

Supporting Information

Lewis Acid-Mediated Synthesis of Mono- and Tris-Indole Adducts from Chiral Aziridines

Lingamurthy Macha, Deepak Singh, Hyong-Jin Rhee and Hyun-Joon Ha*

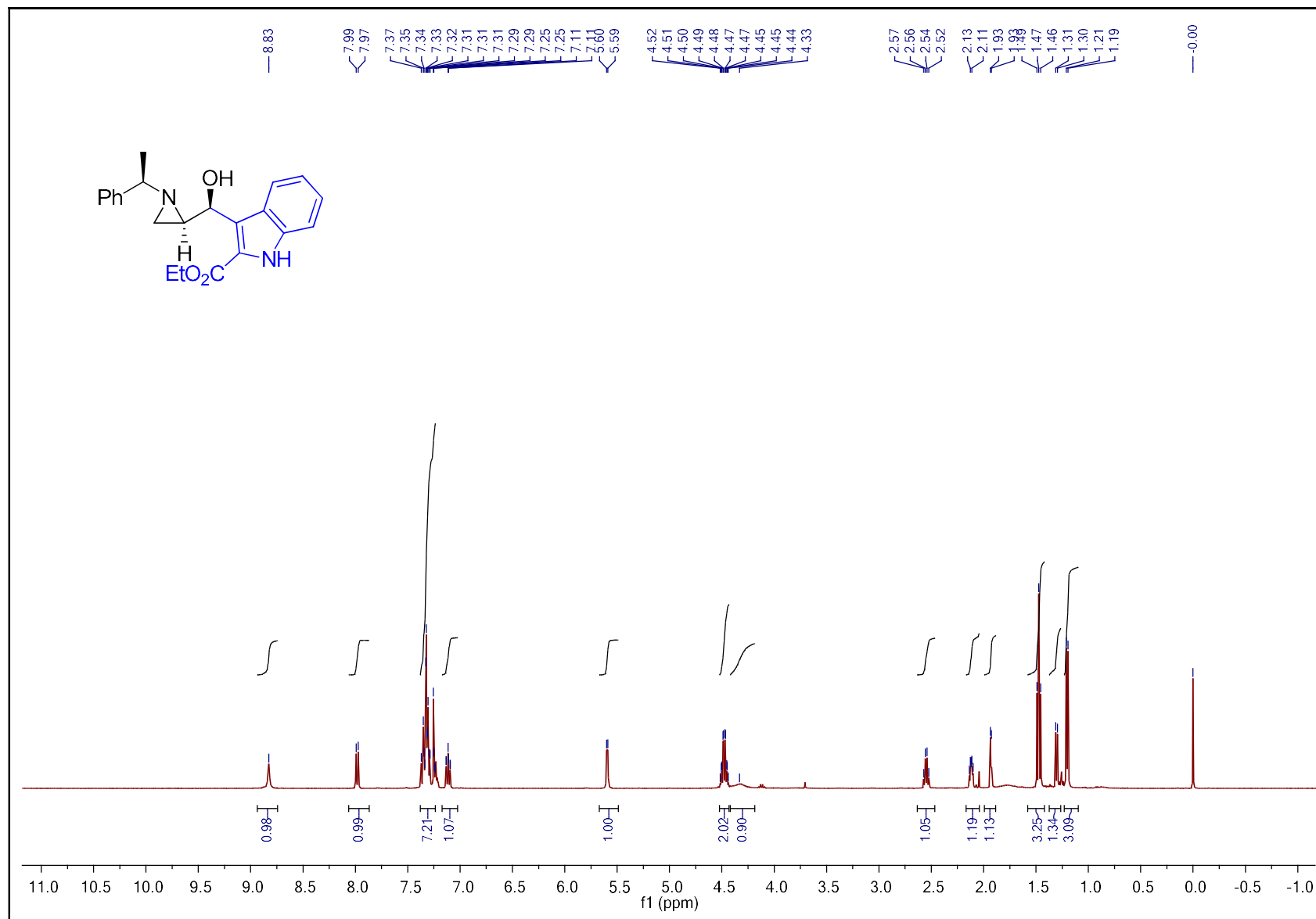
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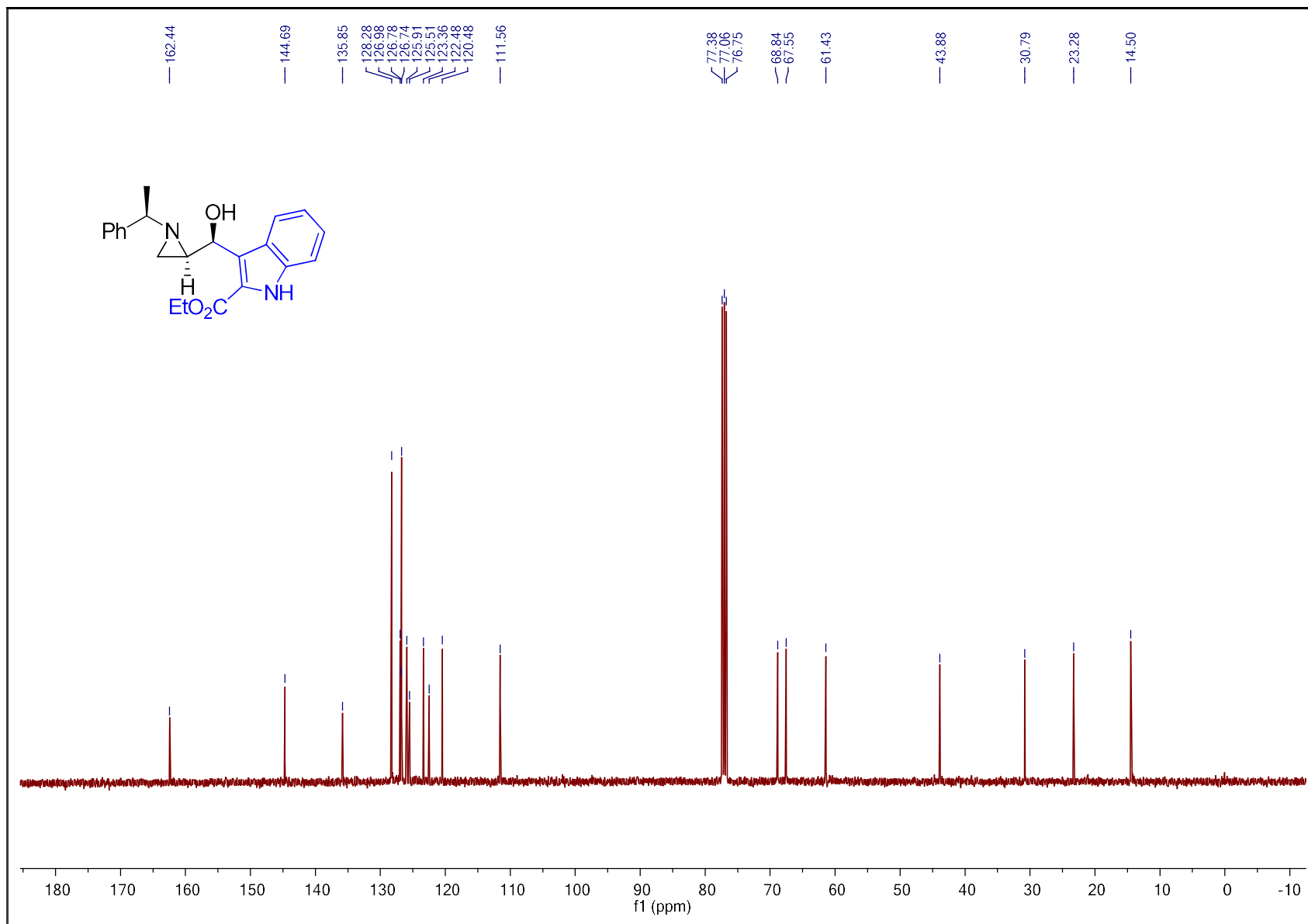
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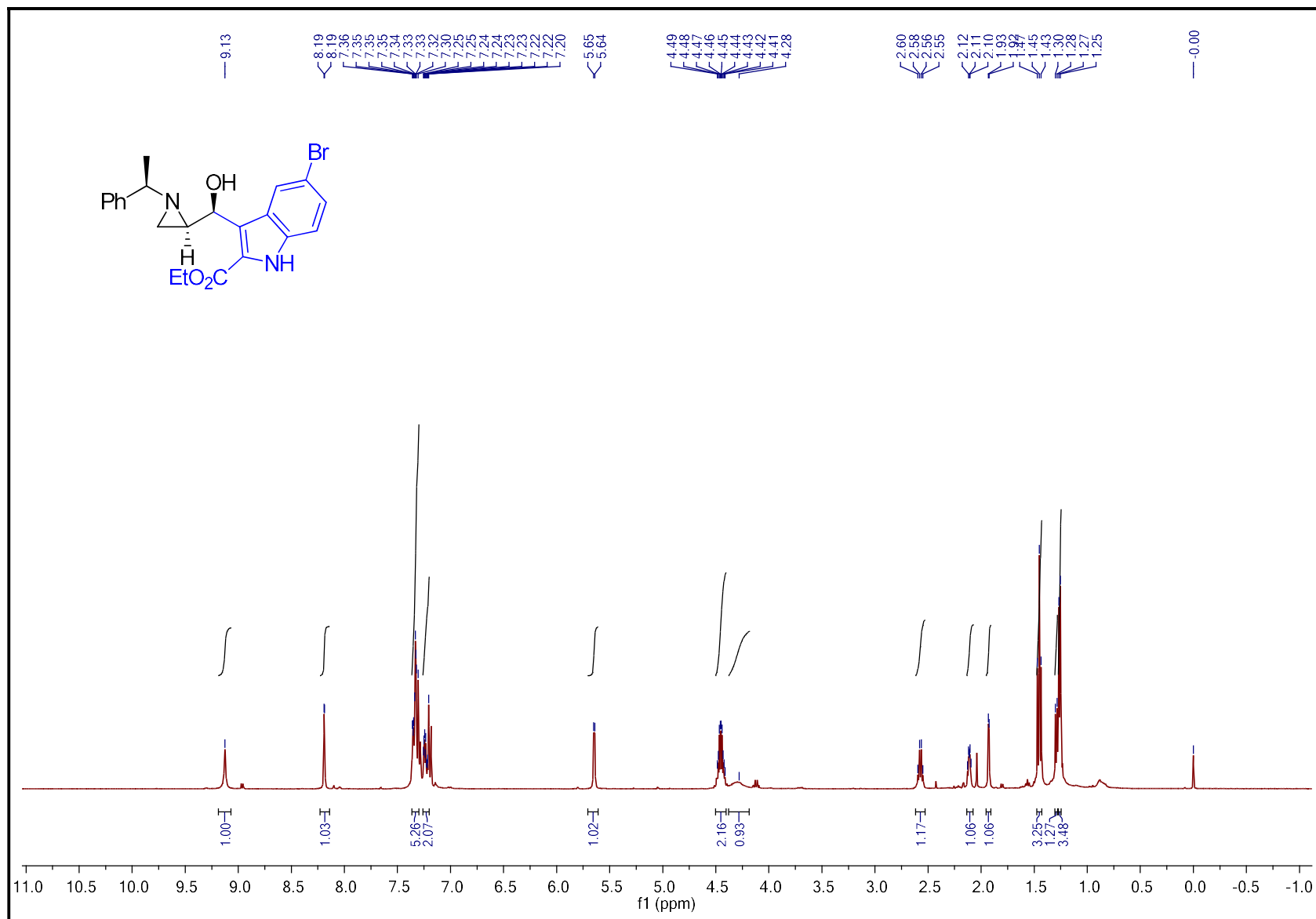
¹H NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4aa):



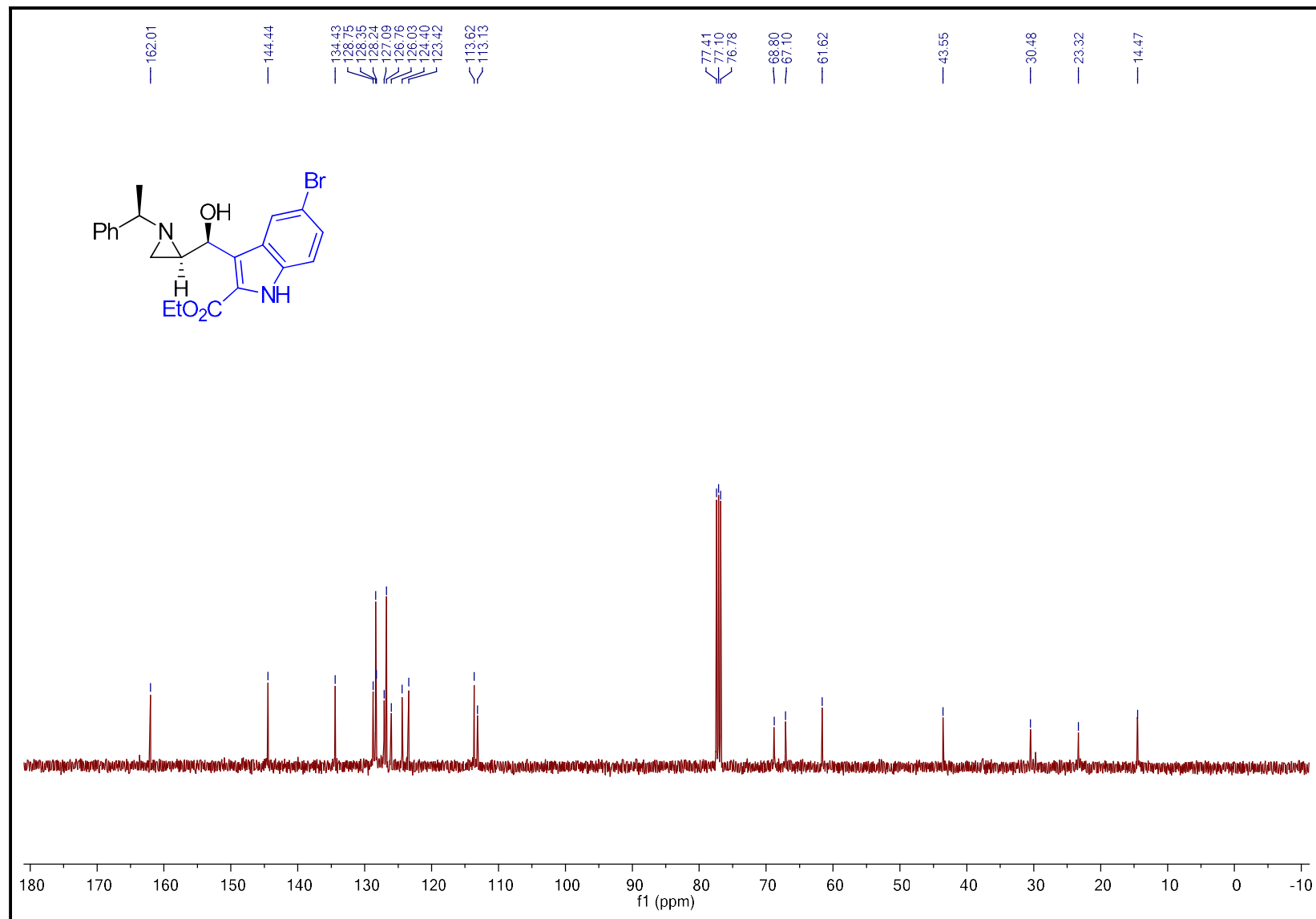
¹³C NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4aa):



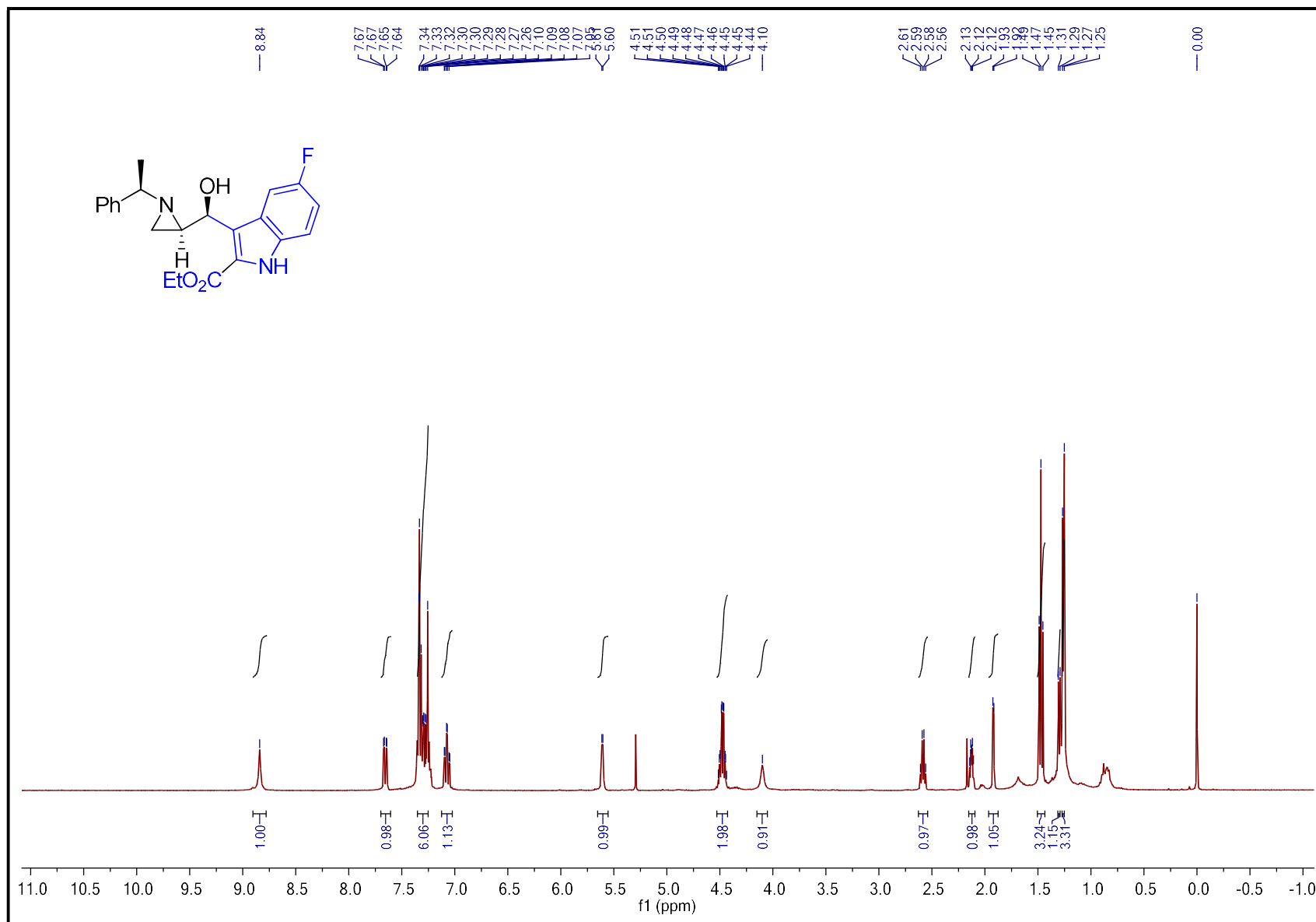
¹H NMR spectrum of Ethyl 5-bromo-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ab):



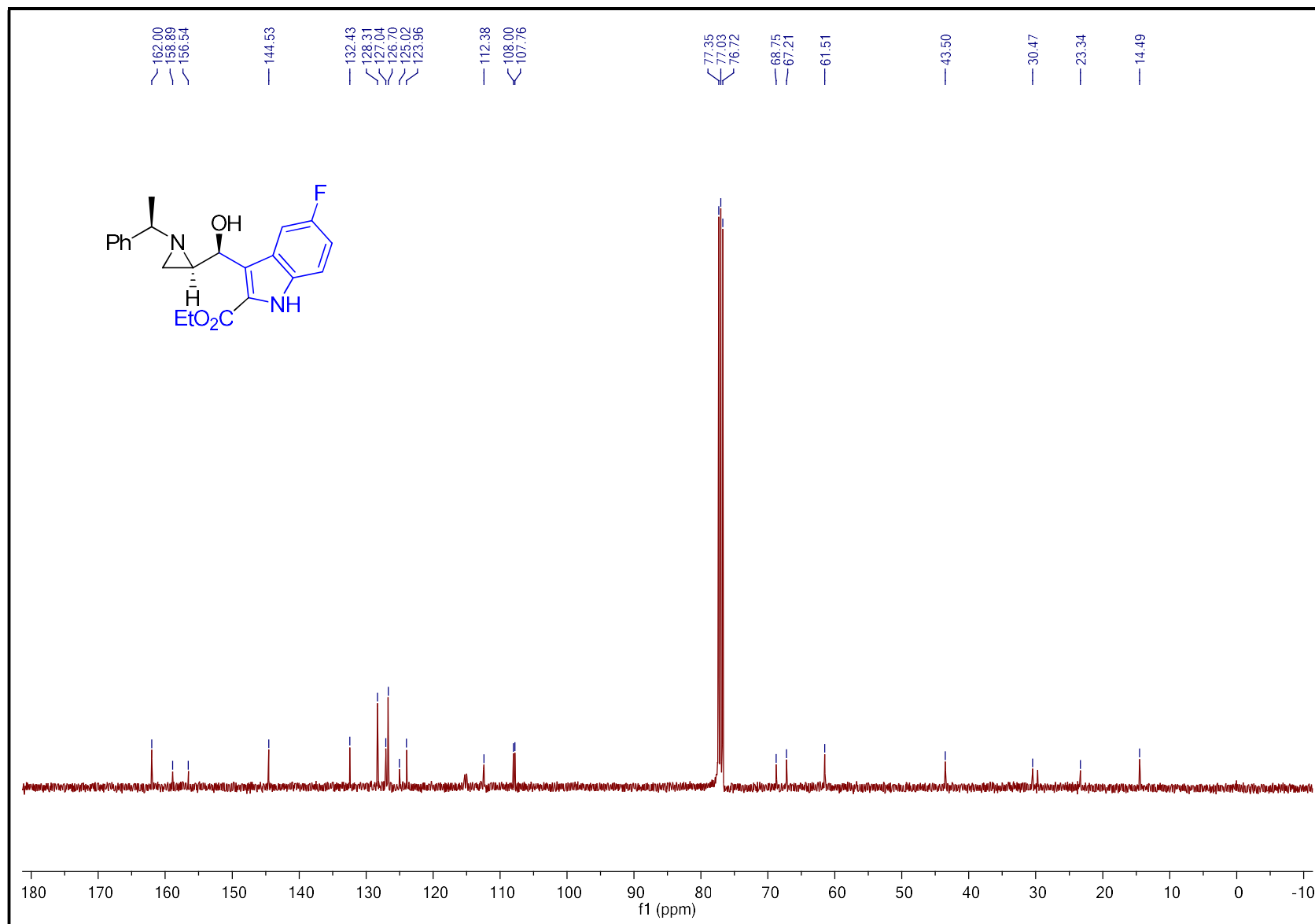
¹³C NMR spectrum of Ethyl 5-bromo-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ab):



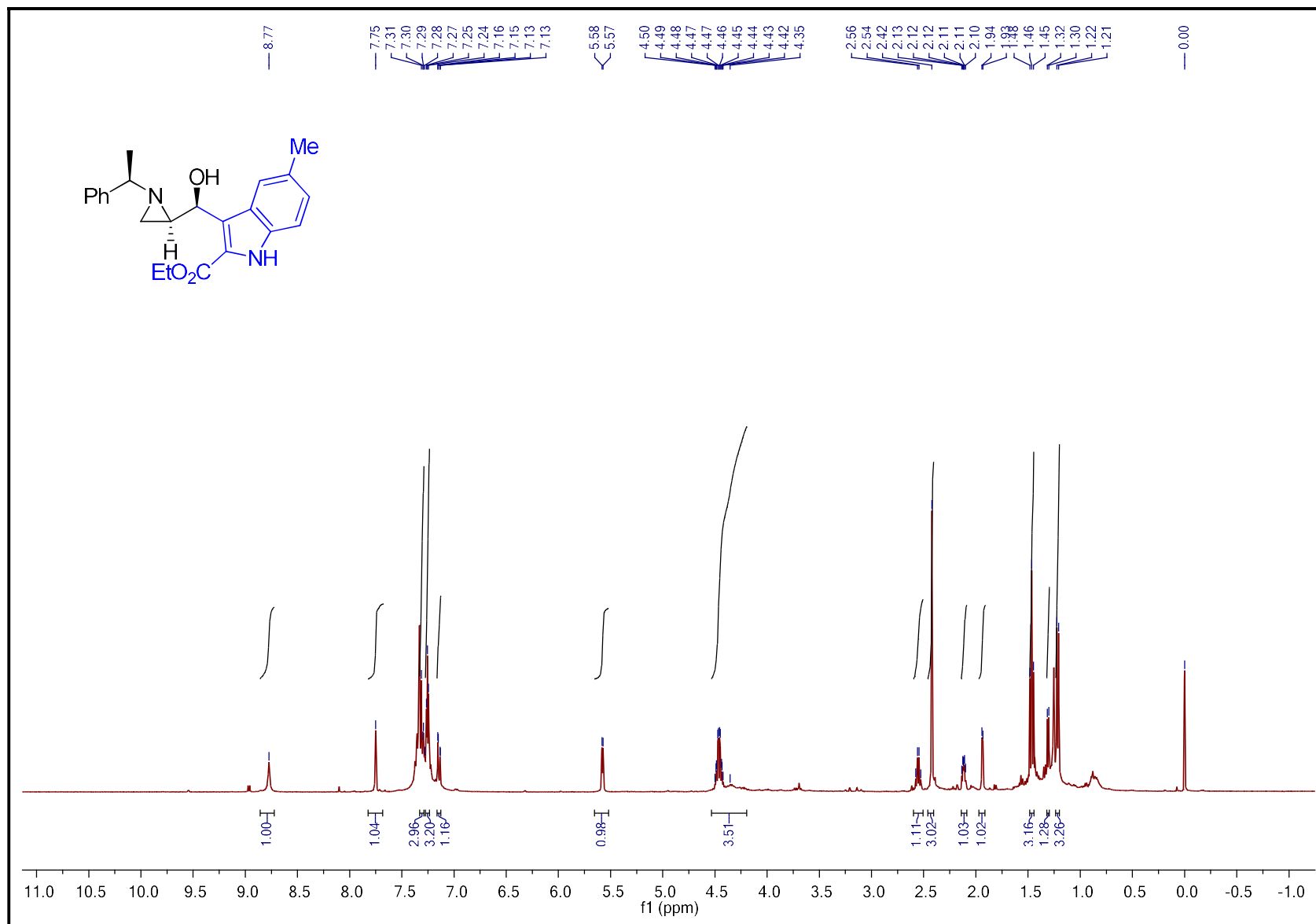
¹H NMR spectrum of Ethyl 5-fluoro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ac):



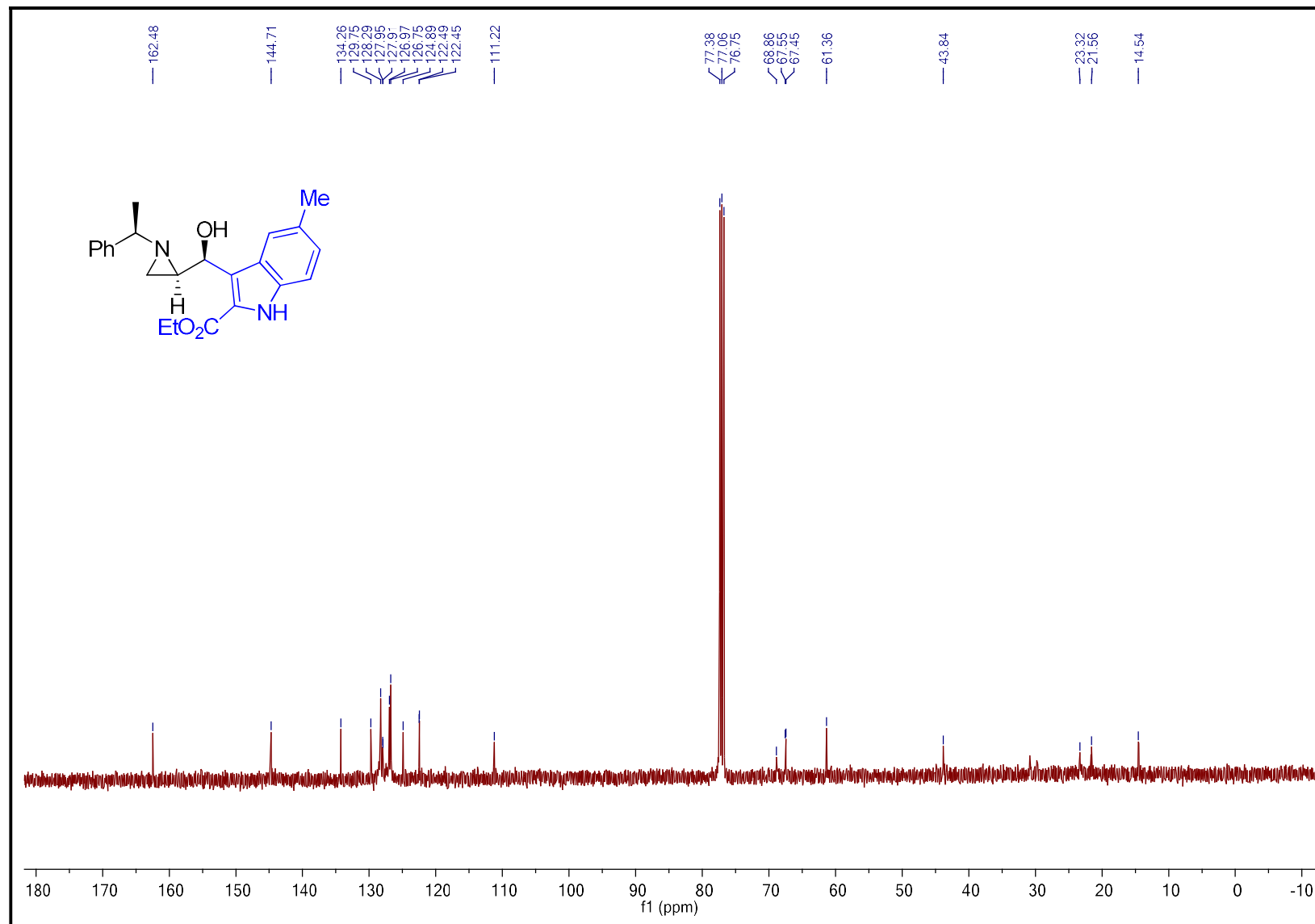
¹³C NMR spectrum of Ethyl 5-fluoro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ac):



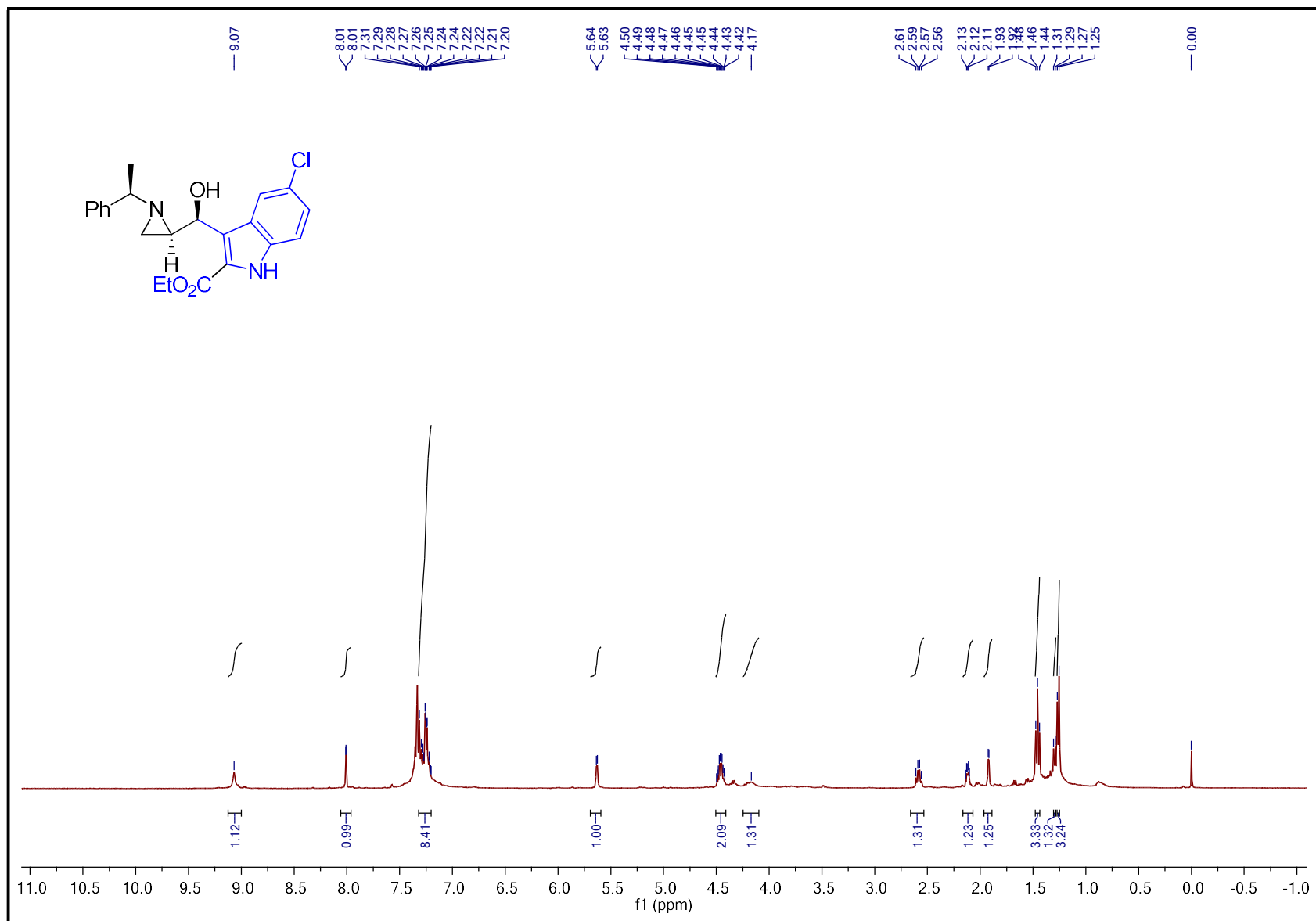
¹H NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-5-methyl-1H-indole-2-carboxylate (4ad):



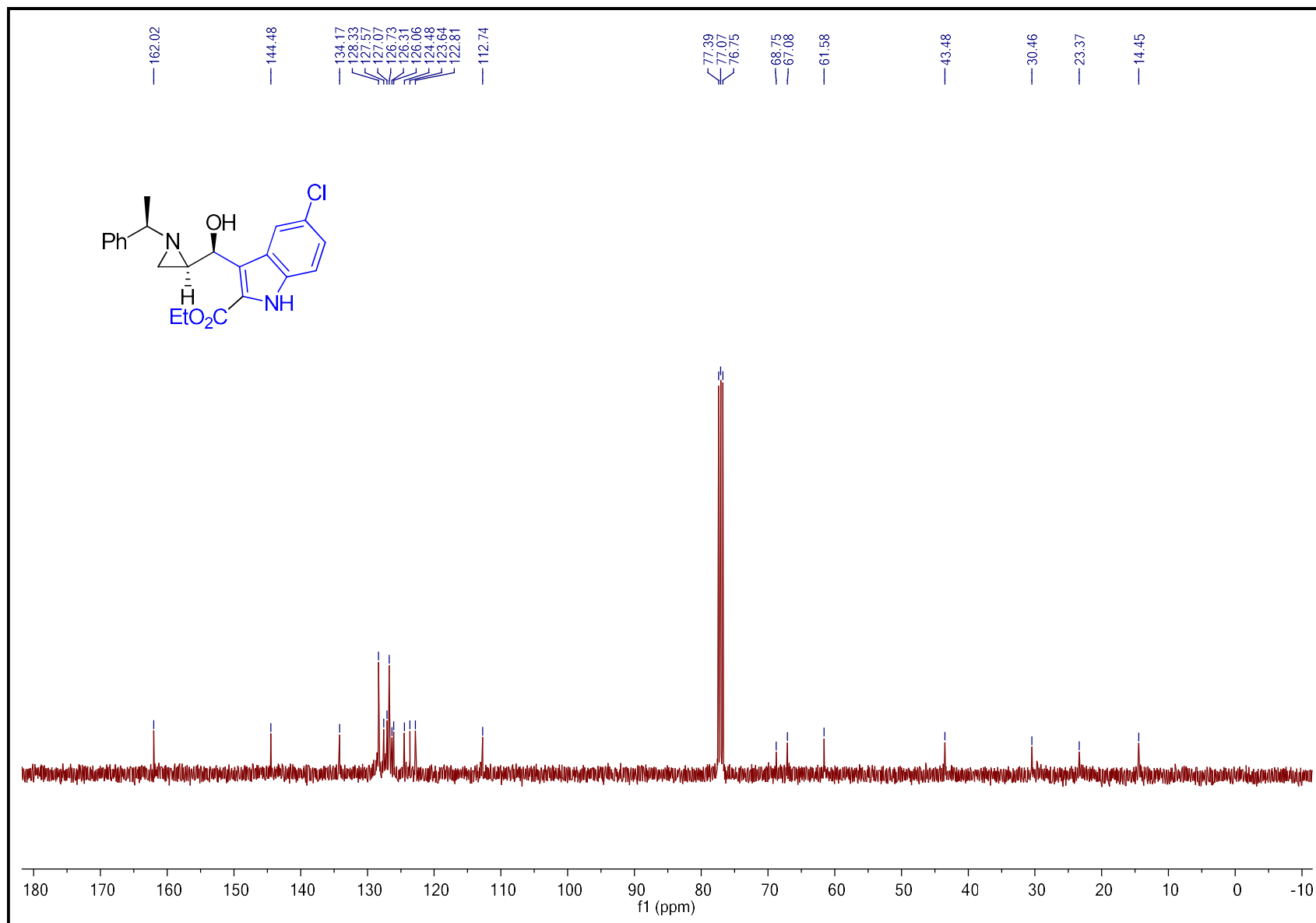
¹³C NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-5-methyl-1H-indole-2-carboxylate (4ad):



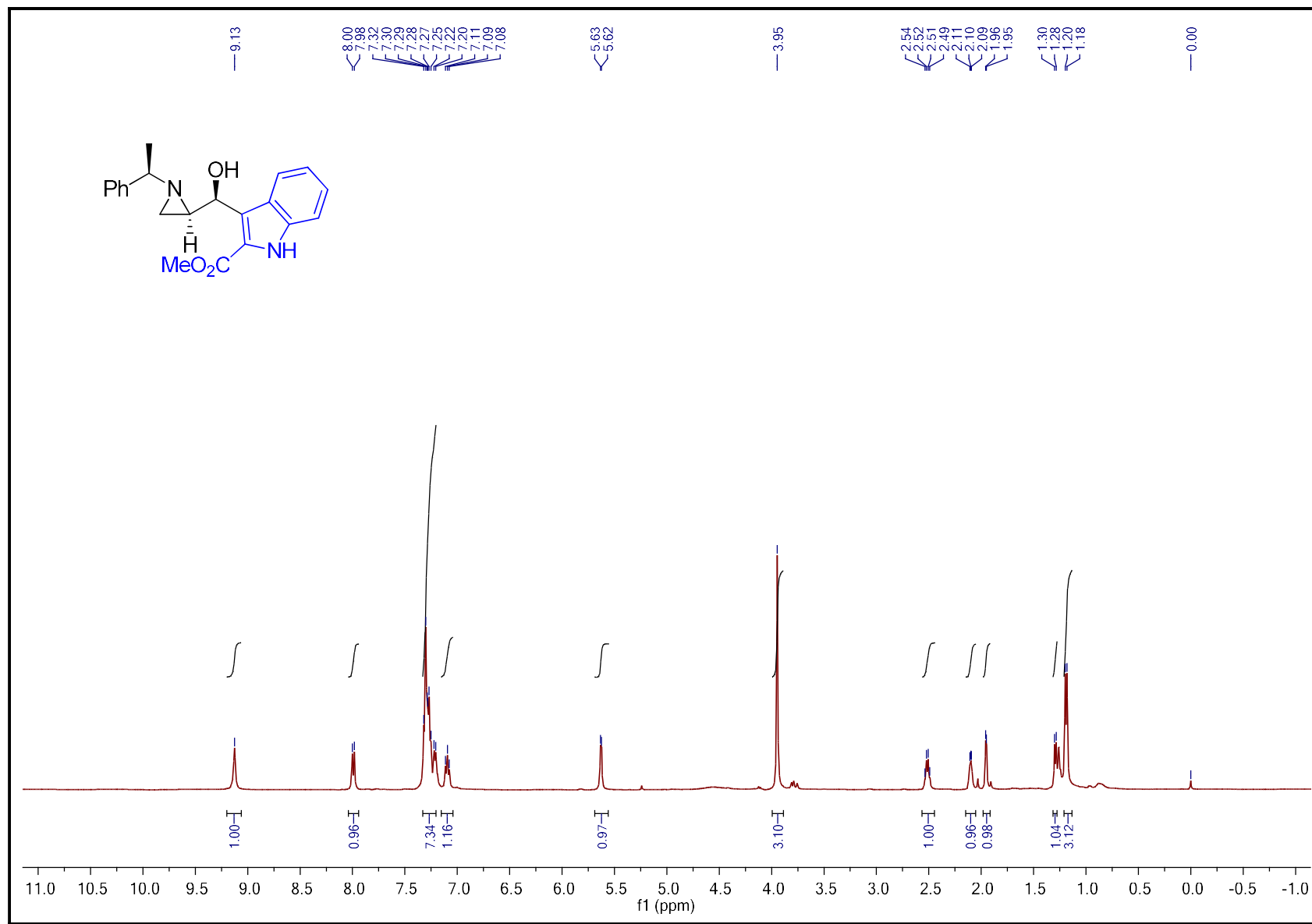
¹H NMR spectrum of Ethyl 5-chloro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ae):



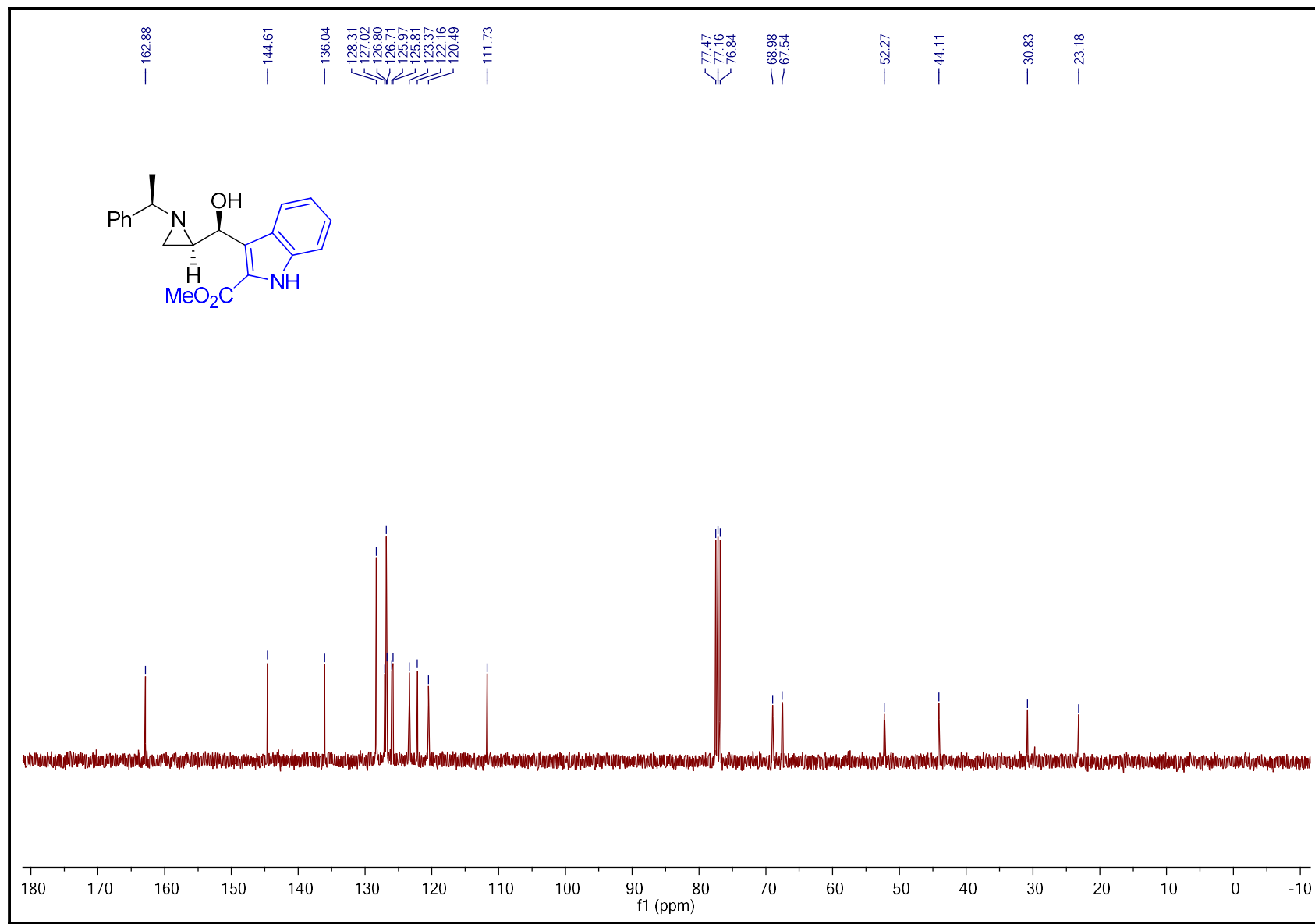
¹³C NMR spectrum of Ethyl 5-chloro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ae):



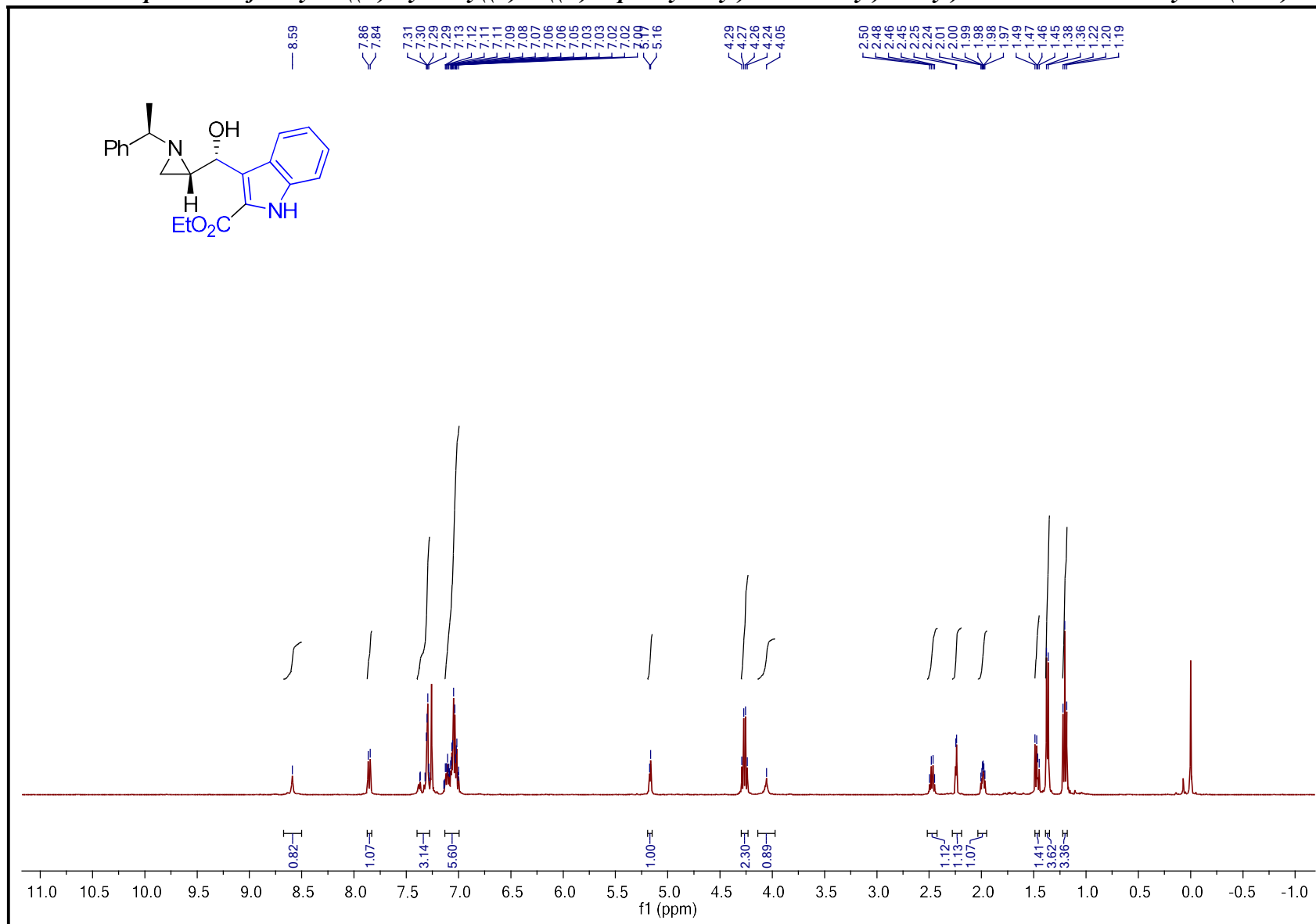
¹H NMR spectrum of Methyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4af):



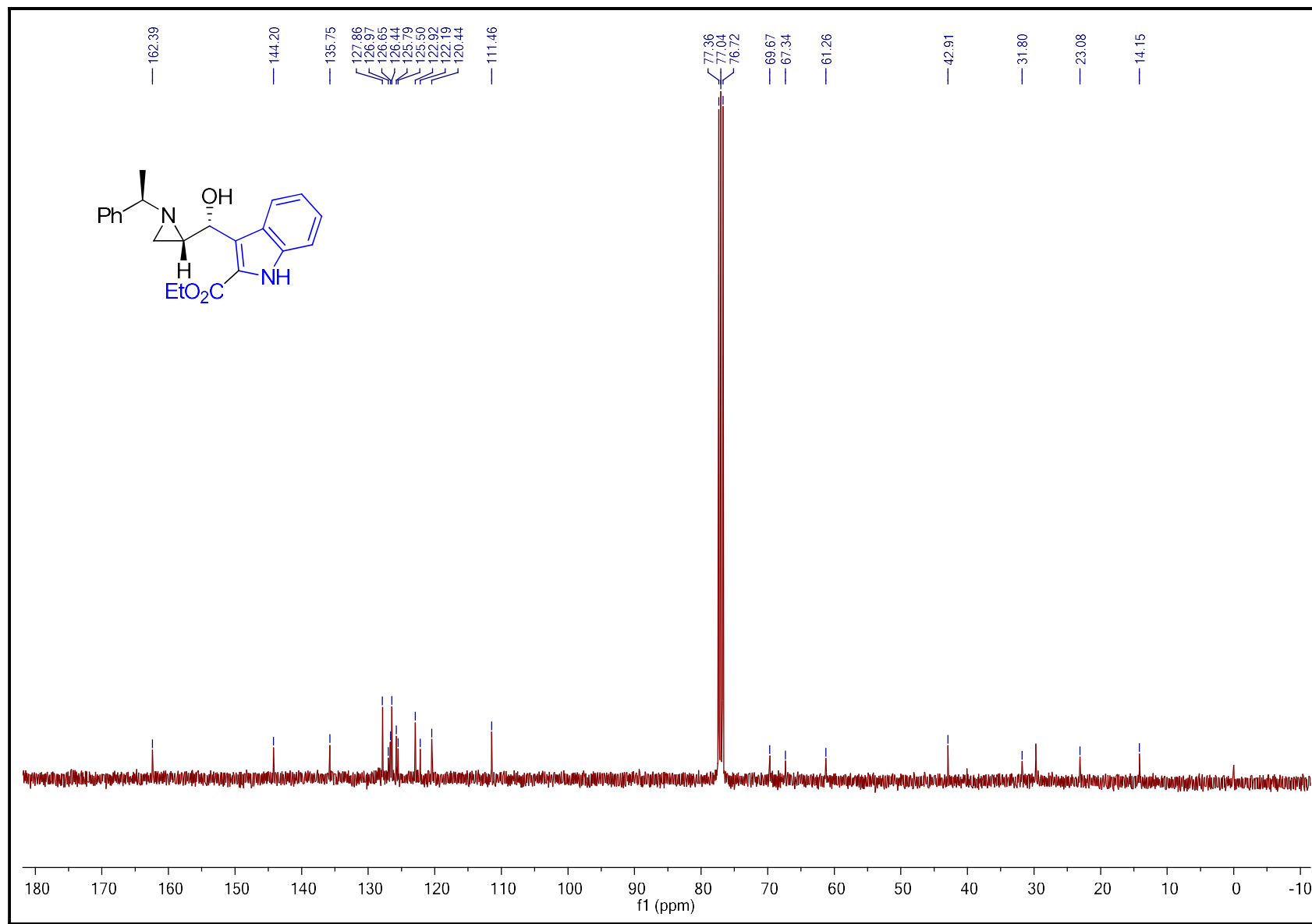
¹³C NMR spectrum of Methyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4af):



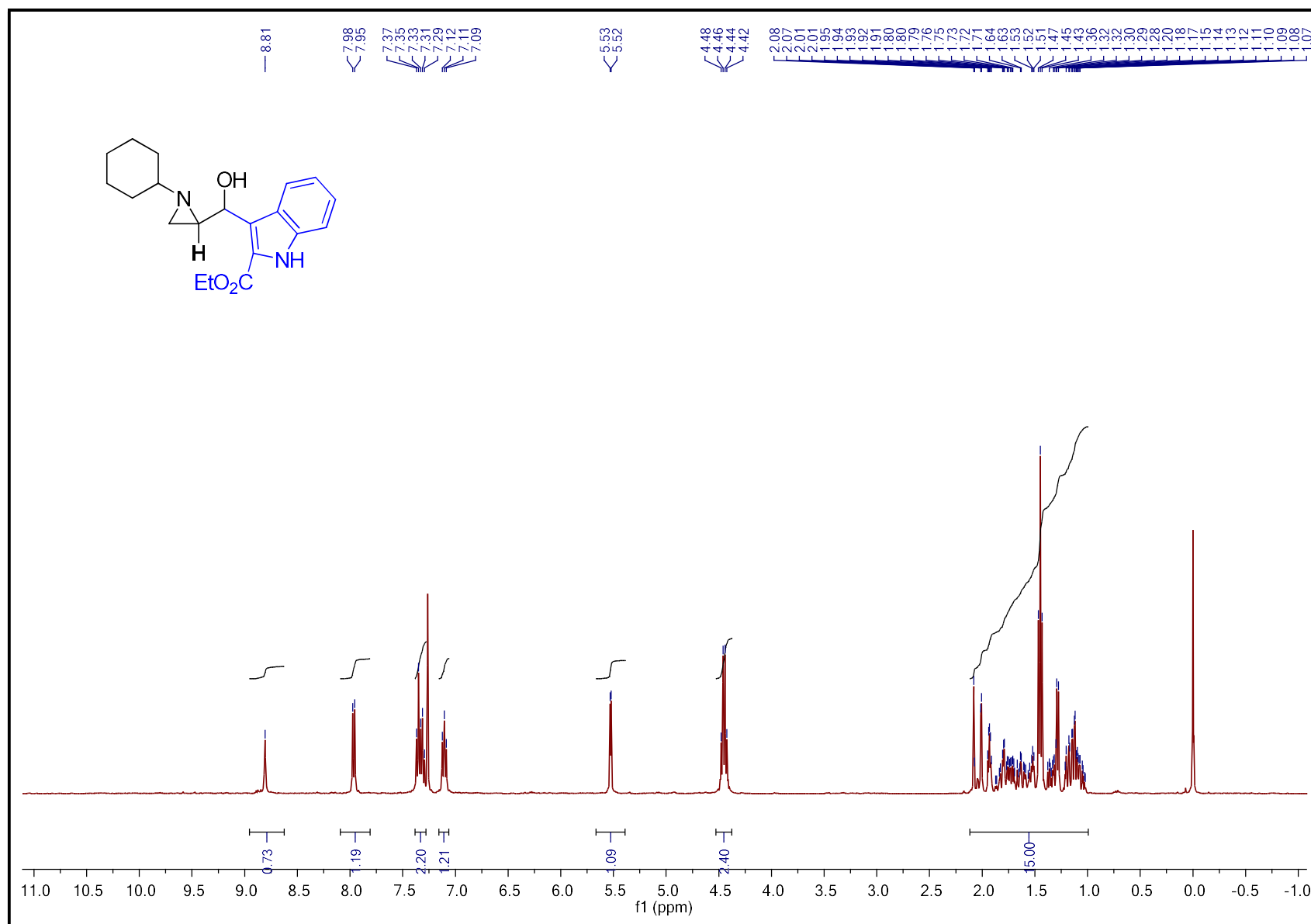
¹H NMR spectrum of Ethyl 3-((R)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4a'a):



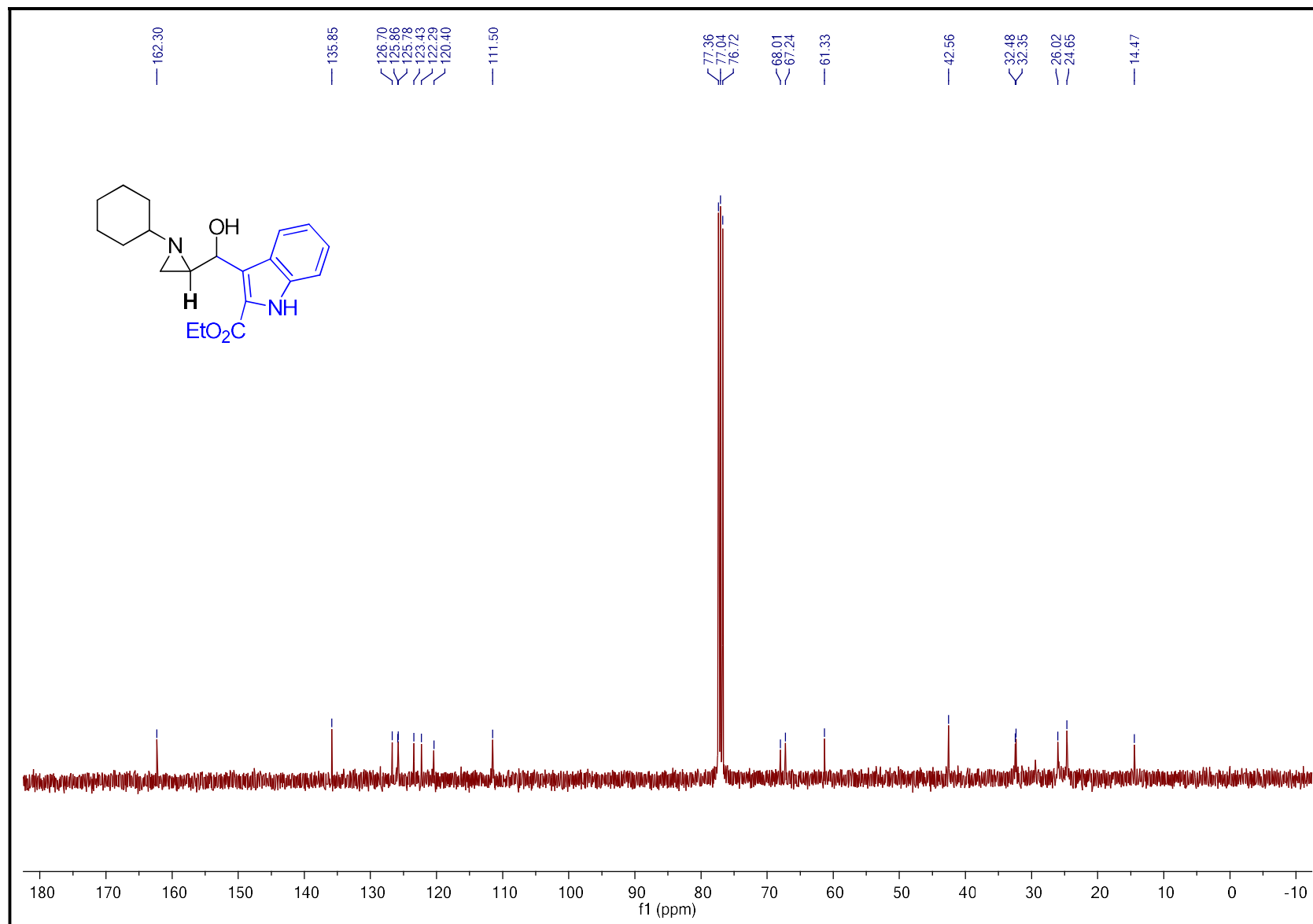
¹³C NMR spectrum of Ethyl 3-((R)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4a'a):



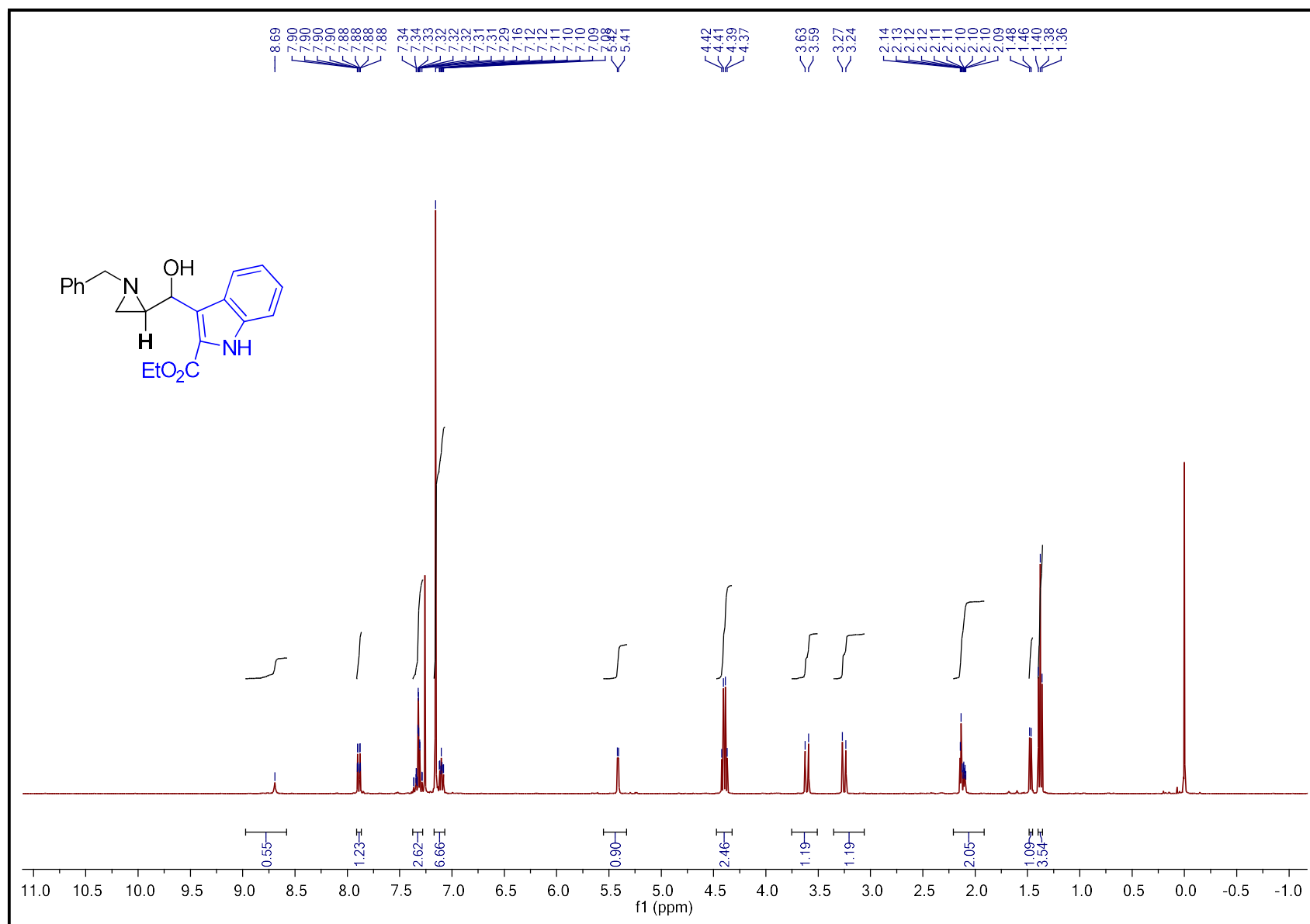
¹H NMR spectrum of Ethyl 3-((1-cyclohexylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ba):



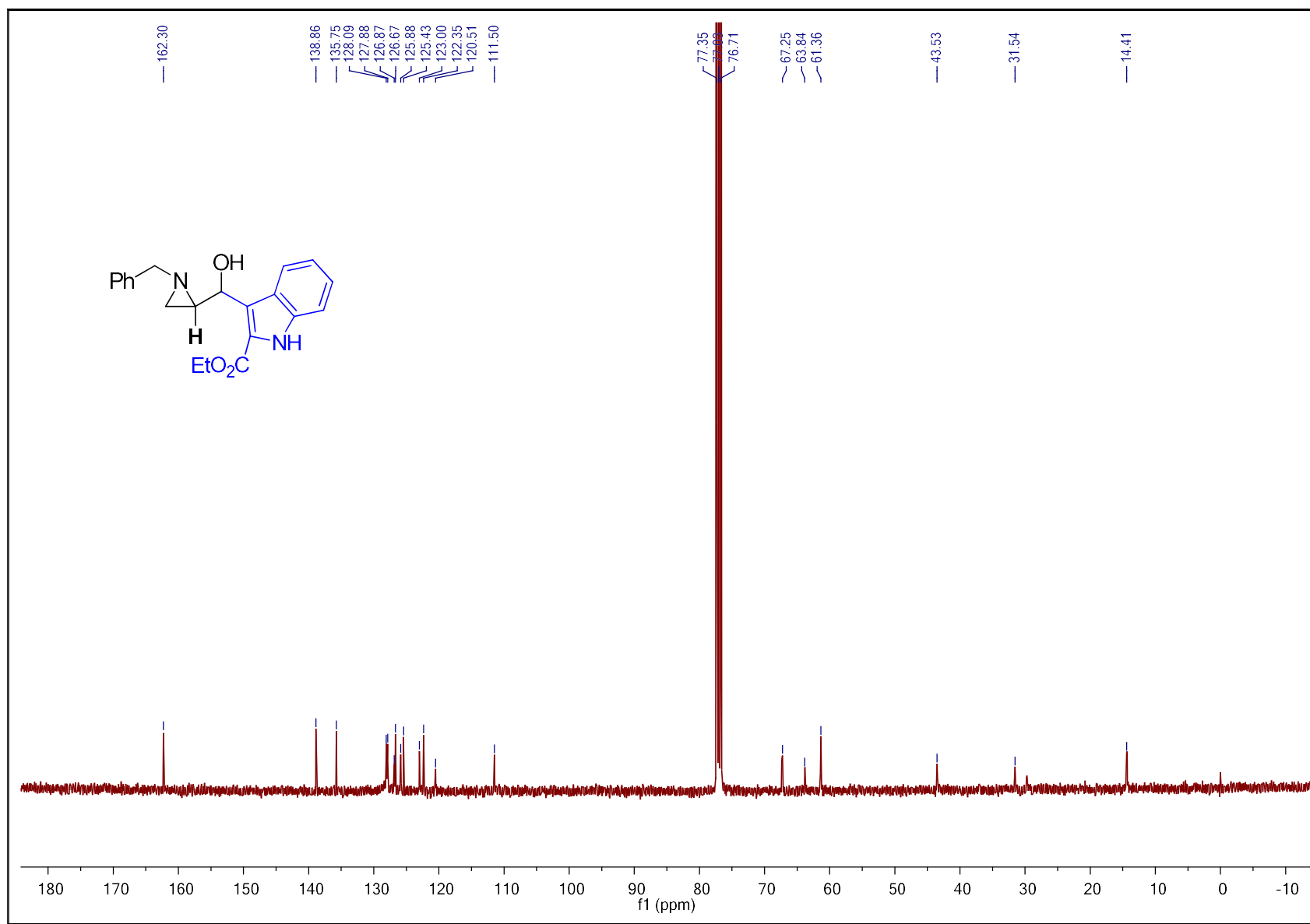
¹³C NMR spectrum of Ethyl 3-((1-cyclohexylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ba):



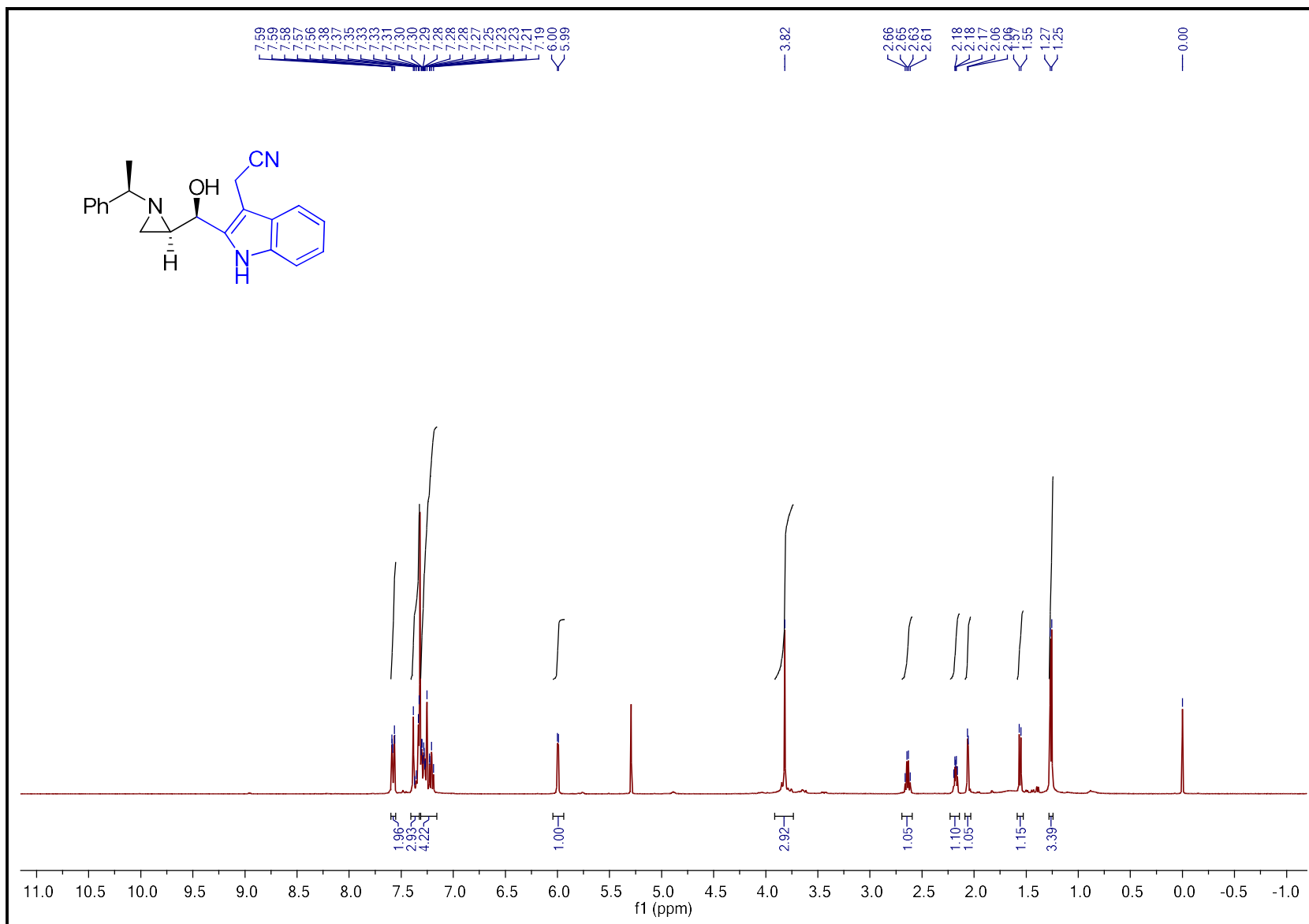
¹H NMR spectrum of Ethyl 3-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ca):



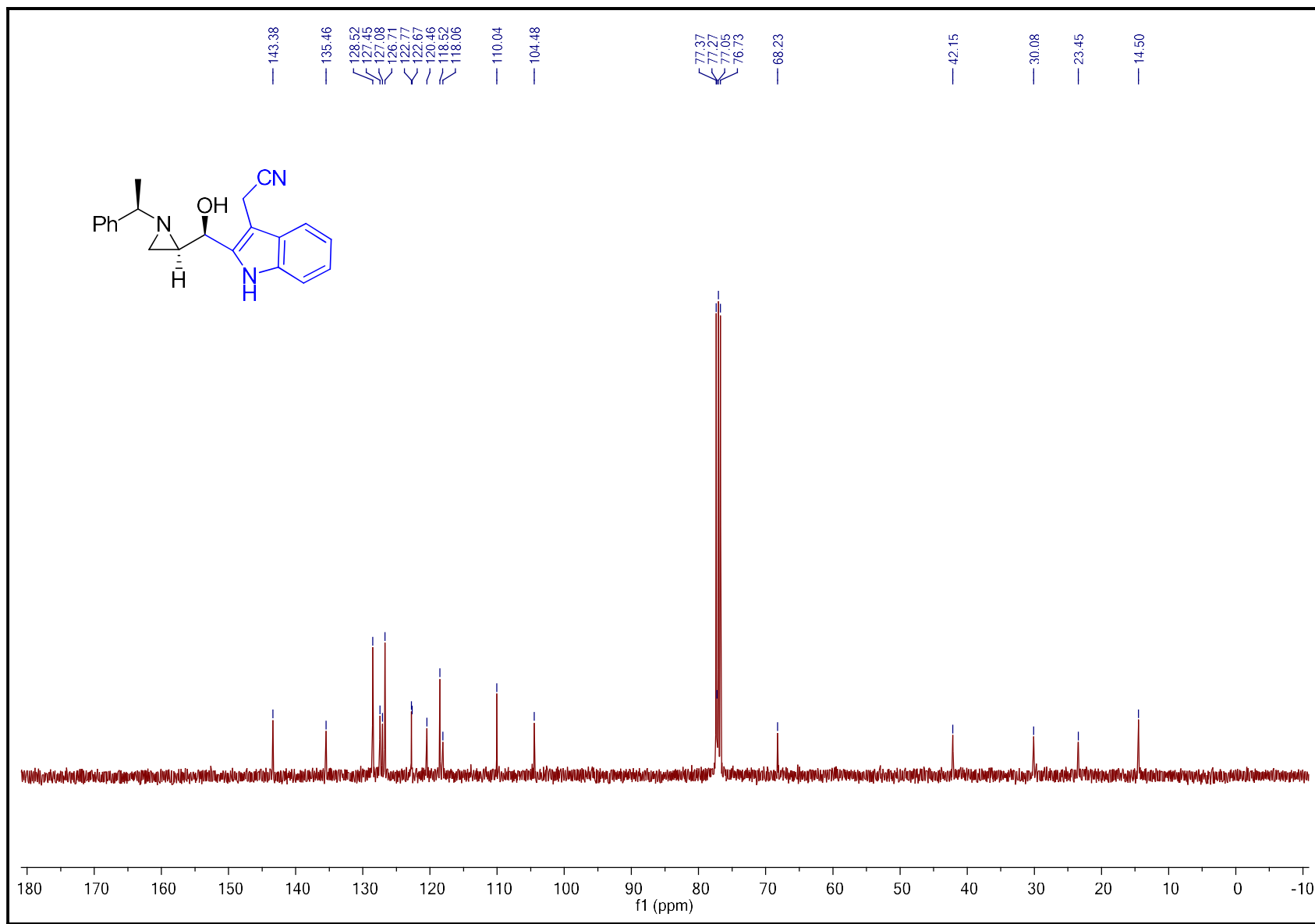
¹³C NMR spectrum of Ethyl 3-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ca):



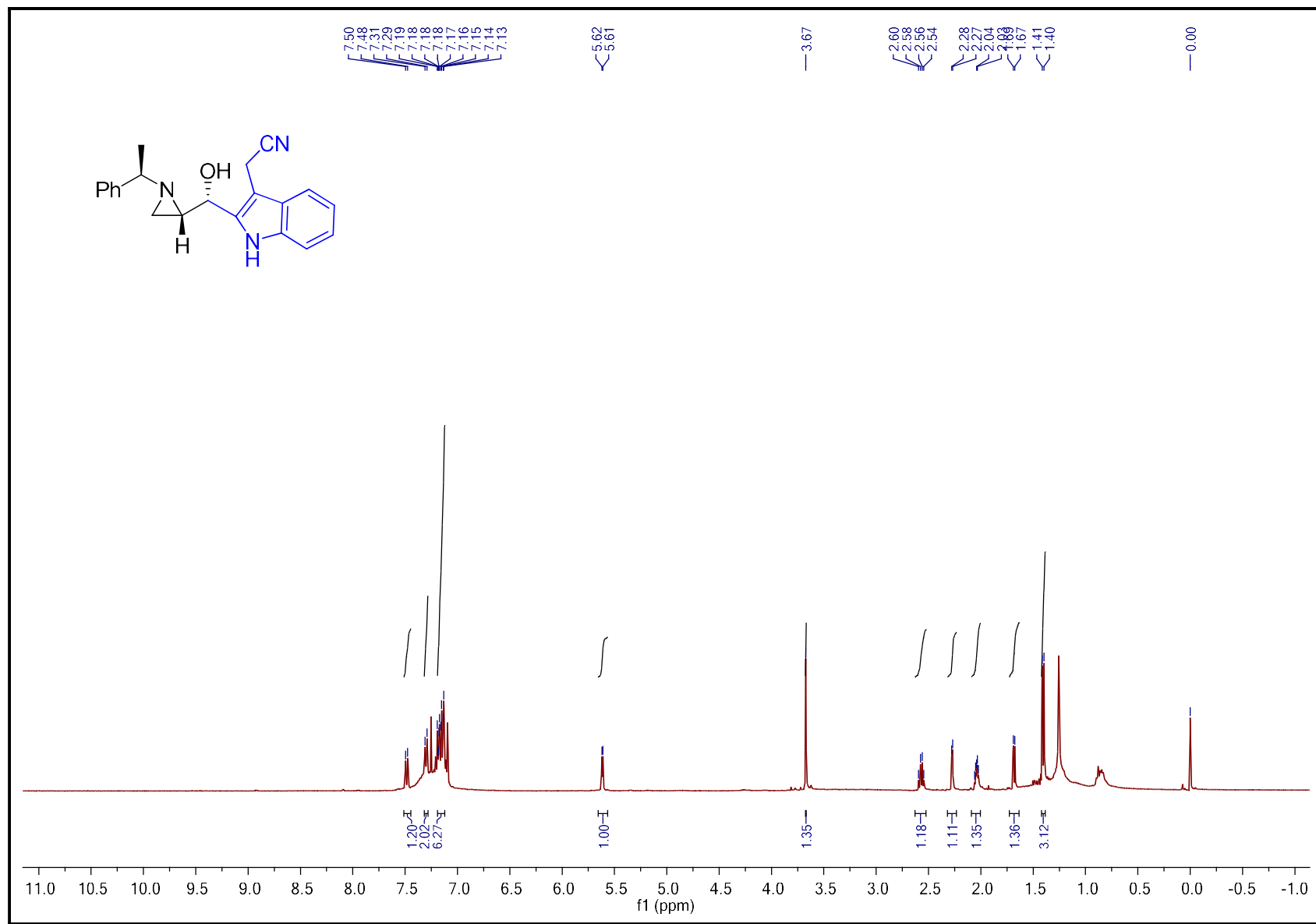
¹H NMR spectrum of 2-(2-((R)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4ag):



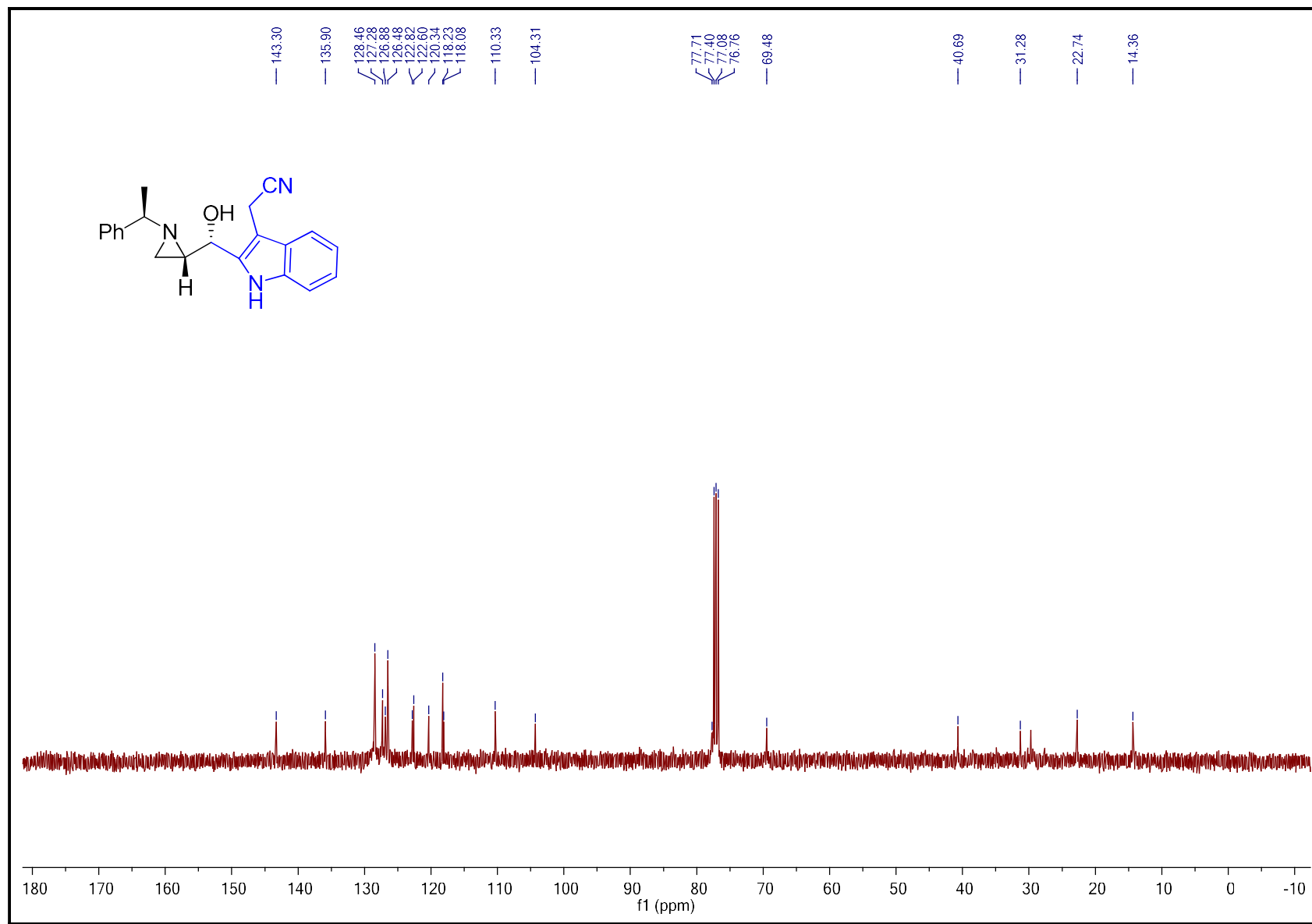
¹³C NMR spectrum of 2-(2-((R)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4ag):



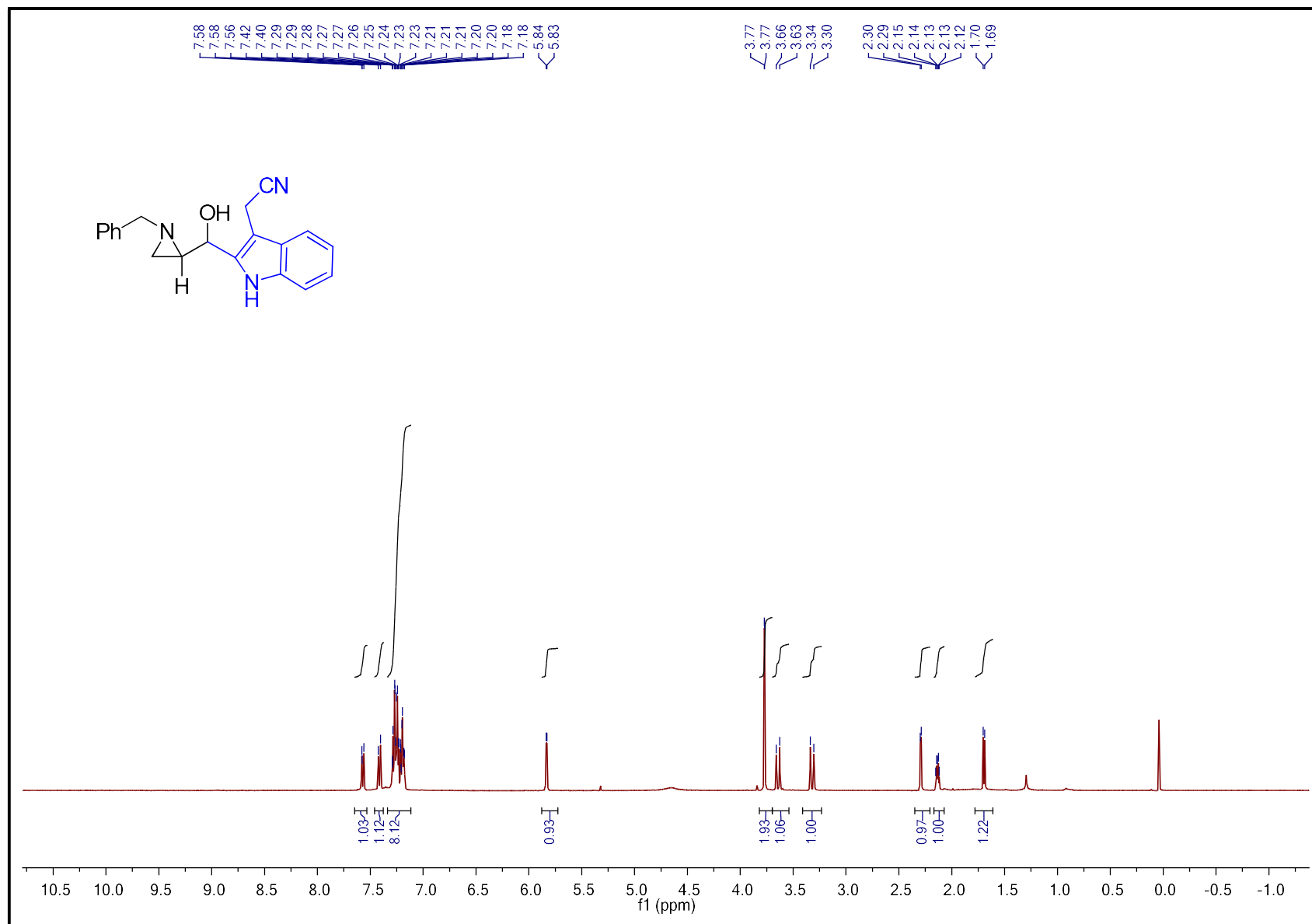
¹H NMR spectrum of 2-(2-((S)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4a''g):



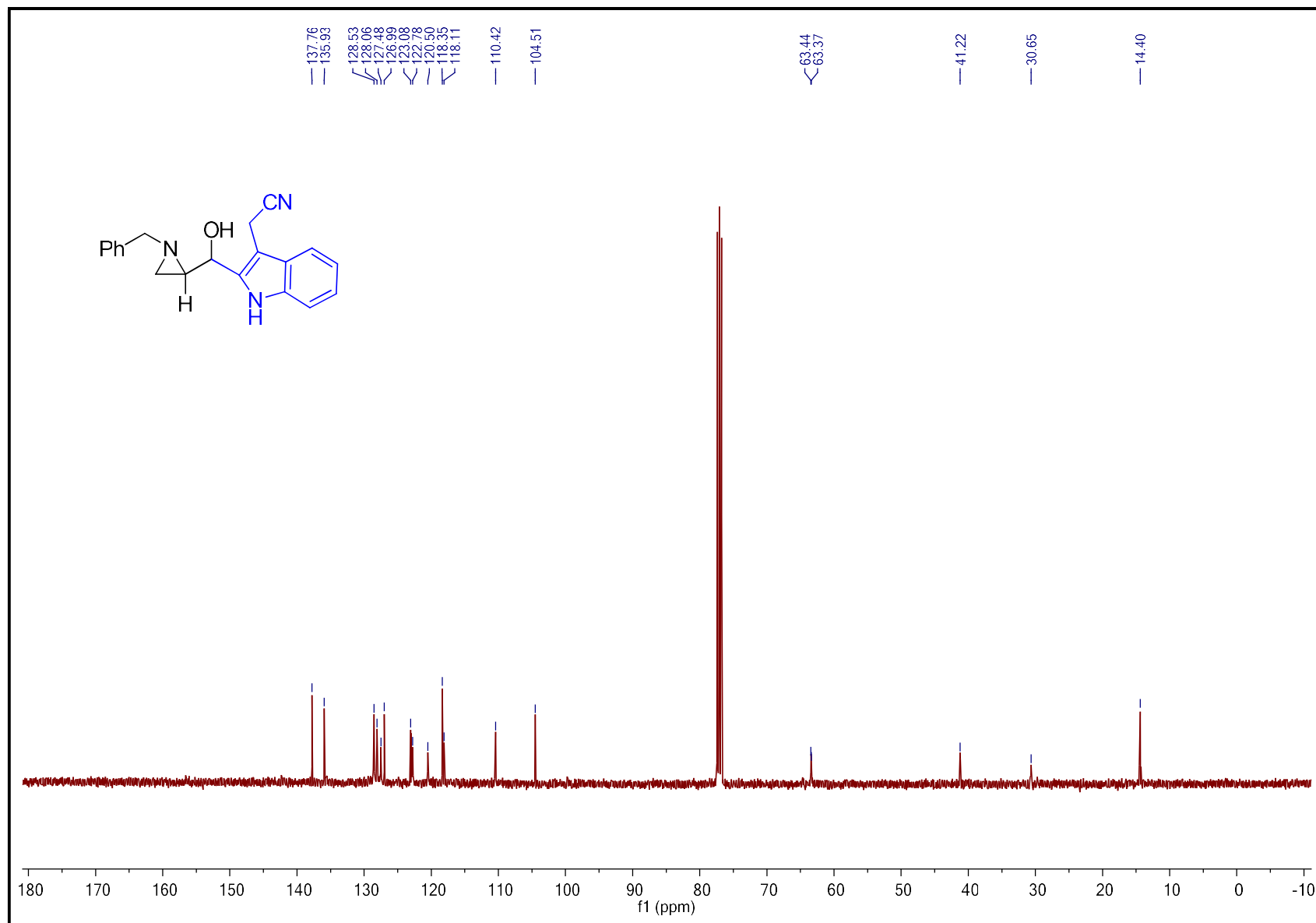
¹³C NMR spectrum of 2-(2-((S)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4a''g):



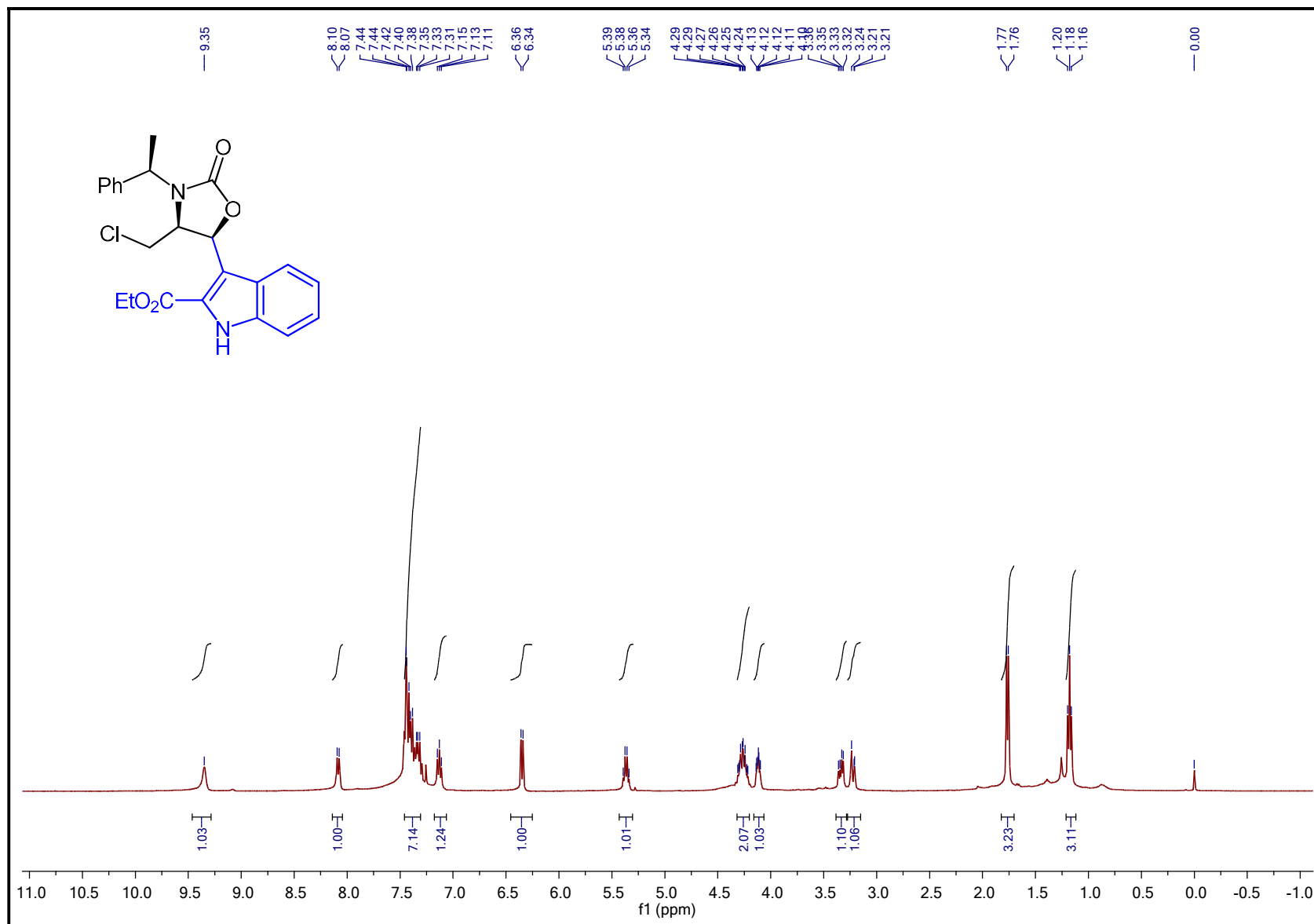
¹H NMR spectrum of 2-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indol-3-yl)acetonitrile (4cg):



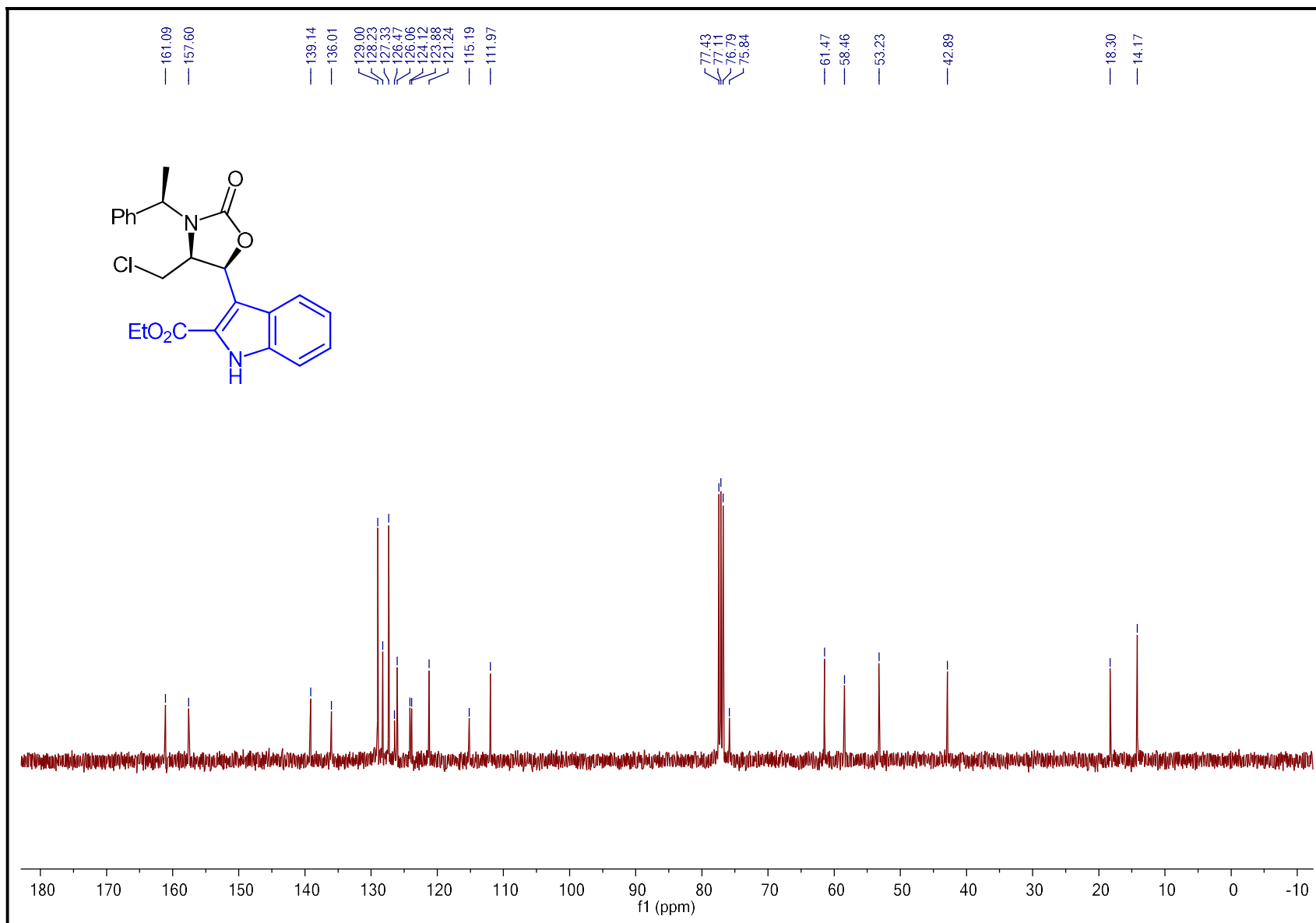
¹³C NMR spectrum of 2-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indol-3-yl)acetonitrile (4cg):



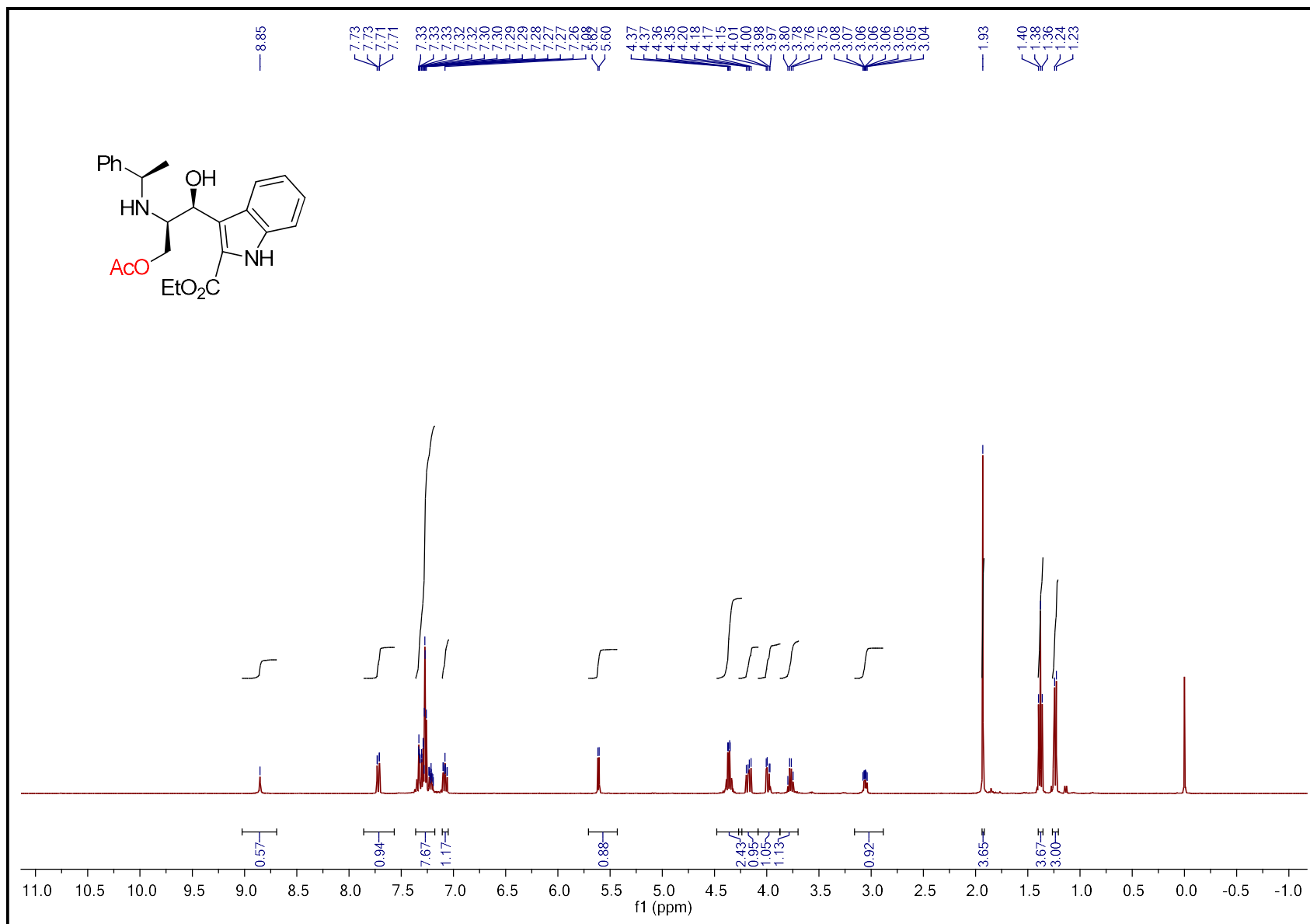
¹H NMR spectrum of Ethyl 3-((4S,5S)-4-(chloromethyl)-2-oxo-3-((R)-1-phenylethyl)oxazolidin-5-yl)-1H-indole-2-carboxylate (7):



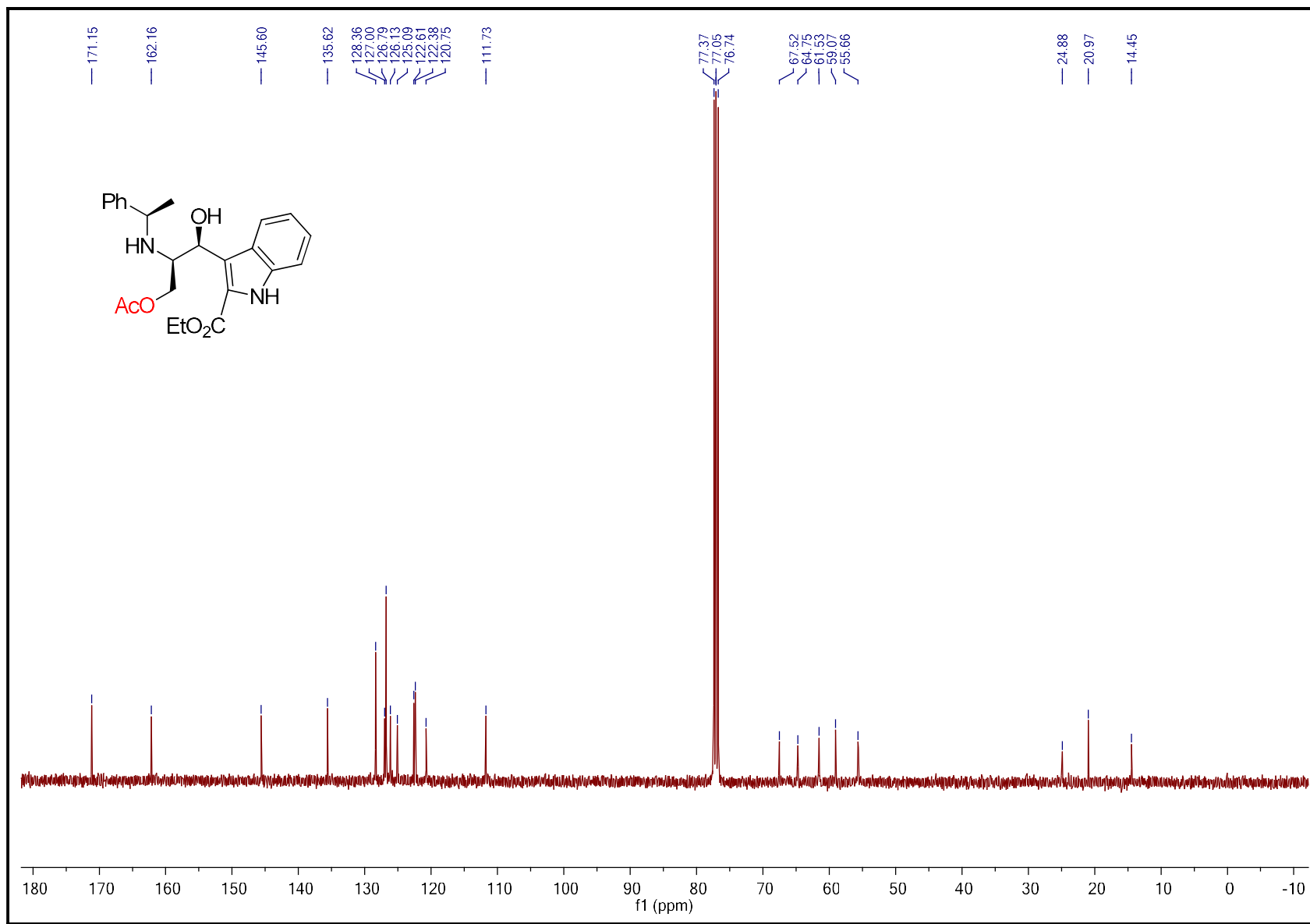
¹³C NMR spectrum of Ethyl 3-((4*S*,5*S*)-4-(chloromethyl)-2-oxo-3-((*R*)-1-phenylethyl)oxazolidin-5-yl)-1*H*-indole-2-carboxylate (7):



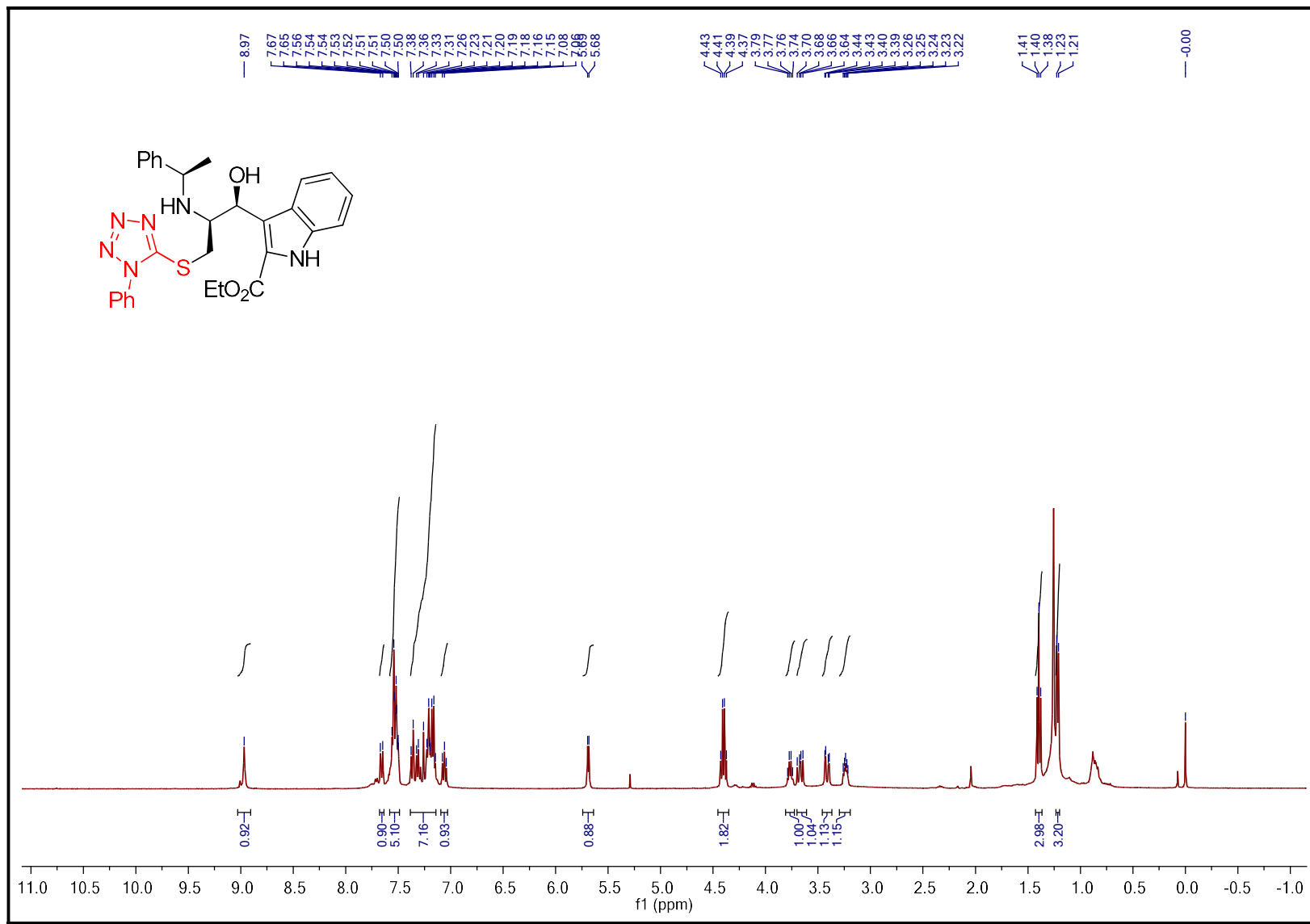
¹H NMR spectrum of Ethyl 3-((1S,2R)-3-acetoxy-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (8):



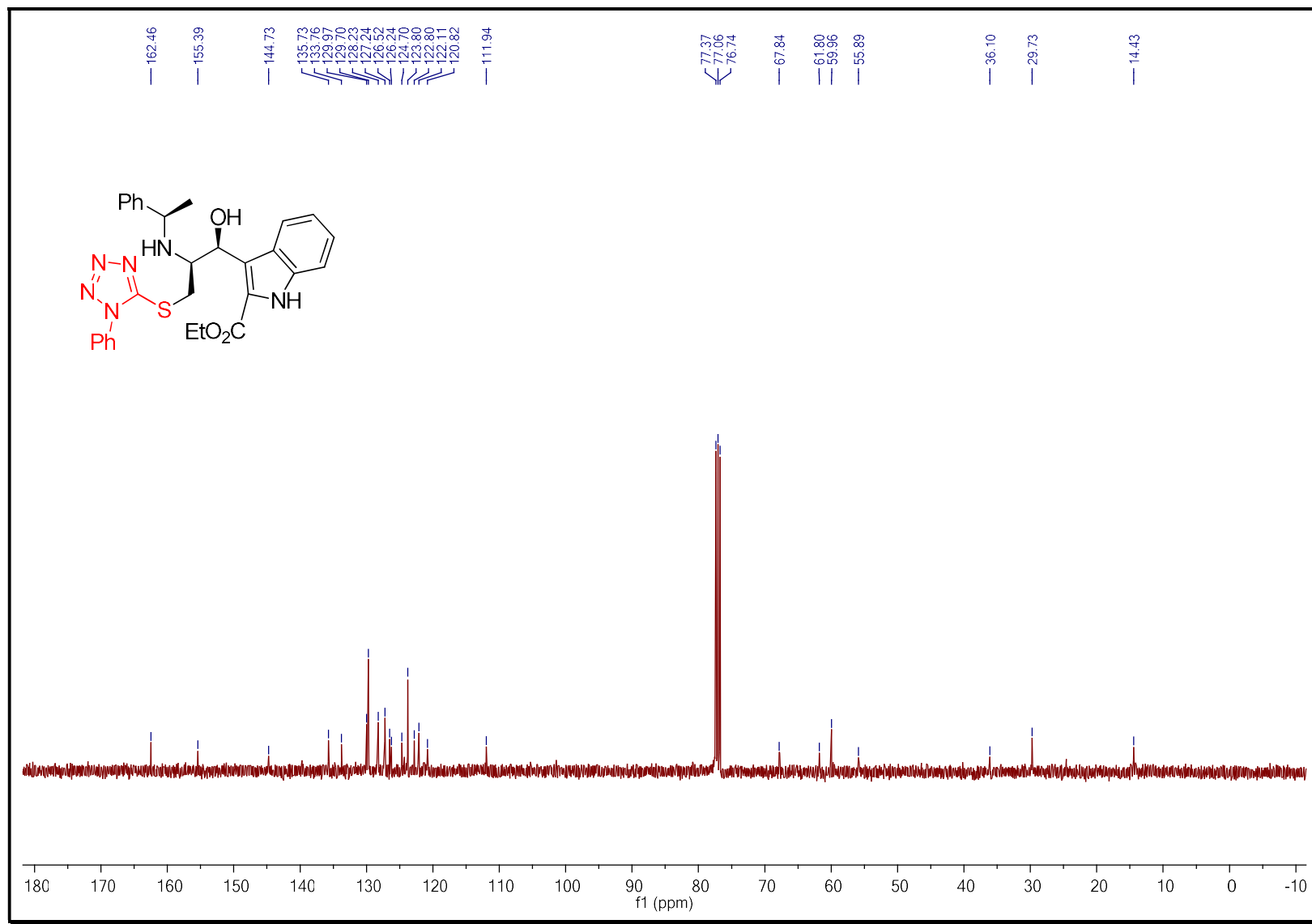
¹³C NMR spectrum of Ethyl 3-((1S,2R)-3-acetoxy-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (8):



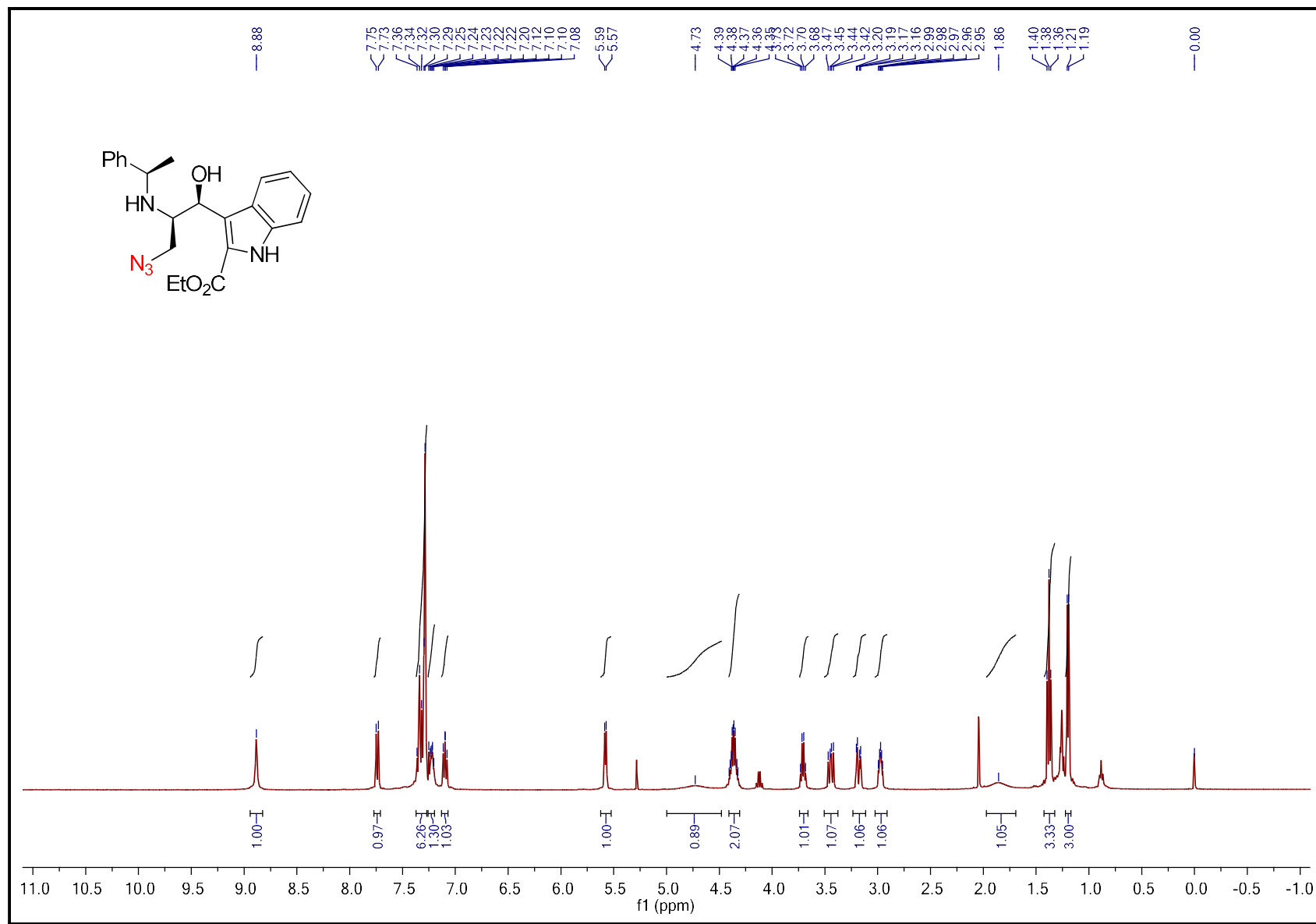
¹H NMR spectrum of Ethyl 3-((1*S*,2*S*)-1-hydroxy-3-((1-phenyl-1*H*-tetrazol-5-yl)thio)-2-(((*R*)-1-phenylethyl)amino)propyl)-1*H*-indole-2-carboxylate (9):



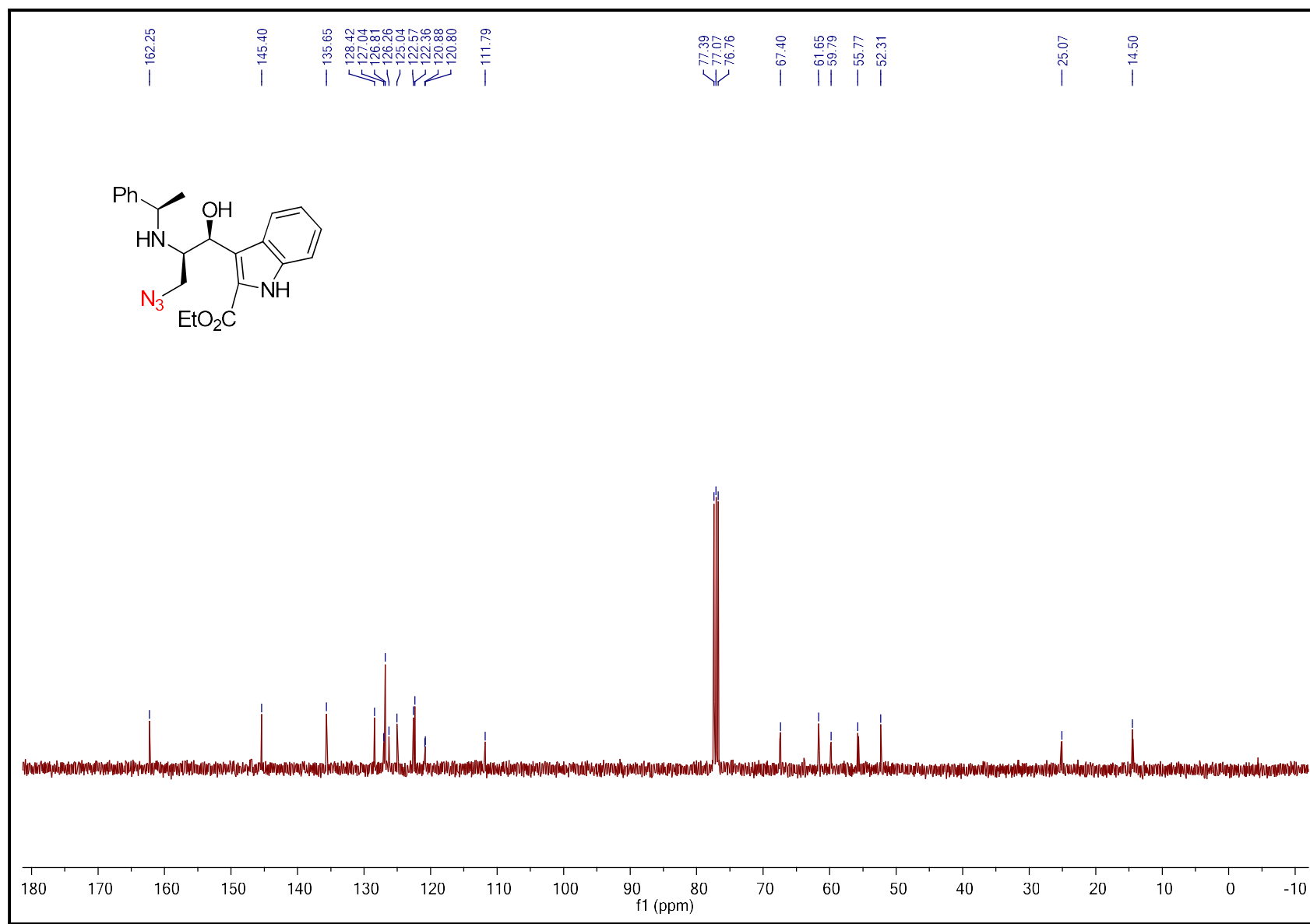
¹³C NMR spectrum of Ethyl 3-((1S,2S)-1-hydroxy-3-((1-phenyl-1H-tetrazol-5-yl)thio)-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (9):



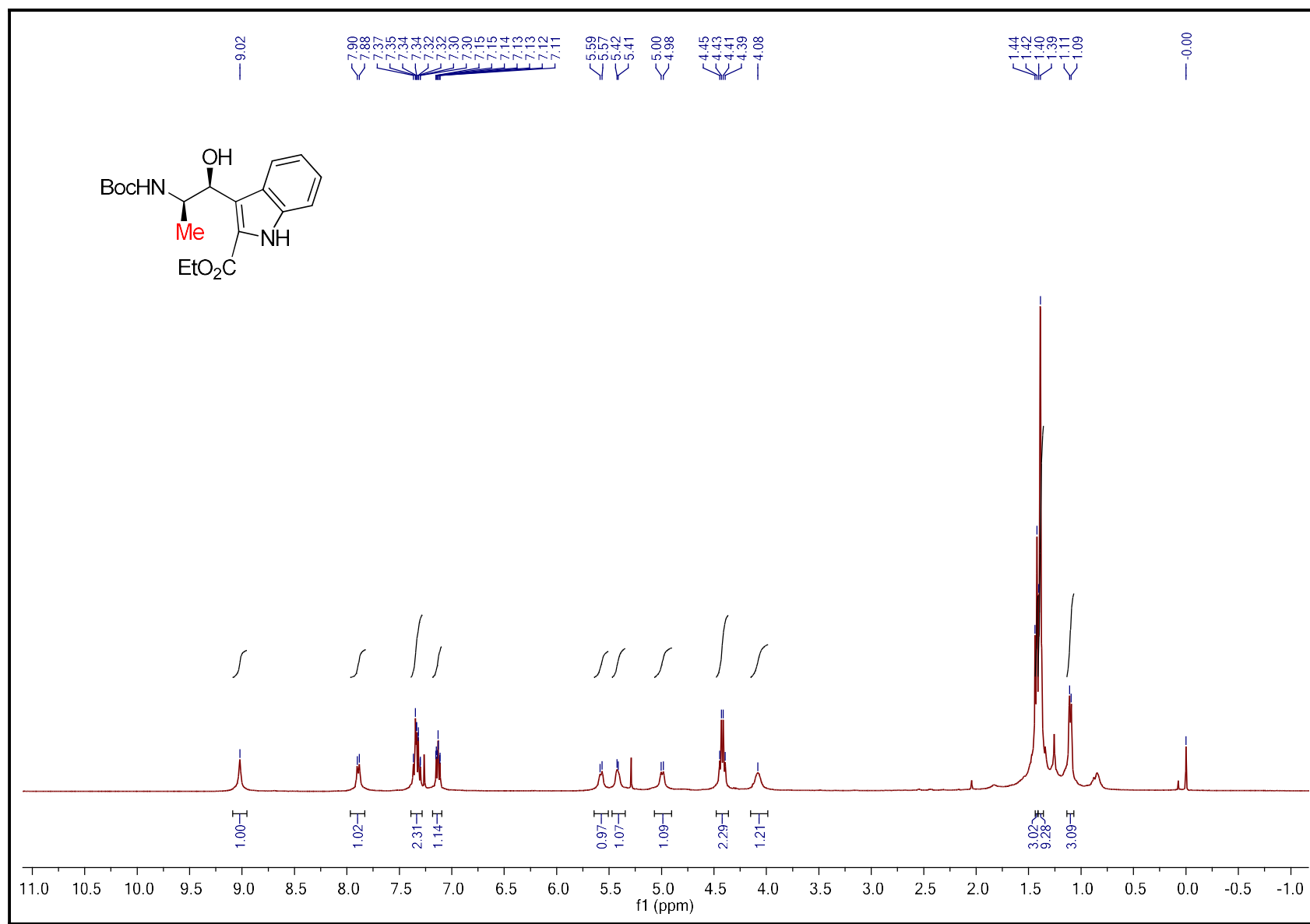
¹H NMR spectrum of Ethyl 3-((1S,2R)-3-azido-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (10):



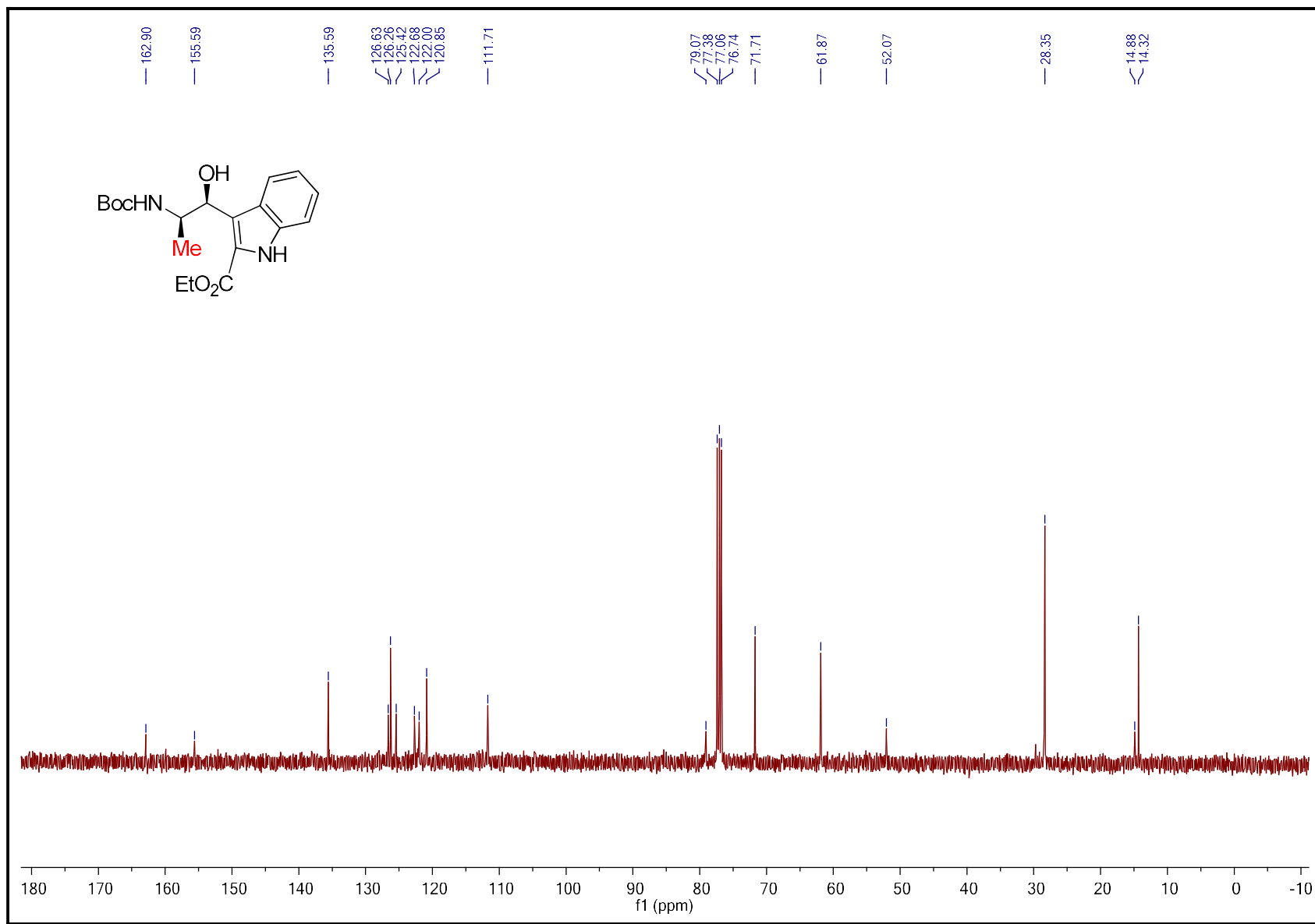
¹³C NMR spectrum of Ethyl 3-((1S,2R)-3-azido-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (10):



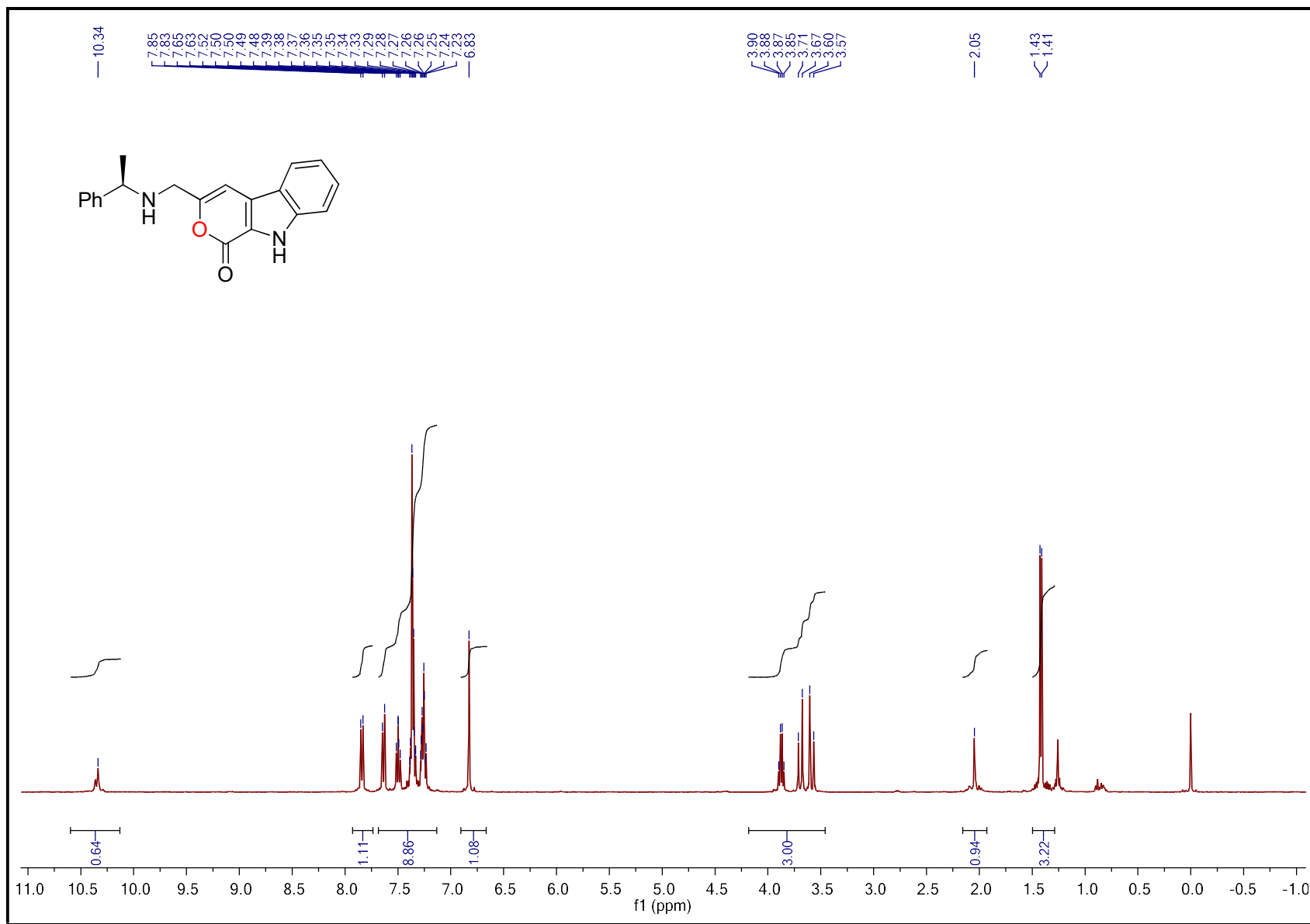
¹H NMR spectrum of Ethyl 3-((1S,2R)-2-((tert-butoxycarbonyl)amino)-1-hydroxypropyl)-1H-indole-2-carboxylate (11):



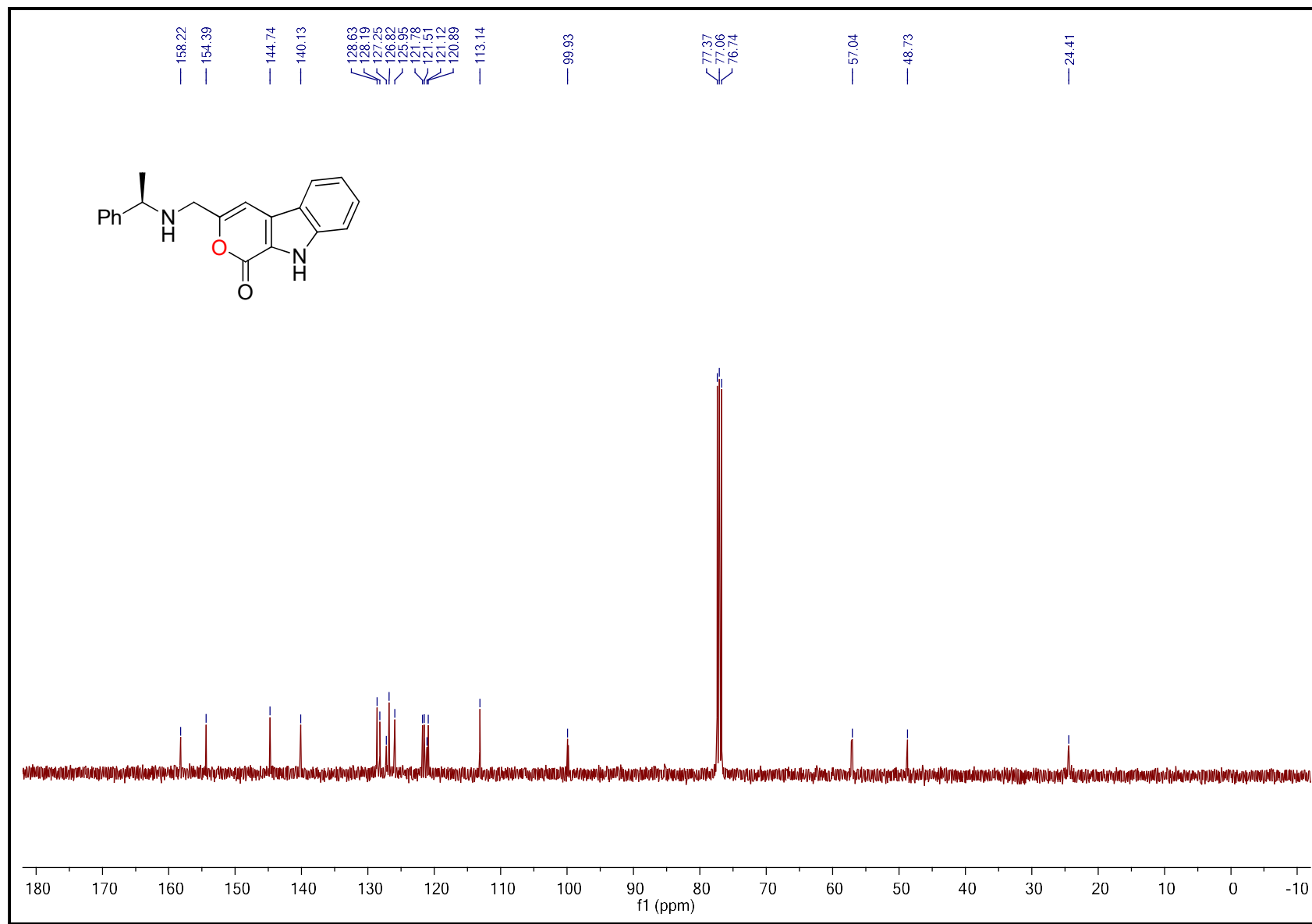
¹³C NMR spectrum of Ethyl 3-((1S,2R)-2-((tert-butoxycarbonyl)amino)-1-hydroxypropyl)-1H-indole-2-carboxylate (11):



¹H NMR spectrum of (R)-3-(((1-phenylethyl)amino)methyl)pyrano[3,4-b]indol-1(9H)-one (12):



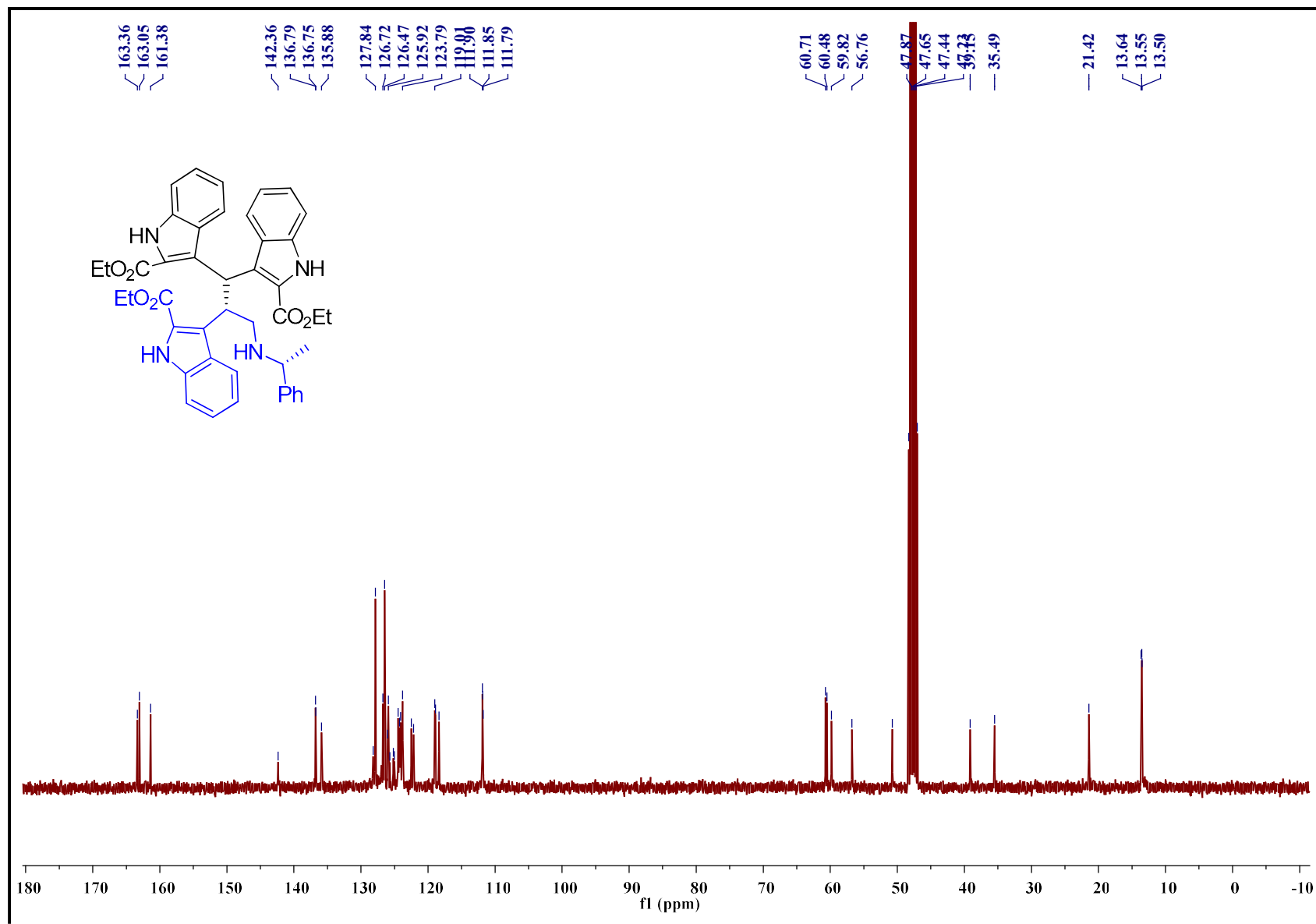
¹³C NMR spectrum of (R)-3-(((1-phenylethyl)amino)methyl)pyrano[3,4-b]indol-1(9H)-one (12):



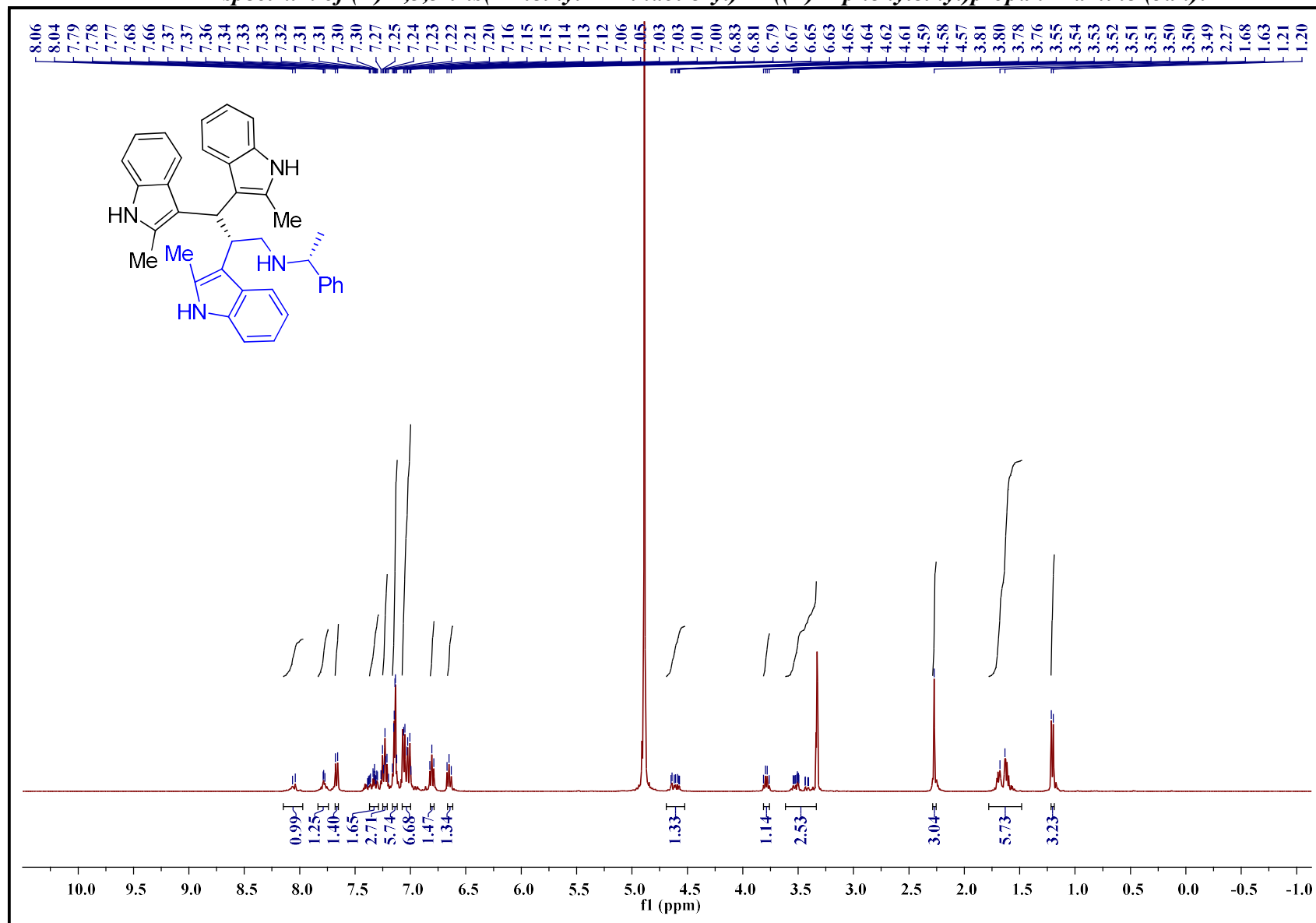
Chemical structure of compound 10 is shown in the top left corner. The structure is a complex molecule featuring a central chiral center (a carbon atom bonded to a hydrogen atom, an ethyl ester group, and two indole rings). The indole rings are further substituted with ethyl ester groups and a phenyl group. The structure is drawn in blue.

The ^1H NMR spectrum (400 MHz, CDCl_3) is displayed below the structure. The x-axis represents the chemical shift in ppm, ranging from 10.0 to -0.5. The y-axis represents the intensity of the signal. The spectrum shows several peaks, with integration values provided below the peaks: 3.07, 16.42, 1.97, 0.96, 4.03, 2.05, 1.08, 1.02, 1.01, 3.01, 3.20, 3.31, 3.14. The peaks are labeled with their corresponding chemical shifts in ppm: 8.31, 8.29, 7.43, 7.41, 7.32, 7.31, 7.29, 7.25, 7.23, 7.19, 7.17, 7.16, 7.15, 7.14, 7.12, 7.10, 7.09, 7.08, 7.04, 7.03, 7.02, 7.01, 7.01, 7.01, 7.00, 6.94, 6.92, 6.90, 6.89, 6.86, 6.84, 6.57, 6.55, 4.55, 4.53, 4.52, 4.51, 4.50, 4.49, 4.49, 4.48, 4.47, 4.25, 4.23, 4.21, 3.76, 3.75, 3.34, 3.33, 3.33, 3.33, 3.32, 3.25, 3.22, 3.14, 3.14, 1.51, 1.49, 1.44, 1.42, 1.41, 1.29, 1.27, 1.25, 1.18, 1.16.

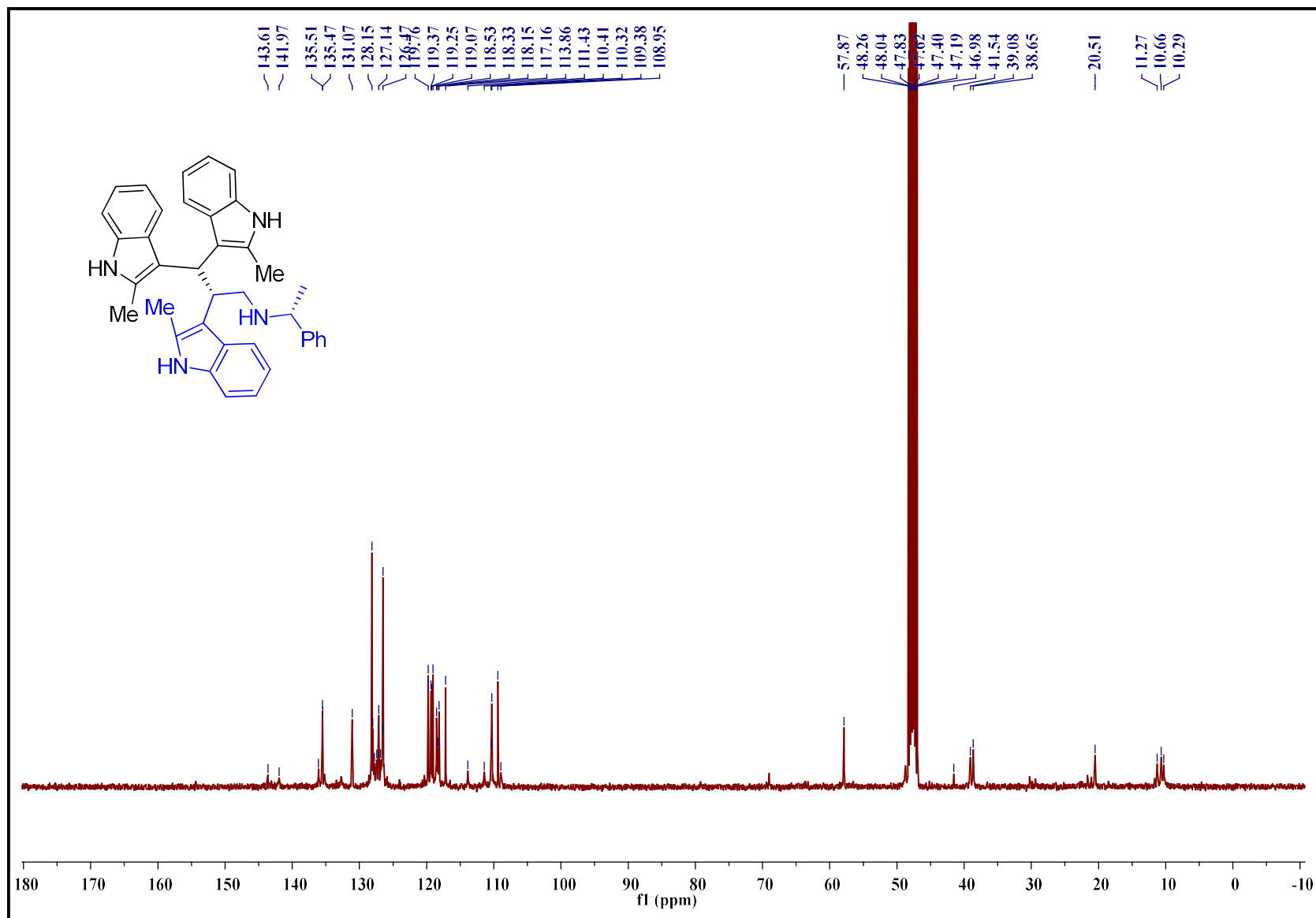
¹³C NMR spectrum of Triethyl 3,3',3''-((S)-3-(((R)-1-phenylethyl)amino)propane-1,1,2-triyl)tris(1H-indole-2-carboxylate) (5aa):



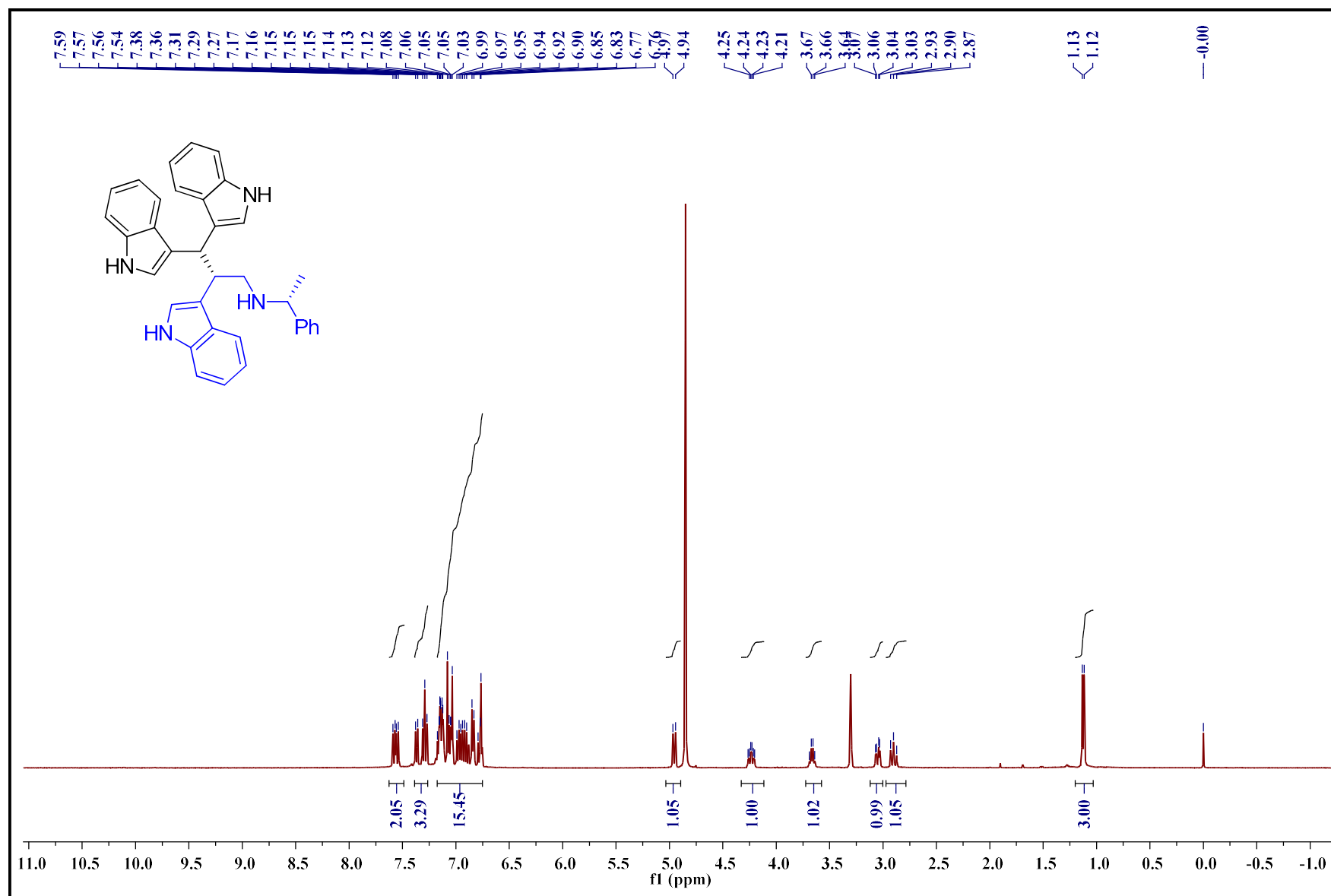
¹H NMR spectrum of (R)-2,3,3-tris(2-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ah):



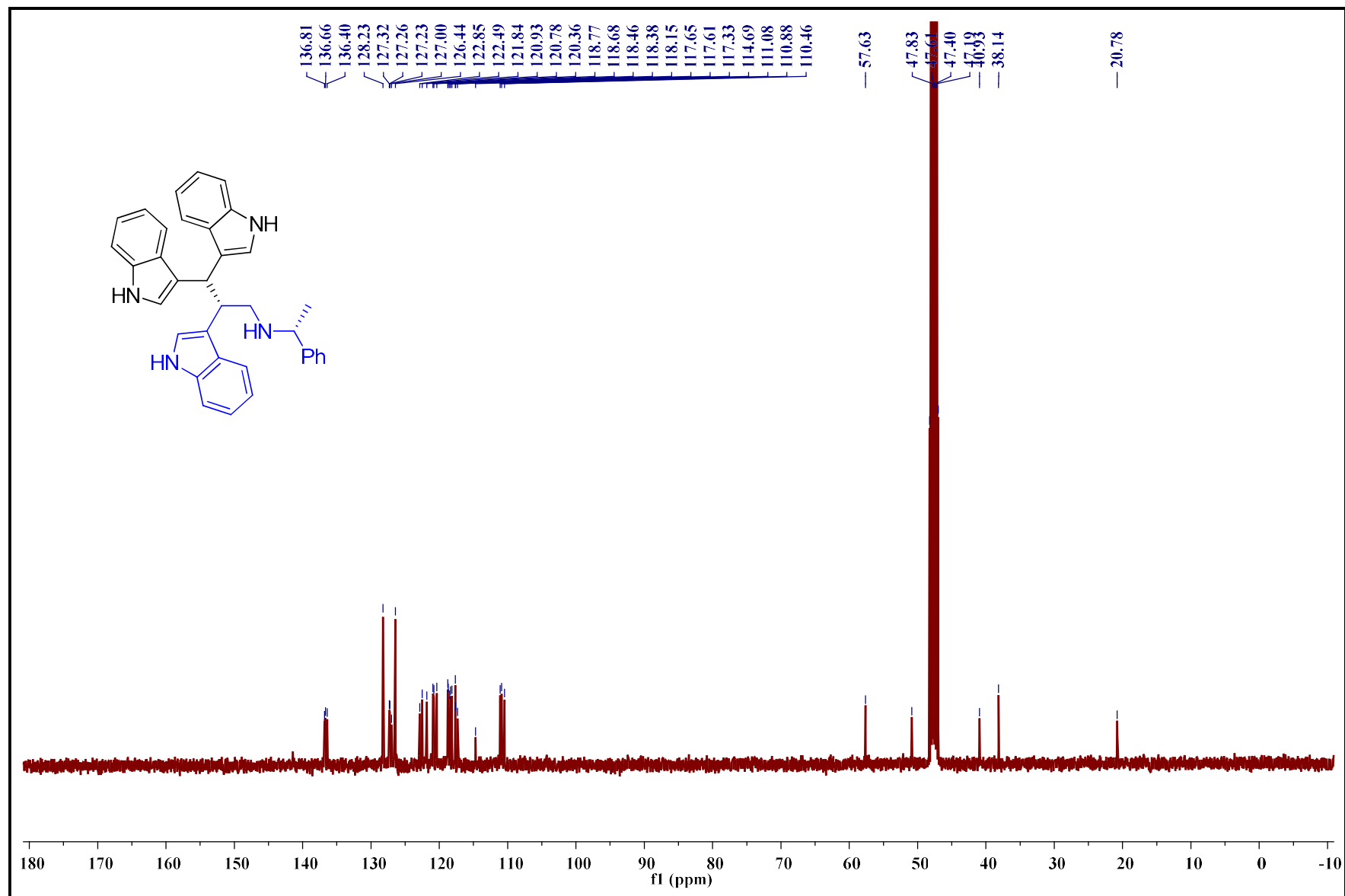
¹³C NMR spectrum of (R)-2,3,3-tris(2-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ah):



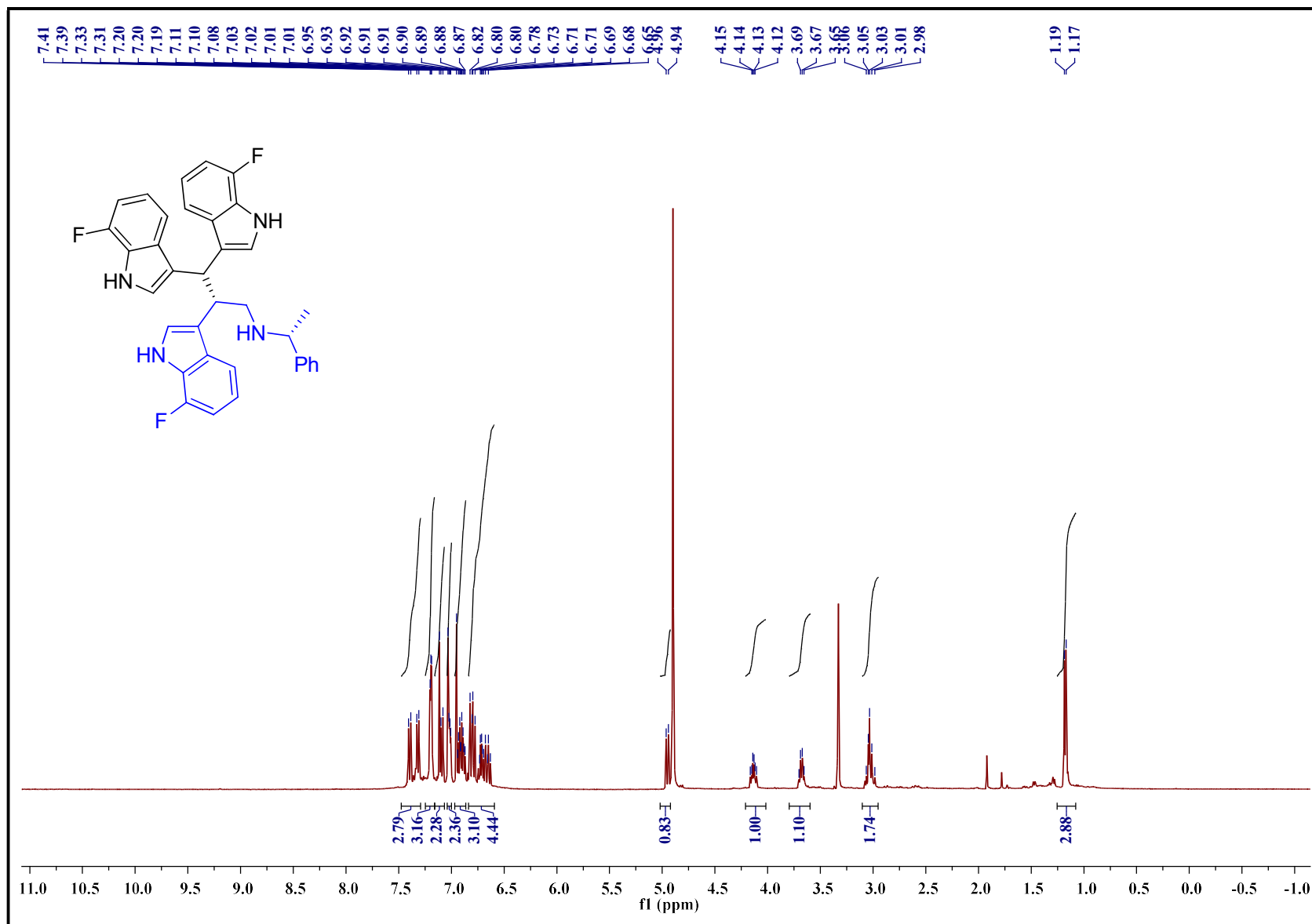
¹H NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ai):



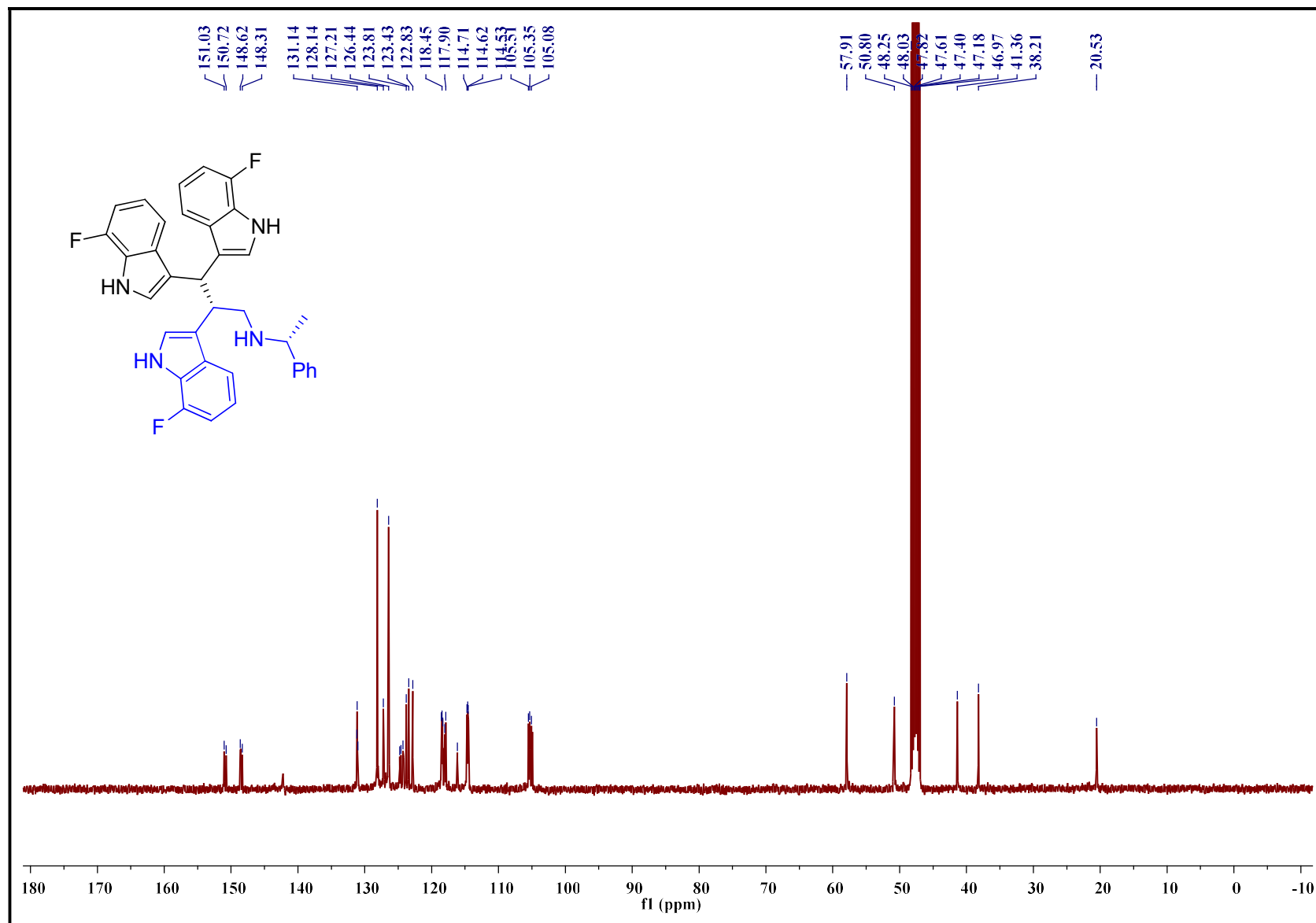
¹³C NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ai):



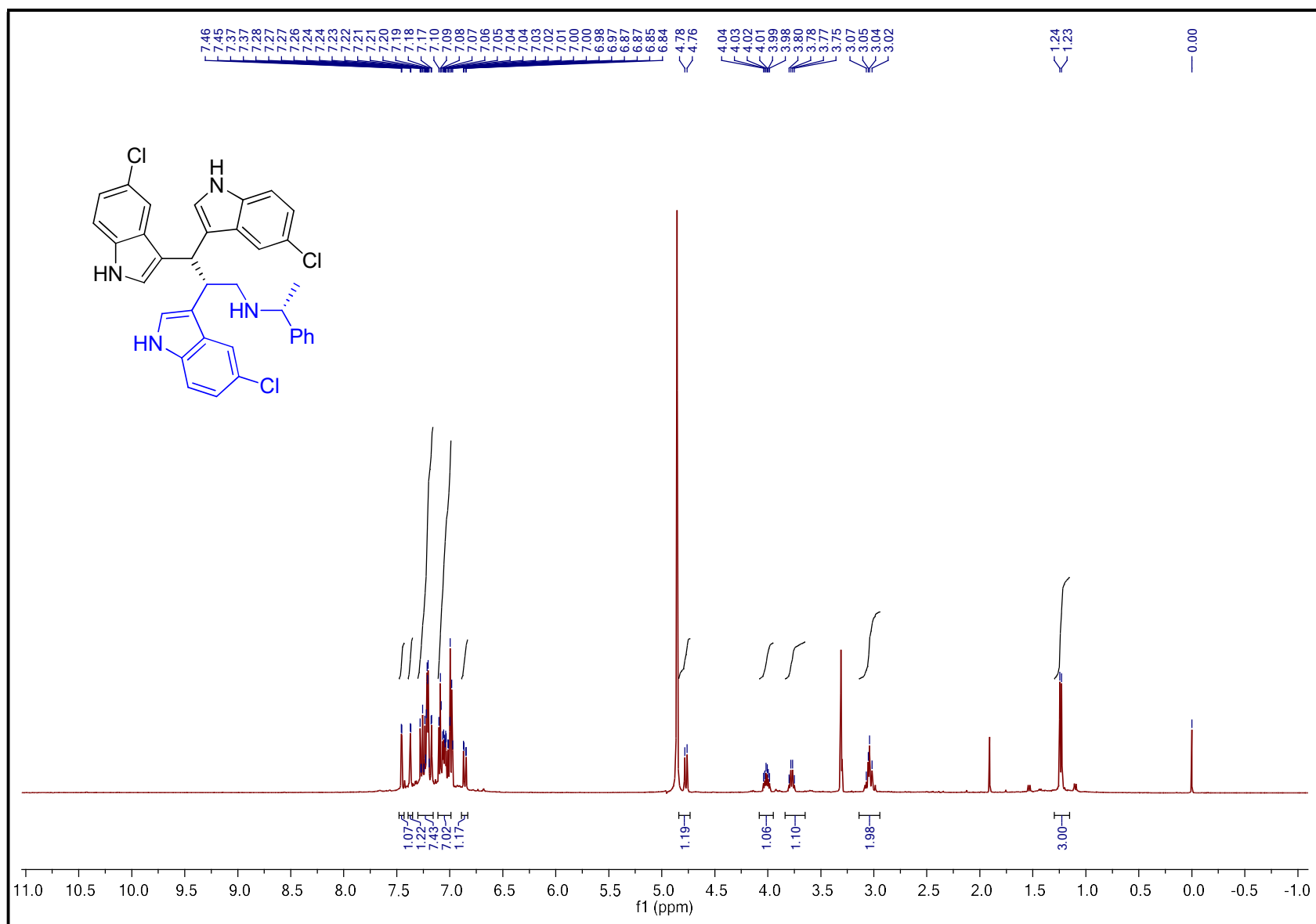
¹H NMR spectrum of (S)-2,3,3-tris(7-fluoro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5aj):



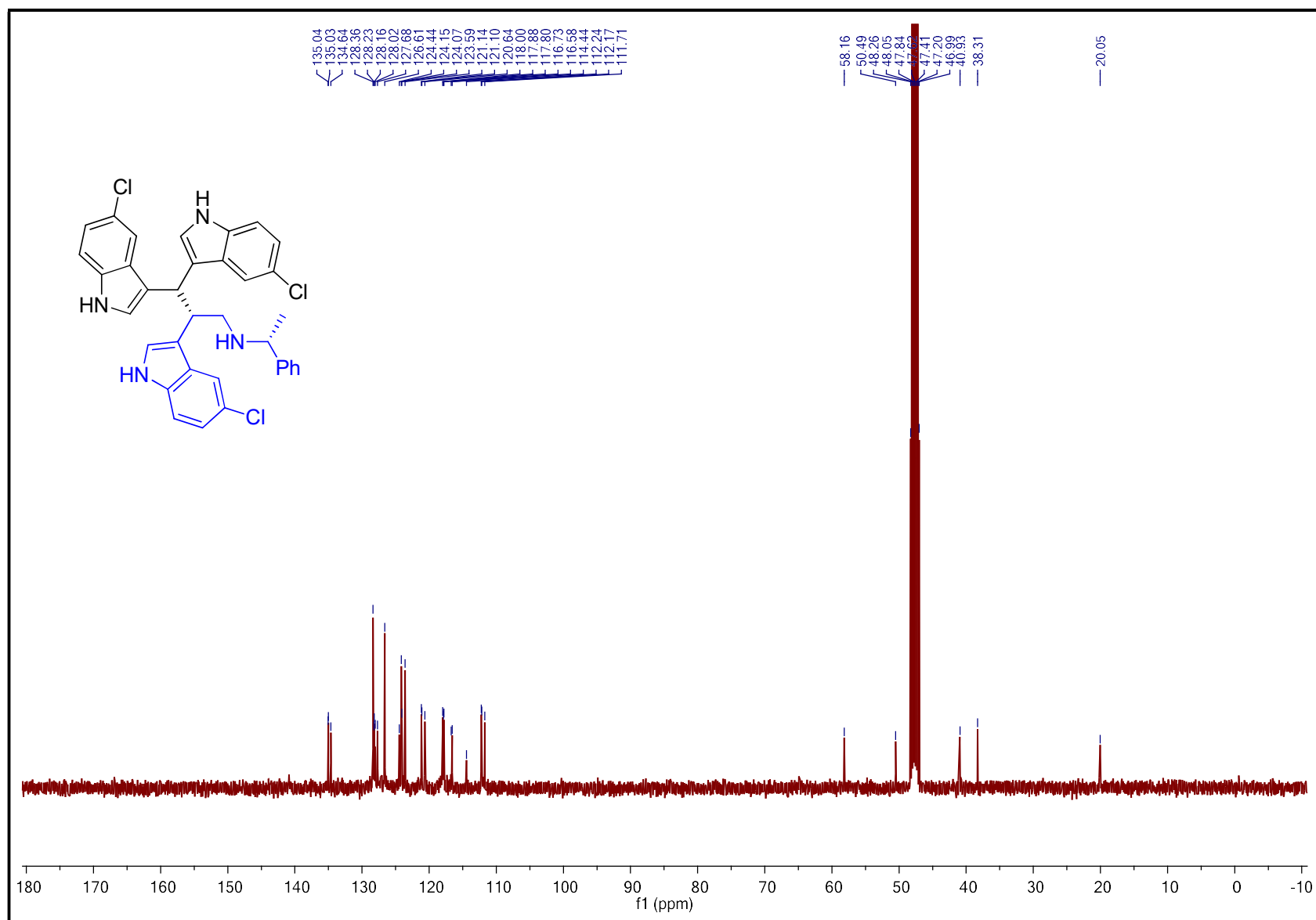
¹³C NMR spectrum of (S)-2,3,3-tris(7-fluoro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5aj):



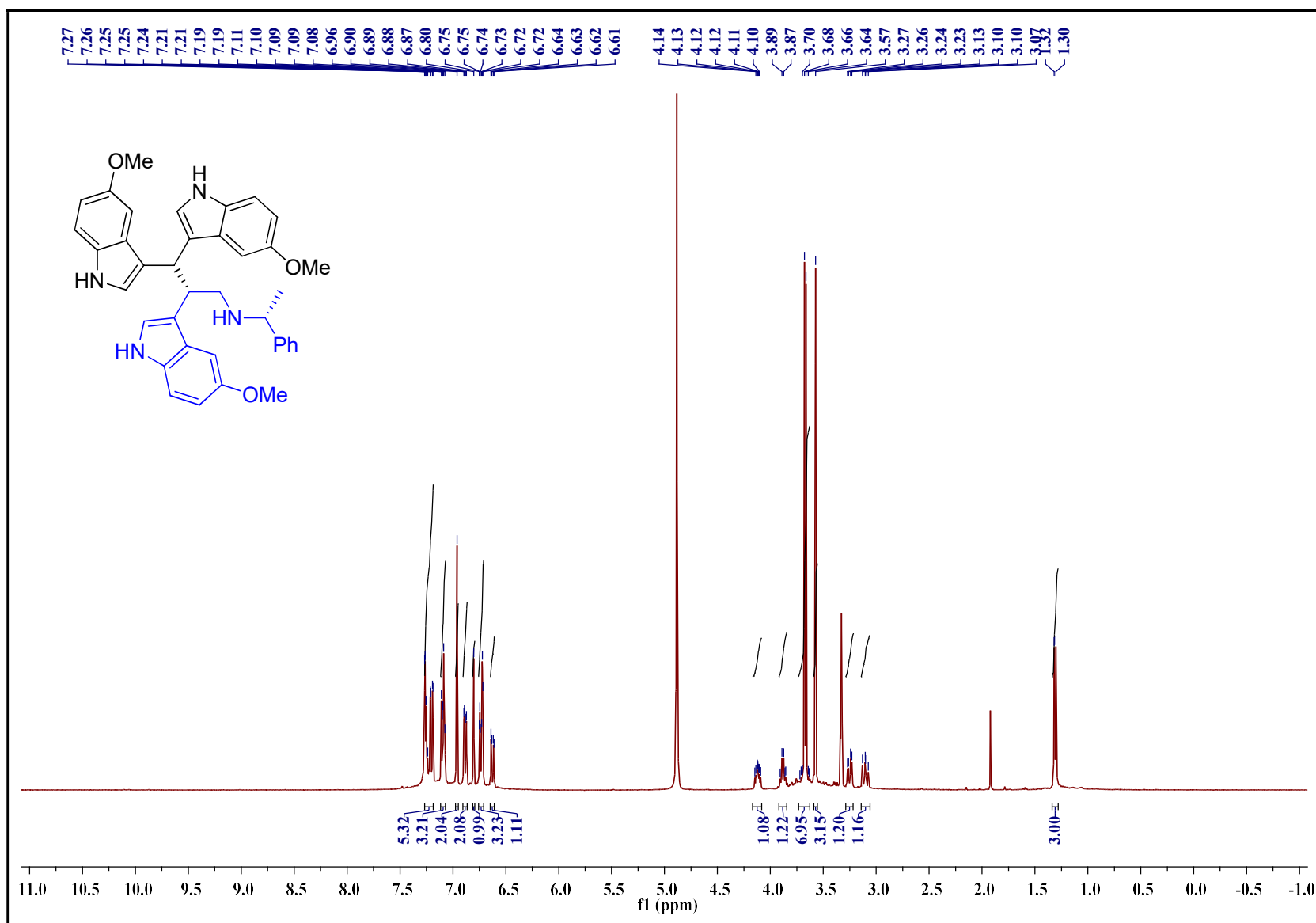
¹H NMR spectrum of (S)-2,3,3-tris(5-chloro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ak):



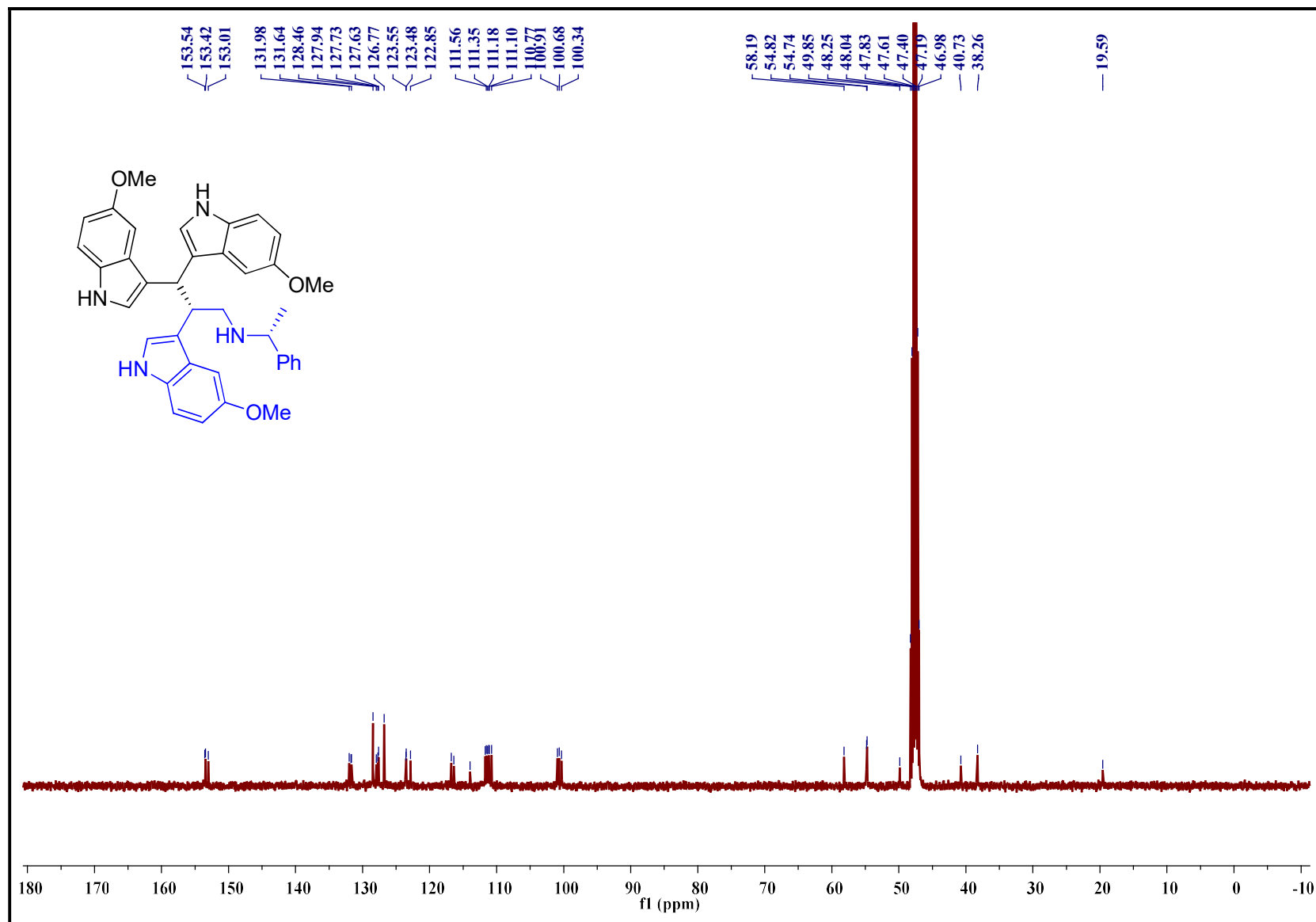
¹³C NMR spectrum of (S)-2,3,3-tris(5-chloro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ak):



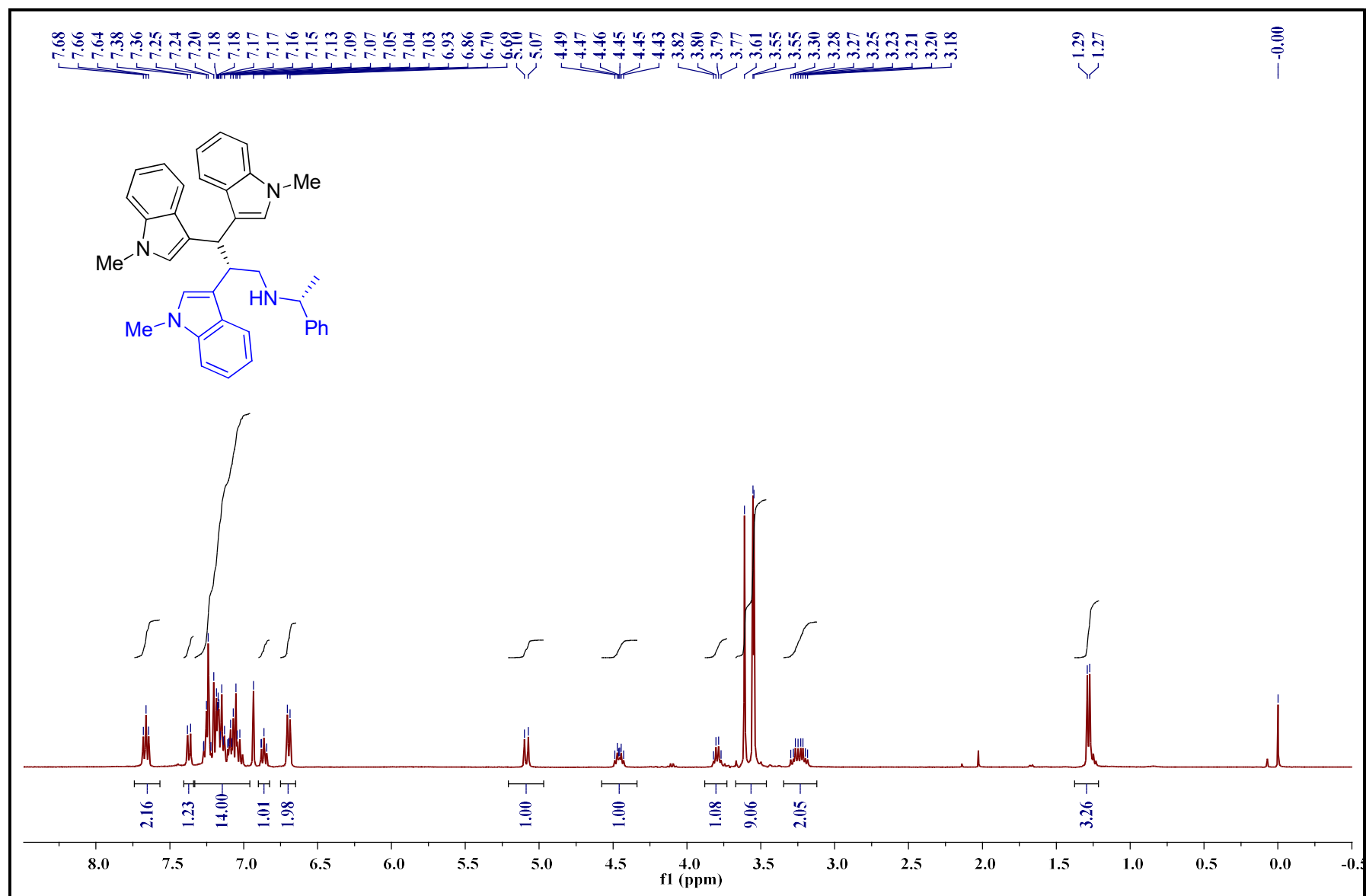
¹H NMR spectrum of (S)-2,3,3-tris(5-methoxy-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5a1):



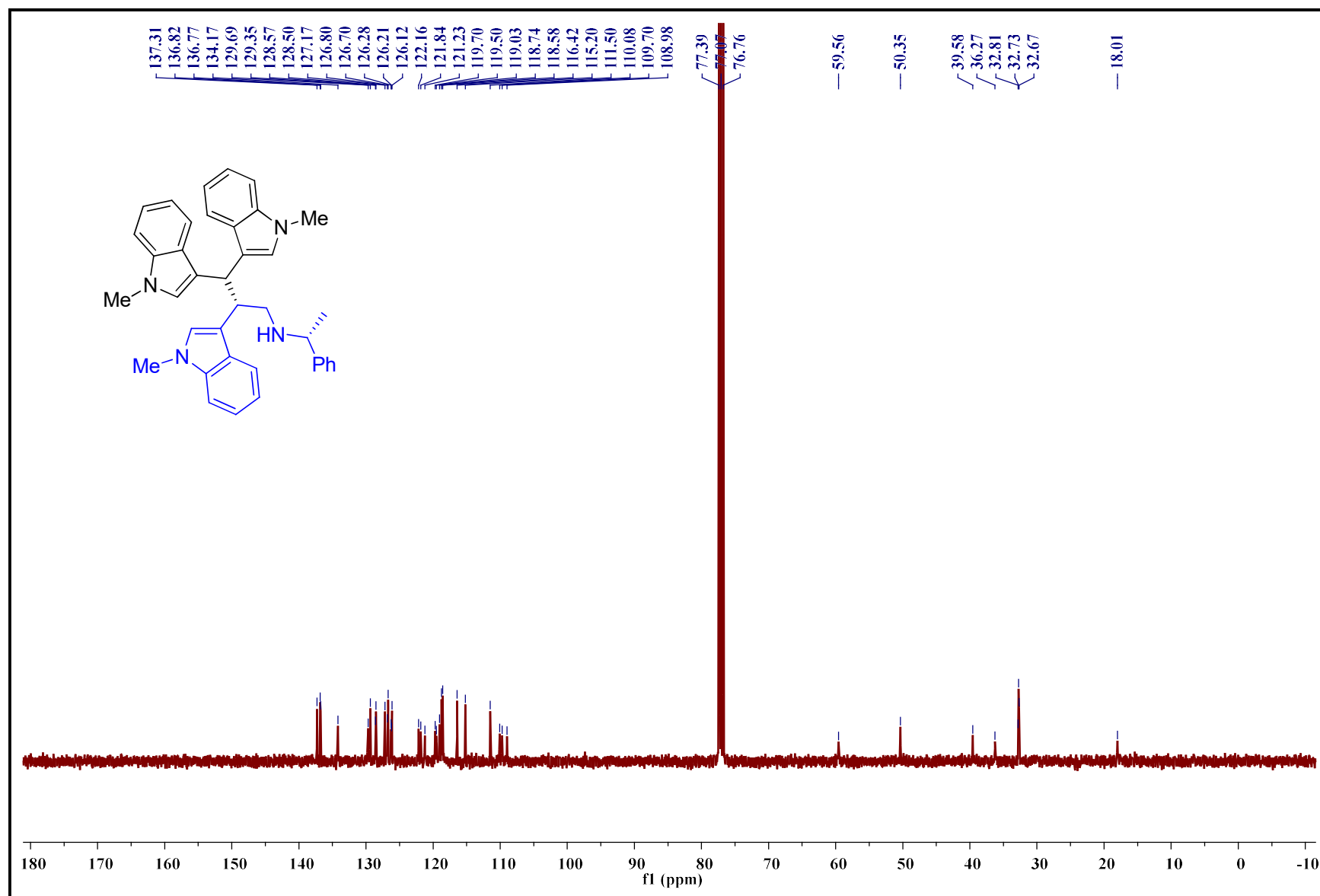
¹³C NMR spectrum of (S)-2,3,3-tris(5-methoxy-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5aI):



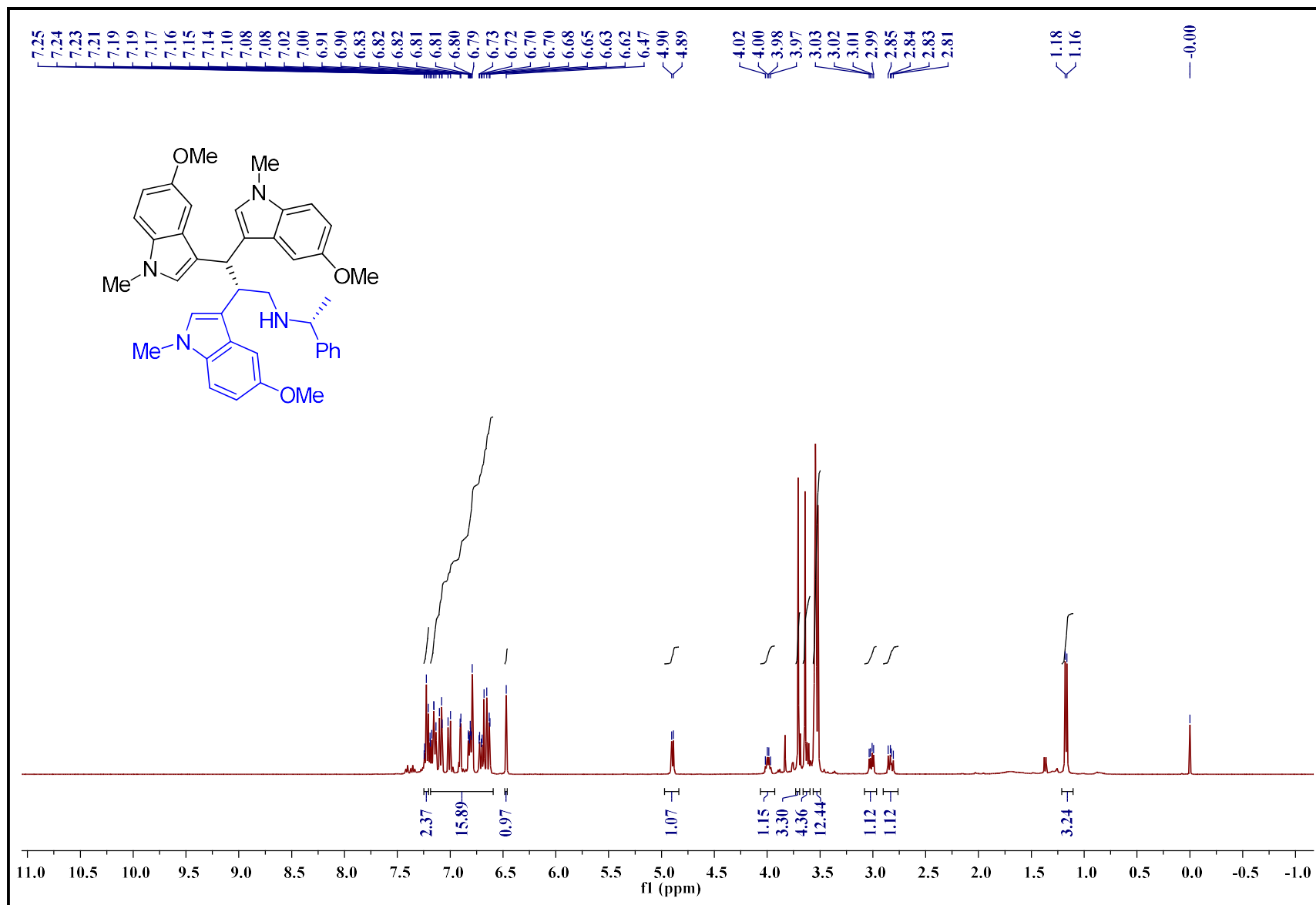
¹H NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5am):



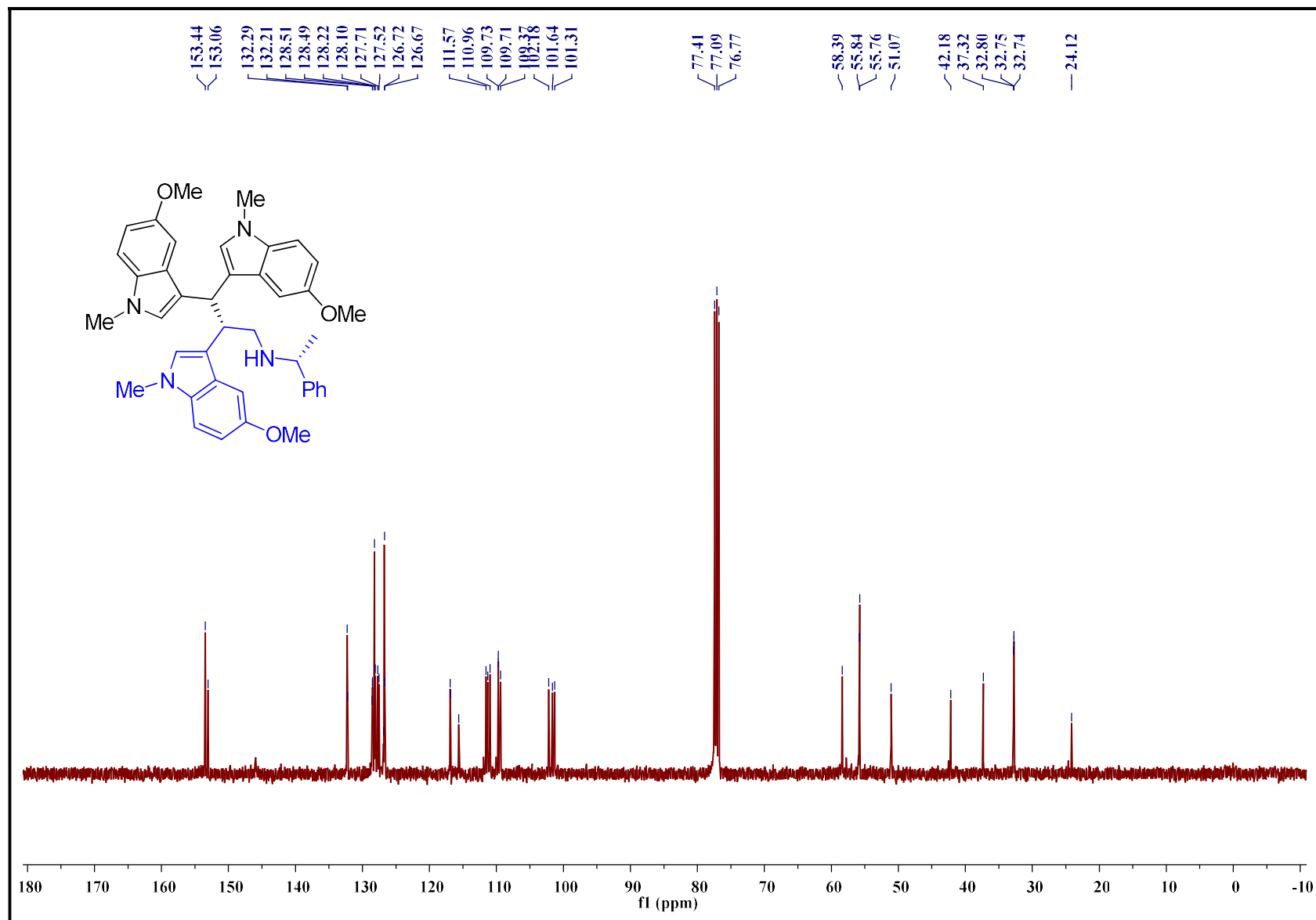
¹³C NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5am):



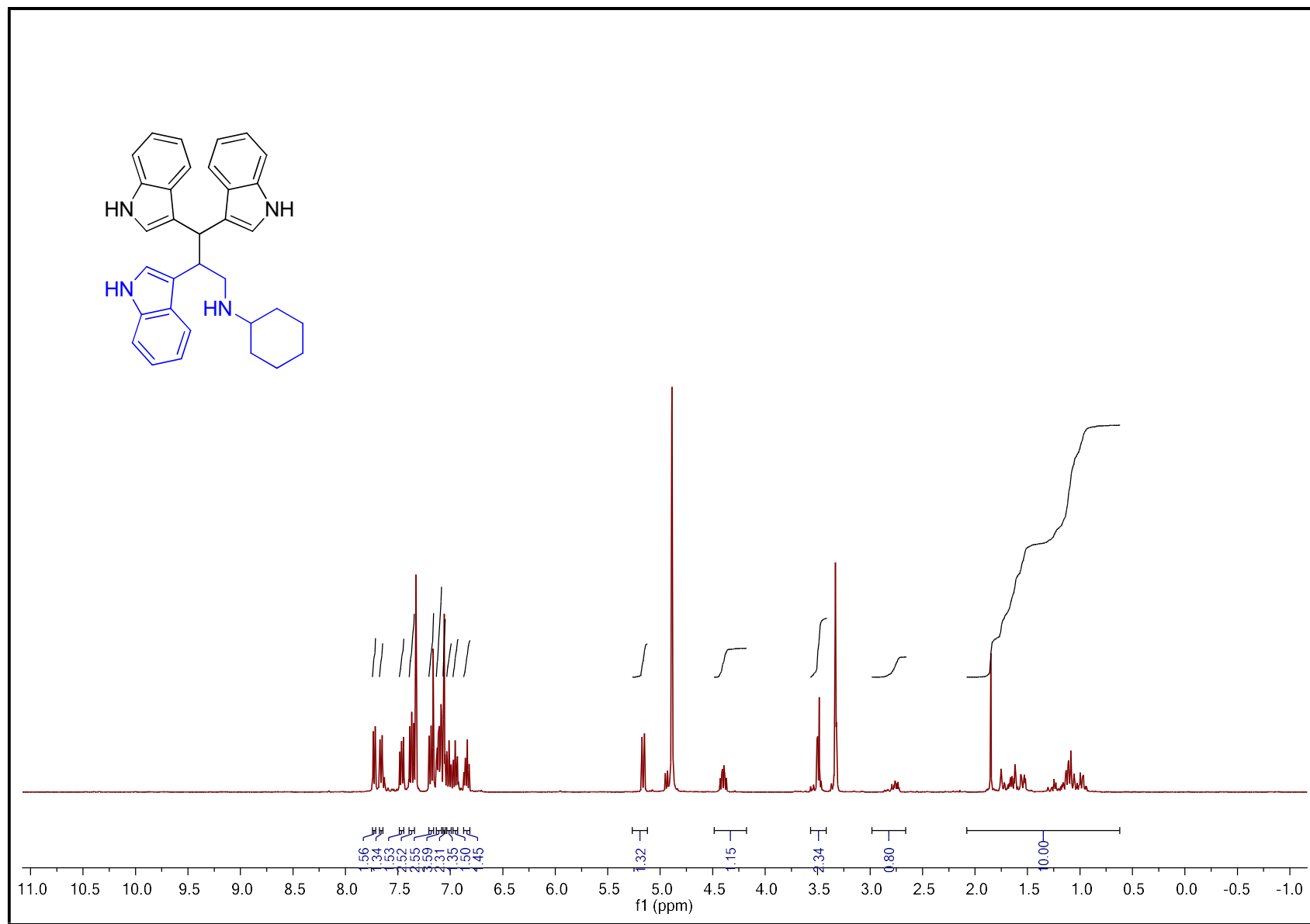
¹H NMR spectrum of (S)-2,3,3-tris(5-methoxy-1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5an):



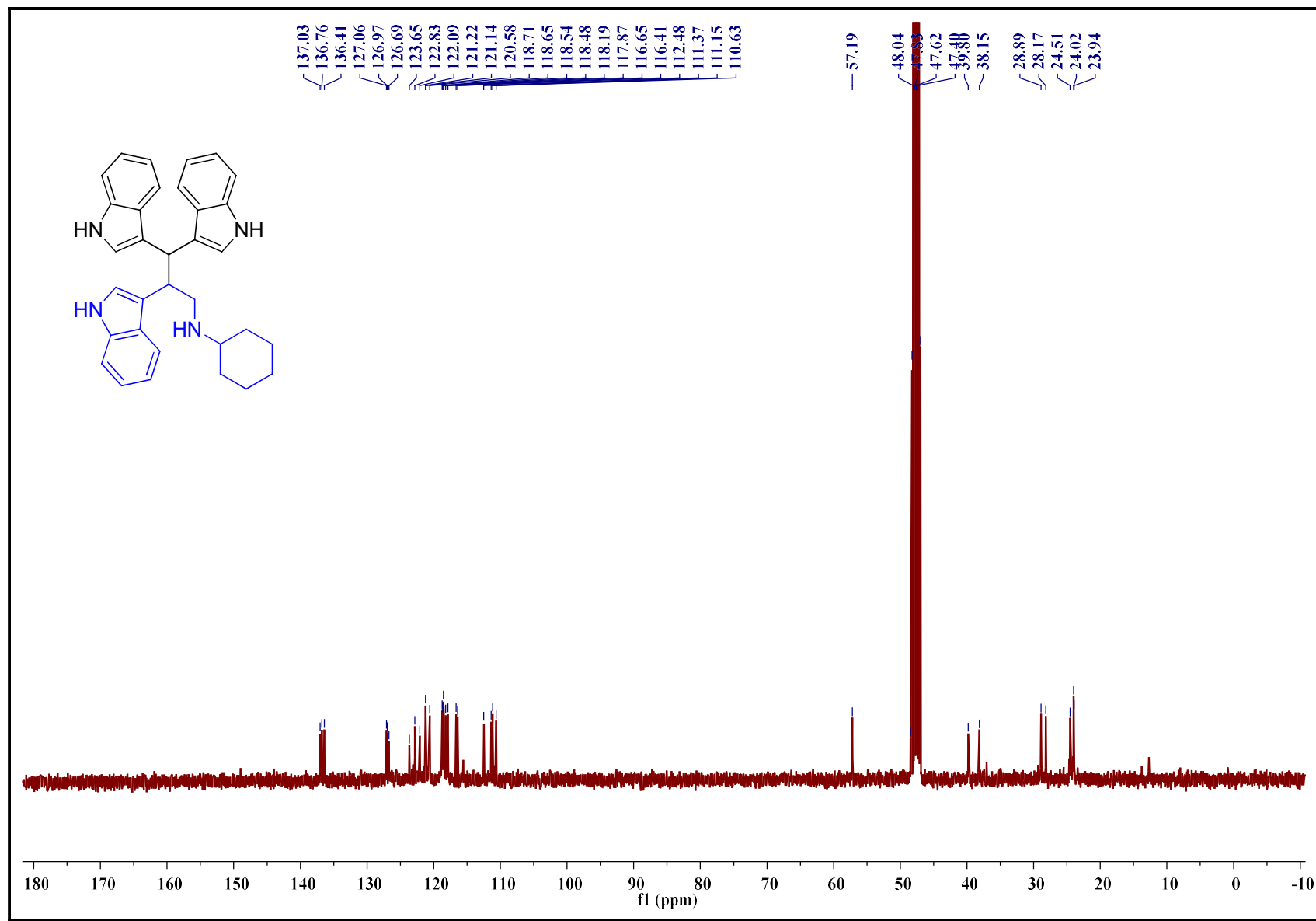
¹³C NMR spectrum of (S)-2,3,3-tris(5-methoxy-1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5an):



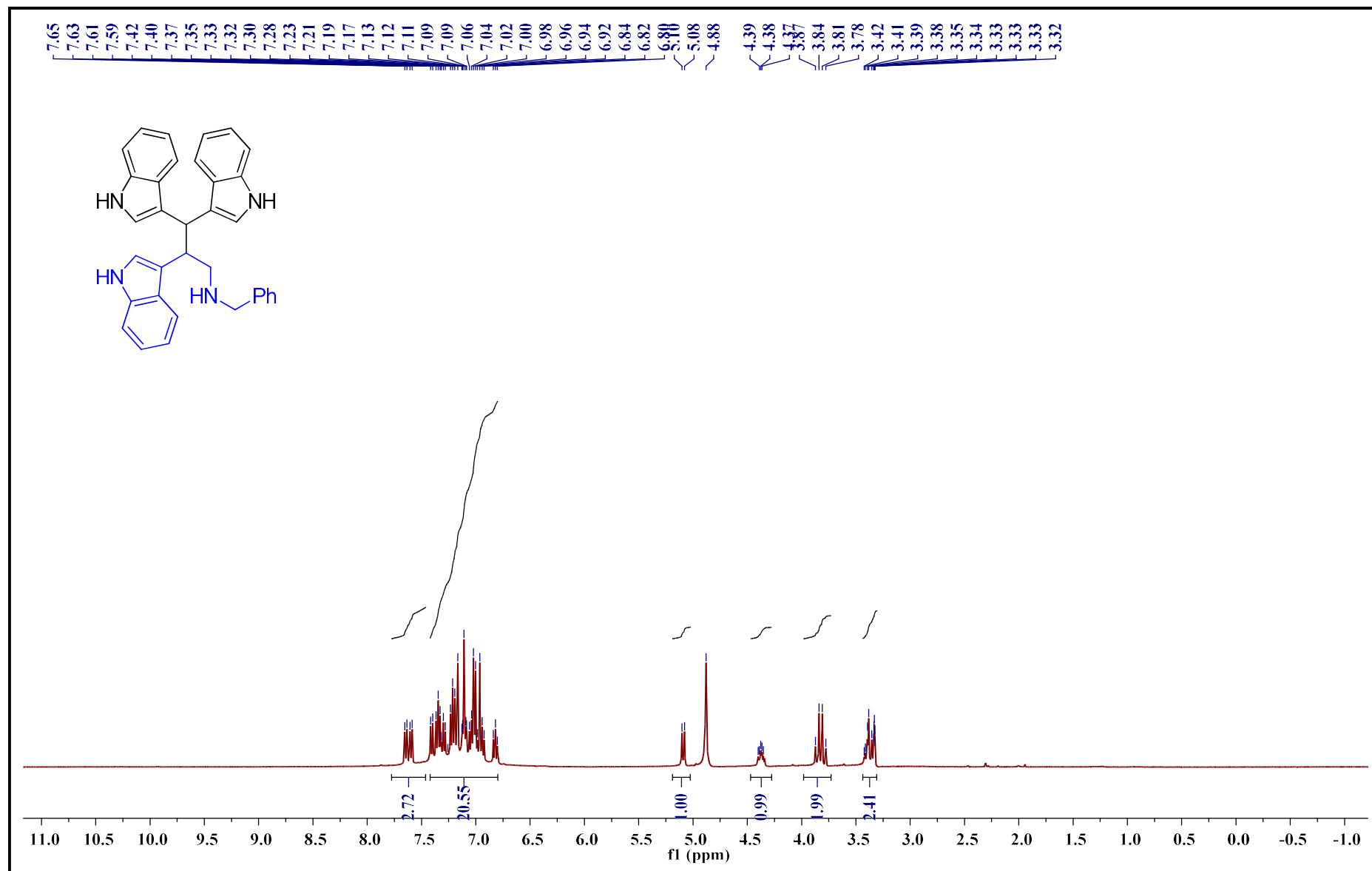
¹H NMR spectrum of N-(2,3,3-tri(1H-indol-3-yl)propyl)cyclohexanamine (5bi):



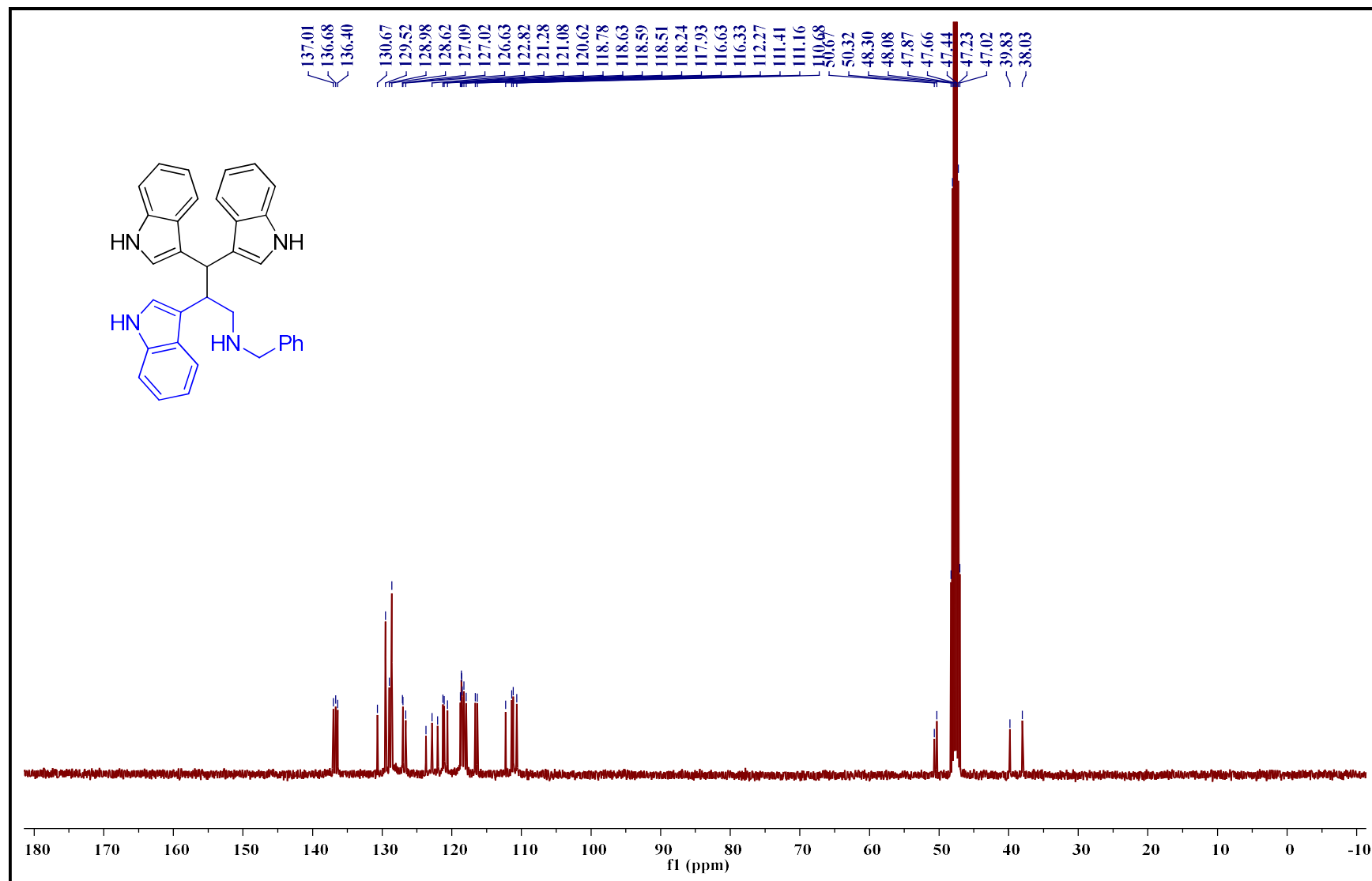
¹³C NMR spectrum of N-(2,3,3-tri(1H-indol-3-yl)propyl)cyclohexanamine (5bi):



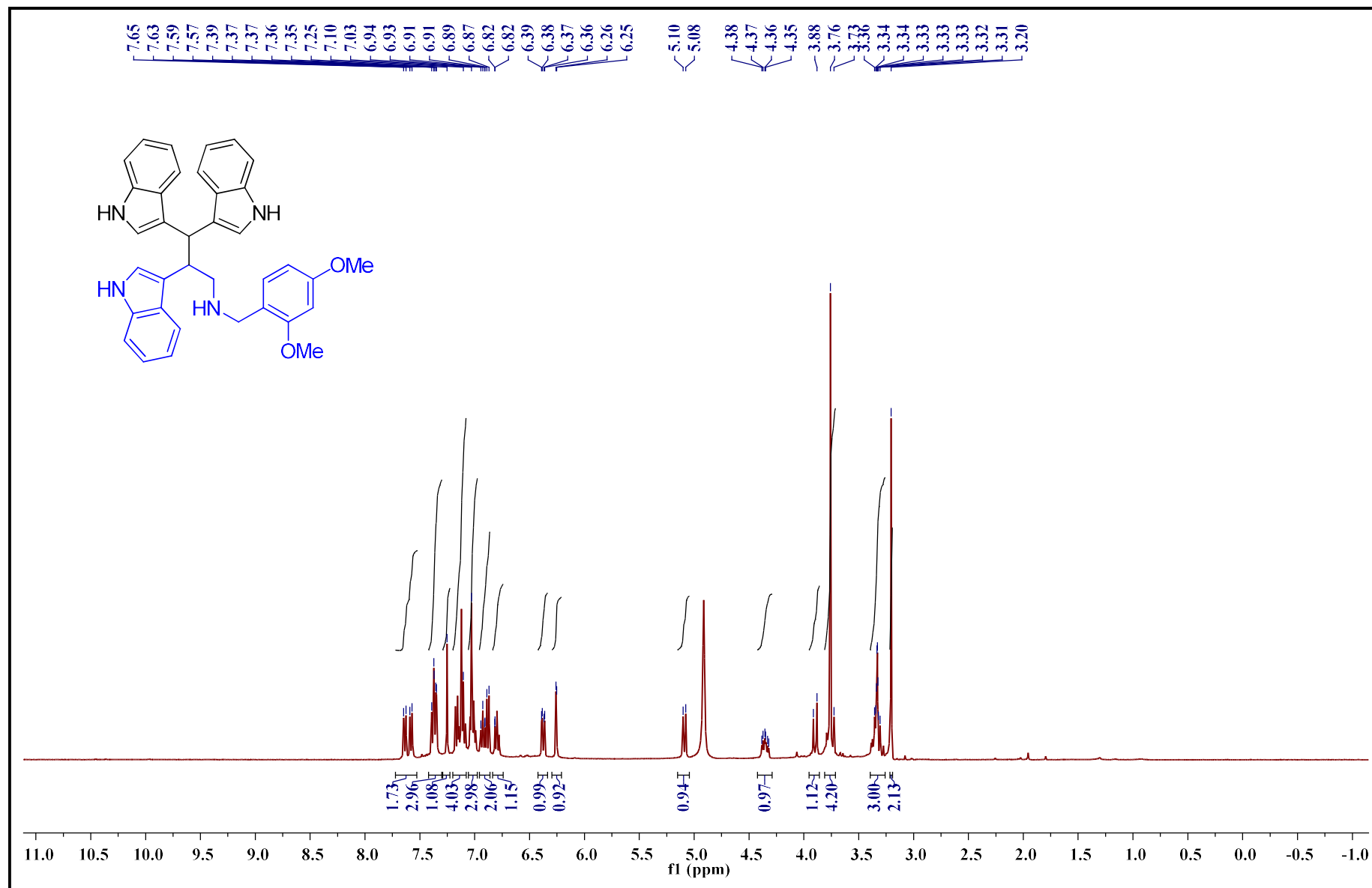
¹H NMR spectrum of N-benzyl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ci):



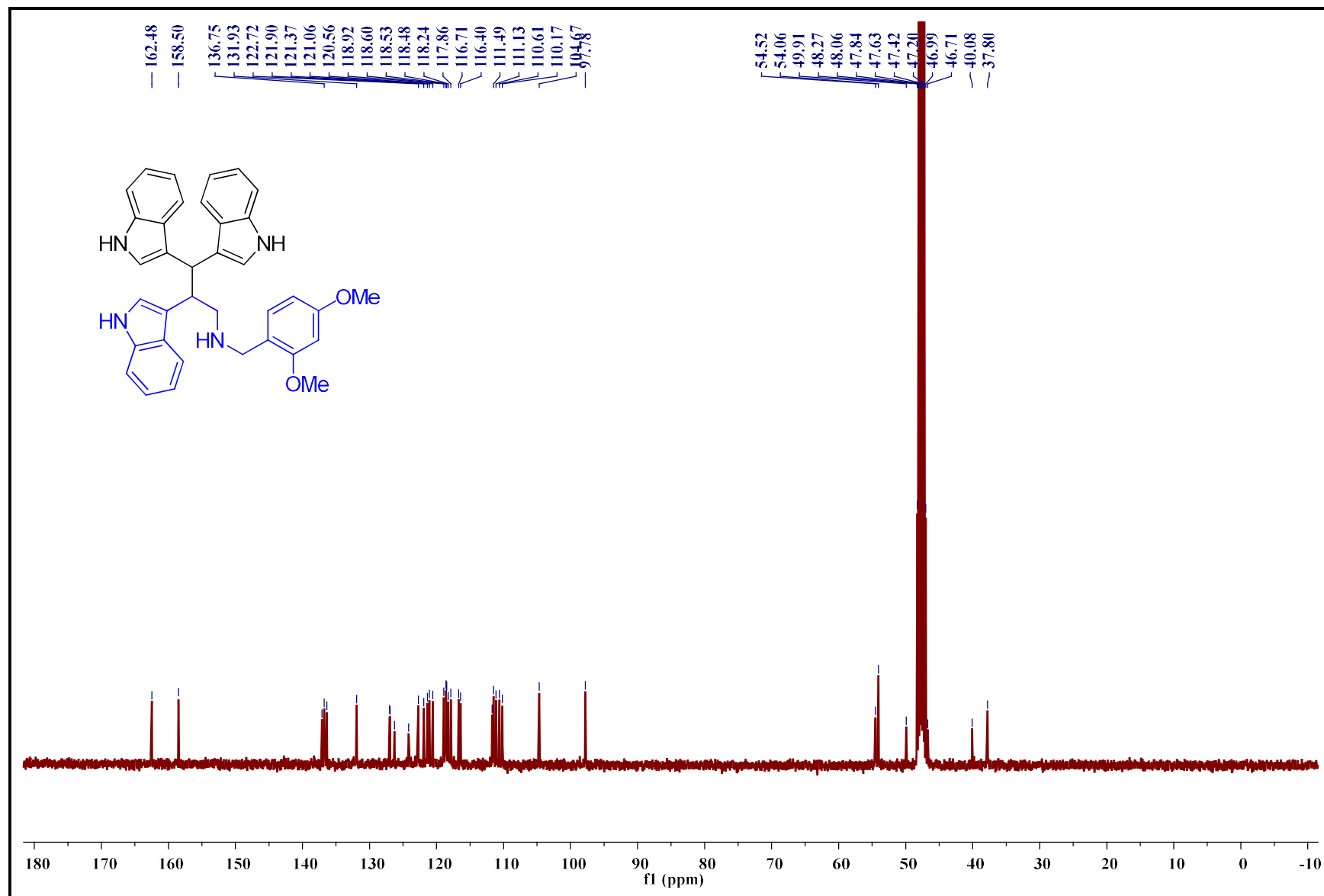
¹³C NMR spectrum of *N*-benzyl-2,3,3-tri(1*H*-indol-3-yl)propan-1-amine (5ci)



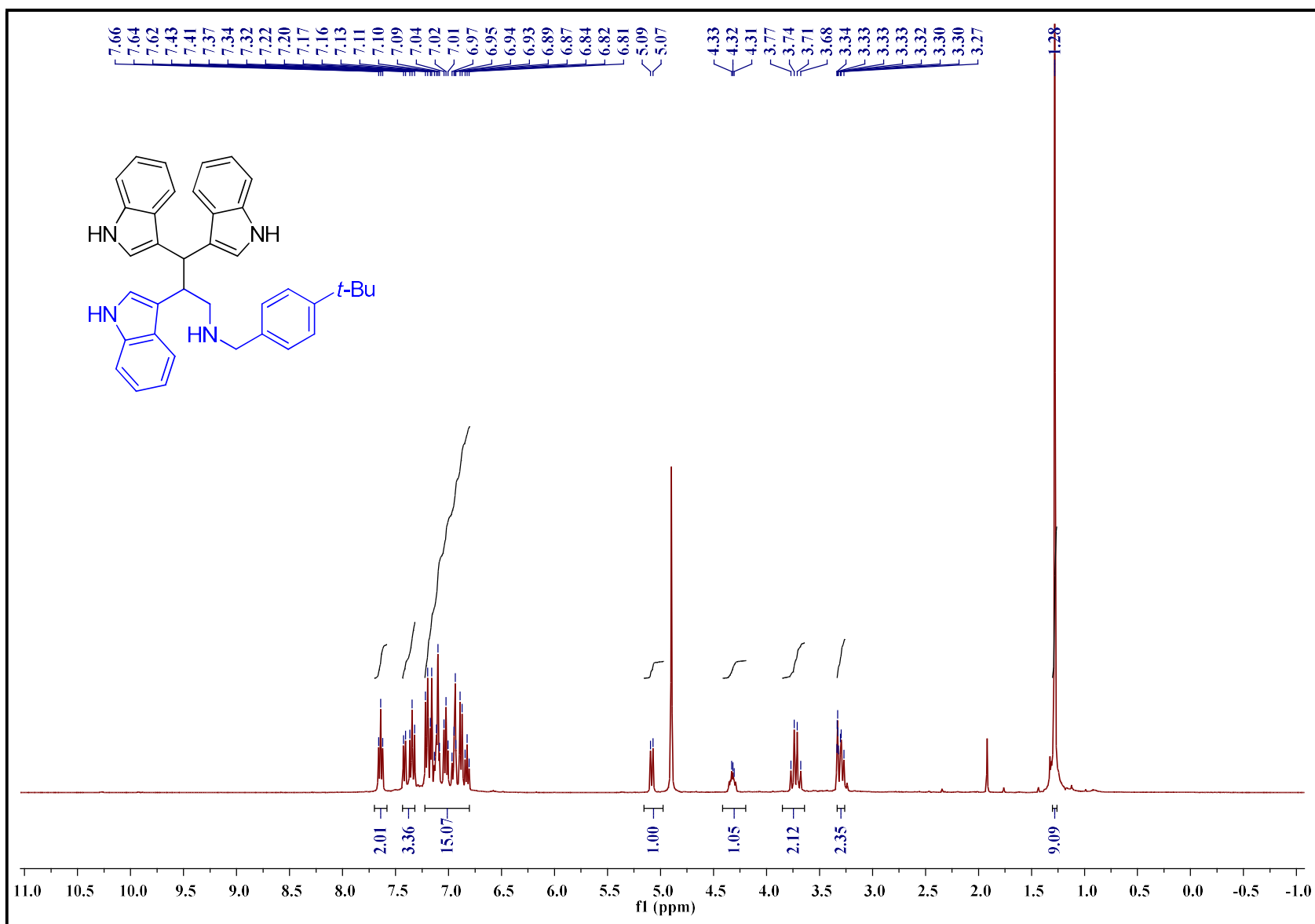
¹H NMR spectrum of N-(2,4-dimethoxybenzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5di):



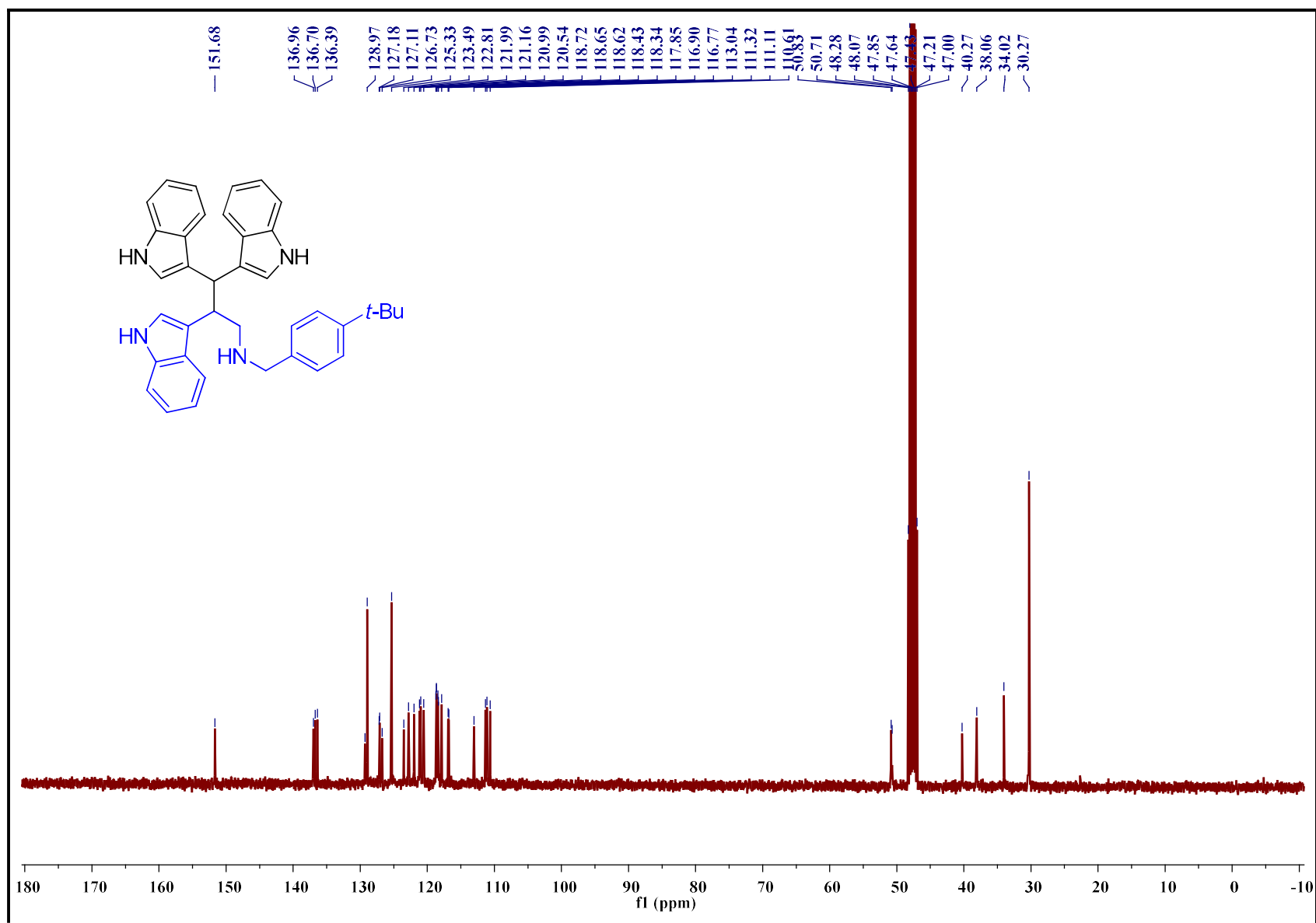
¹³C NMR spectrum of N-(2,4-dimethoxybenzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5di):



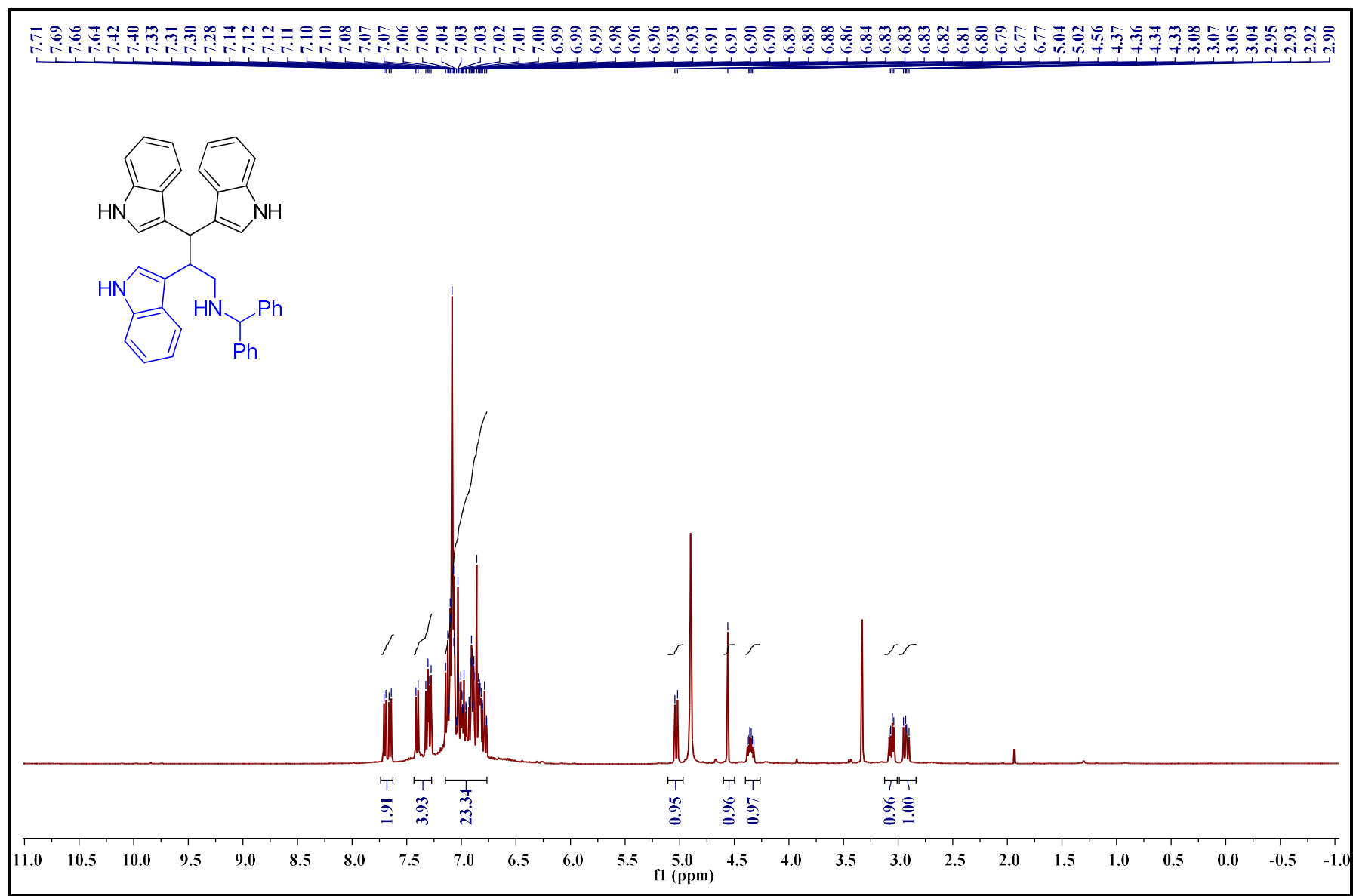
¹H NMR spectrum of N-(4-(tert-butyl)benzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ei):



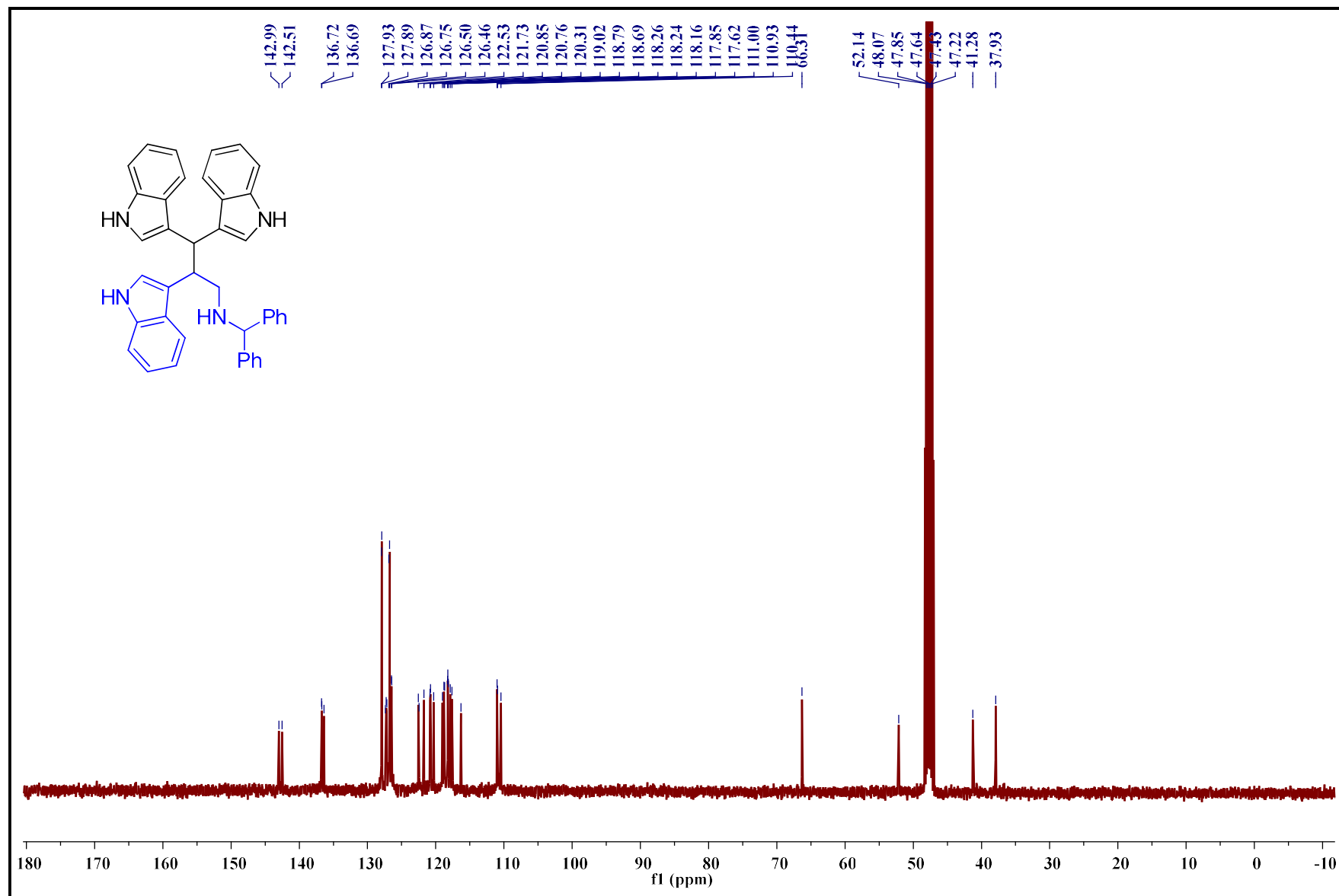
¹³C NMR spectrum of N-(4-(tert-butyl)benzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ei):



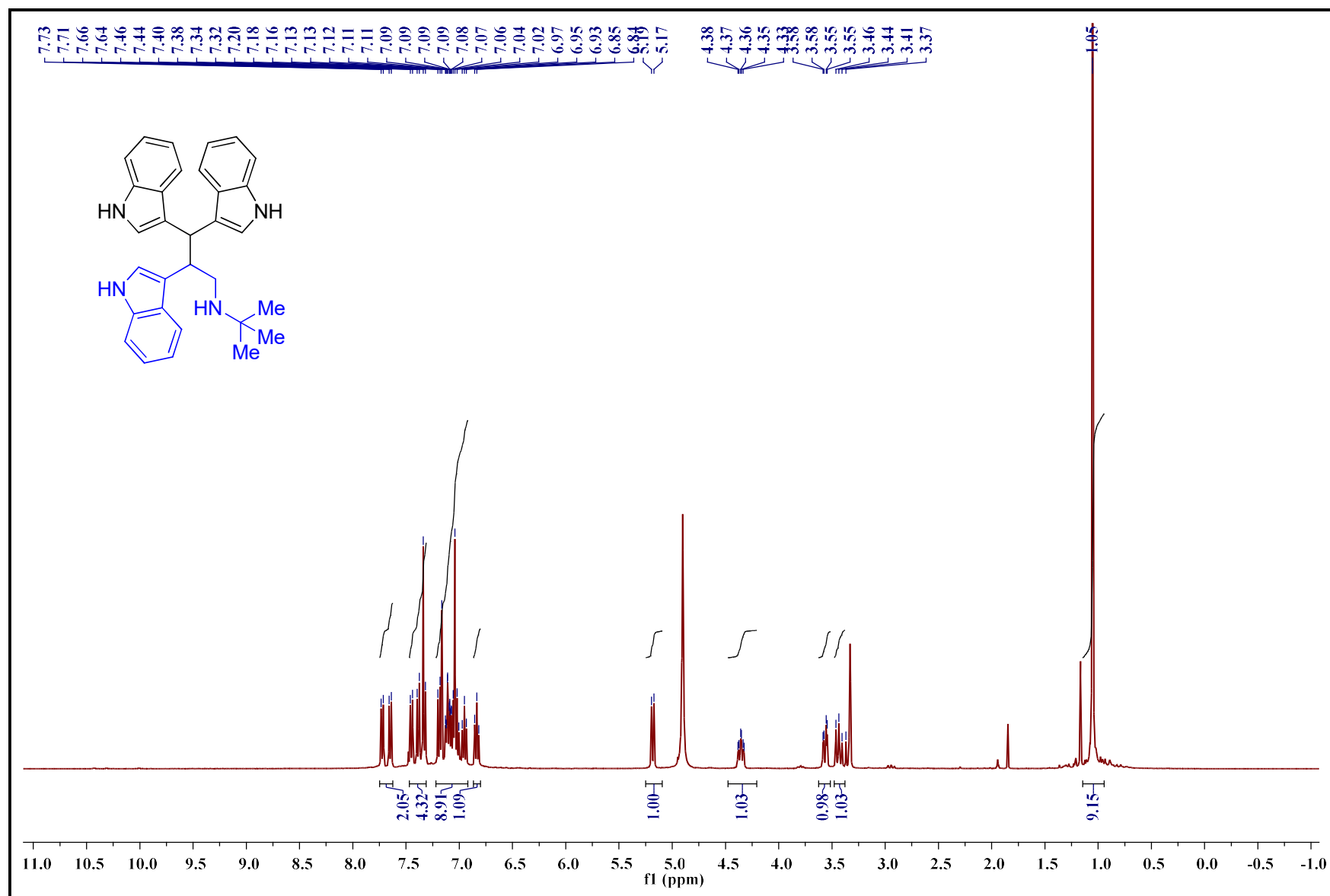
¹H NMR spectrum of N-benzhydryl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5fi):



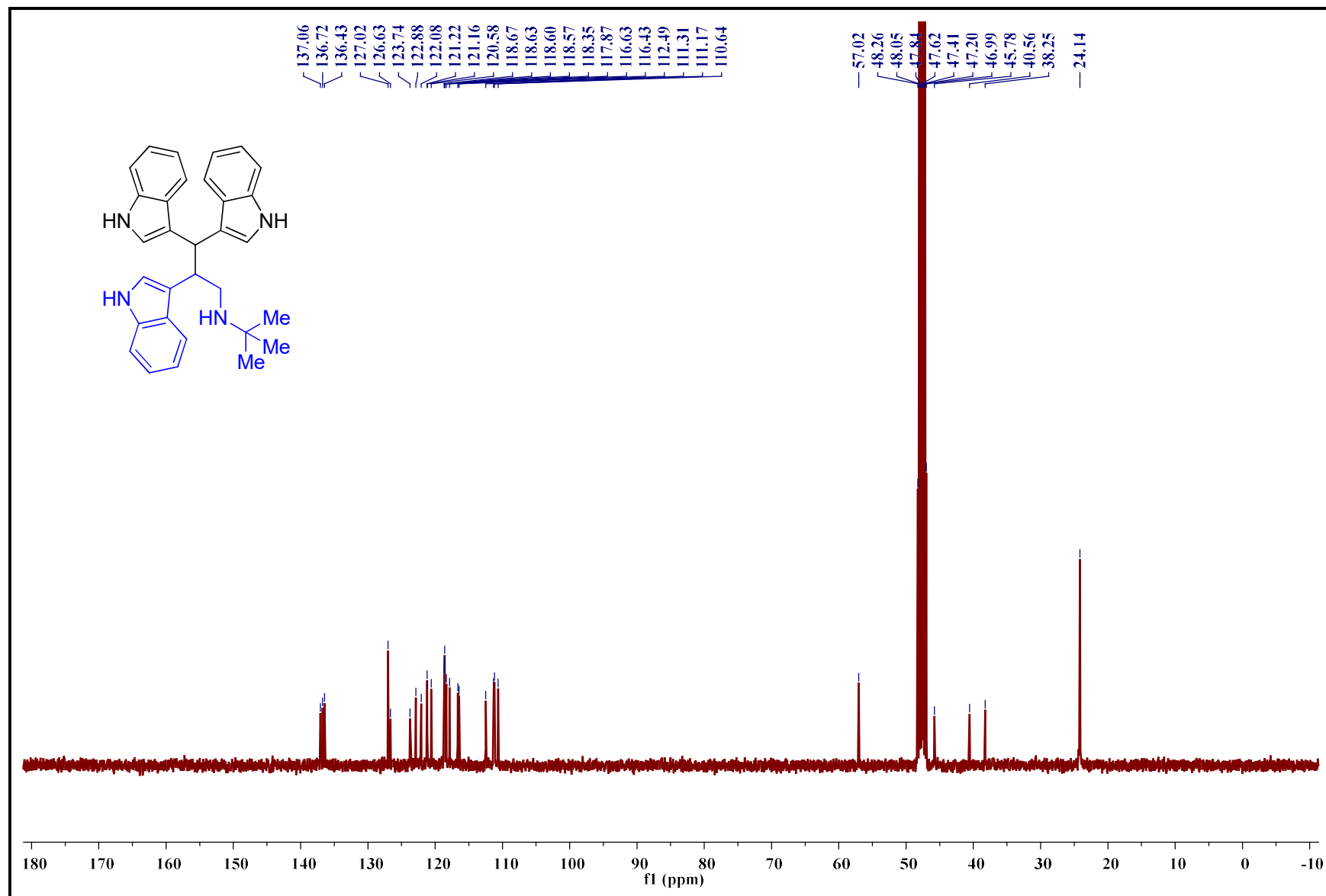
¹³C NMR spectrum of N-benzhydryl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5fi):



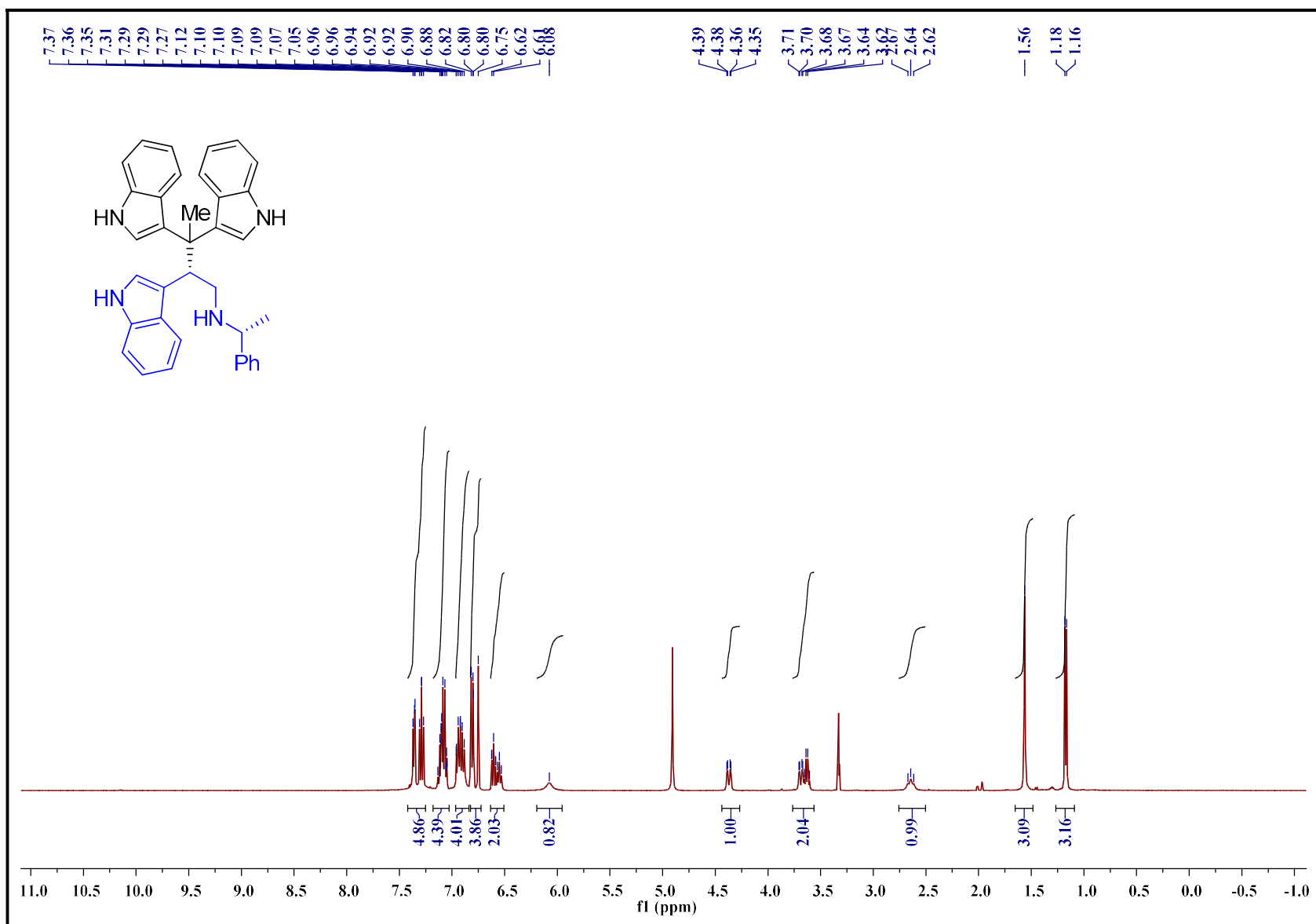
¹H NMR spectrum of N-(tert-butyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5gi):



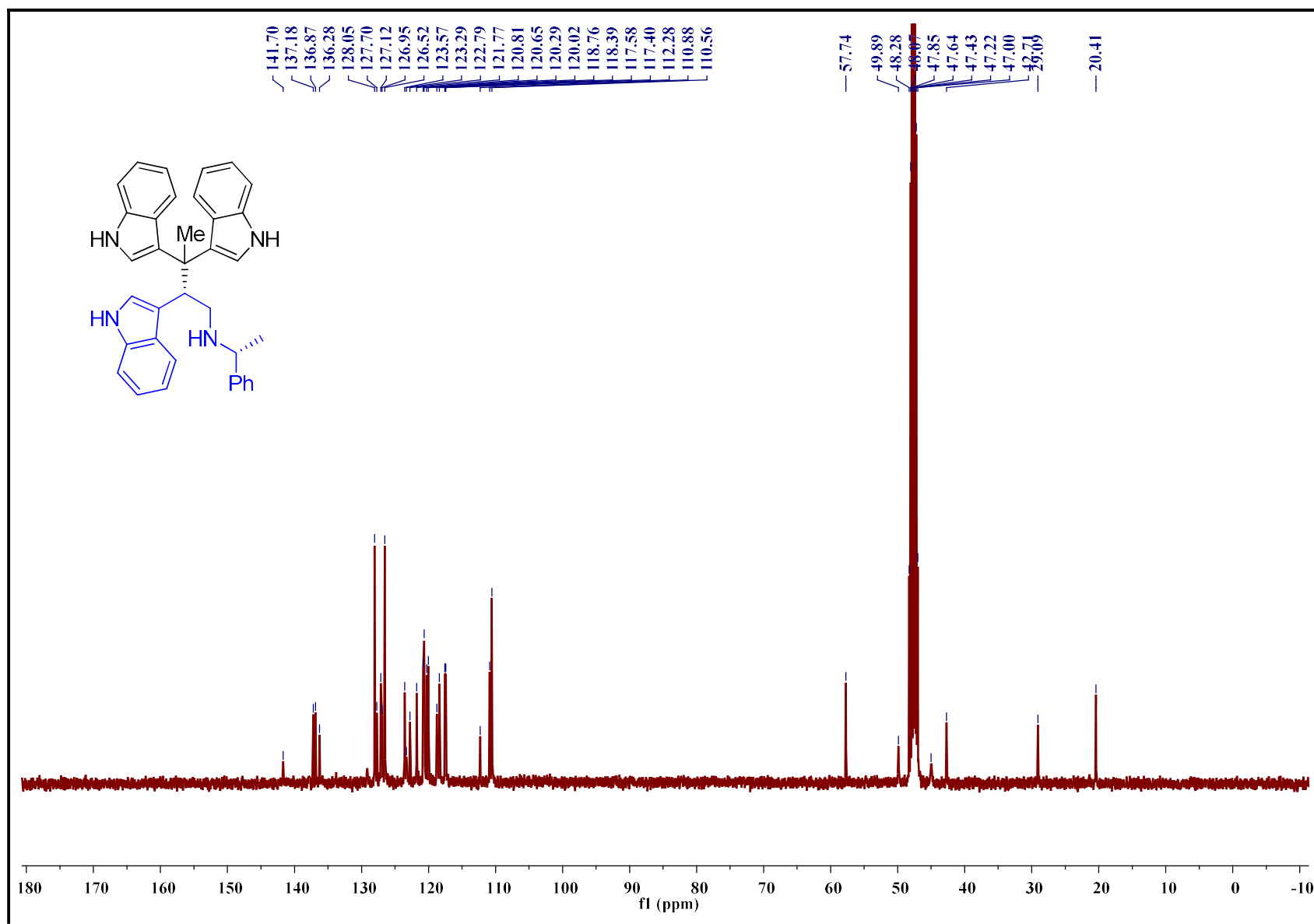
¹³C NMR spectrum of N-(tert-butyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5gi):



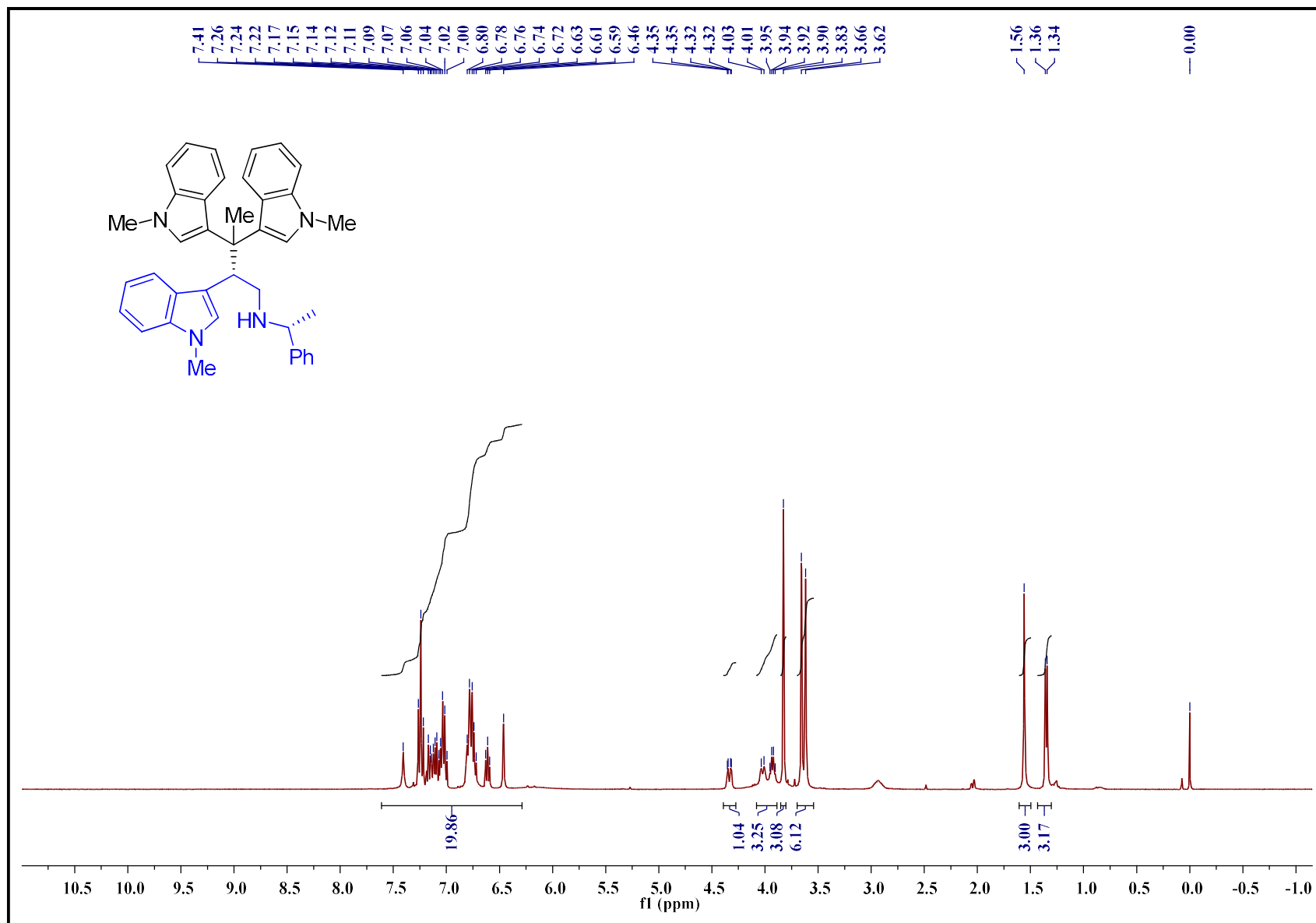
¹H NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6ai):



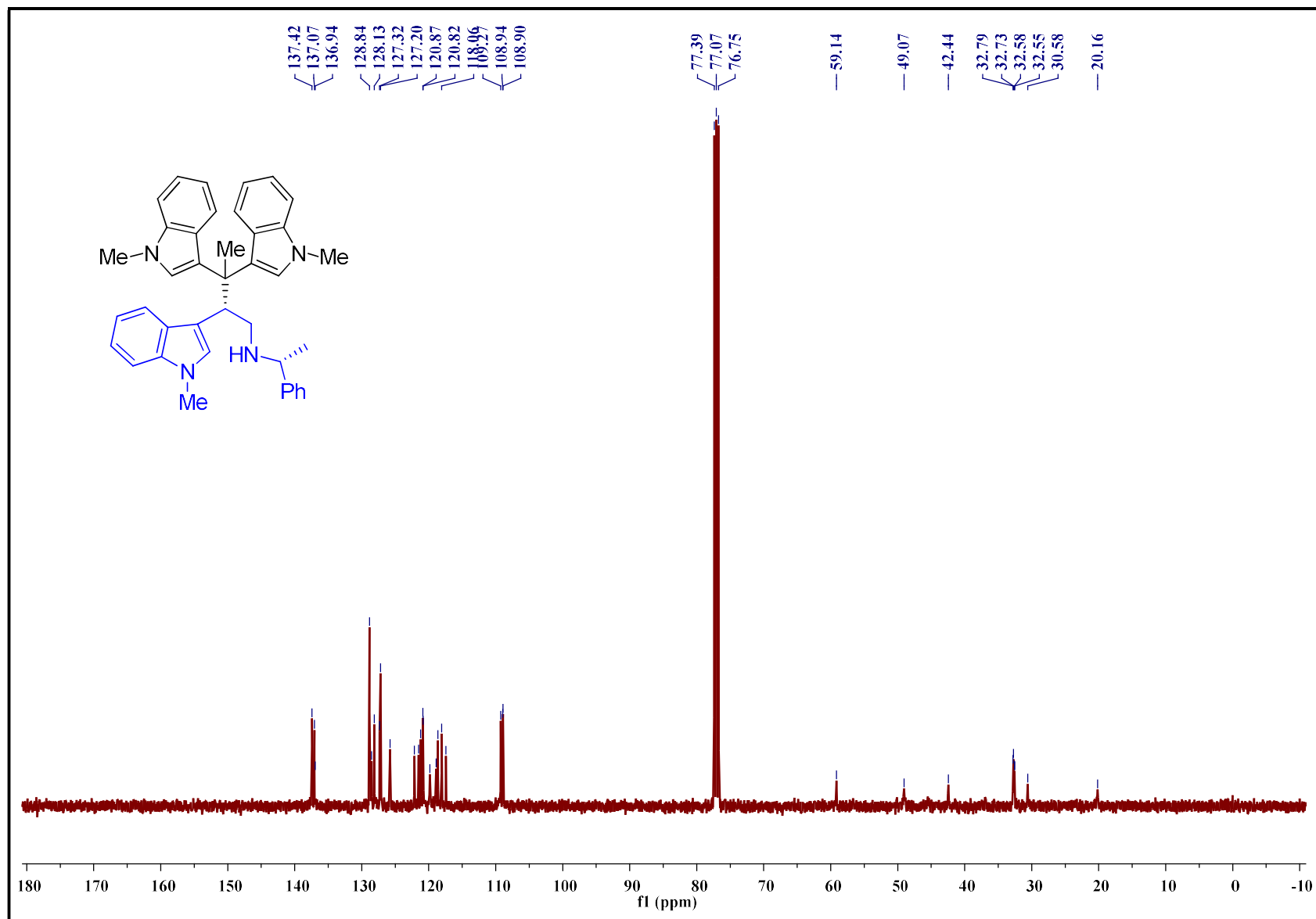
¹³C NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6ai):



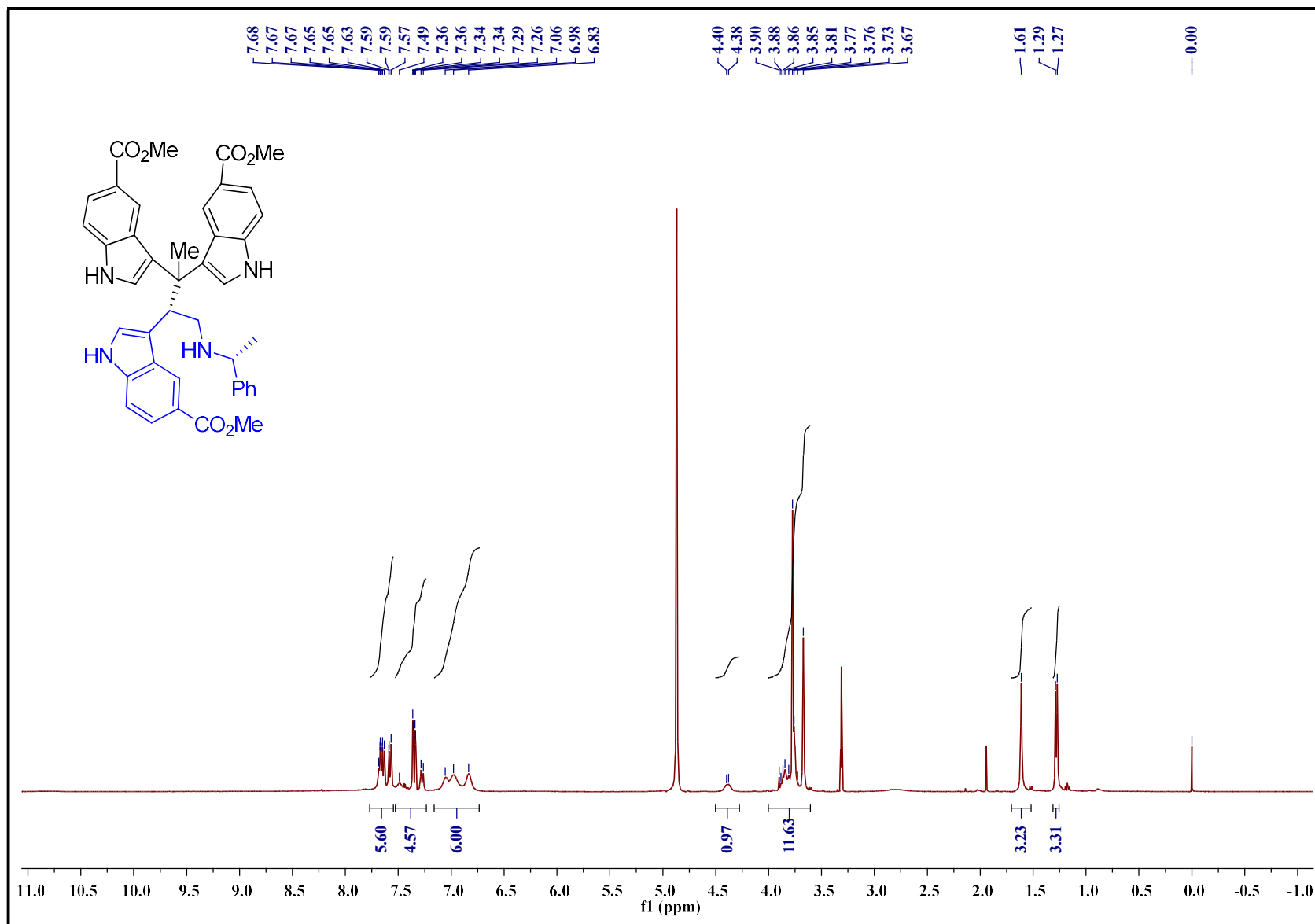
¹H NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6am):



¹³C NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6am):



¹H NMR spectrum of Trimethyl 3,3',3''-((S)-4-(((R)-1-phenylethyl)amino)butane-2,2,3-triyl)tris(1H-indole-5-carboxylate) (6ao):



¹³C NMR spectrum of Trimethyl 3,3',3''-((S)-4-(((R)-1-phenylethyl)amino)butane-2,2,3-triyl)tris(1H-indole-5-carboxylate) (6ao):

