

Supporting Information

An Efficient Palladium Catalyzed Mizoroki-Heck Cross-Coupling in Water

Sanjay N. Jadhav, Chandrashekhar V. Rode*

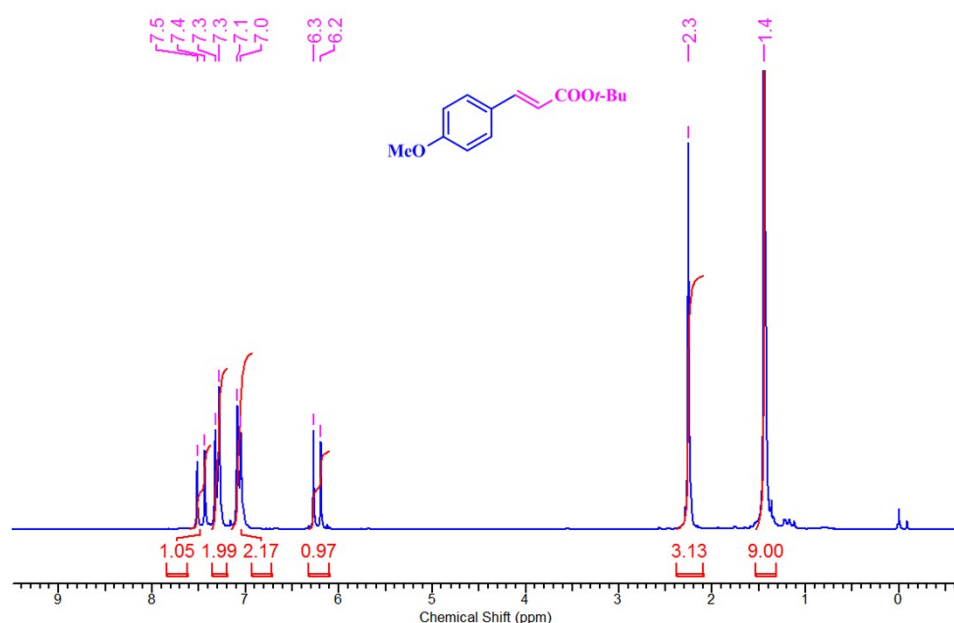
Chemical Engineering and Process Development Division, CSIR-National Chemical Laboratory, Pune 411008,

M. S. India.

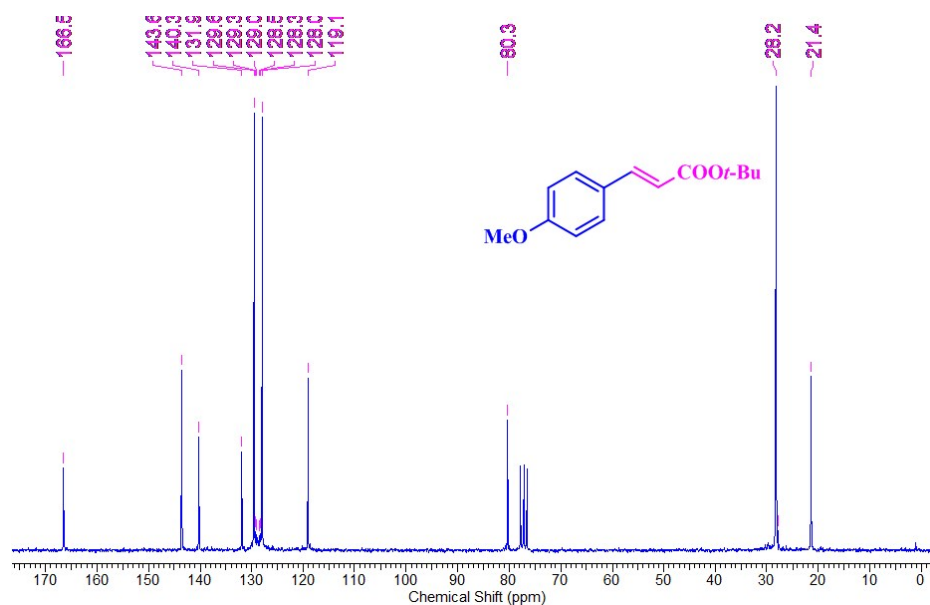
E-mail: cv.rode@ncl.res.in

1. ^1H and ^{13}C Characterization Data for Mizoroki-Heck Coupling Reaction:

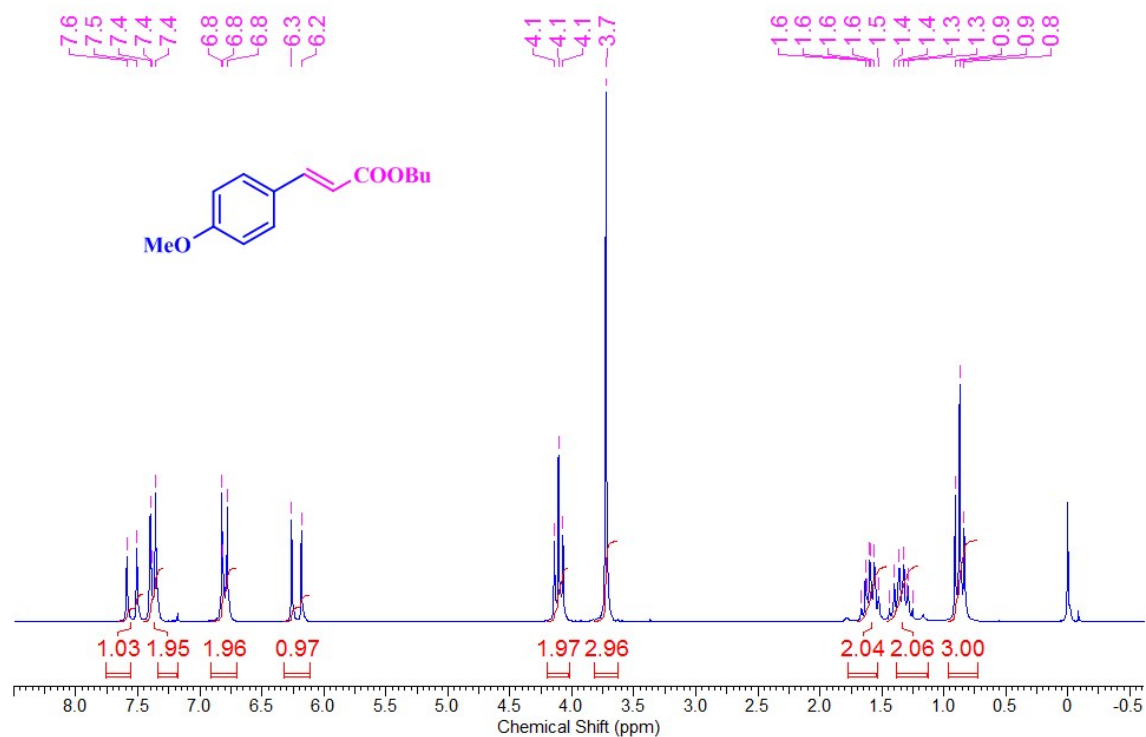
^1H NMR spectrum of tert-butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 1):



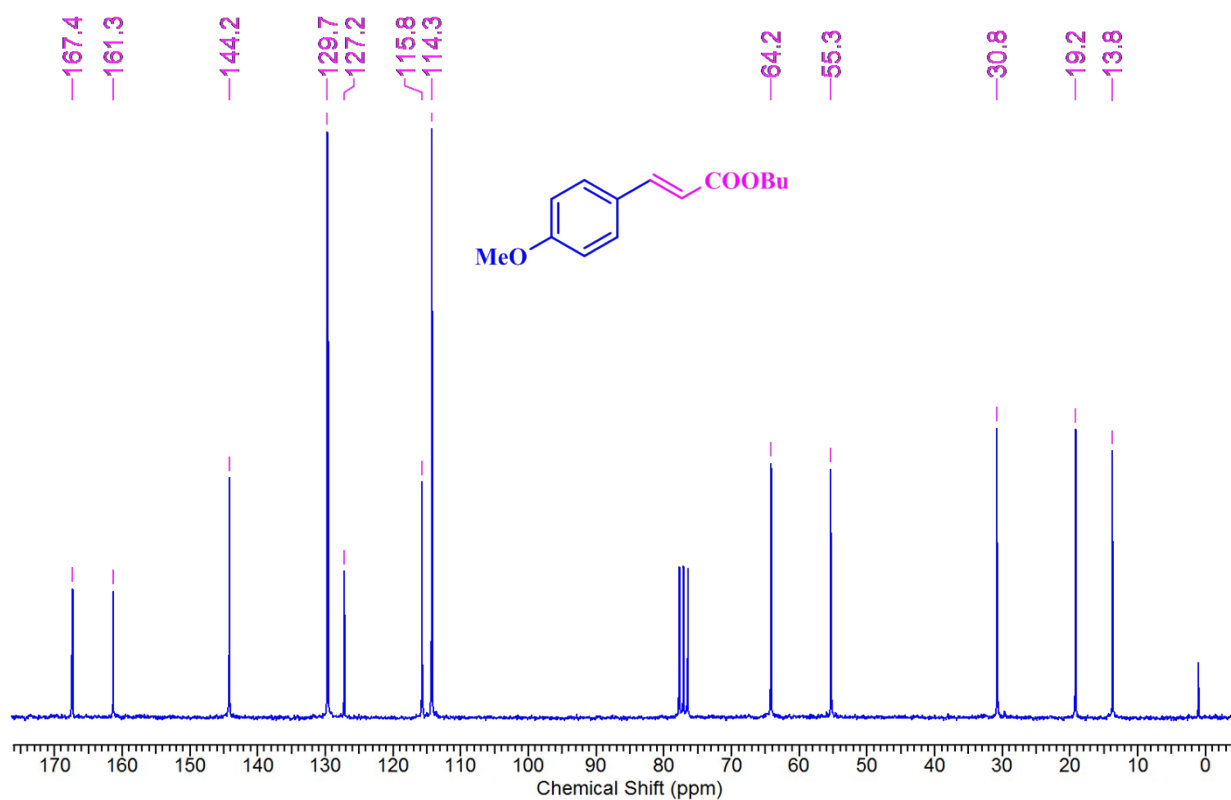
^{13}C NMR spectrum of tert-butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 1):



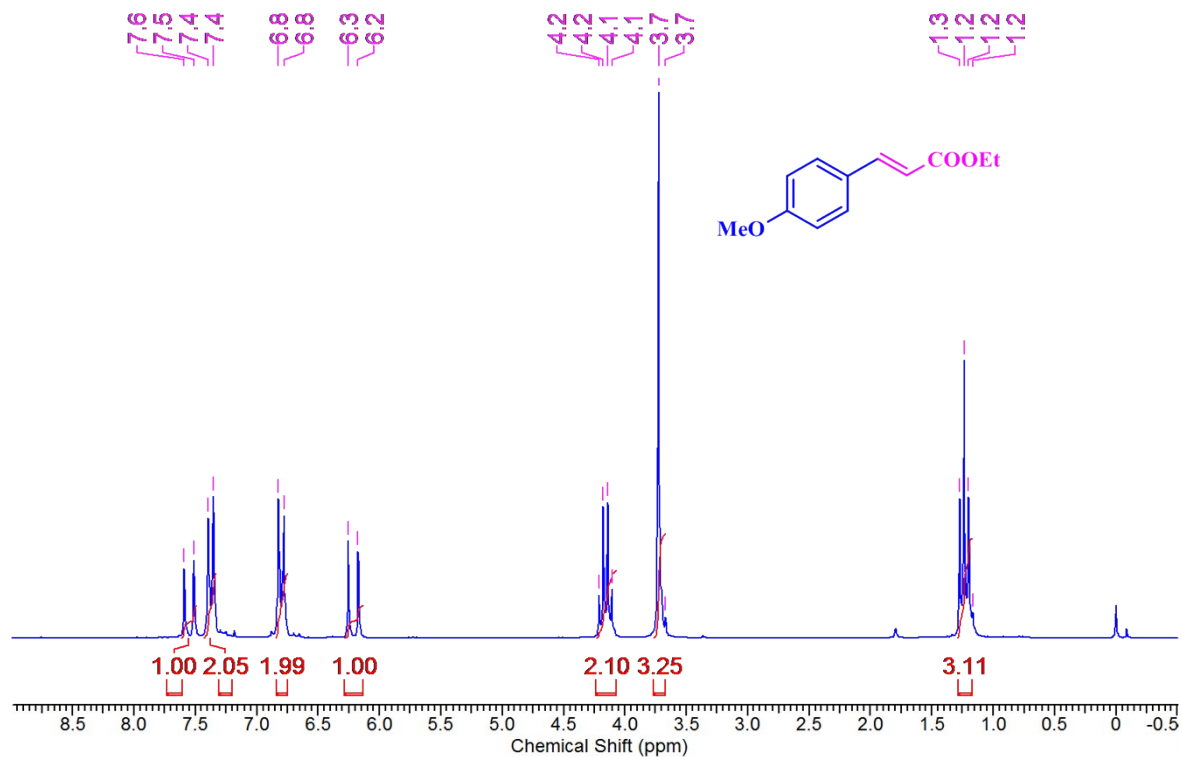
¹H NMR spectrum of butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 2):



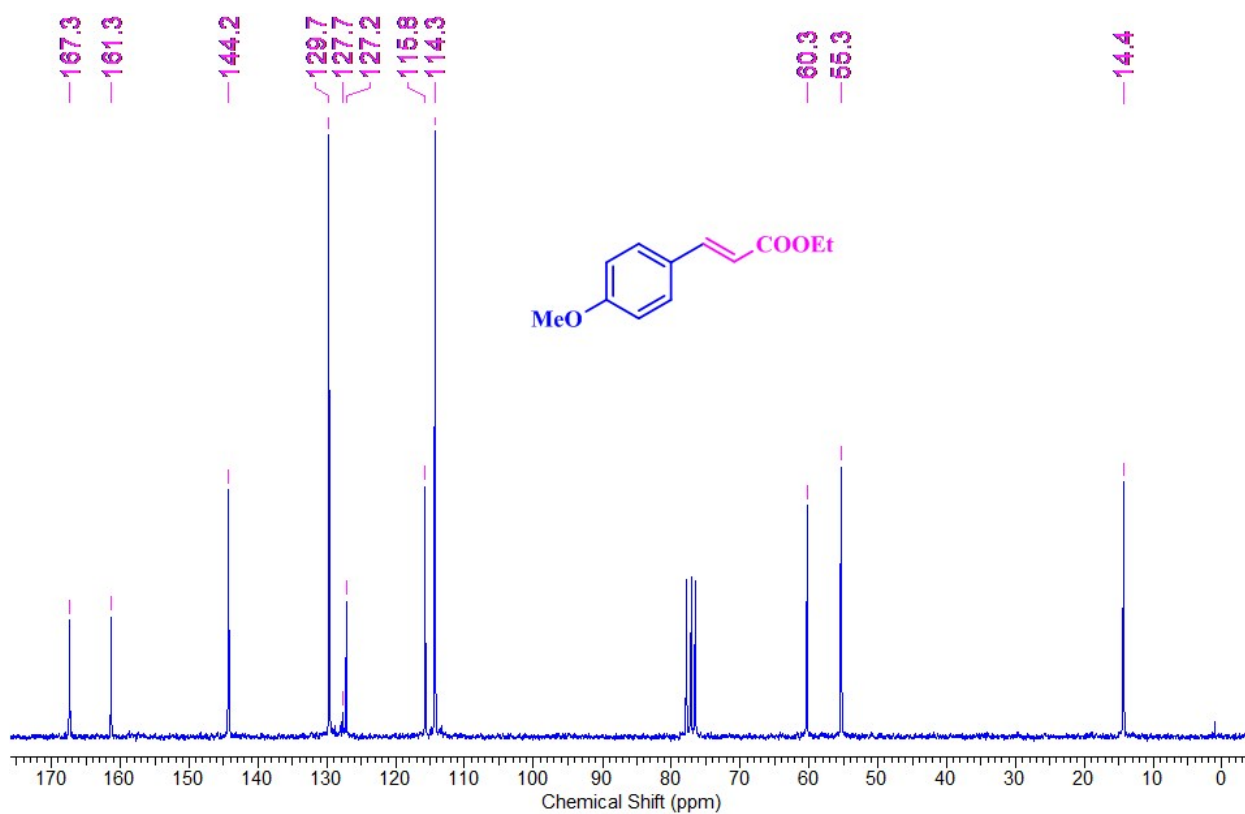
¹³C NMR spectrum of butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 2):



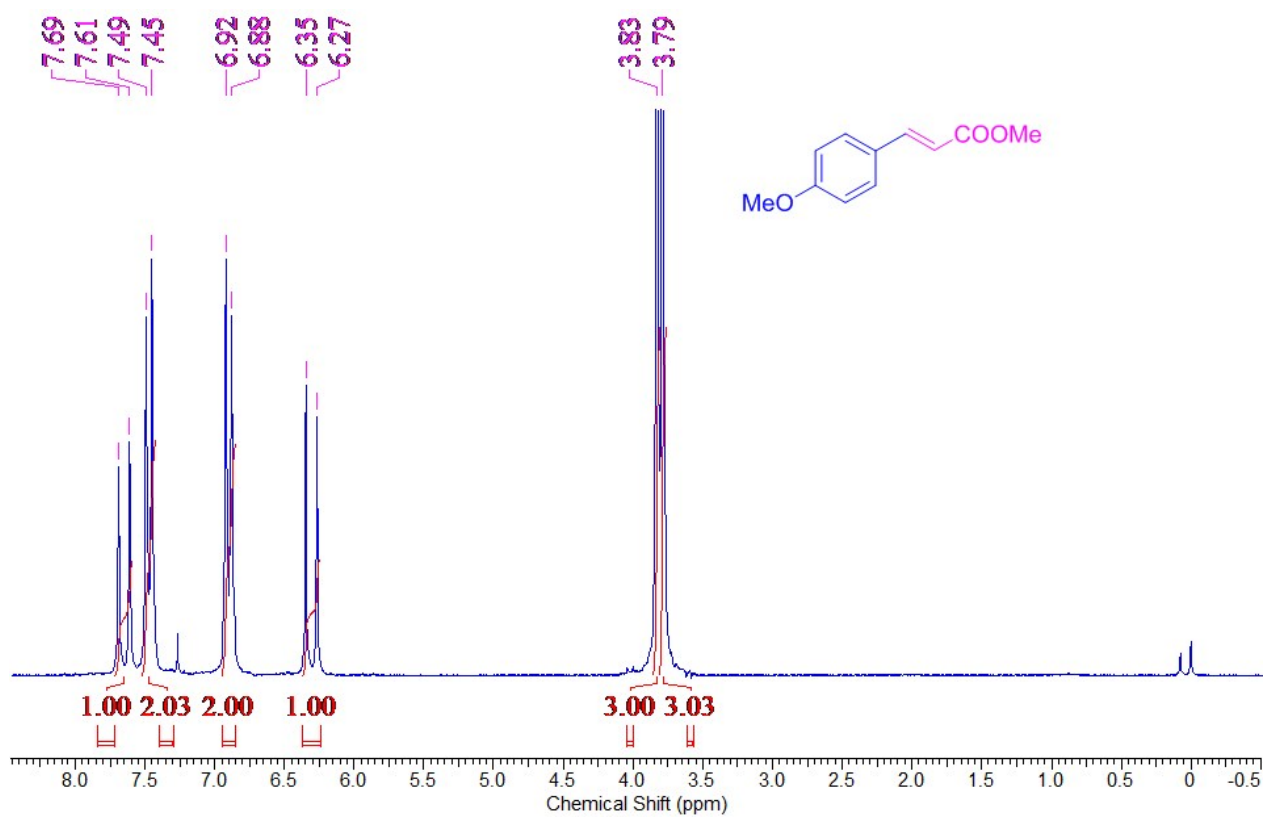
¹H NMR spectrum of ethyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 3):



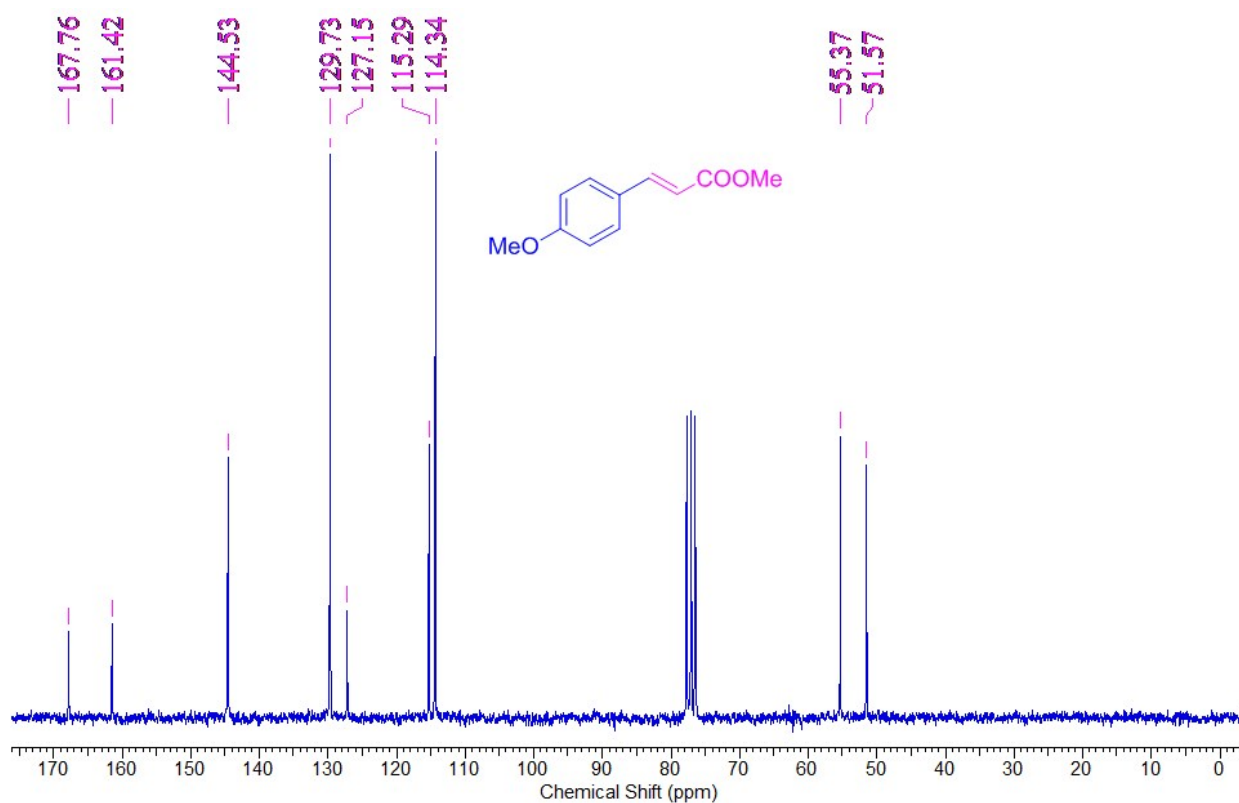
¹³C NMR spectrum of ethyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 3):



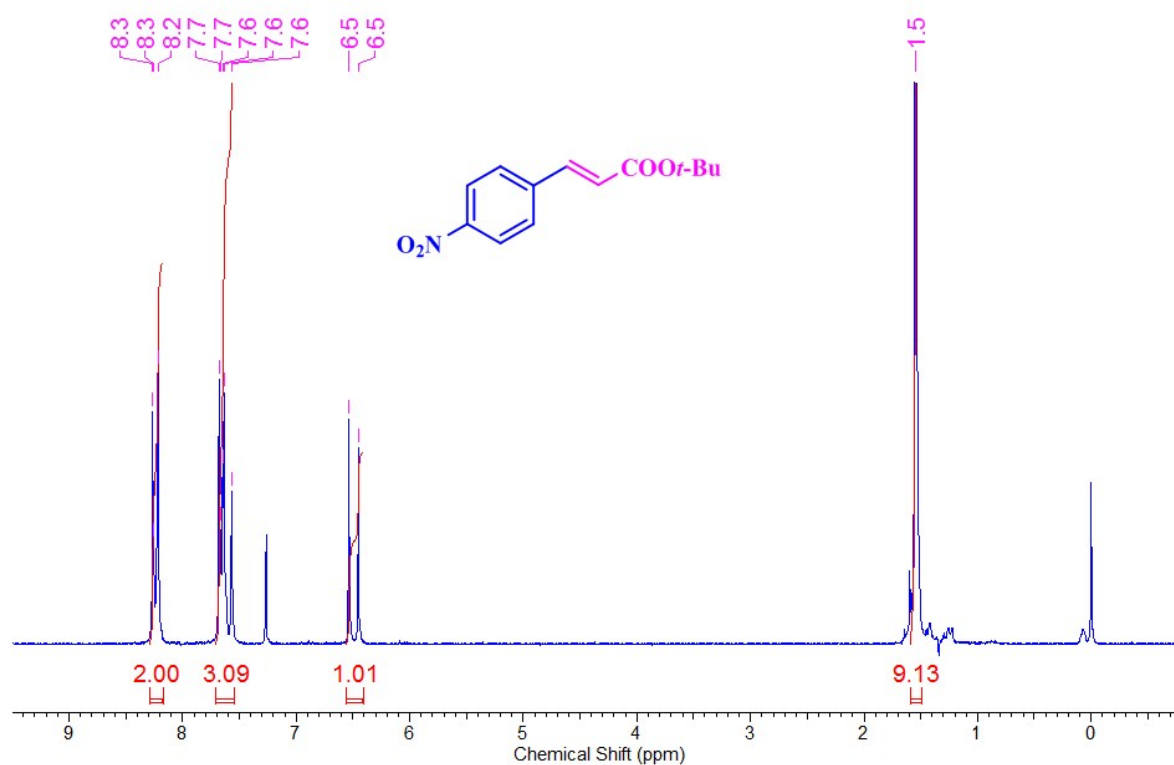
¹H NMR spectrum of methyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 4):



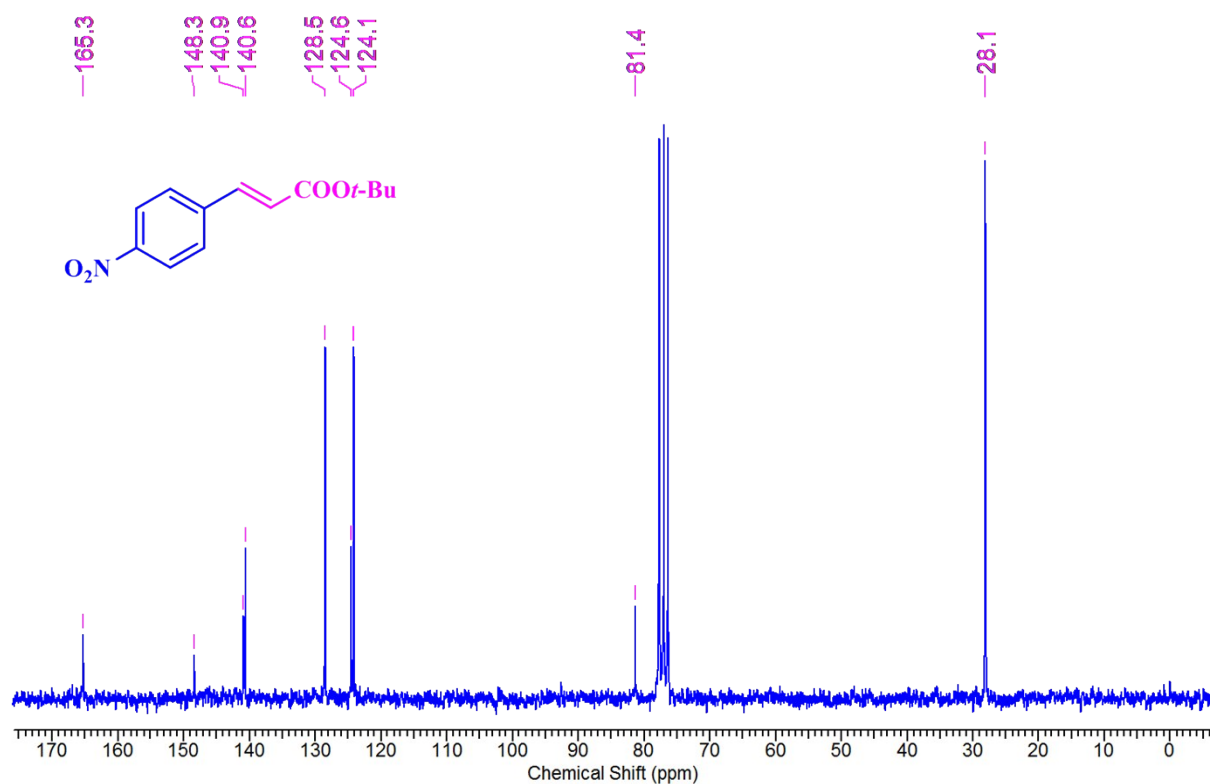
^{13}C NMR spectrum of methyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 4, entry 4):



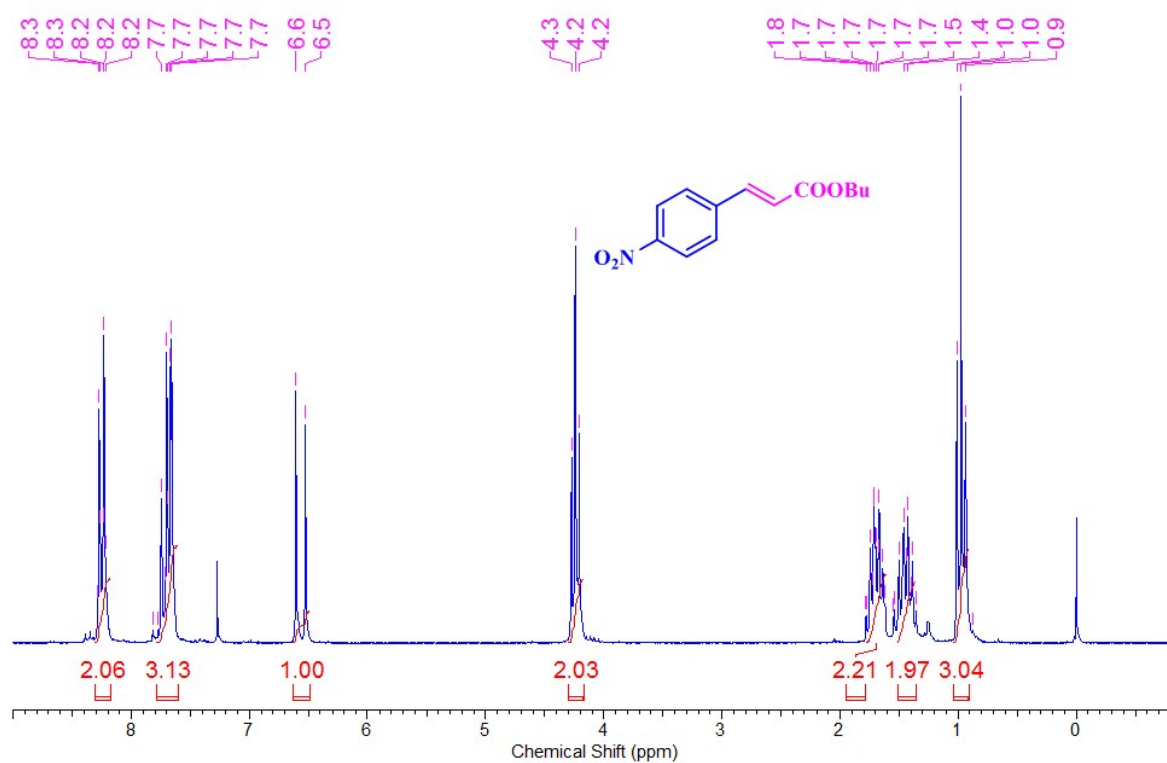
^1H NMR spectrum of tert-butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 5):



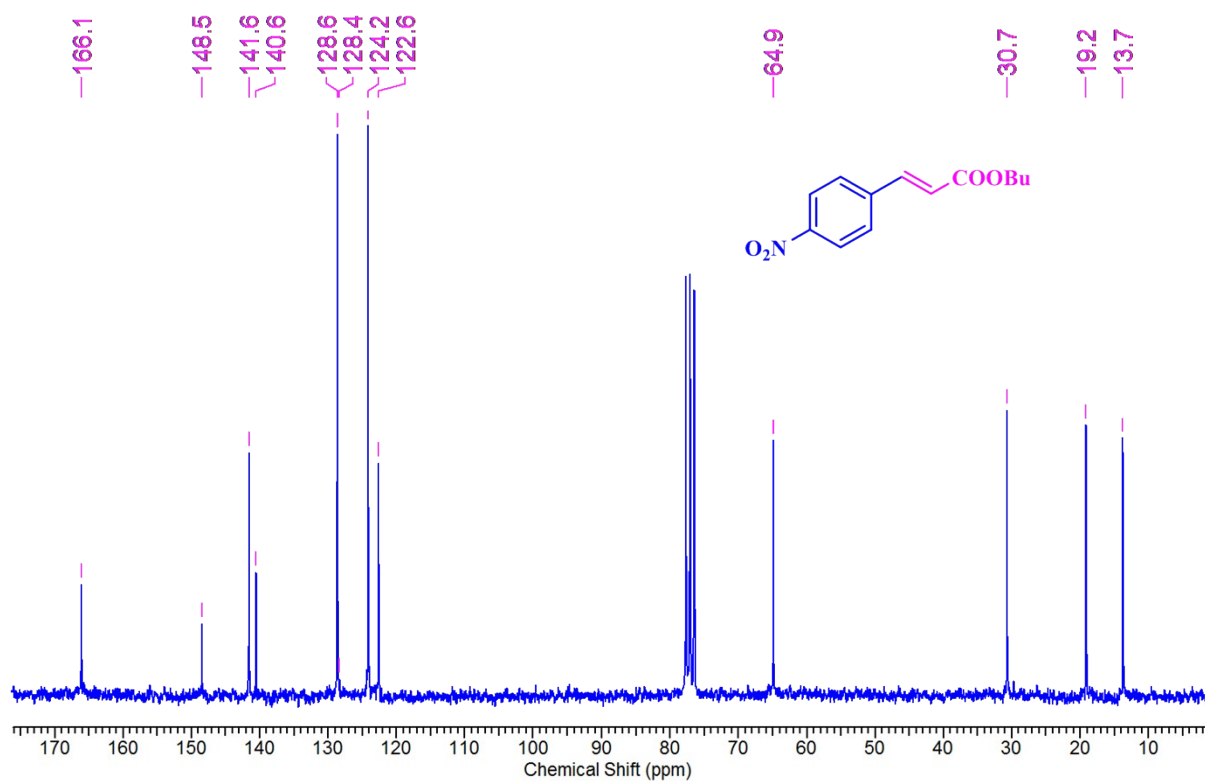
^{13}C NMR spectrum of tert-butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 5):



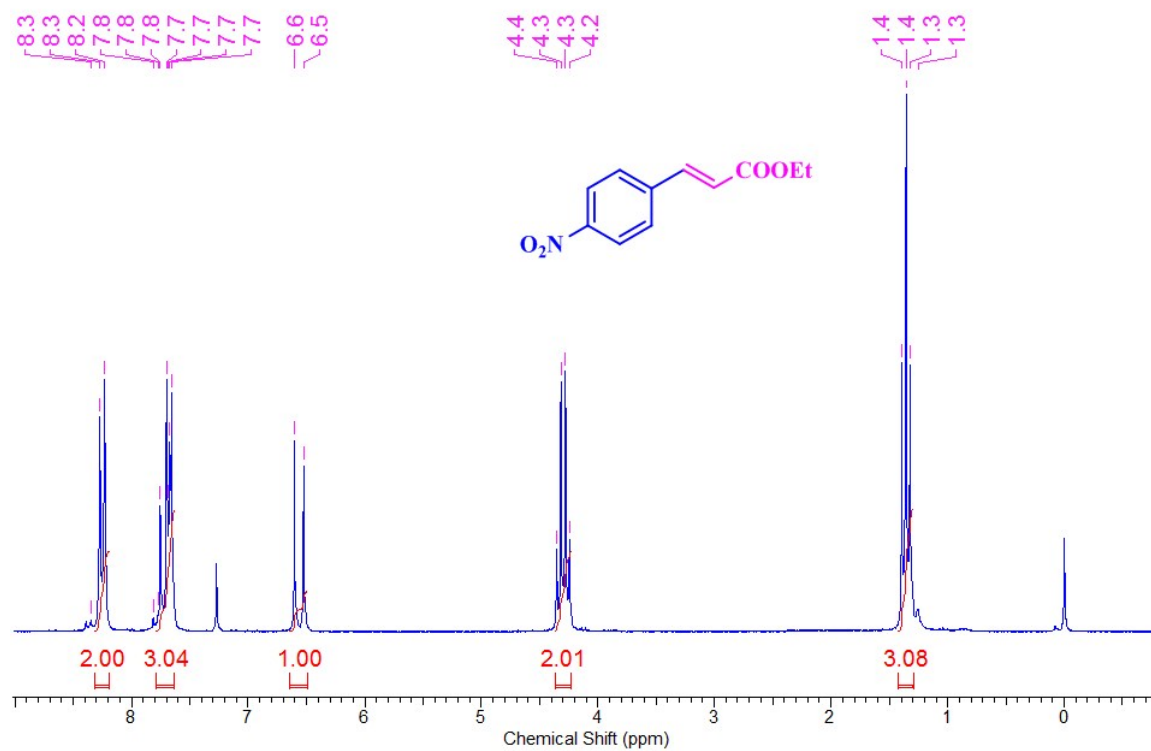
^1H NMR spectrum of butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 6):



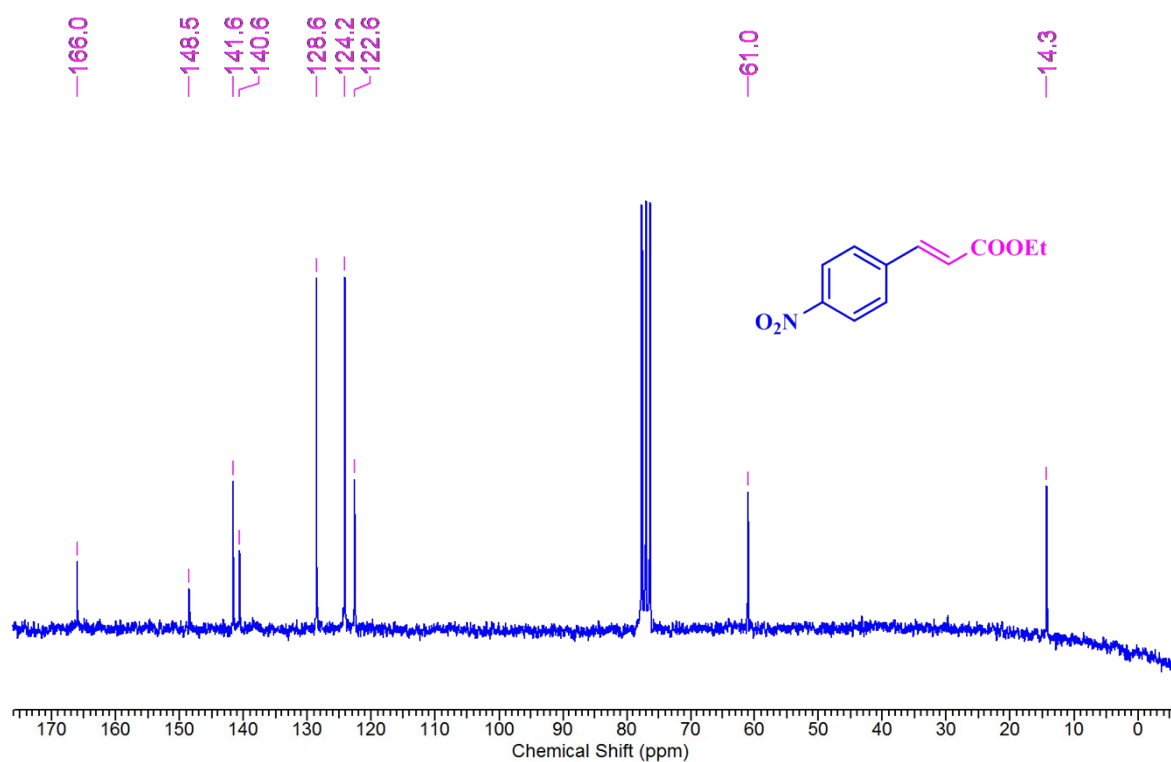
^{13}C NMR spectrum of butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 6):



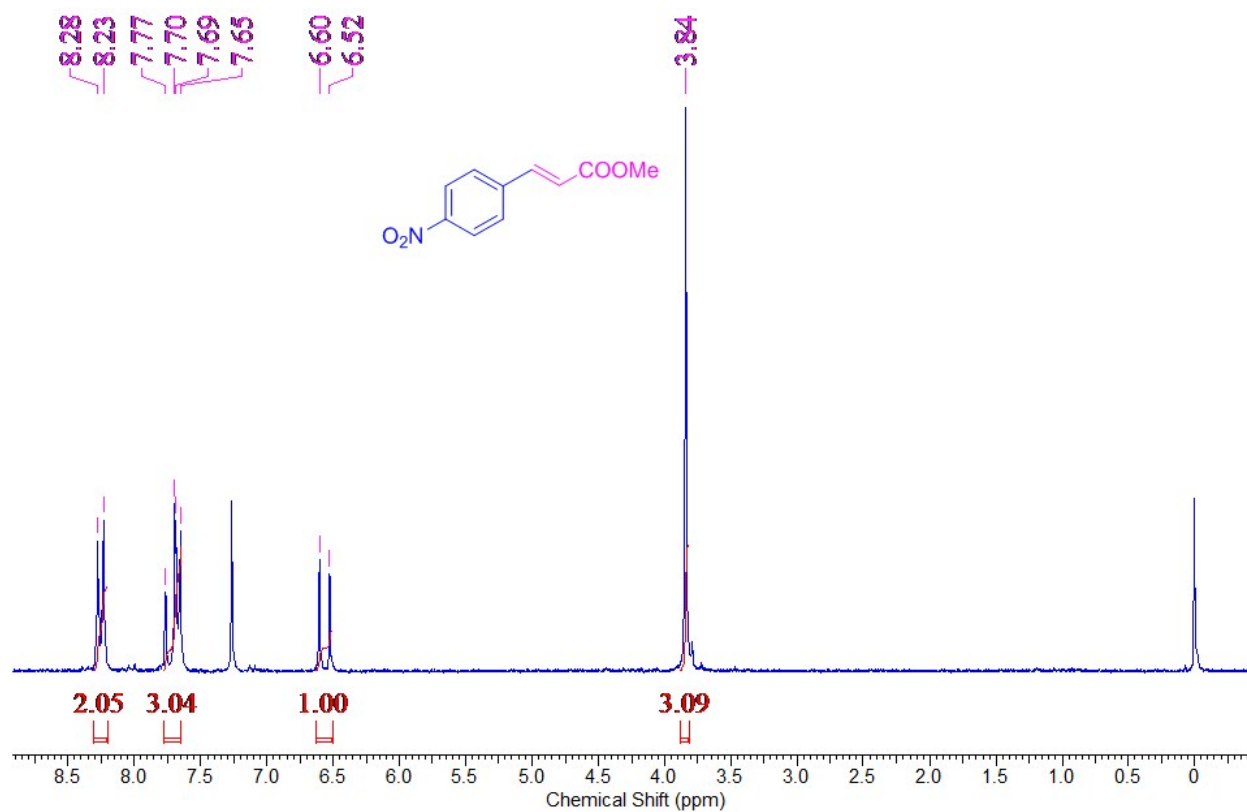
¹H NMR spectrum of ethyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 7):



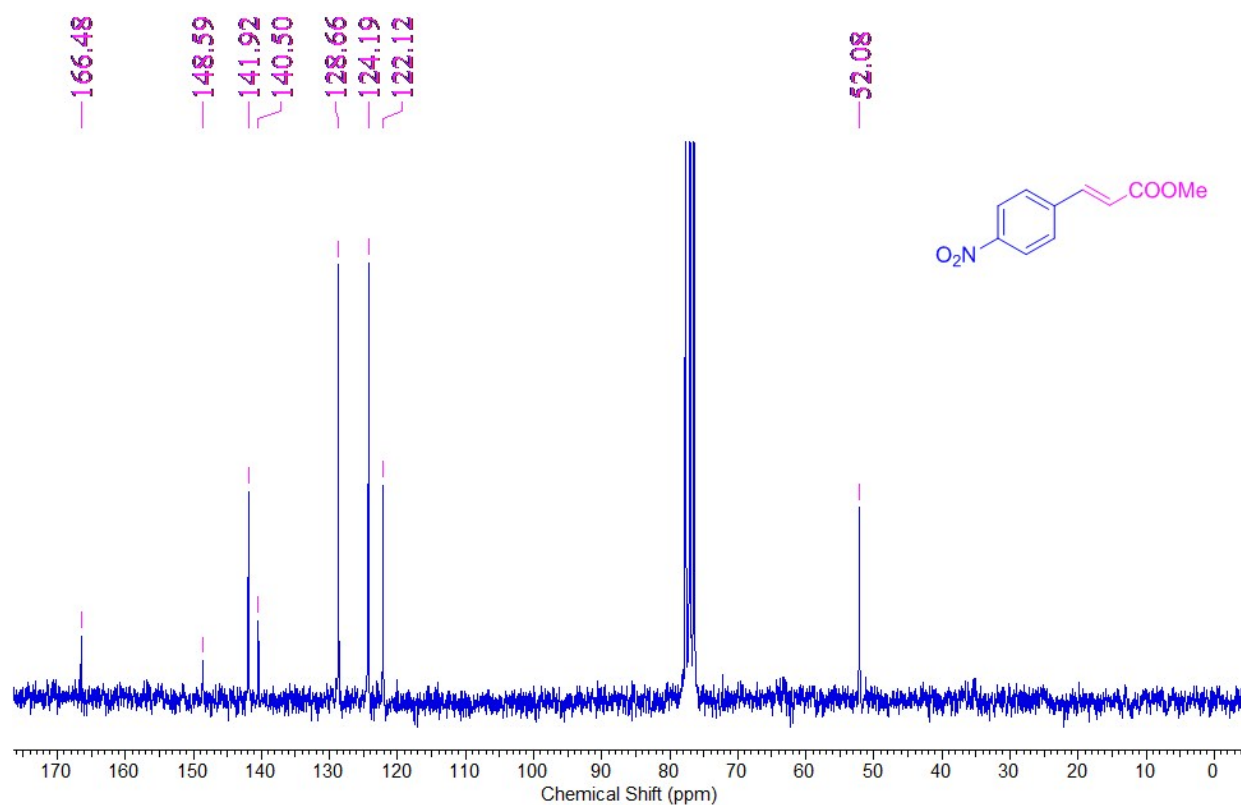
^{13}C NMR spectrum of ethyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 7):



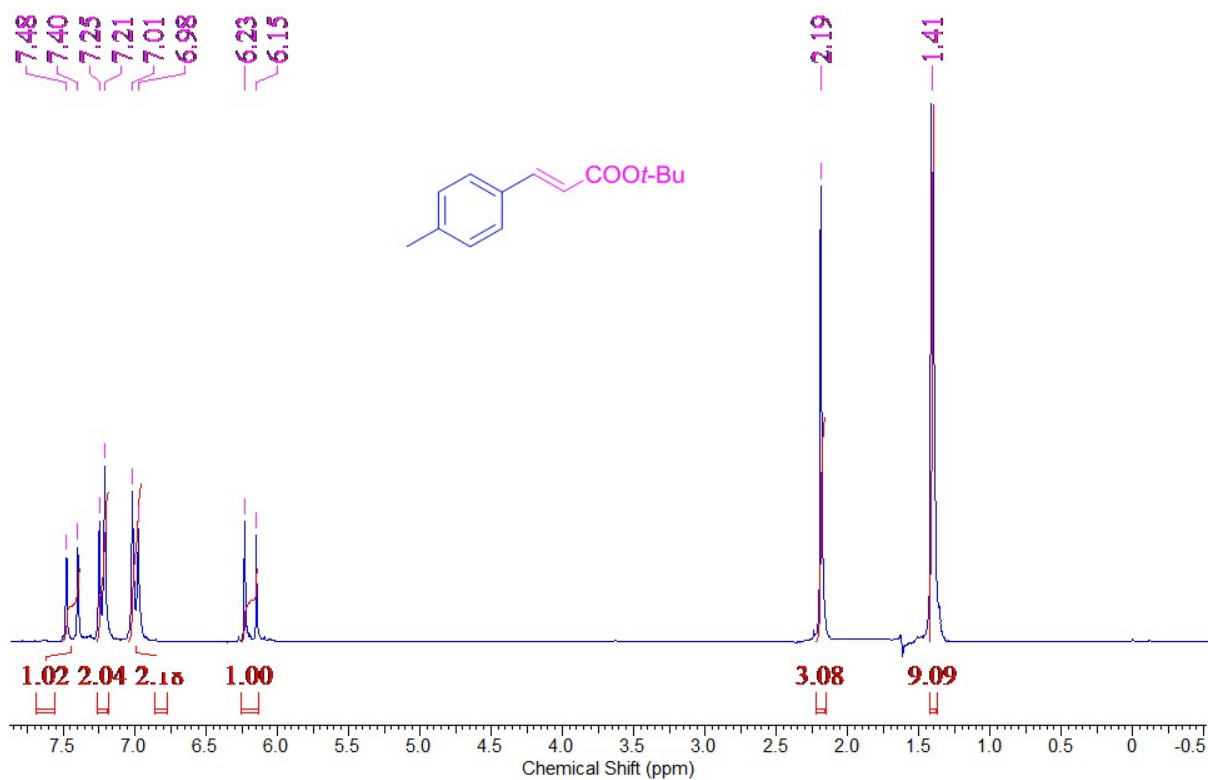
^1H NMR spectrum of methyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 8):



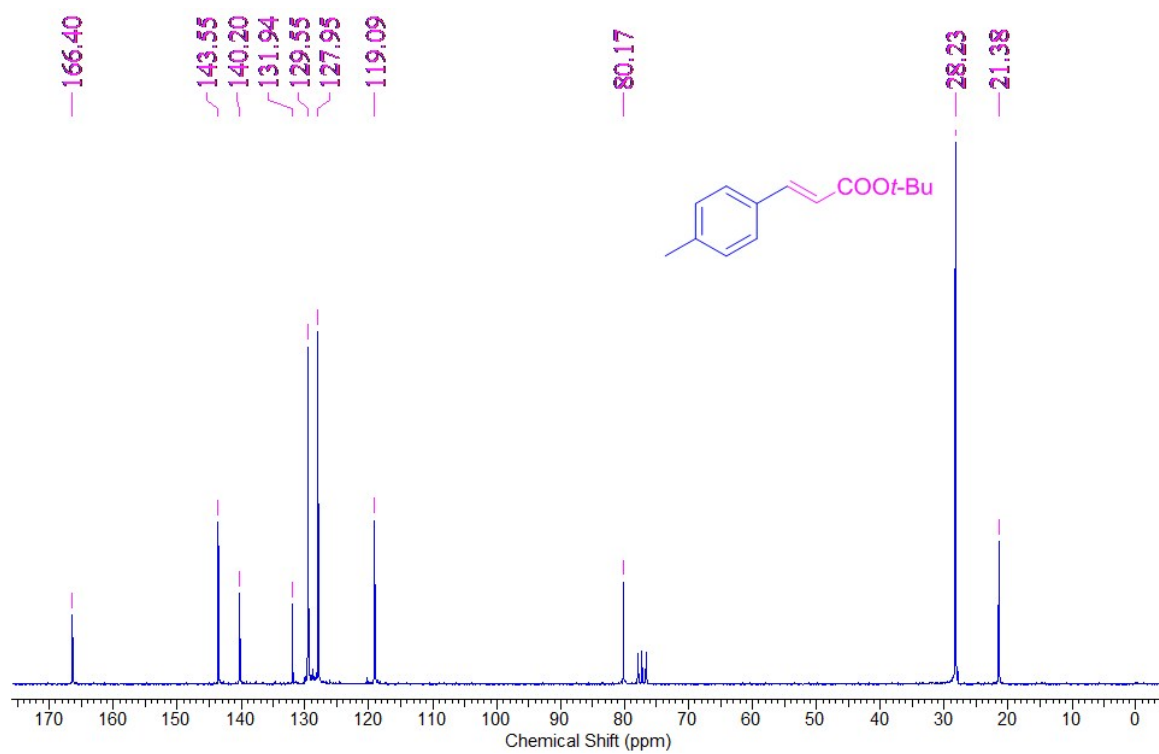
^{13}C NMR spectrum of methyl(*E*)-3-(4-nitrophenyl)acrylate (Table 4, entry 8):



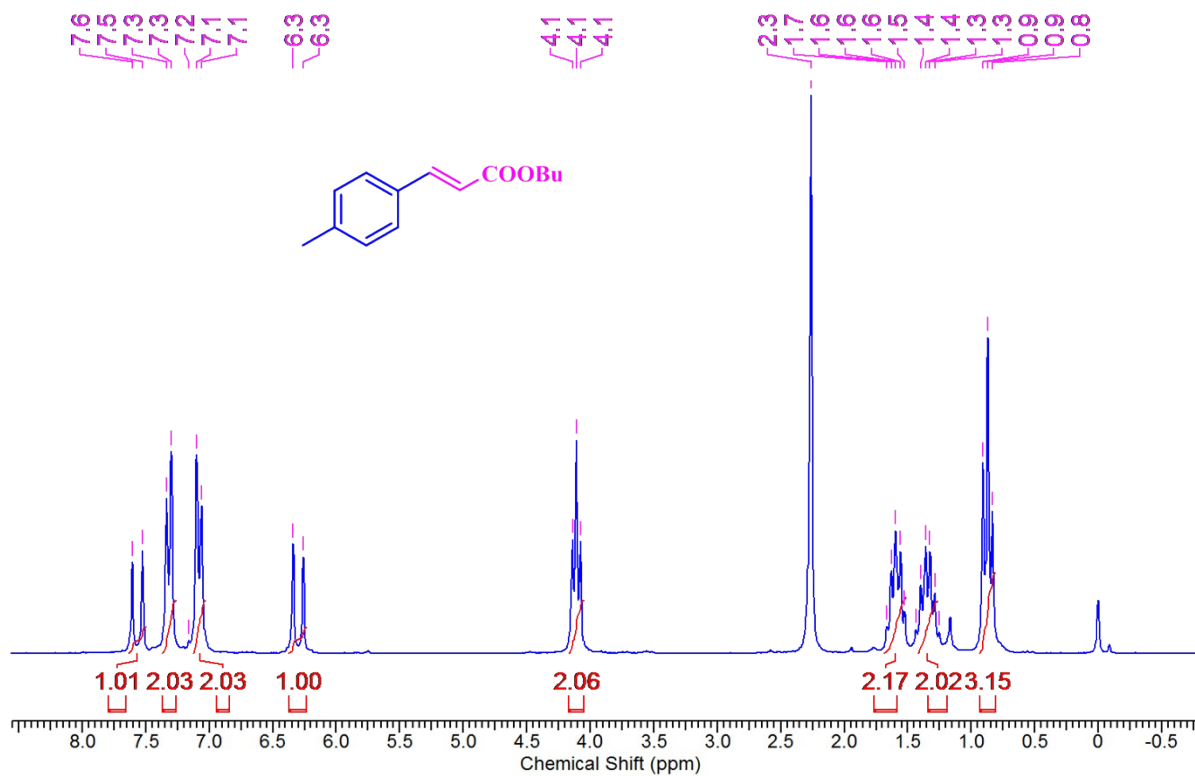
¹H NMR spectrum of tert-butyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 9):



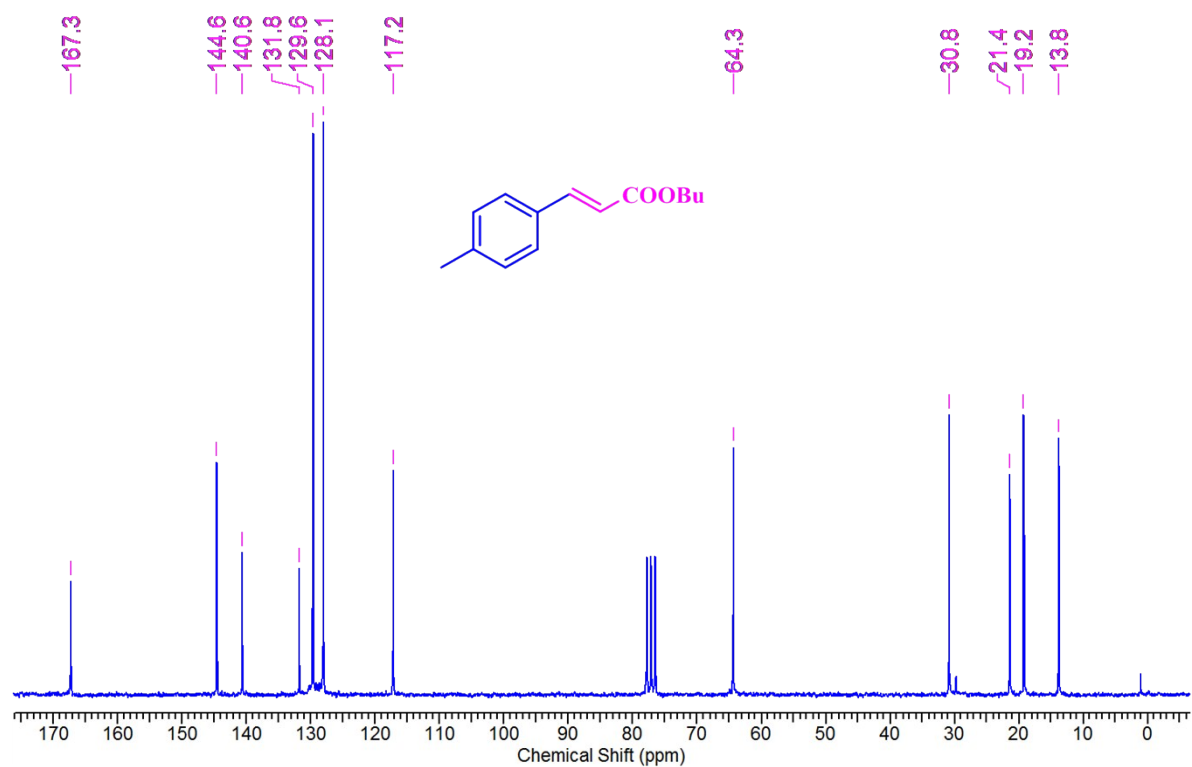
¹³C NMR spectrum of tert-butyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 9):



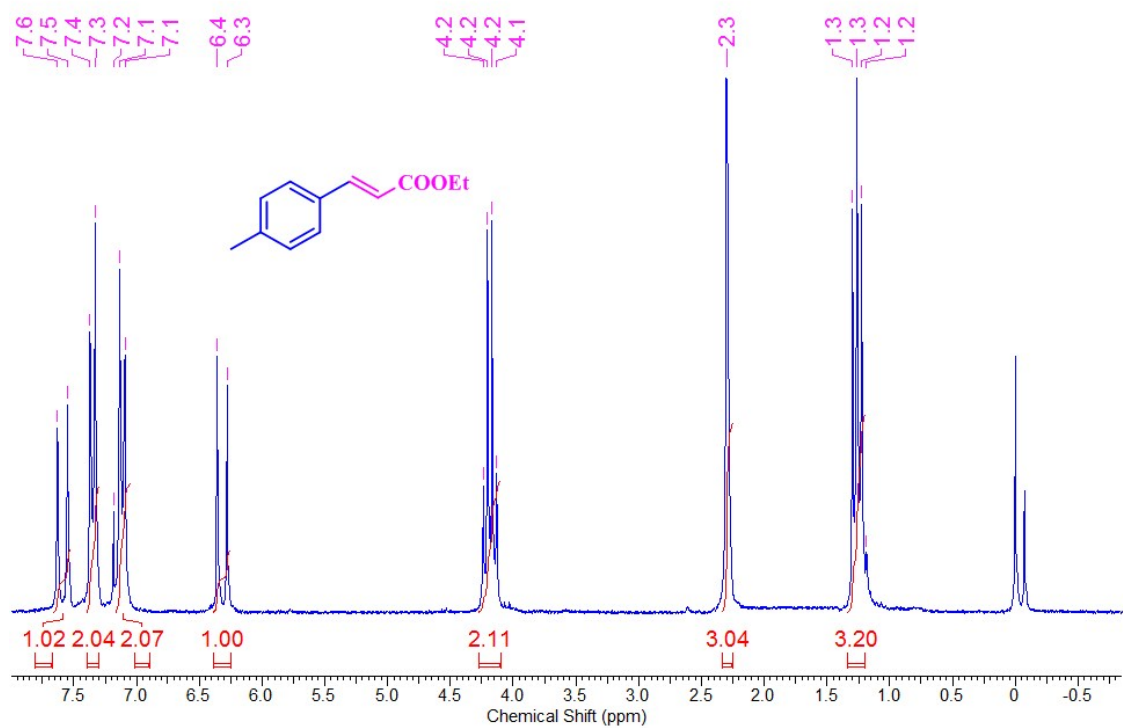
¹H NMR spectrum of butyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 10):



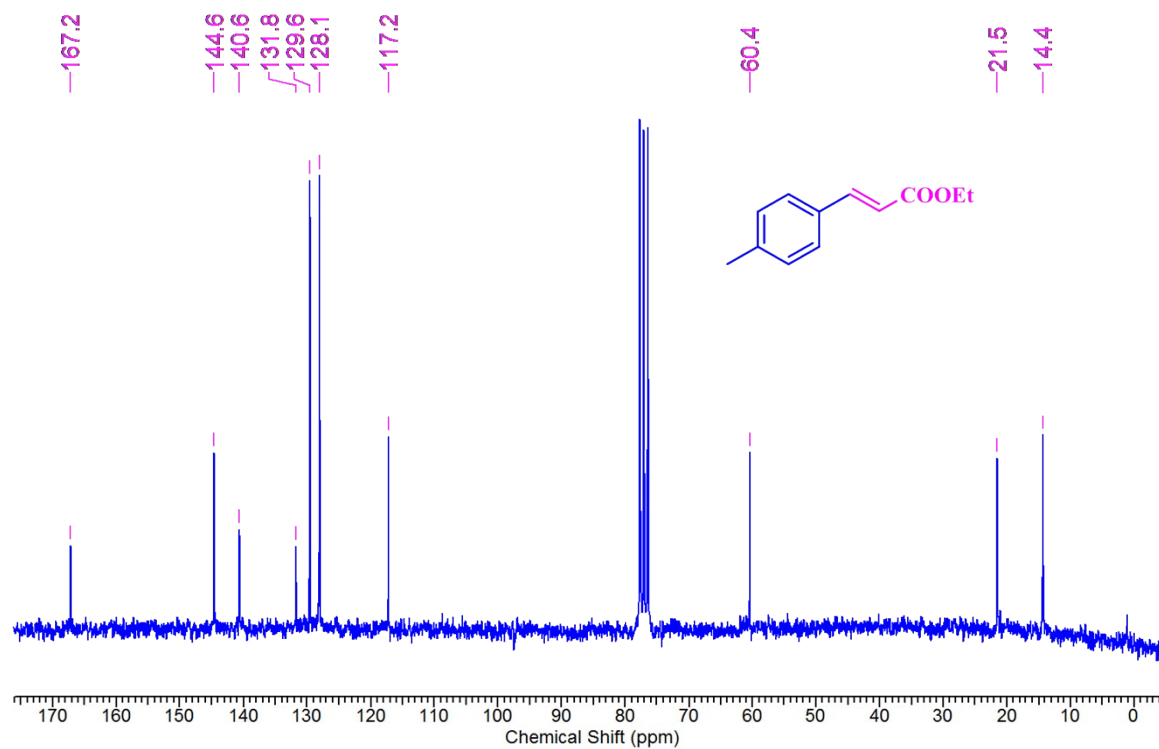
^{13}C NMR spectrum of butyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 10):



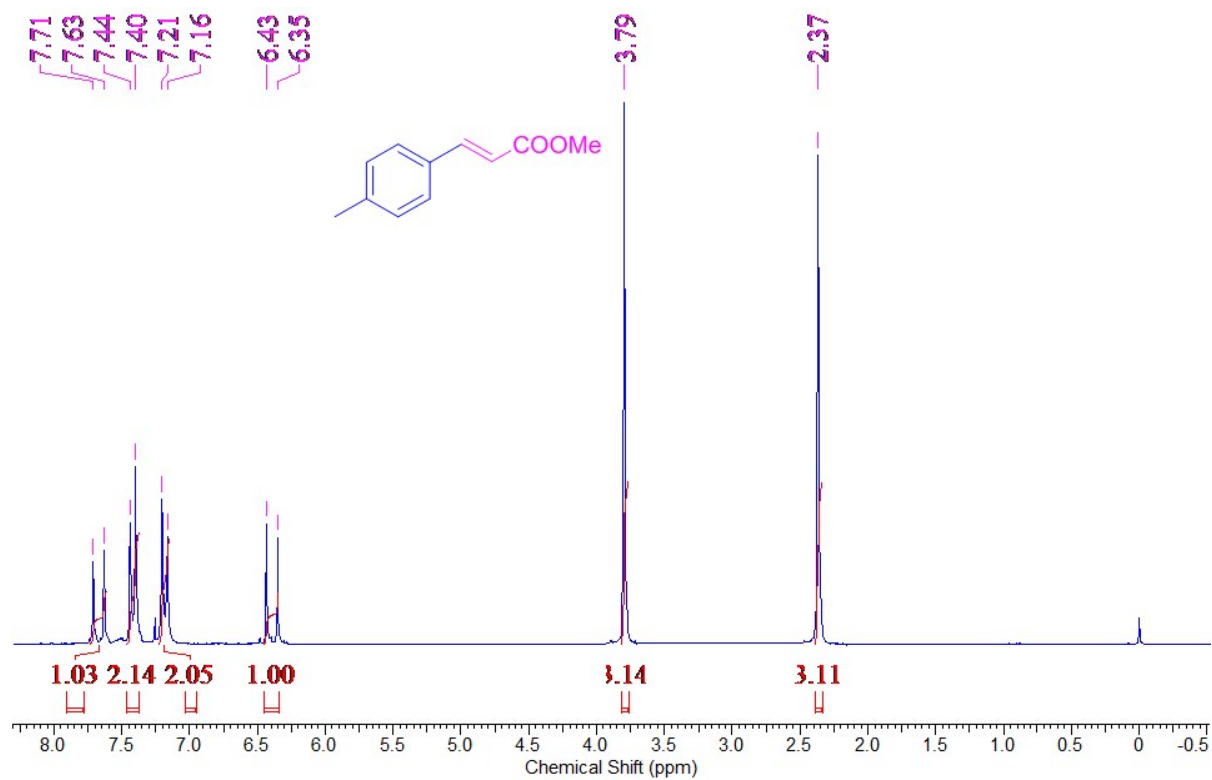
^1H NMR spectrum of ethyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 11):



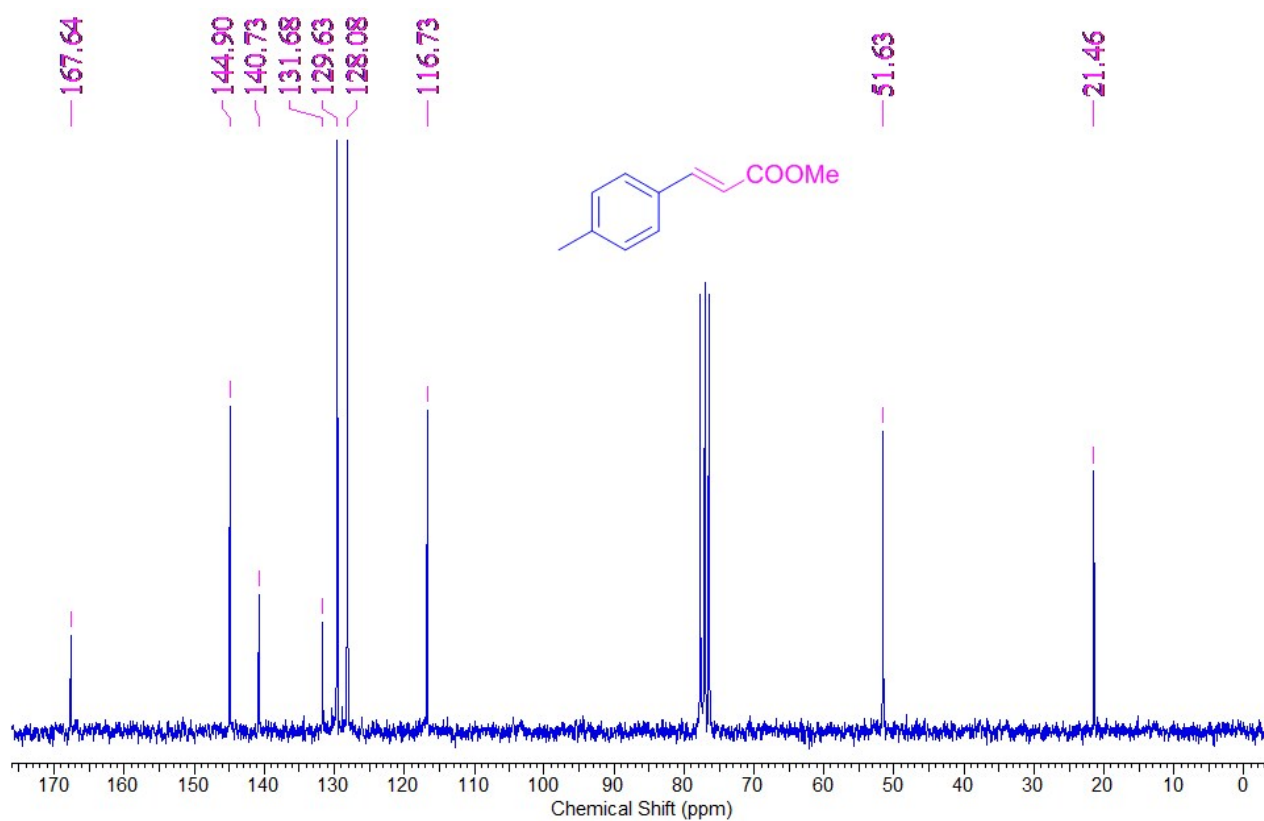
^{13}C NMR spectrum of ethyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 11):



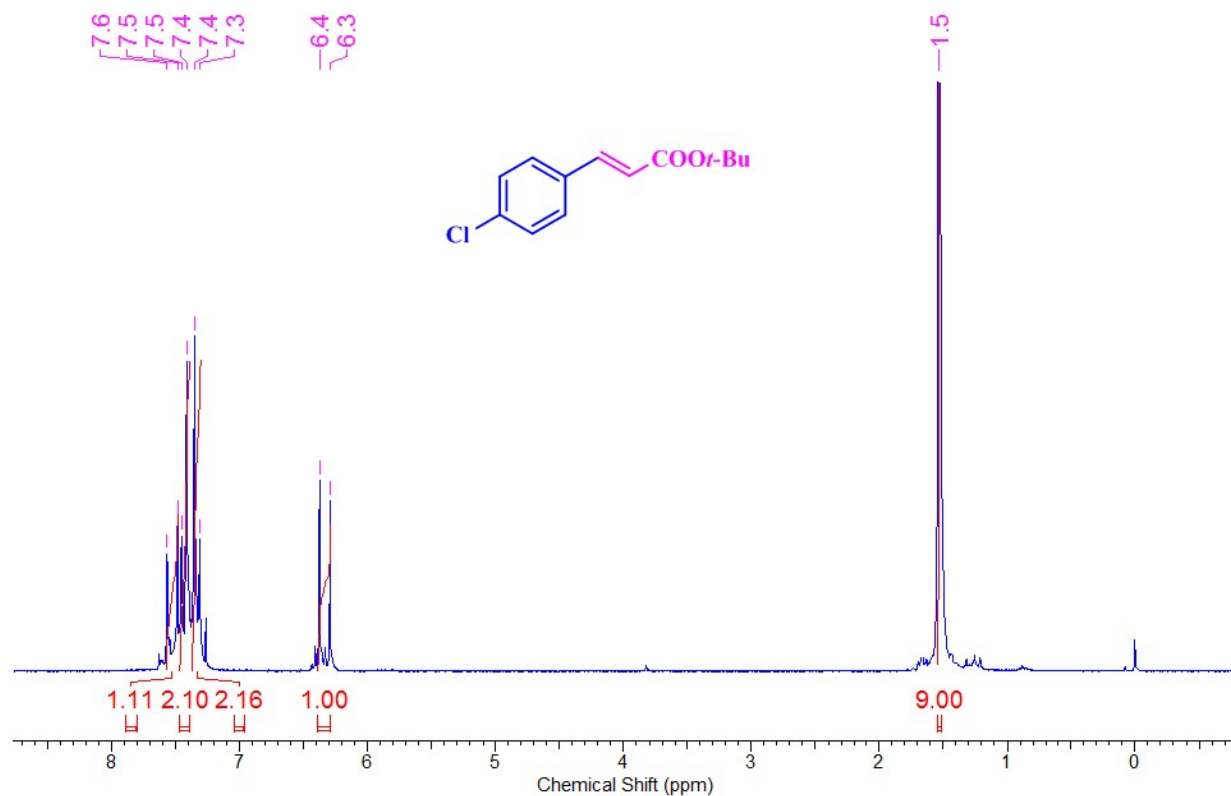
^1H NMR spectrum of methyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 12):



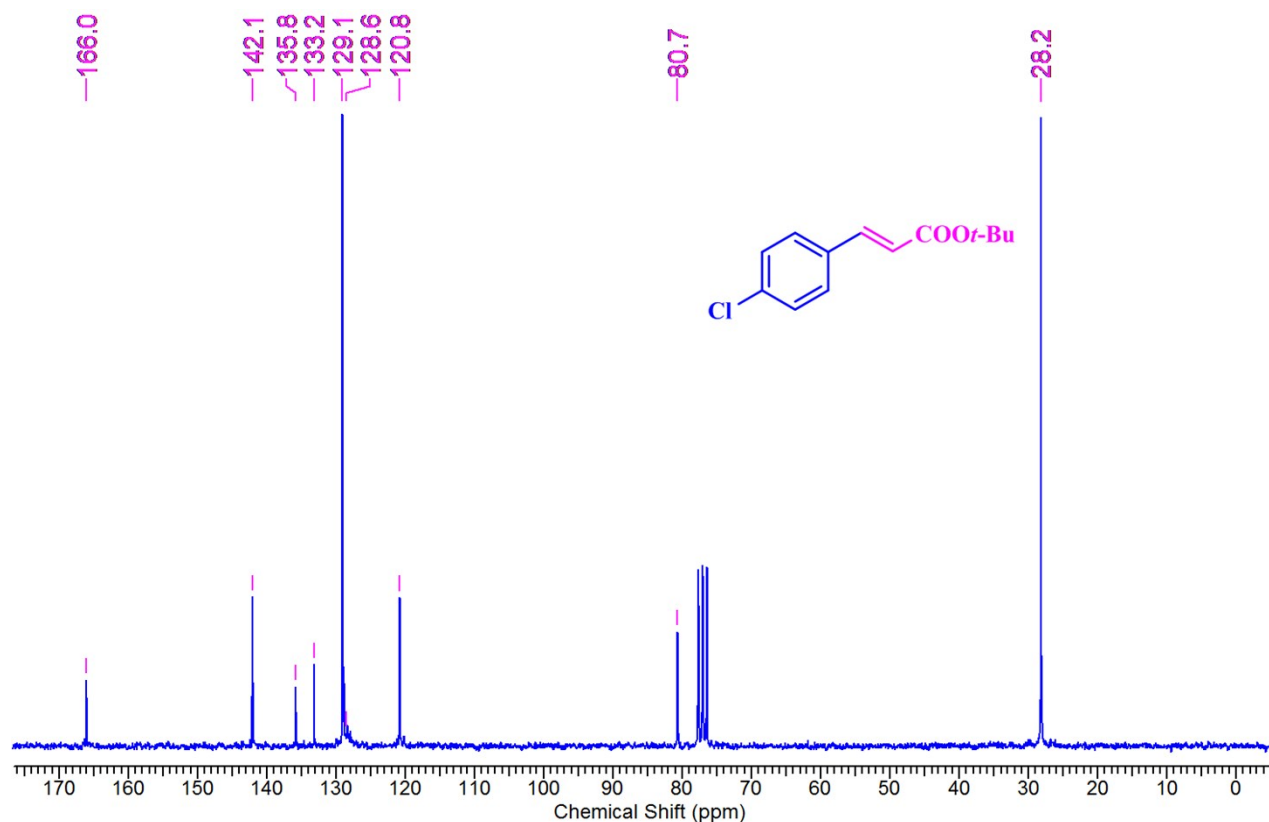
^{13}C NMR spectrum of methyl(*E*)-3-(*p*-tolyl)acrylate (Table 4, entry 12):



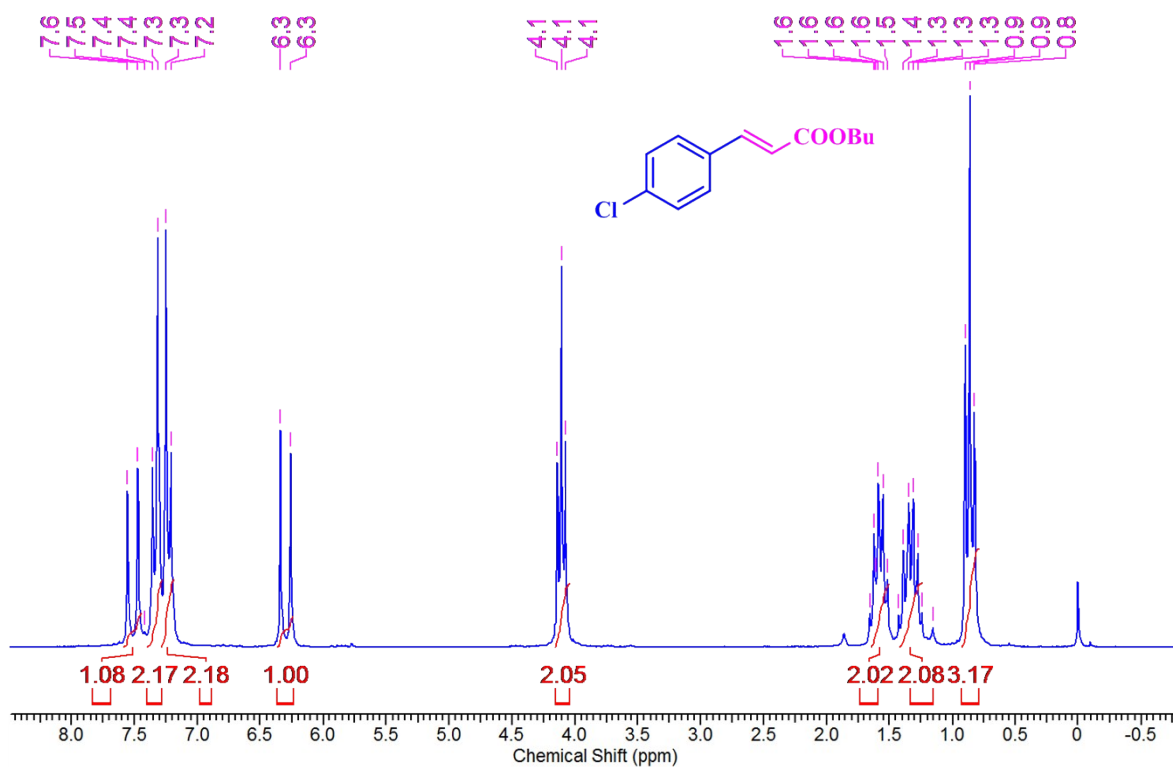
^1H NMR spectrum of tert-butyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 13):



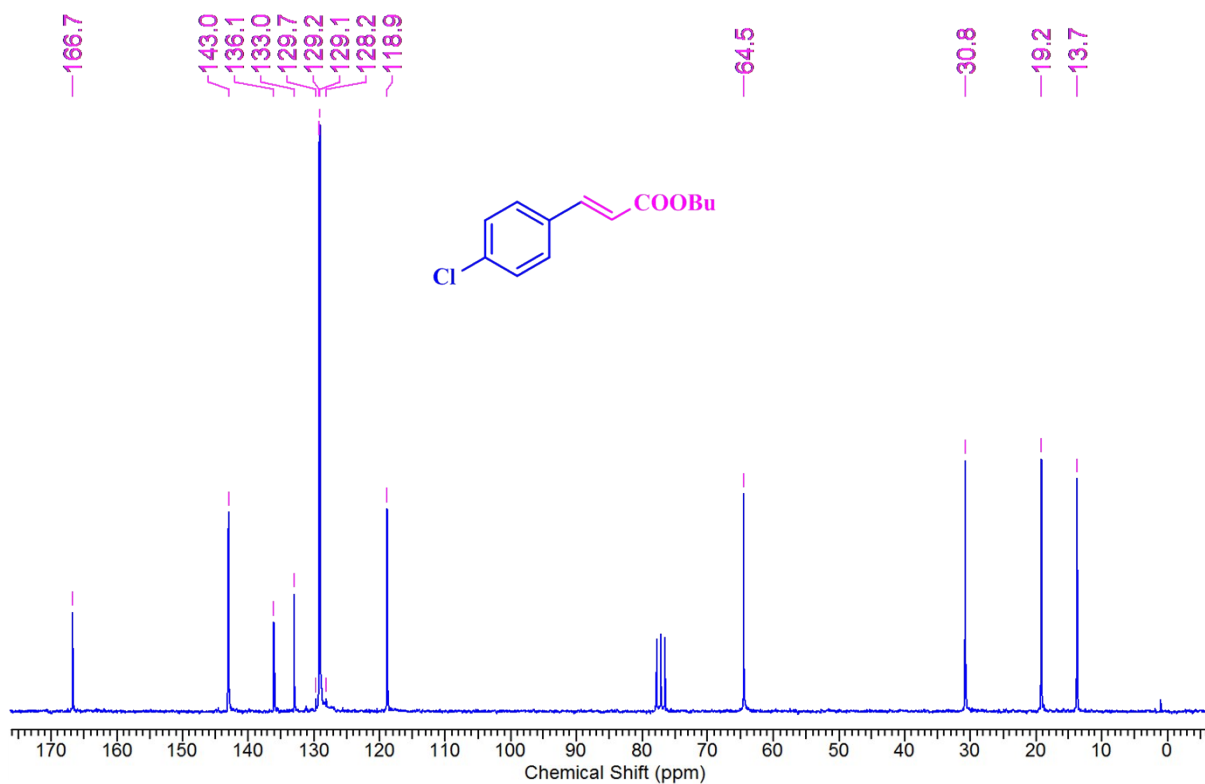
^{13}C NMR spectrum of tert-butyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 13):



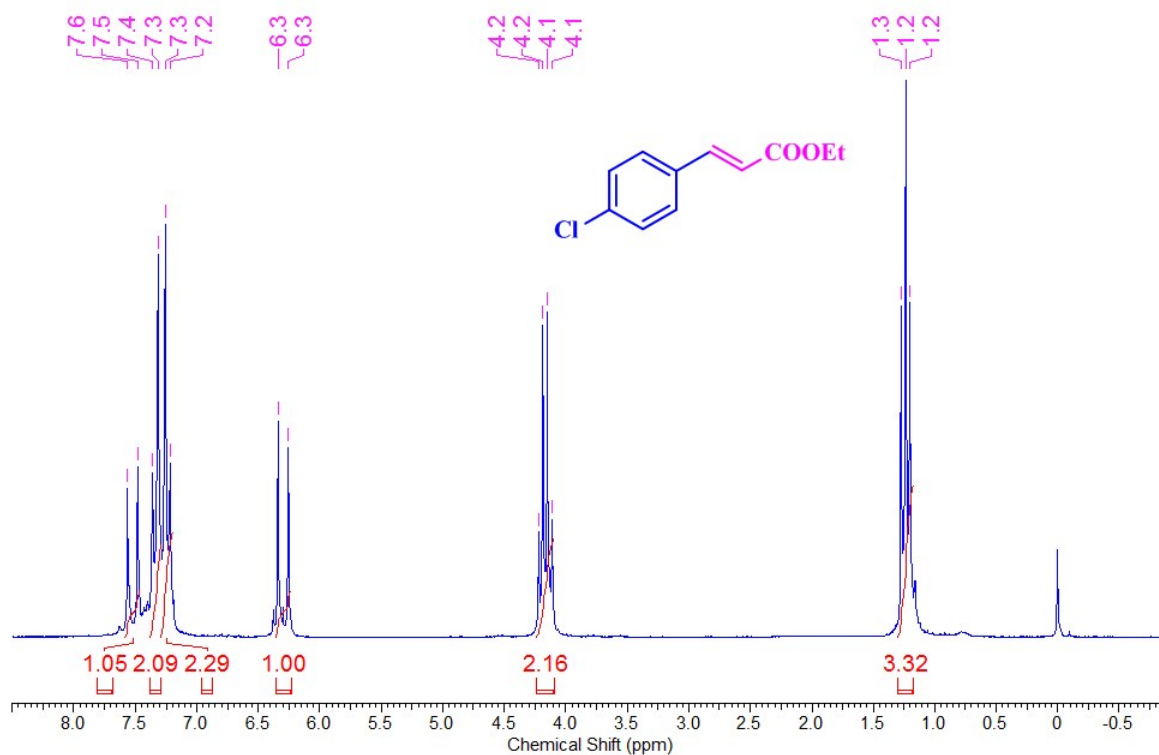
^1H NMR spectrum of butyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 14):



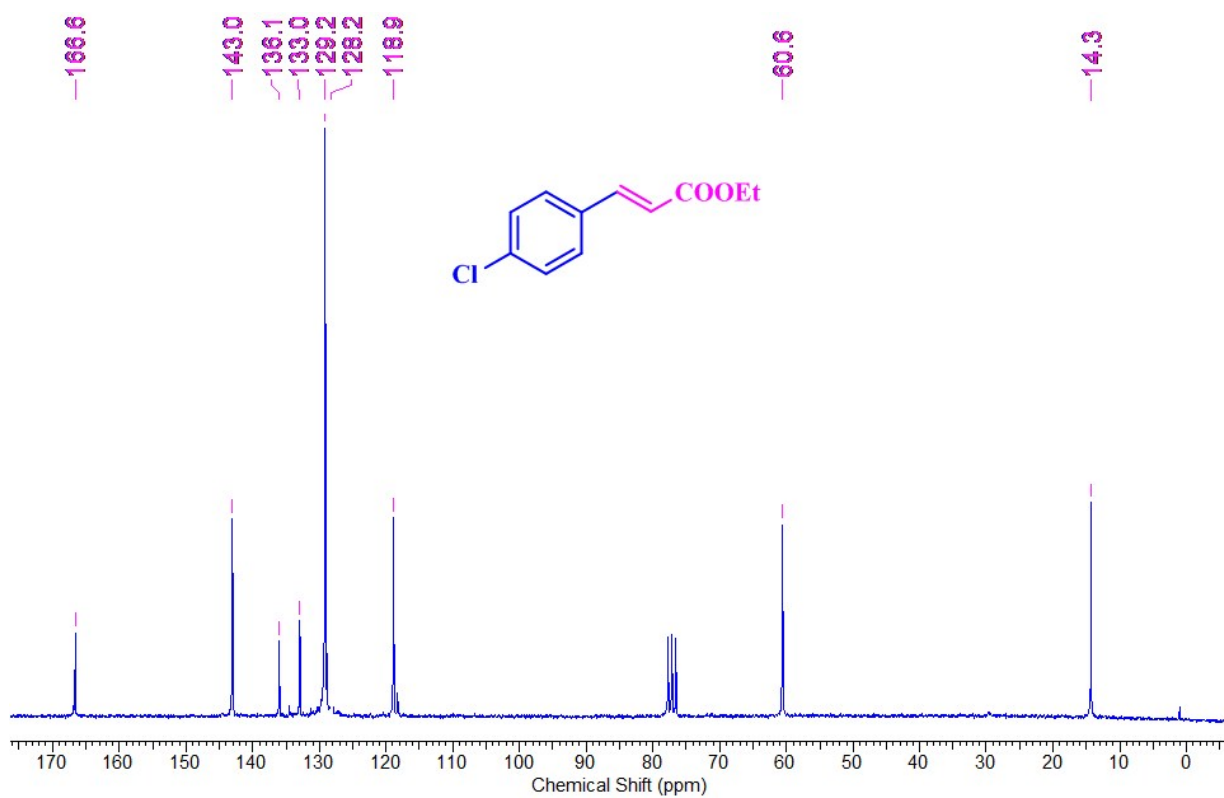
^{13}C NMR spectrum of butyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 14):



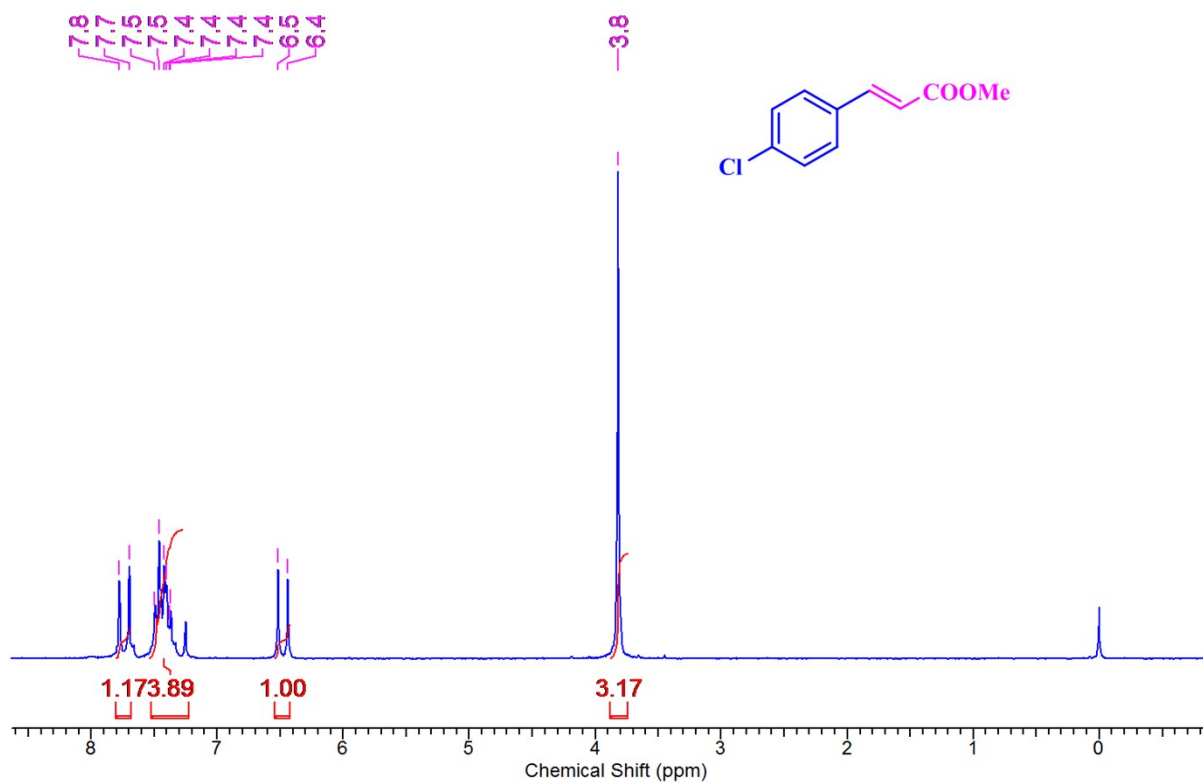
^1H NMR spectrum of ethyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 15):



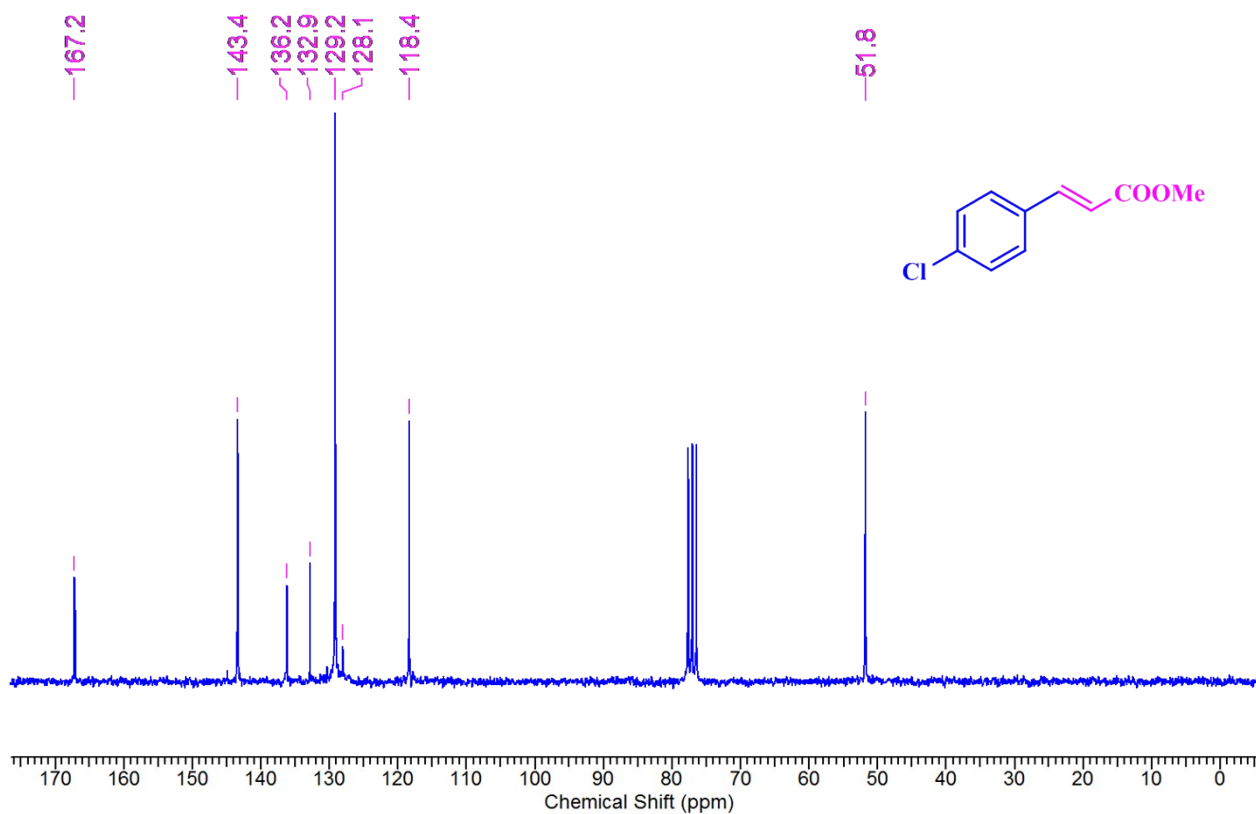
^{13}C NMR spectrum of ethyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 15):



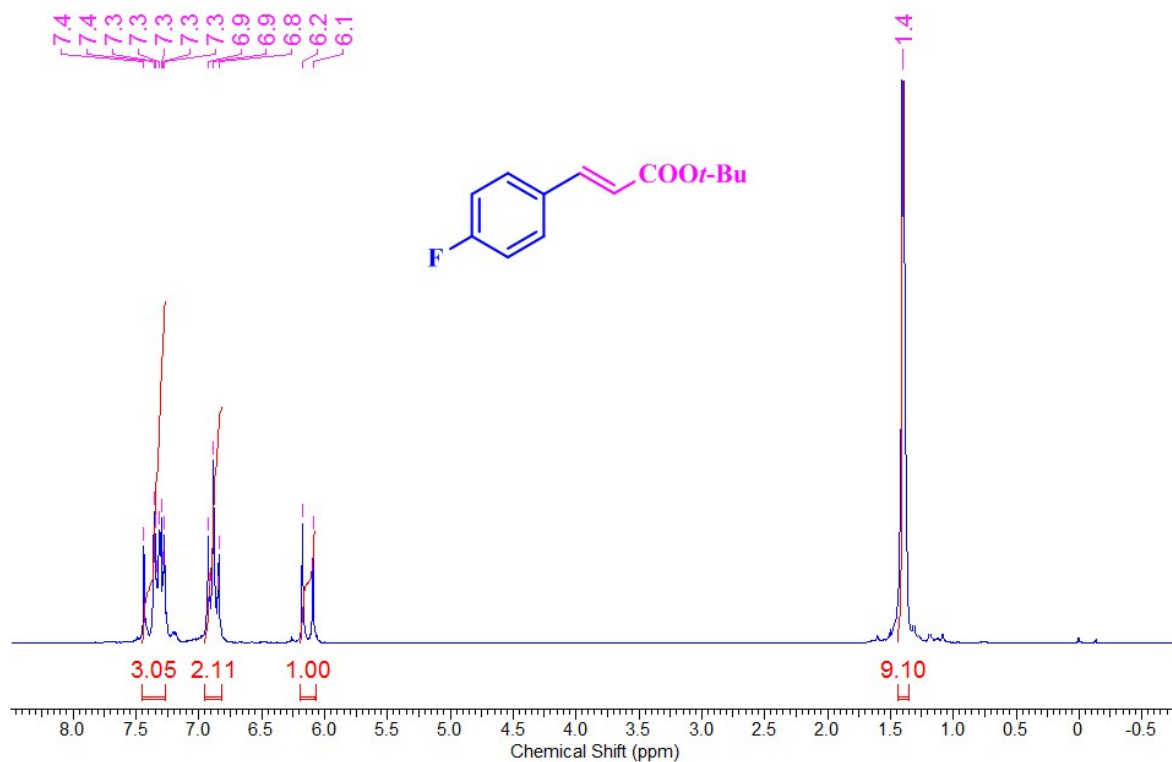
¹H NMR spectrum of methyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 16):



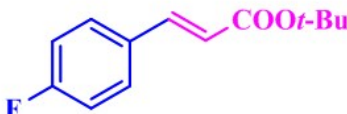
^{13}C NMR spectrum of methyl(*E*)-3-(4-chlorophenyl)acrylate (Table 4, entry 16):



^1H NMR spectrum of tert-butyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 17):



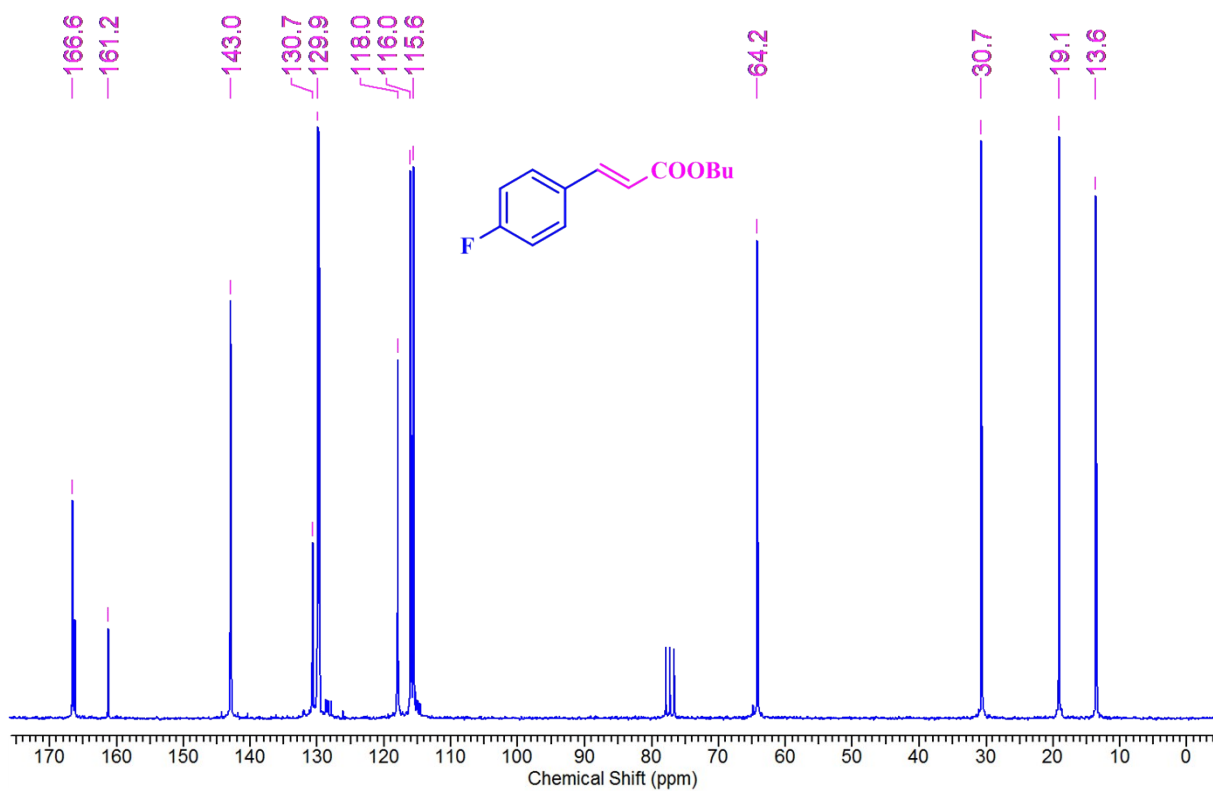
^{13}C NMR spectrum of tert-butyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 17):



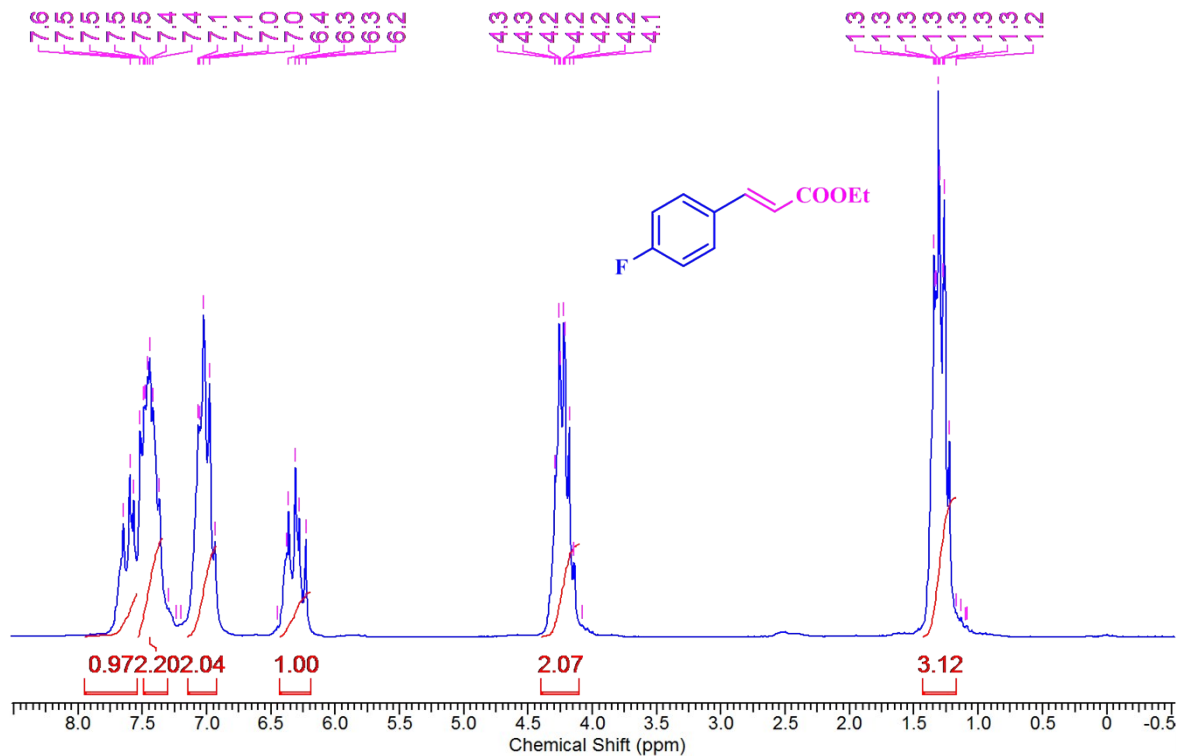
Chemical structure: CCCC(=O)/C=C/c1ccc(F)cc1

¹H NMR spectrum (CDCl₃) showing peaks at 7.4-7.3 ppm (aromatic, 7H), 6.9-6.2 ppm (aromatic, 6H), 4.1 ppm (CH₂, 4H), 2.05 ppm (CH₂, 2H), 1.5-1.3 ppm (CH₂, 4H), and 0.9 ppm (CH₃, 3H). Integration values are shown below the peaks: 1.01, 2.11, 2.13, 1.00, 2.05, 2.04, 2.13, 3.07.

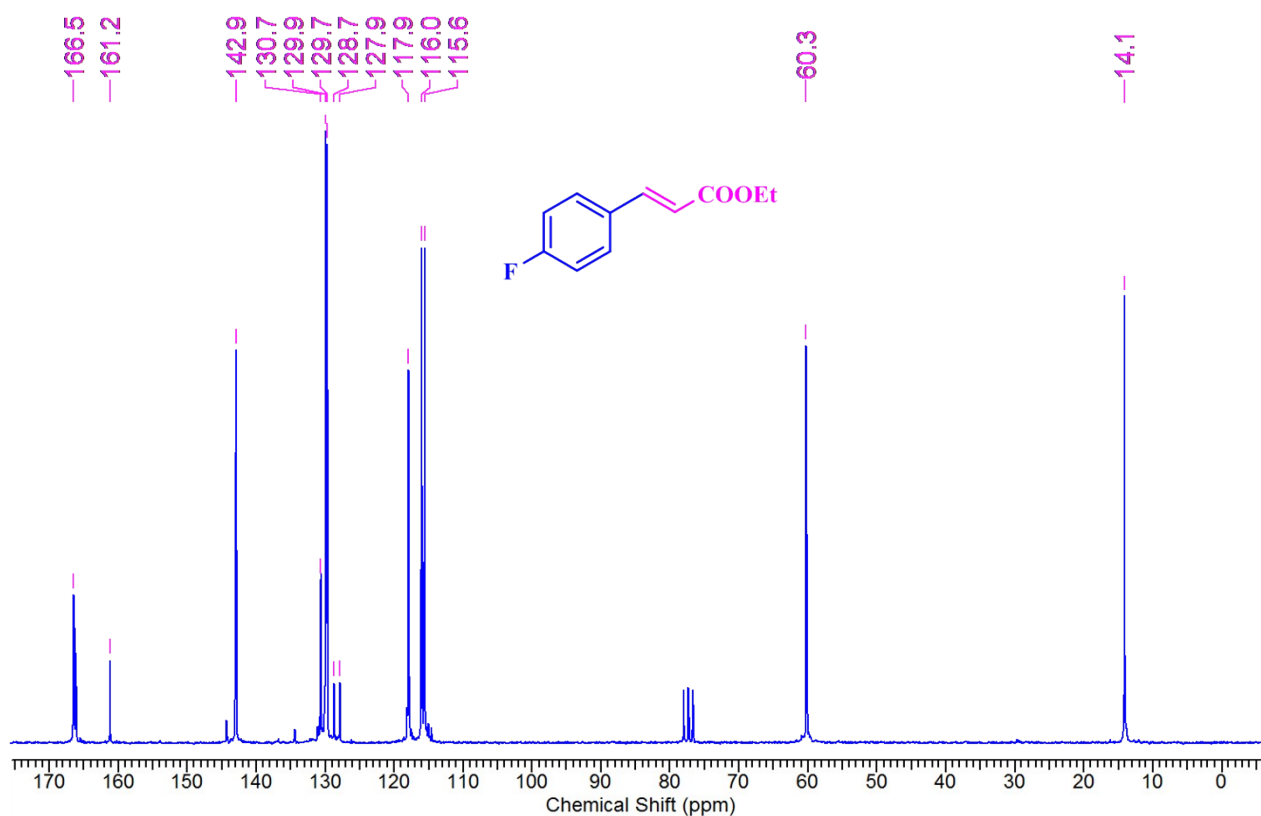
18



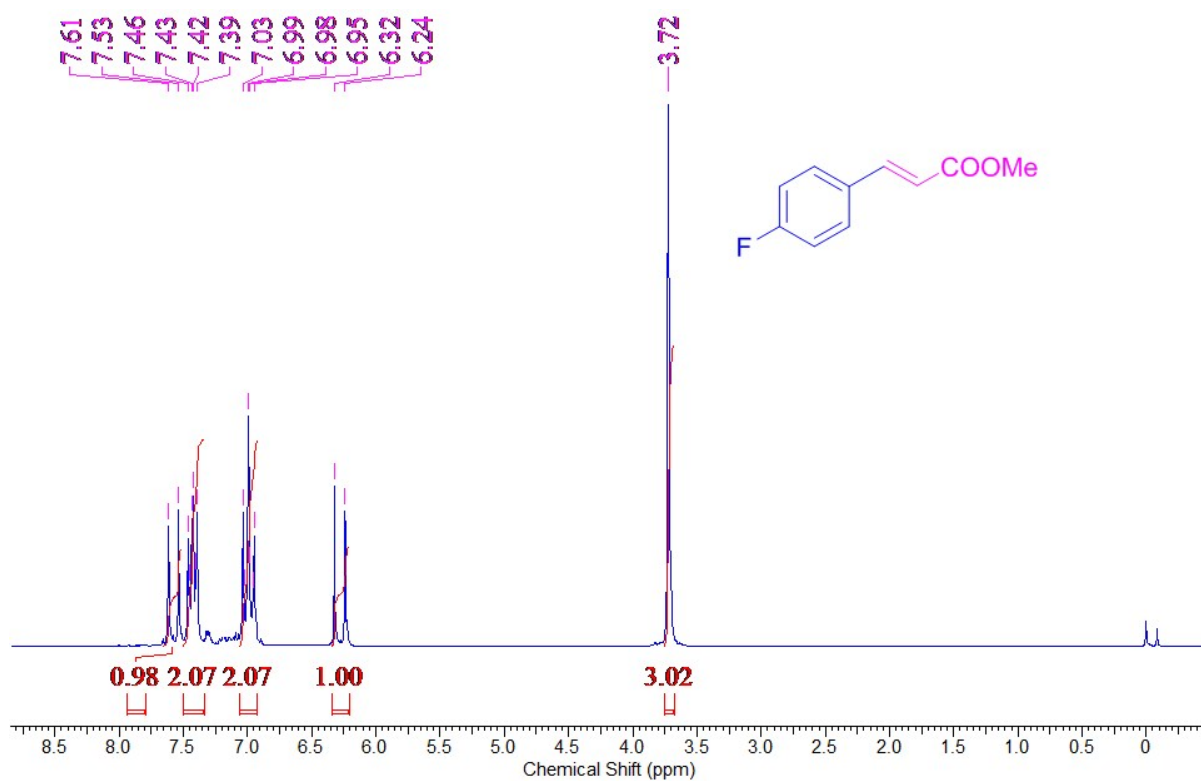
¹H NMR spectrum of ethyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 19):



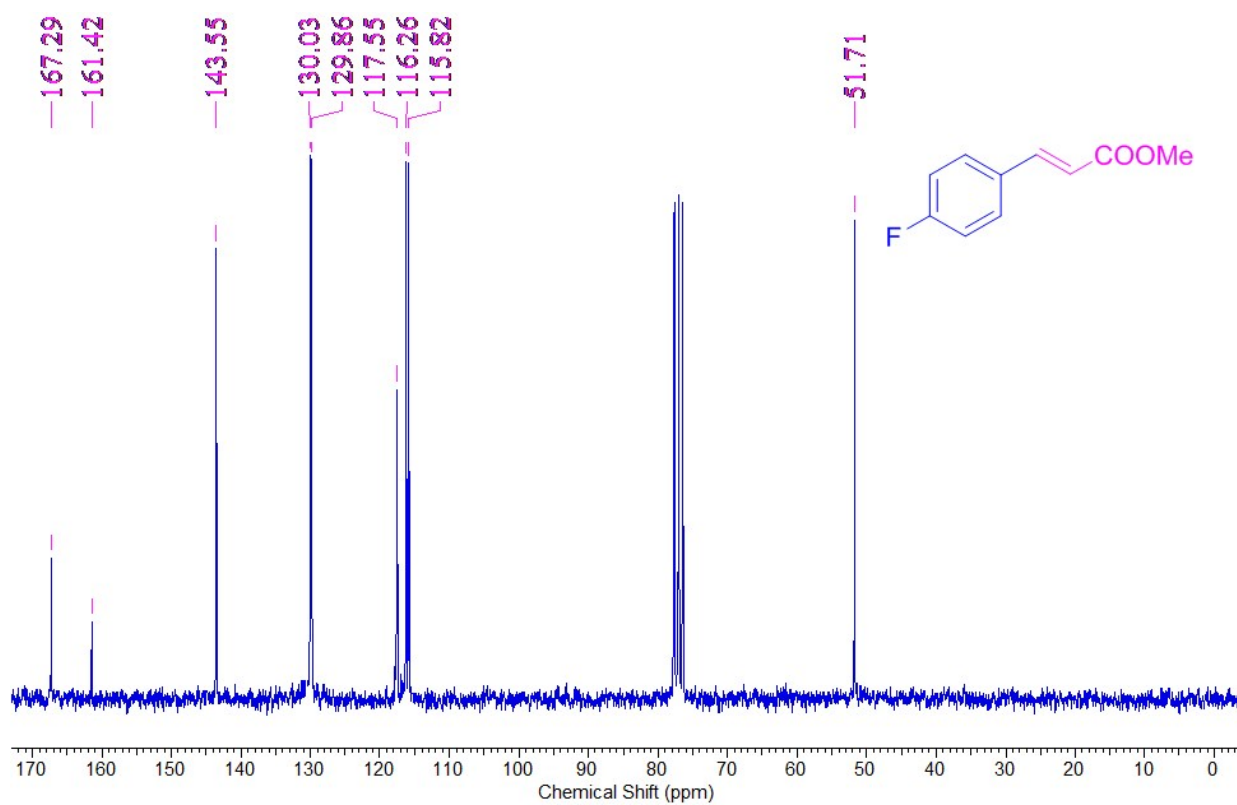
¹³C NMR spectrum of ethyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 19):



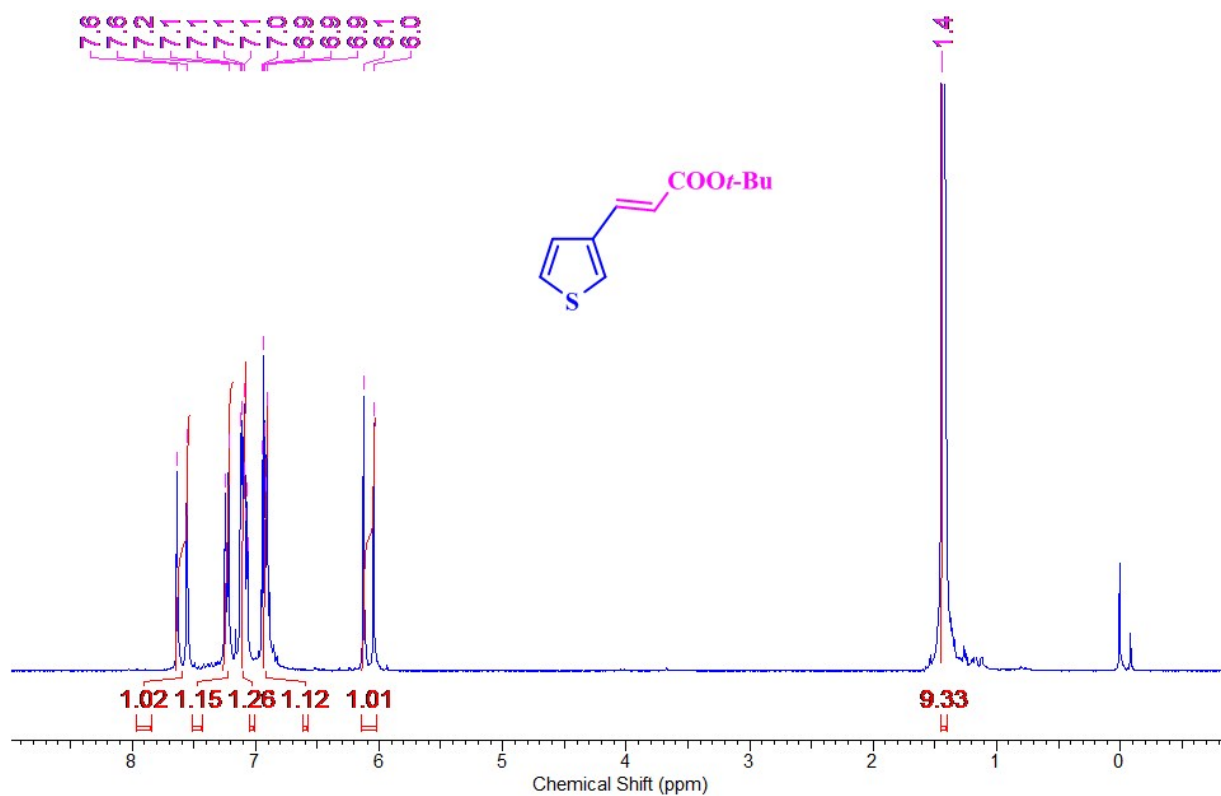
¹H NMR spectrum of methyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 20):



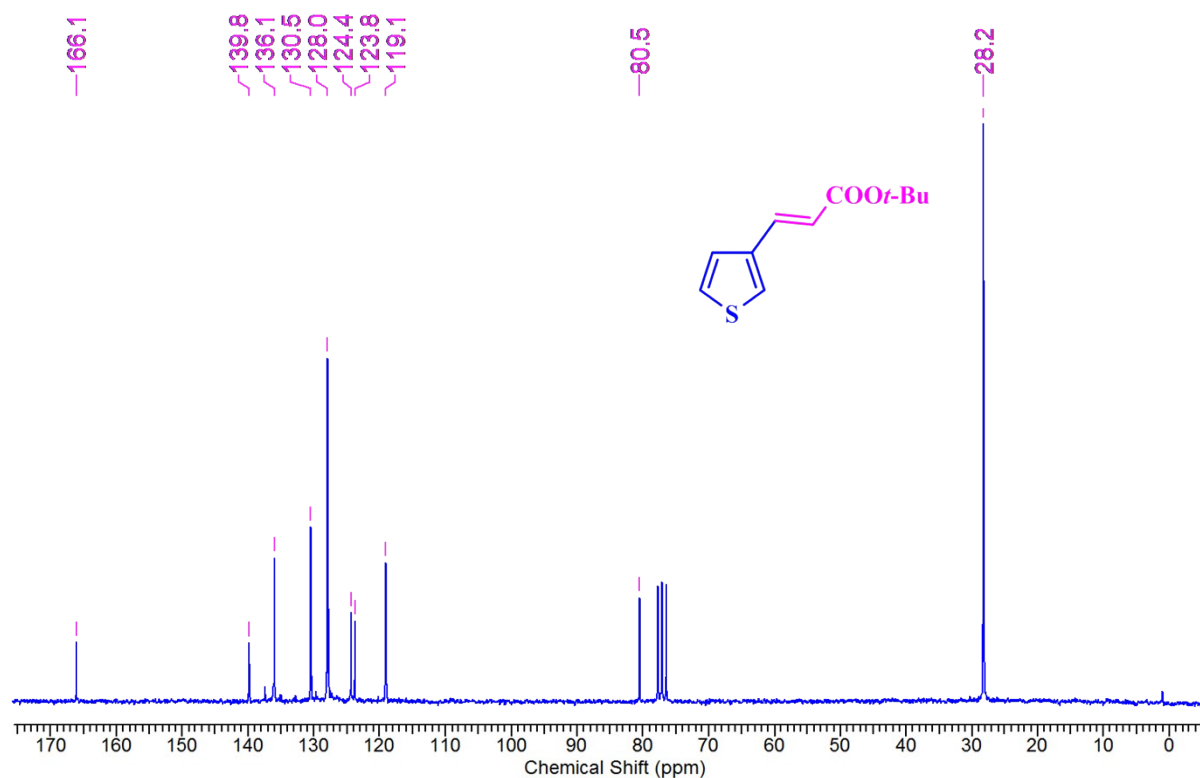
¹³C NMR spectrum of methyl(*E*)-3-(4-fluorophenyl)acrylate (Table 4, entry 20):



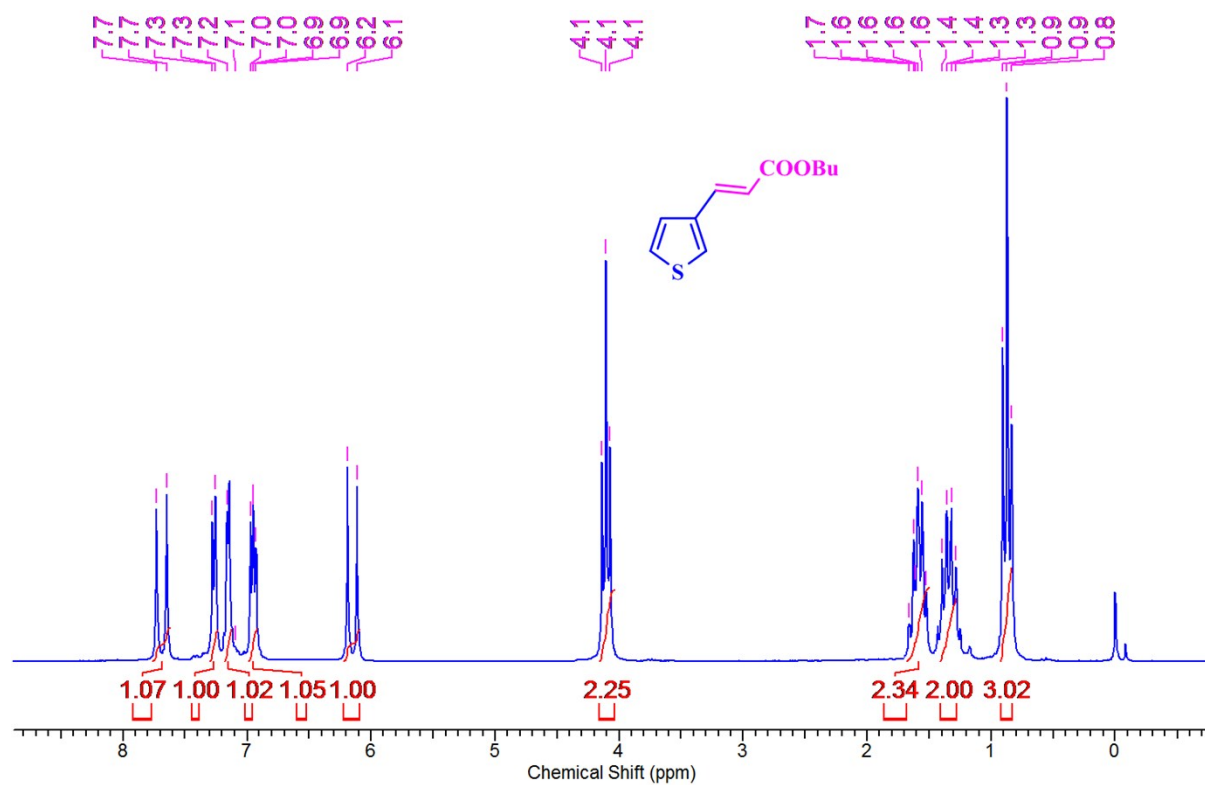
¹H NMR spectrum of tert-butyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 21):



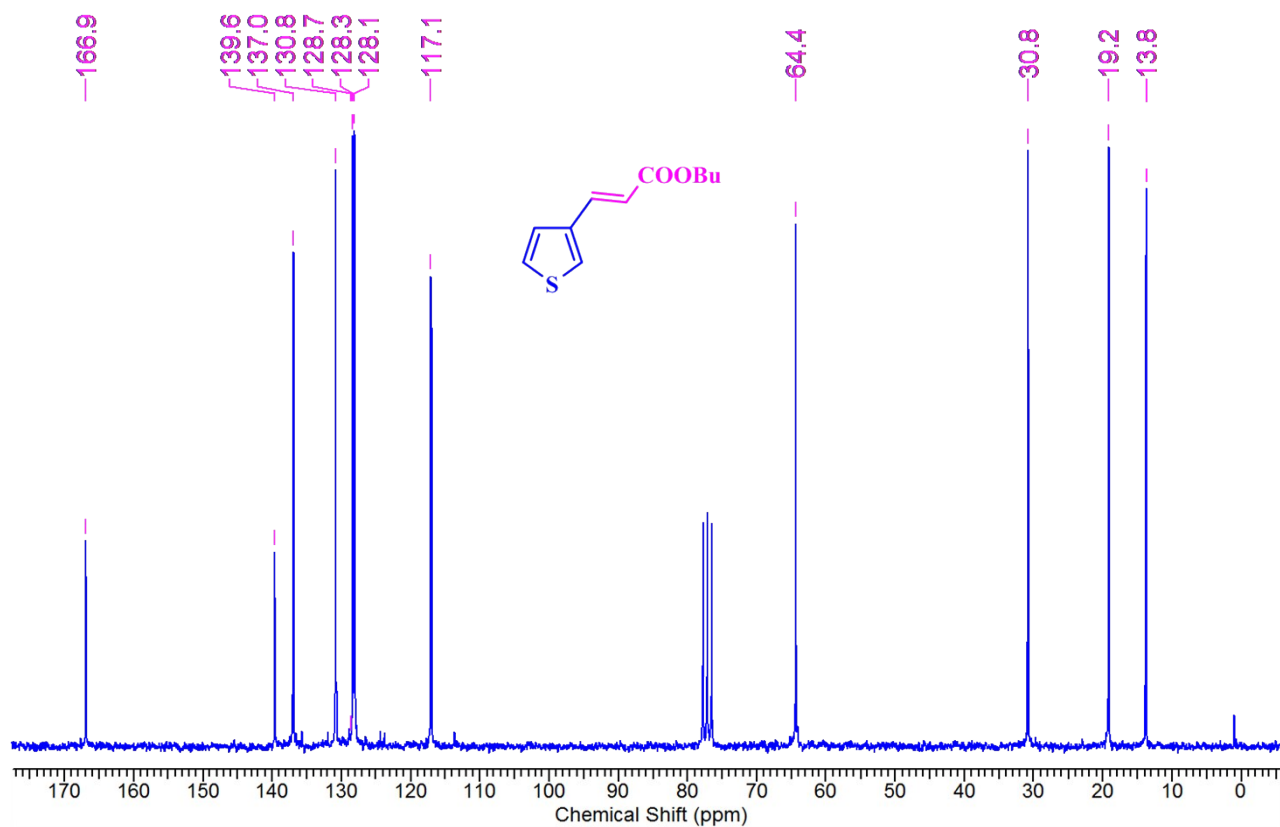
^{13}C NMR spectrum of tert-butyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 21):



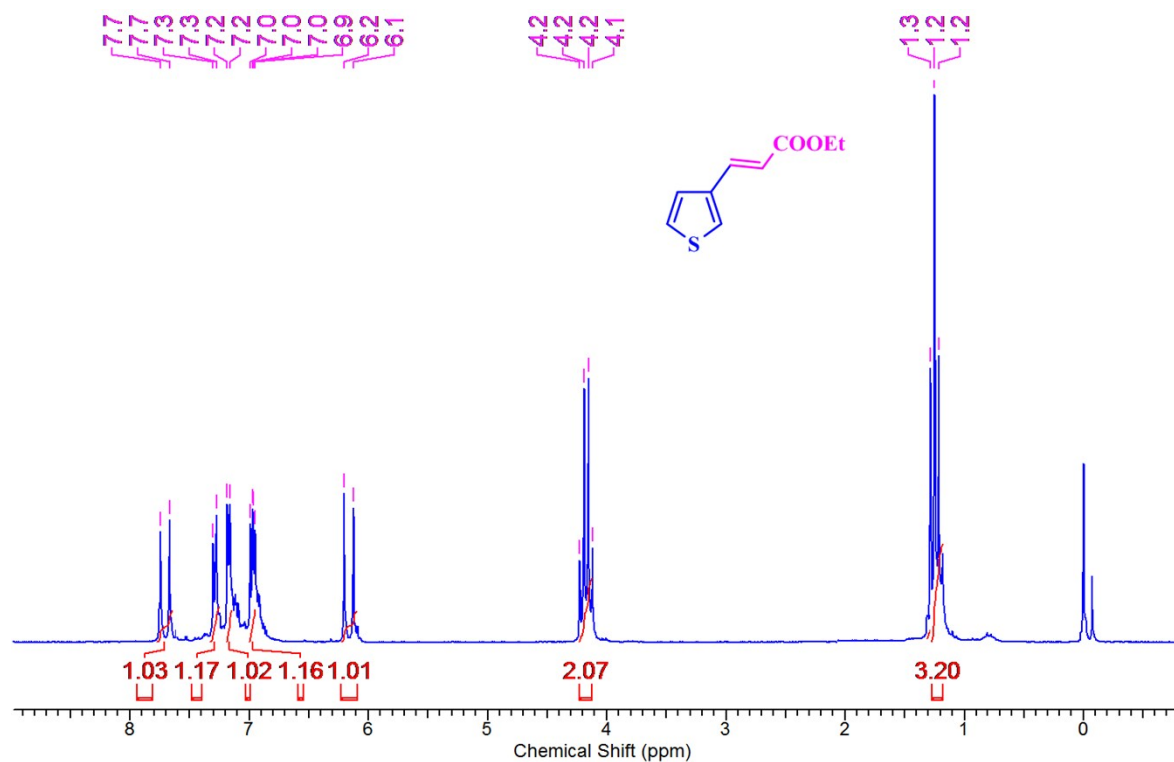
^1H NMR spectrum of butyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 22):



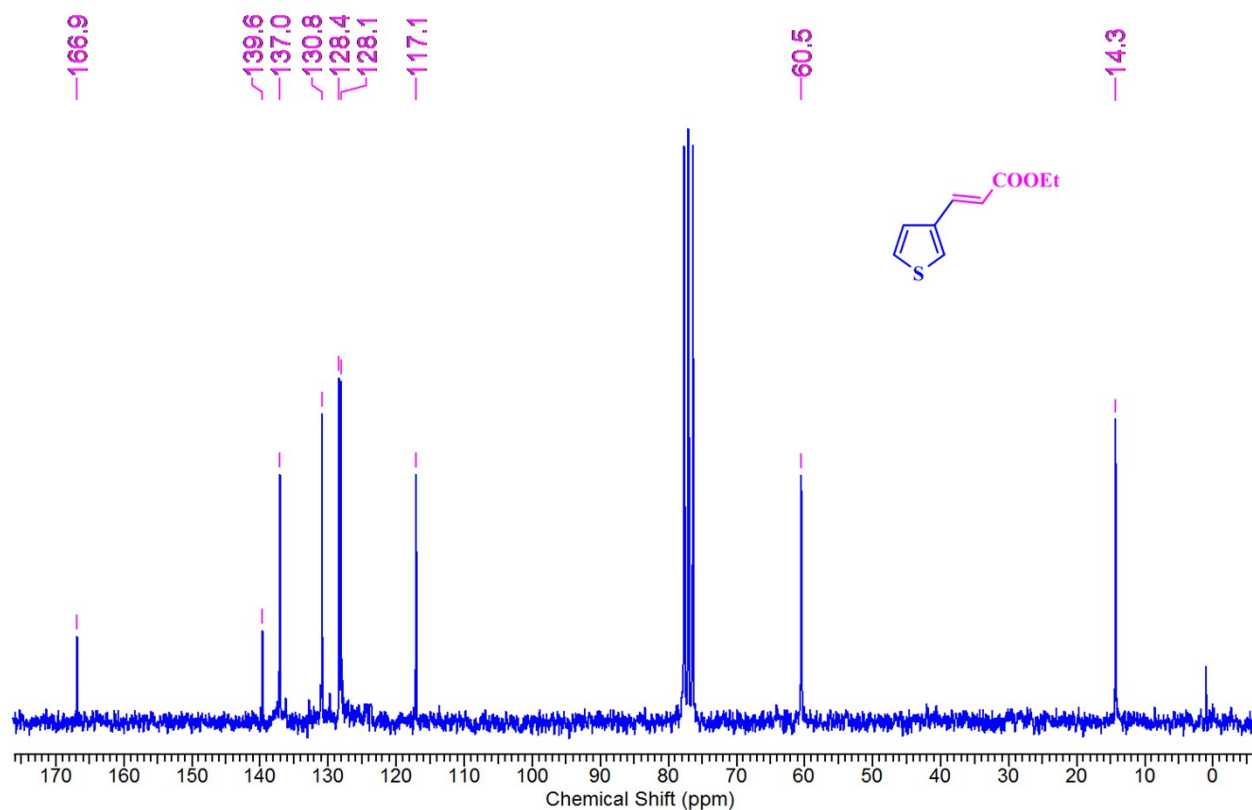
^{13}C NMR spectrum of butyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 22):



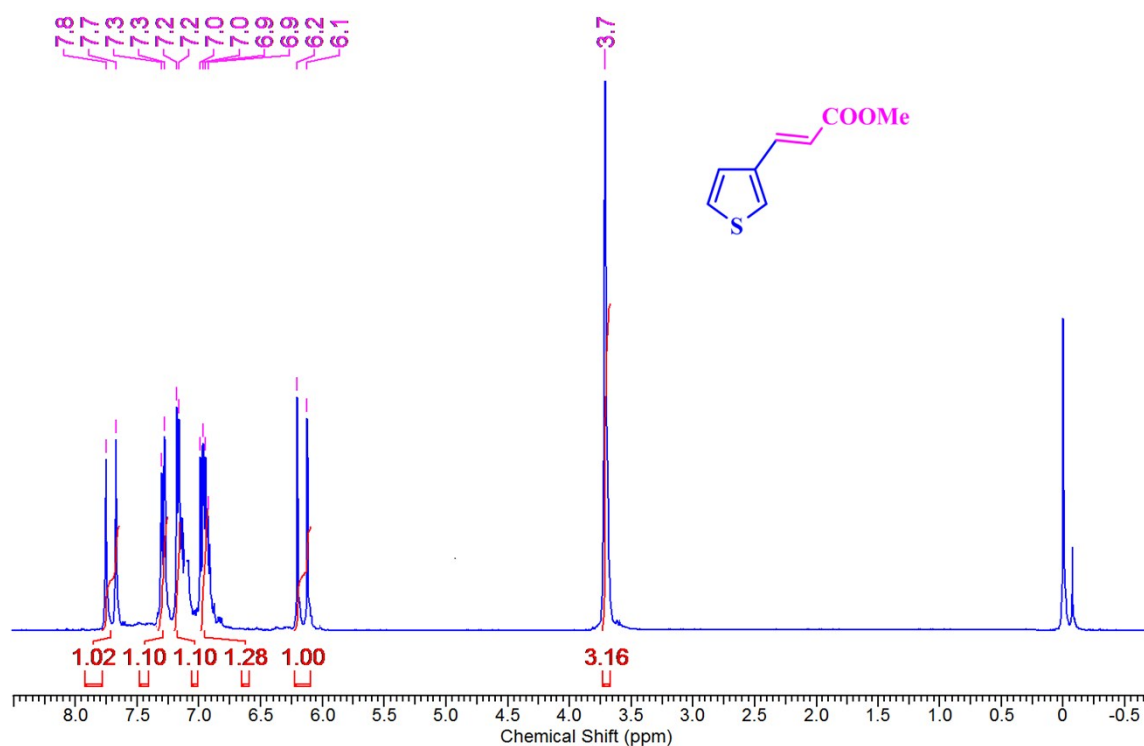
^1H NMR spectrum of ethyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 23):



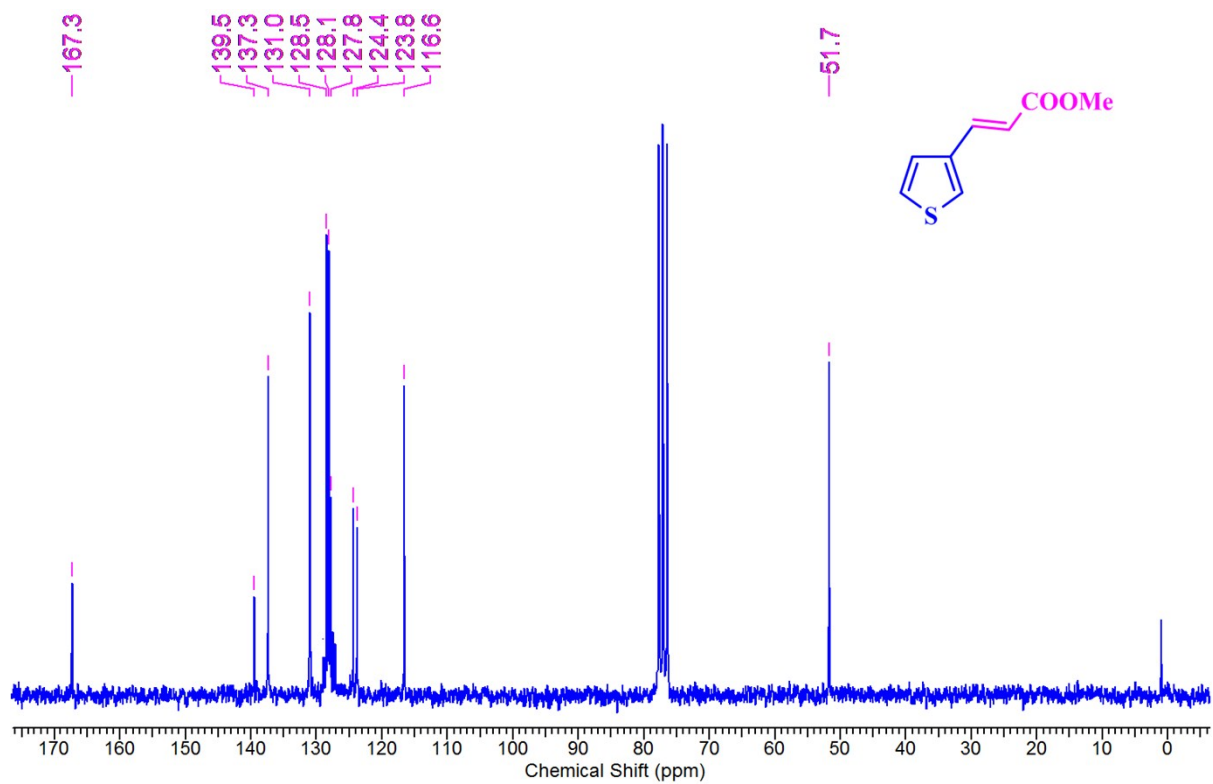
^{13}C NMR spectrum of ethyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 23):



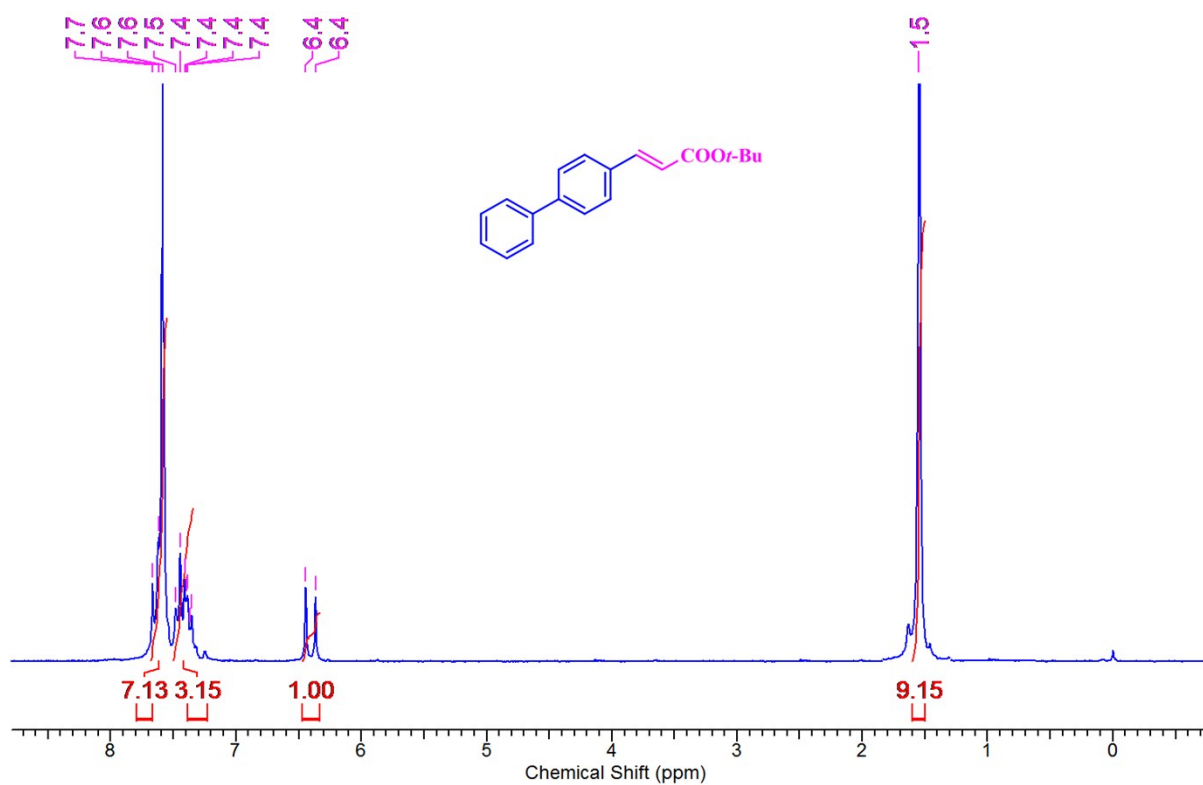
^1H NMR spectrum of methyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 24):



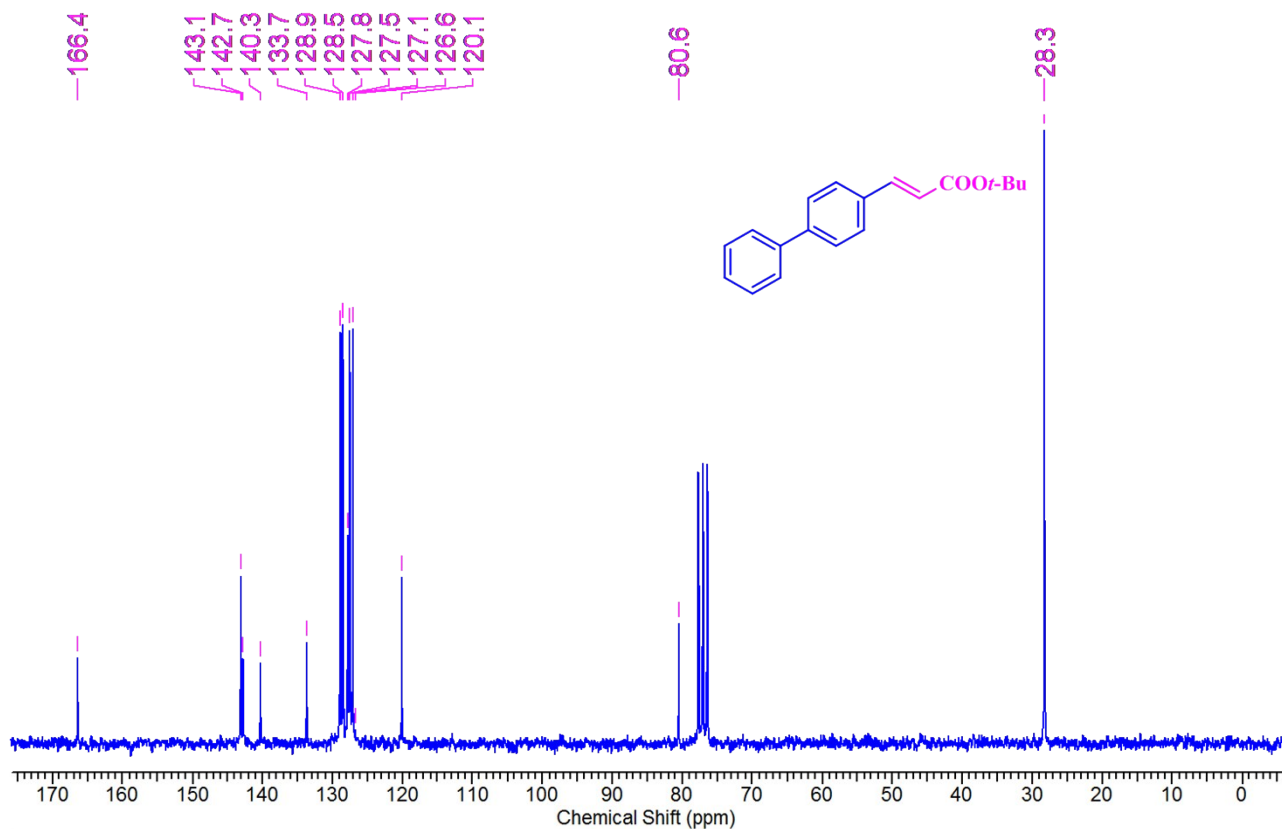
^{13}C NMR spectrum of methyl(*E*)-3-(thiophen-3-yl)acrylate (Table 4, entry 24):



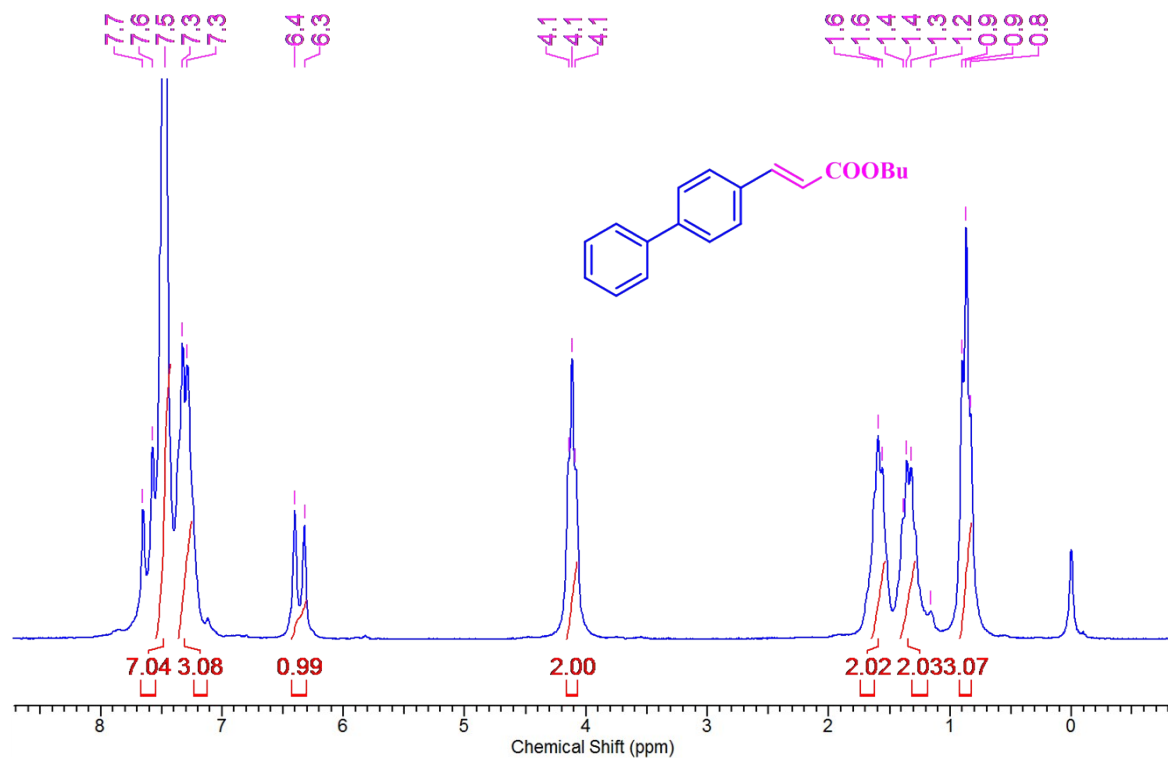
^1H NMR spectrum of tert-butyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 25):



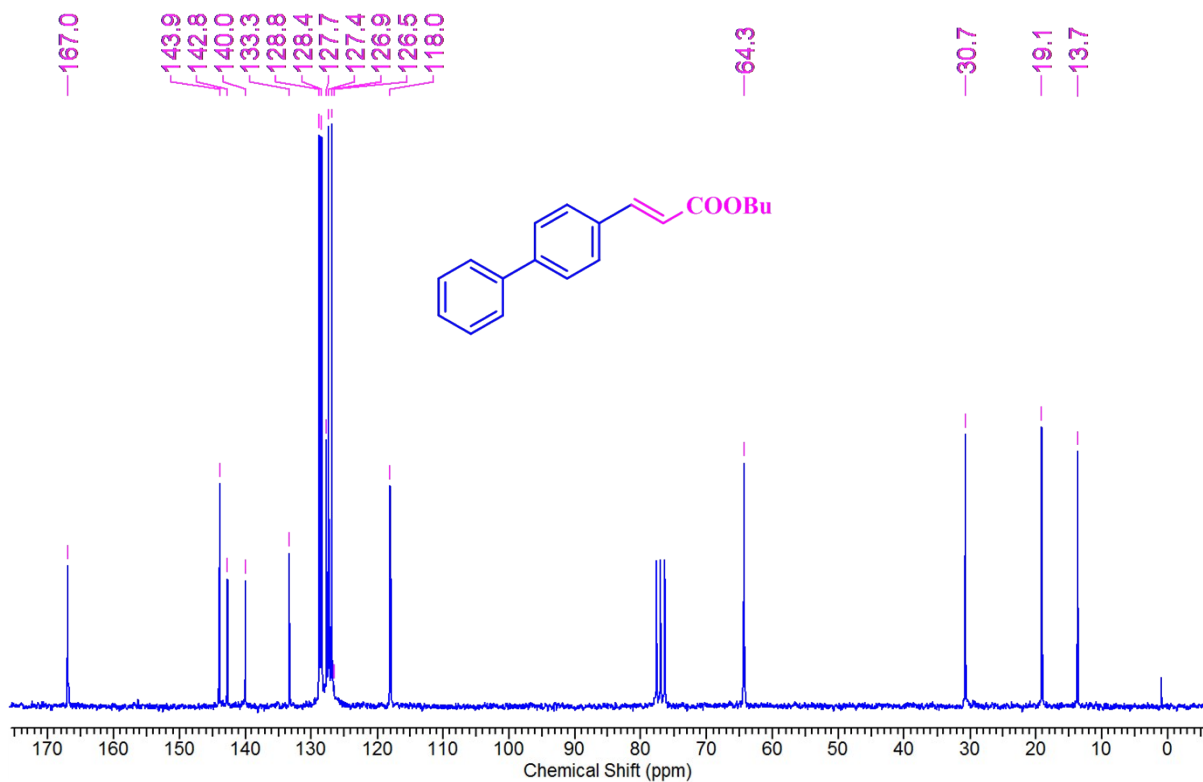
¹³C NMR spectrum of tert-butyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 25):



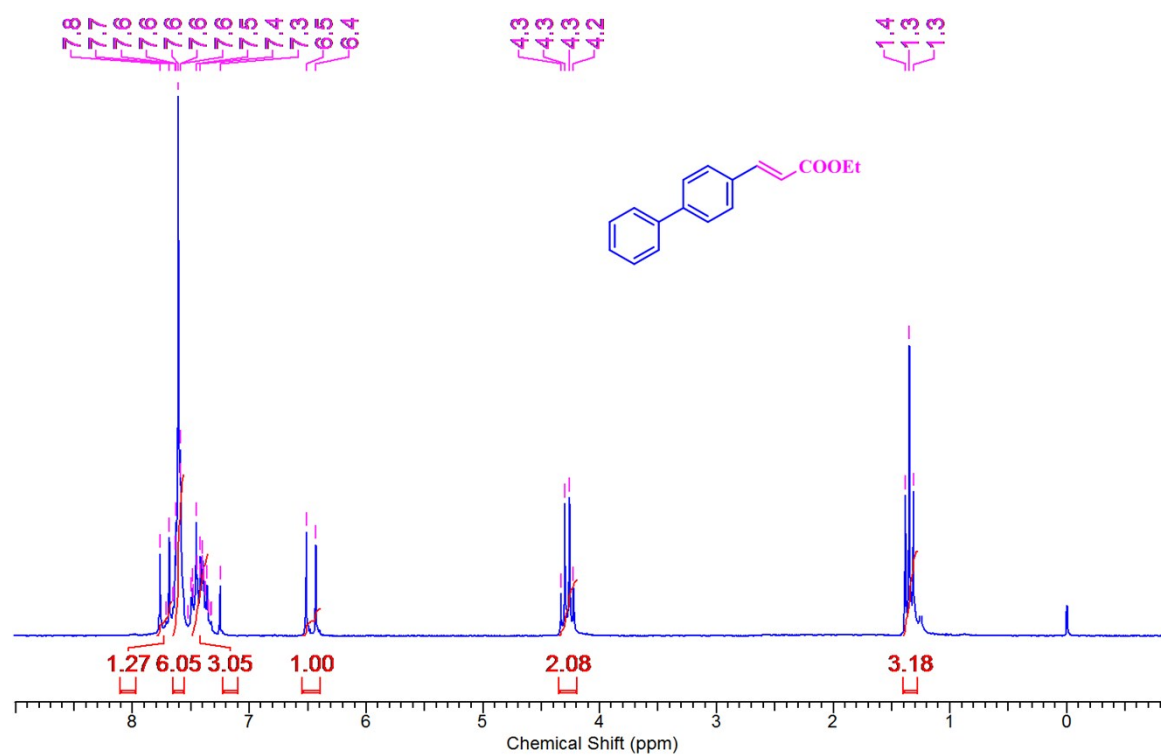
¹H NMR spectrum of butyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 26):



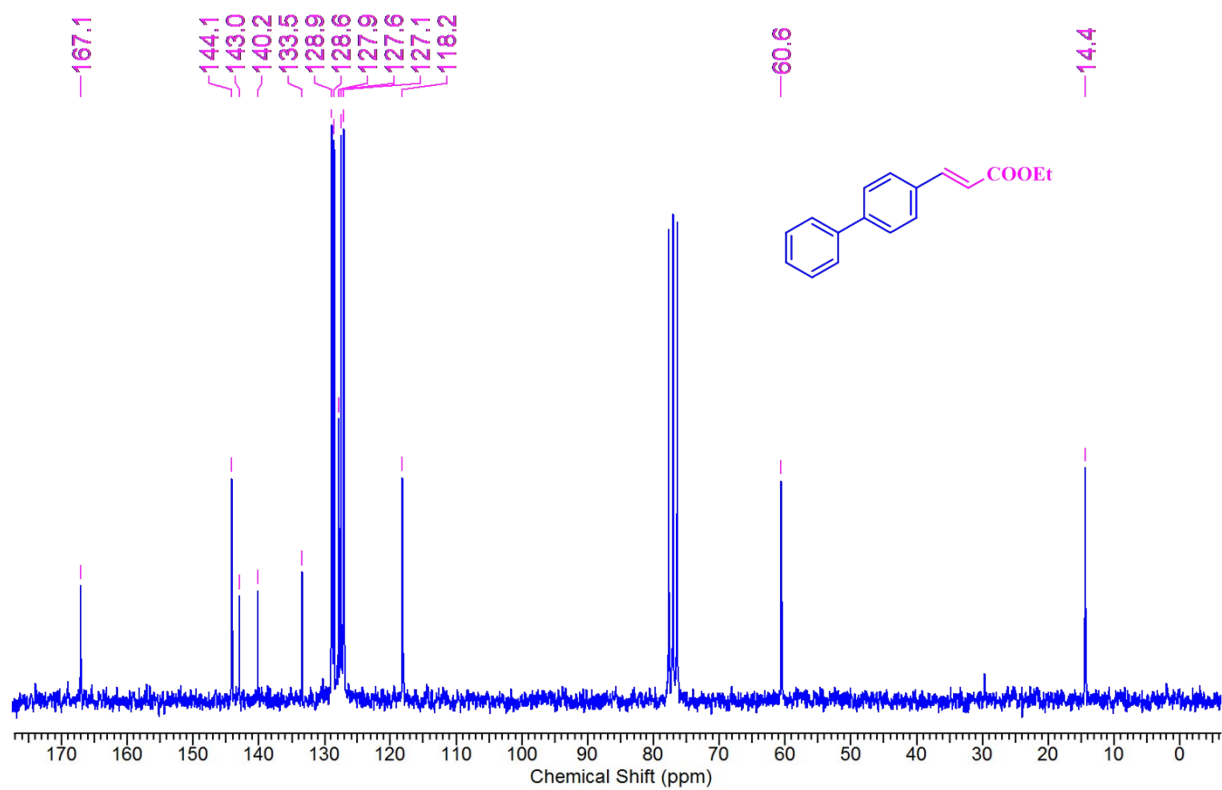
¹³C NMR spectrum of butyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 26):



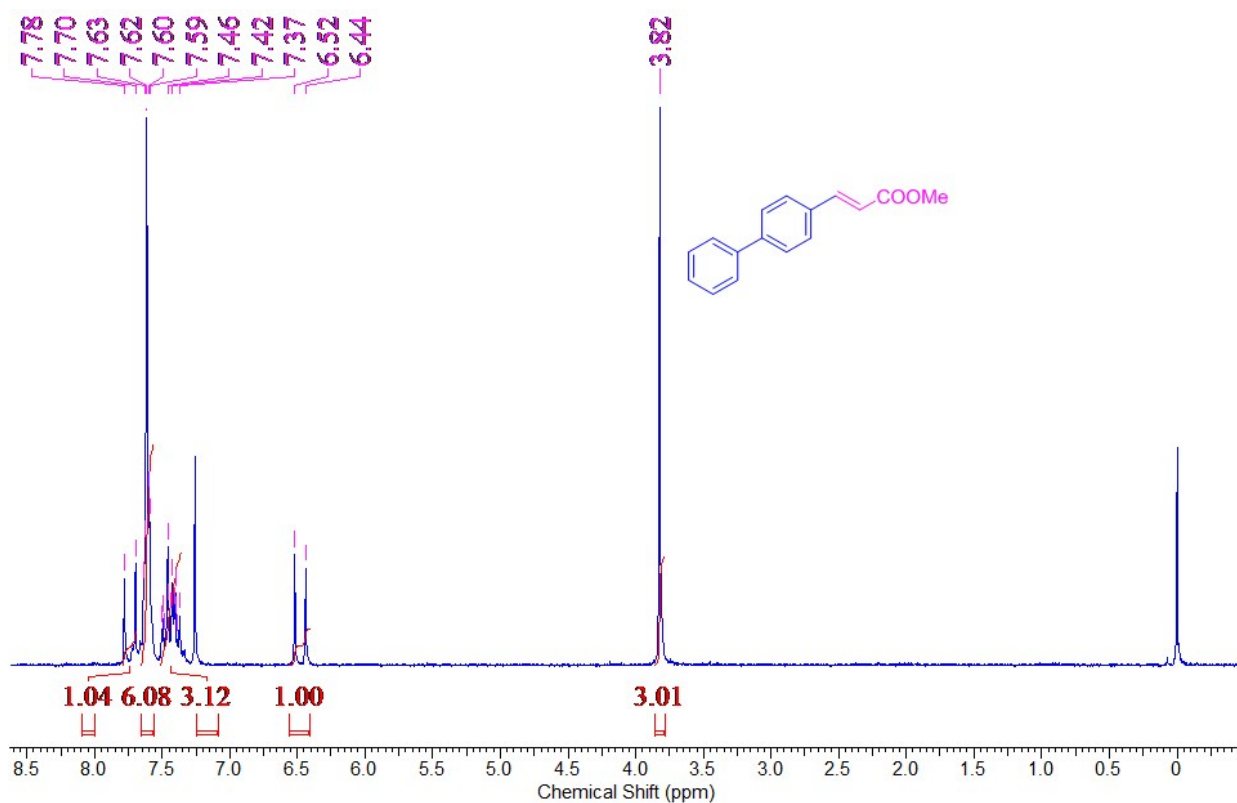
¹H NMR spectrum of ethyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 27):



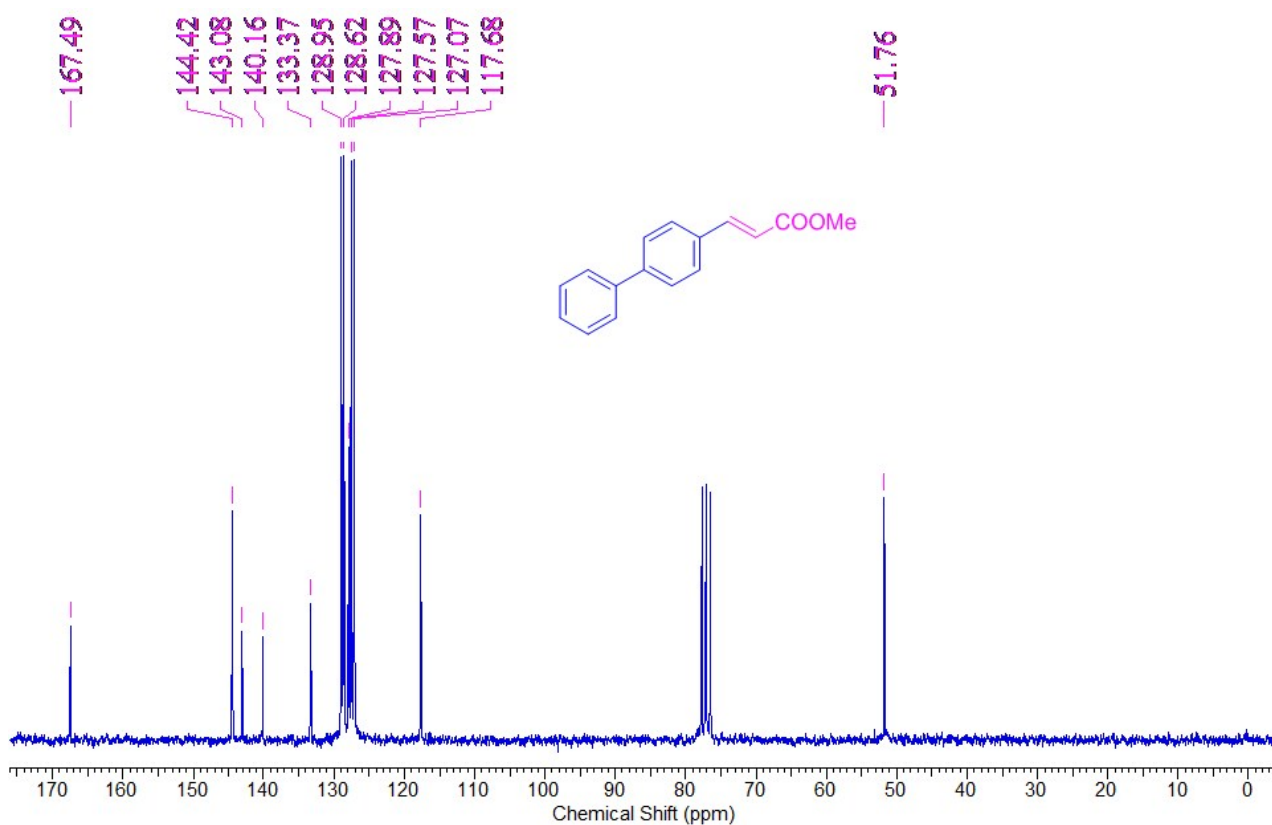
¹³C NMR spectrum of ethyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 27):



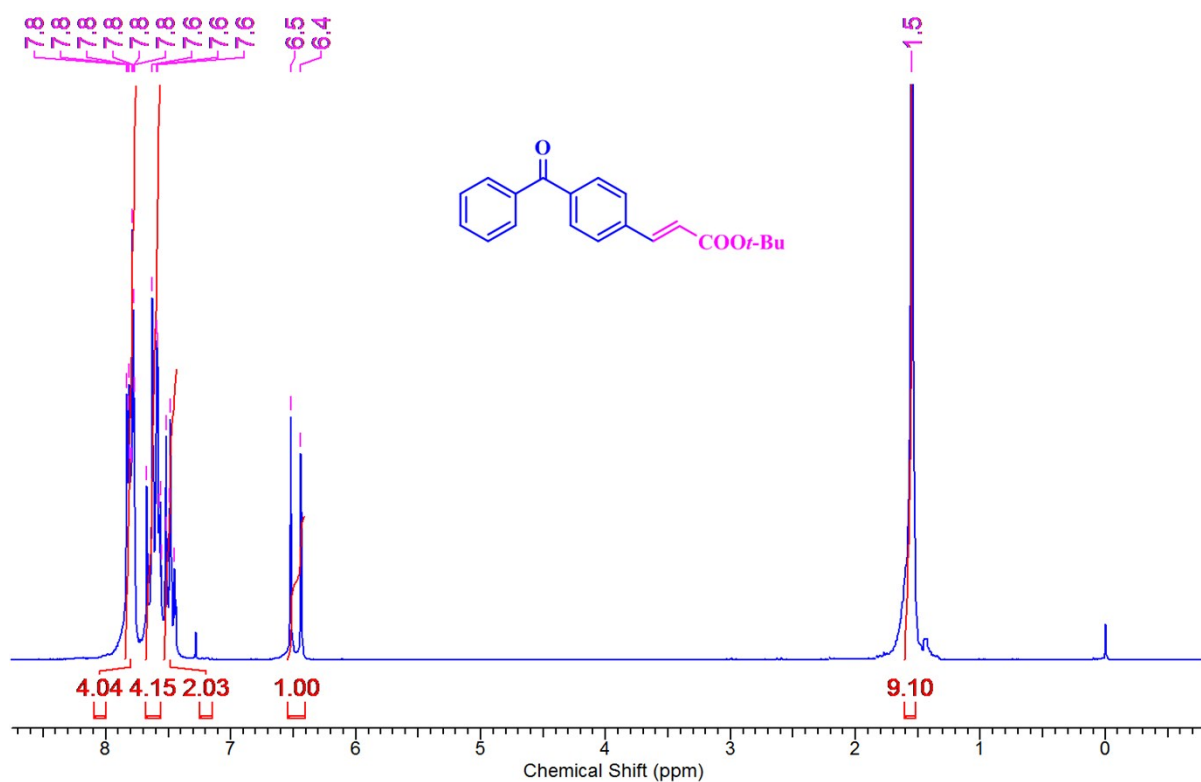
¹H NMR spectrum of methyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 28):



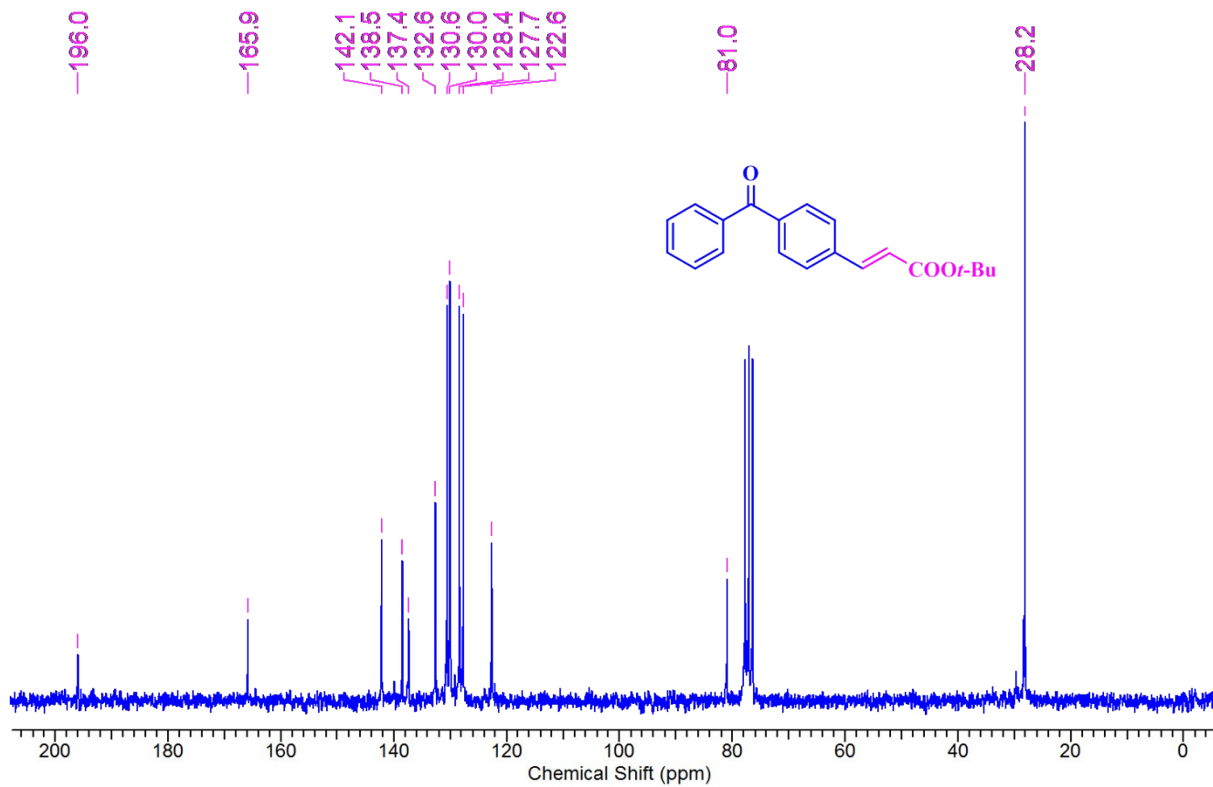
¹³C NMR spectrum of methyl(*E*)-3-([1,1'-biphenyl]-4-yl)acrylate (Table 4, entry 28):



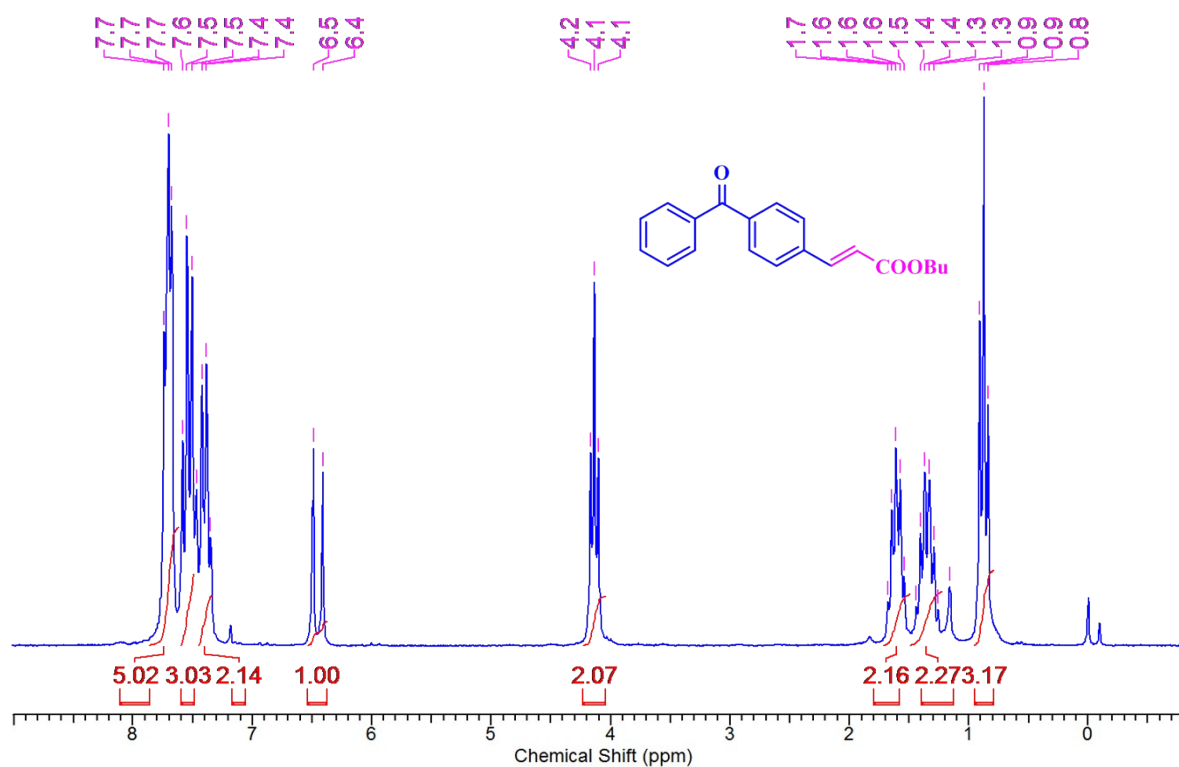
¹H NMR spectrum of tert-butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 29):



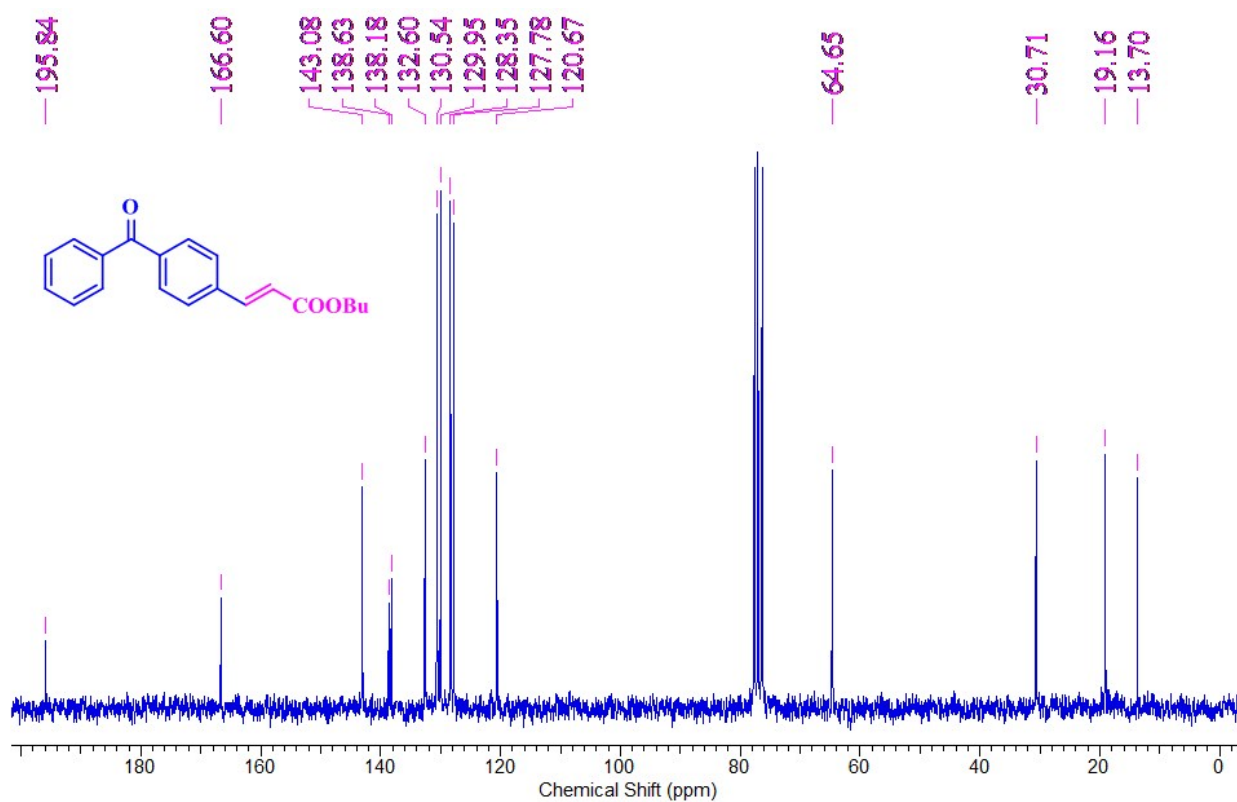
¹³C NMR spectrum of tert-butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 29):



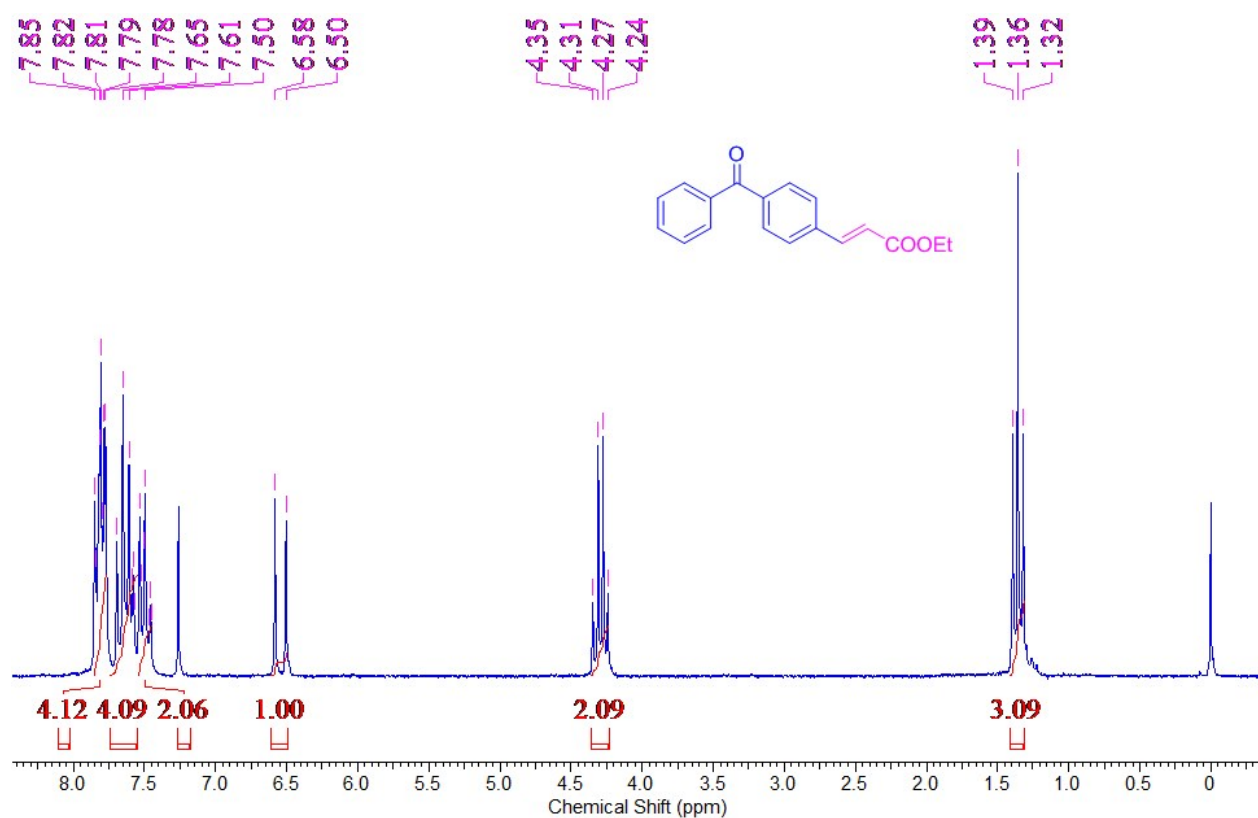
¹H NMR spectrum of butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 30):



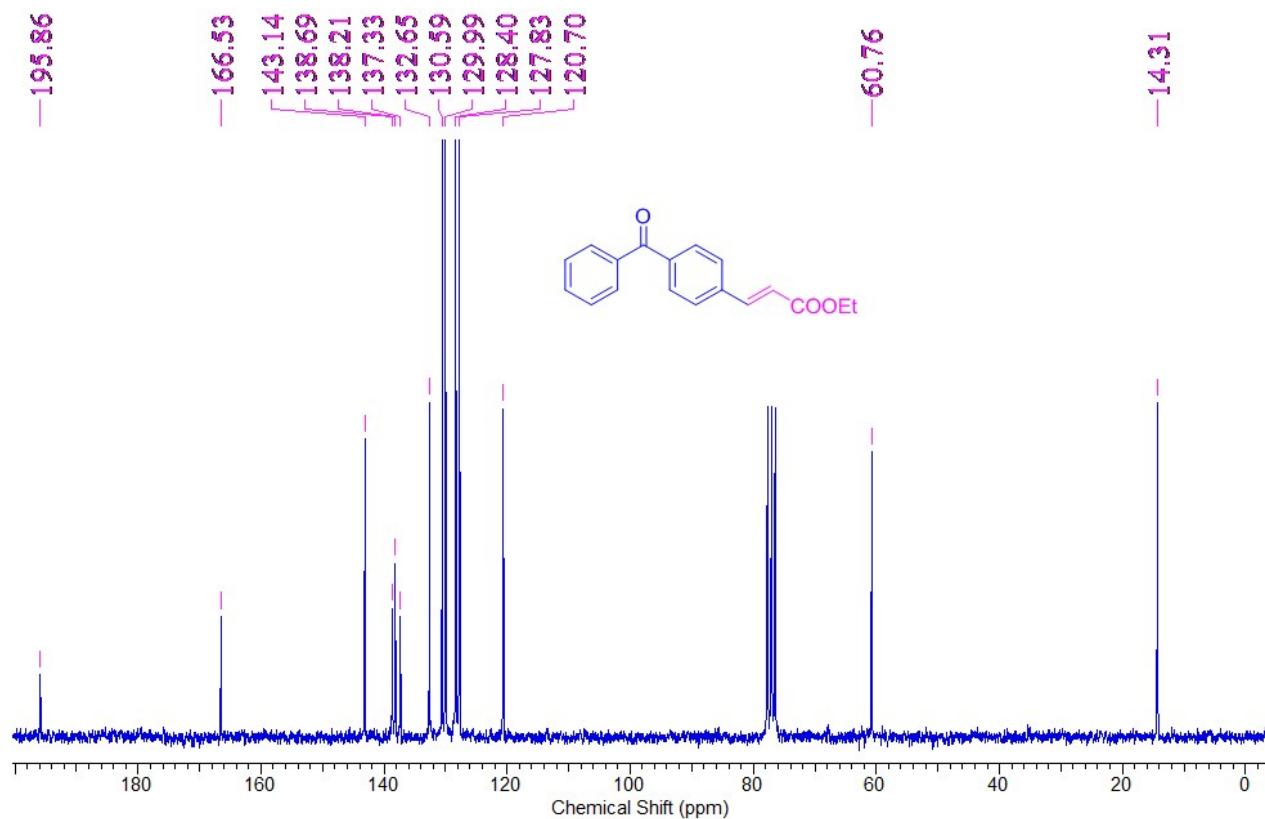
¹³C NMR spectrum of butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 30):



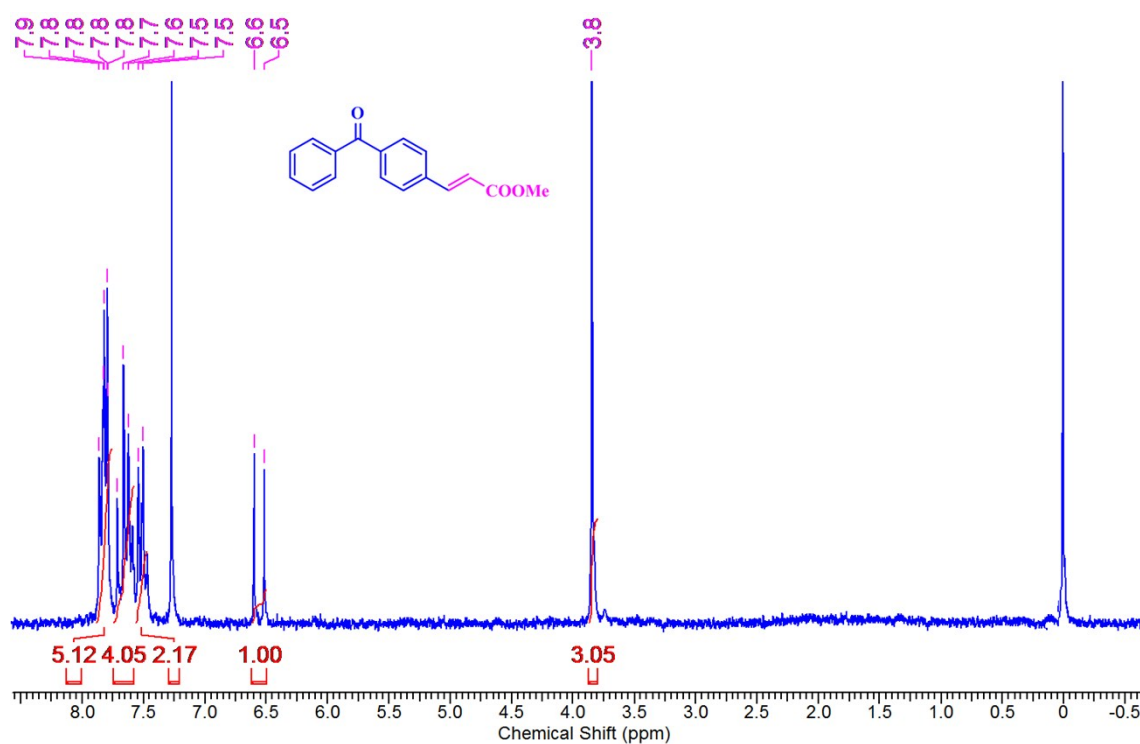
¹H spectrum of ethyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 31):



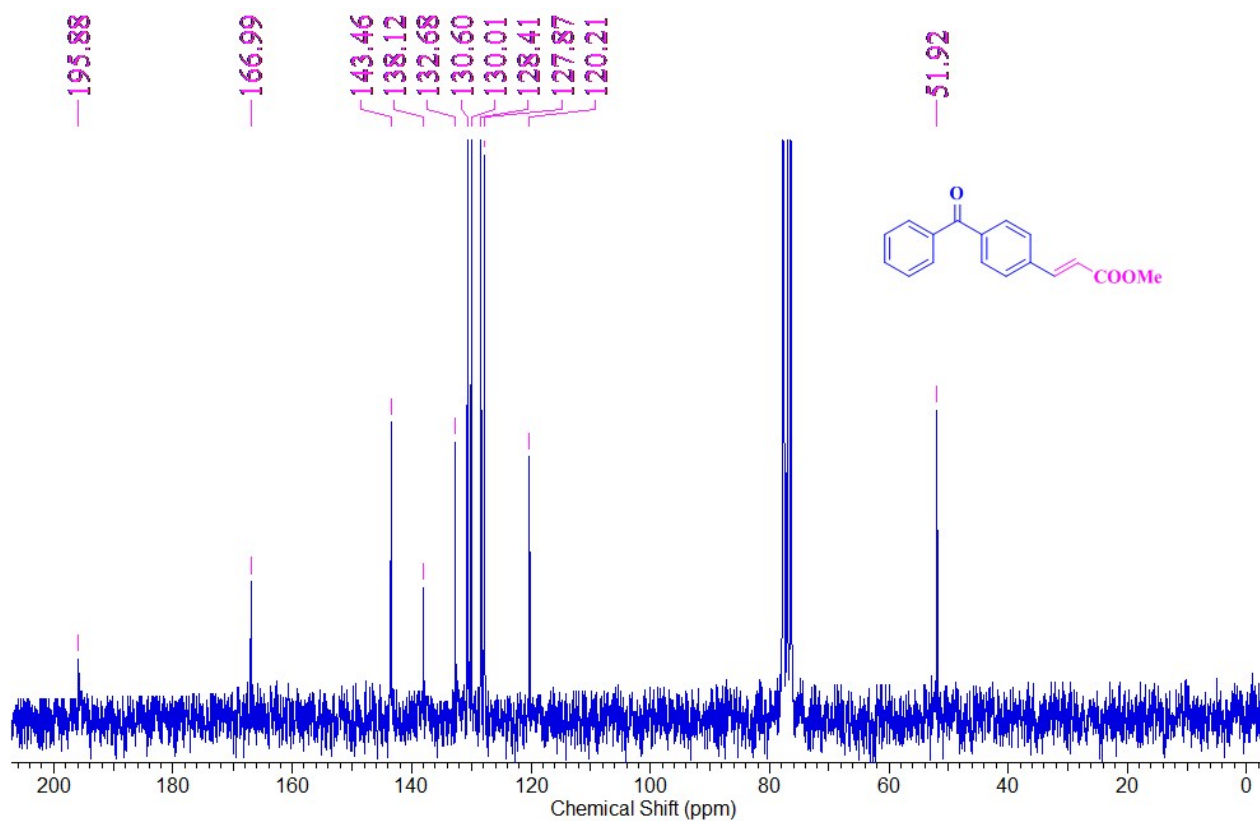
¹³C spectrum of ethyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 31):



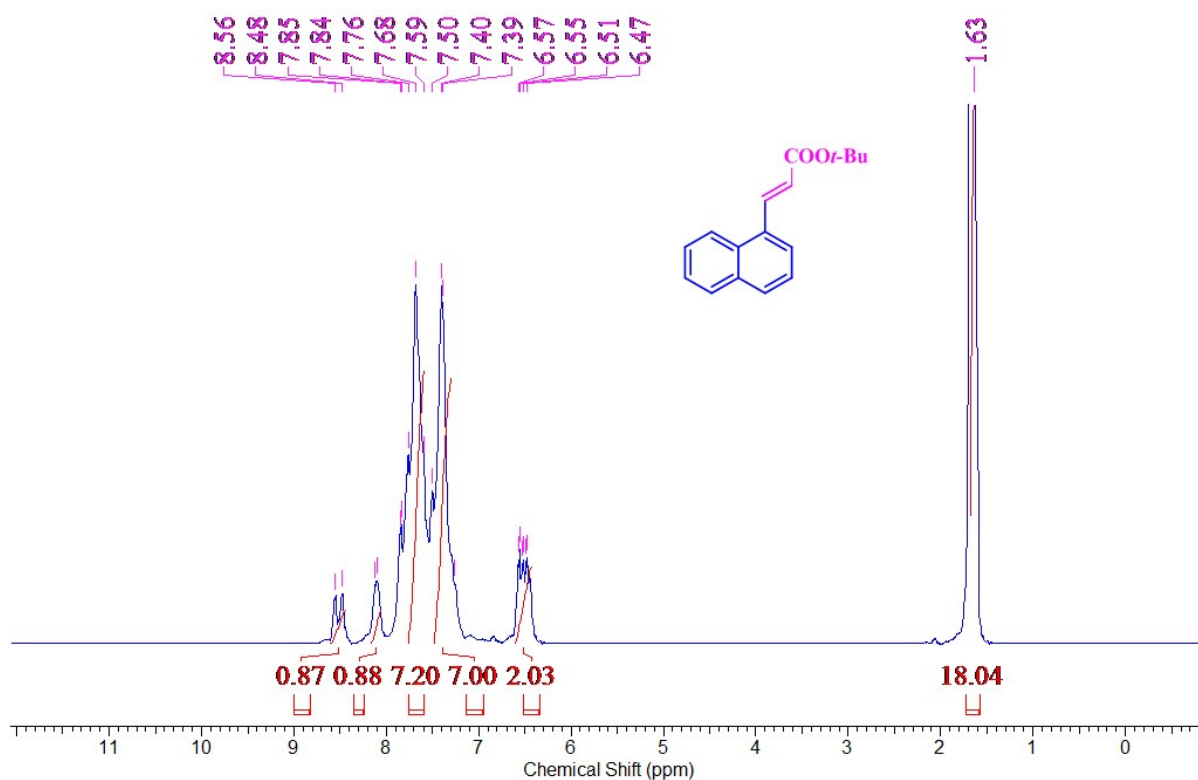
¹H NMR spectrum of methyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 32):



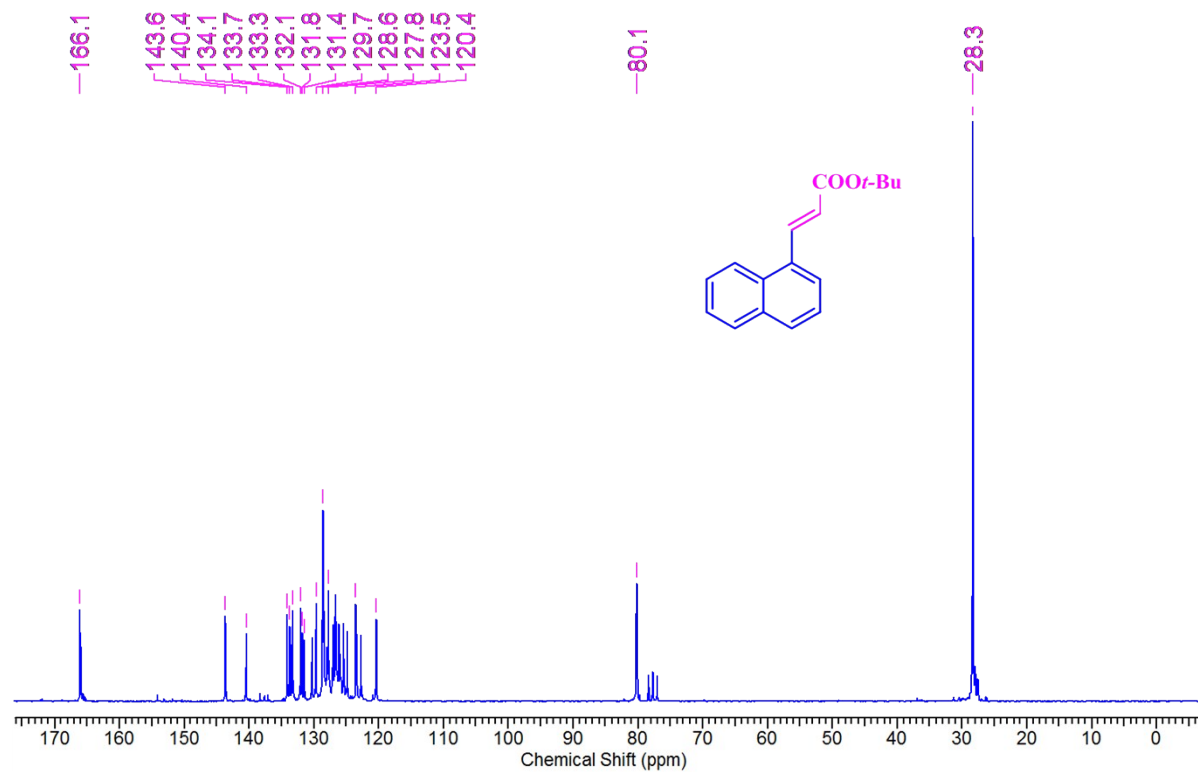
¹³C NMR spectrum of methyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 4, entry 32):



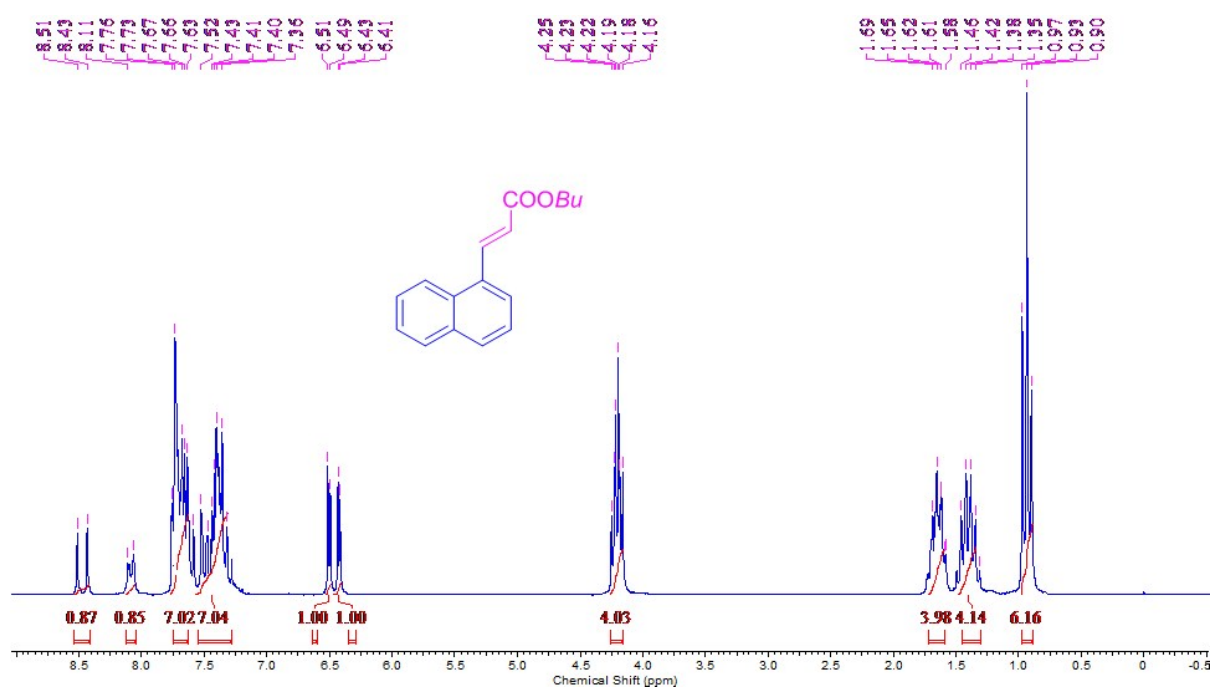
¹H NMR spectrum of tert-butyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 33):



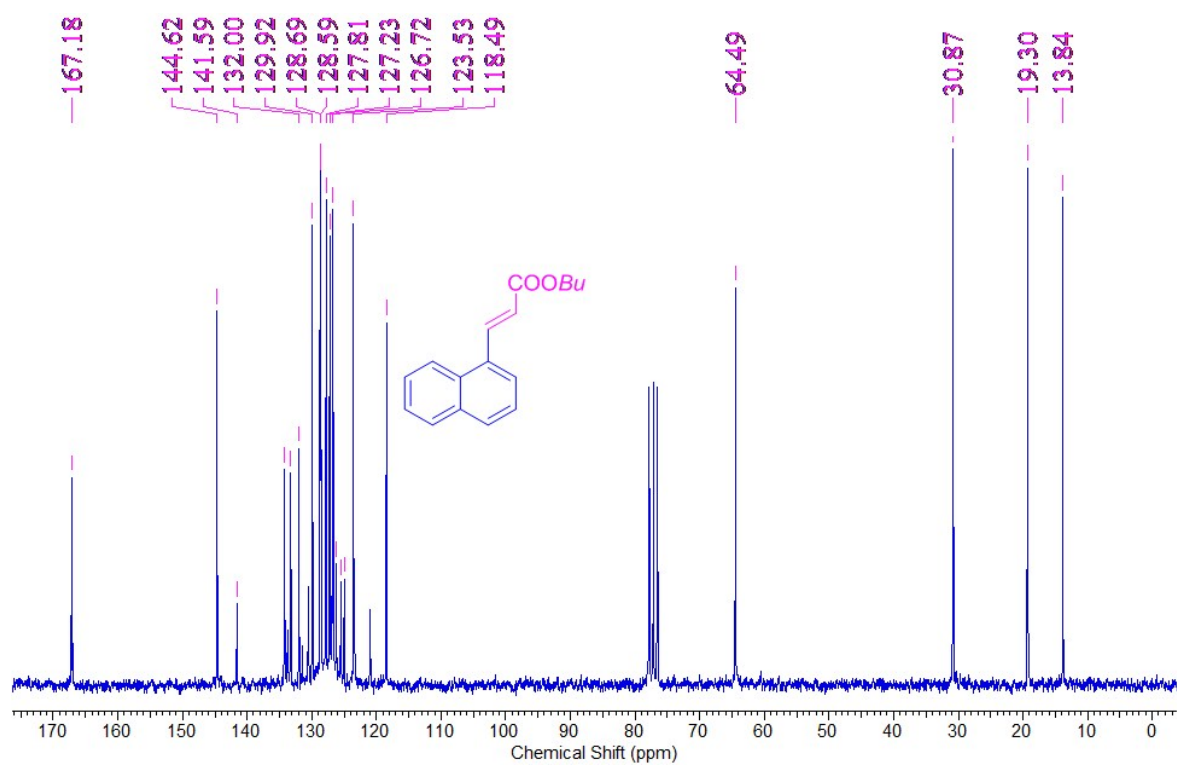
¹³C NMR spectrum of tert-butyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 33):



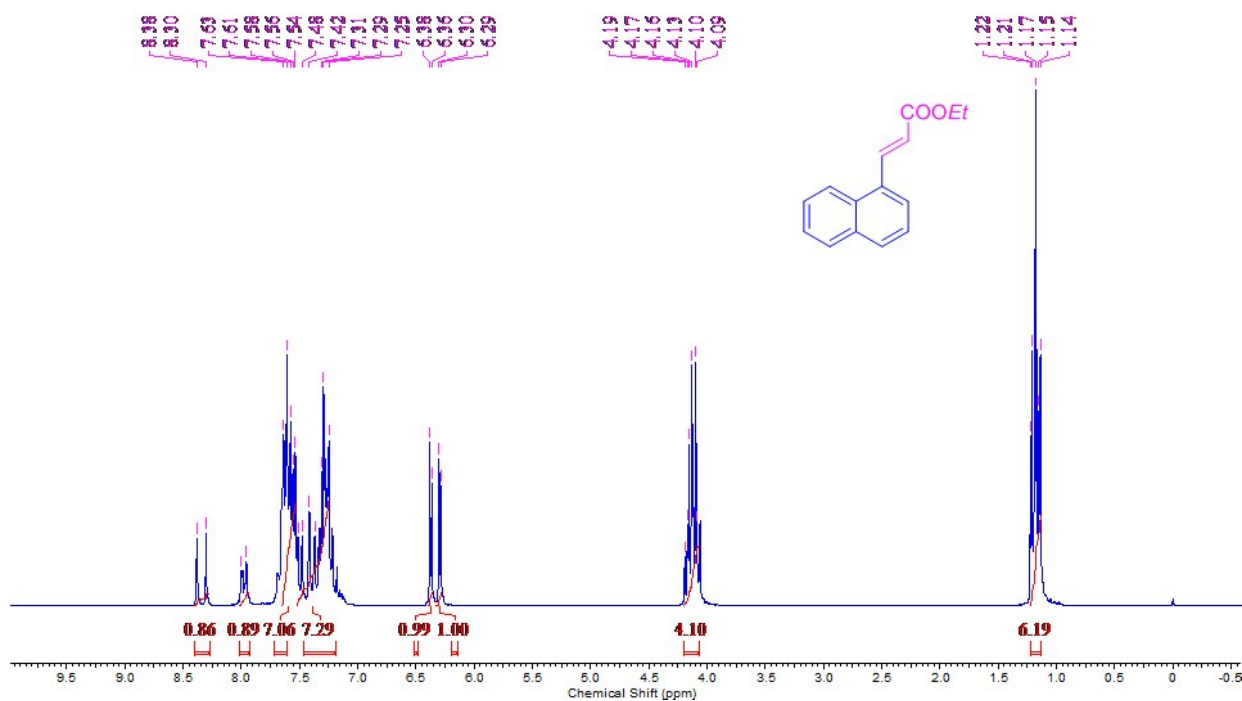
¹H NMR spectrum of butyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 34):



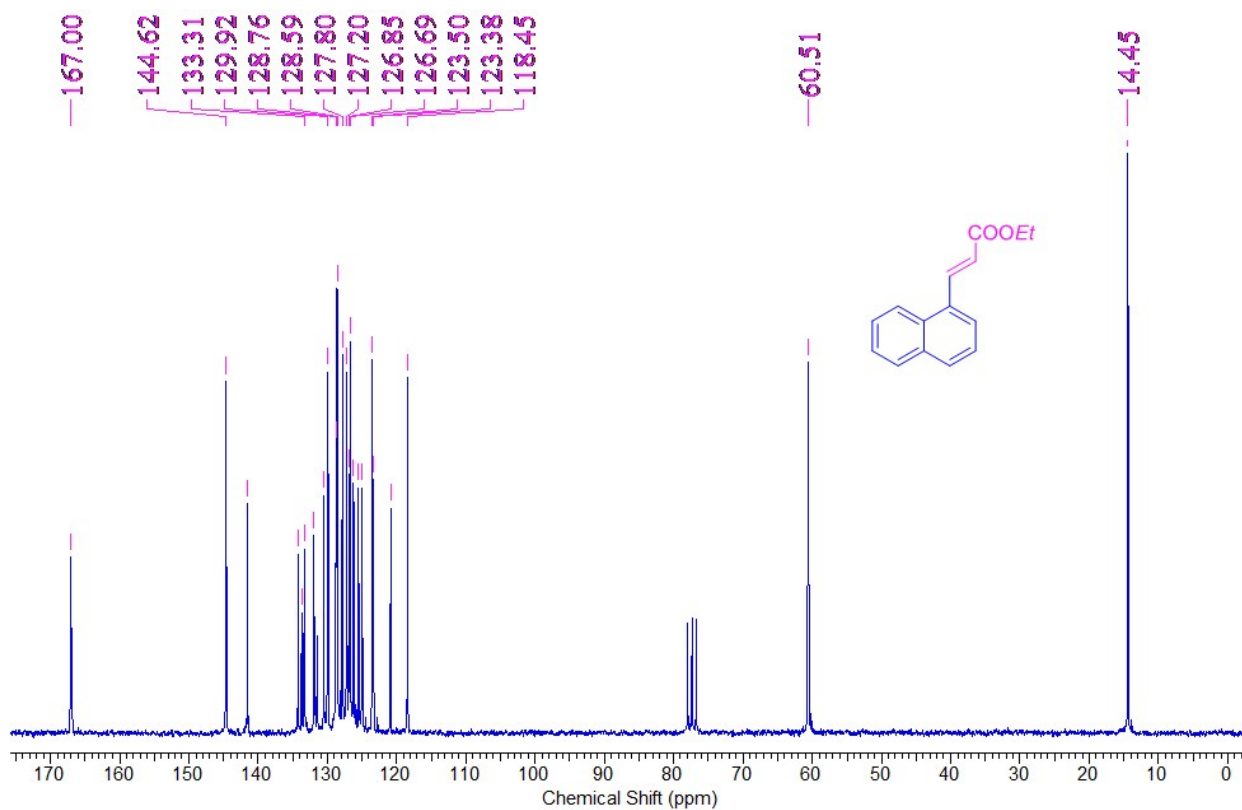
¹³C NMR spectrum of butyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 34):



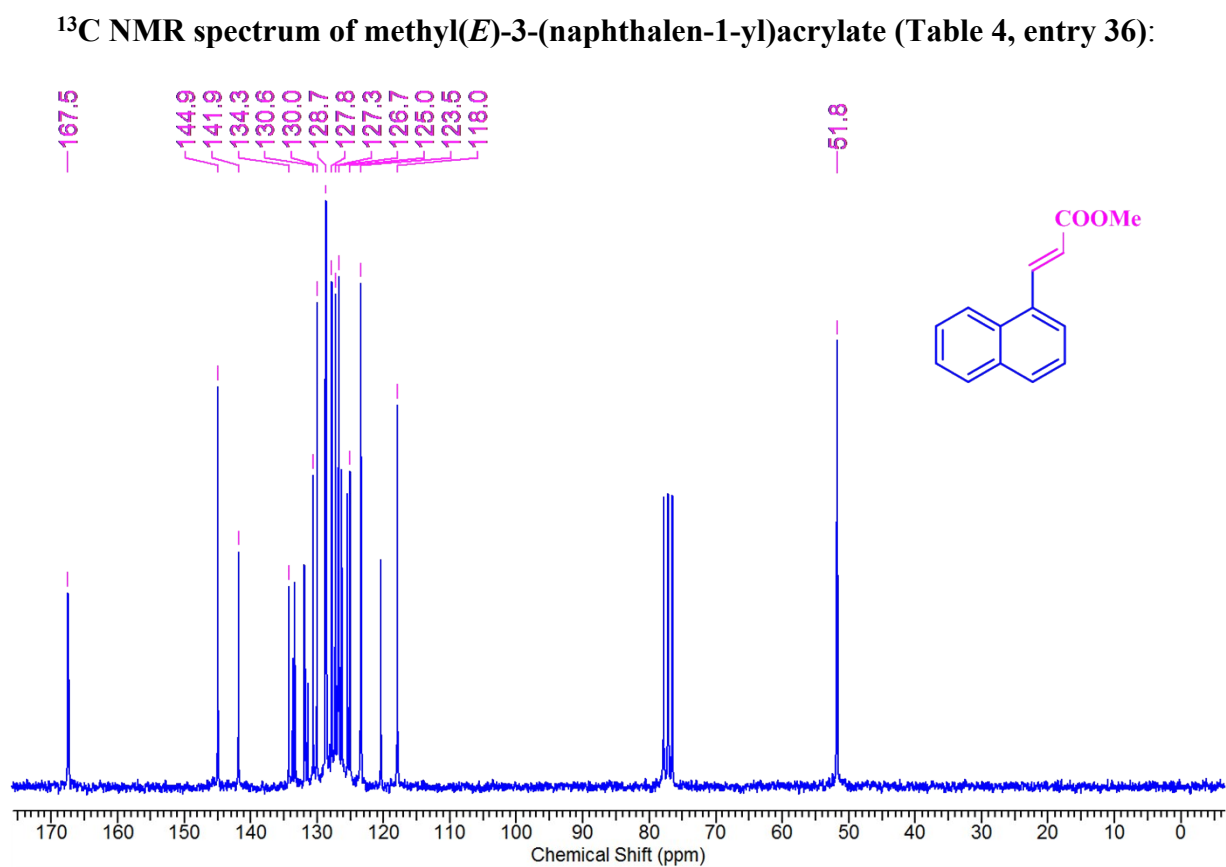
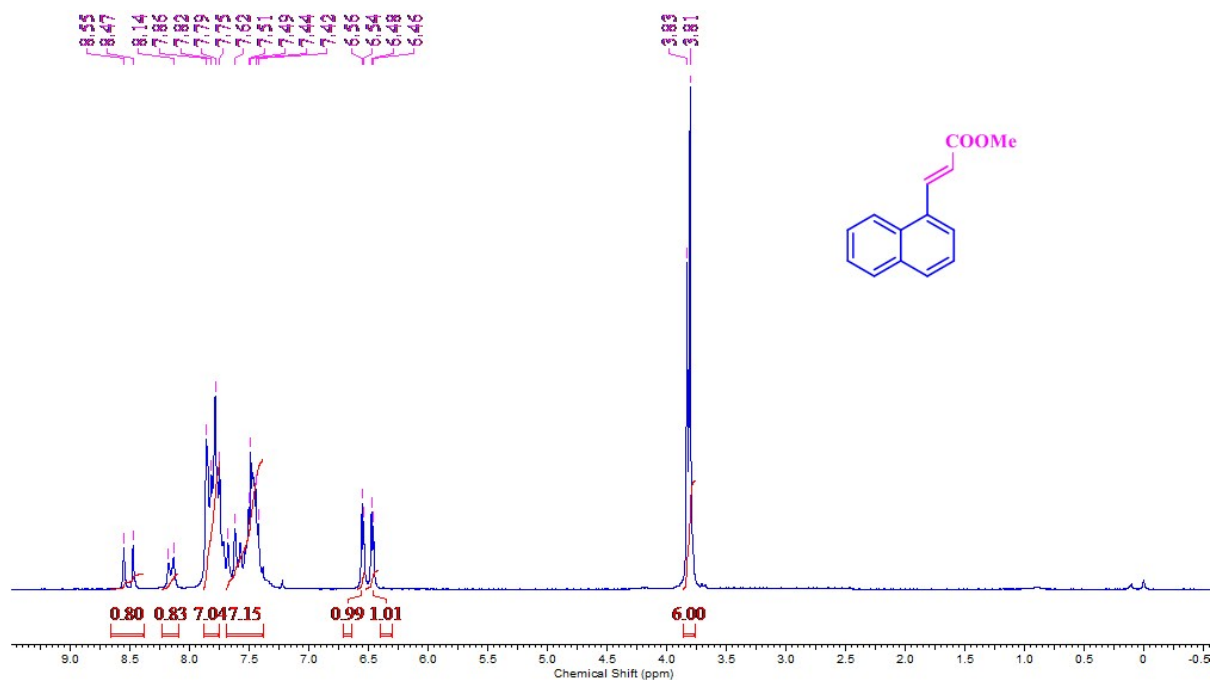
¹H NMR spectrum of ethyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 35):



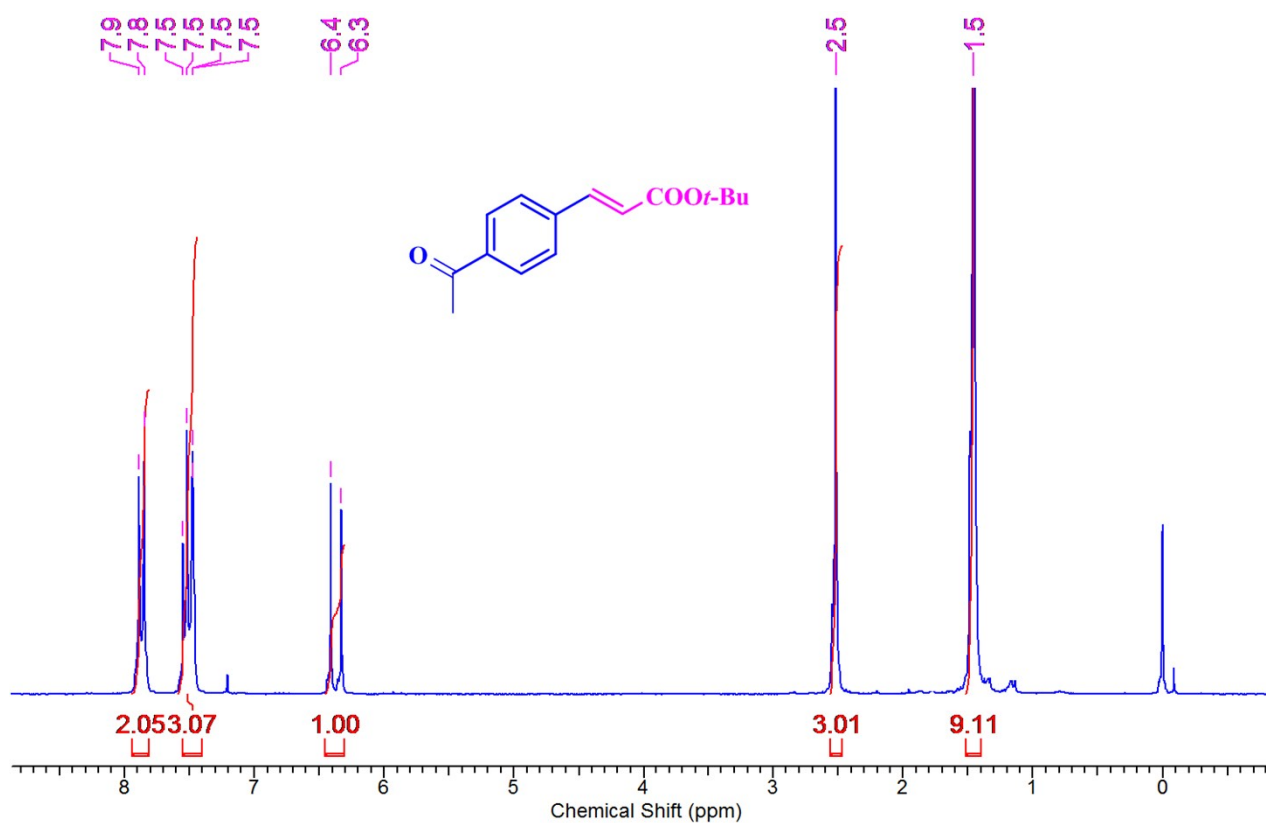
¹³C NMR spectrum of ethyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 35):



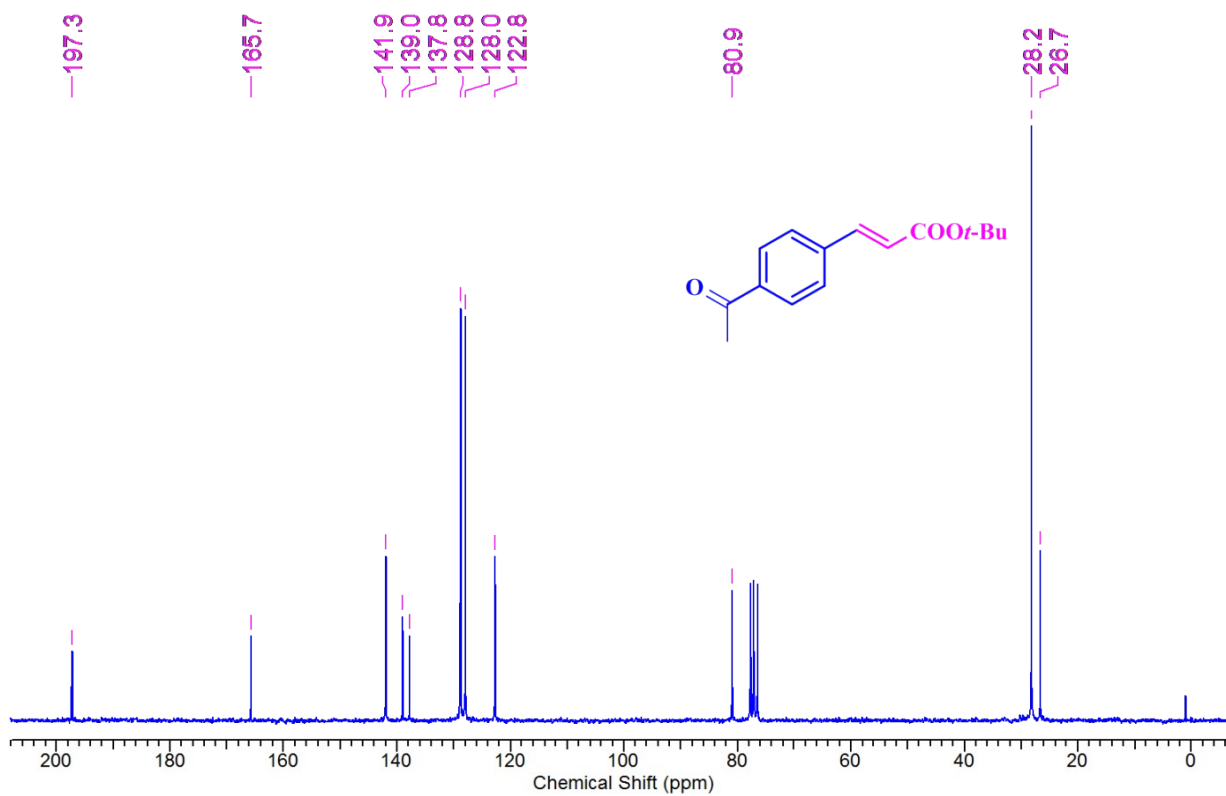
¹H NMR spectrum of methyl(*E*)-3-(naphthalen-1-yl)acrylate (Table 4, entry 36):



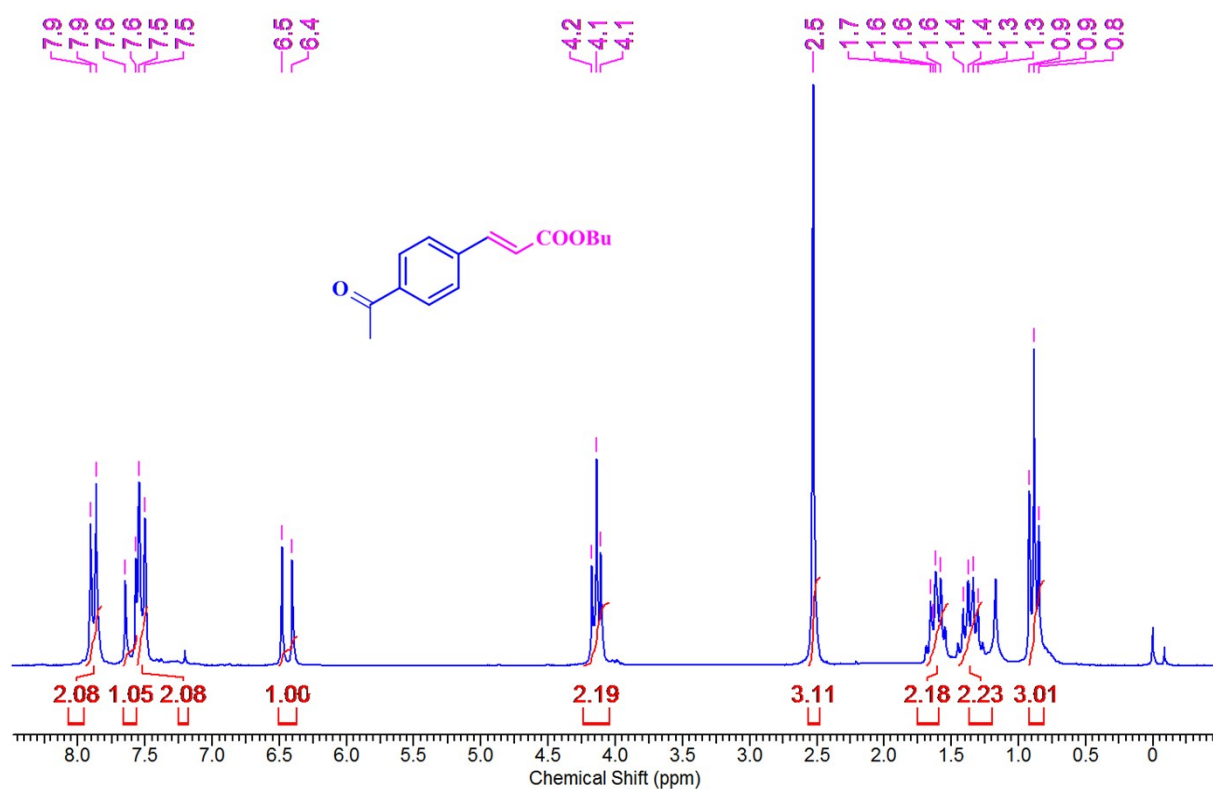
¹H NMR spectrum of tert-butyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 37):



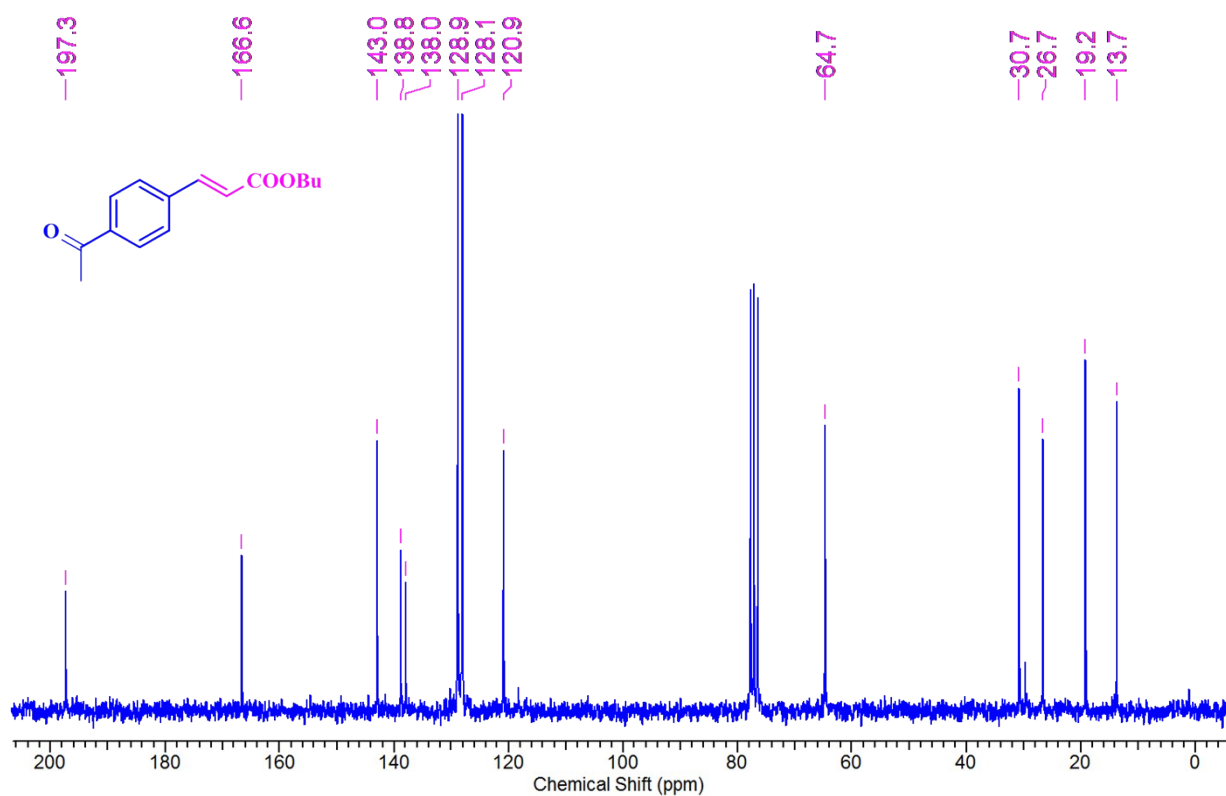
¹³C NMR spectrum of tert-butyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 37):



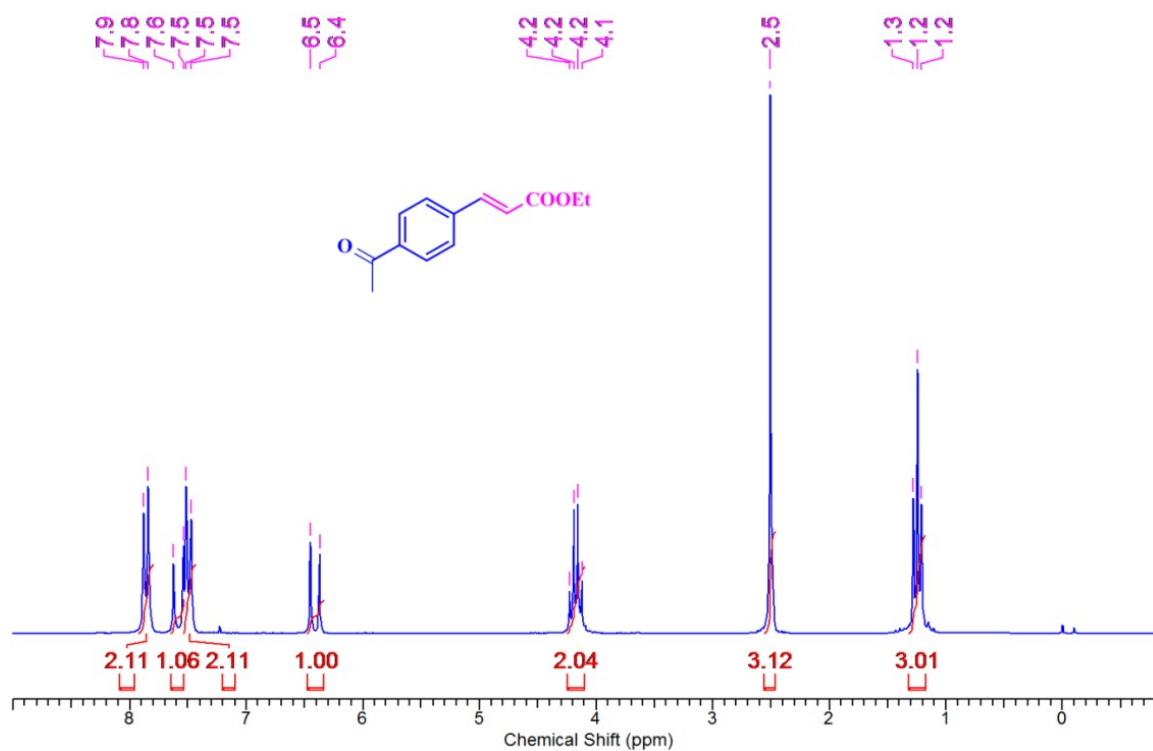
¹H NMR spectrum of butyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 38):



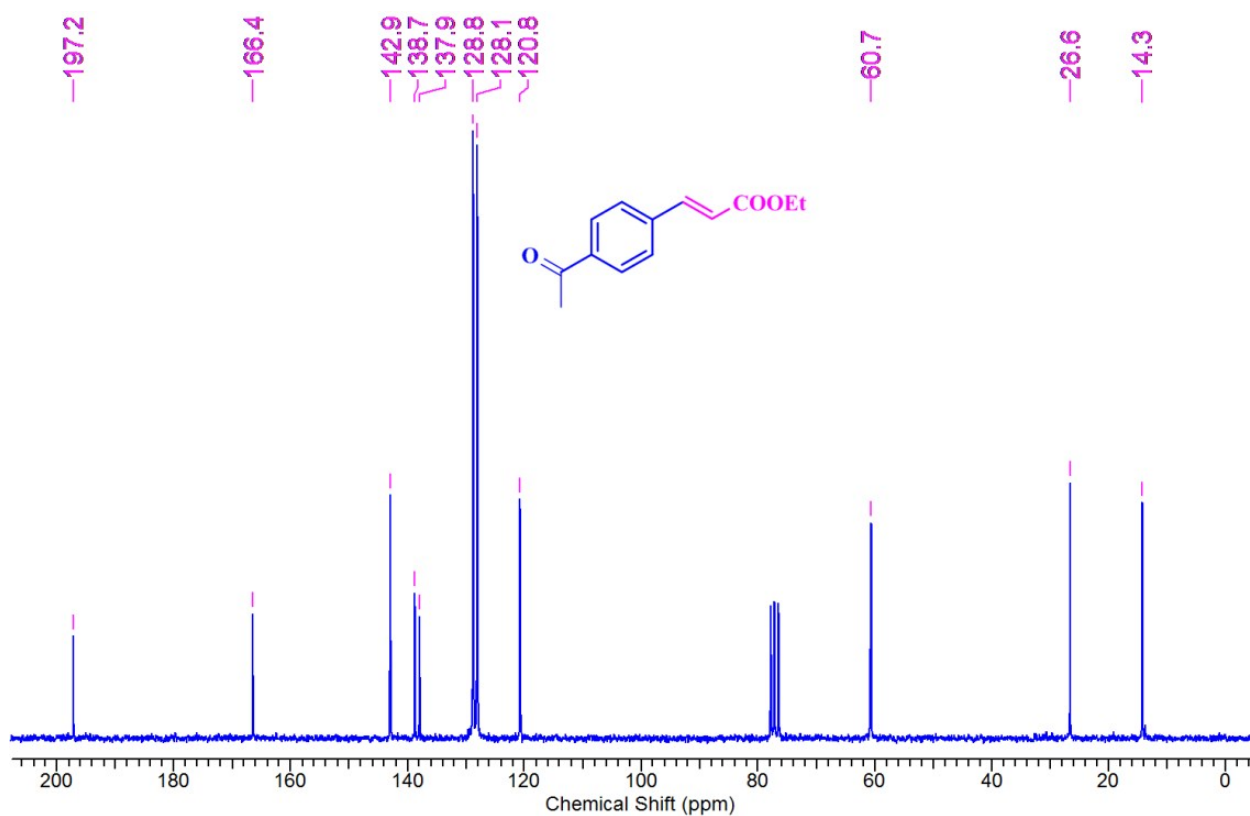
¹³C NMR spectrum of butyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 38):



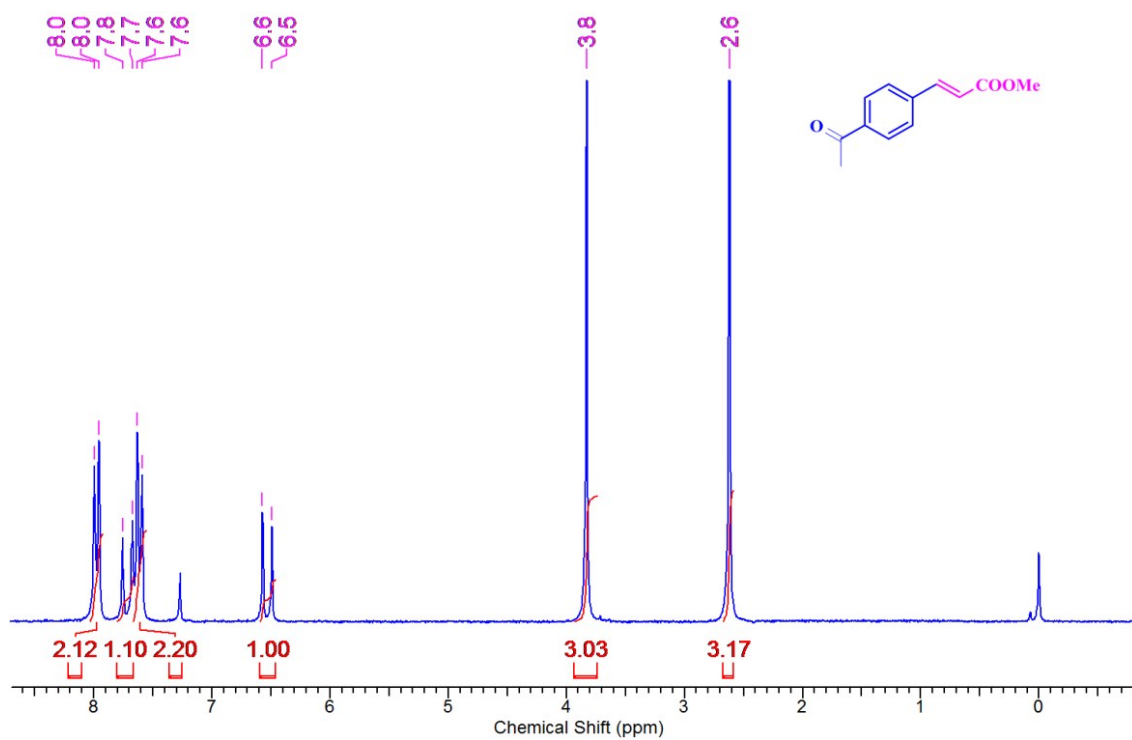
¹H NMR spectrum of ethyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 39):



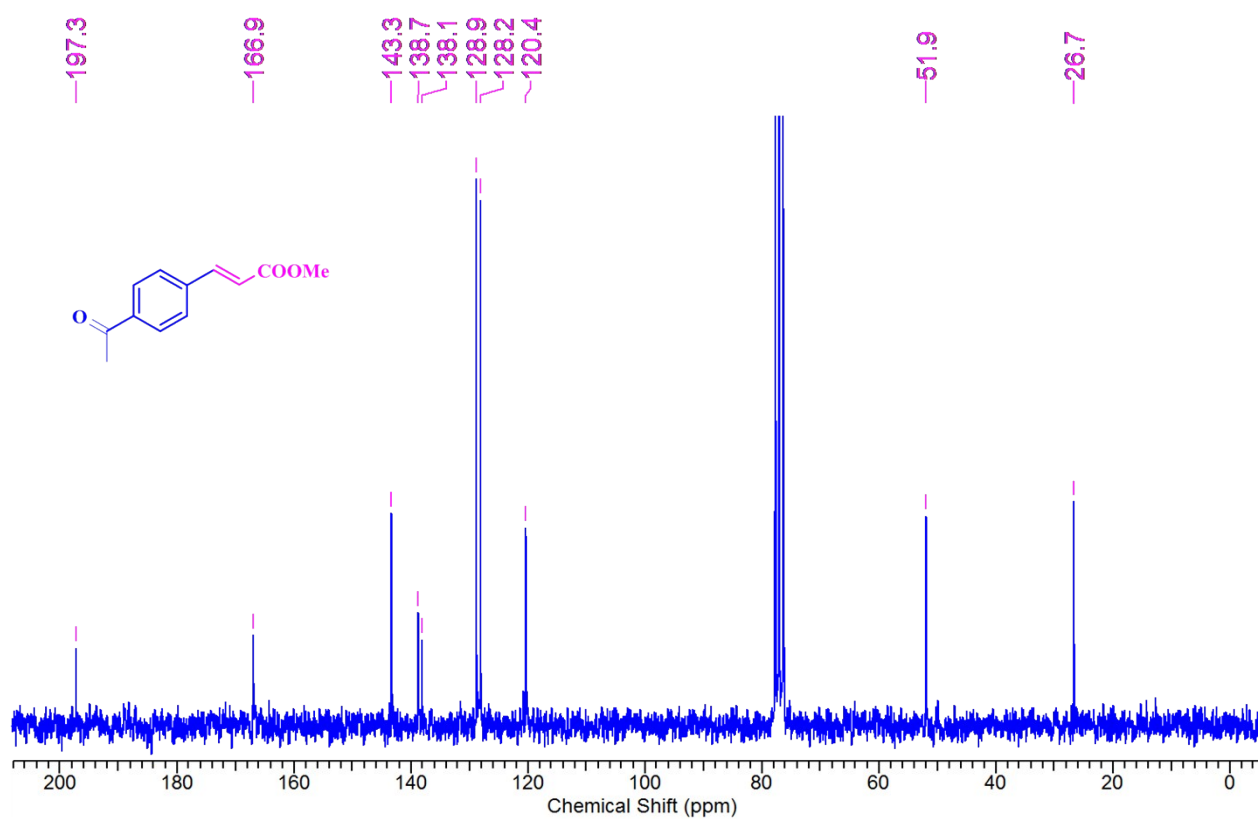
¹³C NMR spectrum of ethyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 39):



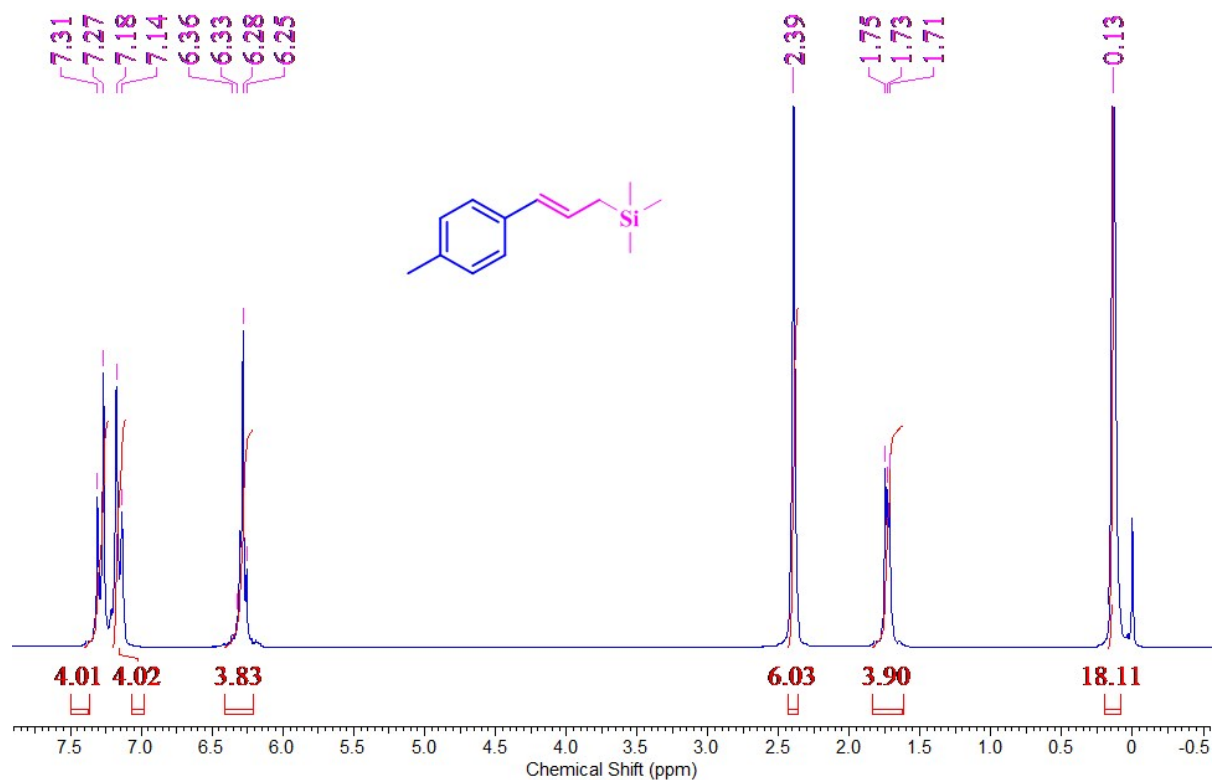
¹H NMR spectrum of methyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 40):



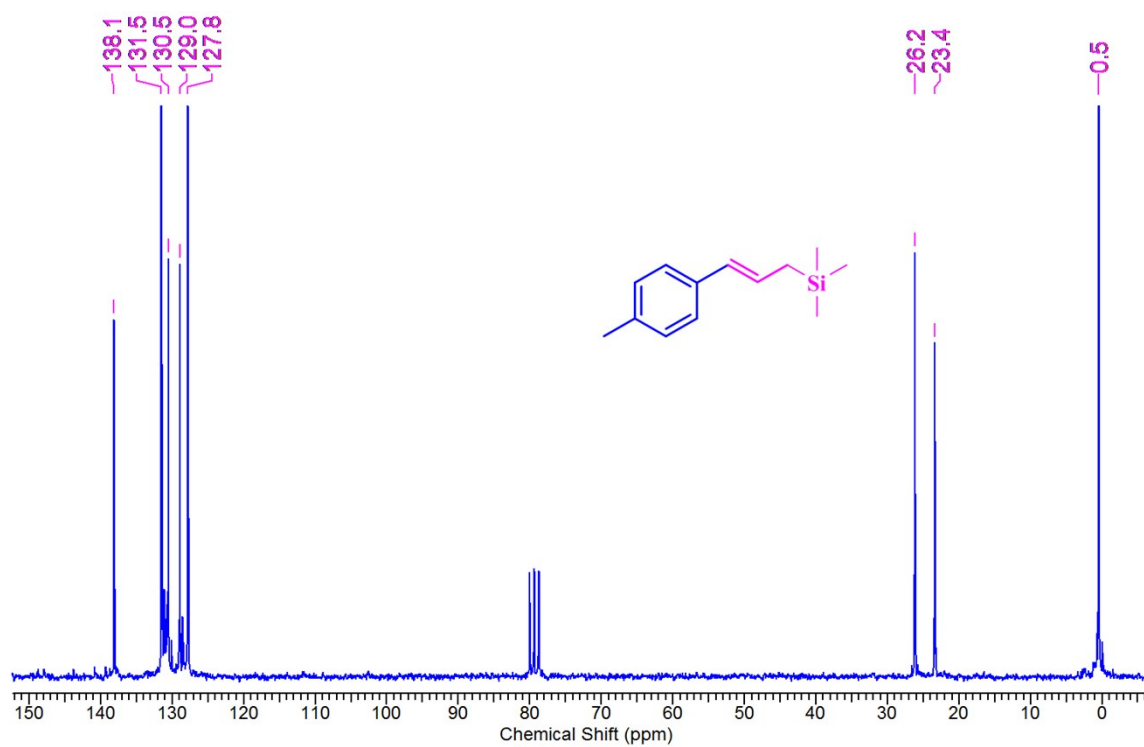
¹³C NMR spectrum of methyl(*E*)-3-(4-acetylphenyl)acrylate (Table 4, entry 40):



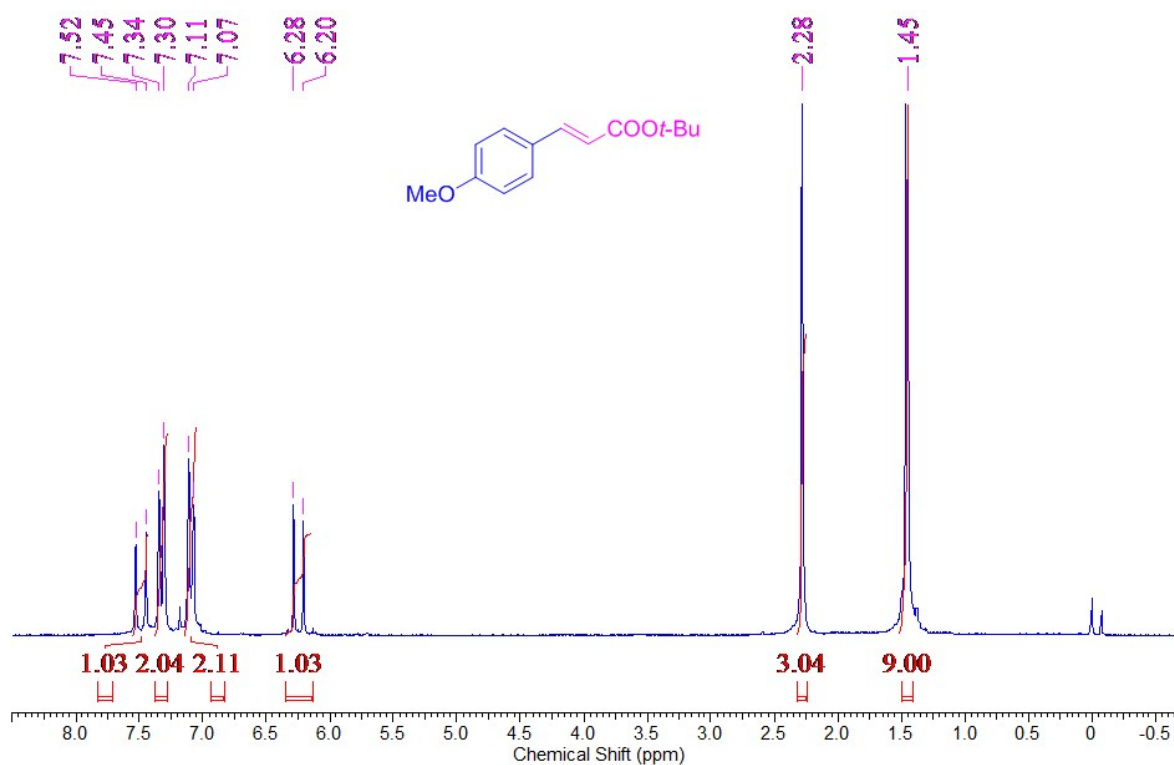
¹H NMR spectrum of (*E*)-trimethyl(3-(*p*-tolyl)allyl)silane (Scheme 1):



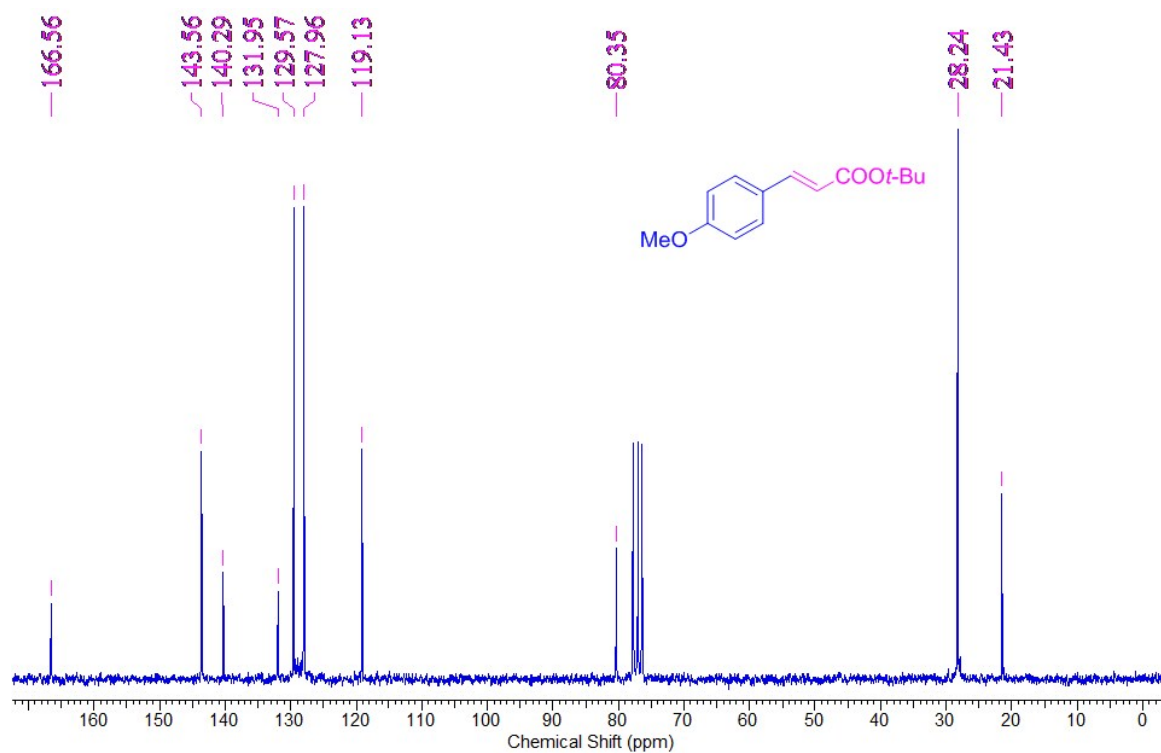
¹³C NMR spectrum of (E)-trimethyl(3-(p-tolyl)allyl)silane (Scheme 1):



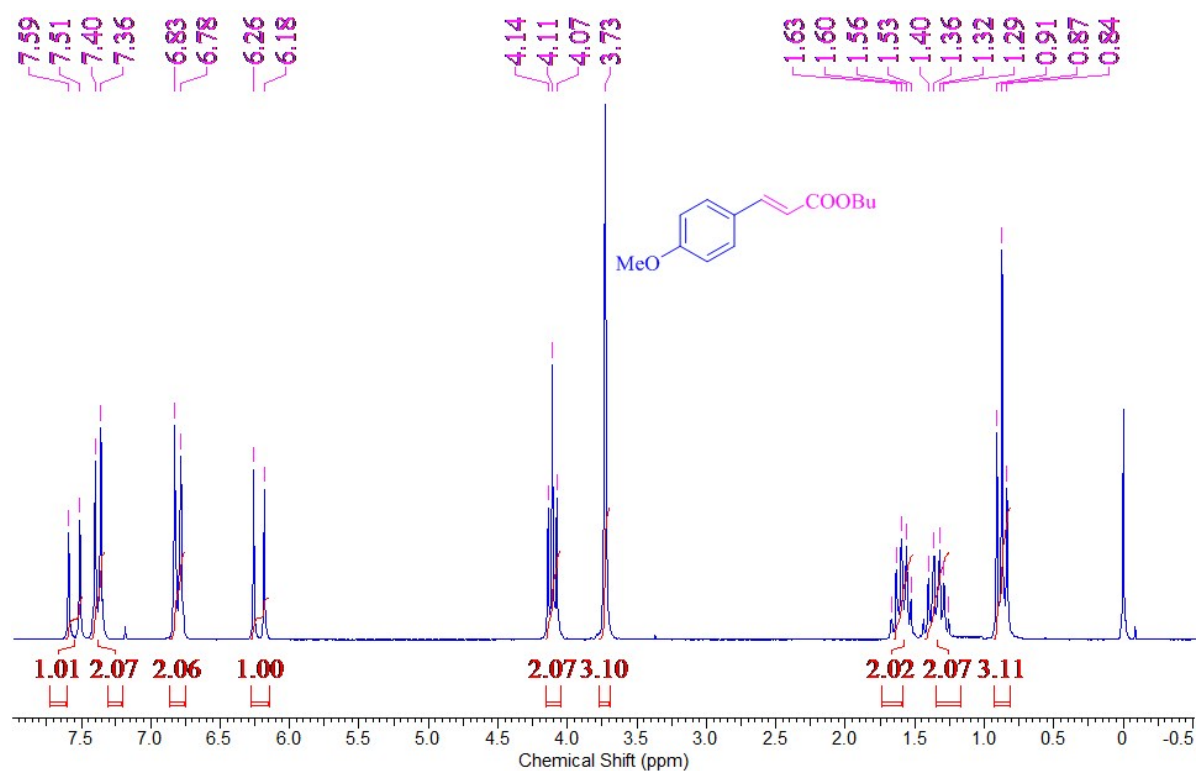
¹H NMR spectrum of tert-butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 1):



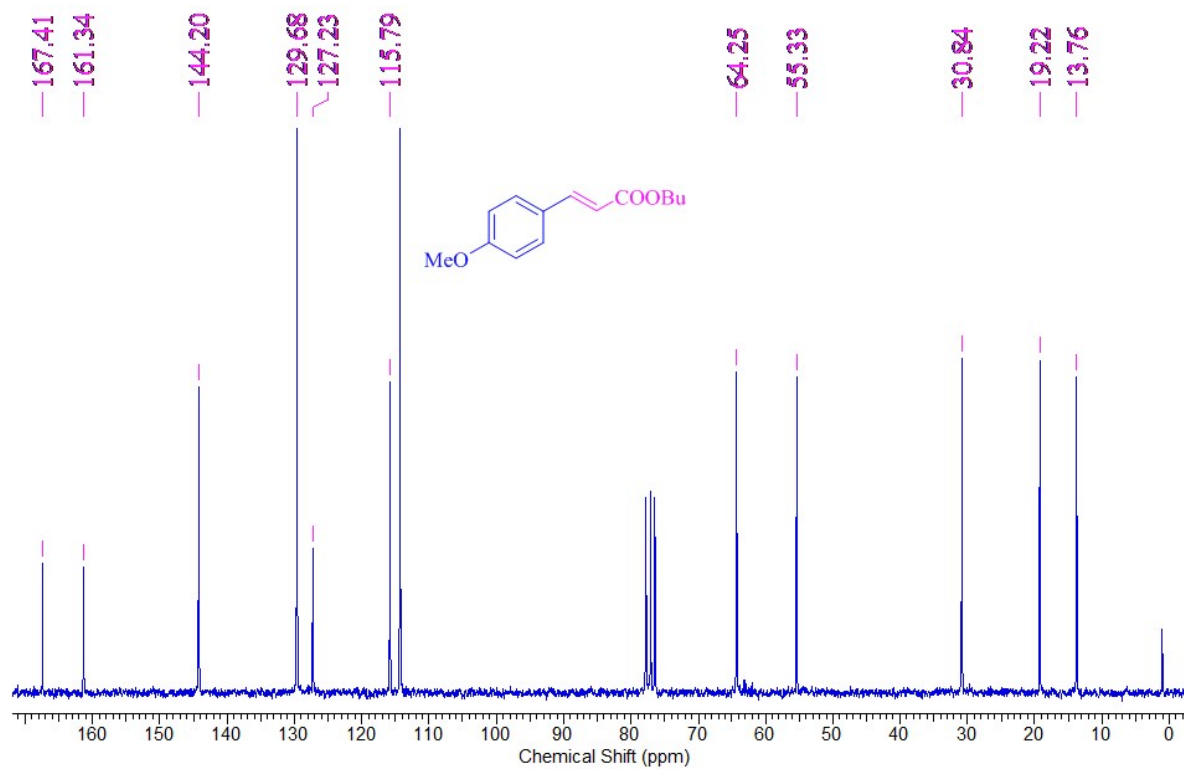
¹³C NMR spectrum of tert-butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 1):



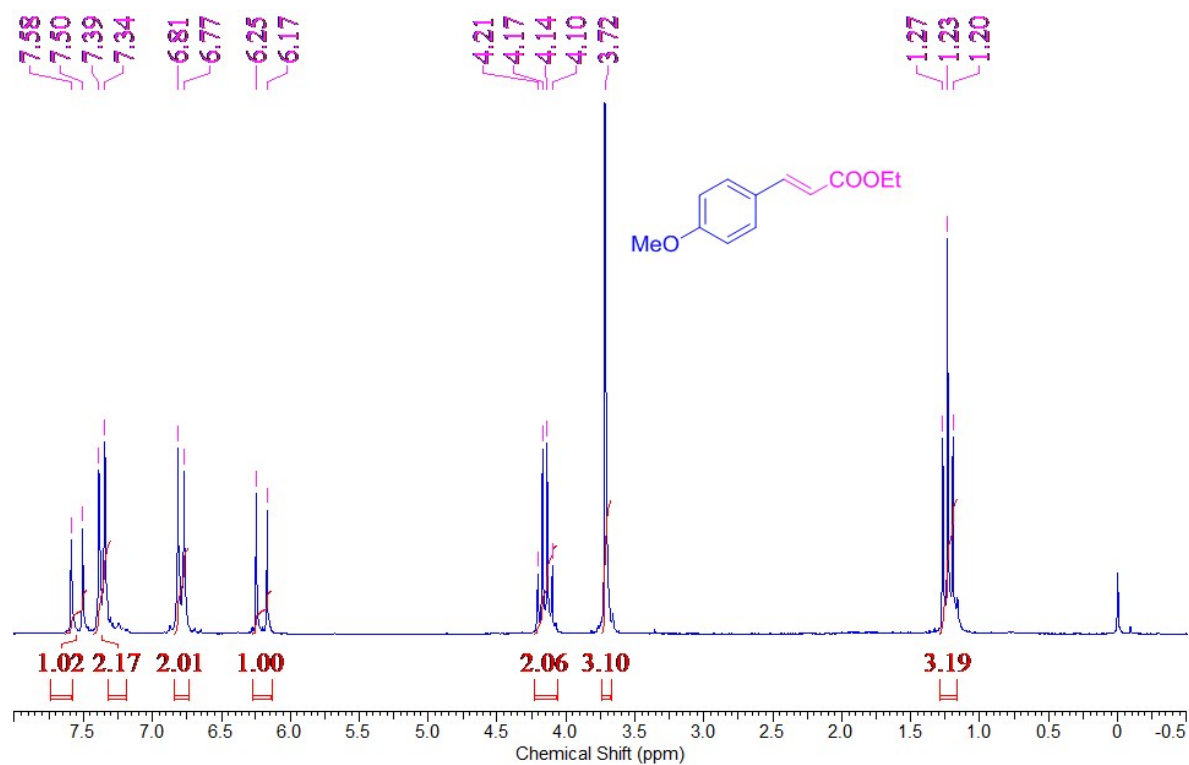
¹H NMR spectrum of butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 2):



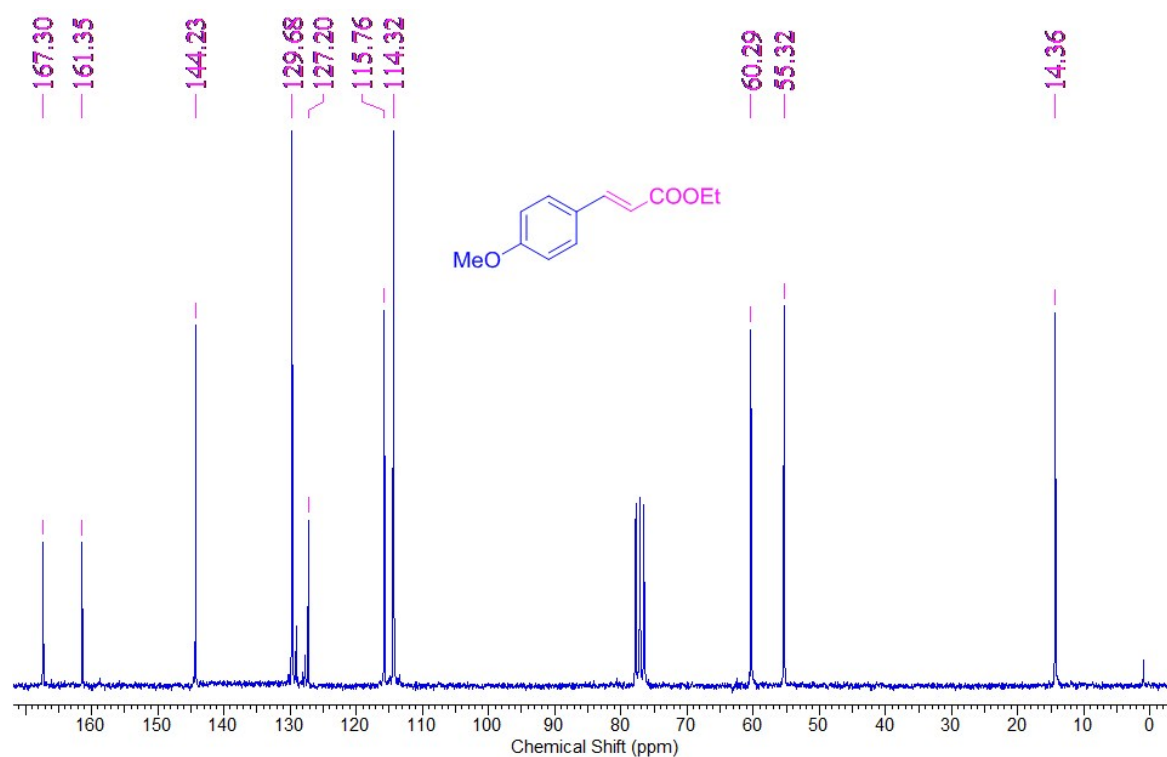
¹³C NMR spectrum of butyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 2):



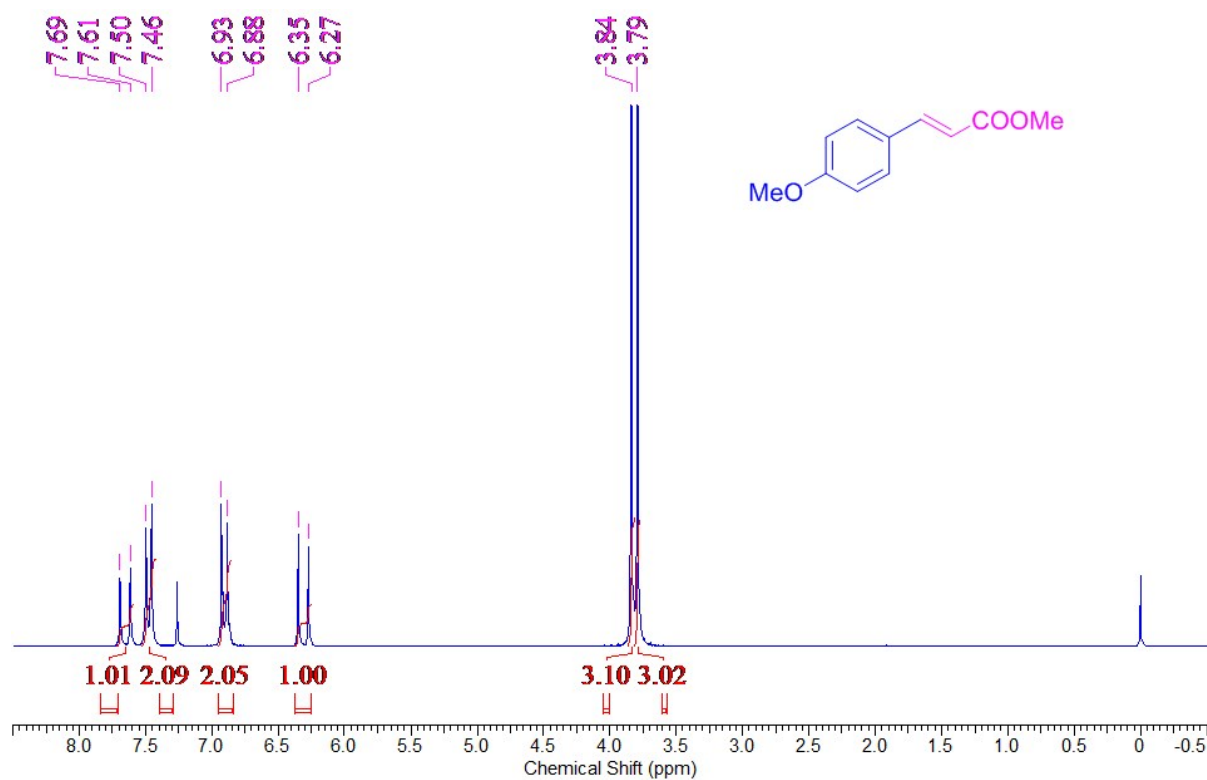
¹H NMR spectrum of ethyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 3):



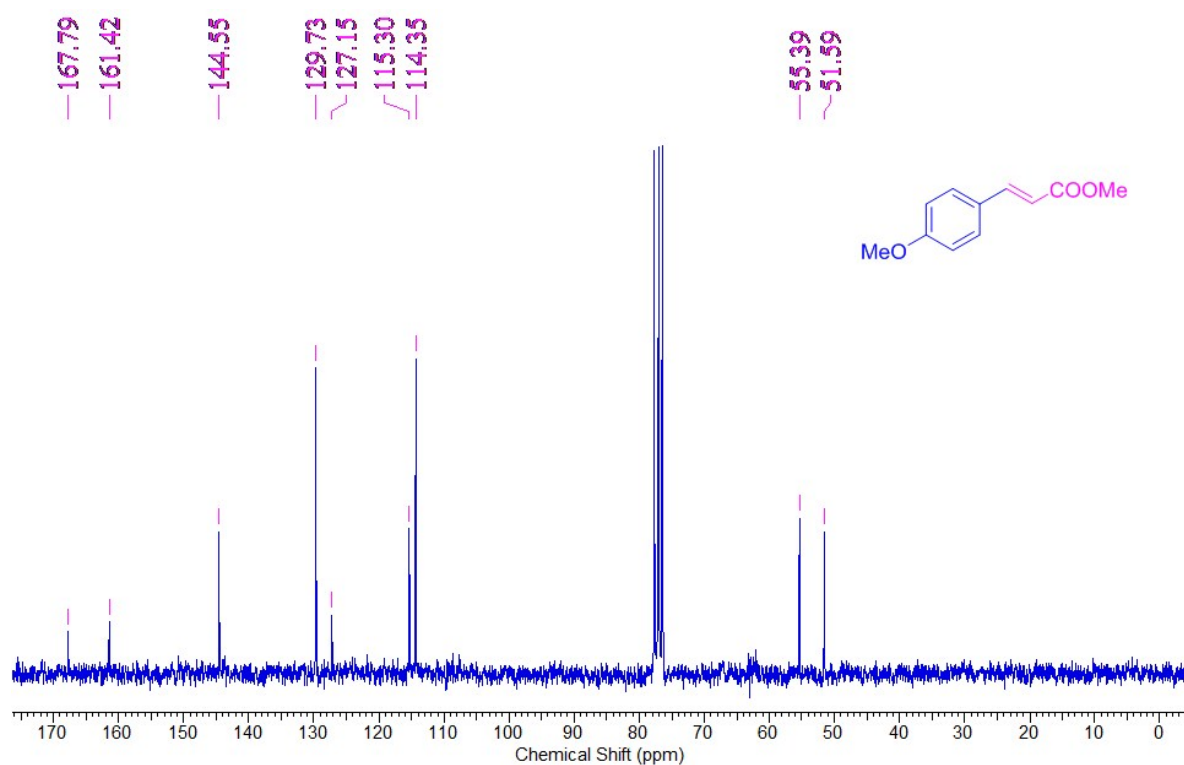
¹³C NMR spectrum of ethyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 3):



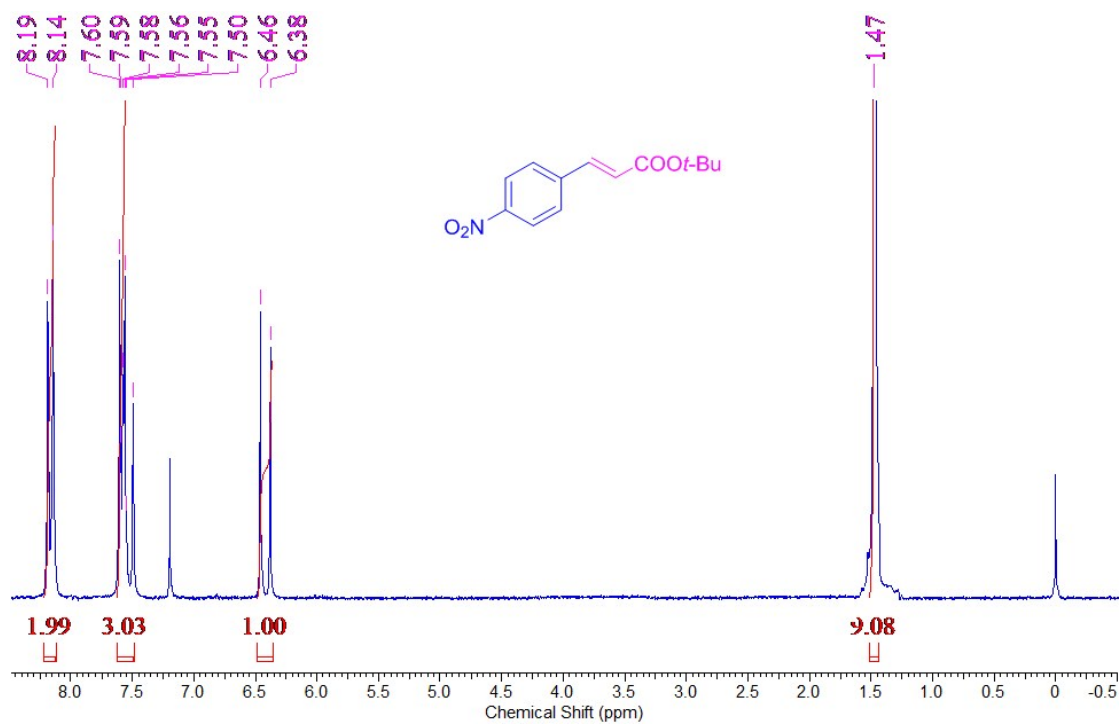
¹H NMR spectrum of methyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 4):



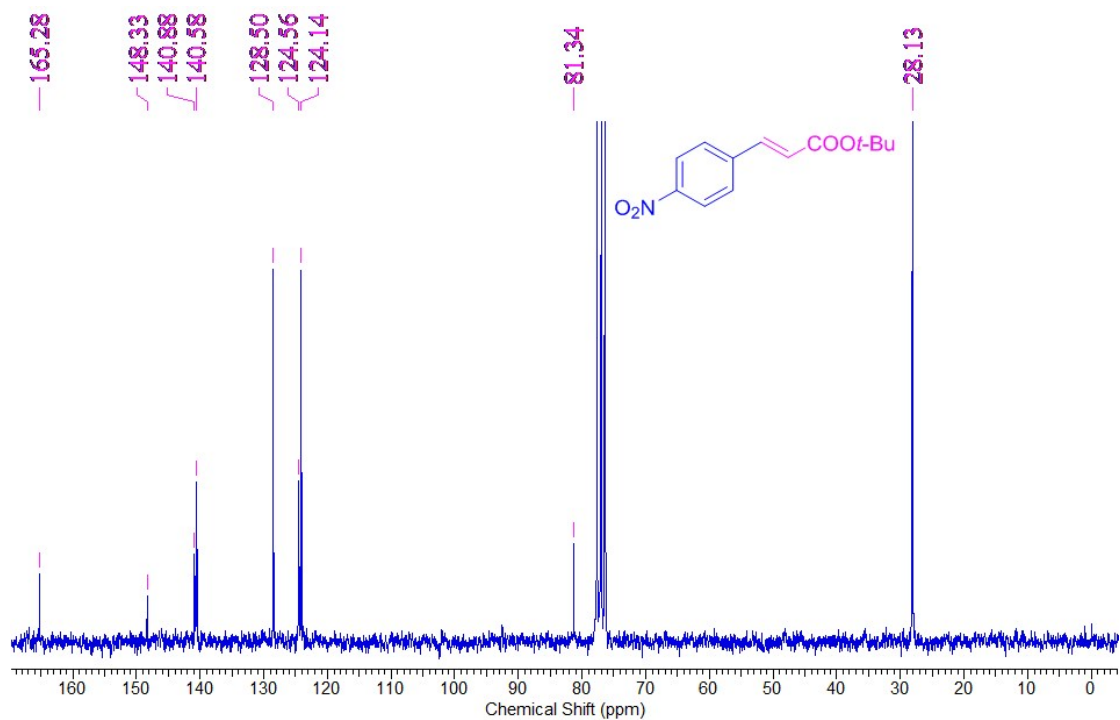
¹³C NMR spectrum of methyl(*E*)-3-(4-methoxyphenyl)acrylate (Table 5, entry 4):



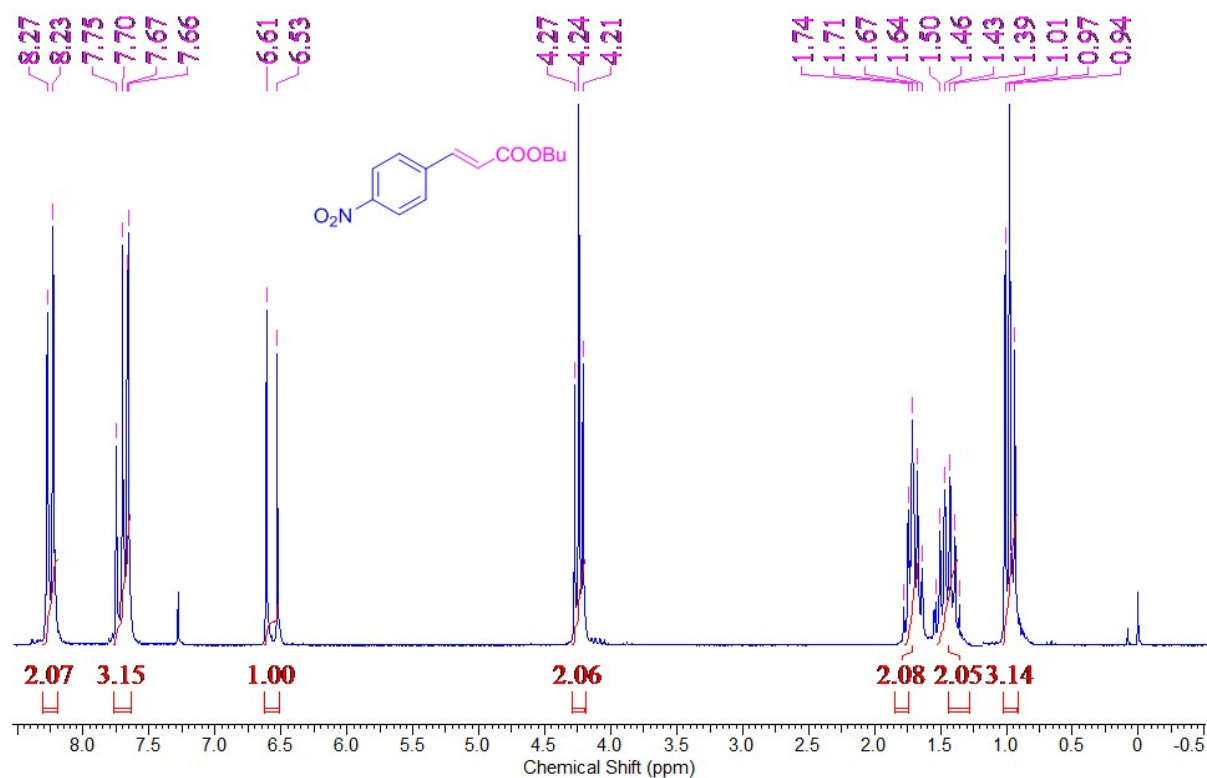
¹H NMR spectrum of tert-butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 5):



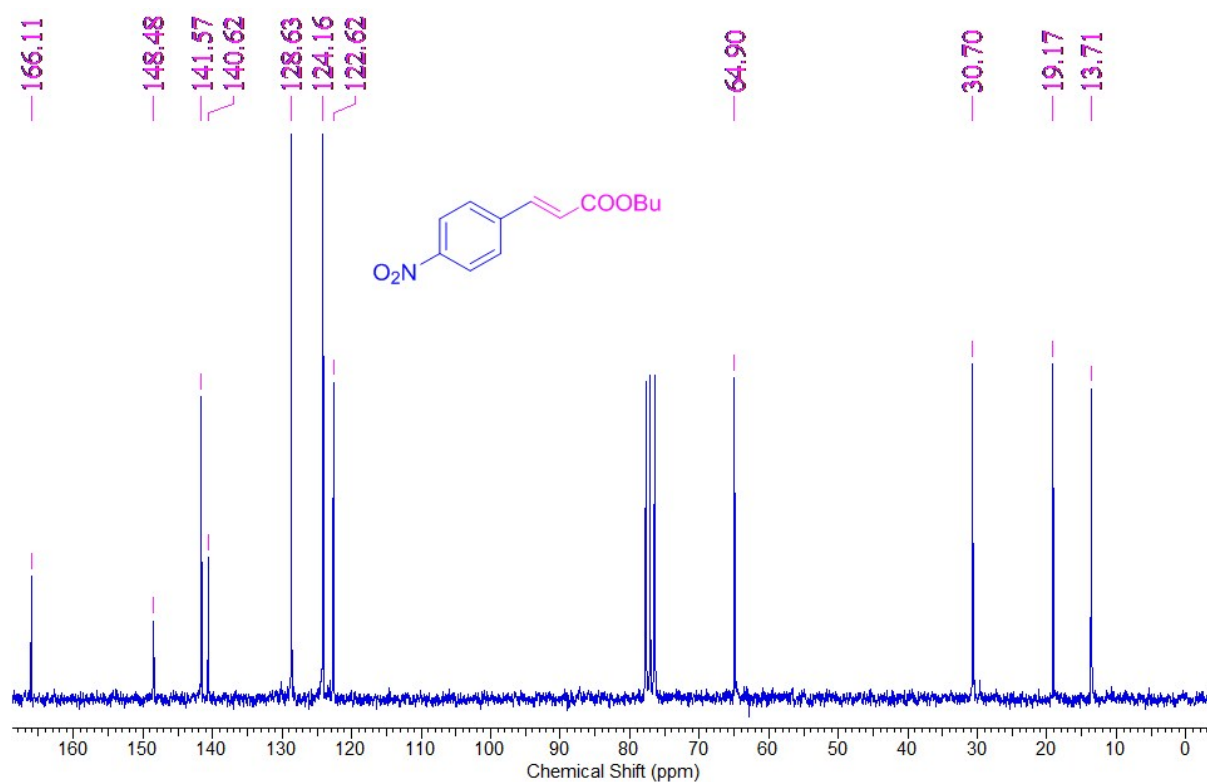
¹³C NMR spectrum of tert-butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 5):



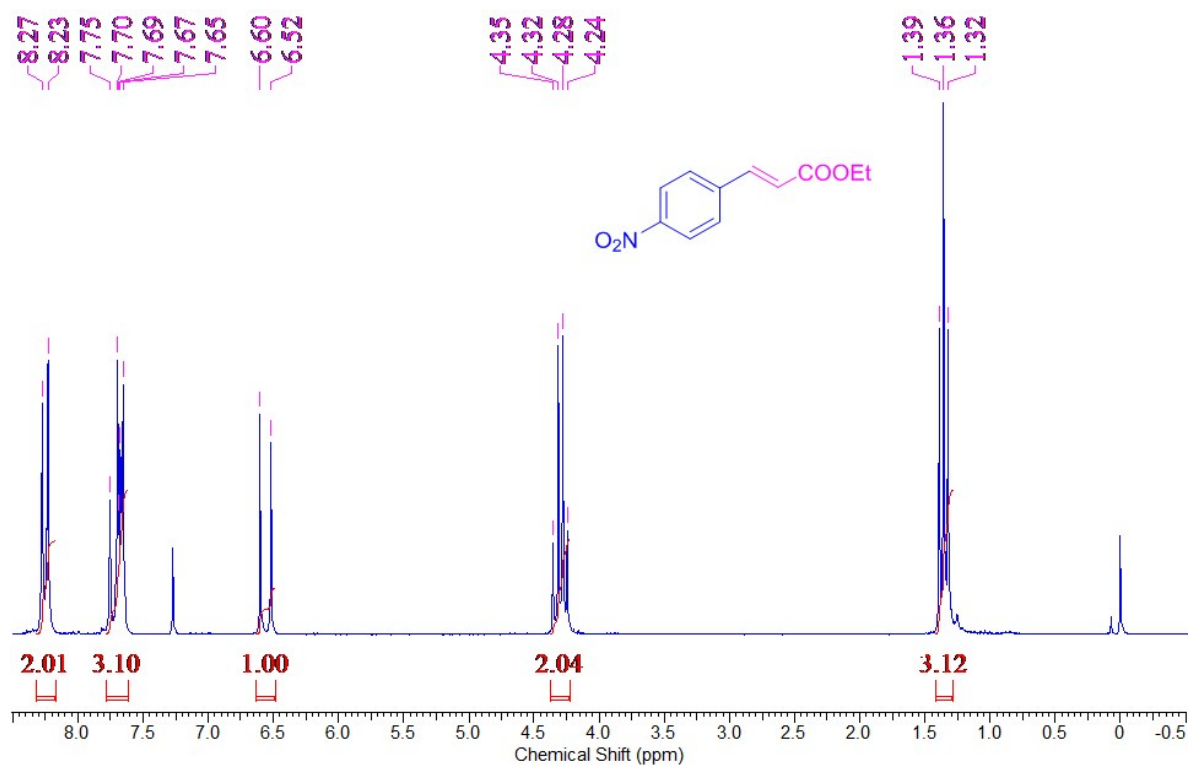
¹H NMR spectrum of butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 6):



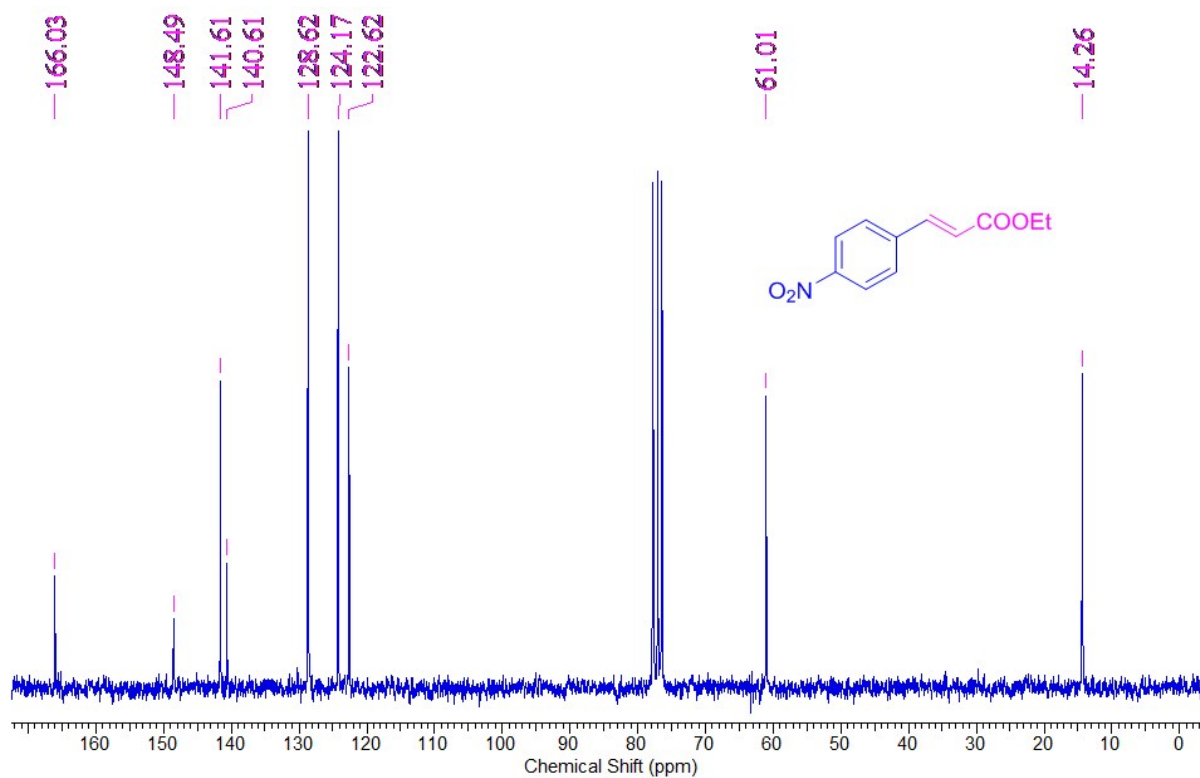
¹³C NMR spectrum of butyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 6):



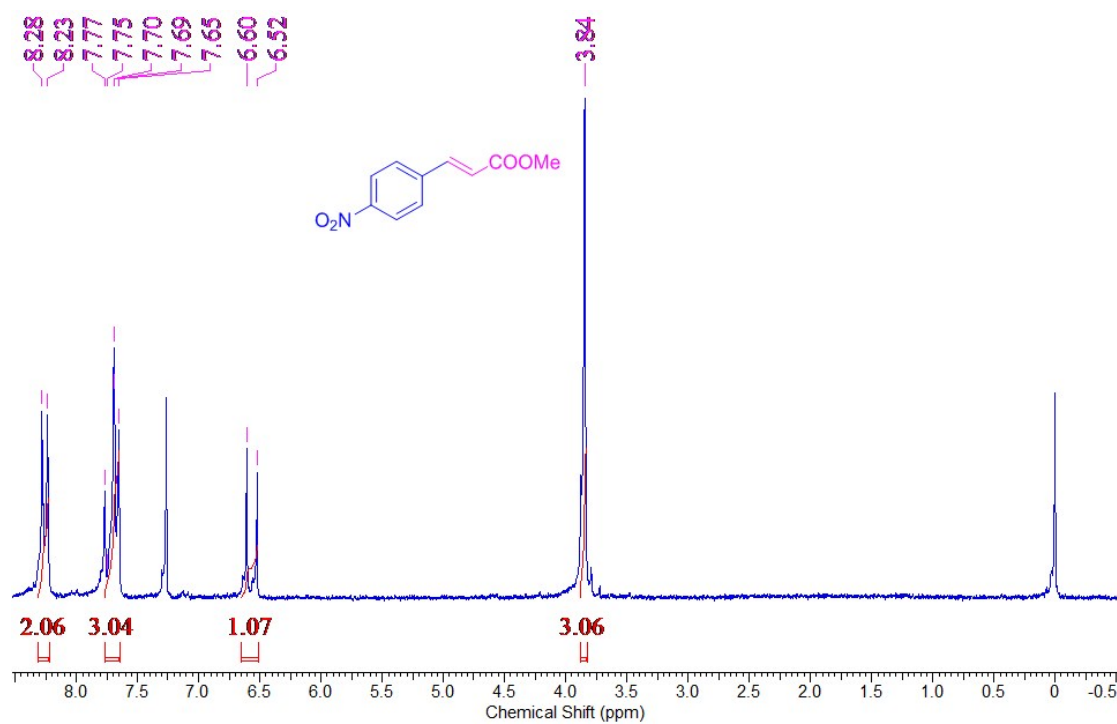
¹H NMR spectrum of ethyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 7):



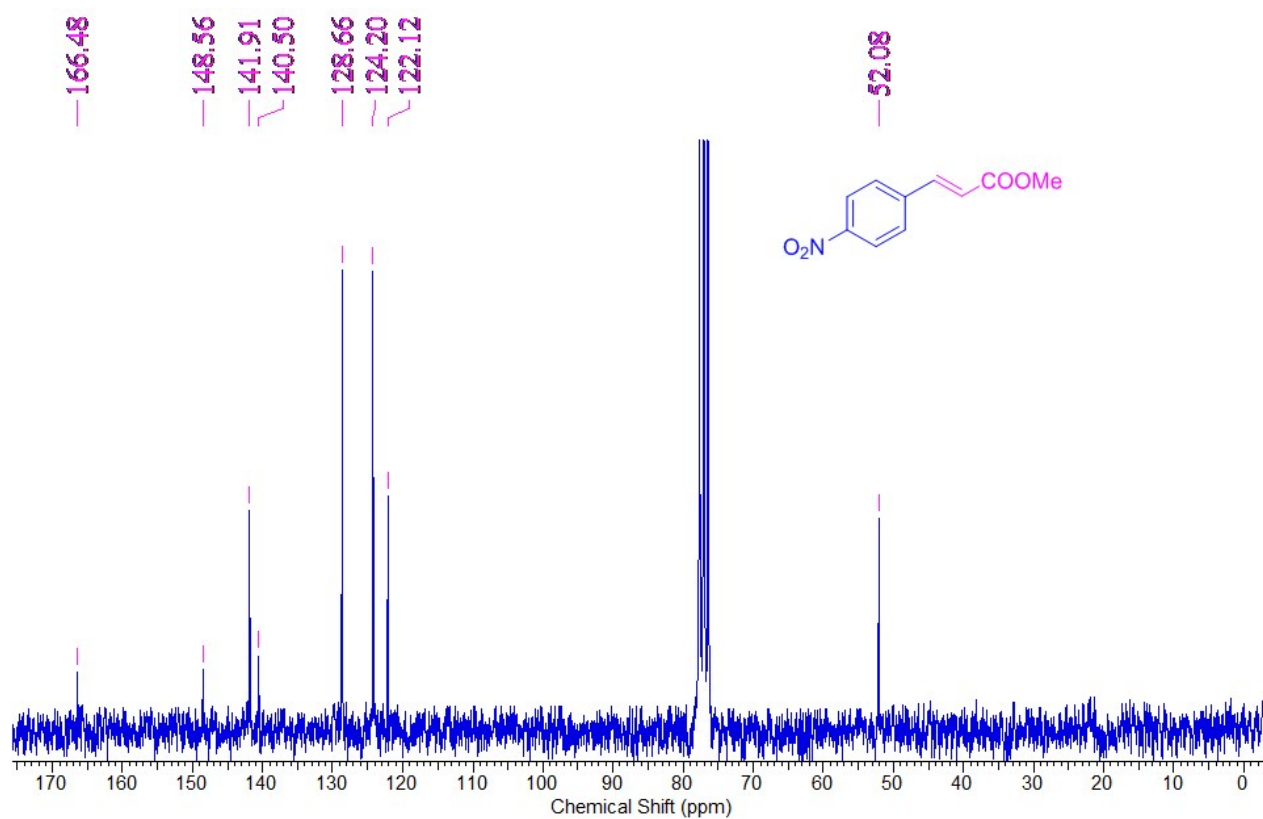
¹³C NMR spectrum of ethyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 7):



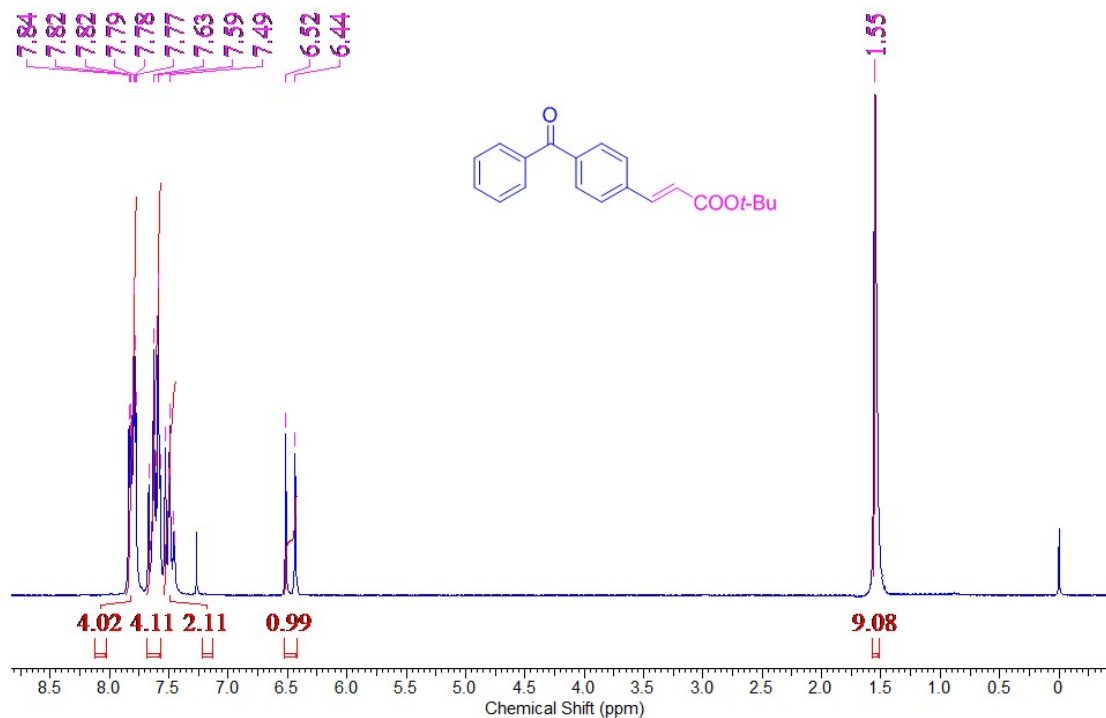
¹H NMR spectrum of methyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 8):



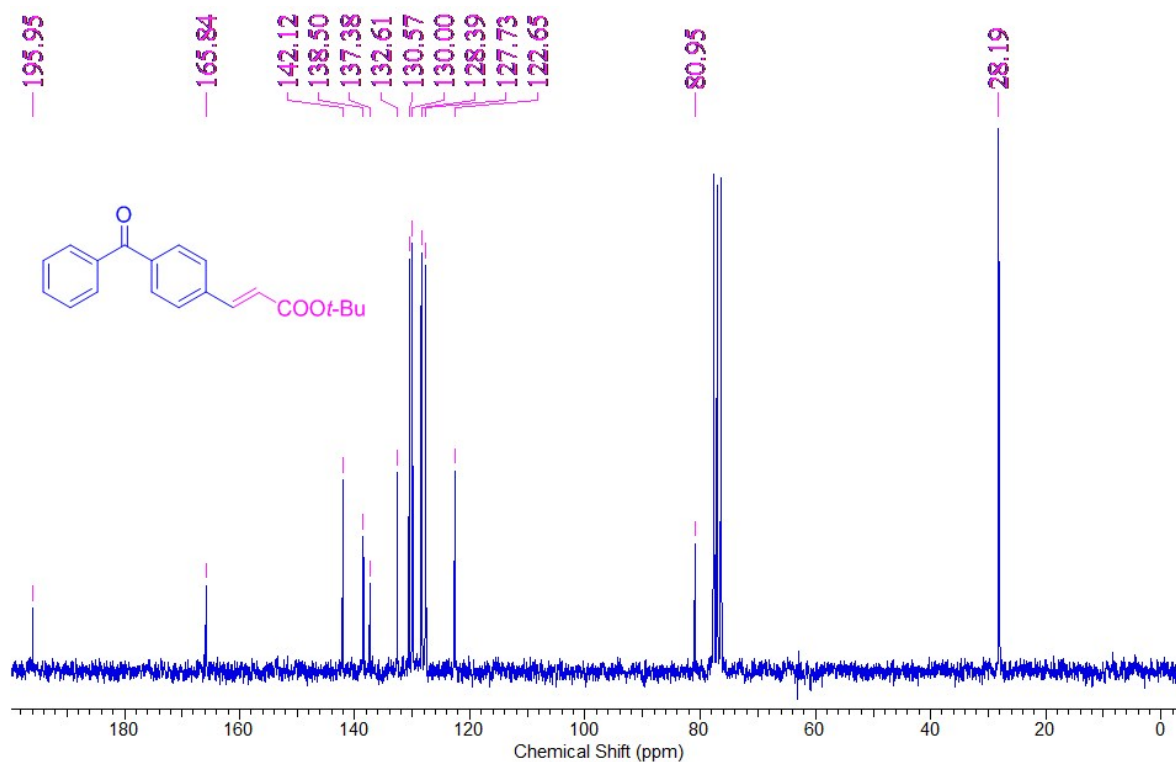
¹³C NMR spectrum of methyl(*E*)-3-(4-nitrophenyl)acrylate (Table 5, entry 8):



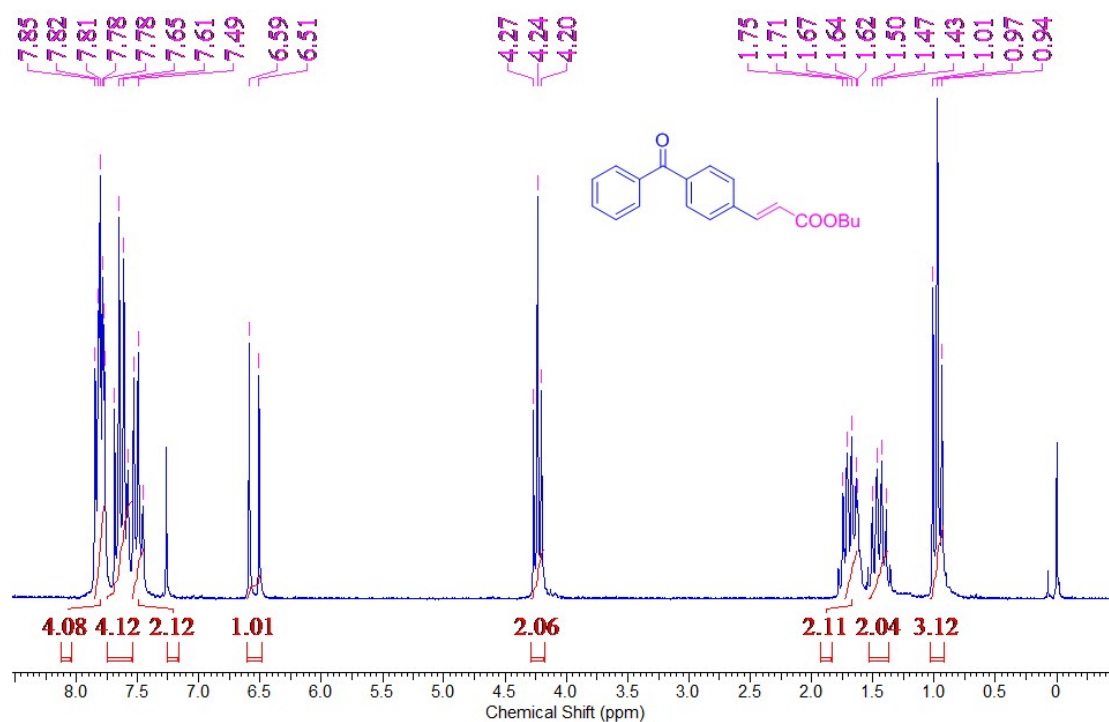
¹H NMR spectrum of tert-butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 9):



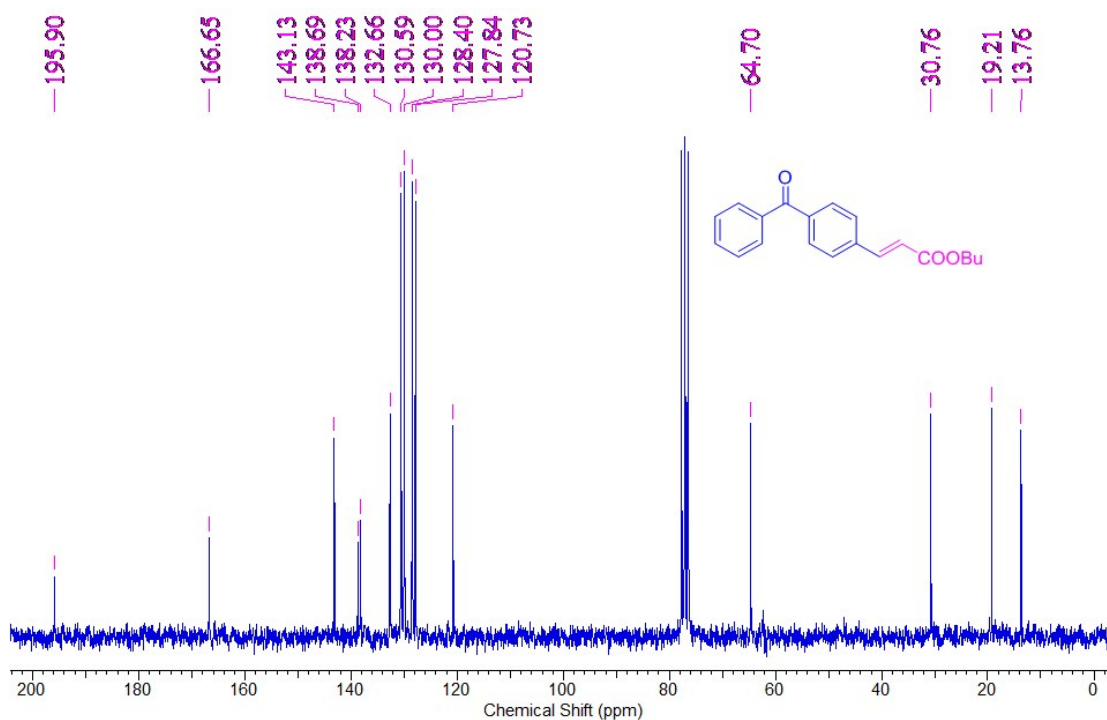
¹³C NMR spectrum of tert-butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 9):



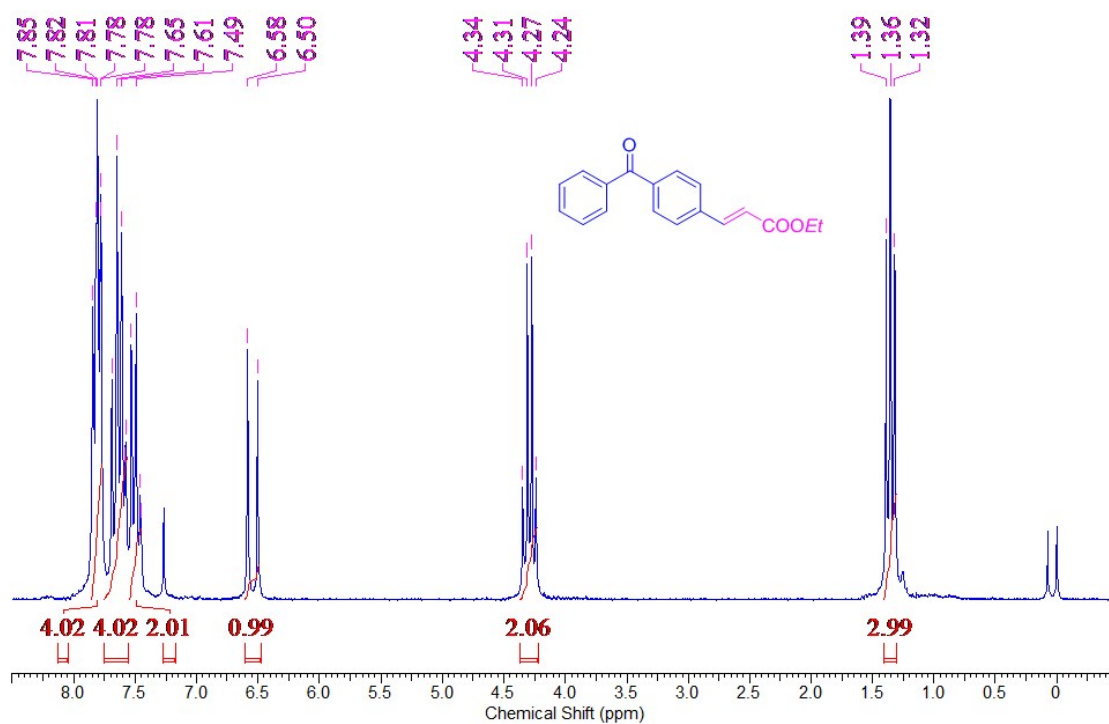
¹H NMR spectrum of butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 10):



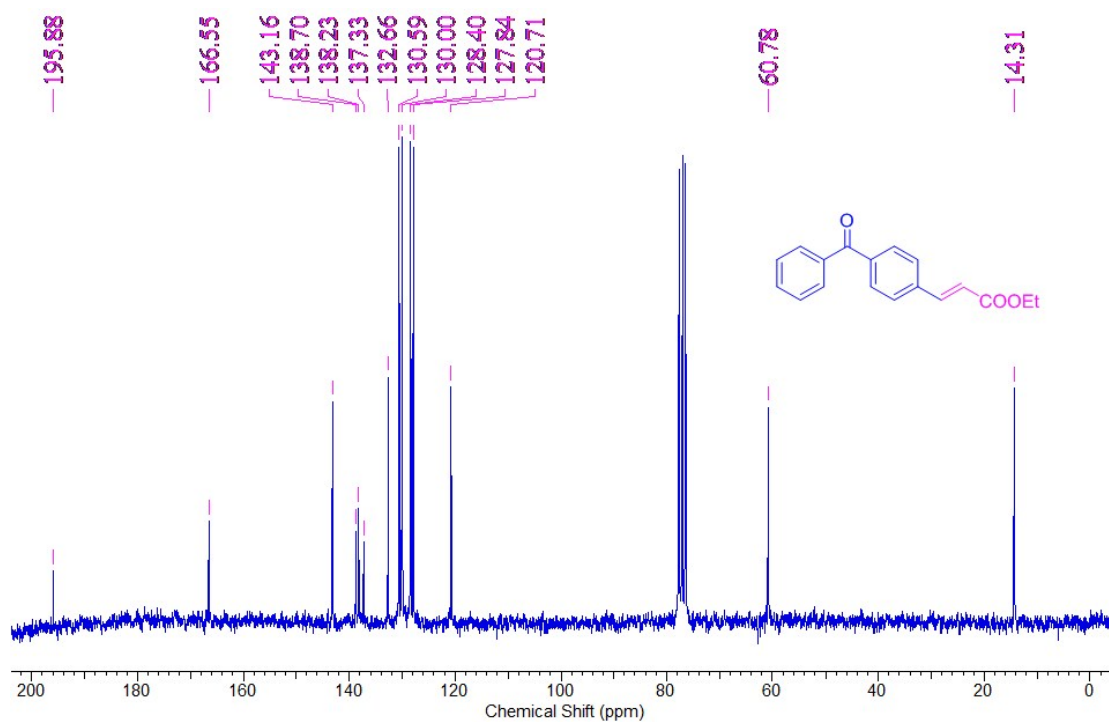
¹³C NMR spectrum of butyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 10):



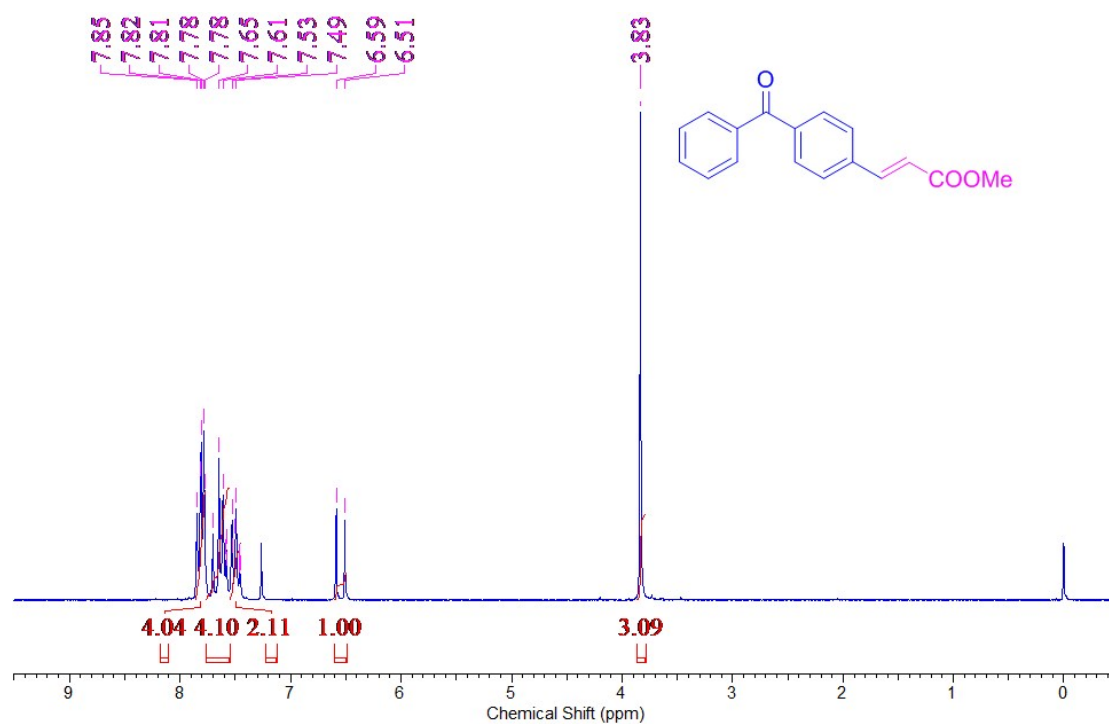
¹H NMR spectrum of ethyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 11):



¹³C NMR spectrum of ethyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 11):



¹H NMR spectrum of methyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 12):



¹³C NMR spectrum of methyl(*E*)-3-(4-benzoylphenyl)acrylate (Table 5, entry 12):

