

Supplementary Material

Synthesis of Substituted Oxazoles from Metal-free Cyclization of Enamides

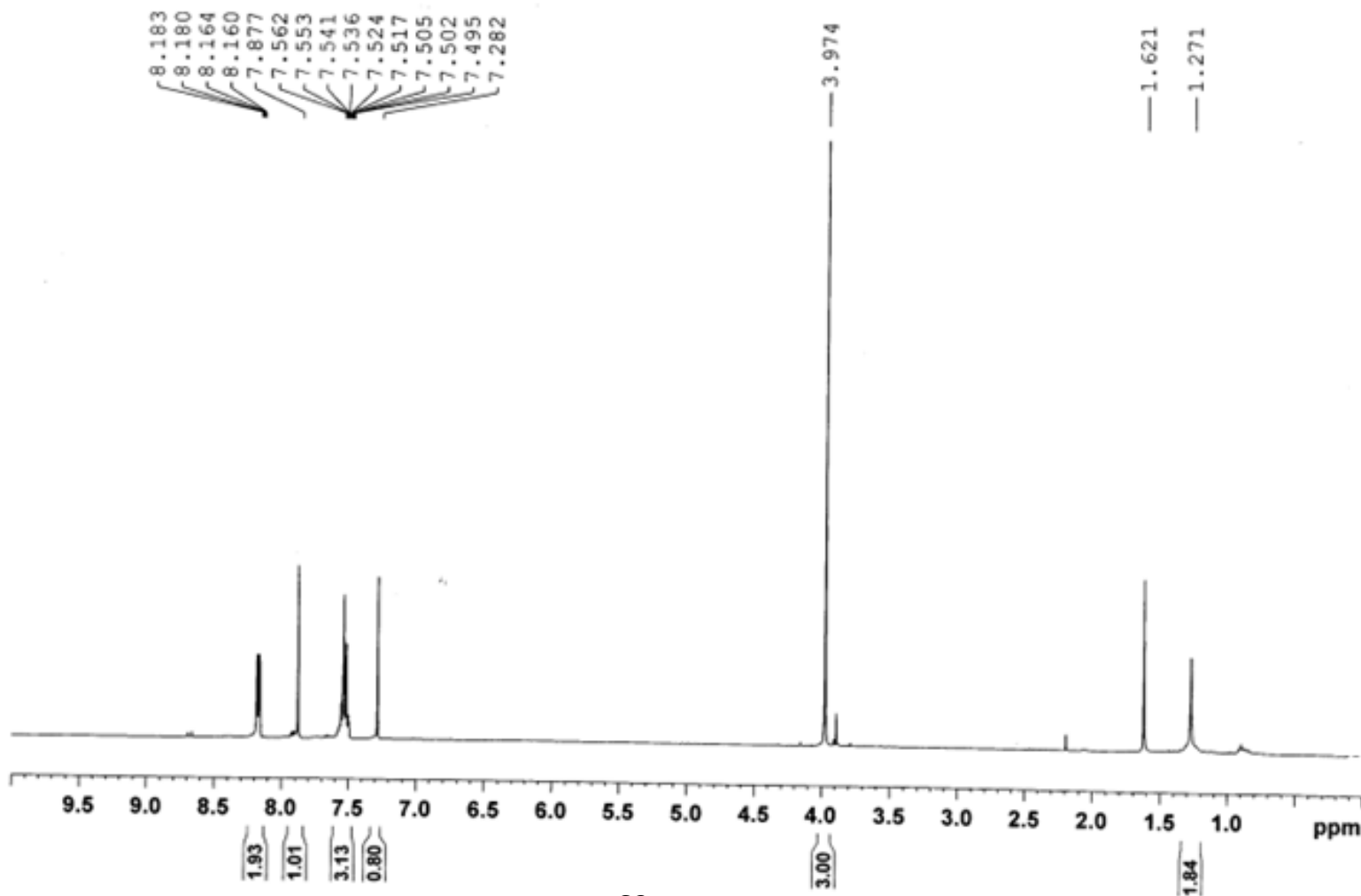
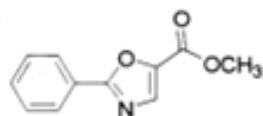
Niranjan Panda,^{*} and Raghavender Mothkuri

*Department of Chemistry, National Institute of Technology, Rourkela-769008
Odisha, India*

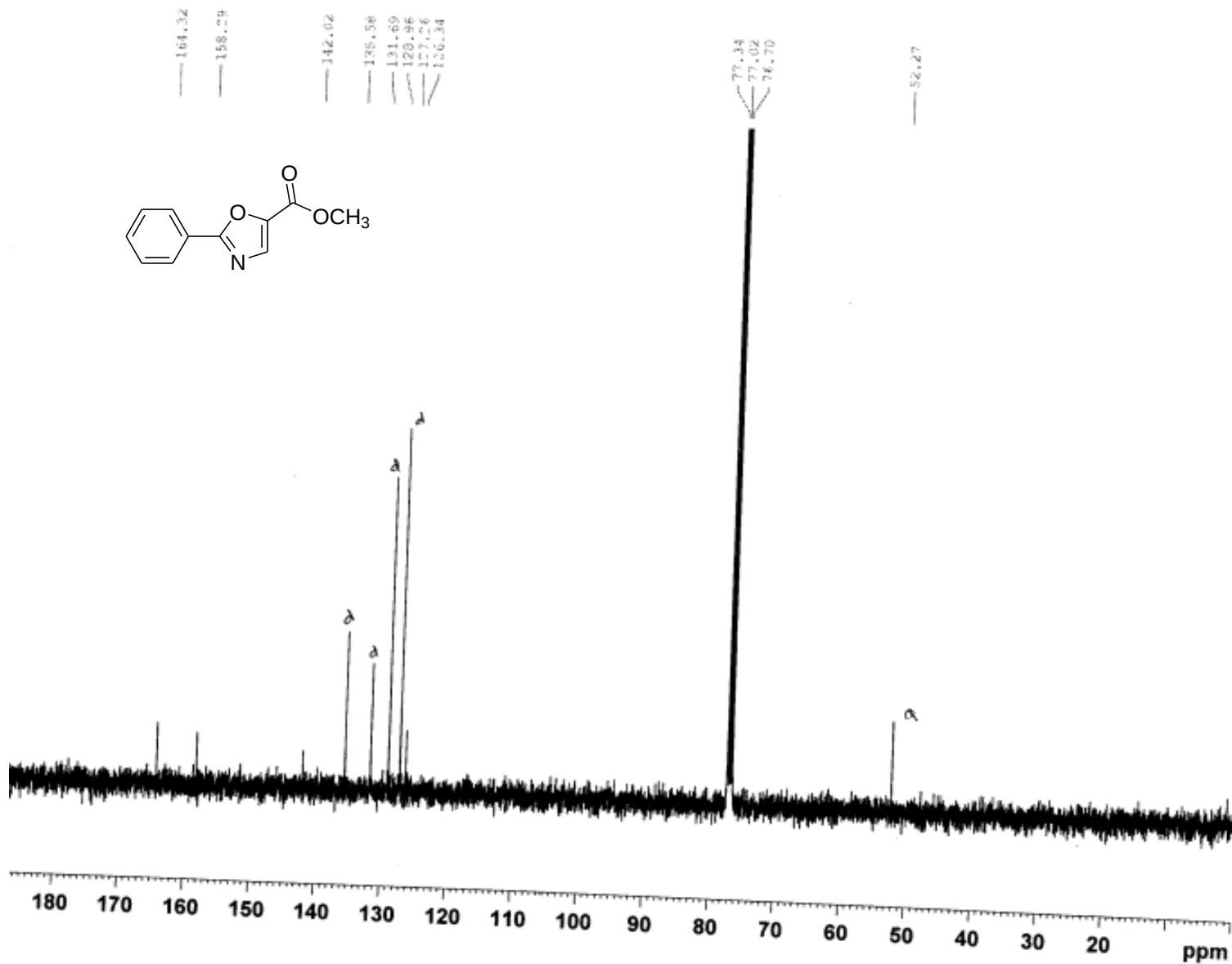
NMR spectra of oxazoles

Methyl 2-phenyloxazole-5-carboxylate (2a)

NP-MR-407-A

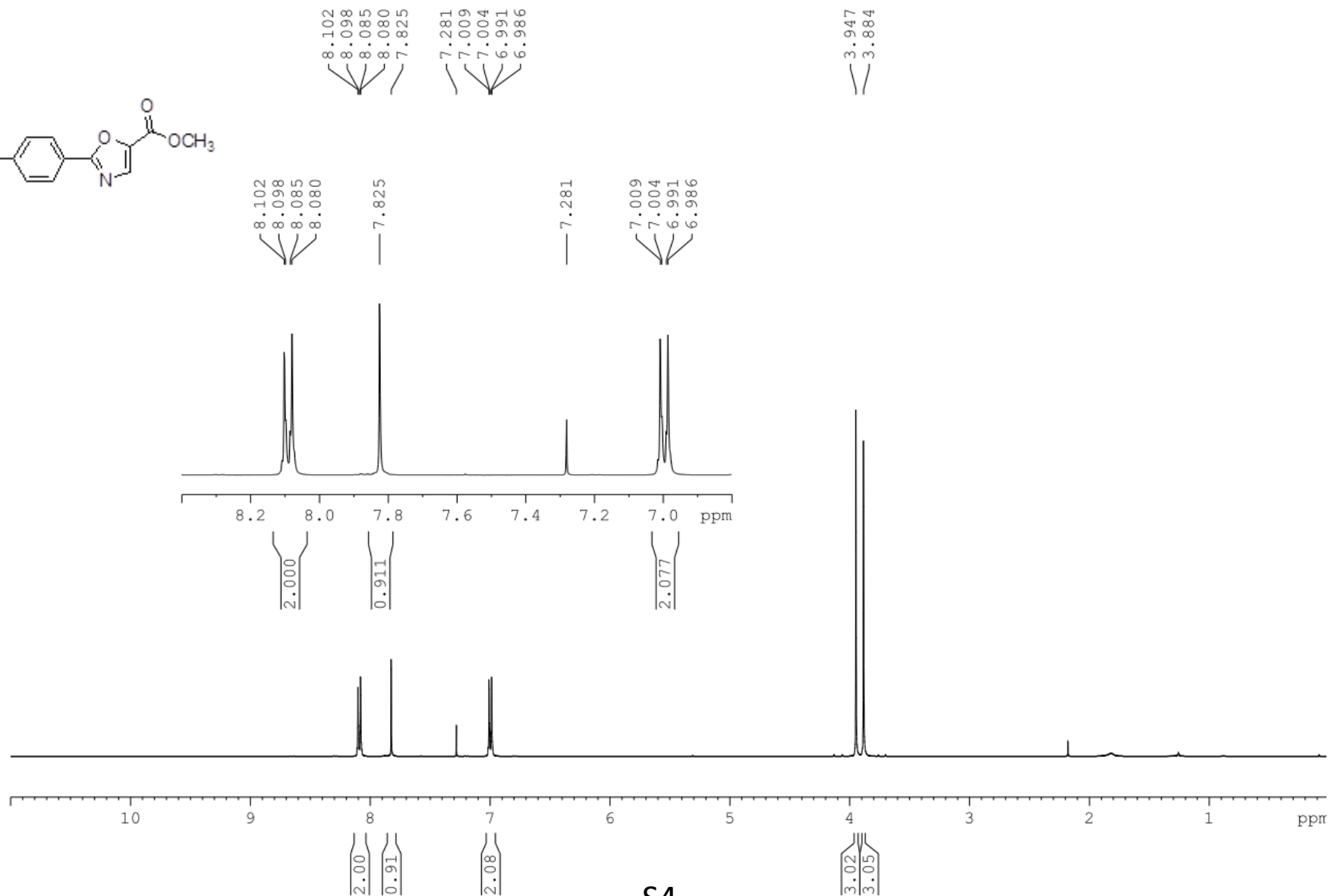
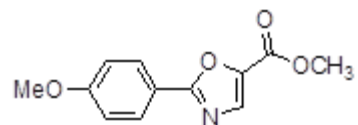


Methyl 2-phenyloxazole-5-carboxylate (2a)



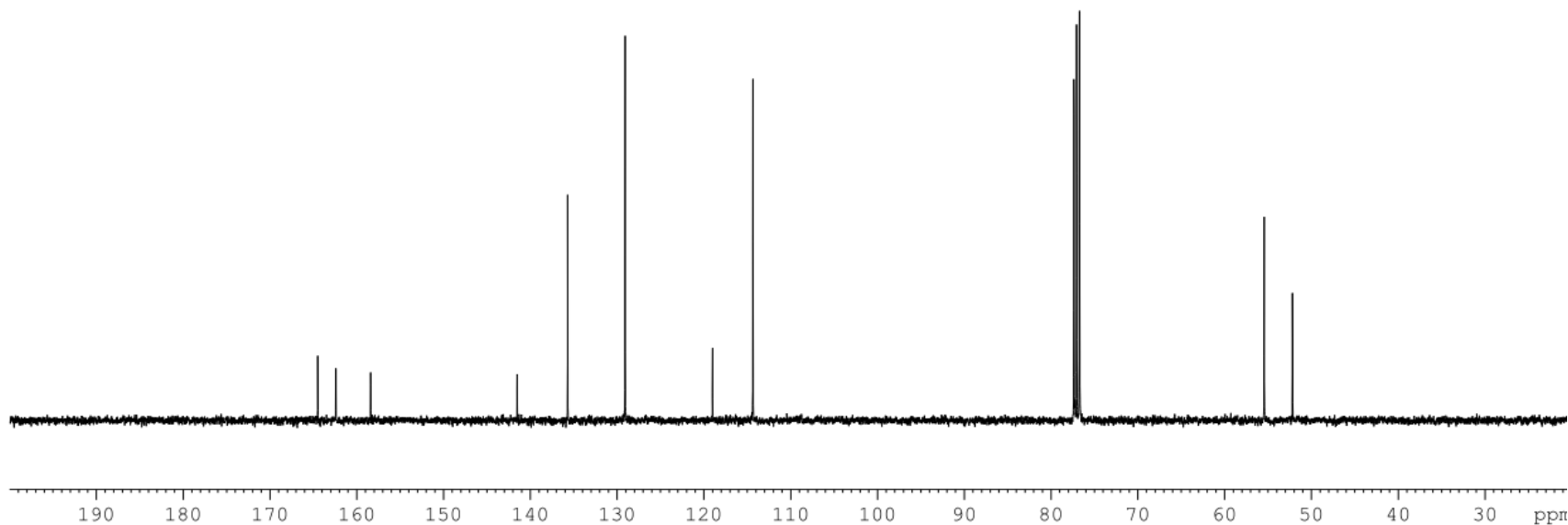
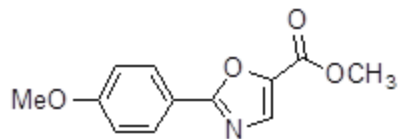
NP-DN-X 1H

Methyl 2-(4-methoxyphenyl)oxazole-5-carboxylate(2b)



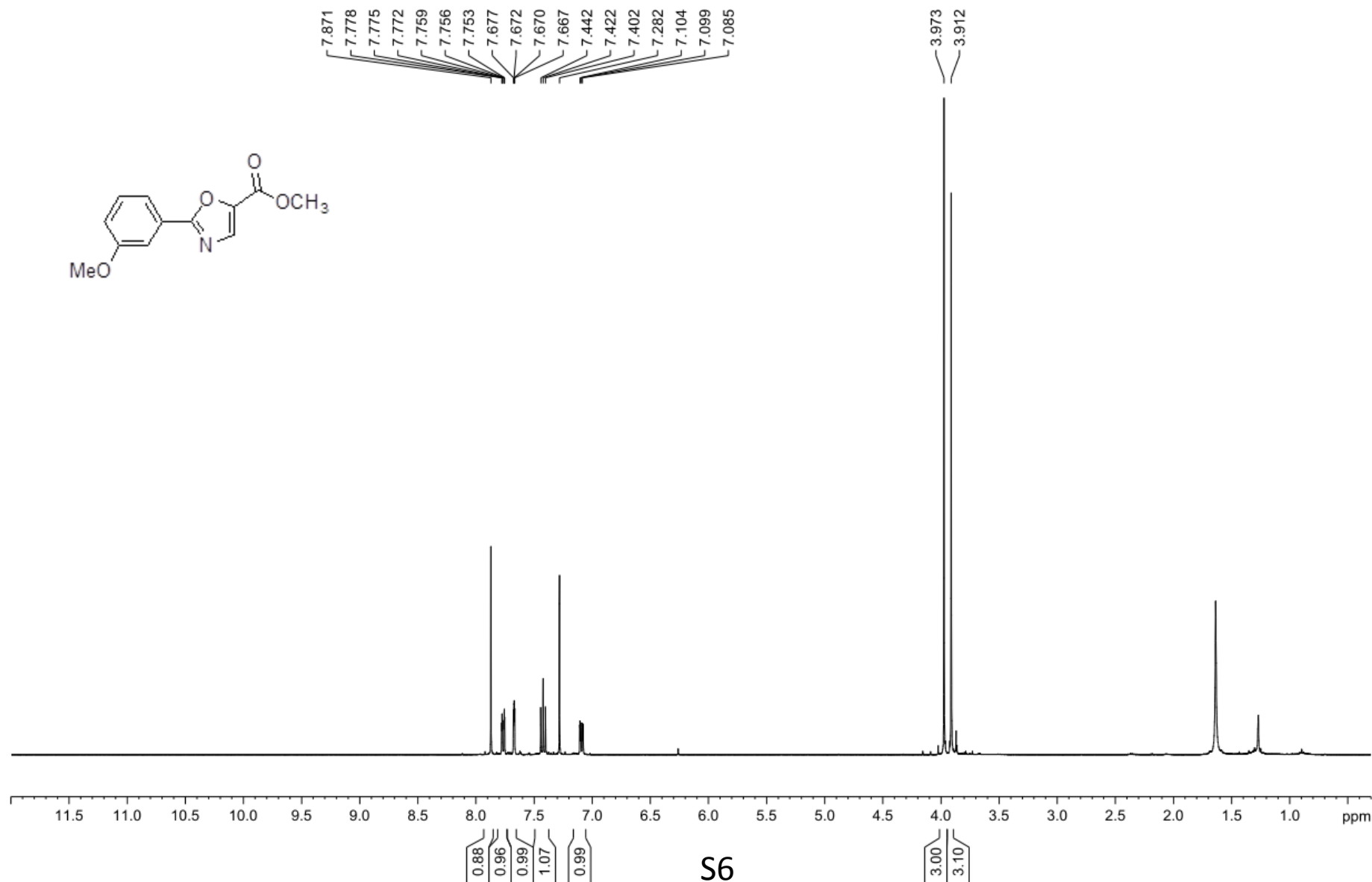
NP-DN-X 13C

Methyl 2-(4-methoxyphenyl)oxazole-5-carboxylate(2b)



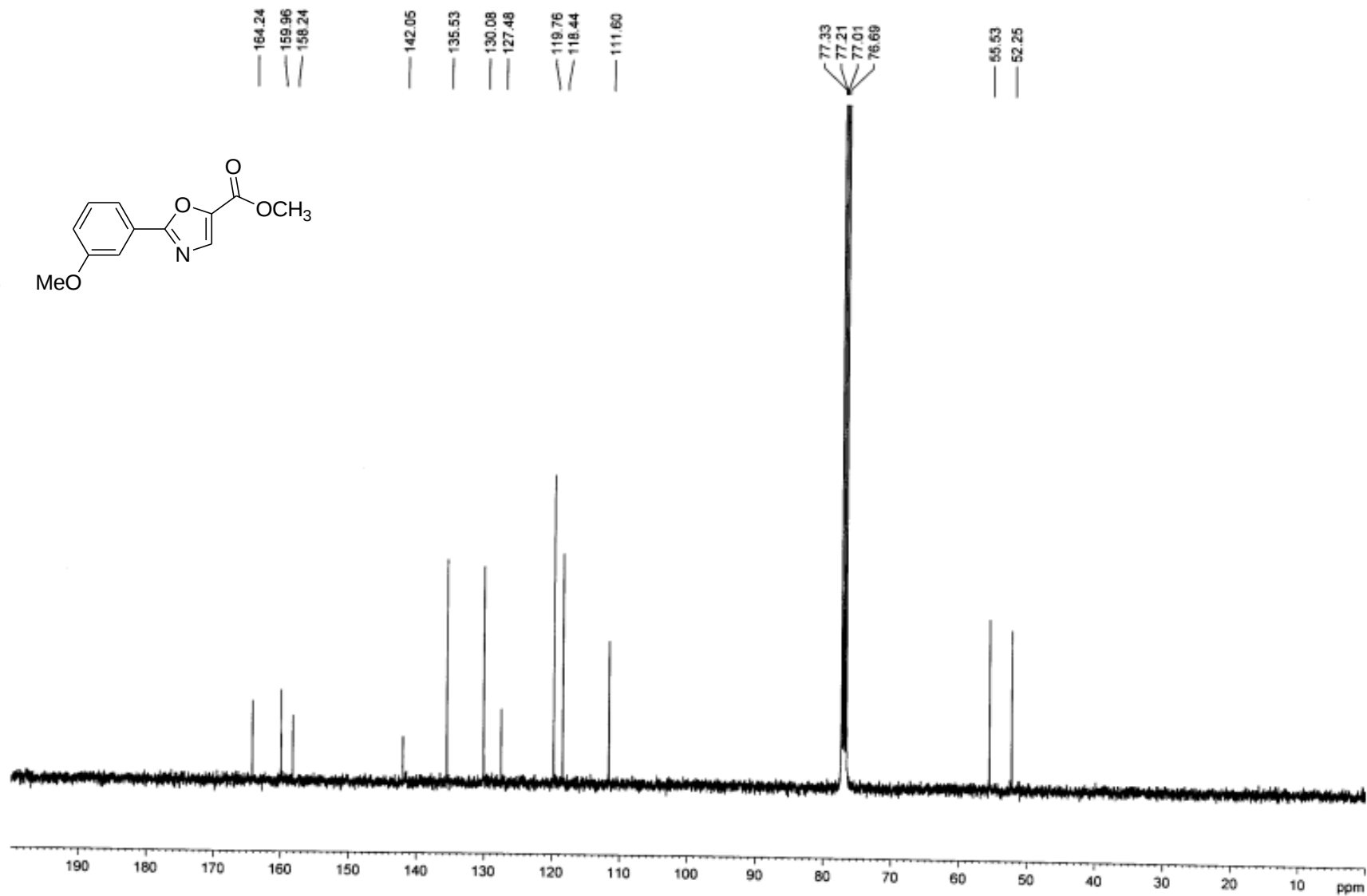
NP-DN-156

Methyl 2-(3-methoxyphenyl)oxazole-5-carboxylate(2c)

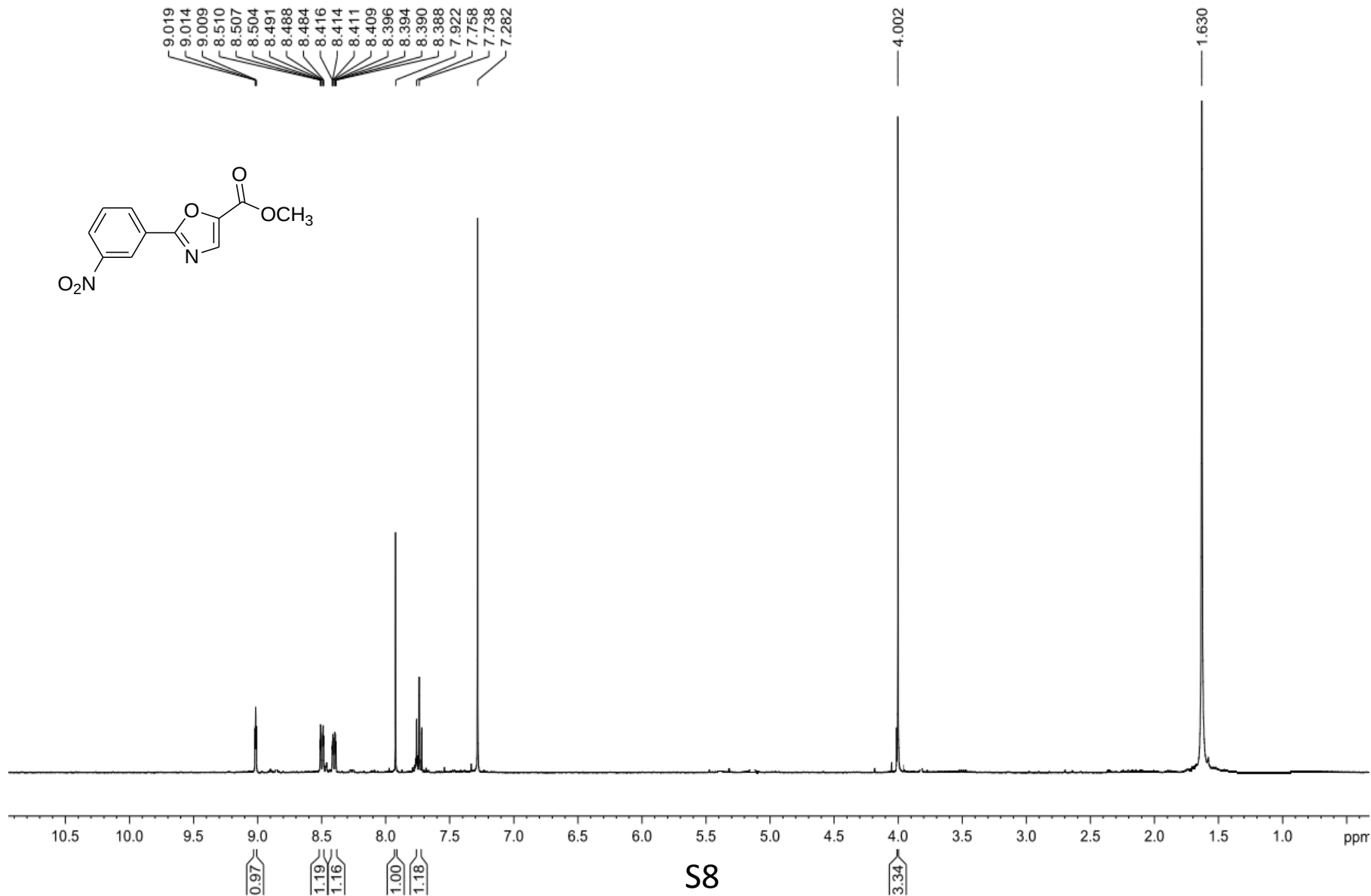
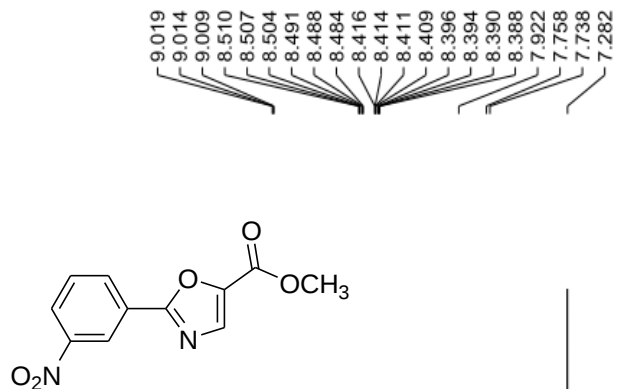


NP-DN-156-13C-2

Methyl 2-(3-methoxyphenyl)oxazole-5-carboxylate(2c)

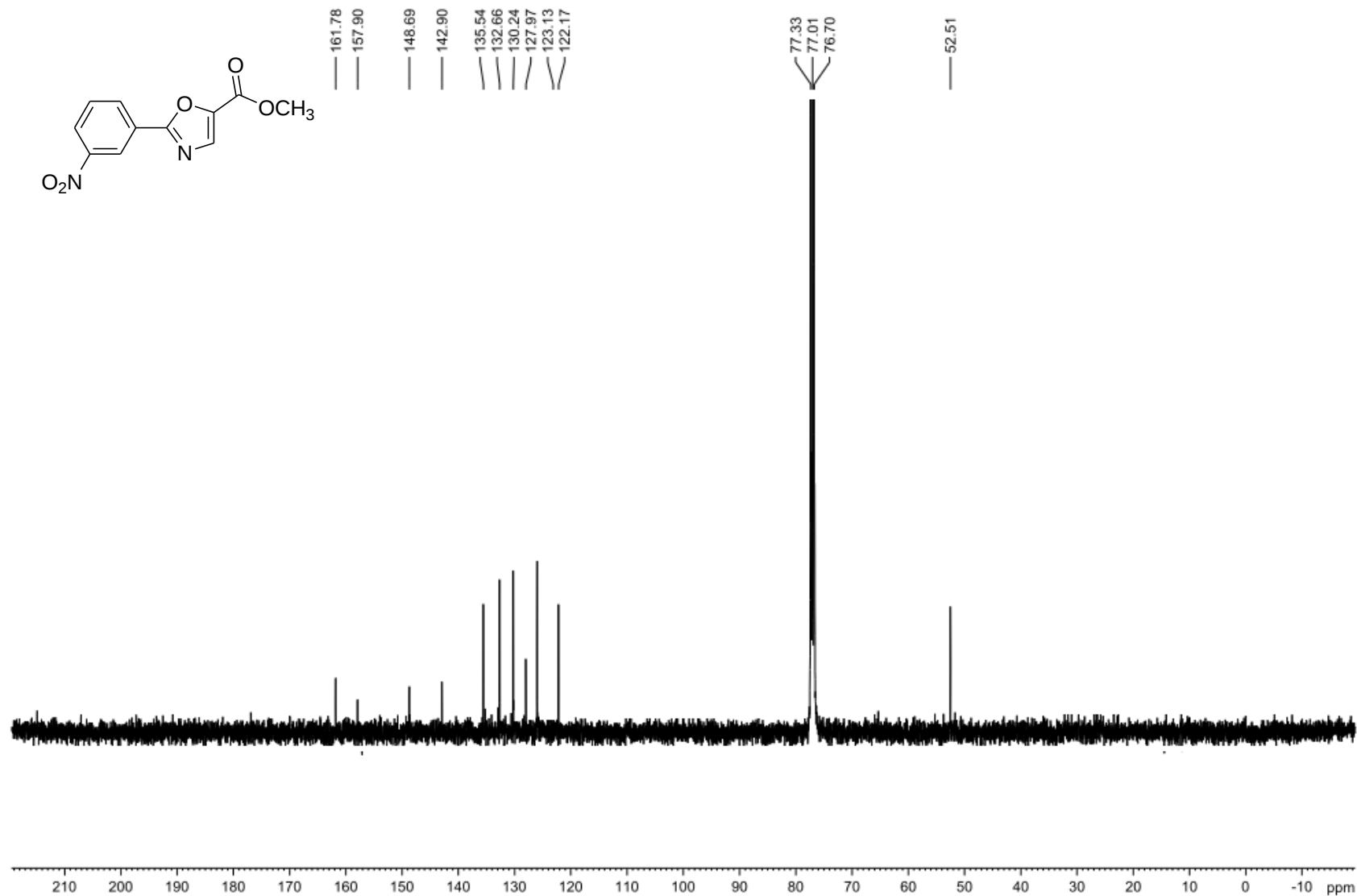
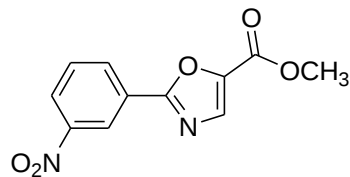


Methyl 2-(3-nitrophenyl)oxazole-5-carboxylate(2d)

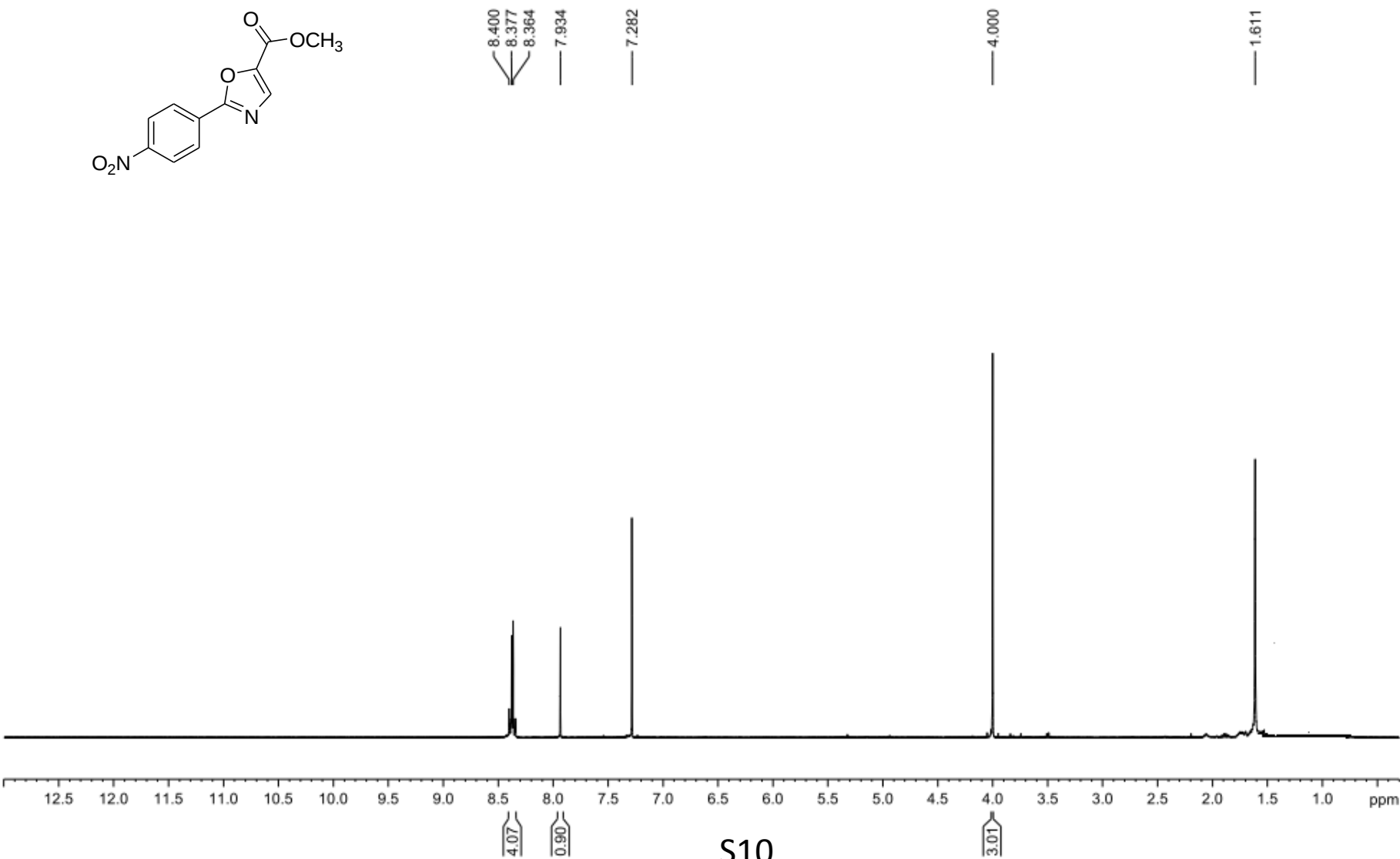
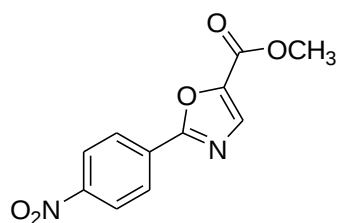


NP-DN-129 13C

Methyl 2-(3-nitrophenyl)oxazole-5-carboxylate(2d)

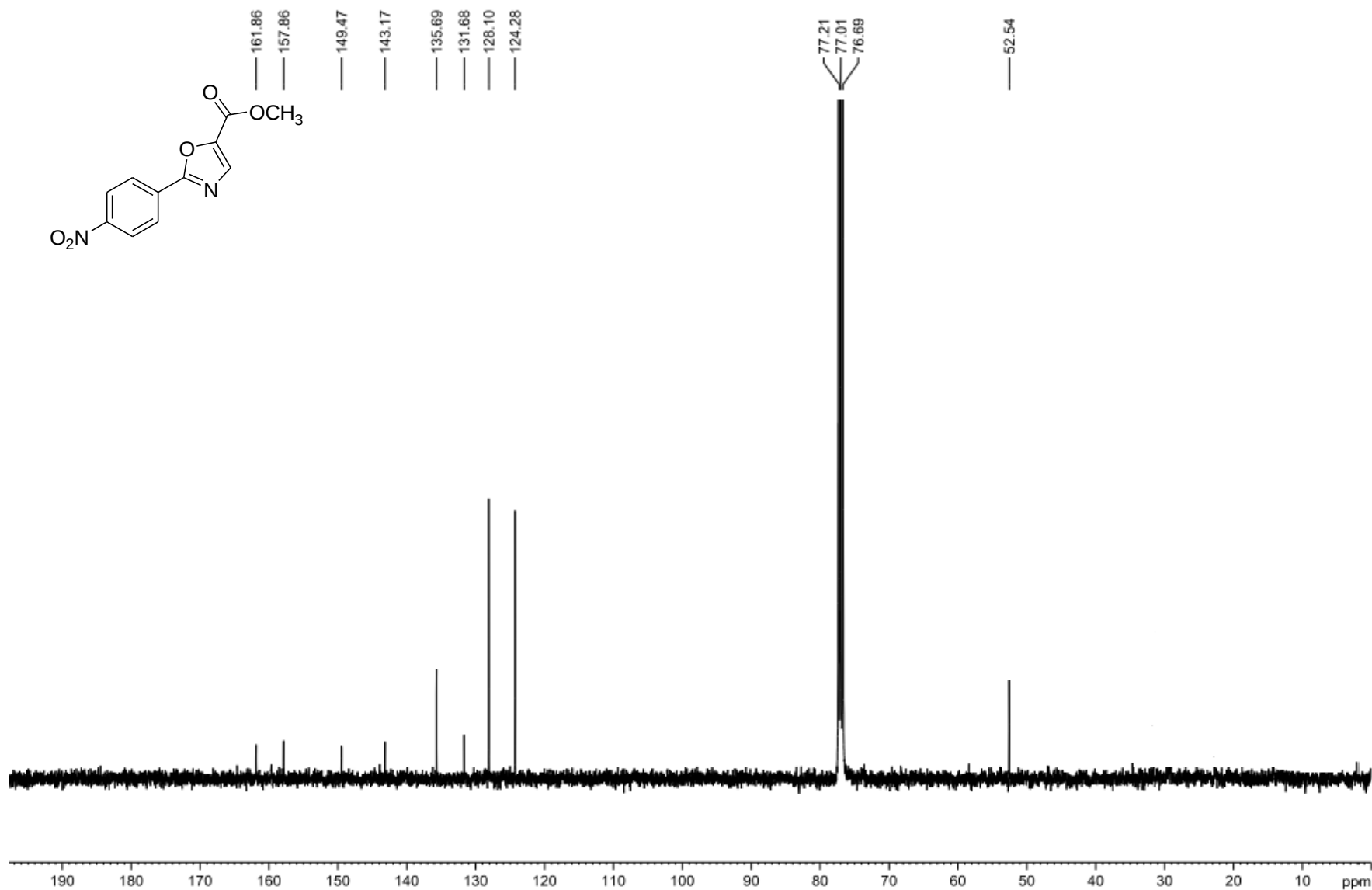
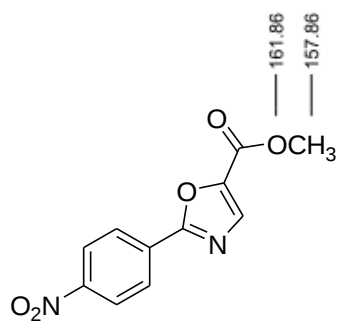


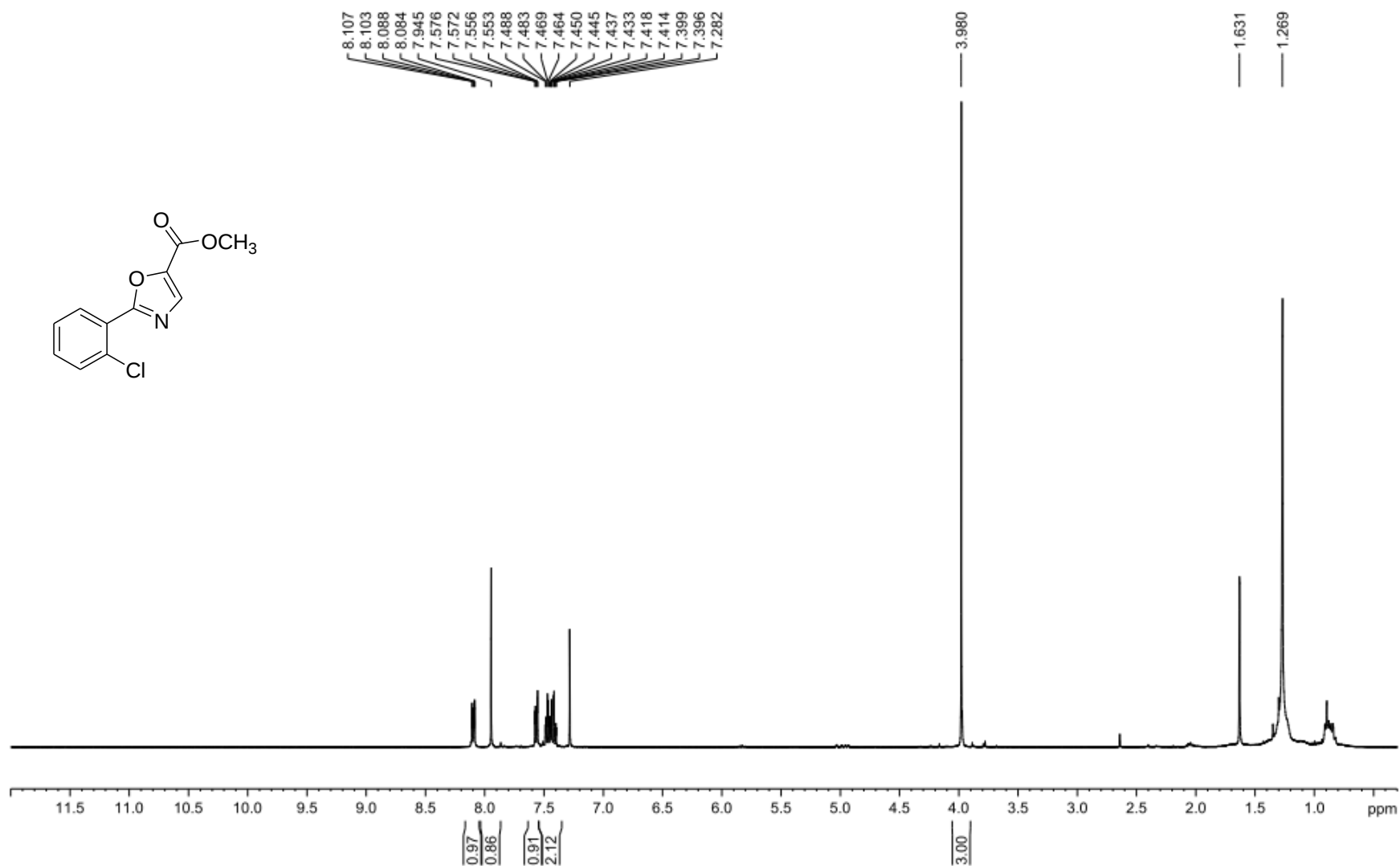
Methyl 2-(4-nitrophenyl)oxazole-5-carboxylate(2e)



S10

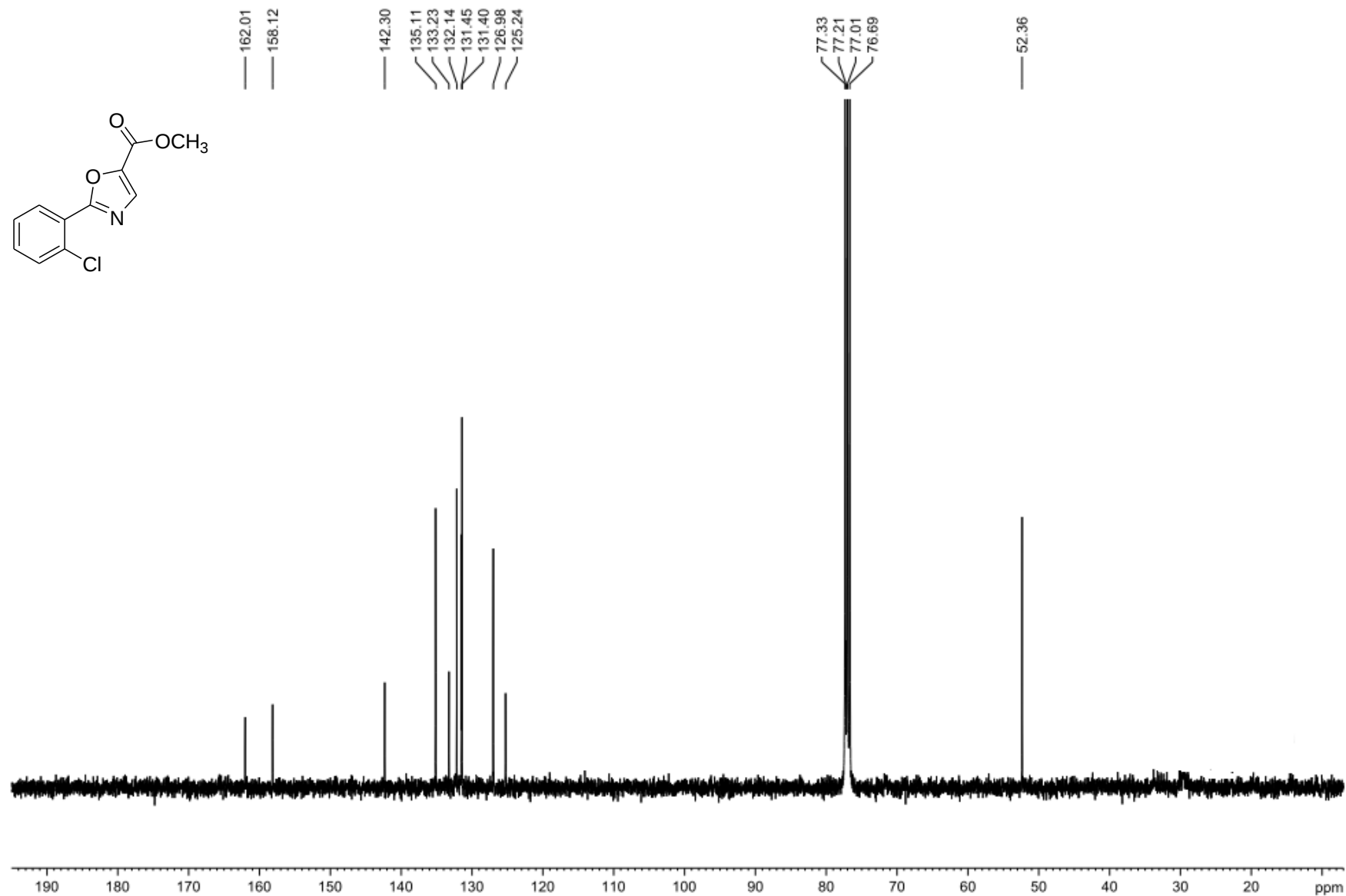
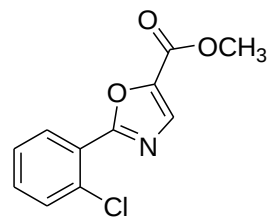
Methyl 2-(4-nitrophenyl)oxazole-5-carboxylate(2e)



Methyl 2-(2-chlorophenyl)oxazole-5-carboxylate(2f)

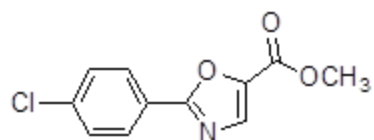
NP-MR-417-13C

Methyl 2-(2-chlorophenyl)oxazole-5-carboxylate(2f)



NP-DN-101

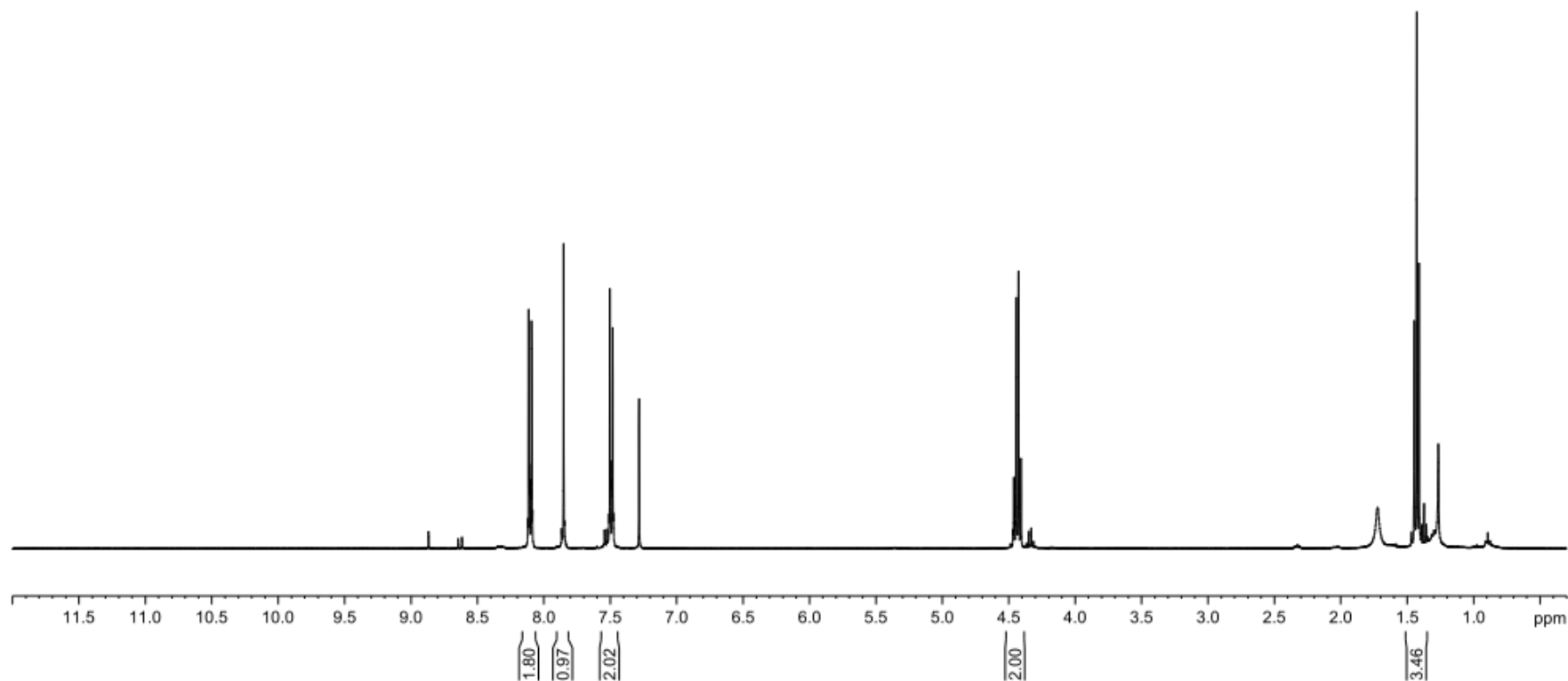
Ethyl 2-(4-chlorophenyl)oxazole-5-carboxylate(2g)



8.113
8.108
8.096
8.091
7.850
7.502
7.497
7.485
7.480
7.282

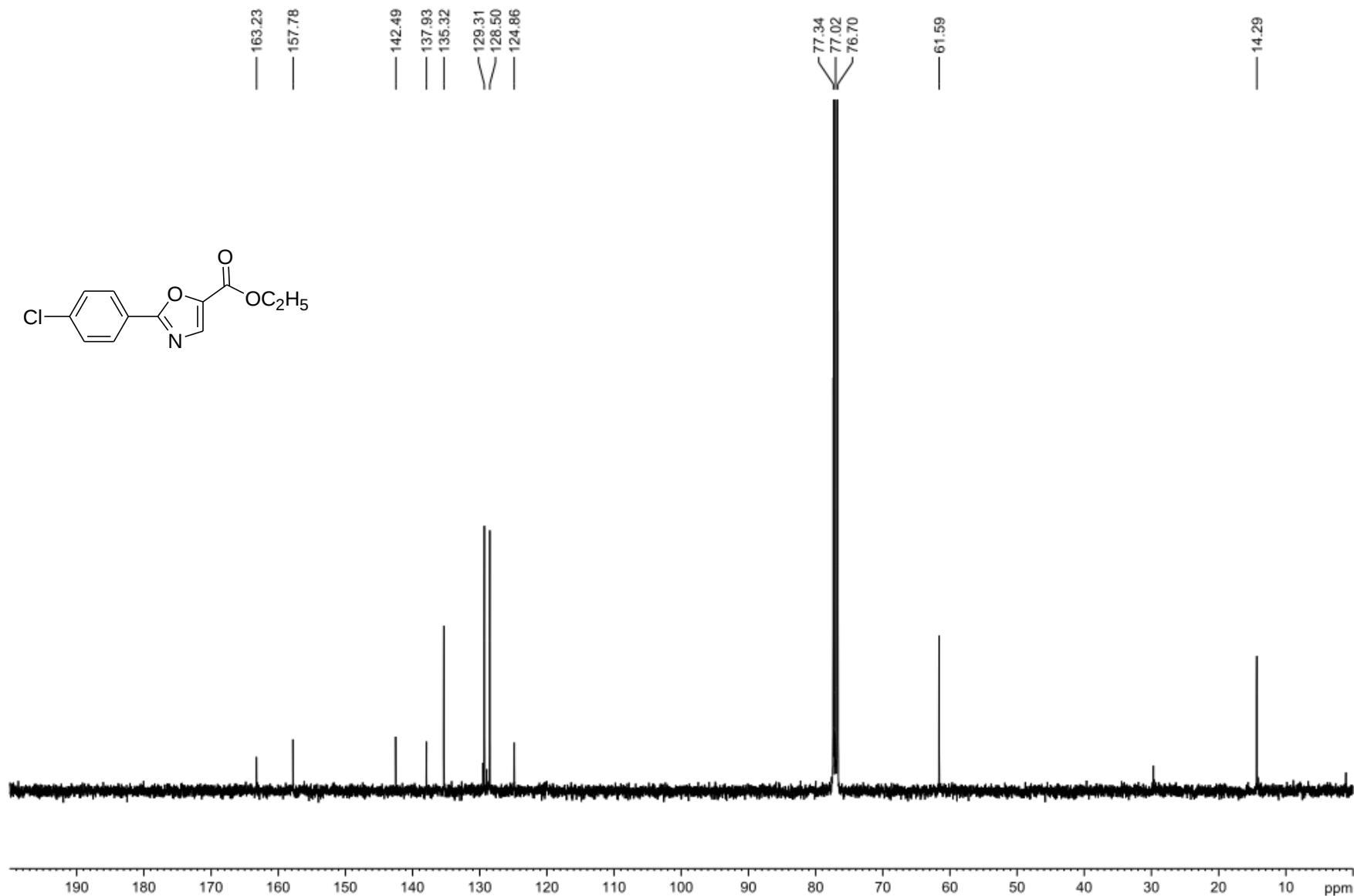
4.462
4.444
4.426
4.409

1.446
1.429
1.411



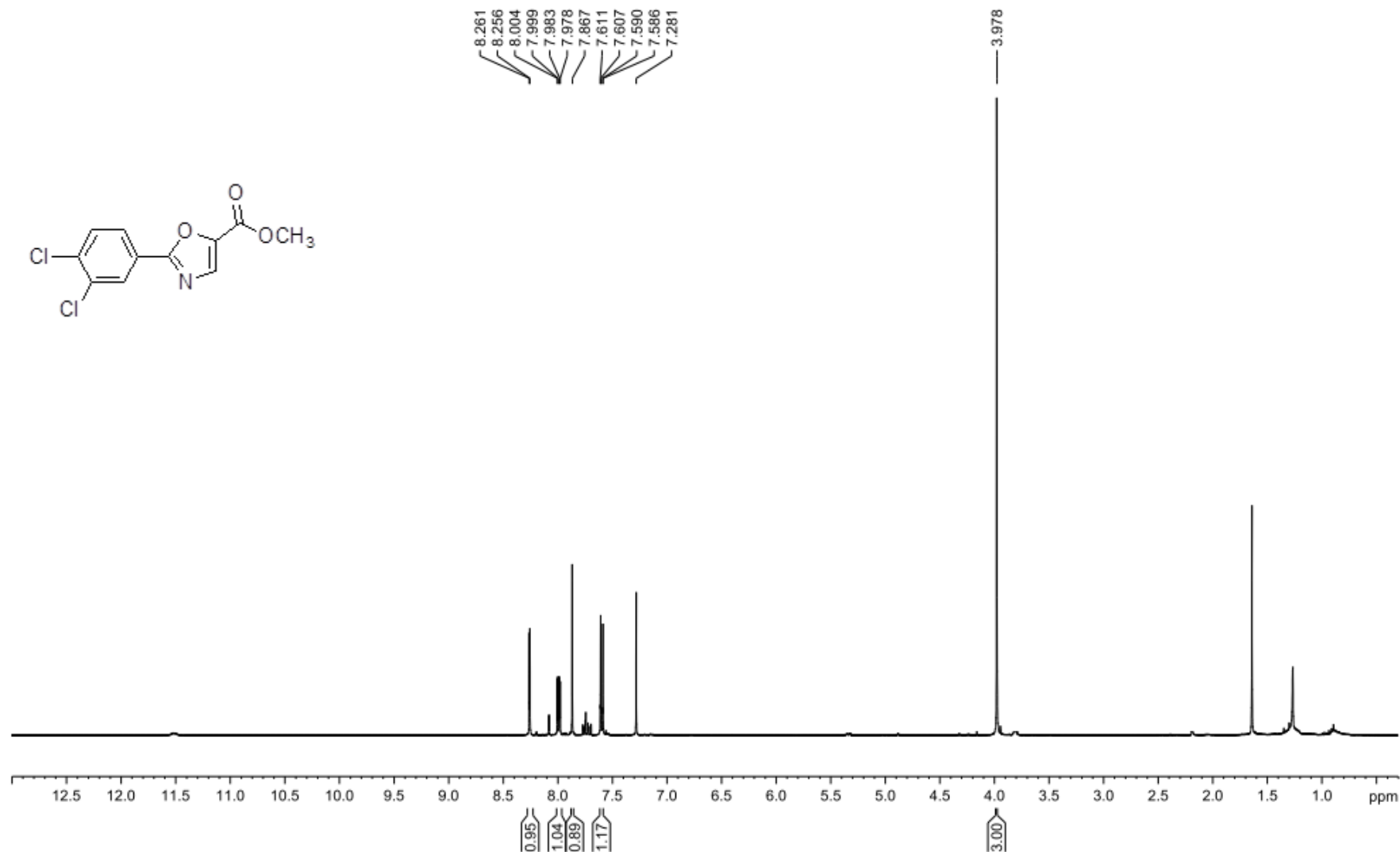
NP-DN-101-13C

Ethyl 2-(4-chlorophenyl)oxazole-5-carboxylate(2g)



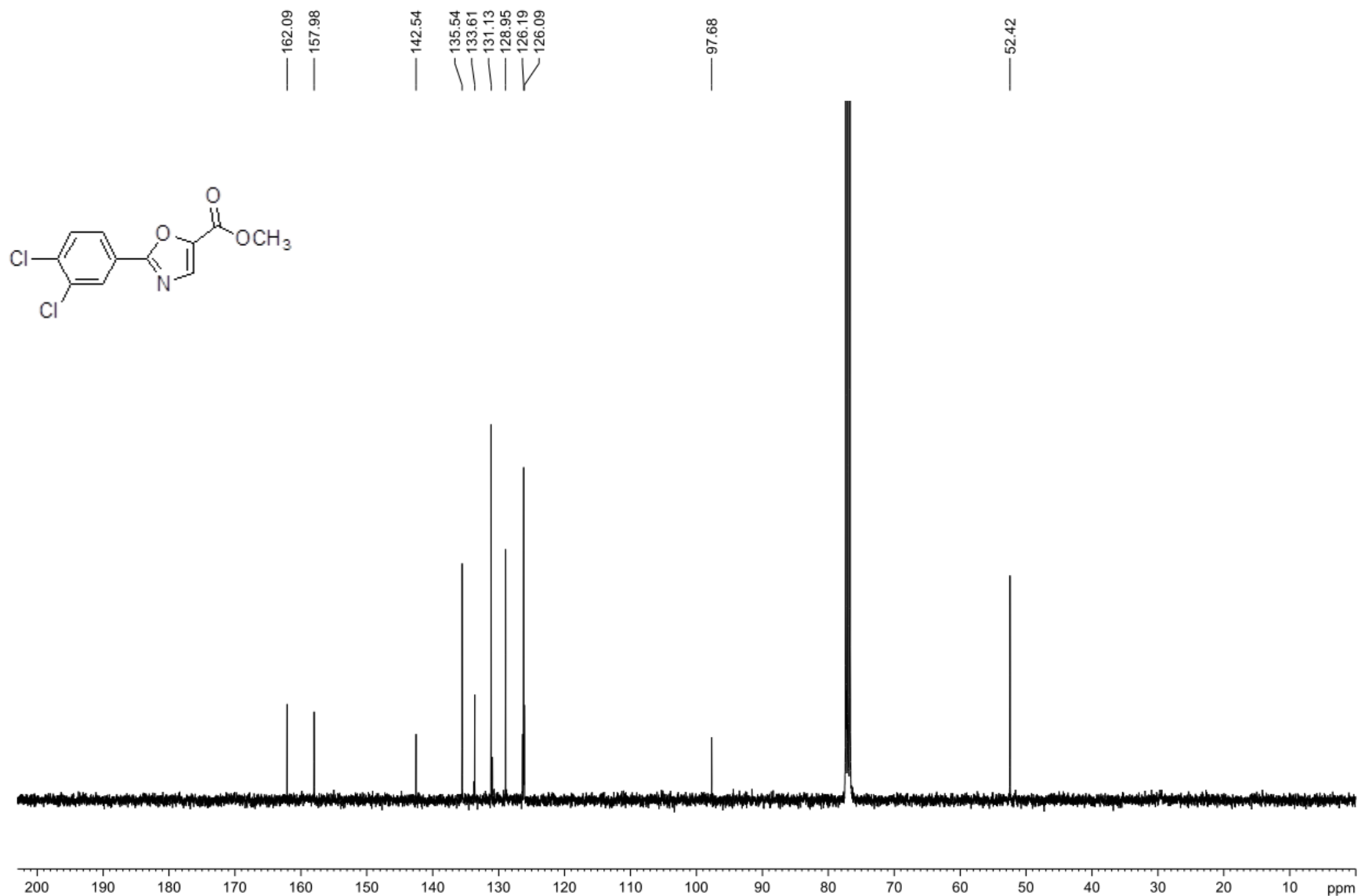
NP-MR-672 1H

Methyl 2-(3,4-dichlorophenyl)oxazole-5-carboxylate(2h)



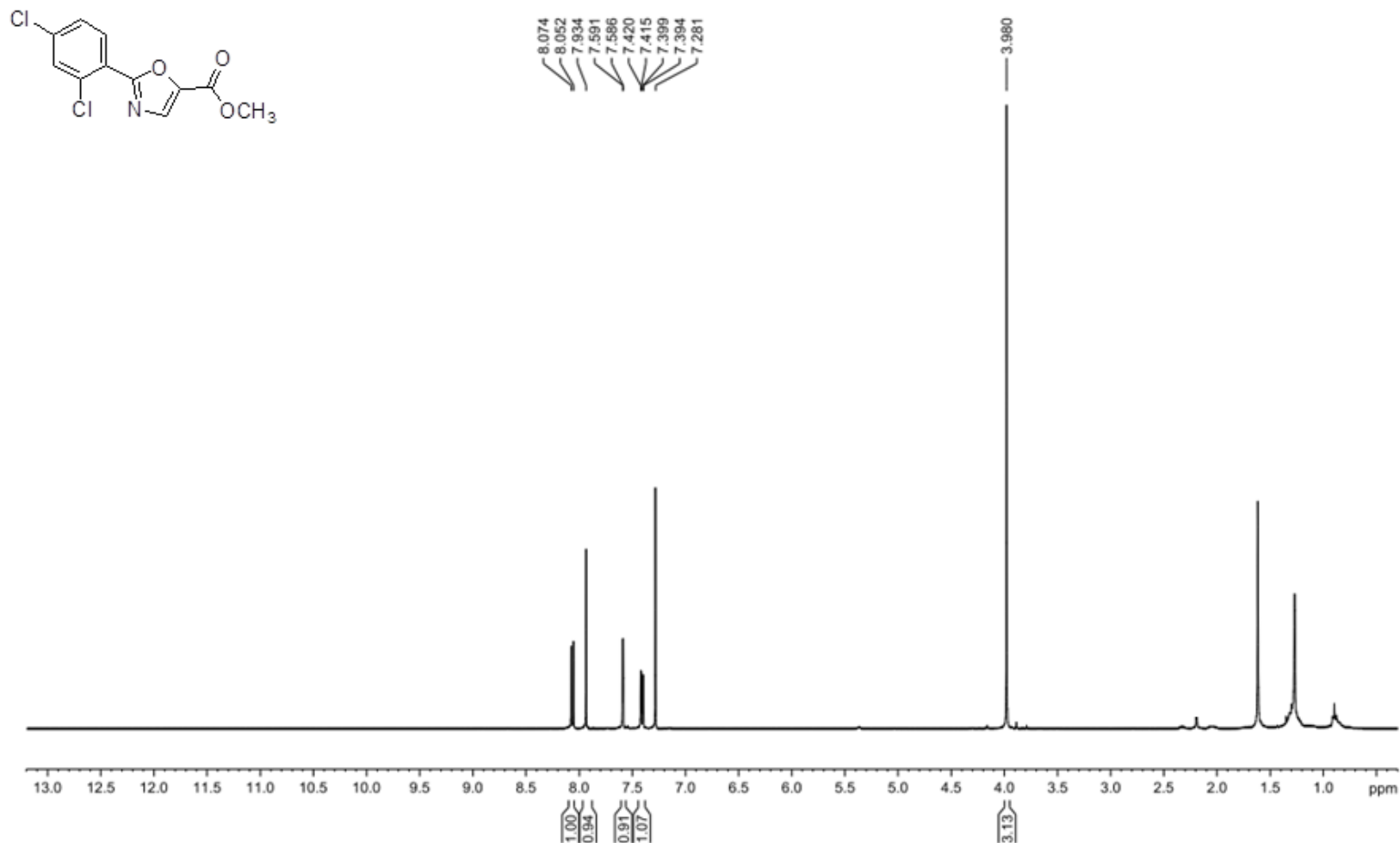
Methyl 2-(3,4-dichlorophenyl)oxazole-5-carboxylate(2h)

NP-MR-67213C



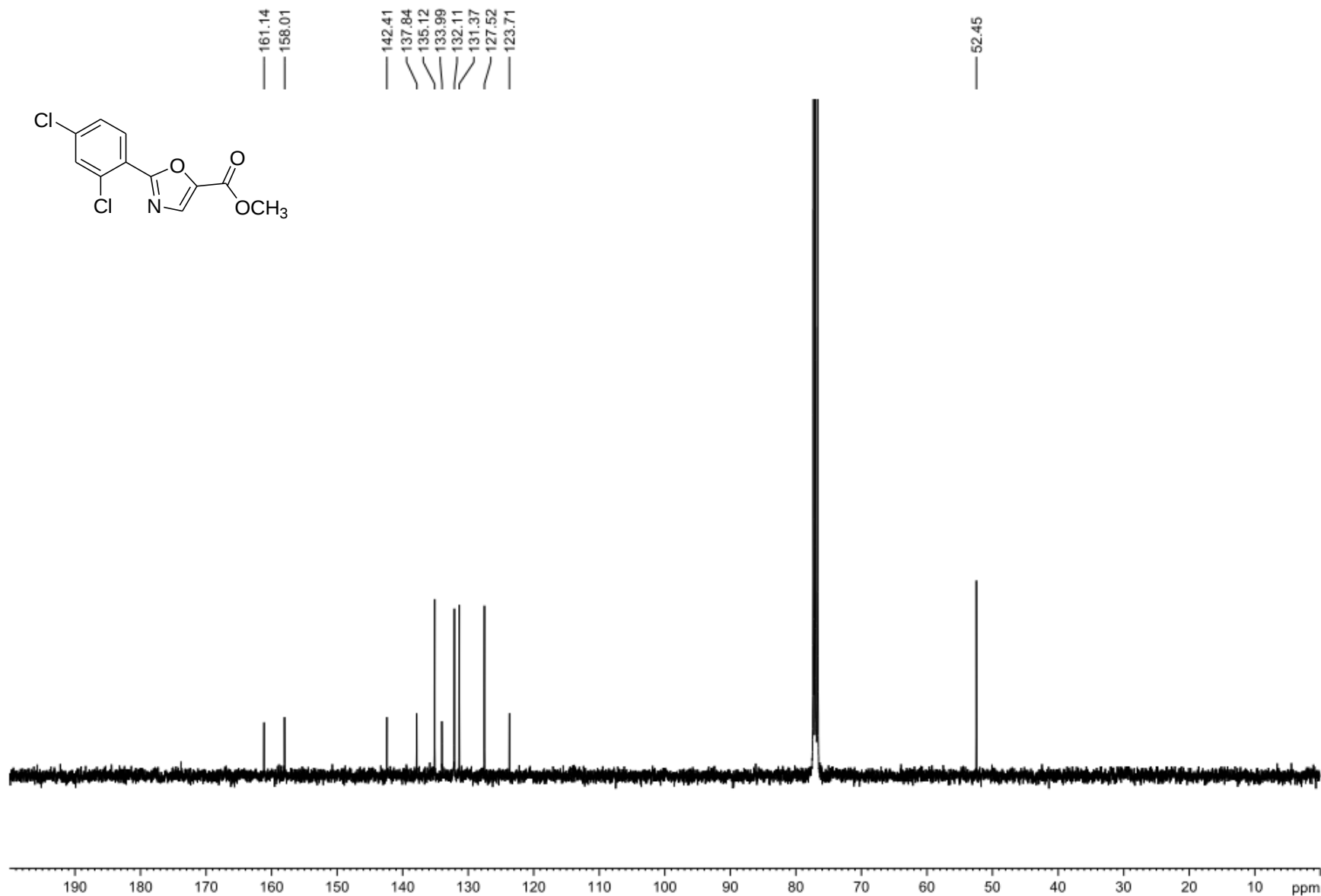
Methyl 2-(2,4-dichlorophenyl)oxazole-5-carboxylate(2i)

NP-MR-674 1H

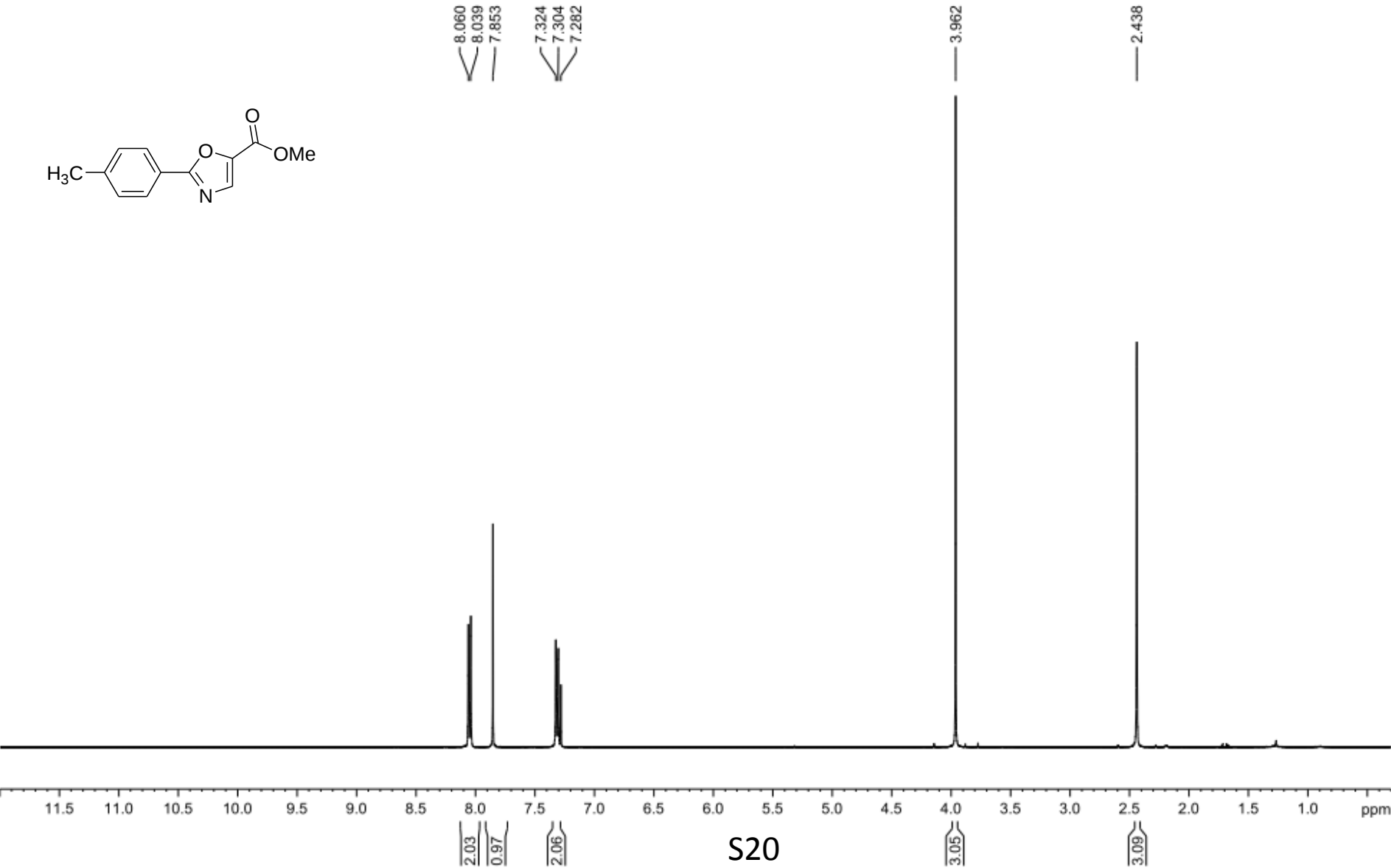
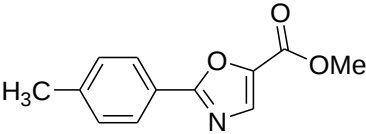


NP-MR-674 13C

Methyl 2-(2,4-dichlorophenyl)oxazole-5-carboxylate(2i)

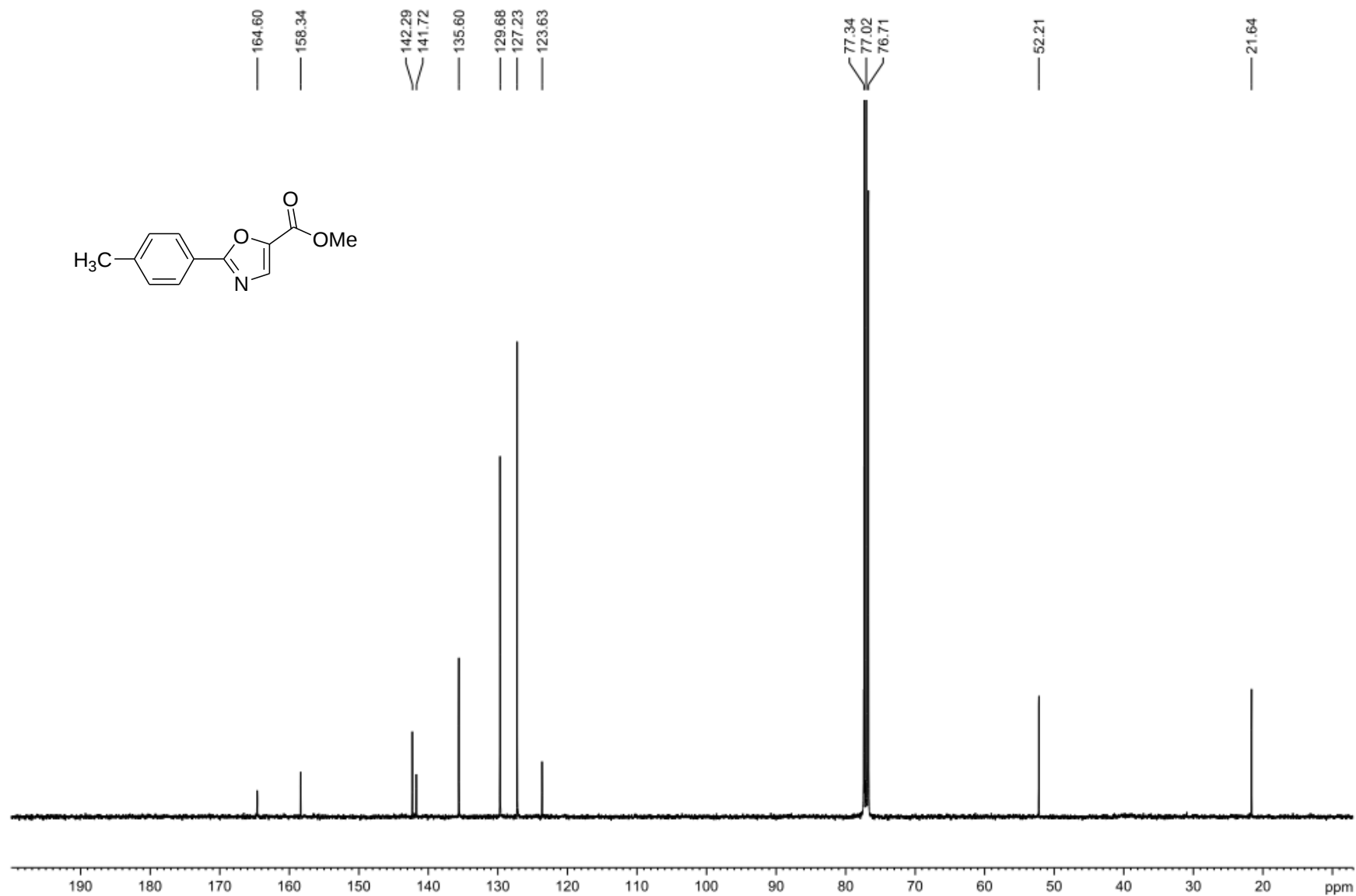


Methyl 2-p-tolylloxazole-5-carboxylate(2j)



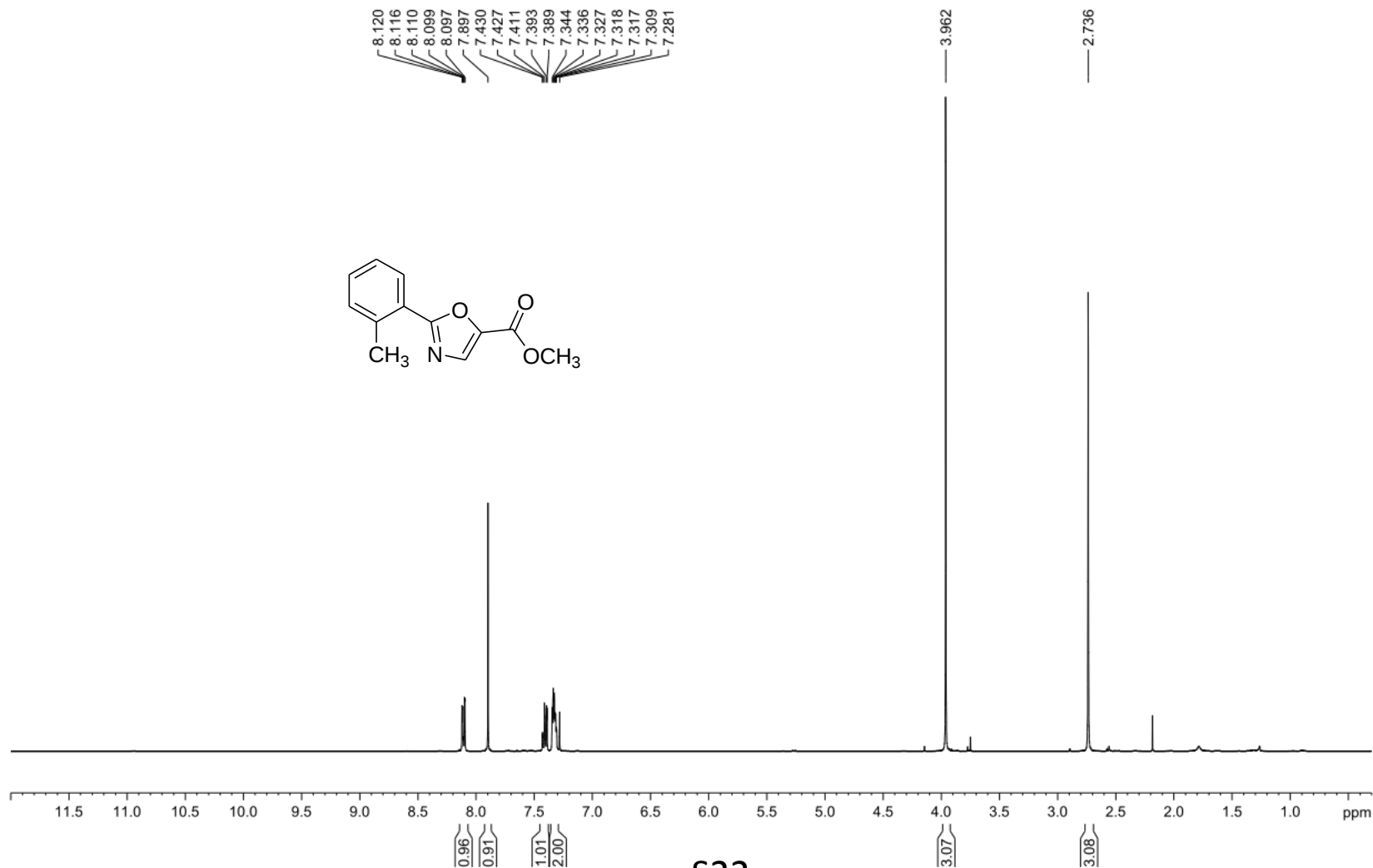
NP-MR-666-A 13C

Methyl 2-p-tolylloxazole-5-carboxylate(2j)



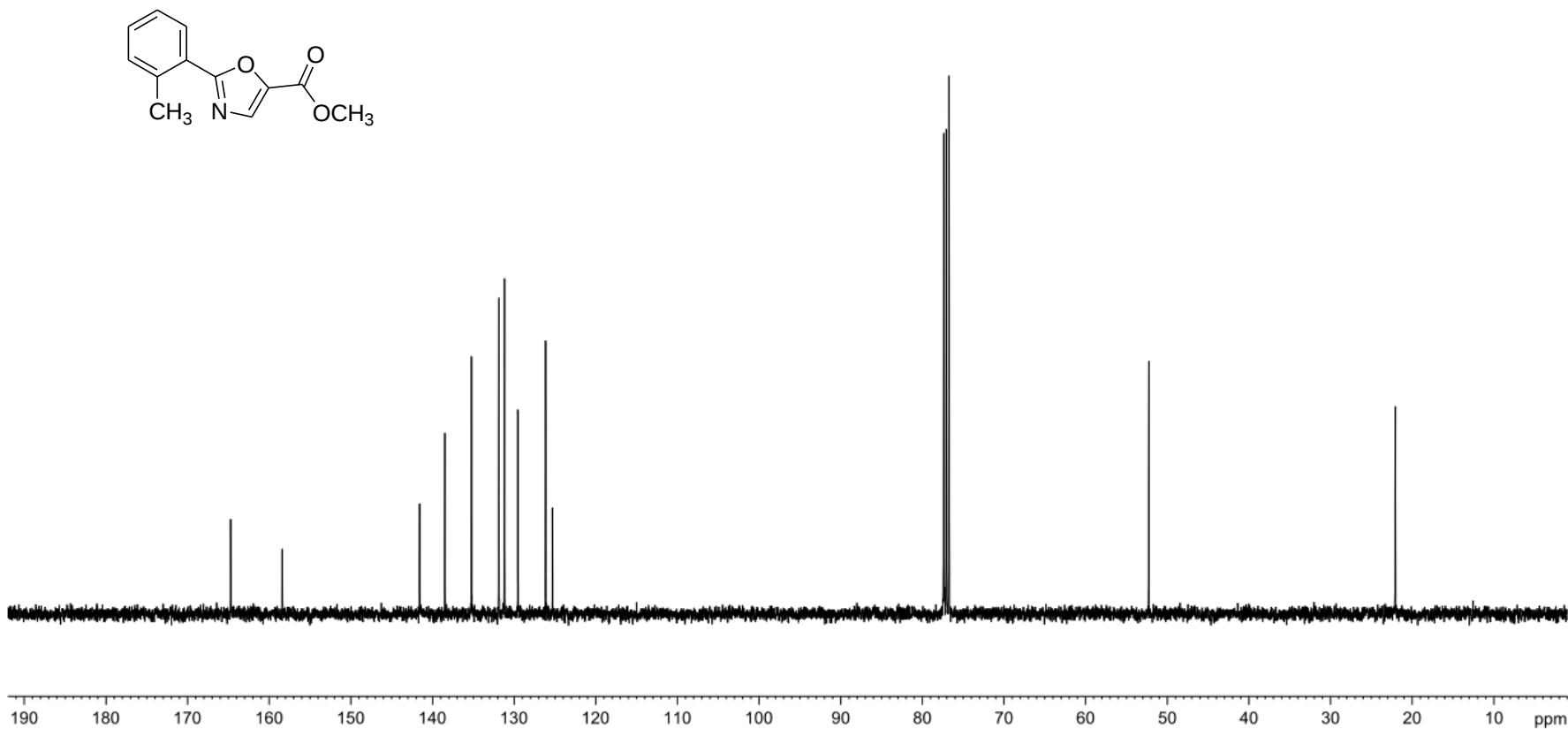
Methyl 2-o-tolylloxazole-5-carboxylate(2k)

NP-MR-tolumide oxazole



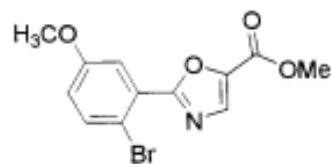
NP-MR-tolumide oxazole 13C

Methyl 2-o-tolyloxazole-5-carboxylate(2k)



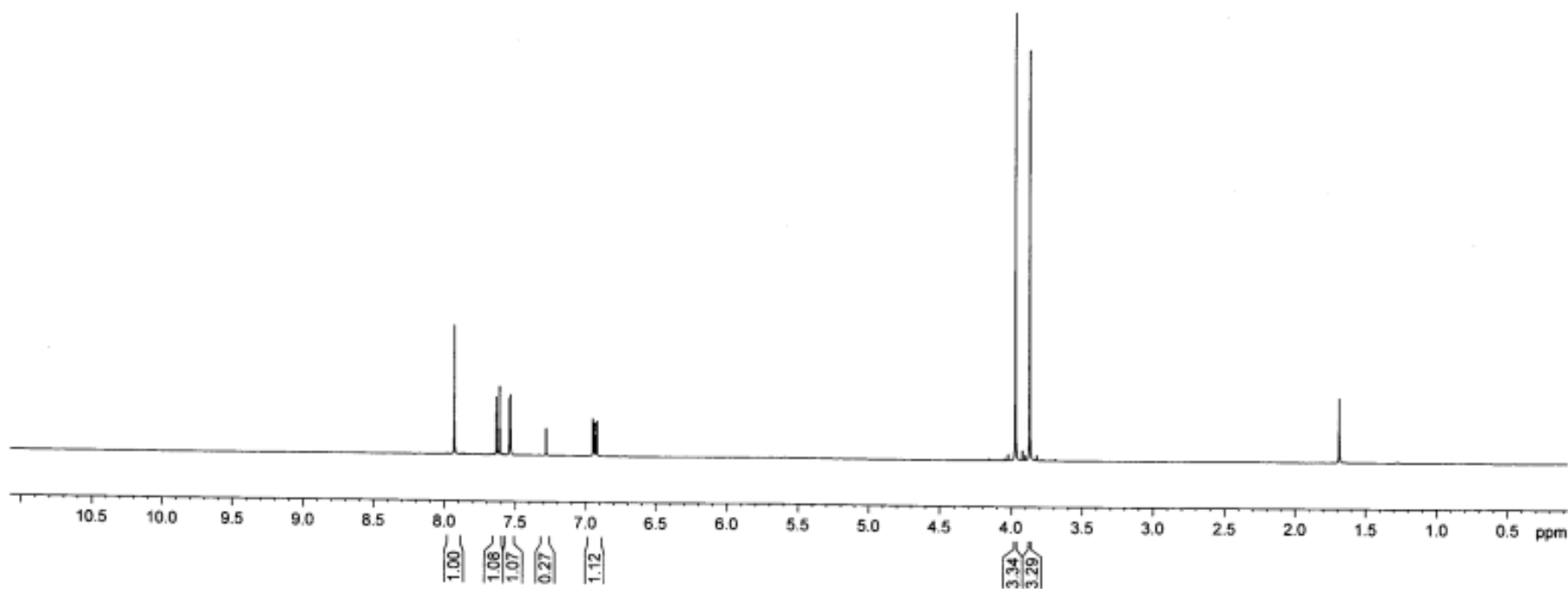
NP-DN-170-1H

Methyl 2-(2-bromo-5-methoxyphenyl)oxazole-5-carboxylate(2I)



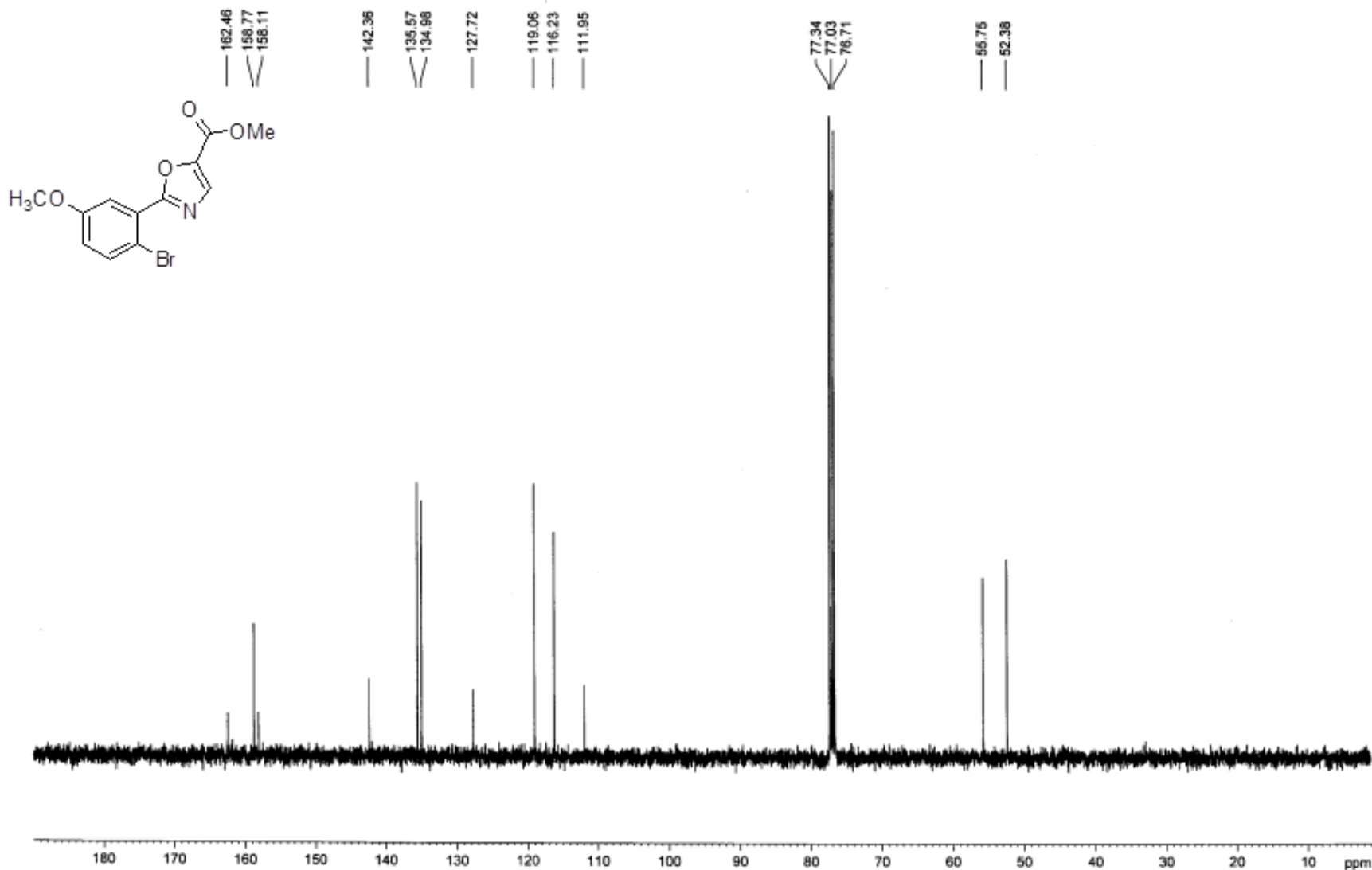
7.930
7.633
7.611
7.541
7.533
7.262
6.949
6.941
6.926
6.919

3.972
3.872

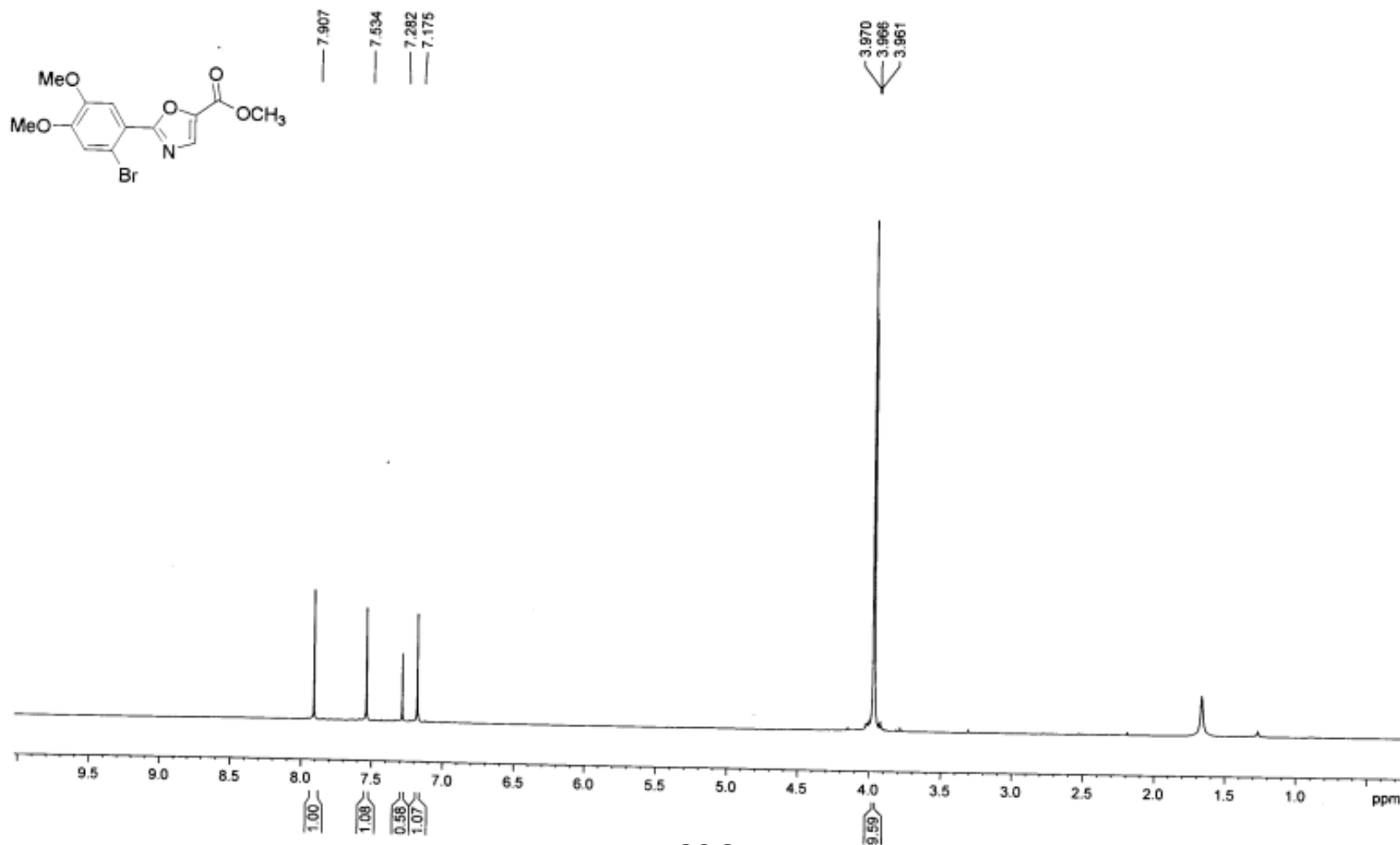


NP-DN-170-13C

Methyl 2-(2-bromo-5-methoxyphenyl)oxazole-5-carboxylate(2I)

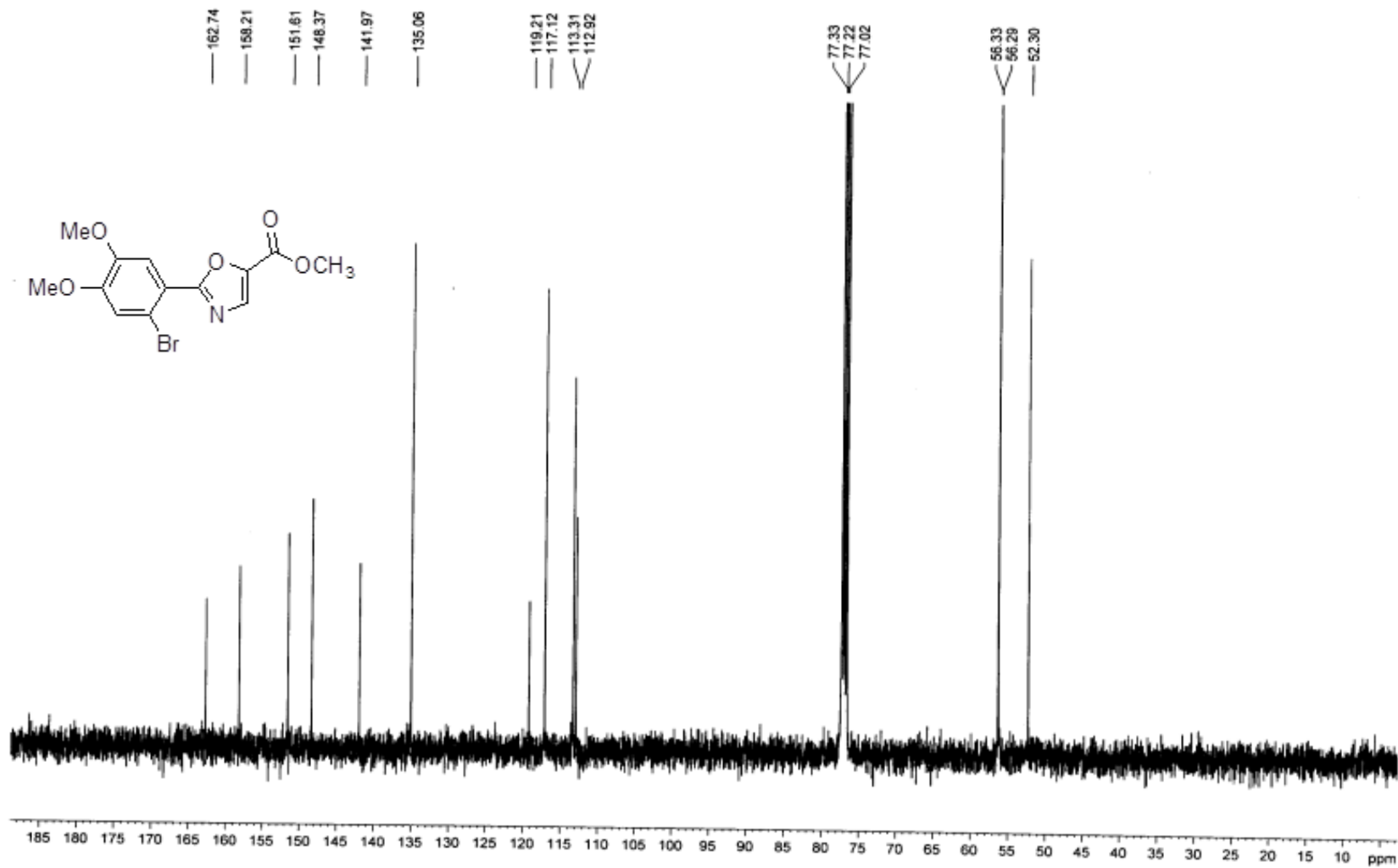


NP-DN-171-1H-CDC13 **Methyl 2-(2-bromo-4,5-dimethoxyphenyl)oxazole-5-carboxylate(2m)**

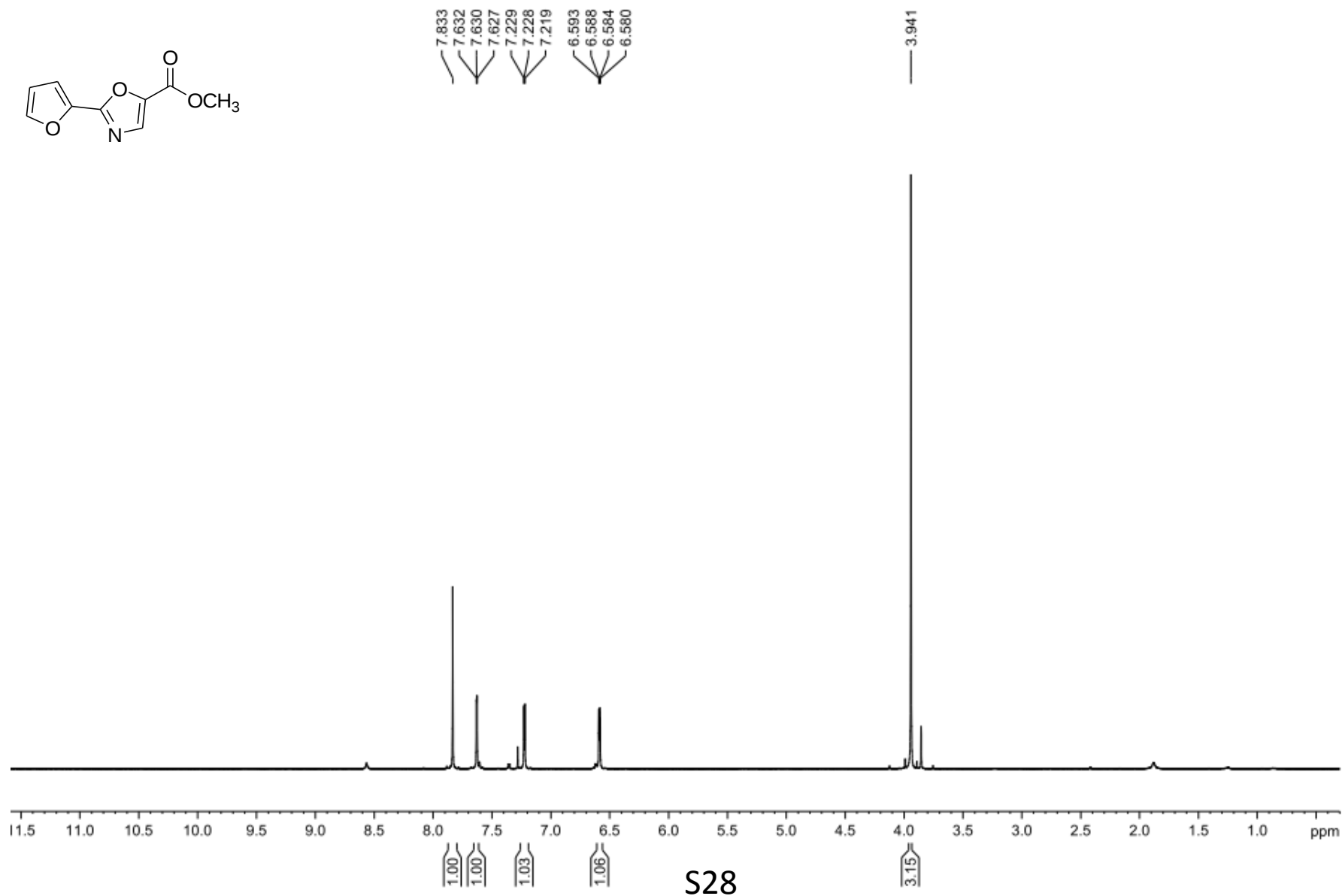
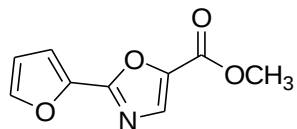


NP-DN-171-13C

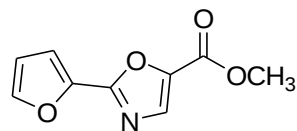
Methyl 2-(2-bromo-4,5-dimethoxyphenyl)oxazole-5-carboxylate(2m)



Methyl 2-(furan-2-yl)oxazole-5-carboxylate(2n)



Methyl 2-(furan-2-yl)oxazole-5-carboxylate(2n)



158.02
156.54

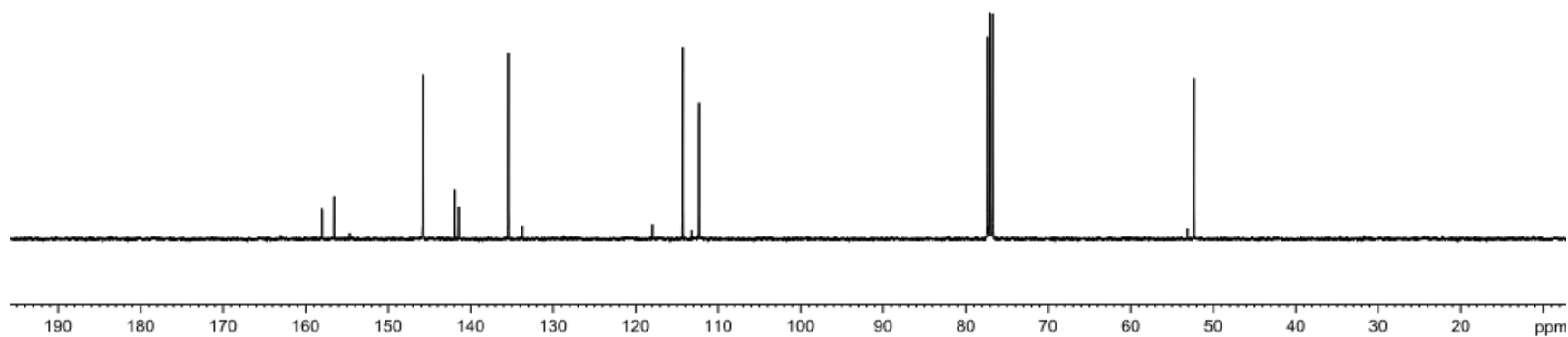
145.79
141.90
141.43

135.44

114.29
112.29

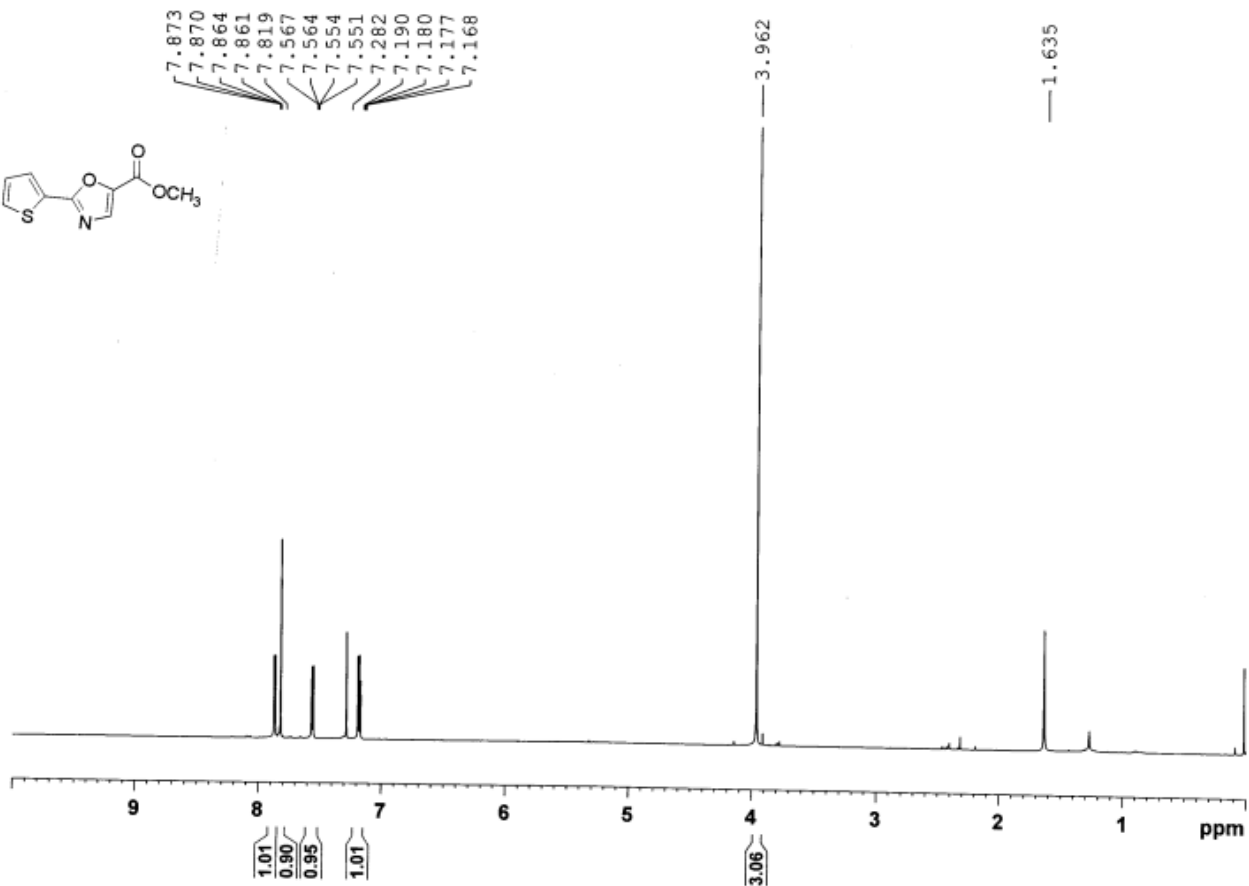
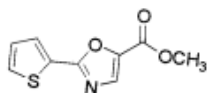
77.38
77.06
76.75

52.34



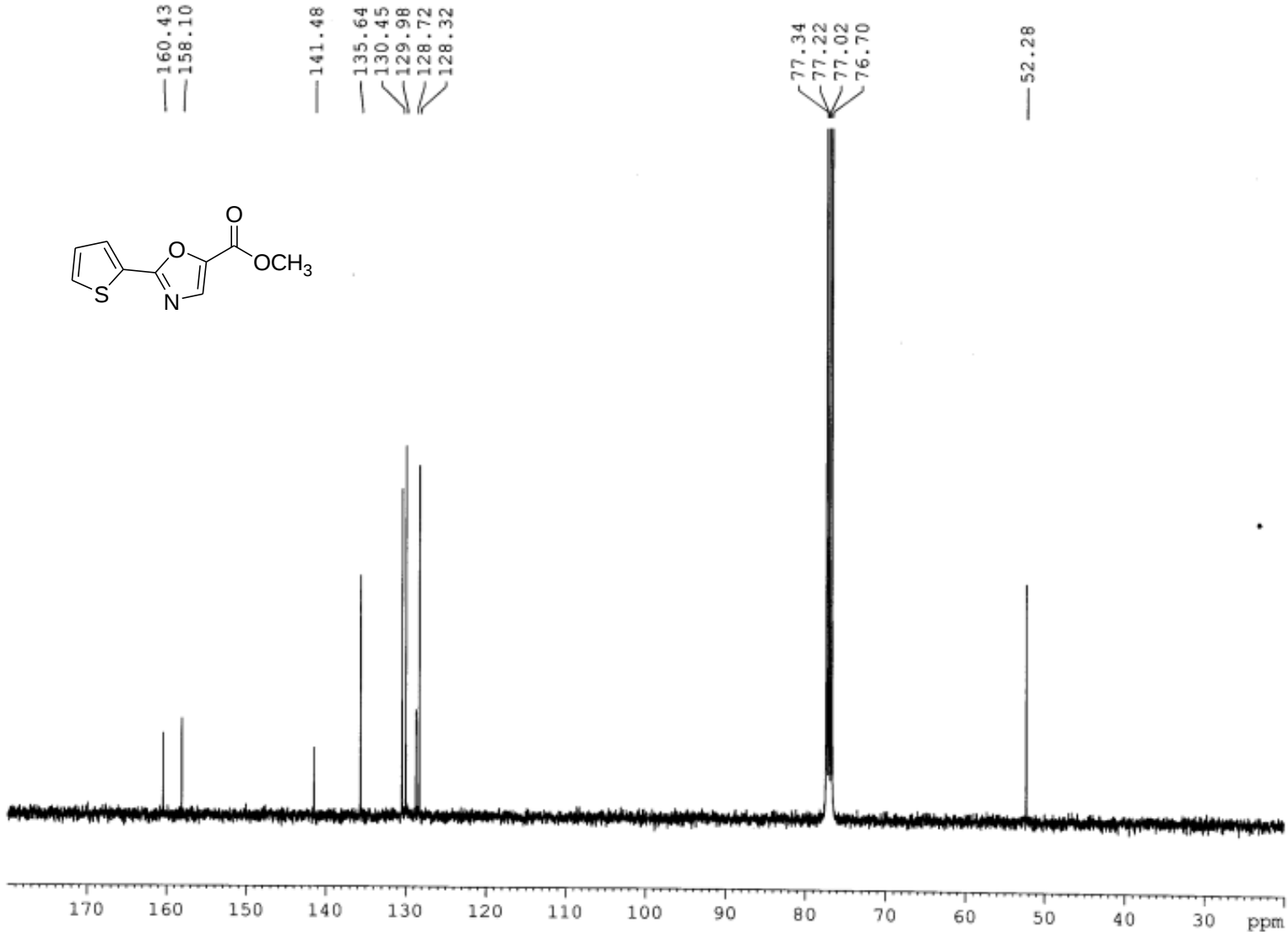
Methyl 2-(thiophen-2-yl)oxazole-5-carboxylate(2o)

NP-MR-417-A



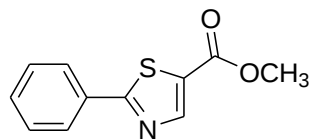
Methyl 2-(thiophen-2-yl)oxazole-5-carboxylate(2o)

NP-MR-417-A-13C



NP-MR-Thioxazole 1H

Methyl 2-phenylthiazole-5-carboxylate(2p)

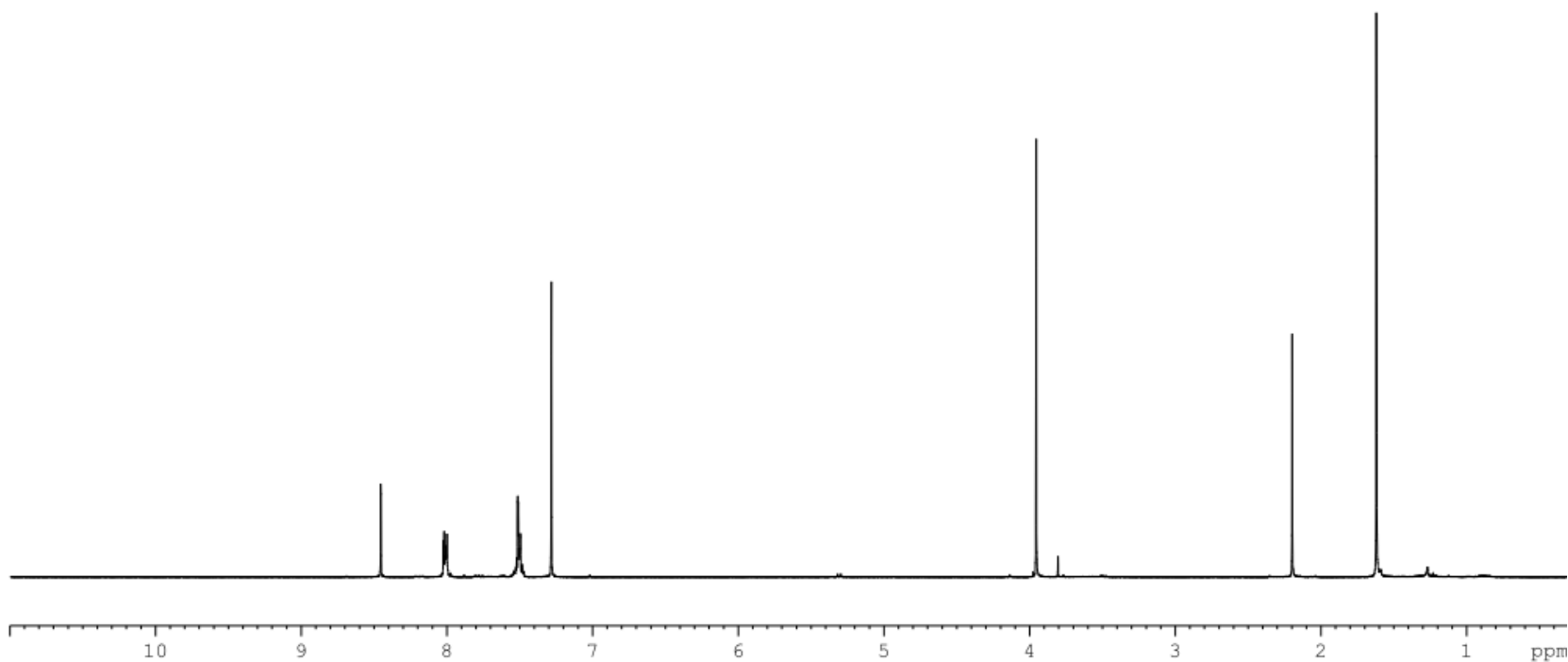


8.452
8.022
8.018
8.012
8.009
8.005
7.998
7.520
7.512
7.508
7.502
7.498
7.494
7.282

3.955

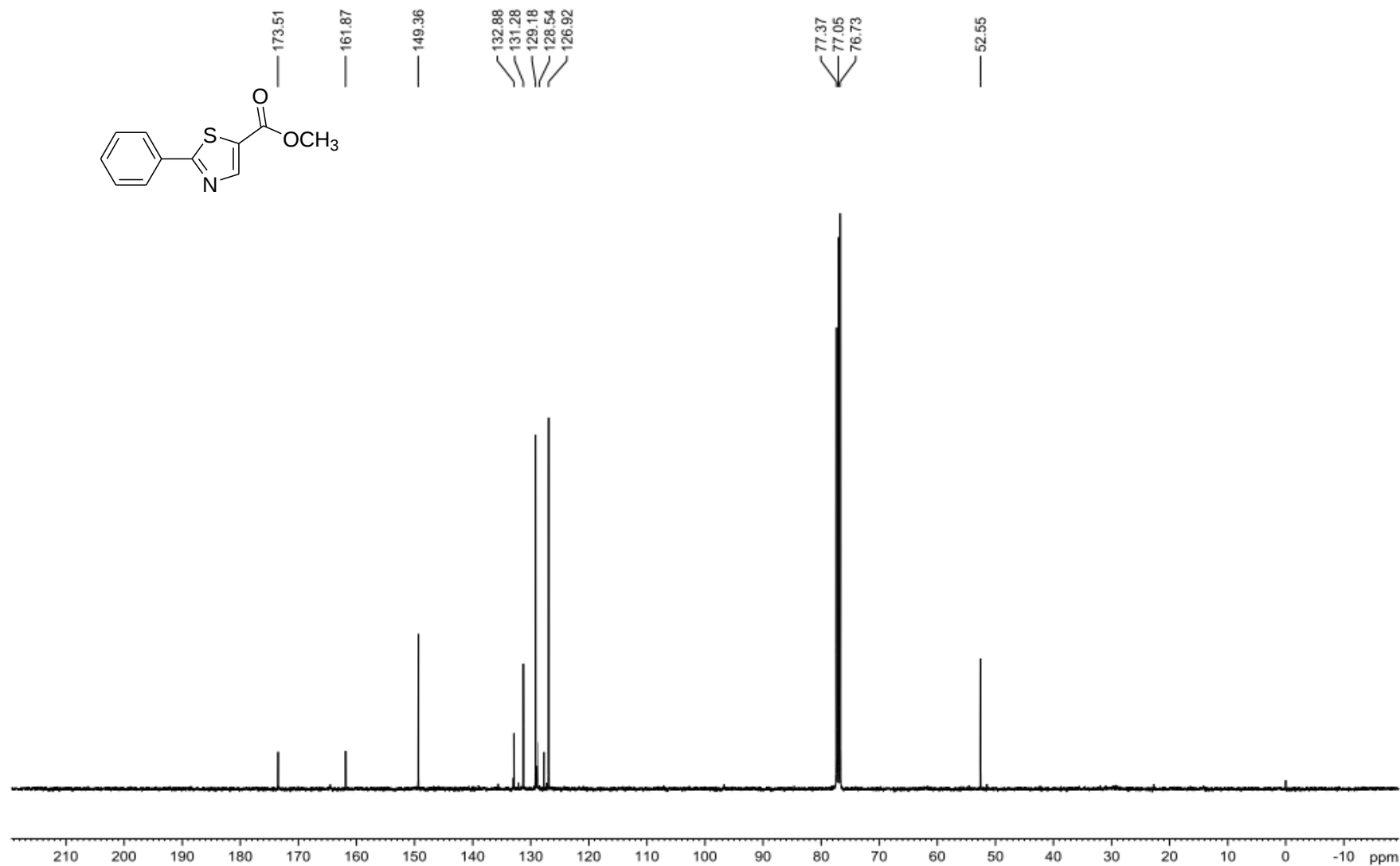
2.196

1.619



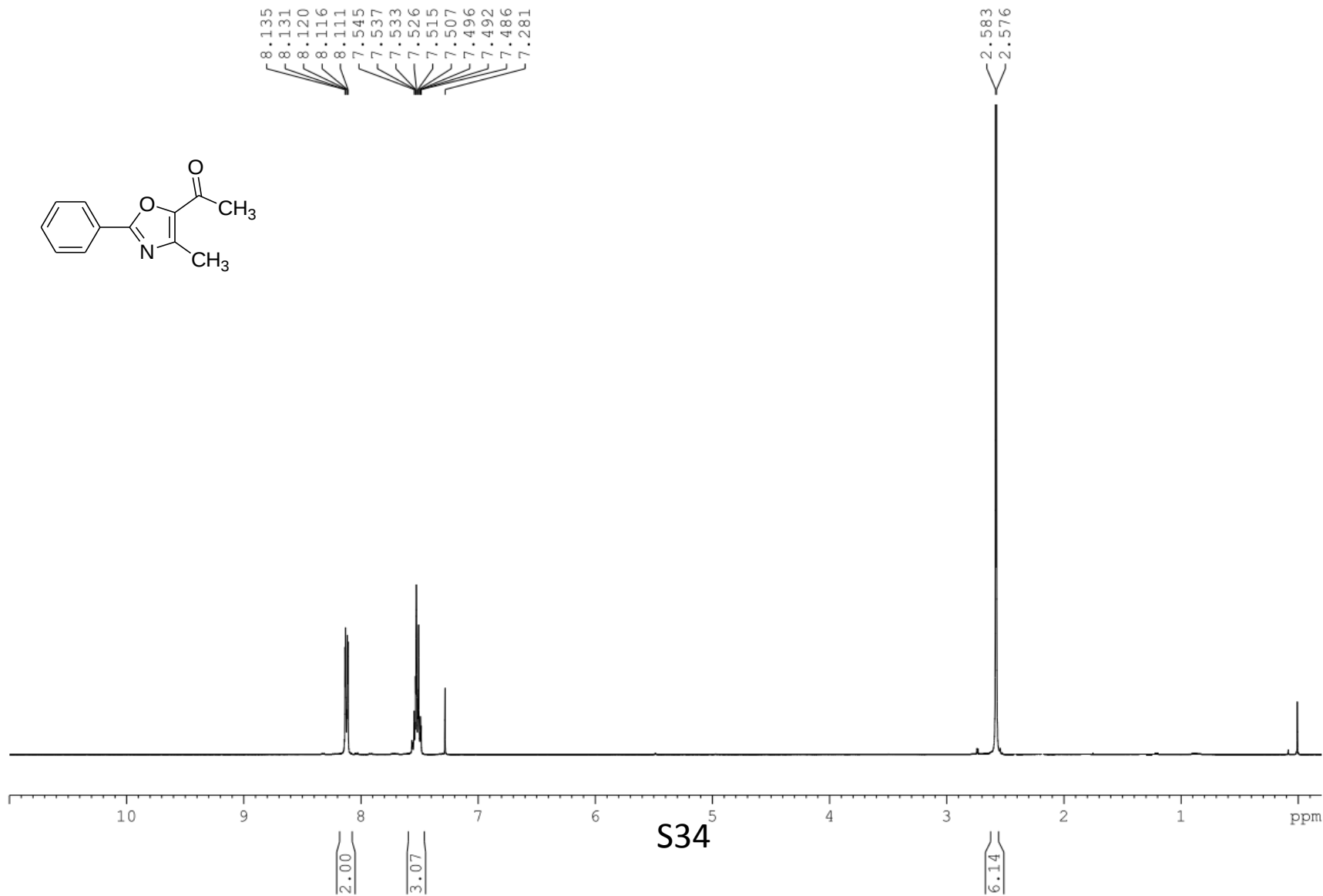
NP-MR-Thiocarbzole -R 13C

Methyl 2-phenylthiazole-5-carboxylate(2p)



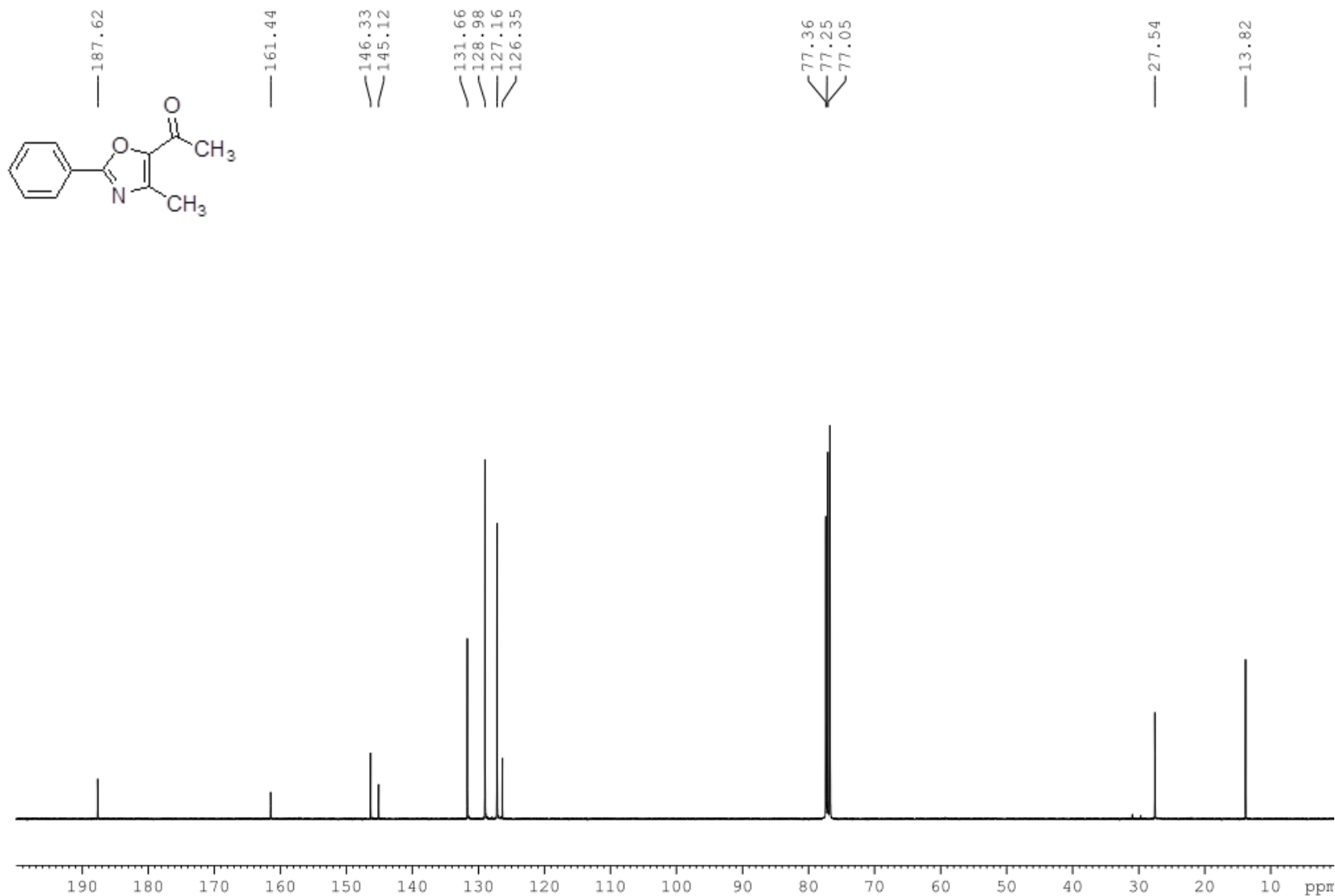
1-(4-methyl-2-phenyloxazol-5-yl)ethanone(6a)

NP-MR-663 1H



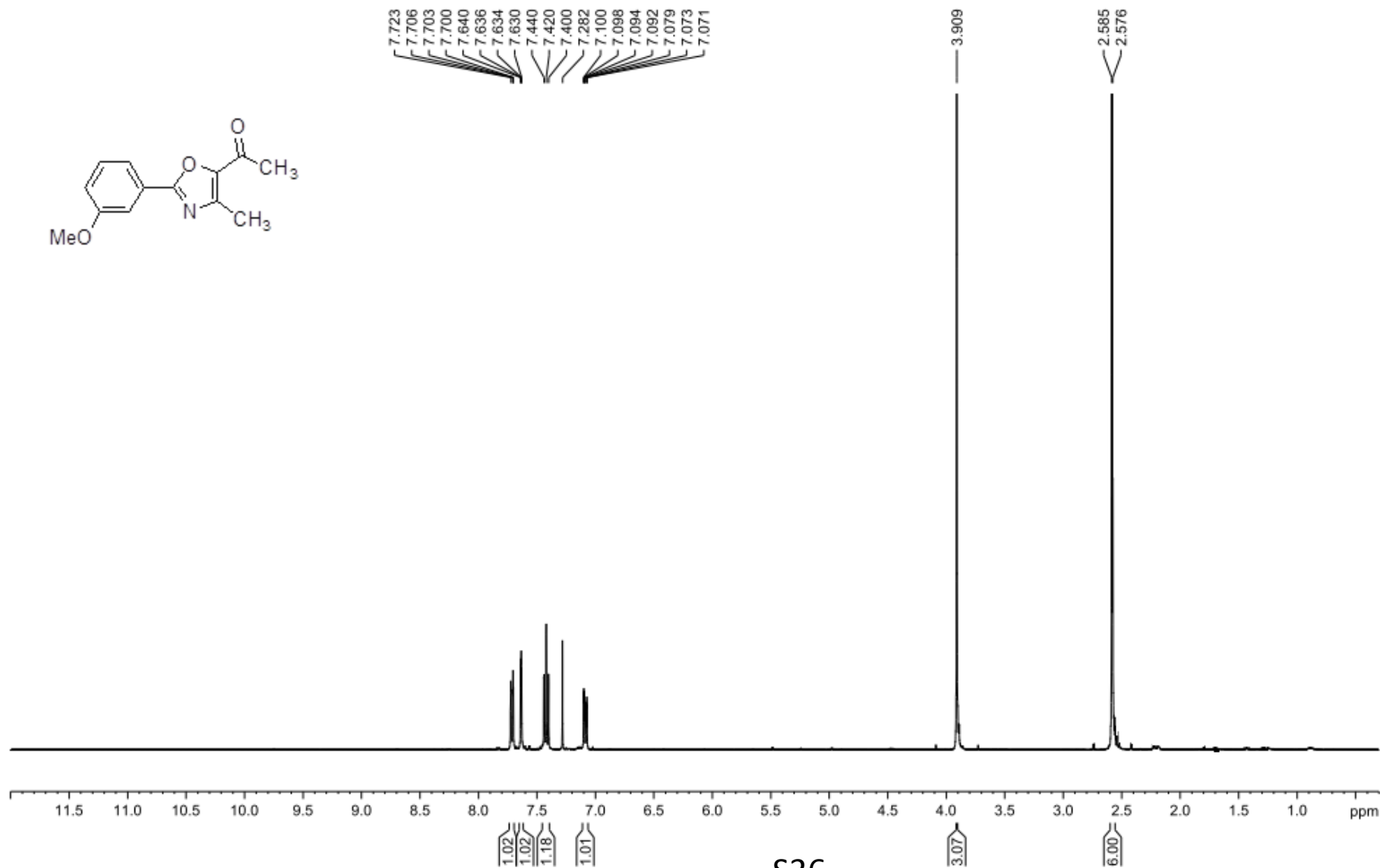
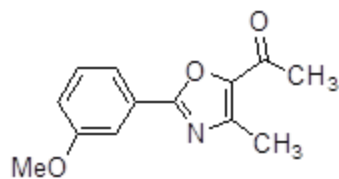
NP-MR-663 13C

1-(4-methyl-2-phenyloxazol-5-yl)ethanone(6a)

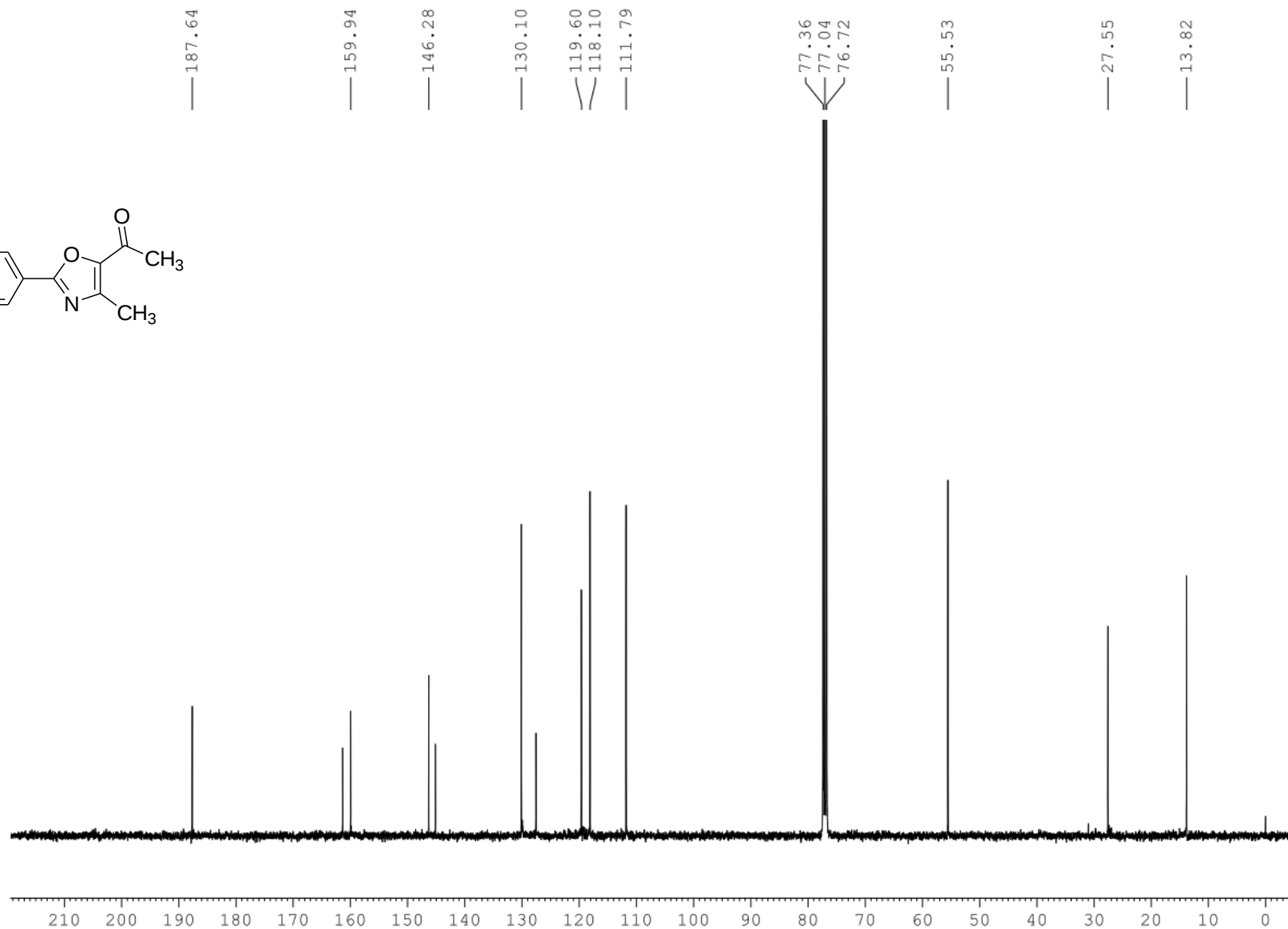
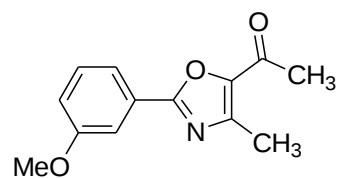


NP-MR-666

1-(2-(3-methoxyphenyl)-4-methyloxazol-5-yl)ethanone(6b)

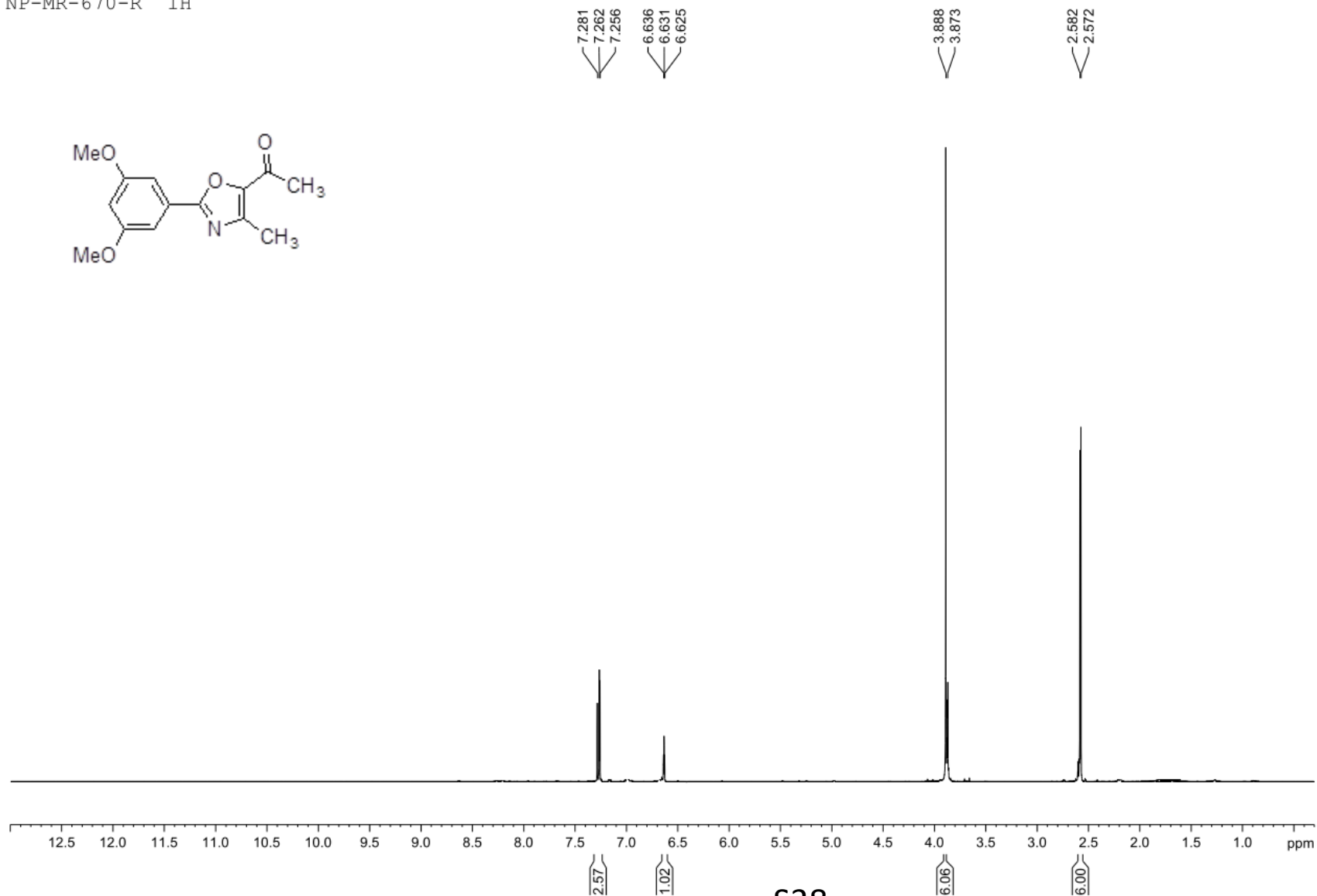


NP-MR-666 13C **1-(2-(3-methoxyphenyl)-4-methyloxazol-5-yl)ethanone(6b)**

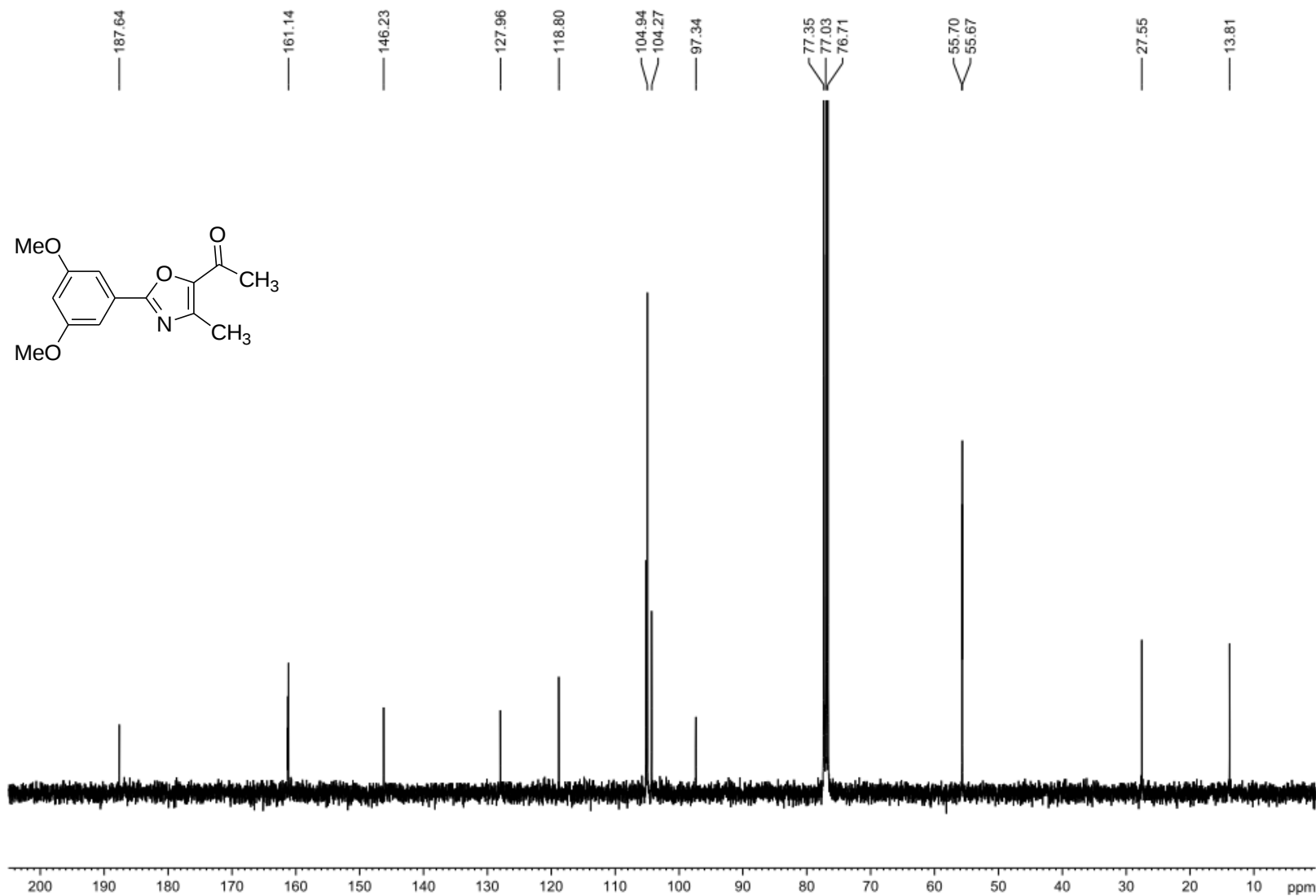


1-(2-(3,5-dimethoxyphenyl)-4-methyloxazol-5-yl)ethanone(6c)

NP-MR-670-R 1H

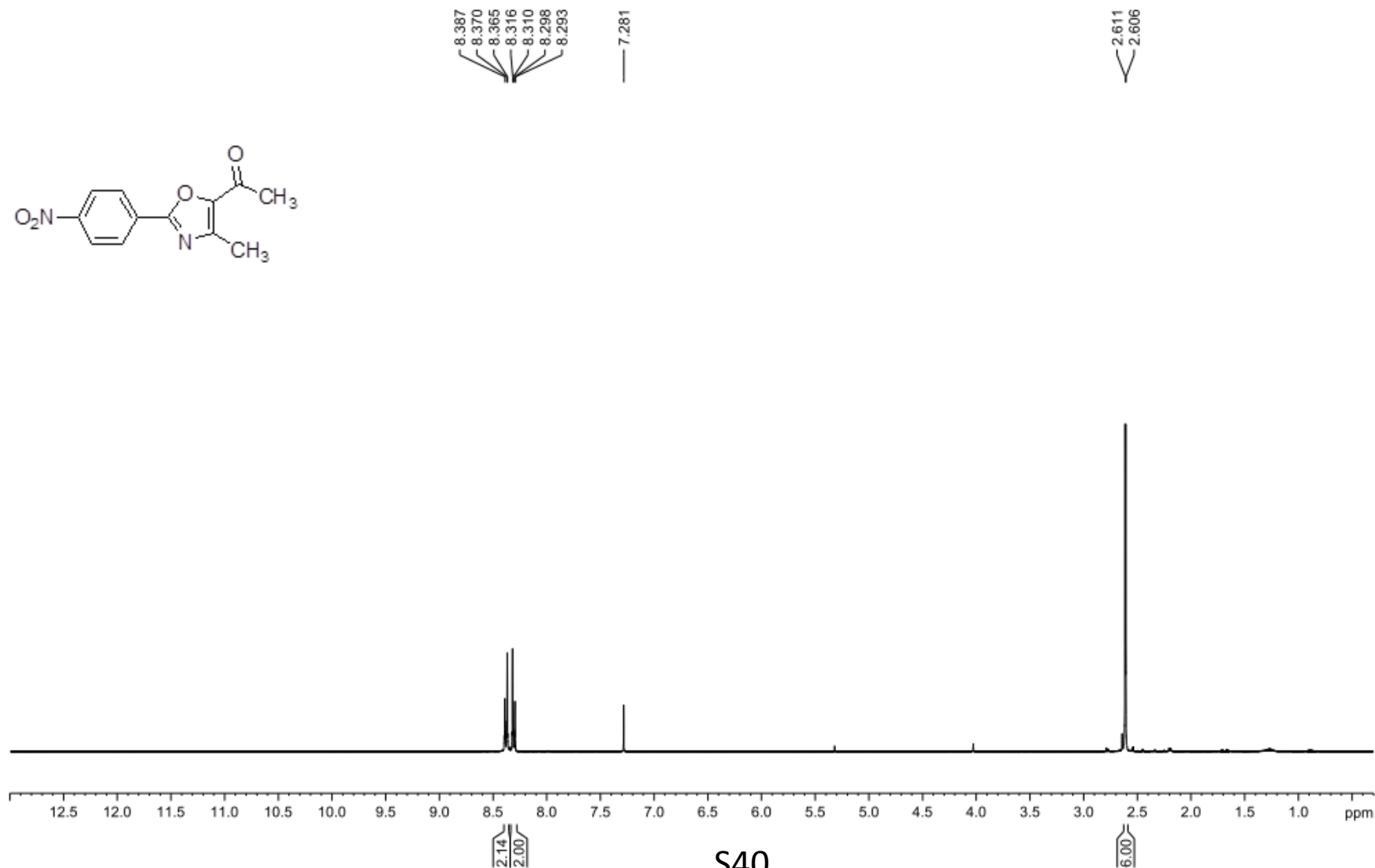


NP-MR-670

¹³C**1-(2-(3,5-dimethoxyphenyl)-4-methyloxazol-5-yl)ethanone(6c)**

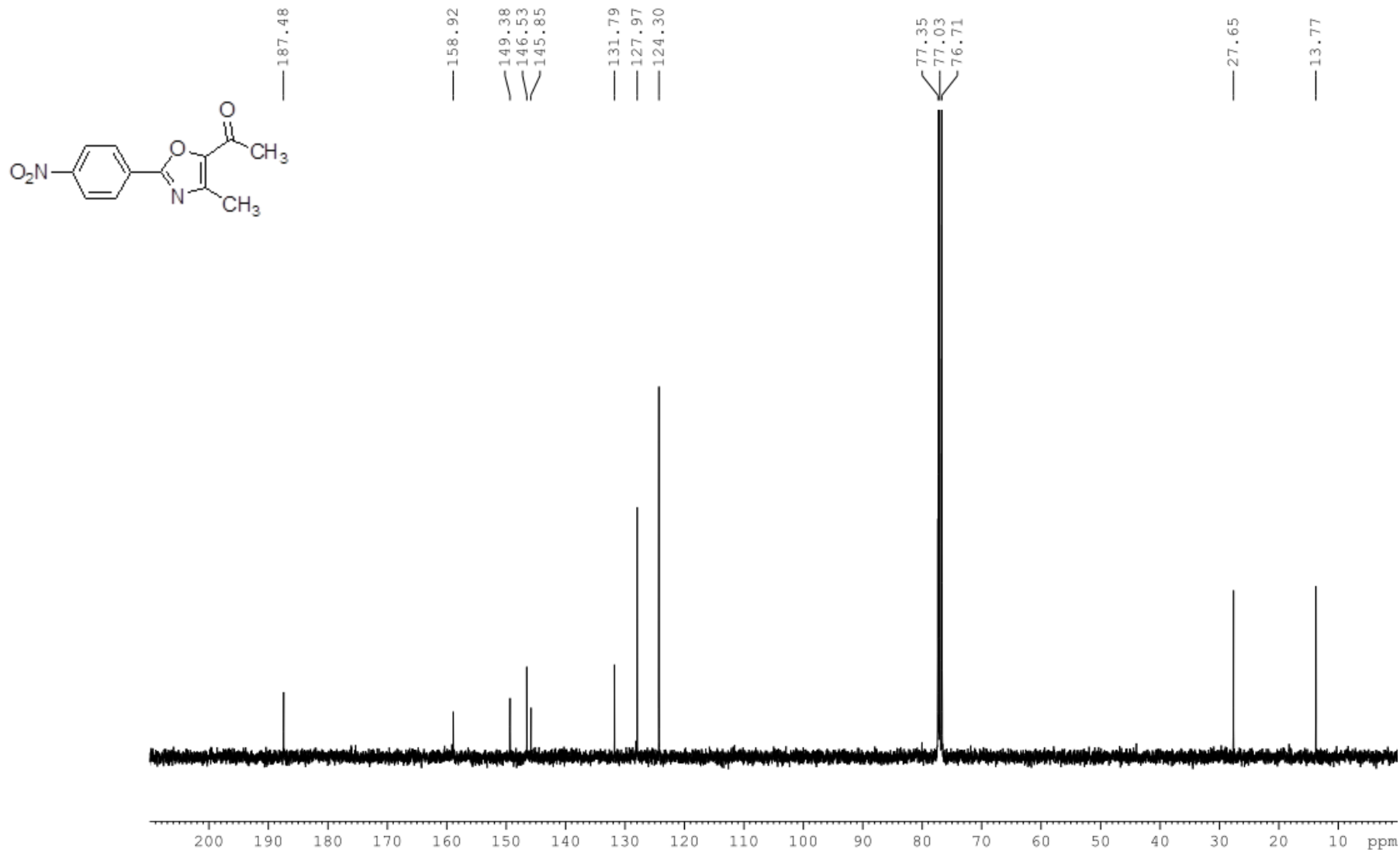
1-(4-methyl-2-(4-nitrophenyl)oxazol-5-yl)ethanone(6d)

NP-MR-667 1H

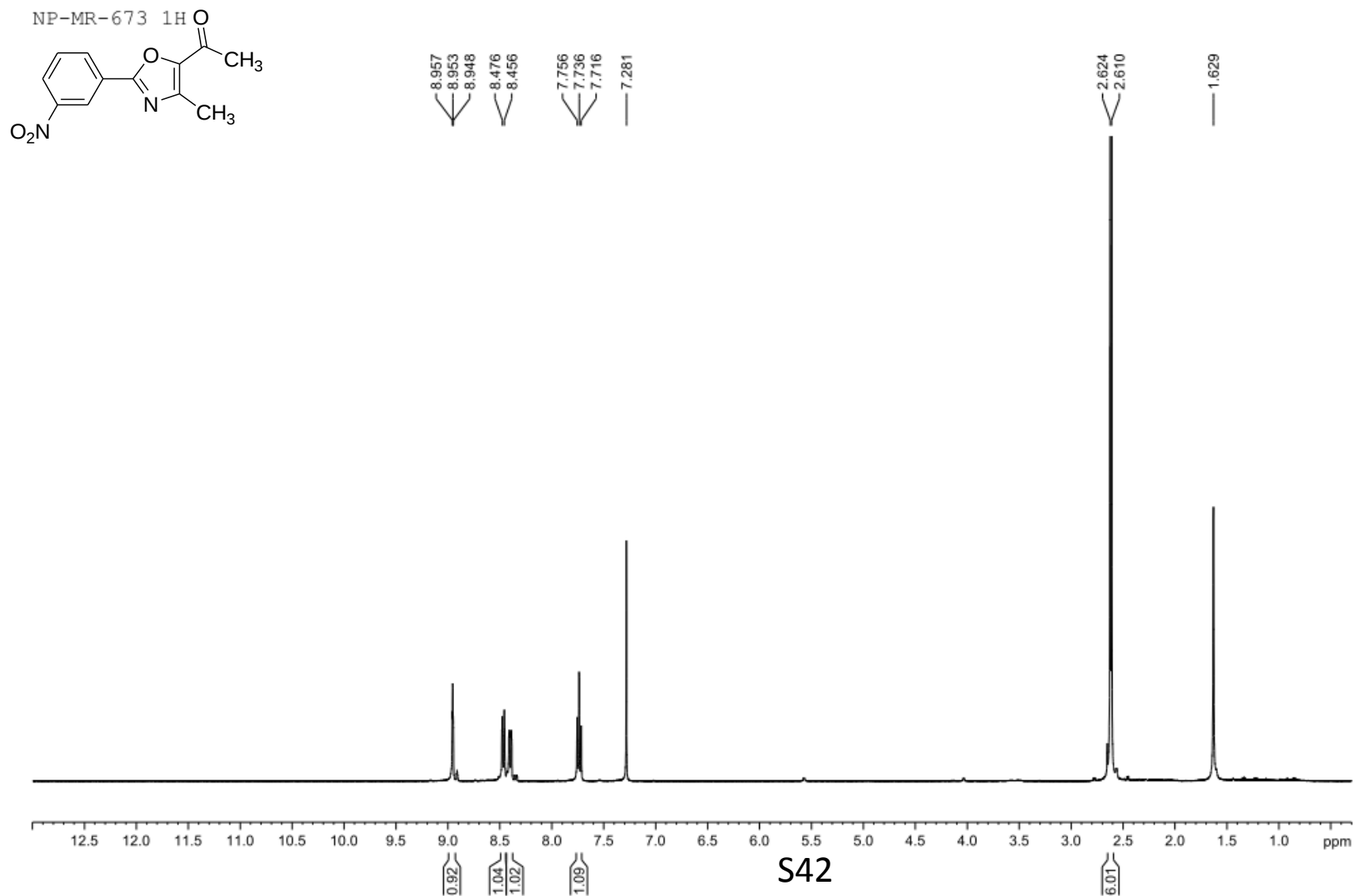


1-(4-methyl-2-(4-nitrophenyl)oxazol-5-yl)ethanone(6d)

NP-MR-667 13C

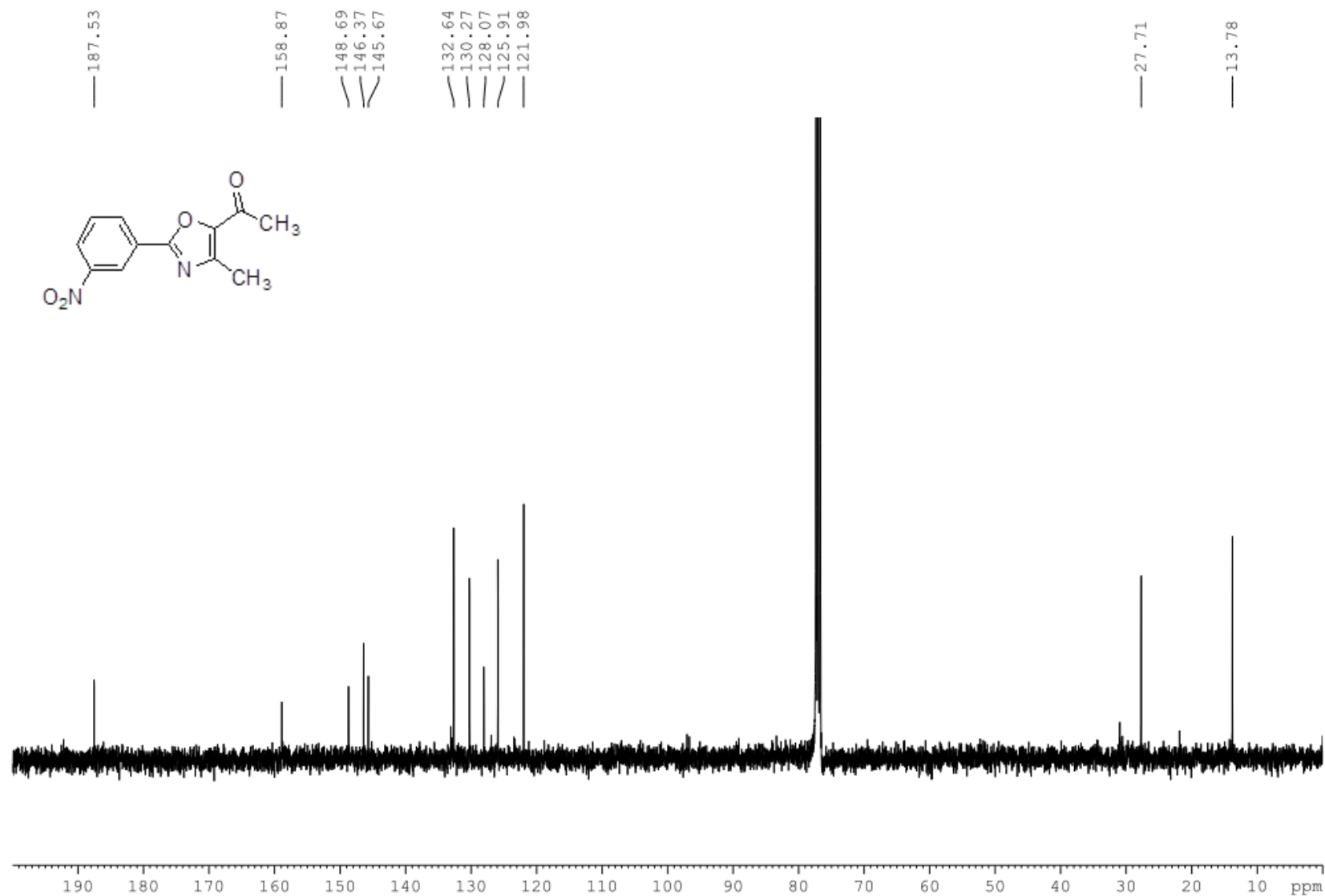


1-(4-methyl-2-(3-nitrophenyl)oxazol-5-yl)ethanone(6e)



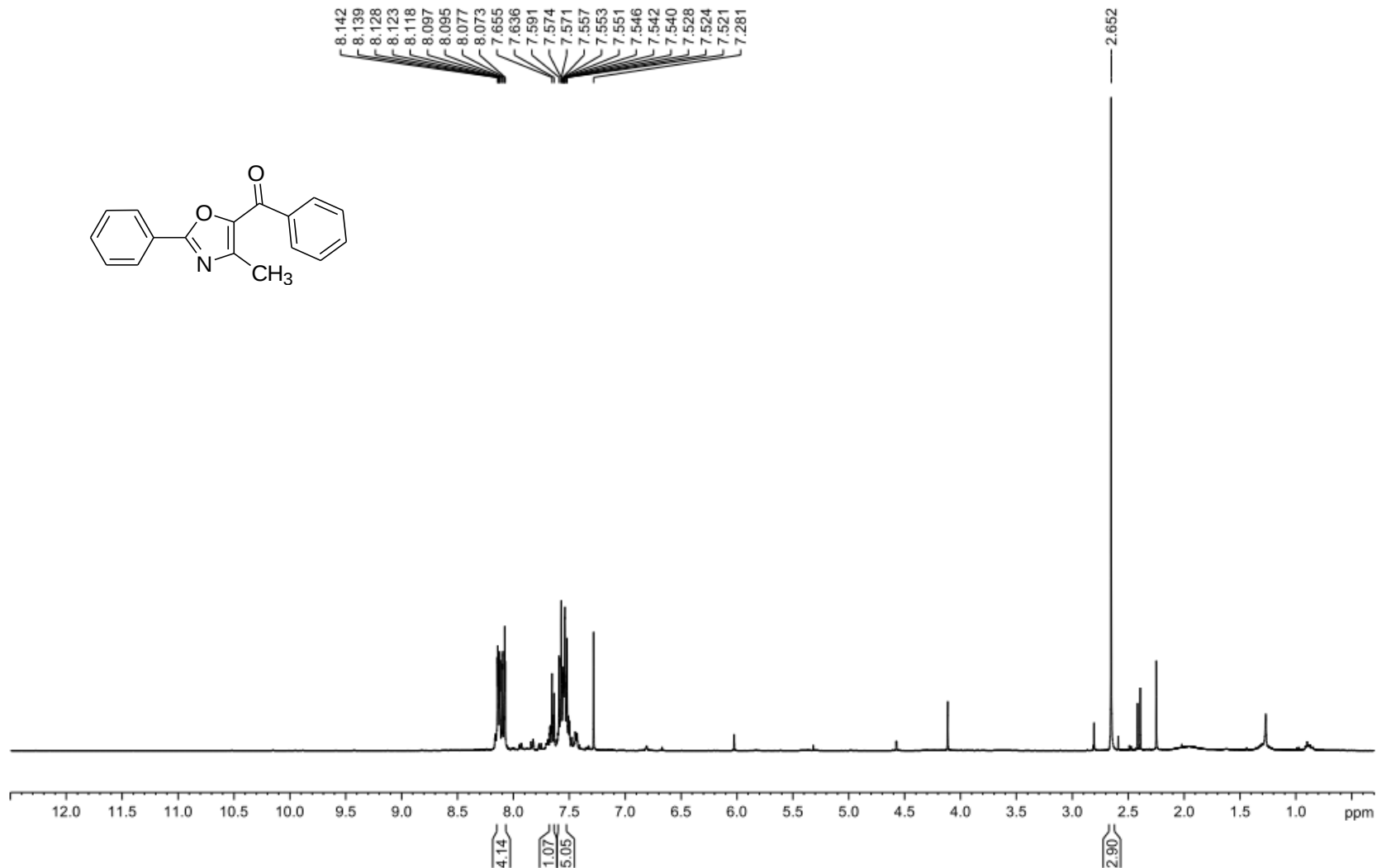
NP-MR-673 13C

1-(4-methyl-2-(3-nitrophenyl)oxazol-5-yl)ethanone(6e)



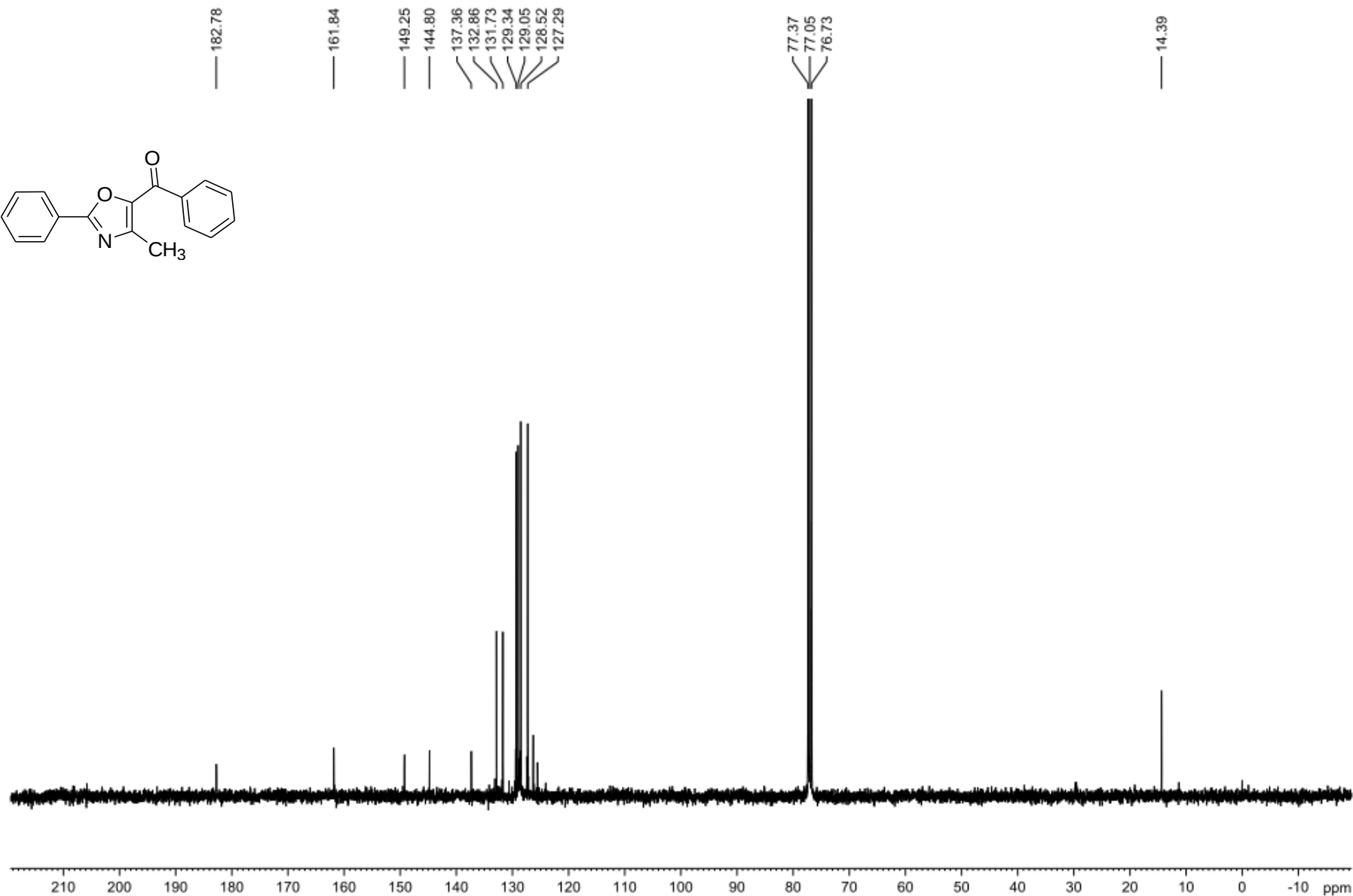
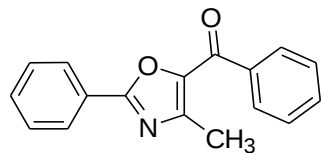
NP-MR-701 1H

(4-methyl-2-phenyloxazol-5-yl)(phenyl)methanone(6f)



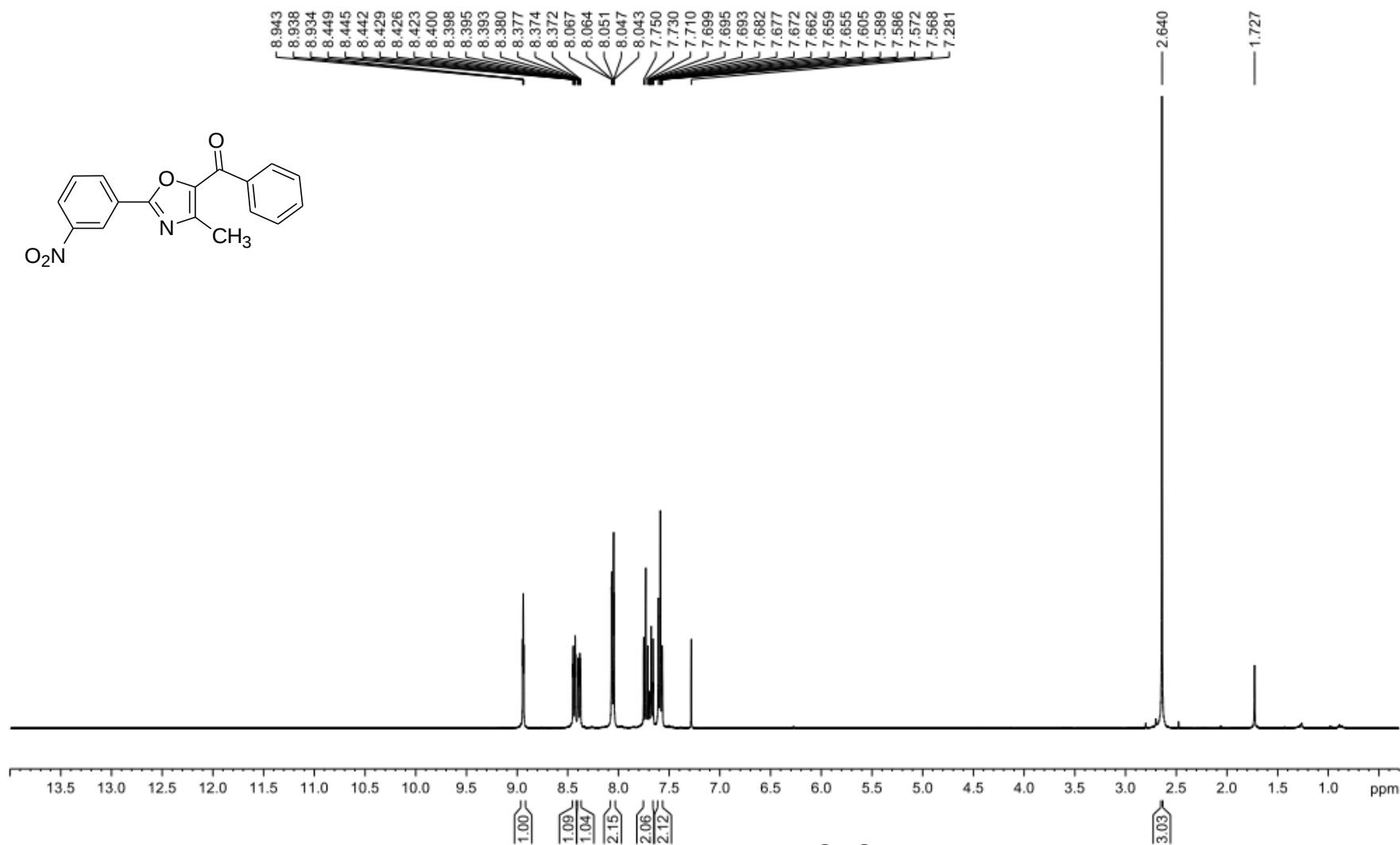
NP-MR-701 13C

(4-methyl-2-phenyloxazol-5-yl)(phenyl)methanone(6f)



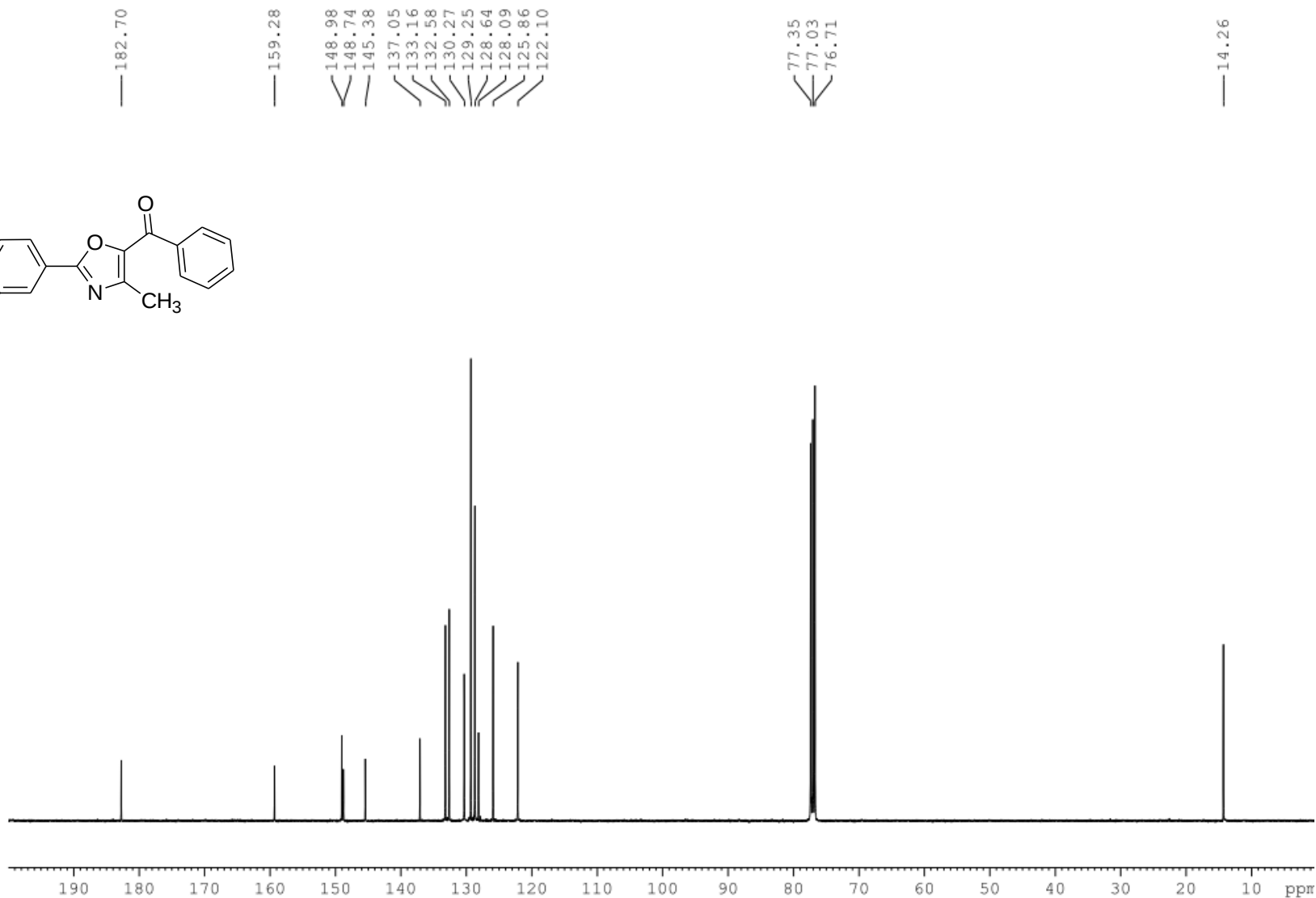
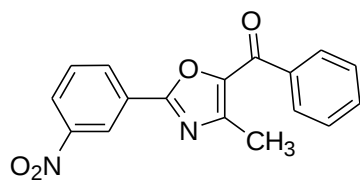
NP-MR-707 1H

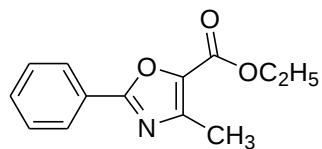
(4-methyl-2-(3-nitrophenyl)oxazol-5-yl)(phenyl)methanone(6g)



MP-MR-707 13c

(4-methyl-2-(3-nitrophenyl)oxazol-5-yl)(phenyl)methanone(6g)



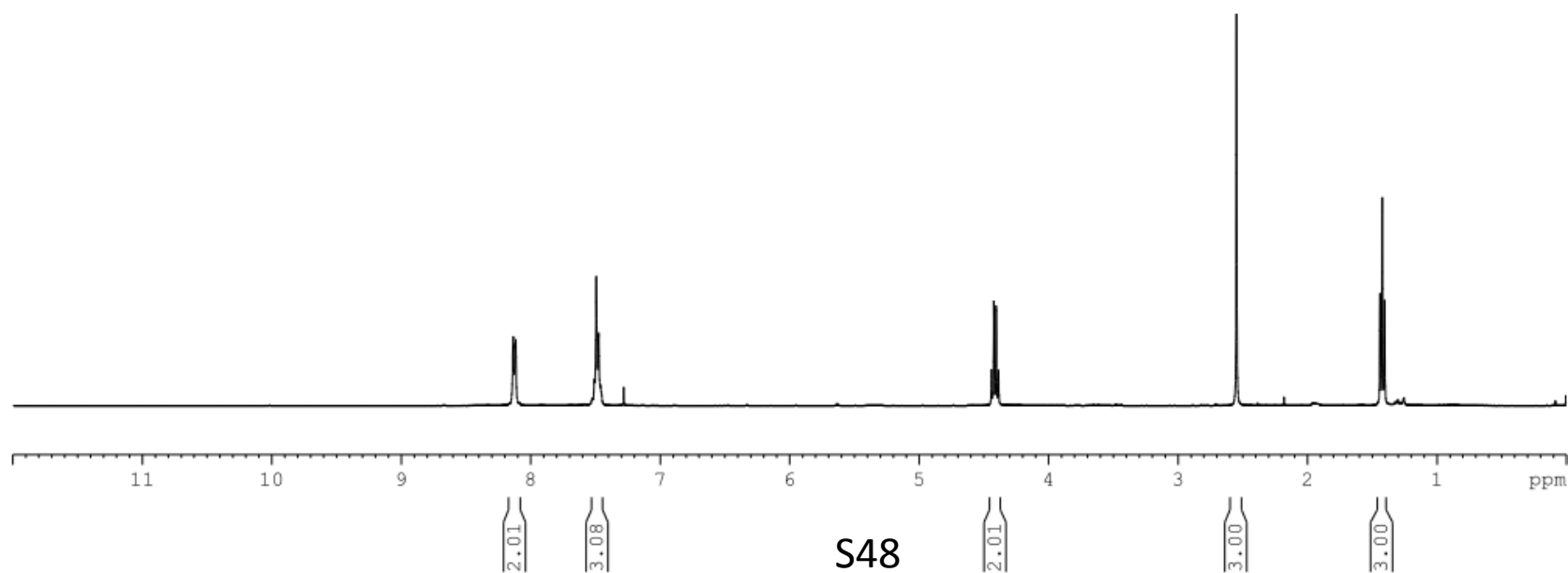
Ethyl 4-methyl-2-phenyloxazole-5-carboxylate(6h)

8.137
8.134
8.119
8.114
7.507
7.493
7.474
7.281

4.441
4.423
4.406
4.388

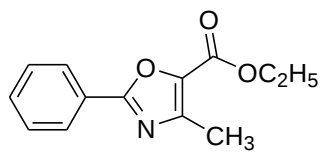
2.549

1.441
1.423
1.405



NP-MR-EAA Oxazole 13C

Ethyl 4-methyl-2-phenyloxazole-5-carboxylate(6h)



—162.22
—158.87

—147.06

—137.43

—131.44

—128.85

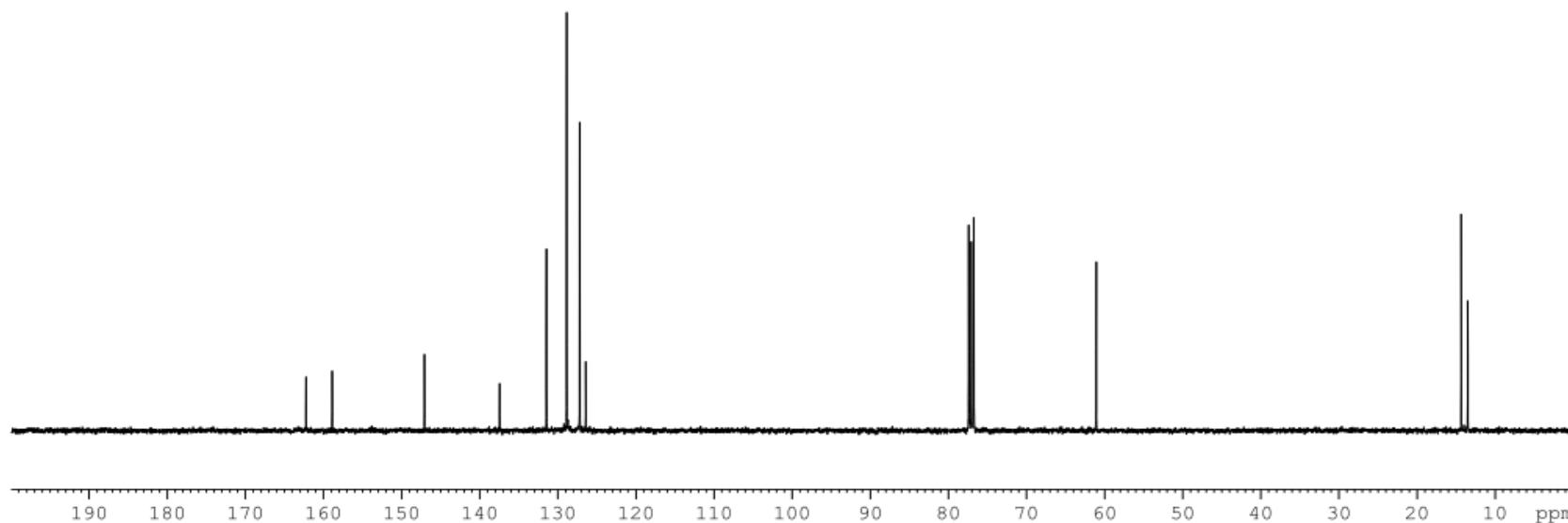
—127.18

—126.41

77.37
77.06
76.74

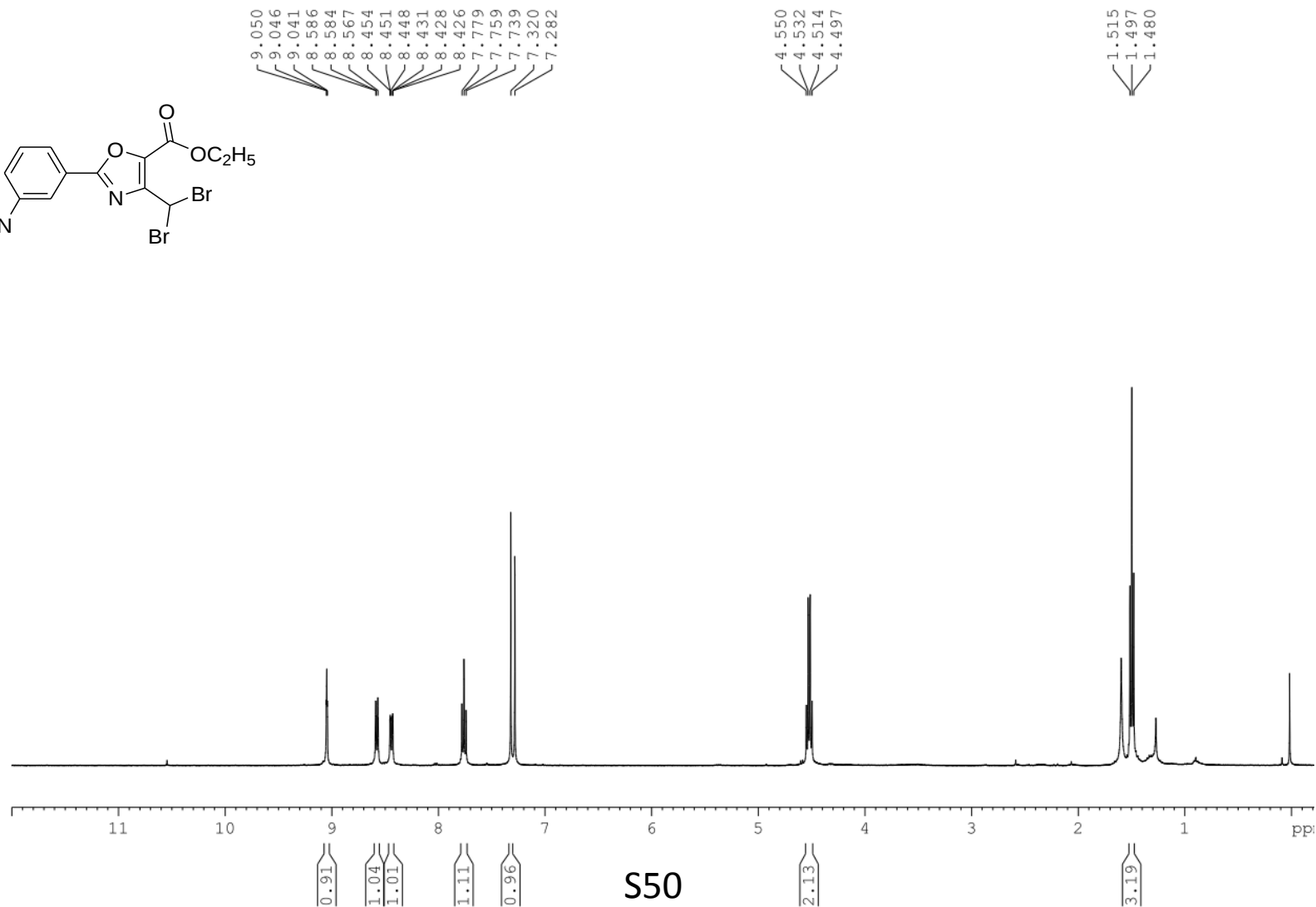
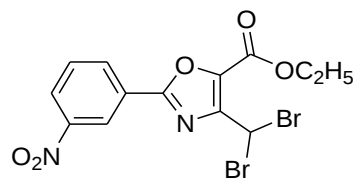
—61.07

14.36
13.53



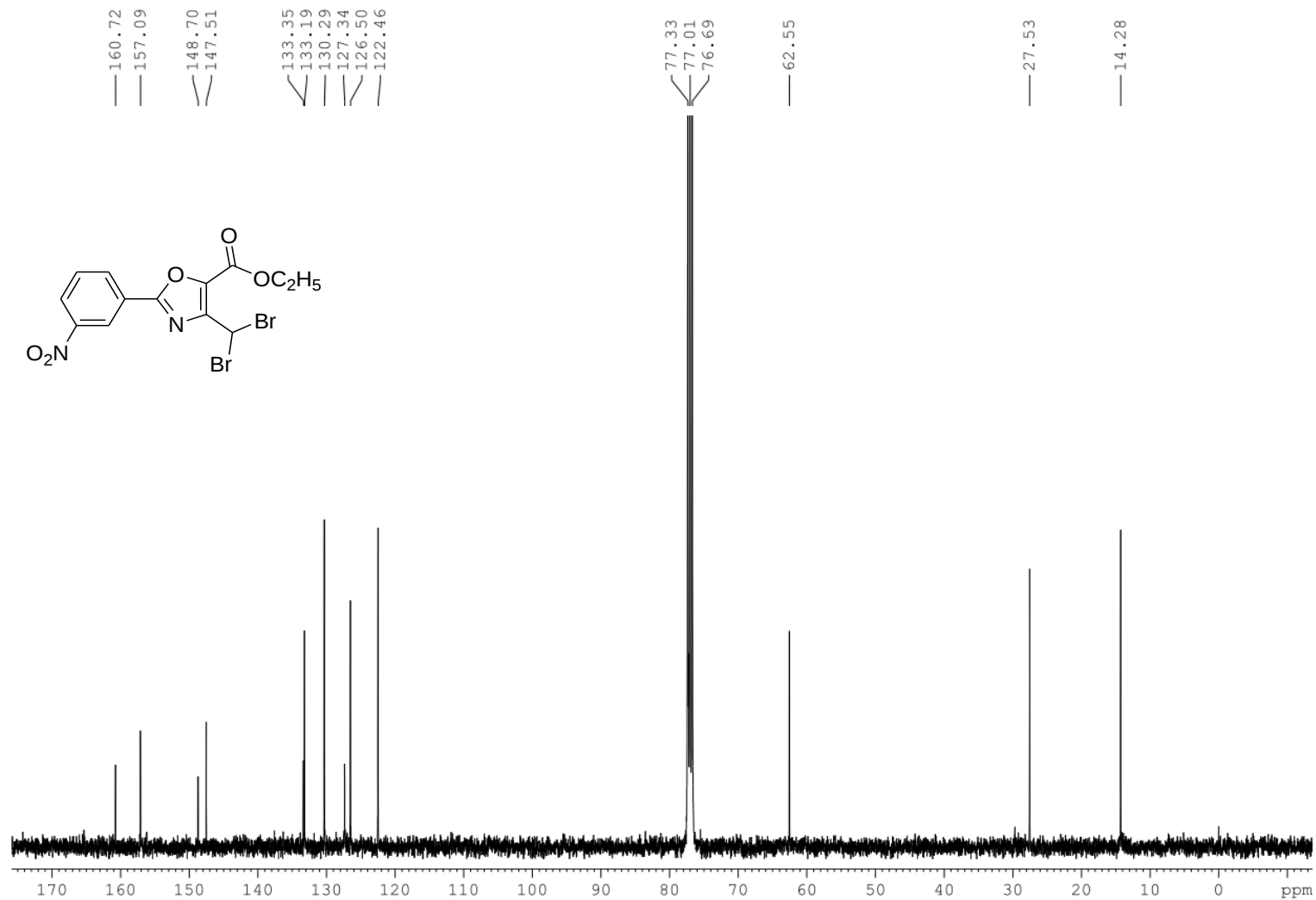
NP-MR-719 1H

Ethyl 4-(dibromomethyl)-2-(3-nitrophenyl)oxazole-5-carboxylate (6i)



Ethyl 4-(dibromomethyl)-2-(3-nitrophenyl)oxazole-5-carboxylate (6i)

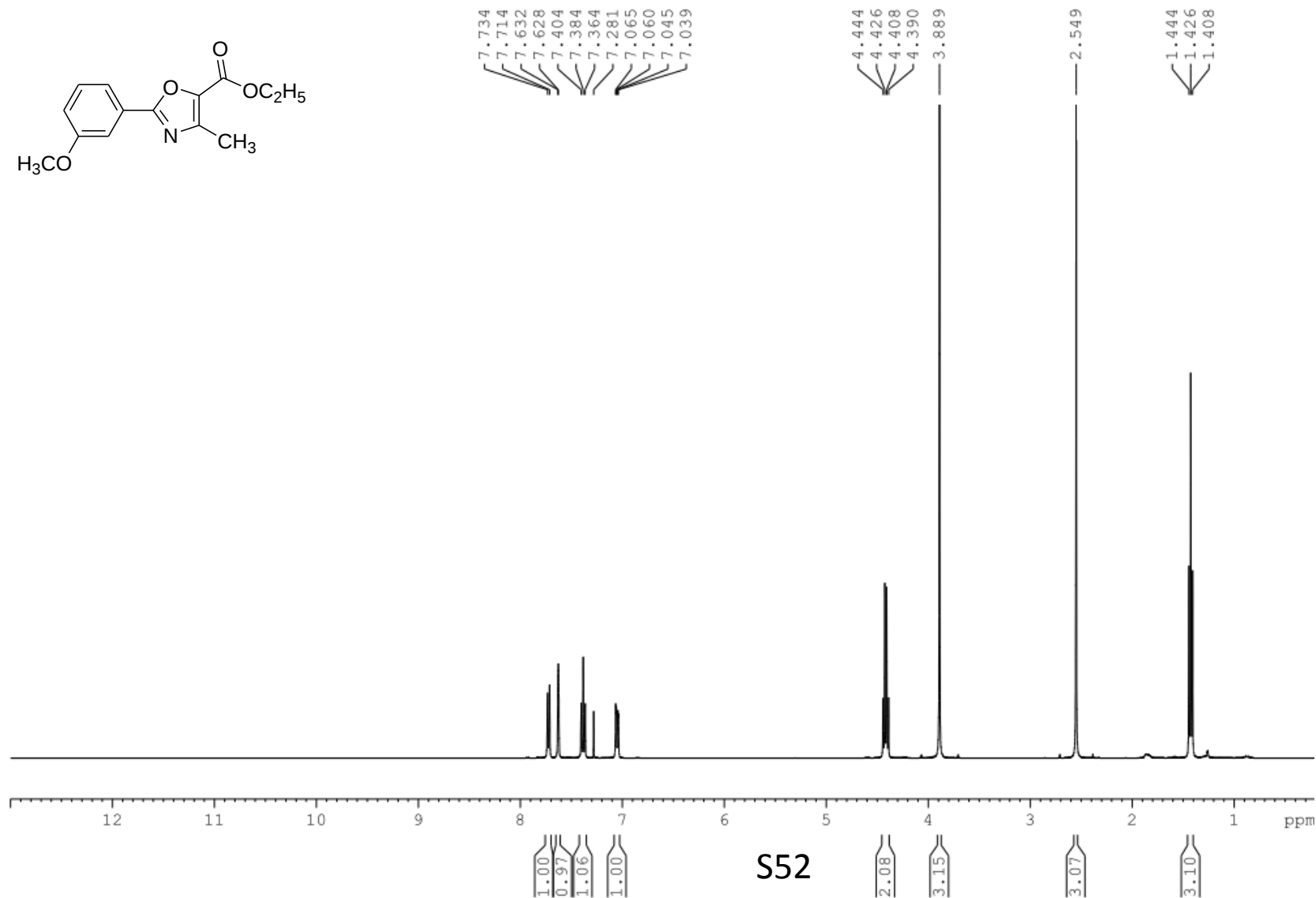
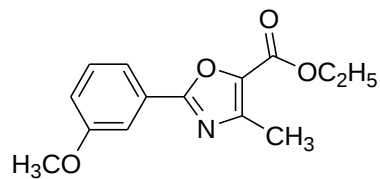
NP-MR-719 13C



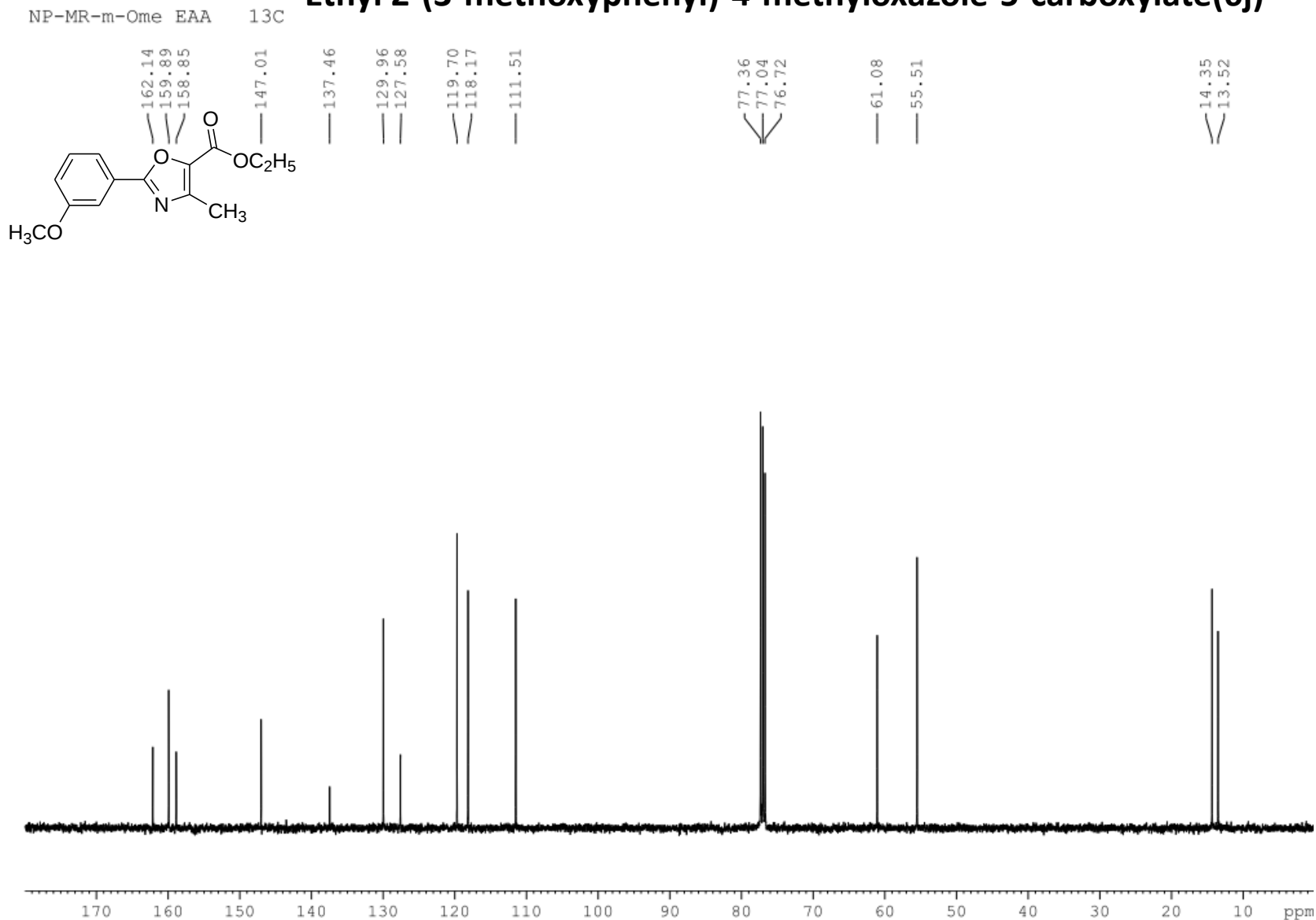
S51

NP-MR-m-Ome EAA 1H

Ethyl 2-(3-methoxyphenyl)-4-methyloxazole-5-carboxylate(6j)

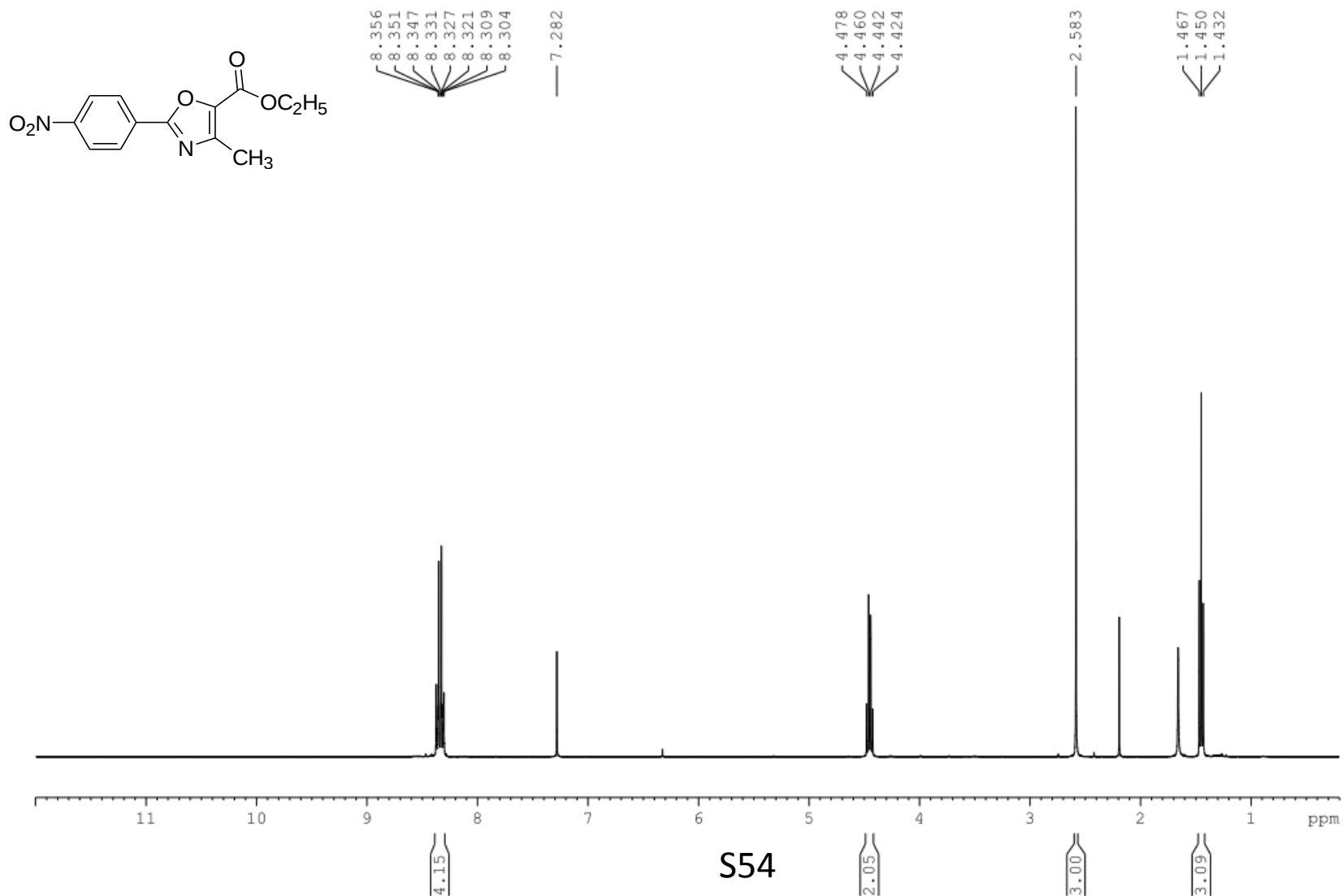


Ethyl 2-(3-methoxyphenyl)-4-methyloxazole-5-carboxylate(6j)



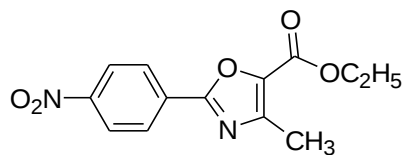
NP-MR-708 1H

Ethyl 4-methyl-2-(4-nitrophenyl)oxazole-5-carboxylate(6k)



NP-MR-708 13C

Ethyl 4-methyl-2-(4-nitrophenyl)oxazole-5-carboxylate(6k)

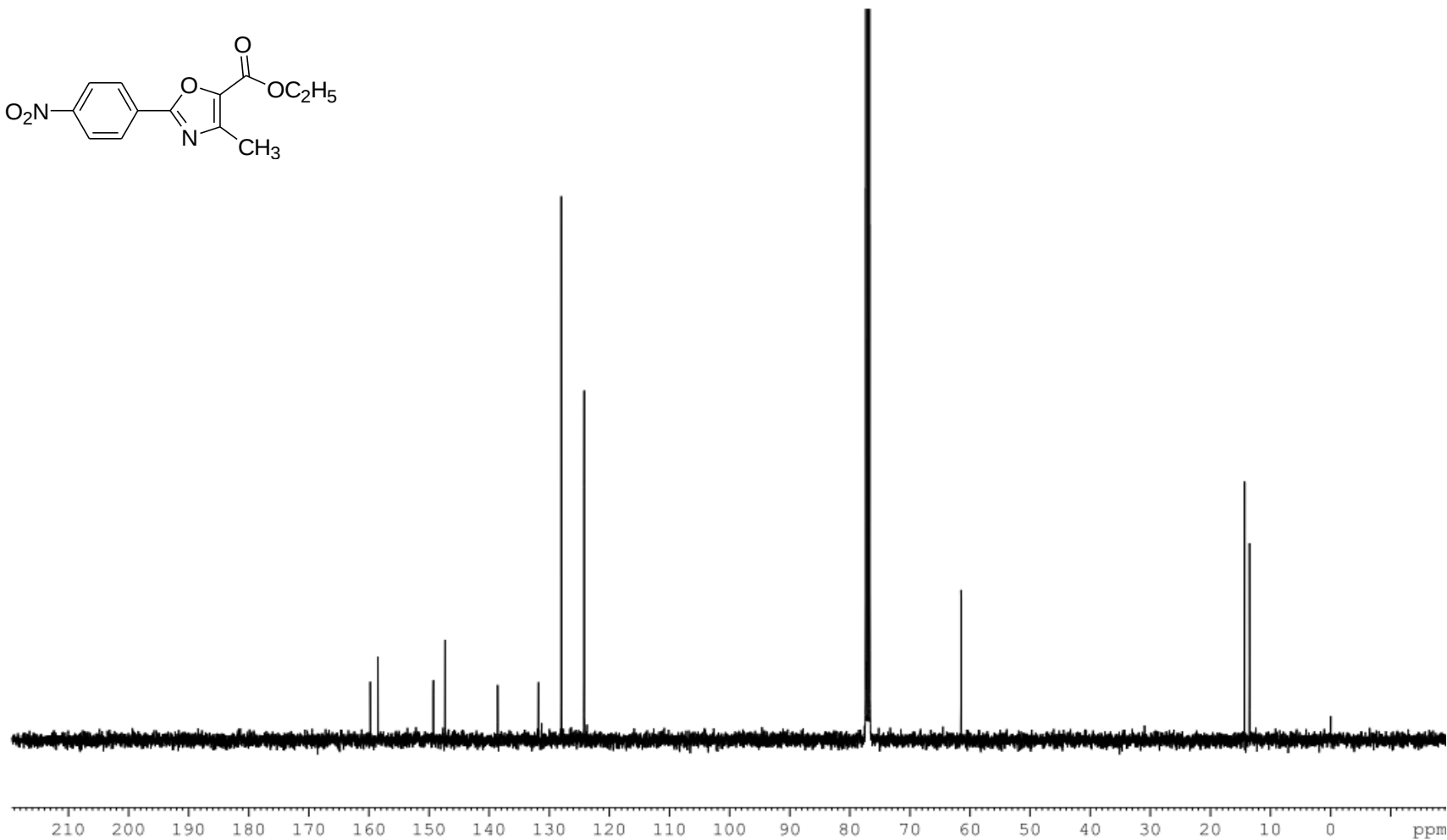


159.79
158.52
149.29
147.34
138.60
131.81
128.00
124.21

77.34
77.03
76.71

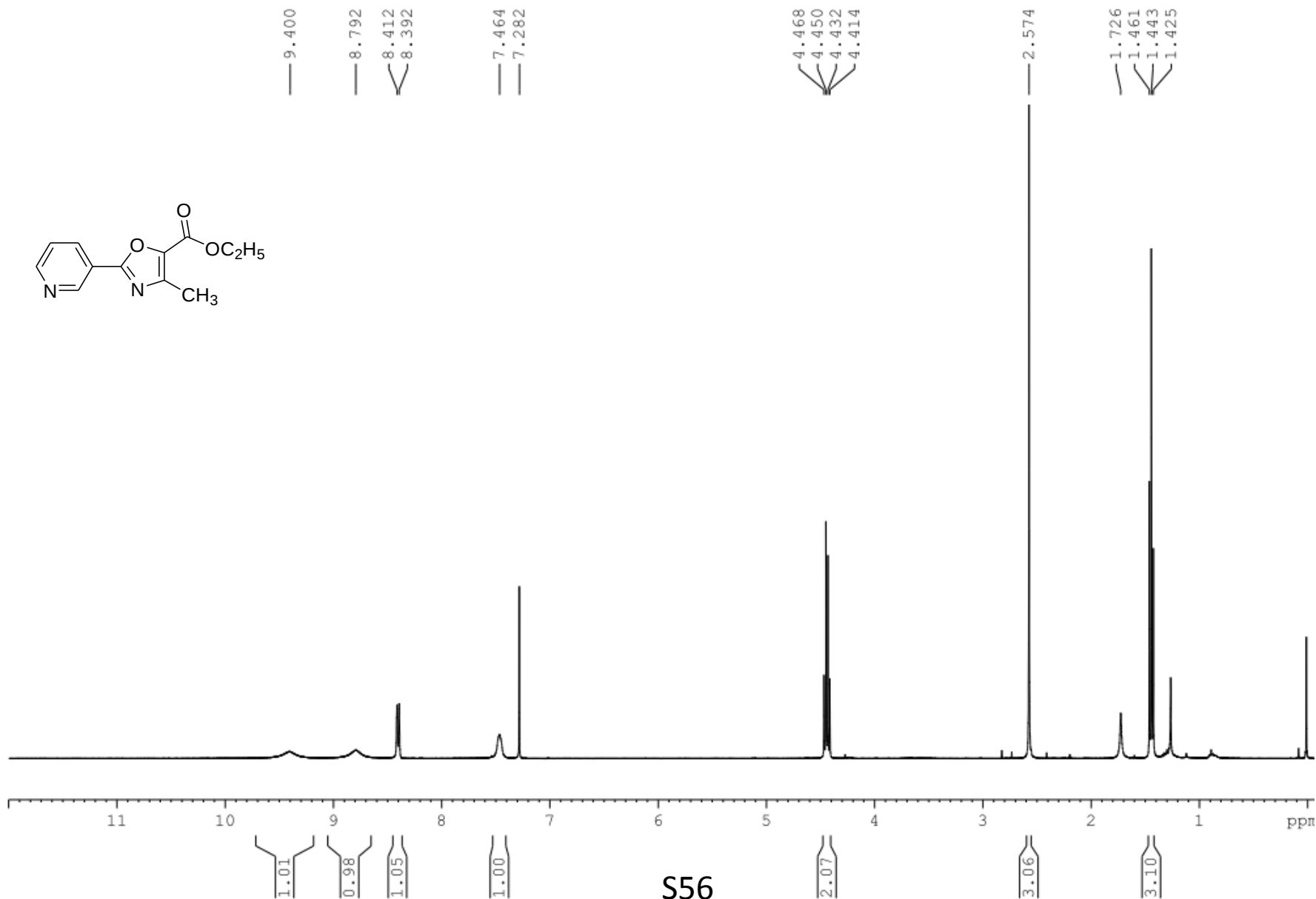
61.49

14.35
13.49



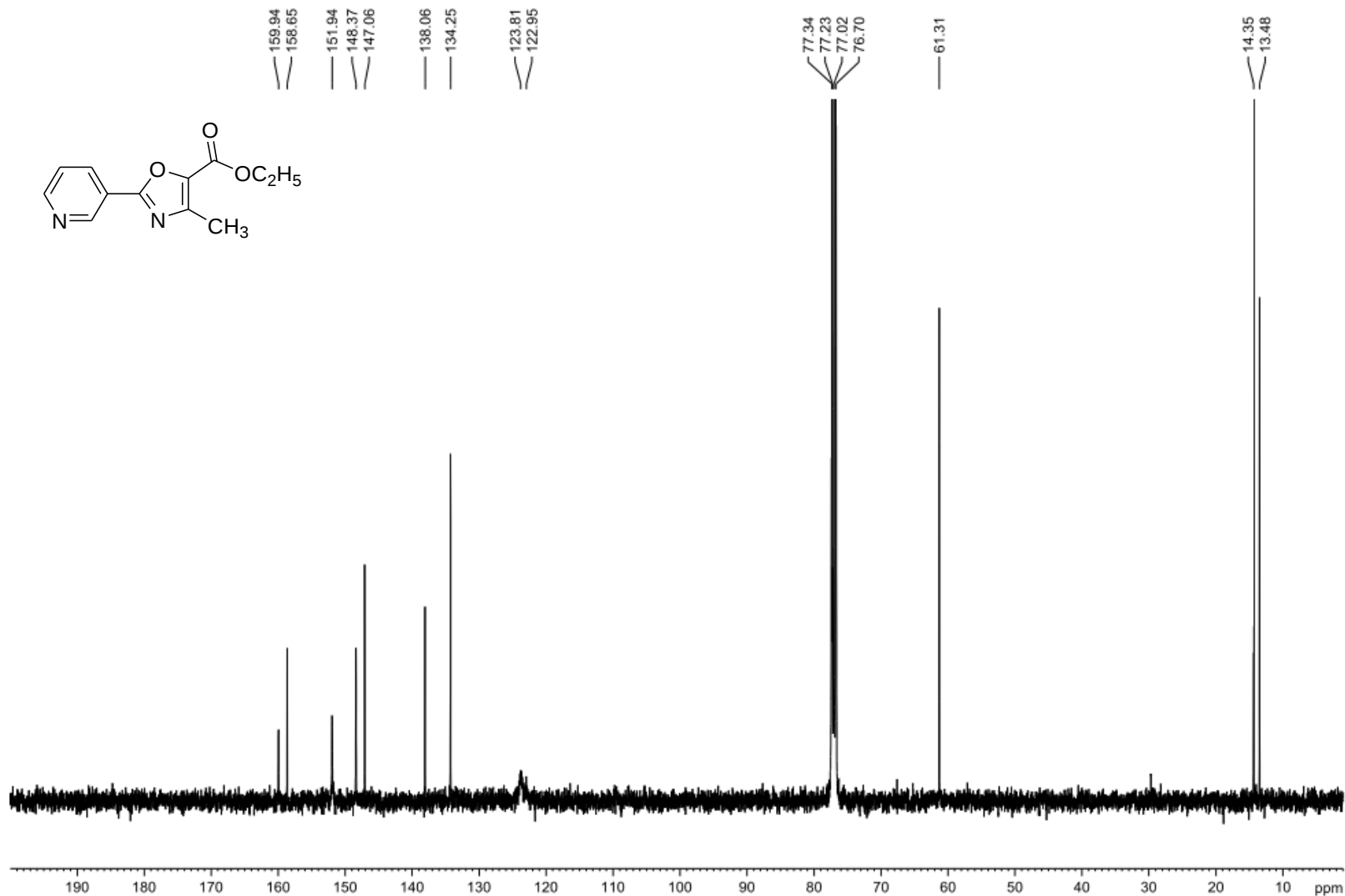
Ethyl 4-methyl-2-(pyridin-3-yl)oxazole-5-carboxylate(6l)

NP-MR-Ni+EAA Oxazole 1H



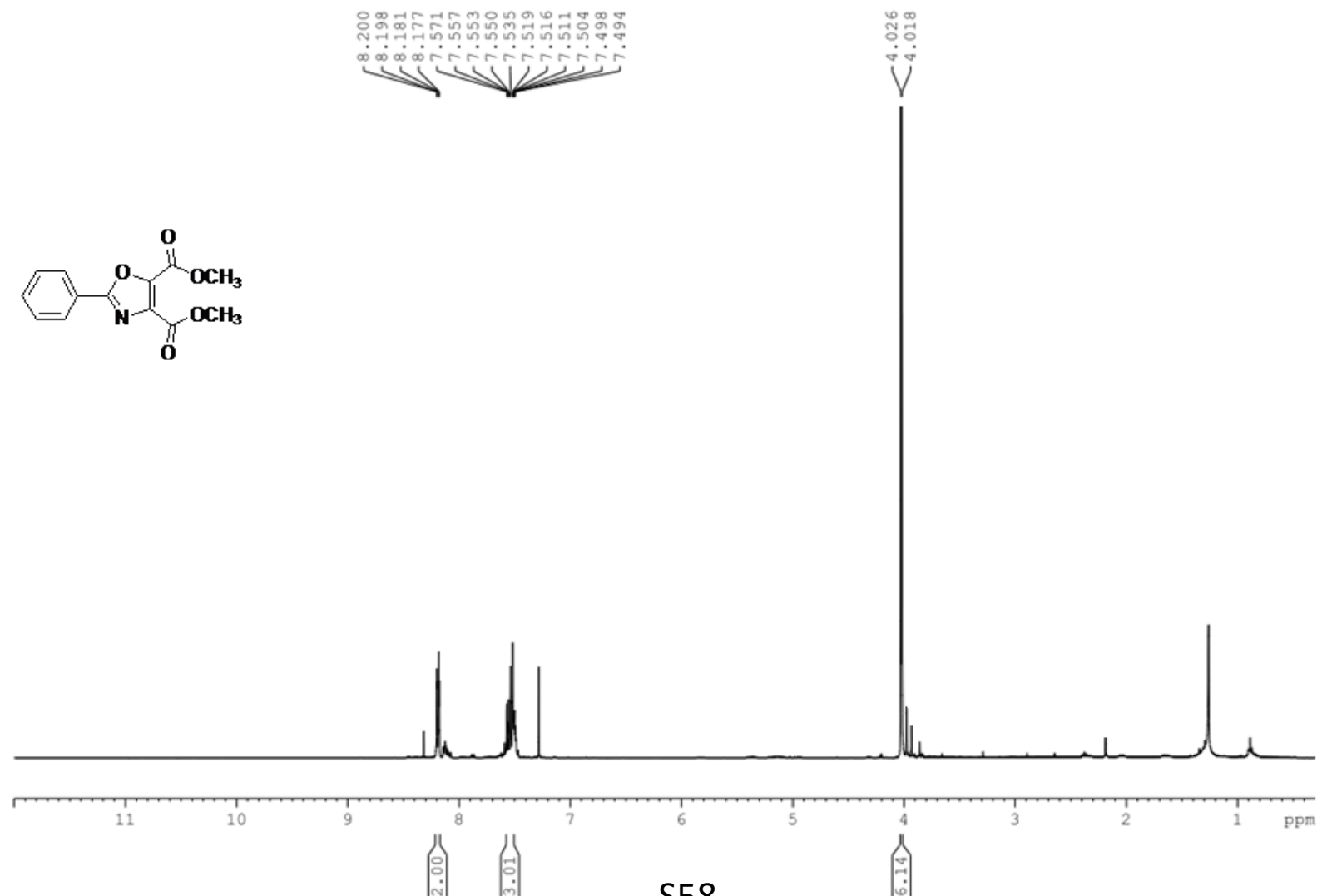
Ethyl 4-methyl-2-(pyridin-3-yl)oxazole-5-carboxylate(6I)

NP-MR-Ni+EAA Oxazole 13C



2-Phenyl-oxazole-4,5-dicarboxylic acid dimethyl ester(6m)

NP-MR-707 1H



NP-MR-707 **2-Phenyl-oxazole-4,5-dicarboxylic acid dimethyl ester(6m)**

