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Cellulose Acetate-Supported Copper as an Efficient Sustainable Heterogenous Catalyst for Azide-Alkyne Cycloaddition Click Reactions in Water

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Supporting Information

1-Benzyl-4-phenyl-1H-1,2,3-triazole (3a)

White solid. ^1H NMR (300 MHz, CDCl_3 , δ ppm): 5.59 (s, 2H, CH_2), 7.28-7.44 (m, 8H, CH_{ar}), 7.69 (s, 1H, $\text{CH}_{\text{triazole}}$), 7.81-7.84(d, 2H, CH_{ar}). ^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 54.6 (CH_2); 120.0 (CH_{ar}); 126.1 (CH_{ar}); 128.5 (2 CH_{ar}); 128.6 (2 CH_{ar}); 129.2 (C_{ar}); 129.6 ($\text{CH}_{\text{triazole}}$); 130.9 (C_{ar}); 135.1 (C_{ar}).

1- Benzyl-4-p-tolyl-1H-1,2,3-triazole (3b)

White solid. ^1H NMR (300 MHz, CDCl_3 , δ ppm): 2.38 (s, 3H, CH_3), 5.59 (s, 2H, CH_2), 7.22-7.42 (m, 7H, CH_{ar}), 7.66 (s, 1H, $\text{CH}_{\text{triazole}}$), 7.70-7.73 (d, 2H, CH_{ar}). ^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 21.7 (CH_3), 54.6 (CH_2), 126.0 (CH_{ar}), 128.2 (2 CH_{ar}), 128.5 (2 CH_{ar}), 129.2 (2 CH_{ar}), 129.5 (2 CH_{ar}), 129.9 (C_{ar}), 131.7 ($\text{CH}_{\text{triazole}}$), 135.1 (2 C_{ar}), 138.4 ($\text{C}_{\text{triazole}}$).

1-benzyl-4-(phenoxyethyl)-1H-1,2,3-triazole (3c)

White solid. ^1H NMR (300 MHz, CDCl_3 , δ ppm): 5.21 (s, 2H, CH_2); 5.55 (s, 2H, OCH_2); 6.96-7.00 (m, 3H, CH_{ar}); 7.28-7.41 (m, 7H, CH_{ar}); 7.57 (s, 1H, $\text{CH}_{\text{triazole}}$). ^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 54.7 (CH_2); 62.5 (CH_2); 115.2 (2 CH_{ar}); 116.6 (CH_{ar}); 121.7 ($\text{CH}_{\text{triazole}}$); 128.5 (CH_{ar}); 129.2 (2 CH_{ar}); 129.5 (4 CH_{ar}); 129.9 (C_{ar}); 134.9 ($\text{C}_{\text{triazole}}$); 158.6 (C_{ar}).

(1-benzyl-1H-1,2,3-triazol-4-yl)methyl benzoate (3d)

White solid. ^1H NMR (300MHz, CDCl_3 , δ ppm): 5.47 (s, 2H, CH_2); 5.54 (s, 2H, CH_2); 7.28-7.38 (m, $J=30$ Hz, 5H, CH_{ar}); 7.40 (s, 1H, CH_{ar}); 7.43 (s, 1H, CH_{ar}); 7.46 (s, 1H, $\text{CH}_{\text{triazole}}$); 7.57 (s, 1H, CH_{ar}); 8.03-8.05 (d, 2H, CH_{ar}). ^{13}C NMR (75 MHz, CDCl_3 , δ ppm) : 54.8 (CH_2); 58.4 (CH_2); 128.5 ($\text{CH}_{\text{triazole}}$); 128.8 (2 CH_{ar}); 129.3 (2 CH_{ar}); 129.6 (2 CH_{ar}); 130.1 (4 CH_{ar}); 133.6 (C_{ar}); 134.8 ($\text{C}_{\text{triazole}}$); 153.2 (C_{ar}); 166.8 ($\text{C}_{\text{carbonyle}}$).

1-benzyl-1H-1,2,3-triazole-4-carboxylic acid (3e)

White solid. ^1H NMR (300 MHz, CD₃OD, δ ppm): 8.48 (s, 1H, CH_{triazole}); 7.33-7.40 (m, J=21 Hz, 5H, CH_{ar}); 5.94 (s, 1H, OH); 5.64 (s, 2H, CH₂). ^{13}C NMR (75 MHz, CD₃OD, δ ppm): 55.6 (CH₂); 129.7-129.9 (5CH_{ar}); 130.2 (CH_{triazole}); 130.5 (C_{ar}); 136.7 (C_{triazole}); 162.3 (C_{carbonyle}).

4-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)pyridine (3f)

White solid. ^1H NMR (300 MHz, CDCl₃, δ ppm): 5.73 (s, 2H, CH₂); 7.25-7.36 (m, 2H, CH_{ar}); 7.41-7.46 (m, 3H, CH_{ar}); 7.69-7.75 (m, 1H, CH_{ar}); 7.83-7.87 (m, 1H, CH_{ar}); 7.96 (s, 1H, CH_{triazole}); 8.64 (s, 2H, CH_{ar}). ^{13}C NMR (75 MHz, CDCl₃, δ ppm): 56.1 (CH₂); 120.6 (2 CH_{ar}); 124.0 (2 CH_{ar}); 126.1 (CH_{ar}); 128.6 (2 CH_{ar}); 129.2 (C_{ar}); 130.9 (CH_{triazole}); 137.8 (C_{ar}); 150.1 (C_{triazole}); 154.9 (2 CH_{ar}).

4-((4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)methyl)pyridine (3g)

White solid. ^1H NMR (300 MHz, CDCl₃, δ ppm): 3.85 (s, 3H, CH₃); 5.51 (s, 2H, CH₂); 6.95-6.98 (d, 2H, CH_{ar}); 7.70-7.72 (d, 2H, CH_{ar}); 7.76-7.79 (d, 2H, CH_{ar}); 7.87 (s, 1H, CH_{triazole}); 8.63 (s, 2H, CH_{ar}). ^{13}C NMR (75 MHz, CDCl₃, δ ppm): 55.7 (CH₂); 56.1 (CH₃); 114.6 (2 CH_{ar}); 119.8 (C_{ar}); 123.7 (2 CH_{ar}); 127.4 (2 CH_{ar}); 130.7 (CH_{triazole}); 137.8 (C_{ar}); 148.5 (C_{triazole}); 154.9 (2 CH_{ar}); 160.0 (O-C_{ar}).

1-(4-methoxyphenyl)-4-phenyl -1H-1,2,3-triazole (3h)

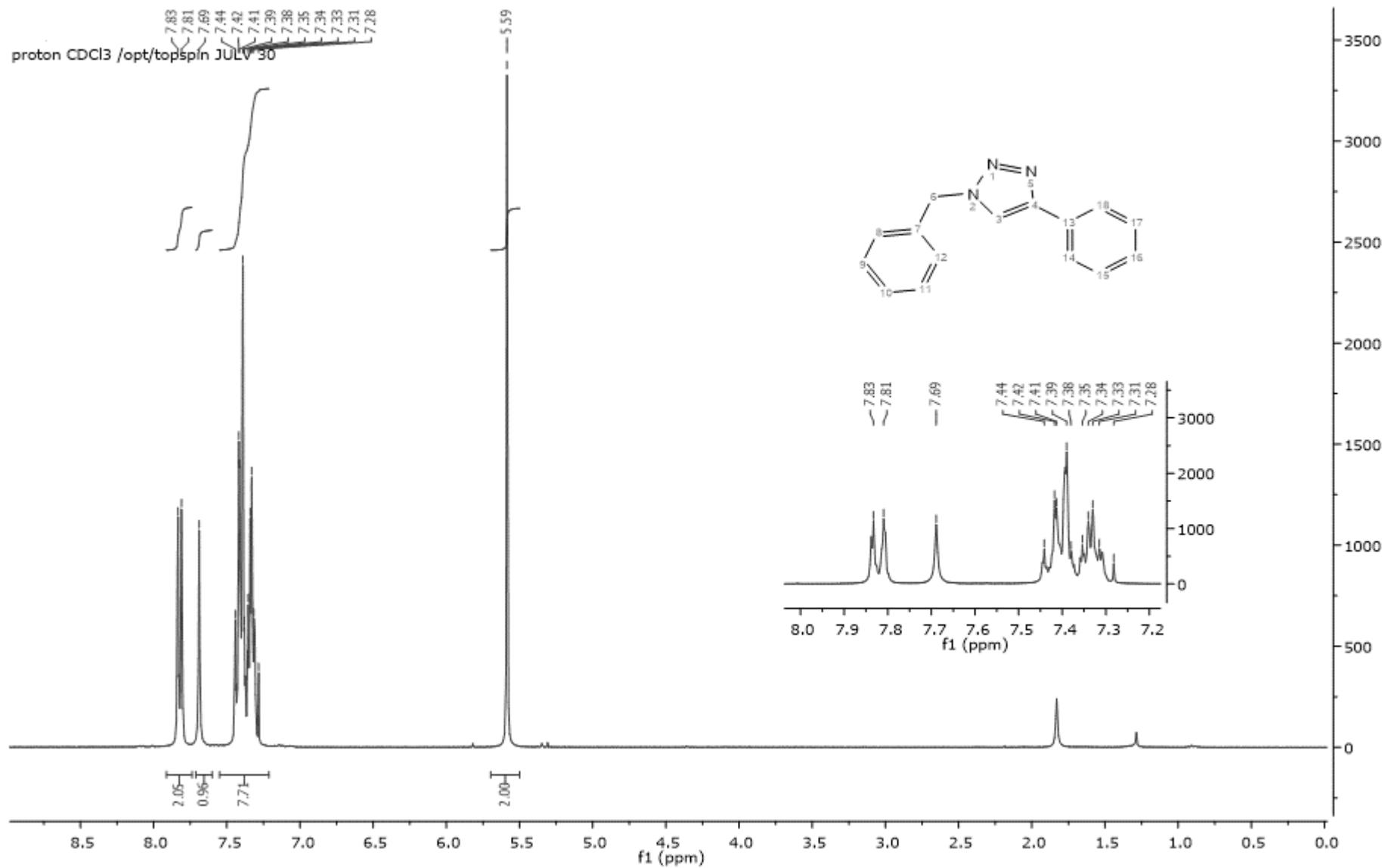
White solid. ^1H NMR (300 MHz, CDCl₃, δ ppm): 3.90 (s, 3H, OCH₃); 7.05-7.08 (d, 2H, CH_{ar}); 7.40-7.49 (m, 5H, CH_{ar}); 7.51-7.97 (d, 2H, CH_{ar}); 8.26 (s, 1H, CH_{triazole}). ^{13}C NMR (75 MHz, CDCl₃, δ ppm): 56.1 (CH₃); 115.0 (CH_{ar}); 115.3 (C_{ar}); 122.7 (2 CH_{ar}); 126.3 (CH_{ar}); 126.6 (2CH_{ar}); 127.0 (2CH_{ar}); 129.0 (CH_{triazole}); 129.4 (C_{ar}); 146.1 (C_{triazole}); 160.5 (C_{ar}).

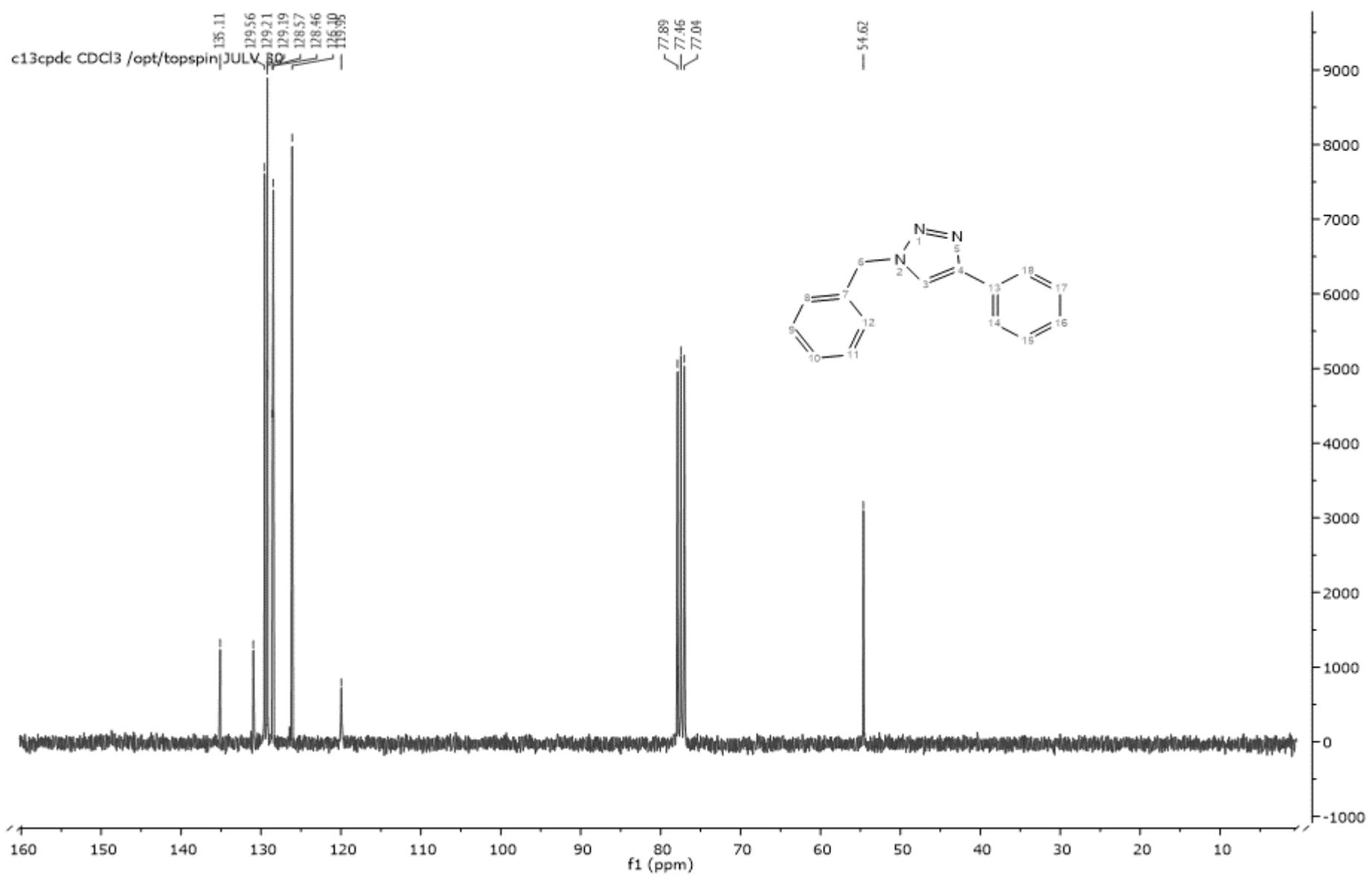
1-(4-isopropylphenyl)-4-phenyl-1H-1,2,3-triazole (3i)

White solid. ^1H NMR (300 MHz, DMSO, δ ppm) : 1.24 (s, 3H,CH₃); 1.26 (s, 3H,CH₃); 2.95-3.04 (m, 1H, CH); 7.36-7.40 (t, 1H, CH_{ar}); 7.48-7.50 (d, 2H, CH_{ar}); 7.51-7.52 (d, 2H,

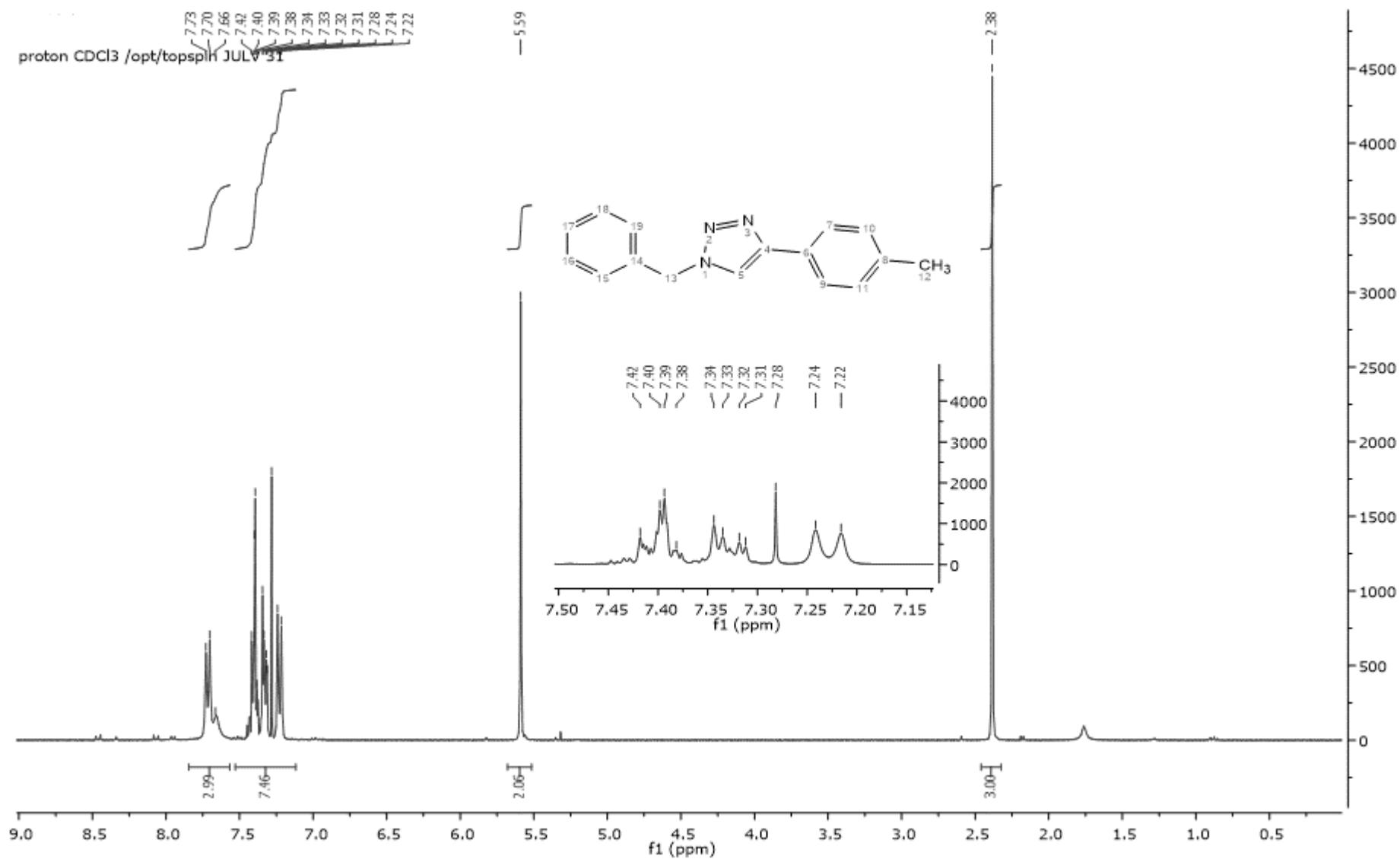
CH_{ar}); 7.84-7.87 (d, 2H, CH_{ar}); 7.94-7.96 (d, 2H, CH_{ar}); 9.24 (s, 1H, $\text{CH}_{\text{triazole}}$). ^{13}C NMR (75 MHz, DMSO, δ ppm): 24.1 (2 CH_3); 33.5 (CH); 119.9 (C_{ar}); 120.4 (2 CH_{ar}); 125.7 (2 CH_{ar}); 128.1 (CH_{ar}); 128.5 (2 CH_{ar}); 129.3 (2 CH_{ar}); 130.7 ($\text{CH}_{\text{triazole}}$); 130.5 (C_{ar}); 148.0 ($\text{C}_{\text{triazole}}$); 149.5 (C_{ar}).

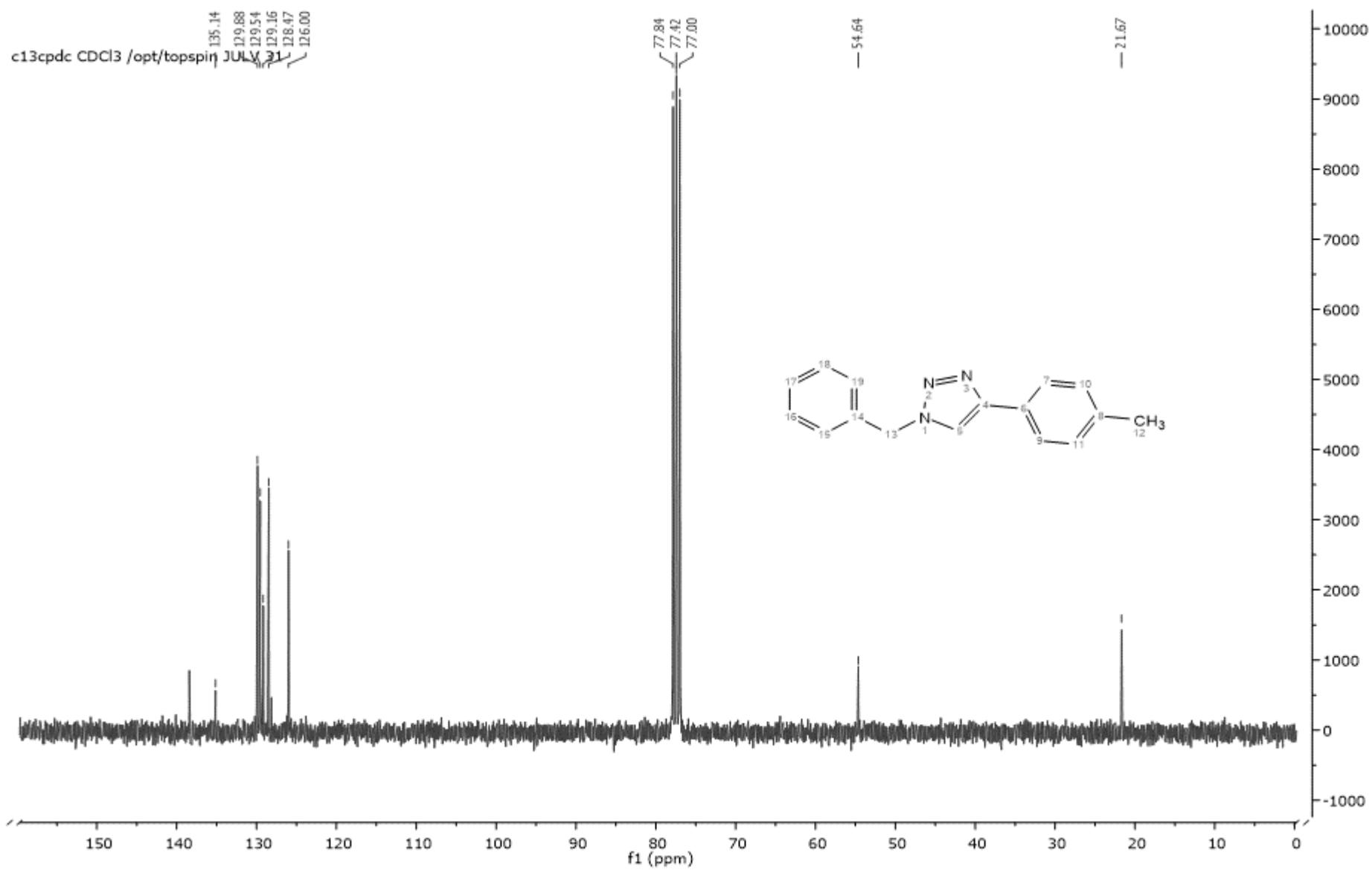
1-Benzyl-4-phenyl-1H-1,2,3-triazole (3a)



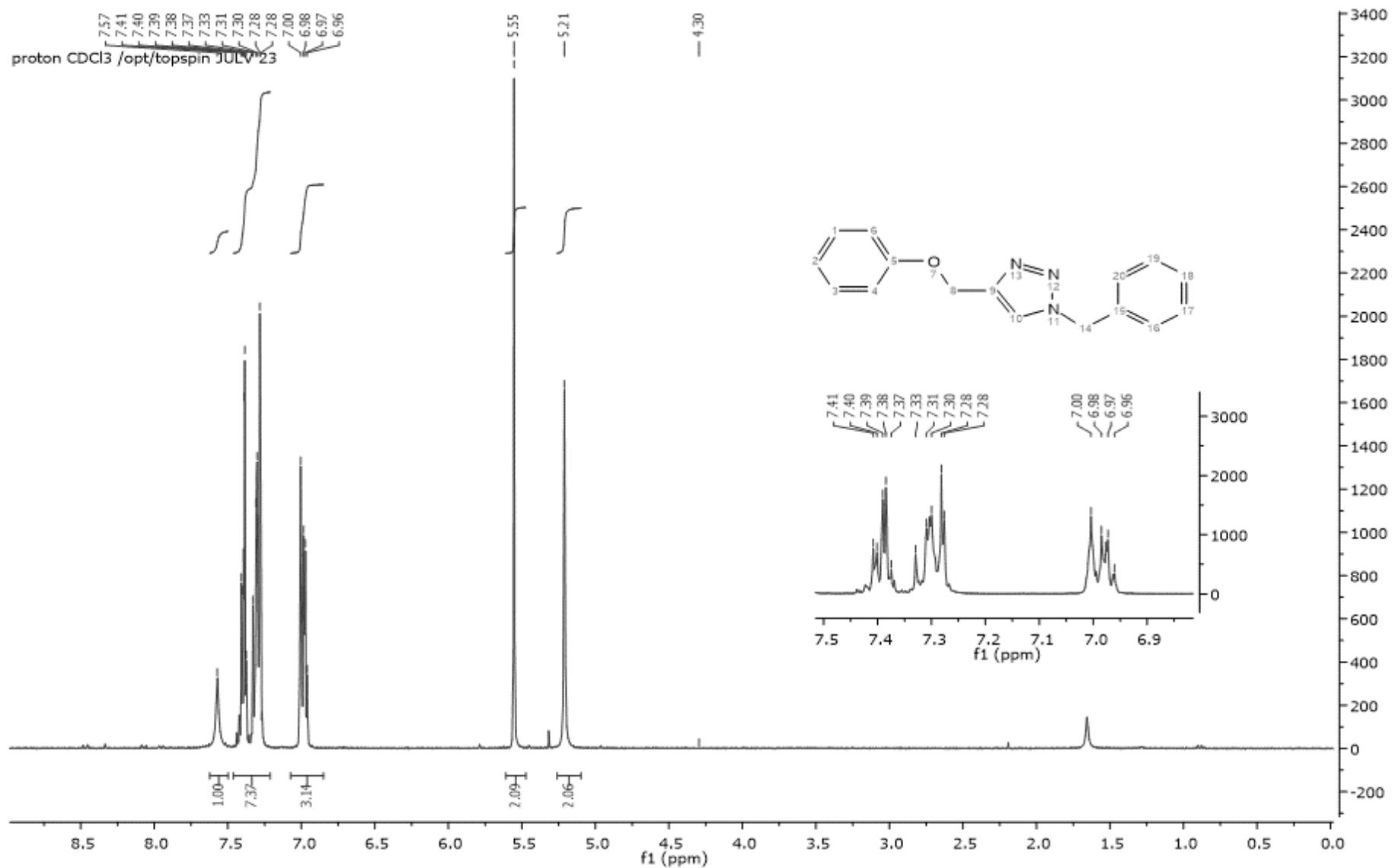


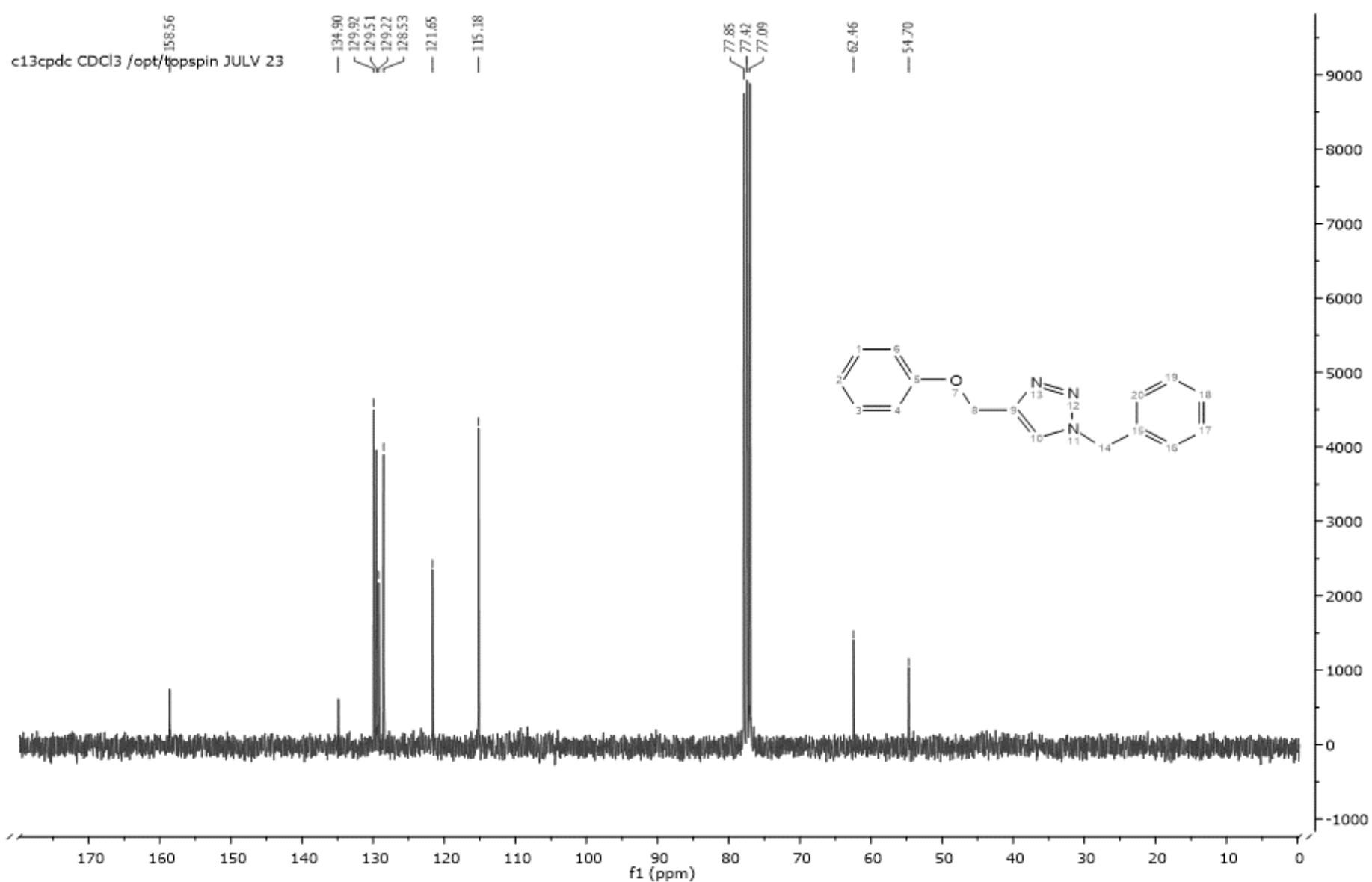
1-(4-methylbenzyl)-4-phenyl-1H-1,2,3-triazole (3b)



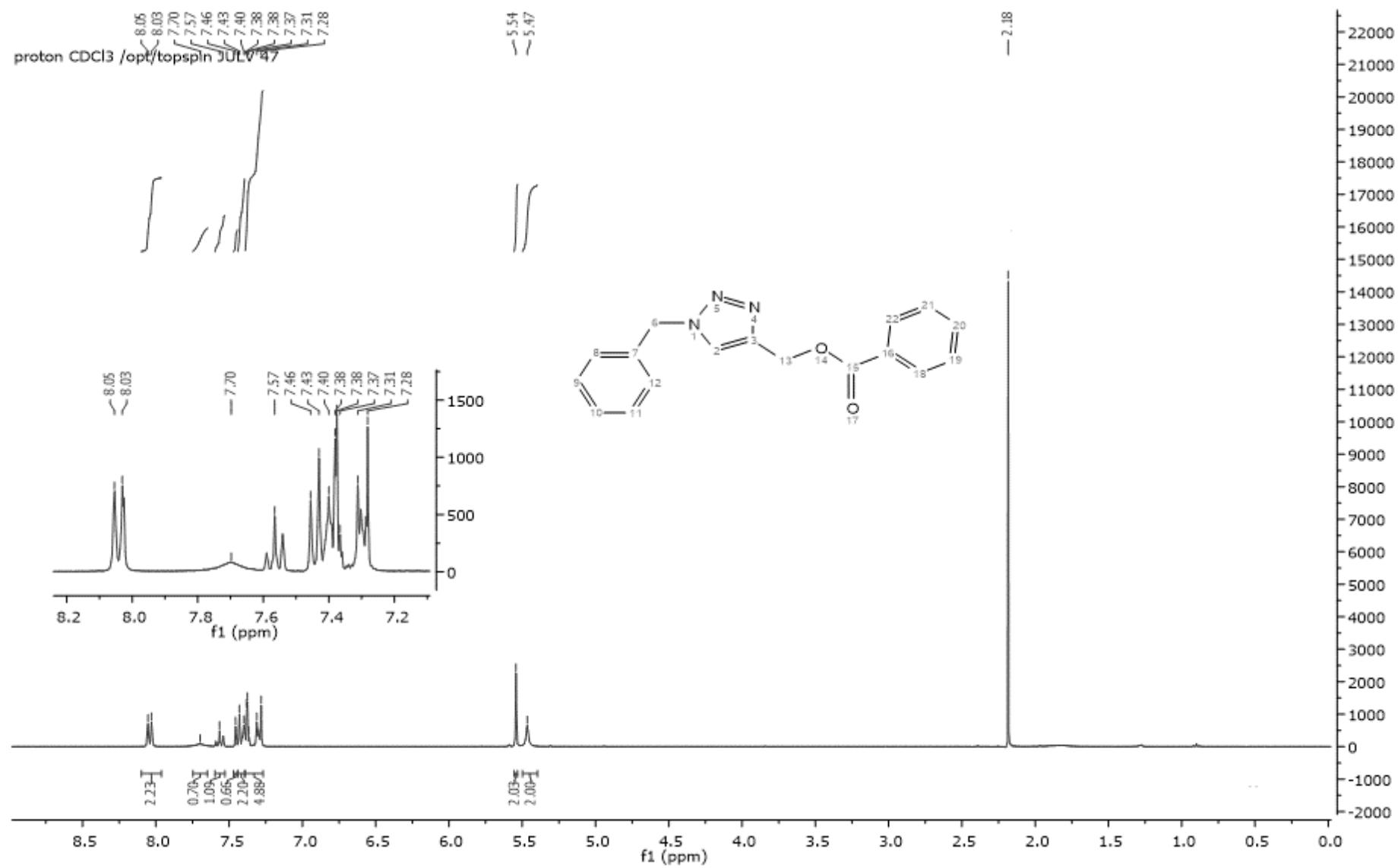


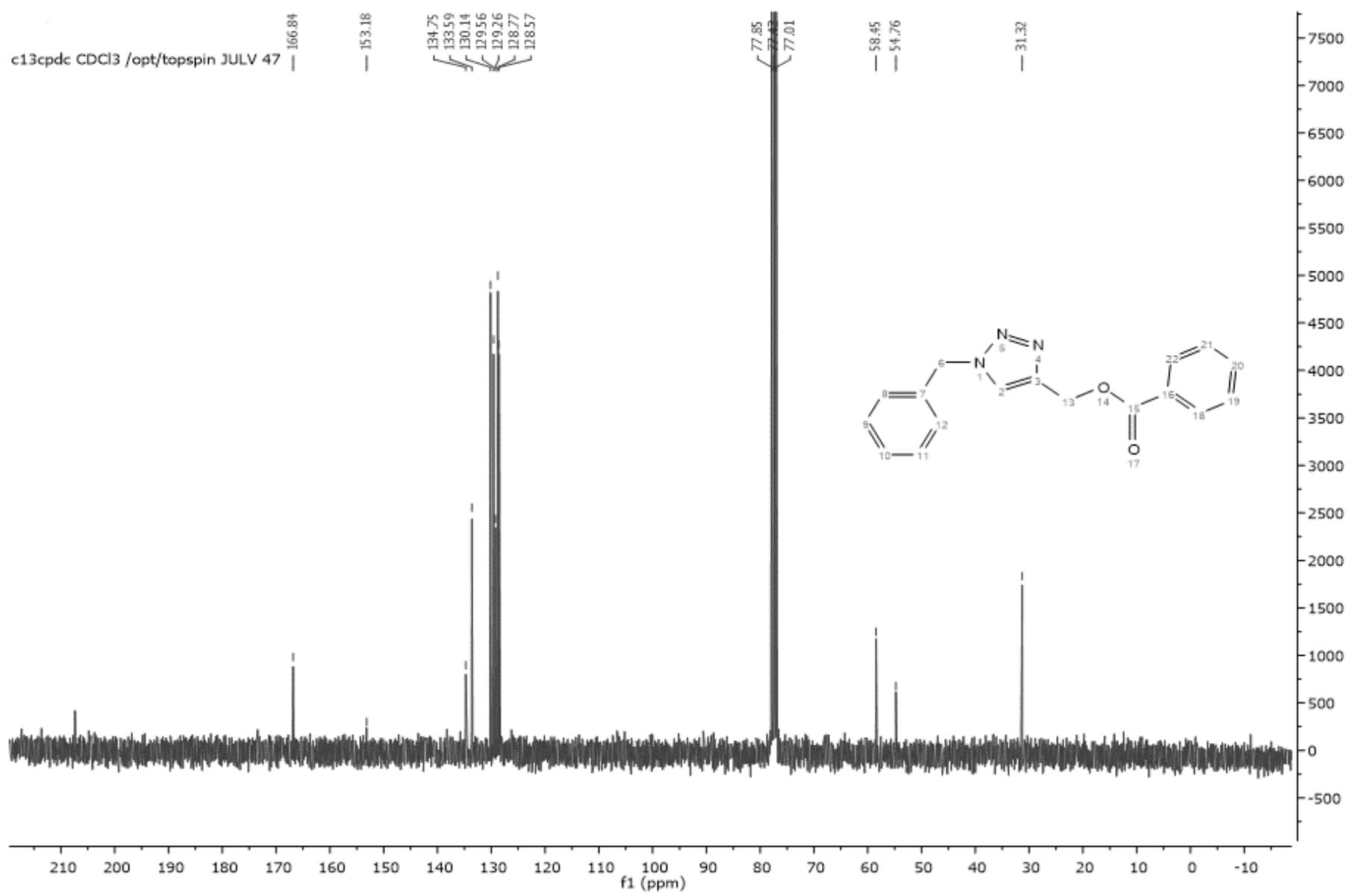
1-benzyl-4-(phenoxy)methyl)-1H-1,2,3-triazole (3c)



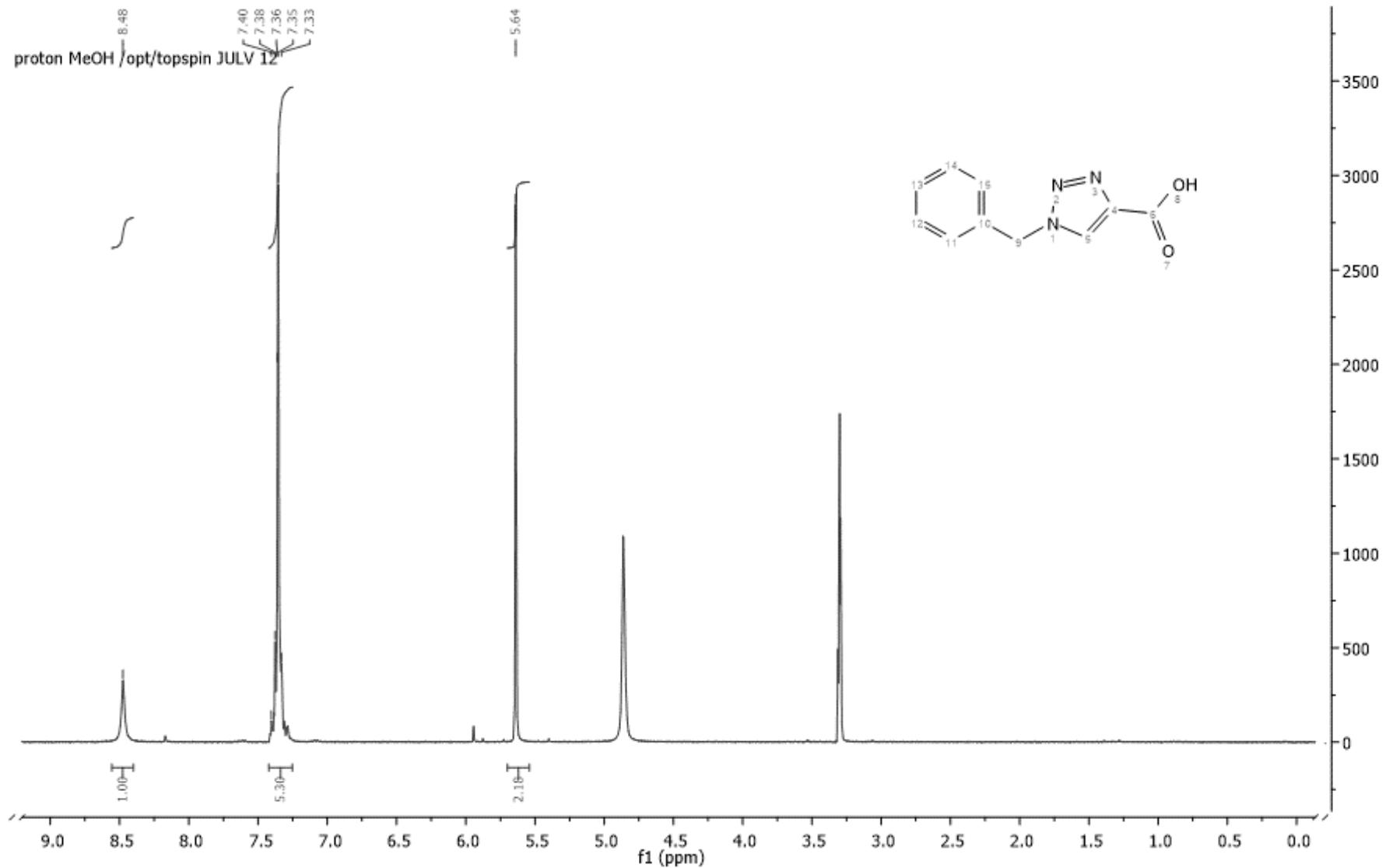


(1-benzyl-1H-1,2,3-triazol-4-yl)methyl benzoate (3d)



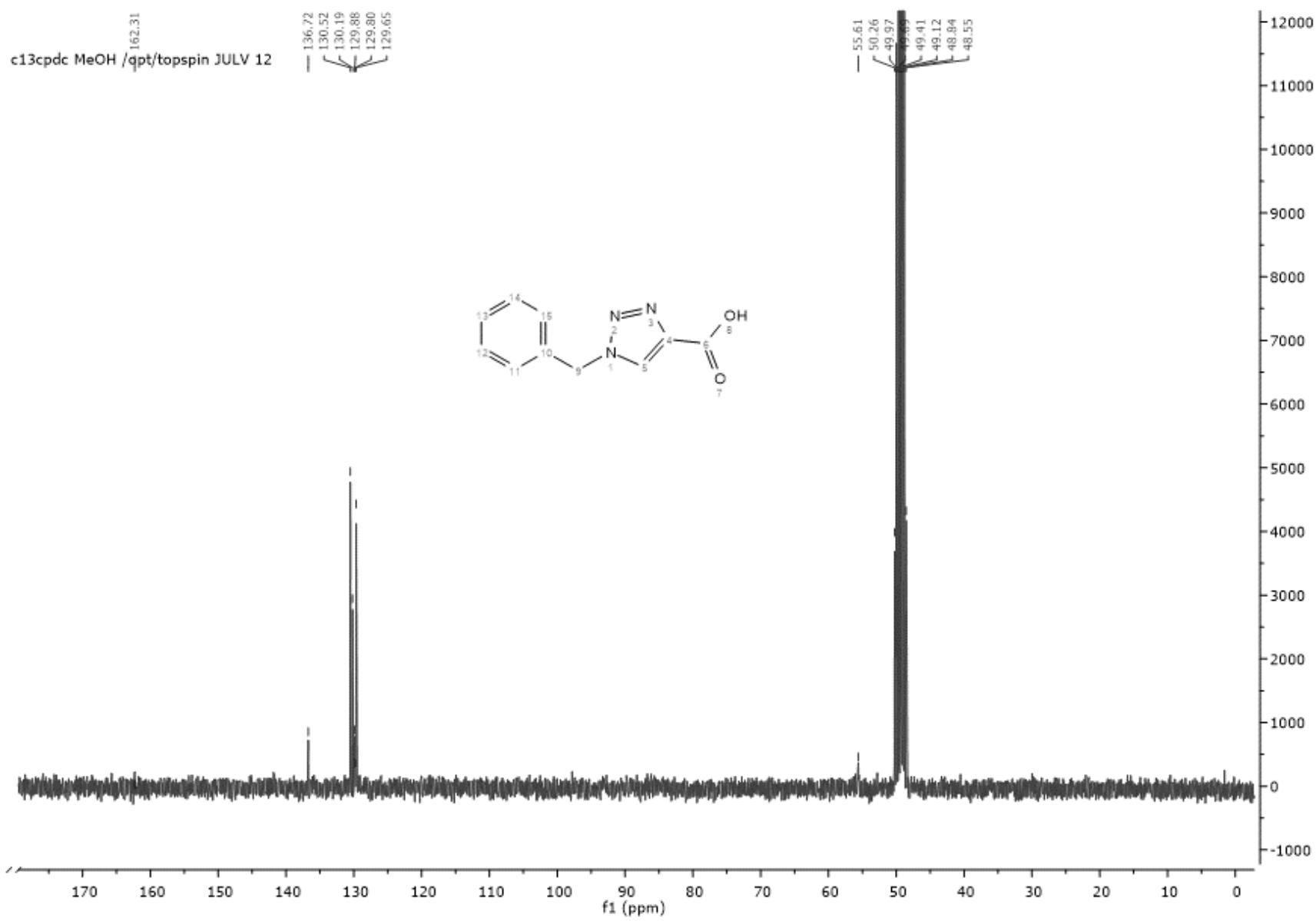
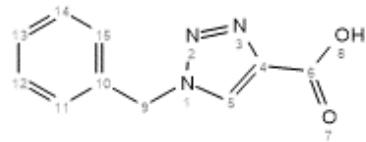


1-benzyl-1H-1,2,3-triazole-4-carboxylic acid (3e)

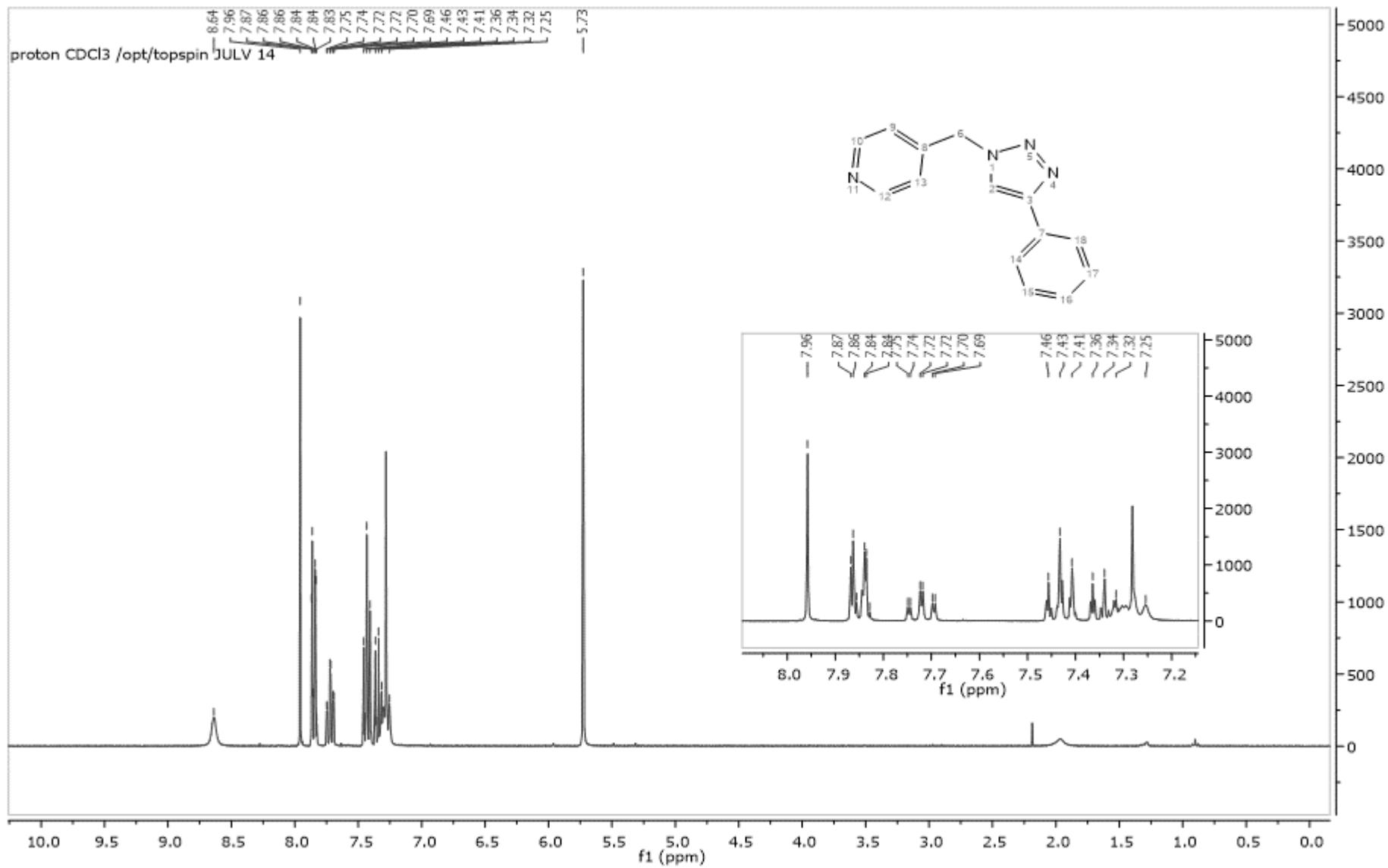


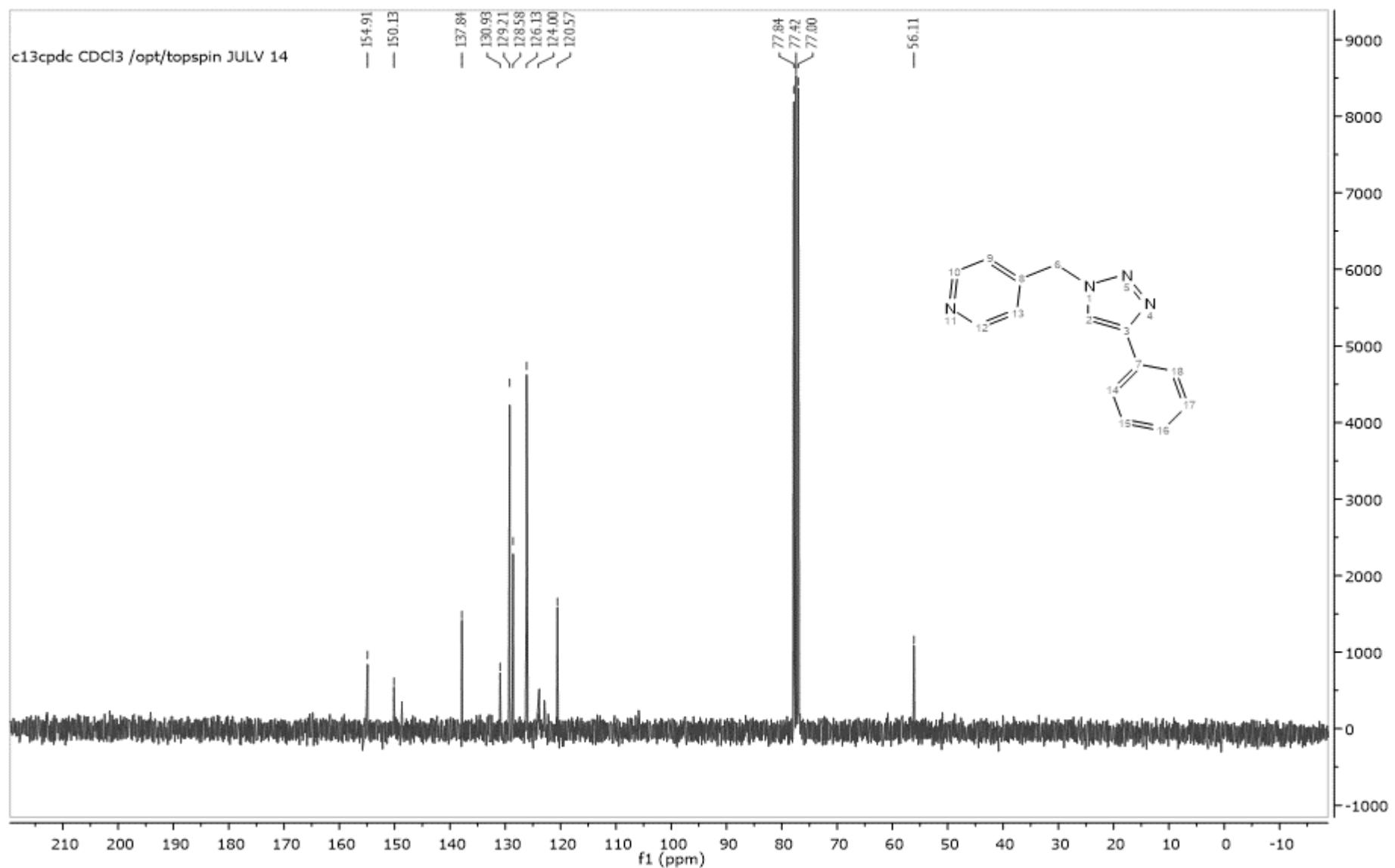
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162.31

136.72
130.52
130.19
129.88
129.80
129.65

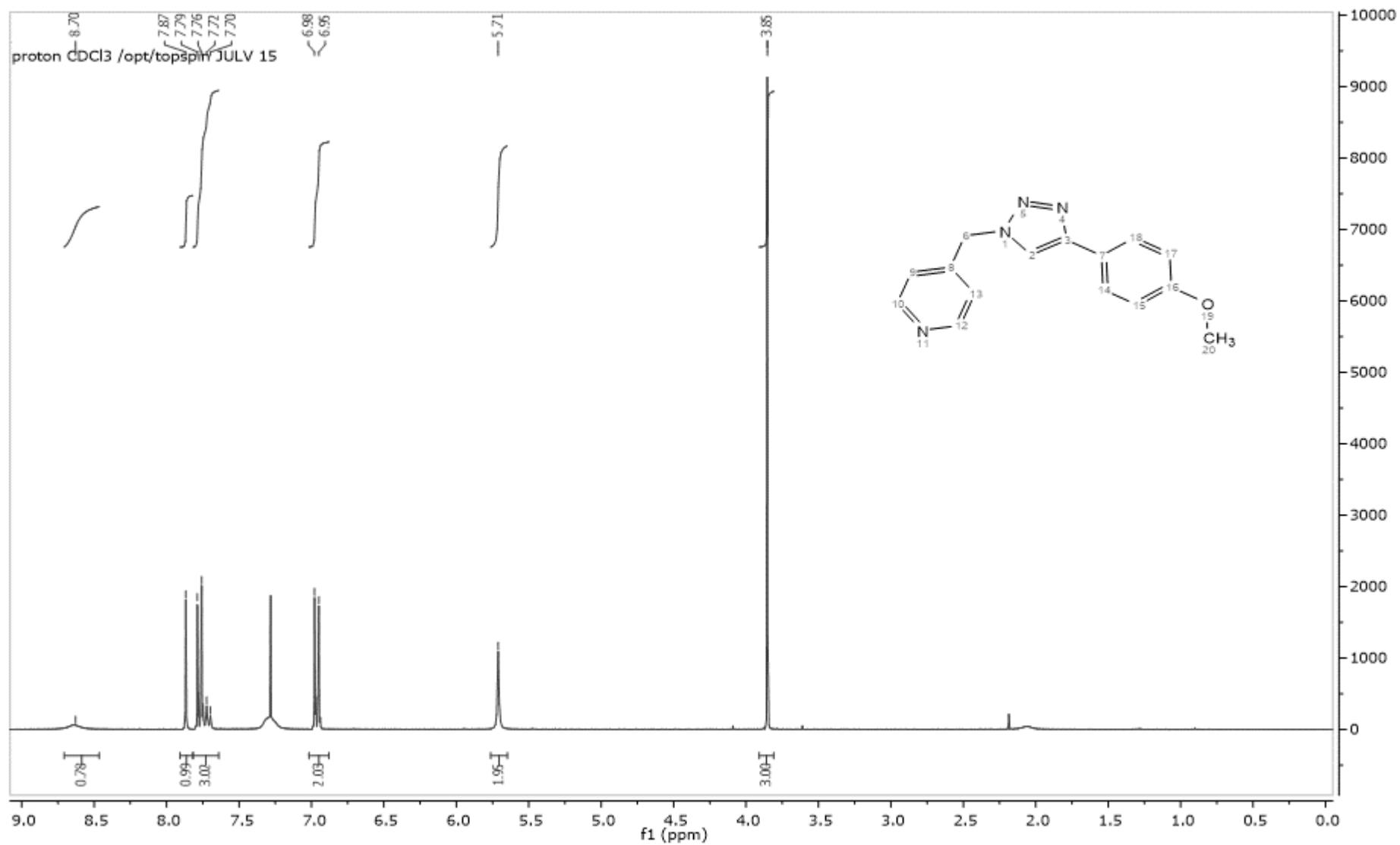


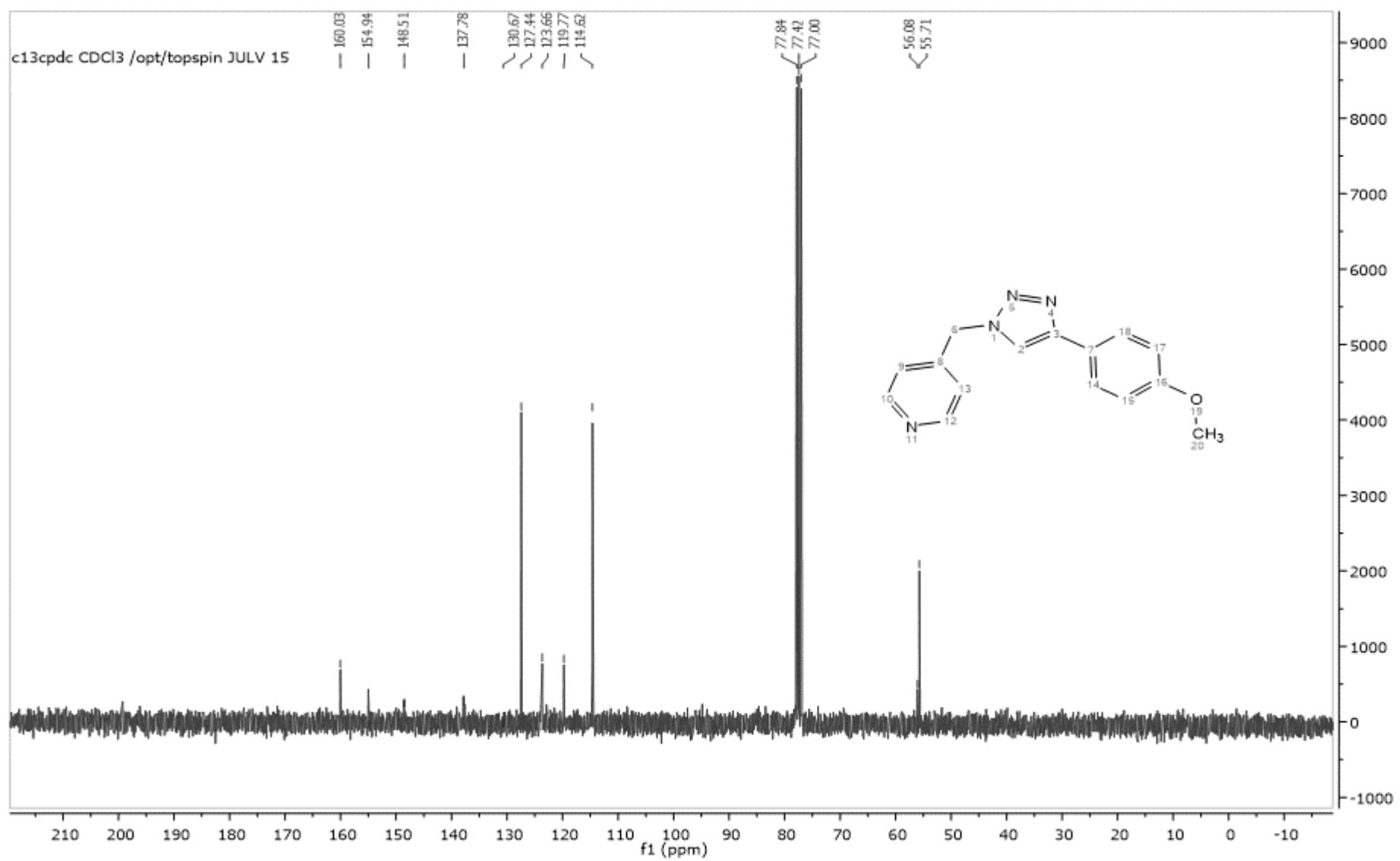
4-(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)pyridine (3f)



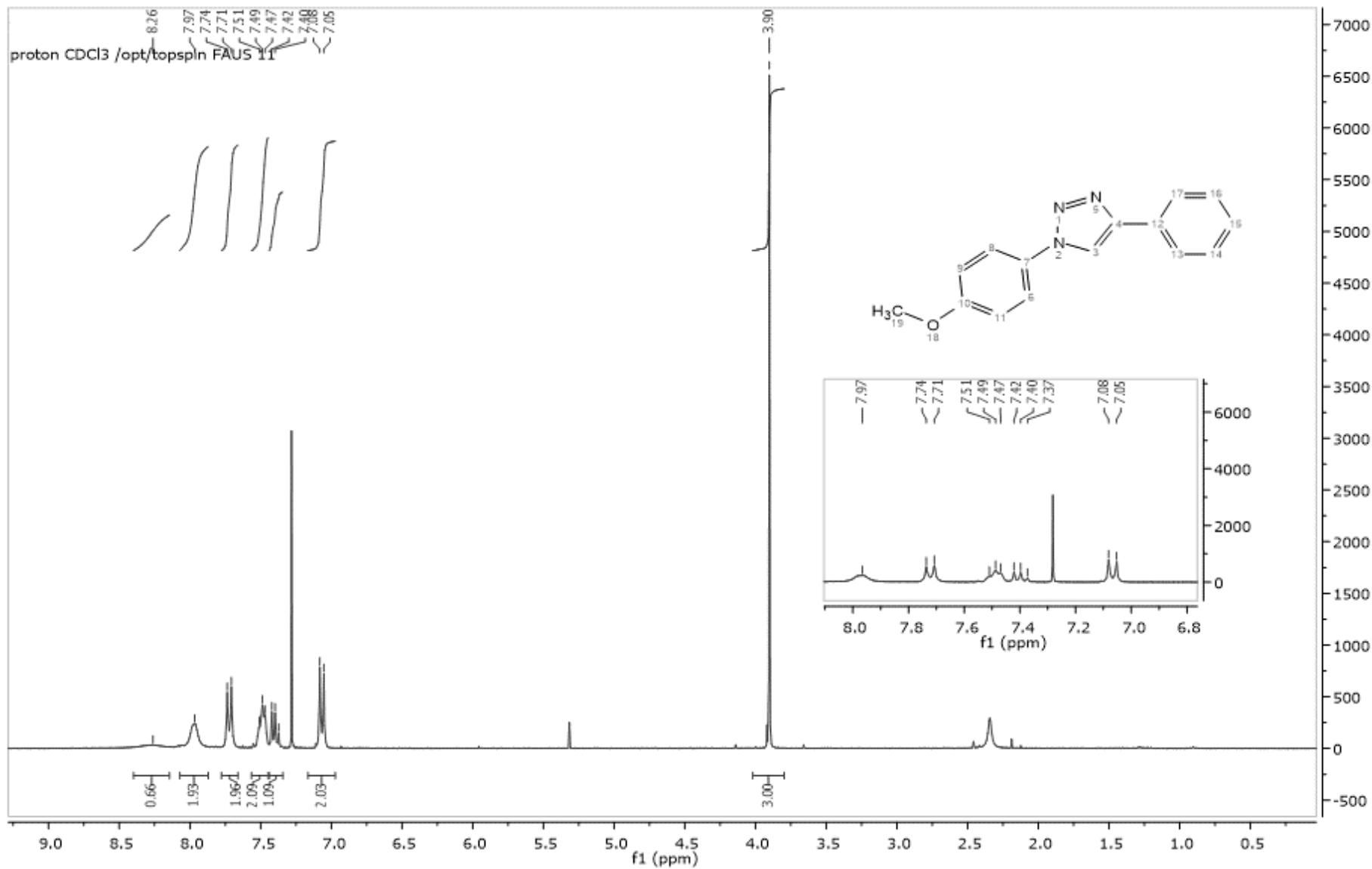


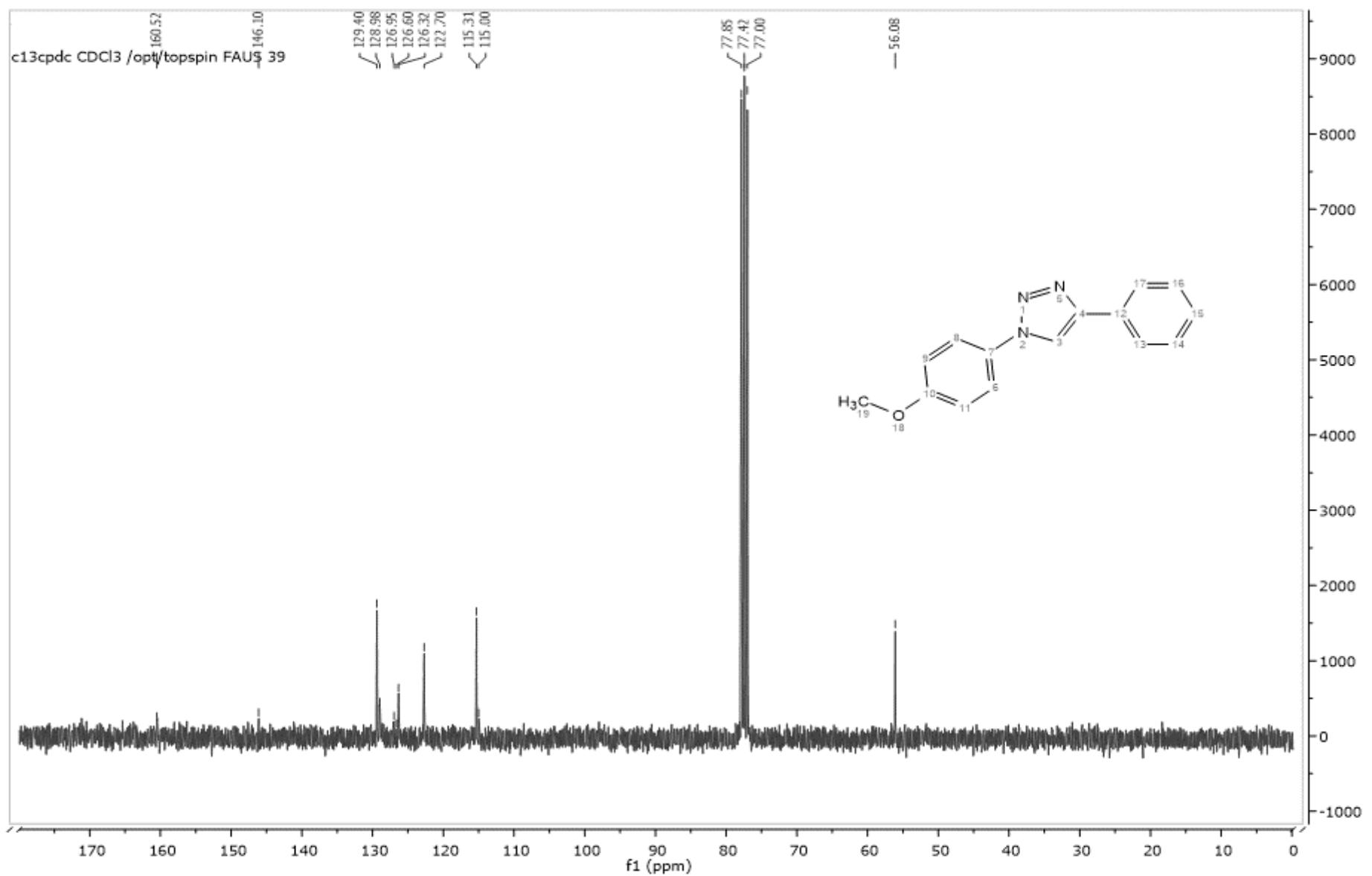
4-((4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)methyl)pyridine (3g)





1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole (3h)





1-(4-isopropylphenyl)-4-phenyl-1H-1,2,3-triazole (3i)

