ELECTRONIC SUPPLEMENTARY MATERIAL

6-Bromoindole- and 6-bromoindazole-based inhibitors of bacterial cystathionine γ-lyase containing 3-aminothiophene-2-carboxylate moiety

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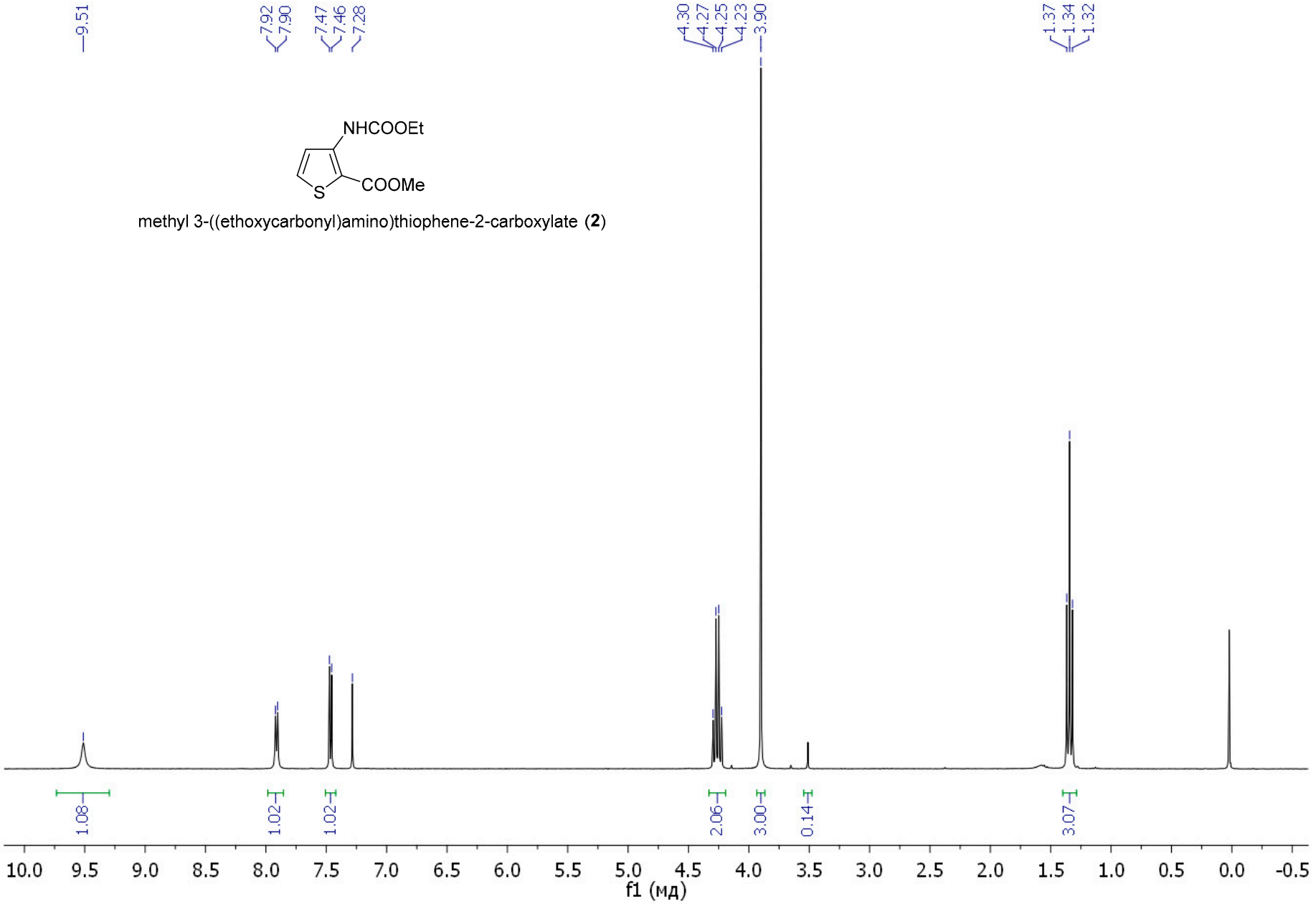
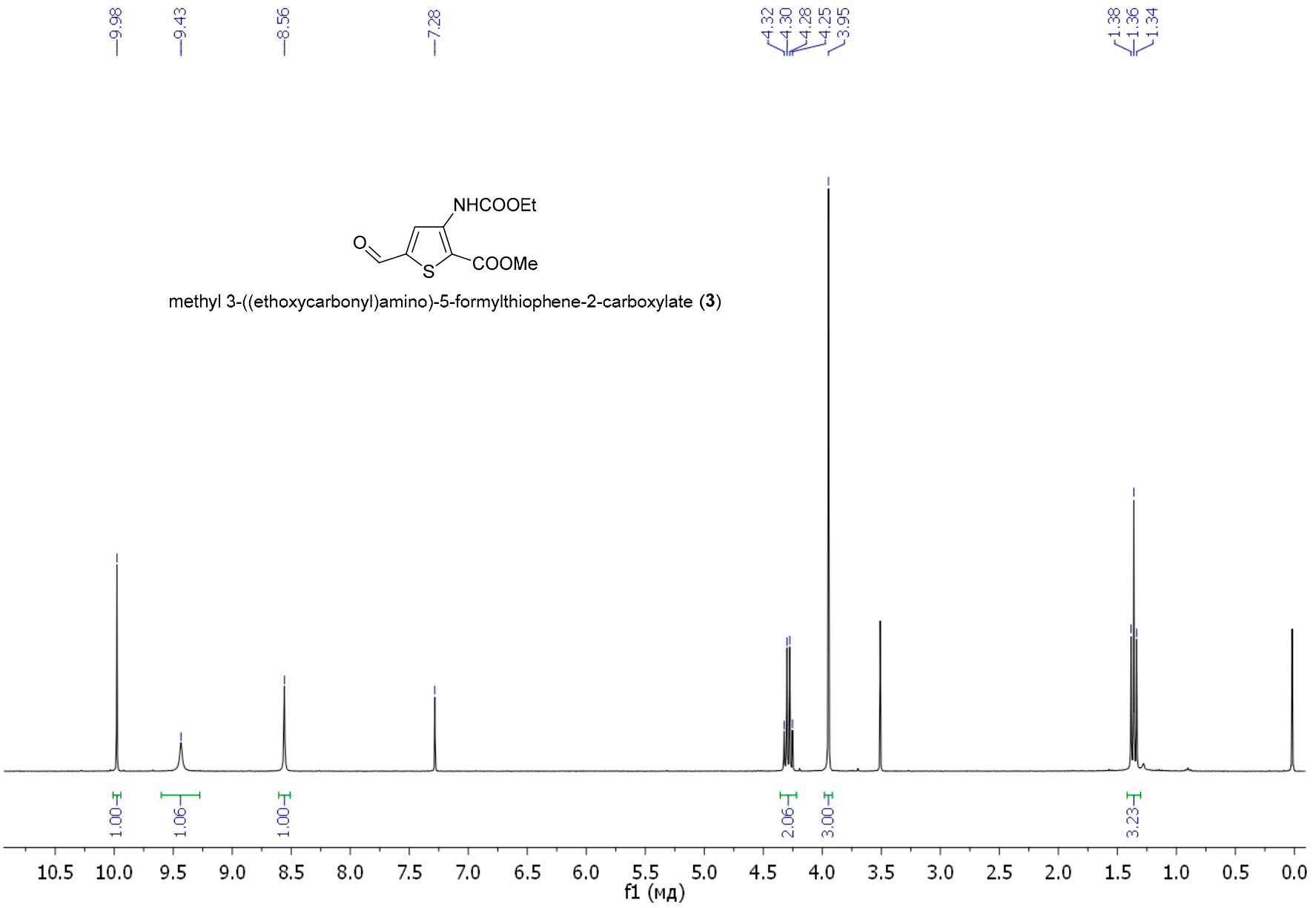
NMR spectral data for compounds

^{1}H NMR (300 MHz) in $CDCl_3$

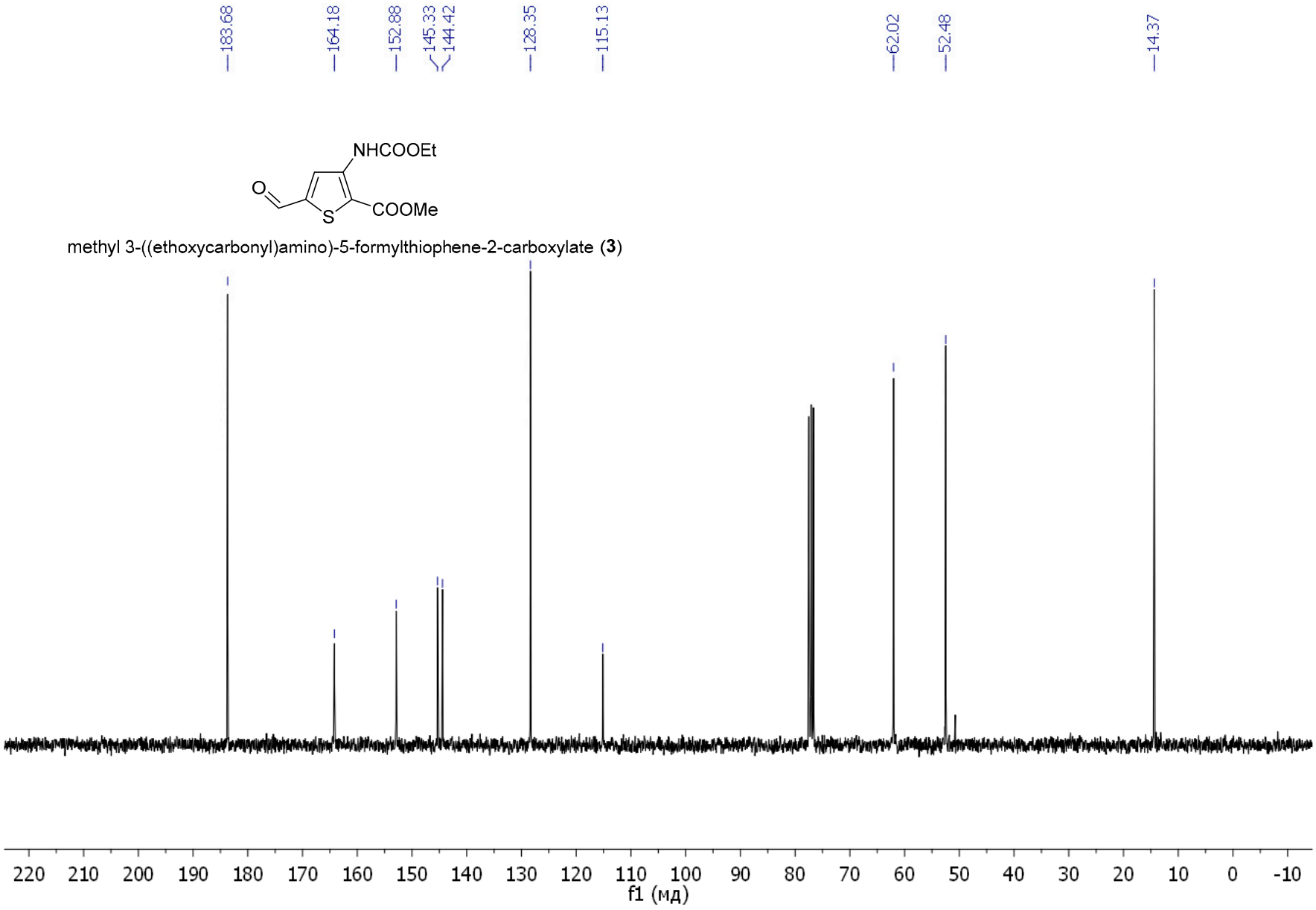


methyl 3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**2**)

^{1}H NMR (300 MHz) in $CDCl_3$

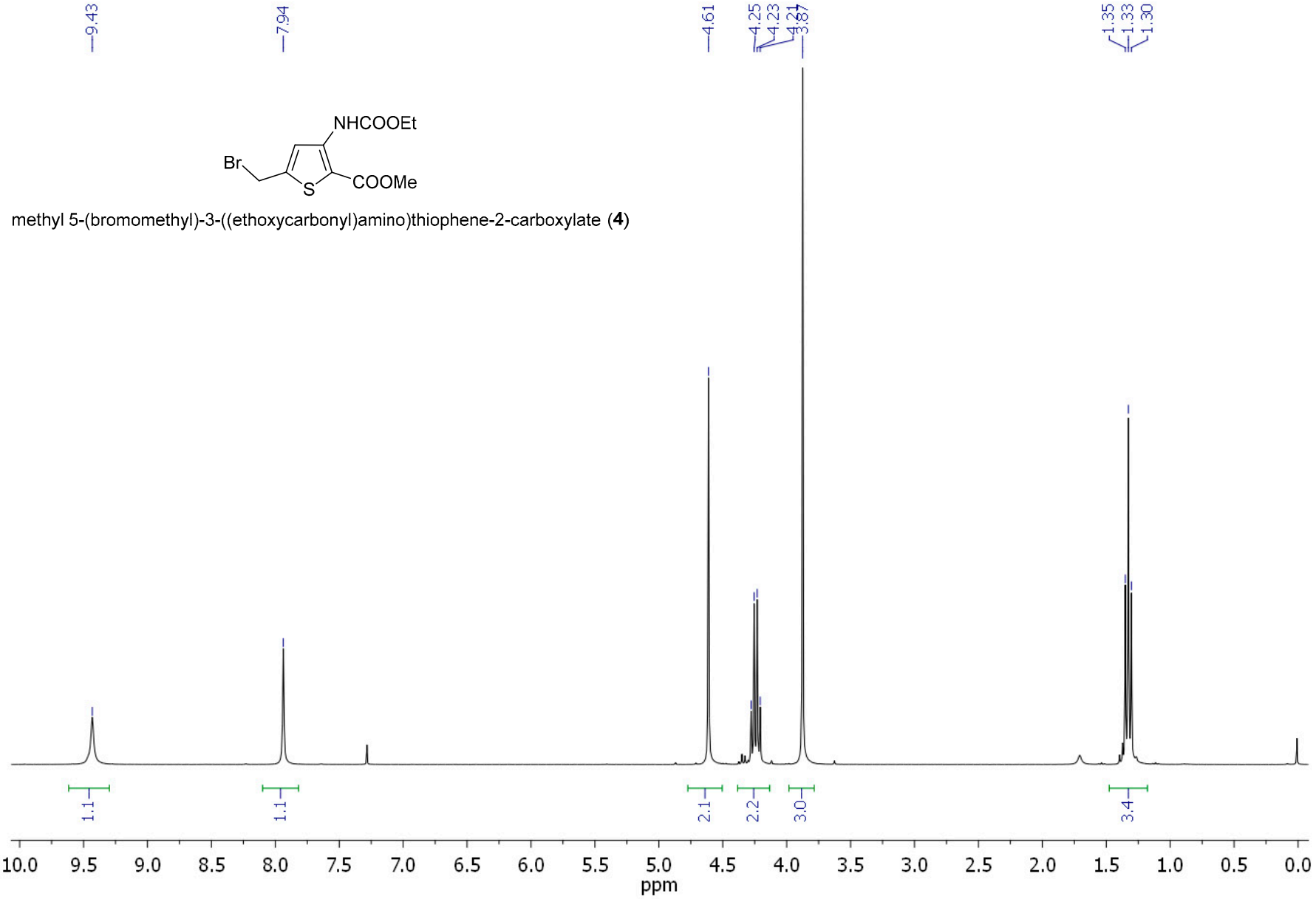


^{13}C NMR (75.5 MHz) in $CDCl_3$



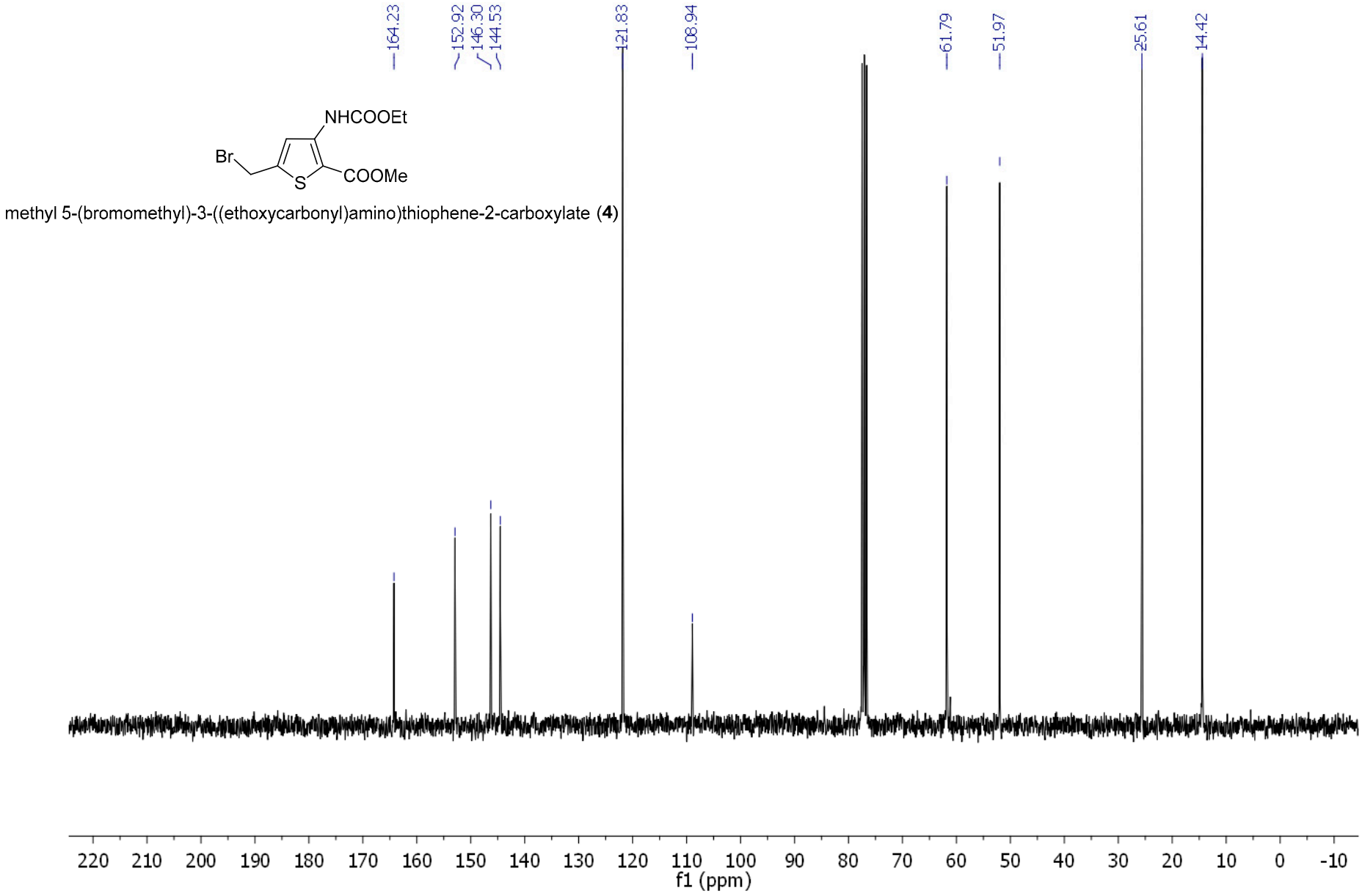
methyl 3-((ethoxycarbonyl)amino)-5-formylthiophene-2-carboxylate (**3**)

^{1}H NMR (300 MHz) in $CDCl_3$



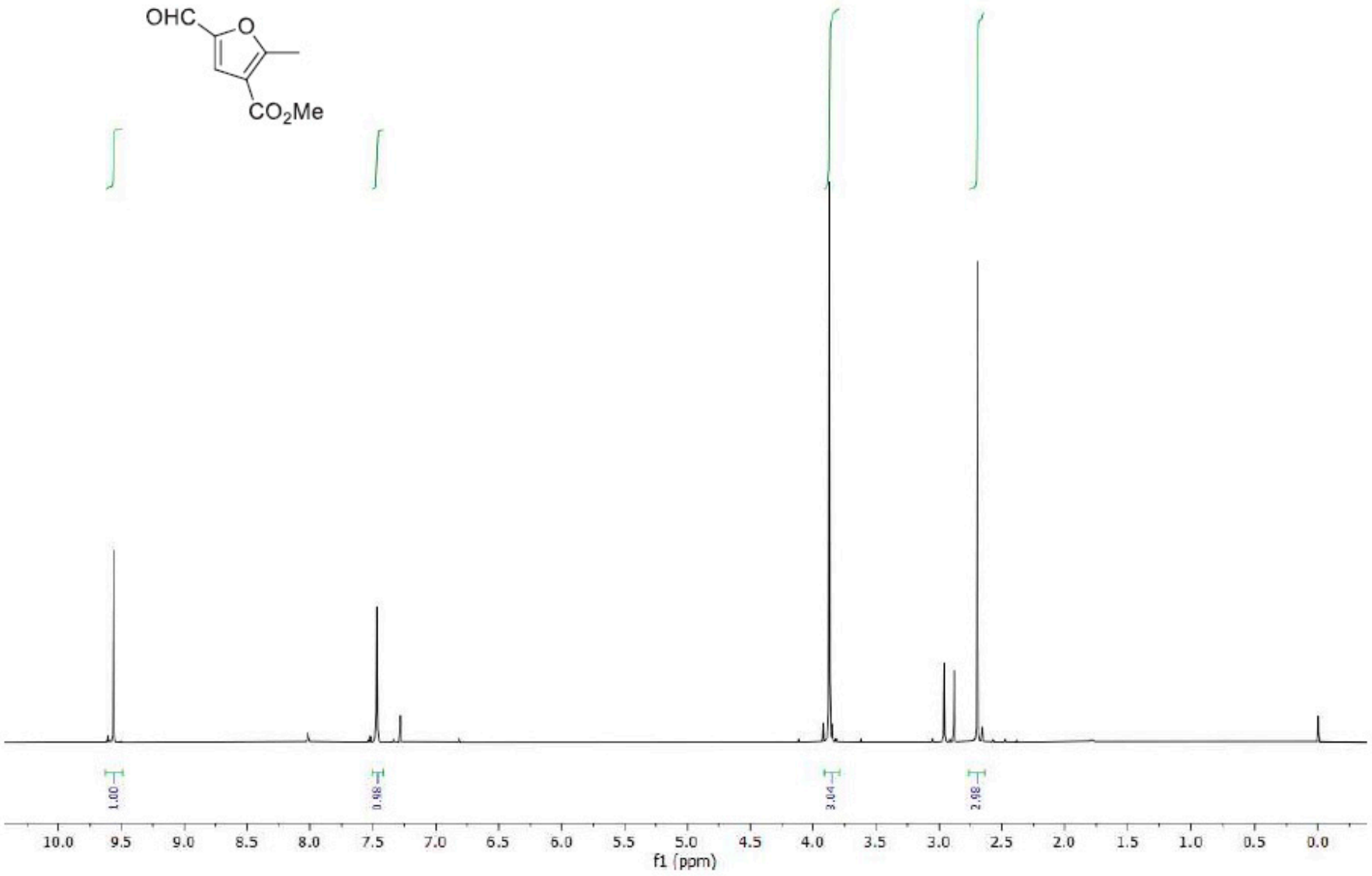
methyl 5-(bromomethyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**4**)

^{13}C NMR (75.5 MHz) in $CDCl_3$

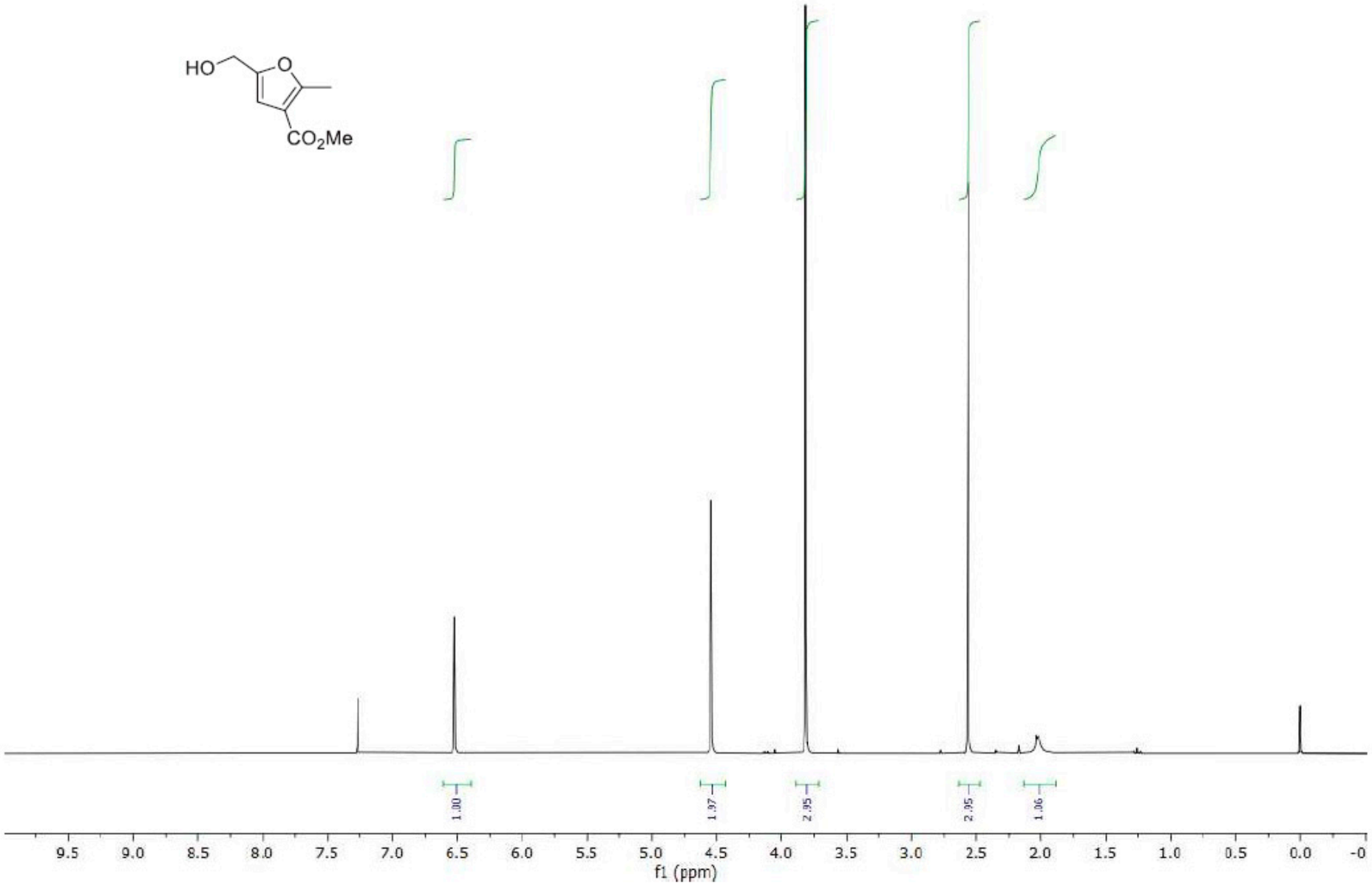


methyl 5-(bromomethyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**4**)

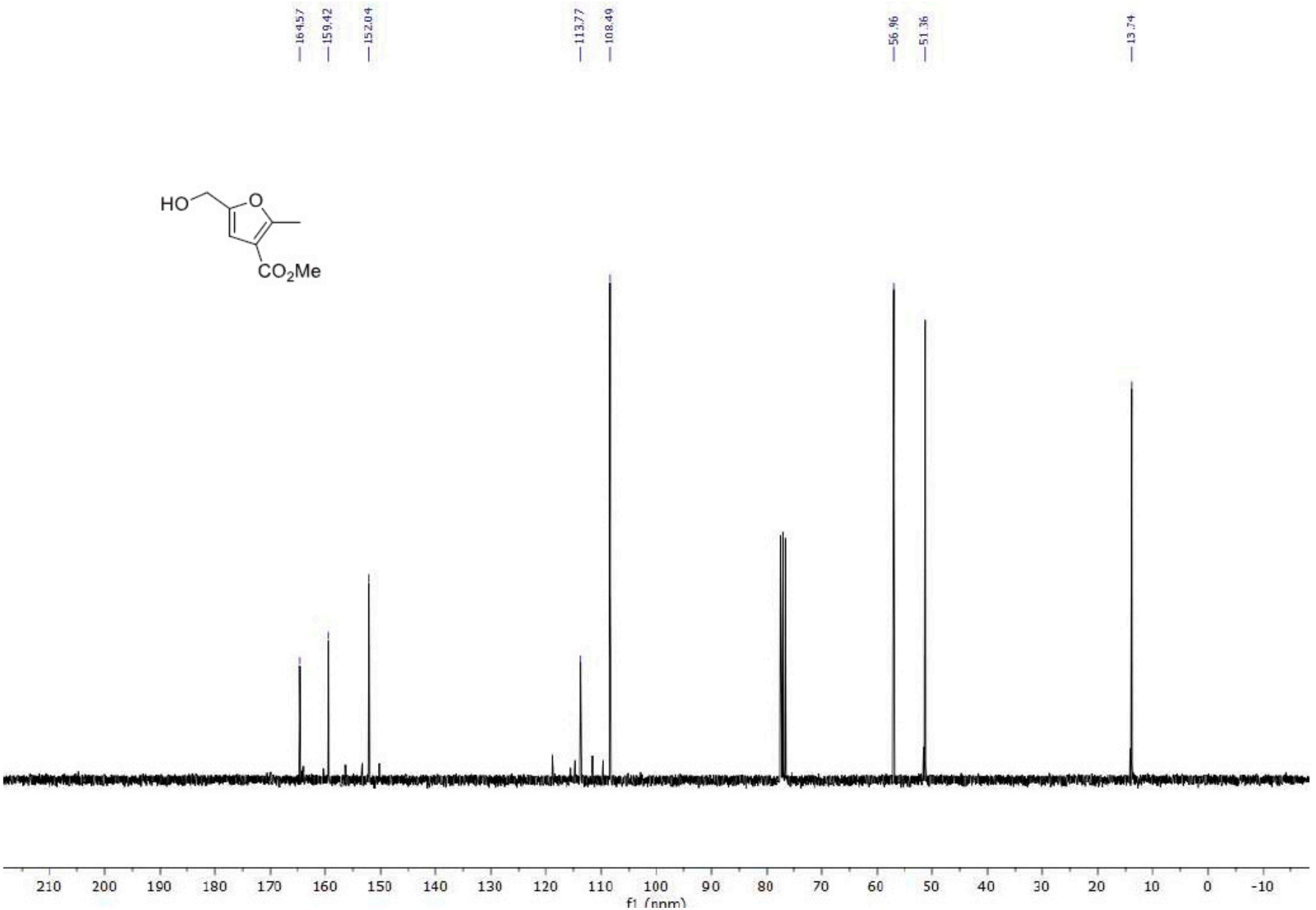
^{1}H NMR (300 MHz) in $CDCl_3$



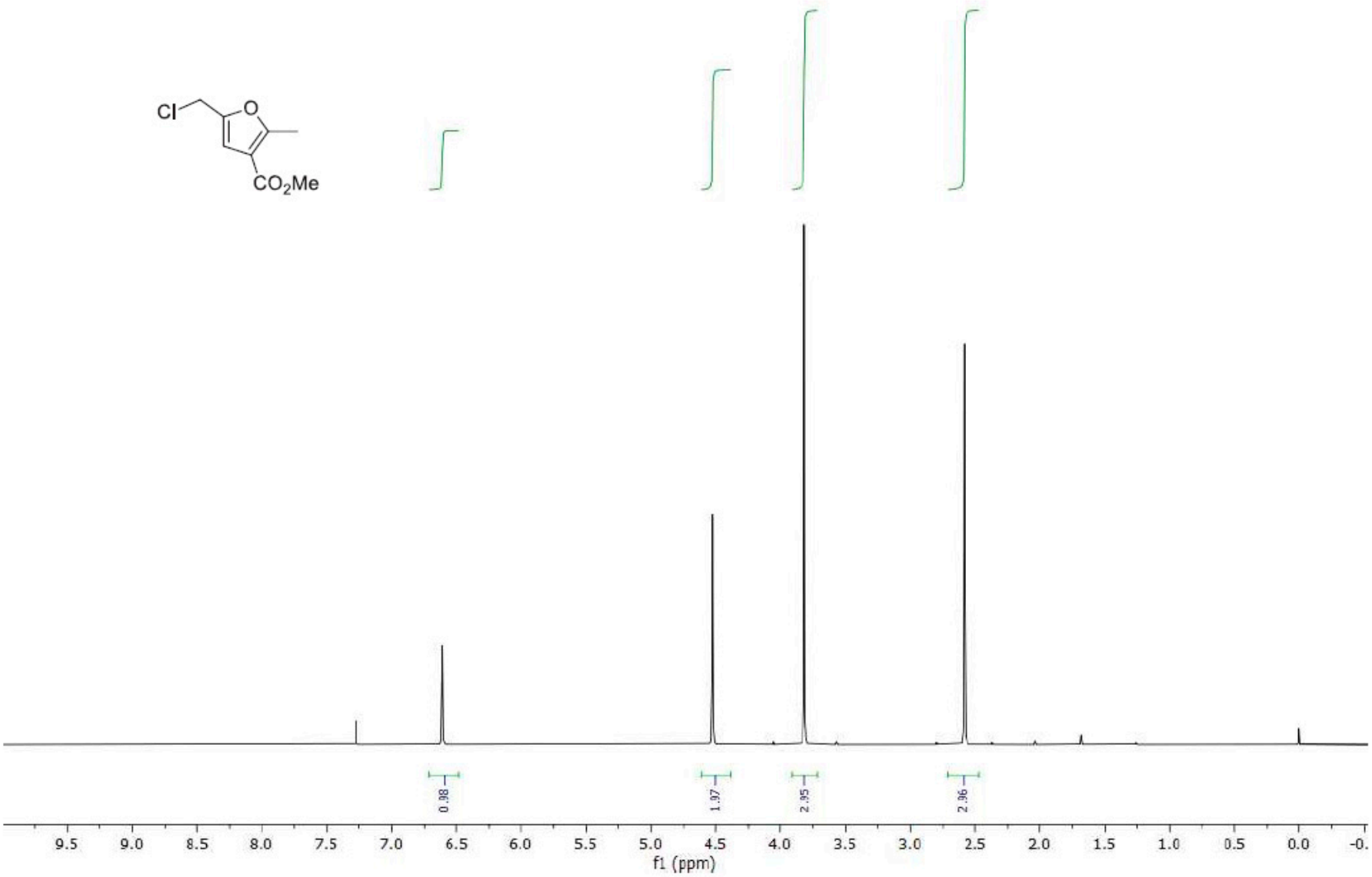
^{1}H NMR (300 MHz) in $CDCl_3$



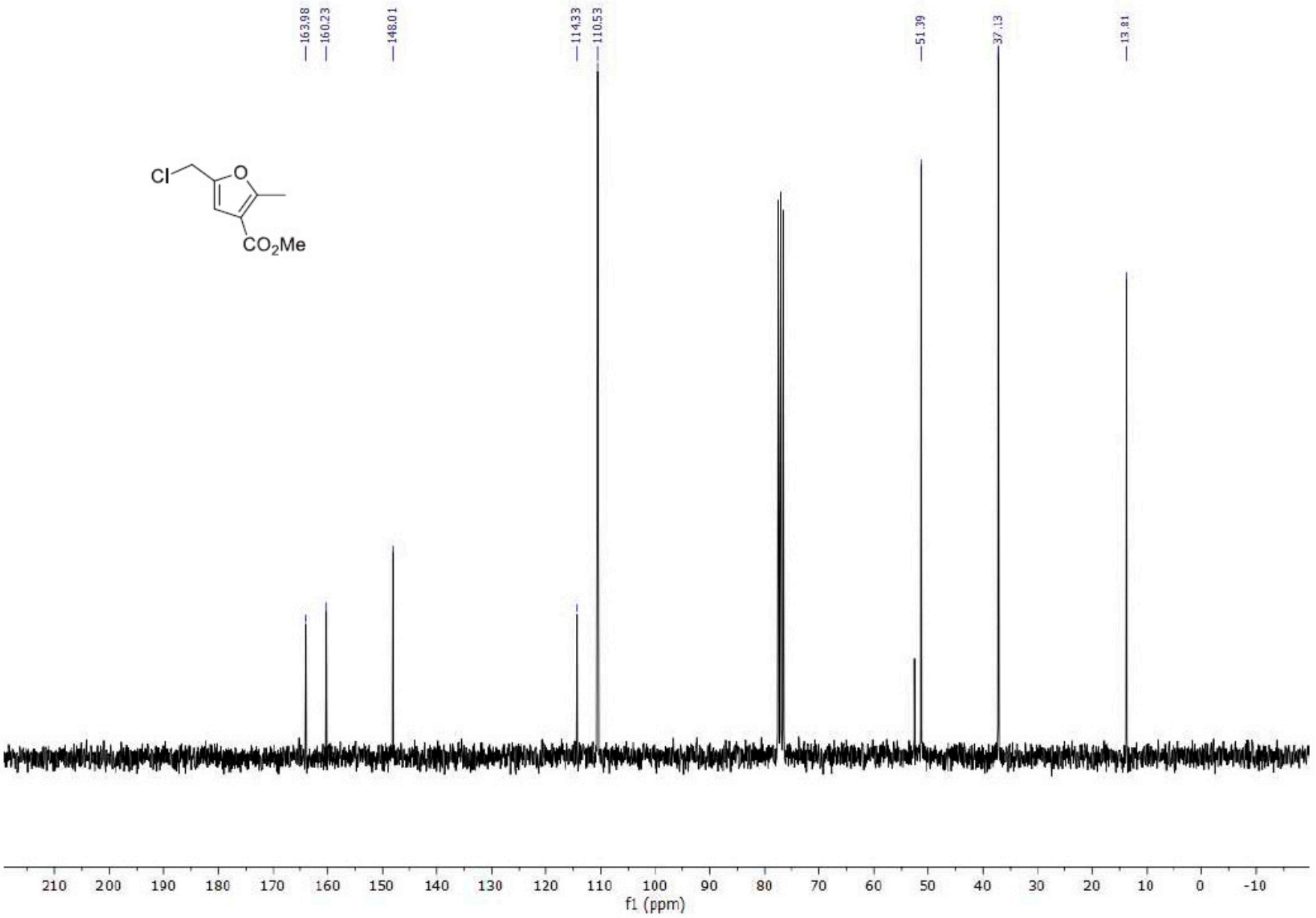
^{13}C NMR (75.5 MHz) in $CDCl_3$



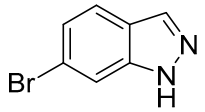
^{1}H NMR (300 MHz) in $CDCl_3$



^{13}C NMR (75.5 MHz) in $CDCl_3$

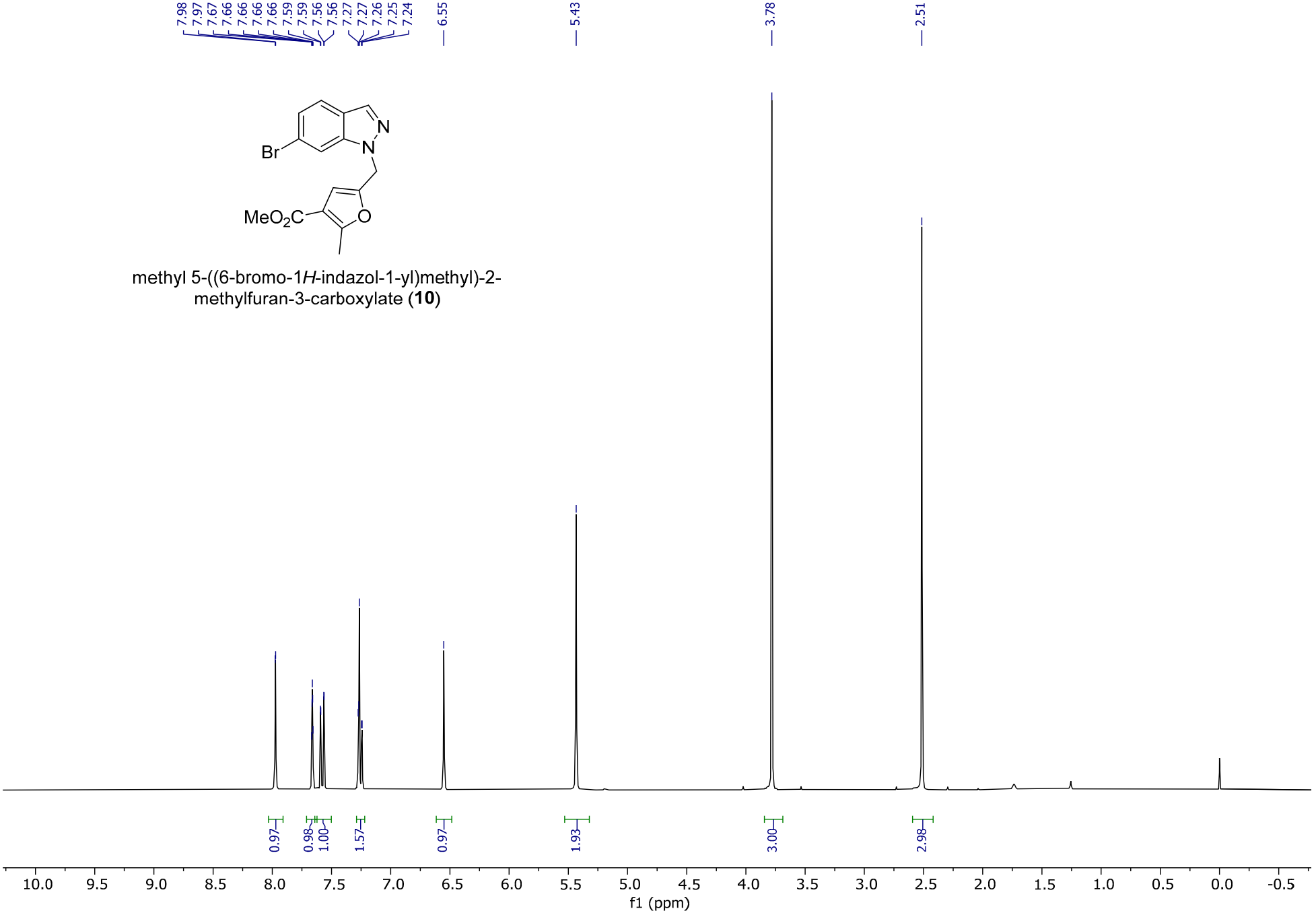


^{1}H NMR (300 MHz) in DMSO-d6



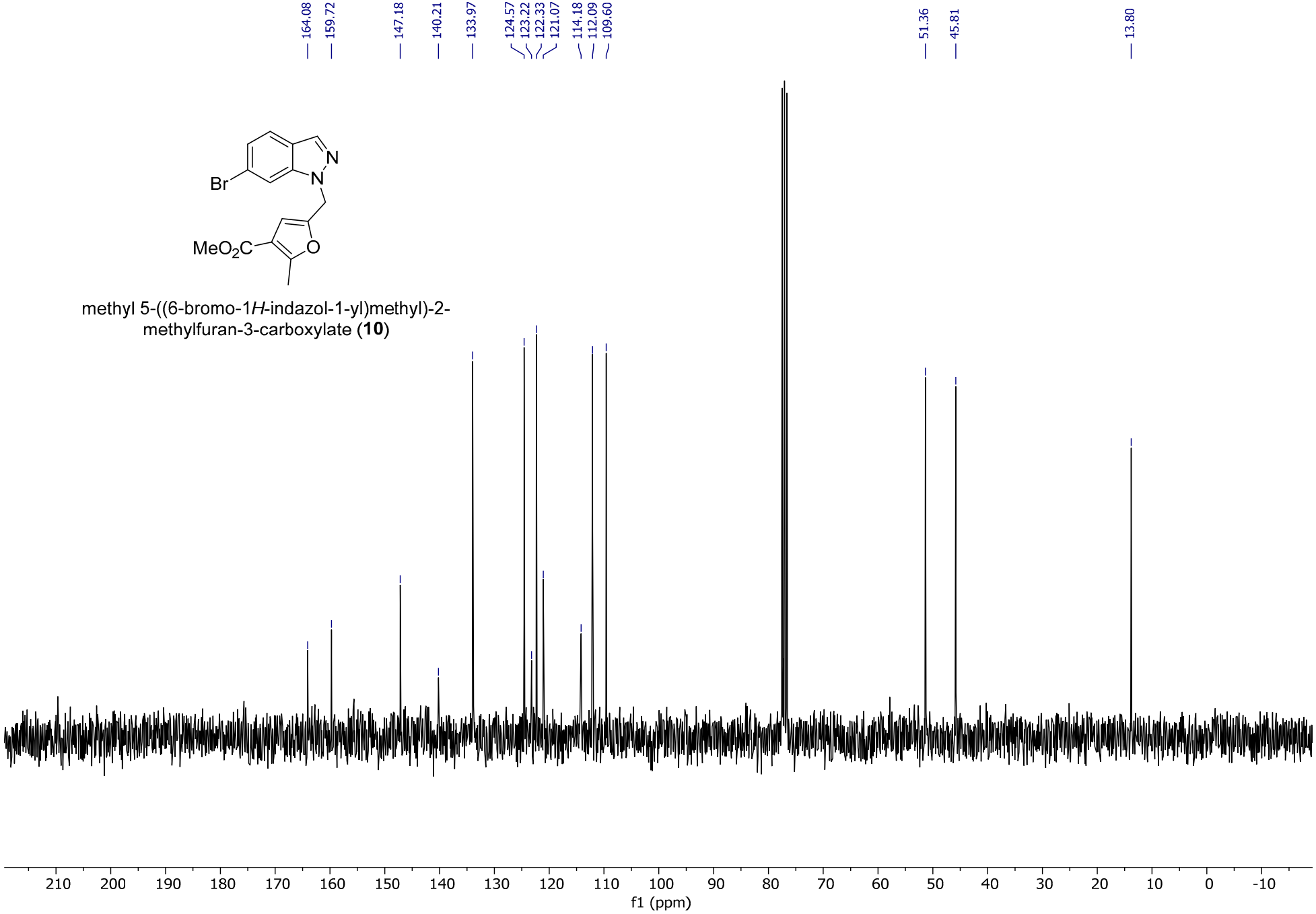
6-bromo-1*H*-indazole (6)

^{1}H NMR (300 MHz) in $CDCl_3$



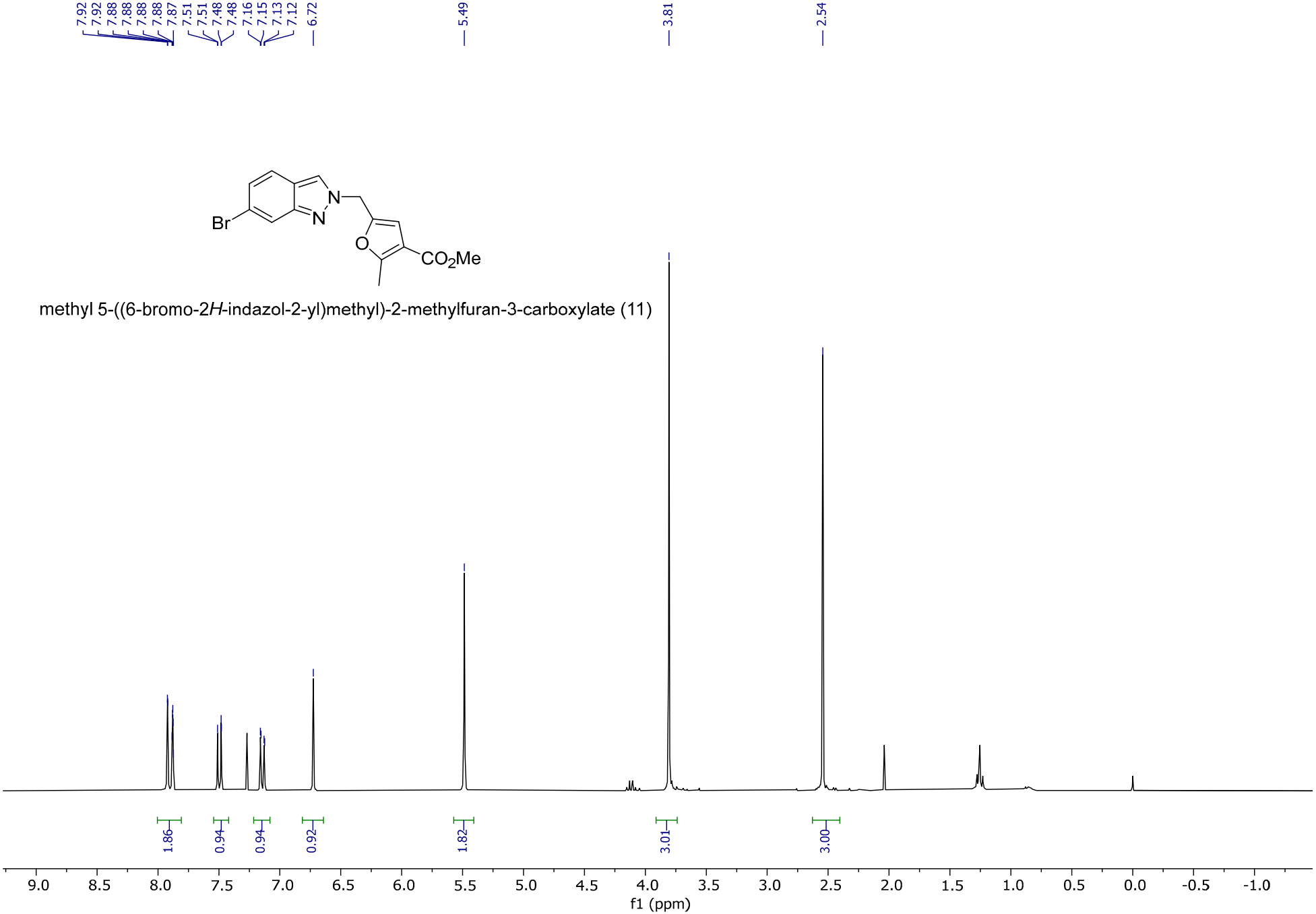
methyl 5-((6-bromo-1*H*-indazol-1-yl)methyl)-2-methylfuran-3-carboxylate (**10**)

^{13}C NMR (75.5 MHz) in $CDCl_3$



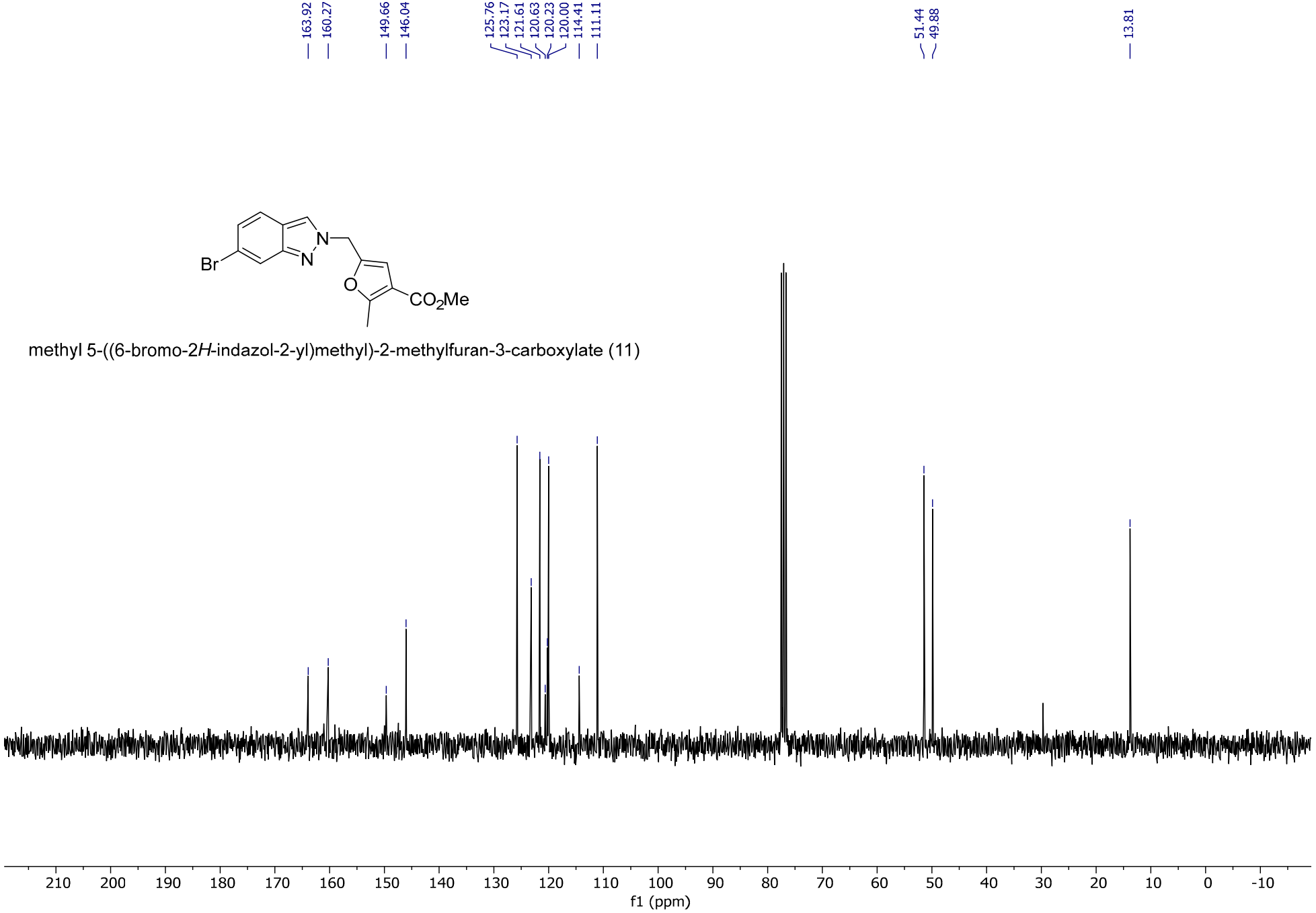
methyl 5-((6-bromo-1*H*-indazol-1-yl)methyl)-2-methylfuran-3-carboxylate (**10**)

^{1}H NMR (300 MHz) in $CDCl_3$



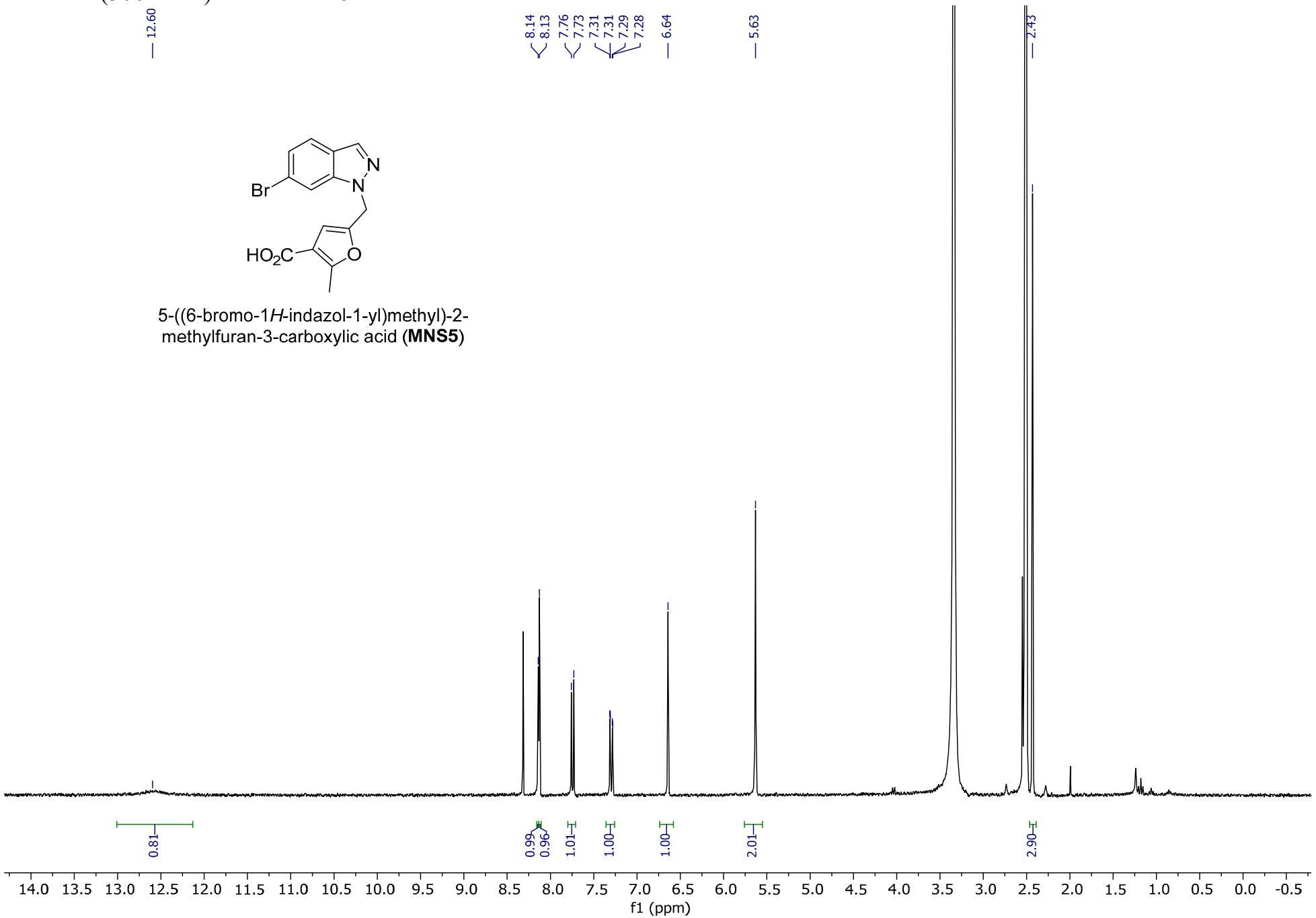
methyl 5-((6-bromo-2*H*-indazol-2-yl)methyl)-2-methylfuran-3-carboxylate (11)

^{13}C NMR (75.5 MHz) in $CDCl_3$



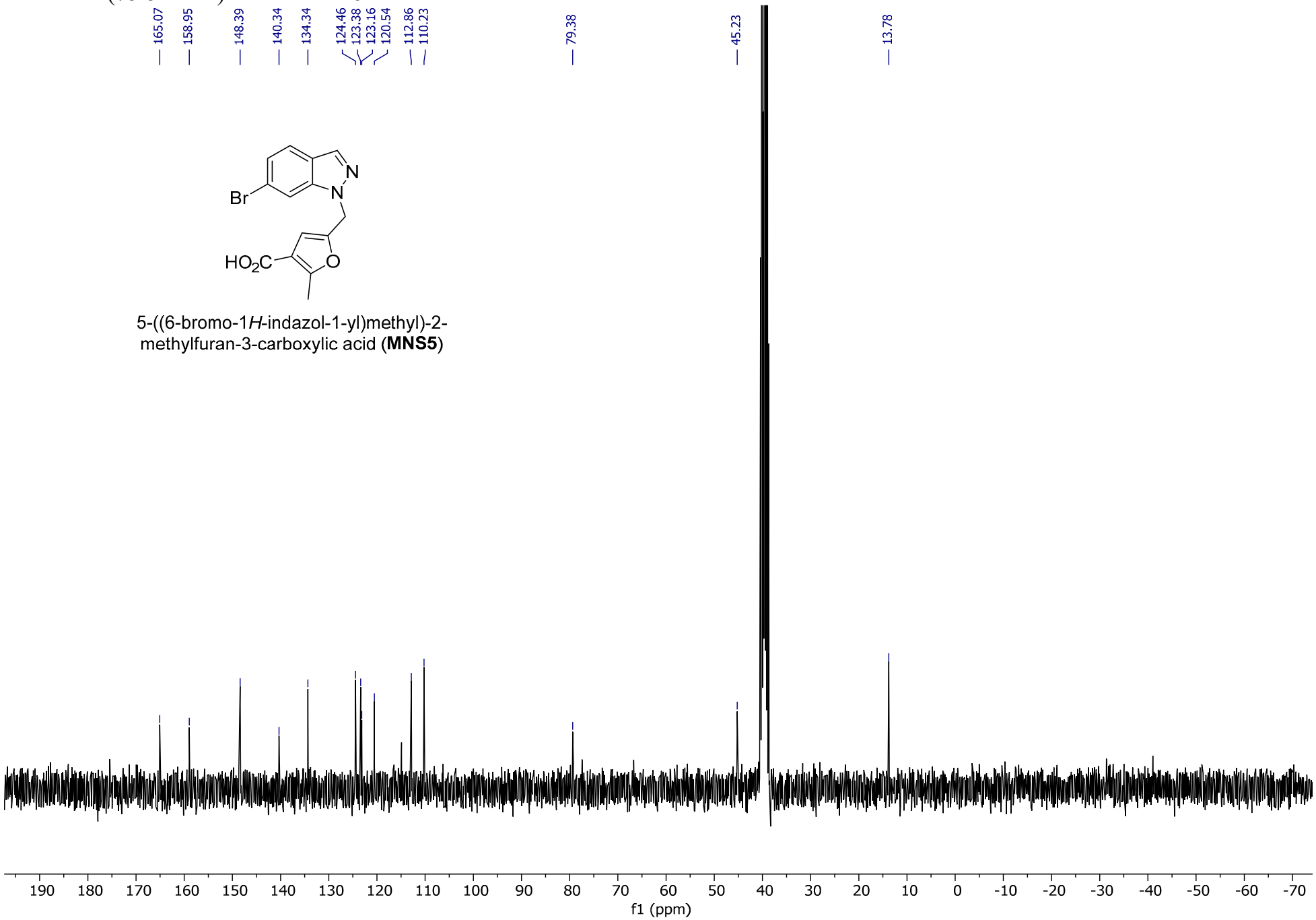
methyl 5-((6-bromo-2*H*-indazol-2-yl)methyl)-2-methylfuran-3-carboxylate (11)

^{1}H NMR (300 MHz) in DMSO-d6



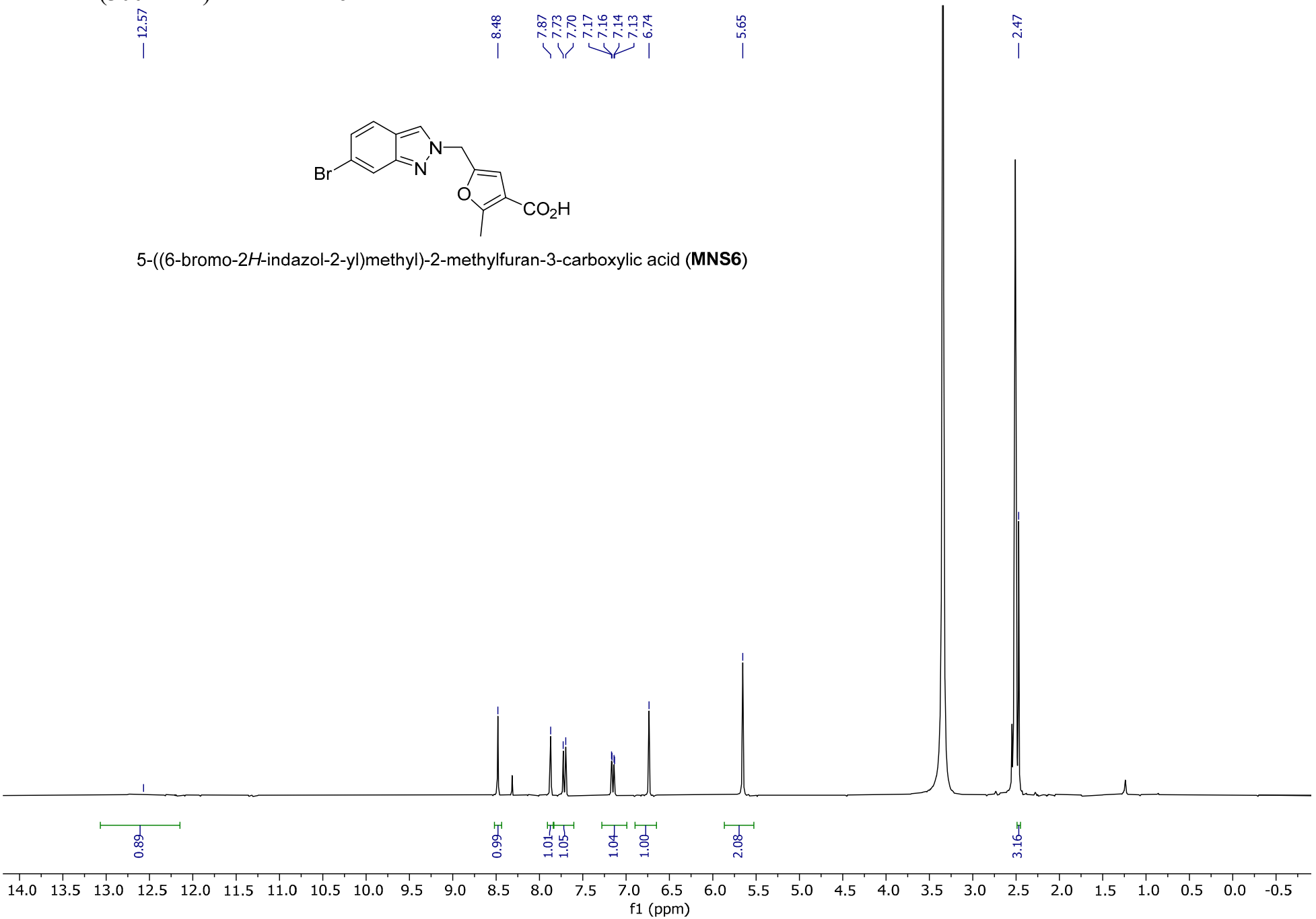
5-((6-bromo-1*H*-indazol-1-yl)methyl)-2-methylfuran-3-carboxylic acid (**MNS5**)

^{13}C NMR (75.5 MHz) in DMSO-d6



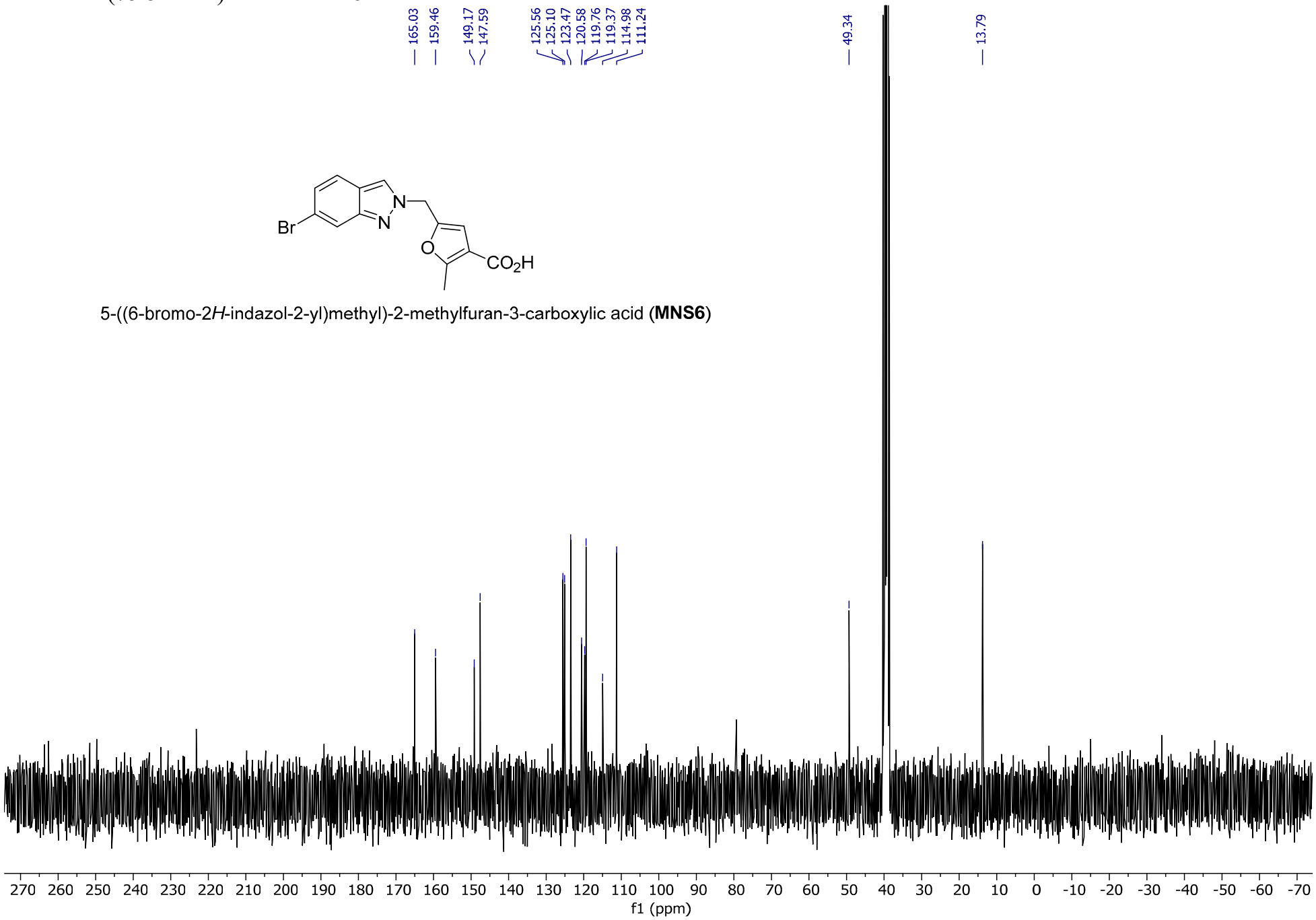
5-((6-bromo-1*H*-indazol-1-yl)methyl)-2-methylfuran-3-carboxylic acid (**MNS5**)

^{1}H NMR (300 MHz) in DMSO-d6



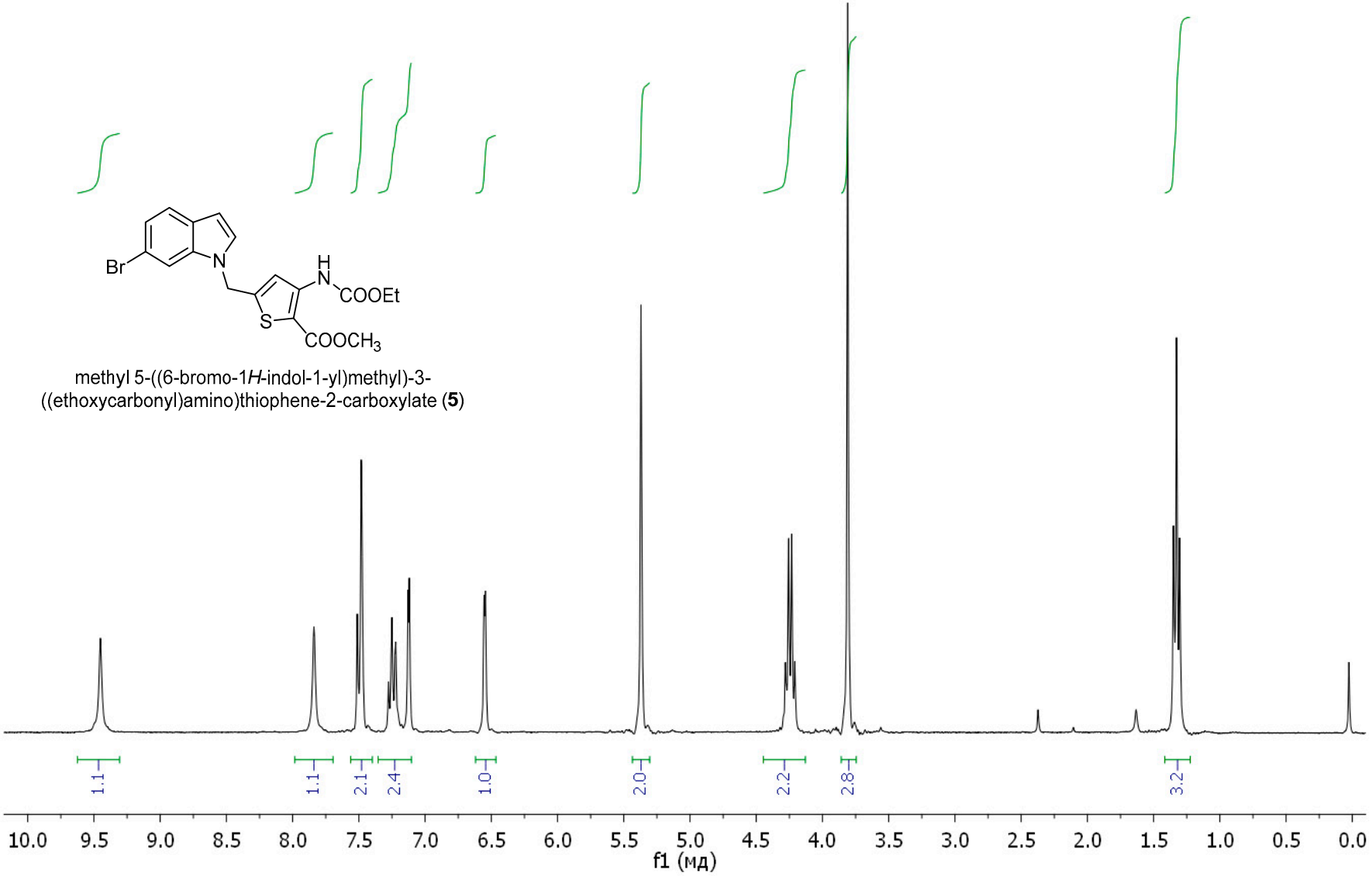
5-((6-bromo-2*H*-indazol-2-yl)methyl)-2-methylfuran-3-carboxylic acid (**MNS6**)

^{13}C NMR (75.5 MHz) in DMSO-d6



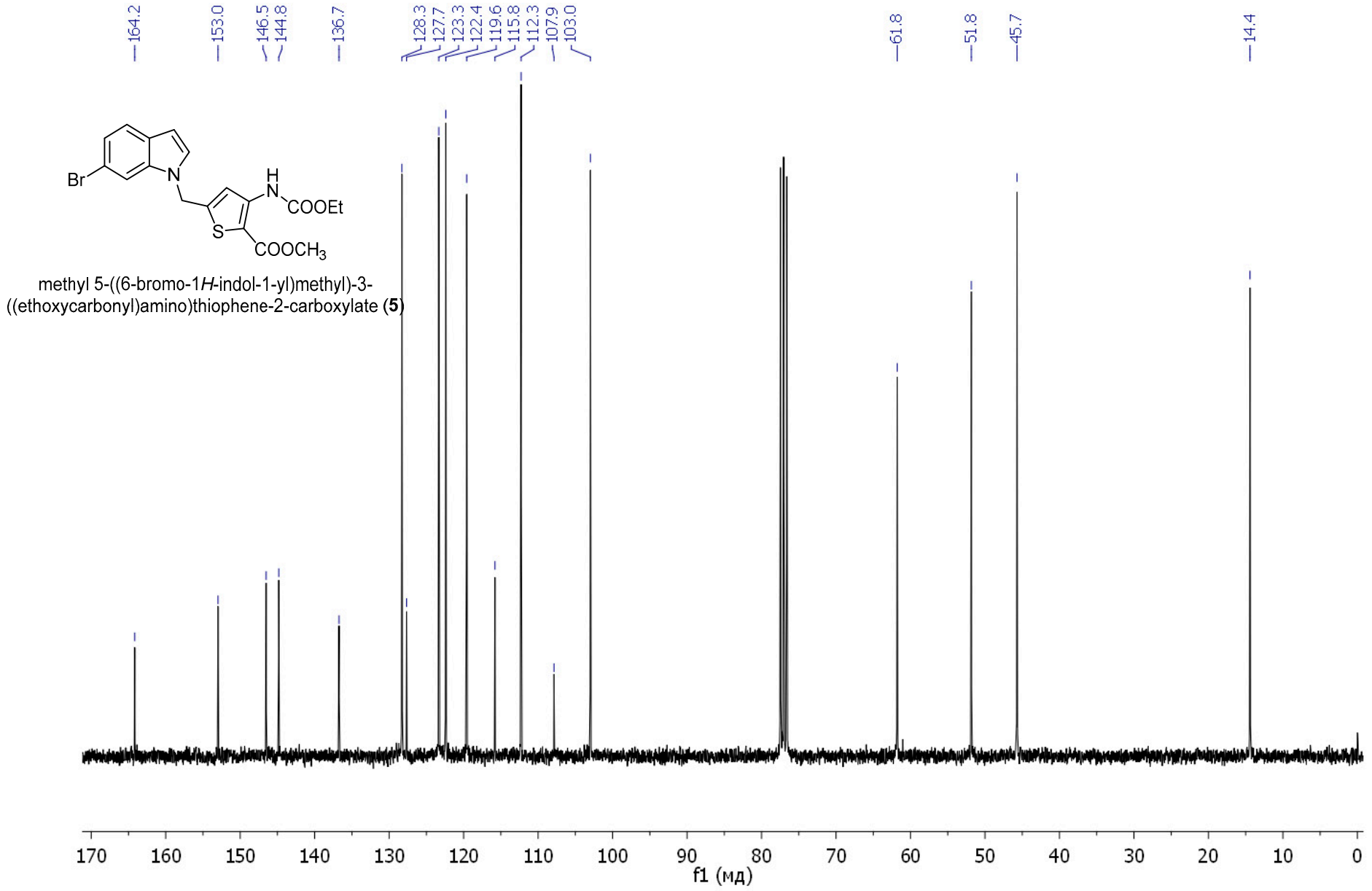
5-((6-bromo-2*H*-indazol-2-yl)methyl)-2-methylfuran-3-carboxylic acid (**MNS6**)

^{1}H NMR (300 MHz) in $CDCl_3$



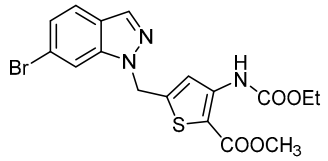
methyl 5-((6-bromo-1*H*-indol-1-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**5**)

^{13}C NMR (75.5 MHz) in $CDCl_3$



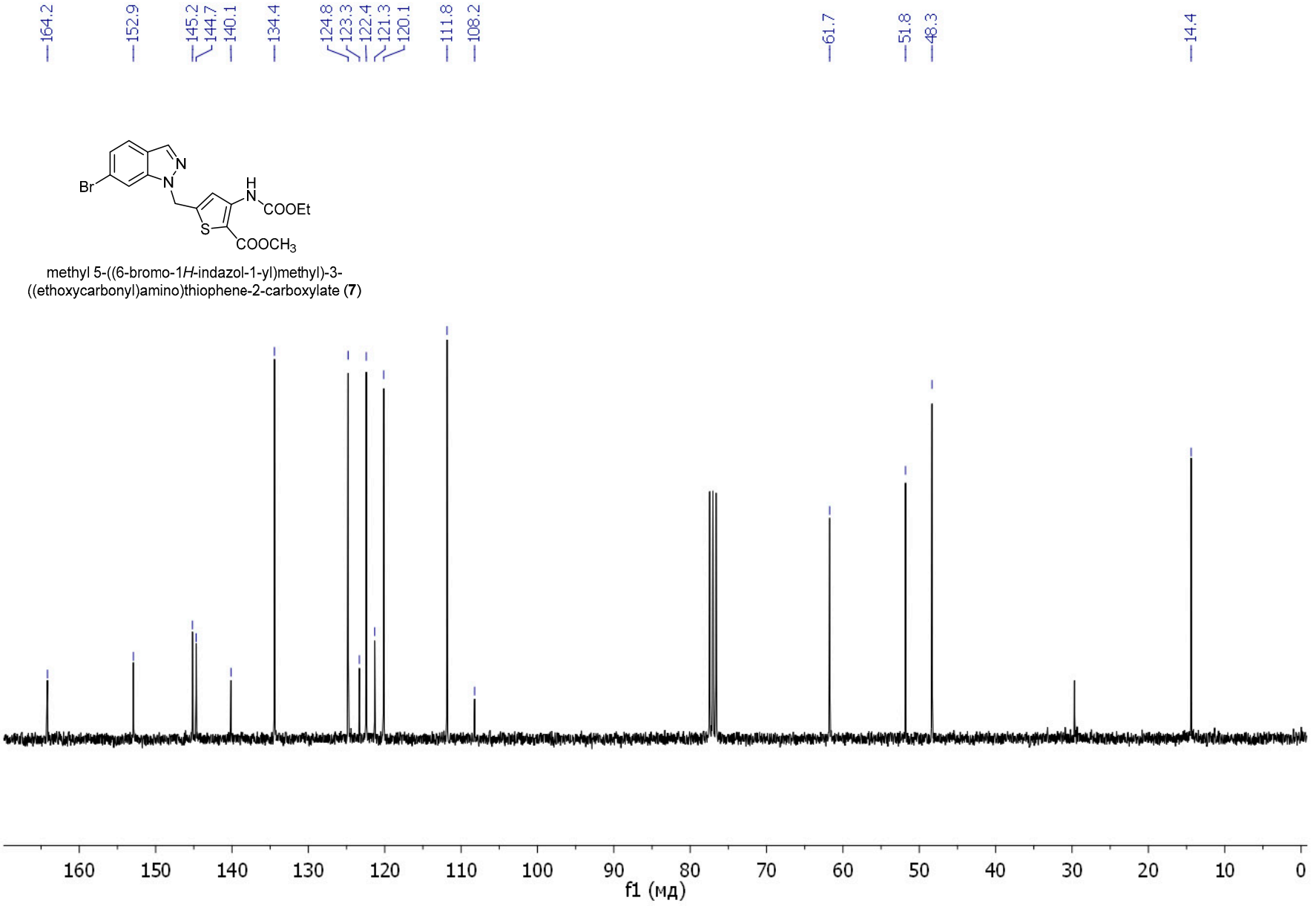
methyl 5-((6-bromo-1*H*-indol-1-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**5**)

^{1}H NMR (300 MHz) in $CDCl_3$



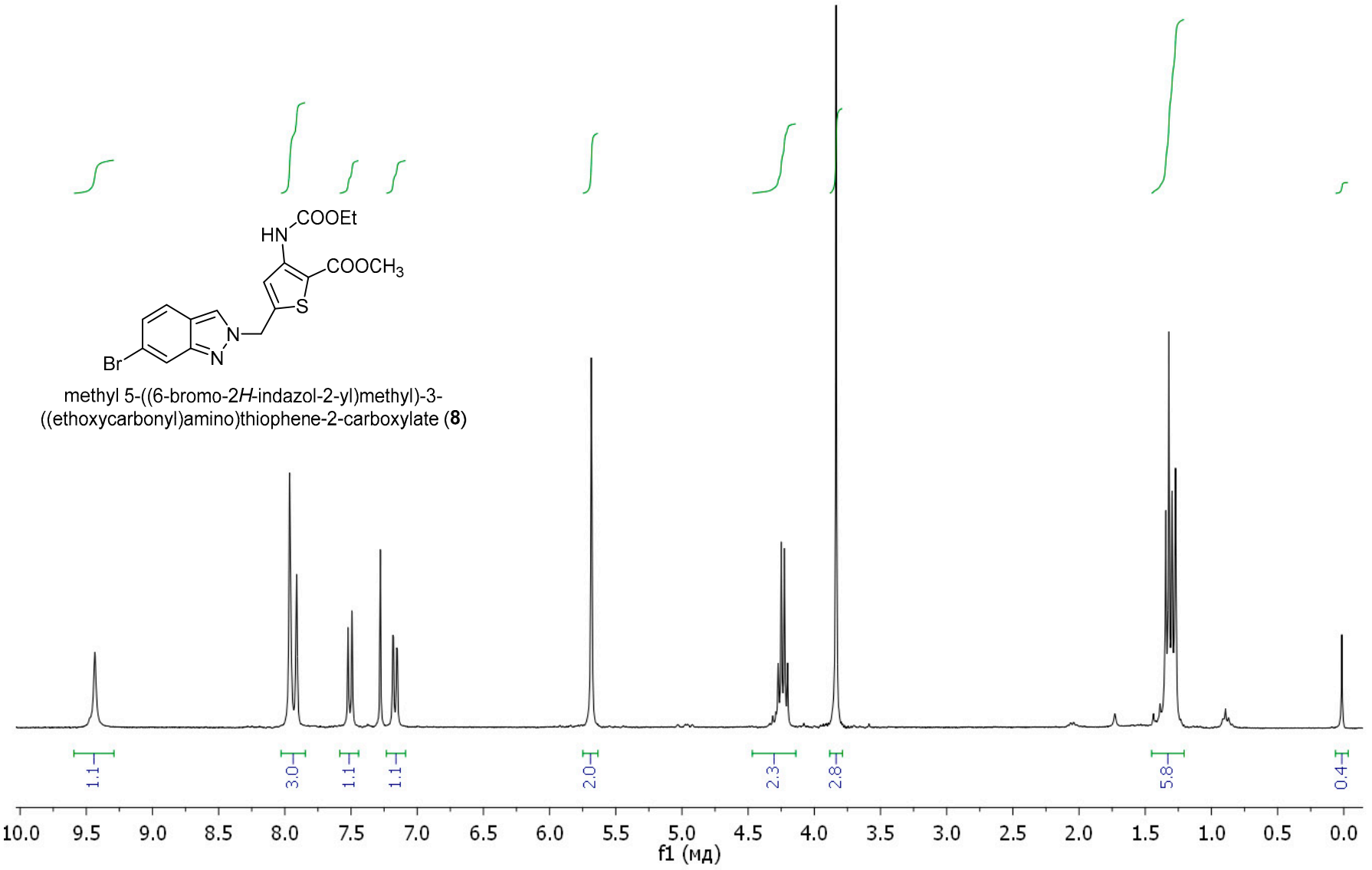
methyl 5-((6-bromo-1*H*-indazol-1-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**7**)

^{13}C NMR (75.5 MHz) in $CDCl_3$



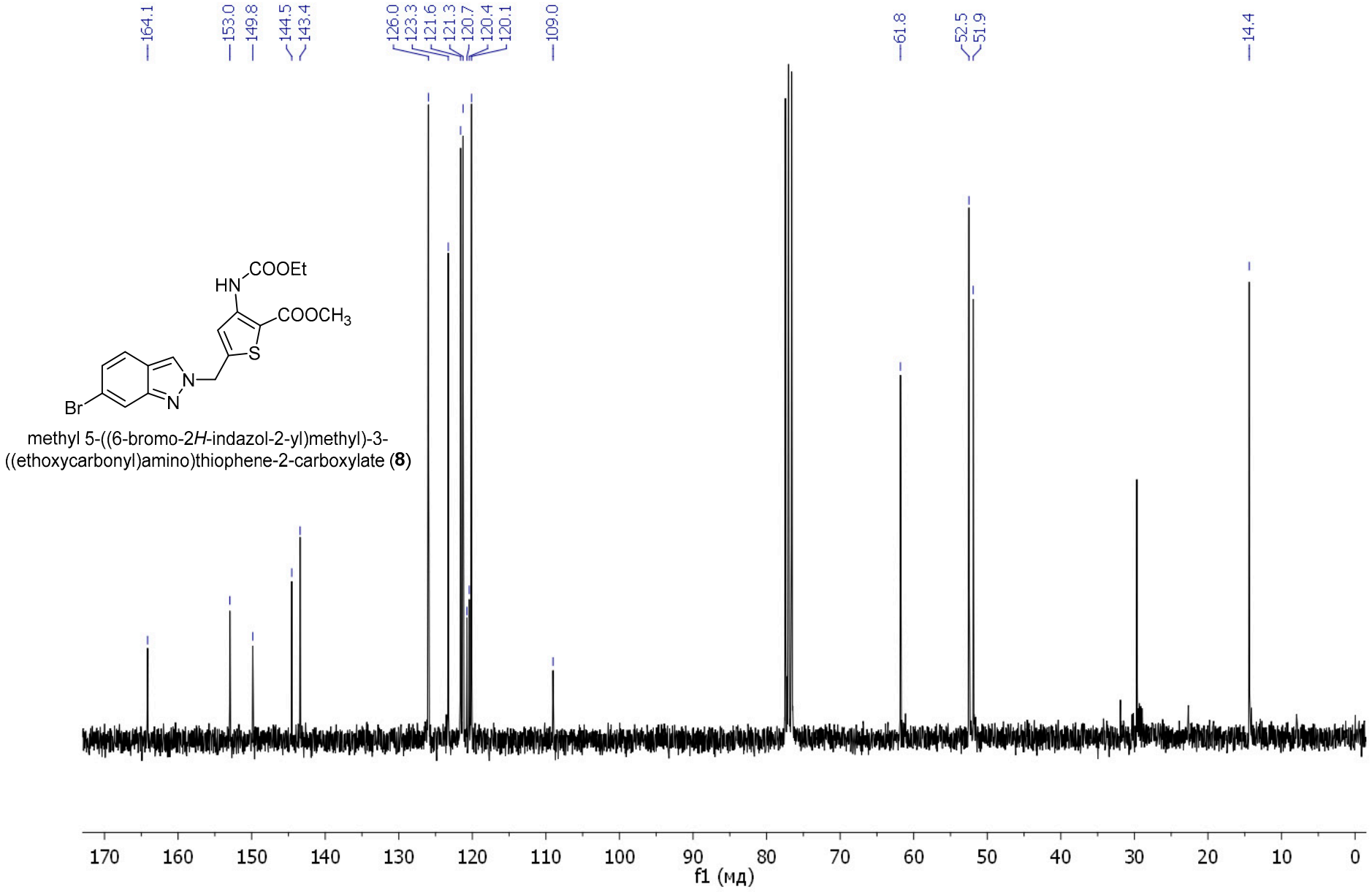
methyl 5-((6-bromo-1*H*-indazol-1-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**7**)

^{1}H NMR (300 MHz) in $CDCl_3$



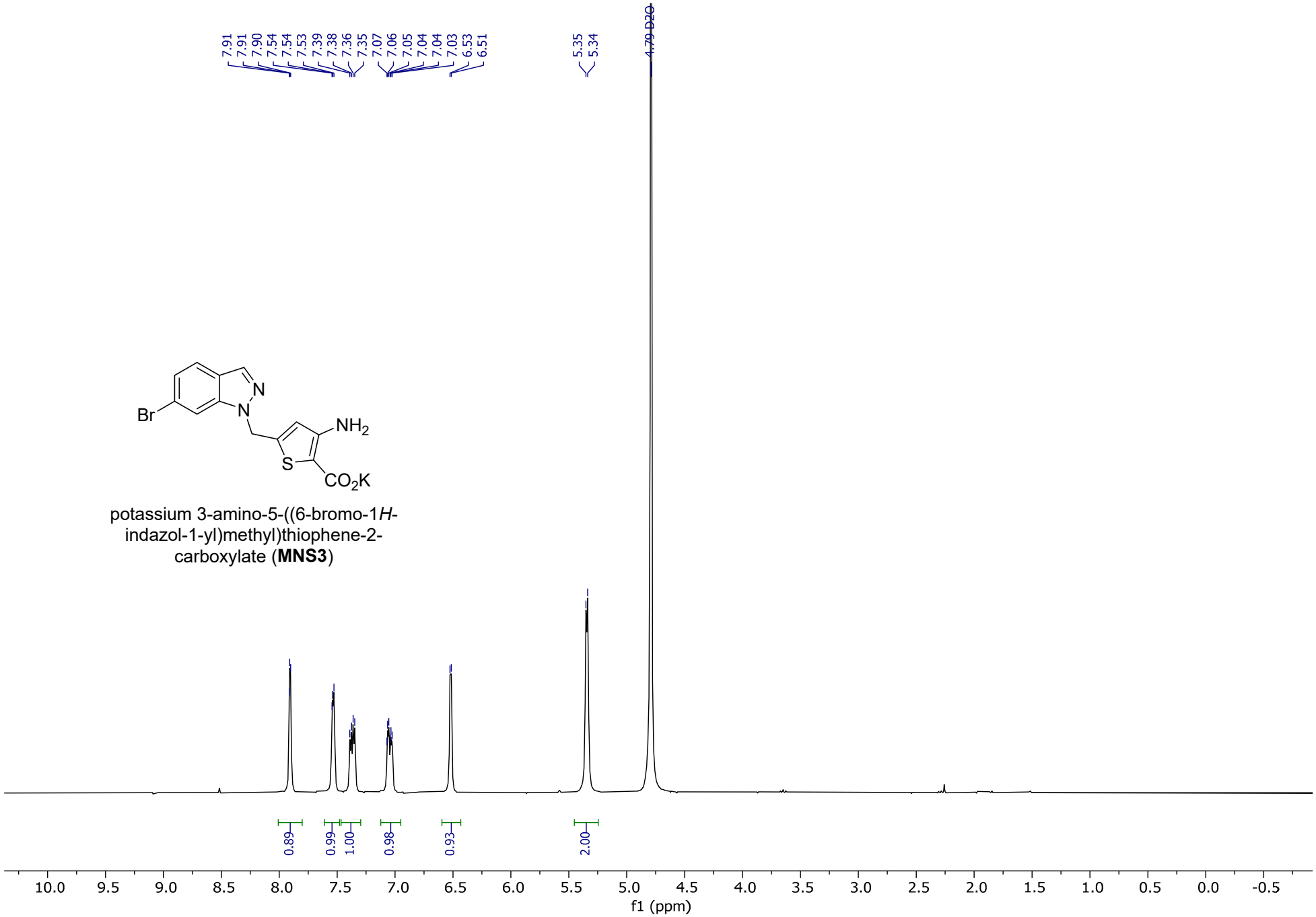
methyl 5-((6-bromo-2*H*-indazol-2-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**8**)

^{13}C NMR (75.5 MHz) in $CDCl_3$



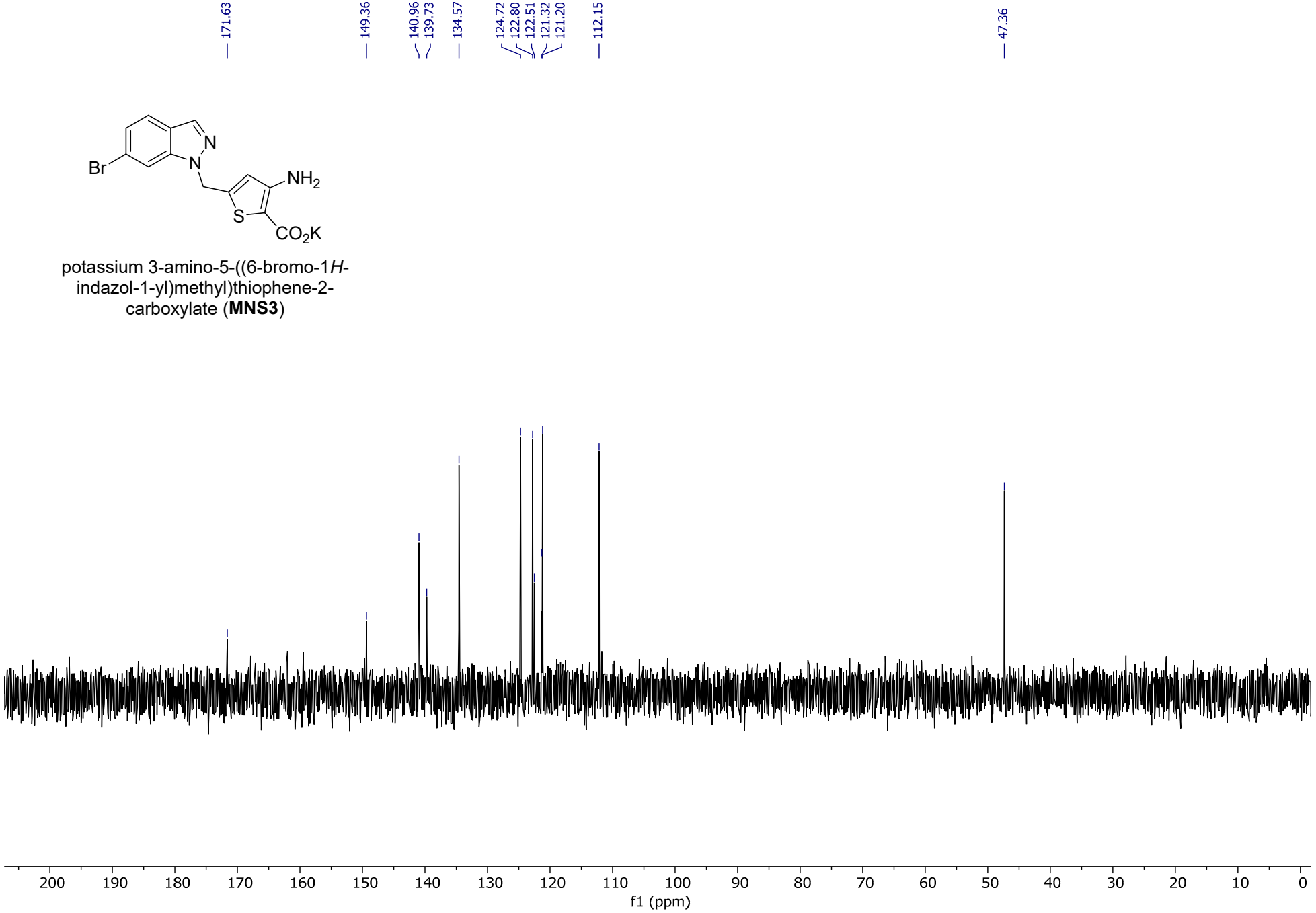
methyl 5-((6-bromo-2*H*-indazol-2-yl)methyl)-3-((ethoxycarbonyl)amino)thiophene-2-carboxylate (**8**)

^{1}H NMR (300 MHz) in D_2O



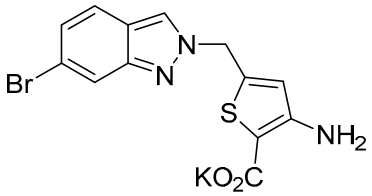
potassium 3-amino-5-((6-bromo-1*H*-indazol-1-yl)methyl)thiophene-2-carboxylate (**MNS3**)

^{13}C NMR (75.5 MHz) in D_2O



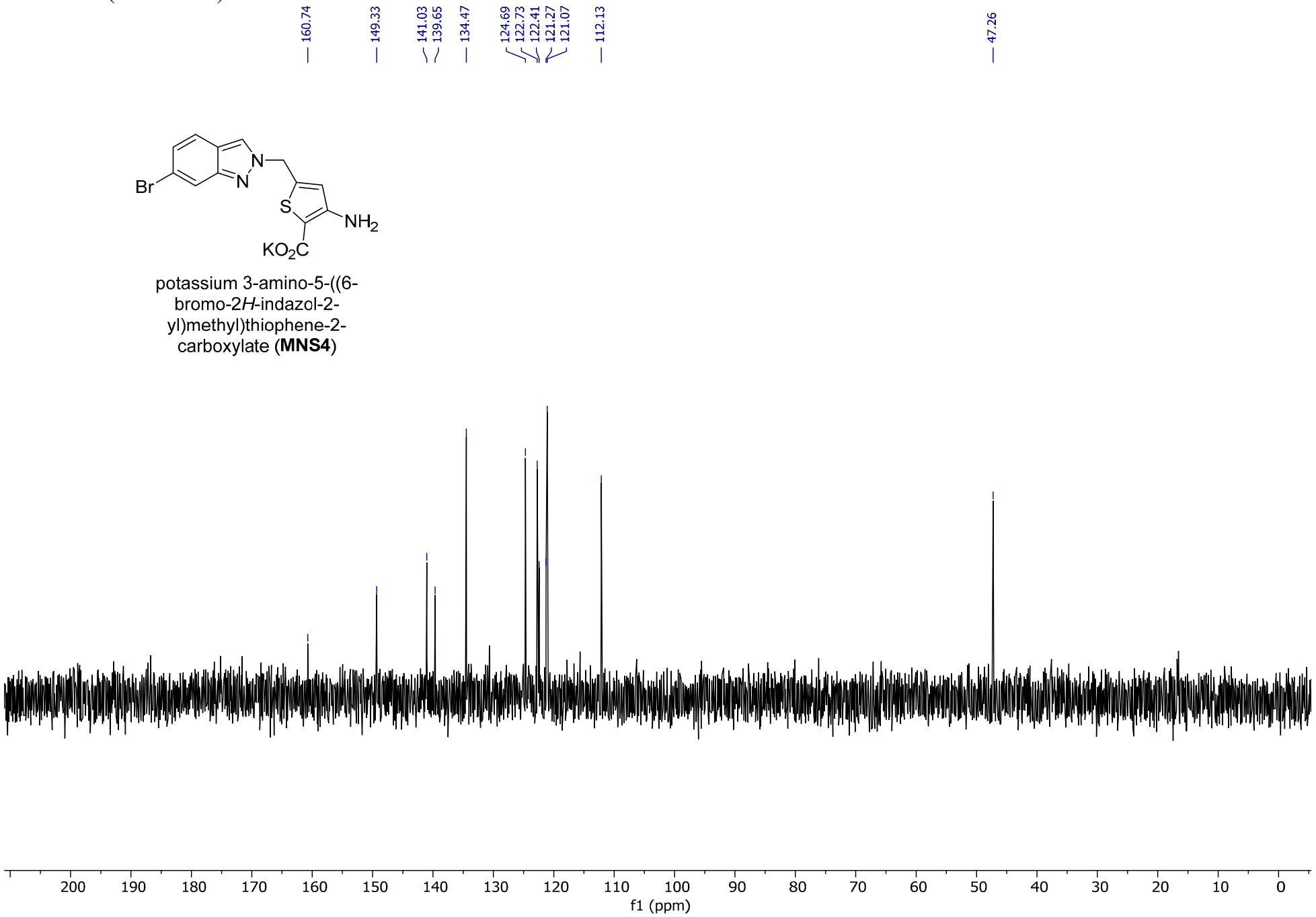
potassium 3-amino-5-((6-bromo-1*H*-indazol-1-yl)methyl)thiophene-2-carboxylate (**MNS3**)

^{1}H NMR (300 MHz) in D_2O



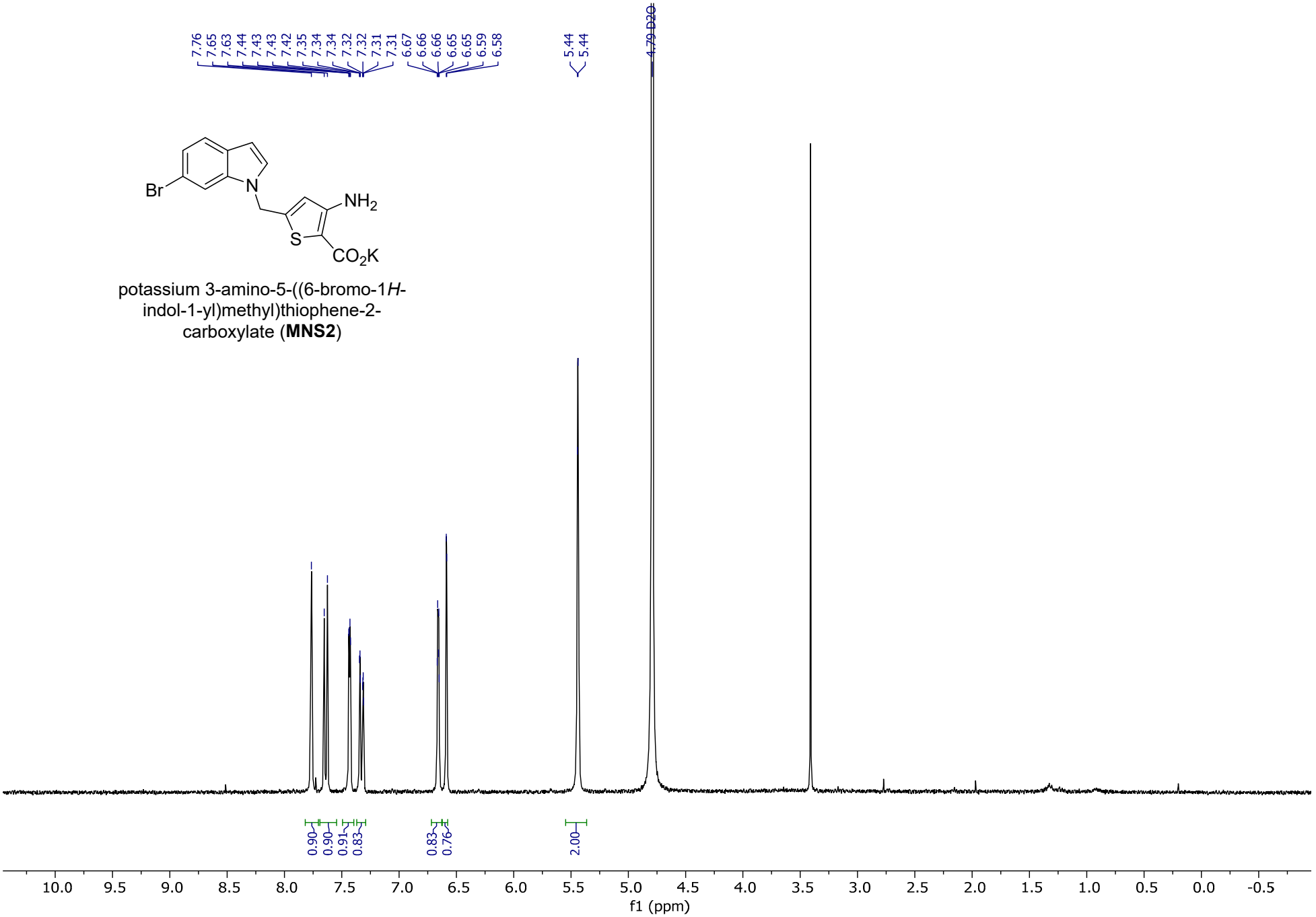
potassium 3-amino-5-((6-bromo-2*H*-indazol-2-yl)methyl)thiophene-2-carboxylate (**MNS4**)

^{13}C NMR (75.5 MHz) in D_2O



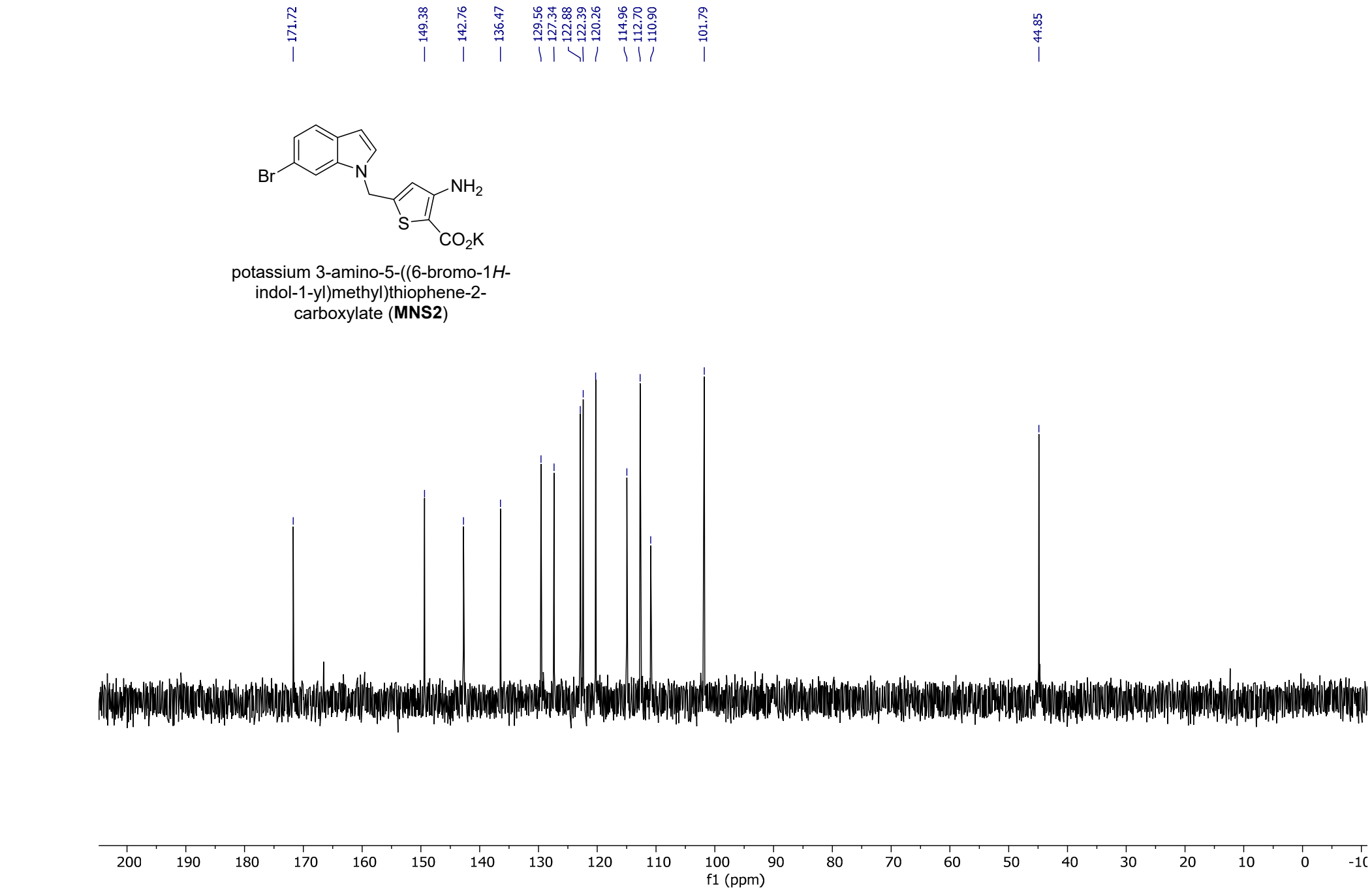
potassium 3-amino-5-((6-bromo-2*H*-indazol-2-yl)methyl)thiophene-2-carboxylate (**MNS4**)

^{1}H NMR (600 MHz) in D_2O



potassium 3-amino-5-((6-bromo-1*H*-indol-1-yl)methyl)thiophene-2-carboxylate (**MNS2**)

^{13}C NMR (151 MHz) in D_2O



potassium 3-amino-5-((6-bromo-1*H*-indol-1-yl)methyl)thiophene-2-carboxylate (**MNS2**)