

Synthesis and evaluation of novel iminosugars prepared from natural amino acids

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Figure S1: ¹H-NMR (400 MHz, CDCl₃) of **1a**.

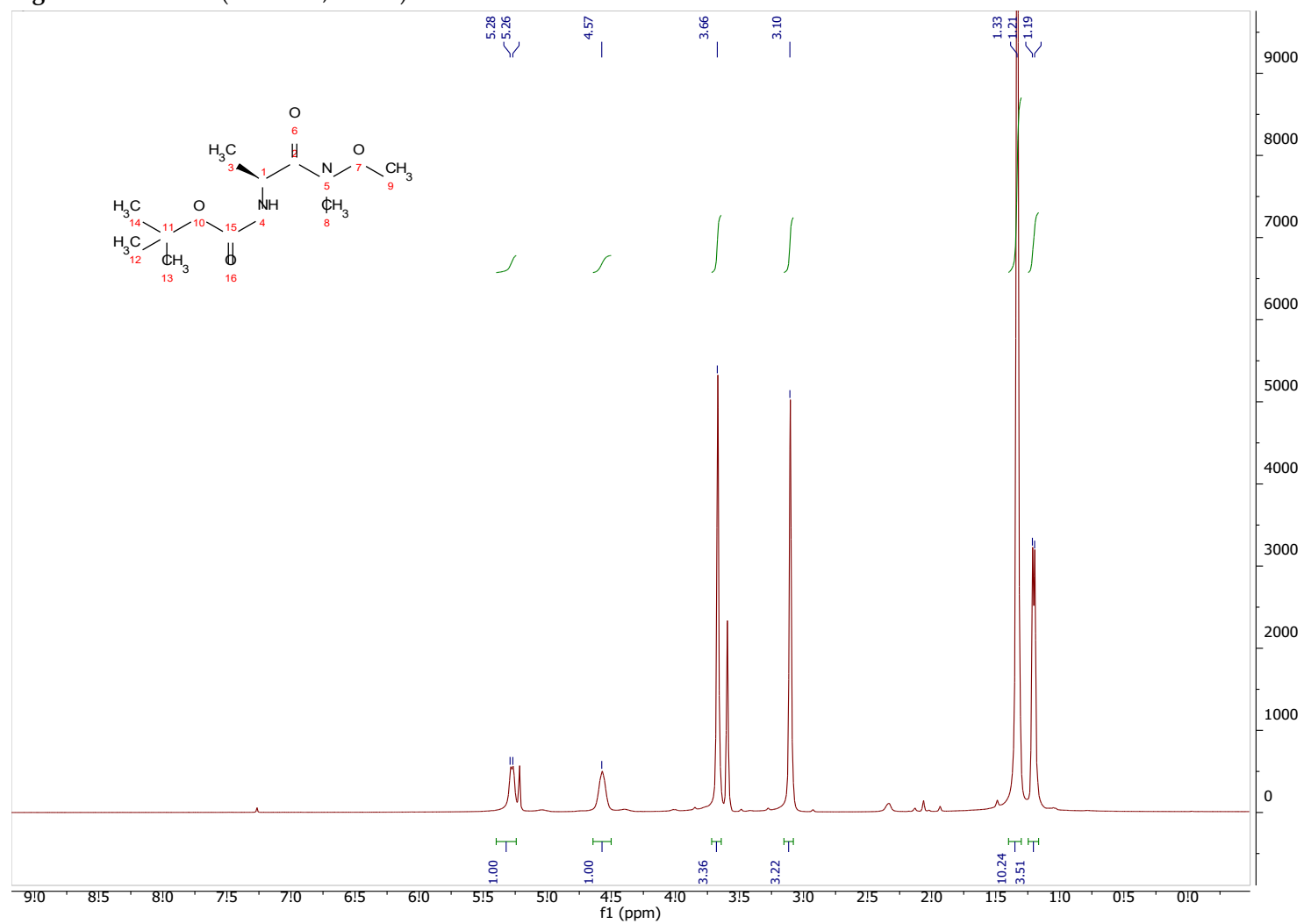


Figure S2: ^{13}C -NMR (100 MHz, CDCl_3) of **1a**.

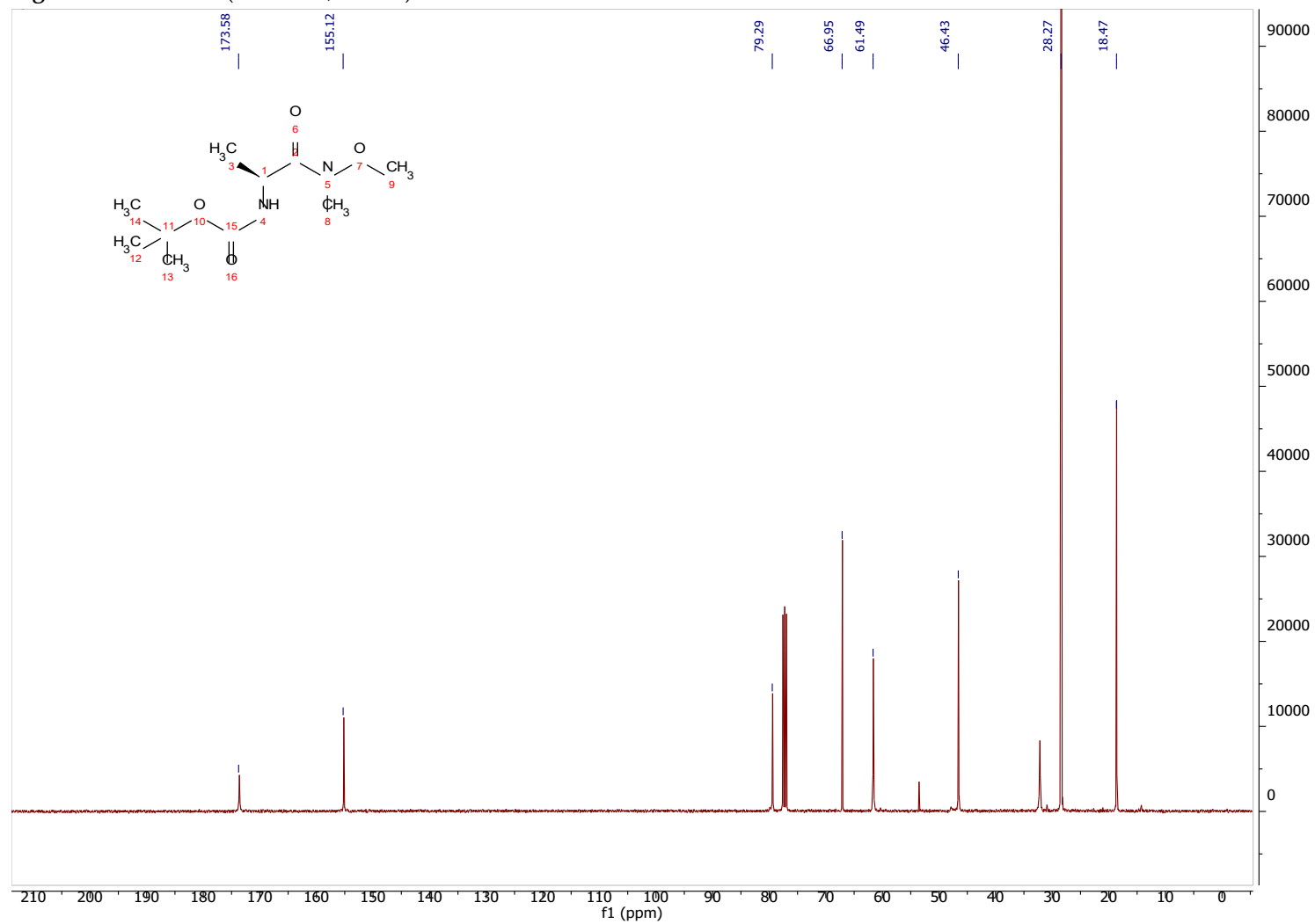


Figure S3: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (S)-allyl(1-(methoxy(methyl)amino)-1-oxopropan-2-yl)carbamate.

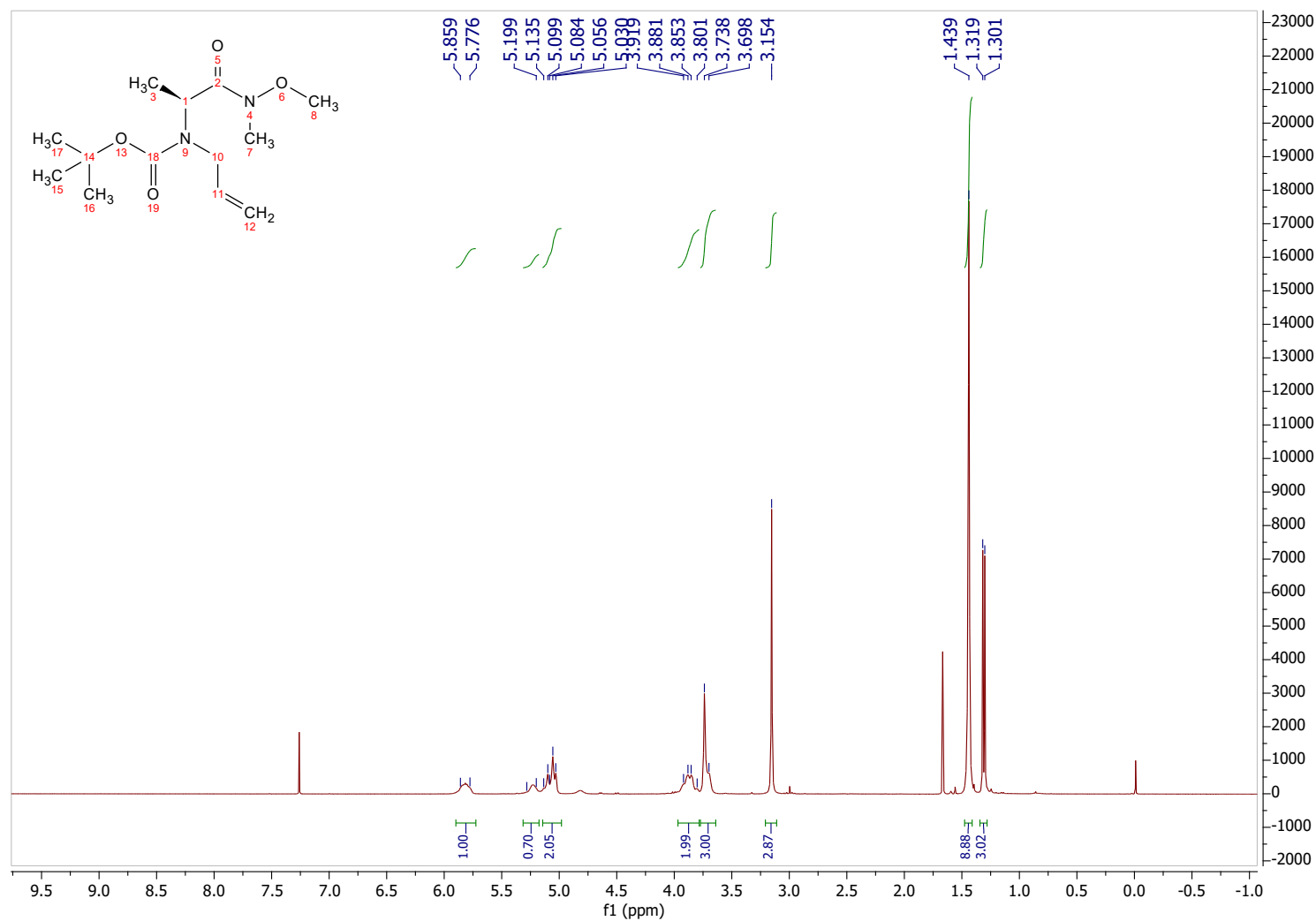


Figure S4: ^{13}C -NMR (100 MHz, CDCl_3) of *tert*-butyl (S)-allyl(1-(methoxy(methyl)amino)-1-oxopropan-2-yl)carbamate.

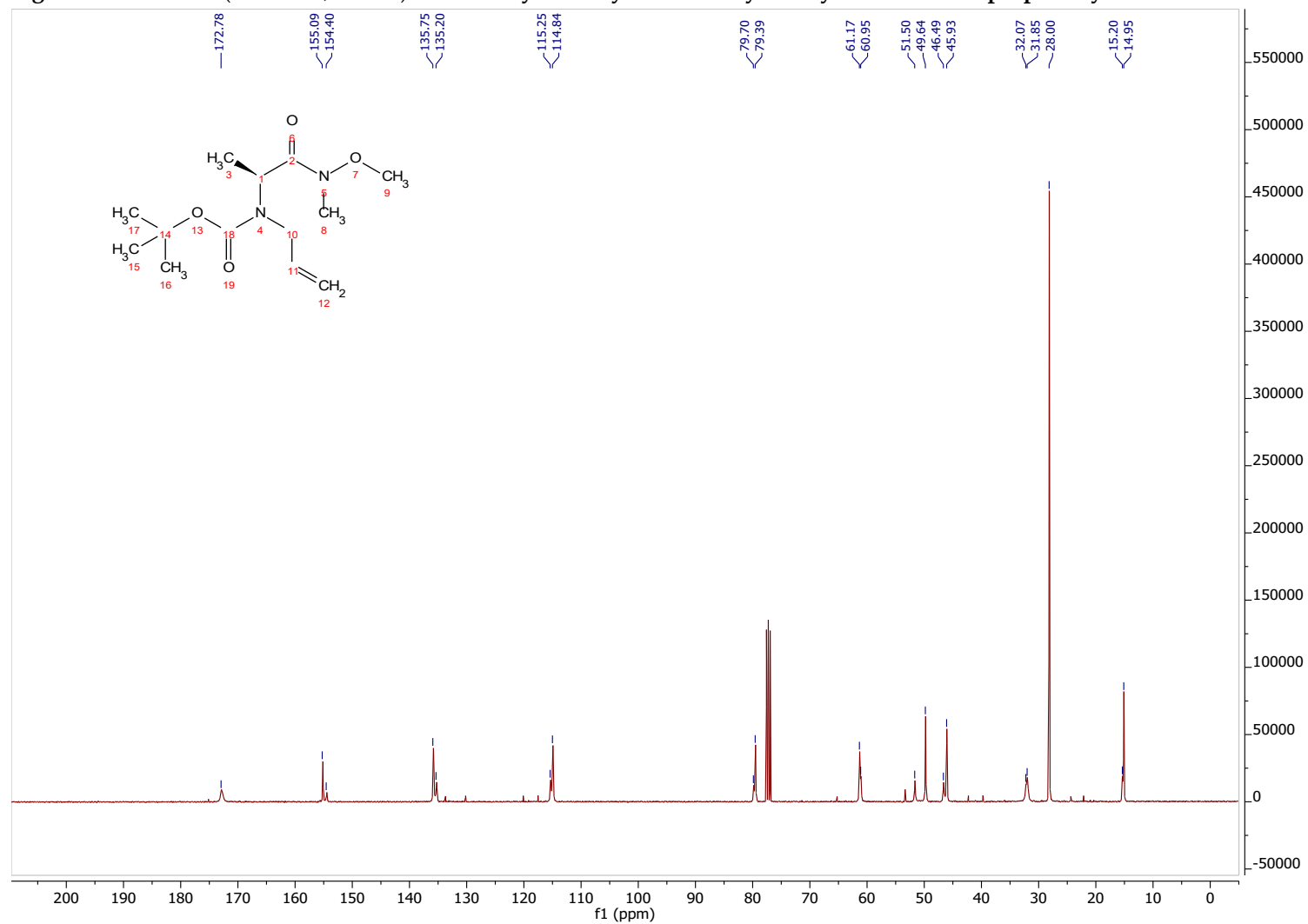
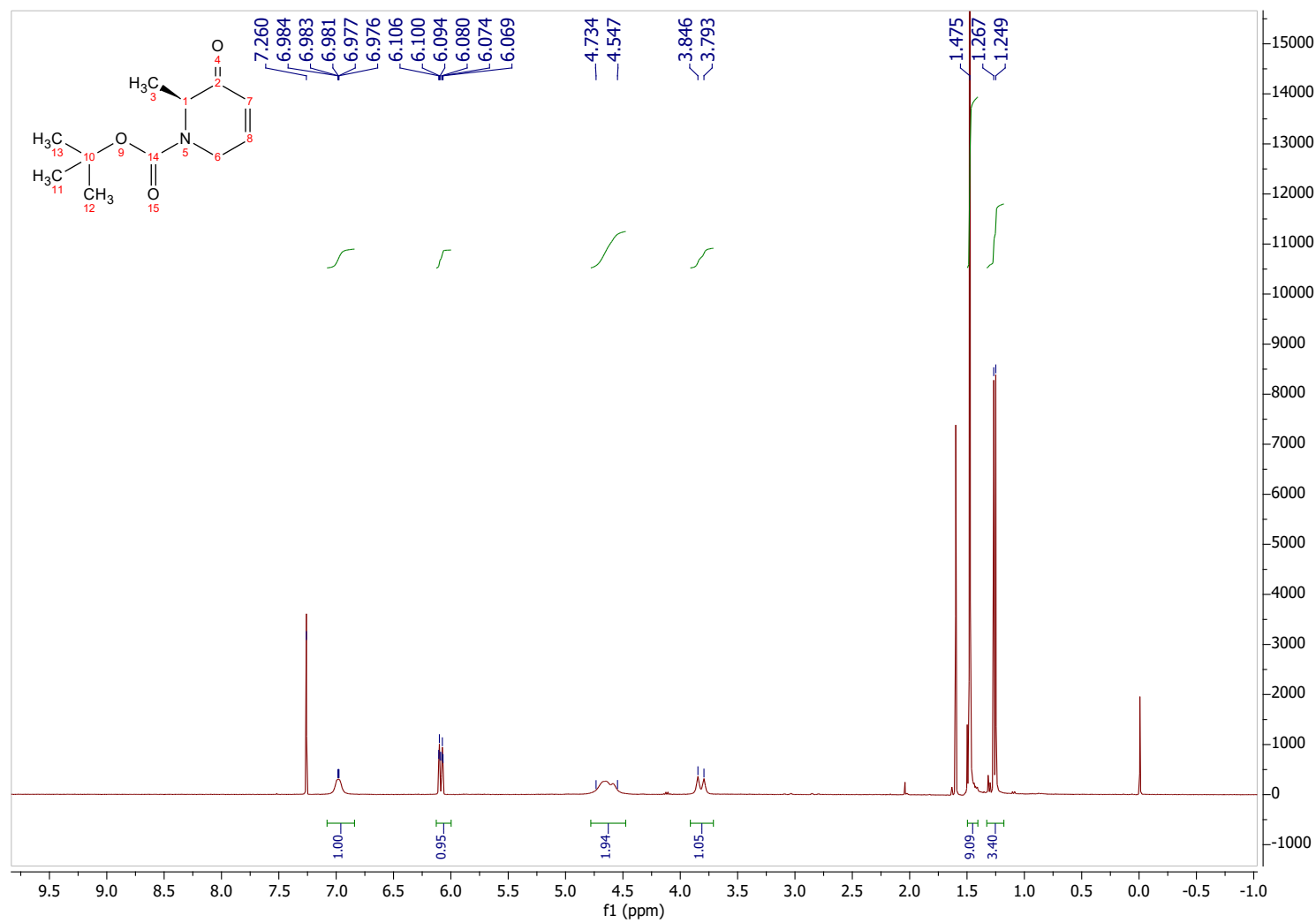


Figure S5: ^1H -NMR (400 MHz, CDCl_3) of **2a**.



2a

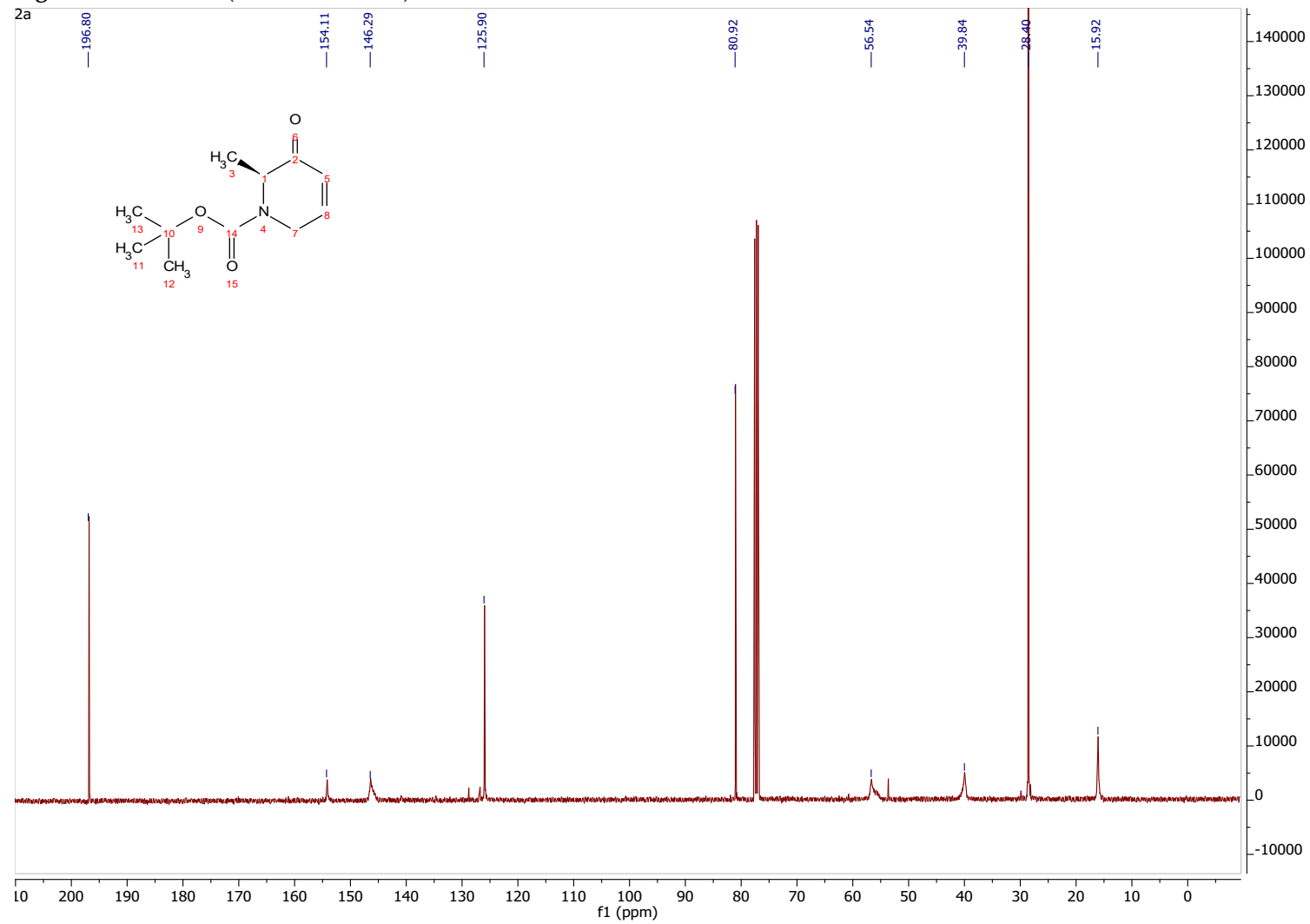


Figure S7: ^1H -NMR (400 MHz, CDCl_3) of **3a**.

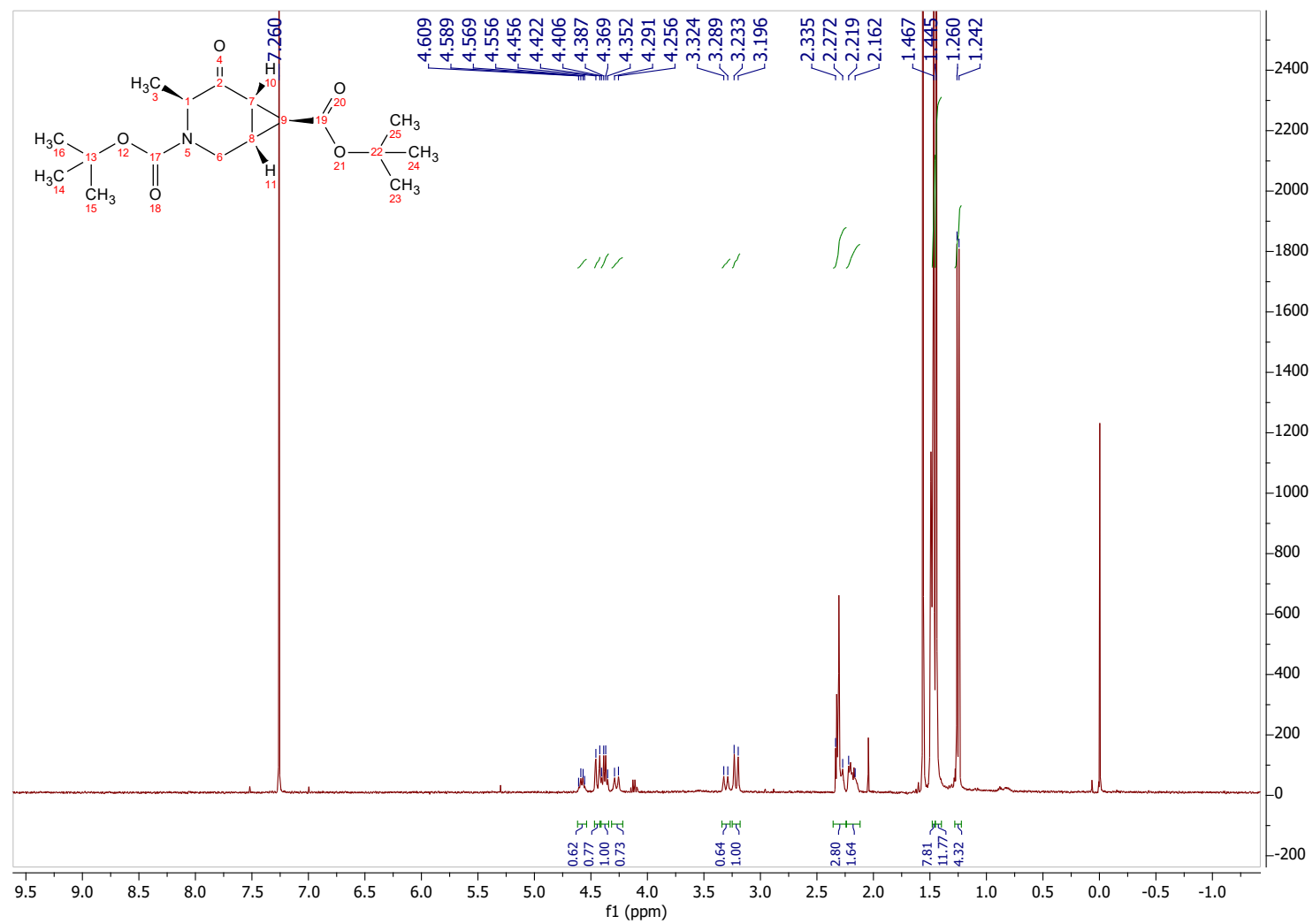


Figure S8: ^{13}C -NMR (100 MHz, CDCl_3) of **3a**.

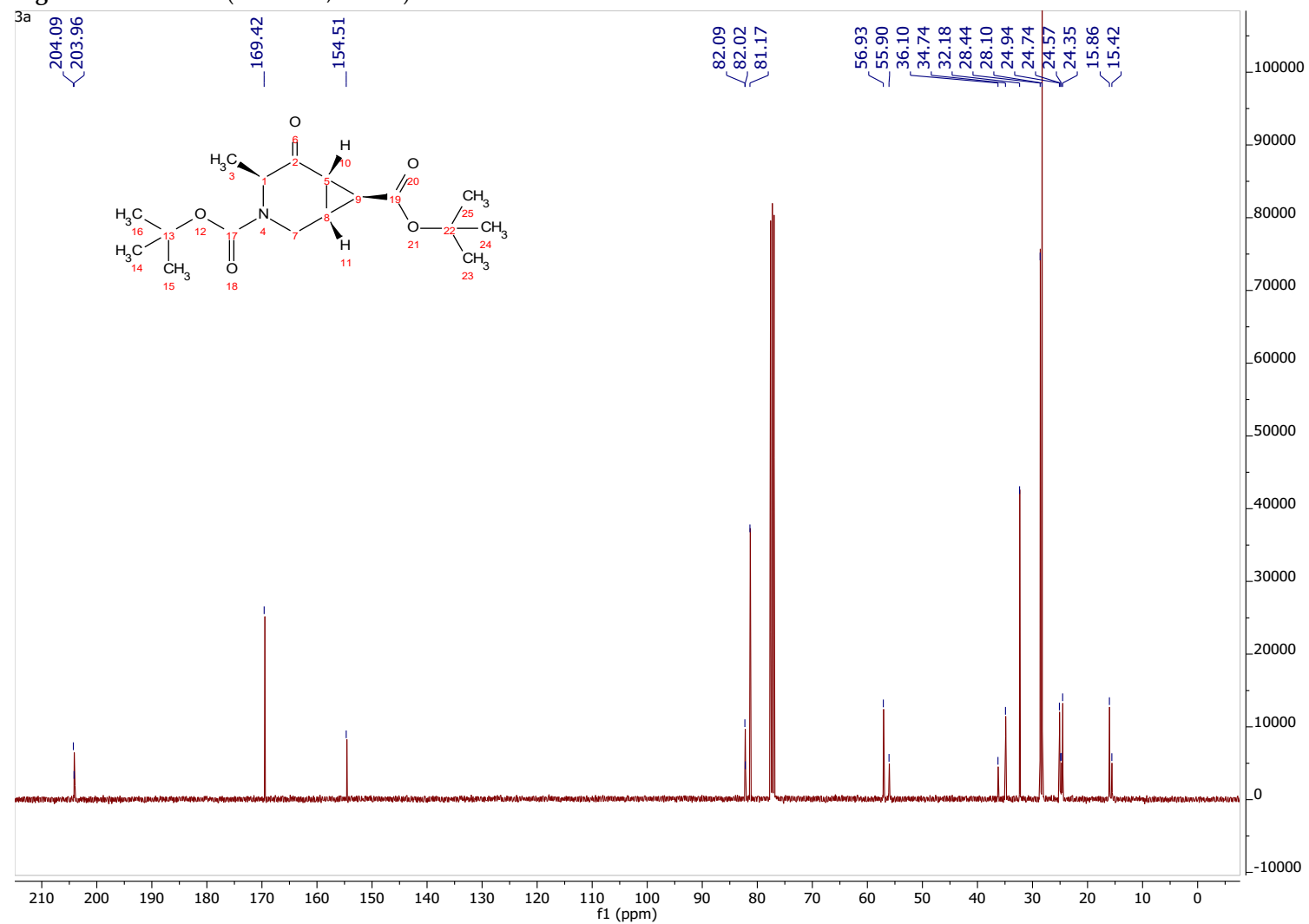


Figure S9: HMQC (400 MHz, CDCl₃) of 3a.

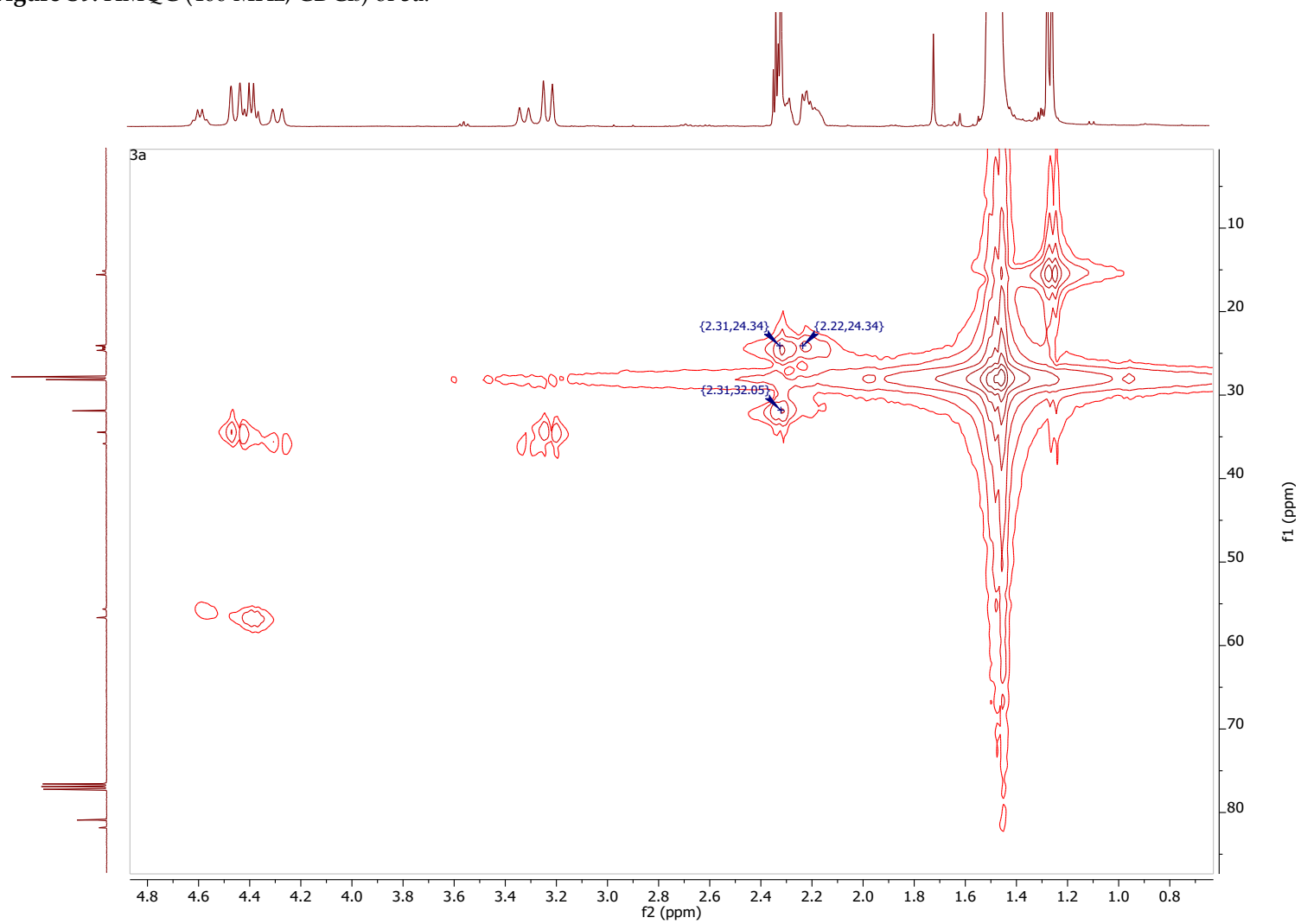


Figure S10: ^1H -NMR (400 MHz, CDCl_3) of **4a**.

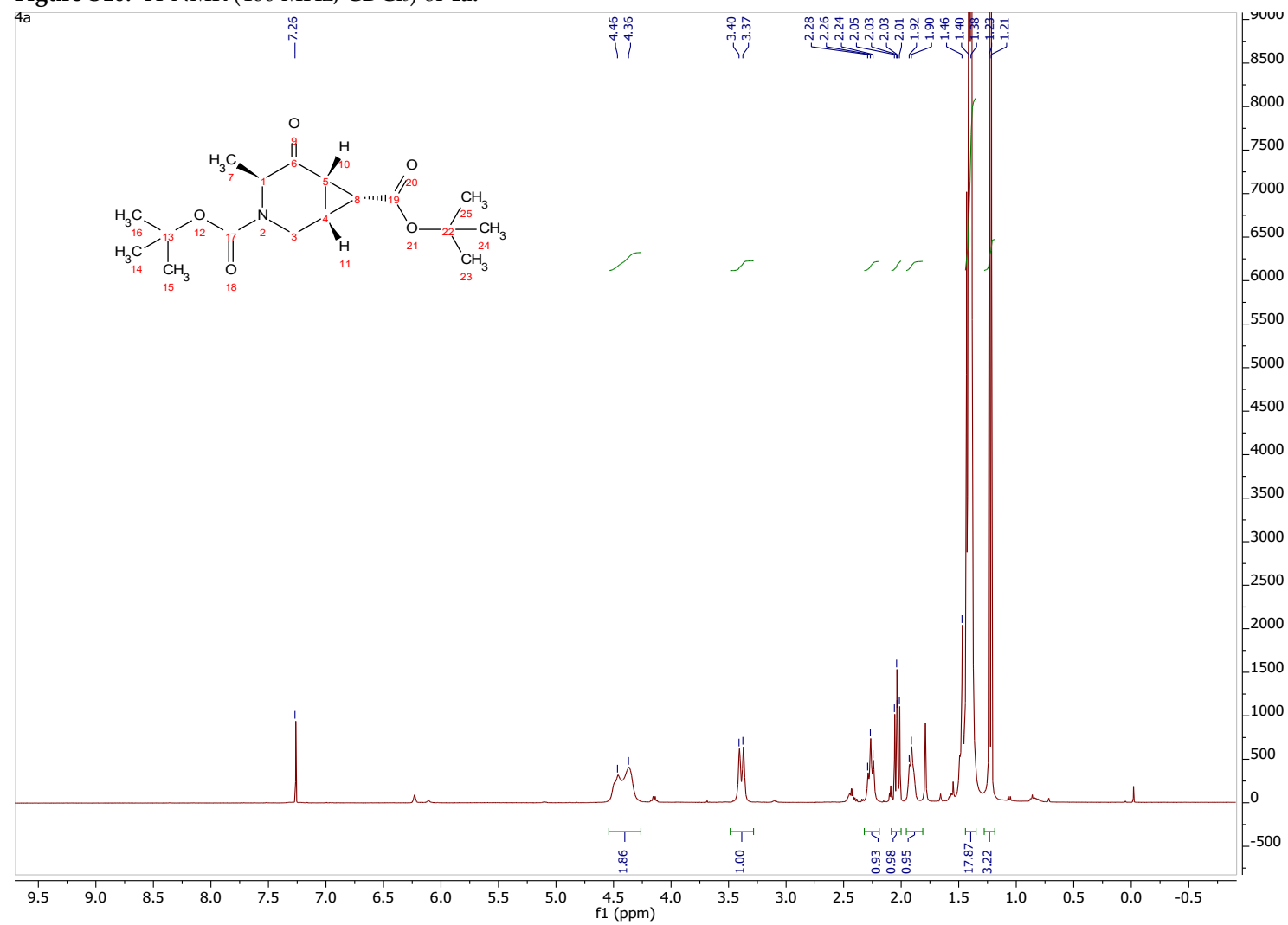


Figure S11: ^{13}C -NMR (100 MHz, CDCl_3) of **4a**.

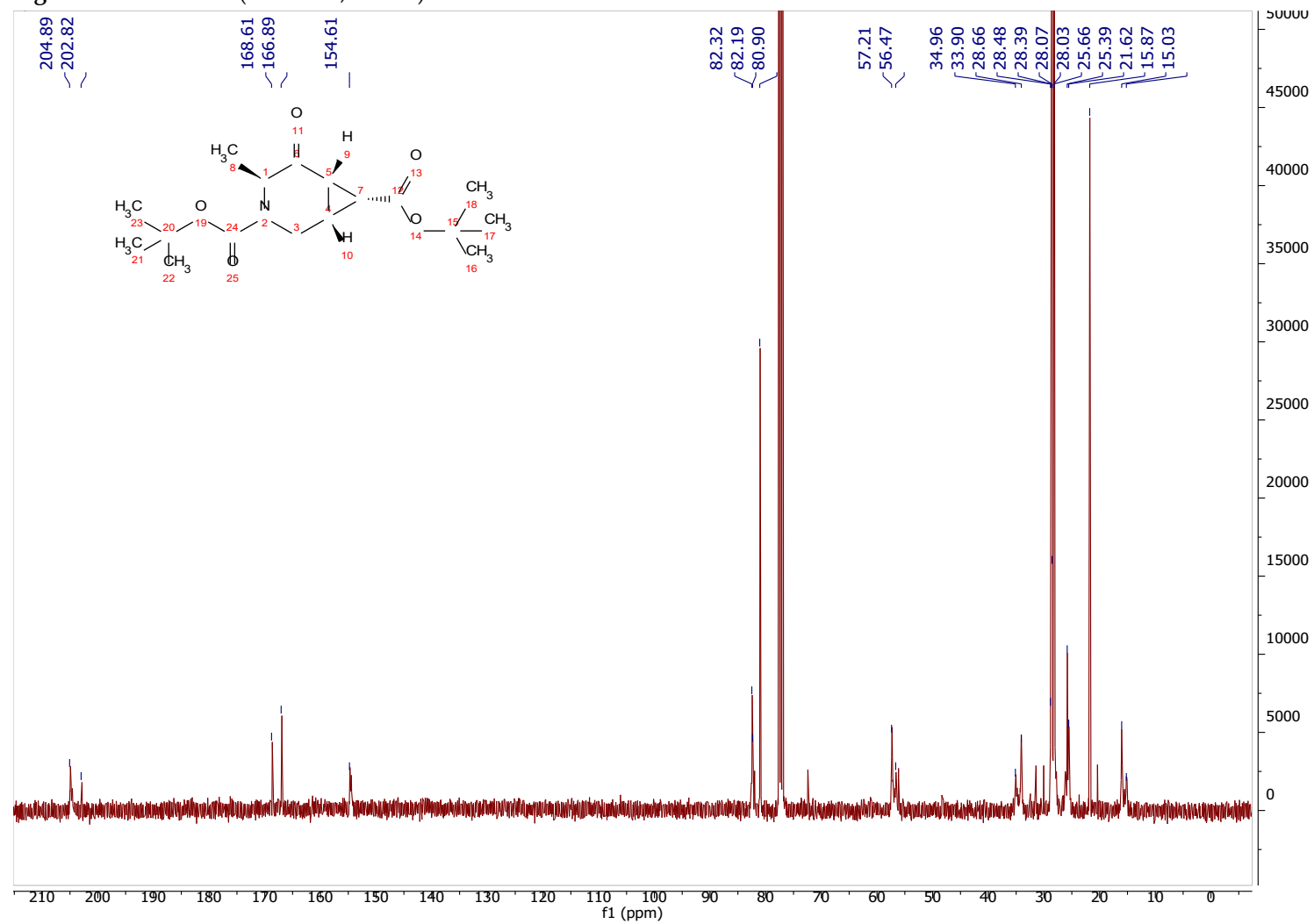


Figure S12: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (S)-(3-hydroxy-1-(methoxy(methyl)amino)-1-oxopropan-2-yl)carbamate.

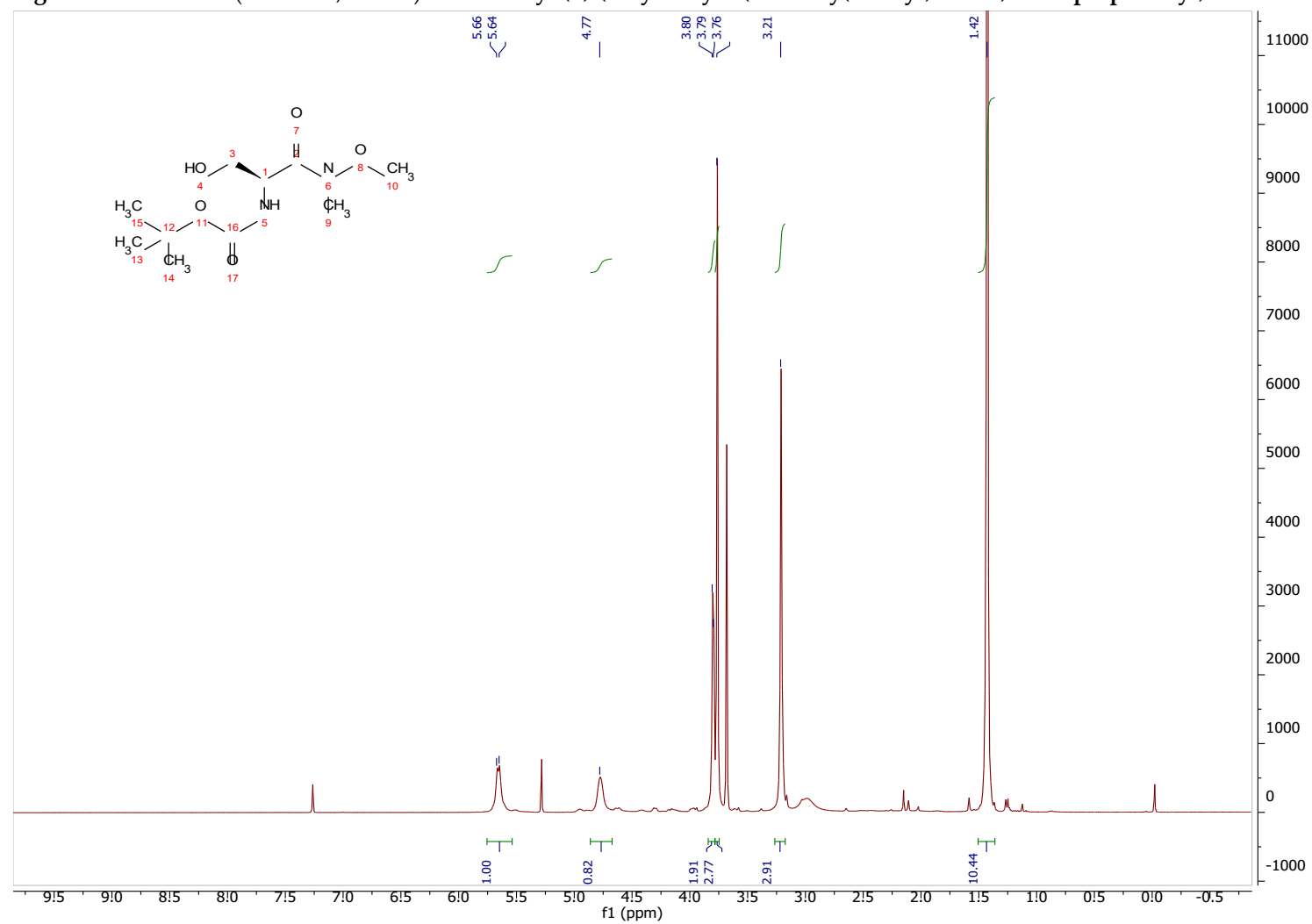


Figure S13: ^{13}C -NMR (100 MHz, CDCl_3) of *tert*-butyl (*S*)-(3-hydroxy-1-(methoxy(methyl)amino)-1-oxopropan-2-yl)carbamate.

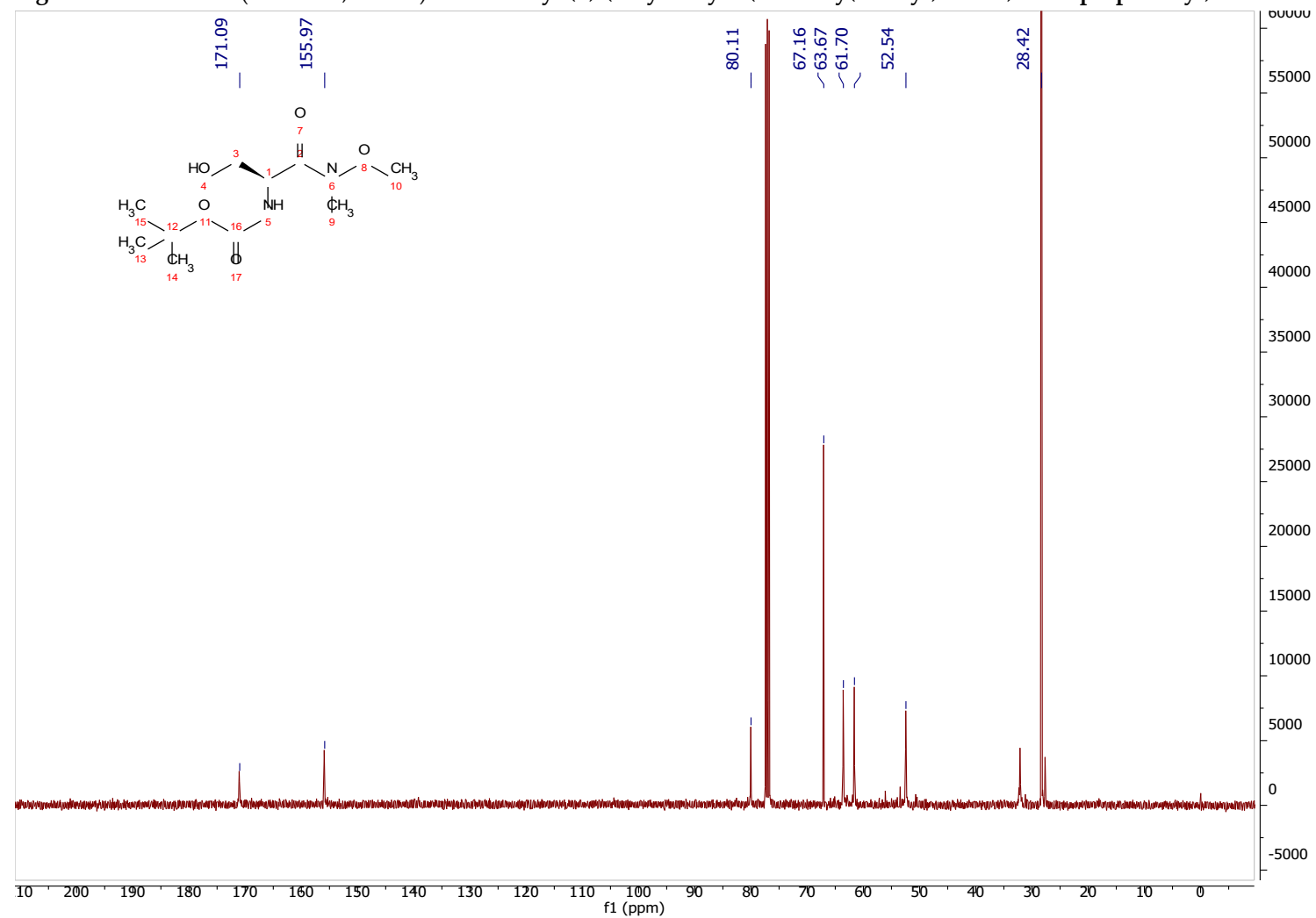


Figure S14: ^1H -NMR (400 MHz, CDCl_3) of **1b**.

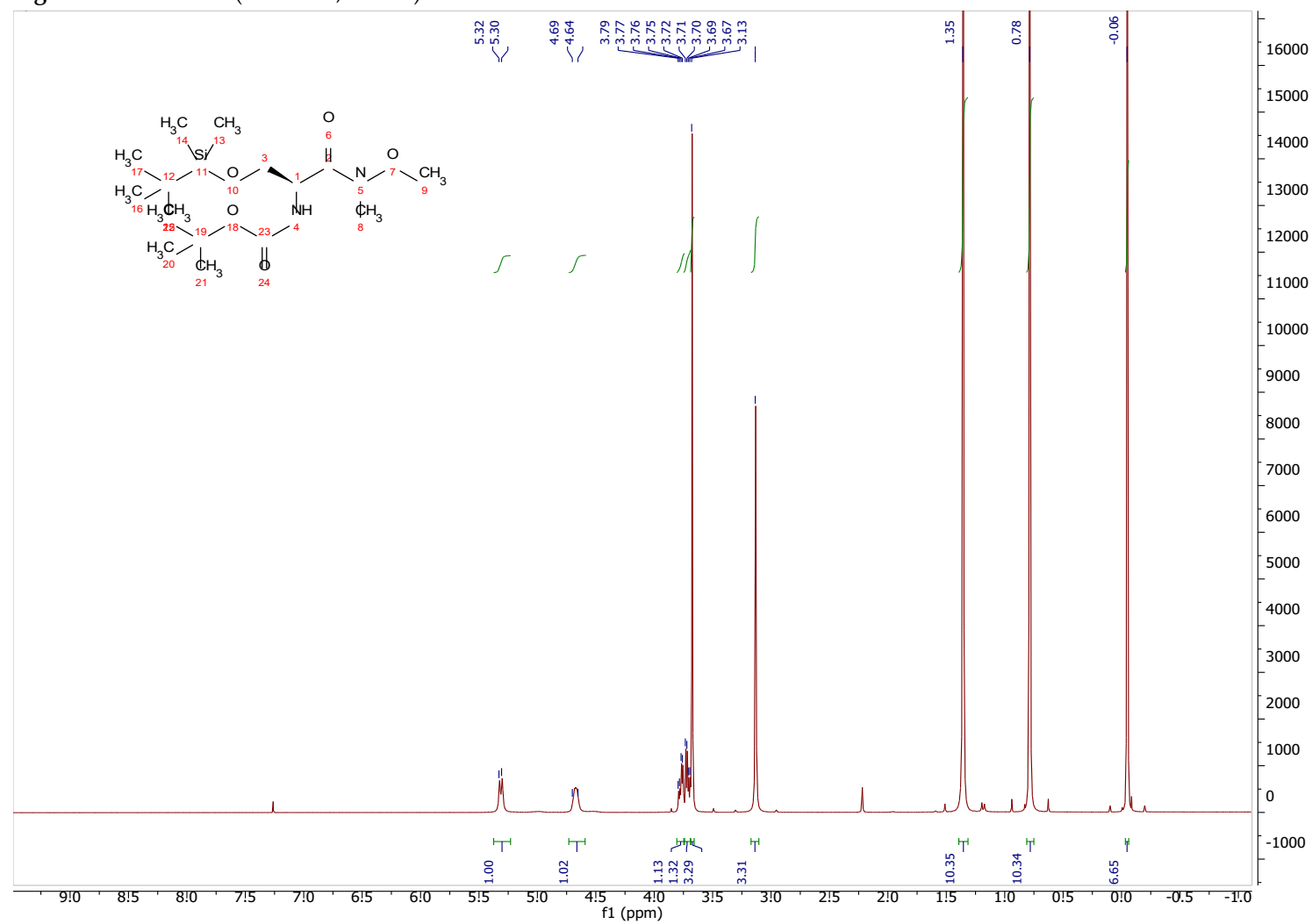


Figure S15: ^{13}C -NMR (100 MHz, CDCl_3) of **1b**.

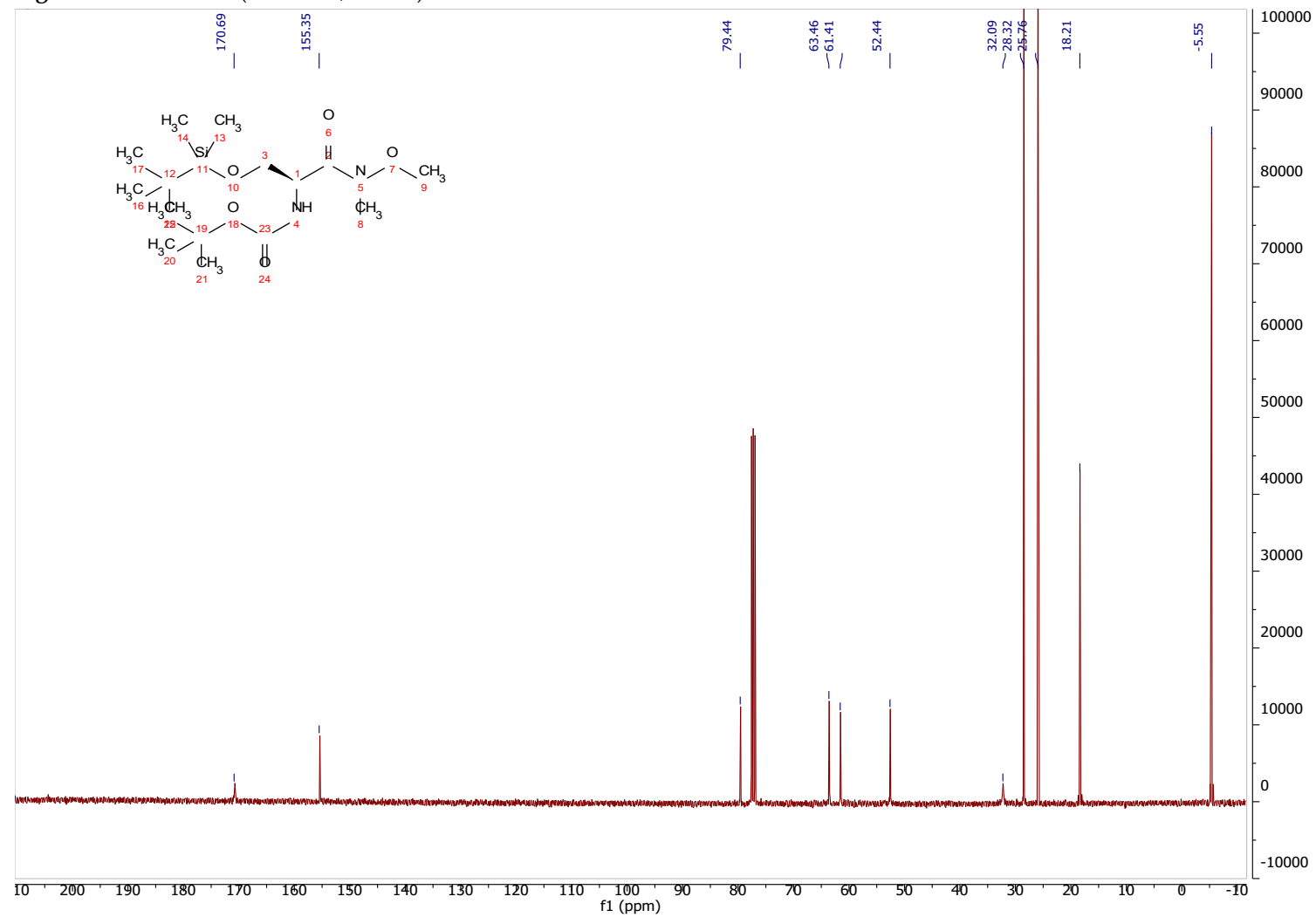


Figure S16: ^1H -NMR (300 MHz, CDCl_3) of *tert*-butyl (S)-allyl(3,8,8,9,9-pentamethyl-4-oxo-2,7-dioxa-3-aza-8-siladecan-5-yl)carbamate.

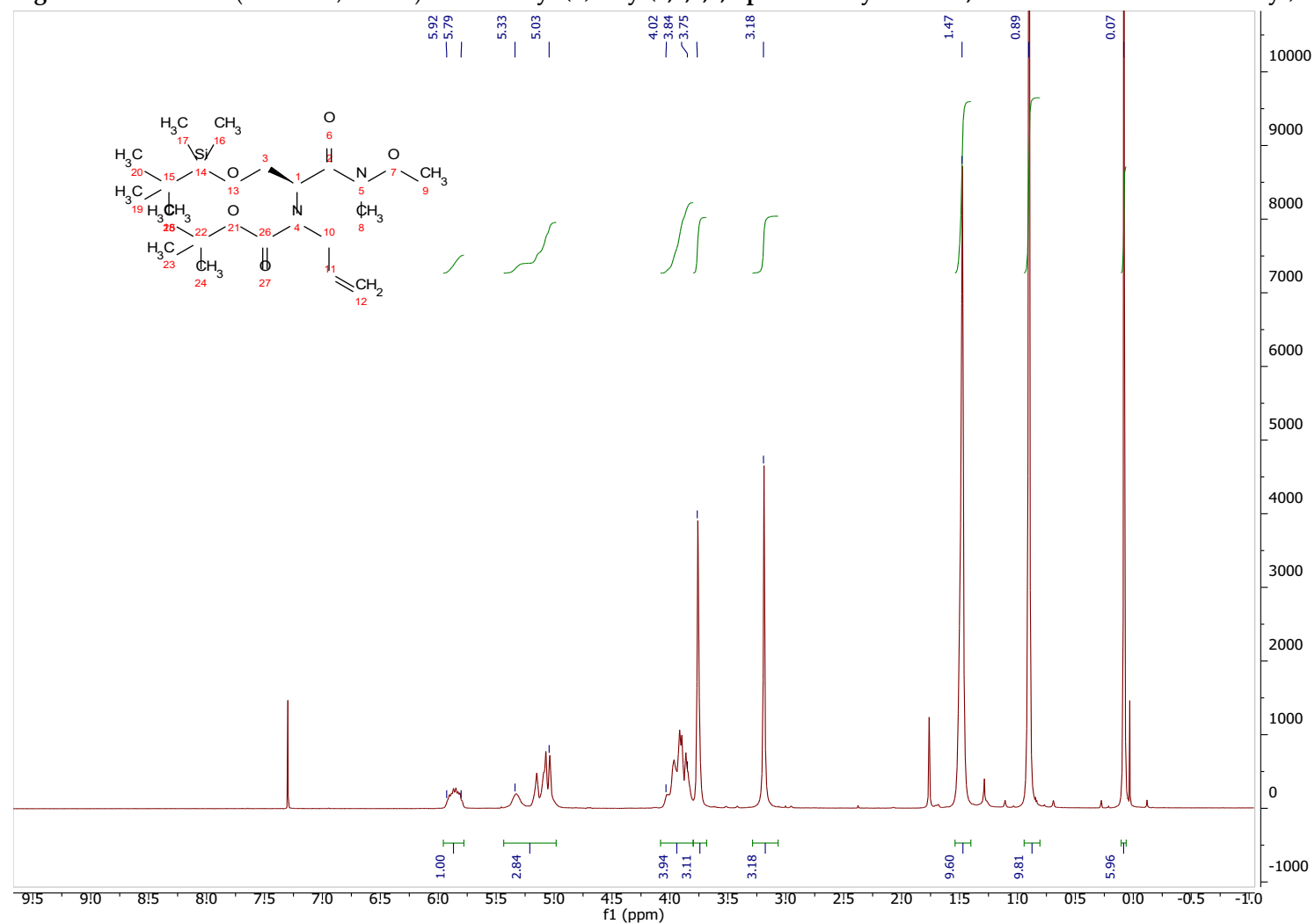


Figure S17: ^{13}C -NMR (75 MHz, CDCl_3) of *tert*-butyl (S)-allyl(3,8,8,9,9-pentamethyl-4-oxo-2,7-dioxo-3-aza-8-siladecan-5-yl)carbamate.

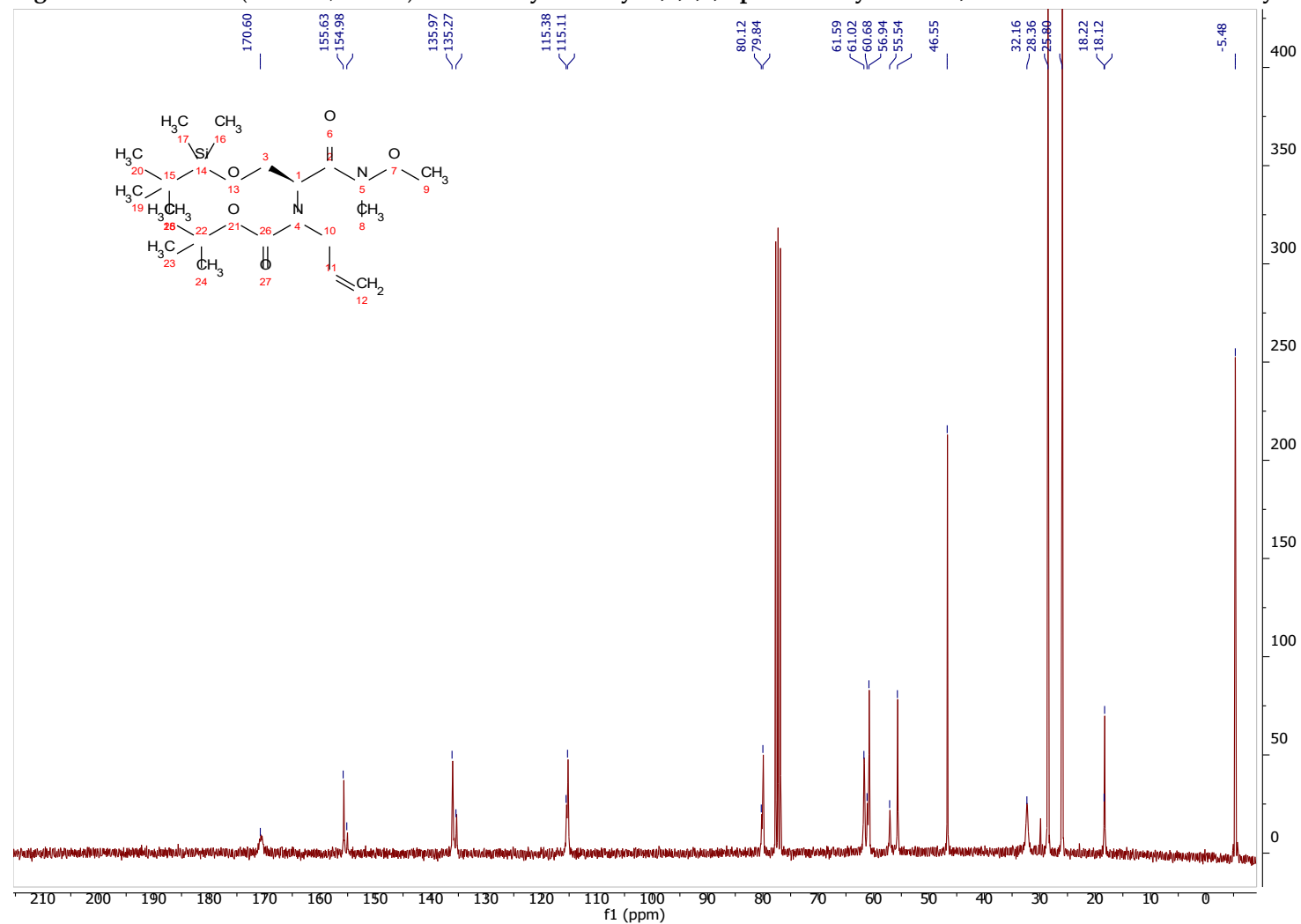


Figure S18: ^1H -NMR (400 MHz, CDCl_3) of **2b**.

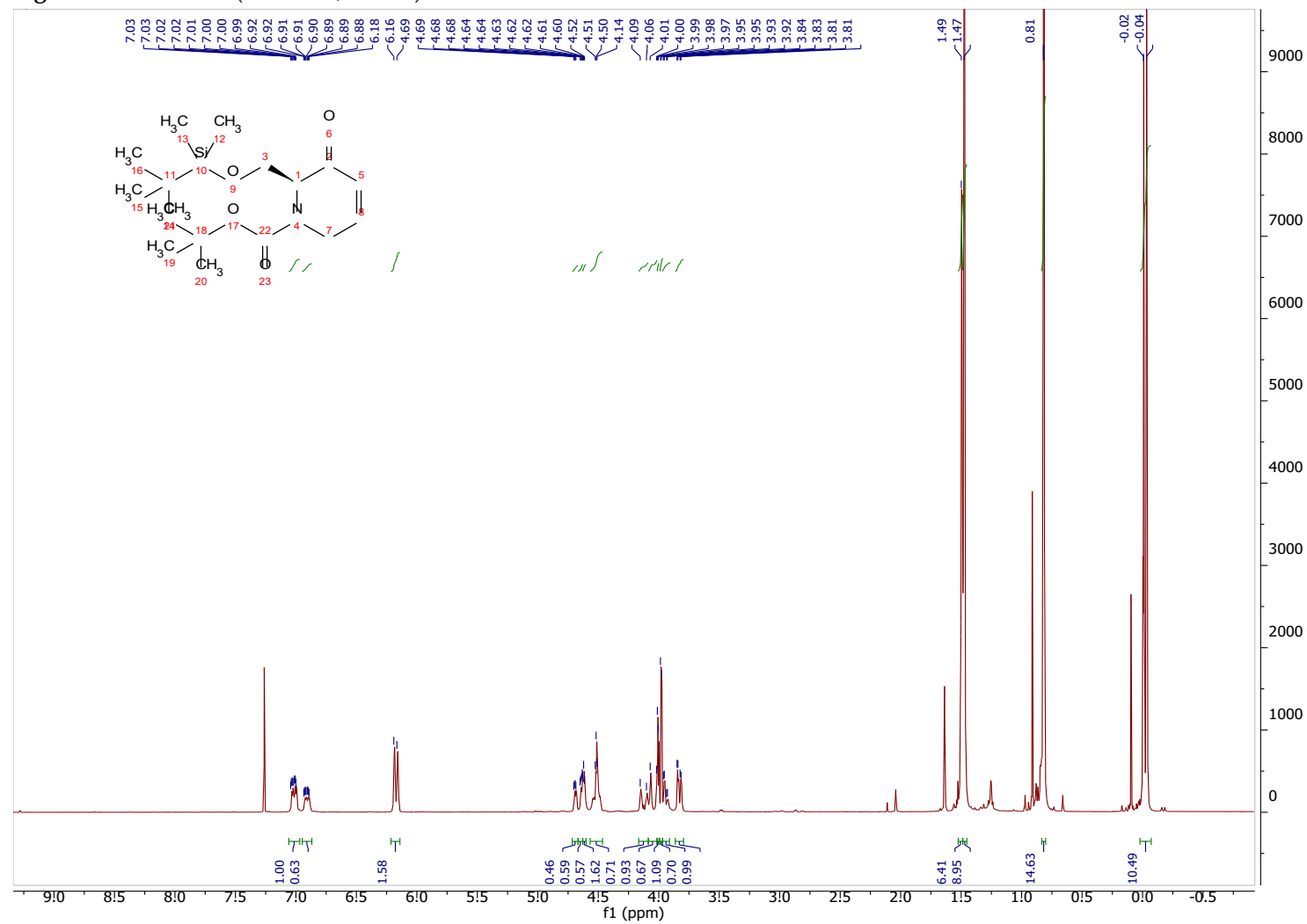


Figure S19: ^{13}C -NMR (100 MHz, CDCl_3) of **2b**.

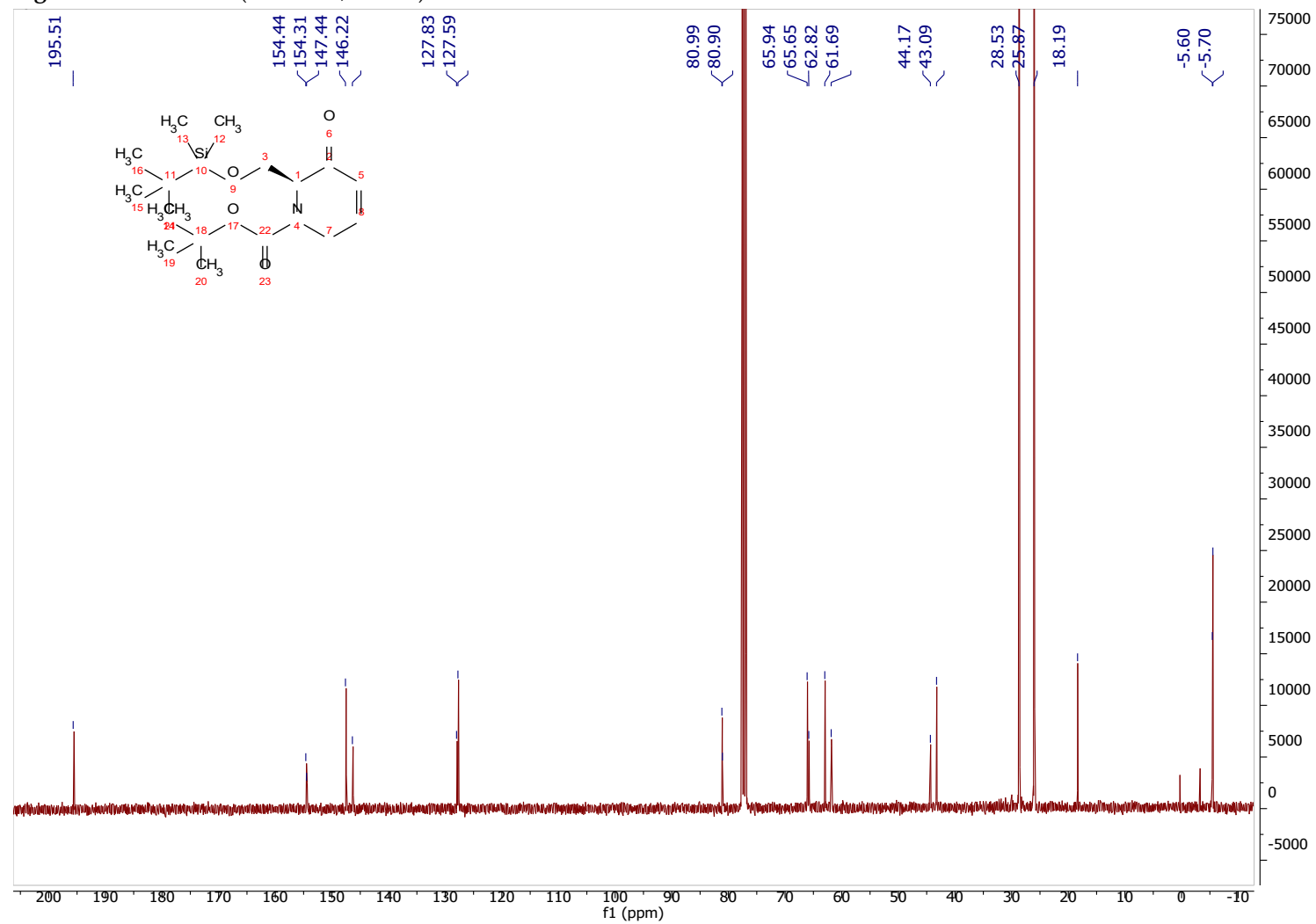


Figure S20: ^1H -NMR (400 MHz, CDCl_3) of **3b**.

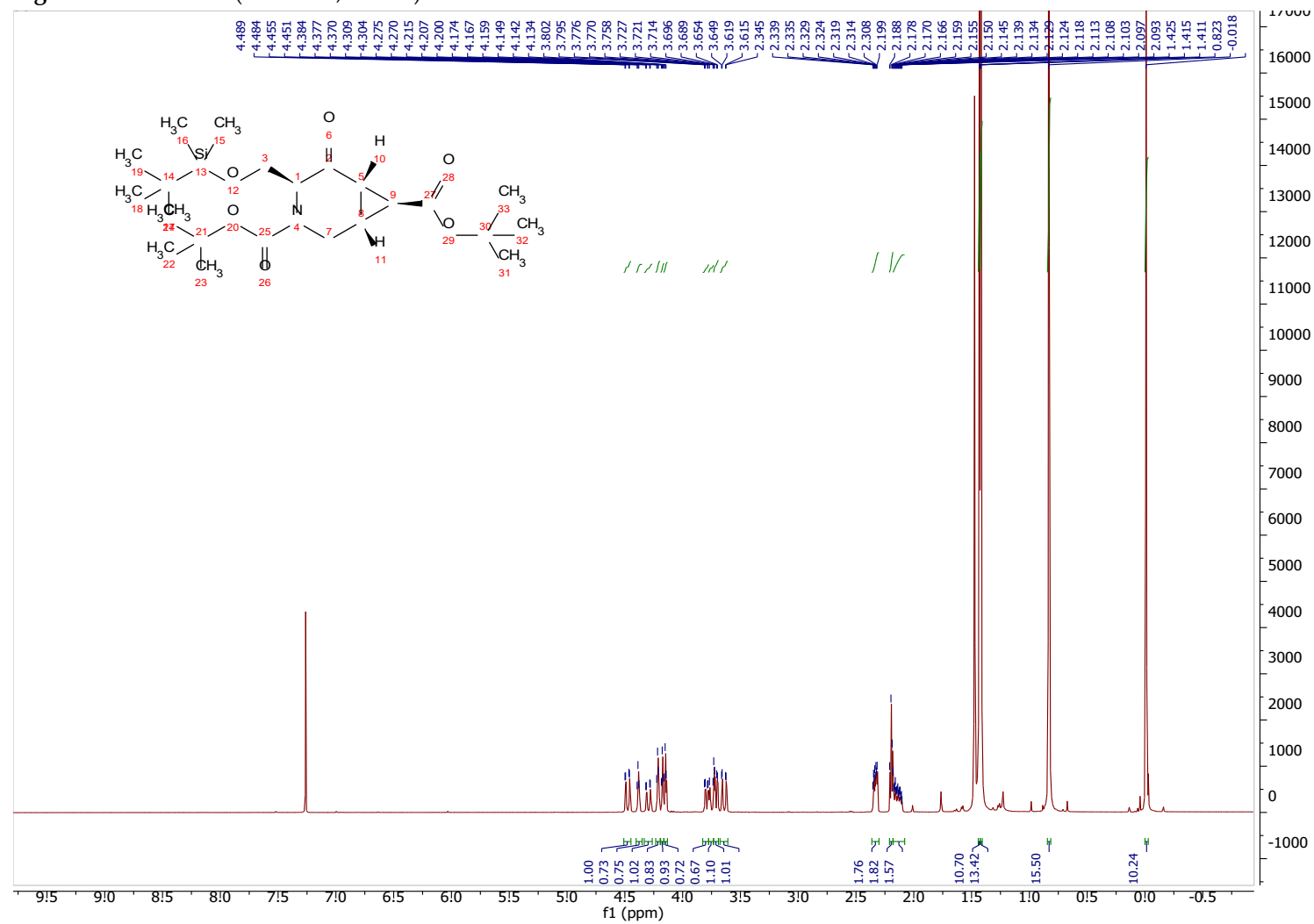


Figure S21: ^{13}C -NMR (100 MHz, CDCl_3) of **3b**.

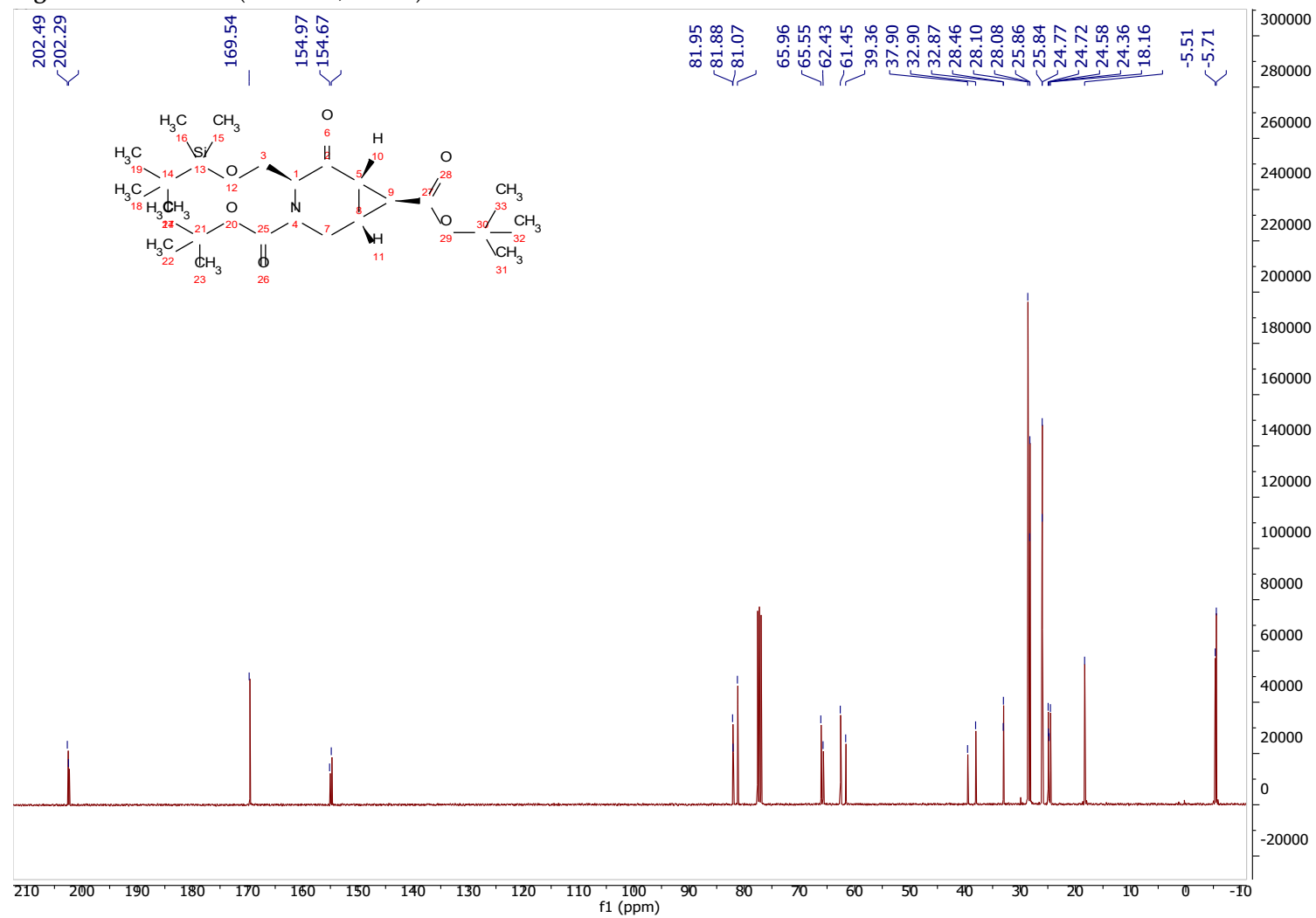


Figure S22: ^1H (400 MHz CDCl_3) bidimensional NOESY of **3b**.

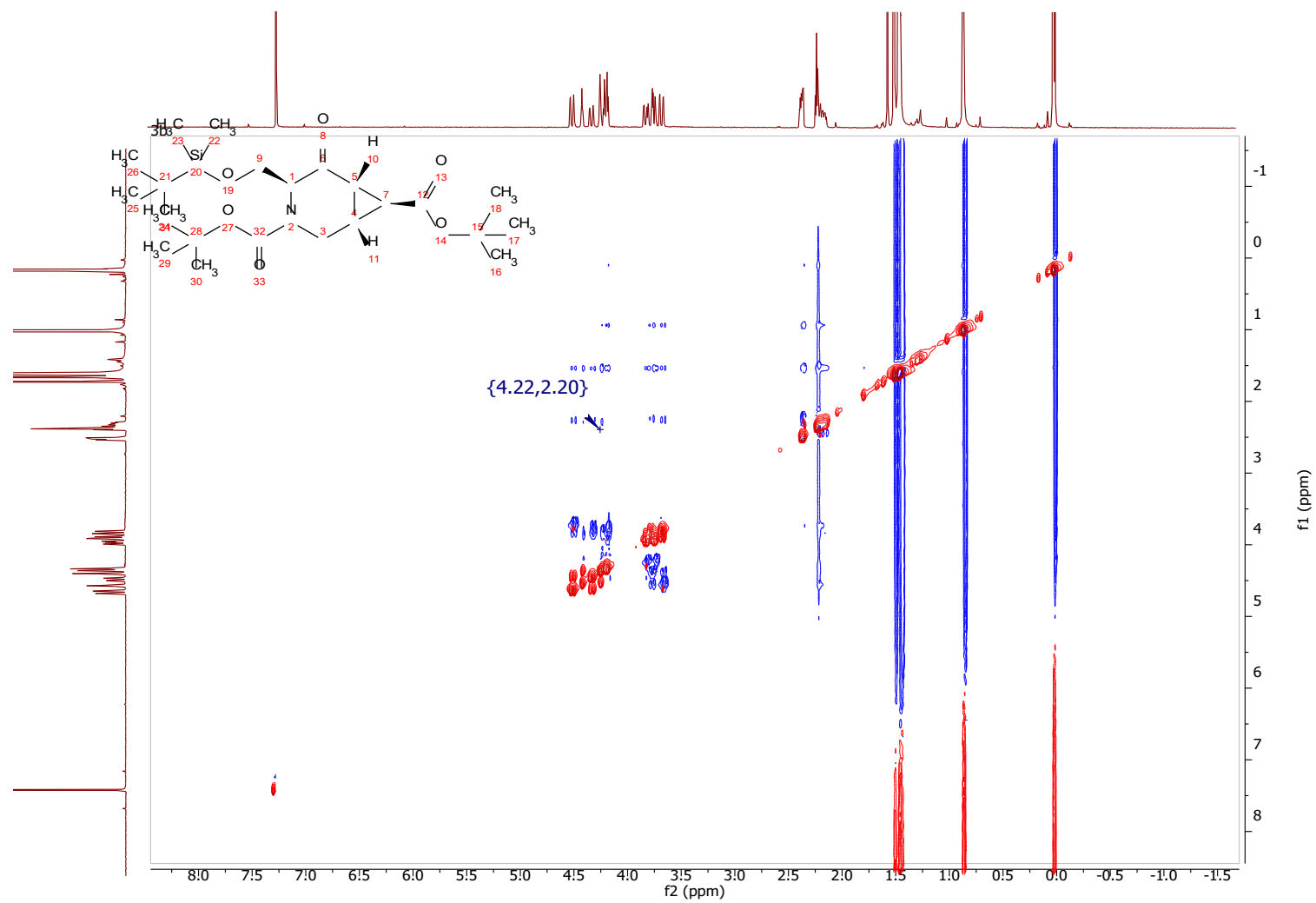


Figure S23: ^1H -NMR (400 MHz, CDCl_3) of **3b** in $\text{DMSO}-d_6$.

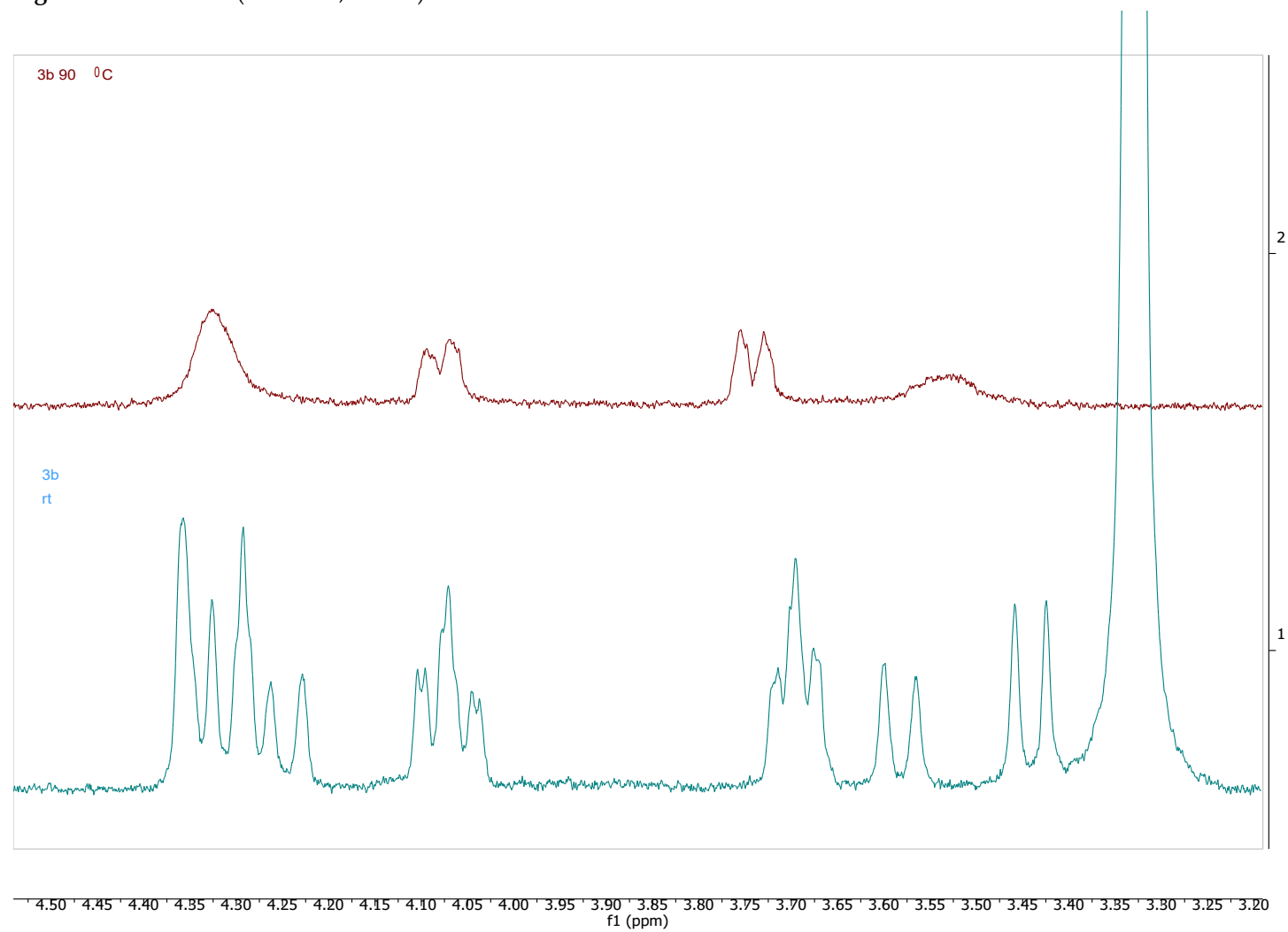


Figure S24: ^1H -NMR (400 MHz, CDCl_3) of **4b**.

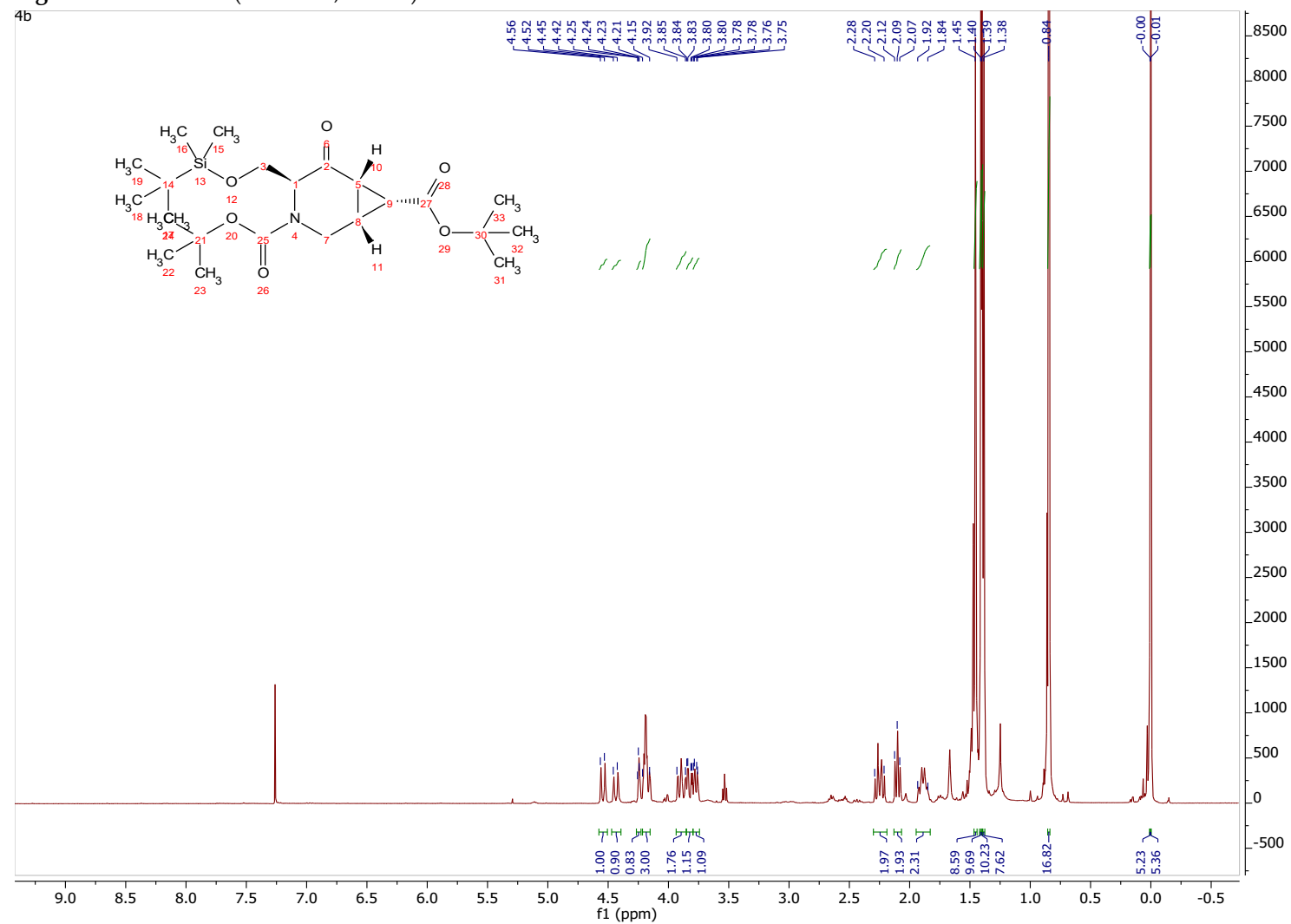


Figure S25: ^{13}C -NMR (100 MHz, CDCl_3) of **4b**.

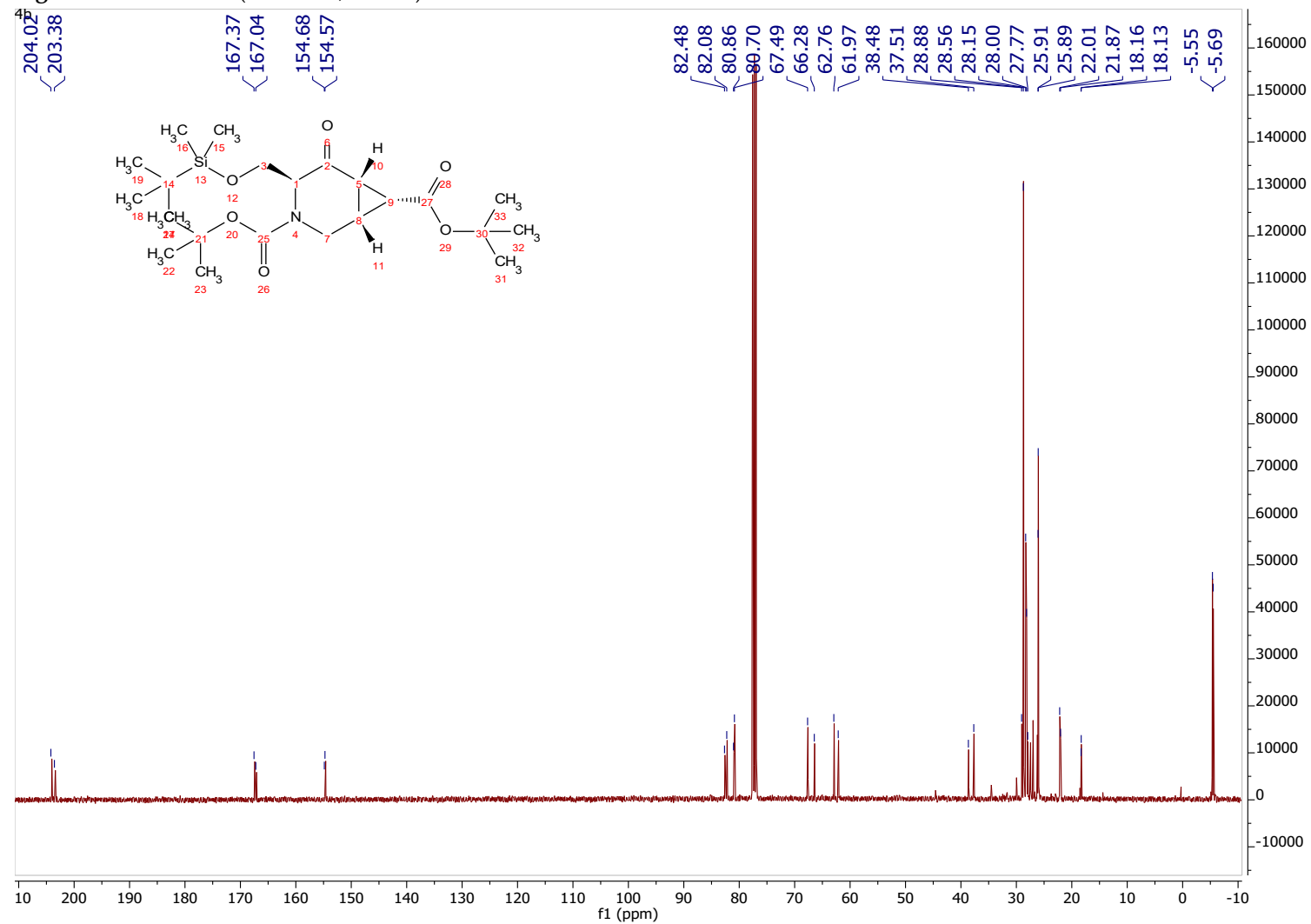


Figure S26: ^1H (400 MHz CDCl_3) bidimensional NOESY of **4b**.

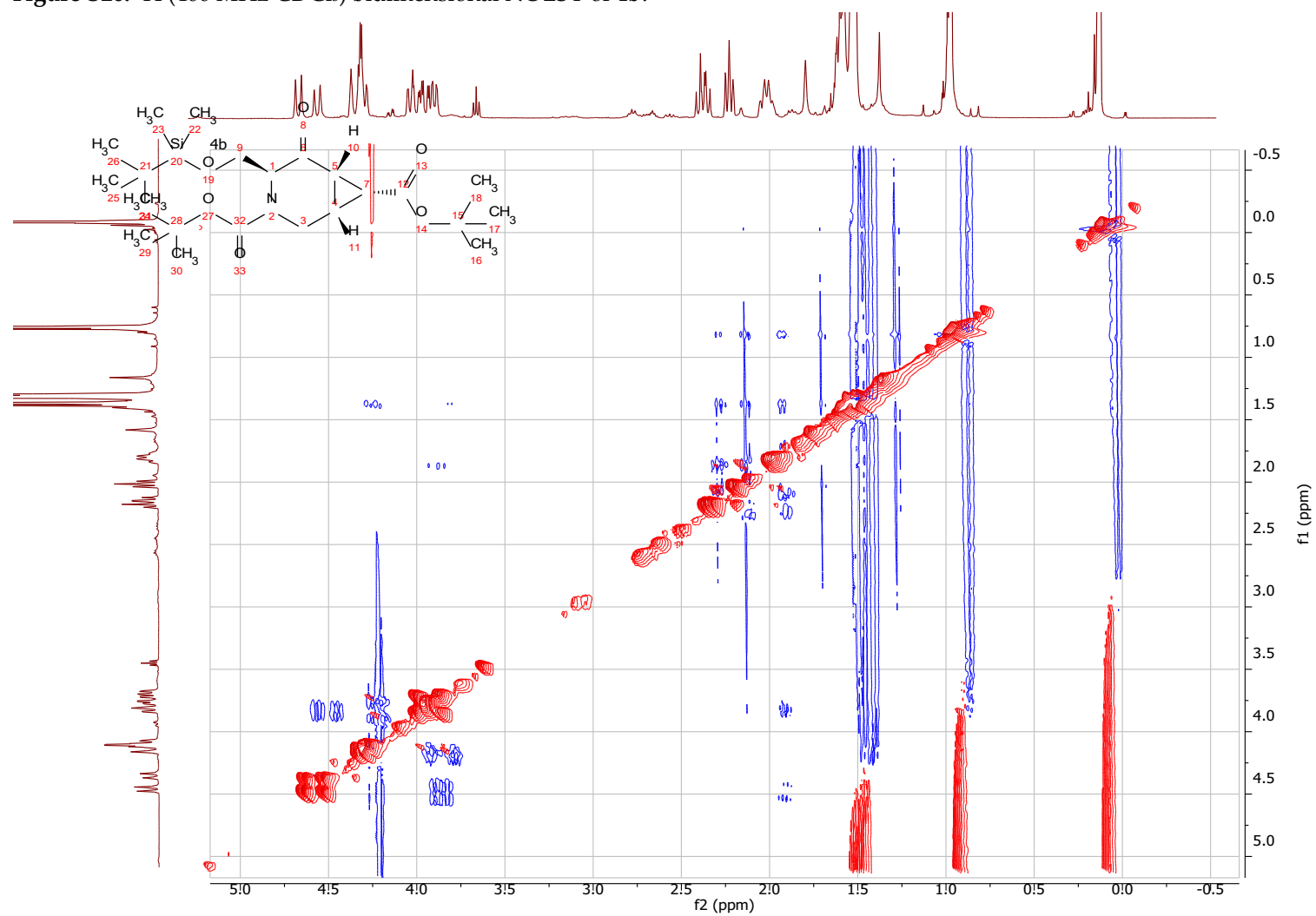


Figure S27: ^1H -NMR (400 MHz, CDCl_3) of 5a.

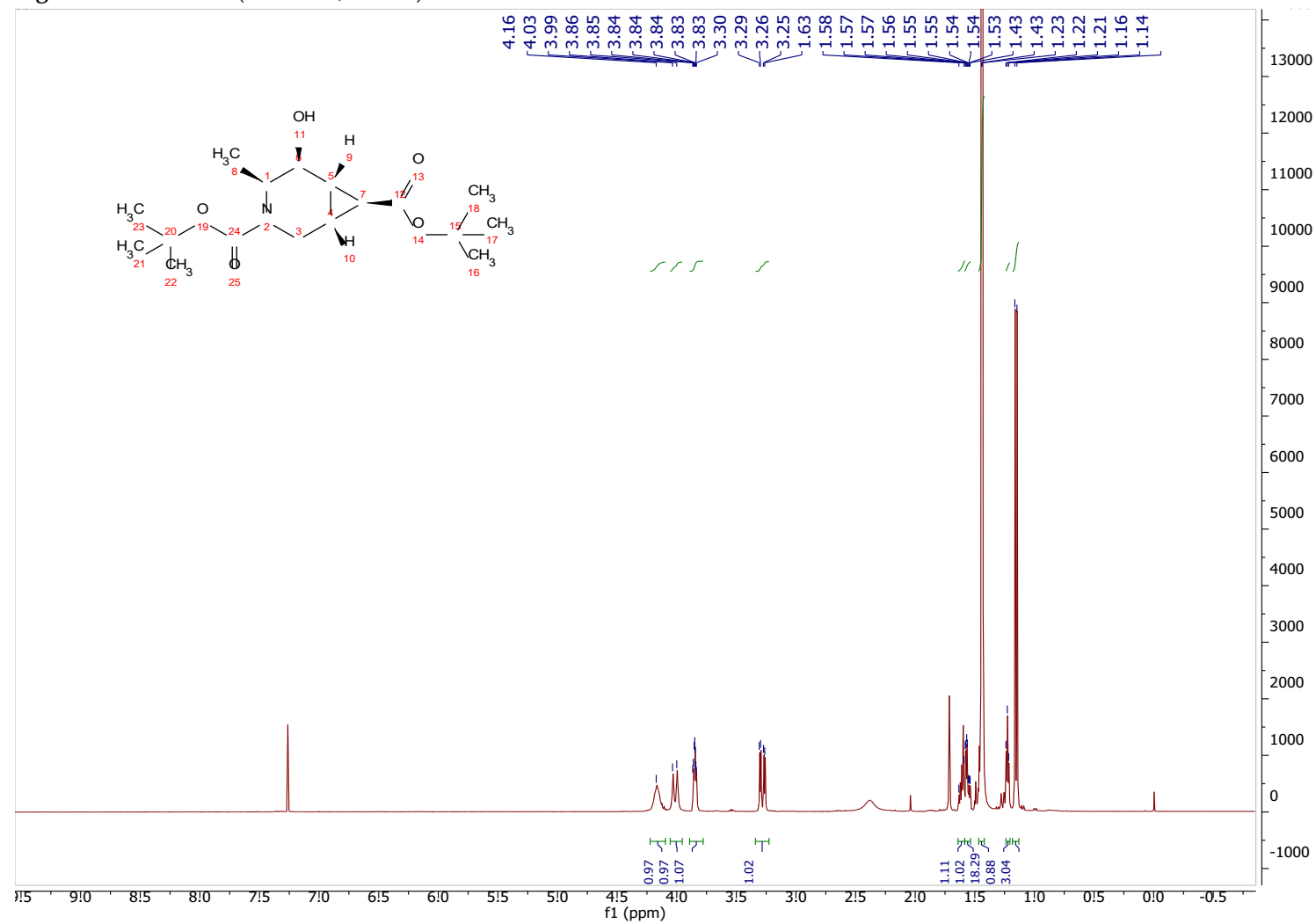


Figure S28: ^{13}C -NMR (100 MHz, CDCl_3) of **5a**.

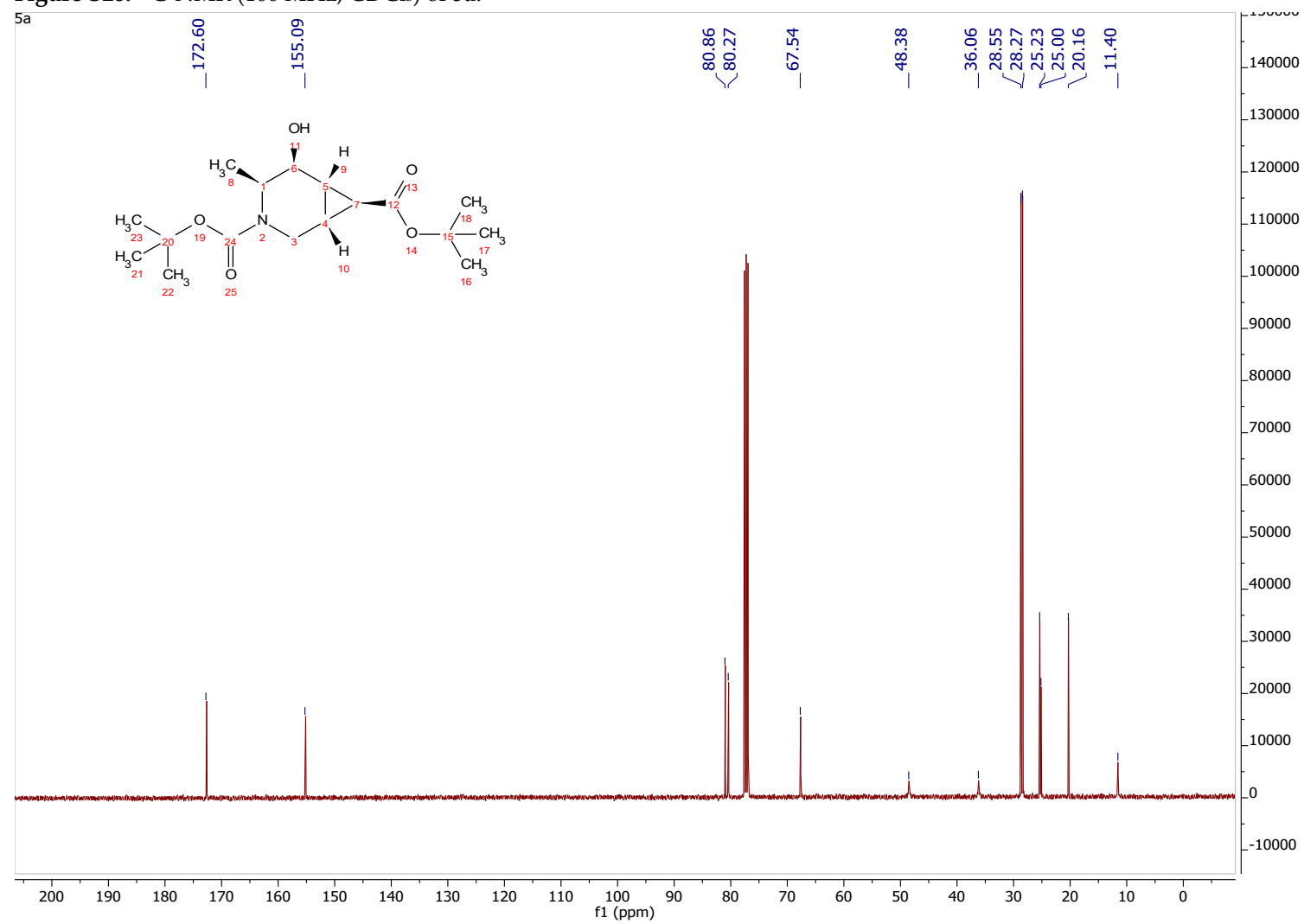
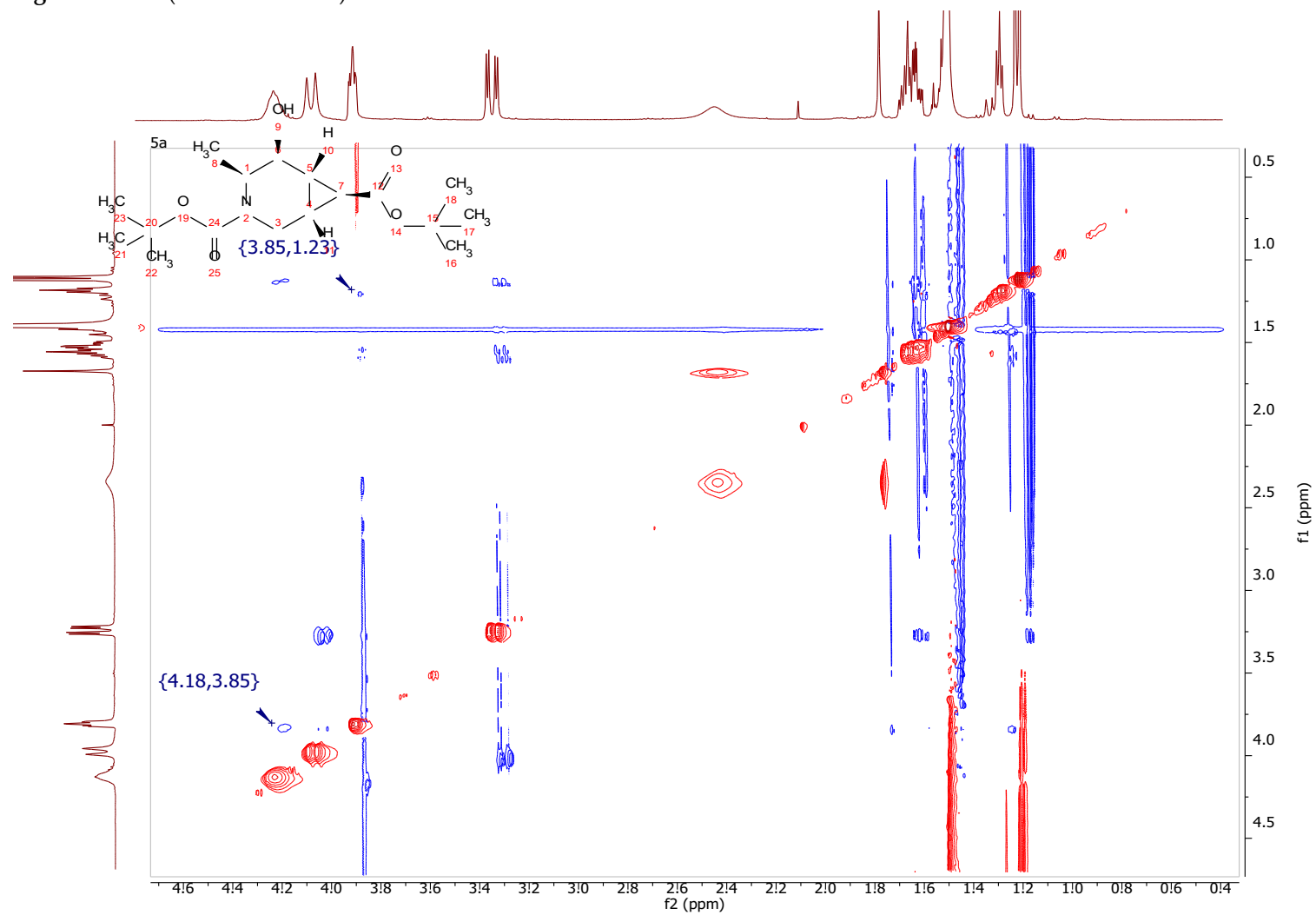


Figure S29: ^1H (400 MHz CDCl_3) bidimensional NOESY of 5a.



Chemical structure of 1-(4-isopropyl-2-methyl-5-oxo-1,2,3,4-tetrahydropyridin-3-yl)ethan-1-ol is shown. The structure is numbered 1 through 25. The NMR spectrum displays peaks corresponding to the protons in the molecule. The x-axis represents the chemical shift in ppm (f1), ranging from 9.5 to -0.5. The y-axis represents the intensity, ranging from 0 to 13000. Key peaks are labeled with their chemical shifts: 7.260, 4.176, 4.064, 3.988, 3.965, 3.222, 3.189, 1.955, 1.935, 1.920, 1.902, 1.674, 1.632, 1.458, 1.442, 1.136, 1.118. Integration values are provided for several peaks: 1.45, 0.92, 0.87, 1.00, 2.07, 16.17, 2.72.

Figure S31: ^{13}C -NMR (100 MHz, CDCl_3) of **5b**.

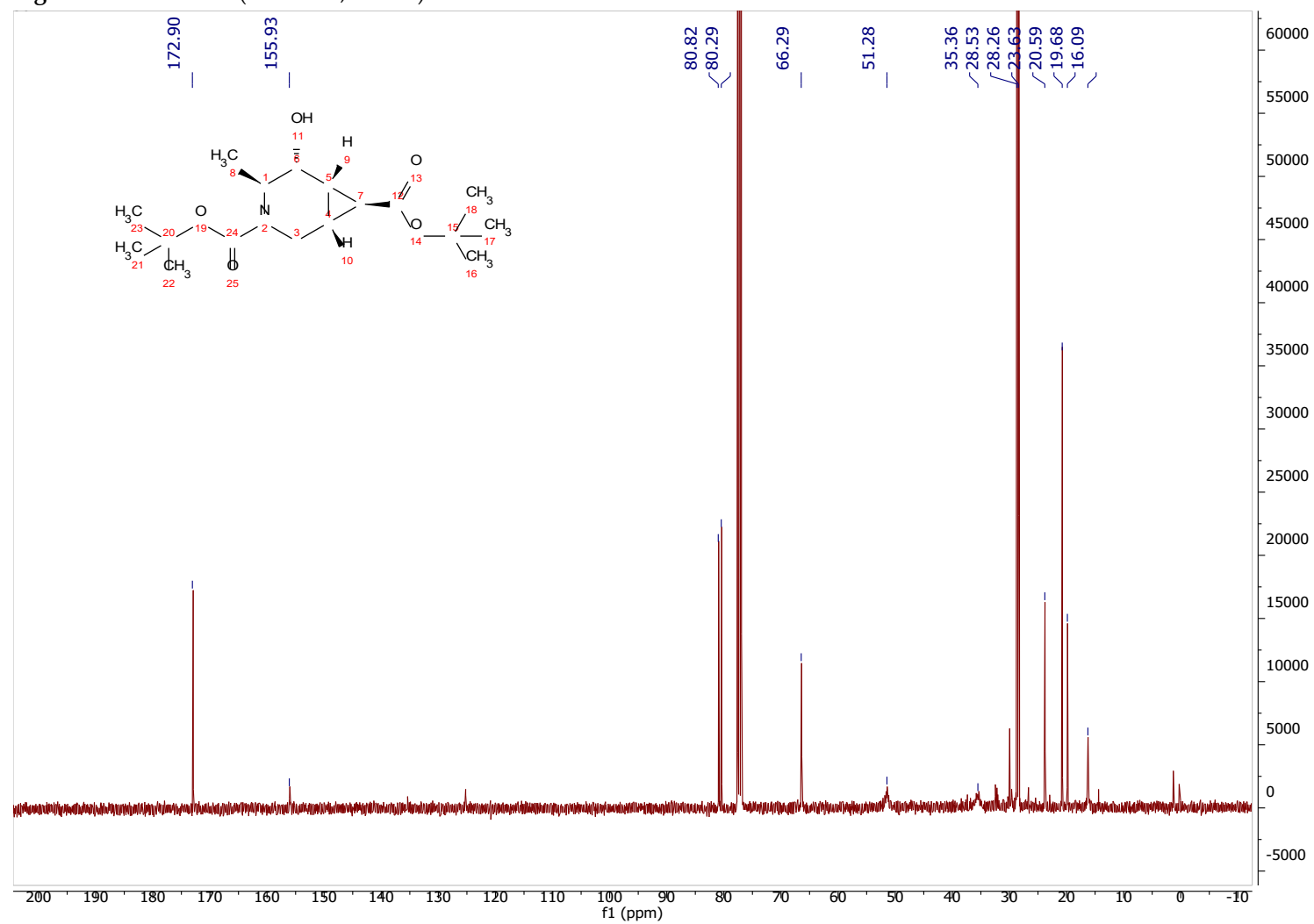


Figure S32: ^1H (400 MHz CDCl_3) bidimensional NOESY of **5b**.

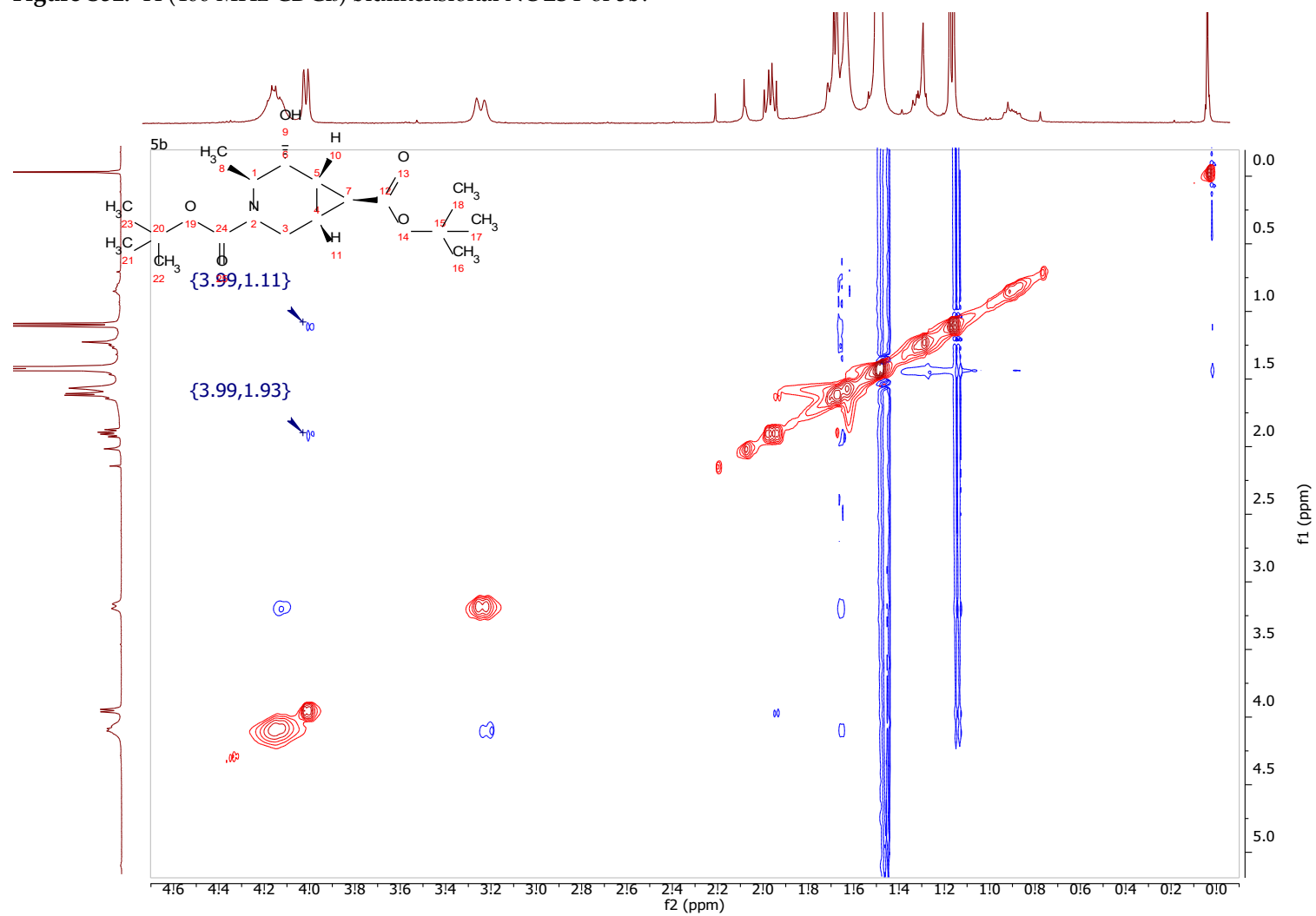


Figure S33: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,6*S*,7*S*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0]heptane-3- carboxylate.

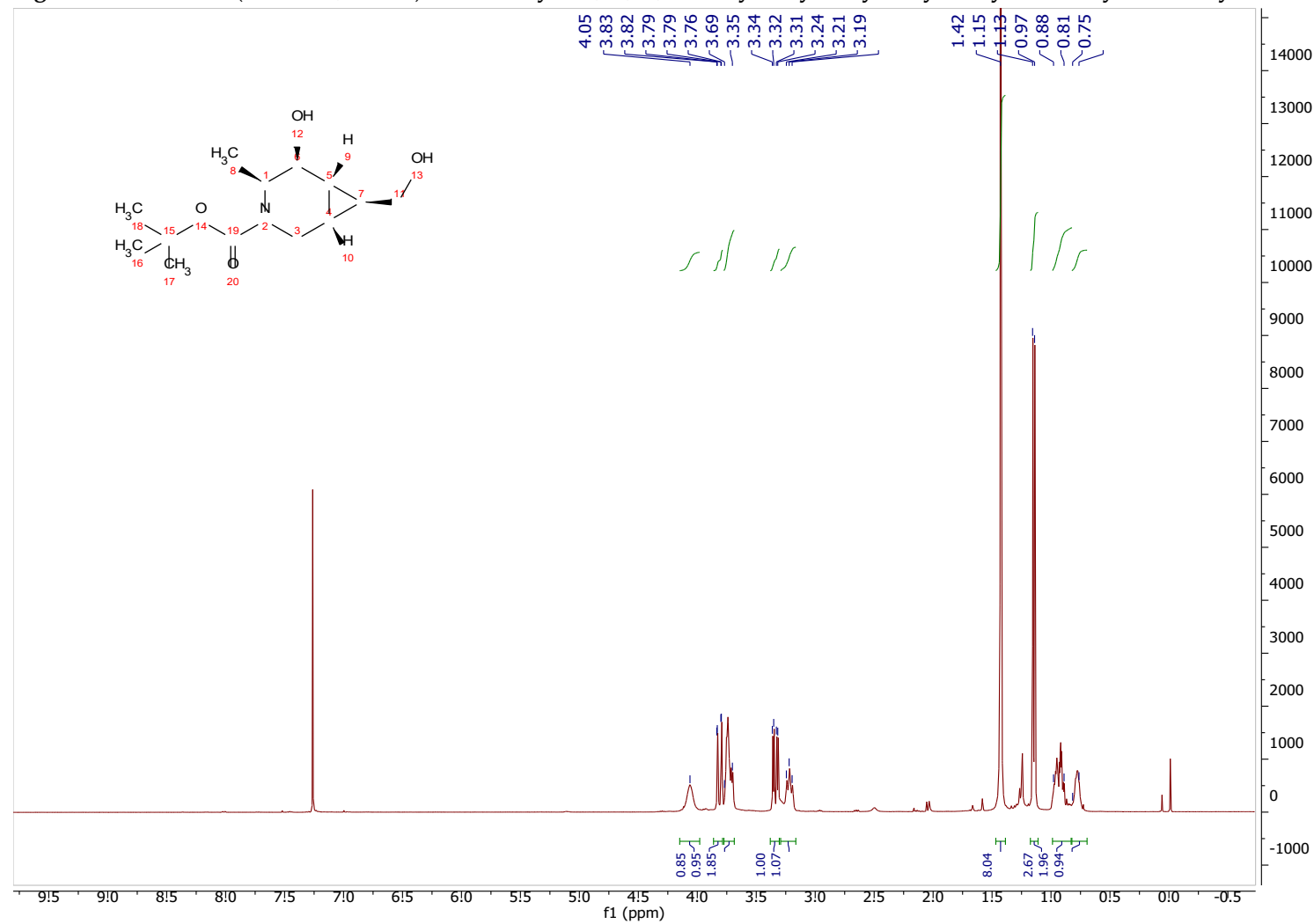


Figure S34: ^{13}C -NMR (100 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,6*S*,7*S*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0]heptane-3- carboxylate.

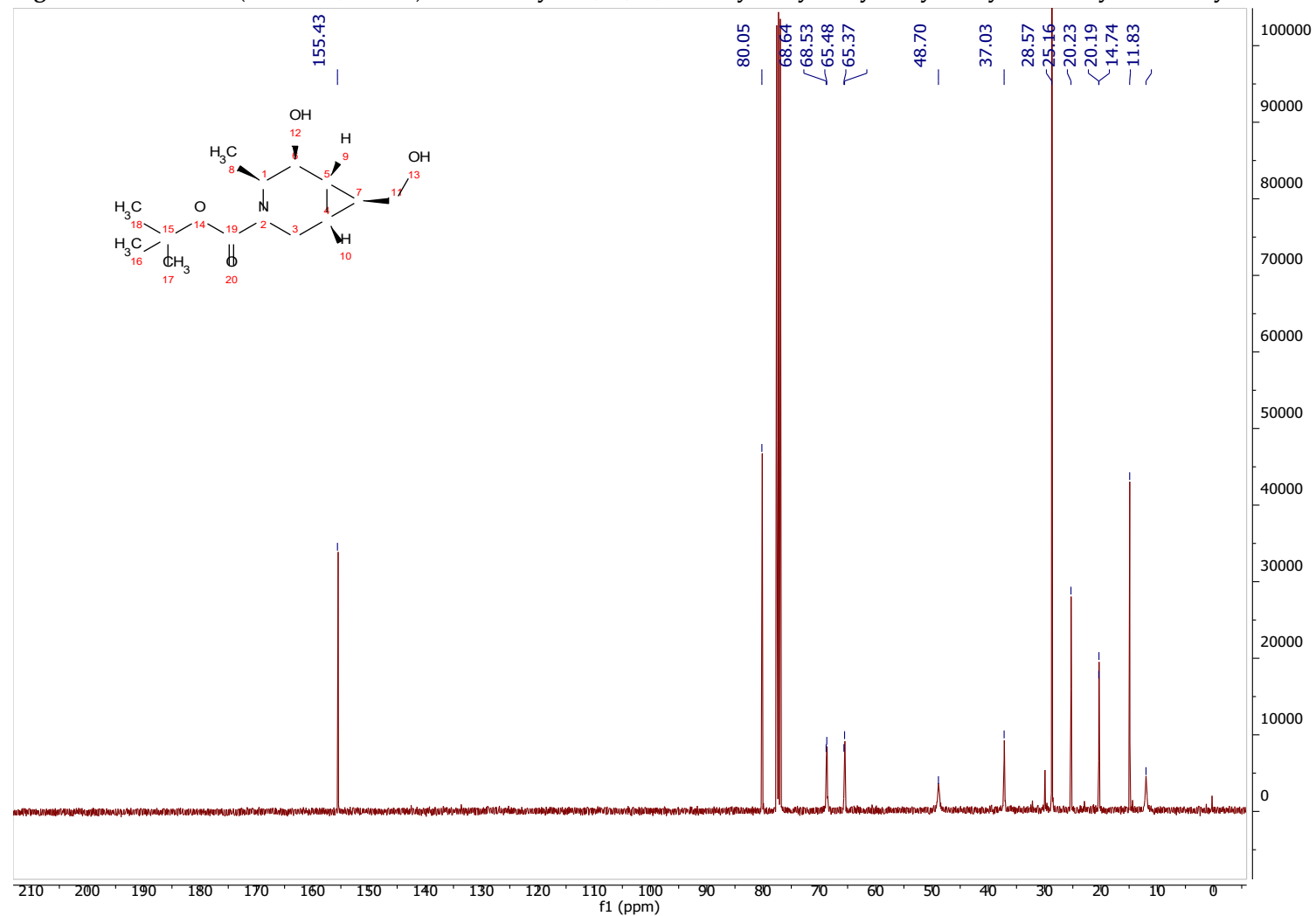


Figure S35: ^1H -NMR (300 MHz, MeOD) of **6a**.

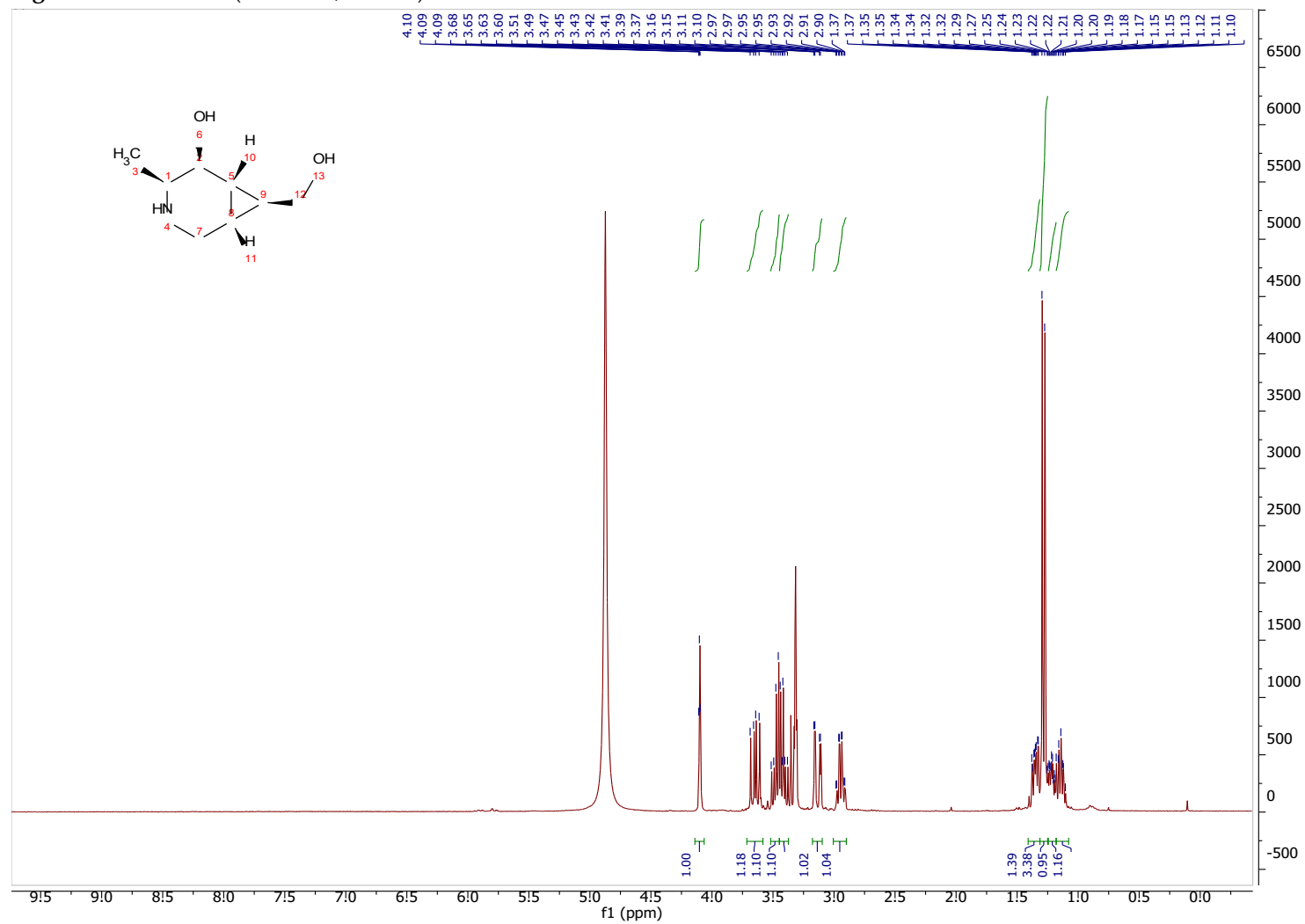


Figure S36: ^{13}C -NMR (75 MHz, MeOD) of **6a**.

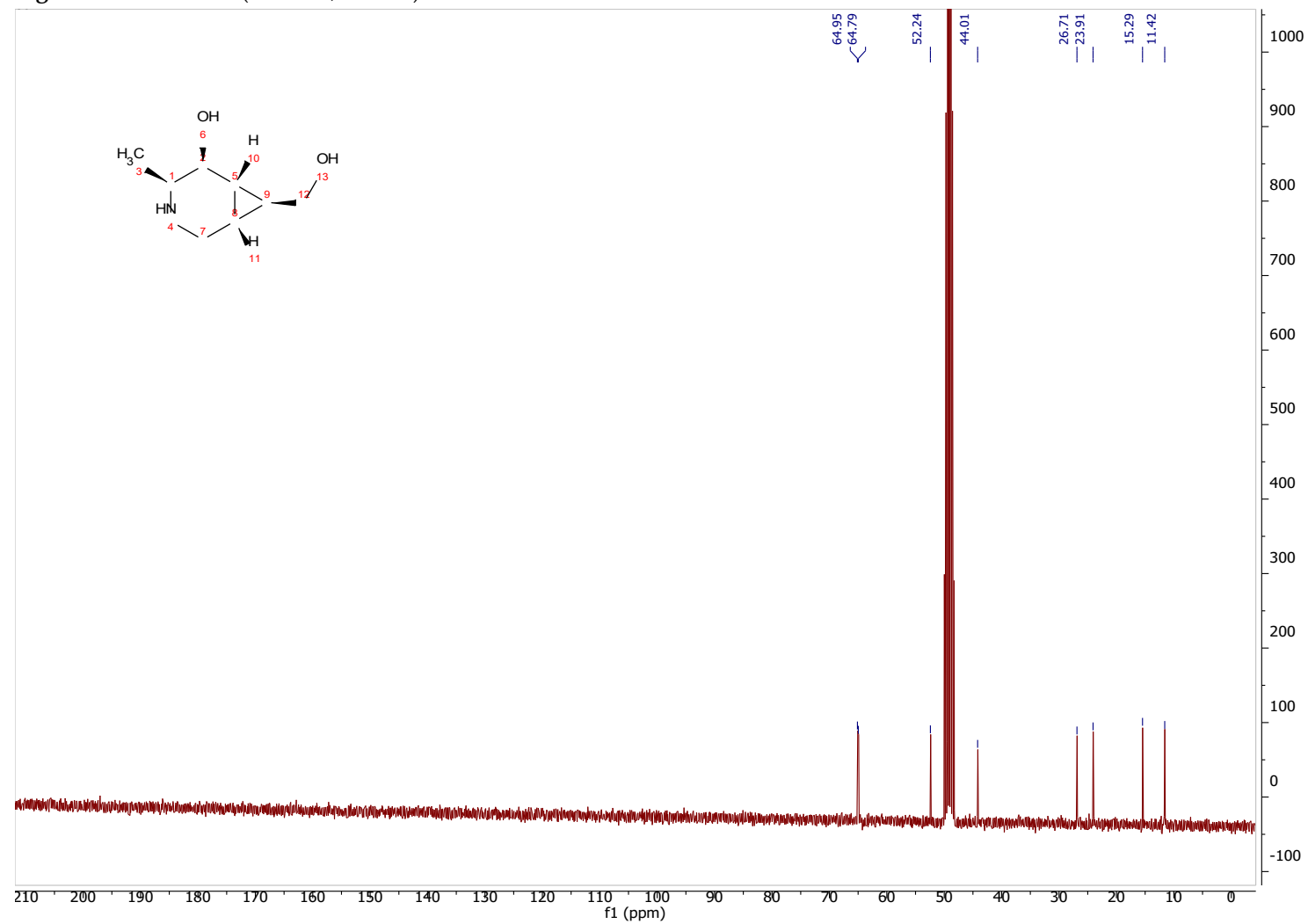


Figure S37: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,5*R*,6*S*,7*S*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0] heptane-3-carboxylate.

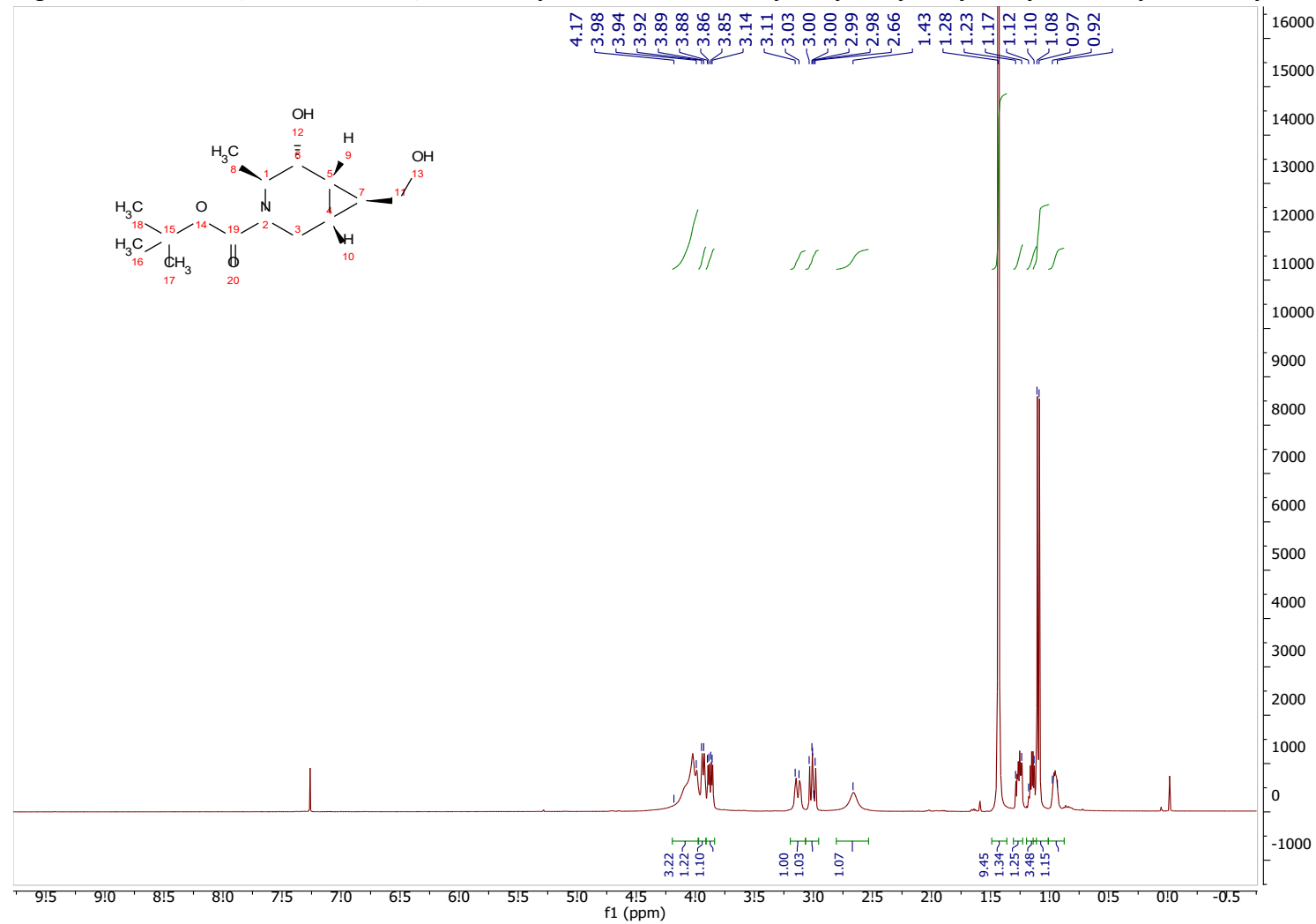


Figure S38: ^{13}C -NMR (100 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,5*R*,6*S*,7*S*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0] heptane-3-carboxylate.

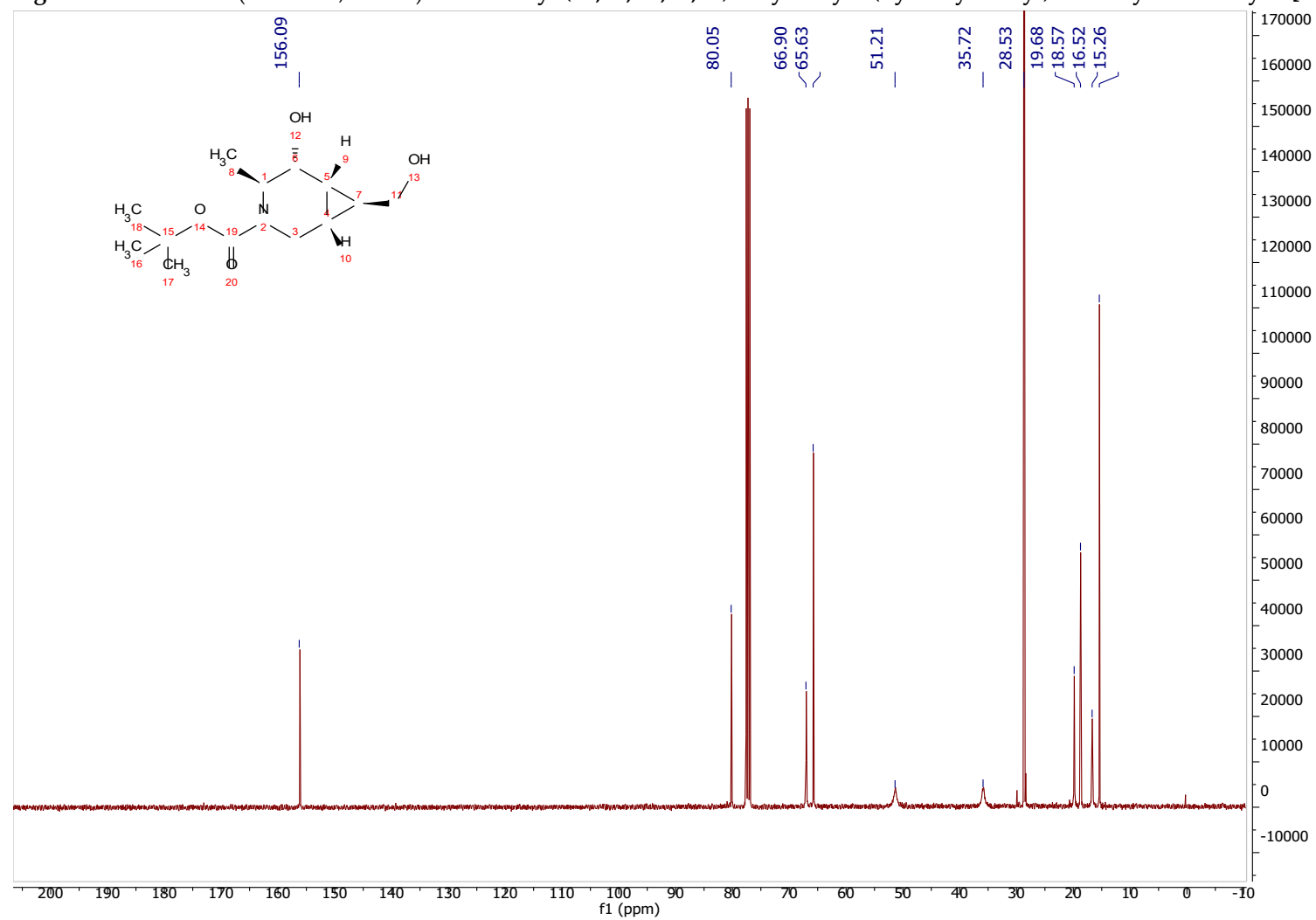


Figure S39: ¹H-NMR (400 MHz, MeOD) of **6b**.

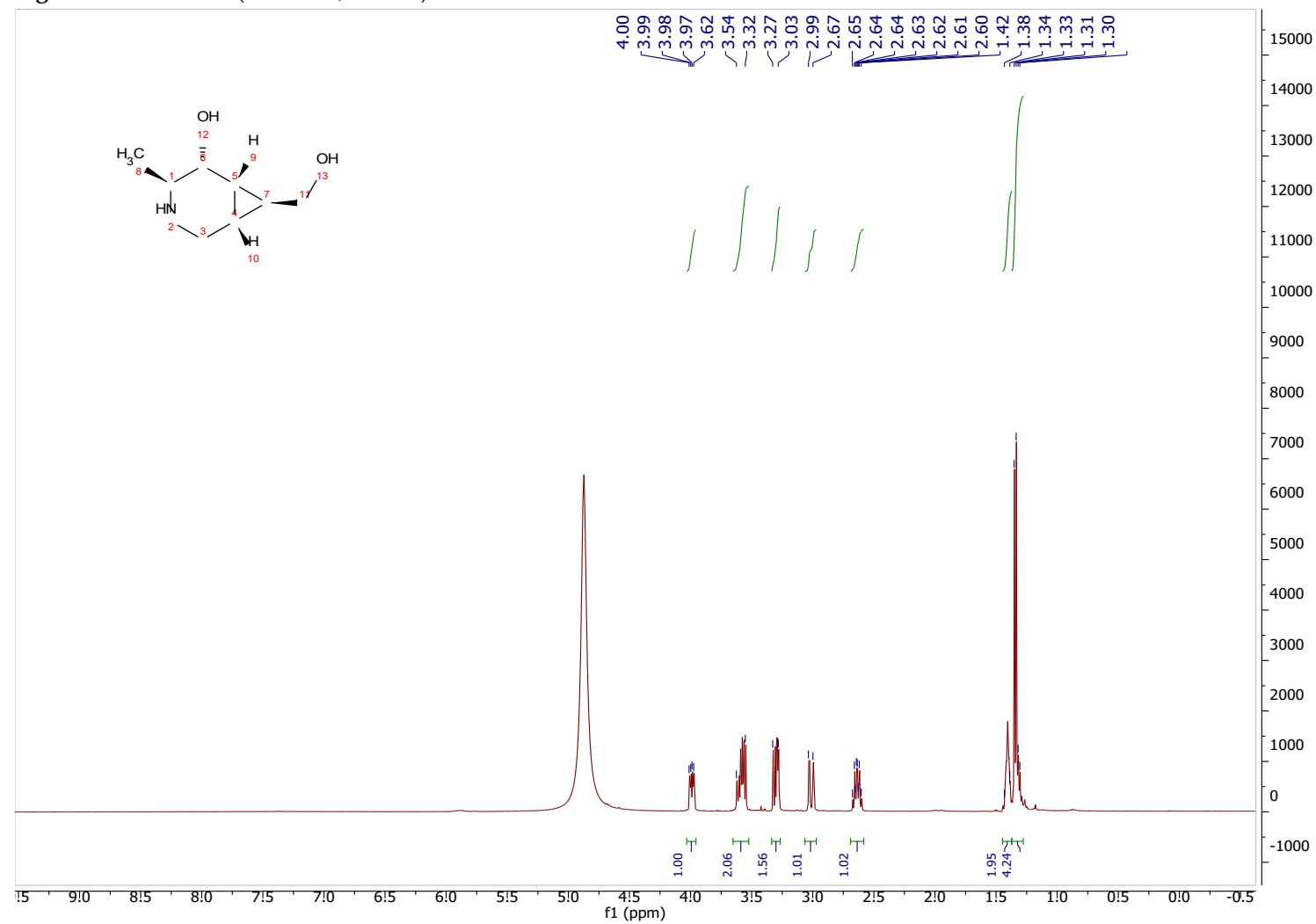


Figure S40: ^{13}C -NMR (100 MHz, MeOD) of **6b**.

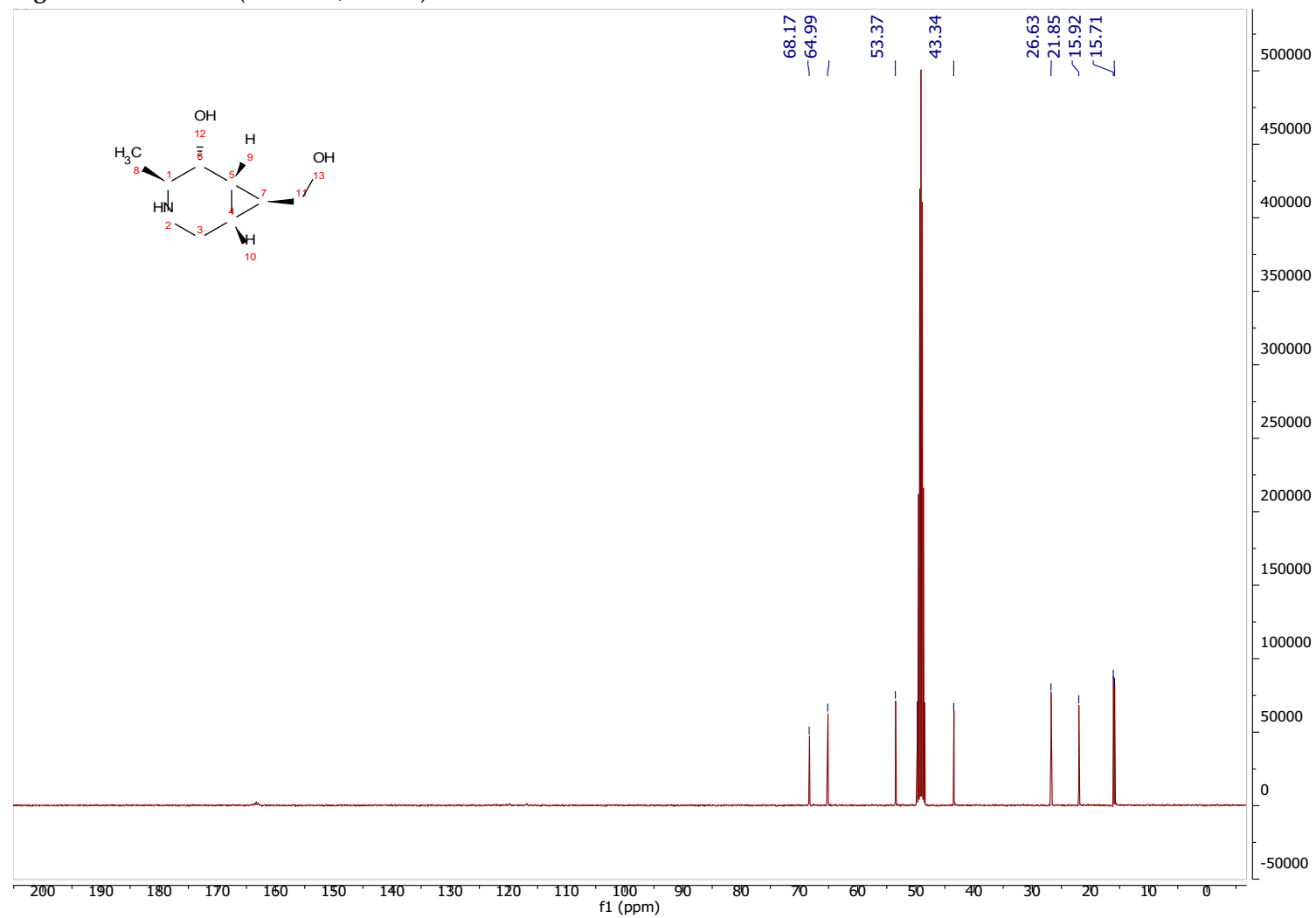


Figure S41: ^1H -NMR with water suppression (500 MHz, D_2O) of PNP-galactose, mixture of PNP-gal with galactosidase after 1 hour and mixture of PNP-gal, galactosidase and **6b** after 12 hours of enzymatic reaction respectively.

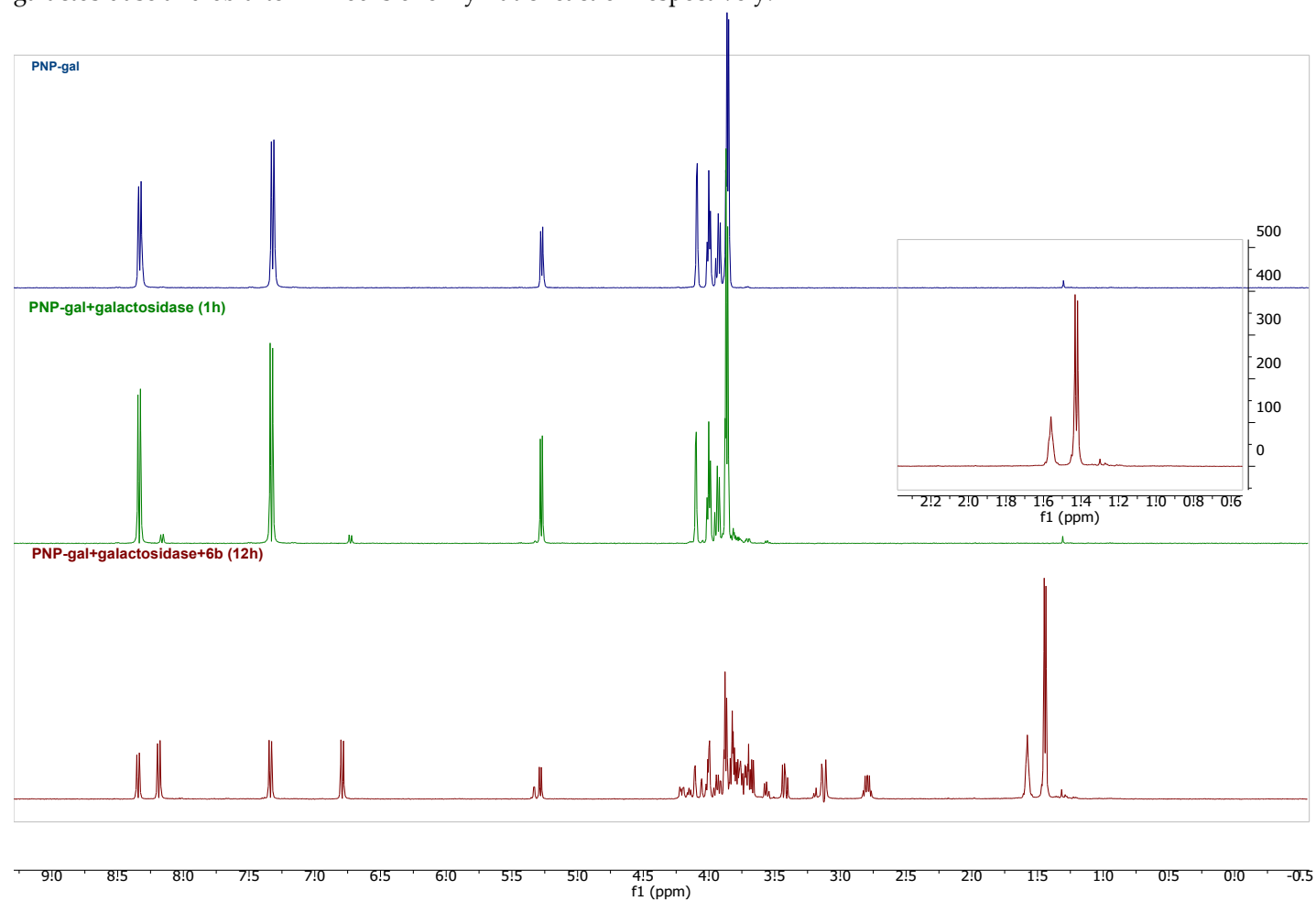


Figure S42: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,5*R*,6*S*,7*R*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0]heptane-3-carboxylate.

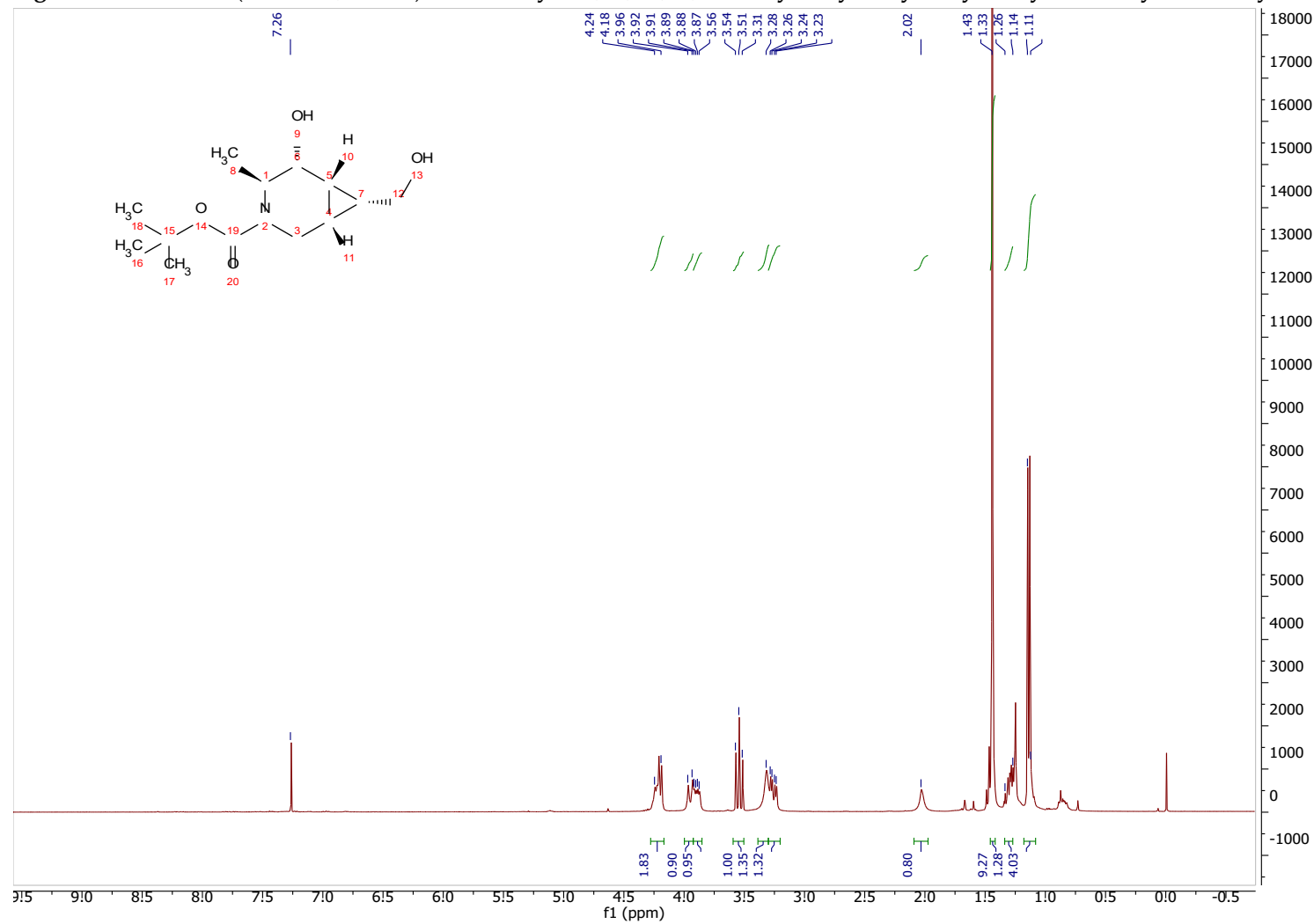


Figure S43: ^{13}C -NMR (100 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,5*R*,6*S*,7*R*)-5-hydroxy-7-(hydroxymethyl)-4-methyl-3-azabicyclo[4.1.0]heptane-3-carboxylate.

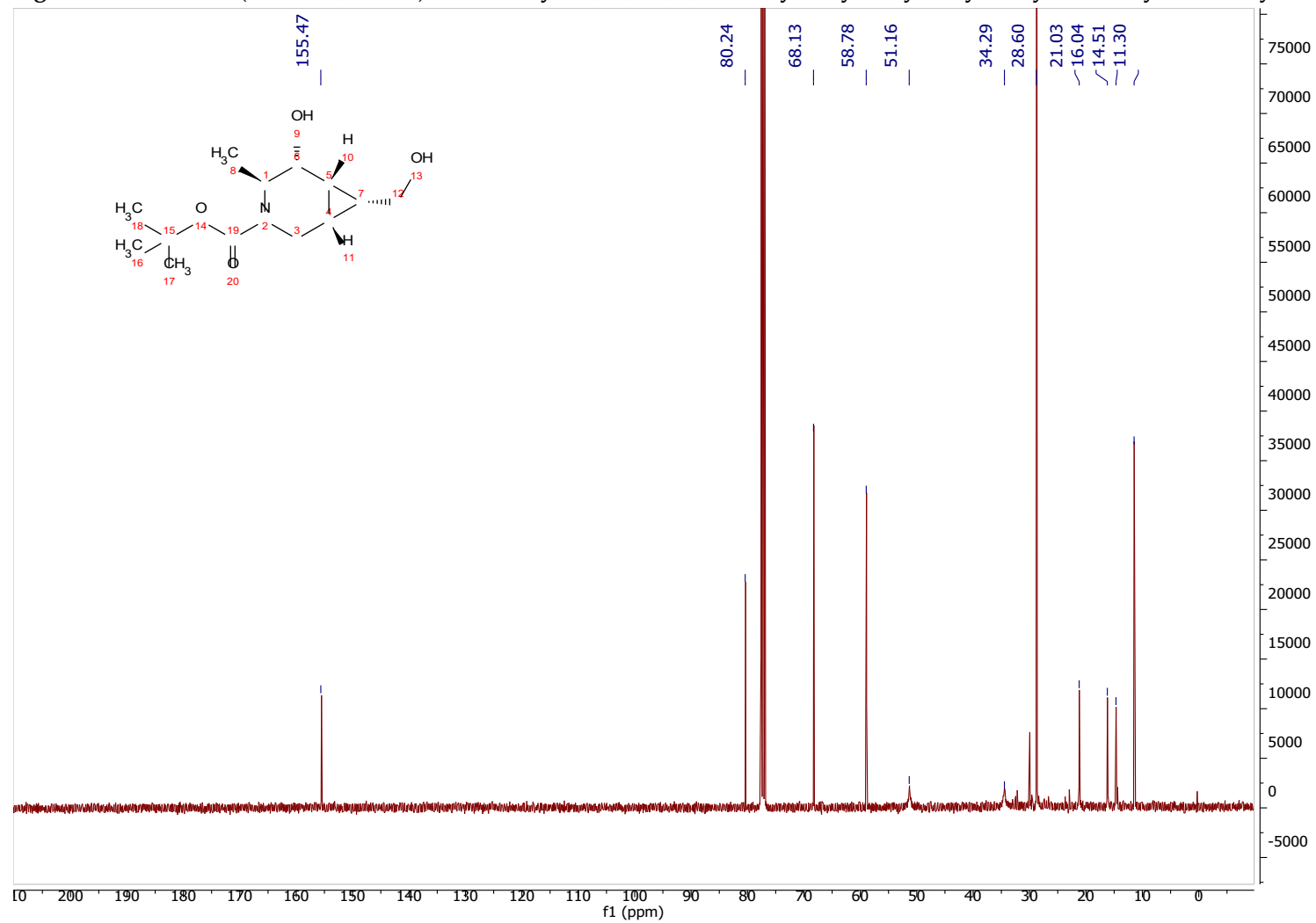


Figure S44: ^1H -NMR (400 MHz, MeOD) of **6c**.

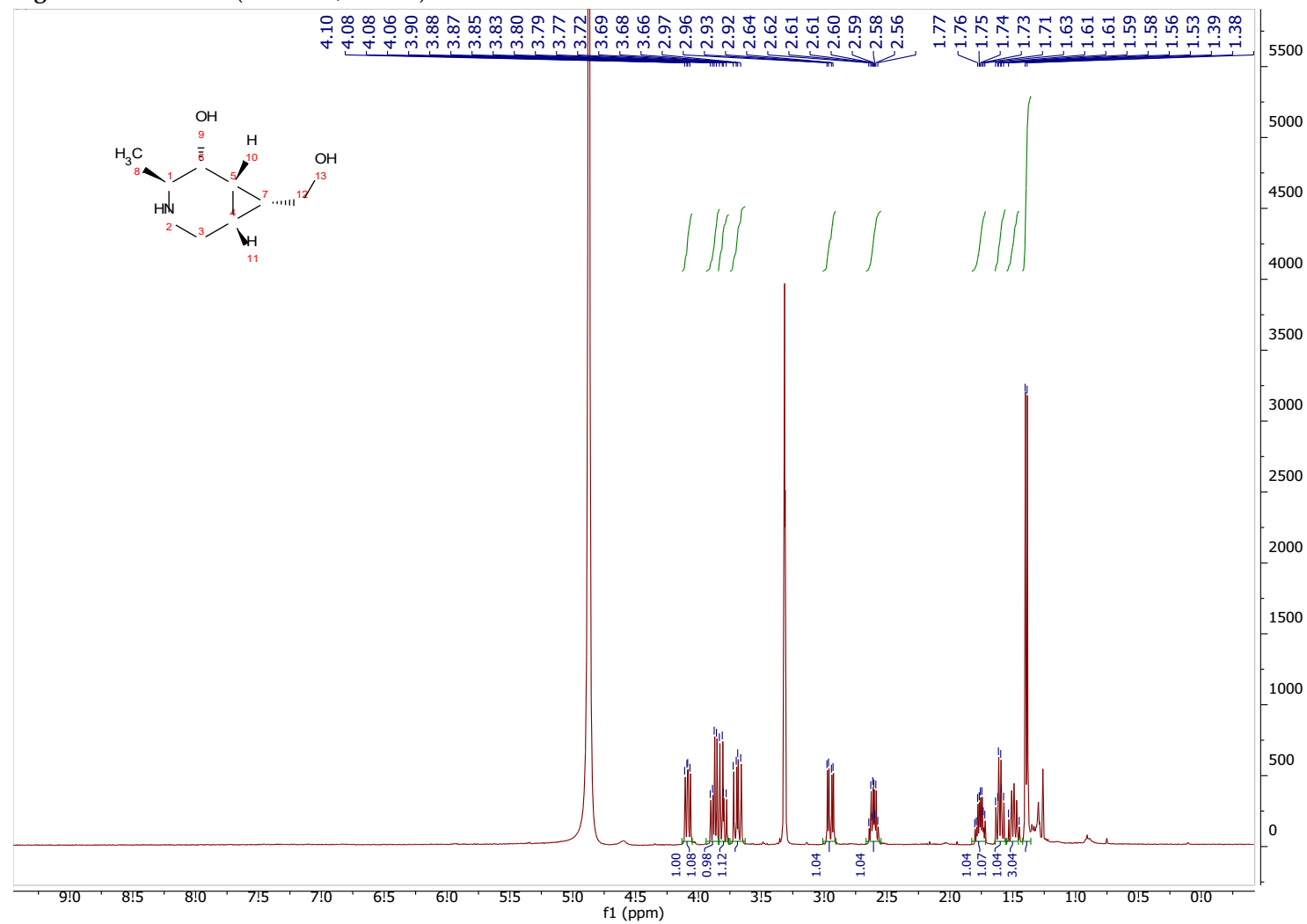


Figure S45: ^{13}C -NMR (100 MHz, MeOD) of **6c**.

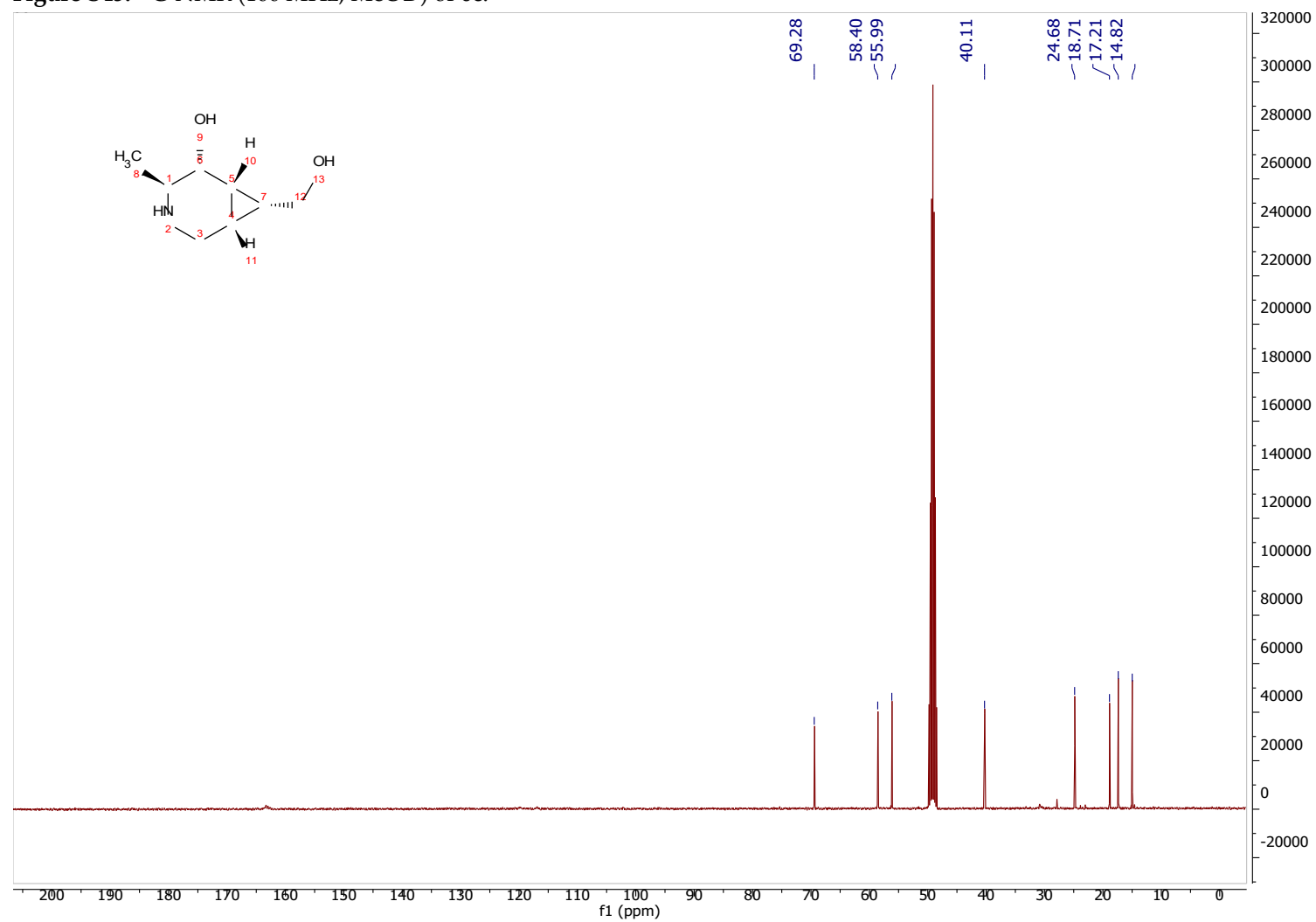


Figure S46: ^1H (400 MHz MeOD) bidimensional NOESY of **6c**.

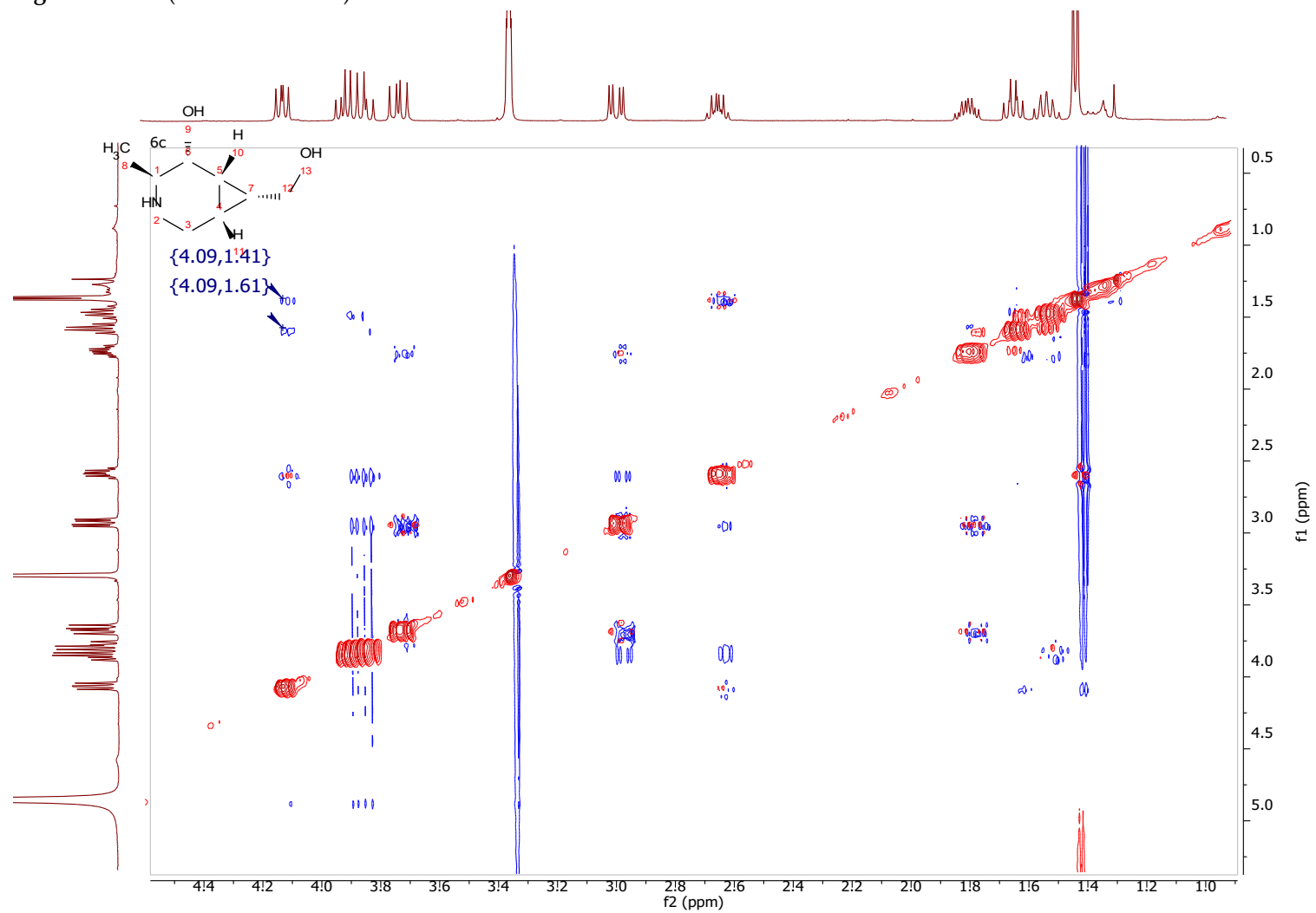


Figure S47: ^1H -NMR (400 MHz, CDCl_3) of 7.

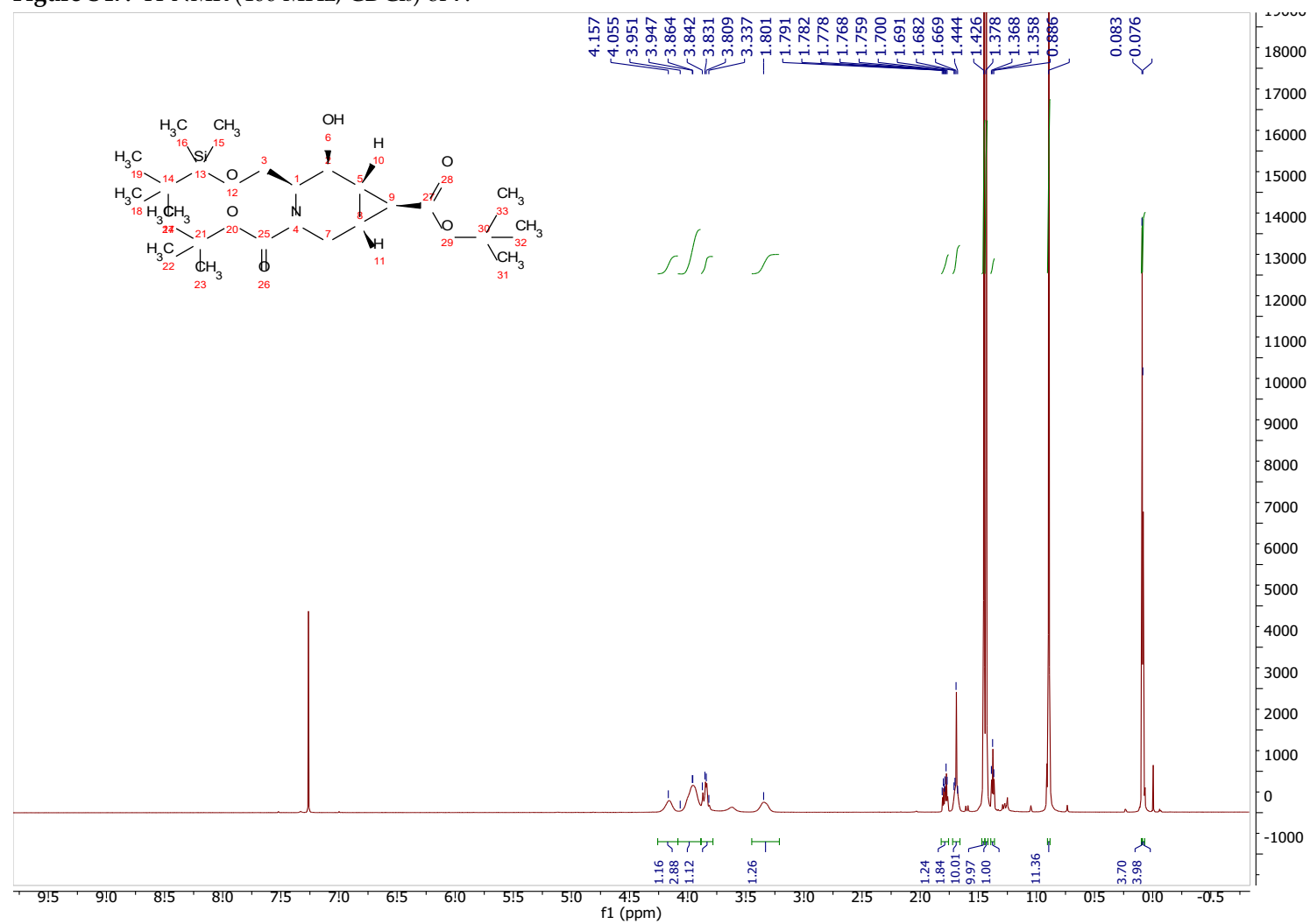


Figure S48: ^{13}C -NMR (100 MHz, CDCl_3) of **7**.

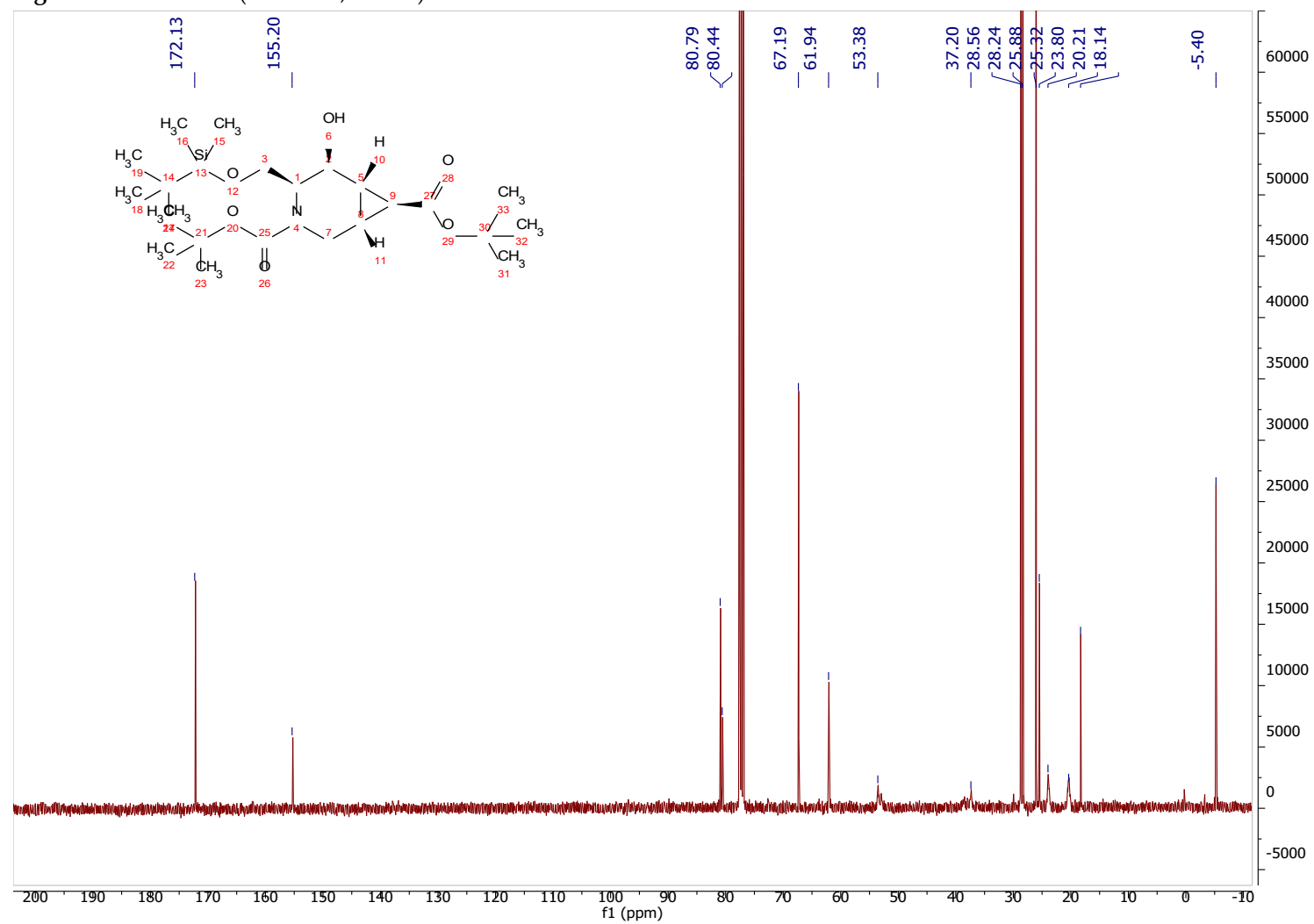


Figure S49: ^1H -NMR (400 MHz, MeOD) of di-*tert*-butyl (1*R*,4*S*,5*S*,6*S*,7*S*)-5-hydroxy-4-(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3,7- dicarboxylate.

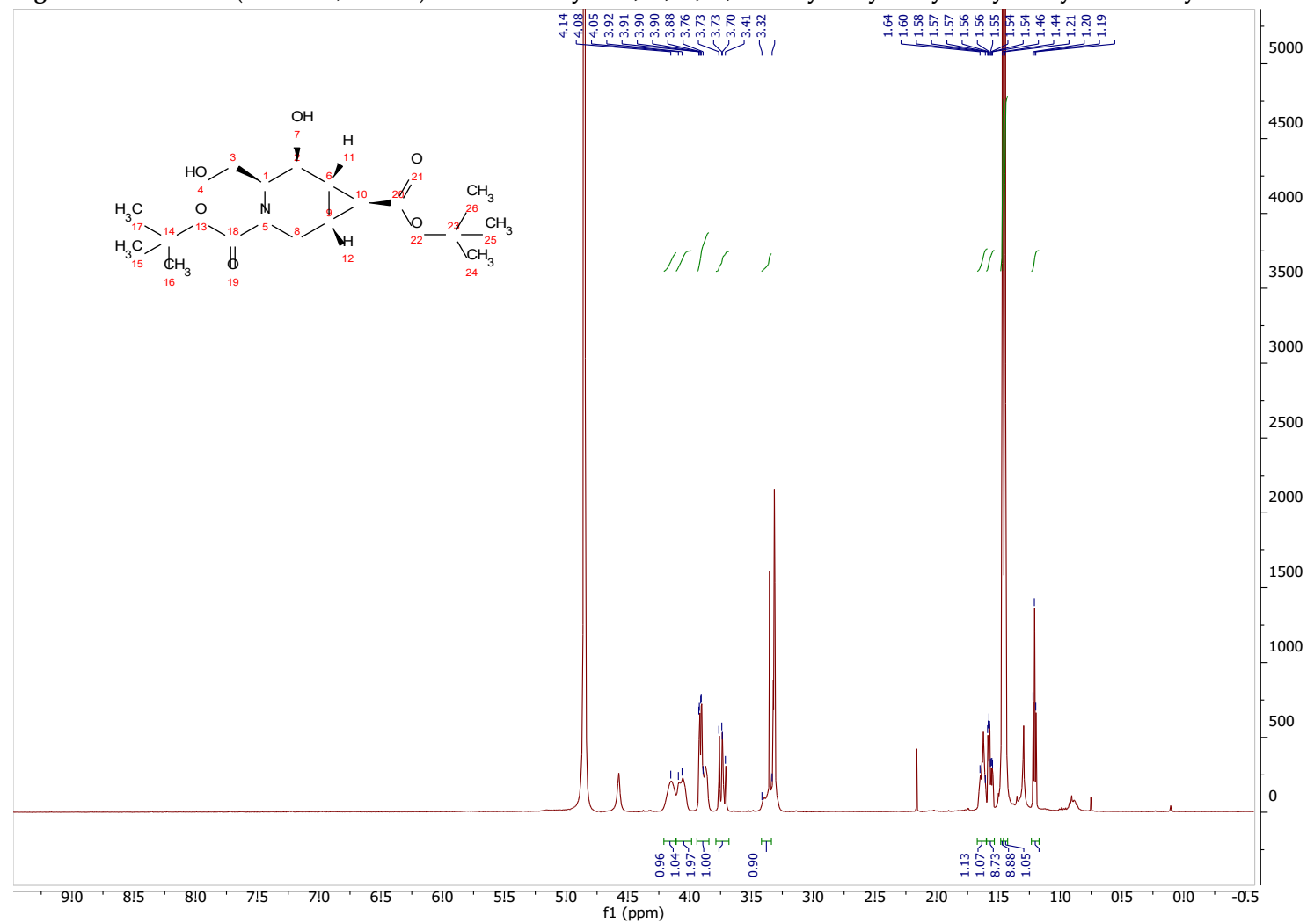


Figure S50: ^{13}C -NMR (100 MHz, MeOD) of di-*tert*-butyl (1R,4S,5S,6S,7S)-5-hydroxy-4-(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3,7- dicarboxylate.

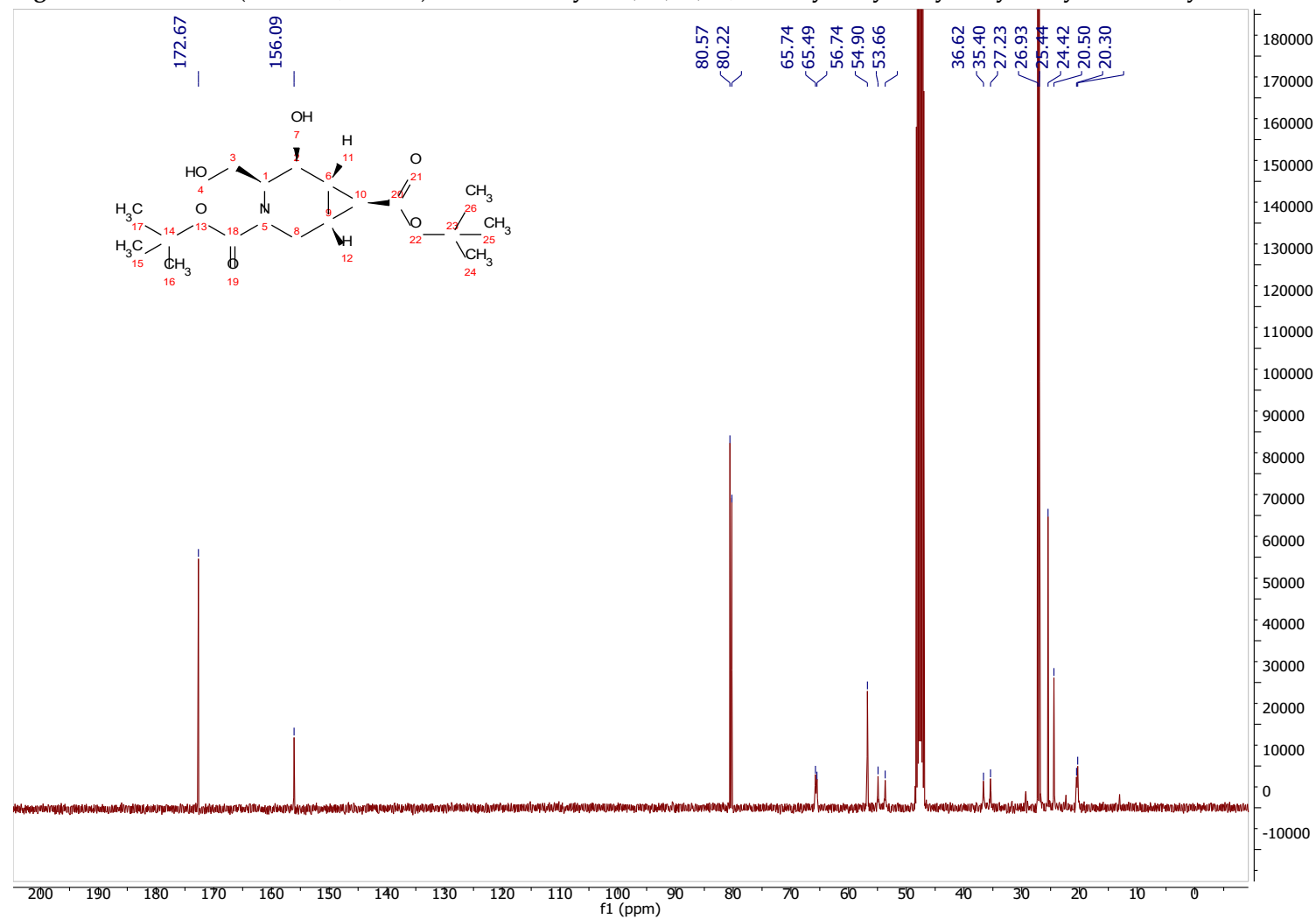


Figure S51: ^1H (400 MHz CDCl_3) bidimensional NOESY of di-*tert*-butyl (1*R*,4*S*,5*S*,6*S*,7*S*)-5-hydroxy-4-(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3,7-dicarboxylate.

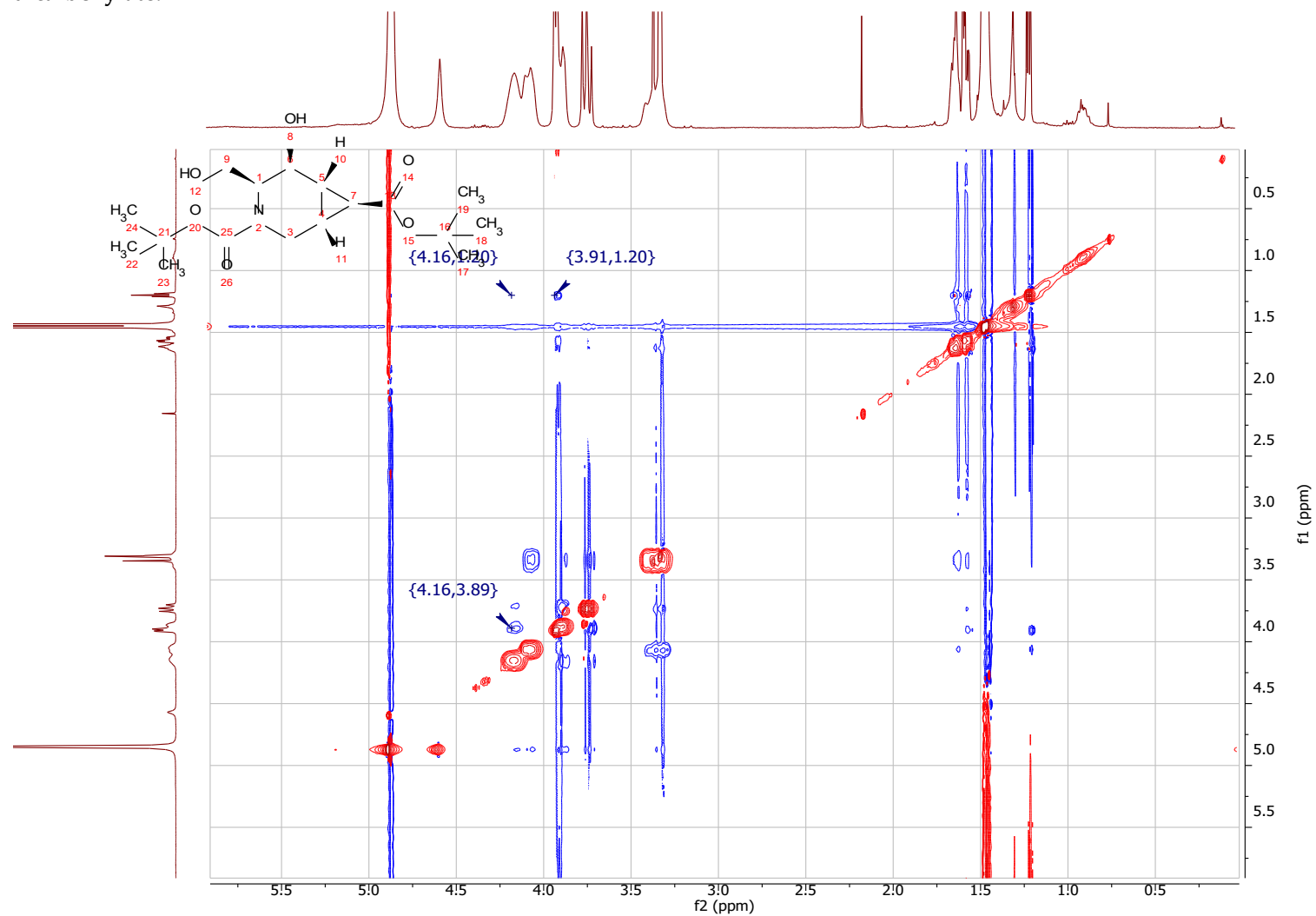


Figure S52: ^1H -NMR (400 MHz, D_2O) of 10a.

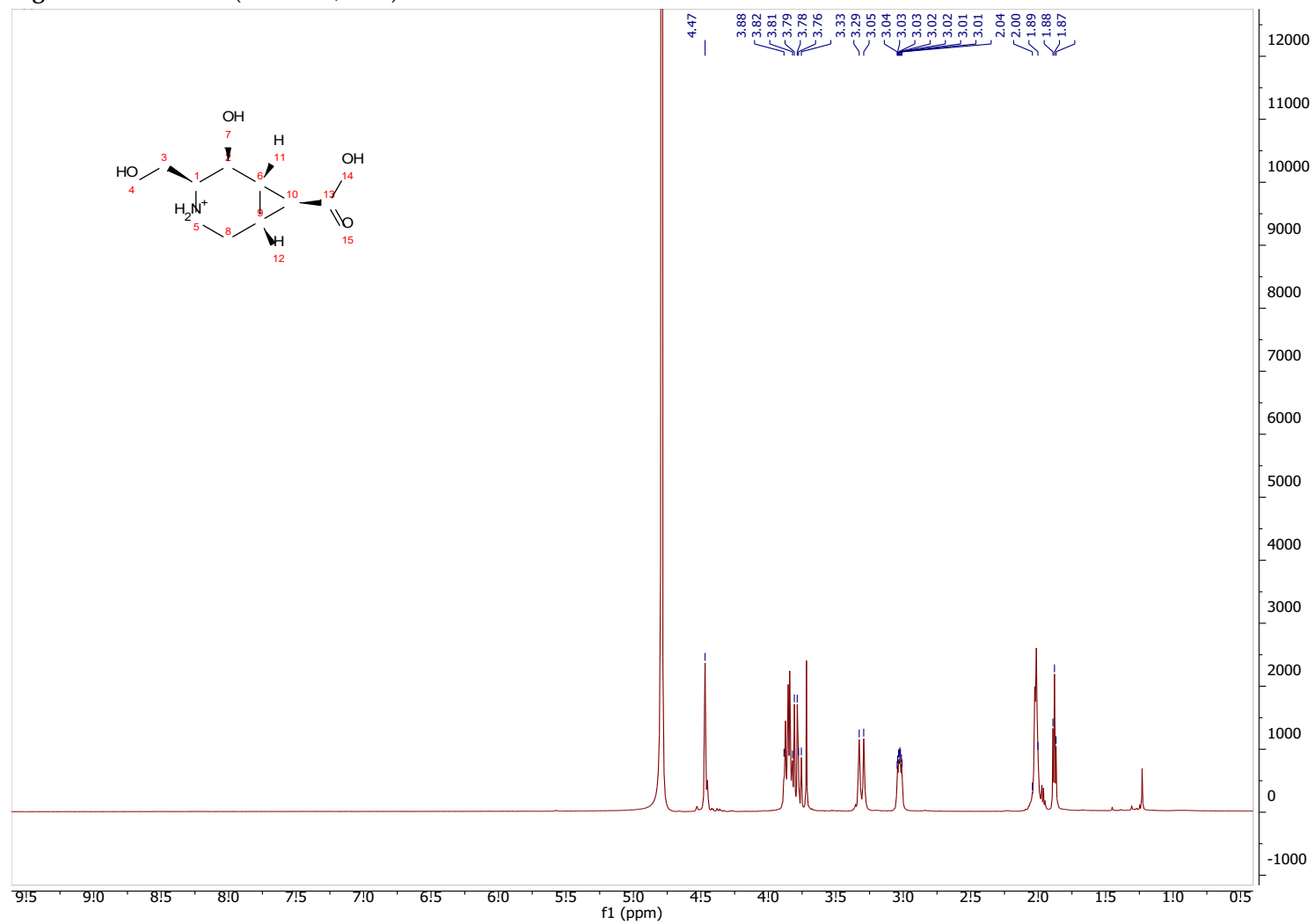


Figure S53: ^{13}C -NMR (100 MHz, D_2O) of 10a.

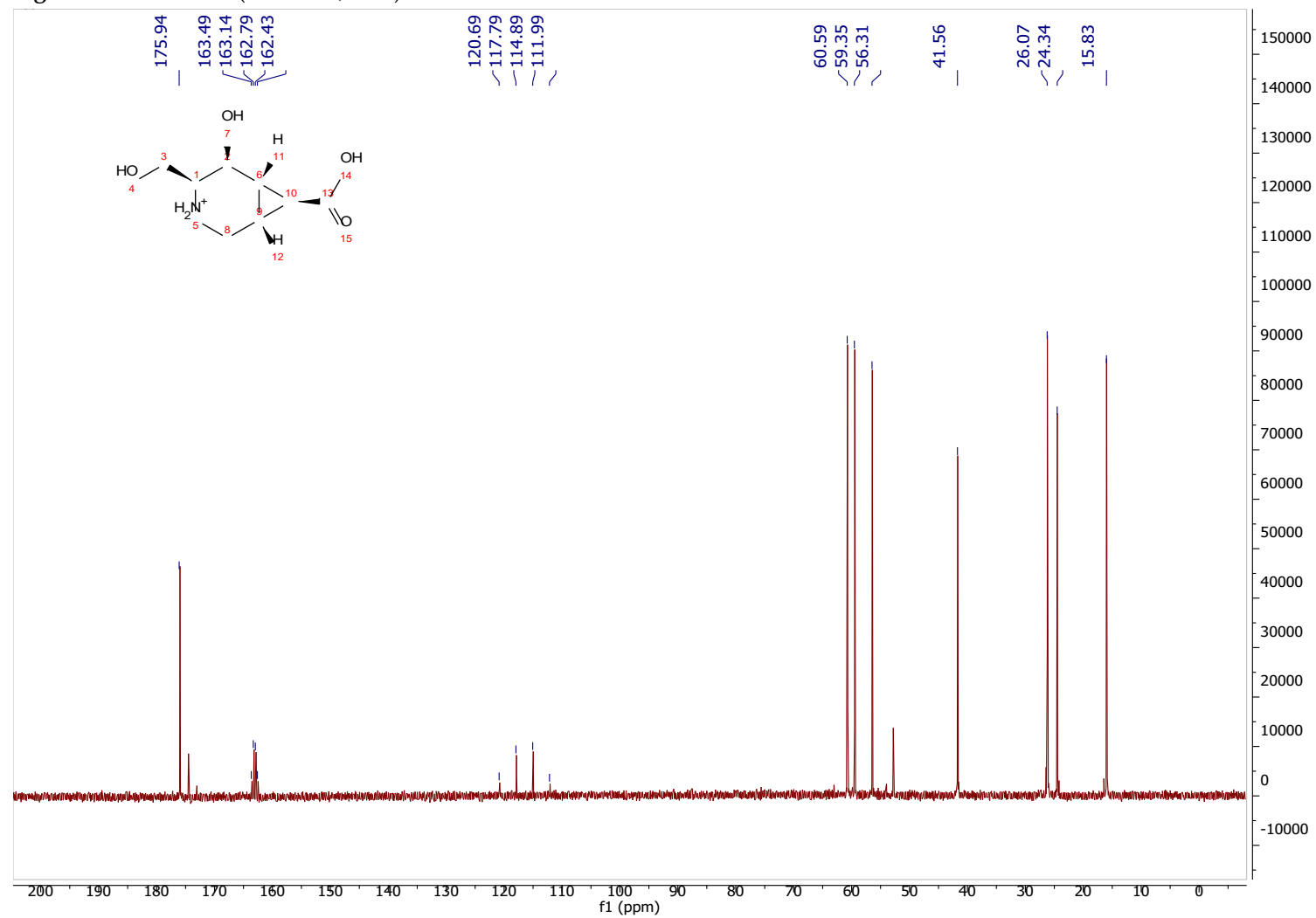


Figure S54: ^1H -NMR (400 MHz, CDCl_3) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*S*)-4-(((*tert*-butyldimethylsilyl)oxy)methyl)-5-hydroxy-7- (hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3-carboxylate.

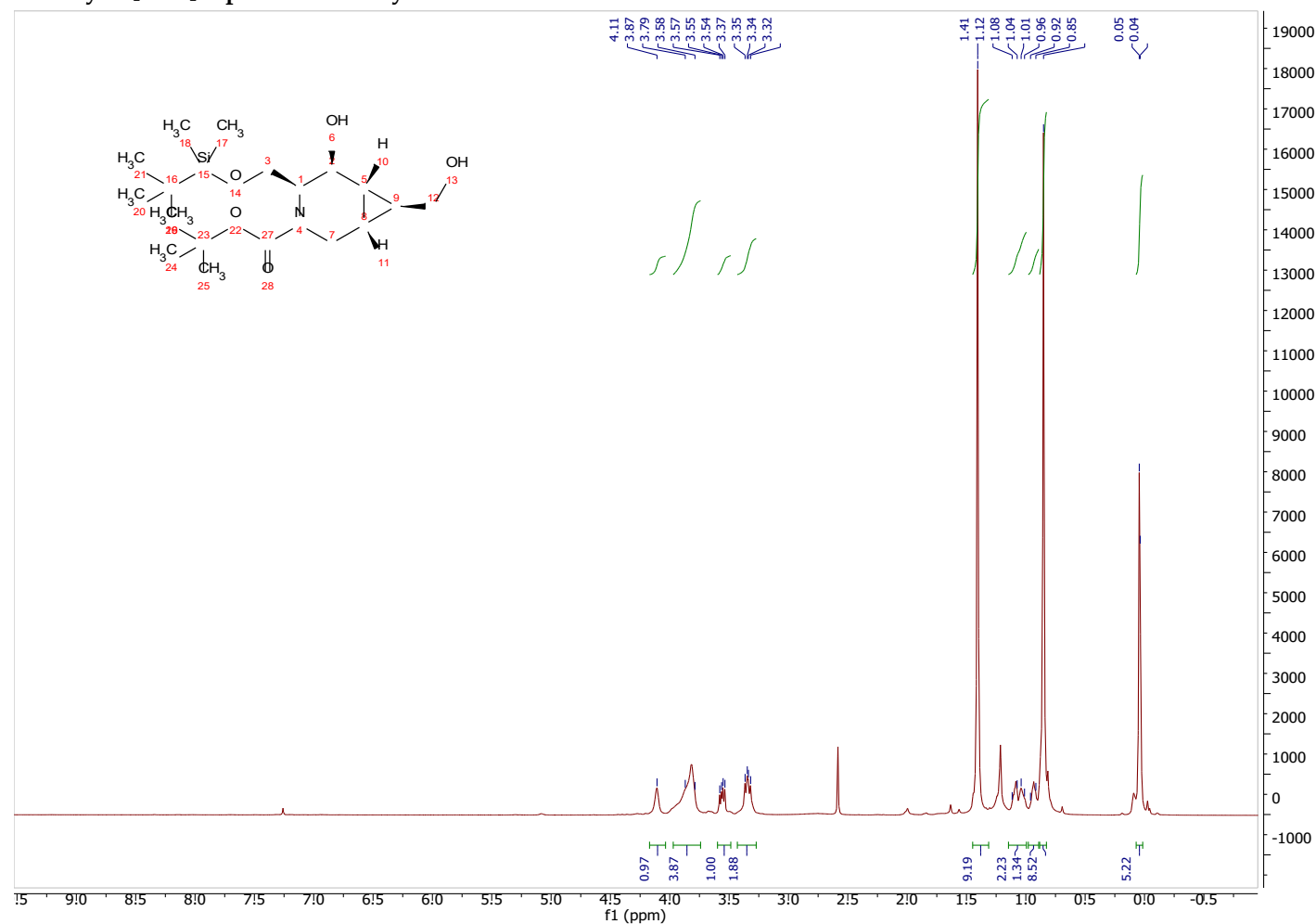


Figure S55: ^{13}C -NMR (100 MHz, MeOD) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*S*)-4-(((*tert*-butyldimethylsilyl)oxy)methyl)-5-hydroxy-7- (hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3-carboxylate.

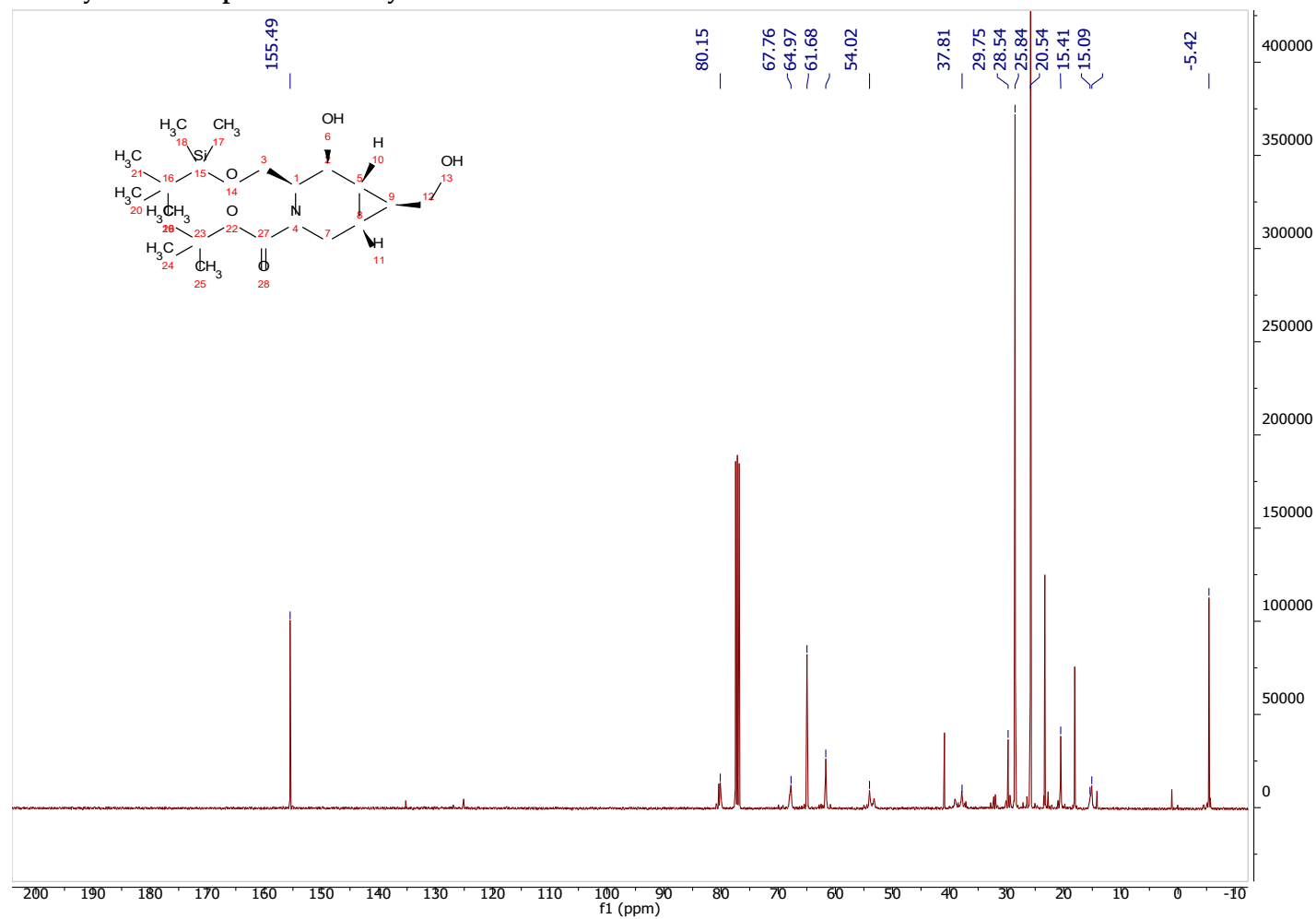


Figure S56: ^1H -NMR (400 MHz, MeOD) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*S*)-5-hydroxy-4,7-bis(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3- carboxylate.

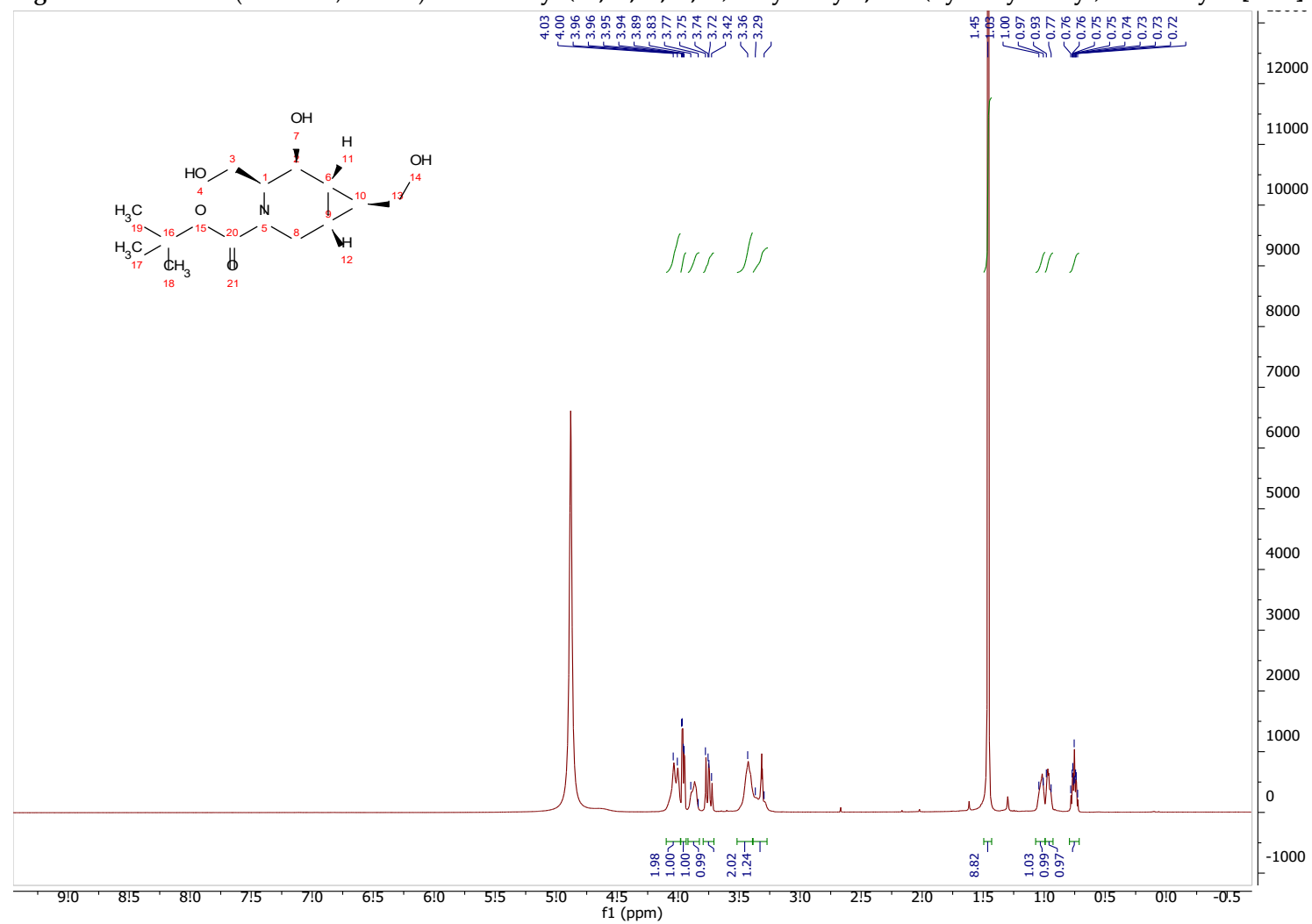


Figure S57: ^{13}C -NMR (100 MHz, MeOD) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*S*)-5-hydroxy-4,7-bis(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3- carboxylate.

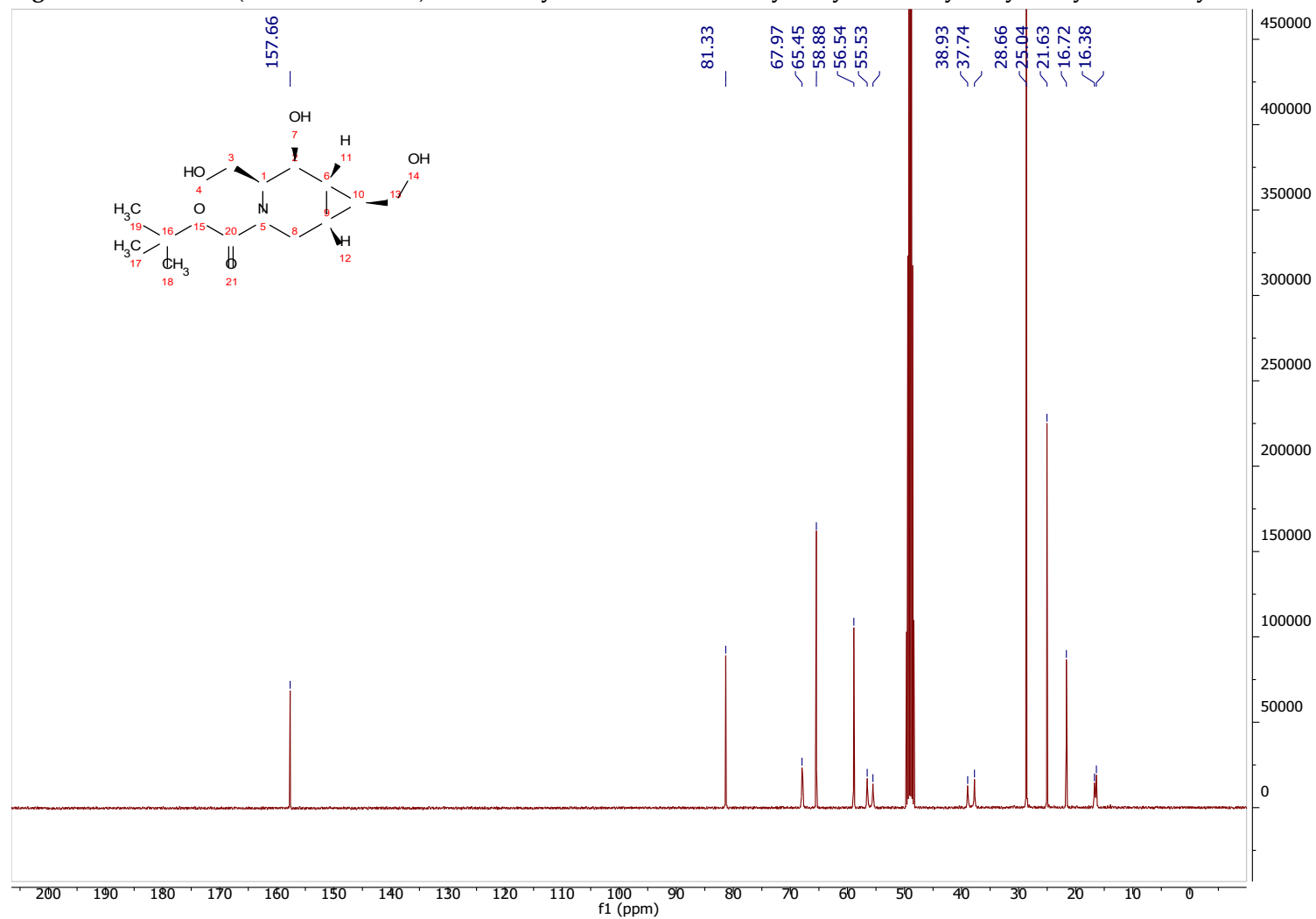


Figure S58: ^1H -NMR (400 MHz, MeOD) of **11a**.

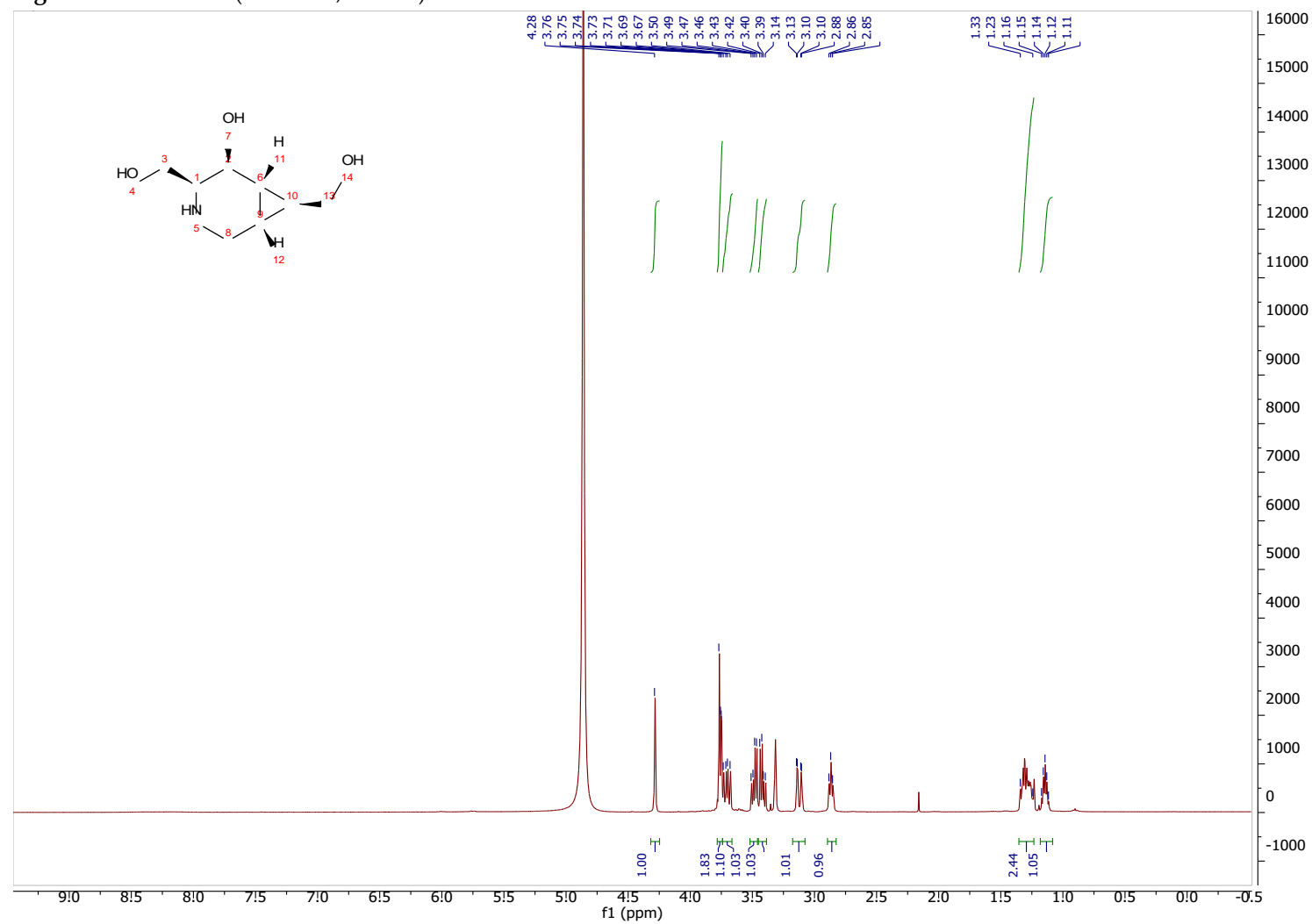


Figure S59: ^{13}C -NMR (100 MHz, MeOD) of **11a**.

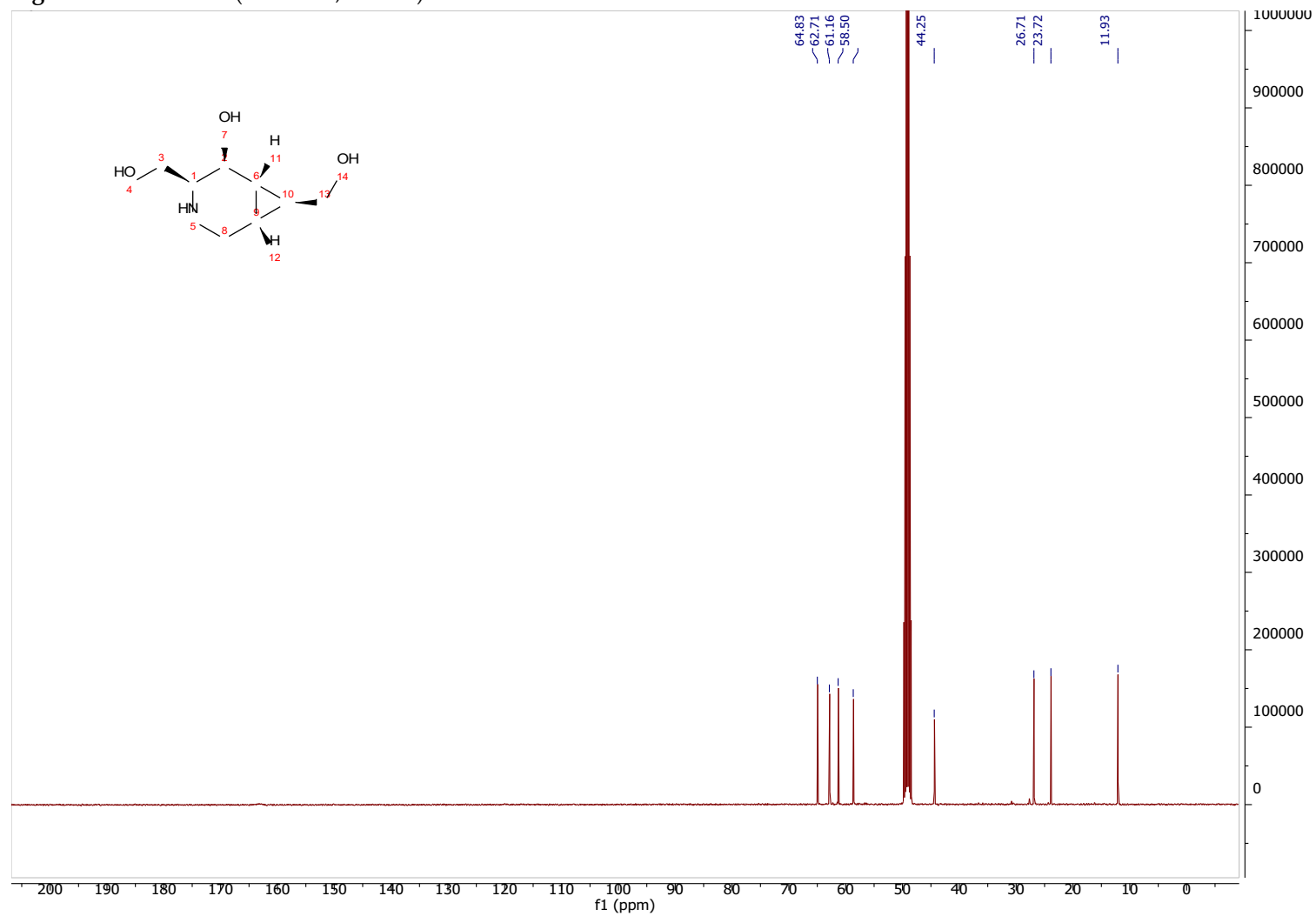


Figure S60: ^1H -NMR (400 MHz, CDCl_3) of **8**.

The chemical structure of compound **8** is shown in the top left, with atoms numbered 1 through 29. The structure includes a pyrazole ring, a sulfone group, and a carboxylic acid group. The ^1H -NMR spectrum (400 MHz, CDCl_3) is displayed below the structure, showing peaks from 0 to 5.5 ppm. The spectrum includes integration values (e.g., 2.01, 1.00, 5.02, 2.01, 2.03, 2.06, 20.12, 19.24, 12.50) and peak labels (e.g., 5.04, 4.18, 4.12, 4.11, 4.10, 4.10, 4.08, 3.82, 3.80, 3.77, 3.76, 3.74, 3.73, 3.68, 3.66, 3.64, 3.58, 3.55, 3.51, 3.48, 2.53, 2.51, 2.50, 2.24, 2.22, 2.20, 1.80, 1.78, 1.78, 1.76, 1.74, 1.74, 0.89, 0.07, 0.06).

Figure S61: ^{13}C -NMR (100 MHz, CDCl_3) of 8.

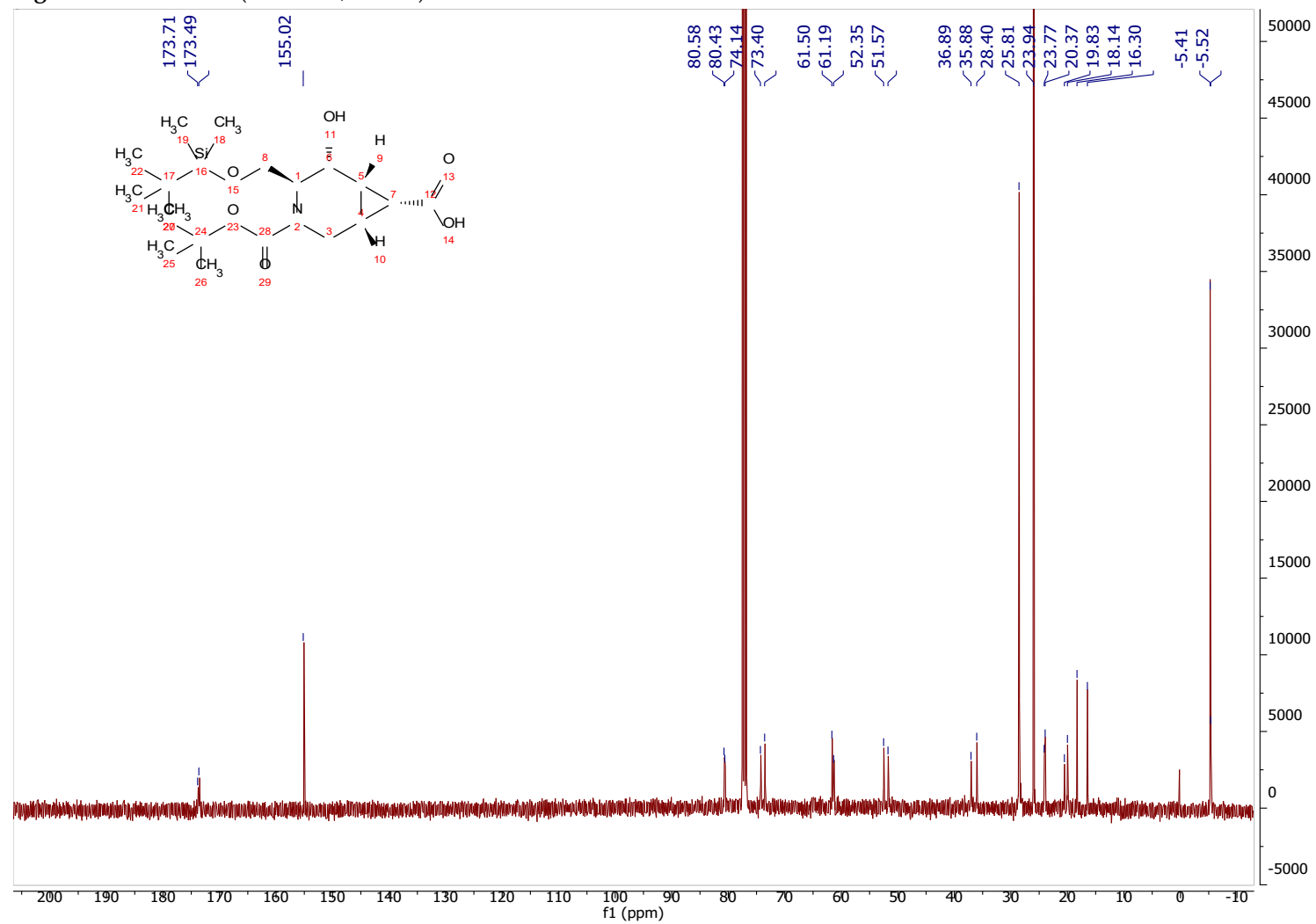


Figure S62: ^1H -NMR (400 MHz, CDCl_3) of (1*R*,4*S*,5*S*,6*S*,7*R*)-3-(*tert*-butoxycarbonyl)-5-hydroxy-4-(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-7-carboxylic acid.

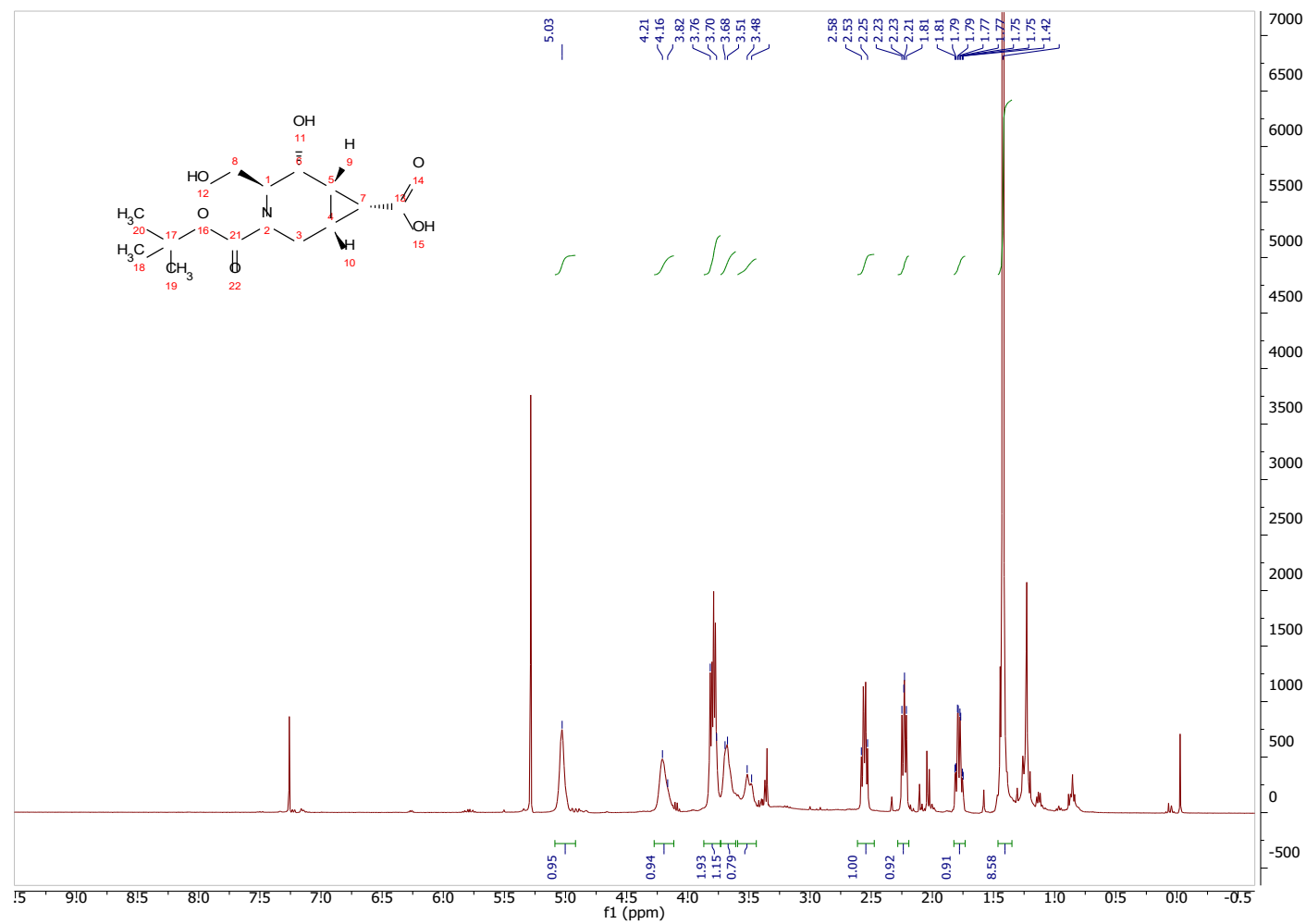


Figure S63: ^{13}C -NMR (100 MHz, CDCl_3) of (1*R*,4*S*,5*S*,6*S*,7*R*)-3-(*tert*-butoxycarbonyl)-5-hydroxy-4-(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-7-carboxylic acid.

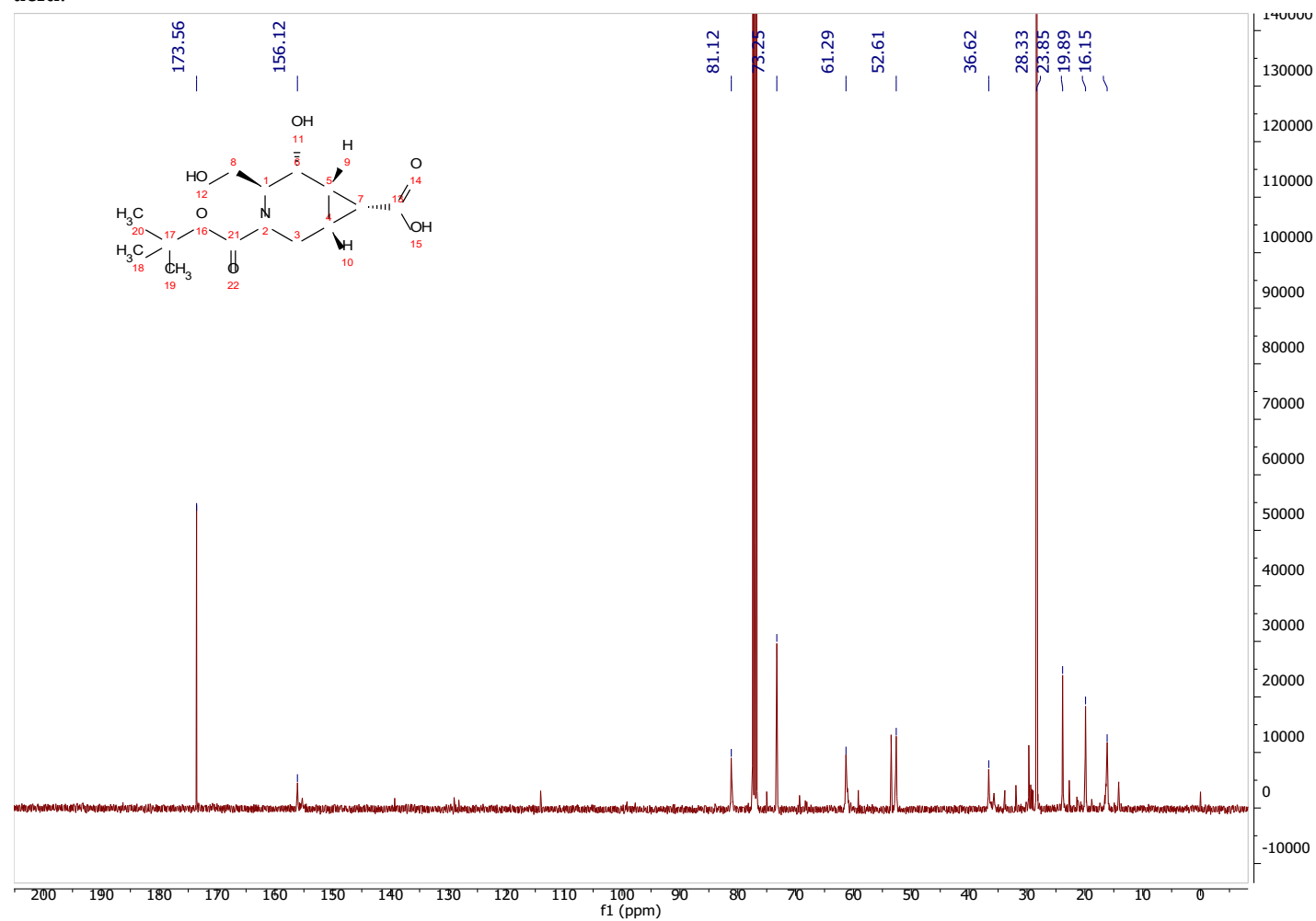


Figure S64: ^1H -NMR (400 MHz, D_2O) of **10b**.

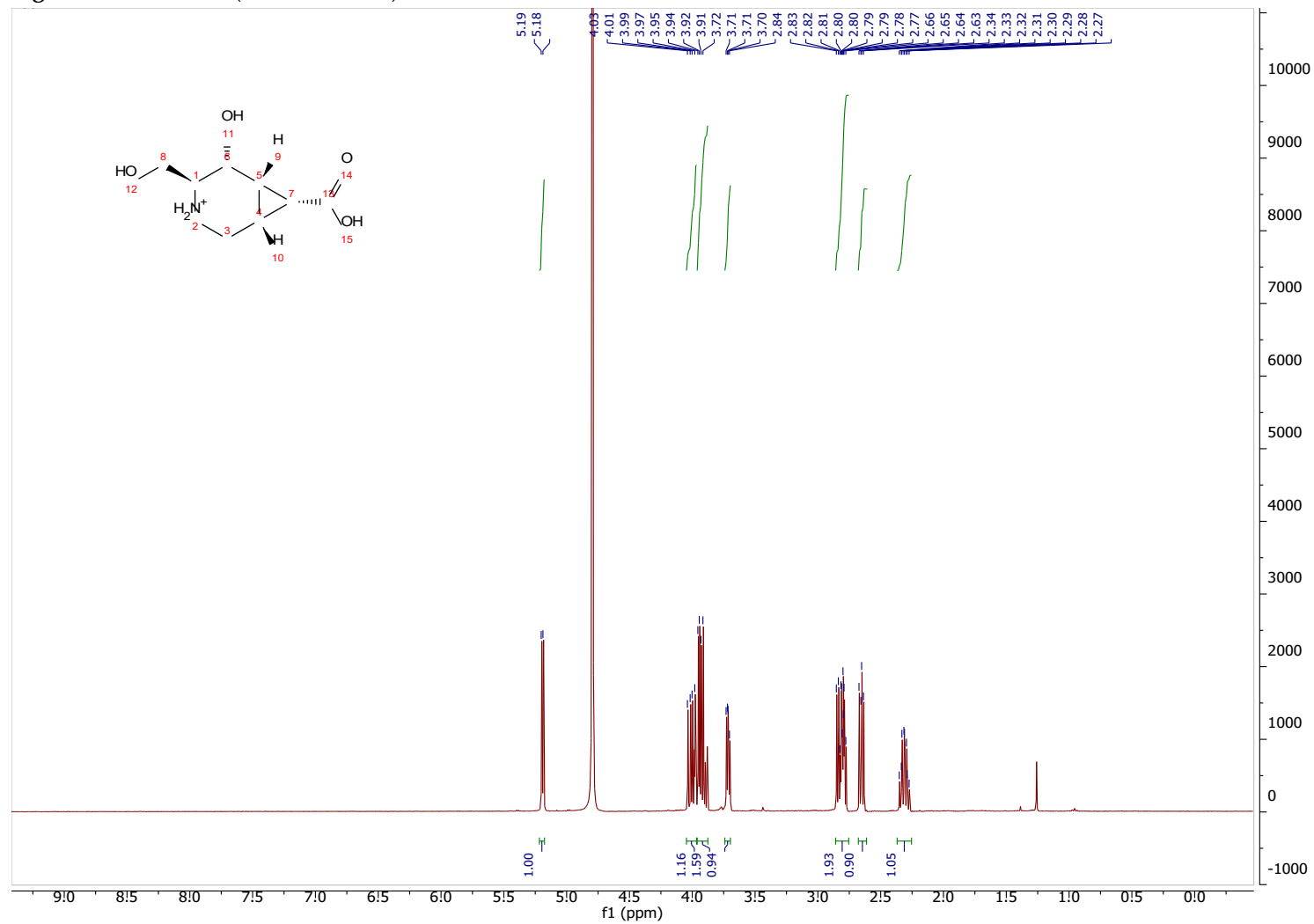


Figure S65: ^{13}C -NMR (100 MHz, D_2O) of **10b**.

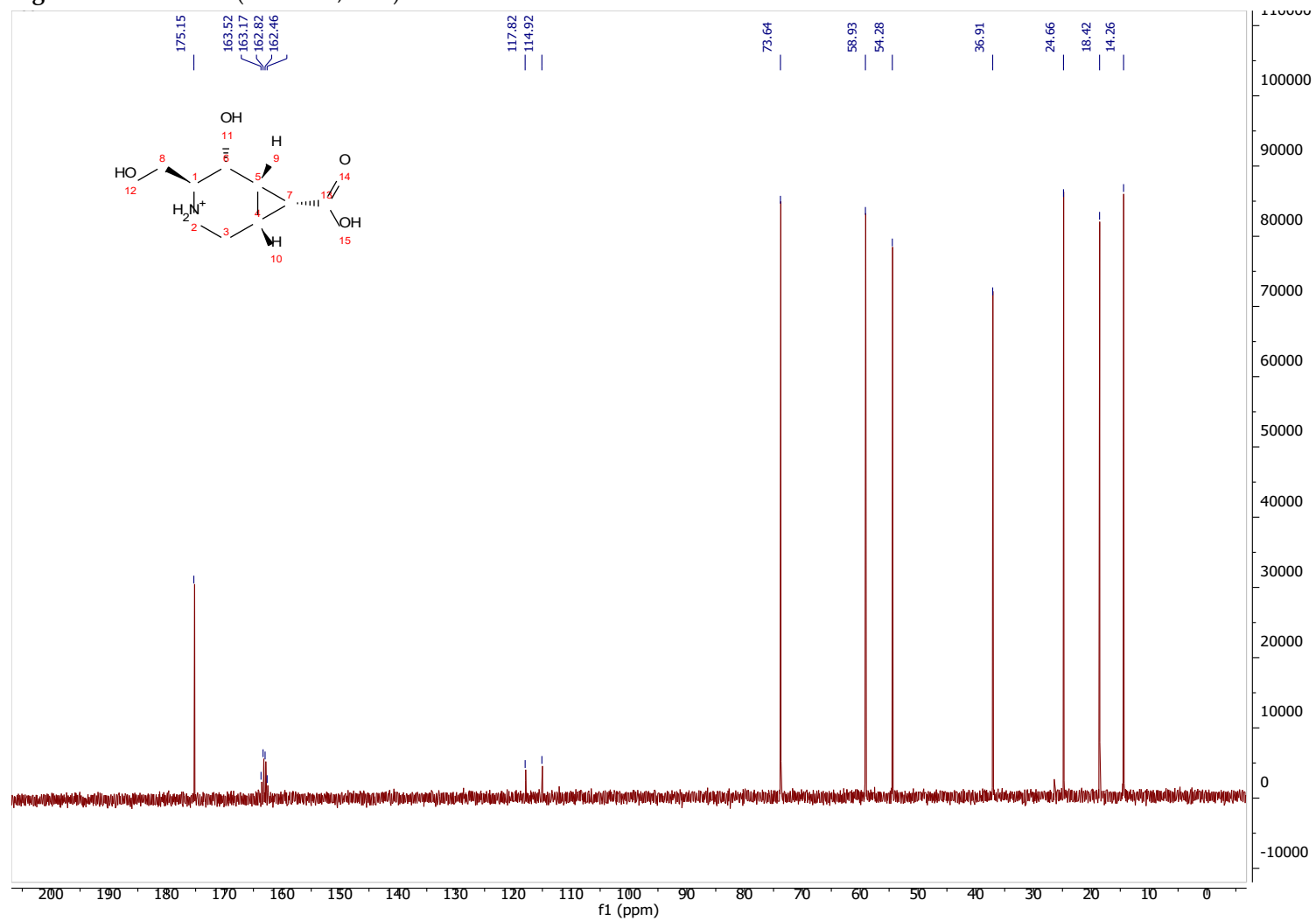


Figure S66: ^1H -NMR (400 MHz, CDCl_3) of **9**.

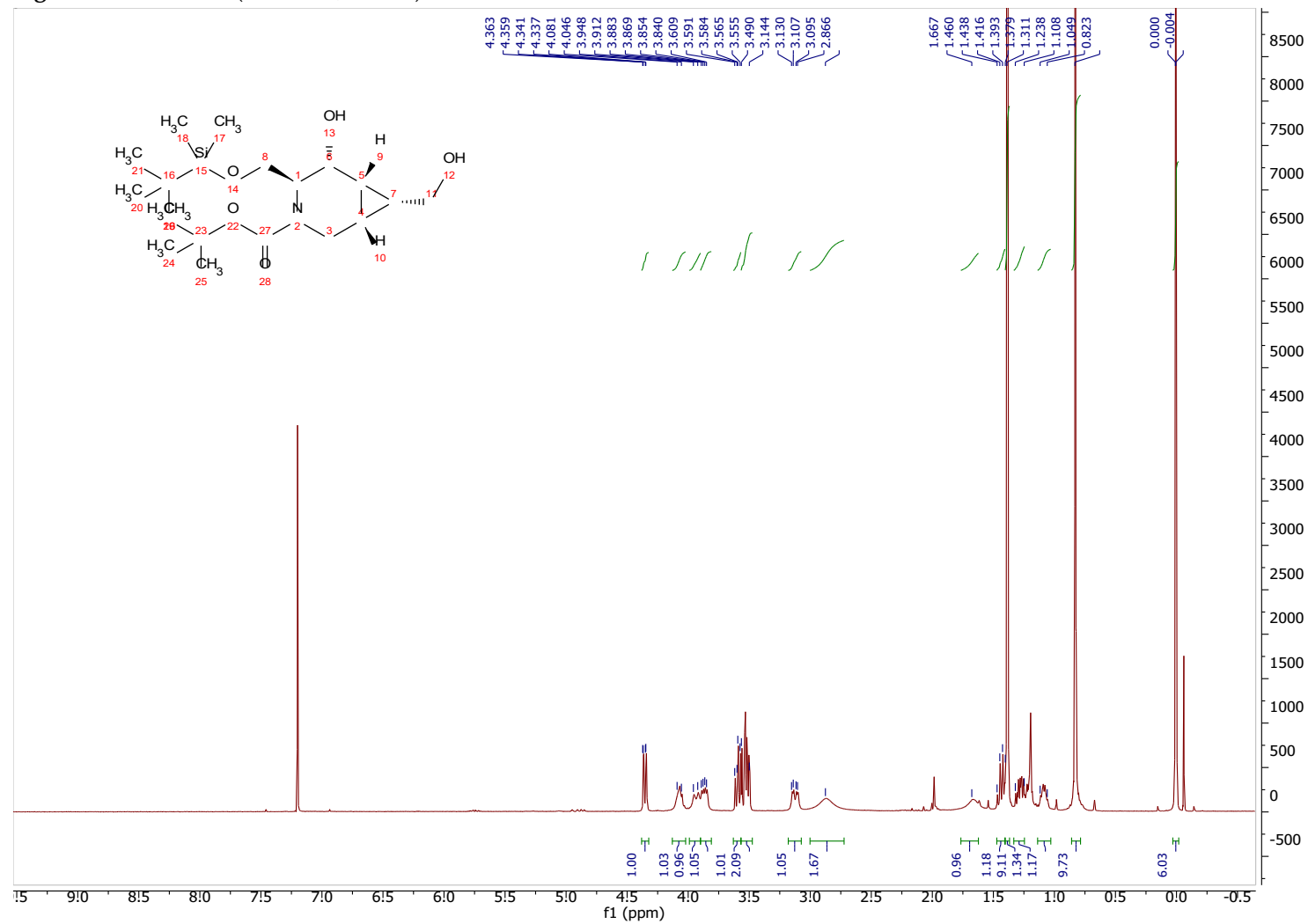


Figure S67: ^{13}C -NMR (100 MHz, CDCl_3) of **9**.

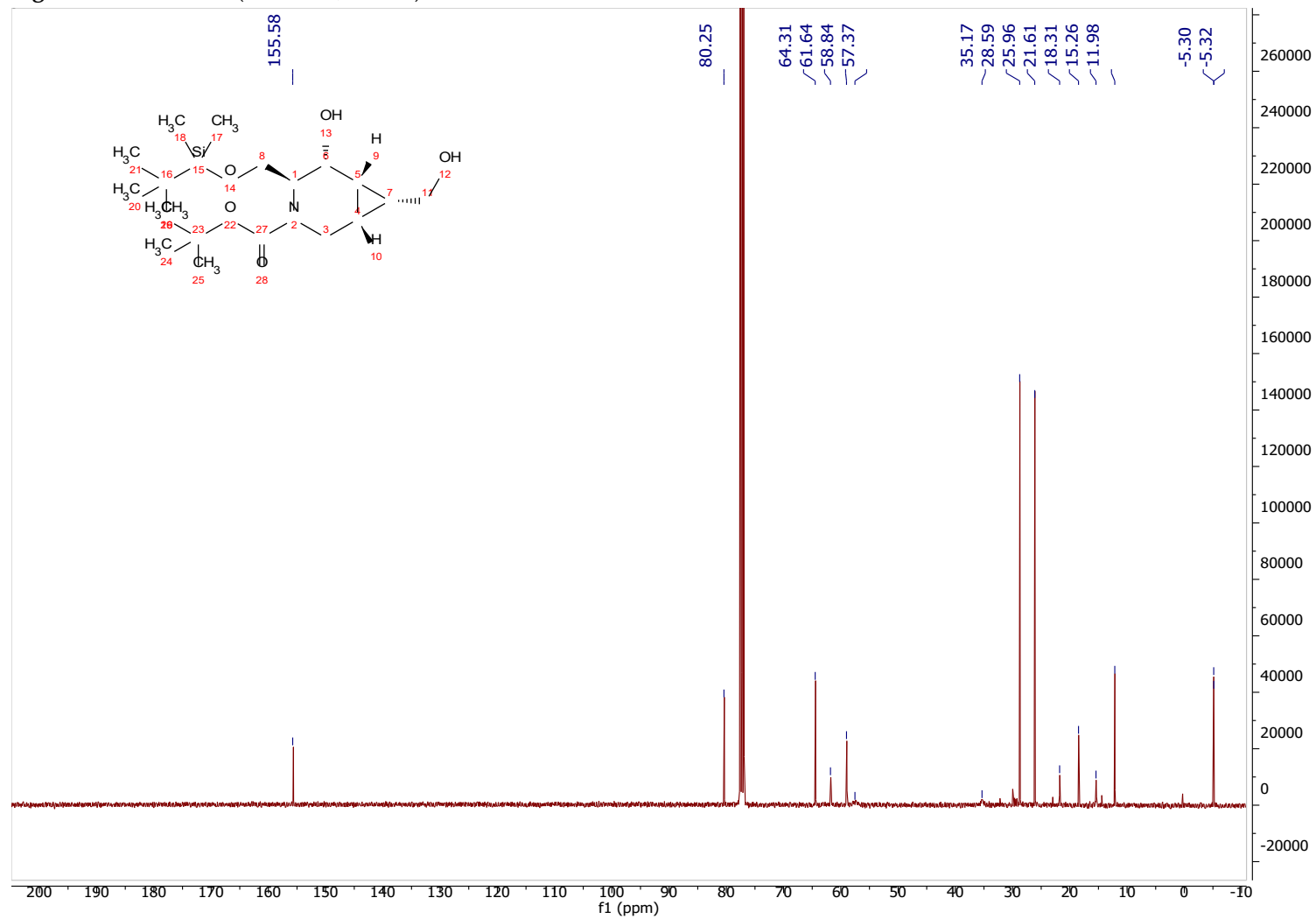


Figure S68: ^1H -NMR (400 MHz, MeOD) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*R*)-5-hydroxy-4,7-bis(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3- carboxylate.

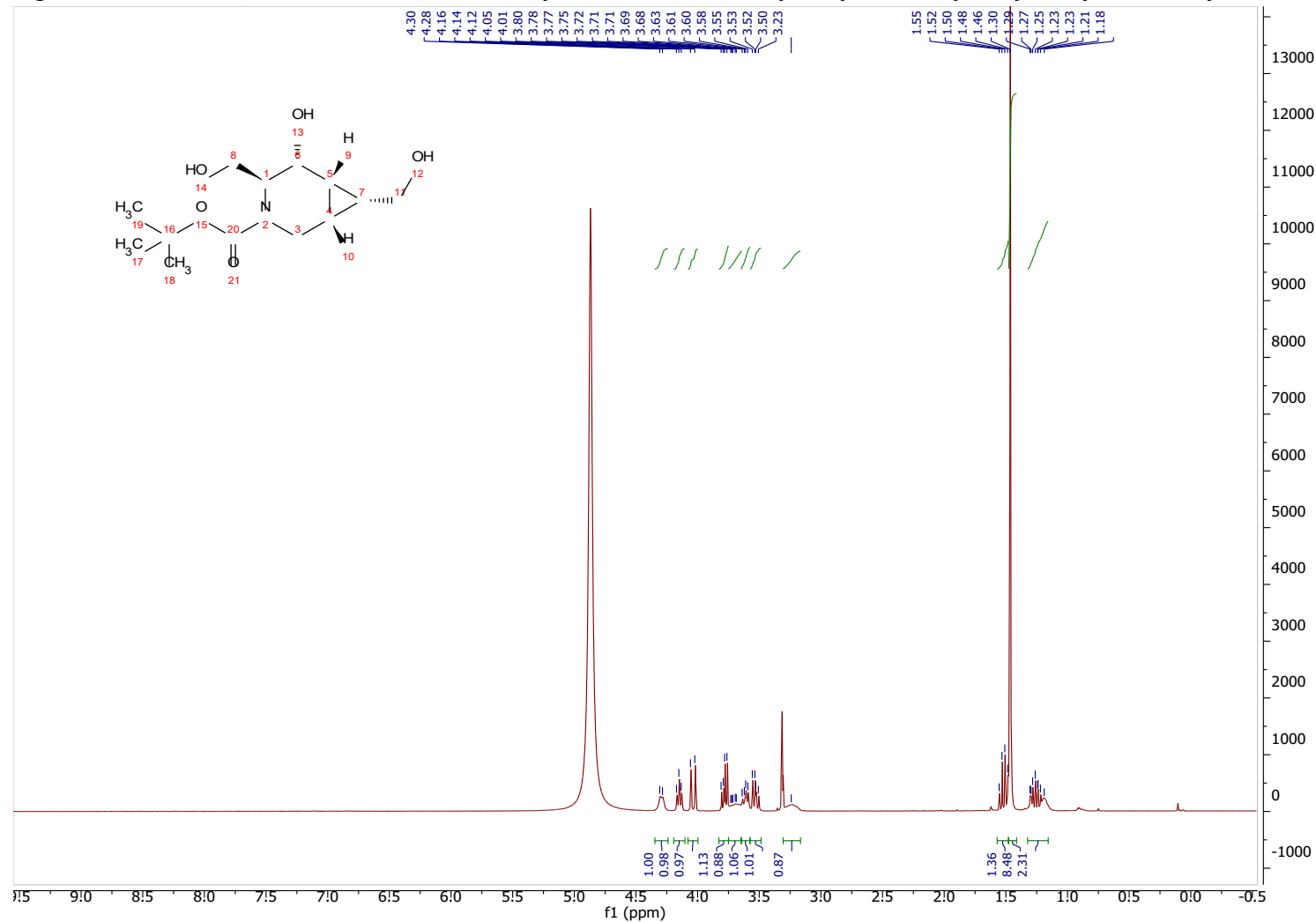


Figure S69: ^{13}C -NMR (100 MHz, MeOD) of *tert*-butyl (1*S*,4*S*,5*S*,6*S*,7*R*)-5-hydroxy-4,7-bis(hydroxymethyl)-3-azabicyclo[4.1.0]heptane-3- carboxylate.

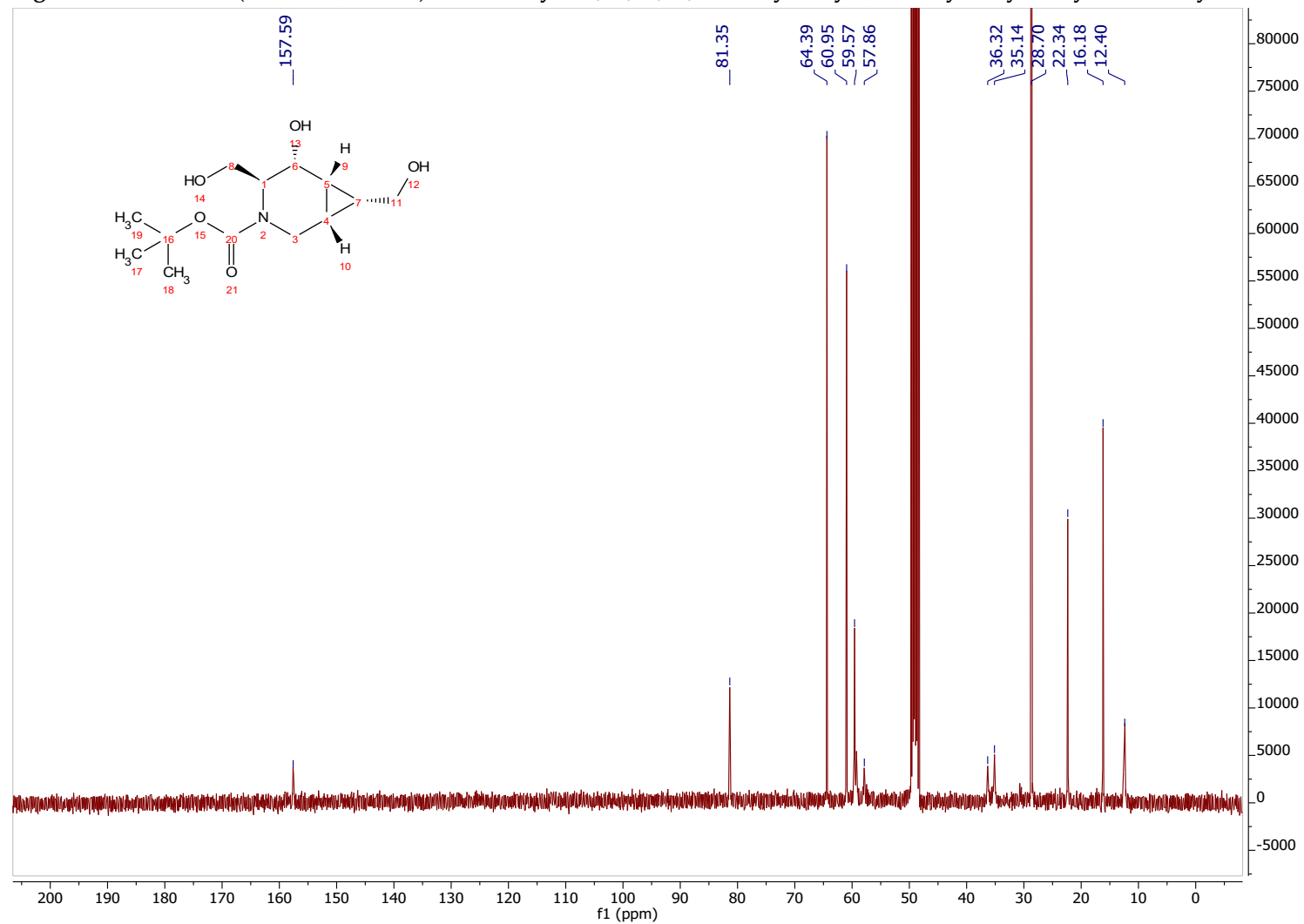


Figure S70: ^1H -NMR (400 MHz, MeOD) of **11b**.

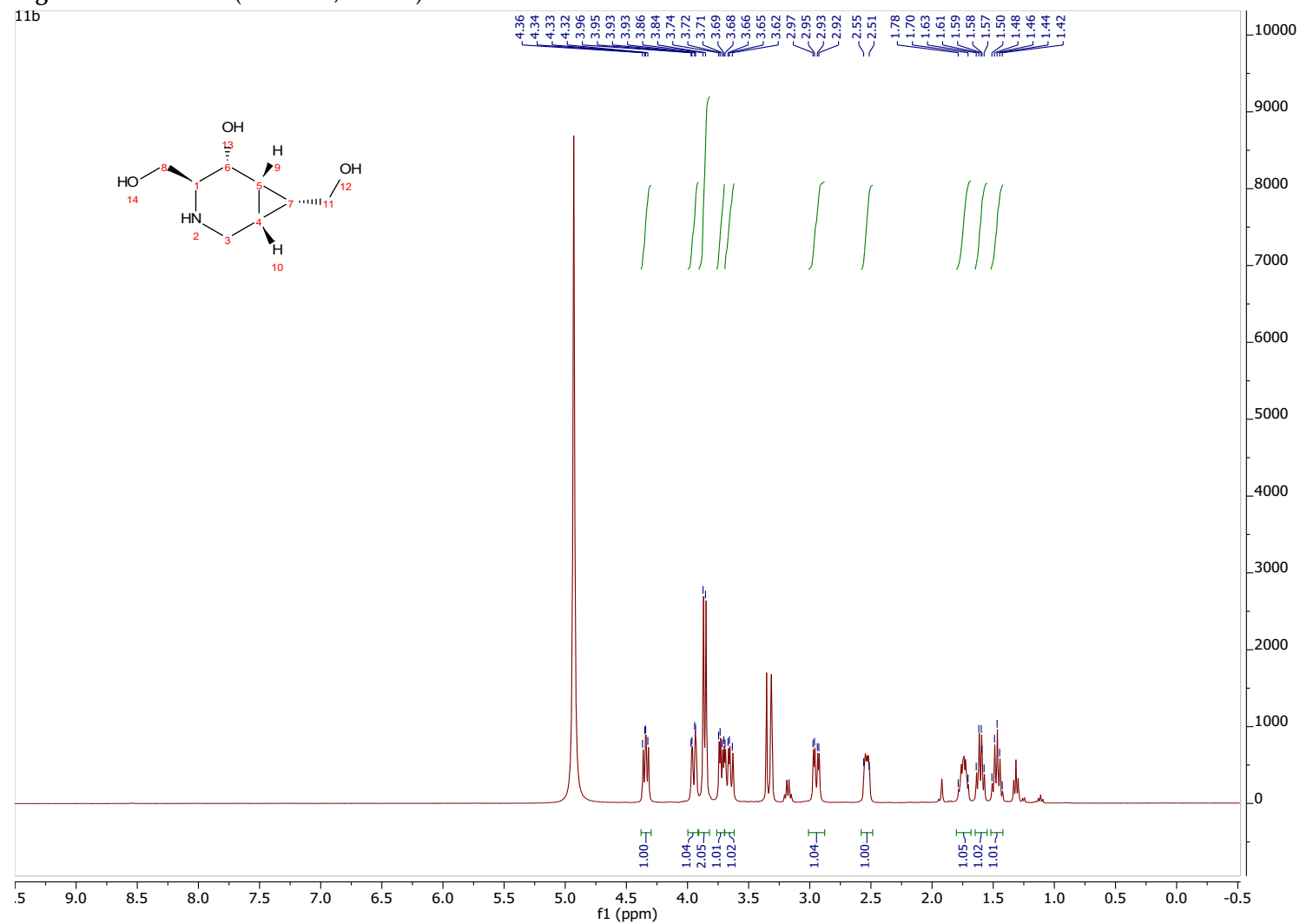


Figure S71: ^{13}C -NMR (100 MHz, MeOD) of **11b**.

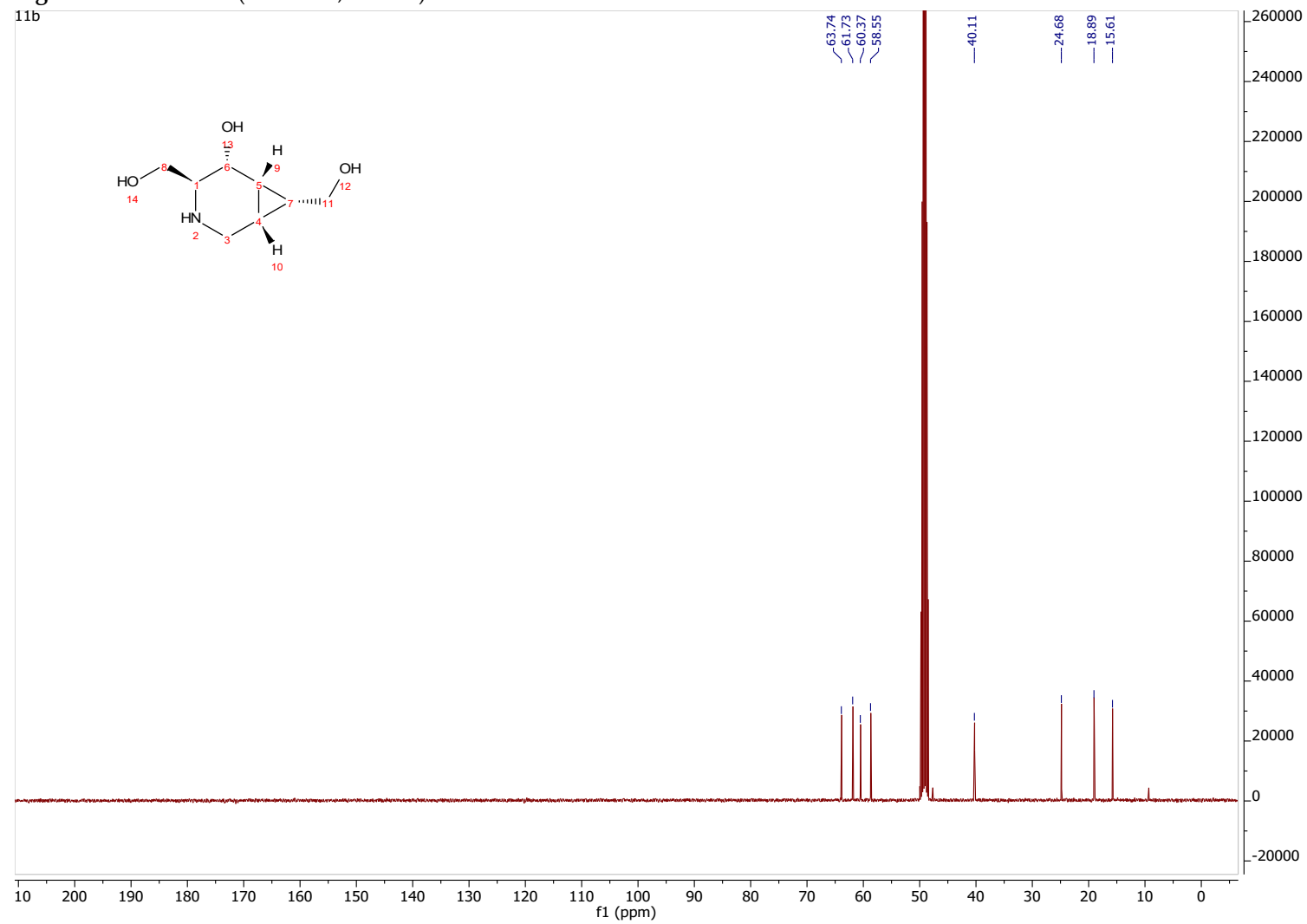


Figure S72: ^1H (400 MHz MeOD) bidimensional NOESY of **11b**.

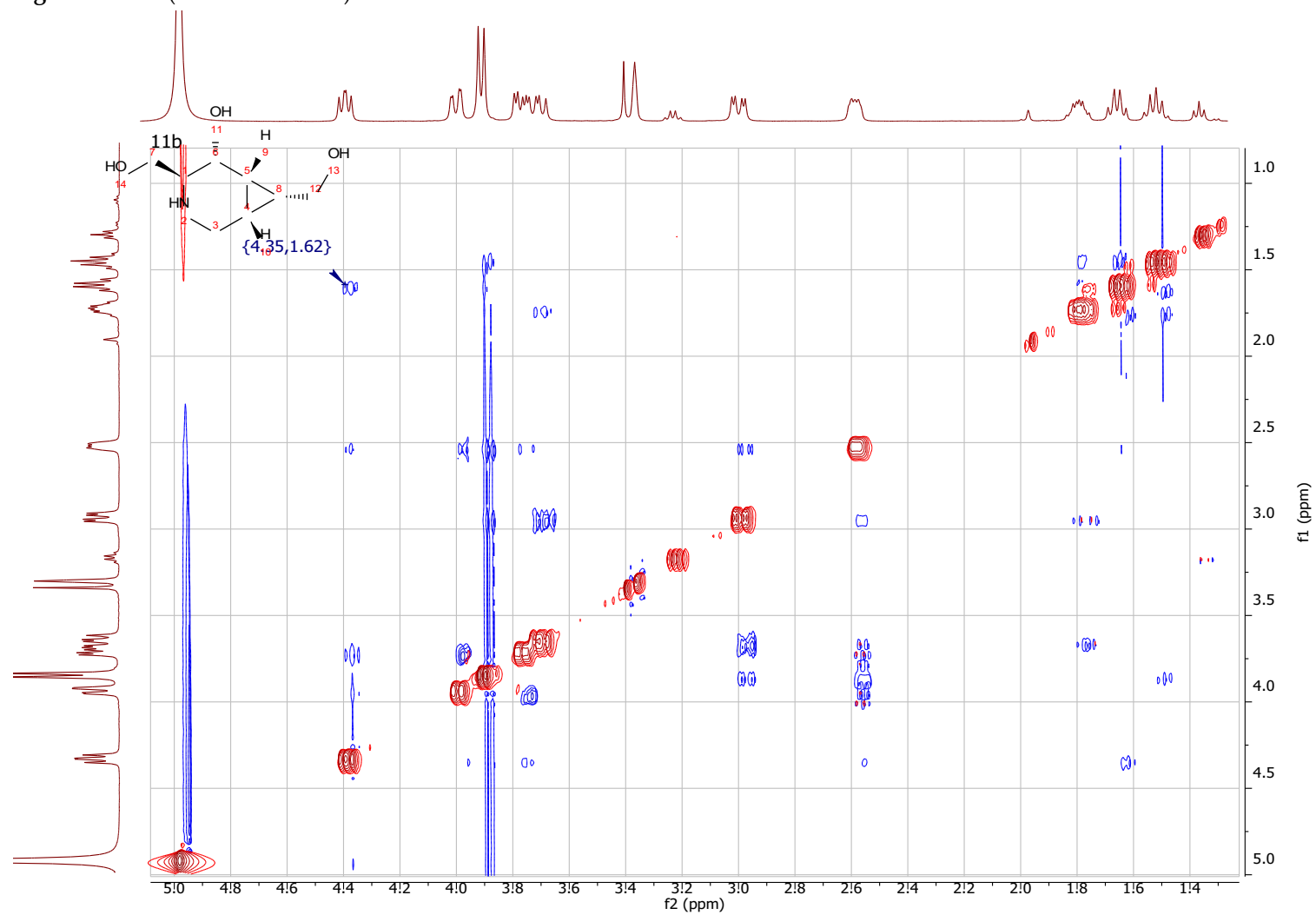
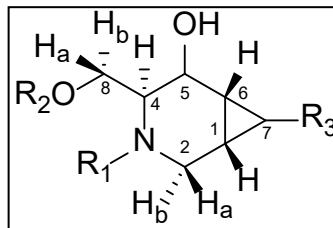


Table S1: Measured constant coupling from products derived from L-serine.



	3b	4b	7	10a	11a	8	28	10b	9	25b	11b
J_{8a-8b}	10.0	10.4		12.2				10.7	11.5	7.6	11.9
J_{8a-4}	2.9	2.7		8.5	6.4			5.4	5.7	7.6	5.1
J_{8b-4}	2.9	2.7		1.5	1.7			5.4	5.7	7.3	3.0
J_{4-5}				4.4	5.5			0	1.4		10.1
J_{5-6}			1.8					5.5	8.8	8.9	7.6
J_{6-7}	4.4	8.6	4.1	4.6	5.6	6.2	6.2	5.9	8.9	9.1	8.9
J_{6-1}		8.6	9.3				8.0	8.3	8.9	9.1	8.9
J_{7-1}	4.4	8.6	4.1	4.6	5.6	8.5	8.0	8.4			8.4
J_{1-2a}	1.9	3.2			8.3		8.0	8.7	5.3		9.6
J_{1-2b}	0	0		0	2.4		2.5	6.4	0	0	5.0
J_{2a-2b}	13.5	13.4		13.5	13.7		14.5	14.7	14.2	14.1	14

