

Supplementary Material

Benzimidazolinone synthesis through hypervalent iodine-mediated cycloaddition between aryl isocyanates and *O*-substituted hydroxylamines

Hiroataka Sasa^a, Haruki Shimada^b, Kyohei Kitamura^b, Keita Mizushima^b, Soshi Yamamoto^b, Shotaro Hamatani^b, and Toshifumi Dohi^{b*}

^a*School of Pharmacy and Pharmaceutical Sciences, Mukogawa Women's University, 11-68 Koshien Kyu-ban-cho, Nishinomiya 663-8179, Hyogo, Japan*

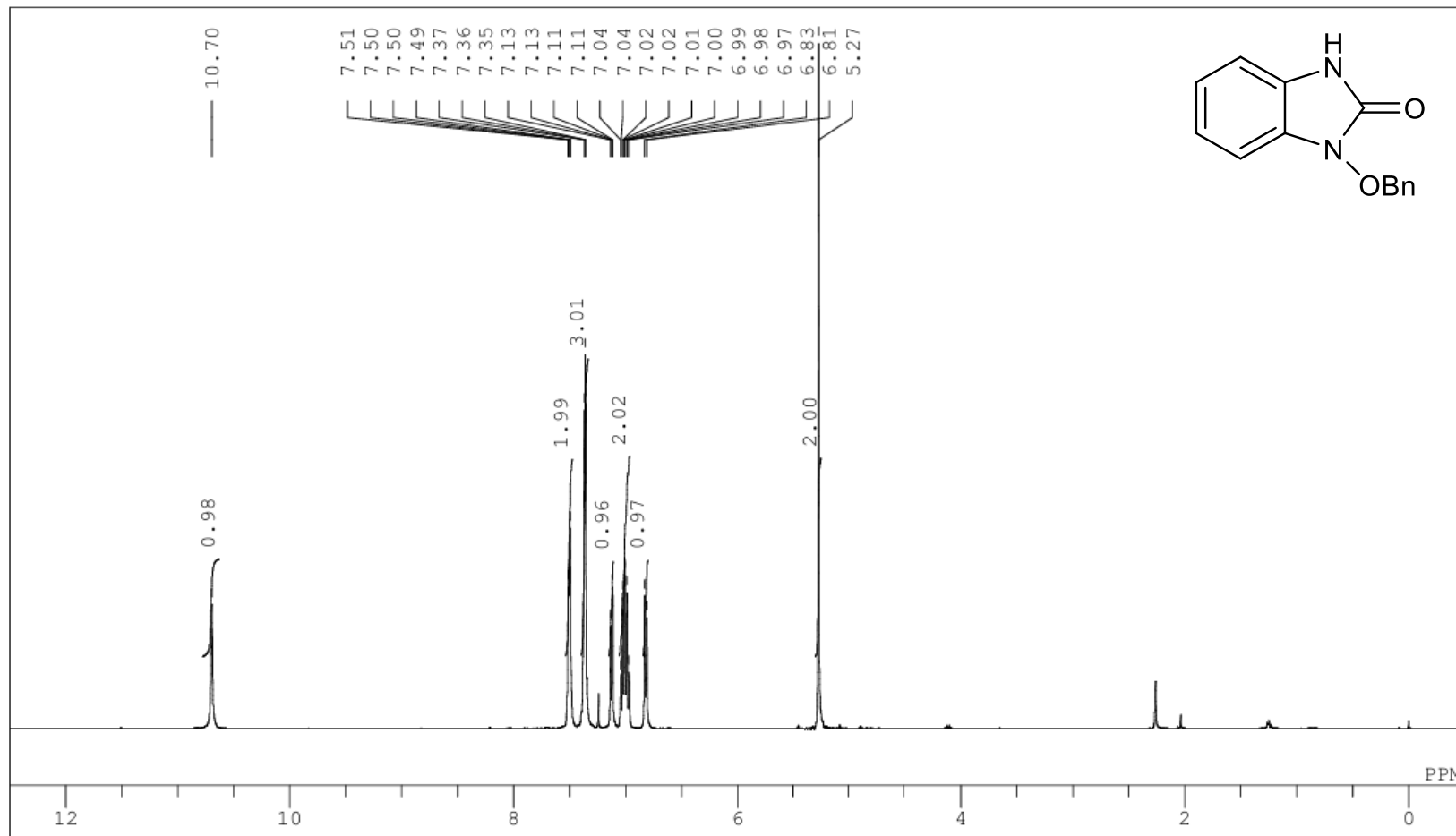
^b*Graduate School of Pharmaceutical Sciences, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu 525-8577, Shiga, Japan*

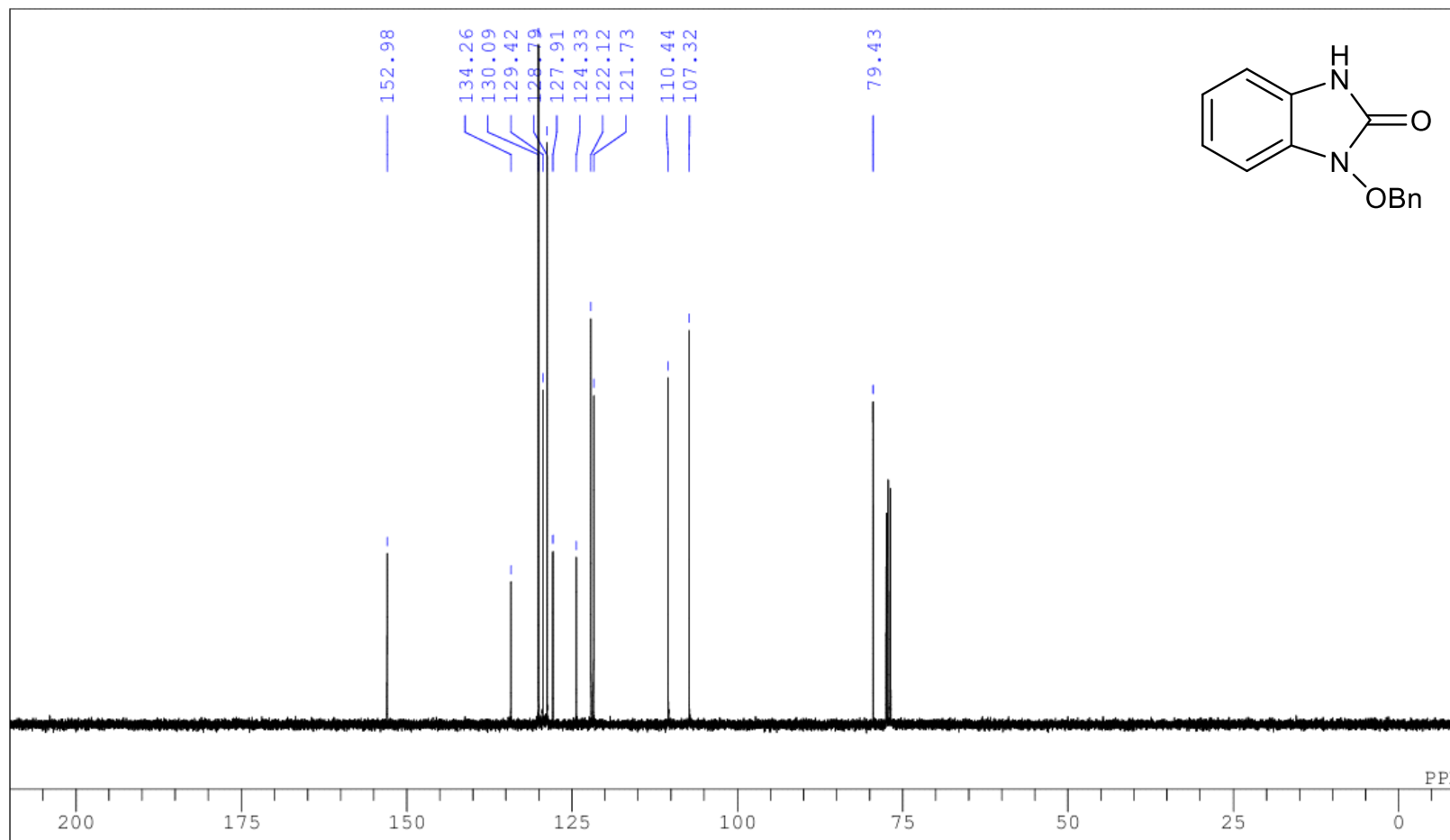
Email: td1203@ph.ritsumei.ac.jp

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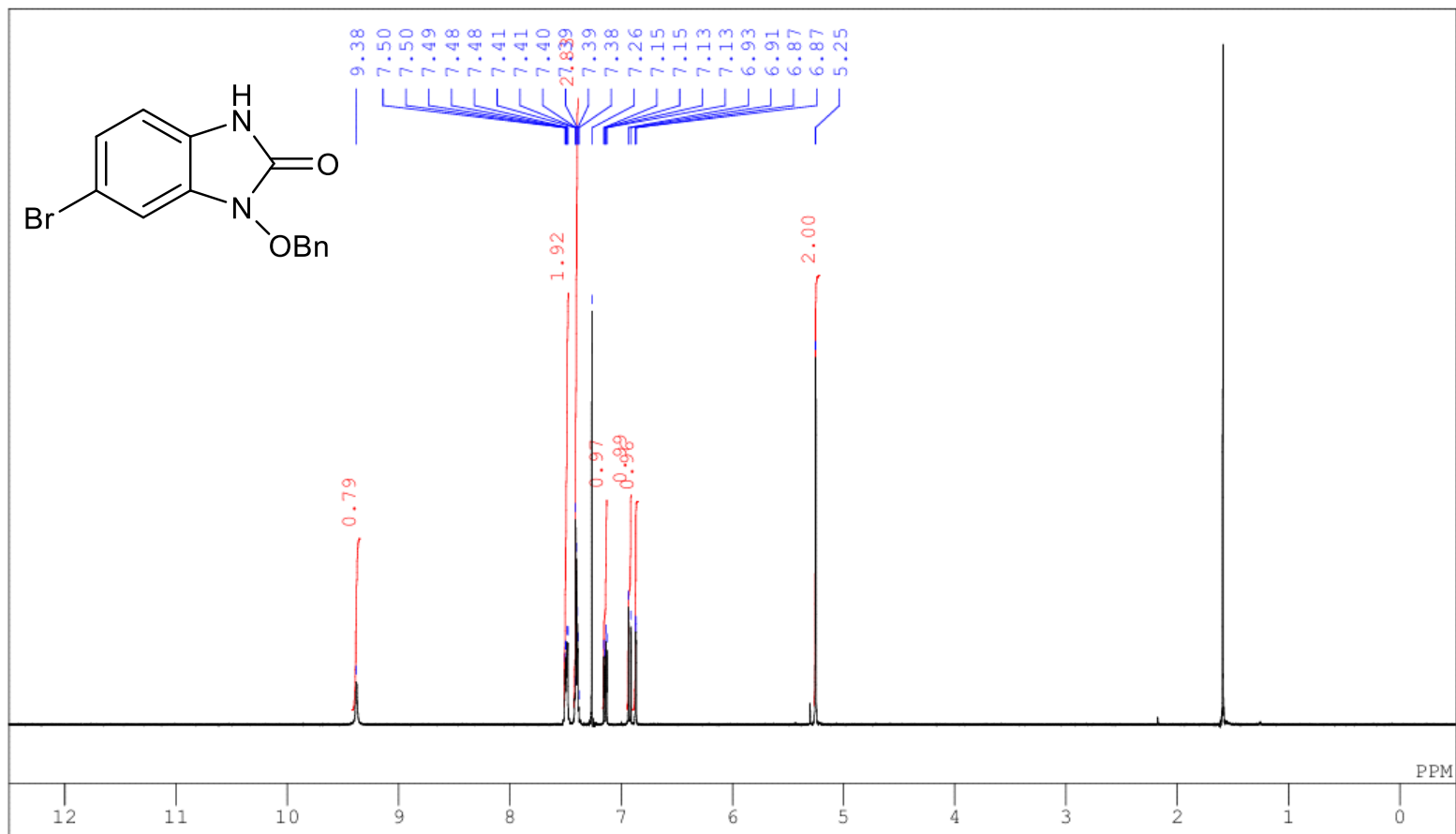
¹H-NMR, ¹³C-NMR, ¹⁹F-NMR spectra-----S2

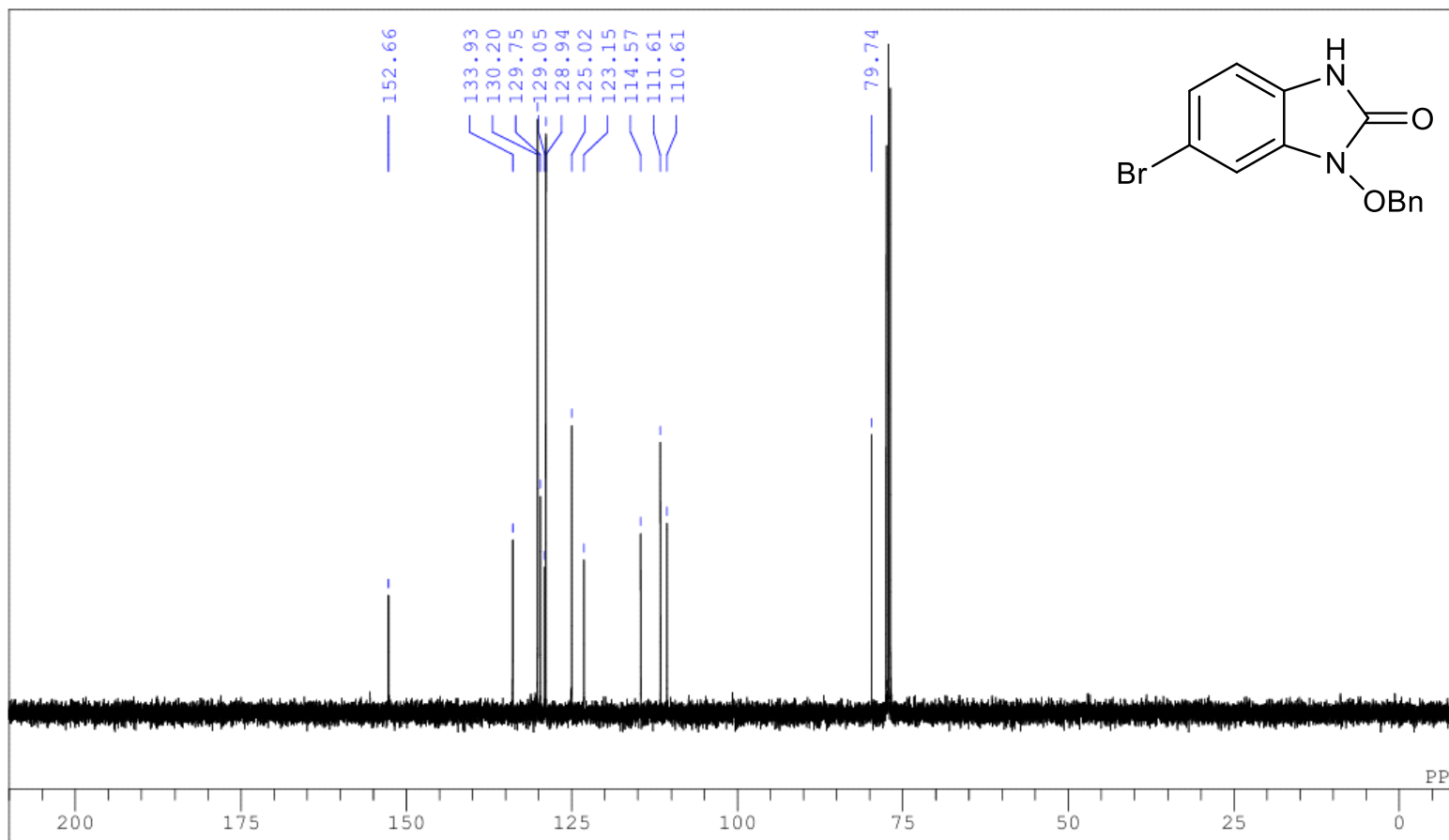
1-(Benzyloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a)

 ^1H NMR (400 MHz, CDCl_3)

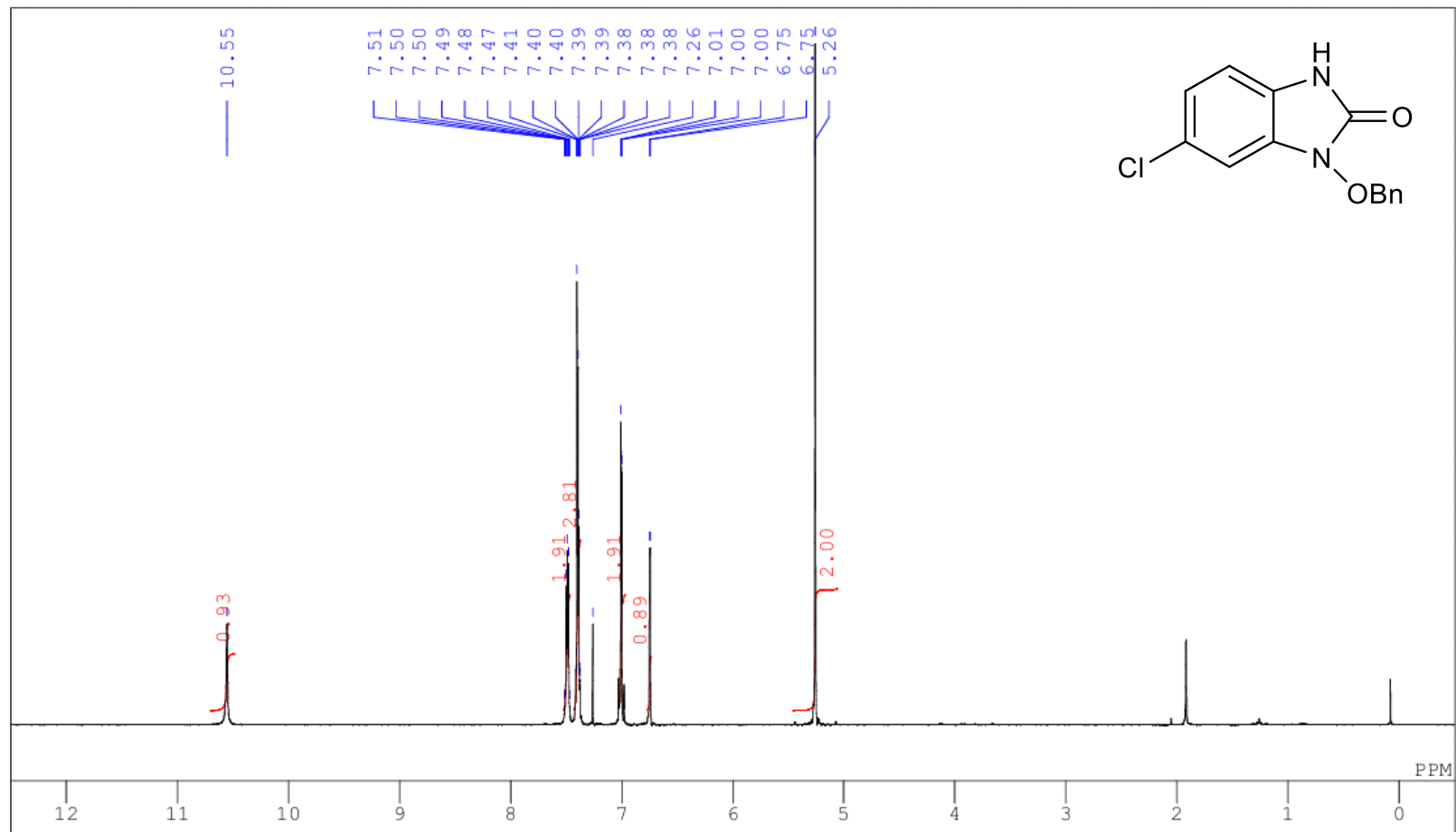
^{13}C NMR (100 MHz, CDCl_3)

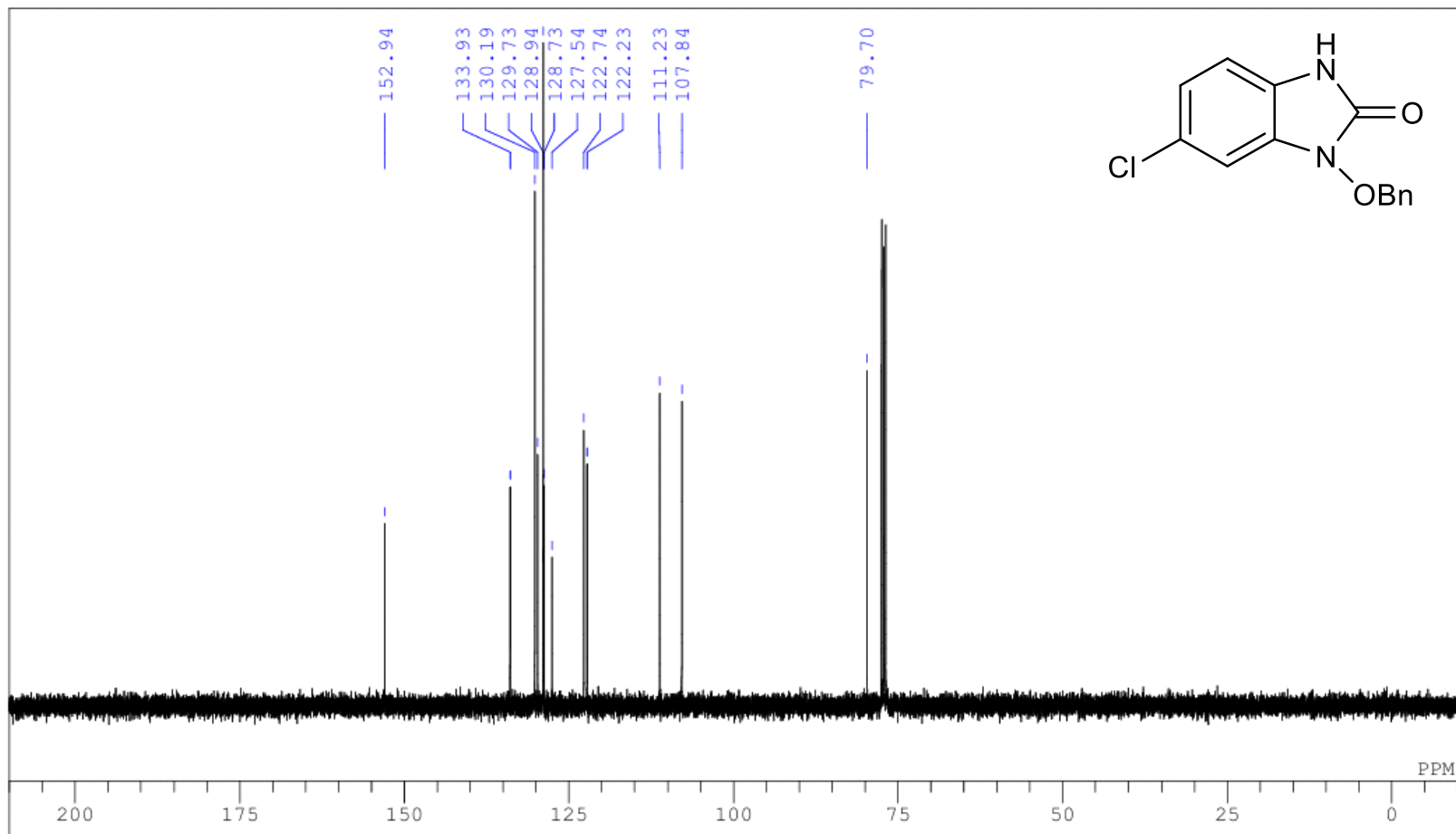
1-(Benzyloxy)-6-bromo-1,3-dihydro-2H-benzo[d]imidazol-2-one (2b)

 ^1H NMR (400 MHz, CDCl_3)

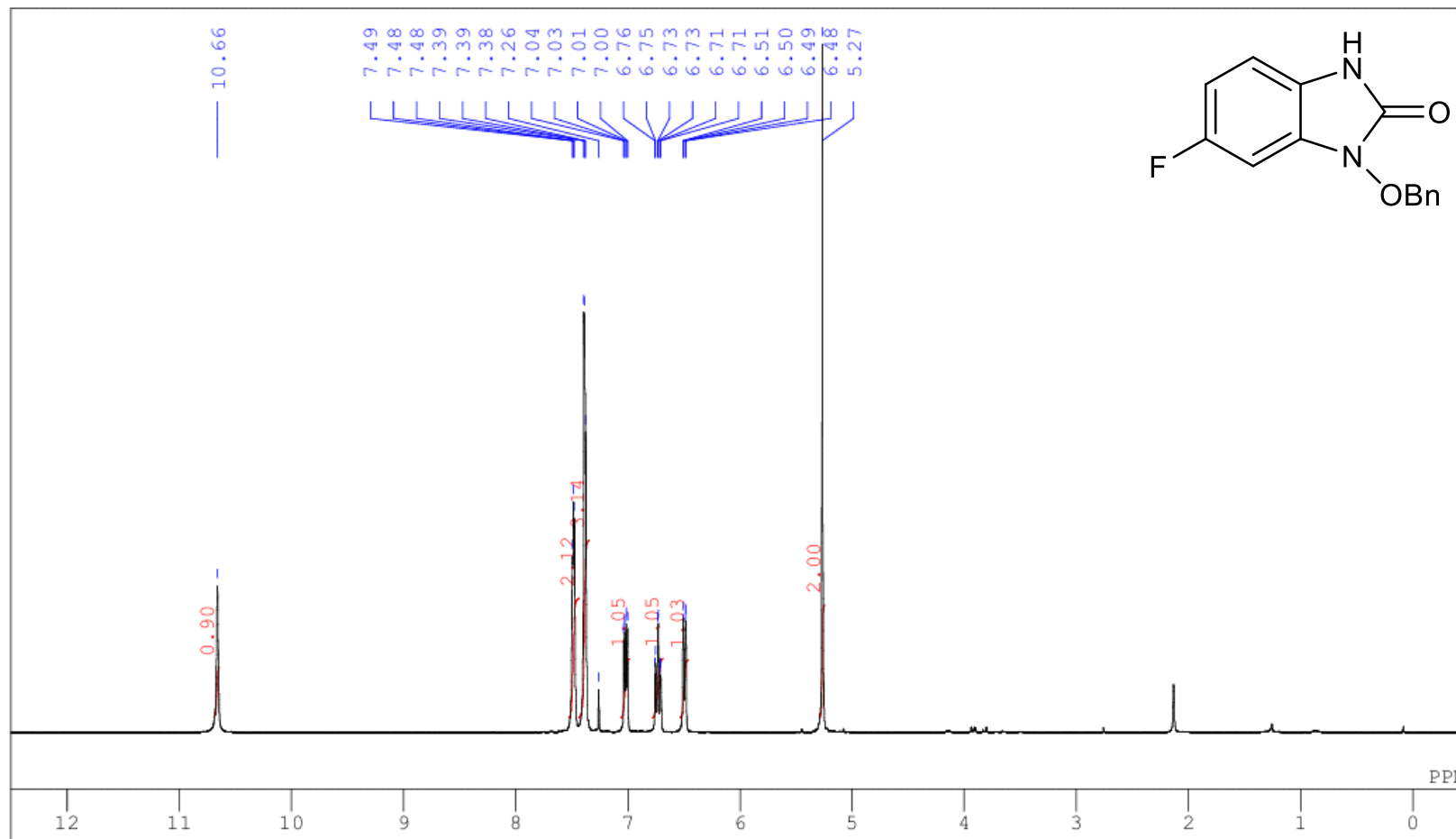
^{13}C NMR (100 MHz, CDCl_3)

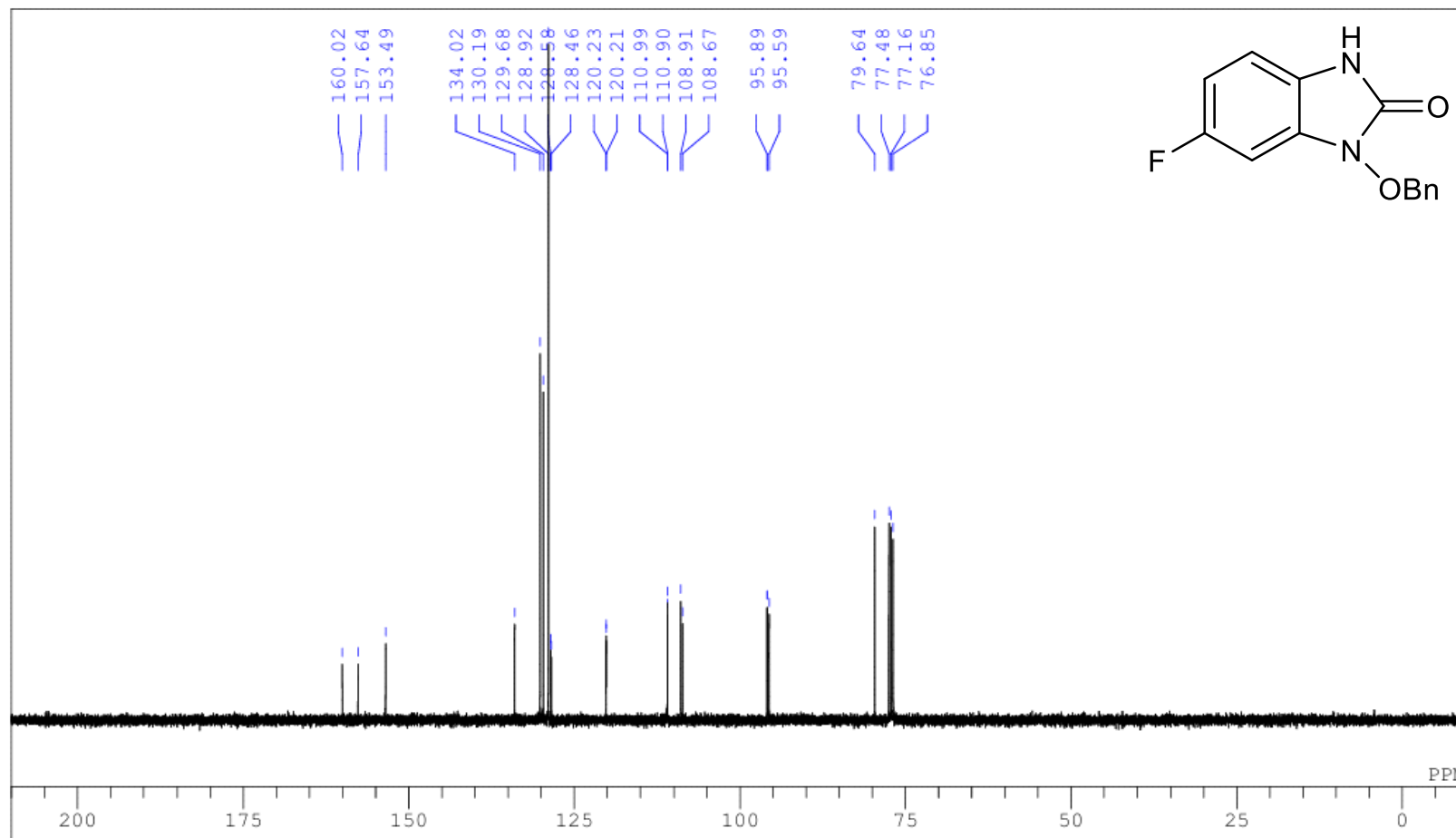
1-(Benzyloxy)-6-chloro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2c)

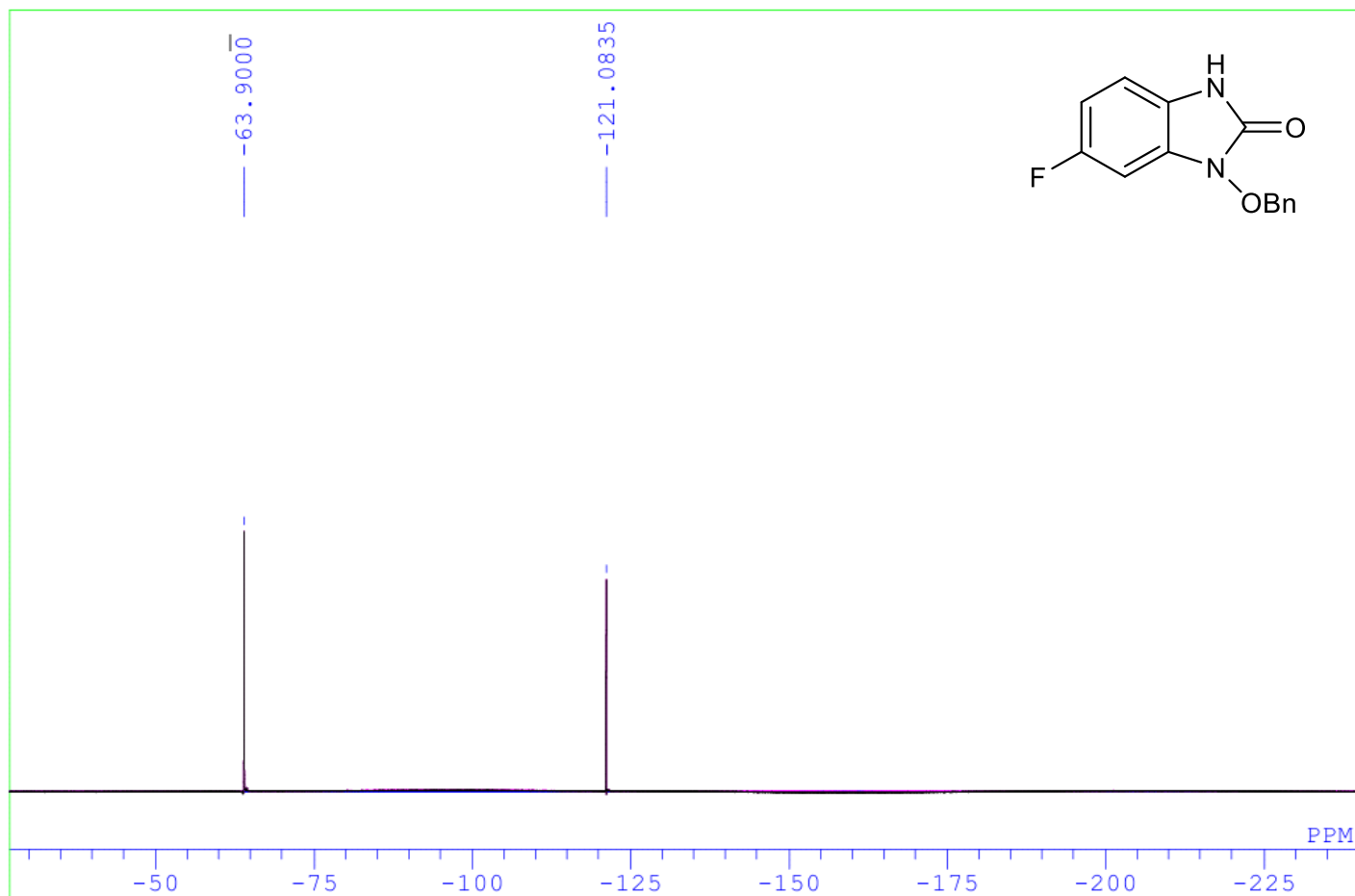
 ^1H NMR (400 MHz, CDCl_3)

^{13}C NMR (100 MHz, CDCl_3)

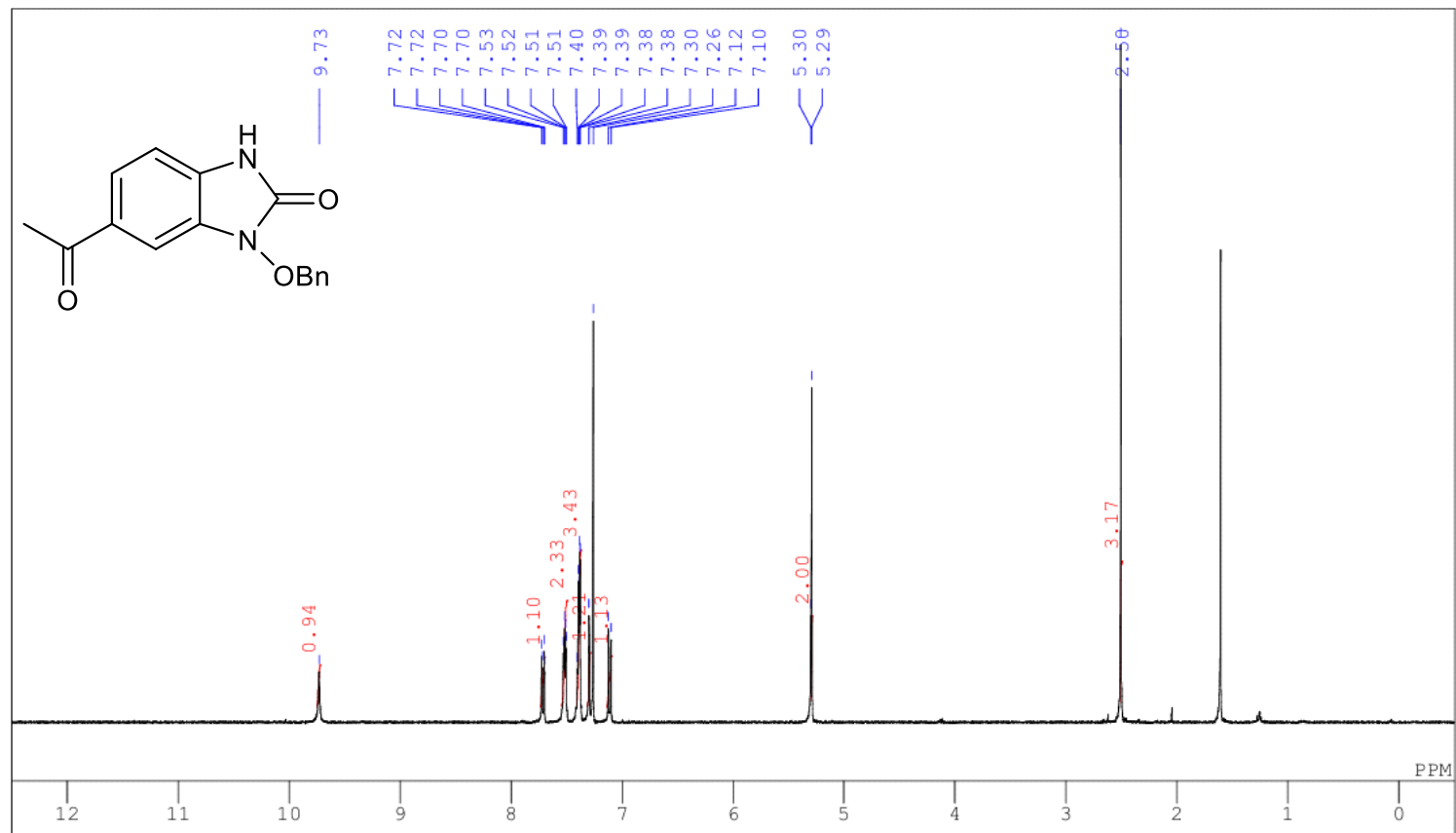
1-(Benzyloxy)-6-fluoro-1,3-dihydro-2H-benzo[d]imidazol-2-one (2d)

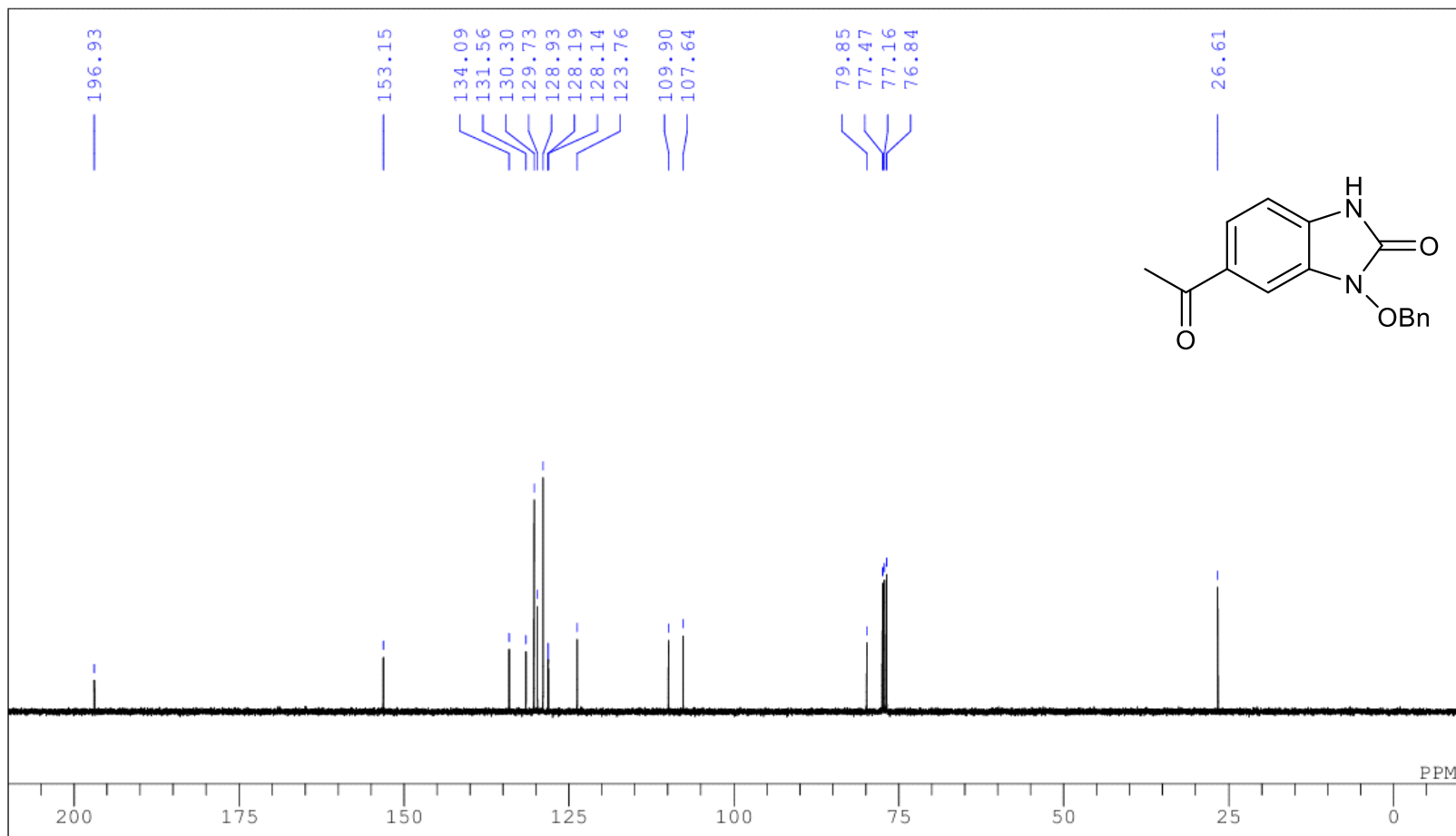
 ^1H NMR (400 MHz, CDCl_3)

¹³C NMR (100 MHz, CDCl₃)

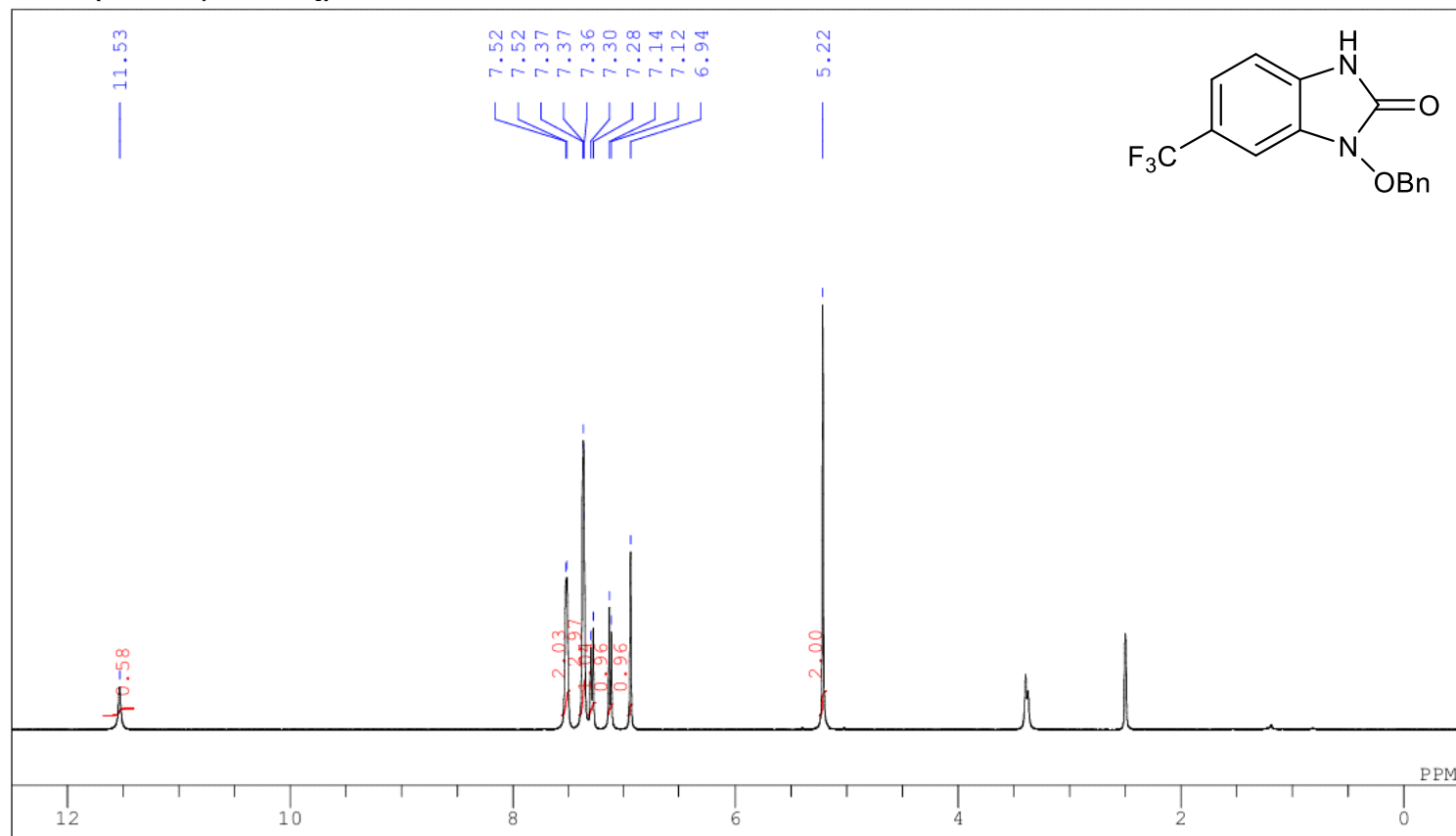
¹⁹F NMR (376 MHz, CDCl₃)

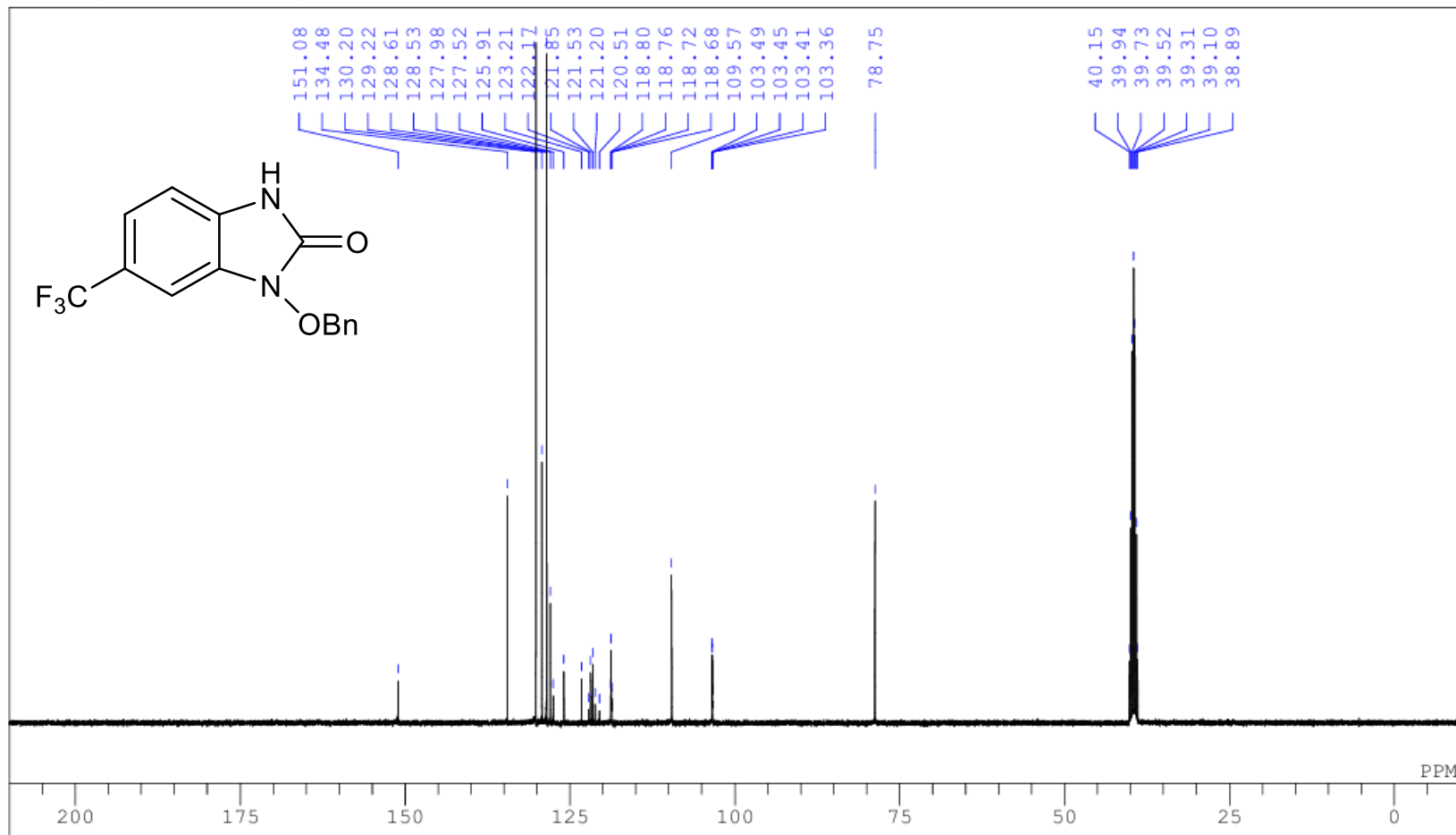
6-Acetyl-1-(benzyloxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2i)

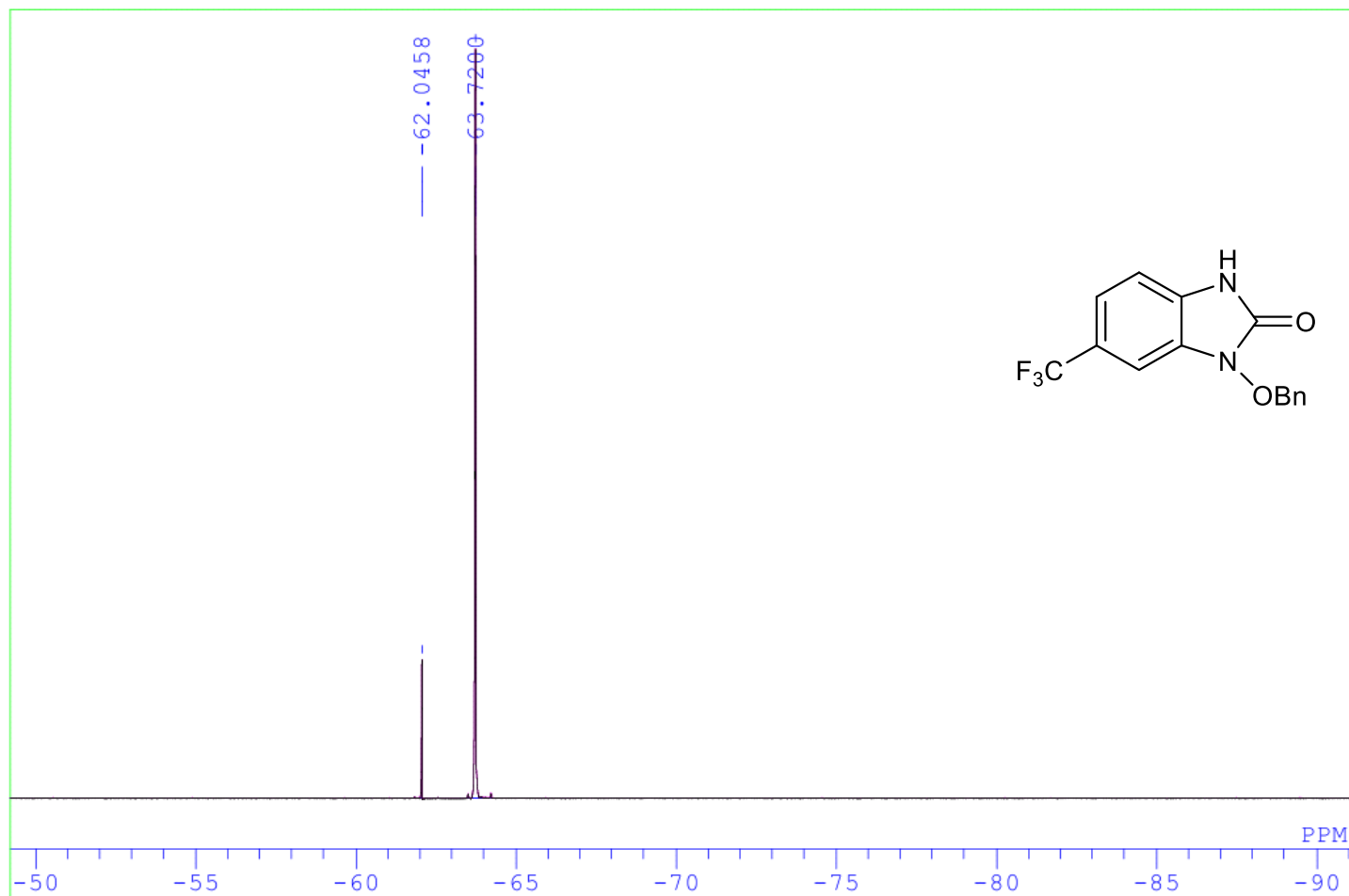
 ^1H NMR (400 MHz, CDCl_3)

^{13}C NMR (100 MHz, CDCl_3)

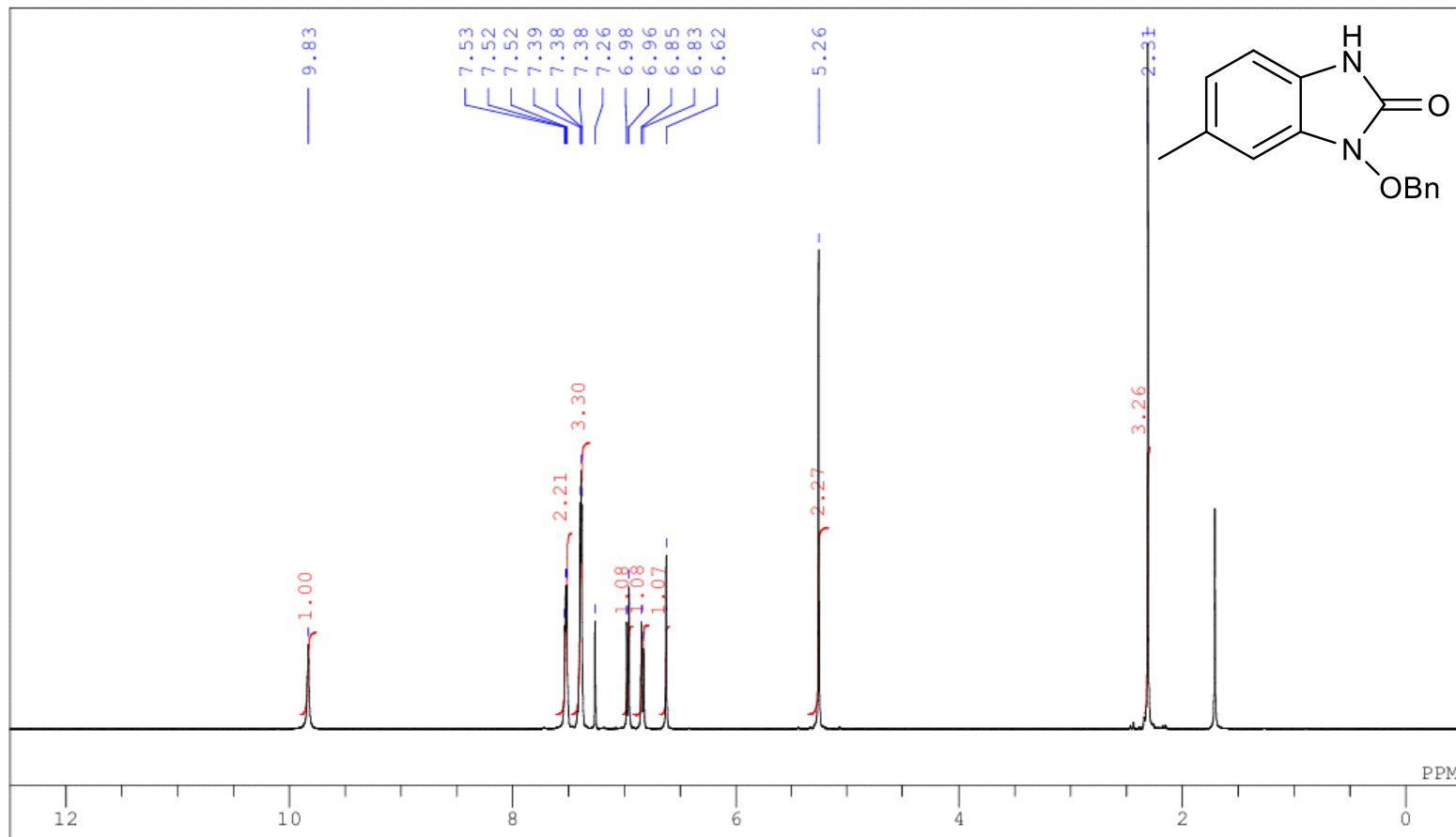
1-(Benzyloxy)-6-(trifluoromethyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2k)

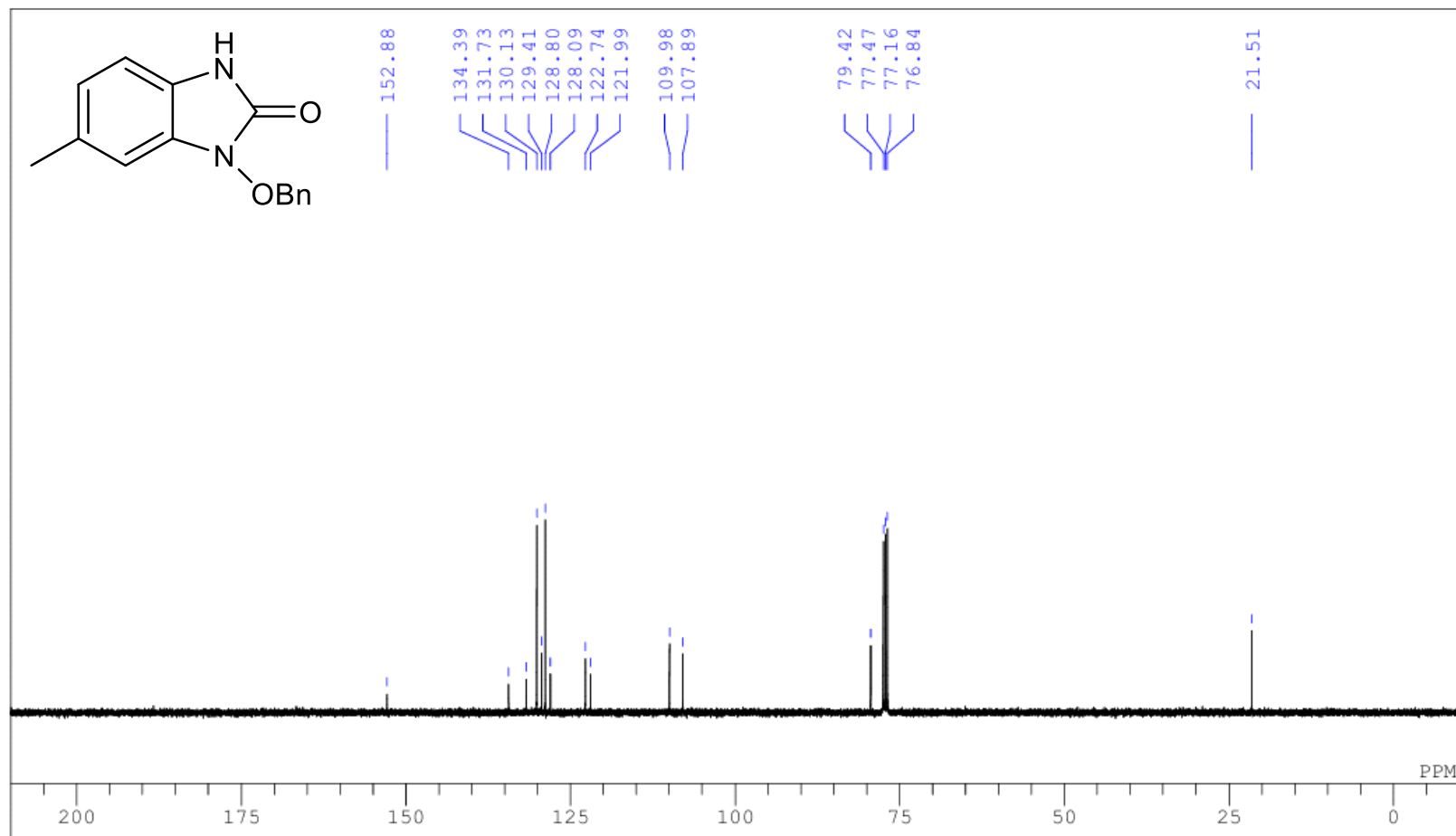
¹H NMR (400 MHz, DMSO-D₆)

^{13}C NMR (100 MHz, DMSO- D_6)

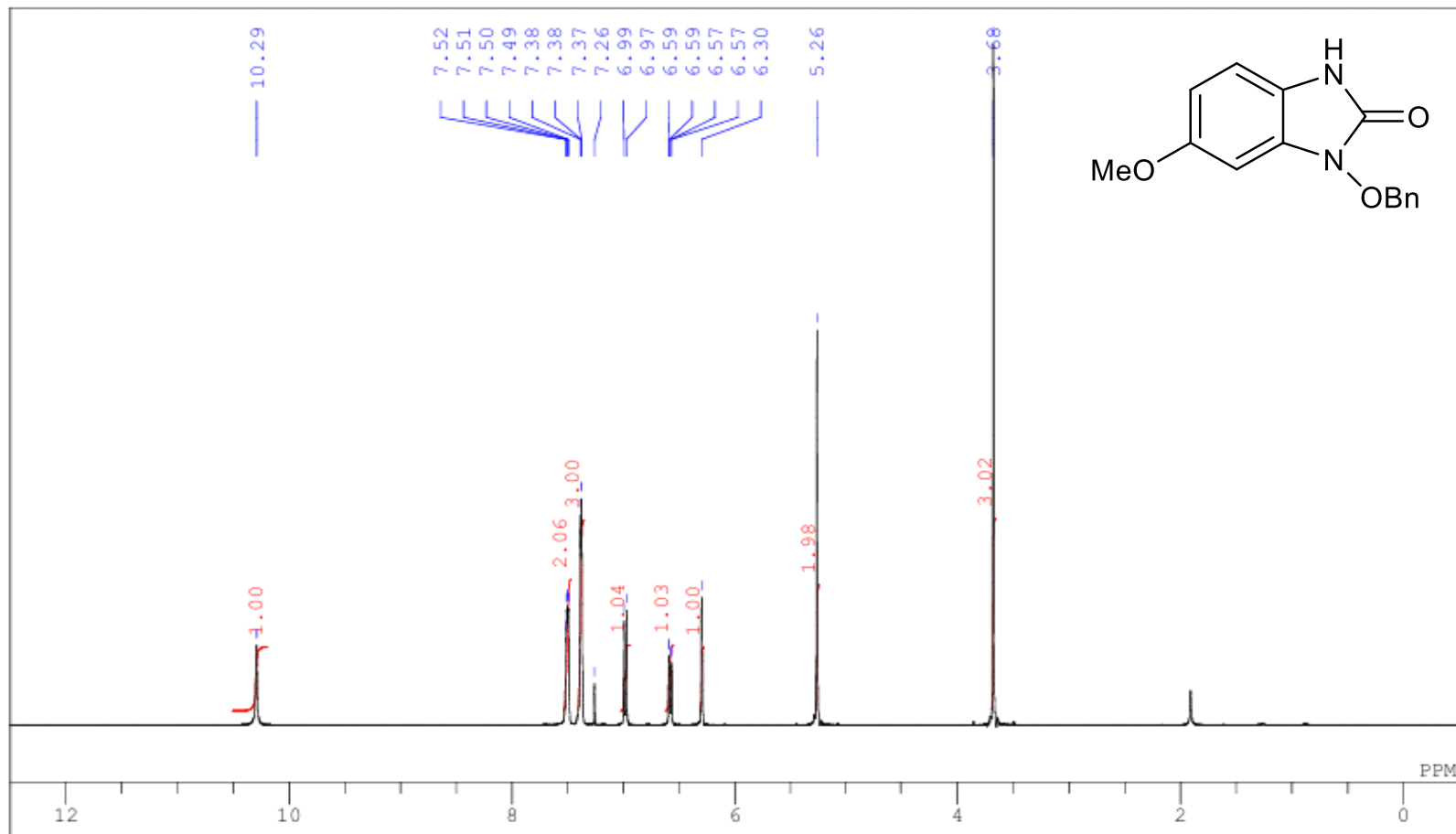
¹⁹F NMR (376 MHz, DMSO-D6)

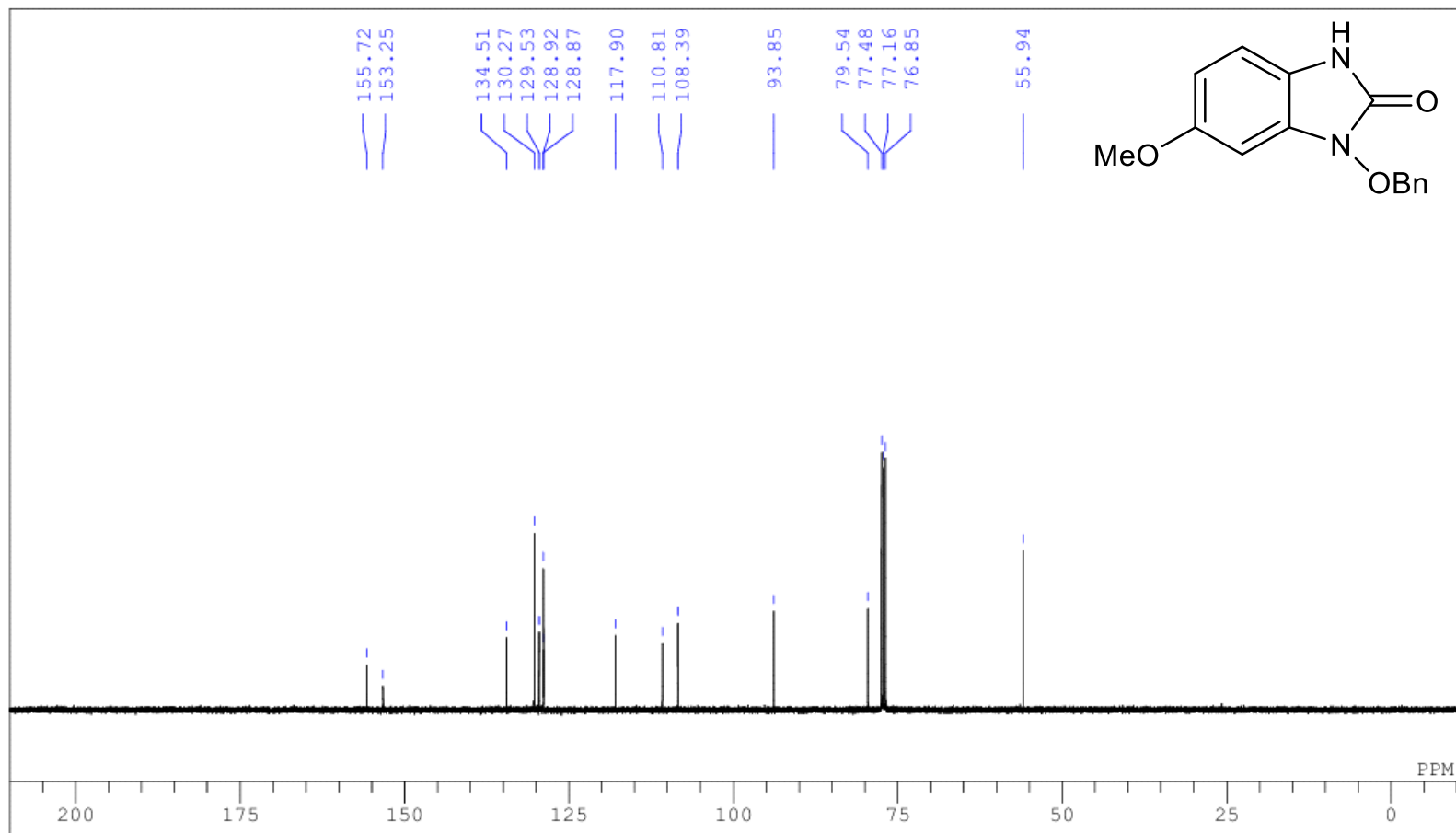
1-(Benzyloxy)-6-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2g)

 ^1H NMR (400 MHz, CDCl_3)

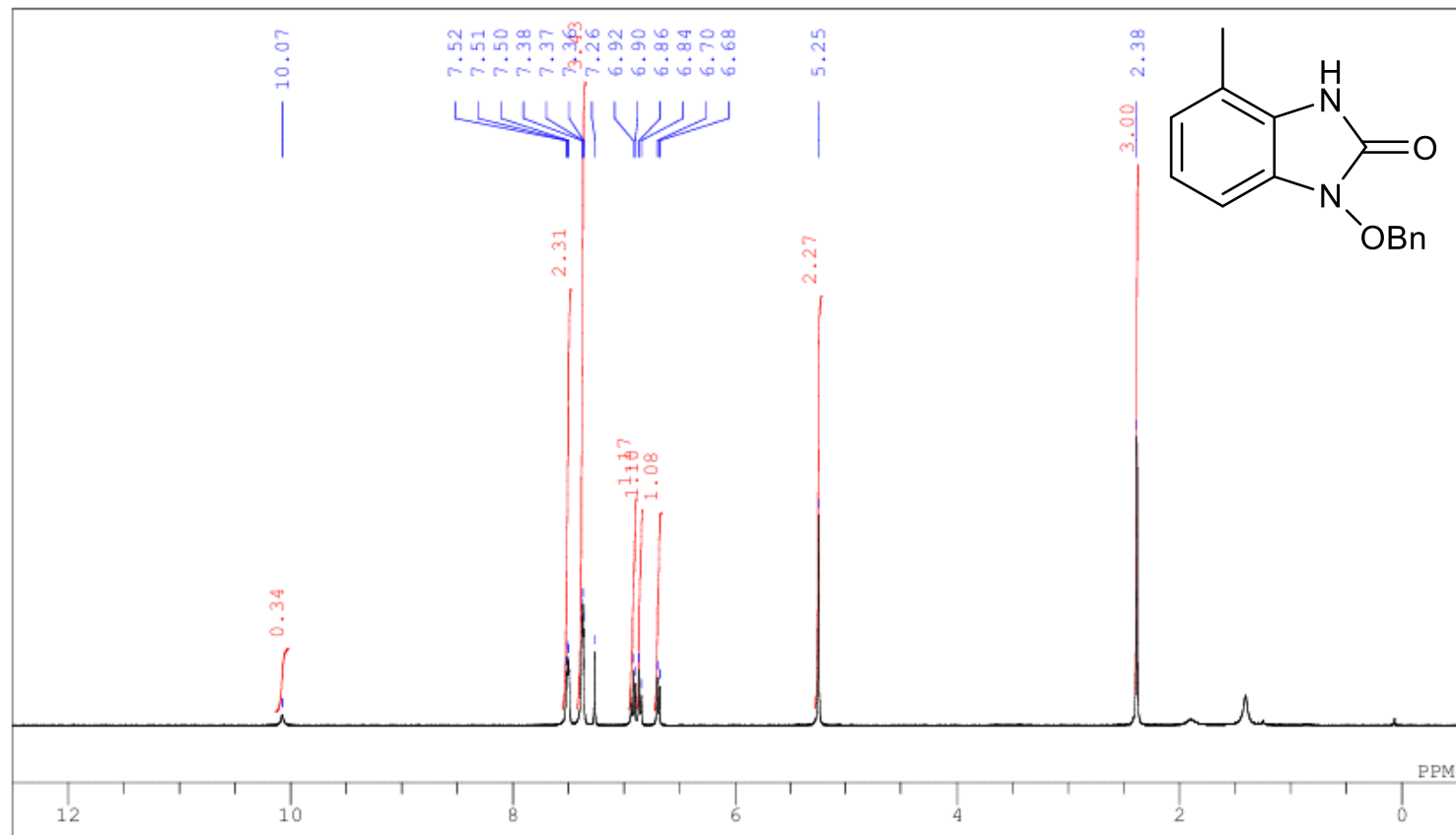
¹³C NMR (100 MHz, CDCl₃)

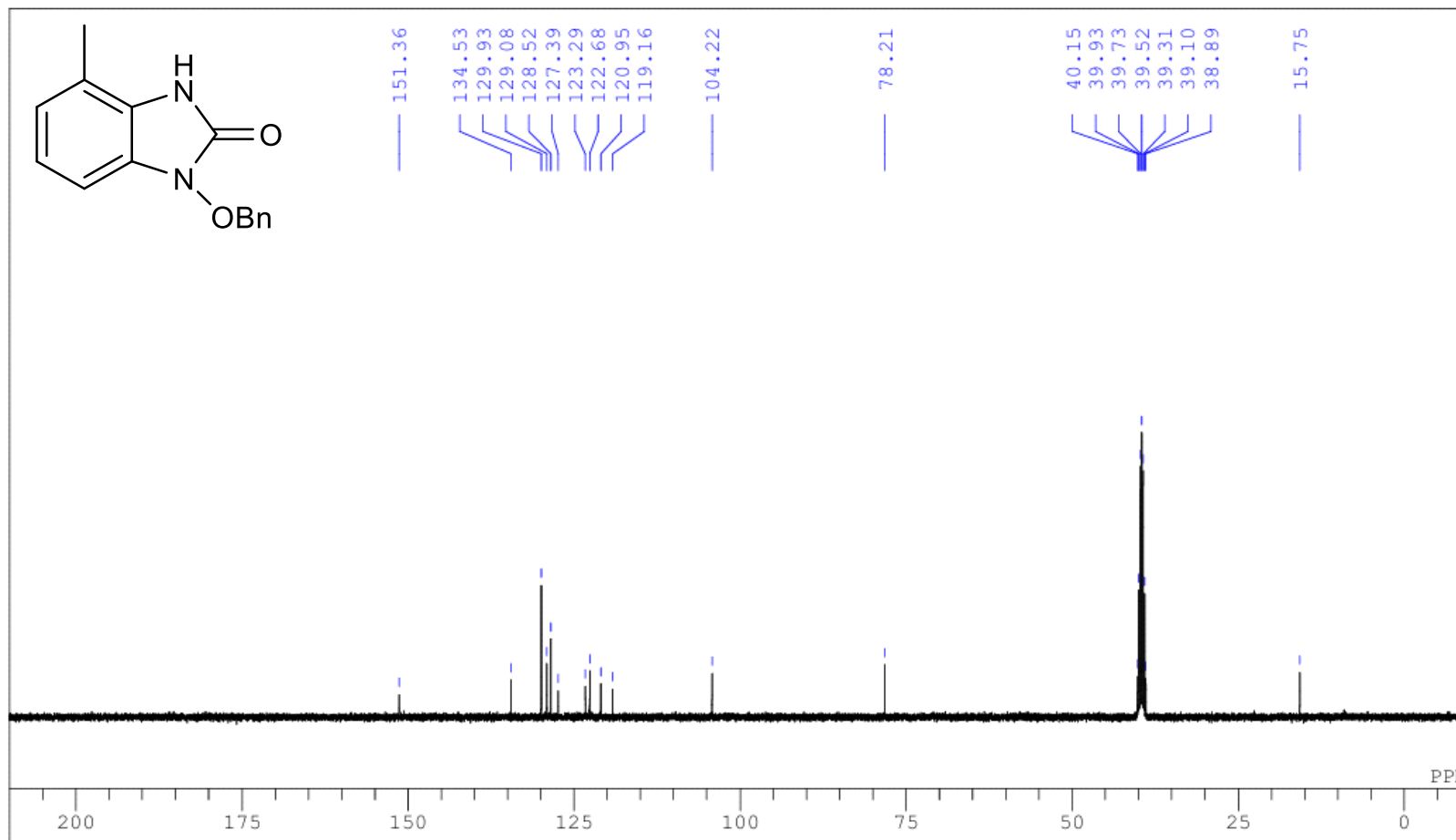
1-(Benzyloxy)-6-methoxy-1,3-dihydro-2H-benzo[d]imidazol-2-one (2j)

 ^1H NMR (400 MHz, CDCl_3)

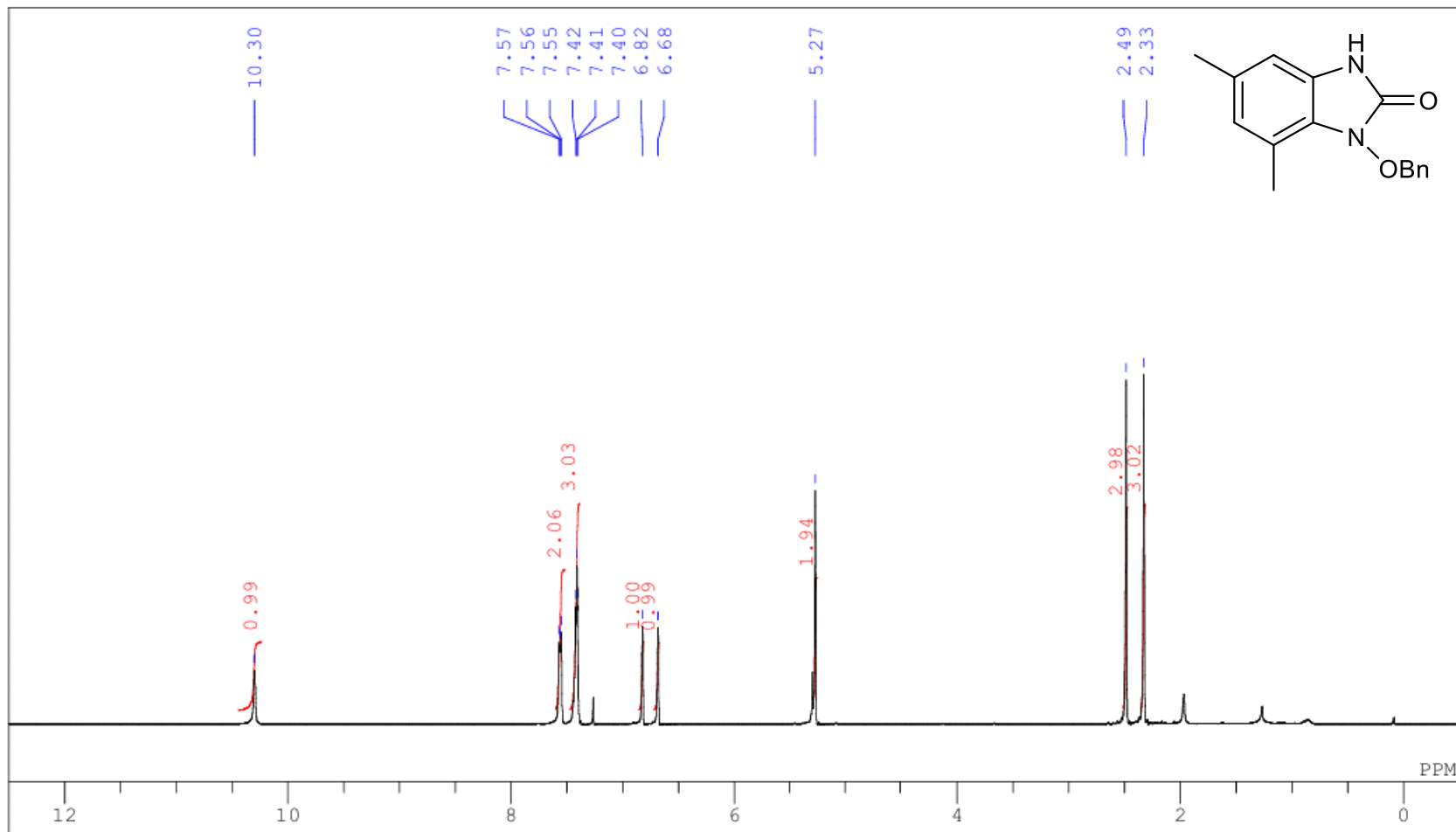
^{13}C NMR (100 MHz, CDCl_3)

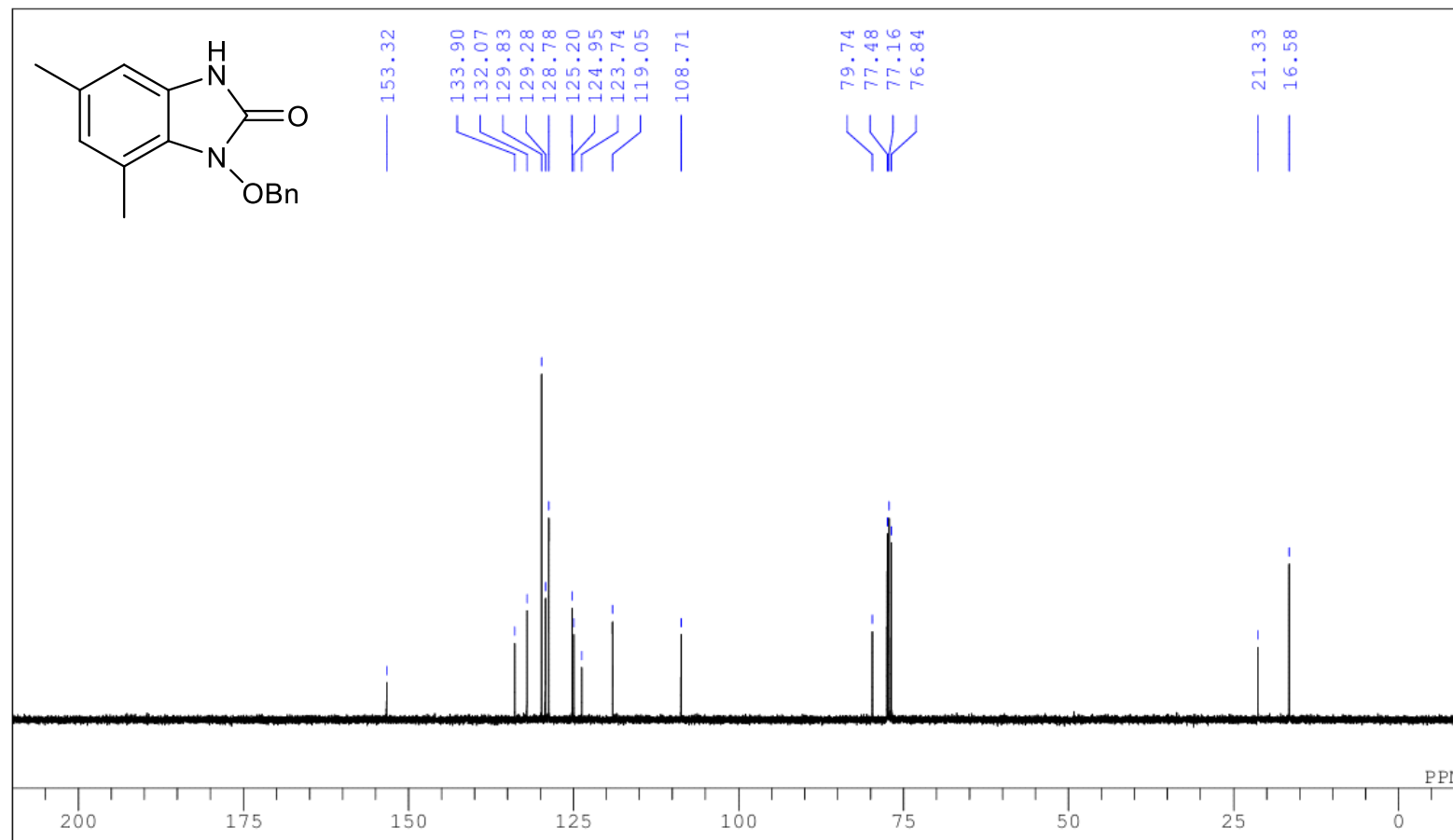
1-(Benzyloxy)-4-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2f)

 ^1H NMR (400 MHz, CDCl_3)

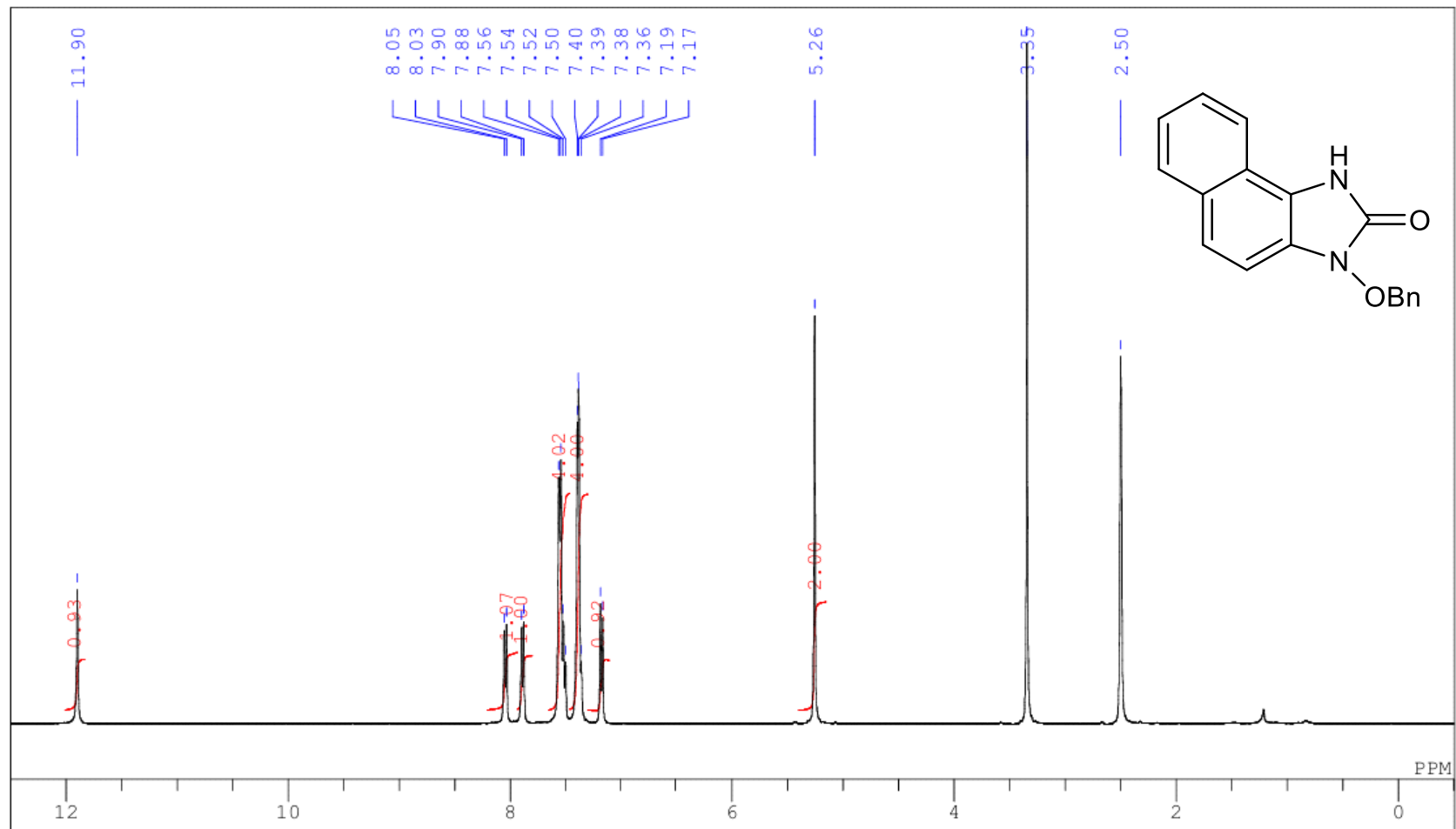
^{13}C NMR (100 MHz, DMSO- D_6)

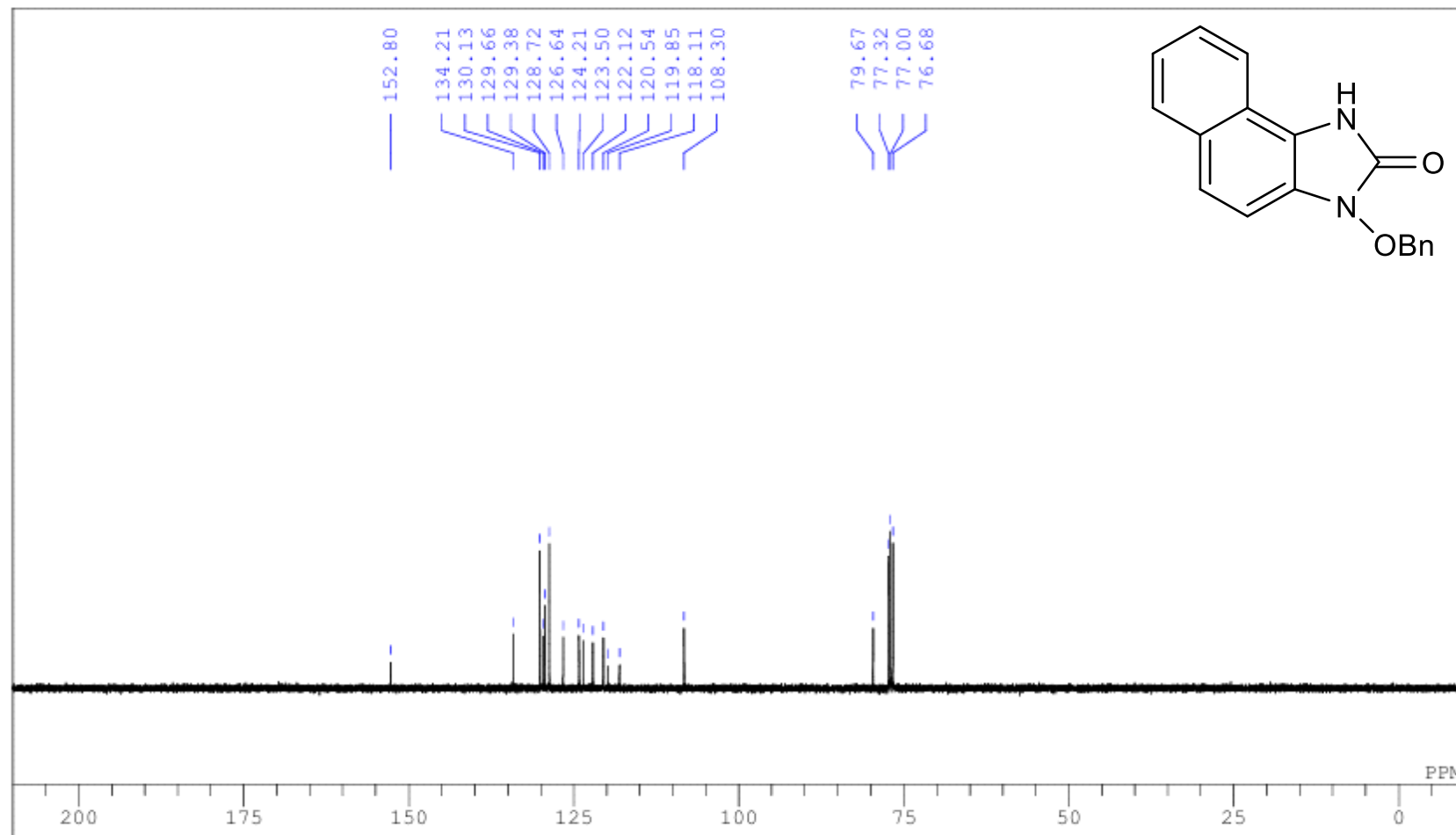
1-(Benzyloxy)-5,7-dimethyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2h)

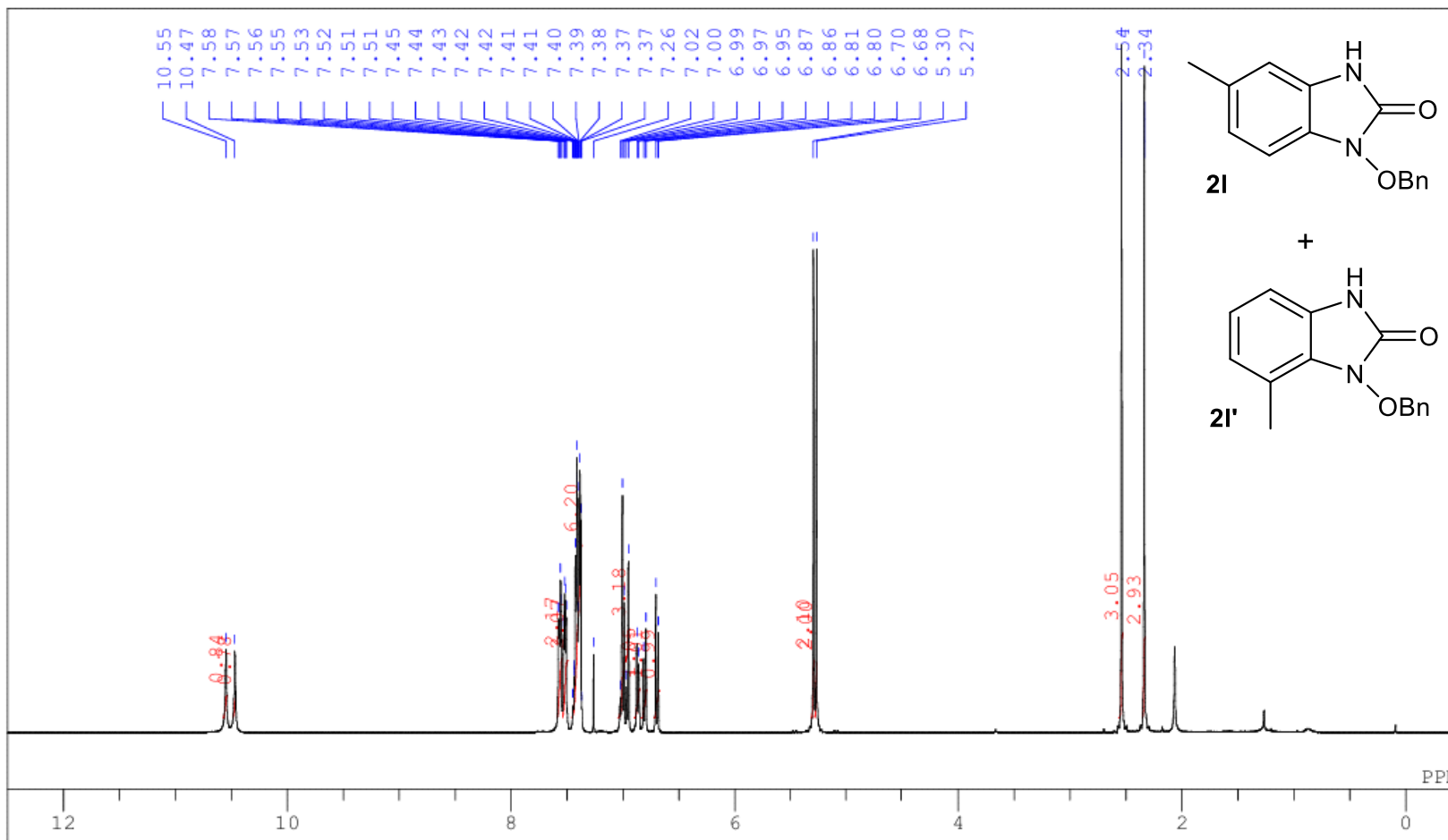
 ^1H NMR (400 MHz, CDCl_3)

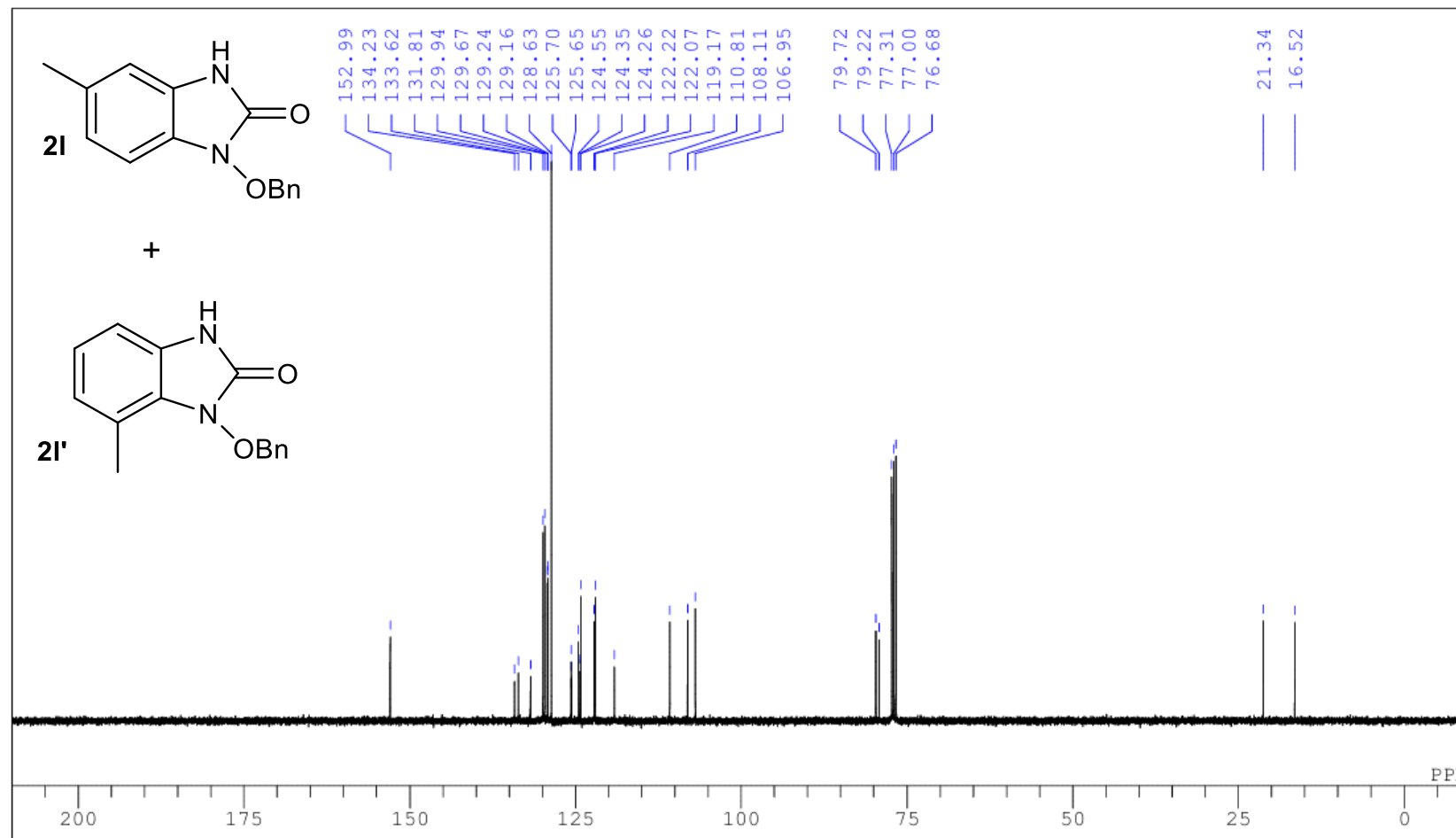
^{13}C NMR (100 MHz, CDCl_3)

3-(Benzyloxy)-1,3-dihydro-2H-naphtho[1,2-d]imidazol-2-one (2k)

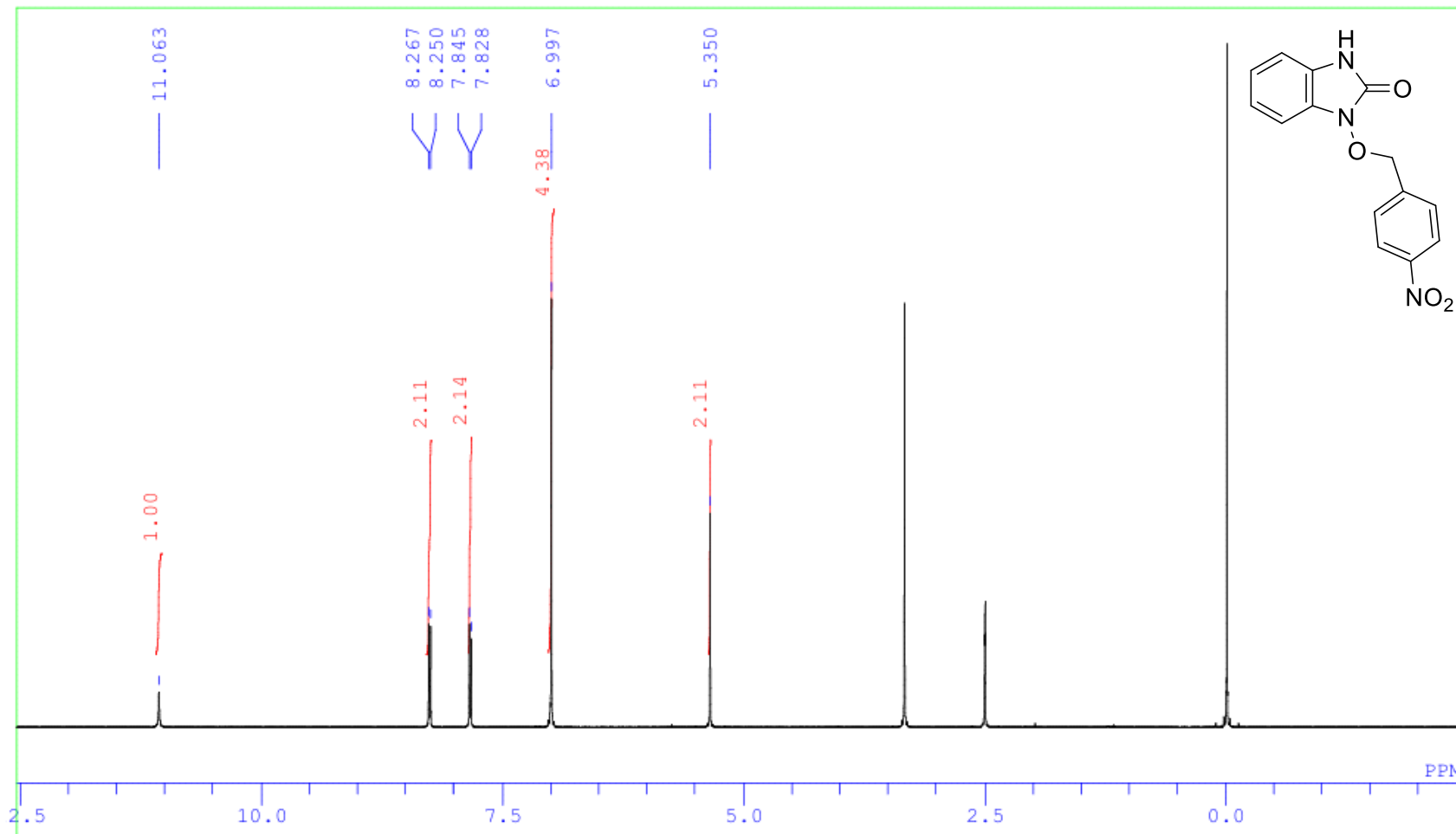
 ^1H NMR (400 MHz, DMSO- D_6)

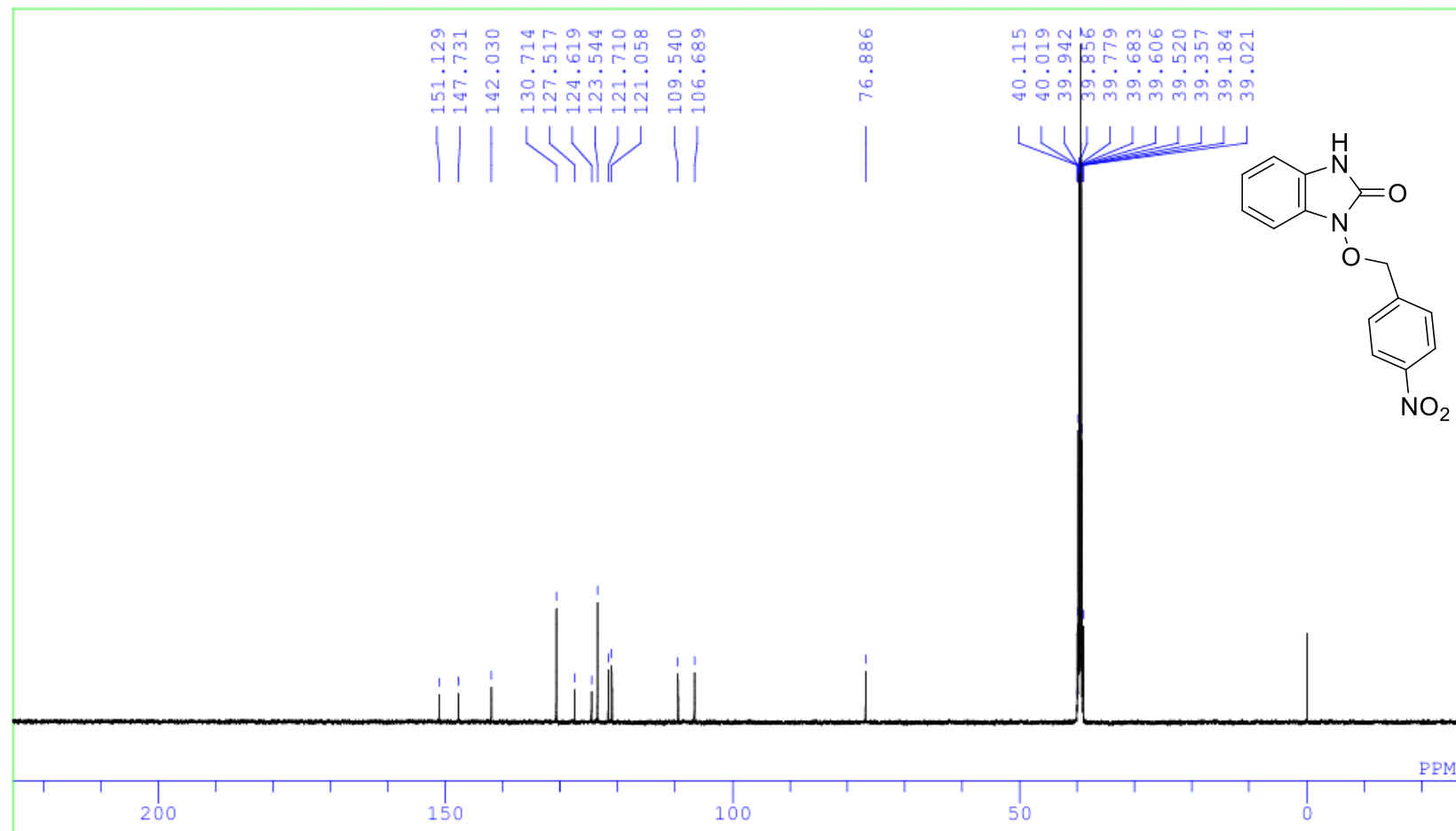
^{13}C NMR (100 MHz, CDCl_3)

1-(Benzyloxy)-5-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2I) and 1-(Benzyloxy)-7-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2I') (mixture)**¹H NMR (400 MHz, CDCl₃)**

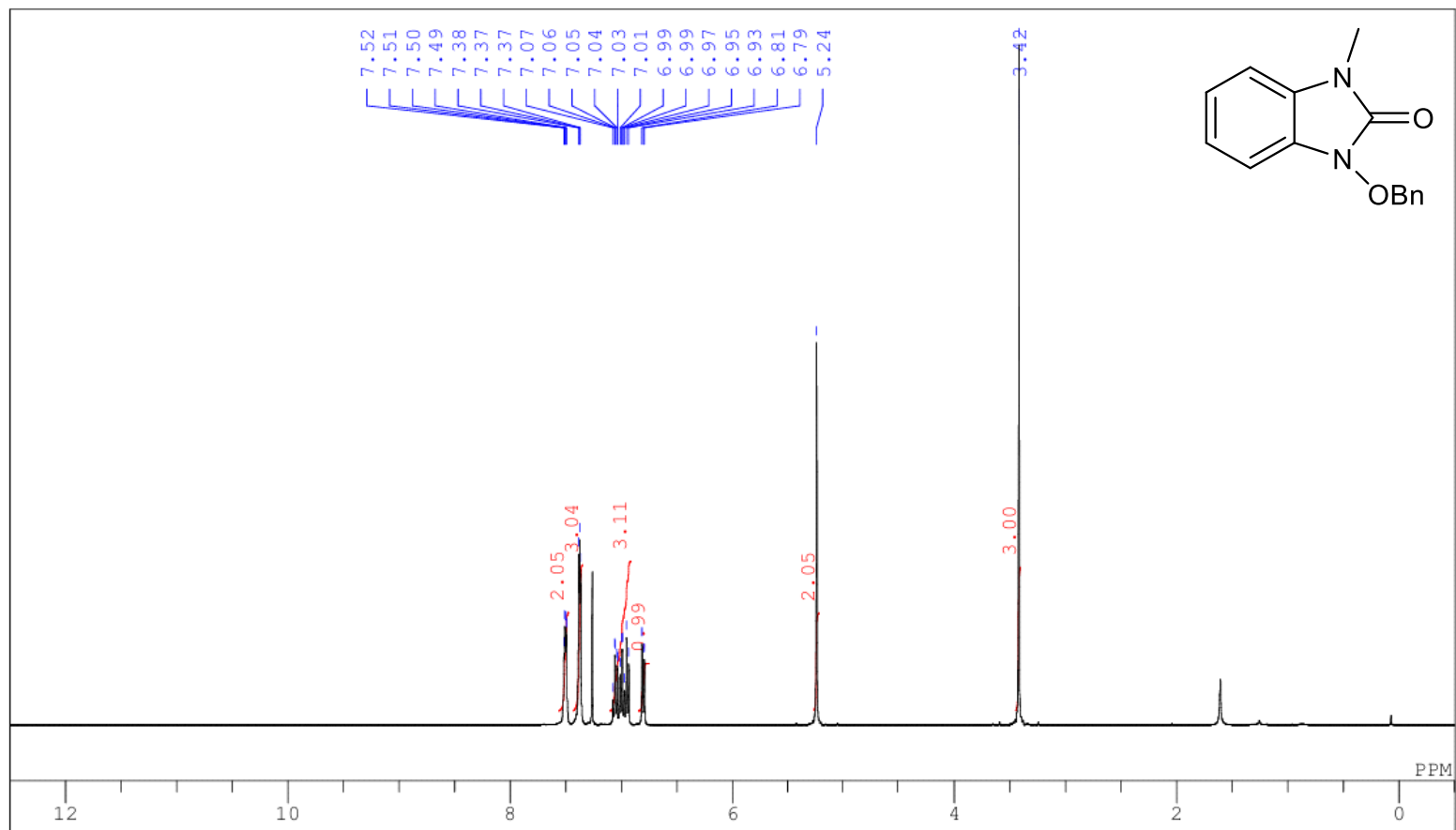
^{13}C NMR (100 MHz, CDCl_3)

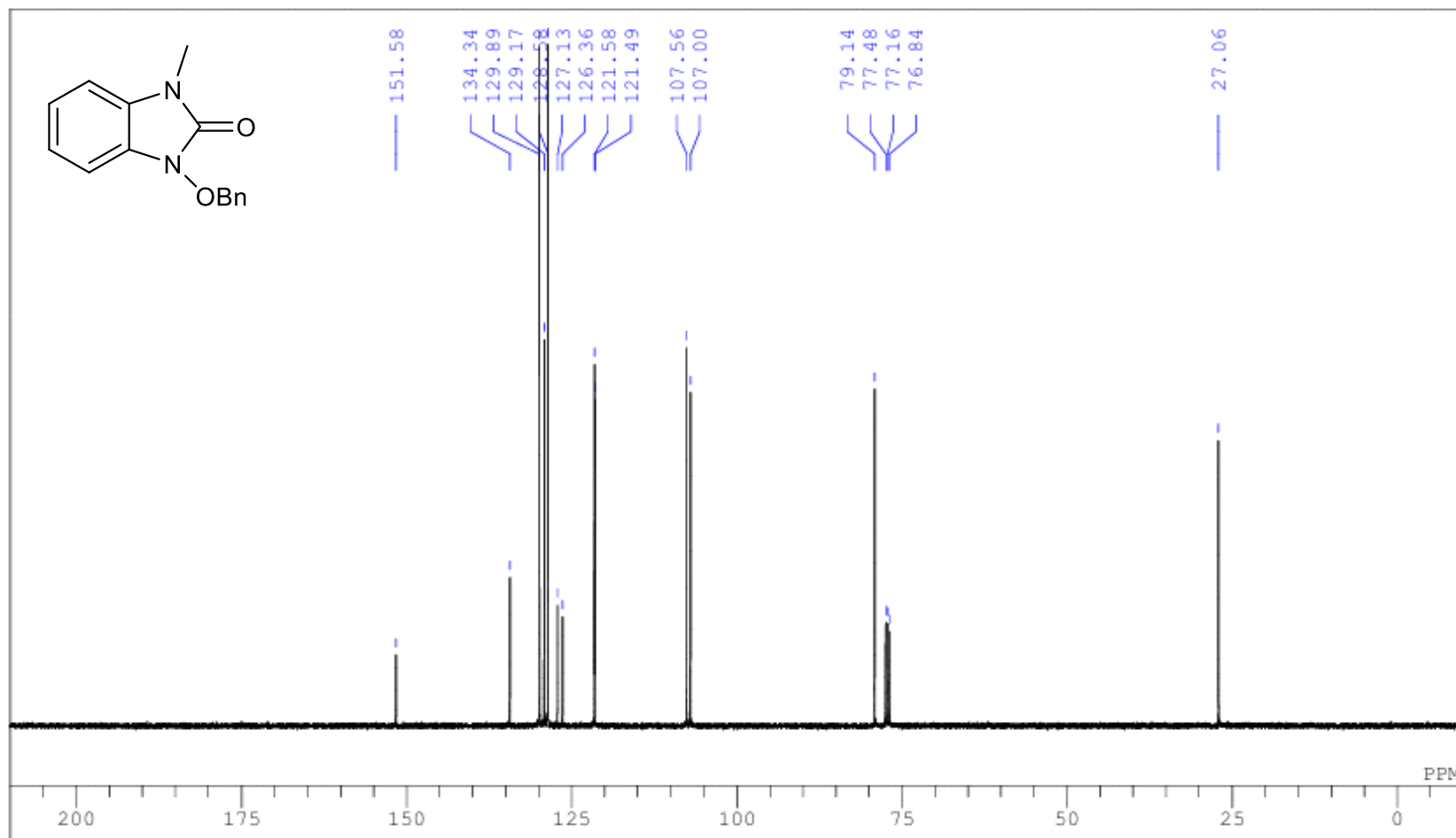
1-((4-Nitrobenzyl)oxy)-1,3-dihydro-2H-benzo[d]imidazol-2-one (2m)

¹H NMR (400 MHz, DMSO-D₆)

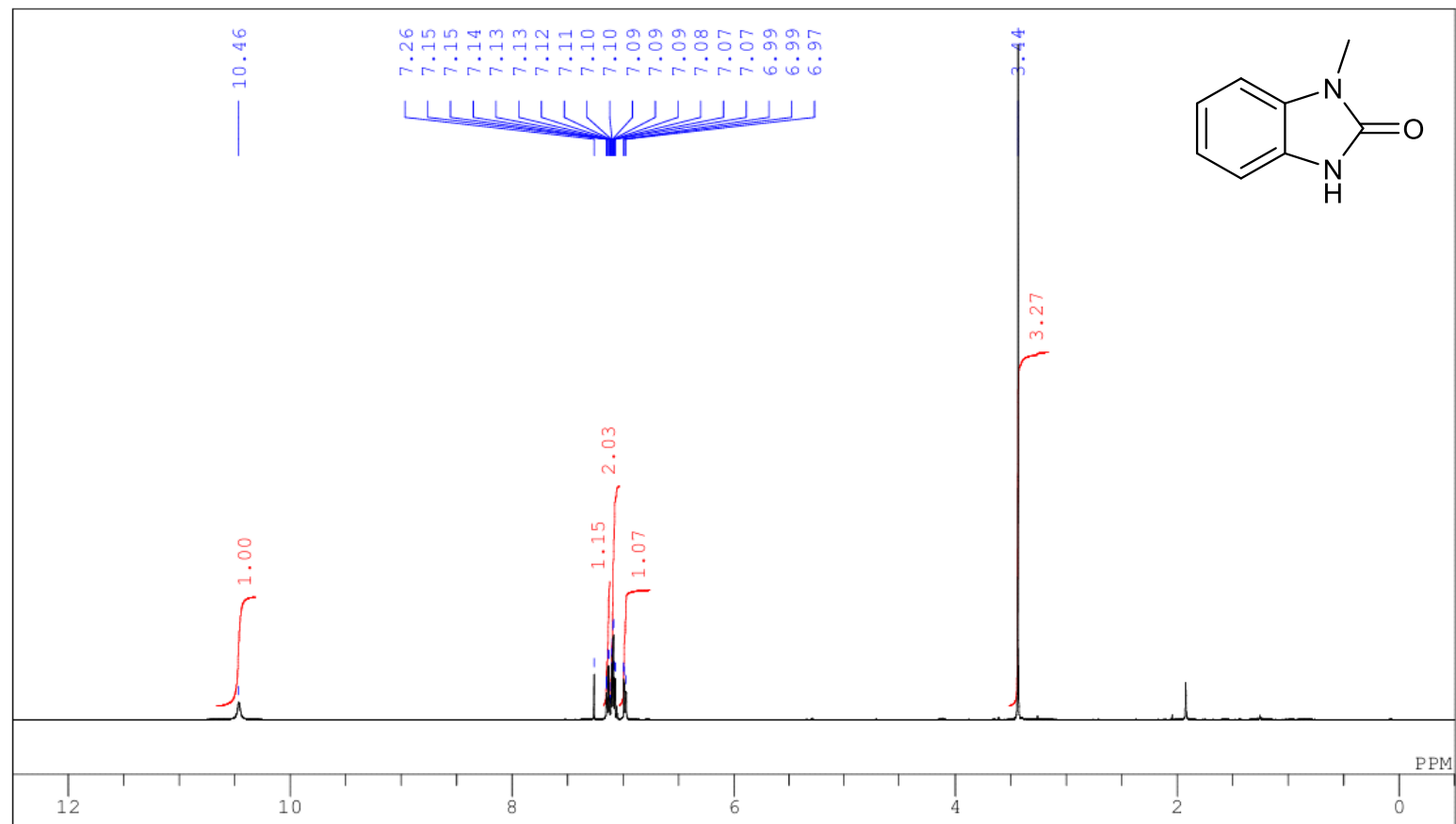
¹³C NMR (100 MHz, DMSO-D₆)

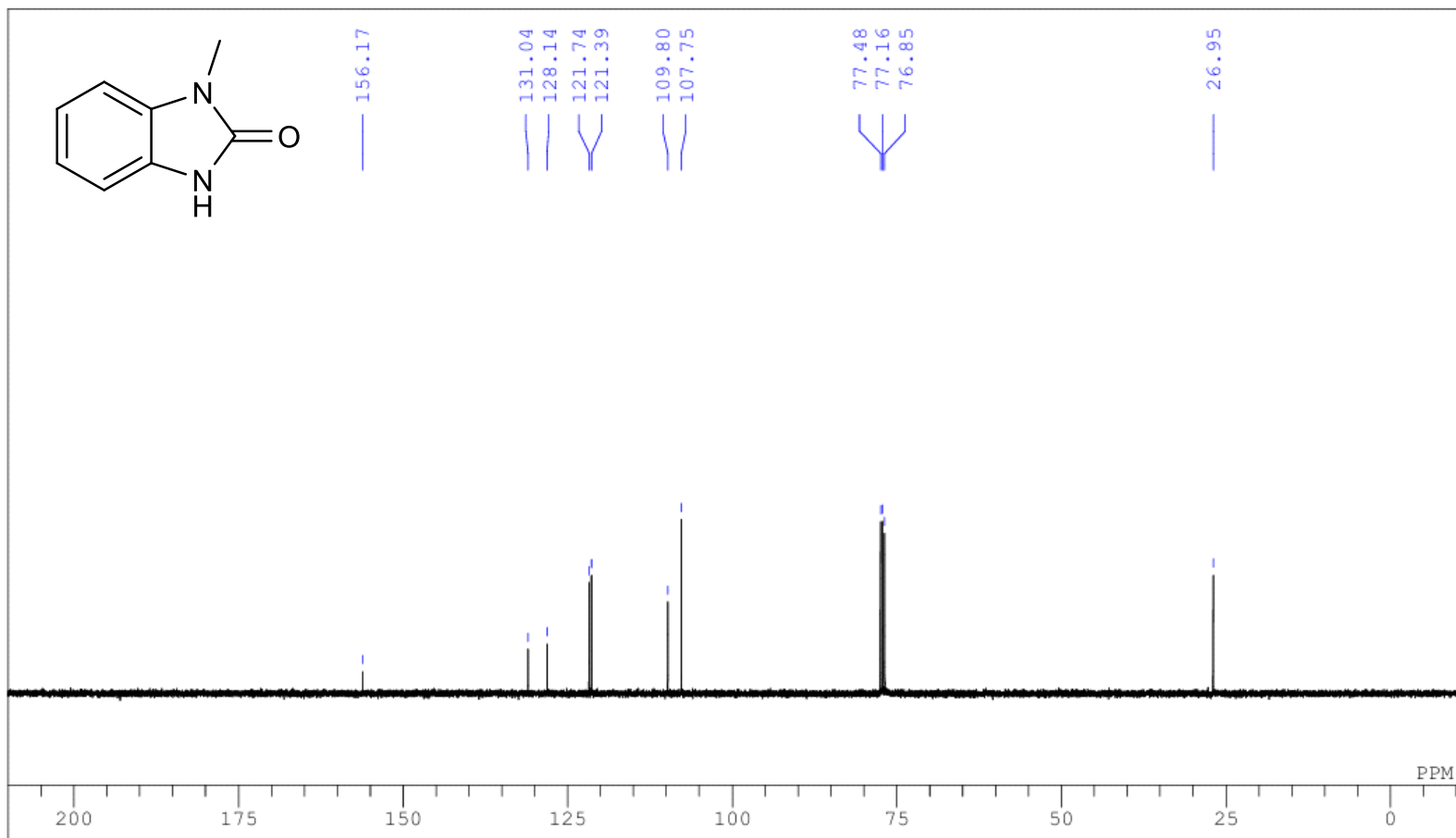
1-(Benzyloxy)-3-methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a')

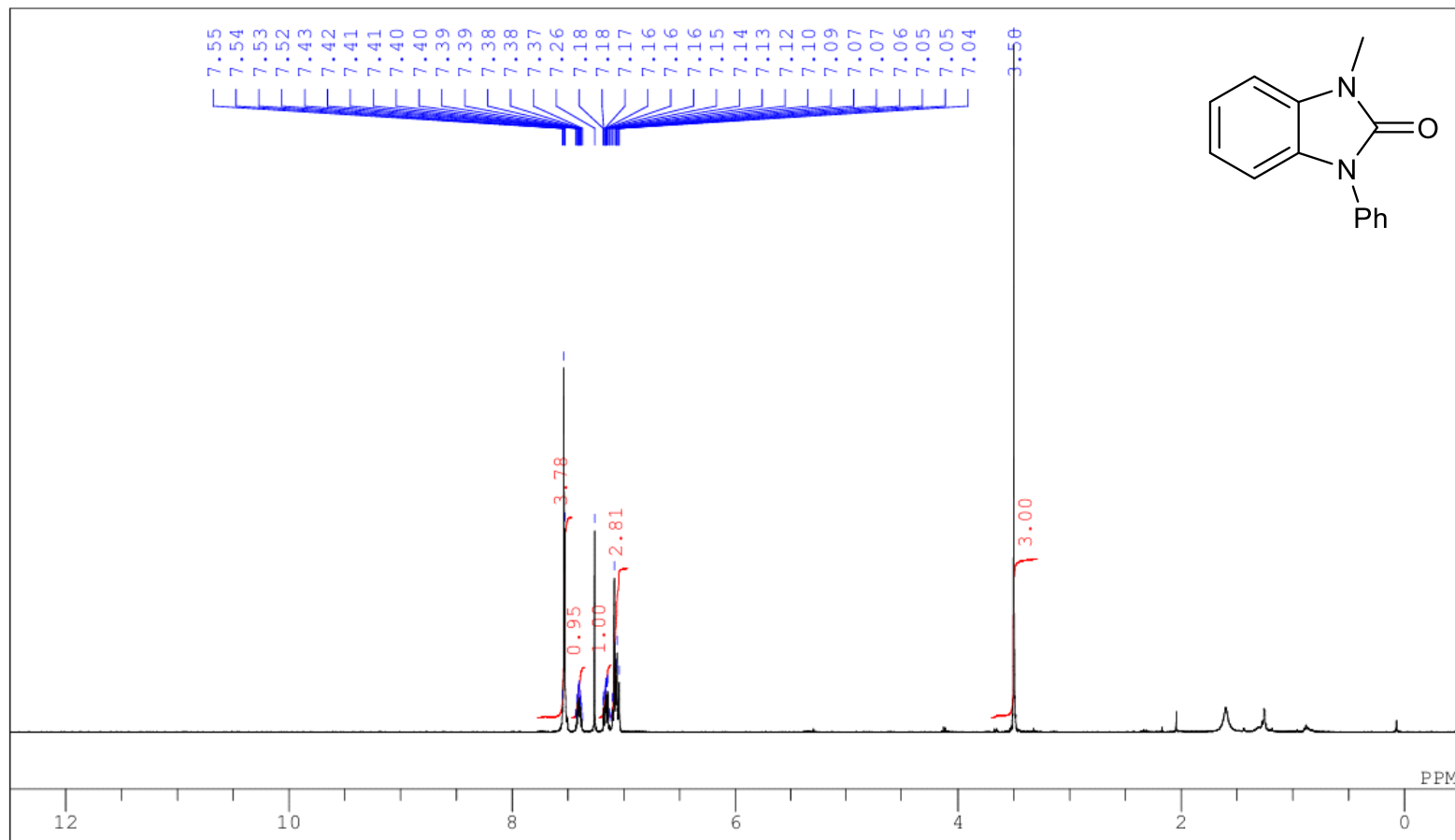
 ^1H NMR (400 MHz, CDCl_3)

¹³C NMR (100 MHz, CDCl₃)

1-Methyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (2a'')

 ^1H NMR (400 MHz, CDCl_3)

^{13}C NMR (100 MHz, CDCl_3)

1-Methyl-3-phenyl-1,3-dihydro-2H-benzo[d]imidazol-2-one (3a)¹H NMR (400 MHz, CDCl₃)

^{13}C NMR (100 MHz, CDCl_3)