

2018-12-21

Diastereodivergent synthesis of chiral tetrahydropyrrolodiazepinediones via a one-pot intramolecular aza-Michael/lactamization sequence

Spandan Chennamadhavuni, James S Panek, John A Porco, Lauren E Brown. 2018.
"Diastereodivergent Synthesis of Chiral Tetrahydropyrrolodiazepinediones via a One-Pot Intramolecular aza-Michael/Lactamization Sequence." JOURNAL OF ORGANIC CHEMISTRY, Volume 83, Issue 24, pp. 15449 - 15462 (14). <https://doi.org/10.1021/acs.joc.8b02724>
<https://hdl.handle.net/2144/39203>

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Diastereodivergent syntheses of chiral tetrahydropyrrolodiazepinediones via a one-pot intramolecular *aza*-Michael/lactamization sequence

Spandan Chennamadhavuni, James S. Panek, John A. Porco, Jr., and Lauren E. Brown

Department of Chemistry and Center for Molecular Discovery, Life Science and Engineering Building, Boston University,
24 Cummington Mall, Boston, Massachusetts, 02215.

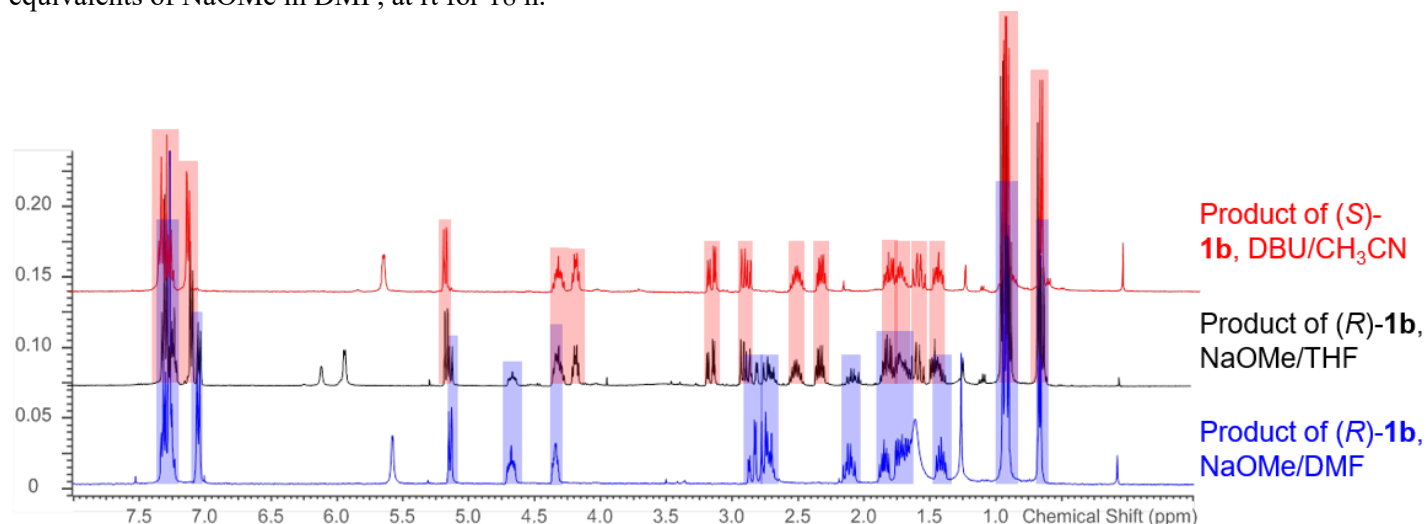
Supporting Information

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1. Diastereodivergence analysis

Stacked comparison of ^1H NMR spectra (400 MHz, CDCl_3) obtained for reactions of diastereomers (*S*)-**1b**/(*R*)-**1b** under three different reaction conditions to afford products (*S,S*)-**3b** and/or (*R,R*)-**3b**. The top (red) spectrum is the major product (*S,S*)-**3b** obtained when (*S*)-**1b** was reacted with 5 equiv. of DBU in CH_3CN at 100 °C for 2 h. The middle (black) spectrum is the product mixture (*S,S*)-**3b** and (*R,R*)-**3b** obtained when (*R*)-**1b** was reacted with two equivalents of NaOMe in THF, -78 °C to rt over 18 h. The bottom (blue) spectrum is the product (*R,R*)-**3b**, obtained when (*R*)-**1b** was reacted with two equivalents of NaOMe in DMF, at rt for 18 h.

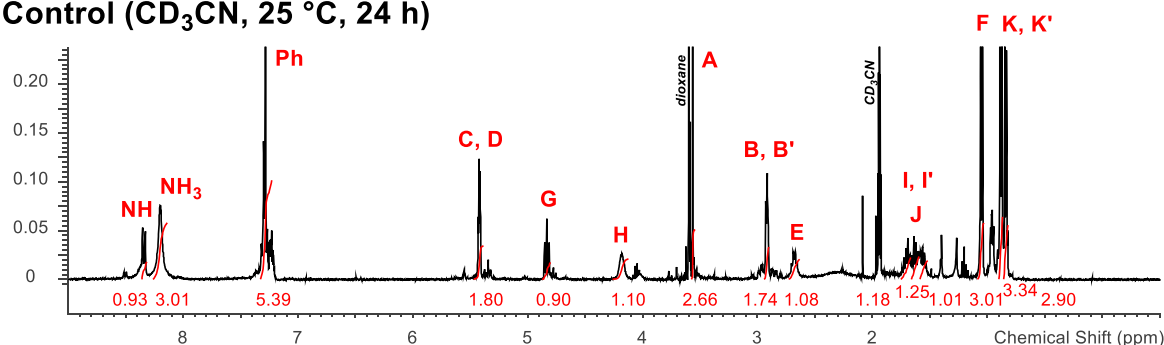


2. Mechanistic Studies: *in situ* NMR analysis

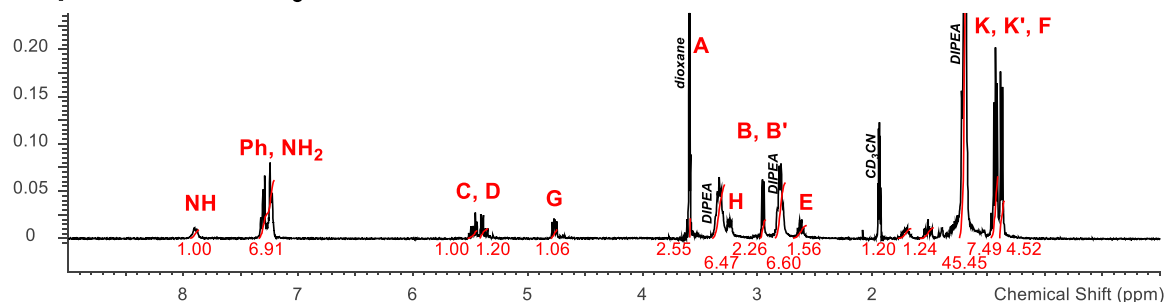
Procedure: Compound (*S*)-**10b** (106 mg, 0.14 mmol) was dissolved in anhydrous dichloromethane (2.0 mL) under an atmosphere of nitrogen. A solution of hydrochloric acid in dioxane (0.135 mL, 4.0 M, 4.0 equiv.) was added and the reaction was stirred at rt until LC/MS analysis indicated full deprotection, approximately 1 h. The solvent was removed *in vacuo* and the residue was dried under high vacuum for 2 h. The residue was then re-dissolved in CD_3CN (2.1 mL) and split into three 0.7 mL portions, each transferred to a separate septa-capped, nitrogen-flushed NMR tube, labeled Reactions A-C. To Reaction A was added DBU (22 μL , 2.0 equiv.). To Reaction B was added Hunig's base (25 μL , 2.0 equiv.). Reaction C was kept as a control. The three tubes were allowed to stand at room temperature for 24 h, after which time ^1H NMR and UPLC/MS data were acquired. The tubes were then placed in a sand bath heated to 60 °C and held at this temperature for an additional 24 h. A second series of ^1H NMR and UPLC/MS data were then acquired.

Incubation at room temperature

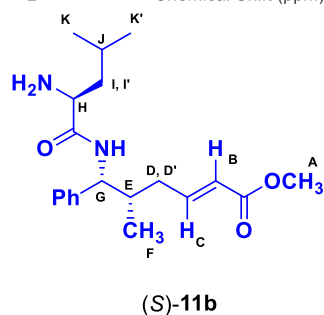
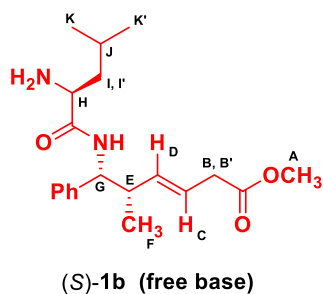
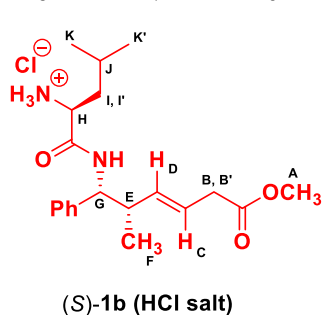
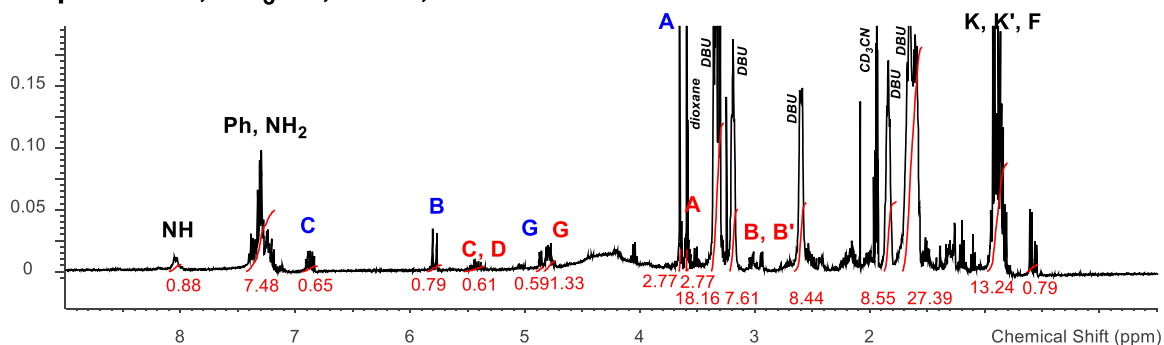
Control (CD₃CN, 25 °C, 24 h)



2 equiv. DIPEA, CD₃CN, 25 °C, 24 h



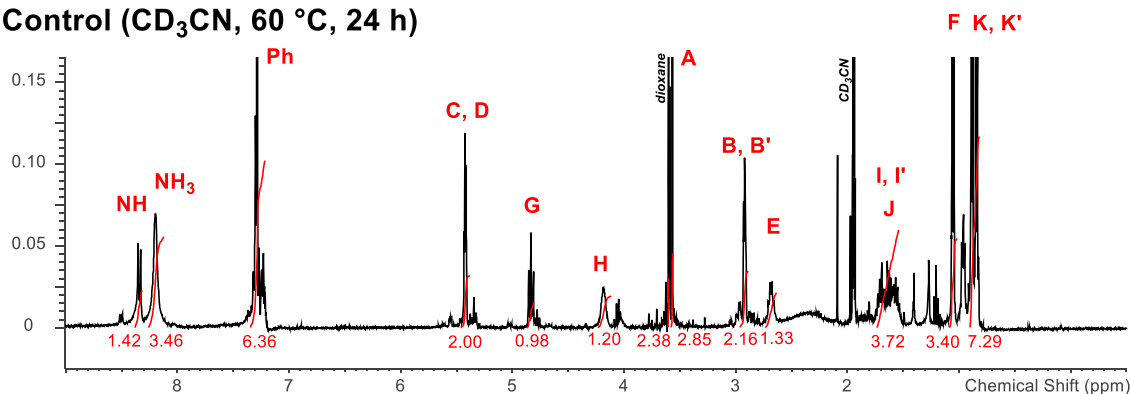
2 equiv. DBU, CD₃CN, 25 °C, 24 h



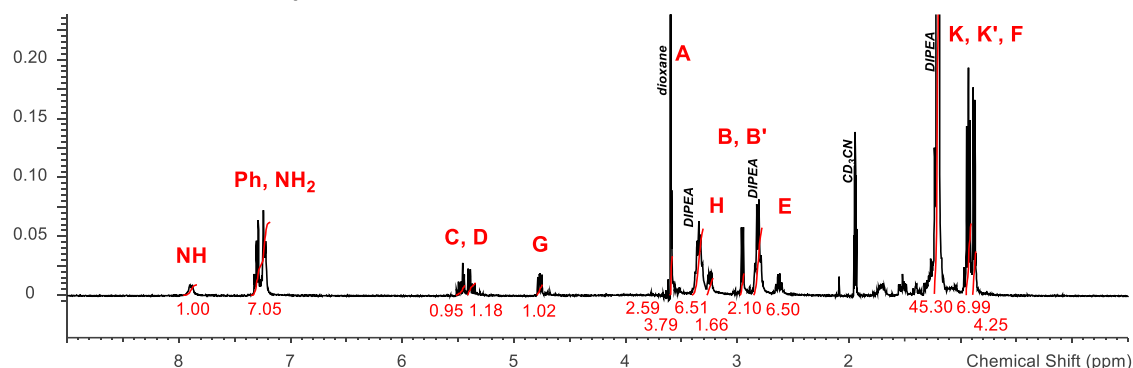
Discussion. Following room temperature incubation, only minor changes in the NMR spectrum of compound (S)-1b were observed upon addition of DIPEA, presumably attributable to the conversion of the hydrochloride salt to the free base. In contrast, on treatment with DBU, an additional compound is generated which was assigned as (S)-11b, due to the olefinic protons **B** and **C**. The macrolactam enone (S)-12b (not shown, see manuscript text) was excluded due to the emergence of a new methyl ester shift at 3.66 ppm (**A**), and lack of a mass ion corresponding to loss of methanol by UPLC/MS analysis (not shown). For the DBU experiments, the highly upfield methyl doublets emerging between 0.5 and 0.6 ppm also indicate partial cyclization to the five-membered ring, and are likely attributable to pyrrolidine **11b** rather than the product **3b** due to the aforementioned LC/MS observations.

Incubation at 60 °C

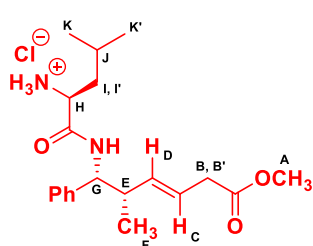
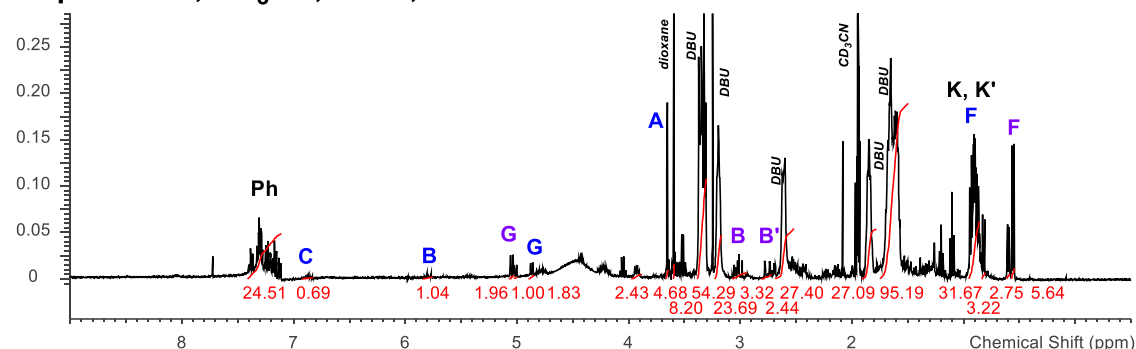
Control (CD₃CN, 60 °C, 24 h)



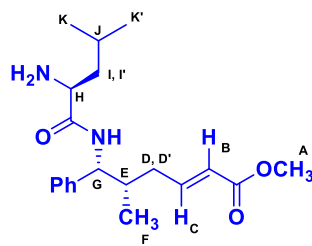
2 equiv. DIPEA, CD₃CN, 60 °C, 24 h



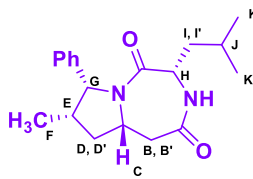
2 equiv. DBU, CD₃CN, 60 °C, 24 h



(S)-1b (HCl salt)



(S)-11b



(S,S)-3b

Discussion. Relative to the room temperature incubation, no changes were observed in either the control or Hunig's base samples after heating to 60 °C for 24 h. In contrast, the heated reaction with DBU indicated full consumption of the starting material (S)-1b (absence of protons C, D and A), with a portion of intermediate (S)-11b remaining (presence of protons C, B, G). In addition, proton signals characteristic of product (S,S)-3b (mixture of diastereomers, major product stereochemistry indicated, protons G, B, B', F) also emerged. UPLC/MS analysis (not shown) also indicated a mixture of open ester (M) and lactamized (M-CH₃OH) compounds.

3. Computational Methods

a. Energy Analysis Workflow: All calculations were performed using Schrödinger's Maestro software within the Small Molecule Drug Discovery Suite,^{S1} using MacroModel^{S2} for all force field calculations and Jaguar^{S3} for all DFT calculations. The computational workflow was as follows:

- 1) For each pyrrolidine (**13**) and pyrrolidiazepinone (**3**), a MacroModel conformational search was performed on each of the four possible diastereomers. Each conformational search output was examined for unique conformers within a ~5 kcal/mol (20 kJ/mol) window. For each diastereomer, each unique conformer was then subjected to DFT optimization using Jaguar (B3LYP-6-31g**, Accurate SCF, no solvent).
- 2) From these optimizations, the lowest energy conformers with acceptable geometry convergence scores (scores of 0, 1, 2, or 3 with an acceptable difference between intermediate and final structure of <0.01 kcal/mol) were selected for single point energy calculations as described below; in cases of failed convergence, optimizations were re-run with Ultrafast or Fully Analytic SCF until acceptable convergence was obtained.

Pyrrolidines: For each pyrrolidine diastereomer, only the top four conformers from the optimization output (ranked by gas phase energy) were carried forward to single point energy calculations.

Pyrrolidiazepinones: For each pyrrolidiazepinone diastereomer, all unique conformers from the optimization output were carried forward to single point energy calculations.

- 3) The selected DFT-optimized structures from above were next subjected to Jaguar DFT single point energy calculations with vibrational frequencies applied to arrive at the final Gibbs free energies used for the thermodynamic comparisons in the manuscript.

Pyrrolidines:

Table S1. Absolute DFT (B3LYP-6-31g**) Gibbs free energies ("GFE," in kcal/mol) from which pyrrolidine **13** relative energy differences (Table 2) are calculated.

Pyrrolidine	(S,2S) GFE	(S,2R) GFE	(R,2R) GFE	(R,2S) GFE
13a	-770669.8364	-770671.2671	-770670.3679	-770669.3682
13b	-699690.5420	-699690.6512	-699693.1575	-699692.5883
13c	-675036.1533	-675034.8888	-675037.3662	-675035.7090
13d	-625727.4932	-625727.4762	-625727.3934	-625727.8408

Pyrrolidiazepinones:

Table S2. Absolute DFT (B3LYP-6-31g**) Gibbs free energies ("GFE," in kcal/mol) from which tetrahydropyrrolidiazepinone **3** relative energy differences (Table 4) are calculated.

Pyrrolidiazepinone	(S,S) GFE	(S,R) GFE	(R,R) GFE	(R,S) GFE
3a	-698072.1655	-698070.7586	-698072.5458	-698071.3918
3b	-627092.7333	-627090.8847	-627093.1901	-627090.6487
3c	-602436.8147	-602436.0749	-602437.3355	-602436.4263
3d	-553128.8491	-553127.1235	-553129.1202	-553127.9091

b. Examination of solvent effects. Single point energy calculation of the Gibbs free energies with vibrational frequencies applied and either acetonitrile, DMF, or THF solvation (PBF solvation model) were run on pyrrolidines (*S*,2*S*)-**13b**, (*R*,2*R*)-**13b**, (*S*,2*R*)-**13b** and (*R*,2*S*)-**13b** as well as for pyrrolidiazepinones (*S*,*S*)-**3b**, (*R*,*R*)-**3b**, (*R*,*S*)-**3b**, and (*S*,*R*)-**3b**. For the pyrrolidines, solvent did not appear to significantly affect the relative energy differences between the diastereomers as compared to the free energy differences calculated with no solvent (see Table S3). For the final product pyrrolidiazepinones,

S1. Small-Molecule Drug Discovery Suite 2018-3, Schrödinger, LLC, New York, NY, **2018**.

S2. Schrödinger Release 2013-1: MacroModel, Schrödinger, LLC, New York, NY, **2018**

S3. (a) Schrödinger Release 2018-3: Jaguar, Schrödinger, LLC, New York, NY, **2018**. (b) Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A. Jaguar: A High-Performance Quantum Chemistry Software Program with Strengths in Life and Materials Sciences. *Int. J. Quantum Chem.*, **2013**, *113*, 2110-2142.

aside from a more pronounced de-stabilization of the (*S,R*) diastereomer in CH₃CN and DMF as compared to no solvent/THF, the overall general trend of a significant thermodynamic stabilization of the major product (*R,R*) and (*S,S*) diastereomers relative to the not observed (*R,S*) and (*S,R*) diastereomers. While it is likely that solvent effects do contribute to the observed reaction outcomes, for the purpose of simplification all of the energy calculations for analyses in the manuscript text were performed in the absence of solvent.

Table S3. Examination of solvent effects on relative Gibbs free energy calculations

DFT-optimized structure	Relative Gibbs free energy (no solvent)	Relative Gibbs free energy (CH ₃ CN)	Relative Gibbs free energy (DMF)	Relative Gibbs free energy (THF)
(<i>S,2S</i>)- 13b	+2.6 kcal/mol	+2.5 kcal/mol	+2.4 kcal/mol	+2.4 kcal/mol
(<i>R,2R</i>)- 13b	0 kcal/mol	0 kcal/mol	0 kcal/mol	0 kcal/mol
(<i>S,2R</i>)- 13b	+2.5 kcal/mol	+3.6 kcal/mol	+3.4 kcal/mol	+3.2 kcal/mol
(<i>R,2S</i>)- 13b	+0.5 kcal/mol	+1.1 kcal/mol	+0.9 kcal/mol	+0.8 kcal/mol
(<i>S,S</i>)- 3b	+0.5 kcal/mol	+0.3 kcal/mol	+10.4 kcal/mol	+0.3 kcal/mol
(<i>R,R</i>)- 3b	0 kcal/mol	0 kcal/mol	0 kcal/mol	0 kcal/mol
(<i>R,S</i>)- 3b	+2.5 kcal/mol	+2.3 kcal/mol	+2.4 kcal/mol	+2.2 kcal/mol
(<i>S,R</i>)- 3b	+2.3 kcal/mol	+3.7 kcal/mol	+3.8 kcal/mol	+1.9 kcal/mol

c. Final coordinates and energies for DFT-optimized lowest energy conformers.

(*S,2S*)-**13a**

Optimized geometry:

atom	angstroms		
	x	y	z
C1	0.5267170000	3.6821010000	-1.1445760000
C2	0.3883970000	3.5359860000	0.4053800000
C3	-1.0531520000	3.0422980000	0.5728790000
C4	-1.2386770000	2.0420830000	-0.5751250000
N1	-0.3689920000	2.6113970000	-1.6365310000
C5	-0.1833420000	1.9277210000	-2.8033180000
C6	0.8275340000	2.4964500000	-3.8161200000
N2	2.1598430000	2.0343320000	-3.3981820000
C7	-2.9914540000	0.4560010000	-1.5274850000
C8	-2.7072590000	1.8503680000	-1.0003050000
C9	0.1967090000	5.0674150000	-1.6878660000
C10	-0.3175200000	7.6712330000	-2.6284120000
C11	0.9845700000	7.2848450000	-2.3097570000
C12	1.2364070000	5.9941350000	-1.8476030000
C13	-1.1036510000	5.4645540000	-2.0213300000
C14	-1.3594280000	6.7551540000	-2.4857070000
C15	0.7527380000	4.7606360000	1.2410410000
O1	-0.7901230000	0.8841180000	-3.0474900000
O2	-2.6501610000	-0.5641880000	-0.9691360000
C16	0.4044240000	2.1030720000	-5.2538790000
C17	1.3376780000	2.6672000000	-6.3004010000
H1	-0.8505110000	1.0571660000	-0.2872450000
C18	1.1976810000	3.9909700000	-6.7431570000
C19	2.3926230000	1.9047990000	-6.8206090000
C20	3.2800450000	2.4456080000	-7.7531130000
C21	3.1271040000	3.7631420000	-8.1823470000
C22	2.0804210000	4.5347080000	-7.6744420000
O3	-3.7375710000	0.4887180000	-2.6497960000
C23	-3.9789360000	-0.7927690000	-3.2512200000
H2	1.5516840000	3.4402300000	-1.4396810000
H3	1.0570500000	2.7116090000	0.6883390000
H4	-1.2366940000	2.5779090000	1.5463230000

H5	-1.7531190000	3.8816710000	0.4677540000
H6	0.8332940000	3.5890380000	-3.7484340000
H7	2.1868450000	1.0164170000	-3.4399890000
H8	2.8550870000	2.3697390000	-4.0622620000
H9	-3.0109850000	2.6050710000	-1.7292940000
H10	-3.3376880000	1.9750760000	-0.1106490000
H11	-0.5168520000	8.6742030000	-2.9946410000
H12	1.8063040000	7.9852270000	-2.4299300000
H13	2.2558890000	5.6957060000	-1.6149270000
H14	-1.9183980000	4.7532030000	-1.9380770000
H15	-2.3752990000	7.0426060000	-2.7422500000
H16	0.6588270000	4.5289410000	2.3071830000
H17	1.7847750000	5.0792340000	1.0619100000
H18	0.0991560000	5.6092860000	1.0197180000
H19	-0.6155060000	2.4663780000	-5.4259470000
H20	0.3572660000	1.0116230000	-5.3119030000
H21	0.3839830000	4.5990450000	-6.3545620000
H22	2.5104470000	0.8717810000	-6.5022080000
H23	4.0879150000	1.8349180000	-8.1468300000
H24	3.8146760000	4.1851990000	-8.9097350000
H25	1.9502790000	5.5609680000	-8.0067250000
H26	-3.0318700000	-1.2420730000	-3.5593560000
H27	-4.4824400000	-1.4639810000	-2.5511530000
H28	-4.6100500000	-0.5982870000	-4.1187850000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 298.760 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.699	1.481	-11.548	19.49021
rot.	0.889	2.981	36.123	0.889	-9.881	16.67755
vib.	14.964	95.806	104.437	14.964	-16.174	27.29843
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.741	101.768	184.258	17.334	-37.603	63.46618

Total internal energy, Utot (SCFE + ZPE + U): -1228.054884 hartrees

Total enthalpy, Htot (Utot + pV): -1228.053939 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1228.141487 hartrees

(S,2R)-13a

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-2.4306250000	3.7724510000	1.5758430000
C2	-1.1843390000	3.0668060000	0.9492330000
C3	-0.5388370000	2.3719320000	2.1578470000
C4	-1.7339570000	1.8511780000	2.9702900000
N1	-2.7884050000	2.8499630000	2.6712740000
C5	-3.9503290000	2.8444420000	3.3874160000
C6	-5.0412840000	3.8788490000	3.0753600000
N2	-6.1816380000	3.1121720000	2.5671760000

C7	-1.1919030000	-0.6220470000	3.0157190000
C8	-2.1826890000	0.4341260000	2.5794080000
C9	-2.1737270000	5.2019070000	2.0388990000
C10	-1.6655350000	7.8625210000	2.8022650000
C11	-1.3961710000	6.8141220000	3.6820590000
C12	-1.6494060000	5.4950060000	3.3041090000
C13	-2.4487830000	6.2639770000	1.1676370000
C14	-2.1953010000	7.5831810000	1.5419270000
C15	-0.2391990000	3.9508320000	0.1391330000
O1	-4.1547420000	2.0132970000	4.2758120000
O2	-0.2058280000	-0.4340550000	3.6987190000
C16	-5.3128940000	4.7167230000	4.3615790000
C17	-6.3894030000	5.7553560000	4.1527730000
H1	-1.5339490000	1.8540310000	4.0444330000
C18	-7.7291190000	5.4840180000	4.4638960000
C19	-6.0790890000	7.0020250000	3.5887620000
C20	-7.0753830000	7.9453730000	3.3435210000
C21	-8.4058090000	7.6599700000	3.6554270000
C22	-8.7296600000	6.4261950000	4.2176350000
O3	-1.5501380000	-1.8380480000	2.5467630000
C23	-0.6888790000	-2.9238580000	2.9269370000
H2	-3.2357080000	3.7969870000	0.8335180000
H3	-1.5818820000	2.2909260000	0.2813500000
H4	0.1487010000	1.5714940000	1.8762970000
H5	0.0326530000	3.0987150000	2.7461180000
H6	-4.7266720000	4.5679940000	2.2888380000
H7	-6.4193280000	2.4043910000	3.2603660000
H8	-6.9881050000	3.7259730000	2.4723800000
H9	-2.3444090000	0.3424150000	1.4992950000
H10	-3.1418790000	0.2193290000	3.0604680000
H11	-1.4728390000	8.8891890000	3.0994430000
H12	-0.9934370000	7.0223700000	4.6691250000
H13	-1.4563410000	4.6892180000	4.0054590000
H14	-2.8740750000	6.0558990000	0.1885320000
H15	-2.4192960000	8.3924050000	0.8526860000
H16	0.5681550000	3.3445840000	-0.2843970000
H17	-0.7546660000	4.4428120000	-0.6922760000
H18	0.2126850000	4.7296170000	0.7595420000
H19	-4.3794160000	5.2069040000	4.6631250000
H20	-5.5856790000	4.0190830000	5.1598550000
H21	-7.9880640000	4.5292580000	4.9149510000
H22	-5.0452970000	7.2335130000	3.3430190000
H23	-6.8134470000	8.9068030000	2.9100830000
H24	-9.1823390000	8.3953440000	3.4648550000
H25	-9.7614210000	6.1961970000	4.4690630000
H26	-0.6651620000	-3.0342810000	4.0137800000
H27	-1.1139960000	-3.8129490000	2.4614630000
H28	0.3292280000	-2.7523870000	2.5687360000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 298.732 kcal/mol is not included in U, H, or G in the table below

T =	298.15 K					
	U	Cv	S	H	G	ln(Q)
	-----	-----	-----	-----	-----	-----

trans.	0.889	2.981	43.699	1.481	-11.548	19.49021
rot.	0.889	2.981	36.203	0.889	-9.905	16.71815
vib.	15.014	95.811	105.404	15.014	-16.412	27.70054
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.791	101.772	185.306	17.384	-37.865	63.90891

Total internal energy, Utot (SCFE + ZPE + U): -1228.056666 hartrees
Total enthalpy, Htot (Utot + pV): -1228.055722 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1228.143767 hartrees

(R,2R)-13a

Optimized geometry:

angstroms			
atom	x	y	z
C1	-12.0935000000	-4.2840010000	2.0518000000
C2	-11.0884550000	-4.6466430000	0.9099240000
C3	-10.2963700000	-3.3444560000	0.7196910000
C4	-10.1117440000	-2.8043170000	2.1457710000
N1	-11.3206000000	-3.3053930000	2.8436370000
C5	-11.6416590000	-2.8181990000	4.0782430000
C6	-12.9493840000	-3.2575970000	4.7708840000
N2	-13.7987750000	-2.0904110000	5.0403710000
C7	-7.5876620000	-2.6706880000	2.2202040000
C8	-8.8250120000	-3.2862090000	2.8347250000
C9	-13.4342670000	-3.7517610000	1.5584270000
C10	-15.9195020000	-2.8586530000	0.5853100000
C11	-14.8701850000	-1.9578210000	0.7676090000
C12	-13.6379730000	-2.4000080000	1.2523410000
C13	-14.4991300000	-4.6444180000	1.3798220000
C14	-15.7304100000	-4.2054180000	0.8953990000
C15	-11.6908350000	-5.2154870000	-0.3728710000
O1	-10.9196040000	-1.9910700000	4.6452370000
O2	-7.5743330000	-1.7817730000	1.3936870000
C16	-12.6236210000	-3.9601400000	6.1086890000
C17	-11.9177370000	-5.2862990000	5.9336780000
H1	-10.1131520000	-1.7120280000	2.1741700000
C18	-12.6508850000	-6.4525280000	5.6689820000
C19	-10.5209260000	-5.3787760000	5.9901970000
C20	-9.8749450000	-6.5986440000	5.7851630000
C21	-10.6163740000	-7.7496550000	5.5188170000
C22	-12.0088020000	-7.6734120000	5.4625860000
O3	-6.4654290000	-3.2338850000	2.7214760000
C23	-5.2310160000	-2.6921490000	2.2215300000
H2	-12.2851840000	-5.1789570000	2.6533040000
H3	-10.4113050000	-5.4003790000	1.3334140000
H4	-9.3436070000	-3.4943170000	0.2071460000
H5	-10.8782410000	-2.6370060000	0.1186360000
H6	-13.5241790000	-3.9436840000	4.1468930000
H7	-13.2015210000	-1.3604360000	5.4287300000
H8	-14.1563620000	-1.7261420000	4.1586870000
H9	-8.7331640000	-4.3776820000	2.8118080000
H10	-8.8594570000	-2.9938940000	3.8889140000
H11	-16.8793120000	-2.5122230000	0.2134060000
H12	-15.0102940000	-0.9058410000	0.5352290000
H13	-12.8331910000	-1.6869300000	1.4035510000
H14	-14.3632670000	-5.6940030000	1.6303830000
H15	-16.5443480000	-4.9136110000	0.7687800000
H16	-10.8926440000	-5.4713740000	-1.0775040000
H17	-12.2683830000	-6.1255930000	-0.1824410000

H18	-12.3538220000	-4.4954210000	-0.8611930000
H19	-13.5759920000	-4.0949030000	6.6308520000
H20	-12.0115230000	-3.2770200000	6.7066800000
H21	-13.7371350000	-6.4017390000	5.6340300000
H22	-9.9401390000	-4.4838800000	6.1970680000
H23	-8.7909010000	-6.6500720000	5.8376080000
H24	-10.1144750000	-8.7001640000	5.3614920000
H25	-12.5958770000	-8.5662310000	5.2643470000
H26	-4.4404770000	-3.2558850000	2.7166160000
H27	-5.1678670000	-2.8131910000	1.1372330000
H28	-5.1518240000	-1.6289480000	2.4610390000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 298.755 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.699	1.481	-11.548	19.49021
rot.	0.889	2.981	35.888	0.889	-9.811	16.55931
vib.	14.430	93.824	98.438	14.430	-14.919	25.18108
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.207	99.786	178.024	16.800	-36.278	61.23060

Total internal energy, Utot (SCFE + ZPE + U): -1228.058693 hartrees

Total enthalpy, Htot (Utot + pV): -1228.057749 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1228.142334 hartrees

(R,2S)-13a

Optimized geometry:

	angstroms		
atom	x	y	z
C1	5.0987450000	-4.9042410000	-0.6559650000
C2	4.1903970000	-3.9805680000	-1.5319530000
C3	3.2348900000	-4.9719970000	-2.2063080000
C4	2.9308250000	-6.0038510000	-1.1121600000
N1	4.1777350000	-6.0092880000	-0.3050890000
C5	4.2410200000	-6.7398920000	0.8487370000
C6	5.5515330000	-6.7684150000	1.6651150000
N2	6.1028260000	-8.1299900000	1.6814060000
C7	1.3284600000	-7.4152320000	-2.5228280000
C8	2.5638290000	-7.3971490000	-1.6486610000
C9	6.3892340000	-5.3635510000	-1.3236480000
C10	8.8063110000	-6.1073650000	-2.5590150000
C11	7.6545320000	-6.8703120000	-2.7496340000
C12	6.4568220000	-6.5026560000	-2.1349220000
C13	7.5561960000	-4.6114040000	-1.1320050000
C14	8.7539070000	-4.9756950000	-1.7448630000
C15	4.9086120000	-3.0321780000	-2.4890130000
O1	3.2980210000	-7.4469440000	1.2187440000
O2	1.2081770000	-8.0527590000	-3.5461490000
C16	5.2741550000	-6.3233470000	3.1178650000
C17	4.8605110000	-4.8730810000	3.2355240000

H1	2.1068240000	-5.6589040000	-0.4774040000
C18	3.5137530000	-4.4951460000	3.1368260000
C19	5.8226670000	-3.8681800000	3.4093990000
C20	5.4537740000	-2.5245180000	3.4797640000
C21	4.1100440000	-2.1617210000	3.3768860000
C22	3.1414160000	-3.1518620000	3.2063450000
O3	0.3365480000	-6.6467470000	-2.0087600000
C23	-0.8883300000	-6.6458130000	-2.7611280000
H2	5.3698820000	-4.3557650000	0.2509690000
H3	3.6048320000	-3.3816040000	-0.8216610000
H4	2.3243520000	-4.4965400000	-2.5806600000
H5	3.7321170000	-5.4549990000	-3.0576310000
H6	6.3117770000	-6.1163410000	1.2305910000
H7	5.3394160000	-8.7710720000	1.8966110000
H8	6.4264880000	-8.3752460000	0.7472640000
H9	2.3887450000	-8.0581770000	-0.7940600000
H10	3.3785410000	-7.8190290000	-2.2429440000
H11	9.7395430000	-6.3975350000	-3.0328320000
H12	7.6876750000	-7.7584700000	-3.3744200000
H13	5.5720210000	-7.1150640000	-2.2748160000
H14	7.5264670000	-3.7352430000	-0.4883820000
H15	9.6478670000	-4.3811840000	-1.5790400000
H16	4.1783650000	-2.4120000000	-3.0193440000
H17	5.5898280000	-2.3596010000	-1.9579350000
H18	5.4932380000	-3.5786560000	-3.2347030000
H19	6.1889830000	-6.5112420000	3.6869960000
H20	4.4922200000	-6.9755010000	3.5211420000
H21	2.7577820000	-5.2635840000	3.0002010000
H22	6.8706540000	-4.1451060000	3.4985880000
H23	6.2146660000	-1.7616940000	3.6209040000
H24	3.8199660000	-1.1164120000	3.4350410000
H25	2.0922510000	-2.8789340000	3.1317060000
H26	-1.5617630000	-5.9758140000	-2.2267940000
H27	-0.7158790000	-6.2879760000	-3.7791230000
H28	-1.3088590000	-7.6530700000	-2.8103620000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 298.847 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.699	1.481	-11.548	19.49021
rot.	0.889	2.981	35.907	0.889	-9.817	16.56900
vib.	14.440	93.769	99.031	14.440	-15.086	25.46215
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.218	99.731	178.637	16.810	-36.451	61.52137

Total internal energy, Utot (SCFE + ZPE + U): -1228.056809 hartrees
Total enthalpy, Htot (Utot + pV): -1228.055865 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1228.140741 hartrees

(S,S)-3a

Optimized geometry:

atom	angstroms		
	x	y	z
C1	-5.9578860000	2.1682520000	-0.2960330000
C2	-5.5211020000	0.7087390000	-0.0557670000
C3	-6.8278110000	-0.0703940000	-0.0791500000
C4	-7.6978020000	0.6433850000	-1.1242440000
N1	-7.0942300000	1.9855990000	-1.2208500000
C5	-7.4565800000	2.9496210000	-2.1048860000
C6	-8.5963090000	2.5114350000	-3.0585420000
N2	-9.8114830000	2.5172810000	-2.2428750000
C7	-10.1839550000	1.7272680000	-1.2278900000
C8	-9.2179510000	0.6101550000	-0.8047740000
C9	-6.2668450000	3.0071950000	0.9573790000
C10	-6.7524600000	4.5863780000	3.2141430000
C11	-7.7993370000	3.9183840000	2.5942870000
C12	-7.5586730000	3.1378740000	1.4710060000
C13	-5.2275610000	3.6975830000	1.5794040000
C14	-5.4661490000	4.4778140000	2.7039260000
C15	-4.6513510000	0.4373780000	1.1874920000
O1	-6.9300560000	4.0576940000	-2.1874990000
O2	-11.2568180000	1.8773350000	-0.6575360000
C16	-8.7662320000	3.4963670000	-4.2367340000
C17	-9.8761760000	3.1360920000	-5.2091920000
H1	-7.5265050000	0.1509110000	-2.0837000000
C18	-11.1718540000	3.6722520000	-5.0467660000
C19	-9.6653520000	2.1386540000	-6.1849200000
C20	-12.2025890000	3.2618510000	-5.8817450000
C21	-11.9712250000	2.3053150000	-6.8623240000
C22	-10.7095660000	1.7427490000	-7.0103810000
H2	-5.1599570000	2.6988310000	-0.8221470000
H3	-4.9367070000	0.4038770000	-0.9274780000
H4	-6.6830780000	-1.1255710000	-0.3138080000
H5	-7.2880820000	-0.0206990000	0.9095860000
H6	-8.4115640000	1.5211920000	-3.4732100000
H7	-10.4906090000	3.2289300000	-2.4583300000
H8	-9.3387160000	0.5929870000	0.2775700000
H9	-9.6451260000	-0.3301930000	-1.1478810000
H10	-6.9407920000	5.1976260000	4.0850090000
H11	-8.8048810000	4.0109740000	2.9788190000
H12	-8.3899280000	2.6402600000	0.9981030000
H13	-4.2229070000	3.6306420000	1.1881890000
H14	-4.6513050000	5.0063610000	3.1769990000
H15	-5.1744010000	0.6945640000	2.1098770000
H16	-4.3723070000	-0.6147290000	1.2520160000
H17	-3.7300500000	1.0198220000	1.1583450000
H18	-7.8302420000	3.5359030000	-4.7967490000
H19	-8.9202200000	4.5127220000	-3.8684960000
H20	-11.3689270000	4.4081360000	-4.2803430000
H21	-8.6923070000	1.6828440000	-6.2982040000
H22	-13.1903710000	3.6838520000	-5.7634510000
H23	-12.7797030000	1.9901870000	-7.5063690000
H24	-10.5421410000	0.9892970000	-7.7664950000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 264.773 kcal/mol

is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.437	1.481	-11.469	19.35822
rot.	0.889	2.981	35.525	0.889	-9.703	16.37701
vib.	12.259	82.468	83.186	12.259	-12.543	21.16992
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.037	88.430	162.148	14.629	-33.715	56.90515

Total internal energy, Utot (SCFE + ZPE + U): -1112.372472 hartrees

Total enthalpy, Htot (Utot + pV): -1112.371527 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1112.448569 hartrees

(R,R)-3a

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-1.9589390000	-5.2943420000	-2.8329490000
C2	-1.3140080000	-5.8549700000	-4.1168000000
C3	-0.7527710000	-4.6219490000	-4.8113320000
C4	-0.2591380000	-3.7249290000	-3.6701400000
N1	-1.0913300000	-4.1387760000	-2.5258410000
C5	-1.0932590000	-3.5417510000	-1.3067170000
C6	-0.2019540000	-2.2767770000	-1.2472450000
N2	1.1774910000	-2.7683330000	-1.1841530000
C7	1.9155230000	-3.4518220000	-2.0714880000
C8	1.2620070000	-3.8568320000	-3.4025980000
C9	-3.4567090000	-4.9556400000	-2.9318790000
C10	-6.1896470000	-4.3890660000	-3.0612830000
C11	-5.2638240000	-3.4469880000	-3.4886010000
C12	-3.9048970000	-3.7271460000	-3.4209590000
C13	-4.3950090000	-5.8890090000	-2.4959550000
C14	-5.7542470000	-5.6095370000	-2.5630270000
C15	-2.2055880000	-6.7321590000	-5.0177400000
O1	-1.7185720000	-3.9446000000	-0.3277260000
O2	3.0803720000	-3.7448450000	-1.8368280000
C16	-0.5166280000	-1.4040800000	-0.0084700000
C17	-0.0055190000	0.0331840000	-0.0328160000
H1	-0.4854130000	-2.6909710000	-3.9371510000
C18	-0.8454110000	1.0730330000	0.4240460000
C19	1.3309460000	0.3459380000	-0.3727680000
C20	1.7776860000	1.6594620000	-0.3142520000
C21	0.9253240000	2.6730700000	0.1027580000
C22	-0.3793850000	2.3799560000	0.4760420000
H2	-1.8539180000	-6.0254340000	-2.0271420000
H3	-0.4698880000	-6.4744060000	-3.8039030000
H4	0.0266310000	-4.8678670000	-5.5342130000
H5	-1.5476750000	-4.1111630000	-5.3581570000
H6	-0.3594000000	-1.6508280000	-2.1243790000
H7	1.6661180000	-2.6071970000	-0.3176190000
H8	1.8162160000	-3.3546110000	-4.1935860000
H9	1.5254300000	-4.9103170000	-3.4946560000
H10	-7.2467310000	-4.1702440000	-3.1092510000
H11	-5.6000930000	-2.4934460000	-3.8690830000
H12	-3.1967000000	-2.9829660000	-3.7519380000
H13	-4.0702620000	-6.8394620000	-2.0979970000
H14	-6.4723150000	-6.3407030000	-2.2208510000

H15	-2.5924730000	-7.5920070000	-4.4699240000
H16	-3.0615770000	-6.1765750000	-5.4036390000
H17	-1.6482740000	-7.1120880000	-5.8744710000
H18	-0.1759860000	-1.8924650000	0.9058460000
H19	-1.6029770000	-1.3545880000	0.0916150000
H20	-1.8590070000	0.8616640000	0.7342670000
H21	2.0250690000	-0.4189510000	-0.6841830000
H22	2.7971680000	1.8920640000	-0.5868450000
H23	1.2826390000	3.6918730000	0.1490980000
H24	-1.0328250000	3.1705540000	0.8159870000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 264.743 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.437	1.481	-11.469	19.35822
rot.	0.889	2.981	35.604	0.889	-9.727	16.41653
vib.	12.279	82.495	83.121	12.279	-12.504	21.10420
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.056	88.457	162.162	14.649	-33.700	56.87895

Total internal energy, Utot (SCFE + ZPE + U): -1112.373071 hartrees

Total enthalpy, Htot (Utot + pV): -1112.372127 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1112.449175 hartrees

(R,S)-3a

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-3.3554820000	-4.5157240000	-2.2483930000
C2	-2.5495750000	-5.6122400000	-2.9919050000
C3	-1.7024950000	-4.8543840000	-4.0046980000
C4	-1.4387430000	-3.5171950000	-3.3216090000
N1	-2.7474450000	-3.2445740000	-2.7006660000
C5	-3.0203190000	-2.0815460000	-2.0603690000
C6	-2.9136650000	-0.8677930000	-3.0108470000
N2	-1.5014960000	-0.4775470000	-3.0150210000
C7	-0.4757580000	-1.1269160000	-3.5764050000
C8	-0.8652470000	-2.4362750000	-4.2606060000
C9	-4.8850660000	-4.5686020000	-2.3850360000
C10	-7.6671360000	-4.6605310000	-2.5914320000
C11	-6.9151740000	-4.0738530000	-3.6006040000
C12	-5.5308170000	-4.0257680000	-3.4966140000
C13	-5.6485430000	-5.1494800000	-1.3750870000
C14	-7.0332750000	-5.1969550000	-1.4783720000
C15	-3.3421190000	-6.7826330000	-3.6097830000
O1	-3.4030620000	-1.9821100000	-0.8959630000
O2	0.6777270000	-0.7181160000	-3.5449700000
C16	-3.7800310000	0.3142300000	-2.5258300000

C17	-3.7700700000	1.5218590000	-3.4467030000
H1	-0.7161980000	-3.6829550000	-2.5172640000
C18	-2.8450990000	2.5689030000	-3.2455790000
C19	-4.5728960000	1.5310190000	-4.6071110000
C20	-2.7791600000	3.6201560000	-4.1504280000
C21	-3.6026290000	3.6342470000	-5.2692940000
C22	-4.4921740000	2.5921250000	-5.4993260000
H2	-3.1425670000	-4.6086190000	-1.1798780000
H3	-1.8678860000	-6.0466220000	-2.2569150000
H4	-0.7807300000	-5.3816660000	-4.2544050000
H5	-2.2600220000	-4.7009640000	-4.9311340000
H6	-3.2474920000	-1.1496930000	-4.0102930000
H7	-1.2503390000	0.3759680000	-2.5435460000
H8	-1.5388190000	-2.2262420000	-5.0897630000
H9	0.0441170000	-2.8210890000	-4.7215790000
H10	-8.7443650000	-4.6955630000	-2.6693150000
H11	-7.4070590000	-3.6529130000	-4.4654710000
H12	-4.9527560000	-3.5687640000	-4.2862240000
H13	-5.1686040000	-5.5626700000	-0.4996840000
H14	-7.6173070000	-5.6469700000	-0.6885290000
H15	-3.9237830000	-7.3083510000	-2.8515830000
H16	-4.0380600000	-6.4381900000	-4.3757180000
H17	-2.6759070000	-7.5103910000	-4.0740180000
H18	-3.4846870000	0.6193880000	-1.5201350000
H19	-4.8129730000	-0.0256710000	-2.4290060000
H20	-2.1898870000	2.5638740000	-2.3864540000
H21	-5.2563340000	0.7174750000	-4.8034940000
H22	-2.0793000000	4.4270610000	-3.9867130000
H23	-3.5431980000	4.4552230000	-5.9694740000
H24	-5.1187260000	2.6041390000	-6.3794860000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 264.864 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.437	1.481	-11.469	19.35822
rot.	0.889	2.981	35.561	0.889	-9.714	16.39472
vib.	12.162	82.293	82.303	12.162	-12.377	20.88996
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	13.939	88.255	161.300	14.532	-33.560	56.64290

Total internal energy, Utot (SCFE + ZPE + U): -1112.371641 hartrees
Total enthalpy, Htot (Utot + pV): -1112.370697 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1112.447336 hartrees

(S,R)-3a

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-3.7577460000	-3.9073460000	-1.9370270000
C2	-4.6411500000	-4.6073560000	-2.9865490000
C3	-5.9503660000	-4.8395170000	-2.2487780000

C4	-6.1207640000	-3.6039220000	-1.3542350000
N1	-4.7465250000	-3.1076270000	-1.1820700000
C5	-4.3560730000	-2.0826620000	-0.3821230000
C6	-5.4826800000	-1.4124230000	0.4380310000
N2	-6.4134500000	-0.7180130000	-0.4557190000
C7	-7.1728980000	-1.1094710000	-1.4870560000
C8	-7.0898720000	-2.5647510000	-1.9595180000
C9	-2.8933110000	-4.8387740000	-1.0674620000
C10	-1.2617920000	-6.4942900000	0.4838700000
C11	-2.5734530000	-6.2532000000	0.8692740000
C12	-3.3834380000	-5.4272820000	0.1002120000
C13	-1.5715780000	-5.0794630000	-1.4375690000
C14	-0.7606930000	-5.9051660000	-0.6690050000
C15	-4.0615120000	-5.8703700000	-3.6536570000
O1	-3.1972000000	-1.6846600000	-0.2881780000
O2	-7.9242120000	-0.3240370000	-2.0494480000
C16	-6.1652920000	-2.2463690000	1.5467520000
C17	-6.6738880000	-1.4096690000	2.7058420000
H1	-6.5072880000	-3.9599550000	-0.4019870000
C18	-7.9390230000	-0.7882030000	2.6343790000
C19	-5.8174050000	-1.0976370000	3.7829460000
C20	-6.2531840000	-0.2498680000	4.7928060000
C21	-7.5192200000	0.3192730000	4.7320650000
C22	-8.3556510000	0.0571920000	3.6540940000
H2	-3.0709350000	-3.2227160000	-2.4415600000
H3	-4.8284210000	-3.8815760000	-3.7818920000
H4	-6.7882000000	-5.0005310000	-2.9290380000
H5	-5.8704500000	-5.7322380000	-1.6254070000
H6	-4.9572420000	-0.6096100000	0.9583050000
H7	-6.5228060000	0.2673700000	-0.2707550000
H8	-8.1042950000	-2.9583940000	-1.9246330000
H9	-6.8578430000	-2.4675170000	-3.0197460000
H10	-0.6295030000	-7.1329810000	1.0838100000
H11	-2.9626970000	-6.7040520000	1.7705700000
H12	-4.3990630000	-5.2453200000	0.4163470000
H13	-1.1653730000	-4.6208530000	-2.3274490000
H14	0.2627960000	-6.0832360000	-0.9658870000
H15	-3.8760680000	-6.6631010000	-2.9273300000
H16	-4.7439360000	-6.2680240000	-4.4054140000
H17	-3.1156130000	-5.6530790000	-4.1508570000
H18	-5.4694140000	-2.9948910000	1.9299960000
H19	-7.0263200000	-2.7887410000	1.1635460000
H20	-8.5875970000	-0.9650710000	1.7877470000
H21	-4.8217580000	-1.5162690000	3.8287430000
H22	-5.6005850000	-0.0241250000	5.6239740000
H23	-7.8491300000	0.9815260000	5.5197000000
H24	-9.3303250000	0.5210210000	3.6031770000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 264.875 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.437	1.481	-11.469	19.35822

rot.	0.889	2.981	35.520	0.889	-9.701	16.37417
vib.	12.334	82.481	84.687	12.334	-12.915	21.79800
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.112	88.442	163.643	14.704	-34.086	57.53039

Total internal energy, Utot (SCFE + ZPE + U): -1112.369519 hartrees
 Total enthalpy, Htot (Utot + pV): -1112.368575 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -1112.446327 hartrees

(S,2S)-13b

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-2.7608780000	-2.4886980000	0.5183680000
C2	-1.9045160000	-3.4654400000	1.3885010000
C3	-2.6289010000	-3.4483920000	2.7389700000
C4	-4.1171890000	-3.4093040000	2.3659130000
N5	-4.1204020000	-2.6894160000	1.0652080000
C6	-5.2833810000	-2.6199310000	0.3408690000
C7	-5.3027090000	-1.9056680000	-1.0297700000
N8	-6.1494230000	-2.6279670000	-1.9839200000
C9	-4.9648670000	-3.4176730000	4.7738740000
C10	-5.0109370000	-2.7377860000	3.4222540000
C11	-2.2901920000	-1.0405410000	0.5237650000
C12	-1.3142780000	1.5991640000	0.4986500000
C13	-2.1785440000	1.1774200000	1.5089510000
C14	-2.6642330000	-0.1302660000	1.5194970000
C15	-1.4294680000	-0.6019000000	-0.4907730000
C16	-0.9425080000	0.7046870000	-0.5050910000
C17	-0.4066130000	-3.1769940000	1.4548580000
O18	-6.3363390000	-3.0870040000	0.7813950000
O19	-4.8747810000	-2.8490130000	5.8402770000
C20	-5.8477620000	-0.4749880000	-0.8167670000
C21	-6.0505070000	0.3478400000	-2.1043410000
H22	-4.4994840000	-4.4227990000	2.2007480000
C23	-6.6791400000	1.7062060000	-1.7595520000
O24	-5.0585020000	-4.7649400000	4.6589500000
C25	-5.0539150000	-5.4897380000	5.9000590000
H26	-2.7266560000	-2.8386000000	-0.5180320000
H27	-2.0467450000	-4.4612750000	0.9467190000
H28	-2.3890930000	-4.3160890000	3.3592490000
H29	-2.3519400000	-2.5494570000	3.3044250000
H30	-4.2983710000	-1.8391340000	-1.4550640000
H31	-5.7198110000	-3.5245370000	-2.2057730000
H32	-7.0146900000	-2.8603270000	-1.4953130000
H33	-6.0429290000	-2.7559480000	3.0588980000
H34	-4.7223300000	-1.6958050000	3.5806810000
H35	-0.9418780000	2.6192980000	0.4875780000
H36	-2.4828560000	1.8695580000	2.2888070000
H37	-3.3555110000	-0.4384980000	2.2964660000
H38	-1.1429620000	-1.2890880000	-1.2838650000
H39	-0.2803690000	1.0252800000	-1.3043250000
H40	0.0972220000	-3.9441750000	2.0518720000
H41	0.0503640000	-3.1790140000	0.4597920000
H42	-0.2044600000	-2.2043380000	1.9120610000
H43	-5.1696350000	0.0617270000	-0.1399270000
H44	-6.8081250000	-0.5636170000	-0.2917060000
H45	-6.0073430000	2.3067840000	-1.1333240000
H46	-4.1359580000	-5.2923970000	6.4592250000

H47	-5.9086940000	-5.2012040000	6.5164290000
H48	-5.1181850000	-6.5427710000	5.6262490000
H49	-7.6216410000	1.5853770000	-1.2138880000
H50	-6.8903510000	2.2842450000	-2.6660210000
H51	-6.7510080000	-0.2082250000	-2.7379880000
C52	-4.7505400000	0.5344770000	-2.8994000000
H53	-4.9200170000	1.1726910000	-3.7740830000
H54	-3.9721020000	1.0074560000	-2.2876380000
H55	-4.3617460000	-0.4208120000	-3.2652730000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 300.916 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.420	1.481	-11.464	19.34976
rot.	0.889	2.981	35.420	0.889	-9.672	16.32409
vib.	14.810	92.988	102.302	14.810	-15.692	26.48419
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.587	98.950	181.142	17.180	-36.828	62.15804

Total internal energy, Utot (SCFE + ZPE + U): -1114.943574 hartrees

Total enthalpy, Htot (Utot + pV): -1114.942630 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1115.028696 hartrees

(S,2R)-13b

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-3.9034580000	5.7233480000	6.8629650000
C2	-2.5563110000	6.0044280000	7.6013970000
C3	-2.2238990000	4.6470370000	8.2412110000
C4	-2.6479960000	3.6203220000	7.1779750000
N5	-3.7466970000	4.3104980000	6.4645710000
C6	-4.5358490000	3.6074180000	5.5922080000
C7	-5.6481320000	4.3265190000	4.7991690000
N8	-5.4598560000	4.1063000000	3.3576870000
C9	-0.3851050000	2.5239680000	6.9280530000
C10	-1.5034100000	3.2373860000	6.2033180000
C11	-5.1457030000	5.9917970000	7.7036390000
C12	-7.3913220000	6.5914420000	9.2893890000
C13	-6.7633120000	5.3506920000	9.3994750000
C14	-5.6515600000	5.0521050000	8.6111500000
C15	-5.7904450000	7.2302670000	7.5960230000
C16	-6.9028410000	7.5310650000	8.3814330000
C17	-2.5460560000	7.1879400000	8.5657000000
O18	-4.3382390000	2.4068880000	5.3884570000
O19	0.6626150000	3.0285620000	7.2772830000
C20	-7.0168360000	3.7697150000	5.2407750000
C21	-8.2273160000	4.2862590000	4.4393090000
H22	-3.0348620000	2.6940080000	7.6122320000
C23	-9.5066800000	3.5838840000	4.9182040000

O24	-0.7140590000	1.2397290000	7.1925300000
C25	0.2674350000	0.4903680000	7.9280610000
H26	-3.9564180000	6.3608260000	5.9734390000
H27	-1.8139510000	6.1975180000	6.8157390000
H28	-1.1658230000	4.5597470000	8.5009690000
H29	-2.8072740000	4.5128810000	9.1591830000
H30	-5.6237500000	5.4044770000	4.9748830000
H31	-4.5934050000	4.5475100000	3.0539630000
H32	-5.3206610000	3.1048910000	3.2217500000
H33	-1.0811670000	4.1345230000	5.7444170000
H34	-1.9237890000	2.5877130000	5.4334490000
H35	-8.2609420000	6.8201730000	9.8984340000
H36	-7.1437470000	4.6082200000	10.0951450000
H37	-5.1882400000	4.0734890000	8.6887540000
H38	-5.4221920000	7.9649760000	6.8835960000
H39	-7.3916410000	8.4956190000	8.2783720000
H40	-1.5441740000	7.3171080000	8.9876160000
H41	-2.8160020000	8.1222760000	8.0624200000
H42	-3.2461410000	7.0403480000	9.3928470000
H43	-7.1593720000	3.9963960000	6.3059030000
H44	-6.9655950000	2.6763820000	5.1603790000
H45	-9.7233700000	3.8264160000	5.9663040000
H46	-0.1576540000	-0.5048860000	8.0557960000
H47	1.2068250000	0.4385970000	7.3723740000
H48	0.4594810000	0.9547050000	8.8986180000
H49	-9.4189110000	2.4943970000	4.8415440000
H50	-10.3729740000	3.8918420000	4.3222370000
H51	-8.0601720000	4.0231630000	3.3883720000
C52	-8.3816010000	5.8116670000	4.5187440000
H53	-9.2825350000	6.1389590000	3.9876640000
H54	-8.4665910000	6.1496320000	5.5592040000
H55	-7.5307670000	6.3275650000	4.0629750000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 301.064 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.420	1.481	-11.464	19.34976
rot.	0.889	2.981	35.463	0.889	-9.685	16.34578
vib.	14.775	92.817	102.442	14.775	-15.768	26.61259
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.553	98.778	181.325	17.145	-36.917	62.30812

Total internal energy, Utot (SCFE + ZPE + U): -1114.943606 hartrees
Total enthalpy, Htot (Utot + pV): -1114.942662 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1115.028815 hartrees

(R,2R)-13b

Optimized geometry:

		angstroms	
atom	x	y	z

C1	-4.6287010000	3.0080260000	6.6080140000
C2	-5.5573950000	2.9139700000	5.3553990000
C3	-5.9530620000	1.4293680000	5.3334330000
C4	-6.1451540000	1.0655670000	6.8148760000
N5	-5.2279890000	2.0033340000	7.5059690000
C6	-4.9436090000	1.8295940000	8.8317640000
C7	-4.0174490000	2.8388830000	9.5453970000
N8	-3.2627040000	2.1914390000	10.6198450000
C9	-8.5082020000	0.1647050000	6.7598420000
C10	-7.5877450000	1.2275390000	7.3184640000
C11	-3.1501130000	2.7712450000	6.3170420000
C12	-0.4246780000	2.4131300000	5.7169630000
C13	-0.9723640000	3.6956720000	5.7499010000
C14	-2.3226890000	3.8702300000	6.0494220000
C15	-2.5872600000	1.4890400000	6.2900770000
C16	-1.2359740000	1.3119780000	5.9901490000
C17	-4.9850660000	3.4430080000	4.0423930000
O18	-5.4469930000	0.9054940000	9.4759140000
O19	-8.1689220000	-0.7742290000	6.0692310000
C20	-4.8898980000	3.9752360000	10.1287510000
C21	-4.1014010000	5.0825660000	10.8541750000
H22	-5.8337220000	0.0397930000	7.0272960000
C23	-3.2192920000	5.8964280000	9.8961520000
O24	-9.7867800000	0.3846240000	7.1380770000
C25	-10.7394600000	-0.5906990000	6.6817750000
H26	-4.7253750000	4.0070220000	7.0470140000
H27	-6.4523180000	3.5021580000	5.6006960000
H28	-6.8498540000	1.2349080000	4.7410010000
H29	-5.1432720000	0.8339780000	4.8981610000
H30	-3.2993340000	3.2577400000	8.8372460000
H31	-3.9049960000	1.5475090000	11.0834160000
H32	-2.5422360000	1.6005560000	10.2092630000
H33	-7.9960260000	2.2149000000	7.0729400000
H34	-7.5961630000	1.1426010000	8.4095870000
H35	0.6283900000	2.2740500000	5.4905930000
H36	-0.3468790000	4.5615620000	5.5523190000
H37	-2.7392230000	4.8742720000	6.0857990000
H38	-3.2023040000	0.6253510000	6.5232930000
H39	-0.8155980000	0.3103770000	5.9768190000
H40	-5.7351400000	3.3628300000	3.2487630000
H41	-4.6971060000	4.4966610000	4.1198780000
H42	-4.1021550000	2.8776840000	3.7309160000
H43	-5.5992420000	3.5141330000	10.8289060000
H44	-5.4975000000	4.4203560000	9.3267770000
H45	-3.8264990000	6.4001570000	9.1320660000
H46	-11.7037430000	-0.2645600000	7.0711290000
H47	-10.7592060000	-0.6291180000	5.5897910000
H48	-10.4872790000	-1.5829470000	7.0635770000
H49	-2.4811340000	5.2723900000	9.3826360000
H50	-2.6674700000	6.6717530000	10.4386560000
H51	-3.4467820000	4.5815640000	11.5766900000
C52	-5.0597700000	6.0060090000	11.6199070000
H53	-4.5094470000	6.7747570000	12.1736130000
H54	-5.7472820000	6.5209770000	10.9366770000
H55	-5.6655420000	5.4452310000	12.3398720000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 300.771 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.420	1.481	-11.464	19.34976
rot.	0.889	2.981	35.597	0.889	-9.725	16.41332
vib.	14.836	93.069	102.894	14.836	-15.842	26.73777
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.614	99.030	181.912	17.206	-37.031	62.50084

Total internal energy, Utot (SCFE + ZPE + U): -1114.947376 hartrees

Total enthalpy, Htot (Utot + pV): -1114.946432 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1115.032864 hartrees

(R,2S)-13b

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-2.0009660000	0.2766500000	-1.3864240000
C2	-1.1824920000	1.0417760000	-0.2966600000
C3	0.0567180000	0.1582950000	-0.1123880000
C4	0.3934490000	-0.3176600000	-1.5324850000
N5	-0.9327740000	-0.3364060000	-2.2034060000
C6	-1.0228940000	-0.5811140000	-3.5464060000
C7	-2.4006290000	-0.4920910000	-4.2401310000
N8	-2.5446040000	-1.5498160000	-5.2446720000
C9	2.5014480000	-1.5966330000	-0.9986780000
C10	1.1121310000	-1.6695640000	-1.5930280000
C11	-3.0245700000	-0.7175880000	-0.8499350000
C12	-4.9676220000	-2.4672980000	0.1915440000
C13	-5.3039410000	-1.1486880000	-0.1149020000
C14	-4.3401290000	-0.2851870000	-0.6328520000
C15	-2.7029920000	-2.0461750000	-0.5497560000
C16	-3.6651550000	-2.9130700000	-0.0307280000
C17	-1.9231290000	1.3894730000	0.9922670000
O18	-0.0311460000	-0.8811440000	-4.2161350000
O19	3.0819260000	-0.5829850000	-0.6683510000
C20	-2.5255650000	0.8888610000	-4.9234480000
C21	-3.8627860000	1.1301860000	-5.6499060000
H22	1.0292660000	0.4189340000	-2.0375390000
C23	-5.0501240000	1.2100510000	-4.6794280000
O24	3.0438910000	-2.8297430000	-0.8926170000
C25	4.3838870000	-2.8699650000	-0.3732540000
H26	-2.5453960000	1.0115680000	-1.9866930000
H27	-0.8568970000	1.9772650000	-0.7720160000
H28	0.8976210000	0.6840910000	0.3431010000
H29	-0.1886960000	-0.6989830000	0.5287690000
H30	-3.2010440000	-0.6187020000	-3.5072160000
H31	-1.6552520000	-1.6069690000	-5.7423670000
H32	-2.6492480000	-2.4465150000	-4.7735600000
H33	1.2039680000	-1.9843510000	-2.6368950000
H34	0.5487460000	-2.4515310000	-1.0713080000
H35	-5.7174690000	-3.1446470000	0.5895550000
H36	-6.3189270000	-0.7940700000	0.0400340000
H37	-4.6142710000	0.7373720000	-0.8818250000
H38	-1.6998820000	-2.4110850000	-0.7435240000

H39	-3.3967140000	-3.9416210000	0.1934960000
H40	-1.2652410000	1.9550110000	1.6601450000
H41	-2.8069550000	2.0062560000	0.7988080000
H42	-2.2529930000	0.4914000000	1.5223160000
H43	-1.6986190000	0.9697250000	-5.6410610000
H44	-2.3622550000	1.6858220000	-4.1824460000
H45	5.0631110000	-2.3043670000	-1.0157080000
H46	4.4198620000	-2.4479040000	0.6341300000
H47	4.6612430000	-3.9238290000	-0.3569750000
H48	-5.9868760000	1.3735700000	-5.2231510000
H49	-5.1698480000	0.2920230000	-4.0956060000
H50	-4.9295570000	2.0449820000	-3.9761300000
H51	-4.0221530000	0.2711070000	-6.3117830000
C52	-3.7817250000	2.4010210000	-6.5080930000
H53	-4.7127170000	2.5629460000	-7.0625940000
H54	-3.6090950000	3.2898820000	-5.8877890000
H55	-2.9654930000	2.3409300000	-7.2360440000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 300.810 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.420	1.481	-11.464	19.34976
rot.	0.889	2.981	35.587	0.889	-9.722	16.40830
vib.	14.819	93.068	102.137	14.819	-15.633	26.38572
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	16.597	99.030	181.145	17.189	-36.819	62.14378

Total internal energy, Utot (SCFE + ZPE + U): -1114.946833 hartrees

Total enthalpy, Htot (Utot + pV): -1114.945889 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1115.031957 hartrees

(S,S)-3b

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-11.0584400000	-17.2825200000	0.5565310000
C2	-10.9597530000	-18.5968090000	-0.2441590000
C3	-9.5021140000	-19.0056020000	-0.0920620000
C4	-9.1156310000	-18.5734200000	1.3300450000
N1	-10.1150370000	-17.5400310000	1.6625260000
C5	-10.2460140000	-16.9289150000	2.8678330000
C6	-9.2134420000	-17.4157470000	3.9163940000
N2	-7.9471270000	-16.8039930000	3.5124940000
C7	-7.1638430000	-17.0593360000	2.4565520000
C8	-7.6262530000	-18.1514800000	1.4794370000
C9	-10.8004320000	-15.9827870000	-0.2269910000
C10	-10.4206280000	-13.5973520000	-1.6364520000
C11	-9.3486330000	-14.2071360000	-0.9996260000
C12	-9.5383210000	-15.3895250000	-0.2961200000
C13	-11.8715380000	-15.3510560000	-0.8570950000

C14	-11.6834240000	-14.1688830000	-1.5623150000
C15	-11.4526330000	-18.5609860000	-1.7041790000
O1	-11.1021260000	-16.0891820000	3.1390680000
O2	-6.1156610000	-16.4542770000	2.2731570000
C16	-9.5733950000	-16.9459550000	5.3465820000
C17	-8.6052920000	-17.4315490000	6.4516020000
H1	-9.3110620000	-19.4198550000	1.9916620000
C18	-8.5587150000	-18.9712560000	6.5616750000
C19	-8.9324050000	-16.7617890000	7.8040500000
H2	-12.0662130000	-17.1899110000	0.9697980000
H3	-11.5692370000	-19.3362690000	0.2812210000
H4	-9.3461740000	-20.0724330000	-0.2562160000
H5	-8.9055470000	-18.4740120000	-0.8359520000
H6	-9.1425420000	-18.5019070000	3.9157970000
H7	-7.6166330000	-16.0342960000	4.0725870000
H8	-7.2846790000	-17.7654290000	0.5198610000
H9	-7.0103840000	-19.0299340000	1.6616670000
H10	-10.2738370000	-12.6748210000	-2.1794720000
H11	-8.3662900000	-13.7591350000	-1.0425480000
H12	-8.6937410000	-15.8383410000	0.2016800000
H13	-12.8617550000	-15.7788950000	-0.7999790000
H14	-12.5220150000	-13.6902940000	-2.0469400000
H15	-11.3703250000	-19.5420910000	-2.1727940000
H16	-10.8746600000	-17.8598840000	-2.3082790000
H17	-12.4985780000	-18.2578220000	-1.7591570000
H18	-10.5848030000	-17.2805250000	5.5861330000
H19	-9.6238080000	-15.8548770000	5.3556100000
H20	-7.6015290000	-17.0978970000	6.1821350000
H21	-7.6561860000	-19.3626420000	6.0906430000
H22	-9.4121310000	-19.4442080000	6.0750840000
H23	-8.5492320000	-19.3208030000	7.5942640000
H24	-9.7058330000	-15.9985310000	7.7088010000
H25	-9.2868230000	-17.4698350000	8.5533840000
H26	-8.0508130000	-16.2699170000	8.2169410000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 266.887 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.131	1.481	-11.378	19.20417
rot.	0.889	2.981	34.799	0.889	-9.487	16.01169
vib.	12.075	79.827	80.232	12.075	-11.846	19.99431
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	13.852	85.789	158.162	14.445	-32.711	55.21017

Total internal energy, Utot (SCFE + ZPE + U): -999.261464 hartrees
Total enthalpy, Htot (Utot + pV): -999.260520 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -999.335668 hartrees

(R,R)-3b

Optimized geometry:

atom	angstroms		
	x	y	z
C1	-7.0579310000	0.6823340000	3.5554510000
C2	-6.5752270000	-0.1541130000	2.3532770000
C3	-6.3455340000	0.8781180000	1.2582820000
C4	-5.8047580000	2.1105470000	1.9923730000
N1	-6.3403040000	1.9577960000	3.3568260000
C5	-6.2069070000	2.8691540000	4.3536350000
C6	-5.5520110000	4.1929700000	3.8800540000
N2	-4.1213240000	3.8974890000	3.7678080000
C7	-3.4528440000	3.0628030000	2.9561620000
C8	-4.2588310000	2.2210250000	1.9523160000
C9	-8.5829750000	0.8306120000	3.6998620000
C10	-11.3471920000	1.0698840000	4.0306610000
C11	-10.6687490000	1.9486990000	3.1971700000
C12	-9.2940230000	1.8318260000	3.0352150000
C13	-9.2734480000	-0.0382410000	4.5423330000
C14	-10.6483720000	0.0775240000	4.7047070000
C15	-7.4665530000	-1.3362680000	1.9245000000
O1	-6.5496720000	2.6872120000	5.5203060000
O2	-2.2332490000	2.9715020000	3.0034470000
C16	-5.7474530000	5.3662020000	4.8733840000
C17	-7.2073110000	5.8560980000	5.0376790000
H1	-6.2383980000	2.9937950000	1.5200210000
C18	-7.8262600000	6.3405680000	3.7087120000
C19	-7.3091010000	6.9229600000	6.1491090000
H2	-6.6971290000	0.2247700000	4.4801600000
H3	-5.6029400000	-0.5706230000	2.6279750000
H4	-5.6778740000	0.5152720000	0.4753190000
H5	-7.2951500000	1.1270520000	0.7807310000
H6	-5.9395430000	4.5096950000	2.9145260000
H7	-3.5143670000	4.3537600000	4.4303020000
H8	-3.9401930000	2.5242580000	0.9566260000
H9	-3.8514390000	1.2195830000	2.0893590000
H10	-12.4158580000	1.1625080000	4.1608560000
H11	-11.2093840000	2.7269330000	2.6784640000
H12	-8.7788900000	2.5256530000	2.3887170000
H13	-8.7405950000	-0.8089970000	5.0800820000
H14	-11.1724100000	-0.6014950000	5.3616820000
H15	-7.6094850000	-2.0386140000	2.7463300000
H16	-8.4539770000	-1.0023050000	1.6024170000
H17	-7.0201960000	-1.8867880000	1.0958450000
H18	-5.1294720000	6.2090780000	4.5612930000
H19	-5.3679310000	5.0611800000	5.8511330000
H20	-7.8055290000	5.0094250000	5.3804390000
H21	-8.4809150000	5.5747870000	3.2906010000
H22	-8.4333960000	7.2378410000	3.8302970000
H23	-7.0675910000	6.5694080000	2.9599940000
H24	-6.3680480000	7.0489630000	6.6856390000
H25	-7.5869540000	7.9064160000	5.7698290000
H26	-8.0582490000	6.6381170000	6.8890740000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 266.968 kcal/mol
is not included in U, H, or G in the table below

T =	298.15 K					
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.131	1.481	-11.378	19.20417
rot.	0.889	2.981	34.741	0.889	-9.469	15.98239
vib.	12.053	79.772	79.758	12.053	-11.726	19.79182
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	13.831	85.733	157.630	14.423	-32.574	54.97838

Total internal energy, Utot (SCFE + ZPE + U): -999.262445 hartrees
 Total enthalpy, Htot (Utot + pV): -999.261501 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -999.336396 hartrees

(R,S)-3b

Optimized geometry:

atom	angstroms		
	x	y	z
C1	-9.1596480000	-12.1954900000	2.6124870000
C2	-8.7010930000	-12.5269620000	1.1788870000
C3	-7.8627240000	-13.7822140000	1.3548390000
C4	-8.5641980000	-14.5688800000	2.4716380000
N1	-9.3353100000	-13.5430820000	3.1930280000
C5	-10.2235940000	-13.7625670000	4.1963180000
C6	-10.3446400000	-15.2327010000	4.6733840000
N2	-9.0727110000	-15.6077680000	5.2937990000
C7	-7.8309410000	-15.7344880000	4.8094630000
C8	-7.5979640000	-15.4316390000	3.3242850000
C9	-8.2450330000	-11.2602410000	3.4238930000
C10	-6.6507310000	-9.4997930000	4.8997520000
C11	-6.4469780000	-10.8694120000	4.9959010000
C12	-7.2417480000	-11.7439170000	4.2661200000
C13	-8.4497640000	-9.8833820000	3.3490620000
C14	-7.6549240000	-9.0072340000	4.0776360000
C15	-7.9938140000	-11.4029280000	0.3966410000
O1	-10.9160260000	-12.8862680000	4.7093770000
O2	-6.9029610000	-16.0851710000	5.5266730000
C16	-10.9127070000	-16.3151630000	3.7103900000
C17	-12.0618730000	-15.8632460000	2.7765690000
H1	-9.2911710000	-15.2138890000	1.9799280000
C18	-13.2783830000	-15.3204380000	3.5587260000
C19	-12.4526030000	-16.9902950000	1.7959020000
H2	-10.1334430000	-11.7004820000	2.5684630000
H3	-9.5948440000	-12.7995360000	0.6120560000
H4	-7.7755380000	-14.3609010000	0.4345400000
H5	-6.8524280000	-13.4960610000	1.6537870000
H6	-11.0475970000	-15.1784430000	5.5056220000
H7	-9.1026150000	-15.7701820000	6.2886330000
H8	-6.6267750000	-14.9386500000	3.3385960000
H9	-7.4201020000	-16.3825340000	2.8259170000
H10	-6.0355290000	-8.8197770000	5.4712980000
H11	-5.6752350000	-11.2583000000	5.6445420000
H12	-7.0740920000	-12.8047000000	4.3654550000
H13	-9.2335600000	-9.4858460000	2.7209220000
H14	-7.8234280000	-7.9422430000	4.0098190000
H15	-7.7360240000	-11.7261710000	-0.6123100000
H16	-8.6327920000	-10.5240280000	0.3065330000
H17	-7.0703690000	-11.0896020000	0.8861340000
H18	-11.2647400000	-17.1511990000	4.3164340000
H19	-10.1120570000	-16.7438560000	3.1110790000

H20	-11.6881320000	-15.0446480000	2.1590510000
H21	-13.2313330000	-15.5670950000	4.6195490000
H22	-13.3265910000	-14.2327060000	3.4866540000
H23	-14.2295680000	-15.7009720000	3.1866710000
H24	-13.4629220000	-17.3649330000	1.9615440000
H25	-12.4057230000	-16.6397170000	0.7641680000
H26	-11.7870650000	-17.8510800000	1.8697070000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 267.263 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
<hr/>						
trans.	0.889	2.981	43.131	1.481	-11.378	19.20417
rot.	0.889	2.981	34.695	0.889	-9.456	15.95938
vib.	11.973	79.536	79.278	11.973	-11.664	19.68596
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	13.751	85.498	157.104	14.343	-32.498	54.84950

Total internal energy, Utot (SCFE + ZPE + U): -999.258645 hartrees
Total enthalpy, Htot (Utot + pV): -999.257701 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -999.332346 hartrees

(S,R)-3b

Optimized geometry:

	angstroms		
atom	x	y	z
C1	3.8143440000	-5.4542990000	-2.5094970000
C2	4.5497980000	-5.6680970000	-1.1727860000
C3	6.0039560000	-5.3703540000	-1.5068110000
C4	5.9448770000	-4.2358110000	-2.5392650000
N1	4.6148520000	-4.3875600000	-3.1478840000
C5	4.1355610000	-3.6826070000	-4.2053500000
C6	5.1020670000	-2.6255550000	-4.8012280000
N2	5.2827330000	-1.5568530000	-3.8150300000
C7	5.7578900000	-1.5296060000	-2.5623290000
C8	6.1937270000	-2.8459880000	-1.9085960000
C9	3.6179320000	-6.7098780000	-3.3766300000
C10	3.2002030000	-8.9757700000	-4.9562490000
C11	4.4555180000	-8.3850390000	-4.9069250000
C12	4.6622250000	-7.2576540000	-4.1223800000
C13	2.3611880000	-7.3083980000	-3.4373680000
C14	2.1529840000	-8.4362480000	-4.2214770000
C15	4.3271730000	-7.0204730000	-0.4672350000
O1	3.0087080000	-3.8247090000	-4.6752010000
O2	5.8437710000	-0.4768090000	-1.9440670000
C16	6.4300650000	-3.0679690000	-5.4791030000
C17	6.3834580000	-4.3901570000	-6.2812130000
H1	6.7093660000	-4.4455790000	-3.2847670000
C18	7.7826910000	-4.7650450000	-6.8151360000
C19	5.3149430000	-4.3732510000	-7.3963060000
H2	2.8178860000	-5.0553270000	-2.3035400000

H3	4.1993160000	-4.8895670000	-0.4906930000
H4	6.5896030000	-5.1178610000	-0.6214530000
H5	6.4714680000	-6.2490610000	-1.9539400000
H6	4.5127530000	-2.1612860000	-5.5930280000
H7	4.9701180000	-0.6432650000	-4.1056280000
H8	7.2498320000	-2.7418020000	-1.6666140000
H9	5.6772690000	-2.8200230000	-0.9493740000
H10	3.0364930000	-9.8502690000	-5.5694230000
H11	5.2708700000	-8.8002180000	-5.4812450000
H12	5.6427640000	-6.8103600000	-4.0910920000
H13	1.5340080000	-6.8928850000	-2.8802700000
H14	1.1728450000	-8.8887790000	-4.2645440000
H15	4.6865160000	-7.8558130000	-1.0699300000
H16	4.8493430000	-7.0576090000	0.4892670000
H17	3.2680350000	-7.1906700000	-0.2708370000
H18	6.7428680000	-2.2676120000	-6.1512360000
H19	7.2299690000	-3.1177710000	-4.7430840000
H20	6.1042070000	-5.1834350000	-5.5894370000
H21	7.8425440000	-4.7336310000	-7.9032410000
H22	8.5593760000	-4.0964580000	-6.4422270000
H23	8.0569560000	-5.7748200000	-6.5075080000
H24	5.6804070000	-4.7692860000	-8.3436370000
H25	4.4562530000	-4.9842790000	-7.1120420000
H26	4.9397010000	-3.3693920000	-7.5953290000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 267.219 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.131	1.481	-11.378	19.20417
rot.	0.889	2.981	34.549	0.889	-9.412	15.88585
vib.	12.007	79.595	79.263	12.007	-11.625	19.62151
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	13.784	85.557	156.942	14.377	-32.416	54.71153

Total internal energy, Utot (SCFE + ZPE + U): -999.259097 hartrees
Total enthalpy, Htot (Utot + pV): -999.258153 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -999.332722 hartrees

(S,2S)-13c

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-5.1991270000	-0.8776280000	-1.3959490000
C2	-4.9312840000	-1.0294120000	0.1367320000
C3	-3.5153490000	-0.4663010000	0.2967140000
C4	-3.4865300000	0.7376470000	-0.6532550000
N5	-4.4352760000	0.3455450000	-1.7300950000
C6	-4.8247610000	1.2905960000	-2.6463000000
C7	-5.8195430000	0.9092330000	-3.7632270000
N8	-6.6428600000	2.0560610000	-4.1538490000

C9	-1.1738680000	1.5824600000	-0.0994290000
C10	-2.0977600000	1.0920620000	-1.1928850000
C11	-4.8361970000	-2.0969350000	-2.2324220000
C12	-4.2378500000	-4.4218640000	-3.7016230000
C13	-3.2346670000	-3.4998830000	-3.4026810000
C14	-3.5321110000	-2.3465400000	-2.6768460000
C15	-5.8362050000	-3.0260400000	-2.5472670000
C16	-5.5428210000	-4.1798630000	-3.2735600000
C17	-5.1462990000	-2.4206700000	0.7277000000
O18	-4.3485410000	2.4292340000	-2.6218480000
O19	-1.4987440000	1.8518000000	1.0387370000
C20	-5.0484850000	0.3414180000	-4.9969940000
C21	-4.2070850000	1.4130580000	-5.7057190000
H22	-3.8823070000	1.6267310000	-0.1487280000
O23	0.0909380000	1.7066540000	-0.5586580000
C24	1.0451130000	2.2054250000	0.3941820000
H25	-6.2679870000	-0.6922040000	-1.5383960000
H26	-5.6230510000	-0.3329050000	0.6304190000
H27	-3.2813830000	-0.1716010000	1.3207510000
H28	-2.7761080000	-1.2174400000	-0.0116570000
H29	-6.4909420000	0.1164570000	-3.4205120000
H30	-7.3491650000	2.2209940000	-3.4398020000
H31	-6.0404390000	2.8785240000	-4.1289210000
H32	-2.1911950000	1.8886920000	-1.9373610000
H33	-1.6275380000	0.2390400000	-1.6950300000
H34	-4.0063880000	-5.3160800000	-4.2727930000
H35	-2.2175840000	-3.6738930000	-3.7422700000
H36	-2.7491840000	-1.6234230000	-2.4741120000
H37	-6.8583950000	-2.8412880000	-2.2242020000
H38	-6.3348630000	-4.8842180000	-3.5113170000
H39	-4.9743410000	-2.3985090000	1.8087400000
H40	-6.1681690000	-2.7779450000	0.5621980000
H41	-4.4624330000	-3.1537730000	0.2906350000
C42	-6.0361280000	-0.3167440000	-5.9700940000
H43	-4.3711750000	-0.4345430000	-4.6191660000
H44	0.7546480000	3.1978840000	0.7469860000
H45	1.1181860000	1.5343210000	1.2535990000
H46	1.9952640000	2.2509090000	-0.1377280000
H47	-4.8524400000	2.1747790000	-6.1551830000
H48	-3.5190870000	1.9148930000	-5.0199340000
H49	-3.6194480000	0.9596310000	-6.5109720000
H50	-5.5157580000	-0.6925550000	-6.8577730000
H51	-6.5505940000	-1.1636290000	-5.5020110000
H52	-6.7898350000	0.4082850000	-6.2908580000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 283.080 kcal/mol is not included in U, H, or G in the table below

T =	298.15 K					
	U	Cv	S	H	G	ln (Q)
trans.	0.889	2.981	43.297	1.481	-11.428	19.28777
rot.	0.889	2.981	35.130	0.889	-9.585	16.17812
vib.	13.915	88.182	93.998	13.915	-14.111	23.81593
elec.	0.000	0.000	0.000	0.000	0.000	0.00000

total	15.692	94.144	172.424	16.285	-35.124	59.28182
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Total internal energy, Utot (SCFE + ZPE + U):	-1075.658417 hartrees
Total enthalpy, Htot (Utot + pV):	-1075.657473 hartrees
Total Gibbs free energy, Gtot (Htot - T*S):	-1075.739397 hartrees

(S,2R)-13c

Optimized geometry:

atom	angstroms		
	x	y	z
C1	-6.5870250000	-6.6090450000	-5.5338440000
C2	-5.5070460000	-7.7054980000	-5.7868240000
C3	-4.8593230000	-7.2533980000	-7.1060460000
C4	-4.7965770000	-5.7213440000	-6.9865450000
N5	-5.9407150000	-5.4088400000	-6.1035670000
C6	-6.3358530000	-4.1079270000	-5.9432330000
C7	-7.5159360000	-3.8326980000	-4.9830740000
N8	-7.1339400000	-4.2614580000	-3.6253070000
C9	-2.2996230000	-5.5073500000	-7.2992620000
C10	-3.4629040000	-5.2100170000	-6.3816030000
C11	-7.9491600000	-6.9176440000	-6.1473460000
C12	-10.4704320000	-7.5769380000	-7.2132110000
C13	-10.1649950000	-7.8903780000	-5.8886820000
C14	-8.9169830000	-7.5596360000	-5.3628260000
C15	-8.2712540000	-6.6009430000	-7.4733660000
C16	-9.5202920000	-6.9284410000	-8.0017620000
C17	-5.9899860000	-9.1536870000	-5.7788780000
O18	-5.7643070000	-3.1976440000	-6.5474810000
O19	-1.4838570000	-6.3928060000	-7.1426860000
C20	-8.0394310000	-2.3765610000	-5.1186200000
C21	-7.1099260000	-1.3353470000	-4.4781770000
H22	-4.9371980000	-5.2149140000	-7.9459870000
O23	-2.2991310000	-4.6811280000	-8.3704550000
C24	-1.2610710000	-4.9213740000	-9.3337910000
H25	-6.7265020000	-6.4536980000	-4.4612190000
H26	-4.7636550000	-7.5893380000	-4.9871550000
H27	-3.8716910000	-7.6967330000	-7.2584140000
H28	-5.4921810000	-7.5457770000	-7.9514560000
H29	-8.3301920000	-4.4996370000	-5.2920670000
H30	-6.4124400000	-3.6452080000	-3.2582170000
H31	-7.9330940000	-4.1751060000	-3.0019750000
H32	-3.2668890000	-5.6998890000	-5.4251590000
H33	-3.5529100000	-4.1318020000	-6.2354070000
H34	-11.4443100000	-7.8268040000	-7.6241340000
H35	-10.9018330000	-8.3843450000	-5.2614340000
H36	-8.6904830000	-7.7946340000	-4.3255640000
H37	-7.5499900000	-6.0743730000	-8.0909040000
H38	-9.7529730000	-6.6700750000	-9.0310030000
H39	-5.1429120000	-9.8319110000	-5.9249430000
H40	-6.4642420000	-9.4167330000	-4.8275870000
H41	-6.7152260000	-9.3405400000	-6.5758030000
C42	-9.4621080000	-2.2664240000	-4.5488130000
H43	-8.0825940000	-2.1651760000	-6.1935080000
H44	-1.4096430000	-4.1791050000	-10.1177780000
H45	-0.2759250000	-4.8042530000	-8.8757520000
H46	-1.3395220000	-5.9324470000	-9.7416610000
H47	-7.0533950000	-1.4619060000	-3.3896110000
H48	-7.4880700000	-0.3243560000	-4.6617220000
H49	-6.1042080000	-1.4037550000	-4.8970530000

H50	-9.8542480000	-1.2515610000	-4.6716240000
H51	-10.1535280000	-2.9548590000	-5.0476320000
H52	-9.4853340000	-2.4901780000	-3.4743010000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 283.157 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.297	1.481	-11.428	19.28777
rot.	0.889	2.981	35.215	0.889	-9.611	16.22096
vib.	13.896	88.105	94.596	13.896	-14.307	24.14813
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	15.674	94.066	173.108	16.266	-35.346	59.65687

Total internal energy, Utot (SCFE + ZPE + U): -1075.656077 hartrees

Total enthalpy, Htot (Utot + pV): -1075.655133 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1075.737382 hartrees

(R,2R)-13c

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-9.0438490000	6.1630880000	0.8489700000
C2	-9.3860100000	5.4436830000	-0.4938200000
C3	-8.8451690000	4.0232970000	-0.2673850000
C4	-9.1780800000	3.7200500000	1.2030910000
N5	-9.1870010000	5.0666850000	1.8248310000
C6	-9.2089880000	5.1908400000	3.1866810000
C7	-9.2913630000	6.6008750000	3.8082080000
N8	-8.7156740000	6.6228090000	5.1537250000
C9	-10.5008890000	1.5756940000	0.9364090000
C10	-10.5263030000	3.0124930000	1.4093710000
C11	-7.6745390000	6.8344950000	0.8762480000
C12	-5.1772570000	8.1298280000	0.8492800000
C13	-5.2673280000	6.7819040000	1.1962660000
C14	-6.5058150000	6.1396980000	1.2125760000
C15	-7.5721190000	8.1905500000	0.5388520000
C16	-6.3358720000	8.8346070000	0.5226210000
C17	-8.8967110000	6.1210010000	-1.7715380000
O18	-9.2141900000	4.1933790000	3.9143690000
O19	-9.5303990000	0.9873790000	0.5060040000
C20	-10.7746130000	7.0869520000	3.8376170000
C21	-10.8271420000	8.5882410000	4.1511730000
H22	-8.4062350000	3.1101860000	1.6794260000
O23	-11.7202630000	1.0064770000	1.0614510000
C24	-11.8000200000	-0.3728160000	0.6638960000
H25	-9.7967440000	6.9352060000	1.0390360000
H26	-10.4826650000	5.3893220000	-0.5332120000
H27	-9.2784120000	3.2869990000	-0.9476900000
H28	-7.7607310000	4.0074990000	-0.4225440000
H29	-8.7280690000	7.3059440000	3.1913170000

H30	-8.9230980000	5.7204180000	5.5819100000
H31	-7.7013630000	6.6561540000	5.0792340000
H32	-11.3417710000	3.5380720000	0.8986960000
H33	-10.7696440000	3.0109660000	2.4762650000
H34	-4.2131930000	8.6299110000	0.8434760000
H35	-4.3716410000	6.2276880000	1.4620340000
H36	-6.5643040000	5.0964050000	1.5069190000
H37	-8.4724260000	8.7500870000	0.2950640000
H38	-6.2793110000	9.8882540000	0.2645070000
H39	-9.2305760000	5.5540260000	-2.6466620000
H40	-9.2898920000	7.1386010000	-1.8672980000
H41	-7.8051130000	6.1802940000	-1.8035170000
C42	-11.6277500000	6.2857700000	4.8318490000
H43	-11.1895650000	6.9285610000	2.8312410000
H44	-12.8352270000	-0.6681850000	0.8338790000
H45	-11.5368010000	-0.4861120000	-0.3907240000
H46	-11.1226360000	-0.9859790000	1.2631070000
H47	-10.3454110000	8.7842100000	5.1131850000
H48	-10.3068470000	9.1767710000	3.3863920000
H49	-11.8621390000	8.9436000000	4.2013360000
H50	-12.6759150000	6.5974700000	4.7738090000
H51	-11.5791850000	5.2101410000	4.6399290000
H52	-11.2834580000	6.4615360000	5.8557970000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 283.057 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.297	1.481	-11.428	19.28777
rot.	0.889	2.981	35.208	0.889	-9.609	16.21750
vib.	13.931	88.196	94.199	13.931	-14.154	23.88952
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	15.709	94.157	172.704	16.301	-35.191	59.39479

Total internal energy, Utot (SCFE + ZPE + U): -1075.660216 hartrees
Total enthalpy, Htot (Utot + pV): -1075.659272 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1075.741330 hartrees

(R,2S)-13c

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-2.7455880000	-5.2575320000	0.8045640000
C2	-3.0161340000	-4.4541260000	2.1171290000
C3	-1.7291270000	-3.6402100000	2.2951880000
C4	-1.3391740000	-3.2259190000	0.8683190000
N5	-1.8991380000	-4.3208060000	0.0359670000
C6	-1.8554340000	-4.2395720000	-1.3302540000
C7	-2.5680600000	-5.3233190000	-2.1679630000
N8	-1.8476450000	-5.5793390000	-3.4175840000
C9	0.7283770000	-1.9427220000	1.5779710000

C10	0.1767430000	-3.0252610000	0.6758400000
C11	-2.1328520000	-6.6399880000	0.9997040000
C12	-1.0968630000	-9.2236560000	1.4132650000
C13	-2.4742570000	-9.0295450000	1.3081870000
C14	-2.9841620000	-7.7489060000	1.1009610000
C15	-0.7525830000	-6.8497050000	1.0951650000
C16	-0.2387380000	-8.1299320000	1.3032560000
C17	-3.4359650000	-5.2684030000	3.3382470000
O18	-1.2610400000	-3.3192370000	-1.8984350000
O19	1.6254960000	-2.0823550000	2.3809220000
C20	-4.0412810000	-4.9032620000	-2.4692760000
C21	-4.8235830000	-6.1040560000	-3.0188200000
H22	-1.8347140000	-2.2897470000	0.5861320000
O23	0.0859130000	-0.7660750000	1.3812540000
C24	0.5452070000	0.3291060000	2.1902070000
H25	-3.6999220000	-5.3974150000	0.2890120000
H26	-3.8249110000	-3.7514470000	1.8735600000
H27	-1.8654090000	-2.7738100000	2.9485130000
H28	-0.9438950000	-4.2659980000	2.7375680000
H29	-2.5977050000	-6.2596920000	-1.6031660000
H30	-1.4713080000	-4.6865910000	-3.7361560000
H31	-1.0368290000	-6.1621570000	-3.2220860000
H32	0.3567470000	-2.7531070000	-0.3671620000
H33	0.7248380000	-3.9421810000	0.9040950000
H34	-0.6953670000	-10.2207050000	1.5689370000
H35	-3.1517520000	-9.8758110000	1.3778090000
H36	-4.0587480000	-7.6080550000	1.0082200000
H37	-0.0736560000	-6.0110060000	0.9862790000
H38	0.8359040000	-8.2724030000	1.3729390000
H39	-3.6356050000	-4.6011900000	4.1830880000
H40	-4.3486510000	-5.8423360000	3.1474600000
H41	-2.6556540000	-5.9728680000	3.6396680000
C42	-4.1218320000	-3.7045400000	-3.4260380000
H43	-4.5006660000	-4.6007220000	-1.5163750000
H44	-0.0764870000	1.1805340000	1.9135540000
H45	0.4324770000	0.0991090000	3.2526550000
H46	1.5977030000	0.5413540000	1.9875450000
H47	-4.3430550000	-6.4761050000	-3.9279110000
H48	-5.8548570000	-5.8242720000	-3.2598990000
H49	-4.8591160000	-6.9263460000	-2.2944980000
H50	-5.1634210000	-3.3928360000	-3.5574080000
H51	-3.5499560000	-2.8488120000	-3.0570080000
H52	-3.7290110000	-3.9763890000	-4.4107790000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 283.206 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.297	1.481	-11.428	19.28777
rot.	0.889	2.981	35.180	0.889	-9.600	16.20342
vib.	13.927	88.078	94.970	13.927	-14.388	24.28395
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	15.705	94.040	173.447	16.297	-35.416	59.77515

Total internal energy, Utot (SCFE + ZPE + U): -1075.657223 hartrees
 Total enthalpy, Htot (Utot + pV): -1075.656278 hartrees
 Total Gibbs free energy, Gtot (Htot - T*S): -1075.738689 hartrees

(S,S)-3c

Optimized geometry:

angstroms			
atom	x	y	z
C1	-0.7181370000	-0.8114820000	-0.0410630000
C2	-0.9155740000	-2.3098710000	-0.3476310000
C3	0.3176030000	-2.9677320000	0.2537340000
C4	0.6220890000	-2.1545960000	1.5205010000
N1	-0.0572930000	-0.8668560000	1.2781220000
C5	-0.1420400000	0.1593850000	2.1639250000
C6	0.5413450000	-0.1617760000	3.5268650000
N2	1.9696590000	-0.0359300000	3.2451740000
C7	2.7724240000	-0.8311470000	2.5256790000
C8	2.1368570000	-2.0684990000	1.8695880000
C9	0.0256580000	0.0119920000	-1.1082960000
C10	1.2977580000	1.5554330000	-3.0630920000
C11	2.0378270000	0.9851450000	-2.0366770000
C12	1.4052750000	0.2222520000	-1.0636540000
C13	-0.7078450000	0.6044240000	-2.1351500000
C14	-0.0766460000	1.3668060000	-3.1101510000
C15	-1.1764160000	-2.6910030000	-1.8182060000
O1	-0.6958240000	1.2331270000	1.9327330000
O2	3.9659970000	-0.5925860000	2.3948490000
C16	0.0951020000	0.8488900000	4.6263480000
C17	0.9211020000	0.6820570000	5.9178360000
H1	0.0946810000	-2.6336150000	2.3479510000
C18	-1.4061670000	0.7484530000	4.9715200000
H2	-1.6958370000	-0.3373450000	0.0777930000
H3	-1.7837230000	-2.6412610000	0.2275320000
H4	0.1658460000	-4.0260680000	0.4688530000
H5	1.1403020000	-2.8982710000	-0.4605470000
H6	0.3005610000	-1.1648140000	3.8770510000
H7	2.4284080000	0.7912870000	3.5920670000
H8	2.7042950000	-2.1590450000	0.9441990000
H9	2.4290570000	-2.9339150000	2.4610700000
H10	1.7893700000	2.1532180000	-3.8170380000
H11	3.1059910000	1.1405000000	-1.9872340000
H12	1.9985500000	-0.1996500000	-0.2684780000
H13	-1.7792810000	0.4745620000	-2.1793070000
H14	-0.6569760000	1.8193820000	-3.9010300000
H15	-0.3391130000	-2.4155450000	-2.4613080000
H16	-1.3325430000	-3.7647440000	-1.9260170000
H17	-2.0651730000	-2.1899490000	-2.2028880000
H18	0.2711750000	1.8630940000	4.2602730000
H19	0.8322140000	-0.3279890000	6.3190760000
H20	1.9804810000	0.8798010000	5.7530500000
H21	0.5885170000	1.3752070000	6.6913170000
H22	-1.6747870000	1.4480060000	5.7636300000
H23	-2.0427100000	0.9872180000	4.1191950000
H24	-1.6714750000	-0.2528610000	5.3113500000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature

are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 249.425 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
-----	-----	-----	-----	-----	-----	-----
trans.	0.889	2.981	42.995	1.481	-11.338	19.13572
rot.	0.889	2.981	34.182	0.889	-9.302	15.70080
vib.	11.004	74.501	70.063	11.004	-9.886	16.68518
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	12.781	80.463	147.239	13.373	-30.526	51.52169

Total internal energy, Utot (SCFE + ZPE + U): -959.974956 hartrees
Total enthalpy, Htot (Utot + pV): -959.974011 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -960.043969 hartrees

(R,R)-3c

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-0.6539410000	0.6275630000	-1.0945410000
C2	-1.8862720000	-0.0750610000	-1.6996720000
C3	-1.2932420000	-1.0637670000	-2.6936010000
C4	0.0005130000	-1.5514260000	-2.0317580000
N1	0.3699810000	-0.4361620000	-1.1416230000
C5	1.5118040000	-0.3679840000	-0.4100840000
C6	2.4952470000	-1.5343220000	-0.7228890000
N2	1.9451040000	-2.6858150000	-0.0055620000
C7	0.8023920000	-3.3677130000	-0.1795960000
C8	-0.1605660000	-2.9017270000	-1.2854040000
C9	-0.2316660000	1.9429000000	-1.7721720000
C10	0.5262130000	4.3653840000	-2.9398660000
C11	0.9751520000	3.1656860000	-3.4751900000
C12	0.6011560000	1.9613250000	-2.8925740000
C13	-0.6671170000	3.1536640000	-1.2375760000
C14	-0.2936110000	4.3586980000	-1.8194570000
C15	-2.9826470000	0.8309450000	-2.2938760000
O1	1.7482710000	0.4970990000	0.4319490000
O2	0.5276360000	-4.3376130000	0.5147430000
C16	3.9309230000	-1.1934050000	-0.2213770000
C17	4.5575150000	0.0163140000	-0.9481470000
H1	0.7511510000	-1.6644040000	-2.8159440000
C18	4.8776210000	-2.4040320000	-0.3477420000
H2	-0.8550520000	0.8640180000	-0.0465440000
H3	-2.3494470000	-0.6500220000	-0.8940080000
H4	-1.9823760000	-1.8727780000	-2.9405130000
H5	-1.0532580000	-0.5502310000	-3.6265780000
H6	2.5605800000	-1.7390590000	-1.7901970000
H7	2.4809430000	-3.0170140000	0.7805310000
H8	-0.2307500000	-3.7127490000	-2.0080120000
H9	-1.1254240000	-2.8869820000	-0.7790170000
H10	0.8200370000	5.3029660000	-3.3895470000
H11	1.6196490000	3.1689100000	-4.3421350000
H12	0.9618060000	1.0363270000	-3.3157840000
H13	-1.2980970000	3.1630410000	-0.3606780000
H14	-0.6366230000	5.2911650000	-1.3950050000

H15	-3.3643420000	1.5272350000	-1.5464440000
H16	-2.6091710000	1.4212160000	-3.1319530000
H17	-3.8264420000	0.2433890000	-2.6567970000
H18	3.8778660000	-0.9354850000	0.8389160000
H19	4.6092000000	-0.1474140000	-2.0246920000
H20	5.5710250000	0.2061980000	-0.5937150000
H21	3.9946950000	0.9354870000	-0.7816970000
H22	4.5480280000	-3.2457700000	0.2615590000
H23	4.9458210000	-2.7496130000	-1.3797500000
H24	5.8858160000	-2.1521400000	-0.0168520000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 249.074 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.995	1.481	-11.338	19.13572
rot.	0.889	2.981	34.333	0.889	-9.348	15.77711
vib.	11.201	74.999	72.345	11.201	-10.369	17.50076
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	12.978	80.961	149.672	13.571	-31.054	52.41359

Total internal energy, Utot (SCFE + ZPE + U): -959.974629 hartrees
Total enthalpy, Htot (Utot + pV): -959.973685 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -960.044799 hartrees

(R,S)-3c

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-1.0584070000	-3.4623060000	-0.5144180000
C2	0.0900190000	-2.4404570000	-0.3149950000
C3	1.2068740000	-3.2359260000	0.3443790000
C4	1.0282750000	-4.6409330000	-0.2205220000
N1	-0.4401060000	-4.7746230000	-0.2168500000
C5	-1.0742610000	-5.9258400000	-0.5533230000
C6	-0.6793570000	-7.0895050000	0.3994530000
N2	0.5675290000	-7.6584510000	-0.1122960000
C7	1.7873060000	-7.1116990000	-0.0936880000
C8	1.8373860000	-5.7183870000	0.5289210000
C9	-2.3646450000	-3.1914010000	0.2483320000
C10	-4.7591640000	-2.7042080000	1.5976120000
C11	-4.6187460000	-2.3248710000	0.2691810000
C12	-3.4274130000	-2.5692650000	-0.4027170000
C13	-2.5171850000	-3.5757370000	1.5810820000
C14	-3.7078990000	-3.3310130000	2.2533220000
C15	-0.2454500000	-1.1272040000	0.4215850000
O1	-1.9309160000	-6.0201030000	-1.4301110000
O2	2.7815280000	-7.6706720000	-0.5379920000
C16	-1.7952940000	-8.1740880000	0.4785560000
C17	-1.5931230000	-9.0722110000	1.7117420000
H1	1.3594120000	-4.6327040000	-1.2630170000

C18	-1.9637450000	-9.0502730000	-0.7853690000
H2	-1.3222710000	-3.4666310000	-1.5755650000
H3	0.4337110000	-2.1624620000	-1.3140960000
H4	2.1940020000	-2.8244930000	0.1290660000
H5	1.0792280000	-3.2460500000	1.4289410000
H6	-0.5306890000	-6.6842270000	1.4014800000
H7	0.5126150000	-8.5524910000	-0.5728130000
H8	1.5532980000	-5.7766600000	1.5781710000
H9	2.8870510000	-5.4254780000	0.5330890000
H10	-5.6872980000	-2.5166280000	2.1182530000
H11	-5.4385290000	-1.8444520000	-0.2451770000
H12	-3.3343550000	-2.2774440000	-1.4388280000
H13	-1.7042000000	-4.0636440000	2.0981320000
H14	-3.8170360000	-3.6309890000	3.2854300000
H15	-0.5809830000	-1.3122630000	1.4427790000
H16	0.6230410000	-0.4699900000	0.4746100000
H17	-1.0388210000	-0.5805530000	-0.0895730000
H18	-2.7438000000	-7.6509590000	0.6218790000
H19	-2.3919740000	-9.8094200000	1.7993470000
H20	-0.6473830000	-9.6130770000	1.6620650000
H21	-1.5920910000	-8.4870300000	2.6318450000
H22	-2.8025500000	-9.7369190000	-0.6686490000
H23	-2.1683780000	-8.4636960000	-1.6801720000
H24	-1.0799590000	-9.6554900000	-0.9853880000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 249.210 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.995	1.481	-11.338	19.13572
rot.	0.889	2.981	34.341	0.889	-9.350	15.78117
vib.	11.078	74.736	71.093	11.078	-10.119	17.07862
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	12.855	80.698	148.429	13.448	-30.807	51.99550

Total internal energy, Utot (SCFE + ZPE + U): -959.973771 hartrees
Total enthalpy, Htot (Utot + pV): -959.972826 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -960.043350 hartrees

(S,R)-3c

Optimized geometry:

		angstroms		
atom	x	y	z	
C1	-3.3329530000	-0.4723050000	-2.0085150000	
C2	-2.4457890000	0.5284630000	-1.2447320000	
C3	-1.4094840000	0.9488570000	-2.2754960000	
C4	-2.1731760000	0.9812550000	-3.6075910000	
N1	-3.2979060000	0.0590020000	-3.3889110000	
C5	-4.1997420000	-0.3465830000	-4.3215870000	
C6	-4.0533090000	0.2784810000	-5.7380510000	
N2	-4.2995700000	1.7192900000	-5.6577290000	
C7	-3.7278200000	2.7255770000	-4.9852870000	

C8	-2.5919300000	2.4138440000	-4.0070810000
C9	-2.9348640000	-1.9528980000	-1.8789090000
C10	-2.2665810000	-4.6529380000	-1.6181760000
C11	-1.5216940000	-3.8301110000	-2.4520560000
C12	-1.8556780000	-2.4881470000	-2.5828420000
C13	-3.6785100000	-2.7893380000	-1.0489680000
C14	-3.3459920000	-4.1318550000	-0.9175870000
C15	-1.8489040000	0.0469530000	0.0925130000
O1	-5.1156560000	-1.1336450000	-4.0914230000
O2	-4.1050740000	3.8795300000	-5.1414840000
C16	-2.8036900000	-0.1399680000	-6.5748410000
C17	-3.0421760000	0.1528700000	-8.0673920000
H1	-1.5065620000	0.5657780000	-4.3598300000
C18	-2.3785340000	-1.6104630000	-6.3973810000
H2	-4.3577470000	-0.3892860000	-1.6378350000
H3	-3.0678020000	1.3992060000	-1.0229250000
H4	-0.9378250000	1.9002290000	-2.0242500000
H5	-0.6112750000	0.2067100000	-2.3269020000
H6	-4.9199460000	-0.1063840000	-6.2780540000
H7	-5.0710460000	2.0506020000	-6.2153650000
H8	-1.7185300000	2.9622310000	-4.3554030000
H9	-2.9104950000	2.9303580000	-3.1019090000
H10	-2.0108950000	-5.6980750000	-1.5187030000
H11	-0.6842370000	-4.2344850000	-3.0017300000
H12	-1.2677130000	-1.8598680000	-3.2327480000
H13	-4.5273970000	-2.4003370000	-0.5055730000
H14	-3.9329330000	-4.7716430000	-0.2745790000
H15	-2.6338780000	-0.2616920000	0.7837830000
H16	-1.1806350000	-0.8043170000	-0.0450860000
H17	-1.2762800000	0.8383260000	0.5770440000
H18	-1.9568850000	0.4873500000	-6.3090900000
H19	-3.2631850000	1.2079860000	-8.2336140000
H20	-2.1629840000	-0.0892770000	-8.6653850000
H21	-3.8781420000	-0.4266050000	-8.4610750000
H22	-1.5541490000	-1.8694940000	-7.0623100000
H23	-2.0433320000	-1.8178950000	-5.3830880000
H24	-3.2041340000	-2.2899100000	-6.6142950000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 249.255 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.995	1.481	-11.338	19.13572
rot.	0.889	2.981	34.209	0.889	-9.311	15.71452
vib.	11.191	74.823	72.786	11.191	-10.511	17.74003
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	12.968	80.785	149.990	13.561	-31.159	52.59027

Total internal energy, Utot (SCFE + ZPE + U): -959.972469 hartrees
Total enthalpy, Htot (Utot + pV): -959.971525 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -960.042790 hartrees

(S,2S)-13d

Optimized geometry:

atom	angstroms		
	x	y	z
C1	-1.3084440000	-6.3558060000	-3.2207390000
C2	-1.7907920000	-6.7822160000	-1.7962320000
C3	-1.8899040000	-5.4479270000	-1.0491470000
C4	-2.4462940000	-4.4734870000	-2.0958470000
N5	-1.9284360000	-5.0220550000	-3.3772330000
C6	-2.3565390000	-4.4888660000	-4.5649110000
C7	-1.8289800000	-5.0613010000	-5.8999180000
N8	-2.8809370000	-5.1004920000	-6.9191900000
C9	-2.6697330000	-2.4448780000	-0.6134710000
C10	-2.0495940000	-3.0105300000	-1.8723340000
C11	0.2011030000	-6.3691050000	-3.4238910000
C12	2.9910290000	-6.5004620000	-3.7710430000
C13	2.4007620000	-5.3537890000	-3.2396470000
C14	1.0176070000	-5.2882120000	-3.0703710000
C15	0.8053220000	-7.5110760000	-3.9656200000
C16	2.1873210000	-7.5800880000	-4.1370900000
C17	-0.9629230000	-7.8555590000	-1.0935900000
O18	-3.1231230000	-3.5230580000	-4.5946310000
O19	-3.5329350000	-2.9763740000	0.0547600000
C20	-0.6828160000	-4.1646780000	-6.3931680000
H21	-3.5414440000	-4.5210520000	-2.1128370000
O22	-2.1468510000	-1.2336350000	-0.3214530000
C23	-2.6983520000	-0.5891550000	0.8392890000
H24	-1.7413690000	-7.0496600000	-3.9484340000
H25	-2.8120520000	-7.1649700000	-1.9296840000
H26	-2.5299890000	-5.4946710000	-0.1663310000
H27	-0.8917210000	-5.1277260000	-0.7217720000
H28	-1.4437020000	-6.0767070000	-5.7753020000
H29	-3.3506280000	-4.1947880000	-6.8931340000
H30	-3.5935360000	-5.7741200000	-6.6415210000
H31	-2.3925210000	-2.4088390000	-2.7196730000
H32	-0.9620140000	-2.8899990000	-1.8136290000
H33	4.0672460000	-6.5479940000	-3.9092750000
H34	3.0171300000	-4.5032620000	-2.9624560000
H35	0.5668000000	-4.3812910000	-2.6814740000
H36	0.1852440000	-8.3533360000	-4.2646710000
H37	2.6345630000	-8.4727780000	-4.5650850000
H38	-1.4154170000	-8.1044860000	-0.1281210000
H39	-0.9102780000	-8.7776040000	-1.6820540000
H40	0.0614030000	-7.5183490000	-0.9109930000
H41	0.1569180000	-4.1650930000	-5.6925770000
H42	-2.5362520000	-1.1983930000	1.7320140000
H43	-2.1735550000	0.3622390000	0.9246760000
H44	-3.7716530000	-0.4255760000	0.7157930000
H45	-1.0396190000	-3.1357340000	-6.5060180000
H46	-0.3380370000	-4.5231550000	-7.3661340000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 247.437 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
-----	-----	-----	-----	-----	-----	-----
trans.	0.889	2.981	43.034	1.481	-11.349	19.15555
rot.	0.889	2.981	34.662	0.889	-9.446	15.94264
vib.	12.252	77.878	82.561	12.252	-12.363	20.86717
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.029	83.839	160.257	14.622	-33.159	55.96535

Total internal energy, Utot (SCFE + ZPE + U): -997.085787 hartrees

Total enthalpy, Htot (Utot + pV): -997.084843 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -997.160986 hartrees

(S,2R)-13d

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-10.0815140000	1.3855650000	3.8800360000
C2	-9.7036590000	-0.1232240000	3.7417120000
C3	-8.5584190000	-0.0972580000	2.7167890000
C4	-7.7473730000	1.1543220000	3.0899370000
N5	-8.7753500000	2.0433900000	3.6802730000
C6	-8.4650710000	3.3337130000	4.0016670000
C7	-9.5554860000	4.1837730000	4.6873520000
N8	-9.7166080000	3.6685290000	6.0624400000
C9	-5.4629080000	0.1216840000	3.4479970000
C10	-6.6071360000	0.8787890000	4.0841180000
C11	-11.1601200000	1.8524340000	2.9067960000
C12	-13.2230320000	2.6302160000	1.1528030000
C13	-11.8922010000	2.6644280000	0.7357770000
C14	-10.8699170000	2.2815500000	1.6052270000
C15	-12.5001850000	1.8347850000	3.3177160000
C16	-13.5237480000	2.2159120000	2.4507990000
C17	-10.8404190000	-1.0847890000	3.4033010000
O18	-7.3429470000	3.7974640000	3.7895610000
O19	-5.3704720000	-0.1731160000	2.2742280000
C20	-9.2091340000	5.6716230000	4.5952170000
H21	-7.3126870000	1.6380410000	2.2112730000
O22	-4.5201020000	-0.1894310000	4.3665120000
C23	-3.3715010000	-0.8862470000	3.8556360000
H24	-10.4261770000	1.5924020000	4.8973990000
H25	-9.2855000000	-0.4179560000	4.7139740000
H26	-7.9474070000	-1.0025010000	2.7320920000
H27	-8.9652520000	0.0009830000	1.7044240000
H28	-10.5074910000	4.0079680000	4.1753280000
H29	-8.8625300000	3.8567620000	6.5862530000
H30	-10.4534780000	4.1936260000	6.5295360000
H31	-6.9590000000	0.3195990000	4.9588600000
H32	-6.2160180000	1.8318820000	4.4528200000
H33	-14.0171720000	2.9322150000	0.4763640000
H34	-11.6458210000	2.9958890000	-0.2690460000
H35	-9.8372380000	2.3341340000	1.2741220000
H36	-12.7419100000	1.5236550000	4.3314630000
H37	-14.5550210000	2.1965900000	2.7922220000
H38	-10.4646580000	-2.1130110000	3.3741570000
H39	-11.6401490000	-1.0459540000	4.1503430000
H40	-11.2829780000	-0.8594830000	2.4287410000
H41	-9.1593420000	6.0049560000	3.5540040000
H42	-2.8588060000	-0.2836940000	3.1018390000
H43	-2.7234210000	-1.0552230000	4.7155100000

H44	-3.6656360000	-1.8370860000	3.4041730000
H45	-8.2346320000	5.8692880000	5.0491170000
H46	-9.9734130000	6.2651930000	5.1087660000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 247.352 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.034	1.481	-11.349	19.15555
rot.	0.889	2.981	34.648	0.889	-9.441	15.93538
vib.	12.244	77.982	82.485	12.244	-12.349	20.84254
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.021	83.944	160.166	14.614	-33.140	55.93346

Total internal energy, Utot (SCFE + ZPE + U): -997.085803 hartrees

Total enthalpy, Htot (Utot + pV): -997.084859 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -997.160959 hartrees

(R,2R)-13d

Optimized geometry:

atom	x	y	z
C1	-8.8024930000	-3.3502780000	-0.0840670000
C2	-7.6060840000	-3.0875530000	-1.0516680000
C3	-7.6226040000	-1.5584890000	-1.2115100000
C4	-7.9801980000	-1.0381740000	0.1911880000
N5	-8.7737950000	-2.1460840000	0.7669680000
C6	-9.4846170000	-1.9538020000	1.9209690000
C7	-10.2464320000	-3.1485910000	2.5384510000
N8	-11.4128280000	-2.7084770000	3.3026890000
C9	-5.9413360000	0.4210560000	0.4945170000
C10	-6.7411100000	-0.7258410000	1.0692990000
C11	-10.1412330000	-3.5752610000	-0.7799480000
C12	-12.5694280000	-4.0631450000	-2.1151590000
C13	-11.7490720000	-5.1274240000	-1.7406510000
C14	-10.5471990000	-4.8828370000	-1.0778800000
C15	-10.9776240000	-2.5152860000	-1.1522680000
C16	-12.1806630000	-2.7575140000	-1.8161430000
C17	-7.6067520000	-3.8689120000	-2.3631940000
O18	-9.4803250000	-0.8656290000	2.4990750000
O19	-4.9209640000	0.3126020000	-0.1547680000
C20	-9.2896650000	-3.9145610000	3.4679560000
H21	-8.5989480000	-0.1363240000	0.1624440000
O22	-6.5346480000	1.6085720000	0.7510230000
C23	-5.8747200000	2.7597600000	0.1992130000
H24	-8.5835000000	-4.2401570000	0.5165250000
H25	-6.7009590000	-3.3585120000	-0.4923240000
H26	-6.6644800000	-1.1683250000	-1.5645270000
H27	-8.3916980000	-1.2674340000	-1.9358740000
H28	-10.5973120000	-3.8235320000	1.7535000000
H29	-11.1240960000	-1.8873100000	3.8359610000
H30	-12.1193160000	-2.3634340000	2.6548600000

H31	-6.0837050000	-1.5969250000	1.1207800000
H32	-7.0960190000	-0.4683130000	2.0691100000
H33	-13.5094550000	-4.2507690000	-2.6256560000
H34	-12.0489840000	-6.1491250000	-1.9553090000
H35	-9.9197200000	-5.7189420000	-0.7776900000
H36	-10.6990090000	-1.4959670000	-0.9036540000
H37	-12.8183400000	-1.9231030000	-2.0939310000
H38	-6.7036340000	-3.6363650000	-2.9365420000
H39	-7.6186230000	-4.9501720000	-2.1901830000
H40	-8.4743000000	-3.6200910000	-2.9808500000
H41	-8.9322730000	-3.2523510000	4.2632780000
H42	-6.4843000000	3.6154080000	0.4887130000
H43	-4.8640610000	2.8537550000	0.6038300000
H44	-5.8106090000	2.6828220000	-0.8891040000
H45	-8.4159540000	-4.2999270000	2.9315730000
H46	-9.8221990000	-4.7499220000	3.9286260000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 247.608 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.034	1.481	-11.349	19.15555
rot.	0.889	2.981	34.612	0.889	-9.431	15.91765
vib.	12.256	77.748	83.313	12.256	-12.584	21.23895
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.033	83.710	160.960	14.626	-33.364	56.31214

Total internal energy, Utot (SCFE + ZPE + U): -997.085294 hartrees
Total enthalpy, Htot (Utot + pV): -997.084350 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -997.160827 hartrees

(R,2S)-13d

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-11.0195050000	-2.8763820000	-0.8624470000
C2	-11.0067290000	-3.5956220000	0.5249380000
C3	-12.4547080000	-4.0727150000	0.6796250000
C4	-12.8534970000	-4.5275830000	-0.7310890000
N5	-12.0244150000	-3.6614270000	-1.6096630000
C6	-12.0006490000	-3.8700230000	-2.9619390000
C7	-11.0326220000	-3.0384990000	-3.8352610000
N8	-11.6419800000	-2.6922260000	-5.1210690000
C9	-15.1602130000	-5.3828830000	-0.1795390000
C10	-14.3535450000	-4.4233890000	-1.0269170000
C11	-11.3090140000	-1.3804660000	-0.8163250000
C12	-11.7543960000	1.3949060000	-0.6734210000
C13	-12.8299960000	0.5132100000	-0.7760350000
C14	-12.6084610000	-0.8620650000	-0.8499090000
C15	-10.2359250000	-0.4833350000	-0.7245640000
C16	-10.4534100000	0.8916480000	-0.6511840000

C17	-10.4651990000	-2.7920200000	1.7044410000
O18	-12.7322700000	-4.7038570000	-3.5005690000
O19	-14.7089590000	-6.2764180000	0.5076110000
C20	-9.7576200000	-3.8575650000	-4.0935550000
H21	-12.5561940000	-5.5707590000	-0.8902100000
O22	-16.4830130000	-5.1320540000	-0.2938960000
C23	-17.3420980000	-6.0149530000	0.4475100000
H24	-10.0355770000	-3.0036800000	-1.3243020000
H25	-10.3751730000	-4.4848480000	0.3925620000
H26	-12.5677970000	-4.8785840000	1.4068050000
H27	-13.0895710000	-3.2374550000	1.0041460000
H28	-10.7695790000	-2.1044890000	-3.3312840000
H29	-12.1028390000	-3.5350370000	-5.4661940000
H30	-12.3949770000	-2.0245070000	-4.9623940000
H31	-14.5323470000	-4.6624110000	-2.0796290000
H32	-14.7299250000	-3.4078070000	-0.8609100000
H33	-11.9274640000	2.4658990000	-0.6229260000
H34	-13.8460810000	0.8962570000	-0.8066380000
H35	-13.4509550000	-1.5367260000	-0.9572780000
H36	-9.2178210000	-0.8662810000	-0.7194610000
H37	-9.6070260000	1.5695190000	-0.5867910000
H38	-10.4692300000	-3.4080330000	2.6095370000
H39	-9.4349100000	-2.4641000000	1.5326540000
H40	-11.0706170000	-1.9018370000	1.8975300000
H41	-10.0160590000	-4.7975480000	-4.5915890000
H42	-17.1232710000	-5.9574820000	1.5166540000
H43	-18.3577340000	-5.6751120000	0.2457400000
H44	-17.2102200000	-7.0480820000	0.1170970000
H45	-9.2268630000	-4.1038450000	-3.1673060000
H46	-9.0886300000	-3.2912080000	-4.7459990000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 247.466 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	43.034	1.481	-11.349	19.15555
rot.	0.889	2.981	34.682	0.889	-9.452	15.95250
vib.	12.247	77.894	82.302	12.247	-12.291	20.74486
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	14.025	83.855	160.018	14.617	-33.092	55.85291

Total internal energy, Utot (SCFE + ZPE + U): -997.086454 hartrees
Total enthalpy, Htot (Utot + pV): -997.085510 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -997.161540 hartrees

(S,S)-3d

Optimized geometry:

	angstroms		
atom	x	y	z
C1	0.0125730000	-0.6006550000	-0.1241930000
C2	-1.4756990000	-0.1967580000	-0.1021940000
C3	-2.0983780000	-1.1589470000	0.8986810000

C4	-1.0180620000	-1.3718830000	1.9693410000
N1	0.2311600000	-0.9930610000	1.2821260000
C5	1.4557000000	-0.9144460000	1.8620260000
C6	1.4426740000	-1.2725810000	3.3690970000
N2	1.2876400000	-2.7260670000	3.4220650000
C7	0.2354540000	-3.4941120000	3.1076510000
C8	-1.0357070000	-2.7880750000	2.6106780000
C9	0.4197120000	-1.6595130000	-1.1648800000
C10	1.2119450000	-3.5176910000	-3.0991480000
C11	0.8541580000	-3.9462060000	-1.8284010000
C12	0.4649570000	-3.0228650000	-0.8666780000
C13	0.7977110000	-1.2413610000	-2.4399440000
C14	1.1861680000	-2.1636610000	-3.4036110000
C15	-2.2033810000	-0.1458470000	-1.4600290000
O1	2.4852800000	-0.5695990000	1.2856440000
O2	0.2749760000	-4.7127340000	3.2157960000
C16	2.7600230000	-0.8854210000	4.0646930000
H1	-1.1823960000	-0.6274790000	2.7512080000
H2	0.6203450000	0.2819630000	-0.3402380000
H3	-1.5267510000	0.8075100000	0.3257870000
H4	-3.0297120000	-0.7801510000	1.3212780000
H5	-2.3327030000	-2.0963670000	0.3905000000
H6	0.6291230000	-0.7726890000	3.8938260000
H7	2.1006080000	-3.2637770000	3.6790240000
H8	-1.4188010000	-3.4907580000	1.8717770000
H9	-1.7593040000	-2.8162790000	3.4229970000
H10	1.5197890000	-4.2356930000	-3.8456080000
H11	0.8859210000	-4.9977870000	-1.5819550000
H12	0.2047300000	-3.3777920000	0.1175430000
H13	0.7920840000	-0.1902020000	-2.6886590000
H14	1.4755960000	-1.8260200000	-4.3881780000
H15	-3.2378590000	0.1778360000	-1.3416500000
H16	-1.7169620000	0.5528400000	-2.1413160000
H17	-2.2193530000	-1.1224440000	-1.9463810000
H18	2.9168920000	0.1930360000	4.0175300000
H19	2.7573650000	-1.1727780000	5.1159960000
H20	3.6217250000	-1.3550540000	3.5871140000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 213.596 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.702	1.481	-11.251	18.98867
rot.	0.889	2.981	33.667	0.889	-9.149	15.44191
vib.	9.463	64.570	60.637	9.463	-8.616	14.54253
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.240	70.532	137.007	11.833	-29.016	48.97311

Total internal energy, Utot (SCFE + ZPE + U): -881.402589 hartrees
Total enthalpy, Htot (Utot + pV): -881.401645 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -881.466741 hartrees

Optimized geometry:

angstroms			
atom	x	y	z
C1	-3.4309160000	0.5673350000	-1.0825000000
C2	-4.0270020000	-0.8297650000	-1.4396900000
C3	-4.2507980000	-0.7352600000	-2.9601430000
C4	-3.0391640000	0.0668350000	-3.4767170000
N1	-2.7165920000	0.9237500000	-2.3199530000
C5	-1.7706750000	1.9070620000	-2.3136550000
C6	-1.1258870000	2.1964830000	-3.6861590000
N2	-0.2708710000	1.0848960000	-4.1227980000
C7	-0.5173410000	-0.2521310000	-4.2752320000
C8	-1.8739370000	-0.8449390000	-3.8874570000
C9	-4.4476050000	1.6216790000	-0.6634570000
C10	-6.3639780000	3.4983620000	0.1846940000
C11	-6.1259650000	3.3020710000	-1.1752630000
C12	-5.1748710000	2.3720540000	-1.5947090000
C13	-4.6886850000	1.8349120000	0.6986740000
C14	-5.6391700000	2.7623450000	1.1219130000
C15	-5.2551050000	-1.2674330000	-0.6449360000
O1	-1.4696670000	2.5299370000	-1.3027600000
O2	0.3567440000	-0.9991000000	-4.7000510000
C16	-0.2852490000	3.4677330000	-3.6171640000
H1	-3.3300850000	0.6881160000	-4.3327300000
H2	-2.7025450000	0.4737150000	-0.2711960000
H3	-3.2260440000	-1.5590600000	-1.2598840000
H4	-4.3307080000	-1.7160660000	-3.4378730000
H5	-5.1787360000	-0.1902100000	-3.1659540000
H6	-1.9326070000	2.3515390000	-4.4174480000
H7	0.6780190000	1.3237290000	-4.3834330000
H8	-2.1799730000	-1.4542530000	-4.7449410000
H9	-1.6572740000	-1.5530310000	-3.0787270000
H10	-7.0999690000	4.2270350000	0.5117010000
H11	-6.6760830000	3.8796290000	-1.9129530000
H12	-4.9815370000	2.2474440000	-2.6561630000
H13	-4.1140010000	1.2792240000	1.4355930000
H14	-5.8049360000	2.9188140000	2.1839770000
H15	-5.0477830000	-1.2955210000	0.4295650000
H16	-6.0983280000	-0.5893060000	-0.8030440000
H17	-5.5638510000	-2.2729940000	-0.9492390000
H18	0.4922790000	3.3687370000	-2.8562690000
H19	0.1726220000	3.6731520000	-4.5897920000
H20	-0.9108950000	4.3174420000	-3.3392070000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 213.514 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.702	1.481	-11.251	18.98867
rot.	0.889	2.981	33.668	0.889	-9.149	15.44243
vib.	9.488	64.635	60.626	9.488	-8.588	14.49445
elec.	0.000	0.000	0.000	0.000	0.000	0.00000

total	11.265	70.597	136.997	11.858	-28.988	48.92555
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Total internal energy, Utot (SCFE + ZPE + U):	-881.403026 hartrees
Total enthalpy, Htot (Utot + pV):	-881.402082 hartrees
Total Gibbs free energy, Gtot (Htot - T*S):	-881.467173 hartrees

(R,S)-3d

Optimized geometry:

	angstroms		
atom	x	y	z
C1	3.2339910000	-0.2526760000	0.2301500000
C2	1.8146540000	-0.7452560000	0.6142760000
C3	1.9499280000	-2.2551750000	0.7530170000
C4	3.3857200000	-2.4431970000	1.2292360000
N1	4.0958430000	-1.4423390000	0.4123270000
C5	5.4460750000	-1.3227620000	0.4159420000
C6	6.1360990000	-2.6188150000	-0.0668240000
N2	6.2567800000	-3.4804130000	1.1112630000
C7	5.2751690000	-4.1344000000	1.7440100000
C8	3.8861850000	-3.9002540000	1.1526360000
C9	3.3807080000	0.4353320000	-1.1361120000
C10	3.6649580000	1.7169240000	-3.5995160000
C11	3.6726490000	0.3299710000	-3.5334970000
C12	3.5338520000	-0.3076730000	-2.3072030000
C13	3.3807860000	1.8262520000	-1.2119320000
C14	3.5204010000	2.4644980000	-2.4381710000
C15	0.6421470000	-0.3166880000	-0.2921130000
O1	6.0713670000	-0.2954870000	0.6713610000
O2	5.4642410000	-4.8526060000	2.7169730000
C16	7.5377340000	-2.3404990000	-0.6366430000
H1	3.4425700000	-2.1220130000	2.2735410000
H2	3.5461860000	0.4840140000	0.9753380000
H3	1.6073940000	-0.3435360000	1.6087980000
H4	1.2229660000	-2.6761040000	1.4489280000
H5	1.8068560000	-2.7420570000	-0.2139940000
H6	5.5379740000	-3.0934390000	-0.8460250000
H7	7.1628820000	-3.5745260000	1.5425320000
H8	3.8531240000	-4.2829290000	0.1341620000
H9	3.2039230000	-4.5338810000	1.7186820000
H10	3.7763750000	2.2143420000	-4.5523050000
H11	3.7890710000	-0.2532540000	-4.4353580000
H12	3.5401890000	-1.3867810000	-2.2633950000
H13	3.2776290000	2.4193570000	-0.3147650000
H14	3.5219630000	3.5438760000	-2.4865210000
H15	0.5687490000	0.7697480000	-0.3539000000
H16	0.7595180000	-0.6951970000	-1.3082770000
H17	-0.3094530000	-0.6878470000	0.0895510000
H18	8.0238880000	-3.2571690000	-0.9697140000
H19	7.4752250000	-1.6689840000	-1.4942450000
H20	8.1847610000	-1.8598510000	0.0989580000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 213.666 kcal/mol is not included in U, H, or G in the table below

T =	298.15 K					
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.702	1.481	-11.251	18.98867
rot.	0.889	2.981	33.662	0.889	-9.148	15.43929
vib.	9.368	64.380	59.586	9.368	-8.398	14.17347
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.146	70.342	135.951	11.738	-28.796	48.60143

Total internal energy, Utot (SCFE + ZPE + U): -881.401593 hartrees

Total enthalpy, Htot (Utot + pV): -881.400649 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -881.465243 hartrees

(S,R)-3d

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-3.6293960000	0.0958470000	-0.2411470000
C2	-3.3955510000	1.4903510000	0.4171560000
C3	-2.6991090000	2.3386430000	-0.6520350000
C4	-2.0861780000	1.3095580000	-1.5893590000
N1	-3.1535630000	0.2919480000	-1.6274220000
C5	-3.6100660000	-0.4946670000	-2.6440230000
C6	-3.2742370000	-0.0063650000	-4.0770340000
N2	-1.8230310000	-0.0900120000	-4.2524600000
C7	-0.9116640000	0.7713040000	-3.7918110000
C8	-1.5050410000	1.8572930000	-2.9027900000
C9	-3.0572810000	-1.1307720000	0.4952050000
C10	-2.1081860000	-3.3791340000	1.8602450000
C11	-1.3788690000	-2.8462270000	0.8063630000
C12	-1.8521730000	-1.7323090000	0.1246740000
C13	-3.7883980000	-1.6868770000	1.5438970000
C14	-3.3154080000	-2.8004180000	2.2267080000
C15	-2.6259020000	1.4962430000	1.7571630000
O1	-4.3298150000	-1.4774400000	-2.4756120000
O2	0.2858950000	0.6866280000	-4.0285720000
C16	-3.9483330000	-0.8725330000	-5.1575140000
H1	-1.2428410000	0.8500470000	-1.0667230000
H2	-4.7062540000	-0.0857570000	-0.2943260000
H3	-4.3736320000	1.9329710000	0.6161850000
H4	-3.4304640000	2.9468330000	-1.1881870000
H5	-1.9485300000	3.0180920000	-0.2451120000
H6	-3.6465650000	1.0099120000	-4.2013550000
H7	-1.4455600000	-0.8673770000	-4.7715820000
H8	-0.6926040000	2.5436640000	-2.6659110000
H9	-2.2226210000	2.4583660000	-3.4567480000
H10	-1.7417740000	-4.2485400000	2.3869300000
H11	-0.4456290000	-3.3023090000	0.5090890000
H12	-1.2749250000	-1.3465590000	-0.7017130000
H13	-4.7331940000	-1.2518620000	1.8355850000
H14	-3.8907830000	-3.2201480000	3.0391040000
H15	-1.6311400000	1.0612780000	1.6492180000
H16	-2.5030390000	2.5094130000	2.1411820000
H17	-3.1526180000	0.9252290000	2.5222400000
H18	-3.7013870000	-0.5251120000	-6.1606450000
H19	-3.6510130000	-1.9194320000	-5.0778630000
H20	-5.0342360000	-0.8395050000	-5.0570940000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 213.769 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.702	1.481	-11.251	18.98867
rot.	0.889	2.981	33.636	0.889	-9.140	15.42644
vib.	9.326	64.184	60.034	9.326	-8.573	14.46930
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.104	70.145	136.373	11.696	-28.963	48.88441

Total internal energy, Utot (SCFE + ZPE + U): -881.400139 hartrees
Total enthalpy, Htot (Utot + pV): -881.399195 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -881.463991 hartrees

(5aS,11aS)-3g

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-5.4975170000	-2.1764050000	2.1789880000
C2	-5.1567710000	-3.3026910000	1.1815000000
C3	-4.6371080000	-4.4261650000	2.0643050000
C4	-5.4545500000	-4.3303160000	3.3603080000
N1	-5.9670020000	-2.9505850000	3.3469910000
C5	-6.8585840000	-2.4361530000	4.2266640000
C6	-7.3183730000	-3.4703750000	5.2880220000
N2	-6.3020810000	-3.8860870000	6.2711220000
C7	-5.0622390000	-4.3855890000	6.0568020000
C8	-4.6401570000	-4.7174080000	4.6168190000
C9	-4.3866980000	-1.1511360000	2.4747710000
C10	-2.4240110000	0.7823310000	2.9627350000
C11	-2.5915800000	-0.2767760000	3.8438340000
C12	-3.5697650000	-1.2333480000	3.6043980000
C13	-4.2211920000	-0.0699400000	1.6099130000
C14	-3.2426900000	0.8873560000	1.8469490000
C15	-4.2214280000	-2.9446230000	0.0099270000
O1	-7.3058780000	-1.2909910000	4.1659340000
O2	-4.2741480000	-4.6225170000	6.9690640000
C16	-8.4262170000	-2.8266250000	6.1574670000
C17	-6.8066250000	-3.7005010000	7.6344430000
C18	-8.3146280000	-3.5461360000	7.4885660000
H1	-6.3097910000	-5.0024660000	3.2630240000
H2	-6.3355190000	-1.5955650000	1.7844600000
H3	-6.1014700000	-3.6359510000	0.7446580000
H4	-4.7269000000	-5.4053960000	1.5924800000
H5	-3.5759330000	-4.2621240000	2.2628080000
H6	-7.7279570000	-4.3597220000	4.8087840000
H7	-3.6490720000	-4.2730010000	4.5363410000
H8	-4.4576870000	-5.7908890000	4.5958640000
H9	-1.6662410000	1.5290440000	3.1518950000
H10	-1.9678240000	-0.3539700000	4.7227990000
H11	-3.6935190000	-2.0343130000	4.3148780000
H12	-4.8572630000	0.0315690000	0.7427850000
H13	-3.1238790000	1.7179650000	1.1663760000

H14	-4.6390100000	-2.1407720000	-0.5968170000
H15	-3.2412270000	-2.6185870000	0.3612250000
H16	-4.0651730000	-3.8017490000	-0.6457700000
H17	-9.4159540000	-2.9116040000	5.7080330000
H18	-8.2425240000	-1.7647130000	6.3373650000
H19	-6.3604900000	-2.7943120000	8.0477340000
H20	-6.5540560000	-4.5306820000	8.2969020000
H21	-8.7815970000	-4.5299380000	7.4202080000
H22	-8.7758950000	-3.0079780000	8.3177050000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 236.480 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.975	1.481	-11.332	19.12561
rot.	0.889	2.981	34.206	0.889	-9.310	15.71330
vib.	9.995	68.853	64.131	9.995	-9.126	15.40211
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.772	74.815	141.311	12.365	-29.767	50.24102

Total internal energy, Utot (SCFE + ZPE + U): -958.785547 hartrees
Total enthalpy, Htot (Utot + pV): -958.784603 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -958.851744 hartrees

(5aR,11aR)-3g

Optimized geometry:

	angstroms		
atom	x	y	z
C1	-0.3954690000	-1.5321770000	0.5883060000
C2	0.4305950000	-1.9418390000	1.8471640000
C3	-0.2443070000	-1.1496090000	2.9823170000
C4	-1.7472420000	-1.1828710000	2.6351850000
N1	-1.7251480000	-1.2668370000	1.1625890000
C5	-2.8350020000	-1.2531590000	0.3715740000
C6	-4.1467520000	-0.9157250000	1.1091270000
N2	-4.6152650000	-2.0029730000	1.9998950000
C7	-3.9381570000	-2.6840360000	2.9700460000
C8	-2.4687120000	-2.3728700000	3.2827340000
C9	0.1544800000	-0.3473660000	-0.1957470000
C10	1.2664790000	1.7903180000	-1.6475150000
C11	0.4624760000	2.0386240000	-0.5352780000
C12	-0.0889170000	0.9780510000	0.1833490000
C13	0.9551800000	-0.5831810000	-1.3190930000
C14	1.5089020000	0.4739620000	-2.0395010000
C15	1.9436410000	-1.7541160000	1.7563250000
O1	-2.7901500000	-1.4586830000	-0.8362090000
O2	-4.4874960000	-3.5749140000	3.6150520000
C16	-5.3210970000	-0.7156250000	0.1396650000
C17	-6.0337980000	-2.3351640000	1.7650870000
C18	-6.5501950000	-1.1449950000	0.9517120000
H1	-2.2308790000	-0.2499650000	2.9502440000

H2	-0.4755490000	-2.3749870000	-0.1049380000
H3	0.2282050000	-3.0083320000	2.0122440000
H4	-0.0393270000	-1.5703460000	3.9710770000
H5	0.1195710000	-0.1159740000	2.9813040000
H6	-3.9853950000	0.0006430000	1.6955730000
H7	-2.4316230000	-2.2613840000	4.3722120000
H8	-1.9227510000	-3.2973500000	3.0593300000
H9	1.6910390000	2.6162470000	-2.2108410000
H10	0.2581340000	3.0608600000	-0.2289720000
H11	-0.7345190000	1.1858240000	1.0316190000
H12	1.1328710000	-1.6059450000	-1.6423820000
H13	2.1207140000	0.2694220000	-2.9135140000
H14	2.2102310000	-0.7027190000	1.6164590000
H15	2.4245990000	-2.1092150000	2.6738020000
H16	2.3679110000	-2.3187230000	0.9197820000
H17	-5.1655630000	-1.3641150000	-0.7266850000
H18	-5.3704820000	0.3139040000	-0.2235270000
H19	-6.5382720000	-2.4804890000	2.7223180000
H20	-6.1113000000	-3.2773580000	1.2078360000
H21	-7.4036140000	-1.4104960000	0.3223400000
H22	-6.8696350000	-0.3401630000	1.6242360000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 236.466 kcal/mol
is not included in U, H, or G in the table below

T = 298.15						
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.975	1.481	-11.332	19.12561
rot.	0.889	2.981	34.238	0.889	-9.319	15.72928
vib.	10.005	68.837	64.115	10.005	-9.111	15.37837
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.782	74.798	141.328	12.375	-29.762	50.23326

Total internal energy, Utot (SCFE + ZPE + U): -958.786190 hartrees
Total enthalpy, Htot (Utot + pV): -958.785245 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -958.852395 hartrees

(5aR,11aS)-3g

Optimized geometry:

		angstroms		
atom	x	y	z	
C1	-0.4822670000	-6.2889290000	-0.4649340000	
C2	-1.1348910000	-6.6396450000	0.8950660000	
C3	-2.3688970000	-5.7549990000	0.9664880000	
C4	-2.8195590000	-5.6510460000	-0.4870280000	
N1	-1.5271550000	-5.5266570000	-1.1888850000	
C5	-1.4095360000	-5.3002400000	-2.5217270000	
C6	-2.2286060000	-4.0660240000	-2.9762950000	
N2	-3.6678540000	-4.3206680000	-3.1208180000	
C7	-4.5234160000	-4.5489440000	-2.1049420000	
C8	-3.8653240000	-4.5437100000	-0.7241390000	
C9	0.8840500000	-5.5875010000	-0.4101720000	

C10	3.3809130000	-4.3418460000	-0.3343450000
C11	2.2249030000	-3.5905710000	-0.1690860000
C12	0.9822810000	-4.2101340000	-0.2095360000
C13	2.0492510000	-6.3314770000	-0.5812920000
C14	3.2923140000	-5.7120640000	-0.5418490000
C15	-0.2456340000	-6.5601940000	2.1530410000
O1	-0.6749060000	-5.9376670000	-3.2766670000
O2	-5.7282950000	-4.7436050000	-2.2392910000
C16	-1.7952420000	-3.6556350000	-4.4033770000
C17	-4.0868540000	-4.3004970000	-4.5214760000
C18	-2.7902480000	-4.3507190000	-5.3240900000
H1	-3.2661500000	-6.6087750000	-0.7707280000
H2	-0.3241830000	-7.2227800000	-1.0112570000
H3	-1.4787200000	-7.6737630000	0.8168080000
H4	-3.1431190000	-6.1724130000	1.6118720000
H5	-2.1080370000	-4.7679450000	1.3543540000
H6	-2.0266290000	-3.2396380000	-2.2936640000
H7	-3.4610050000	-3.5559880000	-0.5079330000
H8	-4.6770860000	-4.6785490000	-0.0089050000
H9	4.3480200000	-3.8606310000	-0.3067410000
H10	2.2916730000	-2.5238740000	-0.0117350000
H11	0.0876410000	-3.6192110000	-0.0800040000
H12	1.9936950000	-7.3968840000	-0.7519610000
H13	4.1902900000	-6.2971560000	-0.6784500000
H14	0.6226320000	-7.2140660000	2.0633590000
H15	0.1231430000	-5.5478190000	2.3230530000
H16	-0.7939850000	-6.8642430000	3.0451360000
H17	-0.7576440000	-3.8876810000	-4.6525620000
H18	-1.9021590000	-2.5754090000	-4.5058820000
H19	-4.6256410000	-3.3704710000	-4.7086880000
H20	-4.7498070000	-5.1308890000	-4.7711510000
H21	-2.4870690000	-5.3907250000	-5.4613650000
H22	-2.8714870000	-3.8936090000	-6.3107640000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 236.540 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.975	1.481	-11.332	19.12561
rot.	0.889	2.981	34.188	0.889	-9.304	15.70399
vib.	9.902	68.684	63.022	9.902	-8.888	15.00111
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.680	74.646	140.185	12.272	-29.524	49.83071

Total internal energy, Utot (SCFE + ZPE + U): -958.785102 hartrees
Total enthalpy, Htot (Utot + pV): -958.784158 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -958.850765 hartrees

(5aS,11aR)-3g

Optimized geometry:

angstroms

atom	x	y	z
C1	-0.9316030000	5.3668240000	4.5221420000
C2	-1.3013290000	6.3124260000	5.6983480000
C3	-2.4900010000	7.1133260000	5.1796050000
C4	-2.2618220000	7.1752260000	3.6737080000
N1	-1.7935070000	5.8071720000	3.3970320000
C5	-2.0380290000	4.9666270000	2.3503120000
C6	-2.9583150000	5.4814270000	1.2031990000
N2	-2.8595180000	6.8729830000	0.7218750000
C7	-3.1458890000	7.9788910000	1.4332620000
C8	-3.4706100000	7.6937920000	2.8909710000
C9	0.5653080000	5.2283140000	4.1952580000
C10	3.2818210000	4.9138580000	3.6261390000
C11	2.5310790000	5.8540150000	2.9333110000
C12	1.1793170000	6.0081720000	3.2134890000
C13	1.3259190000	4.2803250000	4.8766090000
C14	2.6779420000	4.1256570000	4.5965960000
C15	-0.1699310000	7.2308470000	6.2156610000
O1	-1.6060920000	3.8132430000	2.3157060000
O2	-3.1441200000	9.1229860000	0.9869010000
C16	-2.6019740000	4.6567900000	-0.0606490000
C17	-2.5796970000	6.9284020000	-0.7123490000
C18	-2.9674970000	5.5520090000	-1.2324390000
H1	-1.4262190000	7.8553350000	3.4846280000
H2	-1.2633620000	4.3597160000	4.7891170000
H3	-1.6276040000	5.7036740000	6.5438390000
H4	-3.4207220000	6.5854570000	5.3987280000
H5	-2.5694900000	8.1054120000	5.6270070000
H6	-3.9960490000	5.2831440000	1.4729650000
H7	-3.7885930000	8.6428530000	3.3233830000
H8	-4.3340720000	7.0360880000	2.9799120000
H9	4.3324480000	4.7910730000	3.4055220000
H10	2.9963980000	6.4634310000	2.1722200000
H11	0.6076220000	6.7401750000	2.6626500000
H12	0.8669660000	3.6557900000	5.6291280000
H13	3.2582910000	3.3873670000	5.1307580000
H14	0.2193970000	7.8738190000	5.4251850000
H15	-0.5180660000	7.8747580000	7.0238690000
H16	0.6664070000	6.6497890000	6.6062090000
H17	-3.1118040000	3.6928650000	-0.0873750000
H18	-1.5292190000	4.4517720000	-0.1098580000
H19	-1.5134620000	7.1143220000	-0.8497600000
H20	-3.1286250000	7.7186840000	-1.2282840000
H21	-4.0443340000	5.5143130000	-1.4050510000
H22	-2.4656630000	5.2829370000	-2.1627660000

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 236.568 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

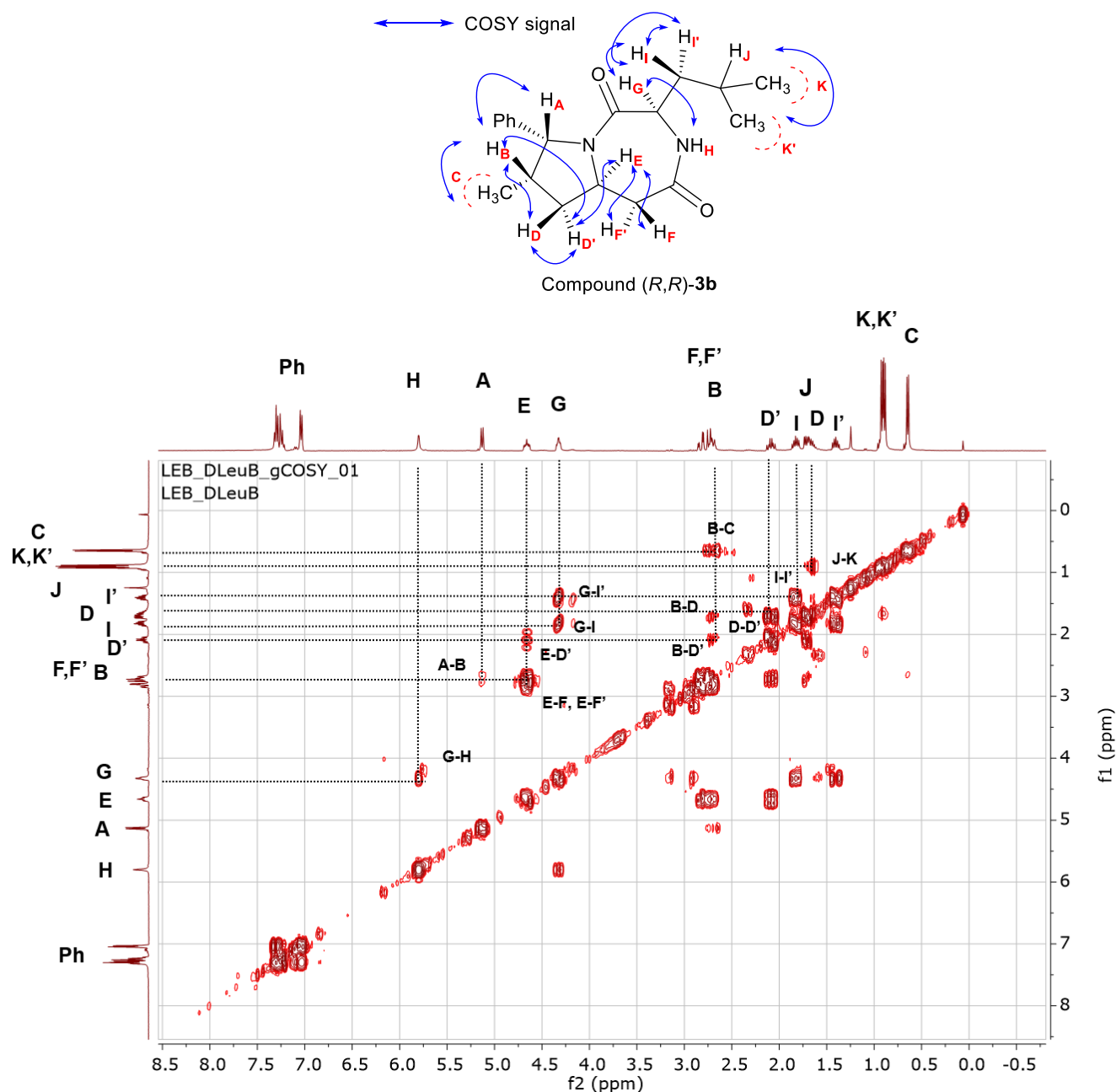
	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	42.975	1.481	-11.332	19.12561
rot.	0.889	2.981	34.174	0.889	-9.300	15.69679
vib.	9.921	68.603	64.163	9.921	-9.210	15.54399

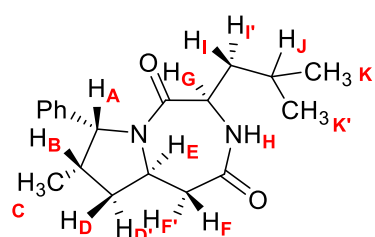
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	11.698	74.565	141.311	12.291	-29.841	50.36639

Total internal energy, Utot (SCFE + ZPE + U): -958.783394 hartrees
Total enthalpy, Htot (Utot + pV): -958.782449 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -958.849591 hartrees

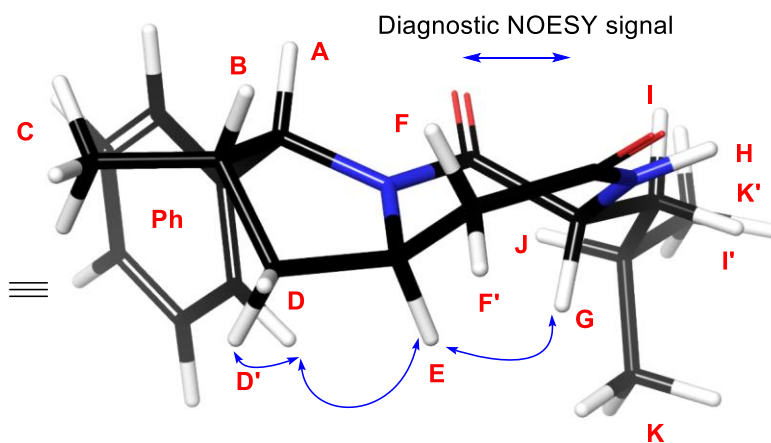
4. Proton and stereochemical assignment for (*R,R*)-**3b**

Proton and stereochemical assignments for pyrrolodiazepinone (*R,R*)-**3b** (NaOMe/DMF major product) was made by diagnostic NOE signals between H_E and H_G as well as between H_E and the phenyl ring *ortho* protons, indicating that all protons sit on the same face of the bicyclic system. The other isolated diastereomer of **3b**, which is the only other diastereomer expected to exhibit the observed diagnostic H_E/H_G NOE ((*S,S*)-**3b**) was separately assigned as the DBU/acetonitrile major product based on ¹H NMR and reactivity correlation to (*S,S*)-**3a**, the structure of which was confirmed using X-ray crystallography.



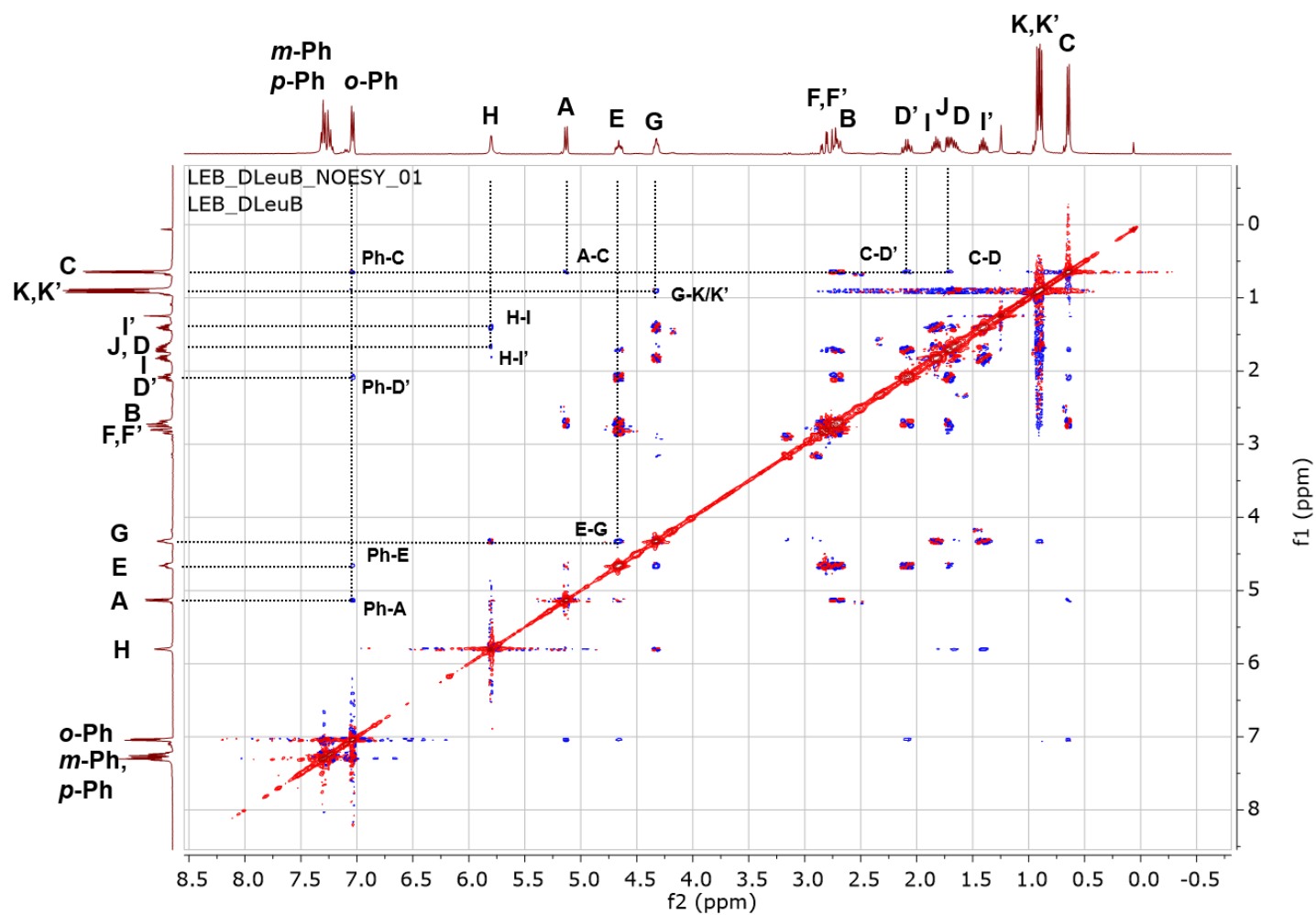


Compound (R,R)-3b



DFT lowest energy conformer (B3LYP-6-31g**)

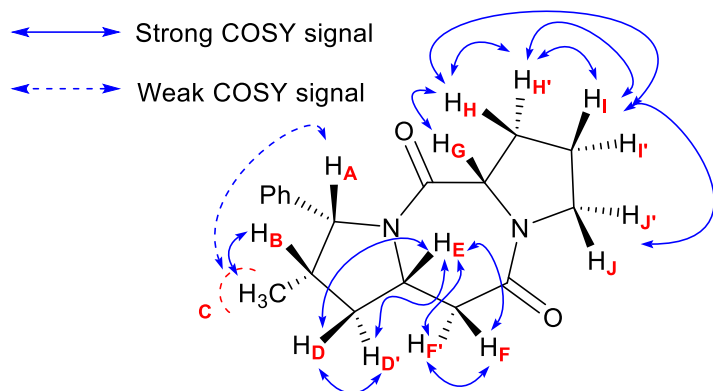
Key NOESY signals for stereochemical assignment:
(Aryl - D') + (Aryl - E) + (E - G) (bottom face)



5. Proton and stereochemical assignment for isolated diastereomers of 3g

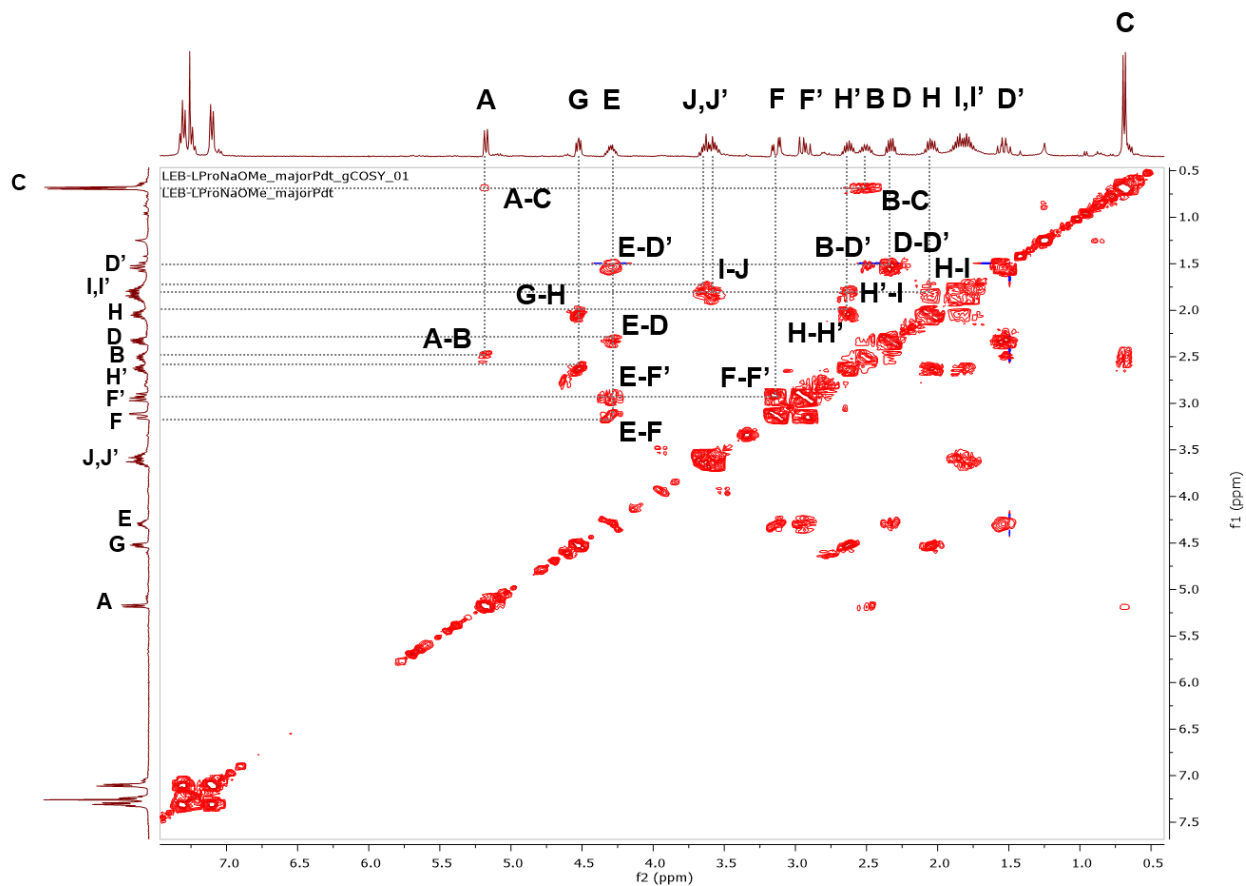
Proton and stereochemical assignments for pyrrolodiazepiniones (*S,S*)-**3g**, (*R,R*)-**3g** and (*R,S*)-**3g** were made using $^3J_{\text{H-H}}$ values, COSY and NOESY relationships between protons. Assignments were further supported by DFT-predicted ^1H NMR spectra

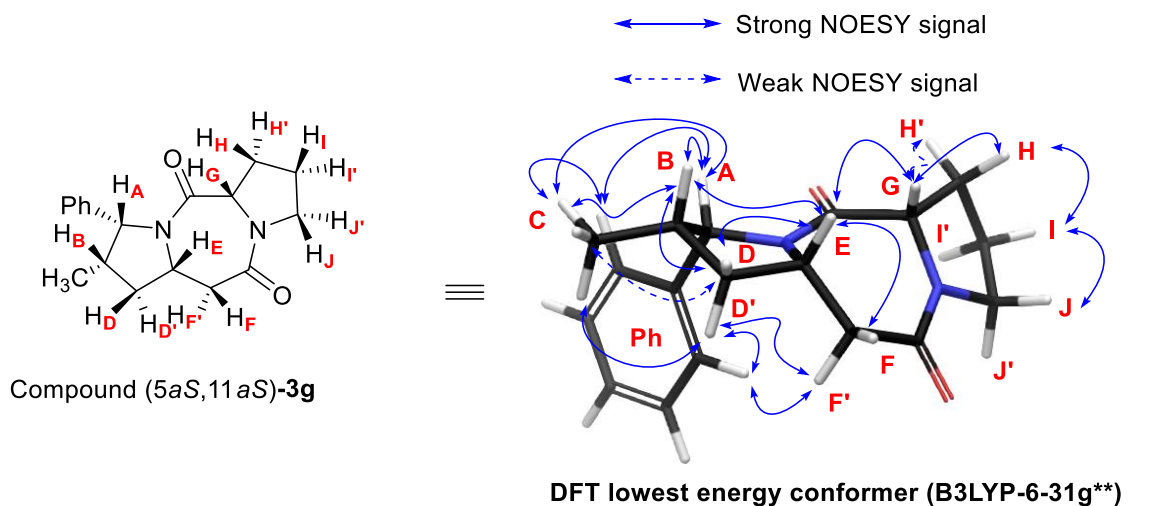
a. Proton and stereochemical assignments for Compound (*5aS,11aS*)-**3g** (COSY + NOESY)



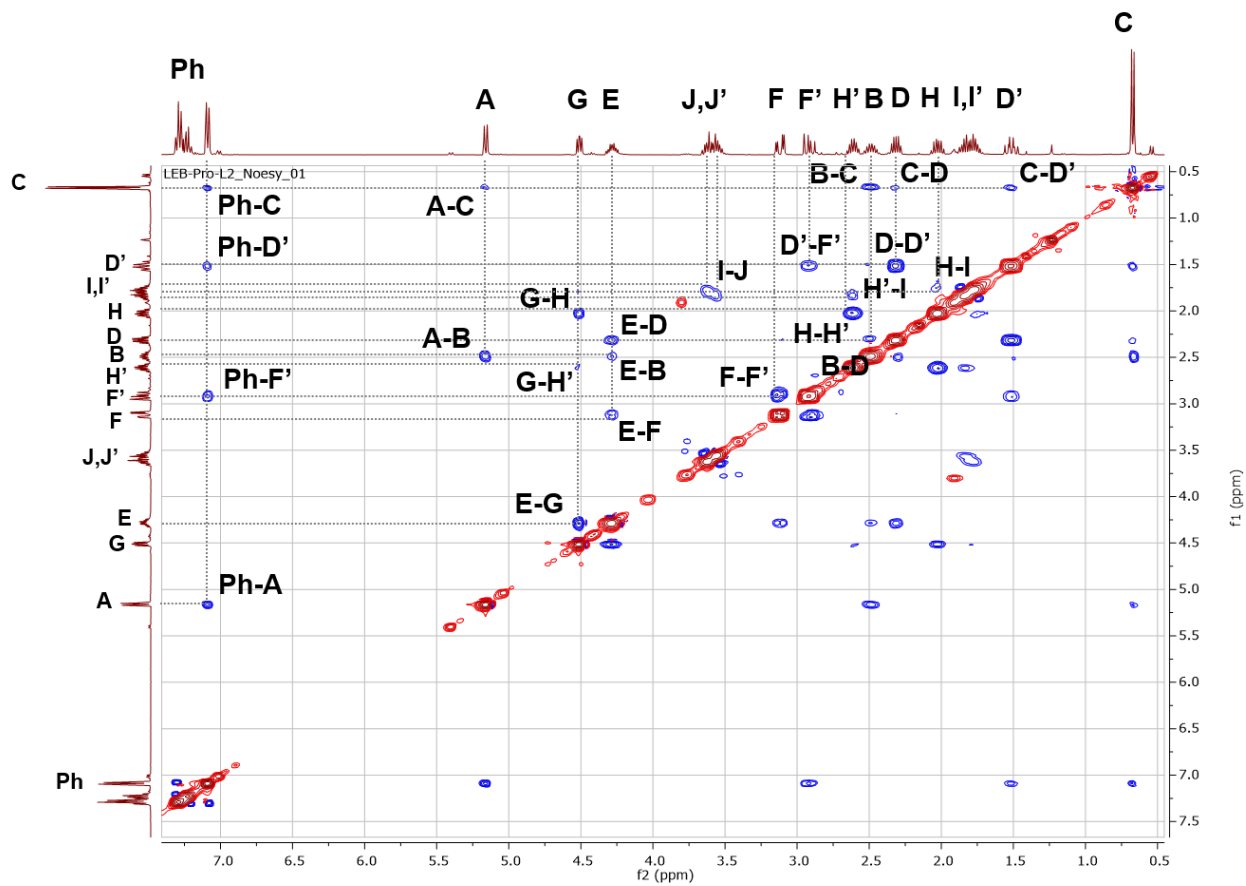
$J_{\text{A-B}}$	8.2 Hz (<i>syn</i>)
$J_{\text{B-D}}$	6.3 Hz (<i>syn</i>)
$J_{\text{B-D'}}$	12.5 Hz (<i>anti</i>)
$J_{\text{D-E}}$	6.3 Hz (<i>syn</i>)
$J_{\text{D'-E}}$	9.8 Hz (<i>anti</i>)
$J_{\text{E-F}}$	4.7 Hz (<i>syn</i>)
$J_{\text{E-F'}}$	11.5 Hz (<i>anti</i>)

Compound (*5aS,11aS*)-**3g**





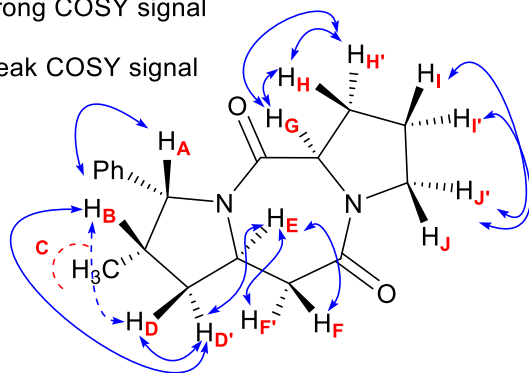
Key NOESY signals for stereochemical assignment:
 (Aryl - D') + (Aryl - F') + (D' - F') (*bottom face*)
 (E - D) + (E - F) + (E - B) + (B - D) + (E - G) (*top face*)



b. Proton assignments for Compound (5a*R*,11a*R*)-3g (COSY + NOESY)

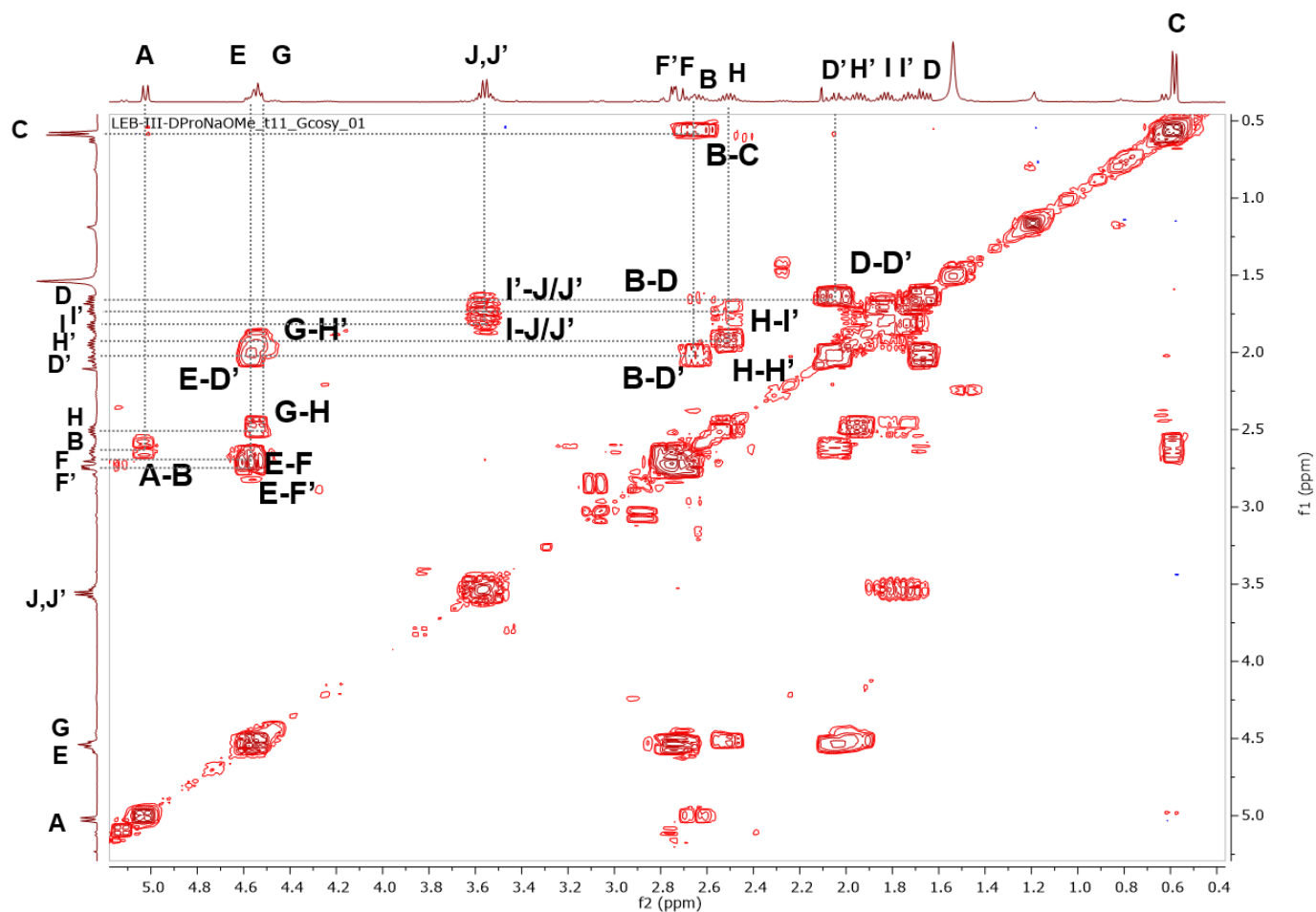
↔ Strong COSY signal

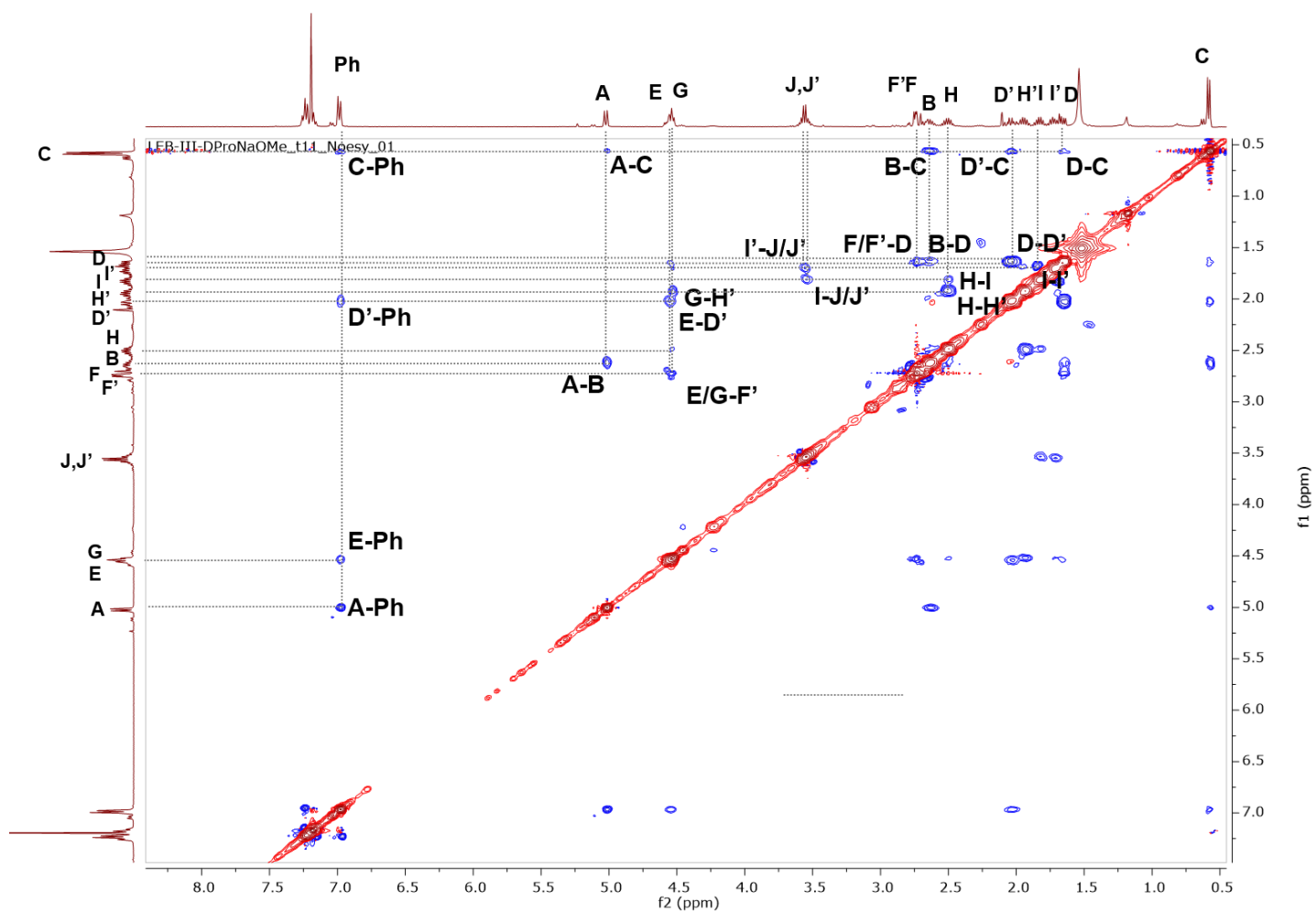
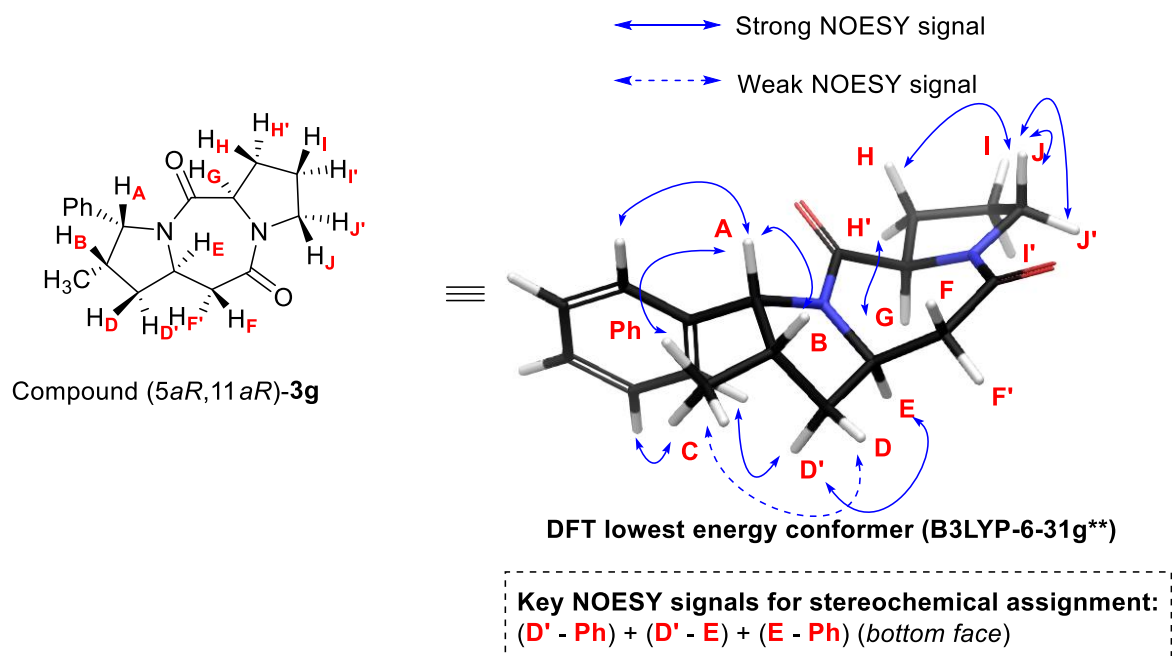
↔ Weak COSY signal



J_{A-B}	7.8 Hz (<i>syn</i>)
J_{B-D}	N/A (<i>syn</i>)
$J_{B-D'}$	13.0 Hz (<i>anti</i>)
J_{D-E}	N/A (<i>anti</i>) ¹
$J_{D'-E}$	8.0 Hz (<i>syn</i>)
J_{E-F}	12.5 Hz (<i>anti</i>)
$J_{E-F'}$	4.0 Hz (<i>syn</i>)
1.91.3° torsion in DFT-optimized structure	

Compound (5a*R*,11a*R*)-3g

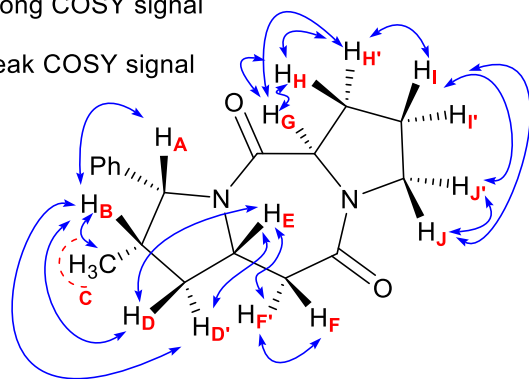




c. Proton assignments for Compound (5*aR*,11*aS*)-3g (COSY + NOESY)

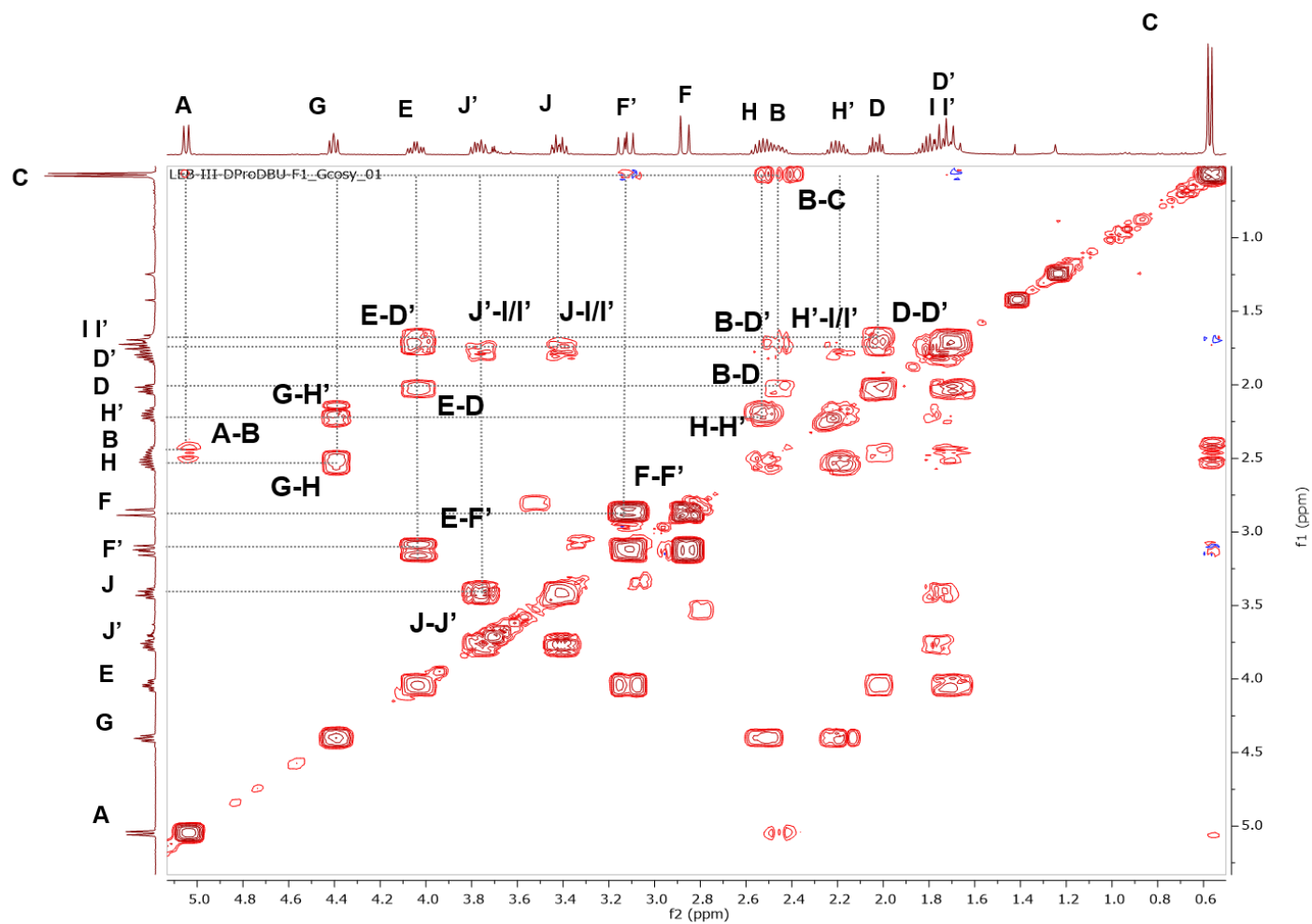
↔ Strong COSY signal

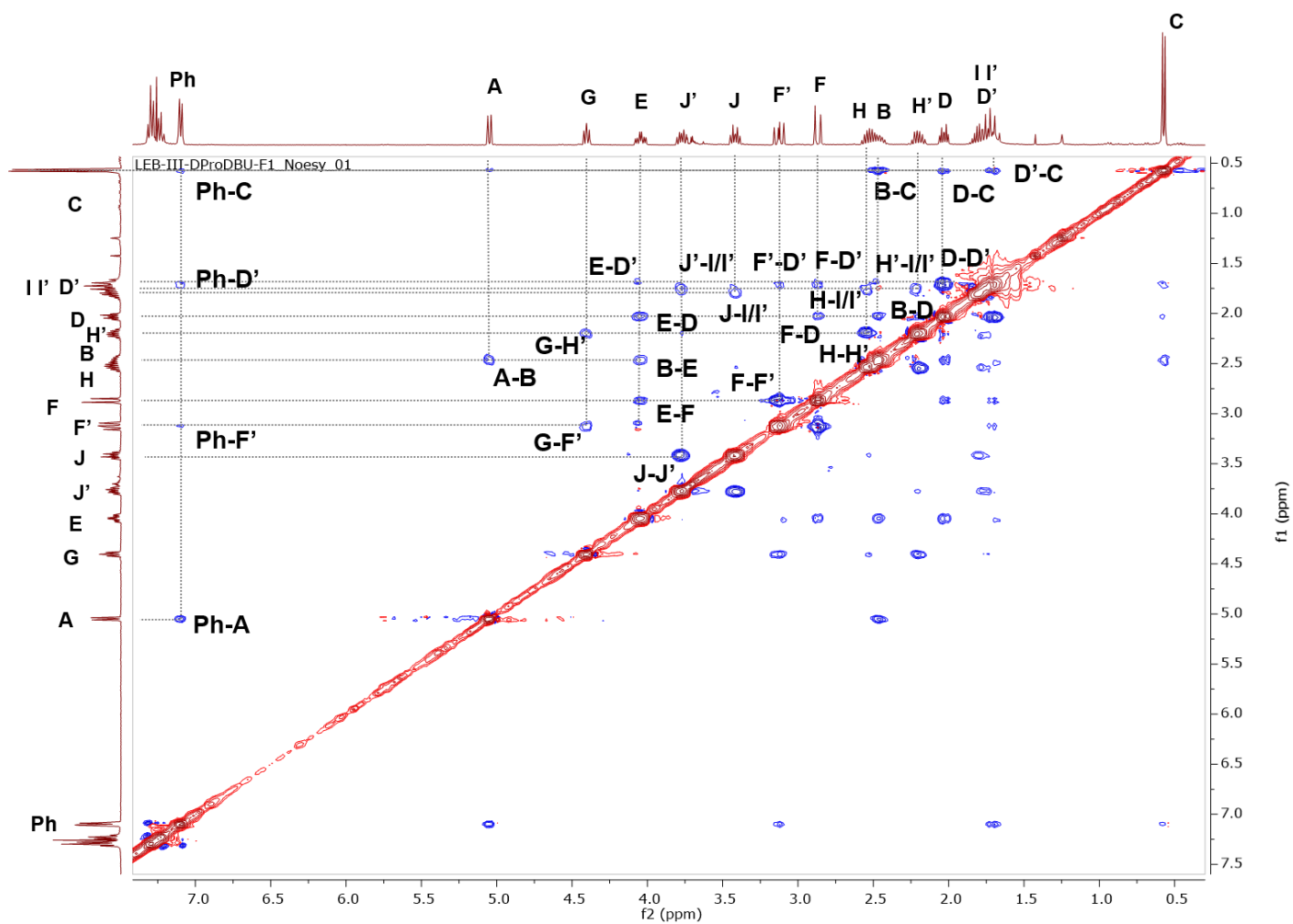
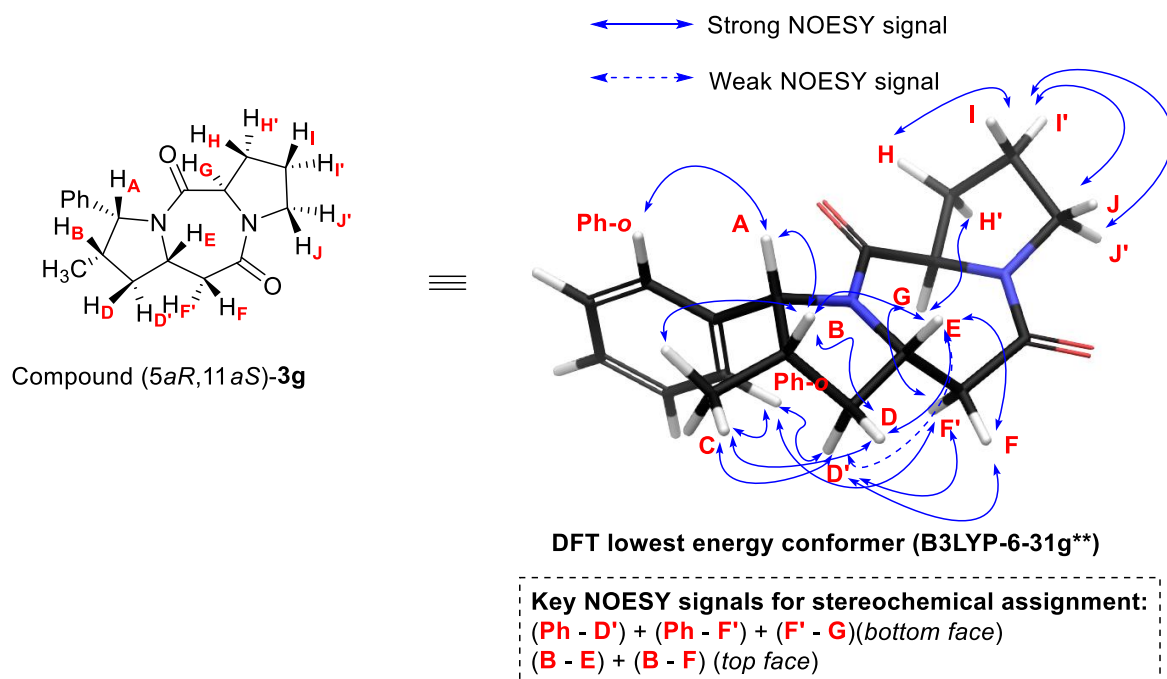
↔ Weak COSY signal



Compound (5*aR*,11*aS*)-3g

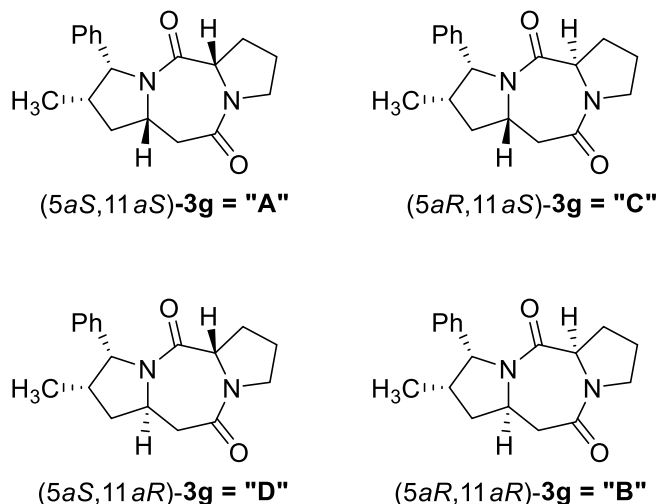
J_{A-B}	9.0 Hz (<i>syn</i>)
J_{B-D}	N/A (<i>syn</i>)
$J_{B-D'}$	13.7 Hz (<i>anti</i>)
J_{D-E}	5.3 Hz (<i>syn</i>)
$J_{D'-E}$	11.3 Hz (<i>anti</i>)
J_{E-F}	N/A (<i>syn</i>)
$J_{E-F'}$	11.1 Hz (<i>anti</i>)





d. DFT NMR Predictions

Based on the proposed epimerization pathways, we envision four possible diastereomers for the proline-derived tetrahydropyrrolodiazepinones, named diastereomers **A–D** for the purpose of this analysis:



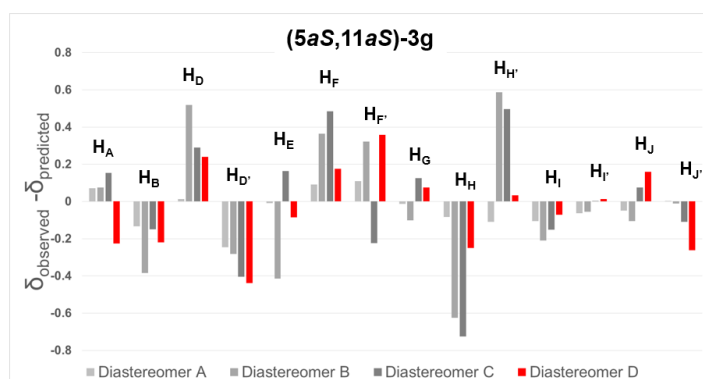
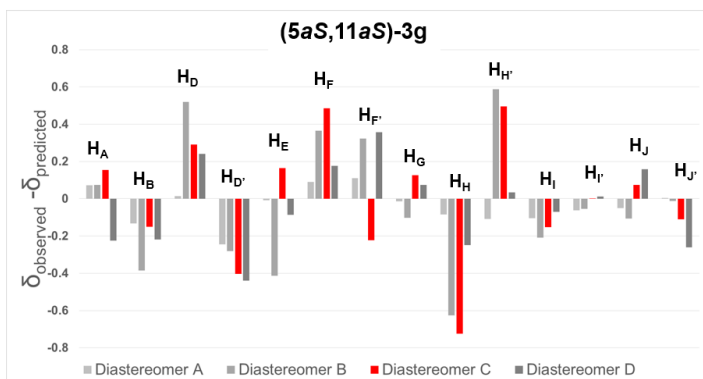
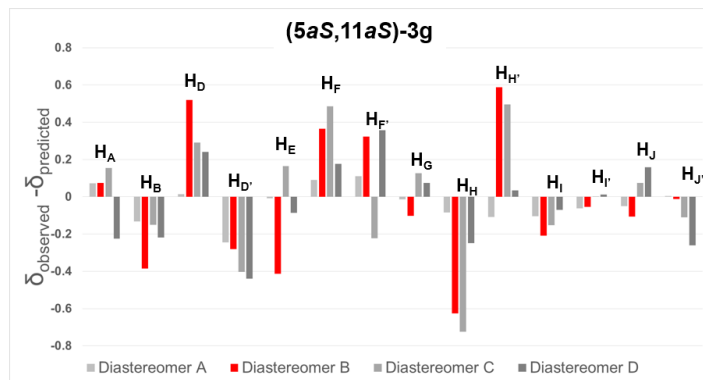
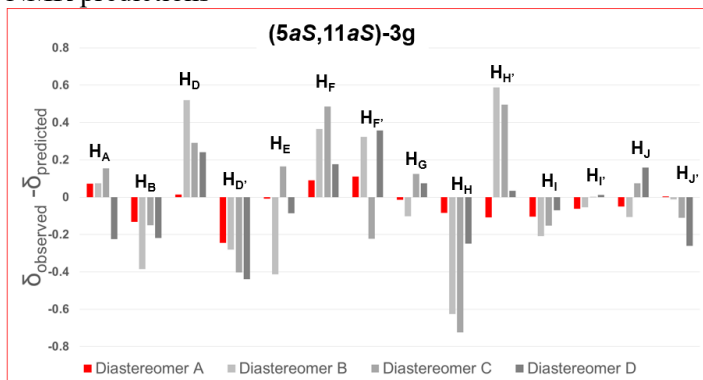
To further support the assignments (made based on *J*-values, COSY and NOESY correlations) for the proline-derived pyrrolodiazepinone diastereomers **A–D**, each diastereomer's cohort of unique DFT-optimized conformers from above were re-subjected to single-point energy DFT calculations (PBE0-6-31g**, PBF solvation in chloroform) with NMR prediction. Predicted chemical shifts for each diastereomer were determined by calculating a Boltzmann-weighted average of the predicted shifts for each unique conformer (Table S4).^{S4}

Table S4. Predicted and observed chemical shifts for pyrrolodiazepinone ring system protons

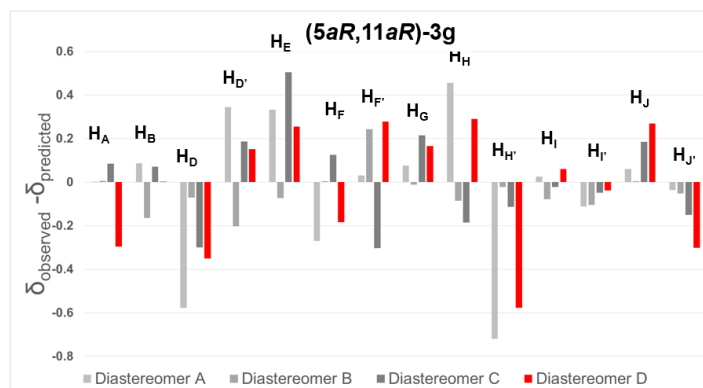
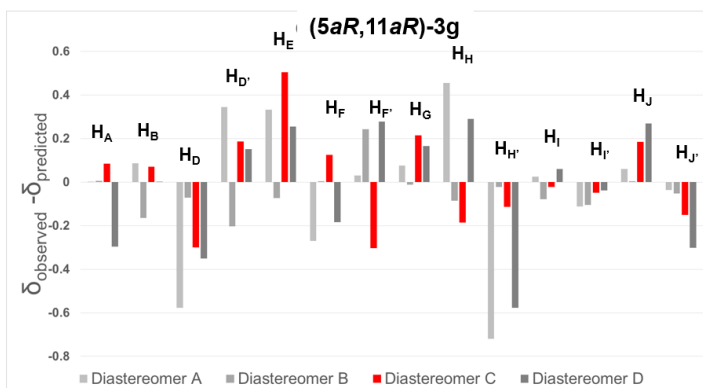
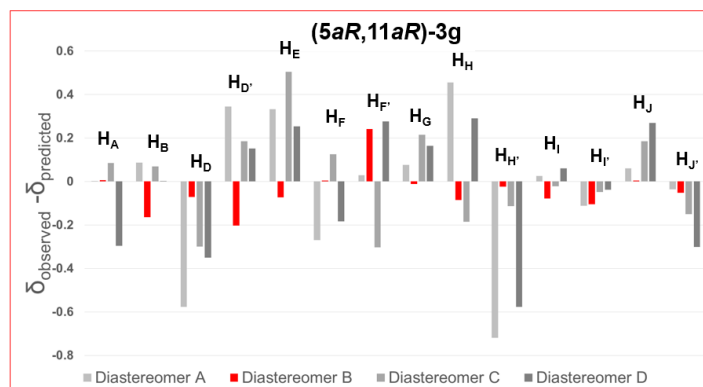
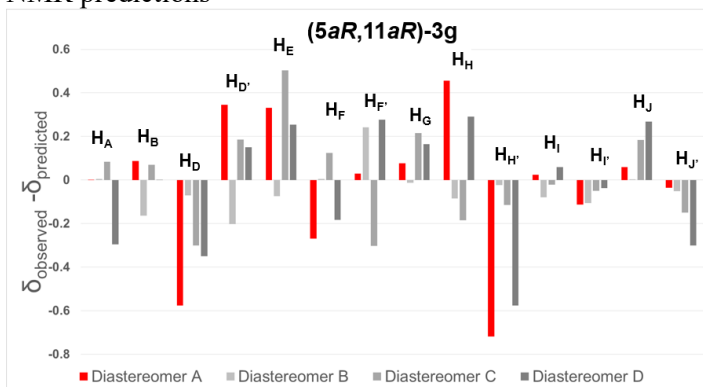
	A <i>predicted</i>	B <i>predicted</i>	C <i>predicted</i>	D <i>predicted</i>	(5aS,11aS)-3g <i>observed</i>	(5aR,11aR)-3g <i>observed</i>	(5aR,11aS)-3g <i>observed</i>
H _A	5.10	5.09	5.01	5.40	5.17	5.10	5.06
H _B	2.63	2.88	2.65	2.72	2.50	2.72	2.44
H _D	2.32	1.81	2.04	2.09	2.33	1.74	2.04
H _{D'}	1.78	2.32	1.93	1.97	1.53	2.12	1.80
H _E	4.31	4.71	4.14	4.39	4.30	4.64	4.06
H _F	3.04	2.77	2.64	2.95	3.13	2.77	2.88
H _{F'}	2.82	2.60	3.15	2.57	2.93	2.85	3.14
H _G	4.53	4.62	4.39	4.45	4.52	4.61	4.42
H _H	2.12	2.67	2.77	2.29	2.04	2.58	2.55
H _{H'}	2.74	2.04	2.13	2.59	2.63	2.02	2.21
H _I	1.88	1.98	1.92	1.84	1.77	1.90	1.80
H _{I'}	1.91	1.91	1.85	1.84	1.77	1.80	1.80
H _J	3.61	3.67	3.49	3.40	3.56	3.67	3.43
H _{J'}	3.64	3.65	3.75	3.90	3.64	3.60	3.79

S4. Willoughby, P. H.; Jansma, M. J.; Hoye, T. R. A Guide to Small-Molecule Structure Assignment Through Computation of (¹H and ¹³C) NMR Chemical Shifts. *Nat. Protoc.*, **2014**, 9, 643-660.

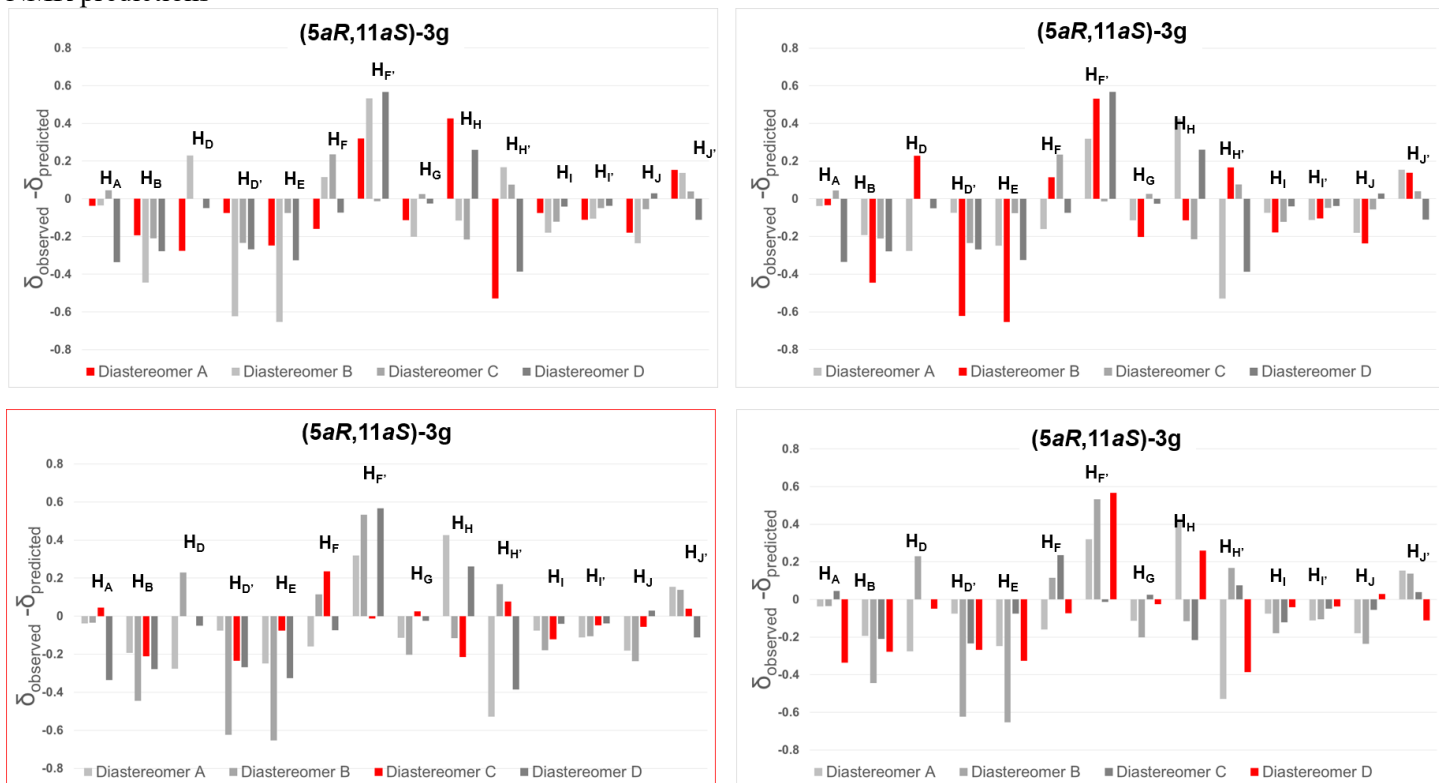
(5*aS*,11*aS*)-**3g**: Assigned as Diastereomer A (5*aS*,11*aS*) based on observed NOESY signals, further supported by DFT ¹H NMR predictions



(5*aR*,11*aR*)-**3g**: Assigned as Diastereomer B (5*aR*,11*aR*) based on observed NOESY signal, further supported by DFT ¹H NMR predictions



(5*aR*,11*aS*)-**3g**: Assigned as Diastereomer C (5*aR*,11*aS*) based on observed NOESY signal, further supported by DFT ¹H NMR predictions



6. X-ray crystallographic data for (*S,S*)-**3a**

X-ray quality crystals of compound (*S,S*)-**3a** were grown by dissolving the compound in dichloromethane, gently layering an equal volume of isooctane. Crystals formed at the interface upon slow evaporation of the dichloromethane. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC# 1866531). Copies of the data can be obtained free of charge through application to the CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)-1223-336-033; email: deposit@ccdc.cam.ac.uk).

Computing details

Data collection: APEX3;^{S5} cell refinement: SAINT v7.68A;^{S6} data reduction: SAINT v7.68A;^{S6} program(s) used to solve structure: SHELXT;^{S7} program(s) used to refine structure: SHELXL;^{S7} molecular graphics: Olex2;^{S8} software used to prepare material for publication: Olex2.^{S8}

S5. APEX3. Bruker Analytical X-ray Instruments Inc., Madison, Wisconsin, USA, **2009**.

S6. SAINT. Bruker Analytical X-ray Instruments Inc., Madison, Wisconsin, USA, **2009**.

S7. Sheldrick, G.M. Crystal Structure Refinement with SHELXL. *Acta Cryst.*, **2015**, C71, 3-8.

S8. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.*, **2009**, 42, 339–341.

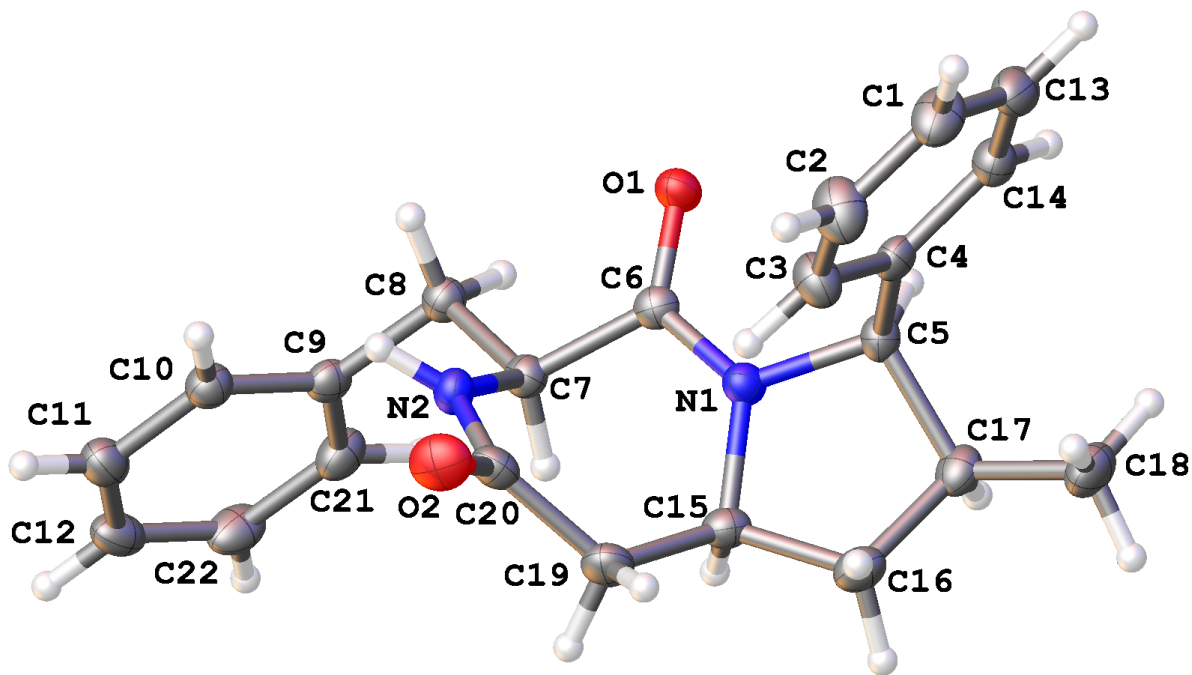


Figure S1. X-ray crystal structure of (*S,S*)-**3a** showing the atom numbering scheme. Atomic displacement ellipsoids are represented at the 50% contour probability level.

Crystal data

$C_{22}H_{24}N_2O_2$	$D_x = 1.250 \text{ Mg m}^{-3}$
$M_r = 348.43$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
Orthorhombic, $P2_12_12_1$	Cell parameters from 9476 reflections
$a = 6.5750 (3) \text{ \AA}$	$\theta = 4.8\text{--}65.5^\circ$
$b = 9.8384 (6) \text{ \AA}$	$\mu = 0.64 \text{ mm}^{-1}$
$c = 28.6228 (15) \text{ \AA}$	$T = 100 \text{ K}$
$V = 1851.54 (17) \text{ \AA}^3$	Block, colorless
$Z = 4$	$0.14 \times 0.09 \times 0.08 \text{ mm}$
$F(000) = 744$	

Data collection

Bruker X8 Proteum-R diffractometer	3214 independent reflections
Radiation source: rotating anode	3189 reflections with $I > 2\sigma(I)$
Montel monochromator	$R_{\text{int}} = 0.042$
ω and ϕ scans	$\theta_{\text{max}} = 66.0^\circ$, $\theta_{\text{min}} = 4.8^\circ$
Absorption correction: multi-scan <i>SADABS2008/1</i> ^{S9} was used for absorption	$h = -7 \rightarrow 7$

S9. SADABS. Bruker Analytical X-ray Instruments Inc., Madison, Wisconsin, USA, 2008.

correction. wR2(int) was 0.0807 before and 0.0571 after correction. The Ratio of minimum to maximum transmission is 0.9128. The $\lambda/2$ correction factor is 0.0015.	
$T_{\min} = 0.687$, $T_{\max} = 0.753$	$k = -11 \rightarrow 10$
86745 measured reflections	$l = -33 \rightarrow 33$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.6802P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.070$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.03$	$\Delta_{\max} = 0.14 \text{ e } \text{\AA}^{-3}$
3214 reflections	$\Delta_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$
239 parameters	Absolute structure: Flack x determined using 1301 quotients $[(I+)-(I-)]/[(I+)+(I-)]^{S10}$
0 restraints	Absolute structure parameter: 0.01 (4)

Special details

<i>Geometry.</i> All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
--

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (spandan1_0m)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6767 (2)	0.27836 (13)	0.04526 (4)	0.0239 (3)
O2	1.2840 (2)	0.56579 (15)	0.02101 (5)	0.0349 (4)
N1	0.7311 (3)	0.49113 (16)	0.07226 (5)	0.0212 (3)
N2	1.0013 (3)	0.47346 (17)	-0.00986 (5)	0.0221 (3)
H2	1.075 (4)	0.408 (2)	-0.0187 (8)	0.027*
C1	1.0912 (4)	0.2772 (2)	0.21215 (7)	0.0351 (5)
H1	1.186749	0.239257	0.233346	0.042*
C2	1.1548 (3)	0.3623 (3)	0.17682 (8)	0.0376 (5)
H2A	1.295470	0.382288	0.173663	0.045*
C3	1.0171 (3)	0.4192 (2)	0.14578 (7)	0.0300 (5)

S10. Parsons, S.; Flack, H.D.; Wagner, T. Use of Intensity Quotients and Differences in Absolute Structure Refinement. *Acta Cryst.* **2013**, B69, 249-259.

H3	1.064345	0.476294	0.121326	0.036*
C4	0.8112 (3)	0.39309 (19)	0.15026 (6)	0.0219 (4)
C5	0.6541 (3)	0.4598 (2)	0.11924 (6)	0.0216 (4)
H5	0.533448	0.398426	0.116451	0.026*
C6	0.7211 (3)	0.39796 (18)	0.03782 (6)	0.0203 (4)
C7	0.7806 (3)	0.45199 (19)	-0.01025 (6)	0.0212 (4)
H7	0.712211	0.541656	-0.015149	0.025*
C8	0.7165 (3)	0.3558 (2)	-0.04958 (6)	0.0229 (4)
H8A	0.801436	0.272757	-0.048419	0.027*
H8B	0.573075	0.328373	-0.044863	0.027*
C9	0.7384 (3)	0.42167 (19)	-0.09703 (6)	0.0225 (4)
C10	0.9244 (3)	0.4220 (2)	-0.12064 (7)	0.0249 (4)
H10	1.039274	0.378919	-0.107018	0.030*
C11	0.9425 (3)	0.4851 (2)	-0.16403 (7)	0.0299 (5)
H11	1.069774	0.485302	-0.179720	0.036*
C12	0.7758 (4)	0.5474 (2)	-0.18437 (7)	0.0313 (5)
H12	0.788169	0.590096	-0.214007	0.038*
C13	0.8864 (3)	0.2478 (2)	0.21636 (7)	0.0309 (5)
H13	0.840787	0.188136	0.240245	0.037*
C14	0.7476 (3)	0.3054 (2)	0.18574 (6)	0.0260 (4)
H14	0.607040	0.284995	0.188952	0.031*
C15	0.7624 (3)	0.63776 (19)	0.06359 (6)	0.0239 (4)
H15	0.653605	0.671522	0.042125	0.029*
C16	0.7298 (3)	0.6987 (2)	0.11209 (7)	0.0283 (4)
H16A	0.859861	0.703863	0.129419	0.034*
H16B	0.671078	0.791069	0.109774	0.034*
C17	0.5823 (3)	0.6022 (2)	0.13631 (7)	0.0269 (4)
H17	0.442754	0.619185	0.123677	0.032*
C18	0.5767 (4)	0.6220 (2)	0.18930 (7)	0.0358 (5)
H18A	0.713504	0.609012	0.202137	0.054*
H18B	0.483676	0.555555	0.203226	0.054*
H18C	0.529378	0.714113	0.196477	0.054*
C19	0.9735 (3)	0.6731 (2)	0.04260 (7)	0.0282 (5)
H19A	0.952893	0.748958	0.020388	0.034*
H19B	1.058516	0.708599	0.068392	0.034*
C20	1.0979 (3)	0.5652 (2)	0.01743 (7)	0.0244 (4)
C21	0.5730 (3)	0.4856 (2)	-0.11785 (7)	0.0292 (5)
H21	0.445754	0.487137	-0.102138	0.035*
C22	0.5913 (4)	0.5471 (2)	-0.16127 (7)	0.0328 (5)
H22	0.476335	0.589292	-0.175188	0.039*

Atomic displacement parameters (\AA^2) for (spandan1_0m)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0267 (7)	0.0212 (7)	0.0239 (7)	-0.0041 (6)	0.0011 (6)	0.0005 (5)
O2	0.0233 (8)	0.0350 (8)	0.0464 (9)	-0.0062 (6)	-0.0042 (6)	-0.0022 (7)
N1	0.0234 (8)	0.0206 (8)	0.0195 (7)	-0.0016 (7)	-0.0001 (7)	0.0003 (6)
N2	0.0218 (8)	0.0220 (8)	0.0226 (8)	0.0004 (7)	0.0017 (7)	-0.0014 (7)
C1	0.0346 (12)	0.0426 (13)	0.0281 (11)	0.0140 (11)	-0.0050 (10)	0.0004 (10)
C2	0.0243 (11)	0.0530 (15)	0.0356 (12)	0.0039 (10)	-0.0013 (9)	0.0043 (10)
C3	0.0261 (10)	0.0369 (12)	0.0271 (10)	-0.0004 (9)	0.0011 (8)	0.0055 (9)
C4	0.0237 (10)	0.0223 (9)	0.0196 (9)	0.0023 (8)	0.0011 (8)	-0.0050 (7)
C5	0.0204 (9)	0.0259 (10)	0.0185 (9)	-0.0002 (8)	0.0010 (7)	-0.0014 (8)
C6	0.0164 (9)	0.0215 (9)	0.0231 (9)	-0.0004 (7)	-0.0021 (8)	-0.0008 (7)
C7	0.0205 (10)	0.0207 (9)	0.0224 (9)	0.0002 (8)	0.0003 (8)	0.0005 (8)
C8	0.0225 (10)	0.0235 (9)	0.0226 (9)	-0.0005 (8)	0.0008 (8)	-0.0012 (7)
C9	0.0257 (10)	0.0198 (9)	0.0220 (9)	-0.0003 (8)	-0.0023 (8)	-0.0041 (7)
C10	0.0261 (10)	0.0240 (10)	0.0246 (10)	0.0009 (9)	-0.0014 (8)	-0.0015 (8)
C11	0.0368 (12)	0.0272 (11)	0.0257 (10)	-0.0031 (9)	0.0020 (9)	0.0005 (8)
C12	0.0480 (13)	0.0224 (10)	0.0235 (9)	-0.0014 (10)	-0.0045 (10)	0.0031 (8)
C13	0.0404 (13)	0.0297 (11)	0.0224 (9)	0.0057 (9)	0.0018 (9)	0.0024 (8)
C14	0.0263 (10)	0.0274 (10)	0.0242 (9)	0.0013 (9)	0.0024 (8)	-0.0019 (8)
C15	0.0269 (10)	0.0194 (9)	0.0256 (9)	0.0012 (8)	-0.0029 (9)	-0.0004 (8)
C16	0.0323 (11)	0.0227 (10)	0.0298 (10)	0.0028 (9)	-0.0018 (9)	-0.0037 (8)
C17	0.0253 (10)	0.0297 (11)	0.0258 (10)	0.0077 (9)	-0.0002 (8)	-0.0020 (8)
C18	0.0465 (13)	0.0331 (12)	0.0279 (11)	0.0083 (10)	0.0023 (10)	-0.0068 (9)
C19	0.0323 (11)	0.0203 (9)	0.0319 (11)	-0.0058 (8)	0.0003 (9)	-0.0011 (8)
C20	0.0263 (10)	0.0221 (10)	0.0249 (10)	-0.0058 (8)	-0.0008 (8)	0.0039 (8)
C21	0.0313 (11)	0.0304 (11)	0.0258 (10)	0.0067 (9)	-0.0022 (9)	-0.0061 (8)
C22	0.0410 (12)	0.0293 (11)	0.0280 (10)	0.0119 (10)	-0.0106 (10)	-0.0015 (9)

Geometric parameters (\AA , $^\circ$) for (spandan1_0m)

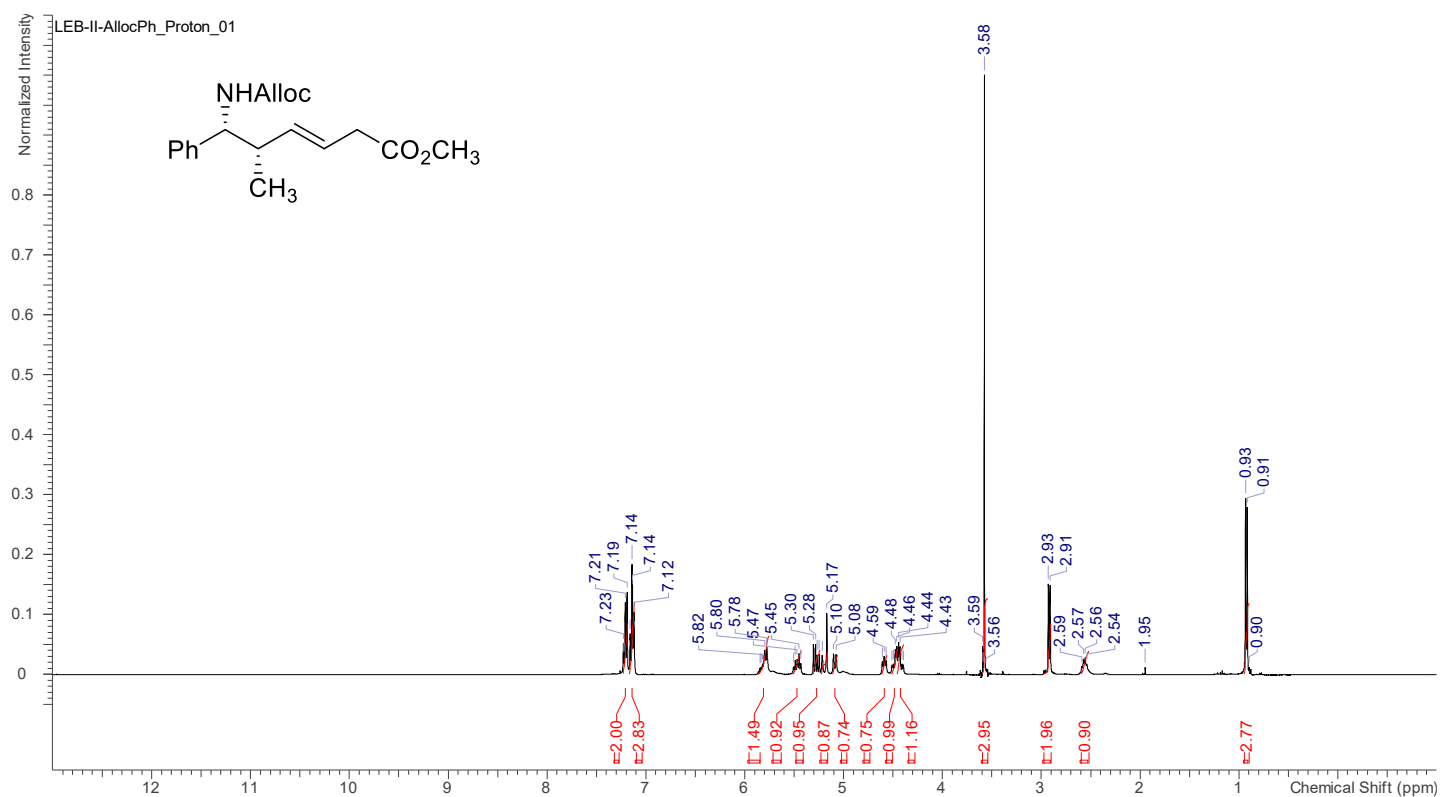
O1—C6	1.231 (2)	C10—H10	0.9500
O2—C20	1.227 (3)	C10—C11	1.393 (3)
N1—C5	1.470 (2)	C11—H11	0.9500
N1—C6	1.348 (2)	C11—C12	1.384 (3)
N1—C15	1.478 (2)	C12—H12	0.9500
N2—H2	0.85 (2)	C12—C22	1.381 (3)
N2—C7	1.467 (2)	C13—H13	0.9500

N2—C20	1.352 (3)	C13—C14	1.387 (3)
C1—H1	0.9500	C14—H14	0.9500
C1—C2	1.378 (3)	C15—H15	1.0000
C1—C13	1.382 (3)	C15—C16	1.527 (3)
C2—H2A	0.9500	C15—C19	1.551 (3)
C2—C3	1.386 (3)	C16—H16A	0.9900
C3—H3	0.9500	C16—H16B	0.9900
C3—C4	1.384 (3)	C16—C17	1.524 (3)
C4—C5	1.512 (3)	C17—H17	1.0000
C4—C14	1.397 (3)	C17—C18	1.530 (3)
C5—H5	1.0000	C18—H18A	0.9800
C5—C17	1.557 (3)	C18—H18B	0.9800
C6—C7	1.526 (3)	C18—H18C	0.9800
C7—H7	1.0000	C19—H19A	0.9900
C7—C8	1.530 (3)	C19—H19B	0.9900
C8—H8A	0.9900	C19—C20	1.521 (3)
C8—H8B	0.9900	C21—H21	0.9500
C8—C9	1.512 (3)	C21—C22	1.388 (3)
C9—C10	1.397 (3)	C22—H22	0.9500
C9—C21	1.390 (3)		
C5—N1—C15	113.98 (15)	C11—C12—H12	120.2
C6—N1—C5	120.62 (15)	C22—C12—C11	119.52 (18)
C6—N1—C15	123.23 (15)	C22—C12—H12	120.2
C7—N2—H2	117.0 (16)	C1—C13—H13	120.0
C20—N2—H2	114.4 (16)	C1—C13—C14	120.1 (2)
C20—N2—C7	124.44 (17)	C14—C13—H13	120.0
C2—C1—H1	120.4	C4—C14—H14	119.5
C2—C1—C13	119.1 (2)	C13—C14—C4	121.0 (2)
C13—C1—H1	120.4	C13—C14—H14	119.5
C1—C2—H2A	119.4	N1—C15—H15	109.1
C1—C2—C3	121.2 (2)	N1—C15—C16	102.17 (14)
C3—C2—H2A	119.4	N1—C15—C19	114.08 (16)
C2—C3—H3	119.8	C16—C15—H15	109.1
C4—C3—C2	120.3 (2)	C16—C15—C19	112.96 (17)
C4—C3—H3	119.8	C19—C15—H15	109.1
C3—C4—C5	122.26 (17)	C15—C16—H16A	110.7
C3—C4—C14	118.36 (18)	C15—C16—H16B	110.7
C14—C4—C5	119.35 (18)	H16A—C16—H16B	108.8
N1—C5—C4	113.14 (15)	C17—C16—C15	104.99 (16)

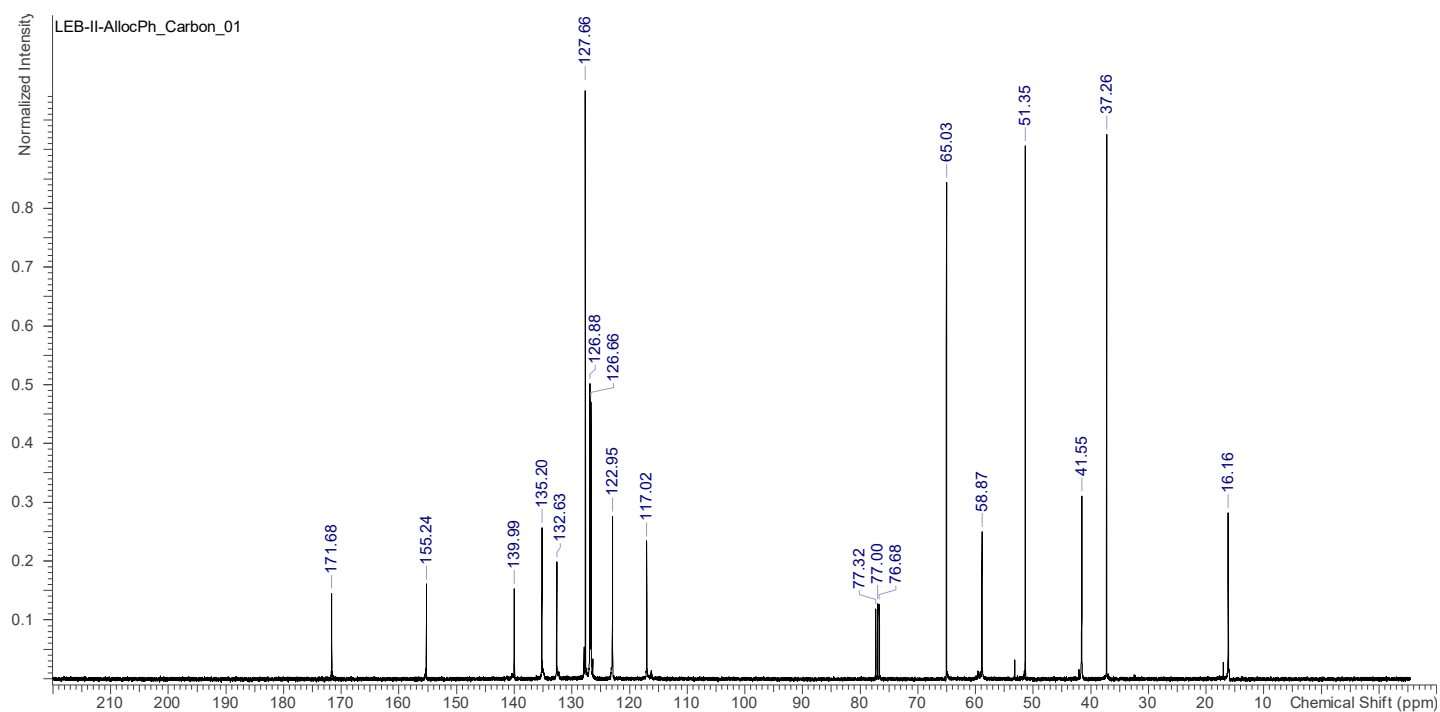
N1—C5—H5	109.1	C17—C16—H16A	110.7
N1—C5—C17	101.69 (15)	C17—C16—H16B	110.7
C4—C5—H5	109.1	C5—C17—H17	108.4
C4—C5—C17	114.41 (15)	C16—C17—C5	102.97 (15)
C17—C5—H5	109.1	C16—C17—H17	108.4
O1—C6—N1	122.38 (17)	C16—C17—C18	112.76 (18)
O1—C6—C7	123.34 (16)	C18—C17—C5	115.66 (17)
N1—C6—C7	114.20 (15)	C18—C17—H17	108.4
N2—C7—C6	107.27 (15)	C17—C18—H18A	109.5
N2—C7—H7	108.6	C17—C18—H18B	109.5
N2—C7—C8	111.54 (15)	C17—C18—H18C	109.5
C6—C7—H7	108.6	H18A—C18—H18B	109.5
C6—C7—C8	112.18 (15)	H18A—C18—H18C	109.5
C8—C7—H7	108.6	H18B—C18—H18C	109.5
C7—C8—H8A	109.3	C15—C19—H19A	107.2
C7—C8—H8B	109.3	C15—C19—H19B	107.2
H8A—C8—H8B	107.9	H19A—C19—H19B	106.8
C9—C8—C7	111.68 (15)	C20—C19—C15	120.56 (16)
C9—C8—H8A	109.3	C20—C19—H19A	107.2
C9—C8—H8B	109.3	C20—C19—H19B	107.2
C10—C9—C8	121.27 (17)	O2—C20—N2	121.3 (2)
C21—C9—C8	120.28 (18)	O2—C20—C19	119.57 (18)
C21—C9—C10	118.44 (17)	N2—C20—C19	119.09 (17)
C9—C10—H10	119.8	C9—C21—H21	119.6
C11—C10—C9	120.46 (19)	C22—C21—C9	120.9 (2)
C11—C10—H10	119.8	C22—C21—H21	119.6
C10—C11—H11	119.8	C12—C22—C21	120.4 (2)
C12—C11—C10	120.3 (2)	C12—C22—H22	119.8
C12—C11—H11	119.8	C21—C22—H22	119.8

7. ^1H and ^{13}C NMR spectra for all new compounds

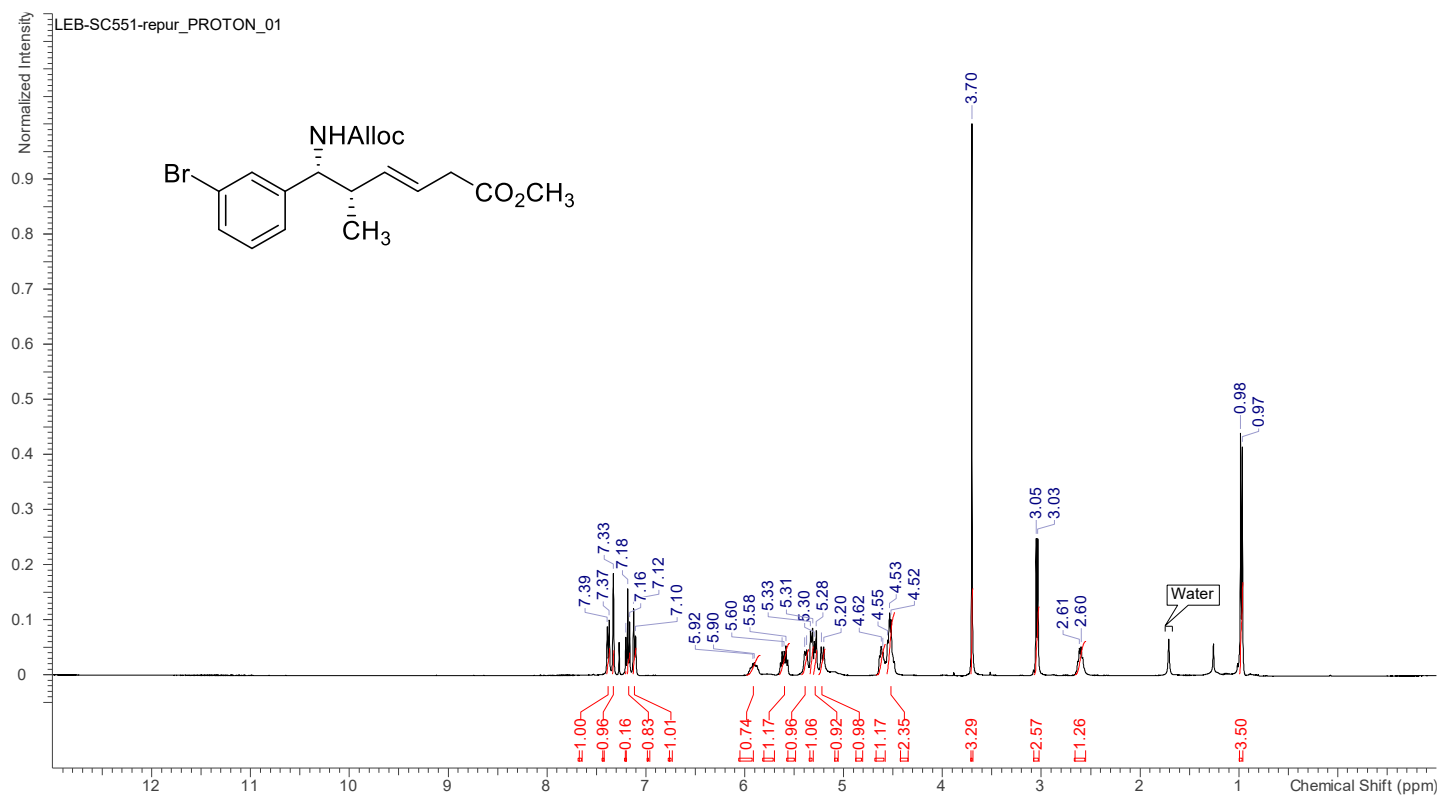
^1H NMR for Compound 7.



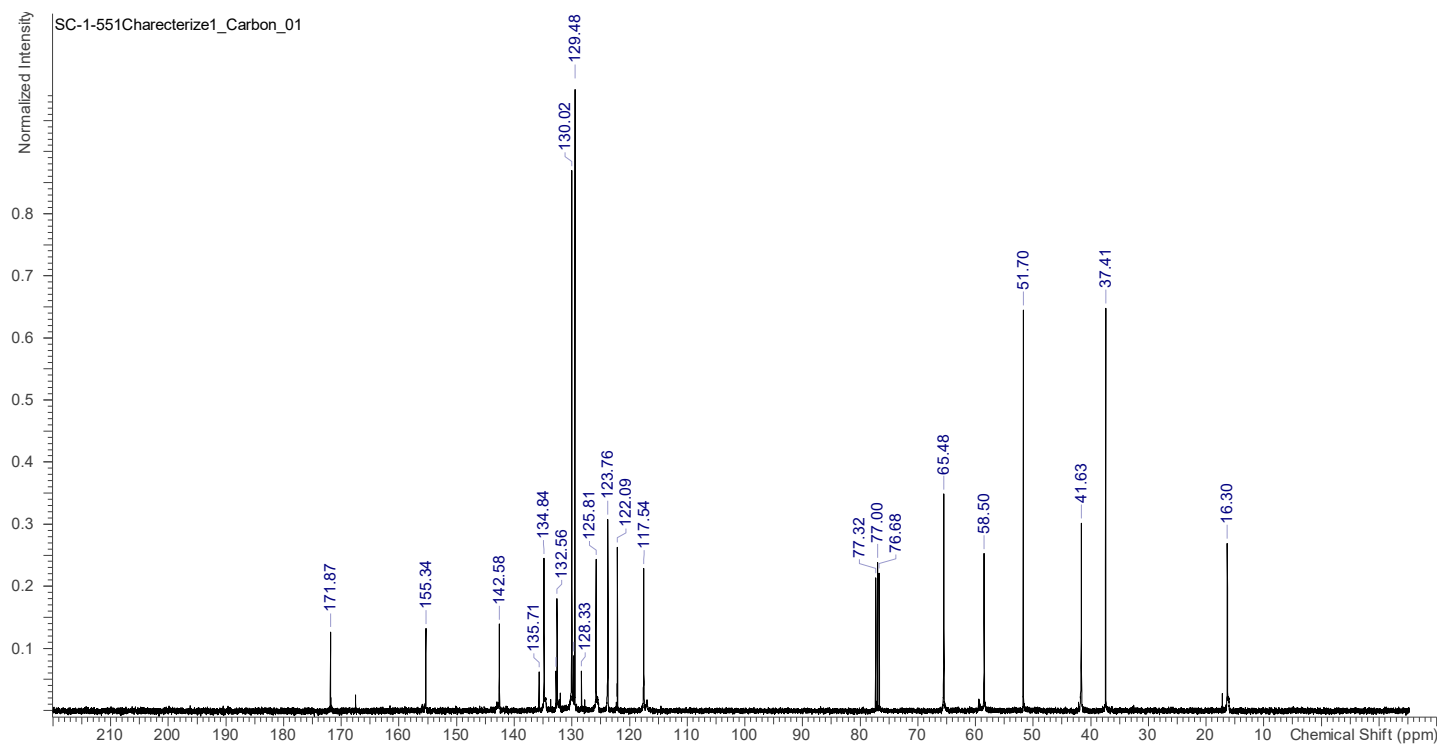
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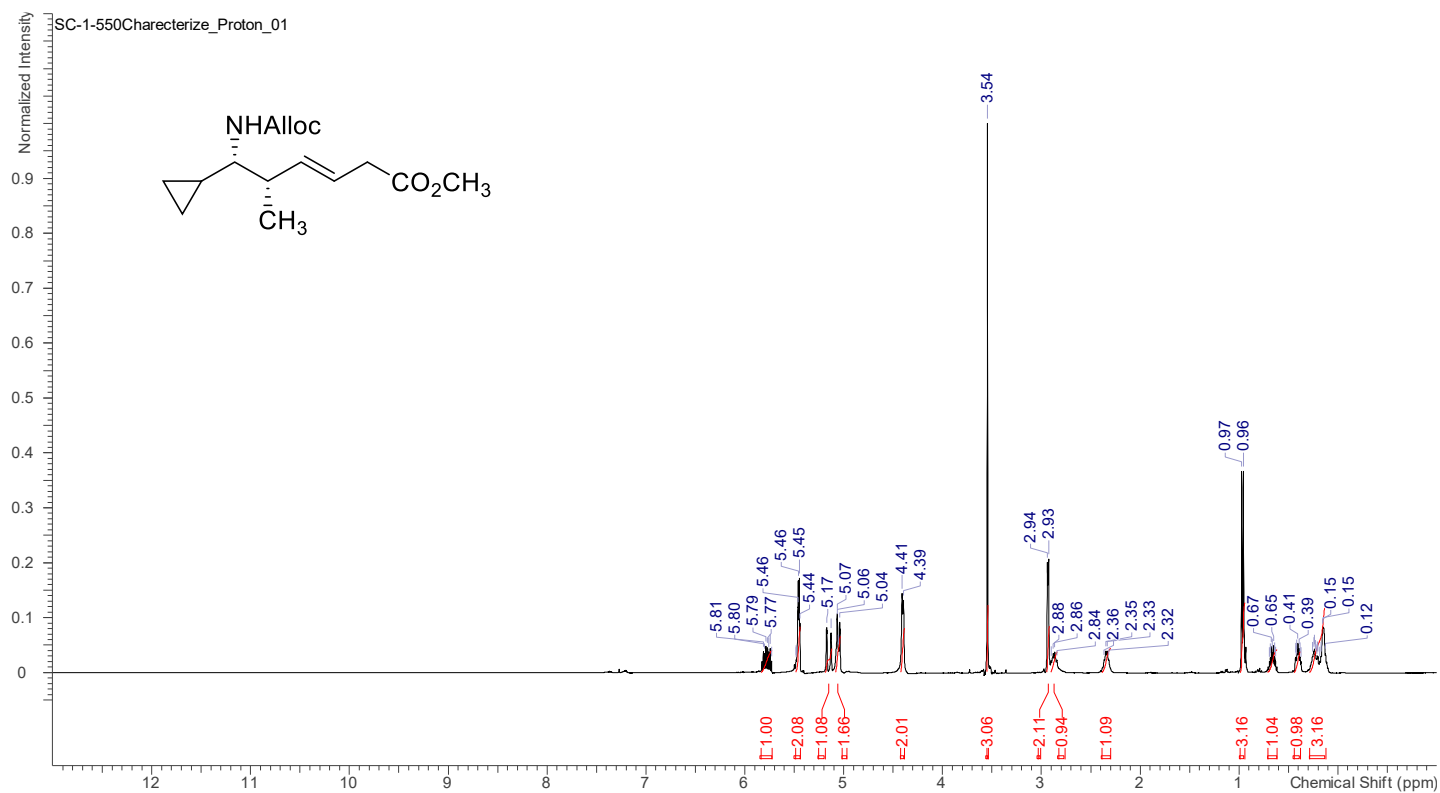
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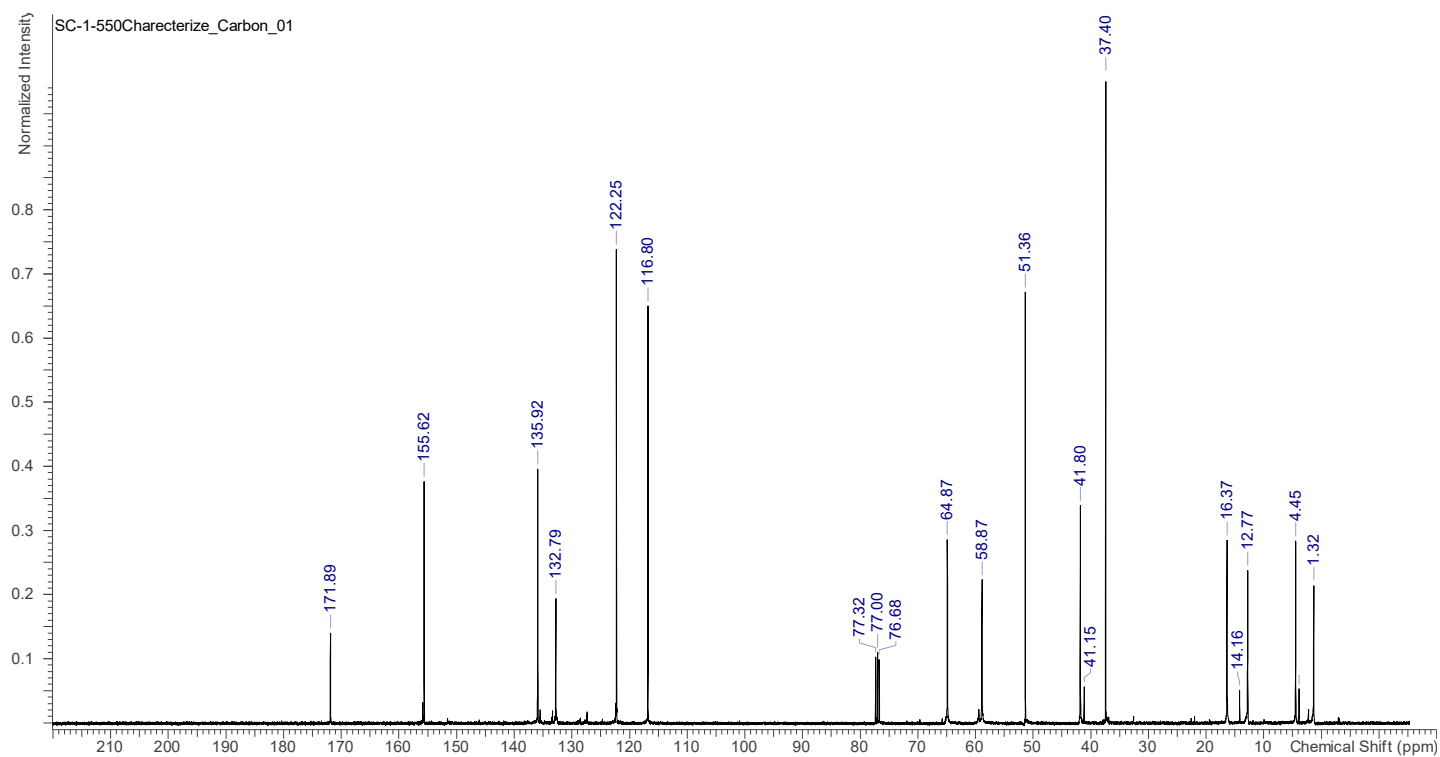
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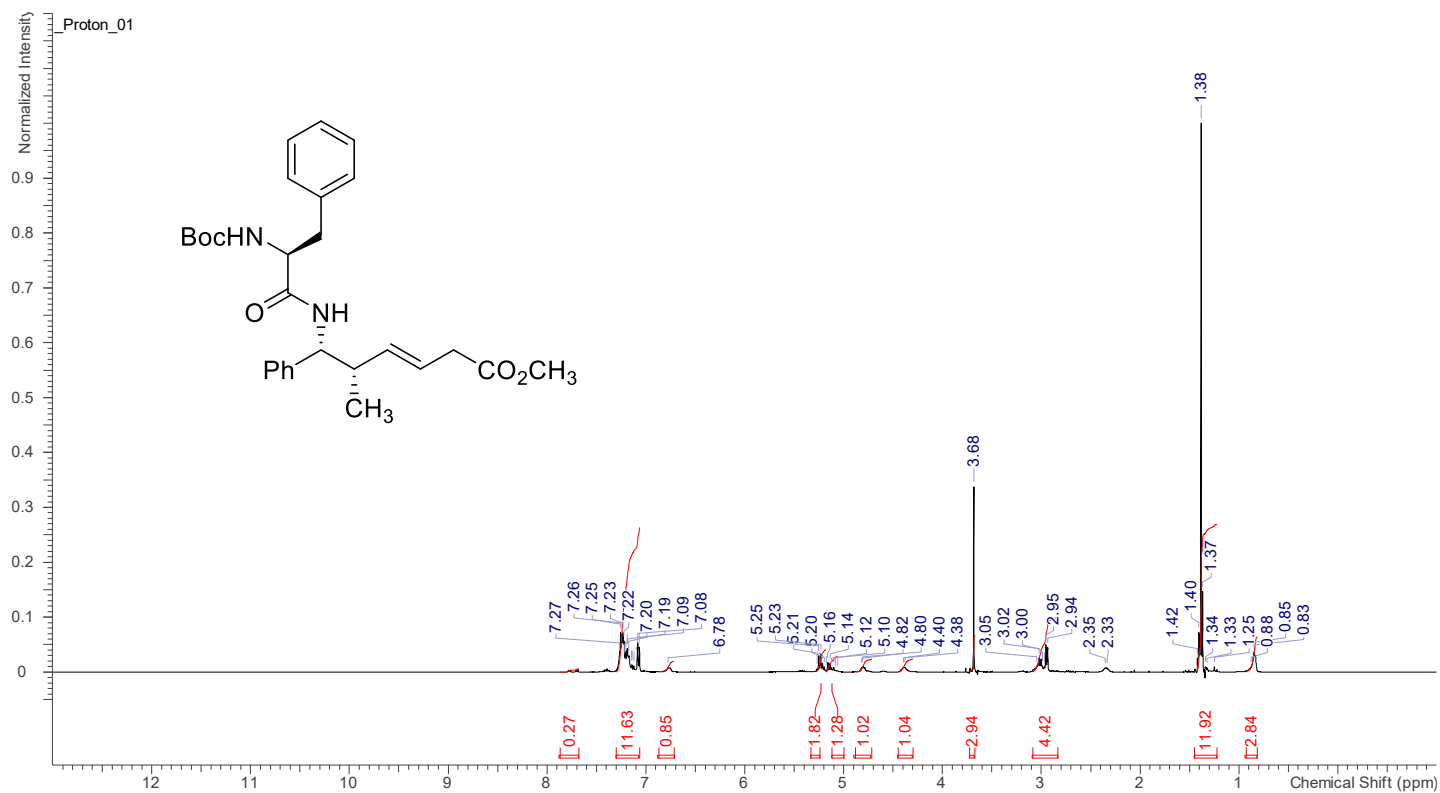
¹H NMR for Compound 9.



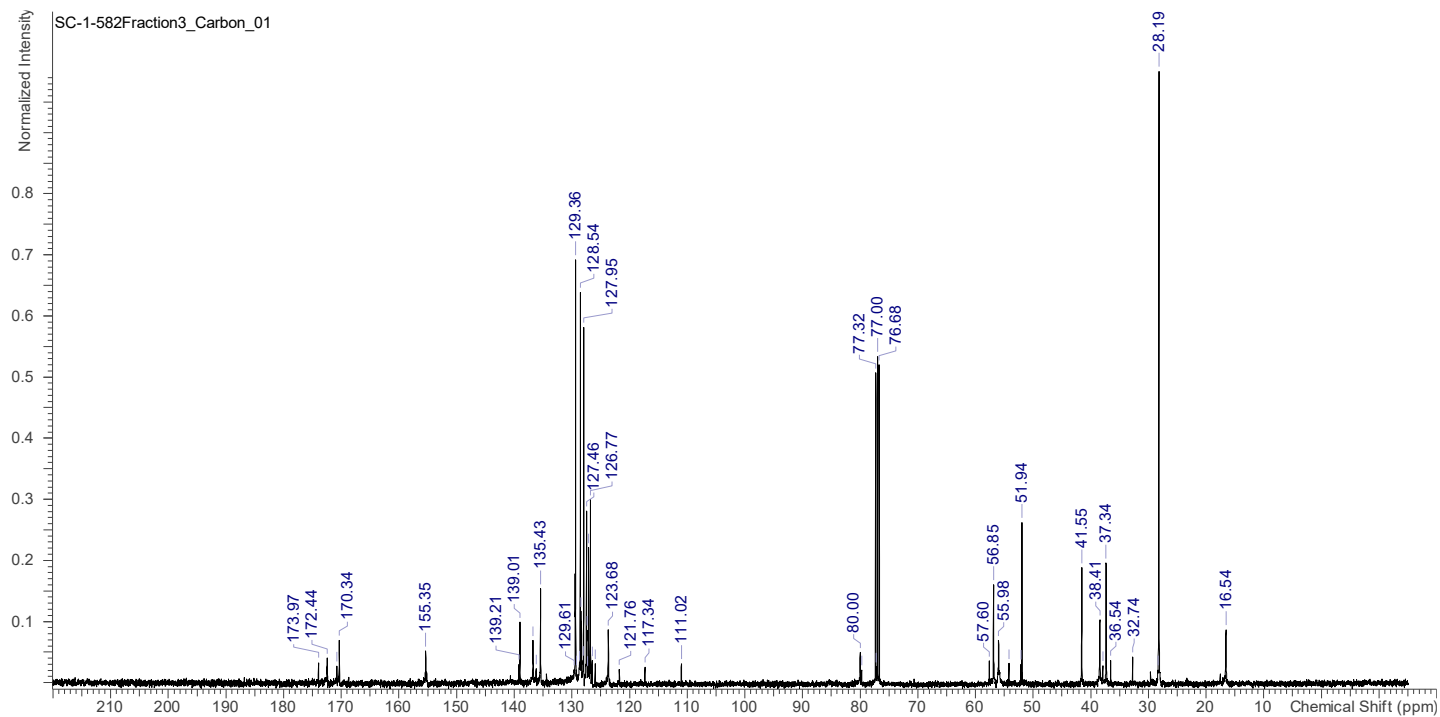
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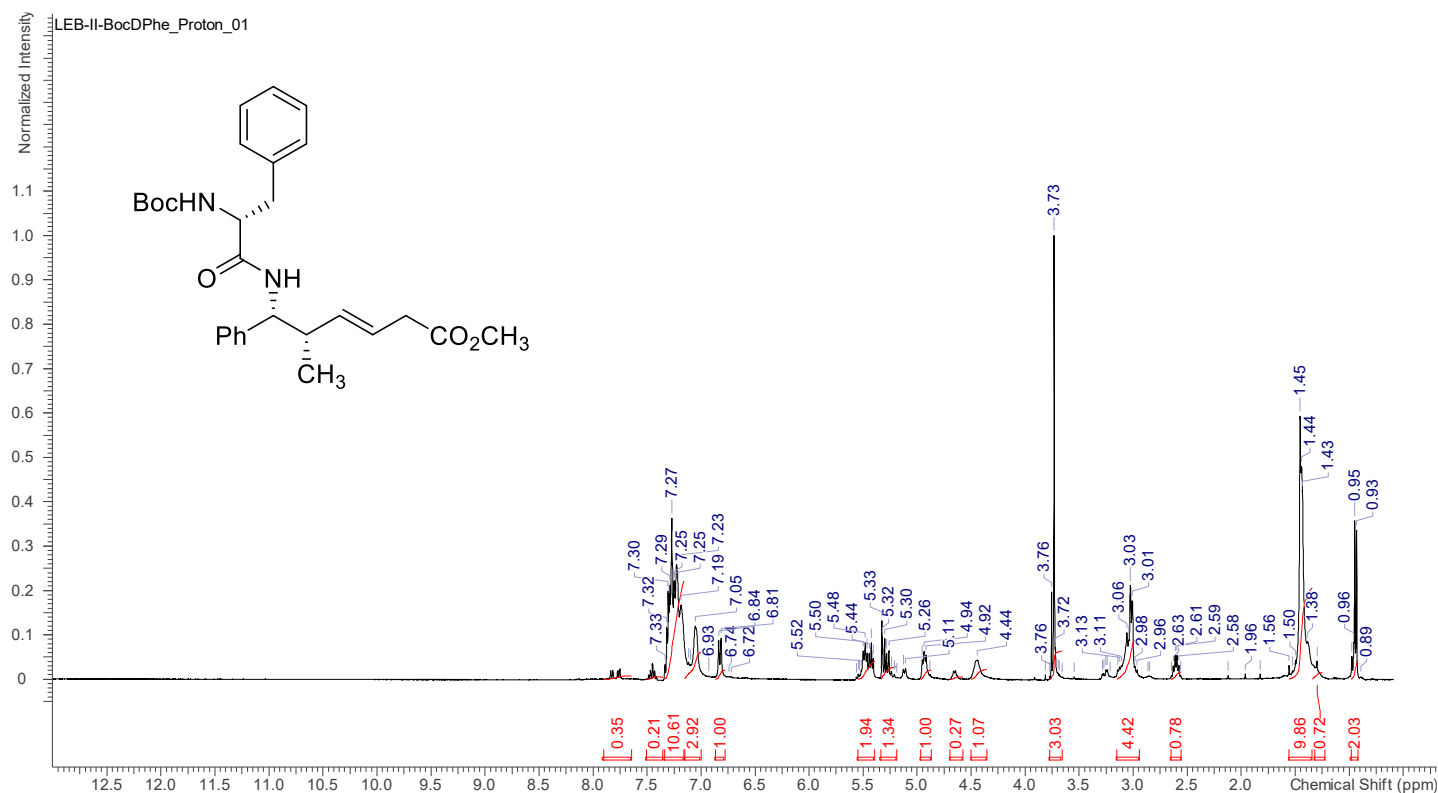
¹H NMR for Compound (*S*)-**10a**.



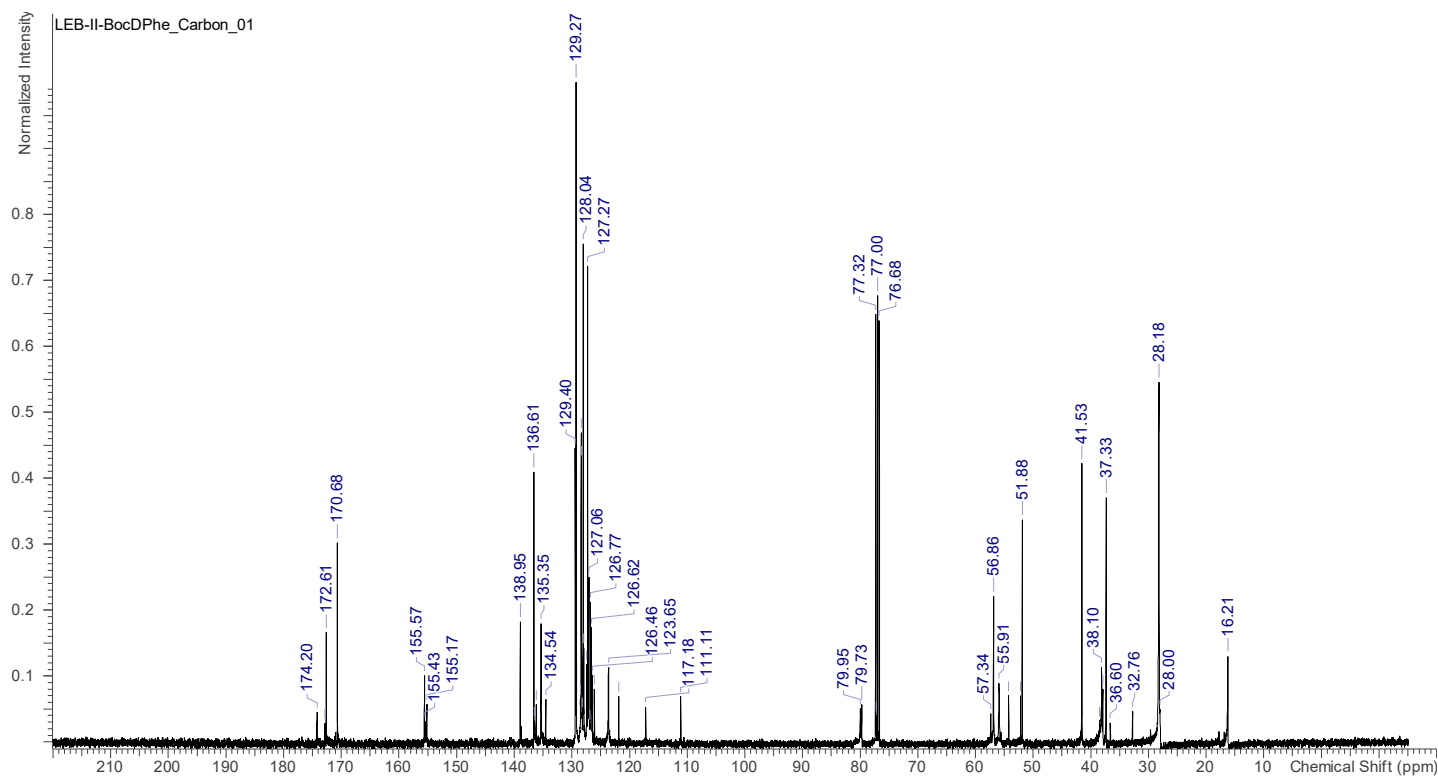
¹³C NMR for Compound (*S*)-**10a**.



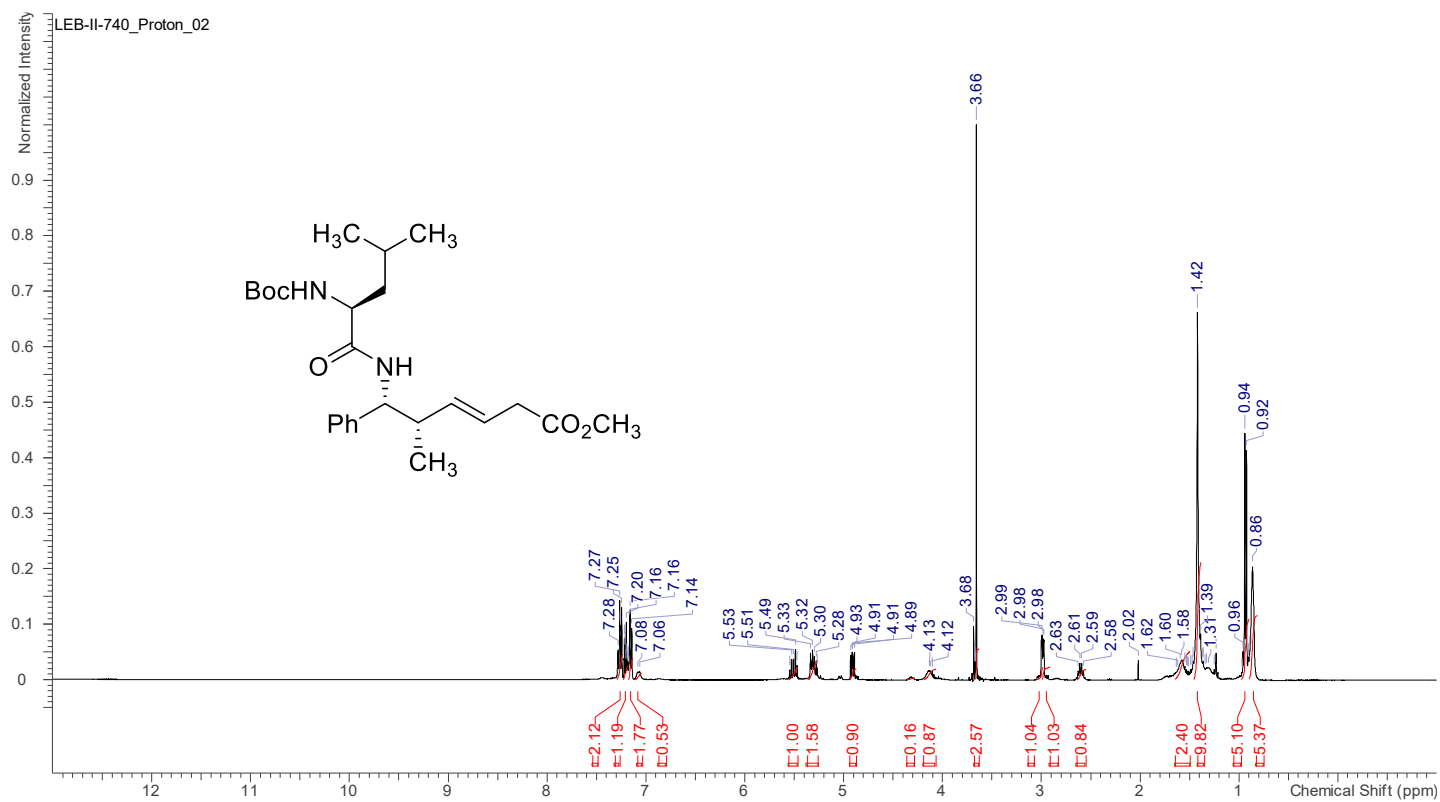
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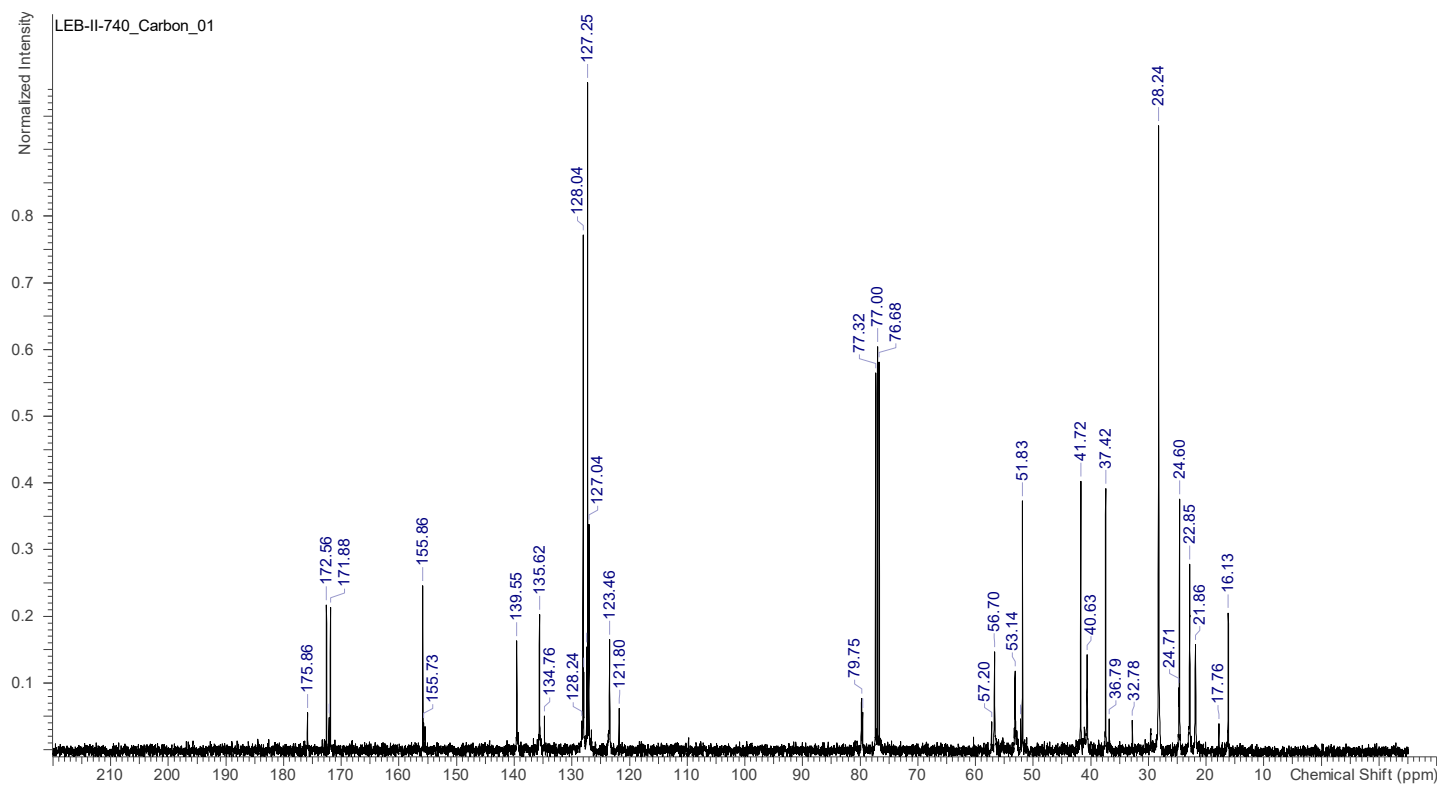
¹³C NMR for Compound (*R*)-10a.



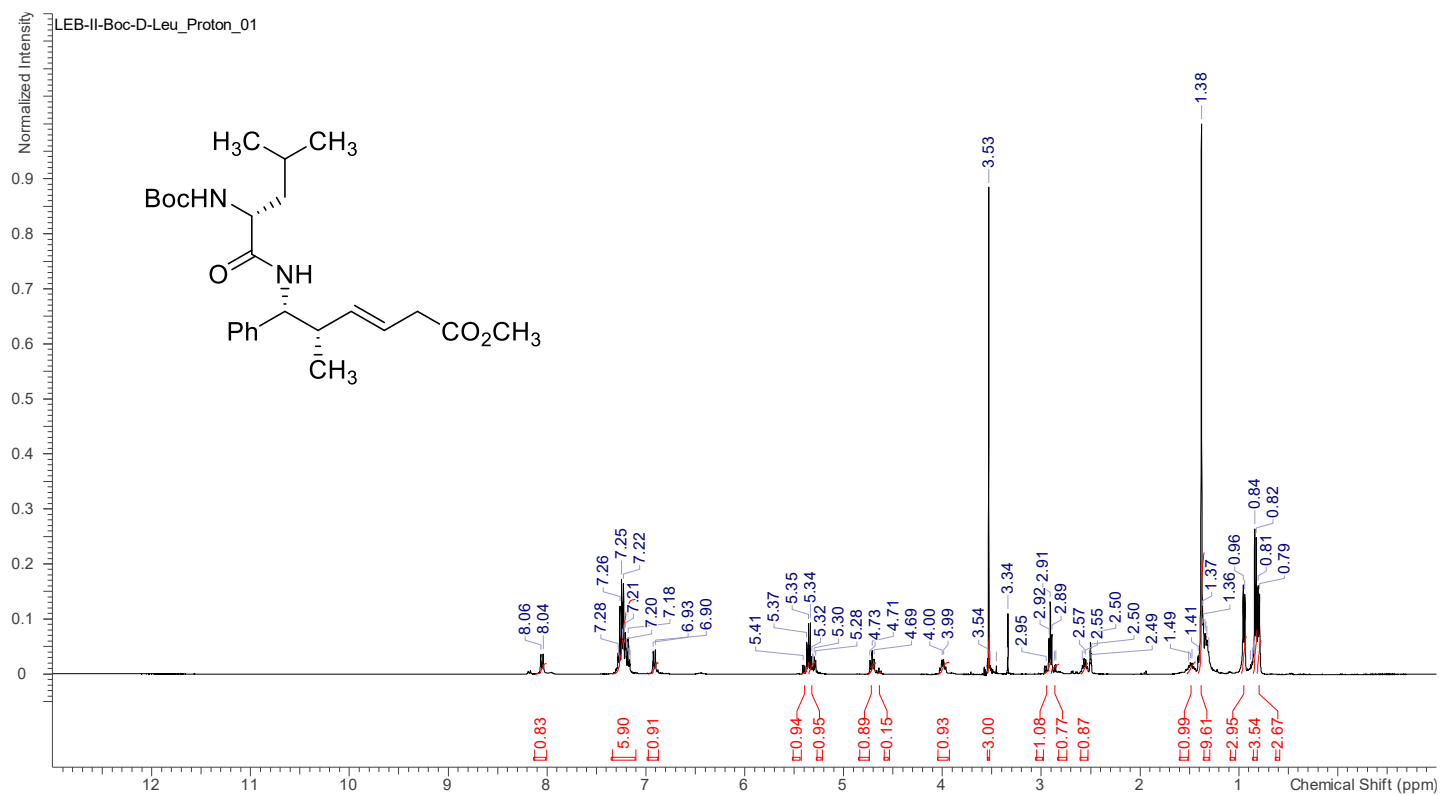
¹H NMR for Compound (*S*)-10b.



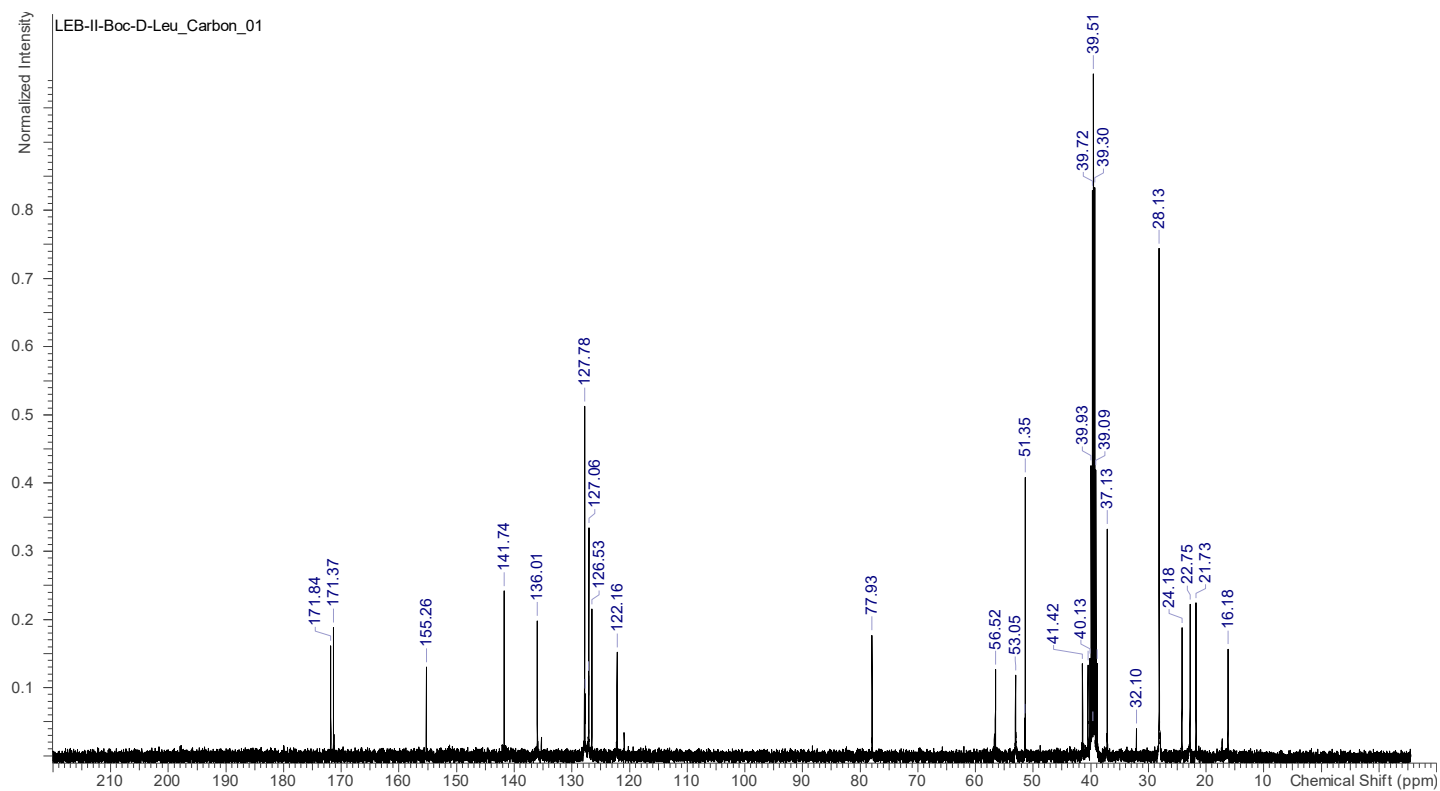
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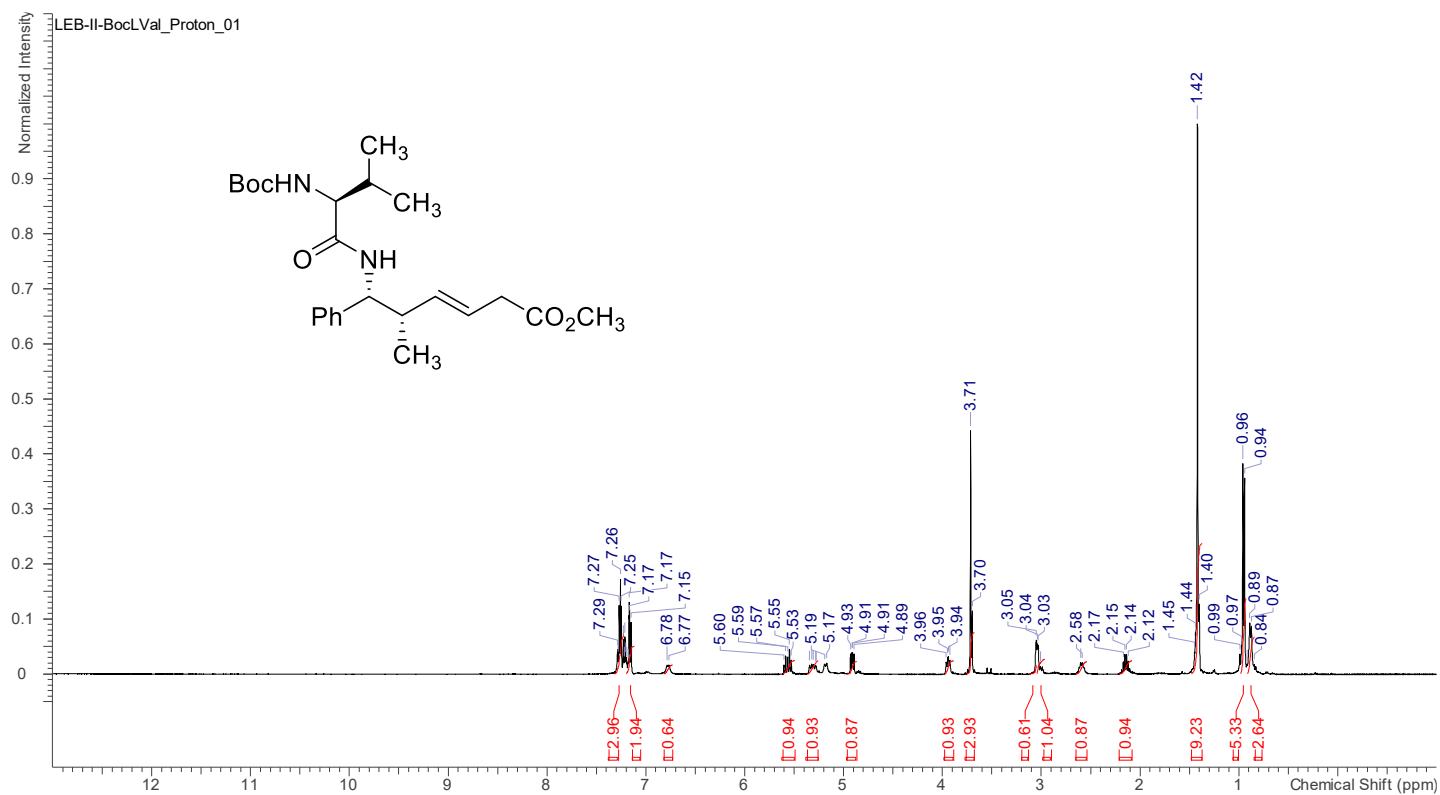
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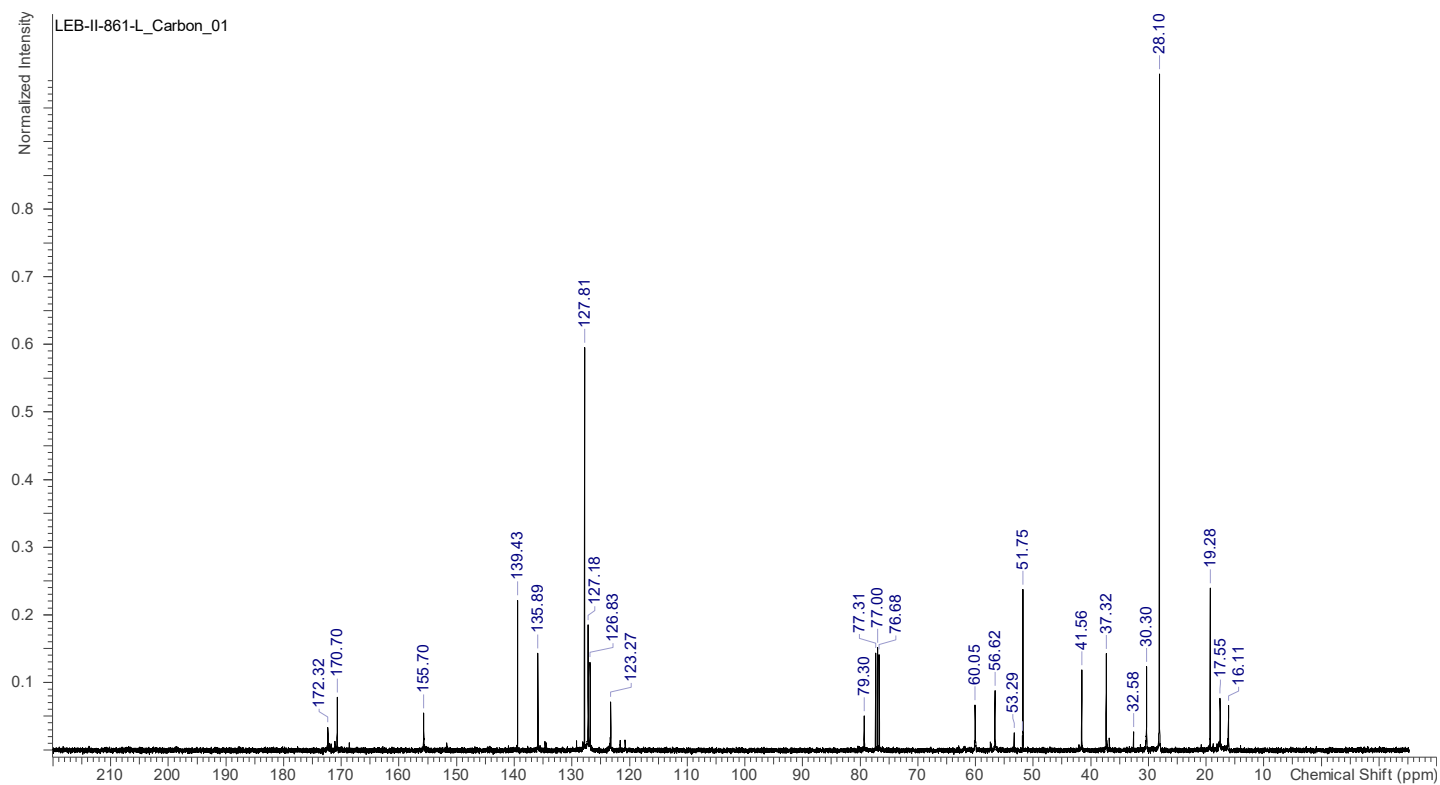
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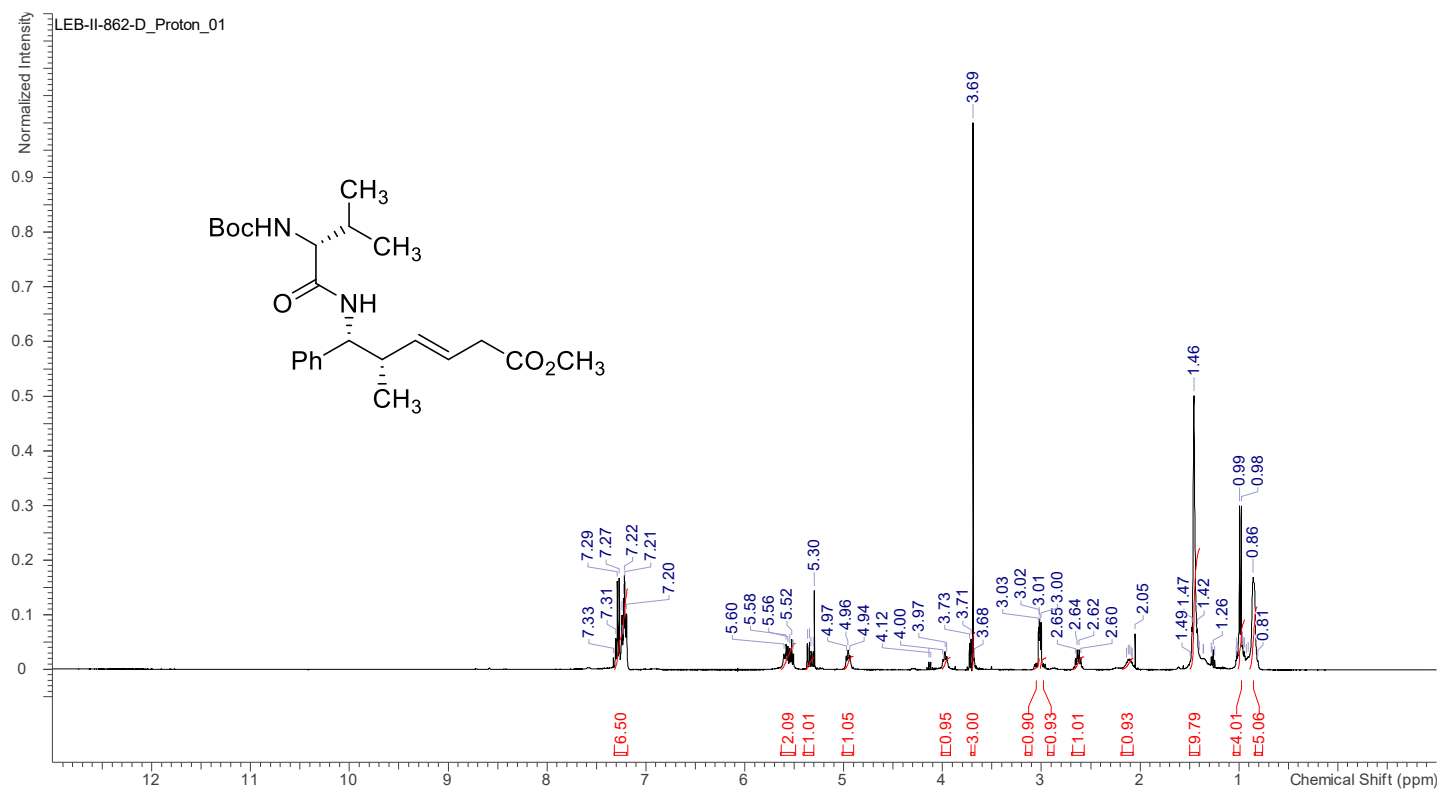
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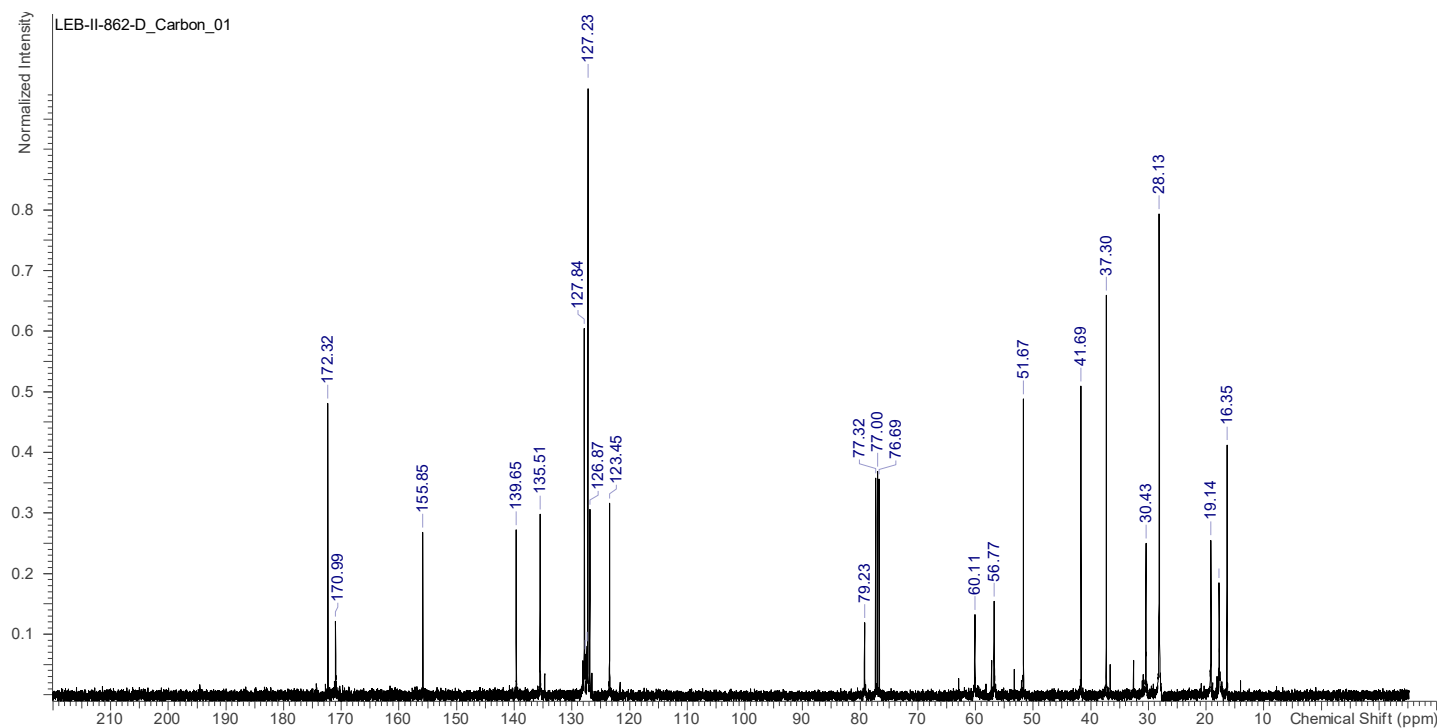
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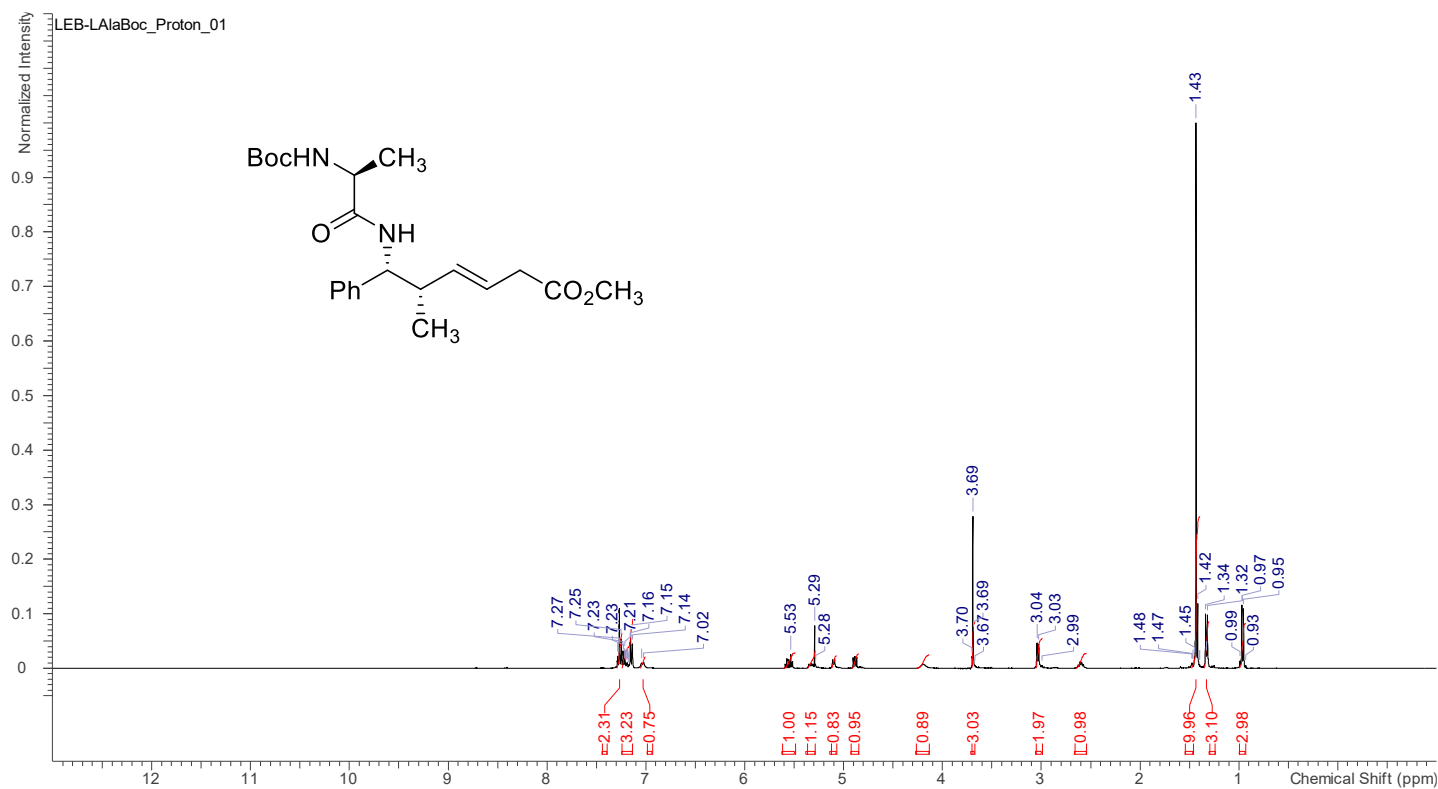
¹H NMR for Compound (*R*)-10c.



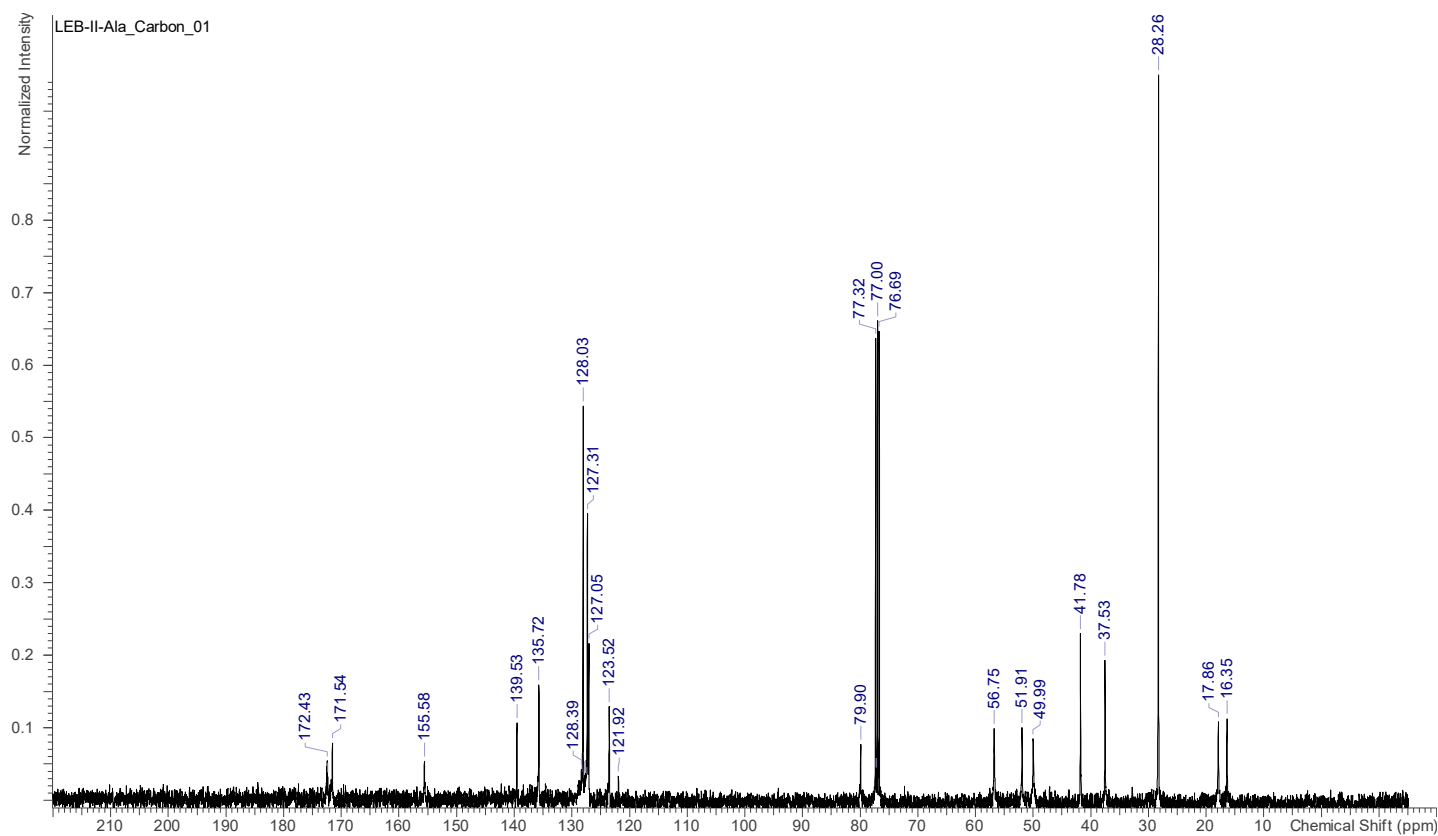
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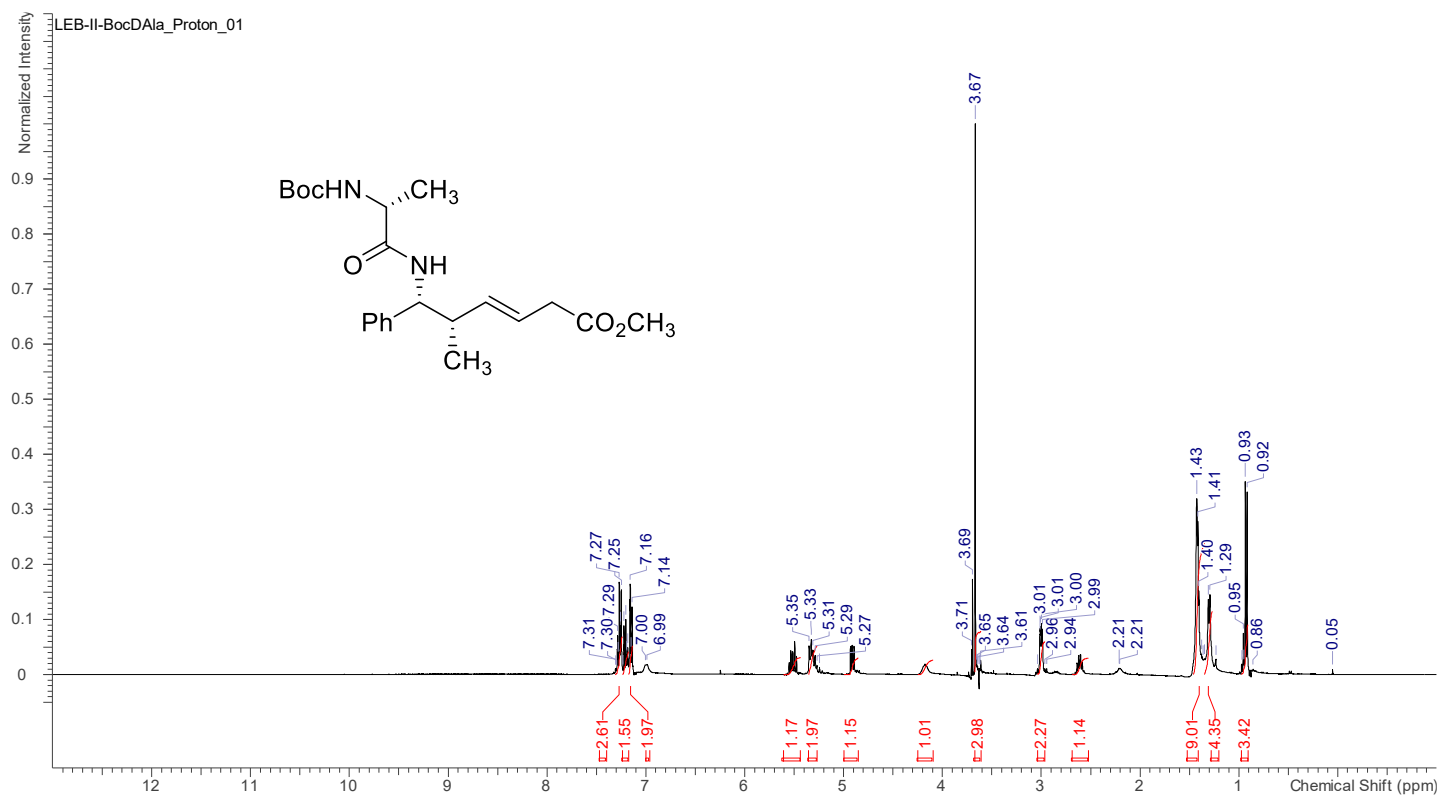
¹H NMR for Compound (S)-10d.



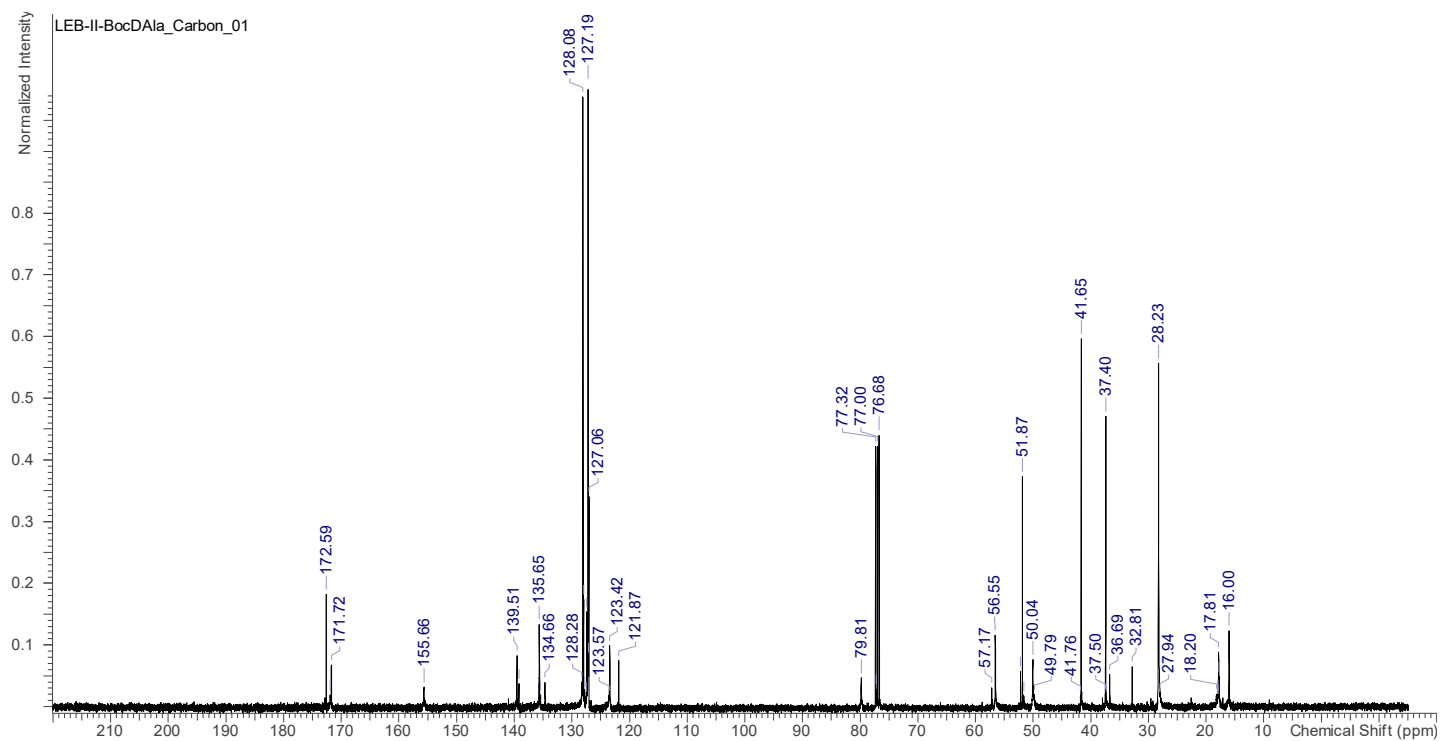
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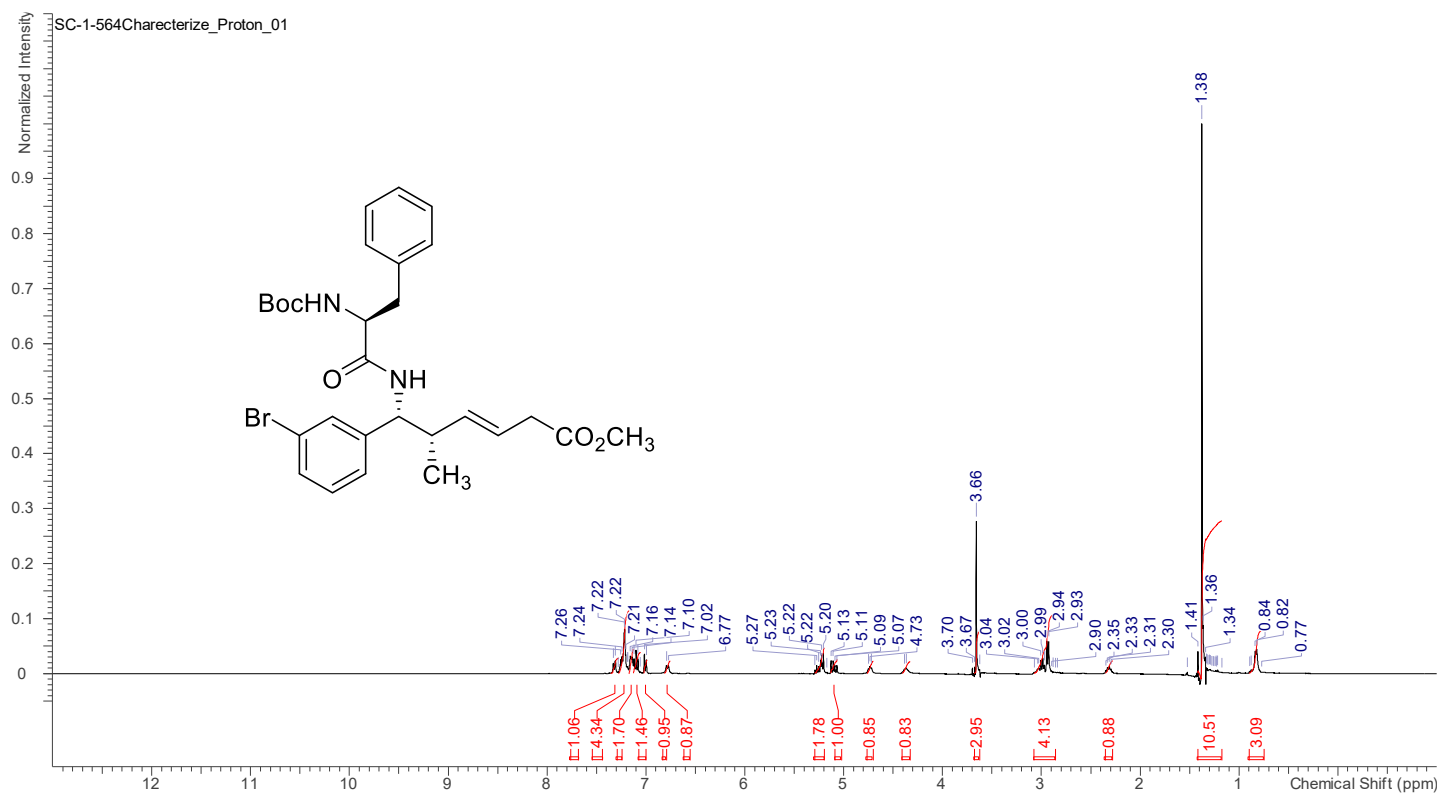
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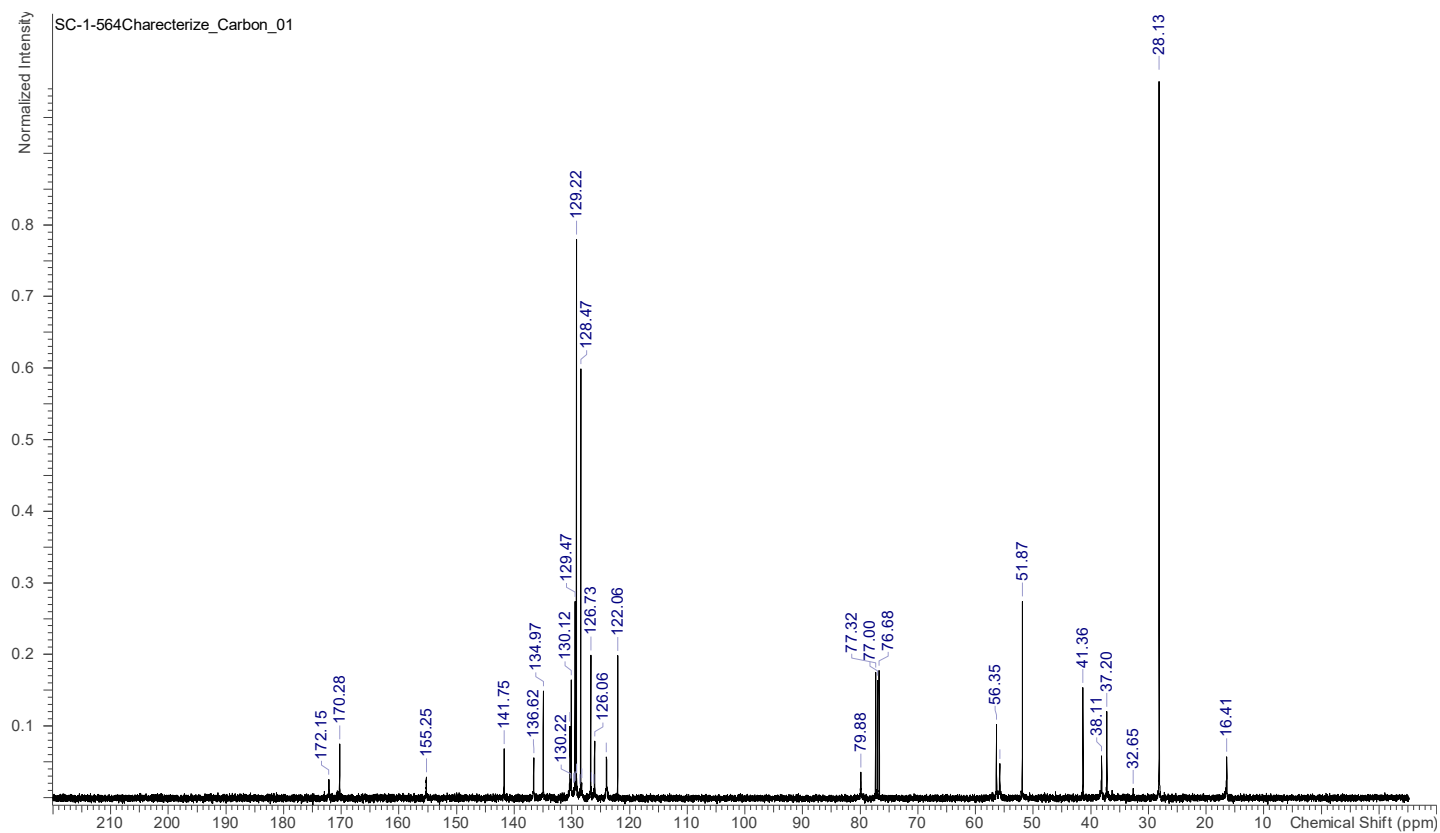
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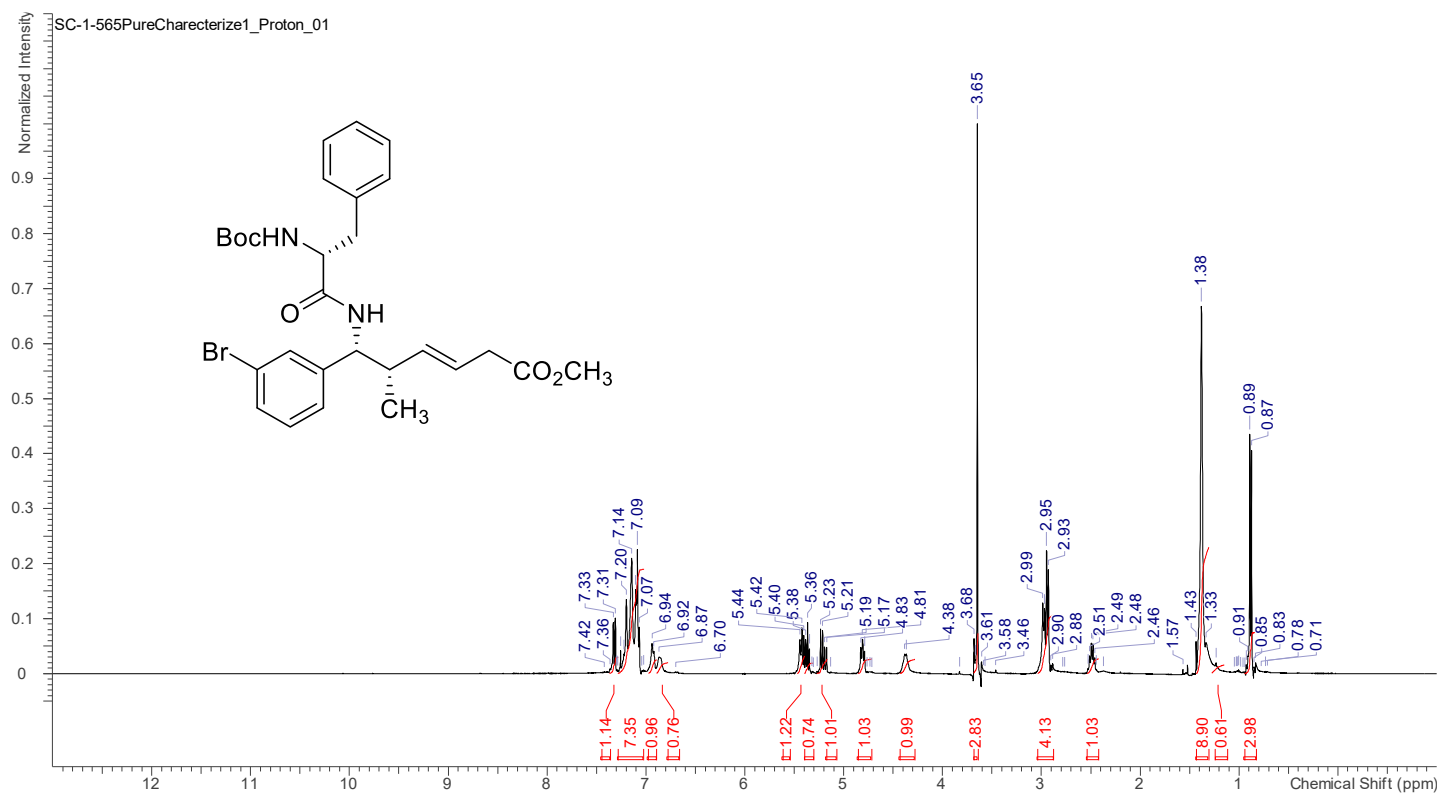
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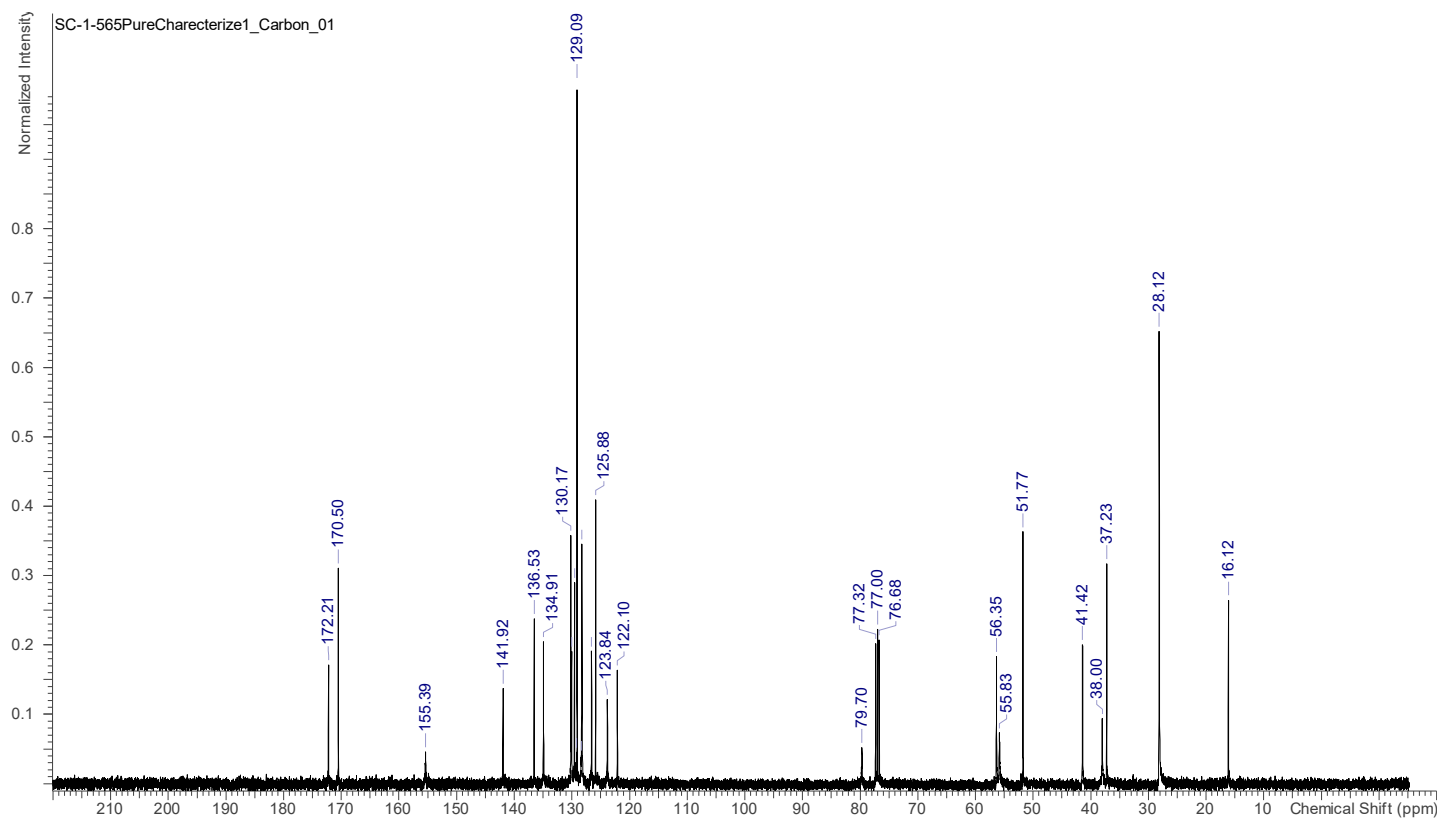
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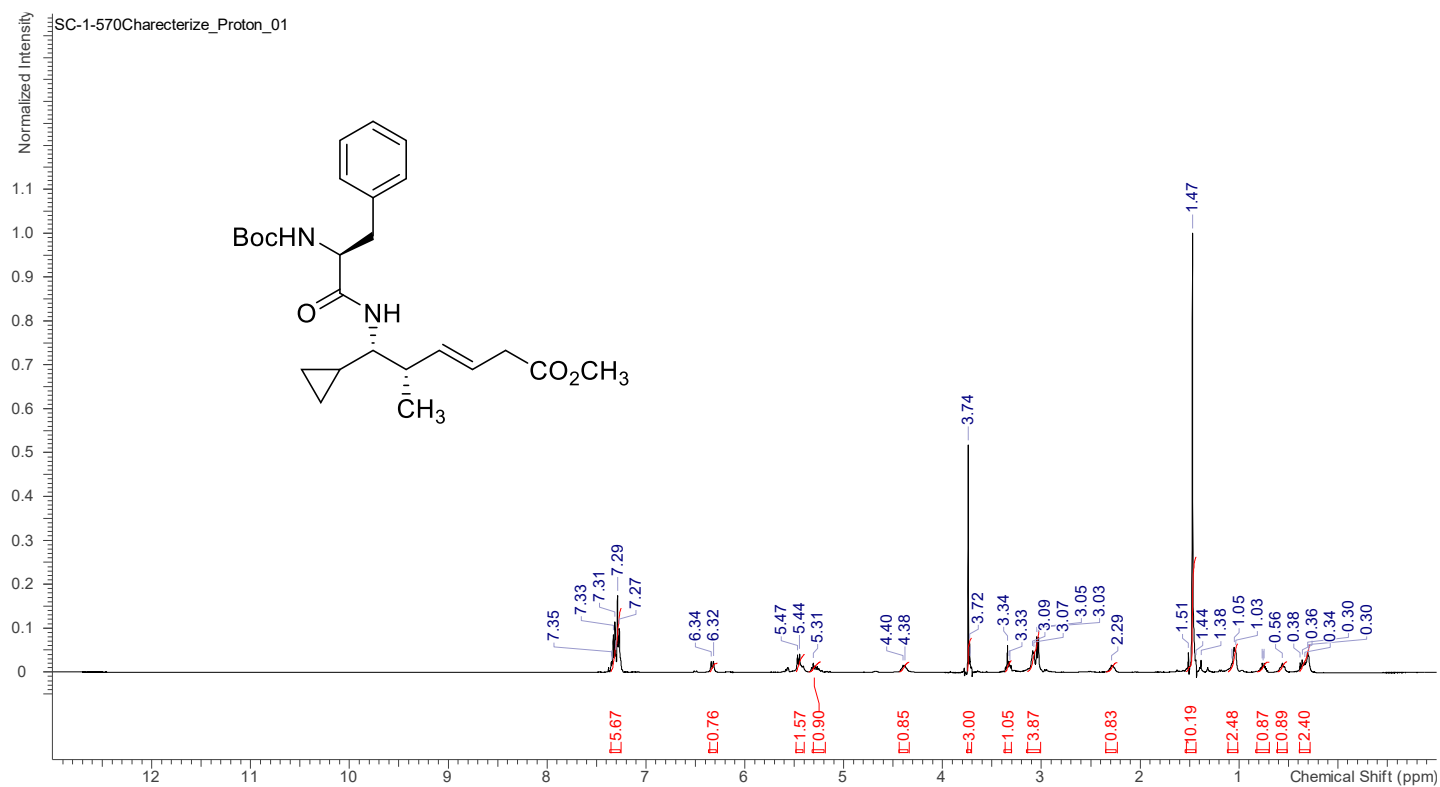
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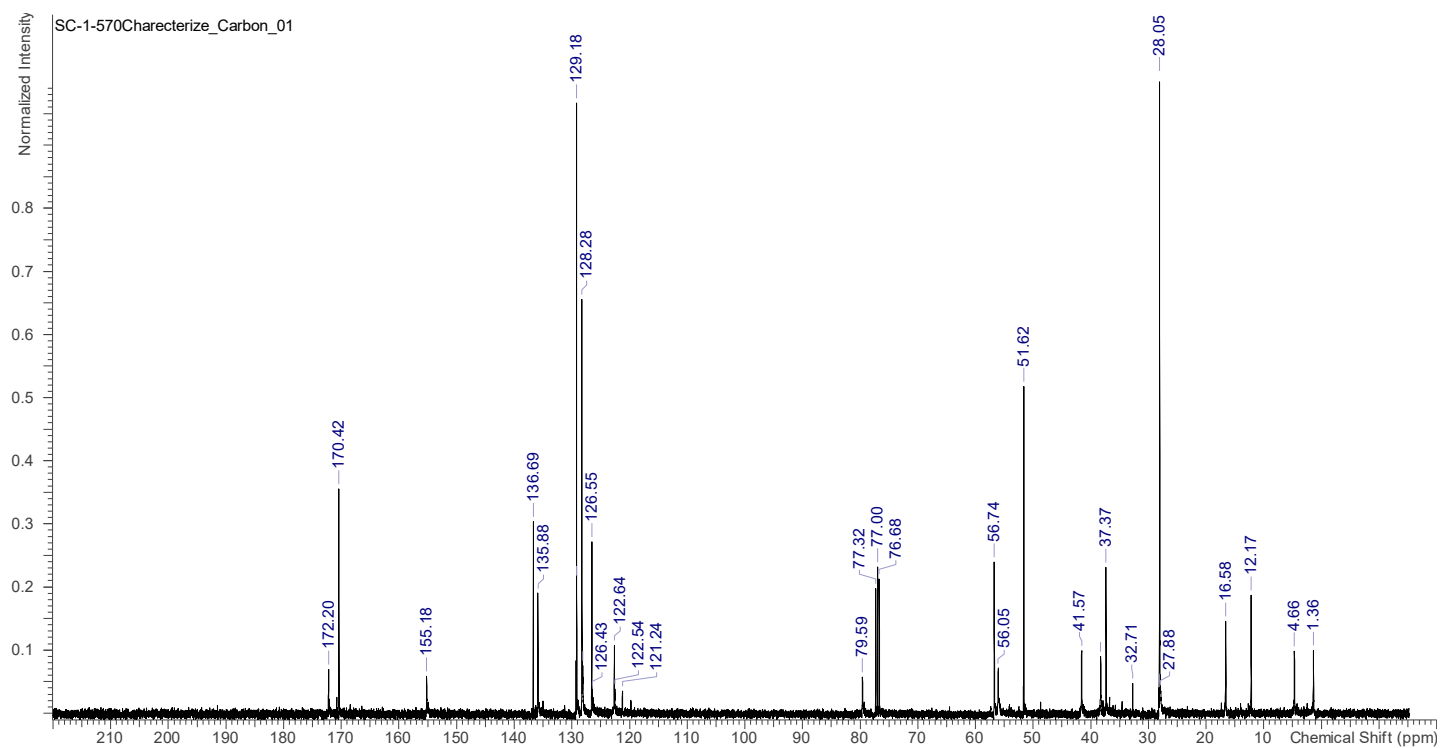
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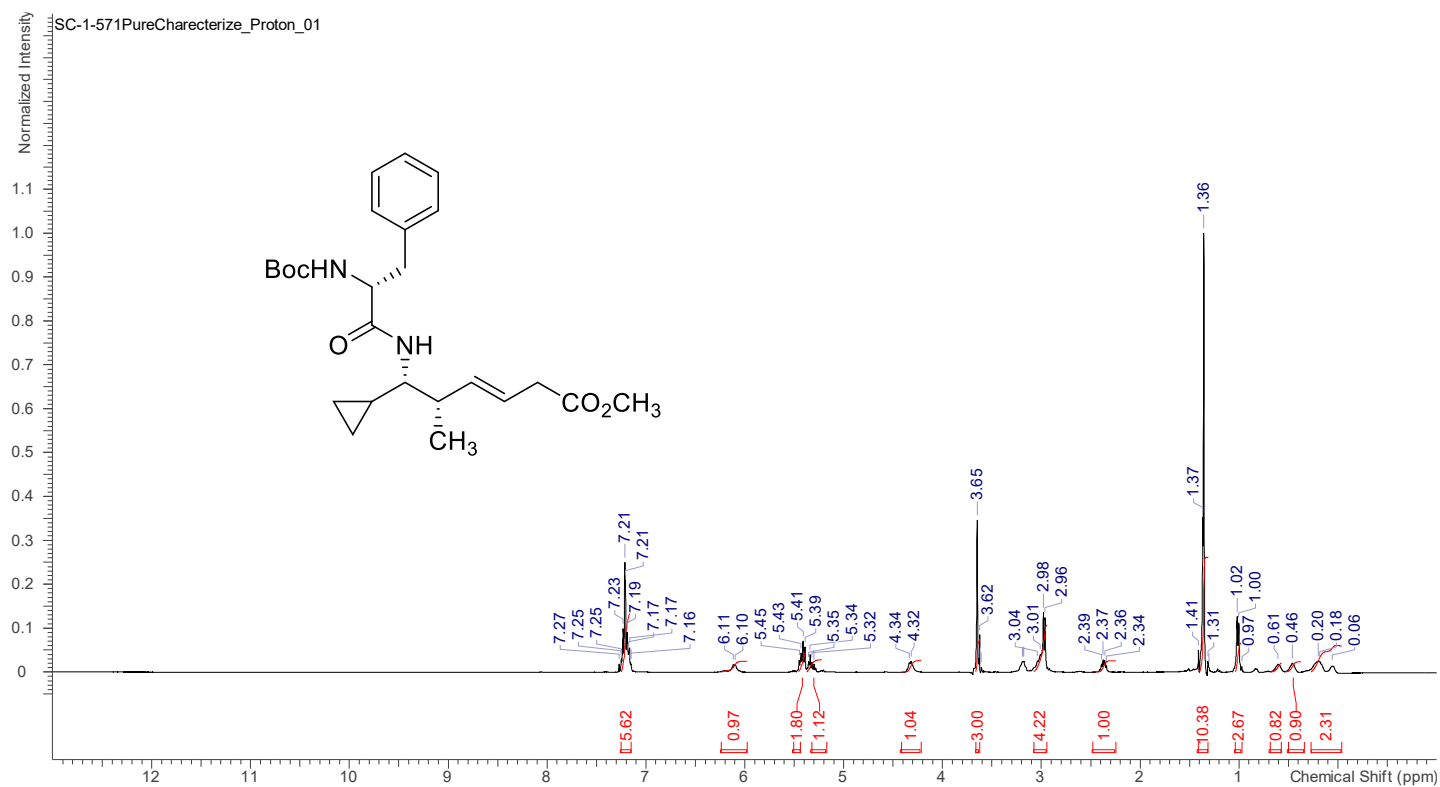
¹H NMR for Compound (*S*)-**10f**.



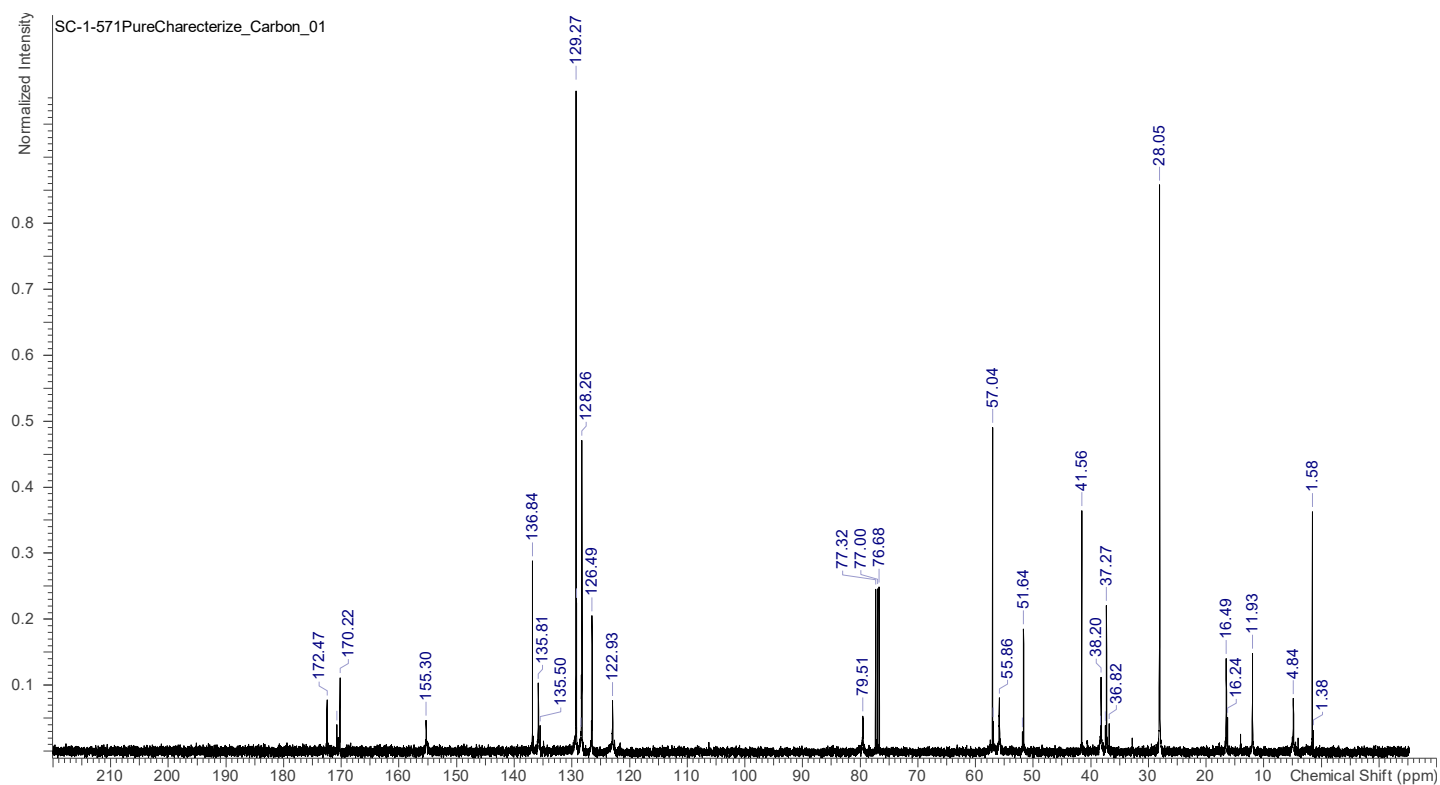
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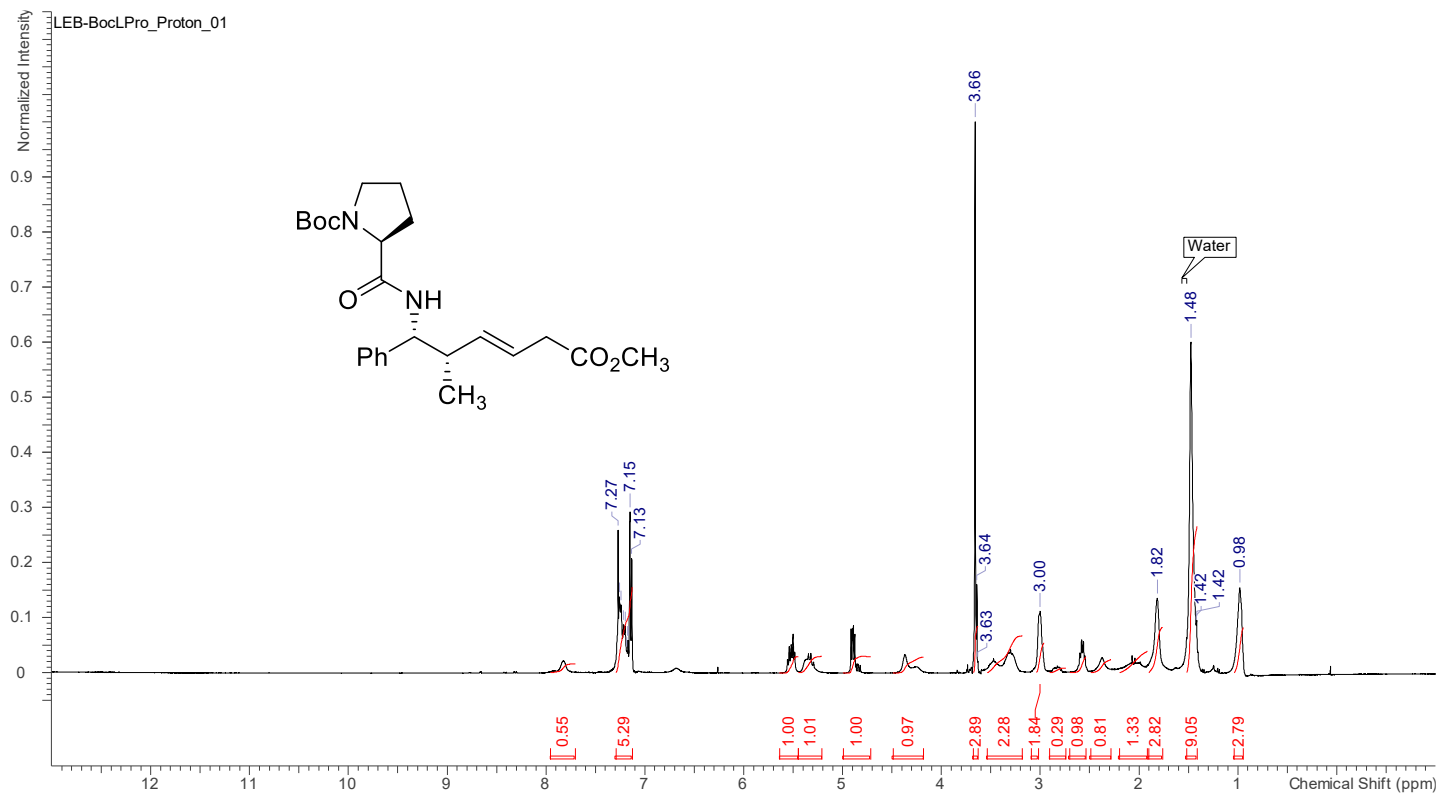
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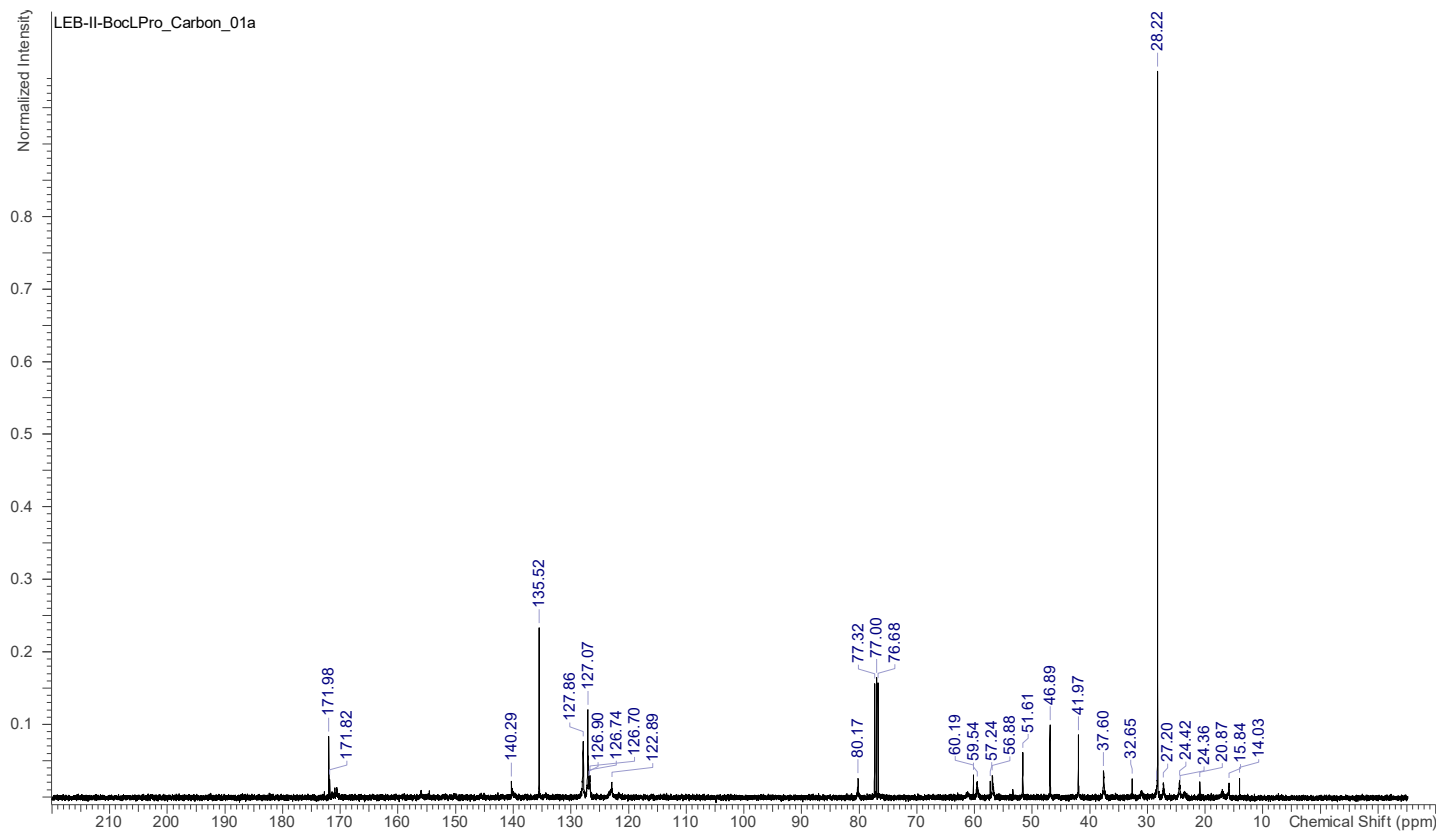
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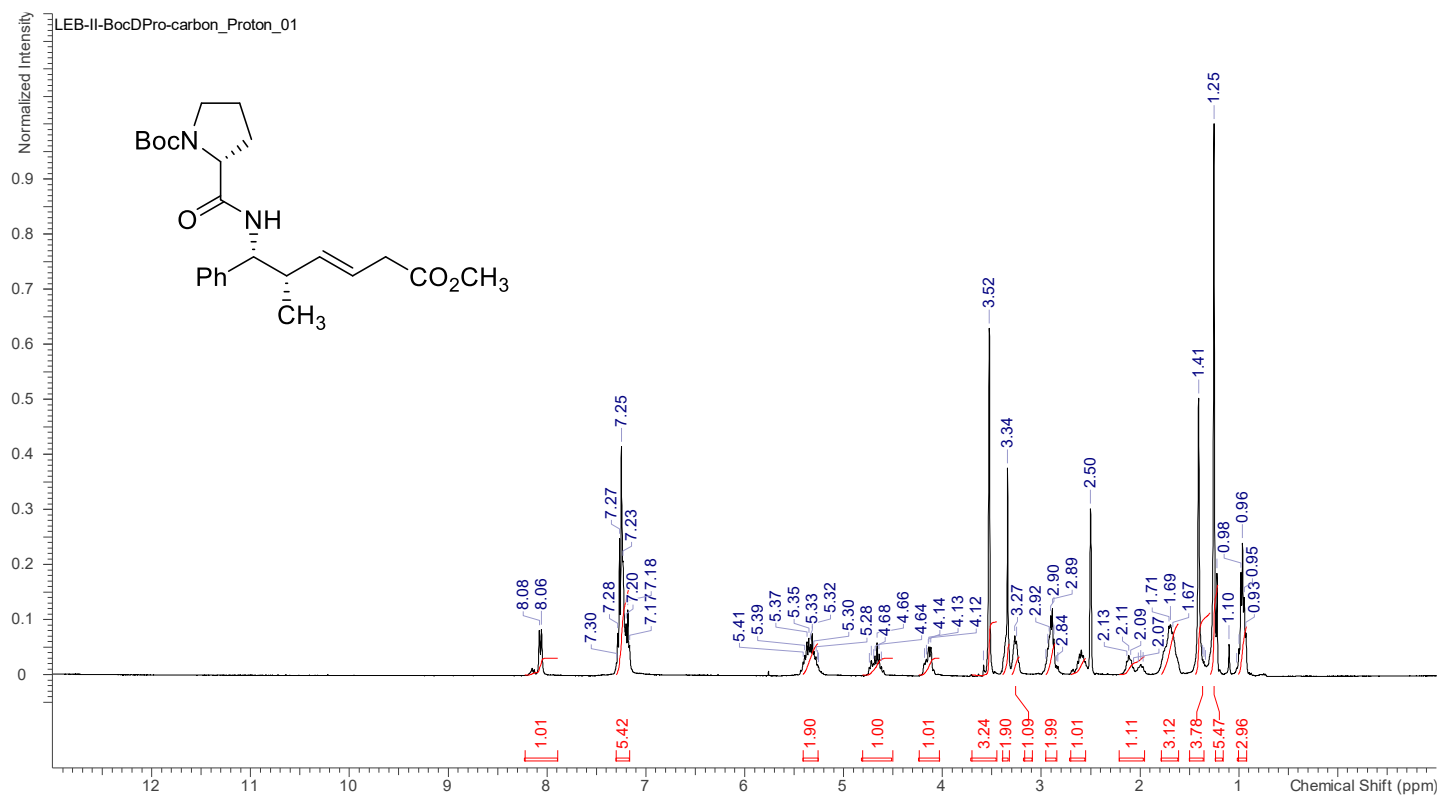
¹H NMR for Compound (S)-**10g**.



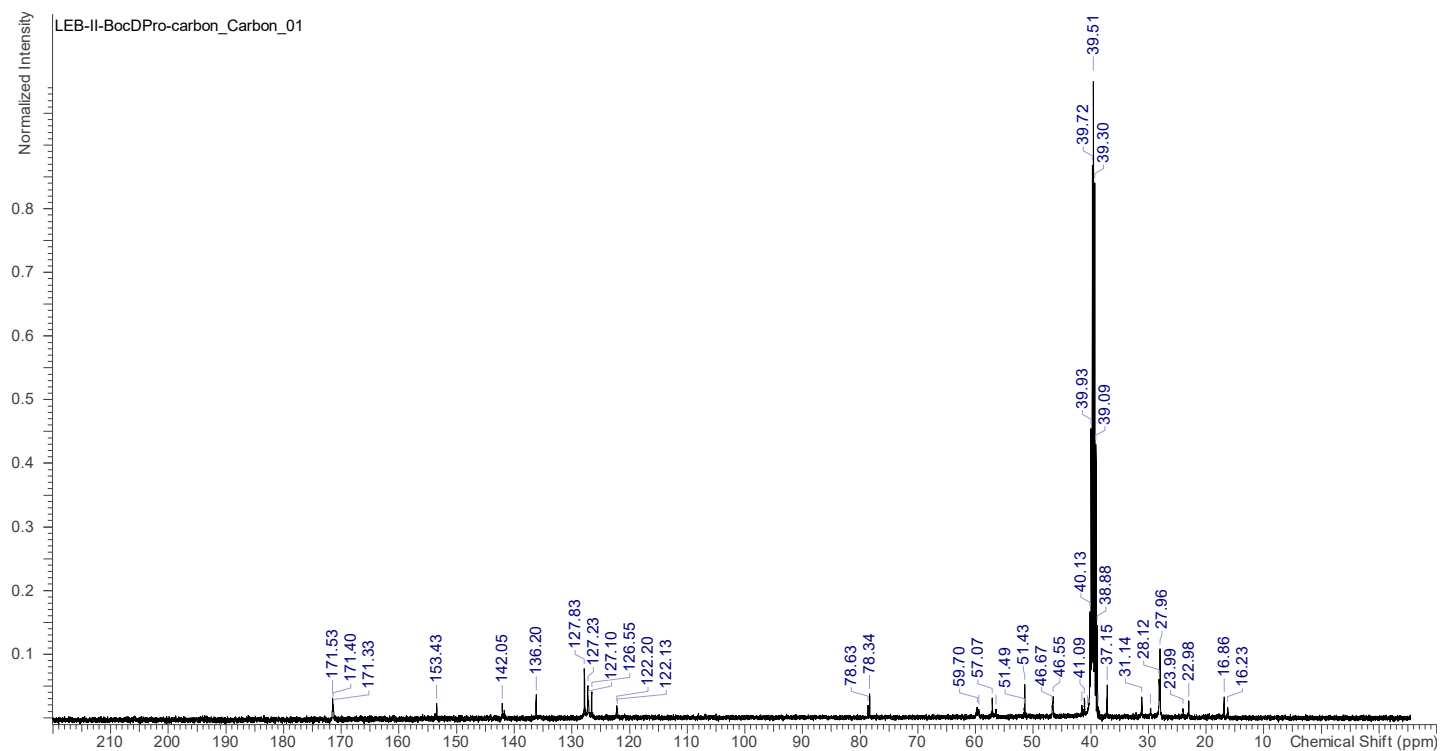
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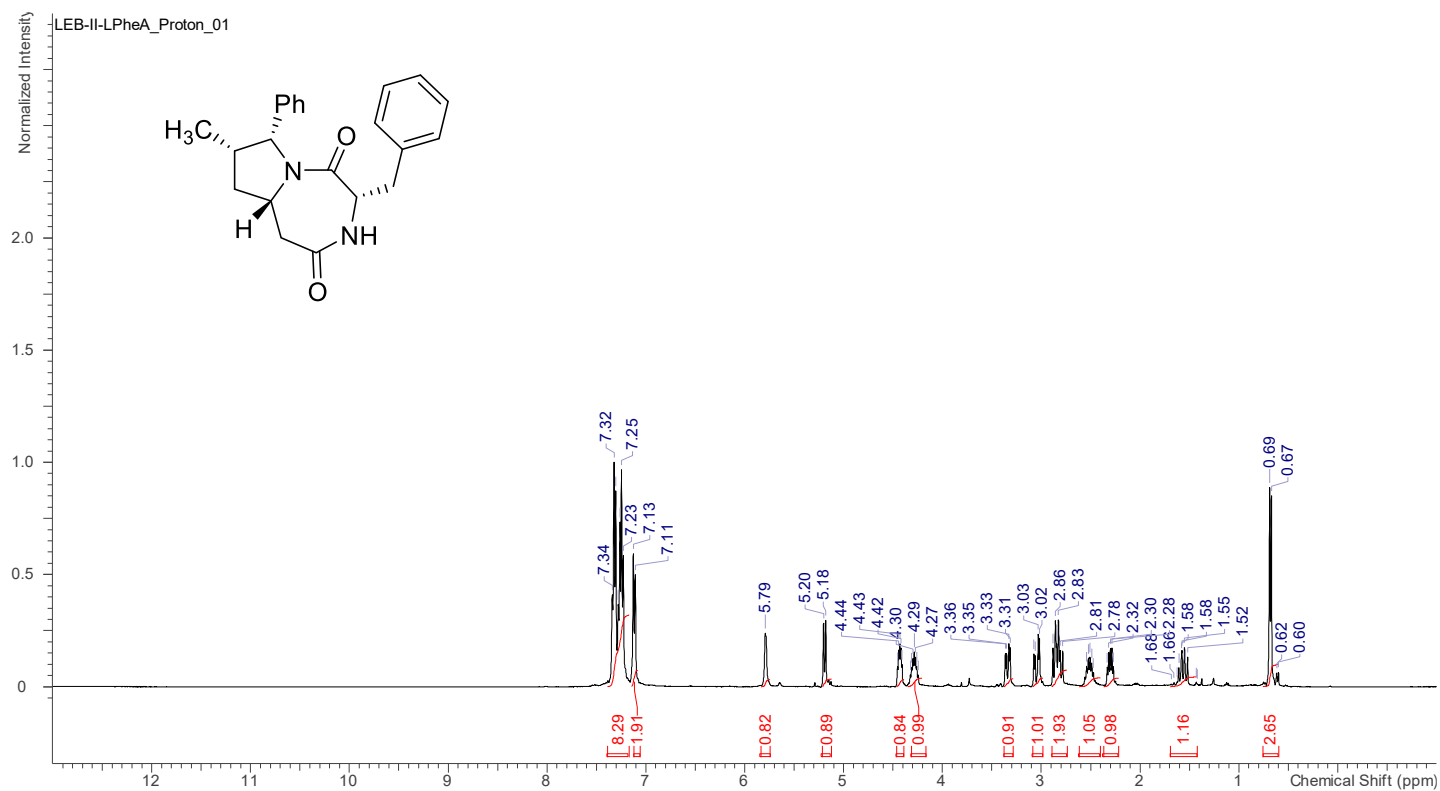
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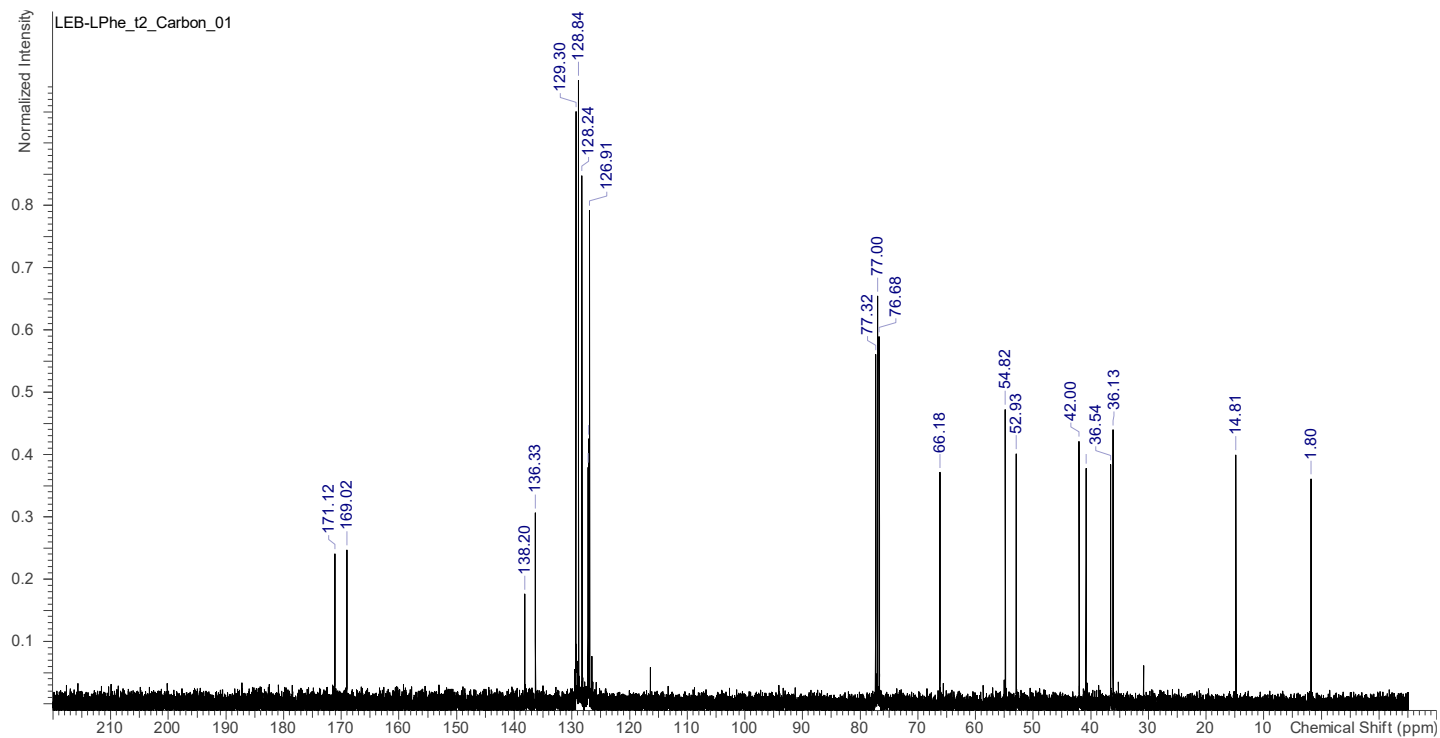
¹³C NMR for Compound (R)-10g.



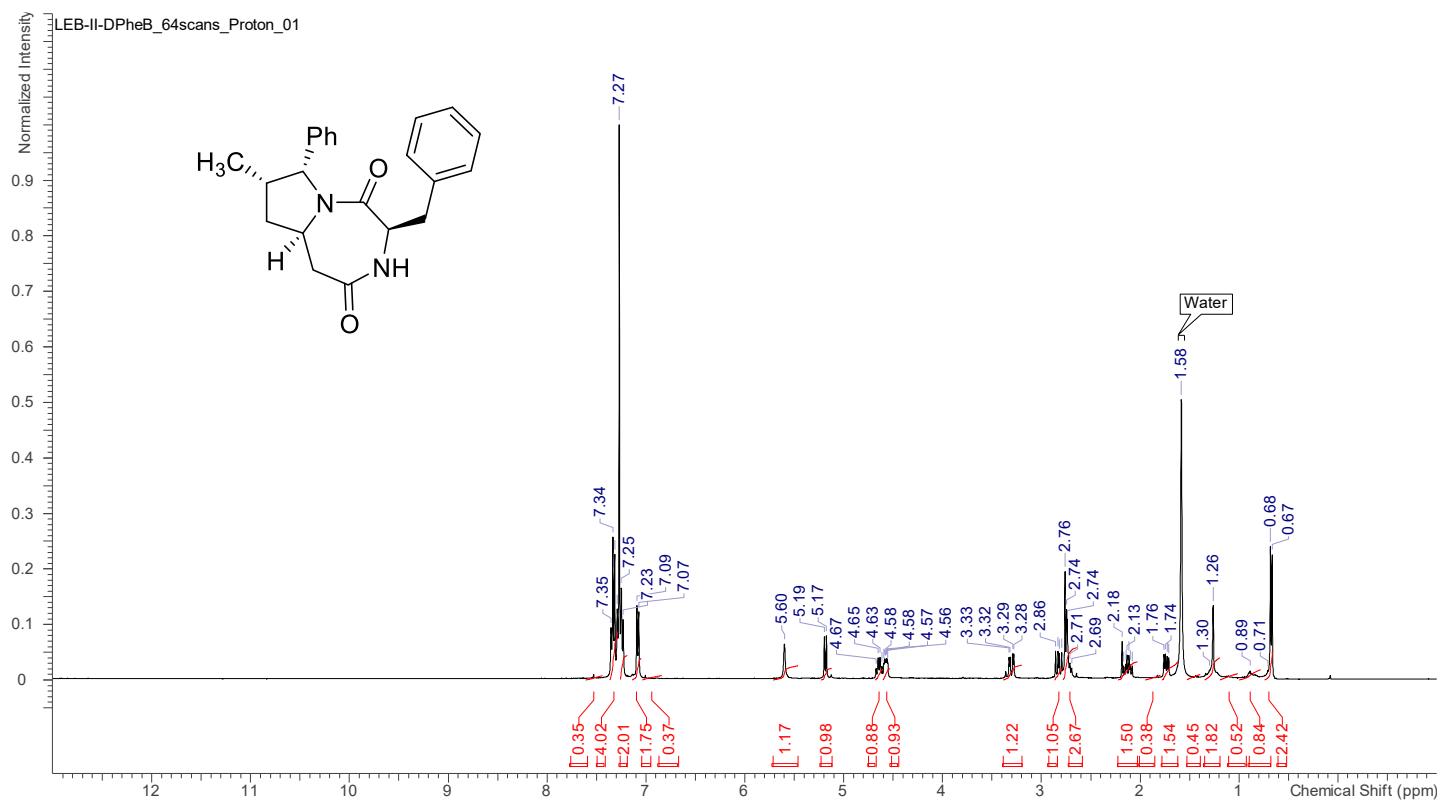
¹H NMR for Compound (*S,S*)-**3a**.



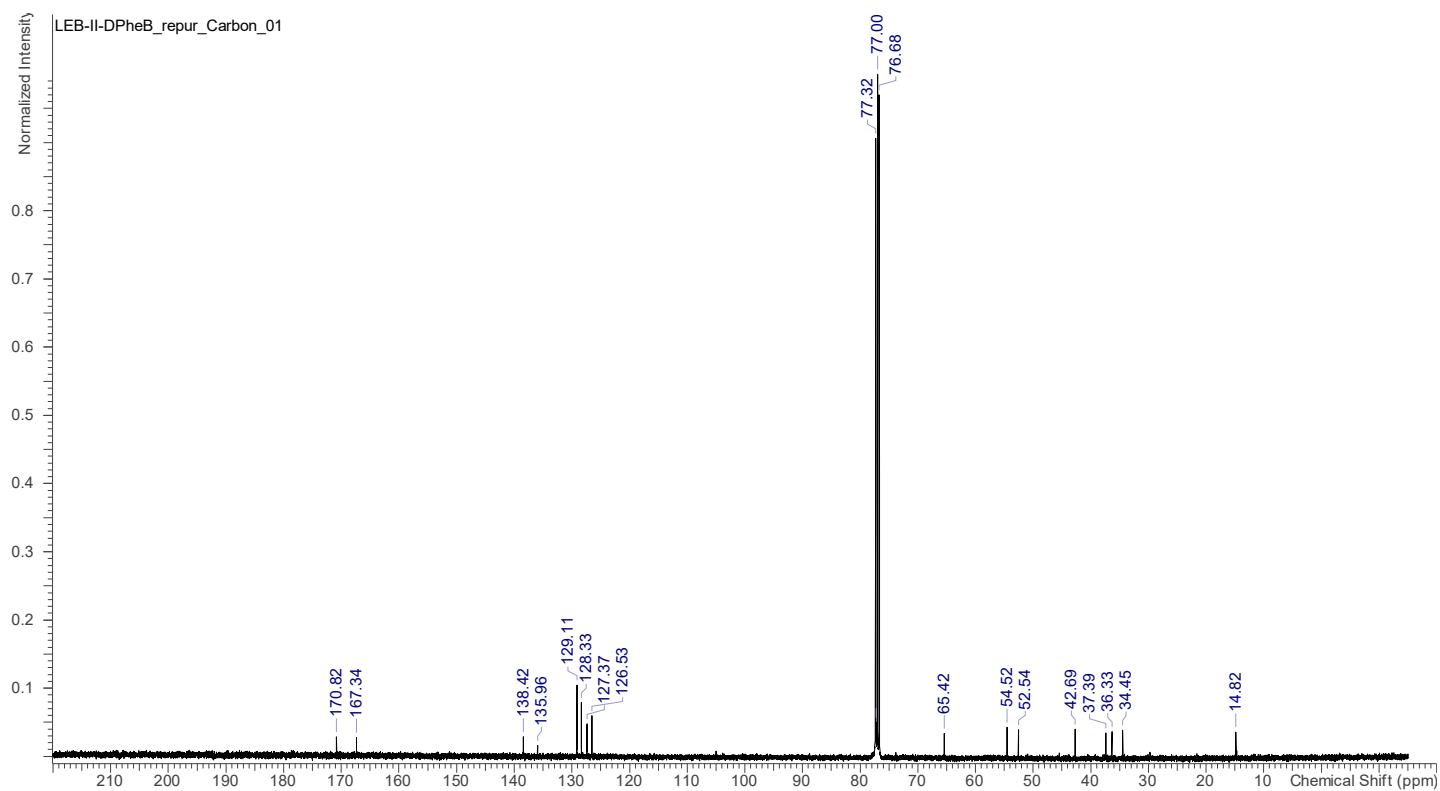
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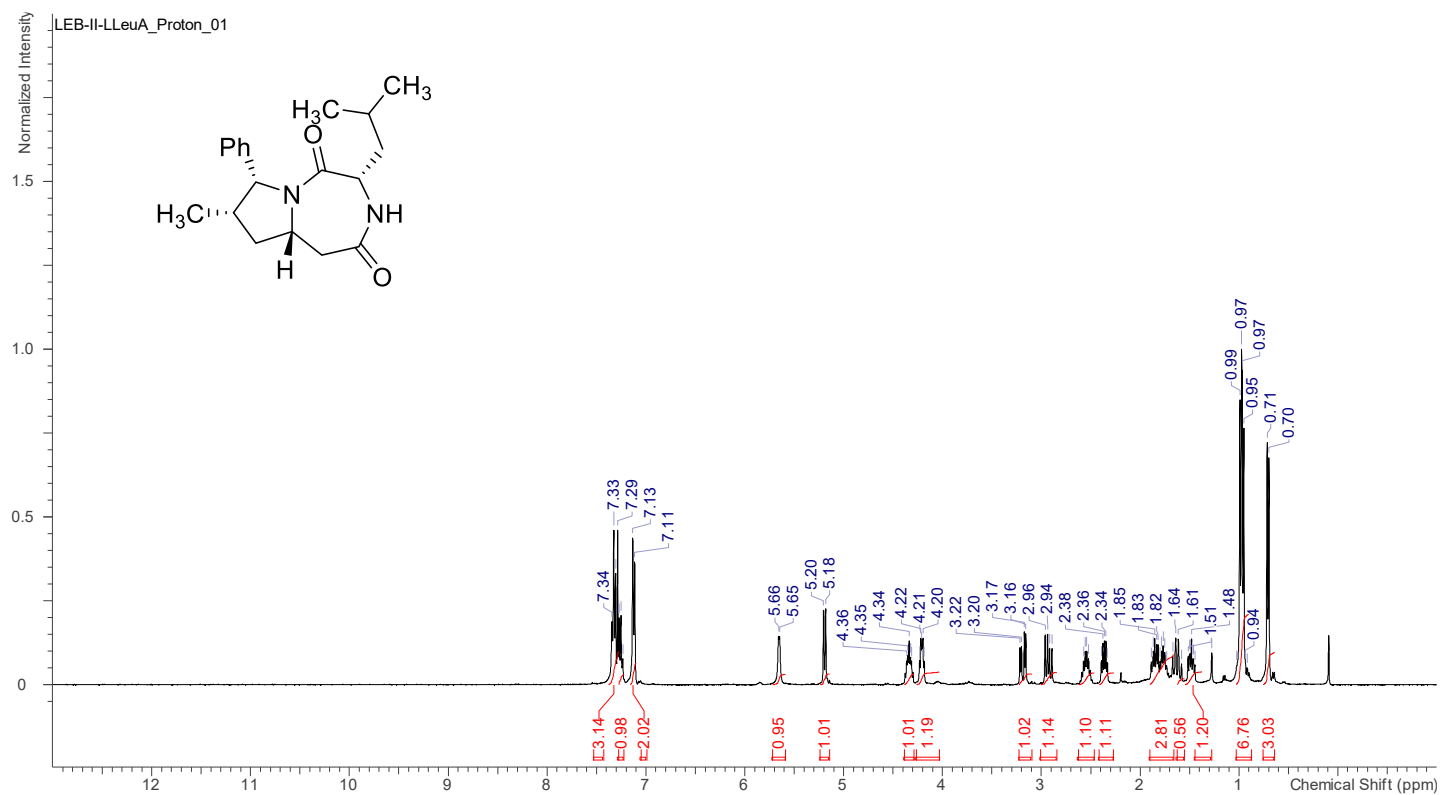
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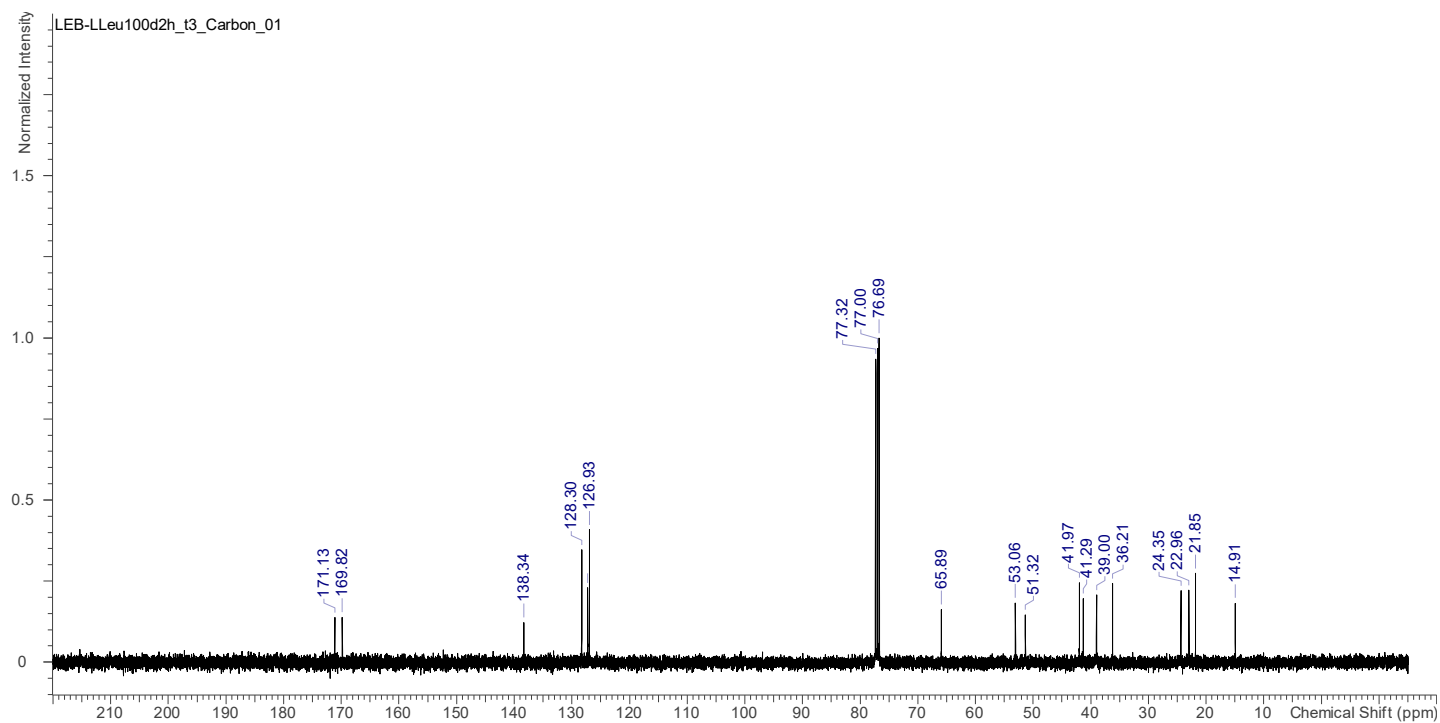
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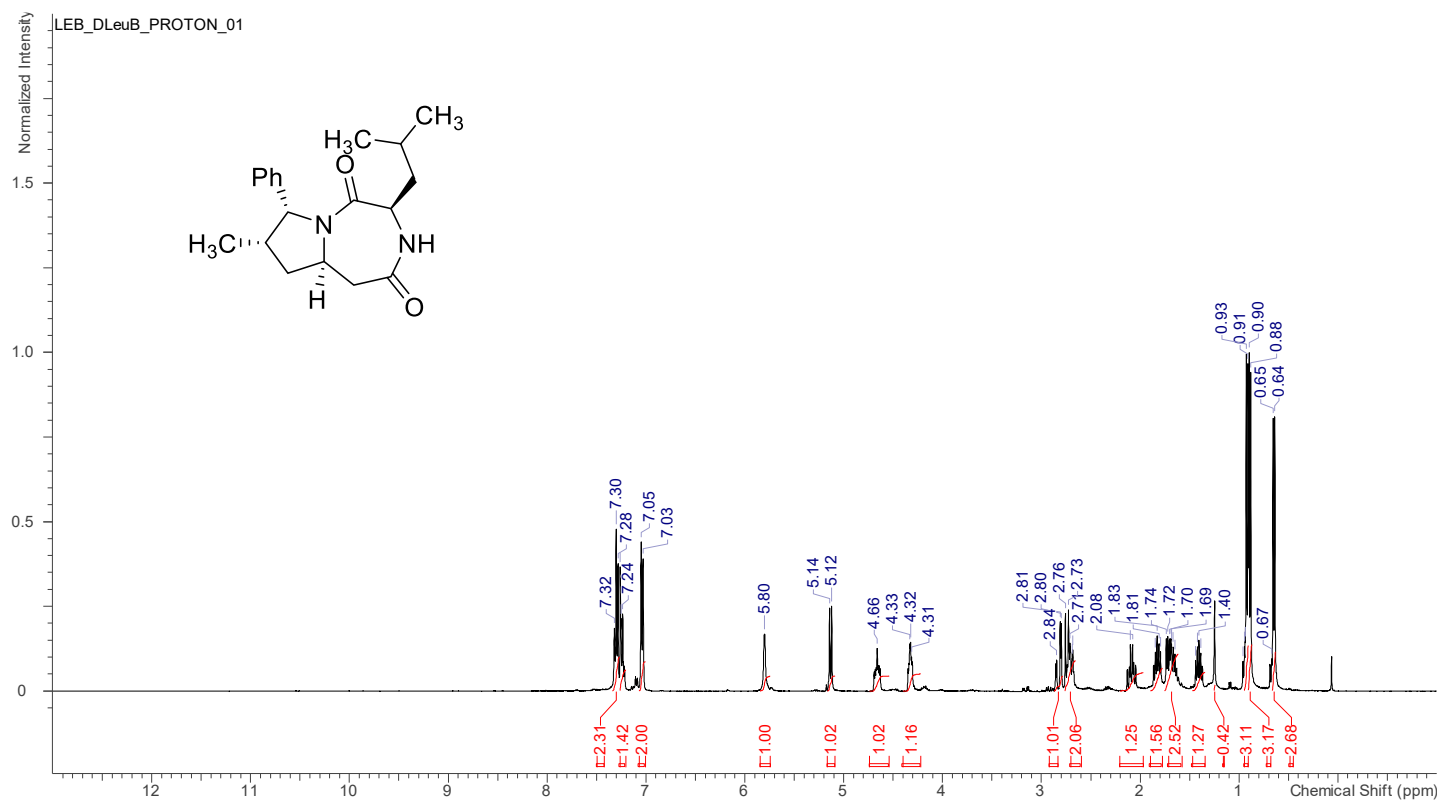
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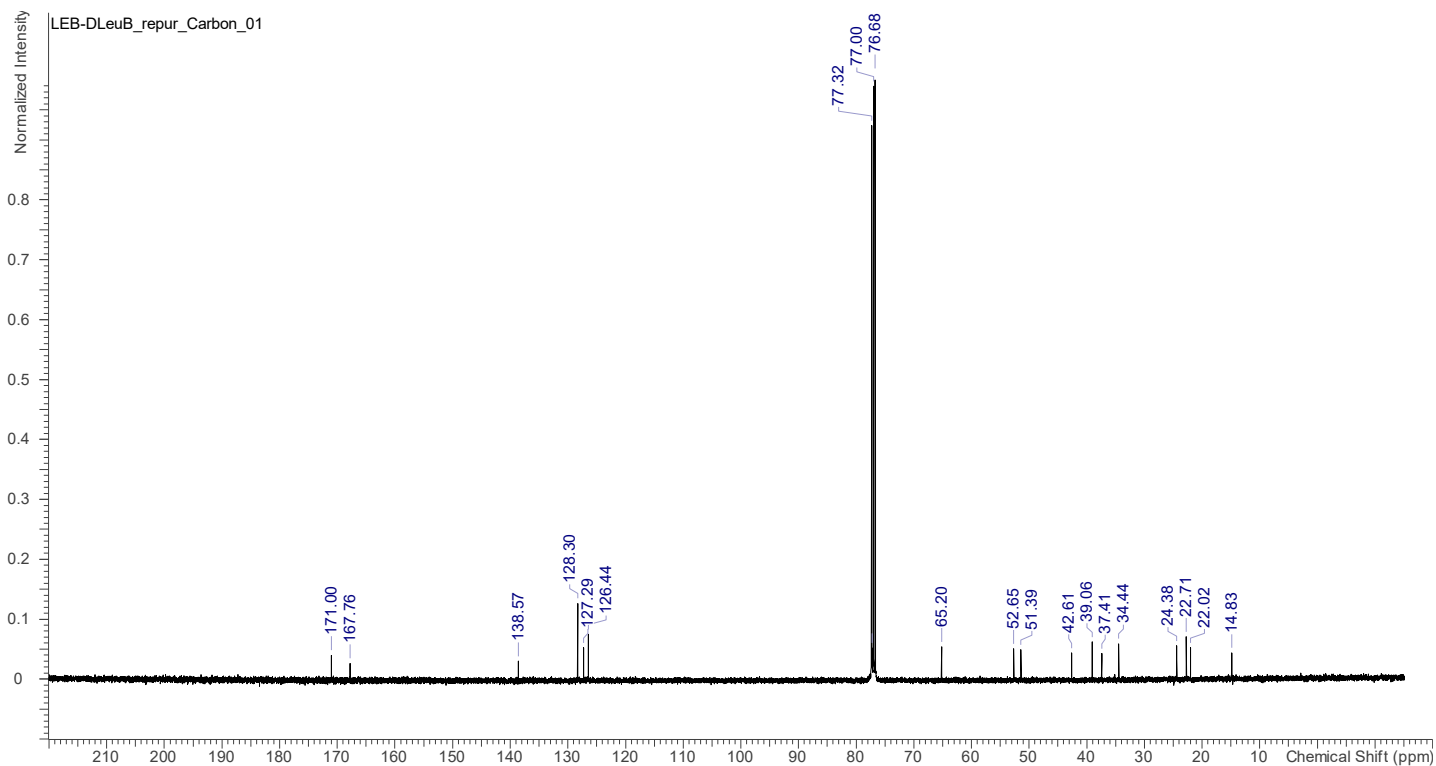
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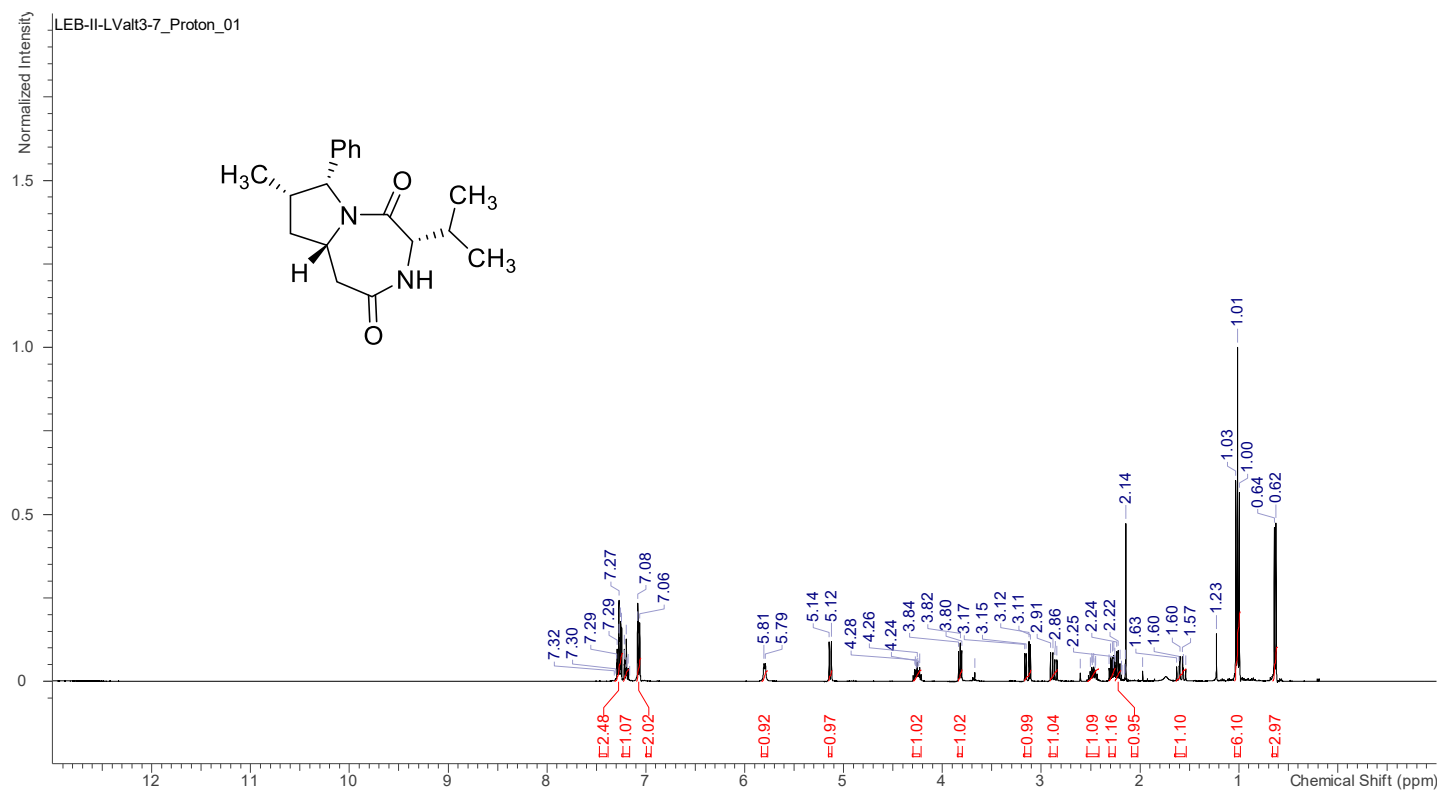
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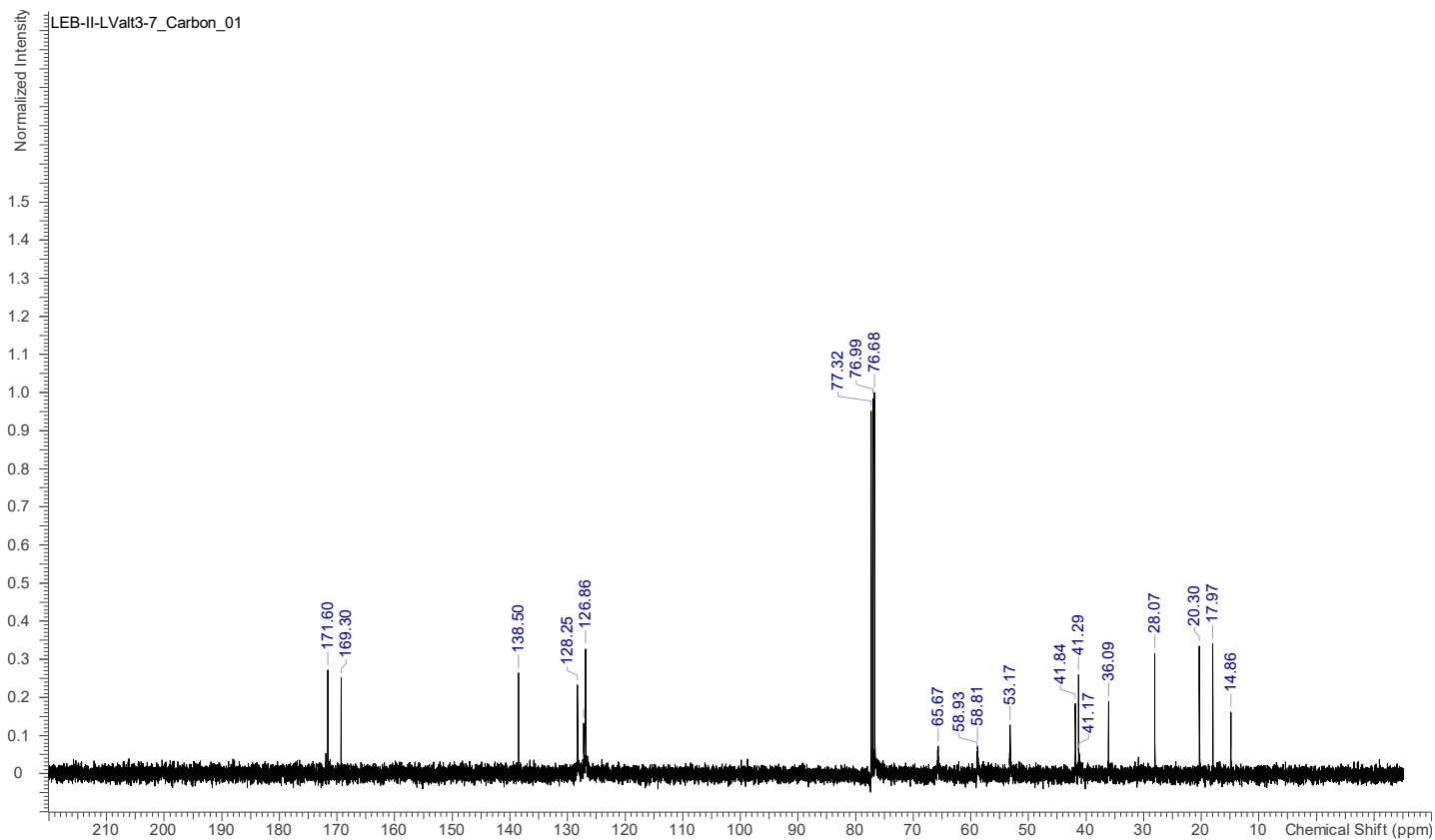
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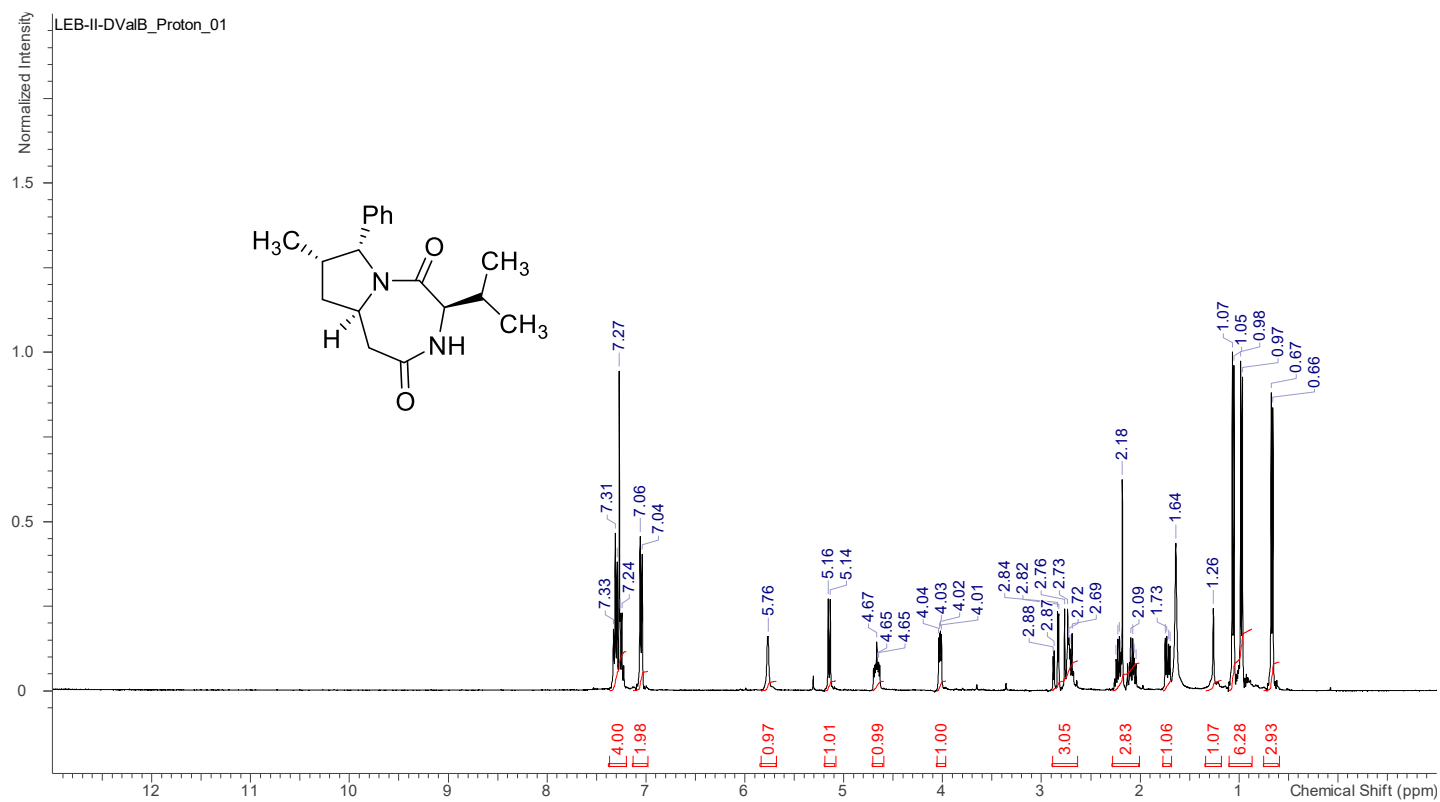
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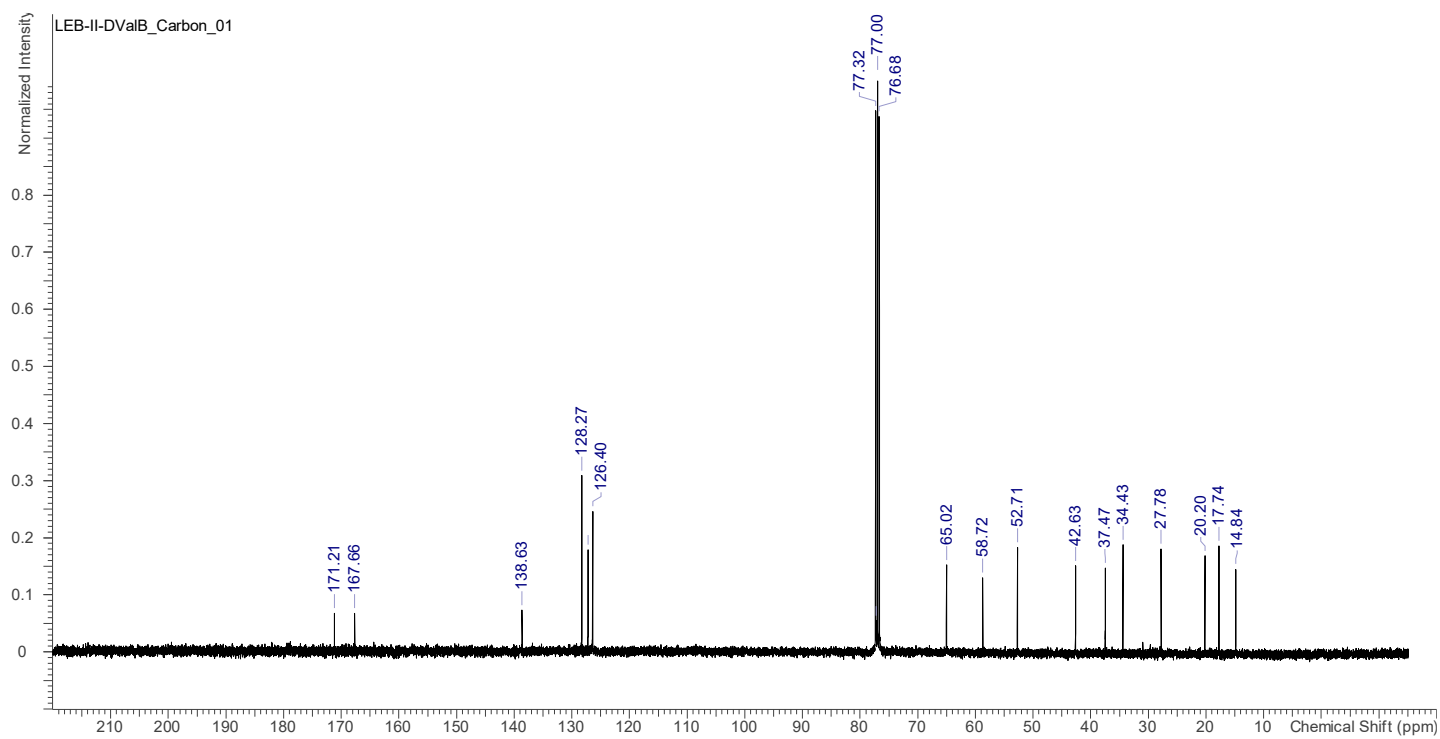
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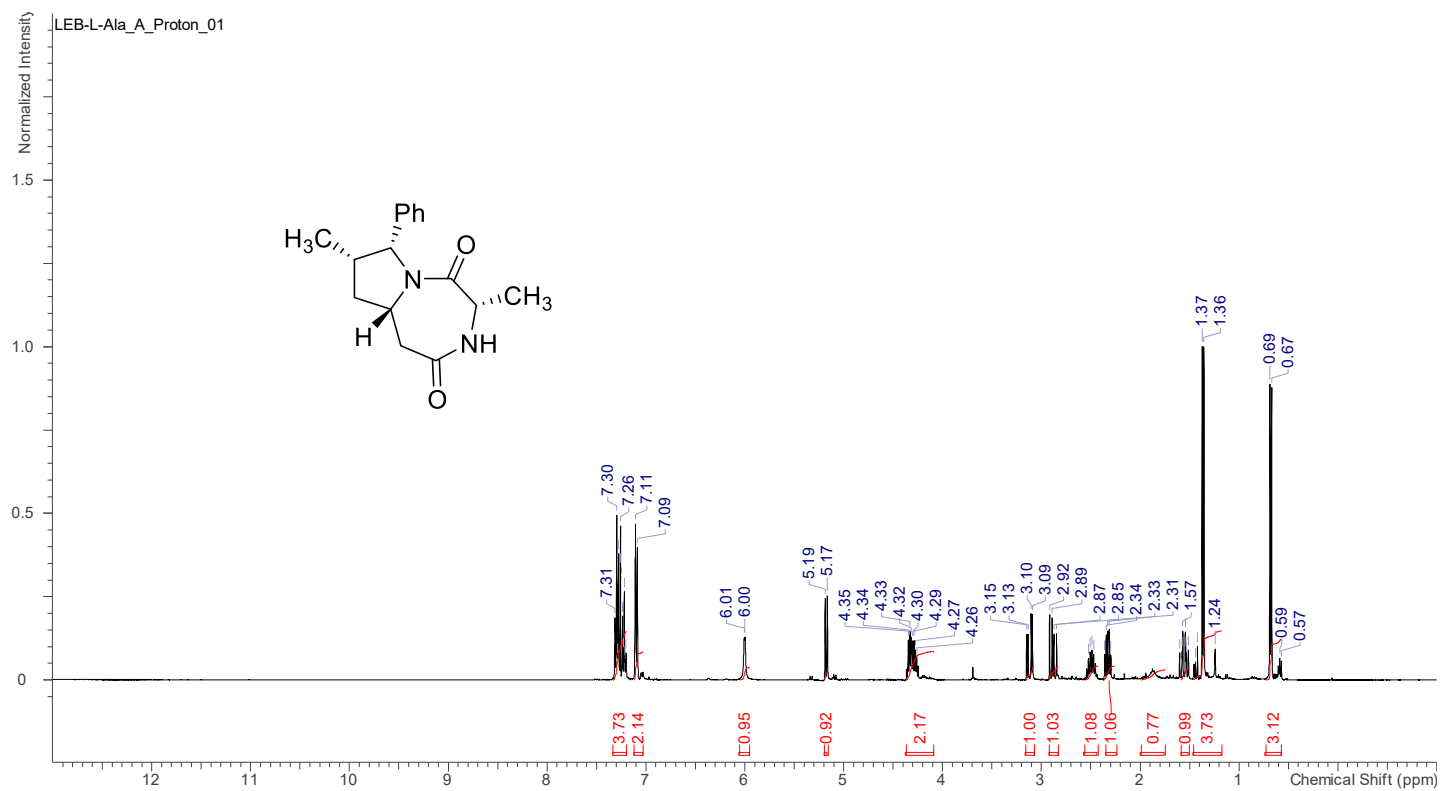
^1H NMR for Compound (*R,R*)-**3c**.



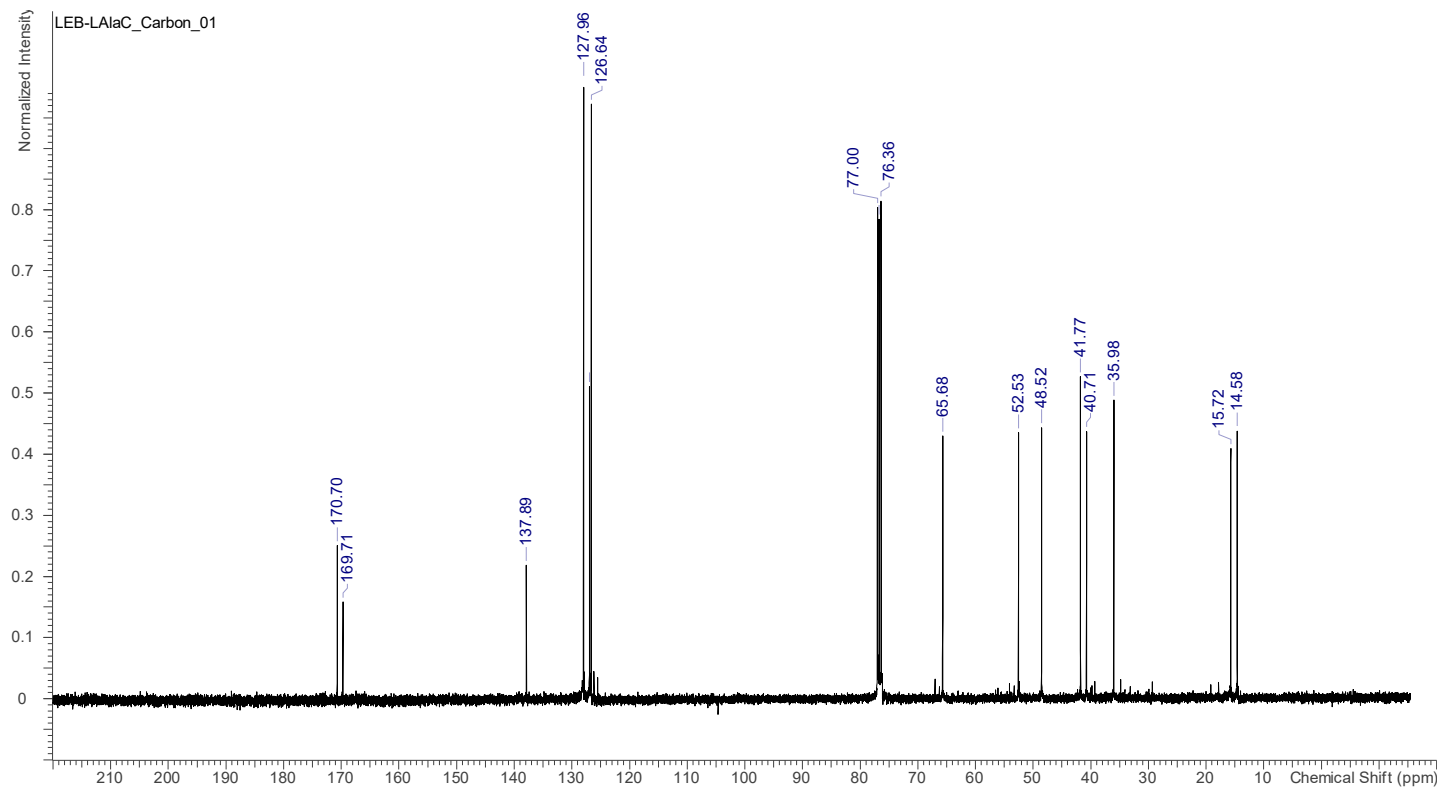
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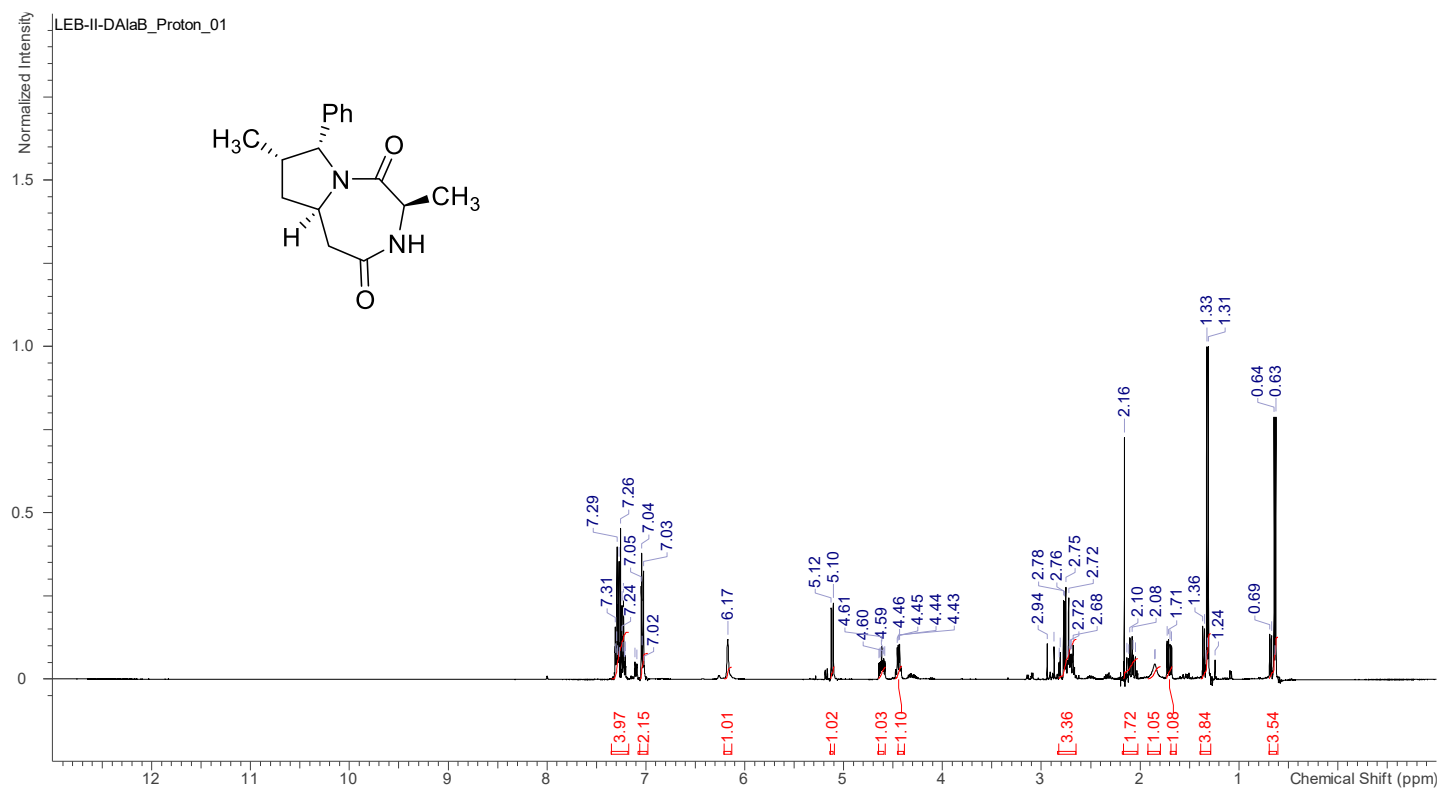
¹H NMR for Compound (*S,S*)-**3d**.



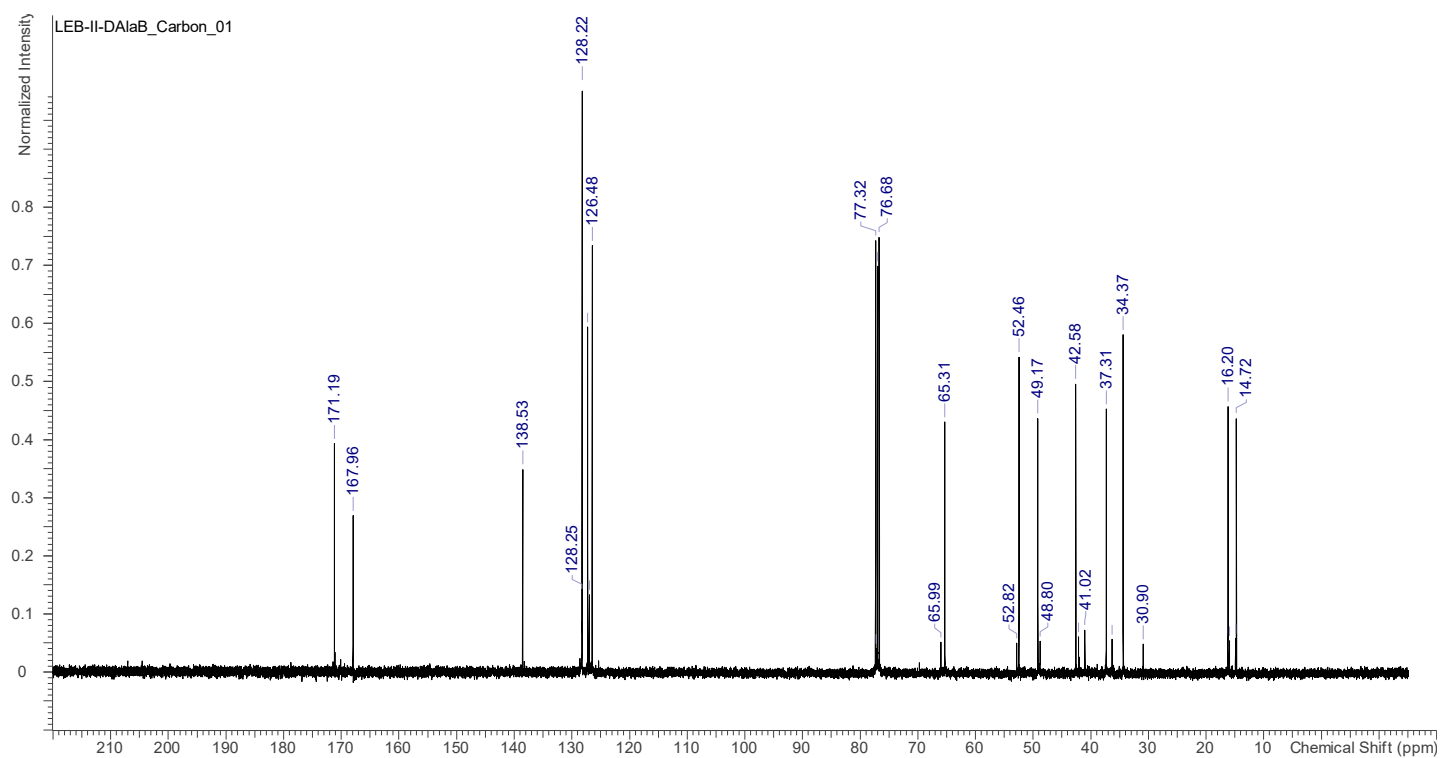
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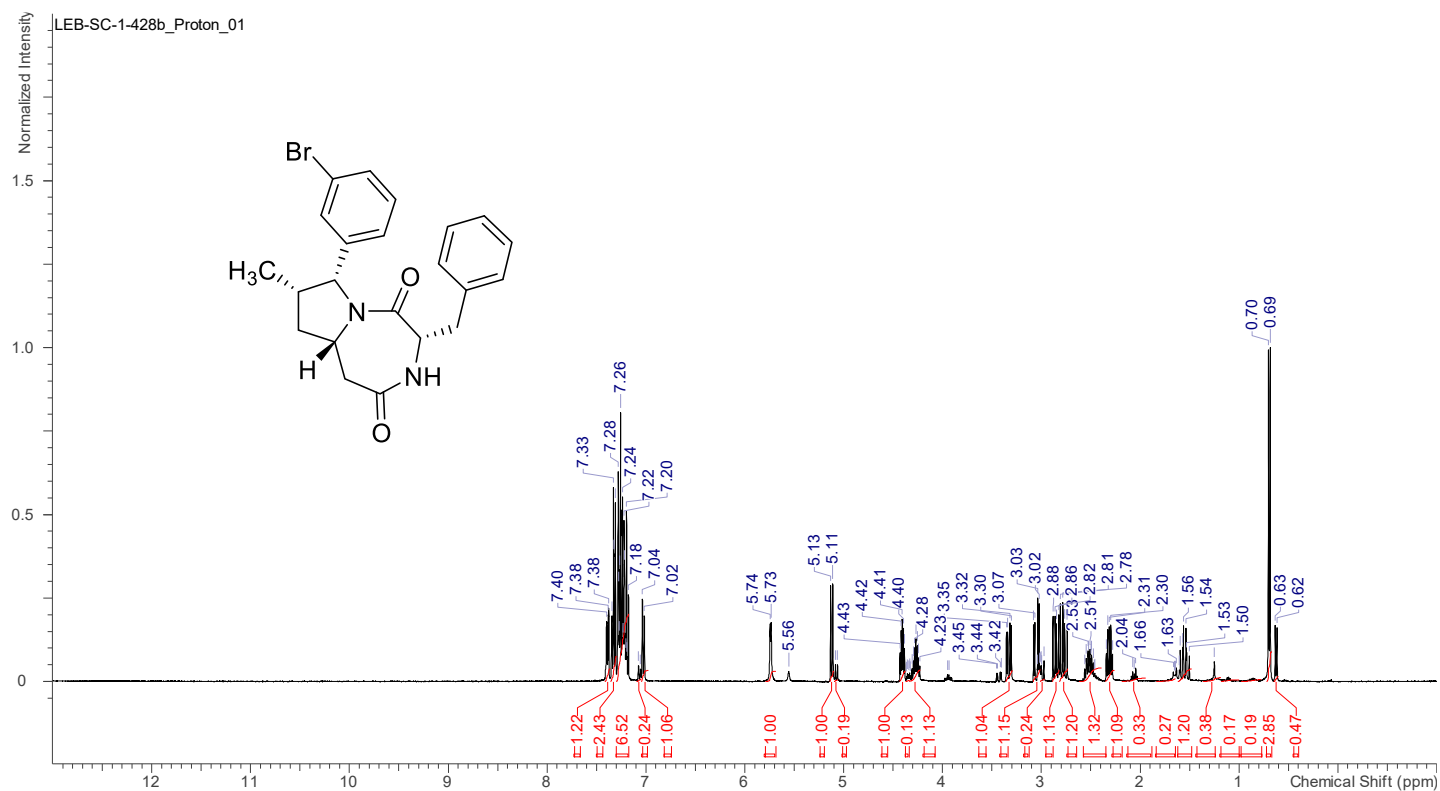
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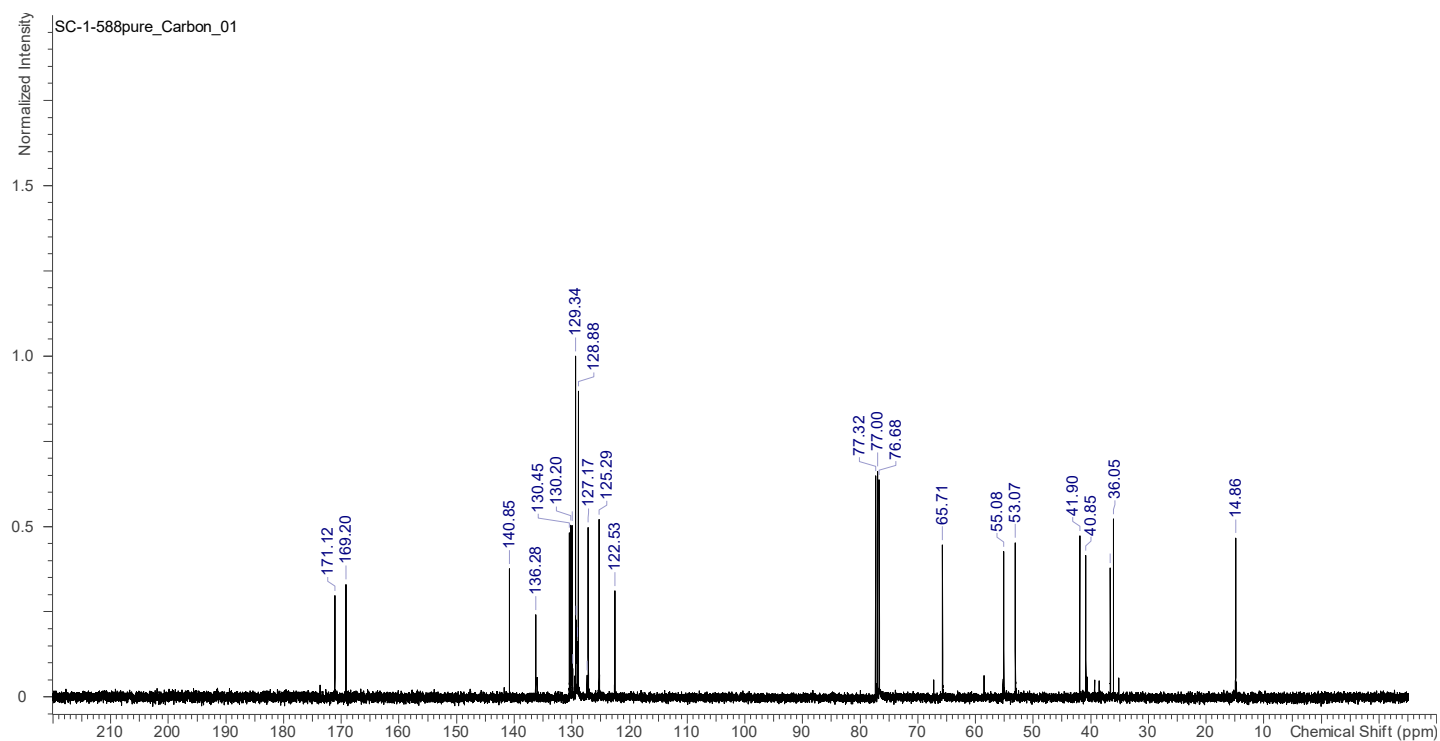
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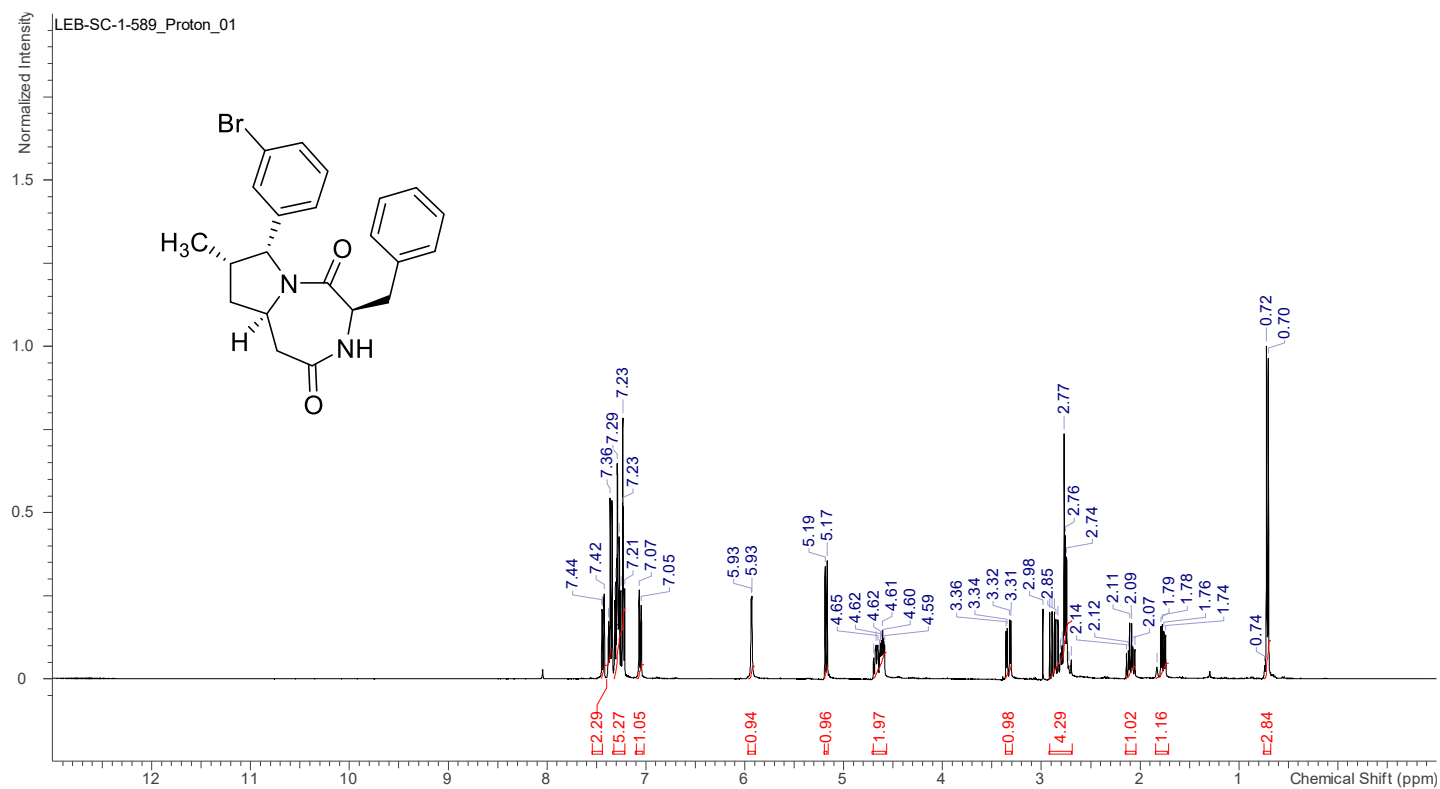
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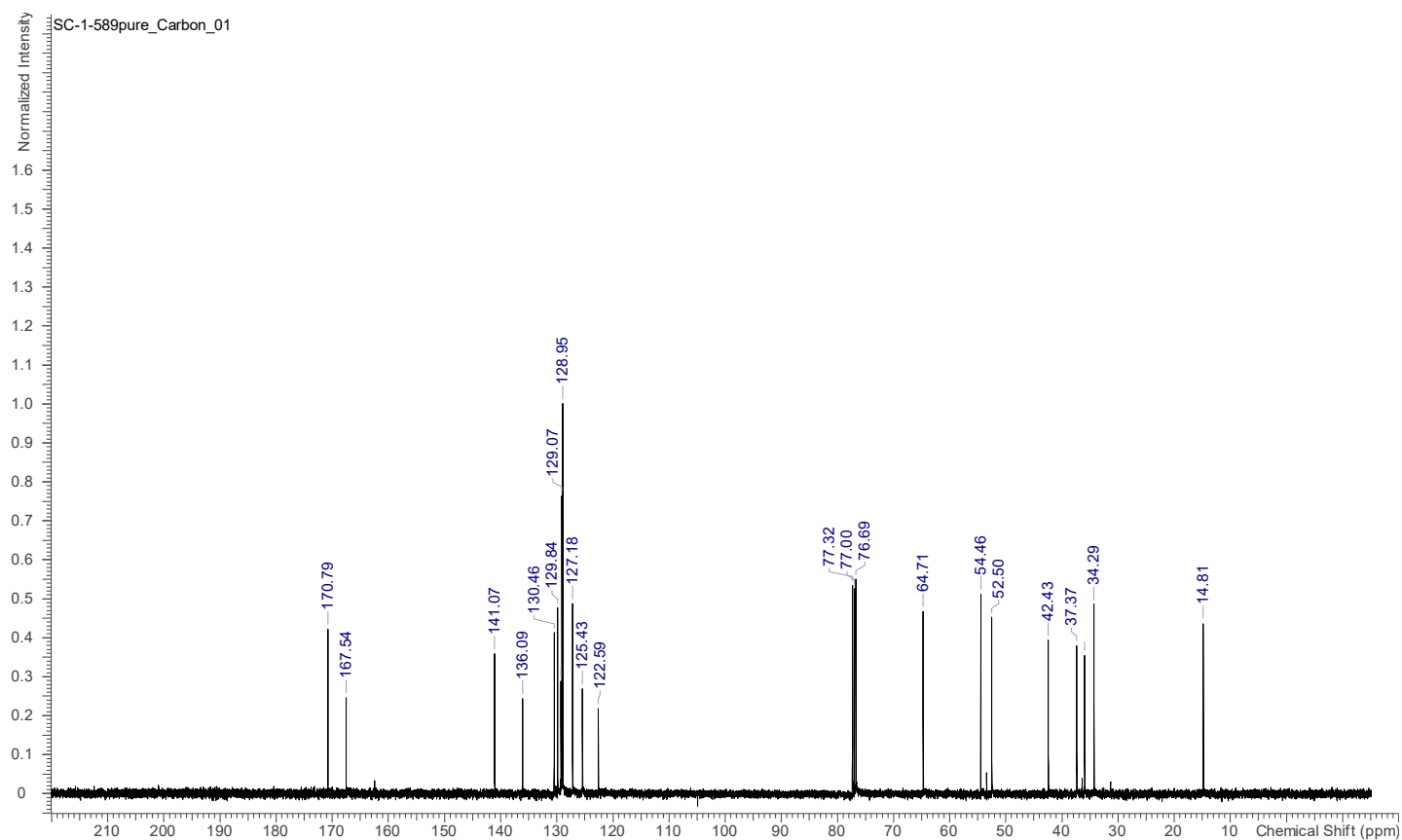
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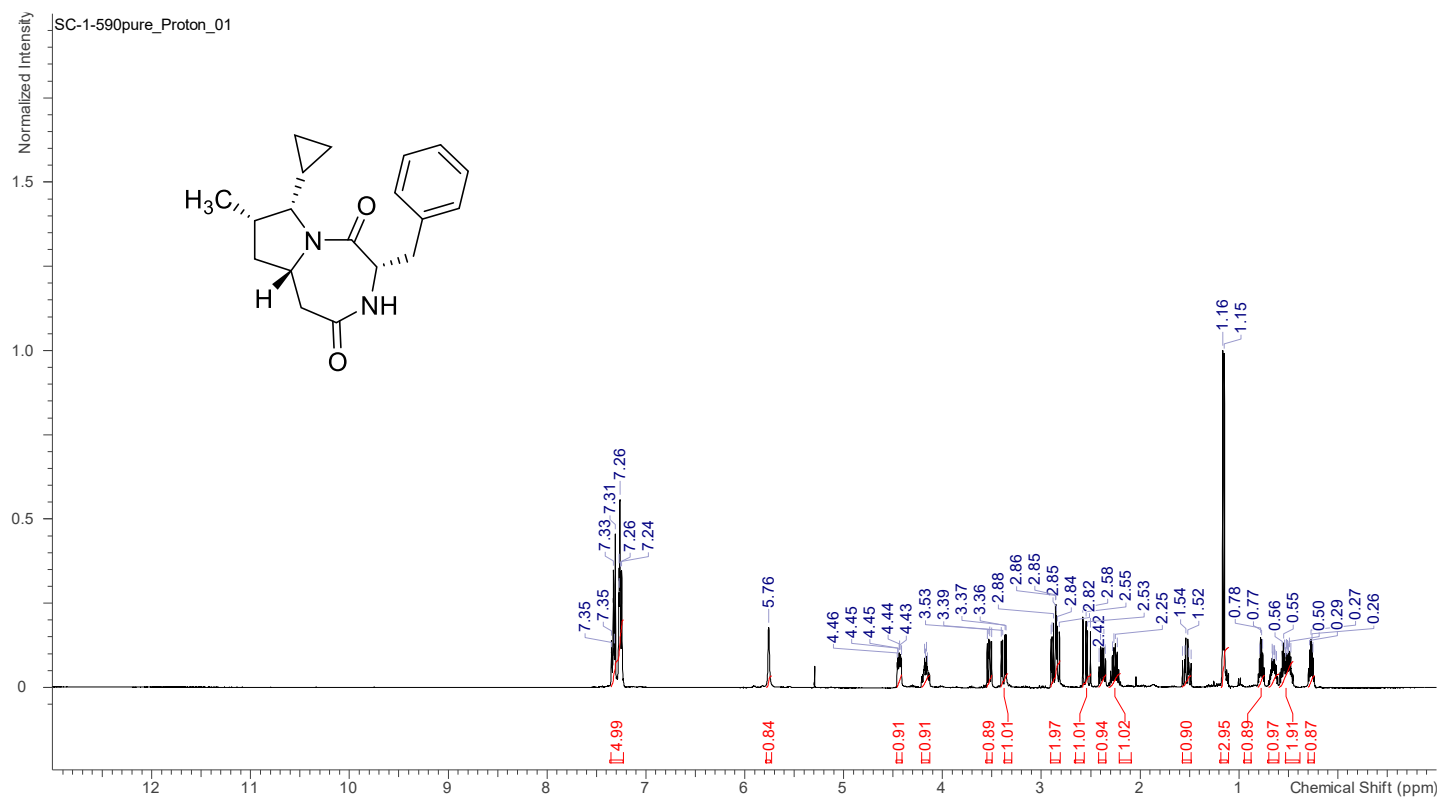
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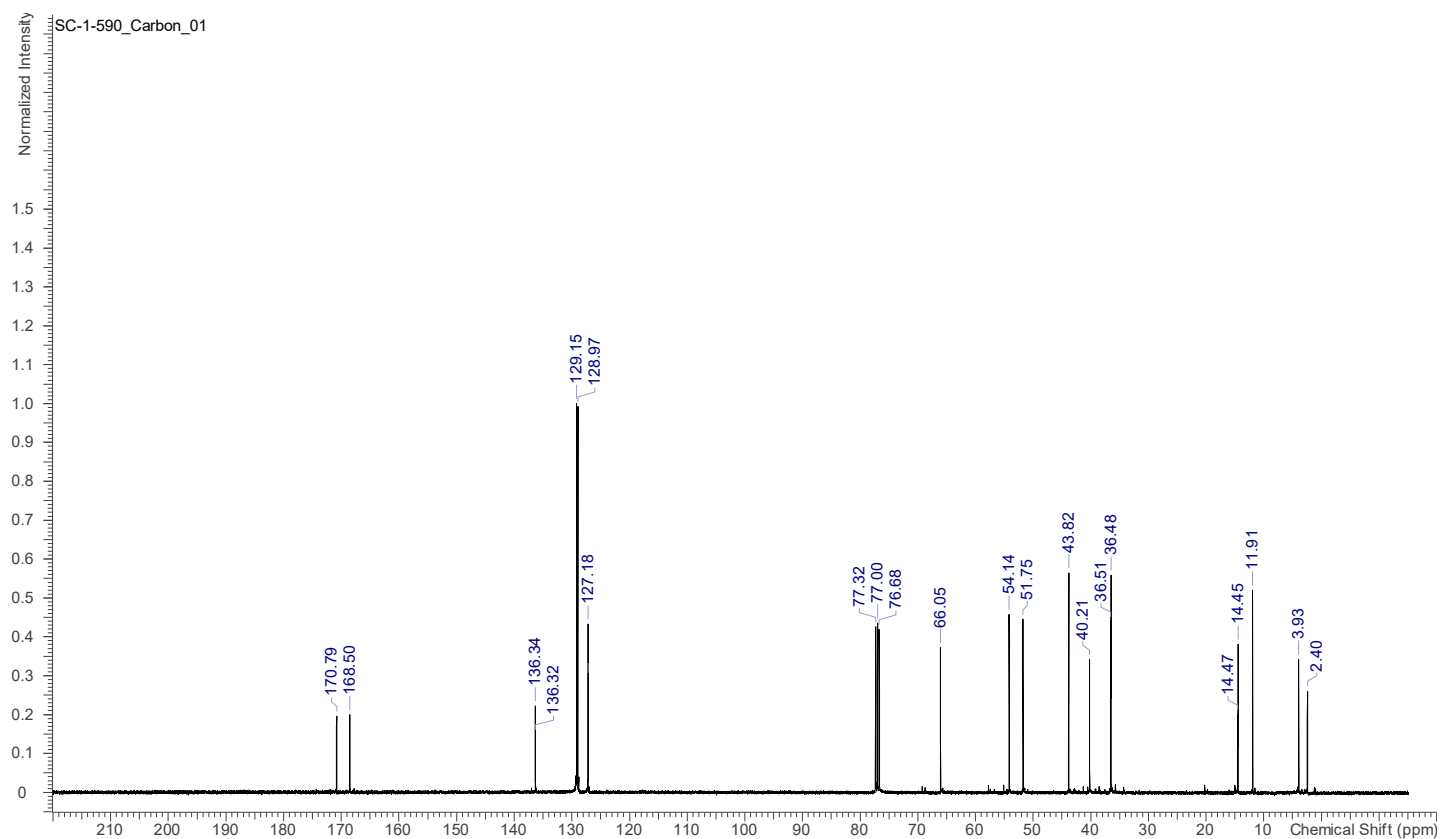
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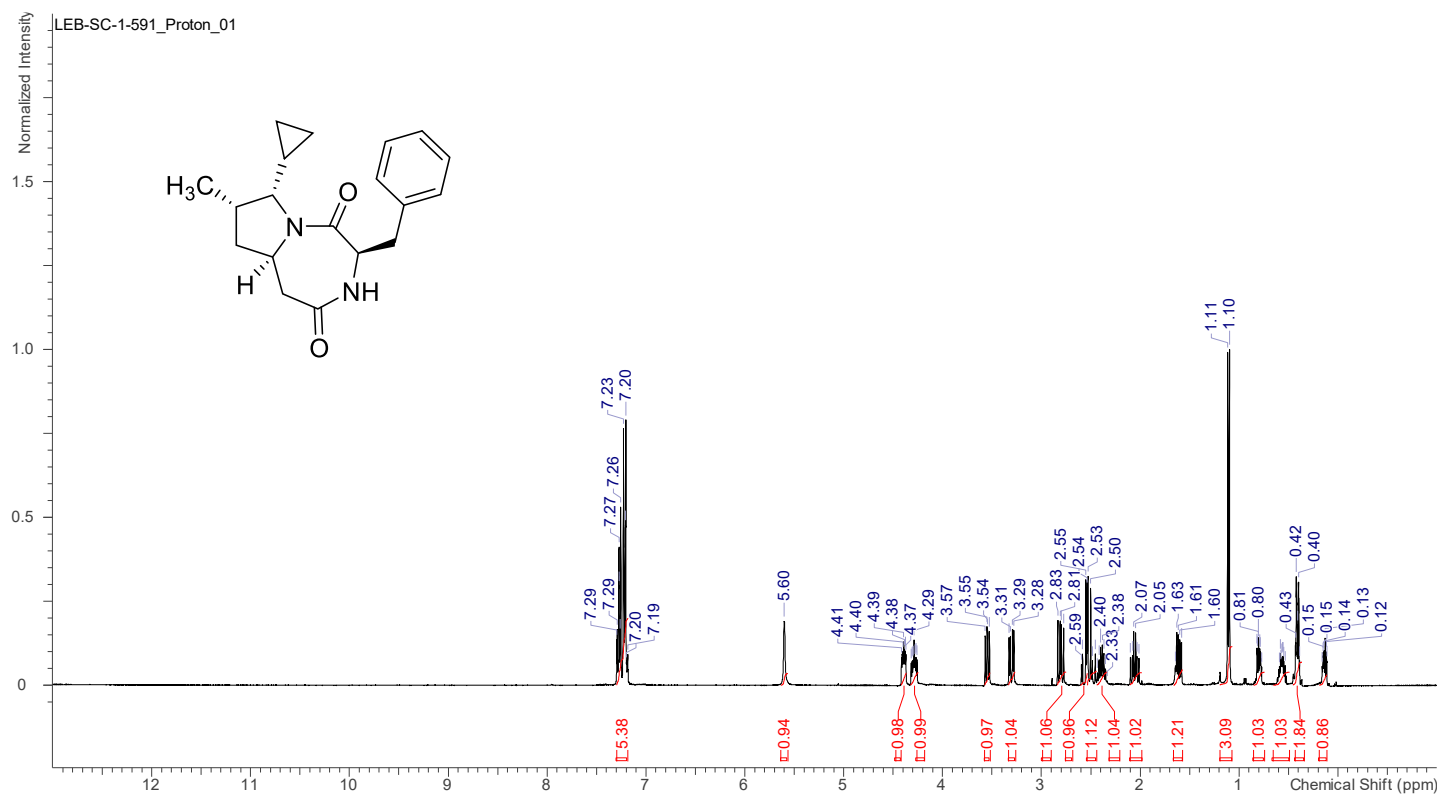
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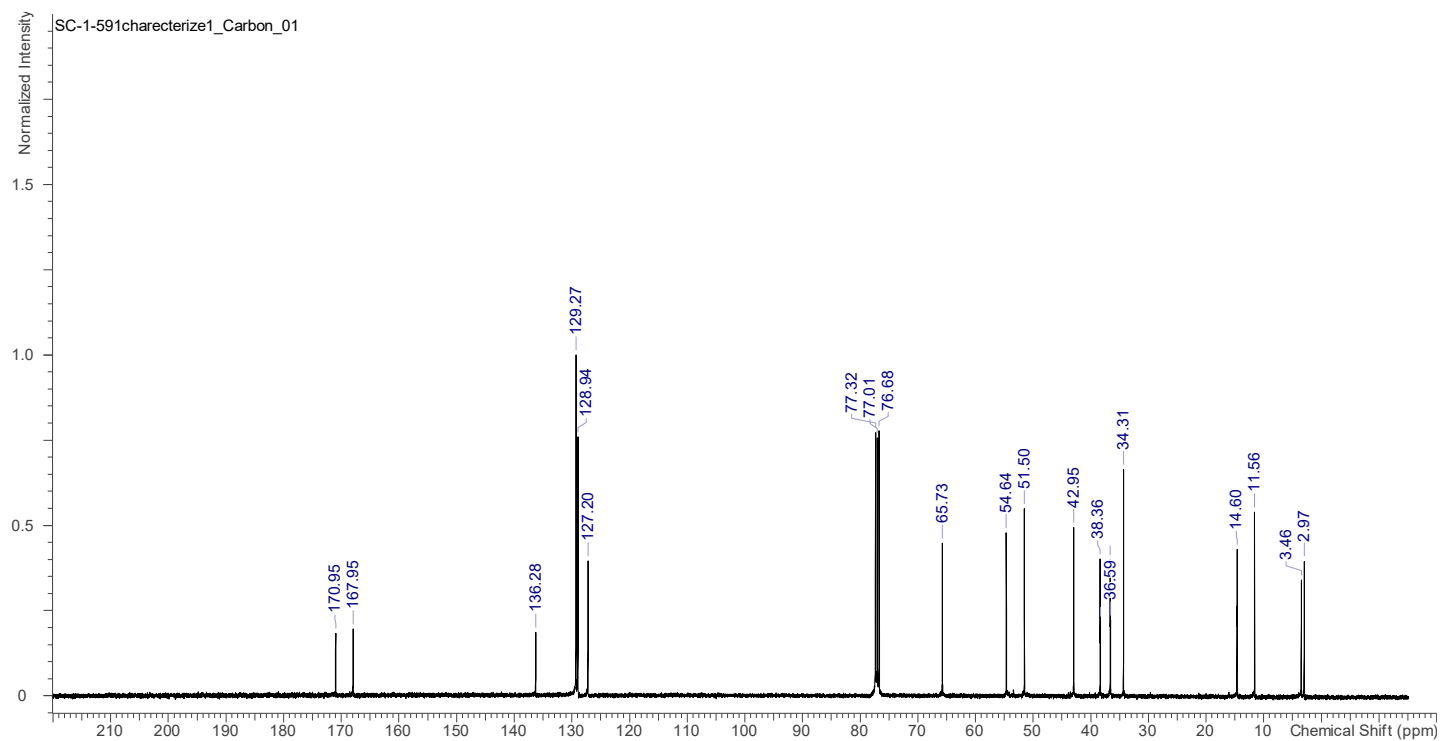
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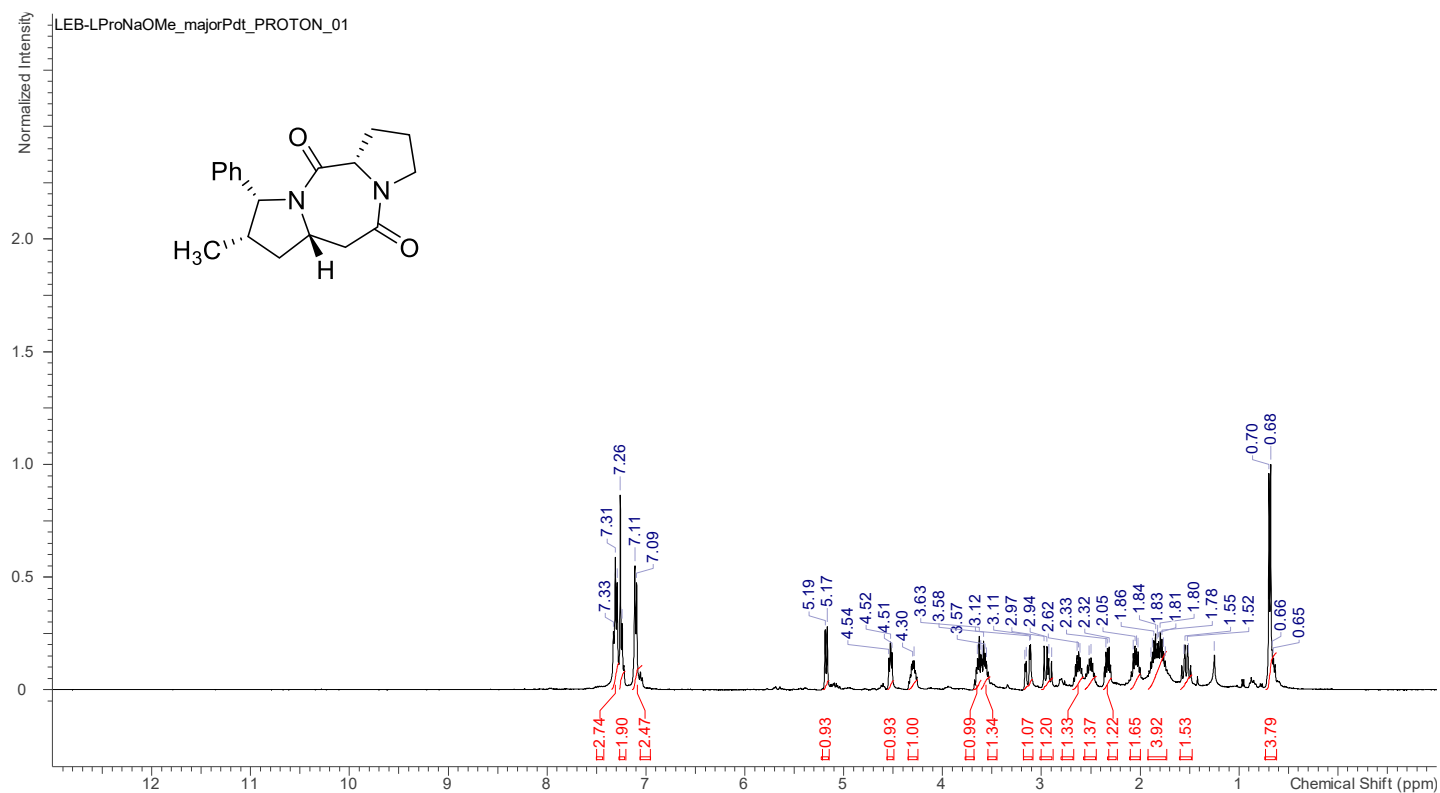
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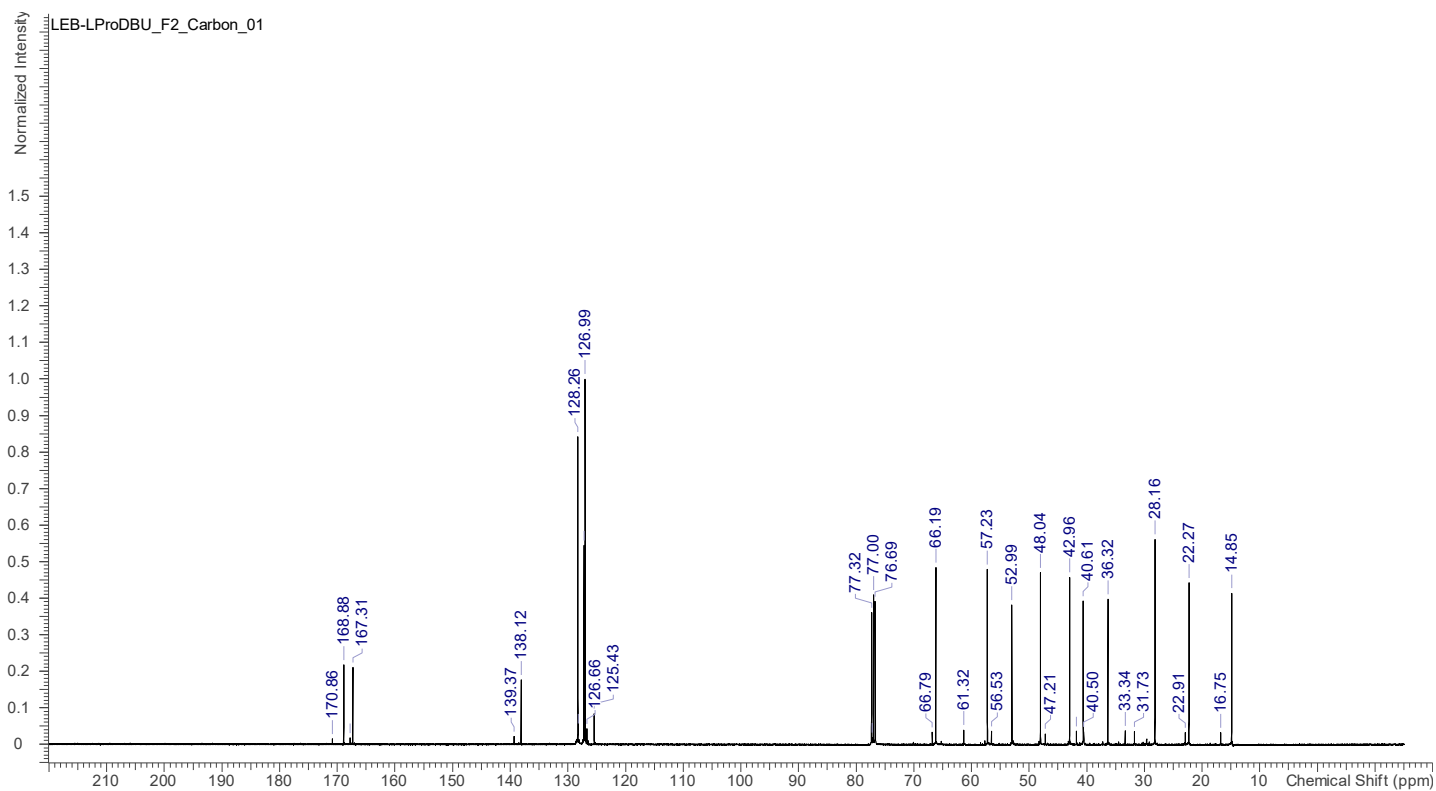
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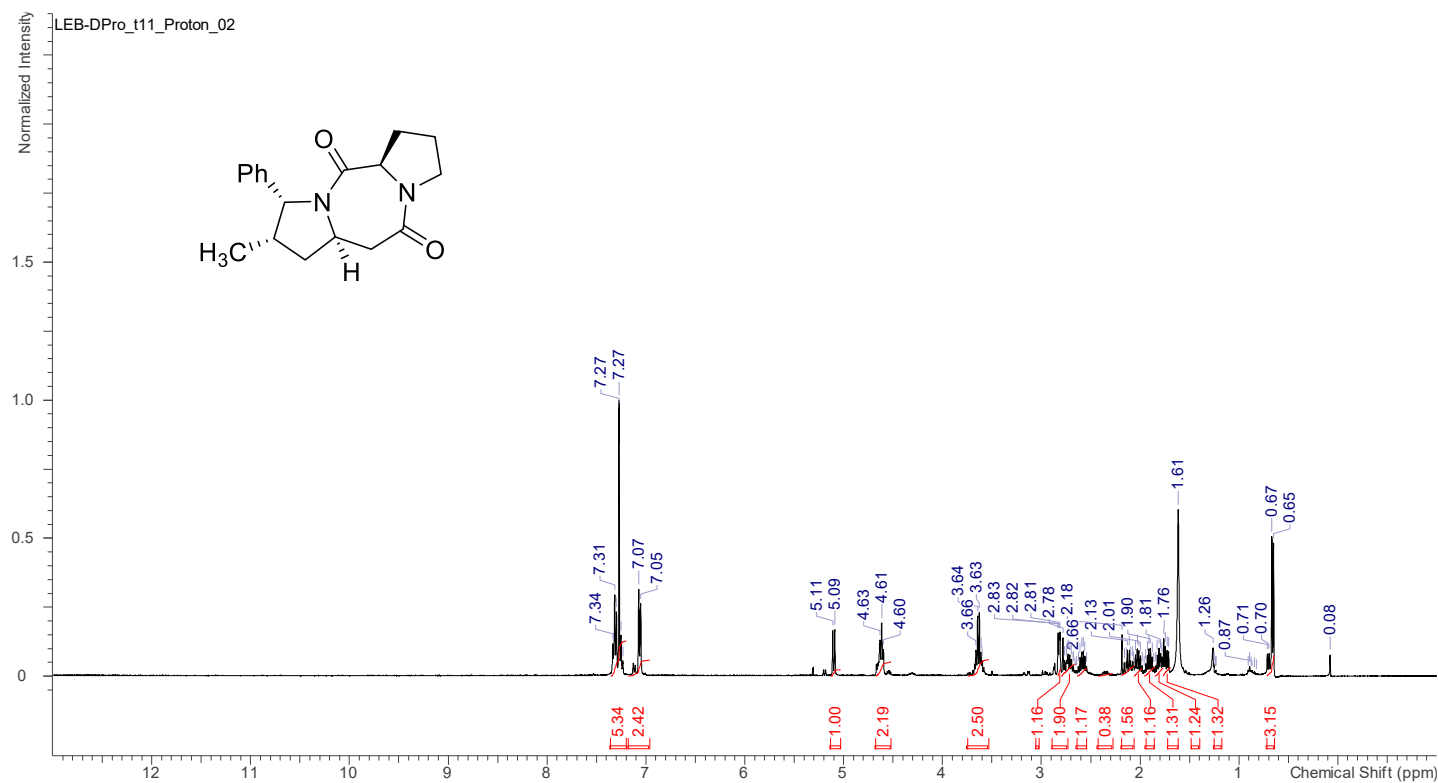
¹H NMR for Compound (5*aS*,11*aS*)-**3g**.



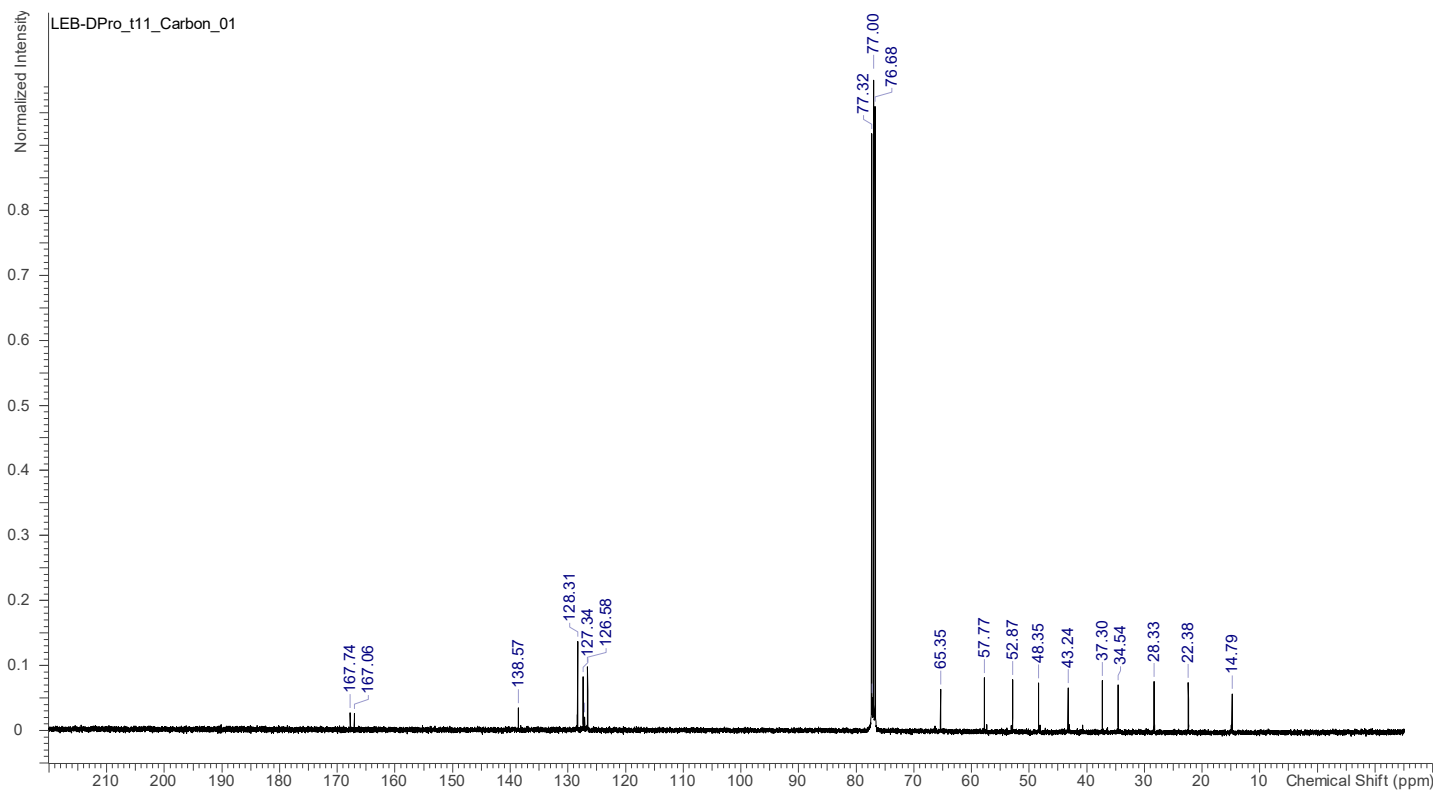
¹³C NMR for Compound (5*aS*,11*aS*)-**3g**.



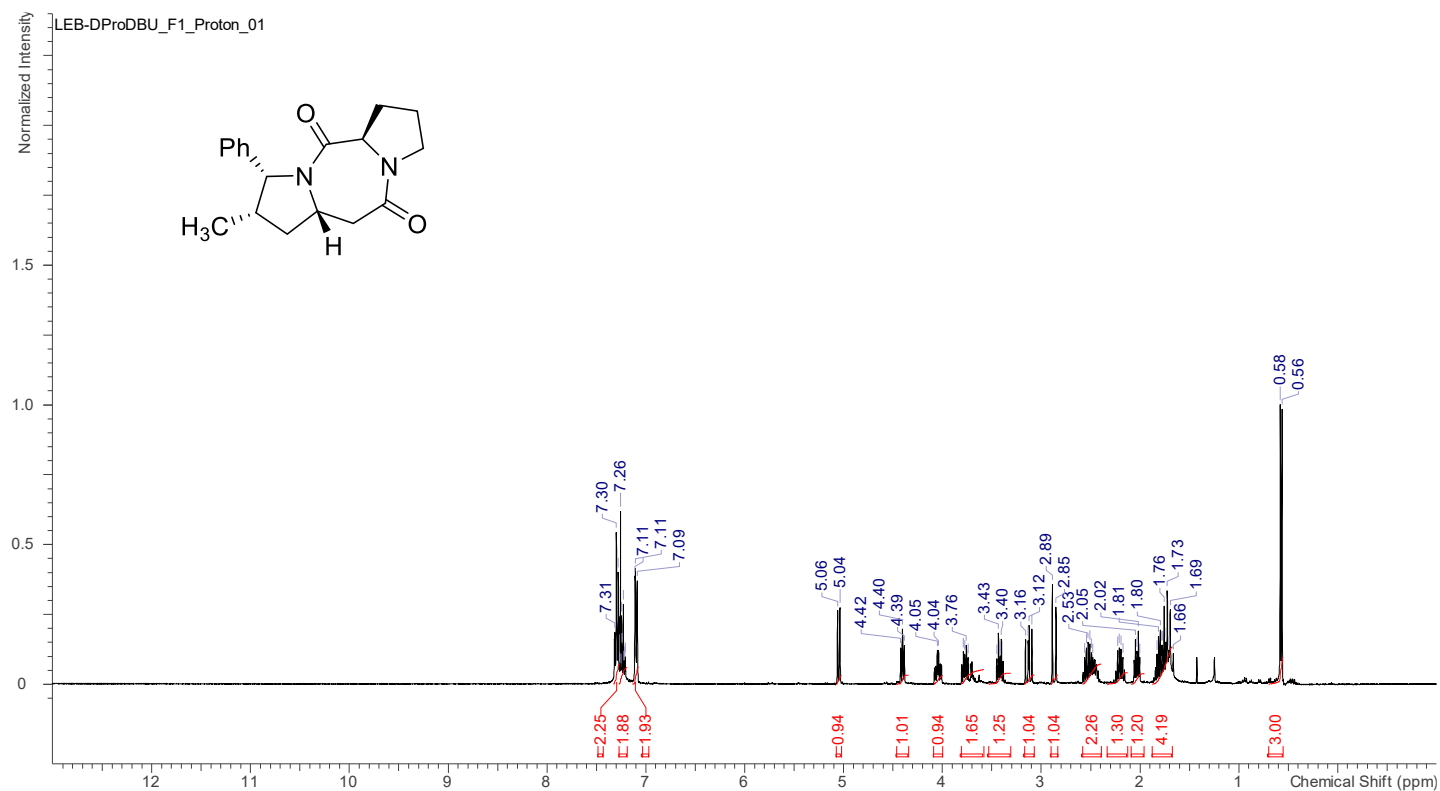
¹H NMR for Compound (5*aR*,11*aR*)-**3g**.



¹³C NMR for Compound (5*aR*,11*aR*)-**3g**.



¹H NMR for Compound (5*aR*,11*aS*)-**3g**.



¹³C NMR for Compound (5*aR*,11*aS*)-**3g**.

