

Supporting Information

The Effect of RO3201195 and a Pyrazolyl Ketone P38 MAPK Inhibitor Library on the Proliferation of Werner Syndrome Cells

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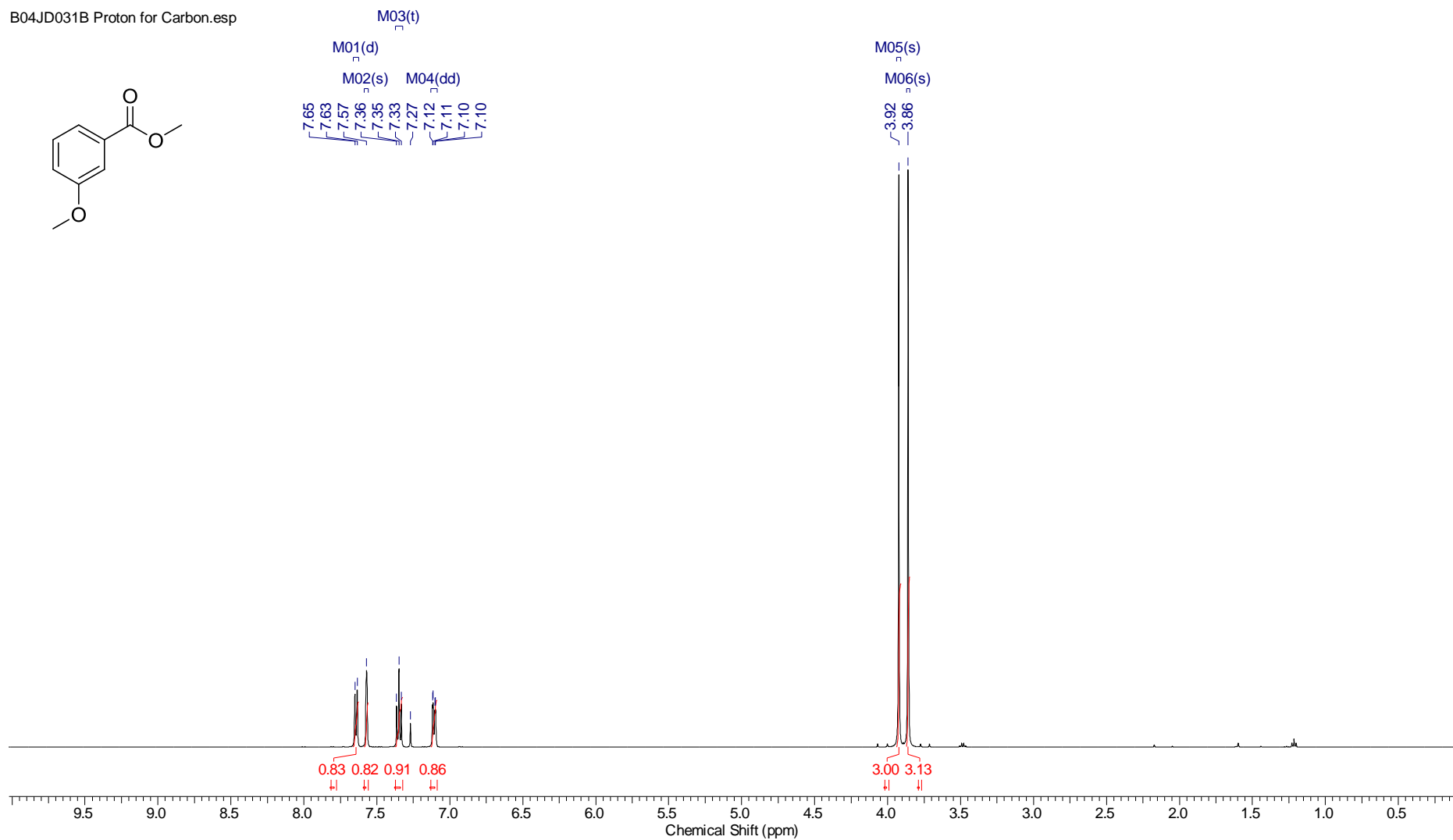
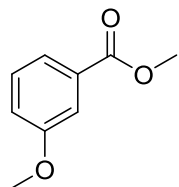
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S18 ¹H NMR spectrum for 5-amino-1-(4-fluorophenyl)-4-{3-[2(*S*)-3-dihydroxypropoxy]benzoyl}pyrazole (RO3201195) (**1**)
S19 ¹³C NMR spectrum for 5-amino-1-(4-fluorophenyl)-4-{3-[2(*S*)-3-dihydroxypropoxy]benzoyl}pyrazole (RO3201195) (**1**)

Spectra published using ACD/NMR Processor Academic Edition and ACD/Chemsketch (Freeware), version 12.01, Advanced Chemistry Development, Inc., Toronto, On, Canada, www.acdlabs.com, 2015

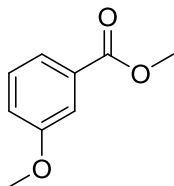
¹H NMR Spectrum (500 MHz, CDCl₃) for methyl 3-methoxybenzoate (**9**)

B04JD031B Proton for Carbon.esp



¹³C NMR spectrum (126 MHz, CDCl₃) for methyl 3-methoxybenzoate (9)

B04JD031B CARBON_01.esp



— 166.93

— 159.61

— 131.51

— 129.34

— 121.98

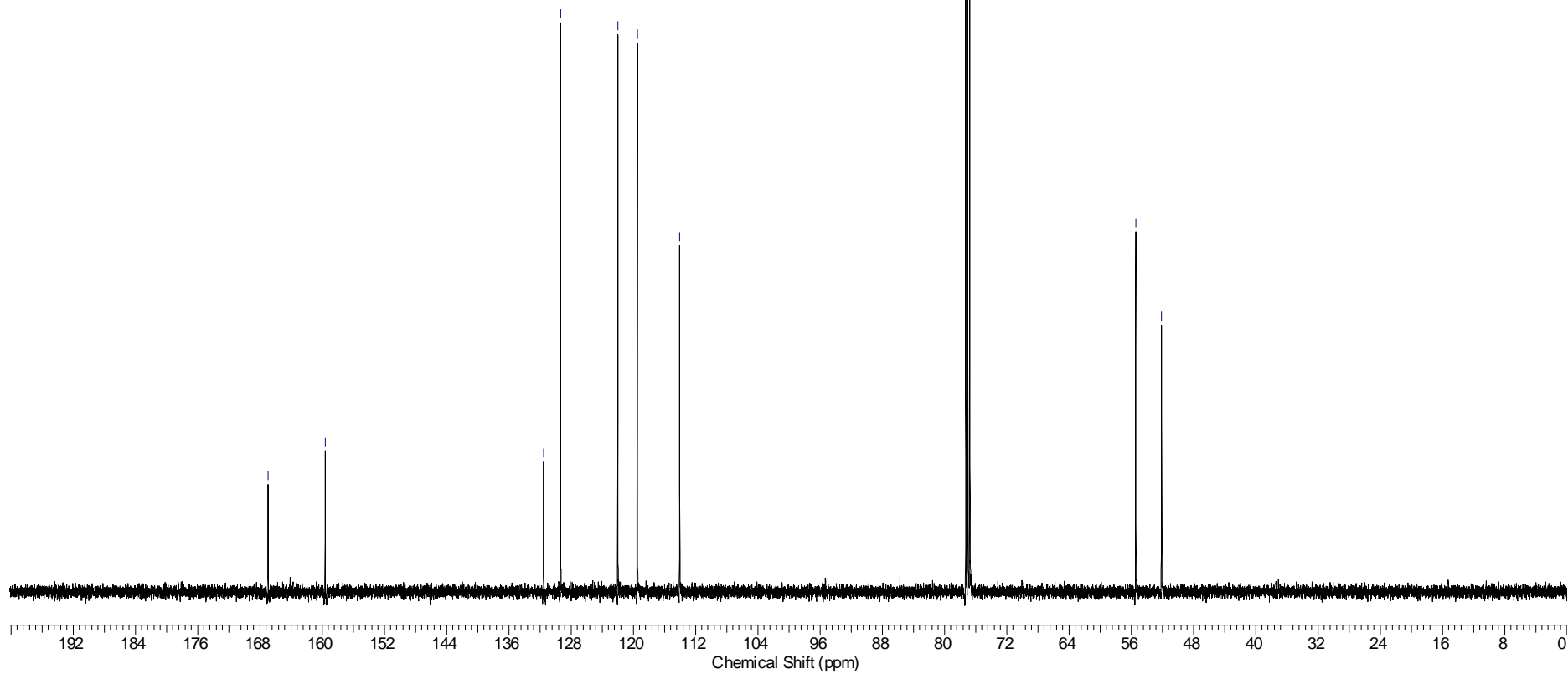
— 119.48

— 114.04

— 77.00

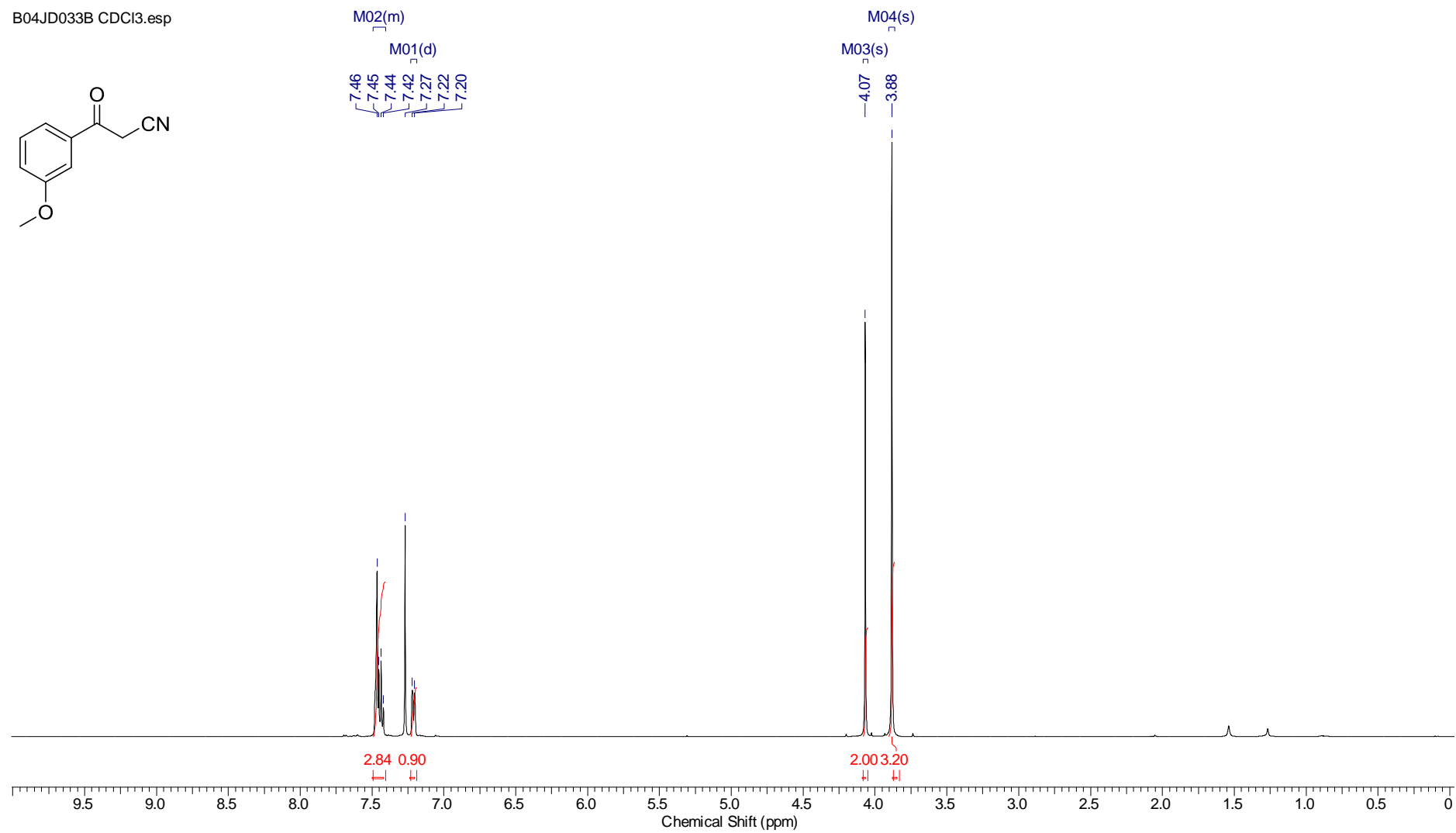
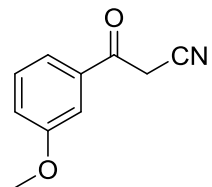
— 55.41

— 52.09



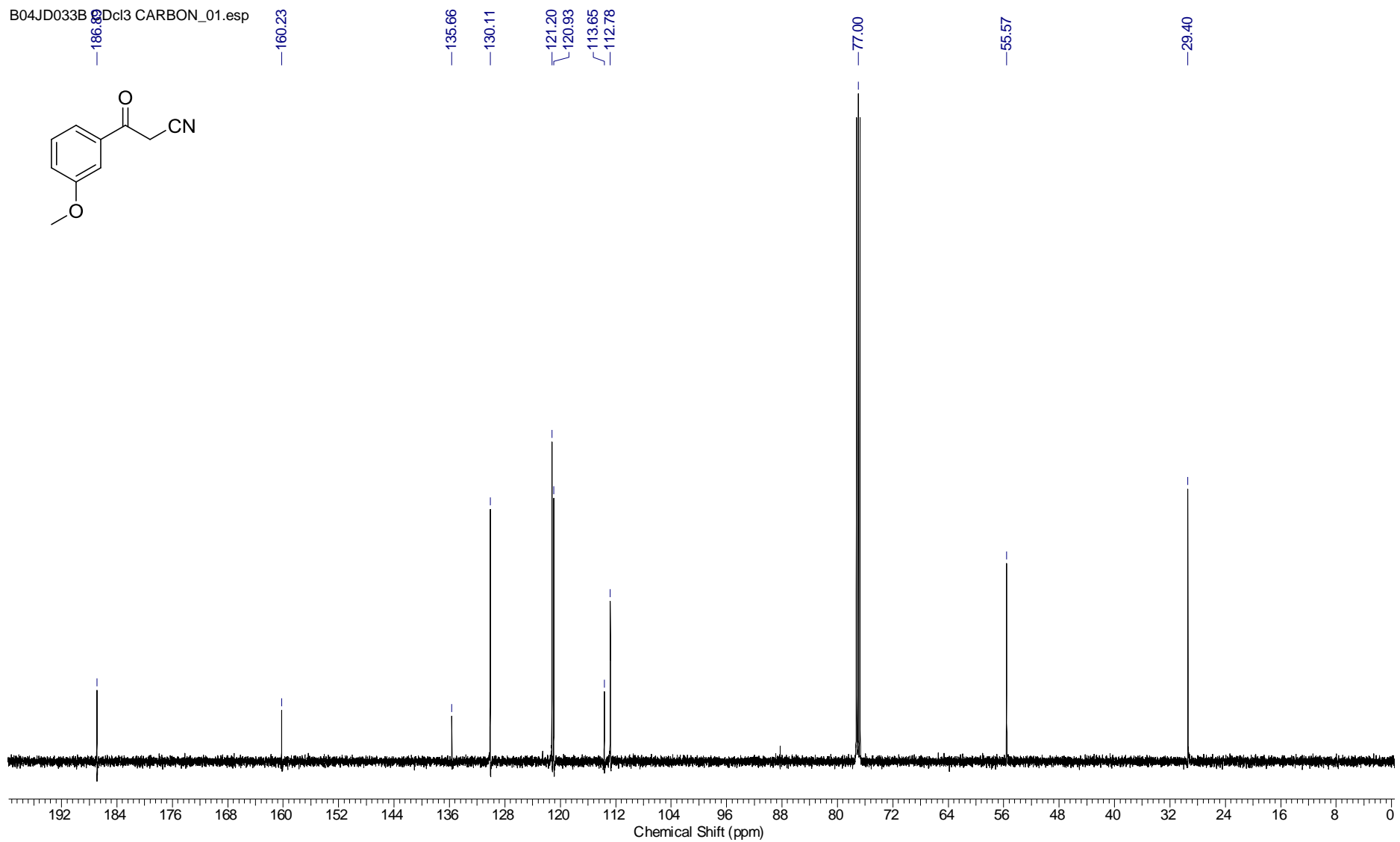
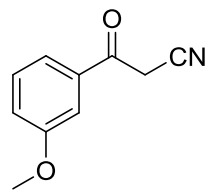
¹H NMR Spectrum (500 MHz, CDCl₃) for methyl 3-methoxybenzoylacetonitrile (6)

B04JD033B CDCl₃.esp



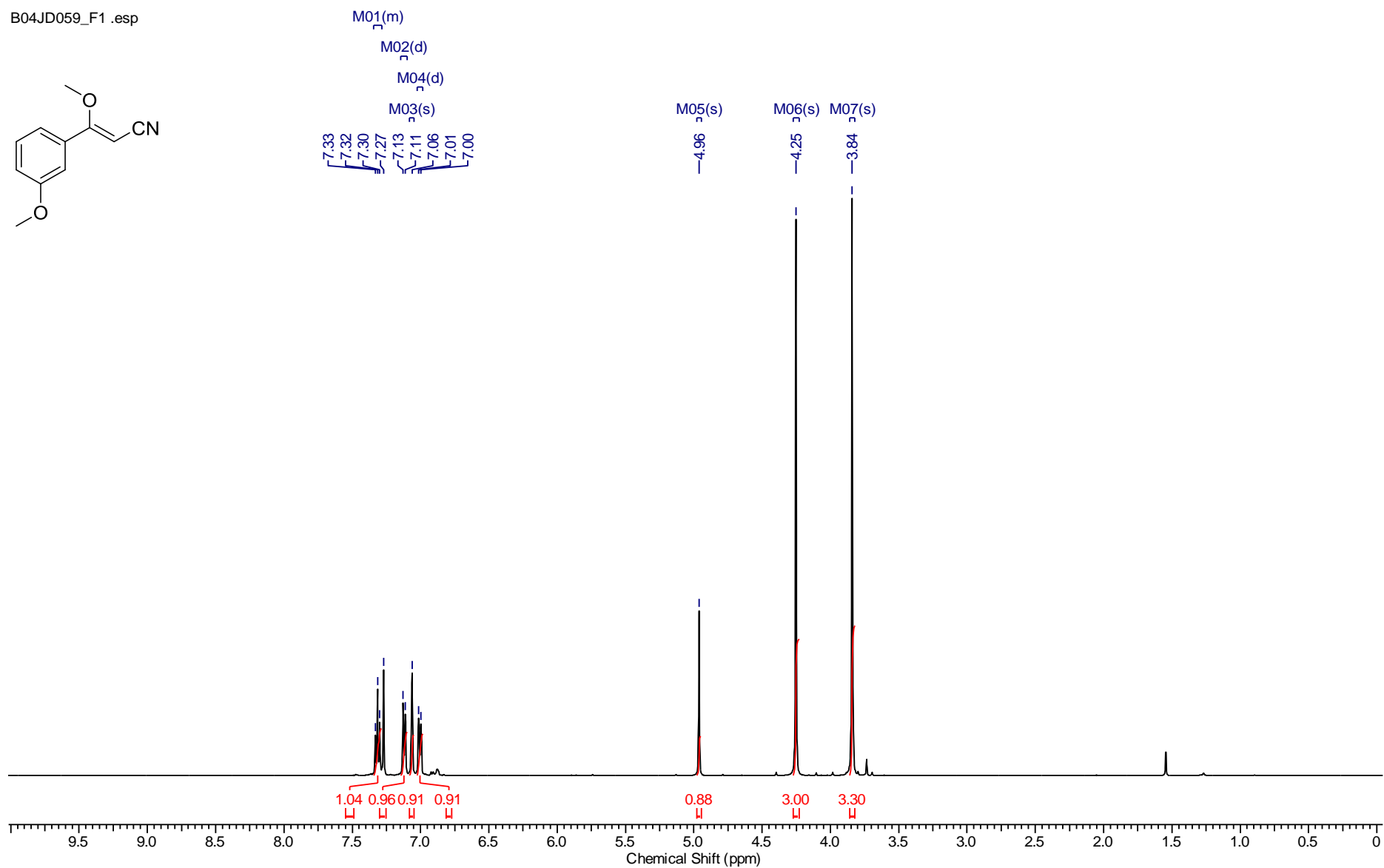
¹³C NMR Spectrum (126 MHz, CDCl₃) for methyl 3-methoxybenzoylacetonitrile (**6**)

B04JD033B DCl3 CARBON_01.esp



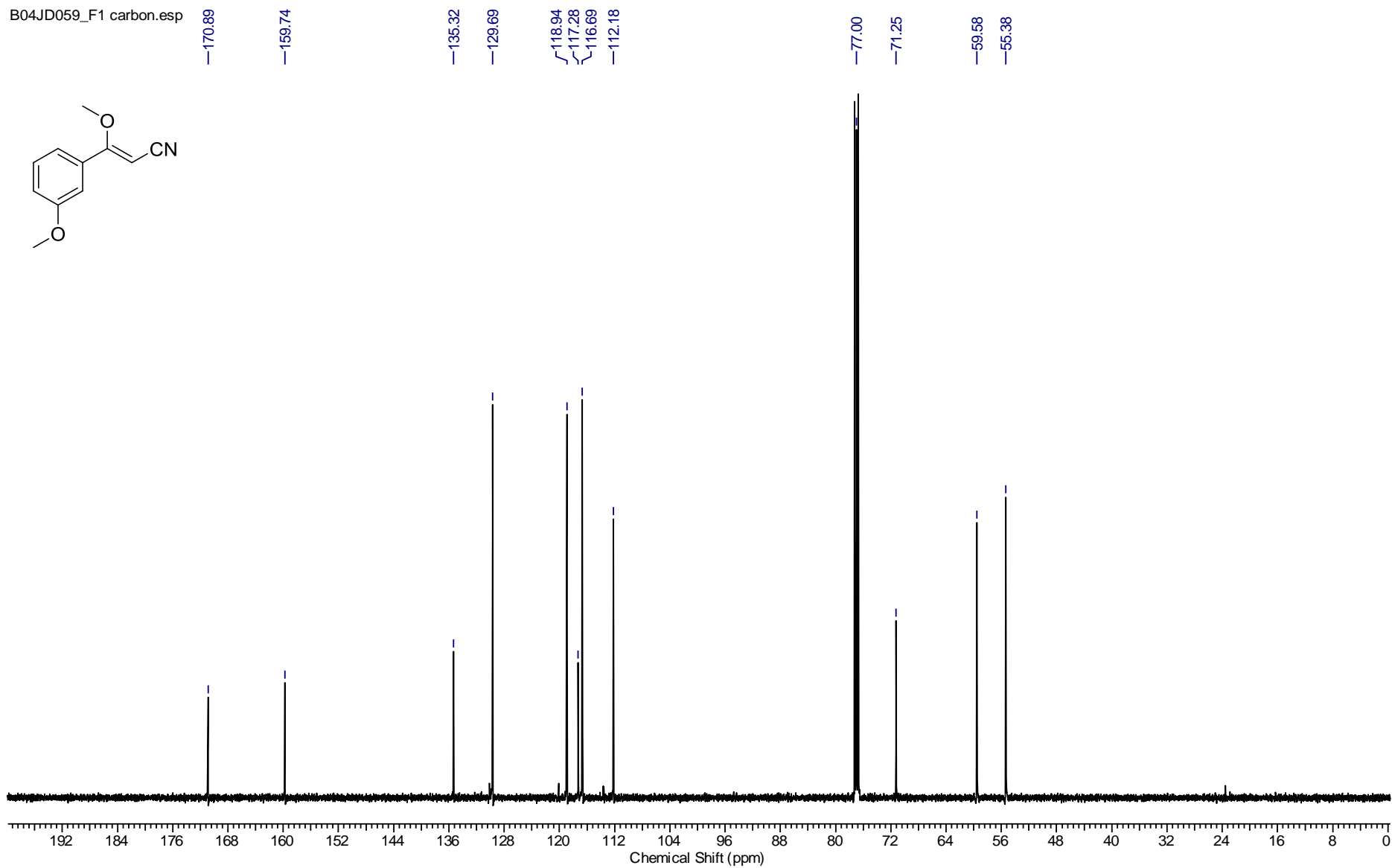
¹H NMR Spectrum (500 MHz, CDCl₃) for (Z)-3-methoxy-3-(3-methoxyphenyl)prop-2-enitrile (**7**)

B04JD059_F1 .esp



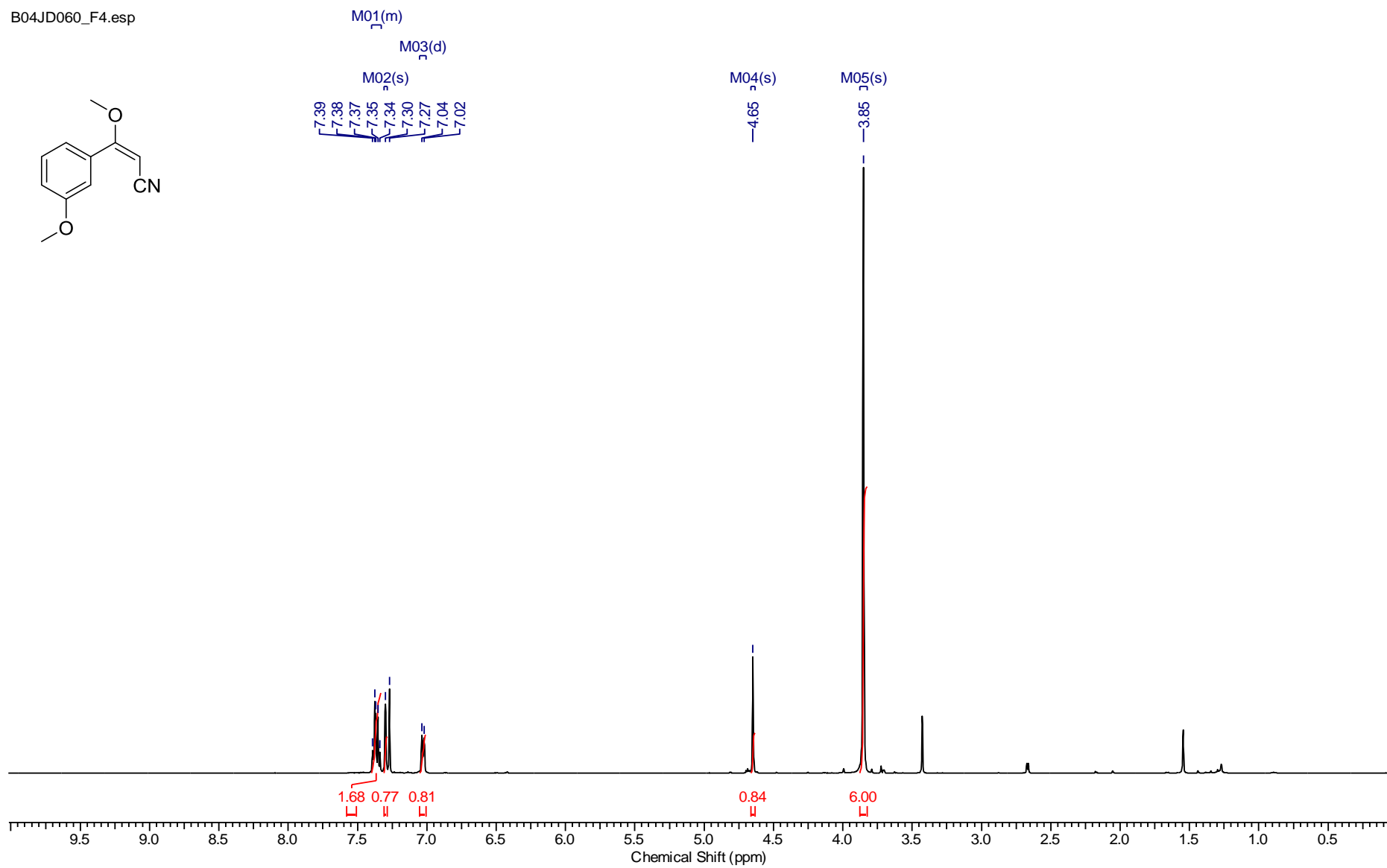
¹³C NMR Spectrum (126 MHz, CDCl₃) for (Z)-3-methoxy-3-(3-methoxyphenyl)prop-2-enitrile (**7**)

B04JD059_F1 carbon.esp



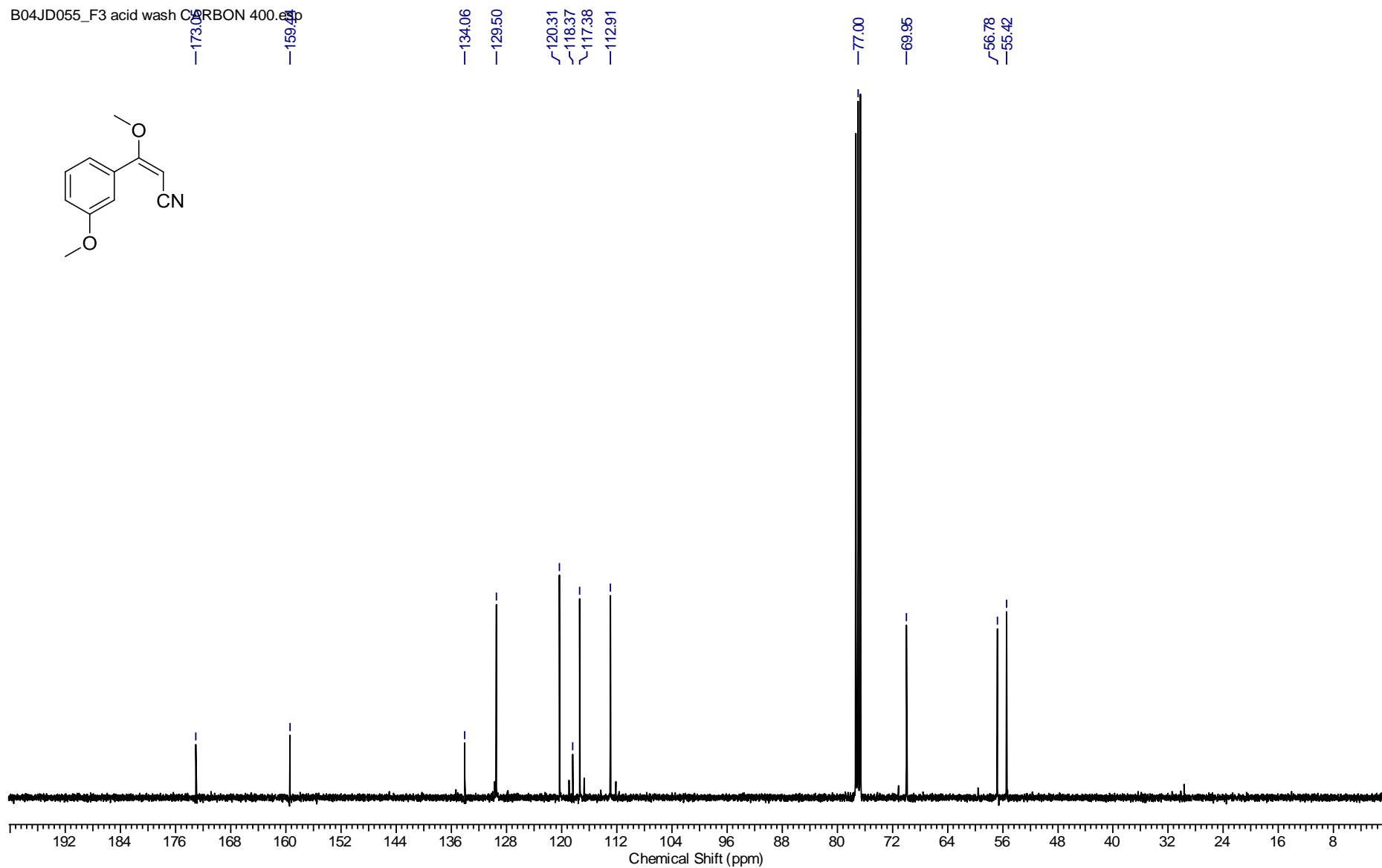
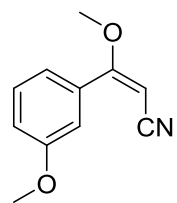
¹H NMR Spectrum (500 MHz, CDCl₃) for (*E*)-3-methoxy-3-(3-methoxyphenyl)prop-2-enitrile (**7**)

B04JD060_F4.esp



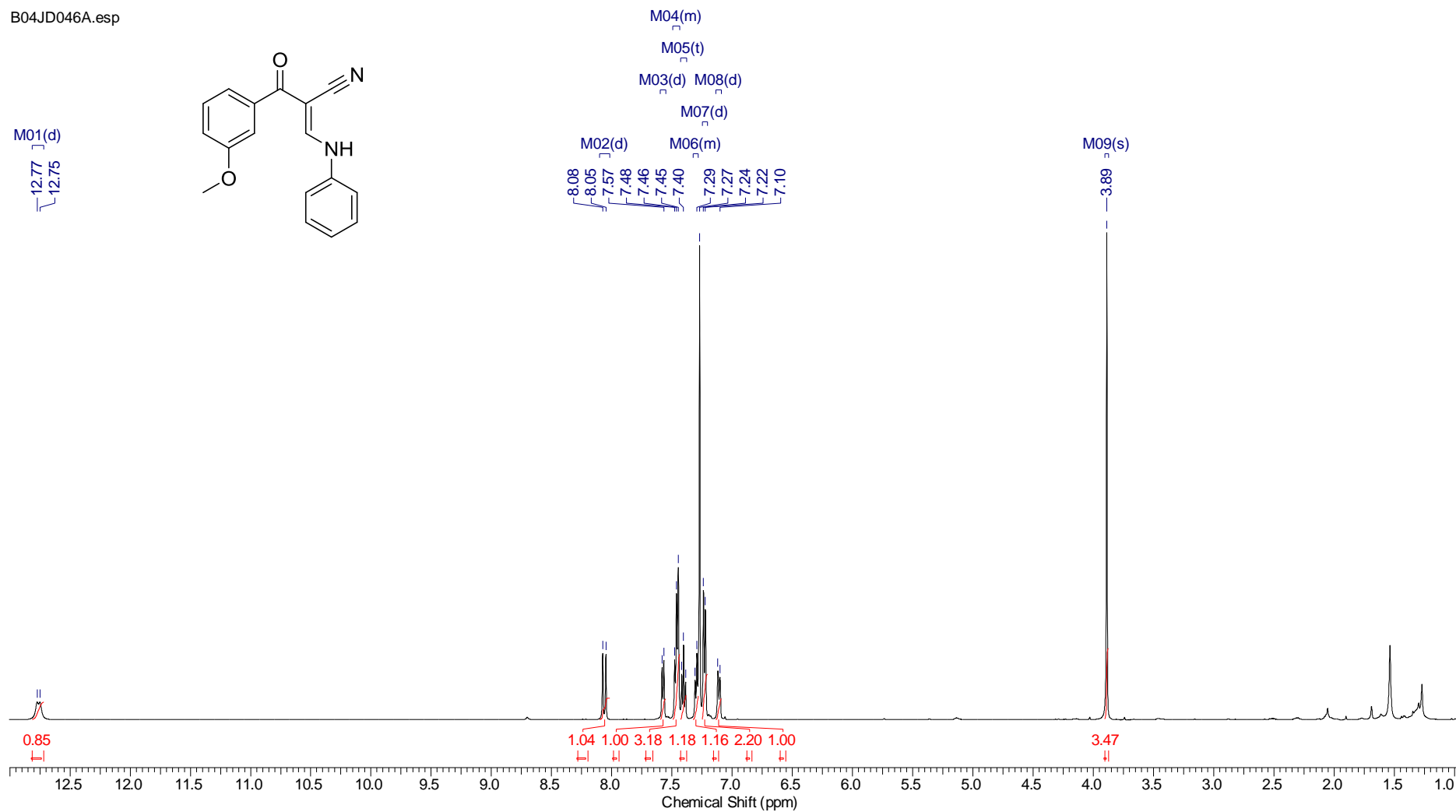
¹³C NMR Spectrum (126 MHz, CDCl₃) for (*E*)-3-methoxy-3-(3-methoxyphenyl)prop-2-enitrile (**7**)

B04JD055_F3 acid wash CARBON 400.01p



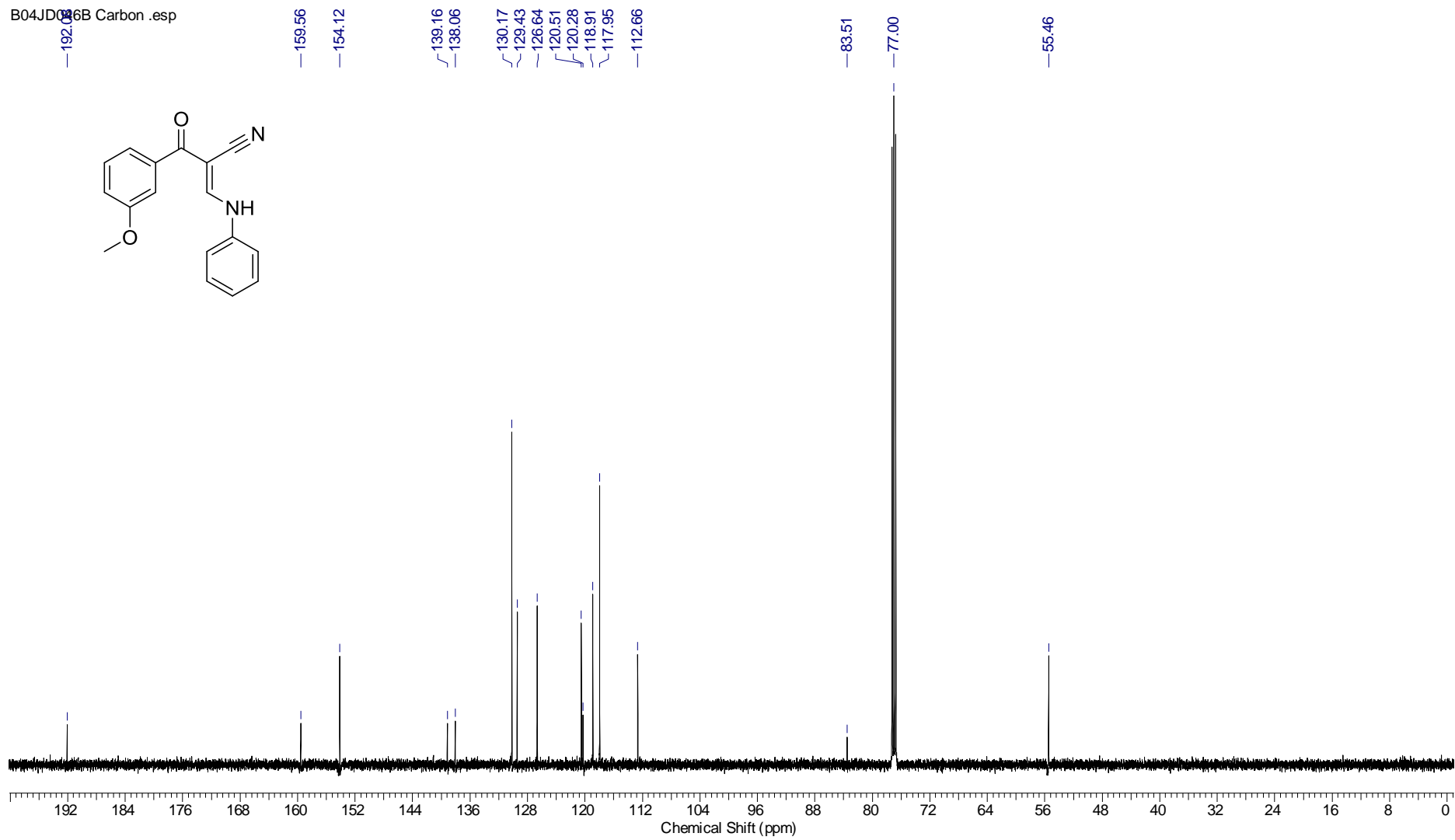
¹H NMR Spectrum (500 MHz, CDCl₃) for 2-(3-methoxybenzoyl)-3-(phenylamino)prop-2-enitrile (**11**)

B04JD046A.esp



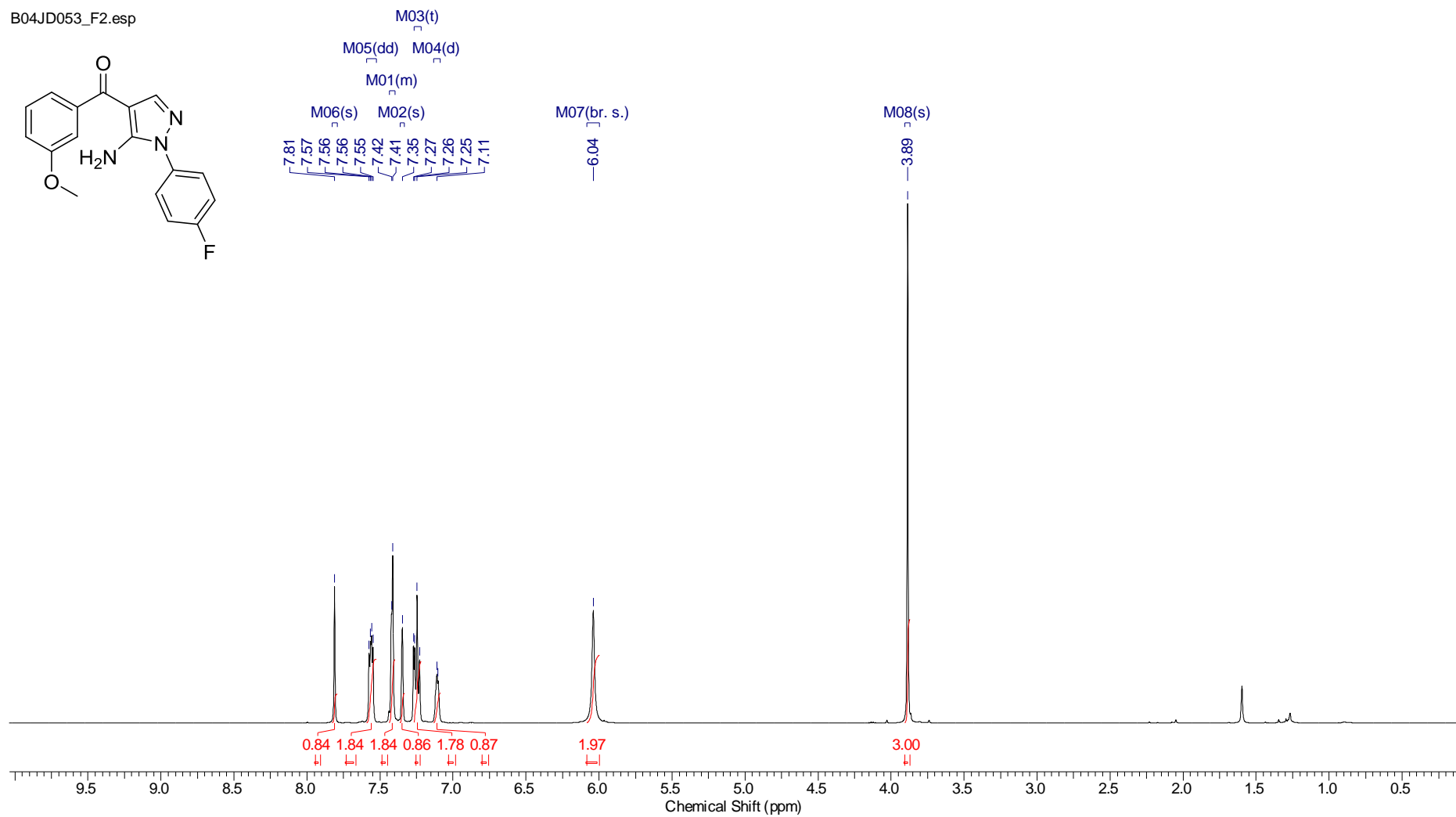
¹³C NMR Spectrum (126 MHz, CDCl₃) for 2-(3-methoxybenzoyl)-3-(phenylamino)prop-2-enitrile (**11**)

B04JD006B Carbon .esp



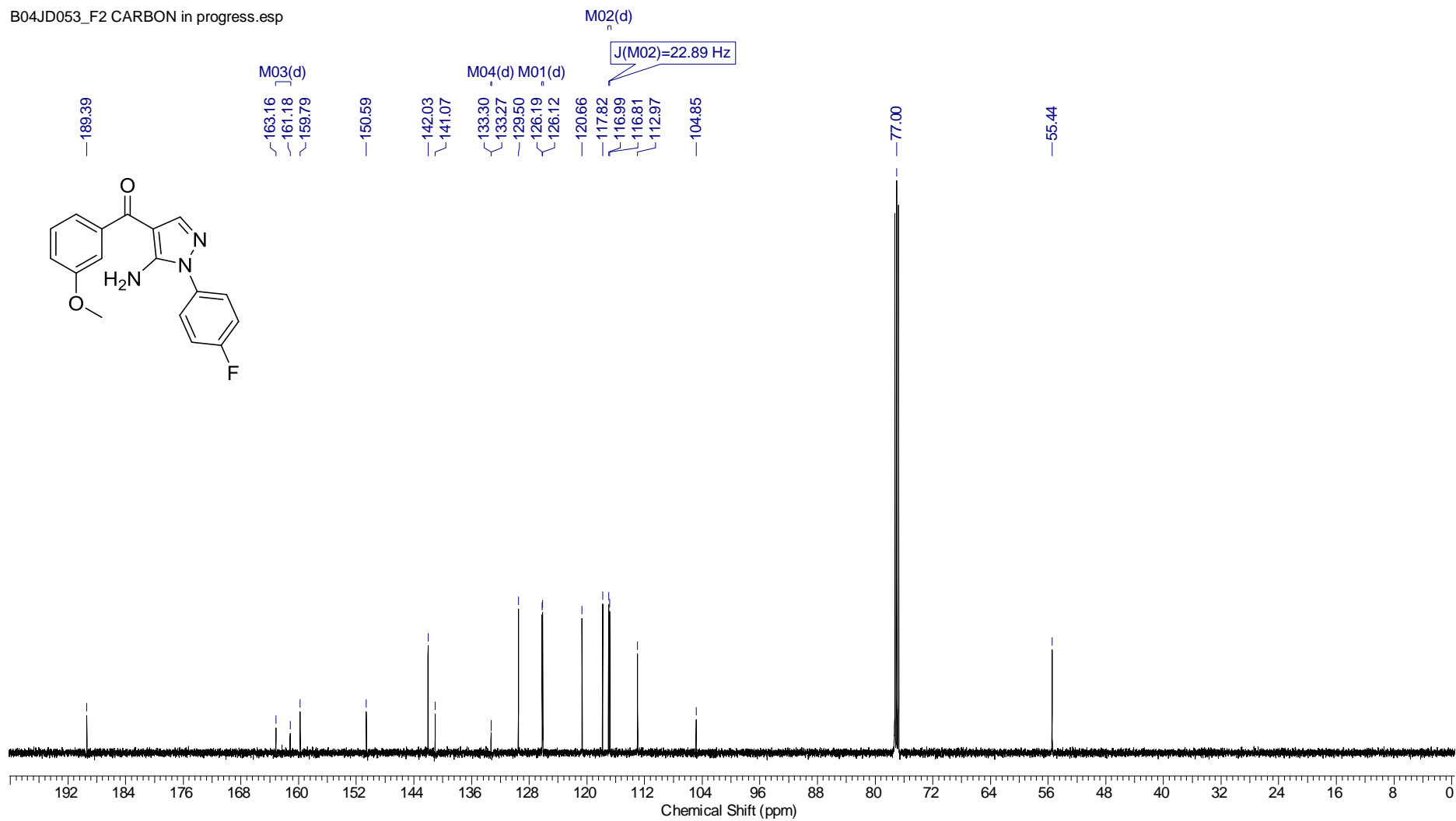
¹H NMR spectrum (500 MHz, CDCl₃) for [5-amino-1-(4-fluorophenyl)-1H-pyrazol-4-yl]-3-methoxyphenyl ketone (**12**)

B04JD053_F2.esp



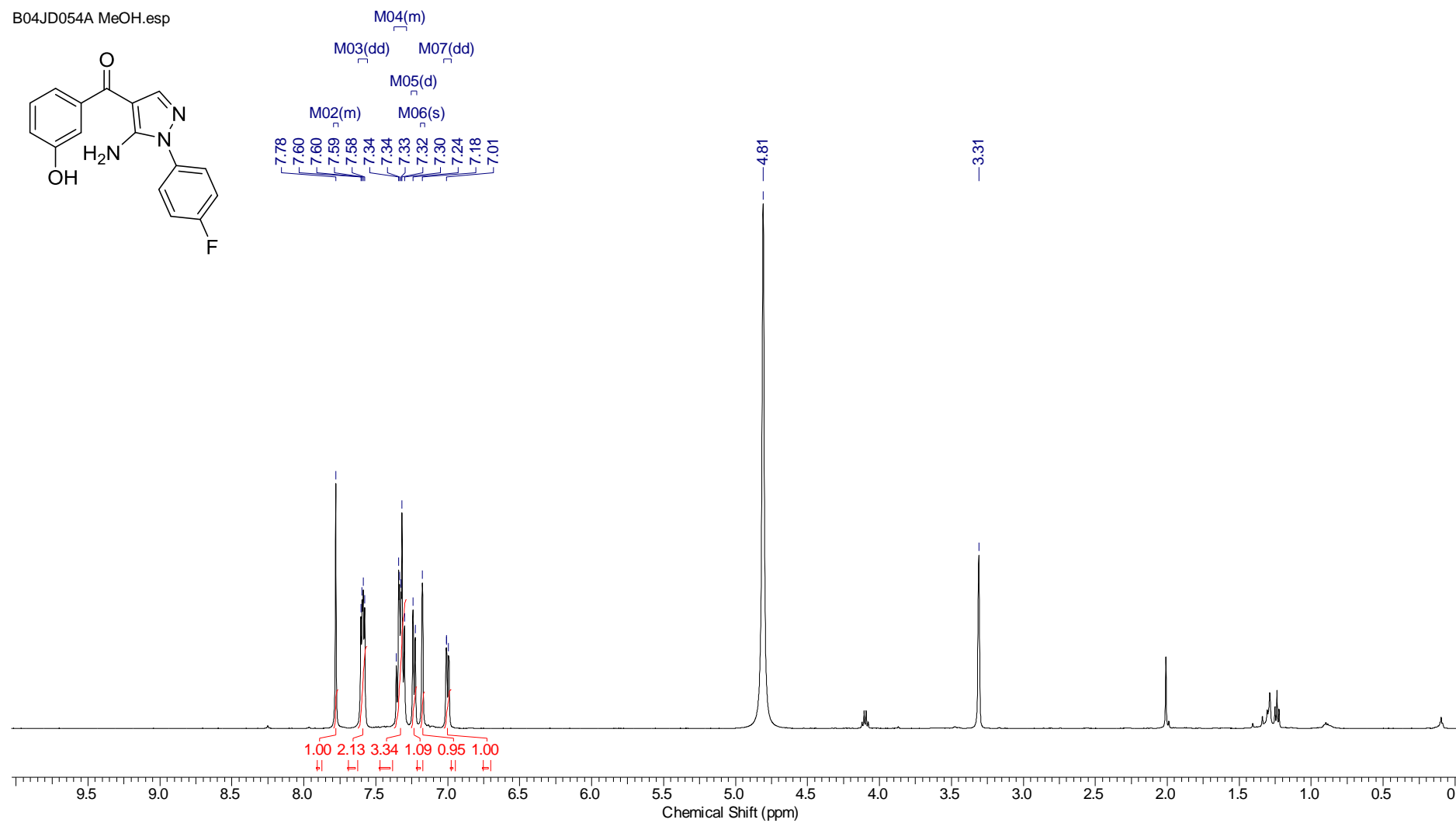
¹³C NMR spectrum (126 MHz, CDCl₃) for [5-amino-1-(4-fluorophenyl)-1H-pyrazol-4-yl]-3-methoxyphenyl ketone (**12**)

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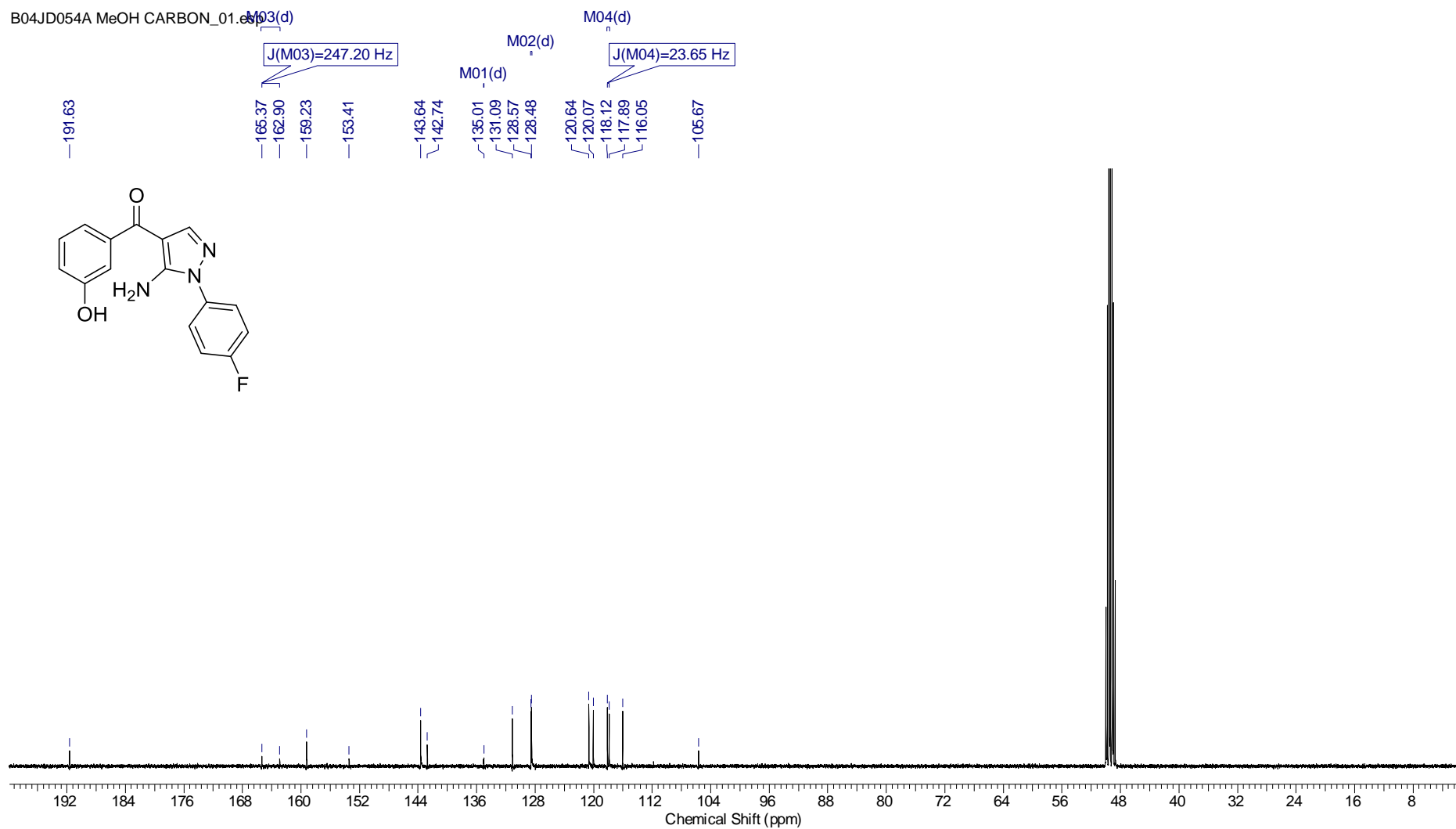
¹H NMR spectrum (500 MHz, CD₃OD) for [5-amino-1-(4-fluorophenyl)-1H-pyrazol-4-yl]-3-hydroxyphenyl ketone (**13**)

B04JD054A MeOH.esp



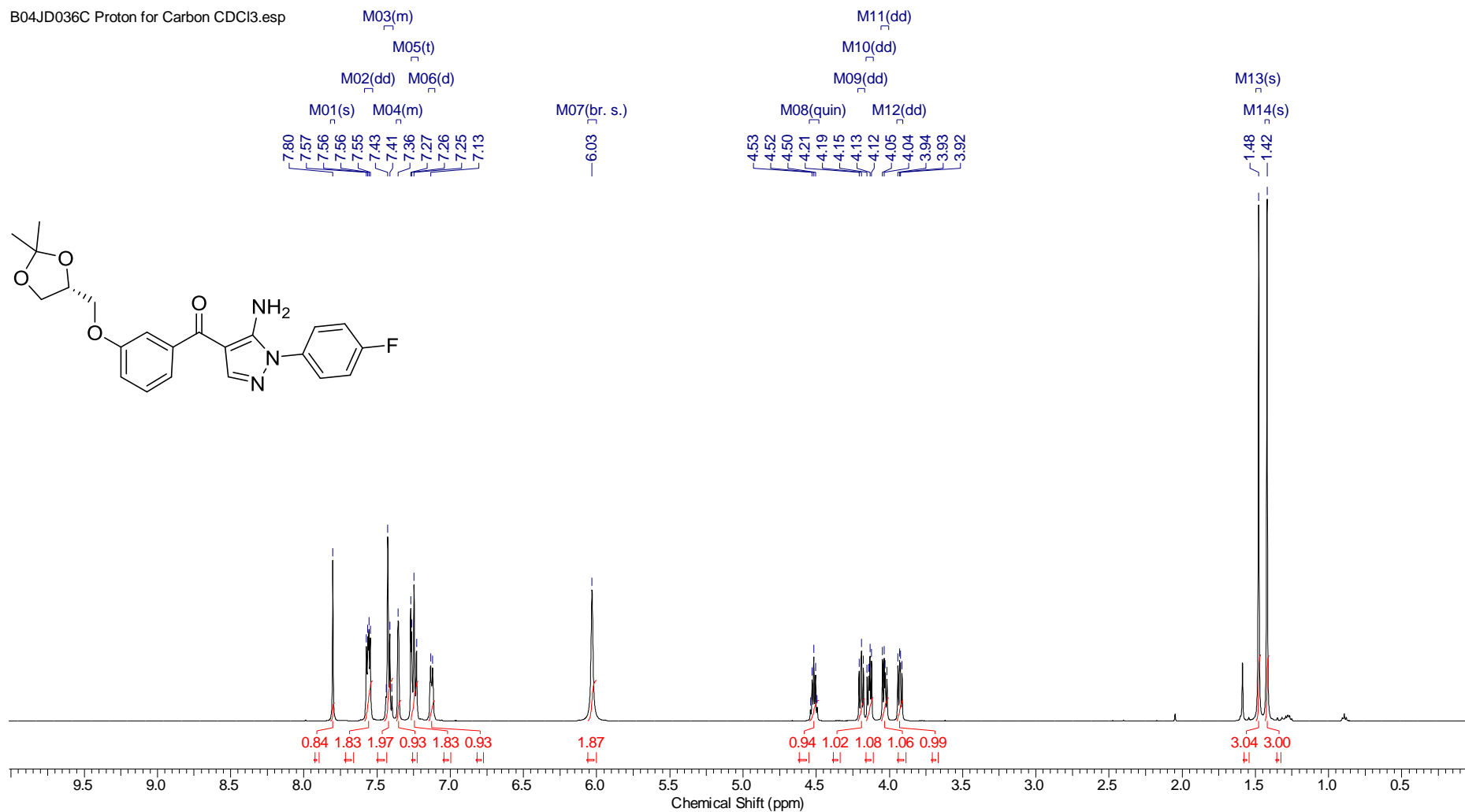
¹³C NMR spectrum (100 MHz, CD₃OD) for [5-amino-1-(4-fluorophenyl)-1H-pyrazol-4-yl]-3-hydroxyphenyl ketone (**13**)

B04JD054A MeOH CARBON_01.esy



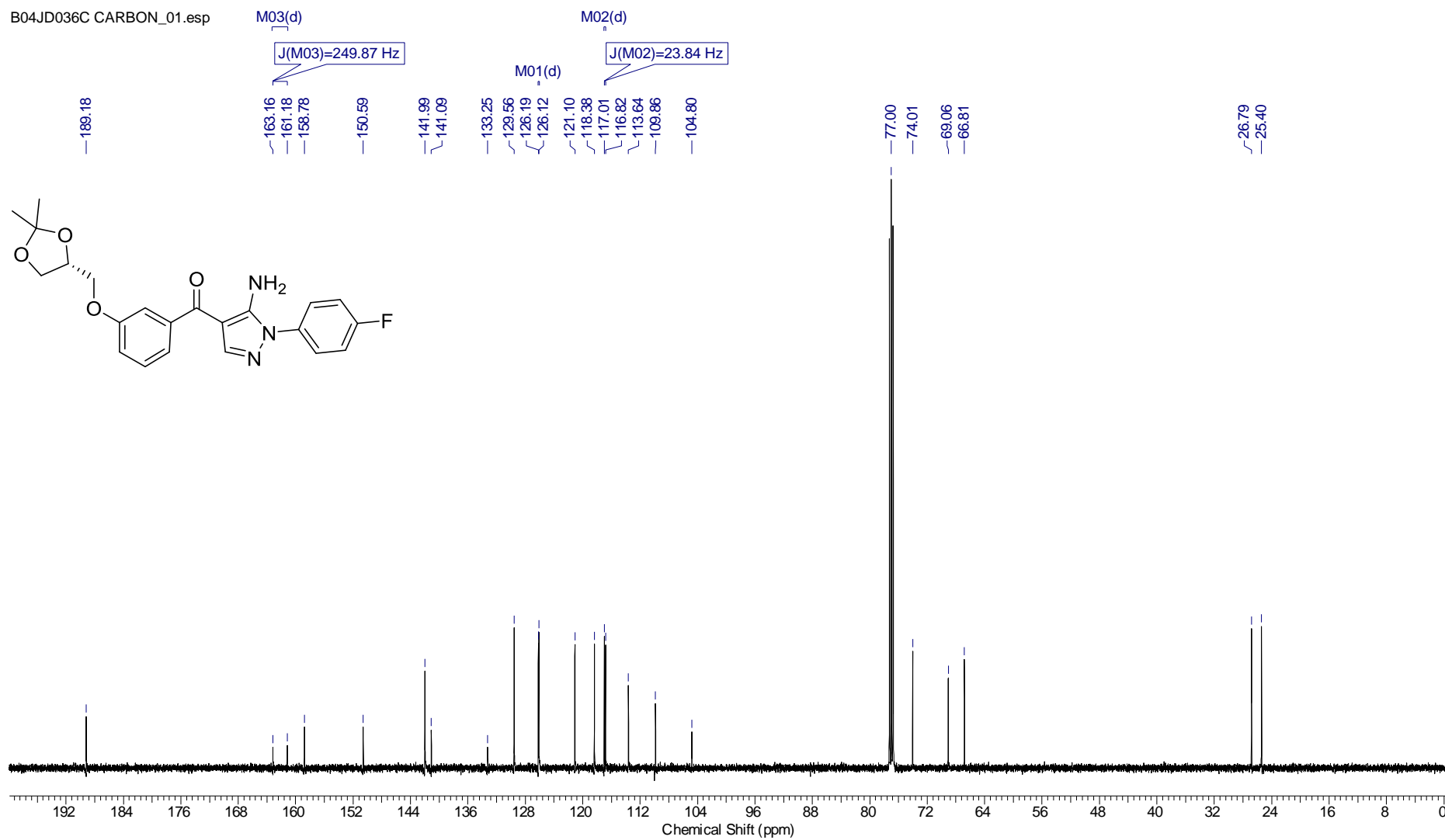
¹H NMR spectrum (500 MHz, CDCl₃) for [5-amino-1-(4-fluorophenyl)-1*H*-pyrazol-4-yl]{3-[(*R*)-2,2-dimethyl-1,3-dioxolan-4-yl]methoxy}phenyl} ketone (**15**)

B04JD036C Proton for Carbon CDCl₃.esp



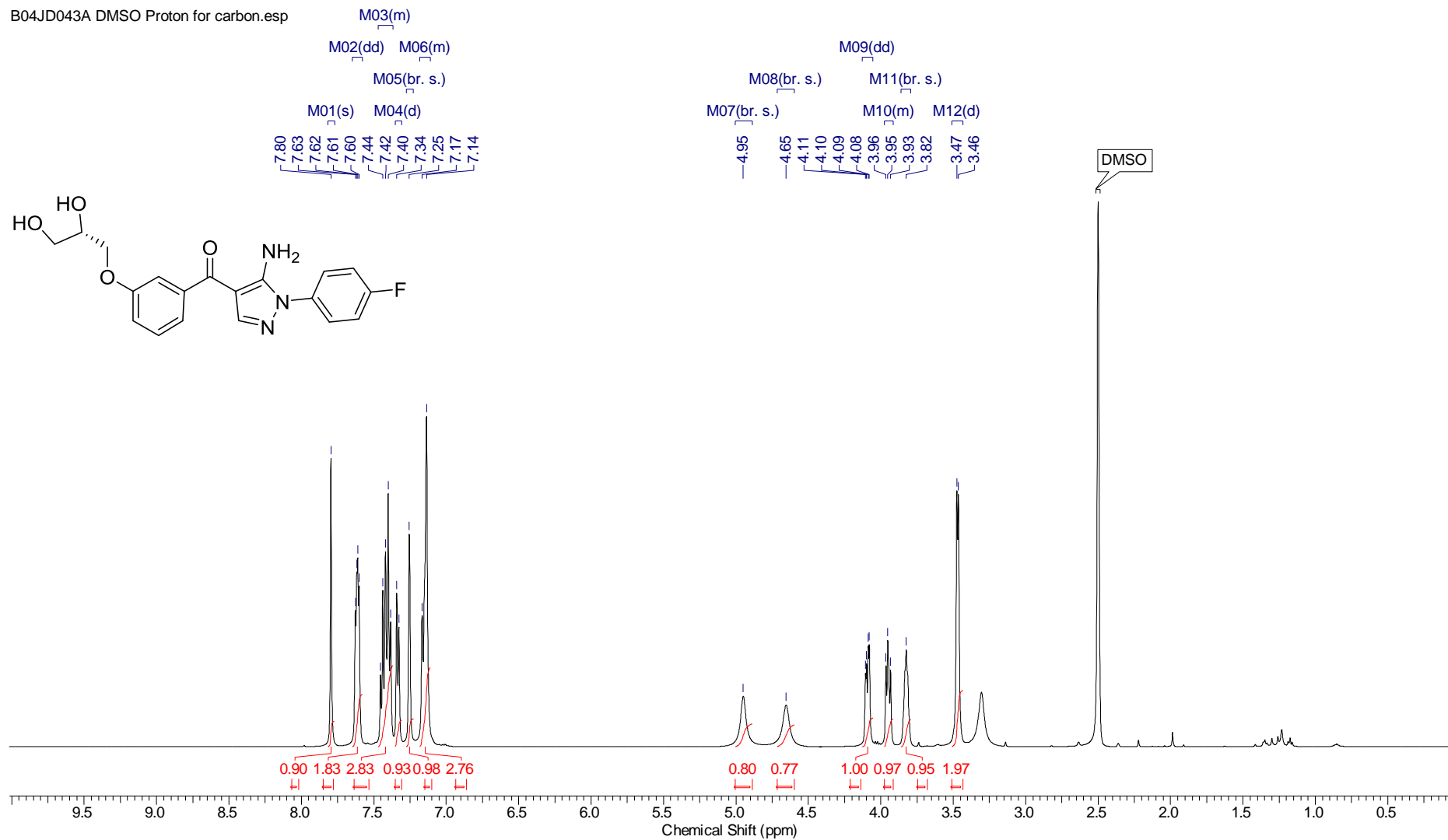
¹³C NMR spectrum (126 MHz, CDCl₃) for [5-amino-1-(4-fluorophenyl)-1*H*-pyrazol-4-yl]{3-[[*R*]-2,2-dimethyl-1,3-dioxolan-4-yl)methoxy]phenyl} ketone (**15**)

B04JD036C CARBON_01.esp



¹H NMR (500 MHz, DMSO-d₆) for 5-amino-1-(4-fluorophenyl)-4-{3-[2(S)-3-dihydroxypropoxy]benzoyl}pyrazole (RO3201195) (**1**)

B04JD043A DMSO Proton for carbon.esp



¹³C NMR (126 MHz, DMSO-*d*₆) for 5-amino-1-(4-fluorophenyl)-4-{3-[2(*S*)-3-dihydroxypropoxy]benzoyl}pyrazole (RO3201195) (1)

B04JD043A DMSO CARBON .esp

