Electronic Supplementary Information: Structure and biosynthesis of the unusual polyketide alkaloid coelimycin P1, a metabolic product of the *cpk* gene cluster of *Streptomyces coelicolor* M145

Juan Pablo Gomez-Escribano,[†,§] *Lijiang Song,*[‡,§] *David J. Fox,*[‡] *Valerie Yeo,*[‡] *Mervyn J. Bibb**[,†] *and Gregory L. Challis**[,‡]

[†]Department of Molecular Microbiology, John Innes Centre, Norwich NR4 7UH, U.K.

[‡]Department of Chemistry, University of Warwick, Coventry CV4 7AL, U.K.

[§]These authors contributed equally.

Proposed functions of proteins encoded by genes within the *cpk* cluster

Table S1. Proposed functions of proteins encoded by genes within the *cpk* gene cluster

Gene product	CDS number	Proposed function
ScbR	SCO6265	Butyrolactone-responsive repressor protein
ScbA	SCO6266	Butenolide synthase involved in SCB1 biosynthesis
ScbB	SCO6267	Reductase involved in SCB1 biosynthesis
CpkM	SCO6268	Two-component system histidine kinase
CpkPβ	SCO6269	α-Ketoacid-dependent ferredoxin reductase β-subunit
CpkPα	SCO6270	α-Ketoacid-dependent ferredoxin reductase α-subunit
AccA1	SCO6271	Acyl-CoA carboxylase α-subunit (biotinylated)
ScF	SCO6272	Secreted flavin-dependent epoxidase/dehydrogenase
CpkC	SCO6273	Polyketide synthase module 5
CpkB	SCO6274	Polyketide synthase modules 3 and 4
CpkA	SCO6275	Polyketide synthase loading module, and modules 1 and 2
CpkD	SCO6276	Secreted flavin-dependent epoxidase/dehydrogenase
CpkE	SCO6277	Isomerase? (α, β-hydrolase fold)
CpkF	SCO6278	Transmembrane efflux protein
CpkG	SCO6279	Pyridoxal-dependent aminotransferase
CpkO	SCO6280	SARP-family transcriptional activator
CpkH	SCO6281	Secreted flavin-dependent epoxidase/dehydrogenase
CpkI	SCO6282	Nicotinamide-dependent dehydrogenase
CpkJ	SCO6283	NmrA-family protein (unknown function)
CpkK	SCO6284	Acyl-CoA carboxylase β-subunit
CpkL	SCO6285	Hypothetical protein (unknown function)
ScbR2	SCO6286	Butyrolactone-responsive repressor protein
ScoT	SCO6287	Type II thioesterase
CpkN	SCO6288	SARP-family transcriptional activator

Experimental Procedures and Spectroscopic/Chromatographic Data

Strains and growth conditions. The strains used in this study are listed in Table S2. *S. coelicolor* strains were grown on SFM[1] agar (for preparation of spore stocks and mycelial growth); DNA[1] agar (for yellow pigment production); in liquid TSB:YEME[1] 50:50 (for genomic DNA extraction); and SMM[1], R3 and R4[2] (to test for yellow pigment production). 50 ml liquid cultures of *S. coelicolor* were grown from an inoculum of germinated spores[1] in 250 ml siliconized flasks containing stainless steel springs at 30 ºC and 250 rpm.

Table S2. Strains used in this study.

Strain	Genotype or Comments	Source
Micrococcus luteus ATCC 4698	Bioassay indicator microorganism	ATCC
S. coelicolor M1148	Δ*act* Δ*red* Δ*cda*	ref. 4
S. coelicolor M1152	Δ*act* Δ*red* Δ*cpk* Δ*cda rpoB*(C1298T)[†]	ref. 5
S. coelicolor M1157	Δ*act* Δ*red* Δ*cda rpoB*(A1310G)[§]	This work*

*Selected as a spontaneous rifampicin resistant mutant of M1148; [†]RpoB(S433L); [§]RpoB(H437R)

Isolation of rpoB *mutants*. Spores of *S. coelicolor* M1148 were plated on SFM agar containing 200 μg/ml of rifampicin (about 10^7 spores per plate). After 13 days, 4 colonies had grown. These were streaked on DNA agar (to assess diffusible yellow pigment production) and on SFM agar (for single colony isolation and preparation of spore stocks) without antibiotic selection.

Sequencing of rpoB *mutant alleles*. Nucleic acid manipulations were performed using standard methods[3] or by following the instructions provided by the manufacturers of PCR enzymes and kits. Total DNA was isolated from cultures grown for 48 h (to stationary phase) in TSB:YEME 50:50 using the salting-out protocol[1]. The region of *rpoB* of interest was amplified by PCR with primers rpoBmut_tst1 (5'-GATCCAGAACCAGGTCCGTA-3') and rpoBmut_tst2 (5'-GATGACGAAGCGGTCCTC-3'). The PCR product was purified and sequenced with primer rpoBsq1 (5'-GGTACGGCGTCTCGATGAAG-3'). The sequencing chromatograms confirmed that the rifampicin-resistant mutants contained only the mutant *rpoB* allele.

Assay of antimicrobial activity. 1.5 ml of an overnight culture of *Micrococcus luteus* ATCC4698 grown in Luria-Bertani (LB) medium were added to 150 ml of warm LB-agar medium (at about 45 ºC) and the seeded medium was poured into 10 cm square plates (about 25 ml per plate). 50 μl of *S. coelicolor* culture supernatant or methanolic mycelial extract were added to filter paper discs, which were then placed on the solidified agar. The plates were incubated at 4 ºC for 2 hours, followed by 30 ºC for 24-48 hours, after which the halos of growth inhibition were recorded (Figure S1).

Comparison of the profile of metabolites produced by S. coelicolor *M1157 and M1152 using HPLC*. 10 ml aliquots were removed from liquid cultures after 3 and 7 days of growth and centrifuged at 4000 rpm for 10 min. The resulting culture supernatants were divided in 2 ml aliquots and stored at -80 °C. Mycelial extracts were prepared by re-suspending mycelium from above in 2 ml of methanol and vortexing for one minute, followed by centrifugation at 4000 rpm for 10 min. The extracts were stored at 4 ºC. Immediately before HPLC analysis, samples were cleared by centrifugation at 14000 rpm for 10 min. 100 µl of each sample were analyzed on a Waters Spherisorb ODS2 C18 column (5 µm, 4.6 x 250 mm) attached to an Agilent 1100 HPLC system equipped with a Diode Array detector. The column was eluted at 1 mL/min using 0.1% formic acid in water (solvent A) and methanol (solvent B), and the following program: 0 min - 2% solvent B; 2 min - 2% solvent B; 15 min - 25% solvent B; 19 min - 90% solvent B; 22 min - 90% solvent B; 22.5 min - 2% solvent B; 34 min - 2% solvent B. A comparison of the profile of metabolites in culture supernatants of the M1157 and M1152 strains grown in SMM and R3 media is shown in Figure S1.

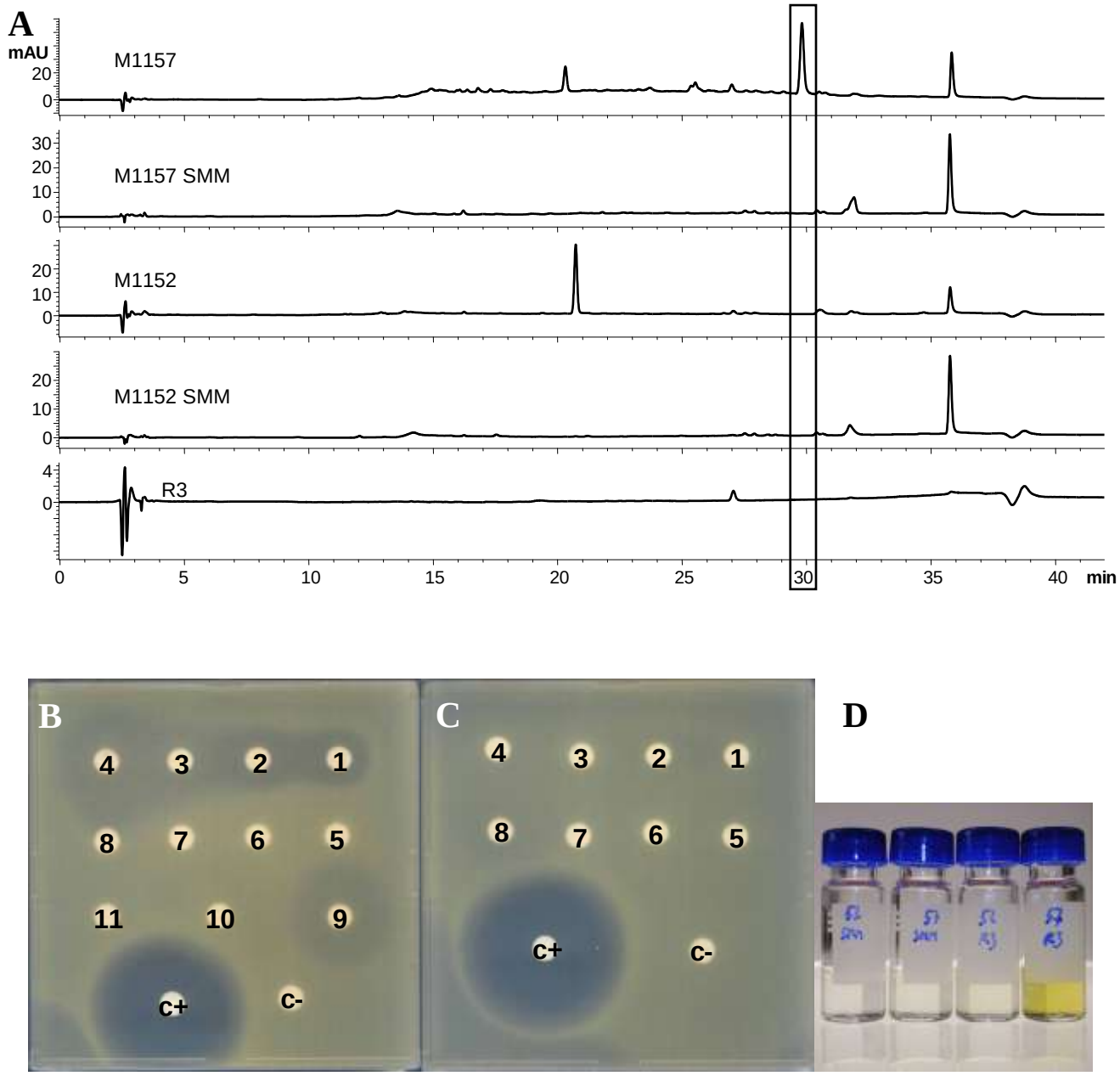


Figure S1. (A) Chromatograms from HPLC analyses monitoring absorbance at 400 nm of culture supernatants of M1157 and M1152 grown in R3 and SMM liquid media, showing that the 30 min peak was exclusive to M1157 and was observed only when the culture was grown in R3 medium. (B) Results of bioassays against *M. luteus* for samples from cultures of M1157 and M1152 grown in R3 medium. (C) Results of bioassays against *M. luteus* for samples from cultures of M1157 and M1152 grown in SMM. Culture supernatants/mycelial extracts applied to the filter paper discs were as follows: **1-4**: M1157 culture supernatant; **5-8**: M1152; **1,5**: 3-day culture; **2,6**: 3-day culture, 5x concentrated; **3,7**: 7-day culture; **4,8**: 7-day culture, 5x concentrated; **9**: 5x concentrated 7-day culture supernatant of M1157 used for HPLC analyses; **10**: 5x concentrated mycelial extract from 7-day culture of M1157; **11**: fraction from HPLC analysis containing the peak eluting after 30 min (equivalent to 100 µl of 5x concentrated culture supernatant, i.e. twice the amount used for disc **9**); **c-**: negative control - R3 medium; **c+**: positive control - hygromycin B (this highlights the difference between clear growth inhibition and the weak growth inhibition observed in **1-4** and **9**). (D) Culture supernatants from M1152 and M1157 grown in SMM and R3 medium for seven days. From left to right: M1152/SMM, M1157/SMM, M1152/R3, M1157/R3.

LC-ESI-TOF-MS analysis of culture supernatants. A Sigma Ascentis C18 column (100 x 2.1mm, 2.7 µm) connected to a Dionex 3000 RS-HPLC coupled with a Bruker MaXis UHR-Q-TOF mass spectrometer was used. The flow rate was 0.2 ml/min and the eluents were water/0.1% formic acid (solvent A) and methanol/0.1% formic acid (solvent B). The elution profile was as follows: 100% solvent A to 100% solvent B in 15.4 minutes, then isocratic at 100% solvent B for 5 minutes, back to 100% solvent A in 3 minutes and equilibrated for 10 minutes before the next injection. The mass spectrometer was calibrated at the beginning of each run with 10 mM sodium formate and the following settings in positive ESI mode were used. Scan range: 50-2000 *m/z*, End plate offset: -500 V, Capillary: -4500 V, Nebulizer gas (N_2): 1.6 bar, Dry gas (N_2): 8 L/min, Dry Temperature: 180 °C. The high resolution mass spectrum of coelimycin P1, which eluted with a retention time of approximately 20 minutes, is shown in Figure S2. The isotope distribution for the $[M+H]^+$ ion indicated that the compound contains a sulfur atom and a molecular formula of $C_{17}H_{20}N_2O_4S$ was deduced for the compound.

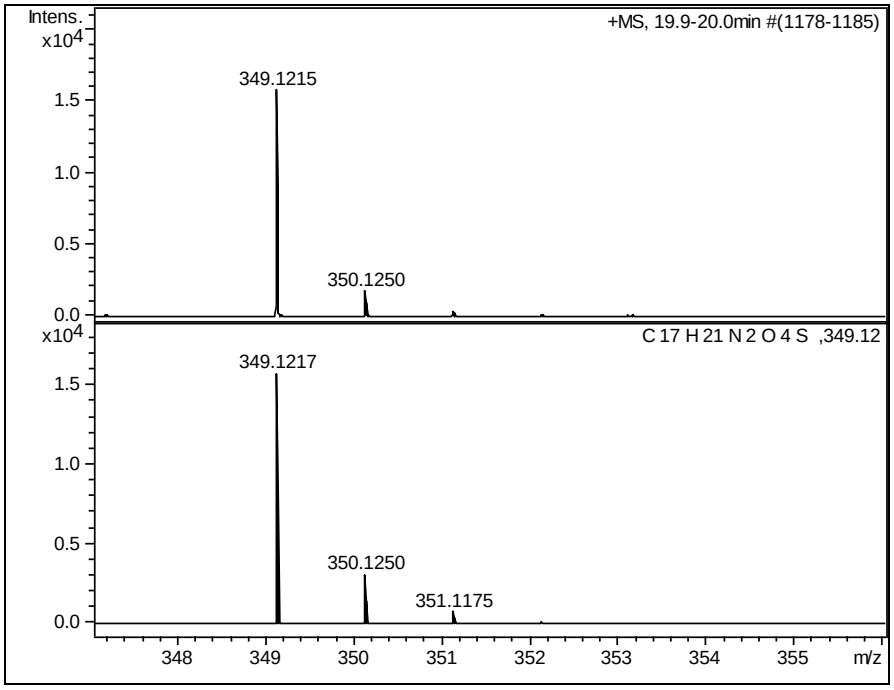


Figure S2. Top panel: High resolution mass spectrum of coelimycin P1 obtained from LC-ESI-TOF-MS analysis of culture supernatants of M1157. Bottom panel: Simulated mass spectrum for the $C_{17}H_{21}N_2O_4S^+$ ion.

Isolation and structure elucidation of coelimycin P1. Cultures of *S. coelicolor* M1157 were grown for 7 days in 4 x 50 mL of R3 medium at 28ºC and 180rpm, after which they were pooled and centrifuged for 10 minutes at 4000 rpm and 4 ºC. The supernatant was decanted and freeze-dried. The residue was dissolved in 2ml of 80% methanol/20% water and centrifuged for 5 minutes at 13000 rpm immediately before HPLC purification, which was carried out on an Agilent Zorbax RP-C18 column (5µm, 21 x 100 mm), equipped with a 21 x 10 mm guard column, attached to an Agilent 1100 instrument. The mobile phases were: water containing 0.05% formic acid (solvent A) and methanol (solvent B). The flow rate was 5ml/min and absorbance at 360 nm was monitored. Initial separation of the supernatant samples was carried out using the following elution profile: 0 min - 30% B; 25 min – 100% B. Fractions containing the yellow pigment were pooled, freeze-dried, resuspended in 80% methanol/20% water and further purified on the same column using the following elution program: 0 min- 40% B; 20 min – 100% B. Fractions containing the yellow pigment were pooled and freeze-dried, typically yielding 3-5 mg of a yellow-orange powder, which was dissolved in 200 µL of $CDCl_3$ for NMR analysis in a 3 mm tube. ^1H, COSY, HSQC, HMBC and NOESY NMR experiments were carried out on a Bruker Avance II 700 MHz NMR spectrometer equipped with TCI cryoprobe. Assignments for the NMR signals and HMBC/key NOESY correlations observed are summarized in Table S3. Spectra are shown in Figures S3-S10.

Table S3. Assignments for ^{1}H and ^{13}C NMR signals and summary of HMBC and key NOESY correlations observed for coelimycin P1 (**1**).

C/H	δ_H/ppm (multiplicity, *J*/ Hz)	δ_C/ppm*	HMBC	Key NOESY
1	4.57 (m)	42.7	C5, C3, C2	
2	2.53 (m)	24.4	C1, C3, C4	
3	6.14 (dt, 4.6, 10.2)	127.4	C5, C1, C2	
4	6.67 (d, 10.2)	117.4	C5, C2	H-3'α
5		138.8		
6		108.8		
7	7.02 (s)	124.8	C5, C6, C8, C9	H-2', H-3'α, H-10, H-1
8		130.6†		
9		180.1		
10	6.71 (d, 13.8)	128.2	C12, C9	H-7, H-12
11	6.99 (dq, 6.7, 13.8)	142.1	C12, C9	
12	1.97 (d, 6.7)	18.4	C9, C10	H-10
1'		171.3		
2'	4.67 (m)	52.4	C1', C3', C4'	H-7
3'β	3.09 (dd, 14.1, 6.0)	37.2	C6, C1', C2'	C2'-N<u>H</u>-C4'
3'α	3.22 (dd, 14.1, 4.5)			H-4, H-7
2'-N<u>H</u>-4'	6.22 (br s)			H-3'β, H-5'
4'		171.9		
5'	2.00 (s)	22.9	C4'	C2'-N<u>H</u>-C4'

*From HMBC/HSQC spectra. †The chemical shift for this carbon atom is approximately 10 ppm upfield of what would be expected for the corresponding carbon atom in a simple enol acetate. This can be attributed to the shielding effect afforded by the lone pair on the nitrogen atom attached to C-5 which is in conjugation with C-8.

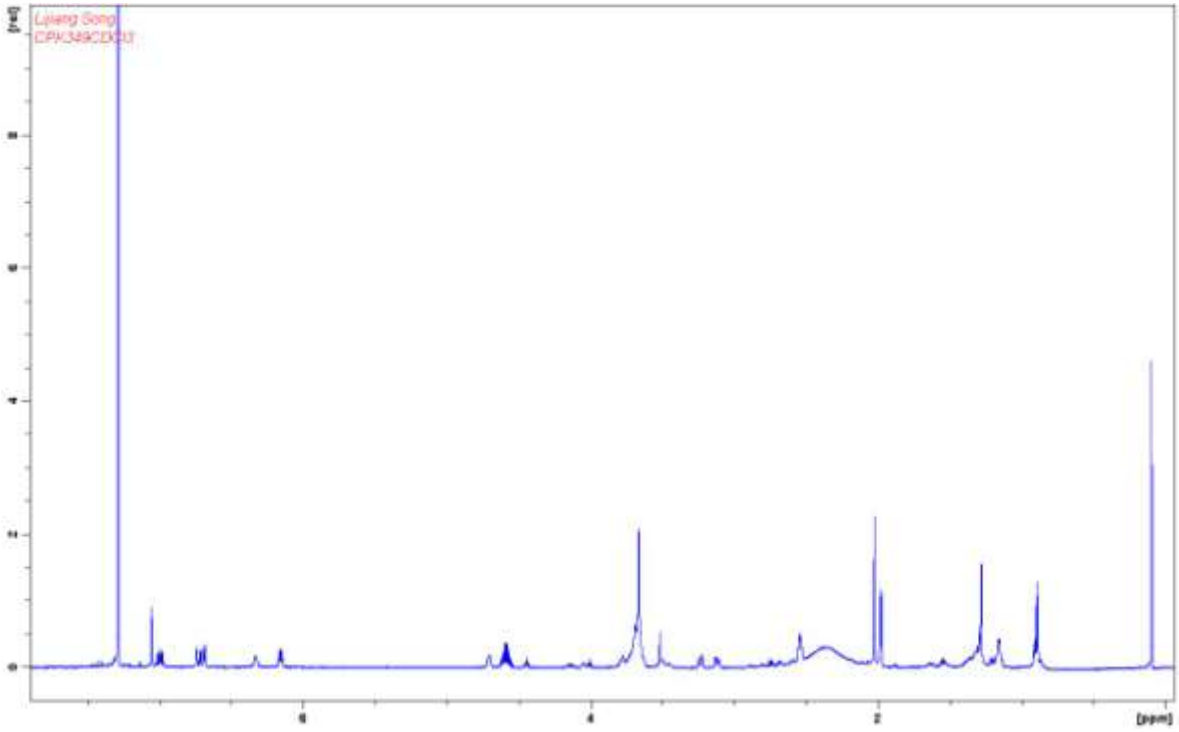


Figure S3. ^{1}H NMR spectrum for coelimycin P1 (**1**)

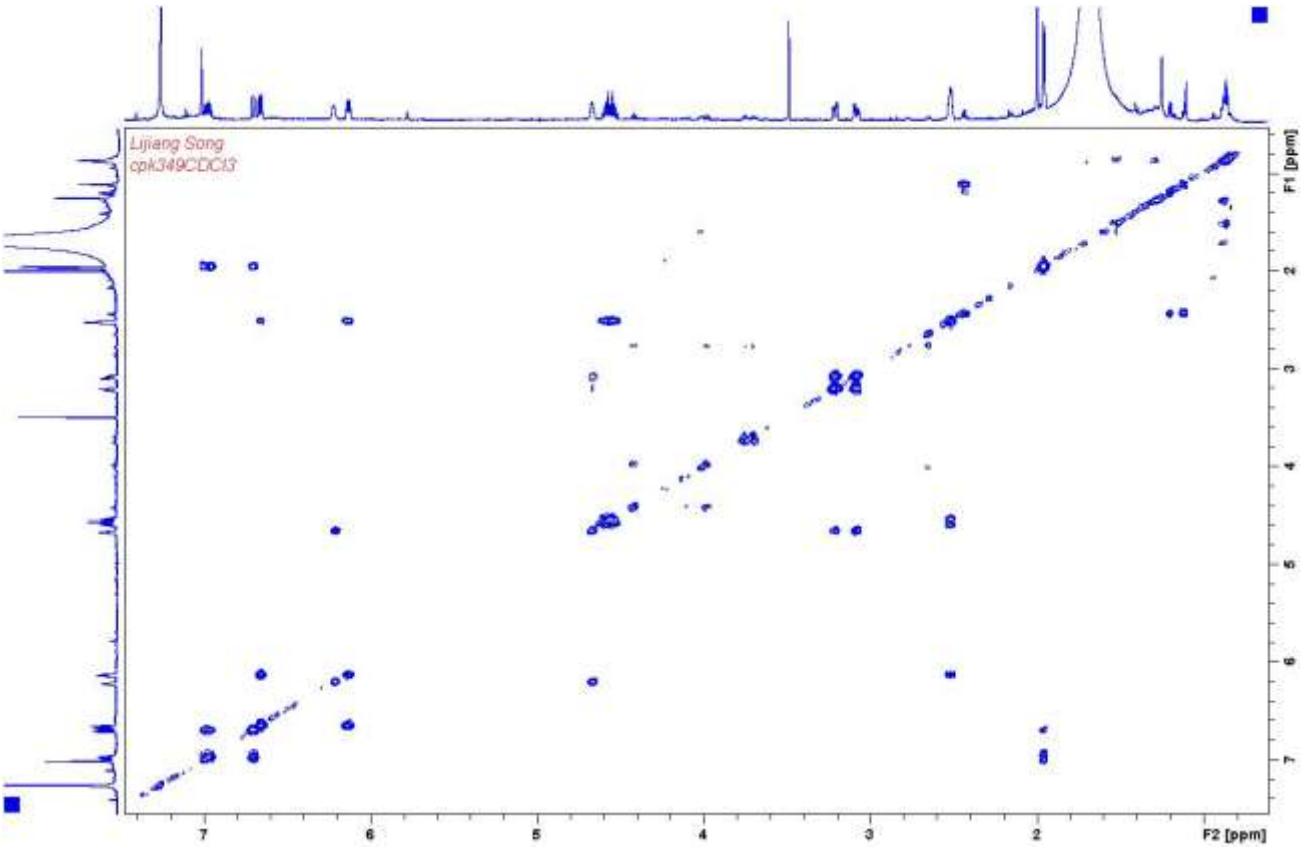


Figure S4. COSY NMR spectrum for coelimycin P1 (**1**)

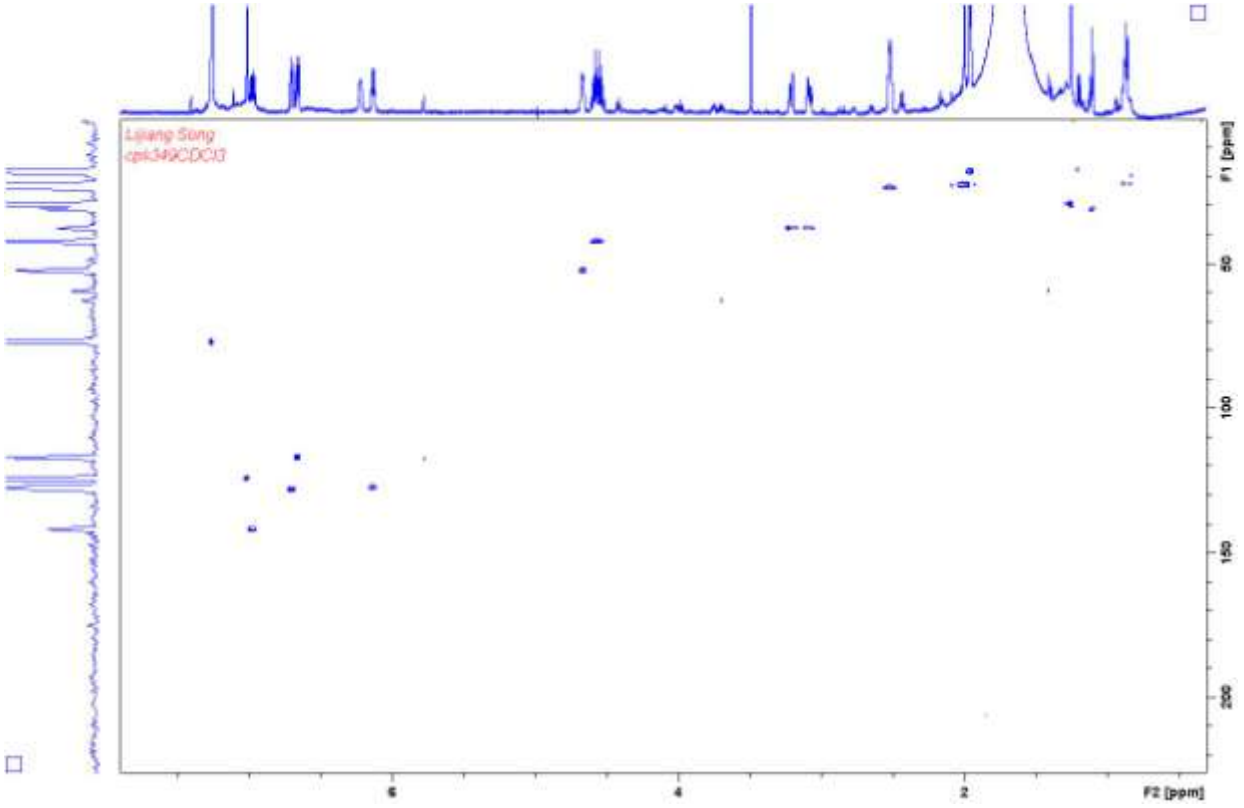


Figure S5. HSQC NMR spectrum for coelimycin P1 (**1**)

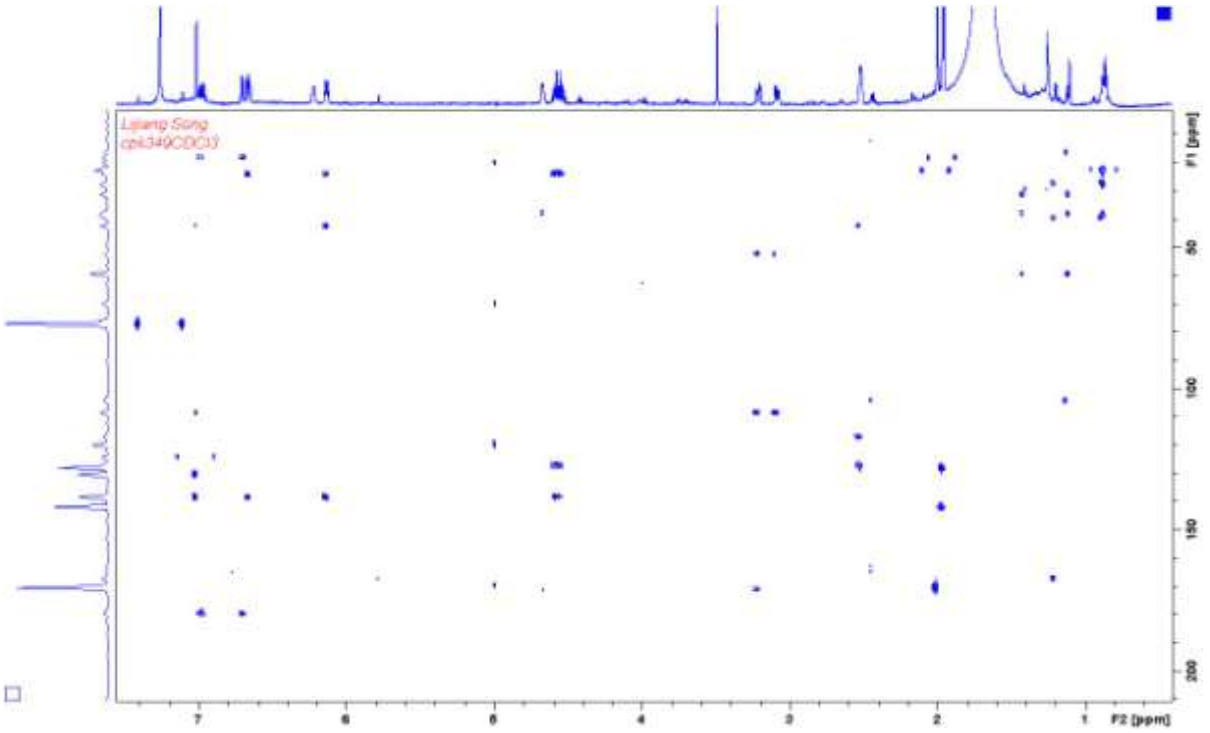


Figure S6. HMBC NMR spectrum for coelimycin P1 (**1**)

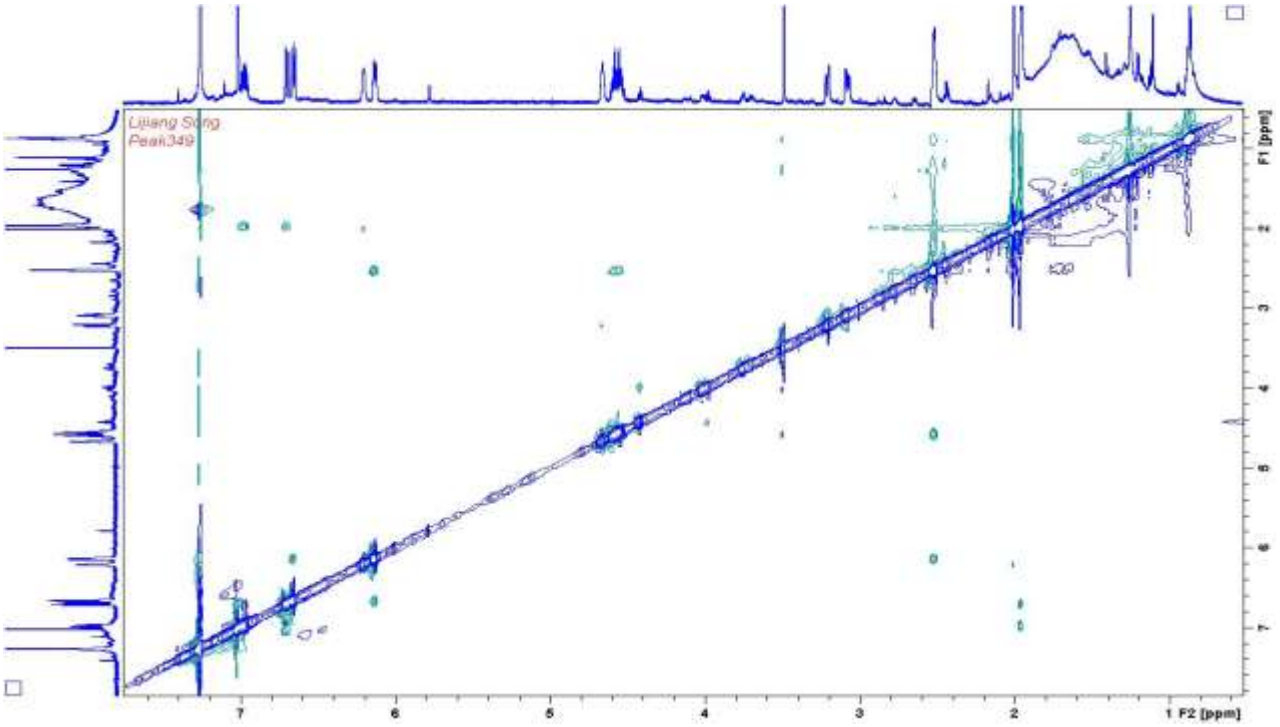


Figure S7. NOESY NMR spectrum for coelimycin P1 (**1**)

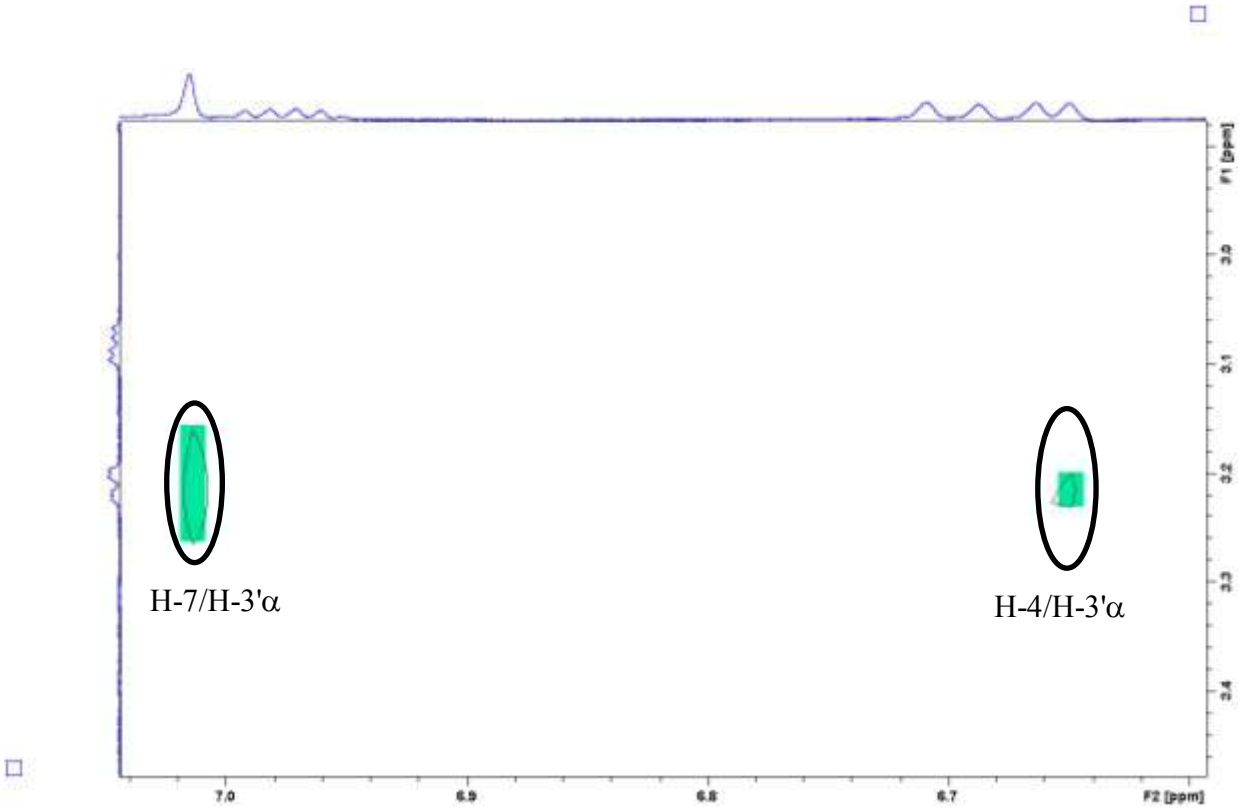


Figure S8. Expansion of the region of the NOESY NMR spectrum for coelimycin P1 (**1**) containing the correlations for H-7/H-3'α and H-4/ H-3'α.

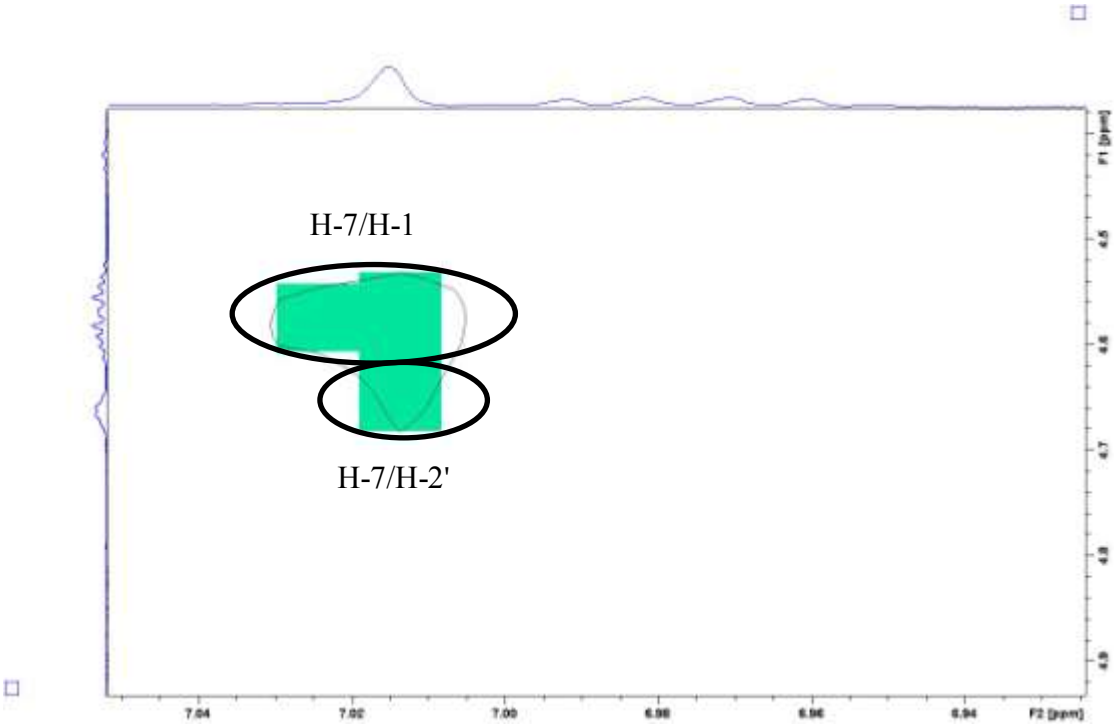


Figure S9. Expansion of the region of the NOESY NMR spectrum for coelimycin P1 (**1**) containing the correlations for H-7/H-1 and H-7/ H-2'.

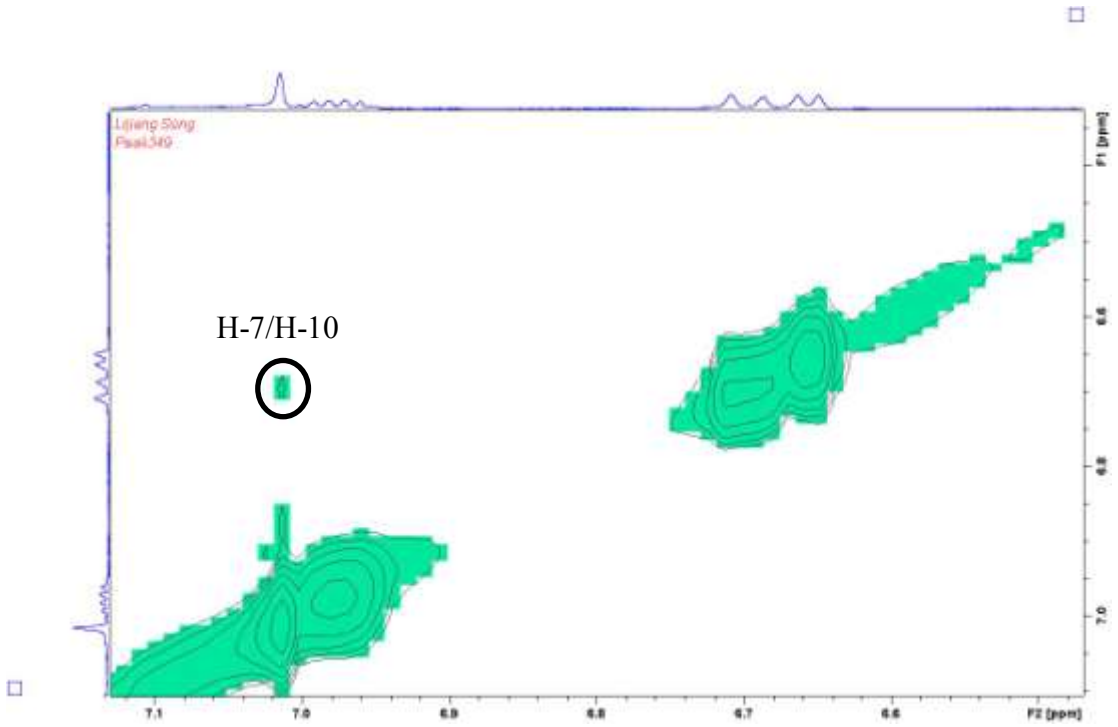


Figure S10. Expansion of the region of the NOESY NMR spectrum for coelimycin P1 (**1**) containing the correlation for H-7/H-10.

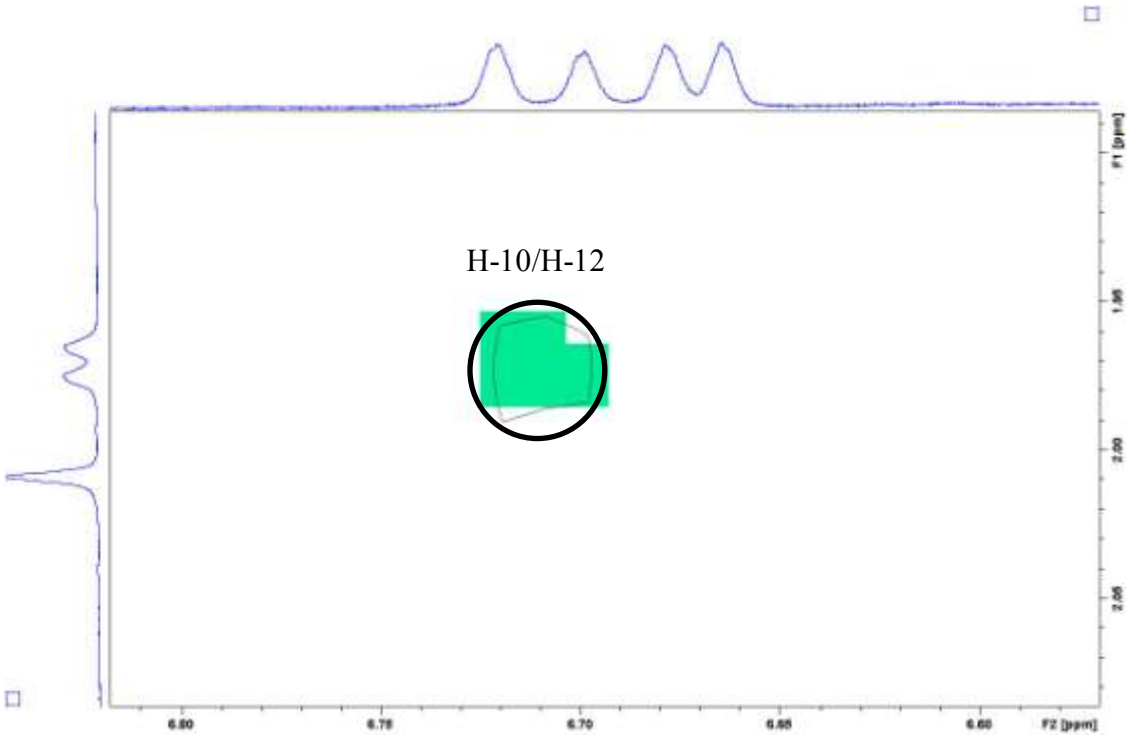


Figure S11. Expansion of the region of the NOESY NMR spectrum for coelimycin P1 (**1**) containing the correlation for H-7/H-12.

Analysis of $^{18}O_2$ incorporation into coelimycin P1. 2μL of M1157 spores were inoculated into 2 mL of R3 liquid medium in a 15 mL centrifuge tube and the culture was saturated with $^{18}O_2$ by sparging for 5 minutes. The cap was placed on the tube and sealed with parafilm. After 4 days incubation at 28 ºC and 180 rpm, the culture was sparged with $^{18}O_2$ for a further 5 minutes and the culture was grown for 3 more days under the same conditions. The culture supernatant was analyzed using LC-ESI-TOF-MS/MS, as described above, which confirmed that a single ^{18}O atom had been incorporated into coelimycin P1 (Figure S12). Comparison of the fragment ions resulting from $[M+H]^+$ parent ion for the ^{18}O-labeled material and a sample of unlabeled coelmycin P confirmed that the ^{18}O label is incorporated into the C-9 keto group (Figure S13).

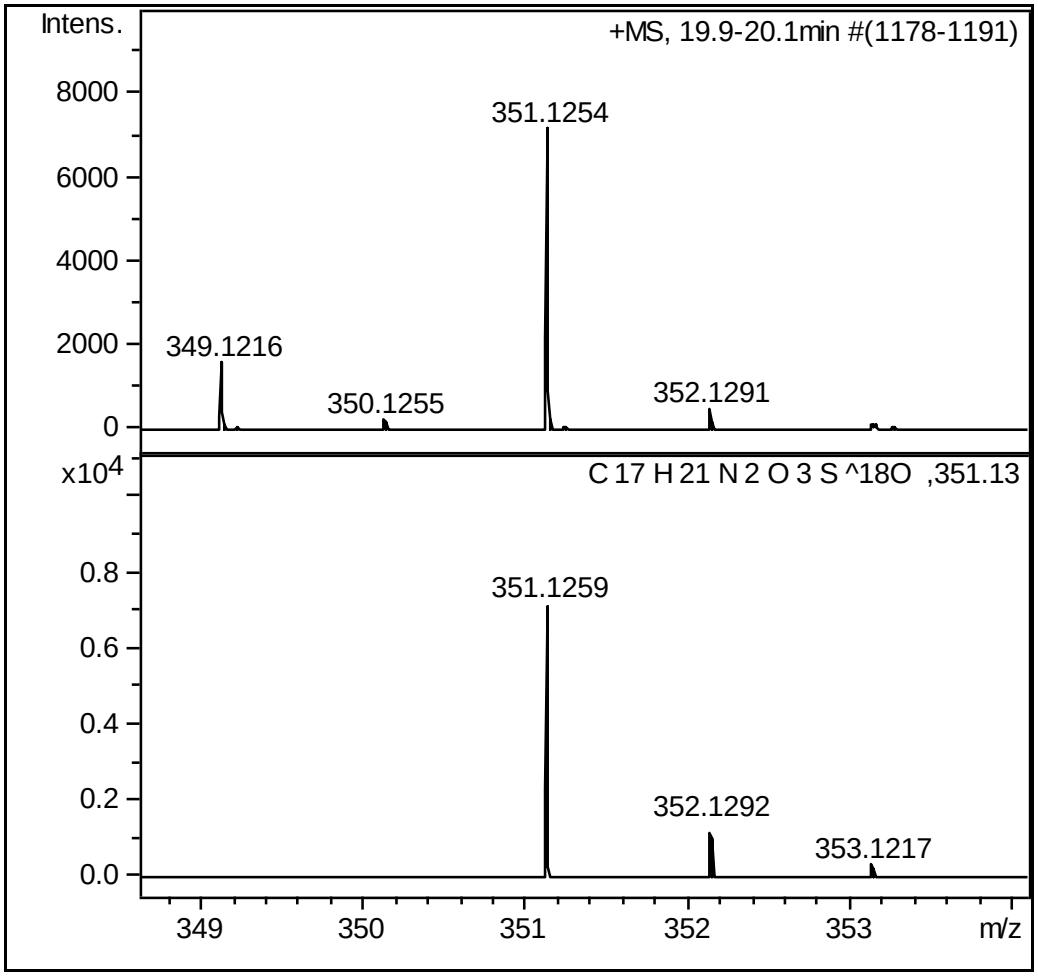
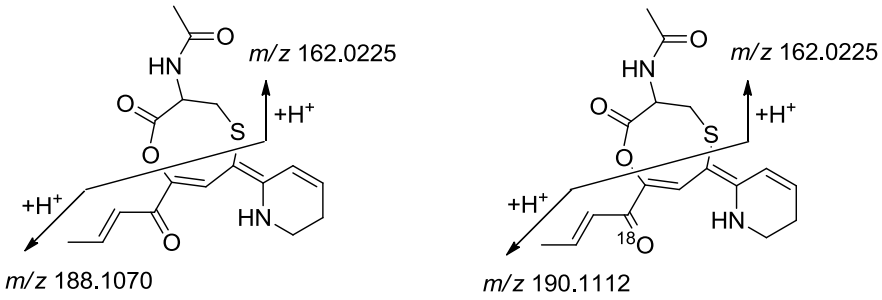


Figure S12. Top panel: High resolution mass spectrum of ^{18}O-labeled coelimycin P1 obtained from LC-ESI-TOF-MS analysis of culture supernatants of M1157 grown in an $^{18}O_2$ atomsphere. The signal for *m/z* = 351.1254 results from the $[M+H]^+$ ion for singly ^{18}O-labeled coelimcyin P, whereas the signal for *m/z* = 349.1216 results from the $[M+H]^+$ ion for unlabeled coelimcyin P. Bottom panel: Simulated mass spectrum for the $C_{17}H_{21}N_2{}^{16}O_3{}^{18}OS^+$ ion.

A



B

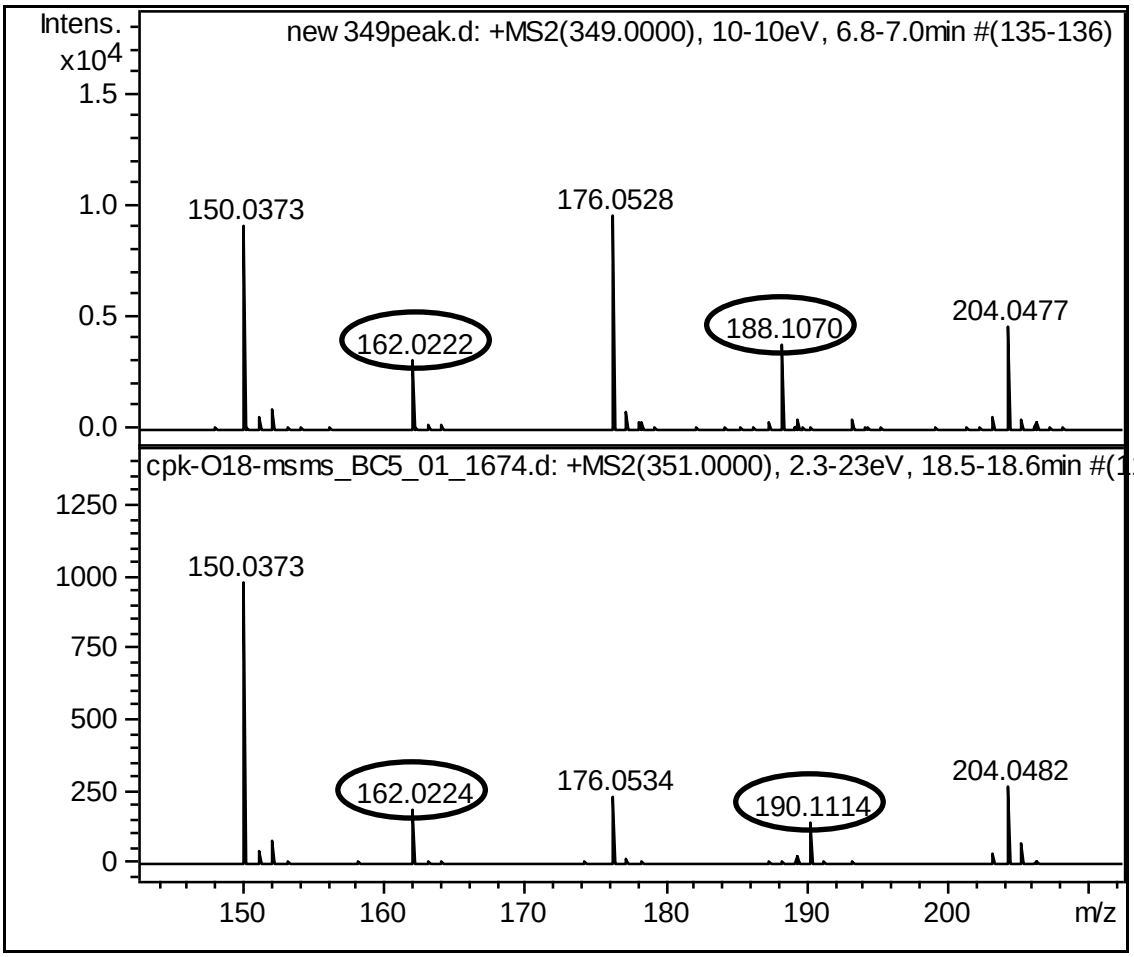


Figure S13. (A) Comparison of fragment ions expected in MS/MS spectra of unlabeled (left) and singly ^{18}O-labeled (right) coelimycin P1. (B) Top panel: region of the MS/MS spectrum resulting from fragmentation of the $[M+H]^+$ ion derived from unlabeled coelimycin P1. Bottom panel: region of the MS/MS spectrum resulting from fragmentation of the $[M+H]^+$ ion derived from singly ^{18}O-labeled coelimycin P1.

*Analysis of deuterium-labeled (2*R*)- and (2*S*)-*N*-acetylcysteine incorporation into coelicmycin P*. Deuterium-labeled (2*R*)- and (2*S*)-*N*-acetylcysteine were synthesized from (2*R*)- and (2*S*)-cysteine and CD_3CN following a literature procedure.[6] After 54 and 72 h growth, 1 ml portions of filter-sterilized 0.5mM aqueous solutions of deuterium-labeled (2*R*)- and (2*S*)-*N*-acetylcysteine were fed to separate cultures of *S. coelicolor* M1157 grown in 50ml of R3 medium at 28 ºC and 180 rpm. Culture supernatants were harvested after 102 h growth by centrifugation for 10 minutes at 13,000rpm and analyzed by LC-ESI-TOF-MS as described above. These analyses confirmed incorporation of deuterium-labeled (2*S*)- and (2*R*)-*N*-acetylcysteine into coelimycin P1 (*m/z* calculated for $C_{17}H_{18}D_3N_2O_4S^+$ = 352.1405; *m/z* found from feeding of (2*S*)-isomer: 352.1407; *m/z* found for feeding of (2*R*)-isomer: 352.1397). The supernatants from cultures to which deuterium-labeled (2*S*)- and (2*R*)-*N*-acetylcysteine had been added, as well as the supernatant from a culture of the M1157 strain to which no labeled precursors had been added, were analyzed on a CHIRALPAL IC column (Chiral Technologies Inc) connected to an Agilent 1200 HPLC coupled with a Bruker HCT-Ultra ETD ion trap mass spectrometer (Figure S14). Water containing 0.1% TFA (solvent A) and acetonitrile containing 0.1% TFA (solvent B) were used as eluents. Gradient elution from 98% solvent A/2% solvent B to 100% solvent B over 45 minutes was used.

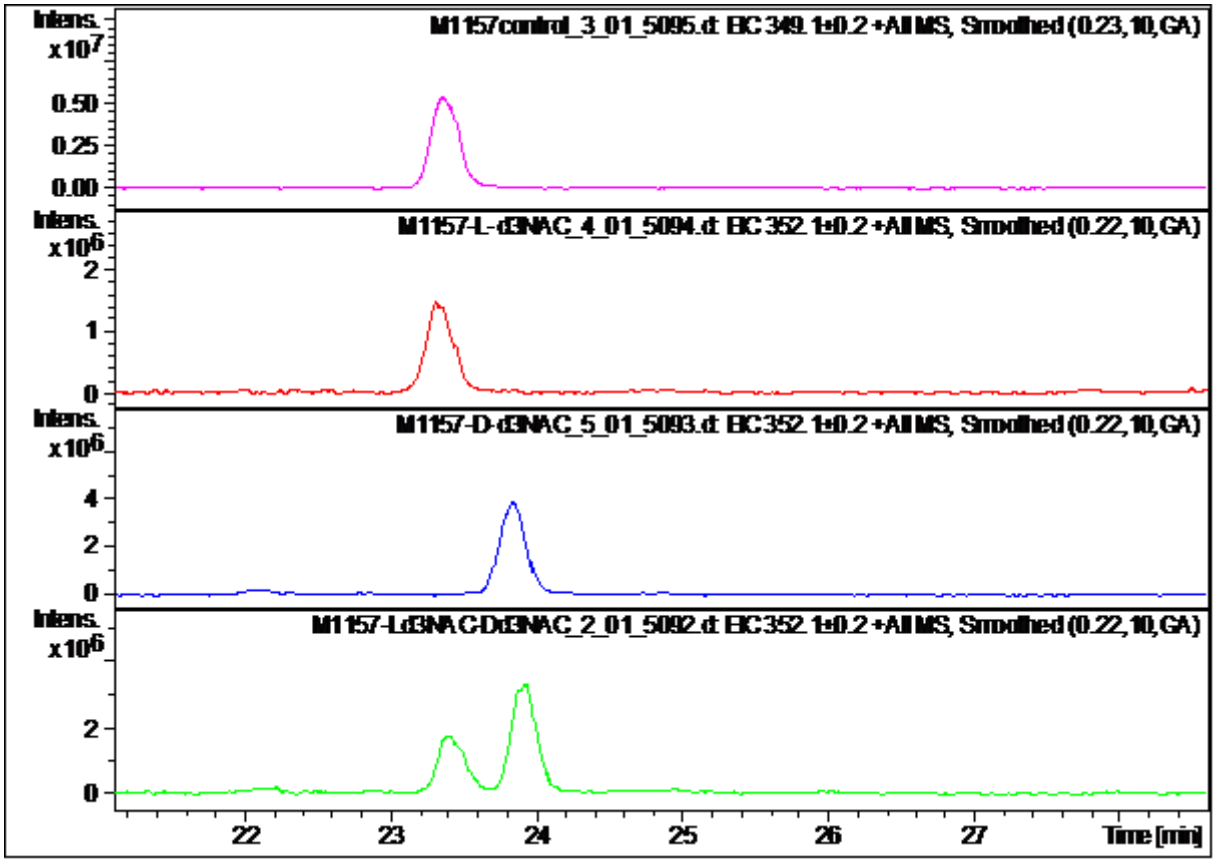


Figure S14. Extracted ion chromatograms (EICs) from LC-MS analyses on a homochiral stationary phase of the incorporation of deuterium-labeled (2*R*)- and (2*S*)-*N*-acetylcysteine into coelimycin P1. Chromatograms from top to bottom are as follows: EIC at *m/z* = 349.0 - unlabeled coelimycin P1 (magenta); EIC at *m/z* = 352.0 - labeled coelimycin P1 derived from deuterium-labeled (2*R*)-*N*-acetylcysteine (red); EIC at *m/z* = 352.0 - labeled coelimycin P1 derived from deuterium-labeled (2*S*)-*N*-acetylcysteine (blue); EIC at *m/z* = 352.0 - a mixture of labeled coelimycin P1 derived from deuterium-labeled (2*S*)- and (2*R*)-*N*-acetylcysteine (green).

LC-ESI-TOF-MS analysis of the yellow pigment produced by S. coelicolor *M145 and M1157 grown in DNB-Glu medium*. The *S. coelicolor* M145, M1157 and M1152 strains were grown in DNB-Glu medium as previously described.[4] LC-ESI-TOF-MS analyses of the culture supernatants using the elution conditions described above showed that coelimycin P1 is not produced, but instead identified a compound with a retention time of ~ 11 minutes and a λ_{max} of ~430 nm in the supernatants from the M145 and M1157 strains that was absent from the M1152 strain (Figure S15). The molecular formula deduced for this compound from the HRMS data was $C_{17}H_{22}N_2O_6$ (Figure S16), which is consistent with a glutamate adduct of **9**.

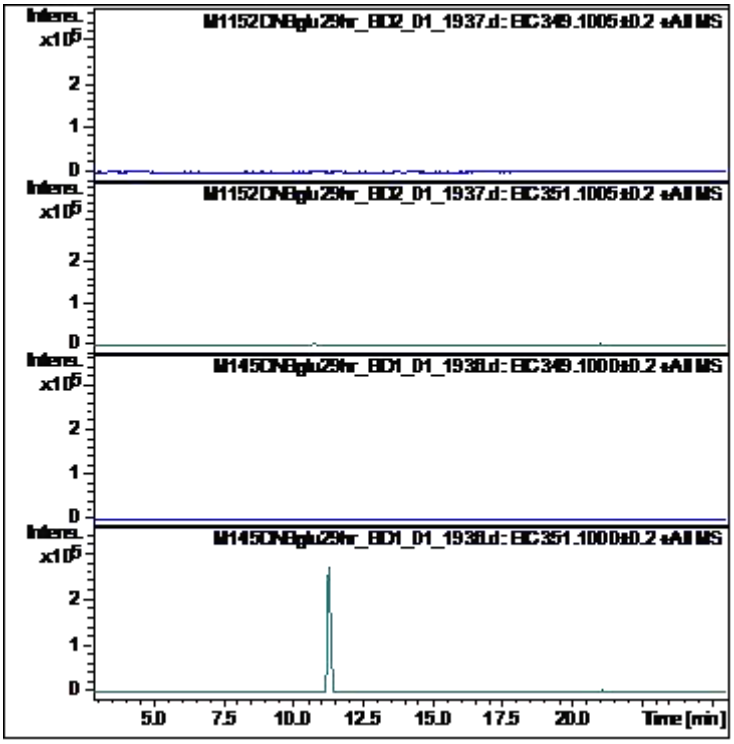


Figure S15. Extracted ion chromatograms (EICs) from LC-ESI-TOF-MS analyses of culture supernatants from *S. coelicolor* M145 and M1152 grown in DNB-Glu medium. The EICs at *m/z* = 349.1 (corresponding to $[M+H]^+$ for coelimycin P1) for the supernatants from the M1152 and M145 strains are shown in the top panel and the third from top panel, respectively. The EICs at *m/z* = 351.1 (corresponding to $[M+H]^+$ for the putative glutamate adduct of **8**) for the supernatants from the M1152 and M145 strains are shown in the second from top panel and the bottom panel, respectively. Similar results were obtained with the M1157 strain.

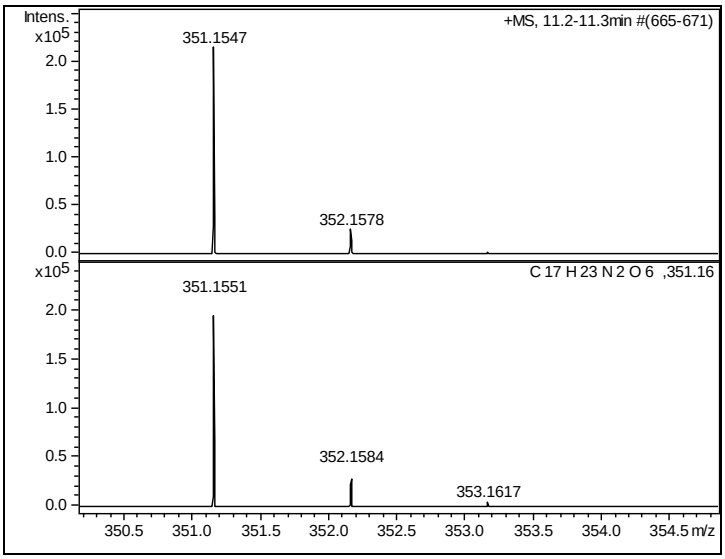


Figure S16. High resolution mass spectrum of the yellow-pigmented metabolic product of the *cpk* gene cluster produced by *S. coelicolor* M145 grown in DNB-Glu medium (top panel). The simulated mass spectrum for the $C_{17}H_{23}N_2O_6^+$ ion is shown in the bottom panel.

DFT Calculations of Ground State Conformations and Energies for Coelimycin P1

DFT calculations were performed using PC-GAMESS at the B3LYP/6-31G(d) level.[7,8] Calculated ground-state structures have a maximum RMS gradient less than or equal to $1x10^{-5}$ Hartree/Bohr. The conformations identified are summarized in Tables S4 and S5. Conformations 3 and 4 include an (*E*)-alkene in the eight-membered ring. Structures 3 and 4 are significantly higher in energy than the (*Z*)-alkene structures 1 and 2. Inter-proton distances for conformation 1a that correspond to key correlations observed in the NOESY spectrum of coelimcyin P are shown in Figure S17.

Table S4. Summary of the eight conformations identified for coelimycin P1 with a (*Z*)-alkene in the eight-membered ring. Energies relative to those of conformation 2d.

Conformation	ester	NHAc	ketone	ΔE (inc ZPE) kJ/ mol	ΔG at 298 K kJ/mol
1a	trans	exo	anti	3.6	1.4
1b	trans	endo	anti	26.9	25.1
1c	trans	exo	syn	20.9	20.8
1d	trans	endo	syn	33.6	34.4
2a	cis	exo	syn	20.1	19.4
2b	cis	endo	syn	15.6	15.3
2c	cis	exo	anti	5.1	3.0
2d	cis	endo	anti	0	0

Table S5. Summary of the eight conformations identified for coelimycin P1 with an (*E*)-alkene in the eight-membered ring. Energies relative to those of conformation 2d.

Conformation	Ring stereo-chemistry	NHAc	ketone	ΔE (inc ZPE) kJ/ mol	ΔG at 298 K kJ/mol
3a	(S)	exo	anti	95.8	97.1
3b	(R)	endo	anti	96.1	95.1
3c	(S)	exo	syn	110.6	112.9
3d	(R)	endo	syn	113.9	114.4
4a	(S)	endo	anti	98.1	101.2
4b	(R)	exo	anti	94.4	94.8
4c	(S)	endo	syn	90.1	93.9
4d	(R)	exo	syn	132.4	132.1

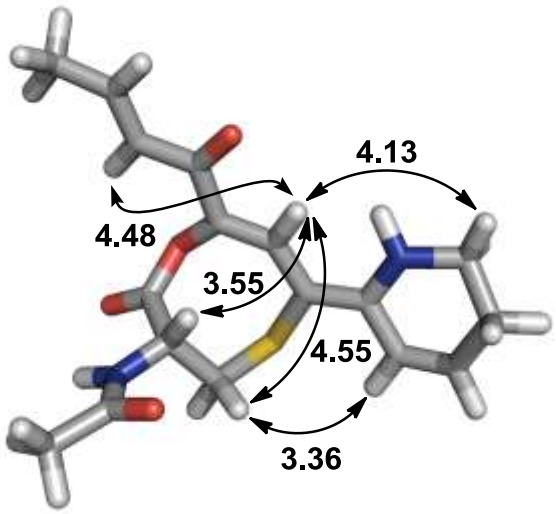


Figure S17. Conformation 1a with inter-proton distances (in Å) corresponding to the key NOESY correlations marked.

Energies and zero point energies (Hartrees/molecule), final gradients (Hartrees/Bohr) Gibbs free energy corrections at 298.15 K (kJ / mol) and Cartesian coordinates (Ångstroms) are given below for each structure. Zero-point energies are based on unscaled vibrational frequencies.

1a

ENERGY = -1468.4018471
MAXIMUM GRADIENT = 0.0000081 RMS GRADIENT = 0.0000031
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352604
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 775.649 kJ / mol

C	6.0	5.1105541336	3.7178310184	-0.3195026996
C	6.0	3.6692336480	3.4463497015	-0.6105496871
C	6.0	2.9081645958	2.5414669153	0.0240248196
C	6.0	1.4826666061	2.3620990884	-0.3492545072
C	6.0	0.7073216426	1.2988745318	0.3516340457
O	8.0	0.9369222407	3.0636930244	-1.2047543777
C	6.0	-0.6162866628	1.1509485829	0.0747401020
O	8.0	1.4271581949	0.6074781226	1.3322940363
C	6.0	-1.6360306975	0.2605369809	0.5419894761
C	6.0	1.8009873227	-0.6945512461	1.2339696878
C	6.0	-2.9598883809	0.4141431661	0.1088766721
C	6.0	1.1084602814	-1.5754526704	0.1977343290
S	16.0	-1.2506725208	-1.0070793750	1.7426009982
C	6.0	-4.0006884978	-0.5777488370	0.3854884512
N	7.0	-3.3571259406	1.4806503268	-0.6609413880
C	6.0	-5.2134400151	-0.5212966453	-0.1924977455
C	6.0	-4.7704562920	1.8402240565	-0.7836575582
O	8.0	2.6319632215	-1.1286358598	1.9970880117
C	6.0	-5.6050436563	0.6032558882	-1.1088681290
C	6.0	-0.1911168133	-2.1765284092	0.7948476736
N	7.0	2.0352211536	-2.6271211487	-0.1760759601
C	6.0	1.9531811879	-3.2647390366	-1.3822401207
C	6.0	3.0212788943	-4.3166303668	-1.6386028797
O	8.0	1.0794517604	-3.0039571149	-2.2020082061
H	1.0	5.2587090838	4.7695859983	-0.0385570939
H	1.0	5.4928002738	3.0869543300	0.4890224845
H	1.0	5.7268809448	3.5489087009	-1.2132182762
H	1.0	3.1985360169	4.0306377719	-1.4009522511
H	1.0	3.3162760468	1.9310792207	0.8232566119
H	1.0	-0.8868139428	1.8480031665	-0.7162547769
H	1.0	0.8563670992	-1.0108735812	-0.7012950509
H	1.0	-3.7272196343	-1.4066176793	1.0244906378
H	1.0	-2.7217129581	2.2643591290	-0.7028097738
H	1.0	-5.9253666839	-1.3260426170	-0.0246143248
H	1.0	-4.8560912606	2.5924673901	-1.5730799895
H	1.0	-5.1381023496	2.2909652785	0.1523215300
H	1.0	-6.6706232032	0.8410770572	-1.0076343339
H	1.0	-5.4490196594	0.2994386824	-2.1553091396
H	1.0	-0.7561774686	-2.6482896671	-0.0122141144
H	1.0	0.0840662360	-2.9416213544	1.5283801431
H	1.0	2.7511864896	-2.8535584100	0.5025231757
H	1.0	3.5825616489	-4.0357882959	-2.5352221467
H	1.0	2.5324269726	-5.2732615873	-1.8466773984
H	1.0	3.7206378730	-4.4456112842	-0.8070211168

1b

ENERGY= -1468.3927965
MAXIMUM GRADIENT = 0.0000079 RMS GRADIENT = 0.0000031
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352446
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 775.547 kJ / mol

C	6.0	5.2037417790	-3.0358801755	0.8567199949
C	6.0	3.8360238290	-2.8375719910	0.2870552093
C	6.0	2.9322357073	-1.9505442686	0.7325848114
C	6.0	1.5987050266	-1.8470345304	0.0950898223
C	6.0	0.6608915985	-0.8090073783	0.6171484191
O	8.0	1.2508442178	-2.5803190931	-0.8357604414
C	6.0	-0.6398468422	-0.8228940315	0.2142713557
O	8.0	1.2025740796	0.0471514131	1.5663054227
C	6.0	-1.7478049472	0.0602249304	0.4439648801
C	6.0	1.4915850165	1.3779334681	1.3701744574
C	6.0	-3.0380307077	-0.3345152109	0.0766088000
C	6.0	1.1053155539	2.0546941483	0.0398687168
S	16.0	-1.5184408754	1.6468866166	1.2301107411
C	6.0	-4.1691419254	0.5901532533	0.0111120537
N	7.0	-3.3047522605	-1.6295586910	-0.3131622942
C	6.0	-5.3514188360	0.2342933729	-0.5226261480
C	6.0	-4.6772371069	-2.1402293483	-0.3153384422
O	8.0	2.0016079998	1.9890298914	2.2698938067
C	6.0	-5.6079856584	-1.1586189979	-1.0249273597
C	6.0	-0.3669811612	2.5502446019	0.1057303082
N	7.0	1.4179401553	1.2979803713	-1.1569016338
C	6.0	2.4631670020	1.6466771995	-1.9848259247
C	6.0	2.6287404816	0.7455594631	-3.1989751470
O	8.0	3.1797913810	2.6144502834	-1.7740863059
H	1.0	5.3346060014	-4.0713658865	1.1997281609
H	1.0	5.4004754642	-2.3643083745	1.6978181114
H	1.0	5.9719569158	-2.8666399777	0.0898724886
H	1.0	3.5493926228	-3.4647050359	-0.5571221371
H	1.0	3.1531135765	-1.2977180772	1.5708029003
H	1.0	-0.8057452734	-1.6373764544	-0.4902684603
H	1.0	1.7589480803	2.9281122767	-0.0121122579
H	1.0	-3.9918266364	1.6043964374	0.3436123534
H	1.0	-2.6130460492	-2.3140000961	-0.0405830792
H	1.0	-6.1372574649	0.9781343626	-0.6309668133
H	1.0	-4.6722422050	-3.1116240701	-0.8184408270
H	1.0	-5.0336807109	-2.2970927991	0.7156060452
H	1.0	-6.6506829978	-1.4527522423	-0.8557372442
H	1.0	-5.4446054749	-1.1955896283	-2.1129274159
H	1.0	-0.7824657216	2.5957594871	-0.9044964016
H	1.0	-0.3769828972	3.5619455921	0.5222365861
H	1.0	0.8642392247	0.4867212162	-1.3874559244
H	1.0	3.6836709759	0.7314876771	-3.4796939060
H	1.0	2.2840319045	-0.2778281934	-3.0175165468
H	1.0	2.0612727481	1.1586004288	-4.0414964764

1c

ENERGY= -1468.3953146
MAXIMUM GRADIENT = 0.0000100 RMS GRADIENT = 0.0000017
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352661
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 777.873 kJ / mol

C	6.0	-0.4530432509	-5.4630223710	-1.9753896997
C	6.0	-1.0748610013	-4.2897981535	-1.2882449463
C	6.0	-0.4131063537	-3.3507310802	-0.5966906752
C	6.0	-1.1450905885	-2.2437991257	0.0705165812
C	6.0	-0.3786826742	-1.1337975921	0.7003369104
O	8.0	-2.3737830439	-2.2031771166	0.1103459909
C	6.0	0.8754058341	-0.7578231522	0.3344743782
O	8.0	-1.1143258628	-0.4574423303	1.6643515232
C	6.0	1.6096697253	0.4533633132	0.6013587668
C	6.0	-1.9899033501	0.5297873754	1.3323181100
C	6.0	2.9748132167	0.5087797820	0.3239482015
C	6.0	-1.7464637007	1.2322973297	-0.0010387687
S	16.0	0.8006825893	1.8906114321	1.2825744423
C	6.0	3.7257547902	1.7585436582	0.2282447361
N	7.0	3.6873205477	-0.6455033446	0.0475564219
C	6.0	4.9893985421	1.7968436040	-0.2309583592
C	6.0	5.1496631783	-0.6466560120	0.1453543668
O	8.0	-2.8369915332	0.8790330941	2.1159136605
C	6.0	5.7335259614	0.5470249561	-0.6080500108
C	6.0	-0.5778611426	2.2601354808	0.1140685167
N	7.0	-2.9757909716	1.8972935637	-0.3828706825
C	6.0	-3.2628683555	2.1661767862	-1.6908623384
C	6.0	-4.6503425294	2.7298810727	-1.9534926290
O	8.0	-2.4562545998	1.9589731897	-2.5918413398
H	1.0	-0.6821018468	-5.4498628112	-3.0495391203
H	1.0	0.6348362253	-5.4847038630	-1.8545840010
H	1.0	-0.8635497618	-6.4038246392	-1.5844342530
H	1.0	-2.1578798588	-4.1887876349	-1.3503651089
H	1.0	0.6674078851	-3.4092566035	-0.4907505311
H	1.0	1.3490504387	-1.4284198875	-0.3797036323
H	1.0	-1.4986240113	0.5083514391	-0.7788950317
H	1.0	3.1908982886	2.6688737801	0.4654100463
H	1.0	3.2635924211	-1.4910374092	0.4048606312
H	1.0	5.4803627402	2.7564066947	-0.3744481476
H	1.0	5.5132714541	-1.5905596404	-0.2720123342
H	1.0	5.4684189321	-0.5995455778	1.1993313295
H	1.0	6.8018288495	0.6391519128	-0.3784005232
H	1.0	5.6593377123	0.3855193381	-1.6943986440
H	1.0	-0.1907340328	2.4626019699	-0.8866801985
H	1.0	-0.9902413255	3.1906187613	0.5168594421
H	1.0	-3.6626663804	2.0116719214	0.3525718384
H	1.0	-4.5602900974	3.5962417883	-2.6143078975
H	1.0	-5.1828796973	3.0224894334	-1.0434240364
H	1.0	-5.2439480525	1.9747893338	-2.4799950693

1d

ENERGY= -1468.3904512
MAXIMUM GRADIENT = 0.0000079 RMS GRADIENT = 0.0000031
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352649
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 778.725 kJ / mol

C	6.0	1.2032729611	5.5550745156	0.7520483758
C	6.0	1.6347281088	4.2050826999	0.2773401992
C	6.0	0.8133045235	3.2100404396	-0.0918120194
C	6.0	1.3549467668	1.9214036784	-0.5842272494
C	6.0	0.4268509516	0.8012419776	-0.8725390440
O	8.0	2.5700229702	1.7618108043	-0.7628819196
C	6.0	-0.7964477458	0.6596563066	-0.2880490064
O	8.0	0.8787532483	-0.0668701220	-1.8481290793
C	6.0	-1.6582633456	-0.4906679599	-0.2157876555
C	6.0	1.5867372203	-1.2350186269	-1.6855149706
C	6.0	-3.0058262559	-0.3245767478	0.0899764612
C	6.0	1.8558802151	-1.7570616615	-0.2680992969
S	16.0	-0.9877234481	-2.1395617436	-0.3852761823
C	6.0	-3.8698562189	-1.4044020160	0.5563450173
N	7.0	-3.5827770329	0.9335501597	0.0238175541
C	6.0	-5.1138331613	-1.1722069974	1.0130398267
C	6.0	-5.0406432943	1.0618090787	-0.0629907159
O	8.0	1.9636009745	-1.8075062980	-2.6707900845
C	6.0	-5.7157391451	0.2047821587	1.0067647816
C	6.0	0.5780427765	-1.9867417790	0.5869144324
N	7.0	2.8229184879	-0.8920276310	0.3960474734
C	6.0	3.5960019653	-1.3841429487	1.4098872366
C	6.0	4.6593953365	-0.4312525670	1.9335485095
O	8.0	3.4413282780	-2.5145680354	1.8613929115
H	1.0	1.5927767413	5.7549574553	1.7594019605
H	1.0	0.1137326908	5.6574275271	0.7757727927
H	1.0	1.6112064020	6.3417227255	0.1030303772
H	1.0	2.7055998891	4.0138055206	0.2196656914
H	1.0	-0.2633921529	3.3549536281	-0.0691647754
H	1.0	-1.1130517861	1.5006376522	0.3271863364
H	1.0	2.3305593087	-2.7274073193	-0.4295088629
H	1.0	-3.4365746952	-2.3954234898	0.6020964880
H	1.0	-3.0911595133	1.5784253686	-0.5806788944
H	1.0	-5.6915786613	-1.9885790865	1.4397259276
H	1.0	-5.2937155078	2.1188127418	0.0637421022
H	1.0	-5.3985597767	0.7470976073	-1.0567192996
H	1.0	-6.7947874562	0.1627832712	0.8159127909
H	1.0	-5.5916005213	0.6660456956	1.9986034794
H	1.0	0.4499420461	-1.1774628199	1.3067959219
H	1.0	0.6952370144	-2.9161598932	1.1470854970
H	1.0	3.0024849419	0.0287261449	-0.0018482125
H	1.0	5.6471984036	-0.8265723060	1.6734924218
H	1.0	4.5671878247	0.5817442616	1.5308508643
H	1.0	4.5976969013	-0.3973309069	3.0249764628

2a

ENERGY= -1468.3948526
MAXIMUM GRADIENT = 0.0000096 RMS GRADIENT = 0.0000033
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.351896
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 775.307 kJ / mol

C	6.0	-3.9438821429	5.1173938187	0.6549757410
C	6.0	-2.6213111275	4.5821688466	0.2063921871
C	6.0	-2.1803013109	3.3315102631	0.4019022897
C	6.0	-0.8333991614	2.9205411900	-0.0809222834
C	6.0	-0.4335996607	1.5000773933	0.0476502709
O	8.0	-0.0486588819	3.7269665186	-0.5745341399
C	6.0	-1.2231896667	0.4442298302	0.3745316996
O	8.0	0.9149879396	1.2770976334	-0.2098573058
C	6.0	-0.8469080687	-0.9440979856	0.5668519534
C	6.0	1.2411979830	0.4314653134	-1.2400966118
C	6.0	-1.7802981160	-1.9417958915	0.2981742437
C	6.0	2.4304569979	-0.4230790907	-0.8435194546
S	16.0	0.7442706584	-1.3749620855	1.2835244282
C	6.0	-1.6156013965	-3.3440996568	0.6890470512
N	7.0	-2.9231248187	-1.6623973840	-0.4032619856
C	6.0	-2.4517460100	-4.3052545747	0.2603985327
C	6.0	-4.0790484428	-2.5534861126	-0.4124303911
O	8.0	0.5880734807	0.2814634901	-2.2385331809
C	6.0	-3.6311382025	-4.0016369427	-0.6249320203
C	6.0	1.8372842815	-1.6967950484	-0.1770780976
N	7.0	3.3532841478	0.2895458092	0.0169826795
C	6.0	4.6506421969	-0.1201390236	0.1538055327
C	6.0	5.5017115764	0.7069704816	1.1043691884
O	8.0	5.1007116656	-1.0806592213	-0.4622753157
H	1.0	-4.5256253829	5.4862643074	-0.2007539006
H	1.0	-4.5397850326	4.3621135488	1.1776631122
H	1.0	-3.8081259828	5.9755993983	1.3270666688
H	1.0	-1.9561246707	5.2652837757	-0.3209268853
H	1.0	-2.7976397095	2.6152941837	0.9380071820
H	1.0	-2.2806662562	0.6654131005	0.5079064495
H	1.0	2.9663769282	-0.7393632500	-1.7415676292
H	1.0	-0.7701347800	-3.5765471880	1.3235892955
H	1.0	-3.0078372371	-0.7578844680	-0.8406135377
H	1.0	-2.2711527280	-5.3398975355	0.5426051879
H	1.0	-4.7505506095	-2.2263065043	-1.2110036381
H	1.0	-4.6299952348	-2.4787526715	0.5378185530
H	1.0	-4.4664229159	-4.6775827778	-0.4060665949
H	1.0	-3.3591400737	-4.1717157801	-1.6778667540
H	1.0	1.2805589289	-2.2792080631	-0.9165119159
H	1.0	2.6684377552	-2.3016110357	0.1952356062
H	1.0	2.9702351847	1.0139350943	0.6074133508
H	1.0	5.9416767671	0.0425450474	1.8540777389
H	1.0	4.9483498936	1.5036886480	1.6104532544
H	1.0	6.3261918208	1.1527386936	0.5389179180

2b

ENERGY= -1468.3966862
MAXIMUM GRADIENT = 0.0000089 RMS GRADIENT = 0.0000031
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352042
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 776.026 kJ / mol

C	6.0	-5.9607556482	-2.9920996369	-0.1181823444
C	6.0	-4.4713455715	-3.1185803946	-0.1688449726
C	6.0	-3.5963348900	-2.1554065229	0.1525605236
C	6.0	-2.1311315994	-2.4092257727	0.0809440052
C	6.0	-1.2021224406	-1.2825346775	0.3289962822
O	8.0	-1.6766741100	-3.5213600474	-0.1742137360
C	6.0	-1.4983932537	0.0405149558	0.3951702442
O	8.0	0.1235027863	-1.6670689197	0.5045837681
C	6.0	-0.6024155446	1.1457152627	0.6814575444
C	6.0	1.0245384282	-1.3193888182	-0.4476505390
C	6.0	-0.8922683399	2.4095835033	0.1743583286
C	6.0	2.3328084459	-0.9375983774	0.2109592398
S	16.0	0.7818585258	0.9266822839	1.8084771117
C	6.0	-0.2040535012	3.6337360802	0.5922877982
N	7.0	-1.8368825459	2.5819360882	-0.8052539392
C	6.0	-0.4062154434	4.8115054713	-0.0230316165
C	6.0	-2.4536884670	3.8781436985	-1.0725935498
O	8.0	0.7974042347	-1.2240915970	-1.6305225833
C	6.0	-1.3774377747	4.9622392639	-1.1631822445
C	6.0	2.2095418228	0.5375283368	0.7038032135
N	7.0	3.4005312586	-1.0660309235	-0.7592183196
C	6.0	4.7138277855	-1.1138927806	-0.3866965857
C	6.0	5.7098090325	-1.3197437183	-1.5175039991
O	8.0	5.0637947026	-1.0097350343	0.7841786166
H	1.0	-6.4022708830	-3.1817376992	-1.1060523920
H	1.0	-6.2802065558	-2.0004255979	0.2184576461
H	1.0	-6.3911175310	-3.7414694112	0.5599202945
H	1.0	-4.0593157329	-4.0751962137	-0.4886967742
H	1.0	-3.9540430931	-1.1881338022	0.4964116682
H	1.0	-2.5390005473	0.3049644377	0.2148814526
H	1.0	2.5305158937	-1.5810410591	1.0718113514
H	1.0	0.4967056493	3.5412460489	1.4118427761
H	1.0	-2.2651497032	1.7606289582	-1.2040641815
H	1.0	0.1548351111	5.6870058454	0.2956220723
H	1.0	-3.0134911946	3.7984105852	-2.0086757689
H	1.0	-3.1685210858	4.1399169547	-0.2768337457
H	1.0	-1.8516554508	5.9508252731	-1.1426945152
H	1.0	-0.8403637522	4.8927206947	-2.1215132053
H	1.0	2.1762291230	1.2023948873	-0.1641747811
H	1.0	3.1078023462	0.7632102745	1.2843560920
H	1.0	3.1182787080	-1.1364509428	-1.7286596732
H	1.0	6.1920411890	-2.2943820934	-1.3888378995
H	1.0	5.2590354285	-1.2788546250	-2.5138391153
H	1.0	6.4901011303	-0.5570050973	-1.4431608181

2c

ENERGY= -1468.4007137
MAXIMUM GRADIENT = 0.0000077 RMS GRADIENT = 0.0000027
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352039
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 774.296 kJ / mol

C	6.0	4.7601743887	4.2165047273	-0.2464127189
C	6.0	3.3149492681	4.0081500147	0.0756938023
C	6.0	2.6705170024	2.8325595071	0.0330436175
C	6.0	1.2282524511	2.7472917729	0.3713129261
C	6.0	0.5808421403	1.4171797505	0.2982034095
O	8.0	0.5673078890	3.7357125788	0.6989257381
C	6.0	-0.7482864333	1.2527055094	0.5093258377
O	8.0	1.3918595220	0.3120306869	0.0114328682
C	6.0	-1.5440916437	0.0469453788	0.5378761892
C	6.0	1.1097886133	-0.3928068638	-1.1404934670
C	6.0	-2.9079327308	0.1225724301	0.2526353460
C	6.0	1.2025633000	-1.8836043997	-0.8754549449
S	16.0	-0.8392888259	-1.5076147081	1.1053016412
C	6.0	-3.8480435848	-0.9815641090	0.4638707562
N	7.0	-3.4540729827	1.2497893346	-0.3019404900
C	6.0	-5.1250648535	-0.9200704752	0.0488785408
C	6.0	-4.8844996205	1.5354789631	-0.2192718632
O	8.0	0.7143027030	0.1044589131	-2.1605332823
C	6.0	-5.6868462487	0.2999117314	-0.6299401456
C	6.0	-0.2160983087	-2.3359323042	-0.4290904634
N	7.0	2.2272777364	-2.2059989617	0.0967422250
C	6.0	2.8596476506	-3.4213344980	0.0847075232
C	6.0	3.8545591274	-3.6485263638	1.2121162508
O	8.0	2.6506385898	-4.2612767079	-0.7828158066
H	1.0	5.2925268298	4.6474841285	0.6125942614
H	1.0	5.2580355462	3.2836673135	-0.5293048032
H	1.0	4.8751201347	4.9335910991	-1.0707163587
H	1.0	2.7354009835	4.8835059633	0.3683277796
H	1.0	3.1879978828	1.9210775848	-0.2503402817
H	1.0	-1.2541892014	2.2000302963	0.6967129404
H	1.0	1.4445172138	-2.4035027217	-1.8048272180
H	1.0	-3.4598830542	-1.8660982176	0.9516495506
H	1.0	-2.8357687638	2.0220199982	-0.5025695450
H	1.0	-5.7772765791	-1.7789394428	0.1898212450
H	1.0	-5.0967844952	2.3813772957	-0.8788476613
H	1.0	-5.1635544302	1.8303632673	0.8043841185
H	1.0	-6.7410934898	0.4427466937	-0.3642725713
H	1.0	-5.6546723014	0.1649861071	-1.7219371074
H	1.0	-0.9342395742	-2.1792079567	-1.2388163326
H	1.0	-0.1731562703	-3.4043156823	-0.1984350754
H	1.0	2.3142419615	-1.5880971626	0.8913853838
H	1.0	4.8370722938	-3.8545736356	0.7765058634
H	1.0	3.5545659019	-4.5380792153	1.7746251927
H	1.0	3.9403821689	-2.8025429375	1.9007037381

2d

ENERGY= -1468.4028971
MAXIMUM GRADIENT = 0.0000092 RMS GRADIENT = 0.0000031
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352291
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 776.987 kJ / mol

C	6.0	5.2907976438	3.7799909886	0.1542907875
C	6.0	3.7960871889	3.7773110270	0.1141698420
C	6.0	3.0258068005	2.6960224096	-0.0765706860
C	6.0	1.5474147957	2.8148973844	-0.1025929136
C	6.0	0.7605447604	1.5790353255	-0.3157627692
O	8.0	0.9672308047	3.8931014546	0.0458594599
C	6.0	-0.5943430378	1.5758024778	-0.3381336500
O	8.0	1.4531399101	0.3790775710	-0.5307166970
C	6.0	-1.5029942695	0.4857495927	-0.6089659346
C	6.0	1.3596120926	-0.5822752780	0.4301370334
C	6.0	-2.8092659145	0.5441580622	-0.1233276312
C	6.0	1.2027863924	-1.9435316621	-0.2110607442
S	16.0	-1.0193946920	-0.8454149670	-1.7182605850
C	6.0	-3.8668904805	-0.3901066227	-0.5177400392
N	7.0	-3.1791664604	1.4747647626	0.8140152048
C	6.0	-5.0804234373	-0.3798703205	0.0603301502
C	6.0	-4.5762761867	1.8627647482	0.9973591401
O	8.0	1.3263761011	-0.3747726247	1.6197582196
C	6.0	-5.4489281914	0.6138518765	1.1287681651
C	6.0	-0.2936574105	-2.1301569400	-0.6101055535
N	7.0	1.6106682916	-2.9564226267	0.7409846495
C	6.0	1.9335399973	-4.2260856486	0.3521814304
C	6.0	2.3844681033	-5.1585581931	1.4657859583
O	8.0	1.8698622583	-4.5852674942	-0.8185123121
H	1.0	5.6996597311	4.4436321628	-0.6199060960
H	1.0	5.7083768420	2.7790416984	0.0068391805
H	1.0	5.6535524539	4.1687720661	1.1156503254
H	1.0	3.2890305785	4.7323424216	0.2502960252
H	1.0	3.4658578112	1.7141901975	-0.2225399357
H	1.0	-1.0152053547	2.5620556333	-0.1420639921
H	1.0	1.8157513407	-2.0148434733	-1.1130722503
H	1.0	-3.6188112022	-1.1095085560	-1.2871624607
H	1.0	-2.4757003667	2.1294476322	1.1235402500
H	1.0	-5.8224499038	-1.1178107065	-0.2359397904
H	1.0	-4.6375554258	2.4833124632	1.8957032178
H	1.0	-4.9281454400	2.4680070400	0.1471331906
H	1.0	-6.5058363585	0.8956147098	1.0507350206
H	1.0	-5.3196417712	0.1564814206	2.1217290628
H	1.0	-0.9012543741	-2.2045591592	0.2965046774
H	1.0	-0.3640955743	-3.0738904755	-1.1574894506
H	1.0	1.6516347819	-2.6697799586	1.7106834138
H	1.0	3.4108486382	-5.4795734719	1.2615980166
H	1.0	2.3457549447	-4.7068270098	2.4617449255
H	1.0	1.7550561542	-6.0533720981	1.4534442750

3a

ENERGY= -1468.3662180
MAXIMUM GRADIENT = 0.0000078 RMS GRADIENT = 0.0000028
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352106
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 777.792 kJ / mol

C	6.0	0.3190262723	5.4830696485	-1.2645085884
C	6.0	0.8788245700	4.1748221359	-0.8074973674
C	6.0	0.2197246409	3.2623960978	-0.0748196535
C	6.0	0.8749874505	1.9935615807	0.3173551205
C	6.0	0.0868750578	0.9969352099	1.0703309725
O	8.0	2.0519439872	1.7402548272	0.0352465497
C	6.0	0.4118998830	-0.3010460432	1.2889423849
O	8.0	-1.1821754774	1.4289888947	1.4940293086
C	6.0	1.1829782063	-1.1860451668	0.4223421012
C	6.0	-2.3063192912	0.9462600944	0.8774832404
C	6.0	2.5303637974	-1.3016292924	0.2072885539
C	6.0	-2.3474434690	-0.4639859682	0.1981167803
S	16.0	-0.0721447339	-2.1773053228	-0.3954701845
C	6.0	3.0831729301	-2.2581047736	-0.7536410698
N	7.0	3.4415461483	-0.5982684572	0.9826303959
C	6.0	4.4023121088	-2.4958277284	-0.8357850553
C	6.0	4.7903526128	-0.4077647067	0.4413149531
O	8.0	-3.3083372768	1.6157519529	0.9641380623
C	6.0	5.3859726834	-1.7536389706	0.0272045901
C	6.0	-1.2878051897	-0.8603946258	-0.8924645134
N	7.0	-3.6930006806	-0.5673884056	-0.3530191400
C	6.0	-4.2527173017	-1.7935413550	-0.5892336775
C	6.0	-5.7231954558	-1.7773752576	-0.9758648621
O	8.0	-3.6065073148	-2.8322959421	-0.5046633669
H	1.0	0.3394145891	5.5524134281	-2.3607506953
H	1.0	-0.7110652473	5.6314051116	-0.9264630285
H	1.0	0.9304899683	6.3166715367	-0.8929953070
H	1.0	1.9047246637	3.9425496218	-1.0926642815
H	1.0	-0.8020911530	3.4376331612	0.2475092707
H	1.0	-0.2906187145	-0.8279707523	1.9348352990
H	1.0	-2.2555918023	-1.1996400295	1.0093611357
H	1.0	2.3776776218	-2.7931229389	-1.3792921323
H	1.0	3.0412265593	0.2791595730	1.3035226263
H	1.0	4.7760480044	-3.2422749938	-1.5331219667
H	1.0	5.3983107529	0.0635247348	1.2200403073
H	1.0	4.7749072959	0.2678822462	-0.4289215752
H	1.0	6.3286576872	-1.5907576652	-0.5092731709
H	1.0	5.6308026169	-2.3516352443	0.9182767980
H	1.0	-1.8406957235	-1.3295970324	-1.7068551574
H	1.0	-0.7477766862	-0.0053747742	-1.3028710669
H	1.0	-4.2786579616	0.2493926688	-0.2294503227
H	1.0	-6.1203429459	-0.7718064710	-1.1437073853
H	1.0	-6.3027553110	-2.2597961214	-0.1816374392
H	1.0	-5.8554758755	-2.3726262221	-1.8836366814

3b

ENERGY= -1468.3659624
MAXIMUM GRADIENT = 0.0000075 RMS GRADIENT = 0.0000019
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.351959
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 775.117 kJ / mol

C	6.0	-0.0502057177	-5.4049221633	-1.2026242575
C	6.0	0.6467419380	-4.1744626648	-0.7196773552
C	6.0	0.0711051269	-3.1761267196	-0.0300068461
C	6.0	0.8561885584	-1.9961781171	0.3930196330
C	6.0	0.1614853043	-0.9253942305	1.1341181586
O	8.0	2.0620792937	-1.8731776208	0.1471154507
C	6.0	0.6215697416	0.3330740287	1.3713997217
O	8.0	-1.1411506211	-1.1946885425	1.5478663213
C	6.0	1.4528195902	1.1669743930	0.5087778388
C	6.0	-2.0685073961	-0.1892196085	1.3148407354
C	6.0	2.8041596236	1.1872901785	0.2933769474
C	6.0	-2.1303734267	0.5336196976	-0.0810325332
S	16.0	0.2617975600	2.2237839222	-0.3308106072
C	6.0	3.4317520668	2.1189227209	-0.6466739513
N	7.0	3.6545615907	0.3925500626	1.0482078565
C	6.0	4.7654623350	2.2557701436	-0.7205150584
C	6.0	4.9880433433	0.1144322704	0.5074359151
O	8.0	-2.9268205851	-0.0026302223	2.1341426007
C	6.0	5.6858622582	1.4205138900	0.1271457552
C	6.0	-0.9049184203	0.9153741592	-0.9533457703
N	7.0	-3.0145719005	1.6726713681	0.0554658531
C	6.0	-4.3337947839	1.5842561380	-0.3342057230
C	6.0	-5.2176909450	2.7234402782	0.1391074477
O	8.0	-4.7512521935	0.6574328780	-1.0147170339
H	1.0	0.0273174699	-5.4911686001	-2.2950442608
H	1.0	-1.1093900888	-5.4135112801	-0.9282086570
H	1.0	0.4239280731	-6.3054538544	-0.7891360933
H	1.0	1.7084681393	-4.0787975597	-0.9464198468
H	1.0	-0.9812644757	-3.2108568270	0.2344585717
H	1.0	-0.0245624231	0.9158184502	2.0310513500
H	1.0	-2.7030039307	-0.1816707991	-0.6917520466
H	1.0	2.7714267325	2.7221138786	-1.2593967598
H	1.0	3.1851799060	-0.4586930071	1.3465258999
H	1.0	5.1982734622	2.9880424720	-1.3984920645
H	1.0	5.5545877419	-0.4198244414	1.2765680526
H	1.0	4.9271478371	-0.5375846331	-0.3788201868
H	1.0	6.6160337985	1.1996570870	-0.4103543690
H	1.0	5.9708886127	1.9773452198	1.0327967664
H	1.0	-1.3266769789	1.3393647407	-1.8695590107
H	1.0	-0.3120969438	0.0454054688	-1.2399328384
H	1.0	-2.7704719033	2.3572025734	0.7590388347
H	1.0	-4.6701002961	3.6657269171	0.2444627869
H	1.0	-6.0391268567	2.8530349777	-0.5677252258
H	1.0	-5.6424554353	2.4620404679	1.1156914731

3c

ENERGY= -1468.3602309
MAXIMUM GRADIENT = 0.0000084 RMS GRADIENT = 0.0000030
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.351742
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 777.873 kJ / mol

C	6.0	4.1063614376	2.5627497155	-1.9339203395
C	6.0	2.6489213323	2.5904306041	-1.6064489473
C	6.0	2.0685972593	1.9429414171	-0.5832430515
C	6.0	0.6148071247	2.0577447659	-0.3454446094
C	6.0	0.0075349183	1.3094395897	0.8122665520
O	8.0	-0.1222808236	2.7588455873	-1.0327822485
C	6.0	0.3114033551	0.0792960468	1.2634479241
O	8.0	-1.1185360436	1.9535134948	1.3125020942
C	6.0	0.9405537973	-0.9311503243	0.3941827748
C	6.0	-2.3258636087	1.5755842459	0.7881544672
C	6.0	2.2168957810	-1.4015931270	0.4368990977
C	6.0	-2.5046308488	0.1489615773	0.1672897104
S	16.0	-0.3858570469	-1.7324720274	-0.5256540445
C	6.0	2.7340800477	-2.4091325250	-0.4881095545
N	7.0	3.1084691394	-0.9772809050	1.4267650191
C	6.0	3.9733146495	-2.9145401315	-0.3706209866
C	6.0	4.5436511968	-1.0373754106	1.1582363662
O	8.0	-3.2648841821	2.3161702363	0.9340512796
C	6.0	4.9191853184	-2.4519168991	0.7059800241
C	6.0	-1.5426316066	-0.3556138835	-0.9681080071
N	7.0	-3.8837632171	0.1257348018	-0.2991338522
C	6.0	-4.5521889725	-1.0559151952	-0.4614836856
C	6.0	-6.0360926104	-0.9287337554	-0.7696454707
O	8.0	-3.9900057995	-2.1424524701	-0.3726619245
H	1.0	4.5272644396	3.5771891609	-1.9147630023
H	1.0	4.6749037497	1.9377507758	-1.2380160266
H	1.0	4.2660407088	2.1825093325	-2.9519216057
H	1.0	2.0032626852	3.1864011231	-2.2508074622
H	1.0	2.6546594808	1.3359517281	0.0987698351
H	1.0	-0.2652542765	-0.2834217556	2.1175021220
H	1.0	-2.4096178049	-0.5613678119	1.0006526624
H	1.0	2.0675825161	-2.7402020489	-1.2770419062
H	1.0	2.7982911370	-0.1704504545	1.9546786958
H	1.0	4.3133897809	-3.6786071304	-1.0657792946
H	1.0	5.0704417701	-0.7705395391	2.0797074143
H	1.0	4.8500748124	-0.3185565252	0.3781132055
H	1.0	5.9539484390	-2.4580710669	0.3415662129
H	1.0	4.8837075635	-3.1411266314	1.5628314811
H	1.0	-2.1772658703	-0.8507074919	-1.7051256690
H	1.0	-1.0238281486	0.4550552125	-1.4784035550
H	1.0	-4.3928320761	0.9948235647	-0.1924501758
H	1.0	-6.3538263073	0.0986254623	-0.9711252369
H	1.0	-6.6085907245	-1.3164239152	0.0798590790
H	1.0	-6.2712630605	-1.5547031182	-1.6348331446

3d

ENERGY= -1468.3589832
MAXIMUM GRADIENT = 0.0000093 RMS GRADIENT = 0.0000028
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.351768
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 776.131 kJ / mol

C	6.0	4.0661322582	2.8311327143	1.3426716765
C	6.0	2.6533229996	2.8575274790	0.8565770371
C	6.0	2.1139048062	1.9940144001	-0.0181656308
C	6.0	0.6985388784	2.1252682200	-0.4308741199
C	6.0	0.1340589766	1.1093509985	-1.3748357657
O	8.0	-0.0256049245	3.0391341808	-0.0477951081
C	6.0	0.4966176079	-0.1746410458	-1.6098796239
O	8.0	-1.0368536020	1.5347333786	-1.9912650575
C	6.0	1.0822536871	-1.0846518733	-0.6123732759
C	6.0	-2.1113803177	0.7070425909	-1.7776456949
C	6.0	2.3613740721	-1.5357730681	-0.5023252121
C	6.0	-2.4055858296	0.2039507230	-0.3319581135
S	16.0	-0.3228009785	-1.8118022301	0.2518957842
C	6.0	2.8065219205	-2.4486402188	0.5512921331
N	7.0	3.3293033680	-1.1866259998	-1.4440317704
C	6.0	4.0565370346	-2.9392205830	0.5847171780
C	6.0	4.7380690387	-1.1981639006	-1.0568979964
O	8.0	-2.8912839358	0.5095939374	-2.6756703577
C	6.0	5.0872438443	-2.5582498127	-0.4453643363
C	6.0	-1.3273395869	-0.3200251827	0.6649764998
N	7.0	-3.5019445900	-0.7435545143	-0.4564209860
C	6.0	-4.4110514447	-0.9112137035	0.5529287588
C	6.0	-5.6109053591	-1.7805857391	0.2140081146
O	8.0	-4.2612889046	-0.4055991298	1.6612208903
H	1.0	4.5759289977	3.7744275509	1.1041590350
H	1.0	4.6388599363	2.0071101448	0.9053437814
H	1.0	4.0969660185	2.7328166197	2.4361884988
H	1.0	2.0066690021	3.6446698378	1.2434726374
H	1.0	2.7045313345	1.1889660594	-0.4424764036
H	1.0	-0.0683500201	-0.6689082160	-2.4047635918
H	1.0	-2.7861660568	1.1079800648	0.1743749616
H	1.0	2.0767455304	-2.7191420099	1.3062287456
H	1.0	3.0531613238	-0.4544816763	-2.0869510861
H	1.0	4.3437085018	-3.6324619029	1.3718852055
H	1.0	5.3357316955	-1.0089840882	-1.9538314221
H	1.0	4.9719908645	-0.4045206191	-0.3260944803
H	1.0	6.0864291607	-2.5126678889	0.0051588332
H	1.0	5.1329303987	-3.3237604795	-1.2343065305
H	1.0	-1.9053054657	-0.6170603525	1.5446694862
H	1.0	-0.6660488014	0.4831620706	0.9884250485
H	1.0	-3.7638088937	-0.9816647592	-1.4044638066
H	1.0	-5.5576455051	-2.2315584386	-0.7812514520
H	1.0	-5.6933320736	-2.5740566773	0.9623891203
H	1.0	-6.5181862281	-1.1714121937	0.2820342745

4a

ENERGY= -1468.3655684
MAXIMUM GRADIENT = 0.0000095 RMS GRADIENT = 0.0000033
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352329
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 780.201 kJ / mol

C	6.0	2.7575903856	-4.5512453496	-0.6247334052
C	6.0	1.5678846190	-3.6767067215	-0.3931670887
C	6.0	1.5983910680	-2.4619931175	0.1811026070
C	6.0	0.3534157648	-1.6869393844	0.3727613208
C	6.0	0.4405573740	-0.4071075650	1.1197697061
O	8.0	-0.7459673239	-2.0687713818	-0.0372142223
C	6.0	-0.5087623702	0.5556003684	1.2155159288
O	8.0	1.6467851046	-0.1400010033	1.7465585490
C	6.0	-1.5355811508	0.9732577907	0.2709407853
C	6.0	2.1082426711	1.1590329288	1.5612268380
C	6.0	-2.7736323883	0.4549608330	0.0365119183
C	6.0	1.8785051334	1.8693712960	0.1853953394
S	16.0	-0.9140118636	2.4322300131	-0.6459038650
C	6.0	-3.7324561749	1.0893496798	-0.8693309167
N	7.0	-3.2262417453	-0.6687475616	0.7363287244
C	6.0	-4.9889807000	0.6353307203	-1.0073544142
C	6.0	-4.2627277865	-1.4735017733	0.0798600687
O	8.0	2.7205691167	1.7018016818	2.4378525345
C	6.0	-5.4607602801	-0.5964561640	-0.2850792599
C	6.0	0.6906630239	2.8848861029	0.1593519501
N	7.0	1.8560953957	1.0050814081	-0.9685386602
C	6.0	2.9920040277	0.3636911329	-1.3931897809
C	6.0	2.8620937324	-0.4020399574	-2.6984886106
O	8.0	4.0235734435	0.3901916618	-0.7330818963
H	1.0	2.8582229701	-4.7965729100	-1.6907988416
H	1.0	3.6859995353	-4.0823363669	-0.2856738086
H	1.0	2.6389107305	-5.5092684964	-0.1003746225
H	1.0	0.5971920361	-4.0584730590	-0.7098403745
H	1.0	2.5297943942	-2.0262248474	0.5292557462
H	1.0	-0.2588418133	1.3258753169	1.9473329599
H	1.0	2.7891749977	2.4767350704	0.1383928678
H	1.0	-3.4156561683	1.9851698195	-1.3942275227
H	1.0	-2.4404509965	-1.2540573599	1.0083961109
H	1.0	-5.6921577488	1.1711589803	-1.6411138536
H	1.0	-4.5594263848	-2.2644077668	0.7759730161
H	1.0	-3.8772040499	-1.9579965575	-0.8324324794
H	1.0	-6.1623763219	-1.1670081969	-0.9065640582
H	1.0	-6.0104511991	-0.3071788605	0.6235661271
H	1.0	0.5286232107	3.2831869854	1.1634856443
H	1.0	0.9857948728	3.7297278940	-0.4718757550
H	1.0	1.0122568989	1.0006510993	-1.5302503546
H	1.0	2.6260366092	-1.4490493038	-2.4783854075
H	1.0	3.8229137282	-0.3715752973	-3.2165616651
H	1.0	2.0798651734	-0.0039804939	-3.3525511802

4b

ENERGY= -1468.3672404
MAXIMUM GRADIENT = 0.0000090 RMS GRADIENT = 0.0000020
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352587
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 778.207 kJ / mol

C	6.0	-1.9956210463	-5.0979003112	-0.3921356395
C	6.0	-0.9283045388	-4.0674028301	-0.2107111009
C	6.0	-1.0527231778	-2.9403808257	0.5083560399
C	6.0	0.0698738516	-1.9833071285	0.6178886549
C	6.0	-0.1337561381	-0.7687864254	1.4037931707
O	8.0	1.1676604761	-2.1934920450	0.0747781743
C	6.0	0.6621312125	0.3371084997	1.5563485364
O	8.0	-1.3996305052	-0.5977951558	1.9980807760
C	6.0	1.5549722745	1.0711305260	0.6924086845
C	6.0	-2.0355499802	0.5665160433	1.6280140544
C	6.0	2.7287265551	0.7060081254	0.0512173936
C	6.0	-1.7323790075	1.1654505663	0.2242512751
S	16.0	0.8719946453	2.7270221526	0.5858002833
C	6.0	3.4233995537	1.6164323038	-0.8625428590
N	7.0	3.3573696992	-0.4778231311	0.3435986025
C	6.0	4.6650594254	1.3572419372	-1.3052414830
C	6.0	4.3724664110	-0.9913143561	-0.5783303979
O	8.0	-2.8921783058	1.0299024730	2.3395124108
C	6.0	5.3894983981	0.0993813946	-0.9118262200
C	6.0	-0.9370724969	2.5090888226	0.1291648319
N	7.0	-3.0587542594	1.4270976849	-0.3308778183
C	6.0	-3.3129369853	1.3400609523	-1.6732193304
C	6.0	-4.7450207803	1.6432379431	-2.0854089927
O	8.0	-2.4457525001	1.0399909026	-2.4852657681
H	1.0	-2.2359111042	-5.2236548314	-1.4567029538
H	1.0	-2.9147421180	-4.8378219626	0.1419024215
H	1.0	-1.6526755913	-6.0789972164	-0.0361836790
H	1.0	0.0267086465	-4.2438159509	-0.7047139548
H	1.0	-1.9777545839	-2.7054680497	1.0254795458
H	1.0	0.2668226755	0.9852185646	2.3372480287
H	1.0	-1.2576424103	0.4271423724	-0.4214810466
H	1.0	2.9056450898	2.5256004895	-1.1429929037
H	1.0	2.7025268566	-1.2021582396	0.6444517980
H	1.0	5.1687572476	2.0724274404	-1.9516098759
H	1.0	4.8572366264	-1.8454487213	-0.0961737406
H	1.0	3.9033008624	-1.3538243447	-1.5070058540
H	1.0	6.0467146787	-0.2418984942	-1.7203689104
H	1.0	6.0366690584	0.2977114968	-0.0435268456
H	1.0	-1.4530612354	3.2570736114	0.7388310977
H	1.0	-1.0223638406	2.7962430297	-0.9206797944
H	1.0	-3.7742872240	1.7112793094	0.3251295078
H	1.0	-5.4135977001	1.8421420320	-1.2424124016
H	1.0	-4.7446932090	2.5110879113	-2.7525490845
H	1.0	-5.1319061781	0.7937686527	-2.6560592197

4c

ENERGY= -1468.3684619
MAXIMUM GRADIENT = 0.0000095 RMS GRADIENT = 0.0000031
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352185
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 780.472 kJ / mol

C	6.0	2.6310491445	-3.9690565879	2.0278844609
C	6.0	1.3247729647	-3.5035418351	1.4706383810
C	6.0	1.1725297382	-2.5382684518	0.5503080840
C	6.0	-0.1694692932	-2.1631077126	0.0593851496
C	6.0	-0.2646041858	-1.0932226310	-0.9663922275
O	8.0	-1.1916066302	-2.7591105850	0.4184896090
C	6.0	0.6142485030	-0.0806944889	-1.2137690841
O	8.0	-1.4415296864	-1.0866632678	-1.6985346579
C	6.0	1.3507327326	0.6309878768	-0.1863618620
C	6.0	-2.1271161927	0.1263492364	-1.5900458432
C	6.0	2.5786676208	1.2166651561	-0.4239030261
C	6.0	-2.2976355734	0.7266286007	-0.1727228381
S	16.0	0.3282488486	1.0225650258	1.2392760421
C	6.0	3.1749694393	2.2396758199	0.4295896801
N	7.0	3.2884422355	0.8788049671	-1.5619502572
C	6.0	4.3065225005	2.8783409483	0.0835372570
C	6.0	4.7320078987	1.1142953914	-1.6202821604
O	8.0	-2.6425945701	0.6024434801	-2.5633684343
C	6.0	5.0518804591	2.5438871876	-1.1796494209
C	6.0	-1.1966058743	1.6764831408	0.4170613658
N	7.0	-2.7229022100	-0.3132113139	0.7465114300
C	6.0	-3.5182200072	-0.0063935749	1.8145733340
C	6.0	-3.9258591280	-1.1908932093	2.6755899621
O	8.0	-3.8888763835	1.1408184309	2.0510037391
H	1.0	2.7738187805	-5.0417086573	1.8386723779
H	1.0	3.4796418692	-3.4260777700	1.6000385254
H	1.0	2.6533329630	-3.8433365019	3.1188464418
H	1.0	0.4223175651	-3.9892529175	1.8399533960
H	1.0	2.0314916972	-2.0128580701	0.1443145436
H	1.0	0.5132689160	0.4189951338	-2.1829006302
H	1.0	-3.1467659824	1.4056558193	-0.3052349029
H	1.0	2.6289315100	2.5083626437	1.3258599069
H	1.0	2.9819311605	0.0245154868	-2.0100257819
H	1.0	4.6822195681	3.6866850290	0.7063523395
H	1.0	5.0622421602	0.9395960299	-2.6485278168
H	1.0	5.2708597239	0.4054754893	-0.9698817280
H	1.0	6.1340902292	2.6490297384	-1.0364325889
H	1.0	4.7712020090	3.2561955870	-1.9704215289
H	1.0	-0.9072679417	2.4203965246	-0.3315725159
H	1.0	-1.7031633467	2.1977451184	1.2345392277
H	1.0	-2.4049208413	-1.2700868199	0.6003191767
H	1.0	-3.3597211406	-2.0993272562	2.4510881520
H	1.0	-4.9922669178	-1.3908058588	2.5235687520
H	1.0	-3.7886729857	-0.9241583164	3.7270325310

4d

ENERGY= -1468.3521627
MAXIMUM GRADIENT = 0.0000079 RMS GRADIENT = 0.0000027
HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000) = 0.352008
TOTAL GIBBS FREE ENERGY CORRECTION AT 298.15 K = 775.893 kJ / mol

C	6.0	-3.0146014472	-3.1267274975	2.0136731155
C	6.0	-1.7260594234	-3.0028453971	1.2672060930
C	6.0	-1.4448638541	-2.0744616103	0.3393143564
C	6.0	-0.1195493009	-2.0564957132	-0.3187232946
C	6.0	0.1959138054	-0.9751467128	-1.2975345463
O	8.0	0.7397225531	-2.9048372276	-0.0912654300
C	6.0	-0.3460096346	0.2433230777	-1.5512880609
O	8.0	1.4160734951	-1.1774240746	-1.9553110994
C	6.0	-1.0250640375	1.1738840463	-0.6453434853
C	6.0	2.4078135014	-0.3477900236	-1.5032001928
C	6.0	-2.3464886212	1.2914369672	-0.3162693668
C	6.0	2.2764720964	0.2245844640	-0.0629310726
S	16.0	0.1635362776	2.4692989129	-0.3084555573
C	6.0	-2.8440109005	2.2309238330	0.6887019463
N	7.0	-3.3197561872	0.5684483225	-0.9928204699
C	6.0	-4.1581357569	2.4163395546	0.8984672095
C	6.0	-4.6220509591	0.3306305800	-0.3775766376
O	8.0	3.3918363315	-0.1633187267	-2.1756055635
C	6.0	-5.2026250259	1.6564773748	0.1239054086
C	6.0	1.8163508907	1.7053112450	0.1505881759
N	7.0	3.6292983771	0.1445466980	0.4791553084
C	6.0	3.8601075233	-0.0430522033	1.8142431569
C	6.0	5.3182472544	-0.2207894642	2.2055673919
O	8.0	2.9503799775	-0.0736589720	2.6358501882
H	1.0	-3.4619713285	-4.1172633936	1.8546083360
H	1.0	-3.7425121583	-2.3653071279	1.7156834615
H	1.0	-2.8432485305	-3.0364255496	3.0948443980
H	1.0	-0.9452580929	-3.7267605137	1.4978853560
H	1.0	-2.1757368571	-1.3220677770	0.0665506819
H	1.0	0.1469060758	0.7506726444	-2.3822064369
H	1.0	1.6536750588	-0.4287250798	0.5469536362
H	1.0	-2.1008239061	2.7757788735	1.2592960686
H	1.0	-2.9831535957	-0.1282937684	-1.6444732927
H	1.0	-4.4886645002	3.1352827819	1.6443822408
H	1.0	-5.2733450186	-0.1210737992	-1.1316300637
H	1.0	-4.5513876986	-0.3742340228	0.4680171281
H	1.0	-6.0810469234	1.4575438431	0.7499052223
H	1.0	-5.5534483209	2.2604592706	-0.7263063621
H	1.0	2.5253086399	2.3561482937	-0.3687526589
H	1.0	1.9266973908	1.8569269125	1.2258270051
H	1.0	4.3837947041	0.1637959615	-0.1945988059
H	1.0	6.0190115630	-0.0241637355	1.3885144119
H	1.0	5.5428364793	0.4455439406	3.0429676297
H	1.0	5.4647996476	-1.2483488424	2.5547606213

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