Supplementary Material

Synthesis of terminal alkynes based on (1*S*,3*R*,4*R*)- and (1*S*,3*S*,4*R*)-2-azabicyclo[2.2.1]heptane

Franz Steppeler[a], Marcin Górecki[b], Elżbieta Wojaczyńska[a]*

[a]Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50 370 Wrocław, Poland
[b]Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka St. 44/52, 01 224 Warsaw, Poland
Email: elzbieta.wojaczynska@pwr.edu.pl

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Reaction conditions for the attempted elimination of the dichloroalkene (6)

Elimination with methyllithium

To a stirred solution of dichloroalkene **(6)** (421 mg, 1.42 mmol, 1 eq.) in 10 mL THF in a sodium chloride/ice cooling bath there was an 1.6 M methyllithium solution (1.07 mL, 1.71 mmol, 1.2 eq.) dropwise added through a syringe. The reaction mixture was kept stirring for 1 h, was quenched with aq. NH_4Cl solution and extracted with *n*-hexane, dried and the solvent was removed. The crude product was purified on column chromatography using silica gel and a *n*-hexane/ethyl acetate mixture (5:1 v/v); ^{1}H-NMR analysis revealed pure starting material.

Elimination with *n*-butyllithium

To a stirred solution of dichloroalkene **(6)** (538 mg, 1.82 mmol, 1 eq.) in 10 mL THF in a sodium chloride/ice cooling bath there was a solution of *n*-buthyllithium (0.9 mL, 2.18 mmol, 1.2 eq.) in 2 mL THF added dropwise using a syringe. The mixture was stirred for 3 h, quenched with aq. NH_4Cl solution and extracted with *n*-hexane, dried and the solvent was removed. The crude product was purified on column chromatography using silica gel and a *n*-hexane/ethyl acetate mixture (5:1 v/v); ^{1}H-NMR analysis revealed pure starting material.

To a mechanical stirred solution of dichloroalkene **(6)** (487 mg, 1.64 mmol, 1 eq.) in 10 mL *n*-hexane in an cooling bath at -78°C there was a solution of 2.5 M *n*-buthyllithium (1.6 mL, 4.1 mmol, 2.5 eq.) in *n*-hexane added dropwise using a syringe. The mixture was stirred for 3 h, left to reach room temperature, quenched with aq. NH_4Cl solution and extracted with *n*-hexane, dried and the solvent was removed. The crude product was purified on column chromatography using silica gel and a *n*-hexane/ethyl acetate mixture (5:1 v/v); ^{1}H-NMR analysis revealed pure starting material.

^{1}H and ^{13}C NMR spectra

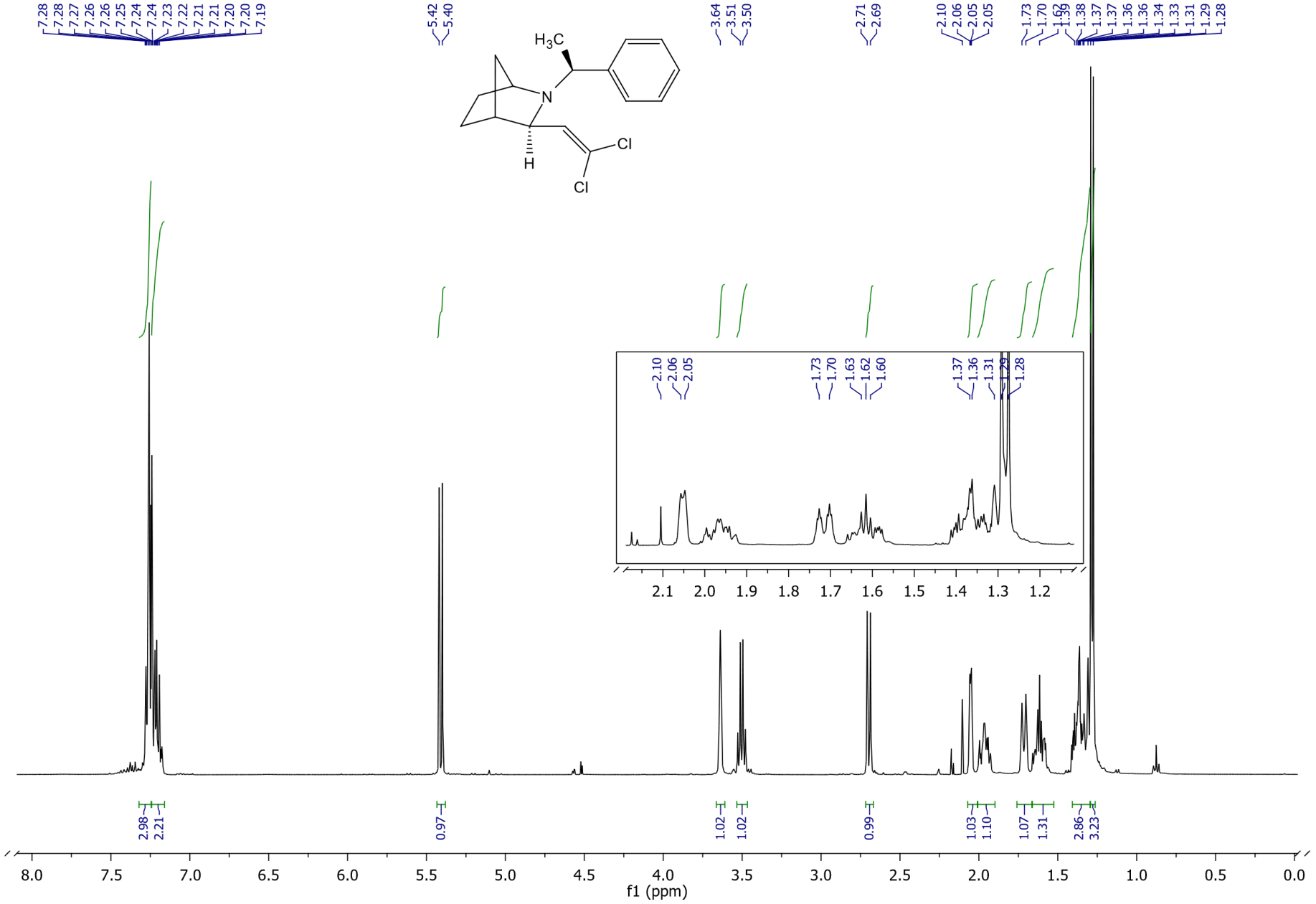


Figure S1. ^{1}H-NMR of **(1*S*,3*R*,4*R*)-3-(2,2-dichlorovinyl)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (6)** at 298 K (400 MHz, $CDCl_3$).

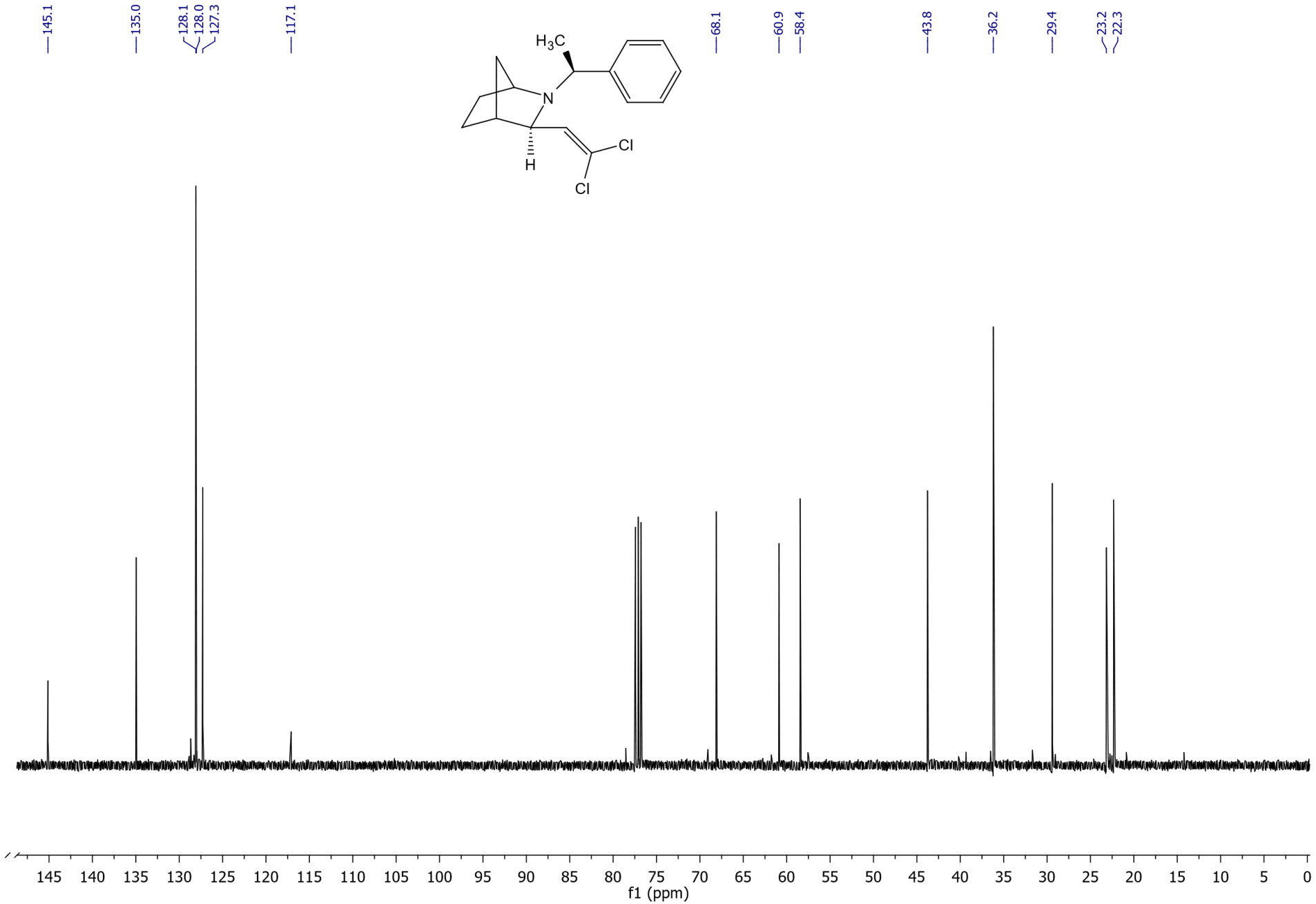


Figure S2. ^{13}C-NMR of **(1*S*,3*R*,4*R*)-3-(2,2-dichlorovinyl)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (6)** at 298 K (100 MHz, $CDCl_3$).

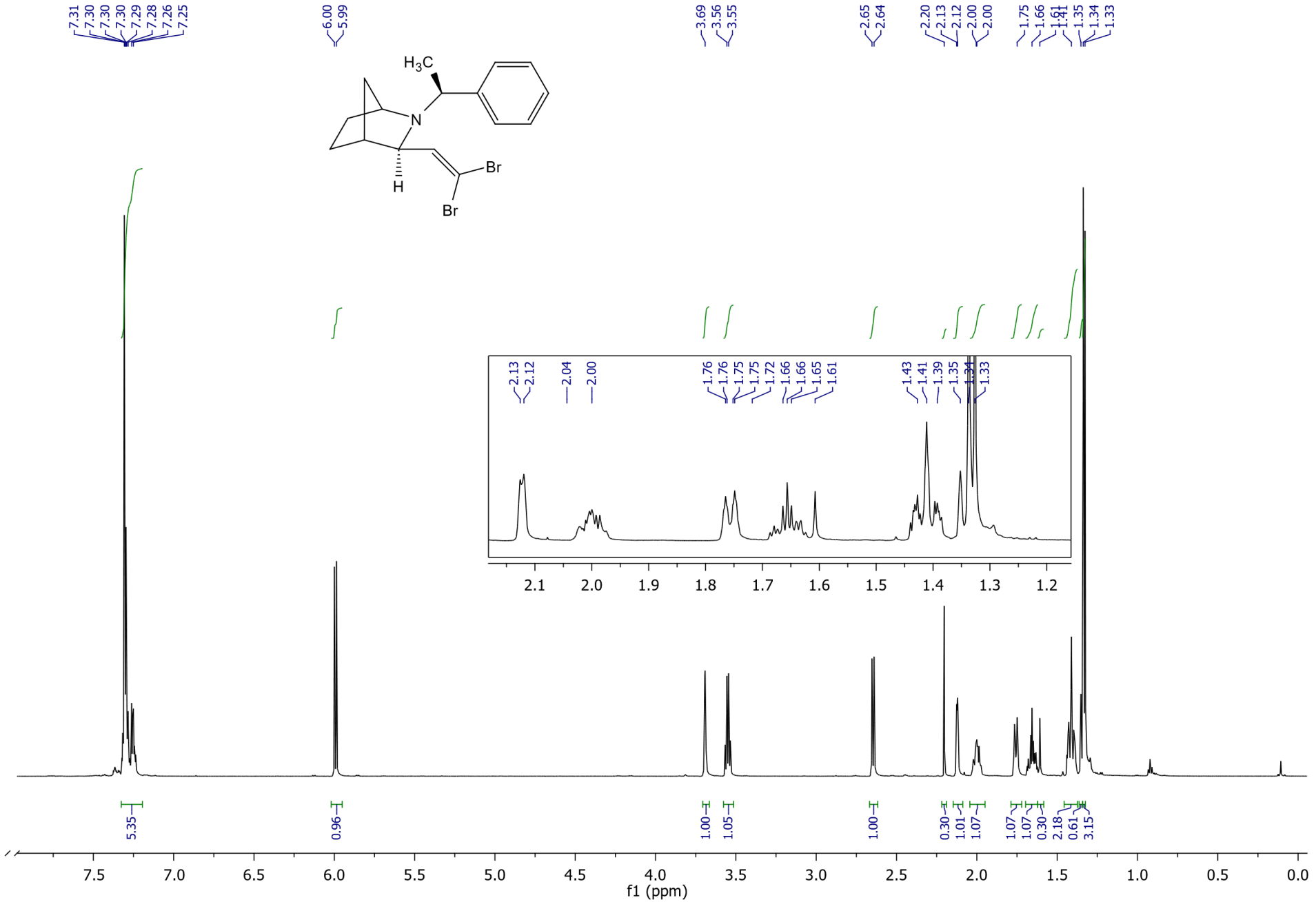


Figure S3. ^{1}H-NMR of **(1*S*,3*R*,4*R*)-3-(2,2-dibromovinyl)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (7)** at 298 K (400 MHz, $CDCl_3$).

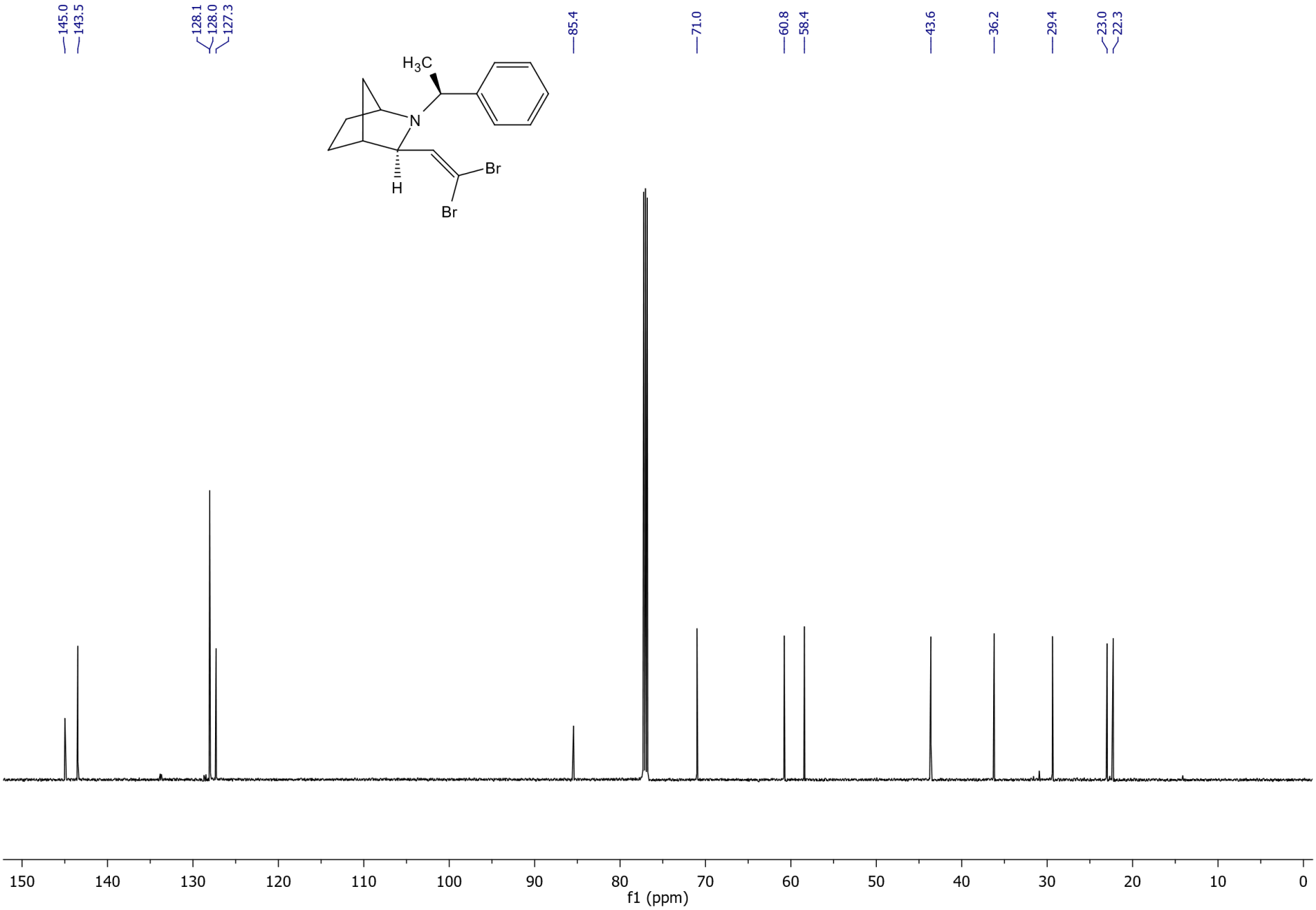


Figure S4. ^{13}C-NMR of **(1*S*,3*R*,4*R*)-3-(2,2-dibromovinyl)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (7)** at 298 K (100 MHz, $CDCl_3$).

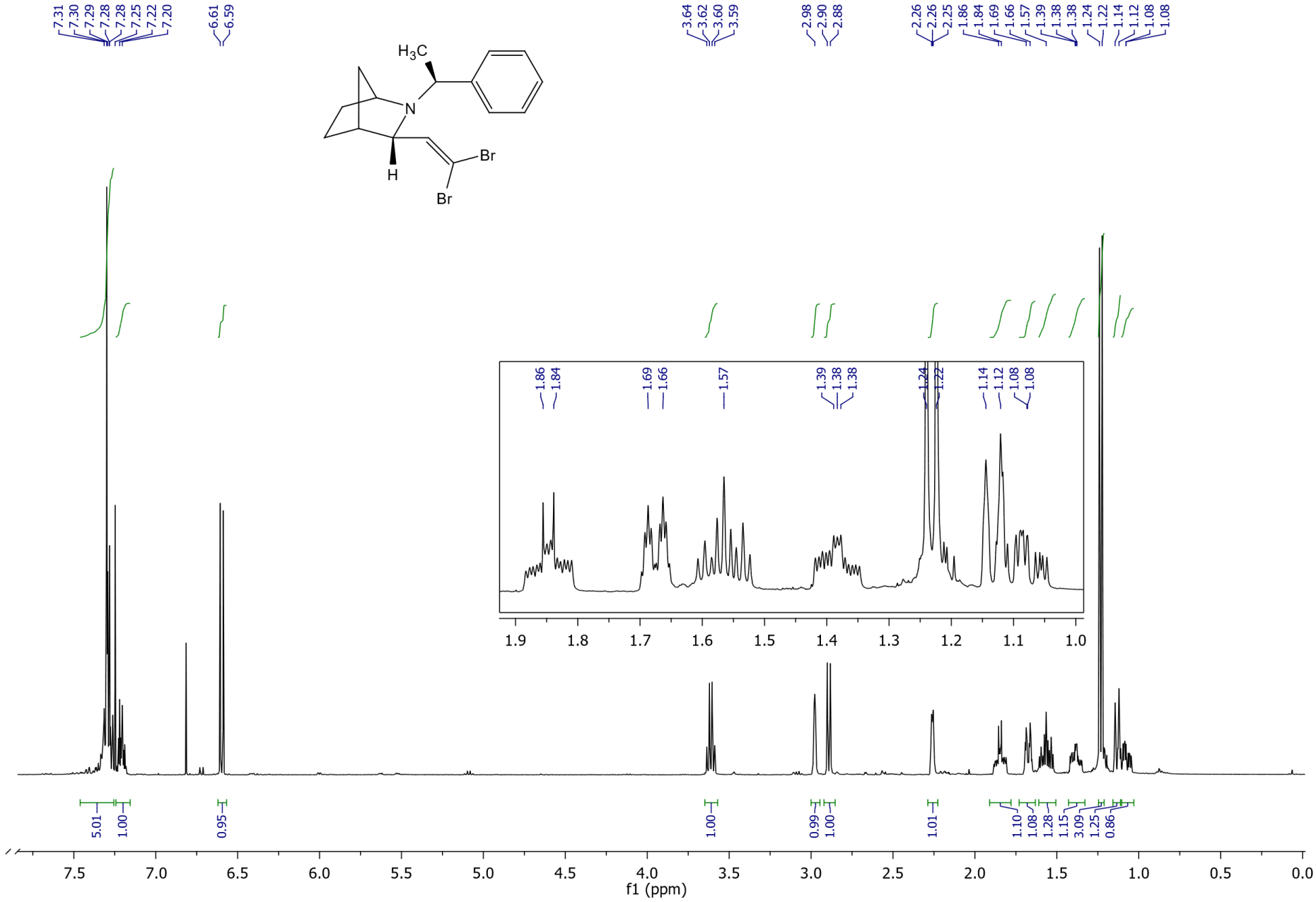


Figure S5. ^{1}H-NMR of **(1S,3S,4R)-3-(2,2-dibromovinyl)-2-((S)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (8)** at 298 K (400 MHz, $CDCl_3$).

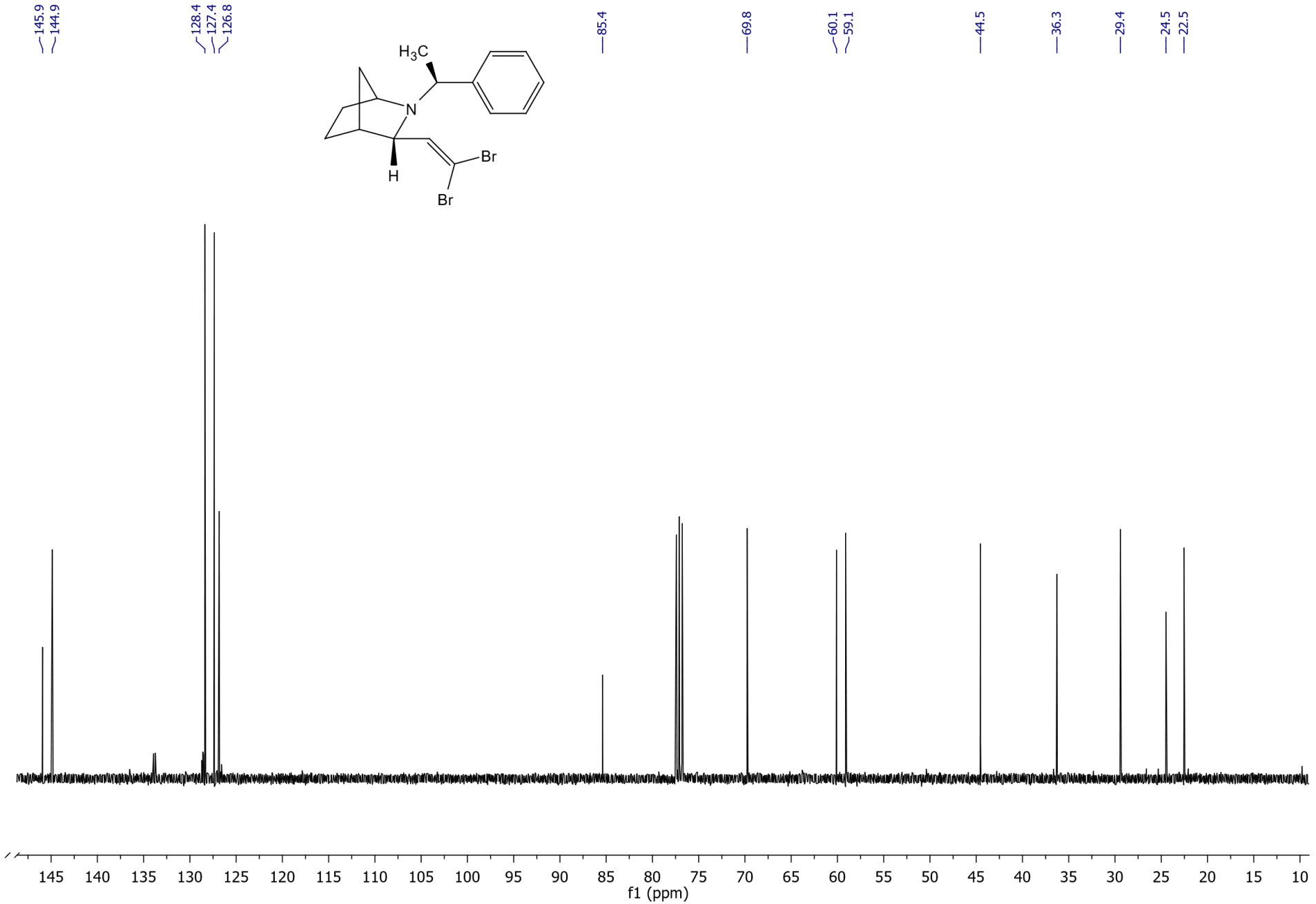


Figure S6. ^{13}C-NMR of **(1S,3S,4R)-3-(2,2-dibromovinyl)-2-((S)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (8)** at 298 K (100 MHz, $CDCl_3$).

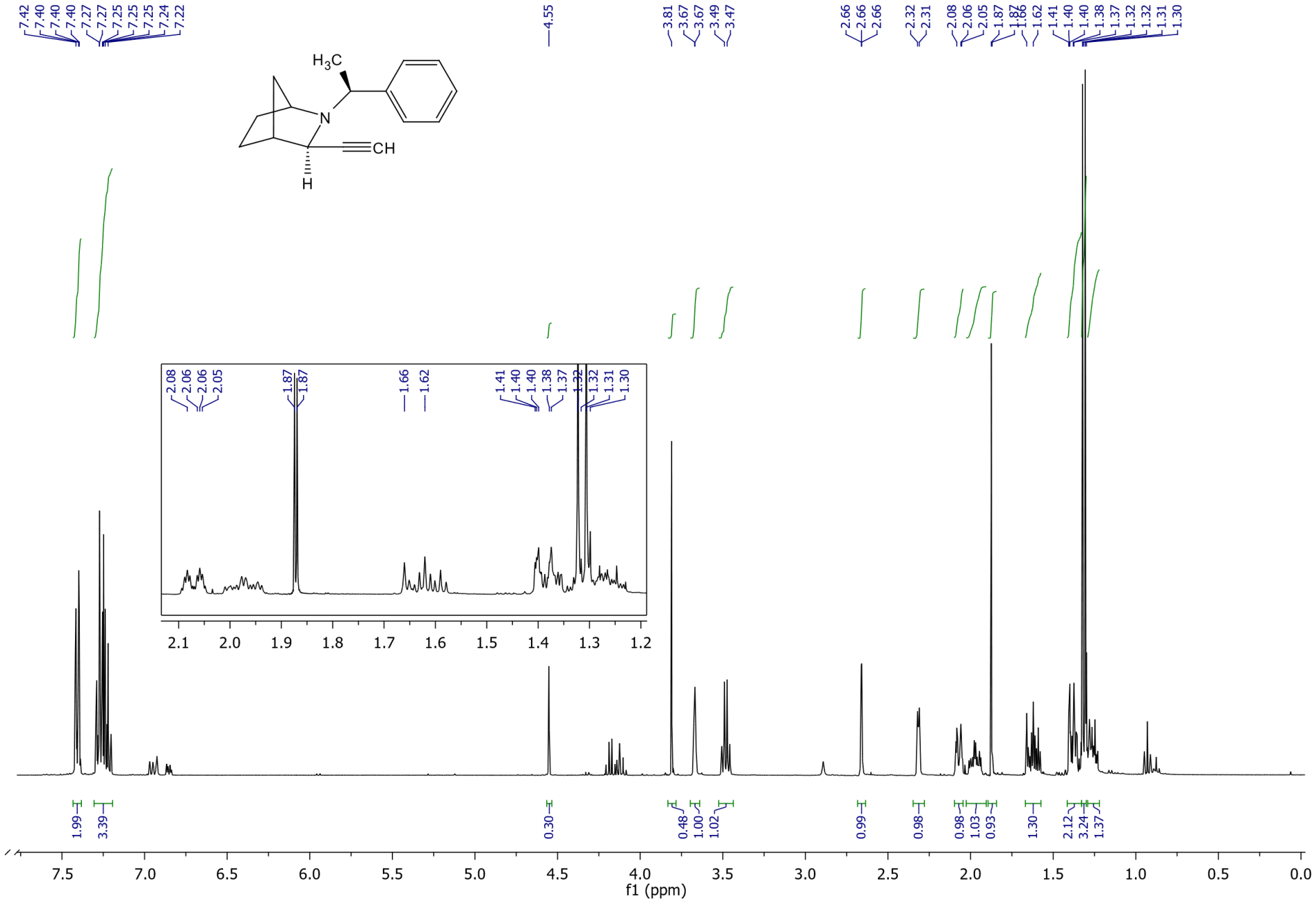


Figure S7. ^{1}H-NMR of **(1*S*,3*R*,4*R*)-3-ethynyl-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (9)** at 298 K (400 MHz, $CDCl_3$).

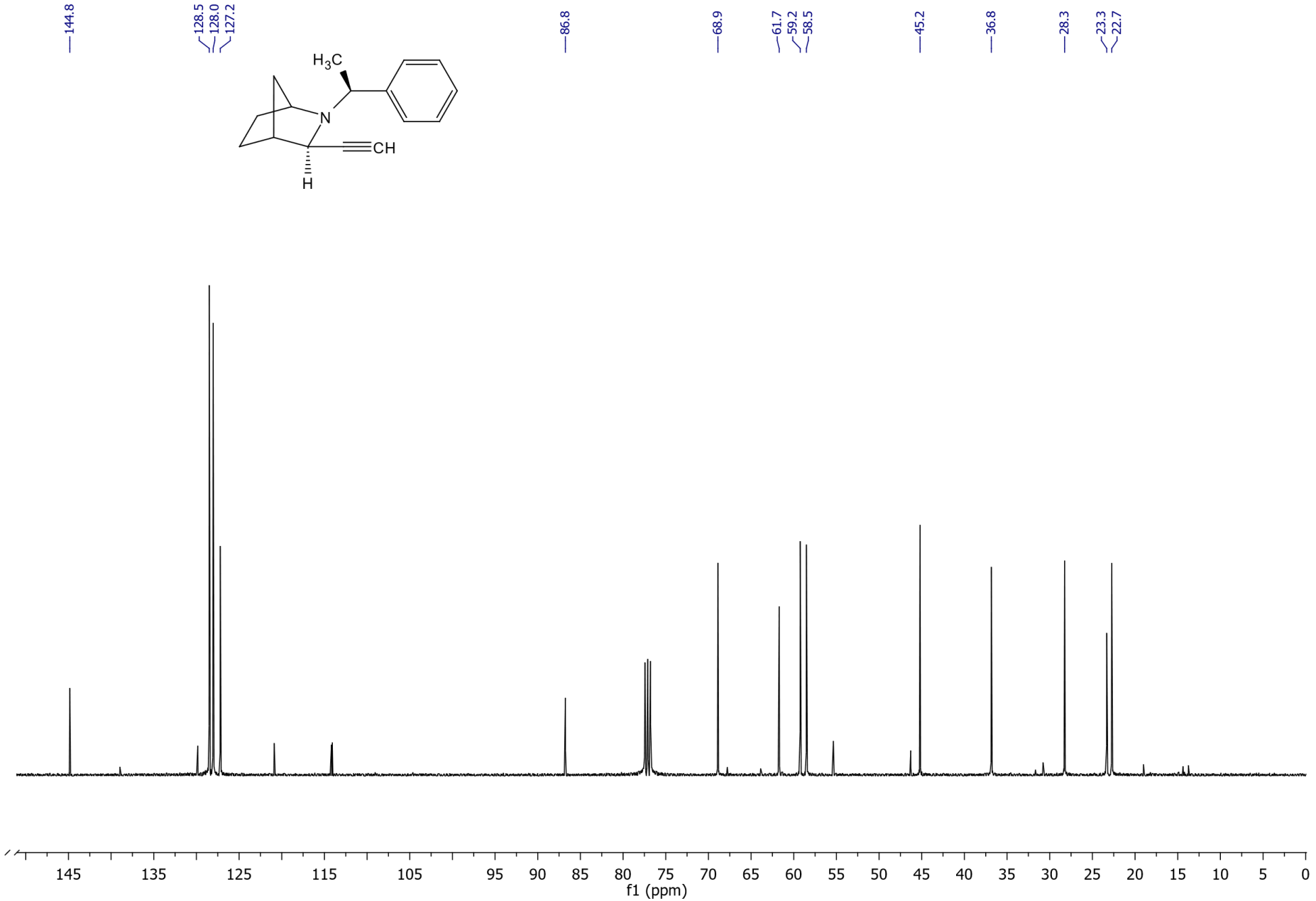


Figure S8. ^{13}C-NMR of **(1*S*,3*R*,4*R*)-3-ethynyl-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (9)** at 298 K (100 MHz, $CDCl_3$).

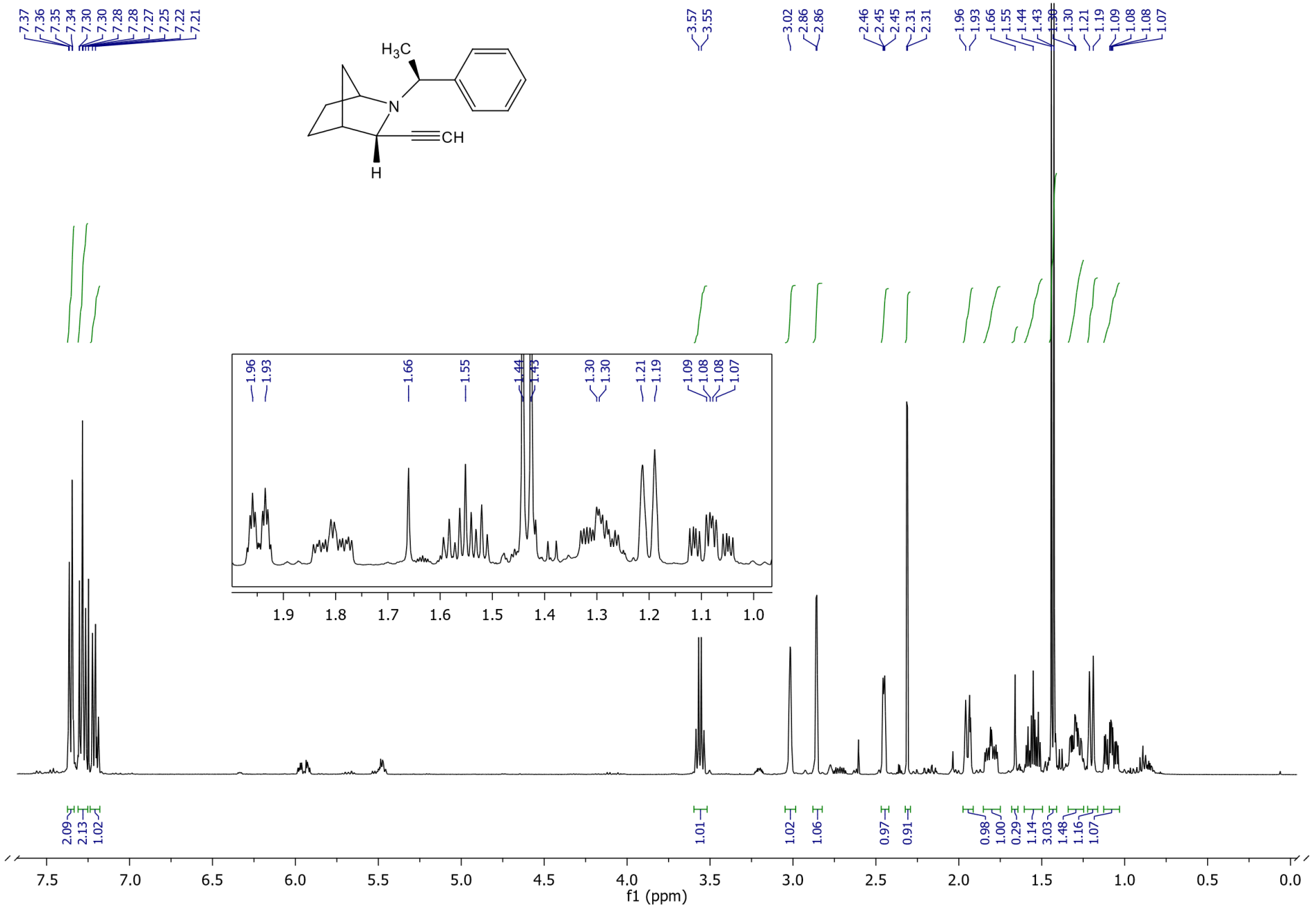


Figure S9. ^{1}H-NMR of **(1*S*,3*S*,4*R*)-3-ethynyl-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (10)** at 298 K (400 MHz, $CDCl_3$).

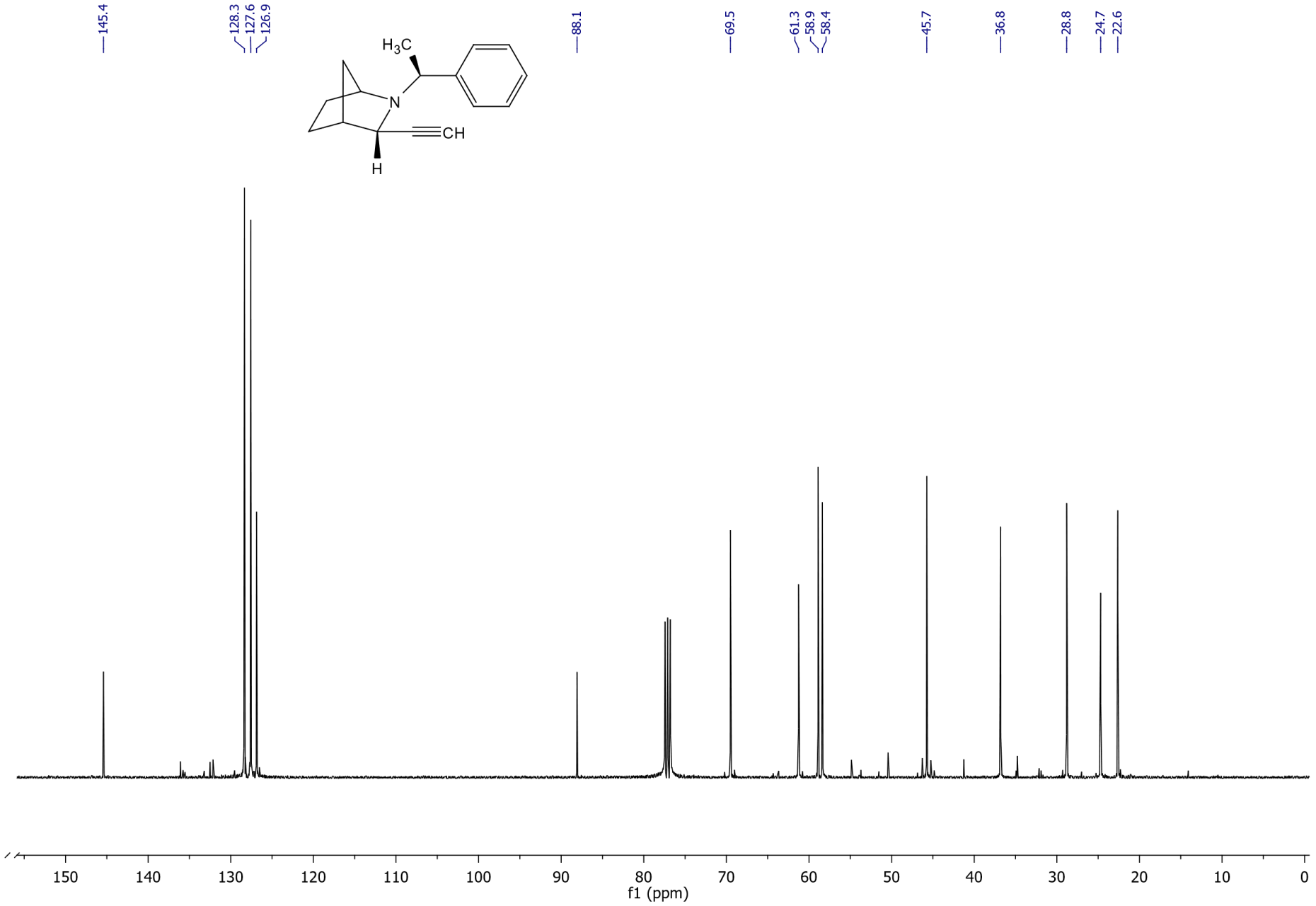


Figure S10. ^{13}C-NMR of **(1*S*,3*S*,4*R*)-3-ethynyl-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptane (10)** at 298 K (100 MHz, $CDCl_3$).

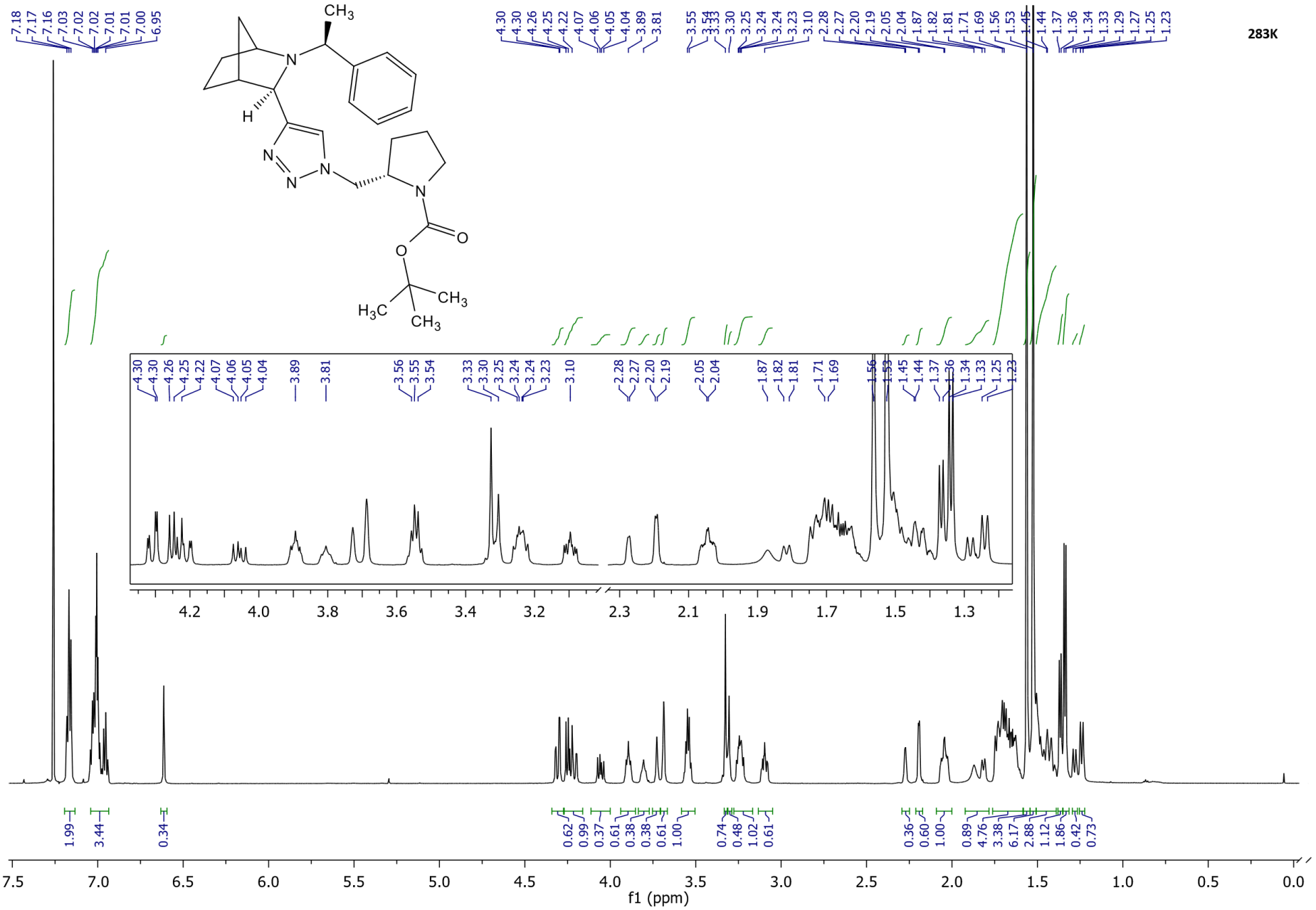


Figure S11. ^{1}H-NMR of **(2S)-tert-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13)** at 283 K (600 MHz, $CDCl_3$).

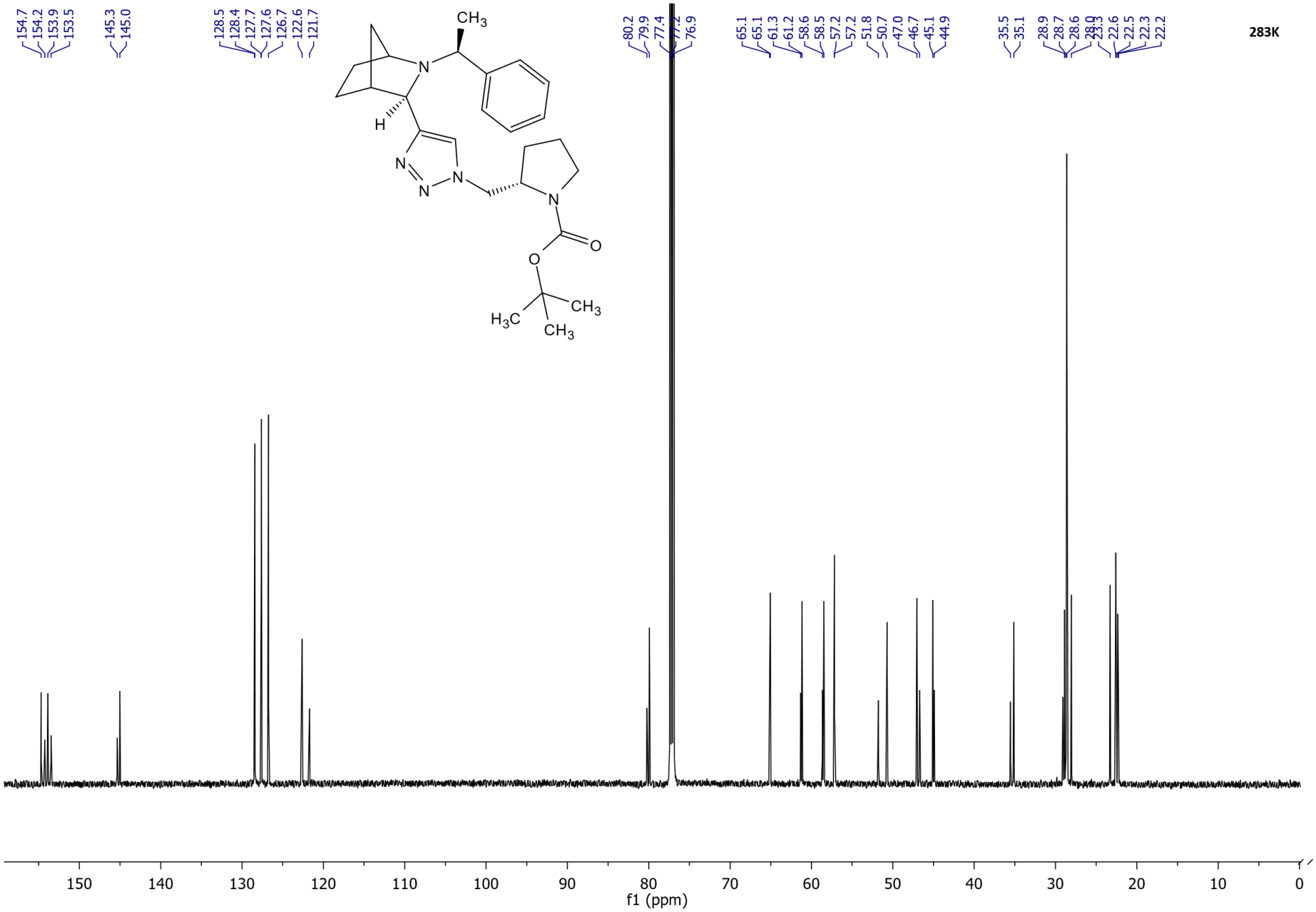


Figure S12. ^{13}C-NMR of **(2S)-tert-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13)** at 283 K (150 MHz, $CDCl_3$).

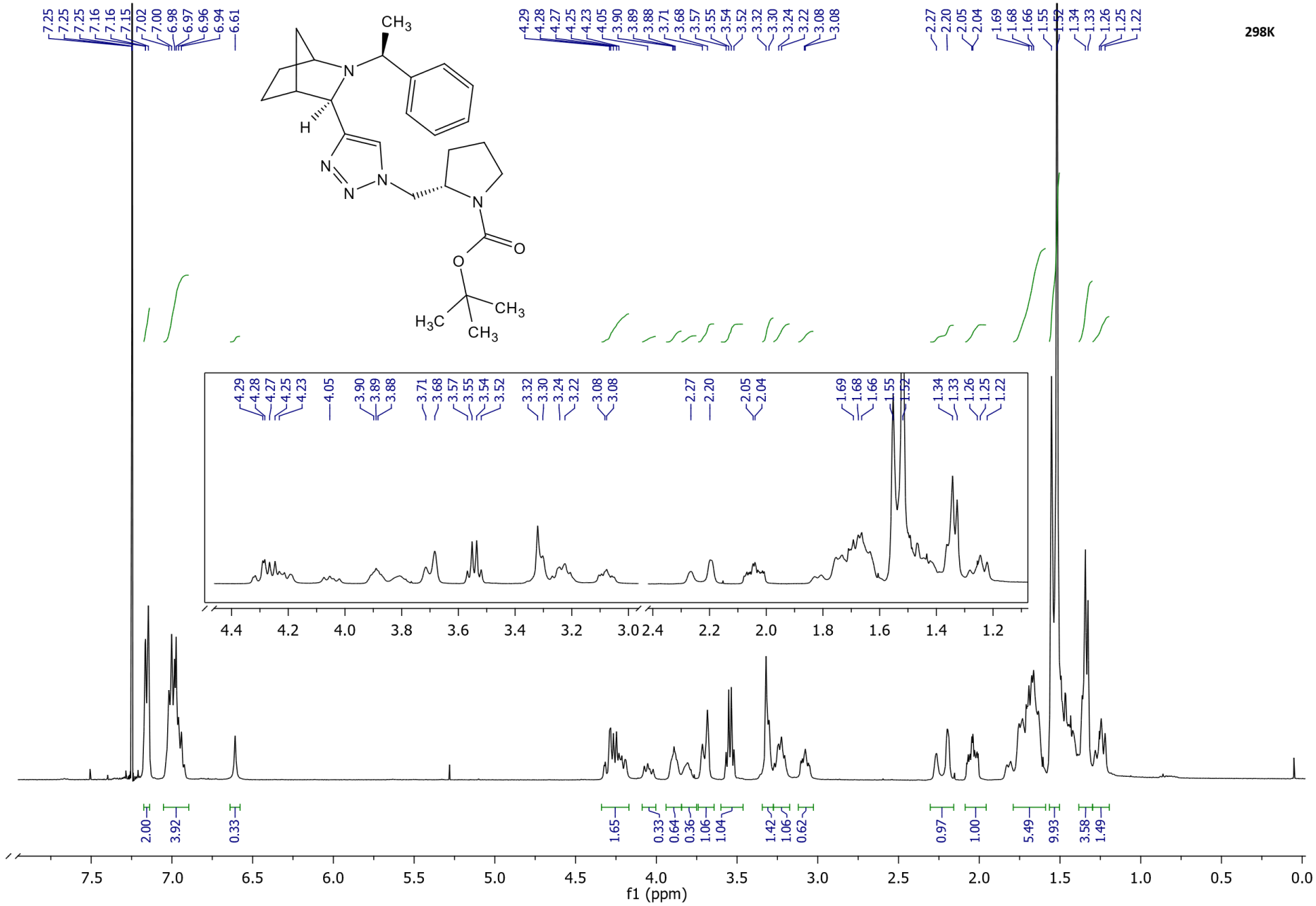


Figure S13. ^{1}H-NMR of **(2S)-tert-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13)** at 298 K (400 MHz, $CDCl_3$).

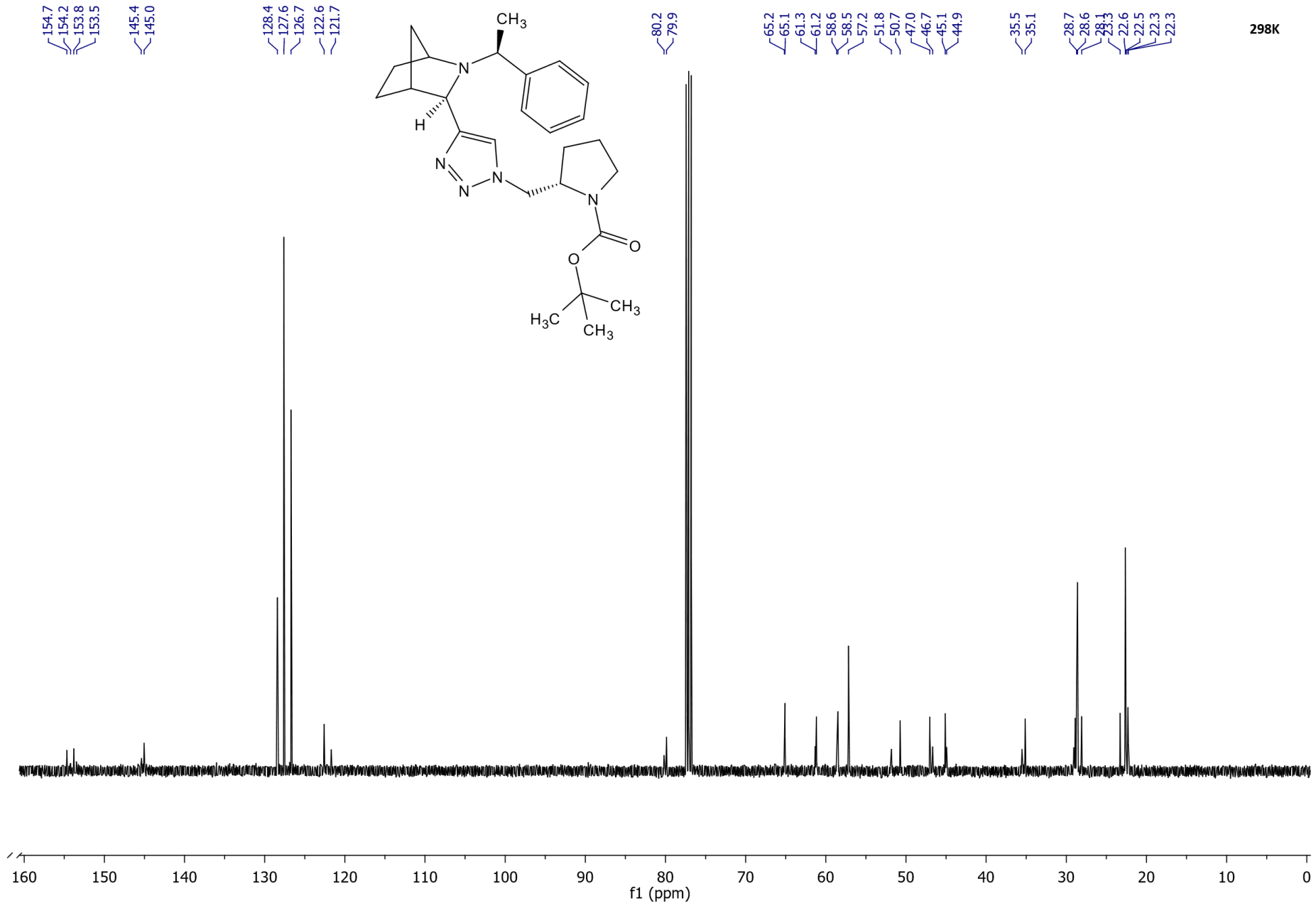


Figure S14. ^{13}C-NMR of **(2S)-tert-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13)** at 298 K (100 MHz, $CDCl_3$).

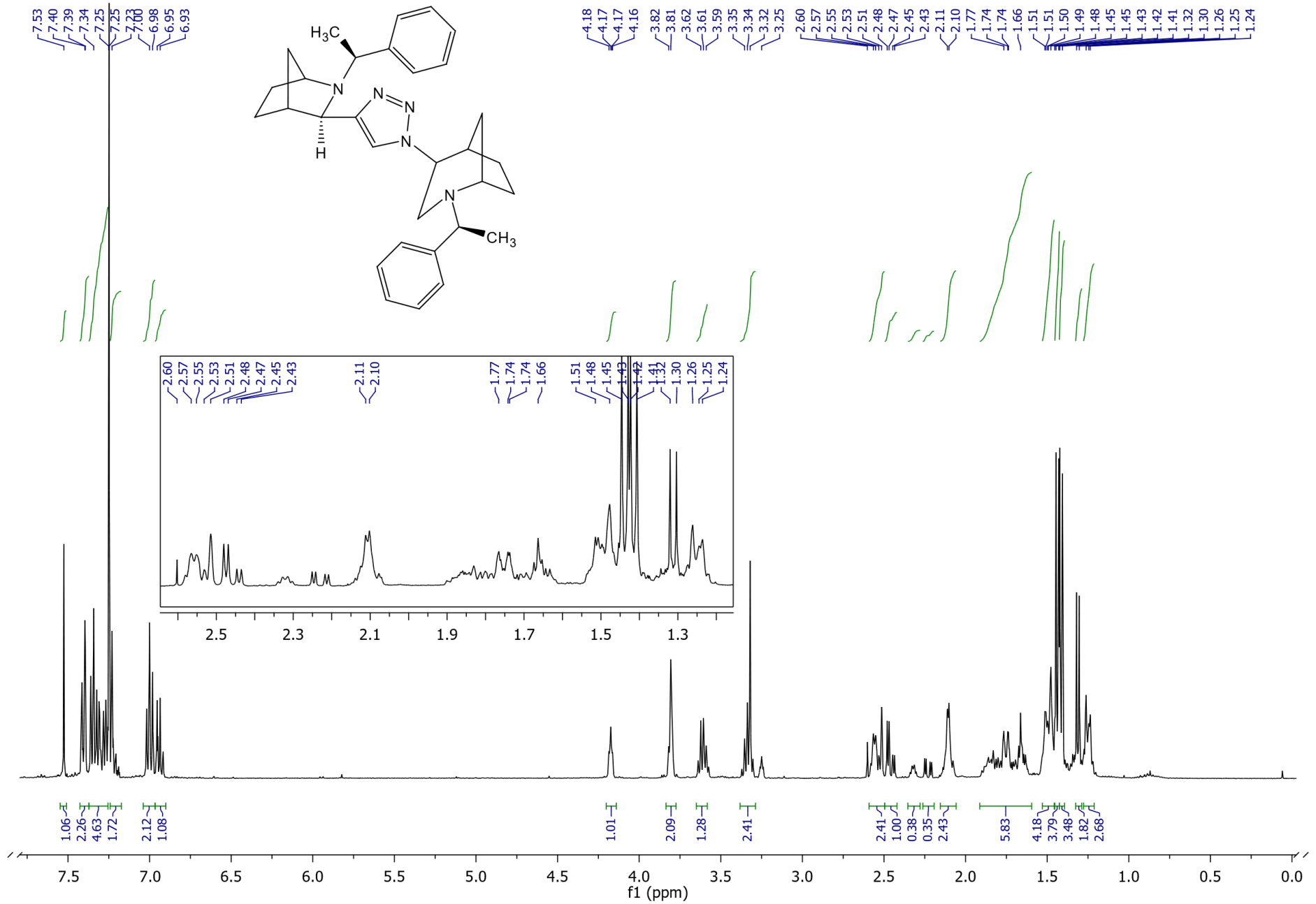


Figure S15. ^{1}H-NMR of **(1*S*,4*S*,5*R*)-2-((*S*)-1-phenylethyl)-4-(4-((1*S*,3*S*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H 1,2,3-triazol-1-yl)-2-azabicyclo[3.2.1]octane (14)** at 298 K (400 MHz, $CDCl_3$).

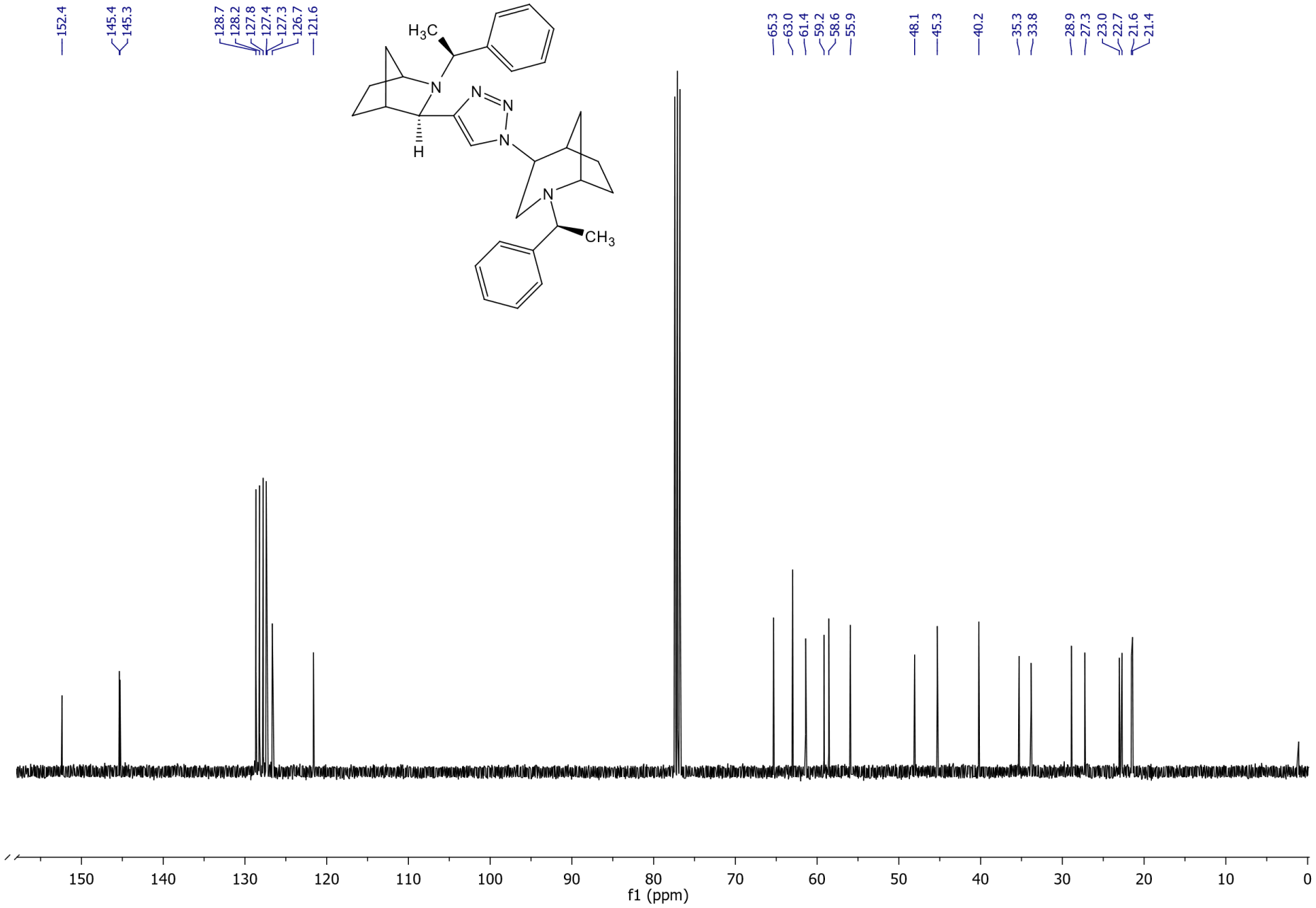


Figure S16. ^{1}H-NMR of **(1*S*,4*S*,5*R*)-2-((*S*)-1-phenylethyl)-4-(4-((1*S*,3*S*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H 1,2,3-triazol-1-yl)-2-azabicyclo[3.2.1]octane (14)** at 298 K (400 MHz, $CDCl_3$).

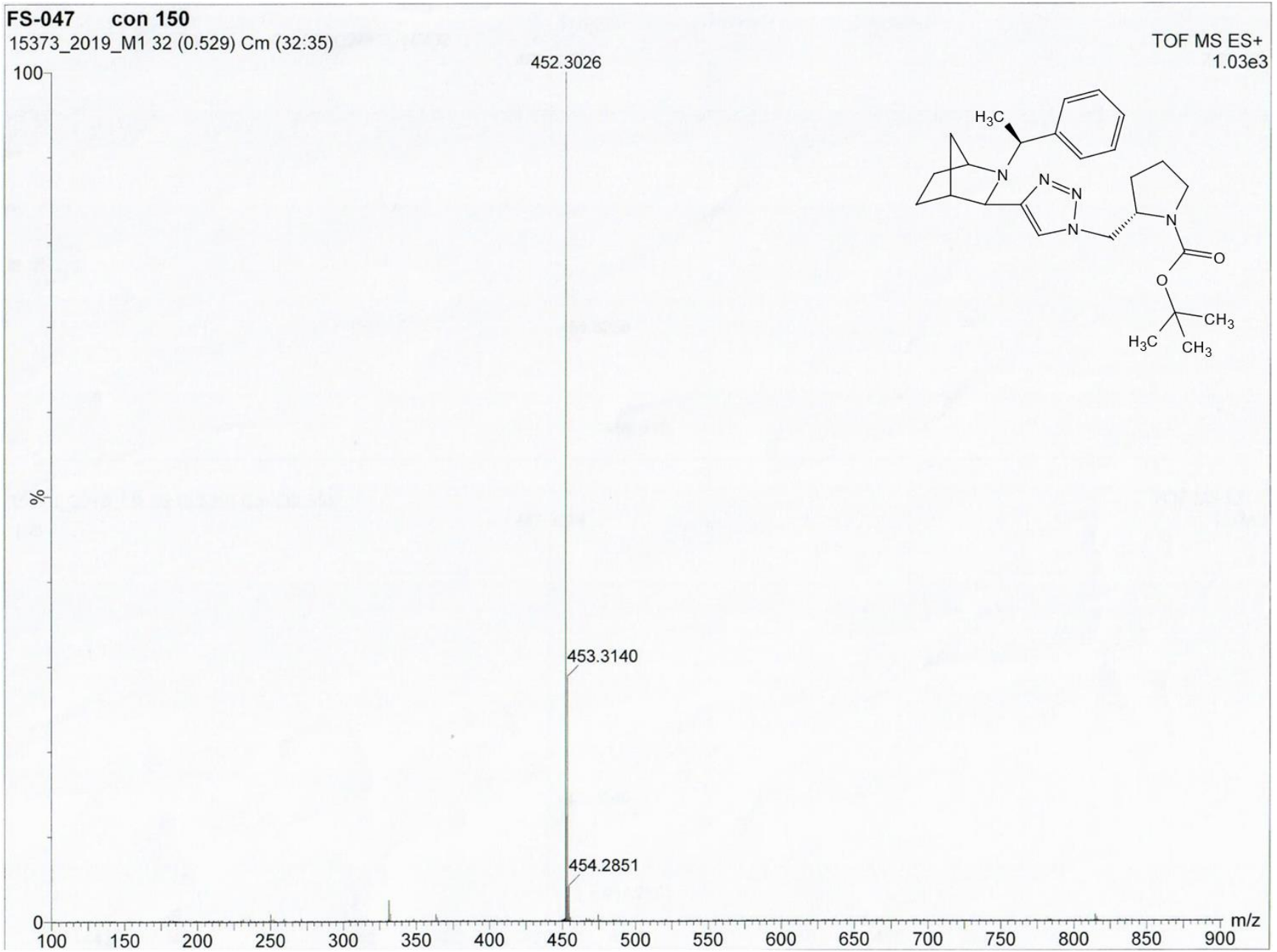


Figure S17. HRMS-spectrum of **(2S)-tert-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13).**

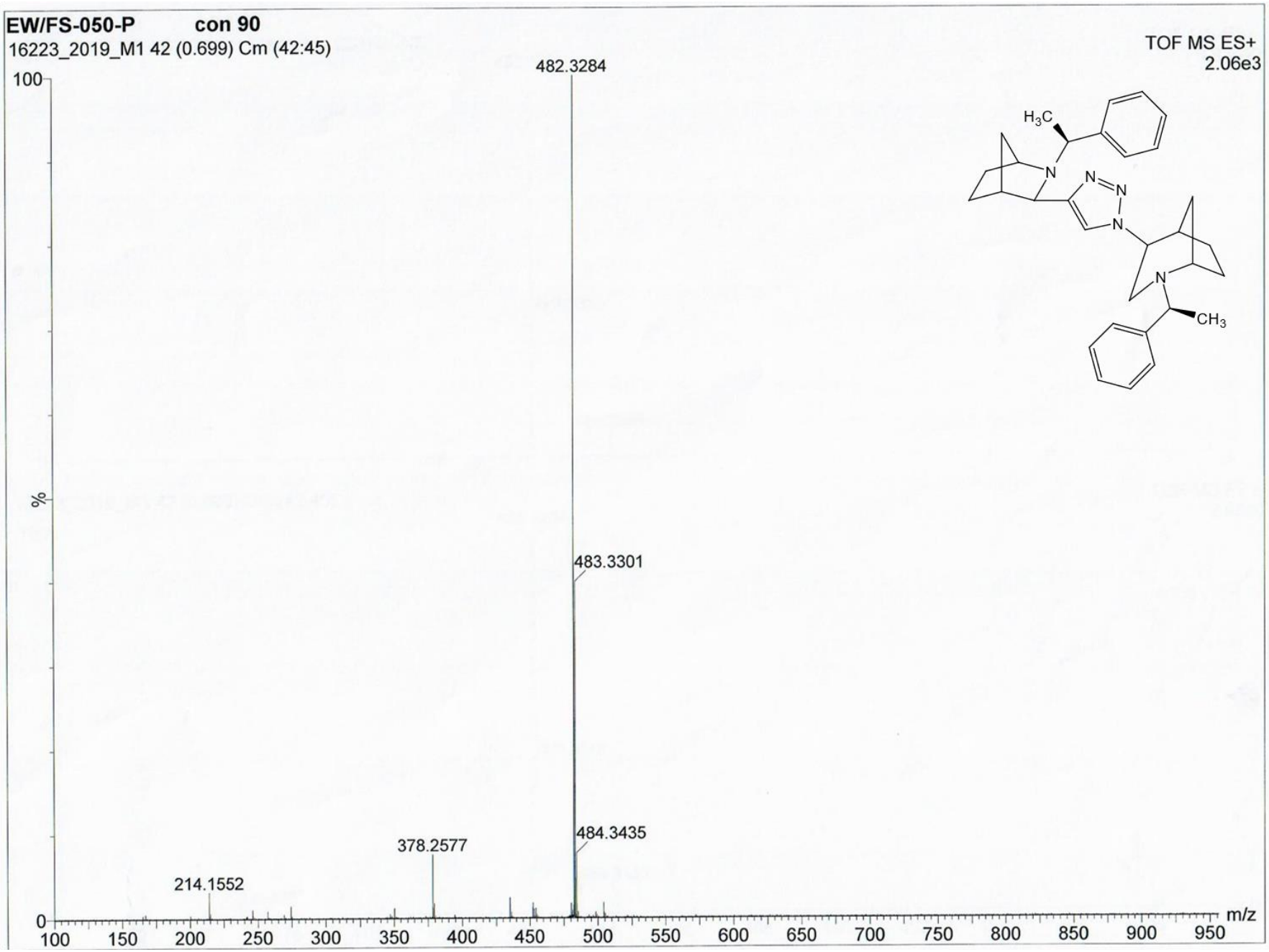
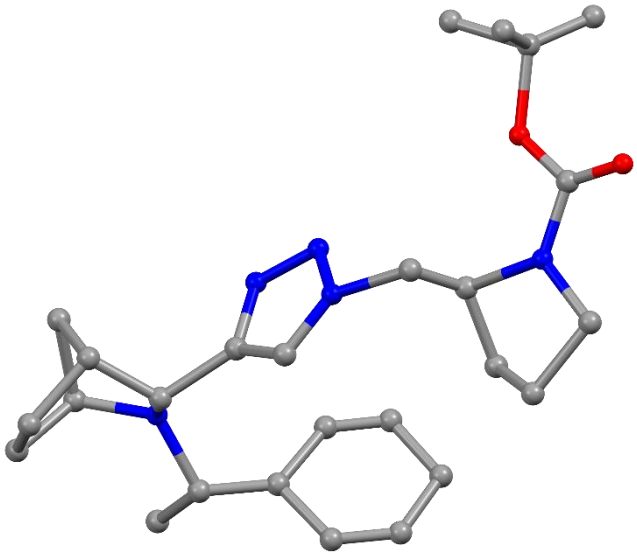


Figure S18. HRMS-spectrum of **(1*S*,4*S*,5*R*)-2-((*S*)-1-phenylethyl)-4-(4-((1*S*,3*S*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1H 1,2,3-triazol-1-yl)-2-azabicyclo[3.2.1]octane (14).



Crystal system: monoclinic, space group: *I*2 (No. 5), Z = 4.
Cell parameters: a = 20.380(4) Å, b = 5.7379(12) Å, c = 21.825(5) Å, β = 104.53(2)°,
V = 2470.5(9) Å^3.

Figure S19. Crystallographic data and X-ray model of **(2*S*)-*tert*-butyl 2-((4-((1*S*,3*R*,4*R*)-2-((*S*)-1-phenylethyl)-2-azabicyclo[2.2.1]heptan-3-yl)-1*H*-1,2,3-triazol-1-yl)-methyl)pyrrolidine-1-carboxylate (13).**

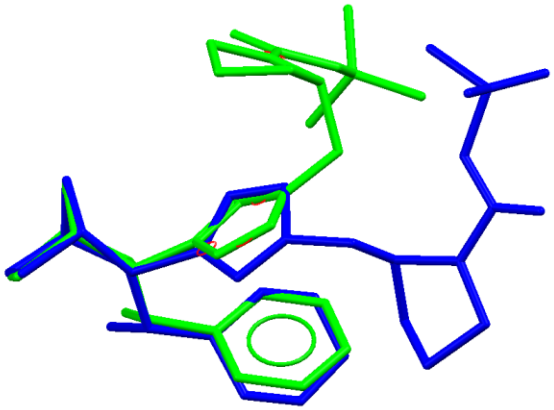


Figure S20. Comparison of the X-ray structure of **13** (blue) with the structure of the lowest energy conformer **13a** (green) calculated at the ωB97X-D/6-311+G(d,p) level of theory. Hydrogen atoms are omitted for clarity.

The geometry in the solid state determined by the X-ray analysis is different in the flexible part of molecule from the geometry of most stable DFT structure(s) in solution equilibrium (conf. **13a–13c**). This can be explained by an impact of intermolecular interactions and a role of vicinal effects in solid state on the geometry of **13**.

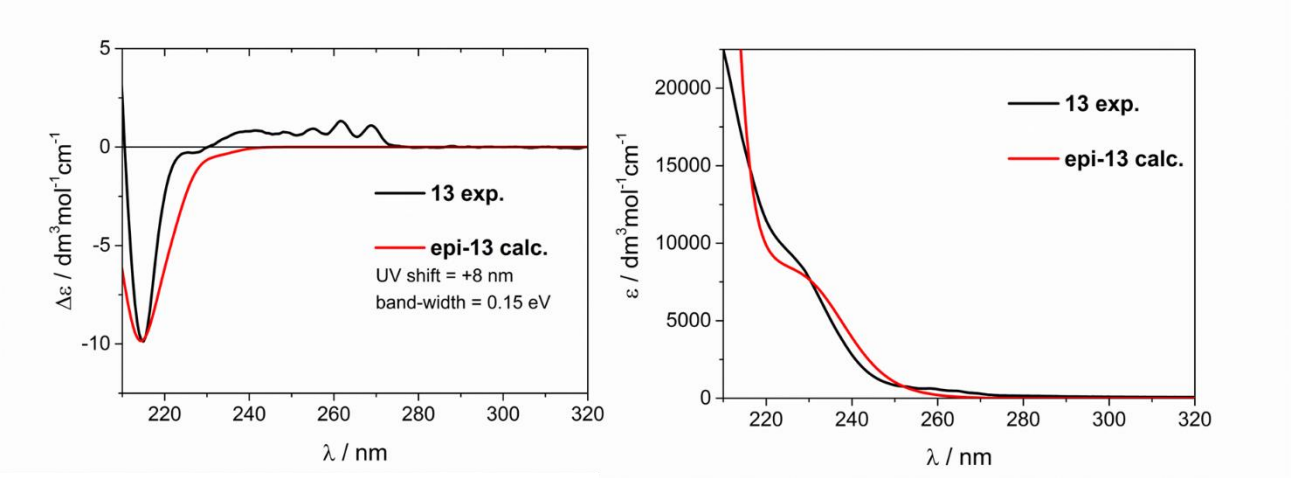


Figure S21. Experimental ECD (left) and UV (right) spectra of **13** recorded in hexane at room temperature (black lines) confronted with TDDFT simulations for ***epi*-13** performed at the CAM-B3LYP/def2-TZVP level of theory (red lines). Enantiomeric Similarity Index Δ equals 0.845.

Table S1. Simulated $[\alpha]_D$ value for individual conformers of **13** at 298 K

	$[\alpha]_D$ /deg cm^2 g^{-1}			
Conformer	CAM-B3LYP/ aug-cc-pVDZ/ PCM(CH_2Cl_2)	CAM-B3LYP/ def2-TZVP/ PCM(CH_2Cl_2)	B3LYP/ aug-cc-pVDZ/ PCM for CH_2Cl_2	B3LYP/ def2-TZVP/ PCM(CH_2Cl_2)
13a	+43	+40	+49	+46
13b	+38	+42	+49	+55
13c	-27	-34	-44	-49
13d	-61	-73	-75	-88
13e	+64	+58	+69	+62
13f	-12	-13	-16	-16

Table S2. Simulated $[\alpha]_D$ value for ***epi*-13** at 298 K

	$[\alpha]_D$ /deg cm^2 g^{-1}			
Experiment* in CH_2Cl_2 for **13**	TDDFT Boltzmann-weighted value			
	CAM-B3LYP/aug-cc-pVDZ/PCM(CH_2Cl_2)	CAM-B3LYP/def2-TZVP/PCM(CH_2Cl_2)	B3LYP/aug-cc-pVDZ /PCM for CH_2Cl_2	B3LYP/def2-TZVP/PCM(CH_2Cl_2)
+45	-56	-55	-79	-75

*) in CH_2Cl_2 (c = 0.23 g/100 cm^3) at 298 K

Table S3. Simulated $[\alpha]_D$ value for individual conformers of ***epi*-13** at 298 K

	$[\alpha]_D$ /deg cm^2 g^{-1}			
Conformer	CAM-B3LYP/ aug-cc-pVDZ/ PCM(CH_2Cl_2)	CAM-B3LYP/ def2-TZVP/ PCM(CH_2Cl_2)	B3LYP/ aug-cc-pVDZ/ PCM for CH_2Cl_2	B3LYP/ def2-TZVP/ PCM(CH_2Cl_2)
***epi*-13a**	-54	-54	-76	-74
***epi*-13b**	-49	-44	-67	-57
***epi*-13c**	-127	-129	-176	-179
***epi*-13d**	-139	-136	-181	-178

Table S4. An overview of the conformational search for **13** and ***epi*-13**. Conformer populations were calculated using the SCF energy ΔE (kcal mol^{-1}) at the ωB97X-D/6-311+G(d,p) level of theory; Boltzmann weights are based on the ΔE at 298 K

Conformer	ΔE / kcal mol^{-1}	Population / %	Conformer	ΔE / kcal mol^{-1}	Population / %
13a	0.00	58.79	***epi*-13a**	0.00	76.63
13b	0.92	12.49	***epi*-13b**	0.82	19.25
13c	0.93	12.12	***epi*-13c**	1.82	3.55
13d	1.19	7.92	***epi*-13d**	2.90	0.57
13e	1.24	7.26			
13f	2.20	1.42			

Cartesian coordinates for individual conformers of 13

Conformer 13a

C	4.36098200	-2.21779800	-0.84240700
C	2.87990400	-2.22697300	-0.42257800
C	2.57431400	-0.87289600	0.25503900
N	2.50610400	0.06057500	-0.89310400
C	4.39124500	-1.15754200	-1.97998600
C	2.91004800	-0.72944800	-2.06834900
C	2.17830600	-2.03970900	-1.77431600
C	3.15436600	1.35040100	-0.66125700
C	1.31390000	-0.87743700	1.05765800
N	1.24581600	-1.43230400	2.29569600
N	0.03895600	-1.30469800	2.75502800
N	-0.67979600	-0.66339800	1.82608900
C	0.07689500	-0.38247900	0.74371800
C	-2.10273700	-0.47152800	1.99239200
C	-2.93304700	-1.54043300	1.26212800
N	-2.62582300	-1.61811200	-0.16640500
C	-1.99390600	-2.87370200	-0.56892000
C	-1.61828300	-3.52594700	0.75988300
C	-2.65764700	-2.97520400	1.74368700
C	-2.86115800	-0.65242200	-1.08713700
O	-2.55308800	-0.74294800	-2.25761500
O	-3.46535900	0.41134000	-0.51707500
C	-3.62477700	1.66611700	-1.24318600
C	-4.58386500	1.48626900	-2.41542000
C	-4.22825400	2.58698800	-0.18842700
C	-2.25882000	2.18735600	-1.68270300
C	2.35964200	2.10937300	0.39156200
C	2.79797800	2.16035800	1.71000800
C	2.03131100	2.77329600	2.69640300
C	0.81637400	3.35820600	2.36831800
C	0.37542300	3.32815400	1.04821800
C	1.13970700	2.70552500	0.07221600
H	4.66006400	-3.20282300	-1.20939600
H	5.01886200	-1.96325700	-0.00774200
H	2.58297600	-3.08054500	0.18545000
H	3.39993400	-0.61565500	0.93354100
H	5.04943400	-0.31591300	-1.75258300
H	4.72866000	-1.58556300	-2.92766700
H	2.63212400	-0.22748400	-2.99392500
H	1.09764000	-1.90484100	-1.70323500
H	2.40869400	-2.83181100	-2.49051300
H	-0.28997000	0.14077000	-0.12111700
H	-2.36289500	0.51782400	1.61796700
H	-2.30916800	-0.51320200	3.06248800

H	-3.98245600	-1.26812400	1.40531800
H	-1.13230800	-2.67293500	-1.20712500
H	-2.70177700	-3.48248200	-1.14245700
H	-1.63754900	-4.61480800	0.70057700
H	-0.61204000	-3.22628400	1.05980200
H	-2.30755700	-2.99673200	2.77649400
H	-3.58101900	-3.55761400	1.68203500
H	-4.78709300	2.46015500	-2.86917800
H	-4.16032400	0.82560400	-3.17032200
H	-5.53133700	1.06753300	-2.06656500
H	-4.41308900	3.57488200	-0.61685000
H	-3.54737500	2.69991100	0.65939200
H	-5.17548400	2.18369400	0.17666200
H	-2.36607500	3.19892700	-2.08308400
H	-1.81890600	1.55014500	-2.44919800
H	-1.58450400	2.23171100	-0.82305000
H	3.74103300	1.69343400	1.97722700
H	2.38240800	2.78526000	3.72202300
H	0.21598400	3.83617500	3.13435900
H	-0.56974100	3.79011800	0.78106200
H	0.77248100	2.66227200	-0.94742100
H	4.17039100	1.20243900	-0.25054200
C	3.29537000	2.15156800	-1.95462700
H	2.33814700	2.23820800	-2.47460400
H	3.65556800	3.15661500	-1.72636100
H	4.00742600	1.68225000	-2.63658500

Conformer 13b

C	3.56375700	-2.95348600	-1.02619800
C	2.14700000	-2.60328500	-0.53681000
C	2.22982200	-1.26206700	0.22581000
N	2.37280100	-0.27346600	-0.86771800
C	3.83383400	-1.86810400	-2.10684400
C	2.51410600	-1.06573300	-2.10102500
C	1.47275200	-2.15543200	-1.84129900
C	3.34028400	0.78915100	-0.59940000
C	1.02901200	-0.99783000	1.07450100
N	0.82663100	-1.61457400	2.26799700
N	-0.31552700	-1.23886000	2.75418700
N	-0.85716200	-0.36932000	1.88975200
C	-0.04835000	-0.19471300	0.82238900
C	-2.22033400	0.08889500	2.04409200
C	-3.21835800	-0.84630500	1.33016600
N	-2.80046600	-1.17984500	-0.03218700
C	-2.43399000	-2.58366600	-0.17264500
C	-3.31977100	-3.24942900	0.87497500
C	-3.33582500	-2.22566600	2.01539300
C	-2.64329600	-0.30867500	-1.05681500

O	-2.18052300	-0.60292700	-2.13999000
O	-3.06920800	0.92073200	-0.69645800
C	-2.91629800	2.06821300	-1.58355200
C	-3.70083000	1.86007900	-2.87547300
C	-3.52232700	3.20380900	-0.76628100
C	-1.43446200	2.33006900	-1.83794000
C	2.78523200	1.67014900	0.51040400
C	3.22182400	1.52176900	1.82195700
C	2.64196200	2.25087500	2.85576500
C	1.62113900	3.15103000	2.58407000
C	1.18880600	3.32172500	1.27175700
C	1.76623700	2.58543100	0.24792800
H	3.58087800	-3.95718900	-1.45833000
H	4.29308600	-2.93233800	-0.21247000
H	1.65799300	-3.38700500	0.04064700
H	3.11341000	-1.27054800	0.87963900
H	4.69671100	-1.24261800	-1.86652700
H	4.01644700	-2.30834300	-3.09075200
H	2.34718100	-0.45090300	-2.98428400
H	0.46489600	-1.75393300	-1.72007100
H	1.46990000	-2.93441000	-2.60748200
H	-0.27054500	0.46566900	0.00442900
H	-2.28562400	1.09483900	1.63146800
H	-2.44302800	0.12361200	3.11142900
H	-4.18172500	-0.32932400	1.30089600
H	-1.36820900	-2.72500200	0.05111700
H	-2.61786400	-2.91578300	-1.19352200
H	-4.32417400	-3.39263600	0.46635000
H	-2.93699900	-4.22051700	1.19116600
H	-2.47319200	-2.38401100	2.66673400
H	-4.23501600	-2.28621100	2.63025900
H	-3.70221100	2.79085500	-3.44919500
H	-3.26135400	1.06992000	-3.48171000
H	-4.73749200	1.59839000	-2.64800800
H	-3.45551900	4.14141200	-1.32319100
H	-2.98752800	3.32487900	0.17928000
H	-4.57370700	3.00236800	-0.54896700
H	-1.32208000	3.23567600	-2.43997000
H	-0.96974600	1.49801200	-2.36738200
H	-0.91511500	2.48944500	-0.88896800
H	4.00867700	0.80772800	2.04508800
H	2.98371500	2.10639300	3.87443900
H	1.16521800	3.71815900	3.38796200
H	0.39660900	4.02912900	1.04801800
H	1.40485800	2.70695300	-0.76696000
H	4.29009800	0.36185100	-0.22759800
C	3.66200500	1.59263900	-1.85861000
H	2.75169900	1.94986600	-2.34637400
H	4.27397100	2.45773800	-1.59562900

H	4.21611800	0.99124300	-2.58205400

Conformer 13c

C	-5.54523200	-0.27208800	-1.23128100
C	-4.32608500	-1.18307500	-0.98940200
C	-3.07504600	-0.29509400	-0.86262700
N	-3.27522700	0.36633800	0.46294700
C	-5.75411500	0.41555200	0.14645100
C	-4.57041200	-0.14374600	0.96377300
C	-4.52448200	-1.59022100	0.47788300
C	-3.12944300	1.82140700	0.43313700
C	-1.79726300	-1.08988600	-0.96476400
N	-1.81674500	-2.44714500	-1.05889600
N	-0.60827000	-2.89467100	-1.17736700
N	0.21499200	-1.84038600	-1.16517600
C	-0.48198600	-0.69051500	-1.03574400
C	1.64755900	-2.05825900	-1.18018400
C	2.26168200	-2.23154800	0.21614100
N	2.27237600	-0.98349800	0.98358000
C	1.43161500	-1.03215200	2.18111700
C	0.59188400	-2.29100400	1.97351100
C	1.50382300	-3.19836600	1.13963600
C	3.23846900	-0.03662800	0.87605500
O	3.38758100	0.87453400	1.66575900
O	3.98951200	-0.24801500	-0.22296800
C	5.12422000	0.60904400	-0.54854500
C	6.16746900	0.55404200	0.56386000
C	5.66630000	-0.02731200	-1.82351900
C	4.64766600	2.03218200	-0.82261400
C	-1.70055300	2.20294200	0.09089000
C	-1.39682800	2.78146200	-1.13764600
C	-0.08803600	3.13296600	-1.45813100
C	0.93140700	2.91605900	-0.54060200
C	0.63977600	2.34172800	0.69472400
C	-0.66550100	1.98387400	0.99997600
H	-6.41548900	-0.86832500	-1.51594200
H	-5.36420500	0.44653100	-2.03560100
H	-4.21051200	-1.99194900	-1.70608900
H	-3.06910800	0.46021400	-1.65881400
H	-5.75491800	1.50506800	0.08103500
H	-6.70137300	0.12168400	0.60693300
H	-4.65260100	-0.00443000	2.04131200
H	-3.69038100	-2.16028100	0.88602700
H	-5.46178800	-2.12401300	0.65175200
H	0.00100000	0.27140300	-1.00364400
H	2.12525500	-1.21824300	-1.68491200
H	1.81716500	-2.96398600	-1.76462300
H	3.28903300	-2.56532900	0.05197500

H	0.82893800	-0.12756400	2.26047700
H	2.06108600	-1.09958600	3.07547900
H	0.30260200	-2.74699000	2.92102700
H	-0.32284200	-2.05236800	1.42623600
H	0.95100100	-3.95386600	0.58152300
H	2.22386600	-3.70403600	1.78918700
H	7.06674000	1.08521200	0.24088300
H	5.79550600	1.01511900	1.47767700
H	6.44190700	-0.48324300	0.77343200
H	6.53262800	0.53394900	-2.18141300
H	4.90491600	-0.02611800	-2.60724000
H	5.97377100	-1.05895800	-1.63732800
H	5.48738500	2.63264400	-1.18228100
H	4.24757200	2.49183700	0.08058300
H	3.87581600	2.02576900	-1.59686600
H	-2.19241500	2.95610400	-1.85585000
H	0.13041800	3.57946700	-2.42208000
H	1.95080100	3.19603200	-0.77848100
H	1.43833700	2.16073600	1.40518800
H	-0.88685900	1.51270000	1.95141000
H	-3.76633200	2.25768500	-0.35860100
C	-3.55088100	2.45317200	1.76158100
H	-3.02511400	1.98725900	2.59860300
H	-3.31108600	3.51837600	1.75425200
H	-4.62340000	2.34765900	1.93476500

Conformer 13d

C	-3.33489300	-2.67961600	-0.88620800
C	-2.43758800	-2.22890600	0.28186100
C	-1.99523100	-0.77940800	-0.00121300
N	-3.22729600	0.00040300	0.29824500
C	-4.61679200	-1.81857900	-0.69064500
C	-4.27002300	-1.00235900	0.57463200
C	-3.47086100	-2.01185200	1.39626100
C	-3.52424100	1.04497600	-0.67287300
C	-0.80313200	-0.32965800	0.78831500
N	-0.55974200	-0.71136700	2.06980100
N	0.52245000	-0.13589300	2.49161000
N	0.98827100	0.62432600	1.49400900
C	0.19893900	0.52488900	0.40865500
C	2.20303900	1.38834900	1.65520200
C	3.44151300	0.70376000	1.05982600
N	3.31096500	0.46182700	-0.37590600
C	4.02611300	1.45022600	-1.18673900
C	4.54932400	2.45726600	-0.15849400
C	4.65751900	1.63542400	1.13141100
C	2.96987500	-0.72978000	-0.94958500
O	3.06886300	-0.93538900	-2.14177600

O	2.52582400	-1.59720100	-0.03259100
C	2.06058400	-2.93320200	-0.40188200
C	3.23164100	-3.75239300	-0.93526100
C	1.56337700	-3.48839900	0.92716700
C	0.91635700	-2.84871900	-1.40866900
C	-2.43419300	2.10403900	-0.63702900
C	-2.10898700	2.73805000	0.56237300
C	-1.10287100	3.69138200	0.60790000
C	-0.39962300	4.02404800	-0.54806100
C	-0.71923500	3.40220800	-1.74813900
C	-1.73448800	2.44898600	-1.78844800
H	-3.55798700	-3.74649700	-0.80520500
H	-2.85831400	-2.51586400	-1.85660400
H	-1.60878000	-2.89808700	0.50681800
H	-1.73594800	-0.67537700	-1.06564300
H	-4.83360700	-1.18144000	-1.55118600
H	-5.50012600	-2.43937500	-0.51881100
H	-5.12467900	-0.55102200	1.07706500
H	-3.04604100	-1.58631500	2.30414300
H	-4.03917800	-2.91639600	1.62718500
H	0.38719900	1.07259900	-0.49936100
H	2.34373600	1.52855800	2.72807900
H	2.04495000	2.36597900	1.19193800
H	3.59944200	-0.24061200	1.58026700
H	3.36345000	1.90288000	-1.92734800
H	4.83884400	0.95941000	-1.73095600
H	5.50069800	2.89457500	-0.46294700
H	3.83829300	3.27828400	-0.03003800
H	4.66498600	2.24934900	2.03459600
H	5.57222900	1.03699700	1.12374600
H	2.90583900	-4.78248500	-1.10308000
H	3.59989400	-3.34401200	-1.87632800
H	4.04653900	-3.76735800	-0.20662700
H	1.18368300	-4.50346800	0.78519300
H	0.76484100	-2.86369100	1.33248800
H	2.37599700	-3.52139300	1.65674600
H	0.47269300	-3.84102300	-1.52702400
H	1.26364100	-2.49731000	-2.37890200
H	0.14381600	-2.17285300	-1.03955600
H	-2.62314300	2.44116100	1.46968100
H	-0.85616700	4.16903000	1.54999800
H	0.38855400	4.76865100	-0.51274000
H	-0.17861000	3.65364600	-2.65413000
H	-1.97197000	1.95558800	-2.72630000
H	-3.53621000	0.63444400	-1.70058000
C	-4.88948400	1.68374900	-0.41263400
H	-4.95327500	2.04566300	0.61694000
H	-5.03240000	2.53197500	-1.08538800
H	-5.70277500	0.97455100	-0.58184000

Conformer 13e

C	5.63866800	-0.69633700	-0.99775500
C	4.22714000	-0.85187600	-1.59098800
C	3.21417700	-0.77813600	-0.42781100
N	3.19470300	0.66626100	-0.09368500
C	5.65181400	0.78366200	-0.52083200
C	4.24525500	1.27337300	-0.93112600
C	4.01613600	0.52108300	-2.24238900
C	3.20811800	0.95149600	1.34067400
C	1.86133800	-1.30754300	-0.78014400
N	1.63614500	-2.63934700	-0.92714500
N	0.38806800	-2.83156000	-1.22329300
N	-0.20189300	-1.63344600	-1.28263100
C	0.68236800	-0.64923900	-1.00756400
C	-1.63811600	-1.51648500	-1.42039300
C	-2.29663300	-1.38797300	-0.03820300
N	-3.68705400	-0.95523800	-0.15736300
C	-4.64914400	-1.98704400	0.22494400
C	-3.78734400	-3.24858800	0.28317600
C	-2.41254600	-2.72091900	0.70692200
C	-4.07887800	0.33315900	-0.32281700
O	-5.23107900	0.70747600	-0.27068700
O	-3.00480400	1.11740600	-0.55854200
C	-3.13742500	2.54759700	-0.79885500
C	-3.72046000	3.23968300	0.42982800
C	-1.69117600	2.97726800	-1.02104500
C	-3.97182200	2.79983200	-2.05135100
C	1.88001900	0.52557100	1.95065600
C	1.77954000	-0.64784700	2.68946700
C	0.55925000	-1.05838200	3.21937000
C	-0.57729700	-0.28647000	3.02509100
C	-0.48919200	0.89093700	2.28695700
C	0.72750900	1.28678400	1.75254200
H	6.39699800	-0.87393700	-1.76431300
H	5.81924100	-1.40478800	-0.18551900
H	4.08781600	-1.73243100	-2.21601500
H	3.59091700	-1.37521000	0.41504900
H	5.82539500	0.87690000	0.55338300
H	6.42614000	1.36793700	-1.02506200
H	4.13402500	2.35596600	-0.97644900
H	3.01267800	0.67133800	-2.64407500
H	4.76231000	0.75192200	-3.00621600
H	0.41176200	0.39125800	-0.96745600
H	-1.99150900	-2.40081200	-1.95313200
H	-1.85634600	-0.62943400	-2.01517300
H	-1.72334300	-0.65780300	0.53387700
H	-5.46148200	-2.04547300	-0.50094100
H	-5.08950600	-1.75007600	1.20032900

H	-4.18940500	-3.99316000	0.97093300
H	-3.72769000	-3.70976000	-0.70718800
H	-1.58934800	-3.39526200	0.46657100
H	-2.39299700	-2.53408900	1.78444900
H	-3.69850900	4.32242500	0.28040700
H	-4.74982300	2.92927900	0.60419200
H	-3.12352400	3.00789200	1.31617200
H	-1.64121600	4.05391300	-1.19929800
H	-1.26591700	2.46294100	-1.88669100
H	-1.08580600	2.74017600	-0.14326000
H	-3.94416500	3.86498500	-2.29612600
H	-5.00801600	2.49978800	-1.90103600
H	-3.55943100	2.24512400	-2.89852900
H	2.66377500	-1.25857500	2.84393100
H	0.50097400	-1.98191400	3.78446200
H	-1.52898000	-0.59812800	3.44168700
H	-1.37583800	1.49299000	2.11821700
H	0.78261500	2.19485300	1.16190100
H	3.99387000	0.35728300	1.84246200
C	3.50060800	2.42542200	1.62295700
H	2.82415000	3.07855900	1.06613300
H	3.37208200	2.62671800	2.68823600
H	4.52394500	2.68870000	1.34886500

Conformer 13f

C	5.63812300	-0.40813400	-1.03826700
C	4.24245900	-0.44486600	-1.68611400
C	3.20425600	-0.64849800	-0.56136300
N	3.15123600	0.68359400	0.08798200
C	5.61415800	0.92716900	-0.24139700
C	4.20772200	1.47763100	-0.56536800
C	4.02013900	1.03655900	-2.01745200
C	3.12867600	0.63918900	1.54950700
C	1.86740100	-1.09978600	-1.05367100
N	1.65221100	-2.37612500	-1.46755500
N	0.41375200	-2.50423700	-1.83206900
N	-0.17804000	-1.31678800	-1.67245200
C	0.69344000	-0.40767100	-1.18218100
C	-1.61328800	-1.17247600	-1.80222500
C	-2.27619000	-1.35367400	-0.43312500
N	-3.68082100	-0.93345000	-0.44009800
C	-4.57583100	-2.00293600	-0.00027300
C	-3.64830700	-2.90683200	0.81058200
C	-2.32466000	-2.81158000	0.04806800
C	-4.06096200	0.37055200	-0.34297200
O	-5.19554900	0.74680300	-0.14175100
O	-2.98849600	1.17265500	-0.50894800
C	-3.09517900	2.62423400	-0.46897200

C	-3.58731800	3.08369500	0.90034800
C	-1.65133700	3.06156000	-0.69349100
C	-3.99266800	3.11961800	-1.59882700
C	1.80044200	0.05983700	2.01668800
C	1.71823000	-1.25178800	2.47034800
C	0.50058800	-1.79797600	2.86706700
C	-0.65242500	-1.02726900	2.82586200
C	-0.58245900	0.28864400	2.37581700
C	0.63188800	0.82143800	1.97058100
H	6.41575900	-0.39910800	-1.80599900
H	5.81423700	-1.27848800	-0.40132700
H	4.13275000	-1.16383600	-2.49640300
H	3.57416600	-1.41544000	0.13407200
H	5.76413600	0.77947700	0.83029500
H	6.38768900	1.62001000	-0.58319600
H	4.07735300	2.54110700	-0.36916100
H	3.02288800	1.26025900	-2.39996400
H	4.77786600	1.44318600	-2.69125100
H	0.41666600	0.60495600	-0.94715500
H	-1.96155900	-1.91832700	-2.51809100
H	-1.82187000	-0.17529200	-2.18844100
H	-1.72261600	-0.73980100	0.28085900
H	-4.99047900	-2.53305300	-0.86491600
H	-5.40337100	-1.57931800	0.56752400
H	-3.53635900	-2.50243700	1.82159000
H	-4.02000300	-3.92924000	0.89304500
H	-2.32971200	-3.49018700	-0.81027900
H	-1.45127200	-3.05771000	0.65267600
H	-3.54785600	4.17497500	0.95155700
H	-4.61162700	2.75933700	1.07843400
H	-2.94388000	2.68463600	1.68924000
H	-1.57838200	4.15118900	-0.66560900
H	-1.29110900	2.71565800	-1.66579200
H	-1.00508200	2.64825000	0.08502100
H	-3.95260100	4.21129900	-1.64136700
H	-5.02572100	2.81106300	-1.44364400
H	-3.64422300	2.72814800	-2.55830000
H	2.61542700	-1.86219800	2.50297600
H	0.45727100	-2.82615700	3.20878700
H	-1.60278200	-1.44709200	3.13739000
H	-1.48123400	0.89456000	2.33004900
H	0.67225300	1.84120400	1.60310600
H	3.91878000	-0.03694200	1.92486600
C	3.37897000	2.01757400	2.16175000
H	2.69943100	2.76597300	1.74652300
H	3.22229700	1.97310700	3.24126000
H	4.40155300	2.35431800	1.98104100

Cartesian coordinates for individual conformers of *epi*-13

Conformer *epi*-13a

C	1.46309	-1.95435	2.83487
C	2.33834	-2.65708	1.78211
C	1.926	-2.21757	0.35383
N	2.26751	-0.77879	0.34082
C	1.90762	-0.46747	2.71679
C	2.97538	-0.53487	1.61526
C	3.65728	-1.87936	1.90668
C	2.96865	-0.28846	-0.84242
C	0.49241	-2.42253	-0.00769
N	0.01669	-3.53647	-0.61917
N	-1.26677	-3.41912	-0.78383
N	-1.63256	-2.23502	-0.27768
C	-0.56247	-1.57379	0.2095
C	-3.00311	-1.77811	-0.35885
C	-3.23687	-0.74769	-1.47483
N	-2.35201	0.41749	-1.39189
C	-1.47923	0.56835	-2.55603
C	-1.52602	-0.81179	-3.20158
C	-2.94418	-1.29664	-2.88383
C	-2.29526	1.32085	-0.38358
O	-1.52796	2.2624	-0.36327
O	-3.17882	1.01721	0.58778
C	-3.14005	1.69906	1.87965
C	-3.47155	3.17905	1.71549
C	-4.23686	0.9881	2.66414
C	-1.78154	1.47827	2.54177
C	2.99986	1.22989	-0.81513
C	4.16928	1.93139	-1.09051
C	4.17168	3.32345	-1.11607
C	2.99928	4.02641	-0.86812
C	1.82492	3.3314	-0.5914
C	1.82937	1.94442	-0.56075
H	1.68084	-2.35763	3.82697
H	0.39675	-2.09836	2.65298
H	2.38537	-3.74124	1.88159
H	2.53972	-2.79448	-0.3508
H	1.09698	0.20085	2.42111
H	2.33167	-0.09716	3.65399
H	3.61017	0.34726	1.54888
H	4.40066	-2.1576	1.15492
H	4.10698	-1.93983	2.90087
H	-0.61443	-0.5911	0.64351
H	-3.28039	-1.35002	0.60287
H	-3.61847	-2.65867	-0.54631

H	-4.28082	-0.433	-1.38255
H	-0.4831	0.87844	-2.24028
H	-1.87198	1.34304	-3.22505
H	-1.32341	-0.77425	-4.27238
H	-0.7867	-1.47245	-2.74175
H	-3.03606	-2.38287	-2.92201
H	-3.65596	-0.86817	-3.59469
H	-3.58191	3.63478	2.70318
H	-2.68727	3.7006	1.16977
H	-4.41636	3.29574	1.17846
H	-4.31399	1.41483	3.66681
H	-4.01508	-0.07781	2.76062
H	-5.20116	1.10047	2.16347
H	-1.79771	1.89694	3.55118
H	-0.98173	1.96117	1.98035
H	-1.56866	0.40824	2.62765
H	5.08844	1.38587	-1.2846
H	5.09176	3.8573	-1.32814
H	2.99985	5.11069	-0.88939
H	0.89757	3.86062	-0.40318
H	0.91375	1.41154	-0.33253
H	4.01329	-0.65339	-0.86134
C	2.29114	-0.75158	-2.13522
H	1.24772	-0.4317	-2.14623
H	2.79872	-0.30176	-2.99101
H	2.31625	-1.83655	-2.25529

Conformer *epi*-13b

C	1.66391	-2.53213	2.50875
C	2.11298	-3.15665	1.17747
C	1.41602	-2.43469	-0.00418
N	1.99579	-1.06849	0.03052
C	2.28506	-1.1076	2.43883
C	3.02485	-1.13244	1.09273
C	3.52808	-2.58201	1.02558
C	2.48322	-0.5996	-1.2721
C	-0.07393	-2.40026	0.06928
N	-0.86696	-3.4479	-0.27402
N	-2.10779	-3.13128	-0.0619
N	-2.1308	-1.88391	0.42717
C	-0.87793	-1.38713	0.51738
C	-3.38012	-1.1944	0.67212
C	-3.81861	-0.33474	-0.52776
N	-2.73373	0.48562	-1.06933
C	-2.38076	0.10845	-2.43422
C	-3.69525	-0.45607	-2.9605
C	-4.25929	-1.18376	-1.73762
C	-2.05041	1.44884	-0.40821

O	-1.08417	2.03147	-0.85973
O	-2.58673	1.65866	0.81098
C	-1.98659	2.59279	1.76077
C	-1.94463	4.00336	1.18039
C	-2.95067	2.52981	2.94014
C	-0.60395	2.09736	2.17627
C	3.10221	0.7788	-1.1339
C	4.44987	0.98712	-1.41133
C	5.01812	2.25118	-1.2796
C	4.23775	3.32269	-0.86617
C	2.88689	3.12393	-0.59352
C	2.3233	1.86303	-0.72793
H	2.0714	-3.10498	3.34555
H	0.57831	-2.52061	2.61797
H	2.0005	-4.23901	1.1211
H	1.70273	-2.96263	-0.92426
H	1.53624	-0.3135	2.44504
H	2.98053	-0.92897	3.26317
H	3.76154	-0.34104	0.9771
H	4.00243	-2.83103	0.07266
H	4.1984	-2.85408	1.84473
H	-0.64497	-0.39903	0.87018
H	-3.25155	-0.5691	1.55429
H	-4.13758	-1.95195	0.87775
H	-4.62931	0.31265	-0.17948
H	-1.59539	-0.65675	-2.4269
H	-2.01081	0.97688	-2.97779
H	-4.3534	0.36303	-3.26453
H	-3.55385	-1.11823	-3.81541
H	-3.81708	-2.18091	-1.66371
H	-5.34356	-1.30085	-1.76592
H	-1.655	4.70521	1.96702
H	-1.23226	4.07397	0.36048
H	-2.93428	4.29034	0.81555
H	-2.59906	3.18087	3.74384
H	-3.01929	1.51043	3.32822
H	-3.94844	2.85664	2.6388
H	-0.19055	2.76736	2.93432
H	0.08388	2.07182	1.3317
H	-0.67167	1.09821	2.61652
H	5.06526	0.1498	-1.72742
H	6.07057	2.39576	-1.49809
H	4.67673	4.30878	-0.76153
H	2.26637	3.95768	-0.2827
H	1.26562	1.72235	-0.53604
H	3.26629	-1.27934	-1.65789
C	1.34615	-0.56367	-2.29511
H	0.55578	0.11031	-1.95792
H	1.72698	-0.1991	-3.25197

H	0.9125	-1.5535	-2.45689

Conformer *epi*-13c

C	-1.26648	-2.18716	2.65268
C	-2.31358	-1.07199	2.47167
C	-1.80644	-0.02927	1.45024
N	-1.69438	-0.82388	0.21494
C	-1.32278	-2.94591	1.29358
C	-2.34911	-2.11369	0.50841
C	-3.37257	-1.76645	1.59959
C	-2.00621	-0.11293	-1.02709
C	-0.50889	0.64378	1.74705
N	-0.38865	1.75153	2.5244
N	0.85751	2.11361	2.5613
N	1.55426	1.24492	1.8168
C	0.73747	0.31111	1.28467
C	2.95175	1.47249	1.52083
C	3.1679	2.12081	0.14131
N	2.54561	1.36921	-0.9499
C	1.44736	2.07901	-1.60549
C	1.16554	3.24652	-0.66332
C	2.52139	3.51012	0.00224
C	2.85661	0.10842	-1.33653
O	2.26265	-0.49637	-2.2062
O	3.88847	-0.37465	-0.61591
C	4.26167	-1.78488	-0.68814
C	4.76322	-2.13601	-2.08548
C	5.39368	-1.88263	0.32819
C	3.08171	-2.65448	-0.25942
C	-3.4859	0.20912	-1.20037
C	-3.98219	1.43943	-0.76745
C	-5.34064	1.73039	-0.82904
C	-6.22984	0.79133	-1.33556
C	-5.74778	-0.43138	-1.79046
C	-4.38988	-0.71621	-1.72564
H	-1.54875	-2.83661	3.48485
H	-0.27466	-1.7873	2.87261
H	-2.65535	-0.61258	3.39844
H	-2.5776	0.74994	1.37355
H	-0.36243	-2.96321	0.77557
H	-1.66672	-3.97645	1.42222
H	-2.72833	-2.59664	-0.39006
H	-4.16203	-1.09662	1.25245
H	-3.81695	-2.64461	2.07512
H	1.06704	-0.47614	0.62978
H	3.47476	0.51818	1.56392
H	3.34174	2.12908	2.29932
H	4.25029	2.17073	-0.00736

H	0.59491	1.41063	-1.73346
H	1.76013	2.41766	-2.59941
H	0.78587	4.11967	-1.1951
H	0.42198	2.96188	0.08426
H	2.4246	4.01157	0.96601
H	3.14435	4.13218	-0.64618
H	5.16773	-3.15178	-2.07816
H	3.95988	-2.07896	-2.81798
H	5.56326	-1.45236	-2.38094
H	5.77037	-2.90728	0.36888
H	5.04355	-1.60505	1.32568
H	6.21678	-1.22048	0.05036
H	3.40207	-3.69783	-0.20174
H	2.25788	-2.58269	-0.96921
H	2.73014	-2.35604	0.73294
H	-3.29342	2.18387	-0.37882
H	-5.70243	2.69245	-0.48329
H	-7.28994	1.01319	-1.38542
H	-6.43257	-1.16543	-2.20102
H	-4.03423	-1.67185	-2.0945
H	-1.48754	0.84887	-0.92993
C	-1.38969	-0.83676	-2.22087
H	-0.30641	-0.90255	-2.09826
H	-1.77844	-1.85335	-2.32647
H	-1.60691	-0.30055	-3.1483

Conformer *epi*-13d

C	-1.43021	-2.02031	2.78589
C	-2.38508	-0.84368	2.50982
C	-1.77817	0.09142	1.43876
N	-1.70281	-0.78443	0.25573
C	-1.51411	-2.85512	1.4736
C	-2.45924	-2.00048	0.6141
C	-3.47551	-1.51085	1.65656
C	-1.94961	-0.13224	-1.03402
C	-0.44153	0.68042	1.74016
N	-0.26027	1.80408	2.48218
N	1.00813	2.06587	2.55714
N	1.66102	1.11583	1.87236
C	0.78935	0.23291	1.33946
C	3.08623	1.20574	1.63895
C	3.41183	1.87418	0.29036
N	2.64792	1.32224	-0.83051
C	1.75607	2.30329	-1.43814
C	2.46072	3.61898	-1.12657
C	3.04206	3.37146	0.26773
C	2.69312	0.04865	-1.28906
O	2.00802	-0.37106	-2.19954

O	3.588	-0.6779	-0.58894
C	3.74173	-2.1129	-0.81573
C	4.82743	-2.49254	0.18486
C	2.43753	-2.83648	-0.48778
C	4.2104	-2.38338	-2.24235
C	-3.39531	0.30717	-1.23574
C	-3.78175	1.60295	-0.89127
C	-5.10932	2.00732	-0.98145
C	-6.07763	1.11764	-1.42843
C	-5.70481	-0.17109	-1.79555
C	-4.37734	-0.56874	-1.70255
H	-1.78014	-2.59423	3.64743
H	-0.416	-1.68307	3.00852
H	-2.70884	-0.30144	3.39748
H	-2.48532	0.92002	1.29548
H	-0.54727	-2.97321	0.98125
H	-1.93547	-3.84836	1.65482
H	-2.85635	-2.51101	-0.26096
H	-4.20487	-0.80743	1.24975
H	-3.99424	-2.3224	2.17348
H	1.07696	-0.60699	0.73324
H	3.50037	0.19939	1.66938
H	3.51372	1.7946	2.45165
H	4.48134	1.72582	0.1108
H	0.76527	2.2569	-0.96686
H	1.64091	2.09491	-2.50085
H	3.25816	3.78911	-1.85569
H	1.78417	4.47391	-1.15383
H	2.28224	3.571	1.02798
H	3.90782	3.99653	0.49119
H	5.03198	-3.56396	0.12411
H	5.7515	-1.94959	-0.02626
H	4.51053	-2.26029	1.20476
H	2.58507	-3.91414	-0.59537
H	1.63273	-2.52861	-1.15499
H	2.1424	-2.64279	0.54772
H	5.09946	-1.78788	-2.46556
H	3.43326	-2.1445	-2.96621
H	4.47476	-3.43979	-2.33942
H	-3.03023	2.30862	-0.54945
H	-5.38511	3.01889	-0.70443
H	-7.11405	1.42785	-1.50025
H	-6.45139	-0.86868	-2.15942
H	-4.10683	-1.57512	-2.0023
H	-1.34235	0.78028	-1.00318
C	-1.40516	-0.98695	-2.17471
H	-0.32796	-1.11241	-2.05637
H	-1.86968	-1.97656	-2.20306
H	-1.59285	-0.50304	-3.1364