"Structure and Function of NzeB, a Versatile C–C and C–N Bond Forming Diketopiperazine Dimerase"

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Supporting Information

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Instrumentation

All UV-Visible spectra were acquired using a single beam Molecular Devices Spectra Max M5 spectrophotometer, with a 1cm quartz cuvette. Analytical HPLC data was acquired using a Shimadzu HPLC system comprised of two LC-20AD$_{XR}$ pumps, a SIL-20AC$_{XR}$ autosampler, and a SPD-M20A diode array detector. Preparatory HPLC was performed using a Beckman Coulter stack comprised of a System Gold 125 solvent module, 168 detector, and SC100 fraction collector. ^{1}H NMR spectra were recorded on Varian 600 MHz spectrometers and are reported relative to residual solvent peak (CD_2HOD: δ 3.31). ^{13}C NMR spectra were reported relative to residual solvent peaks (CD_2HOD: δ 49.0).

***Streptomyces* sp. CMBMQ-030 genomic DNA sequencing**

The genomic DNA of *Streptomyces* sp. CMB-MQ030 was extracted and purified as prescribed using the Promega Wizard® Genomic DNA Purification Kit. The genomic DNA (2x250 bp paired-end) was sequenced using Illumina HiSeq 2500 sequencing system at University of Michigan DNA Sequencing Core. Briefly, the genomic DNA sample was first sheared to approximately 500 nucleotide average fragment size, then Illumina-compatible sequencing libraries were prepared from those fragments on an Apollo 324 robotic workstation (WaferGen Biosystems), using the Kapa HTP Library Preparation Kit (KAPABiosystem) according to the manufacturer's protocols. Subsequent libraries were sequenced on an Illumina HiSeq 2000, obtaining paired-end sequence data with 100 nucleotide reads at each end, as per recommended protocols from Illumina, Inc. The generated next-generation sequencing data were then *de novo* assembled using Velvet 1.2.10.

Supplementary Table 1. Summary of genome assembly dataset and parameters

Genome	**Number of reads**	**k-mer**	**Coverage cutoff**	**N50**	**Number of contigs**
Streptomyces sp. (CMB-MQ030)	33,263,004	51	10	66,868	591

Cloning of NascA, NascB, and NznA

The PCR primers were designed to introduce an *Nde*I restriction site at the 5′ end of the fragment and a *Hind*III restriction site 3′ end, respectively. The coding sequences were amplified from the genomic DNA of *Streptomyces sp.* CMB-MQ030 using primers for the associated target gene. The expression constructs were designed in pET28b vector cloning at *Nde*I and *Hind*III restriction sites for NascA, NznA and NascB. NznB+09 and NzeB were cloned into pET28b using Quickchange mutagenesis. The nucleotide sequences were confirmed by automated sequencing (University of Michigan DNA Sequencing Core).

Supplementary Table 2. Primers used in cloning NascA, NasB, NznA, NznB, and extending codon optimized sequence of NznB

Gene	Primer	Rest. Site	5'→3'
NascA	Forward	*Nde*I	CCAACCcatatgGTGAACACTTCCCTCGCTGCGGTGGCCGGC
NascA	Reverse	*Hind*III	CCAACCaagcttGCGTTCGGCCGCCCGGTCCCGCAGCAGGAT
NascB	Forward	*Nde*I	CCAACCcatatgGTGACCACCACCGCCACGCTGACCTACCCC
NascB	Reverse	*Hind*III	CCAACCaagctt CCAGGTGGCGGGAAGCGCCCGCGGACGGCG
NznA	Forward	*Nde*I	CCAACCcatatgATGGCCACACACGCCTCCGCACCCGCACCC
NznA	Reverse	*Hind*III	CCAACCaagcttCTGCTGCGTCACGCGGTCCTTGAGGAG
NznB (CO) +09	Forward		GTGGATCCGTATACCAAAGAATGCCGTACCGTGACCACCGC GCCGGTTCCGCT
NznB (CO) +19	Forward		GTGATTCGTCCGCAGCCGCATCGTAGCCCGGTGGATCCGTA TACCAAAGAATGCCGTACCGTGACCACCGCGCCGGTTCCGC T
NzeB	Forward		ctgagaatctctacttccaaggcgctagcGTGACCACCACCACCGCCACG CTGACCT
NzeB	Reverse		cctttcgggctttgttagcagccggatcTCACCAGGTGGCGGGGATCGCCC GC

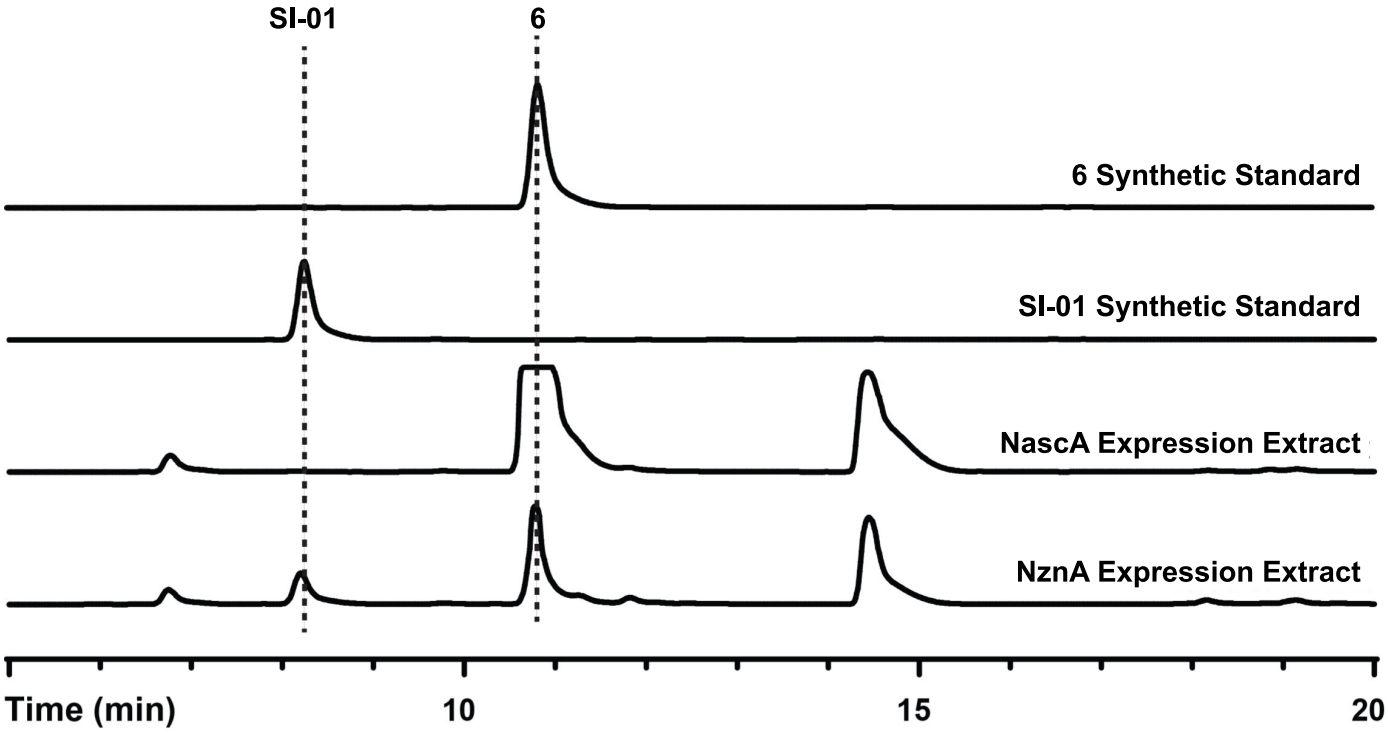
Codon optimized sequence for NznB

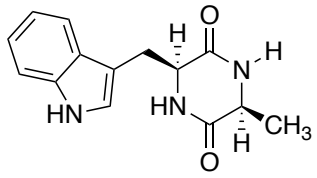
ACCACCGCGCCGGTTCCGCTGACCTTCCCGTTTCACGATTGGAGCCAAGAGCTGAGCCCGCACCATGAG
CGTCTGCGTGAAGCGGATGCGCCGGTGTGCCCGGTGGTTAGCGAGTACACCGGTGACCGTCTGTGGCT
GGTTACCCGTTATGCGACCGCGAAGCGTCTGCTGGAAGATCGTCGTTTCAGCAGCACCGCGGCGATGGC
GCCGGGTGCGCCGCGTCAGGAGCCGGTGGAACTGCGTGCGCCGGGCACCACCGGTGATGGTGTGAGC
GTTCTGCGTGAGGCGGGTCTGCGTACCGTTTTTACCGAAGGTCTGGGTCCGCGTGCGGCGCGTCGTCAC
GGTAAATGGCTGCGTGATCGTGCGGACACCCTGCTGCGTGATGTGGCGGAGTGCGAAGGTCCGGTTGAT
CTGGCGGCGGACTTTGCGCAGCCGCTGGCGGTGGCGATGACCAGCCGTGTTCTGCTGGGTGAACTGAG
CACCGAGGAAGCGGCGCTGCTGCGTGATCGTACCGATCTGGCGCTGCAGTTTTGCGGTGCGACCGCGG
AGGAACAACGTGGTGGCCTGATCGATATTCACCGTTTCTTTACCGCGCATGCGCGTCGTCTGGCGGATG
GTCCGGGTGACCACCTGCTGAAGCGTCTGGCGGAGGCGCCGGCGGAAAACGGTCCGCTGGGTGATGCG
GCGCTGAGCGAAATTGCGGCGCTGCTGCTGATTGCGGGTTTCCCGACCAGCAGCGGCTTTCTGTGCGGT
GCGCTGATCACCCTGCTGCGTCACCCGGAGGCGGTGGGCCGTCTGCGTCGTGATCCGGAACTGATTCC
GGACGCGGTTGAGGAACTGCTGCGTCATACCCCGCTGAGCACCGGTGCGGCGAAACGTATGGCGACCG
AGGACGCGGATATCGACGGCGTGCGTATTCGTCGTGGTGAGGTGGCGATGGTTAGCCTGGAAGCGGCG
AACCACGATCCGGACGCGTTCGACGATCCGGATAGCTTTCGTCCGGAACGTCAAGGTCCGGGTCACCTG
GGTTTTGGCCACGGTCCGAACTTTTGCCCGGGTAACCGTCTGGCGCGTTGCCTGATTGATGCGATGGTG
CGTGCGGTTGCGCGTCGTCCGGGTCTGCACCTGACCGTTGGTCCGGAGGAAATCCGTTGGCACGAAGG
CCTGTTCTTTCGTCGTCCGAAGGCGATTCCGGCGAGCTGG

Overexpression and analysis of CDPSs NascA/NznA.

The expression of CDPS was performed by transforming the plasmid into the competent cell *E. coli* strain C41(DE3) and selected on Luria-Bertani (LB) medium plates containing 50 µg/mL kanamycin. A single colony was grown overnight in 5 mL LB broth containing the same concentration of the antibiotics. The main culture was prepared by inoculating 1% of each overnight culture into a 2 L baffled flask containing 1 L of LB containing 50 µg/mL kanamycin. The cultures were incubated at 37°C and 250 rpm for 3-4 h until the absorbance A_{590nm} = 0.6. The expression of CDPSs was induced by the addition of 1 mM isopropyl β-D-1-thiogalactopyranoside (IPTG). The cultures were incubated further at 18°C for 18 h shaking at 180 rpm. Cells were harvested by centrifugation at 5000×g at 4°C for 15 min and a 1 mL aliquot of the supernatant was extracted with 1 mL $CHCl_3$ (3x). The organic extracts were dried and solvents were removed *en vacuo*. Residue was resuspended in 100 uL of HPLC grade methanol for HPLC analysis in which the samples was resolved using a linear gradient of 5-100% acetonitrile: water (0.1% formic acid) over 30 min (1.5 mL/min flow rate) on a Phenomenex Luna 5µ C-18(2) 100A, 250 × 4.60mm 5 micron column.

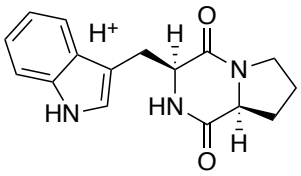
Supplementary Figure 1. HPLC traces for NascA/NznA Expression Extractions



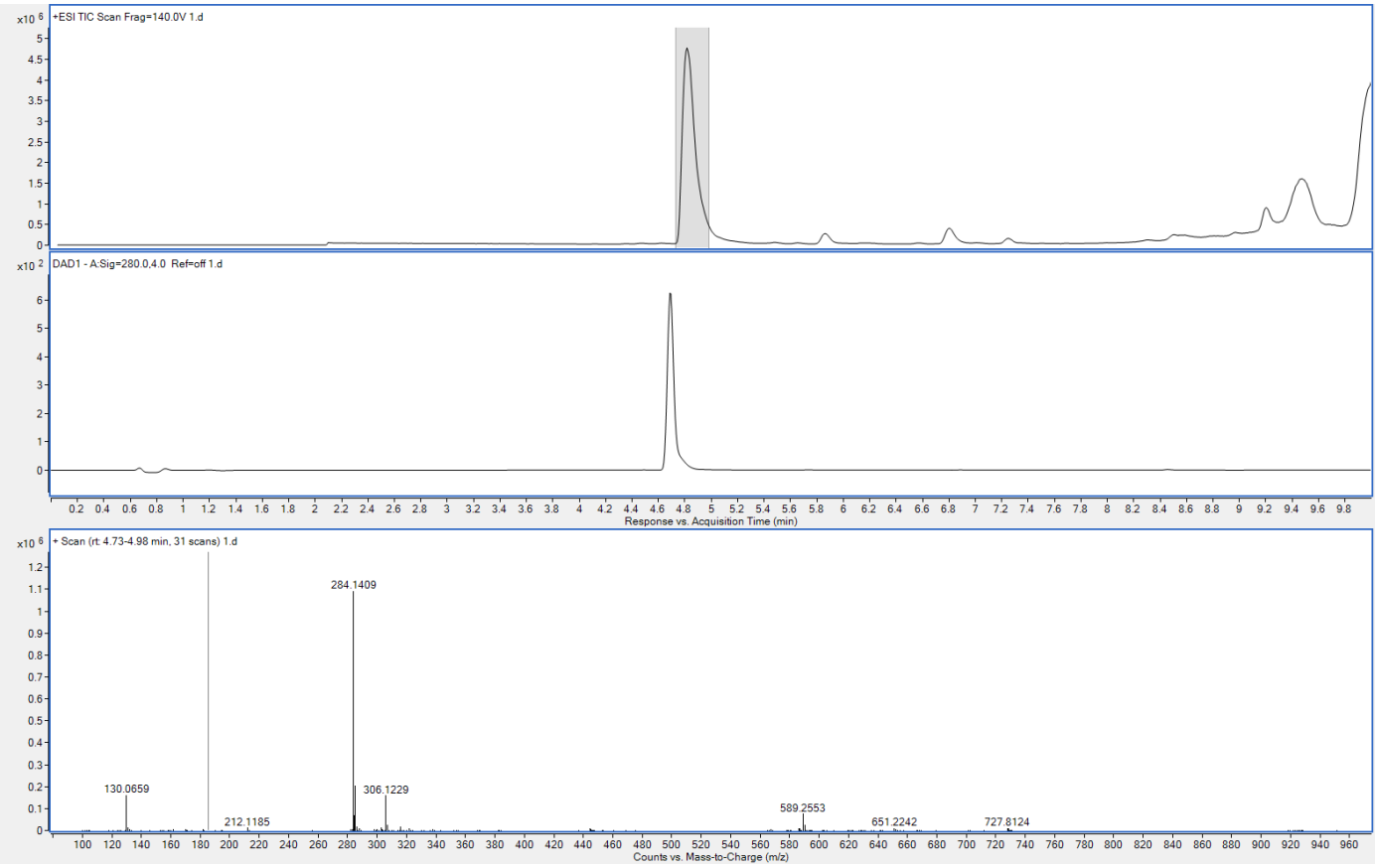


cyclo(*L*-ala-*L*-ala)
SI-01

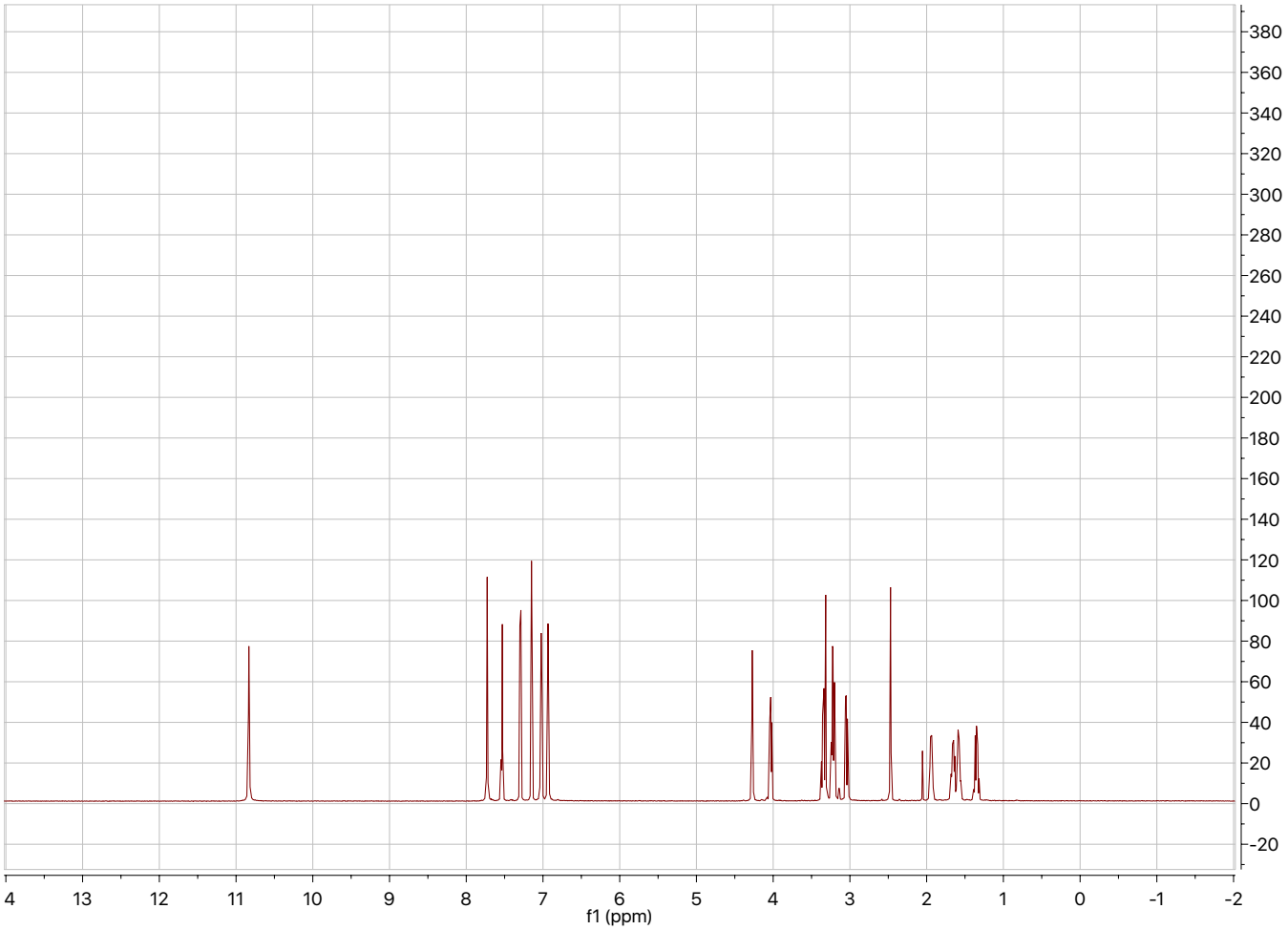
Supplementary Figure 2. HPLC/MS Anaylsis of Diketopiperazine 6 Isolated From CDPS Culture



Exact Mass: 284.1394

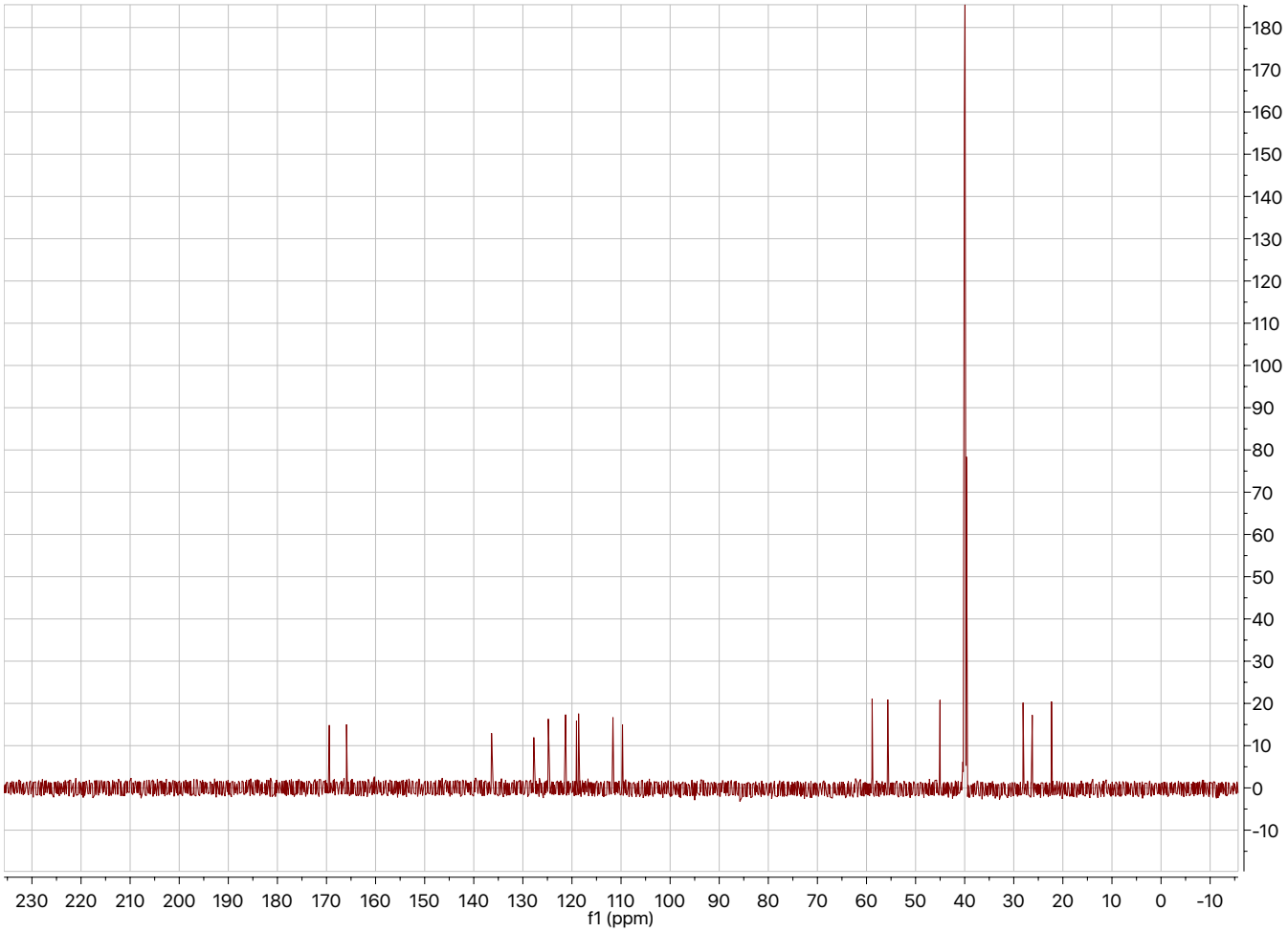


Supplementary Figure 3. [1]H NMR characterization of purified DKP 6 from NascA CDPS overexpression



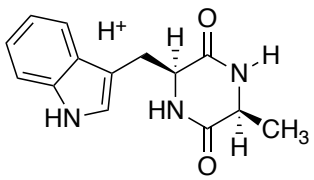
[1]H NMR (599 MHz, DMSO-d_6) δ 10.83 (s, 1H), 7.73 (s, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.15 (d, *J* = 2.2 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.93 (t, *J* = 7.4 Hz, 1H), 1.94 (dtd, *J* = 9.8, 6.9, 2.7 Hz, 1H), 1.66 (ddd, *J* = 19.1, 9.1, 5.6 Hz, 1H), 1.59 (ddp, *J* = 12.2, 8.4, 4.6, 4.1 Hz, 1H), 1.35 (dtd, *J* = 12.1, 10.3, 7.8 Hz, 1H).

Supplementary Figure 4. ^{13}C NMR characterization of purified DKP 6 from NascA CDPS overexpression \

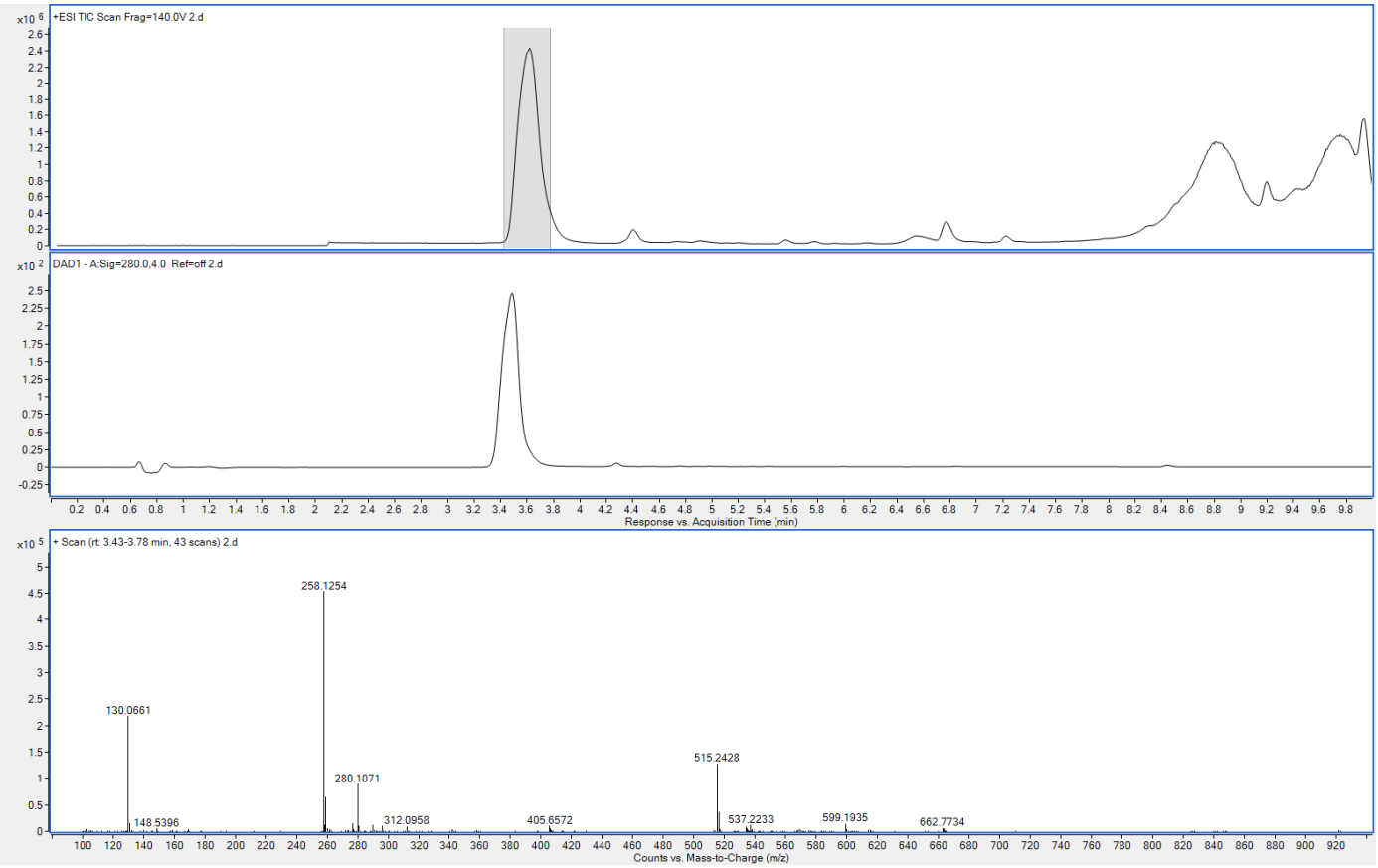


^{13}C NMR (151 MHz, dmso) δ 169.43, 165.92, 136.37, 127.77, 124.82, 121.30, 119.08, 118.65, 111.65, 109.70, 58.85, 55.66, 45.03, 28.11, 26.23, 22.31.

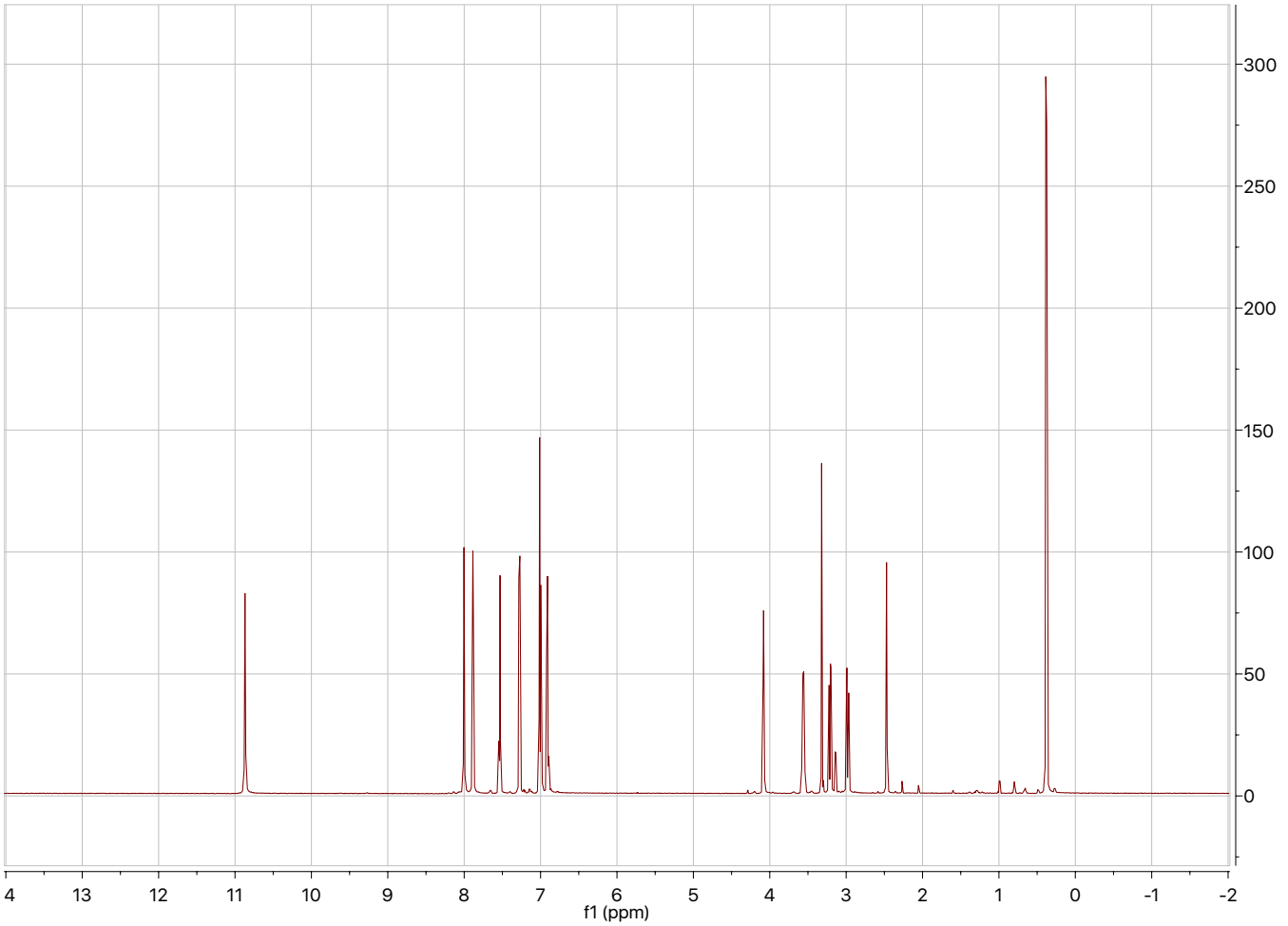
Supplementary Figure 5. HPLC/MS Anaylsis of Diketopiperazine SI-01 Isolated From CDPS Culture



SI-01
Exact Mass: 258.1237

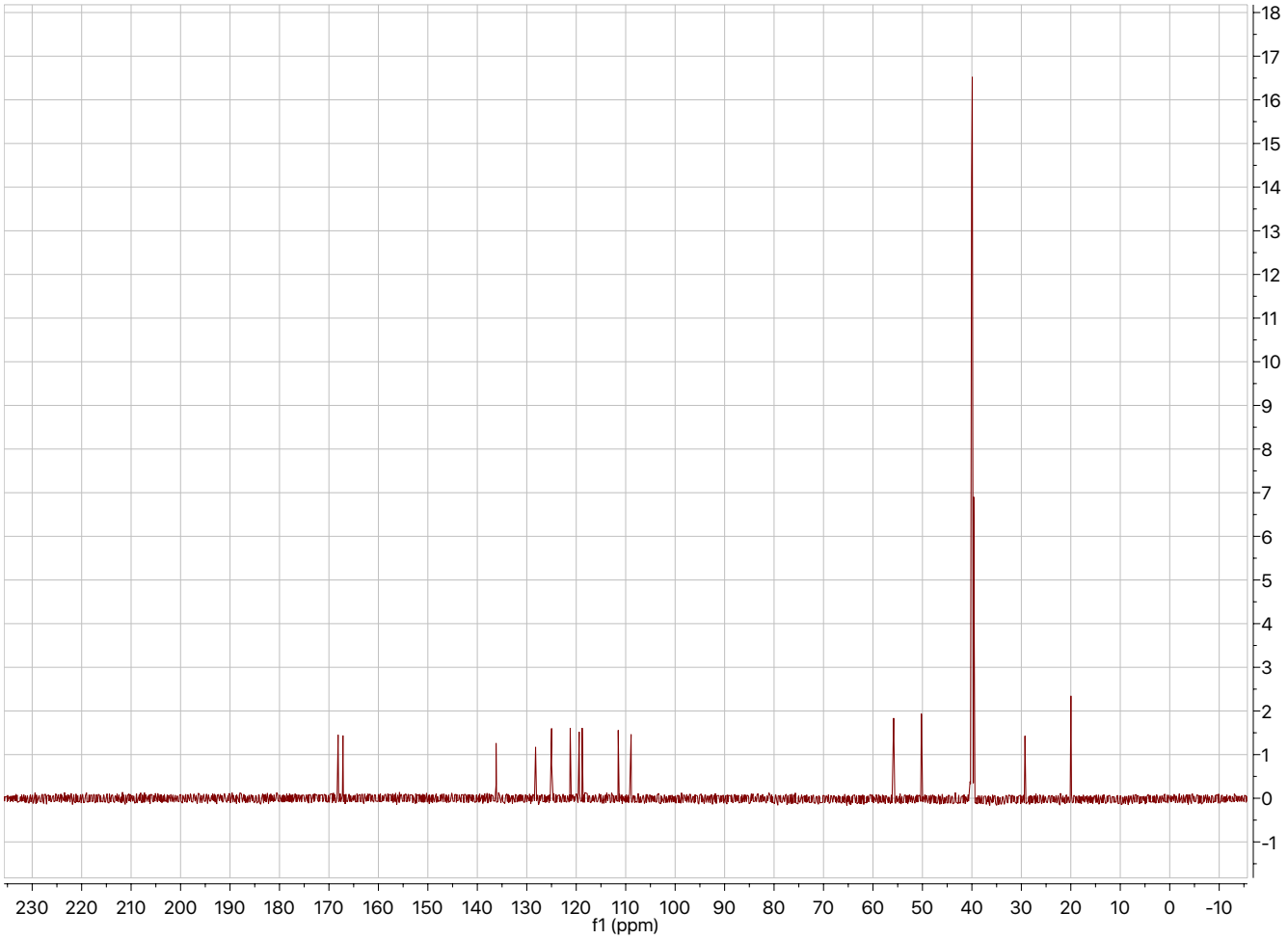


Supplementary Figure 6. ^{1}H NMR characterization of purified DKP SI-01 from NznA expression.



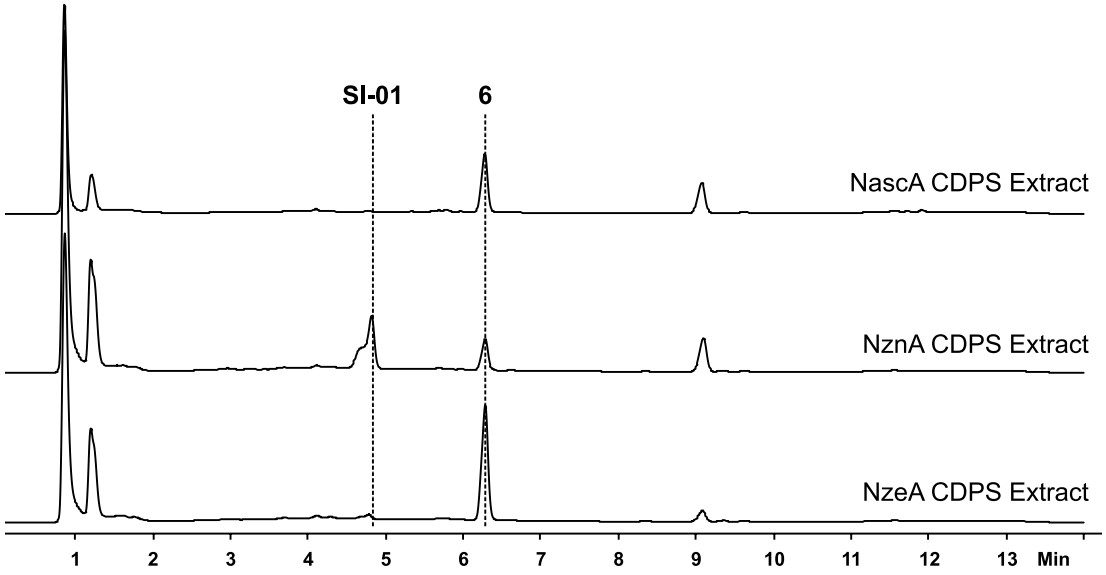
^{1}H NMR (599 MHz, DMSO-d_6) δ 10.87 (s, 1H), 8.00 (s, 1H), 7.89 (s, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 7.04 – 6.97 (m, 2H), 6.91 (t, J = 7.4 Hz, 1H), 4.08 (d, J = 2.7 Hz, 1H), 3.56 (dd, J = 7.0, 2.0 Hz, 1H), 3.32 (s, 1H), 3.21 (dd, J = 14.4, 4.1 Hz, 1H), 2.98 (dd, J = 14.4, 4.6 Hz, 1H), 2.47 (t, J = 1.9 Hz, 1H), 0.38 (d, J = 7.0 Hz, 3H).

Supplementary Figure 7. ^{13}C NMR characterization of purified DKP SI-01 from NznA expression.



^{13}C NMR (151 MHz, dmso) δ 168.14, 167.16, 136.20, 128.22, 124.98, 121.22, 119.40, 118.80, 111.51, 108.91, 55.82, 50.20, 29.27, 19.98.

Supplementary Figure 8. HPLC trace for NzeB CDPS overexpression

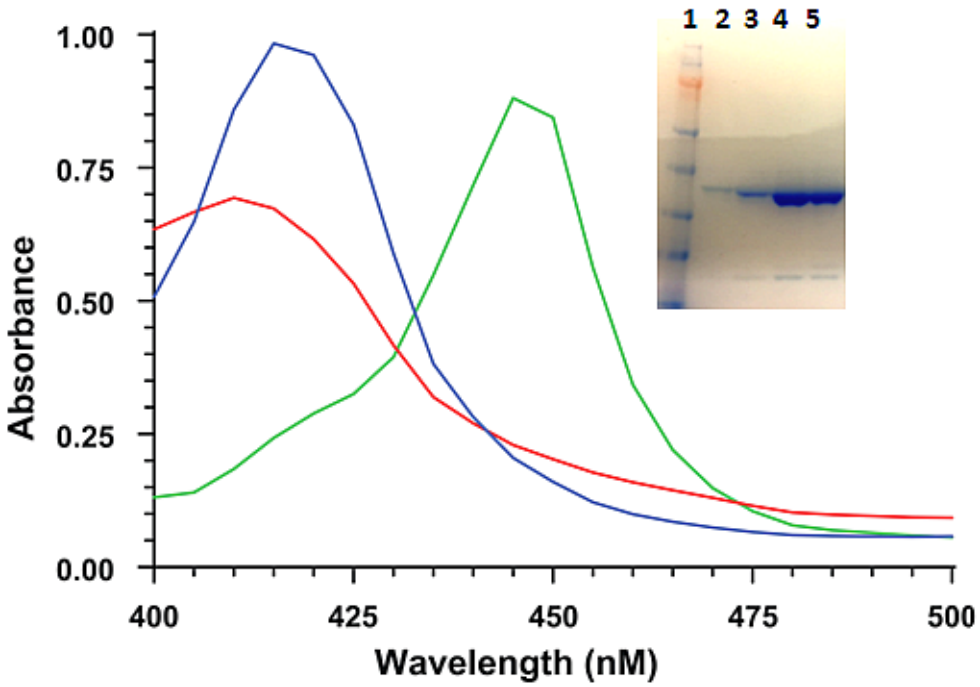


General procedure for overexpression, purification and spectral characterization of cytochrome P450s

The expression of P450s was performed by transforming the plasmid into the competent cell *E. coli* strain C41(DE3) and selected on Luria-Bertani (LB) medium plates containing 50 µg/mL kanamycin. A single colony was grown overnight in LB broth containing the same concentration of the antibiotics. The main culture was prepared by inoculating 1% of each overnight culture into a 2 L baffled flask containing 500 ml of Terrific Broth (TB) containing 50 µg/mL kanamycin. The cultures were incubated at 37°C and 250 rpm for 3-4 h unless the absorbance A_{590nm} = 1. The expression was induced by the addition of 0.8 mM isopropyl β-D-1-thiogalactopyranoside (IPTG) and 1.0 mM delta-5-aminolevulinic acid (w/v). The cultures were incubated further for 36 h, 28°C at 160 rpm. Cells were harvested by centrifugation at 5000×*g* at 4°C for 10 min and the cell pellet was stored at –80°C until purification of the protein.

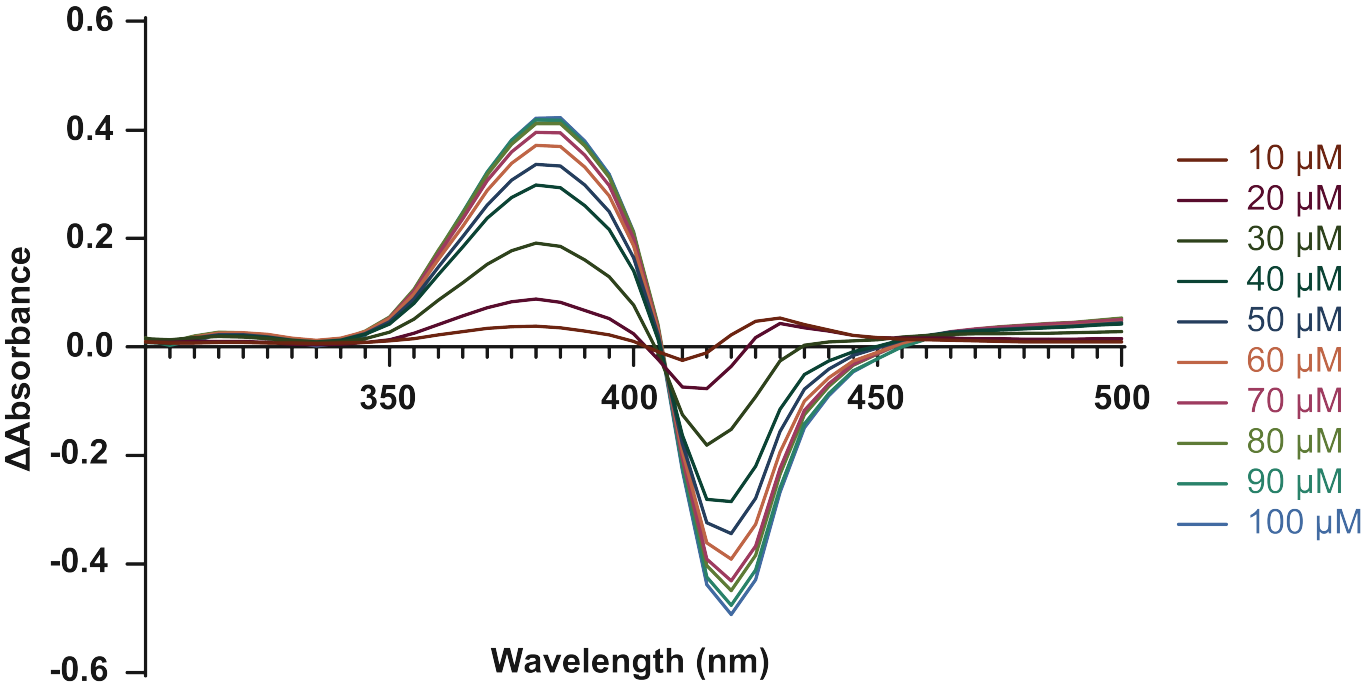
The cell pellet was resuspended in 5% culture volume of lysis buffer (50 mM Tris, pH 7.4 containing 50 mM NaCl, 2% glycerol, 0.5 mM EDTA, 10 mM beta-mercaptoethanol and 1mM phenylmethane sulfonyl fluoride (PMSF) and disrupted by sonication. The cell lysate was centrifugated (35,000 rpm for 35 min) and filtered (0.2 µM Millipore filter). The soluble His_6-tagged NasB was purified by affinity chromatography using Ni-NTA (Qiagen) column and the collected fractions were analyzed by SDS-PAGE. The suitable red fractions were pooled and dialyzed at 4°C three times using 50 mM Tris, pH 7.4 containing 10% glycerol, 50 mM NaCl and 1 mM dithiothreitol (DTT) against a total of 6 L buffer.

Supplementary Figure 9. UV-Visible spectra of NzeB
UV–Vis spectra for the purified NzeB was recorded at room temperature in buffer (50 mM Tris-HCl buffer, pH 7.4 containing 5% glycerol) was used for the spectral measurements of the oxidized and reduced form. NzeB was reduced by the addition of a small amount of sodium dithionite. The concentration of the P450s was estimated by CO-difference spectra, assuming ε(459–490) = 91 mM−1 cm−1 according to the method of Omura and Sato .



The UV-Vis spectra of oxidized (blue line), sodium dithionite reduced (red line) and CO-bound (green line) of purified NzeB are shown. The inset showed the SDS-PAGE of NzeB purification, Lane 1: marker (SeeBlue Plus2, Novex), 2-5: purified NzeB fractions

Supplementary Figure 10. Spin shift titrations with NzeB and brevianamde F (**6**)
The spin-state shift caused by binding of **6** with NzeB was assayed at room temperature under aerobic conditions using an UV–Vis spectrophotometer. The high-spin spectrum of NzeB (5 μM) was obtained by adding 10 to 100 μM of **6**.



The overlaid difference spectra obtained by subtracting the spectrum for ligand-free NzeB from the successive spectra for substrate-bound accumulated during the titration between 10 and 100 μM **6** are shown. The Soret band maximum is gradually shifted from 417 nm to 393 nm during the addition of increasing concentrations of **6**.

General reaction conditions for analytical scale P450 reactions

The conversion of DKPs by P450s were carried out with the heterologous redox electron partners Fdx and FdR from *S. olerecea*. A protein ratio of P450: Fdx: FdR of 10: 20: 6 was used. The *in vitro* reaction mixture included 50 mM Tris-HCl, pH 7.4, 10 μM P450, 20 μM Fdx and 6 μM FdR at the end volume of 250 μL. 3mM of DKP dissolved in DMSO was added, followed by 1 unit of glucose-6-phosphate dehydrogenase (from *S. cerevisiae* and a 500 mM glucose-6-phosphate. The reaction was initiated by adding NADPH (1 mM). Two of the control reactions including all the contents except for NADPH or P450 were used as controls. The reaction was incubated at 30°C for 1 h agitating at 600 rpm in a thermoshaker (Multi-thermoshaker, Benchmark). The conversion was stopped by adding an equal volume of chloroform and was extracted with chloroform for 3 times. The samples were dried under a stream of nitrogen and the residue was resuspended in 100 μL of HPLC grade methanol and analyzed by HPLC in which the reaction mixture was resolved using a linear gradient of 5-100% acetonitrile: water (0.1% formic acid) over 30 min (1.5 mL/min flow rate) on a Phenomenex Luna 5μ C-18(2) 100A, 250 × 4.60mm 5 micron column.

General reaction conditions for preparatory scale P450 reactions

Large scale reaction were performed in 10mL volumes with reaction conditions as described above. After 2 hours, reactions were quenched with 30mL of methanol, transferred to a 50mL conical tube and vortexed on the highest setting for 1 minute. This mixture was then passed through a column of Celite © followed by 20mL of methanol to was the filter cake. Water and solvents were removed en vacuo, and residue was resuspended in HPLC grade methanol with sonication. Insoluble particulates were removed via filtration through 0.2μm syringe filter and products were directly purified by preparatory-HPLC.

Prep-Scale Synthesis of (–)-naseseazine C (4)

Procedure above was followed with DKP **6**, as a substrate and NascB as P450. The filtered solution was then purified via preparative HPLC (Luna preparative HPLC column, C18, 5 μm, 21.2 × 250 mm;) using gradient of 5% to 100% acetonitrile in water containing 0.1% formic acid at the flow of 7.0 mL/min for 60 min. The retention time (t_R) of **4** was 31.2 min. The product fractions were pooled, solvent was removed *en vacuo*, to give 8 mg of (–)-naseseazine C which was used for detailed NMR characterization without any further purification.

Prep-Scale Synthesis of (+)-naseseazine B (2)

Procedure above was followed with DKP **6**, as a substrate and NznB+09 as P450. The filtered solution was then purified via preparative HPLC (Luna preparative HPLC column, C18, 5 μm, 21.2 × 250 mm;) using gradient of 5% to 100% acetonitrile in water containing 0.1% formic acid at the flow of 7.0 mL/min for 60 min. The retention time (t_R) of **2** was 34.1 min. The product fractions were pooled, solvent was removed *en vacuo*, to give 11 mg of (+)-naseseazine B which was used for detailed NMR characterization without any further purification.

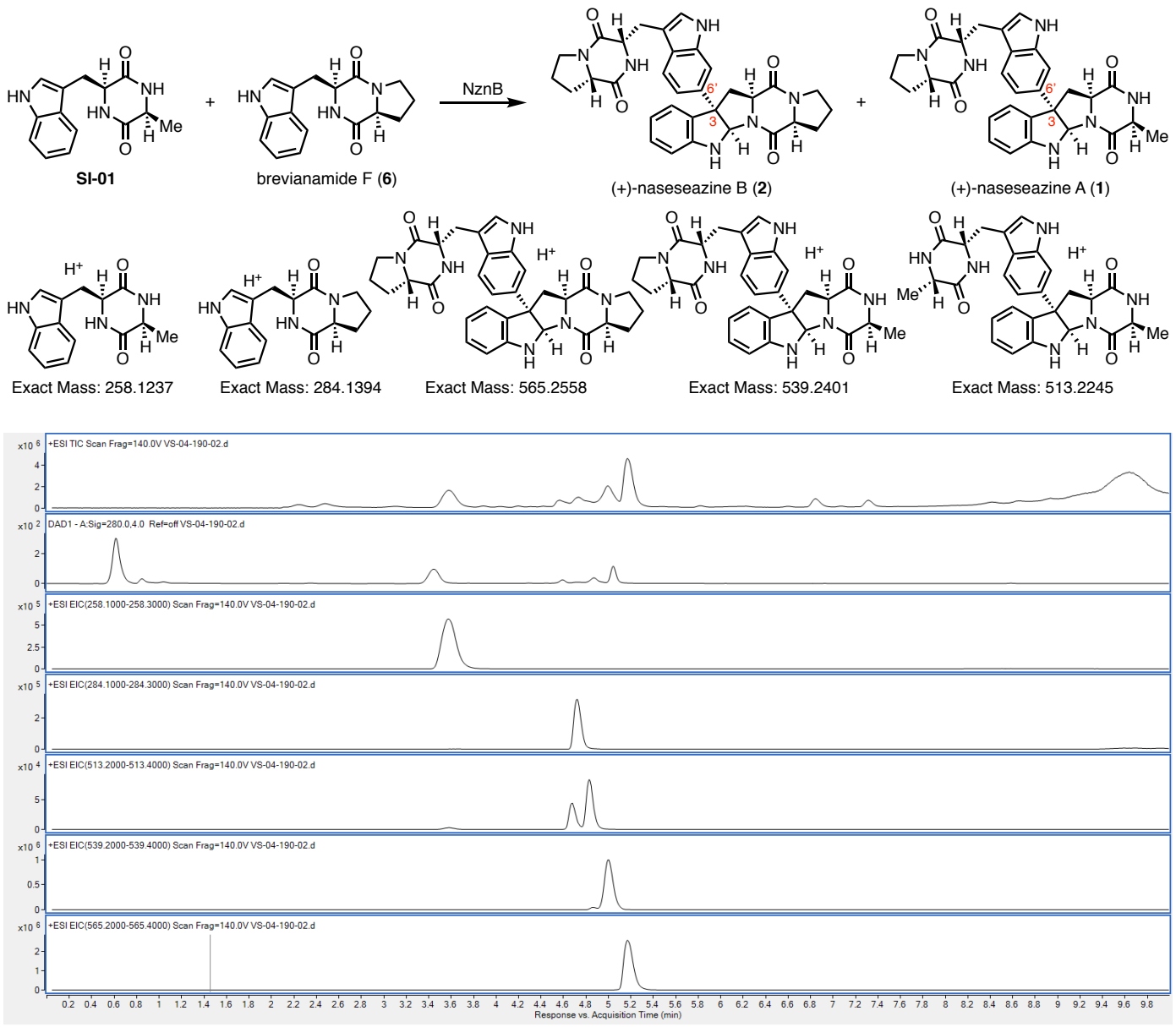
Prep-Scale Synthesis of (–)-aspergilazine A (5)

Procedure above was followed with DKP **6**, as a substrate and NzeB as P450. The filtered solution was then purified via preparative HPLC (Luna preparative HPLC column, C18, 5 μm, 21.2 × 250 mm;) using gradient of 5% to 100% acetonitrile in water containing 0.1% formic acid at the flow of 7.0 mL/min for 60 min. The retention time (t_R) of **5** was 36.6 min. The product fractions were pooled, solvent was removed *en vacuo*, to give 2 mg of (+)-naseseazine B, 6 mg of (–)-naseseazine C, and 3 mg of (–)-aspergilazine A which was used for detailed NMR characterization without any further purification.

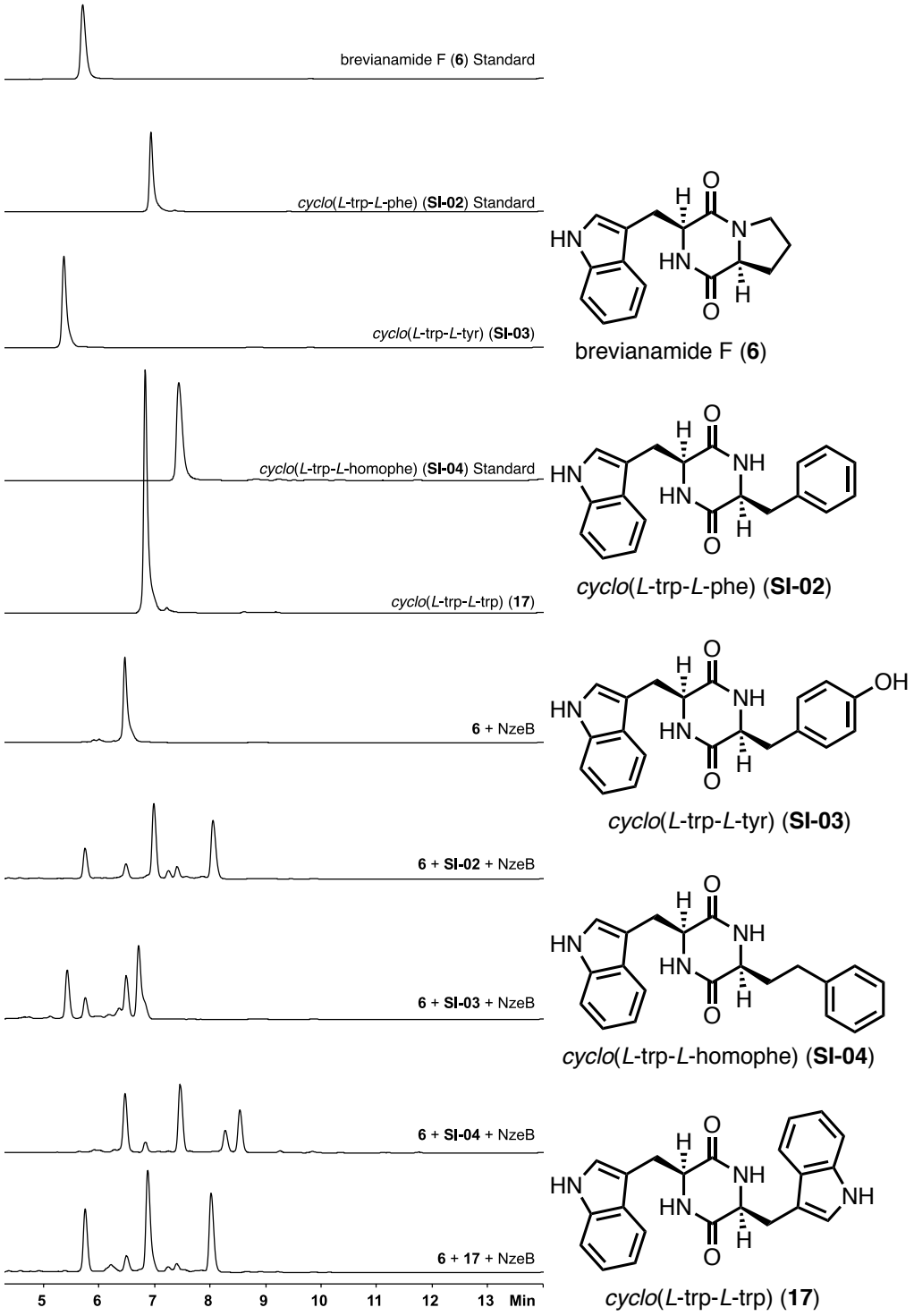
Prep-Scale Synthesis of 18

Procedure above was followed with DKPs **6** and **17**, as a substrates and NzeB as P450. The filtered solution was then purified via preparative HPLC (Luna preparative HPLC column, C18, 5 µm, 21.2 × 250 mm;) using gradient of 5% to 100% acetonitrile in water containing 0.1% formic acid at the flow of 7.0 mL/min for 60 min. The retention time (t_R) of **18** was 42.1 min. The product fractions were pooled, solvent was removed *en vacuo*, to give approximately 1 mg of **18** which was used for detailed NMR characterization without any further purification.

Supplementary Figure 11. HPLC/MS traces with extraction ion chromatograms (EIC) for analytical scale heterodimerization of SI-01 and DKP 6 to form (–)-naseseazine A catalyzed by NznB.

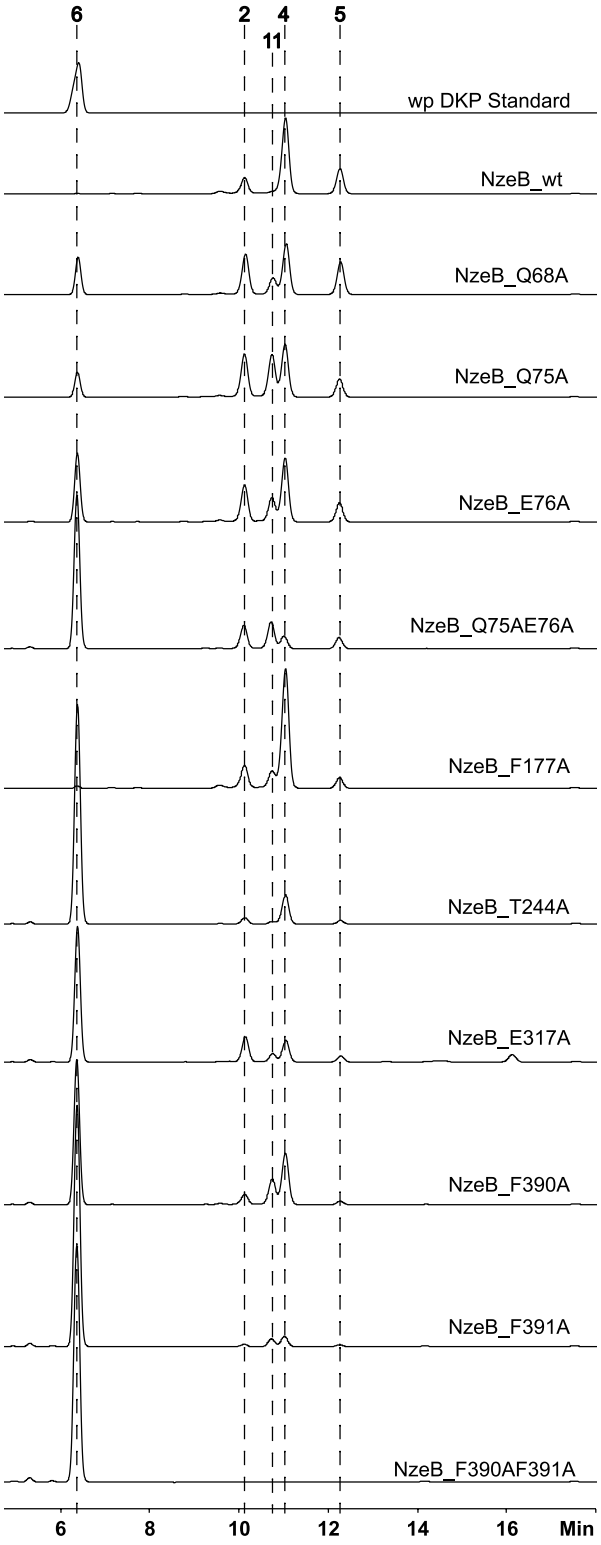


Supplementary Figure 12. HPLC traces from NzeB catalyzed heterodimerizations.

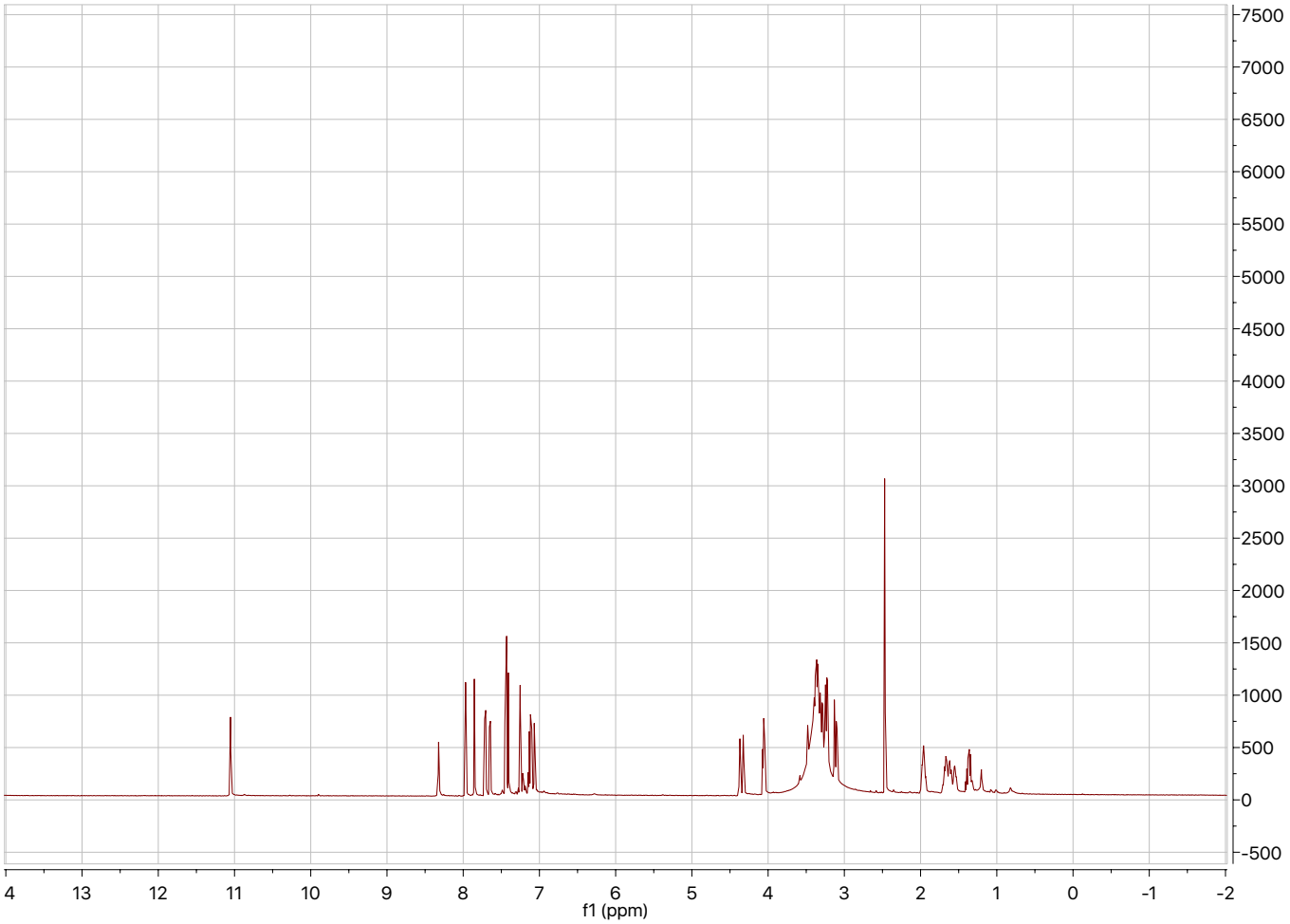


All heterodimerizations of DKP 6 with DKPS **SI-02**-**SI-04** show formation of (–)-naseseazine C (**4**) with the heterodimerization of **6** with *cyclo*(*L*-Trp-*L*-Trp) (**17**) giving the least formation of **4**.

Supplementary Figure 13. HPLC traces from NzeB alanine scanning mutants.

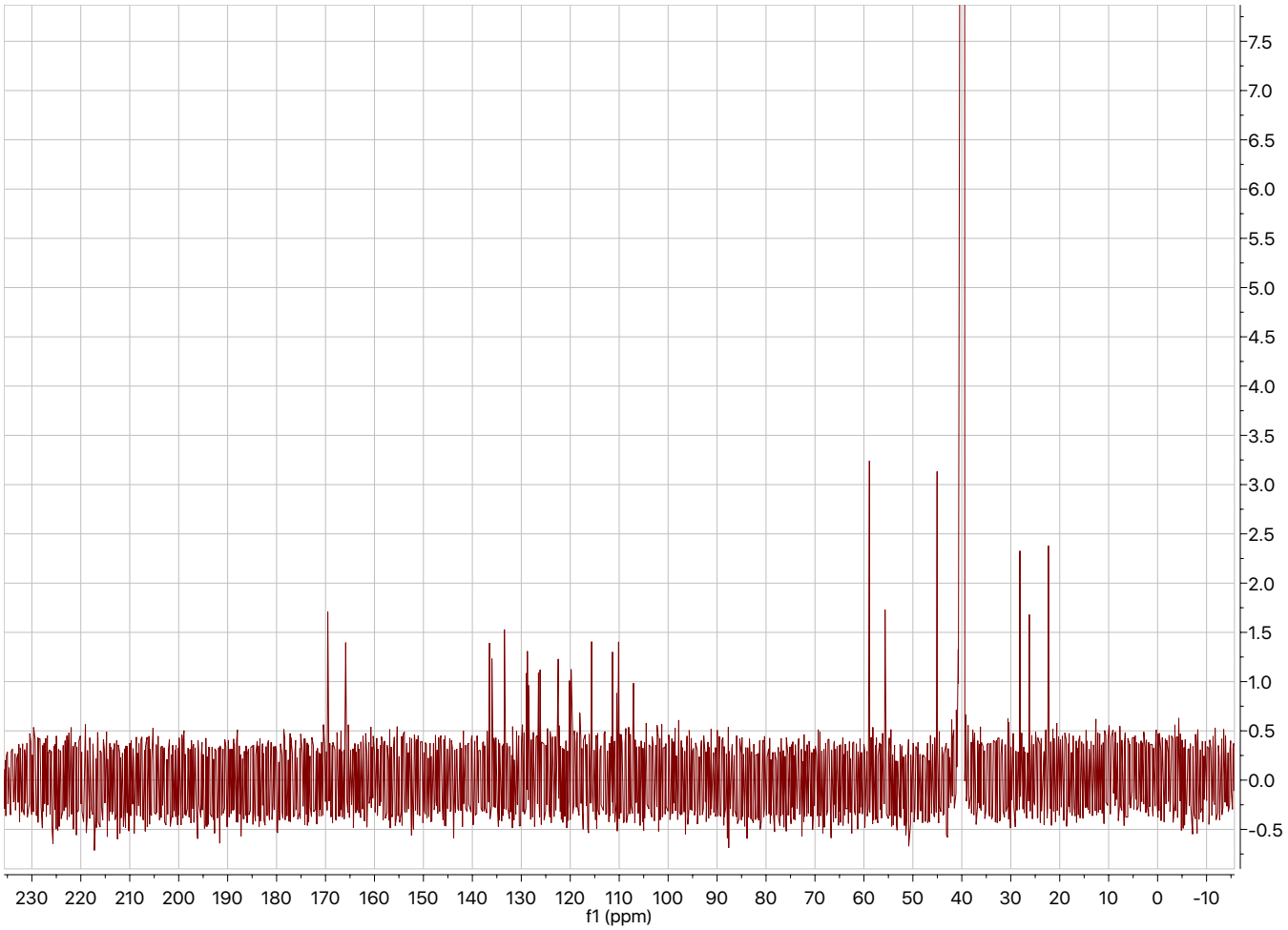


Supplementary Figure 14. ^{1}H NMR spectra for isolated (–)-aspergilazine A (5) from NzeB scale up reaction



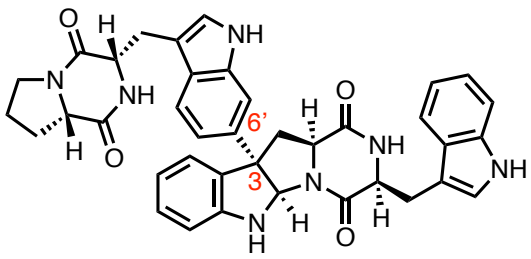
^{1}H NMR (599 MHz, DMSO-d_6) δ 11.05 (s, 1H), 7.97 (s, 1H), 7.85 (s, 1H), 7.71 (d, J = 8.3 Hz, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.45 (d, J = 8.2 Hz, 1H), 7.43 (s, 1H), 7.41 (d, J = 1.9 Hz, 1H), 7.25 (d, J = 2.4 Hz, 1H), 7.15 – 7.12 (m, 1H), 7.10 (d, J = 2.0 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 4.37 (t, J = 5.4 Hz, 1H), 4.33 (t, J = 5.3 Hz, 1H), 4.09 – 4.03 (m, 2H), 3.35 (tdd, J = 19.4, 9.6, 6.3 Hz, 3H), 3.30 – 3.20 (m, 3H), 3.15 – 3.09 (m, 2H), 1.96 (dtt, J = 14.0, 6.9, 3.5 Hz, 2H), 1.75 – 1.51 (m, 4H), 1.36 (ddtd, J = 18.1, 12.4, 10.2, 7.8 Hz, 2H).

Supplementary Figure 15. ^{13}C NMR spectra for isolated (–)-aspergilazine A (5) from NzeB scale up reaction

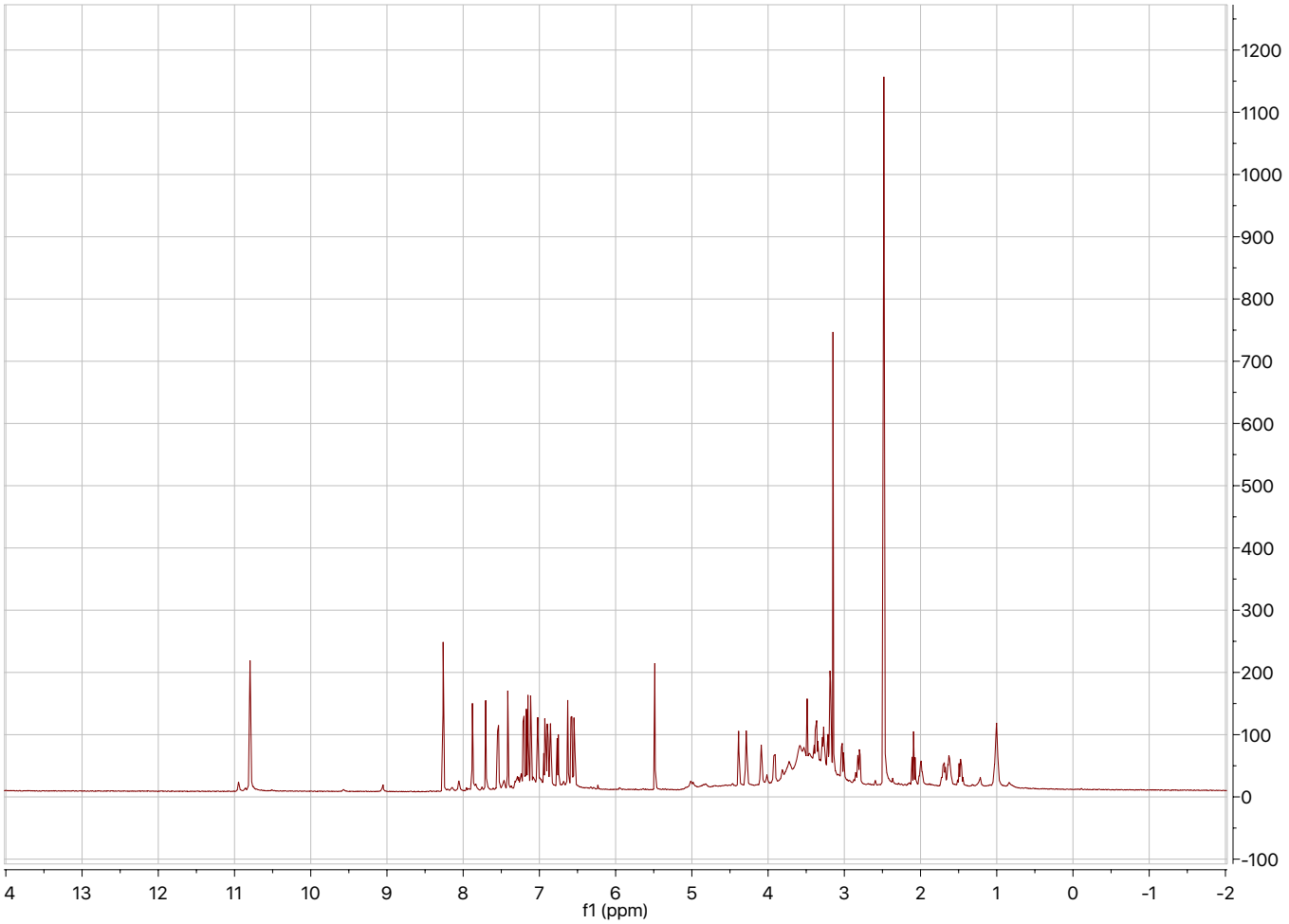


^{13}C NMR (151 MHz, DMSO-d6) δ 169.54, 169.47, 165.88, 165.84, 136.49, 136.01, 133.45, 128.94, 128.76, 128.54, 126.49, 126.17, 122.45, 119.82, 115.63, 111.38, 110.12, 107.09, 58.88, 55.68, 55.59, 45.05, 28.14, 26.20, 22.31, 22.28.

Supplementary Figure 16. ^{1}H NMR spectra for **18** isolated from NzeB scale up

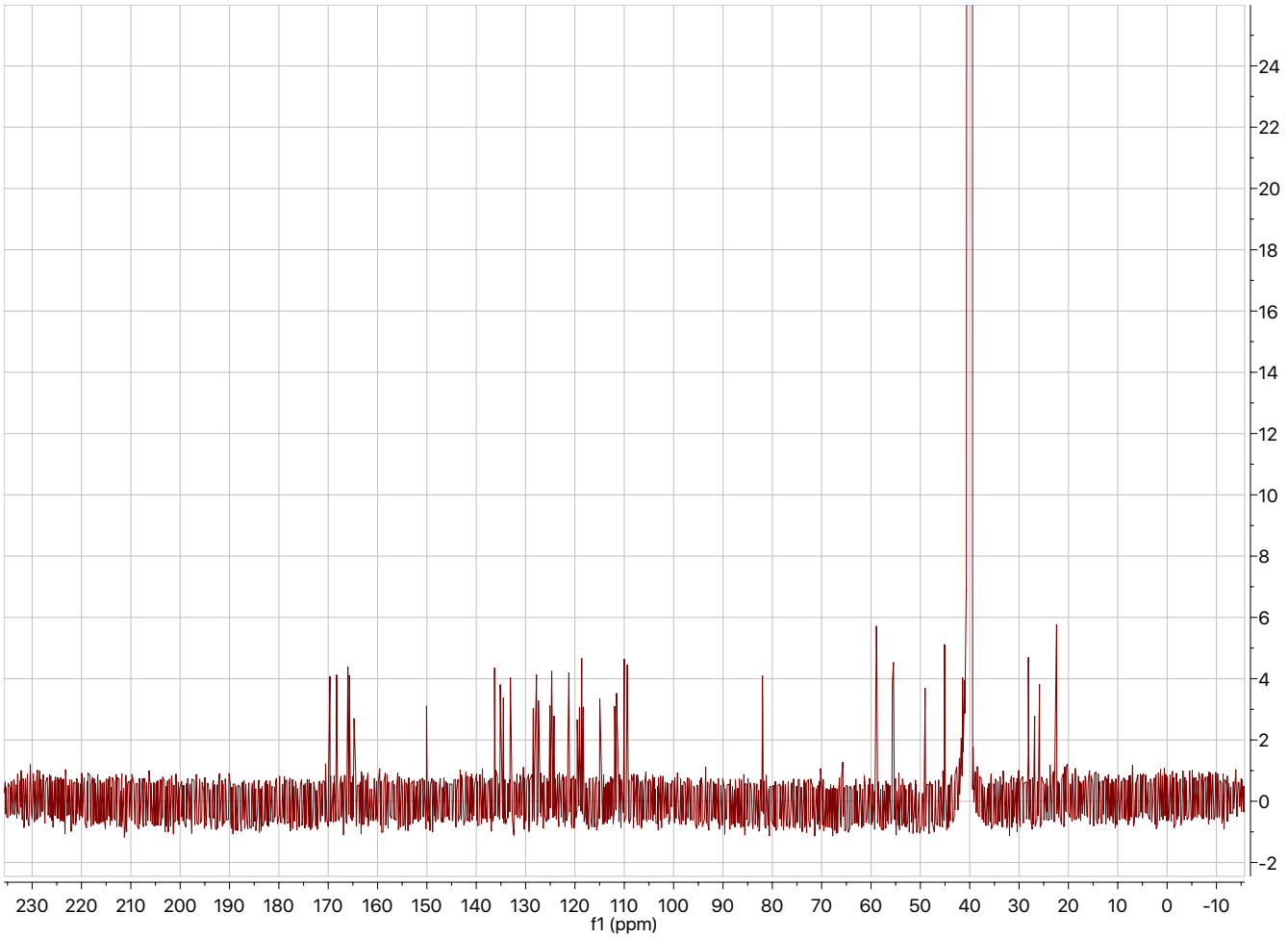


18



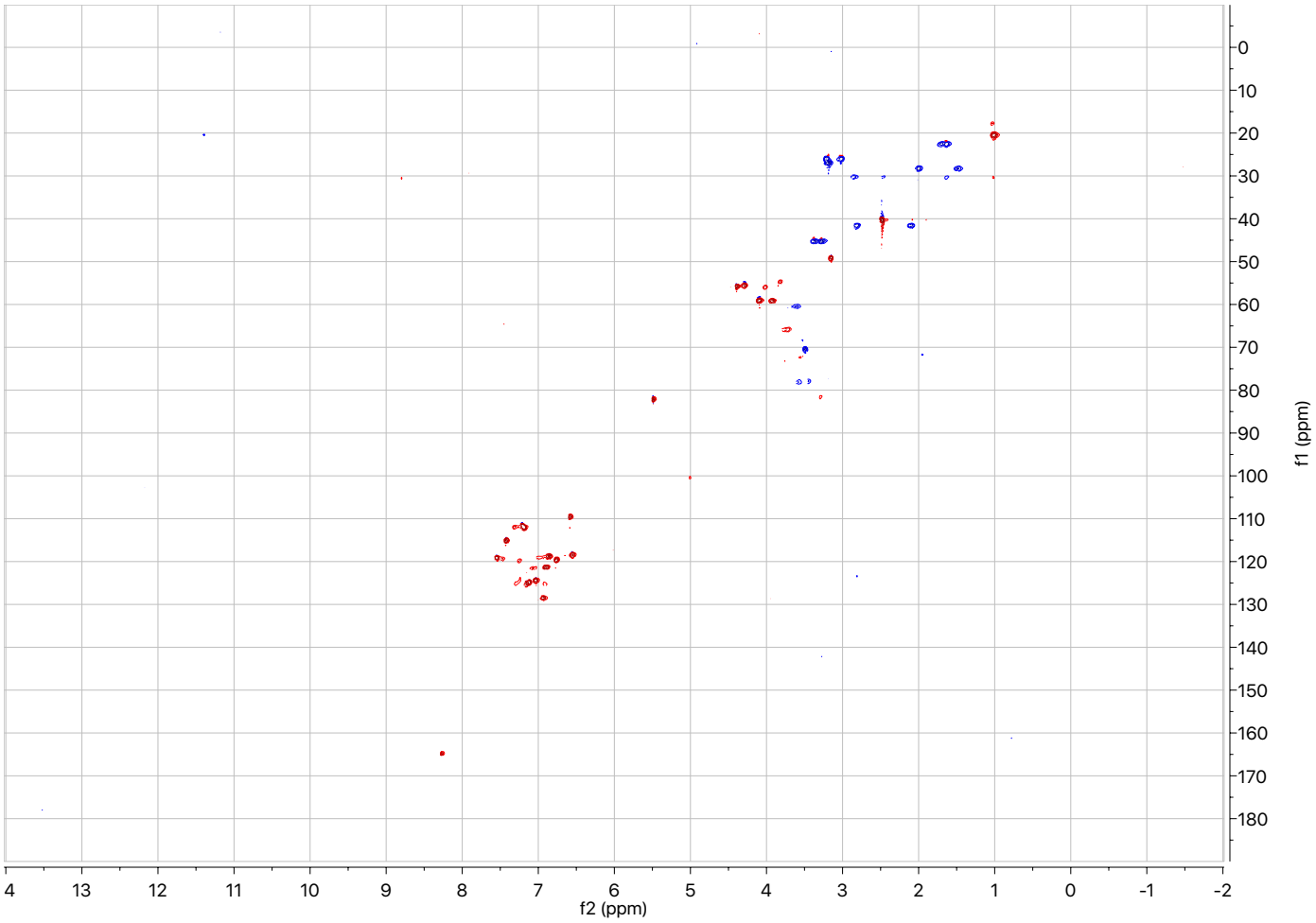
^{1}H NMR (599 MHz, DMSO-d_6) δ 10.80 (s, 2H), 8.26 (s, 1H), 7.88 (s, 1H), 7.70 (s, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.41 (s, 1H), 7.19 (dd, *J* = 17.9, 8.2 Hz, 2H), 7.15 (d, *J* = 2.2 Hz, 1H), 7.12 (d, *J* = 2.3 Hz, 1H), 7.03 (d, *J* = 7.4 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.86 (t, *J* = 7.4 Hz, 1H), 6.76 (dd, *J* = 8.5, 1.7 Hz, 1H), 6.63 (s, 1H), 6.58 (d, *J* = 7.8 Hz, 1H), 6.55 (t, *J* = 7.4 Hz, 1H), 5.49 (s, 1H), 4.38 (d, *J* = 5.1 Hz, 1H), 4.29 (t, *J* = 5.5 Hz, 1H), 4.12 – 4.06 (m, 1H), 3.92 (dd, *J* = 11.8, 5.5 Hz, 1H), 3.37 (dt, *J* = 11.7, 7.9 Hz, 1H), 3.27 (ddd, *J* = 12.2, 8.8, 3.9 Hz, 1H), 3.23 – 3.17 (m, 3H), 3.02 (dd, *J* = 15.0, 6.0 Hz, 1H), 2.81 (dd, *J* = 12.2, 5.6 Hz, 1H), 2.09 (t, *J* = 11.9 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.73 – 1.58 (m, 2H), 1.53 – 1.42 (m, 1H).

Supplementary Figure 17. ^{13}C NMR spectra for **18** isolated from NzeB scale up

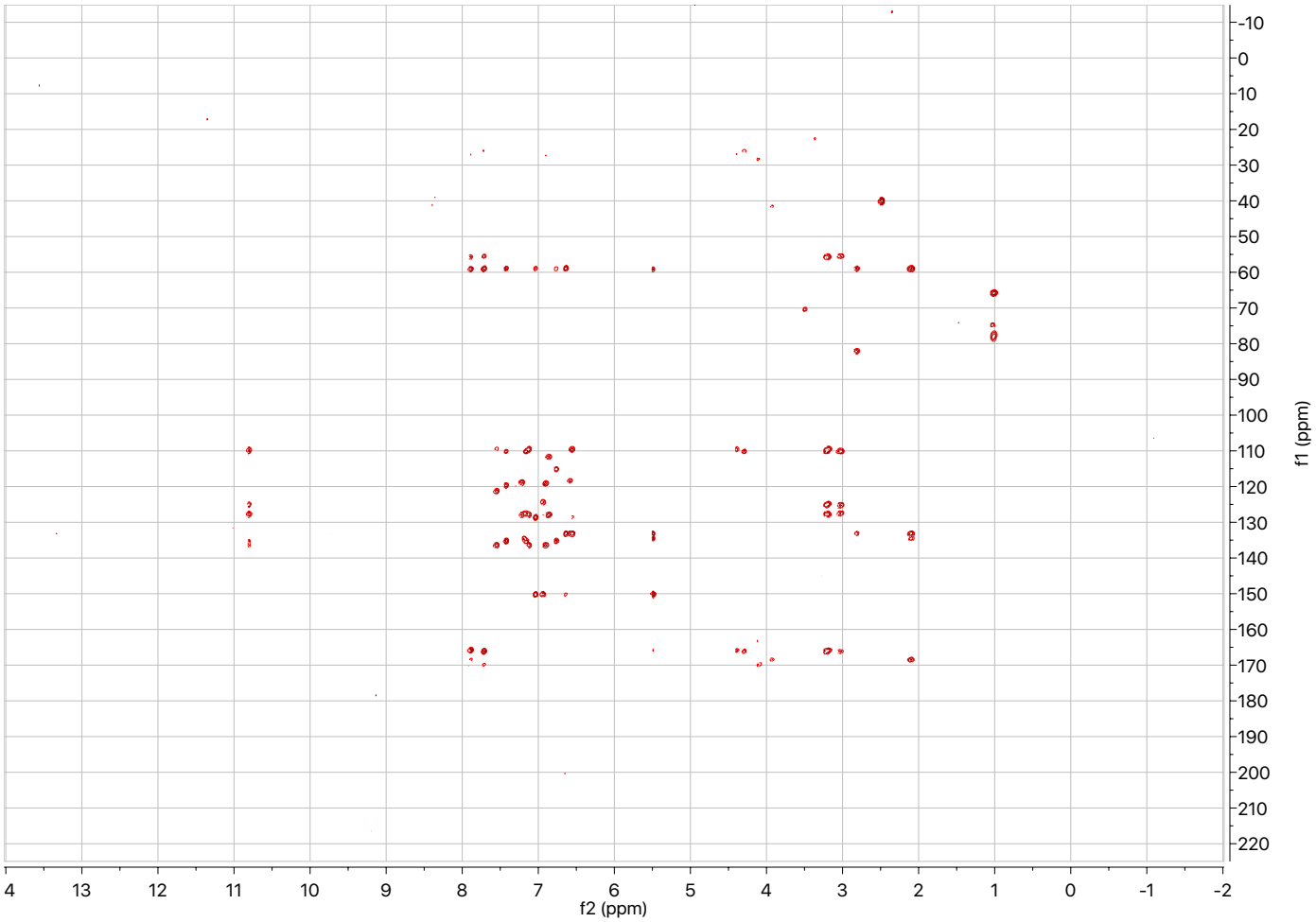


^{13}C NMR (151 MHz, dmso) δ 169.64, 168.30, 166.01, 165.70, 164.76, 150.07, 136.29, 135.14, 134.50, 133.07, 128.45, 127.79, 127.40, 125.08, 124.71, 124.24, 121.22, 119.53, 119.08, 118.63, 118.31, 114.97, 111.94, 111.57, 110.00, 109.45, 109.39, 82.00, 59.02, 58.91, 58.83, 55.68, 55.45, 49.04, 45.09, 41.43, 28.11, 26.83, 25.86, 22.40.

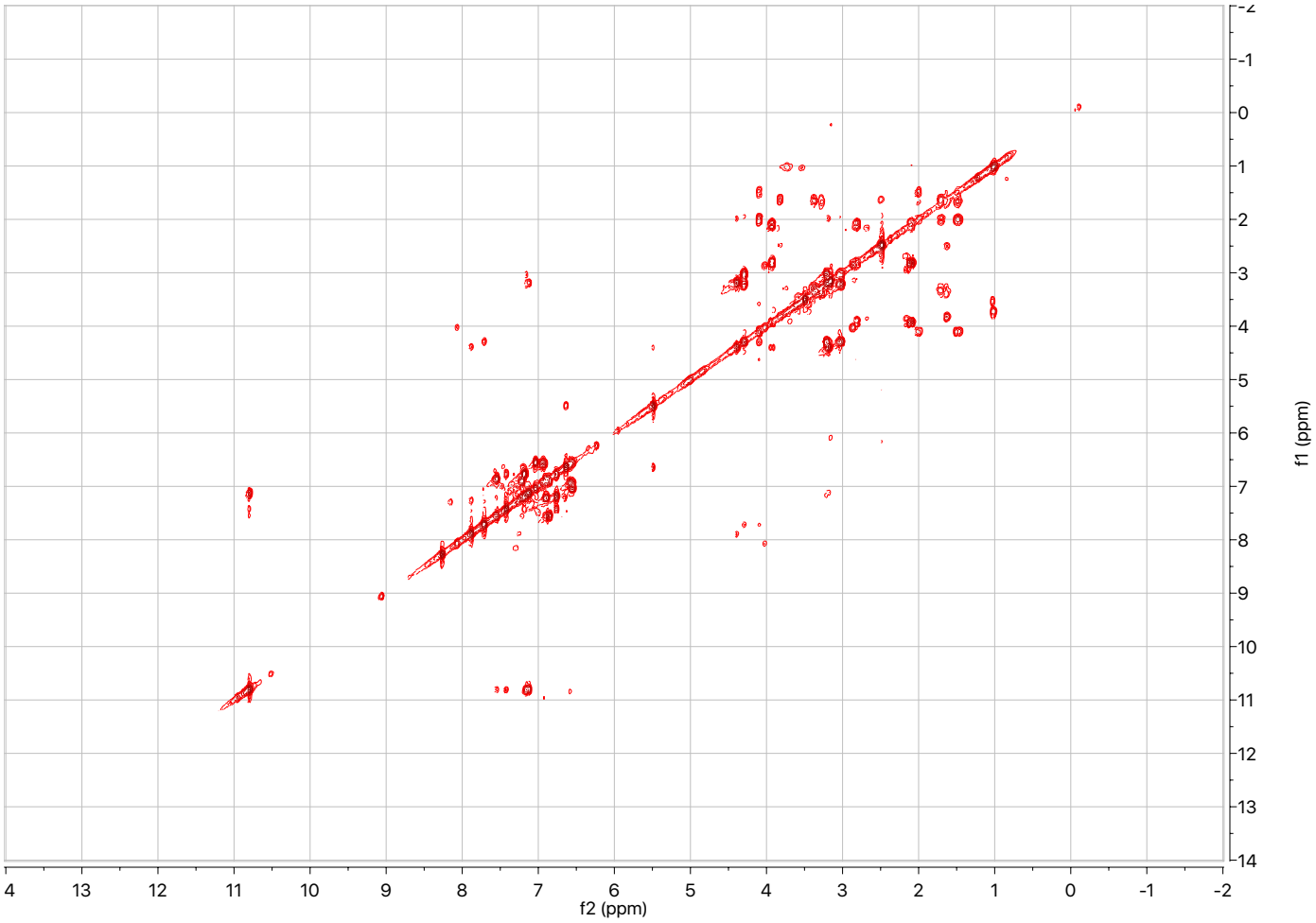
Supplementary Figure 18. gHSQCAD spectra for **18** isolated from NzeB scale up



Supplementary Figure 19. gHMBCAD spectra for **18** isolated from NzeB scale up



Supplementary Figure 20. gCOSY spectra for **18** isolated from NzeB scale up



Supplementary Table 3. Cytochromes P450 used to generate sequence similarity network (SSN)

P450	Organism	Accession	Natural Product	Reference
NascB	*Streptomyces sp.*CMB-MQ030	AWF71596.1	(–)-naseseazine C	Nat. Commun. 2018, 4428
P450NB5737	*S. purpureus* (NRRL B-5737)	WP_019889608	guanitrypmycin C3-1	*Org. Lett.* **2018**, 4921
TxtC	*S. scabies*	6F0C_A	thaxtomin A	*JACS* **2019,** 216
CypX	*B. subtilis*	WP_148962661.1	pulcherrimic acid	Biochemistry, 2010, 7282
BcmD	*S. sapporonensis*	AXQ04975.1	bicyclomycin	*ACIEE* **2018**, 719
CYP121	*M. tuberculosis*	P9WPP7.1	mycocyclosin	J. Biol. Chem. 2003, 5141

Process of crystallization

Crystallization of NzeB.

Single, diffraction quality crystals of the *NzeB* complexes were grown by sitting drop vapor diffusion at 20 °C by mixing 2 µL of 8 mg/mL protein containing 1 mM DKP substrate and 0.2% DMSO with 2 µL of a well solution containing 23% PEG 3350, 100 mM DL-malic acid, 2.5% ethylene glycol. Equimolar concentrations of substrate (0.5 mM) were used for the *NzeB*·**6**·**17** complex. Sitting droplets were nucleated after 4 h from an earlier spontaneous crystallization using a cat whisker. Single crystals grew after 48 hours. 8 µL of a cryoprotecting solution containing 10 mM Tris pH 7.5, 2 % glycerol, 23% PEG 3350, 100 mM DL-malic acid, 18% ethylene glycol, 1 mM DKP substrate, 0.2% DMSO was added directly to the sitting drops and the crystals were harvested using nylon loops and vitrified by rapid plunging into liquid nitrogen. *NzeB* crystallized in space group *P* 1with unit cell dimensions of *a* = 56.1 Å, b = 56.3 Å, *c* = 58.8 Å, α = 91.1°, β = 92.9°, γ = 100.1° and two chains in the asymmetric unit.

Data collection and processing.

X-ray data were collected at 100 K on beamline 23ID-B at the National Institute for General Medical Sciences (NIGMS) and National Cancer Institute (NCI) Structural Biology Facility at the Advanced Photon Source in Argonne, IL, USA. Diffraction data were integrated and scaled using XDS.[1] Data collection statistics are given in Supplementary Table 2.

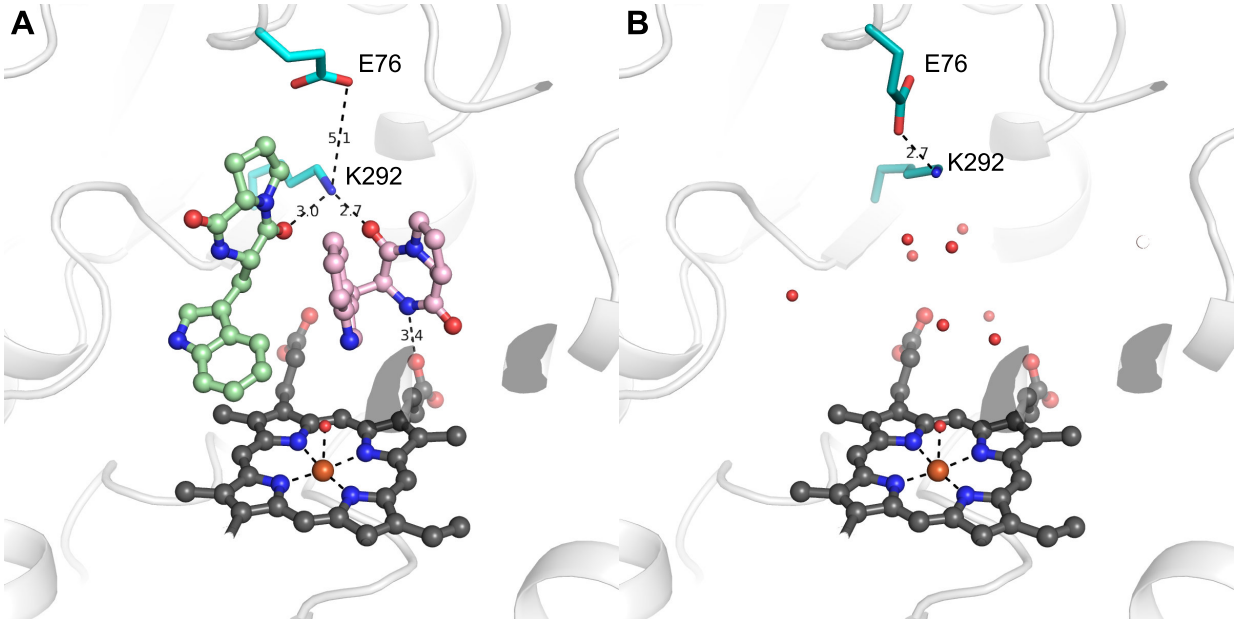
Molecular replacement, model building and refinement.

The structure of NascB-F5053 was solved using Phenix MR-Rosetta.[2] This resulted in an initial model that could be extended by alternating cycles of manual building in *Coot*[3] and least-squares refinement with Phenix.[4] Final models were validated using MolProbity.[5]

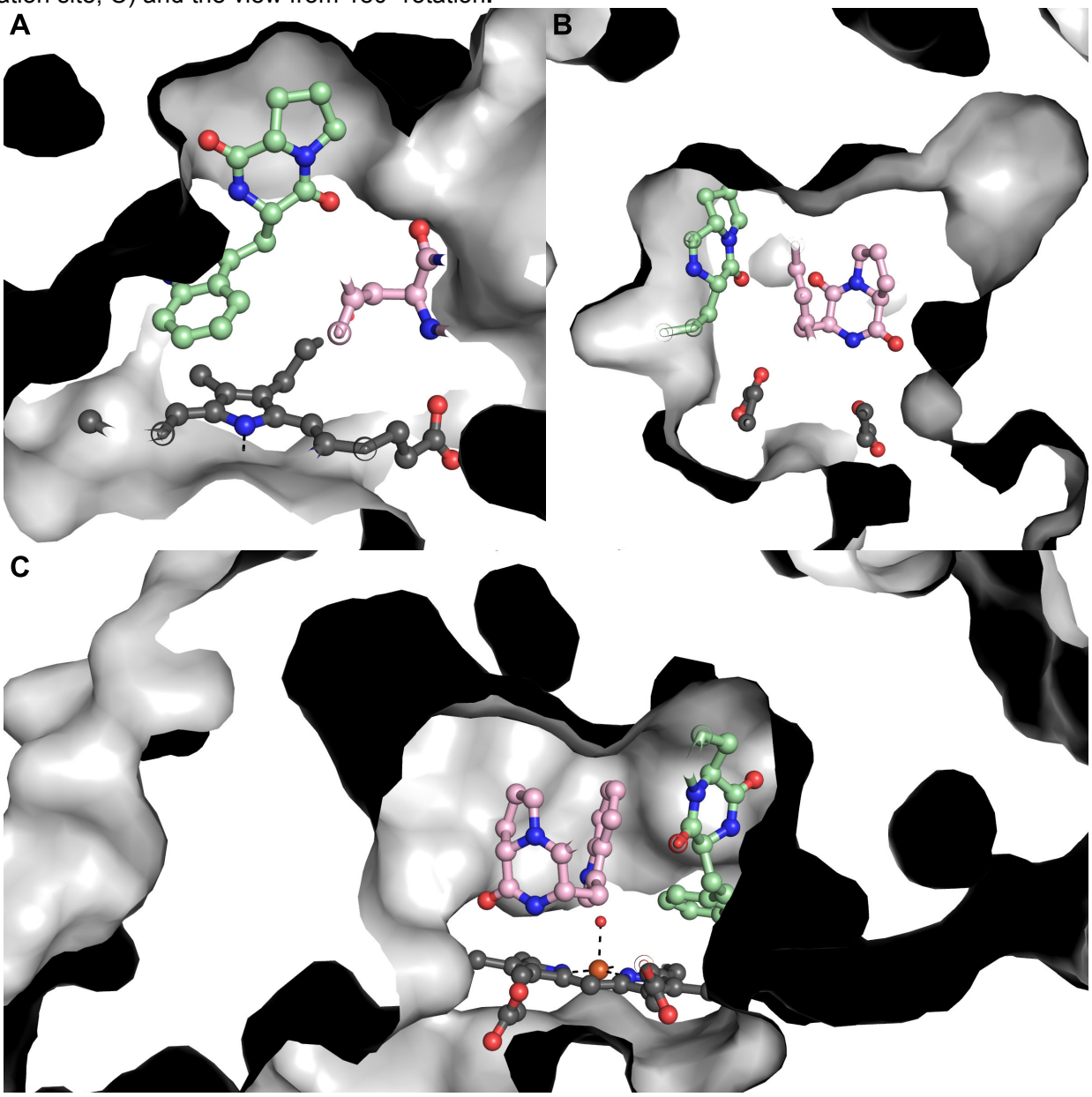
Supplementary Table 4. Data Collection Statistics

	NzeB in complex with **6**	NzeB in complex with **6** and **17**	NzeB ligand free
Wavelength (Å)	1.03	1.03	0.826
Resolution range (Å)	40.83 - 1.49 (1.54 - 1.49)	41.22 - 1.48 (1.53 - 1.48)	39.13 - 1.498 (1.55 - 1.50)
Space group	P 1	P 1	P 2_1
Unit cell	56.12, 56.28, 58.78 Å 91.13, 92.93, 100.10°	56.07, 56.13, 58.48 Å 91.36, 93.04, 101.10°	55.71, 55.81, 56.10 Å 90, 101.92, 90°
Total reflections	382537 (31077)	324387 (4806)	359895 (35646)
Unique reflections	109037 (10046)	94423 (2902)	54058 (5282)
Multiplicity	3.5 (3.1)	3.4 (1.7)	6.7 (6.7)
Completeness (%)	94.48 (87.34)	80.96 (24.95)	99.66 (97.45)
Mean I/sigma(I)	16.78 (2.39)	20.64 (1.81)	14.45 (1.35)
Wilson B-factor (Å2)	19.96	22.24	23.40
R-merge	0.039 (0.361)	0.030 (0.287)	0.056 (1.013)
R-meas	0.046 (0.439)	0.036 (0.398)	0.061 (1.097)
CC1/2	0.998 (0.85)	0.999 (0.851)	0.999 (0.743)
Reflections used in refinement	109025 (10043)	94401 (2902)	54024 (5279)
R-work	0.168 (0.287)	0.192 (0.333)	0.188 (0.292)
R-free	0.211 (0.340)	0.234 (0.410)	0.219 (0.307)
Number of atoms (total):	6989	6995	3441
macromolecules	6108	6079	3021
ligands	190	196	55
solvent	691	720	365
Protein residues	798	793	392
RMS(bonds)	0.005	0.007	0.006
RMS(angles)	0.91	1.23	0.84
Ramachandran favored (%)	97.21	97.56	97.91
Ramachandran allowed (%)	2.79	2.44	2.09
Ramachandran outliers (%)	0.00	0.00	0.00
Average B-factor (Å2)	27.51	28.55	31.52
macromolecules	26.79	28.07	30.84
ligands	19.50	22.09	25.73
solvent	36.01	34.38	37.97

Supplementary Figure 21. Comparison of A) NzeB substrate bound, and B) substrate free active sites.



Supplementary Figure 22. NzeB Active site showing A) steric packing in dimerization site, b) open channel in cyclization site, C) and the view from 180^0 rotation.



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Computational Methods

Conformational searches were performed using the Schrödinger MacroModel[1] software package to identify low-energy conformers for quantum mechanical calculations. All quantum mechanical calculations were performed using the Gaussian 09[2] software package. Structures were optimized at the UB3LYP[3,4]/LanL2DZ(Fe)[5]/6-31G(d) level of theory using the CPCM[6–8] solvent model for diethyl ether, which is intended to model the environment of the enzyme active site; frequency calculations were used to confirm the presence of local minima (no imaginary frequencies) and transition states (one imaginary frequency). Thermochemistry corrections to obtain enthalpies and free energies were computed at 298 K and 1 M, with Truhlar corrections[9] applied to all frequencies below 100 cm^{-1}. To obtain more accurate energetics, single-point energy calculations were performed on the optimized structures at the UB3LYP[3,4]/LanL2DZ(Fe)[5]/6-311++G(2d,2p) level of theory using Grimme's D3(BJ) dispersion correction[10,11] and the CPCM[6–8] solvent model for diethyl ether. For all iron-containing species, all possible spin states were computed separately; the spin state with the lowest free energy is reported and used in the computed reaction pathways.

Supplementary Table 5: Optimized Quantum Mechanical Energies and Geometries

Structure	**Single-Point Energy** (Hartree) UB3LYP/ 6-311++G(2d,2p) CPCM diethylether solvent D3-BJ dispersion correction	**Enthalpy Correction** (Hartree) UB3LYP/6-31G(d) CPCM diethylether solvent	**Gibbs Free Energy Correction** (Hartree) UB3LYP/6-31G(d) CPCM diethylether solvent
Compound **6**	-935.064995353	0.332193	0.267005
Compound **PC-I**	-2560.69811814	0.675898	0.552976
Transition State from **PC-I** to **R-I**	-2560.68200451	0.668580	0.548785
Compound **R-I**	-934.408484774	0.318396	0.252323
Compound **PC-II**	-2560.69111264	0.675486	0.550891
Transition State from **PC-II** to **R-II**	-2560.66865641	0.668467	0.549941
Compound **R-II**	-934.378337774	0.317810	0.251336
Transition State from **R-II** to **R-III**	-934.375022742	0.317227	0.254810
Compound **R-III**	-934.406015167	0.319252	0.257416
3-methylindole	-403.297212617	0.166766	0.125308
Transition State from **R-III** to **R-IV**	-1337.68979078	0.486702	0.403190
Compound **R-IV**	-1337.70558024	0.488372	0.406134
Compound **$PDT_{C–C}$**	-1337.15954501	0.479009	0.398229
Compound **C-III**	-934.228902694	0.321380	0.260447
Transition State from **C-III** to **C-IV**	-1337.54044714	0.489605	0.408473
Compound **C-IV**	-1337.55215821	0.491575	0.410726
Compound **R-V**	-934.408292246	0.318638	0.253313
Transition State from **R-V** to **R-VI**	-1337.69321370	0.486722	0.403322
Compound **R-VI**	-1337.70428197	0.488290	0.400752
Compound **$PDT_{C–N}$**	-1337.15657933	0.478377	0.394108
Compound **C-V**	-934.179753468	0.319454	0.254095
Iron-Oxo Quartet	-1625.60979018	0.341464	0.266017
Iron-Hydroxo Triplet	-1626.26453700	0.352745	0.277069
Iron-Aqua Doublet	-1626.92110182	0.365210	0.288026
Iron-Hydroxo Doublet Anion	-1626.42321553	0.351663	0.276113
Figure 11B Radical C2 TS	-1337.69755972	0.486871	0.403638
Figure 11B Radical C2 Product	-1337.72340783	0.489309	0.407811
Figure 11B Radical C3 TS	-1337.69205782	0.486851	0.405608
Figure 11B Radical C3 Product	-1337.70825431	0.488798	0.408087
Figure 11B Radical C4 TS	-1337.69550474	0.487160	0.405177
Figure 11B Radical C4 Product	-1337.71350934	0.489101	0.407451
Figure 11B Radical C5 TS	-1337.68979078	0.486702	0.403190
Figure 11B Radical C5 Product	-1337.70558024	0.488372	0.406134
Figure 11B Radical C6 TS	-1337.69174411	0.486788	0.403349
Figure 11B Radical C6 Product	-1337.70914756	0.488422	0.405258
Figure 11B Radical C7 TS	-1337.69379606	0.486938	0.404223
Figure 11B Radical C7 Product	-1337.71560829	0.489107	0.407992
Figure 11D Cation C2 TS	-1337.53832625	0.489255	0.407257
Figure 11D Cation C2 Product	-1337.56124772	0.491742	0.410737
Figure 11D Cation C3 TS	-1337.54174717	0.489798	0.408678
Figure 11D Cation C3 Product	-1337.56290761	0.492522	0.413750

Figure 11D Cation C4 TS	-1337.53534315	0.489690	0.408765
Figure 11D Cation C4 Product	-1337.54696654	0.492005	0.412079
Figure 11D Cation C5 TS	-1337.54044714	0.489605	0.408473
Figure 11D Cation C5 Product	-1337.55215821	0.491575	0.410726
Figure 11D Cation C6 TS	-1337.53368503	0.489370	0.406633
Figure 11D Cation C6 Product	-1337.55077701	0.491474	0.409790
Figure 11D Cation C7 TS	-1337.53365020	0.489592	0.407774
Figure 11D Cation C7 Product	-1337.55229112	0.491566	0.411883
Figure 12B Radical C2 TS	-1337.69951164	0.486587	0.402050
Figure 12B Radical C2 Product	-1337.72283996	0.488652	0.402337
Figure 12B Radical C3 TS	-1337.69039795	0.486633	0.404156
Figure 12B Radical C3 Product	-1337.69932417	0.488295	0.403578
Figure 12B Radical C4 TS	-1337.69014921	0.486500	0.401321
Figure 12B Radical C4 Product	-1337.71217497	0.488517	0.401914
Figure 12B Radical C5 TS	-1337.68944354	0.486708	0.404293
Figure 12B Radical C5 Product	-1337.69958304	0.488216	0.400754
Figure 12B Radical C6 TS	-1337.69321370	0.486722	0.403322
Figure 12B Radical C6 Product	-1337.70428197	0.488290	0.400752
Figure 12B Radical C7 TS	-1337.68740315	0.486476	0.401229
Figure 12B Radical C7 Product	-1337.70835455	0.488657	0.402298
Compound **SI-6**	-935.062969833	0.332324	0.268187
Compound **SI-PC-I**	-2560.69153790	0.675829	0.551602
TS from **SI-PC-I** to **SI-R-I**	-2560.67865279	0.668912	0.547686
Compound **SI-R-I**	-934.408292246	0.318638	0.253313
Compound **SI-PC-II**	-2560.69492543	0.676111	0.552240
TS from **SI-PC-II** to **SI-R-II**	-2560.66886329	0.668918	0.548679
Compound **SI-R-II**	-934.380566351	0.317339	0.251457
TS from **SI-R-II** to **SI-R-III**	-934.378935128	0.317125	0.255510
Compound **SI-R-III**	-934.402373050	0.319158	0.257062
TS from **SI-R-III** to **SI-R-IV**	-1337.68947287	0.487089	0.404197
Compound **SI-R-IV**	-1337.70630293	0.488419	0.405430
Compound **SI-PDT$_{c-c}$**	-1337.15713807	0.479196	0.399406
Compound **SI-C-III**	-934.227258143	0.321166	0.259968
TS from **SI-C-III** to **SI-C-IV**	-1337.53149035	0.489508	0.407077
Compound **SI-C-IV**	-1337.54947128	0.491664	0.410192
Figure S23B Radical C2 TS	-1337.69720677	0.486790	0.403187
Figure S23B Radical C2 Product	-1337.72387603	0.489129	0.407753
Figure S23B Radical C3 TS	-1337.69024969	0.486815	0.406062
Figure S23B Radical C3 Product	-1337.70583195	0.488790	0.407690
Figure S23B Radical C4 TS	-1337.69238834	0.487192	0.405409
Figure S23B Radical C4 Product	-1337.71039565	0.488908	0.407710
Figure S23B Radical C5 TS	-1337.68710983	0.486895	0.403027
Figure S23B Radical C5 Product	-1337.70169171	0.488268	0.405240
Figure S23B Radical C6 TS	-1337.68947287	0.487089	0.404197
Figure S23B Radical C6 Product	-1337.70630293	0.488419	0.405430
Figure S23B Radical C7 TS	-1337.69515416	0.487005	0.404216
Figure S23B Radical C7 Product	-1337.71296380	0.488933	0.406893
Figure S23D Cation C2 TS	-1337.53901559	0.489064	0.406499
Figure S23D Cation C2 Product	-1337.56397314	0.491670	0.411416
Figure S23D Cation C3 TS	-1337.54056391	0.489799	0.410016
Figure S23D Cation C3 Product	-1337.56254502	0.492561	0.414297
Figure S23D Cation C4 TS	-1337.53295258	0.489870	0.409363

Figure S23D Cation C4 Product	-1337.54486276	0.491909	0.412625
Figure S23D Cation C5 TS	-1337.53078689	0.489548	0.407453
Figure S23D Cation C5 Product	-1337.54732307	0.491534	0.410373
Figure S23D Cation C6 TS	-1337.53149035	0.489508	0.407077
Figure S23D Cation C6 Product	-1337.54947128	0.491664	0.410192
Figure S23D Cation C7 TS	-1337.53688422	0.489745	0.408768
Figure S23D Cation C7 Product	-1337.54891315	0.491855	0.410992
Compound **6** Radical Cation	-934.841312043	0.332396	0.265895
Iron-Oxo Anion Triplet	-1625.76714766	0.340805	0.266113

Compound **6**

0 1

N	-3.499289	1.573570	-1.088827
C	1.839291	-1.196192	-0.541564
O	1.826066	-2.204846	-1.249758
C	0.556139	-0.411010	-0.221570
C	-5.029522	0.477437	0.591361
C	3.030029	0.481835	0.883470
C	4.482290	0.949079	0.719319
C	5.247060	-0.376807	0.556634
C	4.296107	-1.267749	-0.264702
C	1.970015	1.520484	0.536979
C	-0.483945	-0.581218	-1.349833
C	-1.795276	0.089217	-1.056838
C	-2.259600	1.261651	-1.608940
C	-3.868917	0.603390	-0.181298
C	-2.815166	-0.352831	-0.133412
C	-2.948156	-1.465888	0.717596
C	-4.099105	-1.595235	1.485973
C	-5.128482	-0.631631	1.424408
N	0.848386	1.009082	-0.026565
N	2.965631	-0.703387	0.015475
O	2.130102	2.715542	0.776148
H	-4.050301	2.379233	-1.344403
H	0.136445	-0.835920	0.704576
H	-5.823219	1.217901	0.540913
H	2.854238	0.186240	1.931134
H	4.820264	1.545090	1.569466
H	4.567959	1.564711	-0.182763
H	5.429127	-0.827695	1.538699
H	6.214910	-0.249410	0.064775
H	4.335977	-2.322526	0.023834
H	4.493268	-1.209952	-1.341471
H	-0.615877	-1.656822	-1.501350
H	-0.054730	-0.182839	-2.276257
H	-1.805210	1.896742	-2.357757
H	-2.165671	-2.218741	0.770625
H	-4.211946	-2.451727	2.145046
H	-6.016453	-0.759741	2.037384
H	0.082201	1.657848	-0.179663

Compound **PC-I**

0 4

N	-0.596448	1.739290	-1.534251
C	-6.297386	0.017667	-0.842924
O	-6.959349	0.271436	-1.850792
C	-4.919265	0.650980	-0.599685
C	-0.440828	4.164207	-0.860686
C	-5.986782	-1.152197	1.353302
C	-6.538474	-2.534975	1.726270
C	-8.011209	-2.437386	1.288243
C	-7.971361	-1.597063	-0.002778
C	-4.477612	-1.083105	1.162991
C	-4.211008	0.972500	-1.937796
C	-2.845647	1.566283	-1.741575
C	-1.643315	0.895236	-1.828221
C	-1.101174	2.984314	-1.228719
C	-2.519932	2.918625	-1.355579
C	-3.279769	4.078241	-1.110589
C	-2.626155	5.249747	-0.745722
C	-1.220088	5.290688	-0.619355
N	-4.069035	-0.230024	0.200717
N	-6.725305	-0.823292	0.124869
O	-3.706031	-1.747724	1.862120
H	0.376016	1.440389	-1.432970
H	-5.082677	1.596314	-0.058431
H	0.641680	4.196268	-0.771460
H	-6.240300	-0.429680	2.146679
H	-6.413756	-2.753915	2.788743
H	-6.009787	-3.306060	1.155146
H	-8.596579	-1.918981	2.056020
H	-8.469333	-3.416352	1.125056
H	-8.831287	-0.928556	-0.108017
H	-7.919982	-2.217351	-0.905058
H	-4.868160	1.646328	-2.495555
H	-4.139734	0.046438	-2.519582
H	-1.453402	-0.136177	-2.095880
H	-4.362676	4.061509	-1.208600
H	-3.203368	6.150625	-0.554901
H	-0.737571	6.221287	-0.332628
H	-3.066796	-0.097832	0.096012
Fe	2.698903	-0.358968	-0.034310
N	3.709959	-1.370786	-1.459031
N	1.160416	-1.647815	-0.218547
N	4.373503	0.689376	0.372216
N	1.812282	0.443477	1.586758
C	4.952458	-1.073420	-1.959394
C	-0.010933	-1.643015	0.494156
C	3.230708	-2.402761	-2.231846
C	1.026875	-2.644594	-1.151045
C	5.541406	0.707364	-0.366327
C	0.543208	0.179976	2.052269
C	4.523504	1.666170	1.333597
C	2.292255	1.463535	2.367179
C	5.267568	-1.939232	-3.068861
C	-0.907608	-2.660263	0.001433
C	4.200933	-2.769115	-3.233895
C	-0.260048	-3.283480	-1.023142
C	6.447649	1.694575	0.163457
C	0.224115	1.054708	3.153004
C	5.820971	2.284227	1.218017
C	1.310011	1.852899	3.348350
H	6.192387	-1.906306	-3.630102
H	-1.891581	-2.846697	0.411917
H	4.064950	-3.559828	-3.960304
H	-0.602979	-4.102725	-1.641881
H	7.433361	1.897108	-0.234897
H	-0.712248	1.041121	3.695466
H	6.183772	3.073327	1.863856
H	1.452913	2.632905	4.084941

C	5.806708	-0.095443	-1.461884
C	-0.309839	-0.793917	1.554543
C	3.558668	2.031086	2.259988
C	1.990300	-3.005665	-2.086647
H	6.763308	0.033025	-1.957923
H	-1.285266	-0.910393	2.018369
H	3.807964	2.828703	2.952438
H	1.747310	-3.817396	-2.764801
O	2.081031	0.735586	-1.077832
S	4.000270	-1.995224	1.498491
C	3.902696	-1.437322	3.226359
H	2.866539	-1.367596	3.565672
H	4.459664	-2.139863	3.853112
H	4.369427	-0.449315	3.319768

Transition State from **PC-I** to **R-I**

0 4

N	-0.336737	1.089292	-1.372406
C	-6.282375	0.092394	-1.127643
O	-6.745613	0.279307	-2.253627
C	-4.842179	0.499024	-0.761109
C	-0.082569	3.554161	-0.962505
C	-6.468963	-0.681512	1.242359
C	-7.359104	-1.814134	1.772270
C	-8.713984	-1.519201	1.103141
C	-8.342418	-1.002519	-0.299341
C	-4.972452	-0.968396	1.261612
C	-3.955735	0.531748	-2.027225
C	-2.587327	1.072905	-1.766223
C	-1.385240	0.321217	-1.678930
C	-0.799405	2.403951	-1.254509
C	-2.203731	2.430086	-1.495880
C	-2.892044	3.652359	-1.442625
C	-2.172220	4.816843	-1.146873
C	-0.792856	4.768888	-0.909551
N	-4.282207	-0.420394	0.230042
N	-6.981989	-0.467629	-0.119460
O	-4.449819	-1.629255	2.158155
H	0.872119	0.709942	-1.255216
H	-4.885276	1.517918	-0.344813
H	0.987308	3.520863	-0.781662
H	-6.626873	0.226673	1.847160
H	-7.405227	-1.822615	2.863099
H	-6.959374	-2.778732	1.441175
H	-9.245742	-0.740119	1.660843
H	-9.362570	-2.397741	1.056513
H	-9.016501	-0.222449	-0.665465
H	-8.319935	-1.803041	-1.047816
H	-4.487480	1.144466	-2.762309
H	-3.893390	-0.481860	-2.437434
H	-1.269344	-0.745838	-1.826849
H	-3.960393	3.703908	-1.633859
H	-2.690469	5.769954	-1.103656
H	-0.256411	5.685549	-0.683219
H	-3.272538	-0.522202	0.265552
Fe	2.746783	-0.411197	0.079566
N	3.311397	-1.980796	-1.068114
N	1.020824	-1.372572	0.515138
N	4.530733	0.476025	-0.247502
N	2.262572	1.055009	1.368535
C	4.491209	-2.107276	-1.754011
C	0.043576	-0.951774	1.379418
C	2.560501	-3.083438	-1.387508
C	0.578916	-2.555962	-0.019020
C	5.539705	0.013102	-1.054752
C	1.111322	1.150490	2.107861
C	4.935887	1.702947	0.209228
C	2.969813	2.208445	1.606692
C	4.492469	-3.333171	-2.517269
C	-1.053157	-1.891657	1.389423
C	3.293319	-3.937343	-2.292364
C	-0.720873	-2.884112	0.513567
C	6.618263	0.972796	-1.097790
C	1.098300	2.389771	2.847049
C	6.242525	2.022718	-0.317129
C	2.247950	3.048947	2.530977
H	5.311459	-3.666985	-3.141359
H	-1.956187	-1.794180	1.980779
H	2.922150	-4.873026	-2.690471
H	-1.286449	-3.769528	0.252470
H	7.533094	0.842815	-1.661600
H	0.301703	2.700226	3.510936
H	6.785138	2.934567	-0.102879
H	2.594024	4.011762	2.884550
C	5.533003	-1.187431	-1.750670
C	0.080563	0.217669	2.128705
C	4.208854	2.523293	1.064324
C	1.284006	-3.354262	-0.912739
H	6.405996	-1.420640	-2.351815
H	-0.769660	0.427322	2.769784
H	4.651597	3.473493	1.345097
H	0.807875	-4.269531	-1.249246
O	2.038638	0.402233	-1.241610
S	3.789555	-1.664610	1.855711
C	4.483422	-0.501372	3.087377
H	3.702724	0.114871	3.540846
H	4.965857	-1.095724	3.869873
H	5.233899	0.152763	2.633894

Compound **R-I**

0 2

N	3.546705	-1.709327	-1.054497
C	-1.770616	1.170224	-0.535921
O	-1.700518	2.182332	-1.235014
C	-0.524194	0.322154	-0.214274
C	5.042110	-0.504590	0.559450
C	-3.045978	-0.458726	0.870851
C	-4.515304	-0.861219	0.688192
C	-5.219236	0.498570	0.529315
C	-4.222062	1.354406	-0.274464

C	-2.029734	-1.541771	0.534706
C	0.514329	0.468437	-1.351653
C	1.834196	-0.149151	-1.031519
C	2.356200	-1.393326	-1.534595
C	3.884711	-0.648683	-0.182242
C	2.854690	0.336174	-0.141039
C	3.000655	1.478120	0.651952
C	4.177595	1.623339	1.405494
C	5.178032	0.650570	1.361276
N	-0.880263	-1.084387	-0.027777
N	-2.920240	0.726107	0.009228
O	-2.238901	-2.726276	0.779449
H	-0.084251	0.726633	0.710841
H	5.824291	-1.257066	0.524336
H	-2.869745	-0.174490	1.921348
H	-4.887035	-1.448373	1.530187
H	-4.618304	-1.465007	-0.219947
H	-5.392435	0.948604	1.513245
H	-6.185938	0.417420	0.025792
H	-4.214950	2.406303	0.026361
H	-4.411368	1.317254	-1.353308
H	0.621839	1.542913	-1.532267
H	0.096066	0.025252	-2.262020
H	1.850526	-2.035814	-2.250407
H	2.231602	2.245346	0.686934
H	4.310226	2.503663	2.027218
H	6.080352	0.783244	1.951261
H	-0.151292	-1.778242	-0.156905

Compound **PC-II**

0 4

N	-1.081610	3.574209	-0.367355
C	-4.828508	-1.149960	-0.914314
O	-5.533899	-0.916569	-1.898068
C	-3.788991	-0.146194	-0.375655
C	-2.503315	5.301087	0.802224
C	-4.090212	-2.589002	0.981454
C	-4.153208	-4.119975	1.071138
C	-5.565358	-4.437310	0.546092
C	-5.790792	-3.409935	-0.578320
C	-2.682751	-2.007974	0.859103
C	-3.383093	0.869615	-1.460637
C	-2.691026	2.087988	-0.920902
C	-1.346592	2.367578	-0.983335
C	-2.258739	4.106340	0.114688
C	-3.301821	3.194624	-0.220817
C	-4.622831	3.512460	0.146590
C	-4.869562	4.698582	0.829846
C	-3.819262	5.582916	1.156644
N	-2.616331	-0.858230	0.145078
N	-4.914524	-2.291578	-0.199439
O	-1.716390	-2.557472	1.386847
H	-0.160371	3.978104	-0.266311
H	-4.278730	0.406373	0.442936
H	-1.694789	5.983956	1.049285
H	-4.549691	-2.143610	1.879584
H	-3.977048	-4.479351	2.087230
H	-3.385861	-4.554511	0.421408
H	-6.304170	-4.289377	1.342072
H	-5.662989	-5.465548	0.187722
H	-6.829517	-3.074904	-0.656851
H	-5.489545	-3.794480	-1.560204
H	-4.302966	1.144690	-1.986283
H	-2.746499	0.359645	-2.193737
H	-0.544500	1.782463	-1.409180
H	-5.442277	2.842604	-0.102611
H	-5.886534	4.951748	1.117529
H	-4.041944	6.502124	1.691865
H	-1.699861	-0.415139	0.079551
Fe	2.098308	-0.293750	-0.086056
N	2.380291	-0.311707	-2.085102
N	2.144331	-2.308562	-0.066360
N	2.372321	1.707237	-0.083003
N	2.168517	-0.295910	1.927106
C	2.479199	0.775729	-2.915957
C	2.008865	-3.129074	1.024204
C	2.381265	-1.409693	-2.904159
C	2.179781	-3.141935	-1.160350
C	2.469478	2.528168	-1.182959
C	2.033858	-1.388753	2.761682
C	2.343381	2.538639	1.006300
C	2.190130	0.806509	2.755913
C	2.547440	0.352026	-4.293198
C	1.960915	-4.510913	0.612121
C	2.488075	-1.008496	-4.285768
C	2.071592	-4.519375	-0.743974
C	2.507587	3.910322	-0.772226
C	1.993709	-0.961279	4.137466
C	2.427866	3.916902	0.590348
C	2.094157	0.395672	4.135039
H	2.632824	1.021093	-5.139646
H	1.860643	-5.349915	1.288277
H	2.514152	-1.691718	-5.124758
H	2.081077	-5.366957	-1.416950
H	2.595824	4.751421	-1.447946
H	1.899034	-1.629504	4.983490
H	2.439103	4.764393	1.263702
H	2.097091	1.074079	4.978360
C	2.522218	2.101441	-2.502769
C	1.945703	-2.705591	2.346456
C	2.267085	2.124002	2.333481
C	2.297162	-2.731854	-2.478967
H	2.602051	2.863007	-3.271868
H	1.831470	-3.466370	3.111470
H	2.260522	2.894585	3.097638
H	2.314545	-3.503140	-3.242232
O	0.475589	-0.191946	-0.199320
S	4.643118	-0.622798	0.386079
C	5.389542	0.950848	0.908600
H	4.925309	1.283363	1.844986

H	6.455336	0.788974	1.094717
H	5.251367	1.729051	0.154304

Transition State from **PC-II** to **R-II**

0 4

N	-0.318459	3.592617	-1.955506
C	-4.297482	-0.431363	-0.107857
O	-5.206214	0.390622	0.062278
C	-2.866211	0.051773	-0.406019
C	-1.047106	5.483346	-0.441509
C	-3.494523	-2.784155	-0.345897
C	-4.238724	-3.750085	-1.277739
C	-5.653577	-3.765115	-0.663870
C	-5.866164	-2.330908	-0.119314
C	-2.152716	-2.239268	-0.830166
C	-2.953008	1.004022	-1.683391
C	-2.047600	2.181106	-1.618713
C	-0.849447	2.370649	-2.283529
C	-1.153790	4.232012	-1.053332
C	-2.255162	3.363693	-0.819048
C	-3.270087	3.766380	0.067880
C	-3.164367	5.009036	0.686853
C	-2.067143	5.857687	0.433321
N	-1.852991	-0.947307	-0.595680
N	-4.508309	-1.760540	-0.078755
O	-1.341776	-3.056153	-1.299106
H	0.572040	3.940552	-2.280247
H	-2.584572	0.695945	0.436749
H	-0.205287	6.141314	-0.638726
H	-3.267563	-3.313055	0.594450
H	-3.769687	-4.735519	-1.311988
H	-4.255290	-3.340370	-2.294514
H	-5.695601	-4.489253	0.157164
H	-6.425471	-4.041564	-1.387143
H	-6.326126	-2.324391	0.874813
H	-6.484195	-1.708995	-0.774007
H	-3.990979	1.346846	-1.735864
H	-2.749725	0.392638	-2.567176
H	-0.330880	1.708149	-2.961447
H	-4.114210	3.110934	0.266831
H	-3.939513	5.334485	1.375126
H	-2.014632	6.824100	0.927098
H	-0.402264	-0.593587	-0.782707
Fe	1.805219	-0.484530	0.243709
N	3.082580	-1.452543	-0.989664
N	1.089034	-2.256601	0.870031
N	2.658453	1.274836	-0.251045
N	0.618346	0.473256	1.562763
C	4.020515	-0.881111	-1.813016
C	0.109613	-2.458977	1.805651
C	3.165611	-2.802187	-1.200892
C	1.457774	-3.505289	0.429138
C	3.654813	1.473291	-1.173867
C	-0.318726	-0.097371	2.384964
C	2.296146	2.522510	0.191694
C	0.524598	1.829397	1.761219
C	4.703983	-1.899973	-2.573309
C	-0.138916	-3.870008	1.972559
C	4.172889	-3.094155	-2.192417
C	0.699559	-4.518991	1.119103
C	3.938226	2.880021	-1.305458
C	-1.020969	0.923493	3.124164
C	3.093490	3.532406	-0.456448
C	-0.497003	2.119823	2.737185
H	5.486387	-1.706462	-3.295649
H	-0.864265	-4.288712	2.658107
H	4.426972	-4.088633	-2.535690
H	0.805301	-5.583049	0.952783
H	4.687823	3.296686	-1.965755
H	-1.807527	0.730688	3.842110
H	3.009192	4.595590	-0.271192
H	-0.767514	3.114880	3.065235
C	4.293761	0.475648	-1.902035
C	-0.565822	-1.460008	2.497664
C	1.300922	2.789314	1.125432
C	2.416156	-3.767794	-0.536455
H	5.066640	0.784943	-2.598322
H	-1.335297	-1.770807	3.196852
H	1.114446	3.828106	1.375762
H	2.597631	-4.806384	-0.792699
O	0.619764	-0.338817	-1.011237
S	3.387000	-0.787264	2.002265
C	3.843603	0.832576	2.717955
H	2.966448	1.358701	3.104442
H	4.524823	0.632626	3.551211
H	4.351737	1.467818	1.988249

Compound **R-II**

0 2

N	-3.068676	-1.986608	0.268667
C	1.838962	1.398401	-0.301609
O	1.665946	2.577640	-0.004289
C	0.607305	0.512059	-0.646042
C	-5.137800	-0.593746	-0.114142
C	3.302596	-0.630996	-0.568764
C	4.365301	-1.002555	0.470677
C	5.224630	0.276227	0.523773
C	4.222516	1.436392	0.328523
C	2.003218	-1.437622	-0.538494
C	-0.245983	0.385108	0.668259
C	-1.548222	-0.334046	0.482195
C	-1.738989	-1.696167	0.487635
C	-3.774508	-0.811637	0.116757
C	-2.841906	0.258006	0.241774
C	-3.309897	1.580292	0.126310
C	-4.662564	1.800740	-0.104274
C	-5.567869	0.724173	-0.223784
N	0.969604	-0.774322	-1.162743
N	3.044276	0.790955	-0.282924
O	1.931957	-2.580584	-0.110472

H	-3.461429	-2.915562	0.235496
H	0.012047	1.046565	-1.392574
H	-5.833050	-1.423954	-0.204905
H	3.722580	-0.730006	-1.581282
H	4.930613	-1.891192	0.182063
H	3.883172	-1.198629	1.434275
H	5.955036	0.268919	-0.292160
H	5.776547	0.371921	1.462192
H	4.610832	2.226962	-0.321113
H	3.916338	1.898715	1.272026
H	-0.411680	1.410421	1.013361
H	0.369993	-0.115847	1.424901
H	-1.014399	-2.489144	0.615845
H	-2.624391	2.419496	0.215250
H	-5.032882	2.818356	-0.195049
H	-6.619731	0.928568	-0.403999

Transition State from **R-II** to **R-III**

0 2

N	-2.338248	-1.782052	0.475069
C	1.933448	1.512669	-0.181575
O	2.058894	2.702385	0.125154
C	0.537341	0.908657	-0.369460
C	-4.622182	-1.106776	-0.355875
C	2.890735	-0.756604	-0.645921
C	4.074481	-1.346518	0.129538
C	5.143821	-0.246858	-0.009728
C	4.348934	1.074951	0.039727
C	1.509286	-1.360924	-0.325239
C	-0.365050	1.277650	0.852540
C	-1.488169	0.289379	0.821722
C	-1.219449	-1.105681	0.872291
C	-3.334571	-0.883138	0.124791
C	-2.815449	0.431926	0.331866
C	-3.627429	1.545450	0.025327
C	-4.912735	1.325481	-0.448249
C	-5.404278	0.015046	-0.634552
N	0.470139	-0.538664	-0.518892
N	2.979812	0.675706	-0.327892
O	1.433628	-2.562620	-0.030201
H	-2.427303	-2.787993	0.464407
H	0.099071	1.383704	-1.258702
H	-5.002807	-2.111645	-0.511650
H	3.052683	-0.903312	-1.725400
H	4.389042	-2.311920	-0.272224
H	3.790374	-1.490144	1.178012
H	5.654658	-0.342403	-0.974357
H	5.904913	-0.293345	0.773848
H	4.734002	1.830673	-0.652713
H	4.331330	1.522036	1.039683
H	-0.705282	2.312834	0.785343
H	0.214037	1.178042	1.778839
H	-0.428730	-1.638618	1.377713
H	-3.252609	2.555097	0.166886
H	-5.553270	2.170459	-0.682559
H	-6.414612	-0.124762	-1.007942

Compound **R-III**

0 2

N	-1.825839	-1.536027	0.207325
C	1.975028	1.532017	-0.131974
O	2.210570	2.711006	0.136743
C	0.547036	1.018466	-0.335224
C	-4.258316	-1.392632	-0.397436
C	2.670484	-0.827879	-0.577819
C	3.948188	-1.524530	-0.091778
C	5.039840	-0.475963	-0.371066
C	4.361042	0.868827	-0.056935
C	1.381177	-1.311158	0.085301
C	-0.528403	1.796064	0.475666
C	-1.547686	0.728873	0.721137
C	-0.874169	-0.617174	0.825944
C	-3.038255	-0.875192	0.024054
C	-2.866484	0.530932	0.258928
C	-3.938795	1.410550	-0.002590
C	-5.155799	0.886643	-0.430077
C	-5.317060	-0.498095	-0.613139
N	0.395058	-0.382956	0.116466
N	2.933692	0.593060	-0.285417
O	1.249026	-2.450859	0.530648
H	-1.823790	-2.498270	0.521265
H	0.312492	1.089499	-1.407576
H	-4.383988	-2.457226	-0.573881
H	2.555439	-0.969950	-1.664638
H	4.117559	-2.473966	-0.604246
H	3.865125	-1.729827	0.980713
H	5.333211	-0.510276	-1.426391
H	5.939257	-0.631425	0.230411
H	4.700409	1.686883	-0.699142
H	4.510663	1.177494	0.984630
H	-0.915425	2.650057	-0.084502
H	-0.074420	2.180189	1.398402
H	-0.631596	-0.957224	1.843486
H	-3.817520	2.479030	0.153321
H	-5.993234	1.552469	-0.618361
H	-6.278311	-0.885672	-0.939195

3-methylindole

0 1

N	0.632687	1.814318	0.000440
C	-1.790518	1.108332	0.000038
C	2.641172	-1.314436	0.000037
C	1.608295	-0.226725	-0.000164
C	1.834240	1.127603	-0.000085
C	-0.405047	0.907751	0.000049
C	0.174859	-0.393770	-0.000045
C	-0.675624	-1.514387	0.000006
C	-2.052337	-1.319799	-0.000023
C	-2.603782	-0.020530	-0.000047
H	0.536398	2.818369	-0.001853

H	-2.214783	2.108908	0.000084
H	2.550605	-1.962805	-0.881613
H	3.653333	-0.896375	0.000588
H	2.771096	1.668609	-0.000155
H	-0.261497	-2.519740	0.000054
H	-2.717631	-2.179206	-0.000028
H	-3.683712	0.100979	-0.000093
H	2.549839	-1.963186	0.881338

Transition State from **R-III** to **R-IV**

0 2

N	-5.566010	0.067828	-0.750328
C	-3.454605	0.700912	-1.990373
C	-4.832501	-3.102094	1.047864
C	-4.862720	-1.840573	0.238460
C	-5.927209	-0.991043	0.067570
C	-4.252694	-0.077585	-1.125277
C	-3.766090	-1.271044	-0.515001
C	-2.448732	-1.672261	-0.752188
C	-1.566897	-0.813989	-1.490162
C	-2.154795	0.306253	-2.202178
H	-6.176279	0.822785	-1.025463
H	-3.867343	1.568247	-2.499427
H	-4.064844	-3.062957	1.832136
H	-5.796425	-3.281852	1.535252
H	-6.929326	-1.051219	0.470160
H	-2.068121	-2.601321	-0.336045
H	-0.719156	-1.296211	-1.977442
H	-1.526915	0.877519	-2.879386
H	-4.605915	-3.979222	0.427063
N	0.370239	2.191987	-0.782233
C	3.033387	-1.588206	0.786701
O	2.865040	-2.775631	1.068131
C	1.886553	-0.574303	0.794455
C	-0.928421	3.435362	0.975946
C	4.450511	0.349733	0.084470
C	5.747855	0.295457	-0.733970
C	6.529909	-0.847469	-0.062876
C	5.448422	-1.877127	0.310084
C	3.250176	0.937567	-0.657262
C	0.495758	-1.170169	0.492859
C	-0.249851	-0.002293	-0.133561
C	0.783946	0.807292	-0.931227
C	-0.479647	2.290720	0.321110
C	-0.896340	0.998166	0.725834
C	-1.777322	0.862332	1.800922
C	-2.236110	2.008060	2.462871
C	-1.813846	3.277280	2.051555
N	2.057237	0.441918	-0.260771
N	4.233375	-1.060095	0.456805
O	3.369234	1.804301	-1.526856
H	1.075567	2.898458	-0.953090
H	1.873819	-0.086820	1.781145
H	-0.594050	4.422834	0.669273
H	4.605929	0.956180	0.991746
H	6.278617	1.249778	-0.724339
H	5.511617	0.050567	-1.775019
H	7.026897	-0.481508	0.842661
H	7.296375	-1.275343	-0.714376
H	5.663680	-2.414495	1.238490
H	5.293505	-2.623200	-0.478554
H	0.015751	-1.549716	1.396973
H	0.606425	-2.008434	-0.205451
H	0.881116	0.552887	-1.991896
H	-2.101273	-0.123659	2.122621
H	-2.918971	1.910454	3.302204
H	-2.171186	4.159557	2.576477

Compound **R-IV**

0 2

N	-5.707588	-0.106556	-0.984684
C	-3.514493	0.747008	-1.934977
C	-4.888469	-3.070003	1.101239
C	-4.944779	-1.862661	0.215120
C	-6.064454	-1.160100	-0.159222
C	-4.344925	-0.109478	-1.157341
C	-3.817546	-1.201966	-0.414240
C	-2.448342	-1.453522	-0.410841
C	-1.486476	-0.564979	-1.162549
C	-2.173712	0.531195	-1.950510
H	-6.350730	0.555945	-1.391436
H	-3.952497	1.553633	-2.518845
H	-4.265773	-2.894119	1.988841
H	-5.887756	-3.353622	1.447858
H	-7.101804	-1.324991	0.098605
H	-2.045811	-2.311287	0.120373
H	-0.918361	-1.191505	-1.880610
H	-1.538564	1.179253	-2.547167
H	-4.458452	-3.936931	0.581580
N	0.440190	2.192594	-0.853279
C	2.945619	-1.604629	0.806795
O	2.746688	-2.765072	1.168401
C	1.826344	-0.562040	0.744898
C	-0.594181	3.503371	1.028183
C	4.411405	0.243809	-0.024422
C	5.697867	0.098899	-0.849304
C	6.454800	-1.018436	-0.109762
C	5.349277	-1.989588	0.342068
C	3.223802	0.825641	-0.789041
C	0.434089	-1.139490	0.474653
C	-0.340452	0.004862	-0.222402
C	0.758799	0.783485	-1.023731
C	-0.305836	2.334251	0.323546
C	-0.819854	1.090218	0.732157
C	-1.636557	1.010413	1.853518
C	-1.936942	2.178235	2.571118
C	-1.416667	3.407428	2.157253
N	2.019981	0.369075	-0.376936
N	4.157585	-1.131678	0.440048
O	3.362002	1.657868	-1.688826

H	1.204444	2.833371	-1.036675
H	1.828609	-0.007655	1.695942
H	-0.189497	4.460917	0.711799
H	4.595711	0.901995	0.840492
H	6.254623	1.036435	-0.908040
H	5.443984	-0.208518	-1.869469
H	6.972483	-0.606876	0.764048
H	7.201326	-1.510890	-0.738279
H	5.558649	-2.466591	1.304176
H	5.166973	-2.784081	-0.391378
H	-0.049433	-1.474747	1.393645
H	0.523382	-2.003791	-0.193005
H	0.816040	0.530400	-2.085830
H	-2.038898	0.053708	2.175041
H	-2.571343	2.124434	3.451162
H	-1.647894	4.307559	2.721269

Compound **PDT_{c-c}**

0 1

N	-5.659156	-1.125029	-1.454404
C	-3.636937	0.287975	-2.002739
C	-4.842626	-2.913365	1.701484
C	-4.913807	-2.080493	0.456239
C	-5.964187	-1.998092	-0.424986
C	-4.393358	-0.620818	-1.254922
C	-3.891169	-1.202051	-0.058515
C	-2.598926	-0.858948	0.378889
C	-1.828157	0.039517	-0.358017
C	-2.367123	0.609054	-1.541098
H	-4.025603	0.731838	-2.915406
H	-4.691284	-2.295760	2.596717
H	-5.765336	-3.484911	1.846327
H	-6.922195	-2.500063	-0.401743
H	-2.212353	-1.301169	1.292335
H	-1.770426	1.321956	-2.102336
H	-4.010942	-3.629420	1.665855
N	0.593831	2.105467	-1.321278
C	2.647188	-1.472023	1.206004
O	2.320724	-2.379984	1.971345
C	1.743132	-0.267752	0.930557
C	0.275050	4.133009	0.138959
C	4.222796	-0.371656	-0.394160
C	5.272186	-1.061090	-1.277193
C	5.947897	-2.042169	-0.302816
C	4.797800	-2.540030	0.590544
C	3.031205	0.210497	-1.152344
C	0.246864	-0.561871	1.054812
C	-0.437501	0.466807	0.120186
C	0.602250	0.676218	-1.040318
C	0.173294	2.774577	-0.163366
C	-0.467513	1.882785	0.712514
C	-1.032749	2.345307	1.893174
C	-0.937517	3.708236	2.211029
C	-0.287126	4.585870	1.338651
N	1.870299	0.193038	-0.459589
N	3.823864	-1.437645	0.542030
O	3.135572	0.674322	-2.290391
H	1.409454	2.446032	-1.819171
H	2.032769	0.539380	1.620800
H	0.776938	4.820272	-0.536656
H	4.691019	0.457025	0.161800
H	5.965118	-0.345365	-1.724354
H	4.769942	-1.598617	-2.088684
H	6.693005	-1.515607	0.304226
H	6.455068	-2.864431	-0.814194
H	5.104382	-2.735901	1.622326
H	4.333054	-3.453703	0.201257
H	-0.094246	-0.486164	2.089249
H	0.048146	-1.579994	0.707569
H	0.390496	0.106782	-1.947355
H	-1.542012	1.660460	2.567340
H	-1.369184	4.080411	3.135596
H	-0.213885	5.640391	1.591944
H	-6.269967	-0.895924	-2.223785

Compound **C-III**

1 1

N	-1.843818	-1.512494	0.257149
C	2.006729	1.529724	-0.091016
O	2.224830	2.683849	0.272329
C	0.587546	1.062692	-0.442791
C	-4.287649	-1.445226	-0.199211
C	2.679528	-0.823946	-0.609120
C	3.924232	-1.572061	-0.113030
C	5.040947	-0.524621	-0.271163
C	4.368761	0.804905	0.108496
C	1.361142	-1.300584	-0.007939
C	-0.524615	1.849467	0.315826
C	-1.532267	0.775006	0.511678
C	-0.844548	-0.543404	0.707564
C	-3.020865	-0.894400	0.093849
C	-2.845435	0.556468	0.198926
C	-3.945640	1.432272	-0.082730
C	-5.152305	0.871457	-0.383810
C	-5.313006	-0.557853	-0.432423
N	0.367371	-0.360285	-0.057767
N	2.951094	0.577184	-0.227982
O	1.171001	-2.411728	0.469505
H	-1.729771	-2.508472	0.409070
H	0.442911	1.175059	-1.524728
H	-4.435437	-2.517515	-0.257474
H	2.595197	-0.906573	-1.704048
H	4.103346	-2.486239	-0.682695
H	3.789617	-1.847788	0.937837
H	5.381101	-0.489612	-1.311892
H	5.908373	-0.738371	0.357889
H	4.754814	1.663651	-0.446997
H	4.456646	1.026179	1.178362
H	-0.898201	2.702369	-0.250986
H	-0.125932	2.219624	1.268502

H	-0.625059	-0.772373	1.762091
H	-3.811293	2.507028	-0.026894
H	-6.014871	1.496611	-0.586205
H	-6.295957	-0.950760	-0.674931

Transition State from **C-III** to **C-IV**

1 1

N	-5.209632	0.262283	-0.586504
C	-3.203395	0.840413	-1.976389
C	-4.627184	-3.106813	0.887129
C	-4.614109	-1.782017	0.187942
C	-5.597134	-0.833208	0.186381
C	-3.976616	0.047186	-1.101810
C	-3.546267	-1.243534	-0.632385
C	-2.301151	-1.707898	-1.016250
C	-1.454746	-0.860671	-1.786322
C	-1.968702	0.359614	-2.342749
H	-5.777610	1.083321	-0.746843
H	-3.585522	1.780169	-2.362403
H	-3.799807	-3.193684	1.602521
H	-5.561637	-3.249195	1.437454
H	-6.561623	-0.834086	0.674360
H	-1.941769	-2.682704	-0.699706
H	-0.577471	-1.302144	-2.248819
H	-1.352023	0.925162	-3.032984
H	-4.526682	-3.936026	0.176185
N	0.212167	2.155357	-0.599177
C	3.064318	-1.597984	0.666610
O	2.941516	-2.816807	0.780964
C	1.864309	-0.652221	0.798628
C	-1.371289	3.180726	1.038707
C	4.373960	0.491170	0.248974
C	5.701164	0.624974	-0.510089
C	6.525615	-0.557286	0.029508
C	5.497739	-1.688511	0.199805
C	3.162285	1.087500	-0.463797
C	0.515217	-1.300054	0.400845
C	-0.245062	-0.095669	-0.107465
C	0.745076	0.829190	-0.832893
C	-0.741248	2.118853	0.373120
C	-1.049099	0.759509	0.704185
C	-1.973371	0.475660	1.734178
C	-2.581684	1.527568	2.395690
C	-2.282206	2.863342	2.037875
N	1.982266	0.503264	-0.116804
N	4.232324	-0.967634	0.425187
O	3.227386	2.015536	-1.264898
H	0.721965	2.979367	-0.886630
H	1.813658	-0.299732	1.838190
H	-1.139534	4.211872	0.793522
H	4.449869	0.981310	1.232721
H	6.171736	1.595531	-0.340323
H	5.519506	0.519766	-1.584766
H	6.963572	-0.299222	1.000007
H	7.340634	-0.842364	-0.640232
H	5.713278	-2.349326	1.043872
H	5.407519	-2.308657	-0.699634
H	0.031034	-1.787954	1.247248
H	0.690544	-2.048660	-0.375847
H	0.887564	0.661779	-1.902258
H	-2.193115	-0.551810	2.003906
H	-3.290257	1.334059	3.193926
H	-2.773446	3.671477	2.572534

Compound **C-IV**

1 1

N	-5.647849	-0.163982	-1.064375
C	-3.500934	0.740552	-1.956776
C	-4.894590	-3.074322	1.141437
C	-4.942774	-1.893042	0.225743
C	-6.037991	-1.219164	-0.210976
C	-4.324256	-0.131559	-1.192630
C	-3.798900	-1.219538	-0.384328
C	-2.456582	-1.414697	-0.332673
C	-1.518574	-0.539144	-1.089870
C	-2.160947	0.538712	-1.905149
H	-6.294610	0.473339	-1.515326
H	-3.939724	1.530300	-2.557389
H	-4.317288	-2.850763	2.046276
H	-5.901210	-3.371654	1.446142
H	-7.086674	-1.376641	-0.005002
H	-2.035003	-2.228748	0.249905
H	-1.003861	-1.209824	-1.804330
H	-1.499965	1.188129	-2.468717
H	-4.418714	-3.933438	0.654255
N	0.411151	2.171135	-0.902376
C	2.930070	-1.608562	0.817419
O	2.713867	-2.766109	1.176857
C	1.821497	-0.550925	0.777156
C	-0.570374	3.548170	0.963059
C	4.396394	0.225560	-0.041922
C	5.677309	0.072355	-0.874022
C	6.431205	-1.050119	-0.139169
C	5.322973	-2.015876	0.315540
C	3.204720	0.803108	-0.802065
C	0.421922	-1.128088	0.538595
C	-0.343655	0.013358	-0.170655
C	0.746260	0.759845	-1.015439
C	-0.300573	2.356339	0.289966
C	-0.805694	1.130001	0.756669
C	-1.594022	1.084204	1.900962
C	-1.873019	2.274665	2.585310
C	-1.361803	3.488679	2.114921
N	1.999859	0.370399	-0.353815
N	4.138339	-1.147837	0.431055
O	3.324239	1.606783	-1.726776
H	1.163233	2.810349	-1.137089
H	1.846015	0.006585	1.725035
H	-0.173798	4.493987	0.605835
H	4.585667	0.887280	0.818737

H	6.239544	1.006379	-0.934107
H	5.416362	-0.232292	-1.893098
H	6.955170	-0.643242	0.732794
H	7.171380	-1.545374	-0.772529
H	5.535184	-2.500659	1.272690
H	5.126546	-2.802344	-0.422599
H	-0.048612	-1.432863	1.475099
H	0.499505	-2.011127	-0.104720
H	0.800100	0.467323	-2.067675
H	-1.982723	0.140223	2.275221
H	-2.480487	2.252143	3.484775
H	-1.577357	4.406476	2.655127

Compound **R-V**

0 2

N	-3.049957	1.767668	-0.938990
C	1.226975	-0.379821	1.350606
O	0.668817	-1.205515	2.078688
C	0.891815	1.119025	1.446887
C	-3.937156	-0.528659	-1.404071
C	2.951727	0.232762	-0.356465
C	3.358945	-0.614142	-1.568735
C	3.598159	-1.999161	-0.939197
C	2.528685	-2.114275	0.165686
C	2.191476	1.510604	-0.674993
C	-0.590898	1.344209	1.848498
C	-1.600186	1.142981	0.761433
C	-2.163567	2.189106	-0.058441
C	-3.128193	0.370188	-0.735631
C	-2.247992	-0.055782	0.304737
C	-2.194798	-1.406082	0.671805
C	-3.019767	-2.316515	-0.008681
C	-3.873622	-1.888708	-1.027255
N	1.213738	1.831963	0.211707
N	2.173231	-0.713534	0.453780
O	2.474247	2.204186	-1.647704
H	1.499014	1.511817	2.277799
H	-4.604721	-0.196304	-2.193602
H	3.855768	0.535333	0.197462
H	4.236716	-0.209331	-2.076008
H	2.532376	-0.644972	-2.286978
H	4.599817	-2.040306	-0.497273
H	3.522188	-2.811683	-1.666205
H	2.895304	-2.612983	1.068029
H	1.631644	-2.646631	-0.168840
H	-0.676916	2.370569	2.224488
H	-0.783836	0.667611	2.685956
H	-1.913981	3.244200	0.022986
H	-1.518446	-1.741265	1.451010
H	-2.991264	-3.368044	0.261809
H	-4.502380	-2.611211	-1.539980
H	0.765510	2.726764	0.048899

Transition State from **R-V** to **R-VI**

0 2

N	1.628868	2.371470	0.385167
C	-3.057800	-0.383152	1.292029
O	-3.737536	0.514829	1.793887
C	-1.622581	-0.692437	1.759793
C	0.332875	3.860637	-1.181784
C	-2.761023	-2.328535	-0.245852
C	-3.469395	-2.577941	-1.583383
C	-4.936073	-2.242684	-1.256950
C	-4.846998	-1.048538	-0.289576
C	-1.277190	-2.000168	-0.342929
C	-0.921317	0.532525	2.415086
C	-0.165289	1.417839	1.465689
C	1.205666	1.451723	1.325502
C	0.465431	2.904003	-0.169023
C	-0.678346	2.370905	0.497738
C	-1.957553	2.836098	0.159862
C	-2.081661	3.786109	-0.854961
C	-0.950282	4.288995	-1.522441
N	-0.813341	-1.233708	0.663127
N	-3.519814	-1.205633	0.327785
O	-0.579786	-2.430606	-1.271574
H	-1.728718	-1.460371	2.541819
H	1.205318	4.268784	-1.685649
H	-2.859558	-3.216158	0.400716
H	-3.326397	-3.600416	-1.939099
H	-3.069333	-1.895647	-2.340699
H	-5.413539	-3.093734	-0.758530
H	-5.523112	-2.005611	-2.147886
H	-5.627882	-1.051486	0.476472
H	-4.892440	-0.084966	-0.810284
H	-0.223341	0.150971	3.168011
H	-1.706800	1.077960	2.947712
H	1.941598	0.872288	1.872365
H	-2.834709	2.460448	0.678417
H	-3.068542	4.149615	-1.130270
H	-1.075982	5.029132	-2.308464
H	0.141219	-0.893382	0.590969
N	2.283452	-2.063674	-1.021218
C	2.276500	0.423216	-1.356496
C	5.321341	-2.829177	0.988720
C	4.184181	-2.233125	0.212777
C	3.120222	-2.922849	-0.355244
C	2.766582	-0.773905	-0.864981
C	3.968233	-0.860003	-0.091867
C	4.673715	0.341163	0.210390
C	4.167951	1.544587	-0.201453
C	2.904802	1.638663	-0.916648
H	1.322837	-2.282504	-1.301820
H	1.389518	0.466976	-1.980630
H	5.196008	-3.910690	1.101922
H	6.285879	-2.656927	0.493982
H	2.906609	-3.983242	-0.326546
H	5.612699	0.297331	0.756450
H	4.690834	2.468077	0.027645
H	2.774659	2.511858	-1.546851

H	5.395658	-2.394980	1.993737

Compound **R-VI**

0 2

N	-1.872034	1.532076	0.088560
C	3.904836	0.046474	1.075030
O	4.234756	0.472665	2.183532
C	2.611276	0.503892	0.380565
C	-1.833326	3.853849	-0.921656
C	4.304828	-1.365469	-0.952649
C	5.047536	-2.707464	-0.994375
C	6.325048	-2.411468	-0.188406
C	5.857411	-1.466262	0.934344
C	2.800764	-1.450830	-1.183020
C	1.552130	0.926563	1.422215
C	0.280963	1.435015	0.805328
C	-0.913249	0.757743	0.713912
C	-1.293603	2.739717	-0.263177
C	0.061044	2.716963	0.181557
C	0.871115	3.847261	-0.030497
C	0.334044	4.953610	-0.677650
C	-1.005066	4.953460	-1.120870
N	2.073148	-0.556684	-0.470996
N	4.645378	-0.842134	0.378803
O	2.310969	-2.258975	-1.969424
H	2.863928	1.383060	-0.234113
H	-2.861533	3.868290	-1.270650
H	4.709000	-0.696438	-1.730346
H	5.243779	-3.036362	-2.016867
H	4.441387	-3.475111	-0.500989
H	7.059909	-1.904450	-0.823843
H	6.794989	-3.315586	0.207356
H	6.599003	-0.704592	1.193825
H	5.597840	-2.003950	1.853703
H	2.016525	1.686760	2.057616
H	1.340032	0.065068	2.065603
H	-1.173397	-0.226946	1.078554
H	1.903813	3.857574	0.309654
H	0.951440	5.831622	-0.847058
H	-1.399643	5.829534	-1.628406
H	1.077749	-0.519606	-0.670269
N	-5.051880	-1.572970	1.855717
C	-3.921373	0.466496	0.953583
C	-5.072142	-4.083306	-0.885284
C	-4.925682	-2.897371	0.023114
C	-5.359011	-2.814429	1.339577
C	-4.407755	-0.818460	0.887212
C	-4.324024	-1.647306	-0.280162
C	-3.699024	-1.112289	-1.456058
C	-3.203792	0.148626	-1.459186
C	-3.244329	1.066678	-0.252288
H	-5.259518	-1.265457	2.793862
H	-4.002912	1.074702	1.849323
H	-4.097973	-4.451834	-1.230855
H	-5.577097	-4.909750	-0.375069
H	-5.866236	-3.553292	1.944514
H	-3.625863	-1.726528	-2.350738
H	-2.728537	0.556357	-2.347430
H	-3.769090	1.993874	-0.530962
H	-5.657401	-3.838633	-1.780837

Compound **PDT_{C-N}**

0 1

N	1.356808	0.707155	0.573365
C	-4.081042	0.336718	0.949207
O	-4.341482	1.528507	1.137207
C	-3.008470	-0.408945	1.766030
C	1.096272	2.383042	-1.305989
C	-4.510119	-1.867295	-0.146330
C	-5.062732	-2.108654	-1.555841
C	-6.245956	-1.125921	-1.631076
C	-5.763561	0.113109	-0.853560
C	-3.043113	-2.235749	0.048003
C	-1.917459	0.538487	2.333466
C	-0.748562	0.826435	1.431506
C	0.494137	0.254674	1.560531
C	0.660142	1.614018	-0.219437
C	-0.665674	1.710617	0.291072
C	-1.570271	2.595368	-0.325835
C	-1.141789	3.349713	-1.411588
C	0.179071	3.246737	-1.894550
N	-2.411833	-1.496753	0.992314
N	-4.740787	-0.427444	0.056384
O	-2.502081	-3.137109	-0.588784
H	-3.545340	-0.826325	2.633463
H	2.115685	2.313803	-1.670960
H	-5.095666	-2.444063	0.588558
H	-5.353094	-3.149981	-1.710331
H	-4.295071	-1.857647	-2.295472
H	-7.124714	-1.558408	-1.139529
H	-6.526649	-0.880333	-2.658555
H	-6.559636	0.605398	-0.286949
H	-5.305253	0.864485	-1.506958
H	-1.537527	0.087060	3.256466
H	-2.434722	1.460446	2.616301
H	0.847396	-0.461960	2.290180
H	-2.586256	2.680368	0.046491
H	-1.833111	4.035049	-1.894955
H	0.489639	3.855495	-2.739530
H	-1.416606	-1.660170	1.099554
N	5.259044	-0.997053	-1.940452
C	3.187533	-0.137795	-0.799451
C	7.916480	-1.150499	0.656990
C	6.682845	-0.992579	-0.181149
C	6.548326	-1.273608	-1.518287
C	4.527773	-0.528064	-0.873914
C	5.395085	-0.512776	0.256543
C	4.882918	-0.072616	1.489204
C	3.559723	0.339613	1.571412
C	2.716672	0.303755	0.436455

H	4.913928	-1.125835	-2.879716
H	2.528304	-0.191921	-1.659576
H	7.754077	-1.842854	1.493444
H	8.749271	-1.539320	0.062038
H	7.279620	-1.655734	-2.217705
H	5.516089	-0.040955	2.371856
H	3.159007	0.709255	2.510163
H	8.237153	-0.195091	1.092582

Compound **C-V**

1 1

N	2.390732	-1.819704	-1.422595
C	-1.008776	0.551870	1.251532
O	-0.197445	1.319865	1.779028
C	-0.945713	-0.960549	1.542905
C	3.836111	0.234091	-1.555774
C	-3.002929	0.089168	-0.185243
C	-3.345418	0.815108	-1.493051
C	-3.234871	2.295983	-1.084955
C	-2.061525	2.340070	-0.085488
C	-2.579796	-1.362179	-0.323993
C	0.545899	-1.380014	1.793450
C	1.424478	-1.216982	0.619718
C	1.542912	-2.192876	-0.530695
C	2.909647	-0.559881	-0.953304
C	2.313732	-0.191979	0.296969
C	2.667406	1.015553	0.947923
C	3.618429	1.835931	0.332323
C	4.186644	1.453287	-0.881786
N	-1.550420	-1.760995	0.489326
N	-1.966607	0.949522	0.402982
O	-3.151157	-2.130201	-1.084283
H	-1.445616	-1.134175	2.507029
H	4.297364	-0.029133	-2.500840
H	-3.887882	0.084951	0.470995
H	-4.333305	0.539465	-1.865838
H	-2.605326	0.560458	-2.259565
H	-4.158645	2.618336	-0.593097
H	-3.064821	2.955626	-1.939090
H	-2.230382	3.026922	0.748602
H	-1.111989	2.612101	-0.558233
H	0.539869	-2.435455	2.093546
H	0.897858	-0.772637	2.628174
H	0.983796	-3.119325	-0.605294
H	2.195807	1.295638	1.882198
H	3.915654	2.768208	0.798024
H	4.926974	2.099349	-1.343953
H	-1.443865	-2.768993	0.548216

Iron-Oxo Quartet FeO_quartet

0 4

Fe	0.089141	0.036057	-0.377911
N	1.819494	-0.979714	-0.146250
N	-0.917496	-1.709275	-0.274068
N	1.083957	1.774351	-0.133367
N	-1.657172	1.037712	-0.294031
C	3.081401	-0.442680	-0.039450
C	-2.283740	-1.880043	-0.331182
C	1.995090	-2.338860	-0.207619
C	-0.378864	-2.980953	-0.309906
C	2.440098	1.939745	-0.026959
C	-2.917859	0.504666	-0.369167
C	0.552637	3.037947	-0.164823
C	-1.825001	2.402919	-0.311109
C	4.071808	-1.491461	-0.023063
C	-2.610089	-3.284464	-0.372069
C	3.397629	-2.668854	-0.134568
C	-1.431248	-3.964519	-0.364664
C	2.774252	3.342623	0.015773
C	-3.906480	1.553781	-0.424663
C	1.599634	4.026212	-0.073553
C	-3.227094	2.733367	-0.389255
H	5.138437	-1.328178	0.061663
H	-3.617167	-3.679288	-0.410096
H	3.794198	-3.675647	-0.157896
H	-1.269081	-5.034293	-0.392542
H	3.779796	3.733563	0.102573
H	-4.974948	1.389913	-0.480023
H	1.437863	5.096418	-0.073688
H	-3.621023	3.741304	-0.409414
C	3.374694	0.911083	0.028832
C	-3.216766	-0.854725	-0.375471
C	-0.802078	3.337879	-0.250908
C	0.973072	-3.277374	-0.299936
H	4.419583	1.191446	0.116024
H	-4.263773	-1.135122	-0.431928
H	-1.081791	4.386473	-0.266560
H	1.257039	-4.323926	-0.342683
O	0.174206	0.077727	-2.000977
S	-0.029871	-0.377906	2.210114
C	-1.717070	-0.057908	2.807120
H	-2.414815	-0.741276	2.308018
H	-1.755821	-0.254933	3.882505
H	-2.027517	0.968924	2.599579

Iron-Hydroxo Triplet

0 3

Fe	0.057031	0.006037	-0.226647
N	0.974394	-1.797923	-0.242753
N	-1.731268	-0.907687	-0.220318
N	1.856372	0.908100	-0.084704
N	-0.852320	1.799772	-0.277175
C	2.329800	-2.034563	-0.206678
C	-2.960752	-0.301749	-0.339972
C	0.367226	-3.032337	-0.203144
C	-1.968581	-2.262094	-0.209979
C	3.088172	0.302557	-0.085169
C	-2.199602	2.037186	-0.378754
C	2.088668	2.262332	-0.048308
C	-0.244044	3.029094	-0.224220

C	2.580119	-3.454499	-0.182363
C	-3.998864	-1.300172	-0.375981
C	1.366010	-4.071634	-0.175489
C	-3.385332	-2.513778	-0.289586
C	4.126445	1.301639	-0.022854
C	-2.448488	3.458318	-0.407465
C	3.507320	2.514797	0.003547
C	-1.237045	4.072641	-0.307636
H	3.565438	-3.902074	-0.160285
H	-5.055580	-1.082119	-0.462645
H	1.147003	-5.131360	-0.149657
H	-3.833148	-3.499210	-0.293325
H	5.186599	1.083695	-0.008209
H	-3.429966	3.907778	-0.487049
H	3.953478	3.500219	0.041649
H	-1.015958	5.132094	-0.290082
C	3.319890	-1.065283	-0.147197
C	-3.189691	1.064480	-0.417758
C	1.120128	3.254418	-0.104192
C	-1.000845	-3.257576	-0.181502
H	4.351412	-1.401018	-0.128845
H	-4.218904	1.396951	-0.503597
H	1.456901	4.285330	-0.071754
H	-1.340819	-4.287758	-0.163832
O	0.105832	0.052682	-2.029855
S	0.134786	0.070941	2.082629
C	-1.551017	-0.093903	2.771846
H	-1.987130	-1.064516	2.525644
H	-1.465322	-0.001876	3.858606
H	-2.198792	0.701402	2.395289
H	0.411430	-0.826094	-2.320515

Iron-Aqua Doublet

0 2

Fe	-0.061810	-0.012974	-0.108940
N	-1.440696	1.471790	-0.171790
N	1.426825	1.340160	-0.271464
N	-1.567654	-1.350895	-0.149754
N	1.297105	-1.480332	-0.269235
C	-2.811606	1.352528	-0.123321
C	2.780244	1.098135	-0.365256
C	-1.176848	2.822091	-0.121987
C	1.290574	2.709063	-0.215092
C	-2.919623	-1.107179	-0.115452
C	2.663493	-1.361298	-0.376448
C	-1.428734	-2.716964	-0.114451
C	1.036251	-2.828918	-0.228404
C	-3.424222	2.657030	-0.063240
C	3.509577	2.342040	-0.374909
C	-2.411019	3.567883	-0.059073
C	2.586833	3.340253	-0.276853
C	-3.651620	-2.351266	-0.067339
C	3.277292	-2.667368	-0.409065
C	-2.726705	-3.350030	-0.063671
C	2.268486	-3.577279	-0.312873
H	-4.491511	2.834722	-0.025654
H	4.586746	2.423825	-0.447020
H	-2.475562	4.647925	-0.018730
H	2.751516	4.410129	-0.254024
H	-4.731062	-2.429621	-0.039679
H	4.341759	-2.845496	-0.494230
H	-2.888531	-4.420111	-0.034299
H	2.333066	-4.658000	-0.304806
C	-3.508948	0.151165	-0.110512
C	3.362852	-0.161422	-0.429642
C	-0.224180	-3.408337	-0.145828
C	0.086616	3.400029	-0.138759
H	-4.592712	0.199035	-0.073877
H	4.444266	-0.212462	-0.508450
H	-0.271881	-4.492591	-0.120154
H	0.137795	4.483815	-0.100804
O	-0.145349	0.032792	-2.296283
S	-0.085960	-0.034935	2.133451
C	1.638559	0.015887	2.746327
H	2.132588	0.951395	2.472574
H	1.591581	-0.054151	3.837830
H	2.222347	-0.824329	2.363104
H	-0.898807	0.632536	-2.442733
H	0.640921	0.566030	-2.510789

Iron-Hydroxo Doublet Anion

-1 2

Fe	0.064821	-0.001115	-0.221145
N	1.585262	-1.345021	-0.150582
N	-1.305723	-1.489454	-0.267154
N	1.446338	1.486933	-0.159251
N	-1.443693	1.345391	-0.276697
C	2.931596	-1.096136	-0.097124
C	-2.665785	-1.371806	-0.365284
C	1.443391	-2.708095	-0.142425
C	-1.032427	-2.830214	-0.254517
C	2.810444	1.370747	-0.105622
C	-2.786159	1.094913	-0.373573
C	1.172035	2.829343	-0.161717
C	-1.303741	2.706417	-0.270540
C	3.667576	-2.341348	-0.056227
C	-3.278135	-2.683455	-0.407602
C	2.743649	-3.342022	-0.083157
C	-2.263598	-3.589312	-0.336544
C	3.421566	2.682362	-0.074348
C	-3.524068	2.339897	-0.421777
C	2.404506	3.587718	-0.107798
C	-2.603301	3.341178	-0.355152
H	4.747013	-2.419808	-0.011309
H	-4.343201	-2.866275	-0.482376
H	2.907871	-4.412600	-0.065784
H	-2.322694	-4.670947	-0.342212
H	4.488240	2.865889	-0.030976
H	-4.601947	2.417145	-0.496777
H	2.463382	4.669324	-0.098415

H	-2.767940	4.411805	-0.365729
C	3.512974	0.169140	-0.078506
C	-3.365870	-0.169537	-0.418899
C	-0.096751	3.399739	-0.211639
C	0.236567	-3.400673	-0.190315
H	4.596912	0.222512	-0.034853
H	-4.448002	-0.222606	-0.497209
H	-0.150258	4.484860	-0.211157
H	0.290072	-4.485778	-0.183511
O	0.110636	-0.002976	-2.069830
S	0.066238	-0.018863	2.182733
C	-1.665805	0.046371	2.792667
H	-2.255038	-0.791062	2.406404
H	-1.659807	-0.008823	3.886918
H	-2.159557	0.977055	2.495720
H	1.057433	-0.012378	-2.287687

Figure 11B Radical C2 TS

0 2

N	2.035711	-0.920612	1.727039
C	2.372037	-3.391249	1.368746
C	4.189336	0.763761	-0.802561
C	3.379826	-0.147172	0.065864
C	2.436656	0.243184	1.056341
C	2.556205	-2.033040	1.103180
C	3.406556	-1.572232	0.050721
C	4.089040	-2.522830	-0.737597
C	3.912805	-3.875255	-0.469107
C	3.063223	-4.304924	0.571702
H	1.420774	-0.942104	2.525591
H	1.719648	-3.725291	2.170809
H	3.880152	0.715524	-1.856614
H	4.103793	1.805800	-0.482330
H	2.487971	1.165416	1.623048
H	4.742380	-2.200202	-1.543980
H	4.433374	-4.615938	-1.070007
H	2.944094	-5.368648	0.758460
H	5.252058	0.488585	-0.776539
N	-0.479438	2.379289	1.571440
C	-2.034364	-1.179002	-1.412882
O	-1.542500	-2.038164	-2.145616
C	-1.280255	0.095175	-1.026703
C	0.104475	4.583270	0.515677
C	-3.876945	-0.259676	0.007742
C	-4.967803	-1.054993	0.738210
C	-5.430459	-2.063763	-0.328185
C	-4.139614	-2.442450	-1.075697
C	-2.829692	0.381147	0.918333
C	0.258567	-0.047518	-0.992025
C	0.664288	0.984132	0.038824
C	-0.432701	1.004446	1.109015
C	0.124195	3.194242	0.613673
C	0.838169	2.393779	-0.317131
C	1.528179	3.014941	-1.364245
C	1.513452	4.410286	-1.468951
C	0.811586	5.182611	-0.535799
N	-1.615213	0.530045	0.344067
N	-3.278971	-1.263776	-0.891117
O	-3.083078	0.745757	2.069219
H	-1.326120	2.675432	2.041597
H	-1.560198	0.882542	-1.742760
H	-0.454851	5.185472	1.226517
H	-4.335783	0.547580	-0.586220
H	-5.770313	-0.410498	1.103314
H	-4.528169	-1.568296	1.600071
H	-6.135602	-1.585006	-1.017051
H	-5.926492	-2.937394	0.102781
H	-4.297250	-2.639222	-2.140295
H	-3.650451	-3.323245	-0.642657
H	0.700225	0.126688	-1.975135
H	0.523813	-1.062237	-0.677391
H	-0.304464	0.327653	1.959040
H	2.061144	2.419589	-2.100161
H	2.045030	4.895835	-2.282438
H	0.804682	6.265389	-0.629336

Figure 11B Radical C2 Product

0 2

N	2.021897	-0.812981	1.380367
C	3.475741	-2.854607	1.436932
C	3.688043	1.336042	-1.270884
C	3.175283	0.298457	-0.326469
C	2.050322	0.485176	0.678402
C	3.074558	-1.614212	0.958229
C	3.747670	-0.973253	-0.128925
C	4.826988	-1.641481	-0.755068
C	5.221157	-2.889476	-0.278958
C	4.560355	-3.488268	0.807315
H	1.800037	-0.806017	2.367699
H	2.964921	-3.323651	2.273540
H	3.195911	1.301554	-2.254875
H	3.547794	2.349416	-0.880310
H	2.298025	1.295207	1.385644
H	5.347447	-1.180416	-1.590059
H	6.052401	-3.406840	-0.750372
H	4.888869	-4.459622	1.166566
H	4.759246	1.189607	-1.454013
N	-0.628700	1.996562	1.787857
C	-2.056025	-1.345315	-1.463782
O	-1.549091	-2.096623	-2.297401
C	-1.359476	-0.072008	-0.975772
C	-0.605075	4.291176	0.765246
C	-3.879092	-0.678104	0.111844
C	-4.896036	-1.600332	0.798199
C	-5.351679	-2.521613	-0.347142
C	-4.074839	-2.755885	-1.173090
C	-2.829214	-0.074632	1.043769
C	0.172643	-0.127145	-1.018184
C	0.620261	0.830730	0.102279
C	-0.476397	0.673631	1.207300

C	-0.298999	2.930872	0.798768
C	0.441997	2.316146	-0.229516
C	0.840931	3.070035	-1.327861
C	0.535405	4.438275	-1.379740
C	-0.173014	5.038487	-0.336083
N	-1.646763	0.190966	0.444607
N	-3.270546	-1.552544	-0.907423
O	-3.054254	0.163914	2.232917
H	-1.481104	2.132029	2.320891
H	-1.724799	0.766542	-1.587790
H	-1.178719	4.753052	1.564048
H	-4.403600	0.158402	-0.378316
H	-5.713580	-1.039776	1.256362
H	-4.394655	-2.172258	1.586202
H	-6.105989	-2.014621	-0.959471
H	-5.786580	-3.458450	0.010712
H	-4.264819	-2.860542	-2.245344
H	-3.523013	-3.644316	-0.843321
H	0.560456	0.157519	-1.998437
H	0.513263	-1.143496	-0.799963
H	-0.252525	-0.057497	1.984089
H	1.371184	2.609648	-2.155130
H	0.845026	5.027509	-2.237875
H	-0.408703	6.098494	-0.383328

Figure 11B Radical C3 TS

0 2

N	1.839883	-2.633470	1.532976
C	3.492027	-3.344098	-0.234524
C	2.591438	0.876978	2.235670
C	2.155020	-0.351744	1.458445
C	1.502361	-1.434502	2.123310
C	2.814221	-2.424904	0.569462
C	3.089023	-1.035329	0.531812
C	4.111959	-0.570329	-0.298739
C	4.809425	-1.481030	-1.097377
C	4.493161	-2.849822	-1.070929
H	1.437641	-3.529077	1.768168
H	3.259837	-4.404780	-0.199240
H	2.887521	1.689315	1.566225
H	1.787932	1.249816	2.877810
H	0.797672	-1.405069	2.941892
H	4.363939	0.485654	-0.324688
H	5.607927	-1.128216	-1.744005
H	5.044675	-3.539788	-1.703837
H	3.450043	0.634201	2.873558
N	-0.266893	2.391172	1.215343
C	-2.301233	-1.352517	-1.152531
O	-1.956889	-2.434305	-1.631132
C	-1.316991	-0.203124	-0.920506
C	0.810074	4.128833	-0.246056
C	-3.997217	0.208870	-0.184103
C	-5.300985	-0.167547	0.533070
C	-5.890870	-1.259731	-0.376613
C	-4.662769	-2.050947	-0.860146
C	-2.913375	0.796265	0.720554
C	0.143305	-0.637826	-0.680726
C	0.700853	0.474392	0.194302
C	-0.457701	0.955743	1.084086
C	0.555552	2.826334	0.174214
C	1.172925	1.711173	-0.449840
C	2.043836	1.923960	-1.523597
C	2.307594	3.232078	-1.950336
C	1.698620	4.319356	-1.314873
N	-1.653396	0.546363	0.303697
N	-3.573210	-1.064580	-0.794504
O	-3.178219	1.455580	1.729583
H	-1.082752	2.930917	1.478728
H	-1.367966	0.467138	-1.792297
H	0.322051	4.974807	0.230694
H	-4.204427	0.950434	-0.972875
H	-5.960550	0.693035	0.663026
H	-5.067988	-0.567989	1.525538
H	-6.401815	-0.801868	-1.231279
H	-6.612488	-1.897384	0.140825
H	-4.769085	-2.437407	-1.878142
H	-4.429759	-2.898583	-0.204314
H	0.685205	-0.754768	-1.621031
H	0.147450	-1.602195	-0.164722
H	-0.531050	0.489819	2.071215
H	2.503897	1.081234	-2.031654
H	2.981453	3.401257	-2.785645
H	1.905266	5.329701	-1.658309

Figure 11B Radical C3 Product

0 2

N	2.161406	-2.553138	1.589048
C	3.987615	-3.136642	-0.029161
C	2.564915	0.842287	2.098101
C	1.952142	-0.223774	1.158170
C	1.433696	-1.422899	1.939771
C	3.086421	-2.272960	0.598340
C	3.042404	-0.891966	0.306572
C	3.976169	-0.361955	-0.576248
C	4.897998	-1.211365	-1.209054
C	4.890081	-2.584459	-0.942566
H	1.987209	-3.477400	1.955555
H	3.998785	-4.198624	0.199725
H	2.988301	1.675172	1.526966
H	1.812886	1.249474	2.781242
H	0.981400	-1.375383	2.923297
H	4.006007	0.704473	-0.773827
H	5.622632	-0.797338	-1.904159
H	5.605121	-3.234531	-1.440082
H	3.366367	0.393486	2.693216
N	-0.323586	2.244481	1.395226
C	-2.246010	-1.337030	-1.249517
O	-1.880554	-2.349385	-1.848358
C	-1.285549	-0.196774	-0.900482
C	0.460821	4.099452	-0.105727

C	-3.970786	0.064898	-0.103156
C	-5.246928	-0.427214	0.594132
C	-5.822270	-1.437199	-0.414569
C	-4.581698	-2.129516	-1.006346
C	-2.891477	0.596809	0.838490
C	0.169930	-0.632461	-0.702492
C	0.761520	0.398408	0.286776
C	-0.451285	0.808704	1.193984
C	0.377228	2.768431	0.303338
C	1.056117	1.743134	-0.383417
C	1.787406	2.053693	-1.525603
C	1.879403	3.387553	-1.951231
C	1.226549	4.396590	-1.239091
N	-1.628352	0.415473	0.393146
N	-3.519912	-1.123041	-0.850388
O	-3.161443	1.160334	1.902322
H	-1.171656	2.709542	1.700683
H	-1.353797	0.557753	-1.699032
H	-0.068178	4.881749	0.431761
H	-4.219052	0.876393	-0.806624
H	-5.929909	0.392947	0.825132
H	-4.980990	-0.920362	1.535310
H	-6.369630	-0.909692	-1.203969
H	-6.509071	-2.151304	0.047276
H	-4.699387	-2.402852	-2.059150
H	-4.308225	-3.037015	-0.454747
H	0.715499	-0.666167	-1.647182
H	0.190473	-1.633027	-0.261932
H	-0.503294	0.295303	2.154811
H	2.273418	1.271758	-2.100988
H	2.450444	3.631533	-2.842316
H	1.297264	5.427609	-1.575999

Figure 11B Radical C4 TS

0 2

N	1.620635	-4.001210	0.629230
C	2.220096	-3.150934	-1.665412
C	2.447052	-1.289044	3.023908
C	2.137057	-2.168932	1.845743
C	1.707880	-3.480784	1.902941
C	2.012995	-3.042757	-0.280583
C	2.316723	-1.867312	0.453662
C	2.715423	-0.676594	-0.254214
C	3.075616	-0.862760	-1.634217
C	2.780541	-2.039245	-2.316459
H	1.370546	-4.952881	0.405647
H	2.006109	-4.071093	-2.200993
H	3.527632	-1.113459	3.115482
H	1.973948	-0.303156	2.947642
H	1.467843	-4.089735	2.763819
H	3.247593	0.087841	0.305776
H	3.527212	-0.032211	-2.169301
H	3.008859	-2.111203	-3.376812
H	2.110394	-1.752856	3.957095
N	0.663978	1.696845	1.638795
C	-2.436458	-0.261094	-1.592535
O	-2.384917	-0.960078	-2.605491
C	-1.258223	0.596067	-1.124085
C	1.676579	3.913617	1.017803
C	-3.599933	0.641960	0.428299
C	-4.749711	-0.011105	1.207509
C	-5.693186	-0.491863	0.090445
C	-4.745558	-0.964550	-1.025845
C	-2.260251	0.672878	1.165038
C	0.132812	0.067574	-1.530985
C	1.028871	0.596874	-0.427276
C	0.205790	0.554501	0.864929
C	1.290380	2.597295	0.774909
C	1.543028	1.971917	-0.472553
C	2.196773	2.685614	-1.481079
C	2.590307	4.007793	-1.243653
C	2.331049	4.610550	-0.007039
N	-1.184320	0.650036	0.348741
N	-3.529995	-0.166889	-0.802652
O	-2.179521	0.734392	2.394643
H	0.040445	2.030865	2.364086
H	-1.399122	1.611528	-1.525046
H	1.468278	4.390115	1.971855
H	-3.861415	1.682854	0.176904
H	-5.220877	0.685999	1.903698
H	-4.363263	-0.856925	1.786016
H	-6.307268	0.342344	-0.267512
H	-6.368471	-1.286259	0.419016
H	-5.138578	-0.790389	-2.031914
H	-4.503945	-2.031053	-0.941975
H	0.420460	0.414935	-2.524714
H	0.121289	-1.026742	-1.546593
H	0.284900	-0.365873	1.447391
H	2.386169	2.223722	-2.446689
H	3.094306	4.570155	-2.024547
H	2.636453	5.639491	0.164146

Figure 11B Radical C4 Product

0 2

N	2.339850	-3.871873	0.285473
C	3.077094	-2.534350	-1.705250
C	1.876747	-1.511342	3.099210
C	2.065900	-2.205459	1.774932
C	2.066670	-3.585487	1.599105
C	2.554862	-2.696746	-0.403707
C	2.343935	-1.633887	0.498713
C	2.486395	-0.203790	0.034136
C	3.299653	-0.143072	-1.243021
C	3.492699	-1.226772	-2.062895
H	2.473944	-4.798775	-0.091312
H	3.249502	-3.382704	-2.359777
H	0.830039	-1.503755	3.430702
H	2.454888	-2.008916	3.886351
H	1.899658	-4.375727	2.317741
H	2.985331	0.390146	0.814203

H	3.673344	0.829744	-1.545461
H	4.011680	-1.088257	-3.008901
H	2.207308	-0.468982	3.054755
N	0.418714	1.710266	1.767619
C	-2.242272	-0.541080	-1.636418
O	-2.064050	-1.250178	-2.627615
C	-1.165280	0.404467	-1.096929
C	0.989047	4.055466	1.055934
C	-3.617383	0.310075	0.269551
C	-4.774272	-0.410326	0.975202
C	-5.594185	-0.976580	-0.197936
C	-4.533720	-1.398127	-1.230293
C	-2.343792	0.447253	1.103456
C	0.273889	-0.042680	-1.378492
C	1.096526	0.555259	-0.218894
C	0.129640	0.508015	1.003518
C	0.889023	2.677067	0.869209
C	1.308950	2.066162	-0.327968
C	1.815159	2.848950	-1.359884
C	1.918767	4.237845	-1.188042
C	1.512881	4.827289	0.011783
N	-1.208670	0.489864	0.372104
N	-3.397548	-0.511597	-0.934640
O	-2.362333	0.529836	2.334625
H	-0.297051	1.972439	2.436927
H	-1.344590	1.399831	-1.531387
H	0.657930	4.518922	1.981252
H	-3.931051	1.325376	-0.023322
H	-5.344458	0.262901	1.618843
H	-4.374286	-1.216397	1.599465
H	-6.237171	-0.195378	-0.619114
H	-6.234299	-1.812055	0.097488
H	-4.861523	-1.268733	-2.266021
H	-4.224360	-2.442953	-1.106223
H	0.618807	0.295770	-2.356543
H	0.332821	-1.134743	-1.362420
H	0.219781	-0.375793	1.629515
H	2.115236	2.397240	-2.301419
H	2.309495	4.853914	-1.992683
H	1.592068	5.904108	0.137229

Figure 11B Radical C5 TS

0 2

N	-5.566010	0.067828	-0.750328
C	-3.454605	0.700912	-1.990373
C	-4.832501	-3.102094	1.047864
C	-4.862720	-1.840573	0.238460
C	-5.927209	-0.991043	0.067570
C	-4.252694	-0.077585	-1.125277
C	-3.766090	-1.271044	-0.515001
C	-2.448732	-1.672261	-0.752188
C	-1.566897	-0.813989	-1.490162
C	-2.154795	0.306253	-2.202178
H	-6.176279	0.822785	-1.025463
H	-3.867343	1.568247	-2.499427
H	-4.064844	-3.062957	1.832136
H	-5.796425	-3.281852	1.535252
H	-6.929326	-1.051219	0.470160
H	-2.068121	-2.601321	-0.336045
H	-0.719156	-1.296211	-1.977442
H	-1.526915	0.877519	-2.879386
H	-4.605915	-3.979222	0.427063
N	0.370239	2.191987	-0.782233
C	3.033387	-1.588206	0.786701
O	2.865040	-2.775631	1.068131
C	1.886553	-0.574303	0.794455
C	-0.928421	3.435362	0.975946
C	4.450511	0.349733	0.084470
C	5.747855	0.295457	-0.733970
C	6.529909	-0.847469	-0.062876
C	5.448422	-1.877127	0.310084
C	3.250176	0.937567	-0.657262
C	0.495758	-1.170169	0.492859
C	-0.249851	-0.002293	-0.133561
C	0.783946	0.807292	-0.931227
C	-0.479647	2.290720	0.321110
C	-0.896340	0.998166	0.725834
C	-1.777322	0.862332	1.800922
C	-2.236110	2.008060	2.462871
C	-1.813846	3.277280	2.051555
N	2.057237	0.441918	-0.260771
N	4.233375	-1.060095	0.456805
O	3.369234	1.804301	-1.526856
H	1.075567	2.898458	-0.953090
H	1.873819	-0.086820	1.781145
H	-0.594050	4.422834	0.669273
H	4.605929	0.956180	0.991746
H	6.278617	1.249778	-0.724339
H	5.511617	0.050567	-1.775019
H	7.026897	-0.481508	0.842661
H	7.296375	-1.275343	-0.714376
H	5.663680	-2.414495	1.238490
H	5.293505	-2.623200	-0.478554
H	0.015751	-1.549716	1.396973
H	0.606425	-2.008434	-0.205451
H	0.881116	0.552887	-1.991896
H	-2.101273	-0.123659	2.122621
H	-2.918971	1.910454	3.302204
H	-2.171186	4.159557	2.576477

Figure 11B Radical C5 Product

0 2

N	-5.707588	-0.106556	-0.984684
C	-3.514493	0.747008	-1.934977
C	-4.888469	-3.070003	1.101239
C	-4.944779	-1.862661	0.215120
C	-6.064454	-1.160100	-0.159222
C	-4.344925	-0.109478	-1.157341
C	-3.817546	-1.201966	-0.414240
C	-2.448342	-1.453522	-0.410841

C	-1.486476	-0.564979	-1.162549
C	-2.173712	0.531195	-1.950510
H	-6.350730	0.555945	-1.391436
H	-3.952497	1.553633	-2.518845
H	-4.265773	-2.894119	1.988841
H	-5.887756	-3.353622	1.447858
H	-7.101804	-1.324991	0.098605
H	-2.045811	-2.311287	0.120373
H	-0.918361	-1.191505	-1.880610
H	-1.538564	1.179253	-2.547167
H	-4.458452	-3.936931	0.581580
N	0.440190	2.192594	-0.853279
C	2.945619	-1.604629	0.806795
O	2.746688	-2.765072	1.168401
C	1.826344	-0.562040	0.744898
C	-0.594181	3.503371	1.028183
C	4.411405	0.243809	-0.024422
C	5.697867	0.098899	-0.849304
C	6.454800	-1.018436	-0.109762
C	5.349277	-1.989588	0.342068
C	3.223802	0.825641	-0.789041
C	0.434089	-1.139490	0.474653
C	-0.340452	0.004862	-0.222402
C	0.758799	0.783485	-1.023731
C	-0.305836	2.334251	0.323546
C	-0.819854	1.090218	0.732157
C	-1.636557	1.010413	1.853518
C	-1.936942	2.178235	2.571118
C	-1.416667	3.407428	2.157253
N	2.019981	0.369075	-0.376936
N	4.157585	-1.131678	0.440048
O	3.362002	1.657868	-1.688826
H	1.204444	2.833371	-1.036675
H	1.828609	-0.007655	1.695942
H	-0.189497	4.460917	0.711799
H	4.595711	0.901995	0.840492
H	6.254623	1.036435	-0.908040
H	5.443984	-0.208518	-1.869469
H	6.972483	-0.606876	0.764048
H	7.201326	-1.510890	-0.738279
H	5.558649	-2.466591	1.304176
H	5.166973	-2.784081	-0.391378
H	-0.049433	-1.474747	1.393645
H	0.523382	-2.003791	-0.193005
H	0.816040	0.530400	-2.085830
H	-2.038898	0.053708	2.175041
H	-2.571343	2.124434	3.451162
H	-1.647894	4.307559	2.721269

Figure 11B Radical C6 TS

0 2

N	2.477549	-3.282471	-1.302257
C	2.166737	-0.851400	-1.866568
C	4.390644	-3.390378	1.883507
C	3.633059	-3.060107	0.631191
C	3.097775	-3.958546	-0.268890
C	2.591307	-1.922643	-1.088909
C	3.325192	-1.755535	0.125707
C	3.637505	-0.436012	0.549181
C	3.197071	0.636479	-0.186334
C	2.351196	0.475059	-1.356326
H	1.997614	-3.716455	-2.076185
H	1.687045	-1.011808	-2.827452
H	3.892192	-2.992834	2.777141
H	4.486321	-4.473549	2.011726
H	3.113068	-5.039917	-0.252860
H	4.239408	-0.278233	1.440938
H	3.438027	1.646188	0.132858
H	2.387242	1.275975	-2.092673
H	5.403599	-2.967323	1.869482
N	0.455305	1.530548	1.615077
C	-2.854646	-0.328476	-1.434265
O	-2.938866	-0.623425	-2.627473
C	-1.833216	0.682897	-0.907818
C	0.736354	4.028340	1.615968
C	-3.538558	-0.537764	0.961090
C	-4.203914	-1.746818	1.633697
C	-5.293517	-2.146752	0.623219
C	-4.642629	-1.903015	-0.749574
C	-2.089852	-0.284999	1.380758
C	-0.547084	0.796266	-1.752134
C	0.499723	1.208446	-0.730807
C	0.119804	0.546313	0.599983
C	0.611636	2.776056	1.016175
C	0.668703	2.627853	-0.393237
C	0.866592	3.750732	-1.200279
C	0.998397	5.011138	-0.604483
C	0.932013	5.142145	0.787656
N	-1.331592	0.291925	0.422648
N	-3.650307	-0.852311	-0.475225
O	-1.667490	-0.566948	2.504686
H	0.020613	1.432517	2.523769
H	-2.328604	1.663890	-0.846167
H	0.677656	4.139695	2.695229
H	-4.109326	0.377601	1.187919
H	-4.597700	-1.500191	2.621990
H	-3.466595	-2.547704	1.754548
H	-6.170829	-1.500748	0.741411
H	-5.622880	-3.182192	0.743170
H	-5.351856	-1.570319	-1.513249
H	-4.133691	-2.795669	-1.132953
H	-0.660973	1.516232	-2.565777
H	-0.324026	-0.181050	-2.190973
H	0.611758	-0.406465	0.815146
H	0.906104	3.649845	-2.282554
H	1.148160	5.890243	-1.224737
H	1.030097	6.125732	1.239796

Figure 11B Radical C6 Product

0 2

N	3.212186	-3.043001	-0.990506
C	2.002355	-0.922575	-1.536790
C	5.820712	-2.174360	1.511190
C	4.697764	-2.239450	0.516986
C	4.257976	-3.373054	-0.149783
C	2.943116	-1.687385	-0.881253
C	3.880748	-1.166297	0.066564
C	3.852760	0.242500	0.335240
C	2.941450	1.043375	-0.269118
C	1.880453	0.551684	-1.233564
H	2.708484	-3.693159	-1.574506
H	1.367510	-1.365541	-2.297109
H	5.476279	-1.818550	2.490707
H	6.274623	-3.159887	1.657876
H	4.615723	-4.391570	-0.087667
H	4.579720	0.672219	1.021341
H	2.944071	2.108937	-0.061099
H	1.999145	1.117619	-2.177998
H	6.613890	-1.489565	1.184292
N	0.234056	1.384904	1.607731
C	-2.974968	-0.585873	-1.411653
O	-3.080069	-0.861515	-2.607656
C	-1.947857	0.420880	-0.887118
C	0.086470	3.896370	1.535100
C	-3.613374	-0.836475	0.991838
C	-4.245857	-2.067142	1.657341
C	-5.353808	-2.461514	0.664735
C	-4.737469	-2.184752	-0.717943
C	-2.165382	-0.560197	1.395006
C	-0.685152	0.540830	-1.745891
C	0.421688	0.975253	-0.753845
C	0.007659	0.343774	0.615290
C	0.193099	2.625632	0.967619
C	0.336938	2.461398	-0.422371
C	0.390248	3.571826	-1.255276
C	0.287784	4.855761	-0.698078
C	0.134898	5.006629	0.683001
N	-1.417817	0.007188	0.421718
N	-3.748103	-1.130209	-0.446160
O	-1.735033	-0.815426	2.522157
H	-0.245544	1.259048	2.491864
H	-2.445769	1.398608	-0.797920
H	-0.032445	4.021379	2.607840
H	-4.196824	0.064106	1.244584
H	-4.618713	-1.844582	2.659263
H	-3.496011	-2.860900	1.744036
H	-6.235403	-1.828202	0.815147
H	-5.668324	-3.502816	0.772749
H	-5.467592	-1.843948	-1.457965
H	-4.229312	-3.064517	-1.130742
H	-0.812822	1.256302	-2.561407
H	-0.468810	-0.433801	-2.187807
H	0.552111	-0.564787	0.879051
H	0.500144	3.452460	-2.330980
H	0.322016	5.730326	-1.341140
H	0.048921	6.003156	1.108717

Figure 11B Radical C7 TS

0 2

N	-2.892314	0.454058	-1.848977
C	-1.664756	-1.556181	-0.917054
C	-6.416100	0.240288	-0.687096
C	-4.957892	0.094171	-1.006261
C	-4.180383	0.954574	-1.741089
C	-2.810016	-0.723807	-1.148817
C	-4.089200	-0.987566	-0.606192
C	-4.288594	-2.157098	0.159709
C	-3.206635	-3.024440	0.353660
C	-1.953171	-2.766865	-0.203632
H	-2.086921	1.003447	-2.124869
H	-0.893341	-1.602786	-1.684137
H	-6.595894	0.242032	0.395973
H	-6.815600	1.176655	-1.090529
H	-4.444339	1.889337	-2.216999
H	-5.263719	-2.387556	0.579917
H	-3.353924	-3.941201	0.919202
H	-1.158631	-3.497593	-0.083118
H	-7.011613	-0.581723	-1.106241
N	-0.172638	1.747898	-0.744439
C	3.321457	-1.319006	0.793663
O	3.410660	-2.493549	1.153293
C	2.014226	-0.528146	0.893300
C	-1.427957	2.960829	1.072083
C	4.256405	0.787461	-0.176567
C	5.452465	0.920950	-1.129165
C	6.501724	-0.010902	-0.497375
C	5.679816	-1.196780	0.036970
C	2.895953	1.076692	-0.810771
C	0.731562	-1.384358	0.812287
C	-0.277104	-0.419688	0.217891
C	0.491782	0.451433	-0.785599
C	-0.864157	1.837437	0.475521
C	-0.974520	0.553459	1.063036
C	-1.677332	0.400940	2.261425
C	-2.250963	1.524802	2.866136
C	-2.123897	2.788270	2.276763
N	1.868063	0.413577	-0.234477
N	4.355297	-0.607980	0.290270
O	2.752416	1.860843	-1.751761
H	0.389294	2.533510	-1.054504
H	2.026187	0.029442	1.841697
H	-1.327223	3.944636	0.621803
H	4.376808	1.476154	0.675490
H	5.789500	1.955636	-1.220978
H	5.164855	0.569692	-2.125814
H	7.007172	0.498220	0.331084
H	7.267033	-0.330041	-1.209671
H	6.087935	-1.629386	0.955182
H	5.586588	-2.003715	-0.699815
H	0.437285	-1.767581	1.791111

H	0.912609	-2.242642	0.155853
H	0.533996	0.083953	-1.816376
H	-1.773466	-0.579632	2.720230
H	-2.795332	1.416949	3.799954
H	-2.568985	3.654157	2.759705

Figure 11B Radical C7 Product

0 2

N	-2.749404	0.588212	-1.668534
C	-1.565597	-1.344318	-0.448539
C	-6.417170	0.076139	-1.457907
C	-4.918690	0.058967	-1.384589
C	-4.052147	0.974734	-1.932147
C	-2.758327	-0.553932	-0.912675
C	-4.097646	-0.925722	-0.723321
C	-4.424894	-2.085244	0.034263
C	-3.365106	-2.827857	0.596351
C	-2.041640	-2.496403	0.412502
H	-1.936926	1.194460	-1.762016
H	-1.064385	-1.785654	-1.336005
H	-6.874014	0.097266	-0.459625
H	-6.773922	0.956491	-2.003054
H	-4.253869	1.876710	-2.493605
H	-5.457615	-2.378185	0.195308
H	-3.599647	-3.704781	1.196455
H	-1.275981	-3.136302	0.839368
H	-6.813512	-0.811619	-1.968691
N	-0.221474	1.738705	-0.636559
C	3.265009	-1.345483	0.722345
O	3.375754	-2.501592	1.131233
C	1.955479	-0.559142	0.829930
C	-1.122259	2.970459	1.371492
C	4.148882	0.722686	-0.370206
C	5.299978	0.817075	-1.381510
C	6.381296	-0.080969	-0.754566
C	5.591017	-1.243769	-0.129188
C	2.761873	0.995064	-0.949245
C	0.692749	-1.423211	0.815087
C	-0.410198	-0.503686	0.234456
C	0.364911	0.407509	-0.780747
C	-0.742152	1.826195	0.673436
C	-0.914196	0.543540	1.218969
C	-1.487118	0.394305	2.476986
C	-1.874960	1.536094	3.192069
C	-1.688762	2.807414	2.641416
N	1.763706	0.321535	-0.331895
N	4.273137	-0.651105	0.149561
O	2.572698	1.778927	-1.881969
H	0.378404	2.489460	-0.965938
H	1.994204	0.040806	1.751782
H	-0.982075	3.959768	0.944851
H	4.308826	1.446651	0.445510
H	5.626227	1.847740	-1.535312
H	4.970707	0.418476	-2.347076
H	6.920408	0.468277	0.025620
H	7.115785	-0.430237	-1.484844
H	6.040158	-1.627900	0.791395
H	5.473071	-2.086643	-0.820606
H	0.447227	-1.796289	1.810569
H	0.853750	-2.287814	0.162045
H	0.309191	0.082203	-1.823156
H	-1.632271	-0.594540	2.903601
H	-2.318336	1.431485	4.177981
H	-1.986750	3.687377	3.205323

Figure 11D Cation C2 TS

1 1

N	1.501309	-1.347979	1.780037
C	1.512447	-3.761497	1.061592
C	4.287954	0.271535	-0.064632
C	3.196383	-0.595981	0.464102
C	2.200847	-0.213198	1.396802
C	1.941693	-2.427959	1.053326
C	3.001857	-1.978597	0.206975
C	3.645507	-2.903280	-0.649772
C	3.225392	-4.218768	-0.636694
C	2.169474	-4.639827	0.212388
H	0.806079	-1.386188	2.511643
H	0.705626	-4.093279	1.707043
H	4.479147	0.083232	-1.126610
H	4.069154	1.332748	0.072551
H	2.228907	0.648161	2.050799
H	4.455409	-2.582645	-1.297907
H	3.704572	-4.947439	-1.282749
H	1.866686	-5.682568	0.195750
H	5.222711	0.059943	0.472086
N	-0.140728	2.607873	1.308266
C	-2.153191	-0.987562	-1.305574
O	-1.758441	-1.992945	-1.894588
C	-1.231037	0.212866	-1.058207
C	1.109938	4.511145	0.289322
C	-3.868491	0.359024	-0.080314
C	-5.094182	-0.163580	0.681296
C	-5.669498	-1.221125	-0.277595
C	-4.428616	-1.884146	-0.898948
C	-2.760705	0.929862	0.801917
C	0.268358	-0.165997	-0.955231
C	0.772445	0.886741	-0.007661
C	-0.330496	1.203187	1.016424
C	0.755344	3.162176	0.450316
C	1.323677	2.145385	-0.387144
C	2.200913	2.509504	-1.435413
C	2.533155	3.840359	-1.598411
C	1.997368	4.823959	-0.729361
N	-1.522401	0.861332	0.238639
N	-3.404759	-0.826399	-0.827838
O	-2.951750	1.420239	1.910785
H	-0.731847	3.107768	1.956862
H	-1.373910	0.933694	-1.875078
H	0.686293	5.280500	0.926062

H	-4.169516	1.151529	-0.783799
H	-5.798755	0.636247	0.917963
H	-4.771723	-0.620473	1.622696
H	-6.266515	-0.736990	-1.058230
H	-6.309295	-1.946177	0.231333
H	-4.576814	-2.199618	-1.935332
H	-4.090653	-2.755727	-0.326372
H	0.764122	-0.141847	-1.925878
H	0.354804	-1.176941	-0.547304
H	-0.333060	0.632262	1.946815
H	2.603795	1.751569	-2.099368
H	3.204606	4.142205	-2.395050
H	2.278544	5.862536	-0.878243

Figure 11D Cation C2 Product

1 1

N	1.951542	-1.052607	1.314640
C	3.289477	-3.138505	1.097434
C	3.855563	1.499039	-0.695683
C	3.253263	0.310277	-0.032086
C	1.995487	0.313038	0.800080
C	2.967209	-1.784065	0.852851
C	3.799507	-0.956172	0.005730
C	4.978029	-1.510591	-0.590868
C	5.270753	-2.822686	-0.348182
C	4.425384	-3.624314	0.492814
H	1.249585	-1.393810	1.957627
H	2.667717	-3.759710	1.732119
H	3.595585	1.515810	-1.761963
H	3.512257	2.435856	-0.256262
H	2.140954	1.006621	1.642475
H	5.609921	-0.897258	-1.224109
H	6.150728	-3.280008	-0.787126
H	4.703122	-4.661149	0.657945
H	4.947068	1.452533	-0.635366
N	-0.547363	2.039664	1.738912
C	-2.135124	-1.349285	-1.397643
O	-1.639880	-2.177932	-2.161835
C	-1.379458	-0.086422	-0.968517
C	-0.371422	4.277740	0.603476
C	-3.952377	-0.485322	0.086085
C	-5.050285	-1.300084	0.784206
C	-5.526611	-2.256004	-0.323898
C	-4.241751	-2.618995	-1.087857
C	-2.888918	0.091466	1.018151
C	0.148331	-0.243963	-0.980420
C	0.623207	0.722042	0.122290
C	-0.505346	0.688709	1.210097
C	-0.149918	2.905206	0.714133
C	0.558144	2.196241	-0.274011
C	0.995296	2.853726	-1.420334
C	0.772836	4.230135	-1.548259
C	0.106596	4.930086	-0.536809
N	-1.678199	0.268238	0.429766
N	-3.371937	-1.451294	-0.866898
O	-3.106889	0.385451	2.193067
H	-1.377775	2.262593	2.277487
H	-1.681928	0.735331	-1.633339
H	-0.917946	4.818523	1.370274
H	-4.400640	0.358171	-0.463149
H	-5.844392	-0.662356	1.177857
H	-4.615570	-1.855097	1.622223
H	-6.226196	-1.739943	-0.990753
H	-6.032391	-3.140595	0.071087
H	-4.402066	-2.777387	-2.157969
H	-3.756871	-3.515825	-0.684401
H	0.571278	-0.005307	-1.957886
H	0.410389	-1.278995	-0.745058
H	-0.367159	-0.014679	2.035004
H	1.487398	2.312693	-2.223039
H	1.109249	4.750536	-2.439409
H	-0.063710	5.997519	-0.645747

Figure 11D Cation C3 TS

1 1

N	1.502823	-2.495214	1.567613
C	3.068634	-3.503374	-0.146769
C	2.707532	0.904036	2.192691
C	2.222280	-0.346666	1.511318
C	1.341861	-1.280837	2.112585
C	2.542659	-2.472284	0.627468
C	3.039807	-1.150849	0.597189
C	4.144184	-0.859441	-0.211850
C	4.689199	-1.883313	-0.987658
C	4.154196	-3.183201	-0.961960
H	0.944719	-3.308828	1.799336
H	2.662955	-4.509379	-0.111606
H	3.020163	1.657160	1.462723
H	1.939059	1.344219	2.834156
H	0.610398	-1.118461	2.892657
H	4.576110	0.136074	-0.230072
H	5.547870	-1.675543	-1.618789
H	4.600793	-3.956820	-1.578742
H	3.577475	0.671487	2.817738
N	-0.204073	2.508775	1.000737
C	-2.358858	-1.329471	-1.080285
O	-2.016551	-2.455754	-1.439328
C	-1.357661	-0.170491	-0.984121
C	1.219011	4.097056	-0.298961
C	-4.016307	0.346984	-0.250625
C	-5.336727	0.073783	0.483187
C	-5.939725	-1.095504	-0.315749
C	-4.725739	-1.959466	-0.694398
C	-2.920175	0.973751	0.609427
C	0.100312	-0.630703	-0.740406
C	0.644988	0.507298	0.086560
C	-0.487154	1.087385	0.957775
C	0.765579	2.830294	0.100673
C	1.308391	1.640656	-0.482282
C	2.279113	1.735060	-1.503687

C	2.718834	2.986690	-1.896098
C	2.193555	4.151028	-1.286227
N	-1.660614	0.695274	0.174425
N	-3.618441	-0.988527	-0.738477
O	-3.138966	1.674139	1.593820
H	-0.841471	3.160367	1.436087
H	-1.412284	0.414715	-1.912563
H	0.809820	5.000948	0.139923
H	-4.189386	1.020985	-1.104638
H	-5.978187	0.956950	0.510131
H	-5.125756	-0.222552	1.515995
H	-6.429764	-0.720306	-1.220909
H	-6.680648	-1.658886	0.256790
H	-4.830470	-2.458985	-1.661372
H	-4.508813	-2.725696	0.059239
H	0.642069	-0.767069	-1.676528
H	0.085056	-1.586983	-0.213586
H	-0.587057	0.703866	1.973944
H	2.669789	0.837138	-1.970413
H	3.463090	3.083547	-2.679336
H	2.554010	5.122288	-1.612959

Figure 11D Cation C3 Product

1 1

N	2.179513	-2.543992	1.473199
C	4.140154	-3.043660	-0.036436
C	2.470277	0.742183	2.181264
C	1.939014	-0.265376	1.120859
C	1.478722	-1.510343	1.825871
C	3.184610	-2.209827	0.526538
C	3.086601	-0.832676	0.287164
C	4.043078	-0.238789	-0.530320
C	5.020347	-1.052677	-1.118891
C	5.064564	-2.432959	-0.886717
H	2.035935	-3.482754	1.842409
H	4.175552	-4.106343	0.178381
H	2.852917	1.623539	1.660691
H	1.679053	1.060250	2.862449
H	0.678934	-1.602073	2.550422
H	4.047535	0.829844	-0.707406
H	5.765866	-0.598673	-1.764054
H	5.834689	-3.034672	-1.357836
H	3.285869	0.297531	2.757521
N	-0.302737	2.197058	1.410000
C	-2.307586	-1.351369	-1.230663
O	-1.946534	-2.382760	-1.798233
C	-1.329188	-0.217033	-0.904300
C	0.509883	4.042366	-0.090040
C	-4.002037	0.102914	-0.107344
C	-5.299059	-0.345969	0.580704
C	-5.888891	-1.354118	-0.421414
C	-4.661092	-2.090354	-0.984429
C	-2.915527	0.607572	0.839979
C	0.118571	-0.682850	-0.716630
C	0.723236	0.339994	0.275239
C	-0.477606	0.770154	1.195545
C	0.400588	2.712317	0.317260
C	1.049408	1.678814	-0.383868
C	1.772403	1.969987	-1.538036
C	1.887167	3.300735	-1.959017
C	1.267412	4.321815	-1.231271
N	-1.651905	0.404801	0.388939
N	-3.575770	-1.104728	-0.840756
O	-3.161080	1.166434	1.908748
H	-1.129655	2.684035	1.739100
H	-1.388497	0.531353	-1.707864
H	0.005911	4.835266	0.454547
H	-4.216793	0.915690	-0.819594
H	-5.962178	0.495571	0.790865
H	-5.058363	-0.832676	1.531869
H	-6.409834	-0.823867	-1.226330
H	-6.601510	-2.040961	0.041965
H	-4.772877	-2.383446	-2.032107
H	-4.414323	-2.990266	-0.408660
H	0.662022	-0.717100	-1.662036
H	0.112671	-1.697521	-0.305162
H	-0.549477	0.264597	2.161421
H	2.227703	1.178907	-2.125993
H	2.447715	3.535982	-2.858273
H	1.358038	5.351296	-1.566411

Figure 11D Cation C4 TS

1 1

N	0.892592	-4.090827	0.529078
C	1.777601	-3.249487	-1.664431
C	2.018955	-1.670858	3.109006
C	1.638789	-2.416412	1.862048
C	0.977610	-3.642429	1.812839
C	1.505138	-3.178773	-0.305179
C	1.961217	-2.102077	0.513988
C	2.599192	-0.983953	-0.116549
C	2.961887	-1.132875	-1.495952
C	2.532515	-2.212026	-2.250864
H	0.475488	-4.966373	0.243408
H	1.445933	-4.093877	-2.261628
H	3.098008	-1.743778	3.294257
H	1.778683	-0.603335	3.048373
H	0.578811	-4.230334	2.628357
H	3.183952	-0.310370	0.500948
H	3.548987	-0.349503	-1.964127
H	2.780881	-2.270329	-3.305071
H	1.503908	-2.082405	3.981687
N	0.877277	1.634879	1.617970
C	-2.382668	-0.022189	-1.613931
O	-2.369497	-0.762710	-2.596614
C	-1.138988	0.759152	-1.172129
C	2.252593	3.653000	1.067768
C	-3.466295	1.038283	0.374059
C	-4.680223	0.525629	1.160966
C	-5.652649	0.091806	0.049634

C	-4.743264	-0.512439	-1.033525
C	-2.136050	0.951946	1.120530
C	0.194203	0.087720	-1.573359
C	1.106517	0.527238	-0.451602
C	0.278622	0.566843	0.843150
C	1.664338	2.408851	0.802674
C	1.839407	1.771535	-0.461240
C	2.601426	2.395657	-1.466521
C	3.179385	3.627205	-1.203173
C	3.004446	4.240982	0.057713
N	-1.056540	0.847374	0.299980
N	-3.462614	0.187713	-0.832449
O	-2.036173	0.985581	2.344621
H	0.386834	1.992808	2.427448
H	-1.192480	1.768660	-1.603507
H	2.116861	4.142278	2.026787
H	-3.617183	2.091681	0.089283
H	-5.090898	1.291741	1.821788
H	-4.381381	-0.328306	1.777853
H	-6.181823	0.964177	-0.349233
H	-6.401637	-0.622250	0.400857
H	-5.109518	-0.348997	-2.050759
H	-4.594019	-1.590177	-0.898215
H	0.536205	0.414023	-2.555652
H	0.061352	-0.997003	-1.598591
H	0.239111	-0.356026	1.423676
H	2.728410	1.922409	-2.435738
H	3.767317	4.127582	-1.965340
H	3.466323	5.206774	0.241523

Figure 11D Cation C4 Product

1 1

N	2.499813	-3.824961	0.324475
C	3.240414	-2.474241	-1.628323
C	1.887050	-1.440664	3.087033
C	2.117435	-2.110956	1.761675
C	2.179529	-3.516193	1.589501
C	2.690420	-2.646430	-0.383976
C	2.400054	-1.561244	0.508659
C	2.491217	-0.157926	-0.000060
C	3.235531	-0.069695	-1.295293
C	3.540679	-1.145604	-2.069769
H	2.642710	-4.761672	-0.032626
H	3.494956	-3.325280	-2.253717
H	0.883857	-1.646843	3.477791
H	2.604844	-1.809441	3.827986
H	2.026842	-4.290485	2.329839
H	2.978562	0.478424	0.749469
H	3.472110	0.927466	-1.649524
H	4.029522	-1.013981	-3.028695
H	2.003283	-0.356717	3.016504
N	0.418483	1.663886	1.763658
C	-2.251115	-0.616107	-1.626793
O	-2.046003	-1.355735	-2.589684
C	-1.197493	0.376585	-1.121254
C	0.930396	4.033836	1.089736
C	-3.629823	0.262390	0.261565
C	-4.788755	-0.440914	0.980792
C	-5.597000	-1.049603	-0.179118
C	-4.526932	-1.502278	-1.187023
C	-2.355250	0.412965	1.091204
C	0.248118	-0.042681	-1.419201
C	1.057218	0.571821	-0.260453
C	0.109213	0.485756	0.974583
C	0.850327	2.657944	0.877039
C	1.246130	2.082563	-0.345845
C	1.703295	2.894887	-1.380464
C	1.783943	4.278602	-1.180719
C	1.406325	4.833864	0.046531
N	-1.224347	0.485088	0.346354
N	-3.402703	-0.588546	-0.923013
O	-2.352352	0.477456	2.320872
H	-0.273033	1.900120	2.467776
H	-1.408249	1.357324	-1.571951
H	0.619382	4.471833	2.033510
H	-3.938922	1.270974	-0.056546
H	-5.367264	0.250911	1.596478
H	-4.390612	-1.223584	1.635052
H	-6.239261	-0.286367	-0.632418
H	-6.235637	-1.877045	0.140149
H	-4.847910	-1.419442	-2.229189
H	-4.205314	-2.536578	-1.015837
H	0.575917	0.311442	-2.397865
H	0.319473	-1.134482	-1.417442
H	0.200347	-0.412917	1.579446
H	1.973907	2.475251	-2.345928
H	2.132890	4.920296	-1.983649
H	1.470196	5.908690	0.191401

Figure 11D Cation C5 TS

1 1

N	-5.209632	0.262283	-0.586504
C	-3.203395	0.840413	-1.976389
C	-4.627184	-3.106813	0.887129
C	-4.614109	-1.782017	0.187942
C	-5.597134	-0.833208	0.186381
C	-3.976616	0.047186	-1.101810
C	-3.546267	-1.243534	-0.632385
C	-2.301151	-1.707898	-1.016250
C	-1.454746	-0.860671	-1.786322
C	-1.968702	0.359614	-2.342749
H	-5.777610	1.083321	-0.746843
H	-3.585522	1.780169	-2.362403
H	-3.799807	-3.193684	1.602521
H	-5.561637	-3.249195	1.437454
H	-6.561623	-0.834086	0.674360
H	-1.941769	-2.682704	-0.699706
H	-0.577471	-1.302144	-2.248819
H	-1.352023	0.925162	-3.032984
H	-4.526682	-3.936026	0.176185

N	0.212167	2.155357	-0.599177
C	3.064318	-1.597984	0.666610
O	2.941516	-2.816807	0.780964
C	1.864309	-0.652221	0.798628
C	-1.371289	3.180726	1.038707
C	4.373960	0.491170	0.248974
C	5.701164	0.624974	-0.510089
C	6.525615	-0.557286	0.029508
C	5.497739	-1.688511	0.199805
C	3.162285	1.087500	-0.463797
C	0.515217	-1.300054	0.400845
C	-0.245062	-0.095669	-0.107465
C	0.745076	0.829190	-0.832893
C	-0.741248	2.118853	0.373120
C	-1.049099	0.759509	0.704185
C	-1.973371	0.475660	1.734178
C	-2.581684	1.527568	2.395690
C	-2.282206	2.863342	2.037875
N	1.982266	0.503264	-0.116804
N	4.232324	-0.967634	0.425187
O	3.227386	2.015536	-1.264898
H	0.721965	2.979367	-0.886630
H	1.813658	-0.299732	1.838190
H	-1.139534	4.211872	0.793522
H	4.449869	0.981310	1.232721
H	6.171736	1.595531	-0.340323
H	5.519506	0.519766	-1.584766
H	6.963572	-0.299222	1.000007
H	7.340634	-0.842364	-0.640232
H	5.713278	-2.349326	1.043872
H	5.407519	-2.308657	-0.699634
H	0.031034	-1.787954	1.247248
H	0.690544	-2.048660	-0.375847
H	0.887564	0.661779	-1.902258
H	-2.193115	-0.551810	2.003906
H	-3.290257	1.334059	3.193926
H	-2.773446	3.671477	2.572534

Figure 11D Cation C5 Product

1 1

N	-5.647849	-0.163982	-1.064375
C	-3.500934	0.740552	-1.956776
C	-4.894590	-3.074322	1.141437
C	-4.942774	-1.893042	0.225743
C	-6.037991	-1.219164	-0.210976
C	-4.324256	-0.131559	-1.192630
C	-3.798900	-1.219538	-0.384328
C	-2.456582	-1.414697	-0.332673
C	-1.518574	-0.539144	-1.089870
C	-2.160947	0.538712	-1.905149
H	-6.294610	0.473339	-1.515326
H	-3.939724	1.530300	-2.557389
H	-4.317288	-2.850763	2.046276
H	-5.901210	-3.371654	1.446142
H	-7.086674	-1.376641	-0.005002
H	-2.035003	-2.228748	0.249905
H	-1.003861	-1.209824	-1.804330
H	-1.499965	1.188129	-2.468717
H	-4.418714	-3.933438	0.654255
N	0.411151	2.171135	-0.902376
C	2.930070	-1.608562	0.817419
O	2.713867	-2.766109	1.176857
C	1.821497	-0.550925	0.777156
C	-0.570374	3.548170	0.963059
C	4.396394	0.225560	-0.041922
C	5.677309	0.072355	-0.874022
C	6.431205	-1.050119	-0.139169
C	5.322973	-2.015876	0.315540
C	3.204720	0.803108	-0.802065
C	0.421922	-1.128088	0.538595
C	-0.343655	0.013358	-0.170655
C	0.746260	0.759845	-1.015439
C	-0.300573	2.356339	0.289966
C	-0.805694	1.130001	0.756669
C	-1.594022	1.084204	1.900962
C	-1.873019	2.274665	2.585310
C	-1.361803	3.488679	2.114921
N	1.999859	0.370399	-0.353815
N	4.138339	-1.147837	0.431055
O	3.324239	1.606783	-1.726776
H	1.163233	2.810349	-1.137089
H	1.846015	0.006585	1.725035
H	-0.173798	4.493987	0.605835
H	4.585667	0.887280	0.818737
H	6.239544	1.006379	-0.934107
H	5.416362	-0.232292	-1.893098
H	6.955170	-0.643242	0.732794
H	7.171380	-1.545374	-0.772529
H	5.535184	-2.500659	1.272690
H	5.126546	-2.802344	-0.422599
H	-0.048612	-1.432863	1.475099
H	0.499505	-2.011127	-0.104720
H	0.800100	0.467323	-2.067675
H	-1.982723	0.140223	2.275221
H	-2.480487	2.252143	3.484775
H	-1.577357	4.406476	2.655127

Figure 11D Cation C6 TS

1 1

N	1.379894	-3.637013	-1.373907
C	1.821328	-1.235931	-1.944873
C	3.139838	-4.283304	1.837828
C	2.536687	-3.741532	0.576205
C	1.760788	-4.442501	-0.338054
C	1.898664	-2.372763	-1.170144
C	2.642216	-2.421301	0.061929
C	3.320239	-1.254113	0.498758
C	3.220312	-0.104315	-0.246637
C	2.415827	-0.043266	-1.442852
H	0.812567	-3.924355	-2.159092

H	1.316476	-1.239775	-2.905585
H	2.770154	-3.748907	2.721254
H	2.898096	-5.342637	1.963479
H	1.457412	-5.480661	-0.313096
H	3.913588	-1.274587	1.407704
H	3.732973	0.796623	0.074403
H	2.628675	0.743028	-2.160472
H	4.232254	-4.187711	1.833871
N	0.856189	1.366652	1.603421
C	-2.840085	0.402586	-1.391288
O	-3.000248	0.208750	-2.595803
C	-1.621545	1.162492	-0.851927
C	1.912636	3.628959	1.704735
C	-3.479274	0.169408	1.016139
C	-4.358255	-0.921963	1.642260
C	-5.533341	-1.025757	0.653863
C	-4.885486	-0.829530	-0.727306
C	-2.000253	0.091164	1.387074
C	-0.370407	1.043793	-1.755959
C	0.741080	1.168523	-0.732113
C	0.284477	0.518083	0.577509
C	1.381873	2.497805	1.063005
C	1.317859	2.428317	-0.364505
C	1.768525	3.510759	-1.147381
C	2.283517	4.625237	-0.510648
C	2.355020	4.671782	0.903838
N	-1.170401	0.601116	0.437855
N	-3.691223	-0.017702	-0.432439
O	-1.587841	-0.370302	2.447562
H	0.725152	1.182685	2.587708
H	-1.895665	2.219484	-0.727410
H	1.964765	3.685832	2.786908
H	-3.839473	1.164888	1.321077
H	-4.666397	-0.664652	2.657624
H	-3.797401	-1.861530	1.686459
H	-6.257926	-0.226641	0.845105
H	-6.061040	-1.979895	0.726558
H	-5.531074	-0.310172	-1.440897
H	-4.576453	-1.778114	-1.181795
H	-0.336606	1.825350	-2.515943
H	-0.388192	0.075090	-2.254470
H	0.586660	-0.521057	0.734806
H	1.718772	3.463195	-2.231372
H	2.637675	5.470995	-1.090336
H	2.765062	5.558780	1.378192

Figure 11D Cation C6 Product

1 1

N	3.408693	-3.005977	-0.939452
C	2.053440	-0.970920	-1.398005
C	6.033981	-1.979417	1.484378
C	4.882407	-2.082431	0.529516
C	4.474648	-3.245005	-0.154230
C	3.052001	-1.664323	-0.808390
C	3.996354	-1.078262	0.124837
C	3.878330	0.310349	0.440239
C	2.882710	1.037455	-0.125871
C	1.887275	0.481015	-1.098684
H	2.941379	-3.690966	-1.519809
H	1.389910	-1.447578	-2.110866
H	5.697763	-1.661297	2.477523
H	6.538637	-2.942927	1.593274
H	4.911716	-4.234404	-0.106518
H	4.578348	0.769932	1.130242
H	2.785547	2.091581	0.107871
H	2.065656	1.000661	-2.060092
H	6.773451	-1.249310	1.136897
N	0.177992	1.414163	1.598650
C	-2.947730	-0.723520	-1.426272
O	-2.970913	-1.104816	-2.596910
C	-1.961199	0.341614	-0.934745
C	-0.004084	3.919403	1.407065
C	-3.708189	-0.778640	0.953976
C	-4.381505	-1.948959	1.685247
C	-5.431333	-2.432229	0.668820
C	-4.738131	-2.273312	-0.695260
C	-2.278180	-0.480786	1.401304
C	-0.662961	0.405913	-1.748730
C	0.391645	0.900705	-0.731137
C	-0.069004	0.335500	0.653666
C	0.125706	2.624596	0.902021
C	0.291895	2.399057	-0.476163
C	0.347437	3.467312	-1.364956
C	0.220086	4.771137	-0.869504
C	0.044457	4.984904	0.502525
N	-1.491079	0.036762	0.425616
N	-3.769180	-1.189200	-0.461872
O	-1.880476	-0.675783	2.549978
H	-0.295920	1.327302	2.491272
H	-2.470952	1.315998	-0.947957
H	-0.139409	4.094207	2.470280
H	-4.294332	0.142794	1.100847
H	-4.811618	-1.640823	2.640351
H	-3.639679	-2.729683	1.884632
H	-6.320705	-1.793942	0.714074
H	-5.749956	-3.462009	0.848926
H	-5.424521	-2.003515	-1.502847
H	-4.203194	-3.180952	-0.999167
H	-0.750634	1.075766	-2.606406
H	-0.445116	-0.592752	-2.132576
H	0.438414	-0.574915	0.980758
H	0.477162	3.299686	-2.431696
H	0.252632	5.615199	-1.551273
H	-0.058778	5.999543	0.877244

Figure 11D Cation C7 TS

1 1

N	2.280527	-2.430600	-0.931170
C	1.526461	-0.246925	-1.968903
C	5.685665	-1.855176	0.455900

C	4.328822	-1.825683	-0.178965
C	3.425651	-2.851075	-0.256926
C	2.424075	-1.133962	-1.302518
C	3.711355	-0.709713	-0.860570
C	4.146175	0.568985	-1.209667
C	3.345302	1.396359	-2.027616
C	2.092932	0.981654	-2.441052
H	1.502917	-3.033486	-1.163716
H	0.662988	-0.656668	-2.484142
H	5.766952	-1.118077	1.264067
H	5.896967	-2.841173	0.879499
H	3.497545	-3.868199	0.101155
H	5.124753	0.919562	-0.892927
H	3.727998	2.362159	-2.340229
H	1.487444	1.621811	-3.074637
H	6.474117	-1.626574	-0.271407
N	0.457191	-0.677336	1.534374
C	-3.333659	1.031083	-0.999722
O	-3.515206	1.630097	-2.058927
C	-1.992434	1.096934	-0.259325
C	1.807259	0.915391	2.905820
C	-4.038186	-0.481810	0.864416
C	-5.127443	-1.562265	0.819308
C	-6.287508	-0.847164	0.104583
C	-5.596595	0.021019	-0.960840
C	-2.609768	-1.012227	0.954397
C	-0.781985	1.323424	-1.193798
C	0.326495	0.625171	-0.425850
C	-0.279496	-0.597365	0.291387
C	1.153196	0.479215	1.746535
C	1.117987	1.293231	0.572653
C	1.722880	2.567453	0.582827
C	2.355196	3.002700	1.736577
C	2.399206	2.173307	2.878585
N	-1.679922	-0.182304	0.408211
N	-4.263954	0.273090	-0.383489
O	-2.310573	-2.079180	1.484118
H	0.171910	-1.319850	2.260588
H	-2.045275	1.904235	0.484451
H	1.830820	0.300537	3.799432
H	-4.196449	0.176254	1.733695
H	-5.387168	-1.921897	1.816952
H	-4.771336	-2.415537	0.232579
H	-6.830416	-0.211149	0.812316
H	-7.003803	-1.544135	-0.337192
H	-6.111736	0.966069	-1.153748
H	-5.484594	-0.502820	-1.917222
H	-0.582640	2.383334	-1.353907
H	-0.985565	0.861384	-2.163017
H	-0.231335	-1.554047	-0.233335
H	1.682849	3.199503	-0.297894
H	2.820976	3.981943	1.766712
H	2.901917	2.534176	3.771489

Figure 11D Cation C7 Product

1 1

N	2.749700	-0.468795	-1.547095
C	1.592525	1.327498	-0.154347
C	6.406364	0.244425	-1.669374
C	4.924449	0.167590	-1.472298
C	4.060745	-0.757167	-1.974022
C	2.743545	0.614003	-0.780510
C	4.104266	1.068322	-0.678683
C	4.397929	2.116414	0.162444
C	3.363176	2.772813	0.907461
C	2.064278	2.392673	0.793658
H	1.925055	-1.077314	-1.676379
H	1.151343	1.931965	-0.975306
H	6.939175	0.178365	-0.713454
H	6.755324	-0.572298	-2.306646
H	4.239617	-1.619020	-2.600147
H	5.425334	2.447914	0.287924
H	3.635246	3.588748	1.568136
H	1.300348	2.931396	1.343285
H	6.697293	1.190156	-2.141385
N	0.256657	-1.647046	-0.822564
C	-3.257592	1.263236	0.855727
O	-3.353866	2.366216	1.393103
C	-1.965406	0.440536	0.916788
C	1.070996	-3.166938	1.025488
C	-4.130186	-0.641440	-0.509682
C	-5.252719	-0.596298	-1.556262
C	-6.339607	0.238340	-0.855758
C	-5.552727	1.308992	-0.080875
C	-2.730289	-0.856891	-1.078391
C	-0.696574	1.287321	1.054336
C	0.406003	0.437873	0.377242
C	-0.346400	-0.311137	-0.778093
C	0.720655	-1.931091	0.487494
C	0.880510	-0.743772	1.216879
C	1.407970	-0.776876	2.503855
C	1.764632	-2.012301	3.057834
C	1.592613	-3.190423	2.323442
N	-1.741598	-0.293066	-0.337691
N	-4.252686	0.662711	0.169464
O	-2.508360	-1.500115	-2.103882
H	-0.334473	-2.338269	-1.278023
H	-2.046197	-0.265894	1.755708
H	0.941533	-4.083435	0.457590
H	-4.319547	-1.455875	0.208030
H	-5.587558	-1.596251	-1.839229
H	-4.890930	-0.091867	-2.458538
H	-6.904904	-0.389756	-0.158342
H	-7.049968	0.680701	-1.558523
H	-6.023143	1.595817	0.863712
H	-5.398133	2.220285	-0.670389
H	-0.473009	1.509723	2.099212
H	-0.839783	2.237928	0.529832
H	-0.274273	0.160374	-1.762371
H	1.533813	0.136146	3.080211

H	2.169476	-2.055530	4.064145
H	1.866728	-4.143663	2.766266

Figure 12B Radical C2 TS

0 2

N	4.285907	0.772804	-0.045631
C	4.904886	-1.463709	0.939753
C	1.469529	0.110404	-2.380628
C	2.550238	0.084548	-1.350602
C	3.239943	1.226885	-0.829705
C	4.163016	-0.595537	0.144350
C	3.086290	-1.050405	-0.677592
C	2.757418	-2.423324	-0.682793
C	3.500216	-3.291740	0.108649
C	4.561557	-2.818625	0.906902
H	4.837990	1.381602	0.541294
H	5.720551	-1.105536	1.561000
H	0.714476	-0.658991	-2.184188
H	0.975050	1.085893	-2.410189
H	3.338919	2.175989	-1.335927
H	1.917062	-2.782318	-1.269093
H	3.258450	-4.350618	0.119602
H	5.123970	-3.520648	1.516120
H	1.875202	-0.083637	-3.384559
N	1.900103	2.052854	0.488820
C	-3.055961	-0.224053	1.311536
O	-3.636908	0.741877	1.813652
C	-1.672326	-0.696355	1.799011
C	0.794488	3.733603	-1.021766
C	-2.962811	-2.173453	-0.248316
C	-3.668698	-2.312616	-1.602416
C	-5.092964	-1.814363	-1.296583
C	-4.887071	-0.660721	-0.297782
C	-1.446904	-2.022192	-0.316033
C	-0.847828	0.444949	2.458193
C	-0.001896	1.258278	1.520533
C	1.367320	1.151193	1.389046
C	0.807731	2.724924	-0.050634
C	-0.398600	2.294215	0.583206
C	-1.612984	2.910760	0.253512
C	-1.617812	3.910544	-0.722115
C	-0.429857	4.314052	-1.356968
N	-0.915689	-1.334846	0.720086
N	-3.596364	-0.978734	0.333756
O	-0.782020	-2.505692	-1.234822
H	-1.879921	-1.437204	2.587625
H	1.714280	4.064125	-1.497954
H	-3.179875	-3.053384	0.379399
H	-3.639213	-3.337774	-1.977676
H	-3.175517	-1.668264	-2.337771
H	-5.678547	-2.614449	-0.829816
H	-5.628260	-1.489480	-2.192531
H	-5.676873	-0.594657	0.456434
H	-4.816637	0.314138	-0.794203
H	-0.192695	-0.012638	3.207540
H	-1.570835	1.065841	2.996706
H	2.026677	0.485201	1.935393
H	-2.533542	2.614188	0.747398
H	-2.555362	4.390831	-0.990725
H	-0.463113	5.096279	-2.110883
H	0.079974	-1.142087	0.672604

Figure 12B Radical C2 Product

0 2

N	3.844035	1.208031	0.392991
C	5.979825	0.026852	0.966909
C	2.066650	-1.142762	-1.962229
C	3.000126	-0.435724	-1.039688
C	2.768026	0.991404	-0.574977
C	4.750605	0.158412	0.336072
C	4.213103	-0.884897	-0.491898
C	4.940639	-2.091698	-0.628897
C	6.169757	-2.220855	0.011042
C	6.688163	-1.174479	0.794231
H	4.172928	2.153139	0.544434
H	6.381942	0.827225	1.581875
H	1.117781	-1.413151	-1.474894
H	1.803963	-0.516444	-2.826407
H	2.842330	1.695276	-1.417127
H	4.548778	-2.899226	-1.241099
H	6.739514	-3.139437	-0.098750
H	7.652607	-1.294885	1.279722
H	2.512054	-2.067489	-2.342193
N	1.444723	1.226250	0.007224
C	-3.533280	-0.129704	1.363734
O	-3.985056	0.915990	1.839997
C	-2.247140	-0.766567	1.917209
C	0.510642	3.056465	-1.474559
C	-3.702065	-2.090105	-0.187034
C	-4.305053	-2.080432	-1.596318
C	-5.644268	-1.351322	-1.382075
C	-5.332222	-0.274670	-0.324546
C	-2.190230	-2.251469	-0.120179
C	-1.233719	0.305783	2.411996
C	-0.362705	0.908528	1.344848
C	0.925800	0.515953	1.074252
C	0.475985	2.114281	-0.437185
C	-0.676918	1.941487	0.383658
C	-1.807780	2.746514	0.150780
C	-1.771287	3.682244	-0.876068
C	-0.623890	3.833911	-1.681141
N	-1.611115	-1.664085	0.954180
N	-4.142951	-0.800601	0.366916
O	-1.562198	-2.898852	-0.956976
H	-2.562383	-1.338462	2.804027
H	1.387585	3.186355	-2.101654
H	-4.143306	-2.914172	0.397482
H	-4.419285	-3.088082	-2.001271
H	-3.651645	-1.515131	-2.269430
H	-6.393717	-2.050965	-0.995428

H	-6.040334	-0.915881	-2.303065
H	-6.151085	-0.115730	0.383671
H	-5.086018	0.694771	-0.772079
H	-0.592224	-0.171965	3.161121
H	-1.823171	1.067385	2.930569
H	1.543313	-0.213996	1.581086
H	-2.695993	2.624565	0.762416
H	-2.639825	4.307915	-1.064014
H	-0.622314	4.572646	-2.478131
H	-0.598896	-1.721430	0.978165

Figure 12B Radical C3 TS

0 2

N	-1.367504	-2.194245	-1.417445
C	-0.989037	-2.879502	0.973255
C	-4.437493	-0.173647	-1.409041
C	-3.024797	-0.611376	-1.096303
C	-2.266328	-1.386171	-2.056654
C	-1.600025	-2.150108	-0.045200
C	-2.676354	-1.267717	0.194065
C	-3.199069	-1.167409	1.483573
C	-2.610847	-1.907692	2.514168
C	-1.508852	-2.738778	2.262411
H	-0.493810	-2.539001	-1.813588
H	-0.157926	-3.545046	0.763001
H	-4.480924	0.313878	-2.387122
H	-2.268920	-1.295329	-3.133111
H	-4.053648	-0.531918	1.692058
H	-3.011317	-1.837459	3.521220
H	-1.062355	-3.298924	3.079357
H	-5.108143	-1.040940	-1.421154
N	-2.128709	1.056529	-1.067112
C	2.982124	1.195665	-0.255042
O	3.150924	2.296986	0.272868
C	2.426933	1.084905	-1.682423
C	-2.623481	2.069911	1.195555
C	3.209738	-1.303534	-0.236116
C	3.024921	-2.207772	0.987990
C	3.907436	-1.516631	2.044072
C	3.737519	-0.009930	1.763954
C	2.131030	-1.394779	-1.302253
C	1.335834	2.160024	-1.956246
C	0.001701	1.892822	-1.317166
C	-1.008121	1.139953	-1.869889
C	-1.822735	1.775768	0.083028
C	-0.504623	2.323189	-0.033321
C	-0.000810	3.146953	0.986492
C	-0.796395	3.410324	2.098568
C	-2.097520	2.880335	2.199075
N	1.906496	-0.252401	-1.982111
N	3.294394	0.036407	0.359950
O	1.553682	-2.460824	-1.552065
H	3.271986	1.302780	-2.353019
H	-3.639157	1.695538	1.269980
H	4.163484	-1.550864	-0.731696
H	3.317304	-3.240285	0.785432
H	1.972841	-2.200978	1.291750
H	4.954342	-1.809143	1.906416
H	3.621919	-1.776101	3.066655
H	4.663649	0.558148	1.895163
H	2.970837	0.453162	2.394533
H	1.215897	2.220678	-3.045393
H	1.757207	3.114781	-1.630032
H	-1.011410	0.662208	-2.841853
H	1.000340	3.560597	0.908708
H	-0.414439	4.043563	2.895535
H	-2.706362	3.115062	3.068594
H	1.190629	-0.312012	-2.697214
H	-4.806097	0.535473	-0.662920

Figure 12B Radical C3 Product

0 2

N	4.312527	1.164820	-1.750030
C	4.542382	2.792893	0.148514
C	4.272968	-1.869107	-0.314840
C	3.342897	-0.665966	-0.606490
C	3.715606	-0.069375	-1.953026
C	4.183567	1.574510	-0.430173
C	3.604522	0.531754	0.320371
C	3.382529	0.712228	1.680089
C	3.737655	1.929878	2.279454
C	4.311985	2.953330	1.517530
H	4.609874	1.772308	-2.500012
H	4.982995	3.588816	-0.445067
H	4.087569	-2.668154	-1.040586
H	3.992059	-0.661481	-2.817333
H	2.925877	-0.068848	2.279010
H	3.561862	2.078037	3.340732
H	4.581626	3.892306	1.993452
H	5.312712	-1.543372	-0.413251
N	1.909026	-1.103912	-0.600893
C	-3.580380	-0.585581	-0.867267
O	-3.876331	-1.783690	-0.851375
C	-2.487219	-0.012732	-1.790841
C	1.621370	-2.396346	1.585685
C	-3.936443	1.785607	-0.173889
C	-4.518354	2.297934	1.148973
C	-5.732023	1.376386	1.367507
C	-5.263573	0.002504	0.855260
C	-2.448482	2.055463	-0.380635
C	-1.441295	-1.073918	-2.227519
C	-0.248495	-1.251616	-1.328071
C	1.006845	-0.761254	-1.593018
C	1.214377	-1.830056	0.365258
C	-0.141860	-1.947265	-0.071061
C	-1.067940	-2.663125	0.710433
C	-0.650200	-3.231219	1.906279
C	0.682336	-3.091263	2.340230
N	-1.839889	1.149772	-1.184398
N	-4.217062	0.340336	-0.122523

O	-1.874691	3.016219	0.127380
H	-3.019281	0.300436	-2.704074
H	2.635330	-2.304512	1.953866
H	-4.477184	2.238695	-1.021203
H	-4.781510	3.356652	1.098508
H	-3.777790	2.171160	1.945698
H	-6.581887	1.727721	0.771497
H	-6.051070	1.337284	2.412298
H	-6.059219	-0.578240	0.379285
H	-4.830885	-0.613805	1.652177
H	-1.081470	-0.788848	-3.222082
H	-1.993269	-2.011971	-2.343116
H	1.353218	-0.199463	-2.448999
H	-2.096900	-2.755239	0.376850
H	-1.357434	-3.784974	2.518139
H	0.989424	-3.533306	3.284327
H	-0.832258	1.226309	-1.275306
H	4.146923	-2.276845	0.689539

Figure 12B Radical C4 TS

0 2

N	4.667825	-2.445472	0.666480
C	2.510785	-2.607687	-0.629545
C	5.838701	1.059626	0.315739
C	5.151211	-0.272539	0.286677
C	5.574211	-1.438945	0.902173
C	3.640375	-1.957338	-0.113353
C	3.924487	-0.593911	-0.367220
C	2.988180	0.192686	-1.126304
C	1.916536	-0.528038	-1.760699
C	1.657648	-1.861398	-1.464770
H	4.758690	-3.397934	0.988548
H	2.310627	-3.653187	-0.414748
H	5.179257	1.835282	0.723065
H	6.743096	1.025635	0.931393
H	6.459963	-1.622455	1.494680
H	3.350839	1.094784	-1.606459
H	1.248796	0.017521	-2.419827
H	0.776622	-2.340489	-1.881092
H	6.133009	1.385504	-0.690404
N	2.011978	1.289791	0.226097
C	-3.297860	0.201890	1.322863
O	-3.607835	1.293846	1.806634
C	-2.026045	-0.561626	1.742974
C	1.241373	3.154316	-1.283442
C	-3.753772	-1.782222	-0.121037
C	-4.587890	-1.830645	-1.406617
C	-5.836833	-1.010097	-1.036187
C	-5.297520	0.119500	-0.139765
C	-2.251249	-1.965704	-0.315441
C	-0.931699	0.367254	2.337892
C	0.030014	0.956845	1.346365
C	1.332070	0.540058	1.161819
C	1.073311	2.187611	-0.288031
C	-0.165707	2.046320	0.404955
C	-1.226791	2.913528	0.112320
C	-1.053609	3.874225	-0.886909
C	0.163073	3.990345	-1.580817
N	-1.500012	-1.362346	0.635679
N	-4.064230	-0.450390	0.425479
O	-1.787059	-2.618313	-1.250351
H	-2.347662	-1.232525	2.555940
H	2.186663	3.258655	-1.809853
H	-4.096956	-2.561475	0.579417
H	-4.815942	-2.854686	-1.709958
H	-4.030143	-1.353436	-2.219223
H	-6.541412	-1.631858	-0.472312
H	-6.362727	-0.621792	-1.912285
H	-5.987886	0.406794	0.658893
H	-5.052029	1.023147	-0.710022
H	-0.360437	-0.220160	3.064764
H	-1.465976	1.142846	2.895954
H	1.847984	-0.257606	1.684792
H	-2.166054	2.836112	0.651808
H	-1.871703	4.548122	-1.128492
H	0.270089	4.746879	-2.353846
H	-0.494468	-1.363339	0.491029

Figure 12B Radical C4 Product

0 2

N	-5.664623	-1.505061	-1.029016
C	-4.368672	-2.663947	0.790844
C	-4.419887	1.980691	-1.204769
C	-4.727947	0.539967	-0.915334
C	-5.680310	-0.238864	-1.561069
C	-4.712176	-1.572098	-0.033050
C	-4.112972	-0.302844	0.049099
C	-3.031184	-0.018188	1.054972
C	-2.730438	-1.231637	1.912520
C	-3.356860	-2.441867	1.760379
H	-6.267628	-2.263727	-1.311314
H	-4.852887	-3.629634	0.690682
H	-3.409096	2.105693	-1.612315
H	-5.126640	2.395317	-1.930903
H	-6.361902	0.021451	-2.358742
H	-3.345675	0.811811	1.705652
H	-1.956314	-1.103708	2.664113
H	-3.068601	-3.267153	2.407145
H	-4.474801	2.596057	-0.297900
N	-1.789741	0.484416	0.412421
C	3.393620	0.344507	-1.347710
O	3.465095	1.496649	-1.784438
C	2.231320	-0.602238	-1.704169
C	-1.223812	2.477230	1.864067
C	4.332610	-1.601017	-0.094206
C	5.275344	-1.562910	1.114369
C	6.320372	-0.511983	0.698067
C	5.511263	0.544794	-0.076421
C	2.914950	-2.080519	0.201039
C	0.933324	0.153318	-2.095743

C	0.014689	0.537153	-0.967951
C	-1.152935	-0.120099	-0.652716
C	-1.017638	1.556089	0.826795
C	0.124026	1.627022	-0.026285
C	1.056577	2.663538	0.166518
C	0.846140	3.580391	1.189606
C	-0.281156	3.485790	2.031692
N	1.978813	-1.561253	-0.629573
N	4.344965	-0.206656	-0.567627
O	2.663851	-2.878057	1.101978
H	2.565680	-1.141356	-2.605725
H	-2.085993	2.413384	2.521170
H	4.749977	-2.261047	-0.872583
H	5.706895	-2.542765	1.329361
H	4.719080	-1.236283	1.999369
H	7.068926	-0.966963	0.039579
H	6.847681	-0.078715	1.551943
H	6.062741	0.986029	-0.912011
H	5.169527	1.363459	0.567636
H	0.378782	-0.488271	-2.789357
H	1.255473	1.033307	-2.661079
H	-1.609187	-0.973697	-1.136602
H	1.930300	2.733343	-0.473805
H	1.561889	4.383038	1.347257
H	-0.417801	4.212953	2.827751
H	1.012613	-1.785057	-0.416345

Figure 12B Radical C5 TS

0 2

N	2.236957	-2.686931	-0.632466
C	1.662316	-0.537246	-1.806753
C	5.349938	-2.070473	1.316957
C	4.115946	-2.049460	0.466848
C	3.252491	-3.087456	0.228532
C	2.410568	-1.366402	-0.937084
C	3.581404	-0.909011	-0.254254
C	3.937526	0.431557	-0.348215
C	3.039670	1.346157	-1.018425
C	2.022659	0.780644	-1.898485
H	1.350145	-3.163662	-0.785830
H	0.843812	-0.948408	-2.389519
H	5.305035	-1.313997	2.111241
H	5.483653	-3.047084	1.793139
H	3.277292	-4.101529	0.603968
H	4.811525	0.825544	0.162060
H	3.469106	2.294703	-1.325653
H	1.481145	1.452229	-2.555576
H	6.253039	-1.860268	0.728982
N	1.960608	2.109903	0.357242
C	-2.974004	-0.093844	1.145800
O	-3.541887	0.951474	1.467915
C	-1.644284	-0.545738	1.777681
C	0.930305	3.987277	-0.977513
C	-2.883660	-2.268070	-0.080182
C	-3.515865	-2.602079	-1.437524
C	-4.929010	-2.004766	-1.309200
C	-4.724587	-0.710885	-0.499341
C	-1.361511	-2.200277	-0.072351
C	-0.815116	0.622665	2.374895
C	0.046884	1.399294	1.417846
C	1.397278	1.193408	1.220057
C	0.903479	2.914969	-0.080944
C	-0.301627	2.526955	0.574555
C	-1.481075	3.250658	0.341551
C	-1.448412	4.318537	-0.554812
C	-0.257617	4.680861	-1.211021
N	-0.852886	-1.333306	0.826877
N	-3.486179	-0.967808	0.253559
O	-0.680593	-2.901086	-0.831779
H	-1.928352	-1.190209	2.625048
H	1.851388	4.277271	-1.476651
H	-3.183297	-3.022686	0.666032
H	-3.514204	-3.675363	-1.638395
H	-2.951180	-2.106398	-2.234258
H	-5.578810	-2.693502	-0.757736
H	-5.394798	-1.811538	-2.278889
H	-5.550542	-0.493560	0.184413
H	-4.582697	0.166053	-1.141459
H	-0.173164	0.192527	3.152049
H	-1.535604	1.273704	2.879268
H	2.026523	0.448653	1.692590
H	-2.402677	2.968679	0.841261
H	-2.356996	4.883006	-0.749056
H	-0.260697	5.517253	-1.905227
H	0.148515	-1.171179	0.800912

Figure 12B Radical C5 Product

0 2

N	5.506655	-2.301124	-0.650018
C	3.545351	-1.266604	-1.878345
C	6.429878	0.039847	2.085015
C	5.862558	-0.717985	0.923464
C	6.285557	-1.928739	0.435252
C	4.563612	-1.333758	-0.884671
C	4.748456	-0.308469	0.088363
C	3.925819	0.810659	0.093502
C	2.814537	0.958433	-0.916385
C	2.723145	-0.186013	-1.907288
H	5.622609	-3.151216	-1.181692
H	3.430391	-2.069815	-2.602325
H	5.677161	0.207157	2.866920
H	7.266291	-0.501085	2.539509
H	7.090237	-2.567059	0.773611
H	4.047396	1.608546	0.820172
H	2.960071	1.897331	-1.473934
H	1.936779	-0.111247	-2.653080
H	6.797690	1.029614	1.783326
N	1.503990	1.157945	-0.238449
C	-3.558733	-0.109837	1.391811
O	-3.835493	0.941624	1.975884

C	-2.247248	-0.875291	1.651735
C	0.595669	3.201242	-1.421947
C	-4.136018	-1.997886	-0.139140
C	-5.056816	-1.949772	-1.364346
C	-6.273965	-1.162691	-0.845196
C	-5.671872	-0.106857	0.100799
C	-2.654085	-2.185315	-0.447633
C	-1.104437	0.042465	2.163789
C	-0.271165	0.722511	1.112251
C	0.989247	0.321244	0.731795
C	0.558185	2.129579	-0.518074
C	-0.572571	1.891435	0.319406
C	-1.671223	2.768703	0.248509
C	-1.628937	3.834126	-0.642792
C	-0.507461	4.046295	-1.471375
N	-1.827909	-1.628994	0.470768
N	-4.394810	-0.706843	0.519015
O	-2.261537	-2.803357	-1.435163
H	-2.480053	-1.575876	2.470192
H	1.452498	3.374983	-2.066152
H	-4.442412	-2.822146	0.526025
H	-5.308627	-2.948160	-1.728207
H	-4.555490	-1.410372	-2.174982
H	-6.941639	-1.828766	-0.287101
H	-6.856379	-0.706389	-1.649864
H	-6.300724	0.102934	0.971260
H	-5.475340	0.845076	-0.406007
H	-0.443711	-0.573112	2.784064
H	-1.578175	0.772816	2.826931
H	1.589154	-0.497945	1.106271
H	-2.539446	2.602706	0.878637
H	-2.473186	4.515819	-0.705582
H	-0.502968	4.885061	-2.162460
H	-0.836276	-1.655808	0.258488

Figure 12B Radical C6 TS

0 2

N	1.628868	2.371470	0.385167
C	-3.057800	-0.383152	1.292029
O	-3.737536	0.514829	1.793887
C	-1.622581	-0.692437	1.759793
C	0.332875	3.860637	-1.181784
C	-2.761023	-2.328535	-0.245852
C	-3.469395	-2.577941	-1.583383
C	-4.936073	-2.242684	-1.256950
C	-4.846998	-1.048538	-0.289576
C	-1.277190	-2.000168	-0.342929
C	-0.921317	0.532525	2.415086
C	-0.165289	1.417839	1.465689
C	1.205666	1.451723	1.325502
C	0.465431	2.904003	-0.169023
C	-0.678346	2.370905	0.497738
C	-1.957553	2.836098	0.159862
C	-2.081661	3.786109	-0.854961
C	-0.950282	4.288995	-1.522441
N	-0.813341	-1.233708	0.663127
N	-3.519814	-1.205633	0.327785
O	-0.579786	-2.430606	-1.271574
H	-1.728718	-1.460371	2.541819
H	1.205318	4.268784	-1.685649
H	-2.859558	-3.216158	0.400716
H	-3.326397	-3.600416	-1.939099
H	-3.069333	-1.895647	-2.340699
H	-5.413539	-3.093734	-0.758530
H	-5.523112	-2.005611	-2.147886
H	-5.627882	-1.051486	0.476472
H	-4.892440	-0.084966	-0.810284
H	-0.223341	0.150971	3.168011
H	-1.706800	1.077960	2.947712
H	1.941598	0.872288	1.872365
H	-2.834709	2.460448	0.678417
H	-3.068542	4.149615	-1.130270
H	-1.075982	5.029132	-2.308464
H	0.141219	-0.893382	0.590969
N	2.283452	-2.063674	-1.021218
C	2.276500	0.423216	-1.356496
C	5.321341	-2.829177	0.988720
C	4.184181	-2.233125	0.212777
C	3.120222	-2.922849	-0.355244
C	2.766582	-0.773905	-0.864981
C	3.968233	-0.860003	-0.091867
C	4.673715	0.341163	0.210390
C	4.167951	1.544587	-0.201453
C	2.904802	1.638663	-0.916648
H	1.322837	-2.282504	-1.301820
H	1.389518	0.466976	-1.980630
H	5.196008	-3.910690	1.101922
H	6.285879	-2.656927	0.493982
H	2.906609	-3.983242	-0.326546
H	5.612699	0.297331	0.756450
H	4.690834	2.468077	0.027645
H	2.774659	2.511858	-1.546851
H	5.395658	-2.394980	1.993737

Figure 12B Radical C6 Product

0 2

N	1.436848	1.622912	0.112574
C	-3.604476	-0.172117	1.222682
O	-4.097955	0.886551	1.621131
C	-2.255581	-0.702578	1.745995
C	0.459894	3.367009	-1.436960
C	-3.697515	-2.288584	-0.099461
C	-4.442957	-2.532692	-1.416833
C	-5.814839	-1.883871	-1.157035
C	-5.492909	-0.637326	-0.312355
C	-2.175687	-2.273281	-0.205508
C	-1.331034	0.422865	2.284649
C	-0.445533	1.096732	1.272594
C	0.895642	0.834058	1.108268
C	0.426845	2.412550	-0.410078

C	-0.772964	2.115816	0.302999
C	-1.950070	2.817288	-0.019682
C	-1.913237	3.768918	-1.031877
C	-0.720741	4.038381	-1.735338
N	-1.571193	-1.505695	0.733230
N	-4.219617	-0.983465	0.338954
O	-1.567735	-2.916477	-1.058735
H	-2.511187	-1.340614	2.607608
H	1.371383	3.582601	-1.986652
H	-3.971852	-3.064270	0.634448
H	-4.504921	-3.594936	-1.662792
H	-3.915578	-2.026417	-2.232287
H	-6.451545	-2.568739	-0.585669
H	-6.343498	-1.628614	-2.079131
H	-6.257677	-0.411617	0.436791
H	-5.353255	0.259258	-0.927638
H	-0.695921	-0.019308	3.060005
H	-1.988623	1.143410	2.780611
H	1.532551	0.152188	1.656451
H	-2.872099	2.603165	0.511838
H	-2.817433	4.314260	-1.289613
H	-0.722161	4.784083	-2.525947
H	-0.568118	-1.385495	0.639808
N	4.218573	-1.871805	-1.583379
C	2.976331	0.276843	-1.272523
C	6.743454	-2.045623	1.138391
C	5.649742	-1.716506	0.164408
C	5.249077	-2.495512	-0.912561
C	3.921427	-0.670948	-0.956805
C	4.822370	-0.561871	0.153096
C	4.734396	0.597223	0.994207
C	3.815143	1.562243	0.747877
C	2.828369	1.500281	-0.399410
H	3.747171	-2.238856	-2.396416
H	2.305881	0.170741	-2.120004
H	6.366437	-2.104350	2.167401
H	7.206416	-3.008473	0.899794
H	5.628546	-3.450553	-1.248835
H	5.416107	0.701721	1.835383
H	3.746935	2.440518	1.384119
H	2.959564	2.405961	-1.011627
H	7.535235	-1.285673	1.131104

Figure 12B Radical C7 TS

0 2

N	-2.628234	-0.497297	1.886417
C	-3.844699	0.303962	-0.181696
C	-1.497132	-3.974606	1.227141
C	-2.069454	-2.589328	1.243453
C	-1.976295	-1.662915	2.253534
C	-3.143138	-0.642738	0.628298
C	-2.815957	-1.949175	0.186024
C	-3.275365	-2.379946	-1.071805
C	-4.066239	-1.507232	-1.845761
C	-4.383104	-0.230805	-1.405833
H	-2.617827	0.364504	2.414395
H	-4.382883	1.112494	0.299795
H	-0.659403	-4.040840	0.523207
H	-1.121136	-4.254568	2.216604
H	-1.502167	-1.740486	3.222042
H	-3.048219	-3.378542	-1.433994
H	-4.457837	-1.853008	-2.798484
H	-5.008589	0.416078	-2.013023
H	-2.246966	-4.718987	0.931414
N	-2.461876	1.623527	-0.803679
C	3.084488	0.894715	-0.916491
O	3.347774	2.098162	-0.850916
C	1.999625	0.323760	-1.850563
C	-2.217282	2.895311	1.356540
C	3.508165	-1.494246	-0.344652
C	4.132065	-2.061124	0.936776
C	5.323878	-1.118183	1.182846
C	4.807108	0.267435	0.755765
C	2.023053	-1.795283	-0.534278
C	0.950620	1.375452	-2.292540
C	-0.244749	1.572437	-1.401017
C	-1.527179	1.155518	-1.699769
C	-1.744752	2.276043	0.192721
C	-0.358873	2.307834	-0.153470
C	0.540471	3.006610	0.663752
C	0.064016	3.612645	1.828252
C	-1.297171	3.553547	2.175311
N	1.367041	-0.852556	-1.251847
N	3.753313	-0.047396	-0.221174
O	1.499291	-2.810137	-0.077969
H	2.538657	0.019676	-2.762982
H	-3.274923	2.884547	1.609841
H	4.041094	-1.887636	-1.226202
H	4.423352	-3.107441	0.823008
H	3.405132	-1.999420	1.753508
H	6.170831	-1.412135	0.552616
H	5.662838	-1.127101	2.222048
H	5.576956	0.896452	0.299105
H	4.372567	0.826083	1.593241
H	0.589209	1.076258	-3.282398
H	1.503684	2.311553	-2.423163
H	-1.851245	0.582232	-2.561182
H	1.590288	3.070812	0.393925
H	0.755801	4.147051	2.474397
H	-1.641530	4.038742	3.084861
H	0.361500	-0.952577	-1.344759

Figure 12B Radical C7 Product

0 2

N	-2.852943	-0.675510	1.620853
C	-3.219138	1.210708	-0.070840
C	-4.910853	-3.600901	0.644288
C	-4.185744	-2.298677	0.815185
C	-3.298911	-1.972362	1.814342
C	-3.433299	-0.159537	0.497792

C	-4.278641	-1.137875	-0.038404
C	-5.019761	-0.864899	-1.222400
C	-4.868436	0.403072	-1.830887
C	-4.042682	1.380836	-1.327382
H	-2.163471	-0.208317	2.192710
H	-3.524420	1.979235	0.657362
H	-4.678300	-4.072443	-0.319379
H	-4.637501	-4.309005	1.433370
H	-2.942706	-2.557190	2.650663
H	-5.679523	-1.609766	-1.655532
H	-5.430641	0.617392	-2.736967
H	-3.957455	2.343463	-1.823140
H	-6.000275	-3.469381	0.679706
N	-1.786180	1.504046	-0.321203
C	3.524201	0.336283	-1.055599
O	3.949637	1.491988	-1.138358
C	2.304591	-0.153416	-1.860631
C	-1.177034	2.840207	1.739334
C	3.676003	-2.016308	-0.231743
C	4.281470	-2.502391	1.090403
C	5.602406	-1.715662	1.169875
C	5.259779	-0.334894	0.580443
C	2.158813	-2.137288	-0.336187
C	1.343586	0.997734	-2.260946
C	0.276911	1.356260	-1.262260
C	-1.049148	1.008750	-1.379670
C	-0.923864	2.176390	0.529853
C	0.383930	2.113655	-0.036532
C	1.445236	2.756457	0.628005
C	1.191937	3.419766	1.823026
C	-0.104942	3.458178	2.374747
N	1.591697	-1.213855	-1.149741
N	4.112529	-0.611541	-0.298999
O	1.525565	-3.008363	0.256209
H	2.721722	-0.556356	-2.797982
H	-2.172696	2.882196	2.171467
H	4.111639	-2.581208	-1.072375
H	4.419972	-3.585515	1.104761
H	3.613727	-2.235370	1.916358
H	6.368017	-2.204715	0.557073
H	5.989493	-1.640944	2.189401
H	6.081441	0.109138	0.010585
H	4.960381	0.385355	1.350822
H	0.854010	0.706083	-3.196415
H	1.980598	1.858465	-2.487008
H	-1.546984	0.459104	-2.167598
H	2.446722	2.722601	0.210710
H	2.006028	3.917027	2.343788
H	-0.273527	3.981446	3.312112
H	0.577978	-1.206794	-1.186534

Compound **SI-6**

0 1

N	-3.411545	1.506824	-0.600124
C	1.358177	-0.248240	1.359732
O	0.933925	-1.082974	2.164039
C	0.823028	1.195582	1.318693
C	-3.998417	-0.847060	-1.280641
C	2.945599	0.480348	-0.427680
C	3.579456	-0.396553	-1.514122
C	4.050463	-1.629507	-0.721584
C	2.956197	-1.842449	0.341574
C	1.912163	1.485608	-0.923507
C	-0.632012	1.312448	1.846299
C	-1.729816	1.067741	0.847147
C	-2.486681	2.057690	0.261036
C	-3.279619	0.134434	-0.587631
C	-2.224383	-0.183751	0.315383
C	-1.900592	-1.538844	0.522785
C	-2.614339	-2.515452	-0.161952
C	-3.651366	-2.174342	-1.056257
N	0.944798	1.772342	-0.019162
N	2.352438	-0.507877	0.487718
O	1.976136	1.996010	-2.039887
H	-4.090602	2.027075	-1.135132
H	1.458503	1.758574	2.021697
H	-4.798876	-0.579752	-1.965306
H	3.731268	1.048551	0.097580
H	4.387958	0.117843	-2.037783
H	2.817025	-0.669696	-2.251358
H	5.009386	-1.418559	-0.234994
H	4.184679	-2.511838	-1.352667
H	3.348472	-2.193769	1.300695
H	2.187887	-2.552612	0.014878
H	-0.752821	2.323525	2.250832
H	-0.703840	0.619364	2.690162
H	-2.448788	3.128955	0.409946
H	-1.099900	-1.808675	1.204075
H	-2.371032	-3.563439	-0.007429
H	-4.189824	-2.961729	-1.576910
H	0.203031	2.386955	-0.336186

Compound **SI-PC-I**

0 4

H	0.156796	0.114742	0.205381
Fe	-2.998491	-0.235894	0.008038
N	-3.474594	-2.190562	0.184175
N	-2.222544	-0.595080	-1.817988
N	-4.078481	0.149371	1.666905
N	-2.792431	1.742806	-0.306468
C	-4.067139	-2.802783	1.259344
C	-1.642011	0.318113	-2.660525
C	-3.139187	-3.201730	-0.686097
C	-2.059578	-1.817107	-2.418291
C	-4.604047	-0.776450	2.547968
C	-2.123730	2.346625	-1.347260
C	-4.288463	1.381361	2.249504
C	-3.150039	2.755235	0.545957
C	-4.110441	-4.231010	1.063532
C	-1.101164	-0.342825	-3.821983

C	-3.540646	-4.478082	-0.148008
C	-1.363745	-1.671439	-3.672769
C	-5.177734	-0.106419	3.687593
C	-2.067299	3.773025	-1.143658
C	-4.988367	1.228283	3.500794
C	-2.705897	4.027305	0.031916
H	-4.533443	-4.935121	1.768217
H	-0.594507	0.159842	-4.635577
H	-3.395086	-5.427904	-0.645993
H	-1.118095	-2.488763	-4.338308
H	-5.659137	-0.610381	4.515632
H	-1.597885	4.472442	-1.823081
H	-5.278933	2.048319	4.144559
H	-2.871894	4.979182	0.519431
C	-4.582733	-2.148845	2.372985
C	-1.589188	1.690709	-2.445518
C	-3.859081	2.594125	1.732910
C	-2.494582	-3.033127	-1.902144
H	-5.023357	-2.760310	3.153665
H	-1.091841	2.295557	-3.196783
H	-4.081166	3.488188	2.306612
H	-2.298181	-3.923565	-2.490749
O	-1.566668	-0.383353	0.779155
S	-5.413147	-0.140365	-0.931136
C	-5.971245	1.587188	-1.026737
H	-5.310977	2.184750	-1.659531
H	-6.991641	1.605509	-1.420412
H	-5.983127	2.024731	-0.021115
N	1.107021	0.348551	-0.089892
C	6.505686	0.008094	-0.840995
O	6.664471	1.055633	-1.474254
C	5.418407	-1.021853	-1.204157
C	1.388096	2.609570	0.981445
C	7.184461	-1.631286	0.916681
C	7.899187	-1.336052	2.240820
C	9.012132	-0.359621	1.818290
C	8.364261	0.505702	0.721335
C	5.729757	-2.072420	1.049228
C	4.220685	-0.395834	-1.968472
C	3.115686	0.181156	-1.126609
C	1.903657	-0.435347	-0.891361
C	1.786667	1.507429	0.212969
C	3.062705	1.442261	-0.421689
C	3.948204	2.528370	-0.274418
C	3.552314	3.623163	0.485807
C	2.285872	3.663617	1.109403
N	4.963669	-1.752639	-0.022020
N	7.297742	-0.356639	0.187986
O	5.311604	-2.674635	2.035919
H	5.906537	-1.721997	-1.901921
H	0.411769	2.636213	1.457757
H	7.723262	-2.421849	0.368520
H	8.276376	-2.244489	2.715388
H	7.198043	-0.858220	2.933183
H	9.861767	-0.914705	1.404683
H	9.382792	0.244539	2.650529
H	9.060415	0.790638	-0.073253
H	7.921044	1.424830	1.122308
H	3.796240	-1.179573	-2.606032
H	4.649350	0.361091	-2.632839
H	1.536536	-1.383130	-1.264351
H	4.926492	2.500548	-0.744185
H	4.229274	4.465391	0.605162
H	2.007562	4.533431	1.698896
H	3.969441	-1.937277	0.061203

TS from **SI-PC-I** to **SI-R-I**

0 4

H	0.212881	-0.095237	0.260839
Fe	2.755812	0.248505	-0.018954
N	3.073813	2.234834	0.209025
N	1.894495	0.612618	-1.814512
N	3.745924	-0.115029	1.701589
N	2.591814	-1.733687	-0.333383
C	3.705567	2.843470	1.261672
C	1.440768	-0.323620	-2.707577
C	2.632885	3.241688	-0.610806
C	1.613894	1.837898	-2.362039
C	4.277824	0.820746	2.552374
C	2.036436	-2.347116	-1.426516
C	3.930599	-1.332468	2.303013
C	2.932328	-2.736413	0.541210
C	3.673873	4.278390	1.096538
C	0.852443	0.329265	-3.852857
C	3.004603	4.525599	-0.062788
C	0.954884	1.671067	-3.635923
C	4.827519	0.171359	3.719975
C	2.039686	-3.779304	-1.245453
C	4.607783	-1.163546	3.567994
C	2.588500	-4.020393	-0.022055
H	4.107686	4.986413	1.791029
H	0.423745	-0.187245	-4.702229
H	2.776470	5.478977	-0.522069
H	0.632488	2.485499	-4.272199
H	5.309591	0.688136	4.540018
H	1.661069	-4.490757	-1.968216
H	4.874204	-1.973242	4.235320
H	2.758950	-4.971185	0.466712
C	4.273953	2.194235	2.350870
C	1.509632	-1.700771	-2.539342
C	3.542441	-2.559050	1.776030
C	1.942814	3.067812	-1.803464
H	4.735618	2.811822	3.114675
H	1.103629	-2.322119	-3.331271
H	3.754107	-3.447071	2.362995
H	1.659466	3.959674	-2.353184
O	1.258203	0.321697	0.786757
S	4.875395	0.265719	-1.175643
C	5.781432	-1.282407	-0.802588
H	5.235575	-2.161776	-1.154976

H	6.745971	-1.236476	-1.318420
H	5.964774	-1.386762	0.270695
N	-0.886881	-0.475613	-0.161706
C	-6.100032	-0.177158	-0.646909
O	-6.314447	-1.326261	-1.044886
C	-5.164180	0.766650	-1.422137
C	-1.090980	-2.681852	1.016169
C	-6.543099	1.722981	0.922303
C	-6.786999	1.597455	2.431666
C	-7.867430	0.501842	2.500588
C	-7.502421	-0.476694	1.365110
C	-5.227610	2.370521	0.520930
C	-4.015764	-0.019858	-2.110630
C	-2.917520	-0.496881	-1.209869
C	-1.692665	0.198096	-0.975773
C	-1.540376	-1.663124	0.195092
C	-2.812636	-1.706251	-0.446575
C	-3.644998	-2.822720	-0.252236
C	-3.193245	-3.858540	0.575941
C	-1.942584	-3.791203	1.199523
N	-4.631103	1.831615	-0.575473
N	-6.673486	0.336052	0.456742
O	-4.769363	3.330673	1.132889
H	-5.771496	1.197180	-2.233894
H	-0.119183	-2.633828	1.497020
H	-7.342078	2.337331	0.475455
H	-7.098529	2.544054	2.877360
H	-5.864761	1.272752	2.925922
H	-8.854930	0.938959	2.315968
H	-7.900919	0.003236	3.472560
H	-8.377817	-0.870731	0.839929
H	-6.911801	-1.329618	1.716414
H	-3.585814	0.632455	-2.879681
H	-4.486989	-0.864366	-2.620719
H	-1.384139	1.145522	-1.401398
H	-4.623661	-2.864105	-0.717478
H	-3.825404	-4.726403	0.737604
H	-1.616231	-4.606958	1.837732
H	-3.811043	2.330622	-0.902223

Compound **SI-R-I**

0 2

N	-3.049957	1.767668	-0.938990
C	1.226975	-0.379821	1.350606
O	0.668817	-1.205515	2.078688
C	0.891815	1.119025	1.446887
C	-3.937156	-0.528659	-1.404071
C	2.951727	0.232762	-0.356465
C	3.358945	-0.614142	-1.568735
C	3.598159	-1.999161	-0.939197
C	2.528685	-2.114275	0.165686
C	2.191476	1.510604	-0.674993
C	-0.590898	1.344209	1.848498
C	-1.600186	1.142981	0.761433
C	-2.163567	2.189106	-0.058441
C	-3.128193	0.370188	-0.735631
C	-2.247992	-0.055782	0.304737
C	-2.194798	-1.406082	0.671805
C	-3.019767	-2.316515	-0.008681
C	-3.873622	-1.888708	-1.027255
N	1.213738	1.831963	0.211707
N	2.173231	-0.713534	0.453780
O	2.474247	2.204186	-1.647704
H	1.499014	1.511817	2.277799
H	-4.604721	-0.196304	-2.193602
H	3.855768	0.535333	0.197462
H	4.236716	-0.209331	-2.076008
H	2.532376	-0.644972	-2.286978
H	4.599817	-2.040306	-0.497273
H	3.522188	-2.811683	-1.666205
H	2.895304	-2.612983	1.068029
H	1.631644	-2.646631	-0.168840
H	-0.676916	2.370569	2.224488
H	-0.783836	0.667611	2.685956
H	-1.913981	3.244200	0.022986
H	-1.518446	-1.741265	1.451010
H	-2.991264	-3.368044	0.261809
H	-4.502380	-2.611211	-1.539980
H	0.765510	2.726764	0.048899

Compound **SI-PC-II**

0 4

N	2.776823	-2.902193	-1.761432
C	3.906859	0.961732	1.432361
O	4.633907	0.451003	2.290953
C	2.443526	0.527270	1.299373
C	5.195672	-3.602081	-1.883743
C	3.532782	2.648665	-0.386444
C	4.526529	2.916383	-1.524176
C	5.834046	3.192586	-0.755828
C	5.774178	2.258427	0.473776
C	2.245204	1.943000	-0.779774
C	2.316617	-1.020417	1.402508
C	2.805609	-1.800963	0.212847
C	2.021531	-2.199354	-0.846039
C	4.077690	-2.982504	-1.311833
C	4.137548	-2.293111	-0.064876
C	5.370878	-2.238965	0.614233
C	6.482798	-2.854236	0.049027
C	6.397844	-3.529210	-1.187804
N	1.792775	1.009941	0.085140
N	4.348365	1.907141	0.579551
O	1.646077	2.272368	-1.806272
H	2.425542	-3.302117	-2.618368
H	1.925285	0.942518	2.177500
H	5.124965	-4.121352	-2.836012
H	3.229981	3.612421	0.056255
H	4.212553	3.746071	-2.160699
H	4.618321	2.019623	-2.147218
H	5.861786	4.238930	-0.431940

H	6.725581	3.010340	-1.361579
H	6.128291	2.741223	1.390665
H	6.353131	1.338900	0.338467
H	1.254746	-1.238712	1.563192
H	2.848360	-1.315989	2.311714
H	0.967240	-2.023808	-1.015201
H	5.449920	-1.702904	1.554511
H	7.437795	-2.814383	0.566853
H	7.285134	-3.999134	-1.603943
H	0.893260	0.580749	-0.150261
Fe	-2.316764	0.077543	0.009827
N	-2.689465	1.022754	-1.732504
N	-1.744423	1.827448	0.831512
N	-3.213099	-1.571878	-0.723594
N	-2.236046	-0.786790	1.828617
C	-3.116733	0.453929	-2.905415
C	-1.285613	2.026355	2.108761
C	-2.435659	2.342599	-2.025949
C	-1.620169	3.034990	0.195490
C	-3.582502	-1.799716	-2.035568
C	-1.704154	-0.242602	2.975609
C	-3.418860	-2.765692	-0.064402
C	-2.547789	-2.084806	2.140564
C	-3.133248	1.434561	-3.963028
C	-0.861552	3.393505	2.282887
C	-2.719416	2.609584	-3.414474
C	-1.075151	4.022519	1.093386
C	-4.052641	-3.152965	-2.190654
C	-1.690522	-1.222359	4.033637
C	-3.959153	-3.748506	-0.970313
C	-2.217254	-2.366436	3.515590
H	-3.435425	1.233167	-4.982519
H	-0.463360	3.801911	3.202695
H	-2.605304	3.575148	-3.889672
H	-0.886075	5.055037	0.830045
H	-4.406409	-3.574957	-3.122386
H	-1.326074	-1.039019	5.036092
H	-4.216552	-4.762302	-0.692168
H	-2.375327	-3.319809	4.002873
C	-3.516448	-0.869075	-3.057692
C	-1.257470	1.063569	3.111655
C	-3.114664	-3.007715	1.266338
C	-1.956645	3.285979	-1.130506
H	-3.830526	-1.186843	-4.046581
H	-0.867796	1.360747	4.080029
H	-3.316904	-4.001750	1.652079
H	-1.804748	4.294558	-1.500779
O	-0.800301	-0.368618	-0.400787
S	-4.825981	0.623891	0.373337
C	-5.470722	-0.325365	1.783660
H	-4.904321	-0.121263	2.695363
H	-6.524270	-0.067819	1.926835
H	-5.406894	-1.398018	1.563975

TS from **SI-PC-II** to **SI-R-II**

0 4

N	2.868669	-2.928062	-1.953318
C	3.621599	1.017824	1.222748
O	4.489894	0.498841	1.931676
C	2.210243	0.409313	1.085576
C	5.306654	-3.571247	-1.997780
C	2.819526	2.845064	-0.271095
C	3.667652	3.543926	-1.342572
C	4.930516	3.948770	-0.557919
C	5.152893	2.795409	0.443649
C	1.729144	1.905295	-0.779699
C	2.254088	-1.131969	1.238413
C	2.801522	-1.871745	0.045305
C	2.064530	-2.265000	-1.053266
C	4.154826	-2.990954	-1.456348
C	4.150815	-2.328687	-0.193155
C	5.355940	-2.259554	0.533541
C	6.502441	-2.838574	0.000139
C	6.479943	-3.487951	-1.252481
N	1.493387	0.760749	-0.125260
N	3.830952	2.157811	0.537729
O	1.068883	2.258443	-1.782385
H	2.560068	-3.310608	-2.834475
H	1.647495	0.801762	1.955532
H	5.286068	-4.068911	-2.963764
H	2.312756	3.608412	0.343381
H	3.147536	4.391442	-1.793908
H	3.911683	2.830528	-2.137981
H	4.749413	4.884746	-0.017282
H	5.800028	4.102161	-1.202770
H	5.490681	3.143187	1.425589
H	5.880304	2.058147	0.086022
H	1.226526	-1.463619	1.423186
H	2.836817	-1.362043	2.134488
H	1.013110	-2.111086	-1.254293
H	5.385929	-1.734679	1.482404
H	7.436396	-2.786660	0.553833
H	7.393084	-3.928074	-1.644435
H	0.171342	0.046554	-0.396736
Fe	-2.237524	0.002843	0.045795
N	-2.657373	1.046801	-1.626583
N	-1.421310	1.670421	0.862033
N	-3.128449	-1.623699	-0.725794
N	-1.976109	-0.968611	1.791746
C	-3.295802	0.572216	-2.746433
C	-0.975913	1.825300	2.155099
C	-2.286066	2.330392	-1.915959
C	-1.258419	2.888306	0.257870
C	-3.704036	-1.734323	-1.964927
C	-1.416798	-0.473102	2.940514
C	-3.232456	-2.862628	-0.145476
C	-2.221532	-2.299368	2.033969
C	-3.339193	1.593811	-3.763185
C	-0.509555	3.173927	2.361755
C	-2.706249	2.684785	-3.248803

C	-0.680314	3.832687	1.181731
C	-4.186768	-3.076704	-2.172127
C	-1.323915	-1.507698	3.939273
C	-3.888165	-3.779887	-1.043658
C	-1.817547	-2.644832	3.372746
H	-3.790244	1.470445	-4.739083
H	-0.109847	3.549496	3.294635
H	-2.530500	3.646511	-3.712583
H	-0.454076	4.863908	0.944095
H	-4.682330	-3.419791	-3.070894
H	-0.922212	-1.367003	4.934217
H	-4.090240	-4.819559	-0.821373
H	-1.909301	-3.631864	3.806910
C	-3.795906	-0.712533	-2.904407
C	-0.966628	0.833425	3.123150
C	-2.796395	-3.187541	1.134301
C	-1.615953	3.190579	-1.050092
H	-4.277225	-0.946674	-3.848453
H	-0.569300	1.090650	4.099662
H	-2.936725	-4.211640	1.464787
H	-1.398308	4.190028	-1.409585
O	-0.708696	-0.527651	-0.580195
S	-4.346376	0.809579	0.771725
C	-5.039156	-0.304895	2.049446
H	-4.440599	-0.293232	2.963552
H	-6.043096	0.064705	2.281322
H	-5.120011	-1.330381	1.680053

Compound **SI-R-II**

0 2

N	2.644043	-1.781181	-1.140983
C	-1.130295	0.808909	0.799360
O	-0.283326	1.685774	0.916388
C	-0.917929	-0.637102	1.384117
C	4.381714	0.032908	-1.371507
C	-3.322762	-0.099010	0.076513
C	-4.134917	0.324925	-1.157262
C	-4.111774	1.862295	-1.064586
C	-2.709488	2.196369	-0.519161
C	-2.678551	-1.481357	0.004227
C	0.543061	-0.888083	1.793187
C	1.519784	-0.990193	0.652609
C	1.598576	-2.009132	-0.272380
C	3.276346	-0.604311	-0.796553
C	2.590200	-0.074818	0.333420
C	3.043337	1.136104	0.889126
C	4.143521	1.770833	0.324898
C	4.807152	1.225156	-0.794924
N	-1.380538	-1.611196	0.438871
N	-2.316731	0.965127	0.187870
O	-3.303049	-2.444474	-0.439334
H	2.896872	-2.379485	-1.913237
H	-1.556082	-0.647103	2.288131
H	4.889063	-0.388969	-2.235061
H	-3.971670	-0.095328	0.967502
H	-5.142356	-0.095347	-1.147955
H	-3.629067	-0.019938	-2.066013
H	-4.878412	2.205780	-0.361387
H	-4.300826	2.345534	-2.026451
H	-2.706319	3.050561	0.164191
H	-1.984916	2.399219	-1.315784
H	0.547744	-1.813649	2.381404
H	0.843356	-0.084002	2.470554
H	0.978621	-2.886849	-0.379164
H	2.527822	1.576402	1.737441
H	4.498472	2.706920	0.748002
H	5.663427	1.745647	-1.215417

TS from **SI-R-II** to **SI-R-III**

0 2

N	2.054588	-1.702855	-0.920267
C	-1.285375	0.527119	1.430980
O	-0.896443	1.486723	2.105933
C	-0.832201	-0.921629	1.700817
C	3.141042	0.408001	-1.773276
C	-2.587282	-0.472826	-0.440516
C	-3.056809	0.224715	-1.723386
C	-3.609956	1.566608	-1.209244
C	-2.660827	1.949133	-0.060258
C	-1.436582	-1.483161	-0.612862
C	0.584753	-0.934887	2.333706
C	1.508491	-0.972254	1.156546
C	1.423875	-2.059332	0.237002
C	2.496783	-0.389081	-0.832173
C	2.161418	0.089889	0.471328
C	2.474986	1.422340	0.814730
C	3.126193	2.216795	-0.118700
C	3.457796	1.714810	-1.394976
N	-0.745542	-1.775335	0.508010
N	-2.155522	0.651531	0.409468
O	-1.227853	-2.011393	-1.713728
H	2.124856	-2.289303	-1.739226
H	-1.560154	-1.353338	2.407149
H	3.384922	0.033421	-2.762814
H	-3.431780	-0.996424	0.035195
H	-3.796192	-0.368235	-2.266828
H	-2.197804	0.378683	-2.384721
H	-4.627634	1.432125	-0.825003
H	-3.645947	2.336580	-1.984868
H	-3.157964	2.485818	0.753694
H	-1.821869	2.567573	-0.402367
H	0.706991	-1.828549	2.955336
H	0.723044	-0.051847	2.958568
H	1.233769	-3.099462	0.444966
H	2.202206	1.815093	1.789175
H	3.380256	3.242796	0.130272
H	3.965163	2.361605	-2.104951

Compound **SI-R-III**

0 2

N	-1.634781	-1.658743	-0.712899
C	1.506274	1.567482	-0.154578
O	1.289192	2.670708	0.346353
C	0.755073	1.038723	-1.387324
C	-3.304927	-1.425570	1.142572
C	2.677383	-0.633732	-0.275697
C	3.411967	-1.374954	0.849997
C	4.199742	-0.253039	1.549491
C	3.250679	0.956017	1.502868
C	1.368101	-1.288041	-0.726507
C	-0.635159	1.703001	-1.624591
C	-1.597803	0.590322	-1.339798
C	-0.930233	-0.743561	-1.583446
C	-2.516513	-0.960855	0.094344
C	-2.538967	0.420425	-0.299025
C	-3.374652	1.321822	0.393154
C	-4.168361	0.849252	1.434670
C	-4.133360	-0.507518	1.803256
N	0.474856	-0.406728	-1.227093
N	2.439614	0.703610	0.301756
O	1.162150	-2.500586	-0.626376
H	-1.174033	-2.512178	-0.426085
H	1.408610	1.193394	-2.257627
H	-3.272493	-2.467841	1.446986
H	3.329629	-0.547663	-1.159799
H	4.046275	-2.176432	0.465264
H	2.679024	-1.822222	1.529485
H	5.116531	-0.031114	0.991515
H	4.485357	-0.511679	2.572487
H	3.769873	1.914922	1.417145
H	2.598707	1.005172	2.383523
H	-0.696716	2.068473	-2.657054
H	-0.758934	2.559516	-0.957255
H	-0.943585	-1.108738	-2.620713
H	-3.394087	2.371118	0.111483
H	-4.819868	1.533436	1.970662
H	-4.758319	-0.854737	2.621519

TS from **SI-R-III** to **SI-R-IV**

0 2

N	0.265708	0.489845	-1.431330
C	-3.102061	-0.299133	1.399508
O	-3.569103	0.553118	2.155126
C	-1.626946	-0.733673	1.418794
C	-0.303932	2.861026	-2.044520
C	-3.256682	-1.963198	-0.448991
C	-4.309087	-2.047212	-1.563253
C	-5.628170	-1.769166	-0.820289
C	-5.252241	-0.703634	0.222744
C	-1.859650	-1.542618	-0.916885
C	-0.658815	0.290992	2.059553
C	0.237476	0.763580	0.922416
C	0.185109	-0.276263	-0.201179
C	-0.049512	1.820228	-1.152825
C	-0.055024	2.034553	0.246374
C	-0.303496	3.312377	0.751533
C	-0.553996	4.364950	-0.137298
C	-0.554612	4.135698	-1.518381
N	-1.135600	-0.922788	0.040417
N	-3.829957	-0.971780	0.481196
O	-1.458994	-1.748919	-2.066965
H	-0.111076	0.036184	-2.256286
H	-1.583391	-1.690948	1.959163
H	-0.314333	2.688517	-3.117350
H	-3.161243	-2.938052	0.056518
H	-4.292303	-3.014701	-2.069735
H	-4.108421	-1.272667	-2.310731
H	-5.976438	-2.678506	-0.317294
H	-6.425347	-1.429515	-1.486781
H	-5.828344	-0.778003	1.149628
H	-5.371031	0.315547	-0.165134
H	-0.094538	-0.195297	2.859205
H	-1.231016	1.109055	2.503659
H	0.967053	-1.041636	-0.163663
H	-0.316232	3.486458	1.825023
H	-0.753941	5.361395	0.246319
H	-0.756964	4.958333	-2.199461
N	4.612971	0.341156	-1.222571
C	3.001693	1.230941	0.487554
C	5.364913	-3.165980	-0.245745
C	4.885589	-1.753666	-0.409610
C	5.248712	-0.871348	-1.406146
C	3.807945	0.267939	-0.101945
C	3.969451	-1.046907	0.435380
C	3.288990	-1.369186	1.637875
C	2.470190	-0.435282	2.228870
C	2.195451	0.850824	1.614223
H	4.686095	1.135361	-1.840357
H	2.917798	2.229792	0.070476
H	4.533512	-3.882529	-0.266057
H	6.059179	-3.441529	-1.046287
H	5.921990	-1.016140	-2.240212
H	3.444542	-2.336684	2.109677
H	1.995766	-0.670620	3.177130
H	1.897289	1.653397	2.287298
H	5.886538	-3.310882	0.709442

Compound **SI-R-IV**

0 2

N	0.098901	1.051300	-1.574953
C	-3.065573	-0.584440	1.445621
O	-3.536363	-0.054982	2.452857
C	-1.558598	-0.638766	1.176721
C	-0.102977	3.550690	-1.712833
C	-3.278238	-1.784768	-0.736549
C	-4.466217	-1.720217	-1.707018
C	-5.677065	-1.903360	-0.774946
C	-5.288394	-1.140623	0.504459
C	-2.005637	-1.099597	-1.230571
C	-0.767619	0.515645	1.809384

C	0.387181	0.857149	0.812919
C	0.063664	0.071998	-0.505960
C	0.068491	2.337354	-1.041991
C	0.303493	2.303019	0.343569
C	0.386173	3.484933	1.068556
C	0.226188	4.711746	0.406382
C	-0.020450	4.734052	-0.969459
N	-1.268575	-0.515932	-0.258831
N	-3.816917	-1.169769	0.487644
O	-1.689917	-1.100503	-2.424007
H	-0.416806	0.815927	-2.414236
H	-1.184677	-1.605931	1.548713
H	-0.293906	3.575357	-2.782212
H	-3.016797	-2.837888	-0.540819
H	-4.398846	-2.480233	-2.488047
H	-4.489185	-0.737588	-2.190666
H	-5.819775	-2.966234	-0.549416
H	-6.606690	-1.527118	-1.209823
H	-5.671148	-1.604733	1.418309
H	-5.631258	-0.099353	0.489796
H	-0.401506	0.248634	2.803109
H	-1.427869	1.376228	1.933279
H	0.770914	-0.739261	-0.706337
H	0.561846	3.463945	2.141964
H	0.287716	5.641520	0.964383
H	-0.152437	5.686520	-1.476646
N	4.827437	-0.008359	-0.944487
C	2.918302	0.852849	0.423305
C	5.141064	-3.633303	-0.185239
C	4.788338	-2.179008	-0.302936
C	5.424120	-1.244193	-1.105212
C	3.781910	-0.114483	-0.040617
C	3.749720	-1.484223	0.376989
C	2.773378	-1.867126	1.354234
C	1.887564	-0.960743	1.840349
C	1.818897	0.484585	1.389363
H	5.088543	0.832082	-1.437509
H	2.986814	1.882100	0.085806
H	4.306991	-4.280063	-0.486891
H	5.998766	-3.882851	-0.818355
H	6.260925	-1.369627	-1.778436
H	2.758423	-2.890319	1.724470
H	1.185055	-1.272397	2.608673
H	1.903544	1.126221	2.287369
H	5.399407	-3.906765	0.846009

Compound **SI-PDT$_{c-c}$**

0 1

N	-0.438727	0.477825	-1.938170
C	-2.844336	-0.568978	1.584112
O	-2.782404	0.067747	2.635303
C	-1.645382	-1.304830	0.960532
C	-0.928155	2.910736	-1.510061
C	-4.022475	-1.469358	-0.415412
C	-5.326405	-0.976539	-1.058309
C	-6.223145	-0.671484	0.155027
C	-5.254692	-0.091494	1.198913
C	-2.761785	-1.211069	-1.247230
C	-0.263357	-0.831207	1.436049
C	0.401925	-0.099049	0.235790
C	-0.331410	-0.655094	-1.037150
C	-0.494395	1.635187	-1.148104
C	-0.004895	1.371142	0.141423
C	0.051025	2.386785	1.087698
C	-0.380719	3.675178	0.738967
C	-0.862095	3.926691	-0.549036
N	-1.637367	-1.110858	-0.500239
N	-3.974078	-0.728873	0.860368
O	-2.792362	-1.090933	-2.475260
H	-1.142084	0.360033	-2.661409
H	-1.778140	-2.372384	1.190065
H	-1.313205	3.108633	-2.506587
H	-4.081035	-2.551904	-0.217190
H	-5.753592	-1.717960	-1.737065
H	-5.124951	-0.068661	-1.636075
H	-6.672689	-1.596175	0.534499
H	-7.034364	0.021582	-0.082760
H	-5.534285	-0.323943	2.230508
H	-5.159411	0.998039	1.113778
H	0.339814	-1.687996	1.741830
H	-0.369848	-0.174859	2.302573
H	0.180151	-1.489385	-1.522536
H	0.420133	2.188004	2.090967
H	-0.346015	4.474885	1.472992
H	-1.200853	4.925766	-0.811058
N	5.287597	1.266488	0.116899
C	2.829704	0.721944	0.179606
C	7.093687	-1.977626	-0.077088
C	6.132317	-0.829120	0.003164
C	6.442632	0.508538	0.044949
C	4.196669	0.425539	0.121799
C	4.693061	-0.904573	0.051214
C	3.760983	-1.957778	0.039219
C	2.405941	-1.666100	0.100428
C	1.919985	-0.333098	0.174107
H	2.490303	1.750850	0.225345
H	6.929921	-2.583607	-0.977961
H	8.129501	-1.623207	-0.100683
H	7.410997	0.990461	0.029169
H	4.093022	-2.991383	-0.018608
H	1.696742	-2.490085	0.088676
H	6.994076	-2.653529	0.782519
H	5.253870	2.274163	0.153016

Compound **SI-C-III**

1 1

N	-1.653726	-1.554632	-0.457652
C	1.744958	1.562715	-0.100231
O	1.638618	2.676386	0.408882
C	0.802434	1.074953	-1.212377

C	-3.770019	-1.468938	0.842437
C	2.770709	-0.708030	-0.344519
C	3.588057	-1.483869	0.699652
C	4.519506	-0.404333	1.277999
C	3.645765	0.859707	1.328363
C	1.394802	-1.301192	-0.645228
C	-0.572421	1.806822	-1.245228
C	-1.536262	0.702769	-0.979658
C	-0.911778	-0.627608	-1.292280
C	-2.720259	-0.934950	0.063988
C	-2.655577	0.500486	-0.219783
C	-3.621385	1.386893	0.361522
C	-4.615169	0.844769	1.123256
C	-4.683339	-0.574383	1.351158
N	0.473922	-0.352342	-0.976457
N	2.674684	0.646096	0.239742
O	1.132005	-2.496908	-0.591291
H	-1.505145	-2.556142	-0.493200
H	1.316747	1.184702	-2.175732
H	-3.837361	-2.532144	1.042767
H	3.320315	-0.665772	-1.298334
H	4.122081	-2.325160	0.253641
H	2.917386	-1.877840	1.470523
H	5.371984	-0.244943	0.608806
H	4.910962	-0.670994	2.262627
H	4.205211	1.783673	1.159792
H	3.109848	0.956902	2.279703
H	-0.748162	2.278716	-2.218935
H	-0.609577	2.590263	-0.483680
H	-1.050071	-0.923941	-2.345653
H	-3.562730	2.452737	0.170325
H	-5.375267	1.477656	1.567687
H	-5.495508	-0.952256	1.965084

TS from **SI-C-III** to **SI-C-IV**

1 1

N	0.282788	0.644691	-1.446866
C	-3.035039	-0.389201	1.421128
O	-3.531108	0.407198	2.215769
C	-1.531379	-0.715268	1.398055
C	-0.269550	3.011137	-2.043863
C	-3.112645	-1.999073	-0.483448
C	-4.183456	-2.123295	-1.577146
C	-5.499021	-1.963915	-0.793860
C	-5.175577	-0.904735	0.271996
C	-1.759754	-1.474374	-0.968661
C	-0.636728	0.371172	2.049927
C	0.190495	0.889011	0.886202
C	0.220127	-0.147416	-0.237137
C	-0.018186	1.949740	-1.162944
C	-0.057927	2.147597	0.250339
C	-0.353364	3.418641	0.782611
C	-0.596875	4.464374	-0.090186
C	-0.552690	4.252805	-1.489209
N	-1.066862	-0.816354	-0.001759
N	-3.729250	-1.076520	0.490697
O	-1.346541	-1.626115	-2.116799
H	0.063298	0.197034	-2.328912
H	-1.390797	-1.677693	1.908673
H	-0.249759	2.864305	-3.118668
H	-2.936877	-2.979302	-0.011989
H	-4.109473	-3.071746	-2.112988
H	-4.058485	-1.313680	-2.303678
H	-5.768343	-2.910457	-0.312289
H	-6.333961	-1.662946	-1.431453
H	-5.719284	-1.047853	1.209713
H	-5.373795	0.114107	-0.081442
H	-0.037598	-0.066421	2.846452
H	-1.260423	1.155482	2.483610
H	1.042700	-0.869174	-0.197649
H	-0.386353	3.569928	1.857523
H	-0.827775	5.452743	0.292730
H	-0.754449	5.089075	-2.152370
N	4.420825	0.137988	-1.342505
C	2.951644	1.204971	0.387142
C	5.123178	-3.304831	-0.128381
C	4.678623	-1.892112	-0.363693
C	4.999878	-1.093182	-1.454821
C	3.701266	0.187841	-0.163676
C	3.855940	-1.090782	0.472363
C	3.234678	-1.307586	1.730636
C	2.494841	-0.296450	2.296499
C	2.275395	0.950977	1.616826
H	4.509435	0.887728	-2.014137
H	2.853375	2.168753	-0.102255
H	4.268135	-3.987492	-0.054004
H	5.760536	-3.656043	-0.944905
H	5.616076	-1.332193	-2.311271
H	3.370866	-2.250598	2.251348
H	2.063810	-0.436985	3.282400
H	1.971117	1.806099	2.212811
H	5.693454	-3.396254	0.803823

Compound **SI-C-IV**

1 1

N	0.168642	0.394571	-1.466474
C	-3.072888	-0.431485	1.424746
O	-3.381382	0.357176	2.316885
C	-1.668132	-1.048162	1.294805
C	-0.641526	2.772177	-1.691039
C	-3.515386	-1.785976	-0.618621
C	-4.618686	-1.589365	-1.668184
C	-5.857771	-1.263766	-0.815443
C	-5.306373	-0.403603	0.333660
C	-2.101522	-1.468799	-1.111697
C	-0.555606	-0.271073	2.021804
C	0.352193	0.311056	0.910478
C	0.094140	-0.550155	-0.364885
C	-0.231841	1.646064	-0.976878
C	-0.112376	1.676774	0.422680

C	-0.388286	2.842772	1.128523
C	-0.798885	3.981136	0.423350
C	-0.923516	3.937355	-0.969907
N	-1.259926	-1.080984	-0.119984
N	-3.917616	-0.872197	0.469045
O	-1.773660	-1.547210	-2.296960
H	-0.245371	0.055398	-2.330422
H	-1.730707	-2.073238	1.686633
H	-0.742231	2.744607	-2.772042
H	-3.518144	-2.826036	-0.254411
H	-4.745298	-2.472641	-2.297613
H	-4.356684	-0.747306	-2.317050
H	-6.294573	-2.186115	-0.416554
H	-6.634128	-0.743444	-1.382000
H	-5.844700	-0.536664	1.276164
H	-5.311186	0.665698	0.090407
H	-0.017079	-0.941926	2.691280
H	-0.997211	0.517358	2.634675
H	0.800398	-1.372166	-0.512287
H	-0.302018	2.873679	2.211940
H	-1.028041	4.896268	0.960380
H	-1.250461	4.823887	-1.506250
N	4.779457	0.844622	-1.151920
C	2.714170	0.992737	0.227382
C	6.429390	-2.348788	-0.210321
C	5.543922	-1.148574	-0.366203
C	5.758958	-0.070808	-1.249783
C	3.862599	0.415356	-0.193826
C	4.352643	-0.851884	0.303651
C	3.599154	-1.529113	1.315608
C	2.451074	-0.974347	1.775609
C	1.902901	0.336331	1.294319
H	4.719801	1.701220	-1.687705
H	2.371589	1.940826	-0.173234
H	5.915727	-3.264608	-0.524454
H	7.334612	-2.248246	-0.814988
H	6.578373	0.069944	-1.943049
H	3.956770	-2.473638	1.712877
H	1.905312	-1.482826	2.561932
H	1.937171	1.026408	2.159582
H	6.734403	-2.483403	0.833155

Figure S23B Radical C2 TS

0 2

N	2.714778	-0.758670	1.803598
C	3.944439	-2.701281	0.772631
C	3.440973	2.172721	-0.375352
C	3.276231	0.843215	0.290893
C	2.468096	0.569027	1.427761
C	3.507543	-1.378260	0.861669
C	3.875989	-0.388977	-0.102480
C	4.717248	-0.762373	-1.171968
C	5.159781	-2.077524	-1.256967
C	4.776917	-3.036769	-0.296497
H	2.315984	-1.212909	2.610401
H	3.652981	-3.442190	1.512097
H	2.896273	2.223553	-1.327301
H	3.068620	2.984899	0.255797
H	2.249127	1.288281	2.208969
H	5.012467	-0.030086	-1.918835
H	5.808033	-2.375661	-2.076517
H	5.137357	-4.057695	-0.388453
H	4.497292	2.372197	-0.597641
N	0.237898	0.592625	-1.530339
C	-2.907903	-0.400917	1.474694
O	-3.284239	0.382243	2.346842
C	-1.451716	-0.875370	1.333131
C	-0.345976	3.014071	-1.872188
C	-3.263977	-1.865202	-0.510805
C	-4.400168	-1.801877	-1.540997
C	-5.648013	-1.567559	-0.671164
C	-5.156194	-0.628298	0.442965
C	-1.891573	-1.441454	-1.044418
C	-0.402941	0.059412	1.987616
C	0.384180	0.643635	0.827352
C	0.236410	-0.285853	-0.376624
C	-0.035763	1.893012	-1.105712
C	0.073350	1.972228	0.306369
C	-0.120897	3.199507	0.947371
C	-0.423074	4.332120	0.182392
C	-0.534593	4.235436	-1.210224
N	-1.073428	-0.942483	-0.091731
N	-3.727211	-0.956552	0.555517
O	-1.588171	-1.541287	-2.237306
H	-0.199164	0.223267	-2.367341
H	-1.399270	-1.880670	1.776458
H	-0.444551	2.943542	-2.952049
H	-3.169362	-2.888904	-0.113658
H	-4.456364	-2.710294	-2.144656
H	-4.229093	-0.958139	-2.217519
H	-5.989578	-2.514767	-0.238440
H	-6.480858	-1.137123	-1.233309
H	-5.660140	-0.786924	1.400823
H	-5.271793	0.428904	0.174379
H	0.220693	-0.525185	2.672244
H	-0.909953	0.826679	2.577619
H	1.003690	-1.060712	-0.475237
H	-0.051309	3.271986	2.030270
H	-0.578874	5.289279	0.671972
H	-0.777407	5.120568	-1.792375

Figure S23B Radical C2 Product

0 2

N	1.989245	-1.239008	1.313234
C	3.473386	-3.169335	0.716716
C	3.540872	1.671307	-0.564656
C	3.104180	0.371460	0.027350
C	2.010592	0.216728	1.068173
C	3.051171	-1.848357	0.654952
C	3.701829	-0.886102	-0.182984

C	4.780775	-1.309937	-0.996541
C	5.196149	-2.637831	-0.938317
C	4.557580	-3.557643	-0.089115
H	1.767606	-1.556833	2.248179
H	2.978469	-3.884855	1.367961
H	2.857418	2.025325	-1.348168
H	3.585354	2.465202	0.191765
H	2.289873	0.757330	1.991105
H	5.285297	-0.603088	-1.649460
H	6.027721	-2.967990	-1.555100
H	4.902858	-4.587232	-0.054931
H	4.535298	1.576800	-1.014210
N	0.054983	1.282895	-1.599473
C	-2.825086	-0.758997	1.480920
O	-3.163962	-0.402773	2.610191
C	-1.360601	-0.775411	1.035390
C	-0.075611	3.778144	-1.343442
C	-3.319260	-1.578969	-0.829262
C	-4.605521	-1.332591	-1.630673
C	-5.709313	-1.657777	-0.608692
C	-5.154541	-1.133735	0.728457
C	-2.085615	-0.844045	-1.348495
C	-0.482044	0.268094	1.739982
C	0.580212	0.729453	0.687629
C	0.091414	0.154869	-0.687664
C	0.123273	2.475322	-0.881381
C	0.510267	2.230003	0.447543
C	0.712971	3.287724	1.324982
C	0.529376	4.602623	0.870839
C	0.134092	4.835037	-0.449748
N	-1.229104	-0.431690	-0.386474
N	-3.695847	-1.169960	0.533679
O	-1.899690	-0.662650	-2.555131
H	-0.557035	1.185508	-2.400915
H	-0.961399	-1.786217	1.210227
H	-0.381662	3.966355	-2.368775
H	-3.076206	-2.654331	-0.842107
H	-4.651417	-1.947840	-2.531490
H	-4.650210	-0.281142	-1.934836
H	-5.861322	-2.741590	-0.553016
H	-6.668689	-1.199157	-0.861746
H	-5.442932	-1.748148	1.586592
H	-5.467528	-0.103657	0.935504
H	-0.030474	-0.141514	2.646563
H	-1.101879	1.113139	2.046043
H	0.741093	-0.634175	-1.079566
H	1.000551	3.103364	2.357720
H	0.686573	5.437210	1.547731
H	-0.016360	5.855066	-0.794077

Figure S23B Radical C3 TS

0 2

N	0.447129	-0.050752	-1.463984
C	-2.919196	0.064156	1.391562
O	-3.069446	0.981014	2.199269
C	-1.681680	-0.848689	1.358796
C	0.432169	2.417325	-1.926838
C	-3.624041	-1.350042	-0.533532
C	-4.653126	-1.027837	-1.626119
C	-5.798378	-0.360273	-0.843508
C	-5.080094	0.471348	0.231716
C	-2.167901	-1.383875	-1.012064
C	-0.423670	-0.261870	2.040114
C	0.532824	0.072416	0.904651
C	0.176172	-0.839192	-0.278918
C	0.459264	1.297197	-1.099579
C	0.516954	1.418296	0.311660
C	0.528380	2.693363	0.887576
C	0.505890	3.825073	0.063145
C	0.462844	3.684735	-1.328539
N	-1.276147	-1.106091	-0.035884
N	-3.831531	-0.272010	0.453051
O	-1.863848	-1.627522	-2.184545
H	-0.052308	-0.338151	-2.298742
H	-1.972600	-1.794855	1.839003
H	0.376462	2.311518	-3.007005
H	-3.851476	-2.325535	-0.073554
H	-4.964758	-1.921436	-2.171464
H	-4.211343	-0.331702	-2.346512
H	-6.425497	-1.123445	-0.368620
H	-6.442145	0.254647	-1.477976
H	-5.643138	0.557146	1.165626
H	-4.849992	1.486068	-0.116033
H	-0.000523	-1.012651	2.715608
H	-0.701616	0.611284	2.634449
H	0.703220	-1.796382	-0.313830
H	0.529356	2.810309	1.968158
H	0.510958	4.816278	0.507875
H	0.440197	4.569781	-1.959140
N	3.023256	-2.520003	0.761753
C	4.345167	-1.839888	-1.275953
C	2.595827	0.538547	2.718180
C	2.455057	-0.435447	1.562229
C	2.428802	-1.843286	1.805852
C	3.592786	-1.614714	-0.121489
C	3.315026	-0.312569	0.361432
C	3.842223	0.789425	-0.314993
C	4.611506	0.578233	-1.462746
C	4.850815	-0.721190	-1.939409
H	3.072101	-3.524513	0.675478
H	4.541509	-2.845915	-1.636235
H	2.443103	1.570813	2.393442
H	1.878381	0.321957	3.516206
H	1.992531	-2.384995	2.632677
H	3.655381	1.798087	0.041785
H	5.028020	1.428694	-1.995186
H	5.447623	-0.861390	-2.836713
H	3.602236	0.470984	3.149023

Figure S23B Radical C3 Product

0 2

N	0.442596	0.602631	-1.589954
C	-3.028602	-0.247998	1.423820
O	-3.317107	0.319119	2.478258
C	-1.605899	-0.718472	1.104887
C	0.778510	3.085074	-1.621083
C	-3.598796	-1.165592	-0.829944
C	-4.720882	-0.679973	-1.759144
C	-5.926846	-0.573930	-0.809117
C	-5.323930	-0.061016	0.511068
C	-2.184661	-0.846851	-1.311103
C	-0.503301	0.086440	1.810536
C	0.673967	0.236666	0.788442
C	0.139993	-0.369504	-0.560733
C	0.688146	1.838582	-0.997502
C	0.888949	1.696262	0.387943
C	1.157671	2.821262	1.161748
C	1.257560	4.079353	0.549124
C	1.070580	4.201565	-0.830450
N	-1.305193	-0.565070	-0.323528
N	-3.926054	-0.517894	0.450625
O	-1.892059	-0.862442	-2.510668
H	-0.119223	0.536644	-2.430852
H	-1.529901	-1.780936	1.384798
H	0.618235	3.184245	-2.691149
H	-3.657708	-2.261141	-0.720071
H	-4.883545	-1.361988	-2.596083
H	-4.456806	0.301702	-2.167348
H	-6.373685	-1.563064	-0.657942
H	-6.707652	0.090338	-1.188506
H	-5.821477	-0.462918	1.398775
H	-5.345829	1.032798	0.582921
H	-0.198844	-0.416146	2.729582
H	-0.894146	1.065210	2.094497
H	0.586052	-1.338718	-0.802358
H	1.274154	2.737876	2.238752
H	1.470489	4.958049	1.150914
H	1.141970	5.179421	-1.299917
N	2.532660	-2.803257	0.853636
C	4.300414	-2.486202	-0.902060
C	2.575398	0.132571	2.545264
C	1.971222	-0.536751	1.283901
C	1.633878	-2.000294	1.549537
C	3.333605	-2.051525	0.007668
C	3.055322	-0.683295	0.207902
C	3.788820	0.268137	-0.490486
C	4.768980	-0.148962	-1.404633
C	5.013380	-1.511536	-1.606447
H	2.491810	-3.812027	0.837811
H	4.497850	-3.544313	-1.049953
H	2.948995	1.136265	2.322129
H	1.842098	0.208655	3.356133
H	1.227817	-2.373022	2.483603
H	3.603993	1.327259	-0.339603
H	5.339311	0.591432	-1.958020
H	5.773491	-1.822721	-2.318388
H	3.416936	-0.465251	2.909292

Figure S23B Radical C4 TS

0 2

N	4.424266	-2.387935	-0.475959
C	3.829139	-0.678768	-2.227623
C	3.570014	-0.895868	2.811526
C	3.761834	-1.267700	1.369207
C	4.373517	-2.414673	0.901565
C	3.870874	-1.208372	-0.927611
C	3.418715	-0.493148	0.209947
C	2.756752	0.777899	0.033154
C	2.884204	1.364187	-1.276345
C	3.348154	0.634221	-2.366135
H	4.873999	-3.081719	-1.054529
H	4.204861	-1.236537	-3.080288
H	2.512983	-0.770922	3.075051
H	3.985680	-1.664654	3.471261
H	4.786768	-3.248643	1.452181
H	2.747938	1.457244	0.882528
H	2.531591	2.379965	-1.425442
H	3.358867	1.097370	-3.349539
N	-0.357798	1.494762	-1.668088
C	-2.159326	-1.158956	1.376040
O	-2.162976	-0.887492	2.576758
C	-0.876004	-1.327171	0.545227
C	-1.067118	3.656173	-0.596666
C	-3.265338	-1.654156	-0.800889
C	-4.698325	-1.316620	-1.236205
C	-5.532464	-1.648771	0.014053
C	-4.636573	-1.216548	1.186741
C	-2.174469	-0.846766	-1.513142
C	0.379959	-0.651770	1.144703
C	0.672125	0.528246	0.234648
C	0.071165	0.212965	-1.141978
C	-0.476288	2.393858	-0.607098
C	0.145545	1.863390	0.548933
C	0.185985	2.619626	1.722579
C	-0.400903	3.890530	1.740413
C	-1.019562	4.397864	0.591460
N	-1.045890	-0.707738	-0.783066
N	-3.277668	-1.368299	0.646857
O	-2.339530	-0.363627	-2.637887
H	-1.077210	1.455556	-2.382079
H	-0.710920	-2.408486	0.429422
H	-1.555904	4.052243	-1.482637
H	-3.059256	-2.723719	-0.968918
H	-5.000693	-1.880290	-2.121499
H	-4.761491	-0.250784	-1.478499
H	-5.722245	-2.726957	0.065748
H	-6.499070	-1.138266	0.025124
H	-4.761781	-1.833040	2.081638
H	-4.805484	-0.171172	1.473151
H	1.207346	-1.366087	1.146789

H	0.181184	-0.351989	2.176408
H	0.743163	-0.291778	-1.842301
H	0.655124	2.219821	2.618542
H	-0.380090	4.483189	2.650543
H	-1.476373	5.383781	0.618164
H	4.071011	0.051272	3.050982

Figure S23B Radical C4 Product

0 2

N	0.429591	1.847117	-1.472722
C	-2.415722	-0.558557	1.366240
O	-2.556133	-0.519859	2.589808
C	-1.036369	-0.633979	0.712787
C	0.959831	4.131102	-0.579543
C	-3.311789	-0.588914	-0.969665
C	-4.609809	0.071985	-1.454506
C	-5.633458	-0.379319	-0.397447
C	-4.844692	-0.368508	0.925188
C	-2.026912	0.067444	-1.469099
C	0.065421	0.081498	1.502320
C	1.114058	0.552701	0.448042
C	0.359624	0.504398	-0.931188
C	0.895394	2.736861	-0.512551
C	1.392779	2.042567	0.604859
C	1.973186	2.736980	1.658052
C	2.056489	4.136882	1.598651
C	1.546913	4.818097	0.489617
N	-1.004338	0.051684	-0.586415
N	-3.447917	-0.544599	0.495228
O	-1.948271	0.555433	-2.600695
H	-0.272844	2.105200	-2.153858
H	-0.780719	-1.696406	0.578690
H	0.568745	4.666870	-1.440142
H	-3.284237	-1.637620	-1.309176
H	-4.869931	-0.232050	-2.470414
H	-4.490828	1.160988	-1.445471
H	-5.978583	-1.395307	-0.620109
H	-6.512517	0.269025	-0.355217
H	-5.140368	-1.168554	1.610655
H	-4.940779	0.582463	1.462020
H	0.497702	-0.551977	2.273595
H	-0.369058	0.948983	2.004822
H	0.790957	-0.213523	-1.634662
H	2.353011	2.205306	2.527855
H	2.510188	4.688718	2.416725
H	1.605630	5.902985	0.451149
N	2.237110	-3.722913	-0.951601
C	3.197737	-1.704071	-2.077442
C	1.481124	-2.842750	2.554984
C	1.812794	-2.863470	1.085847
C	1.821338	-4.023461	0.319736
C	2.538940	-2.379789	-1.026546
C	2.239320	-1.803624	0.226398
C	2.450248	-0.319516	0.441137
C	3.378898	0.244682	-0.615751
C	3.651610	-0.390425	-1.800823
H	2.408747	-4.397622	-1.682658
H	3.429284	-2.199806	-3.014666
H	0.422213	-2.637864	2.757524
H	1.708829	-3.812705	3.010419
H	1.572271	-5.037227	0.600879
H	2.887779	-0.148904	1.437860
H	3.754970	1.248708	-0.446791
H	4.254678	0.120049	-2.548351
H	2.067251	-2.086215	3.089210

Figure S23B Radical C5 TS

0 2

N	-0.101160	1.075050	-1.595294
C	-2.634826	-0.841903	1.480686
O	-3.027726	-0.244309	2.482553
C	-1.148922	-1.052269	1.143191
C	-1.143840	3.359616	-1.466511
C	-2.974536	-2.090830	-0.647401
C	-4.215547	-2.114021	-1.550507
C	-5.379202	-2.195177	-0.545996
C	-4.921748	-1.313823	0.627976
C	-1.762490	-1.364260	-1.240176
C	-0.179067	-0.064729	1.833040
C	0.365737	0.814962	0.715844
C	0.206899	0.056678	-0.608475
C	-0.541743	2.221640	-0.932756
C	-0.260862	2.120049	0.450754
C	-0.573972	3.181622	1.301847
C	-1.173034	4.331763	0.772882
C	-1.453912	4.413656	-0.595887
N	-0.925180	-0.865815	-0.303800
N	-3.456099	-1.409659	0.570012
O	-1.594514	-1.242881	-2.457900
H	-0.584483	0.747419	-2.424483
H	-0.903387	-2.087792	1.422180
H	-1.371981	3.426689	-2.526829
H	-2.664056	-3.119299	-0.401385
H	-4.193147	-2.947985	-2.255453
H	-4.259859	-1.185688	-2.129262
H	-5.513833	-3.228780	-0.207261
H	-6.328048	-1.855970	-0.969881
H	-5.287602	-1.657666	1.599832
H	-5.229233	-0.268010	0.504837
H	0.615116	-0.628748	2.329375
H	-0.714090	0.509146	2.593439
H	1.075180	-0.535146	-0.914242
H	-0.369075	3.111510	2.367662
H	-1.425709	5.160453	1.428234
H	-1.925214	5.308032	-0.995249
N	4.964346	-0.875054	-1.497722
C	3.665182	1.247005	-1.033154
C	4.468458	-3.085458	1.449847
C	4.499768	-2.018875	0.396870
C	5.184403	-2.047829	-0.792547

C	4.128358	-0.061665	-0.772783
C	3.803362	-0.750726	0.431810
C	2.982992	-0.127564	1.378388
C	2.357267	1.128773	1.069481
C	2.833059	1.835002	-0.111928
H	5.361869	-0.656211	-2.398983
H	3.975205	1.780143	-1.928220
H	3.445220	-3.433148	1.644847
H	5.063246	-3.954468	1.149868
H	5.818102	-2.821139	-1.205153
H	2.800044	-0.600818	2.338799
H	2.094523	1.756385	1.920948
H	2.467255	2.841954	-0.287431
H	4.867837	-2.724811	2.407226

Figure S23B Radical C5 Product

0 2

N	-0.119646	1.561815	-1.593199
C	-2.566201	-0.986770	1.471354
O	-2.933168	-0.710083	2.613940
C	-1.125206	-0.772092	1.000120
C	-0.637102	3.996132	-1.256340
C	-2.977170	-1.818510	-0.850751
C	-4.302269	-1.755607	-1.623986
C	-5.323195	-2.264699	-0.591097
C	-4.828200	-1.685967	0.746572
C	-1.883920	-0.887723	-1.371243
C	-0.394923	0.368412	1.723824
C	0.544111	1.032546	0.665291
C	0.121809	0.429676	-0.719717
C	-0.223348	2.728643	-0.839826
C	0.217889	2.507042	0.476507
C	0.266436	3.557694	1.383937
C	-0.135379	4.838958	0.976396
C	-0.585870	5.045234	-0.330731
N	-1.079422	-0.373706	-0.413784
N	-3.383874	-1.504345	0.528862
O	-1.757492	-0.647443	-2.575662
H	-0.724940	1.392185	-2.387333
H	-0.579287	-1.719172	1.134956
H	-0.987019	4.163551	-2.271307
H	-2.571036	-2.842574	-0.895829
H	-4.272245	-2.352491	-2.537757
H	-4.512438	-0.717494	-1.903564
H	-5.306588	-3.359902	-0.555162
H	-6.346269	-1.954030	-0.818353
H	-5.008144	-2.348846	1.598187
H	-5.285138	-0.716118	0.976168
H	0.149428	0.000561	2.596088
H	-1.129246	1.091080	2.085058
H	0.881610	-0.231545	-1.148905
H	0.601286	3.390224	2.405337
H	-0.102490	5.666817	1.678685
H	-0.904798	6.037662	-0.639278
N	4.877130	-1.518144	-1.253233
C	3.870665	0.770679	-0.813812
C	3.307284	-3.857672	1.168853
C	3.775887	-2.723282	0.309042
C	4.717496	-2.773547	-0.690004
C	4.036271	-0.631718	-0.626503
C	3.315358	-1.349403	0.368499
C	2.391184	-0.693061	1.177647
C	2.080935	0.773358	0.984825
C	2.968760	1.437387	-0.047111
H	5.511997	-1.295703	-2.005333
H	4.471528	1.300573	-1.549658
H	2.226988	-4.027615	1.064732
H	3.816646	-4.790674	0.905935
H	5.294901	-3.612757	-1.053355
H	1.888266	-1.229156	1.977190
H	2.224874	1.299173	1.948590
H	2.845495	2.508363	-0.176231
H	3.494781	-3.665491	2.233899

Figure S23B Radical C6 TS

0 2

N	0.265708	0.489845	-1.431330
C	-3.102061	-0.299133	1.399508
O	-3.569103	0.553118	2.155126
C	-1.626946	-0.733673	1.418794
C	-0.303932	2.861026	-2.044520
C	-3.256682	-1.963198	-0.448991
C	-4.309087	-2.047212	-1.563253
C	-5.628170	-1.769166	-0.820289
C	-5.252241	-0.703634	0.222744
C	-1.859650	-1.542618	-0.916885
C	-0.658815	0.290992	2.059553
C	0.237476	0.763580	0.922416
C	0.185109	-0.276263	-0.201179
C	-0.049512	1.820228	-1.152825
C	-0.055024	2.034553	0.246374
C	-0.303496	3.312377	0.751533
C	-0.553996	4.364950	-0.137298
C	-0.554612	4.135698	-1.518381
N	-1.135600	-0.922788	0.040417
N	-3.829957	-0.971780	0.481196
O	-1.458994	-1.748919	-2.066965
H	-0.111076	0.036184	-2.256286
H	-1.583391	-1.690948	1.959163
H	-0.314333	2.688517	-3.117350
H	-3.161243	-2.938052	0.056518
H	-4.292303	-3.014701	-2.069735
H	-4.108421	-1.272667	-2.310731
H	-5.976438	-2.678506	-0.317294
H	-6.425347	-1.429515	-1.486781
H	-5.828344	-0.778003	1.149628
H	-5.371031	0.315547	-0.165134
H	-0.094538	-0.195297	2.859205
H	-1.231016	1.109055	2.503659
H	0.967053	-1.041636	-0.163663

H	-0.316232	3.486458	1.825023
H	-0.753941	5.361395	0.246319
H	-0.756964	4.958333	-2.199461
N	4.612971	0.341156	-1.222571
C	3.001693	1.230941	0.487554
C	5.364913	-3.165980	-0.245745
C	4.885589	-1.753666	-0.409610
C	5.248712	-0.871348	-1.406146
C	3.807945	0.267939	-0.101945
C	3.969451	-1.046907	0.435380
C	3.288990	-1.369186	1.637875
C	2.470190	-0.435282	2.228870
C	2.195451	0.850824	1.614223
H	4.686095	1.135361	-1.840357
H	2.917798	2.229792	0.070476
H	4.533512	-3.882529	-0.266057
H	6.059179	-3.441529	-1.046287
H	5.921990	-1.016140	-2.240212
H	3.444542	-2.336684	2.109677
H	1.995766	-0.670620	3.177130
H	1.897289	1.653397	2.287298
H	5.886538	-3.310882	0.709442

Figure S23B Radical C6 Product

0 2

N	0.098901	1.051300	-1.574953
C	-3.065573	-0.584440	1.445621
O	-3.536363	-0.054982	2.452857
C	-1.558598	-0.638766	1.176721
C	-0.102977	3.550690	-1.712833
C	-3.278238	-1.784768	-0.736549
C	-4.466217	-1.720217	-1.707018
C	-5.677065	-1.903360	-0.774946
C	-5.288394	-1.140623	0.504459
C	-2.005637	-1.099597	-1.230571
C	-0.767619	0.515645	1.809384
C	0.387181	0.857149	0.812919
C	0.063664	0.071998	-0.505960
C	0.068491	2.337354	-1.041991
C	0.303493	2.303019	0.343569
C	0.386173	3.484933	1.068556
C	0.226188	4.711746	0.406382
C	-0.020450	4.734052	-0.969459
N	-1.268575	-0.515932	-0.258831
N	-3.816917	-1.169769	0.487644
O	-1.689917	-1.100503	-2.424007
H	-0.416806	0.815927	-2.414236
H	-1.184677	-1.605931	1.548713
H	-0.293906	3.575357	-2.782212
H	-3.016797	-2.837888	-0.540819
H	-4.398846	-2.480233	-2.488047
H	-4.489185	-0.737588	-2.190666
H	-5.819775	-2.966234	-0.549416
H	-6.606690	-1.527118	-1.209823
H	-5.671148	-1.604733	1.418309
H	-5.631258	-0.099353	0.489796
H	-0.401506	0.248634	2.803109
H	-1.427869	1.376228	1.933279
H	0.770914	-0.739261	-0.706337
H	0.561846	3.463945	2.141964
H	0.287716	5.641520	0.964383
H	-0.152437	5.686520	-1.476646
N	4.827437	-0.008359	-0.944487
C	2.918302	0.852849	0.423305
C	5.141064	-3.633303	-0.185239
C	4.788338	-2.179008	-0.302936
C	5.424120	-1.244193	-1.105212
C	3.781910	-0.114483	-0.040617
C	3.749720	-1.484223	0.376989
C	2.773378	-1.867126	1.354234
C	1.887564	-0.960743	1.840349
C	1.818897	0.484585	1.389363
H	5.088543	0.832082	-1.437509
H	2.986814	1.882100	0.085806
H	4.306991	-4.280063	-0.486891
H	5.998766	-3.882851	-0.818355
H	6.260925	-1.369627	-1.778436
H	2.758423	-2.890319	1.724470
H	1.185055	-1.272397	2.608673
H	1.903544	1.126221	2.287369
H	5.399407	-3.906765	0.846009

Figure S23B Radical C7 TS

0 2

N	0.386068	0.191715	-1.353244
C	-3.155271	-0.096339	1.348101
O	-3.382903	0.697709	2.260983
C	-1.871220	-0.937647	1.258417
C	0.545559	2.693855	-1.518248
C	-3.718300	-1.264691	-0.781020
C	-4.700371	-0.816118	-1.872342
C	-5.911273	-0.312555	-1.066863
C	-5.285908	0.370975	0.160883
C	-2.241739	-1.198831	-1.183830
C	-0.672352	-0.371159	2.058354
C	0.348614	0.039240	1.008488
C	0.051977	-0.728508	-0.282873
C	0.452514	1.482184	-0.835397
C	0.454896	1.435447	0.581617
C	0.571753	2.620238	1.315549
C	0.680576	3.839722	0.635385
C	0.664244	3.869736	-0.765316
N	-1.404904	-1.009076	-0.139889
N	-4.011812	-0.342560	0.332770
O	-1.874395	-1.297701	-2.358773
H	-0.058778	0.014665	-2.246798
H	-2.124534	-1.947175	1.614073
H	0.527980	2.726275	-2.604102
H	-3.938046	-2.300766	-0.476181
H	-4.944901	-1.626942	-2.561921

H	-4.250300	-0.004208	-2.452854
H	-6.531190	-1.158601	-0.748981
H	-6.545317	0.370099	-1.638681
H	-5.895747	0.285297	1.064977
H	-5.091386	1.436504	-0.012380
H	-0.287220	-1.143139	2.730313
H	-1.003585	0.471491	2.670054
H	0.588750	-1.675937	-0.396137
H	0.564379	2.596983	2.402858
H	0.767270	4.766195	1.195729
H	0.740351	4.822866	-1.282063
N	3.611321	1.071033	0.338382
C	2.235848	-0.545954	1.722043
C	5.582662	-0.930910	-2.090340
C	4.686470	-0.368282	-1.027344
C	4.502335	0.956822	-0.716133
C	3.193768	-0.177239	0.717077
C	3.853323	-1.114263	-0.114565
C	3.640290	-2.493985	0.096675
C	2.805008	-2.889492	1.149947
C	2.174155	-1.957958	1.976037
H	3.242430	1.939949	0.697934
H	2.093083	0.127752	2.565023
H	5.021293	-1.527583	-2.821324
H	6.093569	-0.132025	-2.637923
H	4.945505	1.840011	-1.155455
H	4.138162	-3.235562	-0.521835
H	2.674044	-3.949330	1.354639
H	1.588711	-2.311218	2.819861
H	6.353788	-1.589169	-1.668442

Figure S23B Radical C7 Product

0 2

N	-0.362704	0.719051	1.495497
C	3.201568	-0.191986	-1.382528
O	3.543373	0.383114	-2.416451
C	1.754289	-0.622229	-1.126212
C	-0.867000	3.177414	1.488855
C	3.663799	-1.163535	0.874552
C	4.766879	-0.727454	1.849619
C	6.007810	-0.642745	0.943242
C	5.466995	-0.090573	-0.387866
C	2.243270	-0.810785	1.310440
C	0.708820	0.252182	-1.833110
C	-0.526245	0.320983	-0.877039
C	-0.041465	-0.275710	0.491478
C	-0.672575	1.930152	0.889578
C	-0.852043	1.757400	-0.495193
C	-1.243049	2.828847	-1.290417
C	-1.457708	4.083574	-0.697873
C	-1.263088	4.246666	0.677283
N	1.404759	-0.500098	0.295569
N	4.054412	-0.504466	-0.382832
O	1.905802	-0.825772	2.497499
H	0.157343	0.672499	2.362990
H	1.651685	-1.671791	-1.443680
H	-0.720895	3.311786	2.556904
H	3.693599	-2.258234	0.746783
H	4.880726	-1.427762	2.679516
H	4.518201	0.254884	2.265795
H	6.430140	-1.642395	0.790885
H	6.794215	-0.008465	1.360424
H	5.982040	-0.493837	-1.264833
H	5.524902	1.003018	-0.440344
H	0.457222	-0.145135	-2.818855
H	1.123314	1.250401	-1.986550
H	-0.513643	-1.232882	0.735495
H	-1.373449	2.703287	-2.363136
H	-1.764204	4.926922	-1.309454
H	-1.420976	5.222280	1.129791
N	-3.683986	0.624760	-0.137445
C	-1.774837	-0.464792	-1.467583
C	-5.652408	-2.021817	1.553105
C	-4.699766	-1.157507	0.780485
C	-4.721926	0.213803	0.679632
C	-2.972690	-0.463597	-0.563089
C	-3.584898	-1.602708	-0.018820
C	-3.101294	-2.901509	-0.345515
C	-2.032672	-2.998430	-1.263092
C	-1.423379	-1.895110	-1.818288
H	-3.443338	1.585701	-0.335334
H	-2.012358	0.082394	-2.398127
H	-5.136082	-2.614338	2.320025
H	-6.411282	-1.415688	2.059158
H	-5.393928	0.936542	1.121045
H	-3.560672	-3.792950	0.069669
H	-1.687158	-3.986279	-1.561264
H	-0.637467	-2.042771	-2.552896
H	-6.177008	-2.733859	0.902216

Figure S23D Cation C2 TS

1 1

N	2.499976	-0.990244	1.891234
C	3.435639	-3.004202	0.701729
C	3.577696	1.963163	-0.087487
C	3.256661	0.622452	0.476312
C	2.484858	0.372334	1.636940
C	3.183815	-1.638333	0.889507
C	3.662650	-0.646611	-0.020789
C	4.413694	-1.049876	-1.150710
C	4.665976	-2.395706	-1.332210
C	4.180834	-3.360826	-0.412445
H	2.148343	-1.428841	2.730211
H	3.069611	-3.748908	1.401218
H	2.786096	2.314671	-0.766134
H	3.682843	2.716738	0.698181
H	2.282227	1.067139	2.440126
H	4.786431	-0.313016	-1.855637
H	5.243533	-2.727758	-2.189123
H	4.401283	-4.409897	-0.586235

H	4.506021	1.930707	-0.665024
N	0.339368	0.613424	-1.506113
C	-2.957120	-0.227594	1.460535
O	-3.345914	0.571139	2.310807
C	-1.490321	-0.680302	1.356446
C	0.188921	3.057604	-2.004183
C	-3.261675	-1.731434	-0.509760
C	-4.377587	-1.687293	-1.563881
C	-5.642378	-1.454917	-0.718666
C	-5.181472	-0.496940	0.392063
C	-1.880927	-1.322386	-1.025795
C	-0.476265	0.300241	2.003848
C	0.356178	0.773043	0.828151
C	0.238298	-0.215373	-0.326998
C	0.283667	1.929148	-1.169915
C	0.299375	2.070341	0.258264
C	0.197518	3.353005	0.844467
C	0.096952	4.453831	0.018286
C	0.095324	4.297870	-1.392938
N	-1.096746	-0.764613	-0.065130
N	-3.748167	-0.807273	0.534380
O	-1.520689	-1.473789	-2.190846
H	0.125153	0.232310	-2.418643
H	-1.412095	-1.670367	1.825868
H	0.173704	2.955172	-3.083959
H	-3.171765	-2.748738	-0.096719
H	-4.413595	-2.603043	-2.157298
H	-4.201745	-0.848667	-2.245604
H	-5.982819	-2.400018	-0.281454
H	-6.467575	-1.038923	-1.301773
H	-5.698058	-0.650937	1.343329
H	-5.301059	0.555521	0.109117
H	0.102851	-0.214479	2.771517
H	-1.007979	1.125549	2.481909
H	0.988024	-1.015051	-0.349455
H	0.202489	3.462863	1.924597
H	0.017104	5.449191	0.441983
H	0.010927	5.183501	-2.015901

Figure S23D Cation C2 Product

1 1

N	2.554474	-0.993042	1.452018
C	4.388018	-2.482461	0.672844
C	3.089784	2.228897	-0.414888
C	3.049797	0.848364	0.130171
C	2.068813	0.353374	1.168725
C	3.621427	-1.296542	0.706688
C	3.953371	-0.164193	-0.130867
C	5.081263	-0.240639	-1.009408
C	5.808749	-1.397695	-1.033949
C	5.457697	-2.506452	-0.193212
H	2.158041	-1.602516	2.154145
H	4.142860	-3.329899	1.303178
H	2.250551	2.403755	-1.098097
H	2.995072	2.969089	0.386605
H	2.179891	0.972384	2.070681
H	5.340179	0.601584	-1.641696
H	6.666616	-1.493142	-1.690514
H	6.069373	-3.402375	-0.244115
H	4.020306	2.410129	-0.956619
N	0.201303	0.498093	-1.561376
C	-2.862096	-0.470295	1.470715
O	-3.145377	0.297484	2.388906
C	-1.447947	-1.042775	1.260581
C	-0.597631	2.884222	-1.685506
C	-3.365621	-1.810403	-0.567264
C	-4.526508	-1.635075	-1.556591
C	-5.730150	-1.362993	-0.636809
C	-5.149118	-0.500952	0.496242
C	-1.989041	-1.441996	-1.125944
C	-0.327222	-0.240940	1.943590
C	0.530149	0.365805	0.800055
C	0.214994	-0.471319	-0.481314
C	-0.156425	1.738016	-1.020982
C	0.055982	1.743130	0.368491
C	-0.160867	2.896898	1.113405
C	-0.598835	4.053677	0.457157
C	-0.814006	4.038301	-0.926157
N	-1.109714	-1.041704	-0.171504
N	-3.740269	-0.924423	0.552994
O	-1.718038	-1.492948	-2.326384
H	-0.262455	0.175547	-2.405761
H	-1.459641	-2.074466	1.639507
H	-0.768665	2.878818	-2.757778
H	-3.317807	-2.854771	-0.218824
H	-4.656638	-2.513045	-2.192631
H	-4.325135	-0.775632	-2.204207
H	-6.115322	-2.304923	-0.230607
H	-6.551152	-0.861210	-1.154987
H	-5.633210	-0.666059	1.462777
H	-5.201891	0.570920	0.270966
H	0.251334	-0.897688	2.596930
H	-0.760742	0.537183	2.574921
H	0.926078	-1.274185	-0.693864
H	-0.006529	2.905454	2.189538
H	-0.780205	4.961182	1.024264
H	-1.161599	4.939391	-1.423547

Figure S23D Cation C3 TS

1 1

N	0.465649	-0.138262	-1.452311
C	-3.020731	0.326576	1.356612
O	-3.203100	1.312602	2.068231
C	-1.734805	-0.517213	1.417682
C	0.917941	2.188723	-2.235191
C	-3.657099	-1.302943	-0.423011
C	-4.683985	-1.118653	-1.550182
C	-5.862549	-0.432496	-0.836938
C	-5.191757	0.519451	0.166591
C	-2.200459	-1.348306	-0.888583

C	-0.514906	0.228332	2.018432
C	0.464403	0.304445	0.859299
C	0.116246	-0.753992	-0.192986
C	0.719866	1.188696	-1.270322
C	0.721316	1.503274	0.125782
C	0.871360	2.844648	0.544105
C	1.060790	3.826429	-0.411374
C	1.091250	3.490281	-1.786578
N	-1.326166	-0.899850	0.050486
N	-3.908309	-0.143382	0.456035
O	-1.857636	-1.743139	-2.001353
H	0.131458	-0.546035	-2.316022
H	-1.956116	-1.417662	2.007000
H	0.915255	1.951418	-3.293842
H	-3.858636	-2.237914	0.123981
H	-4.952221	-2.069050	-2.015908
H	-4.262654	-0.469502	-2.324727
H	-6.465525	-1.175771	-0.303697
H	-6.520796	0.099005	-1.528595
H	-5.763563	0.655743	1.088508
H	-5.002445	1.510051	-0.263478
H	-0.128918	-0.314982	2.881045
H	-0.820462	1.220435	2.357250
H	0.616851	-1.721997	-0.092429
H	0.820990	3.100735	1.597491
H	1.174430	4.863099	-0.112689
H	1.236255	4.281542	-2.516506
N	2.577521	-2.461500	1.181431
C	3.887169	-2.340304	-0.980407
C	2.722199	0.876824	2.671192
C	2.511641	-0.255501	1.700420
C	2.170742	-1.572405	2.100814
C	3.279159	-1.813713	0.155697
C	3.286820	-0.436714	0.469170
C	3.957051	0.450669	-0.378850
C	4.581997	-0.062780	-1.516762
C	4.542659	-1.435256	-1.816167
H	2.405385	-3.459031	1.228852
H	3.862553	-3.402349	-1.202848
H	2.698068	1.844330	2.163160
H	1.970723	0.880621	3.466324
H	1.648351	-1.899309	2.989581
H	4.000646	1.512261	-0.157387
H	5.112453	0.610051	-2.183652
H	5.038022	-1.801634	-2.709910
H	3.707026	0.782766	3.143309

Figure S23D Cation C3 Product

1 1

N	0.408224	0.073579	-1.522427
C	-2.854963	-0.160231	1.394091
O	-2.947450	0.639026	2.324355
C	-1.646641	-1.096461	1.203386
C	0.167977	2.575367	-1.580712
C	-3.636092	-1.281384	-0.686362
C	-4.683848	-0.796182	-1.698397
C	-5.792396	-0.214069	-0.802799
C	-5.028754	0.453764	0.352199
C	-2.195324	-1.276996	-1.205047
C	-0.373100	-0.658629	1.942914
C	0.628587	-0.200716	0.850406
C	0.162081	-0.898565	-0.475339
C	0.327620	1.345161	-0.942956
C	0.468944	1.262655	0.453579
C	0.431641	2.417180	1.231186
C	0.277238	3.658790	0.601542
C	0.151405	3.728808	-0.790044
N	-1.270552	-1.151827	-0.217895
N	-3.792486	-0.339967	0.440849
O	-1.912805	-1.360959	-2.401067
H	-0.111757	-0.101878	-2.377361
H	-1.957658	-2.093882	1.545079
H	0.052760	2.634447	-2.658907
H	-3.872662	-2.305143	-0.354322
H	-5.029841	-1.604305	-2.346227
H	-4.243594	-0.020490	-2.333215
H	-6.426825	-1.019266	-0.415907
H	-6.434772	0.493062	-1.333480
H	-5.565007	0.426276	1.304710
H	-4.780083	1.499417	0.134384
H	0.014316	-1.494854	2.529826
H	-0.614592	0.145234	2.641411
H	0.664440	-1.843185	-0.707420
H	0.497395	2.365827	2.314324
H	0.241478	4.565326	1.197410
H	0.024164	4.695768	-1.268856
N	3.279584	-2.442758	0.540731
C	4.888867	-1.437774	-1.126739
C	2.540973	0.089187	2.592622
C	2.140083	-0.547603	1.227210
C	2.338375	-2.033147	1.335847
C	3.846976	-1.379906	-0.211214
C	3.179343	-0.207039	0.162023
C	3.598298	0.998508	-0.391706
C	4.643688	0.974359	-1.323651
C	5.276941	-0.220747	-1.690378
H	3.584511	-3.412413	0.473612
H	5.378991	-2.370786	-1.384382
H	2.498669	1.176147	2.497745
H	1.869928	-0.224864	3.395512
H	1.818307	-2.727410	1.983821
H	3.130149	1.936965	-0.118850
H	4.973606	1.907201	-1.770033
H	6.085347	-0.201801	-2.413824
H	3.563858	-0.189119	2.859873

Figure S23D Cation C4 TS

1 1

N	4.298010	-2.367940	-0.688516
C	3.702047	-0.471728	-2.221449

C	3.637287	-1.177807	2.764684
C	3.736452	-1.404997	1.283685
C	4.283446	-2.526713	0.665769
C	3.776986	-1.129653	-0.999540
C	3.394066	-0.513970	0.228662
C	2.778545	0.781418	0.185041
C	2.811338	1.475802	-1.070741
C	3.232684	0.856090	-2.237761
H	4.676868	-3.032490	-1.349295
H	4.026271	-0.953745	-3.139256
H	2.614417	-0.953466	3.086130
H	3.971405	-2.061439	3.315923
H	4.681324	-3.424527	1.118914
H	2.762441	1.371969	1.095564
H	2.457115	2.500233	-1.105890
H	3.200367	1.395090	-3.178497
N	-0.281475	1.500890	-1.621422
C	-2.151410	-1.171284	1.371974
O	-2.167042	-0.906769	2.572814
C	-0.849374	-1.330833	0.566313
C	-1.013364	3.664088	-0.593382
C	-3.207514	-1.642838	-0.836442
C	-4.635041	-1.315598	-1.298308
C	-5.489627	-1.666255	-0.067181
C	-4.624080	-1.231463	1.126470
C	-2.112700	-0.817720	-1.518607
C	0.387259	-0.658168	1.210311
C	0.643383	0.535524	0.313311
C	0.120948	0.215207	-1.093667
C	-0.423678	2.393269	-0.585881
C	0.144561	1.857133	0.604630
C	0.123874	2.601471	1.798227
C	-0.459474	3.858361	1.789239
C	-1.019478	4.377460	0.599617
N	-0.996546	-0.682987	-0.754010
N	-3.250271	-1.369807	0.614741
O	-2.239637	-0.317039	-2.634664
H	-0.891608	1.506175	-2.431173
H	-0.669528	-2.406609	0.437006
H	-1.453632	4.072295	-1.497233
H	-2.984763	-2.707397	-1.011383
H	-4.912349	-1.876861	-2.192932
H	-4.705336	-0.248784	-1.533810
H	-5.668683	-2.746368	-0.026562
H	-6.460945	-1.165539	-0.073372
H	-4.760494	-1.853509	2.015213
H	-4.805602	-0.188482	1.412209
H	1.222869	-1.358884	1.210022
H	0.164645	-0.370105	2.239480
H	0.826279	-0.283454	-1.764244
H	0.554153	2.194952	2.708878
H	-0.493068	4.449936	2.698044
H	-1.474594	5.363491	0.619424
H	4.265045	-0.333897	3.076264

Figure S23D Cation C4 Product

1 1

N	-0.182866	1.410408	-1.593239
C	-2.171310	-1.147479	1.284026
O	-2.217552	-0.852837	2.477387
C	-0.856208	-1.408184	0.528025
C	-1.279151	3.375353	-0.458066
C	-3.160174	-1.643646	-0.945902
C	-4.552477	-1.279286	-1.479906
C	-5.470461	-1.542119	-0.272495
C	-4.635725	-1.091128	0.937232
C	-2.002859	-0.886620	-1.604510
C	0.404548	-0.825887	1.184156
C	0.798439	0.397447	0.330407
C	0.227680	0.109735	-1.096243
C	-0.532405	2.196345	-0.489489
C	0.042927	1.667546	0.679076
C	-0.109367	2.321108	1.897820
C	-0.856630	3.503234	1.942752
C	-1.432733	4.017375	0.773893
N	-0.904941	-0.795233	-0.809541
N	-3.251060	-1.310477	0.490554
O	-2.076579	-0.394022	-2.731041
H	-0.809540	1.376116	-2.392315
H	-0.757019	-2.498779	0.432145
H	-1.727391	3.779576	-1.360752
H	-2.974522	-2.722758	-1.068476
H	-4.817957	-1.865850	-2.361981
H	-4.567438	-0.221498	-1.761553
H	-5.695005	-2.611774	-0.194460
H	-6.419585	-1.004535	-0.339966
H	-4.836011	-1.666168	1.845495
H	-4.784017	-0.029615	1.169471
H	1.188474	-1.580168	1.162550
H	0.200699	-0.562538	2.224040
H	0.926097	-0.367175	-1.789098
H	0.329621	1.917156	2.806771
H	-0.995829	4.019449	2.887448
H	-2.015023	4.933262	0.822954
N	4.788363	-1.875832	-0.746704
C	4.120484	0.172593	-1.991158
C	3.321271	-1.578913	2.637634
C	3.686650	-1.444832	1.186448
C	4.594253	-2.295230	0.515444
C	4.046945	-0.721827	-0.948790
C	3.309941	-0.471885	0.251853
C	2.402784	0.714959	0.319814
C	2.643956	1.683686	-0.797651
C	3.423966	1.411815	-1.883103
H	5.429374	-2.291651	-1.410695
H	4.736324	-0.031894	-2.862620
H	2.602951	-2.388307	2.810688
H	4.210732	-1.799914	3.236338
H	5.116615	-3.160867	0.900592
H	2.555121	1.231913	1.276855

H	2.120910	2.630937	-0.740153
H	3.523582	2.138830	-2.681408
H	2.879350	-0.655884	3.022261

Figure S23D Cation C5 TS

1 1

N	0.034211	1.419583	-1.553938
C	-2.595557	-0.899215	1.486292
O	-2.997112	-0.515287	2.583426
C	-1.115574	-0.824743	1.084020
C	-0.469252	3.864005	-1.423320
C	-2.917877	-1.845496	-0.806772
C	-4.194963	-1.789239	-1.658794
C	-5.293459	-2.173880	-0.652290
C	-4.851220	-1.509459	0.662720
C	-1.767698	-0.984009	-1.323921
C	-0.314013	0.259816	1.846706
C	0.381383	1.049315	0.742640
C	0.205039	0.343735	-0.606138
C	-0.123085	2.607672	-0.901368
C	0.104341	2.435434	0.497557
C	-0.027144	3.527469	1.378249
C	-0.365025	4.764652	0.859418
C	-0.580616	4.921468	-0.531523
N	-0.996334	-0.452549	-0.338401
N	-3.386165	-1.420616	0.525506
O	-1.559656	-0.794446	-2.520703
H	-0.308117	1.217663	-2.484368
H	-0.667110	-1.814715	1.250305
H	-0.647885	3.998504	-2.484960
H	-2.545671	-2.881761	-0.759982
H	-4.139812	-2.457698	-2.520147
H	-4.342463	-0.769124	-2.029109
H	-5.327410	-3.262091	-0.530179
H	-6.286180	-1.841188	-0.965251
H	-5.115199	-2.088315	1.552114
H	-5.265699	-0.501714	0.781745
H	0.360629	-0.192023	2.572253
H	-0.998713	0.905981	2.400369
H	1.035039	-0.305973	-0.907057
H	0.139067	3.397478	2.443694
H	-0.470222	5.621999	1.515655
H	-0.849737	5.902322	-0.912799
N	4.399680	-1.598593	-1.501512
C	3.701324	0.759485	-0.995383
C	3.398306	-3.706549	1.400610
C	3.688279	-2.656290	0.372771
C	4.317682	-2.819297	-0.828589
C	3.832431	-0.624353	-0.752889
C	3.355274	-1.247232	0.454646
C	2.747218	-0.459375	1.416868
C	2.516148	0.921574	1.155725
C	3.066017	1.513964	-0.037797
H	4.831063	-1.468101	-2.406814
H	4.093655	1.208688	-1.902077
H	2.322272	-3.790053	1.597413
H	3.755477	-4.686080	1.070177
H	4.725643	-3.711899	-1.281542
H	2.435817	-0.890903	2.363296
H	2.342284	1.570889	2.008838
H	2.945236	2.581638	-0.188259
H	3.884690	-3.477151	2.356679

Figure S23D Cation C5 Product

1 1

N	-0.103391	0.956113	-1.625212
C	-2.710496	-0.836337	1.463792
O	-2.995079	-0.248235	2.505963
C	-1.264673	-1.175376	1.055788
C	-1.213604	3.197802	-1.315998
C	-3.247293	-1.936327	-0.705668
C	-4.514375	-1.785633	-1.559668
C	-5.644248	-1.805854	-0.514655
C	-5.061392	-1.035641	0.681373
C	-1.989766	-1.308456	-1.312004
C	-0.186857	-0.332480	1.760244
C	0.470547	0.536266	0.657624
C	0.131917	-0.145293	-0.708097
C	-0.562189	2.045973	-0.873506
C	-0.222050	1.880673	0.479202
C	-0.514633	2.873286	1.408089
C	-1.165336	4.035669	0.975964
C	-1.508666	4.187247	-0.372316
N	-1.077159	-0.925599	-0.382897
N	-3.613900	-1.274075	0.562188
O	-1.836515	-1.156985	-2.525045
H	-0.609511	0.694943	-2.466453
H	-1.111800	-2.242722	1.269899
H	-1.484723	3.321952	-2.360231
H	-3.036808	-3.002569	-0.523489
H	-4.599819	-2.577808	-2.306402
H	-4.485120	-0.826724	-2.087262
H	-5.869537	-2.837504	-0.221985
H	-6.567889	-1.353141	-0.883857
H	-5.425435	-1.391087	1.649335
H	-5.263120	0.040543	0.619489
H	0.526401	-0.988806	2.260675
H	-0.651165	0.285791	2.531208
H	0.910502	-0.808724	-1.096428
H	-0.256716	2.750453	2.457331
H	-1.409552	4.816104	1.689829
H	-2.019649	5.089693	-0.696356
N	5.589065	-0.220951	-1.100628
C	3.794289	1.486289	-0.790491
C	4.803174	-3.167643	1.044612
C	4.900888	-1.885739	0.280477
C	5.868913	-1.508463	-0.594202
C	4.459141	0.250338	-0.577398
C	3.956516	-0.771852	0.324653
C	2.800321	-0.550817	1.002076

C	2.044199	0.725599	0.855390
C	2.634162	1.697850	-0.117362
H	6.174978	0.268690	-1.767181
H	4.199652	2.224283	-1.474893
H	3.881363	-3.707361	0.797459
H	5.649247	-3.821165	0.817125
H	6.756477	-2.028379	-0.924340
H	2.424275	-1.300720	1.690102
H	2.113034	1.216668	1.846835
H	2.098671	2.629977	-0.255181
H	4.795755	-2.985517	2.125744

Figure S23D Cation C6 TS

1 1

N	0.282788	0.644691	-1.446866
C	-3.035039	-0.389201	1.421128
O	-3.531108	0.407198	2.215769
C	-1.531379	-0.715268	1.398055
C	-0.269550	3.011137	-2.043863
C	-3.112645	-1.999073	-0.483448
C	-4.183456	-2.123295	-1.577146
C	-5.499021	-1.963915	-0.793860
C	-5.175577	-0.904735	0.271996
C	-1.759754	-1.474374	-0.968661
C	-0.636728	0.371172	2.049927
C	0.190495	0.889011	0.886202
C	0.220127	-0.147416	-0.237137
C	-0.018186	1.949740	-1.162944
C	-0.057927	2.147597	0.250339
C	-0.353364	3.418641	0.782611
C	-0.596875	4.464374	-0.090186
C	-0.552690	4.252805	-1.489209
N	-1.066862	-0.816354	-0.001759
N	-3.729250	-1.076520	0.490697
O	-1.346541	-1.626115	-2.116799
H	0.063298	0.197034	-2.328912
H	-1.390797	-1.677693	1.908673
H	-0.249759	2.864305	-3.118668
H	-2.936877	-2.979302	-0.011989
H	-4.109473	-3.071746	-2.112988
H	-4.058485	-1.313680	-2.303678
H	-5.768343	-2.910457	-0.312289
H	-6.333961	-1.662946	-1.431453
H	-5.719284	-1.047853	1.209713
H	-5.373795	0.114107	-0.081442
H	-0.037598	-0.066421	2.846452
H	-1.260423	1.155482	2.483610
H	1.042700	-0.869174	-0.197649
H	-0.386353	3.569928	1.857523
H	-0.827775	5.452743	0.292730
H	-0.754449	5.089075	-2.152370
N	4.420825	0.137988	-1.342505
C	2.951644	1.204971	0.387142
C	5.123178	-3.304831	-0.128381
C	4.678623	-1.892112	-0.363693
C	4.999878	-1.093182	-1.454821
C	3.701266	0.187841	-0.163676
C	3.855940	-1.090782	0.472363
C	3.234678	-1.307586	1.730636
C	2.494841	-0.296450	2.296499
C	2.275395	0.950977	1.616826
H	4.509435	0.887728	-2.014137
H	2.853375	2.168753	-0.102255
H	4.268135	-3.987492	-0.054004
H	5.760536	-3.656043	-0.944905
H	5.616076	-1.332193	-2.311271
H	3.370866	-2.250598	2.251348
H	2.063810	-0.436985	3.282400
H	1.971117	1.806099	2.212811
H	5.693454	-3.396254	0.803823

Figure S23D Cation C6 Product

1 1

N	0.168642	0.394571	-1.466474
C	-3.072888	-0.431485	1.424746
O	-3.381382	0.357176	2.316885
C	-1.668132	-1.048162	1.294805
C	-0.641526	2.772177	-1.691039
C	-3.515386	-1.785976	-0.618621
C	-4.618686	-1.589365	-1.668184
C	-5.857771	-1.263766	-0.815443
C	-5.306373	-0.403603	0.333660
C	-2.101522	-1.468799	-1.111697
C	-0.555606	-0.271073	2.021804
C	0.352193	0.311056	0.910478
C	0.094140	-0.550155	-0.364885
C	-0.231841	1.646064	-0.976878
C	-0.112376	1.676774	0.422680
C	-0.388286	2.842772	1.128523
C	-0.798885	3.981136	0.423350
C	-0.923516	3.937355	-0.969907
N	-1.259926	-1.080984	-0.119984
N	-3.917616	-0.872197	0.469045
O	-1.773660	-1.547210	-2.296960
H	-0.245371	0.055398	-2.330422
H	-1.730707	-2.073238	1.686633
H	-0.742231	2.744607	-2.772042
H	-3.518144	-2.826036	-0.254411
H	-4.745298	-2.472641	-2.297613
H	-4.356684	-0.747306	-2.317050
H	-6.294573	-2.186115	-0.416554
H	-6.634128	-0.743444	-1.382000
H	-5.844700	-0.536664	1.276164
H	-5.311186	0.665698	0.090407
H	-0.017079	-0.941926	2.691280
H	-0.997211	0.517358	2.634675
H	0.800398	-1.372166	-0.512287
H	-0.302018	2.873679	2.211940
H	-1.028041	4.896268	0.960380
H	-1.250461	4.823887	-1.506250

N	4.779457	0.844622	-1.151920
C	2.714170	0.992737	0.227382
C	6.429390	-2.348788	-0.210321
C	5.543922	-1.148574	-0.366203
C	5.758958	-0.070808	-1.249783
C	3.862599	0.415356	-0.193826
C	4.352643	-0.851884	0.303651
C	3.599154	-1.529113	1.315608
C	2.451074	-0.974347	1.775609
C	1.902901	0.336331	1.294319
H	4.719801	1.701220	-1.687705
H	2.371589	1.940826	-0.173234
H	5.915727	-3.264608	-0.524454
H	7.334612	-2.248246	-0.814988
H	6.578373	0.069944	-1.943049
H	3.956770	-2.473638	1.712877
H	1.905312	-1.482826	2.561932
H	1.937171	1.026408	2.159582
H	6.734403	-2.483403	0.833155

Figure S23D Cation C7 TS

1 1

N	-0.527346	0.146970	1.286103
C	3.172773	0.085885	-1.319558
O	3.454134	0.941467	-2.156795
C	1.845911	-0.692482	-1.341597
C	-0.923877	2.576526	1.723200
C	3.611477	-1.279184	0.724723
C	4.571094	-0.960291	1.880368
C	5.829806	-0.455489	1.153495
C	5.279595	0.352766	-0.033354
C	2.127851	-1.198525	1.086885
C	0.706530	0.016135	-2.119050
C	-0.350081	0.271807	-1.055321
C	-0.110613	-0.644707	0.148886
C	-0.700278	1.447219	0.915843
C	-0.605750	1.569557	-0.504236
C	-0.733025	2.834221	-1.116589
C	-0.954194	3.941951	-0.317899
C	-1.046213	3.803730	1.090295
N	1.338490	-0.849788	0.036835
N	3.977120	-0.282273	-0.301119
O	1.695424	-1.419724	2.216437
H	-0.276105	-0.155293	2.219116
H	2.045845	-1.679390	-1.780700
H	-0.989035	2.487699	2.802483
H	3.803394	-2.295378	0.344566
H	4.753631	-1.832904	2.510634
H	4.138383	-0.173717	2.507328
H	6.419676	-1.303320	0.788059
H	6.474122	0.148339	1.797224
H	5.913058	0.307119	-0.923392
H	5.126270	1.408887	0.217919
H	0.355244	-0.616615	-2.933232
H	1.076584	0.948040	-2.551477
H	-0.638048	-1.604183	0.132544
H	-0.655878	2.932906	-2.195503
H	-1.050607	4.926012	-0.764193
H	-1.213348	4.691352	1.693528
N	-3.615715	0.934179	-0.224470
C	-2.238938	-0.350496	-1.901063
C	-5.024906	-1.526235	2.188425
C	-4.349514	-0.751561	1.098394
C	-4.364471	0.601002	0.908829
C	-3.116791	-0.188985	-0.786158
C	-3.552848	-1.291776	0.014268
C	-3.198665	-2.579233	-0.372326
C	-2.431945	-2.775954	-1.545785
C	-2.005459	-1.703170	-2.308078
H	-3.513594	1.872212	-0.588496
H	-2.167527	0.435453	-2.647088
H	-4.300645	-2.095980	2.783297
H	-5.563613	-0.857947	2.866280
H	-4.854184	1.378417	1.477599
H	-3.520538	-3.438635	0.209189
H	-2.195766	-3.787703	-1.859102
H	-1.450000	-1.884123	-3.222397
H	-5.746441	-2.245078	1.781654

Figure S23D Cation C7 Product

1 1

N	-0.389877	0.143650	1.390111
C	3.050916	-0.226684	-1.355094
O	3.194813	0.508531	-2.330615
C	1.825902	-1.140236	-1.163382
C	-0.245296	2.655794	1.321071
C	3.724612	-1.198254	0.837609
C	4.716151	-0.631846	1.864067
C	5.873344	-0.120993	0.987129
C	5.176221	0.450943	-0.258074
C	2.259511	-1.164795	1.279453
C	0.591279	-0.735558	-1.987940
C	-0.469930	-0.264977	-0.962592
C	-0.061694	-0.881347	0.414251
C	-0.312212	1.381815	0.750978
C	-0.378341	1.215857	-0.644451
C	-0.391986	2.323415	-1.489445
C	-0.335968	3.605053	-0.927128
C	-0.260425	3.759227	0.464273
N	1.386110	-1.101225	0.241347
N	3.940743	-0.344539	-0.347884
O	1.915697	-1.178240	2.462180
H	0.062618	0.024631	2.291979
H	2.139437	-2.160216	-1.426563
H	-0.188021	2.784162	2.397611
H	3.979633	-2.243180	0.598366
H	5.023488	-1.384909	2.592571
H	4.243792	0.191911	2.408973
H	6.526924	-0.952840	0.701774
H	6.486921	0.627846	1.494201

H	5.762485	0.343997	-1.174863
H	4.922932	1.511468	-0.141186
H	0.247527	-1.582815	-2.582876
H	0.858476	0.063139	-2.683060
H	-0.557209	-1.822894	0.664650
H	-0.436619	2.202233	-2.568963
H	-0.337830	4.478838	-1.570818
H	-0.209199	4.757879	0.888586
N	-3.309709	1.174502	-0.279515
C	-1.964776	-0.678065	-1.402894
C	-6.045628	-0.332426	1.747708
C	-4.882094	0.032276	0.879481
C	-4.416610	1.276251	0.585506
C	-3.036144	-0.100200	-0.543591
C	-4.018303	-0.884573	0.153046
C	-4.022192	-2.250520	-0.008487
C	-3.064556	-2.885460	-0.866912
C	-2.119253	-2.163820	-1.522970
H	-2.782199	1.967708	-0.629816
H	-2.062438	-0.257351	-2.416648
H	-5.733746	-0.969782	2.583291
H	-6.515751	0.562907	2.162822
H	-4.761147	2.250887	0.898453
H	-4.761619	-2.862981	0.500353
H	-3.112304	-3.961739	-0.992615
H	-1.419111	-2.680493	-2.169513
H	-6.807154	-0.882706	1.182687

Compound **6** Radical Cation
1 2

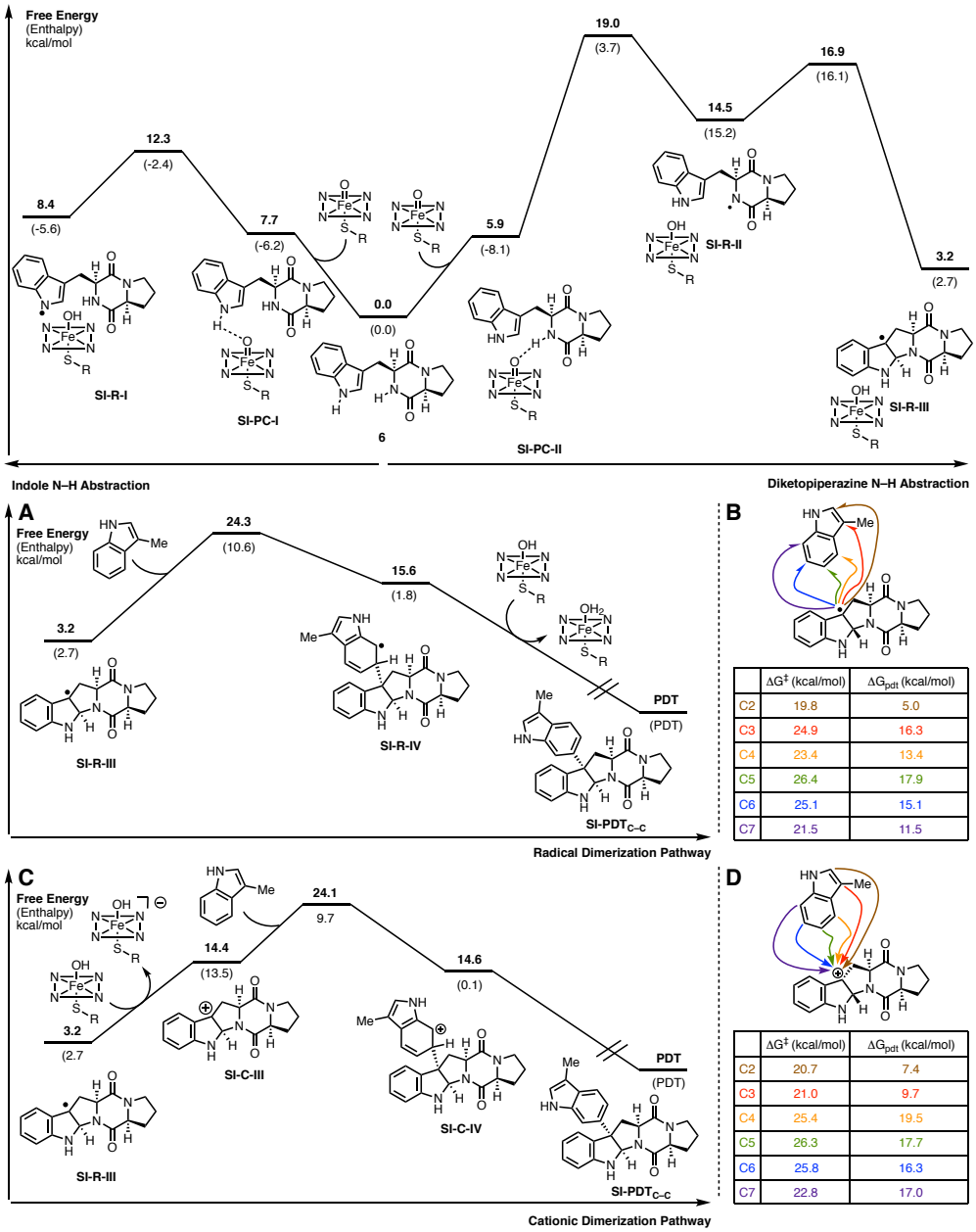
N	3.619127	1.673002	0.931523
C	-1.733273	-1.099358	0.570575
O	-1.580032	-2.071640	1.312202
C	-0.534835	-0.204420	0.182028
C	5.078210	0.312828	-0.611681
C	-3.137632	0.386325	-0.872211
C	-4.610126	0.742506	-0.627587
C	-5.248062	-0.635664	-0.374518
C	-4.176133	-1.421170	0.405296
C	-2.148826	1.522737	-0.668350
C	0.484949	-0.227703	1.351284
C	1.834238	0.285755	0.991920
C	2.402535	1.516279	1.450478
C	3.936560	0.574921	0.111790
C	2.821250	-0.304333	0.147473
C	2.878742	-1.511649	-0.579267
C	4.030813	-1.792945	-1.321724
C	5.106054	-0.901486	-1.340272
N	-0.957245	1.159996	-0.111026
N	-2.916782	-0.741228	0.045410
O	-2.399530	2.672308	-1.009656
H	4.226815	2.465868	1.109906
H	-0.061681	-0.659382	-0.701903
H	5.922524	0.993590	-0.629283
H	-3.011950	0.045210	-1.912663
H	-5.047387	1.275625	-1.473732
H	-4.690320	1.381850	0.258280
H	-5.458007	-1.132239	-1.328077
H	-6.187255	-0.569236	0.179932
H	-4.131840	-2.479203	0.131553
H	-4.313902	-1.360715	1.490264
H	0.548575	-1.276145	1.664838
H	0.070359	0.339949	2.189549
H	1.970350	2.249518	2.118082
H	2.052844	-2.215238	-0.559595
H	4.091014	-2.716637	-1.886685
H	5.990802	-1.139813	-1.921274
H	-0.256931	1.893523	-0.102324

Iron Oxo Anion Triplet
-1 3

Fe	-0.073428	-0.001837	-0.310750
N	-1.285124	1.621577	-0.180319
N	1.550558	1.202948	-0.287649
N	-1.696456	-1.204347	-0.144644
N	1.140382	-1.622091	-0.276528
C	-2.653288	1.625993	-0.140660
C	2.861008	0.816128	-0.389064
C	-0.893012	2.933033	-0.183909
C	1.550140	2.572226	-0.278258
C	-3.008853	-0.817351	-0.108820
C	2.505740	-1.627396	-0.376674
C	-1.694549	-2.574003	-0.127759
C	0.748032	-2.933298	-0.248929
C	-3.145308	2.987235	-0.115666
C	3.719618	1.979164	-0.432436
C	-2.052645	3.798599	-0.140802
C	2.906279	3.069250	-0.359767
C	-3.868012	-1.980310	-0.060118
C	2.996351	-2.988679	-0.404731
C	-3.052198	-3.070631	-0.070422
C	1.905274	-3.799150	-0.322812
H	-4.192029	3.263174	-0.079544
H	4.799621	1.945343	-0.506726
H	-2.013474	4.880896	-0.131048
H	3.178594	4.117521	-0.364451
H	-4.949813	-1.945731	-0.021225
H	4.040958	-3.265924	-0.475557
H	-3.323941	-4.118684	-0.043185
H	1.866285	-4.881470	-0.313659
C	-3.464513	0.497224	-0.110210
C	3.314956	-0.497415	-0.436220
C	-0.565377	-3.384350	-0.172930
C	0.421338	3.383954	-0.223028
H	-4.538521	0.653658	-0.075410
H	4.386730	-0.653329	-0.515941
H	-0.722758	-4.458756	-0.156214
H	0.580286	4.458240	-0.221891
O	-0.140198	-0.004882	-1.957473
S	-0.077129	-0.034934	2.209741

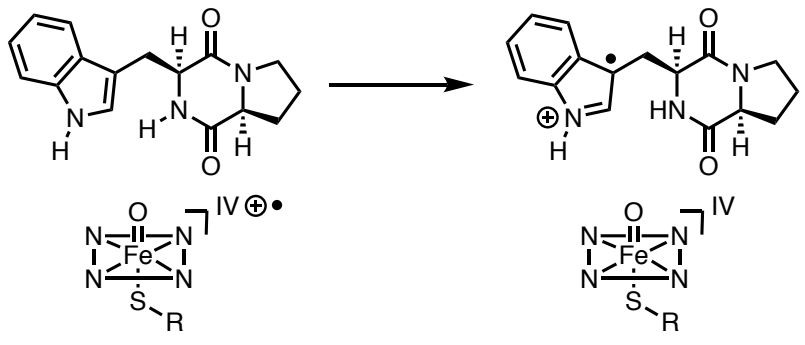
C	1.657207	0.073177	2.813500
H	2.134832	1.007989	2.502419
H	1.660012	0.034311	3.908788
H	2.263352	-0.758495	2.439339

Supplementary Figure 23. Reaction coordinate diagrams for formation of (+)-naseseazine B (**2**), and single electron oxidation to radical cation.



	ΔG‡ (kcal/mol)	ΔG$_{pdt}$ (kcal/mol)
C2	19.8	5.0
C3	24.9	16.3
C4	23.4	13.4
C5	26.4	17.9
C6	25.1	15.1
C7	21.5	11.5

	ΔG‡ (kcal/mol)	ΔG$_{pdt}$ (kcal/mol)
C2	20.7	7.4
C3	21.0	9.7
C4	25.4	19.5
C5	26.3	17.7
C6	25.8	16.3
C7	22.8	17.0



0.0
(0.0)

41.2
(41.3)

Computational References:

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Chemistry

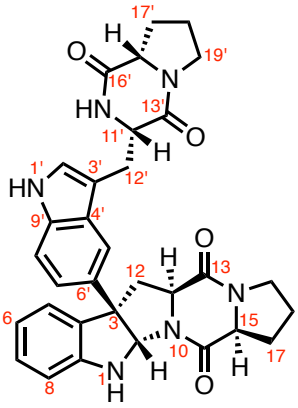
General Procedures:
All reactions were performed in oven-dried or flame-dried round-bottom flasks. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of argon. Gas-tight syringes with stainless steel needles or cannulae were used to transfer air- and moisture-sensitive liquids. Where necessary (so noted), reactions were performed in Schlenk tubes fitted with a PTFE stopcock. Flash column chromatography was performed as described by Still et al. using granular silica gel (60 Å pore size, 40–63 μm, 4–6% H2O content, Zeochem). Analytical thin layer chromatography (TLC) was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). TLC plates were visualized by exposure to short wave ultraviolet light (254 nm) and an aqueous solution of ceric ammonium molybdate (CAM) followed by heating on a hot plate (~250 ºC). Organic solutions were concentrated at 29–30 °C on rotary evaporators capable of achieving a minimum pressure of ~2 torr.

Materials:
Commercial reagents and solvents were used as received with the following exceptions: dichloromethane, acetonitrile, tetrahydrofuran, methanol, pyridine, toluene, and triethylamine were purchased from J.T. Baker (CycletainerTM) and were purified by the method of Grubbs et al. under positive argon pressure. Nitroethane was distilled over calcium hydride and stored over 4 Å molecular sieves. Silver hexafluoroantimonate was purchased from Strem Chemicals, Inc. All other solvents and chemicals were purchased from Sigma–Aldrich.

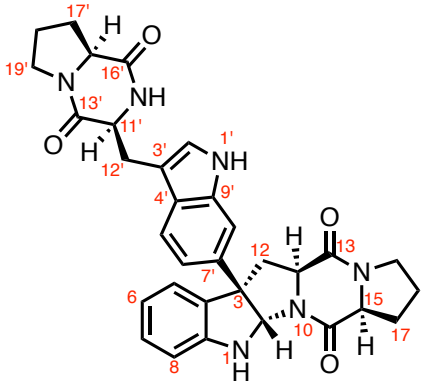
Instrumentation:
Proton nuclear magnetic resonance (1H NMR) spectra were recorded with Varian inverse probe INOVA-500 and Varian INOVA-500 spectrometers, or a Bruker AVANCE III 400 spectrometer. Chemical shifts are reported in parts per million on the δ scale, and are referenced from the residual protium in the NMR solvent (CHCl3: δ 7.26, CD3SOCD2H: δ 2.50, CD2HOD: δ 3.31). Data are reported as follows: chemical shift [multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant(s) in Hertz, integration, assignment]. Carbon-13 nuclear magnetic resonance (13C NMR) spectra were recorded with a Varian INOVA-500 spectrometer or a Bruker AVANCE III 400 spectrometer and are reported in parts per million on the δ scale, and are referenced from the carbon resonances of the solvent (CDCl3: δ 77.16, DMSO-d6: δ 39.52, CD3OD: δ 49.00). Data are reported as follows: chemical shift (assignment). Data are reported as follows: chemical shift (assignment). Infrared data (IR) were obtained with a Perkin-Elmer 2000 FTIR, and are reported as follows: frequency of absorption (cm–1), intensity of absorption (s = strong, m = medium, w = weak, br = broad). Optical rotations were measured on a Jasco-1010 polarimeter. UV-Vis spectrophotometric data were acquired on a Varian Cary 50 Bio UV-Vis spectrophotometer. Preprative HPLC was performed on a Waters system with the 1525 Binary HPLC Pump, 2489 UV/Vis Detector, 3100 Mass Detector, System Fluidics Organizer, and 2767 Sample Manager components. We thank Liam P. Kelly for obtaining the mass spectrometric data at the Department of Chemistry's Instrumentation Facility, Massachusetts Institute of Technology. High resolution mass spectra (HRMS) were recorded on a Bruker Daltonics APEXIV 4.7 Tesla FT-ICR-MS using either an electrospray (ESI) or direct analysis in real time (DART) ionization source.

Positional Numbering System.

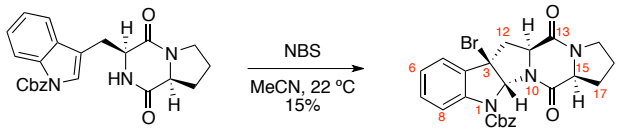
In assigning the ^{1}H and ^{13}C NMR data of all intermediates en route to our total syntheses of (–)-naseseazine C and (–)-iso-naseseazine C, we wished to employ a uniform numbering scheme. This numbering system is also consistent with that employed in the isolation papers of naseseazine C and iso-naseseazine B.[1,2]



(–)-naseseazine C (**4**)

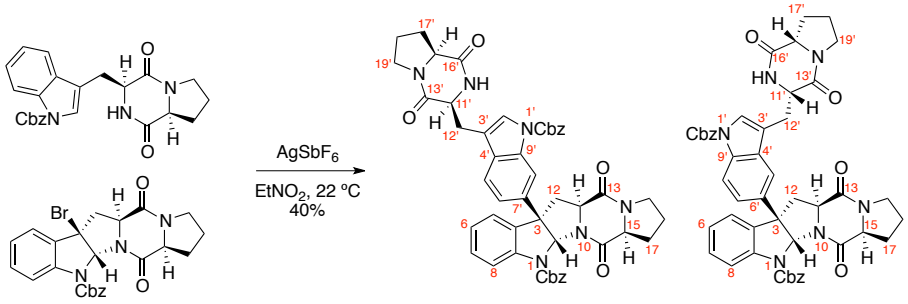


(–)-*iso*-naseseazine C (**11**)



Diketopiperazine bromide (–)-8: A sample of N-bromosuccinimide (641 mg, 3.60 mmol, 3.00 equiv) was added in one portion to a stirred suspension of diketopiperazine **7** (500 mg, 1.20 mmol, 1 equiv) in acetonitrile (60 mL). After 25 min, a solution of saturated aqueous sodium thiosulfate solution (30 mL) was added to the reaction mixture. After 10 min, the reaction mixture was diluted with ethyl acetate (30 mL), and washed with saturated aqueous sodium thiosulfate solution (30 mL). The aqueous layer was extracted with ethyl acetate (3 × 20 mL) and the combined organic layers were dried over anhydrous sodium sulfate, were filtered, and were concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel (eluent: 30→35% ethyl acetate in hexanes), including a second chromatographic purification (eluent: 30→35% ethyl acetate in hexanes) to afford diketopiperazine bromide (-)-**8** (90.5 mg, 14.8%) as an off-white foam.

Structural assignments were made using additional information from gCOSY, HSQC, HMBC and nOe experiments. 1H NMR (MHz, CDCl3, 20 ºC): δ 7.69 (app-br-s, 1H, C8H), 7.48 (app-d, J = 7.3 Hz, 2H, PhCbz-o-H), 7.43 (d, J = 7.7 Hz, 1H, C5H), 7.41–7.30 (m, 4H, C7H, PhCbz-m-H, PhCbz-p-H), 7.16 (app-t, J = 7.5 Hz, 1H, C6H), 6.57 (s, 1H, C2H), 5.43 (d, J = 12.2 Hz, 1H, PhCbzCHa), 5.31 (d, J = 12.3 Hz, 1H, PhCbzCHb), 4.04 (app-t, J = 8.2 Hz, 1H, C15H), 3.97 (dd, J = 5.9, 11.4 Hz, 1H, C11H), 3.62–3.45 (m, 2H, C19H), 3.35 (dd, J = 5.9, 13.2 Hz, 1H, C12Ha), 3.01 (dd, J = 11.0, 13.2 Hz, 1H, C12Hb), 2.35–2.23 (m, 1H, C17Ha), 2.25–2.14 (m, 1H, C17Hb), 2.10–1.97 (m, 1H, C18Ha), 1.95–1.80 (m, 1H, C18Hb). 13C NMR (100 MHz, CDCl3, 20 ºC): δ 165.8 (C16), 164.2 (C13), 153.0 (NC=OCbz), 141.4 (C9), 135.8 (PhCbz-i-C), 132.0 (C4), 131.2 (PhCbz), 128.7 (C7), 128.5 (PhCbz-o-C), 128.4 (PhCbz), 125.1 (C6), 123.9 (C5), 117.7 (C8), 83.3 (C2), 68.6, 60.4 (2C, C11, C15), 59.0 (C3), 45.6 (C19), 43.1 (C12), 27.8 (C17), 23.1 (C18). FTIR (thin film) cm–1: 2957 (w), 2887 (w), 1716 (s), 1674 (s), 1329 (m). HRMS (ESI) (m/z):calc'd for C24H23BrN3O4 [M+H]+: 496.0866, found: 496.0858. [α]D24: –168 (c = 0.46, CH2Cl2). TLC (70% ethyl acetate in hexanes), Rf: 0.22 (UV, CAM).

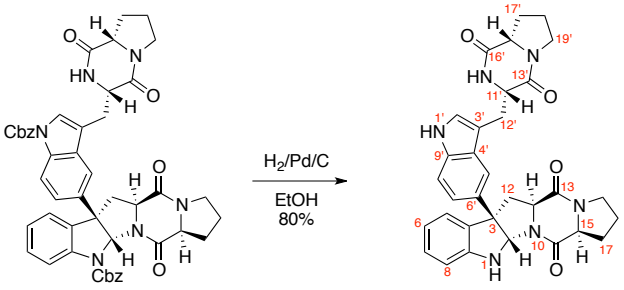


***meta*-(−)-*N*^{in},*N*$^{in'}$-Dicarboxybenzyl *iso*-Naseseazine C (10) and *para*-(−)-*N*^{in},*N*$^{in'}$-Dicarboxybenzyl Naseseazine C (9):** Diketopiperazine bromide **(–)-8** (100 mg, 0.196 mmol, 1 equiv) and proline diketopiperazine **7** (245 mg, 0.588 mmol, 3.00 equiv) were azeotropically dried from anhydrous benzene (3 × 0.5 mL) and the residue was suspended in freshly distilled nitroethane (9.8 mL). Silver hexafluoroantimonate (202 mg, 0.588 mmol, 3.00 equiv) was then added as a solid in a single portion. After 4.5 h, the reaction mixture was diluted with dichloromethane (15 mL) and washed with a mixture of saturated aqueous sodium bicarbonate and saturated aqueous sodium thiosulfate (10:1 v/v, 15 mL). The resulting aqueous layer was extracted with dichloromethane (3 × 10 mL) and the combined organic layers were dried over anhydrous sodium sulfate, were filtered, and were concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel (eluent: 10→50% acetone in dichloromethane) to afford a regioisomeric mixture of (–)-**10** and (–)-**9** (65.6 mg, 40.1%, (−)-**10**:(−)-**9**, 1.4:1) as a white foam. Regioisomers (−)-**10** and (−)-**9** were separated for the purpose of full and independent characterization by preparative HPLC [Luna preparative HPLC column, C18, 5 µm, 21.2 × 250 mm; 7.0 mL/min; gradient, 5%→100% acetonitrile in water with 0.1% formic acid, 60 min; t_R((−)-**10**) = 48.3 min, t_R((−)-**9**) = 50.4 min]. Structural assignments were made using additional information from gCOSY, HSQC, HMBC and nOe experiments.

***para*-(−)-*N*^{in},*N*$^{in'}$-Dicarboxybenzyl Naseseazine C (9):** ^{1}H NMR (500 MHz, $CDCl_3$, 20 ºC): δ 7.99 (br-s, 1H, $C_{8'}$**H**), 7.71 (br-s, 1H, C_8**H**), 7.53 (s, 1H, $C_{2'}$**H**), 7.48–7.43 (m, 3H, $C_{5'}$**H**, Ph_{Cbz}-**H**), 7.43–7.35 (m, 5H, Ph_{Cbz}-**H**), 7.34–7.26 (m, 4H, C_7**H**) Ph_{Cbz}-**H**), 7.22 (d, *J* = 7.4 Hz, 1H, C_5**H**), 7.10 (app-t, *J* = 7.5 Hz, 1H, C_6**H**), 7.04 (d, *J* = 8.8 Hz, 1H, $C_{7'}$**H**), 6.61 (s, 1H, C_2**H**), 5.69 (s, 1H, $N_{10'}$**H**), 5.42 (app-s, 2H, $Ph_{Cbz'}$**C**H_2), 5.39 (d, *J* = 12.2 Hz, 1H, $Ph_{Cbz'}$**C**H_a), 5.28 (d, *J* = 12.3 Hz, 1H, $Ph_{Cbz'}$**C**H_b), 4.31 (dd, *J* = 3.5, 10.7 Hz, 1H, $C_{11'}$**H**), 4.15 (dd, *J* = 5.8, 11.3 Hz, 1H, C_{11}**H**), 4.10 (app-q, *J* = 7.8 Hz, 2H, C_{15}**H**, $C_{15'}$**H**), 3.69–3.47 (m, 5H, $C_{12'}$**H**$_a$, C_{19}**H**, $C_{19'}$**H**), 3.16 (dd, *J* = 5.8, 12.9 Hz, 1H, C_{12}**H**$_a$), 2.91–2.82 (m, 2H, C_{12}**H**$_b$, $C_{12'}$**H**$_b$), 2.36–2.27 (m, 2H, $C_{17'}$**H**), 2.27–2.11 (m, 1H, C_{17}**H**$_a$), 2.11–1.95 (m, 3H, C_{17}**H**$_b$, C_{18}**H**), 1.96–1.84 (m, 2H, $C_{18'}$**H**). ^{13}C NMR (125 MHz, $CDCl_3$, 20 ºC): δ 169.5 (**C**$_{16'}$), 166.0 (**C**$_{16}$), 165.4 (**C**$_{13}$), 164.9 (**C**$_{13'}$), 153.1 (**C**$_{Cbz}$=O), 150.4 (**C**$_{Cbz'}$=O), 141.5 (**C**$_9$), 136.6 (**C**$_{6'}$), 136.1 (Ph_{Cbz}-*i*-**C**), 135.1 (**C**$_4$), 134.8 (2C, **C**$_{9'}$, $Ph_{Cbz'}$-*i*-**C**), 130.0 (**C**$_{4'}$), 129.3 (**C**$_7$), 129.0 (2C, Ph_{Cbz}-**C**), 128.8 (Ph_{Cbz}-**C**), 128.6 (Ph_{Cbz}-**C**), 128.3 (2C, Ph_{Cbz}-**C**), 125.0 (**C**$_{2'}$), 124.8 (**C**$_6$), 124.0 (**C**$_5$), 123.6 (**C**$_{7'}$), 117.6 (**C**$_8$), 116.3 (**C**$_{8'}$), 116.0 (**C**$_{3'}$), 115.4 (**C**$_{5'}$), 81.9 (**C**$_2$), 69.2 ($Ph_{Cbz'}$-**C**H_2), 68.3 (Ph_{Cbz}-**C**H_2), 60.7 (**C**$_{11}$ or **C**$_{15'}$), 60.6 (**C**$_{11}$ or **C**$_{15'}$), 59.3 (**C**$_{15}$), 58.2 (**C**$_3$), 53.9 (**C**$_{11'}$), 45.6 (**C**$_{19}$ or **C**$_{19'}$), 45.5 (**C**$_{19}$ or **C**$_{19'}$), 39.6 (**C**$_{12}$), 28.4 (**C**$_{17'}$), 27.9 (**C**$_{17}$), 26.5 (**C**$_{12'}$), 23.1 (**C**$_{18'}$), 22.8 (**C**$_{18}$). FTIR (thin film) cm^{-1}: 3472 (br-m), 2956 (w), 1716 (s), 1668 (s), 1479 (m), 1401 (m). HRMS (ESI) (*m*/*z*): calc'd for $C_{48}H_{45}N_6O_8$ $[M+H]^+$: 833.3293, found: 833.3286. $[\alpha]_D^{24}$: –128 (*c* = 0.24, CH_2Cl_2). TLC (70% acetone in hexanes), R*f*: 0.24 (UV, CAM).

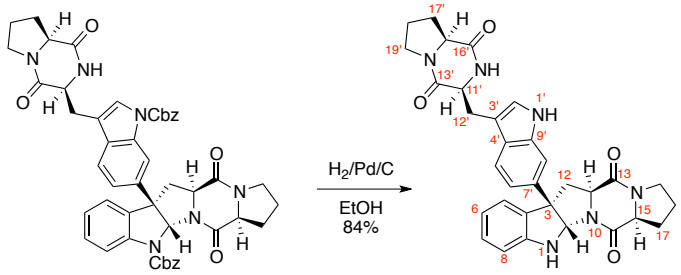
***meta*-(−)-*N*^{in},*N*$^{in'}$-Dicarboxybenzyl *iso*-Naseseazine C (10):** ^{1}H NMR (MHz, $CDCl_3$, 20 ºC): δ 8.19 (br-s, 1H, $C_{8'}$**H**), 7.73 (br-s, 1H, C_8**H**), 7.50 (s, 1H, $C_{2'}$**H**), 7.48–7.38 (m, 6H, Ph_{Cbz}-**H**), 7.38–7.34 (m, 2H, $C_{5'}$**H**, Ph_{Cbz}-**H**), 7.34–7.26 (m, 4H, C_7**H**, Ph_{Cbz}-**H**), 7.19 (d, *J* = 7.5 Hz, 1H, C_5**H**), 7.08 (d, *J* = 7.5 Hz, 1H, $C_{6'}$**H**), 7.07–7.02 (m, 1H, C_6**H**), 6.64 (s, 1H, C_2**H**), 5.57 (s, 1H, $N_{10'}$**H**), 5.41 (d, *J* = 12.3 Hz, 1H, Ph_{Cbz}**C**H_a), 5.39 (app-s, 2H, $Ph_{Cbz'}$**C**H_2), 5.28 (d, *J* = 12.3 Hz, 1H, Ph_{Cbz}**C**H_b), 4.29 (dd, *J* = 2.9, 10.2 Hz, 1H, $C_{11'}$**H**), 4.18–4.14 (m, 1H, C_{11}**H**), 4.14–4.08 (m, 1H, $C_{15'}$**H**), 4.05 (app-t, *J* = 8.0 Hz, 1H, C_{15}**H**), 3.67–3.50 (m, 5H, $C_{12'}$**H**$_a$, C_{19}**H**, $C_{19'}$**H**), 3.15 (dd, *J* = 5.8, 12.9 Hz, 1H, C_{12}**H**$_a$), 2.92–2.81 (m, 2H, C_{12}**H**$_b$, $C_{12'}$**H**$_b$), 2.37–2.28 (m, 2H), 2.27–2.15 (m, 1H, $C_{17'}$**H**), 2.11–1.98 (m, 3H, C_{17}**H**$_b$, C_{18}**H**), 1.98–1.85 (m, 2H, $C_{18'}$**H**). ^{13}C NMR (MHz, $CDCl_3$, 20 ºC): δ 169.4 (**C**$_{16'}$), 166.0 (**C**$_{16}$), 165.4 (**C**$_{13}$), 165.0 (**C**$_{13'}$), 153.1 (**C**$_{Cbz}$=O), 150.3 (**C**$_{Cbz'}$=O), 141.5 (**C**$_9$), 138.8 (**C**$_{7'}$), 136.2 (2C, **C**$_{4'}$, Ph_{Cbz}-*i*-**C**), 134.9 (3C, **C**$_4$, **C**$_{9'}$, $Ph_{Cbz'}$-*i*-**C**), 129.3 (**C**$_7$), 129.0 (2C, Ph_{Cbz}-**C**), 128.8 (Ph_{Cbz}-**C**), 128.6 (Ph_{Cbz}-**C**),

128.3 (Ph_{Cbz}-**C**), 128.2 (Ph_{Cbz}-**C**), 124.8 (**C**$_{2'}$), 124.7 (**C**$_{7'}$), 124.0 (**C**$_5$), 121.1 (**C**$_6$), 119.5 (**C**$_{5'}$), 117.6 (**C**$_8$), 115.7 (**C**$_{3'}$), 113.0 (**C**$_{8'}$), 81.8 (**C**$_2$), 69.1 ($Ph_{Cbz'}$-**C**H_2), 68.3 (Ph_{Cbz}-**C**H_2), 60.7 (**C**$_{11}$ or **C**$_{15'}$), 60.6 (**C**$_{11}$ or **C**$_{15'}$), 59.3 (**C**$_{15}$), 58.6 (**C**$_3$), 54.0 (**C**$_{11'}$), 45.6 (**C**$_{19}$ or **C**$_{19'}$), 45.5 (**C**$_{19}$ or **C**$_{19'}$), 39.4 (**C**$_{12}$), 28.4 (**C**$_{17'}$), 28.0 (**C**$_{17}$), 26.5 (**C**$_{12'}$), 23.1 (**C**$_{18'}$), 22.7 (**C**$_{18}$). FTIR (thin film) cm^{-1}: 3472 (br-m), 2955 (w), 1713 (s), 1667 (s), 1480 (m), 1398 (m). HRMS (ESI) (*m*/*z*): calc'd for $C_{48}H_{45}N_6O_8$ $[M+H]^+$: 833.3293, found: 833.3278. $[\alpha]_D^{24}$: –166 (*c* = 0.26, $CHCl_3$). TLC (70% acetone in hexanes), R*f*: 0.28 (UV, CAM).



(−)-Naseseazine C (4): Palladium on activated charcoal (3.3 mg, 3.1 µmol, 20 mol%) was added to a solution of para(−)-Nin,Nin'-dicarboxybenzyl naseseazine C (–)-**9** (12.9 mg, 30.4 mmol, 1 equiv) in degassed (N_2 stream, 5 min) ethanol (1.6 mL). A stream of hydrogen gas was passed through the heterogeneous mixture for 2 min by discharge of a balloon equipped with a needle extending into the reaction mixture. After stirring the reaction mixture at 22 °C for 21 h under an atmosphere of hydrogen gas, the solution was degassed (N_2 stream, 5 min) and filtered through Celite. The filter cake was washed with methanol (3 × 2 mL) and the combined filtrates were concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel (eluent: 70→ 90% acetone in dichloromethane) to afford **(–)-4** (7.0 mg, 80%). Structural assignments were made using additional information from gCOSY, HSQC, HMBC and nOe experiments.

1H NMR (MHz, CD3OD, 20 ºC): δ 7.64 (d, J = 1.8 Hz, 1H, C5'H), 7.24 (d, J = 8.6 Hz, 1H, C8'H), 7.19 (d, J = 7.4 Hz, 1H, C5H), 7.13 (dd, J = 1.9, 8.6 Hz, 1H, C7'H), 7.08 (s, 1H, C2'H), 7.06 (td, J = 1.2, 7.6 Hz, 1H, C7H), 6.75 (td, J = 1.0, 7.5 Hz, 1H, C6H), 6.71 (d, J = 8.1 Hz, 1H, C8H), 5.70 (s, 1H, C2H), 4.39 (td, J = 1.8, 4.9 Hz, 1H, C11'H), 4.31–4.23 (m, 2H, C11H, C15H), 3.97 (ddd, J = 1.9, 6.4, 10.9 Hz, 1H, C15'H), 3.54–3.47 (m, 2H, C19H), 3.45–3.39 (m, 1H, C19'Ha), 3.28 (app-d, J = 5.2 Hz, 2H, C12'H), 3.26–3.21 (m, 1H, C19'Hb), 3.12 (dd, J = 6.1, 12.7 Hz, 1H, C12Ha), 2.95–2.88 (m, 1H, C12Hb), 2.33–2.25 (m, 1H, C17Ha), 2.10–2.00 (m, 2H, C17Hb, C18Ha), 1.98–1.87 (m, 2H, C17'Ha, C18Hb), 1.71–1.60 (m, 1H, C18'Ha), 1.48–1.40 (m, 1H, C18'Hb), 0.98–0.88 (m, 1H, C17'Hb). 1H NMR (MHz, DMSO-d6, 20 ºC): δ 10.84 (s, 1H, N1'H), 7.74 (s, 1H, N10'H), 7.63 (s, 1H, C5'H), 7.22, (d, J = 8.6 Hz, 1H, C8'H), 7.17 (s, 1H, C8'H), 7.16 (d, J = 8.7 Hz, 1H, C5H), 7.03 (d, J = 8.6 Hz, 1H, C7'H), 6.98 (app-t, J = 7.7 Hz, 1H, C7H), 6.65 (d, J = 8.6 Hz, C8H), 6.64 (s, 1H, N1H), 6.61 (app-t, J = 7.4 Hz, 1H, C6H), 5.63 (s, 1H, C2H), 4.35–4.27 (m, 2H, C11'H, C15H), 4.16 (dd, J = 6.1, 11.4 Hz, 1H, C11H), 4.09 (app-t, J = 8.4 Hz, 1H, C15'H), 3.45–3.33 (m, 3H, C19H, C19'Ha), 3.33–3.23 (m, 1H, C19'Hb), 3.22 (dd, J = 4.8, 14.9 Hz, 1H, C12'Ha), 3.10–3.02 (m, 2H, C12Ha, C12'Hb), 2.68 (app-t, J = 12.0 Hz, 1H, C12Hb), 2.19–2.08 (m, 1H, C17Ha), 2.04–1.97 (m, 1H, C17'Ha), 1.97–1.86 (m, 2H, C17Hb, C18Ha), 1.85–1.76 (m, 1H, C18Hb), 1.75–1.68 (m, 1H, C18'Ha), 1.68–1.59 (m, 1H, C18'Hb), 1.53–1.42 (m, 1H, C17'Hb). 13C NMR (MHz, CD3OD, 20 ºC): δ 170.7 (C16'), 168.5 (C16), 168.0 (C13), 167.4 (C13'), 150.6 (C9), 136.9 (C9'), 135.3 (C6'), 134.2 (C4), 129.6 (C7), 128.5 (C4'), 126.2 (C2'), 125.2 (C5), 121.1 (C7'), 120.5 (C6), 116.3 (C5'), 112.6 (C8'), 111.1 (C8), 109.9 (C3'), 83.6 (C2), 61.9 (C15), 61.7 (C11), 60.8 (C3), 60.0 (C15'), 57.2 (C11'), 46.3 (C19), 46.0 (C19'), 41.1 (C12), 29.1 (2C, C12', C17'), 28.9 (C17), 23.8 (C18), 22.6 (C18'). 13C NMR (MHz, DMSO-d6, 20 ºC) : δ 169.2 (C16'), 166.0 (C16), 165.6 (C13'), 165.3 (C13), 149.3 (C9), 134.8 (C9'), 134.1 (C6'), 133.0 (C4), 128.1 (C7), 127.1 (C4'), 124.8 (C2'), 123.8 (C5), 119.2 (C7'), 118.1 (C6), 114.6 (C5'), 111.4 (C8'), 109.6 (C3'), 109.5 (C8), 81.1 (C2), 60.1 (C11), 59.7 (C15), 58.7 (C3), 58.5 (C15'), 55.1 (C11'), 44.7 (2C, C19, C19'), 39.9 (C12), 27.7 (C17'), 27.4 (C17), 25.4 (C12'), 22.6 (C18), 22.0 (C18'). FTIR (thin film) cm–1: 3310 (br-m), 2926 (m), 1661 (s), 1435 (s), 1301 (w), 1150 (w). HRMS (ESI) (m/z): calc'd for C32H33N6O4 [M+H]+:565.2558, found: 565.2551. [α]D24: –180 (c = 0.16, CH3OH). TLC (80% acetone in dichloromethane), Rf: 0.11 (UV, CAM).



(−)-iso-Naseseazine C (11): Palladium on activated charcoal (6.5 mg, 6.1 μmol, 20.0 mol%) was added to a solution of meta(−)-Nin,Nin'-dicarboxybenzyl iso-naseseazine C **(–)-10** (25.2 mg, 30.3 μmol, 1 equiv) in degassed (N_2 stream, 5 min) ethanol (3 mL). A stream of hydrogen gas was passed through the heterogeneous mixture for 2 min by discharge of a balloon equipped with a needle extending into the reaction mixture. After stirring the reaction mixture at 22 °C for 64 h under an atmosphere of hydrogen gas, the solution was degassed (N_2 stream, 5 min) and filtered over Celite. The filter cake was washed with methanol (3 × 2 mL) and the combined filtrates were concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel (eluent: 70→ 90% acetone in dichloromethane) to afford **(–)-11** (14.3 mg, 83.6%). Structural assignments were made using additional information from gCOSY, HSQC, HMBC and nOe experiments.

1H NMR (MHz, CD3OD, 20 ºC): δ 7.49 (d, J = 8.4 Hz, 1H, C5'H), 7.31 (d, J = 1.6 Hz, 1H, C8'H), 7.11 –7.01 (m, 2H, C5H, C6'H), 7.06 (s, 1H, C2'H), 7.05 (td, J = 1.1, 7.1 Hz, 1H, C7H), 6.72 (td, J = 1.0, 7.5 Hz, 1H, C6H), 6.70 (d, J = 7.7 Hz, 1H, C8H), 5.64 (s, 1H, C2H), 4.35 (td, J = 1.8, 5.0 Hz, 1H, C11'H), 4.21–4.15 (m, 2H, C11H, C15H), 3.92 (ddd, J = 1.9, 6.5, 11.0 Hz, 1H, C15'H), 3.54–3.44 (m, 2H, C19H), 3.44–3.37 (m, 1H, C19'Ha), 3.26 (app-d, J = 4.5 Hz, 2H, C12'H), 3.24–3.19 (m, 1H, C19'Hb), 3.05 (dd, J = 6.0, 12.6 Hz, 1H, C12Ha), 2.85–2.78 (m, 1H, C12Hb), 2.29–2.21 (m, 1H, C17Ha), 2.08–1.97 (m, 2H, C17Hb, C18Ha), 1.95–1.85 (m, 2H, C17'Ha, C18Hb), 1.67–1.56 (m, 1H, C18'Ha), 1.46–1.30 (m, 1H, C18'Hb), 0.96–0.86 (m, 1H, C17'Hb). 1H NMR (MHz, DMSO-d6, 20 ºC): δ 10.79 (d, J = 2.5 Hz, 1H, N1'H), 7.68 (s, 1H, N10'H), 7.50 (d, J = 8.4 Hz, 1H, C5'H), 7.23 (d, J = 1.6 Hz, 1H, C8'H), 7.17 (d, J = 7.4 Hz, 1H, C5H), 7.15 (d, J = 2.4 Hz, 1H, C2'H), 7.08 (dd, J = 1.8, 8.3 Hz, 1H, C6'H), 6.99 (app-t, J = 7.8 Hz, 1H, C7H), 6.65 (d, J = 4.7 Hz, 1H, C8H), 6.65 (s, 1H, N1H), 6.63 (d, J = 7.5 Hz, 1H, C6H), 5.56 (s, 1H, C2H), 4.31 (ddd, J = 1.8, 6.9, 9.1 Hz, 1H, C15H), 4.26 (app-t, J = 5.3 Hz, 1H, C11'H), 4.17 (ddd, J = 3.2, 6.6, 10.1 Hz, 1H, C11H), 4.05 (dd, J = 6.9, 9.7 Hz, 1H, C15'H), 3.45–3.30 (m, 3H, C19'Ha, C19H), 3.25 (td, J = 4.3, 7.7, 8.3 Hz, 1H, C19'Hb), 3.20 (app-dd, J = 4.9, 15.0 Hz, 1H, C12'Ha), 3.03 (app-ddd, J = 6.1, 13.8, 21.2 Hz, 2H, C12'Hb, C12Ha), 2.70–2.61 (m, 1H, C12Hb), 2.19–2.07 (m, 1H, C17'Ha), 2.01–1.86 (m, 3H, C17H, C18Ha), 1.86–1.73 (m, 1H, C18Hb), 1.73–1.63 (m, 1H, C18'Ha), 1.63–1.56 (m, 1H, C18'Hb), 1.46–1.35 (m, 1H, C17'Hb). 13C NMR (MHz, CD3OD, 20 ºC): δ 170.8 (C16'), 168.5 (C16), 168.0 (C13), 167.4 (C13'), 150.6 (C9), 138.2 (C7'), 137.9 (C9'), 133.8 (C4), 129.7 (C7), 127.6 (C4'), 126.1 (C2'), 125.1 (C5), 120.4 (C5' or C6), 120.3 (C5' or C6), 118.0 (C6'), 111.1 (C8), 109.5 (C3'), 109.3 (C8'), 83.5 (C2), 61.8 (C11), 61.6 (C15), 60.7 (C3), 60.0 (C15'), 57.1 (C11'), 46.3 (C19), 46.0 (C19'), 40.9 (C12), 29.1 (C12' or C17'), 29.0 (C12' or C17'), 28.8 (C17), 23.8 (C18), 22.5 (C18'). 13C NMR (MHz, DMSO-d6, 20 ºC): δ 169.1 (C16'), 166.1 (C16), 165.5 (C13'), 165.3 (C13), 149.4 (C9), 136.8 (C7'), 135.9 (C9'), 132.4 (C4), 128.2 (C7), 126.1 (C4'), 124.8 (C2'), 124.0 (C5), 119.0 (C5'), 118.1 (C6), 116.4 (C6'), 109.5 (C8), 109.2 (C3'), 108.0 (C8'), 81.5 (C2), 60.2 (C11), 59.6 (C15), 58.8 (C3), 58.4 (C15'), 55.2 (C11'), 44.8 (C19 or C19'), 44.6 (C19 or C19'), 39.9 (C12), 27.6 (C17'), 27.4 (C17), 25.7 (C12'), 22.6 (C18), 21.9 (C18'). FTIR (thin film) cm–1: 3310 (br-m), 2955 (w), 1653 (s), 1457 (m), 1340 (w), 1056 (w). HRMS (ESI) (m/z): calc'd for C32H33N6O4 [M+H]+: 565.2558, found: 565.2554. [α]D24: –312 (c = 0.42, CH3OH). TLC (80% acetone in dichloromethane), Rf: 0.11 (UV, CAM).

Supplementary Table 6. Comparison of our ^{13}C NMR data for (–)-naseseazine C (**4**) and (–)-*iso*-naseseazine C (**11**) with literature data (CD_3OD).[1]

Assignment	**Wang Report**[1] *iso*-naseseazine B ^{13}C NMR, 150 MHz, CD_3OD	**This Work** (–)-naseseazine C (**4**) ^{13}C NMR, 125 MHz, CD_3OD, 20 ºC	**This Work** (–)-*iso*-naseseazine C (**11**) ^{13}C NMR, 125 MHz CD_3OD, 20 ºC	**Chemical Shift Difference** Δδ = δ (–)-naseseazine C (this work) – δ (Wang report)[1]	**Chemical Shift Difference** Δδ = δ (–)-*iso*-naseseazine C (this work) – δ (Wang report)[1]
C2	83.6	83.6	83.5	0	–0.1
C3	60.8	60.8	60.7	0	–0.1
C4	134.2	134.2	133.8	0	–0.4
C5	125.2	125.2	125.1	0	–0.1
C6	120.5	120.5	120.4 or 120.3	0	–0.1 or –0.2
C7	129.7	129.6	129.7	–0.1	0
C8	111.2	111.1	111.1	–0.1	–0.1
C9	150.6	150.6	150.6	0	0
C11	62.0	61.9	61.8	–0.1	–0.2
C12	41.1	41.1	40.9	0	–0.2
C13	168.1	168.0	168.0	–0.1	–0.1
C15	61.7	61.9	61.6	0.2	–0.1
C16	168.6	168.5	168.5	–0.1	–0.1
C17	28.9	28.9	28.8	0	–0.1
C18	23.9	23.8	23.8	–0.1	–0.1
C19	46.4	46.3	46.3	–0.1	–0.1
C2'	126.3	126.2	126.1	–0.1	–0.2
C3'	109.8	109.9	109.5	0.1	–0.3
C4'	128.5	128.5	127.6	0	–0.9
C5'	112.6	116.3	120.4 or 120.3	3.7*	7.8 or 7.7
C6'	121.1	135.3	118.0	14.2	–3.1
C7'	135.3	121.1	138.2	–14.2	2.9
C8'	116.3	112.6	109.3	–3.7	–7.0
C9'	136.9	136.9	137.9	0	1.0
C11'	57.3	57.2	57.1	–0.1	–0.2
C12'	29.3	29.1	29.1 or 29.0	–0.2	–0.2 or –0.3
C13'	167.4	167.4	167.4	0	0
C15'	60.1	60.0	60.0	–0.1	0.1
C16'	170.7	170.7	170.8	0	0.1
C17'	29.1	29.1	29.1 or 29.0	0	0 or –0.1
C18'	22.5	22.6	22.5	0.1	0
C19'	46.03	46.0	46.0	0	0

The comparison of the ^{1}H and ^{13}C NMR chemical shifts of the reported isonaseseazine B with both synthetic regioisomers **(–)-4** and **(–)-11** in CD_3OD shows that the data for isonaseseazine B is most consistent with synthetic (–)-naseseazine C (**4**).

* Our assignment of these residues is supported by key HSQC and HMBC correlations

Supplementary Table 7. Comparison of our ^{13}C NMR data for (–)-naseseazine C (4) and (–)-*iso*-naseseazine C (11) with literature data (DMSO-d_6).[2]

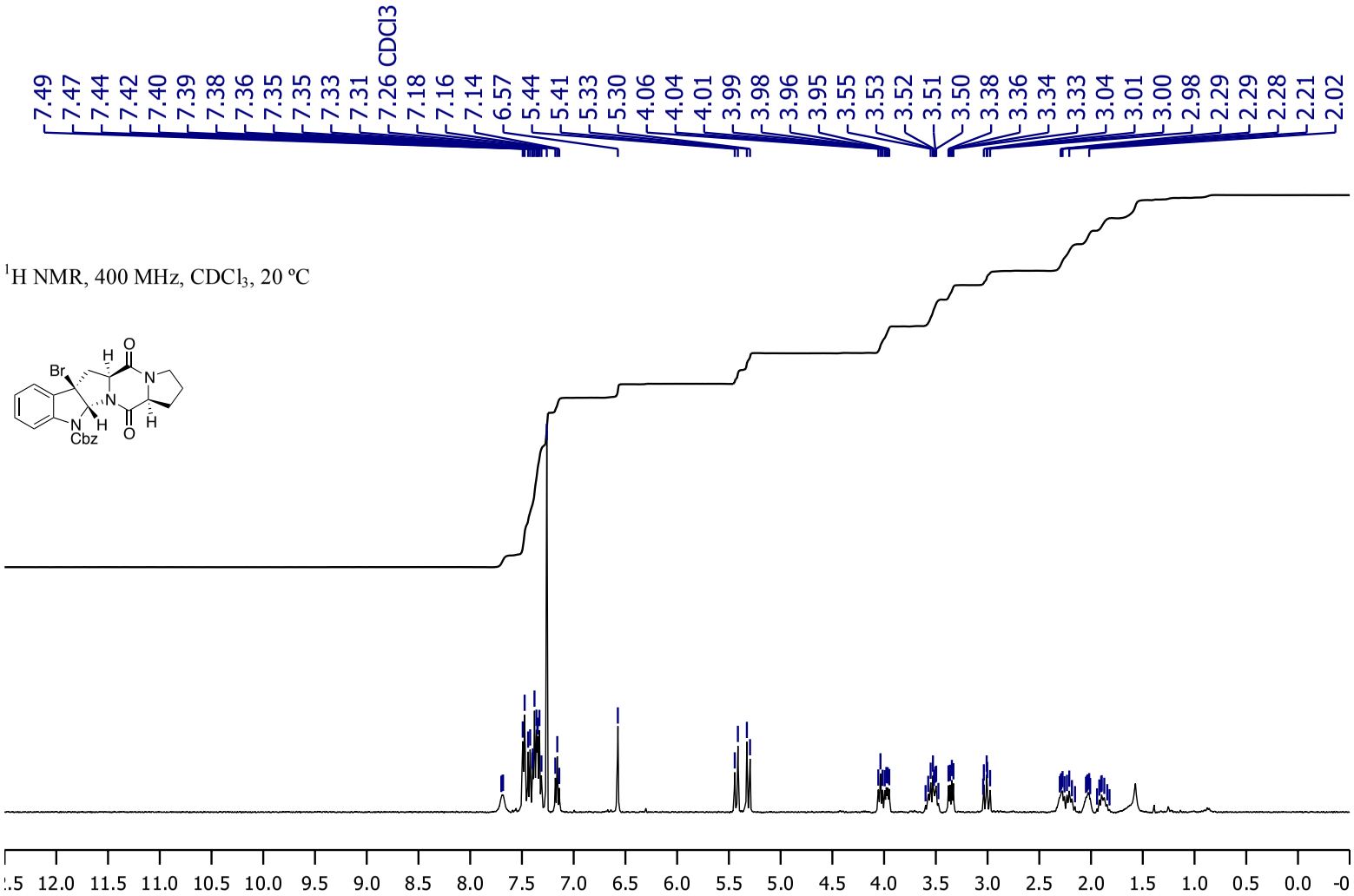
Assignment	**Carroll Report**[2] naseseazine C 13C NMR, 200 MHz, DMSO-d6	**This Work** (–)-naseseazine C (**4**) 13C NMR, 125 MHz	**This Work** (–)-iso-naseseazine C (**11**) 13C NMR, 125 MHz	**Chemical Shift Difference** Δδ = δ (–)-naseseazine C (this work) – δ (Carroll report)[2] DMSO-d6, 20 ºC	**Chemical Shift Difference** Δδ =δ (–)-iso-naseseazine C (this work) – δ (Carroll report)[2] DMSO-d6, 20 ºC
C2	81.1	81.1	81.5	0	–0.4
C3	59.7	58.7	58.8	–1.0*	0.9
C4	134.1	133	132.4	–1.1	1.7
C5	125.8	123.8	124	–2.0	1.8
C6	118.1	118.1	118.1	0	0
C7	128.1	128.1	128.2	0	–0.1
C8	111.4	109.5	109.5	–1.9	1.9
C9	149.3	149.3	149.4	0	–0.1
C11	60.1	60.1	60.2	0	–0.1
C12	40	39.9	39.9	–0.1	0.1
C13	165.3	165.3	165.3	0	0
C15	58.5	59.7	59.6	1.2	–1.1
C16	169.1	166	166.1	–3.1	3
C17	27.4	27.4	27.4	0	0
C18	22.5	22.6	22.6	0.1	–0.1
C19	44.7	44.7	44.8 or 44.6	0	0.1 or –0.1
C2'	124.8	124.8	124.8	0	0
C3'	109.6	109.6	109.2	0	0.4
C4'	127.1	127.1	126.1	0	1
C5'	114.6	114.6	119	0	–4.4
C6'	134.8	134.1	116.4	–0.7	18.4
C7'	119.2	119.2	136.8	0	–17.6
C8'	110.4	111.4	108	1.0	2.4
C9'	135.9	134.8	135.9	–1.1	0
C11'	55.1	55.1	55.2	0	–0.1
C12'	25.4	25.4	25.7	0	–0.3
C13'	166	165.6	165.5	–0.4	0.5
C15'	58.8	58.5	58.4	–0.3	0.4
C16'	165.6	169.2	169.1	3.6	–3.5
C17'	27.7	27.7	27.6	0	0.1
C18'	21.9	22	21.9	0.1	0
C19'	44.7	44.7	44.8 or 44.6	0	0.1 or –0.1

The comparison of the ^{1}H and ^{13}C NMR chemical shifts of the reported naseseazine C with both synthetic regioisomers **(–)-4** and **(–)-11** in DMSO-d6 shows that the data for naseseazine C is most consistent with synthetic (–)-naseseazine C (**4**).

***** Our assignment of these residues is supported by key HSQC and HMBC correlations

Synthetic References:

1. Xiong, Z. Q.; Liu, Q. X.; Pan, Z. L.; Zhao, N.; Feng, Z. X.; Wang, Y., Diversity and bioprospecting of culturable actinomycetes from marine sediment of the Yellow Sea, China. Arch. Microbiol. 2015, 197 (2), 299-309.
2. Buedenbender, L.; Grkovic, T.; Duffy, S.; Kurtboke, D. I.; Avery, V. M.; Carroll, A. R., Naseseazine C, a new anti-plasmodial dimeric diketopiperazine from a marine sediment derived Streptomyces sp. Tet. Lett. 2016, 57 (52), 5893-5895.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7.33
7.31
7.26 CDCl3
7.18
7.16
7.14
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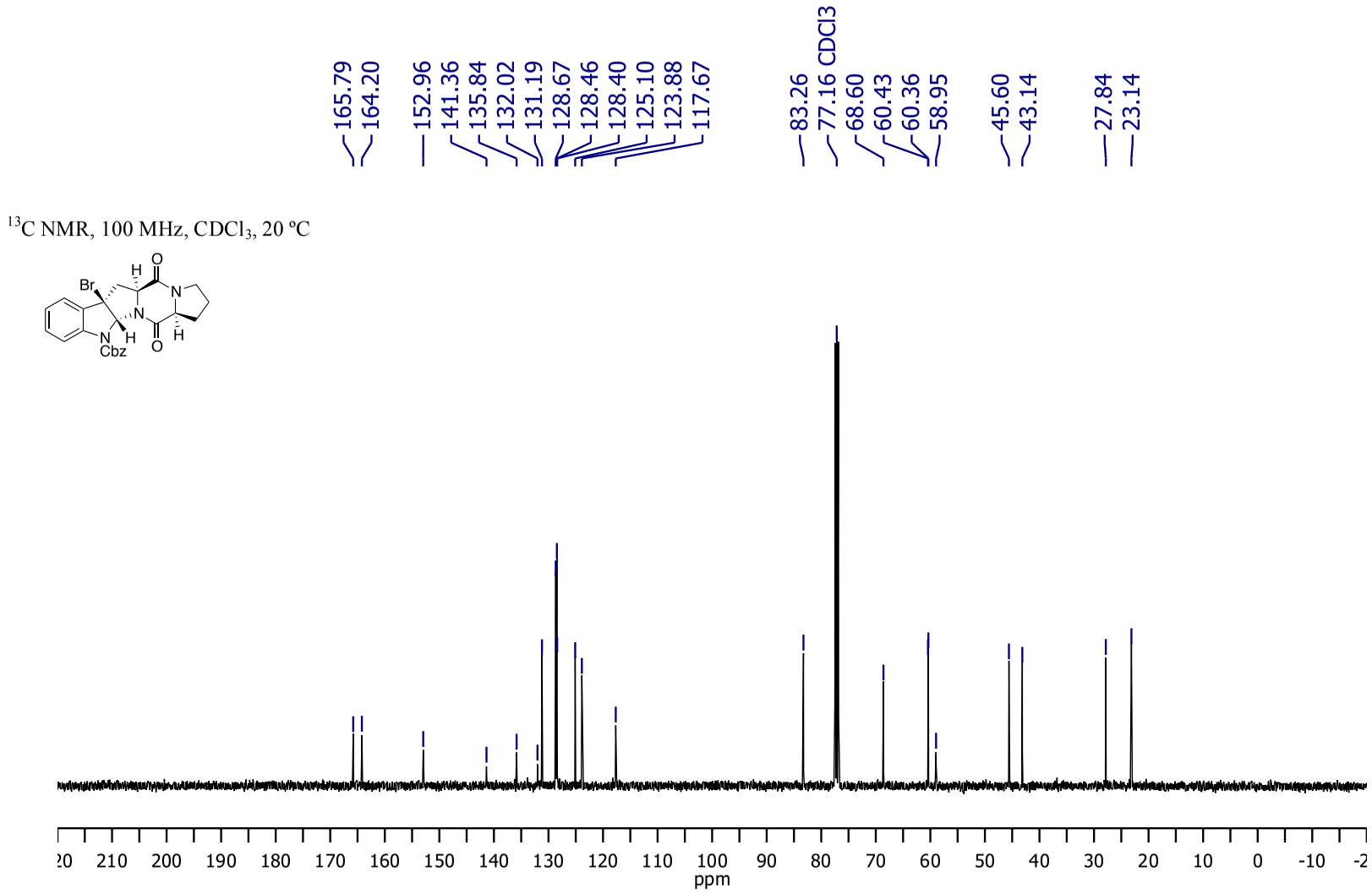
5.44
5.41
5.33
5.30
4.06
4.04
4.01
3.99
3.98
3.96
3.95
3.55
3.53
3.52
3.51
3.50
3.38
3.36
3.34
3.33
3.04
3.01
3.00
2.98
2.29
2.29
2.28
2.21
2.02
1H NMR, 400 MHz, CDCl3, 20 ºC
Br
H
O
N
N
H
N
H
Cbz
O
H
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0



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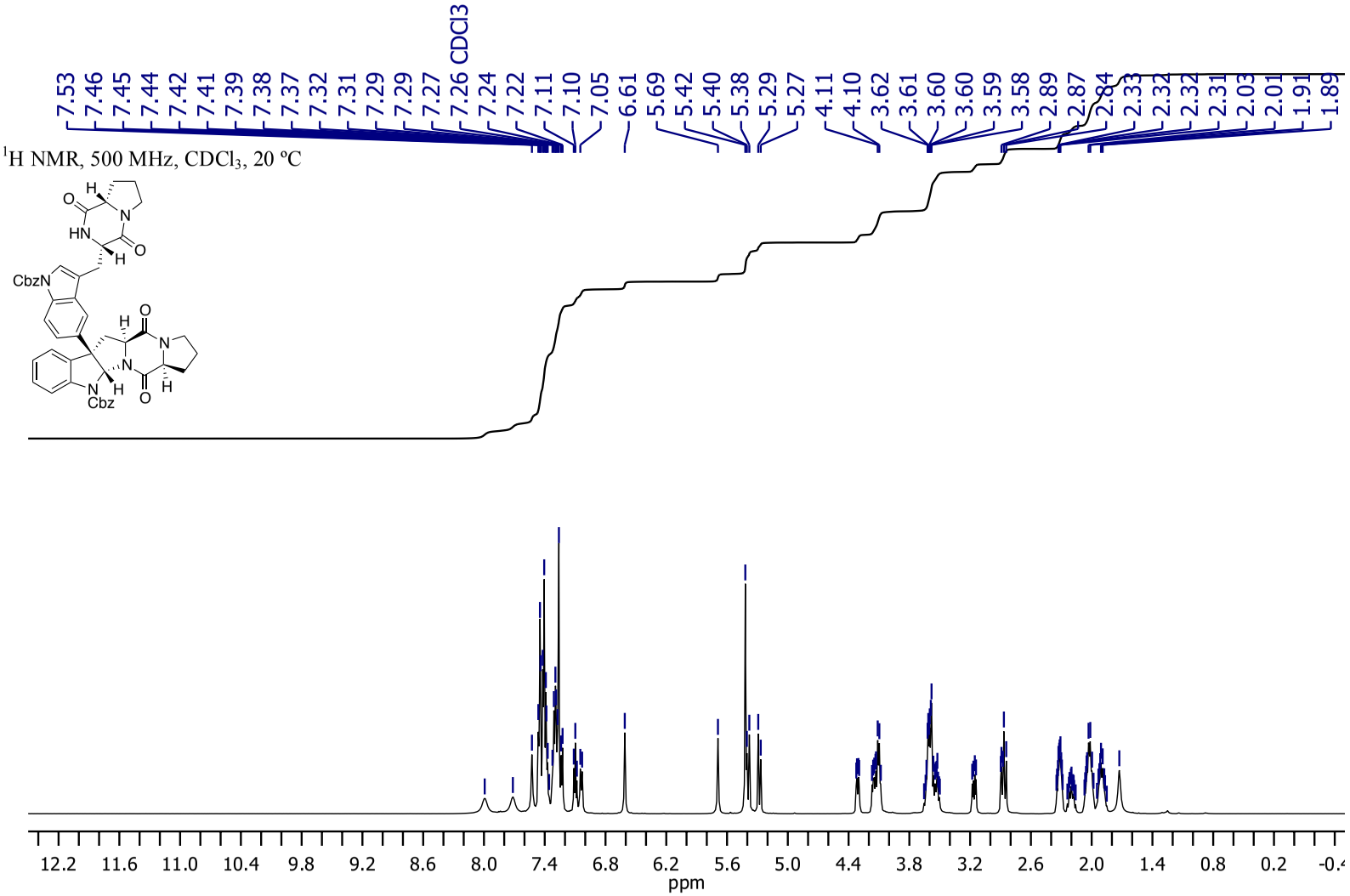
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5.40
5.38
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4.11
4.10
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3.61
3.60
3.60
3.59
3.58
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2.87
2.84
2.33
2.32
2.32
2.31
2.03
2.01
1.91
1.89
1H NMR, 500 MHz, CDCl3, 20 ºC
CbzN
HN
N
Cbz
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11.0
10.4
9.8
9.2
8.6
8.0
7.4
6.8
6.2
5.6
5.0
4.4
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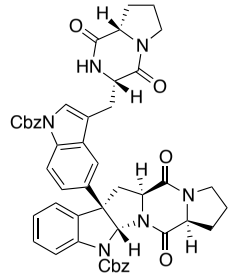
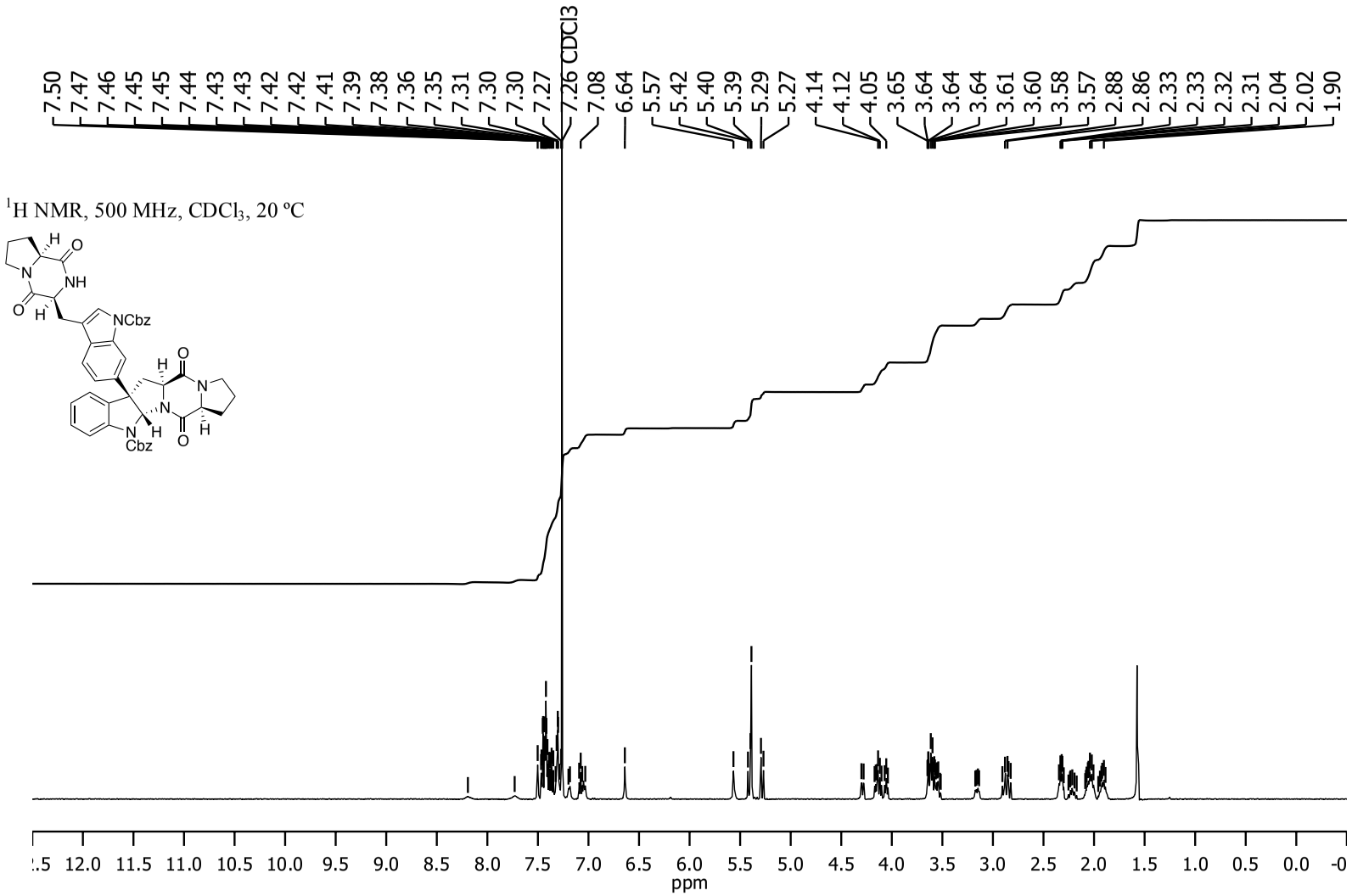
0.2
ppm

^{13}C NMR, 125 MHz, $CDCl_3$, 20 ºC

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7.27
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7.08
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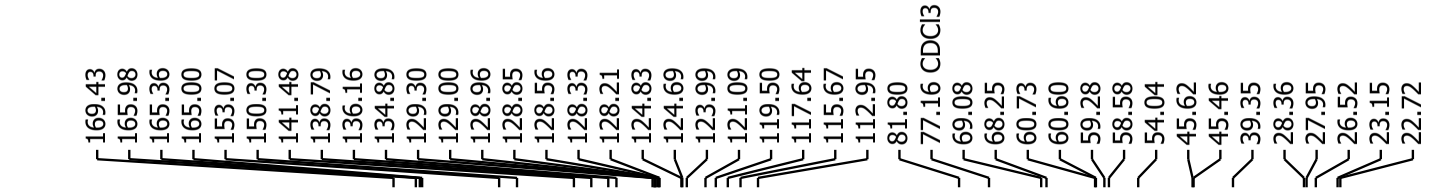

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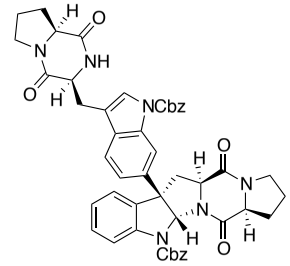

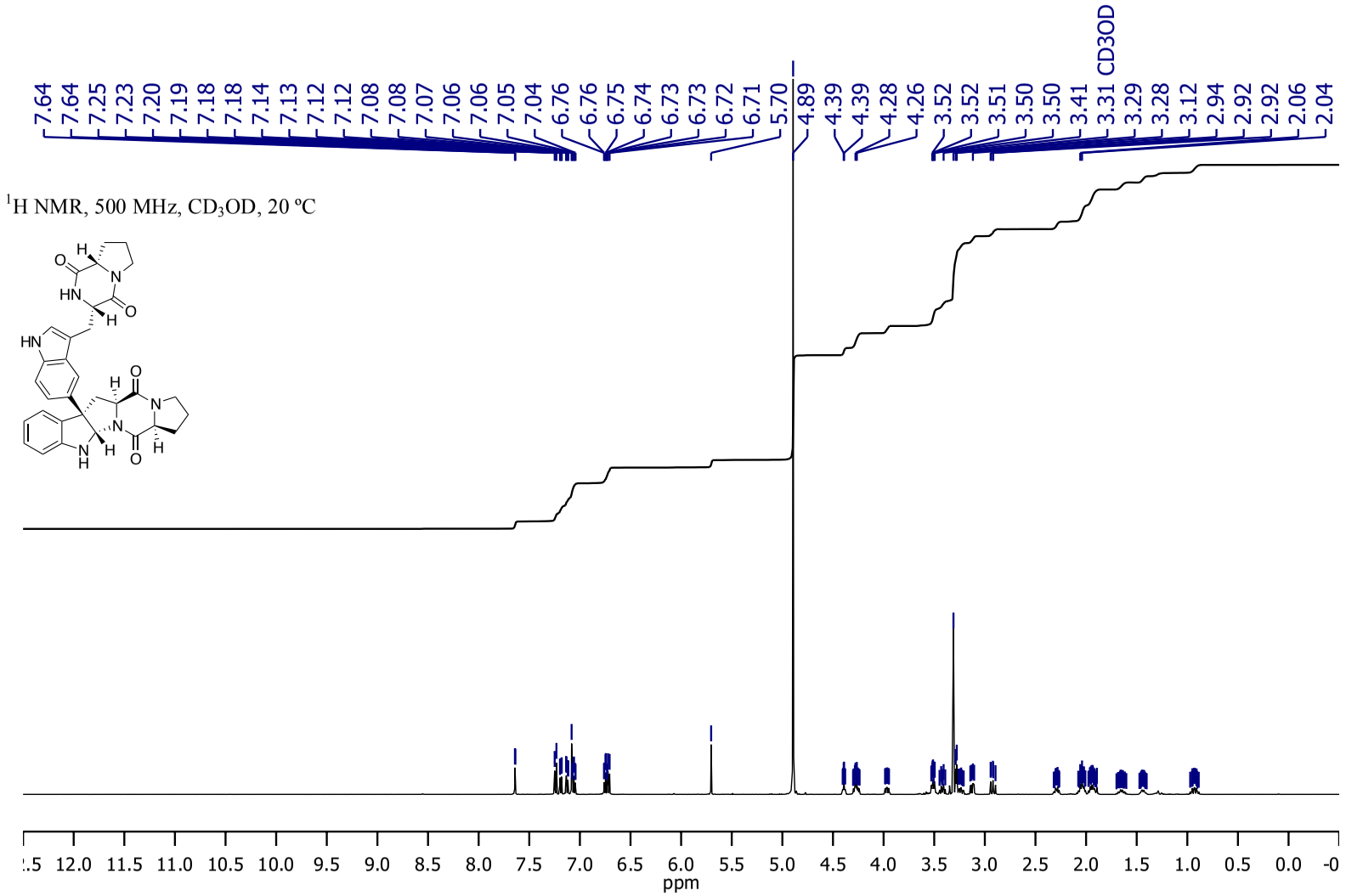
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3.41
3.31 CD3OD
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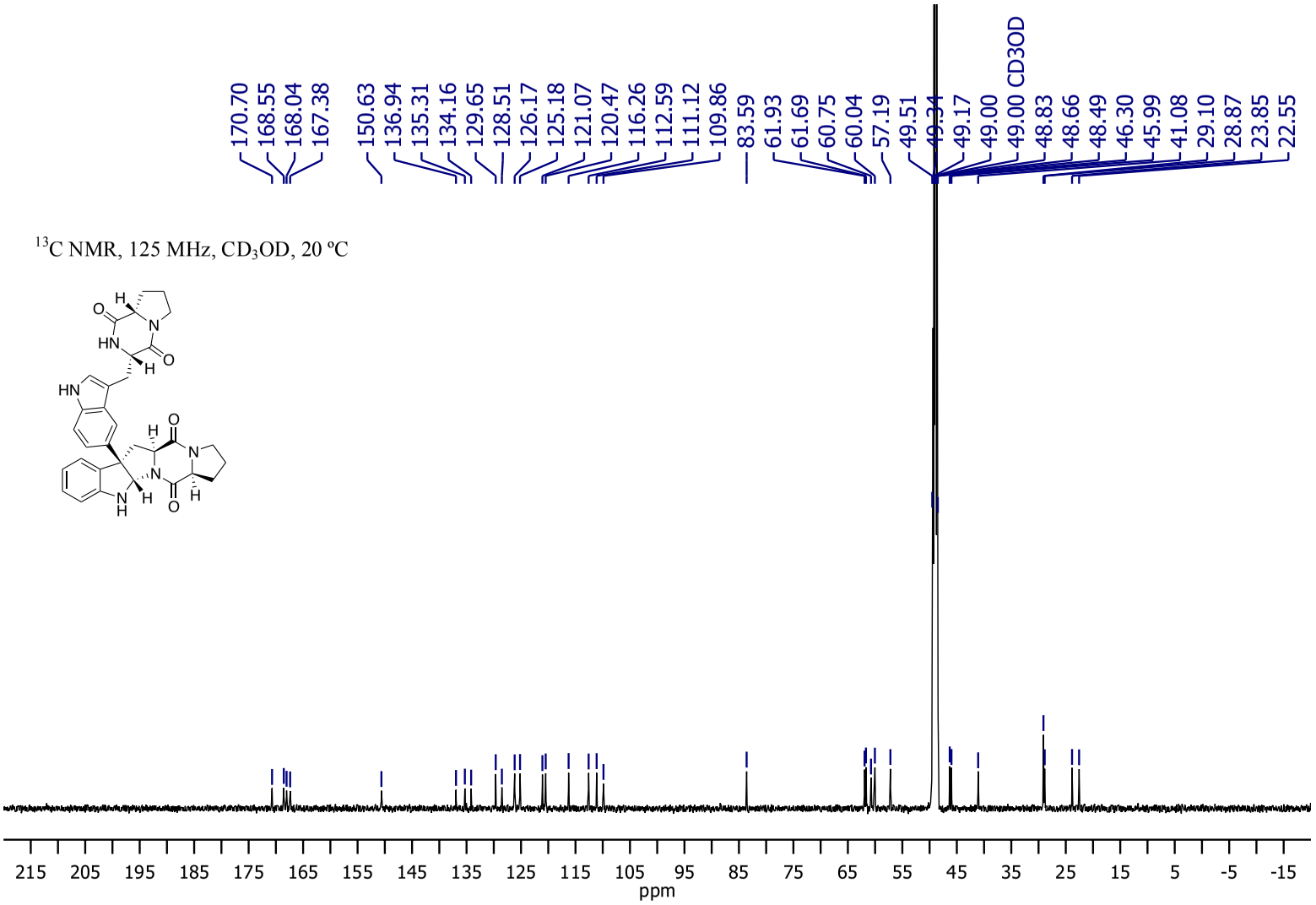
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49.00 CD3OD
48.83
48.66
48.49
46.30
45.99
41.08
29.10
28.87
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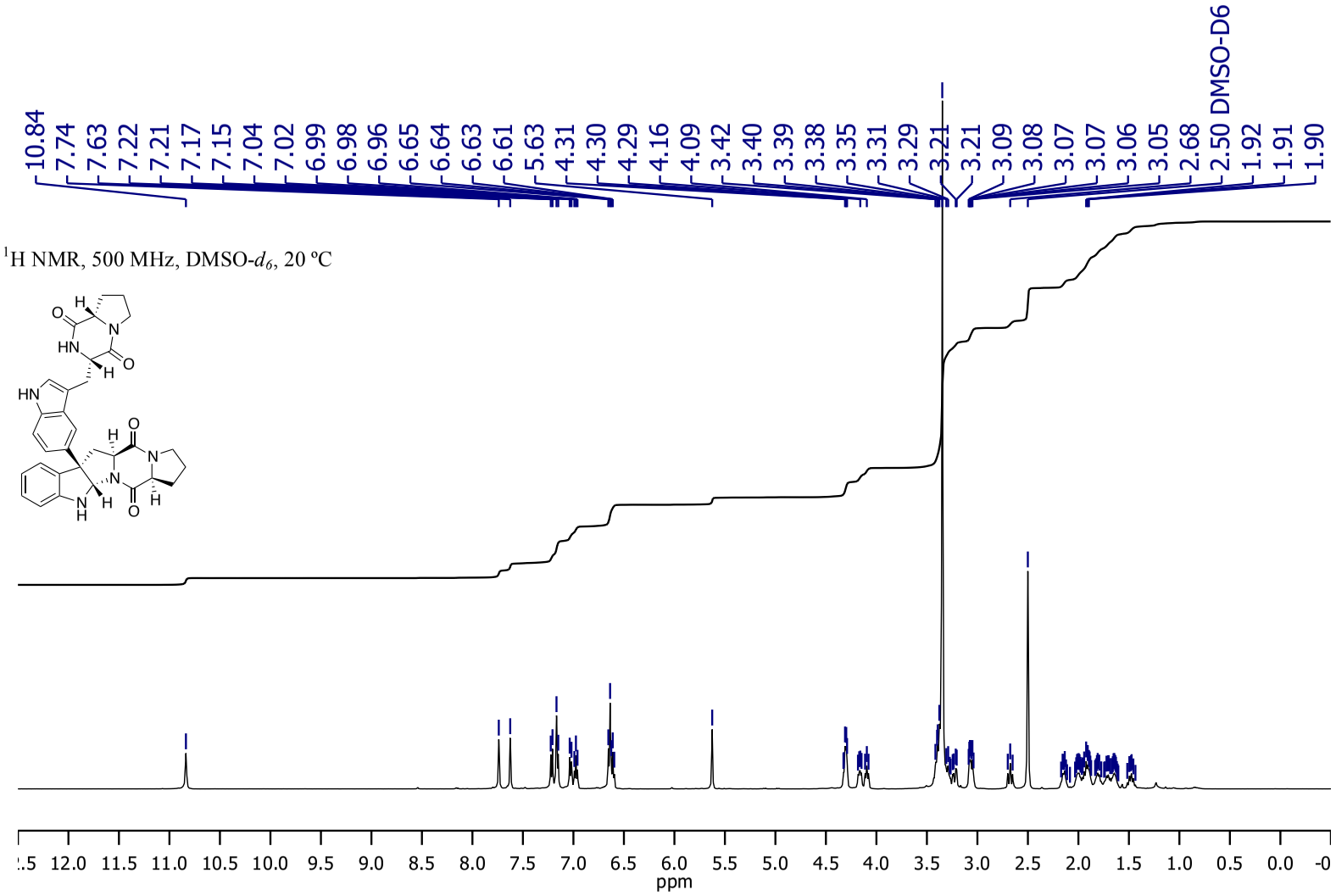
ppm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2.68
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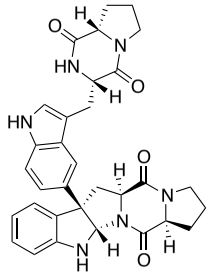
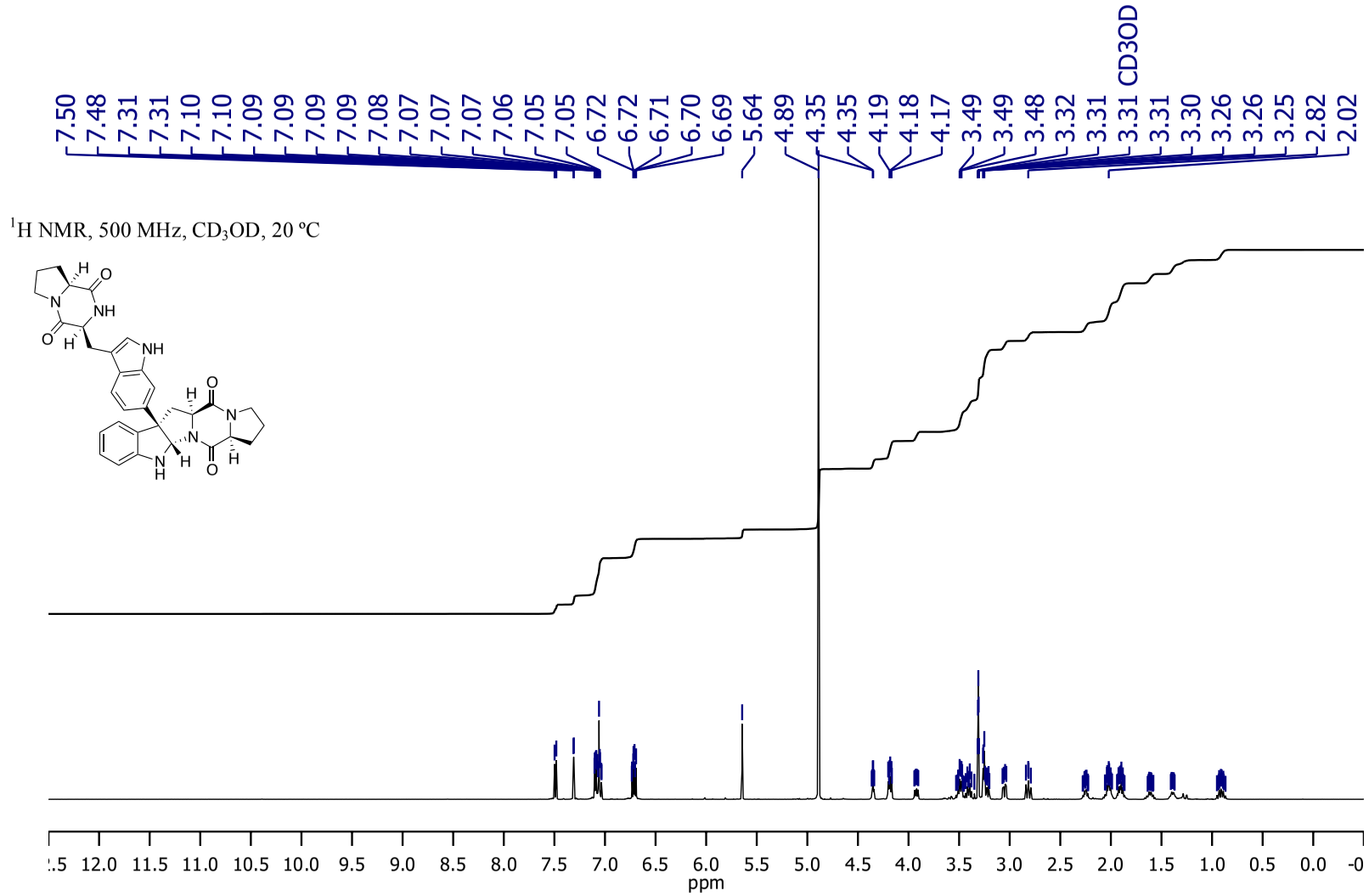
ppm

^{13}C NMR, 125 MHz, DMSO-d_6, 20 ºC

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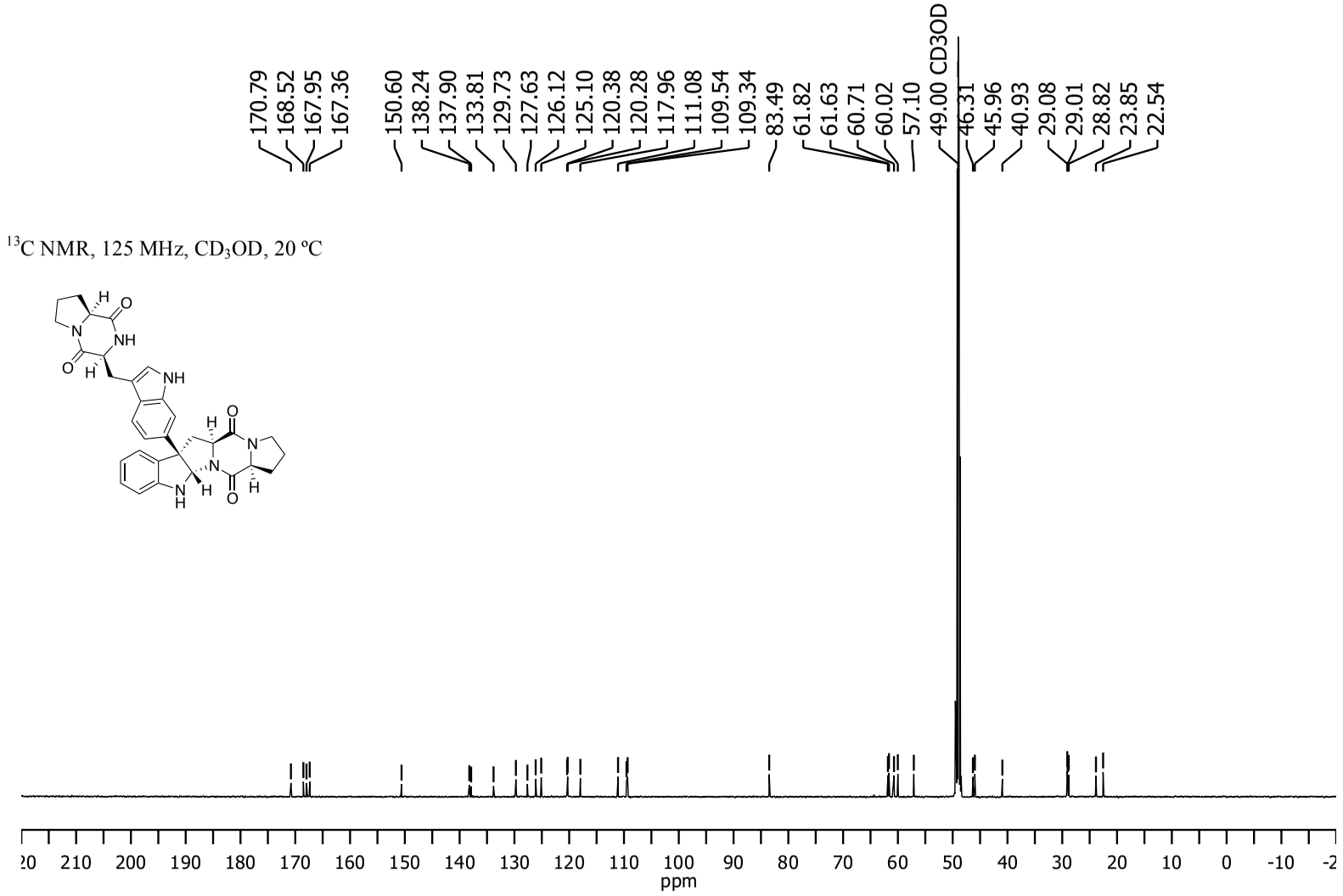
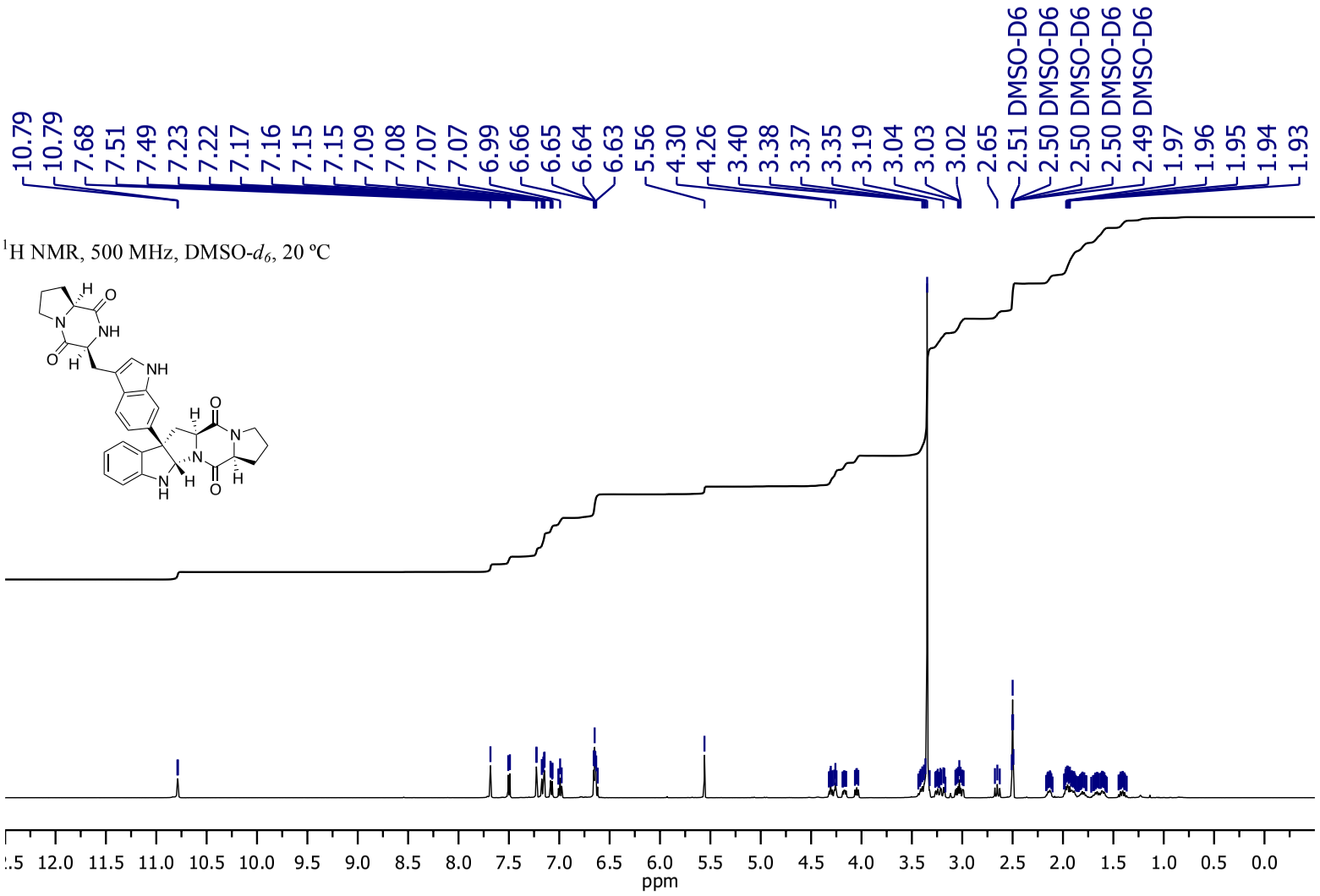
3.48
3.32
3.31
3.31 CD3OD
3.31
3.30
3.26
3.26
3.25
2.82
2.02
^{1}H NMR, 500 MHz, CD_3OD, 20 ºC
ppm



^{13}C NMR, 125 MHz, CD_3OD, 20 ºC


10.79
10.79
7.68
7.51
7.49
7.23
7.22
7.17
7.16
7.15
7.15
7.09
7.08
7.07
7.07
6.99
6.66
6.65
6.64
6.63
5.56
4.30
4.26
3.40
3.38
3.37
3.35
3.19
3.04
3.03
3.02
2.65
2.51 DMSO-D6
2.50 DMSO-D6
2.50 DMSO-D6
2.50 DMSO-D6
2.49 DMSO-D6
1.97
1.96
1.95
1.94
1.93
^{1}H NMR, 500 MHz, DMSO-d_6, 20 ºC
ppm

^{13}C NMR, 125 MHz, DMSO-d_6, 20 ºC