

Preparation of Novel Acyl Pyrazoles and Triazoles by Means of Oxidative Functionalization Reactions

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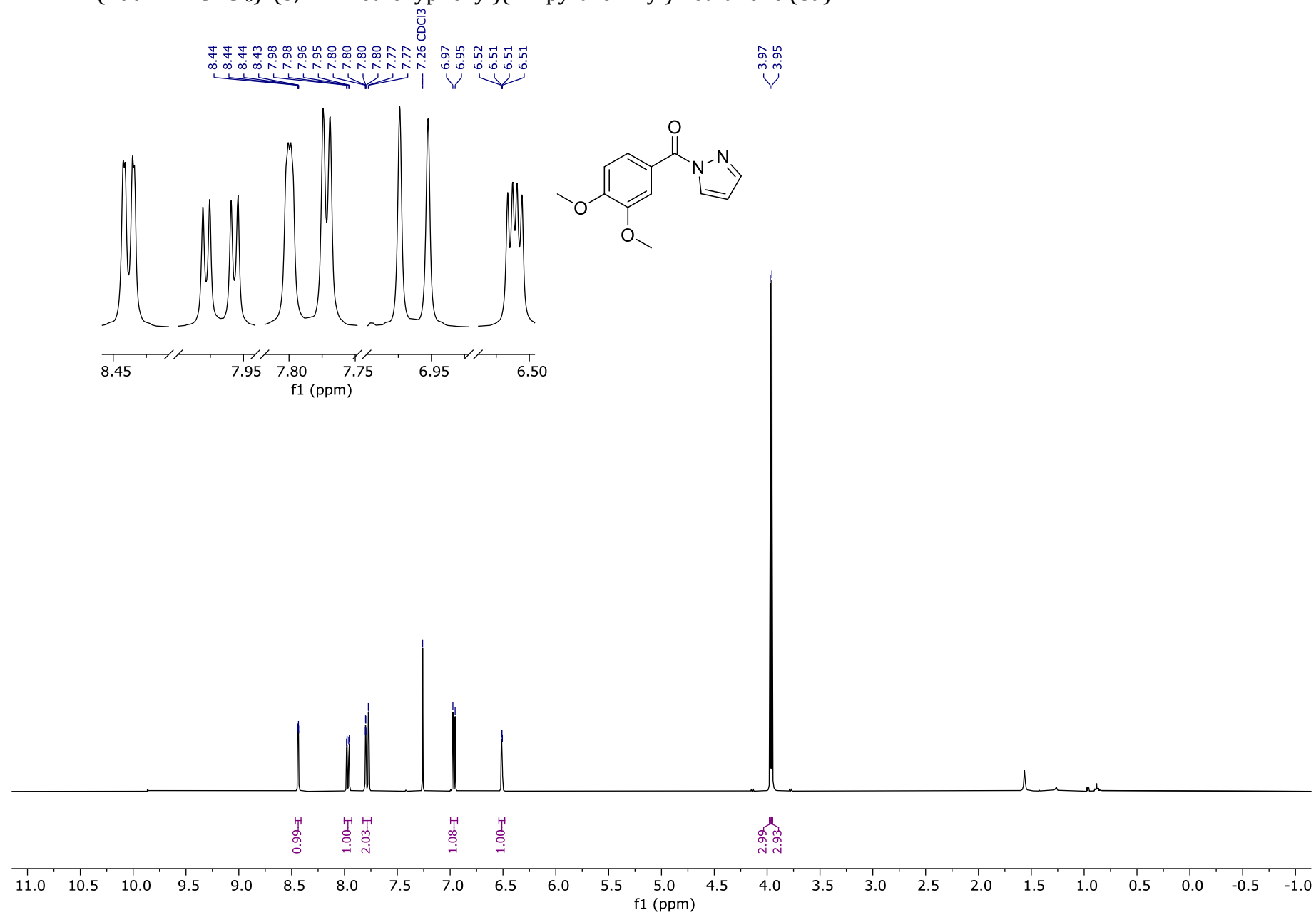
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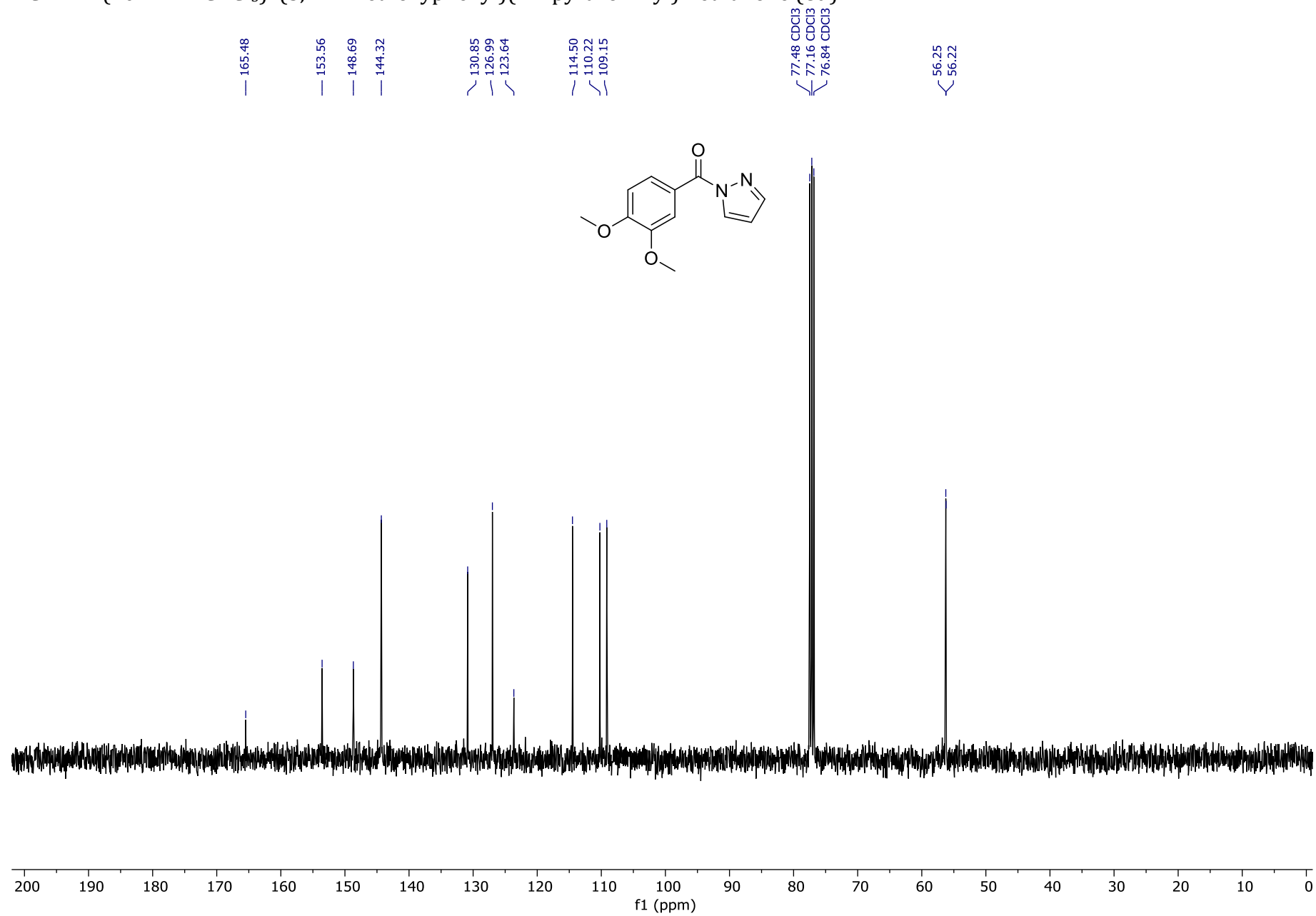
SUPPORTING INFORMATION

^1H -, ^{13}C -, and ^{19}F -NMR spectra of synthesized compounds

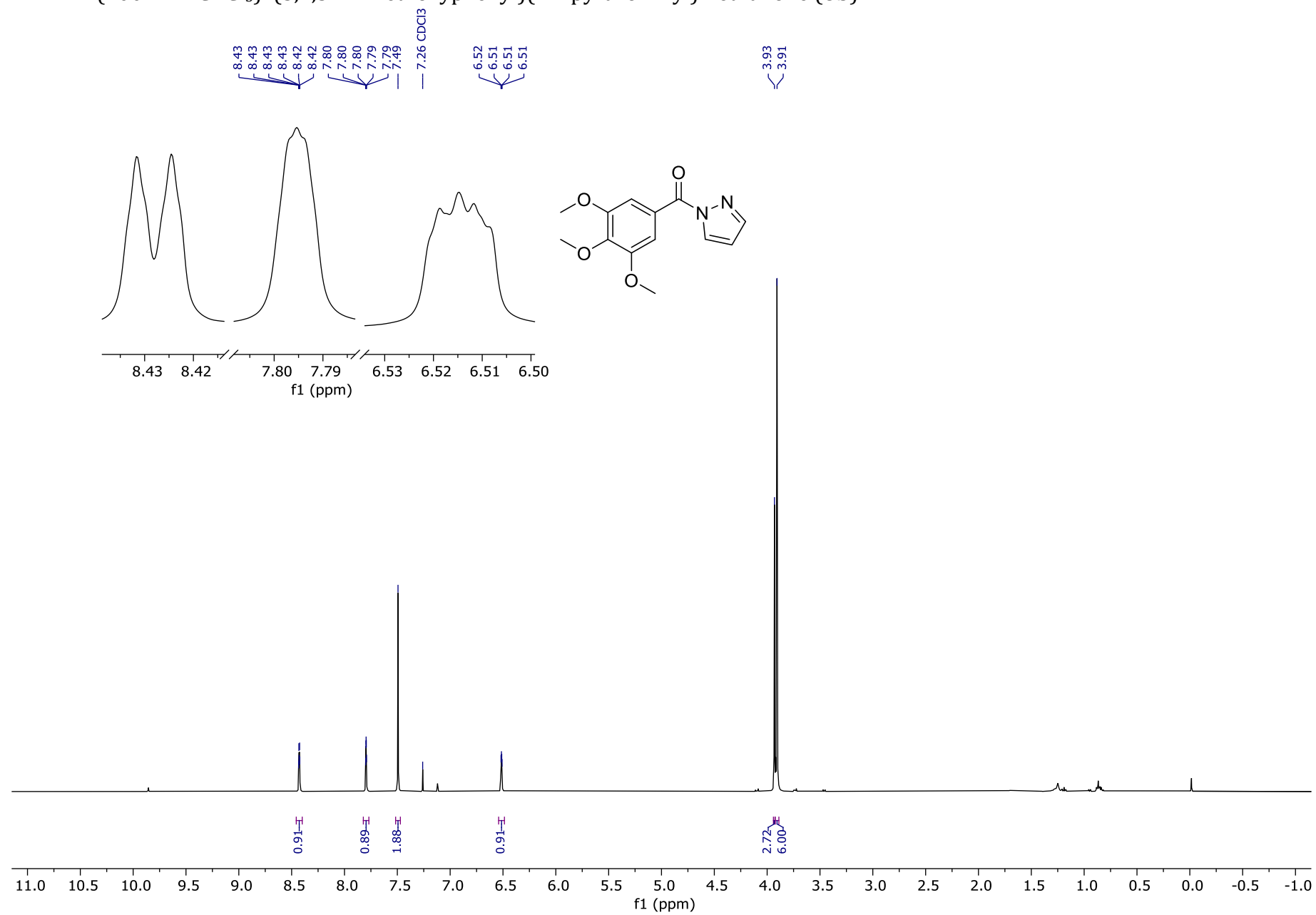
^1H -NMR (400 MHz CDCl_3): (3,4-Dimethoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6a**)



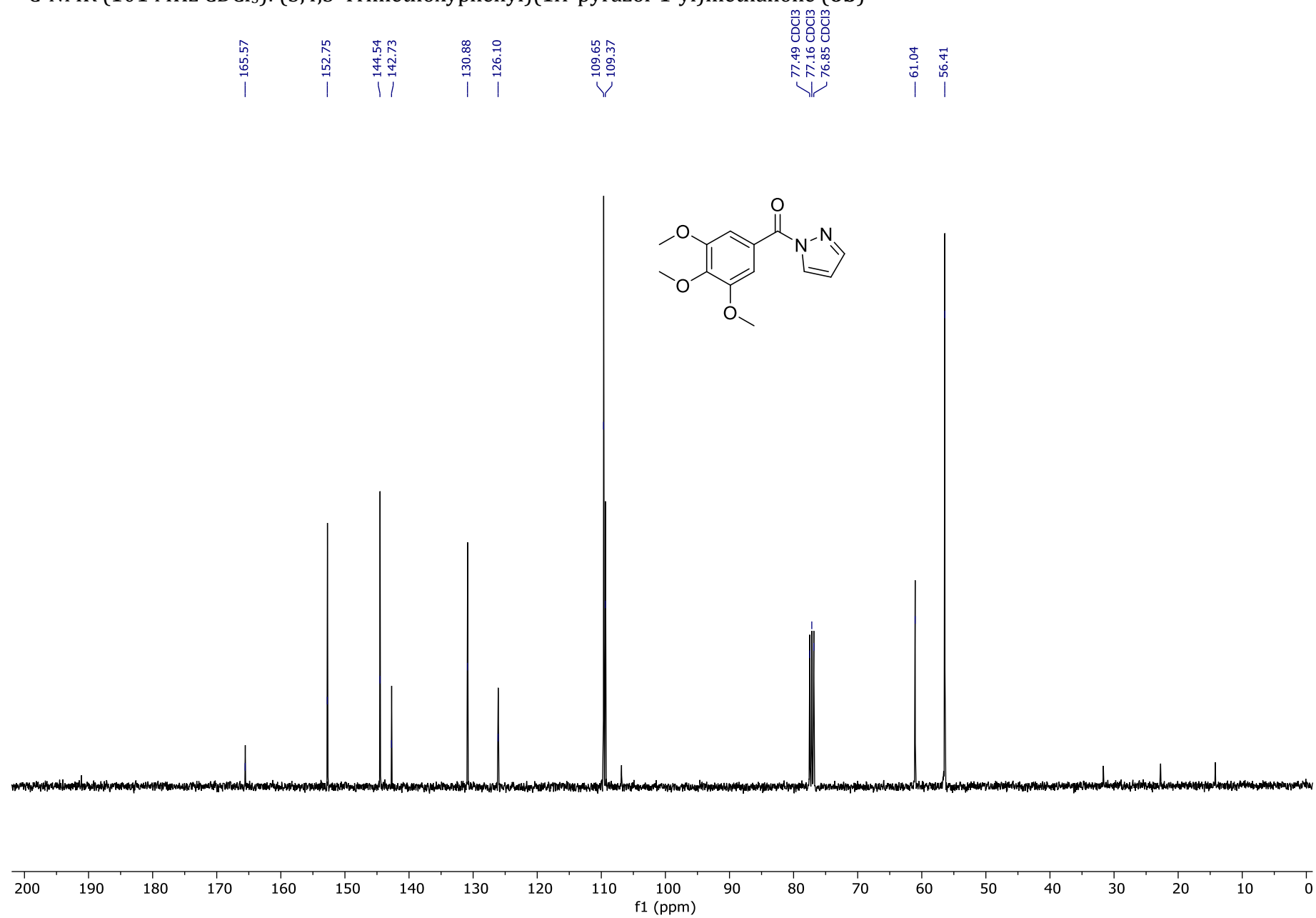
^{13}C -NMR (101 MHz CDCl_3): (3,4-Dimethoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6a**)

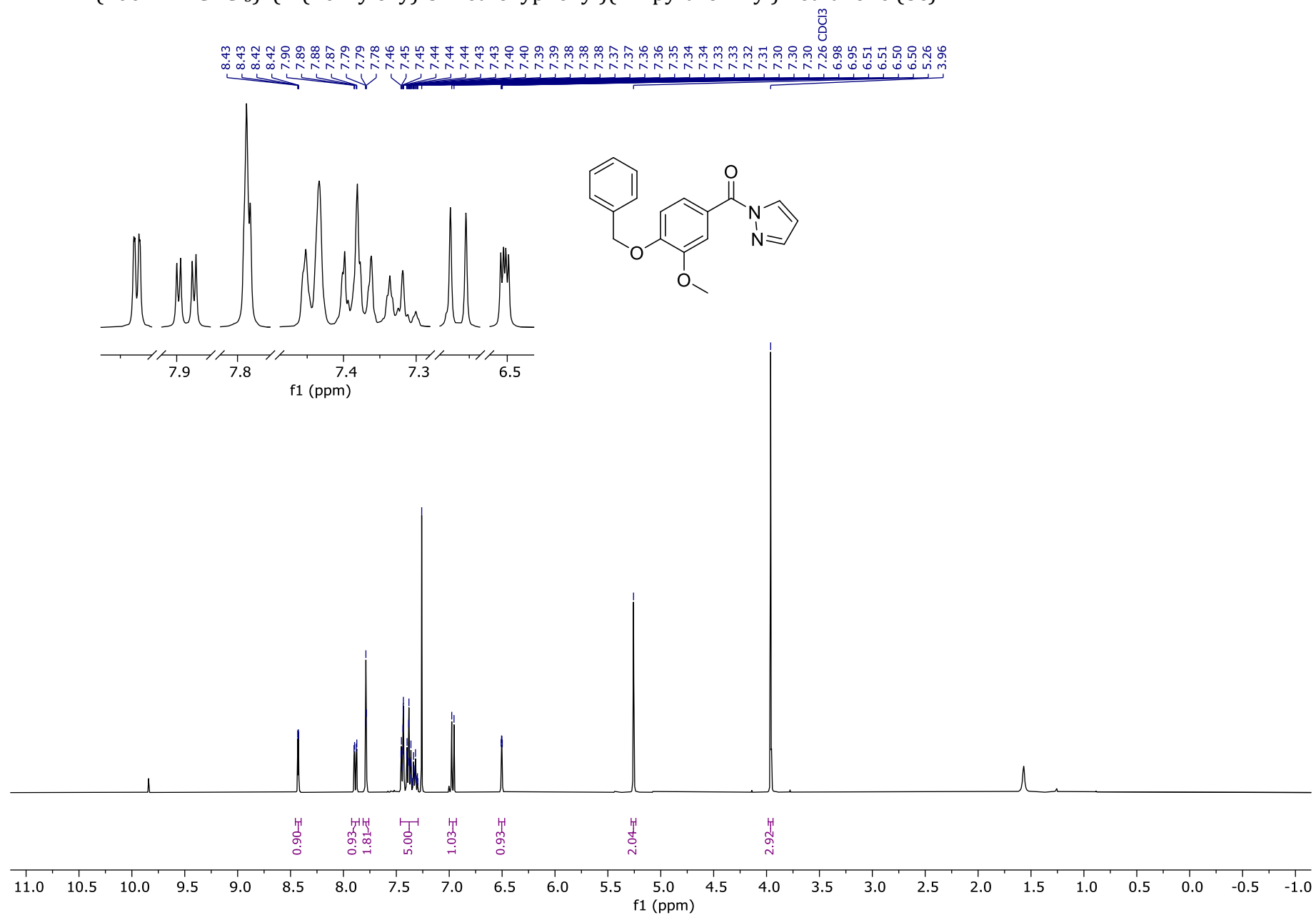


^1H -NMR (400 MHz CDCl_3): (3,4,5-Trimethoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6b**)

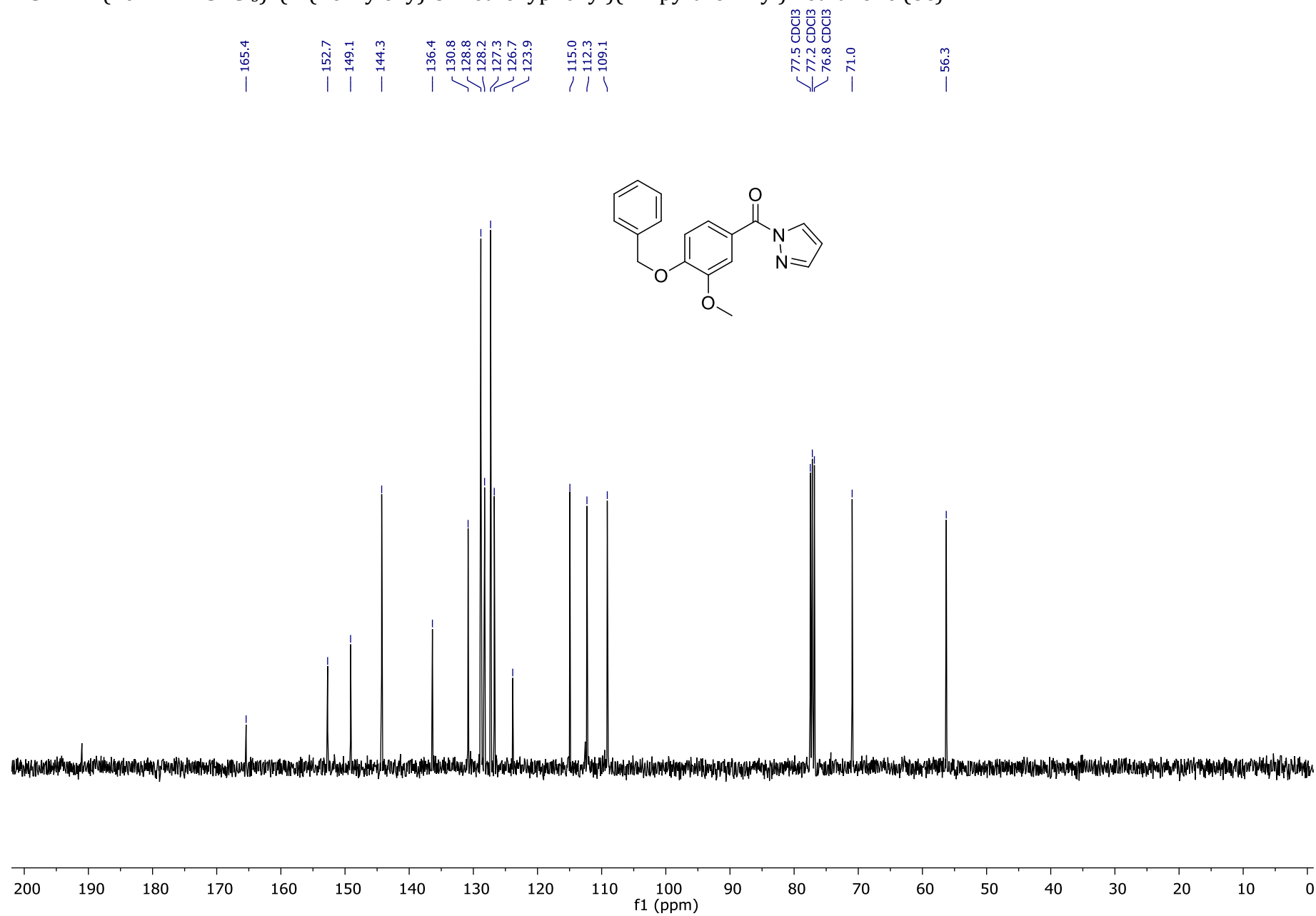


¹³C-NMR (101 MHz CDCl₃): (3,4,5-Trimethoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6b**)

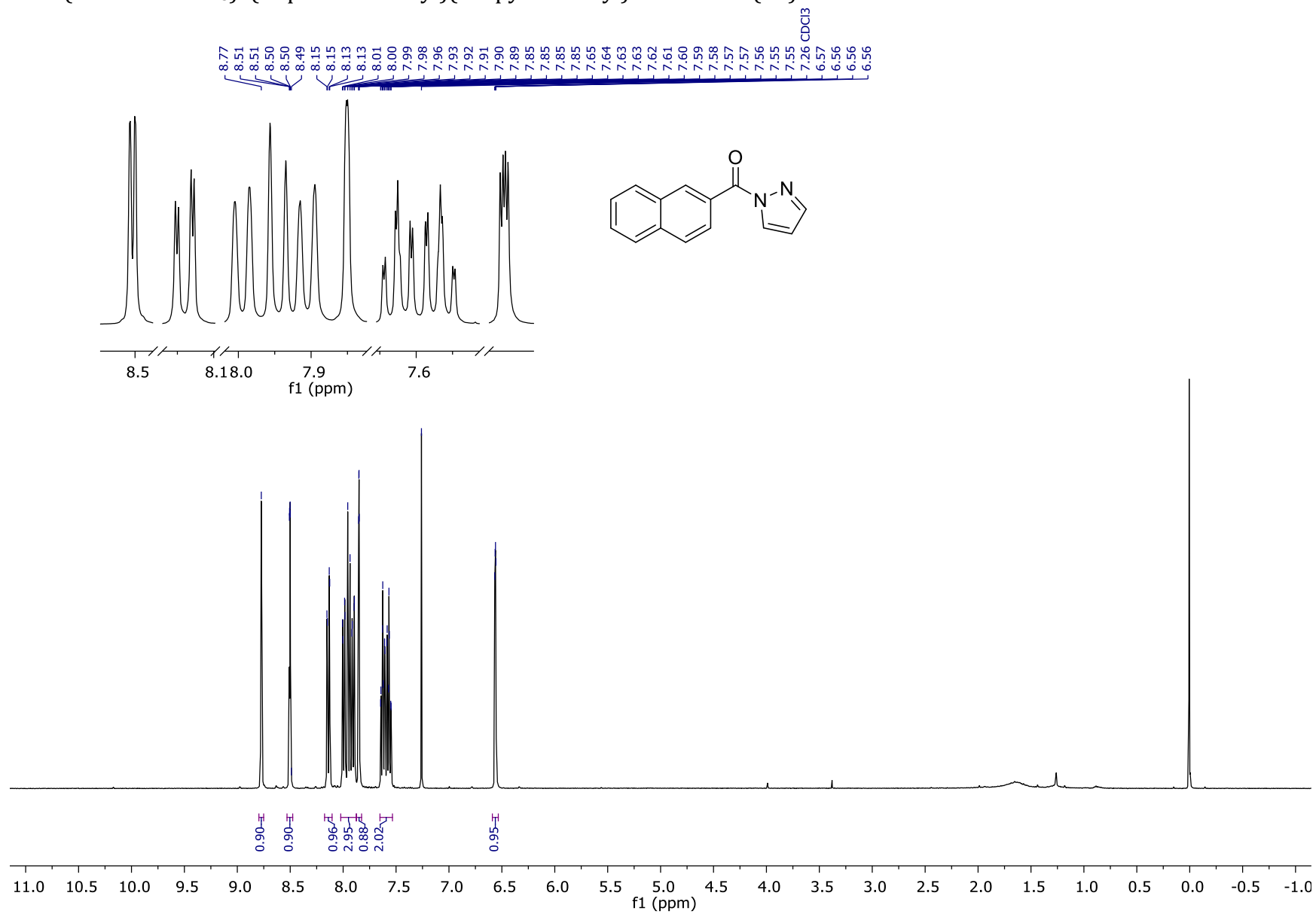


¹H-NMR (400 MHz CDCl₃): (4-(Benzyloxy)-3-methoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6c**)

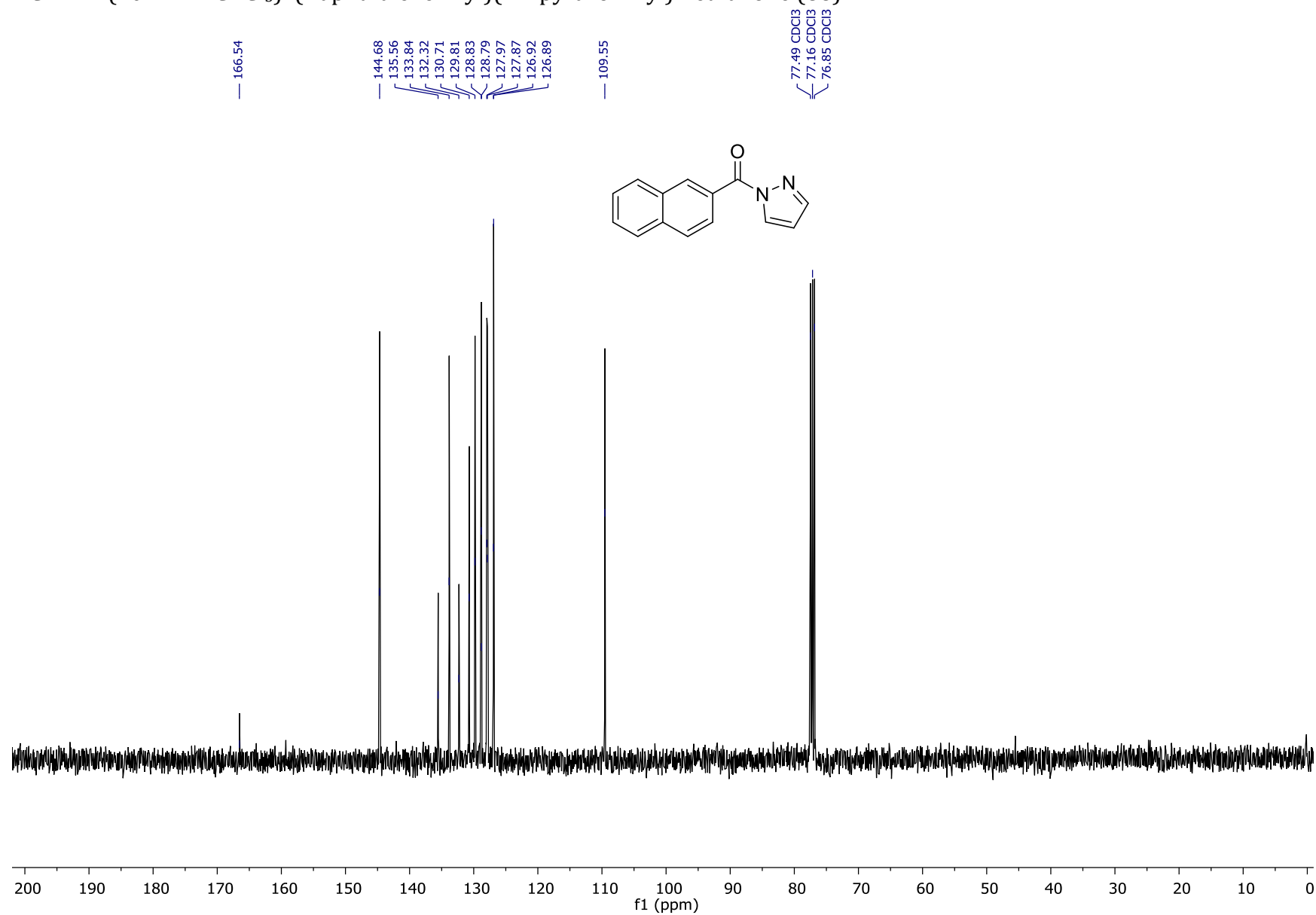
¹³C-NMR (101 MHz CDCl₃): (4-(Benzyloxy)-3-methoxyphenyl)(1*H*-pyrazol-1-yl)methanone (**6c**)



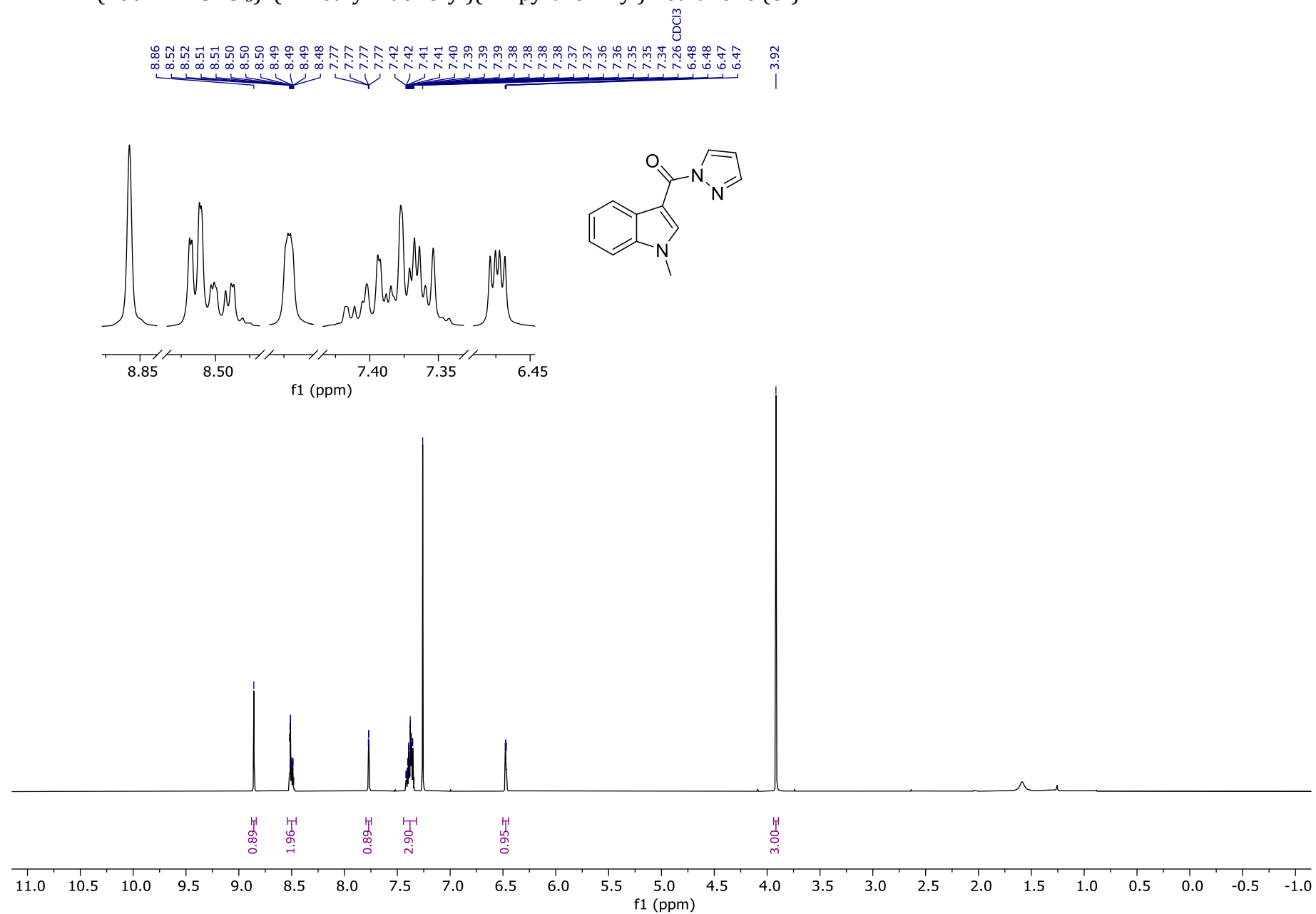
^1H -NMR (400 MHz CDCl_3): (Naphthalene-2-yl)(1*H*-pyrazol-1-yl)methanone (**6e**)



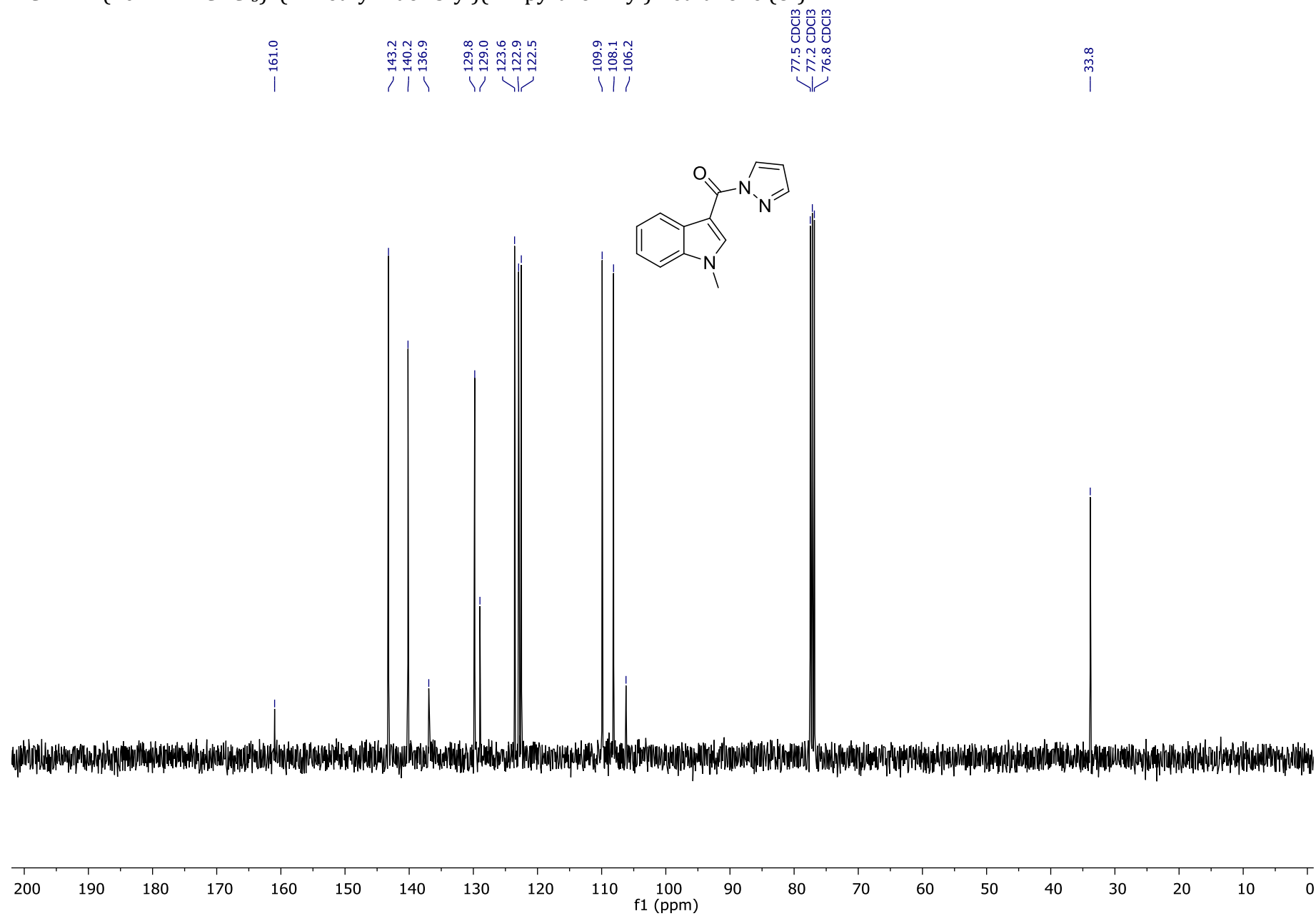
^{13}C -NMR (101 MHz CDCl_3): (Naphthalene-2-yl)(1*H*-pyrazol-1-yl)methanone (**6e**)



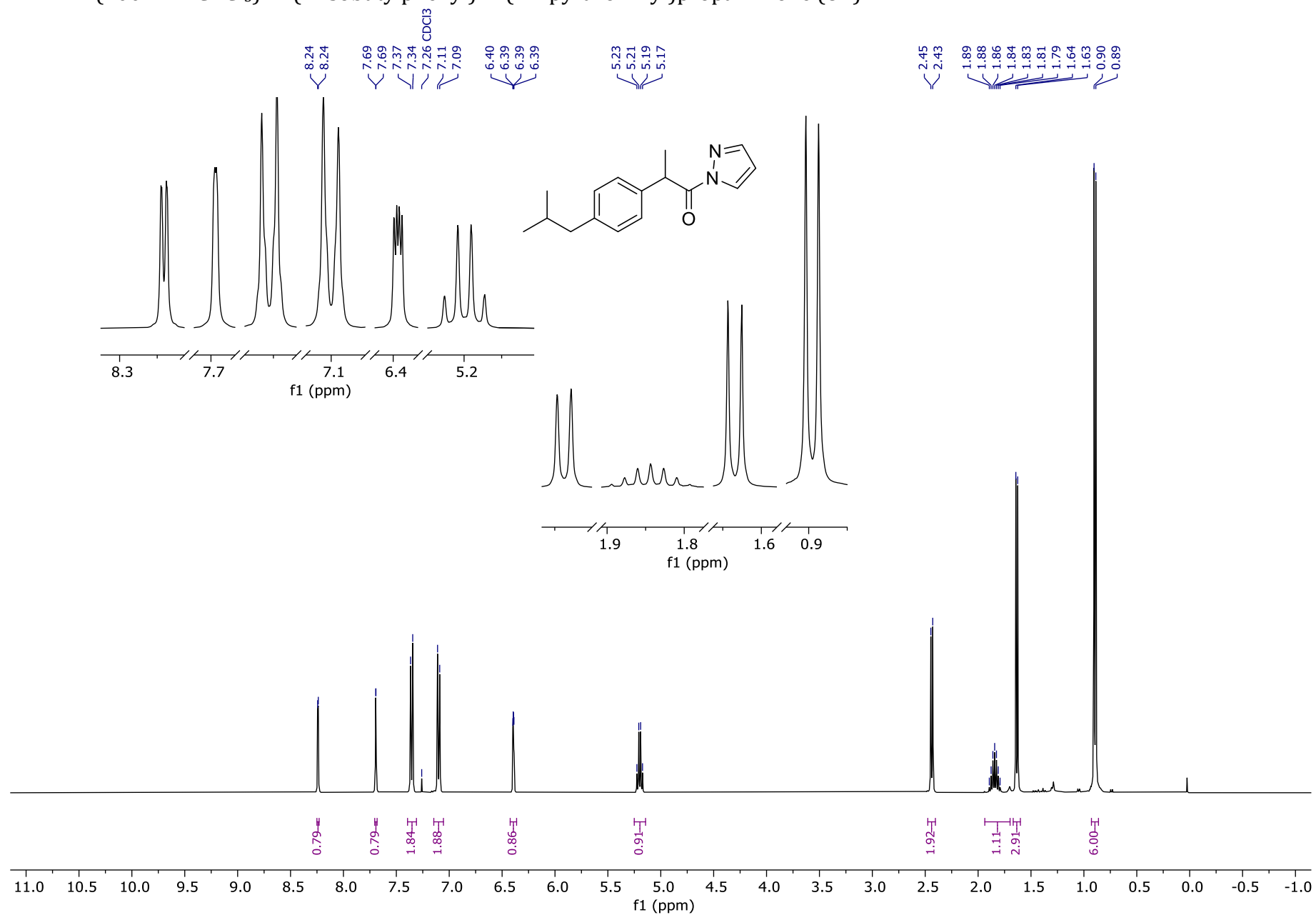
^1H -NMR (400 MHz CDCl_3): (1-Methylindol-3-yl)(1*H*-pyrazol-1-yl)methanone (**6f**)



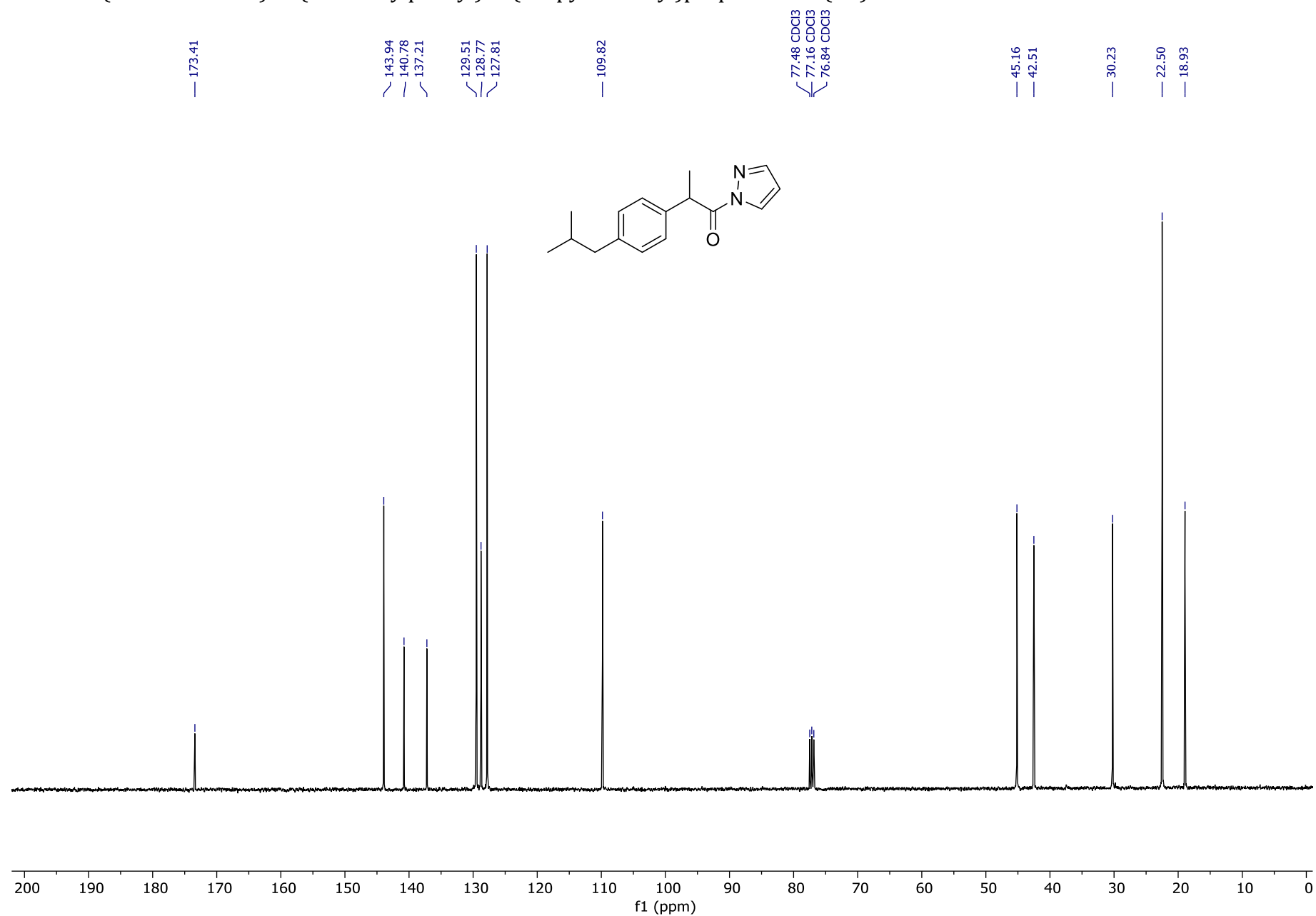
^{13}C -NMR (101 MHz CDCl_3): (1-Methylindol-3-yl)(1*H*-pyrazol-1-yl)methanone (**6f**)



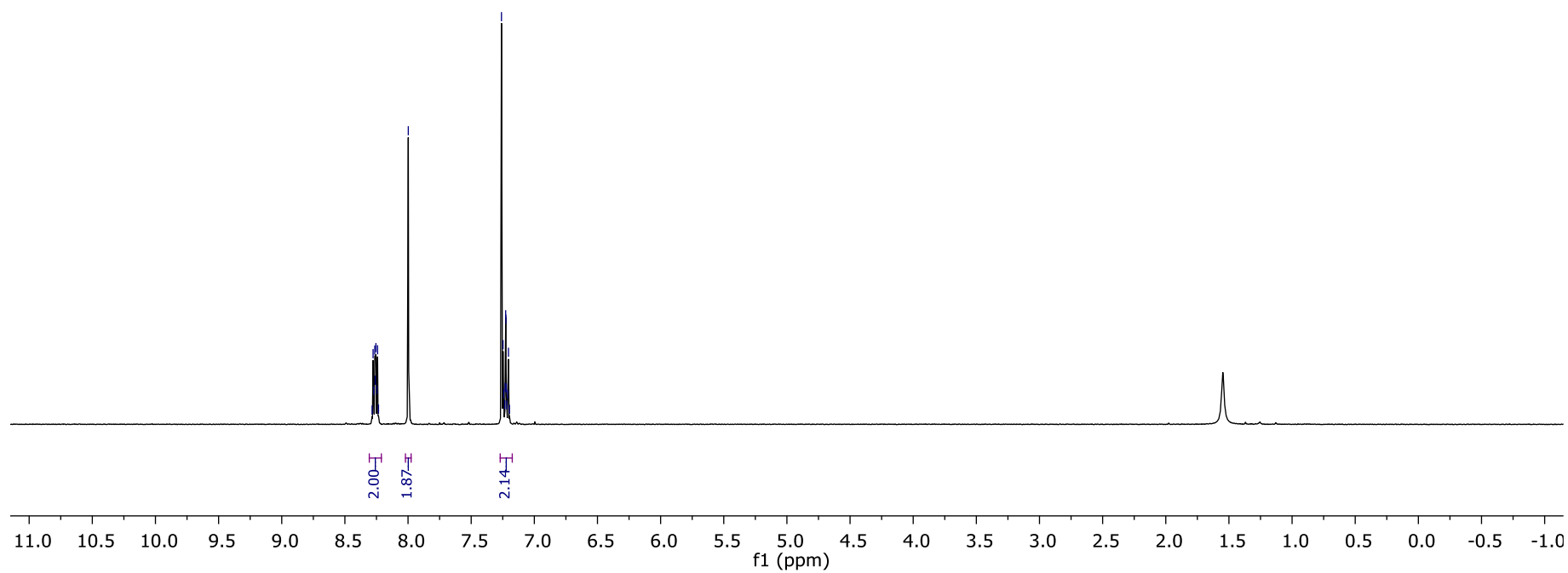
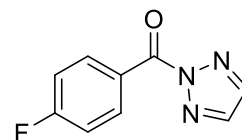
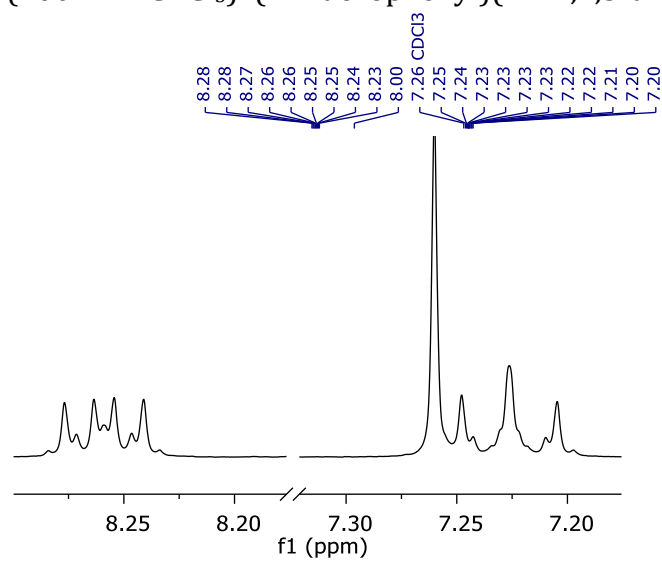
¹H-NMR (400 MHz CDCl₃): 2-(4-Isobutylphenyl)-1-(1*H*-pyrazol-1-yl)propan-1-one (**6h**)



¹³C-NMR (101 MHz CDCl₃): 2-(4-Isobutylphenyl)-1-(1*H*-pyrazol-1-yl)propan-1-one (**6h**)



^1H -NMR (400 MHz CDCl_3): (4-Fluorophenyl)(2H-1,2,3-triazol-2-yl)methanone (**7a''**)



^{13}C -NMR (101 MHz CDCl_3): (4-Fluorophenyl)(2*H*-1,2,3-triazol-2-yl)methanone (**7a''**)

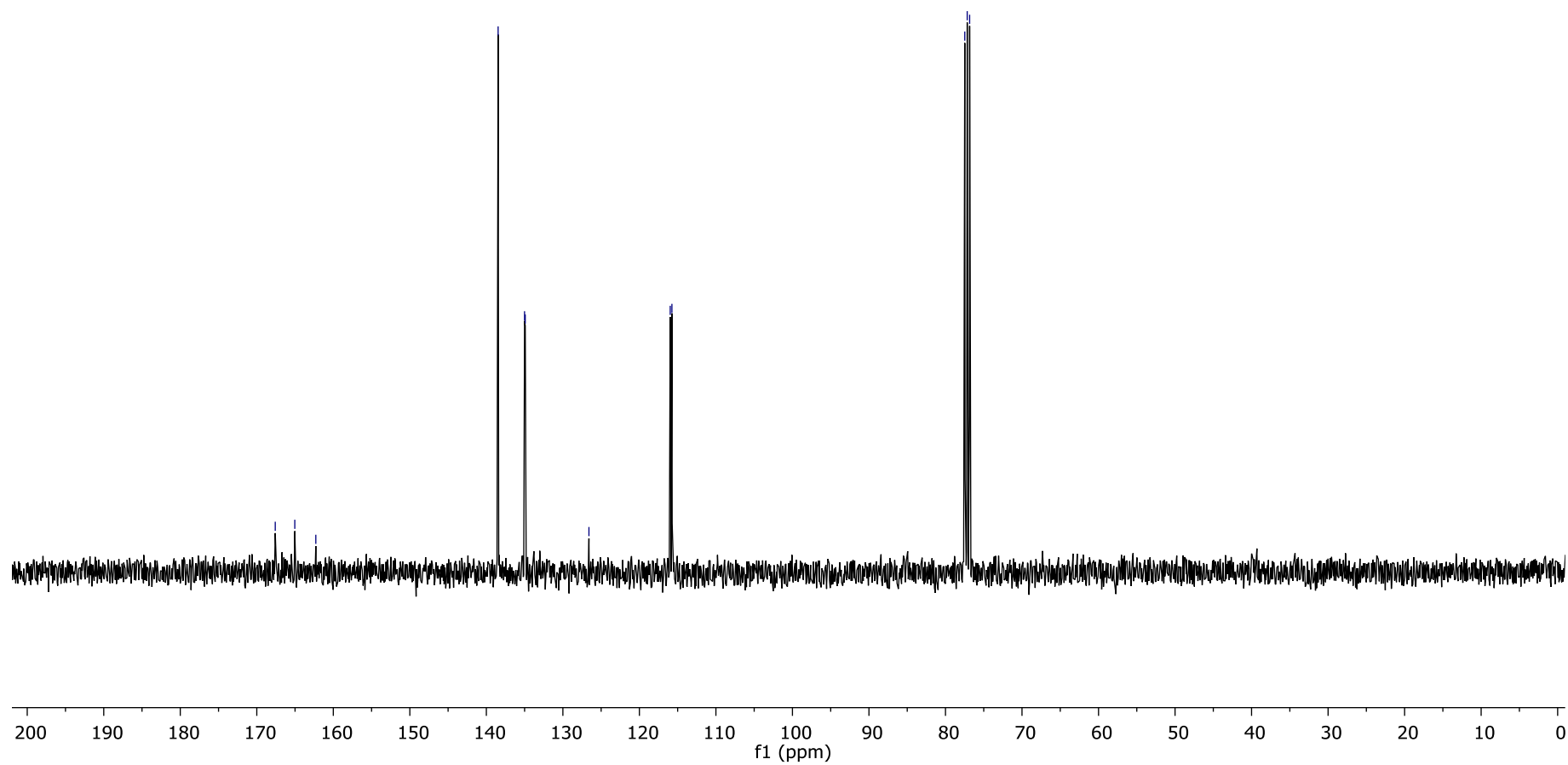
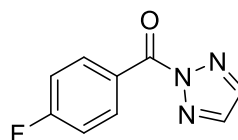
167.6
165.0
162.3

138.5
135.0
134.9

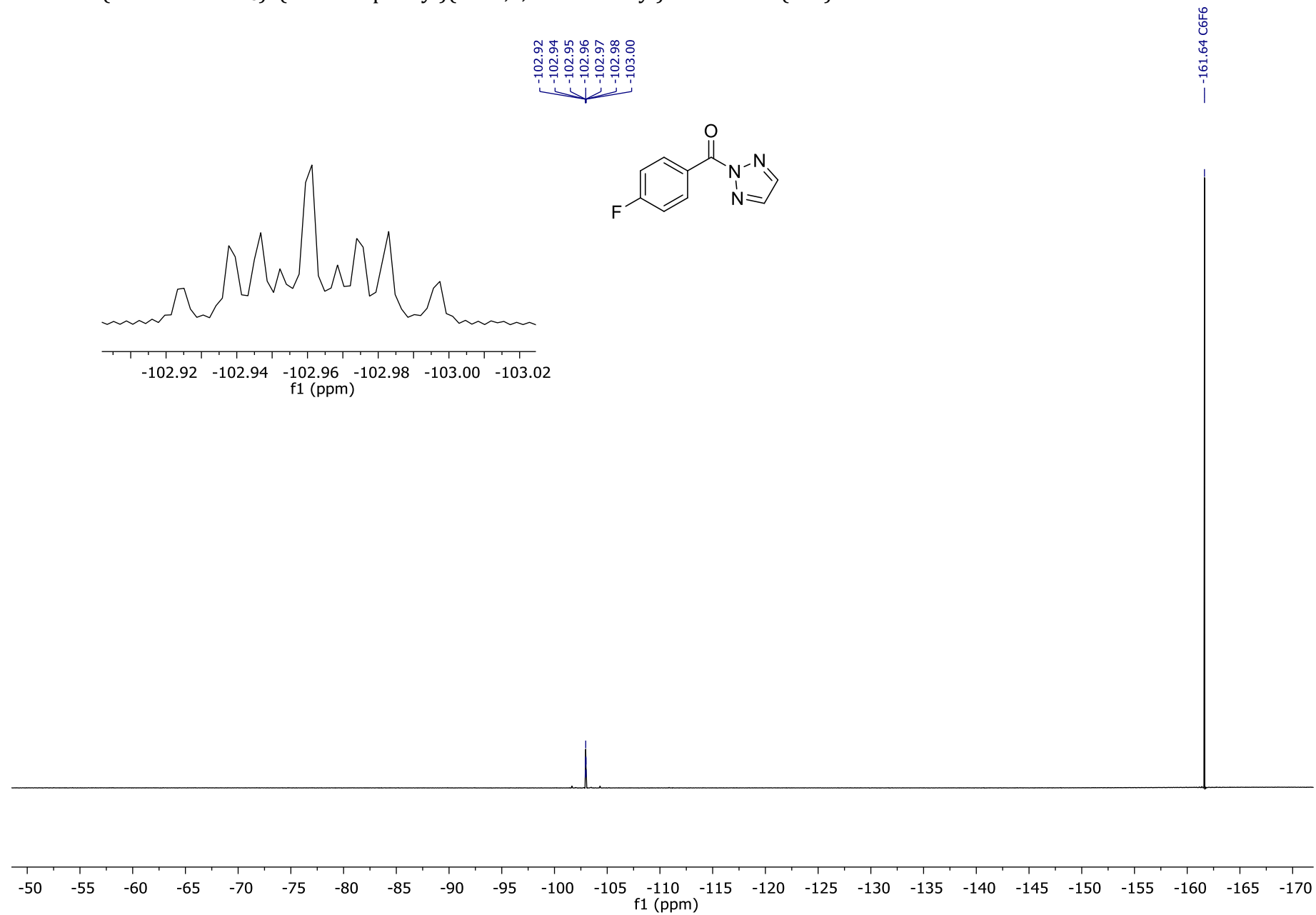
126.6

116.0
115.8

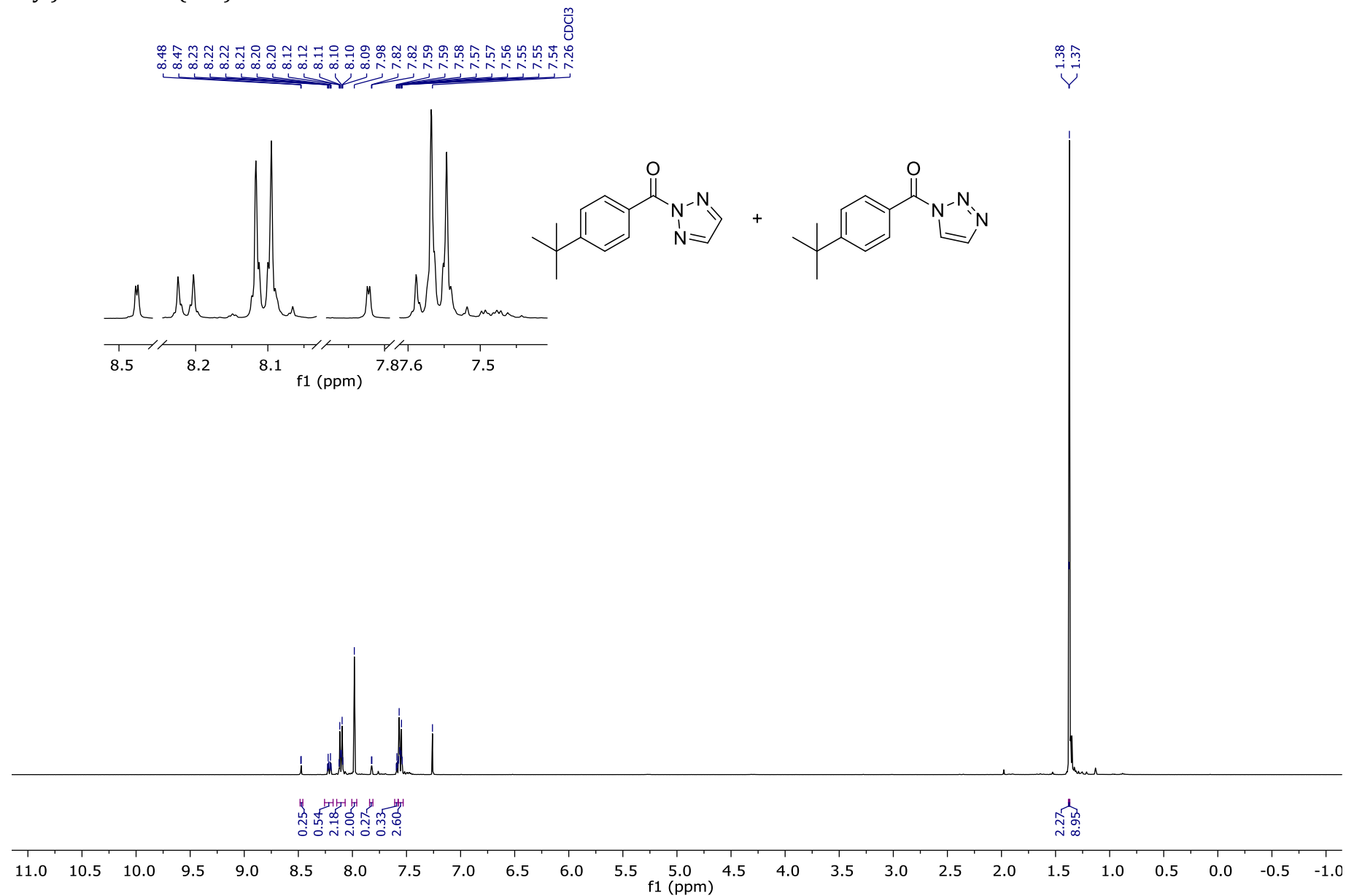
77.5 CDCl_3
77.2 CDCl_3
76.8 CDCl_3



^{19}F -NMR (376 MHz CDCl_3): (4-Fluorophenyl)(2*H*-1,2,3-triazol-2-yl)methanone (**7a''**)



^1H -NMR (400 MHz CDCl_3): (4-(Tert-butyl)phenyl)(1*H*-1,2,3-triazol-2-yl)methanone (**7b'**) and (4-(tert-butyl)phenyl)(2*H*-1,2,3-triazol-2-yl)methanone (**7b''**)



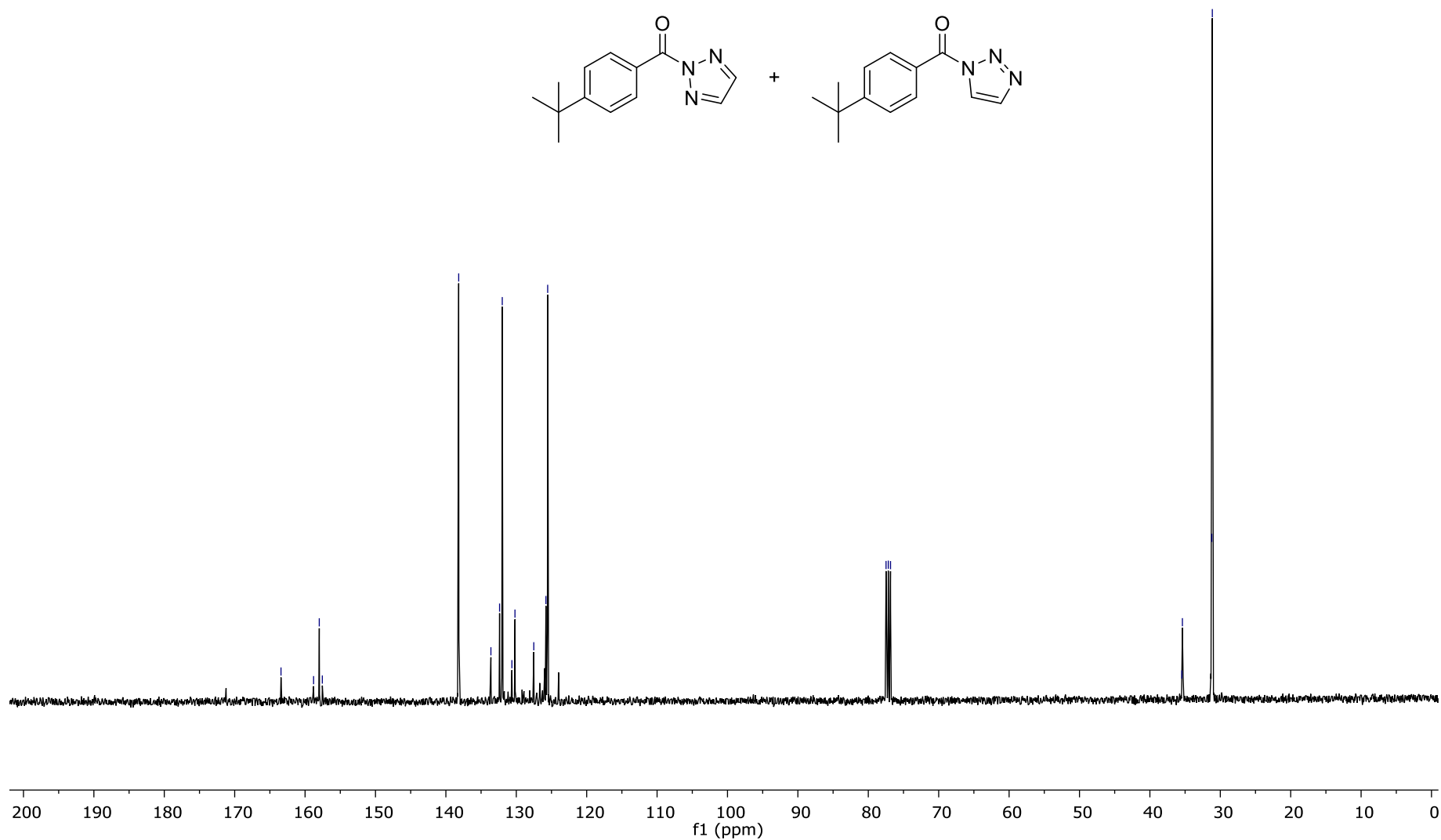
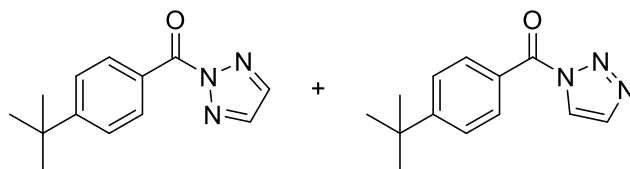
^{13}C -NMR (101 MHz CDCl_3): (4-(Tert-butyl)phenyl)(1*H*-1,2,3-triazol-2-yl)methanone (**7b'**) and (4-(tert-butyl)phenyl)(2*H*-1,2,3-triazol-2-yl)methanone (**7b''**)

163.42
158.79
157.99
157.55

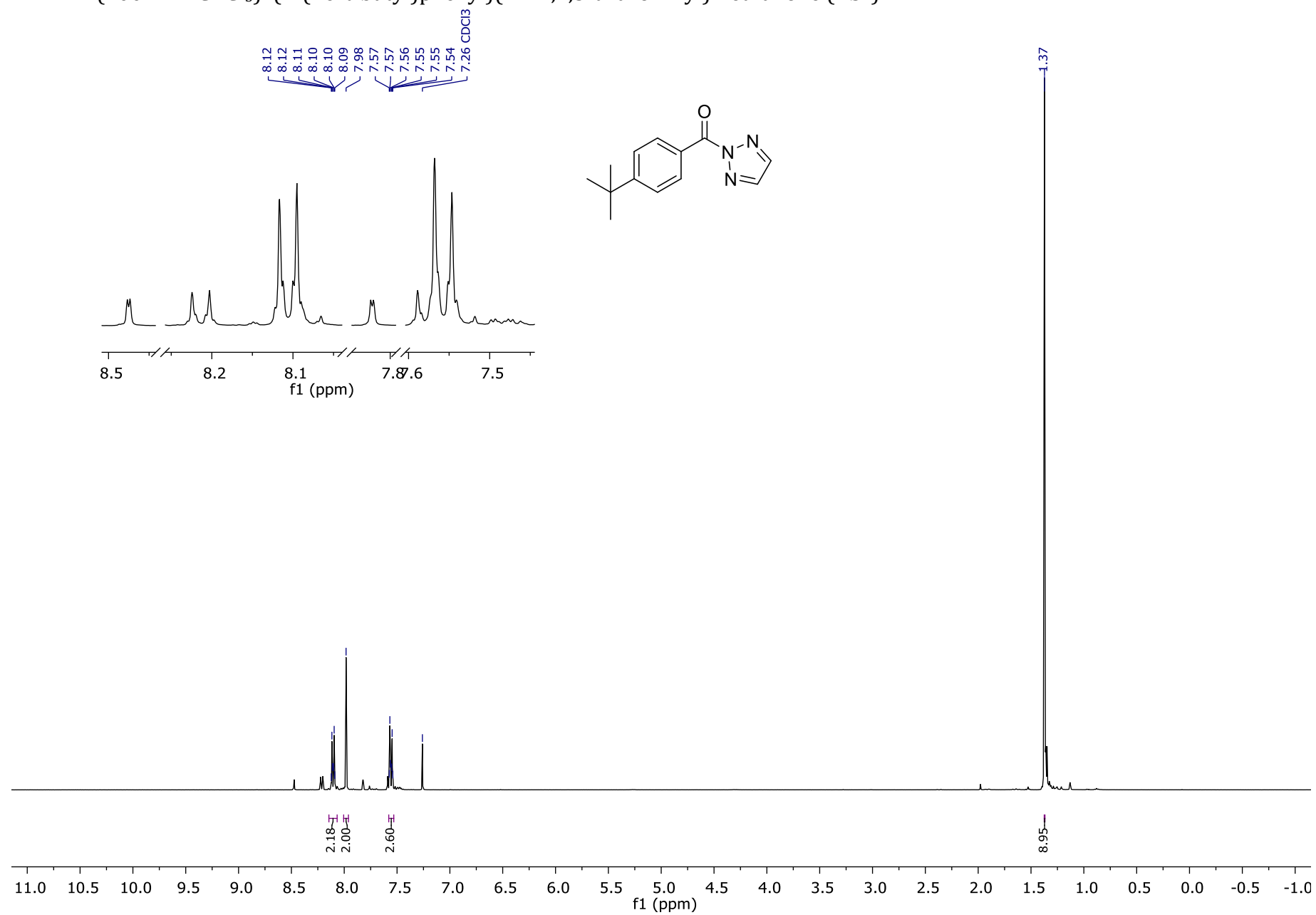
138.18
133.60
132.37
131.99
130.62
130.19
127.51
125.79
125.54

77.48
77.16
76.84

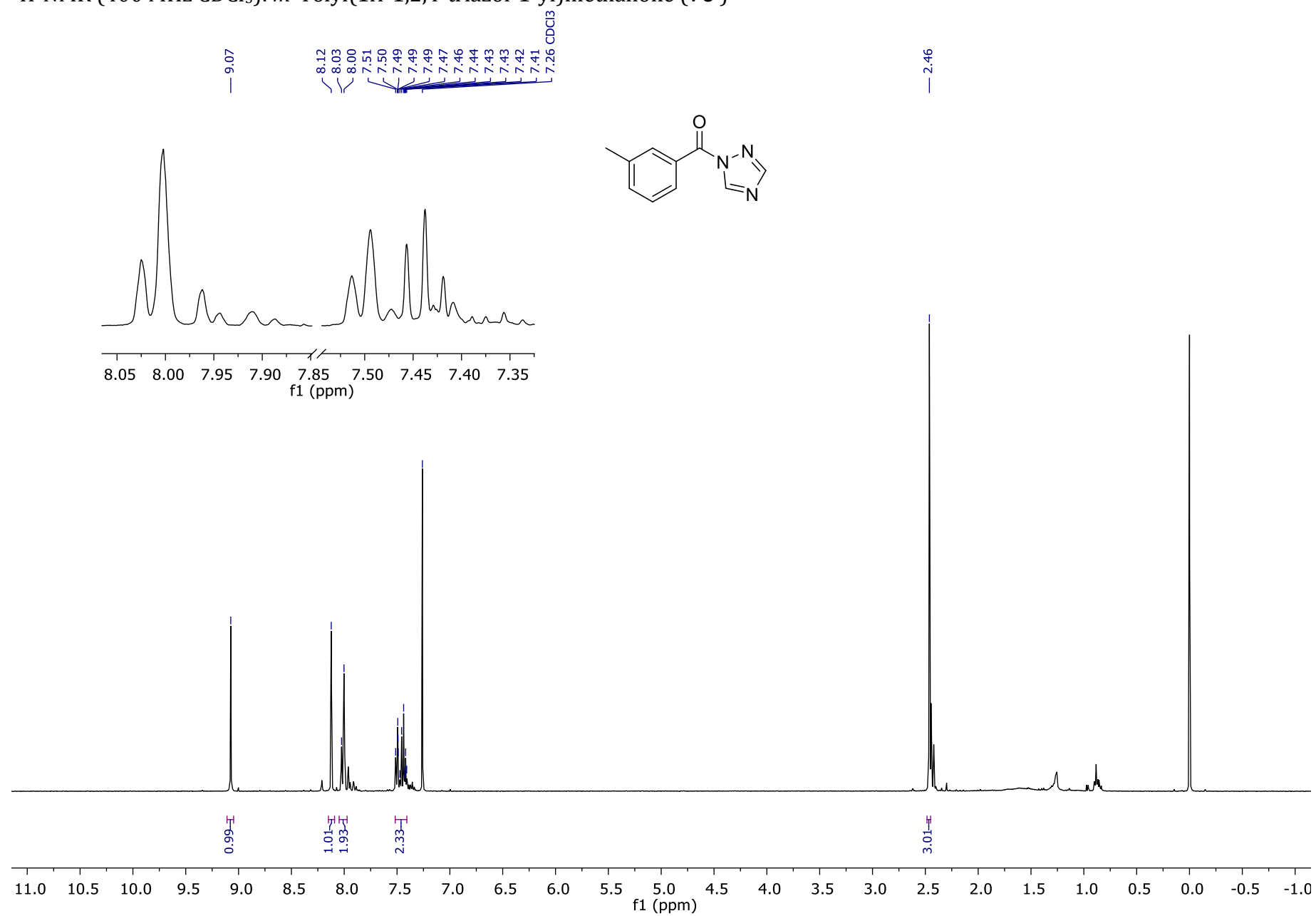
35.46
35.38
31.21
31.13



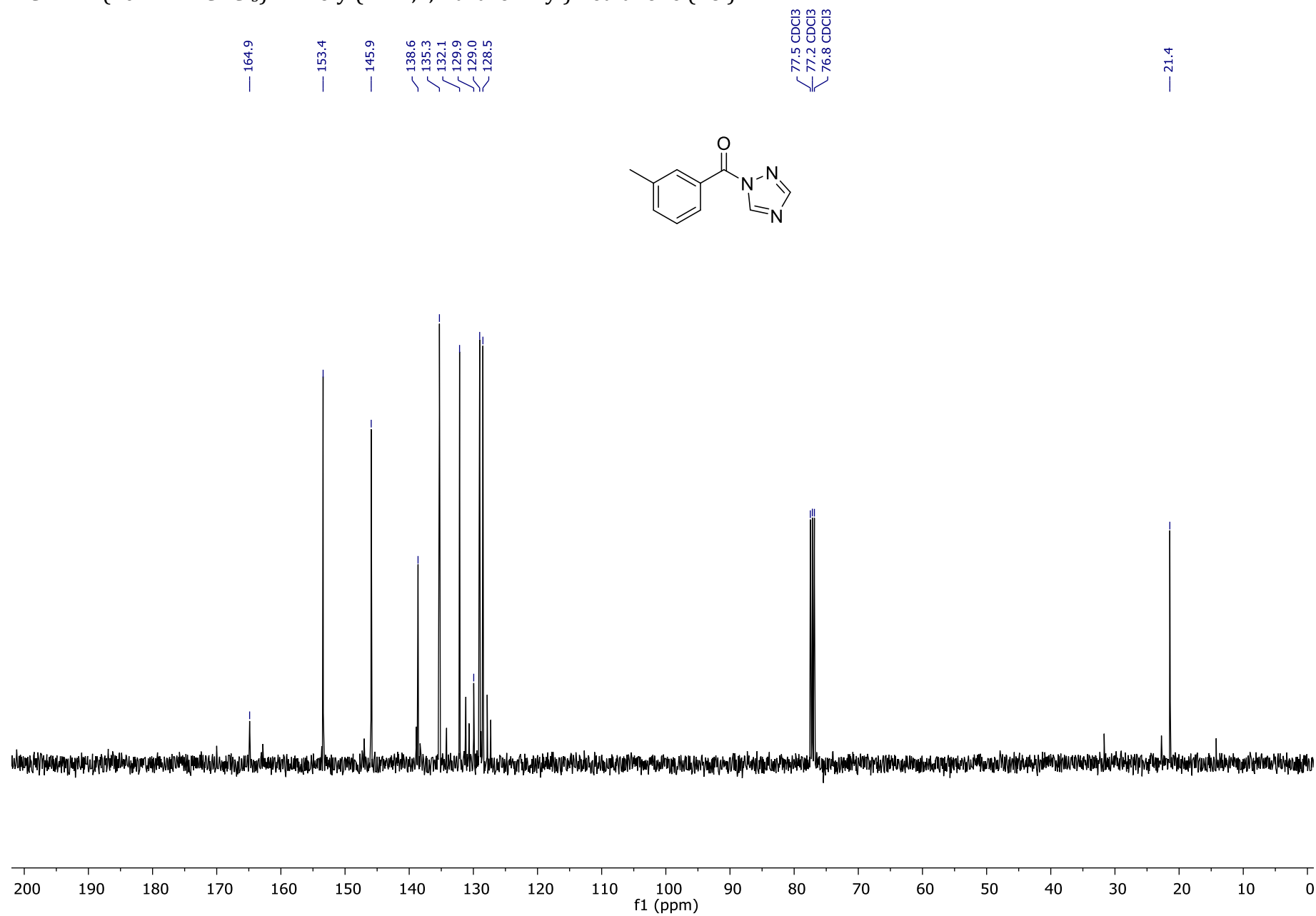
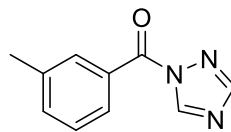
^1H -NMR (400 MHz CDCl_3): (4-(Tert-butyl)phenyl)(2H-1,2,3-triazol-2-yl)methanone (**7b''**)



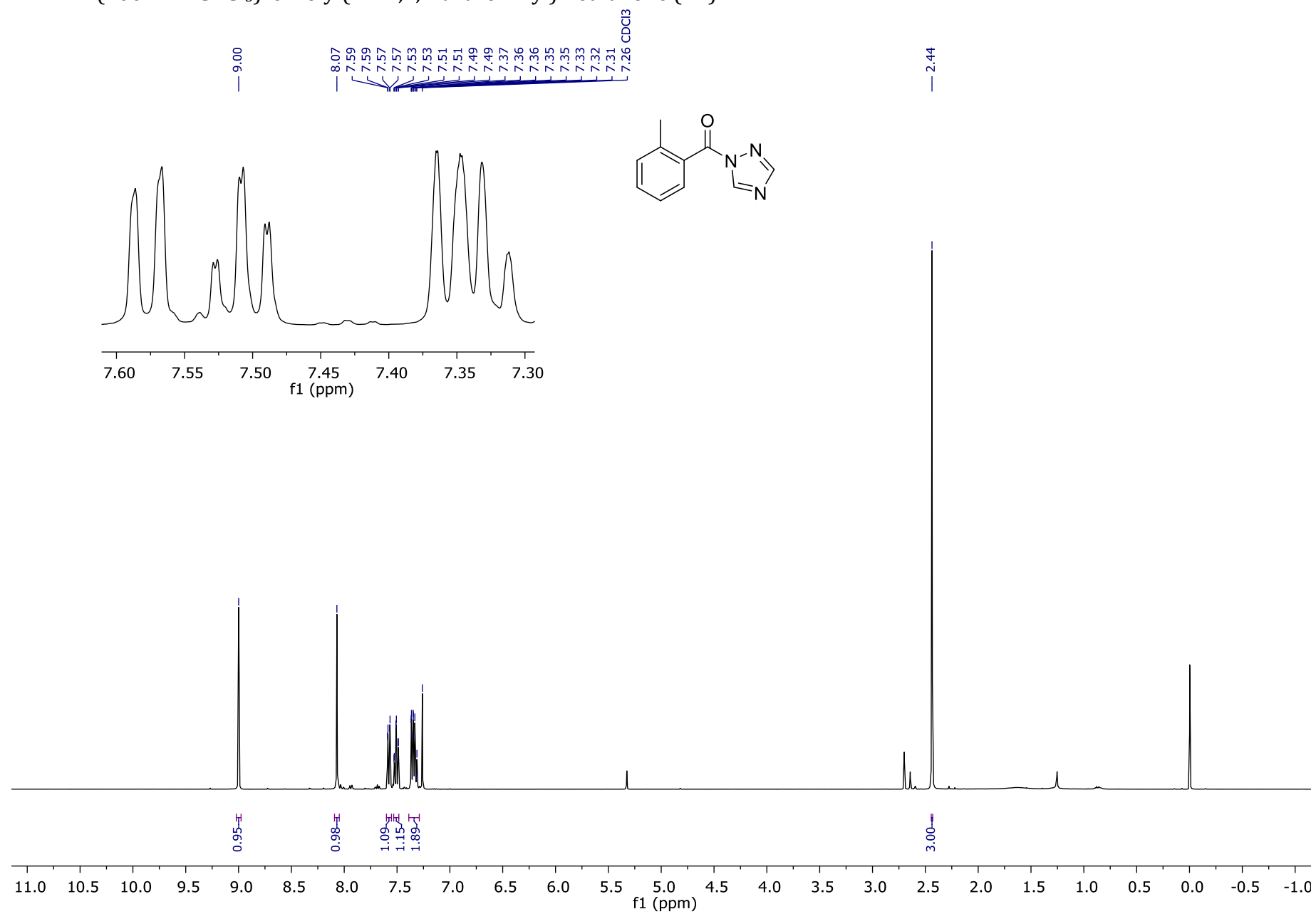
^1H -NMR (400 MHz CDCl_3): *m*-Tolyl(1*H*-1,2,4-triazol-1-yl)methanone (**7e'**)



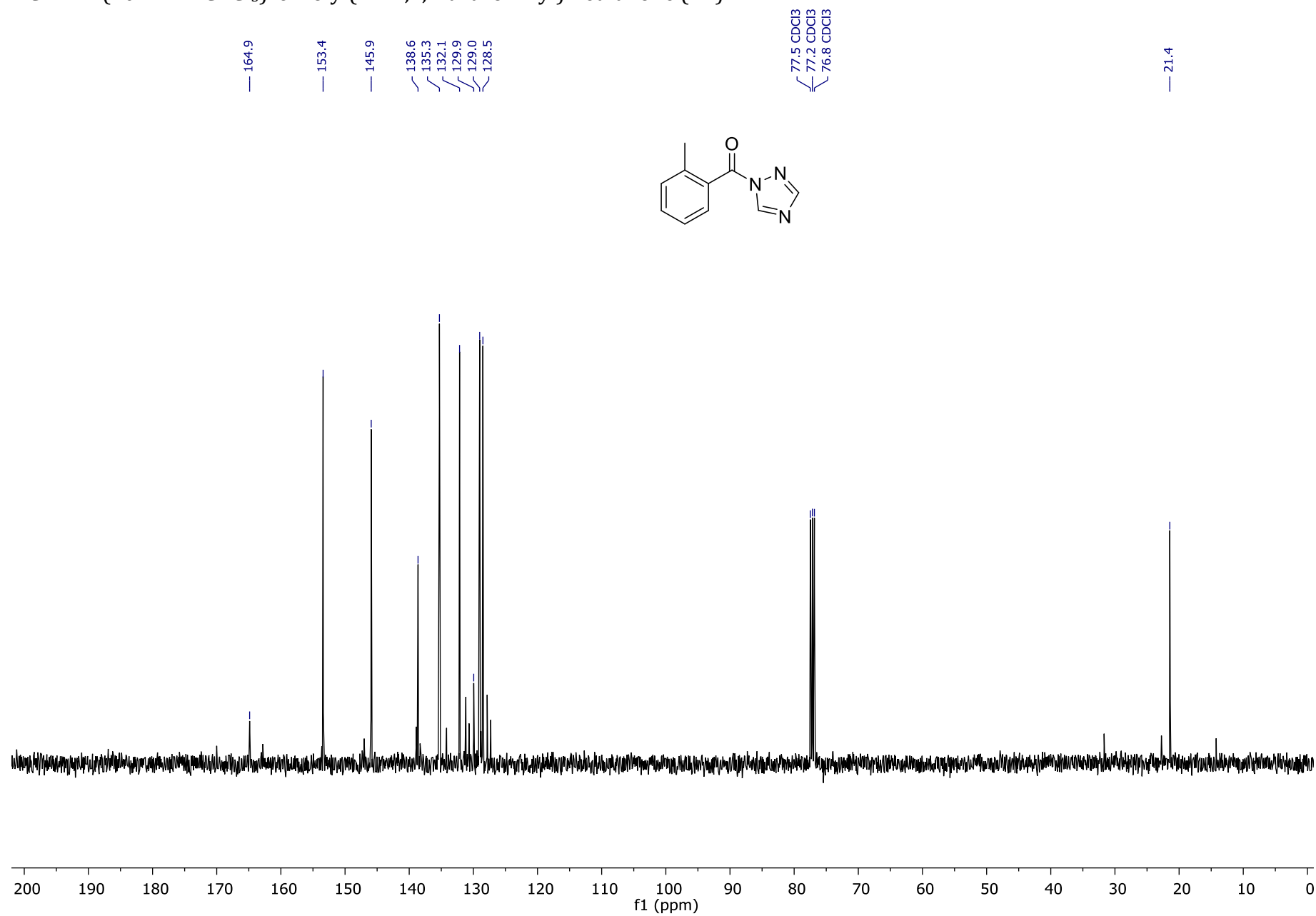
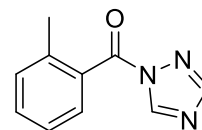
^{13}C -NMR (101 MHz CDCl_3): *m*-Tolyl(1*H*-1,2,4-triazol-1-yl)methanone (**7e'**)



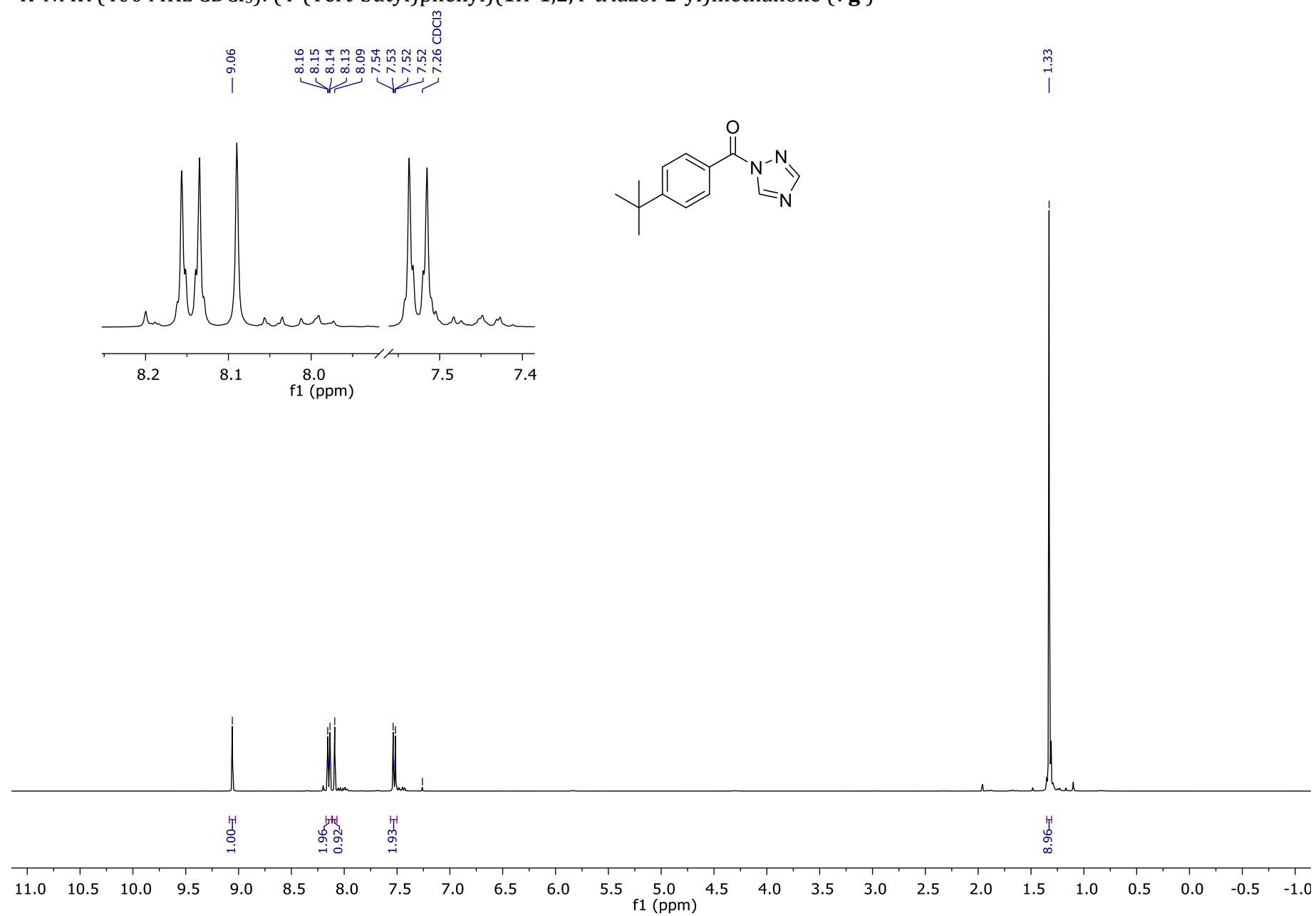
^1H -NMR (400 MHz CDCl_3): *o*-Tolyl(1*H*-1,2,4-triazol-1-yl)methanone (**7f**)



^{13}C -NMR (101 MHz CDCl_3): *o*-Tolyl(1*H*-1,2,4-triazol-1-yl)methanone (**7f**)



^1H -NMR (400 MHz CDCl_3): (4-(Tert-butyl)phenyl)(1*H*-1,2,4-triazol-2-yl)methanone (**7g'**)



^{13}C -NMR (101 MHz CDCl_3): (4-(Tert-butyl)phenyl)(1*H*-1,2,4-triazol-2-yl)methanone (**7g'**)

