Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

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

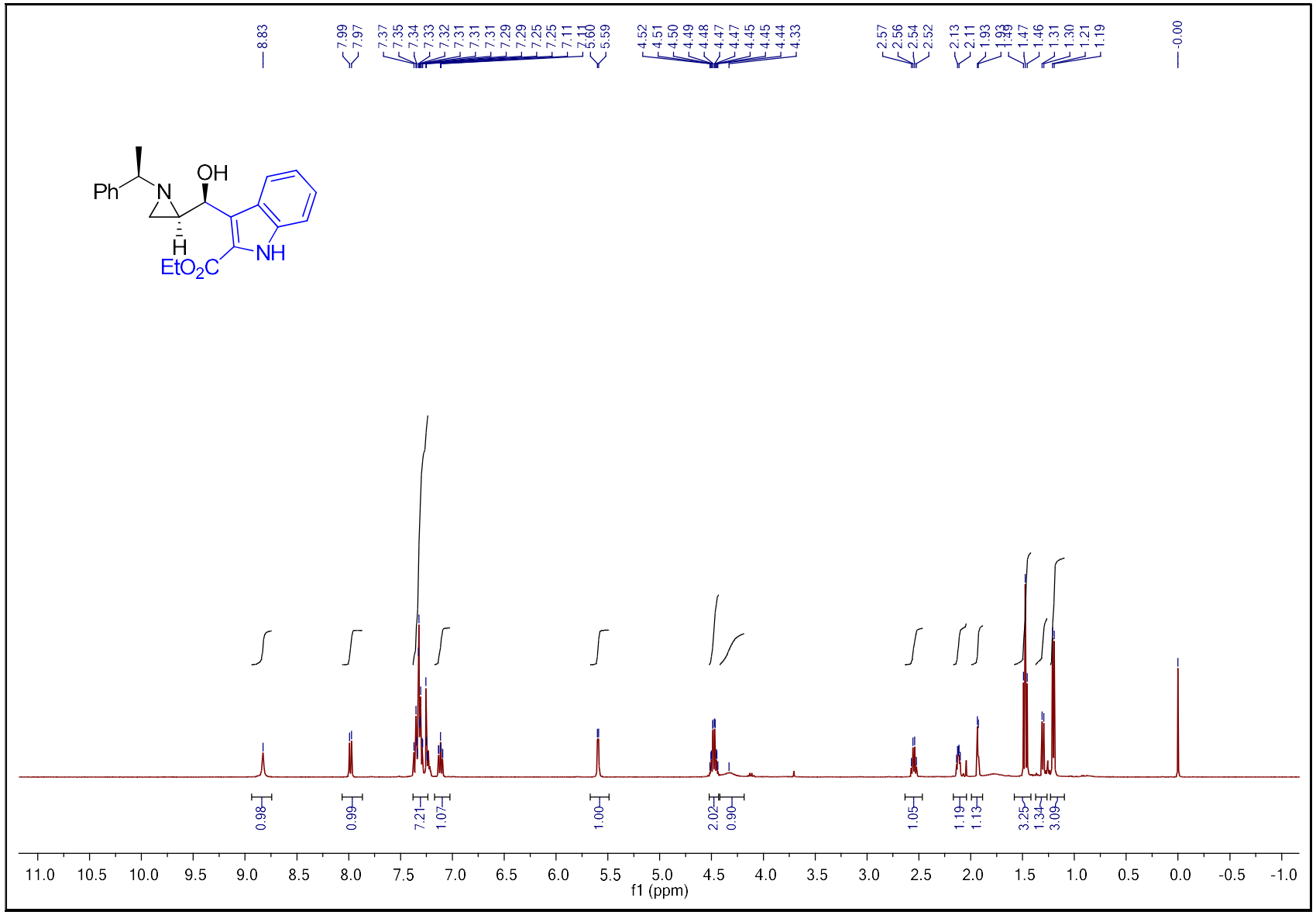
Lingamurthy Macha, Deepak Singh, Hyong-Jin Rhee and Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Yongin 17035, Korea

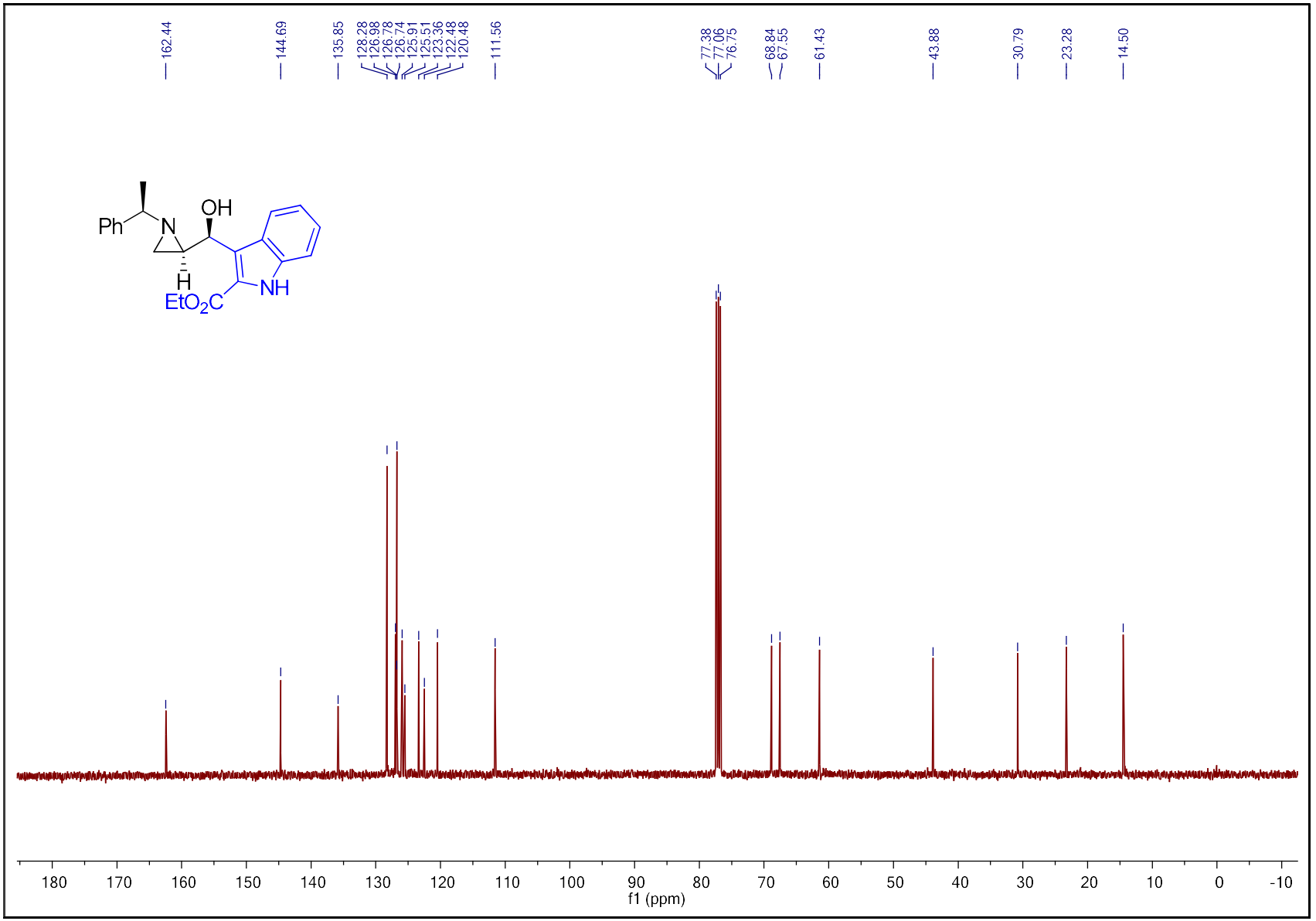
E-mail: hjha@hufs.ac.kr

Table of Contents:

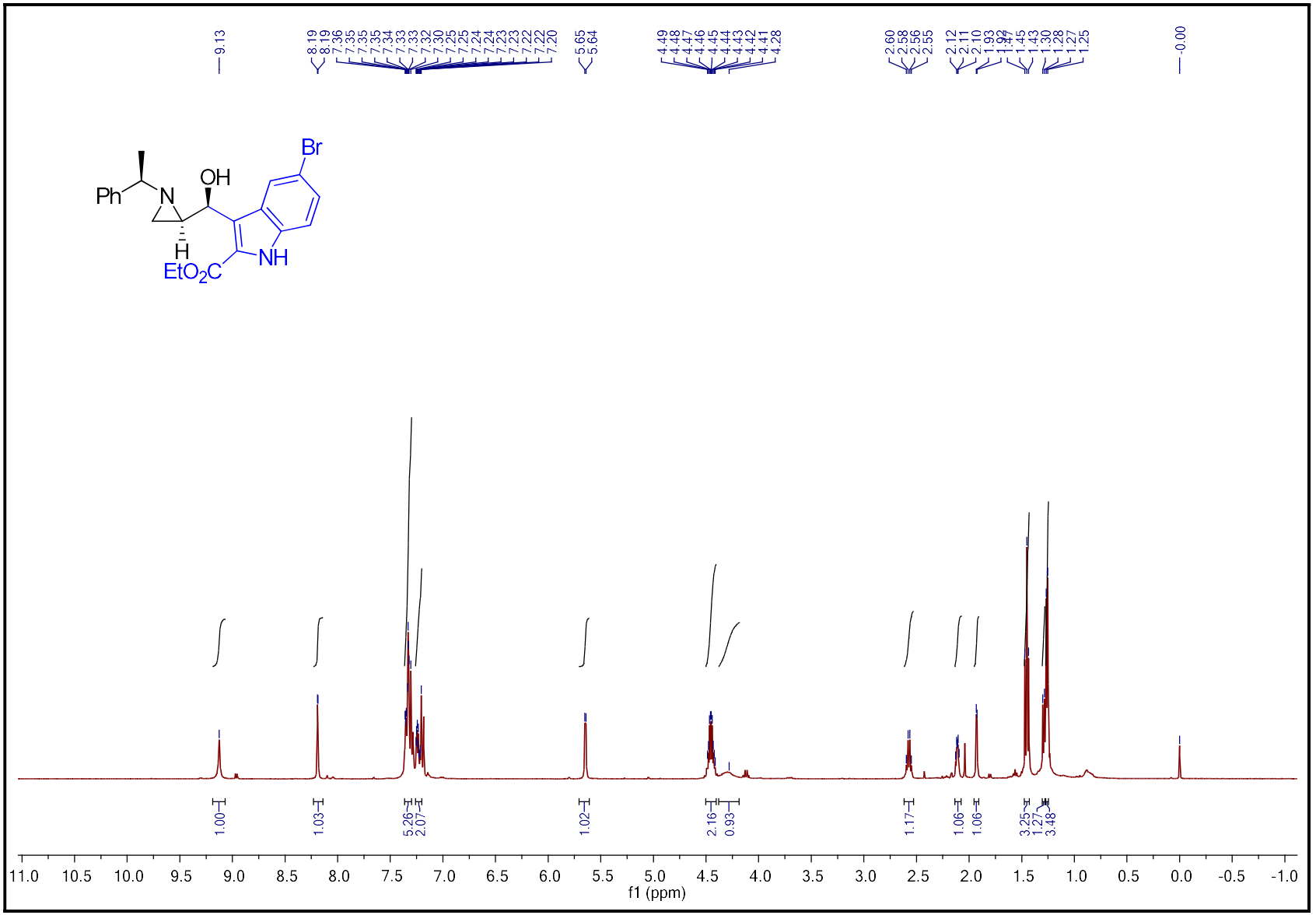
[1]H NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4aa):



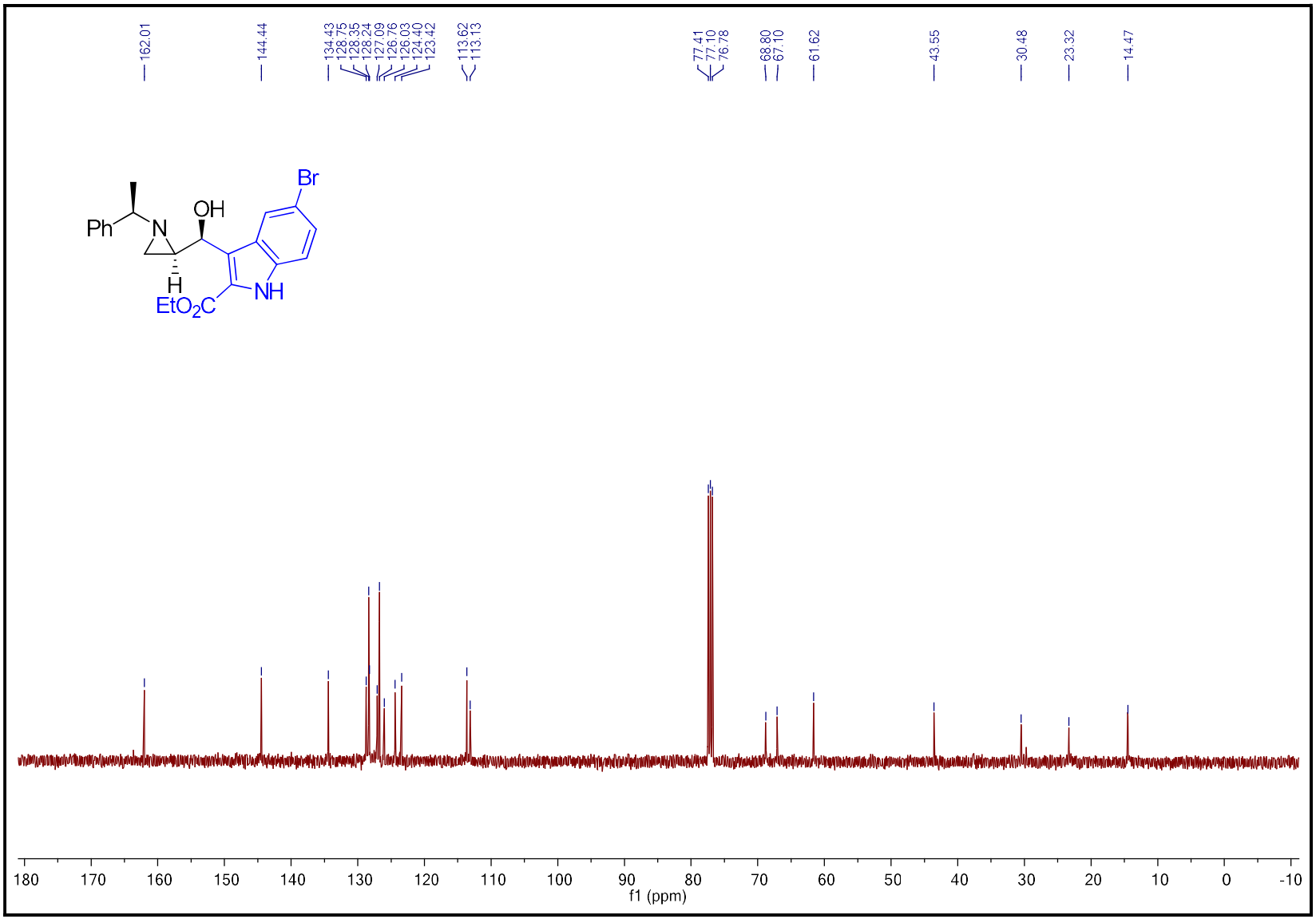
^{13}C NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4aa):



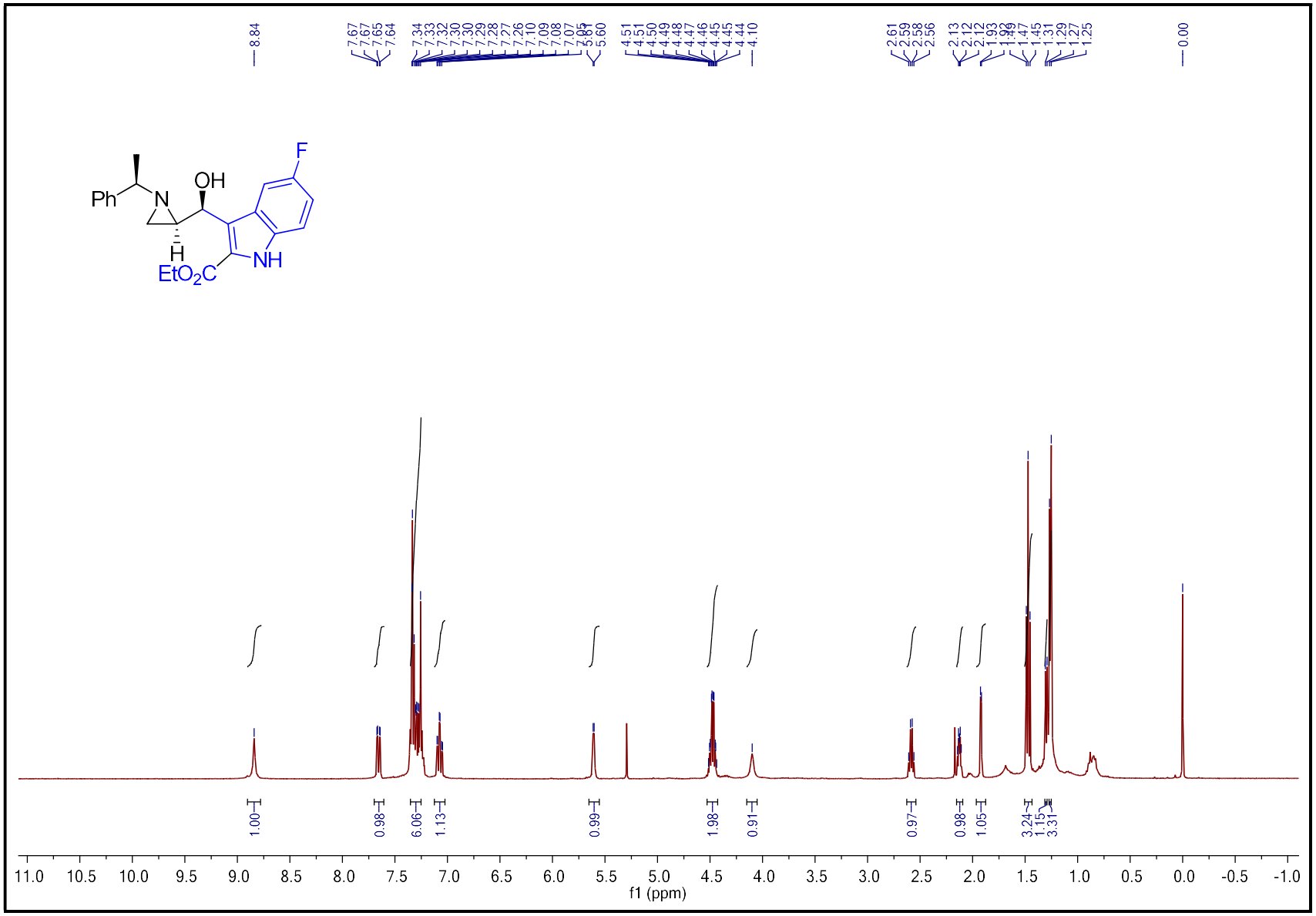
[1]H NMR spectrum of Ethyl 5-bromo-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ab):



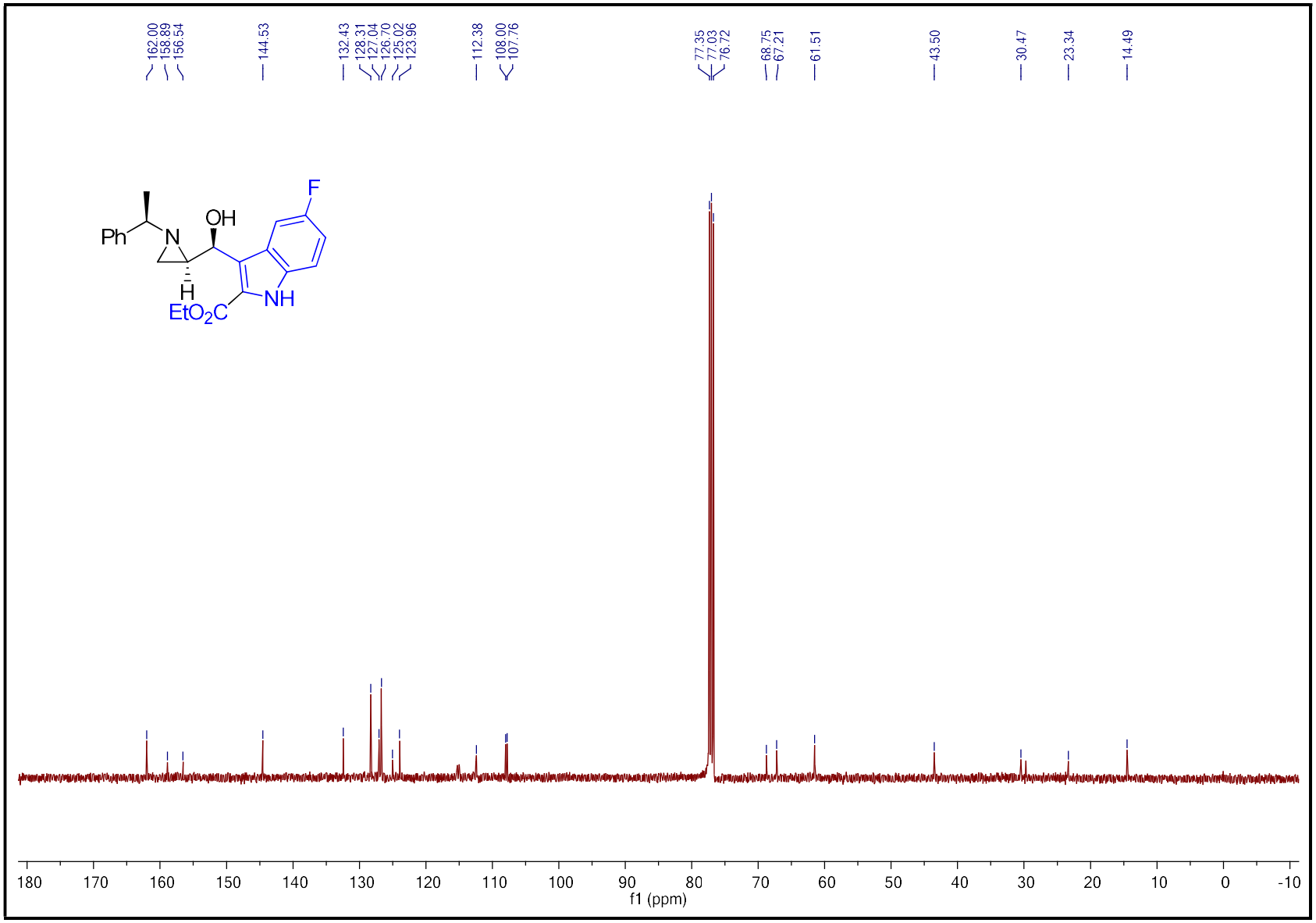
^{13}C NMR spectrum of Ethyl 5-bromo-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ab):



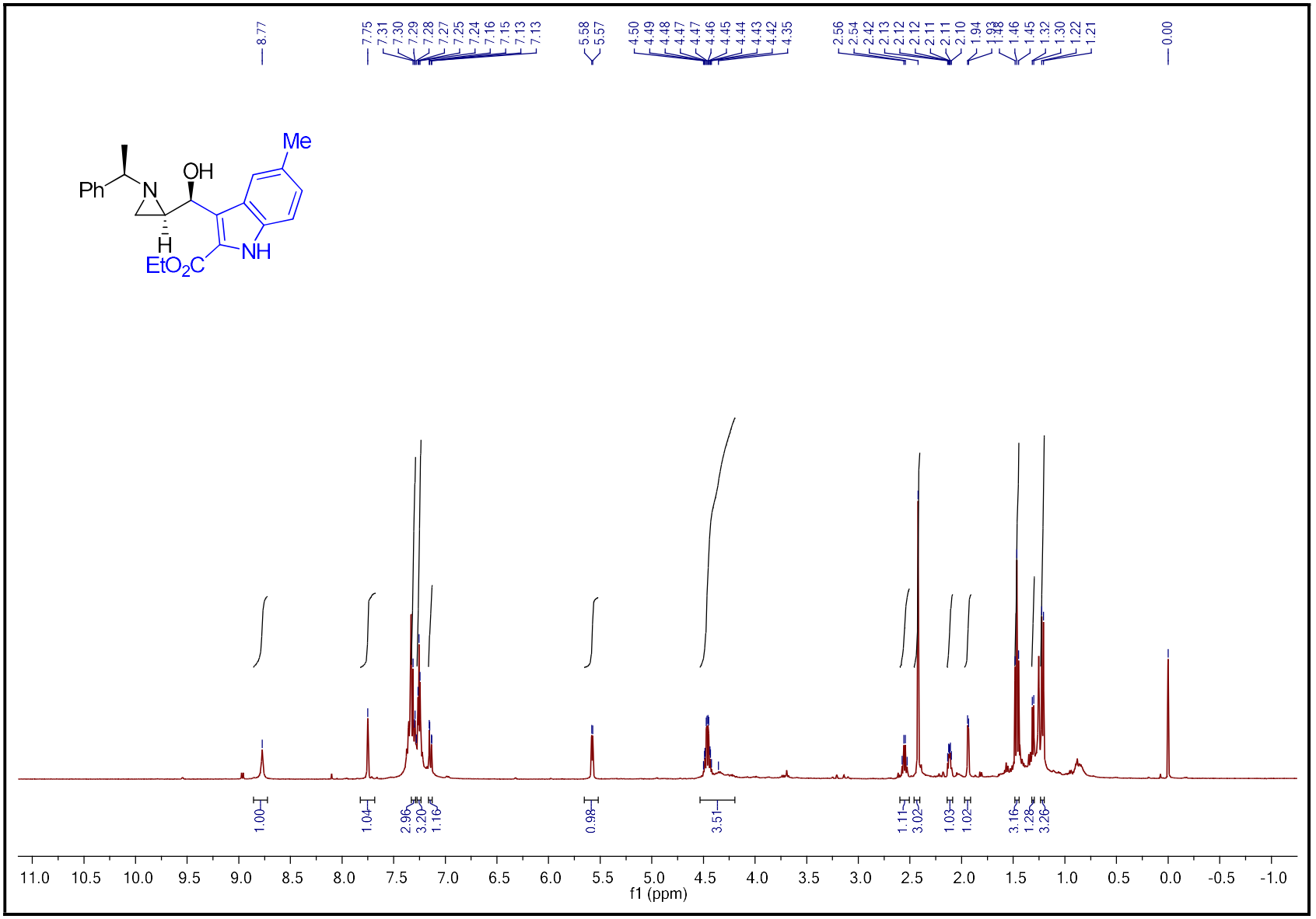
[1]H NMR spectrum of Ethyl 5-fluoro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ac):



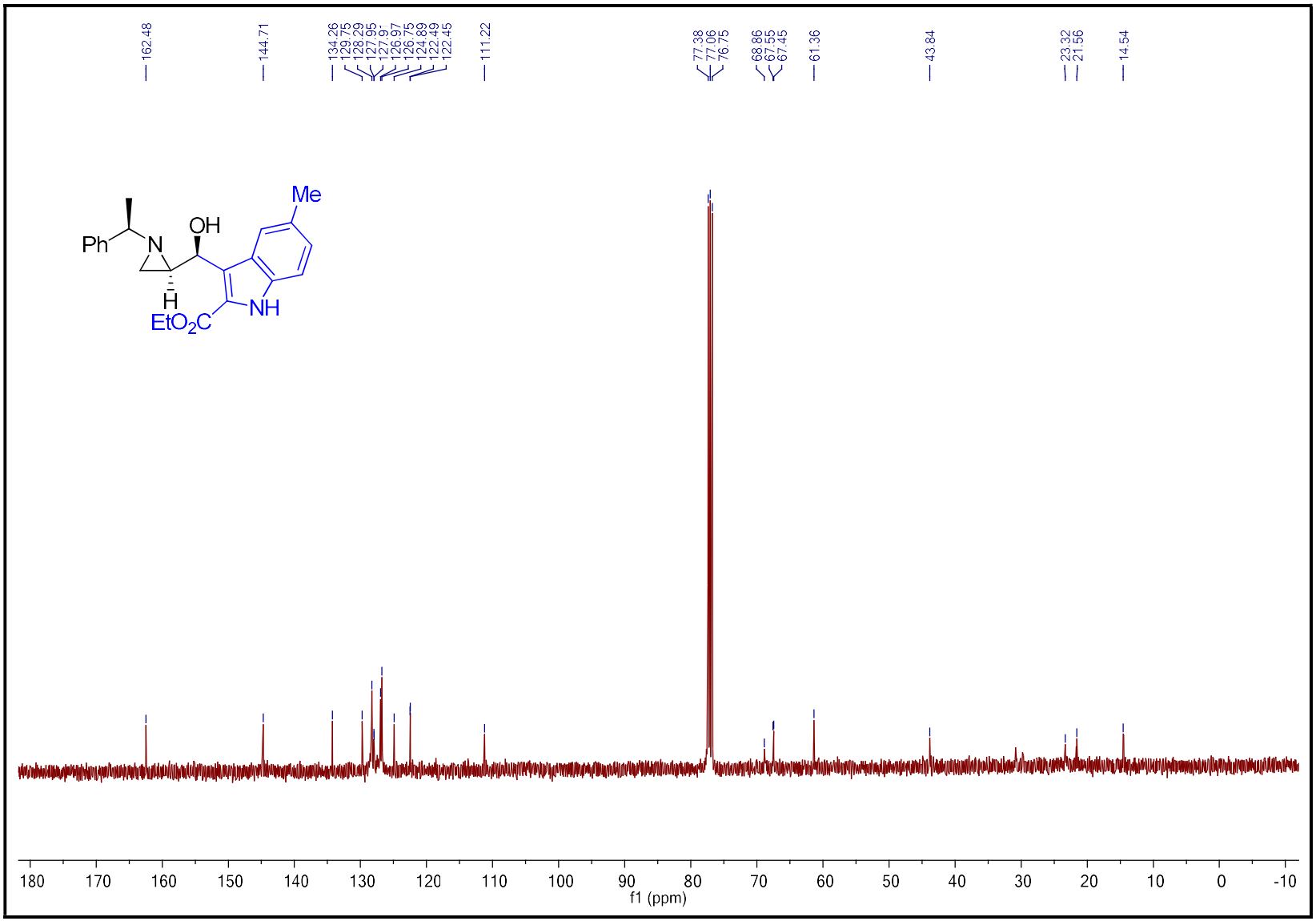
^{13}C NMR spectrum of Ethyl 5-fluoro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ac):



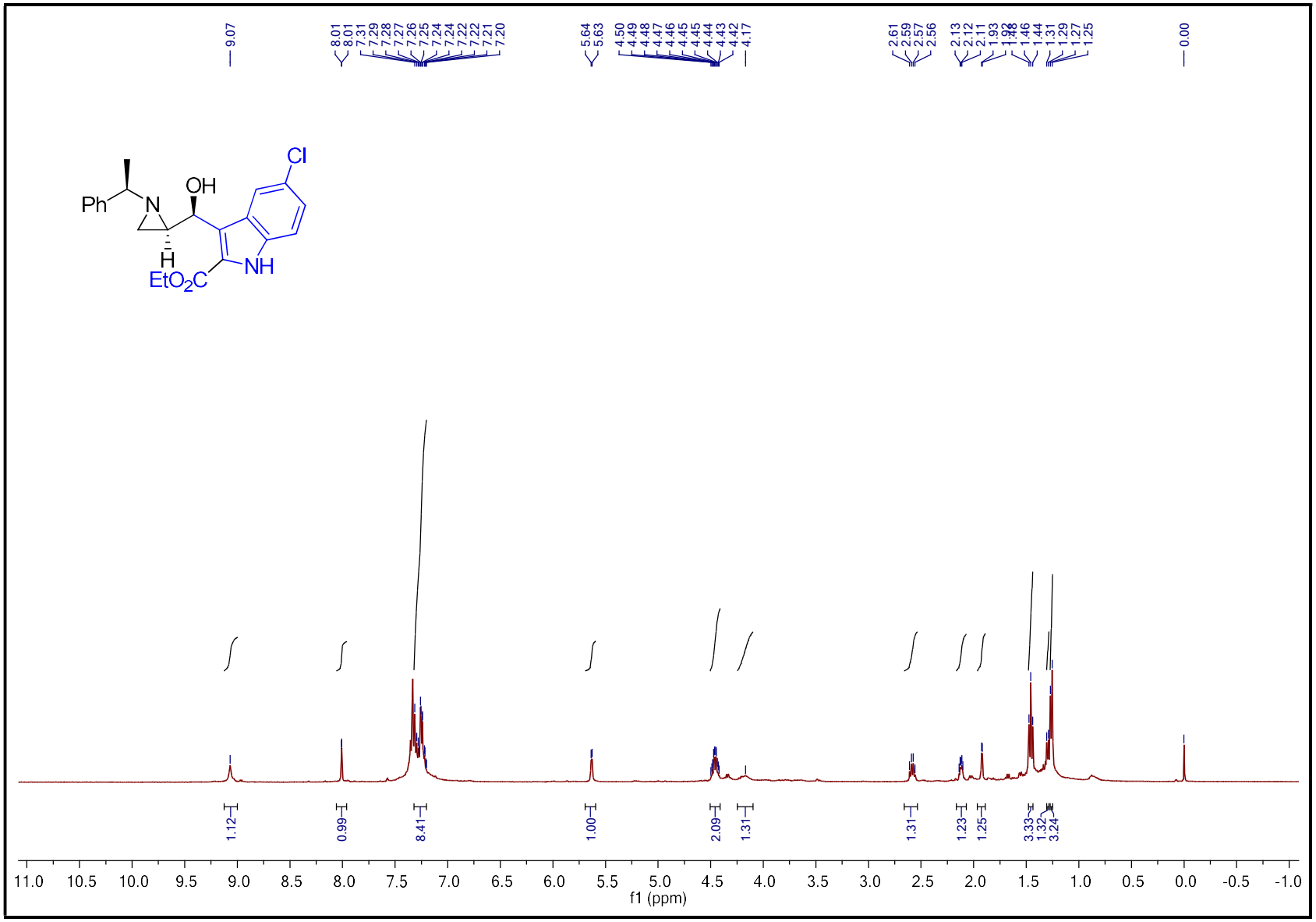
[1]H NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-5-methyl-1H-indole-2-carboxylate (4ad):



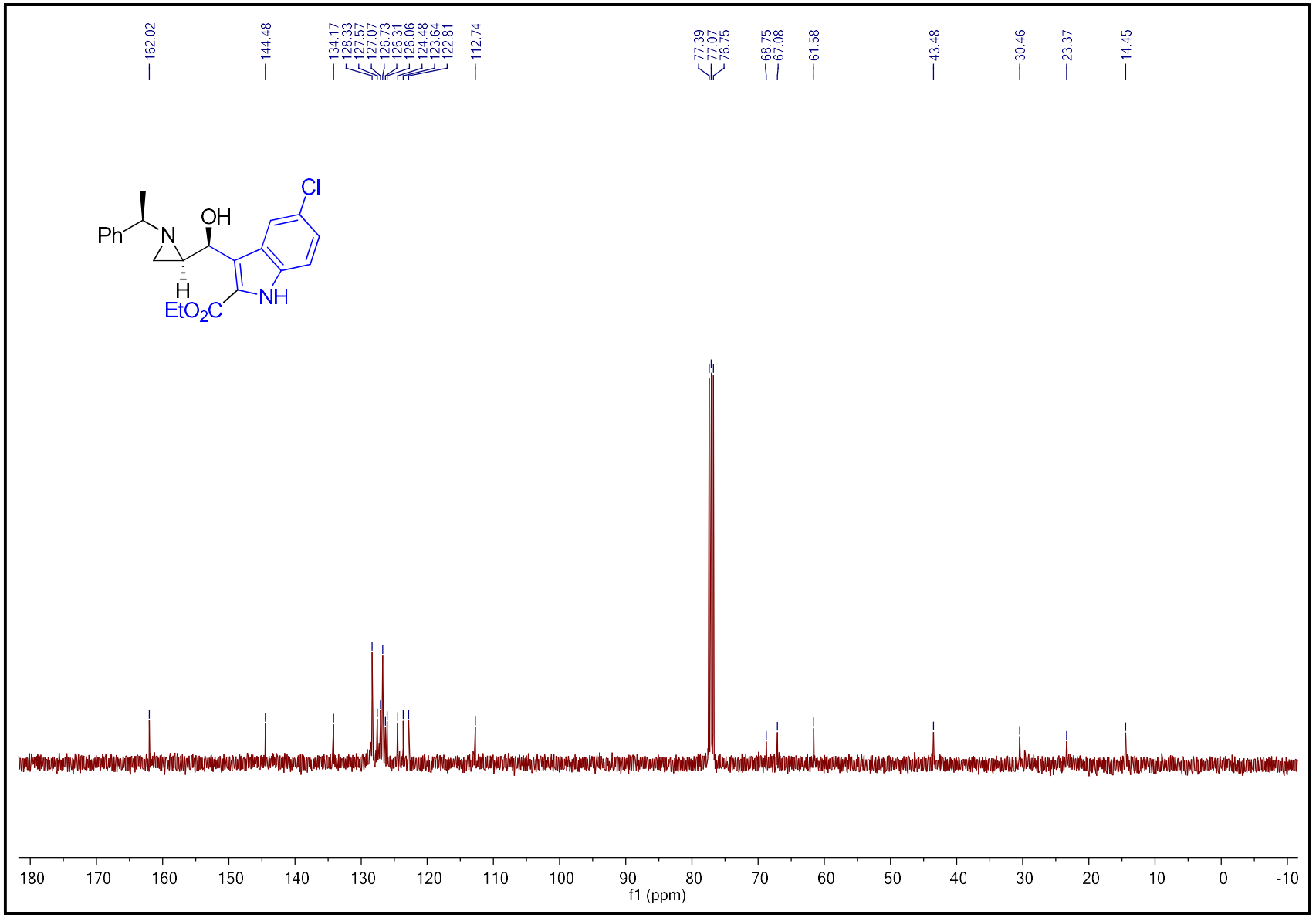
^{13}C NMR spectrum of Ethyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-5-methyl-1H-indole-2-carboxylate (4ad):



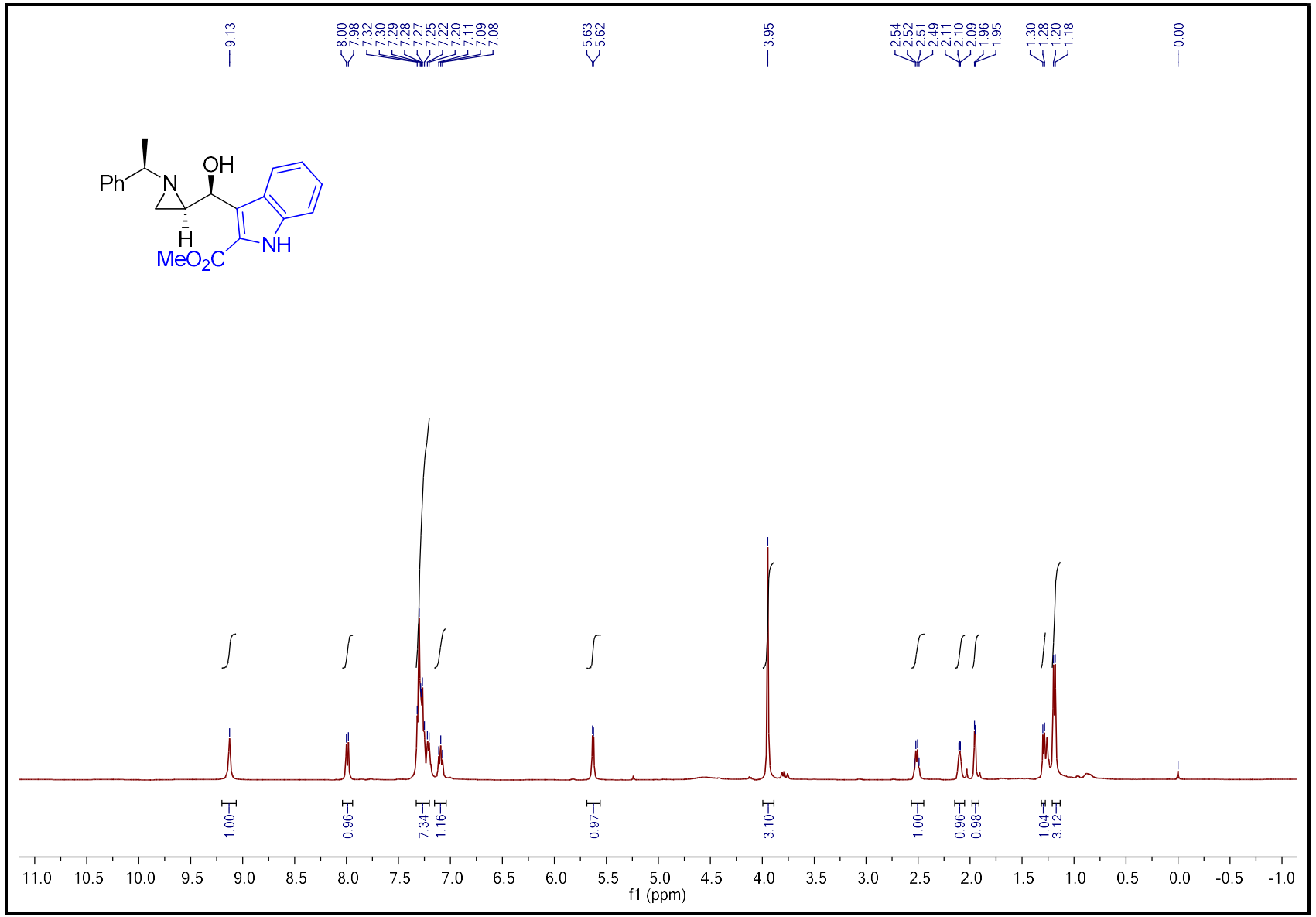
[1]H NMR spectrum of Ethyl 5-chloro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ae):



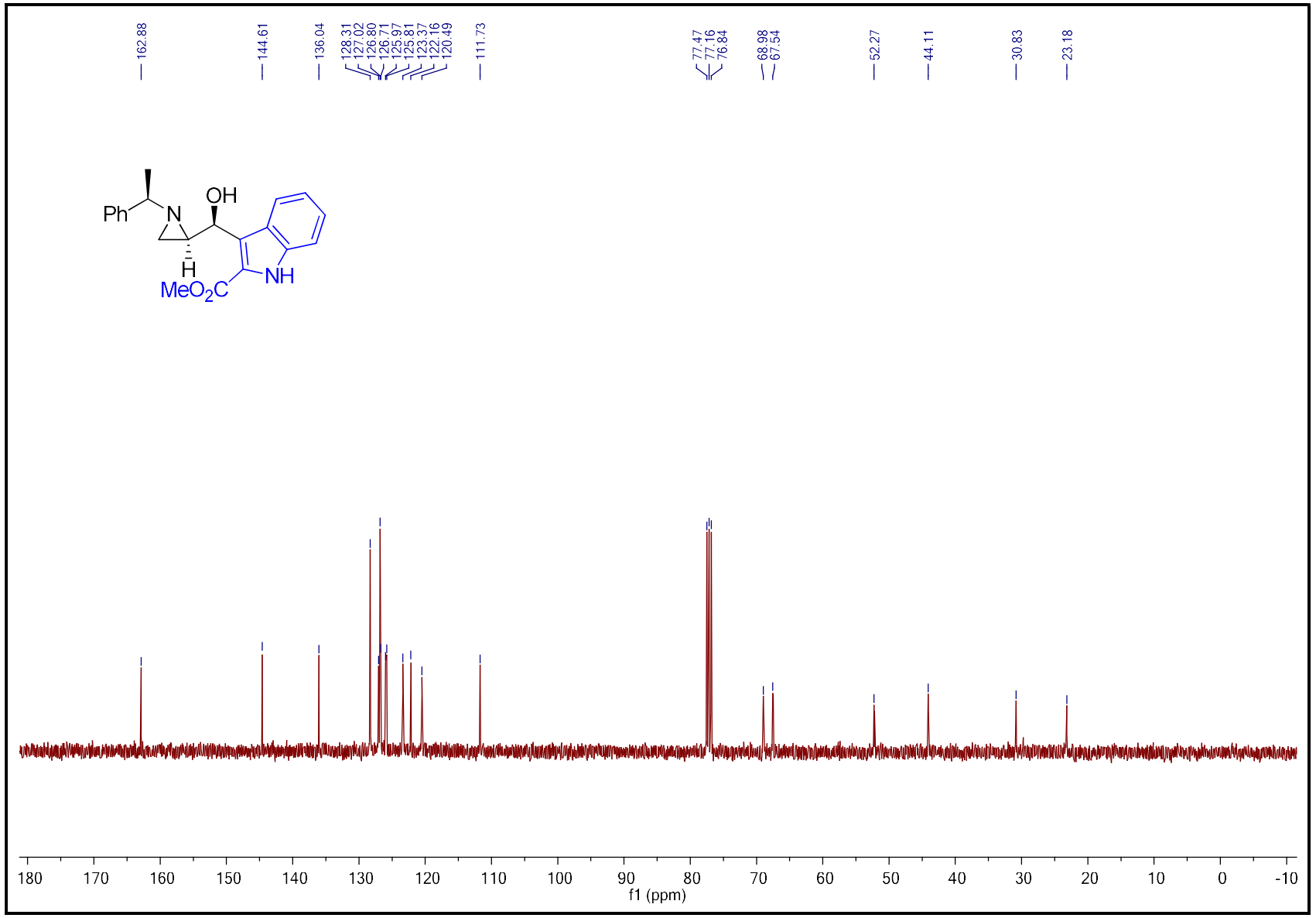
^{13}C NMR spectrum of Ethyl 5-chloro-3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4ae):



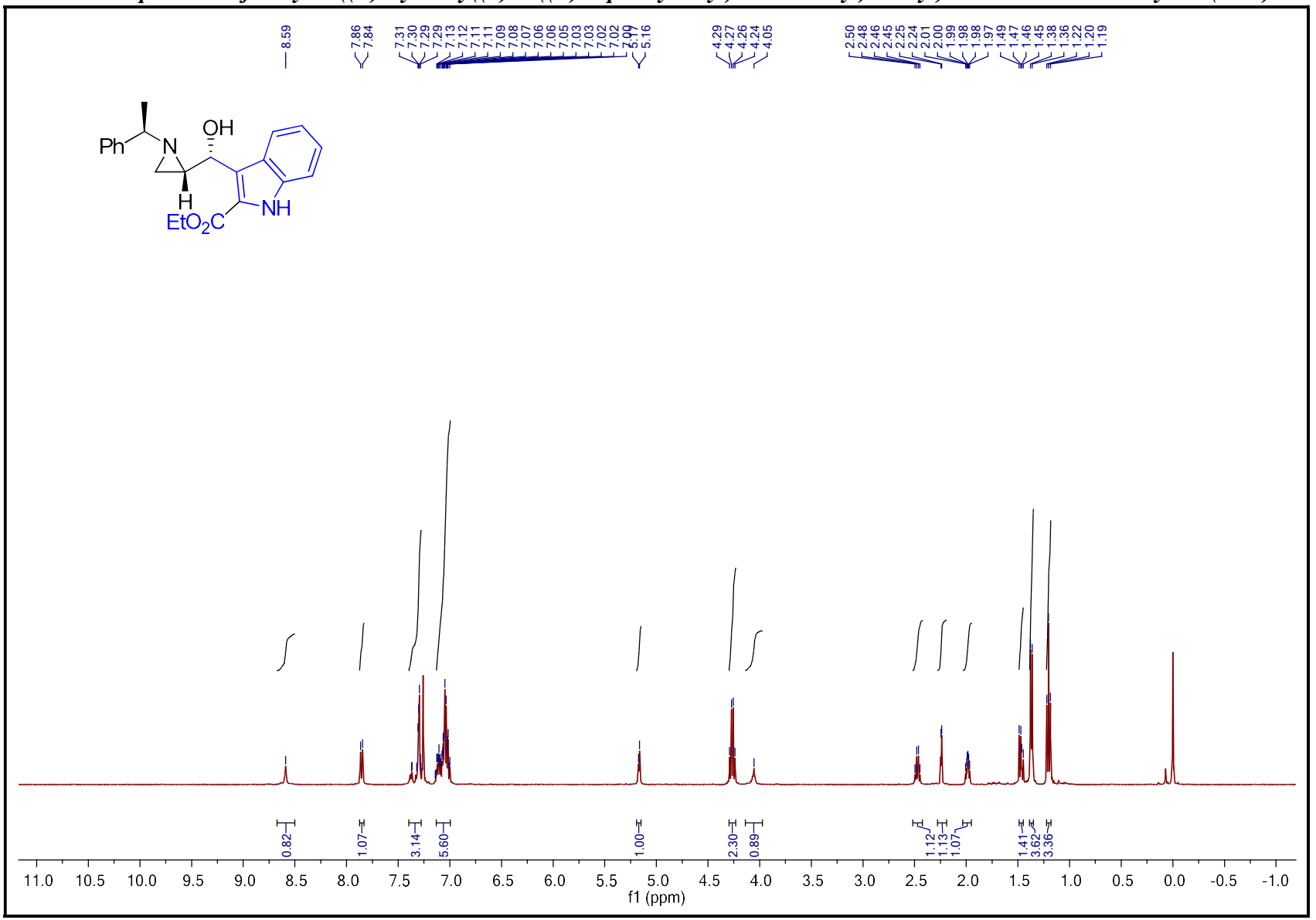
[1]H NMR spectrum of Methyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4af):



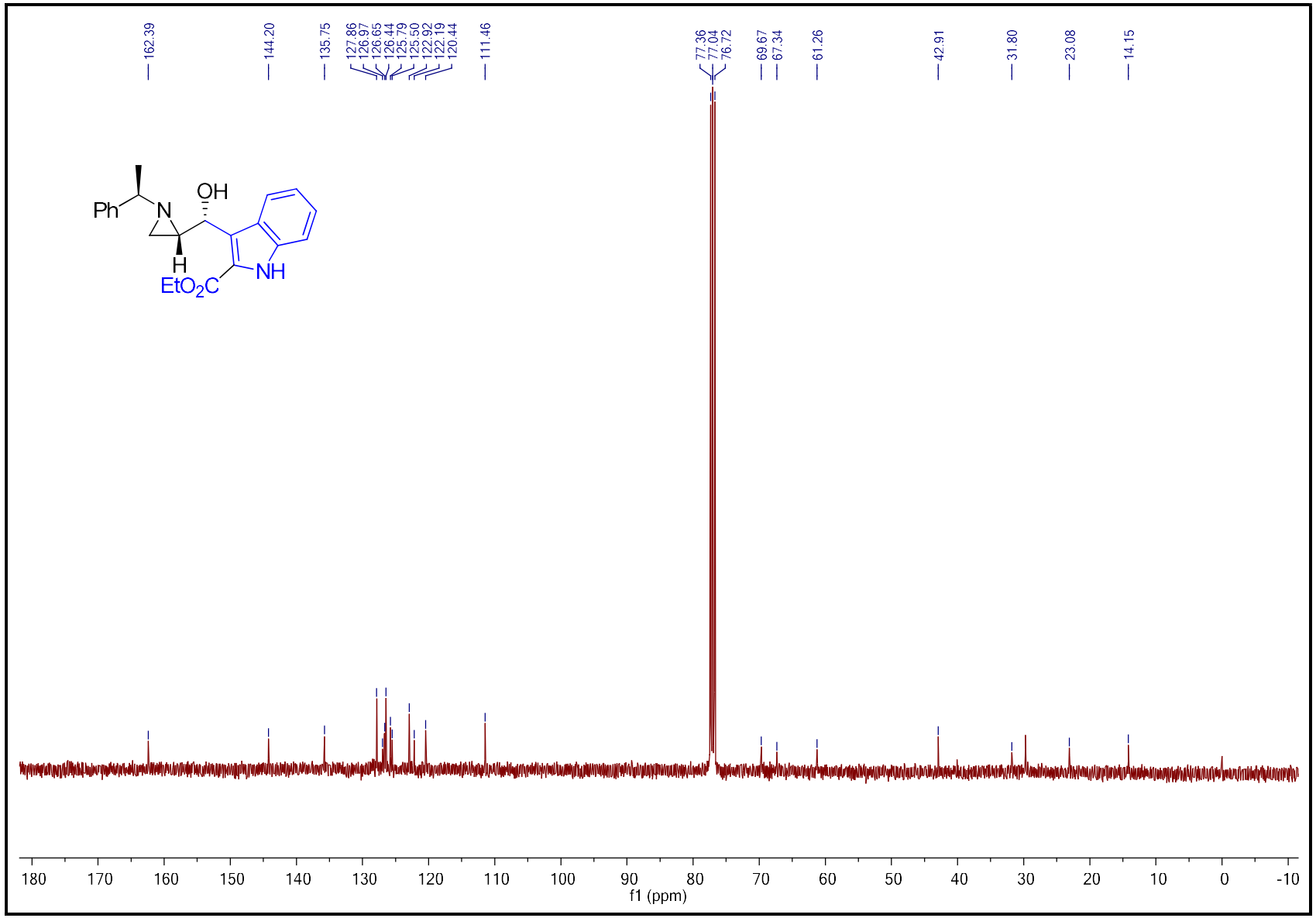
^{13}C NMR spectrum of Methyl 3-((S)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4af):



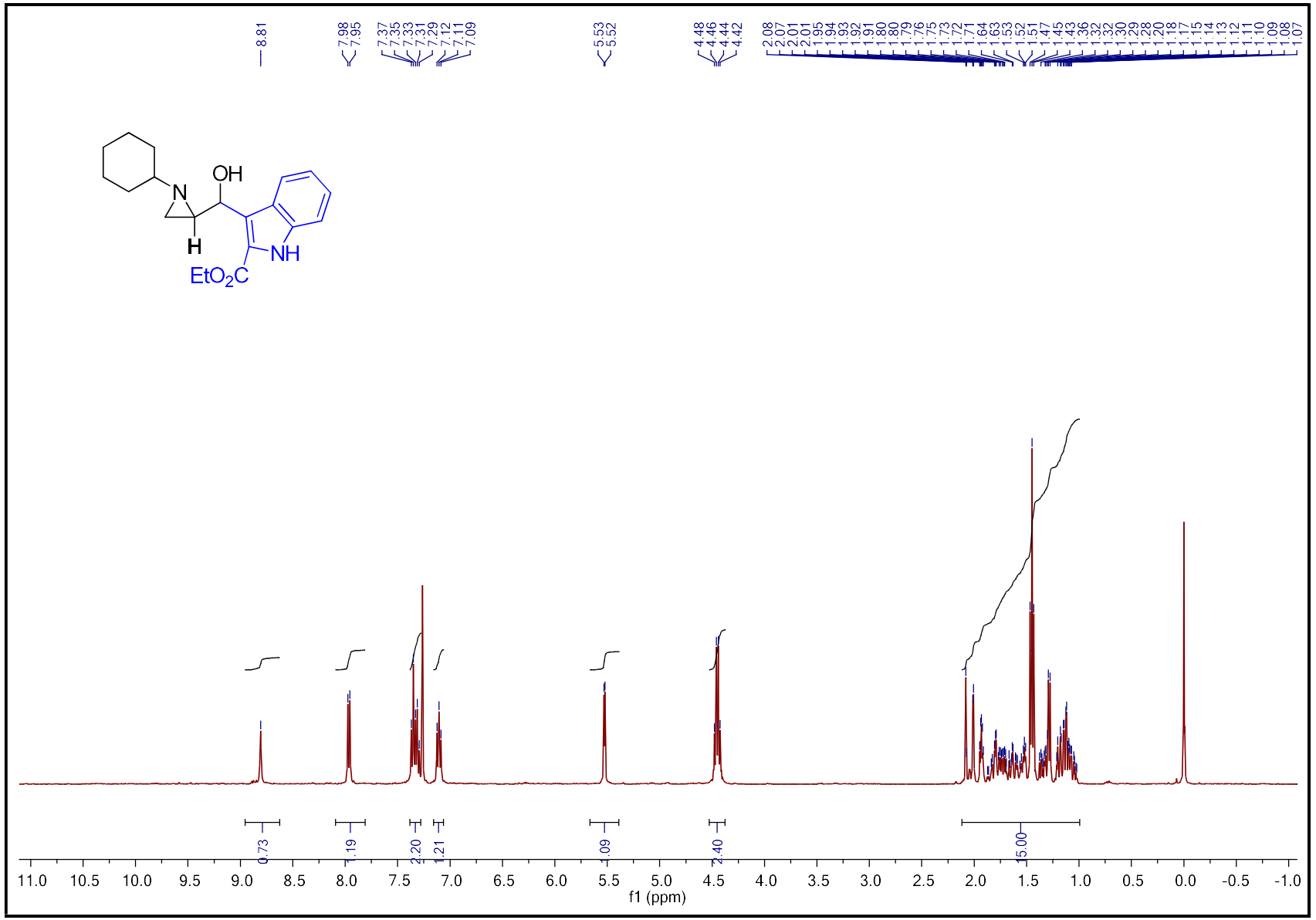
^{1}H NMR spectrum of Ethyl 3-((R)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4a'a):



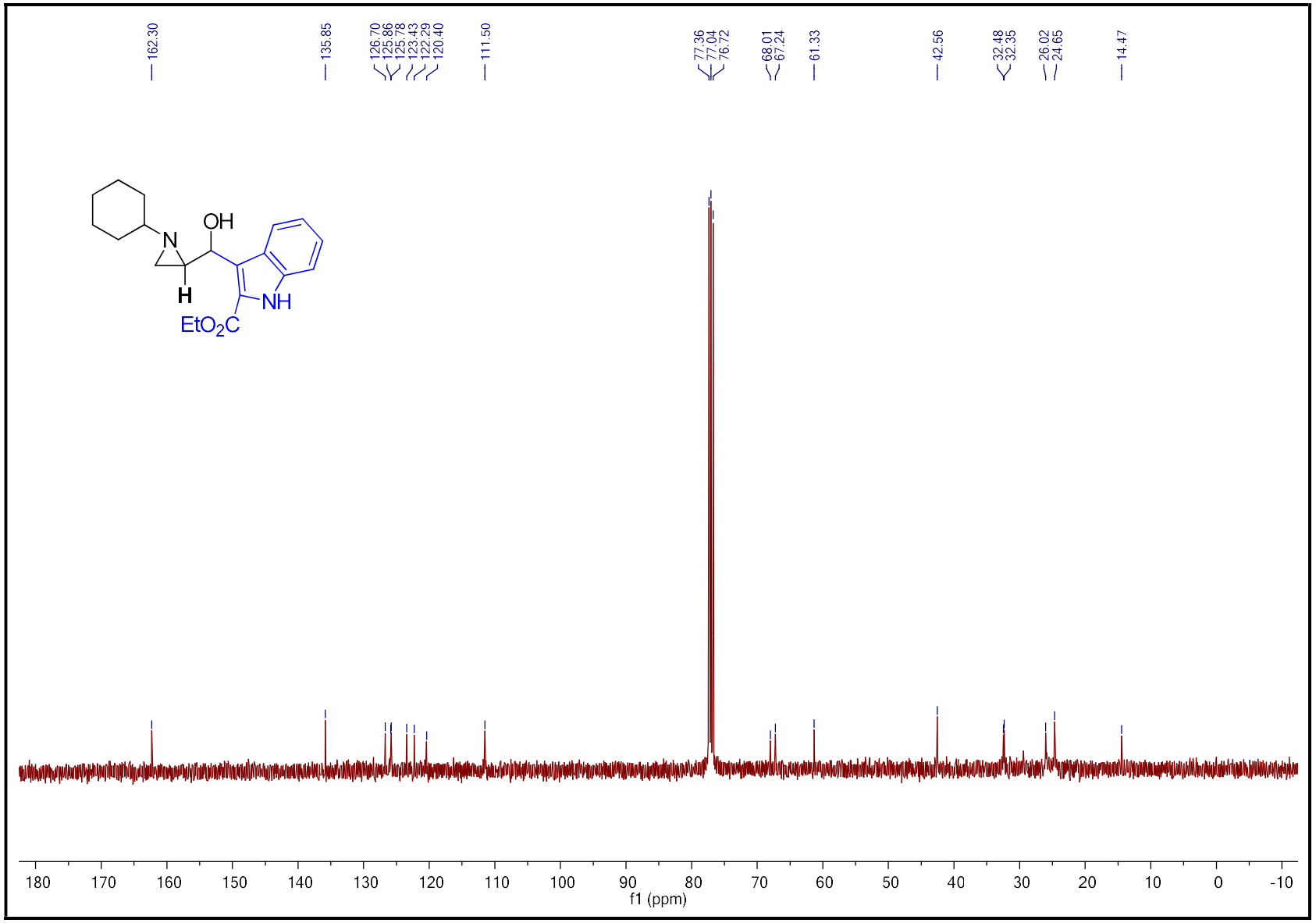
^{13}C NMR spectrum of Ethyl 3-((R)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indole-2-carboxylate (4a'a):



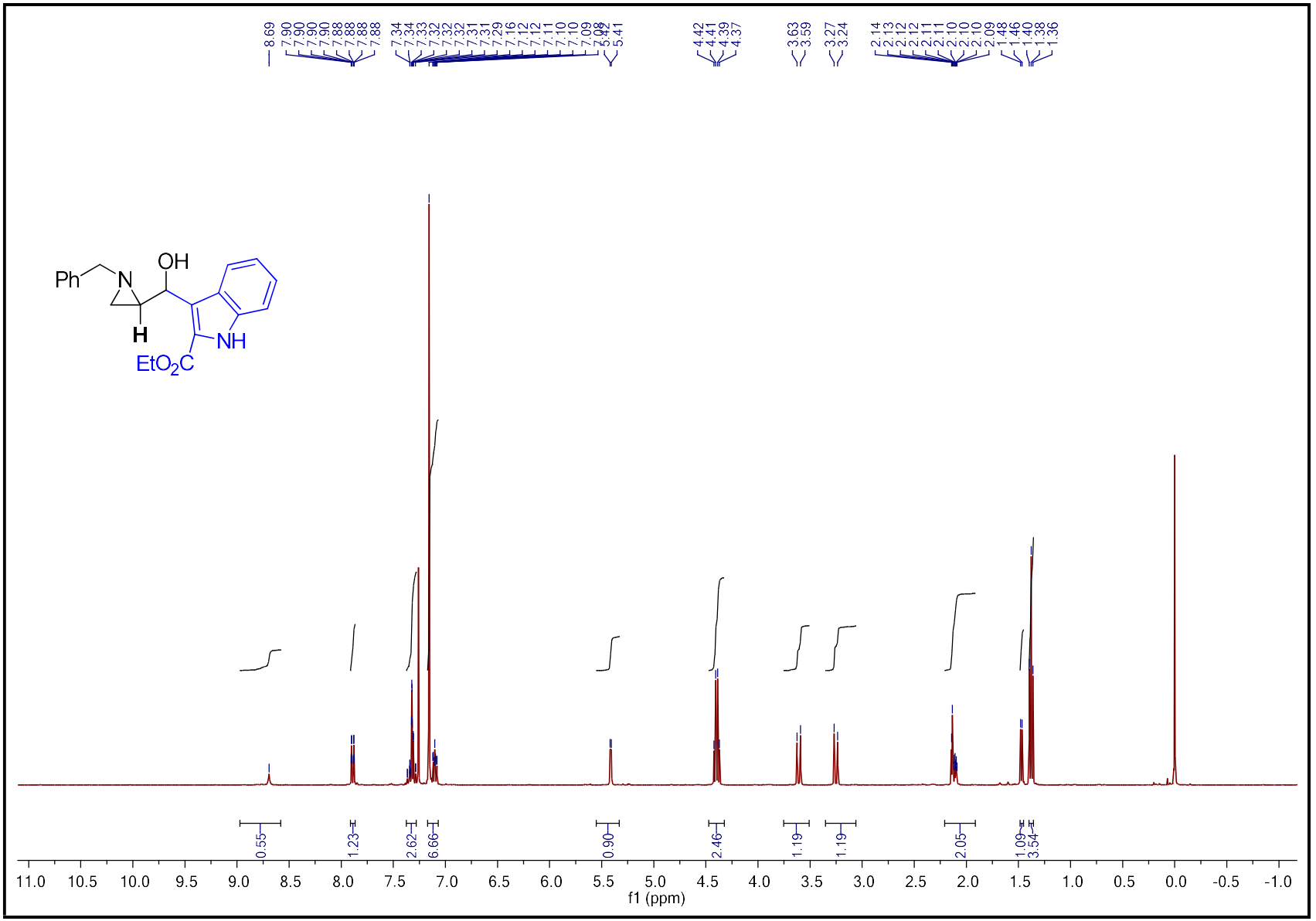
^{1}H NMR spectrum of Ethyl 3-((1-cyclohexylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ba):



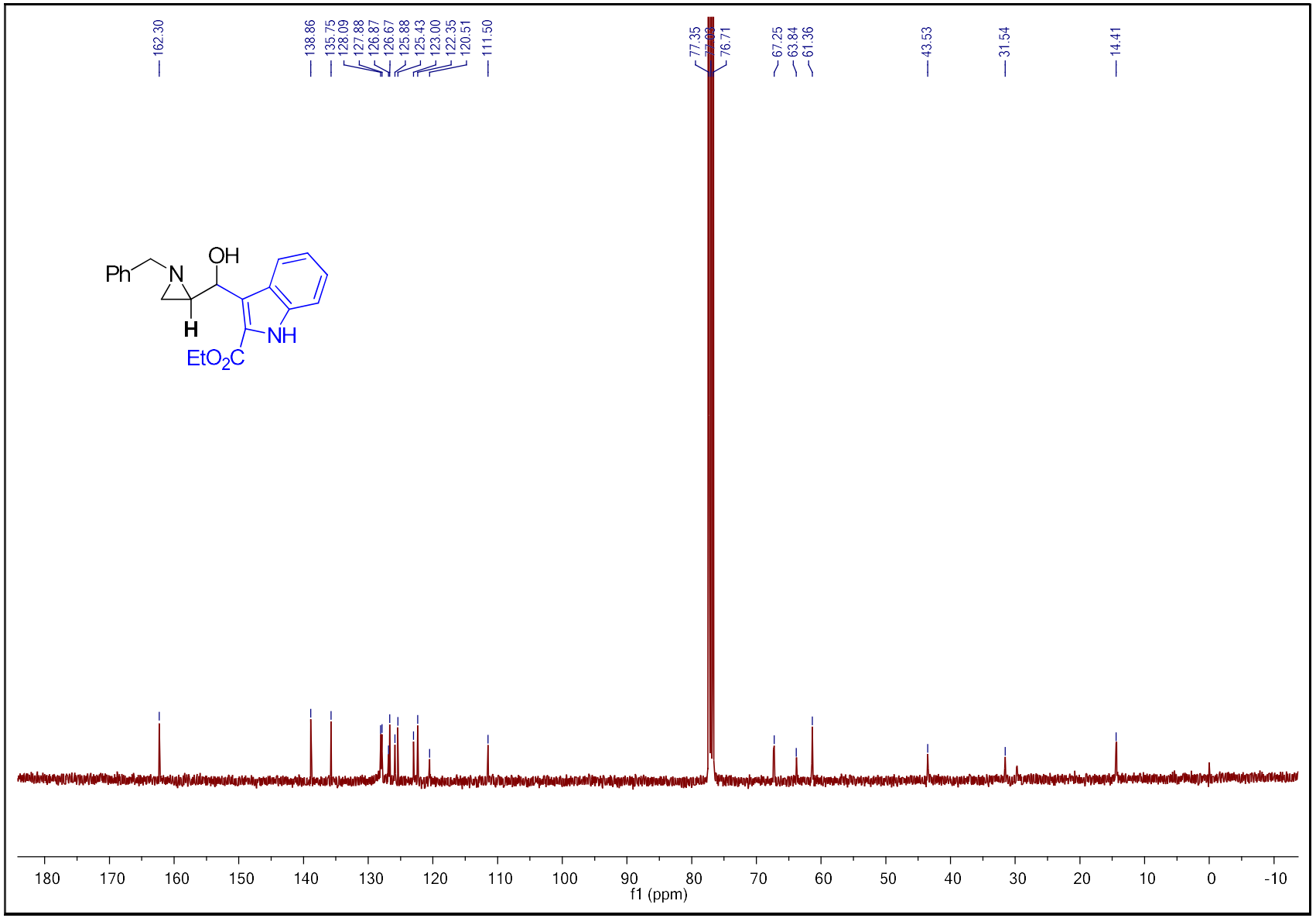
^{13}C NMR spectrum of Ethyl 3-((1-cyclohexylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ba):



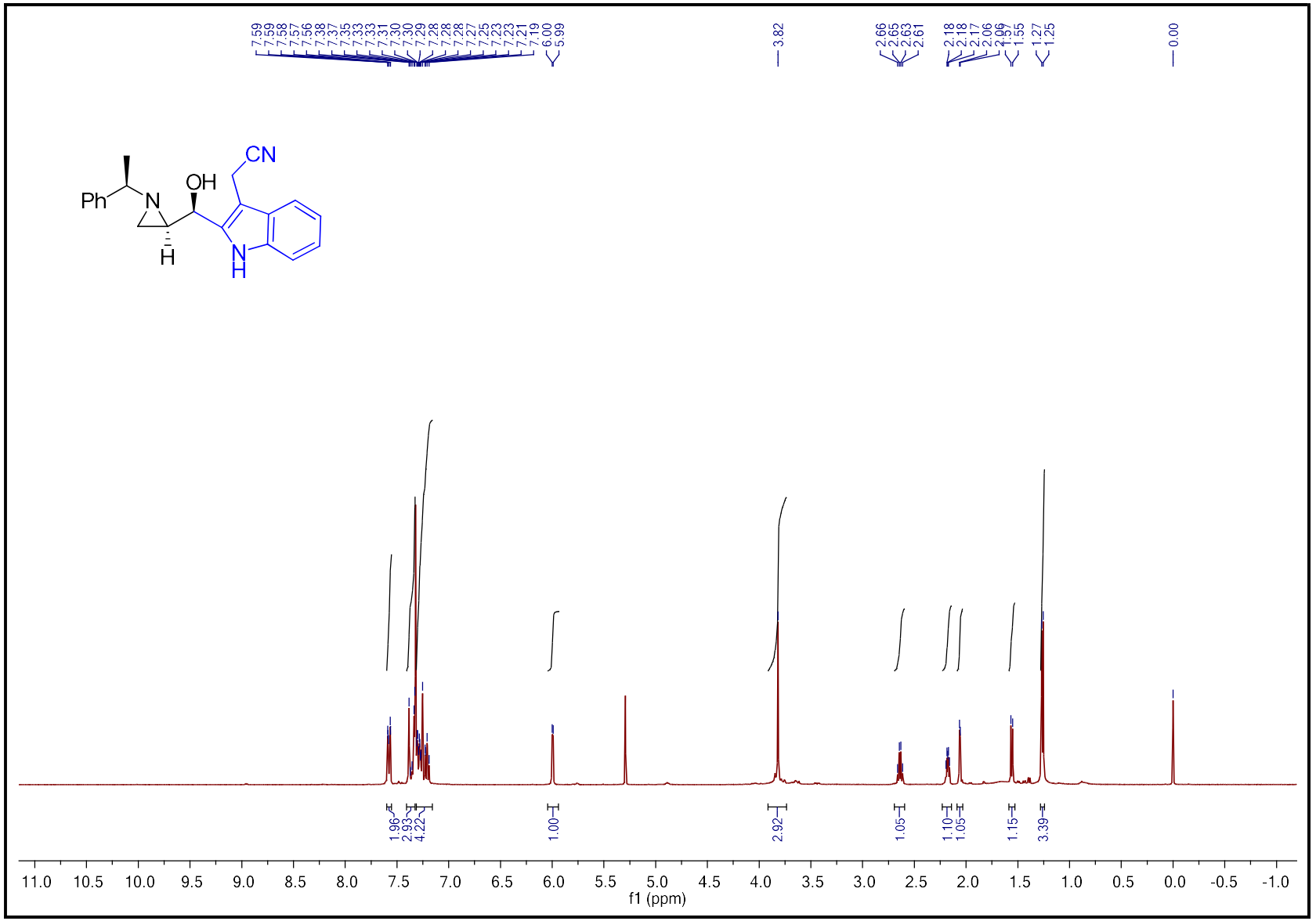
[1]H NMR spectrum of Ethyl 3-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ca):



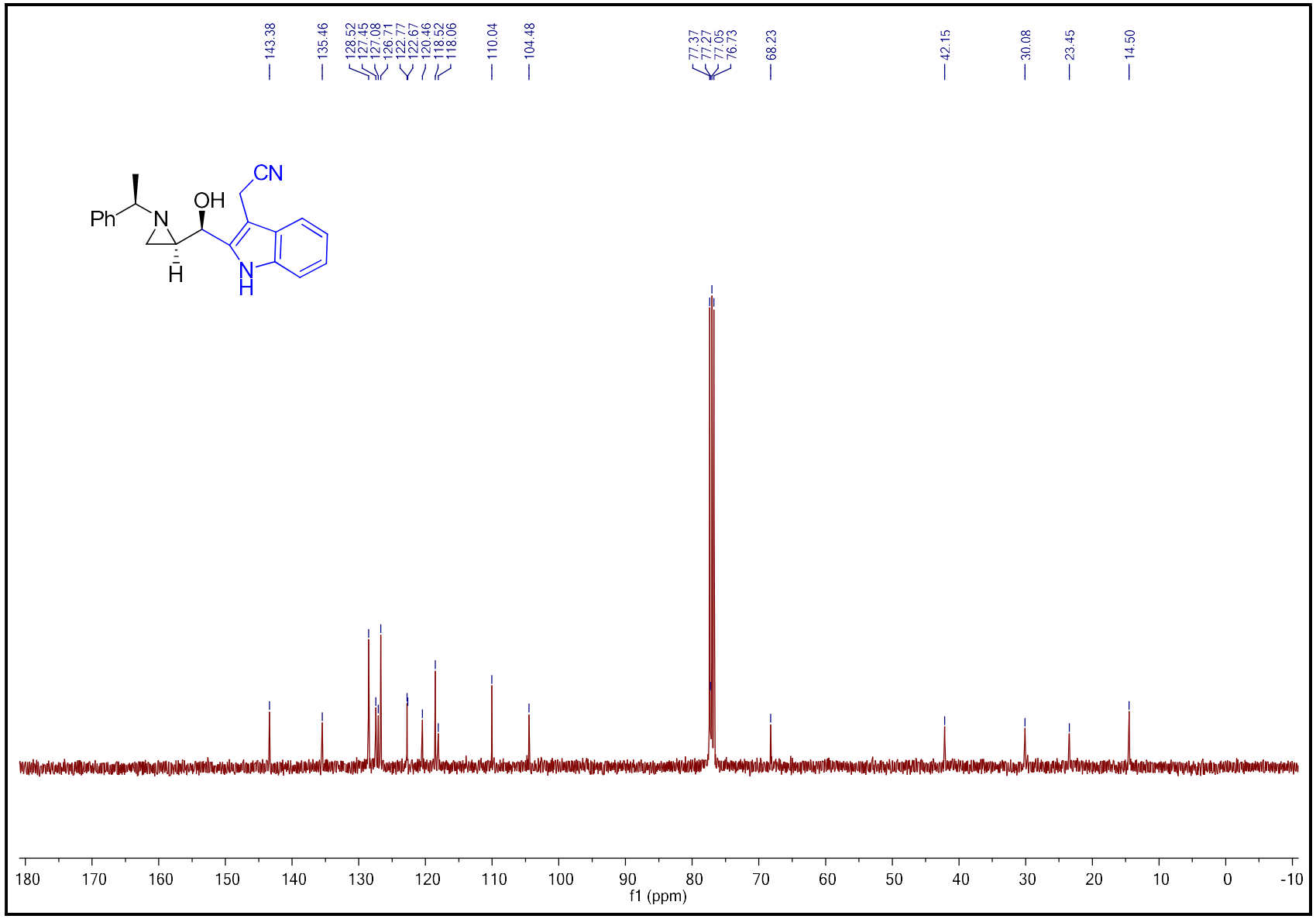
^{13}C NMR spectrum of Ethyl 3-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indole-2-carboxylate (4ca):



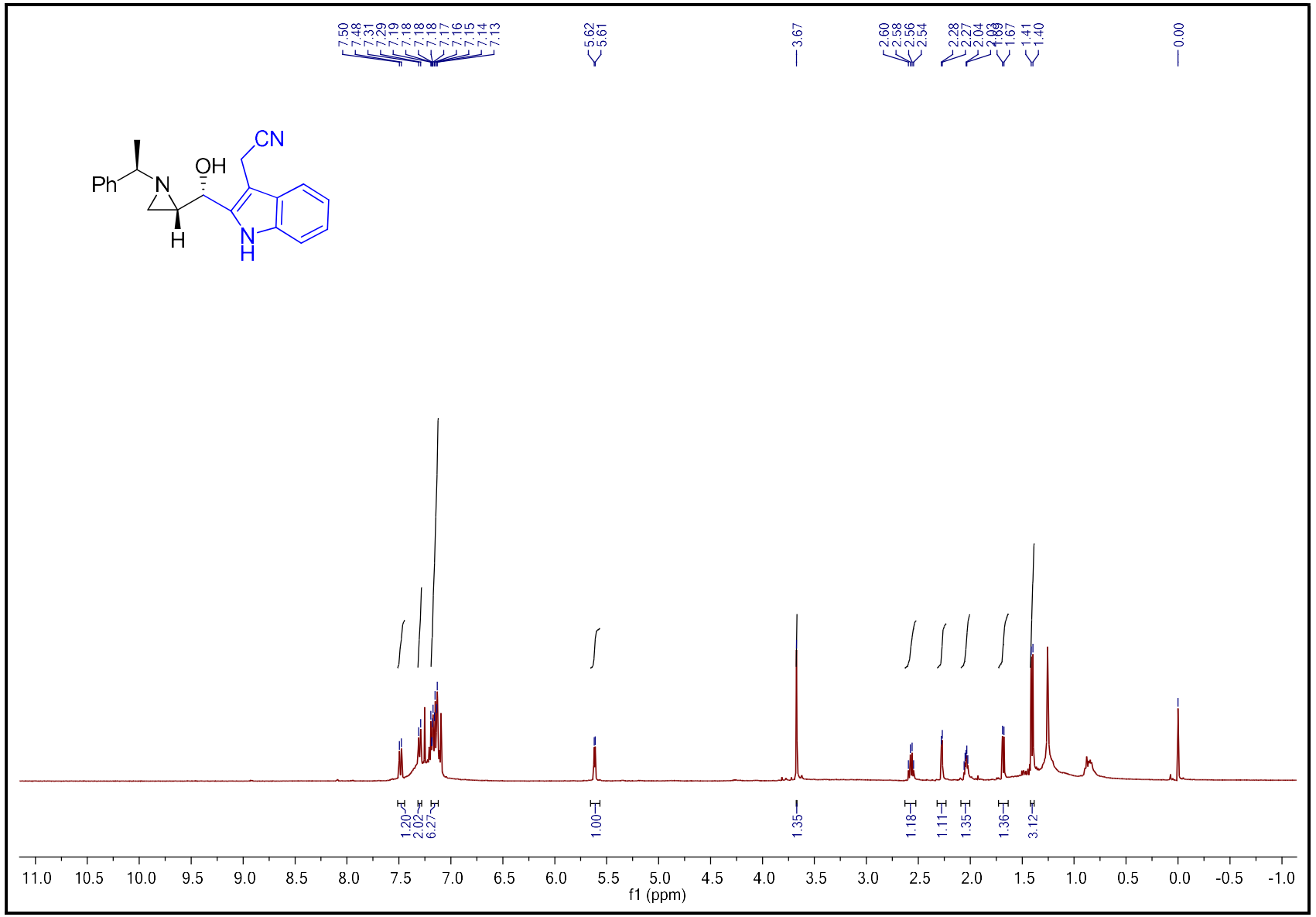
[1]H NMR spectrum of 2-(2-((R)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4ag):



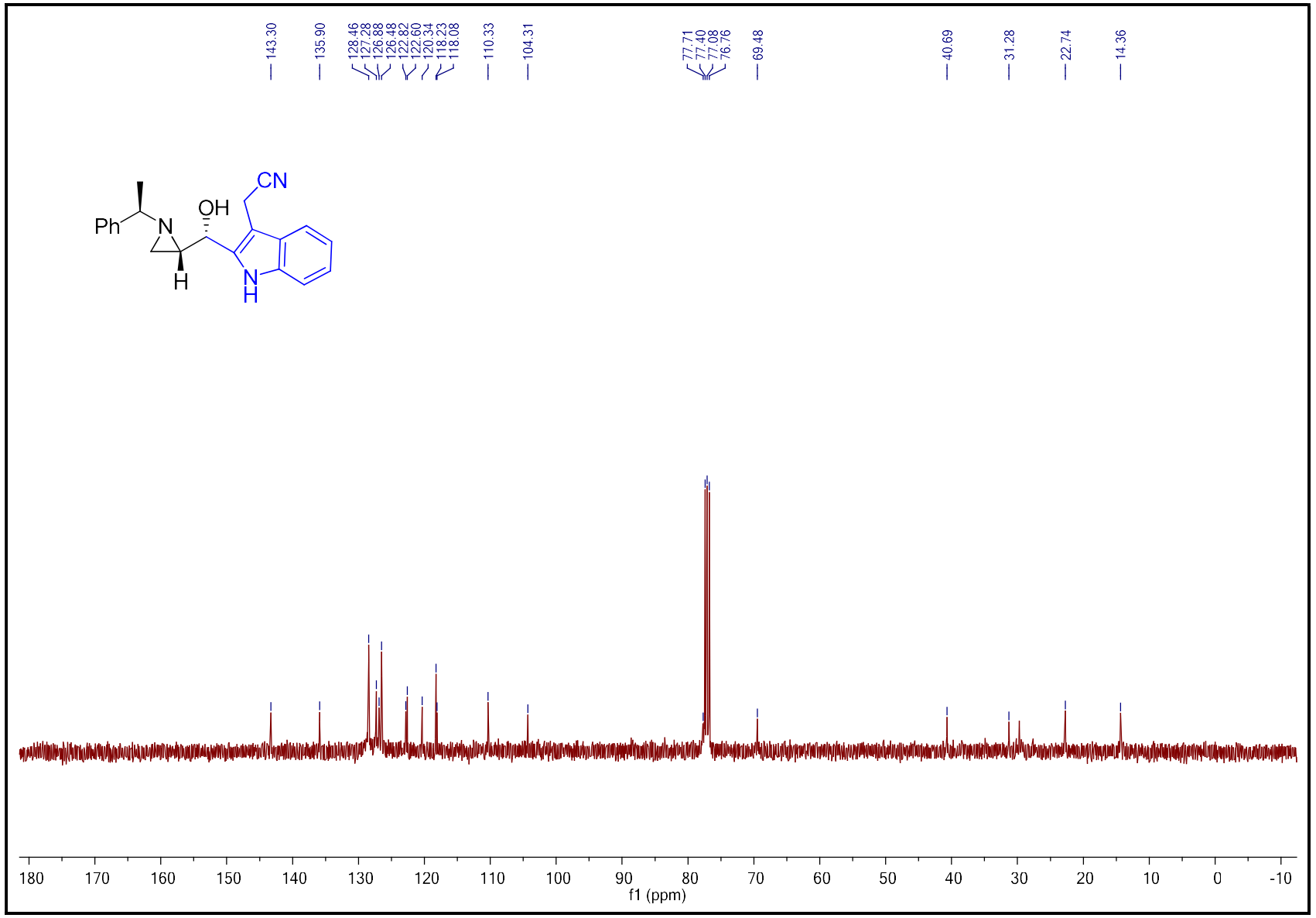
^{13}C NMR spectrum of 2-(2-((R)-hydroxy((R)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4ag):



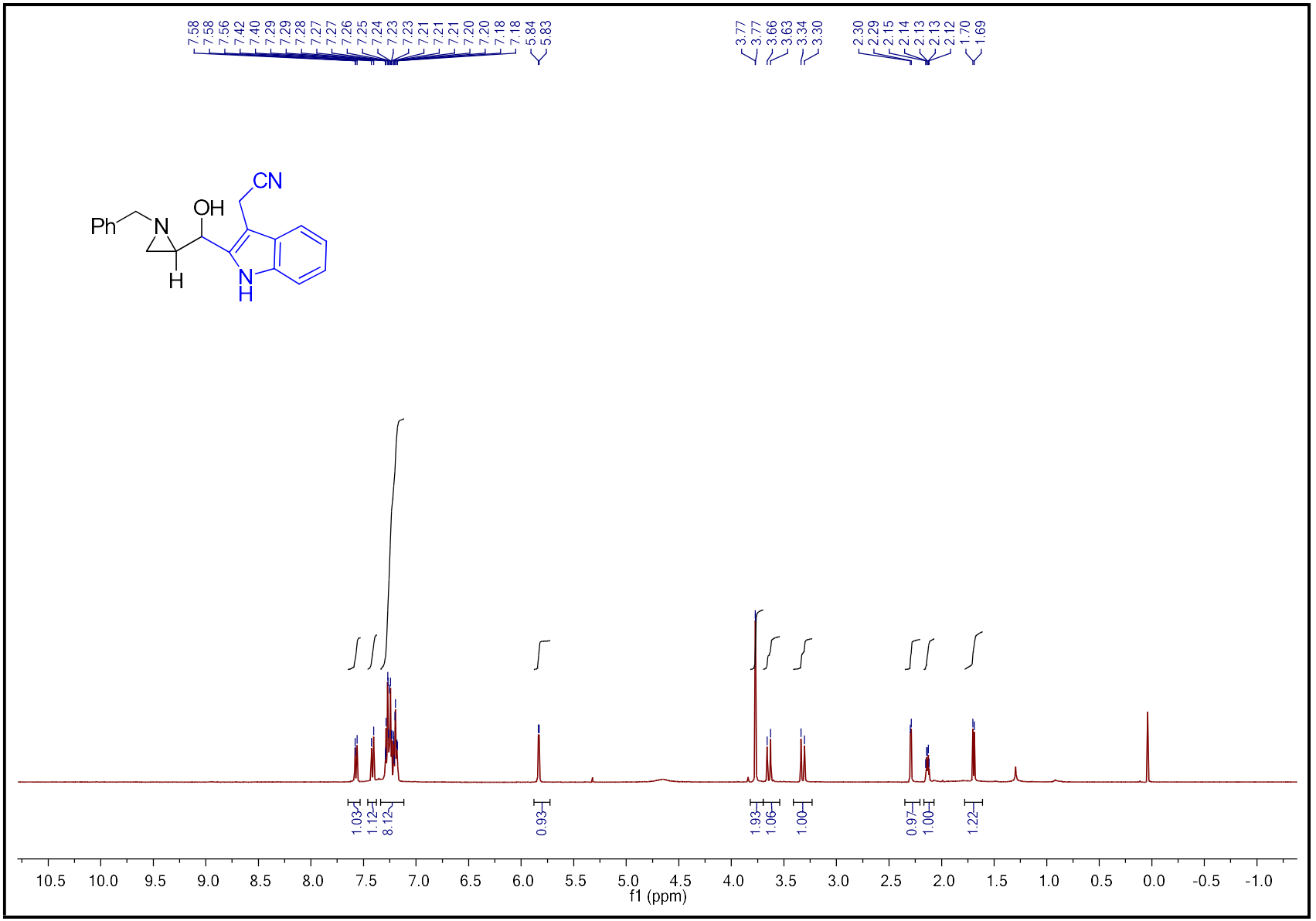
[1]H NMR spectrum of 2-(2-((S)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4a''g):



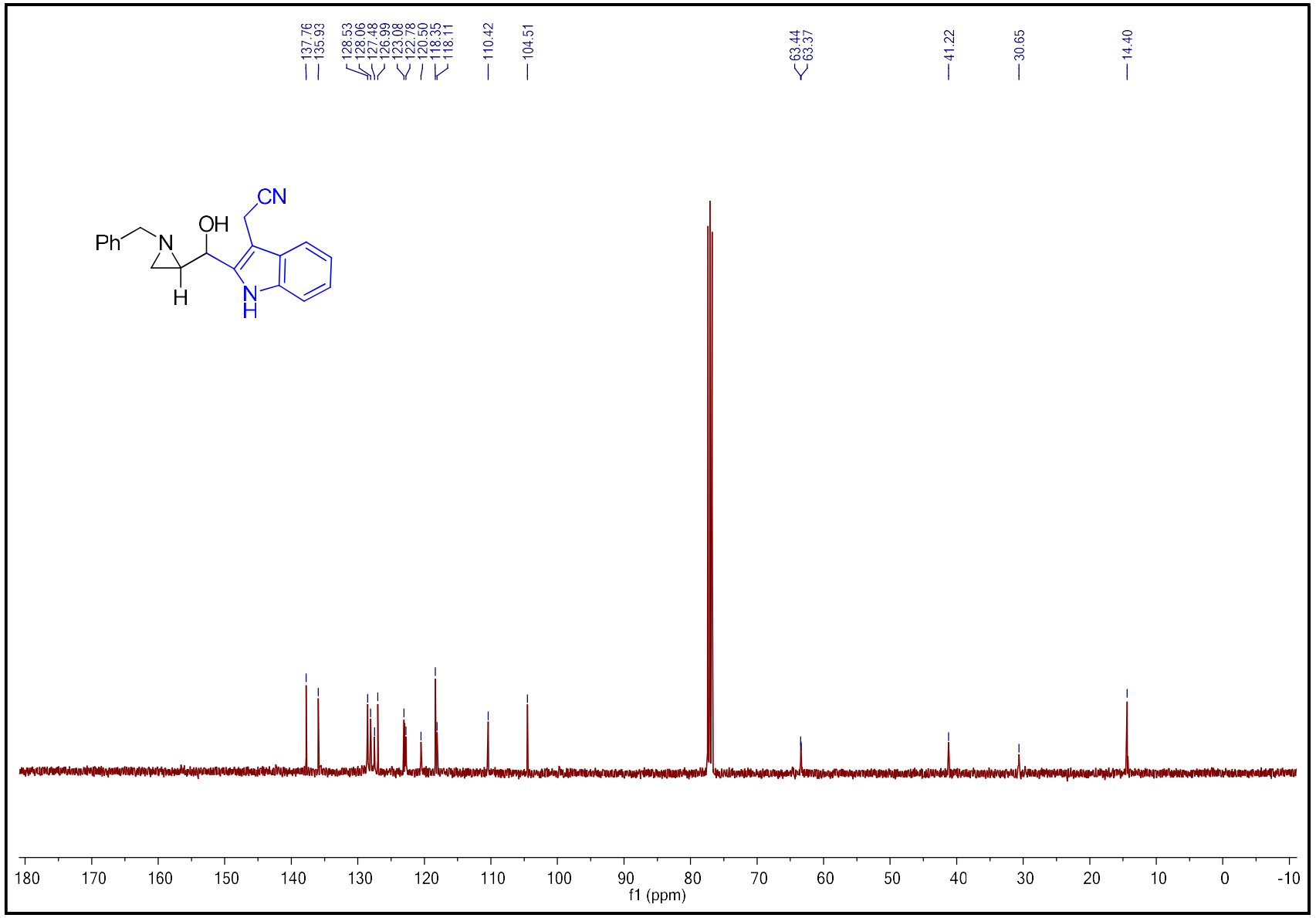
^{13}C NMR spectrum of 2-(2-((S)-hydroxy((S)-1-((R)-1-phenylethyl)aziridin-2-yl)methyl)-1H-indol-3-yl)acetonitrile (4a''g):



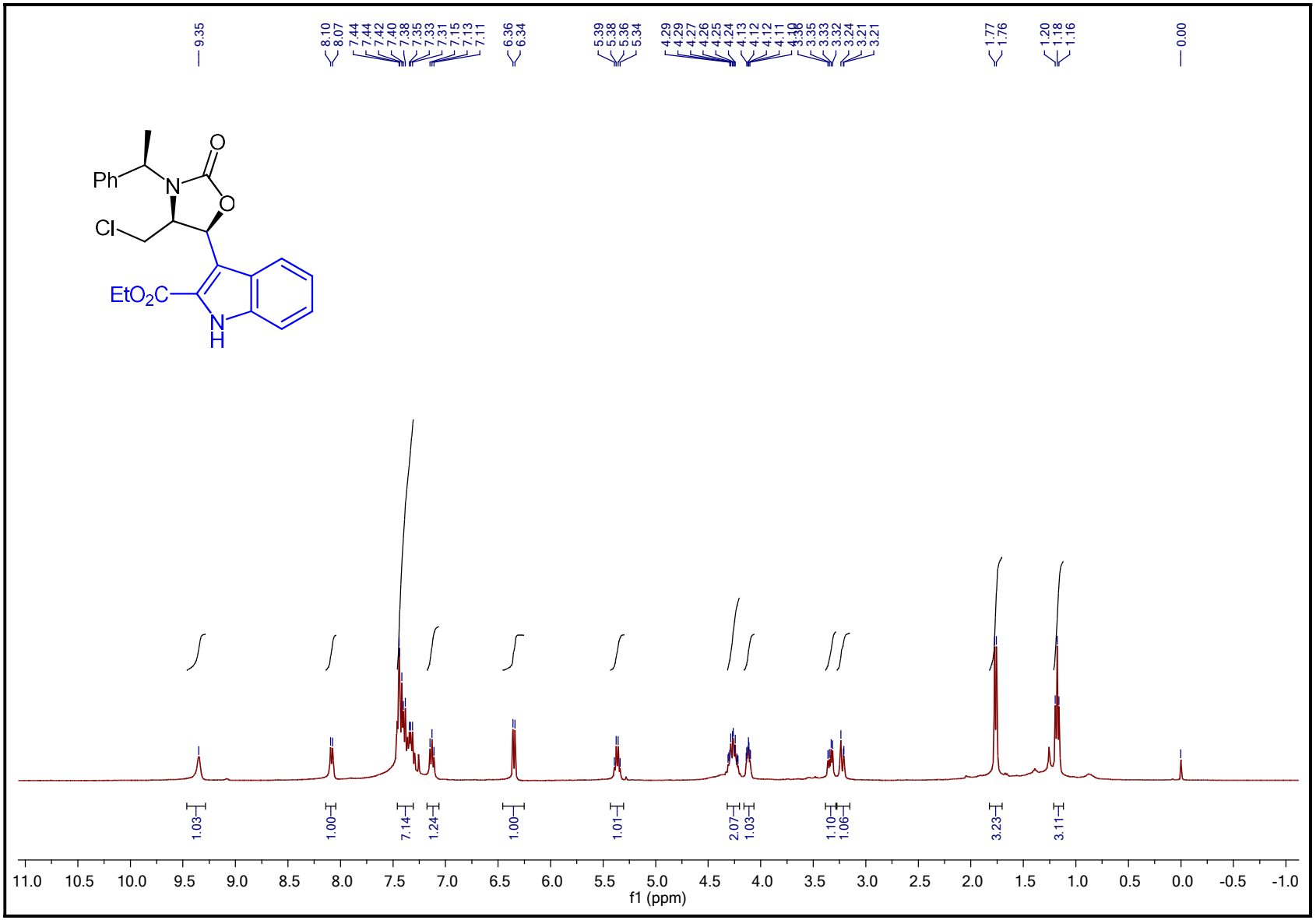
^{1}H NMR spectrum of 2-(2-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indol-3-yl)acetonitrile (4cg):



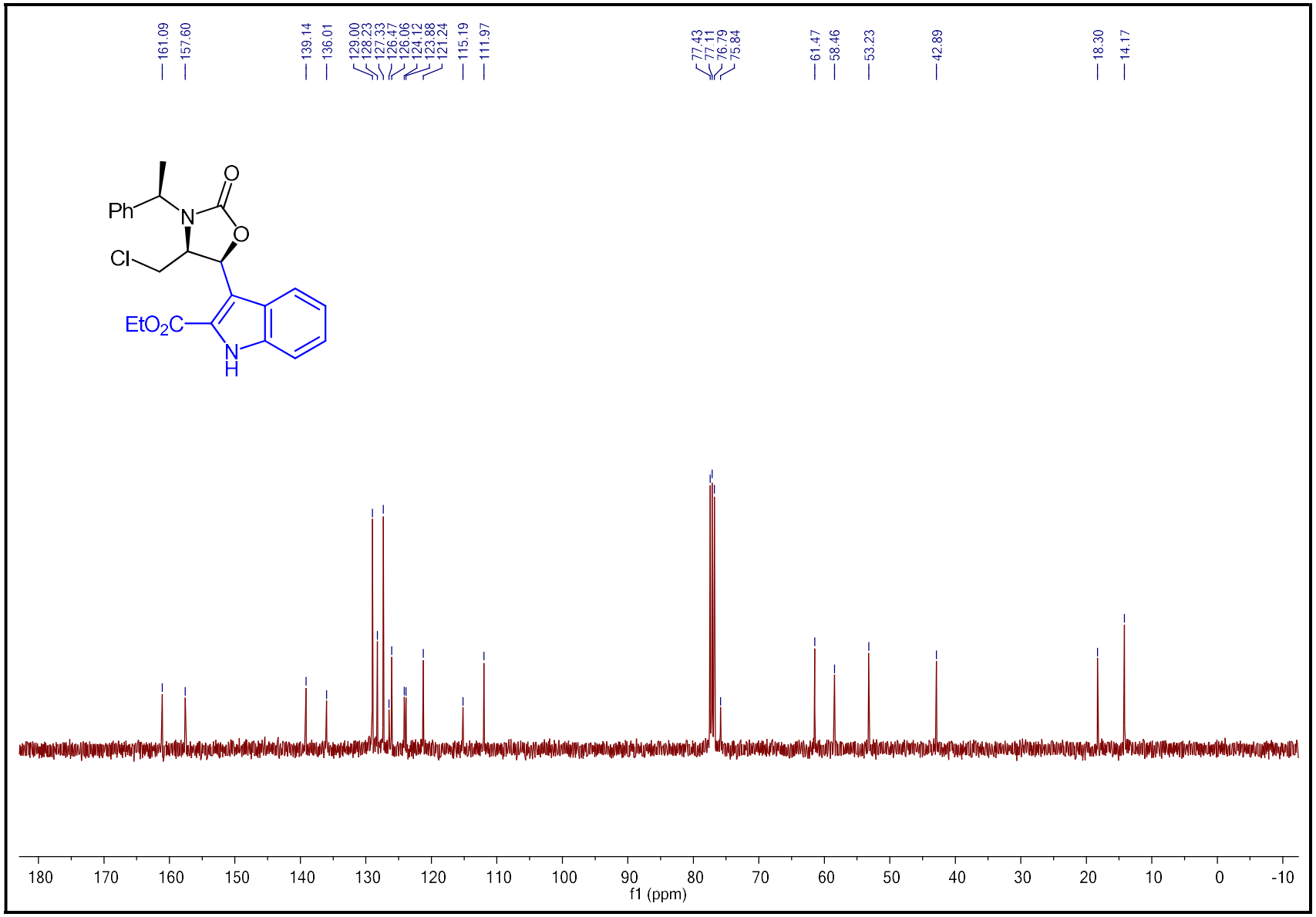
^{13}C NMR spectrum of 2-(2-((1-benzylaziridin-2-yl)(hydroxy)methyl)-1H-indol-3-yl)acetonitrile (4cg):



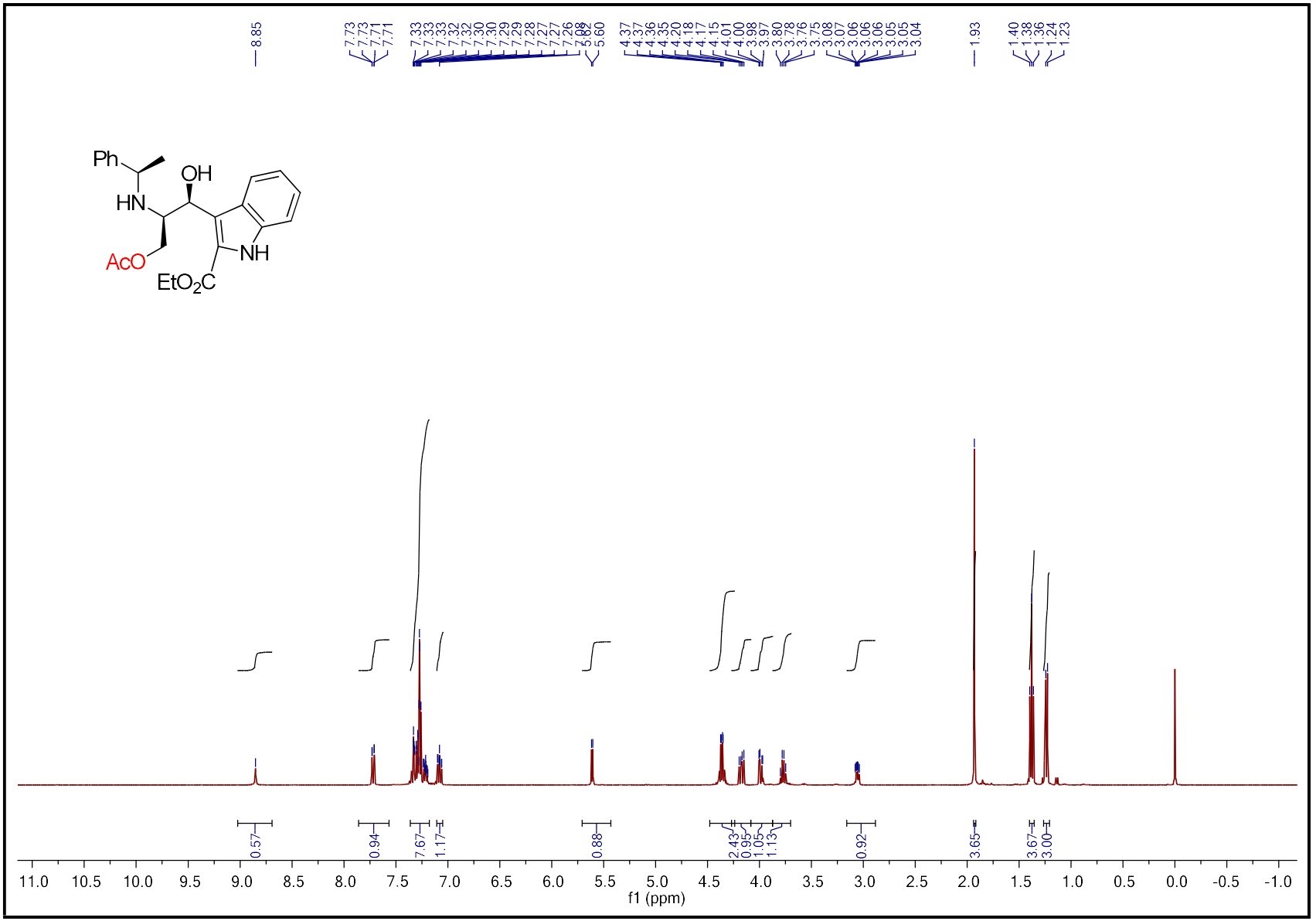
[1]H NMR spectrum of Ethyl 3-((4S,5S)-4-(chloromethyl)-2-oxo-3-((R)-1-phenylethyl)oxazolidin-5-yl)-1H-indole-2-carboxylate (7):



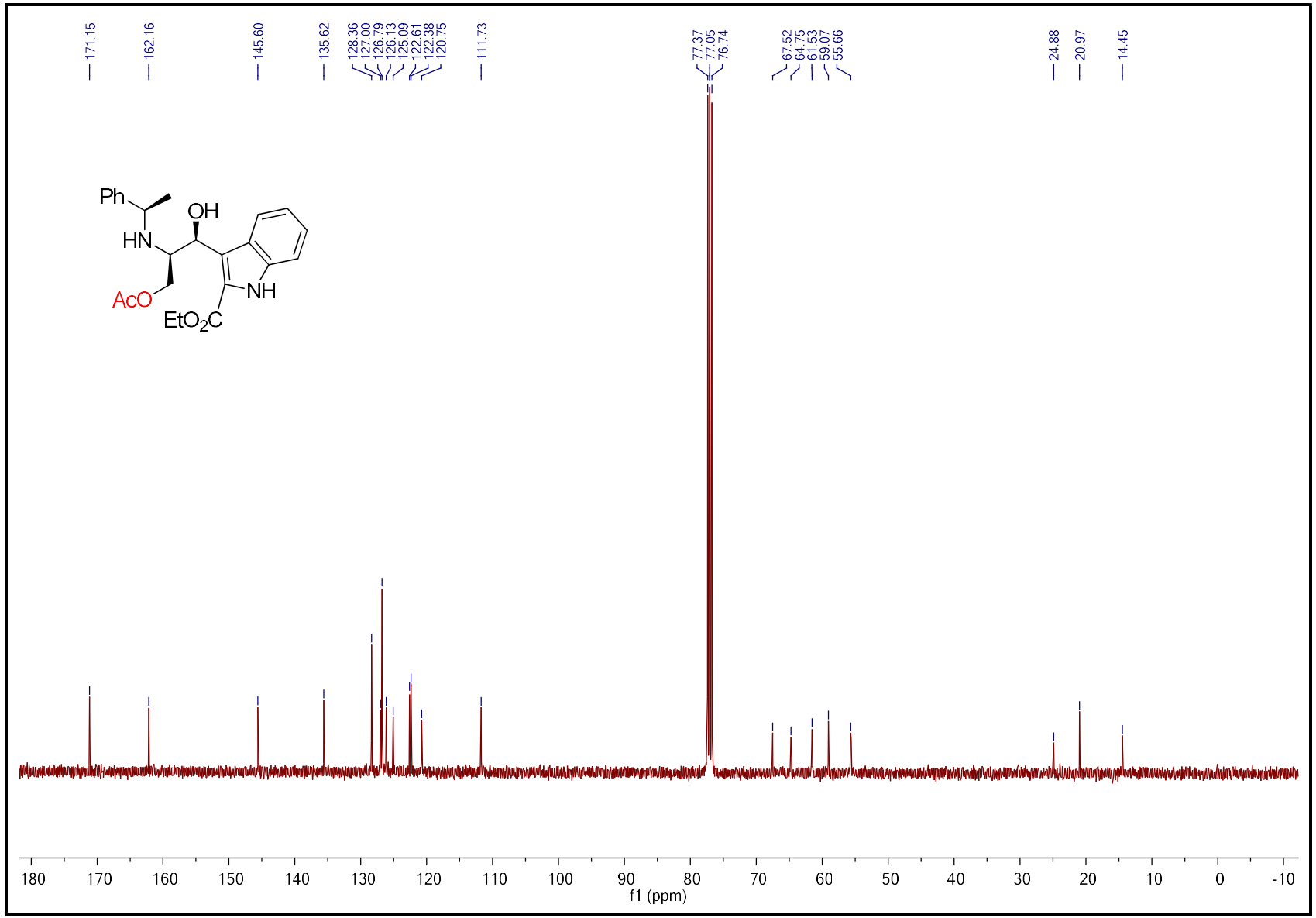
^{13}C NMR spectrum of Ethyl 3-((4S,5S)-4-(chloromethyl)-2-oxo-3-((R)-1-phenylethyl)oxazolidin-5-yl)-1H-indole-2-carboxylate (7):



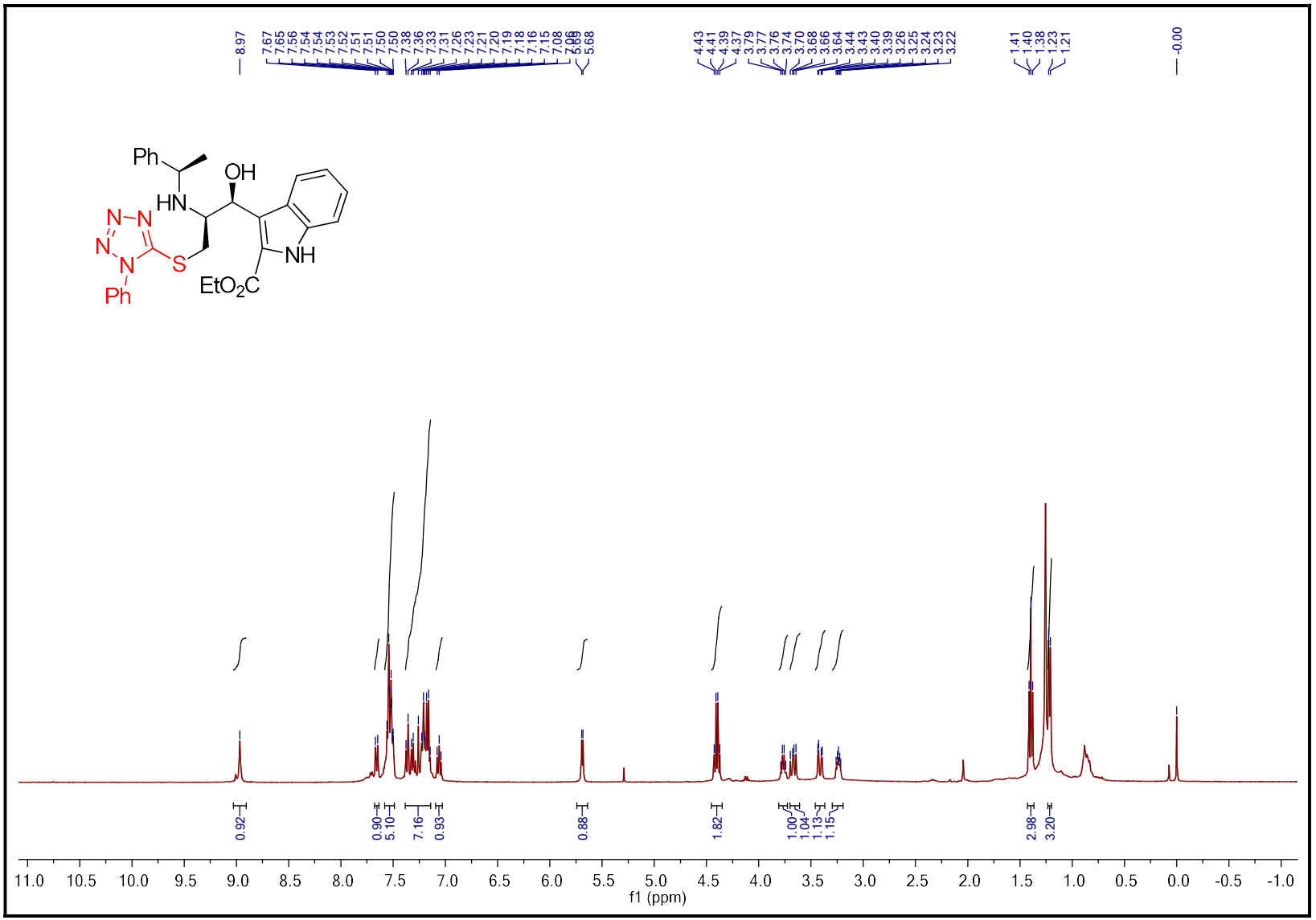
[1]H NMR spectrum of Ethyl 3-((1S,2R)-3-acetoxy-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (8):



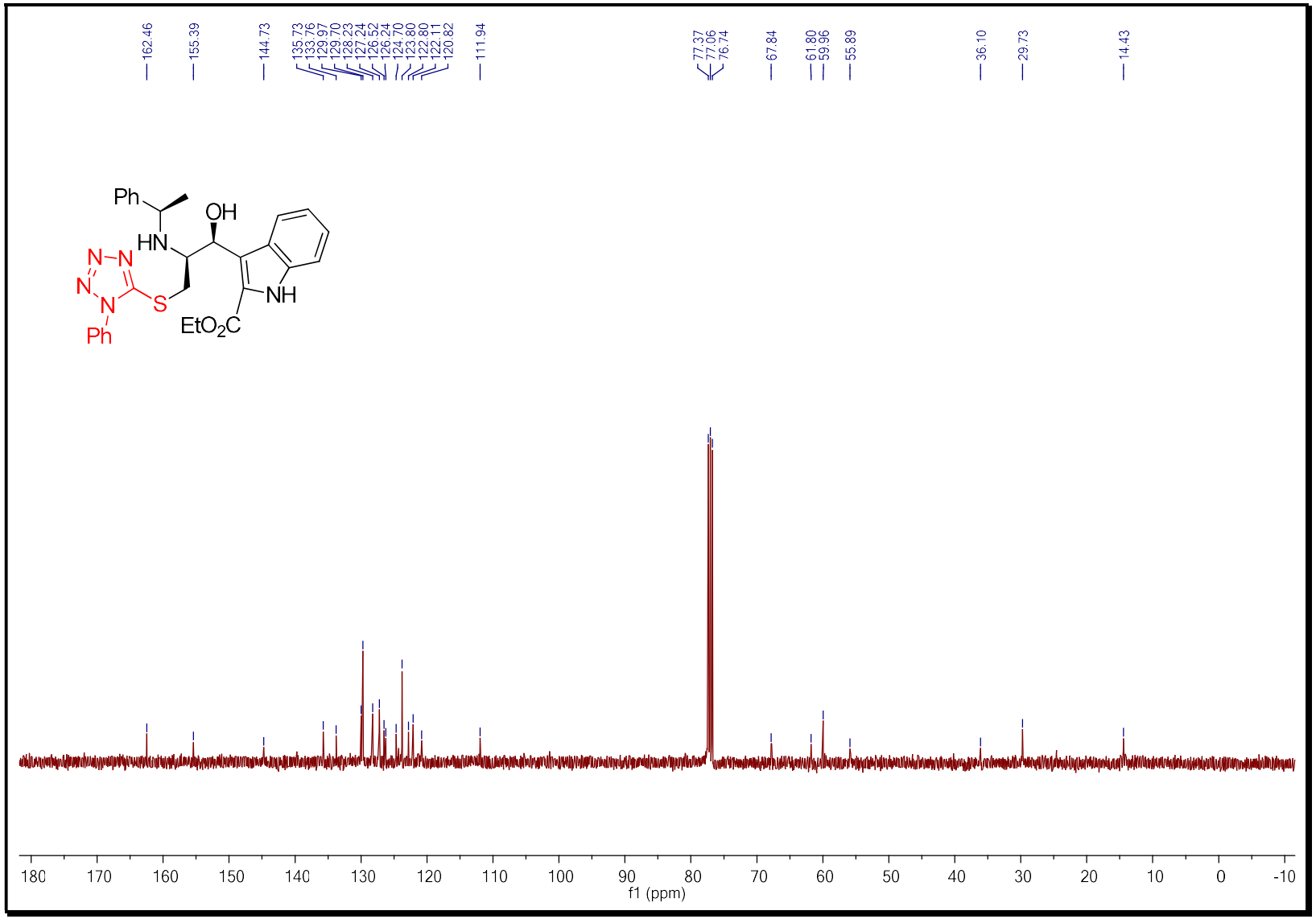
^{13}C NMR spectrum of Ethyl 3-((1S,2R)-3-acetoxy-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (8):



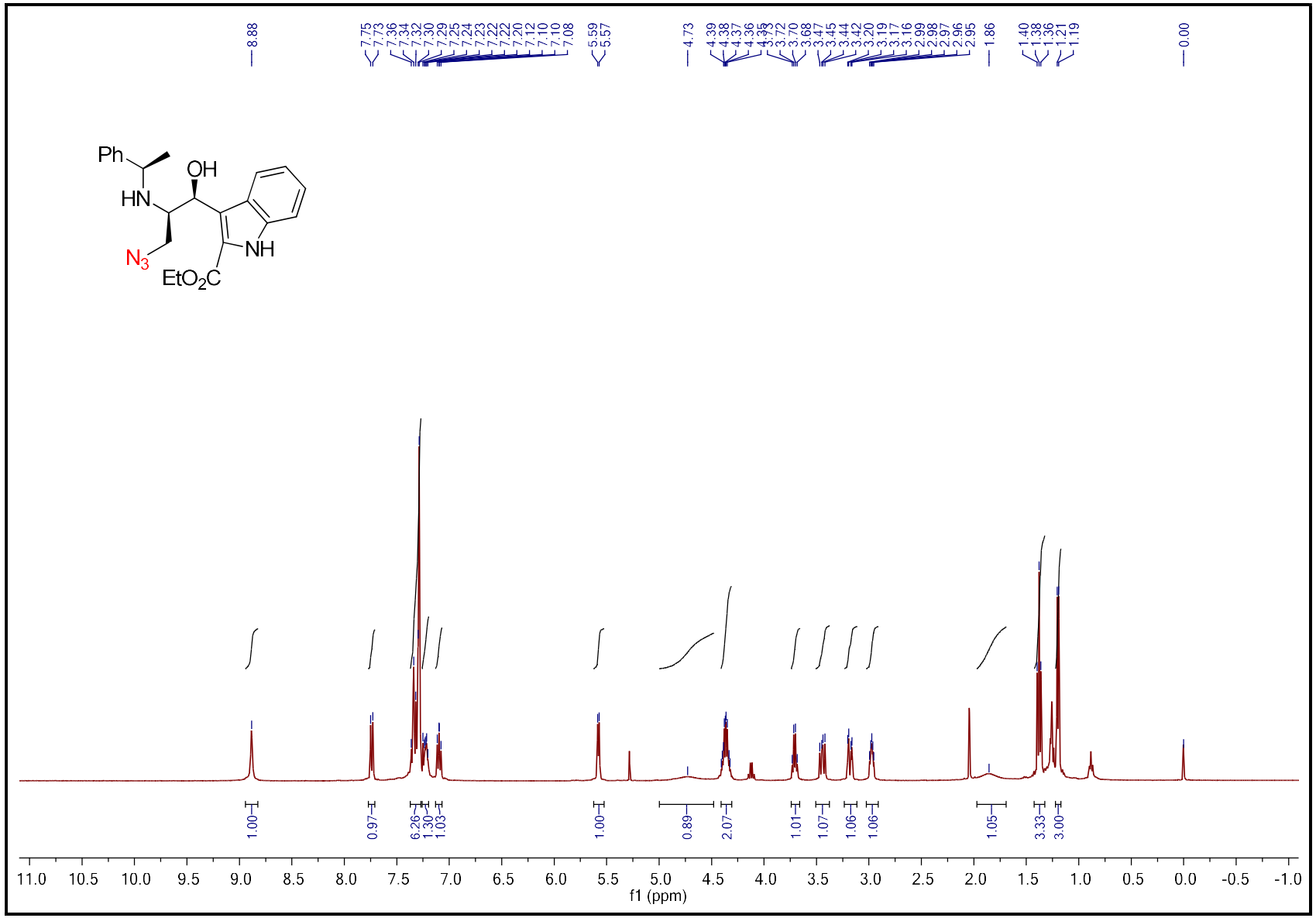
^{1}H NMR spectrum of Ethyl 3-((1S,2S)-1-hydroxy-3-((1-phenyl-1H-tetrazol-5-yl)thio)-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (9):



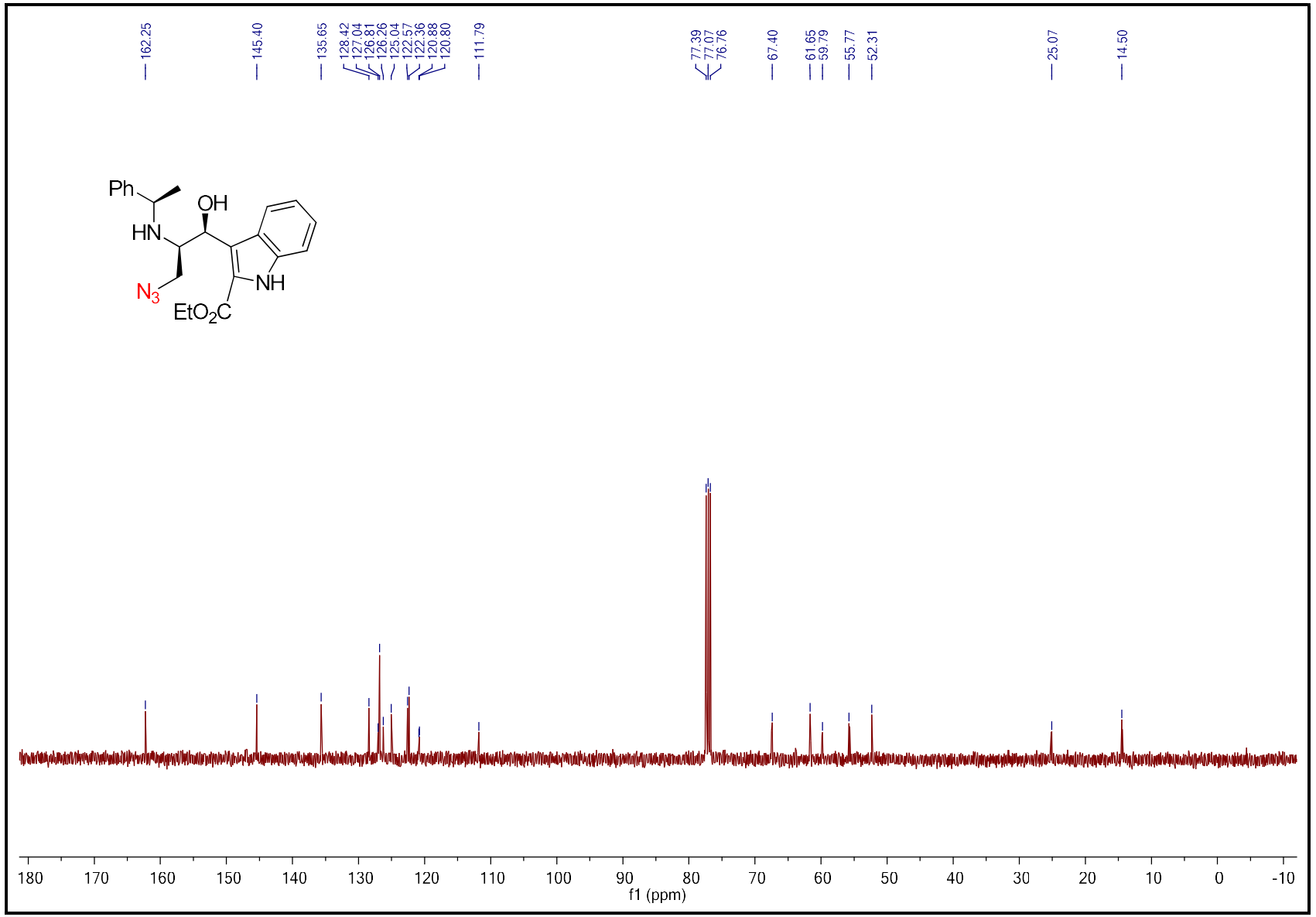
^{13}C NMR spectrum of Ethyl 3-((1S,2S)-1-hydroxy-3-((1-phenyl-1H-tetrazol-5-yl)thio)-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (9):



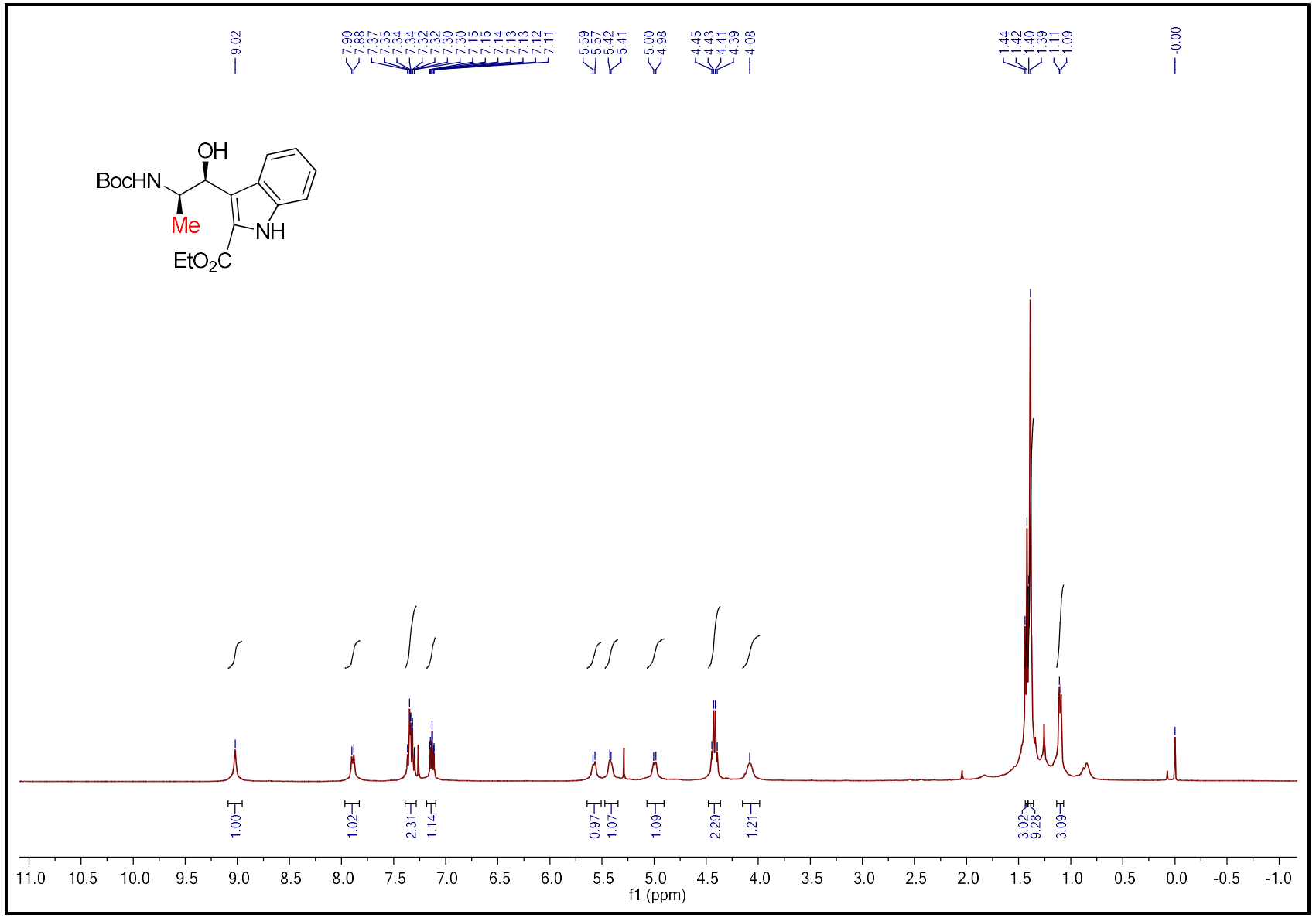
[1]H NMR spectrum of Ethyl 3-((1S,2R)-3-azido-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (10):



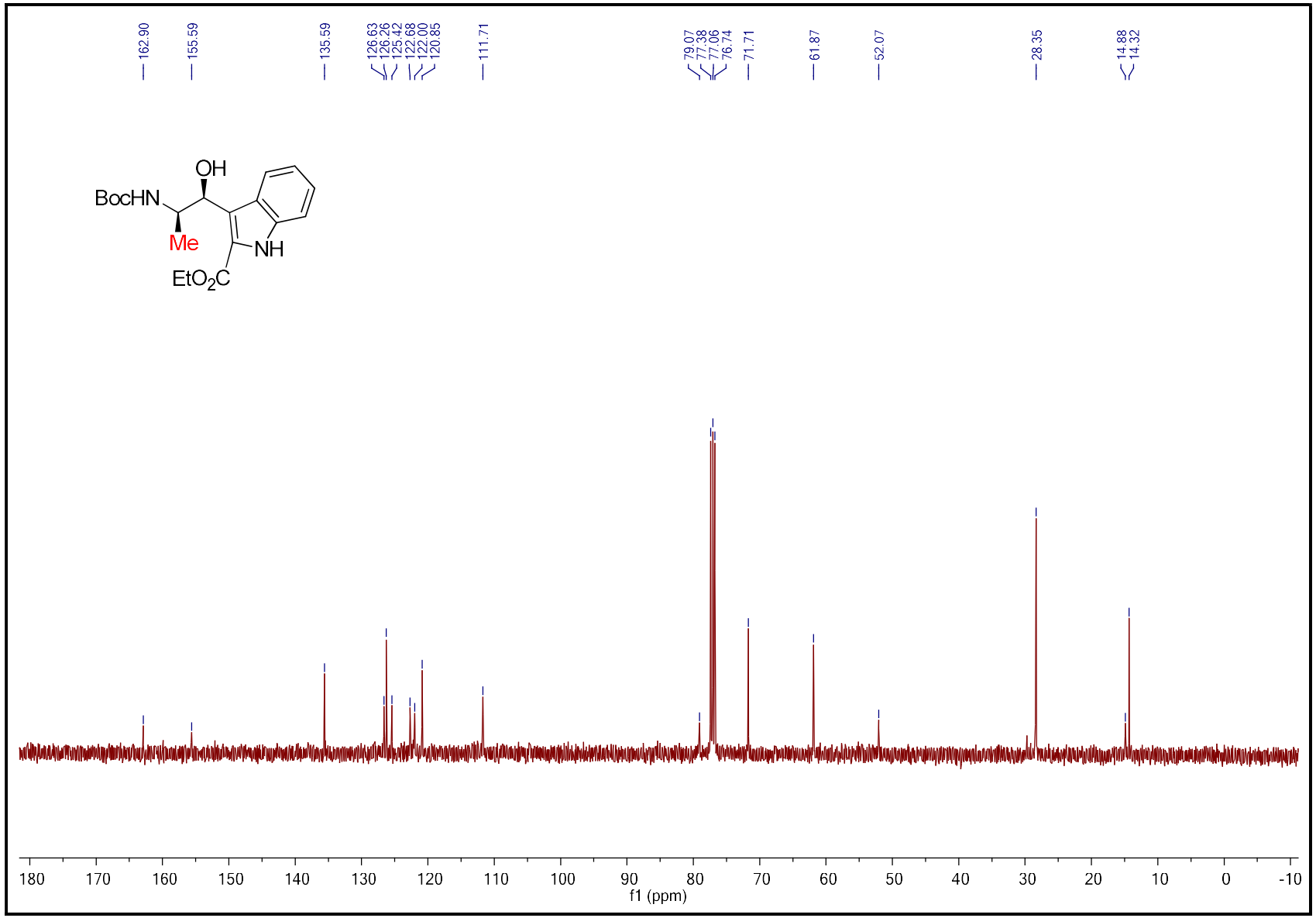
^{13}C NMR spectrum of Ethyl 3-((1S,2R)-3-azido-1-hydroxy-2-(((R)-1-phenylethyl)amino)propyl)-1H-indole-2-carboxylate (10):



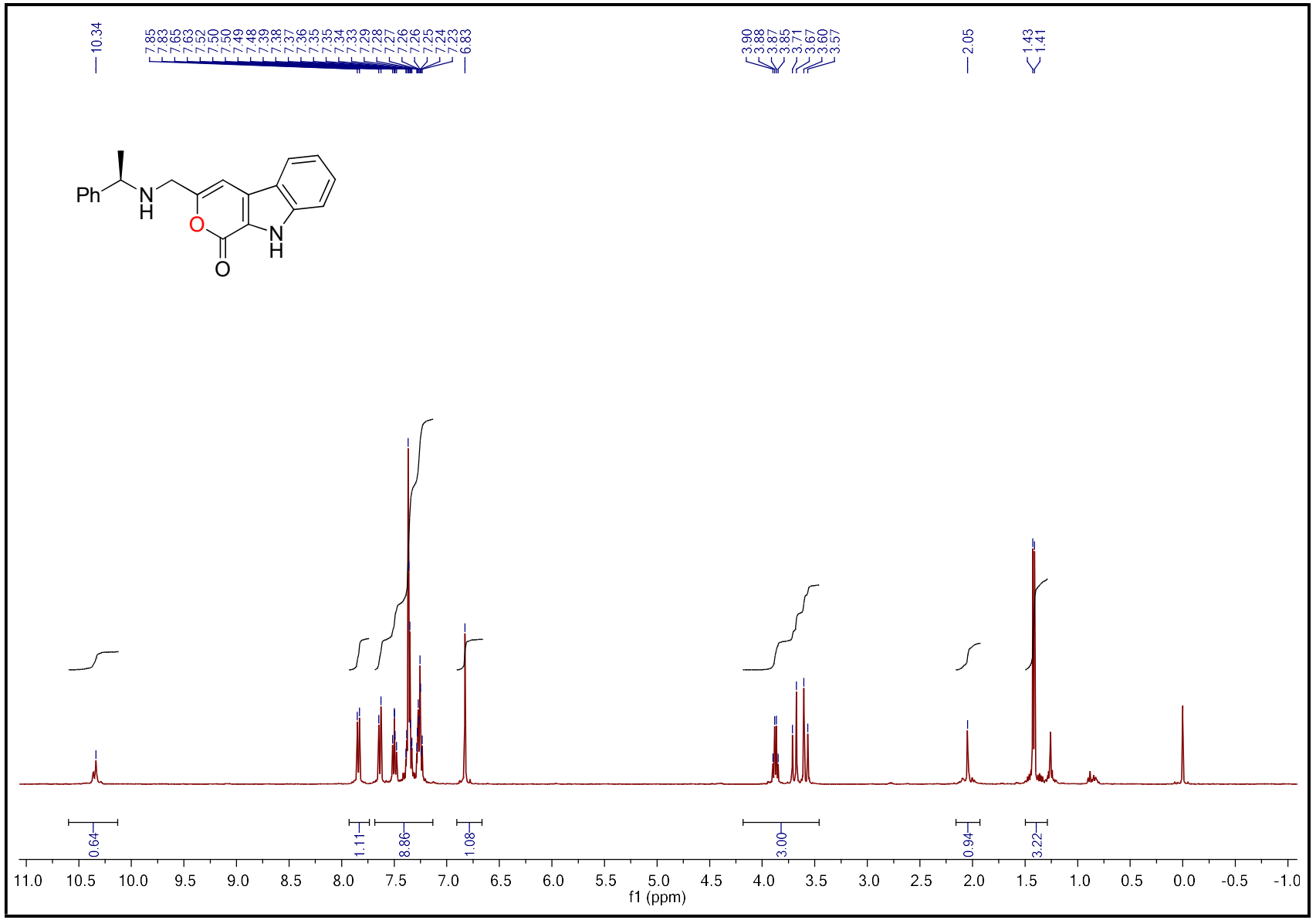
[1]H NMR spectrum of Ethyl 3-((1S,2R)-2-((tert-butoxycarbonyl)amino)-1-hydroxypropyl)-1H-indole-2-carboxylate (11):



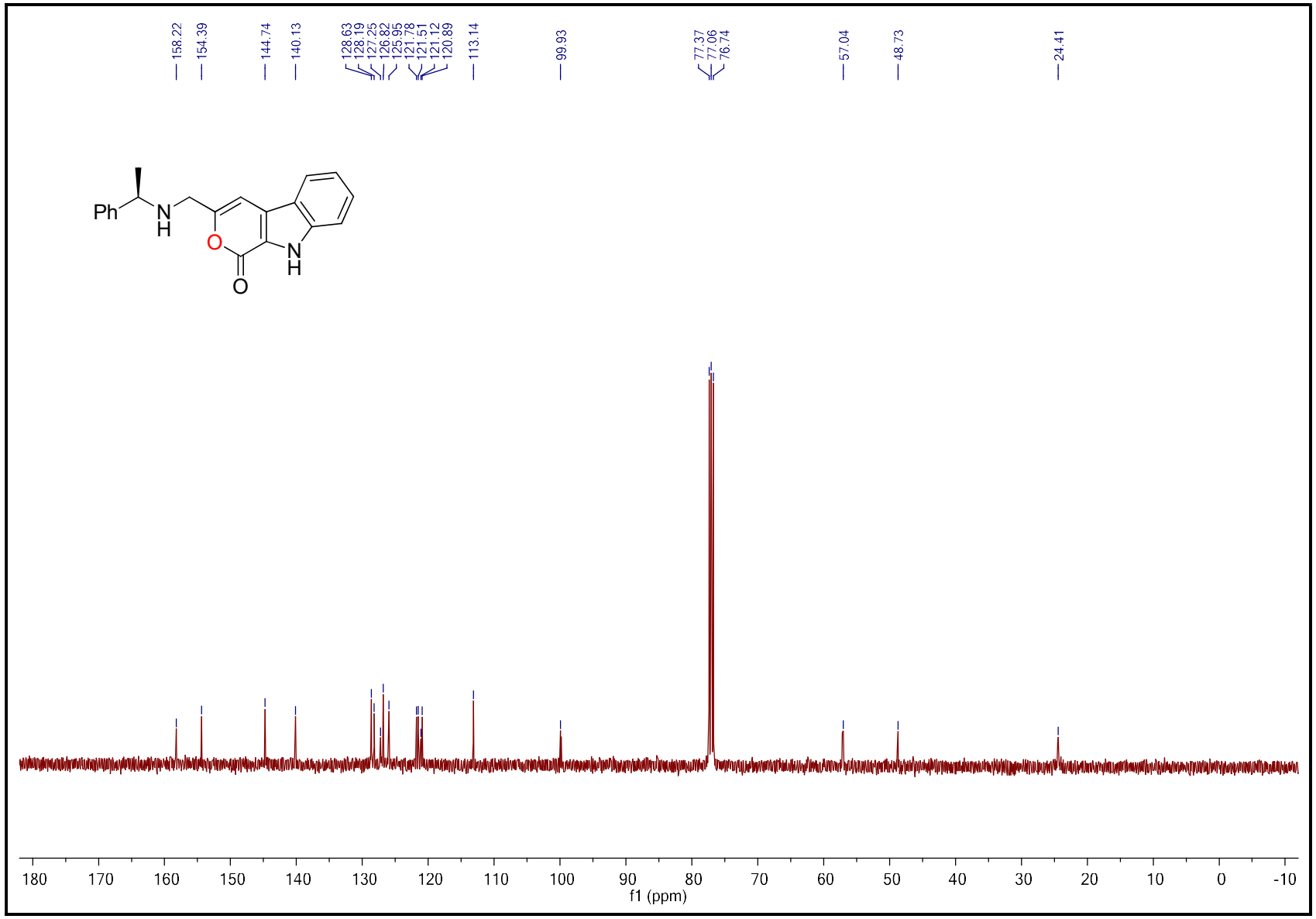
^{13}C NMR spectrum of Ethyl 3-((1S,2R)-2-((tert-butoxycarbonyl)amino)-1-hydroxypropyl)-1H-indole-2-carboxylate (11):



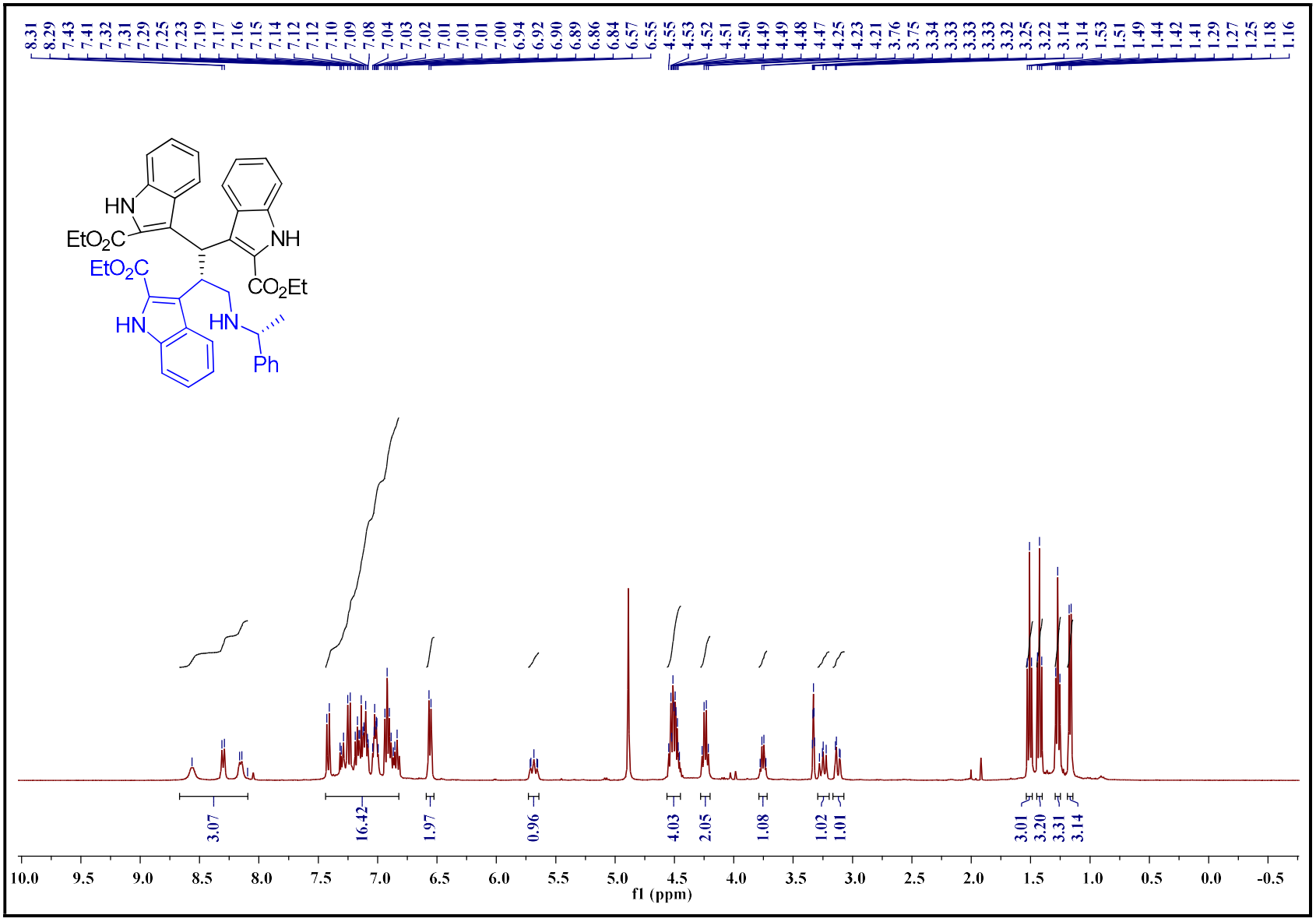
[1]H NMR spectrum of (R)-3-(((1-phenylethyl)amino)methyl)pyrano[3,4-b]indol-1(9H)-one (12):



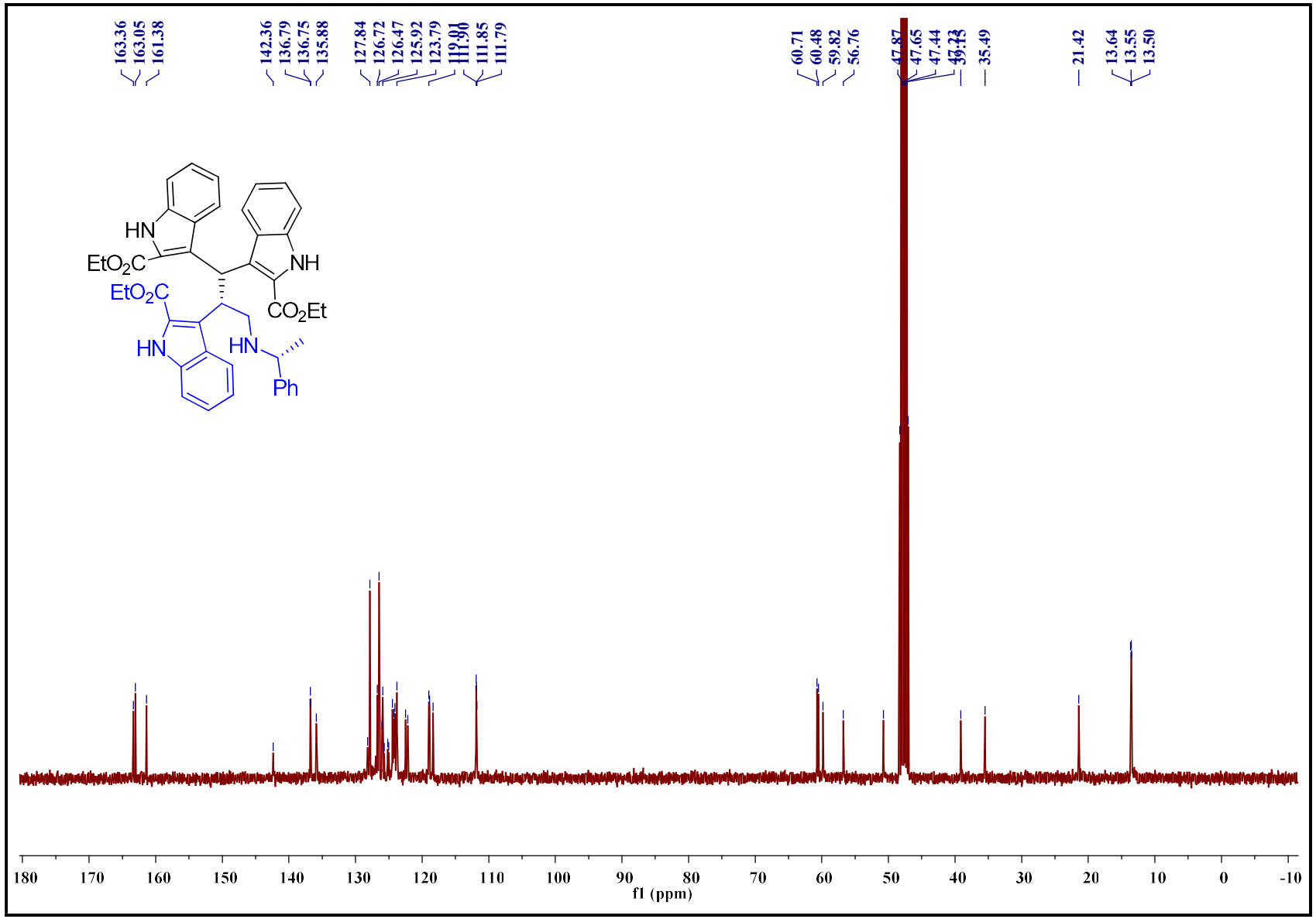
^{13}C NMR spectrum of (R)-3-(((1-phenylethyl)amino)methyl)pyrano[3,4-b]indol-1(9H)-one (12):



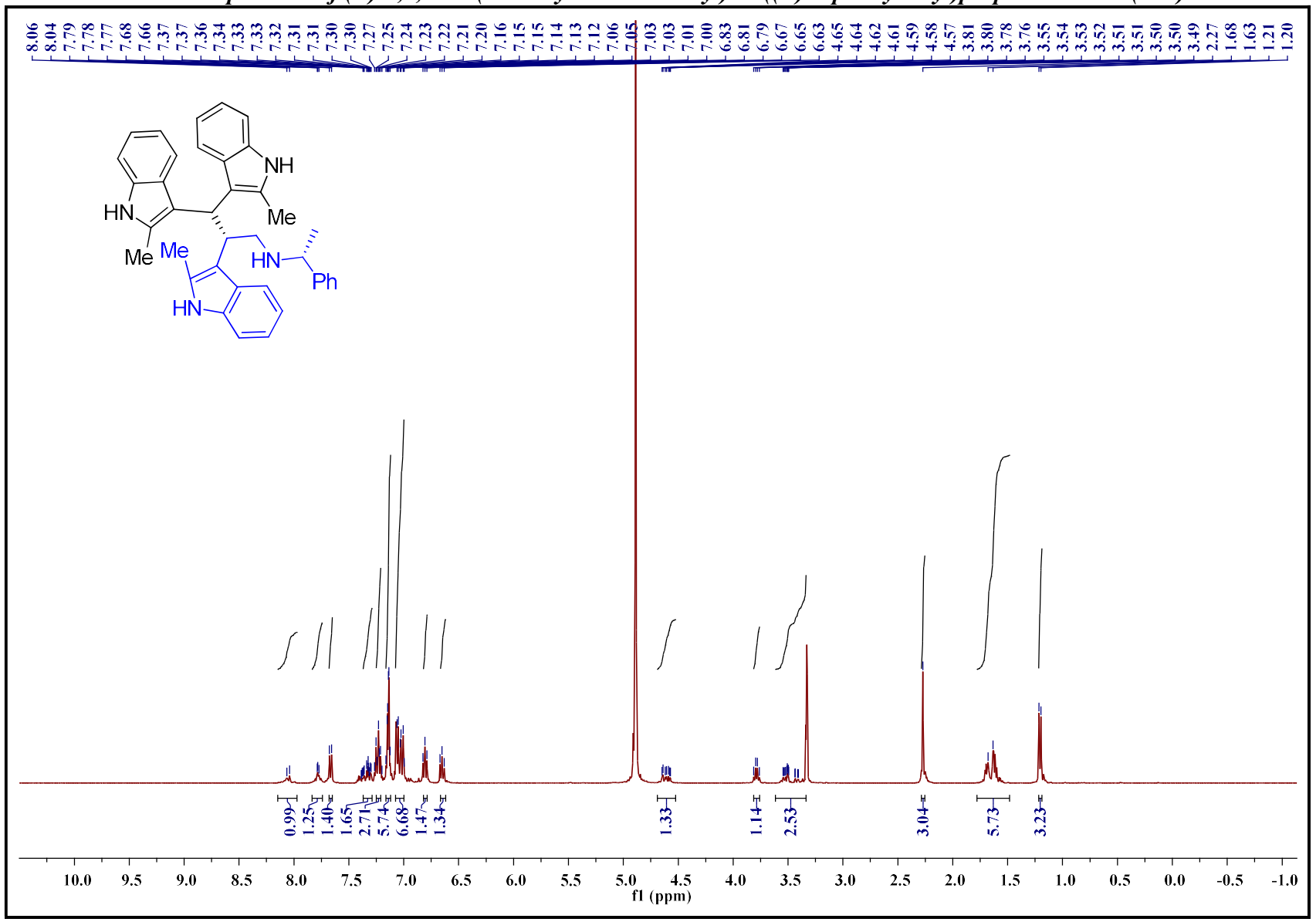
[1]H NMR spectrum of Triethyl 3,3',3''-((S)-3-(((R)-1-phenylethyl)amino)propane-1,1,2-triyl)tris(1H-indole-2-carboxylate) (5aa):



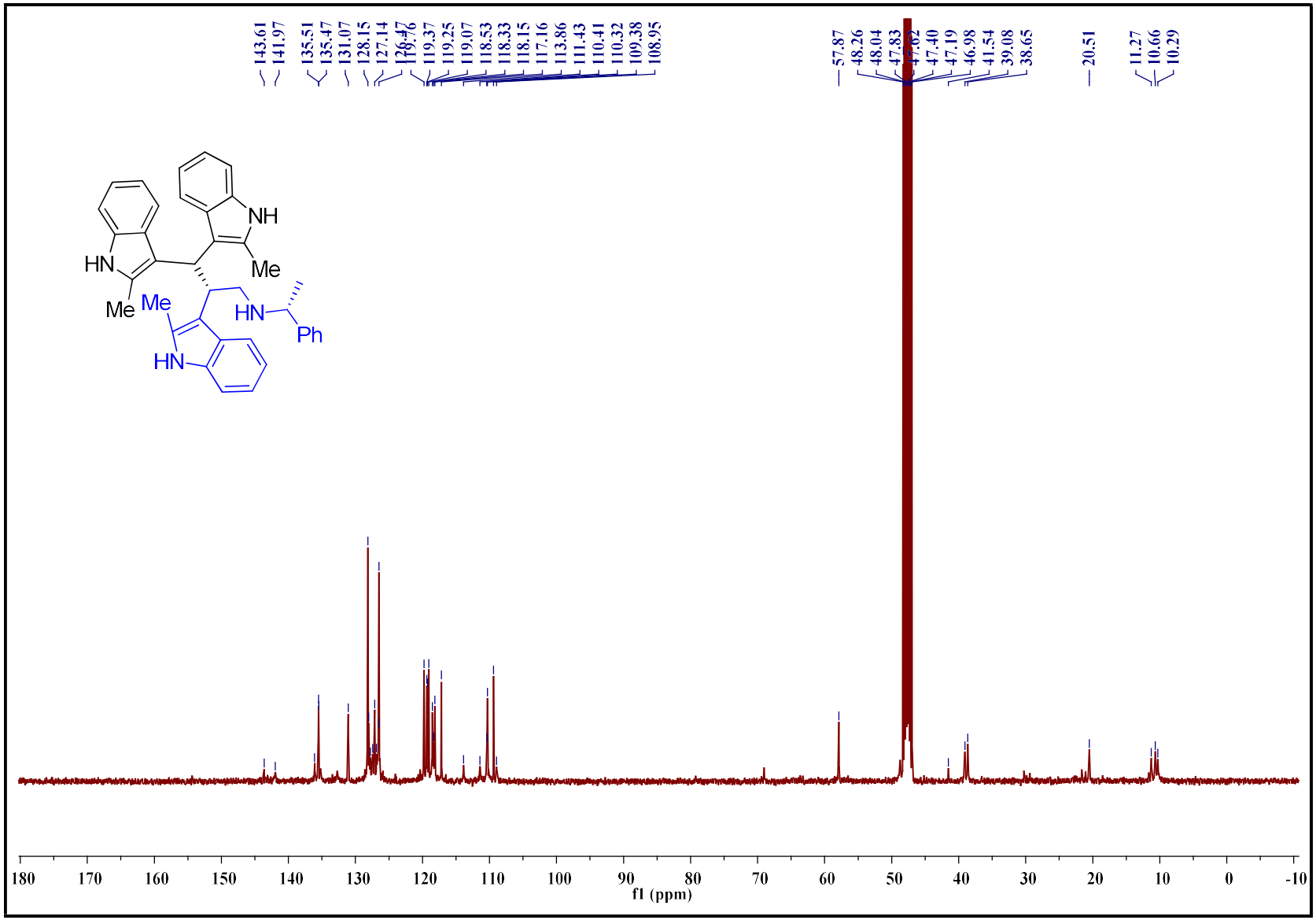
^{13}C NMR spectrum of Triethyl 3,3',3''-((S)-3-(((R)-1-phenylethyl)amino)propane-1,1,2-triyl)tris(1H-indole-2-carboxylate) (5aa):



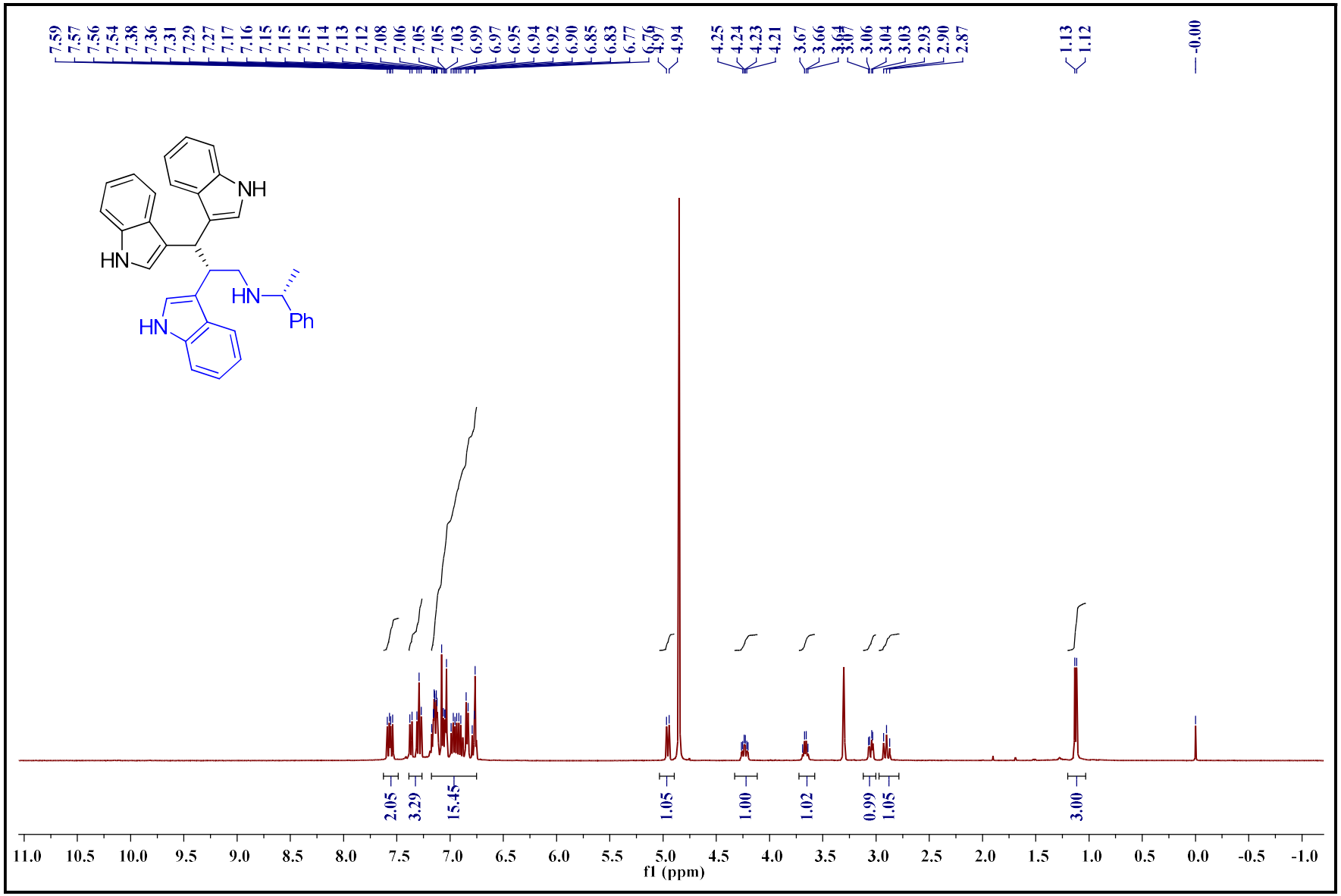
^{1}H NMR spectrum of (R)-2,3,3-tris(2-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ah):



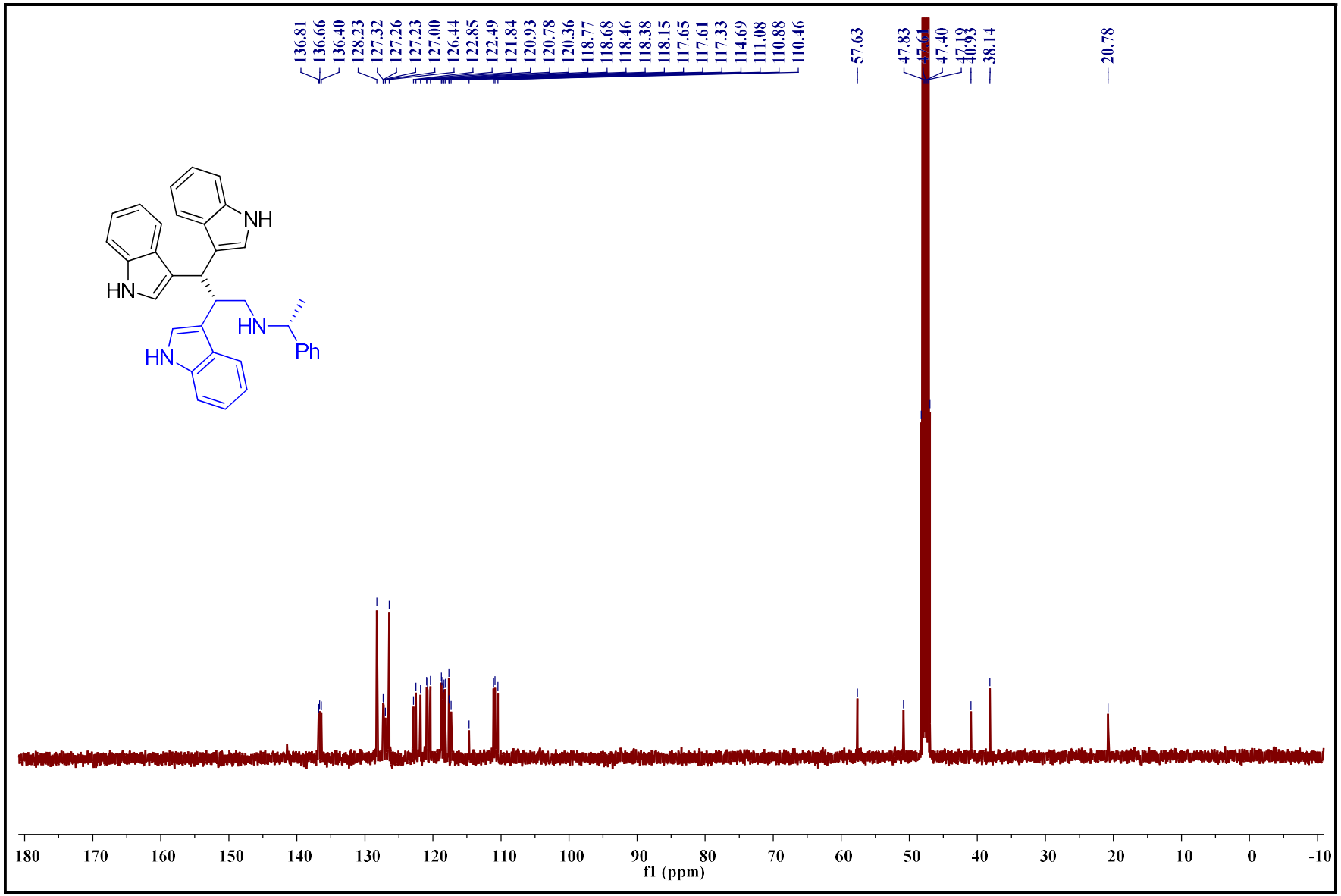
^{13}C NMR spectrum of (R)-2,3,3-tris(2-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ah):



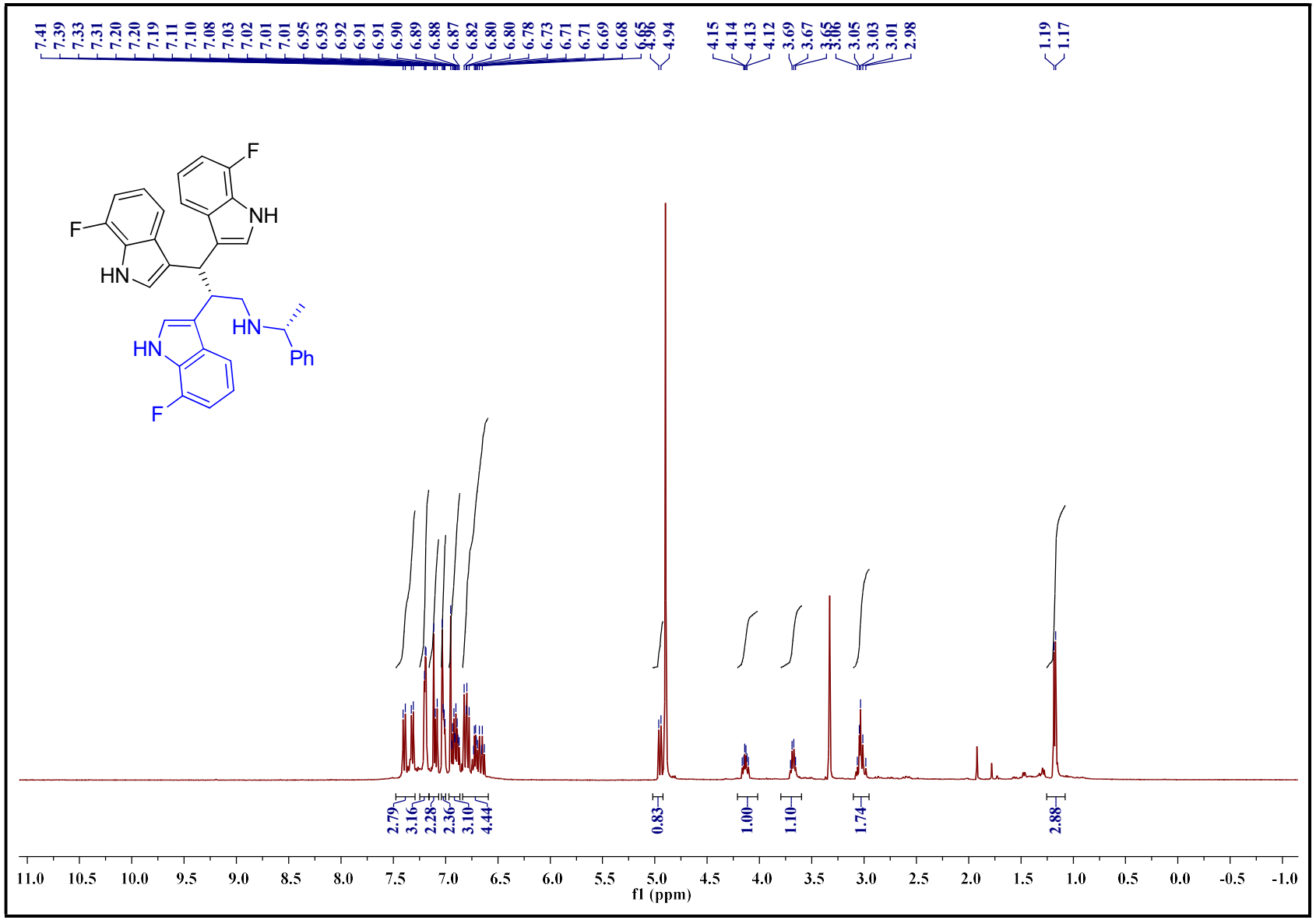
^{1}H NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ai):



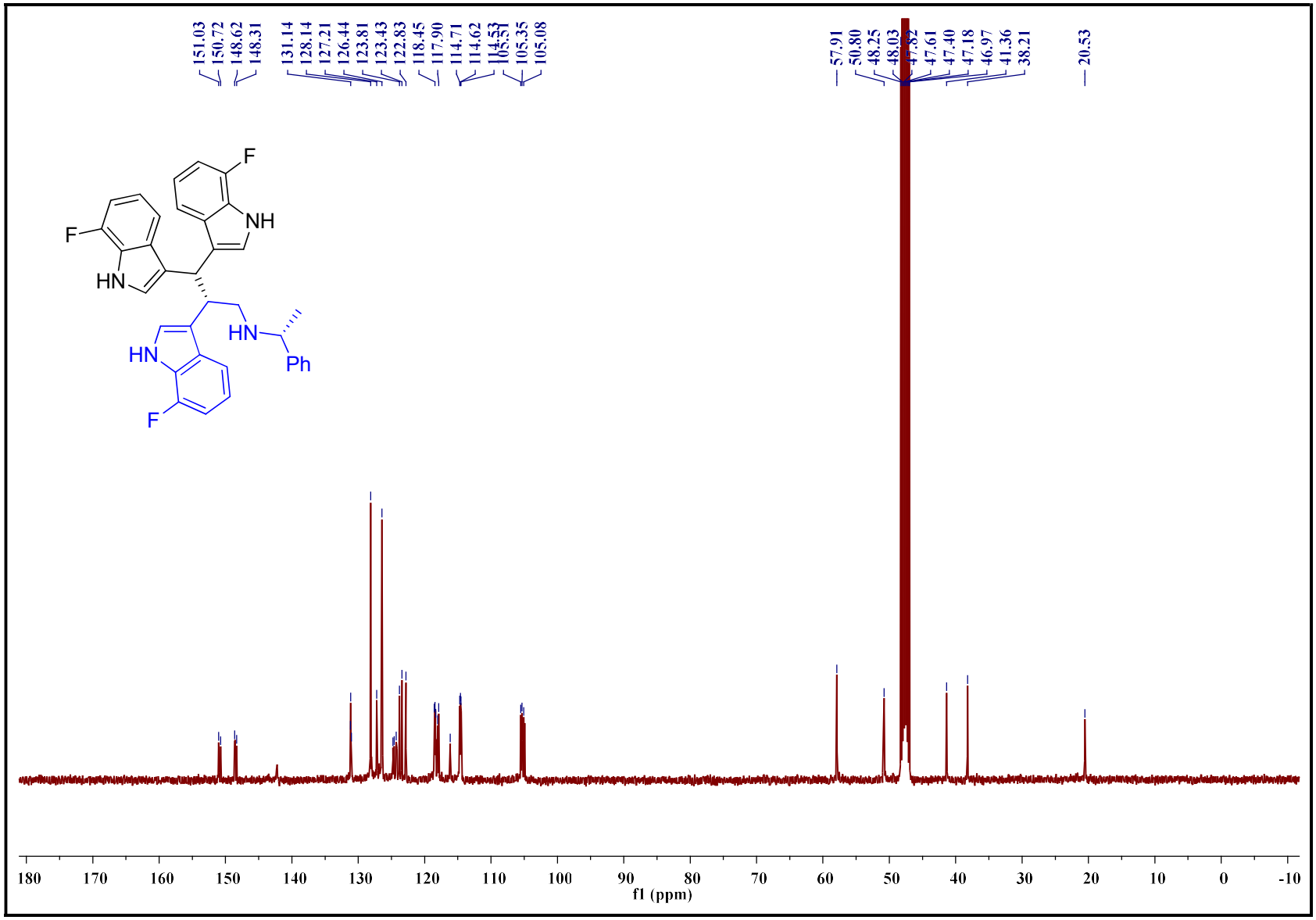
^{13}C NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ai):



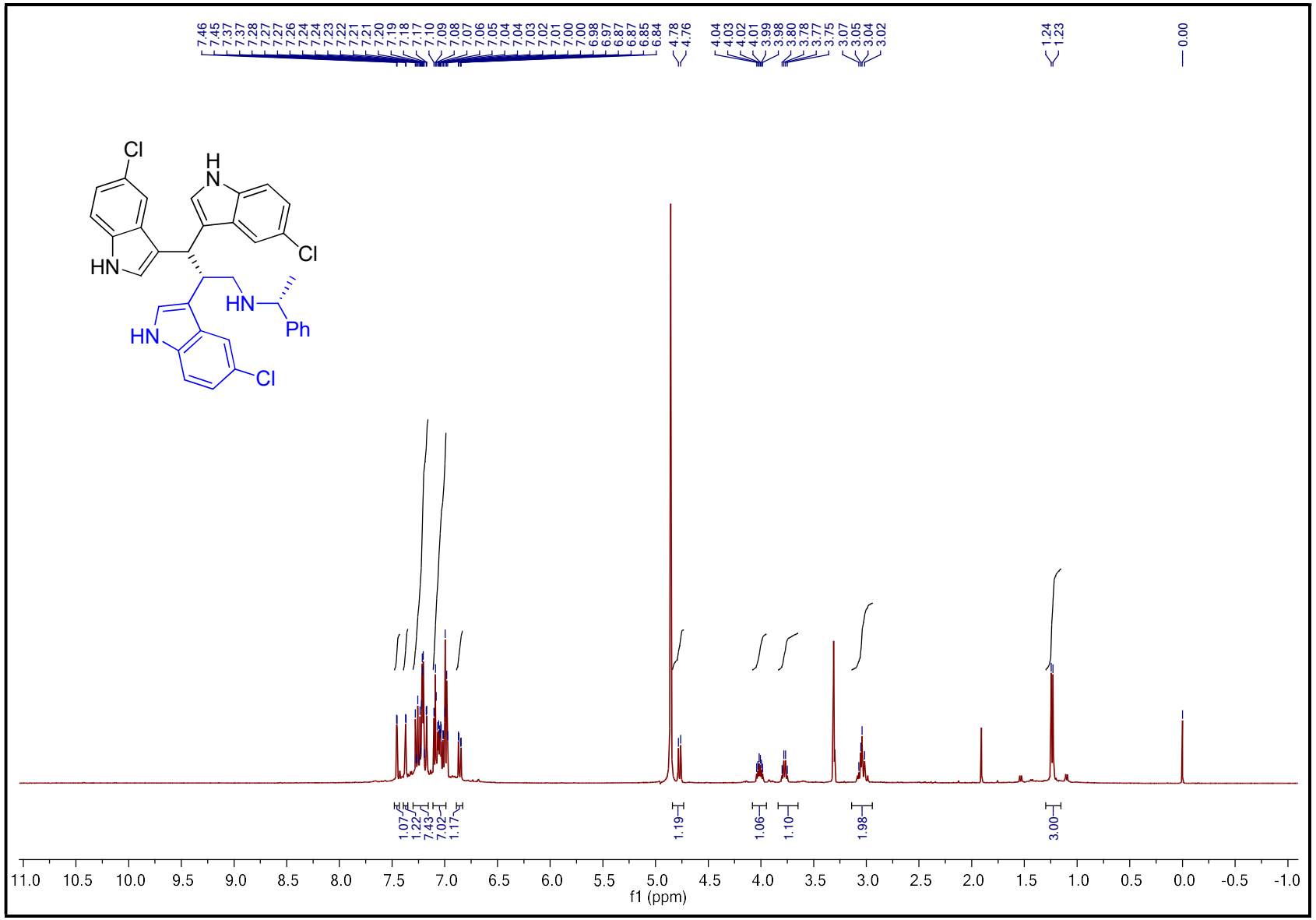
^{1}H NMR spectrum of (S)-2,3,3-tris(7-fluoro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5aj):



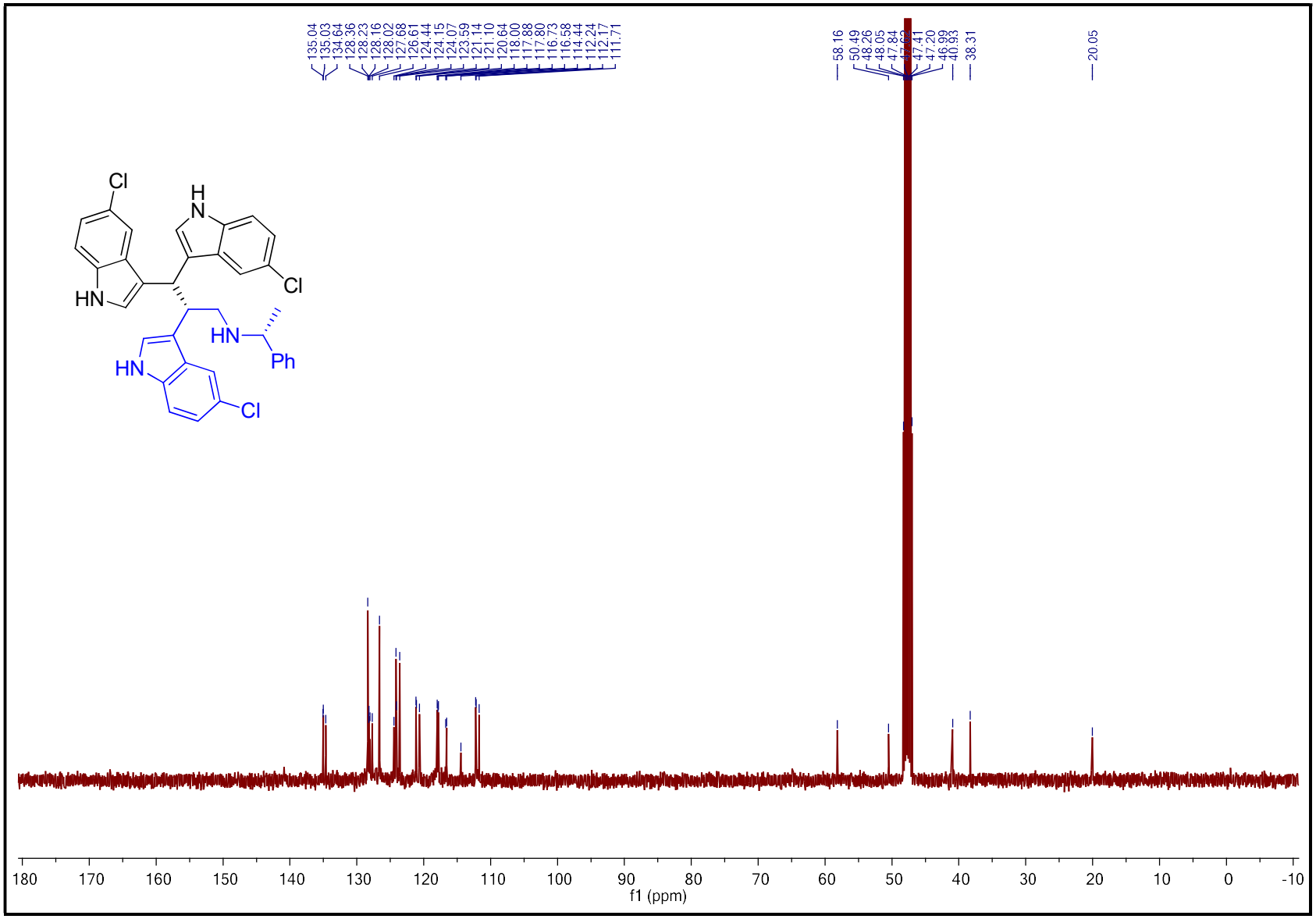
^{13}C NMR spectrum of (S)-2,3,3-tris(7-fluoro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5aj):



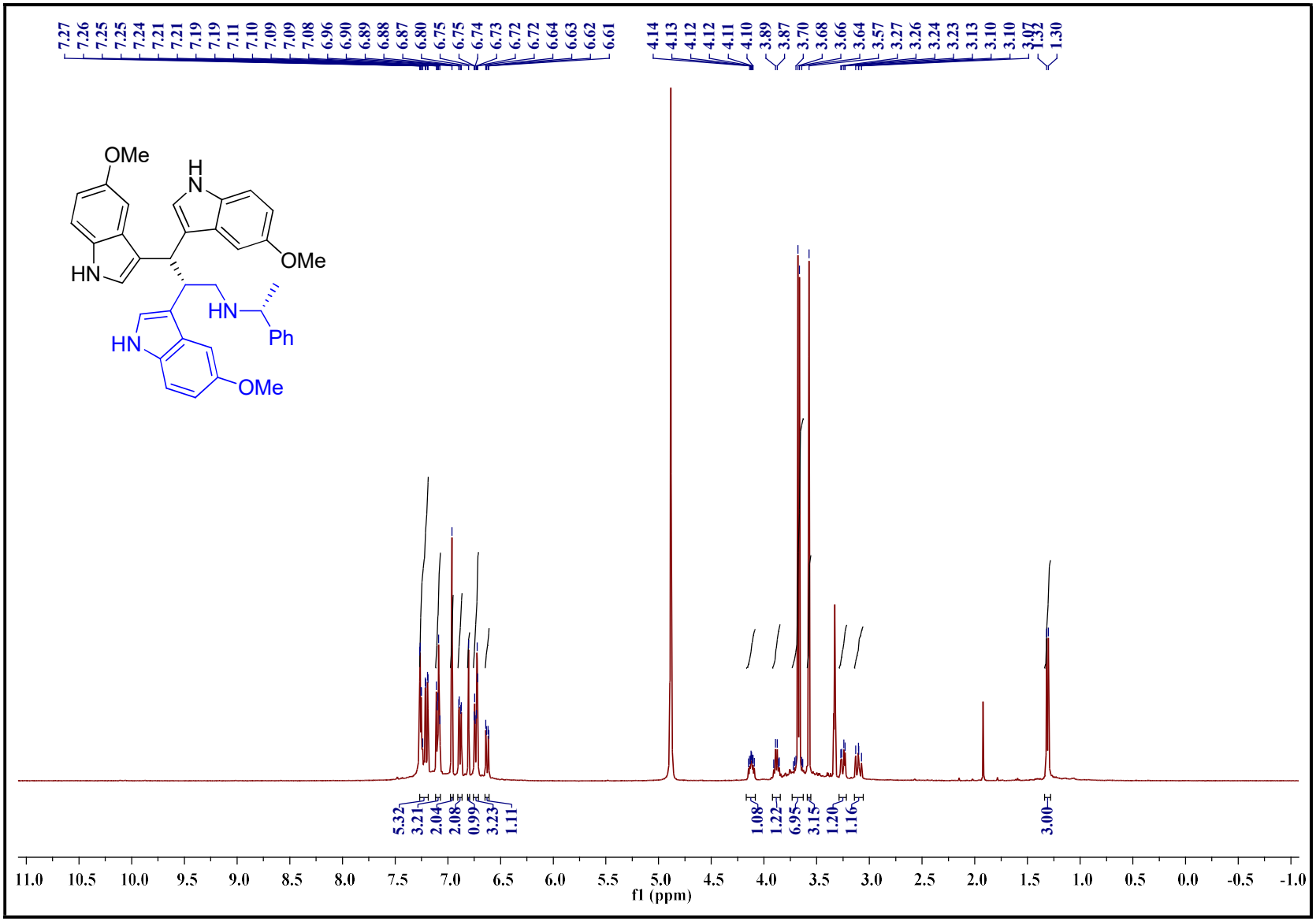
[1]H NMR spectrum of (S)-2,3,3-tris(5-chloro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ak):



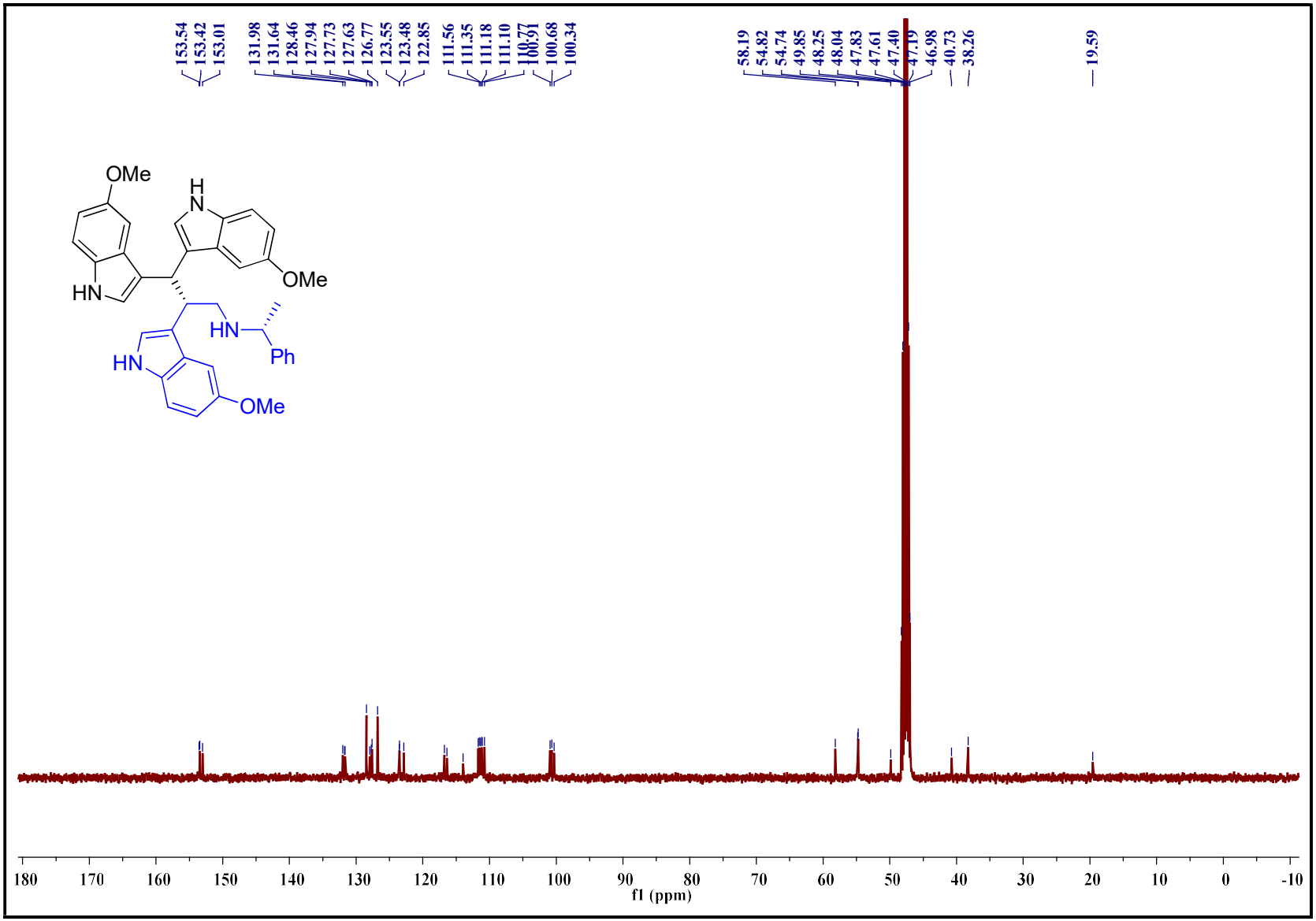
^{13}C NMR spectrum of (S)-2,3,3-tris(5-chloro-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5ak):



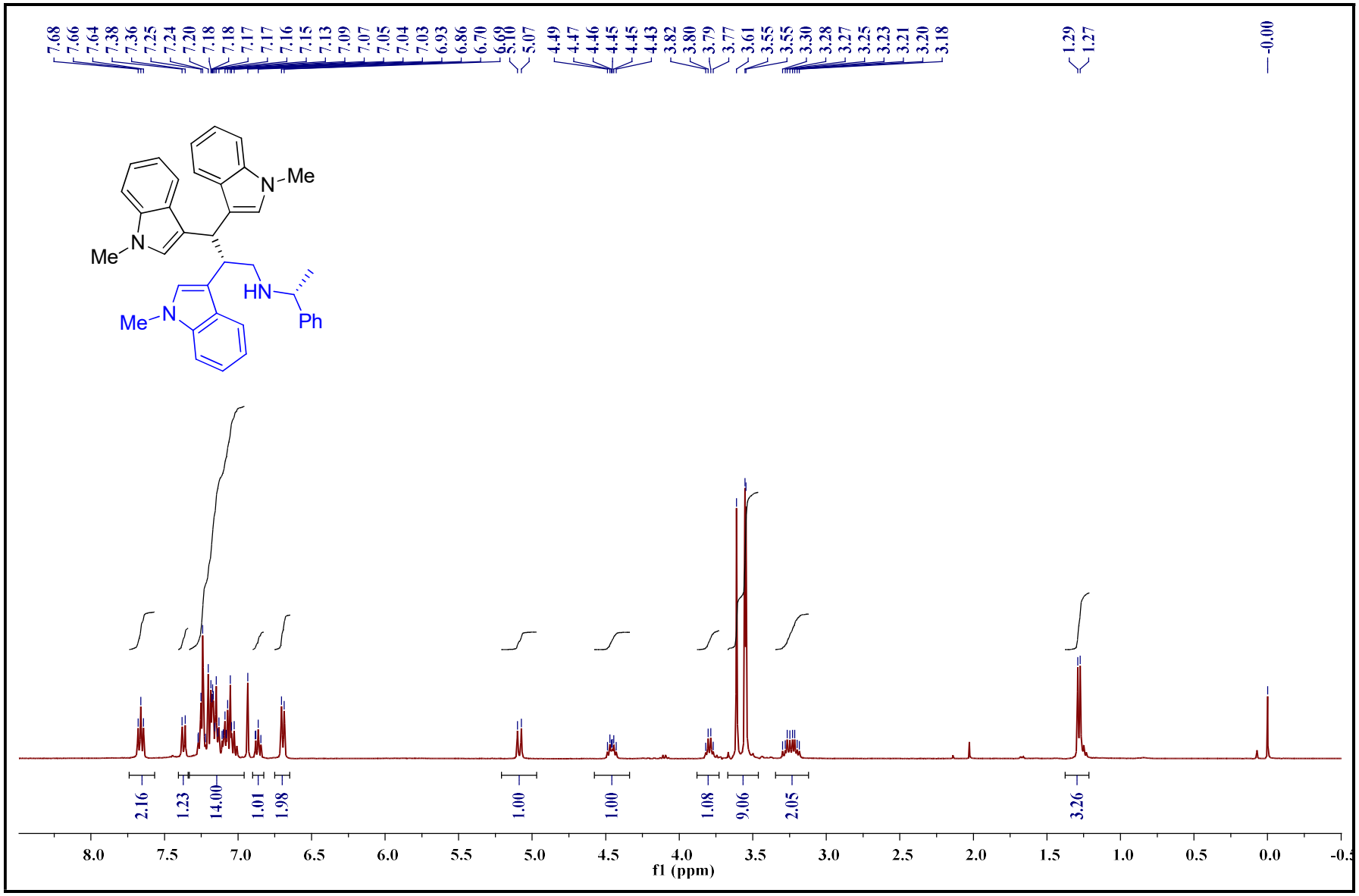
^{1}H NMR spectrum of (S)-2,3,3-tris(5-methoxy-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5al):



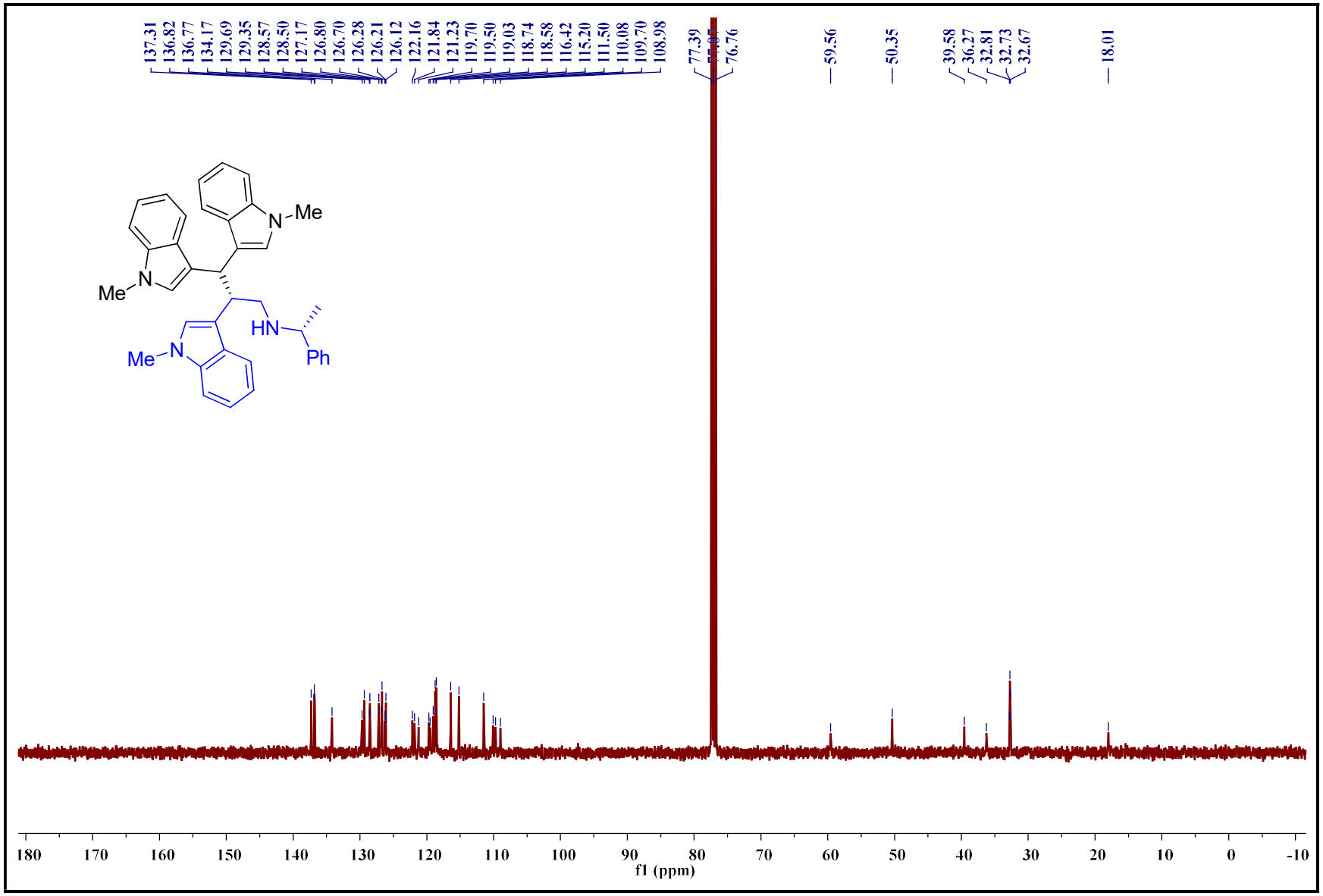
^{13}C NMR spectrum of (S)-2,3,3-tris(5-methoxy-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5al):



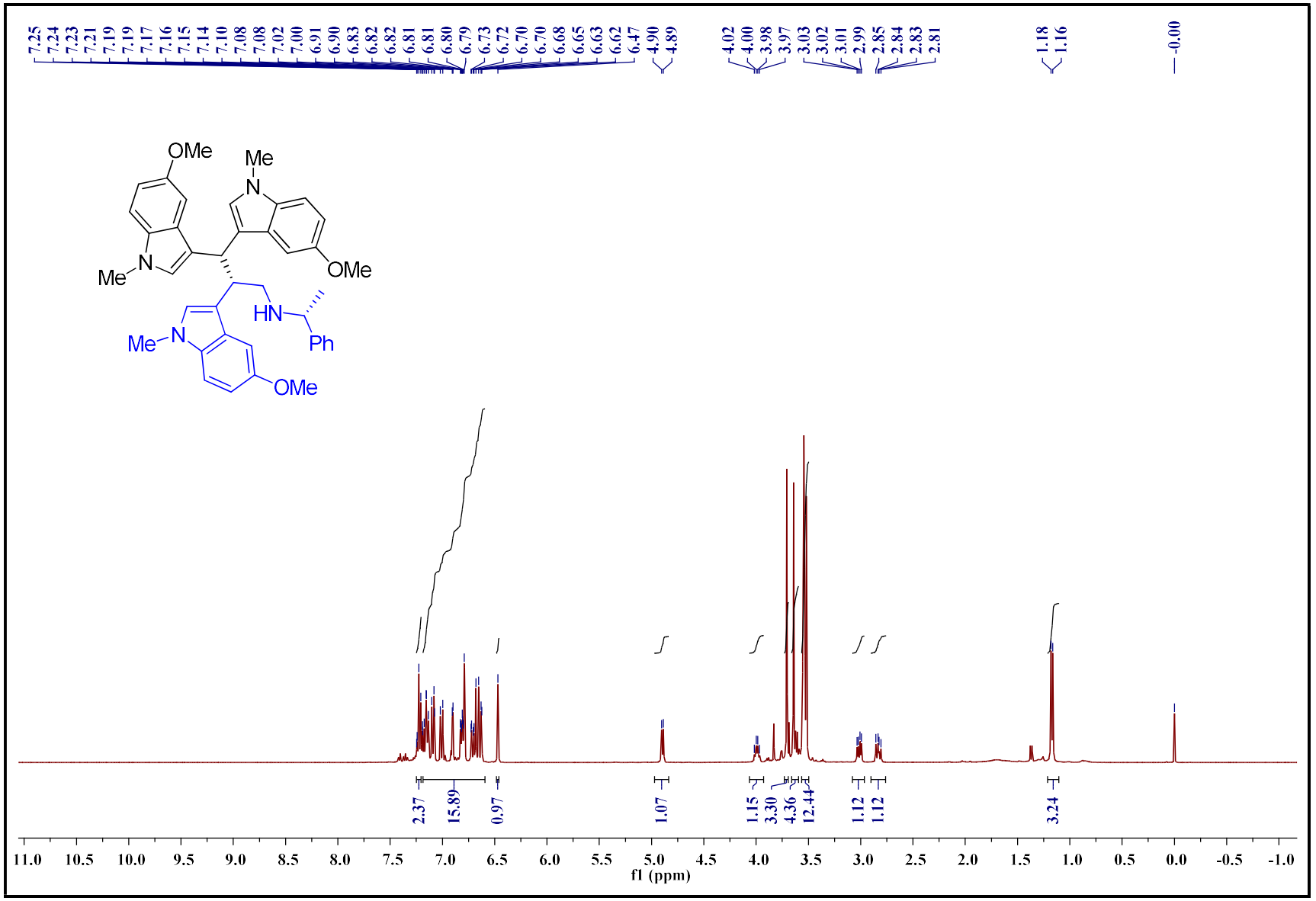
^{1}H NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5am):



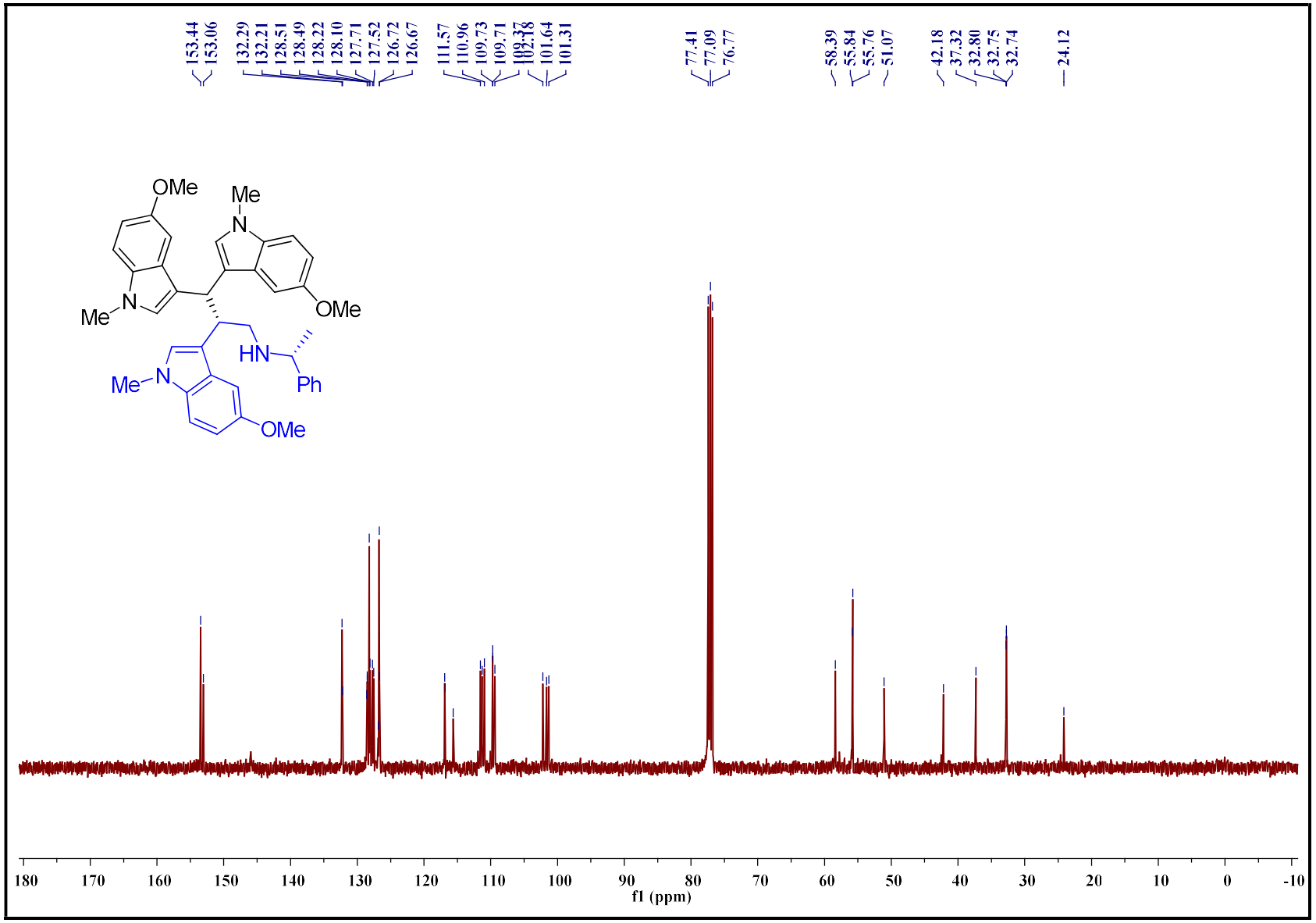
^{13}C NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5am):



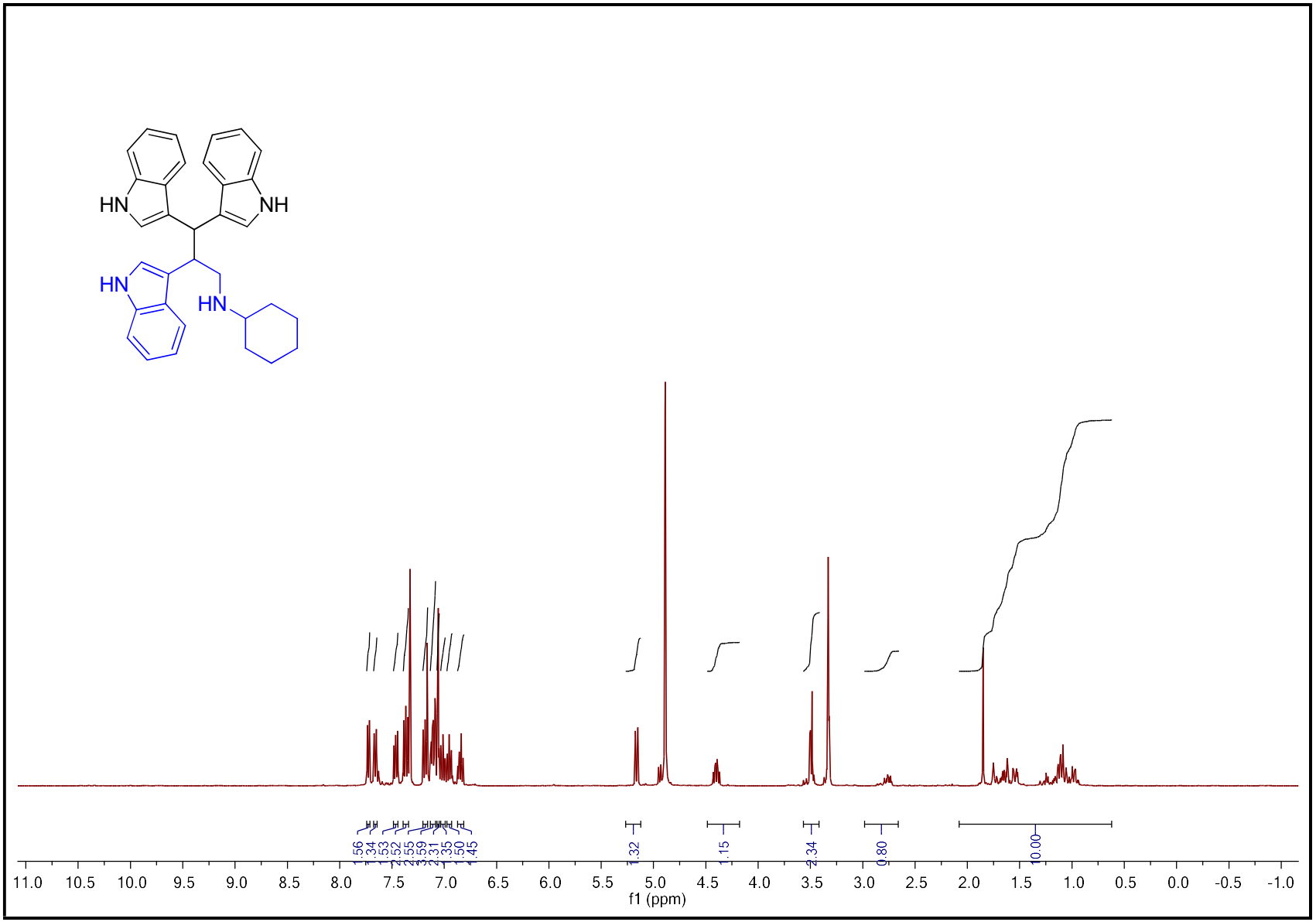
^{1}H NMR spectrum of (S)-2,3,3-tris(5-methoxy-1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5an):



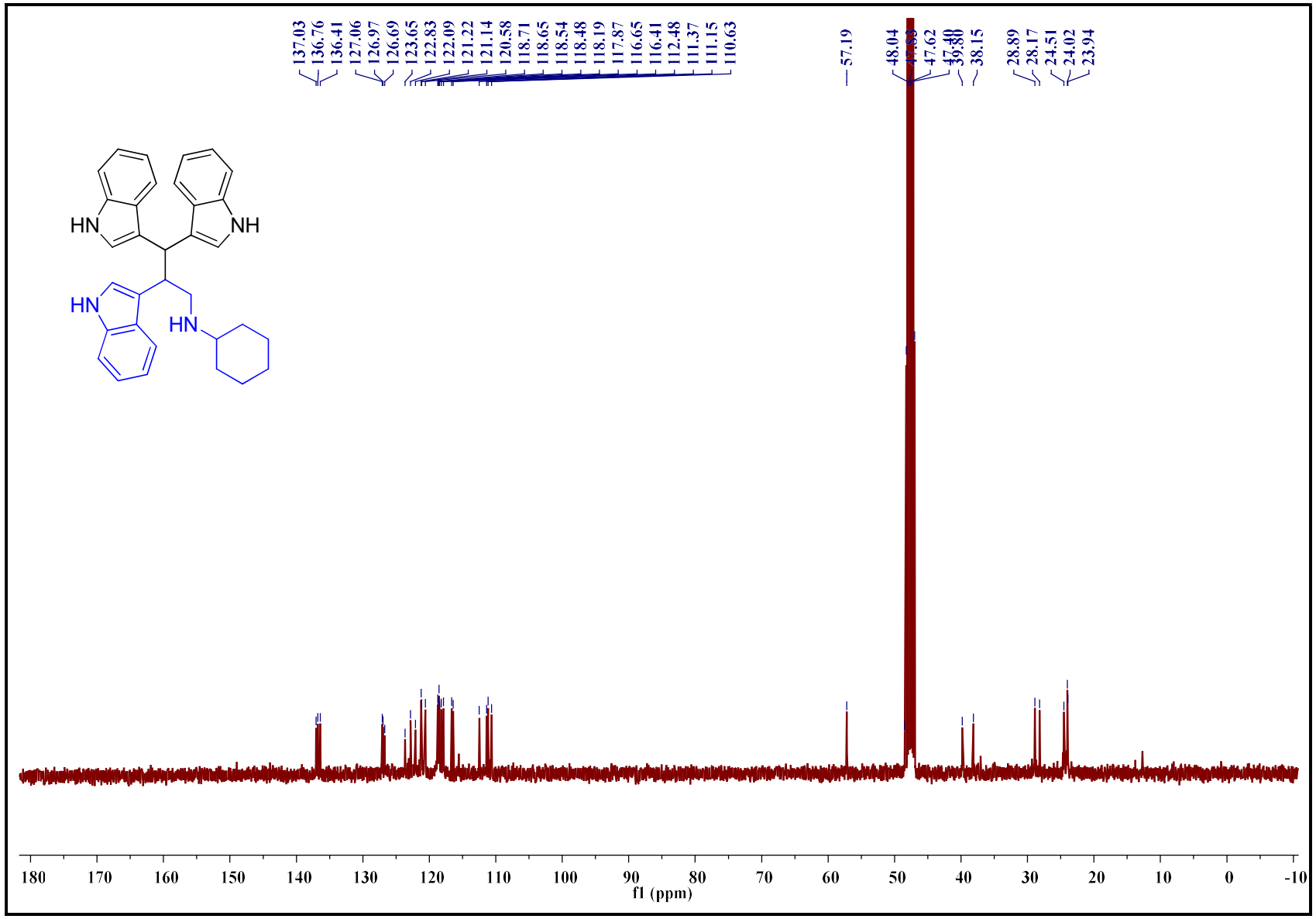
^{13}C NMR spectrum of (S)-2,3,3-tris(5-methoxy-1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)propan-1-amine (5an):



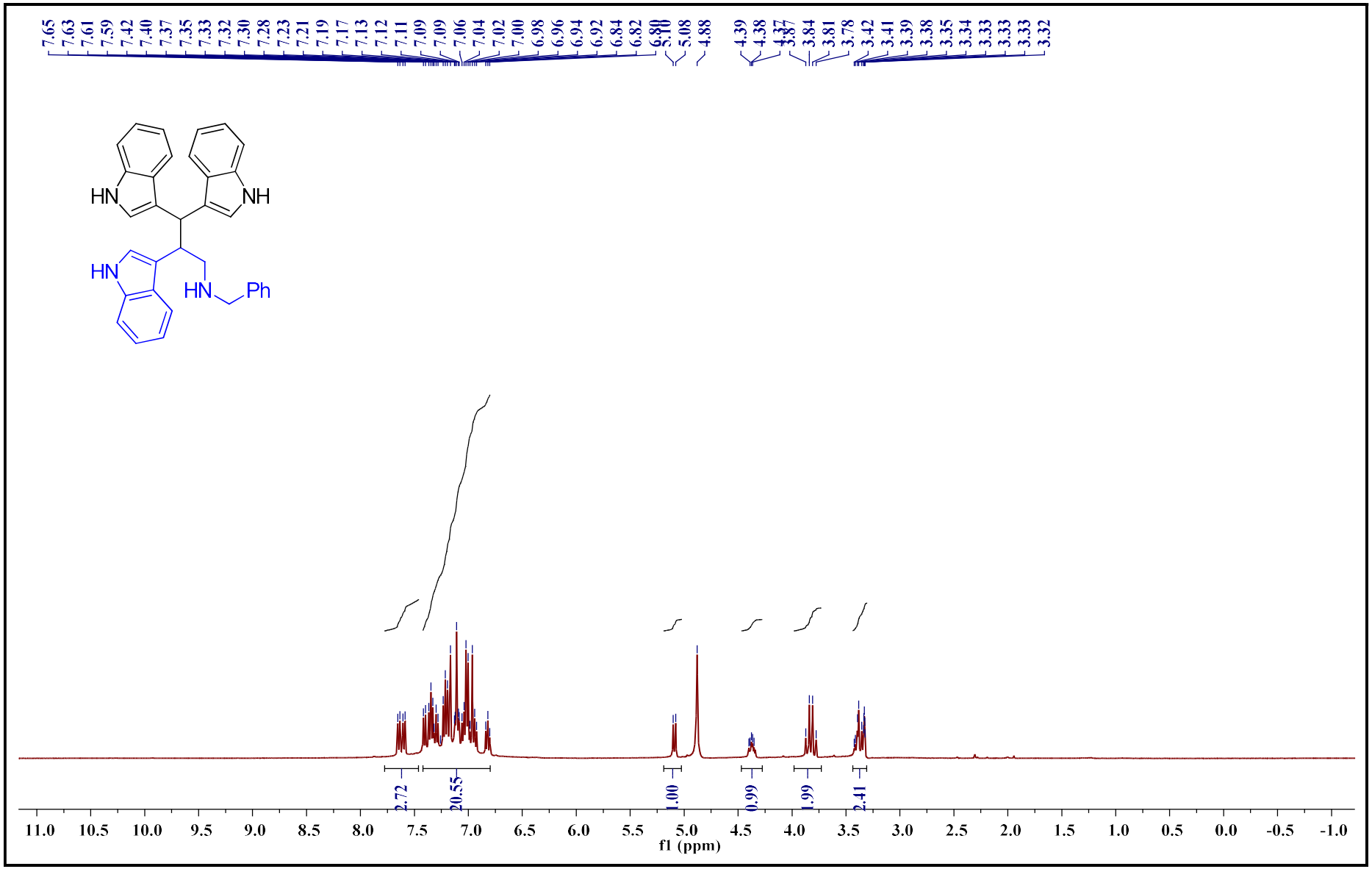
[1]H NMR spectrum of N-(2,3,3-tri(1H-indol-3-yl)propyl)cyclohexanamine (5bi):



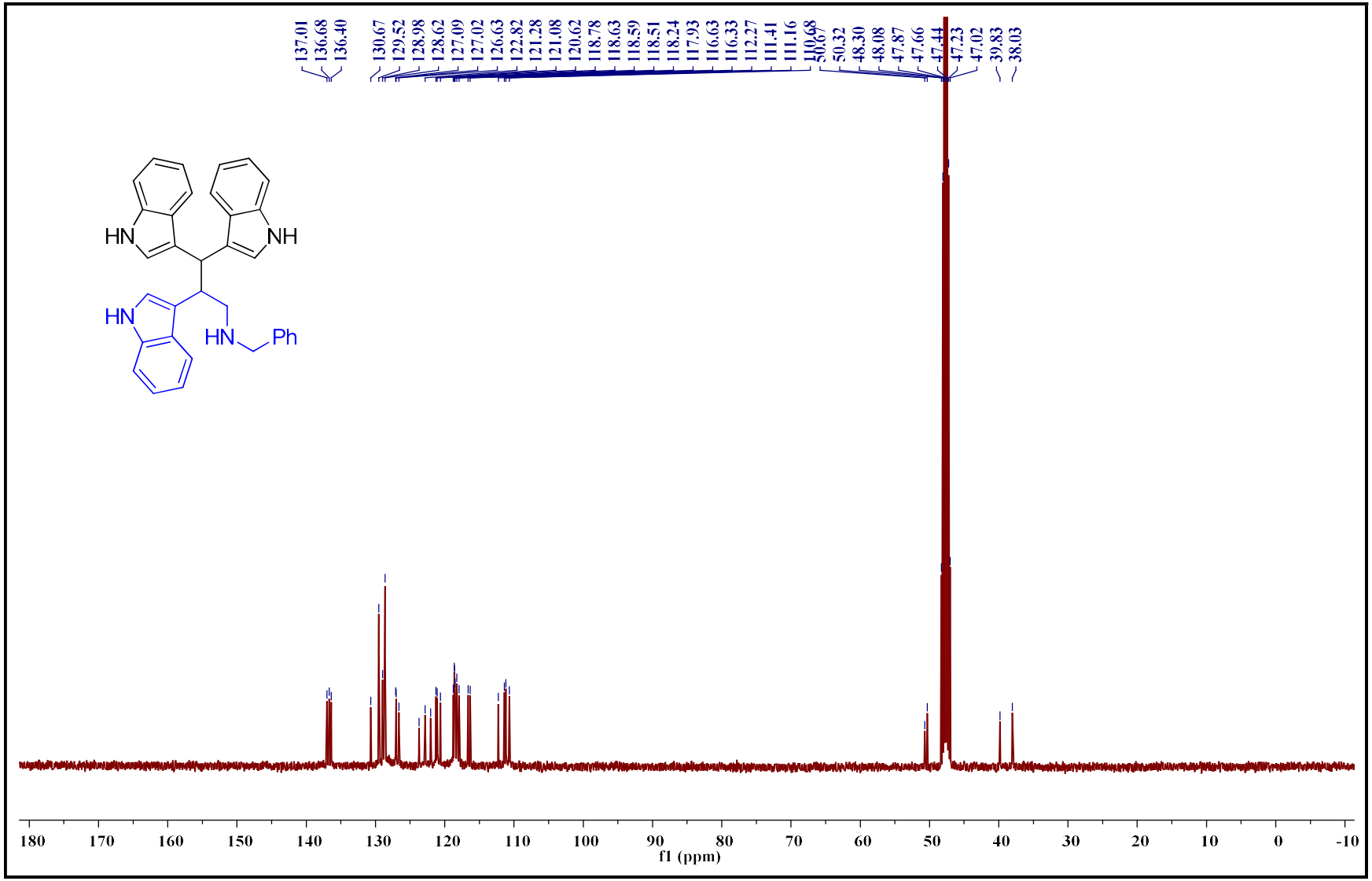
^{13}C NMR spectrum of N-(2,3,3-tri(1H-indol-3-yl)propyl)cyclohexanamine (5bi):



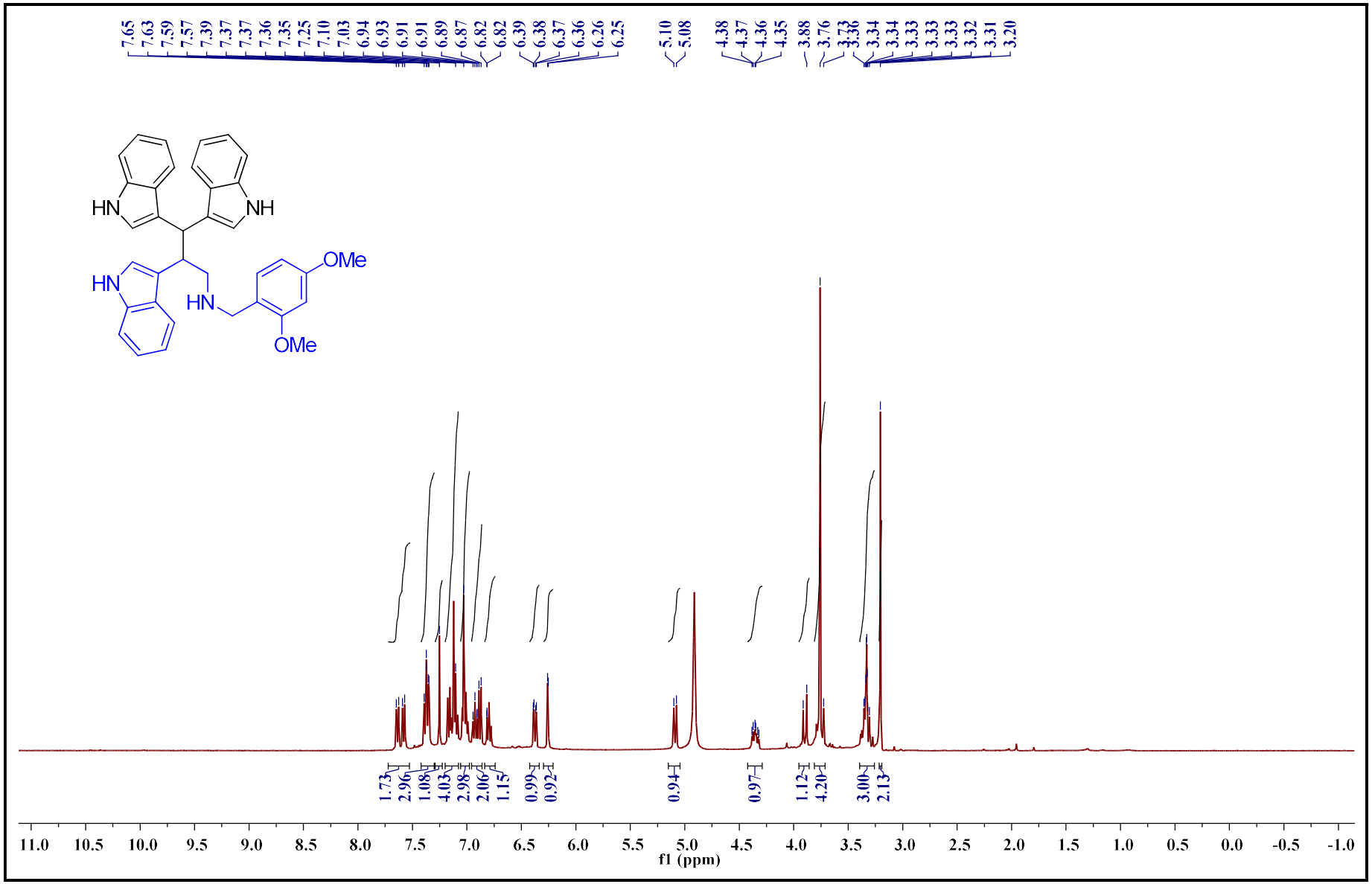
^{1}H NMR spectrum of N-benzyl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ci):



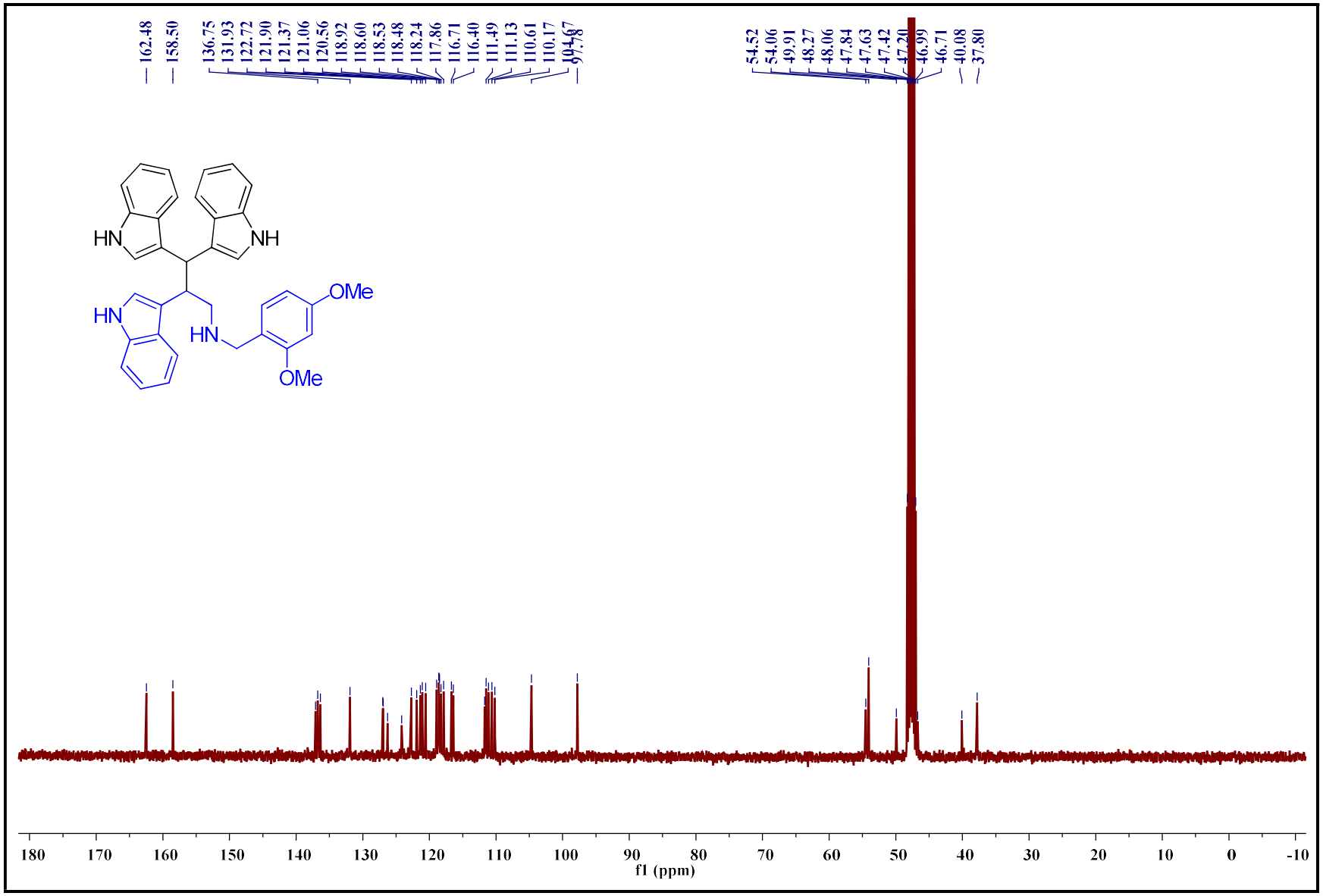
^{13}C NMR spectrum of N-benzyl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ci)



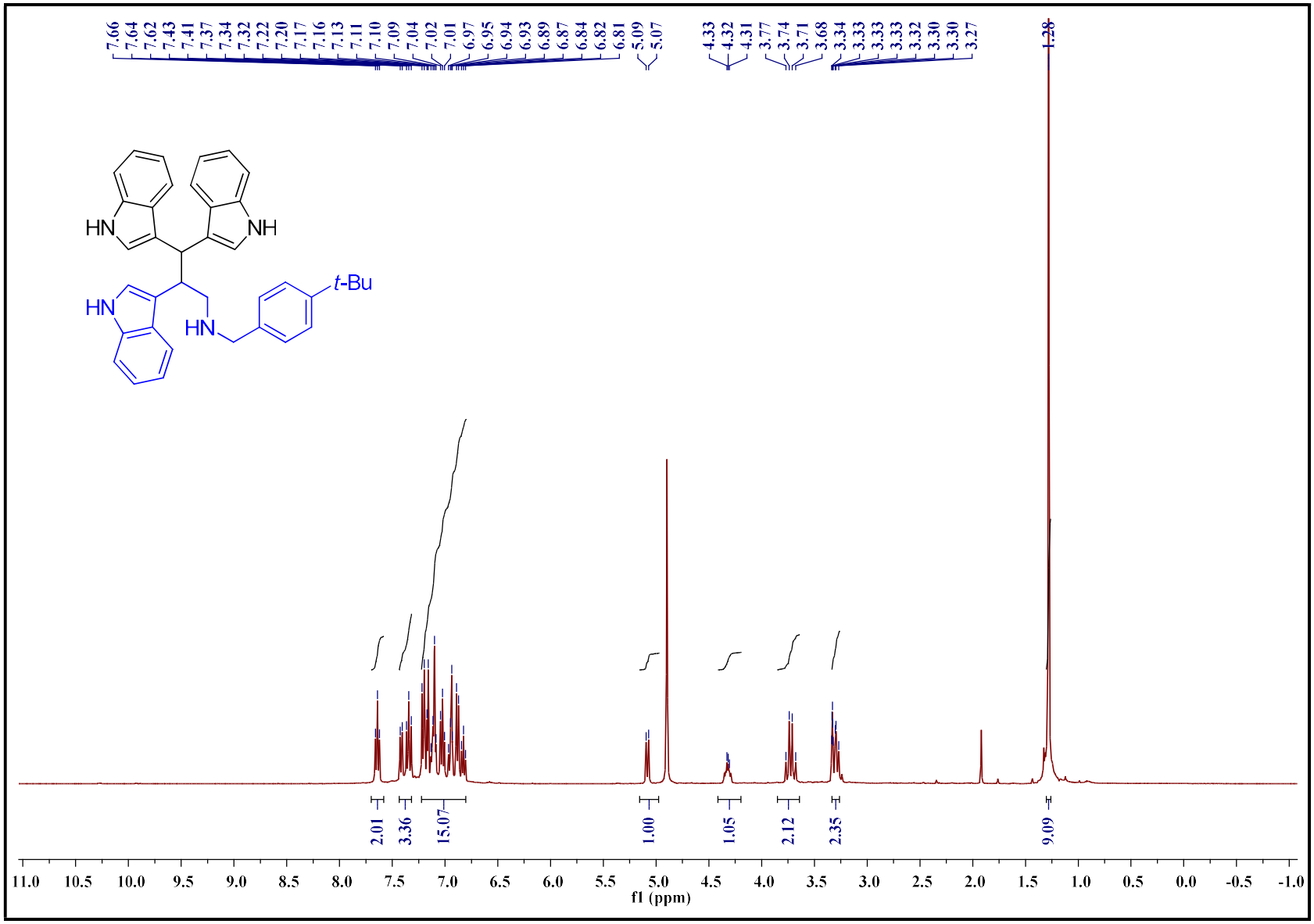
[1]H NMR spectrum of N-(2,4-dimethoxybenzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5di):



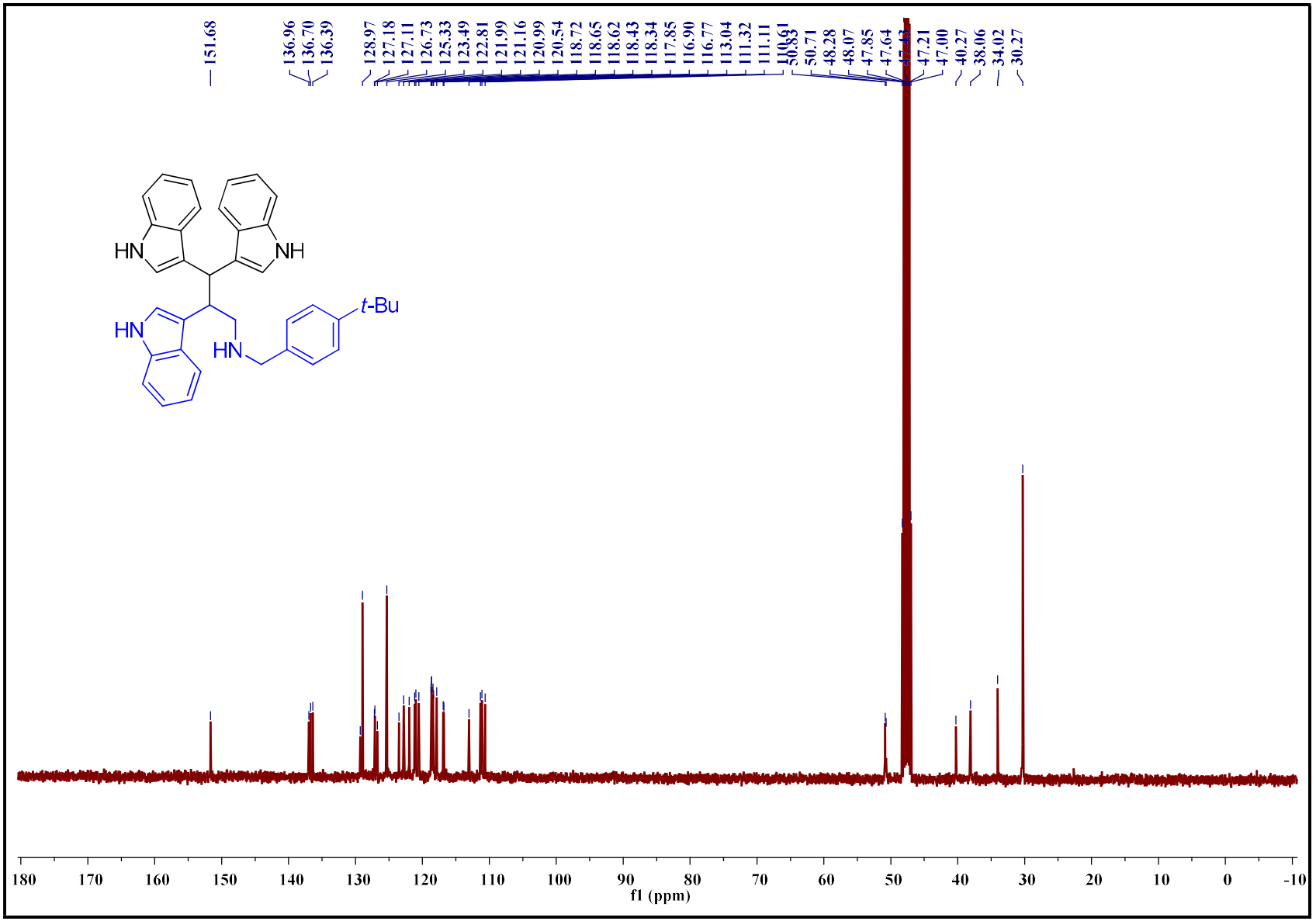
^{13}C NMR spectrum of N-(2,4-dimethoxybenzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5di):



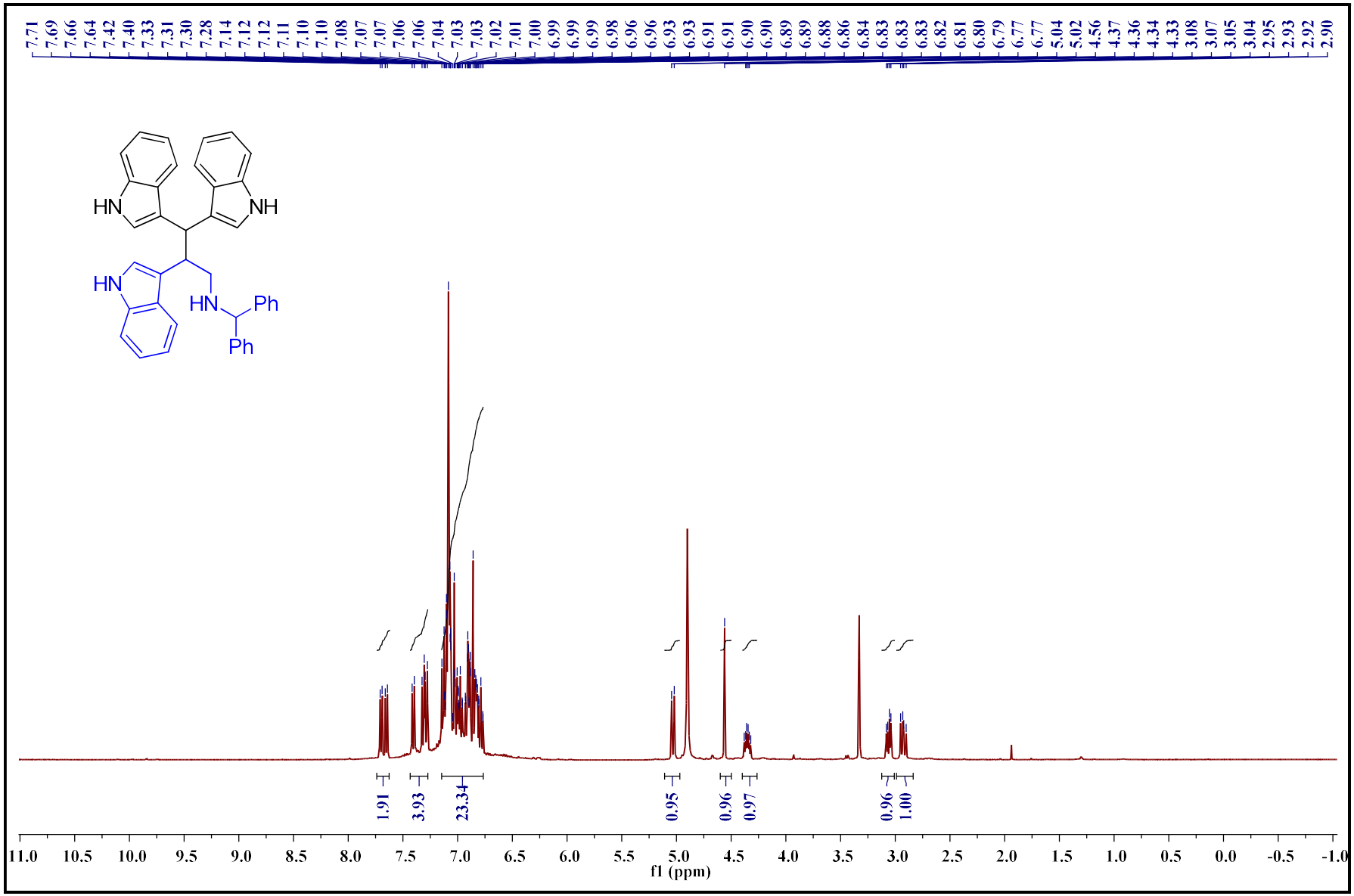
^{1}H NMR spectrum of N-(4-(tert-butyl)benzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ei):



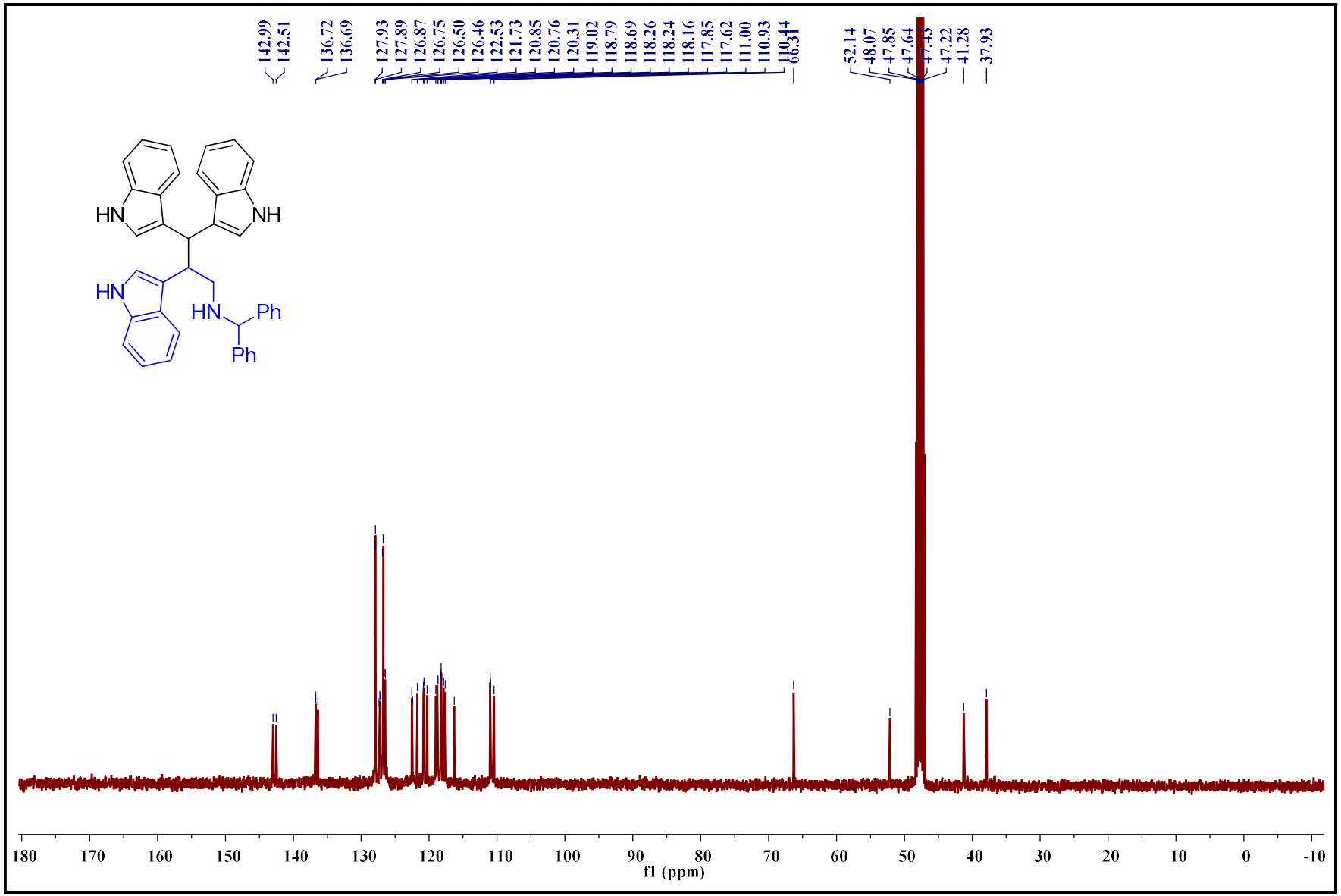
^{13}C NMR spectrum of N-(4-(tert-butyl)benzyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5ei):



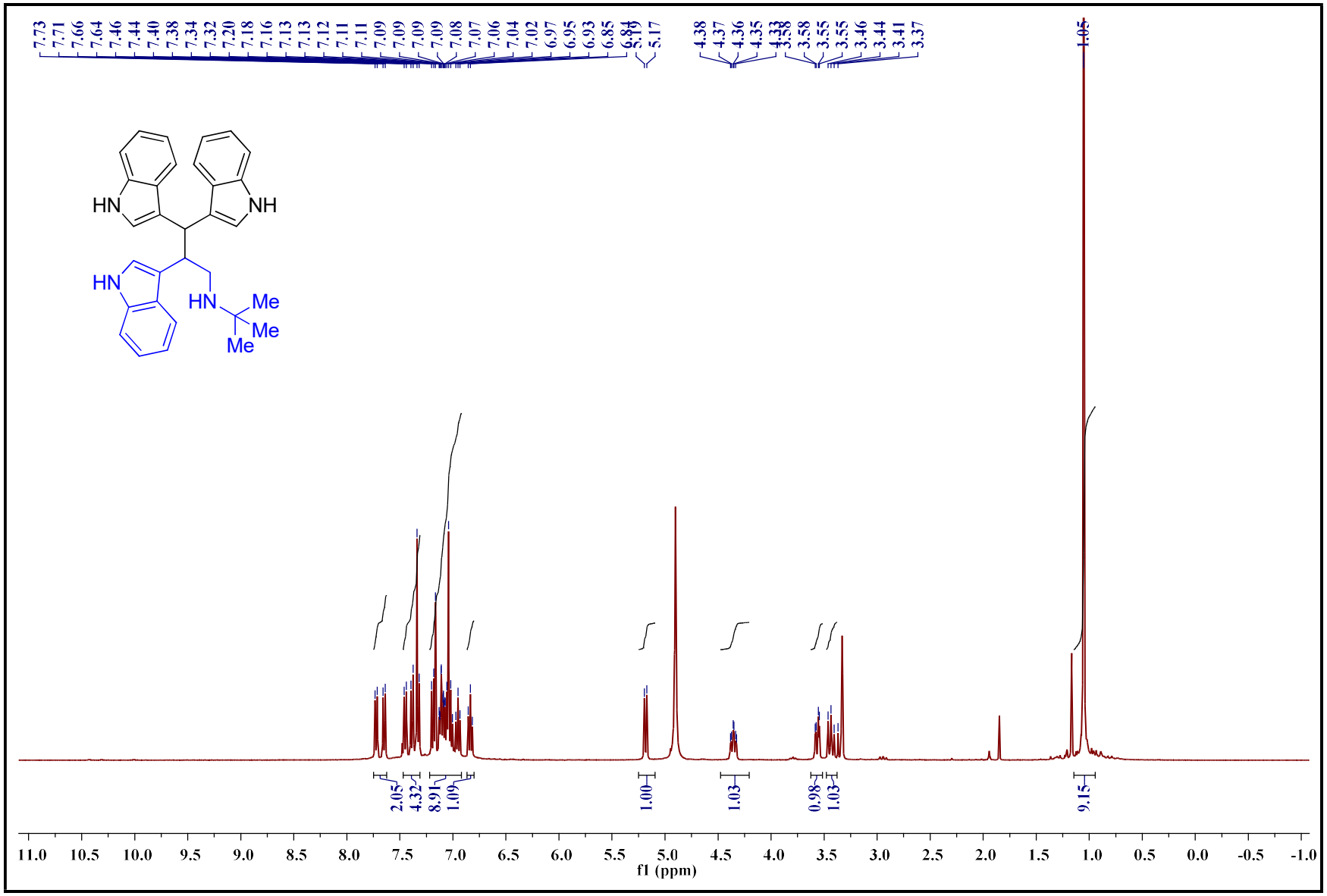
^{1}H NMR spectrum of N-benzhydryl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5fi):



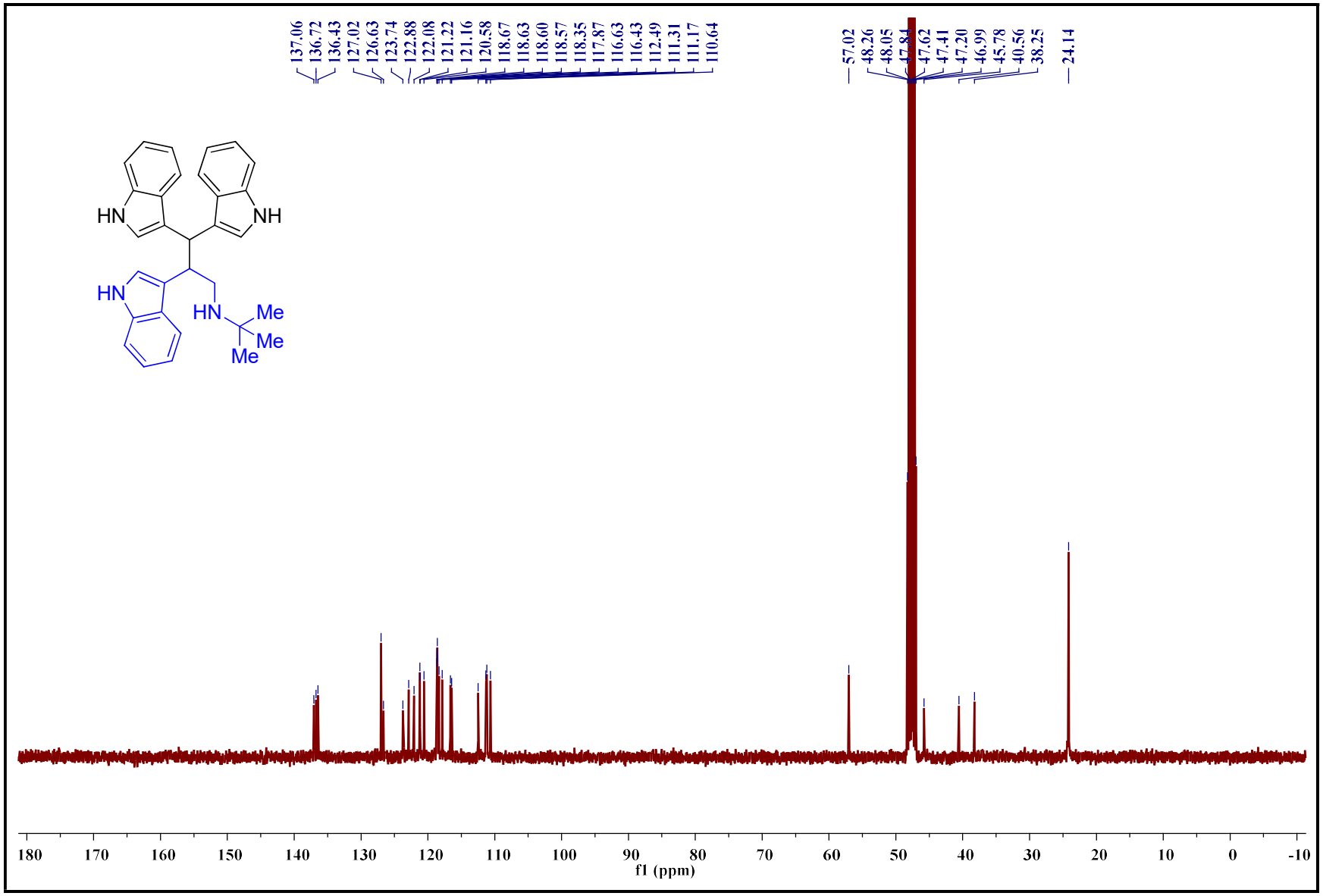
^{13}C NMR spectrum of N-benzhydryl-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5fi):



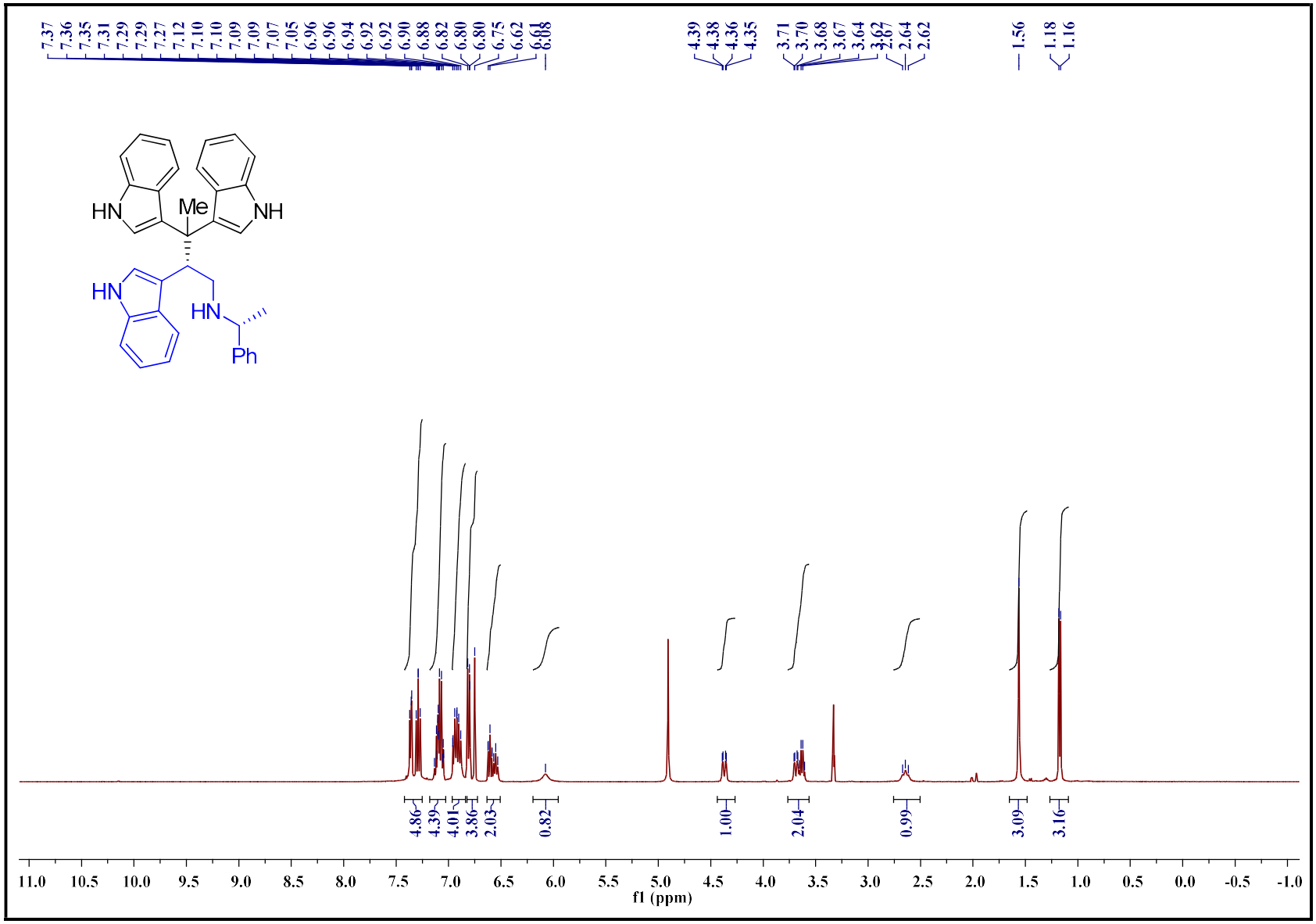
^{1}H NMR spectrum of N-(tert-butyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5gi):



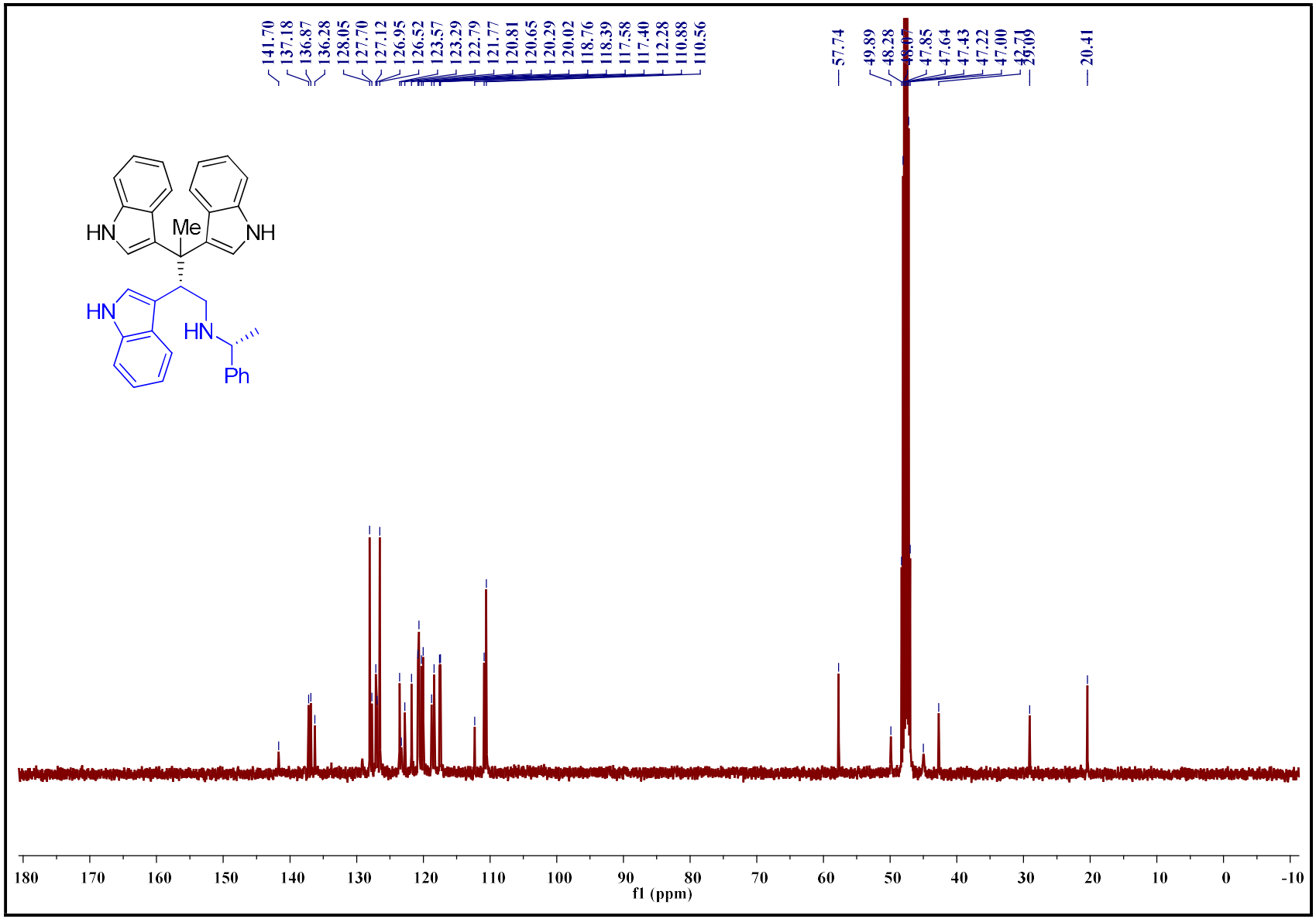
^{13}C NMR spectrum of N-(tert-butyl)-2,3,3-tri(1H-indol-3-yl)propan-1-amine (5gi):



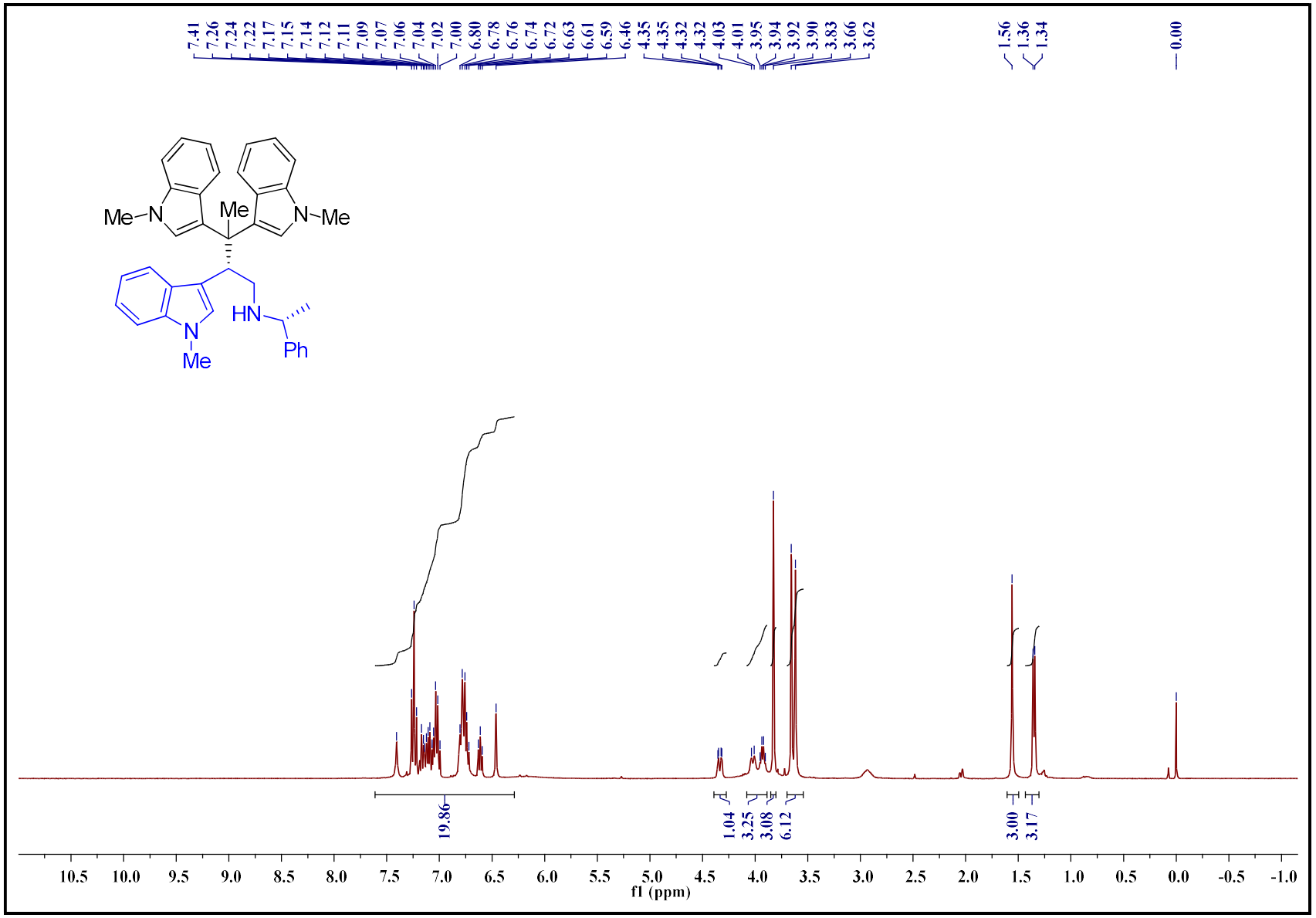
[1]H NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6ai):



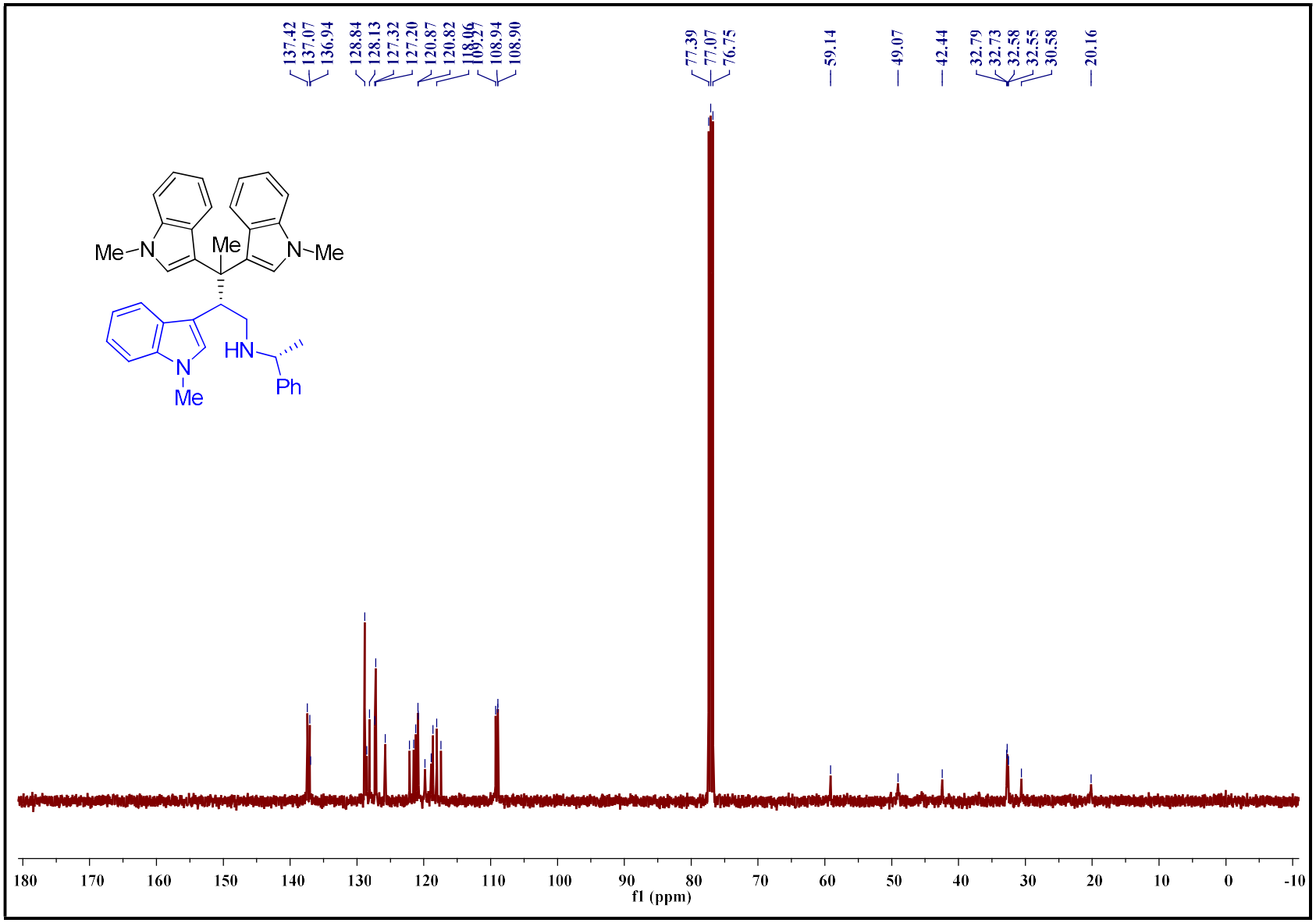
^{13}C NMR spectrum of (S)-2,3,3-tri(1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6ai):



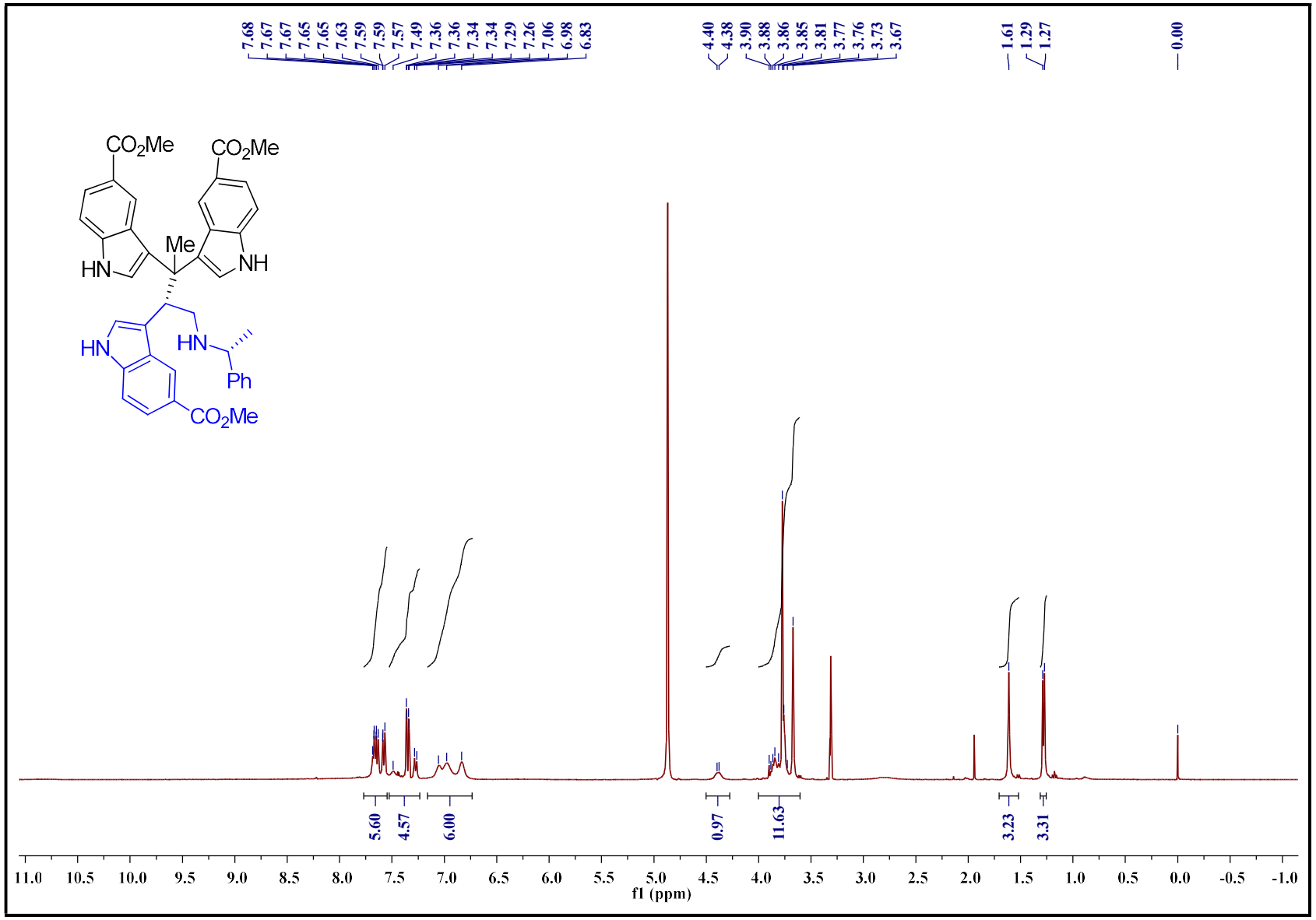
[1]H NMR spectrum of (S)-2,3,3-tris(1-methyl-1H-indol-3-yl)-N-((R)-1-phenylethyl)butan-1-amine (6am):



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



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



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