**Supporting Information**

# Nitrogen positional scanning in tetramines active against HIV-1 as potential CXCR4 inhibitors

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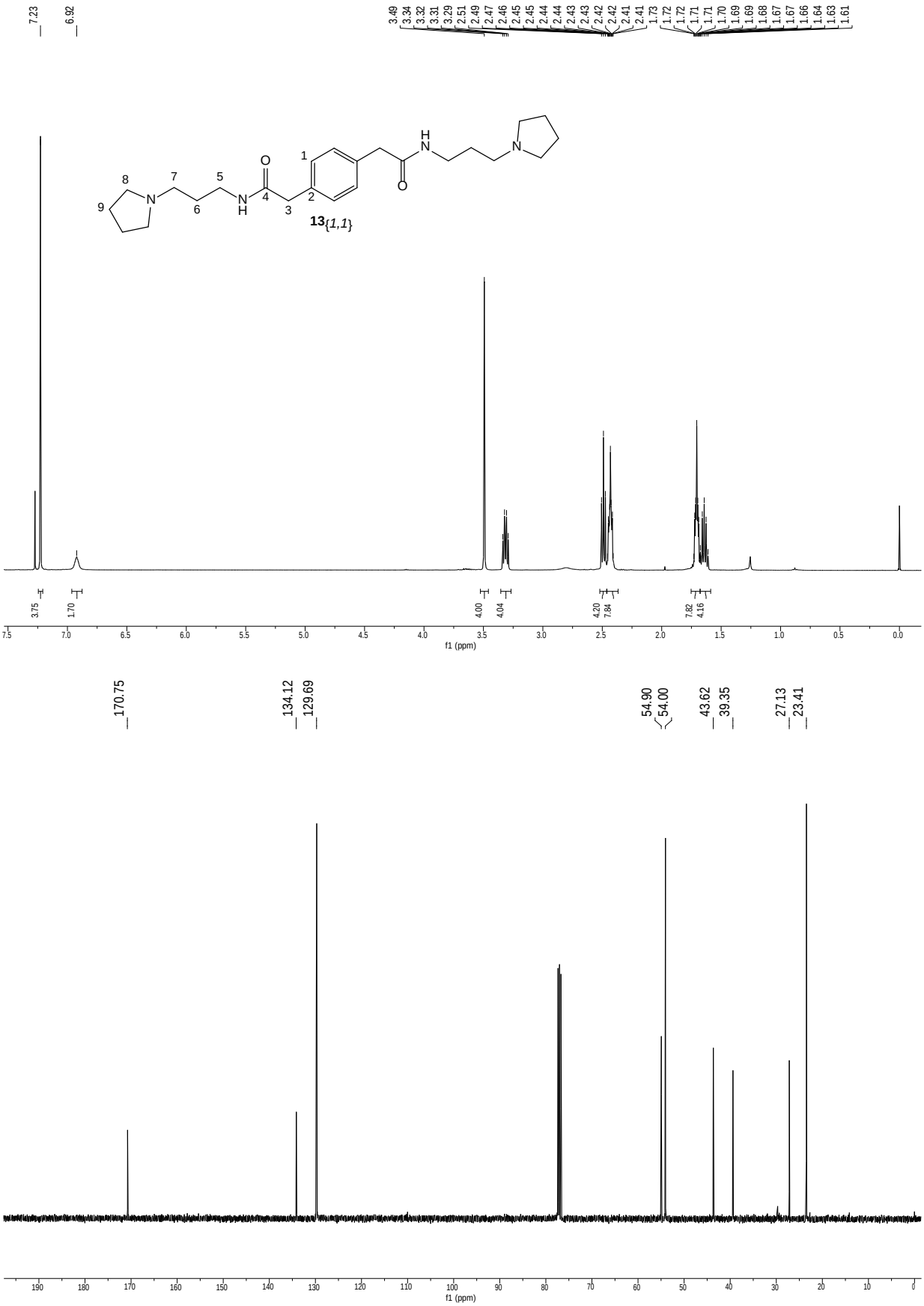


**Fig. S-1:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(3-(pyrrolidin-1-yl)propyl)-1,4-di(amino-carbonylmethyl)benzene (**13**{*1,1*}).

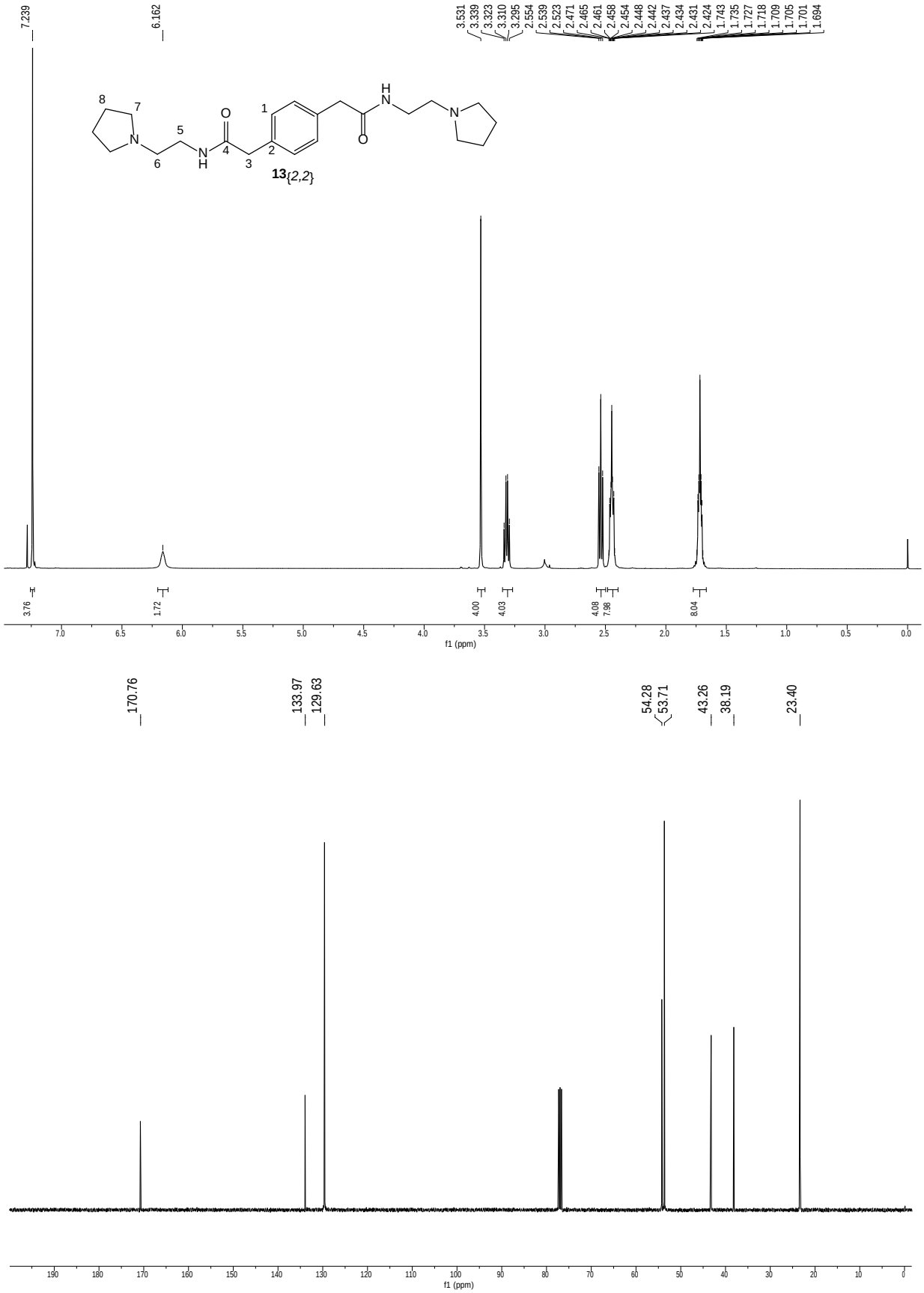


**Fig. S-2:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(2-(pyrrolidin-1-yl)ethyl)-1,4-di(aminocarbonyl-methyl)benzene (**13**{*2*,*2*}).

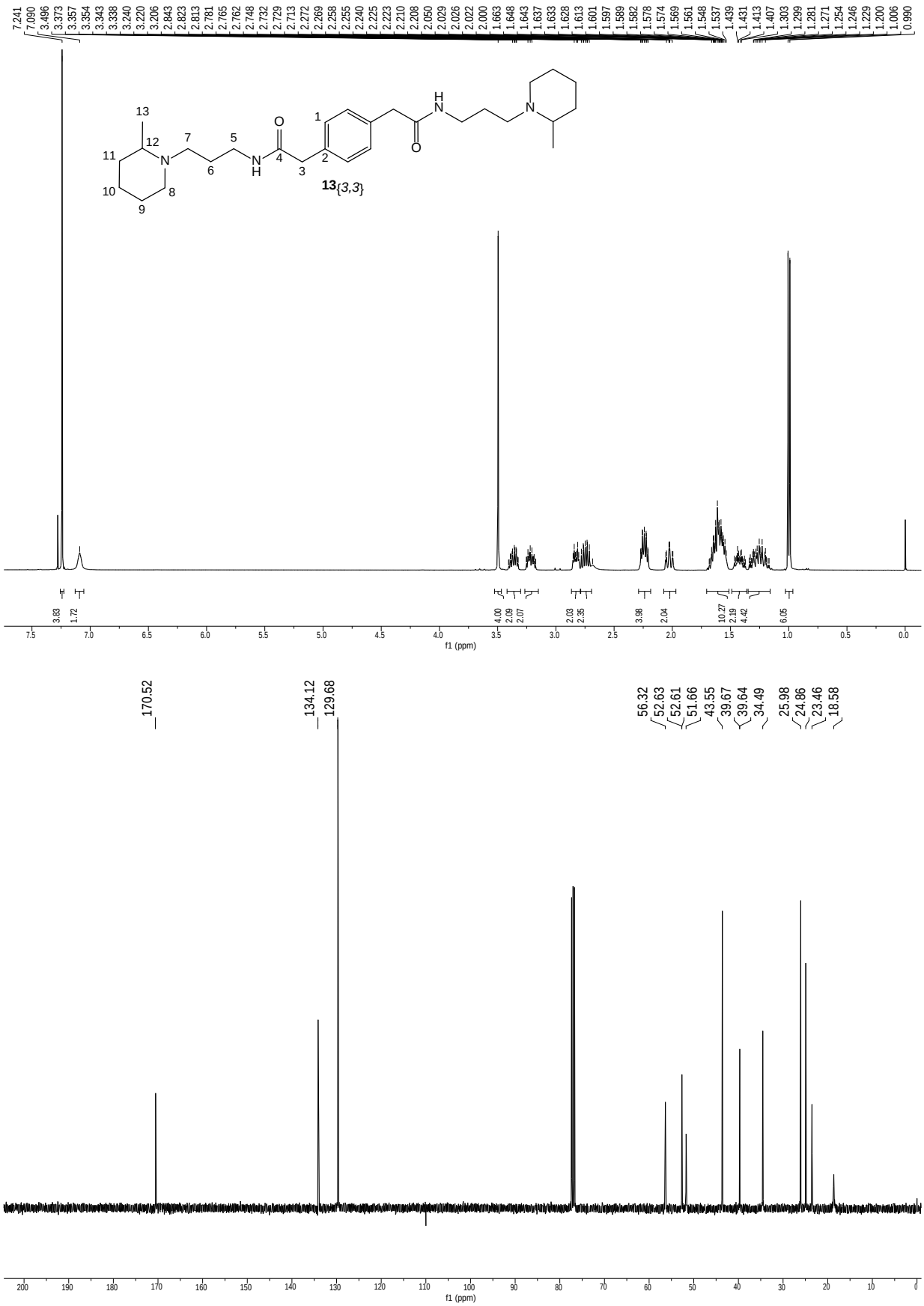


**Fig. S-3:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(3-(2-pipecolin-1-yl)propyl)-1,4-di(amino-carbonylmethyl)benzene (**13**{*3*,*3*}).

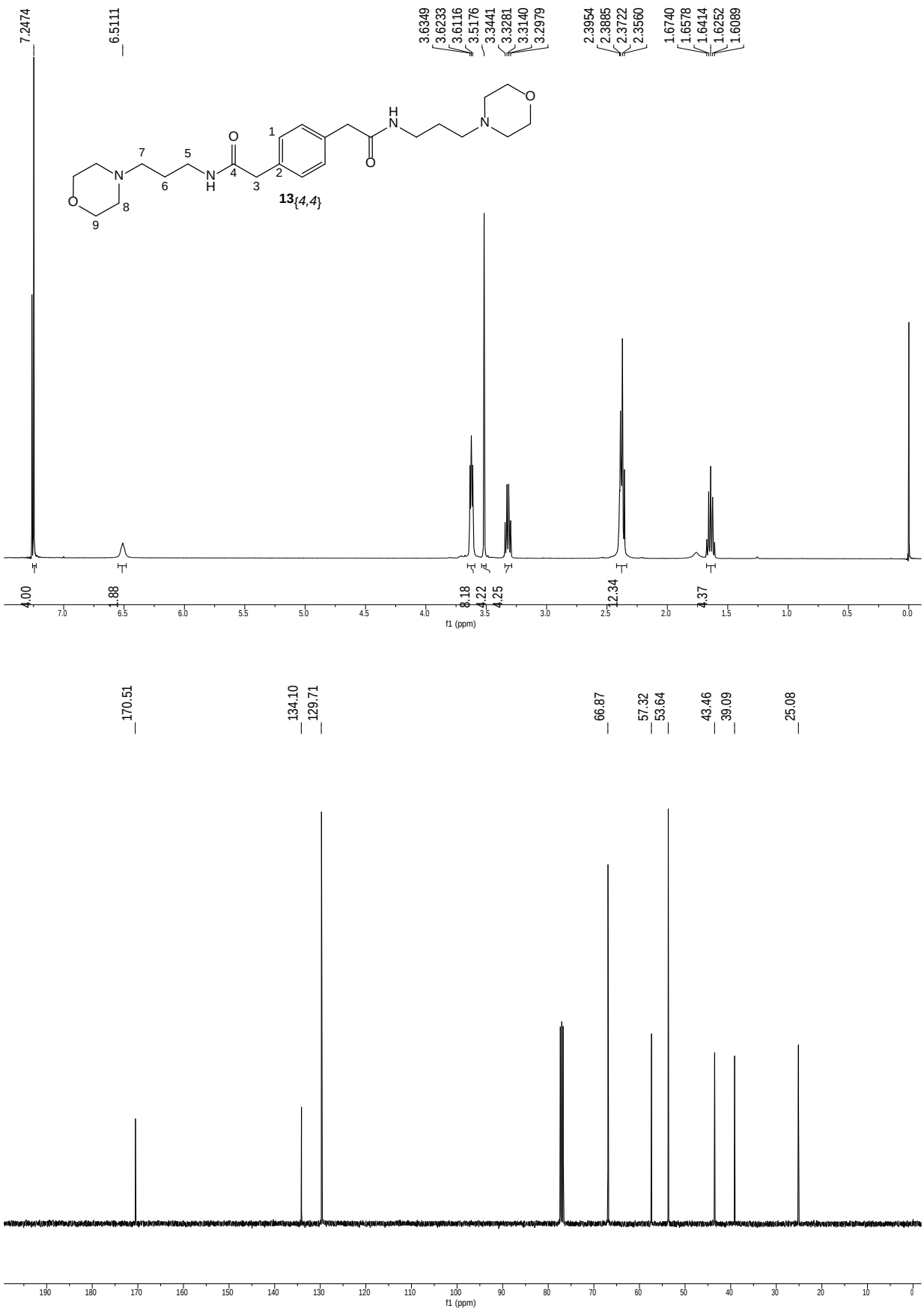


**Fig. S-4:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(3-(morpholin-4-yl)propyl)-1,4-di(amino-carbonylmethyl)benzene (**13**{*4*,*4*}).

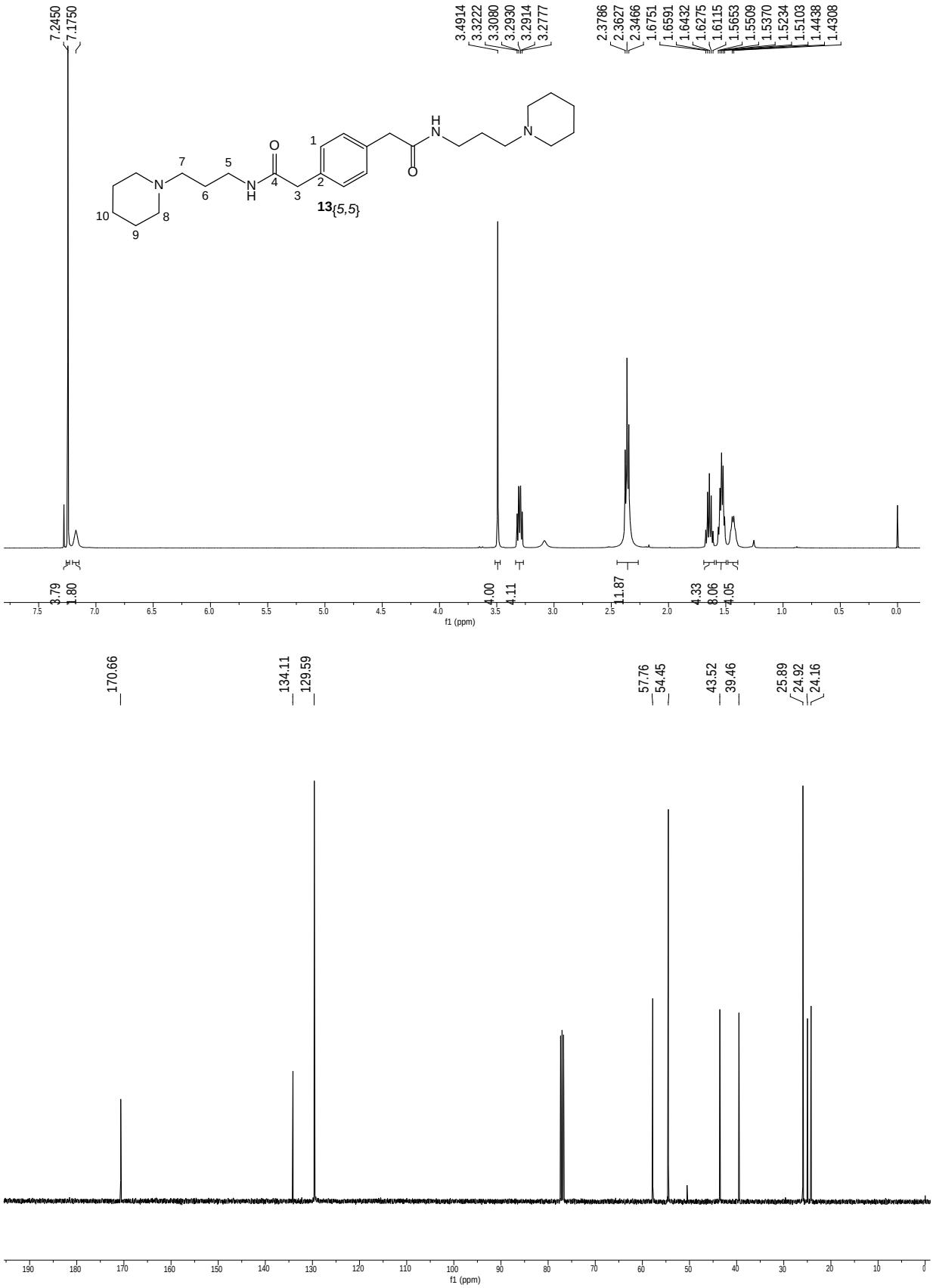


**Fig. S-5:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(piperidin-1-yl)propyl)-1,4-di(aminocarbonyl-methyl)benzene (**13**{*5,5*}).

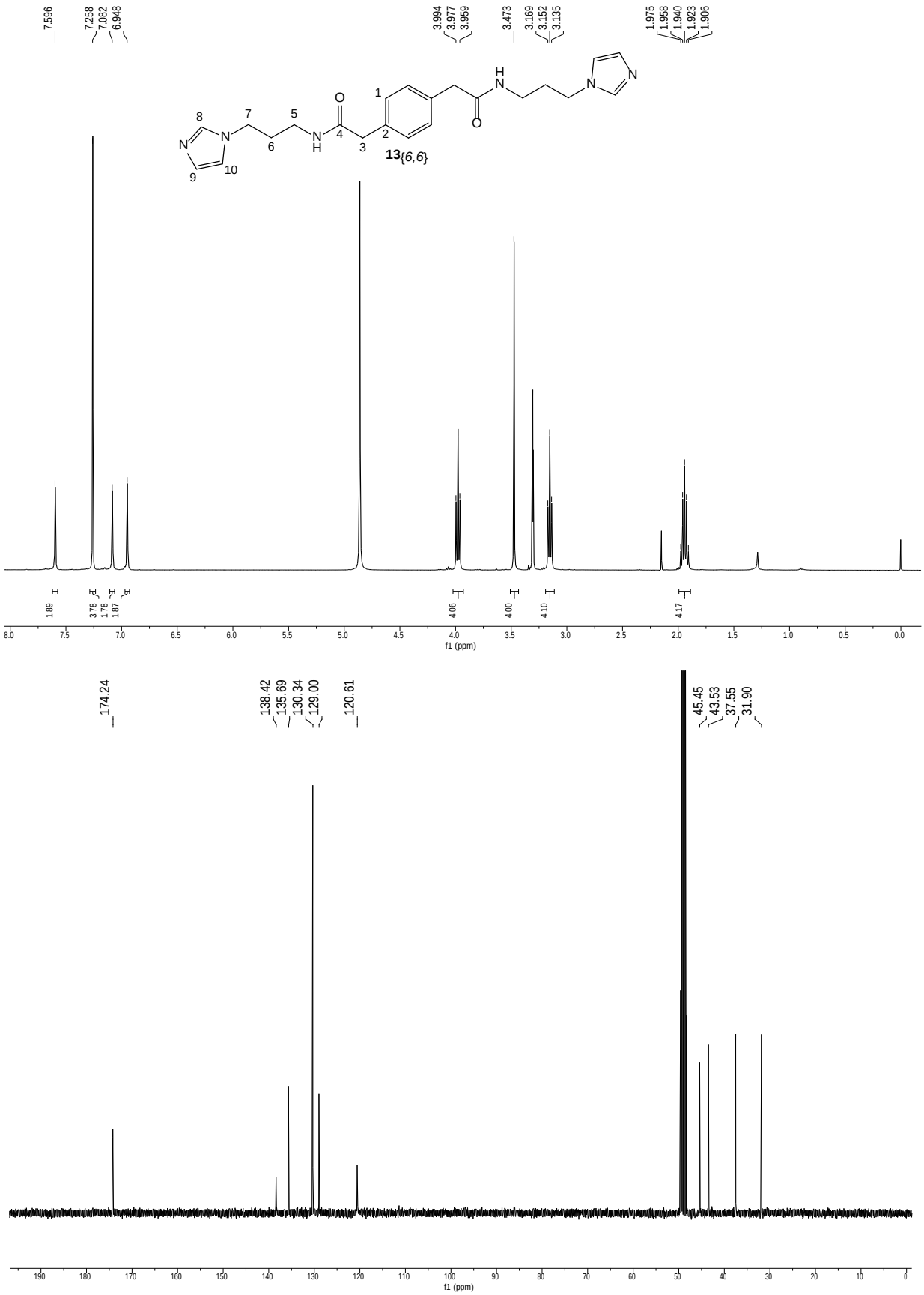


**Fig. S-6:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(imidazol-1-yl)propyl)-1,4-di(aminocarbonyl-methyl)benzene (**13**{*6,6*}).

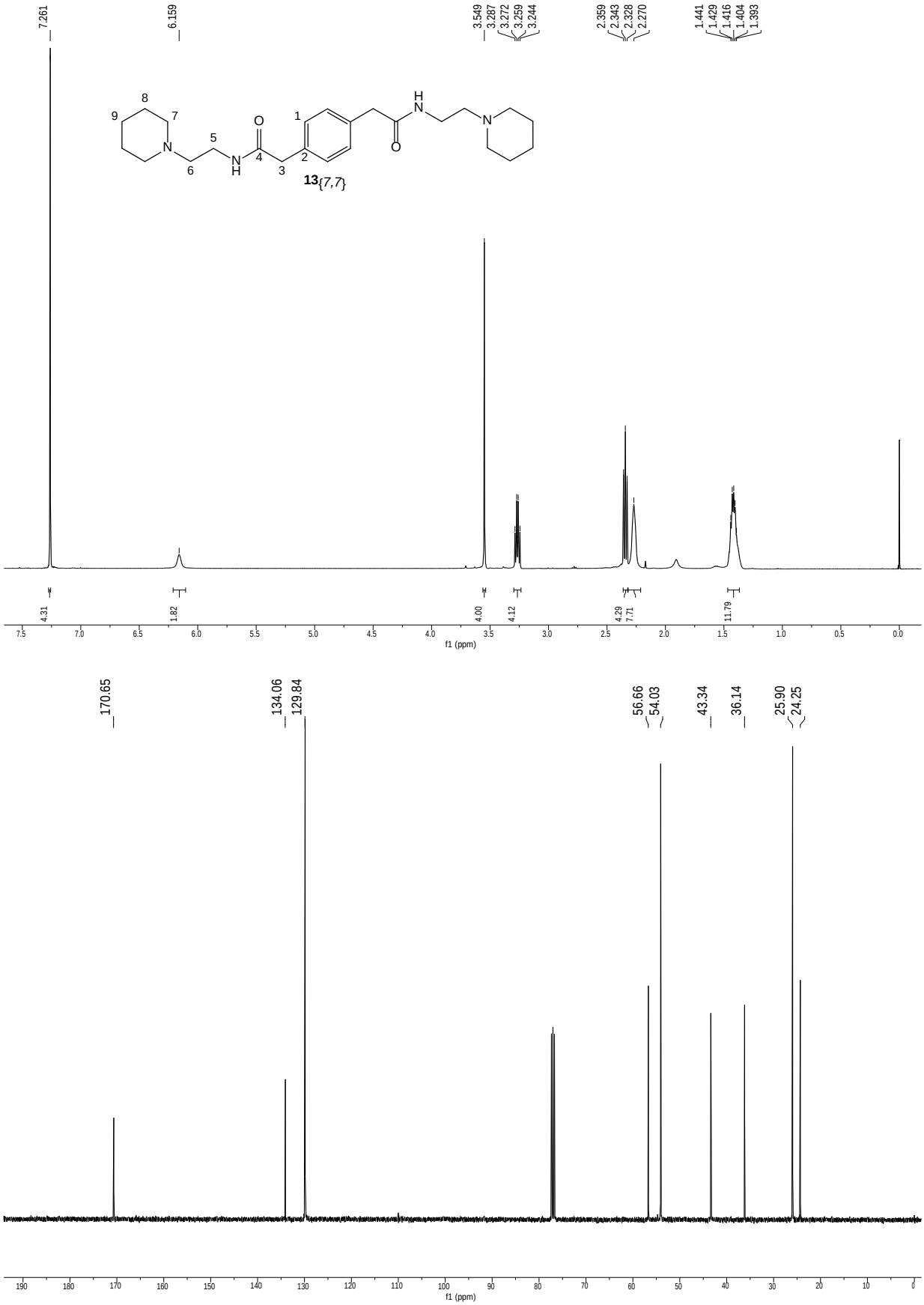


**Fig. S-7:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(2-(piperidin-1-yl)ethyl)-1,4-di(aminocarbonyl-methyl)benzene (**13**{*7,7*}).

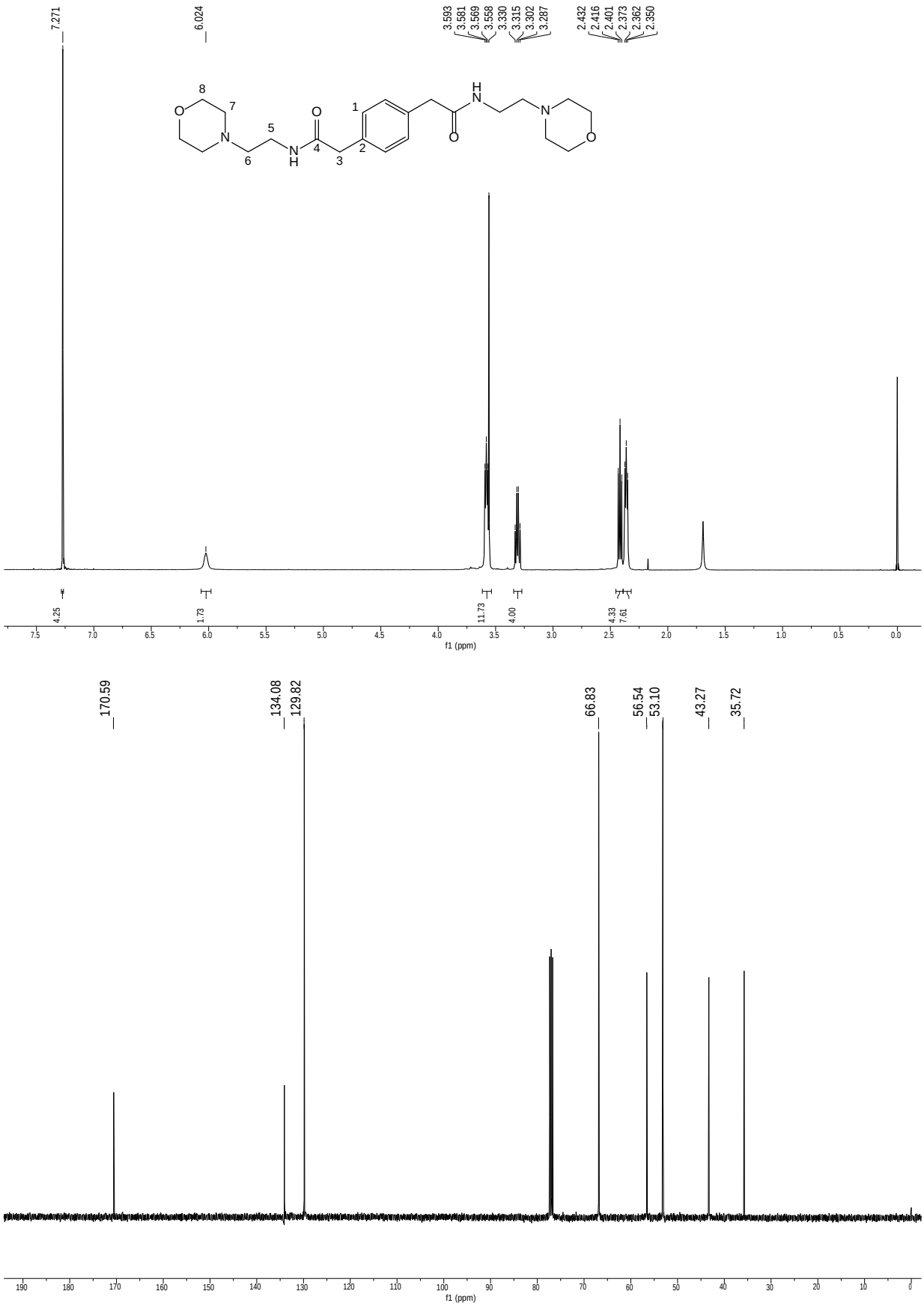


**Fig. S-8:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(2-(morpholin-4-yl)ethyl)-1,4-di(aminocarbonyl-methyl)benzene (**13**{*8,8*}).

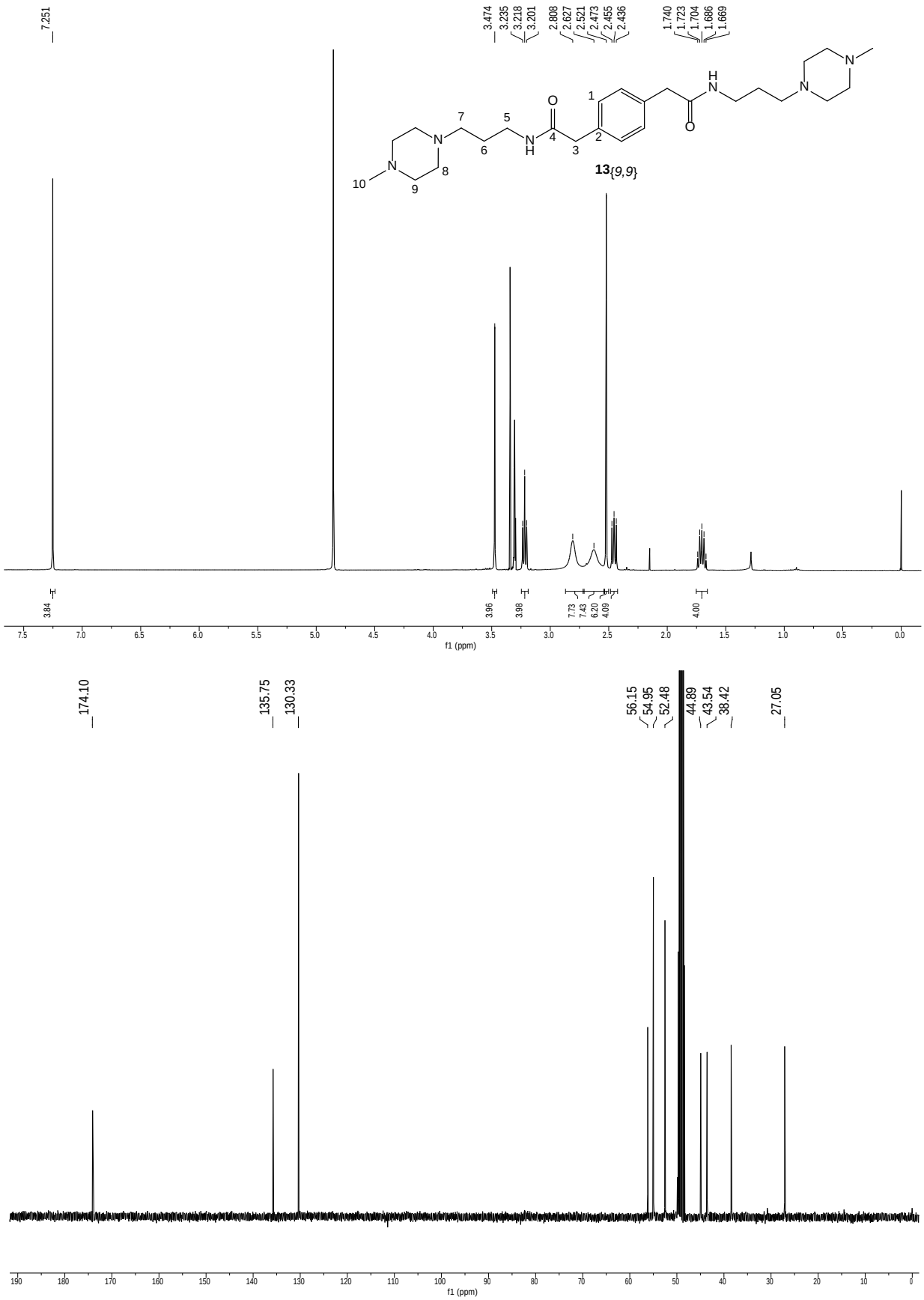


**Fig. S-9:** $^{1}$H and $^{13}$C-NMR of *N*,*N*'-bis(3-(4-methylpiperazin-1-yl)propyl)-1,4-di(aminocarbonylmethyl)benzene (**13**{*9,9*}).

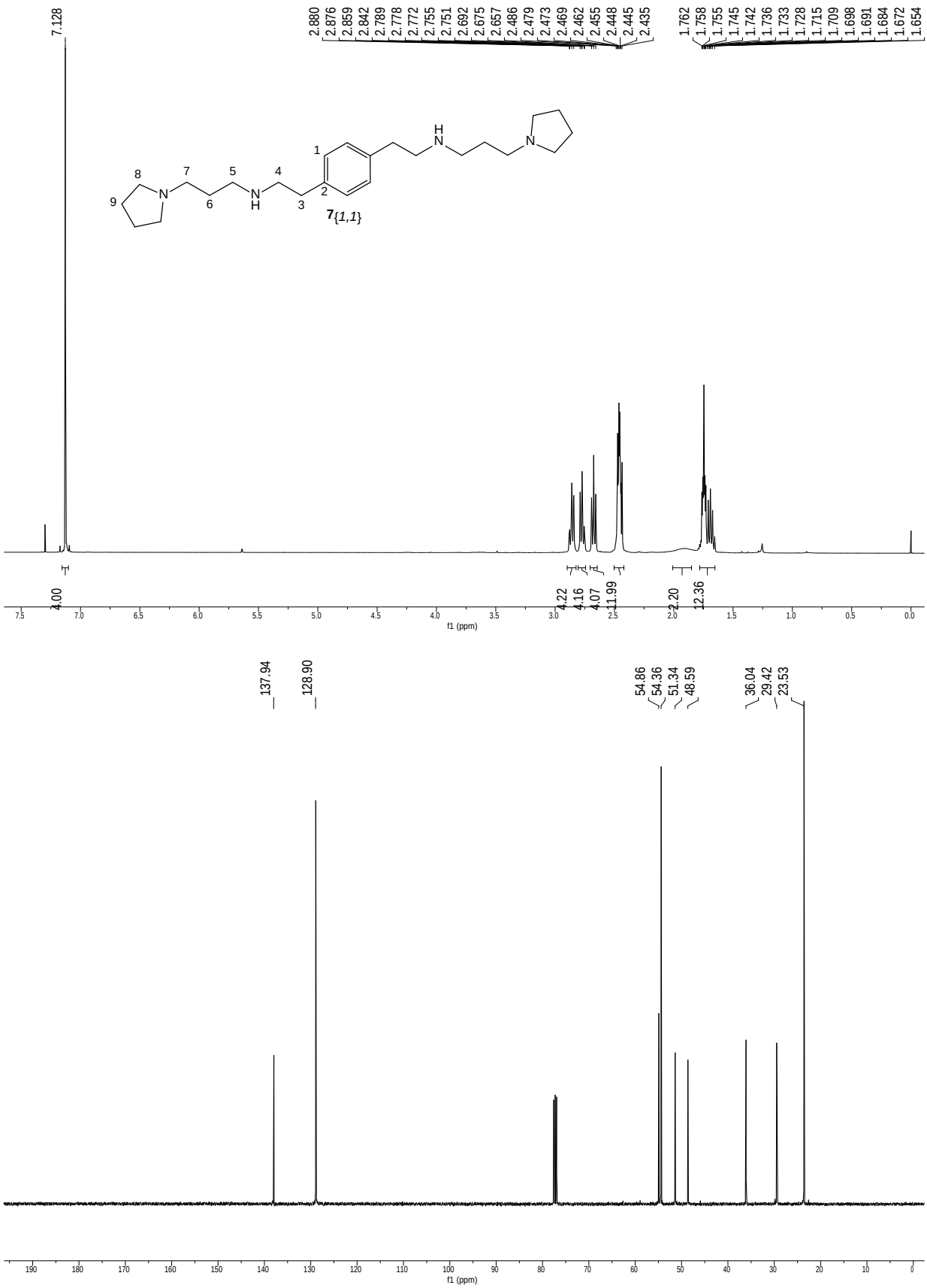


**Fig. S-10:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(pyrrolidin-1-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*1,1*}).

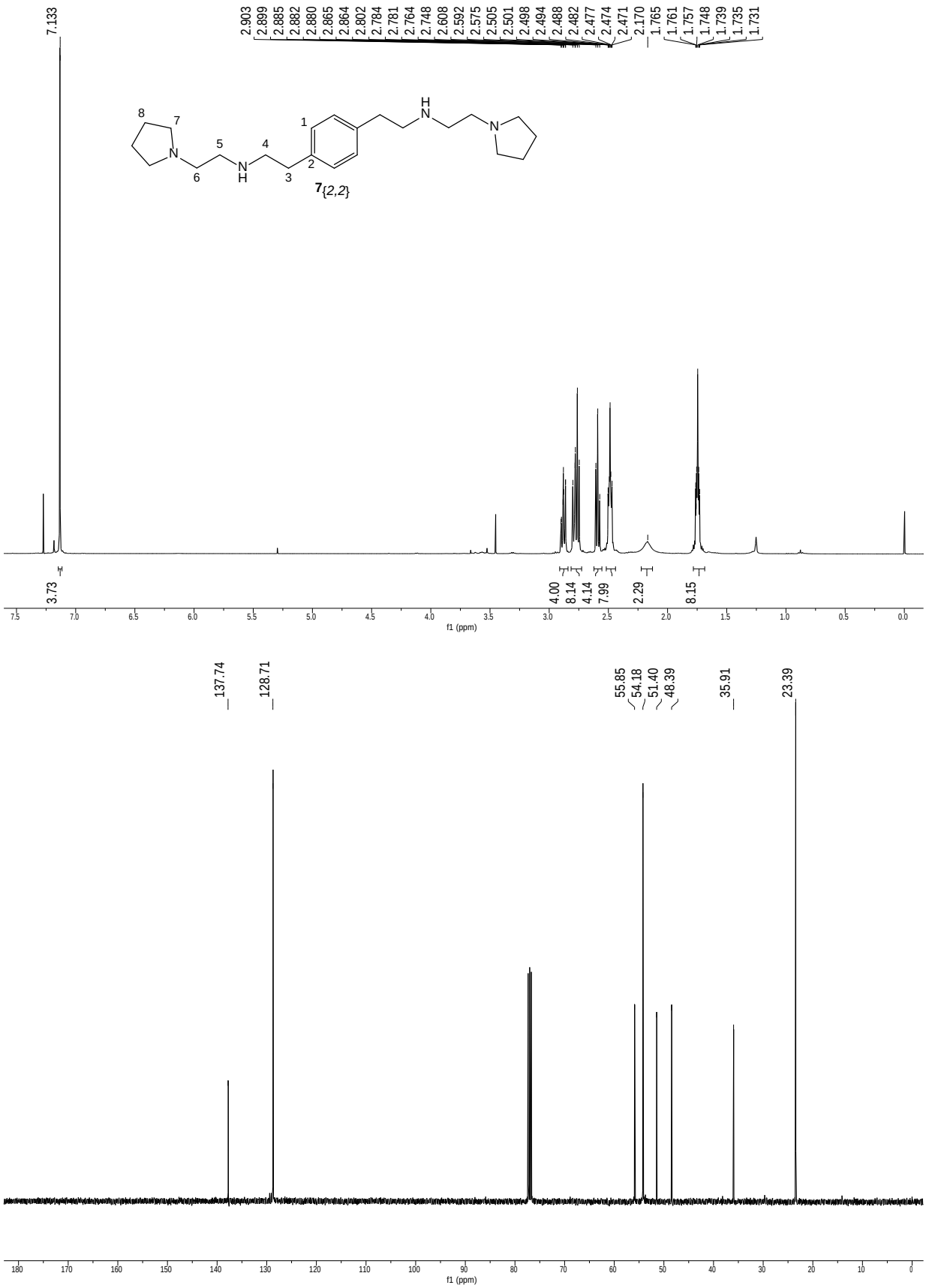


**Fig. S-11:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(2-(pyrrolidin-1-yl)ethyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*2,2*}).

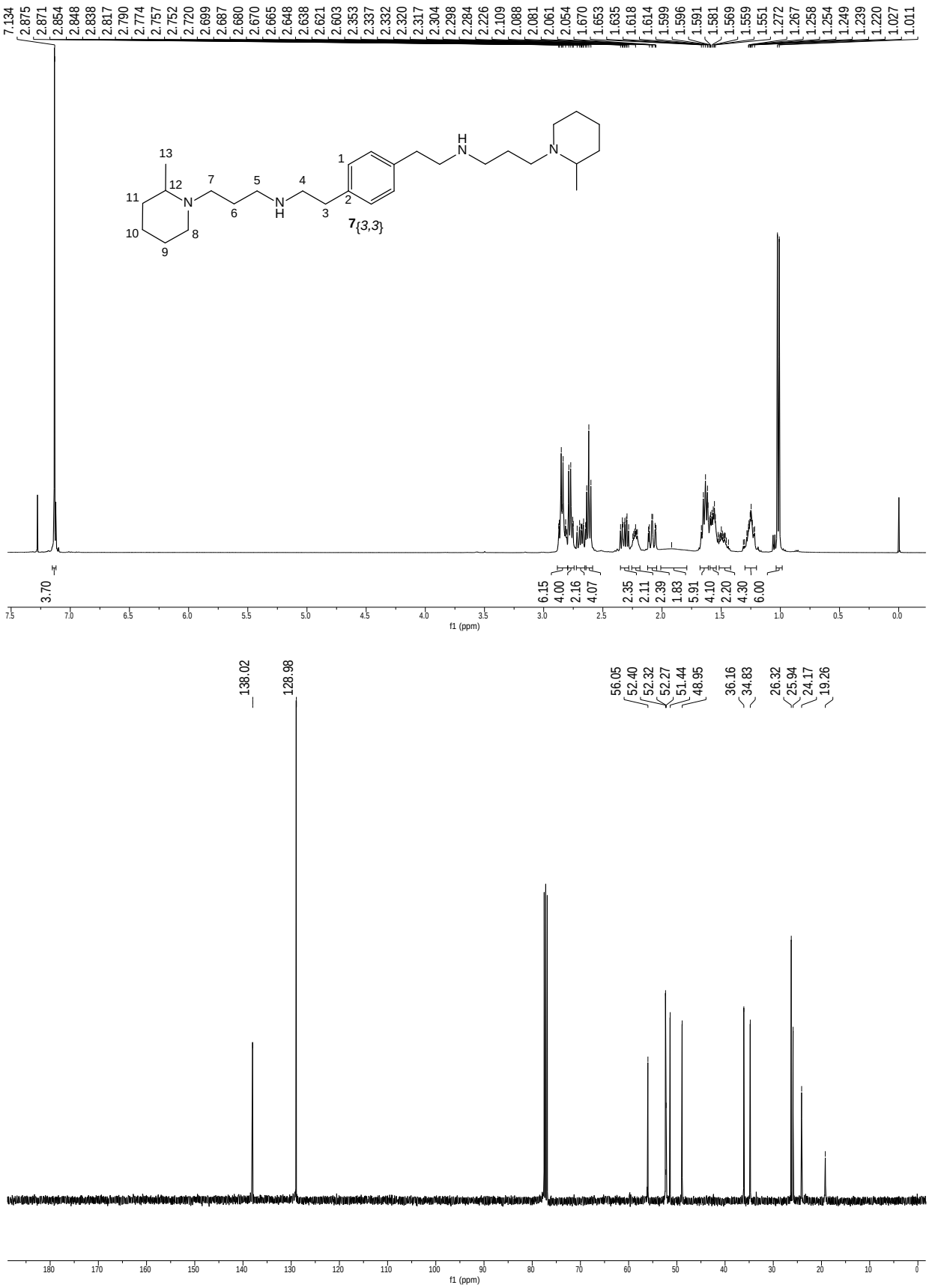


**Fig. S-12:** $^{1}$H and $^{13}$C-NMR of *N*,*N'*-bis(3-(2-pipecolin-1-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*3*,*3*}).

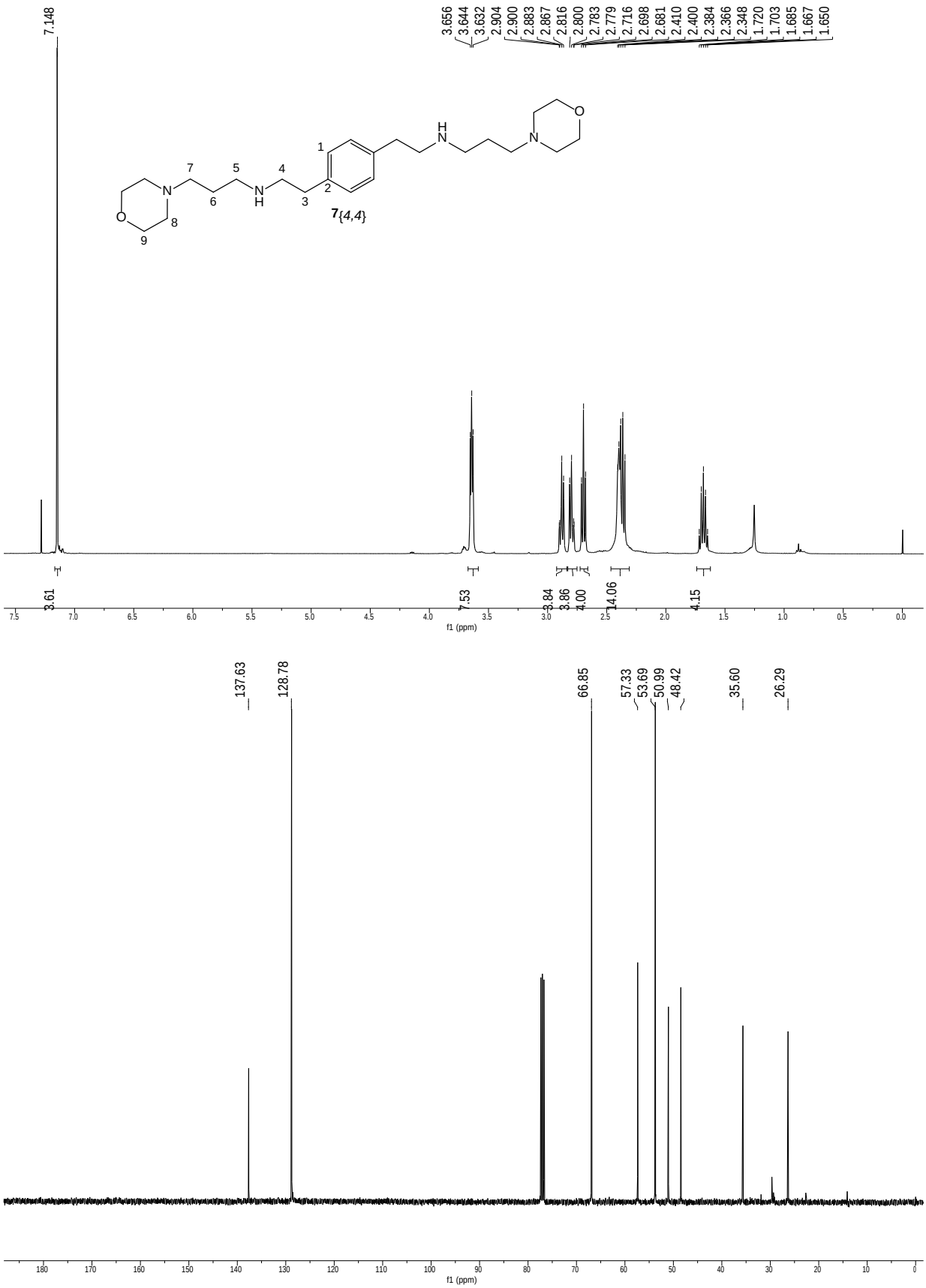


**Fig. S-13:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(morpholin-4-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*4,4*}).

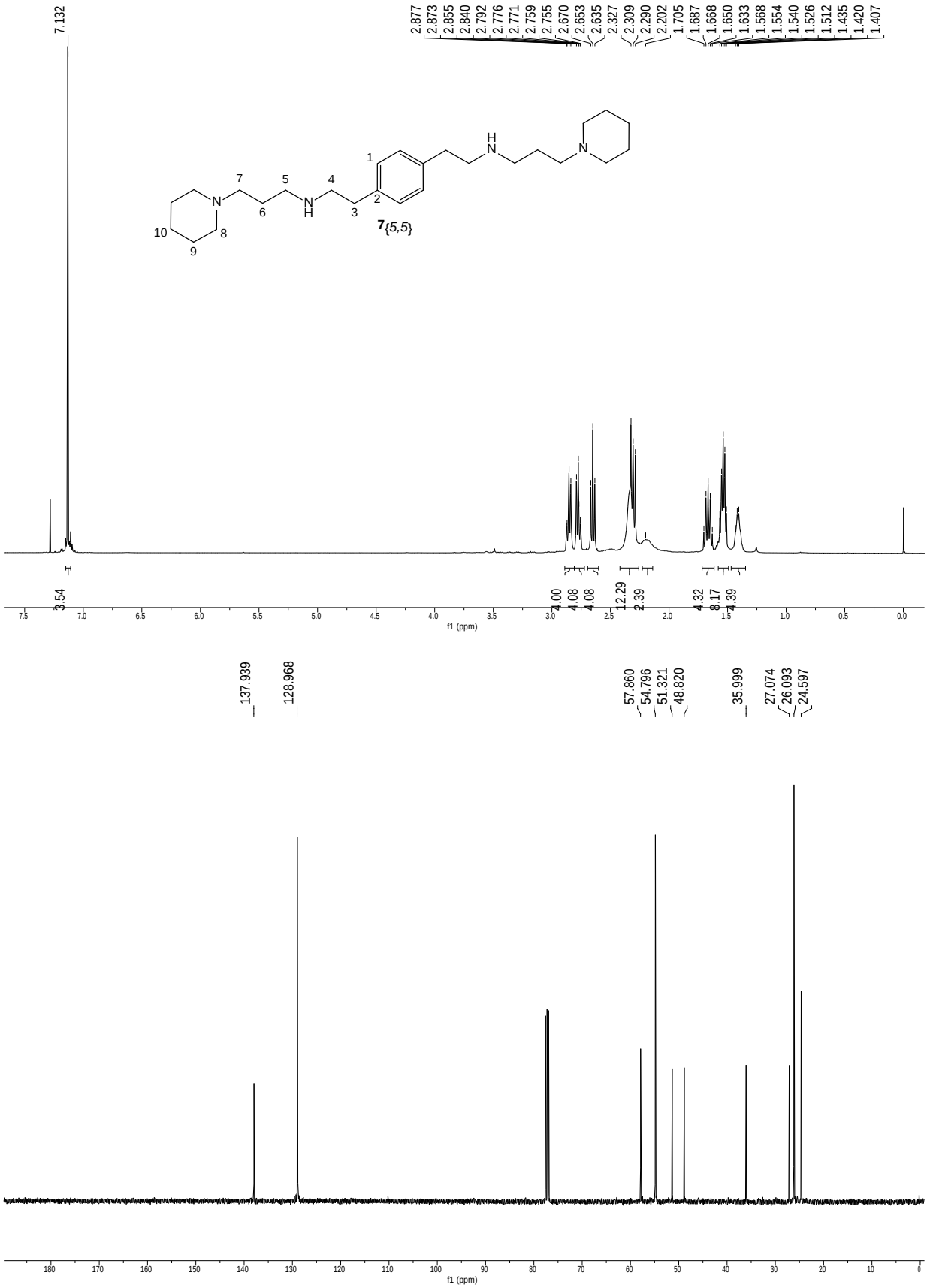


**Fig. S-14:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(piperidin-1-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*5,5*}).

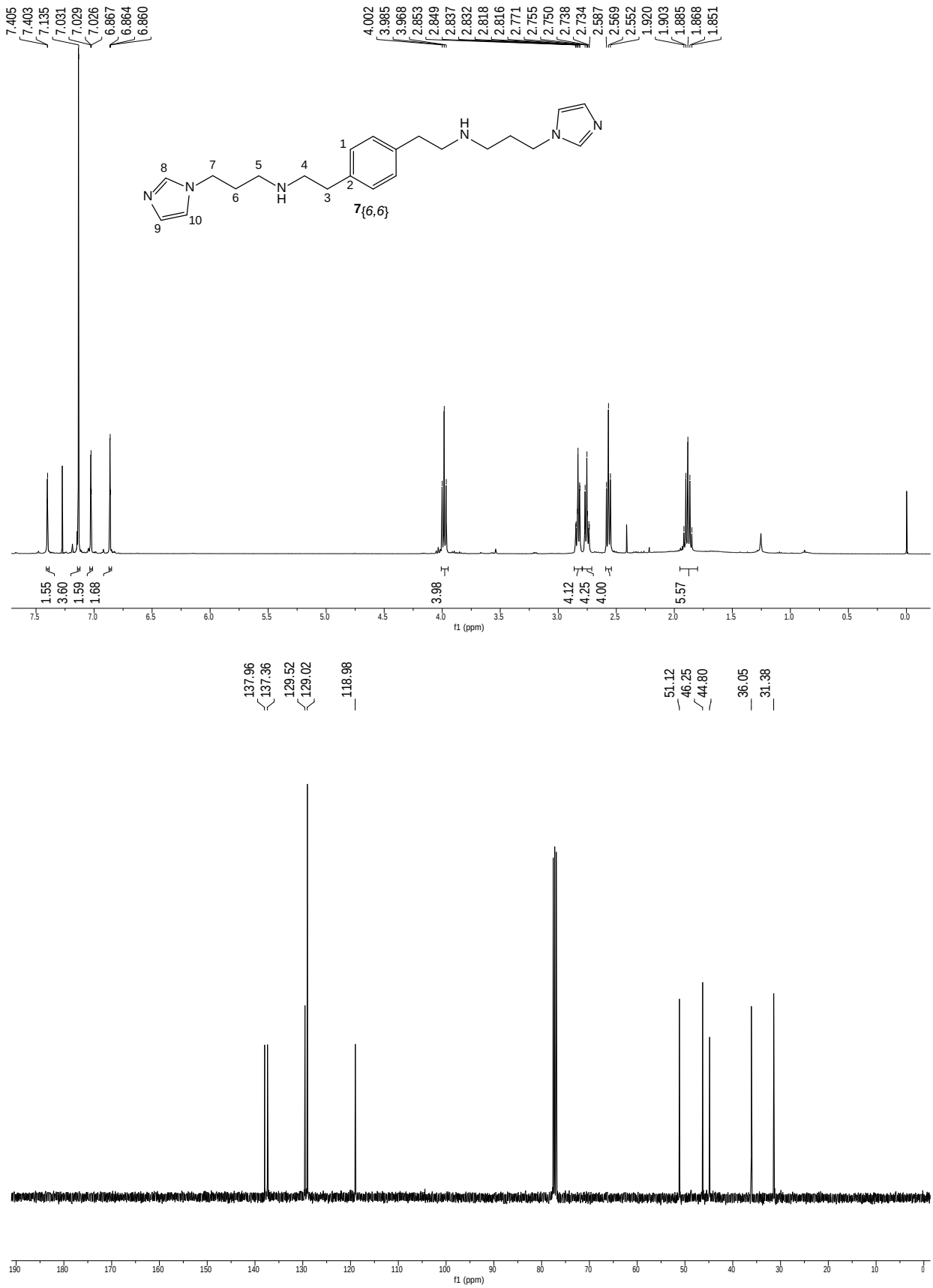


**Fig. S-15:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(imidazol-1-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*6,6*}).

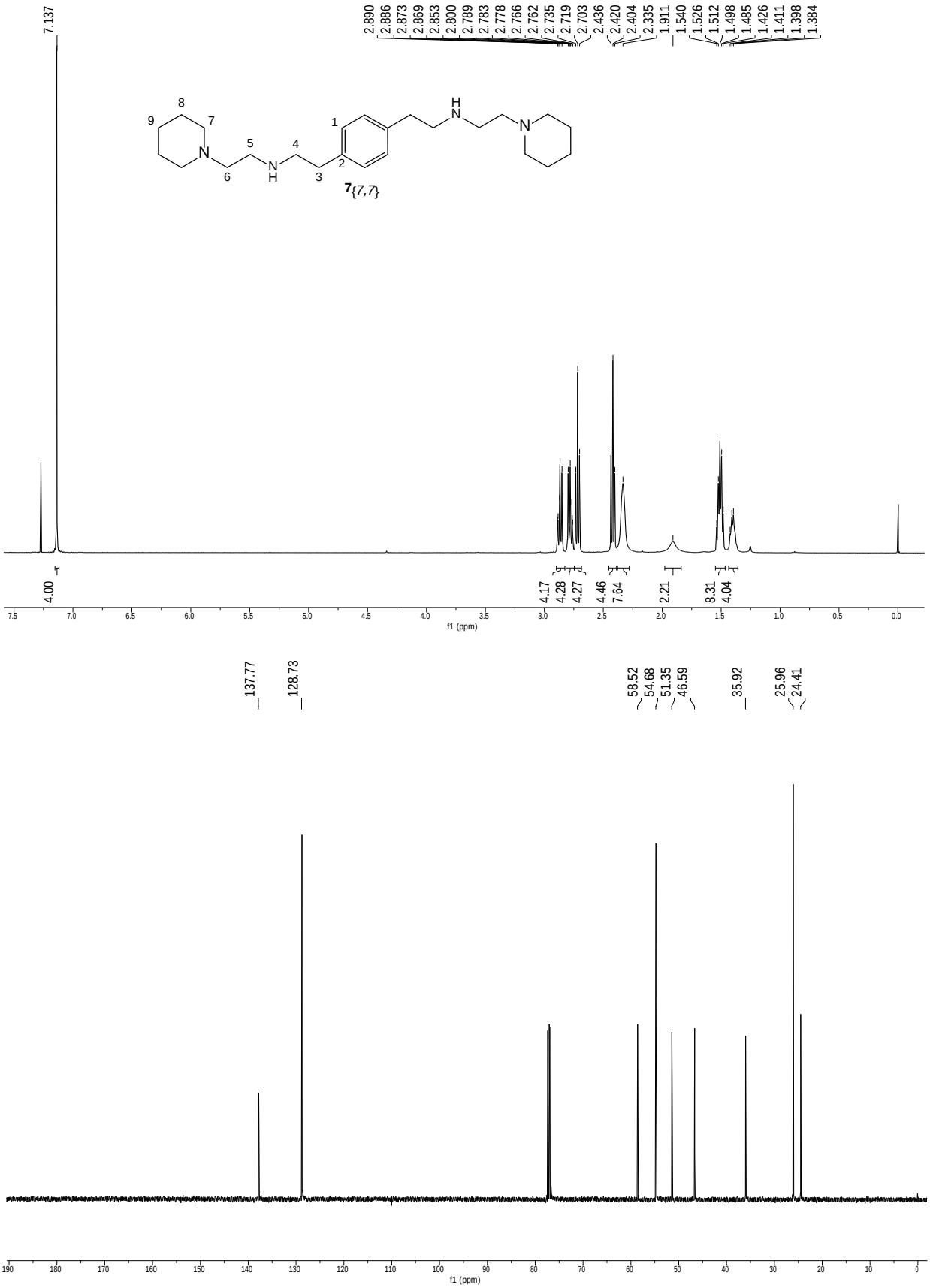


**Fig. S-16:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(2-(piperidin-1-yl)ethyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*7,7*}).

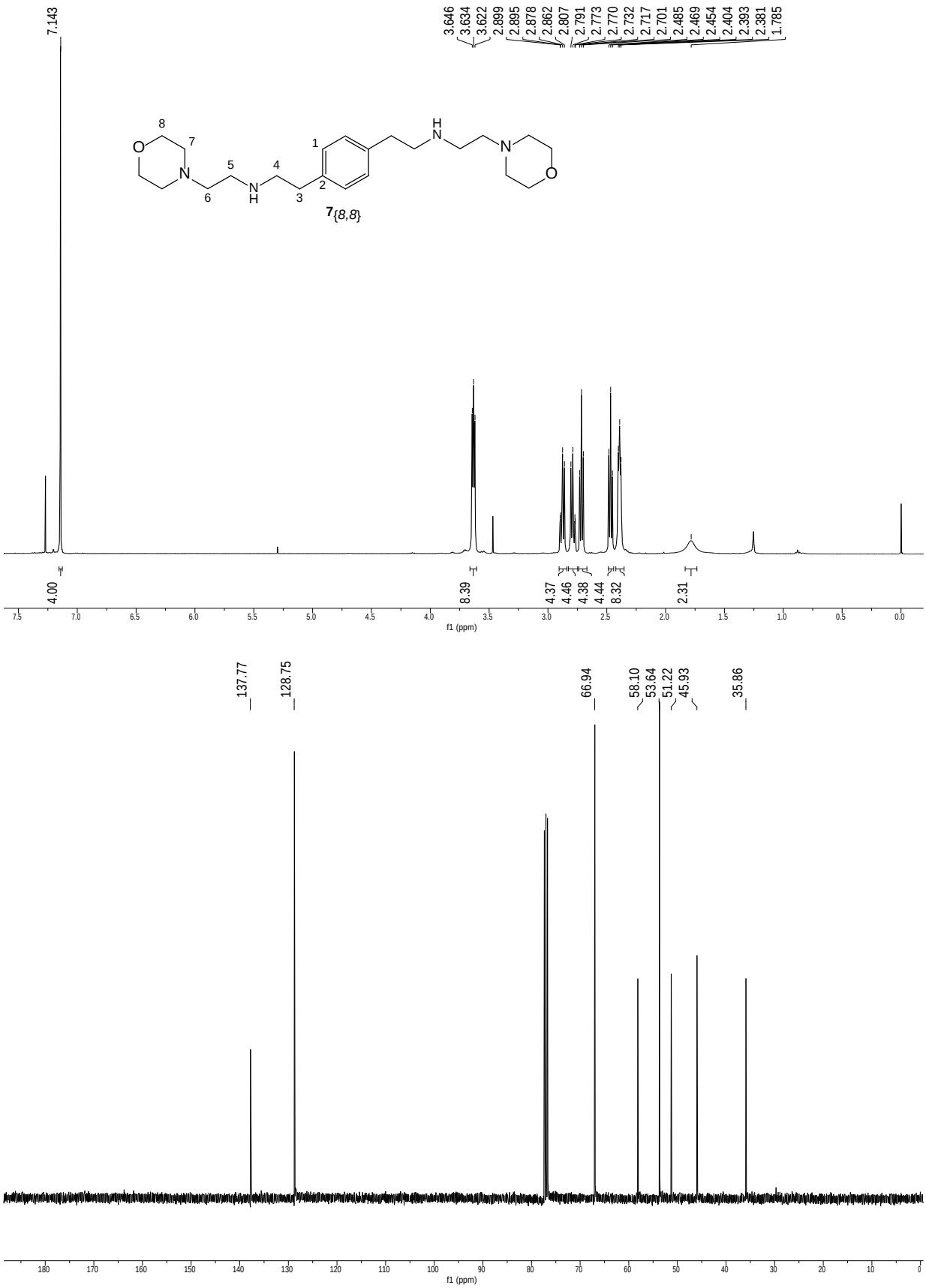


**Fig. S-17:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(2-(morpholin-4-yl)ethyl)-1,4-bis(2-aminoteh-1-yl)benzene (**7**{*8,8*}).

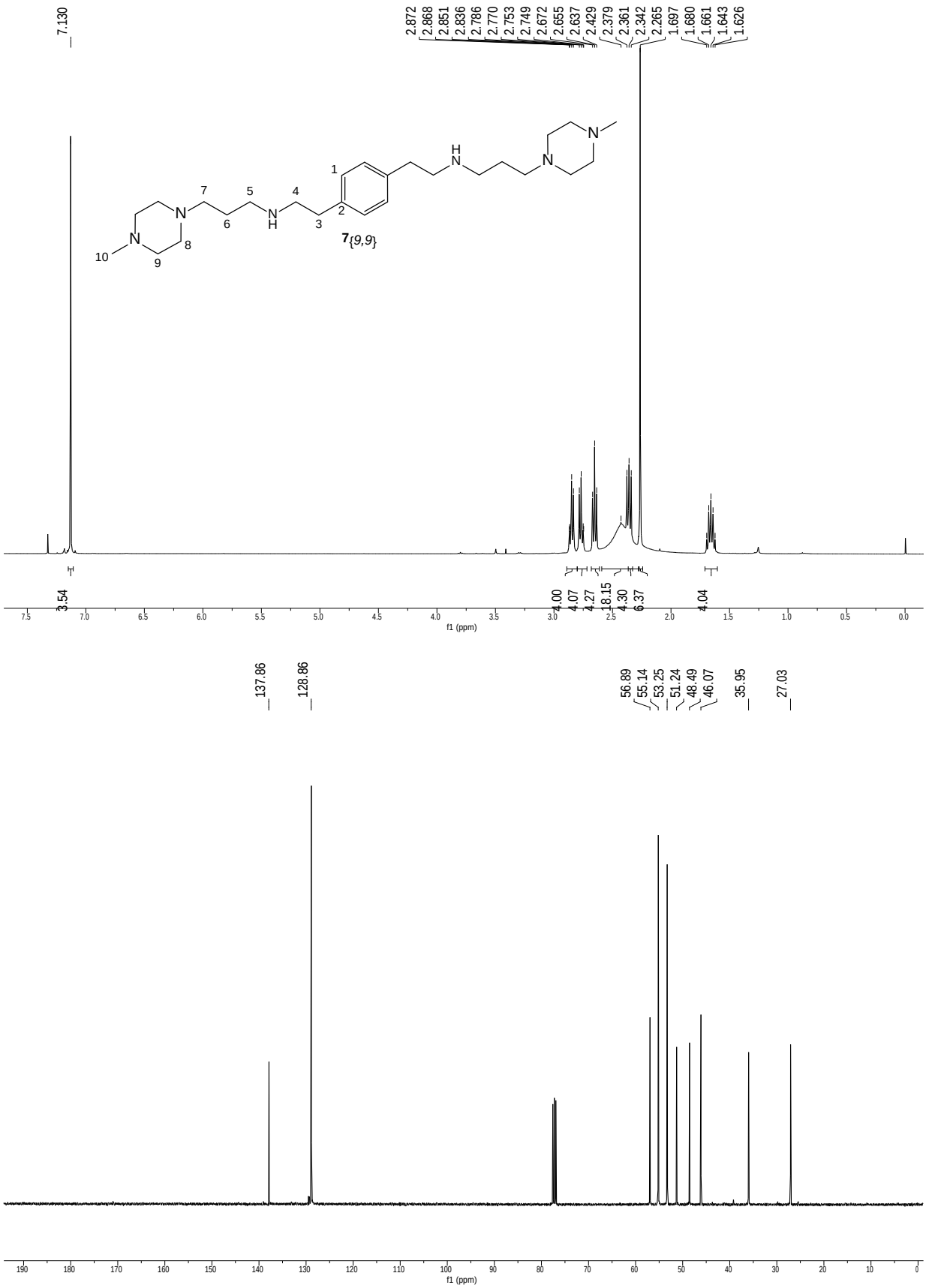


**Fig. S-18:** $^{1}$H and $^{13}$C-NMR of *N,N'*-bis(3-(4-methylpiperazin-1-yl)propyl)-1,4-bis(2-aminoeth-1-yl)benzene (**7**{*9,9*}).

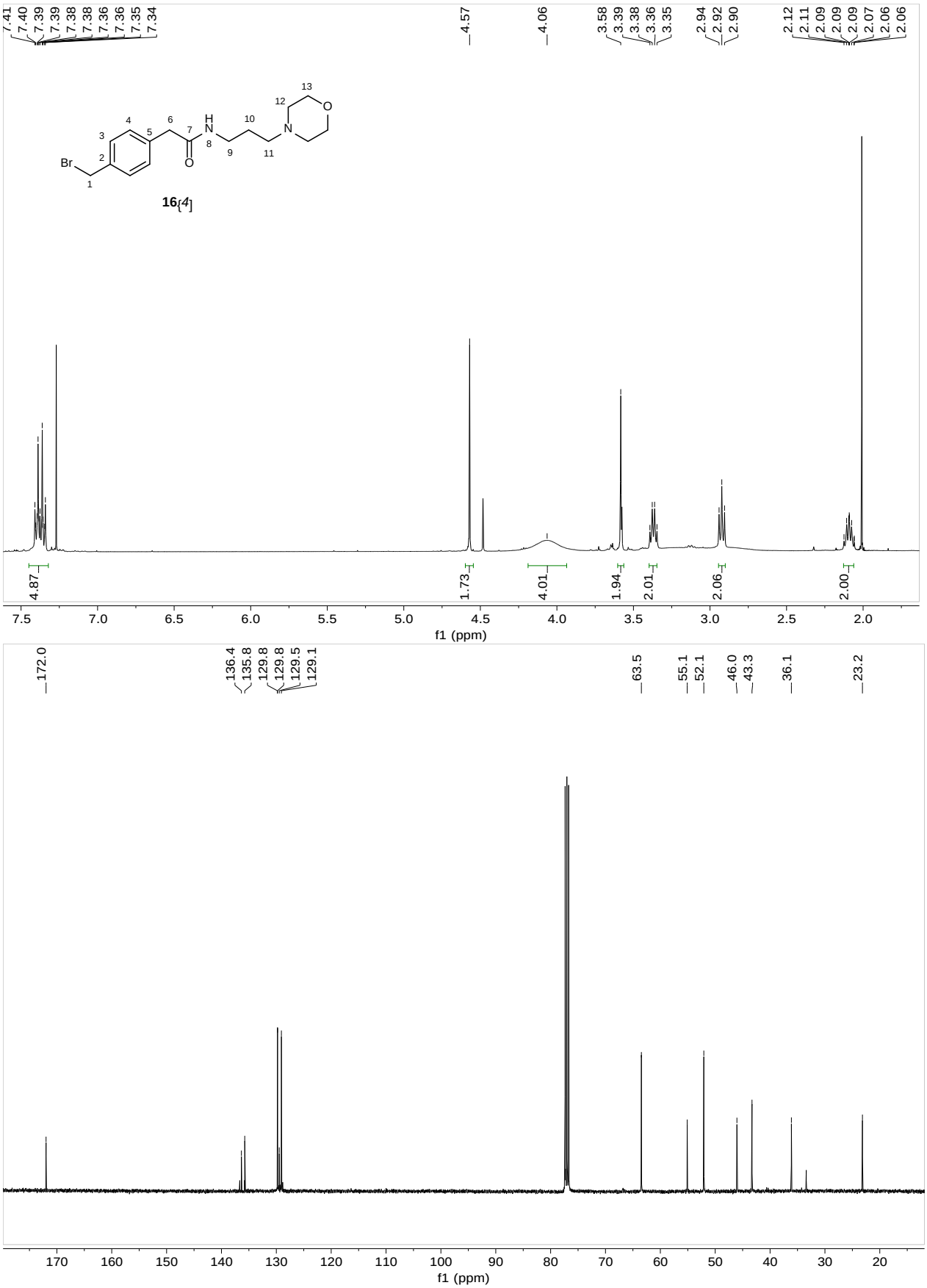


**Fig. S-19:** $^{1}$H and $^{13}$C-NMR of 2-(4-(bromomethyl)phenyl)-*N*-(3-morpholinopropyl)acetamide (**16**{*4*}).

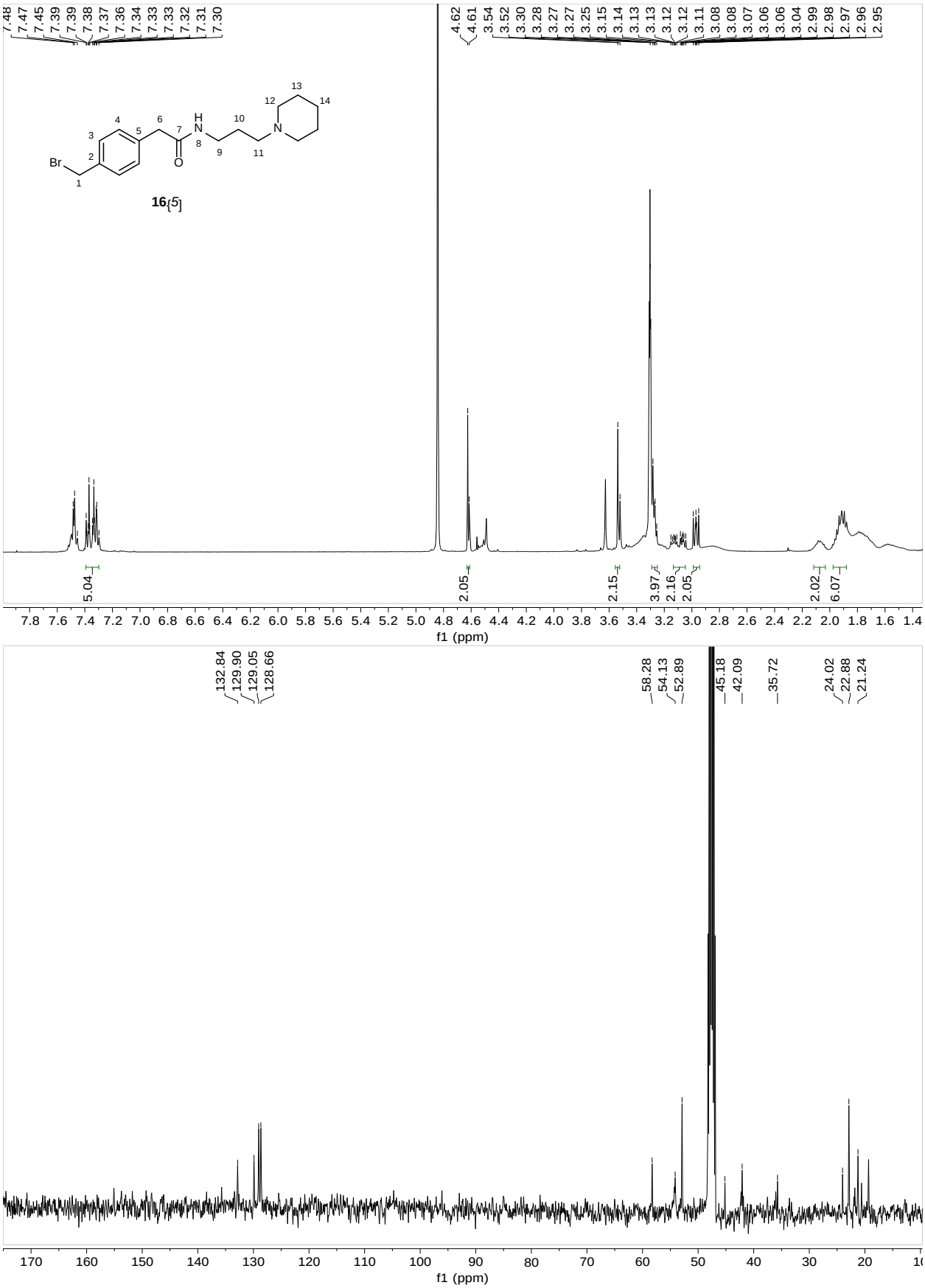


**Fig. S-21:** $^{1}$H and $^{13}$C-NMR of 2-(4-(bromomethyl)phenyl)-*N*-(3-(piperidin-1-yl)propyl)acetamide (**16**{*5*}).

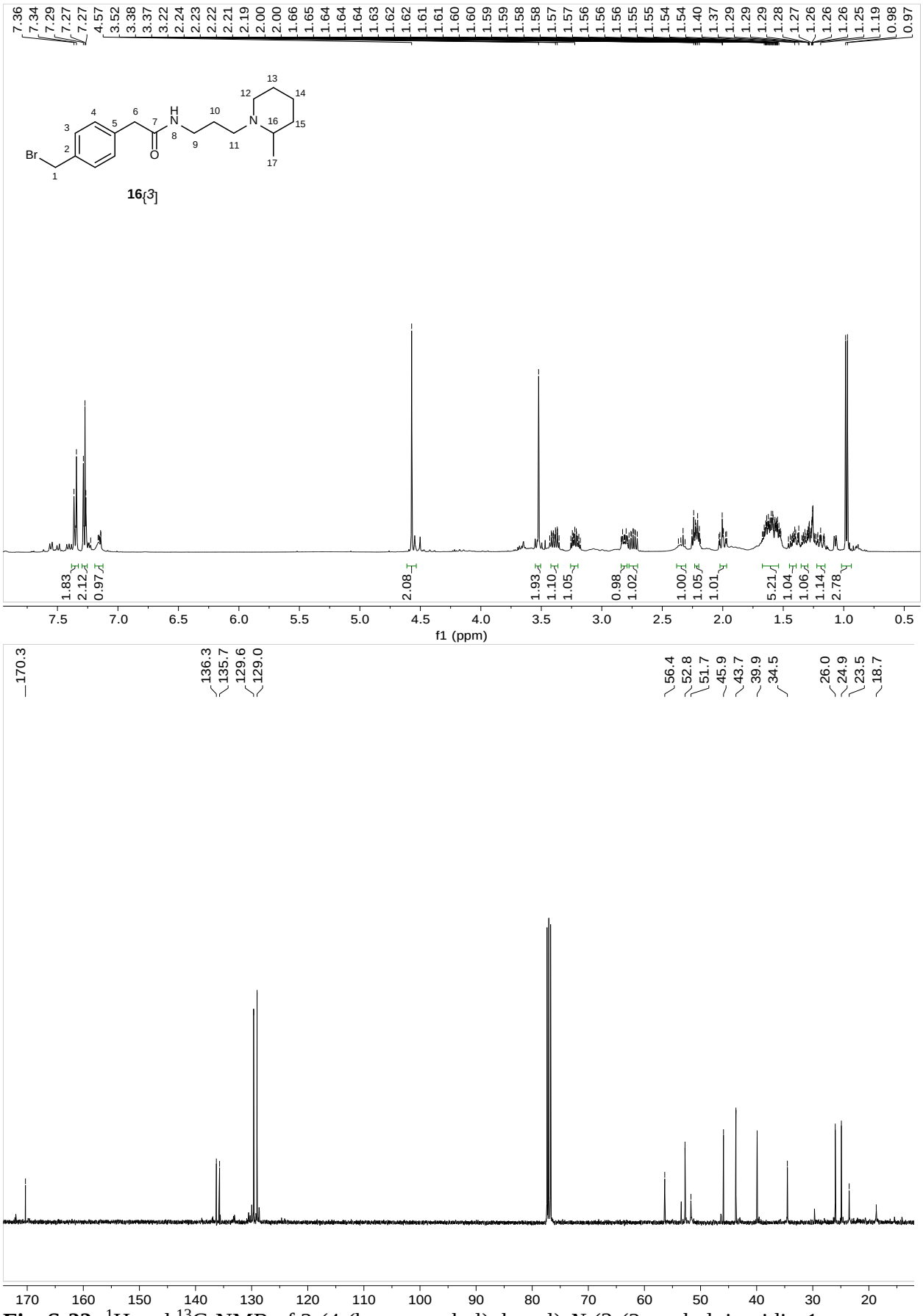


**Fig. S-22:** $^{1}$H and $^{13}$C-NMR of 2-(4-(bromomethyl)phenyl)-*N*-(3-(2-methylpiperidin-1-yl)propyl) acetamide (**16**{*3*}).

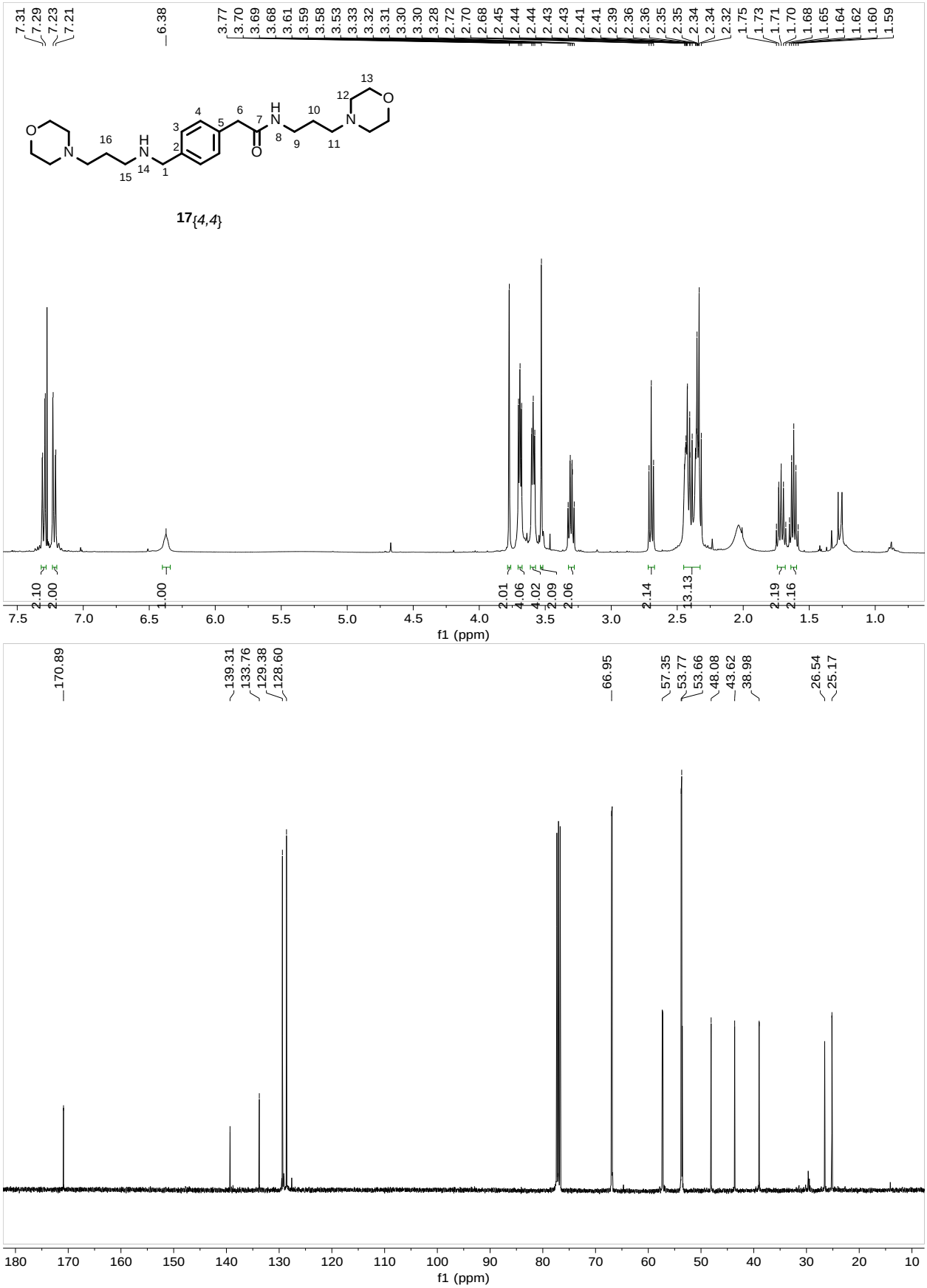


**Fig. S-23:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-morpholinopropylamino)methyl)phenyl)-*N*-(3-morpholinopropyl) acetamide (**17**{*4,4*}).

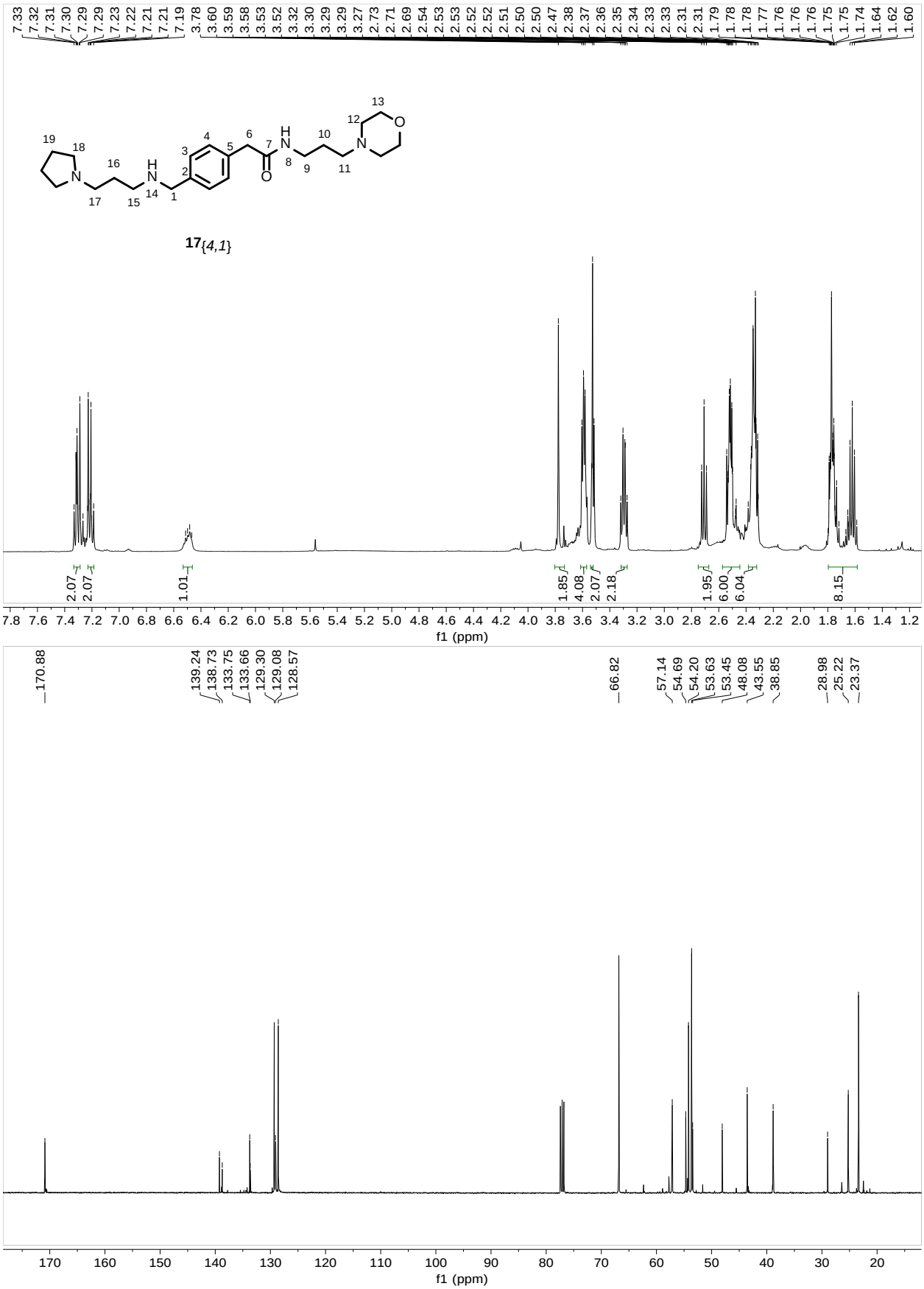


**Fig. S-24:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-(pyrrolidin-1-yl)propylamino)methyl)phenyl)-*N*-(3-morpholino propyl)acetamide (**17**{*4,1*}).

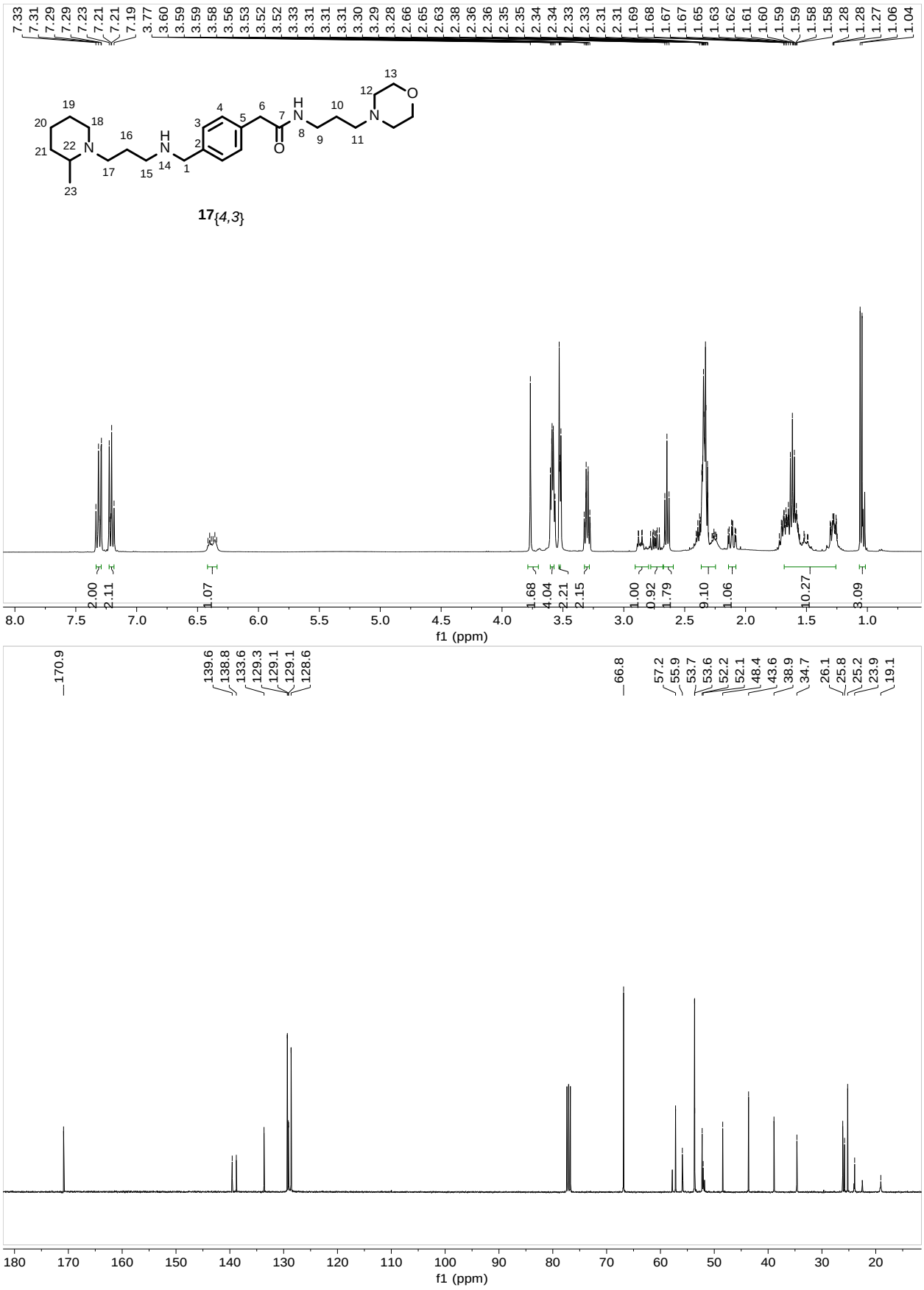


**Fig. S-25:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-(2-methylpiperidin-1-yl)propylamino)methyl)phenyl)-*N*-(3-morpholinopropyl)acetamide (**17**{*4*,*3*}).

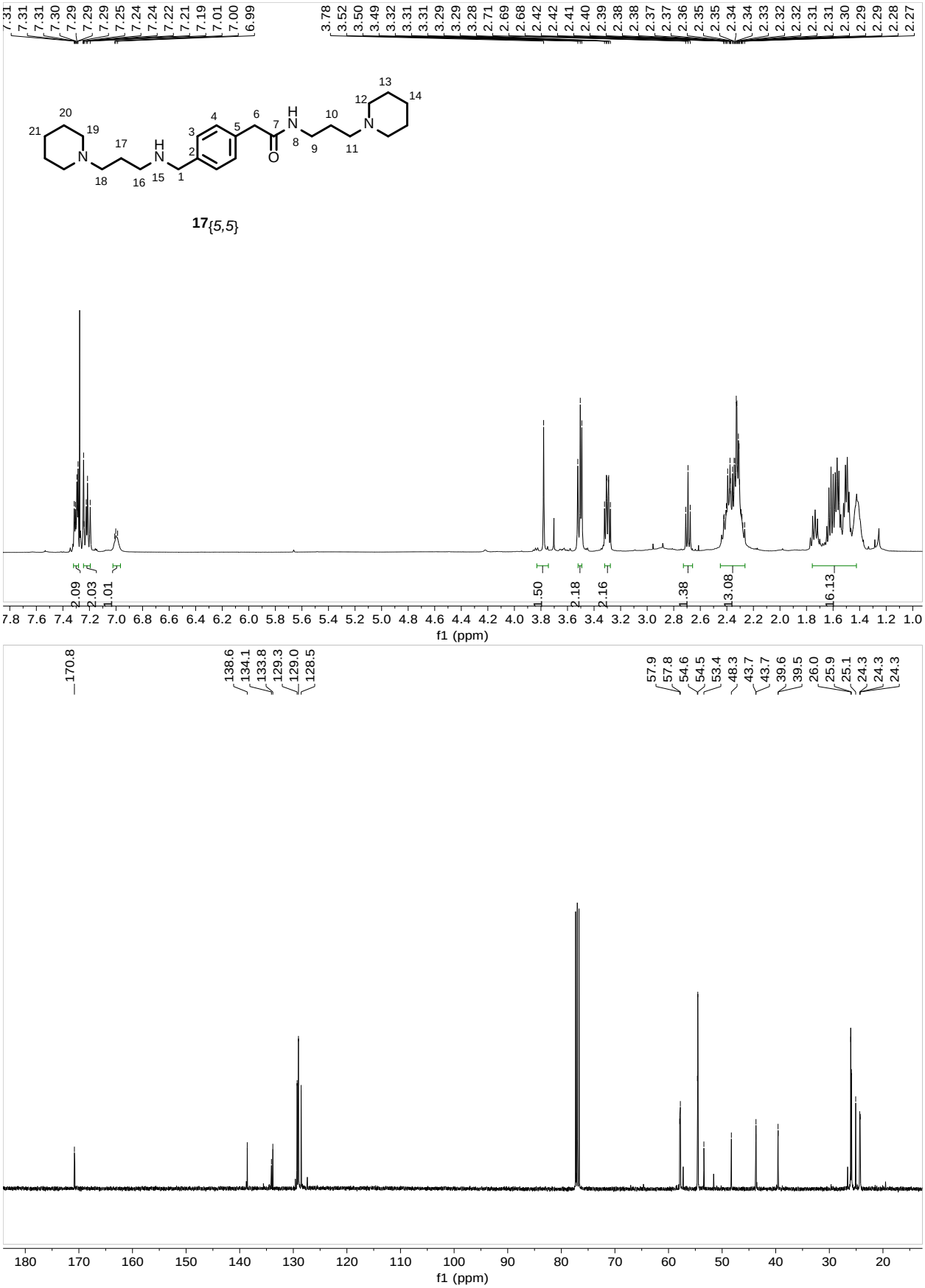


**Fig. S-26:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-(piperidin-1-yl)propylamino)methyl)phenyl)-*N*-(3-(piperidin-1-yl)propyl)acetamide (**17**{*5,5*}).

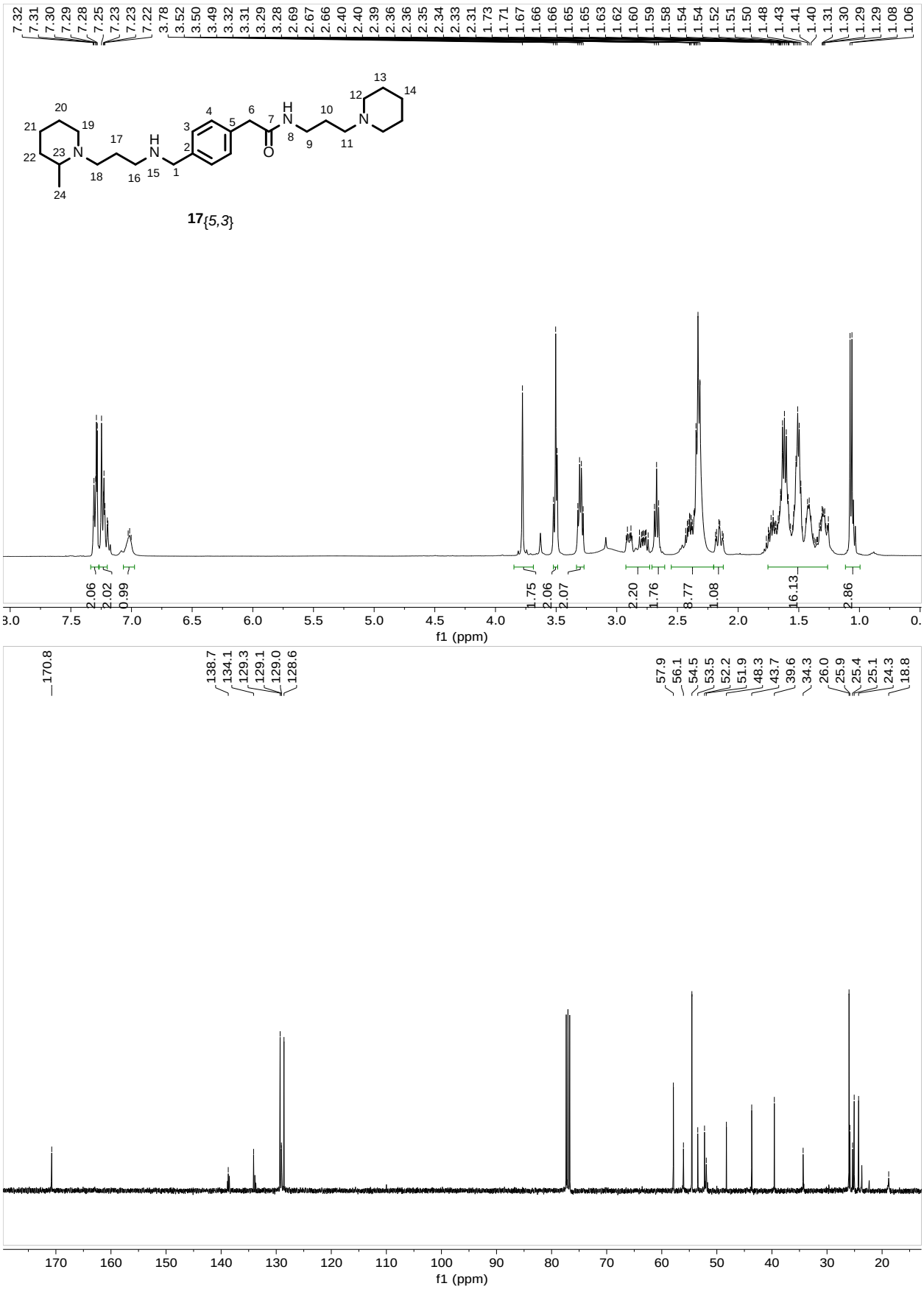


**Fig. S-27:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-(2-methylpiperidin-1-yl)propylamino)methyl)phenyl)-*N*-(3-(piperidin-1-yl)propyl)acetamide (**17**{*5,3*}).

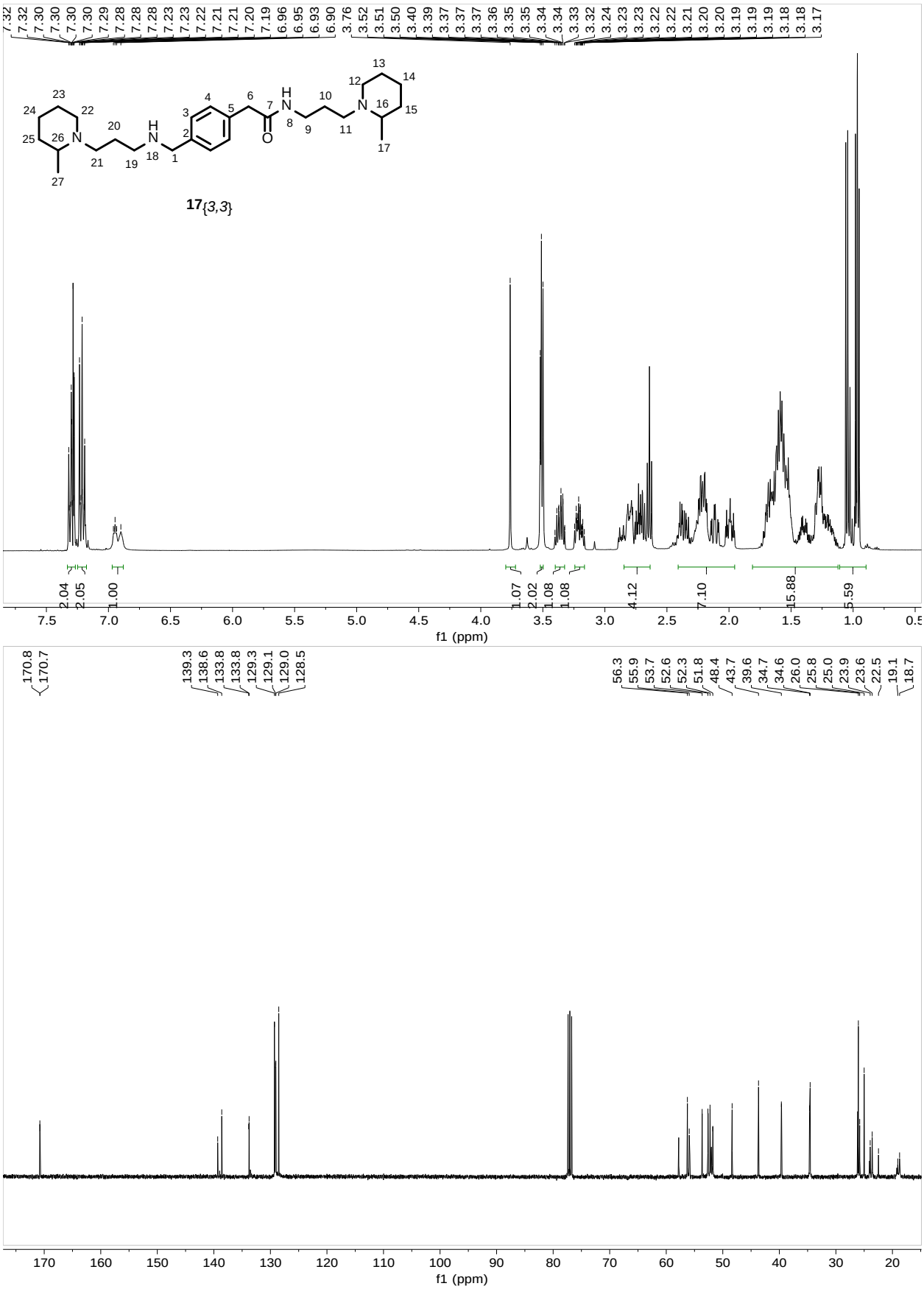


**Fig. S-28:** $^{1}$H and $^{13}$C-NMR of 2-(4-((3-(2-methylpiperidin-1-yl)propylamino)methyl)phenyl)-*N*-(3-(2-methylpiperidin-1-yl)propyl)acetamide (**17**{*3*,*3*}).

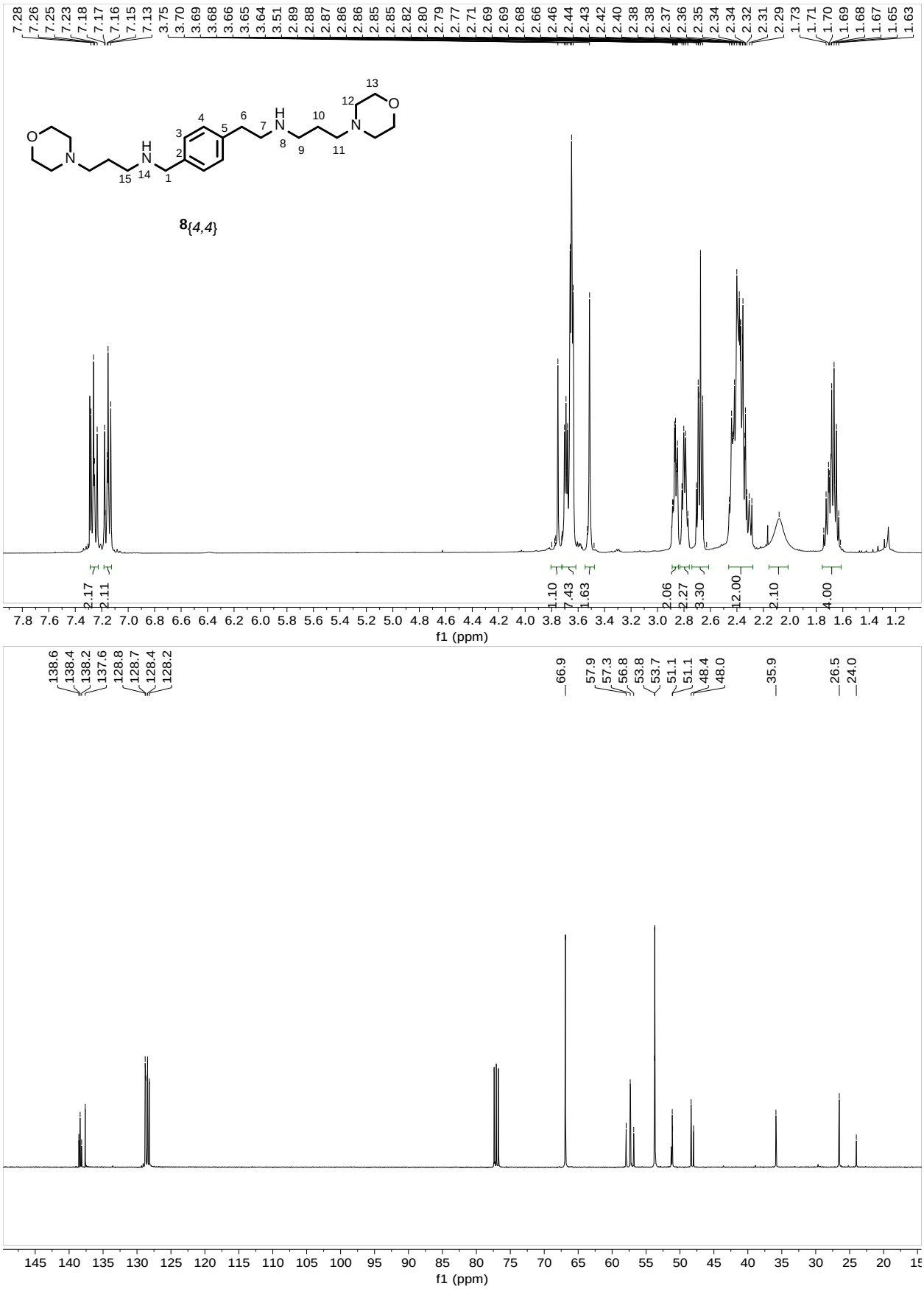


**Fig. S-29:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-morpholinopropylamino)ethyl)benzyl)-3-morpholinopropan-1-amine (**8**{*4,4*}).

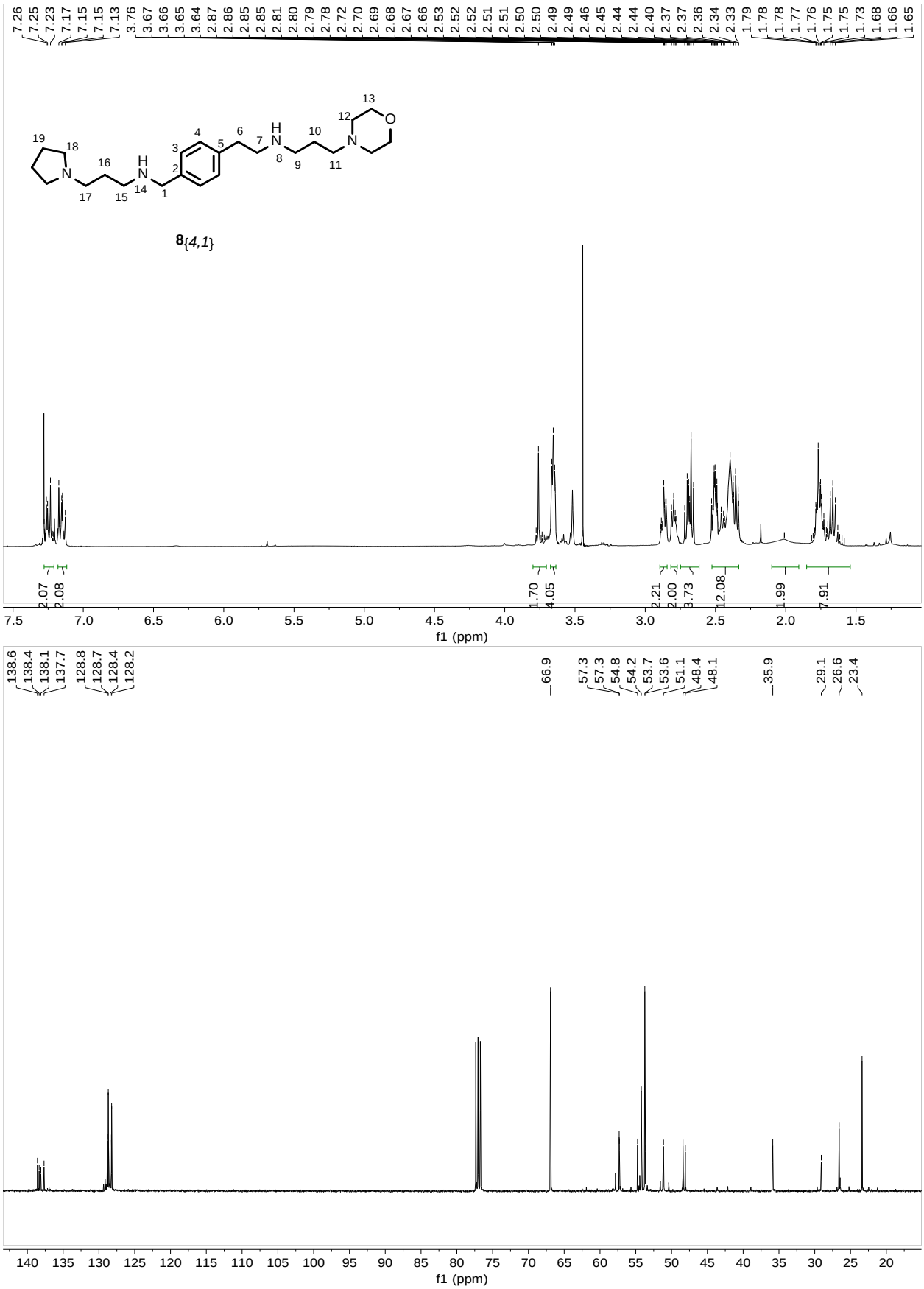


**Fig. S-30:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-morpholinopropylamino)ethyl)benzyl)-3-(pyrrolidin-1-yl)propan-1-amine (**8**{*4,1*}).

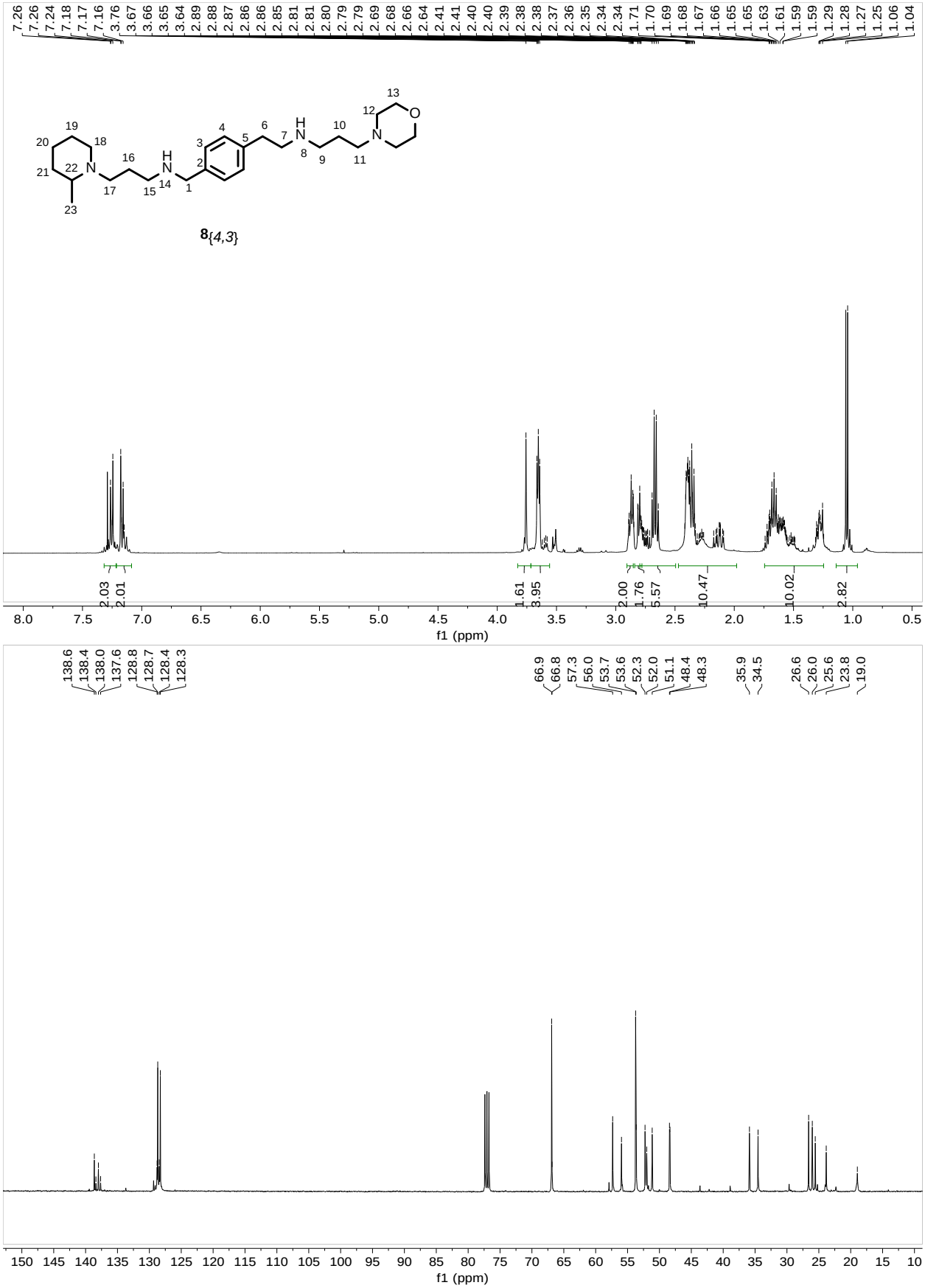


**Fig. S-31:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-morpholinopropylamino)ethyl)benzyl)-3-(2-methylpiperidin-1-yl)propan-1-amine (**8**{*4,3*}).

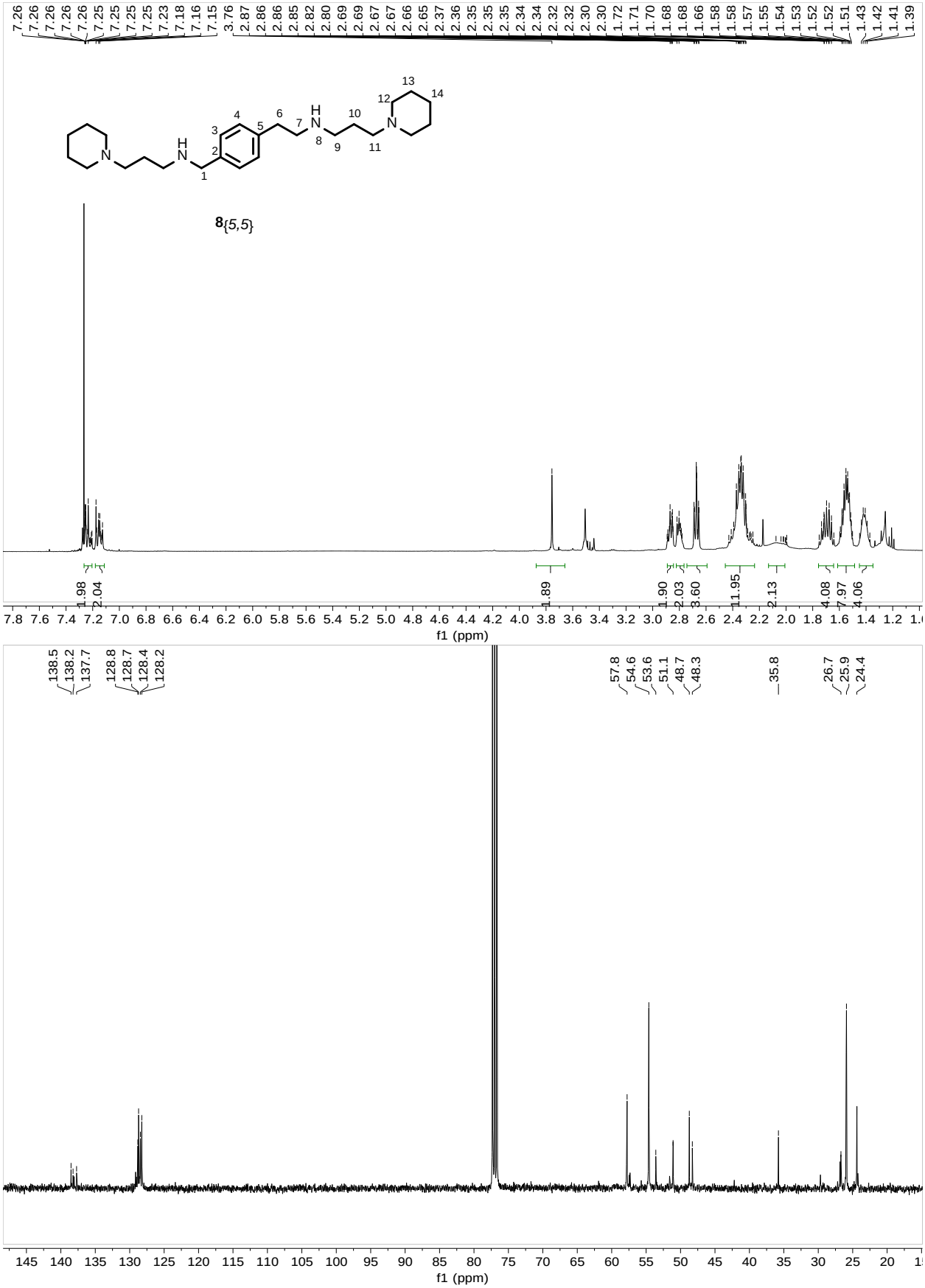


**Fig. S-32:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-(piperidin-1-yl)propylamino)ethyl)benzyl)-3-(piperidin-1-yl)propan-1-amine (**8**{*5,5*}).

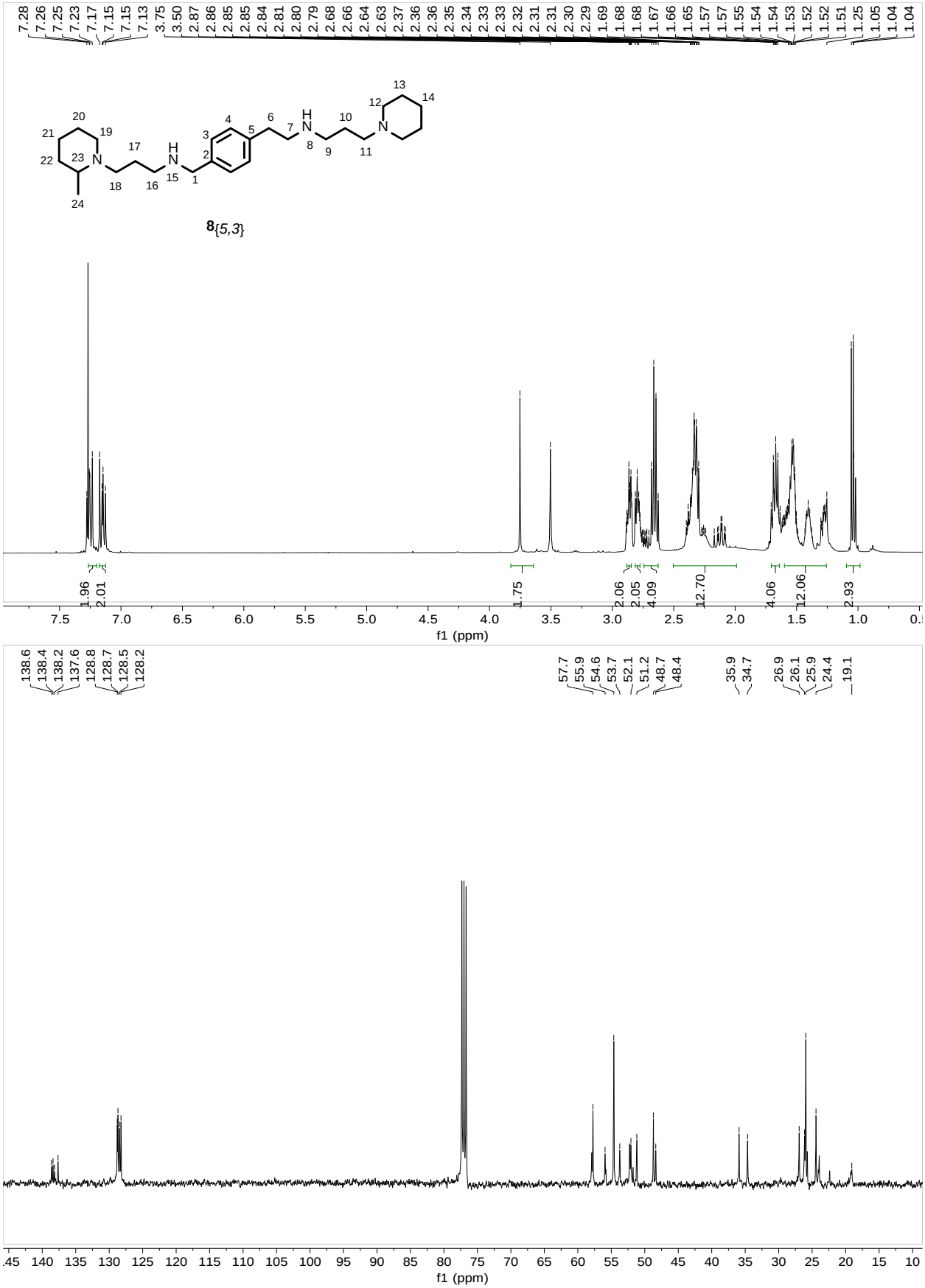


**Fig. S-33:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-(piperidin-1-yl)propylamino)ethyl)benzyl)-3-(2-methyl piperidin-1-yl)propan-1-amine (**8**{*5,3*}).

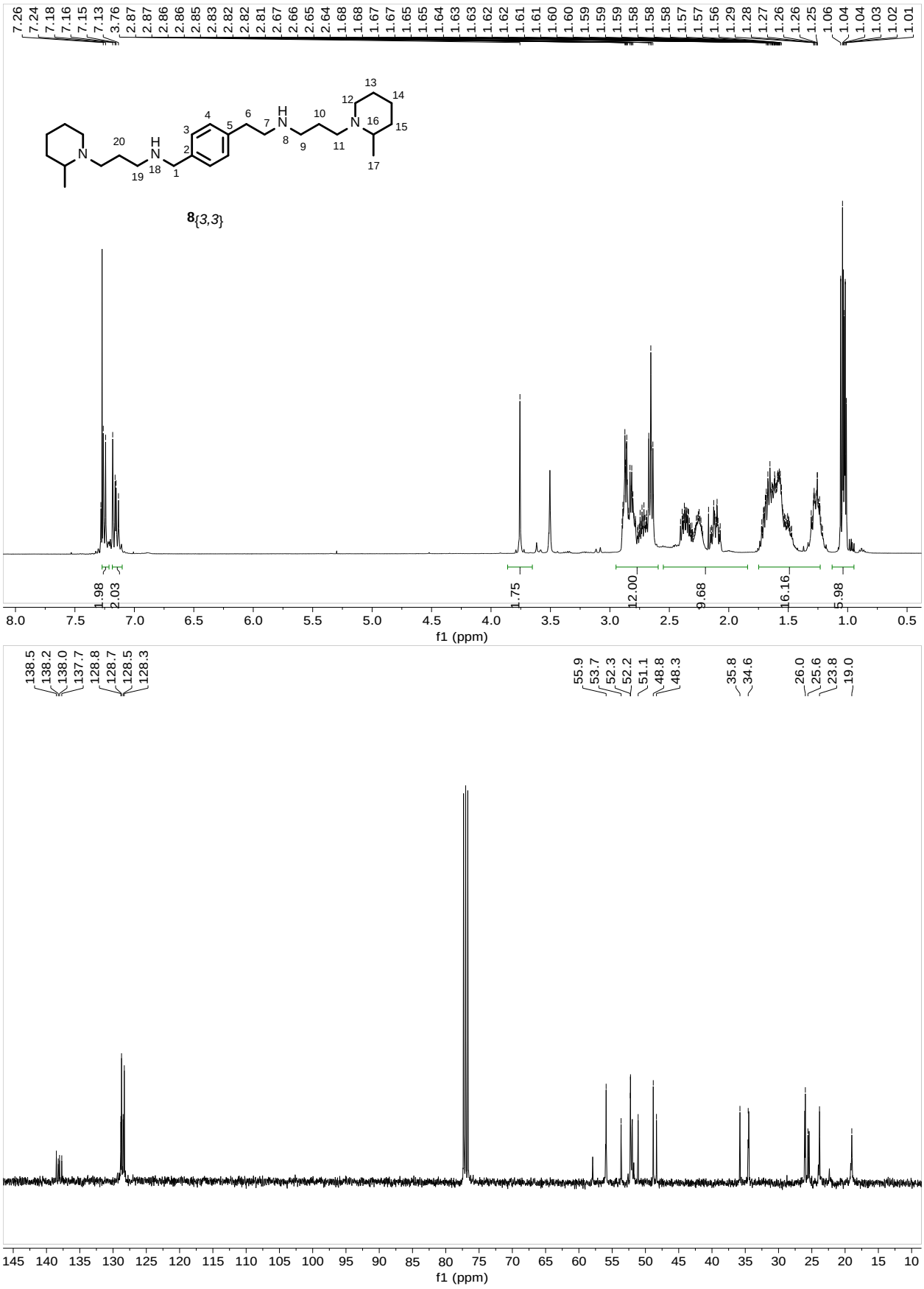


**Fig. S-34:** $^{1}$H and $^{13}$C-NMR of *N*-(4-(2-(3-(2-methylpiperidin-1-yl)propylamino)ethyl)benzyl)-3-(2-methylpiperidin-1-yl)propan-1-amine (**8**{*3,3*}).