

Supporting Information

Simple assembly of polysubstituted pyrazoles and isoxazoles via ring closure–ring opening domino reaction of 3-acyl-4,5-dihydrofurans with hydrazines and hydroxylamine

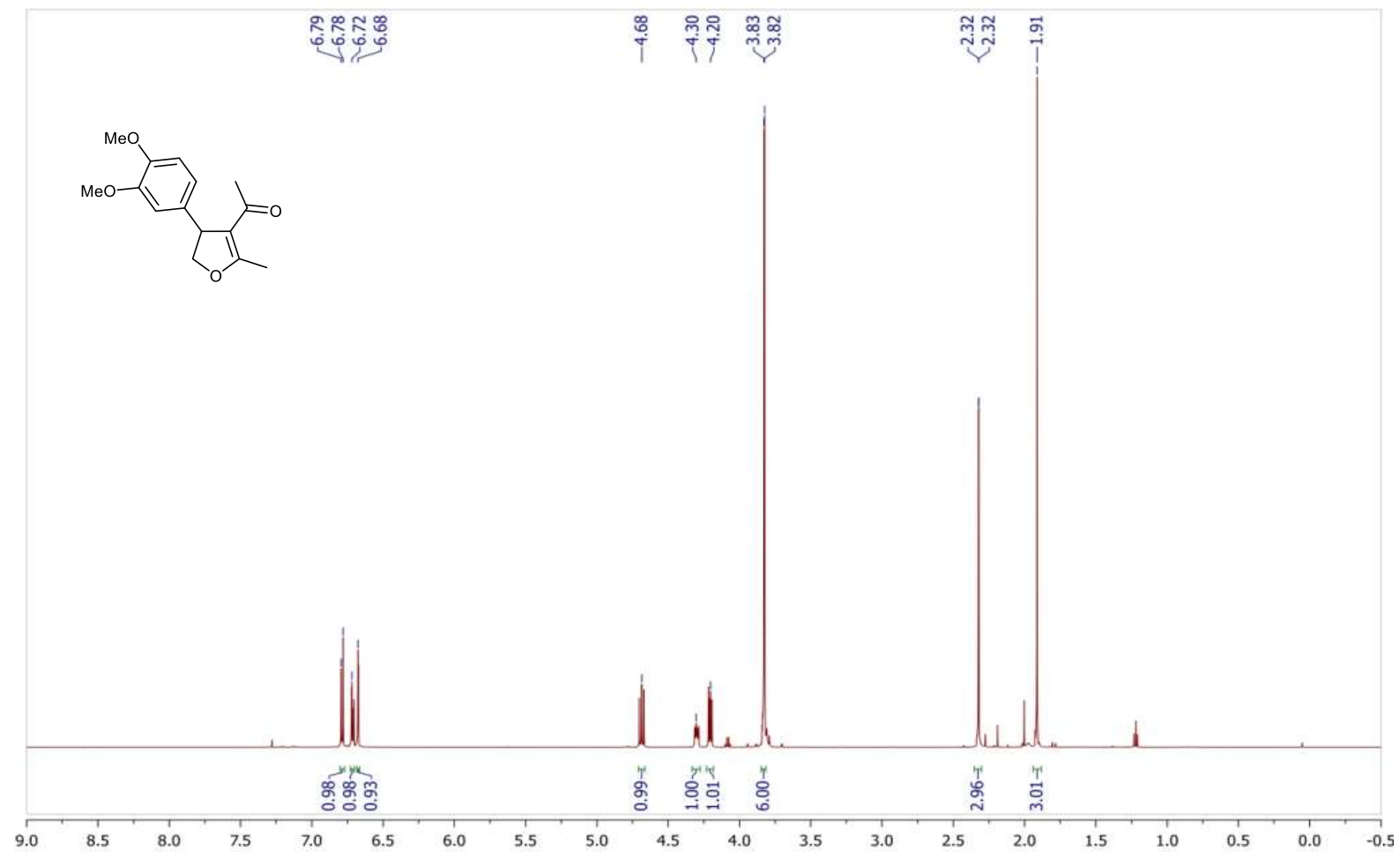
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Igor V. Trushkov,^{†,‡,*} Mikhail Ya. Melnikov[†]

[†]Department of Chemistry, M. V. Lomonosov Moscow State University, Leninskie gory 1-3, Moscow 119991 Russia, e-mail:
trush@phys.chem.msu.ru

[‡]Federal Research Center of Pediatric Hematology, Oncology and Immunology named after Dmitrii Rogachev, Samory Mashela 1, Moscow 117997
Russia

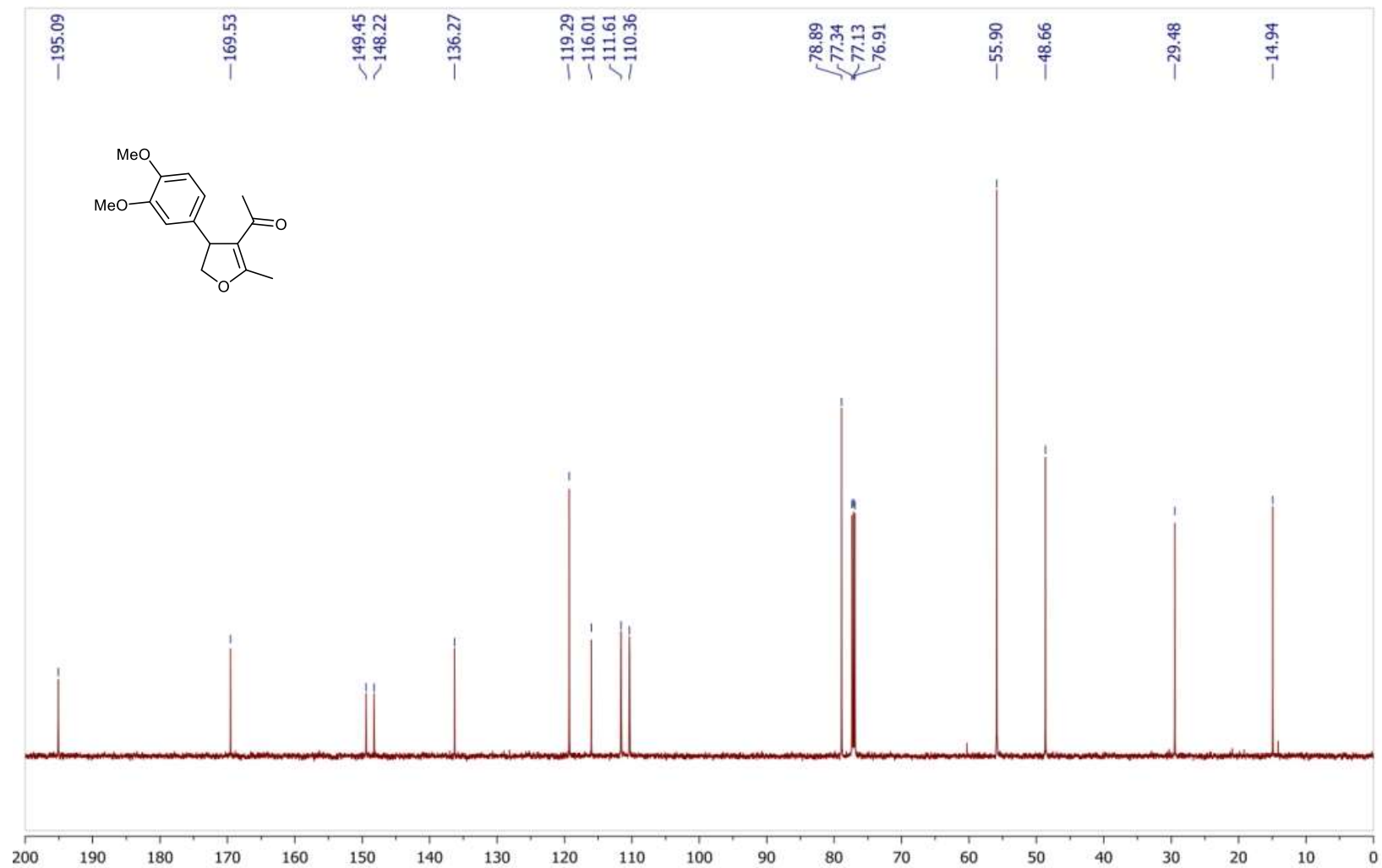
1-[4-(3,4-Dimethoxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethan-1-one (1d)

¹H NMR (CDCl₃, 600 MHz)



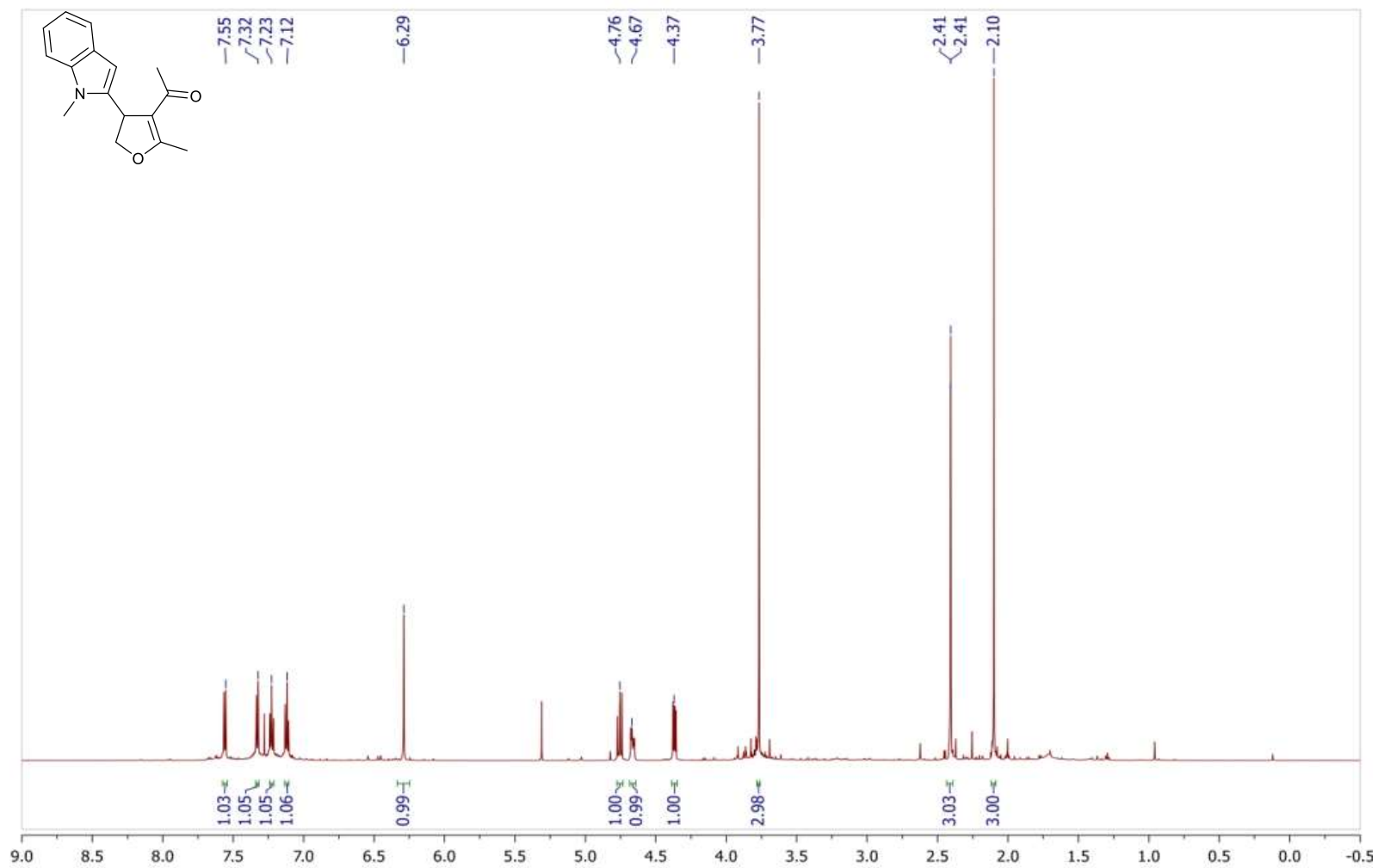
1-[4-(3,4-Dimethoxyphenyl)-2-methyl-4,5-dihydrofuran-3-yl]ethan-1-one (1d)

^{13}C NMR (CDCl_3 , 150 MHz)



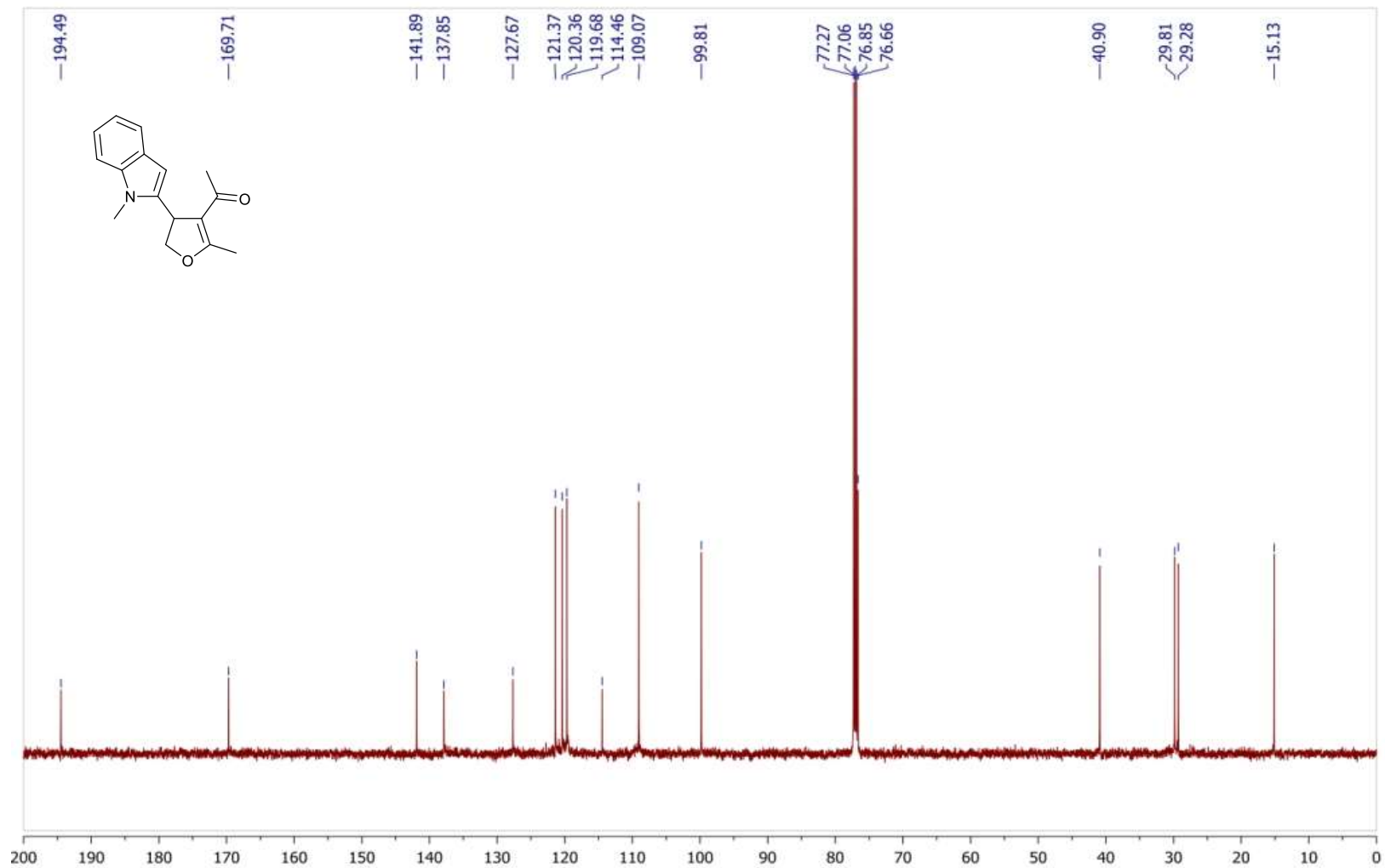
1-[2-Methyl-4-(1-methyl-1H-indol-2-yl)-4,5-dihydrofuran-3-yl]ethan-1-one (1g)

¹H NMR (CDCl₃, 600 MHz)



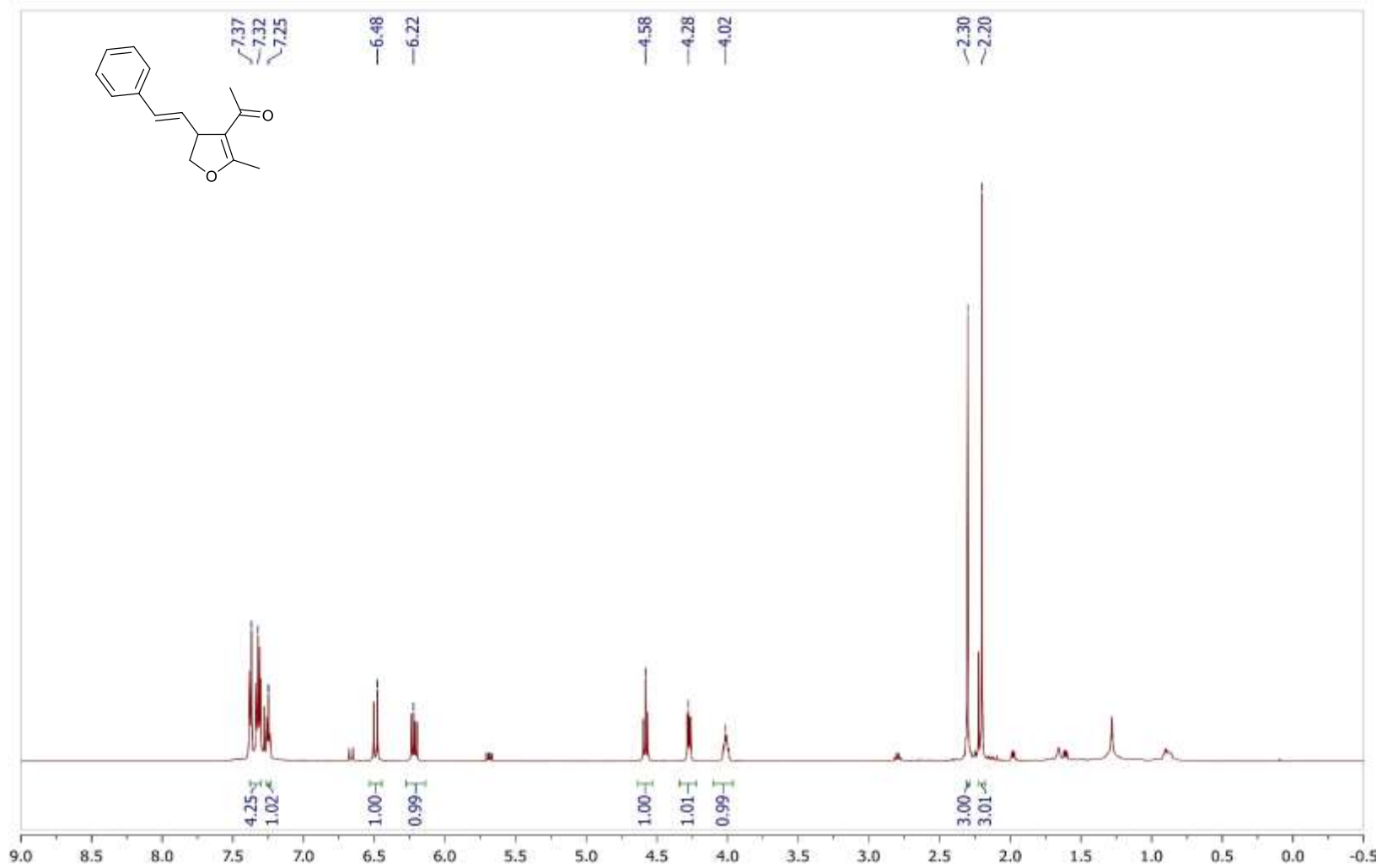
1-[2-Methyl-4-(1-methyl-1H-indol-2-yl)-4,5-dihydrofuran-3-yl]ethan-1-one (1g)

^{13}C NMR (CDCl_3 , 150 MHz)



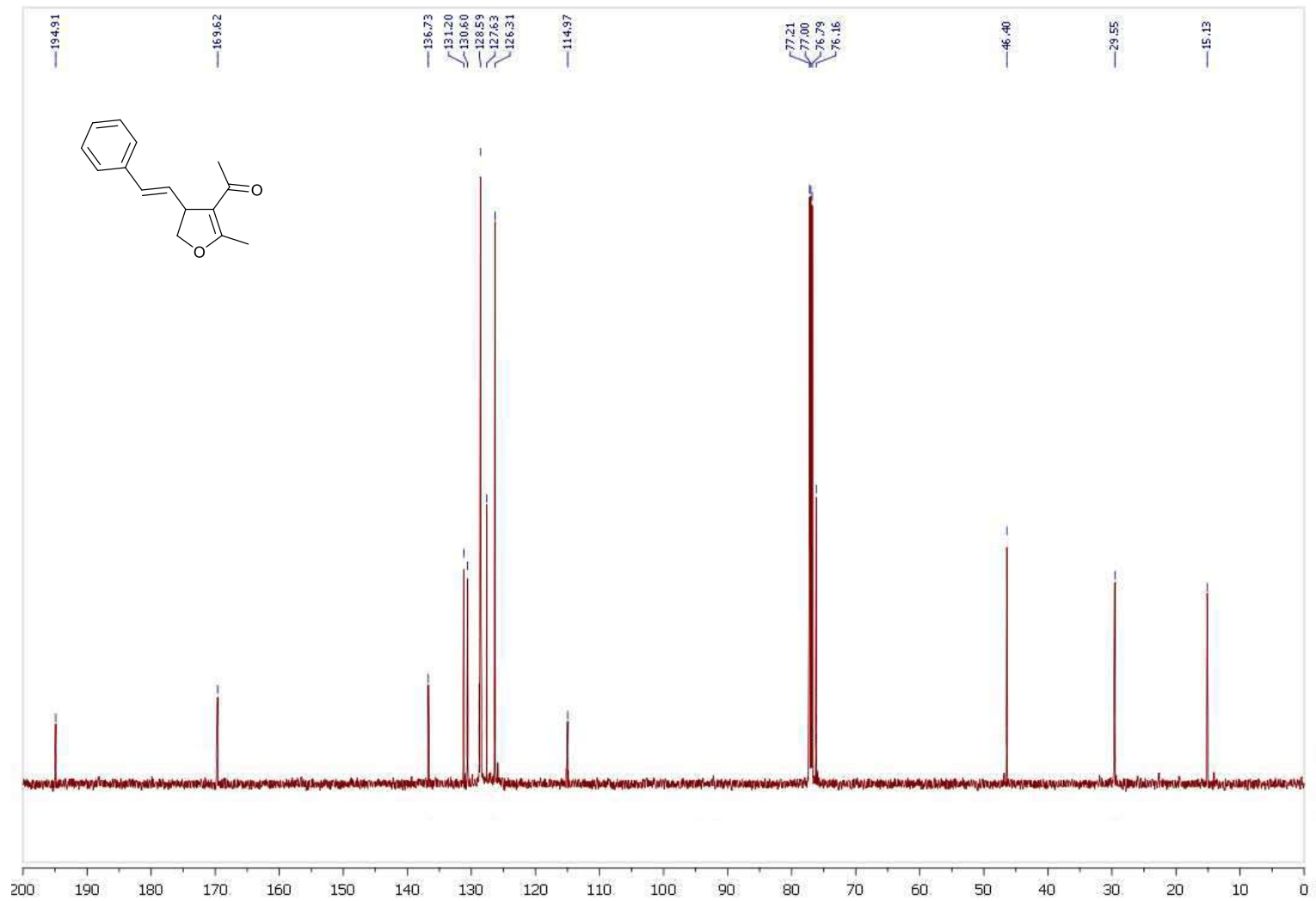
(E)-1-(2-Methyl-4-styryl-4,5-dihydrofuran-3-yl)ethan-1-one (*1h*)

¹H NMR (CDCl₃, 600 MHz)



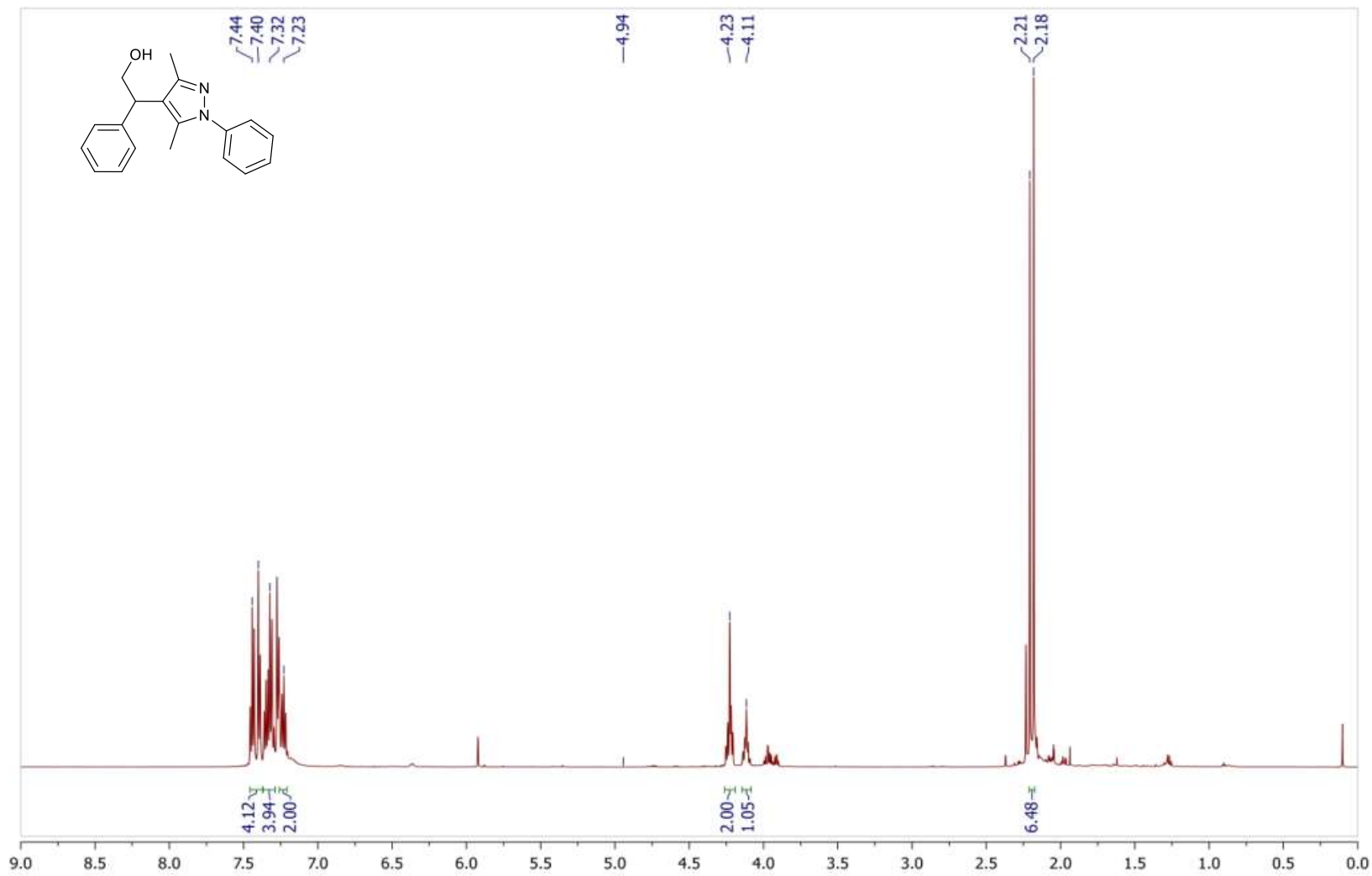
(E)-1-(2-Methyl-4-styryl-4,5-dihydrofuran-3-yl)ethan-1-one (*1h*)

^{13}C NMR (CDCl_3 , 150 MHz)



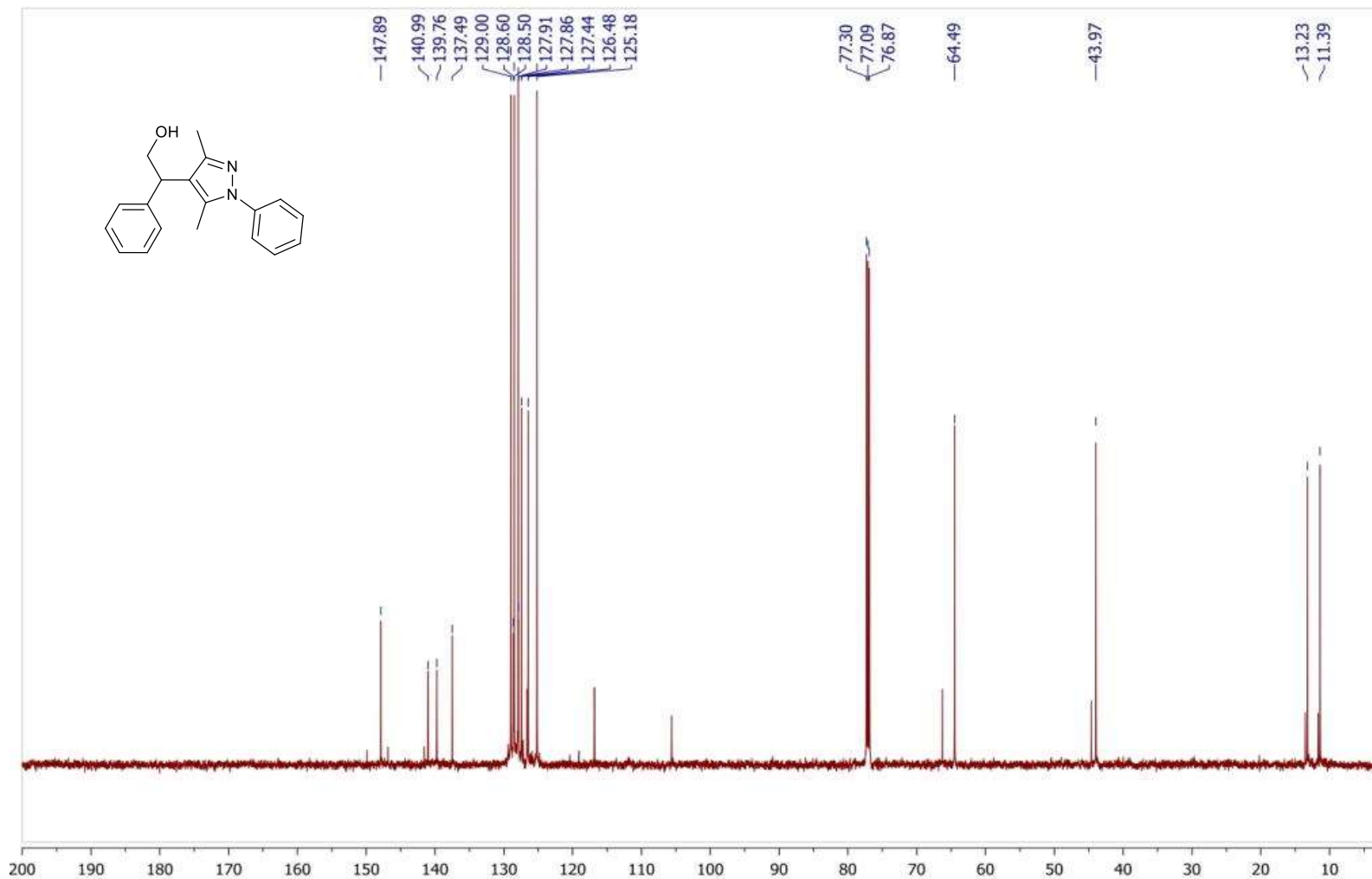
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-phenylethanol (3a)

^1H NMR (CDCl_3 , 600 MHz)



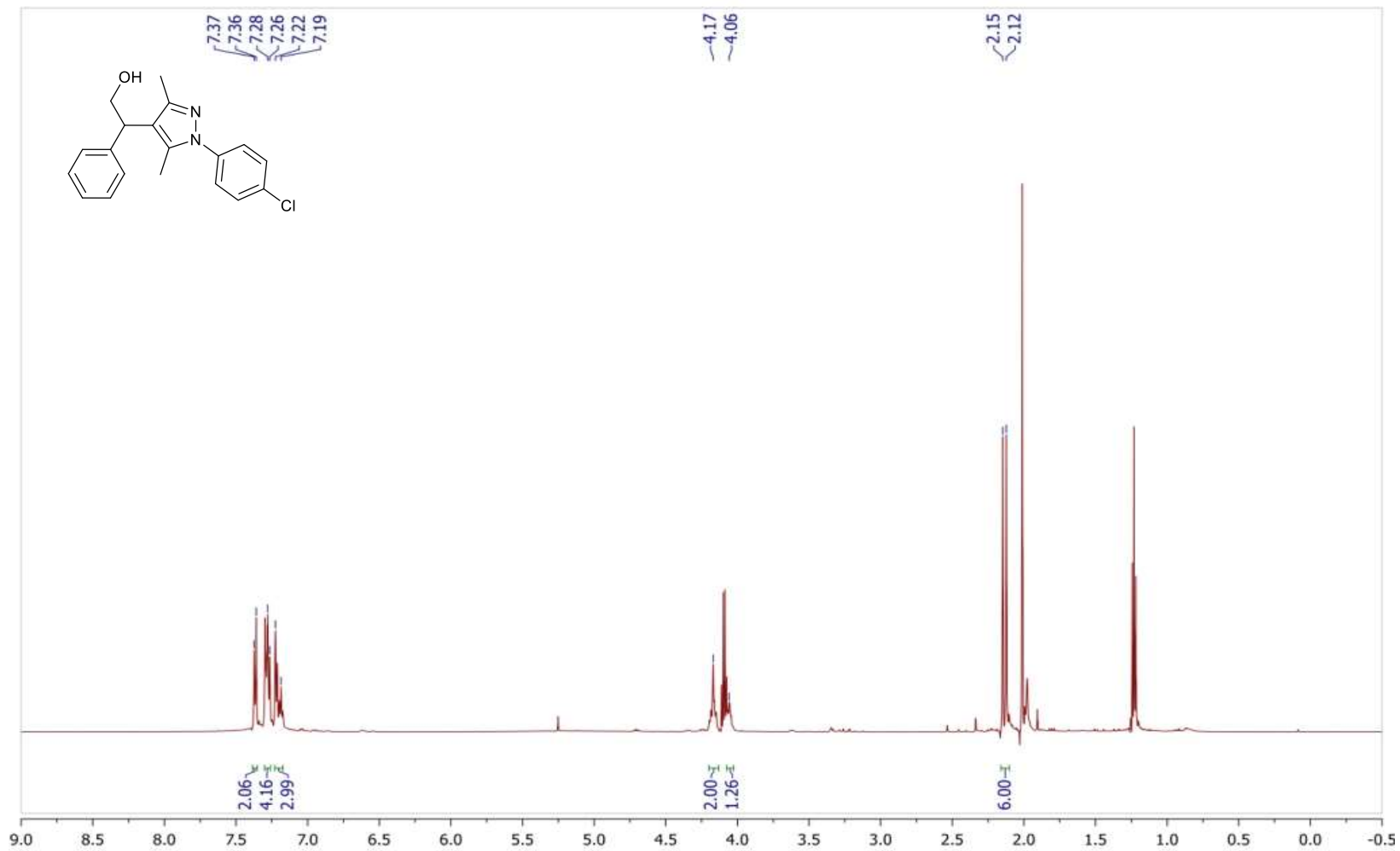
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-phenylethanol (3a)

^{13}C NMR (CDCl_3 , 150 MHz)



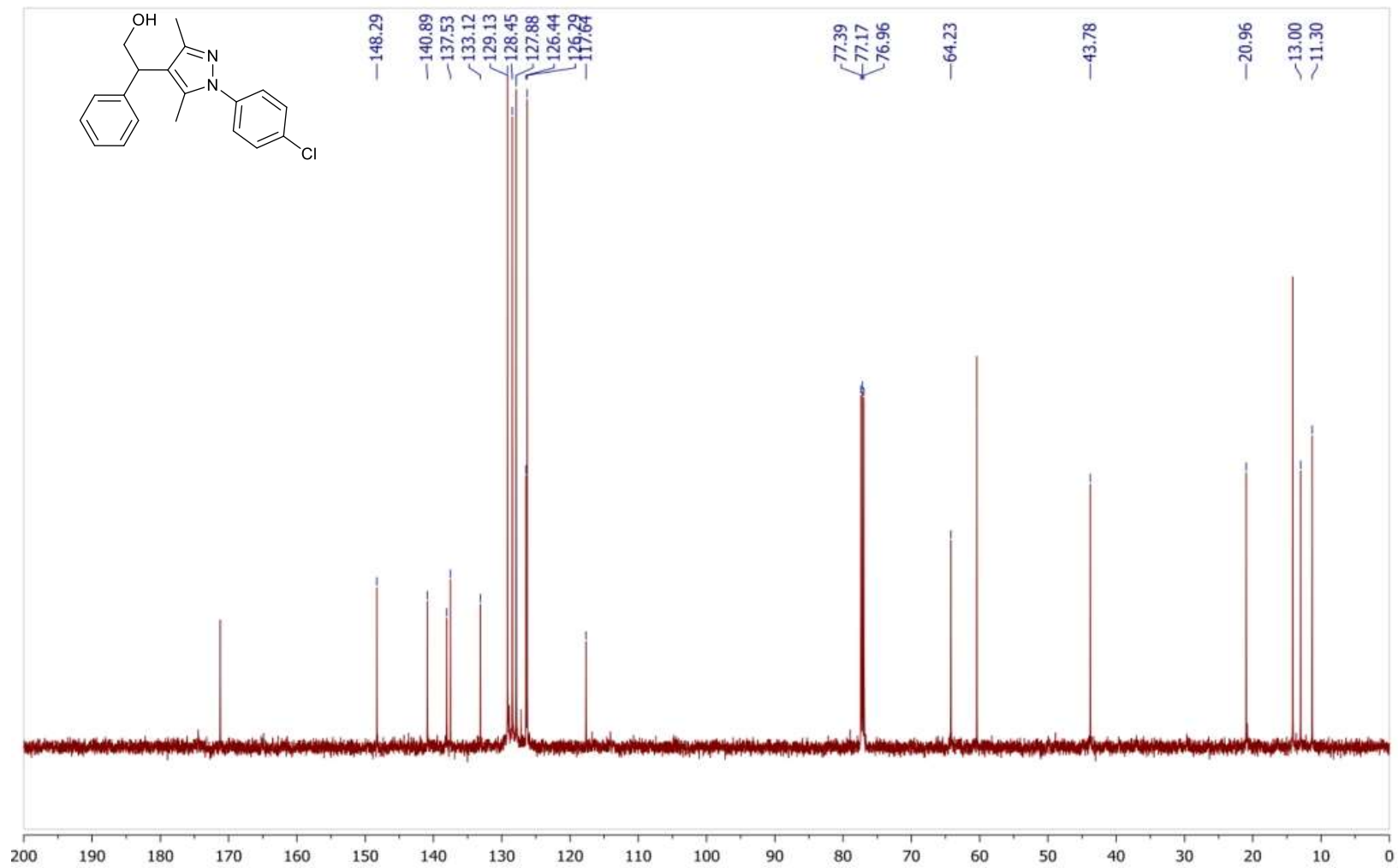
2-[1-(4-Chlorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-phenylethanol (3b)

¹H NMR (CDCl₃, 600 MHz)



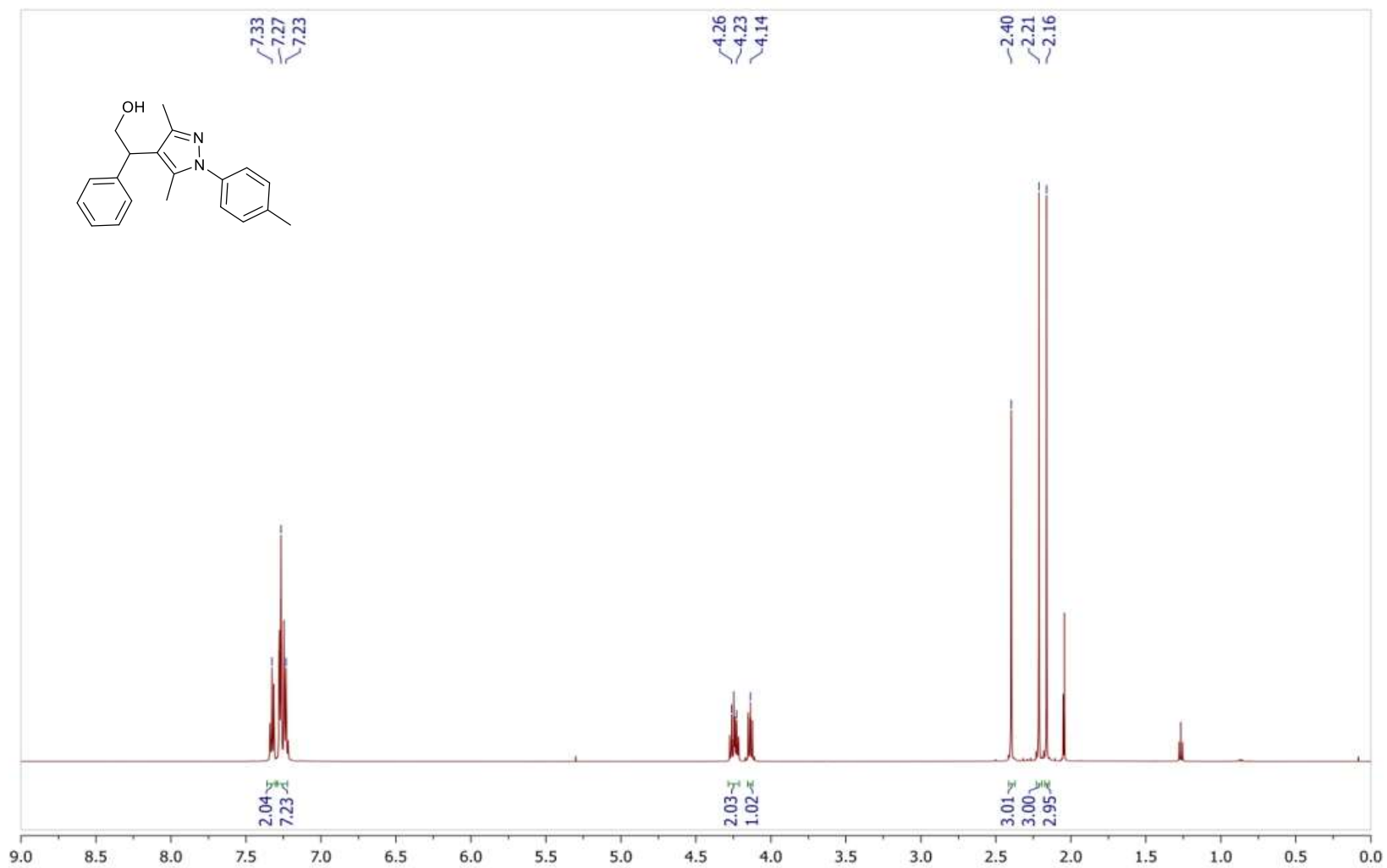
2-[1-(4-Chlorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-phenylethanol (3b)

^{13}C NMR (CDCl_3 , 150 MHz)



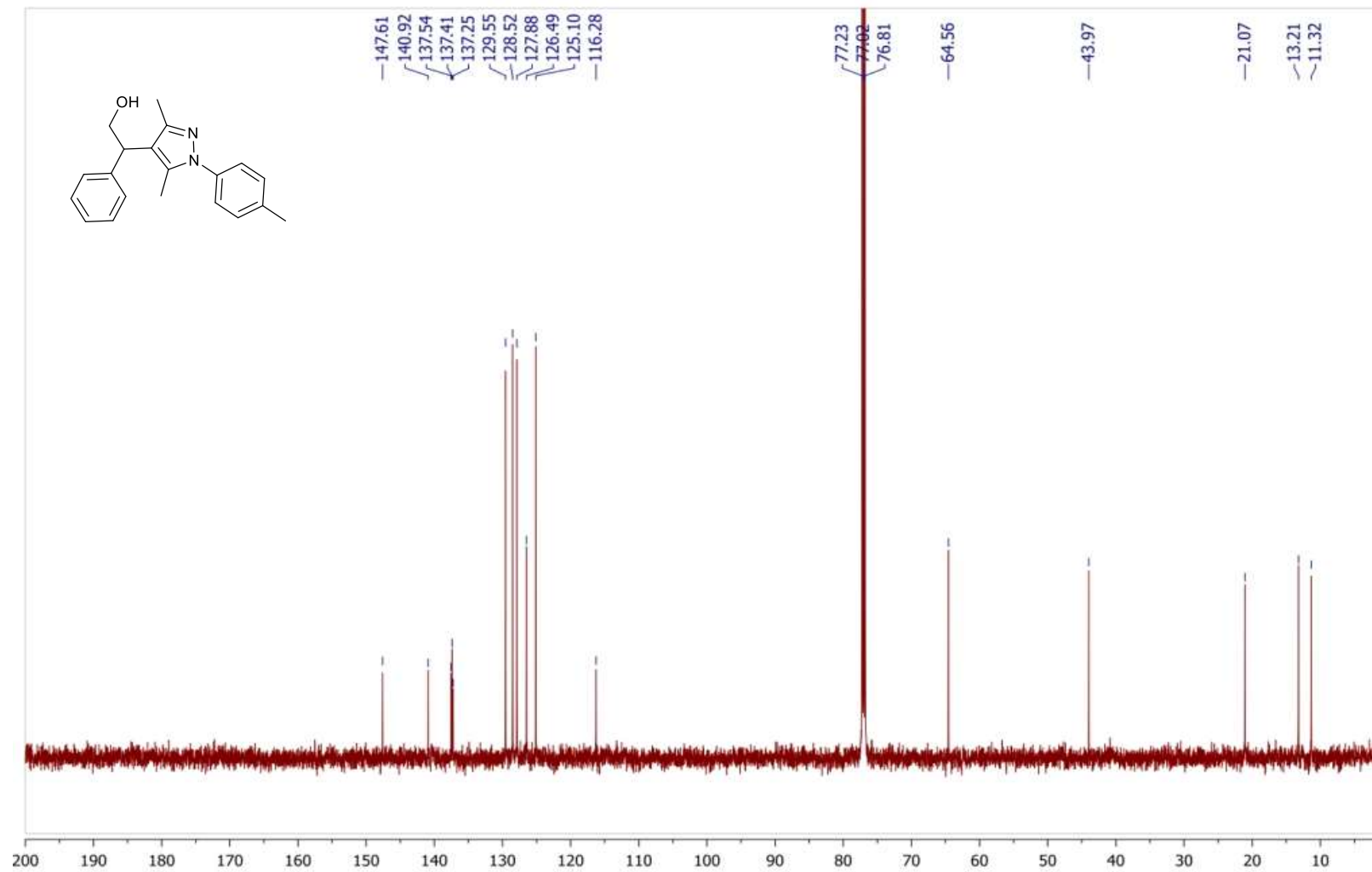
2-[3,5-Dimethyl-1-(4-methylphenyl)-1H-pyrazol-4-yl]-2-phenylethanol (3c)

¹H NMR (CDCl₃, 600 MHz)



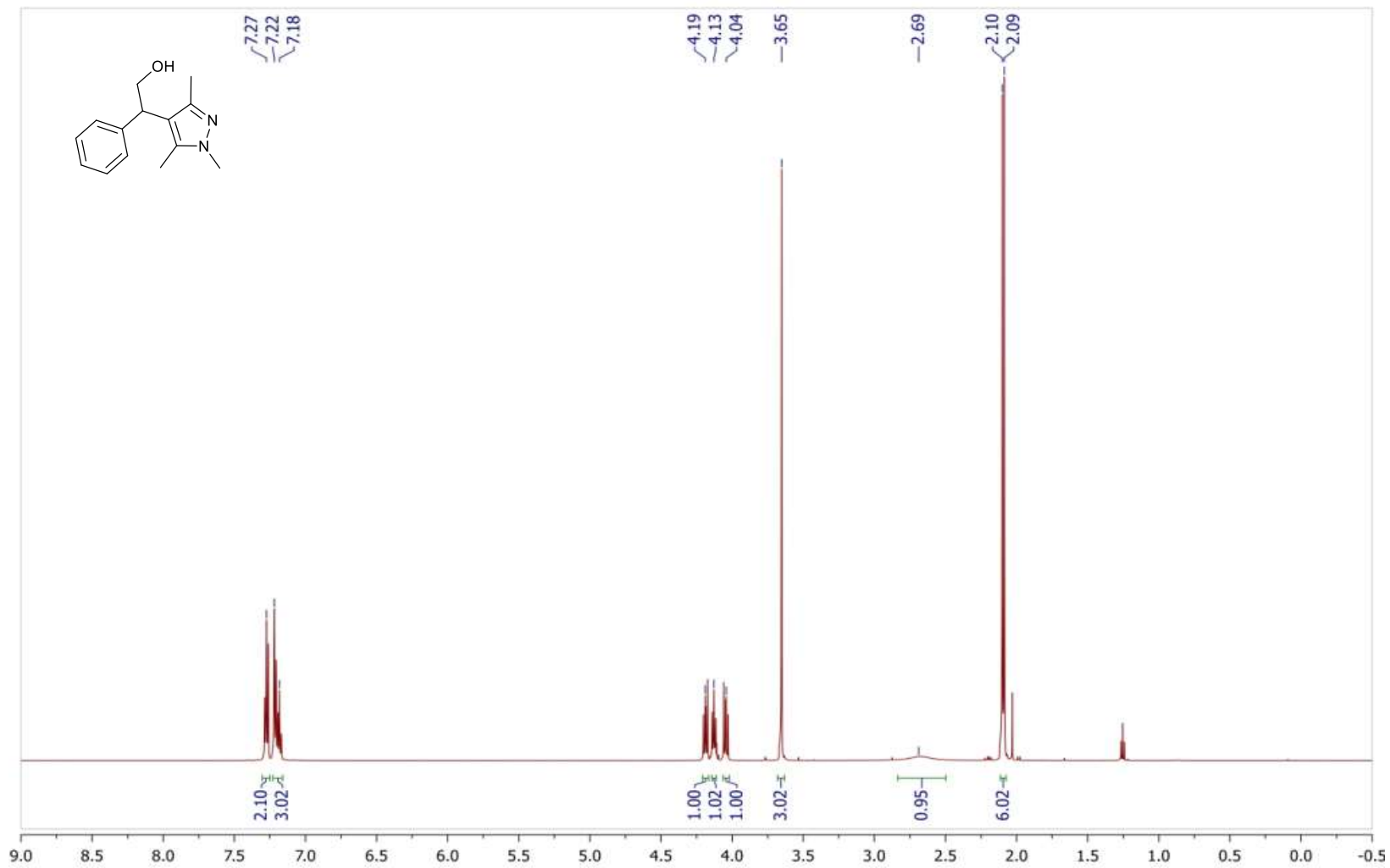
2-[3,5-Dimethyl-1-(4-methylphenyl)-1H-pyrazol-4-yl]-2-phenylethanol (3c)

^{13}C NMR (CDCl_3 , 150 MHz)



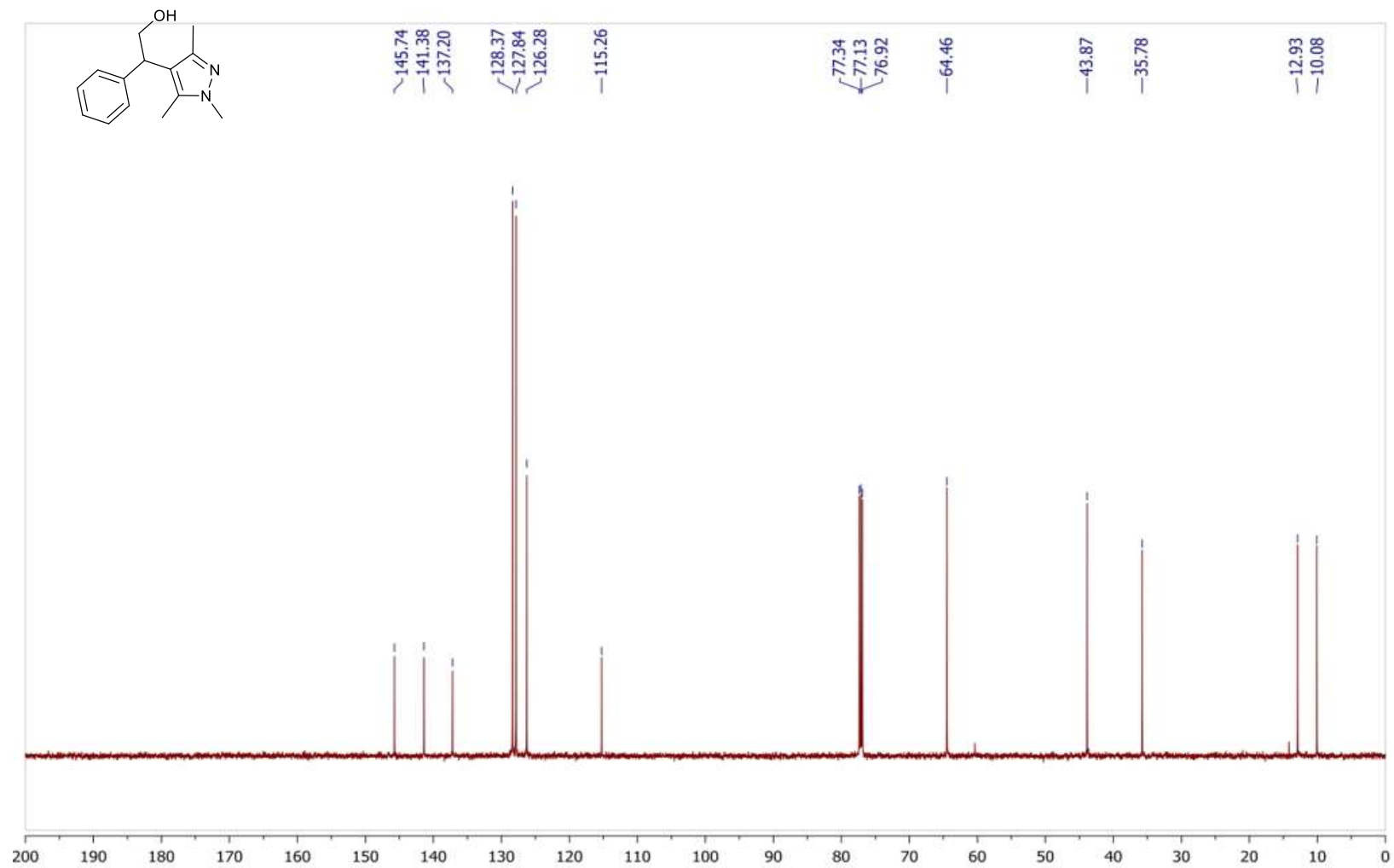
2-Phenyl-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3d)

¹H NMR (CDCl₃, 600 MHz)



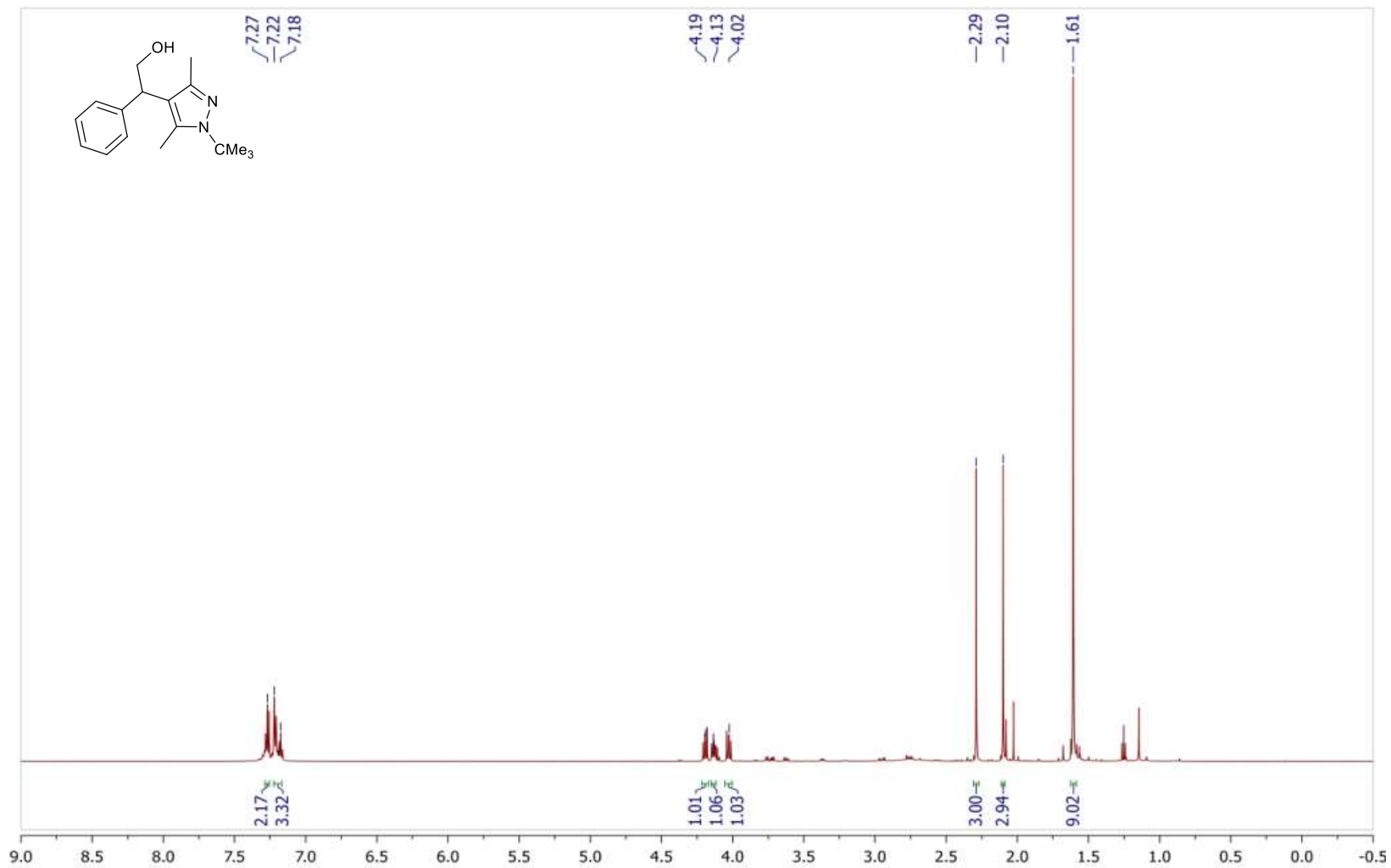
2-Phenyl-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3d)

^{13}C NMR (CDCl_3 , 150 MHz)



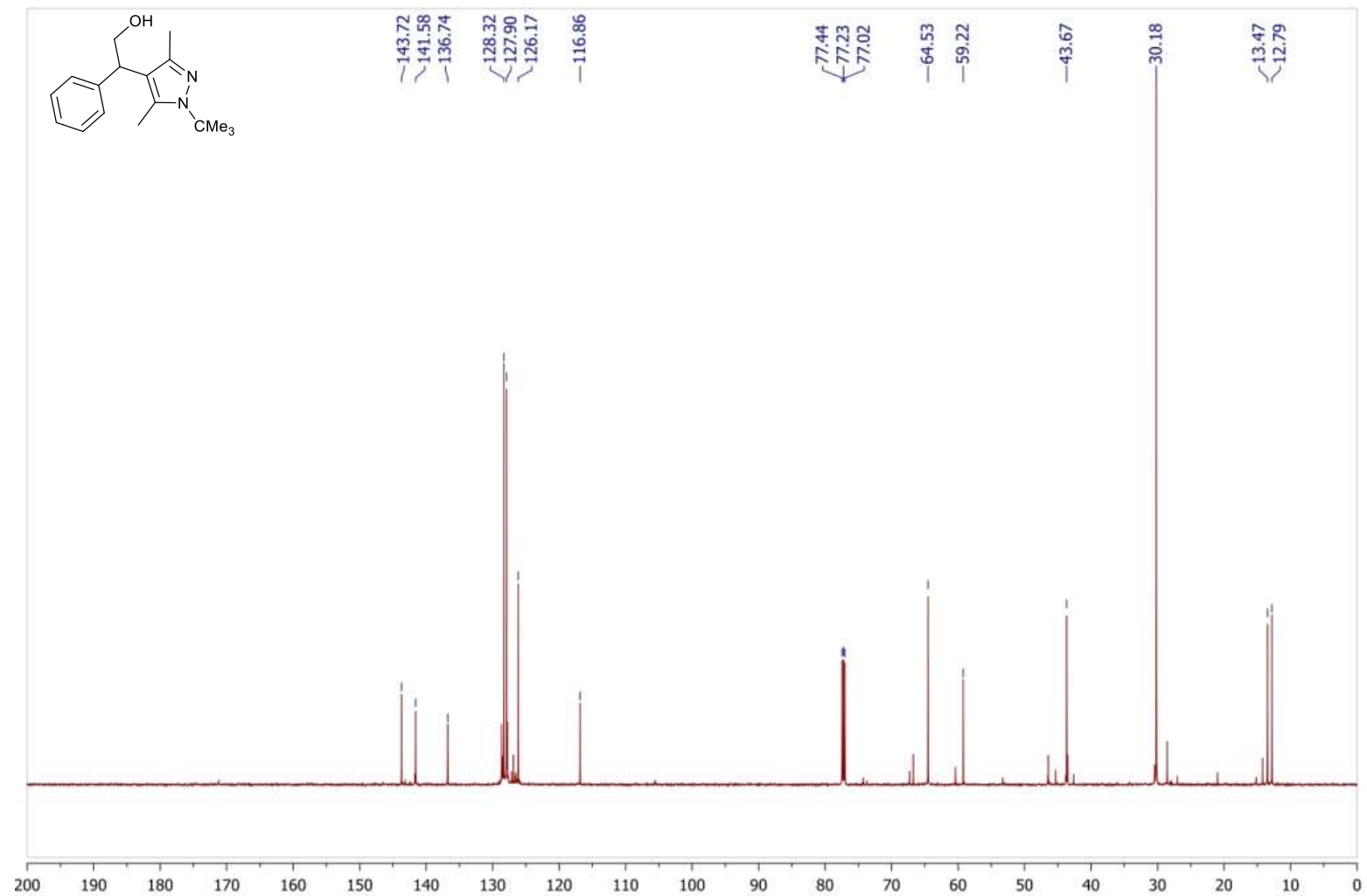
2-[1-(*tert*-Butyl)-3,5-dimethyl-1*H*-pyrazol-4-yl]-2-phenylethanol (**3e**)

^1H NMR (CDCl_3 , 600 MHz)



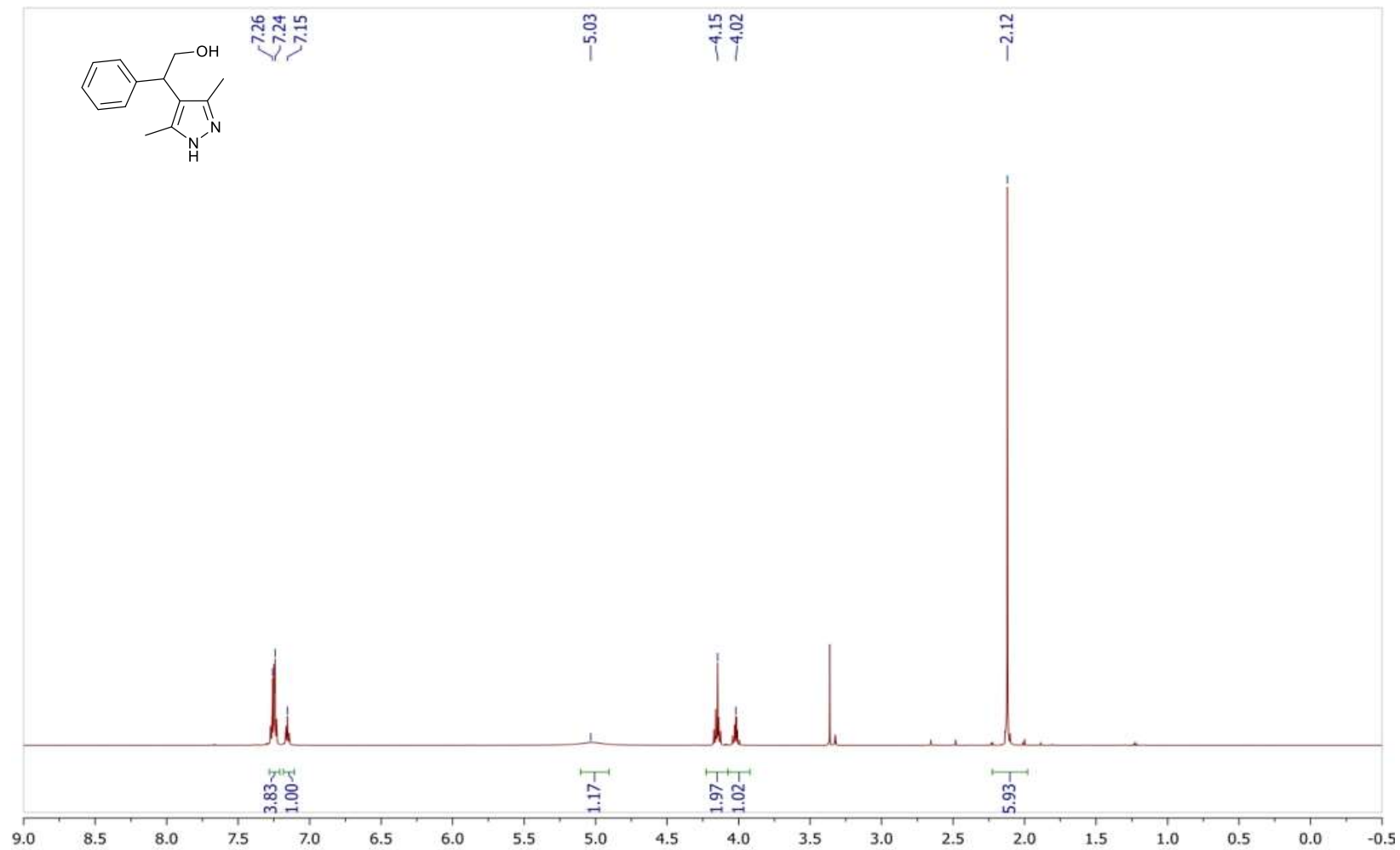
2-[1-(tert-Butyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-phenylethanol (3e)

^{13}C NMR (CDCl_3 , 150 MHz)



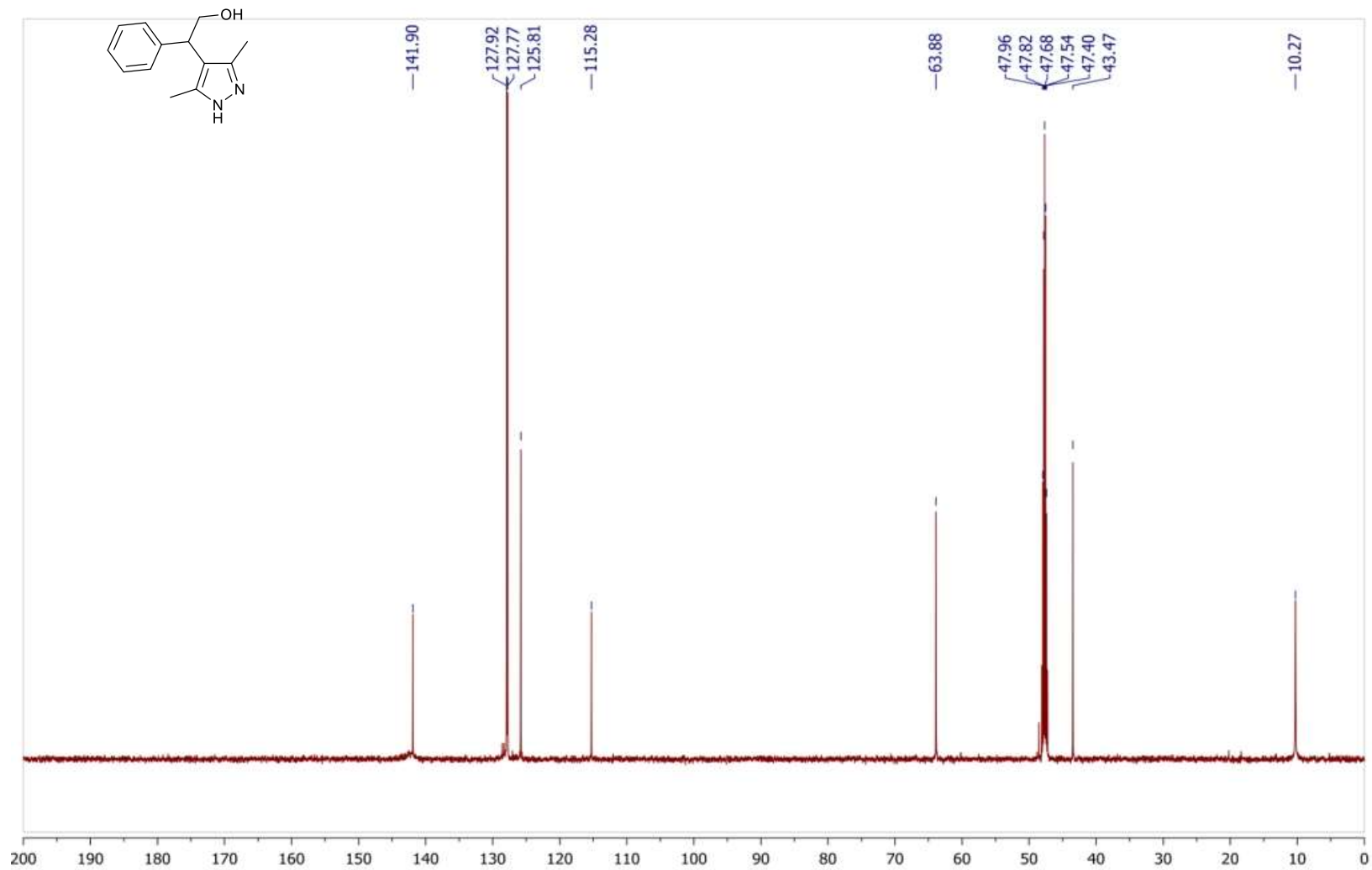
2-(3,5-Dimethyl-1H-pyrazol-4-yl)-2-phenylethanol (3f)

¹H NMR (CDCl₃, 600 MHz)



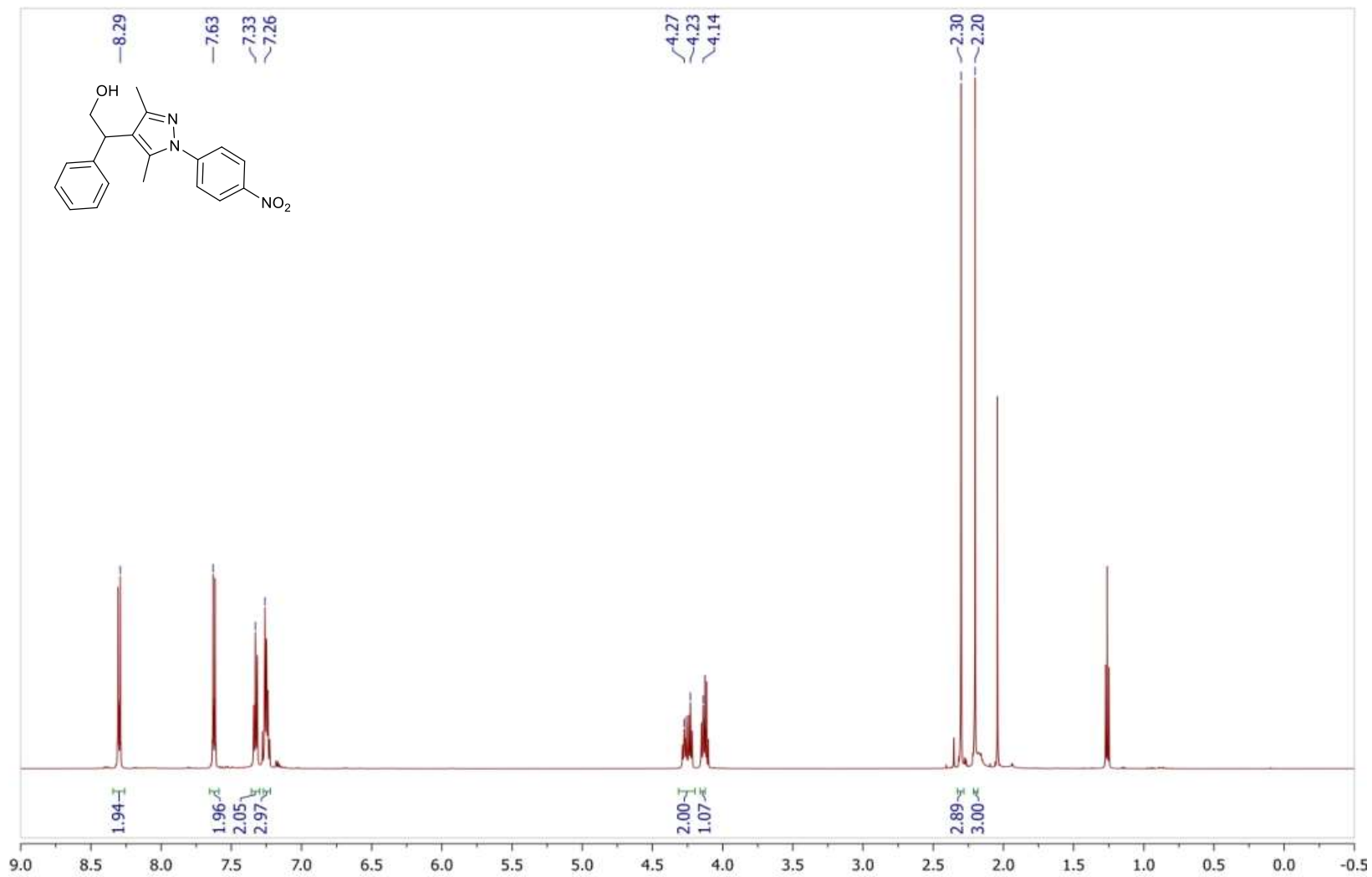
2-(3,5-Dimethyl-1H-pyrazol-4-yl)-2-phenylethanol (3f)

^{13}C NMR (CDCl_3 , 150 MHz)



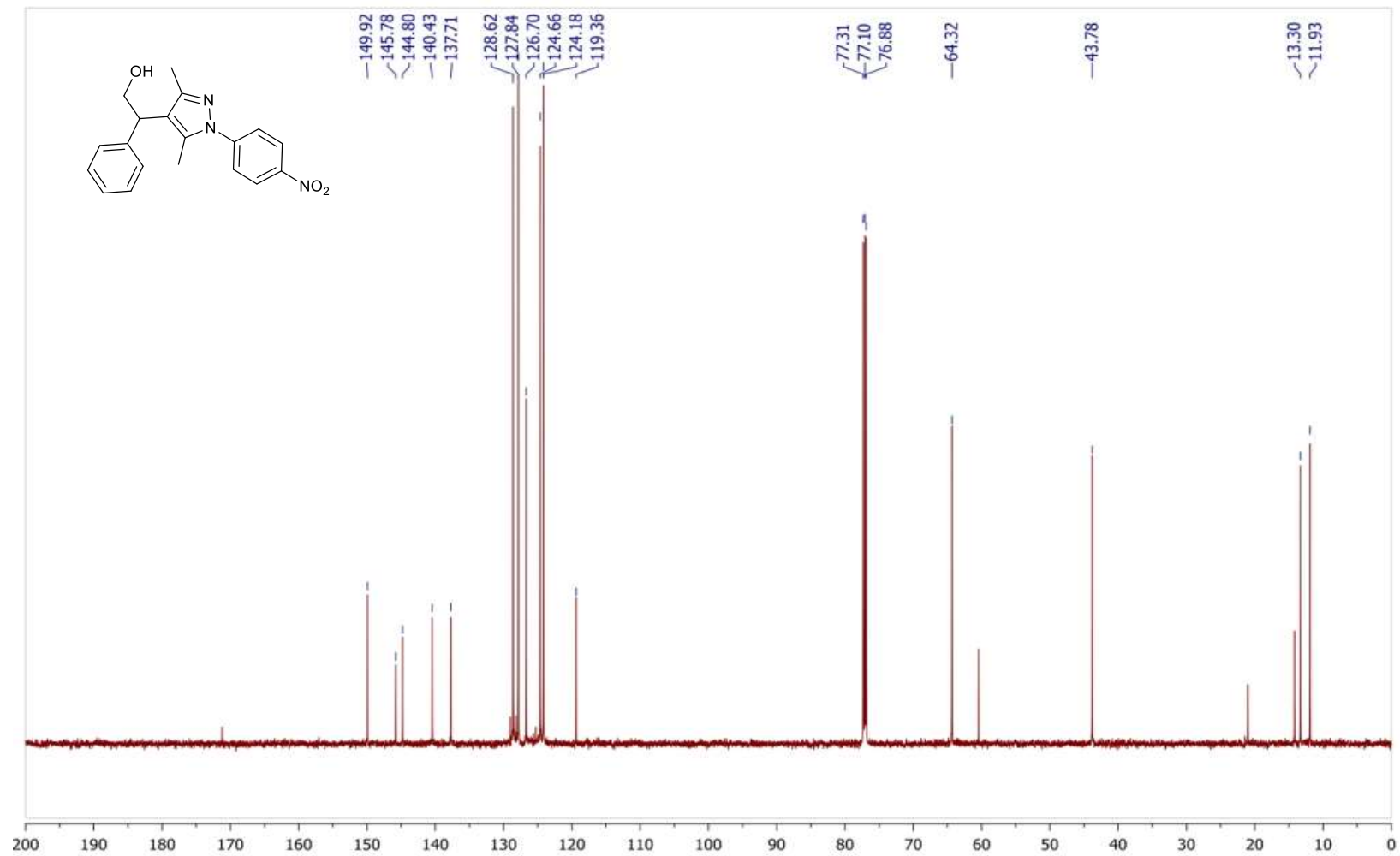
2-[3,5-Dimethyl-1-(4-nitrophenyl)-1H-pyrazol-4-yl]-2-phenylethanol (3g)

¹H NMR (CDCl₃, 600 MHz)



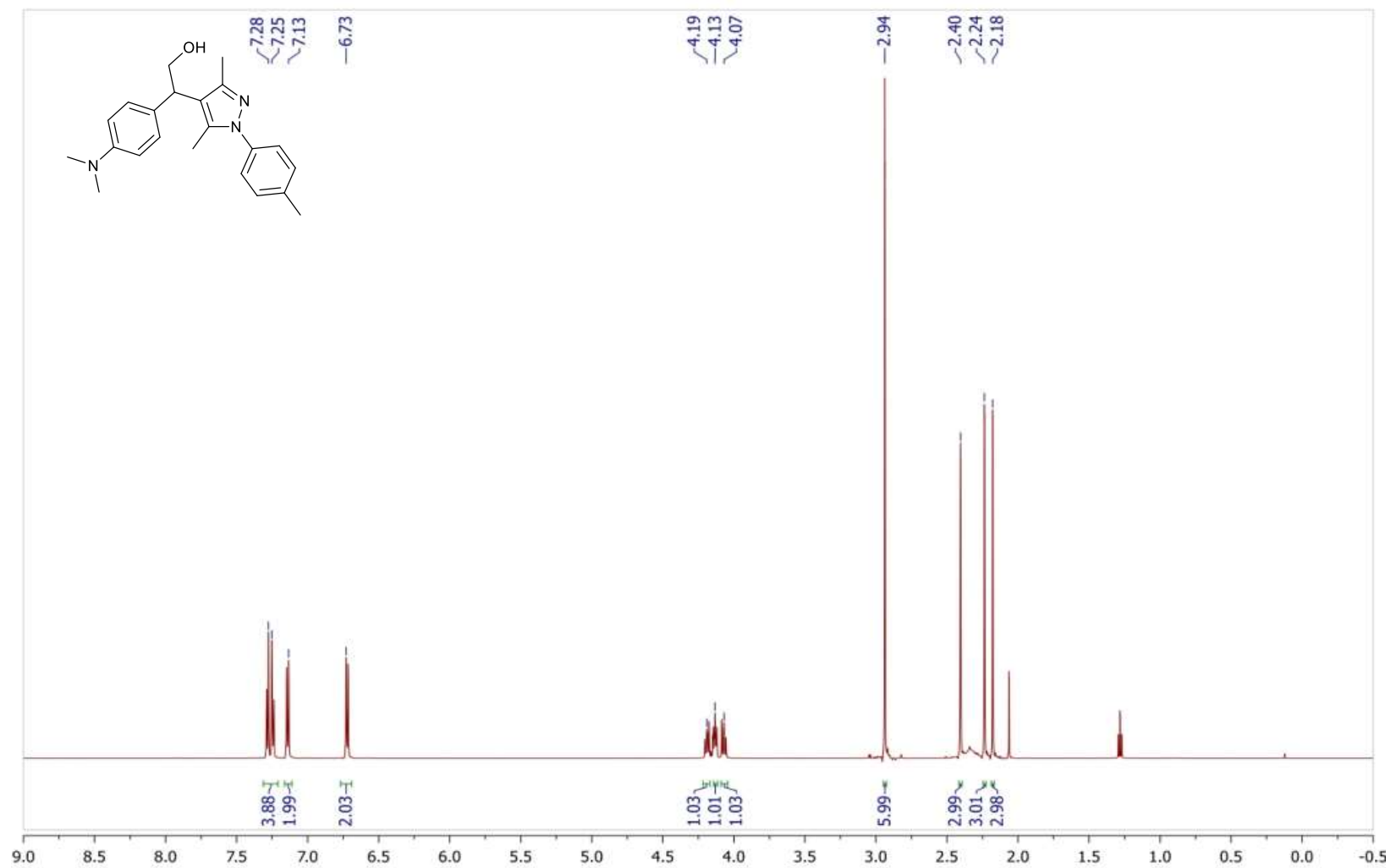
2-[3,5-Dimethyl-1-(4-nitrophenyl)-1H-pyrazol-4-yl]-2-phenylethanol (3g)

^{13}C NMR (CDCl_3 , 150 MHz)



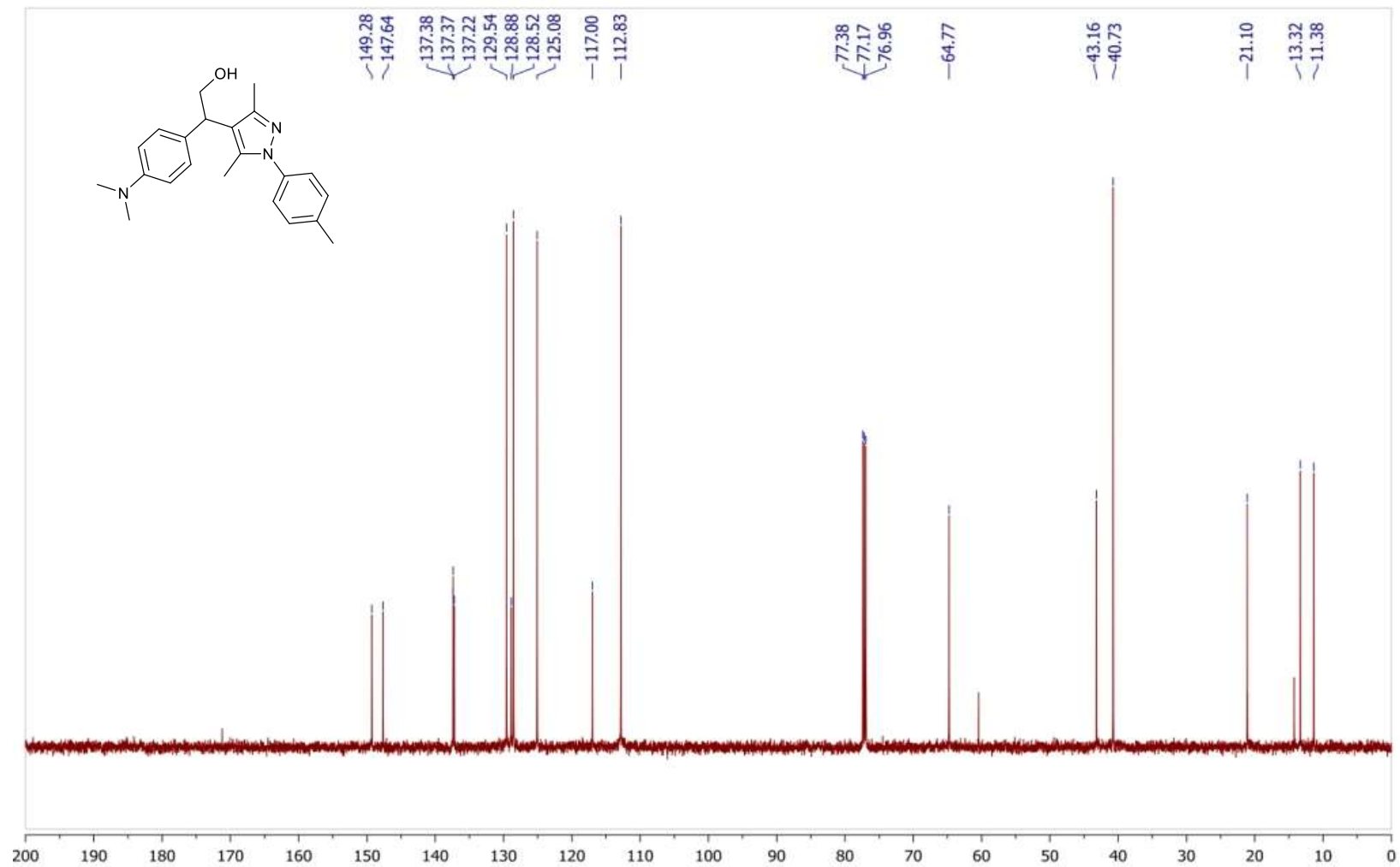
2-[3,5-Dimethyl-1-(4-methylphenyl)-1H-pyrazol-4-yl]-2-[4-(dimethylamino)phenyl]ethanol (3h)

¹H NMR (CDCl₃, 600 MHz)



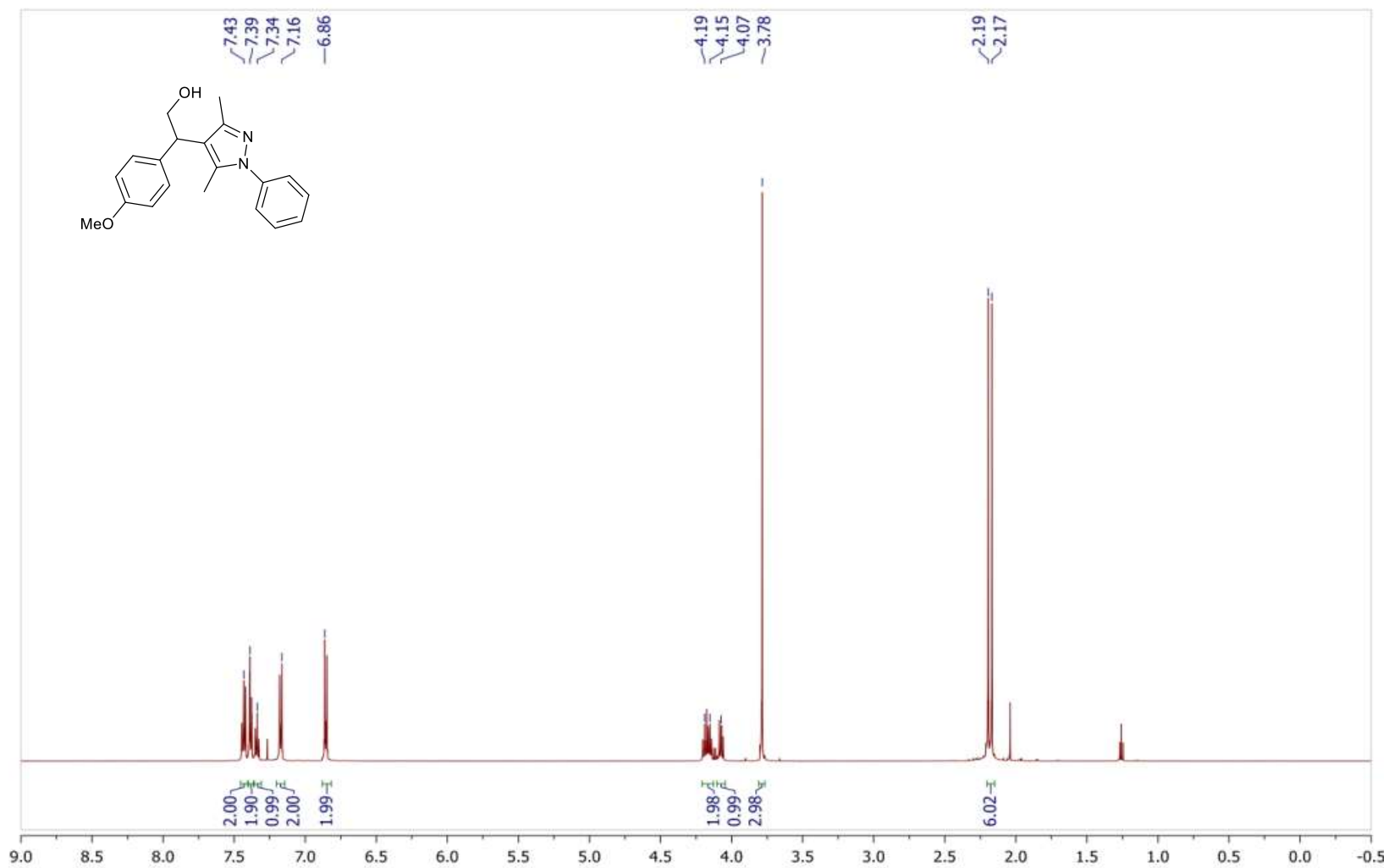
2-[3,5-Dimethyl-1-(4-methylphenyl)-1H-pyrazol-4-yl]-2-[4-(dimethylamino)phenyl]ethanol (3h)

^{13}C NMR (CDCl_3 , 150 MHz)



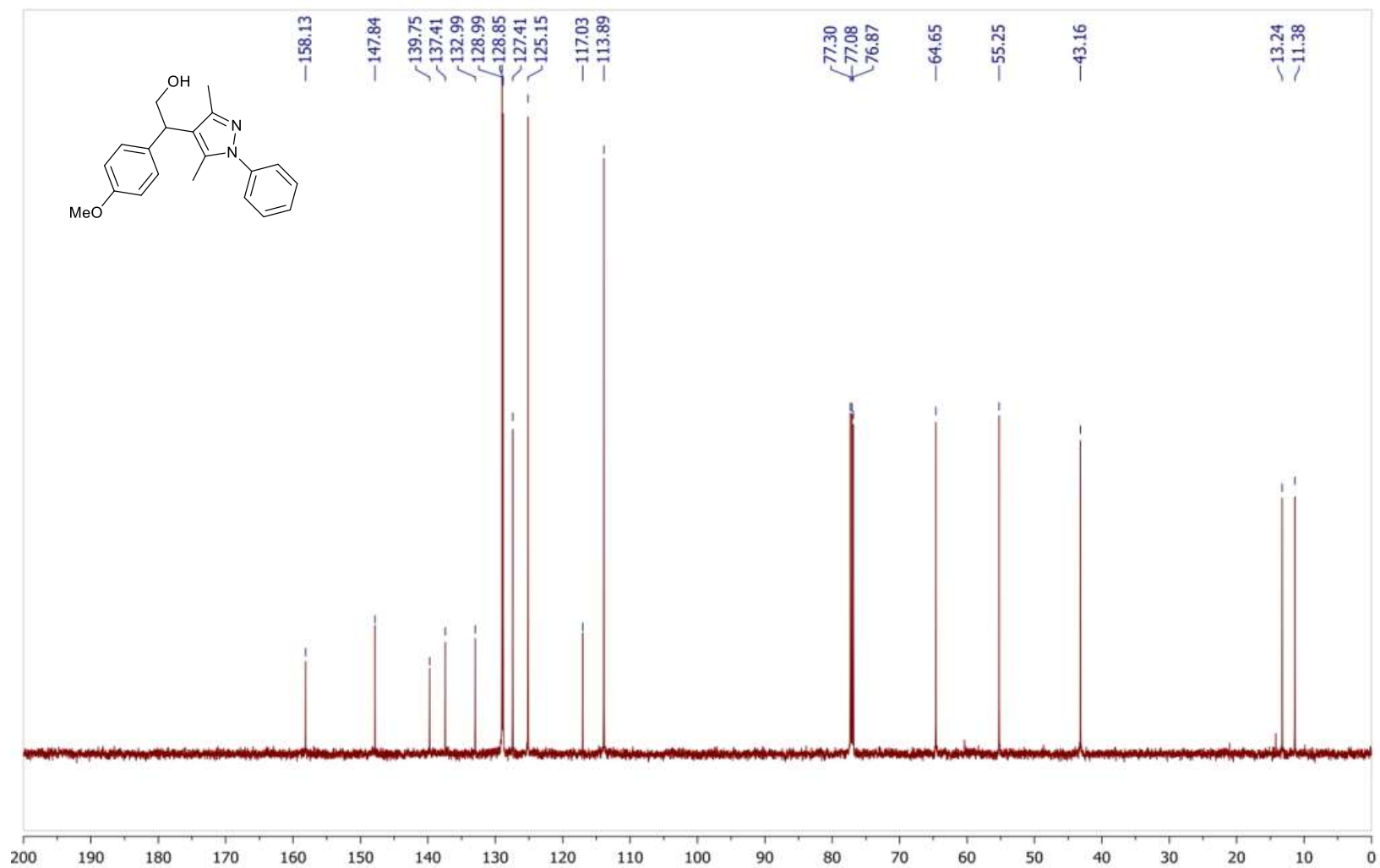
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(4-methoxyphenyl)ethanol (3i)

¹H NMR (CDCl₃, 600 MHz)



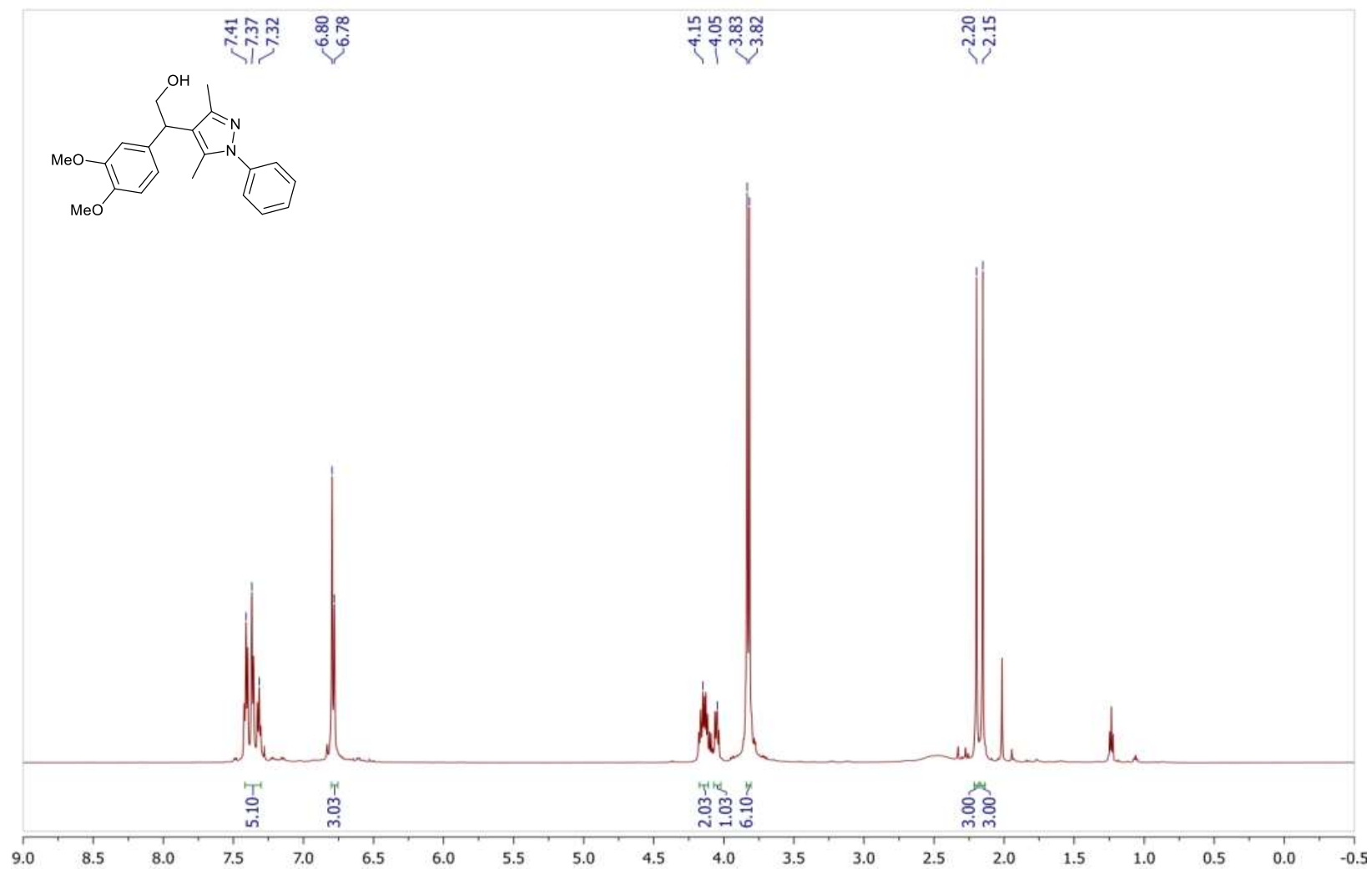
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(4-methoxyphenyl)ethanol (3i)

^{13}C NMR (CDCl_3 , 150 MHz)



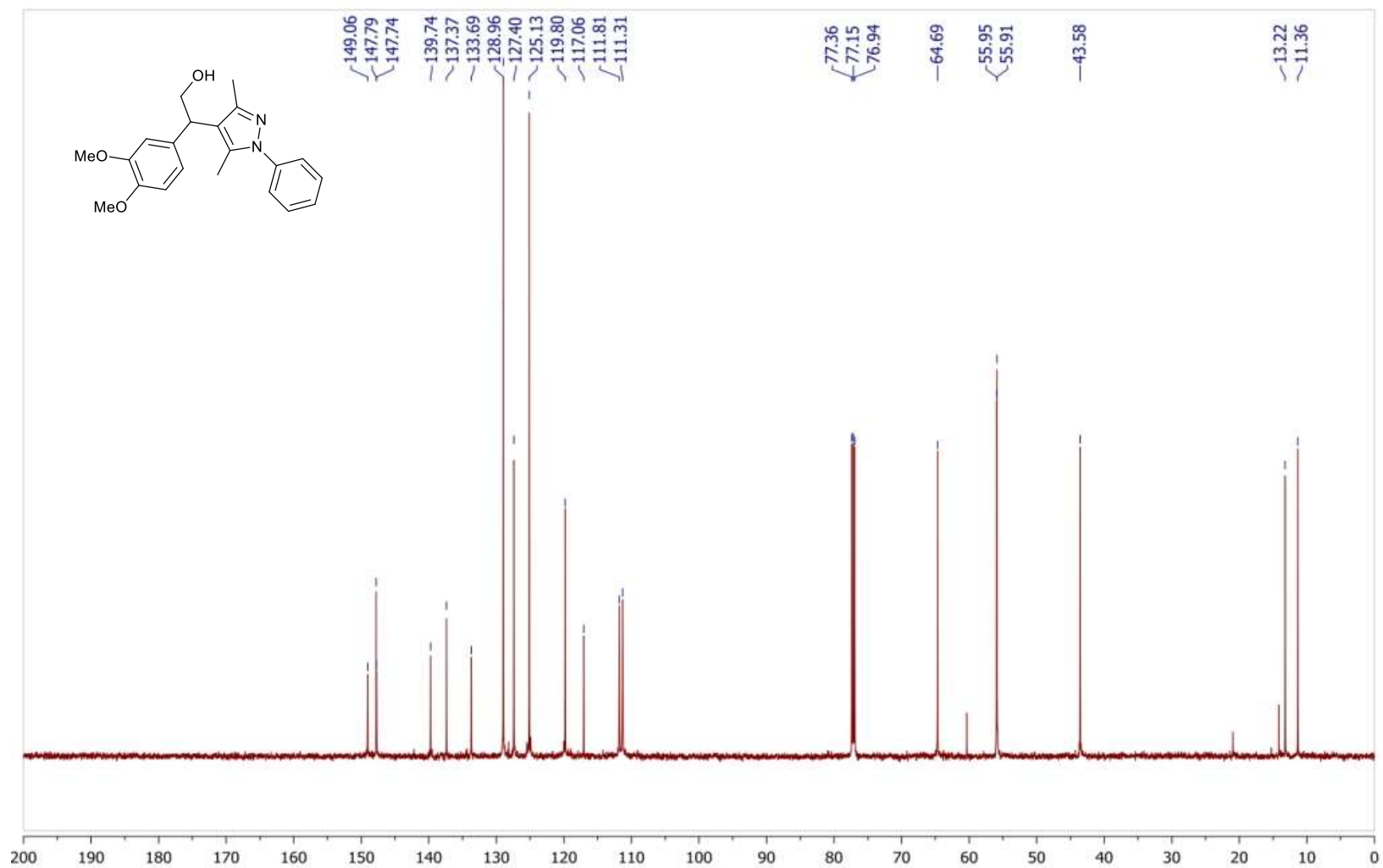
2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethanol (3j)

¹H NMR (CDCl₃, 600 MHz)



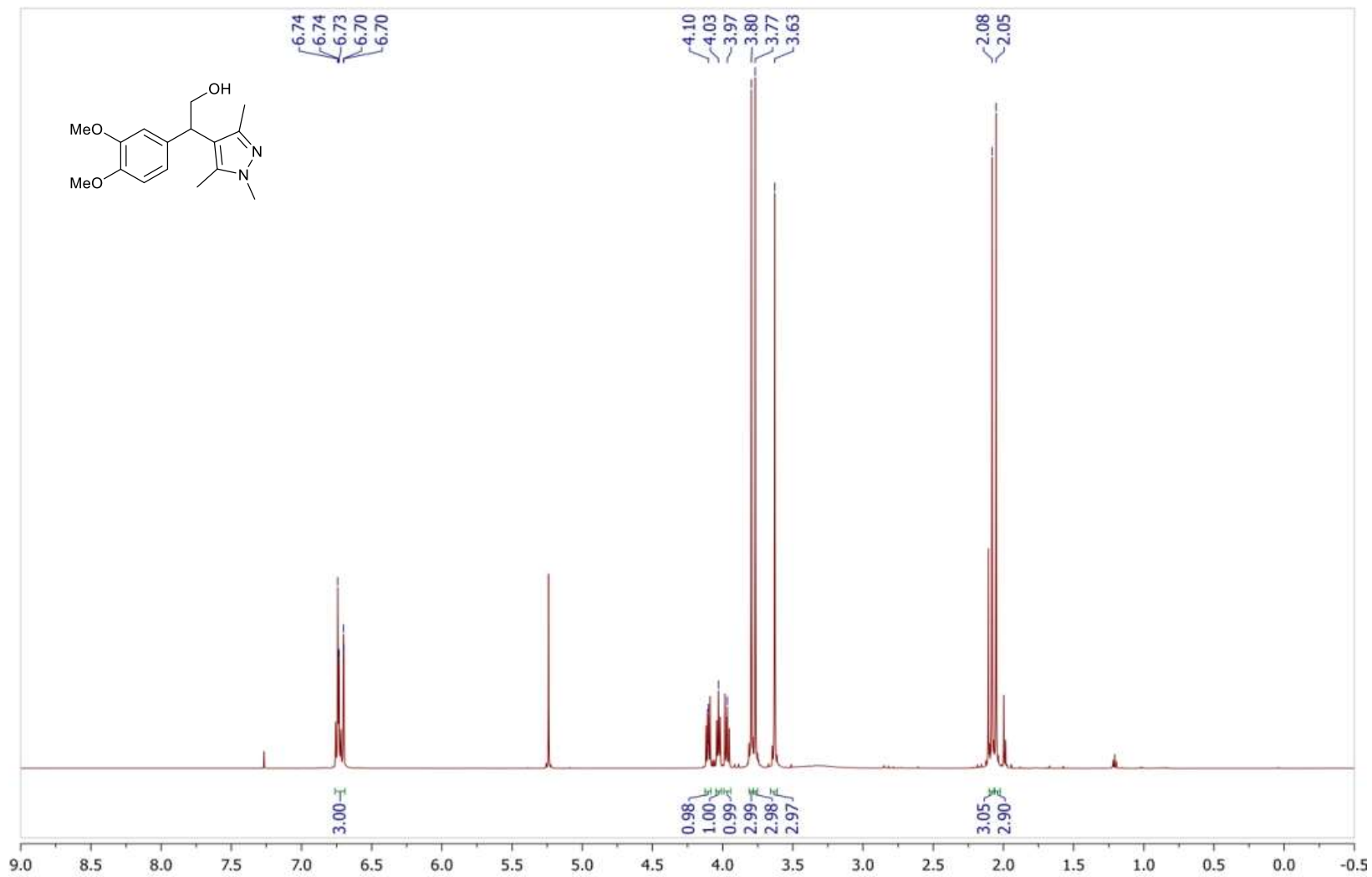
2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethanol (3j)

¹³C NMR (CDCl₃, 150 MHz)



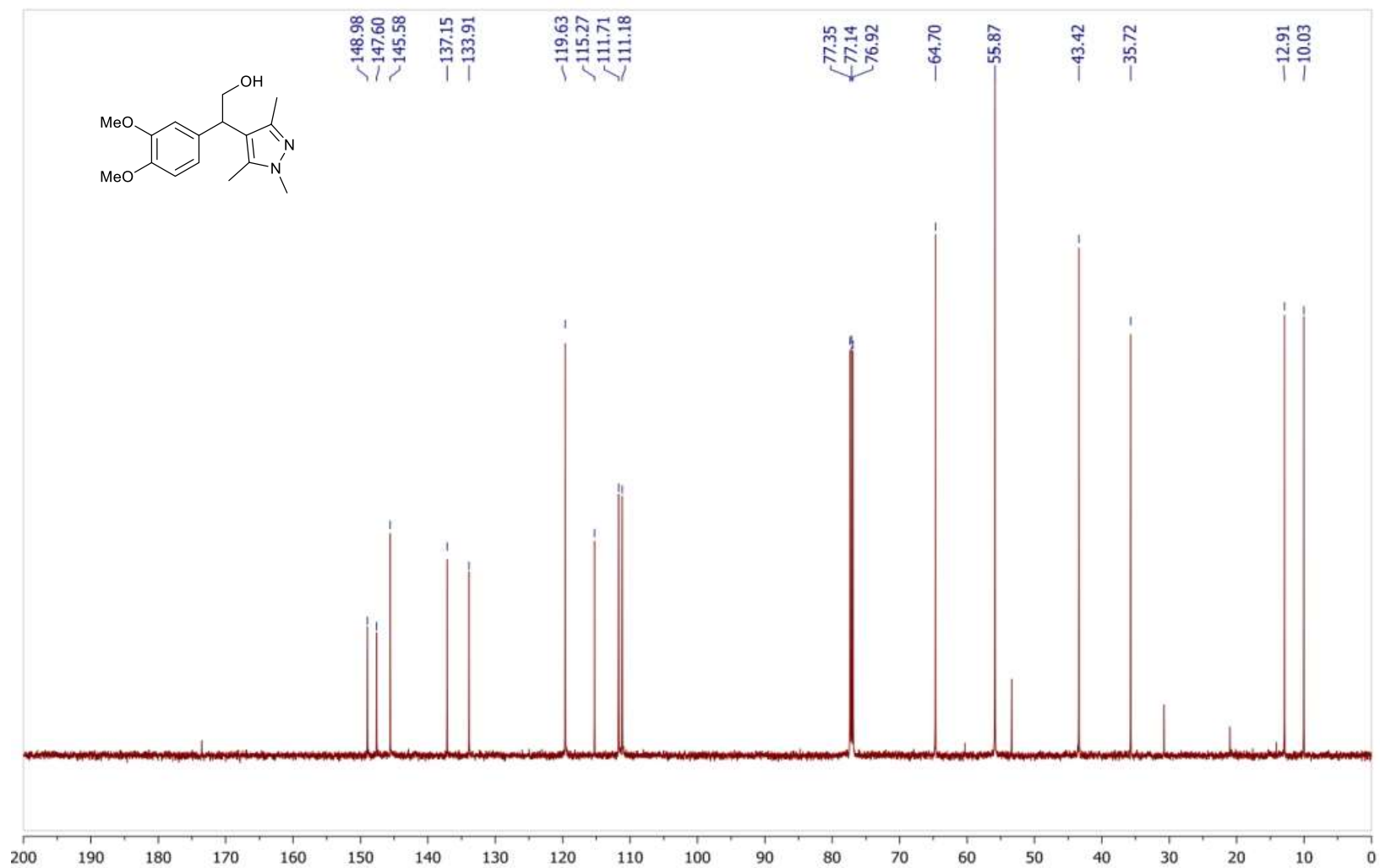
2-(3,4-Dimethoxyphenyl)-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3k)

¹H NMR (CDCl₃, 600 MHz)



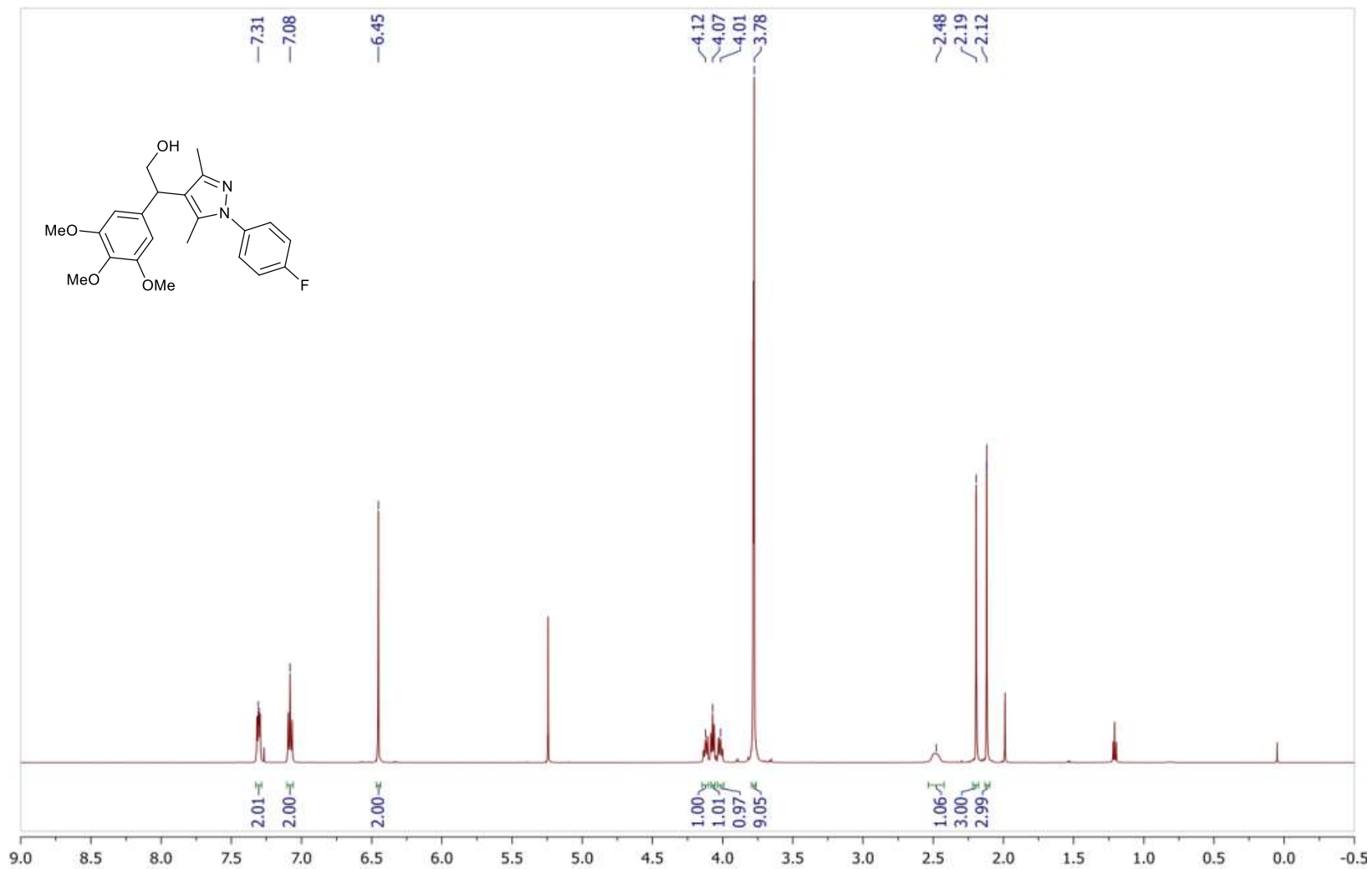
2-(3,4-Dimethoxyphenyl)-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3k)

¹³C NMR (CDCl₃, 150 MHz)



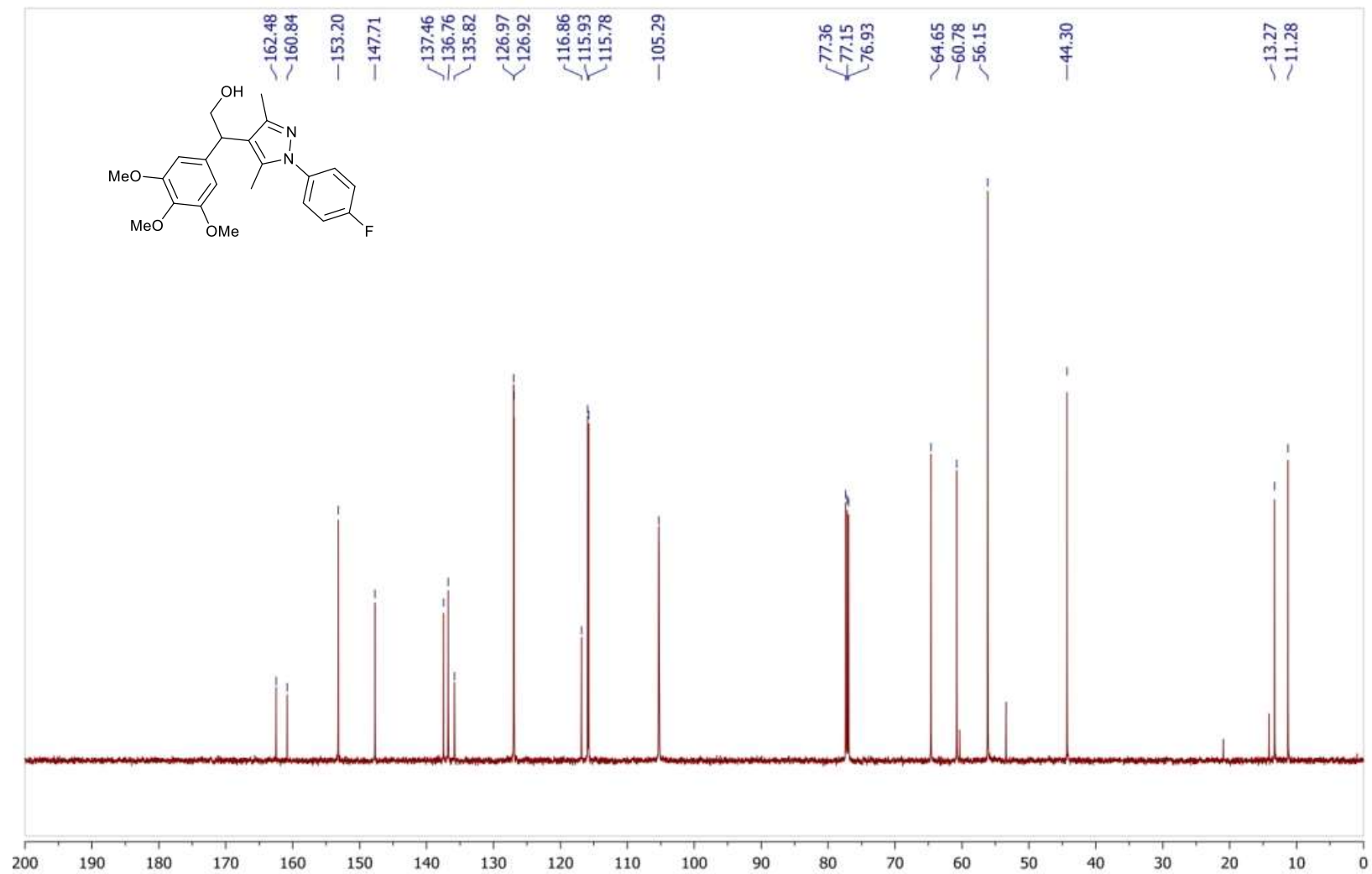
2-[1-(4-Fluorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-(3,4,5-trimethoxyphenyl)ethanol (3l)

¹H NMR (CDCl₃, 600 MHz)



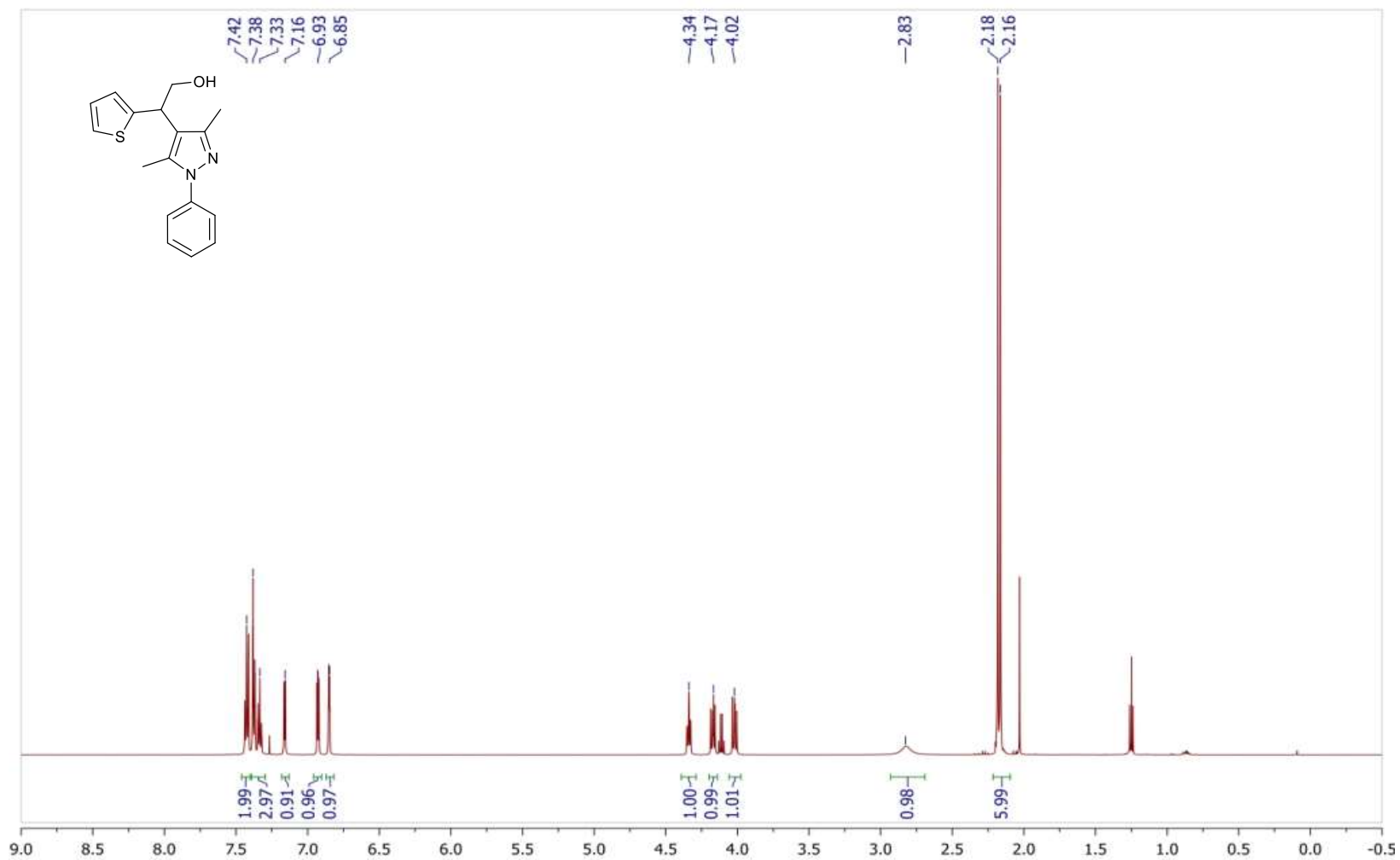
2-[1-(4-Fluorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-(3,4,5-trimethoxyphenyl)ethanol (3l)

¹³C NMR (CDCl₃, 150 MHz)



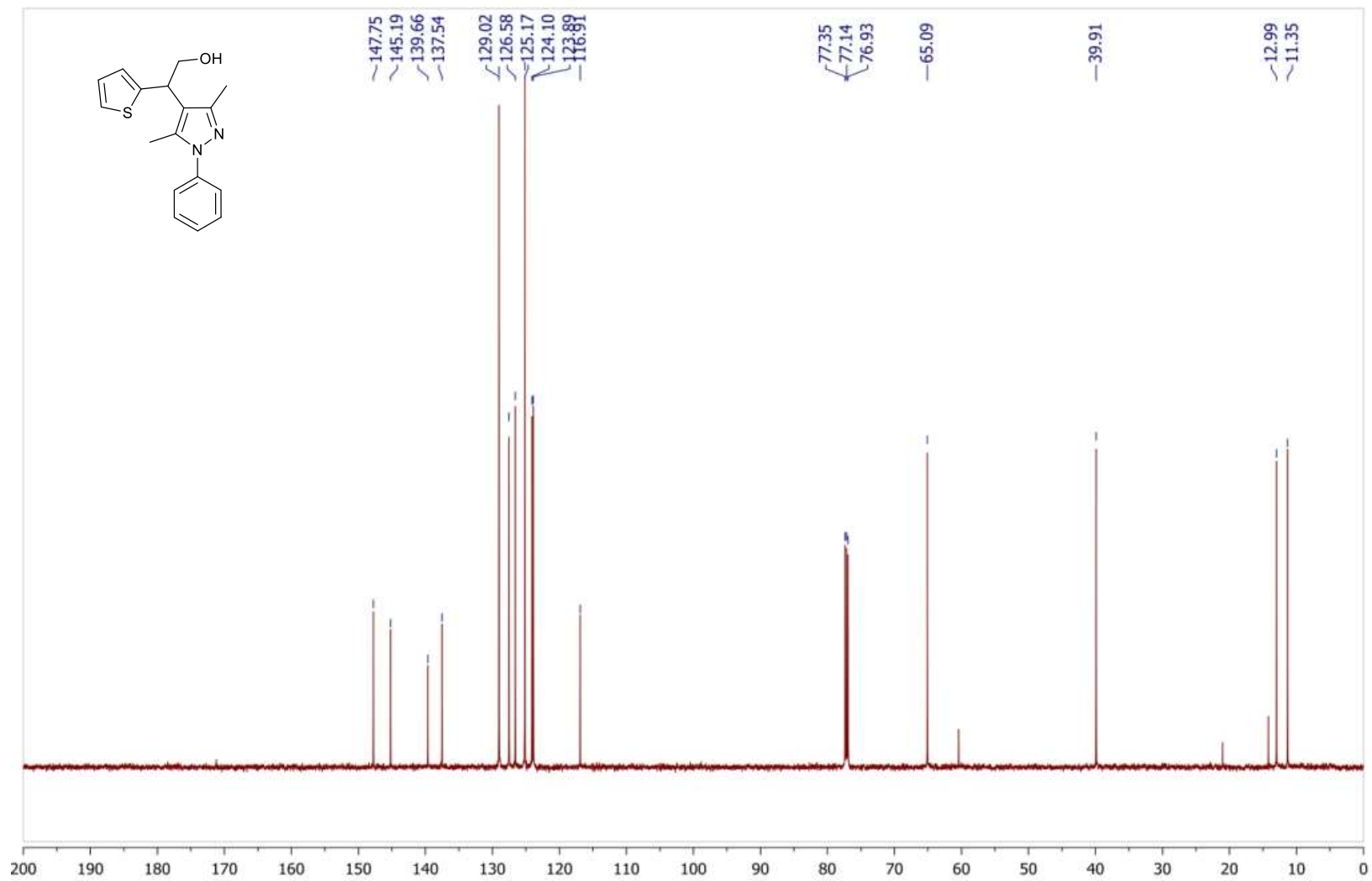
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(thiophen-2-yl)ethanol (3m)

¹H NMR (CDCl₃, 600 MHz)



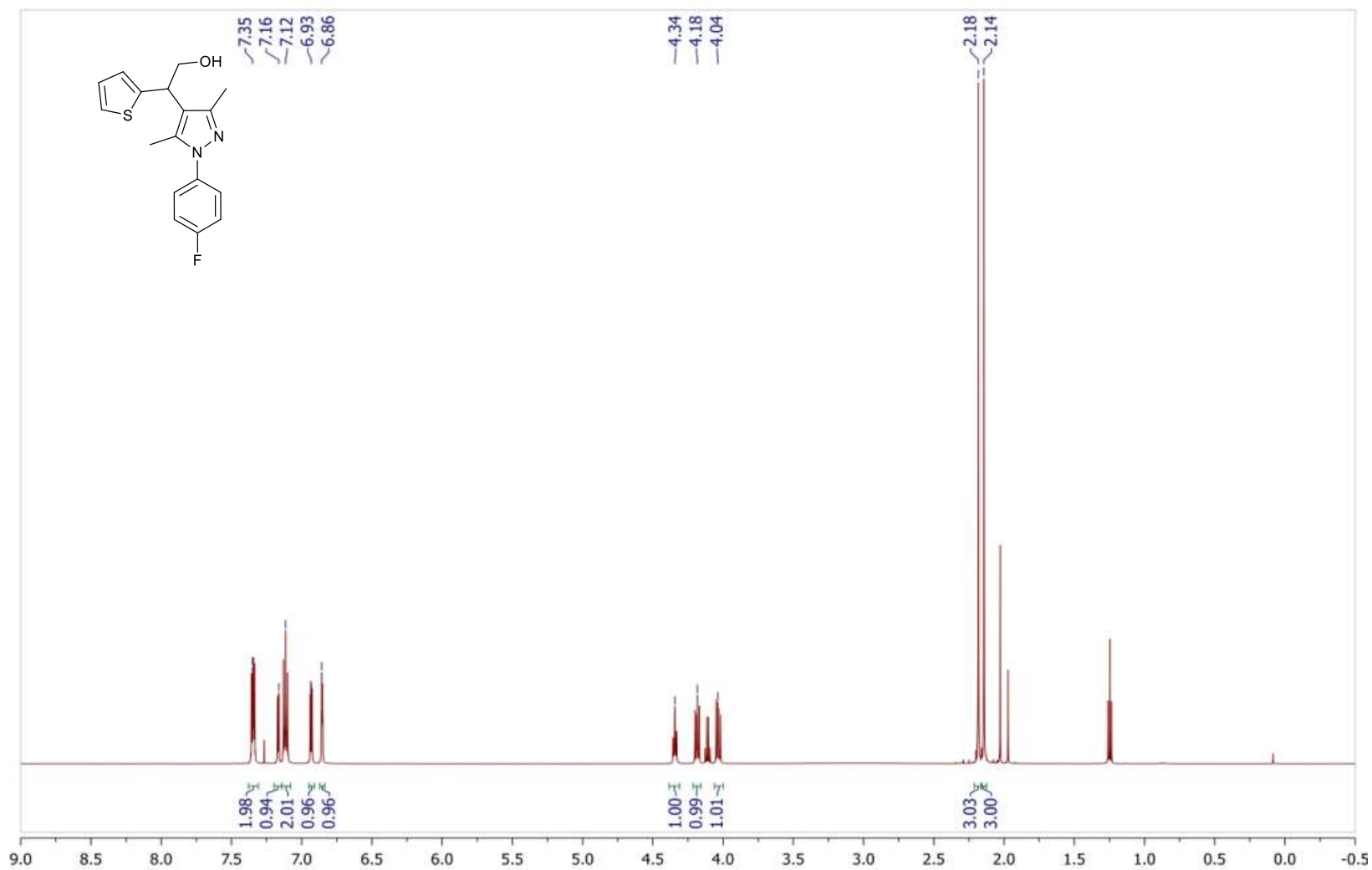
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(thiophen-2-yl)ethanol (3m)

^{13}C NMR (CDCl_3 , 150 MHz)



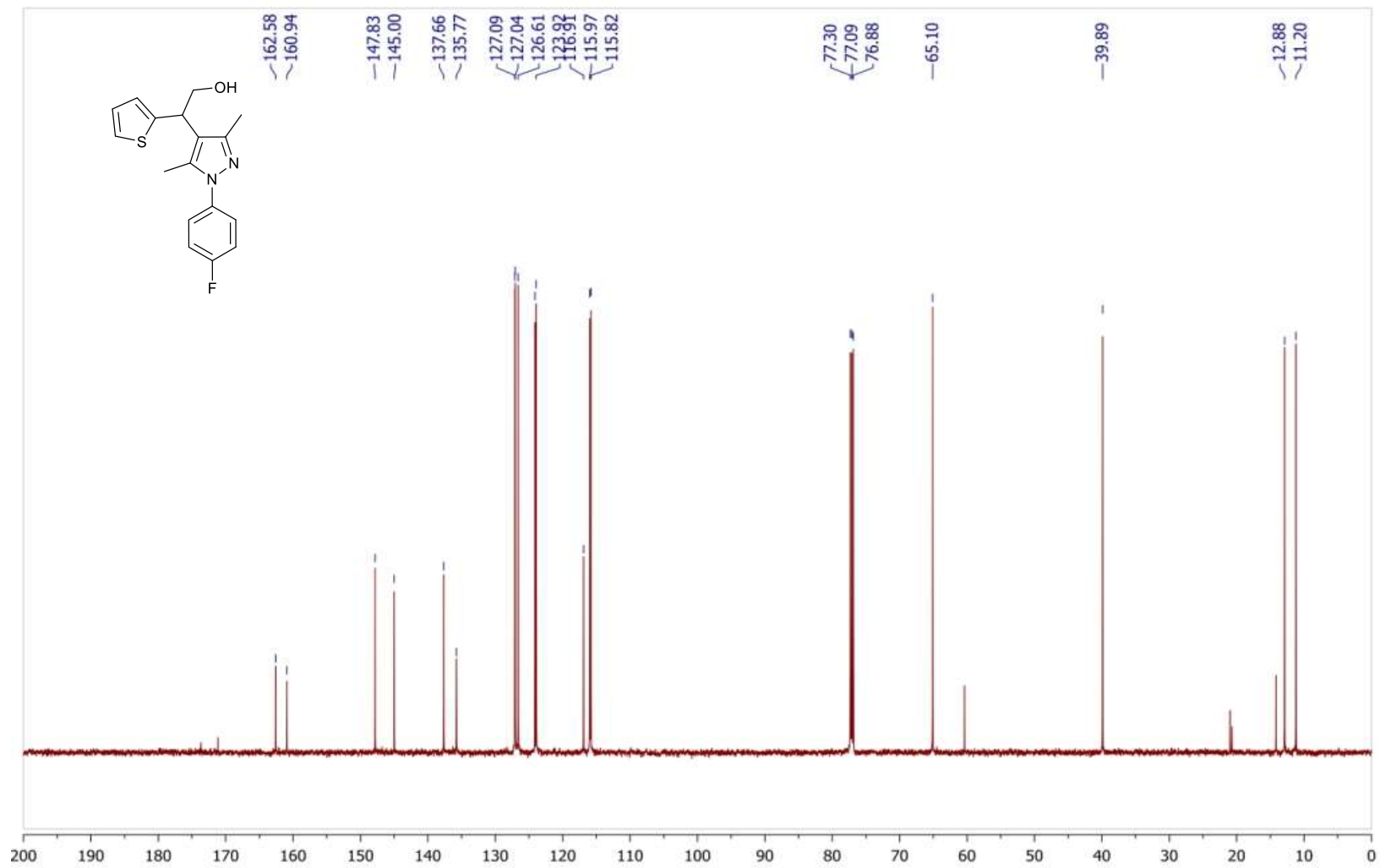
2-[1-(4-Fluorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-(thiophen-2-yl)ethanol (3n)

¹H NMR (CDCl₃, 600 MHz)



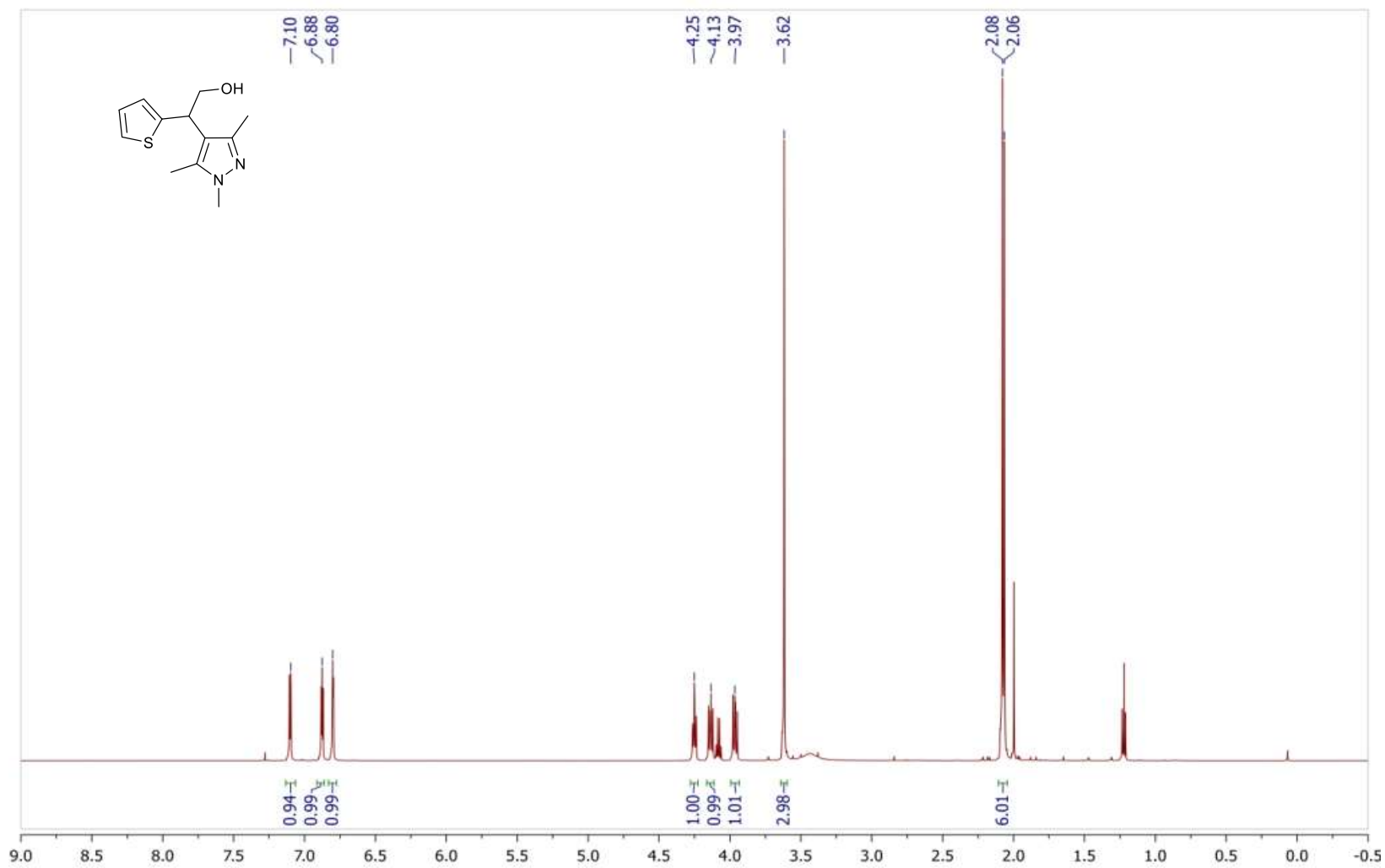
2-[1-(4-Fluorophenyl)-3,5-dimethyl-1H-pyrazol-4-yl]-2-(thiophen-2-yl)ethanol (3n)

^{13}C NMR (CDCl_3 , 150 MHz)



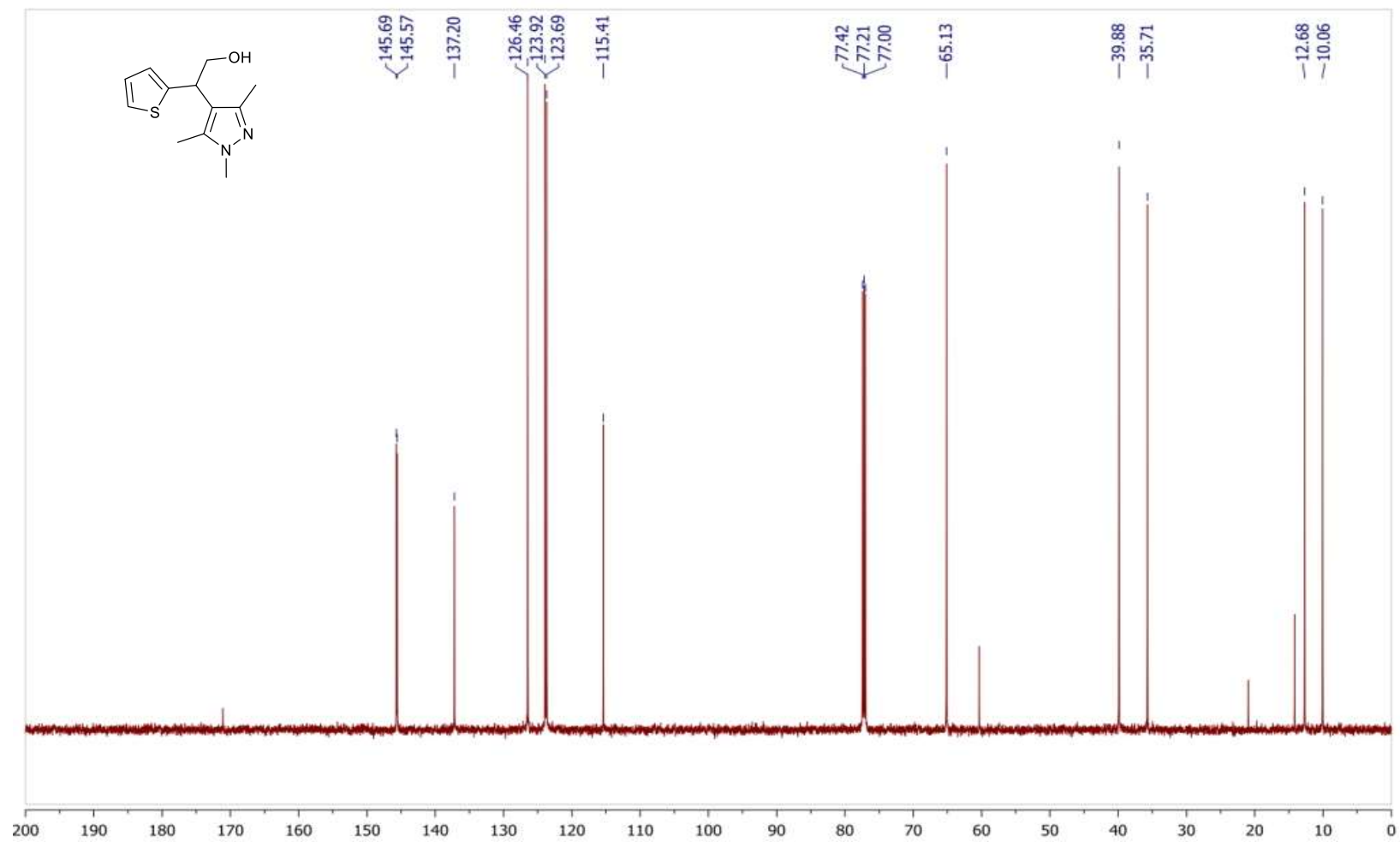
2-(Thiophen-2-yl)-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3o)

¹H NMR (CDCl₃, 600 MHz)



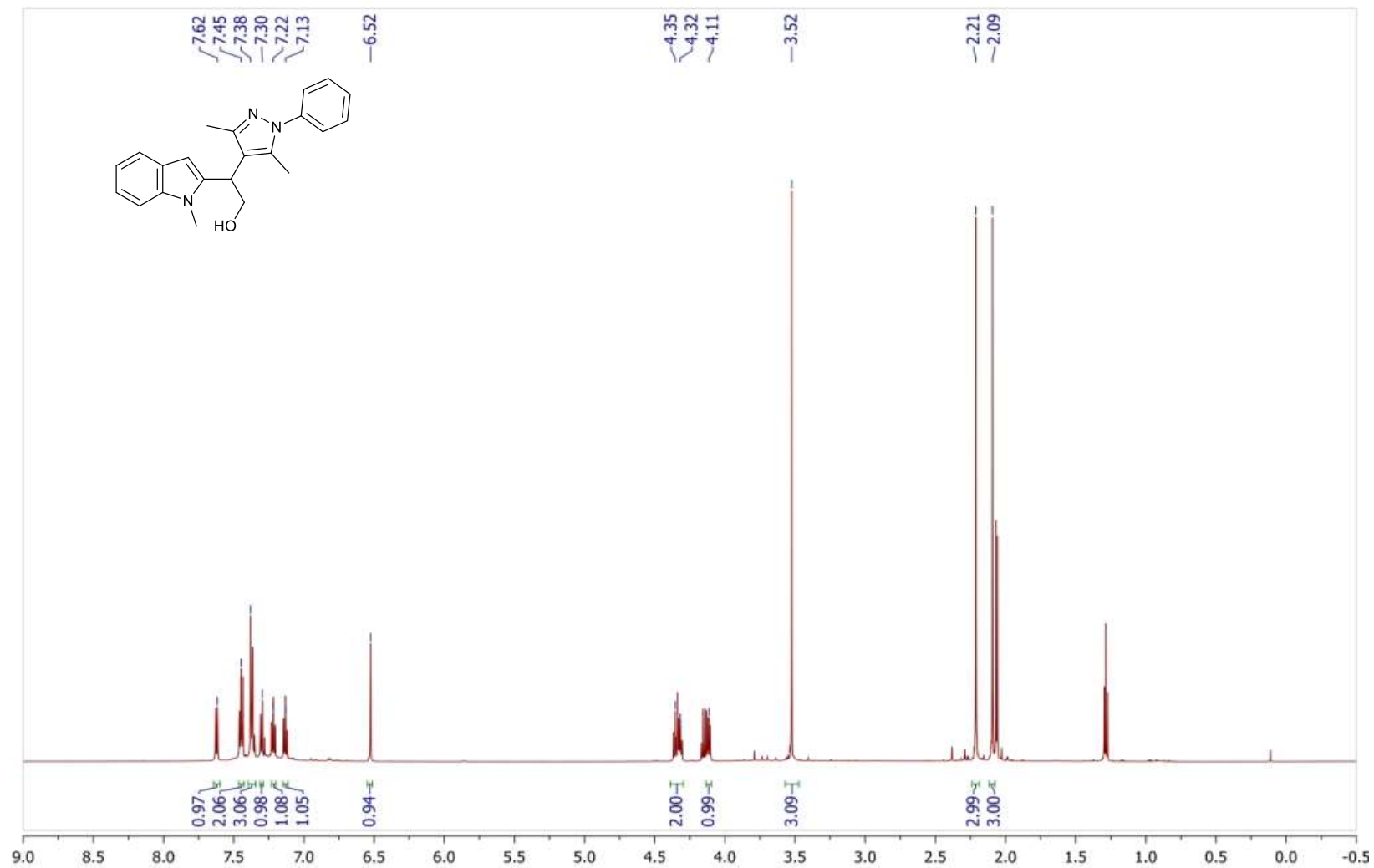
2-(Thiophen-2-yl)-2-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (3o)

^{13}C NMR (CDCl_3 , 150 MHz)



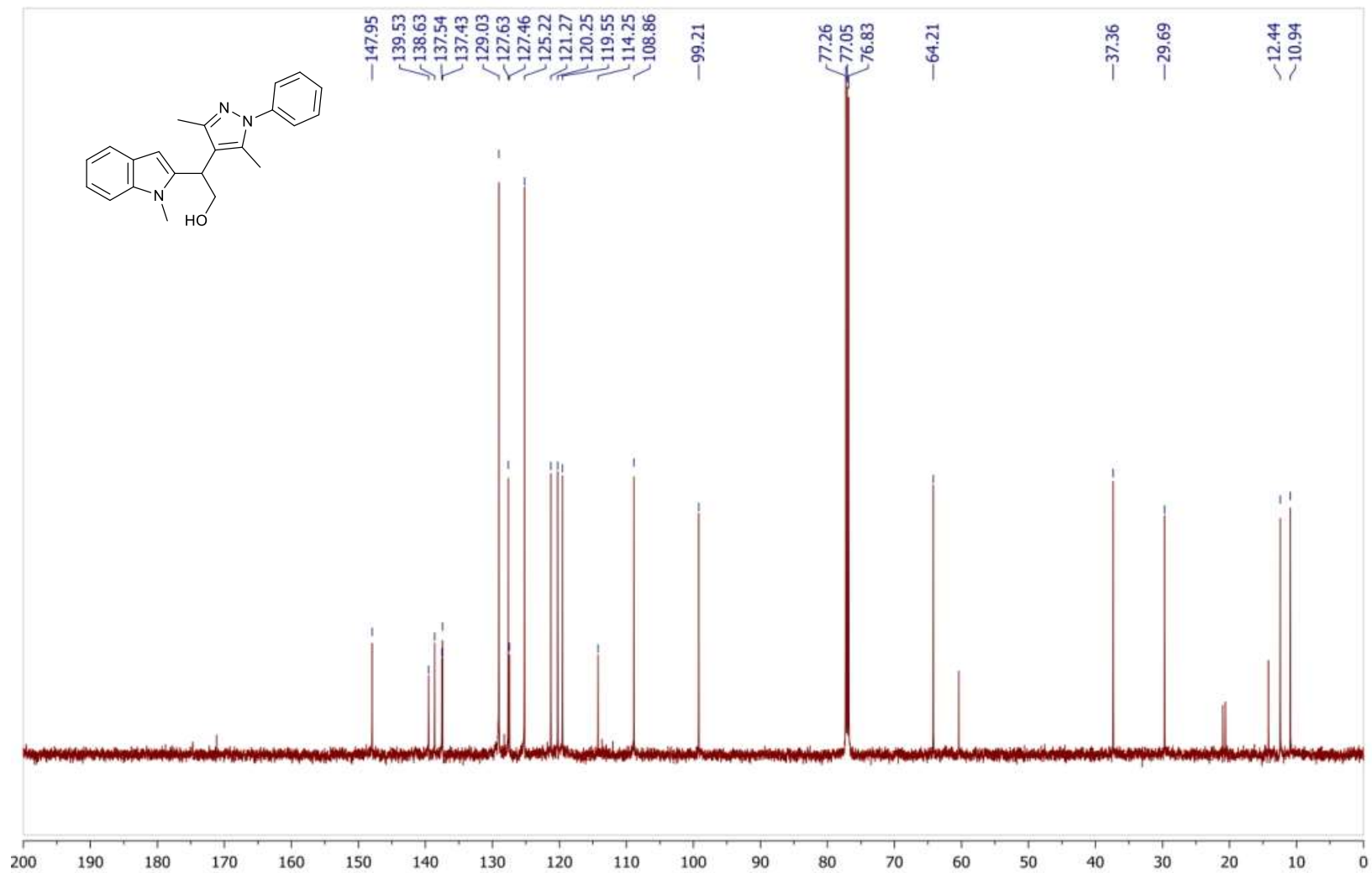
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(1-methyl-1H-indol-3-yl)ethanol (3p)

¹H NMR (CDCl₃, 600 MHz)



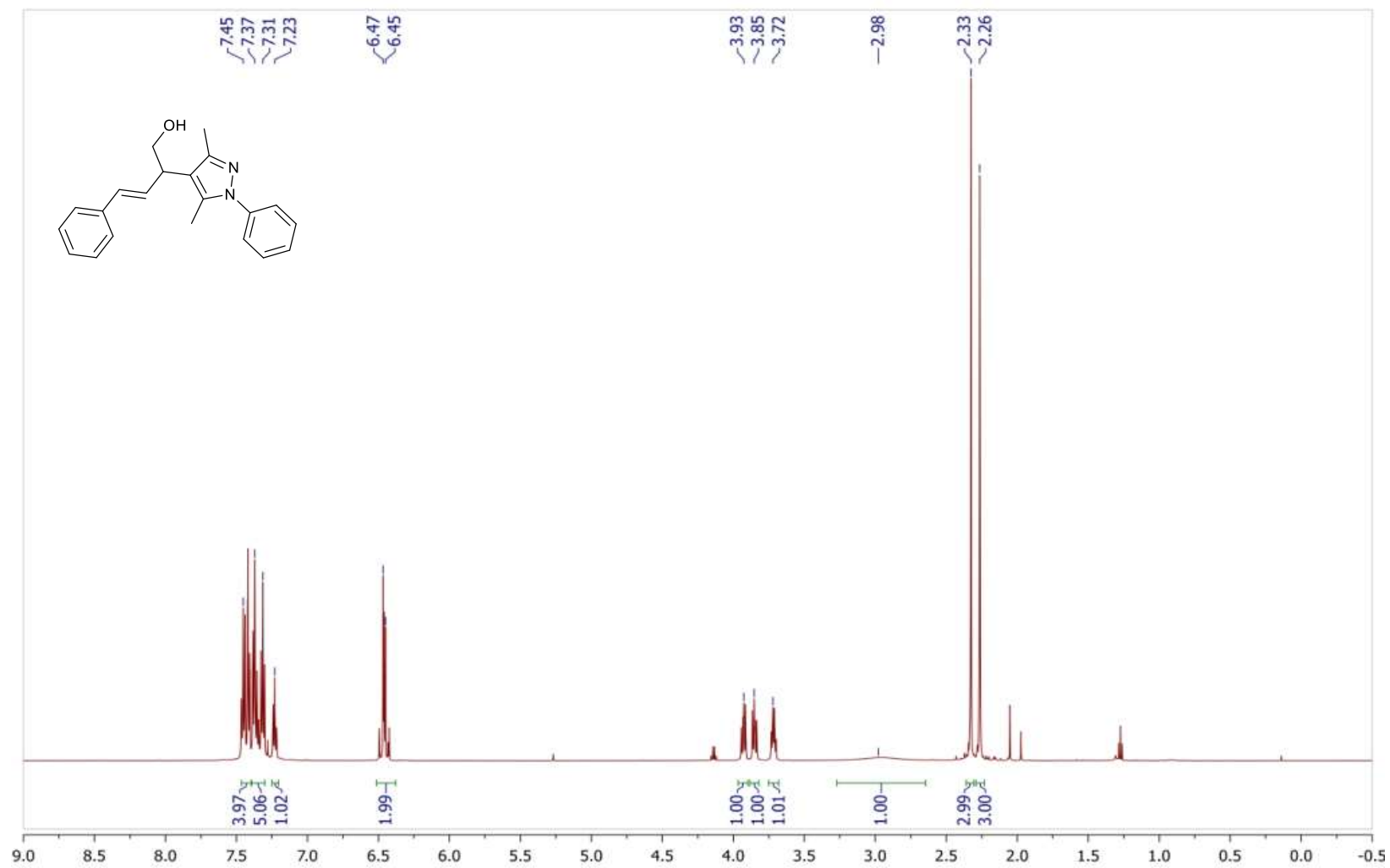
2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-2-(1-methyl-1H-indol-3-yl)ethanol (3p)

¹³C NMR (CDCl₃, 150 MHz)



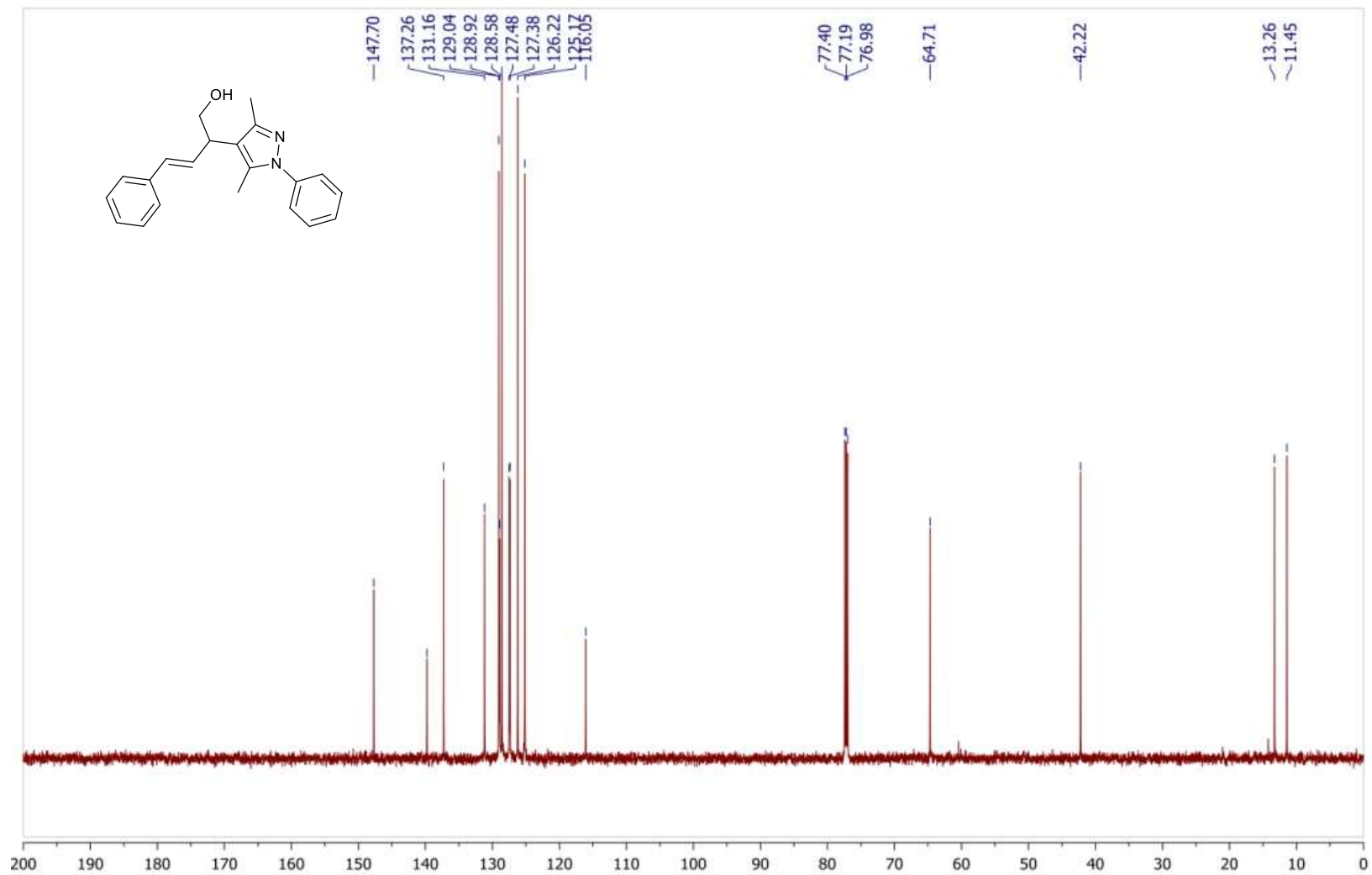
(E)-2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-4-phenylbut-3-en-1-ol (3q)

¹H NMR (CDCl₃, 600 MHz)



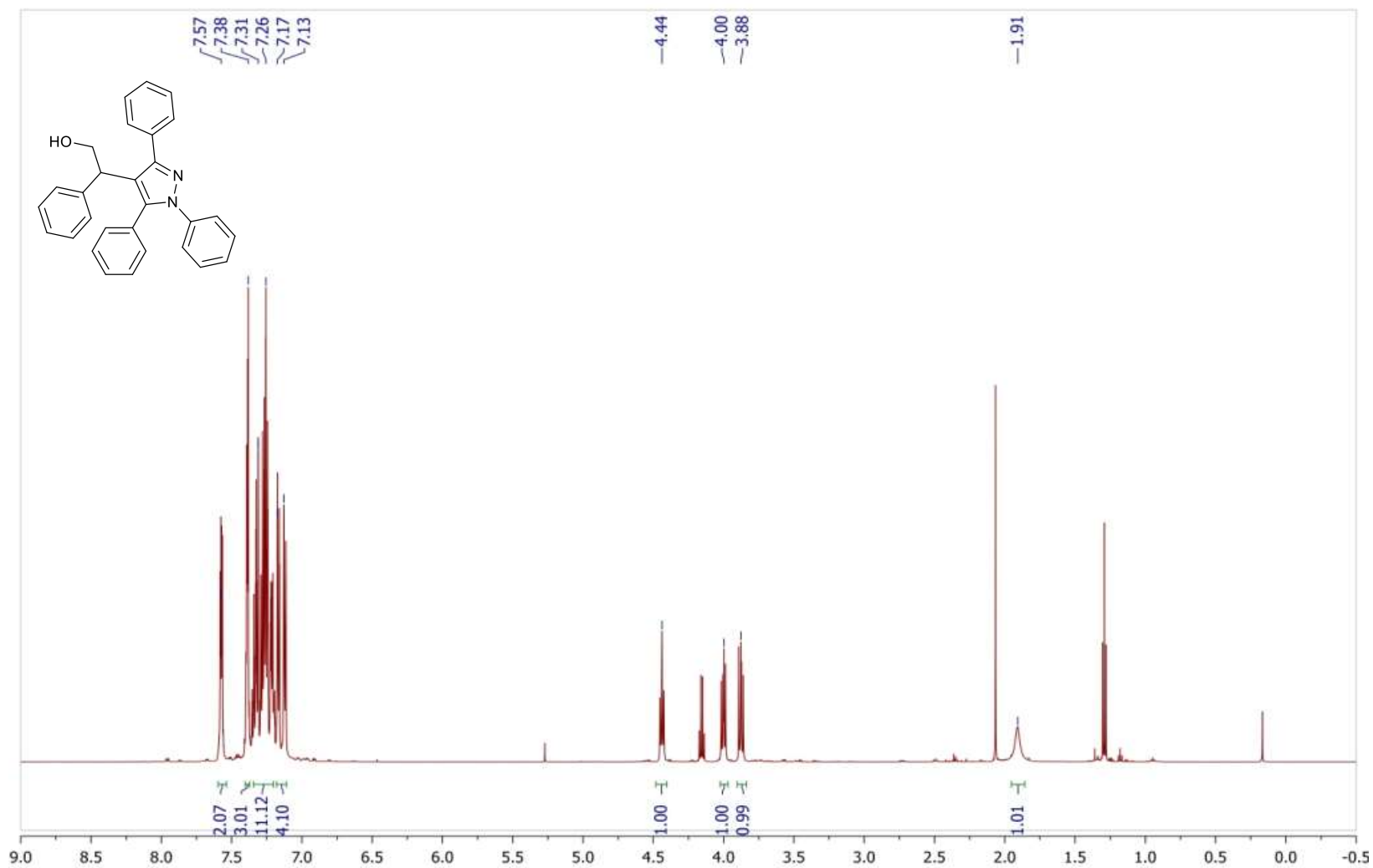
(E)-2-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-4-phenylbut-3-en-1-ol (**3q**)

^{13}C NMR (CDCl_3 , 150 MHz)



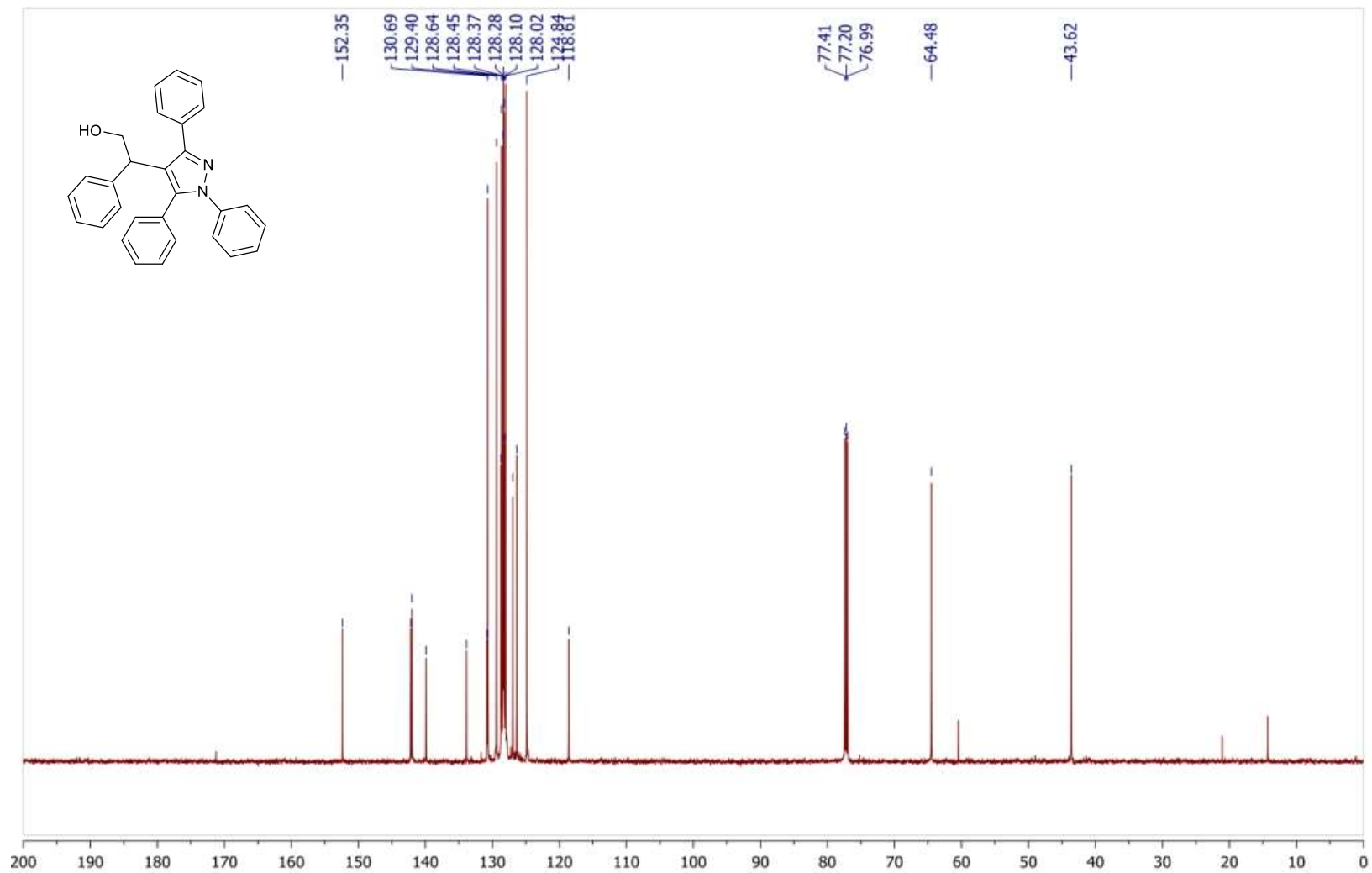
2-Phenyl-2-(1,3,5-triphenyl-1H-pyrazol-4-yl)ethanol (3r)

¹H NMR (CDCl₃, 600 MHz)



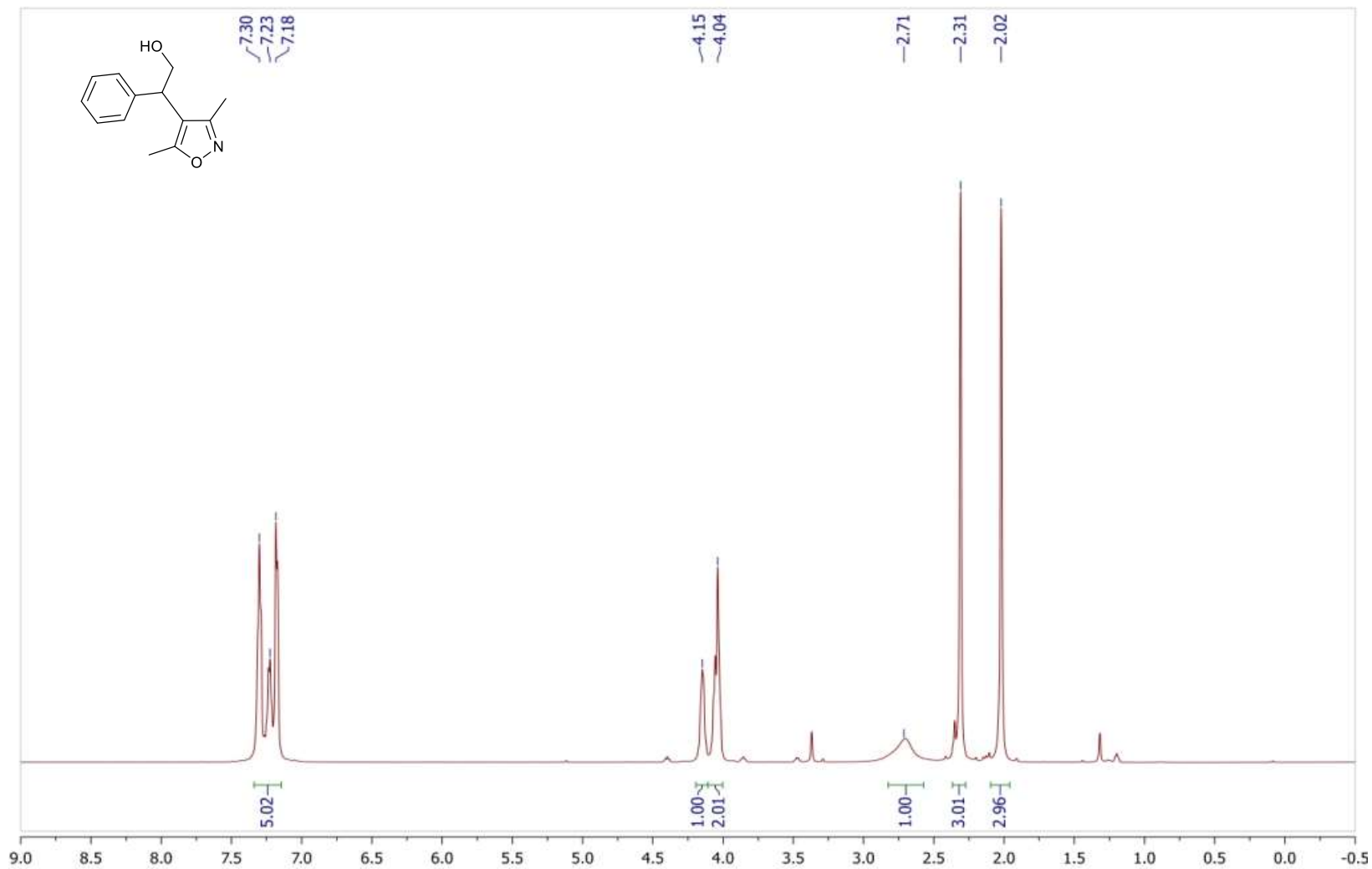
2-Phenyl-2-(1,3,5-triphenyl-1H-pyrazol-4-yl)ethanol (3r)

^{13}C NMR (CDCl_3 , 150 MHz)



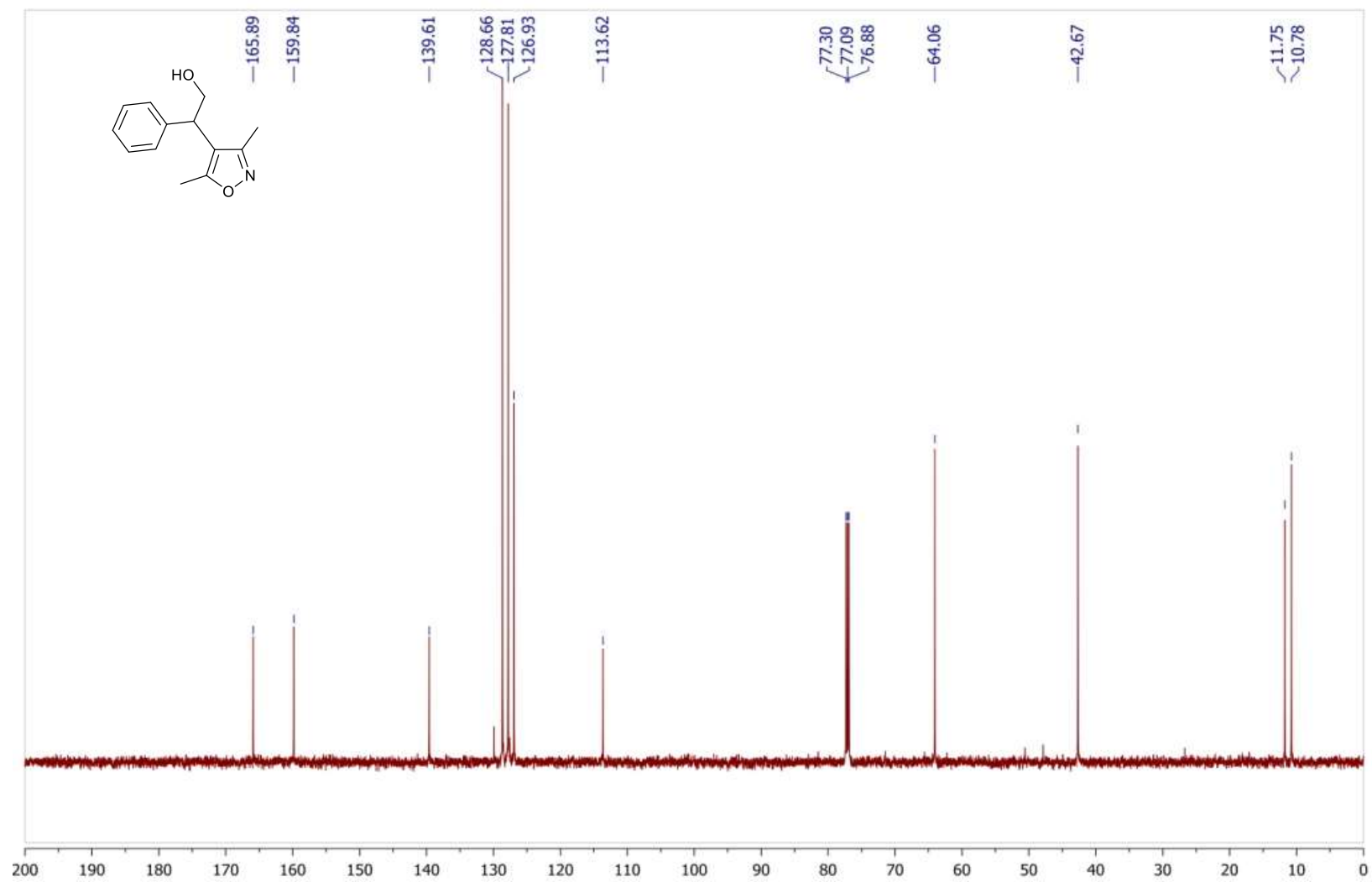
2-(3,5-Dimethylisoxazol-4-yl)-2-phenylethanol (4a)

^1H NMR (CDCl_3 , 600 MHz)



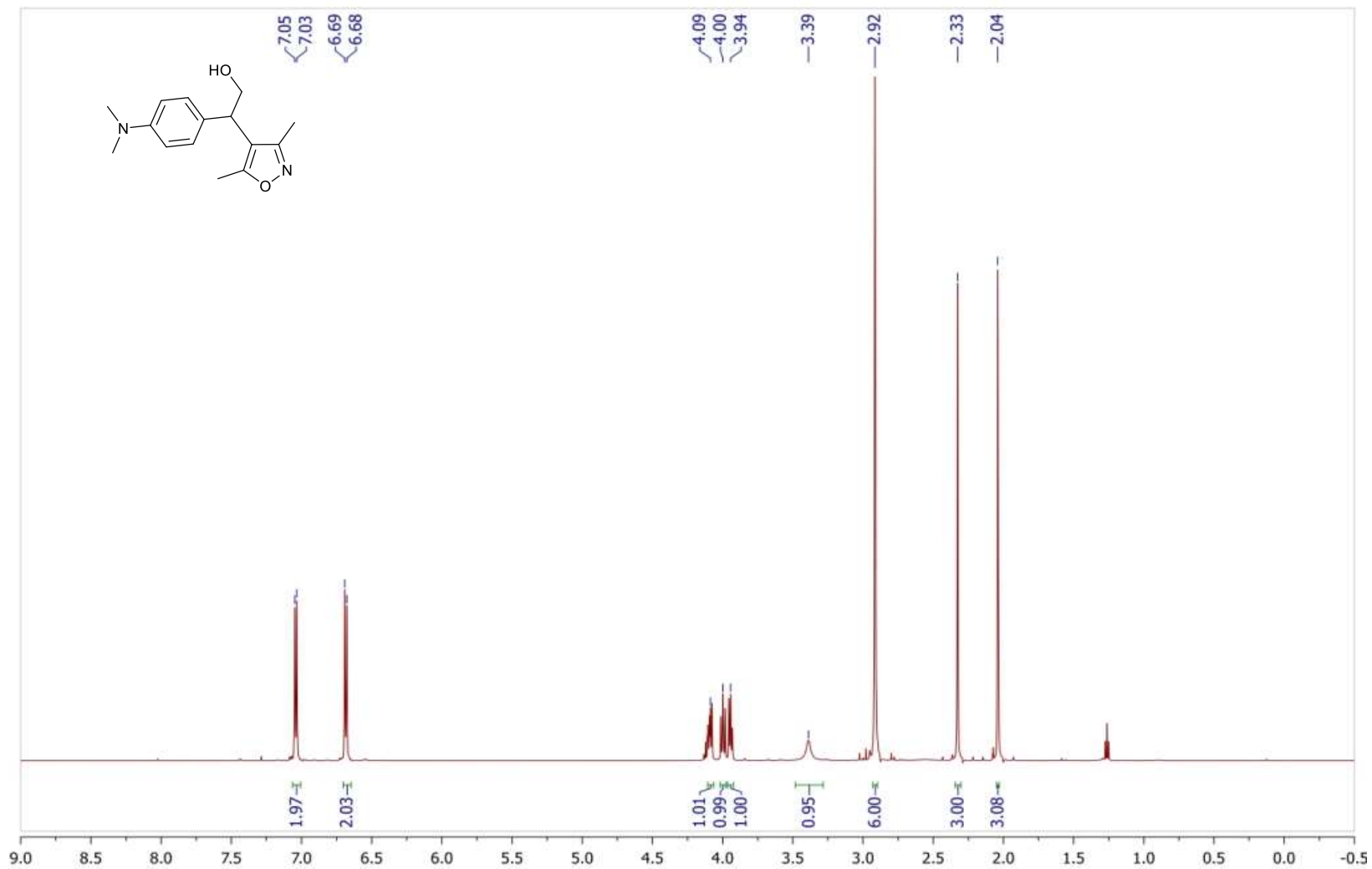
2-(3,5-Dimethylisoxazol-4-yl)-2-phenylethanol (4a)

^{13}C NMR (CDCl_3 , 150 MHz)



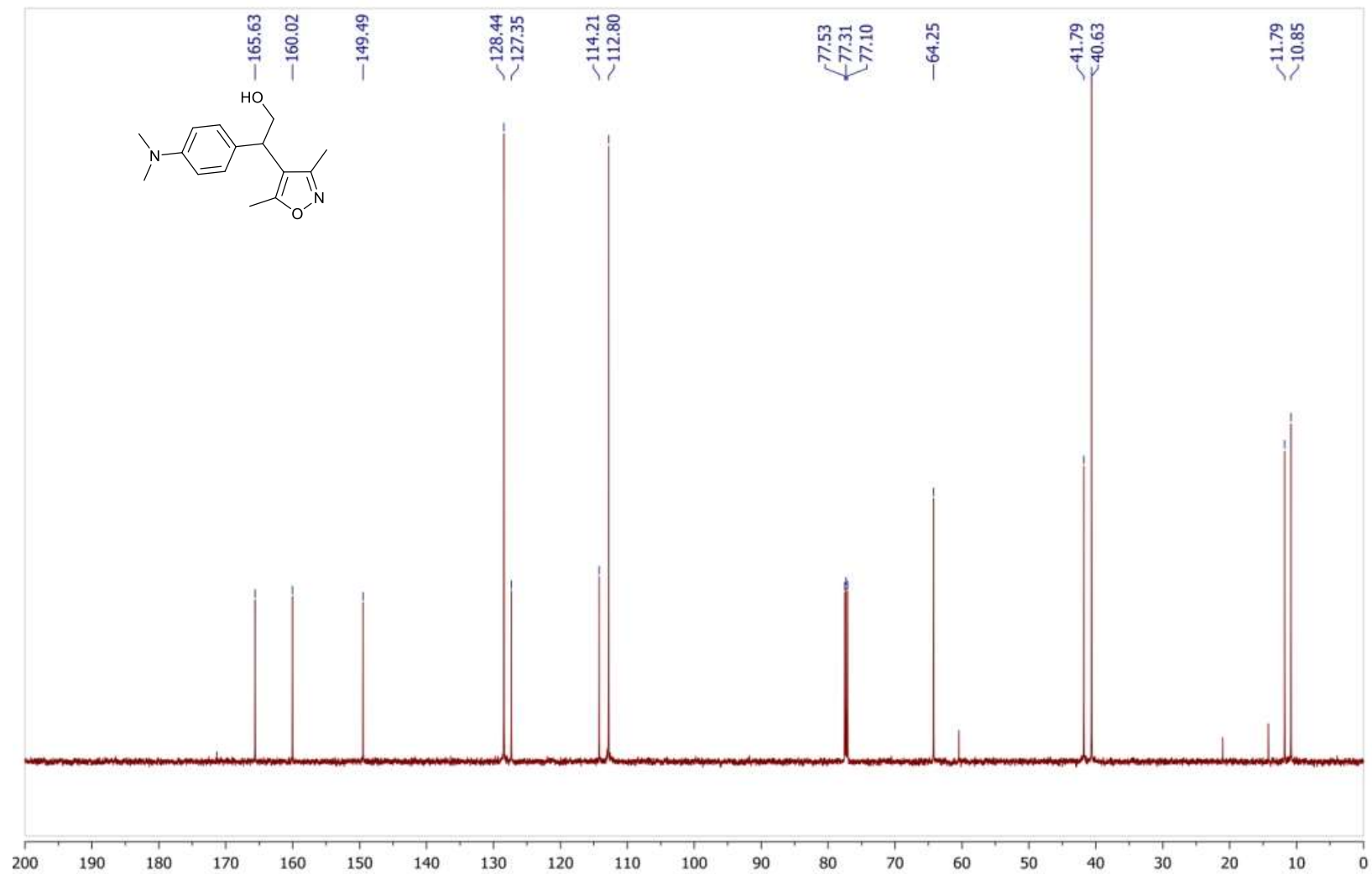
2-[4-(Dimethylamino)phenyl]-2-(3,5-dimethylisoxazol-4-yl)ethanol (4b)

¹H NMR (CDCl₃, 600 MHz)



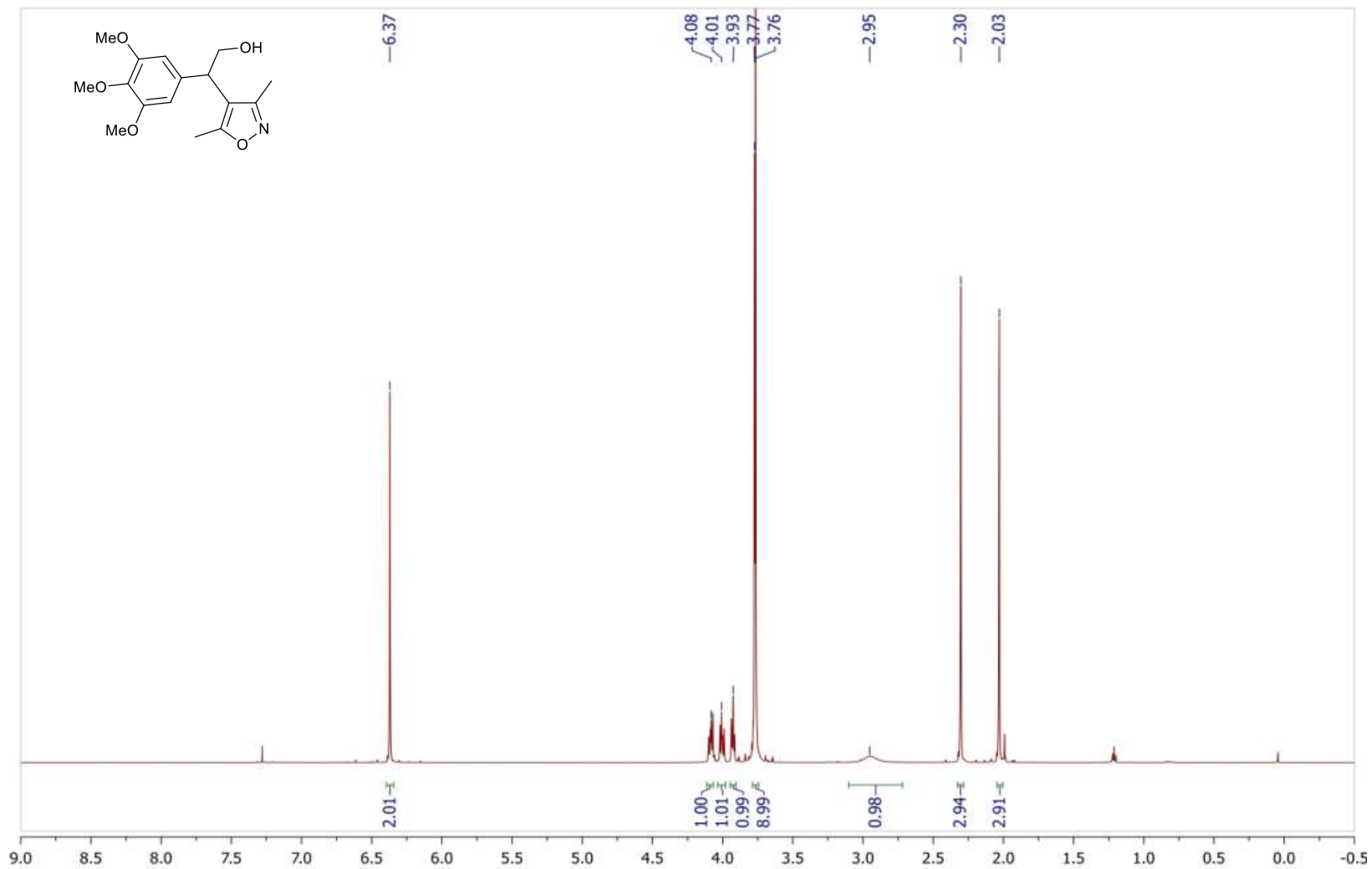
2-[4-(Dimethylamino)phenyl]-2-(3,5-dimethylisoxazol-4-yl)ethanol (4b)

^{13}C NMR (CDCl_3 , 150 MHz)



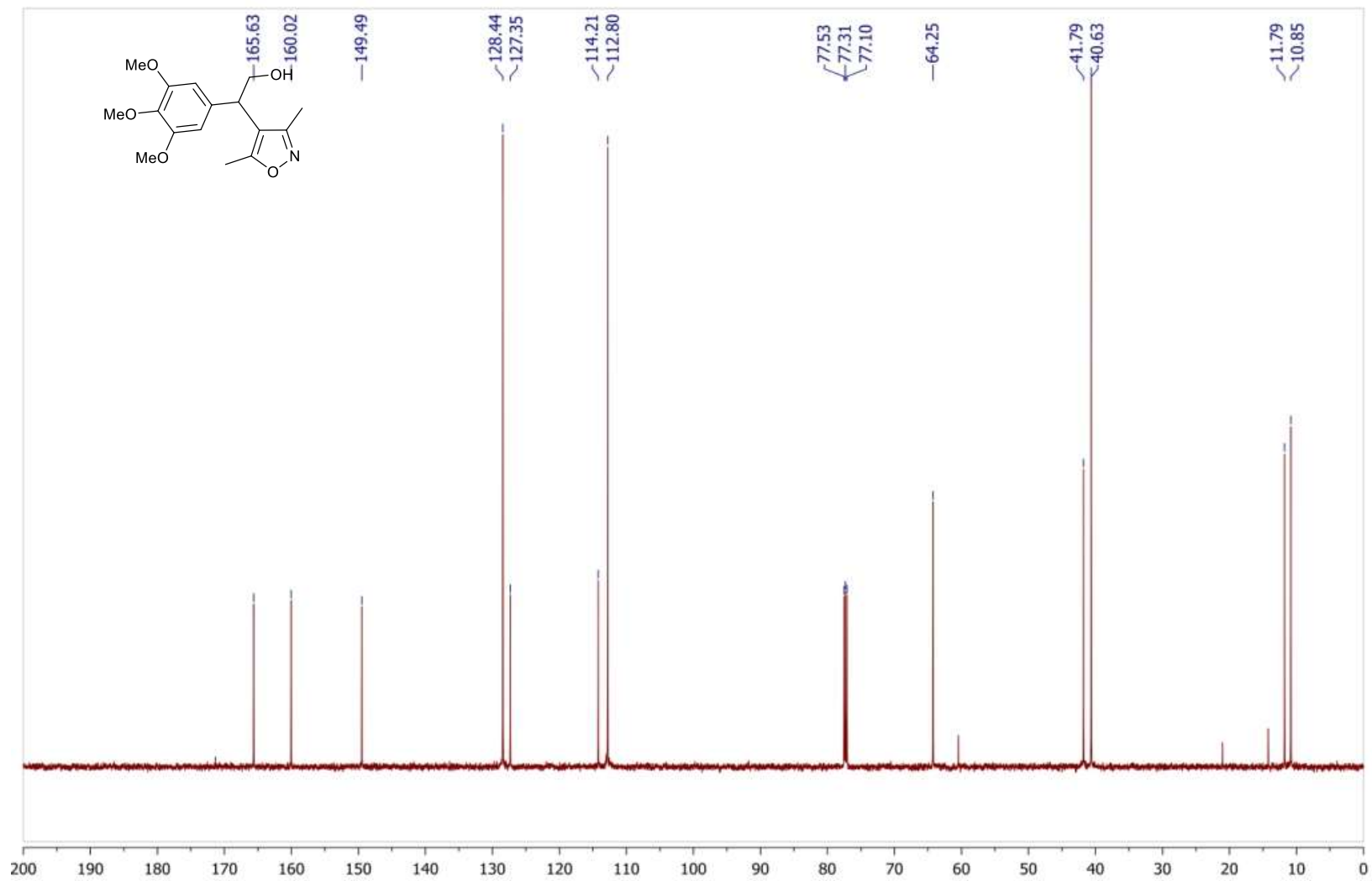
2-(3,5-Dimethylisoxazol-4-yl)-2-(3,4,5-trimethoxyphenyl)ethanol (4c)

^1H NMR (CDCl_3 , 600 MHz)



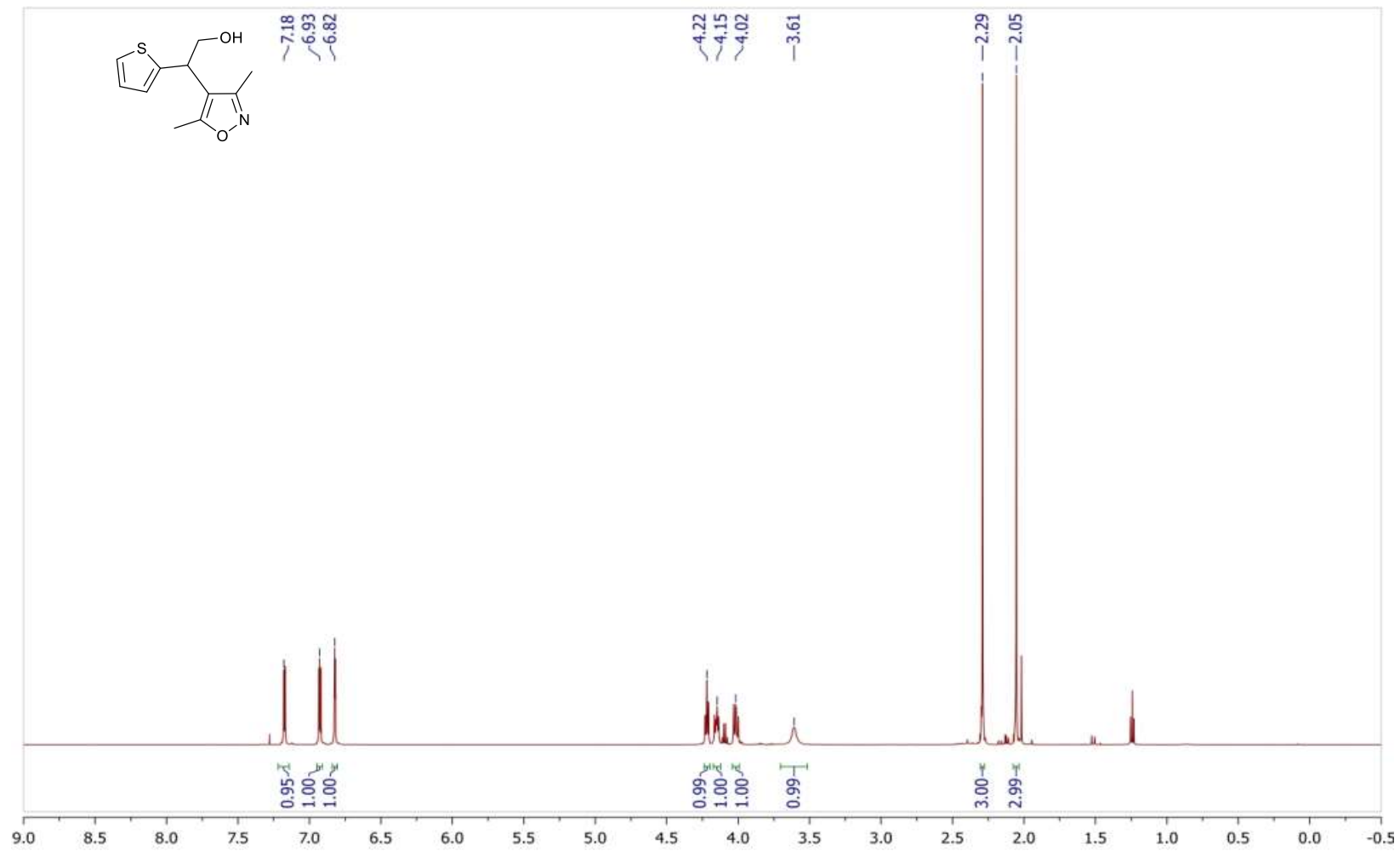
2-(3,5-Dimethylisoxazol-4-yl)-2-(3,4,5-trimethoxyphenyl)ethanol (4c)

^{13}C NMR (CDCl_3 , 150 MHz)



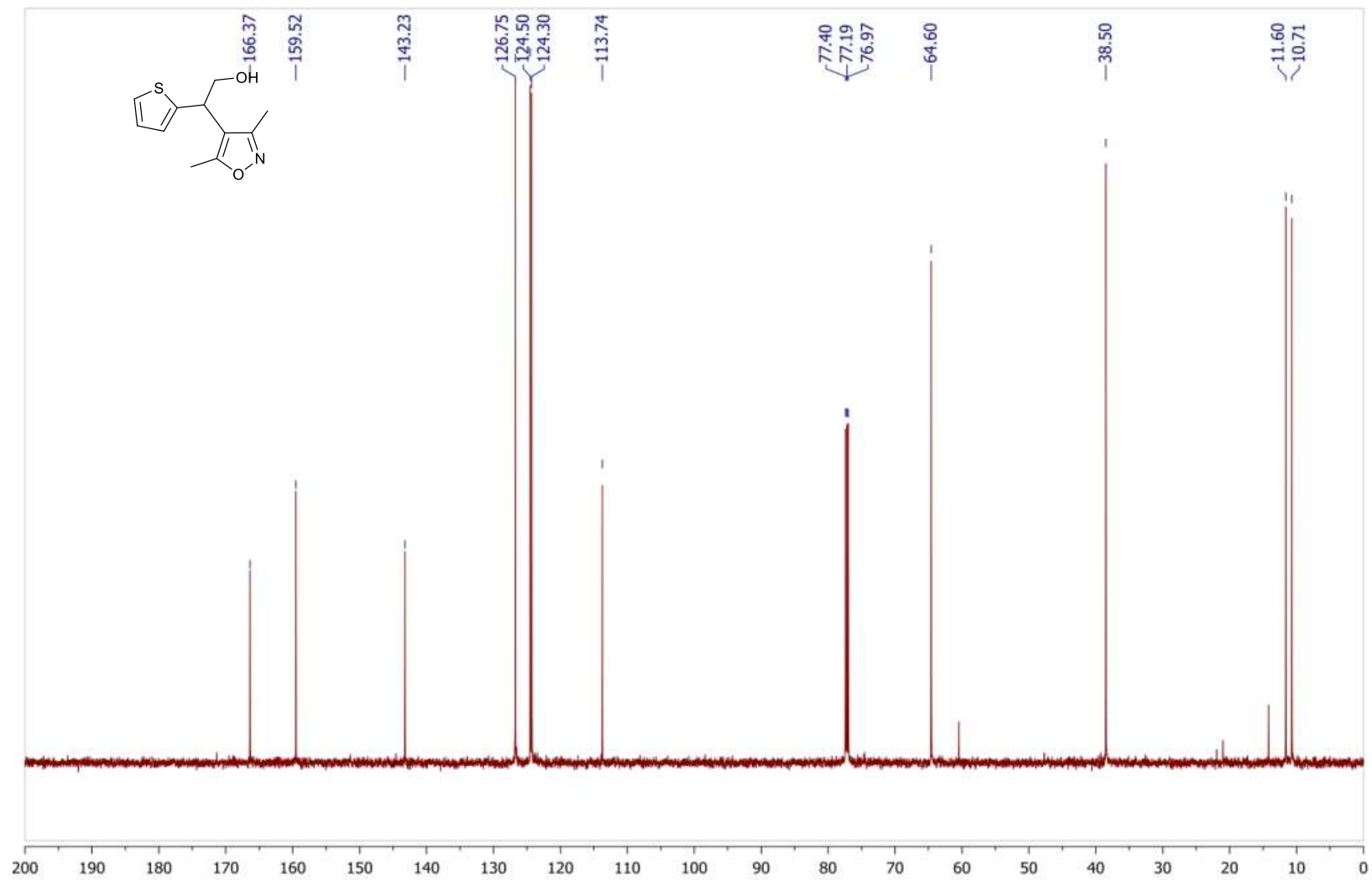
2-(3,5-Dimethylisoxazol-4-yl)-2-(thiophen-2-yl)ethanol (4d)

¹H NMR (CDCl₃, 600 MHz)



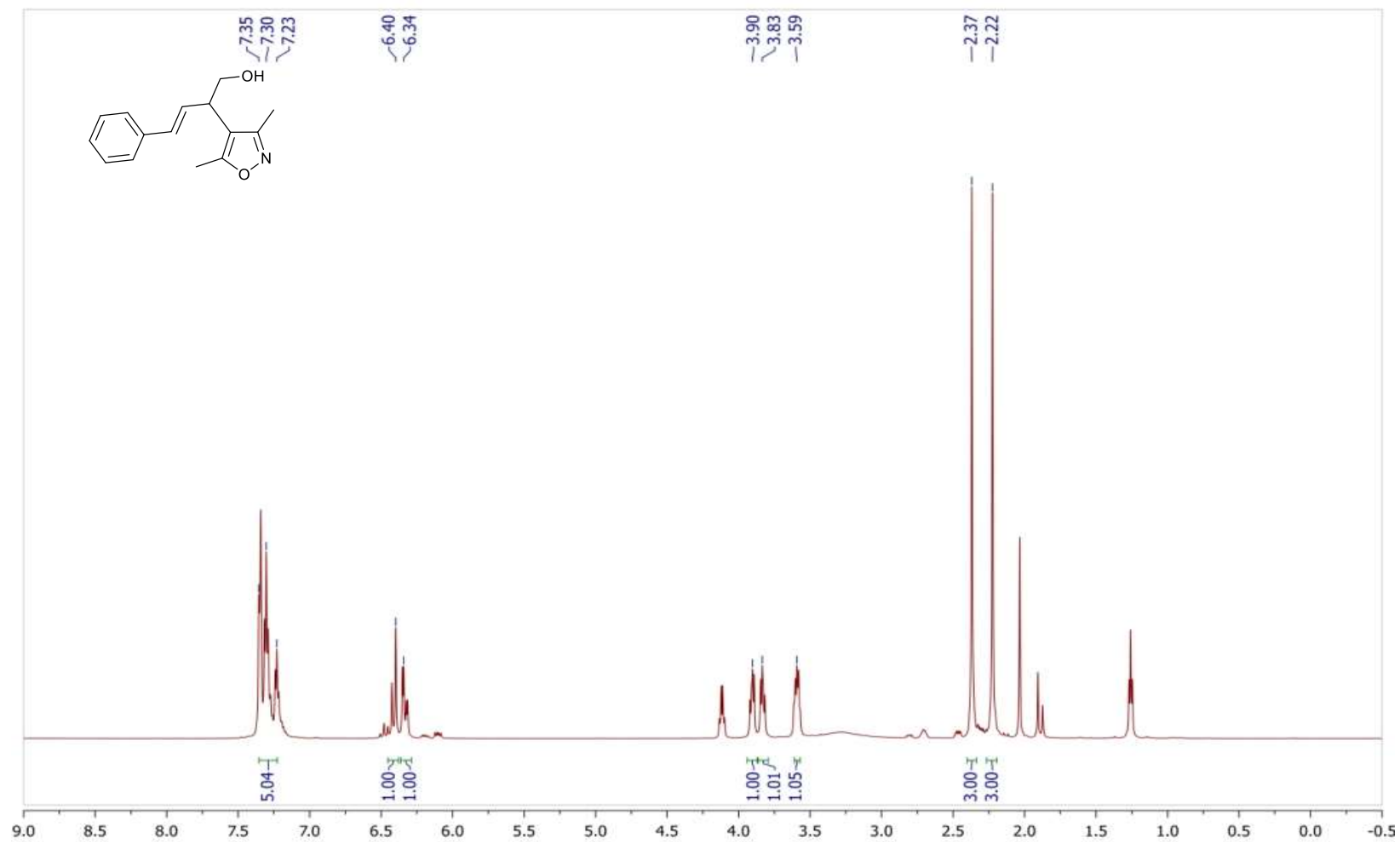
2-(3,5-Dimethylisoxazol-4-yl)-2-(thiophen-2-yl)ethanol (4d)

^{13}C NMR (CDCl_3 , 150 MHz)



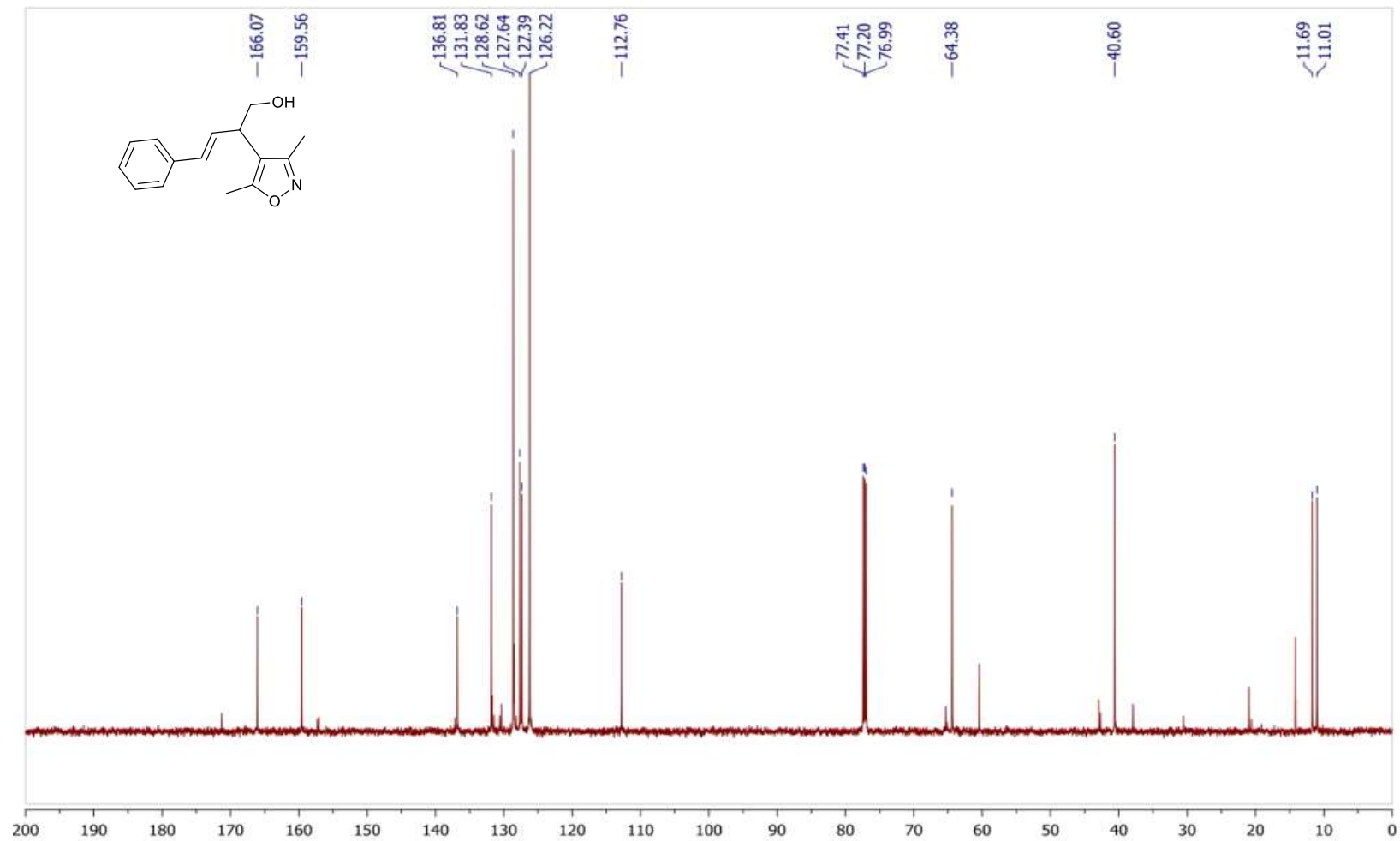
(E)-2-(3,5-Dimethylisoxazol-4-yl)-4-phenylbut-3-en-1-ol (*4e*)

¹H NMR (CDCl₃, 600 MHz)



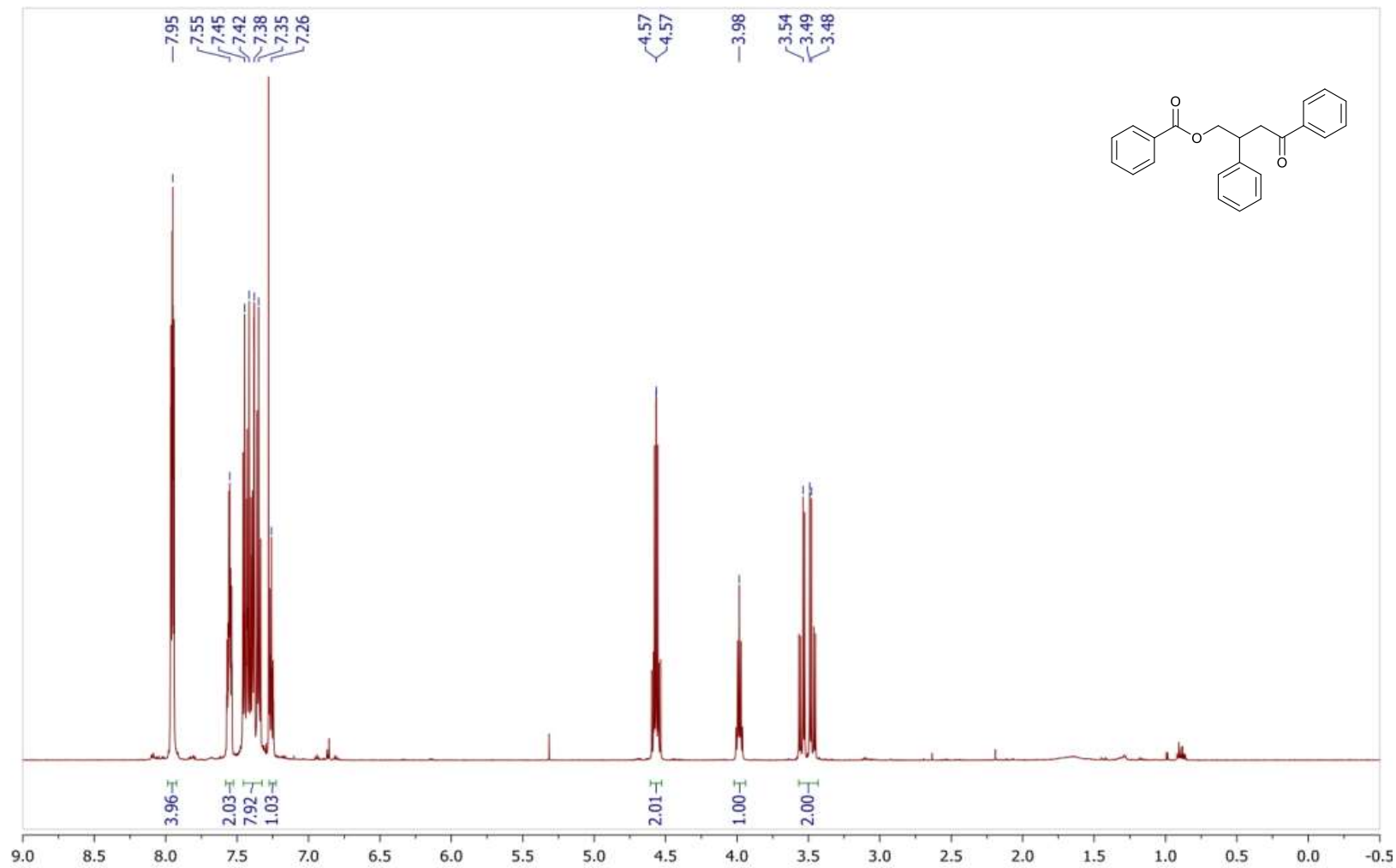
(E)-2-(3,5-Dimethylisoxazol-4-yl)-4-phenylbut-3-en-1-ol (*4e*)

^{13}C NMR (CDCl_3 , 150 MHz)



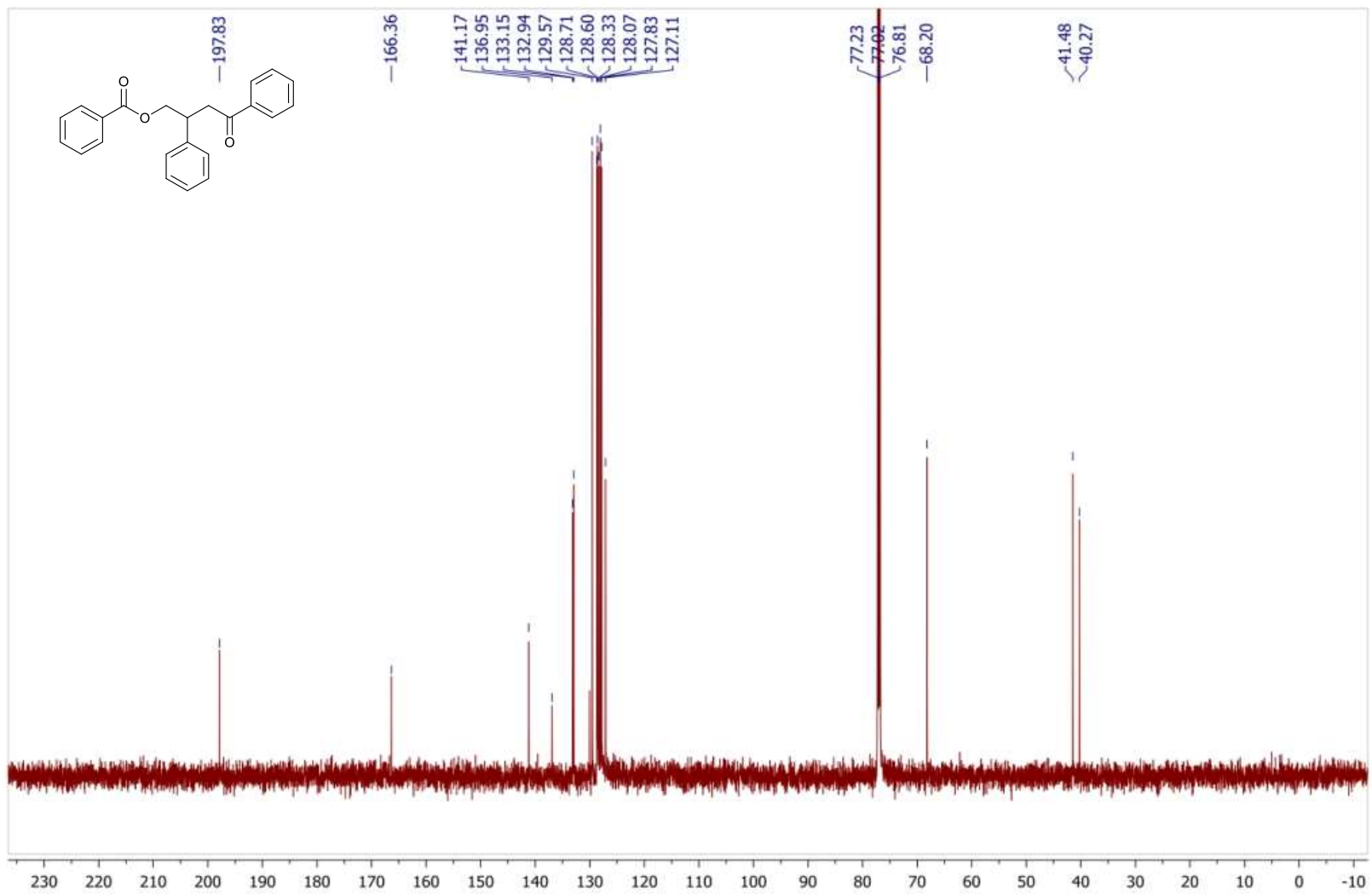
4-Oxo-2,4-diphenylbutyl benzoate (6)

¹H NMR (CDCl₃, 600 MHz)



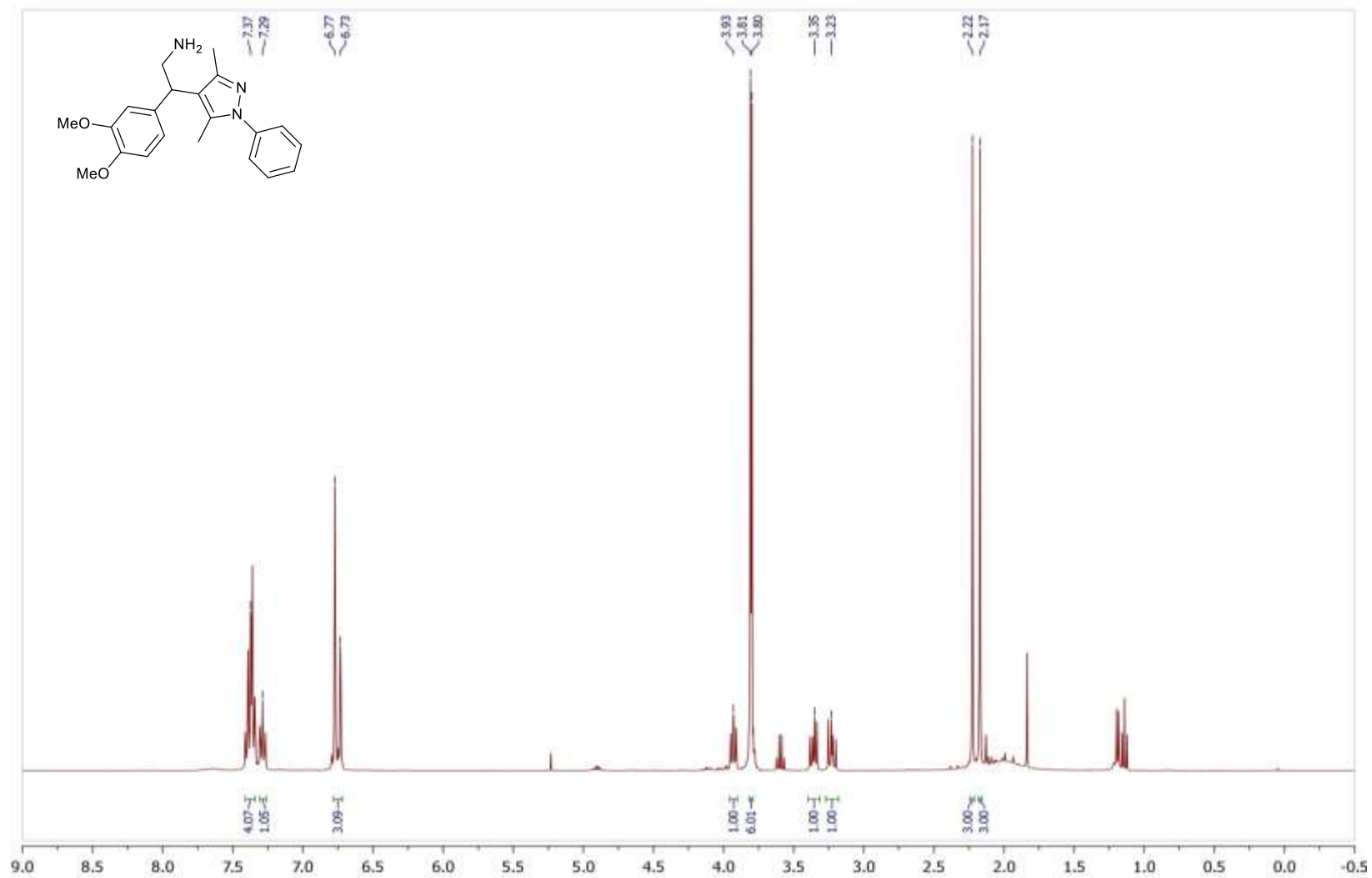
4-Oxo-2,4-diphenylbutyl benzoate (6)

^{13}C NMR (CDCl_3 , 150 MHz)



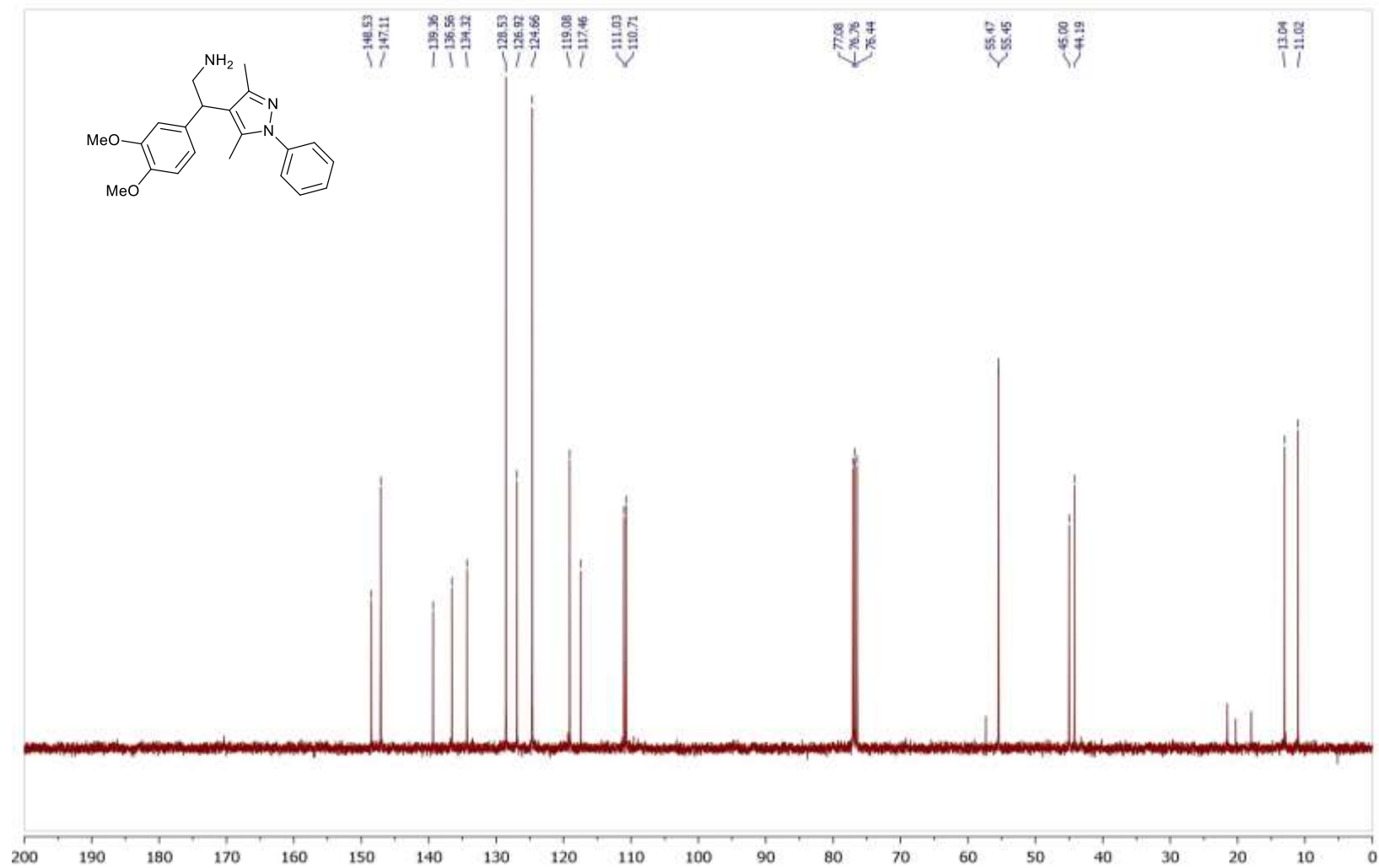
2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethylamine (7)

¹H NMR (CDCl₃, 600 MHz)



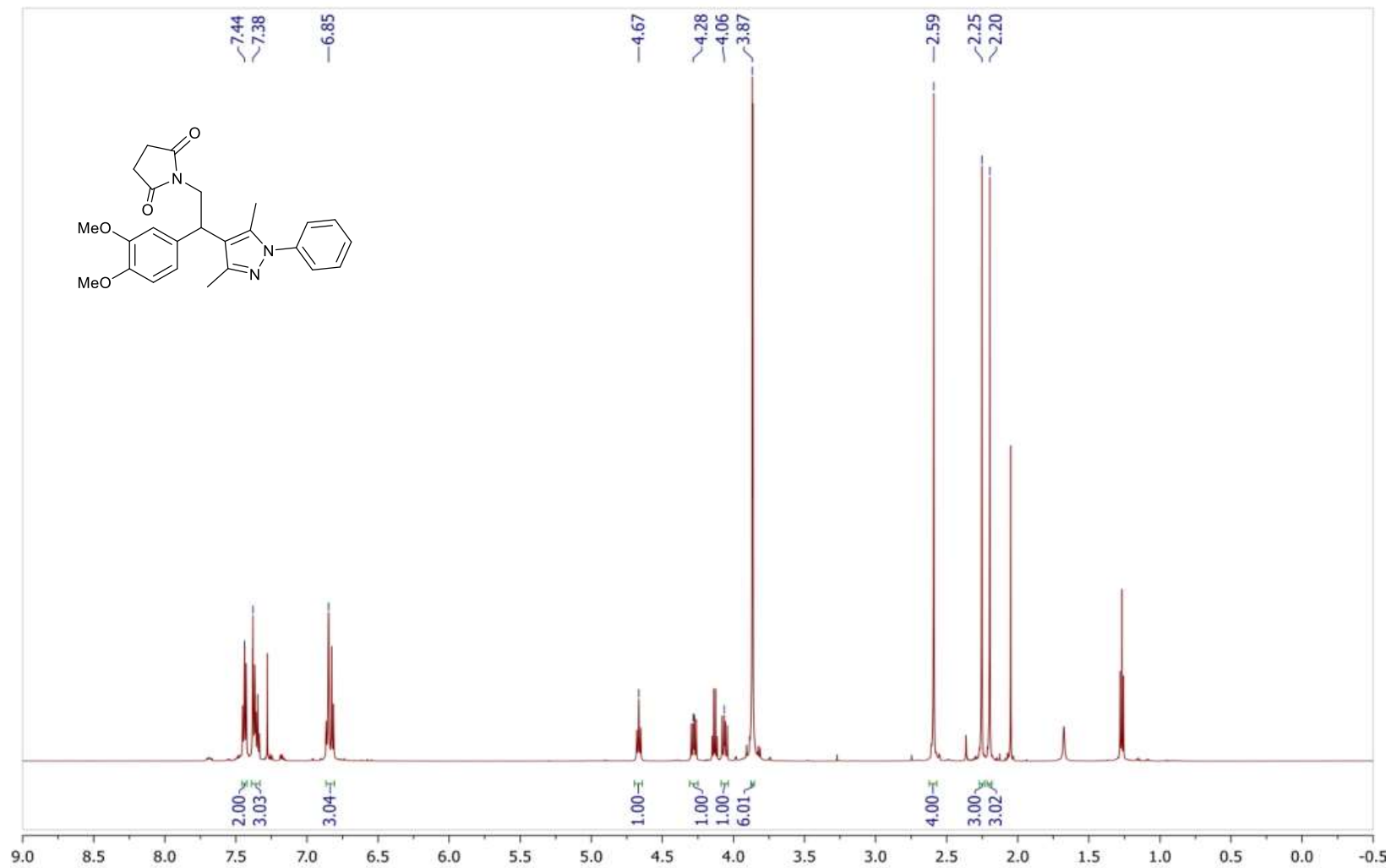
2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethylamine (7)

^{13}C NMR (CDCl_3 , 150 MHz)



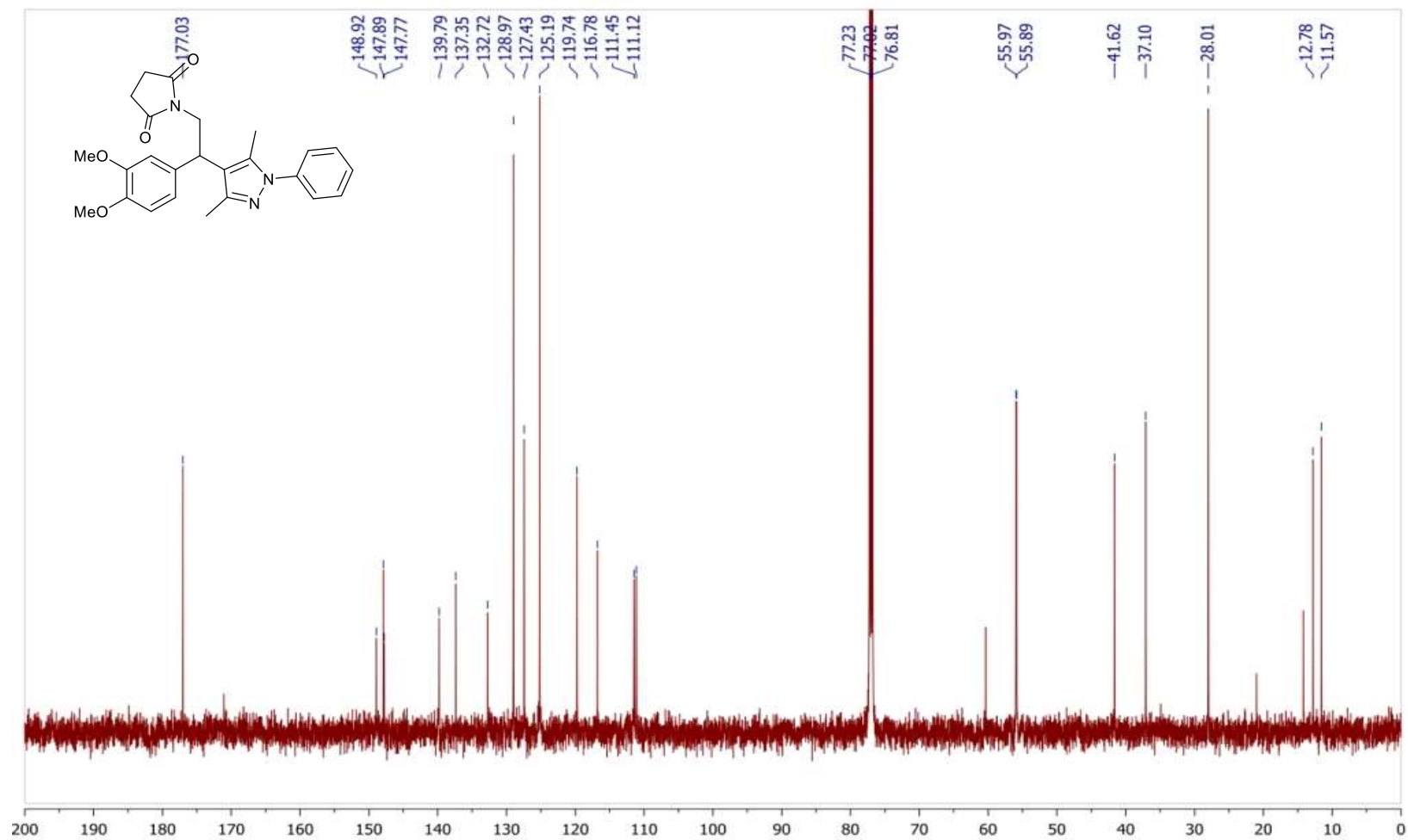
1-[2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethyl]pyrrolidine-2,5-dione (8)

¹H NMR (CDCl₃, 600 MHz)



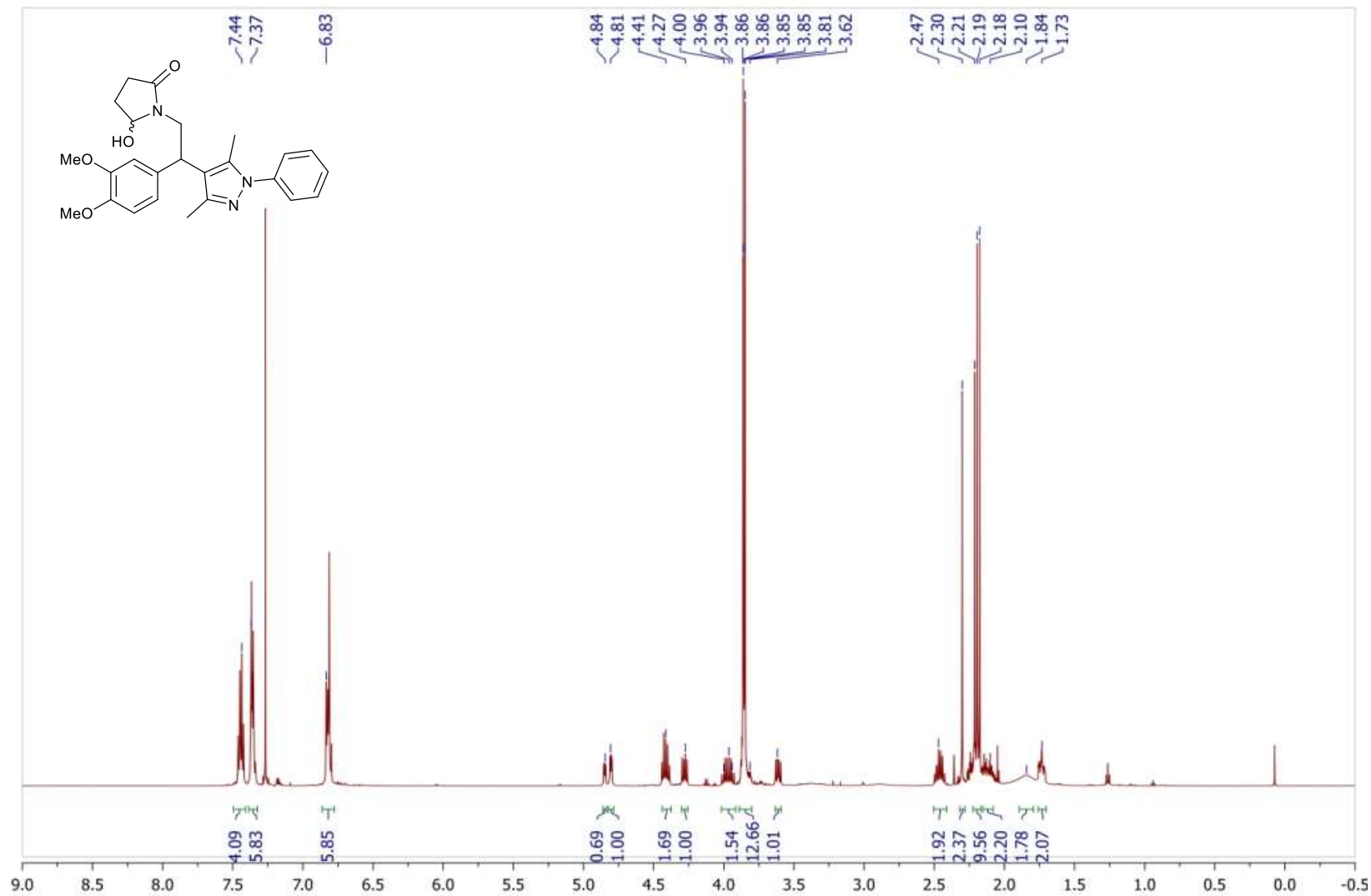
1-[2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethyl]pyrrolidine-2,5-dione (8)

^{13}C NMR (CDCl_3 , 150 MHz)



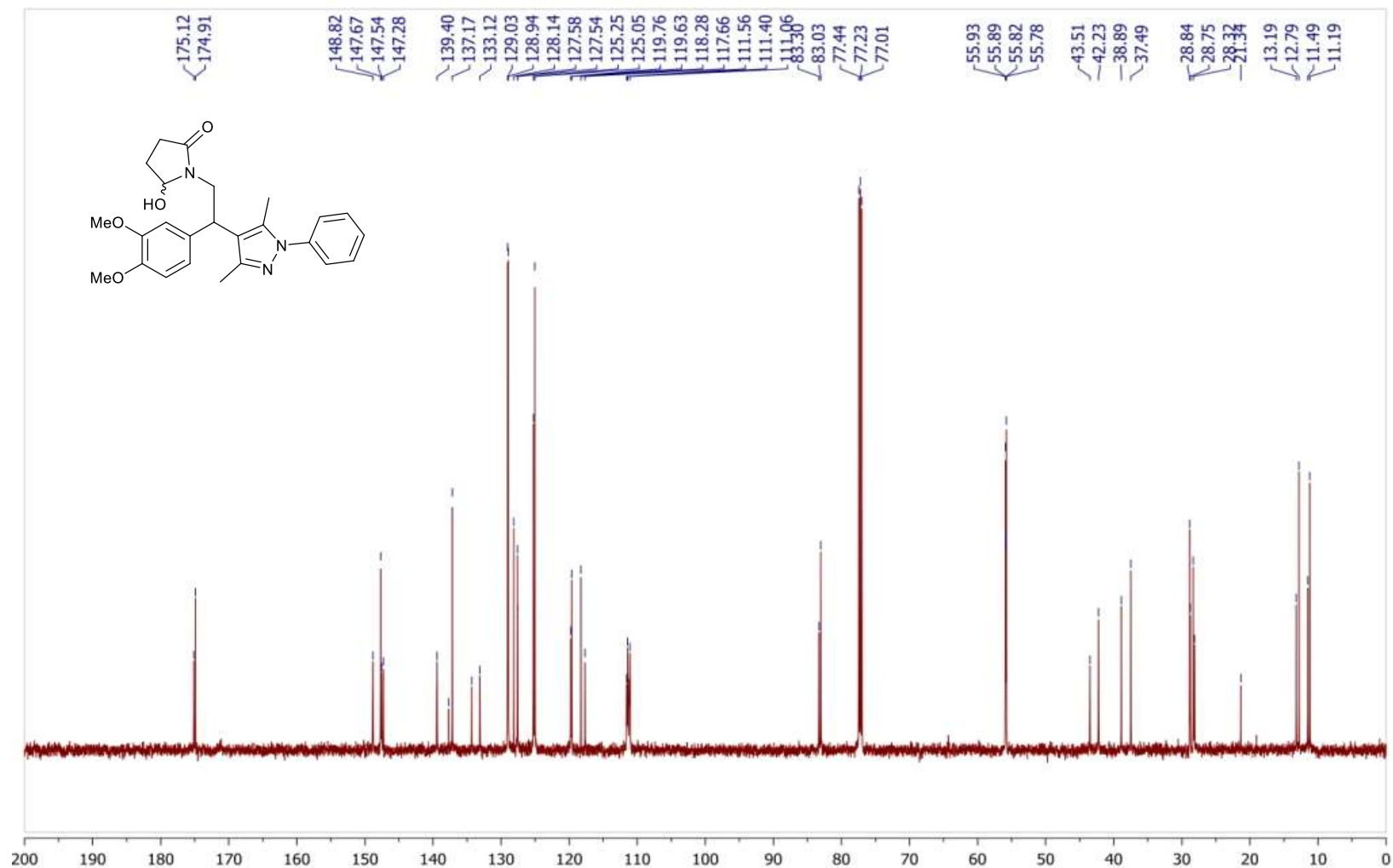
1-[2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethyl]-5-hydroxypyrrolidin-2-one (S1)

¹H NMR (CDCl₃, 600 MHz)



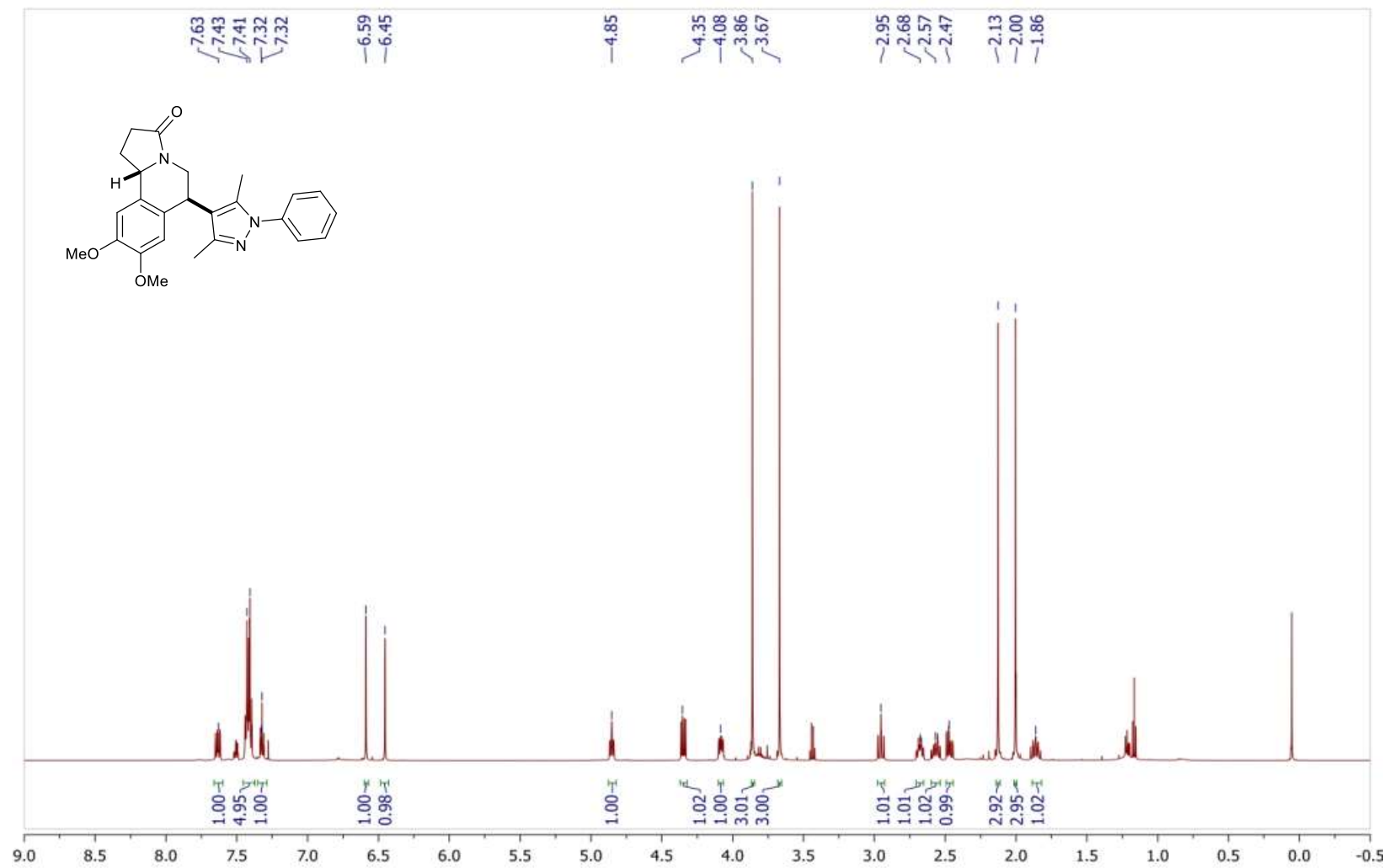
1-[2-(3,4-Dimethoxyphenyl)-2-(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)ethyl]-5-hydroxypyrrolidin-2-one (S1)

¹³C NMR (CDCl₃, 150 MHz)



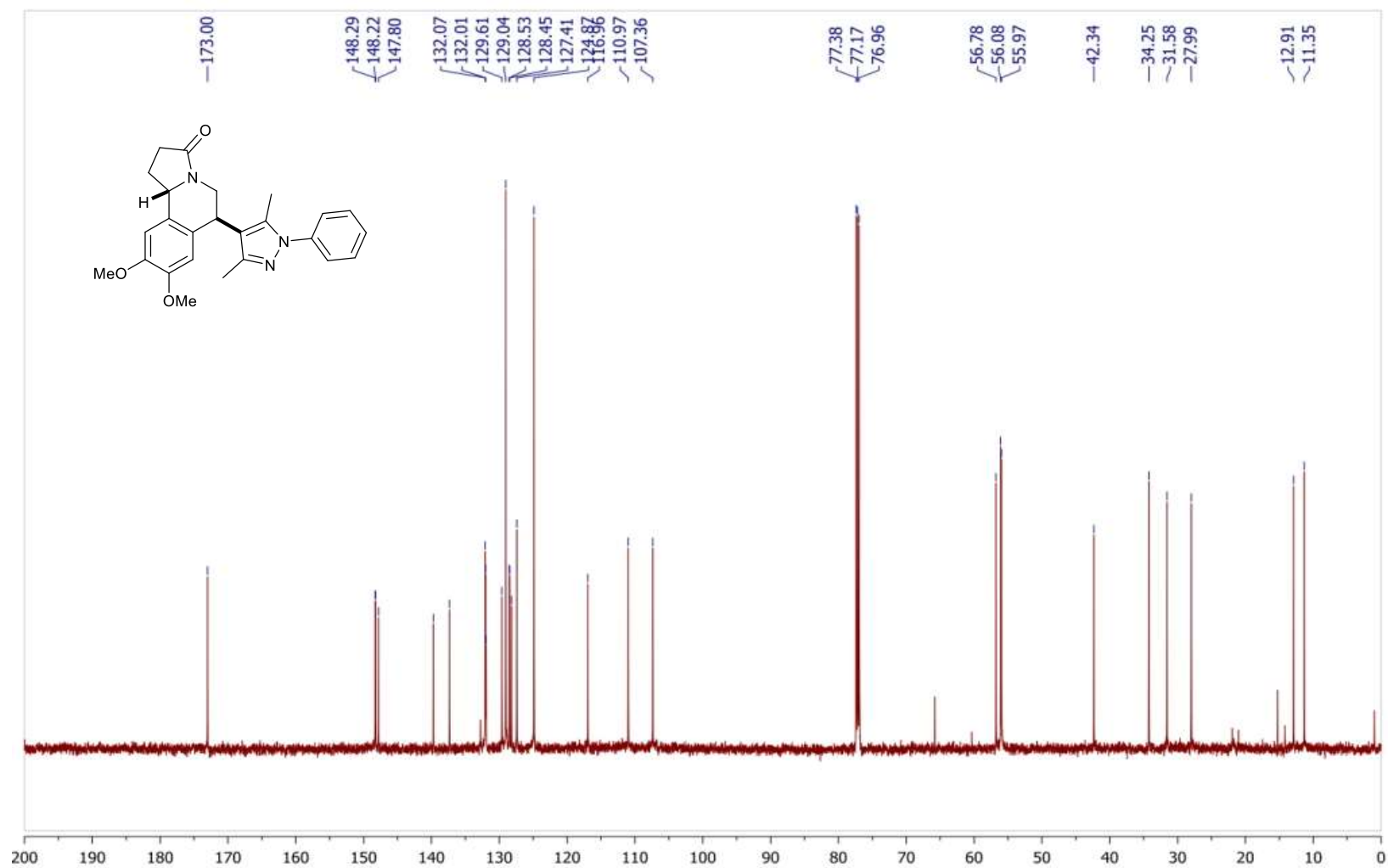
(6RS,10bSR)-6-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-8,9-dimethoxy-1,5,6,10b-tetrahydropyrrolo[2,1-a]isoquinolin-3(2H)-one (9)

¹H NMR (CDCl₃, 600 MHz)

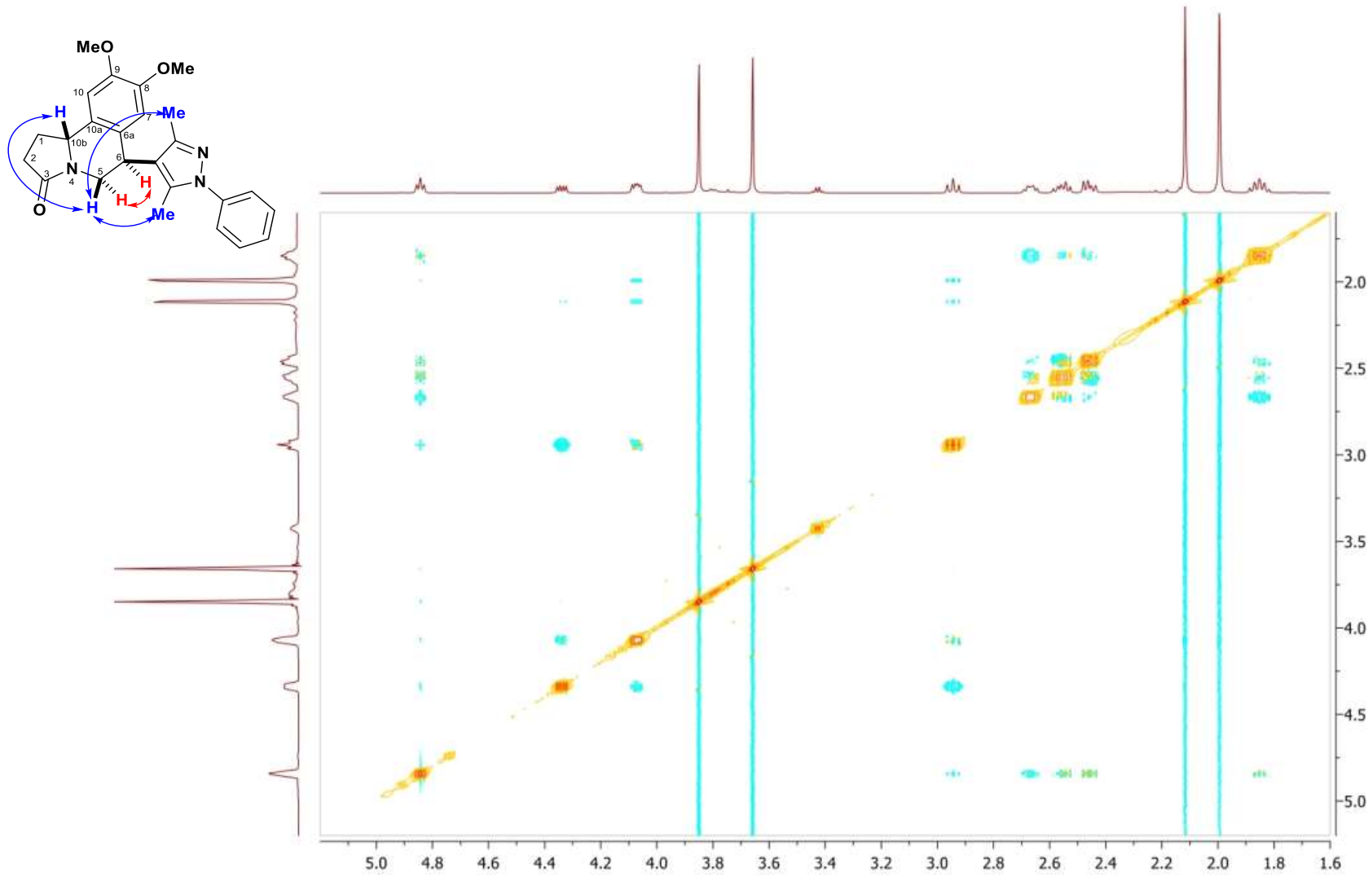


(6RS,10bSR)-6-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-8,9-dimethoxy-1,5,6,10b-tetrahydropyrrolo[2,1-a]isoquinolin-3(2H)-one (9)

^{13}C NMR (CDCl_3 , 150 MHz)

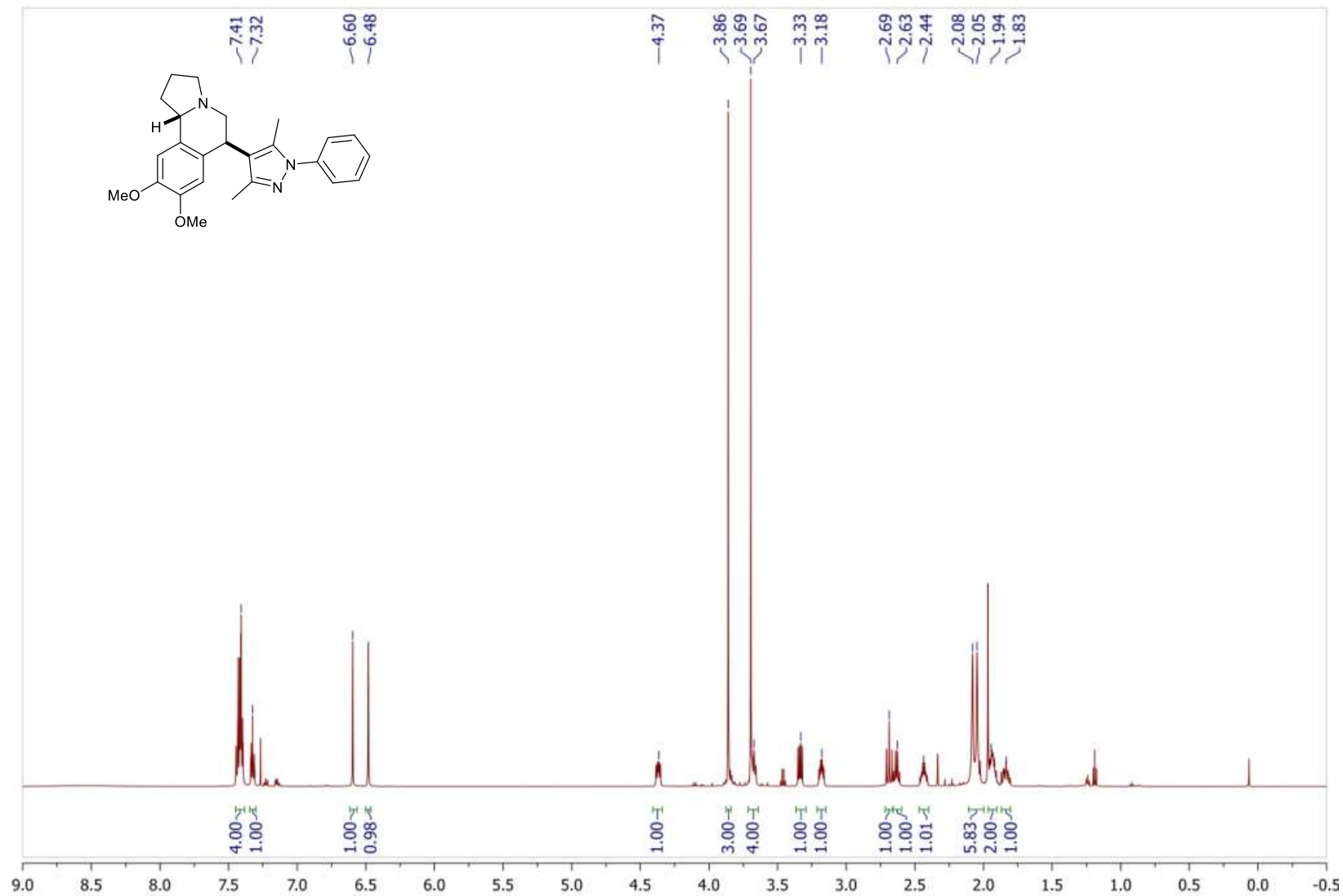


(6R,10bS)-6-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-8,9-dimethoxy-1,5,6,10b-tetrahydropyrrolo[2,1-a]isoquinolin-3(2H)-one (9)



(6RS,10bSR)-6-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-8,9-dimethoxy-1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinoline (10)

¹H NMR (CDCl₃, 600 MHz)



(6R,10bSR)-6-(3,5-Dimethyl-1-phenyl-1H-pyrazol-4-yl)-8,9-dimethoxy-1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinoline (10)

¹³C NMR (CDCl₃, 150 MHz)

