

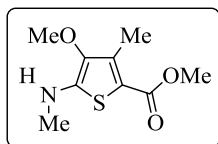
Supporting Information

A One-Pot Assembly of Fully Substituted Alkyl 5-Aminothiophene-2-carboxylates from Allenes, Isothiocyanates, and Alkyl 2-Bromoacetates

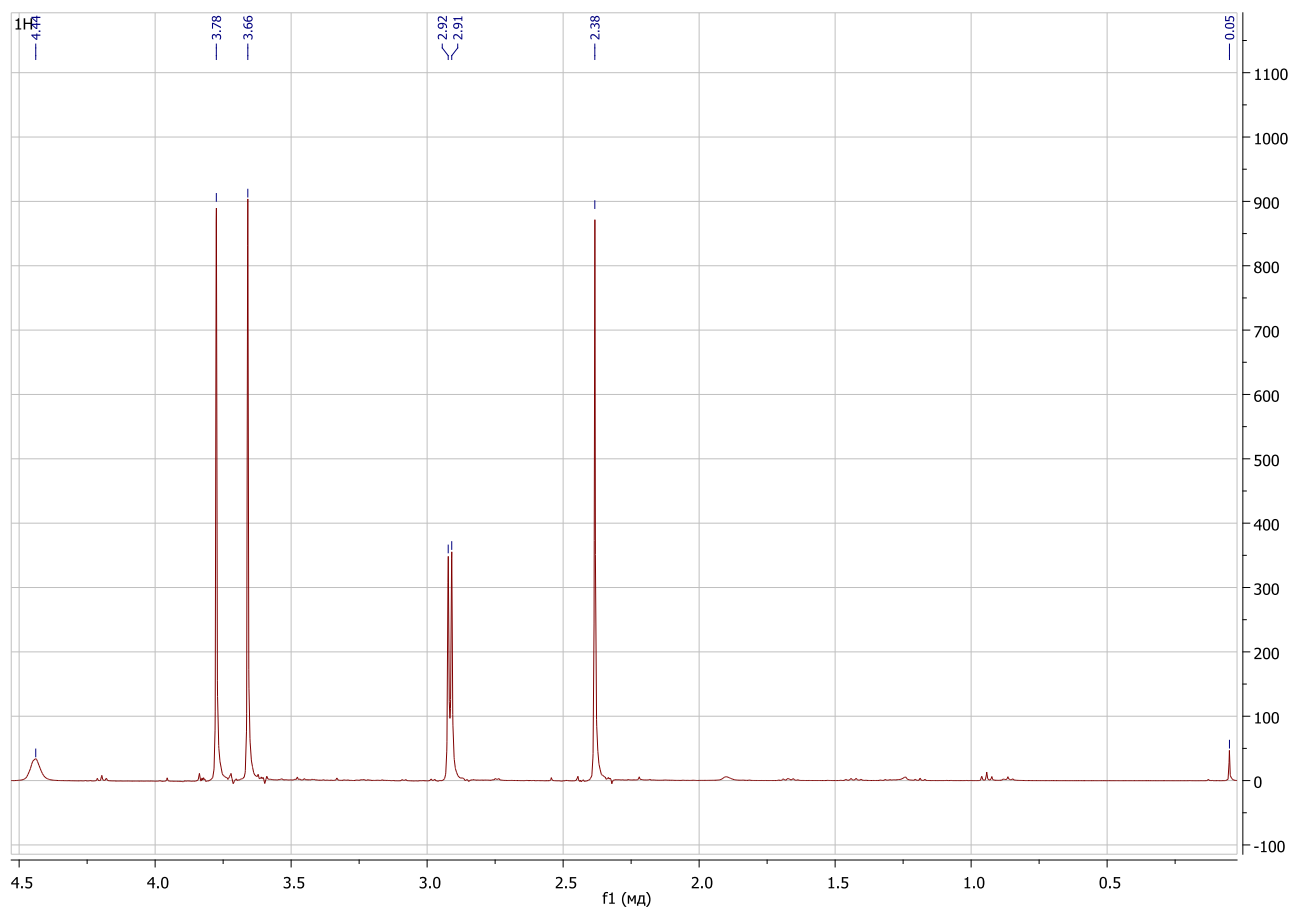
Nina A. Nedolya,* Ol'ga A. Tarasova, Alexander I. Albanov, and Boris A. Trofimov*

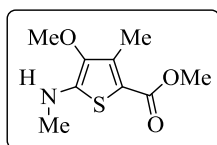
*A. E. Favorsky Irkutsk Institute of Chemistry of the Russian Academy of Sciences, Siberian Branch,
Favorsky Street 1, 664033 Irkutsk, Russia*

Fax +7(3952)419346; E-mails: nina@irioch.irk.ru; boris_trofimov@irioch.irk.ru

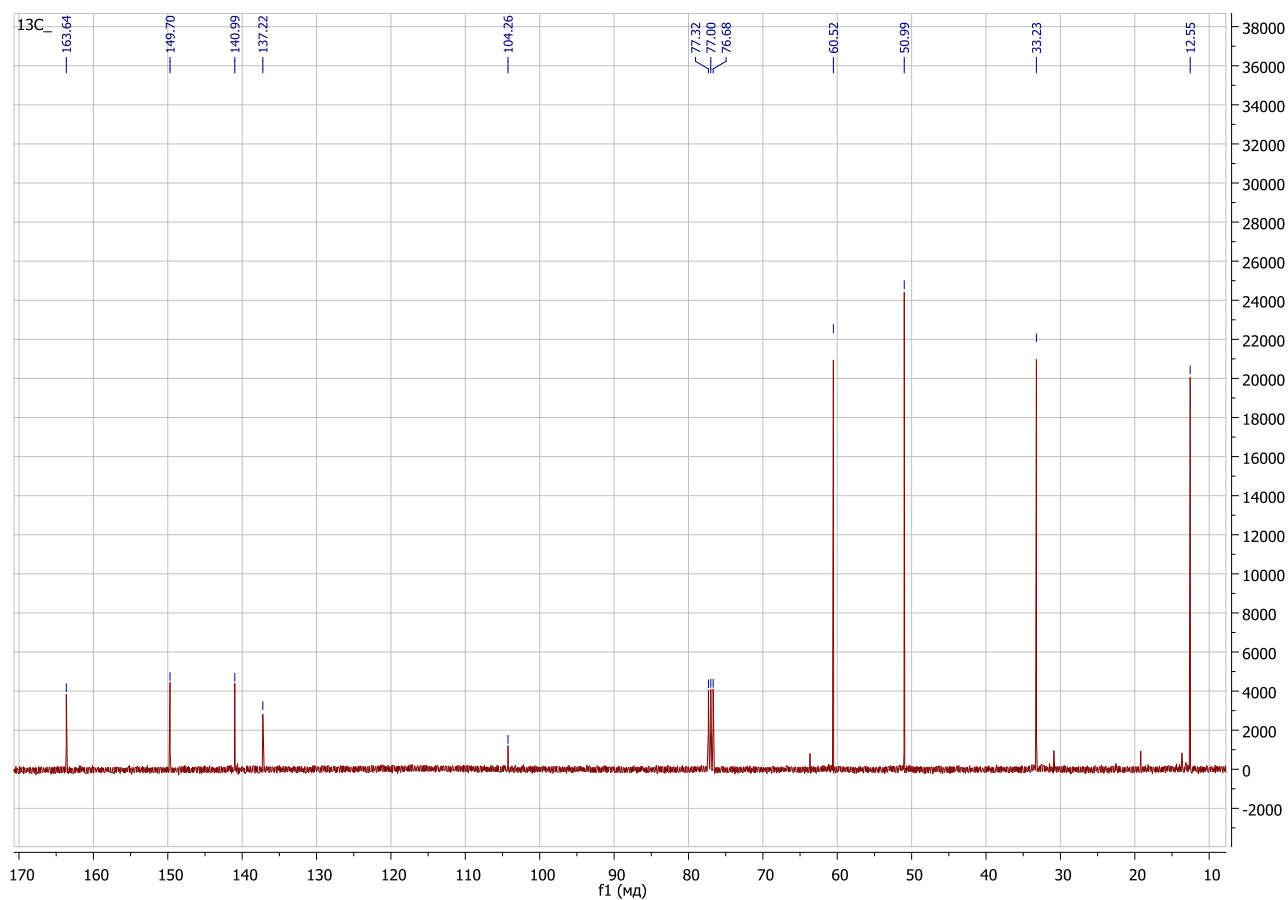


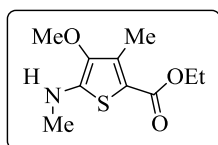
¹H NMR Spectrum of Methyl 4-methoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2a)



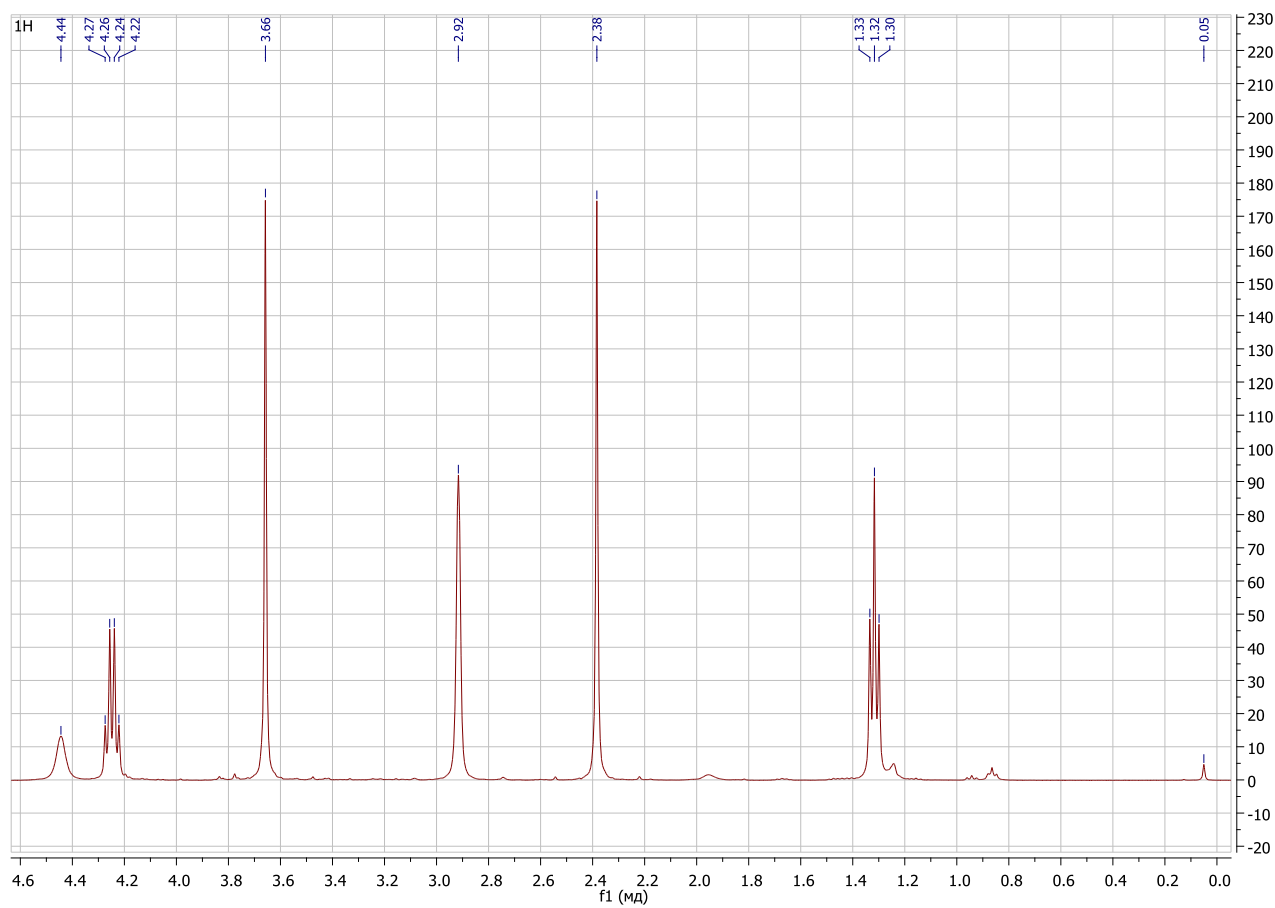


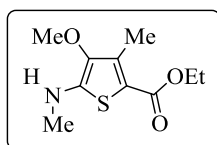
^{13}C NMR Spectrum of Methyl 4-methoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2a)



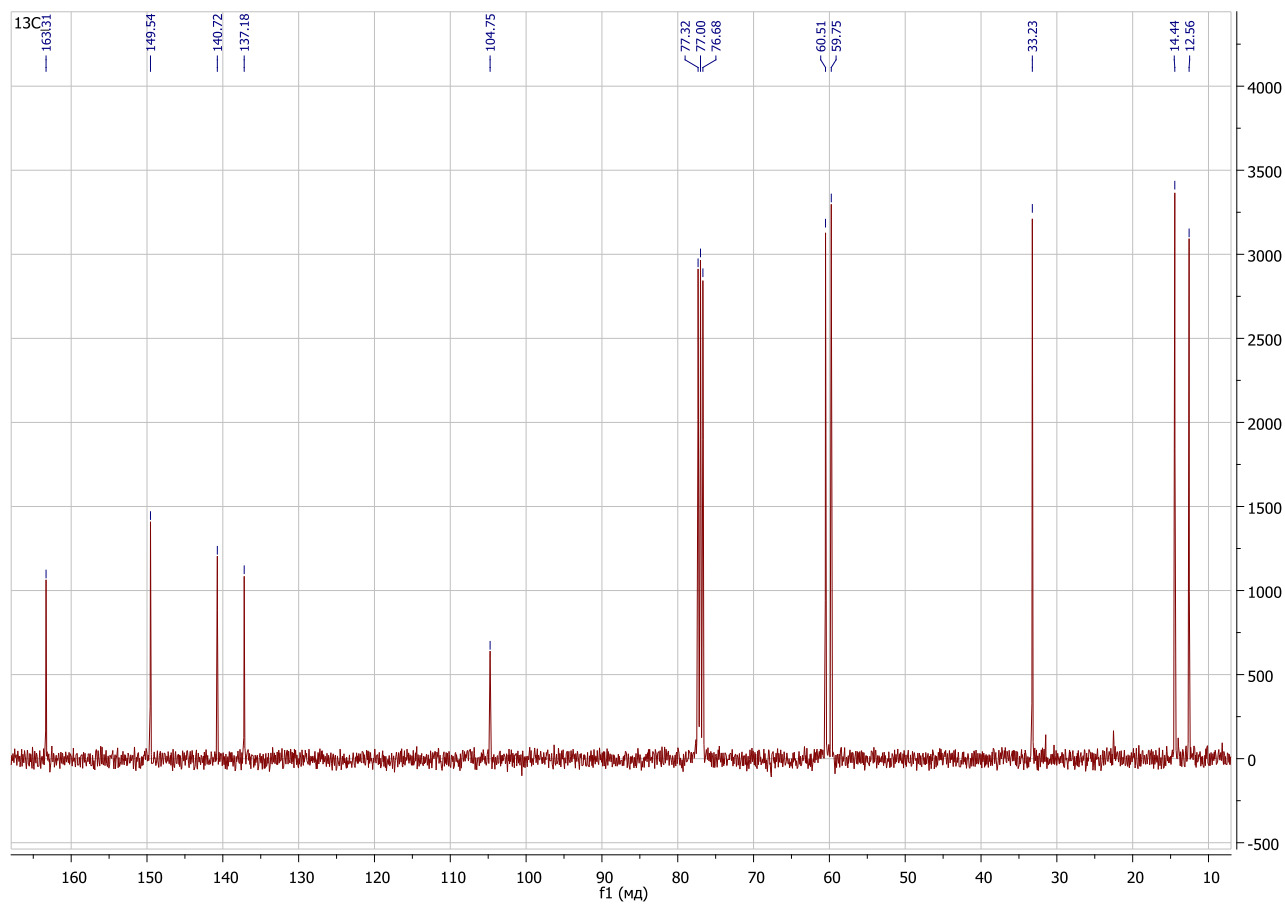


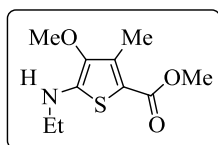
¹H NMR Spectrum of Ethyl 4-methoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2b)



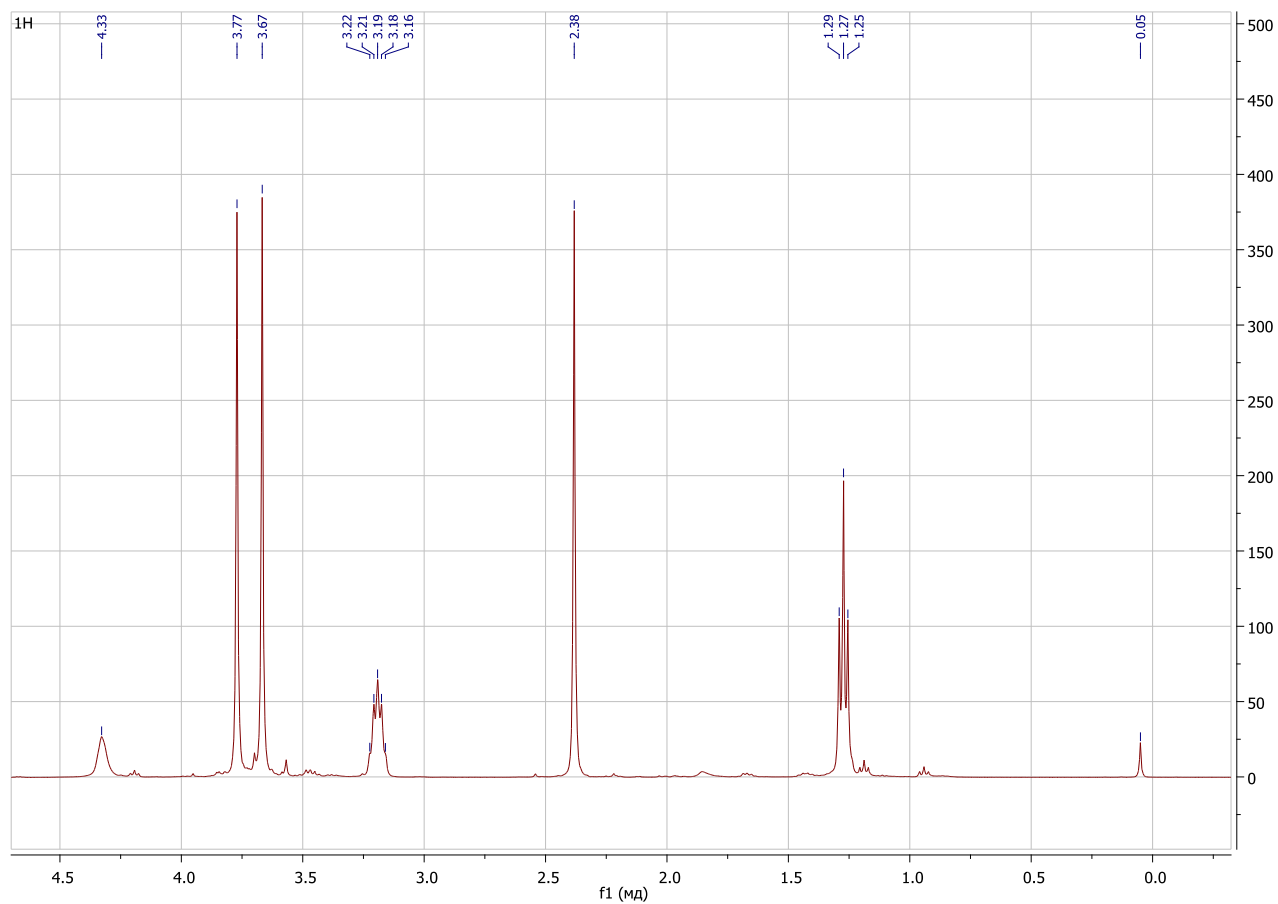


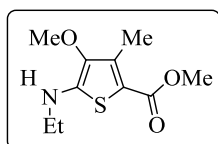
^{13}C NMR Spectrum of Ethyl 4-methoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2b)



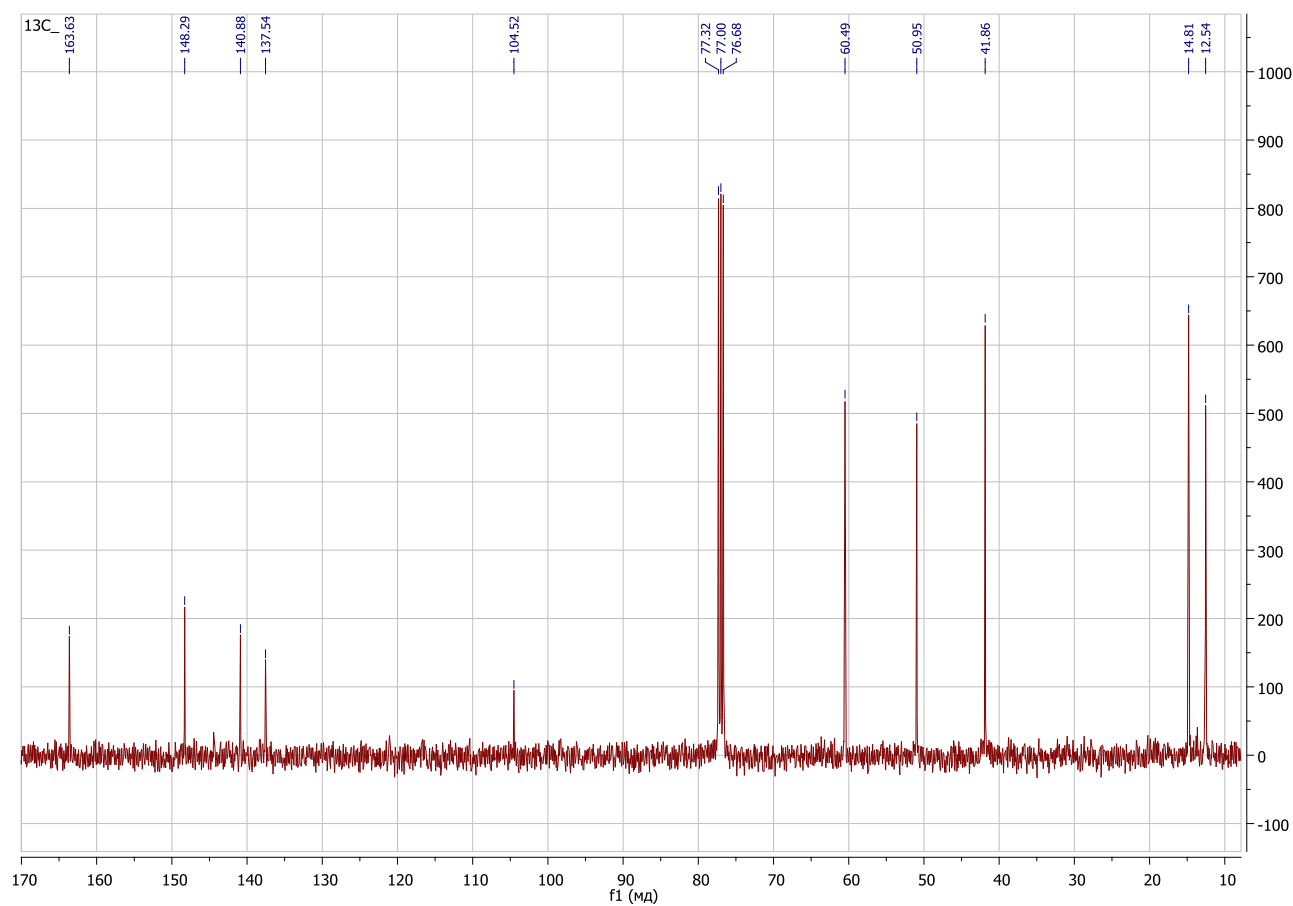


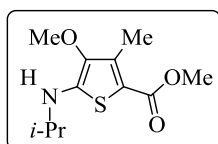
¹H NMR Spectrum of Methyl 5-(ethylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2c)



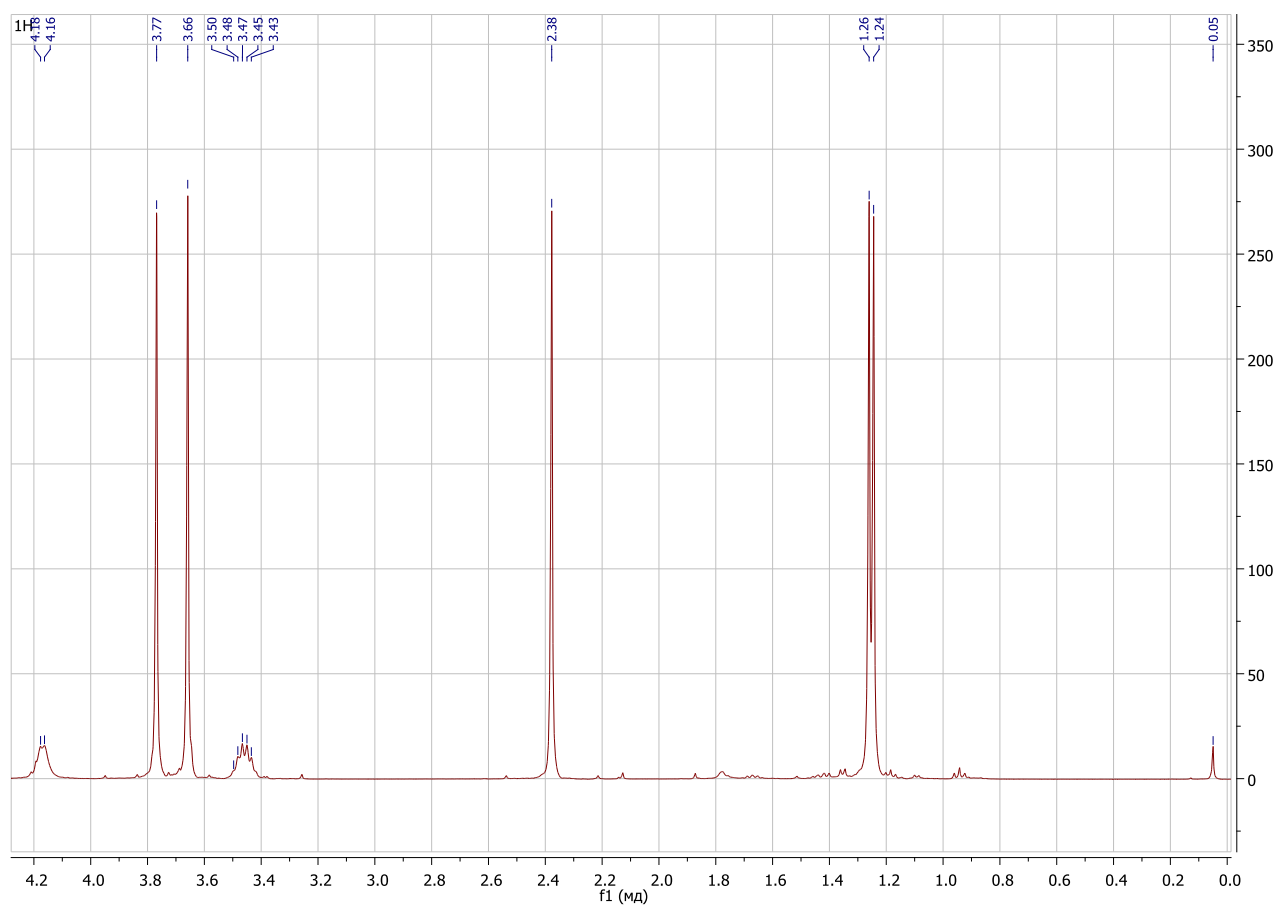


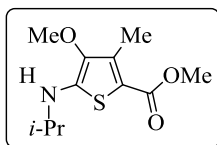
^{13}C NMR Spectrum of Methyl 5-(ethylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2c)



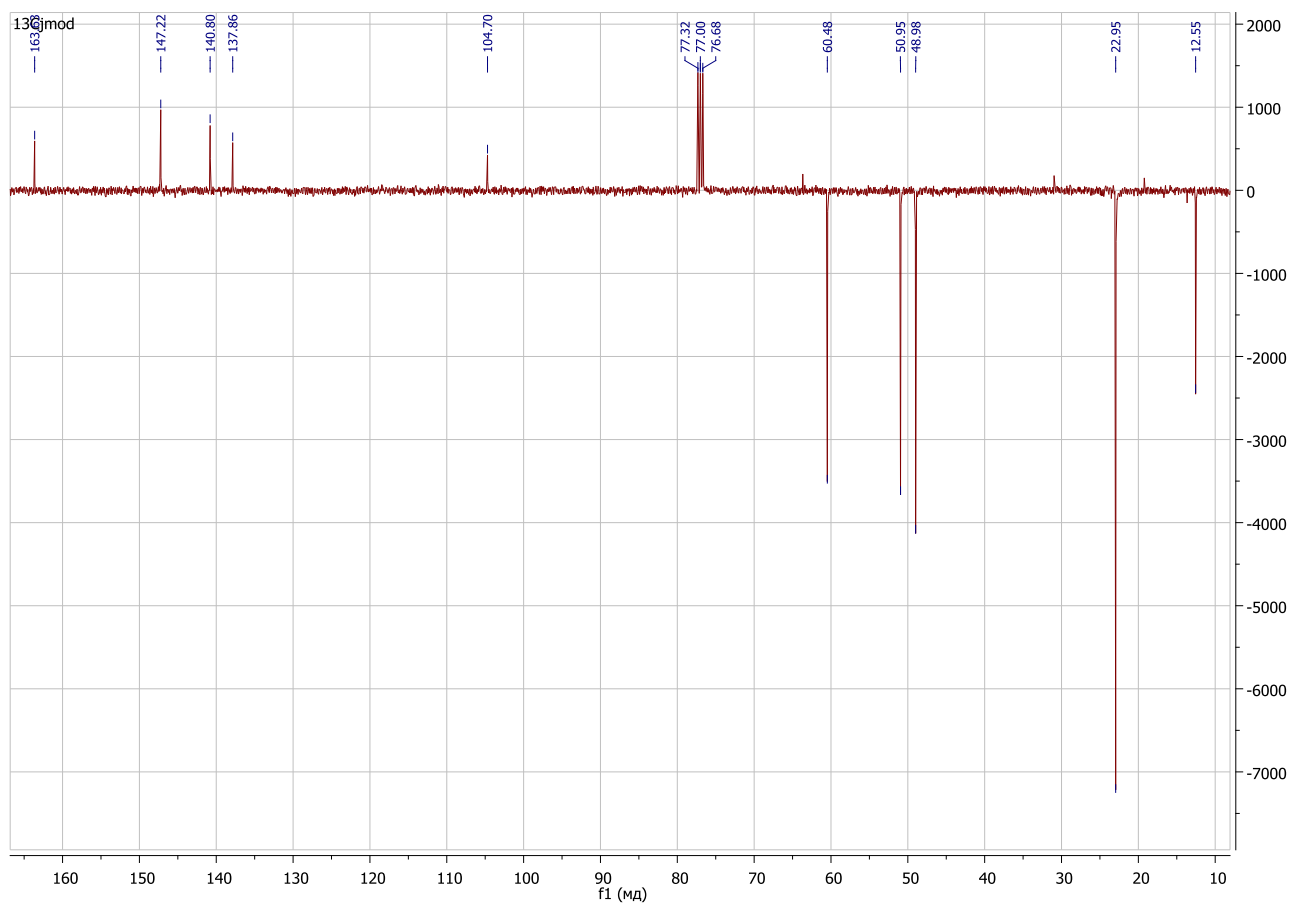


^1H NMR Spectrum of Methyl 5-(isopropylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2d)

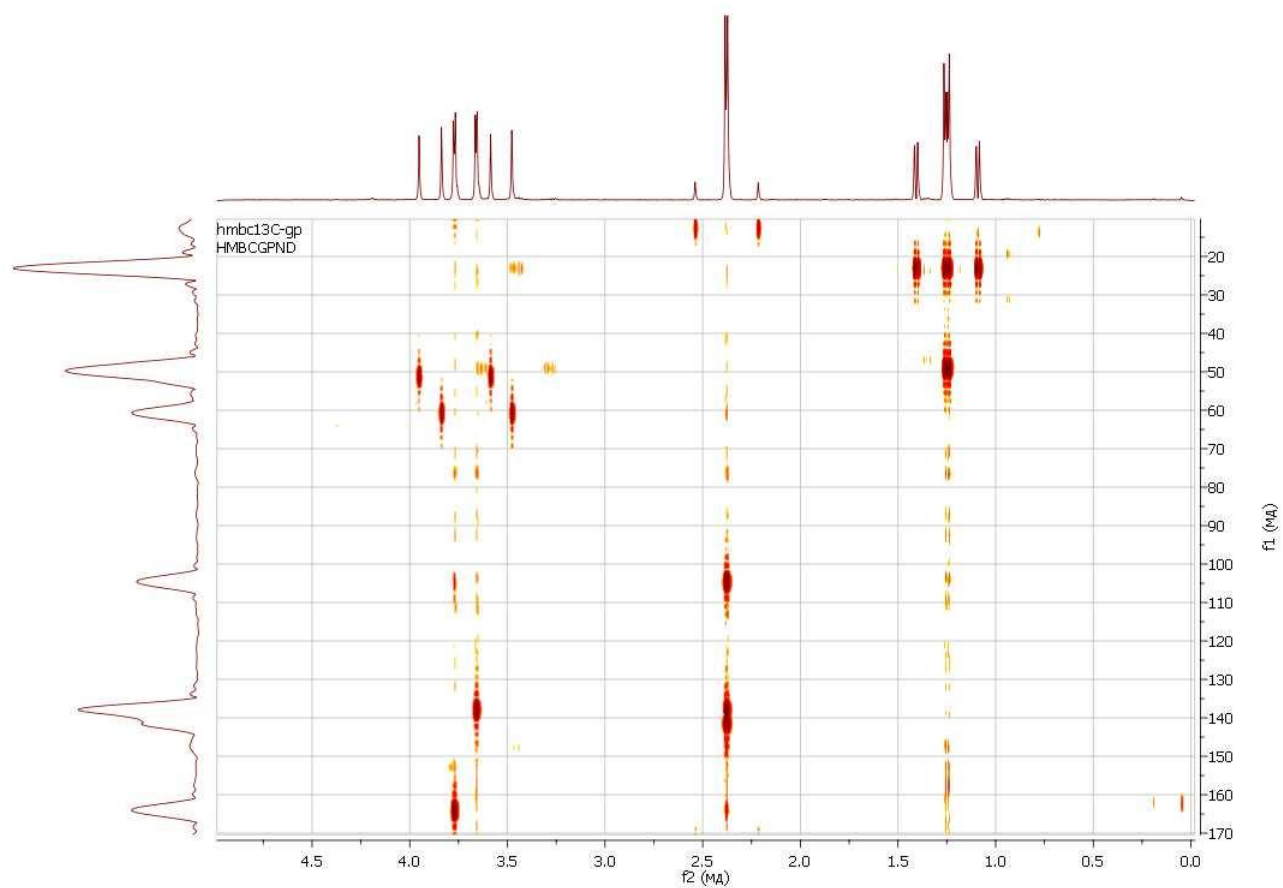


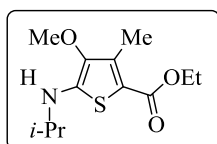


^{13}C NMR Spectrum of Methyl 5-(isopropylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2d)

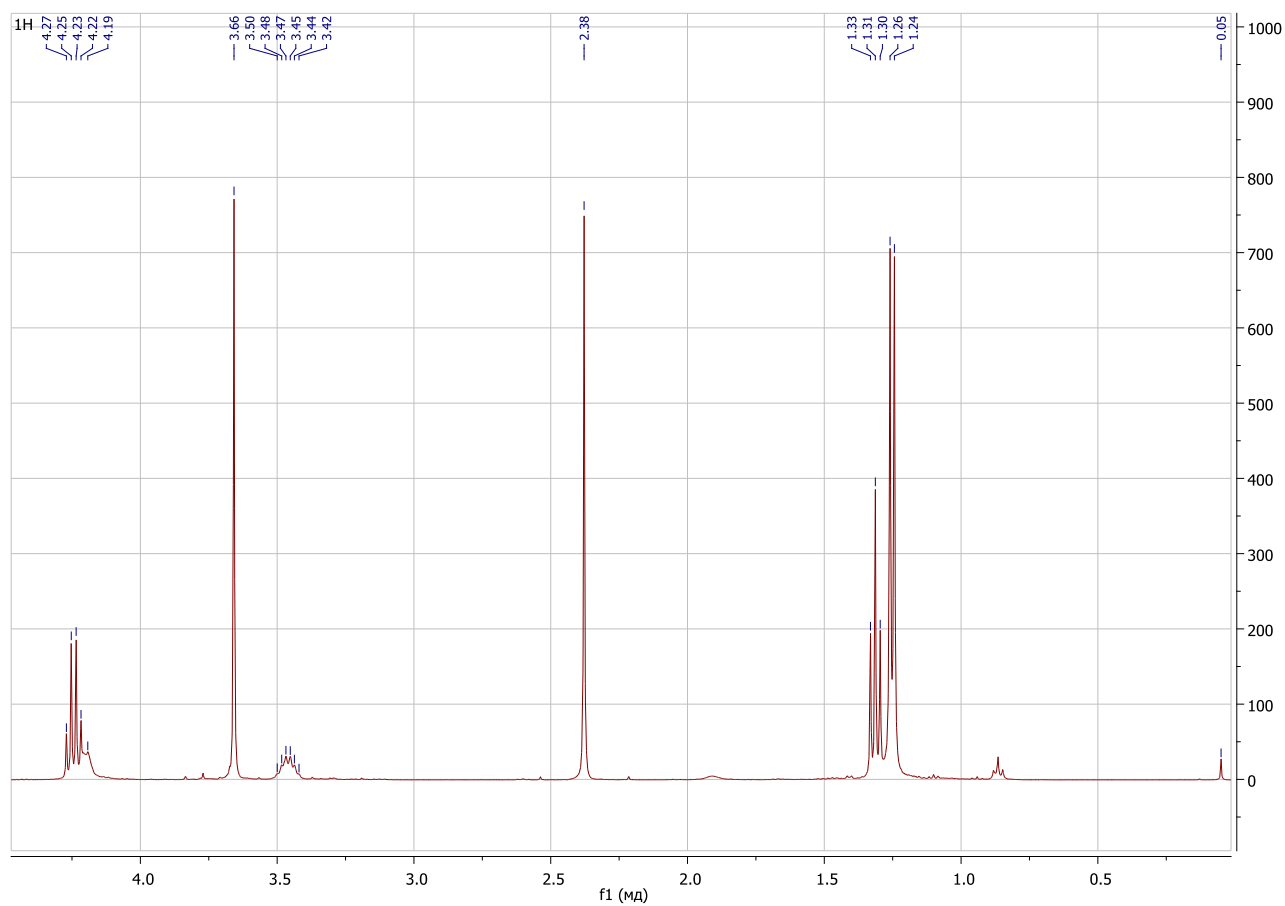


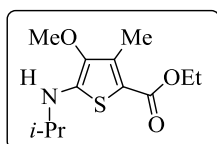
^1H - ^{13}C -HMBC Spectrum of compound **2d**:



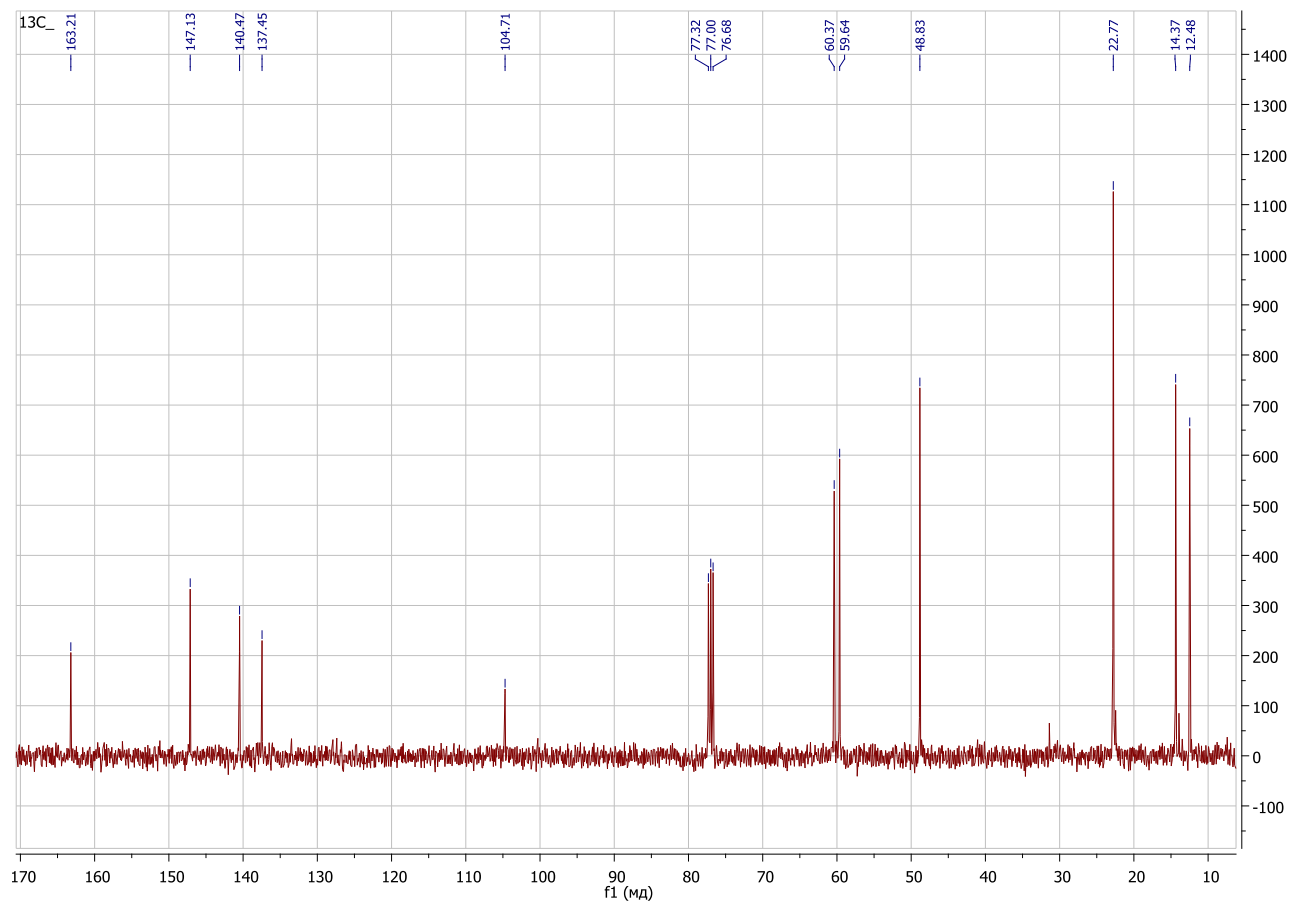


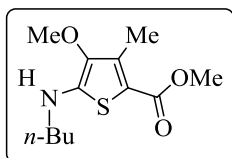
^1H NMR Spectrum of Ethyl 5-(isopropylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2e)



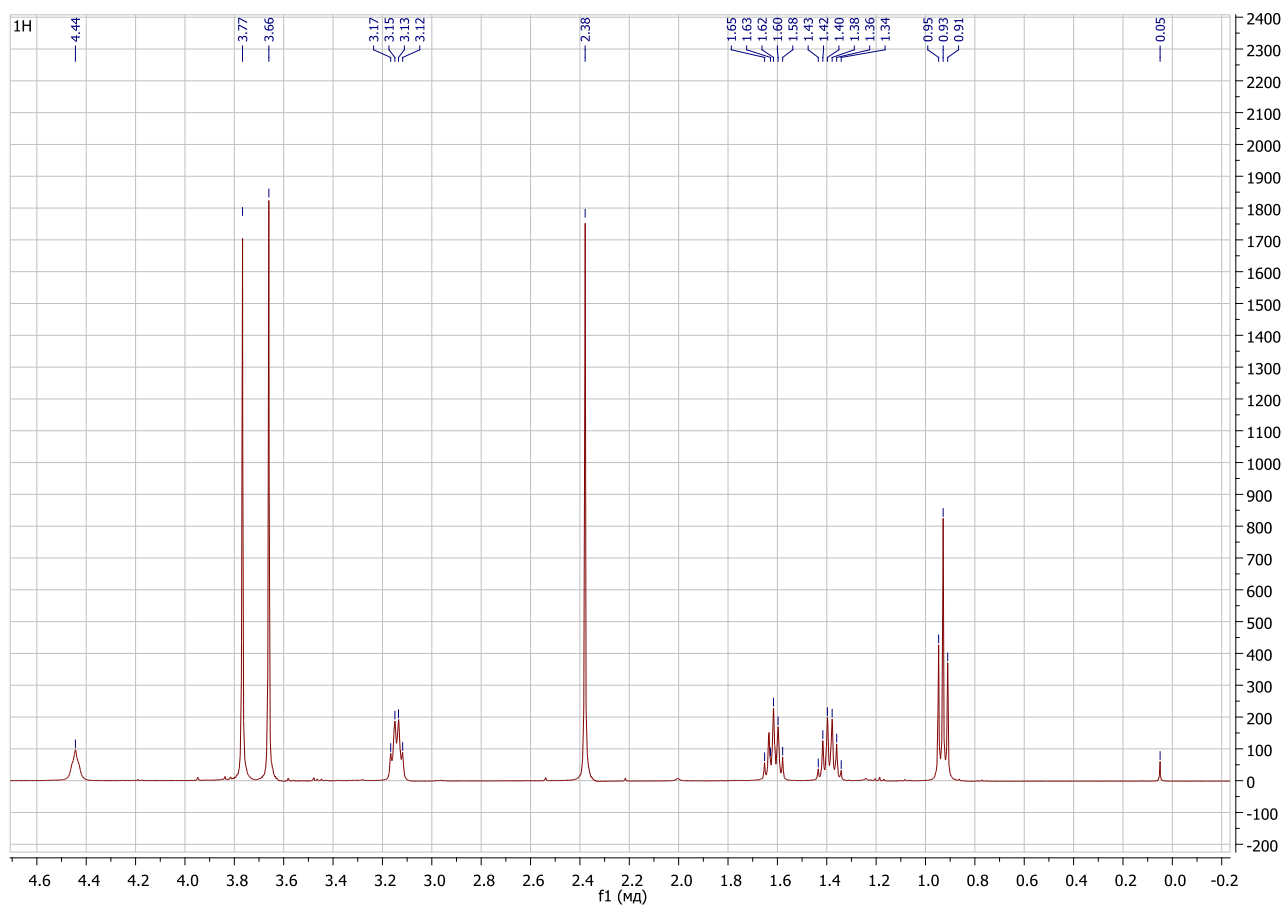


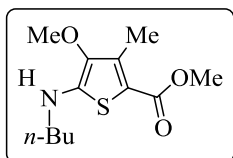
^{13}C NMR Spectrum of Ethyl 5-(isopropylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2e)



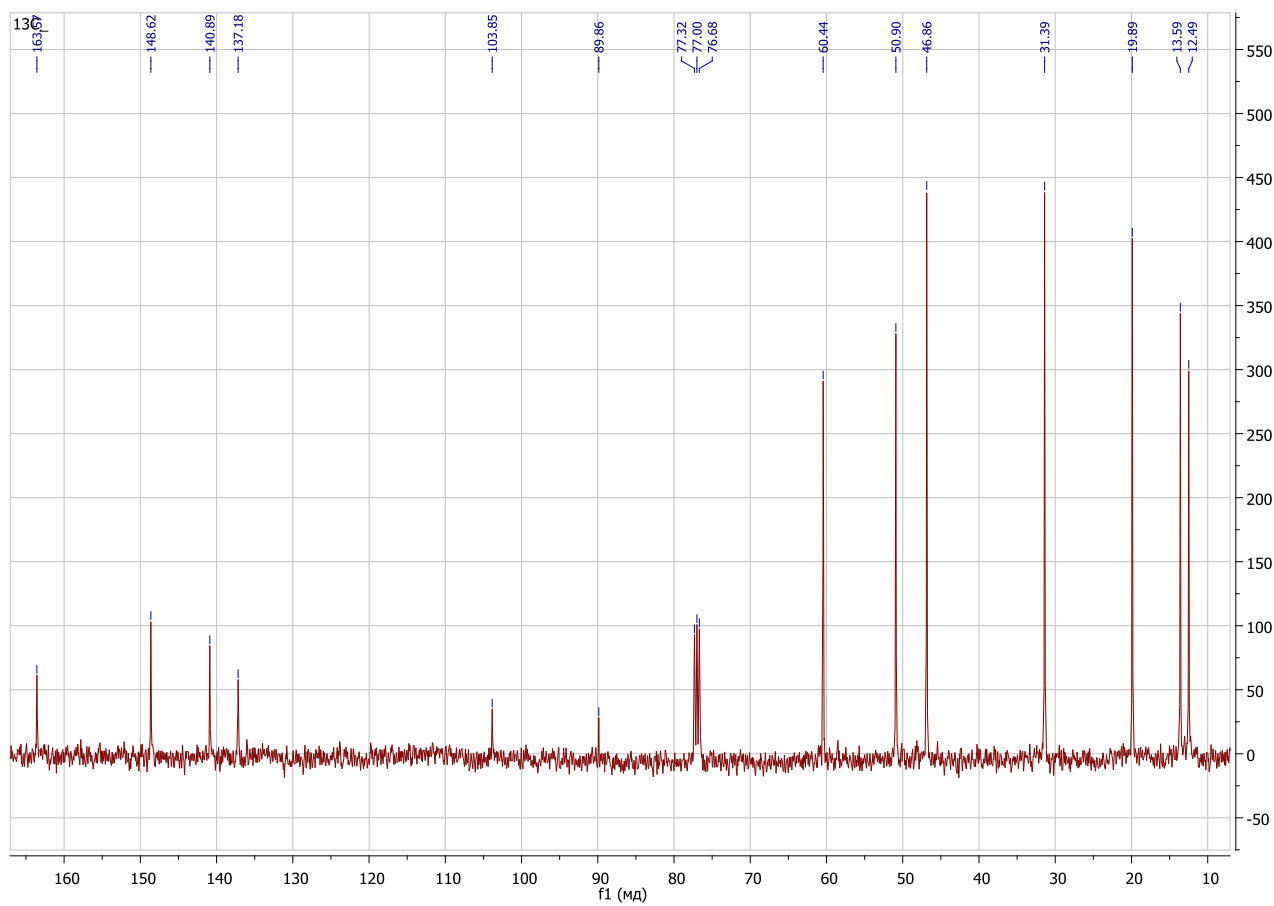


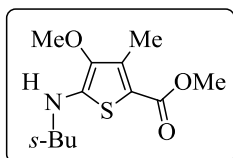
^1H NMR Spectrum of Methyl 5-(*n*-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2f)



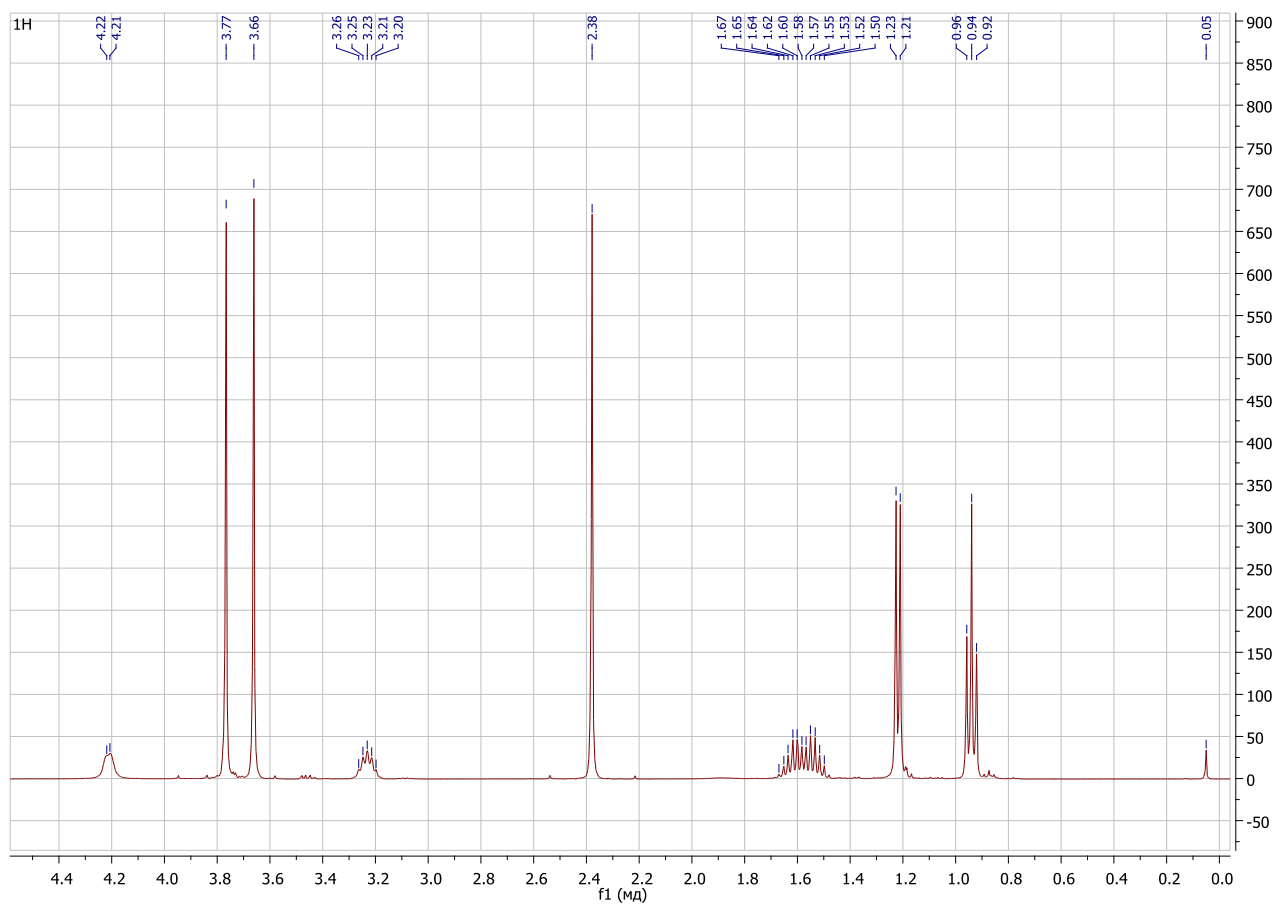


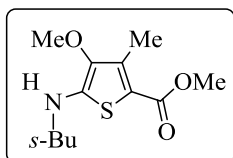
^{13}C NMR Spectrum of Methyl 5-(*n*-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2f)



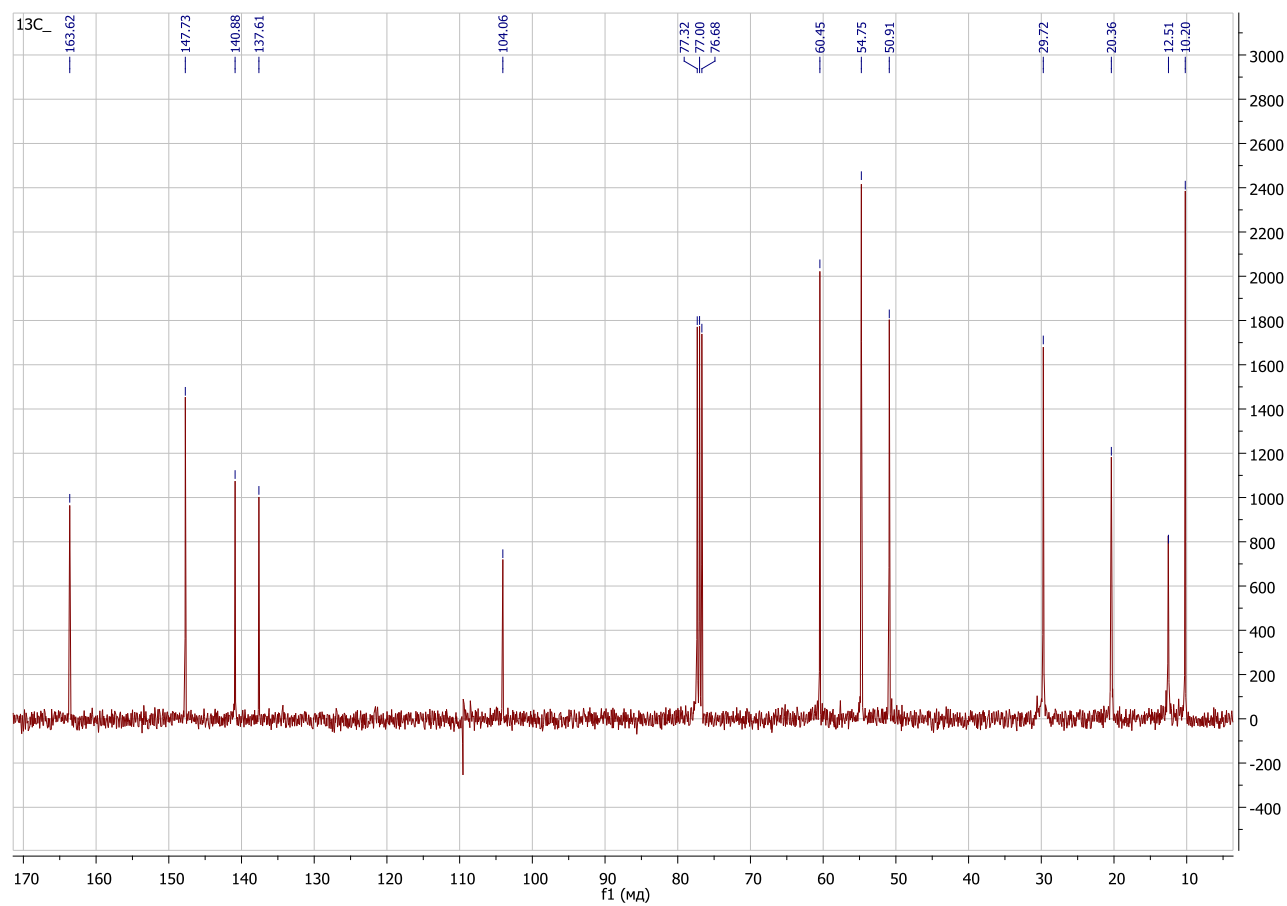


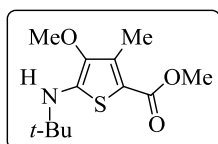
^1H NMR Spectrum of Methyl 5-(s-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2g)



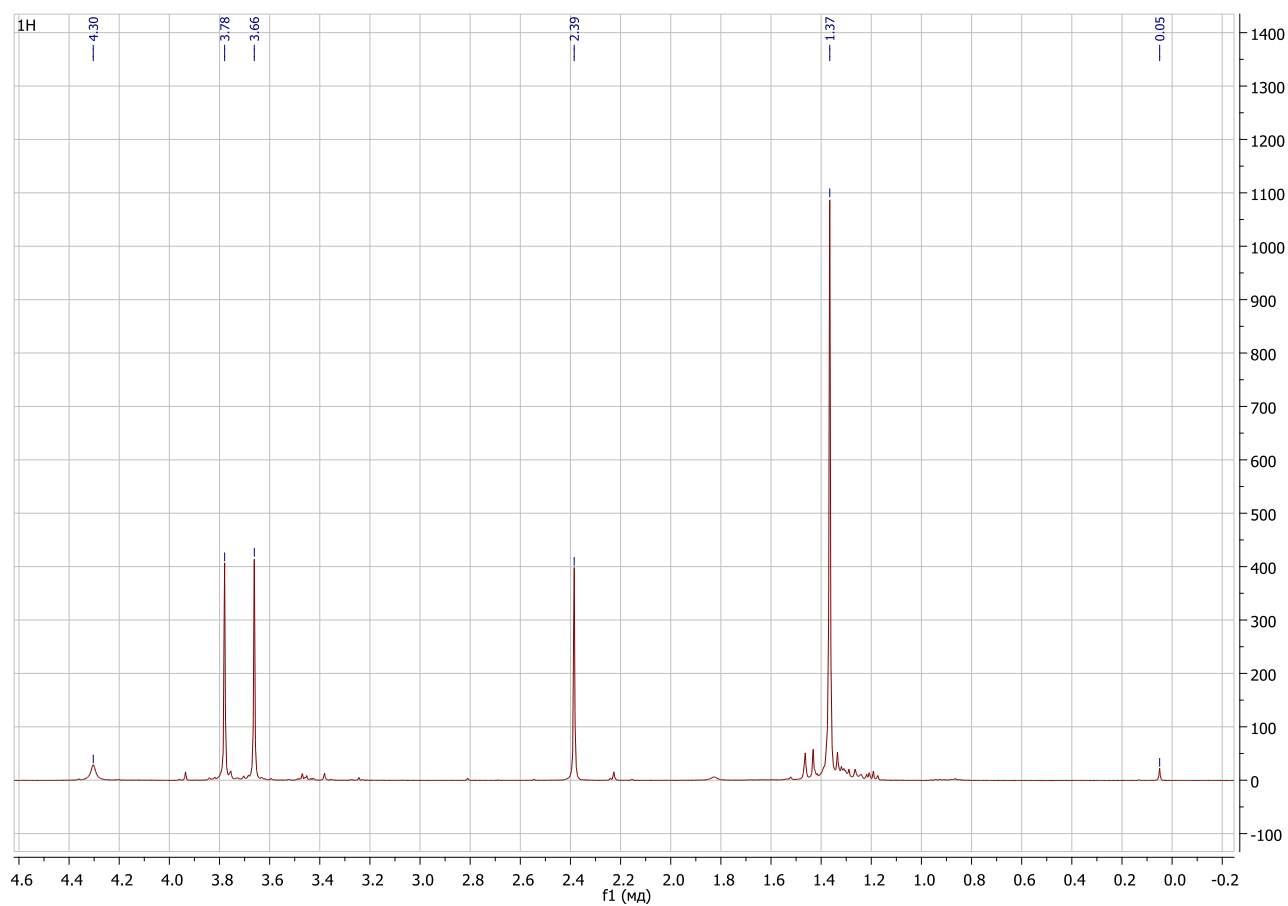


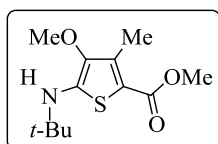
^{13}C NMR Spectrum of Methyl 5-(s-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2g)



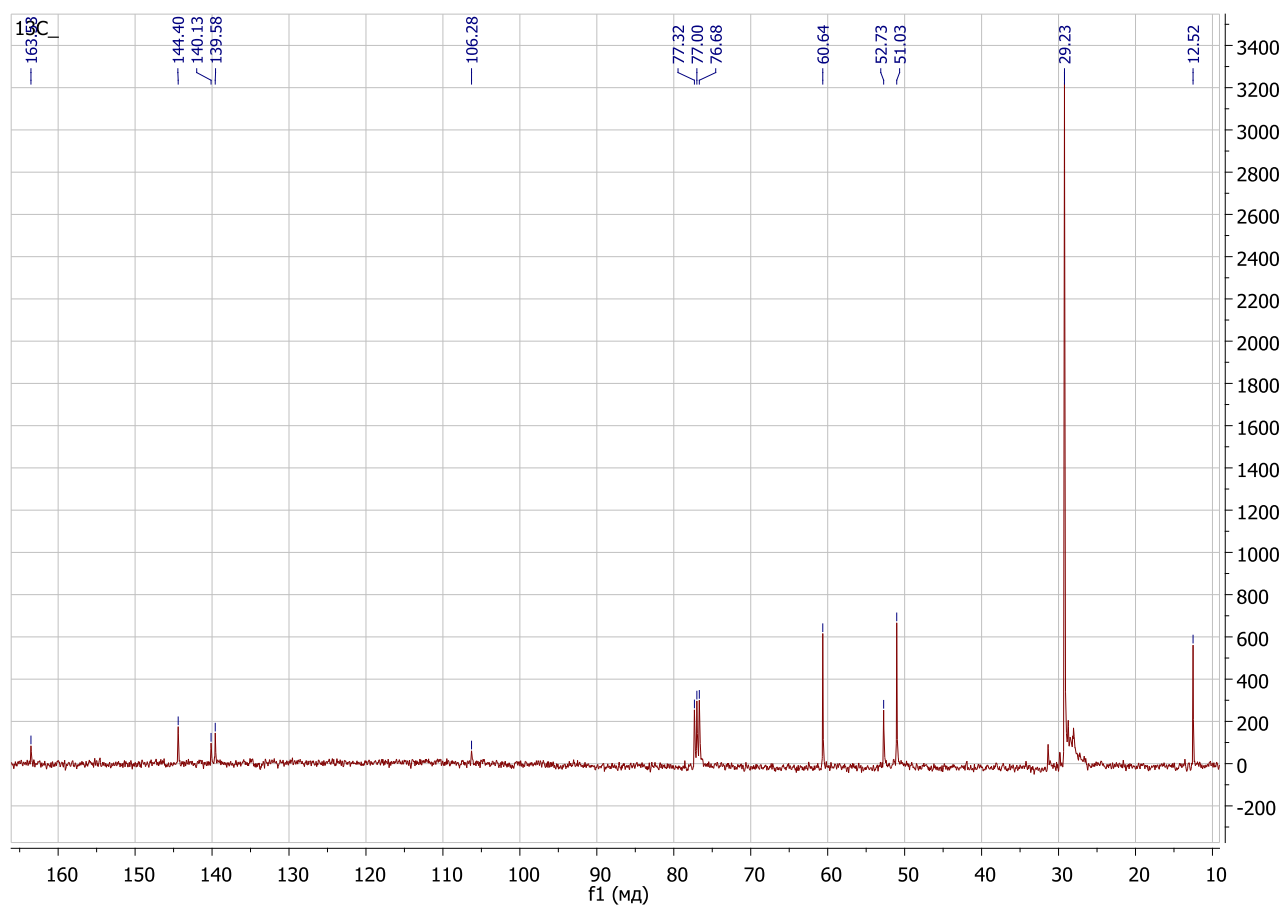


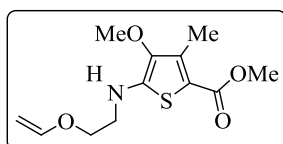
¹H NMR Spectrum of Methyl 5-(*tert*-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2h)



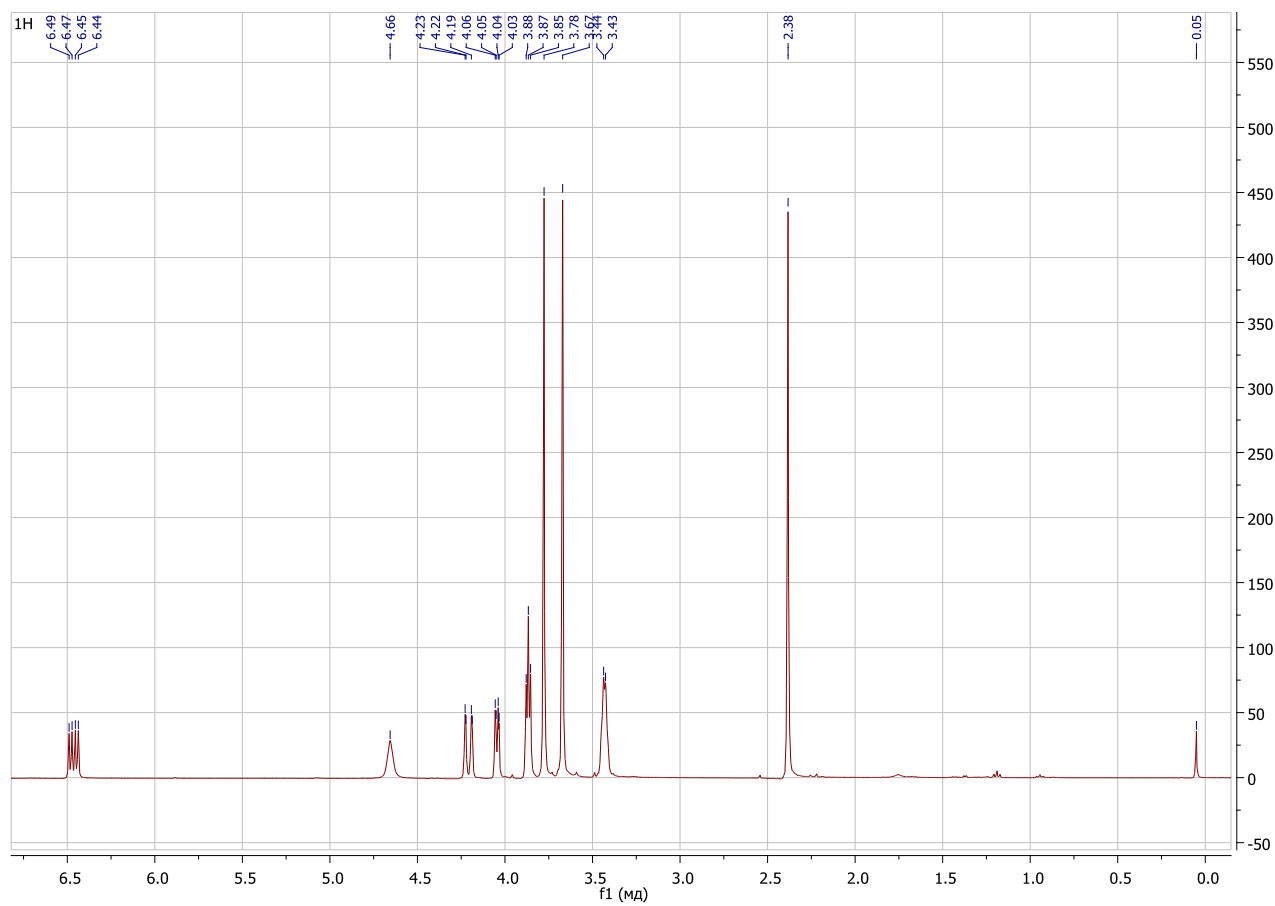


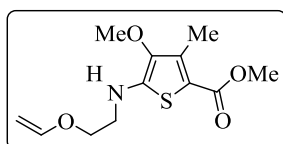
^{13}C NMR Spectrum of Methyl 5-(*tert*-butylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2h)



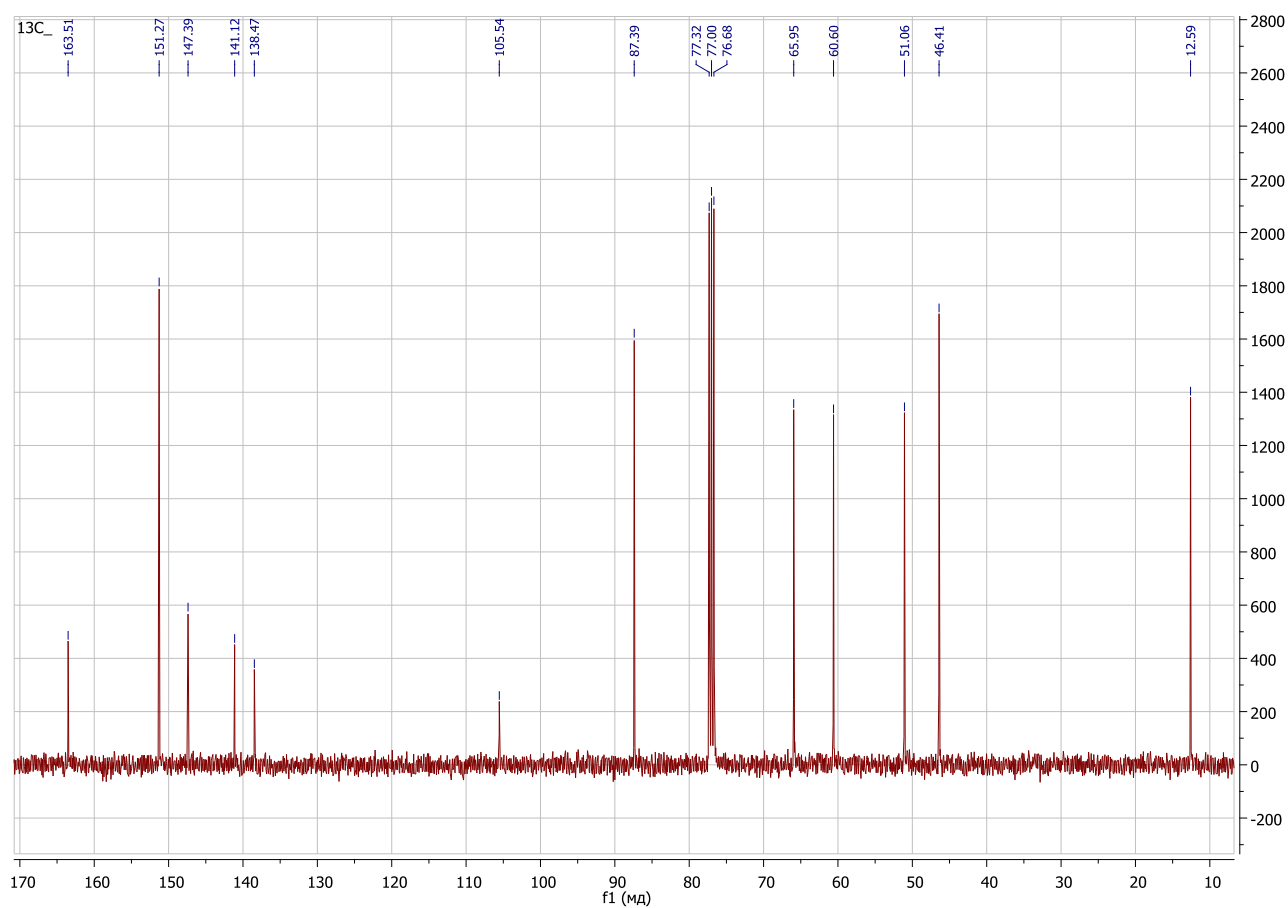


^1H NMR Spectrum of Methyl 4-methoxy-3-methyl-5-([2-(vinylloxy)ethyl]amino)thiophene-2-carboxylate (2i)

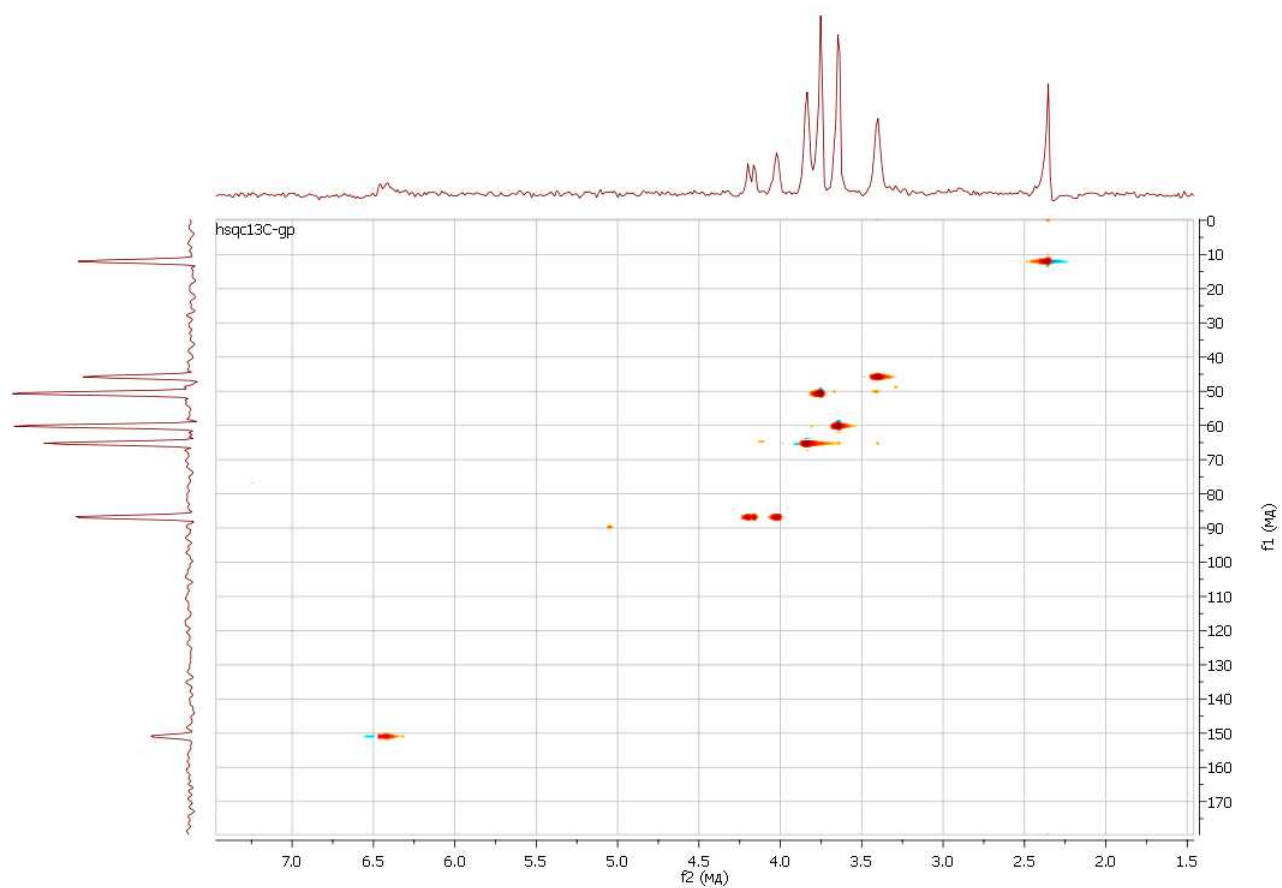


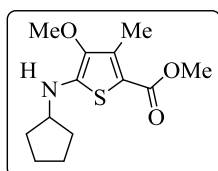


^{13}C NMR Spectrum of Methyl 4-methoxy-3-methyl-5-([2-(vinylloxy)ethyl]amino)thiophene-2-carboxylate (2i)

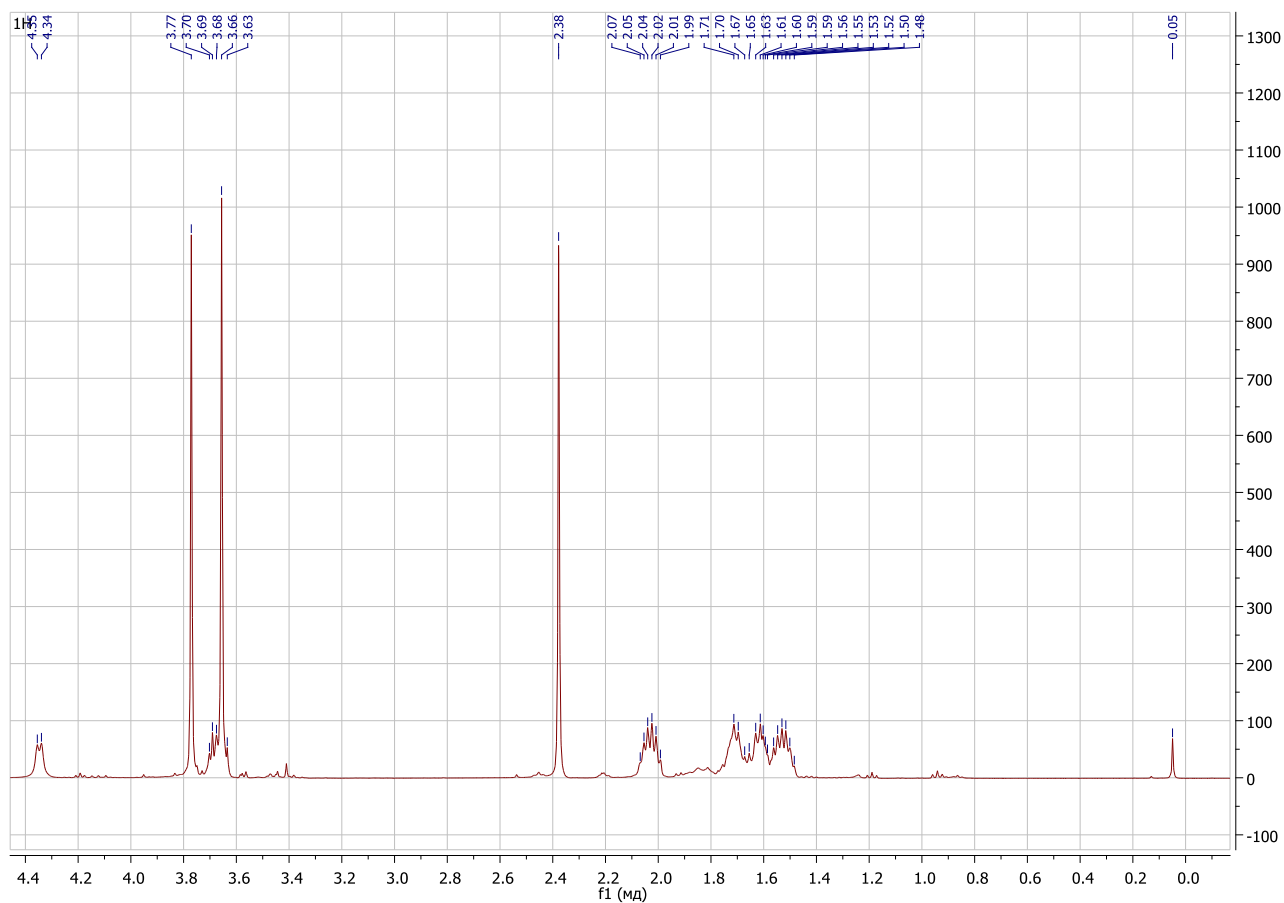


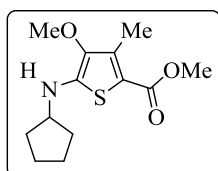
^1H - ^{13}C -HSQC Spectrum of compound **2i**:



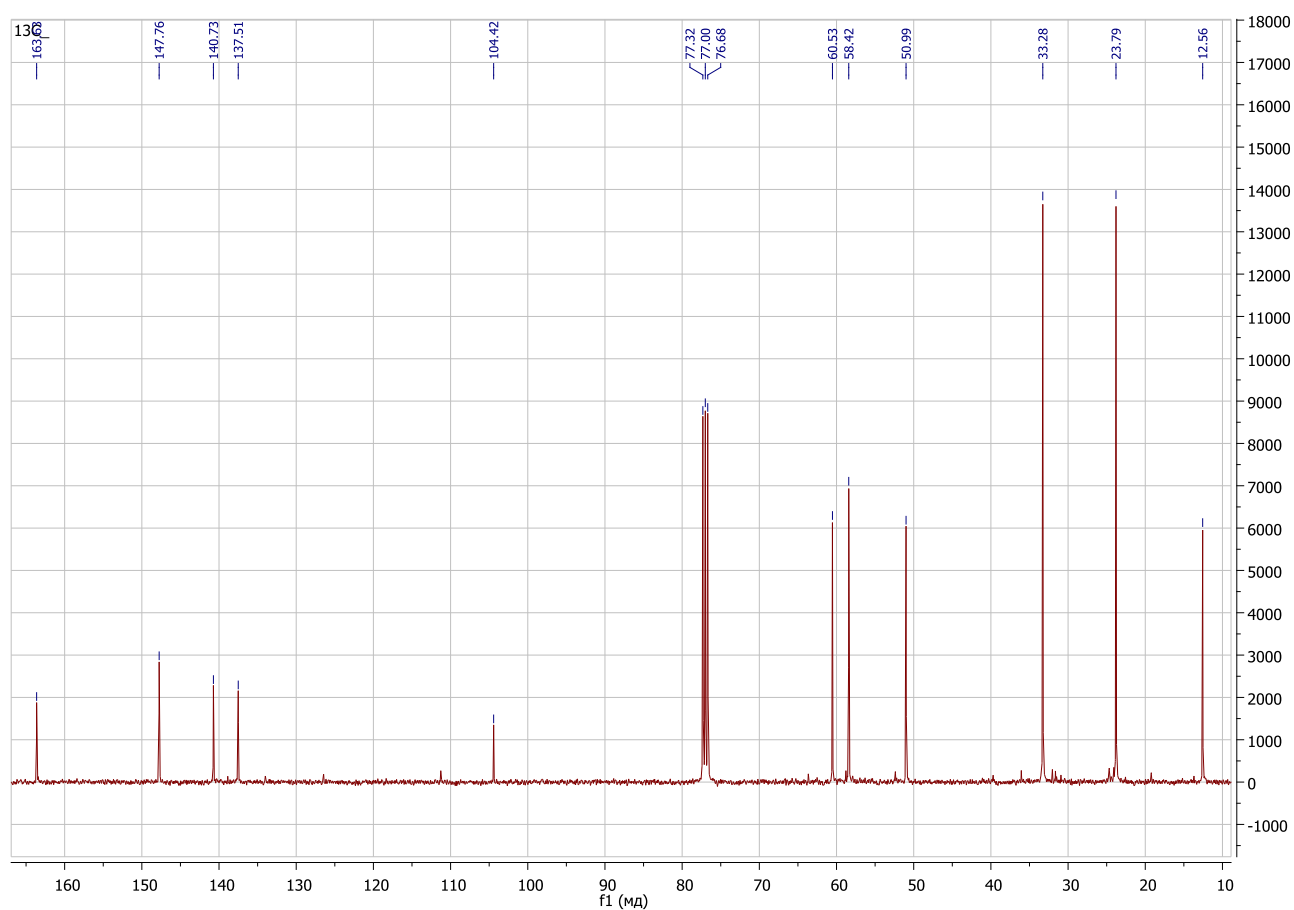


¹H NMR Spectrum of Methyl 5-(cyclopentylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2j)

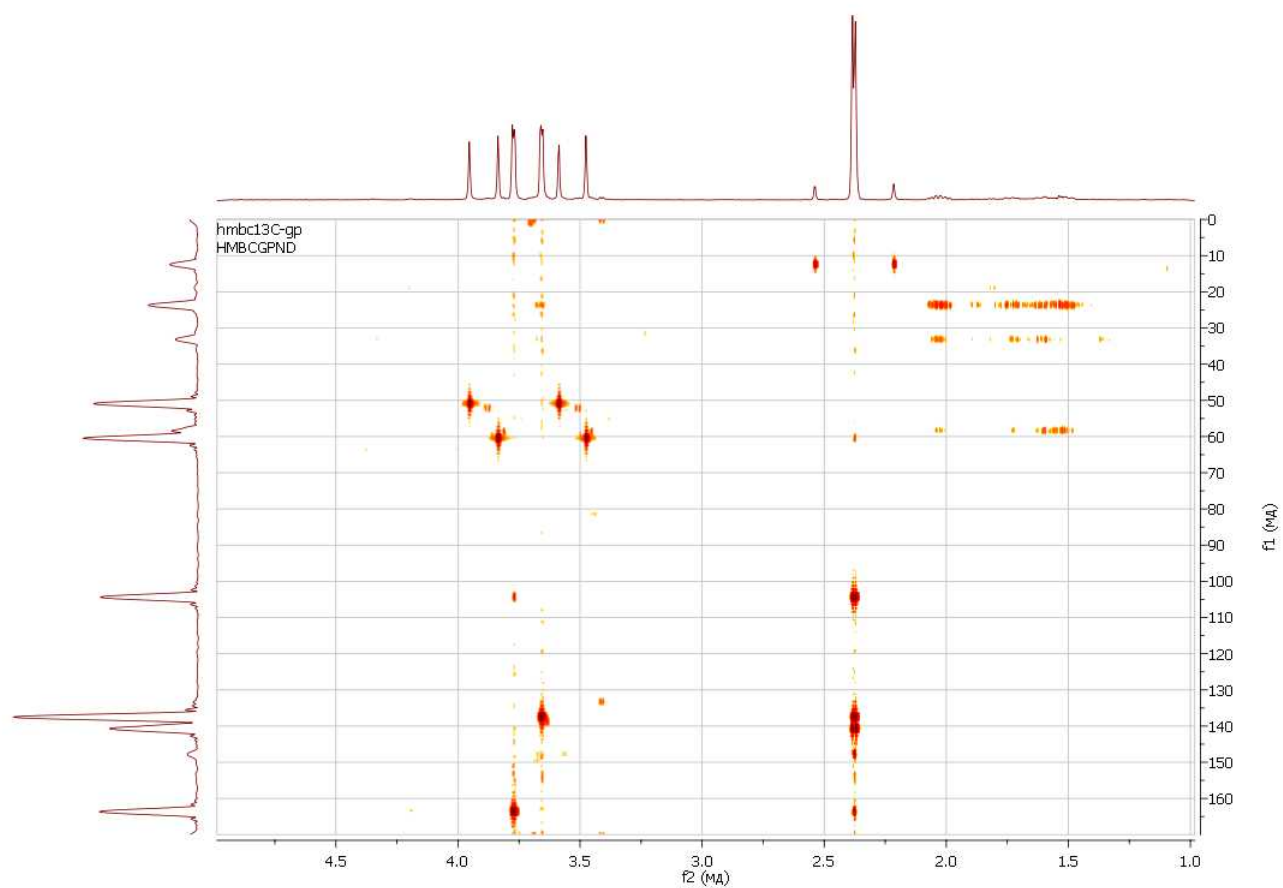


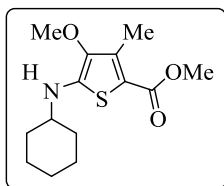


^{13}C NMR Spectrum of Methyl 5-(cyclopentylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2j)

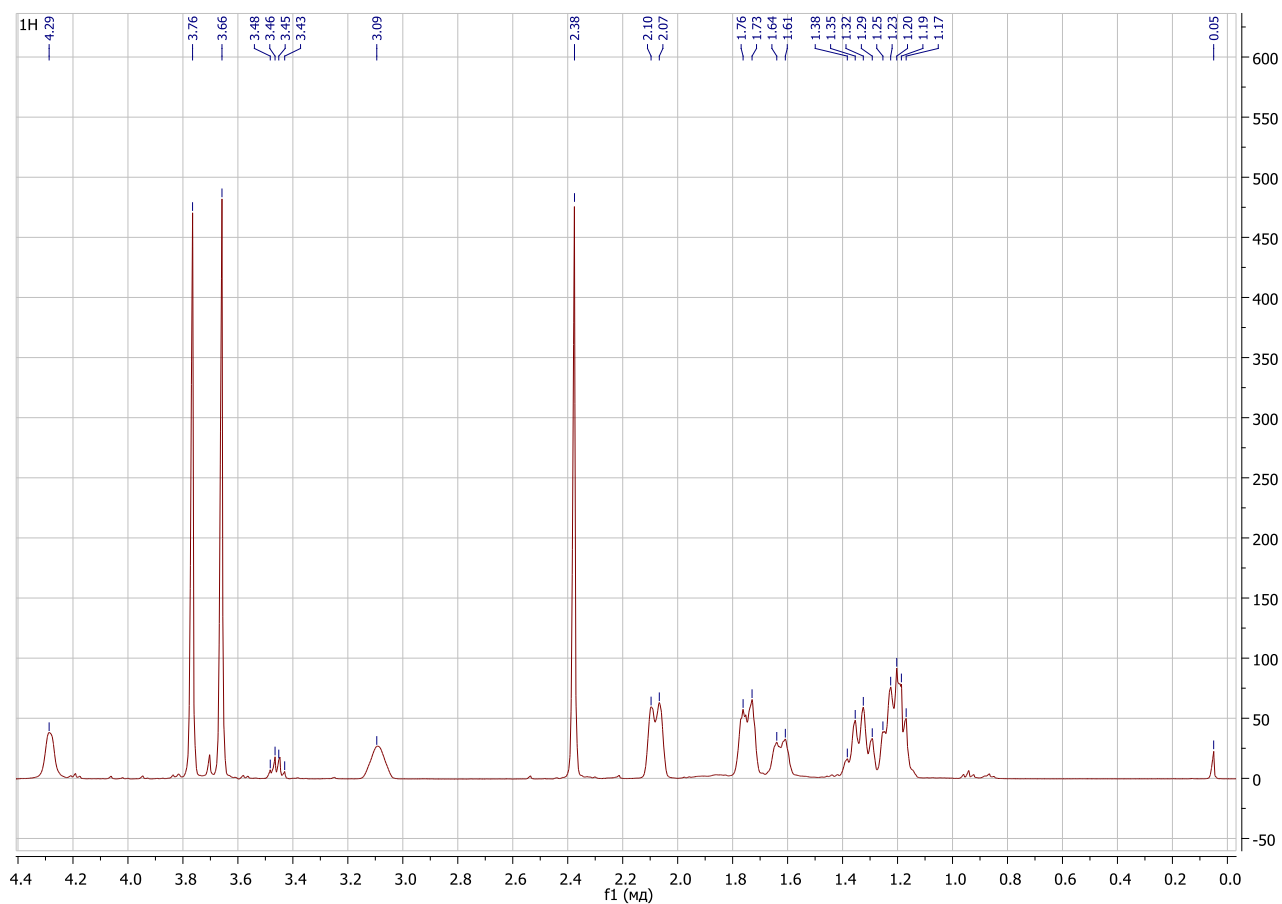


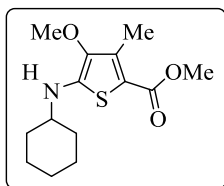
^1H - ^{13}C -HMBC Spectrum of compound **2j**:



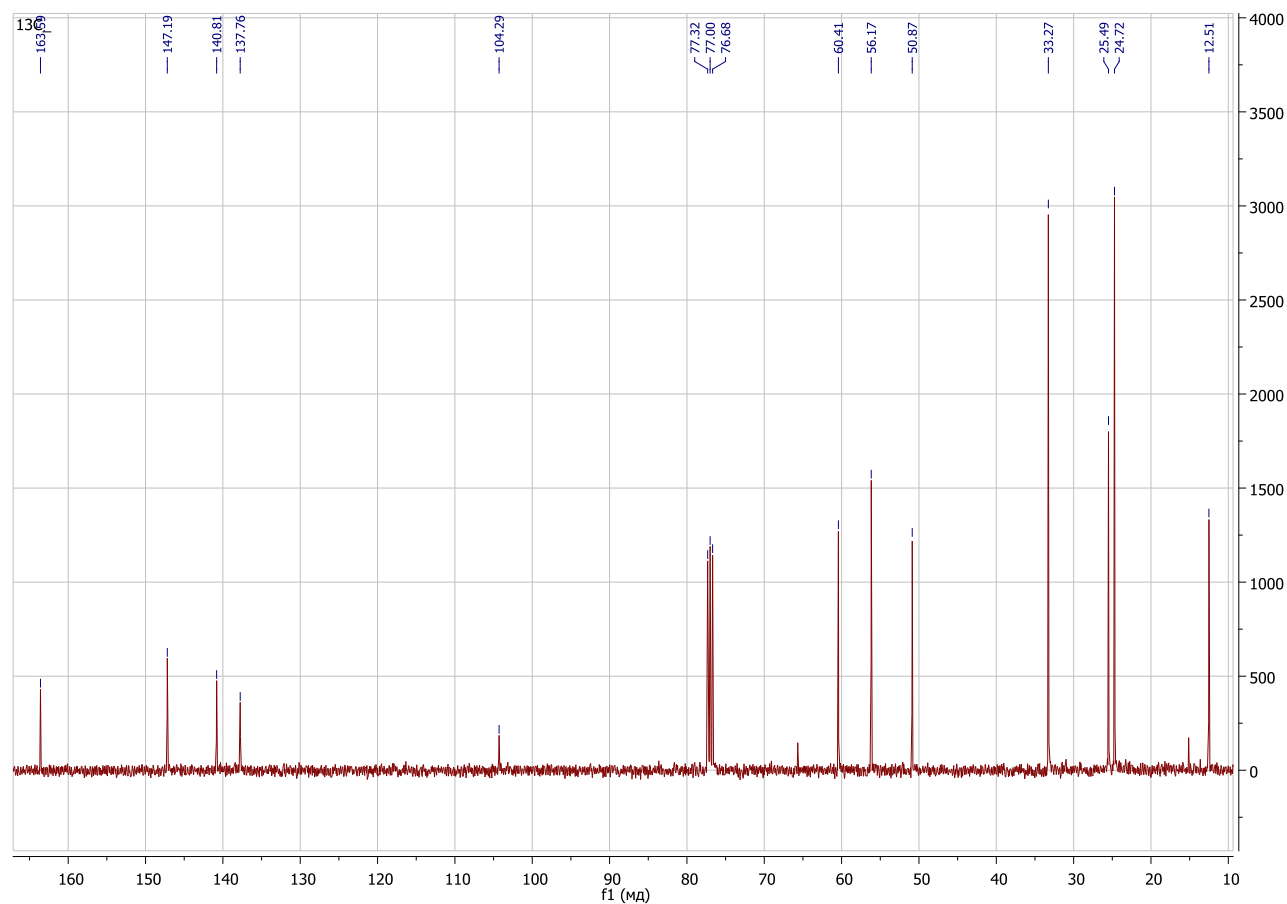


^1H NMR Spectrum of Methyl 5-(cyclohexylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2k)

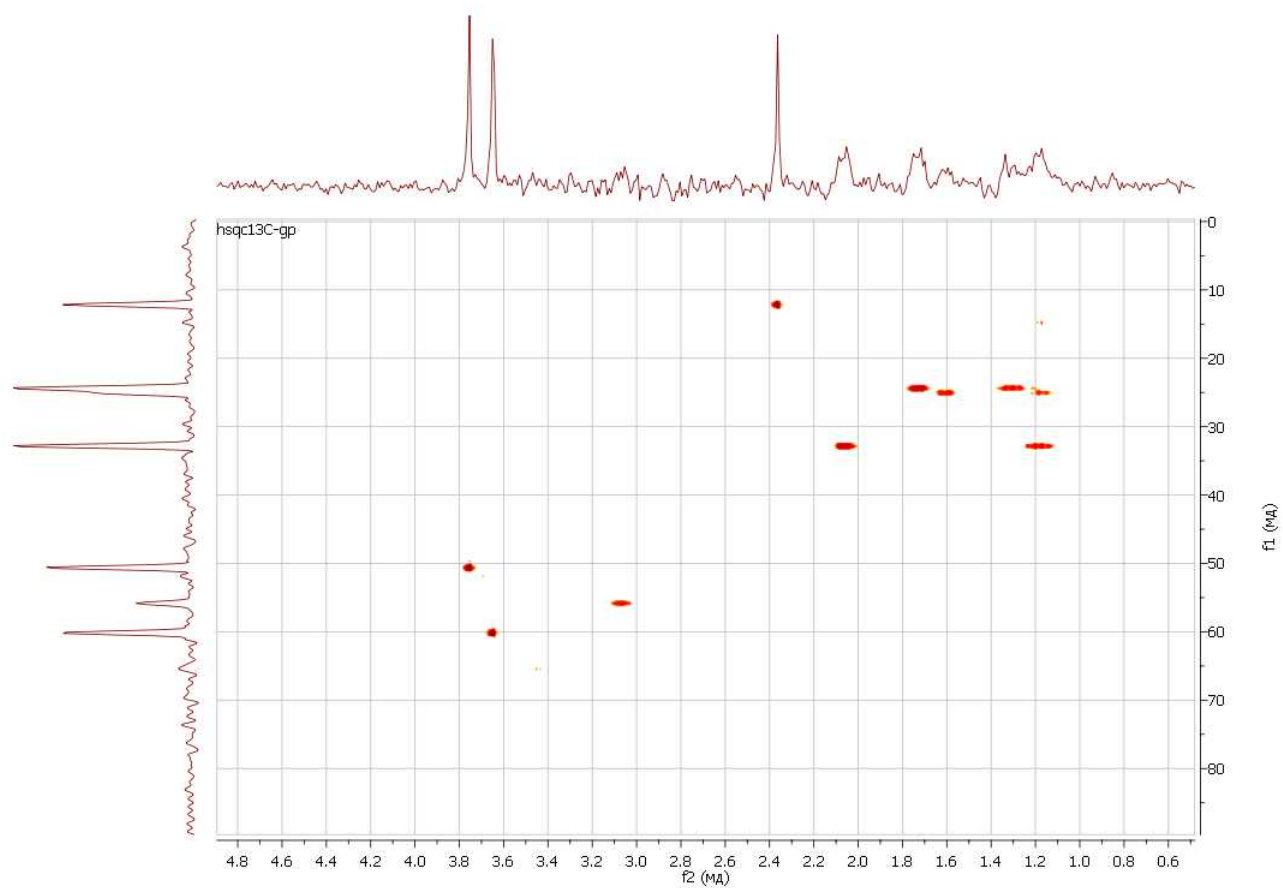


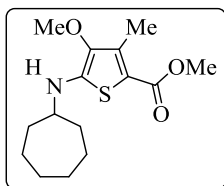


^{13}C NMR Spectrum of Methyl 5-(cyclohexylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2k)

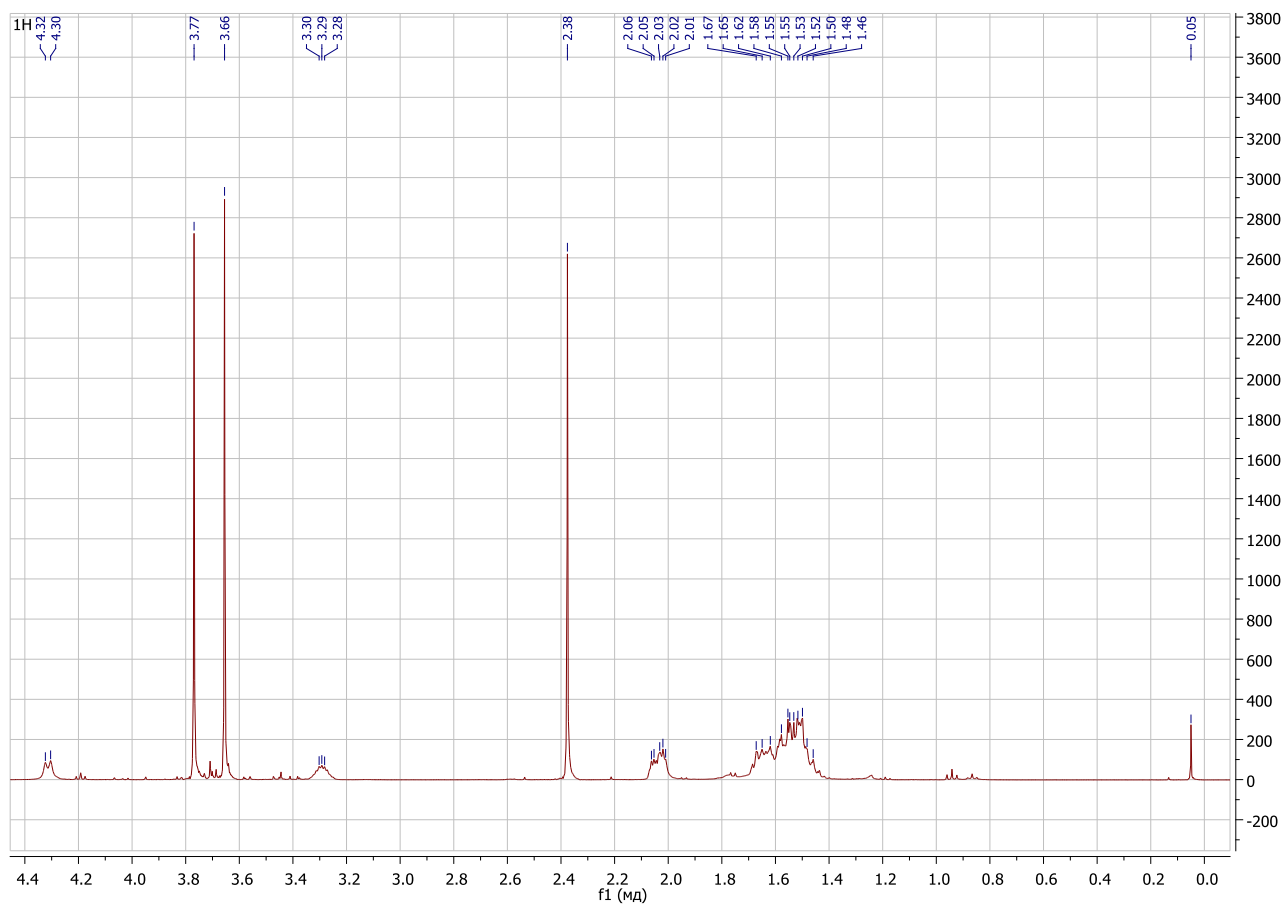


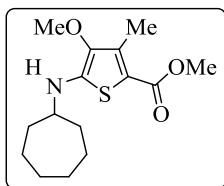
^1H - ^{13}C -HSQC Spectrum of compound **2k**:



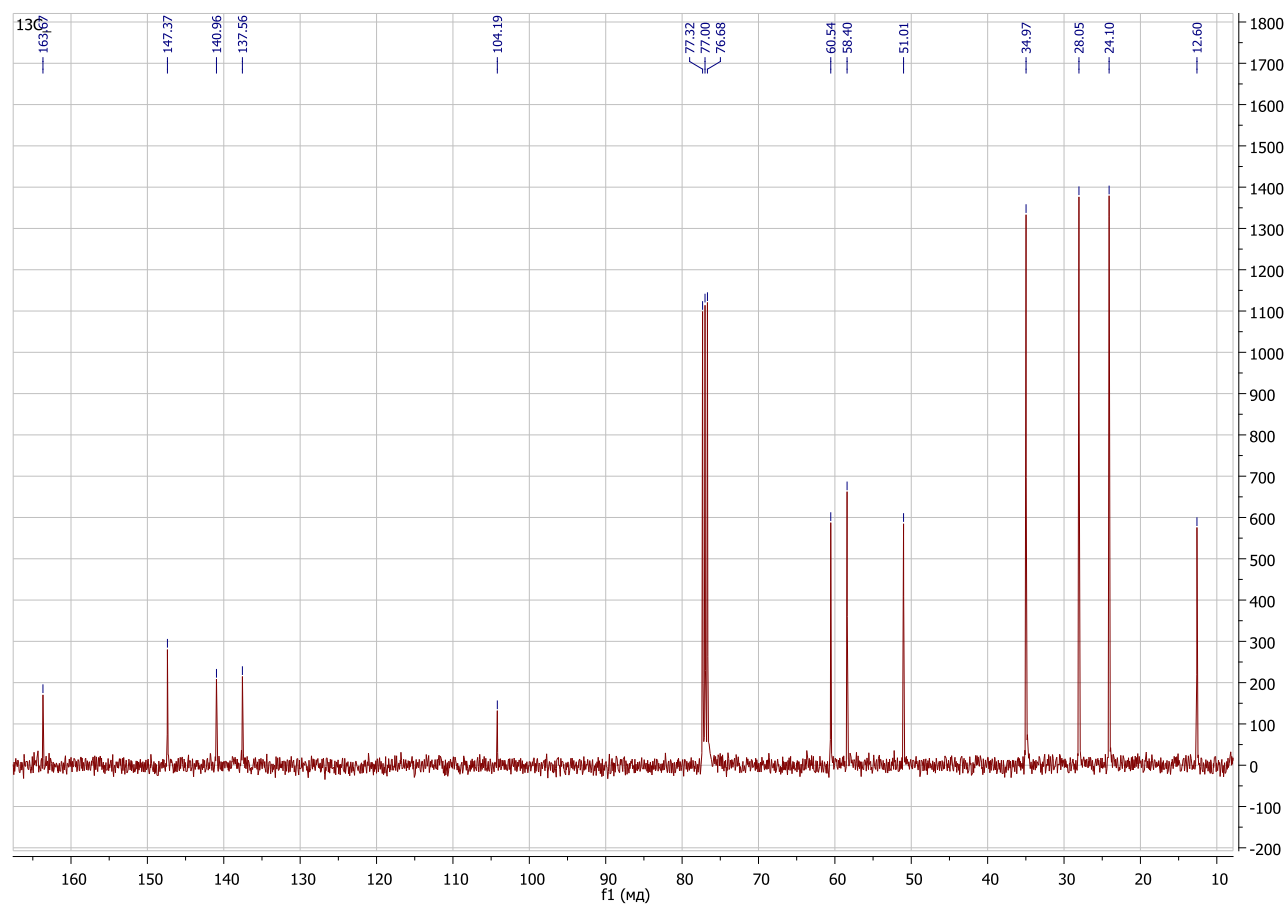


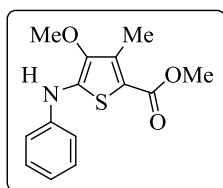
^1H NMR Spectrum of Methyl 5-(cycloheptylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2I)



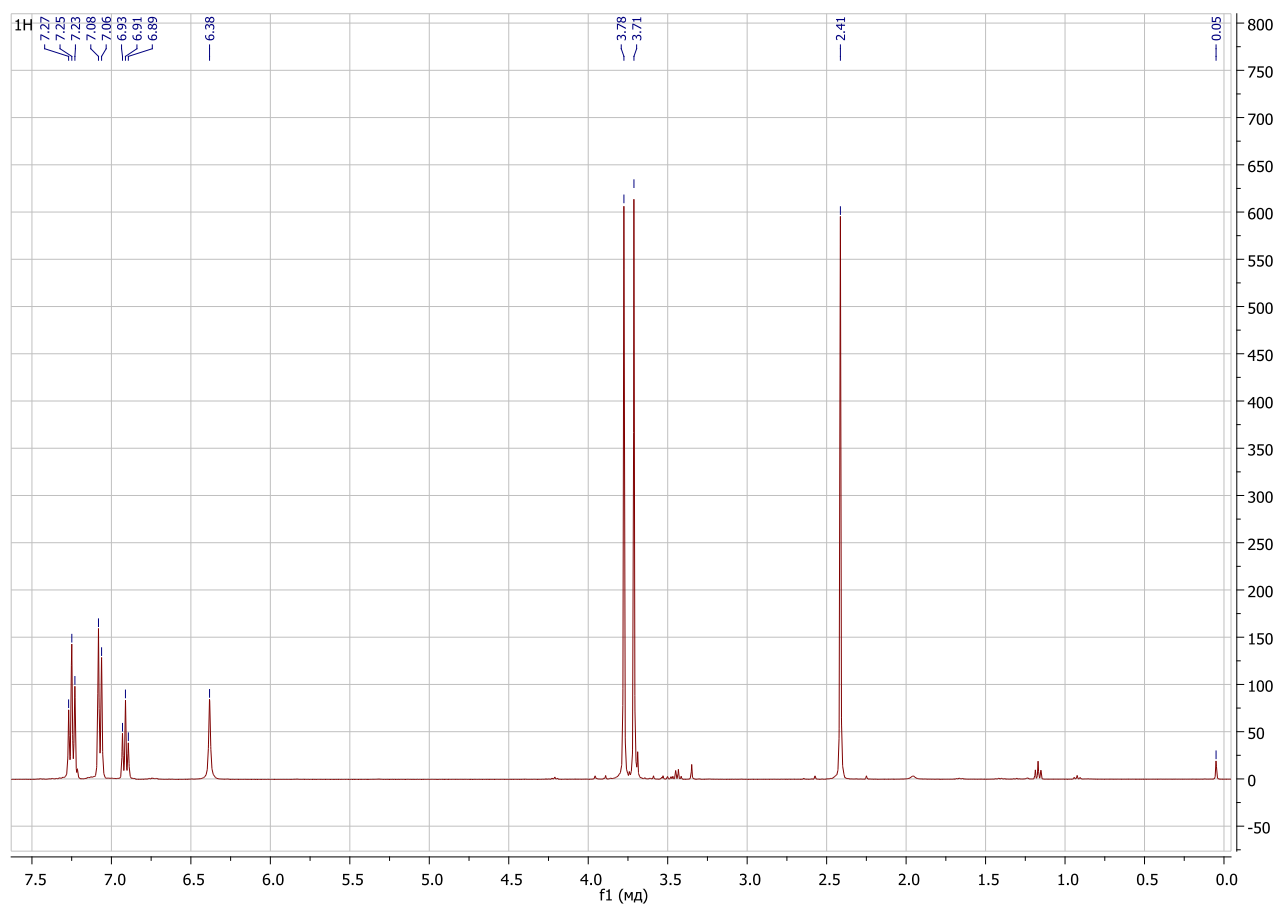


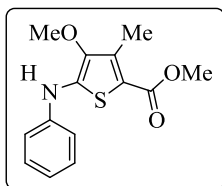
^{13}C NMR Spectrum of Methyl 5-(cycloheptylamino)-4-methoxy-3-methylthiophene-2-carboxylate (2I)



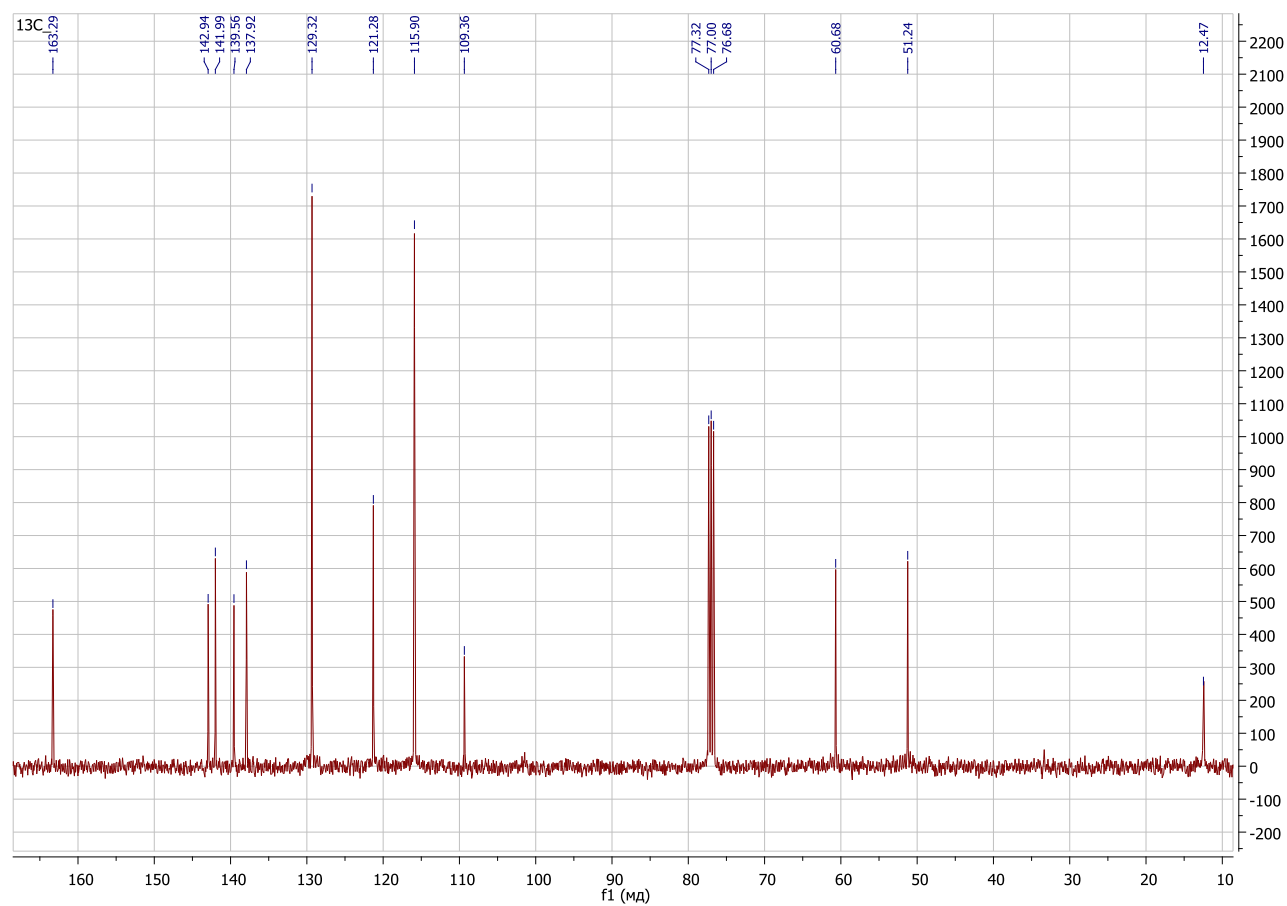


^1H NMR Spectrum of Methyl 5-anilino-4-methoxy-3-methylthiophene-2-carboxylate (2m)

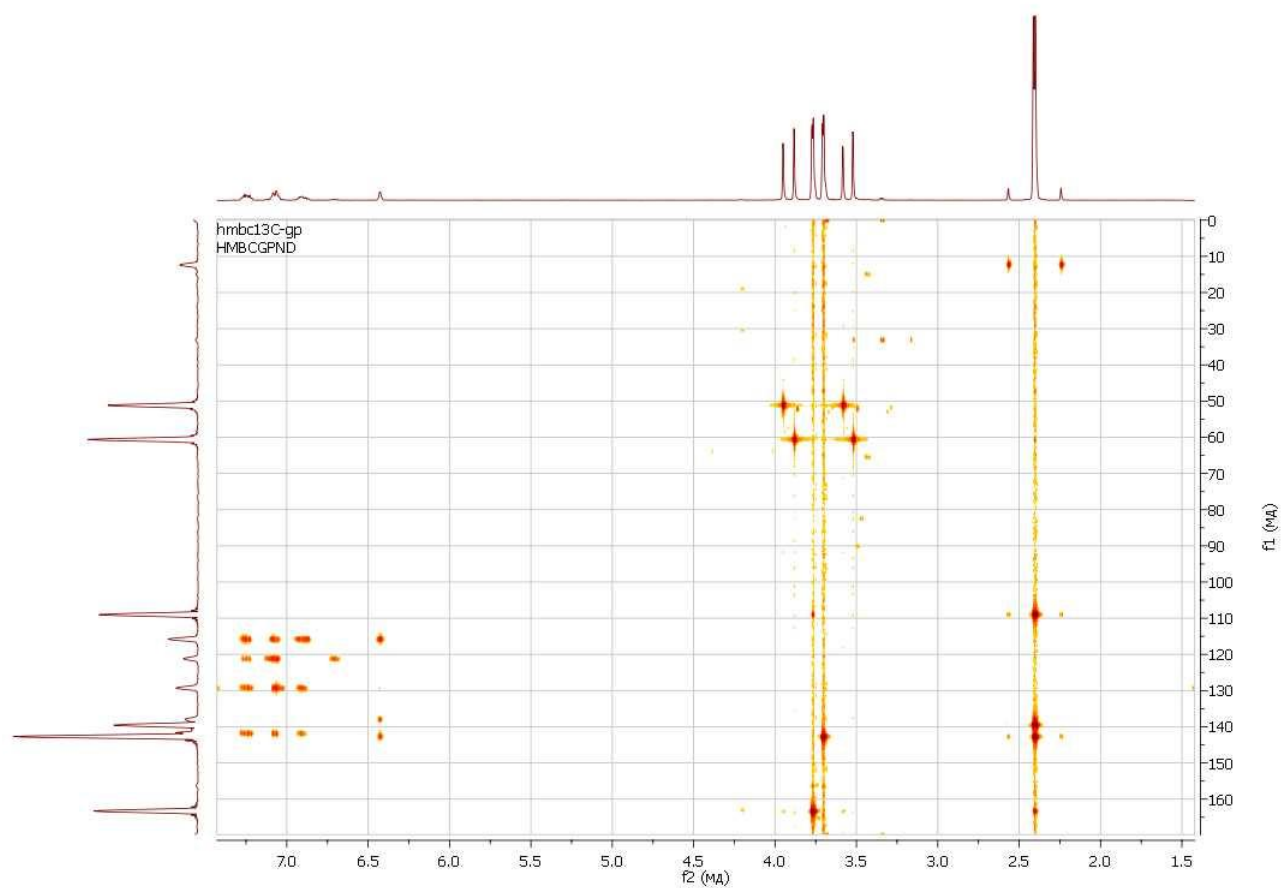




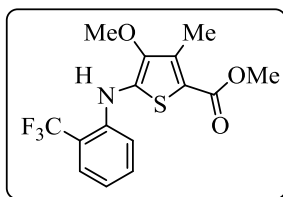
^{13}C NMR Spectrum of Methyl 5-anilino-4-methoxy-3-methylthiophene-2-carboxylate (2m)



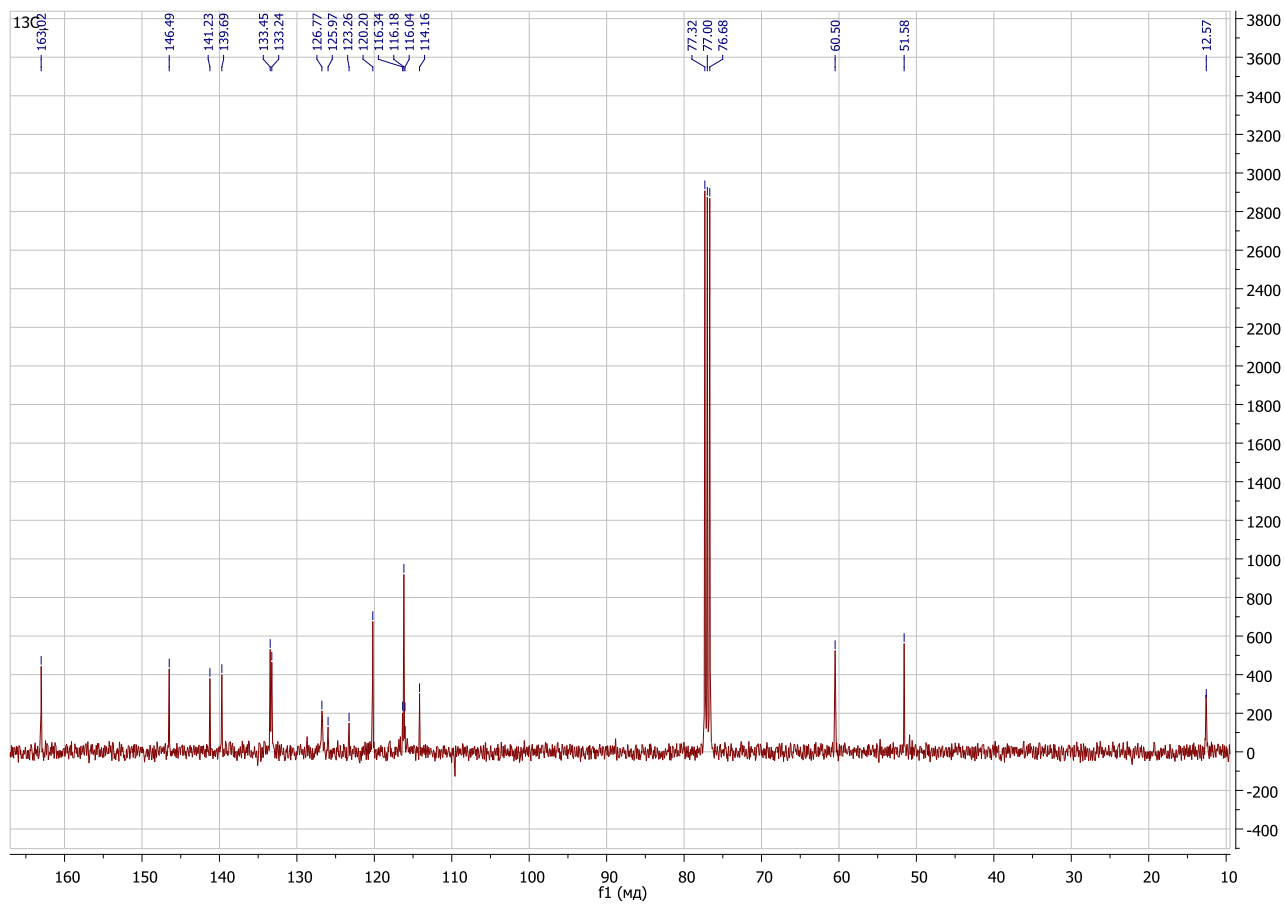
^1H - ^{13}C -HMBC Spectrum of compound **2m**:

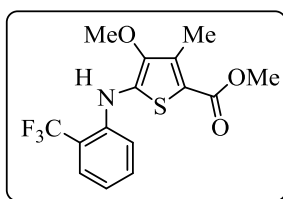




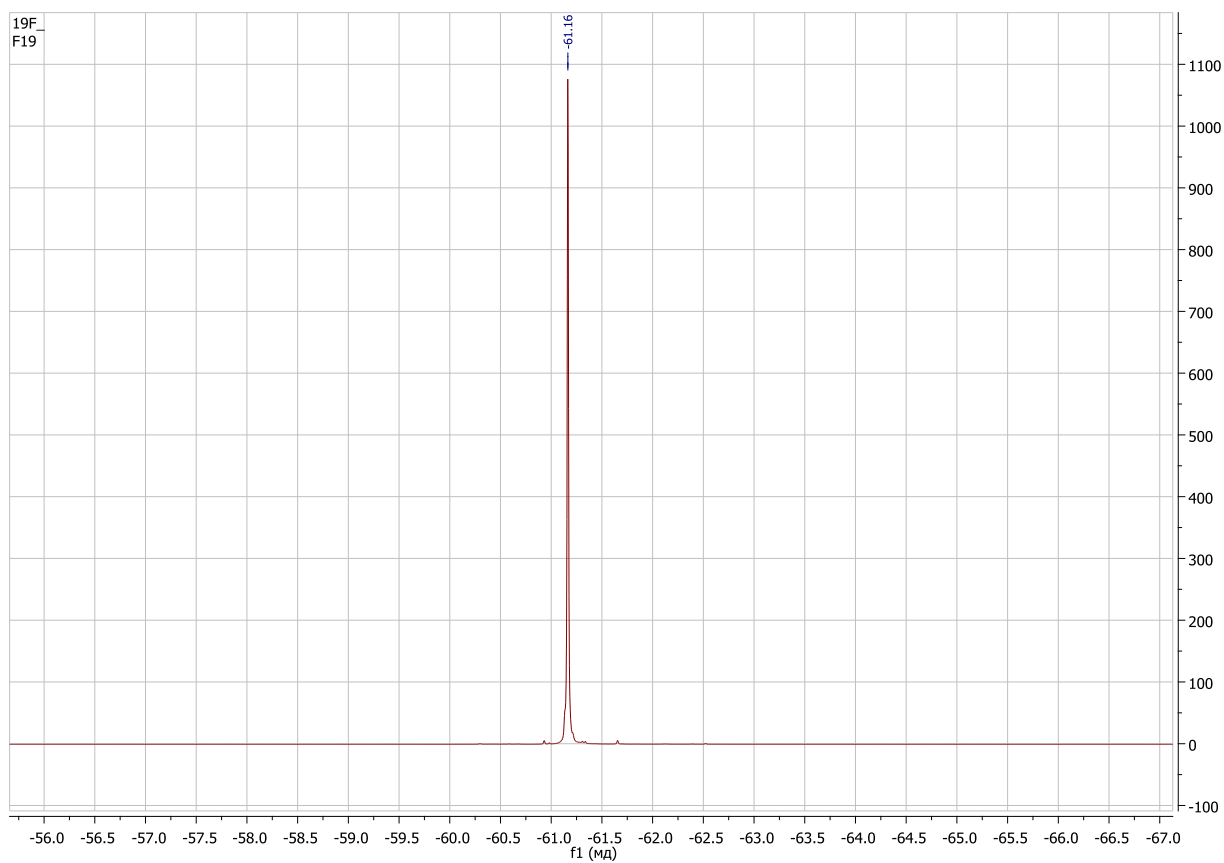


^{13}C NMR Spectrum of Methyl 4-methoxy-3-methyl-5-[2-(trifluoromethyl)anilino]thiophene-2-carboxylate (2n)

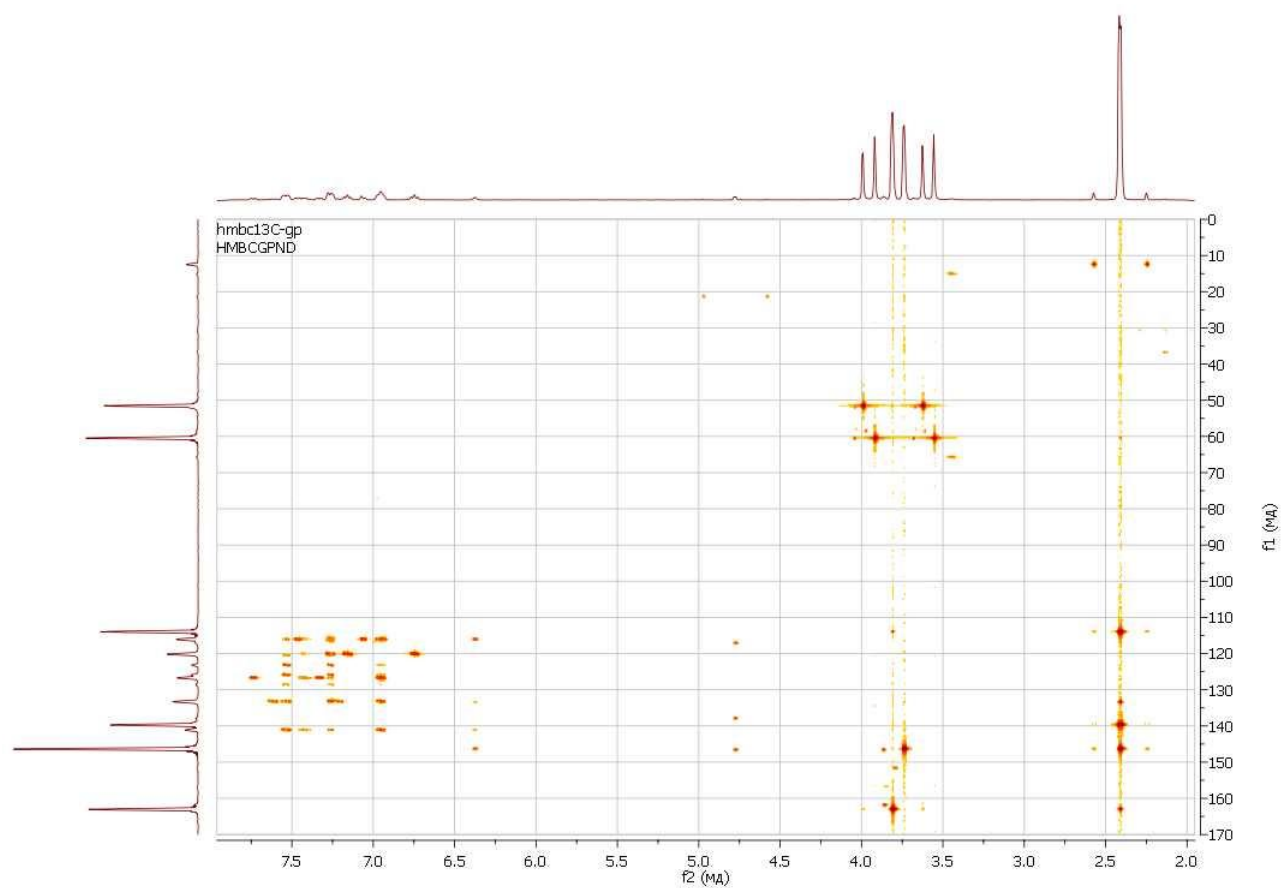




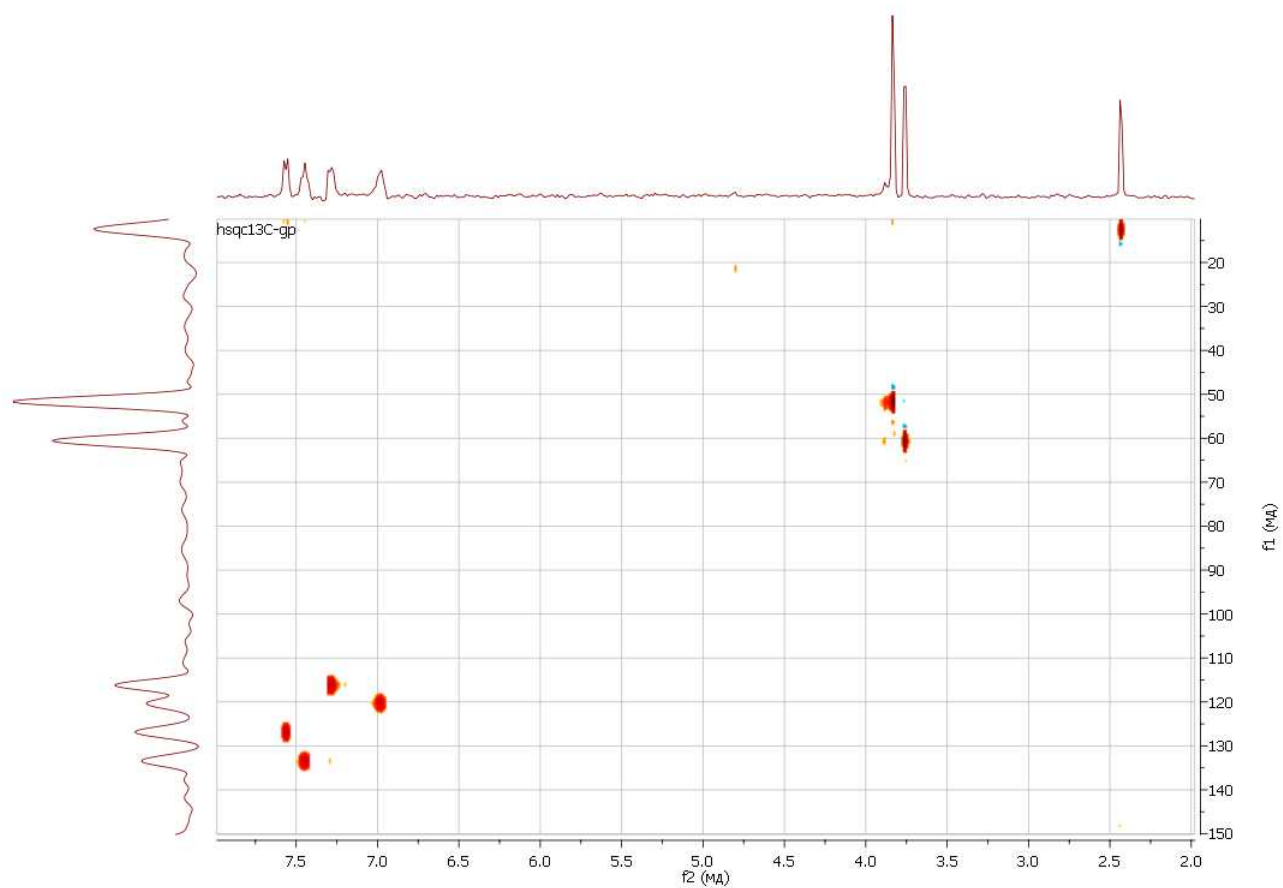
^{19}F NMR Spectrum of Methyl 4-methoxy-3-methyl-5-[2-(trifluoromethyl)anilino]thiophene-2-carboxylate (2n)

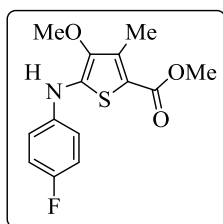


^1H - ^{13}C -HMBC Spectrum of compound **2n**:

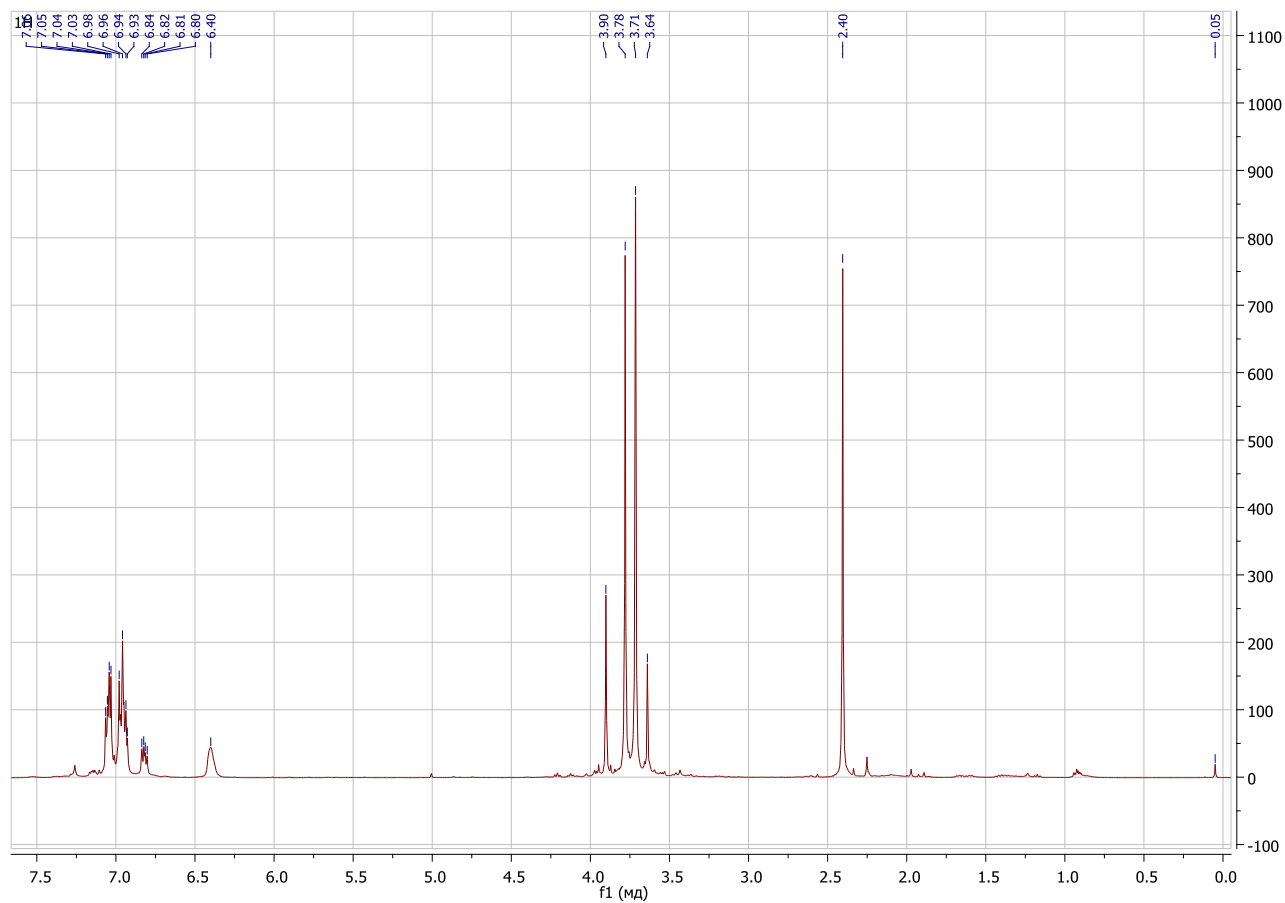


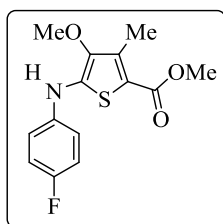
^1H - ^{13}C -HSQC Spectrum of compound **2n**:



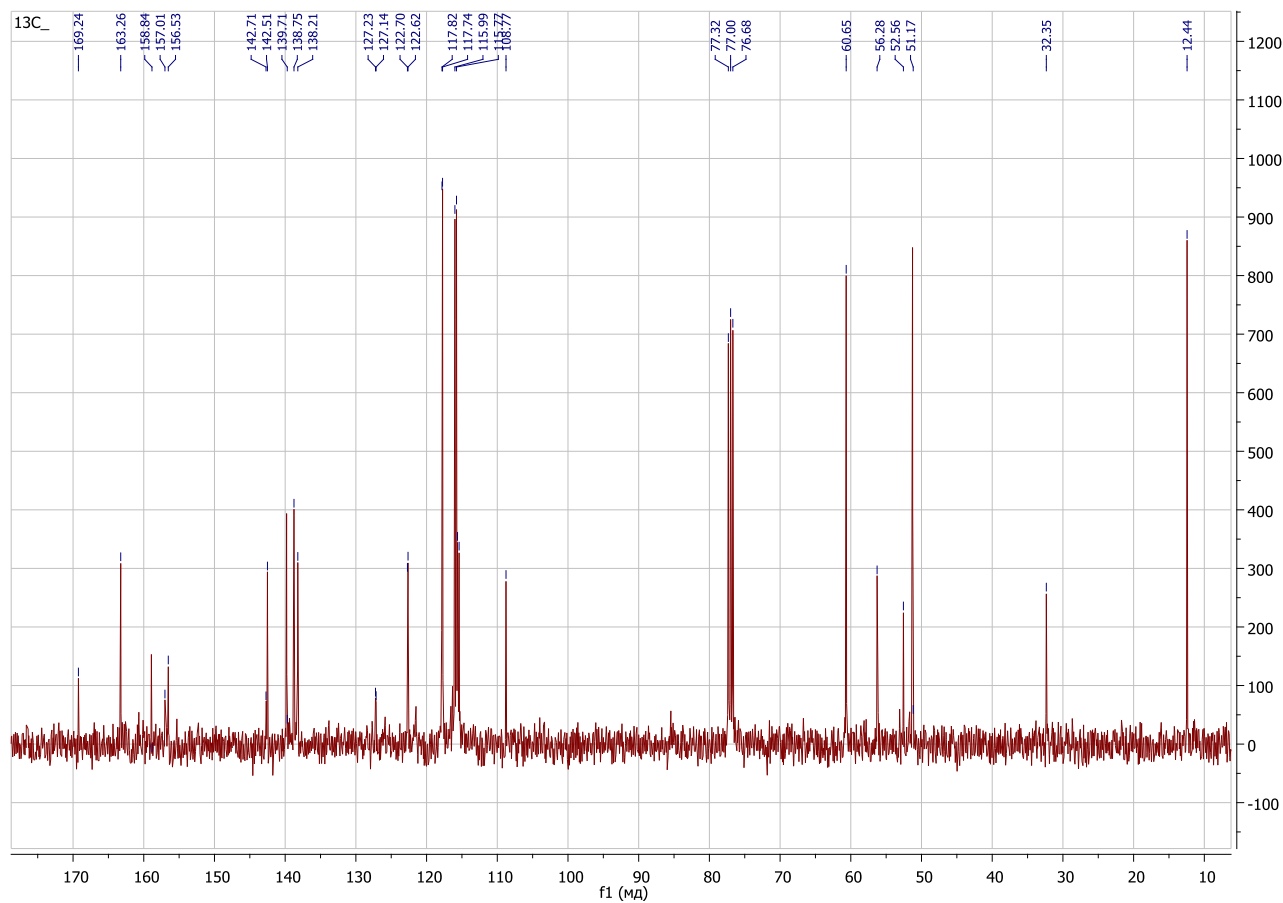


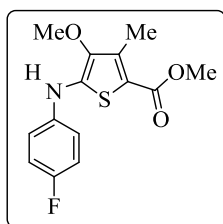
^1H NMR Spectrum of Methyl 5-(4-fluoroanilino)-4-methoxy-3-methylthiophene-2-carboxylate (2o)



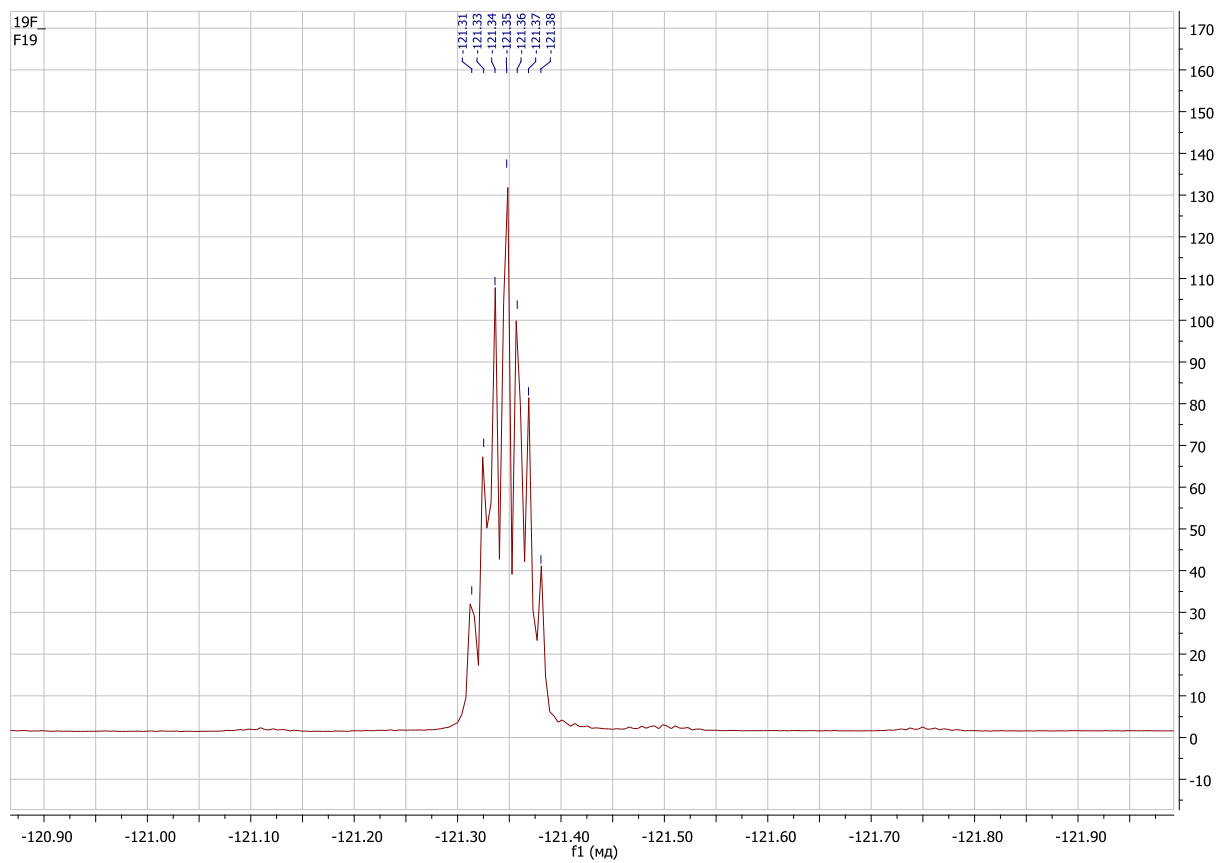


^{13}C NMR Spectrum of Methyl 5-(4-fluoroanilino)-4-methoxy-3-methylthiophene-2-carboxylate (2o)

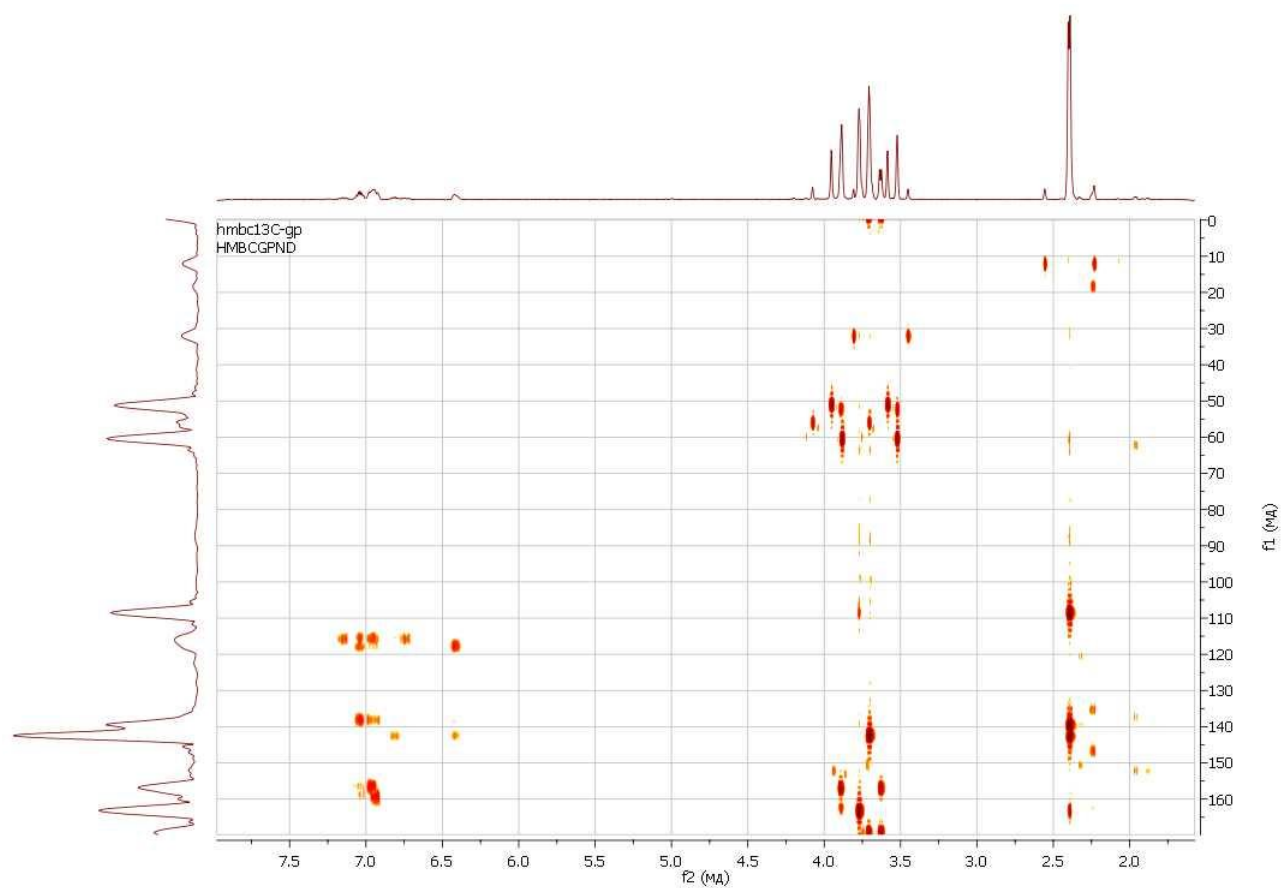


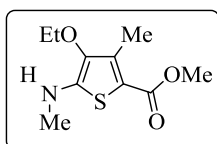


^{19}F NMR Spectrum of Methyl 5-(4-fluoroanilino)-4-methoxy-3-methylthiophene-2-carboxylate (2o)

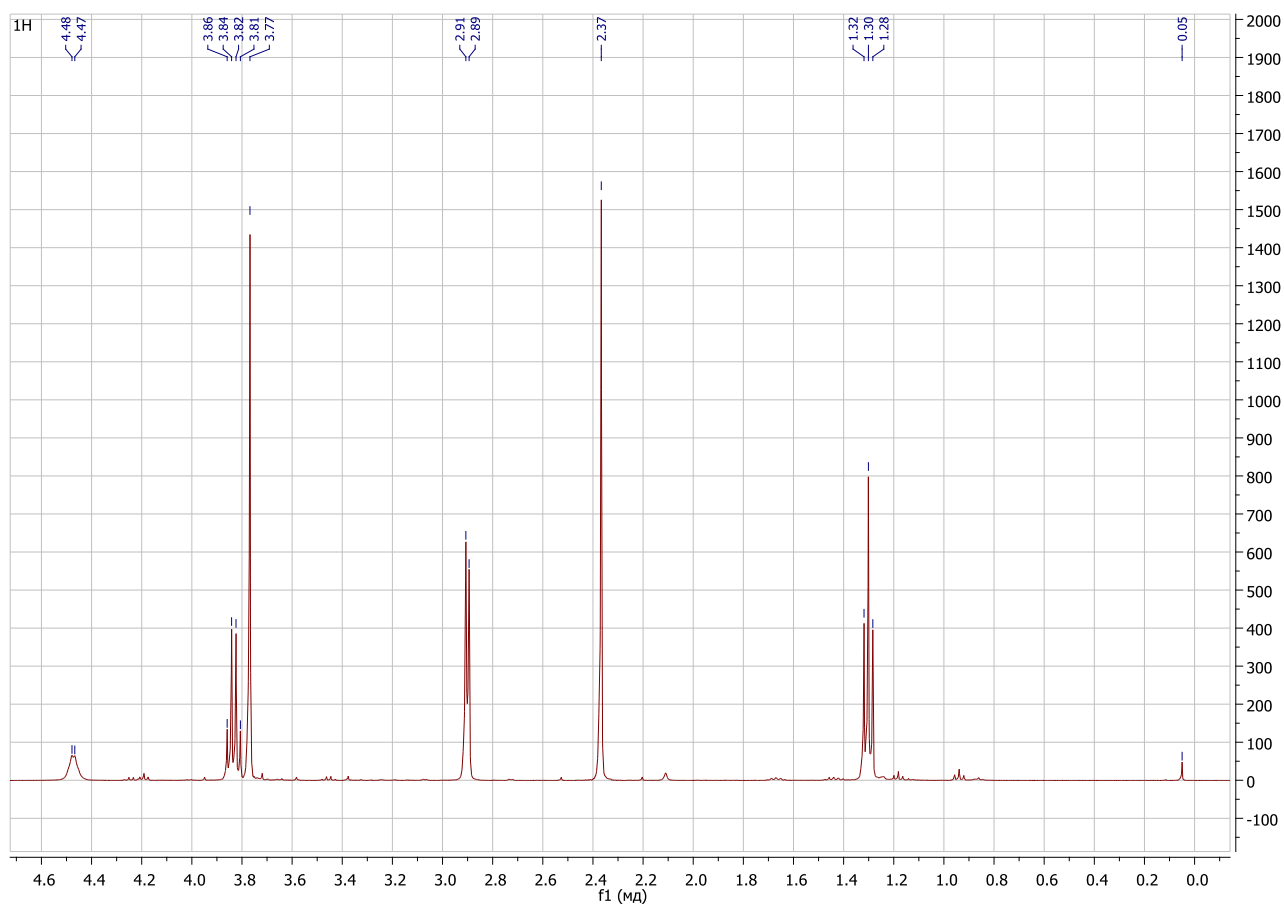


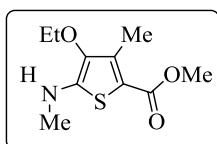
^1H - ^{13}C -HMBC Spectrum of compound **2o**:



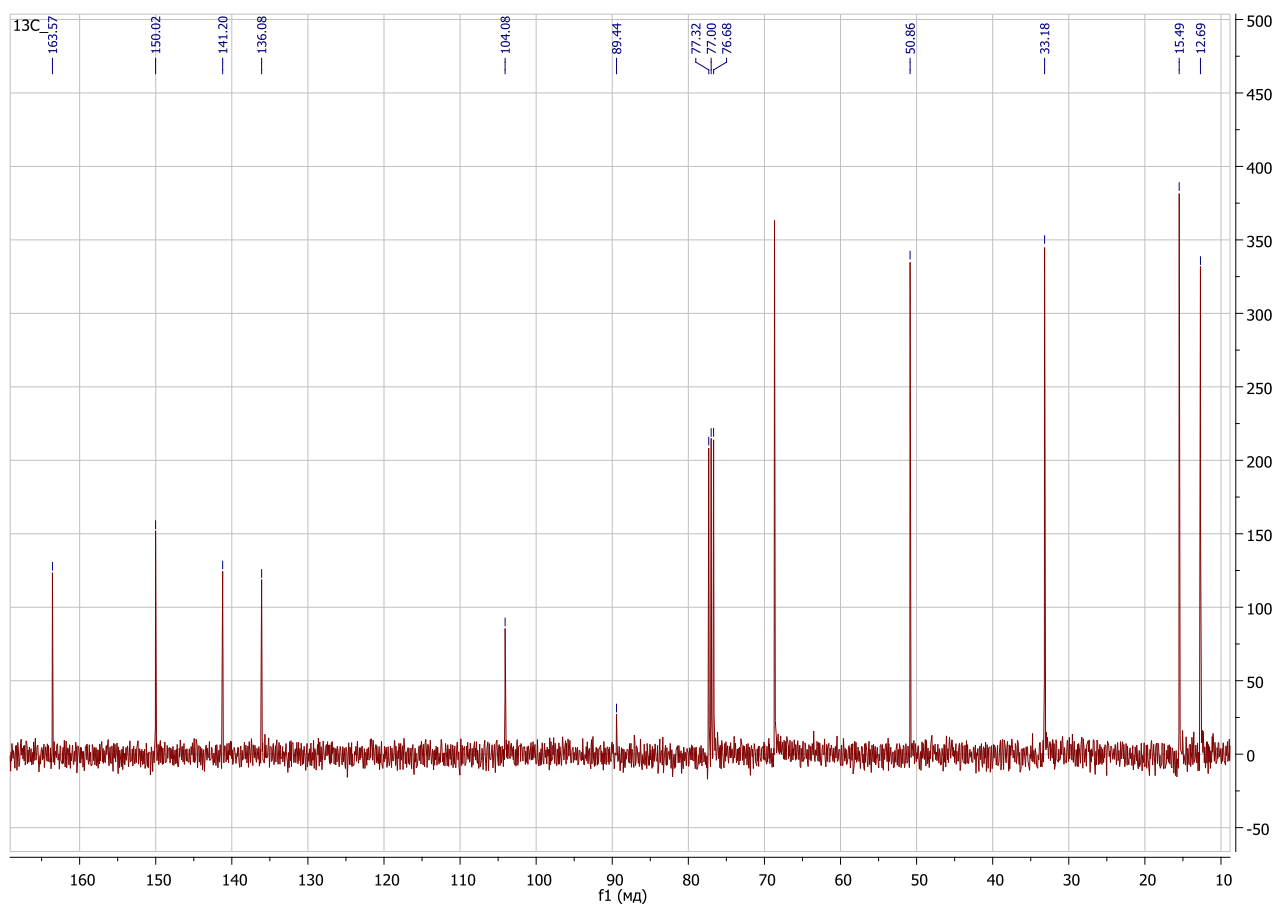


¹H NMR Spectrum of Methyl 4-ethoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2p)

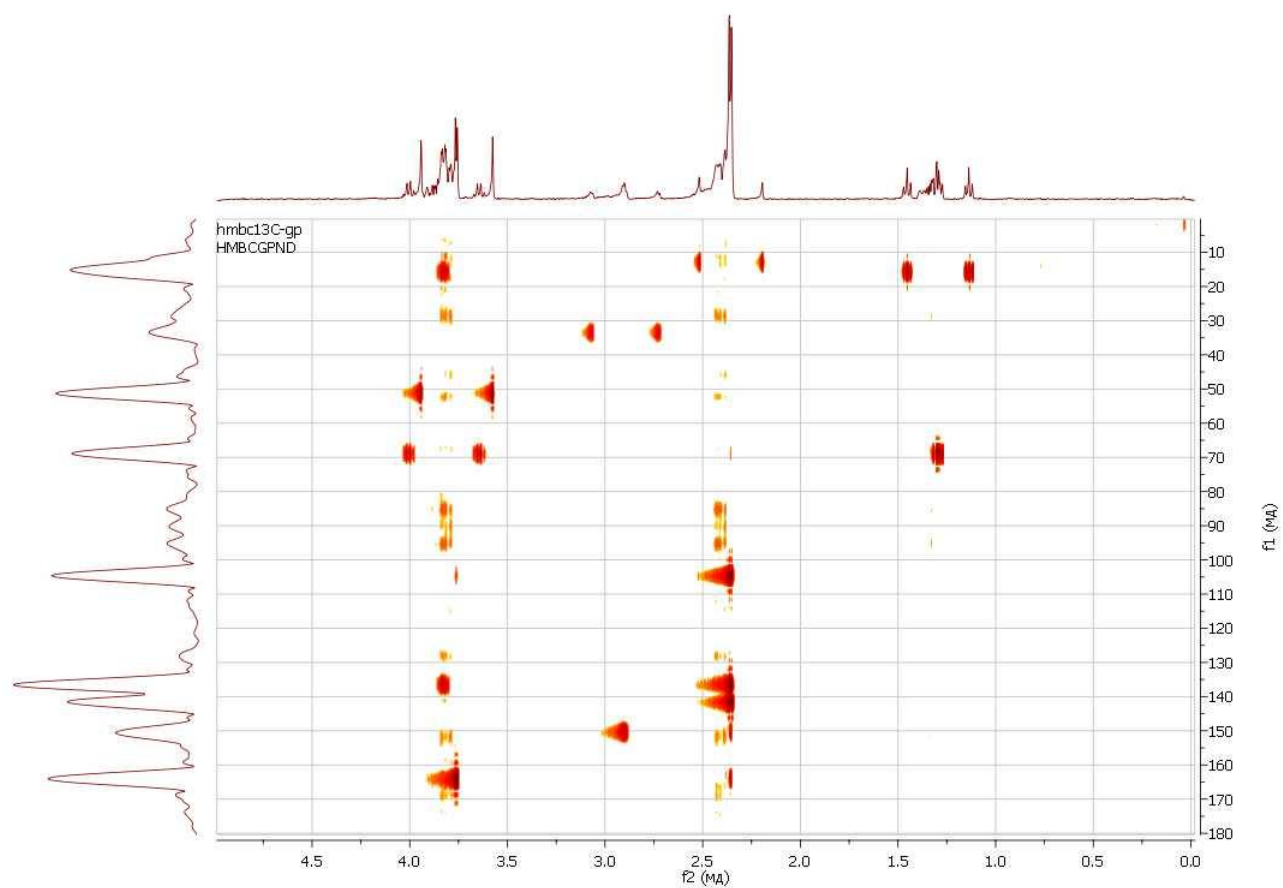


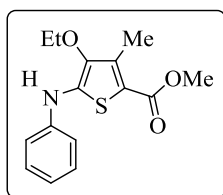


^{13}C NMR Spectrum of Methyl 4-ethoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2p)

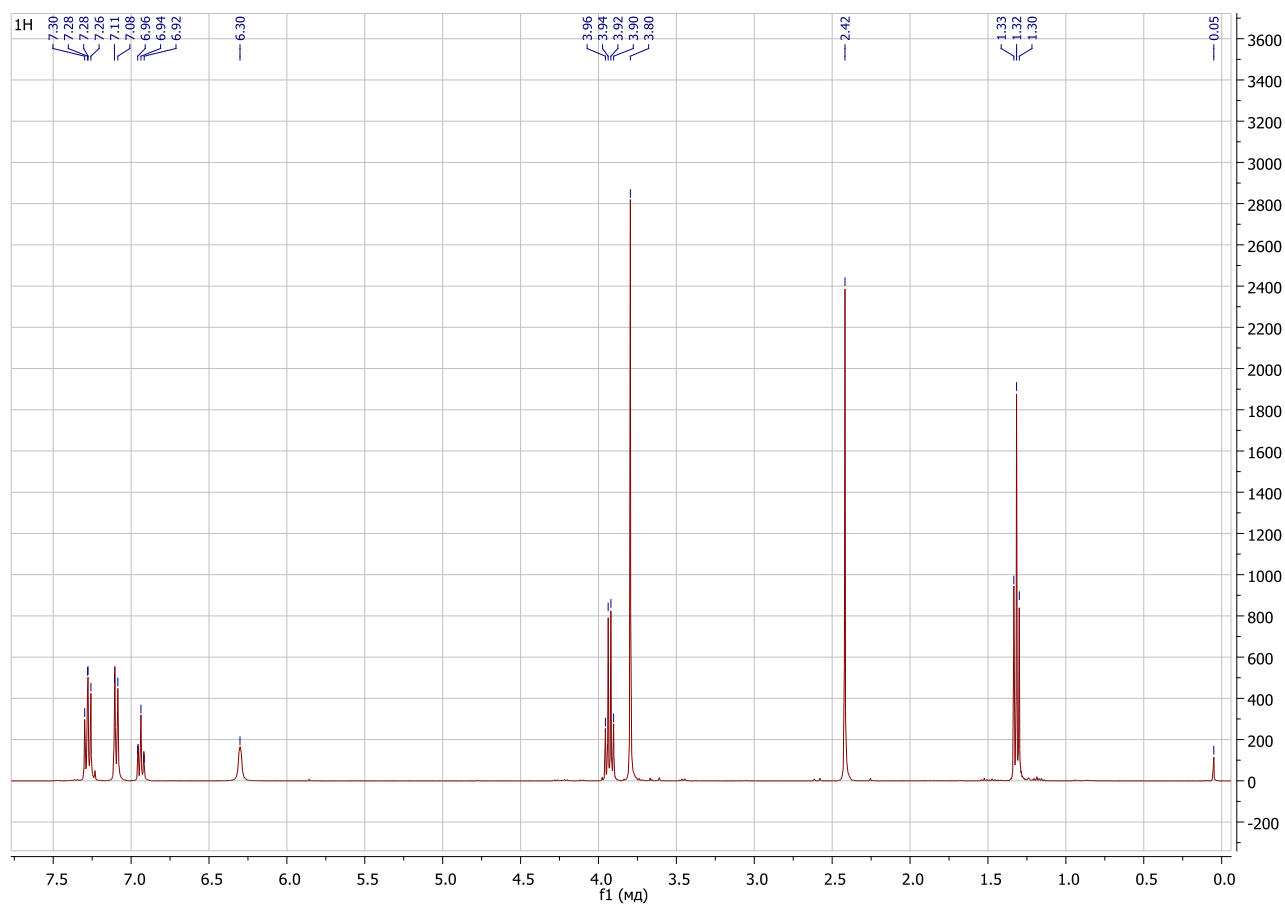


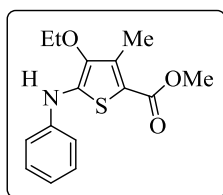
^1H - ^{13}C -HMBC Spectrum of compound **2p**:



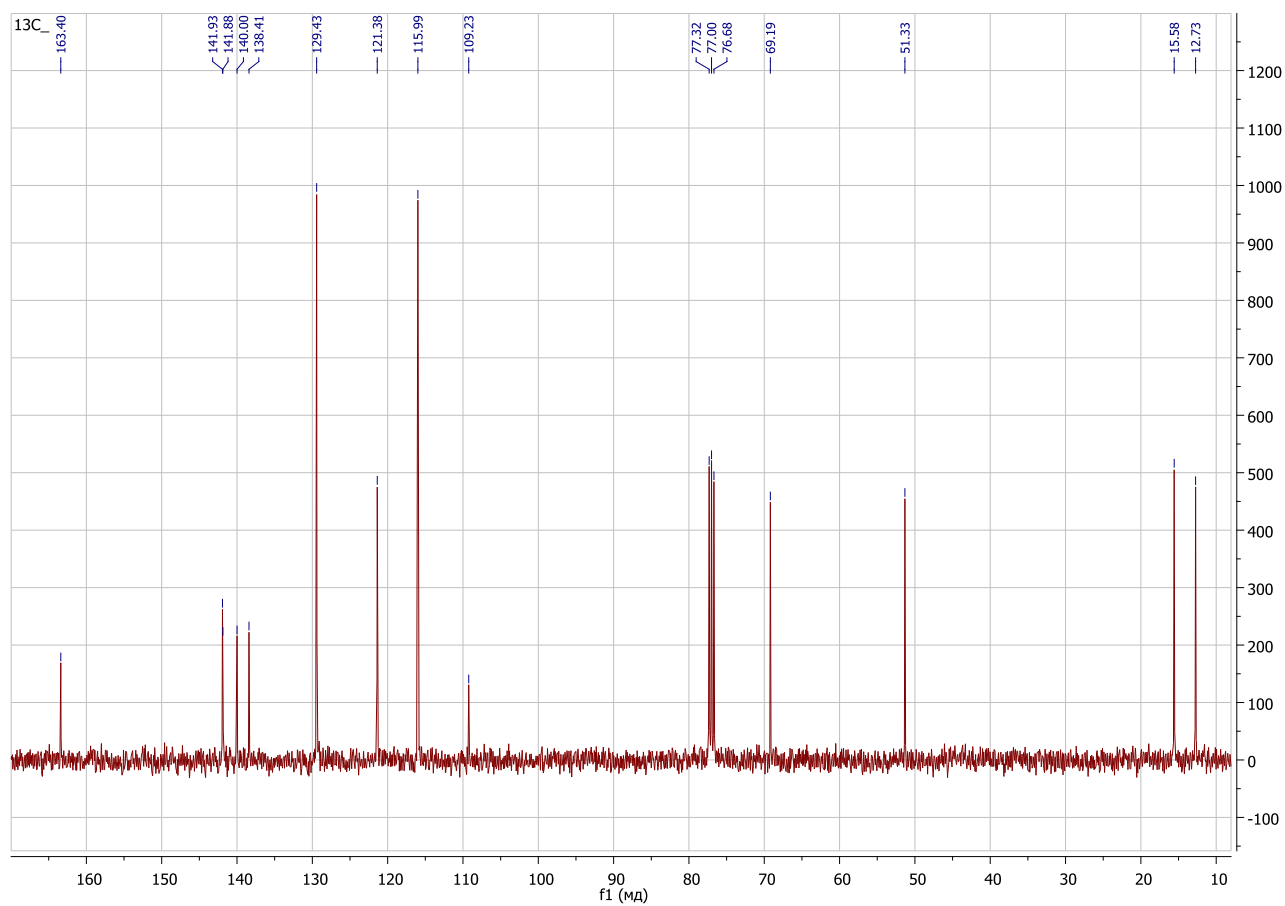


^1H NMR Spectrum of Methyl 5-anilino-4-ethoxy-3-methylthiophene-2-carboxylate (2q)

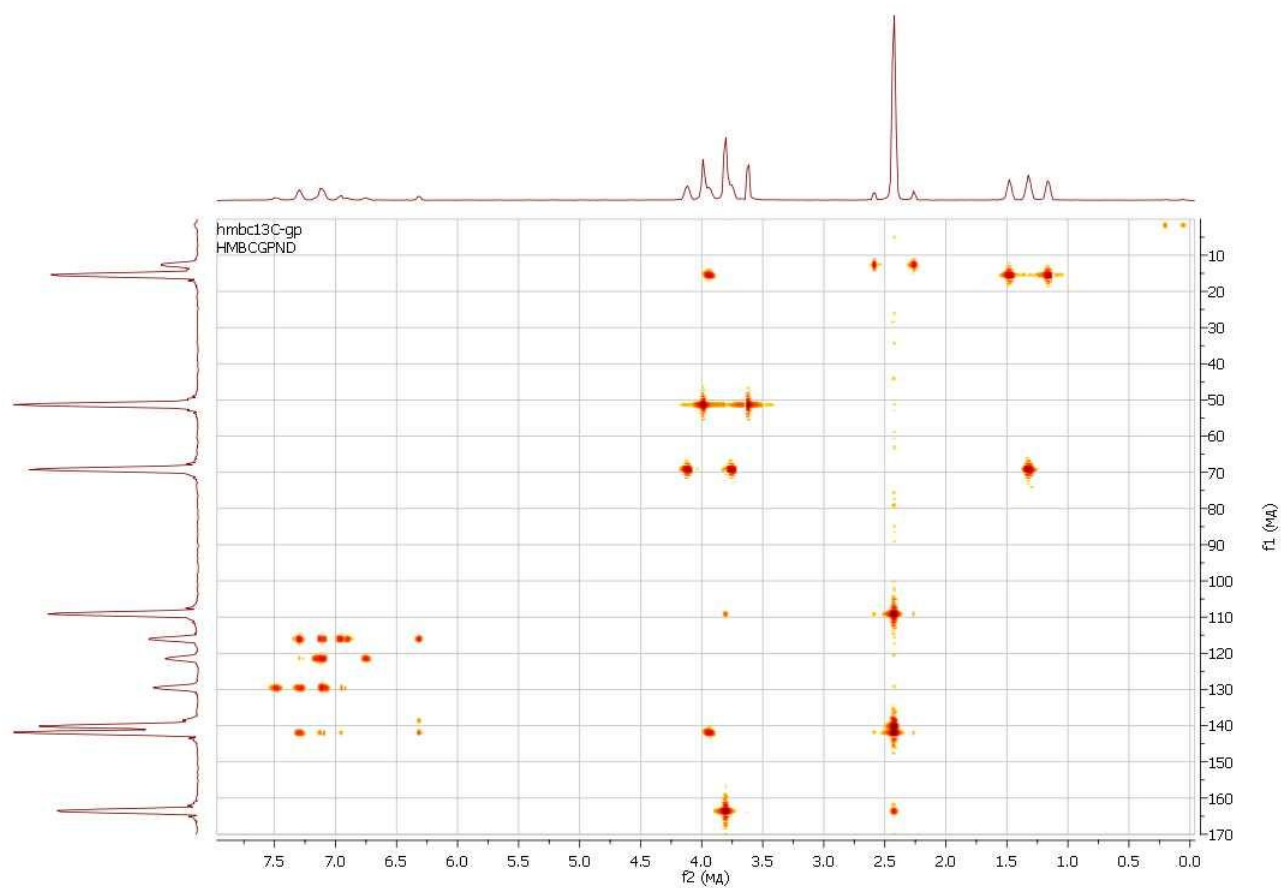


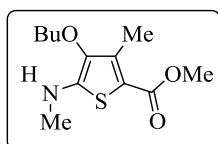


^{13}C NMR Spectrum of Methyl 5-anilino-4-ethoxy-3-methylthiophene-2-carboxylate (2q)

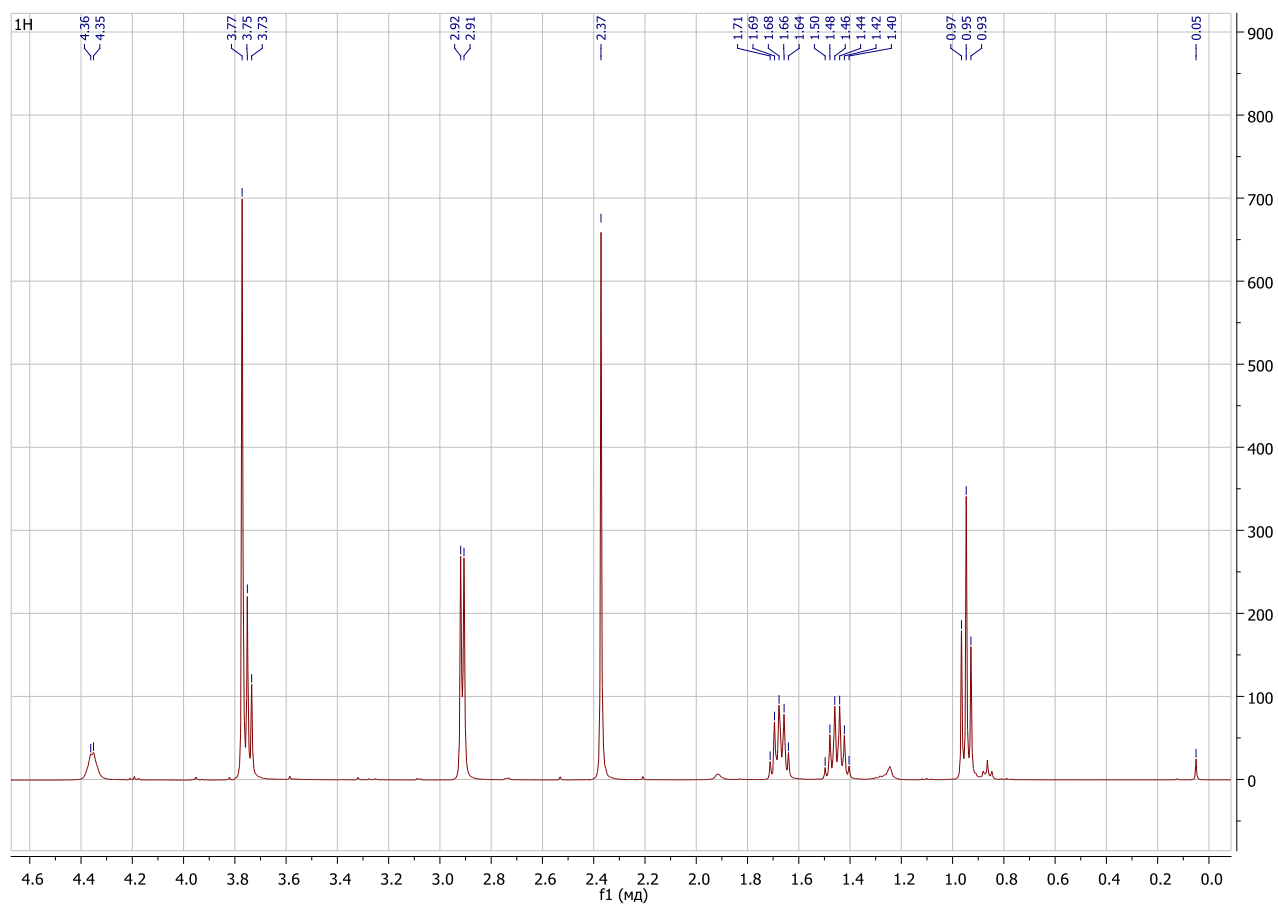


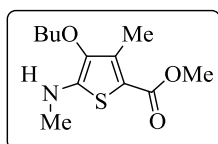
^1H - ^{13}C -HMBC Spectrum of compound **2q**:



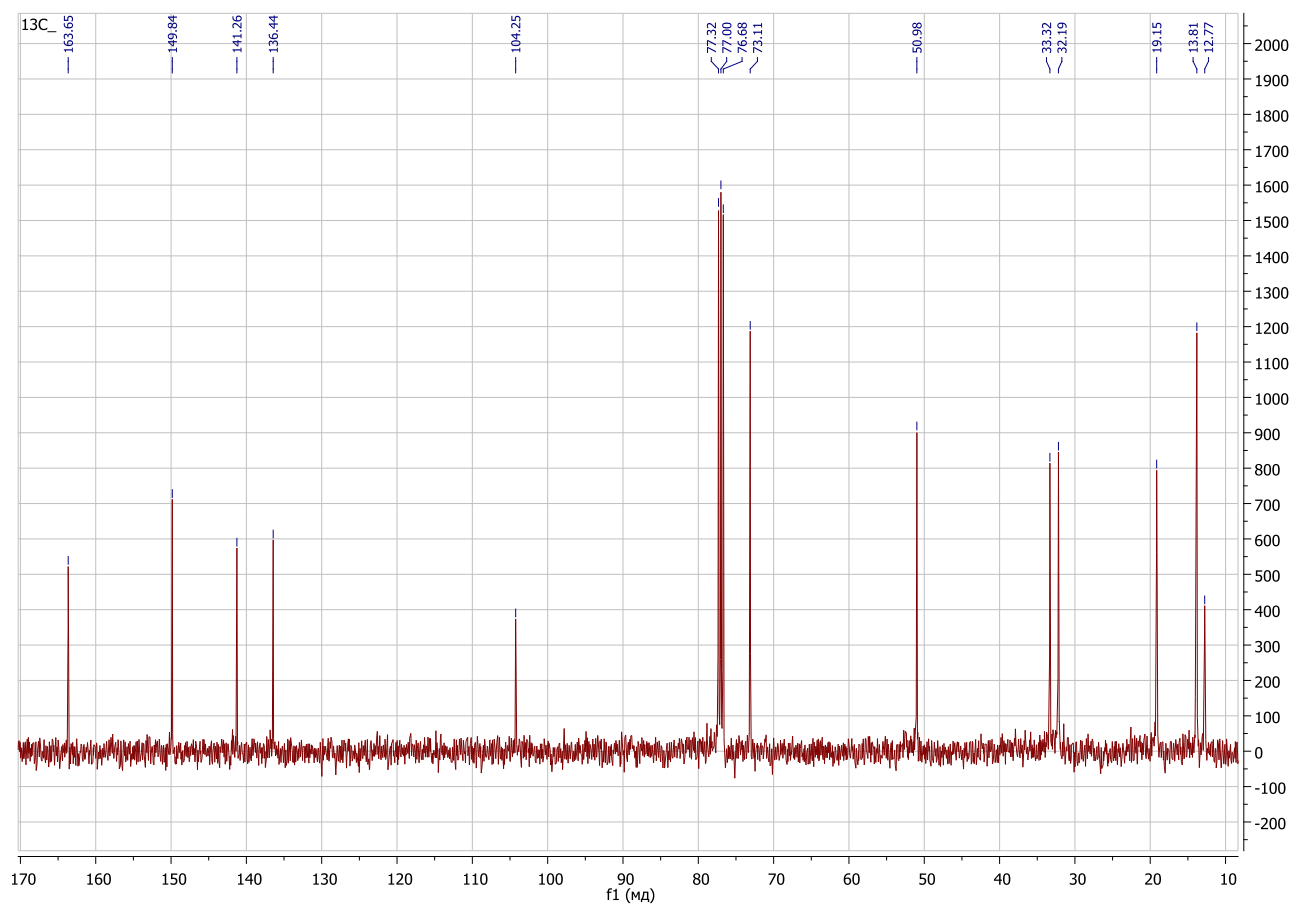


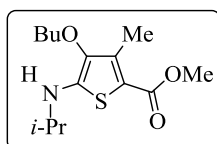
¹H NMR Spectrum of Methyl 4-butoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2r)



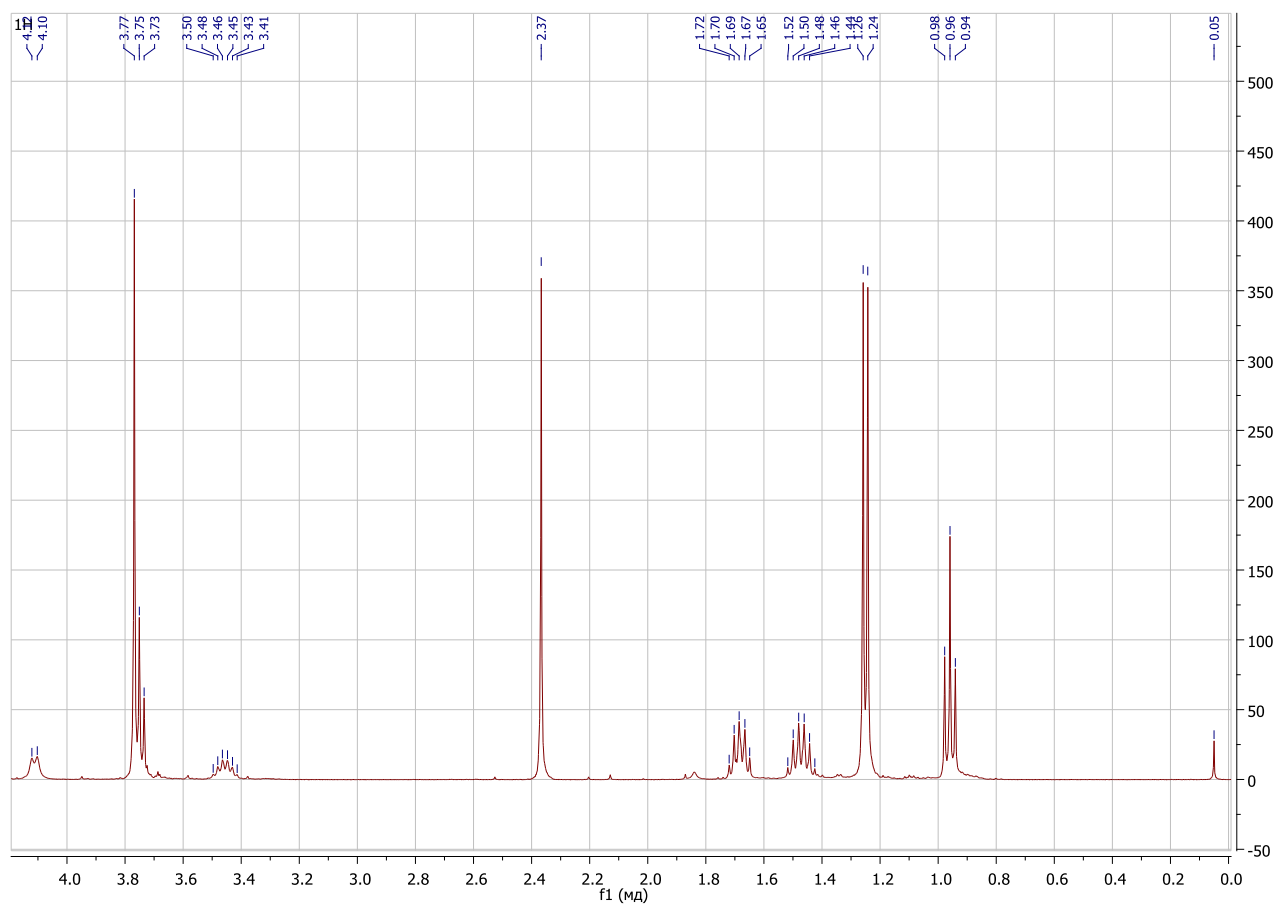


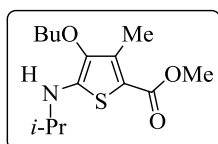
^{13}C NMR Spectrum of Methyl 4-butoxy-3-methyl-5-(methylamino)thiophene-2-carboxylate (2r)



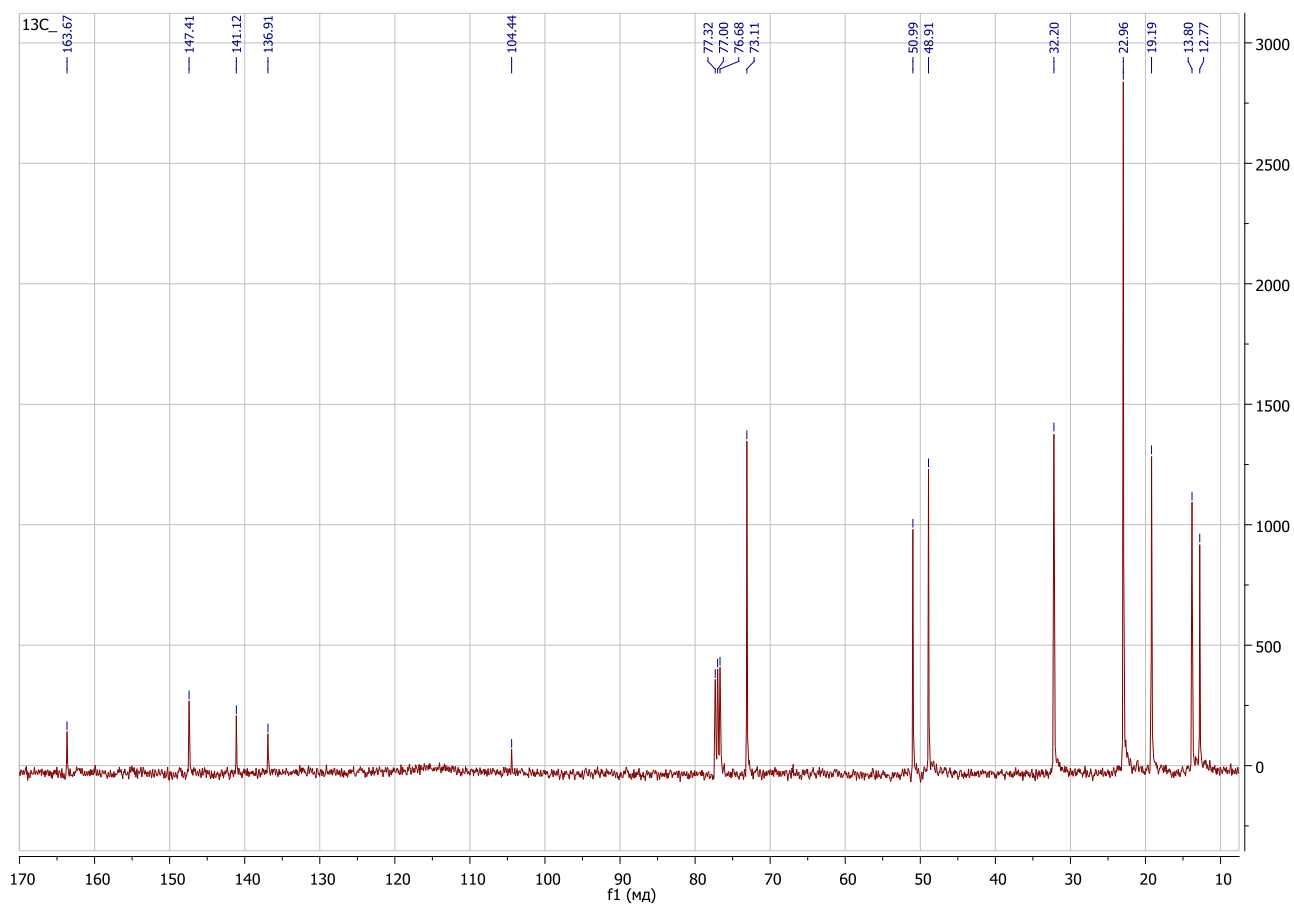


^1H NMR Spectrum of Methyl 4-butoxy-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2s)

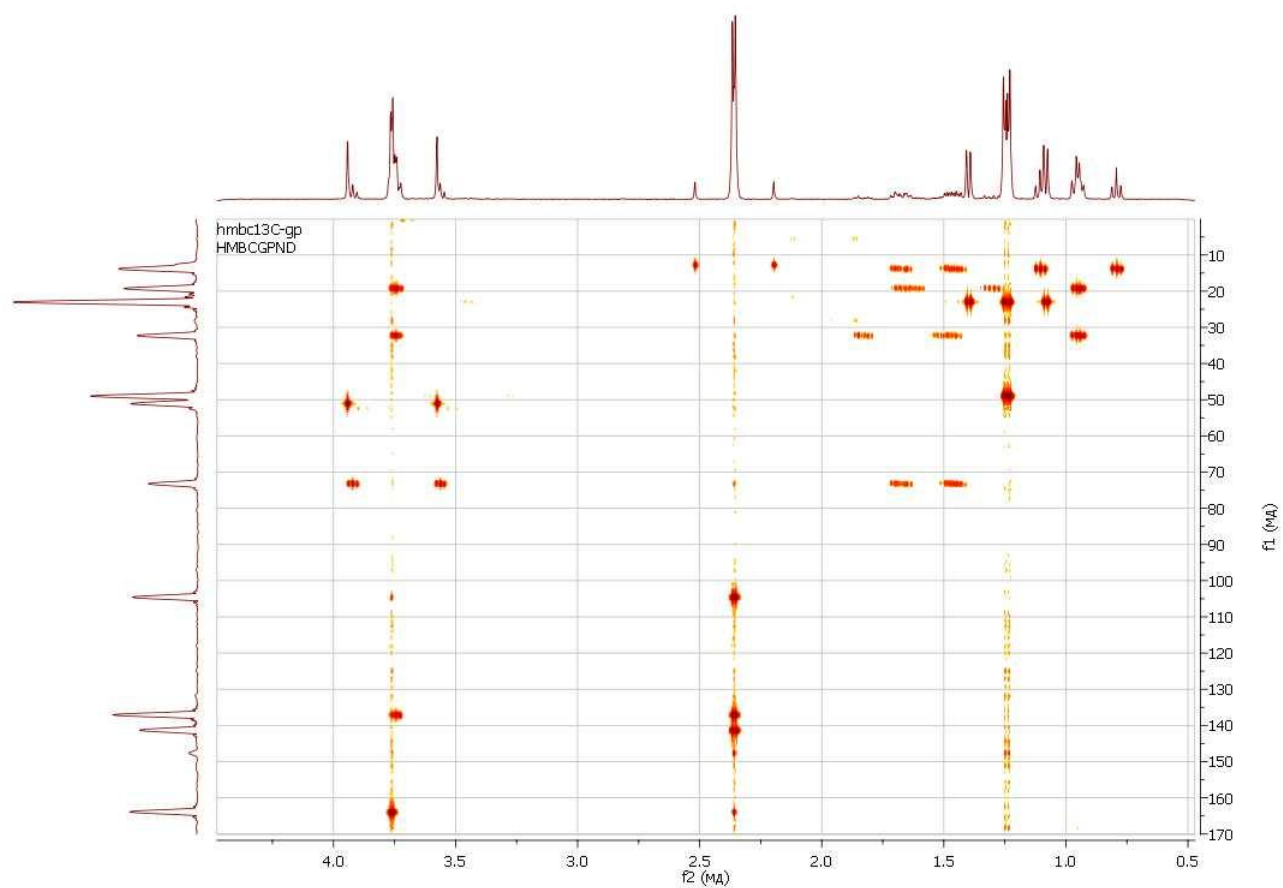




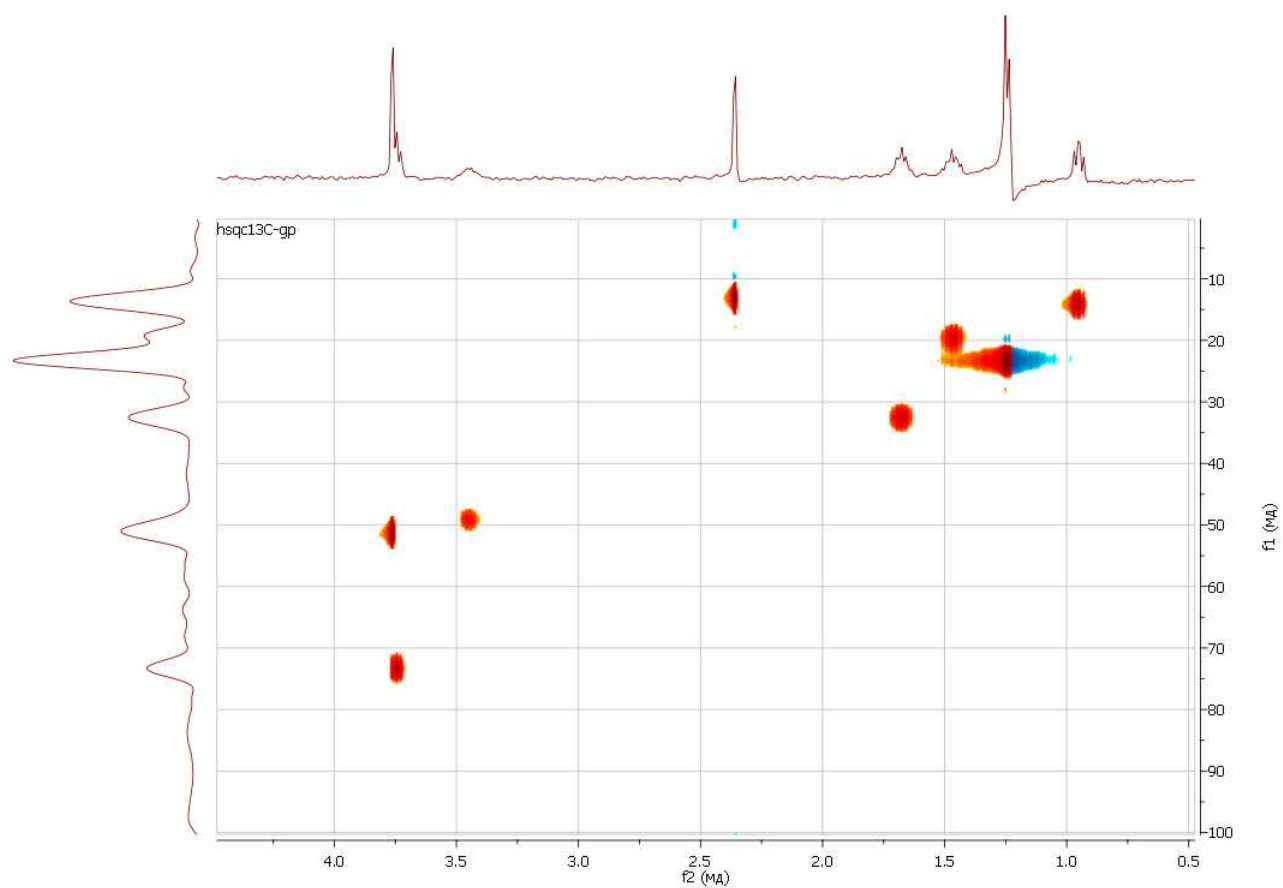
^{13}C NMR Spectrum of Methyl 4-butoxy-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2s)

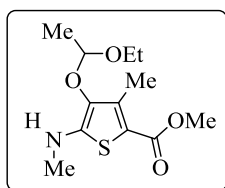


^1H - ^{13}C -HMBC Spectrum of compound **2s**:

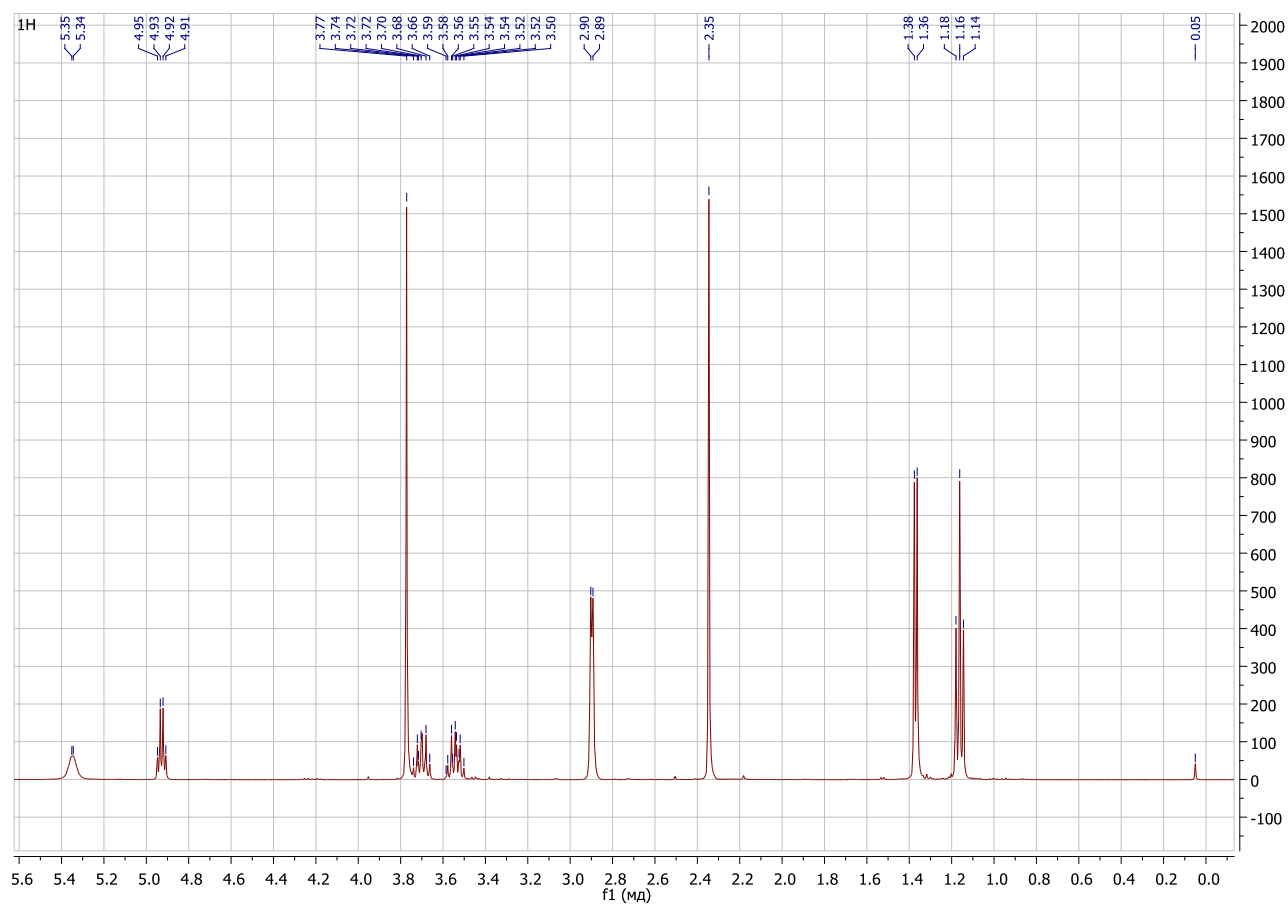


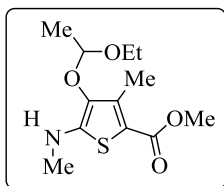
^1H - ^{13}C -HSQC Spectrum of compound **2s**:



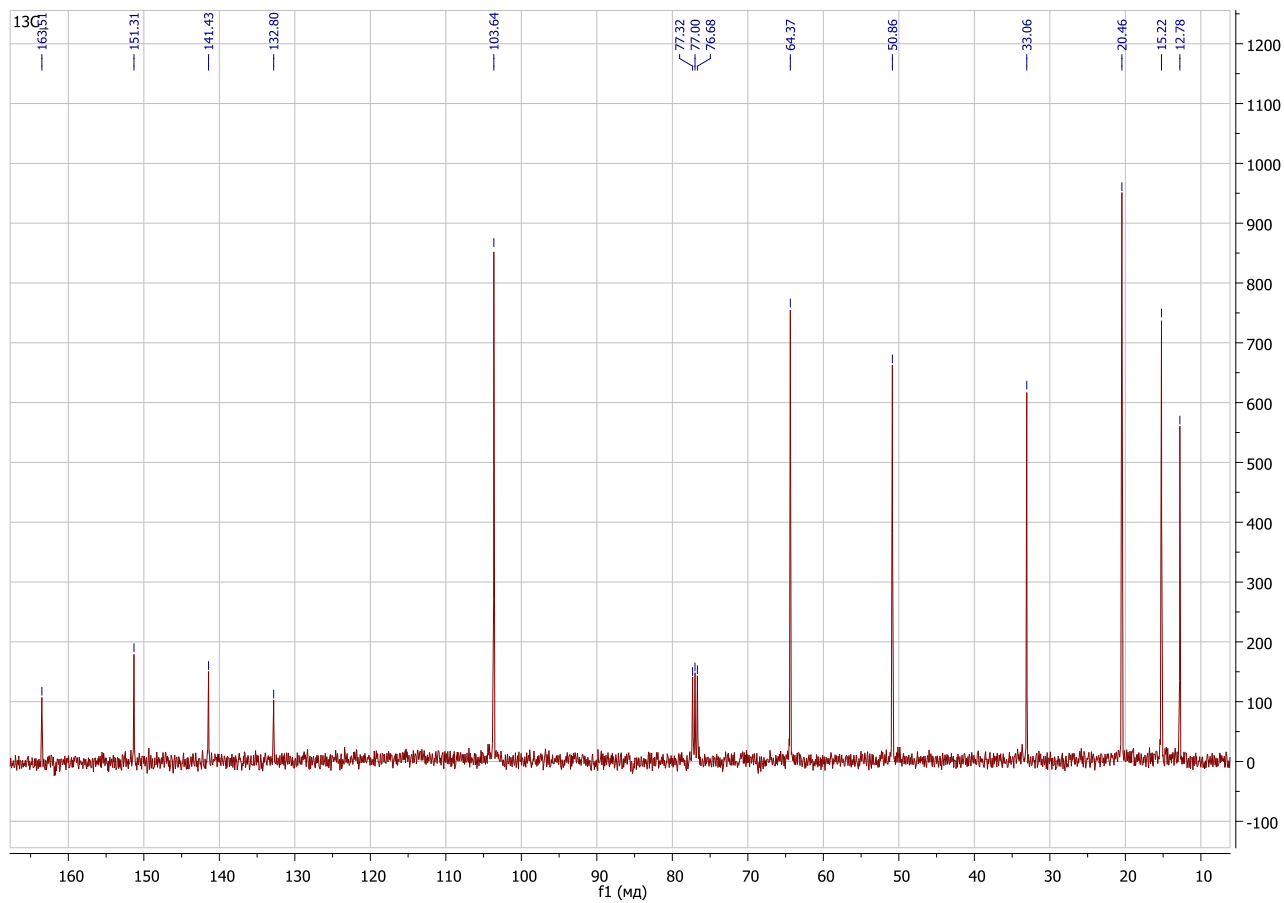


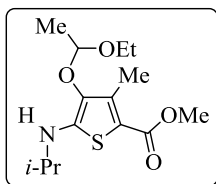
^1H NMR Spectrum of Methyl 4-(1-ethoxyethoxy)-3-methyl-5-(methylamino)thiophene-2-carboxylate (2t)



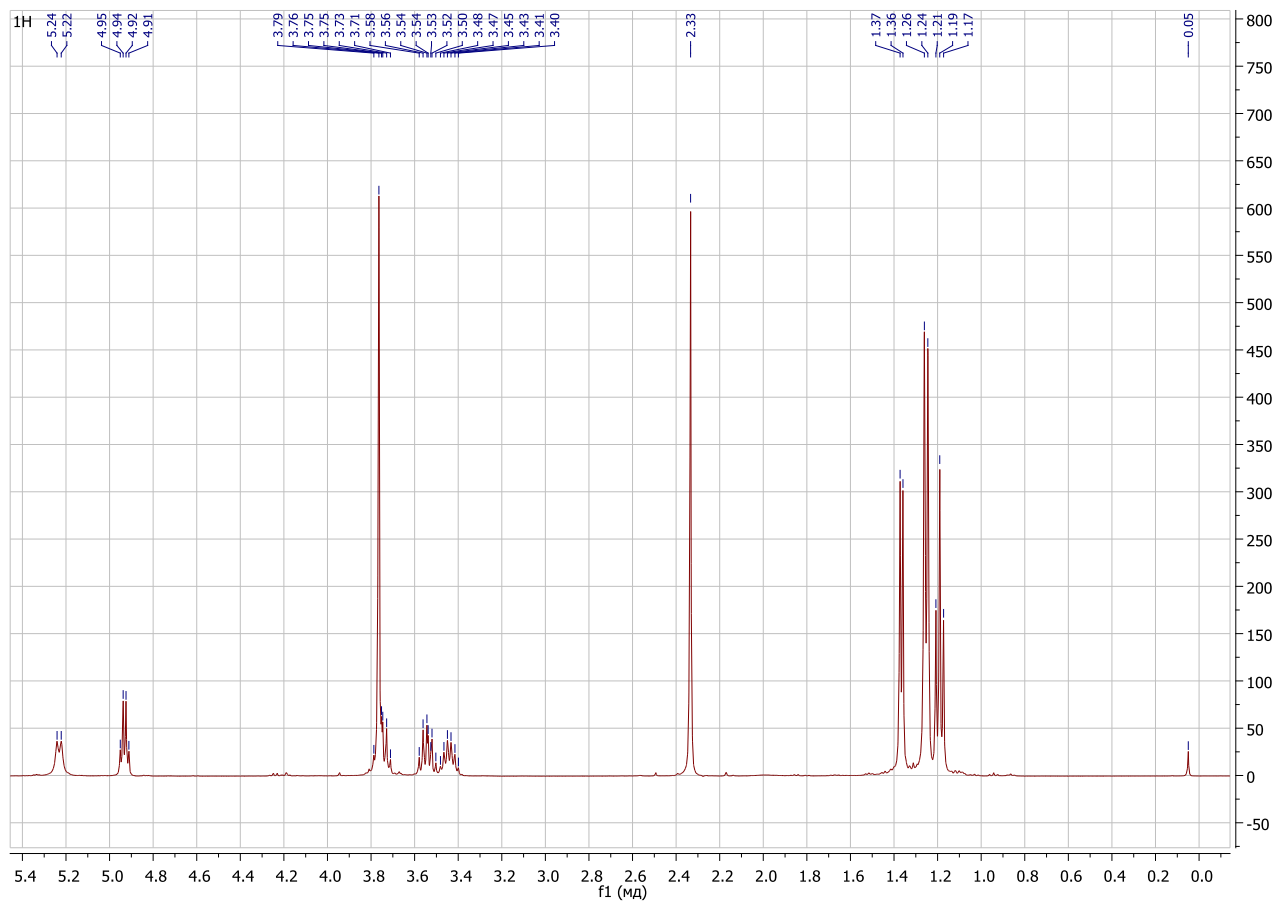


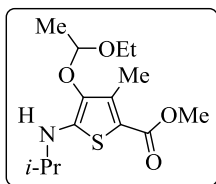
^{13}C NMR Spectrum of Methyl 4-(1-ethoxyethoxy)-3-methyl-5-(methylamino)thiophene-2-carboxylate (2t)



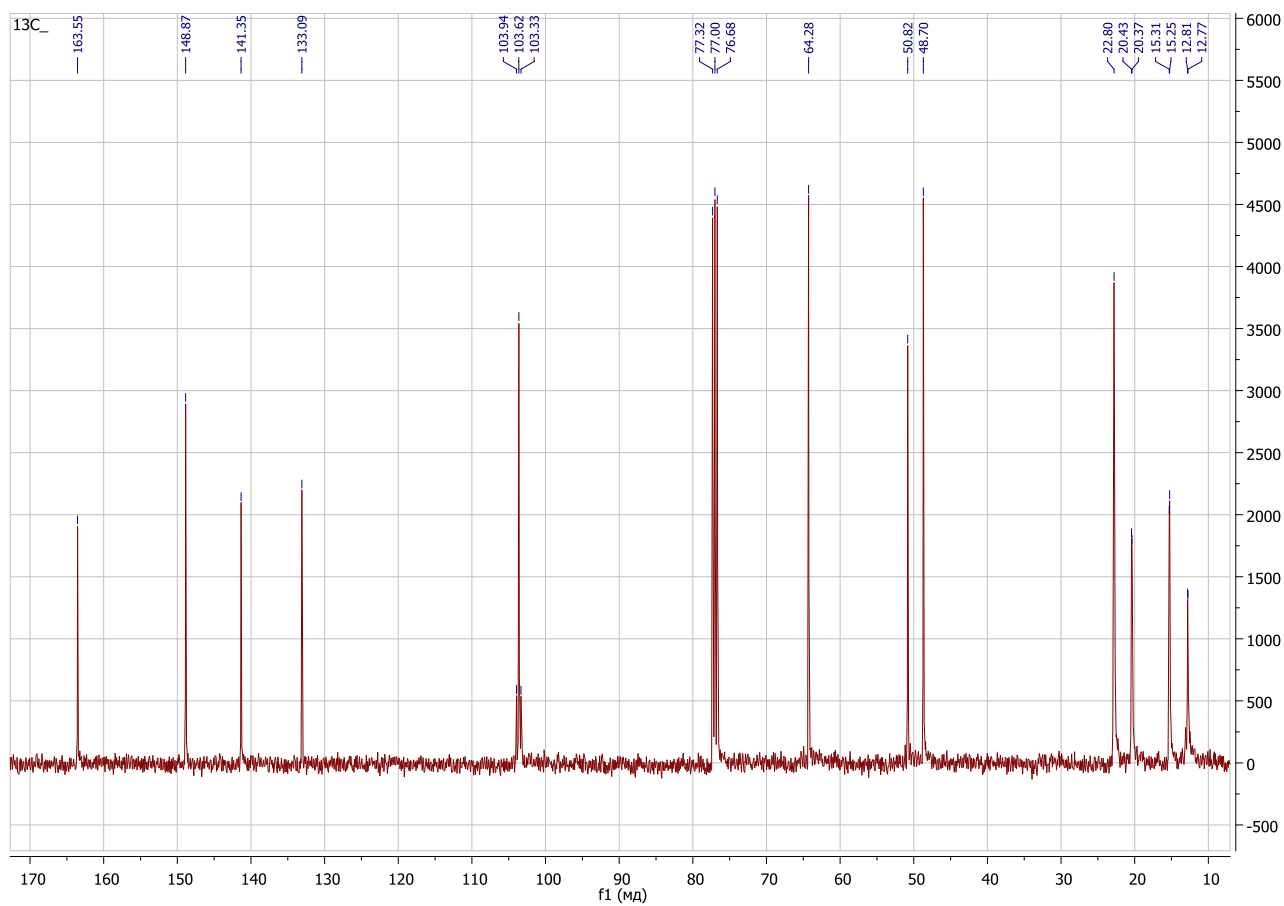


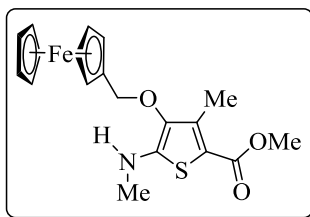
^1H NMR Spectrum of Methyl 4-(1-ethoxyethoxy)-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2u)



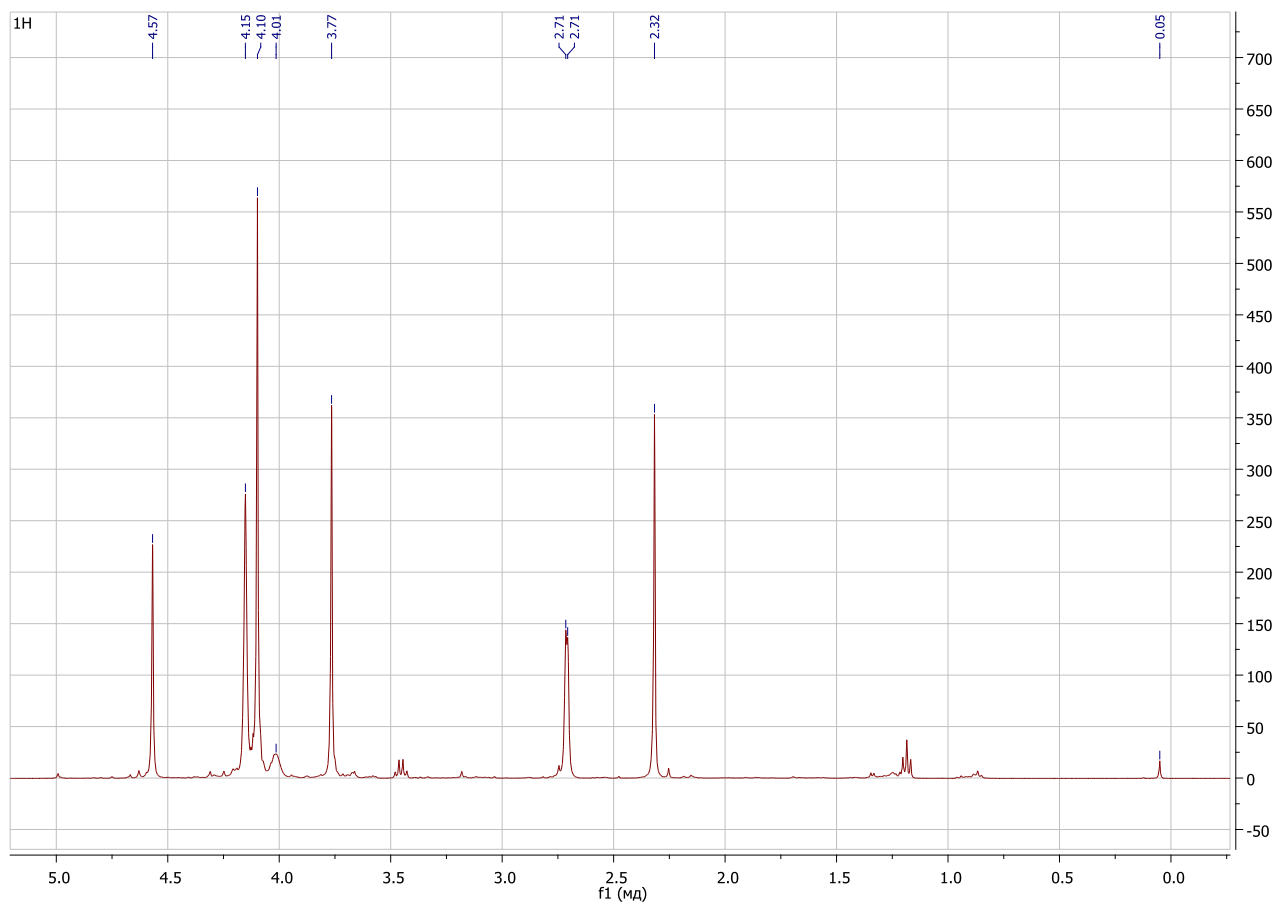


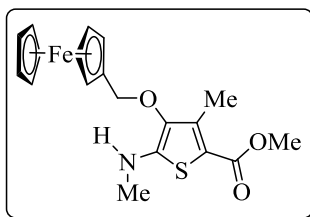
^{13}C NMR Spectrum of Methyl 4-(1-ethoxyethoxy)-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2u)



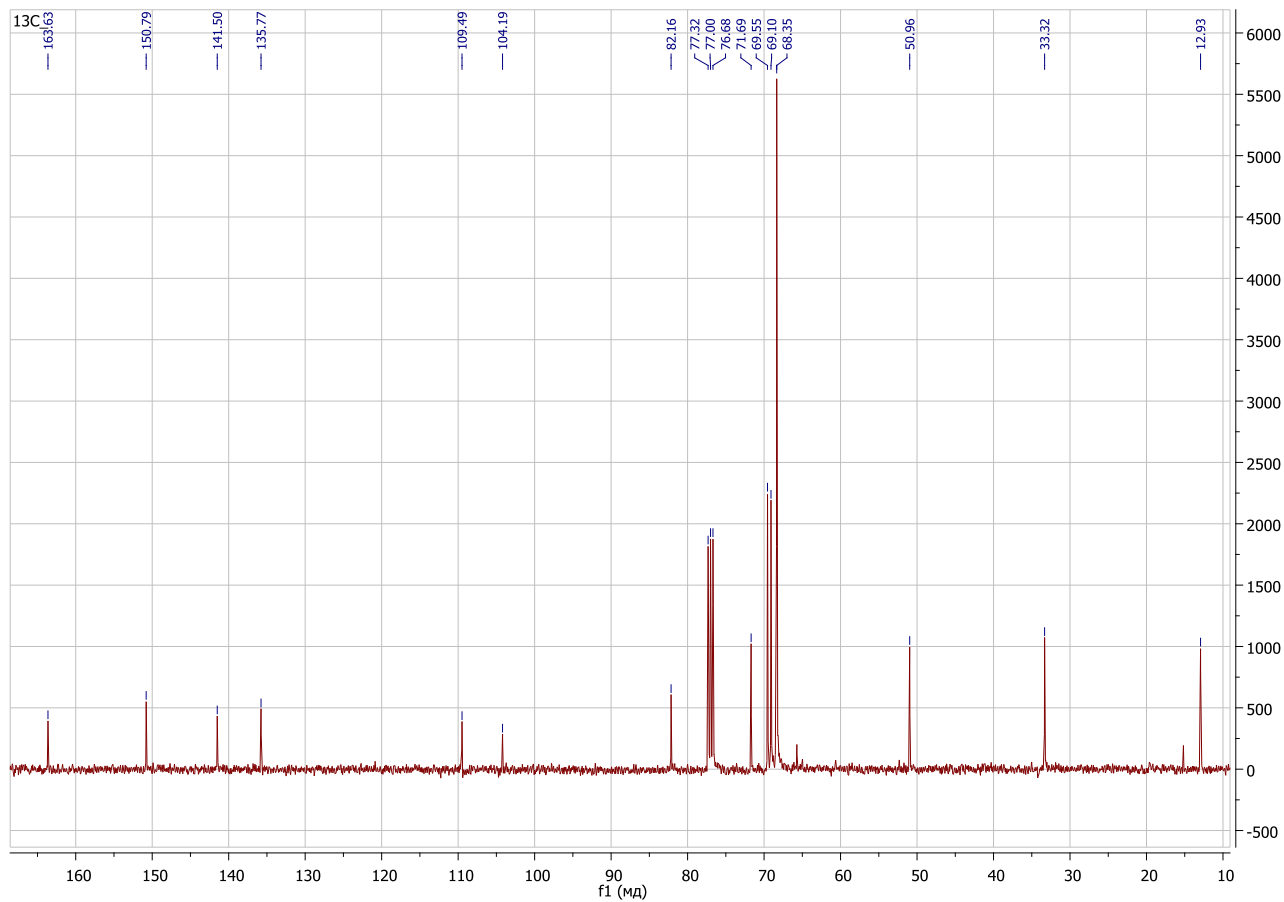


^1H NMR Spectrum of Methyl 4-(ferrocenylmethoxy)-3-methyl-5-(methylamino)thiophene-2-carboxylate (2v)

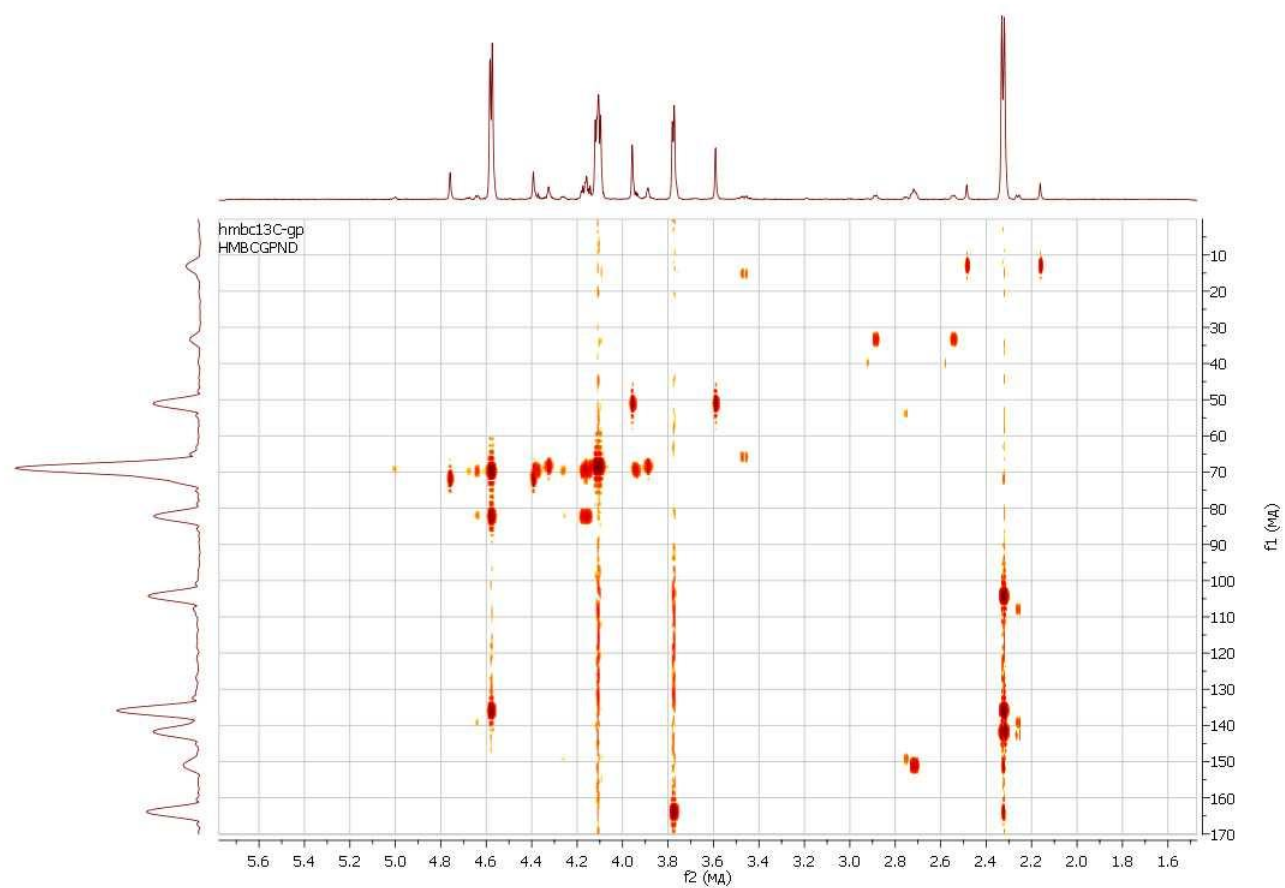




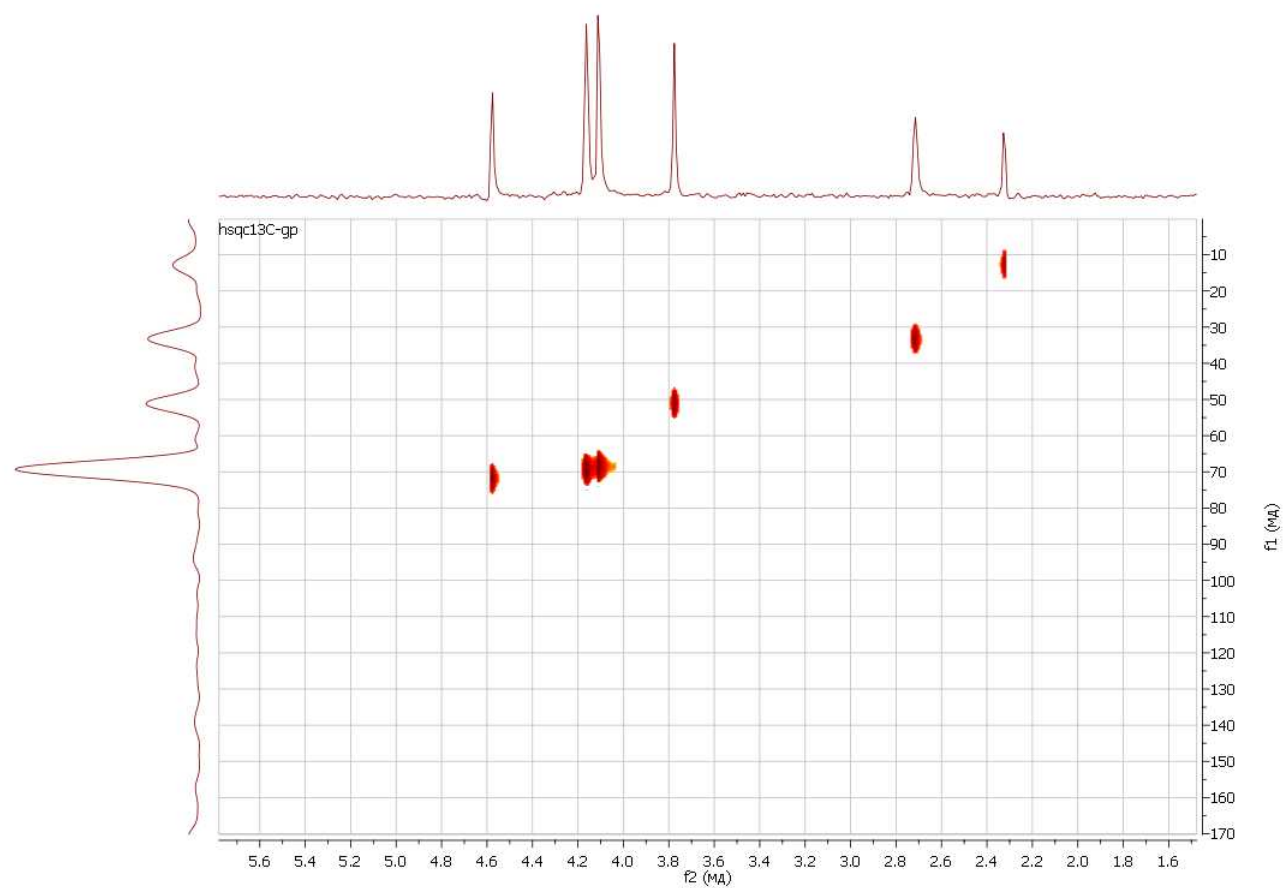
^{13}C NMR Spectrum of Methyl 4-(ferrocenylmethoxy)-3-methyl-5-(methylamino)thiophene-2-carboxylate (2v)

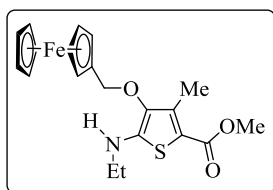


^1H - ^{13}C -HMBC Spectrum of compound **2v**:

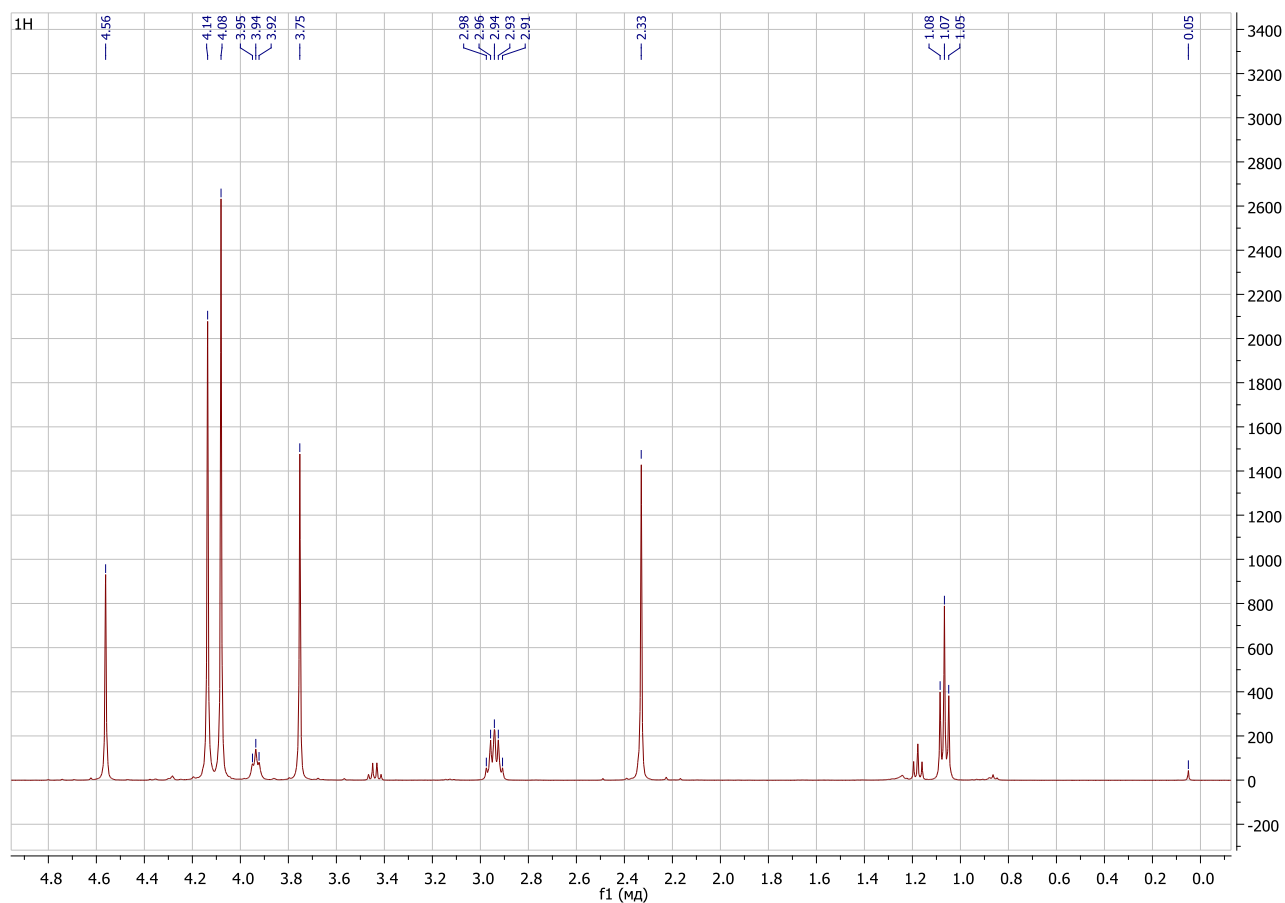


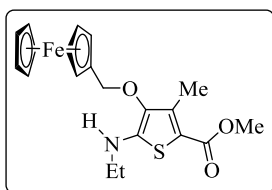
^1H - ^{13}C -HSQC Spectrum of compound **2v**:



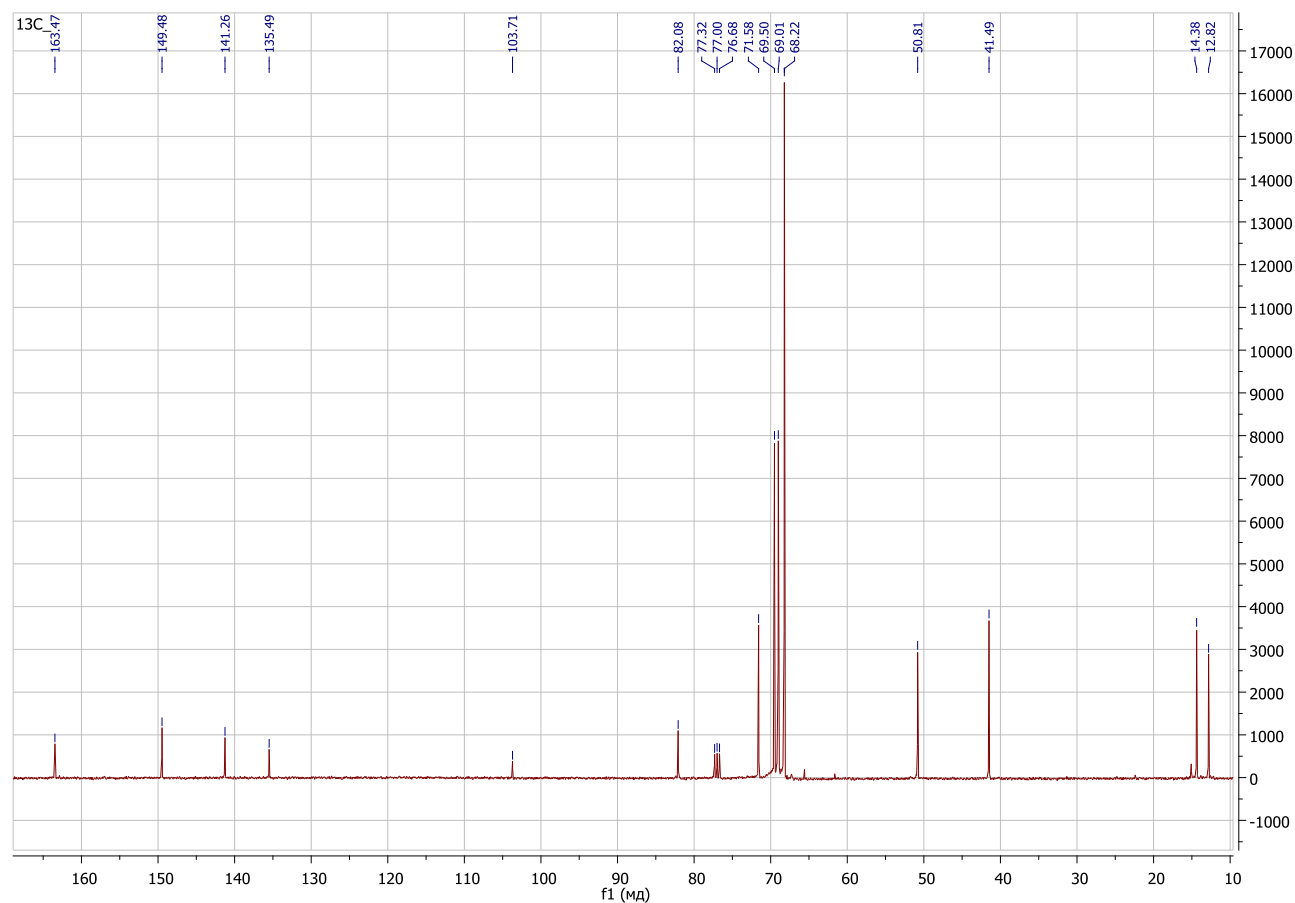


^1H NMR Spectrum of Methyl 5-(ethylamino)-4-(ferrocenylmethoxy)-3-methylthiophene-2-carboxylate (2w)

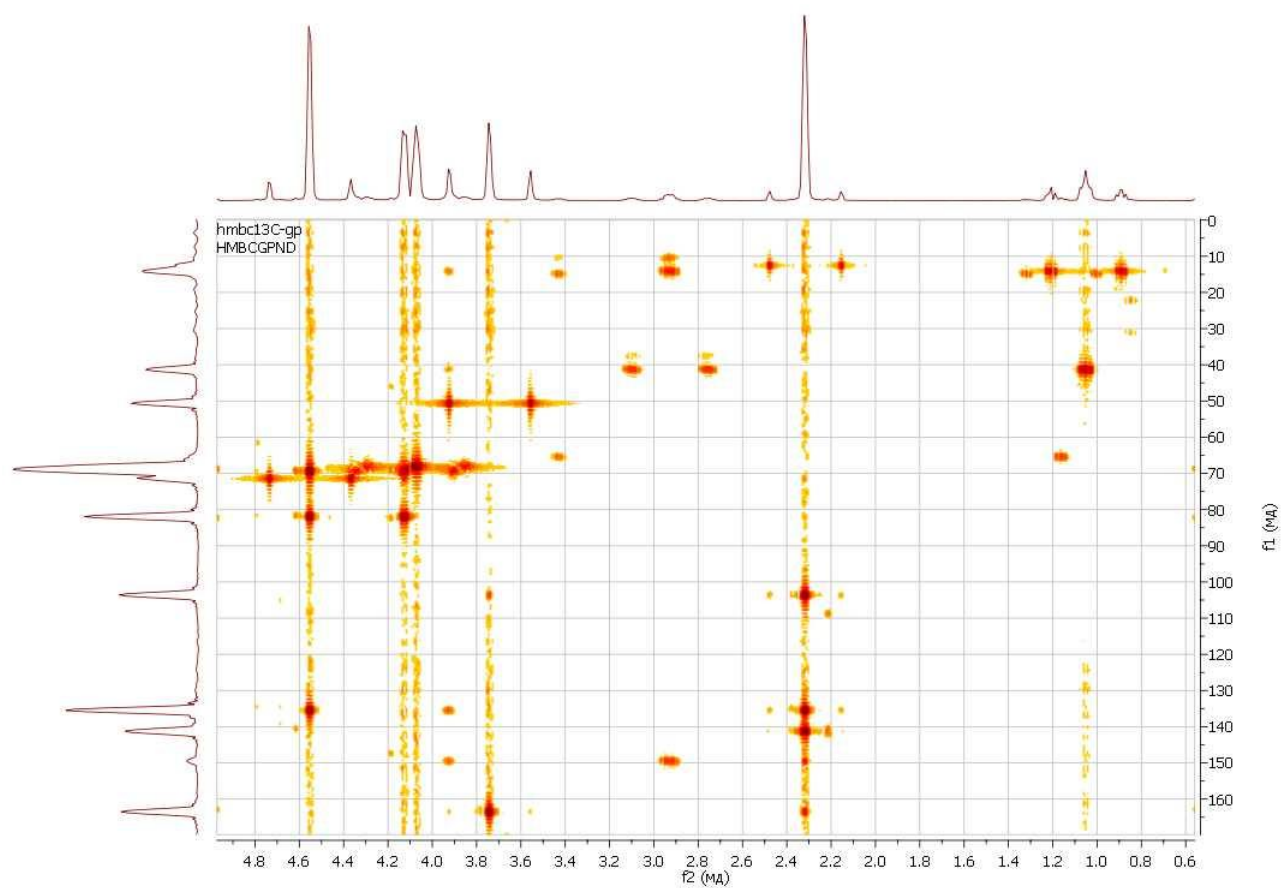




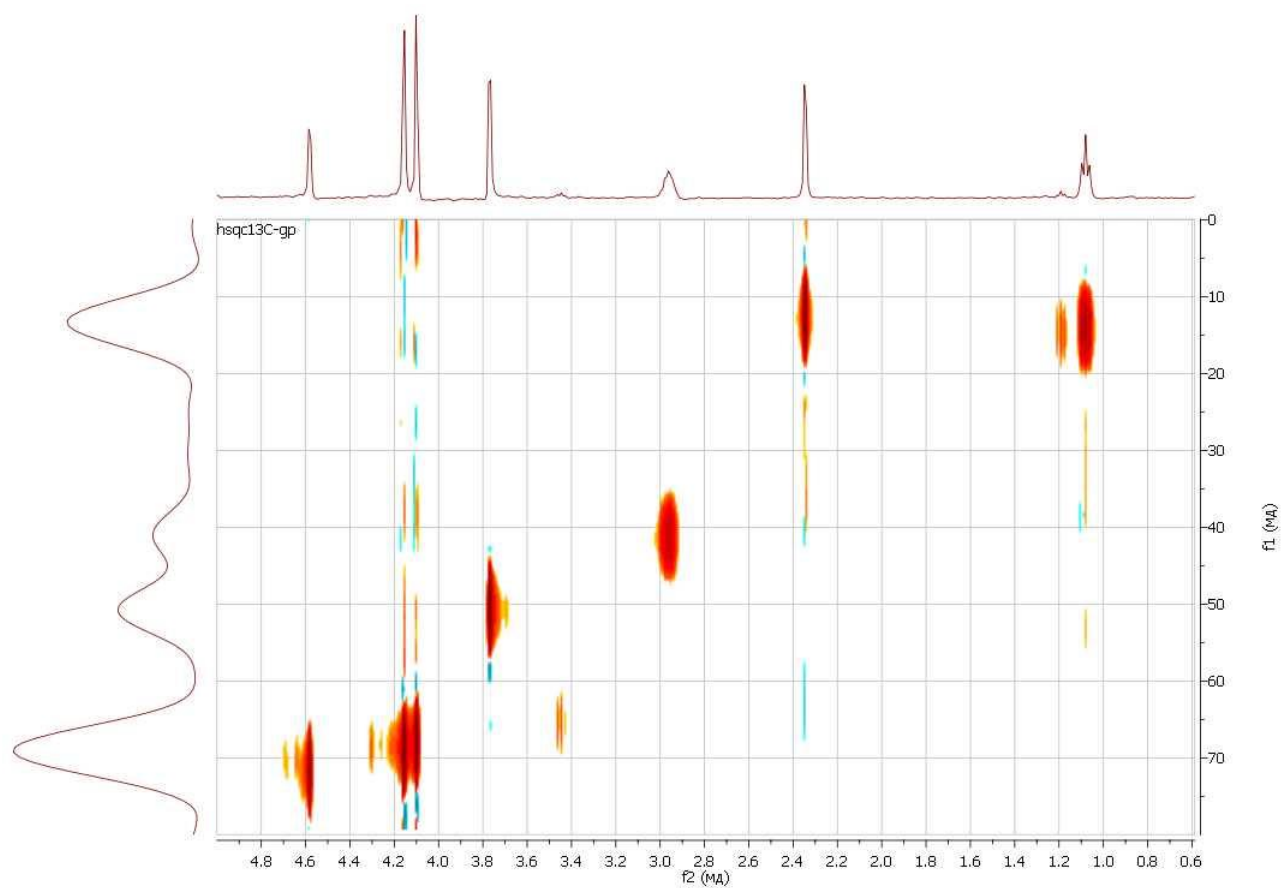
^{13}C NMR Spectrum of Methyl 5-(ethylamino)-4-(ferrocenylmethoxy)-3-methylthiophene-2-carboxylate (2w)

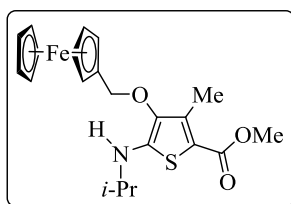


^1H - ^{13}C -HMBC Spectrum of compound **2w**:

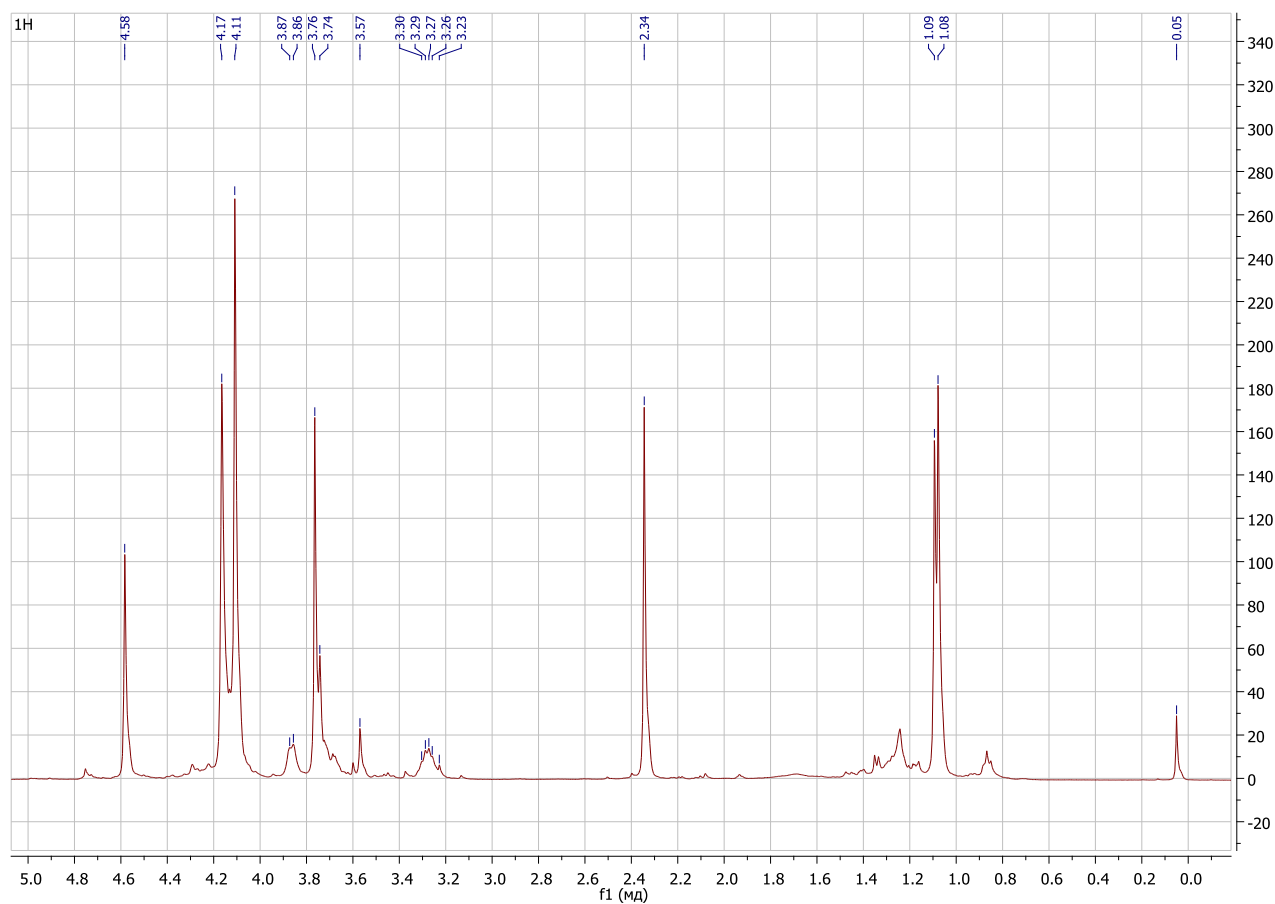


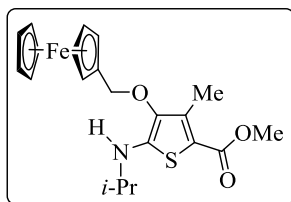
^1H - ^{13}C -HSQC Spectrum of compound **2w**:



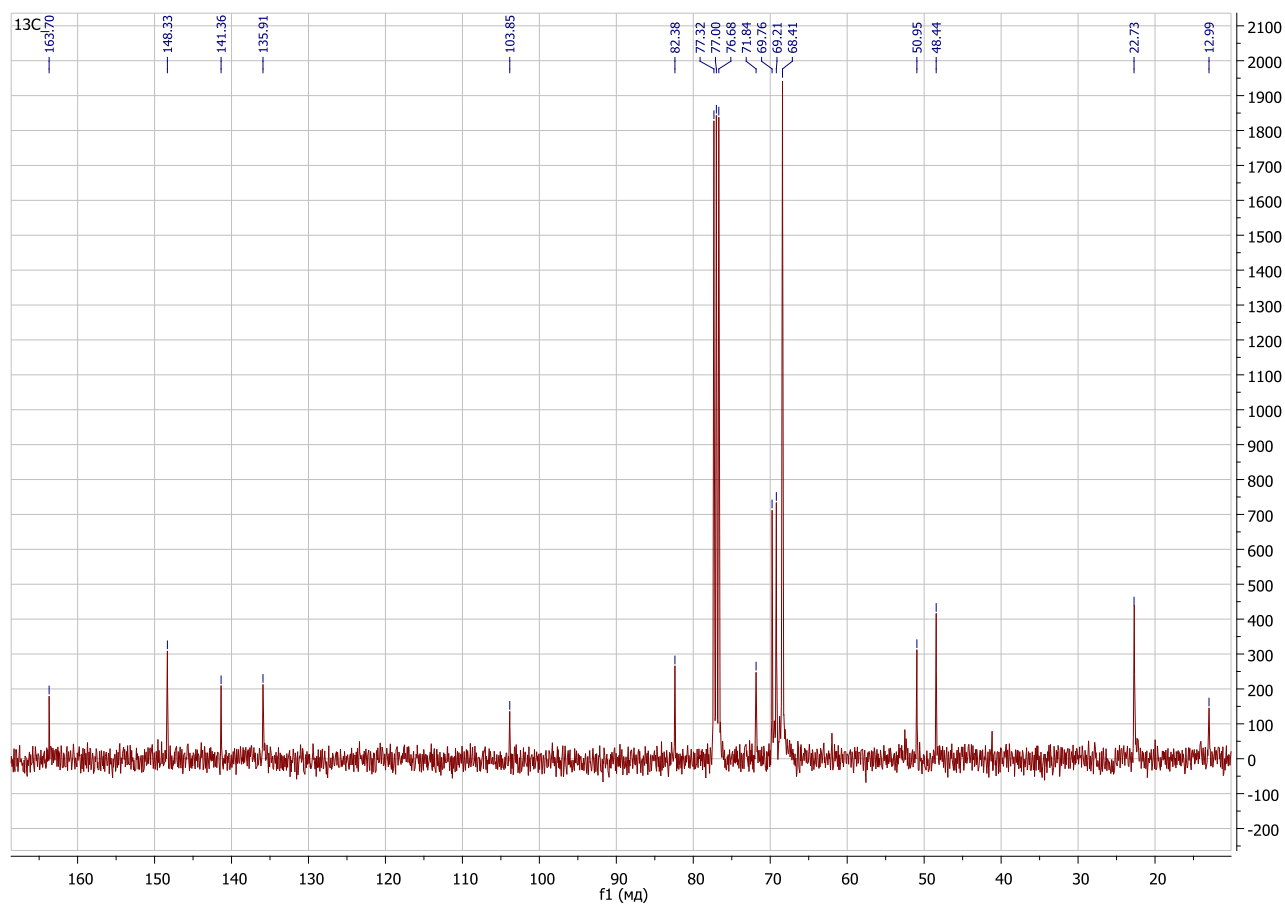


^1H NMR Spectrum of Methyl 4-(ferrocenylmethoxy)-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2x)

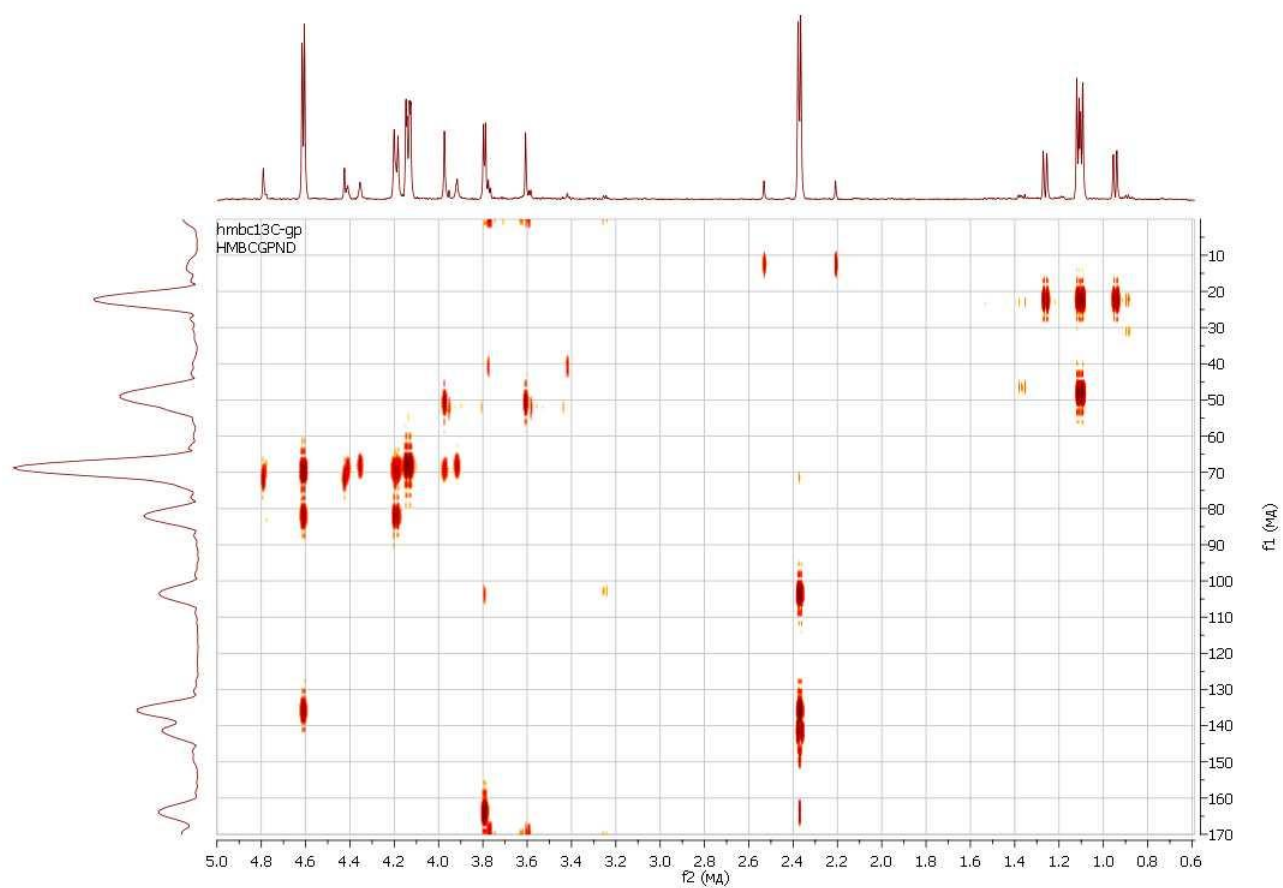


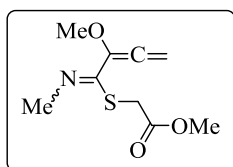


^{13}C NMR Spectrum of Methyl 4-(ferrocenylmethoxy)-5-(isopropylamino)-3-methylthiophene-2-carboxylate (2x)

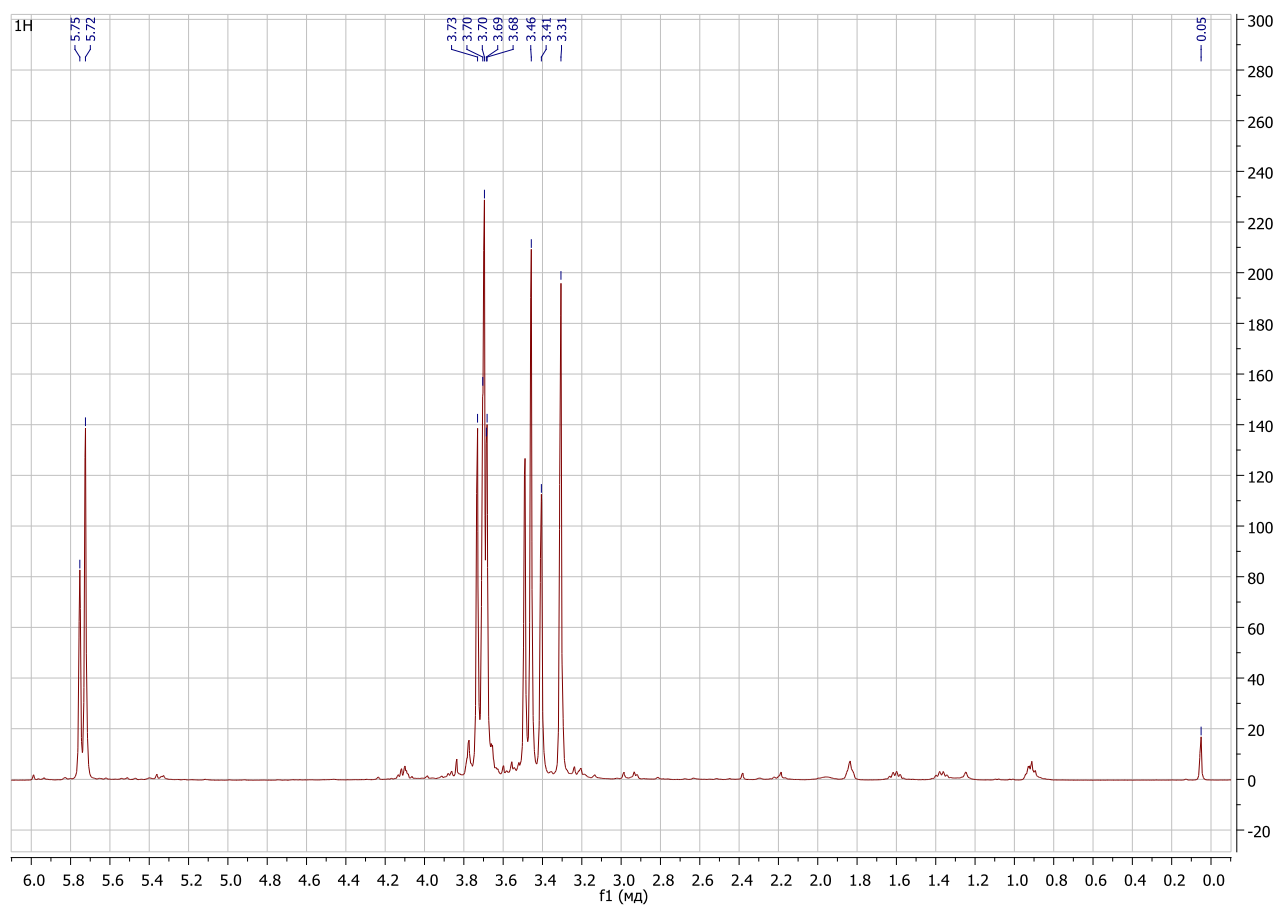


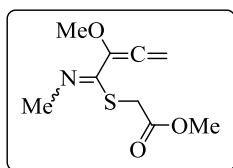
^1H - ^{13}C -HMBC Spectrum of compound **2x**:



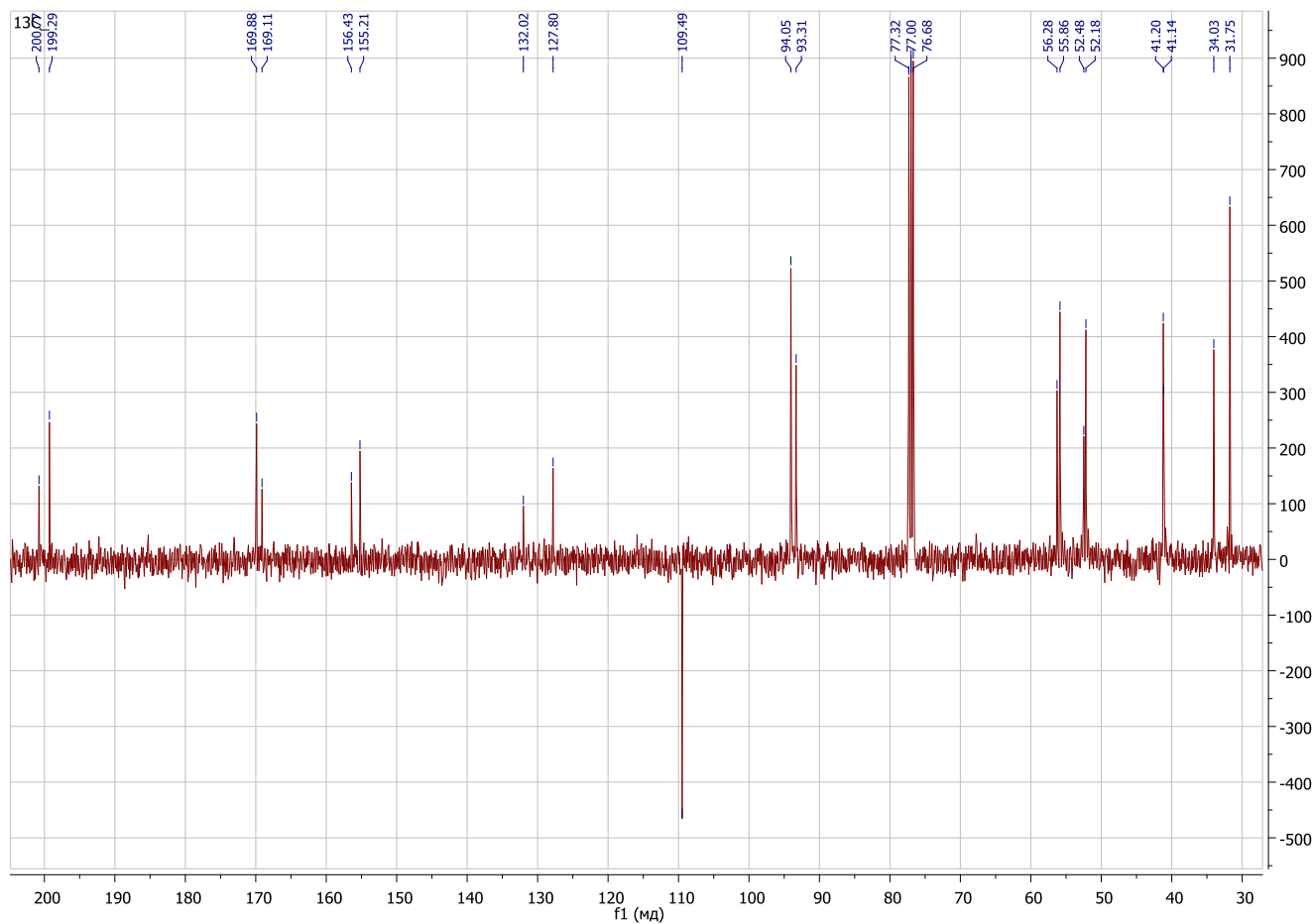


^1H NMR Spectrum of Methyl 2-[[2-methoxy(methyl)buta-2,3-dienimidoyl]sulfanyl]acetate (3a)

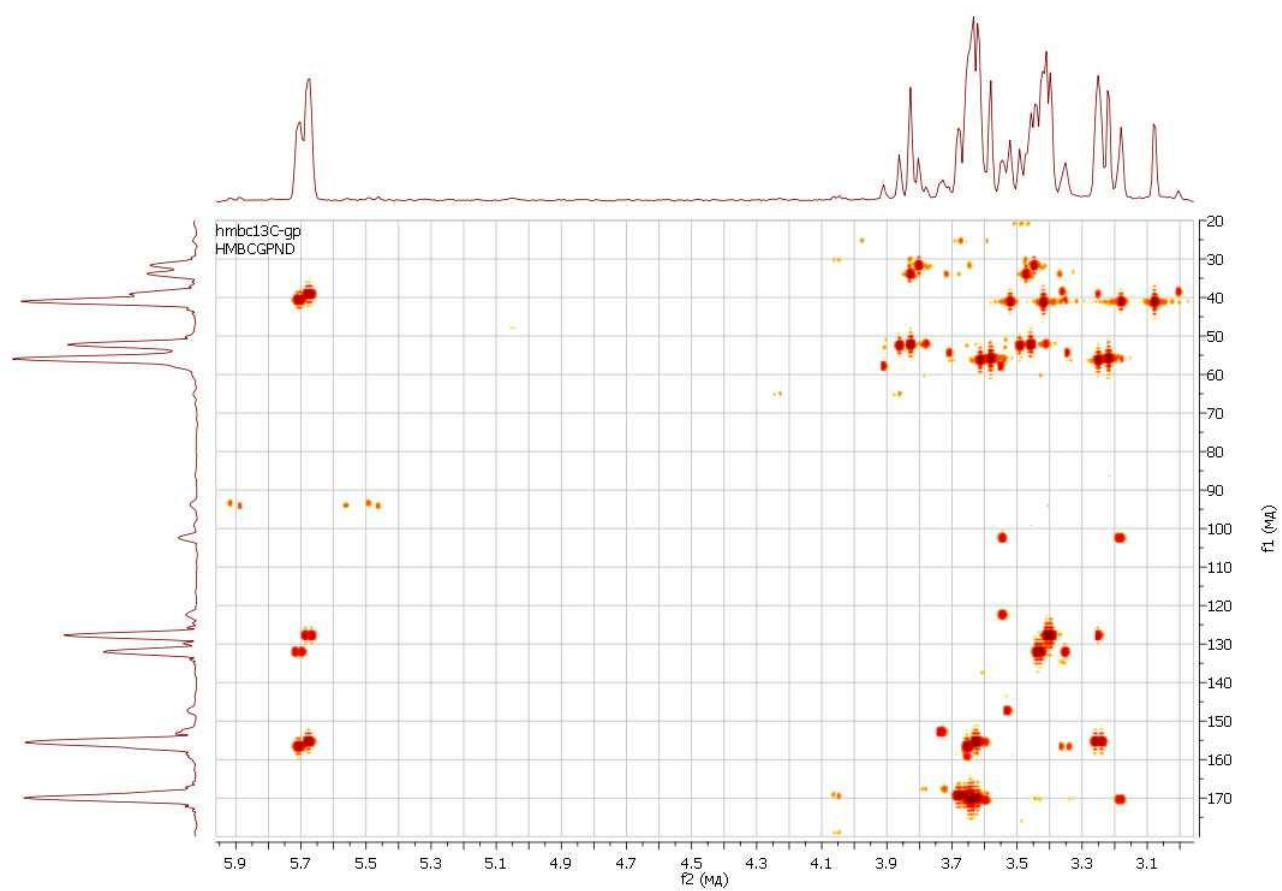




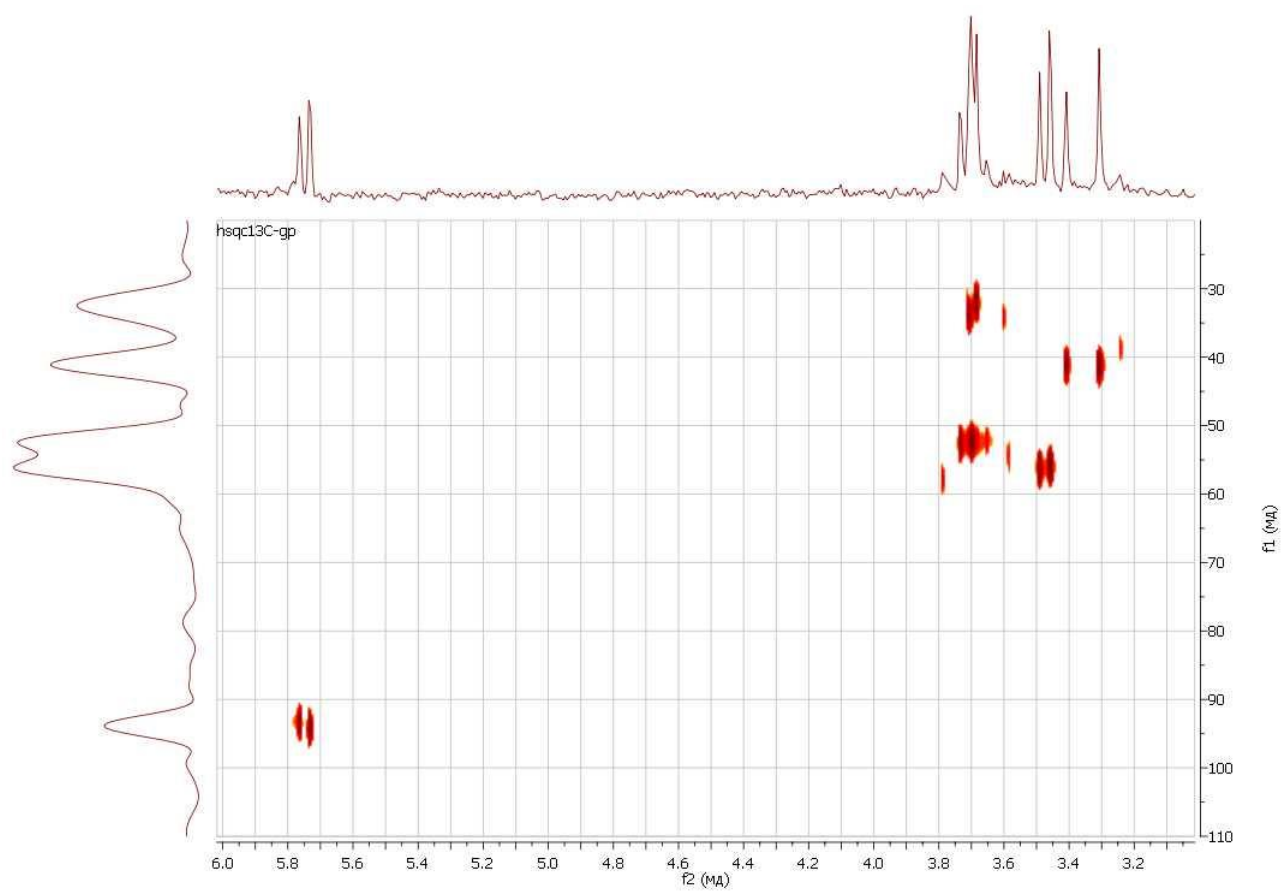
^{13}C NMR Spectrum of Methyl 2-([2-methoxy(methyl)buta-2,3-dienimidoyl]sulfanyl)acetate (3a)

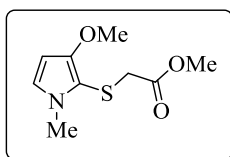


^1H - ^{13}C -HMBC Spectrum of compound **3a**:

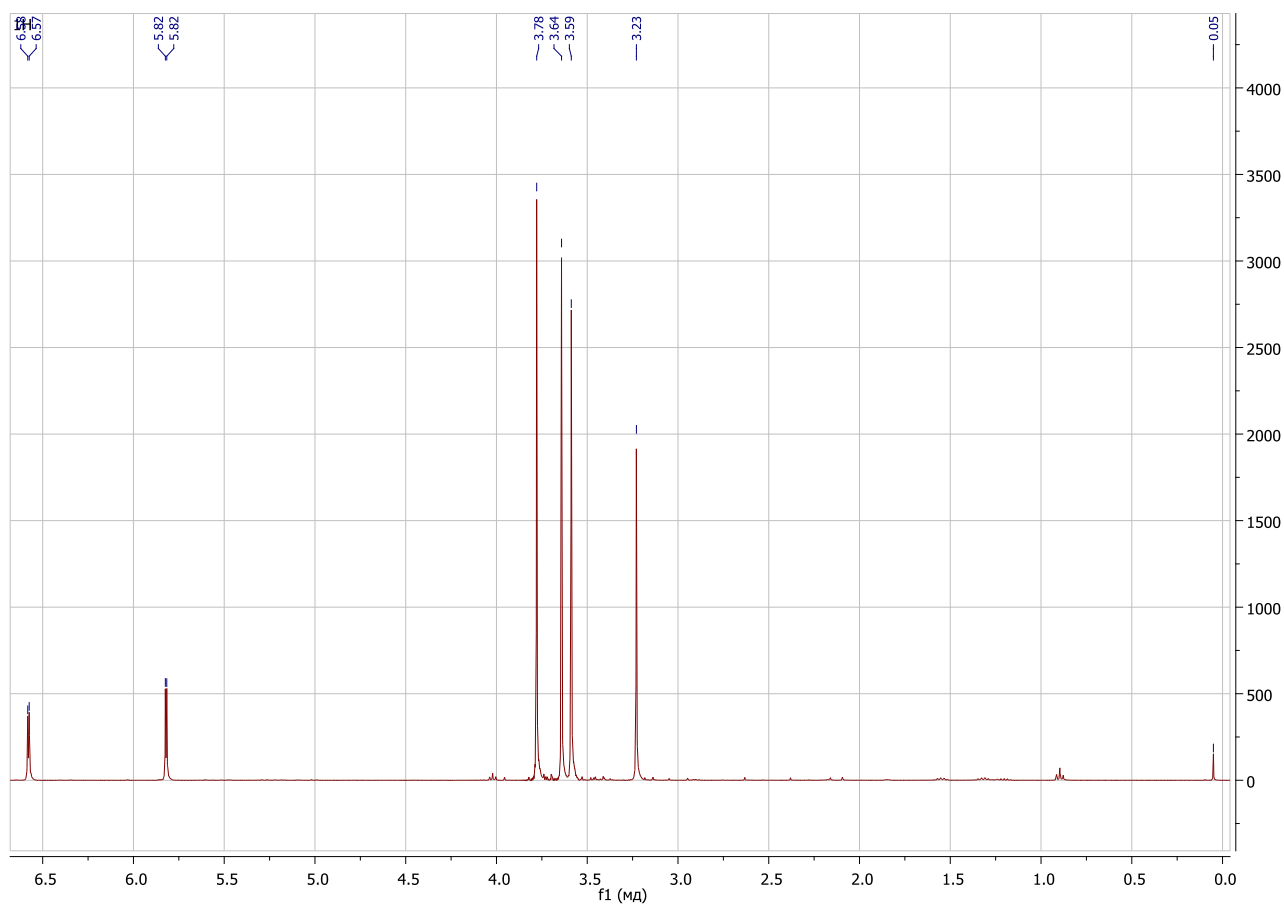


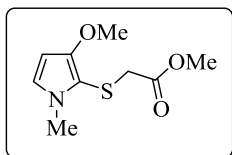
^1H - ^{13}C -HSQC Spectrum of compound **3a**:



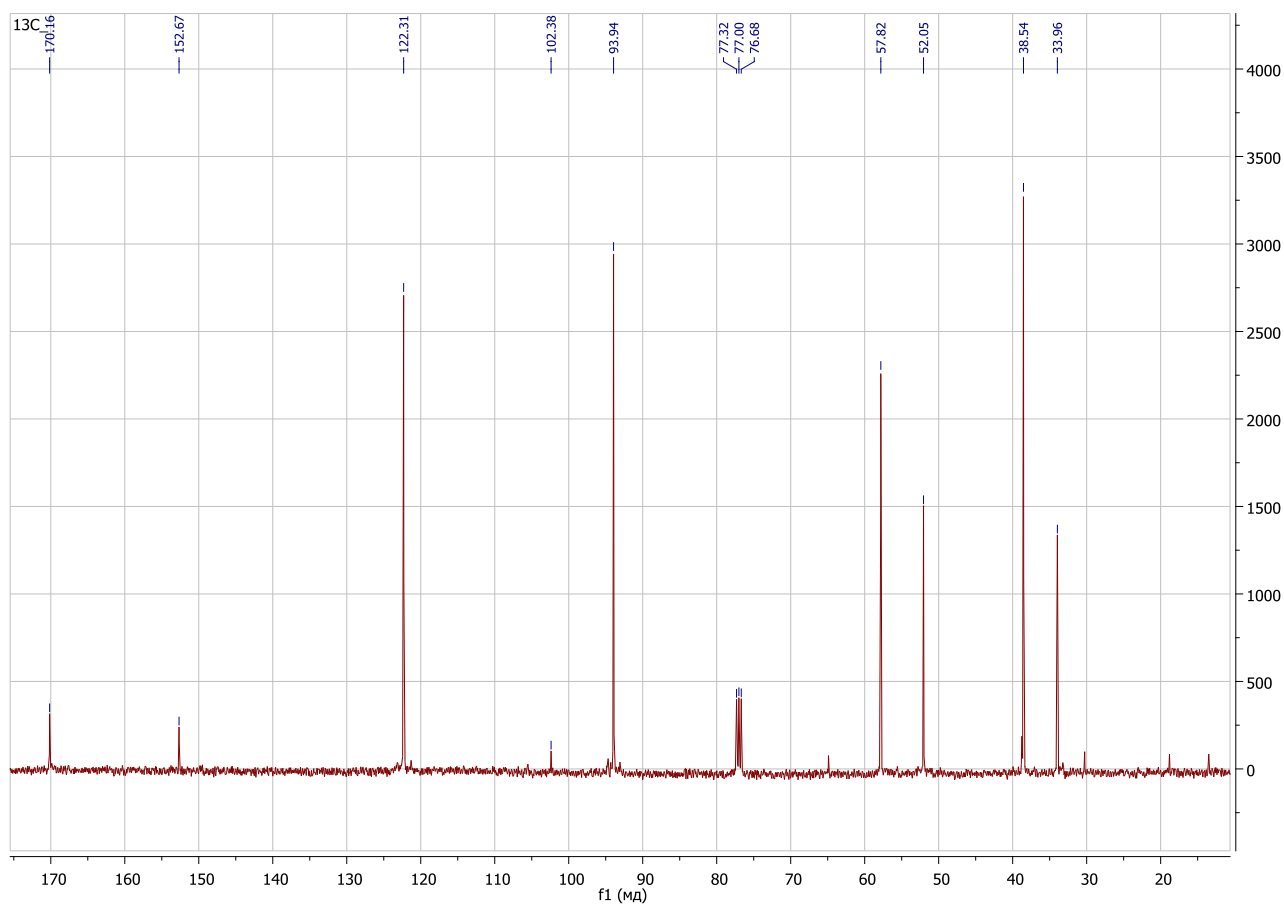


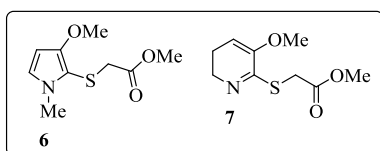
¹H NMR Spectrum of Methyl 2-[(3-methoxy-1-methyl-1*H*-pyrrol-2-yl)sulfanyl]acetate (6)



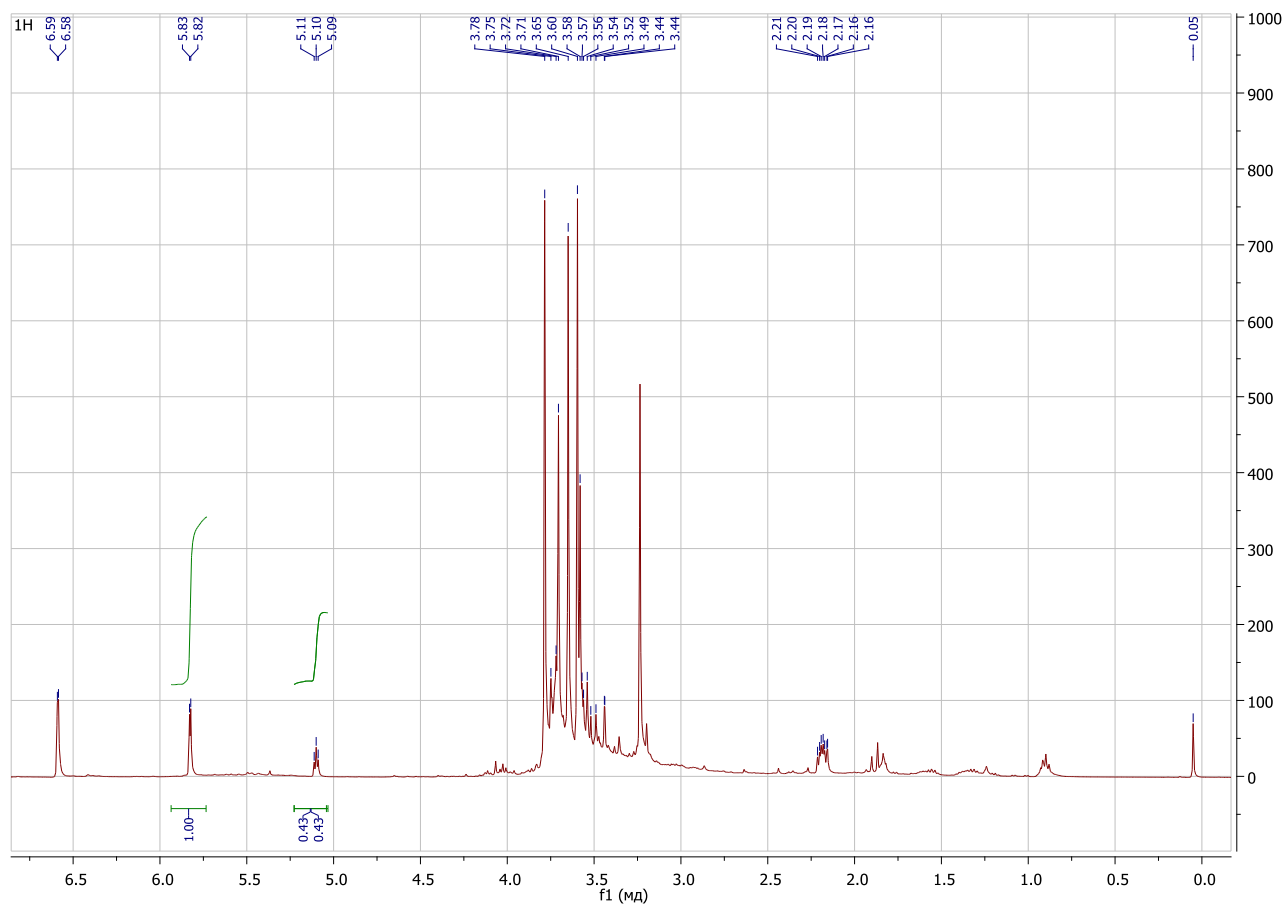


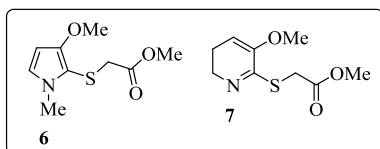
^{13}C NMR Spectrum of Methyl 2-[(3-methoxy-1-methyl-1*H*-pyrrol-2-yl)sulfanyl]acetate (6)



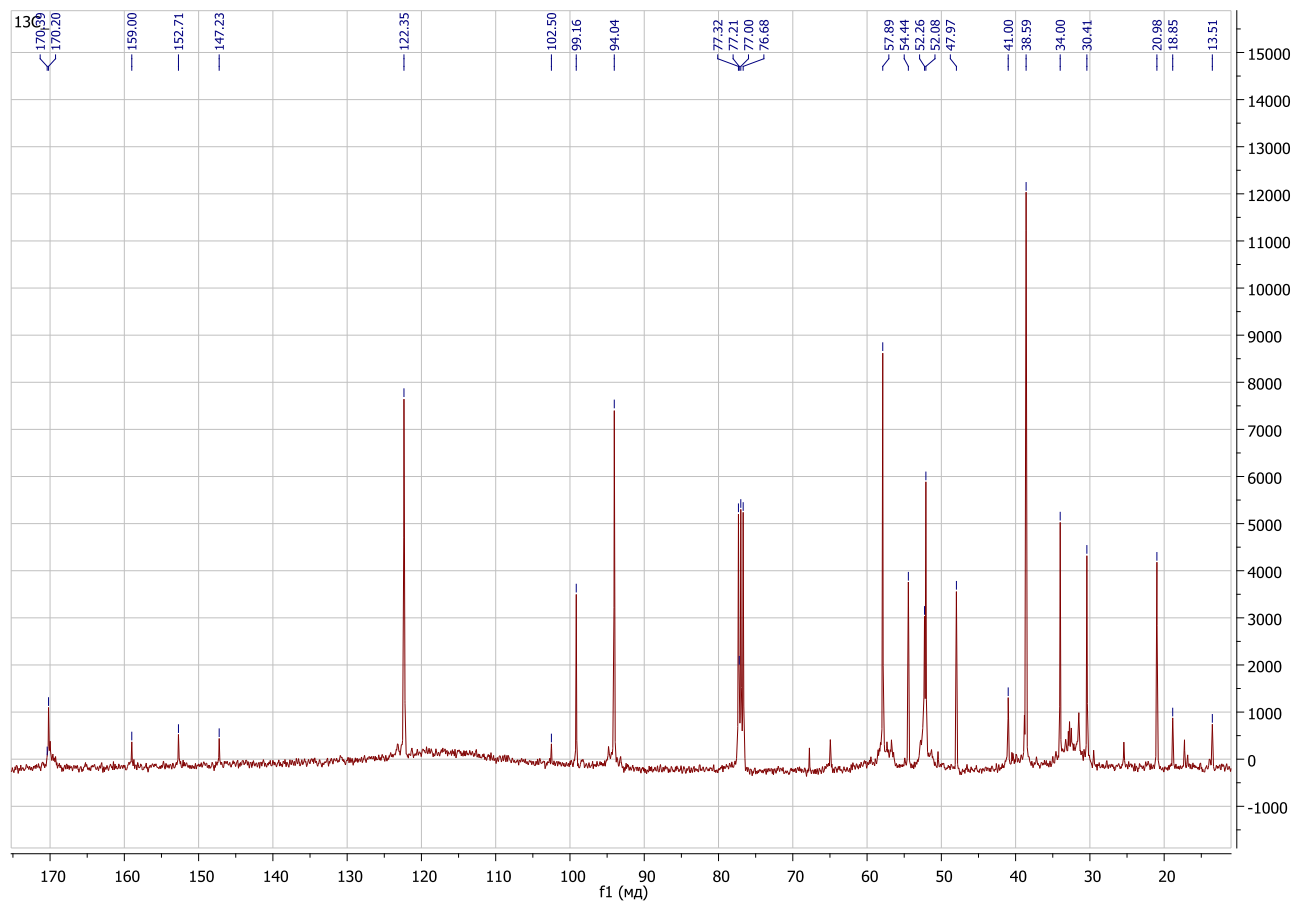


¹H NMR Spectrum of a mixture of 2-[(3-methoxy-1-methyl-1*H*-pyrrol-2-yl)sulfanyl]acetate (6) and methyl 2-[(3-methoxy-5,6-dihydropyridin-2-yl)sulfanyl]acetate (7)

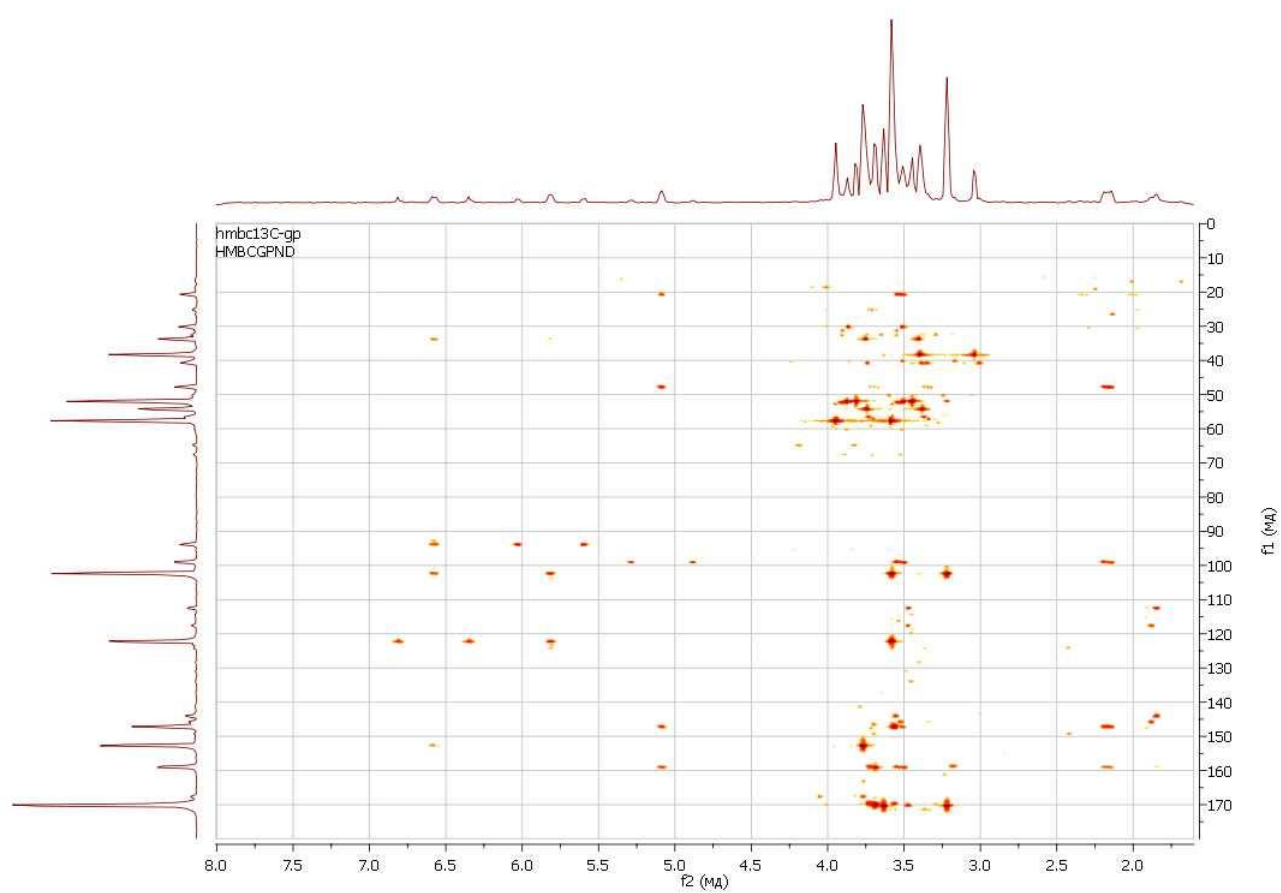




^{13}C NMR Spectrum of a mixture of 2-[(3-methoxy-1-methyl-1*H*-pyrrol-2-yl)sulfanyl]acetate (6) and methyl 2-[(3-methoxy-5,6-dihydropyridin-2-yl)sulfanyl]acetate (7)



^1H - ^{13}C -HMBC Spectrum of a mixture of compounds **6** and **7**:



^1H - ^{13}C -HSQC Spectrum of a mixture of compounds **6** and **7**:

