THF was added dropwise and stirred vigorously for 3 h in room temperature. The obtained solid is filtered, washed with water and dried. The crude reaction mixture was purified by silica gel column chromatography with PE: EtOAC = 1:1) to afford decanamide (66% yield).



5-Bromo-1-pentene (533 uL, 4.5 mmol,1.5 eq.) was added to a solution of decanamide (3 mmol, 1.0 eq.), crushed NaOH (10.5 mmol, 3.5 eq.), potassium carbonate (6 mmol, 2.0 eq.), and tetrabutylammonium hydrogen sulfate (.3 mmol, 0.1 eq.) in toluene (8 mL), and the reaction was stirred for 1.5 h at 120 ºC. The reaction was cooled to r.t, diluted with CH_2Cl_2, and washed with H_2O. The organic layer was dried over $NaHSO_4$, filtered, and concentrated in vacuo. Purification of the residue by silica gel column chromatography using PE: EtOAC = 5:1 as eluent afforded N-(pent-4-en-1-yl)decanamide (54% yield).

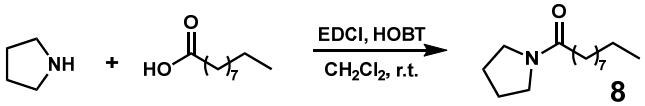


To a solution of N-(pent-4-en-1-yl)decanamide (1.5 mmol, 1.0 eq.) in the mixture of dioxane and H_2O (3:1, v/v; 12 mL), OsO_4 solution in 2,6-lutidine (3.0 mmol, 2.0 eq.) was added at 25 ºC. Then $NaIO_4$ (6 mmol, 4.0 eq.) was added and the resultant mixture was allowed to stir at 25 ºC for 3 h until the material N-(pent-4-en-1-yl)decanamide disappeared monitored by TLC. After completion of the reaction, the saturated aqueous solution of $Na_2S_2O_3$ was added to quench the reaction and the mixture was extracted with EtOAC. The organic layer was dried over $NaHSO_4$, filtered and concentrated under reduced pressure. The crude reaction mixture was purified by silica gel column chromatography with PE: EtOAC = 3:1 to afford N-(4-oxobutyl)decanamide (87% yield).



N-(4-oxobutyl)decanamide (1.0 mmol, 1.0 eq.), TEA (5 mmol, 5.0 eq.) and DMAP (0.2 mmol, 0.2 eq.) were dissolved in DCM (4 mL). Then MsCl (2.5 mmol, 2.5 eq.) was added at 0 ºC and the resultant mixture was allowed to stir at 25 ºC for 5 h. After removing the solvents under reduced pressure, the crude reaction mixture was purified by silica gel column chromatography with PE: EtOAC = 5:1 to afford the final product **7** (30% yield).

Synthesis of compound 8.



Pyrrolidine (1.2 mmol, 1.2 eq.), neo-Decanoic acid (1 mmol, 1.0 eq.), EDCI (1.2 mmol, 1.2 eq.) and HOBT (1.2 mmol, 1.2 eq.) were dissolved in CH_2Cl_2 (10 mL). The reaction mixture was stirred for 3 h in room temperature. The solvent was quenched by water, and extracted three times with CH_2Cl_2, the combined organic phase was dried over anhydrous Na_2SO_4. After removing the solvents under reduced pressure, the residue was purified by silica gel column chromatography with PE: EtOAC = 3:1 as eluent to afford the final product **8** (68% yield).

In situ reduction of imine cation by STAB.

In situ reduction of imine cation by STAB: In situ reduction of iminium cation experiments by STAB, we employed two equivalent experimental methods: one is liquid system followed by reduction capture of the crude extract, and the other is solid plate system followed by direct quenching of the mycelium for reduction capture. The description is as follows:

For liquid system, The fermentation products of *AN-pnltABC* (100 μL spores of *AN-pnltABC* was used to inoculate 25 mL of CD-ST), the feeding products of compound **3**、**4**、**5** to *AN-pnltC* (100 μL spores of *AN-pnltC* were used to inoculate 25 mL of CD-ST) and 2 mM STAB were dissolved in MeOH (7 mL) individually. The reaction mixture was stirred for 25 min in room temperature. The solvent was then quenched by water, then extracted three times with ethyl acetate. The organic phase was dried and dissolved in 200 μL MeOH for LC-MS analysis. For solid plate system, the fermentation of *AN-pnltABC* (5mL in diameter 3cm Petri dish) was inoculating at 28 °C for 3 days, adding compound **3**、**4**、**5** to 25 mL CD-ST solid plate (5mL in diameter 3cm Petri dish) individually, then inoculating with spores of A1145 expressing the *pnltC* at 28 °C for 3 days. The fungal mycelium after solid plate fermentation was dissolved in MeOH (7 mL) containing 2 mM STAB individually. The reaction mixture was stirred for 25 min in room temperature. The solvent was then quenched by water, then extracted three times with ethyl acetate. The organic phase was dried and dissolved in 200 μL MeOH for LC-MS analysis.

In situ reduction of compound 3 by STAB: Compound **3** (0.02 mmol, 1 eq.) and STAB (0.06 mmol, 3 eq.) were dissolved in MeOH (2 mL), The reaction mixture reacted for 25 min in room temperature. The solvent was then quenched by water, then extracted three times with ethyl acetate. The organic phase was dried and dissolved in 200 μL MeOH for LC-MS analysis.

Calculation tools.

AlphaFold2-based local ColabFold v1.5.5 was deployed in activated virtual environment for protein structure prediction combining with MMseqs2. FoldX 5.0 was used to compute the virtual saturation mutagenesis. Autodock vina 1.2.5 was used to subject docking projects. DiscoveryStudio45 and Autodock tool were used to preprocess protein structures. DiscoveryStudio 45, LigPlot 2.2.8 and Pymol were used for visual results of dockings. Chem3D was used to pre-optimization of compounds structures. Spartan 14 was used to pre-minimization of compounds energies. GaussView 5.0.9 was used to set calculation parameters and visualize calculated results. Gaussian 09 and 16 was used to calculate. All the HEME-binding structures were calculated using the Gaussian 16 program package.[3] The geometry of all reactants and transition states were optimized using B3LYP hybrid functional[4,5] in combination with Grimme's dispersion correction (D3)[6] and Becke−Johnson damping factor (BJ)[7] and def2SVP basis set[8,9]. Harmonic vibrational frequency analysis was calculated at the same level to verify that reactants, intermediates, and products have positive frequencies, while transition states have and have only one imaginary frequency.

Table S1. Deduced gene functions in *pnlt* BGC

ORF	Amino acids	Blastp homologue	Identity/coverage [%]
pnltA	3980	Polyketide synthase-nonribosomal peptide synthetase ffsA	39.87/99
pnltB	633	Trans-enoyl reductase calK	38.89/53
pnltC	439	Cytochrome P450 monooxygenase TwmD	34.11/95
pnltD	348	Fusaric acid cluster transcription factor FUB10	98/100

Table S2. Primers used in this study

Primer	Sequence of primer (5'-3')
PANP-PnltA-F	CCCTTCTCTGAACAATAAACCCCACAGAAGGCATTTATGCATACTTCACCTGAACCAG
PANP-PnltA-R	GATGAGACCCAACAACCATGATACCAGGGGATTTAAATGAATGTGCAAGAATAGGGCTG
PANU-PnltB-F	GAGCCTGAGCTTCATCCCCAGCATCATTACACCTCAGCAATGATTCTCCCAAAGGAACG
PANU-PnltB-R	GAGGACATACCCGTAATTTTCTGGGCATTTAAATGAGCTTAACATGCATGAATGCAAAC
PANR-PnltC-F	GACTAACCATTACCCCGCCACATAGACACATCTAAACAATGGCTAACCTAACTATGGCC
PANR-PnltC-R	GGGTATCATCGAAAGGGAGTCATCCAATTTAAATCATGCCAAGCTATCTATGTGCATG
PANP-PnltA-A-F	CTGAACAATAAACCCCACAGAAGGCATTTCATCATCATCATCATCATATCGA
PANP-PnltA-A-R	CAACCATGATACCAGGGGATTTAAATCGAAAGGGGAAGCGAAGC
PANR-PnltC^{Y305A}-F	GGACTCAGTCGCTTTAGTCC
PANR-PnltC^{Y305A}-R	GGACTAAAGCGACTGAGTCCGGCCGGAACATTTGTGTGTAAG
PANR-PnltC^{N302A}-F	GTTCCGTATGGACTCAGTCGC
PANR-PnltC^{N302A}-R	GCGACTGAGTCCATACGGAACGGCTGTGTGTAAGCGTAGTG
PANR-PnltC^{F238A}-F	GCAGATCATTATGAATCCTCGAG
PANR-PnltC^{F238A}-R	CTCGAGGATTCATAATGATCTGCTACCAAATGGGATGCTTG
PANR-PnltC^{F238Y}-F	TATGATCATTATGAATCCTCGAG
PANR-PnltC^{F238Y}-R	CTCGAGGATTCATAATGATCATATACCAAATGGGATGCTTG
PANR-PnltC^{F238W}-F	TGGGATCATTATGAATCCTCGAG
PANR-PnltC^{F238W}-R	CTCGAGGATTCATAATGATCCCATACCAAATGGGATGCTTG
PANR-PnltC^{H235A}-F	GCATTGGTATTTGATCATTATGAATCC
PANR-PnltC^{H235A}-R	GATTCATAATGATCAAATACCAATGCGGATG
PANR-PnltC^{E242A}-F	GCATCCTCGAGTCCAATGACAG
PANR-PnltC^{E242A}-R	CTGTCATTGGACTCGAGGATGCATAATG
PANR-PnltC^{D239A}-F	GCACATTATGAATCCTCGAGTCC
PANR-PnltC^{D239A}-R	GGACTCGAGGATTCATAATGTGCAAATACCAAATGG
PANR-PnltC^{K50A}-F	TCTCATATGCTGGATACAGGTGATAAG
PANR-PnltC^{K50A}-R	CACCTGTATCCAGCATATGAGACGCGATGAAGGCGGGCTTTCGATC
PANR-PnltC^{S51A}-F	CATATGCTGGATACAGGTGATAAGCAC
PANR-PnltC^{S51A}-R	GCTTATCACCTGTATCCAGCATATGTGCCTTGATGAAGGCGGGCTTTC
PANR-PnltC^{H52A}-F	CAATGCTGGATACAGGTGATAAGCAC

PANR-PnltC^{H52A}-R	CGTGCTTATCACCTGTATCCAGCATTGCAGACTTGATGAAGGCG
PANR-PnltC^{M53A}-F	CTGGATACAGGTGATAAGCACGAG
PANR-PnltC^{M53A}-R	CCTCGTGCTTATCACCTGTATCCAGTGCATGAGACTTGATGAAGGCG
PANR-PnltC^{D55A}-F	GCAACAGGTGATAAGCACGAGG
PANR-PnltC^{D55A}-R	GTCCCTCGTGCTTATCACCTGTTGCCAGCATATGAGACTTGATGAAGGC
PANR-PnltC^{T56A}-F	GGTGATAAGCACGAGGGACTTC
PANR-PnltC^{T56A}-R	GGAAGTCCCTCGTGCTTATCACCTGCATCCAGCATATGAGACTTGATG
PANR-PnltC^{L63A}-F	CACCCTCAGAGCGAGACCTAG
PANR-PnltC^{L63A}-R	CATCTAGGTCTCGCTCTGAGGGTGCTCCCTCGTGCTTATCACCTG
PANR-PnltC^{P64A}-F	CATCAGAGCGAGACCTAGATGTG
PANR-PnltC^{P64A}-R	GCACATCTAGGTCTCGCTCTGATGCAAGTCCCTCGTGCTTATCACC
PANR-PnltC^{S65A}-F	GAGCGAGACCTAGATGTGCAC
PANR-PnltC^{S65A}-R	CACGGTGCACATCTAGGTCTCGCTCTGCGGGAAGTCCCTCGTGCTTATC
PANR-PnltC^{L150A}-F	CTTAAGGCTATACAGGTGGTAGGC
PANR-PnltC^{L150A}-R	GCCTACCACCTGTATAGCCTTAAGAGCAGGTTGGGCTTGGCCAC
PANR-PnltC^{V157A}-F	GGCAAATGGCTAACAGTAAAACACTG
PANR-PnltC^{V157A}-R	CAGTGTTTTACTGTTAGCCATTTGCCAGCCACCTGTATAGCCTTAAGTAAAGG
PANR-PnltC^{G158A}-F	CTAAATGGCTAACAGTAAAACACTGCC
PANR-PnltC^{G158A}-R	GCAGTGTTTTACTGTTAGCCATTTAGCTACCACCTGTATAGCCTTAAG
PANR-PnltC^{T162A}-F	GTAAAACACTGCCTTCAGCG
PANR-PnltC^{T162A}-R	CGCTGAAGGCAGTGTTTTACAGCTAGCCATTTGCCTACCACCTG
PANR-PnltC^{K164A}-F	CACTGCCTTCAGCGTTTTCC
PANR-PnltC^{K164A}-R	CAGAGGAAAACGCTGAAGGCAGTGAGCTACTGTTAGCCATTTGCCTACCAC
PANR-PnltC^{H165A}-F	TGCCTTCAGCGTTTTCCTCTG
PANR-PnltC^{H165A}-R	CAGAGGAAAACGCTGAAGGCAAGCTTTTACTGTTAGCCATTTGCCTACC
PANR-PnltC^{S231A}-F	CAAGCATCCCATTTGGTATTTGATC
PANR-PnltC^{S231A}-R	GATCAAATACCAAATGGGATGCTTGAGCGACCAGGAAATCCACAGGTCG
PANR-PnltC^{S234A}-F	GCACATTTGGTATTTGATCATTATGAATCCTC
PANR-PnltC^{S234A}-R	CTCGAGGATTCATAATGATCAAATACCAAATGTGCTGCTTGAGAGACCAGGAAATC
PANR-PnltC^{S245A}-F	CCAATGACAGCTGCTGTTTG
PANR-PnltC^{S245A}-R	GAAACAAACAGCAGCTGTCATTGGAGCCGAGGATTCATAATGATCAAATACC
PANR-PnltC^{V303A}-F	CCGTATGGACTCAGTCGCTTTAG
PANR-PnltC^{V303A}-R	GACTAAAGCGACTGAGTCCATACGGGGCATTTGTGTGTAAGCGTAGTG
PANR-PnltC^{L307A}-F	GCCAGTCGCTTTAGTCCAGG
PANR-PnltC^{L307A}-R	CCCTGGACTAAAGCGACTGGCTCCATACGGAACATTTGTGTG
PANR-PnltC^{S308A}-F	CGCTTTAGTCCAGGGGC
PANR-PnltC^{S308A}-R	CTACCGTGGCCCCTGGACTAAAGCGAGCGAGTCCATACGGAACATTTGTG
PANR-PnltC^{R309A}-F	GCTTTTAGTCCAGGGGCCAC
PANR-PnltC^{R309A}-R	CTACCGTGGCCCCTGGACTAAAAGCACTGAGTCCATACGGAACATTTGTG
PANR-PnltC^{L420A}-F	TGGGCTGTTTGGGACAAGC
PANR-PnltC^{L420A}-R	CAAGGCTTGTCCCAAACAGCCCACGCGCGAAGATCCCGATCCCAG

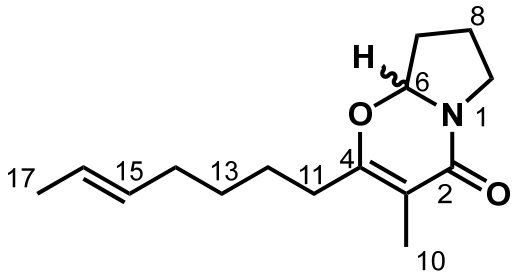
PANR-PnltC^{V423A}-F	TGGGACAAGCCTTGCGTG
PANR-PnltC^{V423A}-R	GTACTTTCACGCAAGGCTTGTCCCACGCAGCCCAGAGGCGAAGATC
PANR-PnltC^{W424A}-F	GACAAGCCTTGCGTGAAAGTACG
PANR-PnltC^{W424A}-R	CGTACTTTCACGCAAGGCTTGTCCGCAACAGCCCAGAGGCGAAG
PYET-PnltC-F	CTATATCGTAATACCATCATCATATGATGGCTAACCTAACTATGGCCG
PYET-PnltC-R	GGAAACTATAAATCGTGAAGGCATGTTTAAACTCAGATTTCCTTCGCAAGAGTG
pET28(a)-PnltA-A-F	CGGCCTGGTGCCGCGCGGCAGCCATATGAAATCAGAATGGCCGCAAACC
pET28(a)-PnltA-A-R	CTCAGTGGTGGTGGTGGTGCTCGAGCGAAAGGGGAAGCGAAGC

Table S3. *S*trains used in this study

Strain	Description
Yeast+PnltC	*S. cerevisiae* RC01+ *pnltC*
A1145+PnltC	*A. nidulans* A1145 + *pnltC*
A1145+PnltABC	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{Y305A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{N302A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{F238A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{F238Y}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{F238W}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{H235A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{E242A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{D239A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{K50A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S51A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{H52A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{M53A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{D55A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{T56A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{L63A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{P64A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S65A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{L150A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{V157A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{G158A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{T162A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{K164A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{H165A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S231A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S234A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S245A}	*A. nidulans* A1145 + *pnltABC*

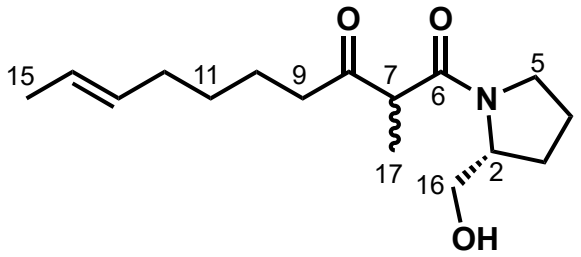
A1145+ PnltABC^{V303A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{L307A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{S308A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{R309A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{L420A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{V423A}	*A. nidulans* A1145 + *pnltABC*
A1145+ PnltABC^{W424A}	*A. nidulans* A1145 + *pnltABC*
A1145+PnltA-A	*A. nidulans* A1145 + PnltA-A
DE3+PnltA-A	*Escherichia coli* + PnltA-A

Table S4. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR Spectroscopic Data of compound **1** in $CDCl_3$. (TMS, δppm).



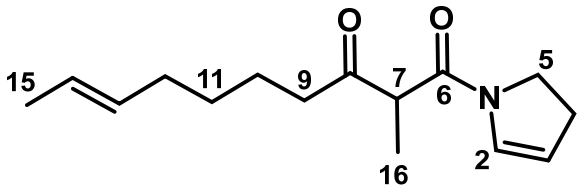
NO.	δ_C	δ_H (*J* in Hz)
1(N)	-	-
2	164.52	-
3	106.4	-
4	164.08	-
5(O)	-	-
6	87.68	5.21 dd (6.0, 4.6)
7	32.39	2.32 m, 2.14 m
8	22.06	2.01 m, 1.87 m
9	44.64	3.74 m, 3.44 m
10	10.2	1.80 s
11	30.62	2.28 m, 2.20 m
12	26.41	1.52 p (7.5)
13	29.29	1.37 dt (15.0, 7.2)
14	31.79	1.98 m
15	131.03	5.41, m
16	125.35	5.41, m
17	18.06	1.64 d (4.9)

Table S5. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **2** in $CDCl_3$. (TMS, δppm).



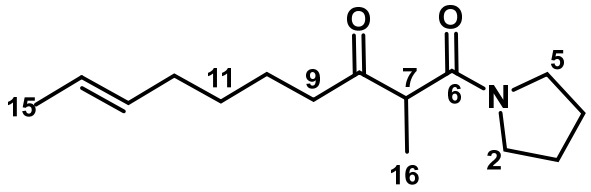
NO.	2a		2b	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1(N)	-	-	-	-
2	61.17	4.17 m	61.34	4.17 m
3	28.10	2.00 m, 1.64 m	28.19	2.00 m, 1.64 m
4	24.44	1.90 m, 1.82 m	24.33	1.90 m, 1.82 m
5	48.30	3.51 m, 3.38 m	48.20	3.51 m, 3.38 m
6	171.05	-	171.50	-
7	53.19	3.51 m	53.17	3.51 m
8	207.13	-	207.16	-
9	39.68	2.44 m	39.43	2.44 m
10	23.02	1.50 m	23.00	1.50 m
11	28.94	1.26 m	28.94	1.26 m
12	32.28	1.90 m	32.28	1.90 m
13	130.87	5.33 m	130.87	5.33 m
14	125.16	5.35 m	125.16	5.35 m
15-Me	17.90	1.57 d (4.6)	17.90	1.57 d (4.6)
16	66.09	3.68 dd (11.4, 3.3)	66.61	3.60 dd (11.4, 3.3)
17-Me	13.00	1.32 dd (12.9, 7.0)	13.71	1.32 dd (12.9, 7.0)

Table S6. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR Spectroscopic Data of compound **3** in $CDCl_3$. (TMS, δppm).



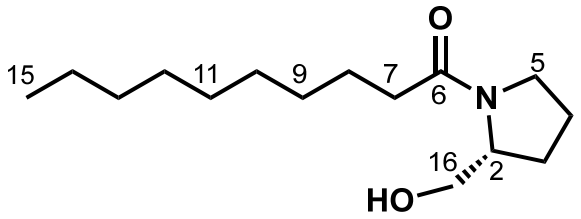
NO.	δ_C	δ_H (J in Hz)
1 (N)	-	-
2	129.45, 128.43	6.94, m, 6.53, m
3	113.19, 111.75	5.27, m
4	32.38	2.46, m
5	45.59	3.85, m
6	165.75	-
7	53.30	3.56, q, (7.1), 3.46, q (7.0)
8	207.17	-
9	39.28	2.76,m, 2.63, m
10	29.00	1.54, m
11	28.23	1.28, m
12	23.11	1.96, m
13	131.03	5.37, m
14	125.21	5.37, m
15	18.03	1.61, m
16	13.27	1.37, dd (7.1, 4.8)

T**able S7.** ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **3c-keto** in $CDCl_3$. (TMS, *δ*ppm).



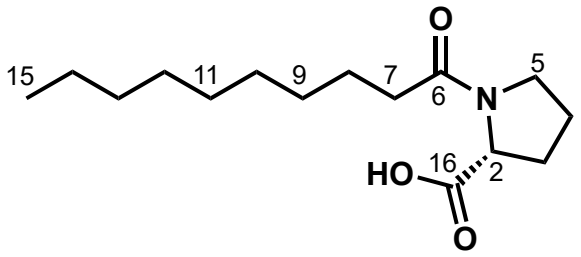
NO.	δ_C	δ_H (*J* in Hz)
1 (N)	-	-
2	46.29	3.47, m
3	29.09	1.94, m
4	32.43	1.96, m
5	47.01	3.50, m
6	168.75	-
7	53.48	3.43, m
8	207.68	-
9	39.36	2.47, m
10	26.25	1.54, m
11	24.41	1.30, m
12	23.17	1.87, q (6.3)
13	131.1	5.38, m
14	125.21	5.38, m
15	18.02	1.62, m
16	13.51	1.35, d (7.0)

T**able S8.** ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **4** in $CDCl_3$. (TMS, δppm).



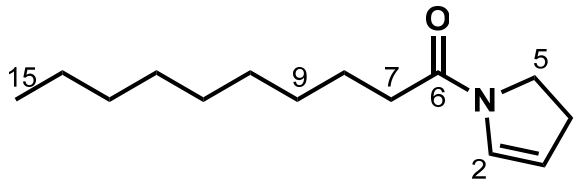
NO.	δ_C	δ_H (J in Hz)
1 (N)	-	-
2	61.06	4.16 m
3	28.27	1.97 m, 1.57 m
4	24.39	1.89 m, 1.81 m
5	48.14	3.48 m, 3.42 m
6	174.68	-
7	35.11	2.24 t (7.7)
8	24.80	1.57 m
9	29.45	1.24 m
10	29.28	1.24 m
11	29.45	1.24 m
12	29.39	1.24 m
13	31.87	1.24 m
14	22.66	1.24 m
15	14.12	0.82 t (6.6)
16	67.35	3.59 dd (11.3, 3.0), 3.52 m

Table S9. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **5** in $CDCl_3$. (TMS, δppm).



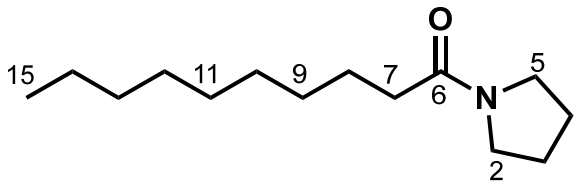
NO.	δ_C	δ_H (*J* in Hz)
1 (N)	-	-
2	59.33	4.50 dd (8.0, 3.3)
3	28.34	2.17 m, 2.06 m
4	24.67	2.06 m, 1.96 m
5	47.56	3.57 m, 3.44 m
6	174.11	-
7	34.46	2.29 m
8	24.59	1.58 m
9	29.44	1.23 m
10	29.27	1.23 m
11	29.39	1.23 m
12	29.31	1.23 m
13	31.85	1.23 m
14	22.65	1.23 m
15	14.10	0.82 t (6.7)
16	174.30	-

Table S10. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **7** in $CDCl_3$. (TMS, δppm).



NO.	δ_C	δ_H (*J* in Hz)
1 (N)	-	-
2	129.50, 129.09	6.95, dt (4.5, 2.3), 6.48, dt (4.4, 2.3)
3	111.45, 110.11	5.20, m
4	29.38	1.64, m
5	44.94	3.82, m
6	169.30	-
7	34.45	2.33, t (7.7), 2.24, t (7.6)
8	25.17	1.64, m
9	28.34	1.26, m
10	29.55	1.26, m
11	29.55	1.26, m
12	29.50	1.26, m
13	31.97	1.26, m
14	22.76	1.26, m
15	14.21	0.87, t (6.8)

Table S11. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data of compound **8** in $CDCl_3$. (TMS, δppm).



NO.	δ_C	δ_H (*J* in Hz)
1 (N)	-	-
2	46.47	3.32, m
3	26.00	1.83, p (6.7)
4	24.28	1.73, p (6.7)
5	45.41	3.32, m
6	171.69	-
7	34.70	2.13, t (7.7)
8	24.82	1.52, p (7.4)
9	29.40	1.17, m
10	29.16	1.17, m
11	29.35	1.17, m
12	29.35	1.17, m
13	31.74	1.17, m
14	22.52	1.17, m
15	13.95	0.76, t (6.7)

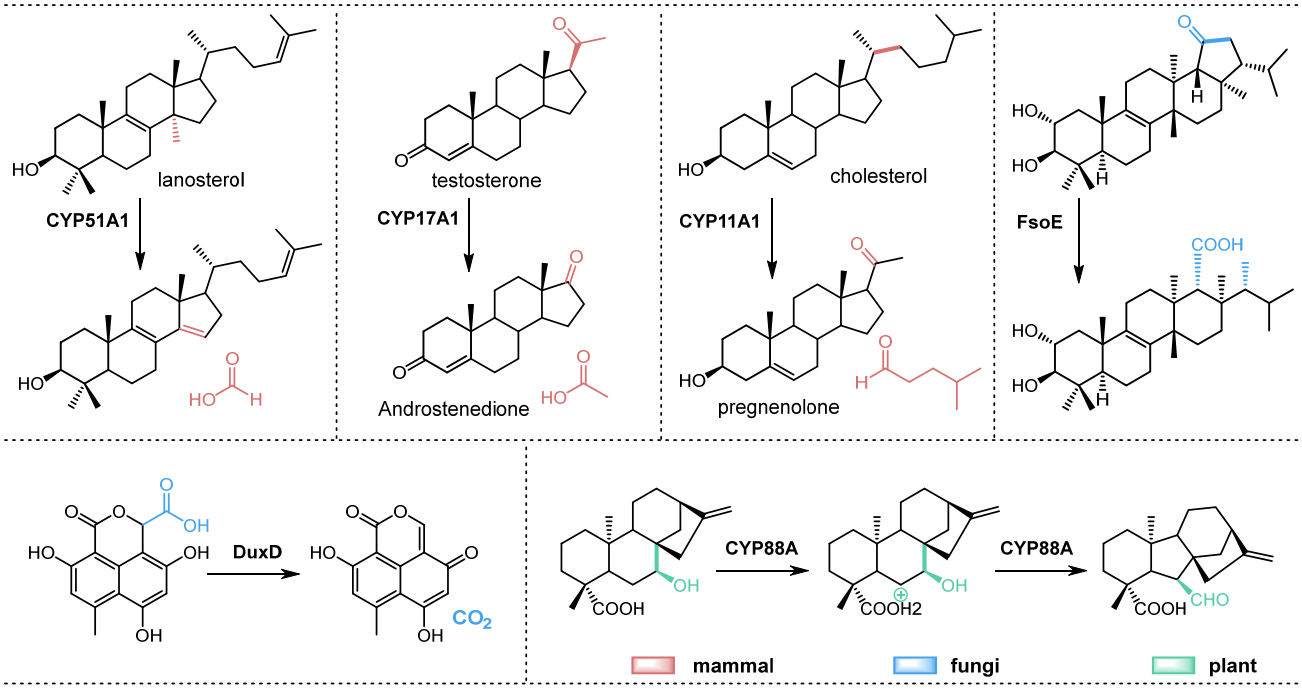


Fig. S1. C–C bond cleavage catalyzed by P450s.

Including but not all C–C bond cleavage mechanisms catalyzed by cytochrome P450 enzymes, highlighting the diversity of radical-mediated pathways in natural product biosynthesis. CYP51A1 catalyzes the oxidative removal of the methyl group in lanosterol as formic acid and generates a C=C bond in situ; CYP17A1 catalyzes the removal of the acetyl group in testosterone as acetic acid and forms a carbonyl group in situ; CYP11A1 catalyzes the cleavage of the non-oxidized C−C bond in cholesterol into two aldehydes; FsoE directly catalyzes the cleavage of the carbonylated C−C bond into non-oxidized and carboxyl forms of C; DuxD catalyzes the cleavage of the carboxyl group and induces in situ electron migration; CYP88A catalyzes continuous proton abstraction and free radical capture to obtain carbon cations and induce rearrangement.

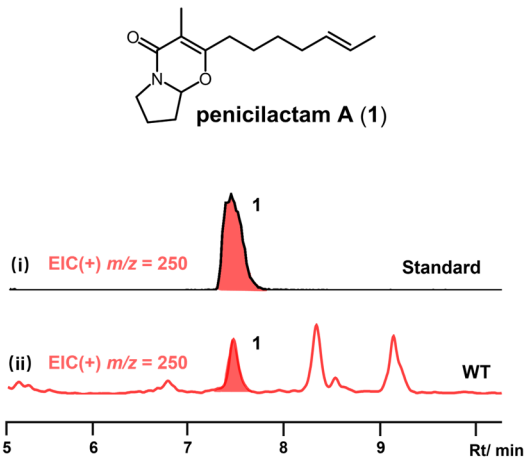


Fig. S2. Strain identification for penicilactam A (**1**) production.

LC-MS analysis revealed metabolites exhibiting a molecular mass corresponding to **1** (*m/z* 250 $[M+H]^+$) in cultures of *Penicillium citrinum* HDN11-186, a fungus isolated from *Suaeda salsa*.

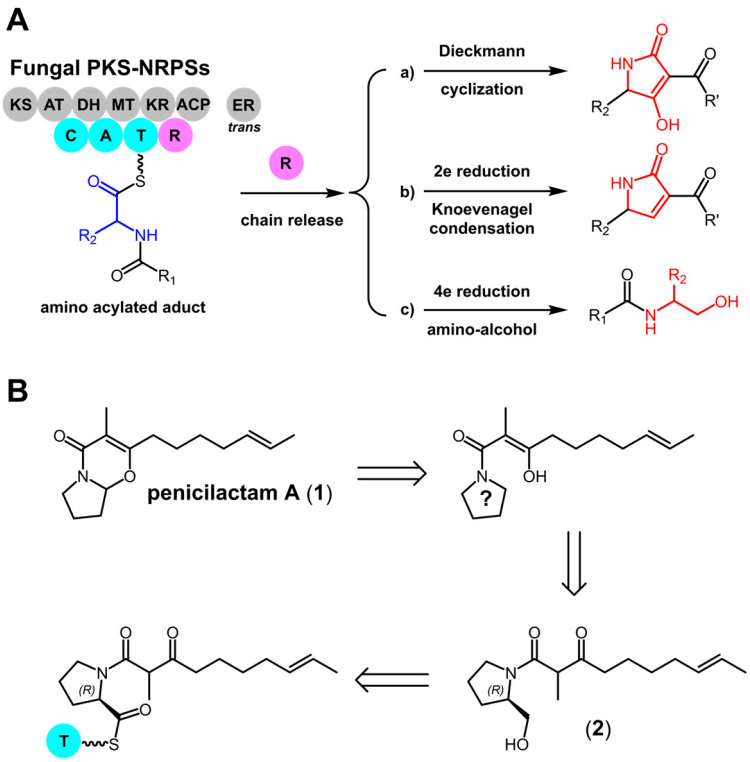


Fig. S3. Mechanistic diversity of R domains and retrobiosynthetic analysis

(A) Comparative release strategies employed by R domains in fungal PKS-NRPS systems. (B) Retrobiosynthetic deconstruction of penicilactam A (**1**), highlighting key transformations. *Note:* Classical R domains mediate thioester reduction and Dieckmann cyclization to form tetramic acids, while R* variants promote alternative pathways such as Knoevenagel condensation, yielding 3,4-dehydrogenated products.

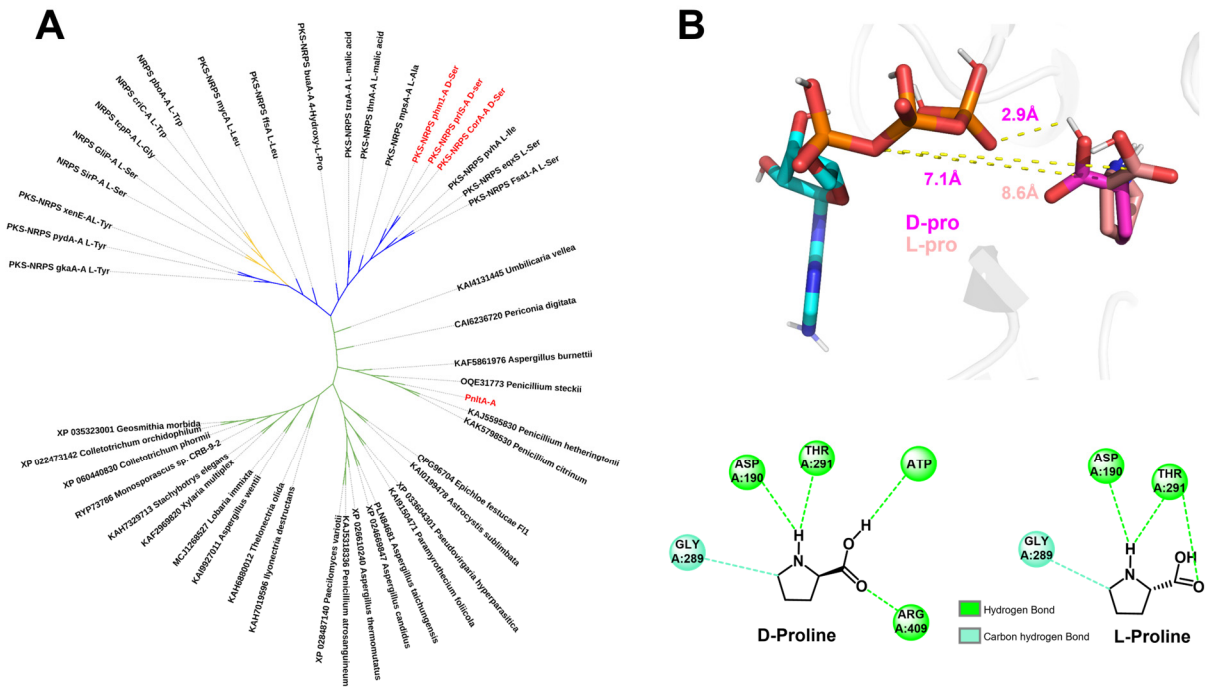


Fig. S4. Phylogenetic analysis and Molecular docking of PnltA-A domain.

(A) Phylogenetic tree of adenylation domains reveals limited resolution for functional prediction of PnltA-A (Neighbor-joining method). Color code: blue = PKS-NRPS hybrids, yellow = NRPS systems, green = uncharacterized NCBI homologs. (B) Molecular docking demonstrates stereochemical preference: *D*-proline exhibits favorable binding interactions with ATP in the PnltA-A catalytic pocket (center coordinates: x=-5.577, y=-0.812, z=-0.376; grid size=33.4Å^3), while *L*-proline shows suboptimal positioning for pyrophosphate interaction.

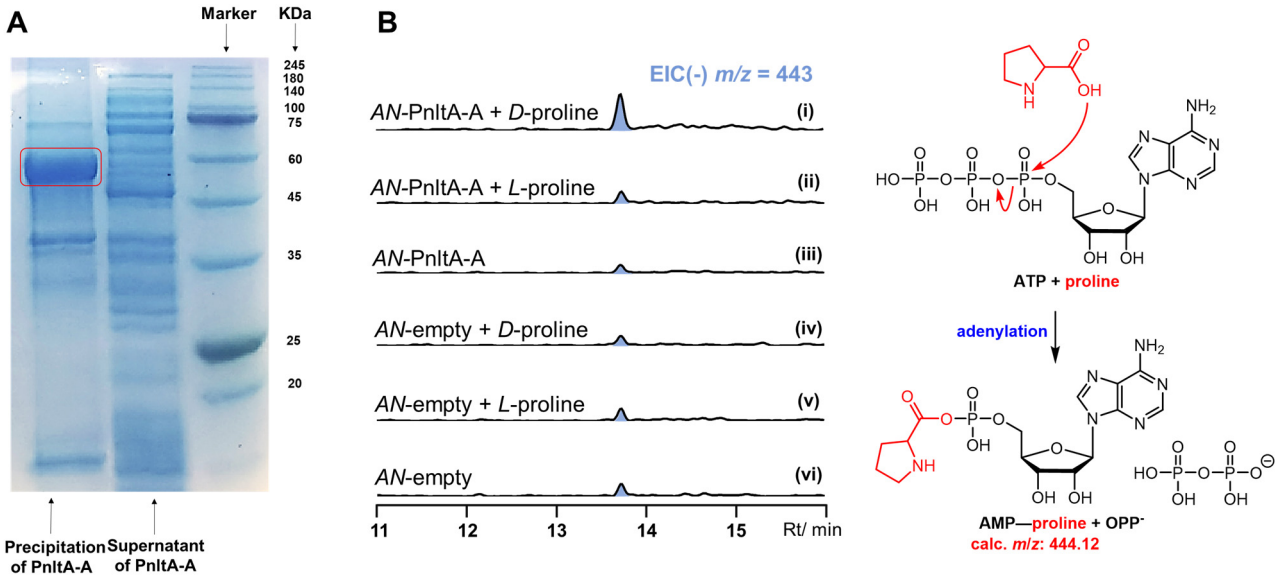


Fig. S5. Functional characterization of PnltA-A domain.

(A) Recombinant expression challenges: Despite extensive optimization efforts, the PnltA-A domain protein remained insoluble. (B) In vitro enzymatic assays with *L*/*D*-proline substrates confirmed adenylation activity through detection of AMP-*D*-proline adducts (LC-MS analysis).

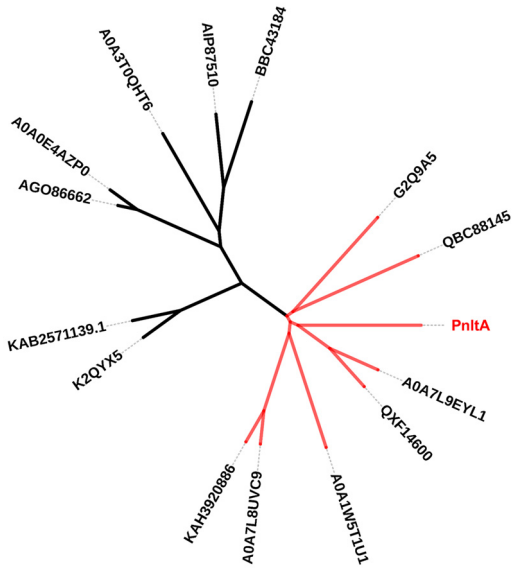


Fig. S6. Phylogenetic tree of PnltA-R domain.

Phylogenetic analysis revealed that the R domains from fungal PKS-NRPSs were separated into two groups (black: Dieckmann cyclization; red: reduction release), and the PnltA-R domain falls into the reduction group.

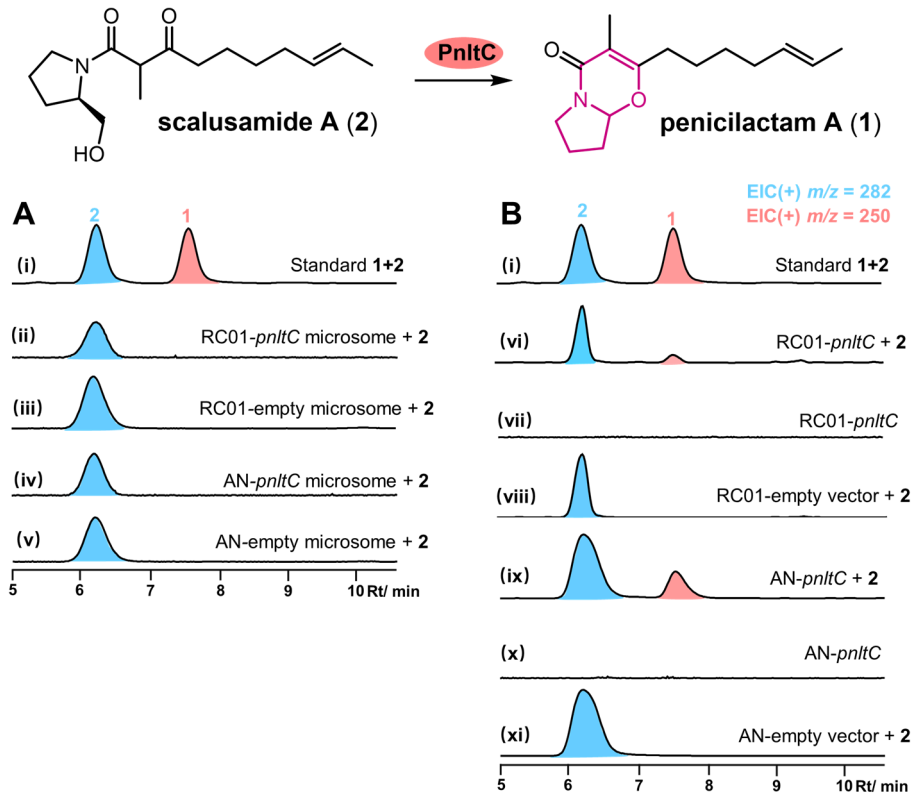


Fig. S7. In vitro and feeding assays of PnltC.

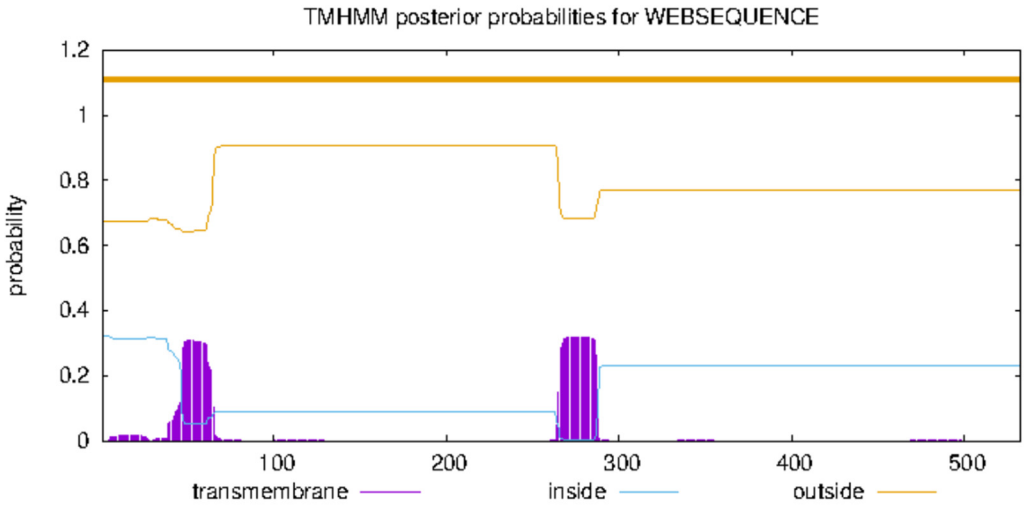


Fig. S8. Transmembrane analysis of PnltC.

Transmembrane domain prediction revealed no canonical membrane-spanning regions, though hydrophobicity profiling indicated membrane-associated propensity. *Note*: Despite this prediction, neither microsomal fractions, cytosolic supernatant, nor crude enzyme extracts exhibited catalytic activity for the **2→1** conversion.

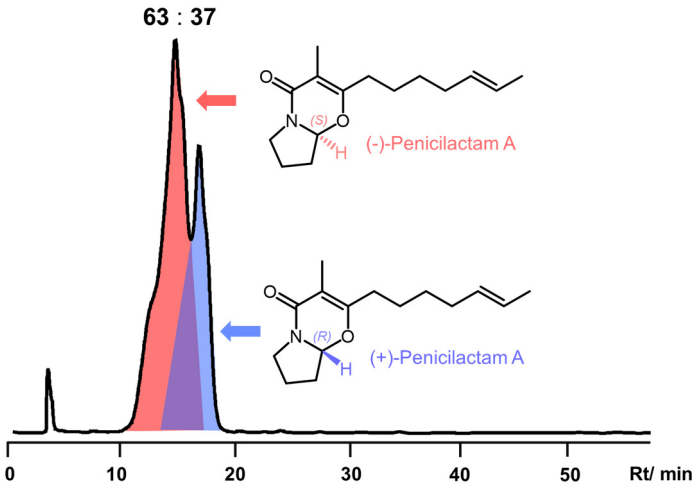


Fig. S9. Chiral resolution of penicilactam A (**1**).

HPLC analysis using a chiral stationary phase revealed enantiomeric separation with peak area ratio 63:37 (isocratic elution with 5% isopropanol in n-hexane, 1 mL/min).[10] The racemic mixture of (+/-)-**1** ($[\alpha]_D^{25}$ = -19.2, *c* 0.3 in MeOH)) showed comparable enantiomeric ratio (7:3) by polarimetric analysis.

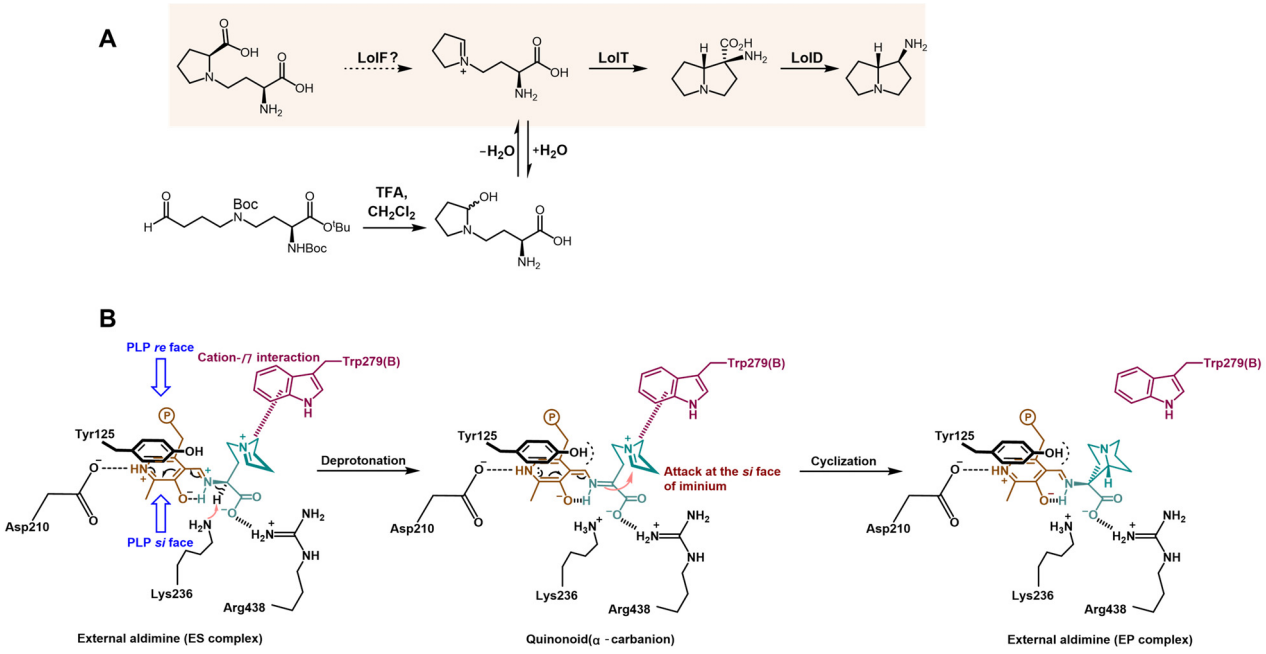


Fig. S10. Biosynthesis of loline.

(A) Reported pathway for the pyrrolizidine formation of loline. (B) Proposed catalytic mechanism of LolT. Dashed straight lines indicate hydrogen-bond or π–π stacking interactions. The conformation of the iminium side chain is favoured by cation–π interaction with Trp279 and its orientation is restricted by Y125. EP, enzyme product complex; ES, enzyme substrate complex.

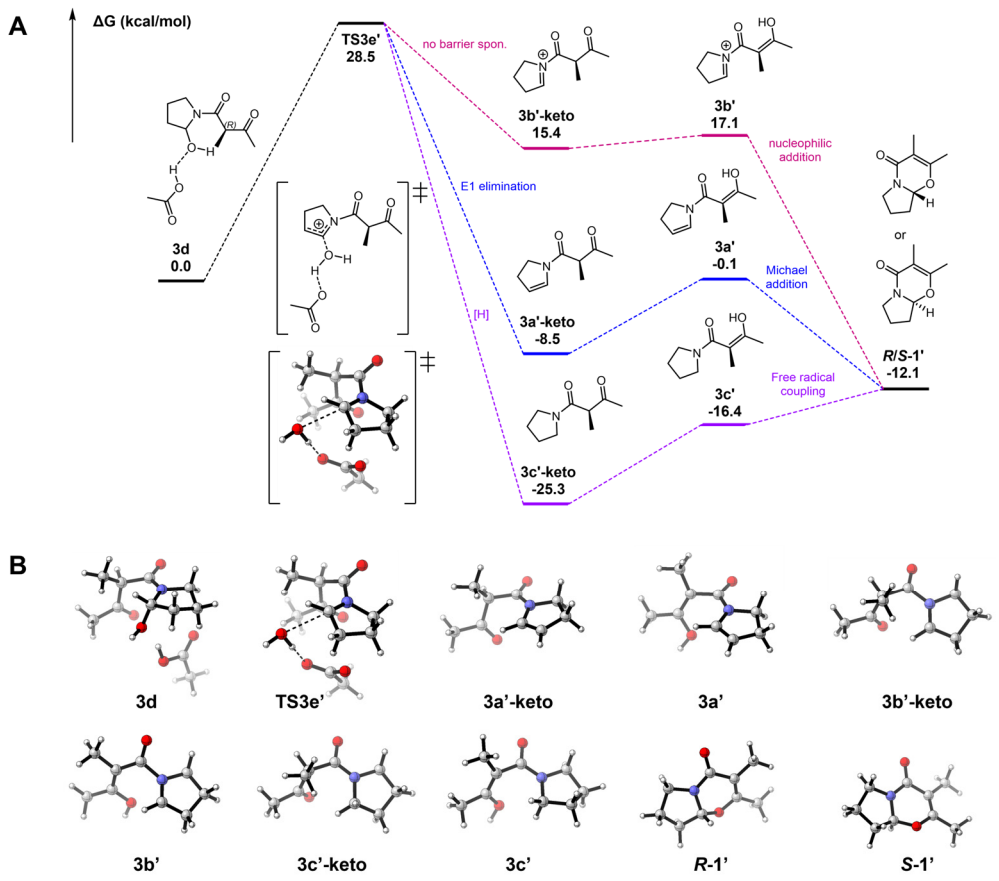


Fig. S11. Computational elucidation of non-enzymatic transformation pathways using simplified model. (A) Proposed mechanistic network originating from C2-hydroxylated precursor **3d**. Dehydration generates reactive C2-carbocation intermediate **3e'** (TS energy barrier: 28.5 kcal/mol), which bifurcates into three distinct pathways: (1) Autoelectronic rearrangement: Barrier-free conversion to iminium species **3b'-keto** (15.4 kcal/mol); (2) Hydrogen abstraction: Forms conjugated enamine **3a'-keto** (-8.5 kcal/mol) (3) Reductive cyclization: Yields pyrrolidine **3c'-keto** (-25.3 kcal/mol). (B) Given the low energy difference between **3a'-keto** and **1'** (-3.6 kcal/mol), the conversion from **3a'-keto** to **1'** is thermodynamically unfavorable, while **3b'-keto** has tendency to convert to **1'** more easily along the potential energy surface. As for **3c'-keto**, its extremely stable energy and the climbing energy barrier required to convert to **1'** mean that it is almost impossible to be a precursor of **1'**. In addition, since **3c'** must generate the new C−O bond through free radical coupling, enzymatic cyclization is necessary if conversion occurs through such process.

The calculated results suggested three distinct competing transformation pathways with significant energy differences. Combining the reported synthetic studies of **1** which showed the generation of mixed products of **3** and **1** followed by a C2-cation ion after C2−C16 bond cleavage, with **3** converting to **1** in low yields only under specific conditions,[11,12] we initially speculated that these three pathways have different requirements for enzymes: (1) Enzymatic electrophilic addition is needed in proposed pathway from **3a** to **1**; (2) The conversion from **3b** to **1** can be partially spontaneous or facilitated by enzymatic stabilization of the iminium intermediate; (3) Enzymatic free radical coupling is required in the process from **3c** to **1** (extremely unfavorable) (See Fig. 2D).

Note: The energies of key species involved in different pathways were calculated and are given in kcal/mol. Method: (opt freq b3lyp/6-31+g(d) scrf=(cpcm,solvent=water) em=gd3; b3lyp/6-311+g(d,p) scrf=(cpcm,solvent=water) em=gd3; opt=modredundant 6-31g(d) em=gd3 m062x; opt=(calcfc,ts,noeigen) freq b3lyp/6-31g(d) em=gd3).

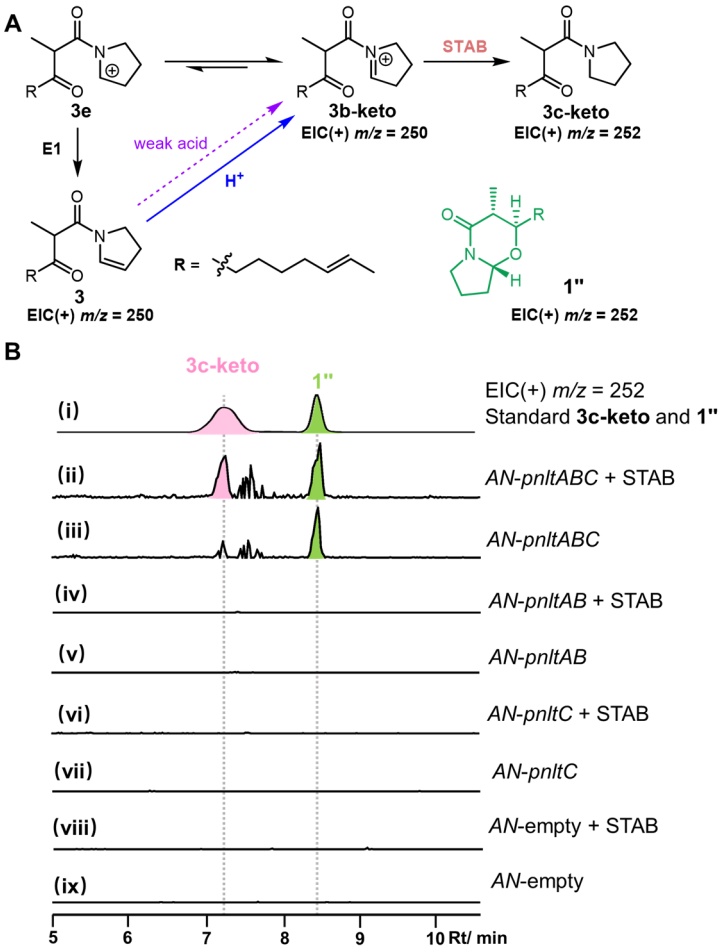


Fig. S12. Trapping of reactive iminium intermediate.

(A) Proposed equilibrium between enamine (**3**), iminium (**3b-keto**), and pyrrolidine (**3c-keto**) states under physiological conditions. Due to the higher energy of the iminium form, such reactions are biased towards the enamine state (**3**) or pyrrolidine state (**3c-keto**) under normal conditions without appropriate acidity. (B) LC-MS detection of STAB-reduced **3c-keto** (*m*/*z* 252 $[M+H]^+$ at 7.25 min) confirms transient iminium formation (Sporadic appearance of the weak peaks in (iii) is due to be reduced in a small amount in the native environment). *Note*: Product **1"** suggests competing bypass pathways.

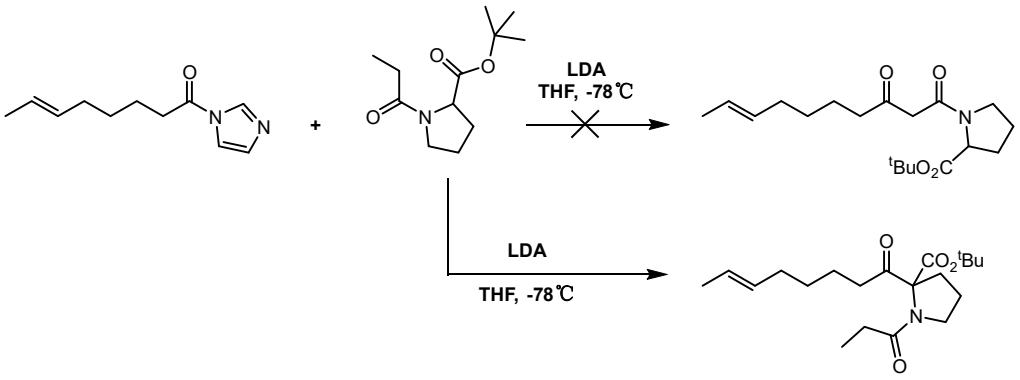


Fig. S13. Attempted synthesis of carboxyl analogue **2c**.

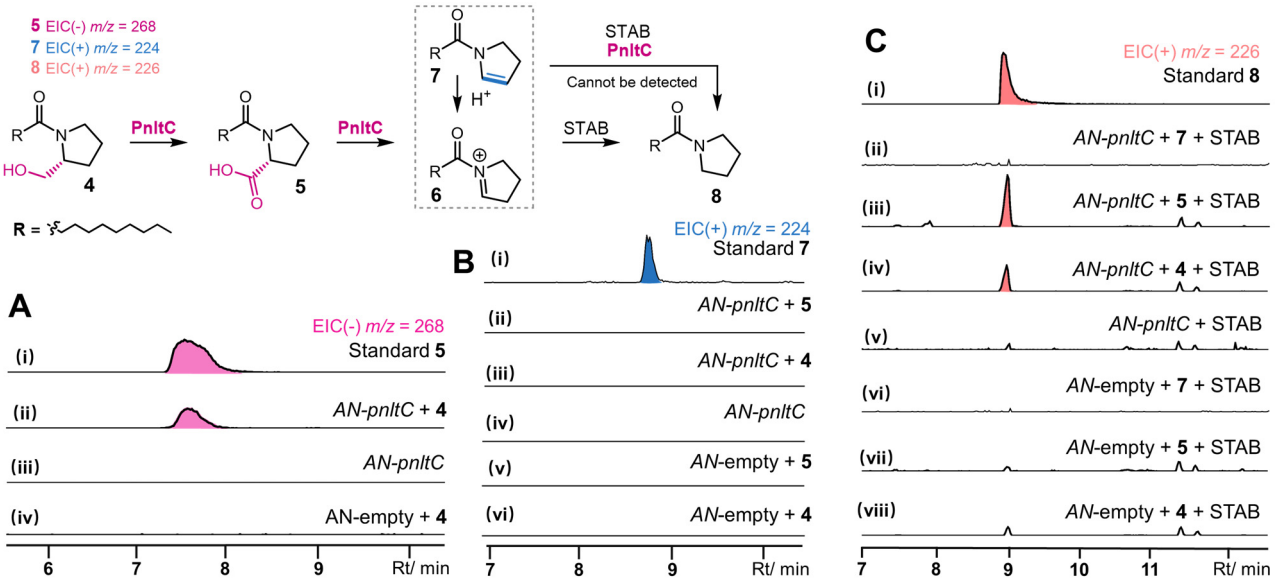


Fig. S14. Analogues feeding assays validate PnltC functionality.

Analysis of *AN-pnltC* fed with synthesized substrates **4**, **5** and **7**, the products of which were further reduced to **8** under the action of STAB, separately. (A) Conversion of **4**→**5** in *AN-pnltC* cultures (LC-MS verification). (B) Absence of **7** detectionafter feeding **4** and **5**. (C) STAB-mediated reduction identifies iminium intermediate **6** through **8** detection.

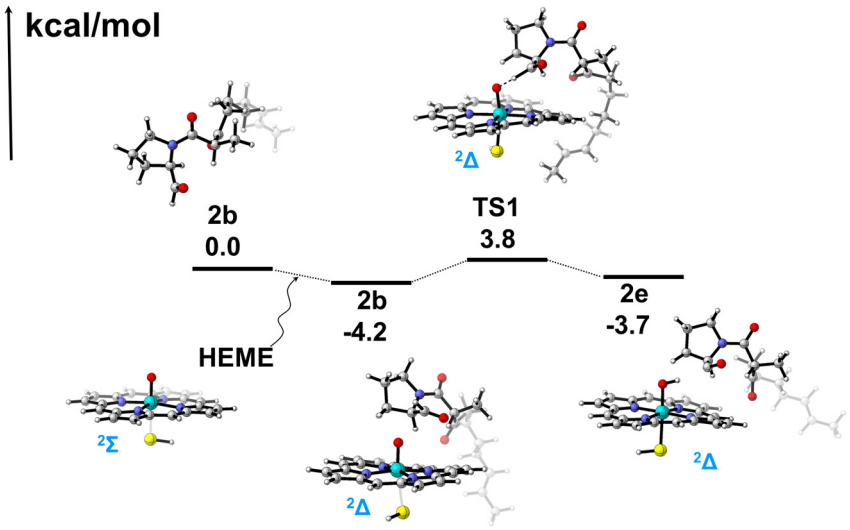


Fig. S15. Proposed mechanism for the first oxidation on C16−OH.

Structural optimization was calculated by: opt/freq/b3lyp/def2svp/empiricaldispersion=gd3bj/scf=xqc;

The transition states (TSs) searching calculations were conduxted by:

freq/ub3lyp/def2svp/empiricaldispersion=gd3bj/scf=xqc and freq/b3lyp/def2svp/empiricaldispersion=gd3bj scf=xqc**;**

The energies of key species involved in different pathways at were calculated by:

b3lyp/def2tzvp/empiricaldispersion=gd3bj;

All energies are given in kcal/mol. The optimized geometries of these key species along the reaction.

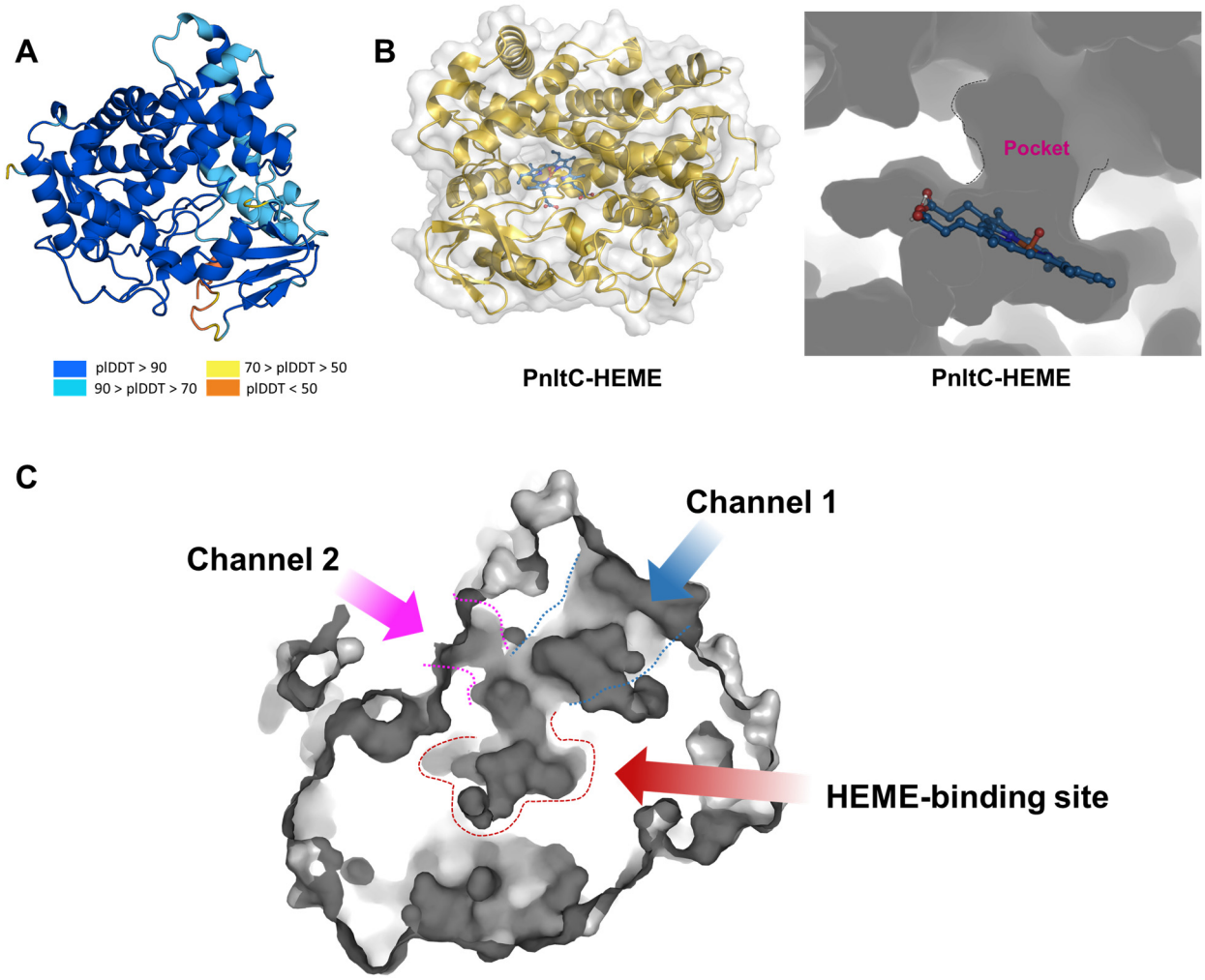


Fig. S16. Structural characterization of PnltC.

(A) Validation metrics for AlphaFold2 model (sequence coverage >90%, pLDDT >85). (B) Heme docking reveals conserved cofactor positioning. (C) Dual substrate access channels: Channel 1 accommodates substrate transit; Channel 2 potentially facilitates electron transfer to maintain P450 catalytic cycling for efficiency multiple oxidations. Docking position parameter: center_x = 0.167; center_y = -6.519; center_z = -2.208; size_x = 18.0; size_y = 18.0; size_z = 18.0.

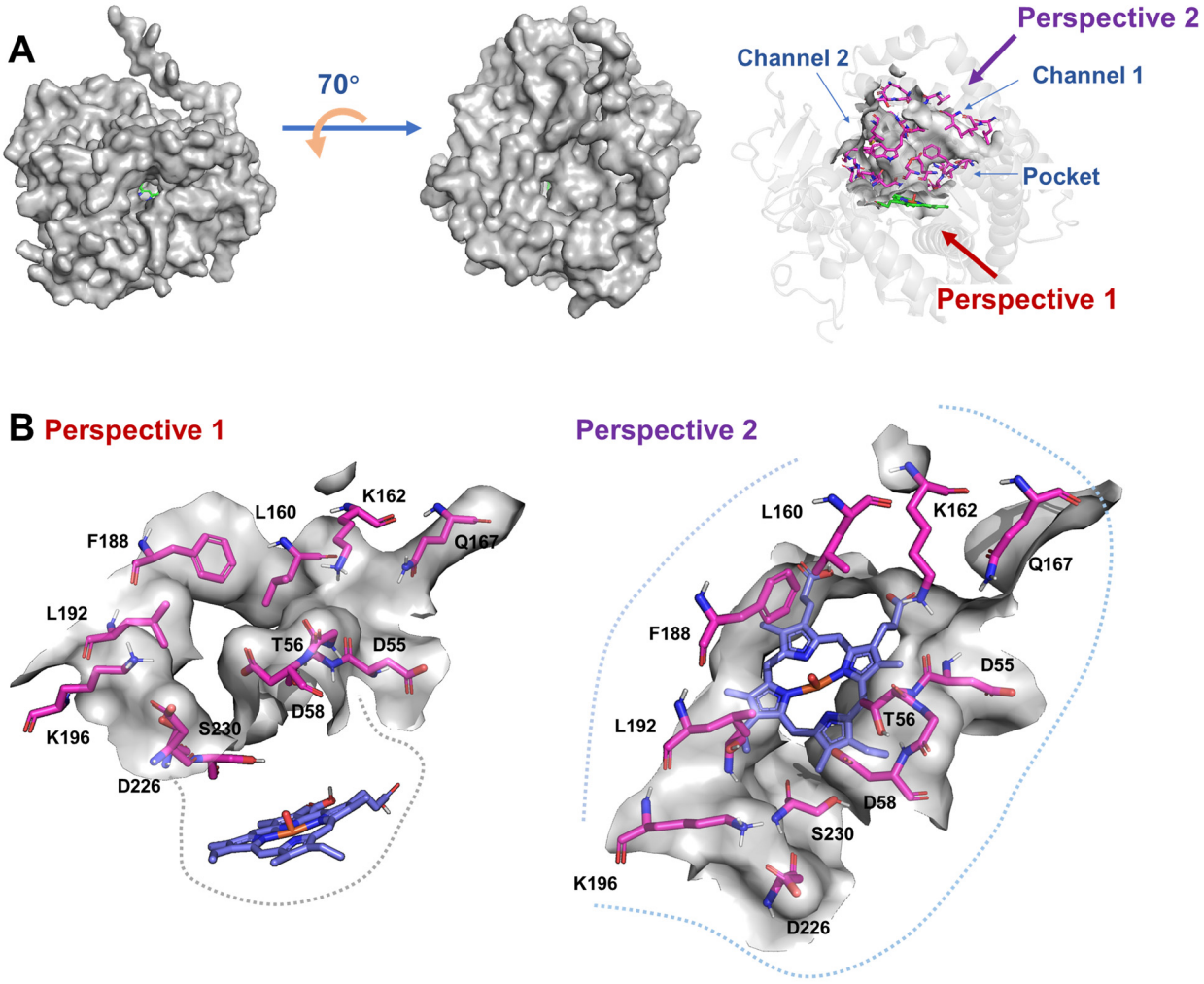


Fig. S17. Analysis of the surface residues of the channel 1.

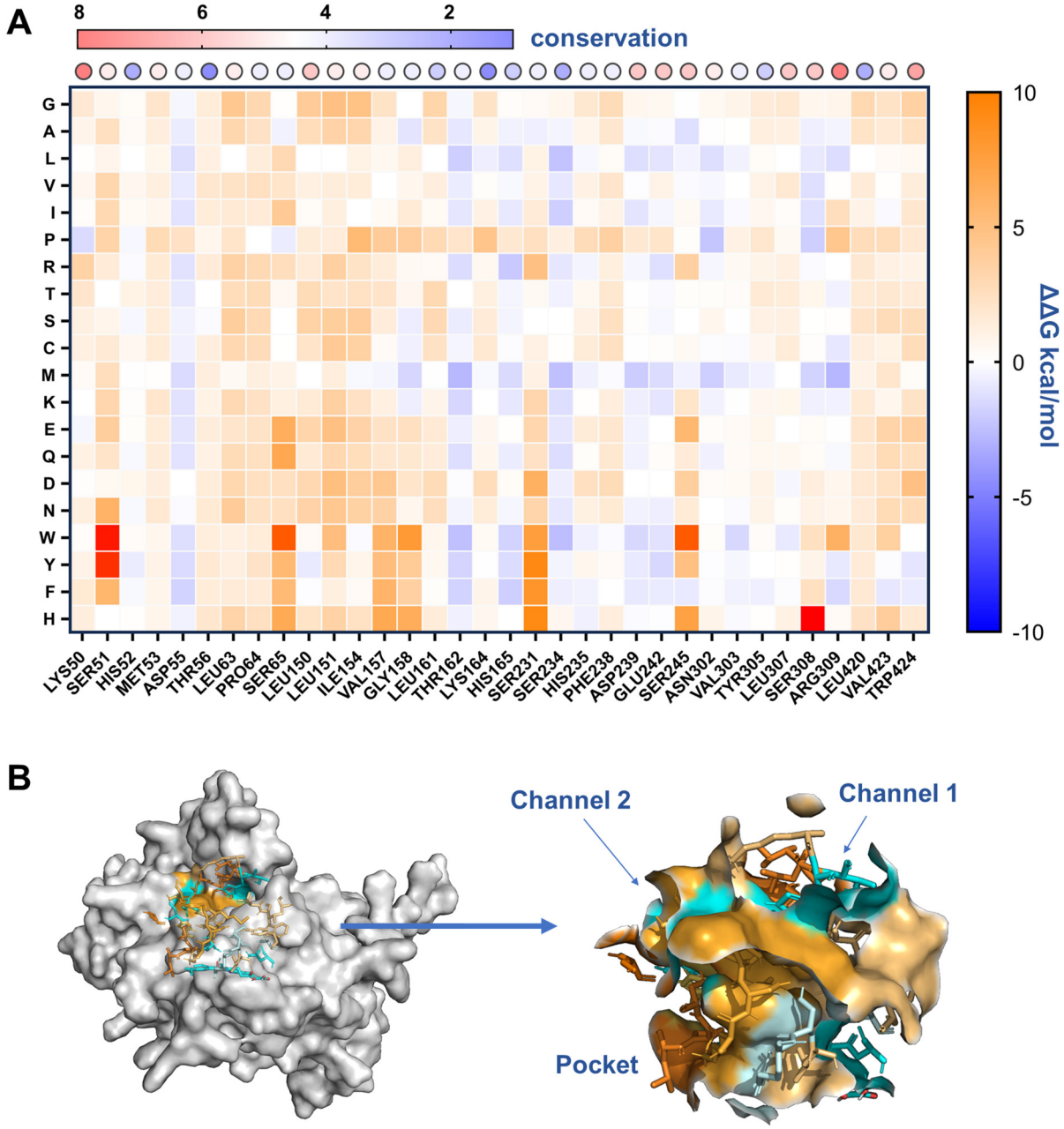


Fig. S18. Computational mutagenesis profiling.

(A) Heatmap displaying ΔΔG values for 34 channel surface residues (x-axis) across 20 amino acid substitutions (y-axis). Color scale: red (ΔΔG >0, destabilizing) to bule (ΔΔG <0, stabilizing). Conservation scores from homologous sequences overlaid (red = high conservation). (B) Mutation tolerance model highlighting residues with average ΔΔG.

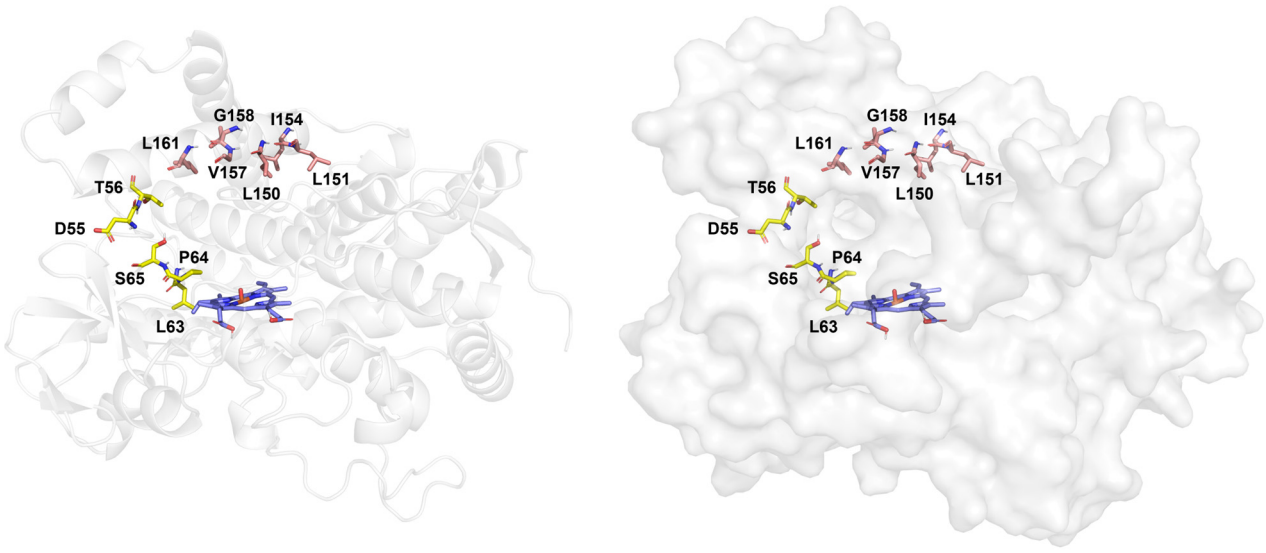


Fig. S19. Energy-based mutagenesis strategy.

Eleven residues increasing protein energy upon mutation (T56/D55/S65/L63/P64 in flexible loop; L150/L151/I154/V157/G158/L161 in α-helical lid). Rational selection criteria: (1) Dynamic control residues (loop region) prioritized for alanine scanning; (2) Structural stabilizers (helical lid) with low conservation partially selected (L150A/V157A/G158A). Final 31-site scanning array established.

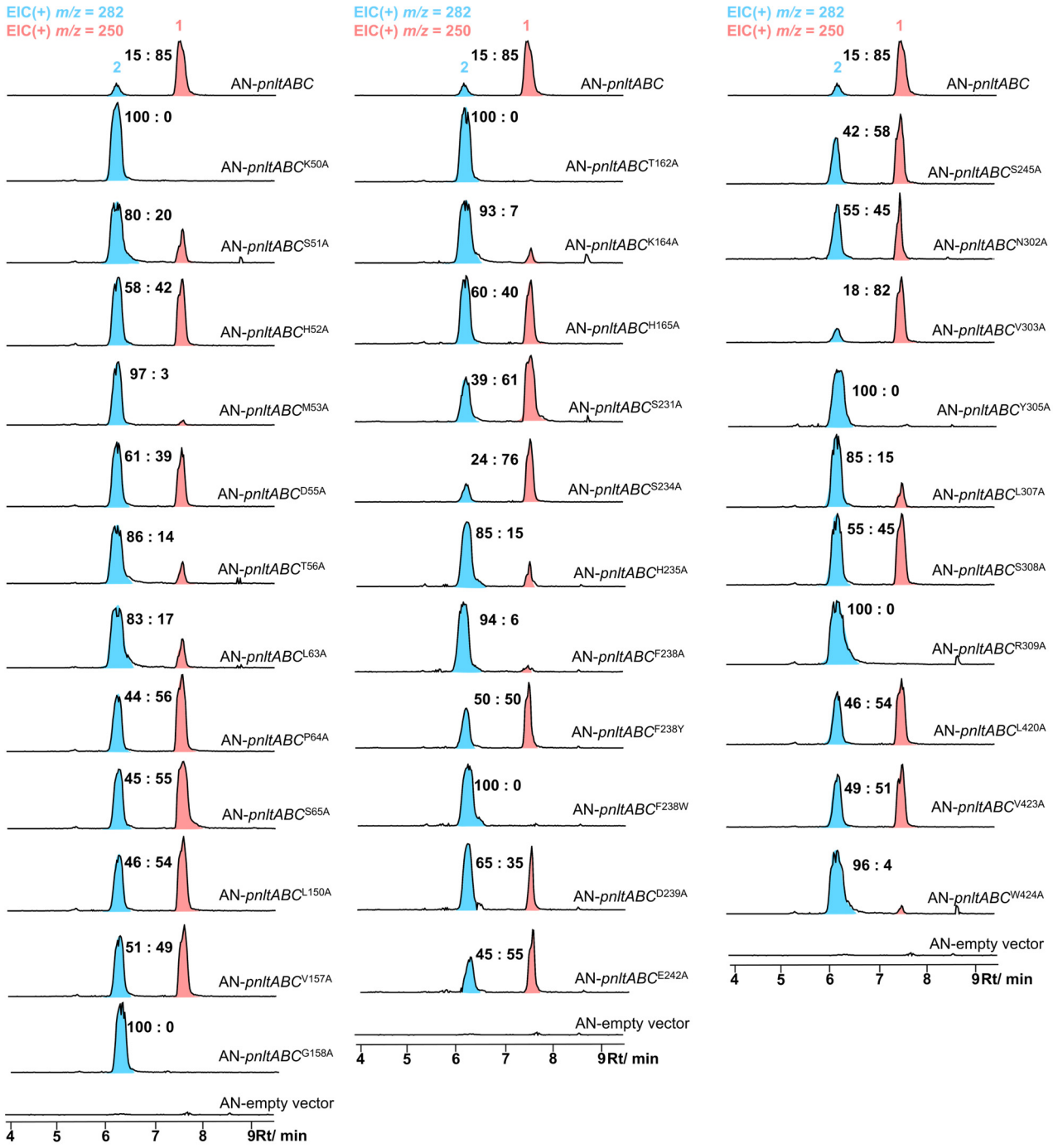
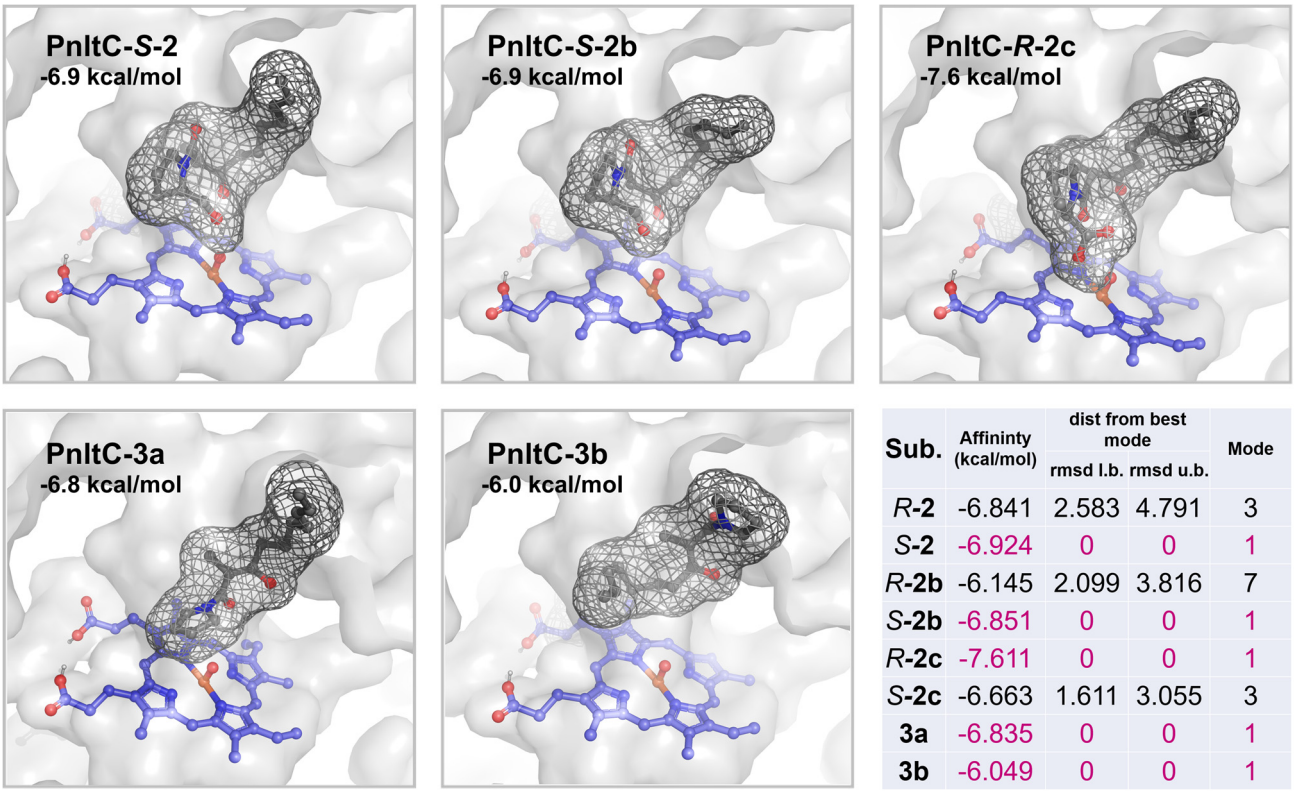


Fig. S20. In vivo assays of scanning mutagenesis of surface residues from the entrance to pocket of PnltC.



Sub.	Affinity (kcal/mol)	dist from best mode		Mode
		rmsd l.b.	rmsd u.b.	
R-**2**	-6.841	2.583	4.791	3
S-**2**	-6.924	0	0	1
R-**2b**	-6.145	2.099	3.816	7
S-**2b**	-6.851	0	0	1
R-**2c**	-7.611	0	0	1
S-**2c**	-6.663	1.611	3.055	3
3a	-6.835	0	0	1
3b	-6.049	0	0	1

Fig. S21. Molecular docking validation.

Binding energies (kcal/mol) and RMSD values for optimal substrates (*R*/*S*-**2**, *R*/*S*-**2b**, *R*/*S*-**2c**, **3a** and **3b**, *R*/*S* represents only the C7 position configuration) conformations. Catalytically competent poses (RMSD=0) selected for **2**, **2b**, **2c**, **3a**, **3b**. Consensus docking parameters: grid center (0.254, 0.197, 1.515 Å), cubic search space 25.0 Å^3.

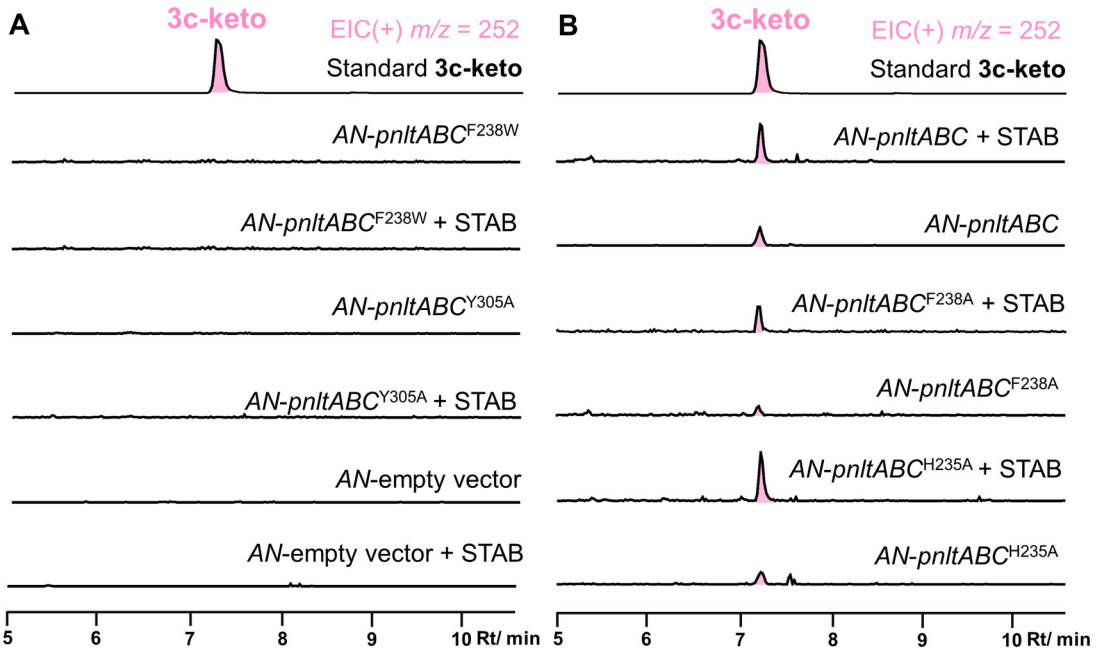


Fig. S22. Detecting the generation of **3c-keto** in mutants through in situ reduction.

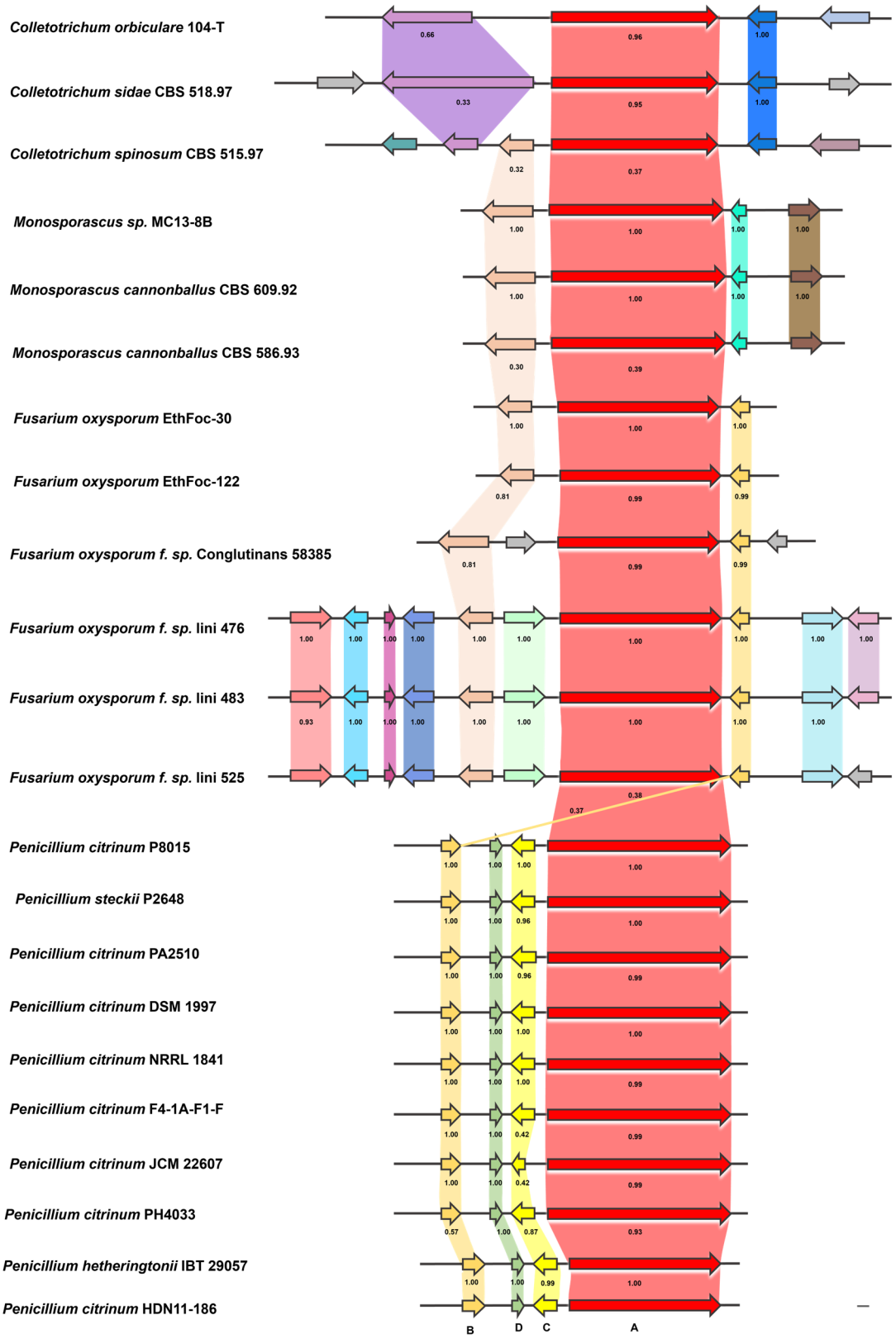


Fig. S23. Homologous BGCs mining among the fungi species.

Data sources: Manual annotation for *Penicillium hetheringtonii* IBT 29057 & HDN11-186; NCBI genome database automated annotation (retrieved July 2022). Phylogenetic distribution reveals BGC conservation within *Penicillium* genus.

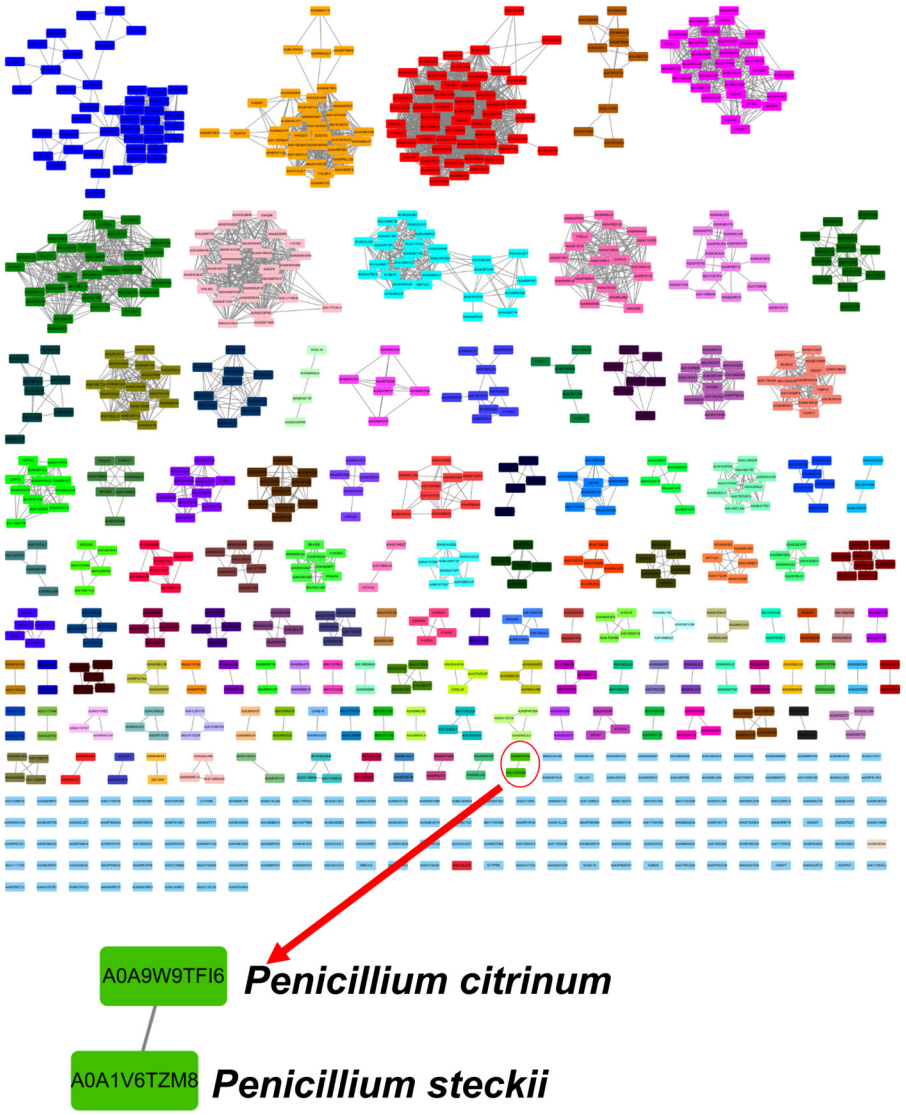


Fig. S24. Similarity Network (SSN) searching of PnltC in Fungi P450s (Uniprot database).

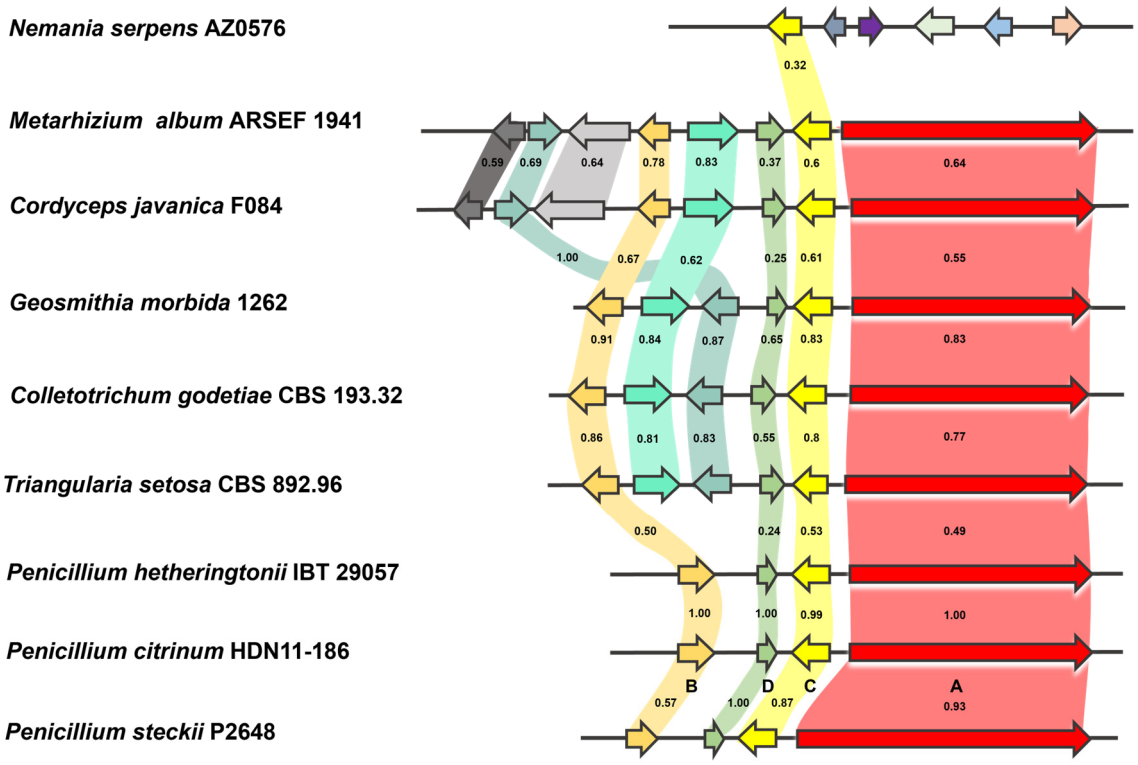


Fig. S25. Display of homologous BGCs using PnltC as a probe in NCBI database.

Using the above homologous P450s as probes, the BGCs were located in the respective local genomes, indicating that the BGC of compound **1** may be highly conserved mainly among *Penicillium* species. Homology probing identifies conserved P450-PKS/NRPS associations across: *Penicillium* spp. (high conservation), *Triangularia-Metarhizium* (moderate), *Nemania* (divergent).

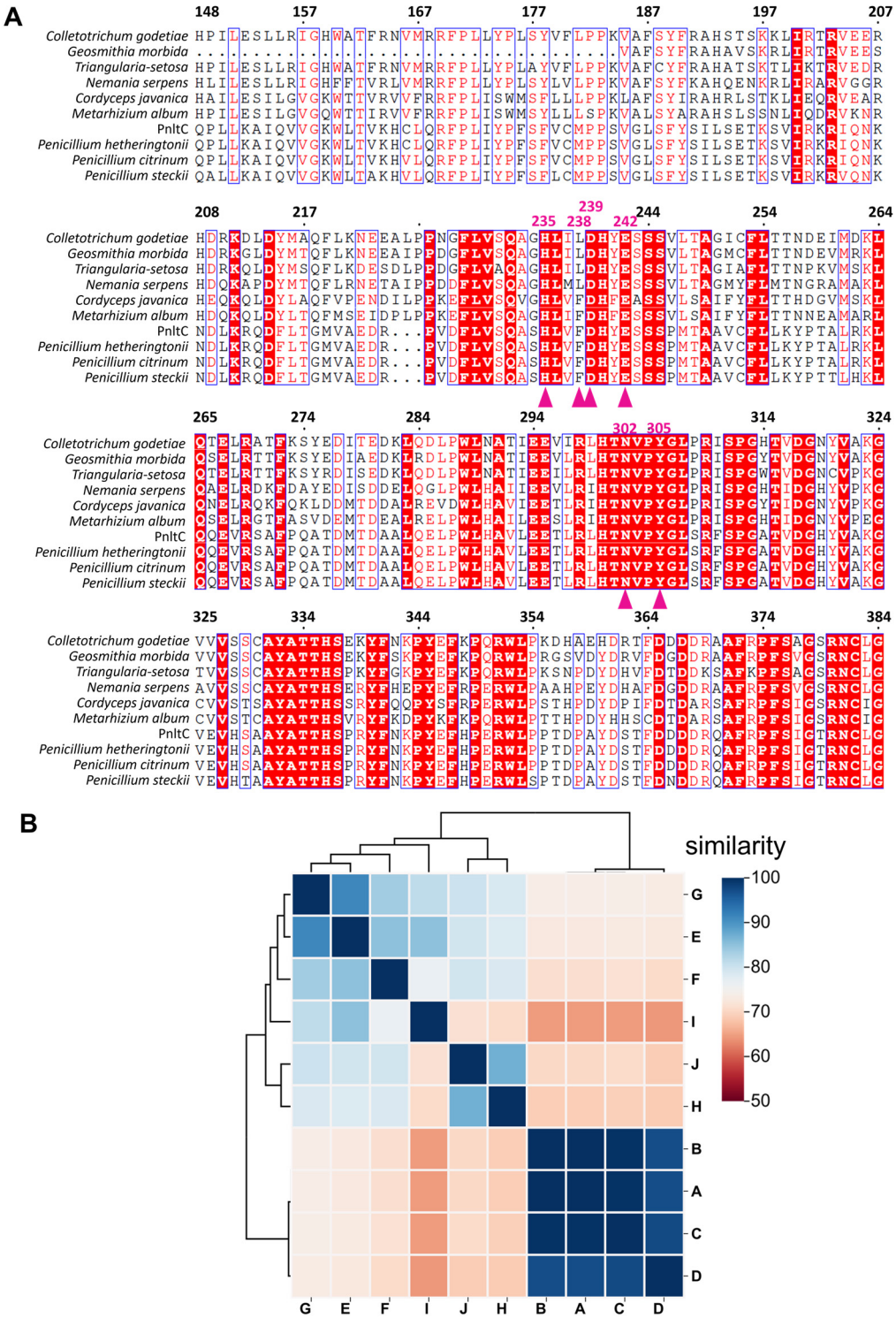


Fig. S26. Multiple sequence alignment of PnltC and its homologues.

(A) The residues in the active pocket of PnltC are indicated by purple arrows, and they are conserved in PnltC homologues except for F238. Multiple sequence alignment of these new homologous revealed that F238 is conserved in a minority of enzymes, whereas other residues are highly conserved in PnltC homologues across species. Specifically, P450s in the BGCs of *Metarhizium album* and *Cordyceps javanica* retain the conserved F238 residue, in contrast to the L238 variant found in strains such as *Colletotrichum godetiae*, *Geosmithia morbida*, *Triangularia-setosa* and a non-BGC-clustered *Nemania serpens*. This suggests a difference in potential cation stabilization. The prevalence of these P450s in *trans*-ER-type PKS-

NRPS hybrid BGCs highlights their evolutionary role in binding to PKS-NRPS and catalyzing potential sequential oxidation reactions. (B) Sequence similarity heat map of the most homologous proteins. The sequence information was obtained from blast based on the NCBI database using the pnltC probe. A-J represent homologues from: A: PnltC; B: *Penicillium hetheringtonii*; C: *P. citrinum*; D: *P. steckii*; E: *Colletotrichum godetiae*; F: *Nemania serpens*; G: *Triangularia setosa*; H: *Cordyceps javanica*; I: *Geosmithia morbida*; J: *Metarhizium album*. Despite over 60% similarity among these homologous proteins, the conservation pattern in *Penicillium* markedly differs from other species.

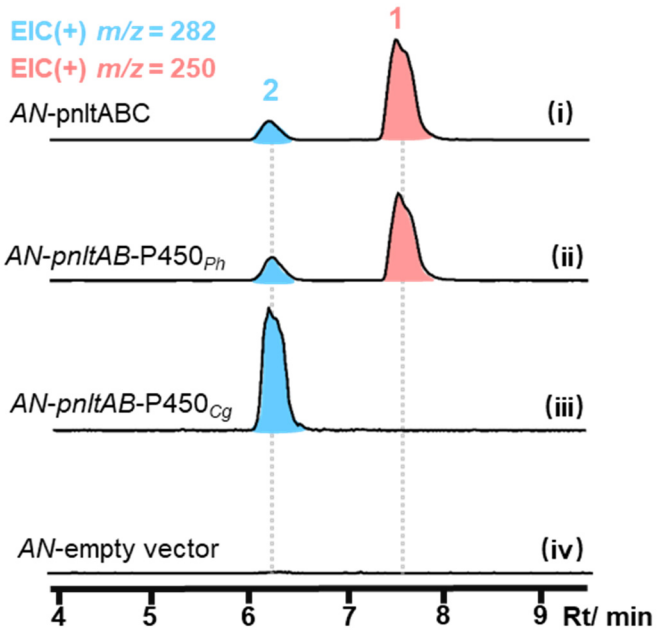


Fig. S27. Functional verification of homologous proteins.

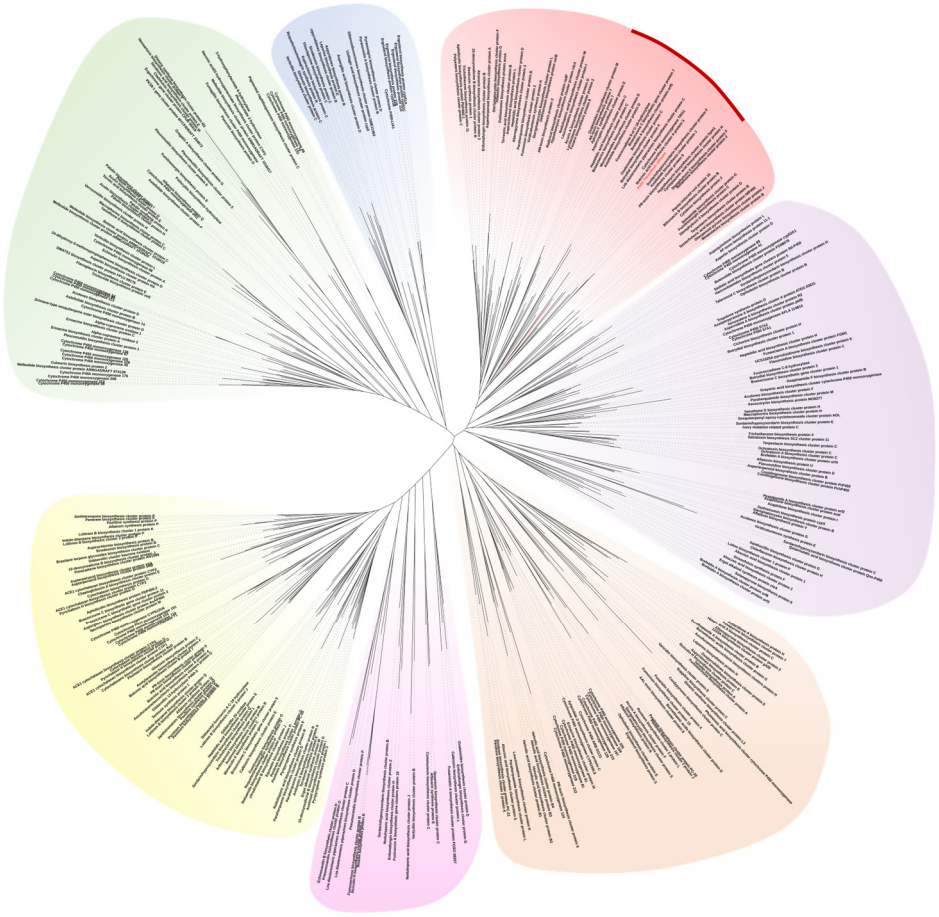


Fig. S28. Phylogenetic tree analysis of PnltC.

In PnltC-located clade, many P450s display multi-oxidized function and un-confirmed oxidation process, such as StnF, tri4, Bet2 and poxC, which implies the potential of P450s in such cluster.[13–16]

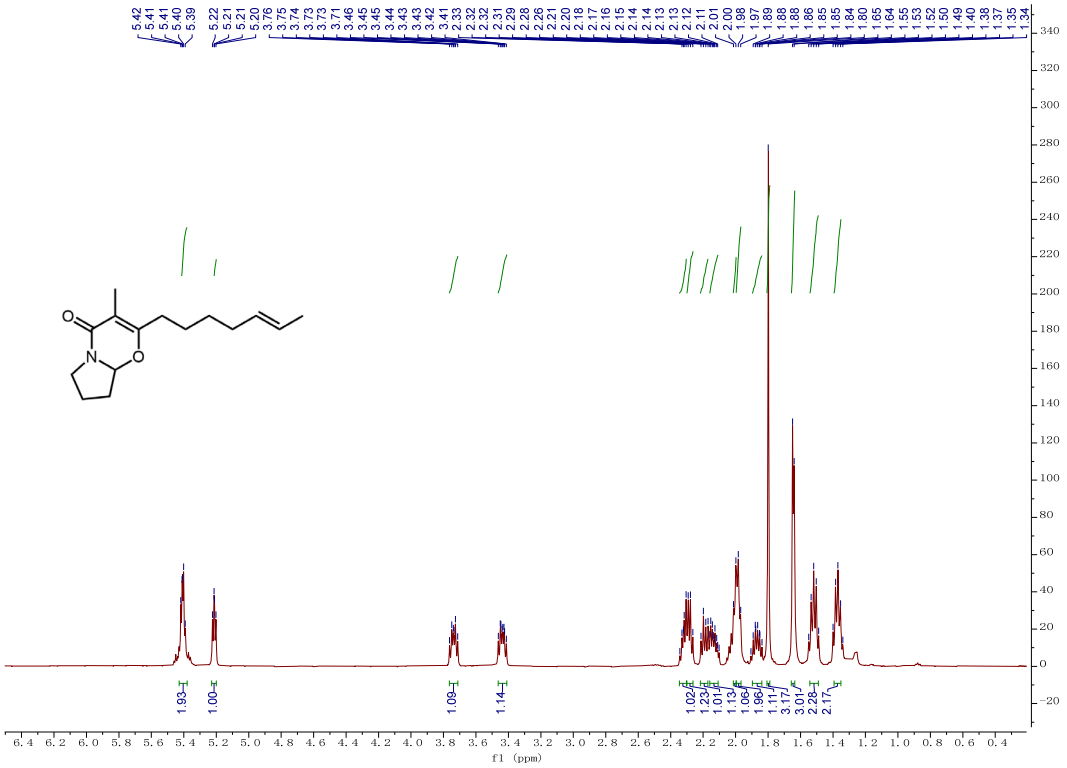


Fig. S29. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$.) of compound **1**.

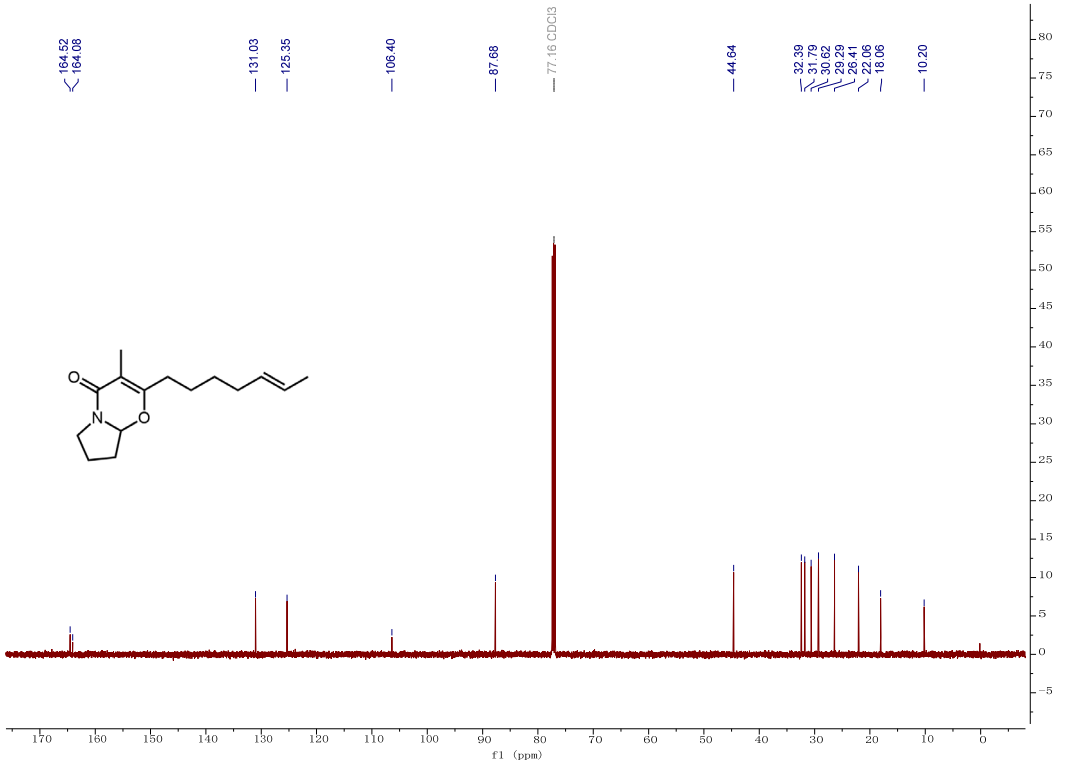


Fig. S30. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$.) of compound **1**.

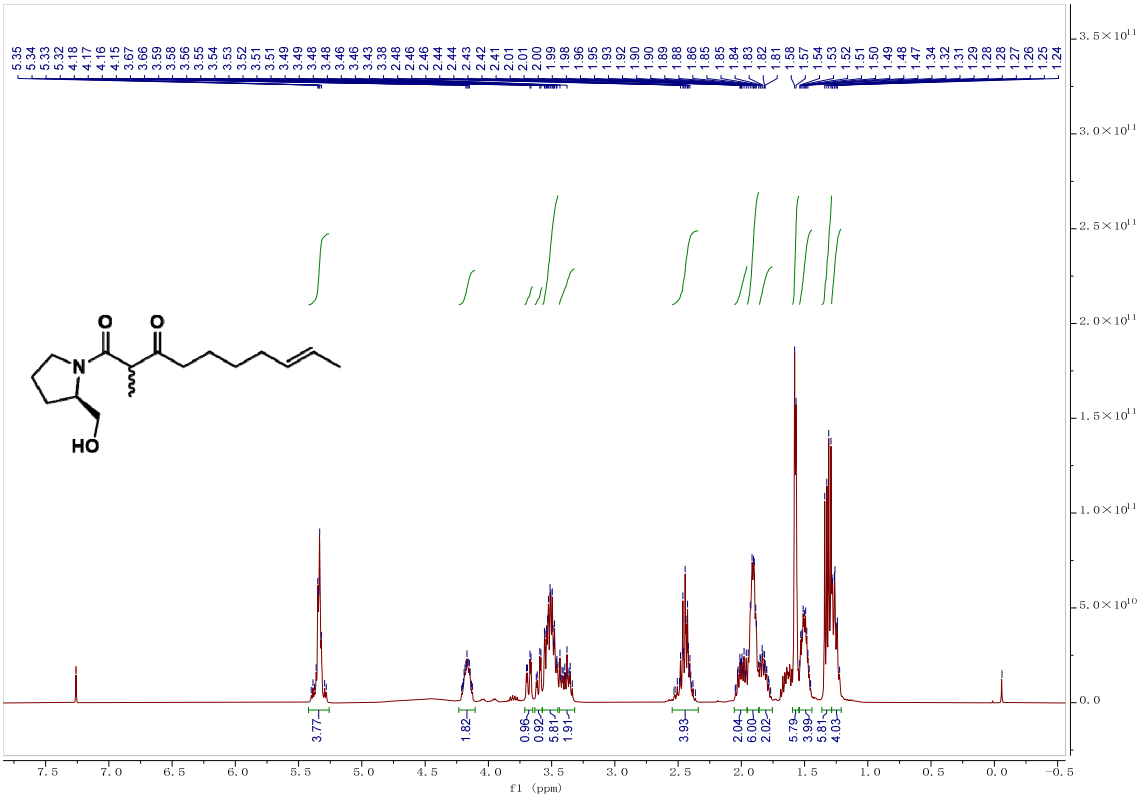


Fig. S31. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **2**.

(As compound **2** is a mixture in the form of a pair of epimers, both configurations, 1:1, consistent with the optical rotation results. Coupled with the support of carbon signal, the integral of H is doubled.)

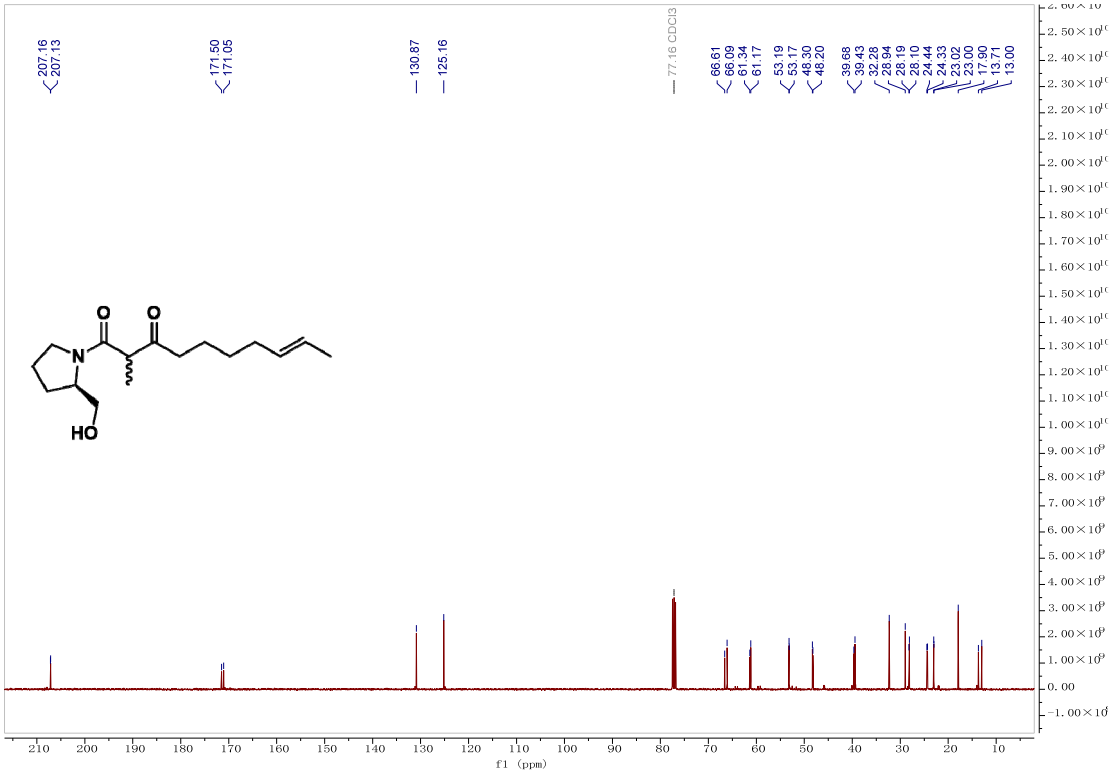


Fig. S32. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **2**.

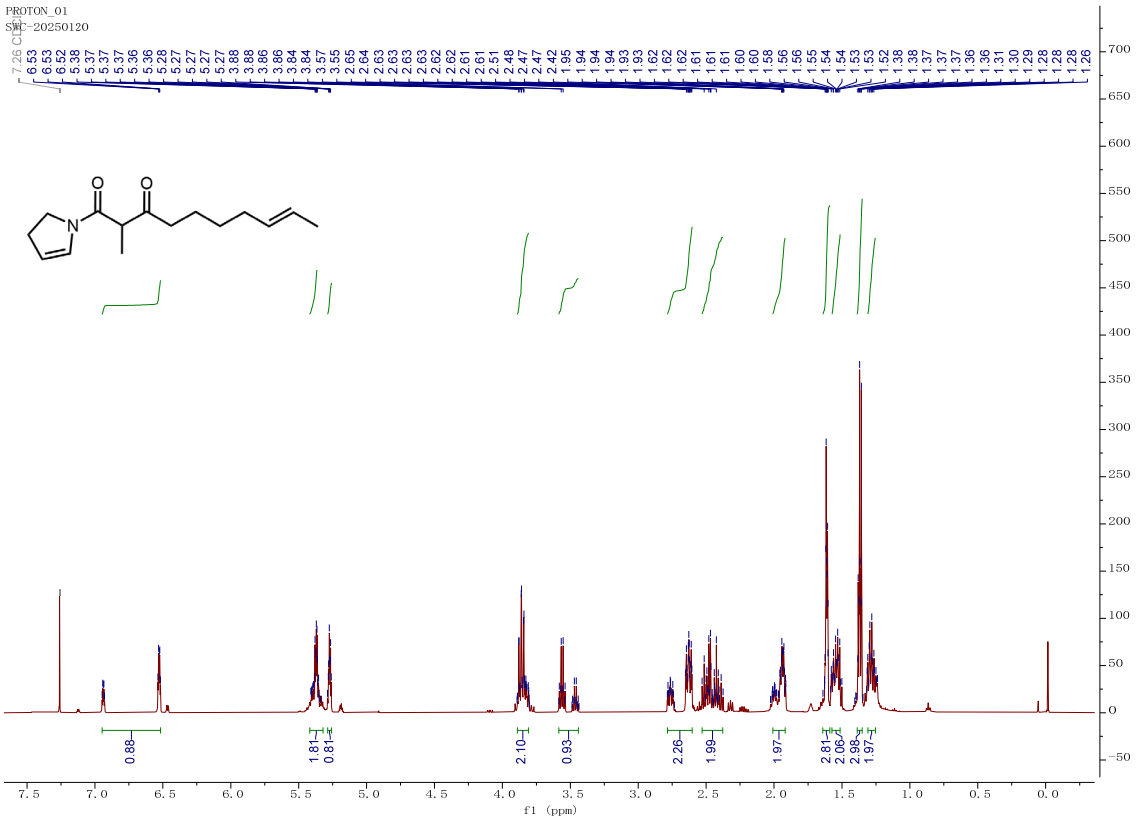


Fig. S33. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$.) of compound **3**.

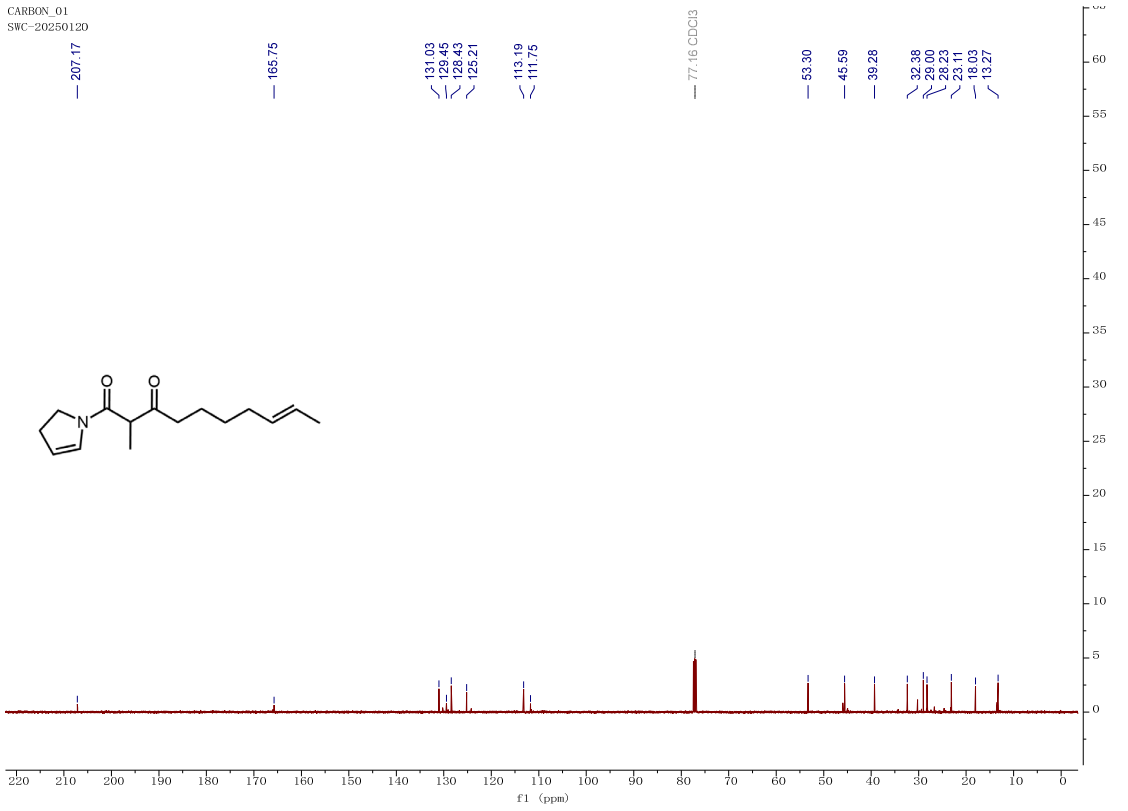


Fig. S34. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$.) of compound **3**.

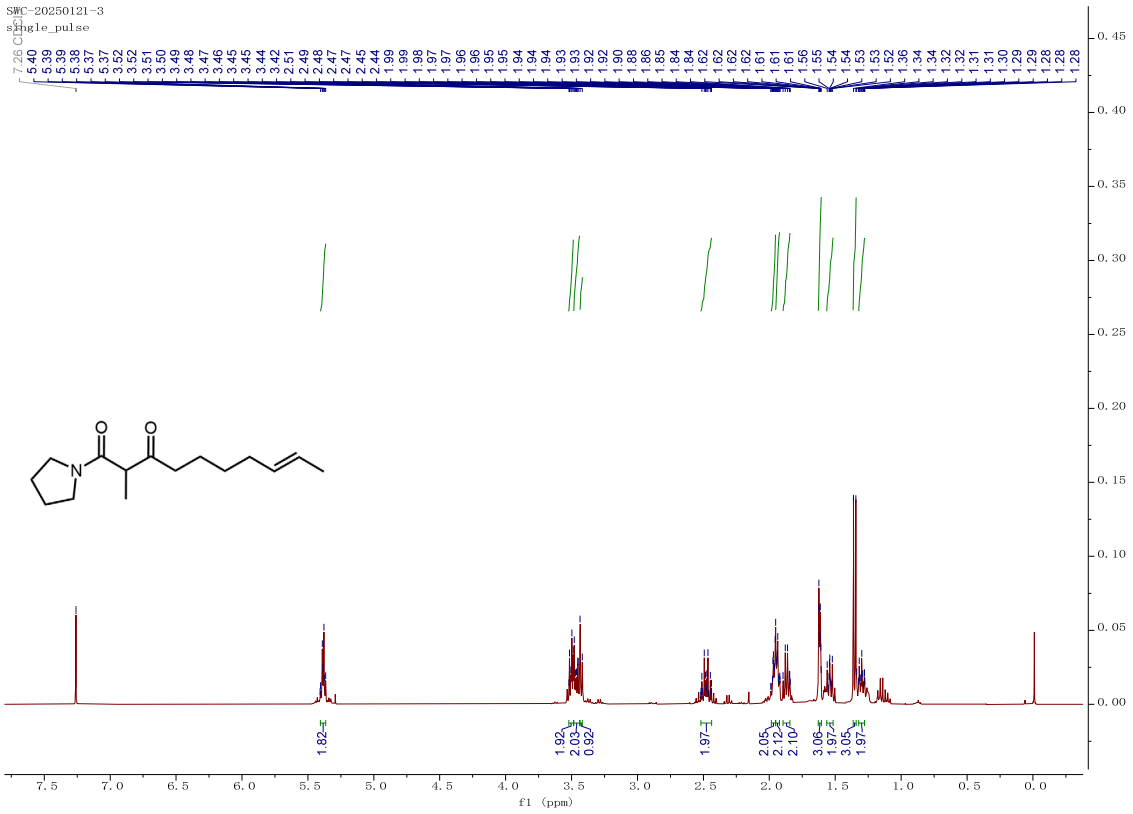


Fig. S35. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **3c-keto**.

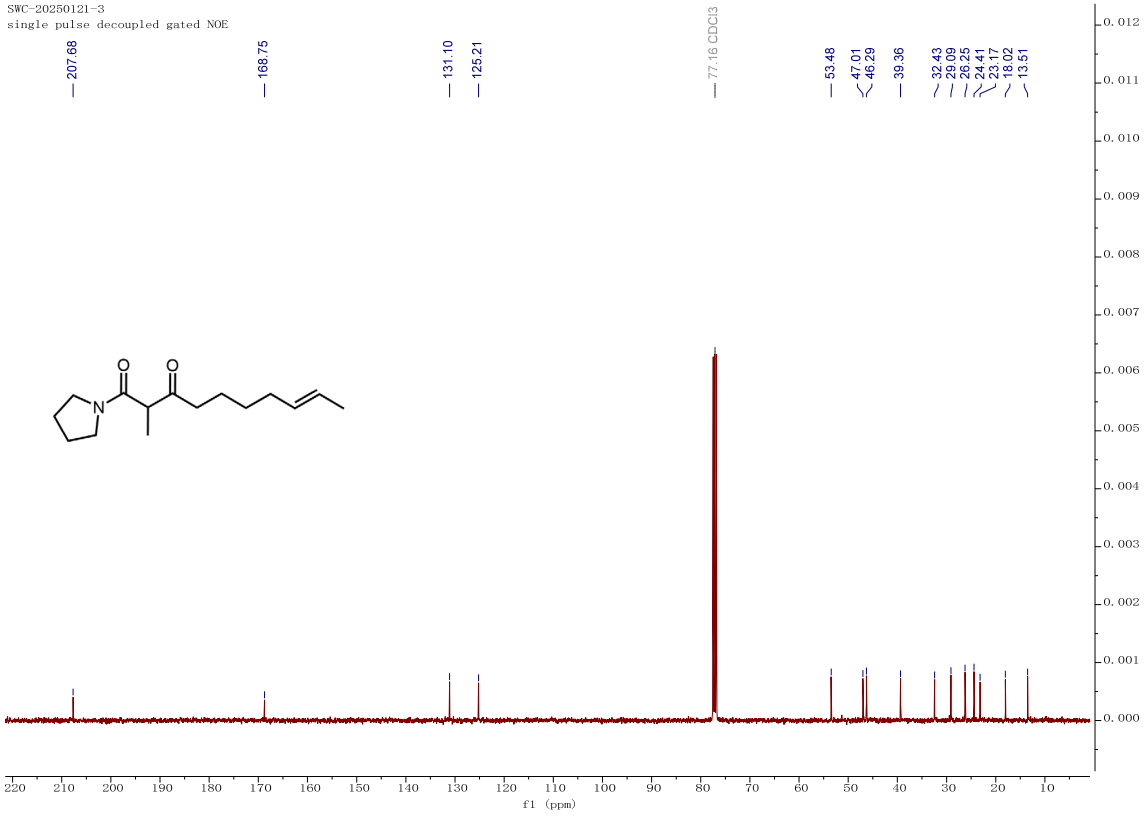


Fig. S36. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **3c-keto**.

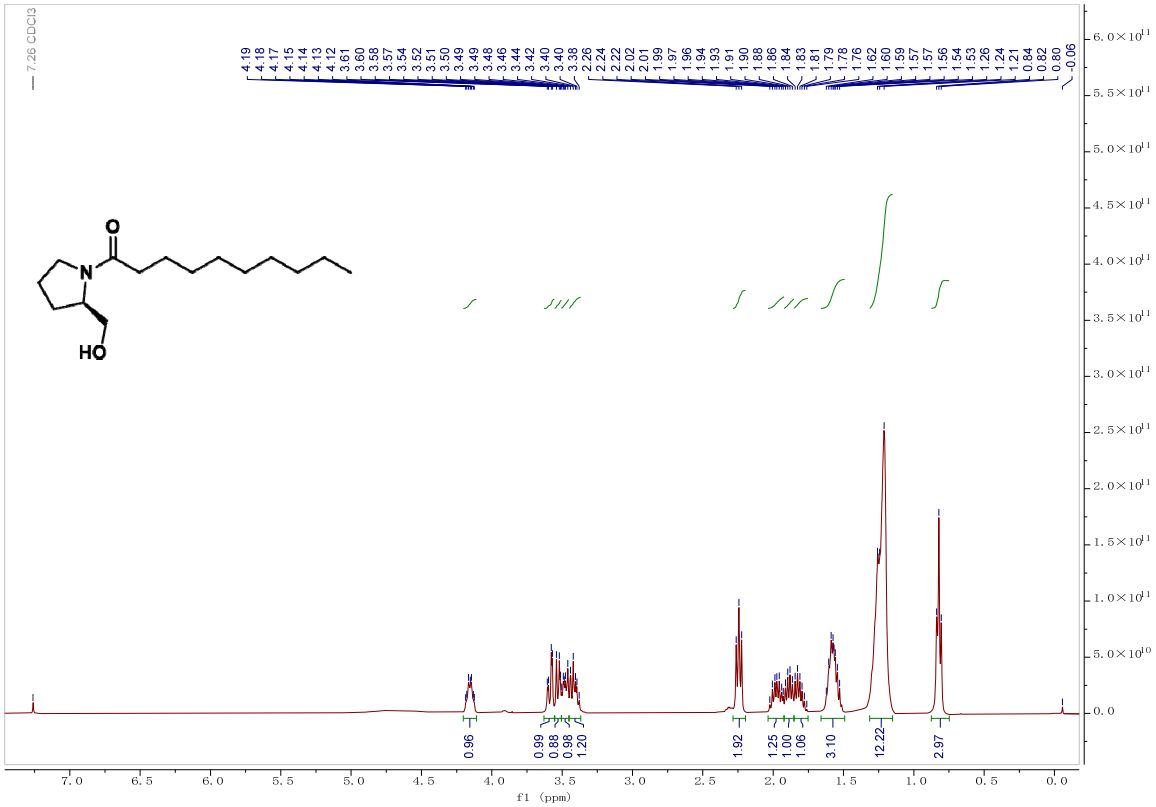


Fig. S37. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **4**.

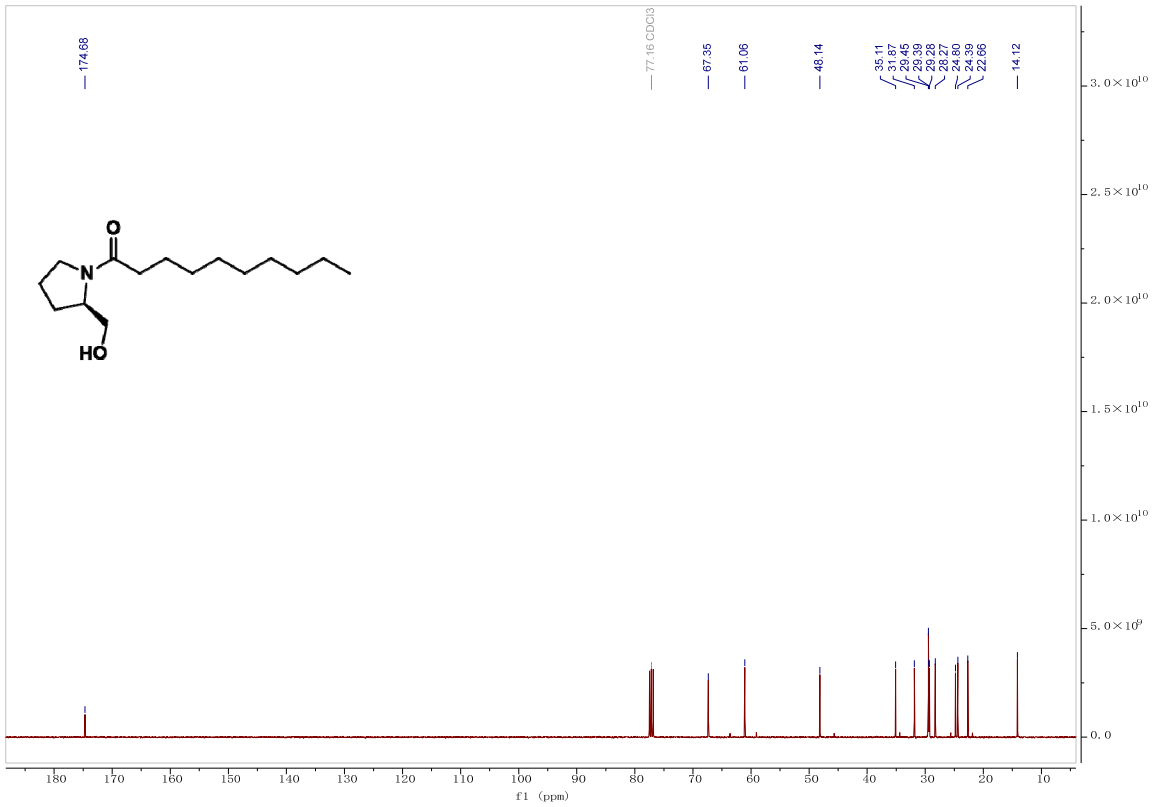


Fig. S38. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **4**.

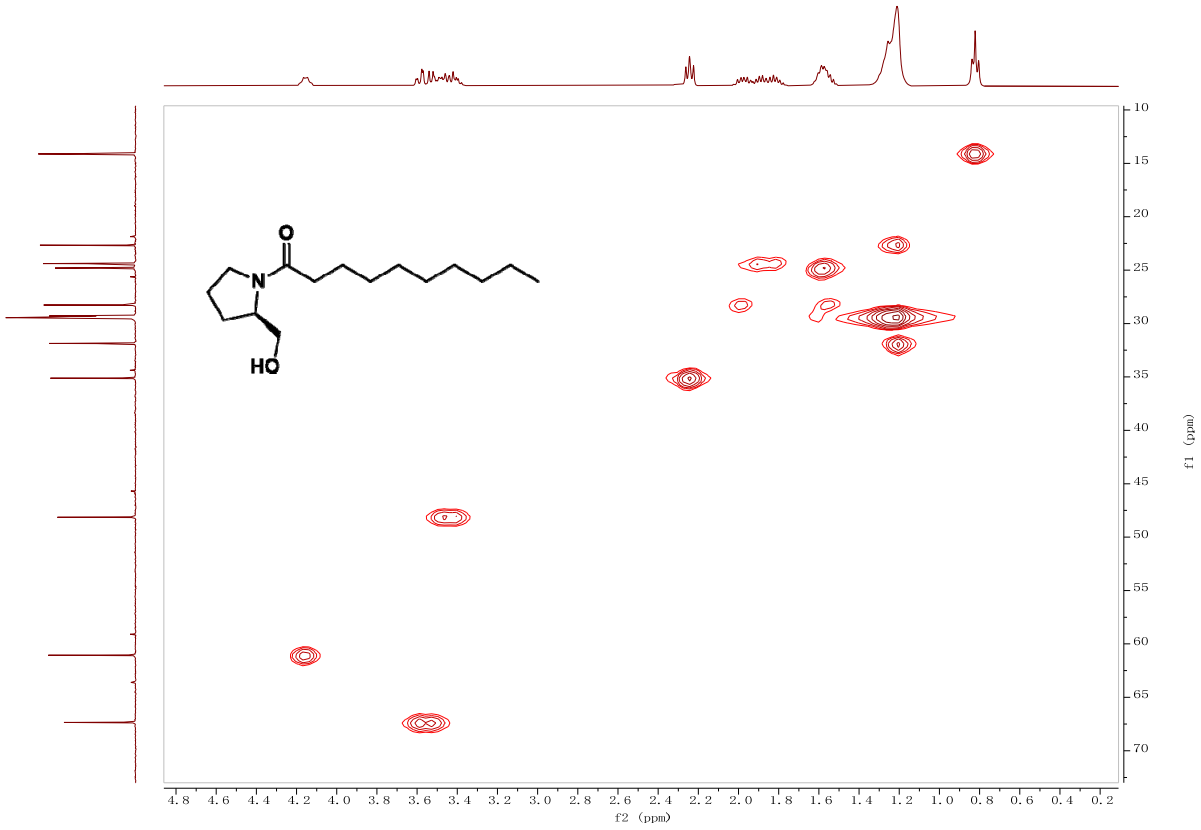


Fig. S39. HSQC spectrum of compound **4**.

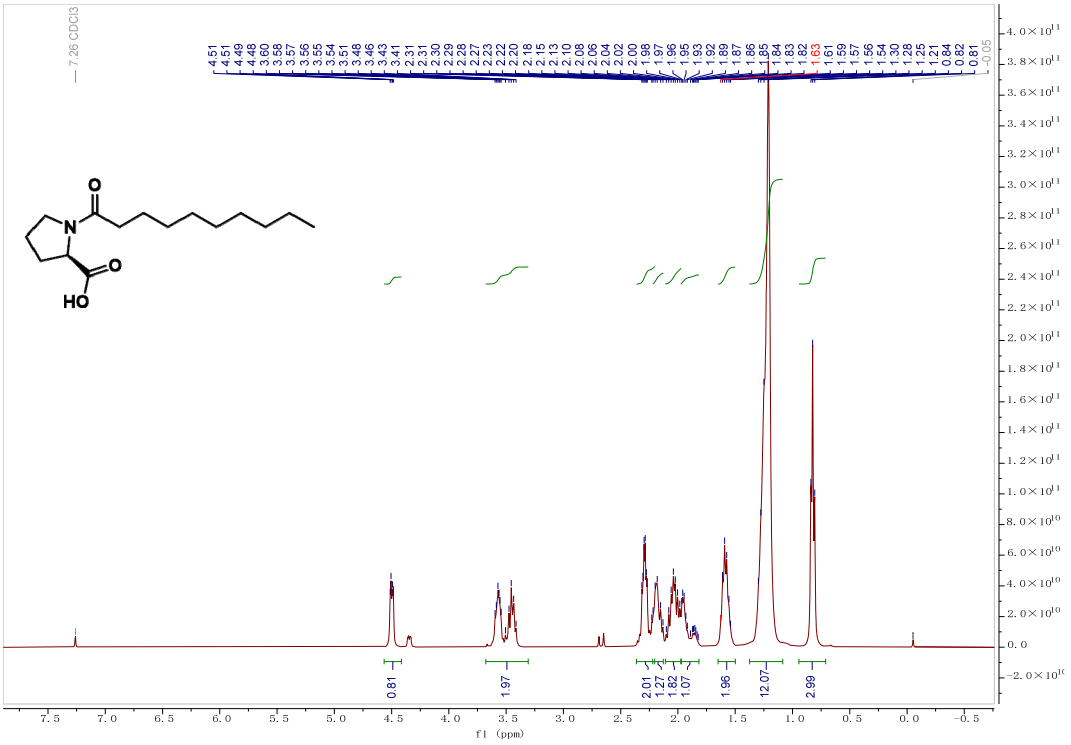


Fig. S40. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **5**.

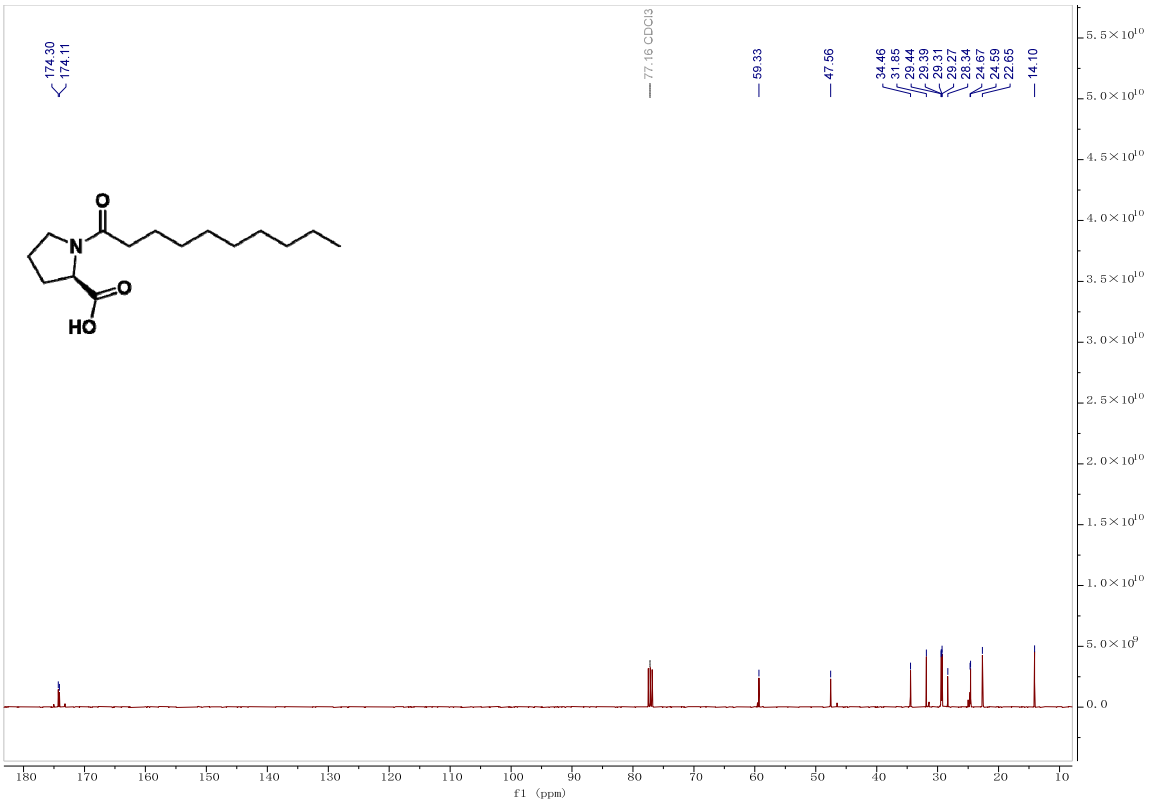


Fig. S41. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **5**.

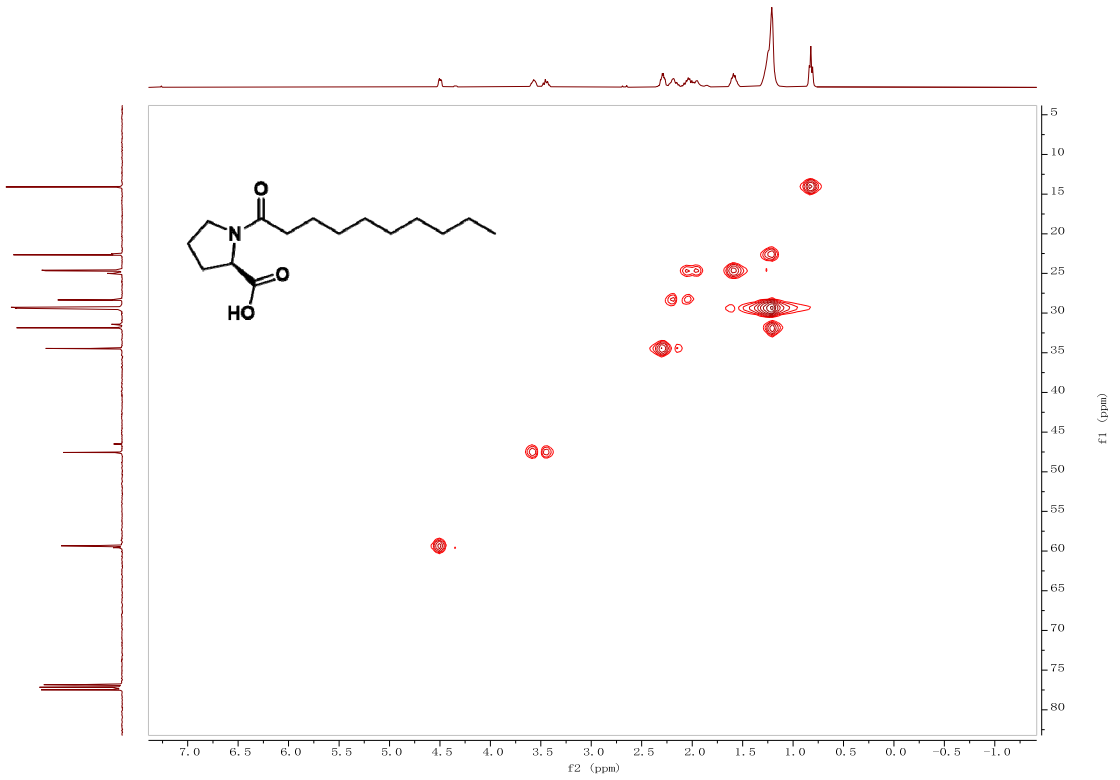


Fig. S42. HSQC spectrum of compound **5**.

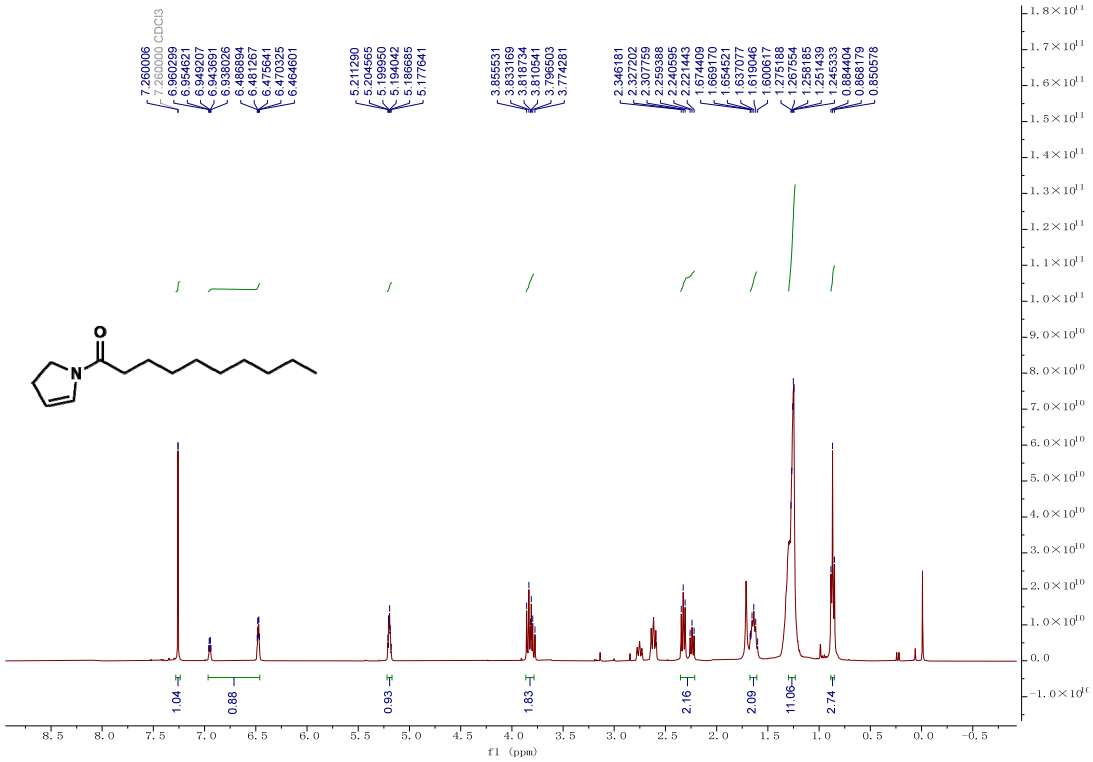


Fig. S43. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **7**.

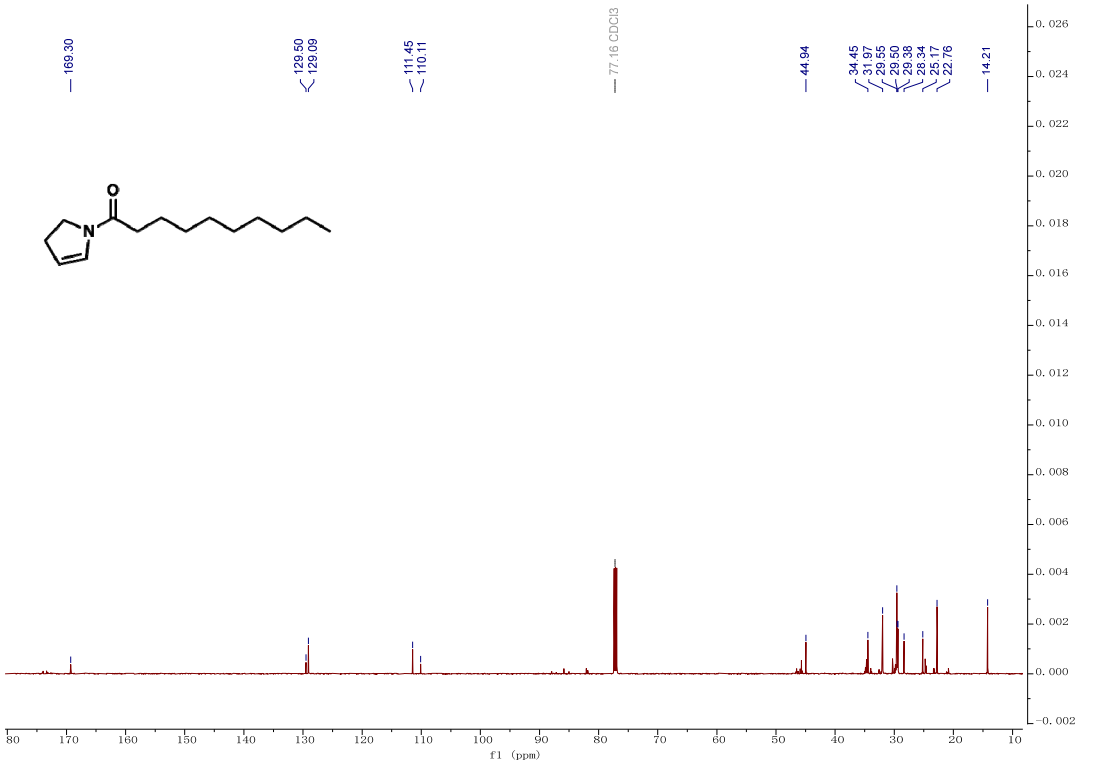


Fig. S44. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **7**.

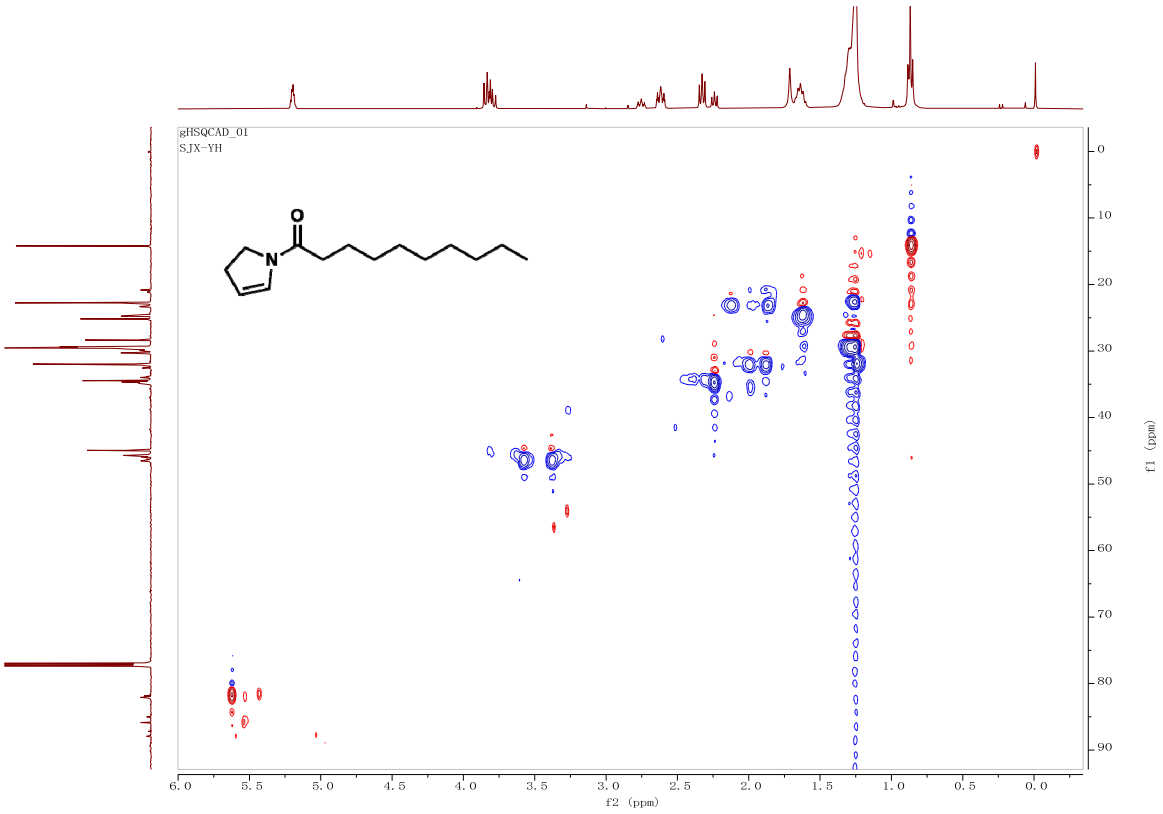


Fig. S45. HSQC spectrum of compound **7**.

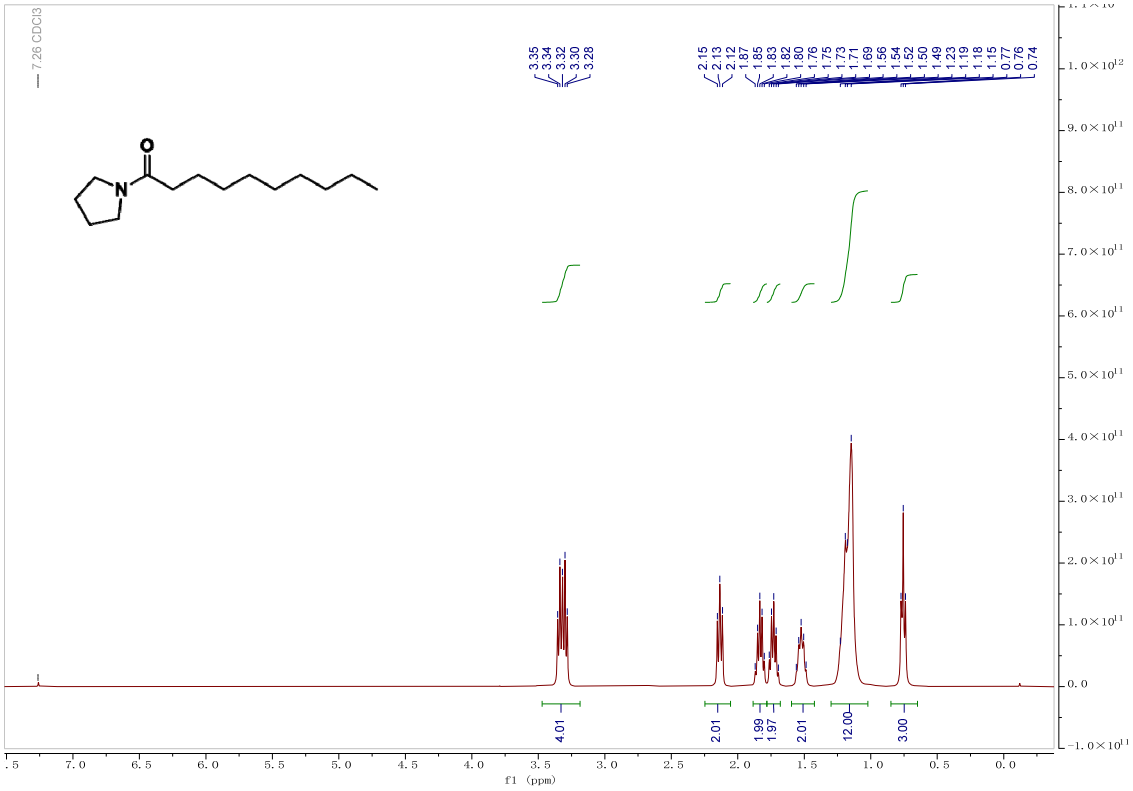


Fig. S46. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$.) of compound **8**.

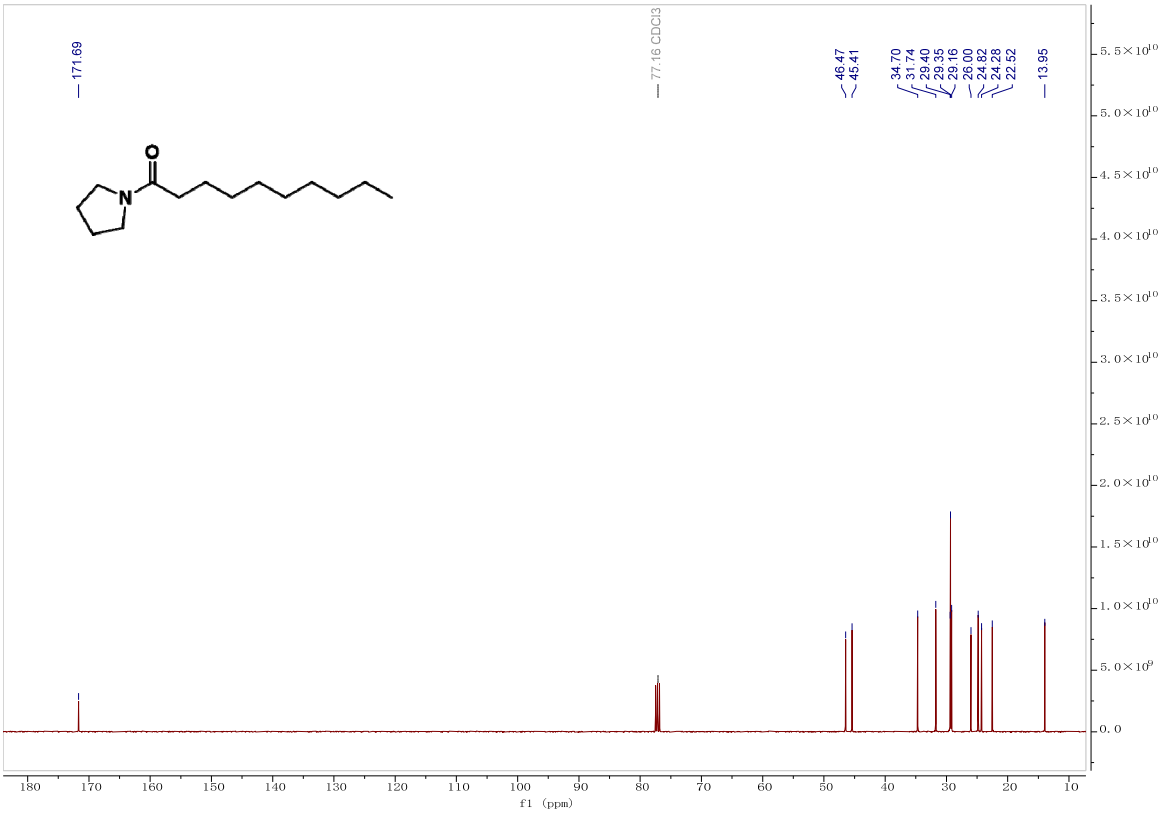


Fig. S47. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$.) of compound **8**.

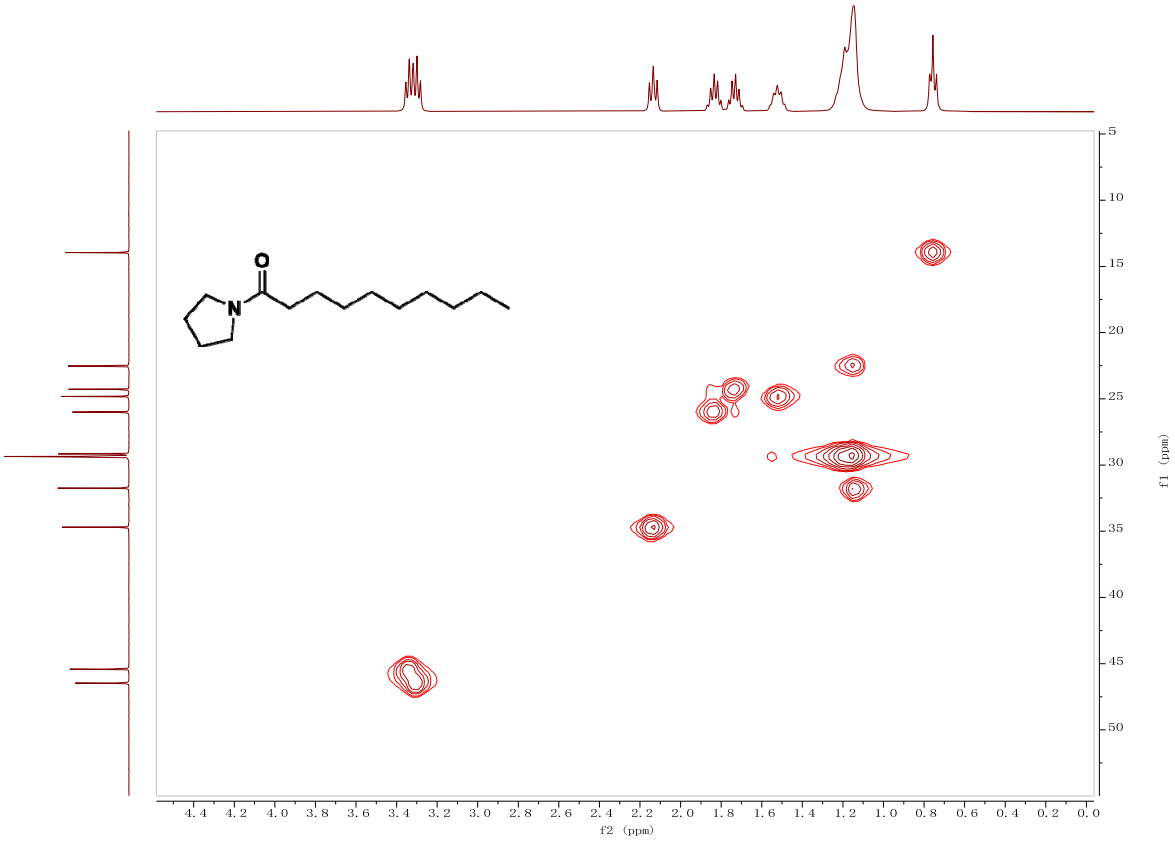


Fig. S48. HSQC spectrum of compound **8**.

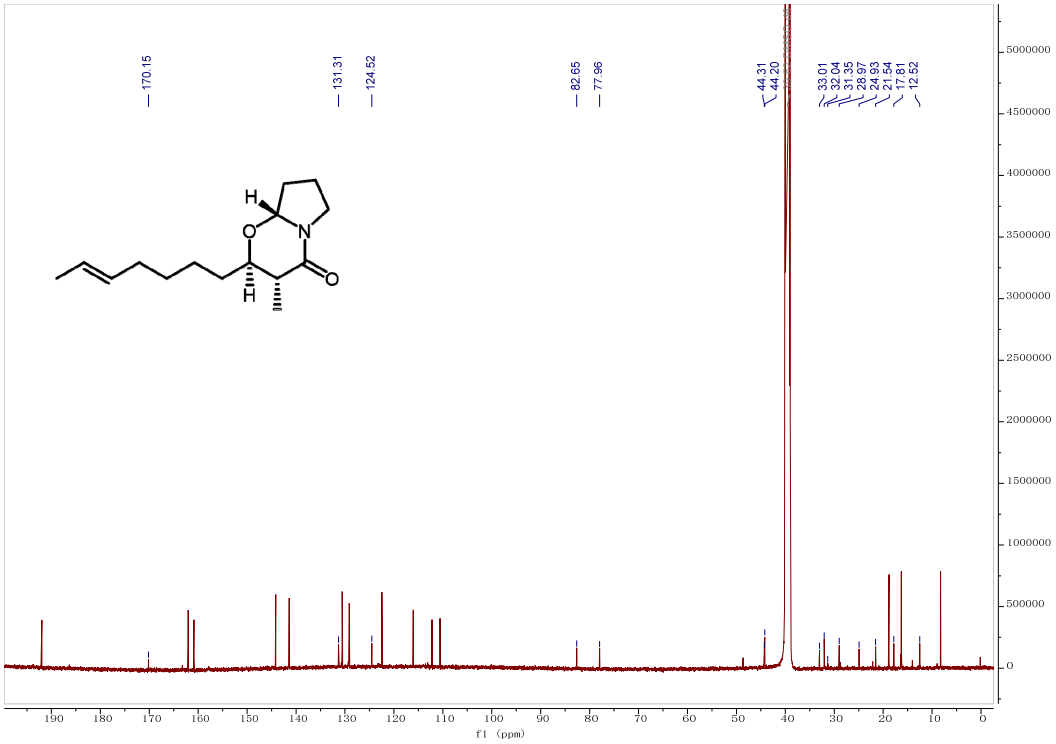


Fig. S49. ^{13}C-NMR spectrum (125 MHz, DMSO-d_6.) of compound **1''**.

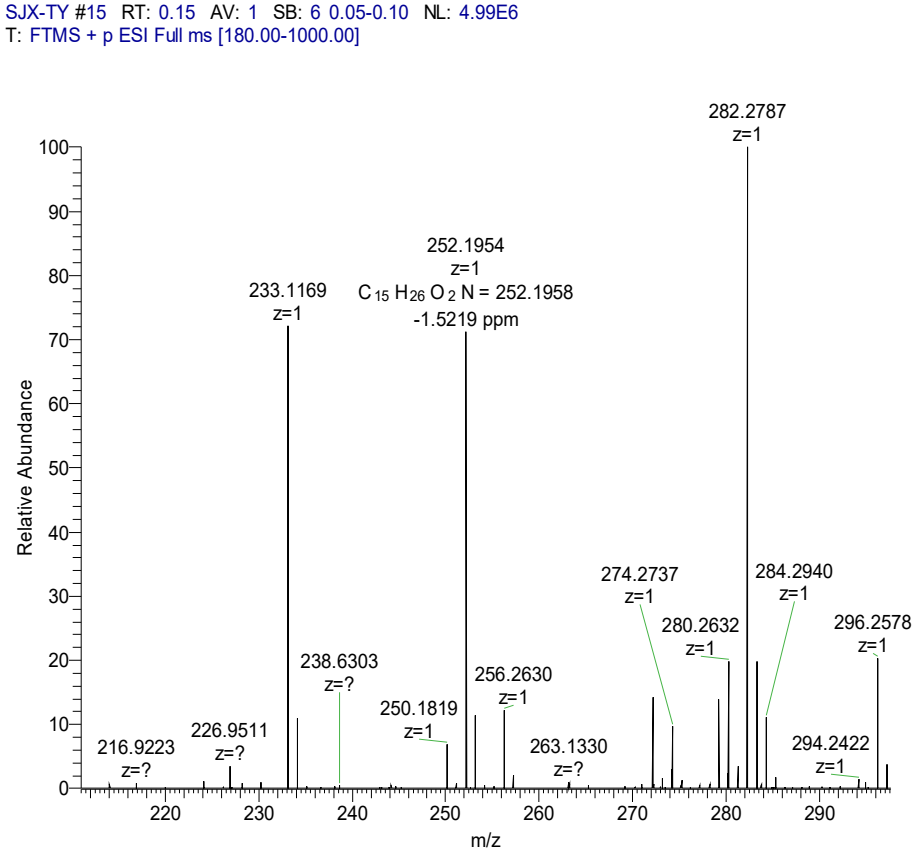


Fig. S50. HRESIMS and UV/vis spectrum of compound **1''**.

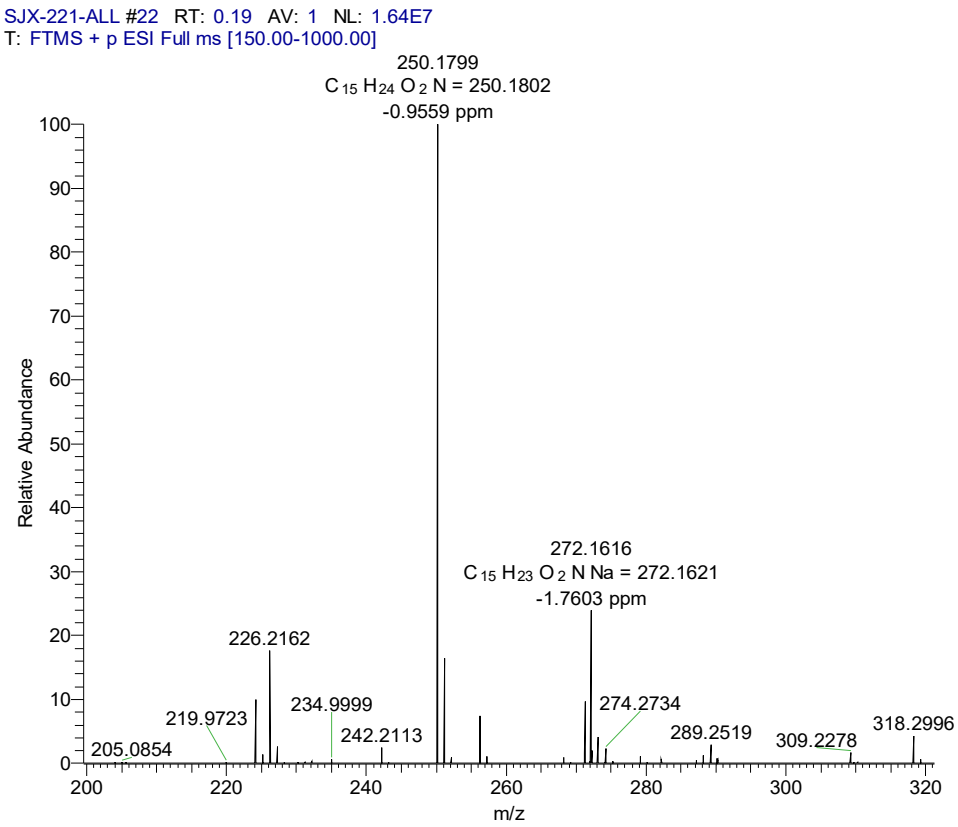


Fig. S51. HRESIMS and UV/vis spectrum of compound **1**.

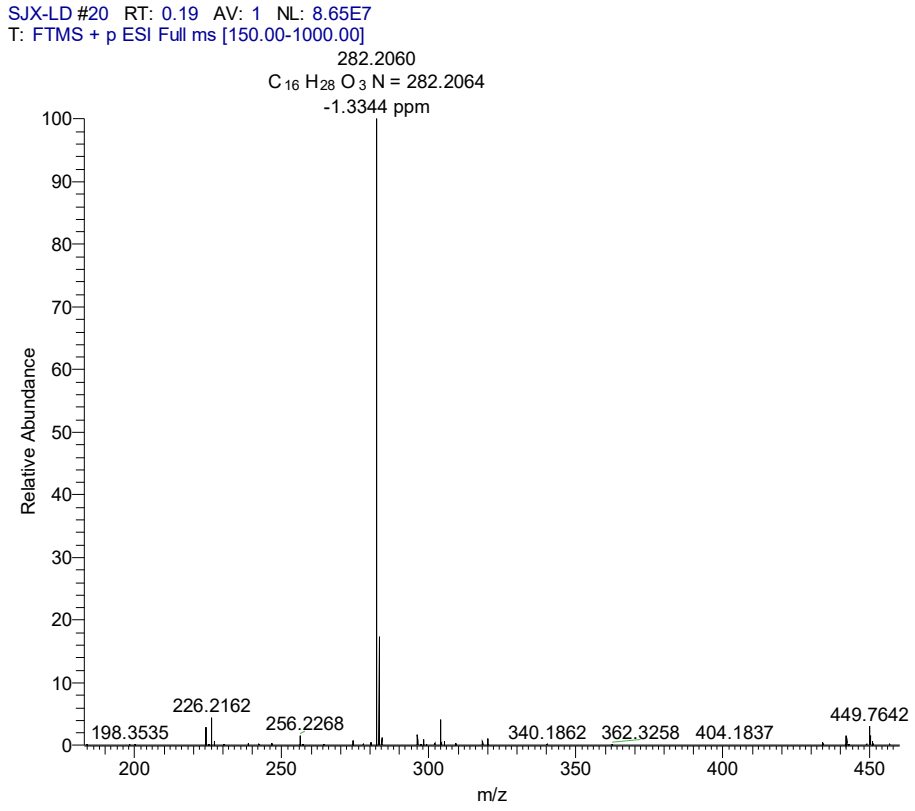


Fig. S52. HRESIMS and UV/vis spectrum of compound **2**.

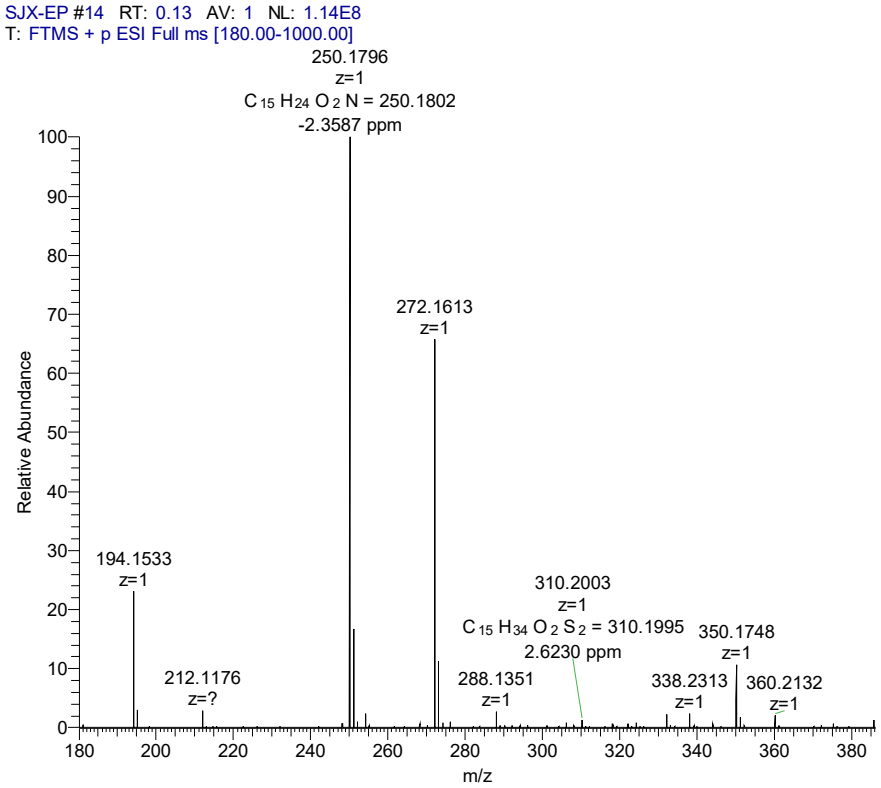


Fig. S53. HRESIMS and UV/vis spectrum of compound **3**.

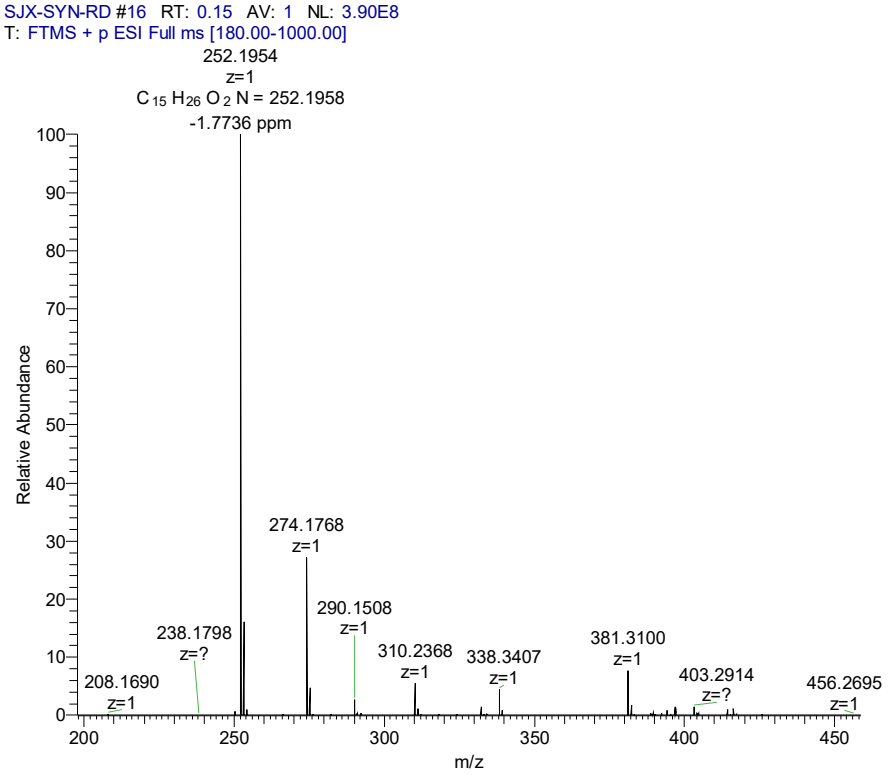


Fig. S54. HRESIMS and UV/vis spectrum of compound **3c-keto**.

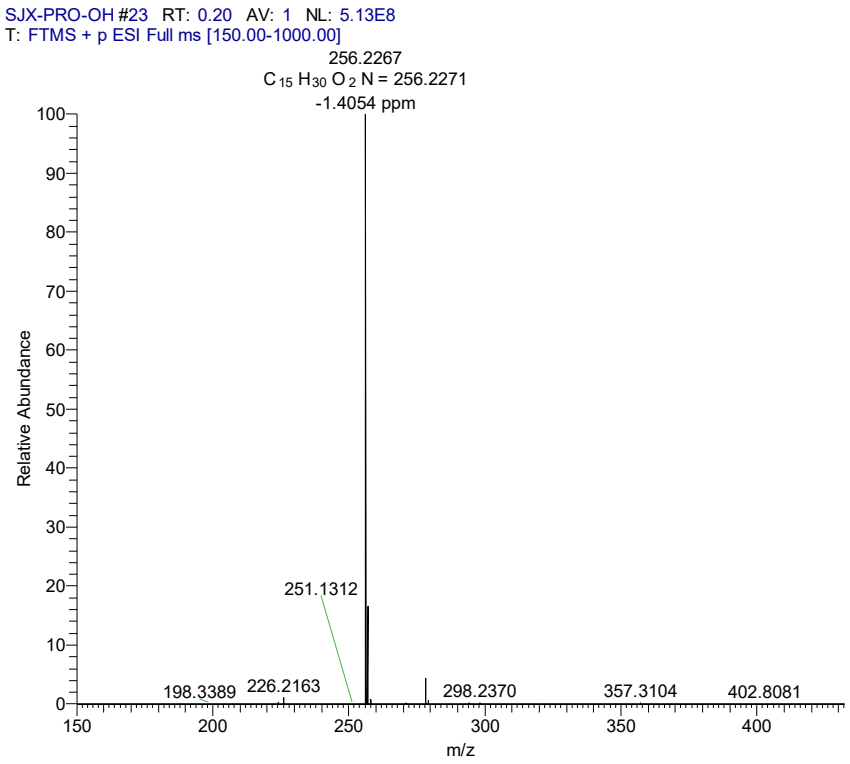


Fig. S55. HRESIMS and UV/vis spectrum of compound **4**.

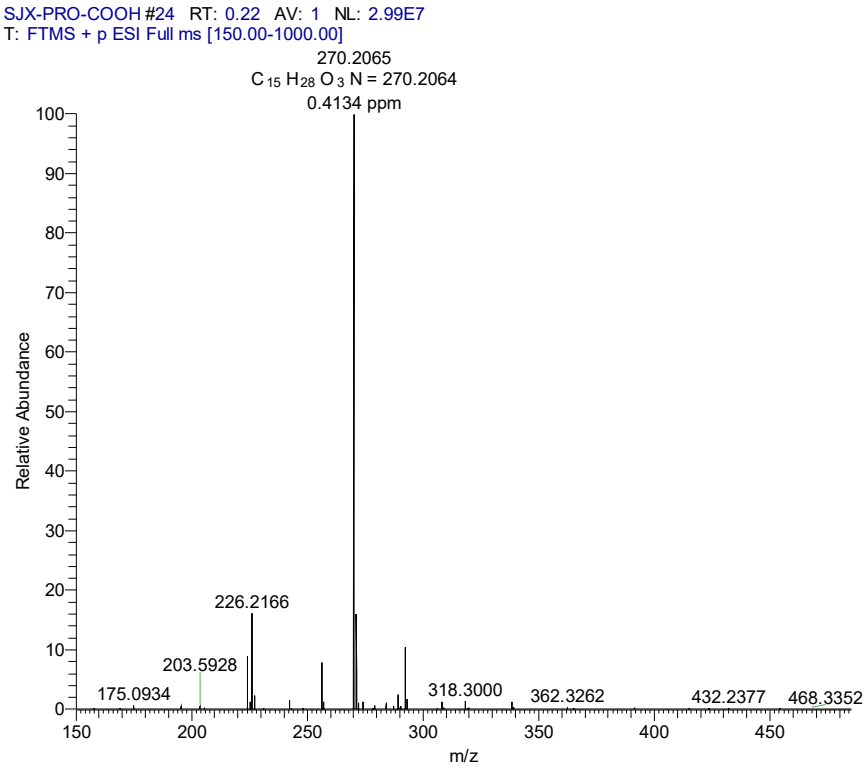


Fig. S56. HRESIMS and UV/vis spectrum of compound **5**.

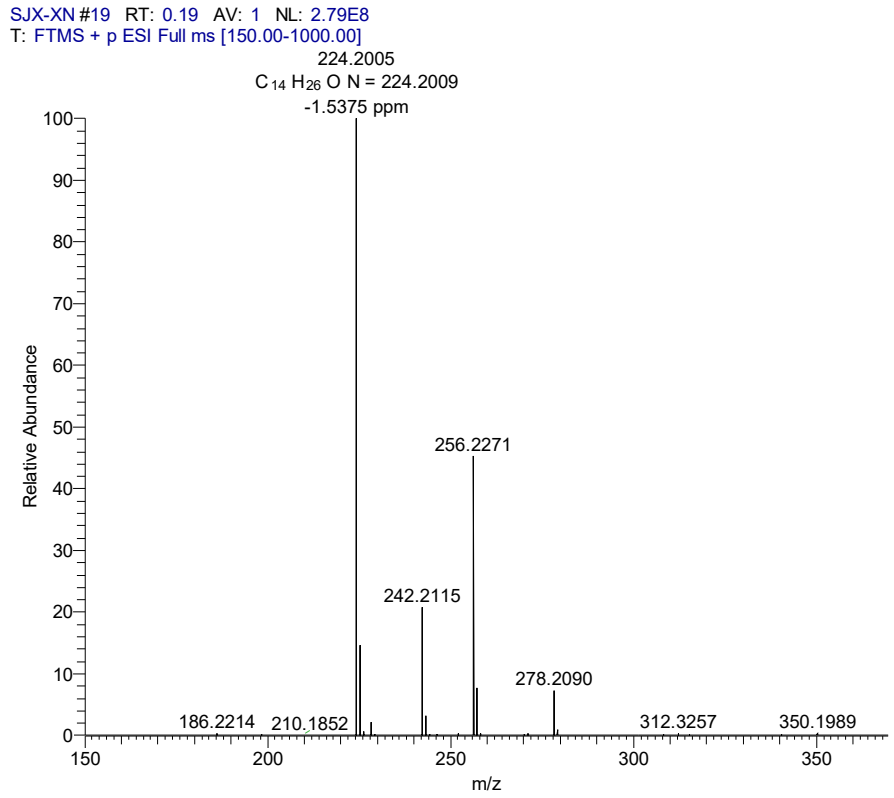


Fig. S57. HRESIMS and UV/vis spectrum of compound **7**.

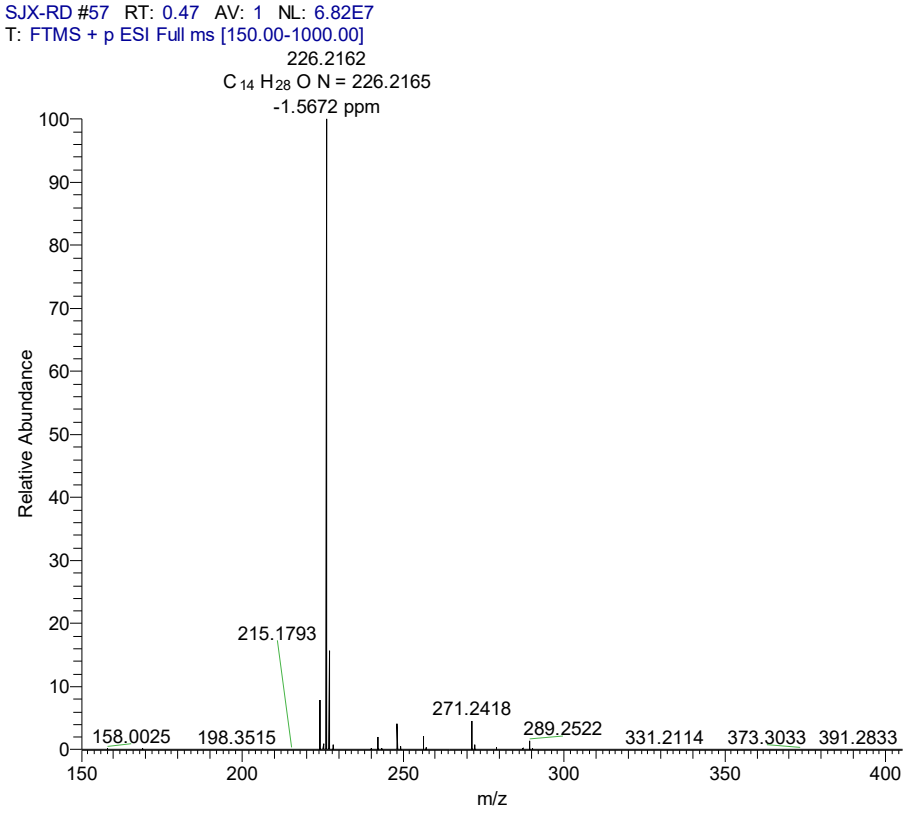


Fig. S58. HRESIMS and UV/vis spectrum of compound **8**.

Molecular Coordinates of Calculated Structures for Pathway Verification

For non-HEME-involved reactions:

DFT-optimizeation: opt freq b3lyp/6-31+g(d) scrf=(cpcm,solvent=water) em=gd3;

Main Single-Point Energy (Hartree): b3lyp/6-311+g(d,p) scrf=(cpcm,solvent=water) em=gd3;

Restrictive optimization: opt=modredundant 6-31g(d) em=gd3 m062x

Transition state calculation: opt=(calcfc,ts,noeigen) freq b3lyp/6-31g(d) em=gd3

For HEME-involved reactions:

DFT-optimizeation: opt freq b3lyp def2svp empiricaldispersion=gd3bj scf=xqc

Main Single-Point Energy (Hartree): b3lyp def2tzvp empiricaldispersion=gd3bj

Transition state calculation: (1) opt=(calcfc,ts,noeigen,gdiis) freq b3lyp def2svp empiricaldispersion=gd3bj; (2) freq b3lyp def2svp empiricaldispersion=gd3bj

Correction (Hartree): ZPE + $\Delta G_{0\to T}$

3d				**TS3e'**			
0 1				0 1			
C	-0.61710000	-0.63510000	4.49560000	C	1.77714800	-0.60919800	1.00124400
N	0.15560000	-0.87920000	5.60580000	N	1.53220100	0.63993500	0.32382700
C	0.32950000	-2.14900000	6.30870000	C	1.68929300	0.88717500	-0.95233900
O	-0.87640000	0.49070000	4.14080000	O	2.23055600	-0.56302200	2.11005300
C	0.86620000	0.17730000	6.31270000	C	1.07002500	1.81689200	1.10207500
C	1.92800000	-0.56620000	7.13300000	C	0.78656900	2.85525200	0.00655000
C	1.18090000	-1.83920000	7.54370000	C	1.55389800	2.34803800	-1.22557200
C	-1.10080000	-1.84270000	3.67800000	C	1.30249600	-1.88137800	0.32236900
O	0.97530000	-3.14210000	5.53600000	O	-0.12965500	0.02645400	-1.95127100
C	0.02790000	-2.57540000	2.94820000	C	-0.24044500	-1.81146000	0.38362100
C	-0.24720000	-3.96900000	2.41170000	C	-1.02183800	-2.68625500	-0.55399600
C	-2.14360000	-2.73020000	4.37360000	C	1.87136600	-2.22646600	-1.06087100
O	1.10190000	-2.04300000	2.77390000	O	-0.75003100	-1.08246800	1.20506900
H	-0.64740000	-2.55730000	6.64880000	H	2.20777100	0.18620900	-1.58844800
H	1.34750000	0.89890000	5.61320000	H	0.16613200	1.53040600	1.64272300
H	0.15440000	0.72230000	6.97590000	H	1.86588900	2.09272500	1.79823700
H	2.79380000	-0.83570000	6.48140000	H	-0.28349800	2.83499600	-0.19692400
H	2.30170000	0.02360000	8.00020000	H	1.09485100	3.85840300	0.30379900
H	0.52190000	-1.60720000	8.41510000	H	2.56973700	2.76264900	-1.28946400
H	1.86380000	-2.66780000	7.83680000	H	1.05189900	2.53260500	-2.17494400
H	-1.65580000	-1.38340000	2.81710000	H	1.59027700	-2.66691700	1.03268300
H	1.28400000	-3.86220000	6.08850000	H	-0.18901100	0.41237700	-2.83758800
H	-1.16000000	-3.96180000	1.77480000	H	-0.62073900	-3.70505300	-0.57096000
H	0.59980000	-4.33500000	1.78880000	H	-2.07019900	-2.68203100	-0.25796600
H	-0.38730000	-4.68820000	3.24900000	H	-0.93554000	-2.24894600	-1.55489300
H	-2.78910000	-3.25810000	3.63440000	H	1.70230100	-3.28760200	-1.26061900
H	-2.81940000	-2.12150000	5.01690000	H	2.95324900	-2.06206000	-1.09578900
H	-1.68750000	-3.52390000	5.00180000	H	1.36617800	-1.64797500	-1.83820300
C	6.06540000	-3.31350000	4.98320000	C	-3.84301800	0.25109900	0.82493900
C	4.78520000	-2.77160000	4.38640000	C	-2.60838900	0.67755000	0.06306900
O	4.67650000	-2.10920000	3.38300000	O	-1.88805700	1.58370700	0.45707800
O	3.71460000	-3.12030000	5.12690000	O	-2.39296300	-0.04144600	-1.00782400
H	6.94190000	-3.01890000	4.36290000	H	-4.16561300	1.04641700	1.49665500
H	6.21610000	-2.91000000	6.01010000	H	-4.64545200	-0.03078700	0.14073300
H	6.03170000	-4.42560000	5.02960000	H	-3.57083500	-0.62859300	1.41724500
H	2.92040000	-2.75160000	4.70630000	H	-1.39421700	0.11034500	-1.40444200
3a'-keto				**3a'**			

0 1			
C	-0.11342300	1.11738900	-0.20775800
N	1.05024000	0.24429500	-0.03766800
C	1.06152800	-1.03147000	0.19223400
O	0.09425900	2.17332100	-0.74923900
C	2.42574300	0.78965600	-0.29564000
C	3.33459600	-0.34660300	0.20247600
C	2.42630400	-1.59837700	0.18691900
C	-1.46185100	0.69563800	0.34907600
C	-2.10936100	-0.42374900	-0.48437600
C	-3.51557000	-0.81176500	-0.11186300
C	-1.43440100	0.39977700	1.86947600
O	-1.49525400	-0.96086500	-1.39512000
H	0.14888900	-1.59666400	0.32763300
H	2.49940900	0.97750800	-1.36939700
H	2.53503500	1.73192600	0.24018900
H	4.21396600	-0.46341000	-0.43209600
H	3.66738000	-0.14286900	1.22334900
H	-2.08863000	1.58269700	0.19615100
H	-4.12023400	0.06086500	0.15446800
H	-3.97526600	-1.35901800	-0.93737900
H	-3.48075500	-1.46723500	0.76831300
H	-2.45997200	0.33402200	2.24025000
H	-0.93557700	1.21536300	2.40037100
H	-0.92368600	-0.53540800	2.11225400
H	2.71655845	-2.62818932	0.17513137

0 1			
C	-0.23487100	1.14897300	-0.02881500
N	1.01519000	0.34541500	0.04667400
C	1.29504700	-0.51518300	0.96321000
O	-0.05554500	2.34453700	-0.18123200
C	2.13280700	0.55262600	-0.92336100
C	3.31395800	-0.17563600	-0.25069000
C	2.65920700	-1.08212200	0.82237500
C	-1.51601500	0.48576700	0.11904500
C	-1.73564200	-0.83590500	-0.18950900
C	-3.07732300	-1.49880000	-0.14106300
C	-2.67093300	1.40294500	0.48907600
O	-0.72084400	-1.61891800	-0.61559600
H	0.56912800	-0.77115500	1.72854500
H	1.82152300	0.10432600	-1.87159300
H	2.28054500	1.62305600	-1.06333800
H	3.89383900	-0.74837700	-0.97592900
H	3.97986800	0.54766700	0.22655400
H	-3.02525500	-2.39679100	0.48783000
H	-3.85618600	-0.84726500	0.25045500
H	-3.36853000	-1.81724700	-1.15083400
H	-2.28814700	2.37842400	0.79383400
H	-3.25034000	0.99725100	1.32426000
H	-3.35424200	1.56505500	-0.35269800
H	-1.03115900	-2.52266200	-0.79816800
H	3.08772231	-1.91618556	1.33775118

3b'-keto			
1 1			
C	-2.09180500	0.32385300	-0.65348200
N	-1.06767000	1.22181200	-0.10674300
C	-0.68661400	1.34479300	1.13207900
O	-2.86277000	0.79671800	-1.44507500
C	-0.31753800	2.14655200	-1.01876200
C	0.32296800	3.13562200	-0.03054100
C	0.39427600	2.31616600	1.27616300
C	-2.04010900	-1.14265600	-0.25209700
C	-0.67817800	-1.68419800	-0.75190400
C	-0.15893000	-2.95915900	-0.15365300
C	-2.40893400	-1.46982200	1.21009300
O	-0.11213100	-1.06200000	-1.63355300
H	-1.07981000	0.71819700	1.91882100
H	0.43289400	1.53121500	-1.52015200
H	-1.01852100	2.57564700	-1.73451700
H	1.31808700	3.42669600	-0.36833800
H	-0.29965900	4.02895300	0.09155900
H	0.39444600	2.86185500	2.22159900
H	1.32040700	1.67294400	1.18574900
H	-2.79340500	-1.60262600	-0.90553100
H	-0.93624300	-3.73373000	-0.14956100
H	0.72172400	-3.28673700	-0.70509500
H	0.13801600	-2.75771900	0.88124500
H	-2.66352700	-2.53147400	1.28014600
H	-3.29199300	-0.90211800	1.52342600
H	-1.57868800	-1.28614800	1.89698300

3b'			
1 1			
C	0.09010000	0.90650000	0.75620000
N	1.00860000	-0.13250000	0.33220000
C	1.19740000	-1.25520000	0.96400000
O	0.58900000	1.73900000	1.48480000
C	1.97470000	0.01740000	-0.82580000
C	3.00660000	-1.08360000	-0.49980000
C	2.26080000	-2.12560000	0.35890000
C	-1.21530000	0.97750000	0.35790000
C	-1.71950000	0.02180000	-0.45230000
C	-3.12050000	0.00210000	-1.01730000
C	-2.02510000	2.15300000	0.87020000
O	-0.96660000	-1.02930000	-0.86240000
H	0.60870000	-1.54660000	1.84410000
H	1.45290000	-0.18410000	-1.78910000
H	2.43130000	1.03270000	-0.85100000
H	3.47480000	-1.52560000	-1.40800000
H	3.82070000	-0.63000000	0.11770000
H	2.92130000	-2.58220000	1.13020000
H	1.78120000	-2.91870000	-0.25930000
H	-3.69930000	-0.82840000	-0.55300000
H	-3.70060000	0.93850000	-0.89610000
H	-3.07330000	-0.18410000	-2.11460000
H	-1.93050000	2.24670000	1.97600000
H	-3.11650000	2.08360000	0.69130000
H	-1.66840000	3.09870000	0.40180000
H	-1.15200000	-1.32410000	-1.76730000

3c'-keto			
0 1			
C	0.00478000	1.13712700	-0.13355800
N	1.03026900	0.26344500	0.01583800
C	1.01366200	-1.10030100	0.38183600
O	0.21130400	2.28709600	-0.55918100
C	2.41946000	0.65542000	-0.33178100
C	3.27513800	-0.58918300	0.02253500
C	2.24211900	-1.62914400	0.39255400
C	-1.40625500	0.71723000	0.29007800
C	-1.98520400	-0.40873300	-0.57469000
C	-3.27078100	-1.04904500	-0.10988600
C	-1.52951700	0.51205700	1.81677600
O	-1.44520700	-0.73710800	-1.62319500
H	2.45973000	0.90408800	-1.39677700
H	2.69494500	1.54816700	0.23405300
H	3.89711300	-0.90528200	-0.82283000
H	3.95588800	-0.38708600	0.85956600
H	-2.02946600	1.58566100	0.03349300
H	-4.00319600	-0.28968200	0.18722100
H	-3.68075500	-1.67658500	-0.90397600
H	-3.07477600	-1.66803300	0.77492200
H	-2.57888300	0.42199400	2.11023600
H	-1.11114400	1.38009800	2.33589600
H	-0.99915800	-0.37828400	2.16505600
H	0.58635020	-1.19324679	1.35839409
H	0.40844858	-1.64043033	-0.31592974
H	2.45539588	-2.00477084	1.37149090
H	2.28517571	-2.43427400	-0.31087460

3c'			
0 1			
C	-0.04104300	1.01992400	-0.25543700
N	1.06392200	0.27759300	0.01047600
C	1.16831400	-0.91868300	0.74784800
O	0.06350400	2.11625400	-0.84200800
C	2.41216400	0.70265300	-0.43487400
C	3.35185800	-0.44436600	0.02711400
C	2.42986200	-1.36205600	0.80040900
C	-1.37943800	0.52808800	0.21613900
C	-1.89906300	-0.61862900	-0.26642300
C	-3.24188400	-1.21627400	0.03878600
C	-2.09136200	1.49359400	1.13477900
O	-1.14075900	-1.34898200	-1.16170100
H	2.40620100	0.84667700	-1.51827600
H	2.65637200	1.66236000	0.03075800
H	3.80965700	-0.95938100	-0.82737700
H	4.17448700	-0.06695600	0.64615300
H	-3.11815000	-2.21886800	0.47052000
H	-3.82059500	-0.61794800	0.74242300
H	-3.82881300	-1.32329500	-0.88304500
H	-1.51463600	1.65081600	2.05644500
H	-3.08677100	1.14888600	1.42138400
H	-2.19725300	2.47243000	0.65141900
H	-1.59326200	-2.17743400	-1.38502500
H	0.81831323	-0.74539200	1.74402554
H	0.55552197	-1.66571515	0.28814276
H	2.74720414	-1.40145782	1.82150716
H	2.47588598	-2.34446654	0.37892196

***R*-1'**			
0 1			
C	-12.96250000	1.00440000	0.59510000
N	-12.94990000	-0.34890000	0.55510000
C	-11.72700000	-1.12570000	0.35940000
O	-10.95280000	-0.58820000	-0.62810000
C	-11.01550000	0.82190000	-0.63500000
C	-11.93080000	1.62940000	-0.03560000
C	-14.12410000	-1.22800000	0.74450000
C	-13.63000000	-2.66070000	0.65210000
C	-12.16170000	-2.60240000	0.13370000
C	-9.81310000	1.34740000	-1.29950000
C	-11.81310000	3.16120000	-0.33260000
O	-13.85120000	1.64260000	1.07480000
H	-11.07260000	-1.07030000	1.24440000
H	-14.70820000	-1.03190000	1.70300000
H	-14.96320000	-0.99770000	0.01000000
H	-14.26410000	-3.28800000	-0.02350000
H	-13.59170000	-3.06270000	1.68200000
H	-11.36350000	-3.30800000	0.54300000
H	-12.14630000	-2.79610000	-0.96300000
H	-10.01450000	1.24810000	-2.40850000
H	-9.40130000	2.41260000	-1.21700000
H	-8.93990000	0.62640000	-1.26640000
H	-11.44740000	3.48820000	-1.39380000

***S*-1'**			
0 1			
C	-0.83840000	0.86220000	0.68870000
N	-0.54300000	-0.46230000	0.80040000
C	0.18010000	-1.20830000	-0.20070000
O	1.09890000	-0.43180000	-0.91390000
C	0.75250000	0.88770000	-1.04260000
C	-0.20500000	1.51900000	-0.32450000
C	-0.90250000	-1.30970000	1.92530000
C	-0.28310000	-2.67940000	1.58550000
C	0.83330000	-2.34310000	0.58050000
C	1.59630000	1.58740000	-2.08920000
C	-0.55940000	2.97940000	-0.52680000
O	-1.60650000	1.39210000	1.45700000
H	-0.56400000	-1.61490000	-0.92860000
H	-0.44260000	-0.89770000	2.85420000
H	-2.00710000	-1.37390000	2.05340000
H	-1.04560000	-3.32280000	1.08360000
H	0.09310000	-3.22130000	2.48270000
H	1.12420000	-3.20570000	-0.06020000
H	1.73310000	-1.97060000	1.12530000
H	2.66170000	1.28230000	-1.97590000
H	1.25970000	1.28840000	-3.10780000
H	1.60180000	2.69480000	-2.02670000
H	-1.65480000	3.15030000	-0.42300000

H	-12.75180000	3.68780000	-0.00060000
H	-11.10020000	3.54740000	0.40530000

H	-0.03070000	3.61310000	0.22130000
H	-0.32820000	3.36050000	-1.54340000

AcOH			
0 1			
C	-11.84810000	-0.55220000	-0.00080000
C	-10.48050000	0.09460000	-0.00090000
O	-9.41230000	-0.46800000	0.00120000
O	-10.57540000	1.43890000	-0.00350000
H	-11.75640000	-1.66180000	-0.00070000
H	-12.41940000	-0.25160000	0.90660000
H	-12.41980000	-0.25170000	-0.90790000
H	-9.67680000	1.80760000	-0.00250000

AcO^-			
-1 1			
C	3.25150600	-0.85100300	-1.42004400
C	2.54137600	-0.30542700	-0.18057100
O	2.38800000	0.94569300	-0.10319100
O	2.12239500	-1.16993200	0.64719000
H	3.88790800	-0.08949900	-1.87823900
H	3.83903600	-1.73847300	-1.16674000
H	2.48072200	-1.14913100	-2.14043000

CO_2			
0 1			
O	0.00000000	0.00000000	-0.59997300
C	0.00000000	0.00000000	0.70132700
O	-0.00000000	0.00000000	1.95972700

O_2			
0 3			
O	0.71381200	-0.08191700	-0.68452200
O	1.15801807	0.52585346	-1.76881718

H_2O			
0 1			
H	-12.41760000	-0.07710000	0.00450000
O	-11.59990000	0.39060000	-0.00640000
H	-10.94640000	-0.28780000	0.00450000

His			
0 1			
N	-3.44030000	-1.67930000	0.12380000
C	-2.73290000	-0.64360000	-0.05300000
C	-3.59050000	0.38470000	0.01180000
N	-4.76290000	-0.04670000	0.22210000
C	-4.63980000	-1.30420000	0.28490000
C	-3.29850000	1.84660000	-0.12650000
H	-3.09550000	-2.66610000	0.13520000
H	-1.65190000	-0.67300000	-0.21780000
H	-5.44970000	-2.02190000	0.45720000
H	-2.20610000	2.02830000	-0.24050000
H	-3.81380000	2.26100000	-1.02260000
H	-3.64850000	2.40150000	0.77340000

$His+H^+$			
1 1			
N	-3.44030000	-1.67930000	0.12380000
C	-2.73290000	-0.64360000	-0.05300000
C	-3.59050000	0.38470000	0.01180000
N	-4.76290000	-0.04670000	0.22210000
C	-4.63980000	-1.30420000	0.28490000
C	-3.29850000	1.84660000	-0.12650000
H	-3.09550000	-2.66610000	0.13520000
H	-1.65190000	-0.67300000	-0.21780000
H	-5.44970000	-2.02190000	0.45720000
H	-2.20610000	2.02830000	-0.24050000
H	-3.81380000	2.26100000	-1.02260000
H	-3.64850000	2.40150000	0.77340000
H	-5.60173294	0.48925813	0.31753678

3a_pre1			
0 1			
C	-5.51150000	3.91980000	5.23790000
N	-5.01900000	4.40040000	4.17180000
C	-5.60330000	5.68380000	3.67240000
O	-5.42460000	1.85730000	3.22800000
C	-5.64530000	1.62020000	4.55010000
C	-5.70950000	2.58600000	5.49920000
C	-4.04940000	4.07950000	3.41750000
C	-3.89120000	4.88300000	2.36230000
C	-4.94160000	5.94590000	2.30580000
C	-5.92500000	0.15260000	4.84740000
C	-6.59080000	-0.63900000	3.70540000
C	-7.98620000	-0.09940000	3.34730000
C	-8.63260000	-0.89640000	2.20370000
C	-9.99140000	-0.33810000	1.85970000
C	-10.28950000	0.23850000	0.68540000

3a_pre2			
0 1			
C	-5.30440000	3.73960000	4.99130000
N	-5.34490000	4.32620000	3.86660000
C	-6.44940000	5.31240000	3.65420000
O	-2.71940000	4.84570000	4.41410000
C	-2.93290000	3.85600000	5.32560000
C	-4.15930000	3.39220000	5.66630000
C	-4.68170000	4.22670000	2.78830000
C	-5.06680000	5.07530000	1.83160000
C	-6.16660000	5.97730000	2.29320000
C	-1.64040000	3.44150000	6.01170000
C	-0.45700000	3.29620000	5.03440000
C	-0.70470000	2.21080000	3.97280000
C	0.48620000	2.06140000	3.01370000
C	0.21490000	0.99460000	1.98180000
C	0.09600000	1.23550000	0.66710000

C	-11.64270000	0.80410000	0.34730000
C	-6.06240000	2.22900000	6.93880000
O	-5.82100000	4.71280000	6.10970000
H	-5.35420000	6.52770000	4.36030000
H	-6.71200000	5.61430000	3.56790000
H	-3.41180000	3.21770000	3.65390000
H	-3.11200000	4.76730000	1.59670000
H	-5.62810000	5.75010000	1.45040000
H	-4.49730000	6.96360000	2.22540000
H	-4.94180000	-0.32180000	5.08270000
H	-6.58910000	0.01980000	5.73020000
H	-6.69370000	-1.70640000	4.01920000
H	-5.93450000	-0.64870000	2.80420000
H	-7.91550000	0.97170000	3.04450000
H	-8.64080000	-0.14320000	4.25030000
H	-8.75250000	-1.96590000	2.49620000
H	-7.96430000	-0.87180000	1.31170000
H	-10.76770000	-0.40970000	2.63950000
H	-9.51230000	0.31710000	-0.09320000
H	-12.37190000	0.68750000	1.17990000
H	-11.55540000	1.89060000	0.11810000
H	-12.05920000	0.28830000	-0.54760000
H	-5.79020000	1.19340000	7.23000000
H	-7.15080000	2.37870000	7.12320000
H	-5.48660000	2.83390000	7.67500000
H	-5.89380000	1.21560000	2.67390000

C	-0.18450000	0.17080000	-0.35920000
C	-4.35190000	2.48790000	6.87860000
O	-6.37170000	3.42820000	5.48960000
H	-6.47830000	6.07490000	4.46810000
H	-7.43850000	4.79600000	3.60320000
H	-3.87800000	3.48600000	2.68530000
H	-4.61400000	5.14230000	0.83290000
H	-7.04140000	5.94910000	1.60510000
H	-5.78150000	7.01800000	2.39410000
H	-1.39590000	4.22100000	6.77240000
H	-1.71920000	2.46480000	6.53600000
H	0.46090000	3.03140000	5.61340000
H	-0.24010000	4.27010000	4.53660000
H	-1.61510000	2.46240000	3.37930000
H	-0.89940000	1.23650000	4.48130000
H	1.40560000	1.78050000	3.57900000
H	0.68890000	3.04000000	2.51960000
H	0.10100000	-0.03690000	2.35470000
H	0.20320000	2.26740000	0.29290000
H	-0.28030000	-0.84130000	0.09370000
H	-1.13480000	0.39770000	-0.89410000
H	0.64010000	0.13470000	-1.10700000
H	-3.45890000	2.33070000	7.51360000
H	-4.70570000	1.48180000	6.55620000
H	-5.08970000	2.91900000	7.59280000
H	-1.94020000	5.36440000	4.67020000

3b_pre1

1 1

C	-5.51150000	3.91980000	5.23790000
N	-5.01900000	4.40040000	4.17180000
C	-5.60330000	5.68380000	3.67240000
O	-5.42460000	1.85730000	3.22800000
C	-5.64530000	1.62020000	4.55010000
C	-5.70950000	2.58600000	5.49920000
C	-4.04940000	4.07950000	3.41750000
C	-3.89120000	4.88300000	2.36230000
C	-4.94160000	5.94590000	2.30580000
C	-5.92500000	0.15260000	4.84740000
C	-6.59080000	-0.63900000	3.70540000
C	-7.98620000	-0.09940000	3.34730000
C	-8.63260000	-0.89640000	2.20370000
C	-9.99140000	-0.33810000	1.85970000
C	-10.28950000	0.23850000	0.68540000
C	-11.64270000	0.80410000	0.34730000
C	-6.06240000	2.22900000	6.93880000
O	-5.82100000	4.71280000	6.10970000
H	-5.35420000	6.52770000	4.36030000
H	-6.71200000	5.61430000	3.56790000
H	-3.41180000	3.21770000	3.65390000
H	-3.94120000	4.29690000	1.46850000
H	-5.62810000	5.75010000	1.45040000
H	-4.49730000	6.96360000	2.22540000
H	-4.94180000	-0.32180000	5.08270000
H	-6.58910000	0.01980000	5.73020000

3b_pre2

1 1

C	-5.13280000	3.30290000	4.51340000
N	-5.45880000	4.47940000	3.73290000
C	-6.66180000	5.37260000	3.95020000
O	-3.18520000	5.21370000	4.37180000
C	-2.99330000	4.07900000	5.09000000
C	-3.94410000	3.12230000	5.16260000
C	-4.78770000	4.84320000	2.67830000
C	-5.32830000	6.07000000	2.00070000
C	-6.27260000	6.60040000	3.09940000
C	-1.64480000	4.02900000	5.77690000
C	-0.51370000	3.73140000	4.77840000
C	-0.65780000	2.35690000	4.10520000
C	0.48700000	2.07460000	3.12010000
C	0.30540000	0.72990000	2.46040000
C	0.06920000	0.56300000	1.15010000
C	-0.11850000	-0.77920000	0.49520000
C	-3.77500000	1.82340000	5.92670000
O	-6.02440000	2.48090000	4.55600000
H	-6.80670000	5.62300000	5.02530000
H	-7.57200000	4.86890000	3.55020000
H	-3.92680000	4.27620000	2.29920000
H	-4.52480000	6.79840000	1.74920000
H	-7.15380000	7.14350000	2.68980000
H	-5.70390000	7.31210000	3.74730000
H	-1.47050000	5.02290000	6.25410000
H	-1.60510000	3.30510000	6.61770000

H	-6.69370000	-1.70640000	4.01920000	H	0.46520000	3.77360000	5.31420000
H	-5.93450000	-0.64870000	2.80420000	H	-0.49020000	4.52780000	3.99690000
H	-7.91550000	0.97170000	3.04450000	H	-1.62620000	2.30830000	3.55270000
H	-8.64080000	-0.14320000	4.25030000	H	-0.67750000	1.56320000	4.88940000
H	-8.75250000	-1.96590000	2.49620000	H	1.46700000	2.07960000	3.65240000
H	-7.96430000	-0.87180000	1.31170000	H	0.52410000	2.88310000	2.35340000
H	-10.76770000	-0.40970000	2.63950000	H	0.36440000	-0.15480000	3.11600000
H	-9.51230000	0.31710000	-0.09320000	H	0.00320000	1.44710000	0.49400000
H	-12.37190000	0.68750000	1.17990000	H	-0.03840000	-1.62020000	1.21970000
H	-11.55540000	1.89060000	0.11810000	H	-1.12330000	-0.83320000	0.01780000
H	-12.05920000	0.28830000	-0.54760000	H	0.65410000	-0.93090000	-0.29260000
H	-5.79020000	1.19340000	7.23000000	H	-2.76070000	1.64270000	6.33400000
H	-7.15080000	2.37870000	7.12320000	H	-3.97450000	0.95170000	5.26240000
H	-5.48660000	2.83390000	7.67500000	H	-4.48270000	1.78630000	6.78620000
H	-5.89380000	1.21560000	2.67390000	H	-2.79270000	6.00810000	4.76560000
H	-2.92910000	5.34770000	2.42030000	H	-5.88060000	5.77040000	1.08070000
3b_act1				**3b_act2**			
0 1				0 1			
C	-5.51150000	3.91980000	5.23790000	C	2.16341400	-0.44872300	1.19068700
N	-5.01900000	4.40040000	4.17180000	N	2.53968200	0.66079900	0.28702200
C	-5.60330000	5.68380000	3.67240000	C	3.95500000	1.13398200	0.20004200
O	-5.42460000	1.85730000	3.22800000	O	1.39274600	-1.03719800	-1.50747300
C	-5.64530000	1.62020000	4.55010000	C	0.73493000	-1.62452400	-0.48092700
C	-5.70950000	2.58600000	5.49920000	C	1.06816800	-1.32719900	0.81687100
C	-4.04940000	4.07950000	3.41750000	C	1.71607600	1.42674900	-0.34397400
C	-3.89120000	4.88300000	2.36230000	C	2.39578600	2.54939600	-1.03271700
C	-4.94160000	5.94590000	2.30580000	C	3.89141300	2.15615000	-0.95006200
C	-5.92500000	0.15260000	4.84740000	C	-0.34925700	-2.58695400	-0.87790400
C	-6.59080000	-0.63900000	3.70540000	C	-1.60735900	-1.86015900	-1.42020900
C	-7.98620000	-0.09940000	3.34730000	C	-2.35386400	-1.04569400	-0.35783100
C	-8.63260000	-0.89640000	2.20370000	C	-3.57869600	-0.31097200	-0.93356000
C	-9.99140000	-0.33810000	1.85970000	C	-4.34814300	0.43940400	0.12086100
C	-10.28950000	0.23850000	0.68540000	C	-4.52233200	1.76710000	0.15483600
C	-11.64270000	0.80410000	0.34730000	C	-5.27905100	2.51837700	1.21620900
C	-6.06240000	2.22900000	6.93880000	C	0.40738300	-2.04711800	1.98139900
O	-5.82100000	4.71280000	6.10970000	O	2.80863600	-0.50345800	2.22272500
H	-5.35420000	6.52770000	4.36030000	H	4.60021600	0.27535800	0.01069500
H	-6.71200000	5.61430000	3.56790000	H	4.21431700	1.57028000	1.16724700
H	-3.41180000	3.21770000	3.65390000	H	0.64767000	1.24200800	-0.31135700
H	-3.94120000	4.29690000	1.46850000	H	2.01035400	2.68214700	-2.04876600
H	-5.62810000	5.75010000	1.45040000	H	4.53806200	3.01443400	-0.76211400
H	-4.49730000	6.96360000	2.22540000	H	4.20265900	1.68629400	-1.88655900
H	-4.94180000	-0.32180000	5.08270000	H	0.05252900	-3.24806600	-1.65778800
H	-6.58910000	0.01980000	5.73020000	H	-0.62527400	-3.22652900	-0.03793500
H	-6.69370000	-1.70640000	4.01920000	H	-2.27455300	-2.62566300	-1.83473100
H	-5.93450000	-0.64870000	2.80420000	H	-1.32880100	-1.20592900	-2.25770900
H	-7.91550000	0.97170000	3.04450000	H	-1.67934300	-0.30801500	0.09772200
H	-8.64080000	-0.14320000	4.25030000	H	-2.67831300	-1.71503100	0.45142800
H	-8.75250000	-1.96590000	2.49620000	H	-4.23645500	-1.05290400	-1.41224100
H	-7.96430000	-0.87180000	1.31170000	H	-3.25262100	0.37966100	-1.72336700
H	-10.76770000	-0.40970000	2.63950000	H	-4.77588200	-0.17028800	0.92141800
H	-9.51230000	0.31710000	-0.09320000	H	-4.08976500	2.37300000	-0.64520300
H	-12.37190000	0.68750000	1.17990000	H	-5.68046500	1.84280200	1.98066900
H	-11.55540000	1.89060000	0.11810000	H	-4.63403600	3.25470900	1.71547400

H	-12.05920000	0.28830000	-0.54760000	H	-6.11784200	3.08012900	0.78223200
H	-5.79020000	1.19340000	7.23000000	H	-0.68224500	-2.01485100	1.90099200
H	-7.15080000	2.37870000	7.12320000	H	0.68500900	-1.56961300	2.92305100
H	-5.48660000	2.83390000	7.67500000	H	0.71527600	-3.09784900	2.04029000
H	-2.92910000	5.34770000	2.42030000	H	2.15730200	3.47273800	-0.48331800
(*R*)-1				**(*S*)-1**			
0 1				0 1			
C	2.10890000	0.00880000	1.11030000	C	1.71380000	0.96990000	1.26090000
N	2.44830000	0.84240000	0.08900000	N	2.52530000	0.75250000	0.18980000
C	3.54860000	1.79180000	0.11090000	C	3.29500000	1.77460000	-0.49980000
O	1.18960000	-0.33730000	-1.53780000	O	1.60850000	-1.38070000	-0.30000000
C	0.80920000	-1.13010000	-0.48610000	C	0.84720000	-1.17380000	0.82140000
C	1.19970000	-0.95900000	0.79900000	C	0.89660000	-0.06790000	1.60130000
C	1.74540000	0.89120000	-1.16920000	C	2.71930000	-0.54030000	-0.41810000
C	2.78680000	1.39980000	-2.15970000	C	3.07820000	-0.22060000	-1.86490000
C	3.52800000	2.43200000	-1.29090000	C	3.96030000	1.02620000	-1.67160000
C	-0.10910000	-2.25190000	-0.94230000	C	-0.10210000	-2.33680000	1.06050000
C	-1.51850000	-1.73820000	-1.28290000	C	-1.29990000	-2.30090000	0.09630000
C	-2.23190000	-1.09790000	-0.08140000	C	-2.18440000	-1.05800000	0.28550000
C	-3.63440000	-0.58990000	-0.44990000	C	-3.38980000	-1.05900000	-0.66720000
C	-4.30410000	0.05020000	0.74100000	C	-4.23900000	0.17090000	-0.46080000
C	-4.62690000	1.35070000	0.81030000	C	-4.41680000	1.12450000	-1.38790000
C	-5.28590000	1.98970000	2.00310000	C	-5.25710000	2.35510000	-1.17550000
C	0.75300000	-1.85100000	1.94170000	C	0.01240000	0.16310000	2.81310000
O	2.60230000	0.13980000	2.20600000	O	1.73080000	2.02910000	1.84330000
H	4.50430000	1.23910000	0.26940000	H	4.04720000	2.24500000	0.17370000
H	3.41930000	2.55110000	0.91560000	H	2.59990000	2.55640000	-0.88670000
H	3.48320000	0.57660000	-2.44660000	H	4.04000000	1.64510000	-2.59380000
H	2.93650000	3.37890000	-1.26310000	H	4.98850000	0.70490000	-1.37700000
H	4.54570000	2.66880000	-1.67590000	H	0.46890000	-3.28390000	0.90850000
H	0.34660000	-2.71400000	-1.85080000	H	-0.46500000	-2.40890000	2.10630000
H	-0.17860000	-3.08900000	-0.21660000	H	-1.92090000	-3.21520000	0.25610000
H	-2.13450000	-2.58950000	-1.66090000	H	-0.93190000	-2.33950000	-0.95650000
H	-1.45330000	-0.99510000	-2.11300000	H	-1.58310000	-0.13610000	0.10230000
H	-1.62860000	-0.24060000	0.30130000	H	-2.54530000	-1.02140000	1.34090000
H	-2.31310000	-1.84760000	0.74110000	H	-4.02370000	-1.95910000	-0.48810000
H	-4.27150000	-1.43450000	-0.80280000	H	-3.02980000	-1.11360000	-1.72080000
H	-3.55640000	0.13780000	-1.29090000	H	-4.72610000	0.27630000	0.52290000
H	-4.52250000	-0.60770000	1.59860000	H	-3.92580000	1.02420000	-2.37040000
H	-4.40320000	2.01140000	-0.04410000	H	-5.71920000	2.38440000	-0.16340000
H	-5.47850000	1.26180000	2.82270000	H	-4.63150000	3.26900000	-1.29270000
H	-4.63710000	2.79880000	2.40930000	H	-6.07770000	2.39150000	-1.92760000
H	-6.26160000	2.43710000	1.70590000	H	-0.67570000	-0.66310000	3.07570000
H	-0.15110000	-2.45780000	1.73620000	H	-0.64000000	1.05190000	2.65210000
H	0.47300000	-1.24240000	2.83150000	H	0.63870000	0.34100000	3.71710000
H	1.57300000	-2.54710000	2.23130000	H	3.60240000	-1.05570000	-2.38140000
H	0.91140000	1.62810000	-1.06740000	H	2.16100000	0.04940000	-2.44040000
H	2.33890000	1.83830000	-3.07960000	H	3.57950000	-1.03460000	0.09610000
3a_act1_ Scan				**HEME**			
0 1				4 2			
C	2.85003900	-0.55631200	0.62473900	S	3.38900000	0.28600000	-1.33200000
N	2.66050000	0.83642200	0.04756200	N	2.11300000	1.60600000	0.95100000
C	2.87378600	1.99994000	0.92944800	C	2.77400000	1.41600000	2.13900000
O	0.35130900	-0.31770200	-1.10339600	C	2.04700000	2.96700000	0.76300000

C	0.68450800	-1.32406800	-0.45726200
C	1.92284300	-1.53673800	0.25968600
C	2.51657500	1.15579800	-1.17876600
C	2.52816300	2.63395700	-1.39297700
C	2.43118200	3.17848800	0.04850500
C	-0.31369500	-2.48962900	-0.41336800
C	-1.69320800	-2.10869100	-0.93904800
C	-2.44331300	-1.16405100	-0.00207600
C	-3.82101700	-0.76987500	-0.54558900
C	-4.57862600	0.11839600	0.39781100
C	-4.97281000	1.36165500	0.13027200
C	-5.71239000	2.25162700	1.08527100
C	2.20867600	-2.88583100	0.88614300
O	3.81053900	-0.58388700	1.38499800
H	3.92982300	2.01066500	1.20695000
H	2.28188900	1.86625600	1.83589300
H	2.41823200	0.38918600	-1.93697600
H	1.70504200	2.94367800	-2.04141500
H	1.39383200	3.43742900	0.27088700
H	3.04624300	4.06498400	0.20587300
H	0.10930000	-3.30890100	-1.01139600
H	-0.38580300	-2.87908800	0.60973200
H	-2.28716400	-3.01986900	-1.08650800
H	-1.58005600	-1.62869900	-1.91683400
H	-1.84499400	-0.26012000	0.15243900
H	-2.56455500	-1.64286400	0.98036300
H	-4.40026100	-1.68485400	-0.73748700
H	-3.70104600	-0.26404400	-1.51186400
H	-4.79452100	-0.30040500	1.38355000
H	-4.75155700	1.77928000	-0.85313900
H	-5.88434900	1.74664400	2.04011900
H	-5.15374100	3.17360700	1.28343800
H	-6.68511900	2.55065600	0.67829300
H	2.02922600	-3.70886000	0.18684800
H	1.59942700	-3.07786400	1.77928400
H	3.25429100	-2.92719000	1.19572400
H	3.46330200	2.91013600	-1.89626800
B 4 7 S 10 -0.120000			

C	3.16000000	2.68900000	2.70500000
C	2.70300000	3.65200000	1.85400000
C	1.44800000	3.60100000	-0.31400000
H	1.46200000	4.69200000	-0.32600000
C	0.86300000	2.95700000	-1.39800000
N	0.74600000	1.59900000	-1.54900000
C	0.15400000	1.40000000	-2.77100000
C	-0.10700000	2.66700000	-3.41200000
C	0.32300000	3.63600000	-2.55300000
C	-0.18100000	0.16400000	-3.30800000
H	-0.64100000	0.15700000	-4.29700000
C	-0.02300000	-1.06000000	-2.66800000
C	-0.45700000	-2.32400000	-3.21500000
C	0.49800000	-2.58900000	-1.19300000
N	0.55000000	-1.24400000	-1.43800000
C	-0.14700000	-3.27700000	-2.28600000
C	1.03000000	-3.22400000	-0.07600000
H	0.92200000	-4.30600000	-0.01500000
C	1.71400000	-2.58700000	0.95300000
C	2.28000000	-3.26900000	2.09100000
N	1.93400000	-1.23900000	1.04800000
C	2.61300000	-1.04500000	2.22400000
C	3.01400000	0.18500000	2.73300000
H	3.54600000	0.18200000	3.68500000
Fe	1.21800000	0.18500000	-0.18100000
C	2.84400000	-2.31000000	2.88100000
O	-0.19500000	0.33100000	0.65000000
H	3.70600000	2.81000000	3.63900000
H	2.79400000	4.73300000	1.93600000
H	-0.56800000	2.78000000	-4.39200000
H	0.29600000	4.71700000	-2.67700000
H	-0.94100000	-2.44600000	-4.18200000
H	-0.32500000	-4.35000000	-2.32200000
H	2.23900000	-4.34600000	2.24800000
H	3.36600000	-2.42700000	3.82900000
H	4.15700000	-0.09800000	-0.28600000

TS1

0 2

S	2.64453600	2.38244100	0.55808300
N	3.42531500	-0.30449200	1.69190400
C	4.79046600	-0.44136300	1.73759300
C	2.96920000	-0.52430900	2.96586100
C	5.21396500	-0.72294400	3.09125300
C	4.08115100	-0.80269700	3.84760300
C	1.64767400	-0.39663500	3.37786500
H	1.42122700	-0.61286100	4.42273700
C	0.61703100	0.08945200	2.58541200
N	0.72630100	0.38940400	1.24977900
C	-0.48334500	0.92846100	0.87200400
C	-1.36879500	0.99638400	2.01209600
C	-0.69775700	0.44764400	3.06558200
C	-0.83837200	1.24082900	-0.42915200

TS2

0 2

S	-1	2.66612758	-3.77591302	1.60513492
N	-1	0.57282358	-2.16908702	0.05938092
C	-1	0.26069458	-2.73937602	-1.15172008
C	-1	-0.60427742	-2.09960802	0.76790392
C	-1	-1.15891042	-3.01162202	-1.21849808
C	-1	-1.69364542	-2.62225302	-0.02374008
C	-1	-0.74246942	-1.57402602	2.04765092
H	-1	-1.74904642	-1.52568402	2.46040392
C	-1	0.30184658	-1.05789302	2.80647292
N	-1	1.62125758	-1.01371502	2.42013092
C	-1	2.31097858	-0.45050302	3.46429692
C	-1	1.39765758	-0.09814502	4.52886692
C	-1	0.15031858	-0.47702002	4.12117192
C	-1	3.68676958	-0.25307602	3.51756492

H	-1.83232400	1.65059500	-0.59546700	H	-1	4.08865258	0.20861698	4.42093592
C	-0.06029600	0.98157600	-1.55588000	C	-1	4.59615358	-0.61795502	2.53205492
C	-0.51976600	1.15513700	-2.91496500	C	-1	6.02770358	-0.42476102	2.63457392
C	1.56172800	0.28962300	-2.85911400	C	-1	5.47385258	-1.39624102	0.67569492
N	1.20237900	0.45867200	-1.54682700	N	-1	4.28537358	-1.20480002	1.33250492
C	0.48343000	0.70706100	-3.72631800	C	-1	6.57309658	-0.91232902	1.48389292
C	2.81523800	-0.12191900	-3.29593600	C	-1	5.61722758	-1.95850102	-0.58749708
H	2.96697700	-0.22303700	-4.37173900	H	-1	6.62874858	-2.05710502	-0.98427808
C	3.91699900	-0.31988700	-2.46986800	C	-1	4.56759658	-2.39937402	-1.38544308
C	5.26653000	-0.53414400	-2.94099400	C	-1	4.71665958	-2.97105602	-2.70417308
N	3.90582300	-0.22225000	-1.10450600	N	-1	3.23775258	-2.34378402	-1.04322208
C	5.20343300	-0.35772600	-0.69454400	C	-1	2.54235258	-2.87779402	-2.10171308
C	5.62921200	-0.41169100	0.63121200	C	-1	1.16375058	-3.04509002	-2.16395608
H	6.70011900	-0.52290200	0.80910200	H	-1	0.75726958	-3.48700302	-3.07506908
Fe	2.29056200	-0.06485600	0.05093900	Fe	0	2.43481258	-1.78269402	0.73901892
C	6.07060000	-0.53338900	-1.83771000	C	-1	3.45966458	-3.26317502	-3.15055908
O	1.90208600	-1.65055100	-0.00578300	O	0	2.19409272	0.36238047	-0.42691002
H	6.24790600	-0.86368700	3.40137500	H	-1	-1.66358342	-3.45528402	-2.07520808
H	3.98974200	-1.01204000	4.91189400	H	-1	-2.72610442	-2.65063402	0.31505392
H	-2.37567300	1.40426400	1.98523600	H	-1	1.69131558	0.37021898	5.46688792
H	-1.04251800	0.30441400	4.08777700	H	-1	-0.79671842	-0.38457602	4.64998492
H	-1.49608000	1.54945700	-3.19028400	H	-1	6.53242258	0.02480098	3.48812892
H	0.51076700	0.66936900	-4.81383000	H	-1	7.62063758	-0.94648002	1.18927392
H	5.54869800	-0.64698800	-3.98628500	H	-1	5.66848258	-3.12205602	-3.21064508
H	7.15098900	-0.65557500	-1.78475200	H	-1	3.16381458	-3.70667302	-4.09986708
H	3.80694200	2.31055100	1.24738600	H	-1	1.45722758	-3.87824902	2.21002592
C	-4.20350800	-2.72531300	-0.10791400	C	-1	-1.96600207	2.90992556	-0.97679576
N	-3.00460600	-2.91188800	-0.71069100	N	-1	-0.76888807	3.13366856	-0.36058276
C	-2.84915200	-3.98138100	-1.70189700	C	-1	-0.38159507	4.50774156	0.00067724
O	-3.99275100	0.00471800	-0.85384700	O	-1	-3.39068107	0.61425156	0.65544224
C	-4.60542900	-0.25990200	0.16481300	C	-1	-3.56599907	1.13052256	-0.43053276
C	-4.33800800	-1.57251100	0.90779500	C	-1	-2.35329307	1.46439956	-1.31484576
C	-1.79580300	-2.11137900	-0.56591000	C	-1	0.25683093	2.16515856	-0.00177676
C	-0.95988500	-2.49443300	-1.80017300	C	-1	1.13732393	2.92763156	1.00140724
C	-1.35065200	-3.96071600	-2.02348400	C	-1	1.06708393	4.36603256	0.47847324
C	-5.62855500	0.71503000	0.72782700	C	-1	-4.93895807	1.52999756	-0.92147476
C	-5.62241900	2.06710700	0.01739300	C	-1	-6.08063407	1.07178756	-0.01904576
C	-4.38131100	2.87963200	0.38869900	C	-1	-6.35976107	-0.42903744	-0.11478776
C	-4.15230900	4.16517200	-0.41811800	C	-1	-7.46154807	-0.90735644	0.84124824
C	-2.83683400	4.79726900	-0.05279300	C	-1	-7.75944207	-2.37257544	0.70513224
C	-1.72380900	4.72863100	-0.79354800	C	-1	-7.55606607	-3.29461444	1.65310224
C	-0.37257400	5.24056600	-0.39814800	C	-1	-7.82978507	-4.76209344	1.51361824
C	-5.36601000	-1.95726200	1.97303300	C	-1	-2.58847807	1.32657056	-2.82312476
O	-5.16727600	-3.43714400	-0.35741000	O	-1	-2.72051207	3.83633956	-1.23692676
C	-1.02165000	-2.35877500	0.71931300	C	0	1.06138993	1.66235456	-1.21837676
O	-1.48230200	-2.86266600	1.71782900	O	-1	0.75748893	1.72626756	-2.37833976
H	-3.46625700	-3.75759300	-2.59004000	H	-1	-1.05089607	4.87757256	0.79564224
H	-3.20889300	-4.93707900	-1.29362800	H	-1	-0.50584007	5.17738156	-0.86211276
H	-3.36775300	-1.42007600	1.40584200	H	-1	-1.57496907	0.76212156	-1.00223376
H	-2.04004100	-1.03843100	-0.58630400	H	-1	-0.15762207	1.25580556	0.45471524
H	-1.27006700	-1.87543900	-2.65504800	H	-1	0.66773593	2.84053656	1.99223224
H	0.11376100	-2.33342900	-1.63116500	H	-1	2.14622793	2.50885556	1.06152724
H	-0.80331500	-4.60522100	-1.31595900	H	-1	1.76321493	4.49074356	-0.36780676
H	-1.13201700	-4.31985900	-3.03954000	H	-1	1.33345393	5.11444956	1.23778924

H	-6.61215700	0.21598500	0.66164500
H	-5.44648300	0.83304800	1.80982500
H	-6.54076800	2.62552400	0.26292600
H	-5.62764700	1.89205100	-1.07006100
H	-3.50256900	2.23739900	0.23809500
H	-4.40378000	3.12066600	1.46758900
H	-4.98706600	4.86727700	-0.24148000
H	-4.16328500	3.92255100	-1.49462000
H	-2.78416100	5.28005000	0.93282800
H	-1.78449400	4.24207000	-1.77669000
H	-0.40302800	5.75976100	0.57209900
H	0.35398900	4.41240000	-0.31600700
H	0.03185900	5.93832500	-1.15167000
H	-5.49239900	-1.16601700	2.72512700
H	-5.02816100	-2.86432900	2.49373000
H	-6.33656400	-2.18410000	1.51209700
H	0.58418142	-1.88113123	0.45331452

H	-1	-4.89643207	2.62951856	-1.02350576
H	-1	-5.07324907	1.15764756	-1.95089276
H	-1	-6.99398207	1.63088056	-0.28417976
H	-1	-5.83937707	1.33391056	1.02396024
H	-1	-5.43827807	-0.99397444	0.09988324
H	-1	-6.64323307	-0.68154644	-1.15356276
H	-1	-8.37985807	-0.32206144	0.64366024
H	-1	-7.16658707	-0.68176944	1.88035824
H	-1	-8.15283107	-2.69686344	-0.26884976
H	-1	-7.15715007	-2.96473144	2.62226024
H	-1	-8.22381607	-5.00892644	0.51550124
H	-1	-6.91421307	-5.35772444	1.67642224
H	-1	-8.56226407	-5.10714544	2.26465524
H	-1	-2.97540907	0.32537656	-3.06526976
H	-1	-1.63727307	1.46289656	-3.35634776
H	-1	-3.29644807	2.08597256	-3.18191676
H	0	2.84543072	0.36249247	-1.14955402

TS3

0 2

S	3.30204500	2.00943300	-2.12955100
N	4.43591000	0.97559300	0.48476200
C	5.65463300	0.35162000	0.41527600
C	4.56081800	1.98190900	1.40730000
C	6.58340600	0.98602000	1.32192700
C	5.90495700	1.99776900	1.93652800
C	3.56164200	2.86285000	1.79317000
H	3.81559800	3.61479300	2.54141800
C	2.26169400	2.85289900	1.30925600
N	1.75660000	1.99323500	0.37087600
C	0.43847400	2.32077700	0.21207900
C	0.09536600	3.43308100	1.06898600
C	1.22809800	3.76526400	1.74997400
C	-0.45776300	1.68067000	-0.62808600
H	-1.49428100	2.01393300	-0.62607800
C	-0.13543700	0.60138800	-1.43694400
C	-1.07736400	-0.05463700	-2.30959600
C	0.96630000	-0.99813500	-2.47539000
N	1.09724100	-0.00038100	-1.53845900
C	-0.39294300	-1.04441000	-2.95699900
C	1.97186500	-1.85532400	-2.89695100
H	1.71619100	-2.60240800	-3.64925400
C	3.27822800	-1.83286500	-2.43058900
C	4.31085100	-2.74551700	-2.86151600
N	3.77704300	-0.97280200	-1.48648900
C	5.08974900	-1.32094100	-1.29570800
C	5.97280000	-0.71456400	-0.41315700
H	6.99002500	-1.10511900	-0.36736800
Fe	2.75759400	0.46514800	-0.52020700
C	5.43544600	-2.42794800	-2.15661700
O	-0.11794400	0.70987300	2.60584200
H	7.62009200	0.68207600	1.45575300
H	6.26549400	2.70349000	2.68282800
H	-0.89601200	3.87791400	1.12954600
H	1.37419900	4.55205000	2.48823300

TS4

0 2

C	-3.41041400	-2.52324900	0.24095600
N	-2.11361200	-2.88024300	-0.01911200
C	-1.87506200	-4.09413200	-0.81912900
O	-4.22482700	-0.12483400	-0.83505600
C	-4.48220700	-0.28552900	0.33778500
C	-3.70150700	-1.33183800	1.15662600
C	-0.92769700	-2.45350500	0.63482400
C	0.14698800	-3.15838100	0.05644200
C	-0.36033000	-4.36094800	-0.67515200
C	-5.53929300	0.55973000	1.02713100
C	-5.94191300	1.77391300	0.19673100
C	-4.80066800	2.80869300	0.12194500
C	-4.57812600	3.42286300	-1.27651800
C	-3.33104100	4.27003900	-1.31448200
C	-2.22975000	3.96207900	-2.01433700
C	-0.92961800	4.70629600	-1.97951700
C	-4.42106500	-1.83248500	2.41732600
O	-4.33017800	-3.15297400	-0.24387100
C	-0.84321400	-3.09548300	2.20557300
O	-1.74399600	-3.84681900	2.46938500
H	-2.17268300	-3.90427100	-1.86237000
H	-2.50074500	-4.91852900	-0.43870200
H	-2.77432200	-0.80176700	1.44709600
H	-0.80850000	-1.37980600	0.85691300
H	1.19072700	-2.93180900	0.25505000
H	2.61452700	-1.45595600	1.61352400
H	-0.15524600	-5.26878400	-0.07787200
H	0.16521900	-4.50087400	-1.63793600
H	-6.40023700	-0.11310200	1.22073300
H	-5.17439300	0.85583300	2.02645500
H	-6.85386900	2.22503900	0.61547900
H	-6.19648700	1.42501300	-0.81776900
H	-3.86200800	2.32274500	0.41992000
H	-4.96312800	3.60975800	0.85648500
H	-5.46726200	4.01911700	-1.55562400

H	-2.12400300	0.22859500	-2.39495200
H	-0.75826000	-1.74798000	-3.70313800
H	4.17272000	-3.52636600	-3.60729500
H	6.41874500	-2.89318900	-2.19825800
H	4.59832000	1.65046500	-2.28314600
O	2.39697000	-0.53973500	0.86334200
C	-3.00946800	-2.22176100	2.07941200
N	-1.68250400	-2.34531800	1.81617700
C	-1.03069000	-3.66251300	1.86657000
O	-3.34642700	0.58080700	0.00327800
C	-3.76172500	-0.46739300	0.45490400
C	-3.60270300	-0.80833000	1.93998500
C	-0.75006700	-1.27318600	1.48417500
C	0.34384700	-2.04589300	0.74805300
C	0.43546800	-3.37512800	1.47954300
C	-4.43860600	-1.50040300	-0.43010700
C	-5.28439800	-0.87900400	-1.54045200
C	-6.57134700	-0.24074400	-1.01312800
C	-7.33320900	0.56121100	-2.07805300
C	-8.65012100	1.08777900	-1.58544200
C	-8.93129100	2.37720700	-1.36513600
C	-10.23374000	2.90733500	-0.84317600
C	-4.96037400	-0.71969300	2.64814000
O	-3.70396900	-3.19105100	2.34803700
C	-0.18364900	-0.62222200	2.74122600
O	0.17149300	-1.21782800	3.72594800
H	-1.53163700	-4.33907100	1.15490700
H	-1.13448600	-4.10565100	2.86789400
H	-2.92182900	-0.04988400	2.35260300
H	-1.19246400	-0.49936600	0.84993400
H	0.09180800	-2.13747800	-0.31645000
H	1.35434700	-1.40323600	0.79756400
H	1.04464000	-3.26427100	2.38739800
H	0.87077700	-4.17099500	0.86041600
H	-3.60667100	-2.08734000	-0.86355900
H	-5.01354300	-2.21062300	0.18205200
H	-5.52982400	-1.65151200	-2.28799300
H	-4.68217600	-0.11414300	-2.05741700
H	-6.33562400	0.42976400	-0.16858600
H	-7.22947000	-1.02665400	-0.60070200
H	-7.49865900	-0.09077800	-2.95649000
H	-6.70216600	1.39738100	-2.42463000
H	-9.42057900	0.33507600	-1.36643200
H	-8.15444800	3.12294200	-1.58369300
H	-10.96075000	2.09956400	-0.66633700
H	-10.09166700	3.45300800	0.10636600
H	-10.68625400	3.62583900	-1.54913500
H	-5.44678400	0.24434600	2.43739200
H	-4.82186300	-0.81006400	3.73532400
H	-5.61979200	-1.53874800	2.33366900
H	0.36664400	1.06702500	3.36941000
TS5			
0 2			
S	3.24182200	2.62301900	1.39767600
H	-4.49241500	2.60370500	-2.00808100
H	-3.31876400	5.15926400	-0.67278000
H	-2.24479000	3.06403900	-2.64398000
H	-0.98389300	5.58747700	-1.32248900
H	-0.11796300	4.06280800	-1.61338100
H	-0.63747900	5.04791500	-2.98672100
H	-4.62808300	-1.01791900	3.11880300
H	-3.79899500	-2.57883100	2.93122100
H	-5.36581900	-2.32130700	2.14100600
H	0.81597500	-2.01780000	2.32891200
S	2.64715200	1.94400500	-1.71788500
N	0.58731300	-0.27524700	-1.26330000
C	-0.71973500	0.16292900	-1.29521400
C	0.67178500	-1.31638800	-2.14783000
C	-1.48111800	-0.61639000	-2.25733300
C	-0.61405700	-1.53338600	-2.78249600
C	1.82454500	-2.06833300	-2.41824300
H	1.73100900	-2.85513500	-3.17126300
C	3.07348700	-1.88512900	-1.84228500
N	3.37921400	-0.95419000	-0.88245600
C	4.70735700	-1.10573000	-0.59661400
C	5.26500100	-2.18249300	-1.39209100
C	4.25146300	-2.67072500	-2.16700200
C	5.43631000	-0.33535900	0.30581200
H	6.49943600	-0.56944800	0.42703900
C	4.92311000	0.71541600	1.06118400
C	5.69207700	1.51340100	1.99180600
C	3.53577400	2.18933700	1.91461400
N	3.61720000	1.14148000	1.03613500
C	4.82979100	2.42965600	2.52400200
C	2.38228800	2.90797700	2.20852400
H	2.47252600	3.71120100	2.94764700
C	1.12107000	2.69692000	1.65961300
C	-0.05595700	3.46916600	2.00298300
N	0.80257600	1.75358100	0.71308100
C	-0.53156300	1.91414500	0.43385600
C	-1.24428000	1.17433800	-0.50024900
H	-2.29582800	1.41342800	-0.64432100
Fe	2.09618700	0.42082000	-0.11996400
C	-1.07984400	2.98387800	1.24718700
O	0.13608800	-2.63738600	2.89542600
H	-2.53929300	-0.48892700	-2.44134100
H	-0.81361700	-2.29349900	-3.53319500
H	6.30271600	-2.51396300	-1.35010800
H	4.27678300	-3.47786000	-2.89825800
H	6.74929400	1.37942900	2.19753800
H	5.03710400	3.20280900	3.25573000
H	-0.07391700	4.27895600	2.72573300
H	-2.11082000	3.31991600	1.20518200
H	1.43253500	2.08506100	-2.29684400
O	1.68129300	-1.29133200	1.37271400
2b			
0 2			
S	7.76650000	0.71400000	0.09570000

N	2.17730500	-0.30659100	1.74375200
C	2.76461100	-1.04333300	2.73567100
C	0.85341800	-0.20235200	2.07358700
C	1.78467900	-1.44190700	3.70540500
C	0.58621100	-0.89935000	3.30461900
C	-0.12739400	0.40006300	1.29219100
H	-1.16958400	0.34740800	1.60930800
C	0.10395600	1.01246000	0.06968100
N	1.33263500	1.24388600	-0.51268600
C	1.08578300	1.86757800	-1.71494700
C	-0.34128900	2.02973500	-1.88341100
C	-0.94652400	1.51797900	-0.78942600
C	2.05207100	2.30763600	-2.61658600
H	1.70016200	2.84632000	-3.49240500
C	3.42602100	2.16145000	-2.44614000
C	4.42611000	2.72791300	-3.30015100
C	5.37901400	1.58182800	-1.60974600
N	4.02323800	1.45146700	-1.43011300
C	5.64674900	2.36539500	-2.78255500
C	6.35579900	1.01870700	-0.79126200
H	7.40324100	1.15624300	-1.08391200
C	6.11911000	0.26443700	0.35575400
C	7.14064400	-0.40847100	1.11271300
N	4.88382200	0.02445000	0.92326700
C	5.10728100	-0.82174500	1.98735600
C	4.12685600	-1.33731100	2.83578400
H	4.44952900	-1.97511200	3.66438000
Fe	3.10130200	0.64266500	0.20831700
C	6.51095500	-1.08367500	2.11469700
O	0.59762300	-1.54608600	-1.50661800
H	1.97698200	-2.05499900	4.58158300
H	-0.38773500	-0.96981000	3.77734800
H	-0.79379900	2.49364400	-2.76720200
H	-2.00066500	1.42506800	-0.54609200
H	4.21744600	3.32638200	-4.17730700
H	6.63836500	2.61679800	-3.15334600
H	8.20037600	-0.38489800	0.86778200
H	6.94757000	-1.73083700	2.87900700
H	4.10560200	2.14847700	2.32772000
O	2.97527800	-1.29147700	-0.98724000
C	-3.42762100	-3.12953300	0.08152600
N	-2.69062200	-3.29606500	-1.02939200
C	-2.86522600	-4.50220000	-1.85104500
O	-3.85499800	0.27862500	-0.37195600
C	-4.27028700	-0.77105800	0.06982600
C	-3.31718700	-1.75649500	0.78378700
C	-1.85655600	-2.35081800	-1.74309500
C	-1.53074200	-2.98130200	-3.06744800
C	-1.66458800	-4.48572500	-2.77058400
C	-5.72224600	-1.19227400	-0.11302200
C	-6.60851900	-0.09214200	-0.69024300
C	-6.94824700	1.01106200	0.33544000
C	-7.63242000	2.21469000	-0.31580900
C	-8.26731000	3.14940600	0.68616700

N	5.71630000	-1.38090000	1.08460000
C	5.91500000	-2.64550000	0.59590000
C	5.77280000	-1.50210000	2.44870000
C	6.11490000	-3.59680000	1.68470000
C	6.02520000	-2.88570000	2.83730000
C	5.62020000	-0.45070000	3.35690000
H	5.68790000	-0.69190000	4.41990000
C	5.40530000	0.88740000	3.01520000
N	5.31370000	1.36590000	1.73550000
C	5.14470000	2.71860000	1.86570000
C	5.12750000	3.11060000	3.27300000
C	5.28760000	1.97010000	3.98870000
C	5.02720000	3.61880000	0.80290000
H	4.91340000	4.67660000	1.05060000
C	5.04800000	3.27450000	-0.55090000
C	4.92150000	4.23850000	-1.63970000
C	5.13620000	2.12650000	-2.40280000
N	5.18380000	2.00030000	-1.03970000
C	4.97300000	3.52370000	-2.79210000
C	5.24160000	1.06850000	-3.31050000
H	5.18120000	1.31180000	-4.37330000
C	5.43670000	-0.27220000	-2.96820000
C	5.57700000	-1.35190000	-3.94180000
N	5.54990000	-0.75040000	-1.68970000
C	5.75050000	-2.09890000	-1.81950000
C	5.92880000	-2.99030000	-0.75810000
H	6.09640000	-4.04040000	-1.00670000
Fe	5.28210000	0.28450000	0.02490000
C	5.77450000	-2.48780000	-3.22730000
O	3.68270000	0.05290000	0.05290000
H	6.30260000	-4.66240000	1.55740000
H	6.12290000	-3.23880000	3.86350000
H	5.01860000	4.13210000	3.63660000
H	5.34010000	1.84780000	5.07010000
H	4.81190000	5.31510000	-1.51200000
H	4.91580000	3.88460000	-3.81840000
H	5.53740000	-1.22690000	-5.02340000
H	5.93250000	-3.50180000	-3.59290000
H	8.21860000	0.03830000	-0.99450000
C	-1.63350000	2.35310000	2.21390000
N	-1.23040000	1.84030000	0.93130000
C	-2.22060000	1.13970000	0.10200000
O	-0.09960000	4.89860000	1.27060000
C	-0.74710000	4.67850000	2.27390000
C	-0.67600000	3.28170000	2.95780000
C	0.02220000	1.99670000	0.27550000
C	-0.27100000	1.68350000	-1.18990000
C	-1.41370000	0.66090000	-1.10530000
C	-1.77630000	5.64450000	2.80650000
C	-1.91320000	6.96590000	2.04860000
C	-0.93920000	8.05750000	2.51850000
C	-1.20790000	9.39860000	1.87930000
C	-0.54690000	10.59250000	2.42620000
C	-0.71660000	11.87920000	1.87350000

C	-8.30347300	4.49134400	0.59573100
C	-9.00522600	5.38304500	1.57688000
C	-3.63921900	-1.90256000	2.27808800
O	-4.23587600	-3.95995700	0.47950100
C	-0.27487000	-2.12176000	-0.76616700
O	-0.17415400	-2.44036600	0.41307000
H	-3.81419800	-4.42496400	-2.42420900
H	-2.96546600	-5.40243700	-1.20446800
H	-2.30699100	-1.34843500	0.66636100
H	-2.25181700	-1.36086600	-1.79009700
H	-2.31363700	-2.65538900	-3.77734900
H	-0.55690300	-2.69697100	-3.47877100
H	-0.76740600	-4.83967500	-2.23780200
H	-1.79727300	-5.12194000	-3.67251500
H	-5.71811600	-2.09042500	-0.75936300
H	-6.10700800	-1.56483600	0.85731300
H	-7.55619300	-0.53887000	-1.05106200
H	-6.10629800	0.35840900	-1.56077300
H	-6.01380000	1.33928700	0.82187500
H	-7.58460100	0.58568500	1.11385600
H	-8.43343700	1.84589700	-0.99326700
H	-6.92070700	2.78033400	-0.93783800
H	-8.76704300	2.62730900	1.56498600
H	-7.79435600	5.00293200	-0.25645200
H	-9.56688400	4.78687700	2.37136000
H	-8.28467400	6.05311400	2.10241900
H	-9.74976900	6.04258100	1.05904500
H	-3.40200200	-0.96643500	2.81577400
H	-3.03554500	-2.71205500	2.70725500
H	-4.69524600	-2.15671900	2.46255800
H	1.71330000	-1.45893100	-1.17820900

C	-0.09810000	13.09400000	2.38990000
C	-1.02030000	3.27160000	4.44120000
O	-2.71400000	2.01910000	2.61540000
C	1.11000000	0.96940000	0.90370000
O	1.46840000	1.03000000	2.02990000
H	-2.99710000	1.88150000	-0.16720000
H	-2.72990000	0.36540000	0.69540000
H	0.35190000	2.92620000	2.80450000
H	0.45310000	2.99860000	0.49610000
H	-0.60100000	2.61120000	-1.68380000
H	0.61640000	1.32480000	-1.73220000
H	-1.02030000	-0.35170000	-0.91820000
H	-2.02190000	0.61230000	-2.01750000
H	-2.73390000	5.08900000	2.80260000
H	-1.56860000	5.79850000	3.87810000
H	-2.94530000	7.32440000	2.19170000
H	-1.78940000	6.79350000	0.96710000
H	0.09980000	7.74920000	2.30490000
H	-1.01030000	8.16190000	3.61530000
H	-2.30000000	9.69310000	1.94680000
H	-1.12660000	9.39280000	0.76850000
H	0.07130000	10.51630000	3.33100000
H	-1.37480000	11.96740000	0.99740000
H	0.59910000	12.94480000	3.22410000
H	0.37470000	13.67040000	1.56810000
H	-0.91660000	13.78490000	2.70700000
H	-0.36640000	3.96110000	4.99200000
H	-0.86590000	2.26080000	4.84530000
H	-2.07090000	3.53590000	4.62260000
H	1.45540000	0.16680000	0.19250000

2e			
0 2			
S	3.38900000	0.28600000	-1.33200000
N	2.11300000	1.60600000	0.95100000
C	2.77400000	1.41600000	2.13900000
C	2.04700000	2.96700000	0.76300000
C	3.16000000	2.68900000	2.70500000
C	2.70300000	3.65200000	1.85400000
C	1.44800000	3.60100000	-0.31400000
H	1.46200000	4.69200000	-0.32600000
C	0.86300000	2.95700000	-1.39800000
N	0.74600000	1.59900000	-1.54900000
C	0.15400000	1.40000000	-2.77100000
C	-0.10700000	2.66700000	-3.41200000
C	0.32300000	3.63600000	-2.55300000
C	-0.18100000	0.16400000	-3.30800000
H	-0.64100000	0.15700000	-4.29700000
C	-0.02300000	-1.06000000	-2.66800000
C	-0.45700000	-2.32400000	-3.21500000
C	0.49800000	-2.58900000	-1.19300000
N	0.55000000	-1.24400000	-1.43800000
C	-0.14700000	-3.27700000	-2.28600000
C	1.03000000	-3.22400000	-0.07600000

2c-b			
0 2			
S	3.38900000	0.28600000	-1.33200000
N	2.11300000	1.60600000	0.95100000
C	2.77400000	1.41600000	2.13900000
C	2.04700000	2.96700000	0.76300000
C	3.16000000	2.68900000	2.70500000
C	2.70300000	3.65200000	1.85400000
C	1.44800000	3.60100000	-0.31400000
H	1.46200000	4.69200000	-0.32600000
C	0.86300000	2.95700000	-1.39800000
N	0.74600000	1.59900000	-1.54900000
C	0.15400000	1.40000000	-2.77100000
C	-0.10700000	2.66700000	-3.41200000
C	0.32300000	3.63600000	-2.55300000
C	-0.18100000	0.16400000	-3.30800000
H	-0.64100000	0.15700000	-4.29700000
C	-0.02300000	-1.06000000	-2.66800000
C	-0.45700000	-2.32400000	-3.21500000
C	0.49800000	-2.58900000	-1.19300000
N	0.55000000	-1.24400000	-1.43800000
C	-0.14700000	-3.27700000	-2.28600000
C	1.03000000	-3.22400000	-0.07600000

H	0.92200000	-4.30600000	-0.01500000
C	1.71400000	-2.58700000	0.95300000
C	2.28000000	-3.26900000	2.09100000
N	1.93400000	-1.23900000	1.04800000
C	2.61300000	-1.04500000	2.22400000
C	3.01400000	0.18500000	2.73300000
H	3.54600000	0.18200000	3.68500000
Fe	1.21800000	0.18500000	-0.18100000
C	2.84400000	-2.31000000	2.88100000
O	-0.19500000	0.33100000	0.65000000
H	3.70600000	2.81000000	3.63900000
H	2.79400000	4.73300000	1.93600000
H	-0.56800000	2.78000000	-4.39200000
H	0.29600000	4.71700000	-2.67700000
H	-0.94100000	-2.44600000	-4.18200000
H	-0.32500000	-4.35000000	-2.32200000
H	2.23900000	-4.34600000	2.24800000
H	3.36600000	-2.42700000	3.82900000
H	4.15700000	-0.09800000	-0.28600000
C	-5.54870000	2.49300000	3.87710000
N	-5.34180000	2.14450000	2.56290000
C	-6.43090000	1.78290000	1.66460000
O	-2.67050000	4.47210000	4.01540000
C	-3.82650000	4.29170000	4.32640000
C	-4.31440000	2.88840000	4.69320000
C	-4.05960000	2.08280000	1.85890000
C	-4.44860000	2.14250000	0.37080000
C	-5.75770000	1.34430000	0.35560000
C	-4.85250000	5.41660000	4.31940000
C	-4.26670000	6.82680000	4.49600000
C	-3.61810000	7.02330000	5.87650000
C	-3.05500000	8.44280000	6.04740000
C	-2.43190000	8.61790000	7.41020000
C	-1.12950000	8.86870000	7.61330000
C	-0.50950000	9.03780000	8.97440000
C	-4.52920000	2.78640000	6.21360000
O	-6.65400000	2.51670000	4.36300000
C	-3.27560000	0.80340000	2.15110000
O	-3.64160000	0.00540000	2.98370000
H	-7.06830000	2.68140000	1.48880000
H	-7.05740000	0.96440000	2.08800000
H	-3.50130000	2.16080000	4.45960000
H	-3.40600000	2.95110000	2.09610000
H	-4.65570000	3.19890000	0.07350000
H	-3.67630000	1.73020000	-0.31630000
H	-5.52870000	0.25210000	0.38980000
H	-6.38130000	1.54570000	-0.54460000
H	-5.38610000	5.35720000	3.34080000
H	-5.60860000	5.23880000	5.11740000
H	-5.08740000	7.57470000	4.37460000
H	-3.52420000	7.03470000	3.69020000
H	-2.79300000	6.28610000	6.01780000
H	-4.37780000	6.82500000	6.67000000
H	-3.86910000	9.19670000	5.93430000

H	0.92200000	-4.30600000	-0.01500000
C	1.71400000	-2.58700000	0.95300000
C	2.28000000	-3.26900000	2.09100000
N	1.93400000	-1.23900000	1.04800000
C	2.61300000	-1.04500000	2.22400000
C	3.01400000	0.18500000	2.73300000
H	3.54600000	0.18200000	3.68500000
Fe	1.21800000	0.18500000	-0.18100000
C	2.84400000	-2.31000000	2.88100000
O	-2.77160000	3.48040000	1.55880000
H	3.70600000	2.81000000	3.63900000
H	2.79400000	4.73300000	1.93600000
H	-0.56800000	2.78000000	-4.39200000
H	0.29600000	4.71700000	-2.67700000
H	-0.94100000	-2.44600000	-4.18200000
H	-0.32500000	-4.35000000	-2.32200000
H	2.23900000	-4.34600000	2.24800000
H	3.36600000	-2.42700000	3.82900000
H	4.15700000	-0.09800000	-0.28600000
O	-0.37150000	0.67500000	0.92950000
C	-5.82240000	2.53490000	4.95920000
N	-4.64940000	2.04530000	4.43400000
C	-3.61660000	1.42870000	5.25680000
O	-7.59330000	2.04610000	1.98510000
C	-7.56150000	2.01910000	3.19500000
C	-6.83490000	3.12040000	3.97030000
C	-4.24600000	2.04600000	3.02670000
C	-3.14600000	0.97170000	2.95410000
C	-2.44370000	1.14900000	4.30560000
C	-8.18380000	0.88420000	3.99680000
C	-9.32600000	0.14090000	3.28560000
C	-10.54950000	1.04060000	3.04350000
C	-11.69090000	0.28020000	2.35060000
C	-12.88410000	1.17700000	2.13070000
C	-13.35810000	1.51230000	0.92110000
C	-14.46560987	2.23081080	0.46448886
C	-7.85750000	4.06280000	4.62940000
O	-6.06160000	2.48180000	6.14170000
C	-3.70090000	3.39550000	2.55930000
O	-3.73530000	4.37790000	3.26470000
H	-4.01060000	0.47270000	5.67560000
H	-3.30530000	2.09630000	6.09300000
H	-6.27560000	3.75360000	3.24130000
H	-5.07900000	1.75570000	2.34900000
H	-3.60810000	-0.04390000	2.90750000
H	-2.45920000	1.08430000	2.08560000
H	-1.76700000	2.03590000	4.26050000
H	-1.84170000	0.26120000	4.60440000
H	-7.36090000	0.16570000	4.22630000
H	-8.55970000	1.27490000	4.96940000
H	-9.63720000	-0.72730000	3.91570000
H	-8.96270000	-0.28080000	2.31900000
H	-10.26060000	1.91450000	2.41340000
H	-10.90810000	1.44250000	4.02130000

H	-2.30630000	8.64320000	5.24600000
H	-3.10560000	8.52380000	8.27800000
H	-0.45280000	8.95890000	6.74700000
H	-1.25300000	8.93340000	9.79590000
H	0.28320000	8.27110000	9.13050000
H	-0.04480000	10.04660000	9.05940000
H	-3.59430000	3.03910000	6.76510000
H	-4.82000000	1.75110000	6.50620000
H	-5.32320000	3.47390000	6.58040000
H	-1.05580000	0.78380000	0.76290000

H	-12.01310000	-0.58520000	2.97610000
H	-11.32670000	-0.13140000	1.38070000
H	-13.37730000	1.57450000	3.03340000
H	-12.86370000	1.11960000	0.01670000
H	-14.90950987	2.58631080	1.42118886
H	-14.16400987	3.12551080	-0.12631114
H	-15.25780987	1.68751080	-0.09951114
H	-8.54420000	4.49940000	3.86790000
H	-7.34590000	4.90960000	5.14220000
H	-8.49010000	3.54630000	5.38480000
H	-2.28760000	4.23870000	1.86150000

2c-a

0 2

S	3.38900000	0.28600000	-1.33200000
N	2.11300000	1.60600000	0.95100000
C	2.77400000	1.41600000	2.13900000
C	2.04700000	2.96700000	0.76300000
C	3.16000000	2.68900000	2.70500000
C	2.70300000	3.65200000	1.85400000
C	1.44800000	3.60100000	-0.31400000
H	1.46200000	4.69200000	-0.32600000
C	0.86300000	2.95700000	-1.39800000
N	0.74600000	1.59900000	-1.54900000
C	0.15400000	1.40000000	-2.77100000
C	-0.10700000	2.66700000	-3.41200000
C	0.32300000	3.63600000	-2.55300000
C	-0.18100000	0.16400000	-3.30800000
H	-0.64100000	0.15700000	-4.29700000
C	-0.02300000	-1.06000000	-2.66800000
C	-0.45700000	-2.32400000	-3.21500000
C	0.49800000	-2.58900000	-1.19300000
N	0.55000000	-1.24400000	-1.43800000
C	-0.14700000	-3.27700000	-2.28600000
C	1.03000000	-3.22400000	-0.07600000
H	0.92200000	-4.30600000	-0.01500000
C	1.71400000	-2.58700000	0.95300000
C	2.28000000	-3.26900000	2.09100000
N	1.93400000	-1.23900000	1.04800000
C	2.61300000	-1.04500000	2.22400000
C	3.01400000	0.18500000	2.73300000
H	3.54600000	0.18200000	3.68500000
Fe	1.21800000	0.18500000	-0.18100000
C	2.84400000	-2.31000000	2.88100000
O	-2.26430000	1.80140000	2.15370000
H	3.70600000	2.81000000	3.63900000
H	2.79400000	4.73300000	1.93600000
H	-0.56800000	2.78000000	-4.39200000
H	0.29600000	4.71700000	-2.67700000
H	-0.94100000	-2.44600000	-4.18200000
H	-0.32500000	-4.35000000	-2.32200000
H	2.23900000	-4.34600000	2.24800000
H	3.36600000	-2.42700000	3.82900000
H	4.15700000	-0.09800000	-0.28600000
O	-0.52170000	0.23800000	0.76360000

2f

0 2

S	-5.42540000	0.36540000	1.40660000
N	-2.61660000	0.01150000	1.94990000
C	-2.07590000	1.03520000	2.68870000
C	-2.39660000	-1.13020000	2.68070000
C	-1.44100000	0.52290000	3.88320000
C	-1.66110000	-0.81920000	3.88860000
C	-2.75390000	-2.41360000	2.30060000
H	-2.49720000	-3.22410000	2.98420000
C	-3.39540000	-2.75470000	1.11360000
N	-3.77540000	-1.88090000	0.12580000
C	-4.37610000	-2.64300000	-0.85160000
C	-4.35830000	-4.03810000	-0.47540000
C	-3.74920000	-4.10750000	0.74500000
C	-4.91180000	-2.15370000	-2.03710000
H	-5.35910000	-2.87400000	-2.72370000
C	-4.92200000	-0.81320000	-2.41430000
C	-5.49660000	-0.30980000	-3.64090000
C	-4.62960000	1.35800000	-2.39300000
N	-4.40250000	0.21550000	-1.67480000
C	-5.31620000	1.04430000	-3.62640000
C	-4.26360000	2.64600000	-2.00700000
H	-4.52780000	3.46090000	-2.68320000
C	-3.61040000	2.98730000	-0.82870000
C	-3.26900000	4.34200000	-0.45090000
N	-3.19880000	2.11120000	0.14250000
C	-2.63570000	2.86840000	1.13360000
C	-2.10730000	2.36800000	2.32420000
H	-1.61280000	3.07230000	2.99430000
Fe	-3.45430000	0.11200000	0.11760000
C	-2.66310000	4.26690000	0.77080000
O	0.73780000	-0.93030000	-3.53400000
H	-0.88800000	1.13090000	4.59750000
H	-1.33670000	-1.55720000	4.61870000
H	-4.77090000	-4.84760000	-1.07520000
H	-3.56320000	-4.98590000	1.36070000
H	-5.97380000	-0.92370000	-4.40290000
H	-5.61500000	1.77630000	-4.37490000
H	-3.48730000	5.22650000	-1.04740000
H	-2.27870000	5.07510000	1.39020000
H	-4.99720000	1.42350000	2.13290000
O	-1.73450000	-0.21210000	-0.87900000

C	-5.80000000	3.52160000	4.66450000	C	4.27860000	-0.19950000	-0.67620000
N	-5.23600000	3.65230000	3.41700000	N	3.23070000	-1.07070000	-0.81320000
C	-6.02640000	3.90870000	2.21980000	C	3.35670000	-2.40930000	-0.21170000
O	-2.90810000	4.59980000	6.30610000	O	2.70280000	2.10130000	1.00380000
C	-4.11610000	4.58250000	6.22710000	C	3.82400000	1.88000000	0.58960000
C	-4.84330000	3.29330000	5.83860000	C	4.05850000	1.32560000	-0.83030000
C	-3.81380000	3.56990000	3.07990000	C	1.92830000	-0.87980000	-1.44220000
C	-3.71440000	4.26760000	1.71140000	C	1.24980000	-2.22040000	-1.13700000
C	-5.03340000	3.85100000	1.04960000	C	1.92490000	-2.84310000	0.07080000
C	-4.96070000	5.82900000	6.45300000	C	5.05350000	2.12160000	1.44020000
C	-4.30840000	6.89920000	7.34290000	C	4.75570000	2.56810000	2.86860000
C	-4.10120000	6.41370000	8.78730000	C	4.27910000	4.01790000	2.97440000
C	-3.46740000	7.49960000	9.67070000	C	3.96350000	4.44400000	4.41500000
C	-3.28120000	7.00720000	11.08460000	C	3.55220000	5.88340000	4.52790000
C	-2.08640000	6.86260000	11.67770000	C	2.35580000	6.31730000	4.94050000
C	-1.65875695	6.51761605	12.97776056	C	1.93690000	7.75380000	5.03670000
C	-5.52760000	2.68200000	7.07400000	C	5.27570000	1.93680000	-1.52840000
O	-6.99190000	3.61100000	4.83690000	O	5.40080000	-0.61380000	-0.41610000
C	-3.30280000	2.13260000	2.98060000	C	1.92460000	-0.61180000	-2.97650000
O	-3.99280000	1.18630000	3.28440000	O	2.85010000	-0.22870000	-3.64450000
H	-6.47640000	4.92680000	2.29460000	H	4.01980000	-2.34150000	0.65670000
H	-6.83840000	3.15570000	2.09520000	H	3.73580000	-3.06110000	-0.95630000
H	-4.08210000	2.54220000	5.51980000	H	3.16110000	1.53780000	-1.42070000
H	-3.17500000	4.11470000	3.80970000	H	1.42010000	-0.00440000	-1.00460000
H	-3.70310000	5.37580000	1.84890000	H	0.18360000	-2.32970000	-1.33180000
H	-2.81720000	3.97880000	1.11950000	H	-2.05650000	-1.01380000	-1.32290000
H	-4.94660000	2.80390000	0.67200000	H	1.79280000	-3.93260000	0.04140000
H	-5.32220000	4.50950000	0.19940000	H	1.55160000	-2.46270000	1.03860000
H	-5.16860000	6.26180000	5.44530000	H	5.63290000	1.18120000	1.41160000
H	-5.94120000	5.54180000	6.89590000	H	5.69520000	2.85550000	0.92120000
H	-4.96470000	7.80300000	7.35800000	H	5.66580000	2.43730000	3.47870000
H	-3.33500000	7.21960000	6.90250000	H	3.98980000	1.90170000	3.29920000
H	-3.44580000	5.51120000	8.79520000	H	3.37930000	4.15380000	2.35440000
H	-5.08600000	6.11060000	9.21690000	H	5.05370000	4.68770000	2.55670000
H	-4.11940000	8.40410000	9.69730000	H	4.86040000	4.26710000	5.03950000
H	-2.49050000	7.81010000	9.23260000	H	3.16870000	3.79620000	4.82300000
H	-4.19640000	6.75050000	11.64370000	H	4.30390000	6.62490000	4.22200000
H	-1.16930000	7.11430000	11.11900000	H	1.60640000	5.57140000	5.23910000
H	-2.62665695	6.28481605	13.47536056	H	2.74230000	8.43380000	4.71850000
H	-1.04175695	5.59031605	12.97836056	H	1.05120000	7.95610000	4.40870000
H	-1.13605695	7.28841605	13.58896056	H	1.65270000	8.02120000	6.06990000
H	-4.78740000	2.49210000	7.88520000	H	5.21670000	3.03580000	-1.53350000
H	-6.00550000	1.70710000	6.82310000	H	5.30760000	1.58900000	-2.57210000
H	-6.31630000	3.34300000	7.49690000	H	6.20970000	1.62350000	-1.04590000
H	-2.53490000	0.92490000	1.90960000	H	0.82530000	-0.81950000	-4.49850000
2g				**2h**			
0 2				0 2			
C	0.08435000	4.19843900	-1.72104200	S	3.15349900	1.08444000	2.69193400
N	0.77167600	4.27722800	-0.54249000	N	1.56790200	-1.12831800	1.35532800
C	1.30372300	5.57610400	-0.08042200	C	1.99317000	-2.41380700	1.57426200
O	-1.39878400	1.36492100	-0.52690500	C	0.28387900	-1.05246700	1.83329600
C	-1.53933300	2.35470100	-1.22636600	C	0.92793400	-3.18959200	2.16631100
C	-0.40608300	2.80454400	-2.14903400	C	-0.13074800	-2.34192600	2.33396000
C	1.07969800	3.28303700	0.40727600	C	-0.51576200	0.08234600	1.84232200

C	1.85625700	3.76371400	1.38812800
C	2.18942200	5.21487200	1.13569400
C	-2.79342900	3.19765800	-1.20243300
C	-3.84086900	2.80555100	-0.16124400
C	-4.62445600	1.53349900	-0.49178800
C	-5.72699800	1.24589900	0.53743900
C	-6.49173200	-0.01712100	0.26298900
C	-6.69698400	-1.00799000	1.13931700
C	-7.45147200	-2.27349400	0.86281900
C	-0.83514300	2.81417200	-3.62001200
O	-0.14090500	5.19672000	-2.38801300
C	3.91897100	2.14544500	-0.37083600
O	4.67110400	2.82107500	0.19739100
H	0.46176900	6.23322800	0.19114200
H	1.84178200	6.06670100	-0.90244600
H	0.40663700	2.07792200	-2.01348300
H	0.69226100	2.27369500	0.30551500
H	2.21970900	3.17608300	2.22734000
H	-0.02178000	0.30179700	-0.80183200
H	3.26472000	5.33523900	0.91410700
H	1.97393800	5.85749900	2.00406200
H	-2.46772900	4.24459000	-1.07080300
H	-3.22245900	3.17527100	-2.22066000
H	-4.54907800	3.64535700	-0.05788700
H	-3.34701200	2.68584000	0.81730900
H	-3.93603000	0.67698300	-0.54692900
H	-5.08330500	1.63531000	-1.49269300
H	-6.42782200	2.10324700	0.54577300
H	-5.28787100	1.20174600	1.54876500
H	-6.90294700	-0.11880100	-0.75120900
H	-6.28323300	-0.90386100	2.15167300
H	-7.83120200	-2.30274000	-0.17024800
H	-6.81237000	-3.16043500	1.01822600
H	-8.31087500	-2.38614100	1.54659700
H	-1.27731400	1.84603600	-3.89867200
H	0.03924200	2.99331300	-4.26127900
H	-1.55356400	3.62054400	-3.81556400
H	1.54719500	0.27491000	-0.90102000
S	0.99908300	-3.52652500	1.73804300
N	2.56450400	-0.98306800	1.01911800
C	2.68299700	-0.03940600	2.00994600
C	3.84400200	-1.30575800	0.63839400
C	4.07572300	0.26136400	2.24724200
C	4.79773600	-0.53115000	1.39785900
C	4.19007000	-2.21305600	-0.35625500
H	5.25359700	-2.36615300	-0.54654800
C	3.29176500	-2.91629600	-1.14815300
N	1.92575700	-2.84996900	-1.06167300
C	1.43926000	-3.65194200	-2.05912300
C	2.52989300	-4.24502200	-2.80381600
C	3.68231000	-3.79371200	-2.23226700
C	0.09542400	-3.89016400	-2.31726400
H	-0.15124300	-4.55130100	-3.14946700
C	-0.95475900	-3.37987900	-1.56587500
H	-1.53205700	-0.01083900	2.22244800
C	-0.14268700	1.31195000	1.31992000
N	1.07107900	1.61256500	0.75124000
C	0.97114000	2.89232400	0.26874800
C	-0.34648300	3.41756500	0.54025100
C	-1.03567300	2.44054900	1.20138400
C	1.97785100	3.59428900	-0.38242300
H	1.75084300	4.60615000	-0.72070100
C	3.26611500	3.12080400	-0.58546200
C	4.34196500	3.91025600	-1.14608500
C	5.07348700	1.87607000	-0.50171500
N	3.73432200	1.88707200	-0.21958600
C	5.46658800	3.14217300	-1.08219500
C	5.93902000	0.81344000	-0.28702900
H	6.98678400	0.95083800	-0.55721000
C	5.55776600	-0.43037200	0.19972900
C	6.44298700	-1.56855800	0.29719700
N	4.29353200	-0.78768700	0.58946500
C	4.34040500	-2.12372300	0.89781000
C	3.27407600	-2.89566900	1.33706100
H	3.46736800	-3.94725800	1.55357600
Fe	2.66244800	0.39081700	0.59136500
C	5.68516900	-2.62195000	0.71965500
O	0.74933000	-2.83387800	-1.39419100
H	1.00136900	-4.24359300	2.42875500
H	-1.11249200	-2.55122000	2.75526400
H	-0.68531900	4.41100400	0.25091900
H	-2.06579900	2.44281900	1.55035600
H	4.23178800	4.92661500	-1.52067100
H	6.47868400	3.38923000	-1.39844300
H	7.50292300	-1.54929200	0.04914800
H	5.99060600	-3.65179700	0.89754600
H	4.13881800	0.19382700	2.95252800
O	2.24400600	-0.11746800	-1.08711900
C	-2.27631800	-1.64955700	-2.02655300
N	-1.35493400	-0.73486100	-2.48545800
C	-0.81241000	-0.86846600	-3.85229700
O	-3.52870500	0.43871400	0.66050800
C	-3.56299400	-0.14376500	-0.40412200
C	-2.78803600	-1.45135800	-0.60119100
C	-0.80352200	0.35475900	-1.83890800
C	0.03251400	1.14783100	-2.78732800
C	0.37747100	0.10084900	-3.86613800
C	-4.41221000	0.34030800	-1.56571800
C	-5.52160000	1.30714600	-1.16121100
C	-6.64954600	0.63069000	-0.37994700
C	-7.74861100	1.60700500	0.06157300
C	-8.87841400	0.93275400	0.78517100
C	-9.21921900	1.14982300	2.06077300
C	-10.33438700	0.46780900	2.79172600
C	-3.70366600	-2.61071900	-0.18011900
O	-2.64250900	-2.57812600	-2.73998800
C	-0.02116200	-3.57367300	-0.93252400
O	-0.78626500	-4.31518400	-0.47122900

C	-2.34934000	-3.69146400	-1.79611100	H	-1.59896400	-0.59177500	-4.57498900
C	-2.09420400	-2.34325700	-0.00577800	H	-0.54899200	-1.91770500	-4.03861700
N	-0.82699900	-2.55037400	-0.48231700	H	-1.92756300	-1.41438800	0.08537700
C	-3.05801700	-3.05259200	-0.82189000	H	-1.15699000	0.66978800	-0.86225400
C	-2.43353000	-1.54358700	1.07744500	H	-0.54014700	1.99936100	-3.21134000
H	-3.48786500	-1.48556800	1.34006900	H	0.92724300	1.55635800	-2.29940000
C	-1.54449900	-0.77451900	1.81532800	H	1.29609400	-0.42320300	-3.56218100
C	-1.93982000	0.12982000	2.87232600	H	0.54490800	0.53638400	-4.86138800
N	-0.18951400	-0.71039600	1.62042600	H	-3.70580800	0.82185900	-2.26663400
C	0.28700300	0.19959300	2.53104300	H	-4.80695500	-0.53463900	-2.11018200
C	1.62465200	0.52761100	2.71189000	H	-5.93327500	1.78466600	-2.06665800
H	1.86518100	1.24998100	3.49333100	H	-5.08283000	2.11062400	-0.54756600
Fe	0.87187800	-1.84538800	0.32898000	H	-6.23418200	0.13574600	0.51377700
C	-0.80242100	0.74408300	3.31094500	H	-7.09552000	-0.16959400	-0.99917200
O	3.17349800	1.48691800	-0.97865100	H	-8.14094100	2.12456600	-0.83507700
H	4.44145900	0.98264300	2.97619600	H	-7.30750000	2.38876300	0.70389900
H	5.87909200	-0.59605600	1.28757800	H	-9.44515500	0.18841200	0.20784700
H	2.40821500	-4.92067800	-3.64886500	H	-8.64649000	1.89070200	2.63498800
H	4.71158300	-4.01617900	-2.50919700	H	-10.85493800	-0.25631500	2.14603100
H	-2.71759600	-4.32528500	-2.60122400	H	-9.96061700	-0.07177700	3.68002500
H	-4.13284700	-3.03650200	-0.65730900	H	-11.07864400	1.19649100	3.15932700
H	-2.96307600	0.26808200	3.21742600	H	-4.03554700	-2.46540900	0.85822800
H	-0.69093300	1.49217000	4.09414100	H	-3.16282300	-3.56267500	-0.25662500
H	1.29641200	-2.82609000	2.85992100	H	-4.58491400	-2.67489800	-0.83423300
O	0.75036500	-0.25463600	-1.06053600	H	1.36438860	0.16041003	-1.39207849
2i				***R*-2b**			
0 4				0 1			
S	3.15151800	1.80410900	-2.38828500	C	2.22955100	-1.12679000	0.15198900
N	0.71884300	2.16482500	-0.58655000	N	2.91206600	-0.06448100	-0.36198500
C	0.83755800	3.30797200	0.16079400	C	4.05209200	-0.29965100	-1.25750200
C	-0.53378700	2.18814100	-1.14721300	O	-0.39607700	0.78882500	-0.00158900
C	-0.36593100	4.09757300	0.04295100	C	-0.12277300	-0.38752400	0.14079000
C	-1.22276700	3.39505700	-0.75520500	C	1.02803200	-0.80763800	1.06457300
C	-1.07201900	1.21343800	-1.97588200	C	2.77982700	1.33723000	0.01087800
H	-2.10209900	1.33697200	-2.30669000	C	3.59797800	2.06170600	-1.07550200
C	-0.38534600	0.09508900	-2.42675700	C	4.73556400	1.06937700	-1.35206700
N	0.90417200	-0.23997000	-2.09685000	C	-0.82865600	-1.47566400	-0.64407900
C	1.22738100	-1.34441300	-2.84430000	C	-2.09719200	-1.01140700	-1.35408500
C	0.09775600	-1.73231700	-3.65714700	C	-3.25273000	-0.70899000	-0.39838800
C	-0.91009100	-0.85229900	-3.38100800	C	-4.51889900	-0.22433700	-1.11852300
C	2.43108300	-2.03488500	-2.78803600	C	-5.66812900	0.02608100	-0.18557300
H	2.55518600	-2.89080500	-3.45256500	C	-6.24442500	1.21376400	0.03168000
C	3.44876100	-1.77067100	-1.88062800	C	-7.37935000	1.47060600	0.97713000
C	4.60561800	-2.61348800	-1.68664200	C	0.71245200	-1.99768600	1.97064900
C	4.56605000	-0.93621200	-0.17624200	O	2.50288500	-2.27476500	-0.16358800
N	3.45794500	-0.75168200	-0.96205000	C	3.34246700	1.62780400	1.39796800
C	5.28889000	-2.10591400	-0.61850800	O	3.77015800	0.78845300	2.16252800
C	4.96802000	-0.11463500	0.86866400	H	3.68801300	-0.65310900	-2.23775600
H	5.87141100	-0.39375100	1.41197600	H	4.69957900	-1.08957400	-0.85094300
C	4.33902400	1.06829900	1.22996400	H	1.24964500	0.07337700	1.67737200
C	4.84567700	1.98960200	2.22398200	H	1.72706600	1.66790900	0.01061500
N	3.20243900	1.57759200	0.66035100	H	2.96933100	2.20034100	-1.96854900
C	2.98471200	2.79949100	1.23895500	H	3.94405400	3.05530100	-0.75276700
C	1.90616100	3.63291300	0.98590200	H	5.50977000	1.15944600	-0.57303500

H	1.85754000	4.57807800	1.52752900
Fe	2.06729800	0.68673200	-0.73976200
C	4.01470600	3.07130500	2.21686800
H	-0.52711900	5.05406600	0.53694100
H	-2.23404500	3.65459500	-1.06323600
H	0.09001400	-2.58185700	-4.33796800
H	-1.92232900	-0.82418600	-3.77858500
H	4.83889700	-3.49048100	-2.28803200
H	6.20643100	-2.47335500	-0.16219300
H	5.73521900	1.81860200	2.82771000
H	4.06932000	3.97523400	2.82086700
H	2.09428400	2.53136100	-2.81835700
O	1.26275300	-0.26222300	0.56348800
C	-1.25635900	-1.41198600	2.02422300
N	-0.56254000	-2.45708400	1.43167300
C	0.23882400	-3.38031400	2.25952600
O	-3.31010300	-0.79407900	-0.82723900
C	-3.11802100	-0.99865200	0.35412800
C	-1.89665100	-0.41539300	1.06876100
C	-0.32418200	-2.66677600	0.08682400
C	0.61863600	-3.81445600	-0.08505100
C	1.32019300	-3.86246600	1.28667700
C	-4.07706100	-1.82553200	1.19249600
C	-5.47491700	-1.94728500	0.59311300
C	-6.26057400	-0.63563200	0.63928900
C	-7.65430900	-0.74269500	0.00514200
C	-8.43713600	0.53579900	0.08546100
C	-8.84414300	1.26136500	-0.96234700
C	-9.60949300	2.54832400	-0.88525200
C	-2.29191500	0.87168300	1.80396800
O	-1.32371900	-1.32615400	3.24076200
H	-0.40868000	-4.20281300	2.60940500
H	0.62268600	-2.84701500	3.13567500
H	-1.16142000	-0.15915100	0.29731400
H	-0.97026200	-2.23716000	-0.67663800
H	0.06858100	-4.75742100	-0.28714400
H	1.31174200	-3.66507600	-0.92635800
H	2.15840500	-3.14853100	1.29733700
H	1.70856700	-4.85684100	1.54622300
H	-3.60131200	-2.82057000	1.28256300
H	-4.09896800	-1.42903400	2.22073200
H	-6.03380400	-2.73187600	1.13072400
H	-5.38199400	-2.27946100	-0.45359800
H	-5.69308300	0.15226800	0.11715800
H	-6.35868800	-0.30343600	1.68914300
H	-8.21257300	-1.55044500	0.51605500
H	-7.55404700	-1.05308600	-1.04907400
H	-8.66510900	0.89879100	1.09776800
H	-8.60791700	0.89607300	-1.97131400
H	-9.80238700	2.84452100	0.15753900
H	-9.06158700	3.37081100	-1.37817200
H	-10.58179100	2.46900300	-1.40296300
H	-2.74592100	1.58133900	1.09815400
H	-1.39291900	1.33216600	2.23449400
H	5.22177900	1.23175300	-2.32432100
H	-0.07862500	-1.84682500	-1.36736700
H	-1.02503300	-2.33745900	0.01345200
H	-2.40957200	-1.78924300	-2.07149300
H	-1.86630300	-0.10895200	-1.94322200
H	-2.94076200	0.05933000	0.32726100
H	-3.48962700	-1.61584800	0.18843100
H	-4.81091000	-0.98485100	-1.86794100
H	-4.28929700	0.69577400	-1.68278700
H	-6.03684700	-0.84757800	0.37064100
H	-5.86712900	2.08417000	-0.52257800
H	-7.69512000	0.55026400	1.49255400
H	-7.10075100	2.21372200	1.74509600
H	-8.25662000	1.88403500	0.44875300
H	-0.24966000	-1.85743300	2.48650400
H	1.50005400	-2.10052200	2.73130100
H	0.68828800	-2.93115700	1.39358800
H	3.32364300	2.71710000	1.67264300

H	-2.99579400	0.66898200	2.62312300
H	0.93761700	-1.10822400	0.19320000

***R*-2g**			
0 1			
C	2.35674600	1.12363400	0.18959600
N	3.34902500	0.22095200	-0.04285900
C	4.53483000	0.15545800	0.83320500
O	-0.03449100	-0.86017700	-1.45355700
C	0.31057900	-0.16414100	-0.52656100
C	1.16573500	1.08287200	-0.76746200
C	3.43566300	-0.77815800	-1.02523300
C	4.56800400	-1.46882400	-0.93147800
C	5.41991500	-0.94188800	0.19593600
C	-0.06824200	-0.48018400	0.90672500
C	-1.40145800	-1.20858100	1.03959800
C	-2.59360400	-0.31692100	0.70093500
C	-3.93525300	-1.04901100	0.81037300
C	-5.10636100	-0.15811800	0.53381900
C	-5.95671400	-0.30201800	-0.47568200
C	-7.11449600	0.60022500	-0.76539600
C	0.30053100	2.33798400	-0.62345000
O	2.42014400	1.90083800	1.12925800
H	4.21624600	-0.09363700	1.84582200
H	5.01330900	1.13218700	0.87366100
H	1.52345800	1.00896300	-1.79500200
H	2.63197100	-0.91425600	-1.72980700
H	4.84921800	-2.28186800	-1.58146400
H	6.36364900	-0.53304400	-0.17524700
H	5.67794600	-1.71970700	0.91773900
H	0.74863400	-1.10513200	1.28923000
H	-0.04573600	0.43091300	1.50739500
H	-1.50243000	-1.57982600	2.06321900
H	-1.39726800	-2.08006800	0.38164400
H	-2.48719800	0.07105500	-0.31567600
H	-2.59861500	0.55275000	1.36746000
H	-4.02341600	-1.46806700	1.82025000
H	-3.94387200	-1.89558400	0.11797200
H	-5.23722300	0.68377600	1.21219000
H	-5.81688100	-1.13933900	-1.15658900
H	-7.18129300	1.40937200	-0.03635000
H	-7.02896900	1.04496800	-1.76140500
H	-8.05948800	0.04871900	-0.74888500
H	-0.54701300	2.28741100	-1.30756000
H	0.88870100	3.22446000	-0.85792600
H	-0.06739200	2.45002300	0.39419600

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1 1			
C	2.99130700	-0.77437200	0.26668800
N	3.03673400	0.68467900	0.18888500
C	3.95221800	1.34161500	-0.78900100
O	0.30980900	0.18476300	-0.22722800
C	0.50433900	-0.98623400	0.03247300
C	1.75679800	-1.38249800	0.89852700
C	2.20664100	1.51912200	0.74004400
C	2.39253400	2.90088900	0.24614400
C	3.74488700	2.83700900	-0.49927500
C	-0.39757500	-2.08692500	-0.45229100
C	-1.66502000	-1.60592100	-1.15556000
C	-2.70249400	-1.00410400	-0.20481400
C	-3.96708100	-0.51927100	-0.92768900
C	-5.00272200	0.03129600	0.01038600
C	-5.44468000	1.29424300	0.01330200
C	-6.47846000	1.85286700	0.94282900
C	1.97201100	-2.87597700	1.13771300
O	3.88659400	-1.37790400	-0.24607800
H	3.63260200	1.03270200	-1.79631500
H	4.97195700	0.97145200	-0.62847100
H	1.57560900	-0.88187200	1.86662700
H	1.49782800	1.21233200	1.50563600
H	1.53015400	3.10510700	-0.42009600
H	2.33278800	3.64466700	1.05538700
H	4.54725700	3.21484700	0.15035100
H	3.74993700	3.43720500	-1.41736500
H	0.22646000	-2.71535200	-1.11622900
H	-0.63482600	-2.74484700	0.40128300
H	-2.10688900	-2.46527200	-1.68492400
H	-1.39359400	-0.86858800	-1.92838100
H	-2.26275400	-0.15593200	0.34598100
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H	-5.41033600	-0.67382300	0.74798400
H	-5.03512800	1.99042400	-0.73195000
H	-6.83439500	1.09712000	1.65944300
H	-6.08184800	2.70993500	1.51462100
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H	1.11438600	-3.31439700	1.66271300
H	2.86579300	-3.03131400	1.75742500
H	2.12865700	-3.41577500	0.19478100

Genes sequence

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