

Direct conversion of secondary propargyl alcohol into 1,3-di-arylpropanone via DBU promoted redox isomerization and palladium assisted chemoselective hydrogenation in a single pot operation.

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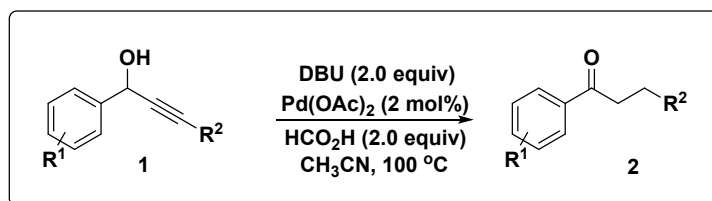
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Supporting Information

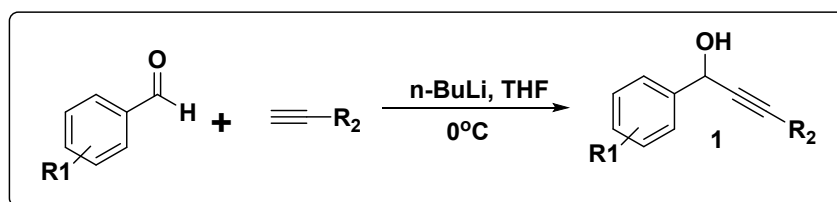
Table of content

Schematic representation of 1, 3-diarylpropanone synthesis	03
Synthetic procedure of secondary propargyl alcohol	03
NMR spectra of compounds	04 - 26

Schematic representation of 1, 3-diarylpropanone synthesis from secondary propargyl alcohol



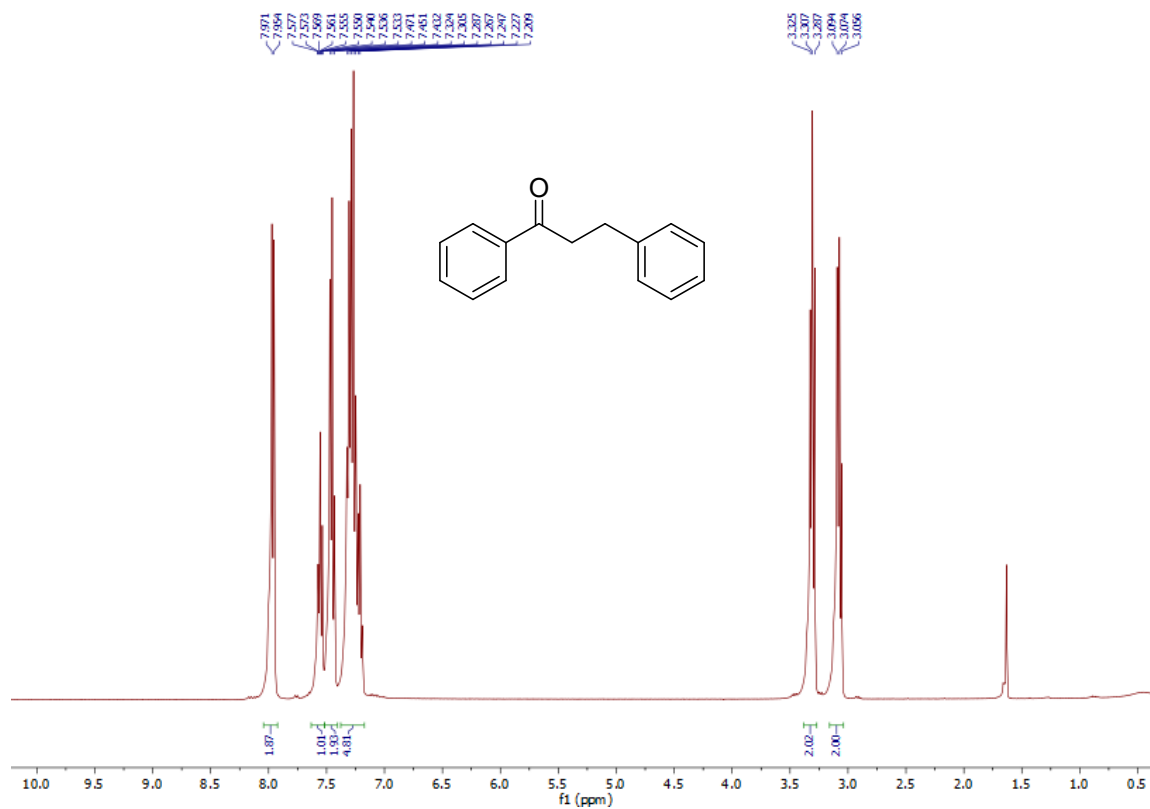
Synthetic procedure of secondary propargyl alcohols



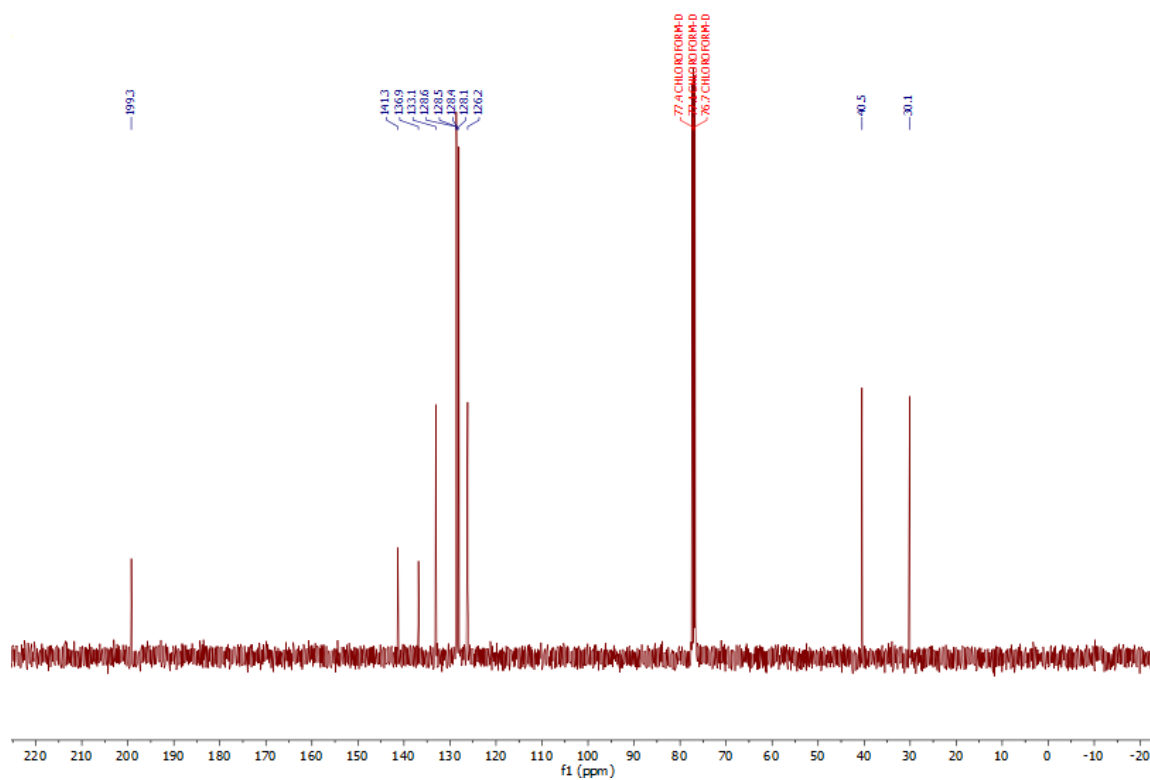
A series of secondary propargyl alcohol (**1a-1w**) were prepared according to the previously reported method (Reference no. 22b in the manuscript).

At first, 2.0 M solution of *n*-butyl lithium in hexane (1.1 mmol) was added to THF solution of phenyl acetylene (1.2 mmol) at 0 °C through septa- syringe system under N₂ atmosphere. After 20 mins, THF solution of aromatic aldehyde (1.0 mmol) was added to this reaction mixture and stirred for another 30 mins at same temperature. After completion of the reaction confirmed by TLC, the reaction mixture was quenched by adding saturated aqueous solution of ammonium chloride and extracted thrice with ethyl acetate (25ml x 3). Then the combined organic layer was dried over sodium sulphate and the solvent was reduced under vacuo. After purification of crude product on silica gel column chromatography (100-200 Mess, Pet ether: ethyl acetate=4:1), a series of secondary propargyl alcohols (**1a - 1w**) were obtained with good to excellent yields.

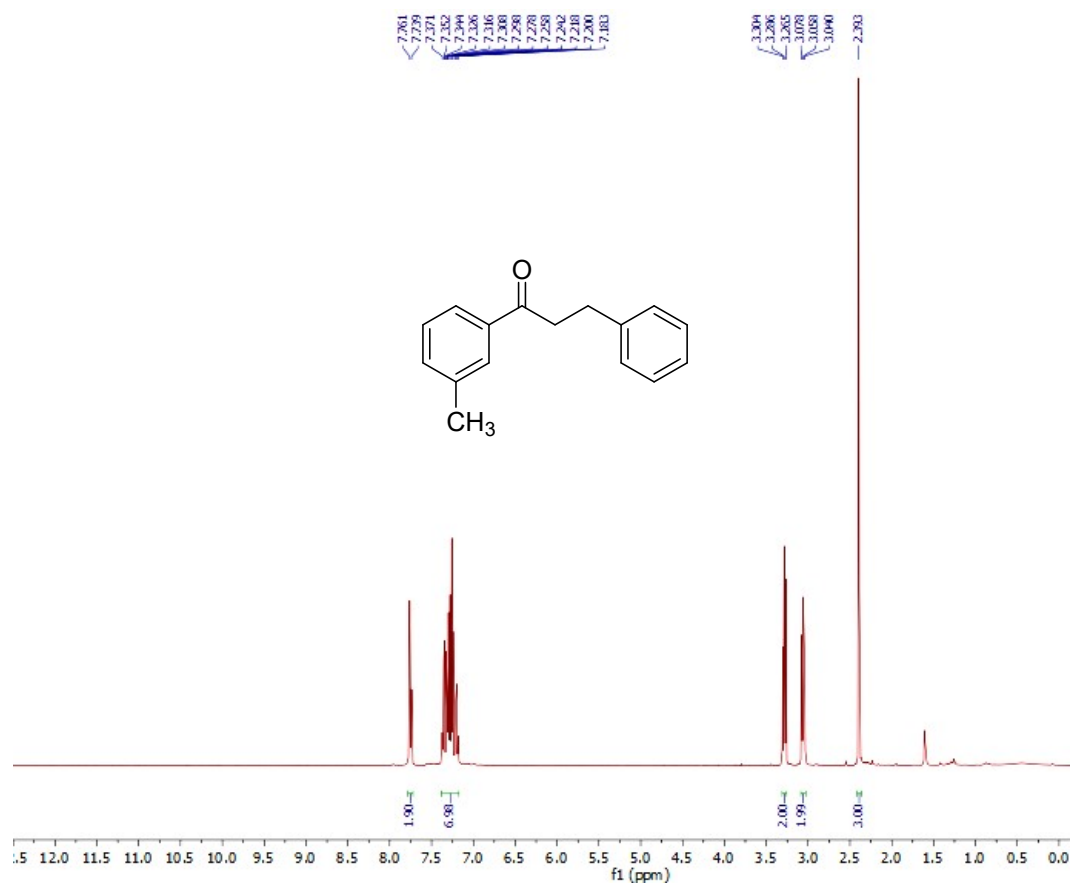
¹H NMR of 1, 3- Diphenylpropan-1-one (2a):



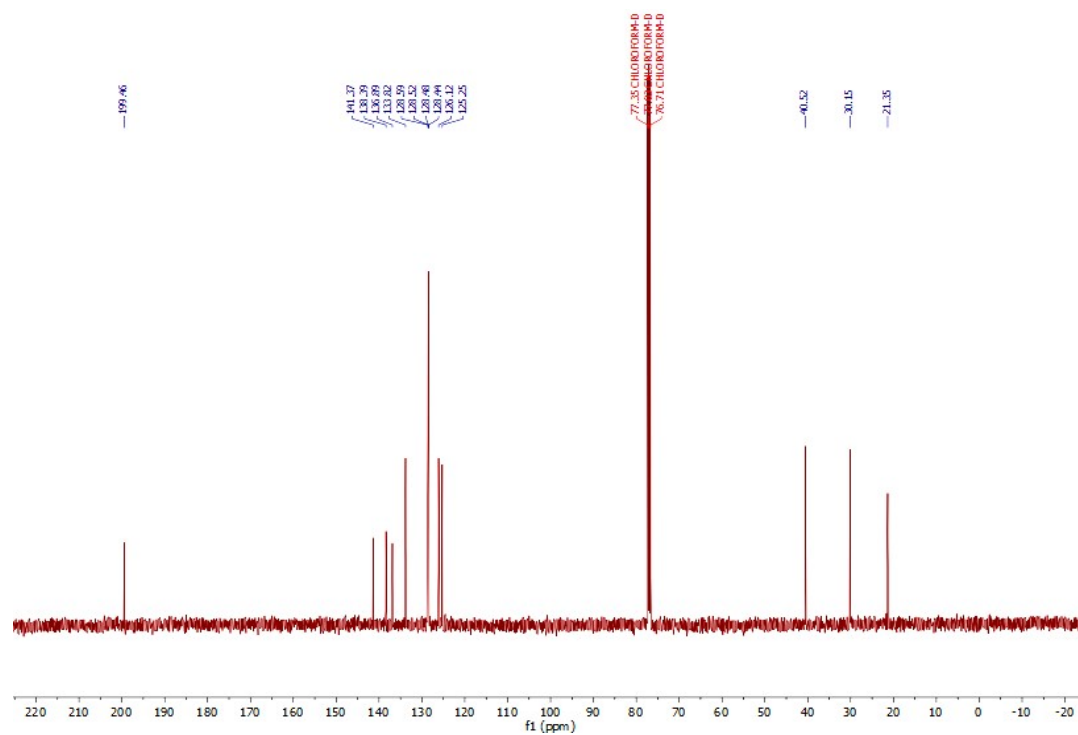
¹³C NMR of 1, 3- Diphenylpropan-1-one (2a):



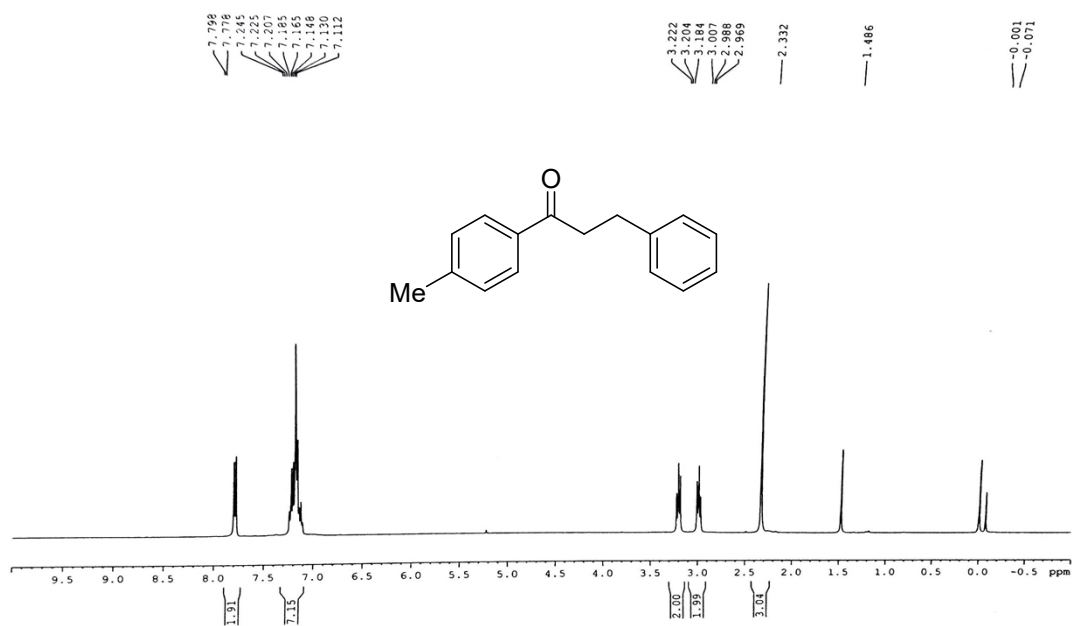
¹H NMR of 3-phenyl-1-(m-tolyl) propan-1-one (2b):



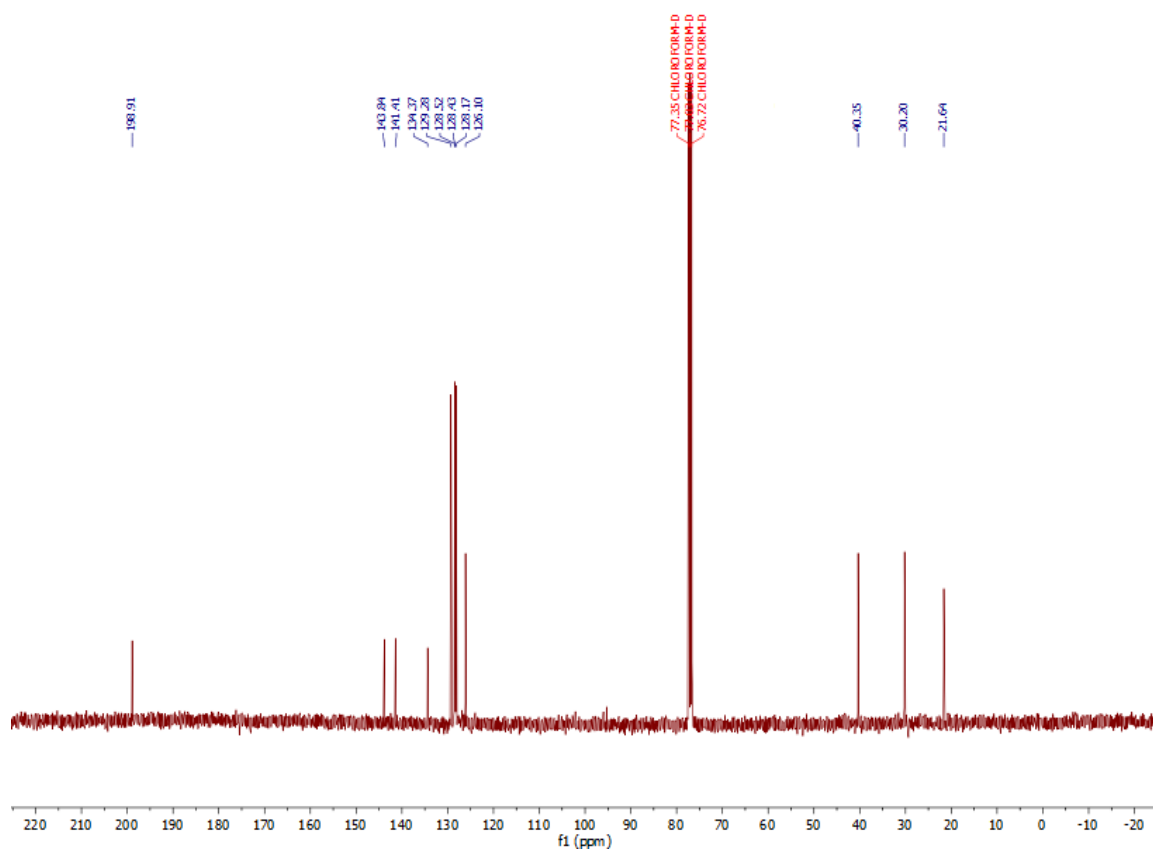
¹³C NMR of 3-phenyl-1-(m-tolyl) propan-1-one (2b):



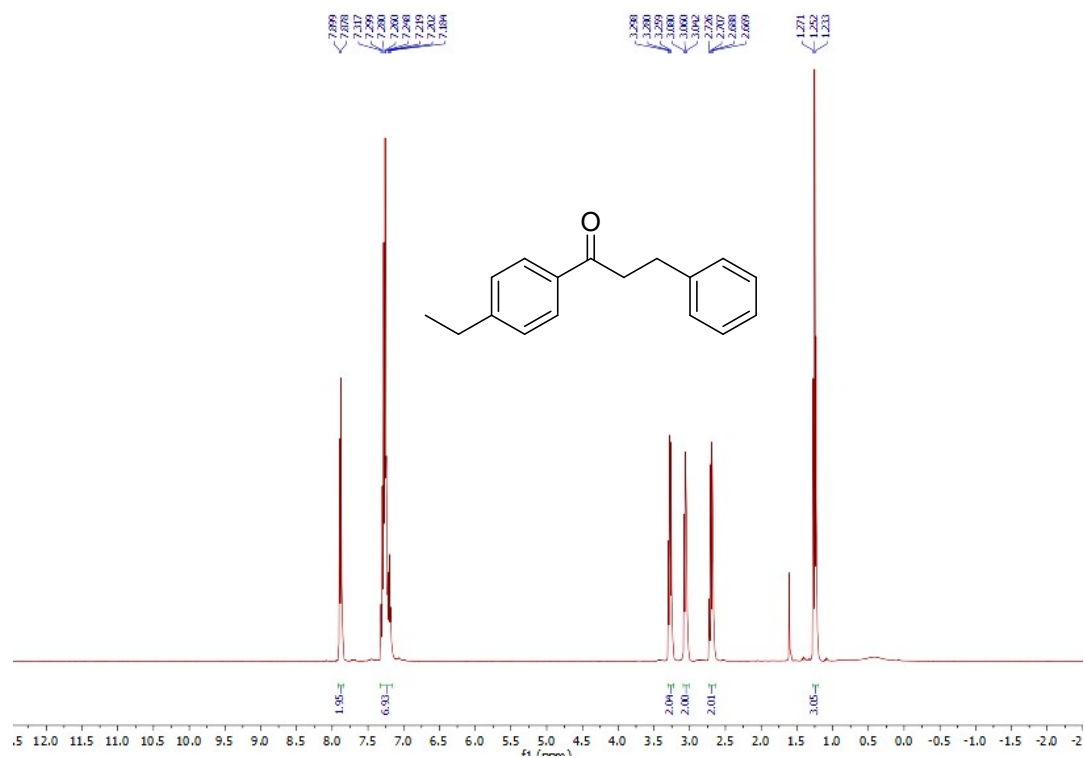
¹H NMR of 3-phenyl-1-(p-tolyl) propan-1-one (2c):



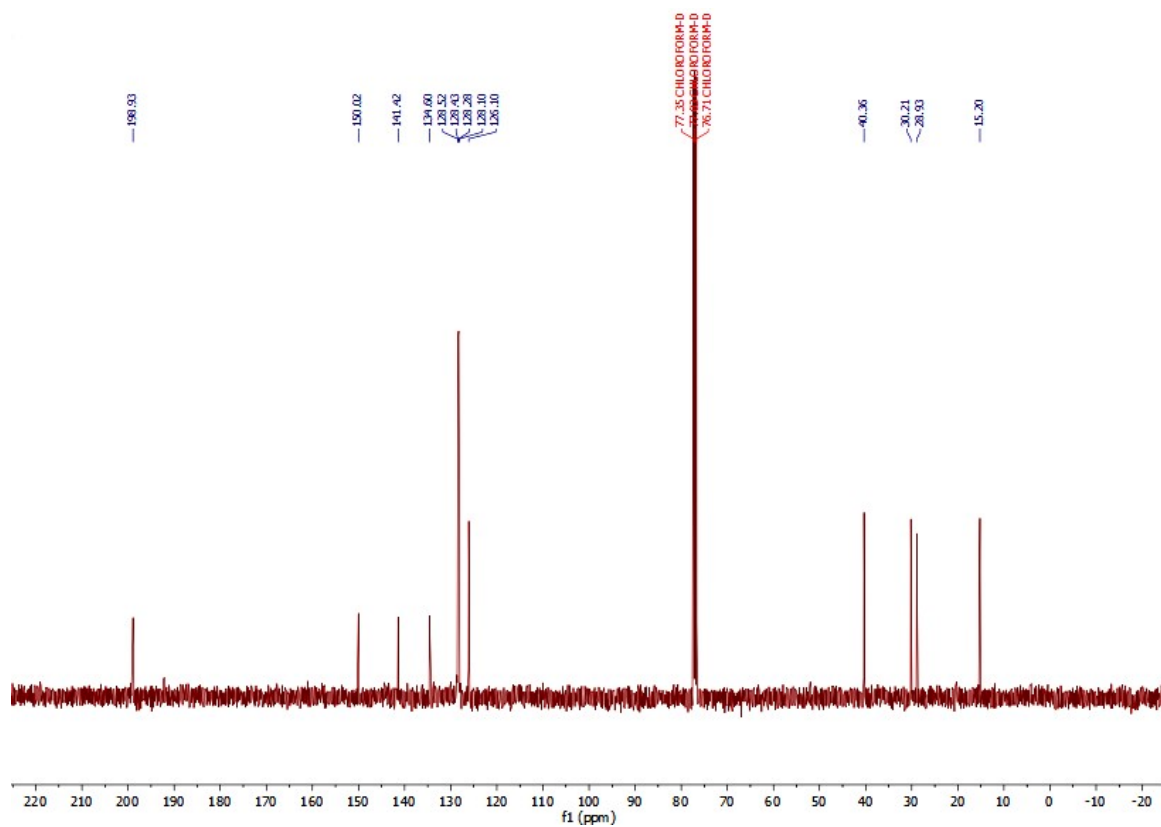
¹³C NMR of 3-phenyl-1-(p-tolyl) propan-1-one (2c):



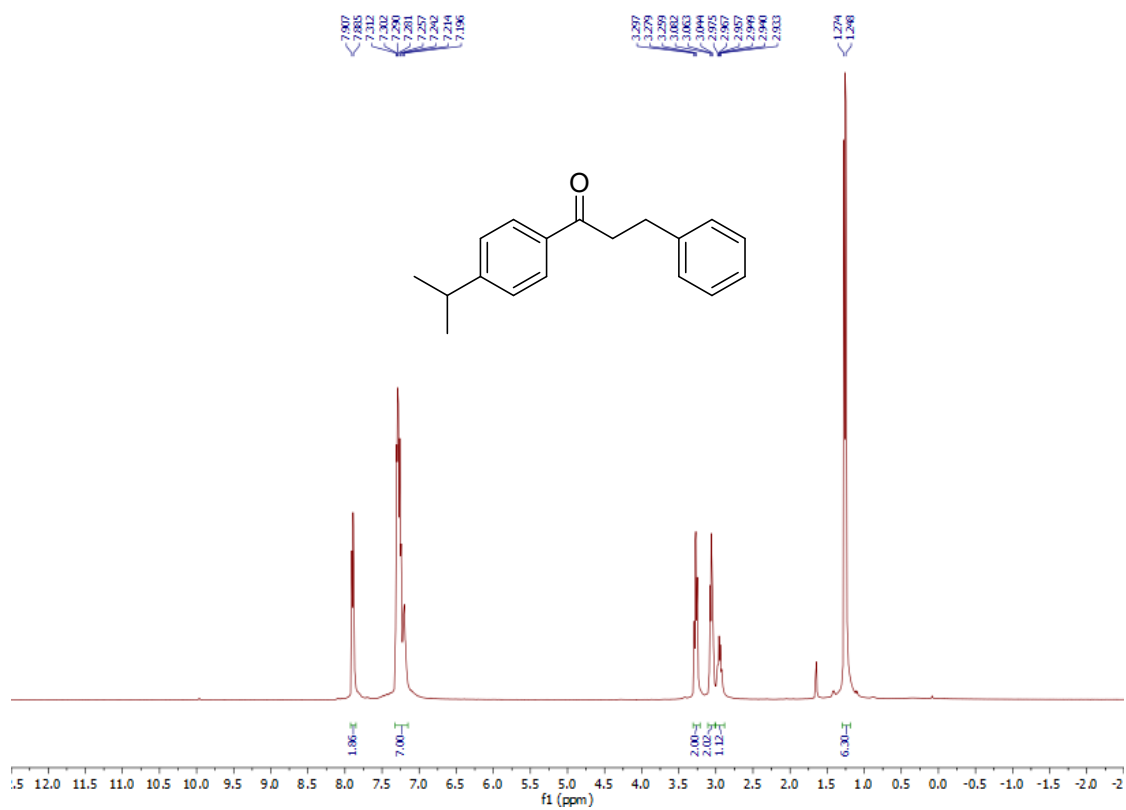
¹H NMR of 1-(4-ethylphenyl)-3-phenylpropane-1-one (2d):



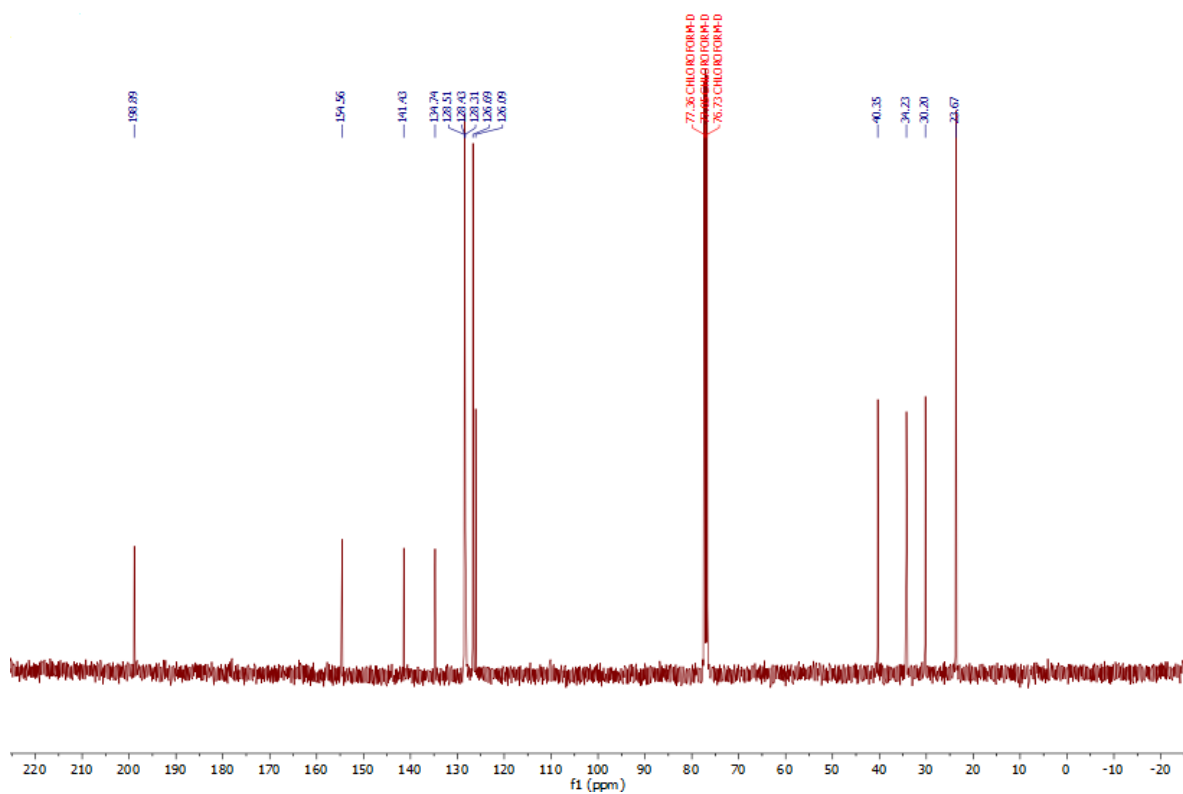
¹³C NMR of 1-(4-ethylphenyl)-3-phenylpropane-1-one (2d):



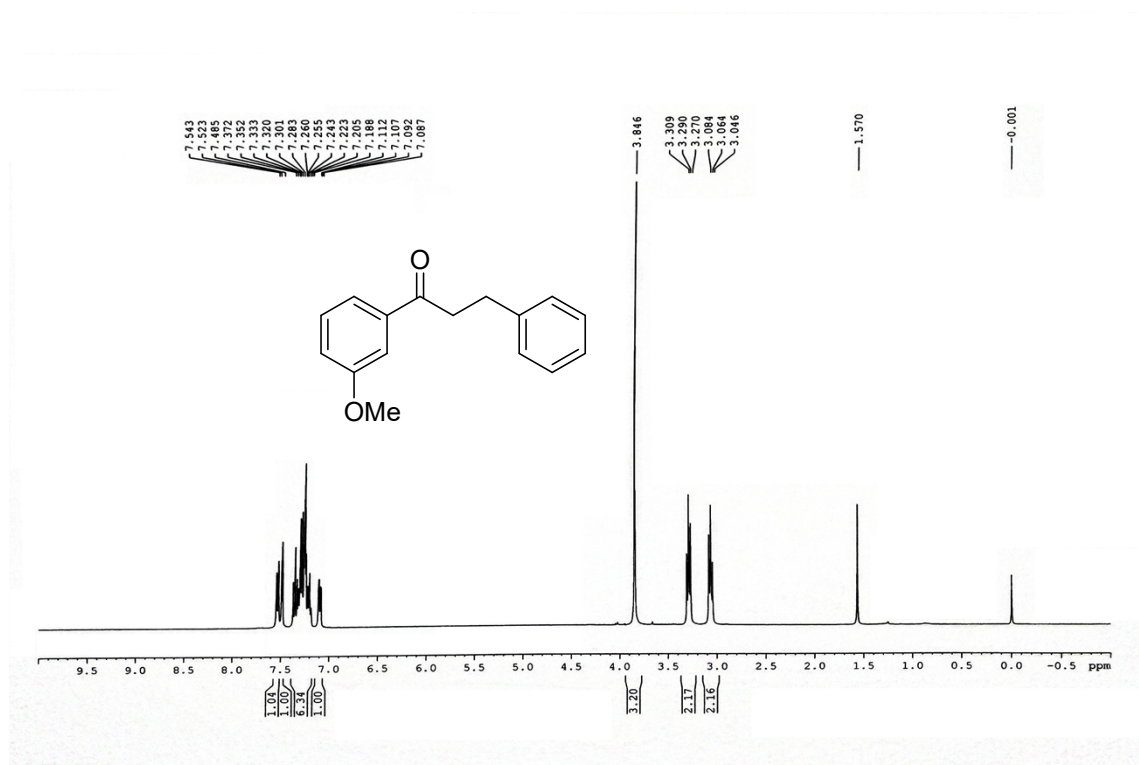
¹H NMR of 1-(4-isopropylphenyl)-3-phenylpropane-1-one (2e):



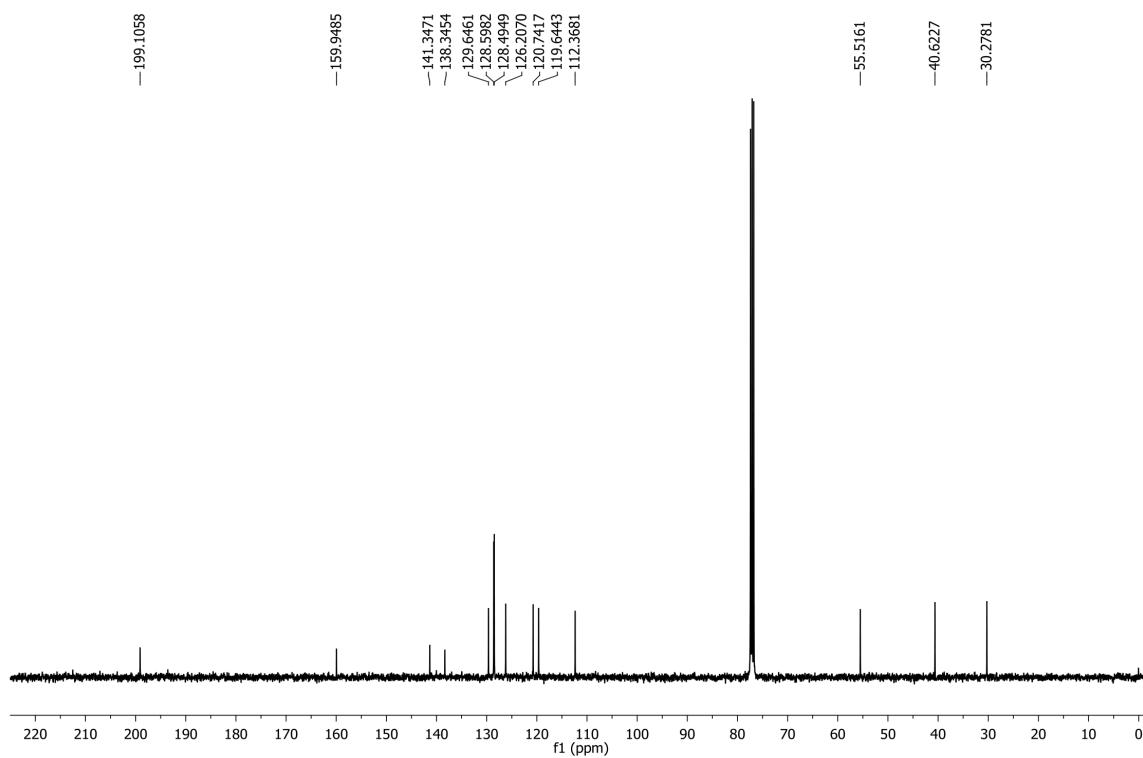
¹³C NMR of 1-(4-isopropylphenyl)-3-phenylpropane-1-one (2e):



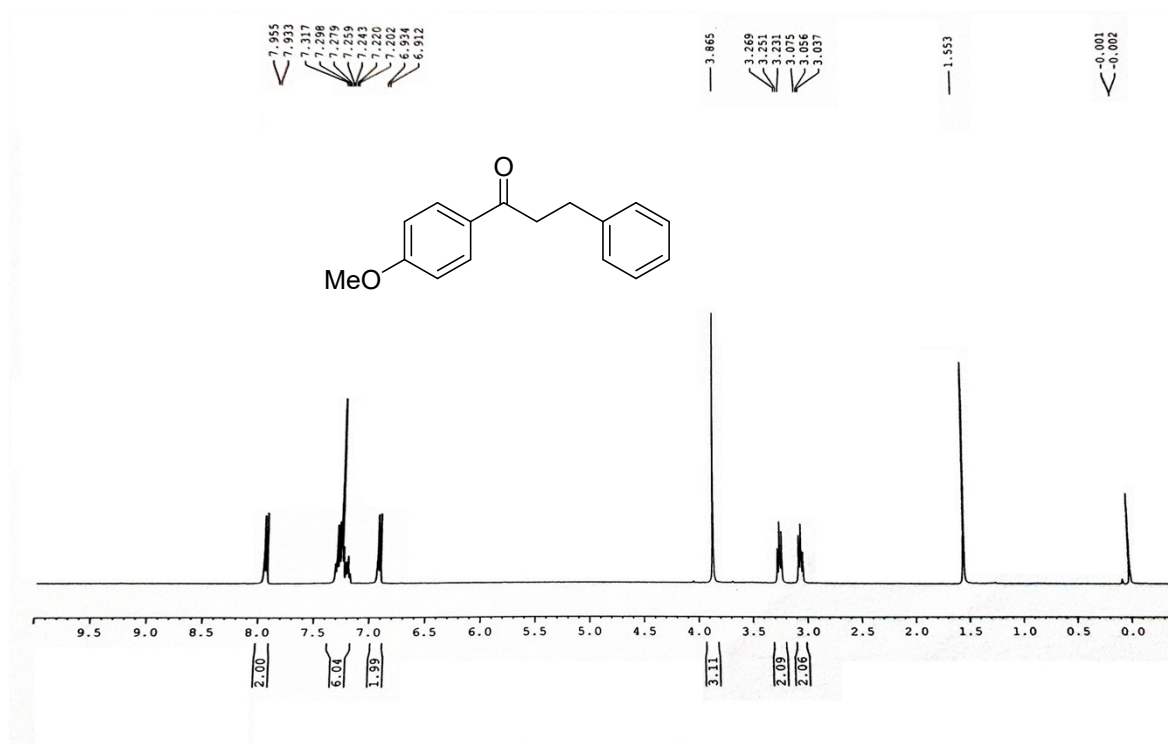
¹H NMR of 1-(3-methoxyphenyl)-3-phenylpropane-1-one (2g):



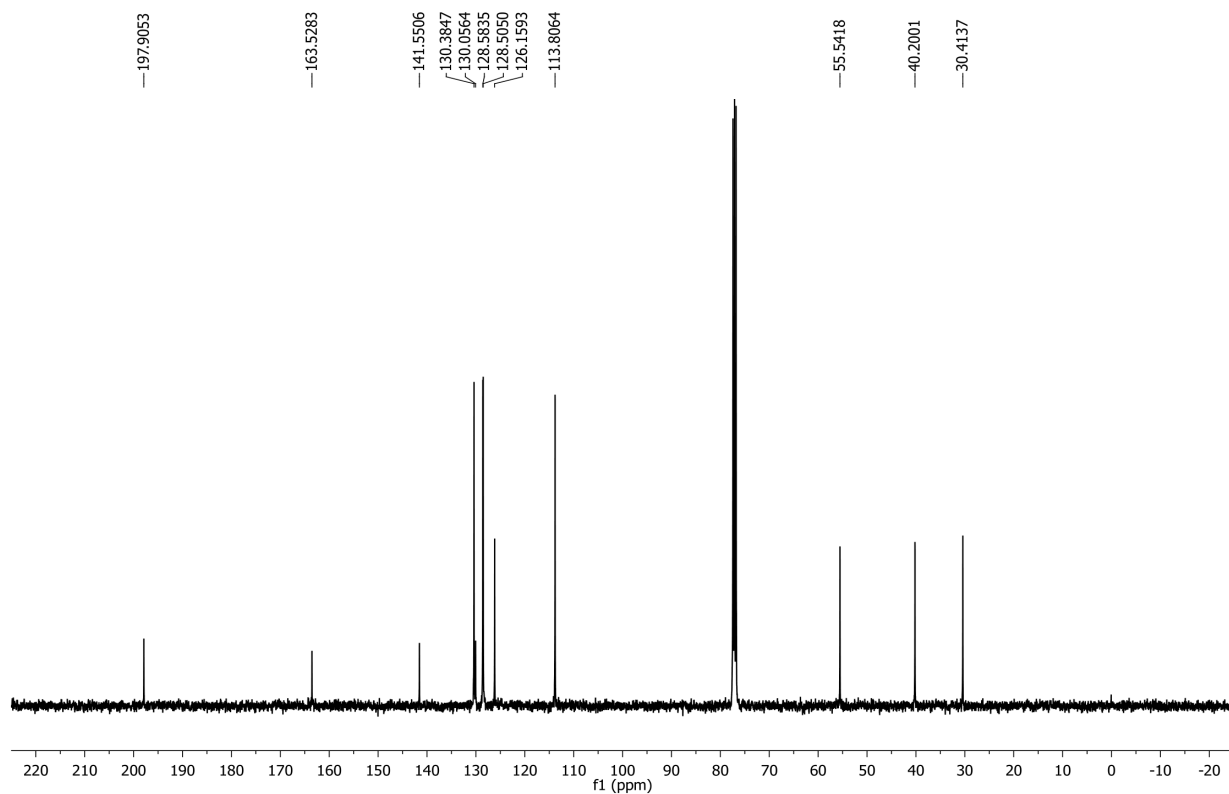
¹³C NMR of 1-(3-methoxyphenyl)-3-phenylpropane-1-one (2g):



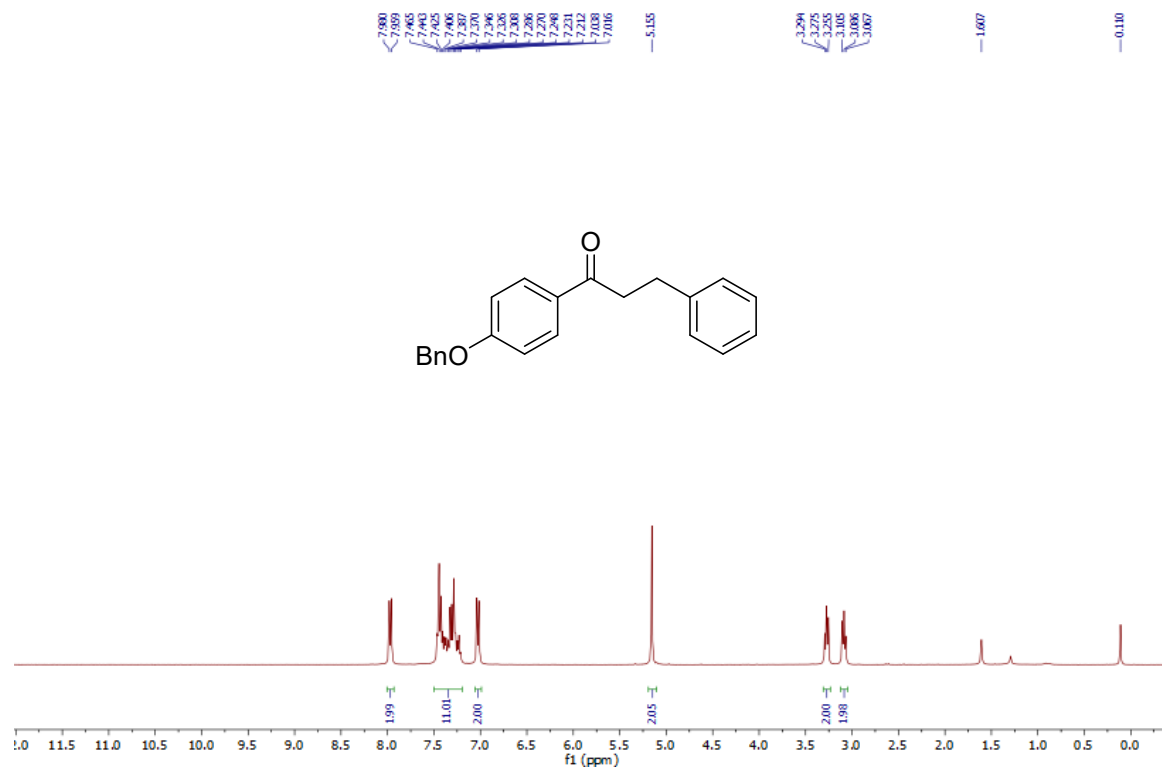
¹H NMR of 1-(4-methoxyphenyl)-3-phenylpropane-1-one (2h):



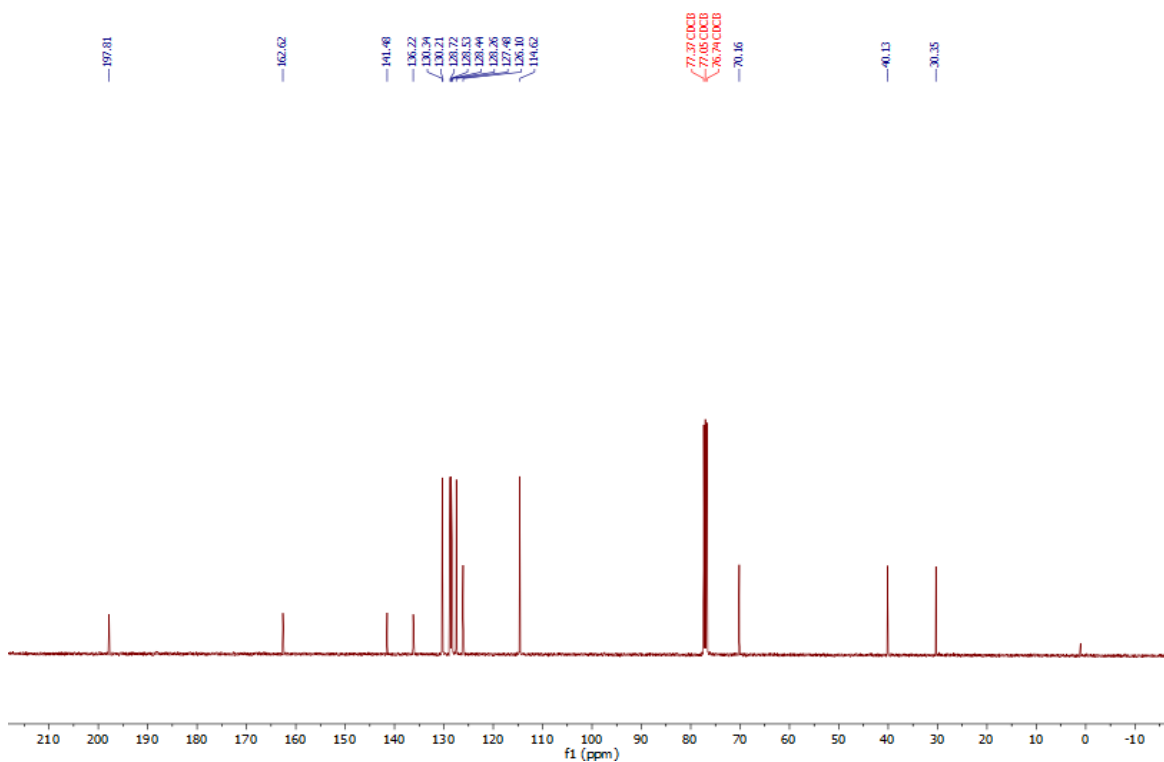
¹³C NMR of 1-(4-methoxyphenyl)-3-phenylpropane-1-one (2h):



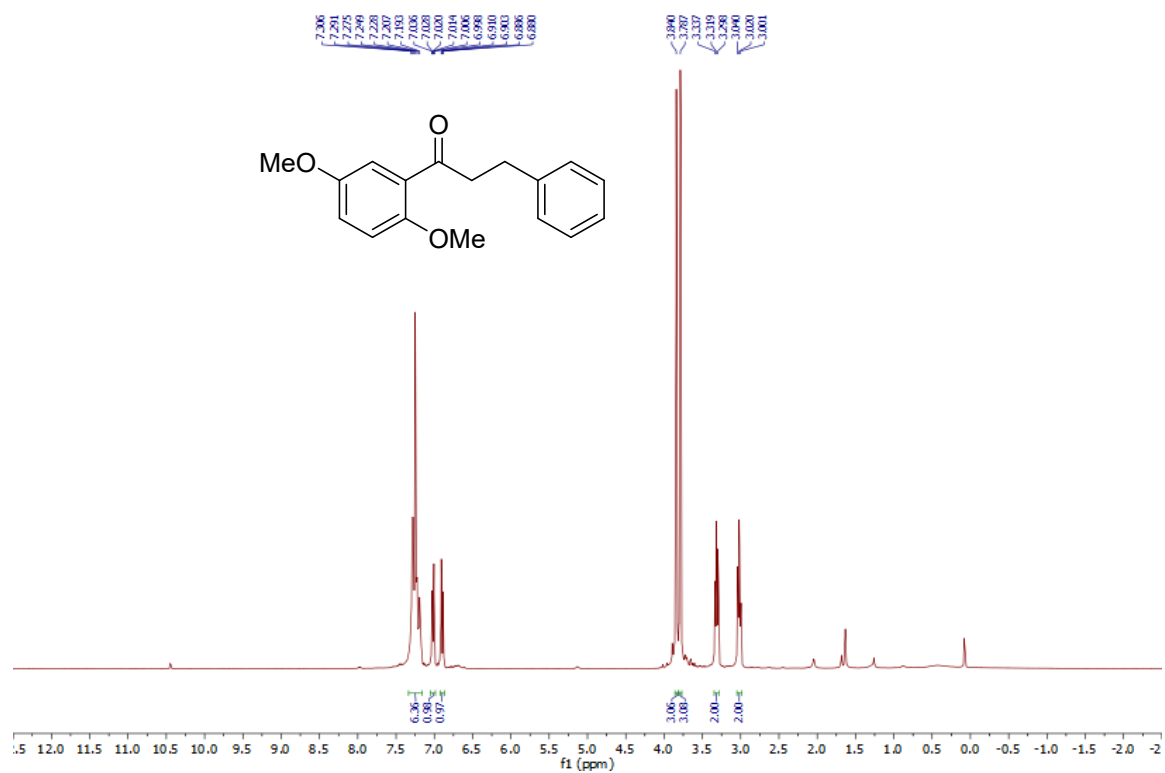
¹H NMR of 1-(4-(benzyloxy)phenyl)-3-phenylpropan-1-one (2i):



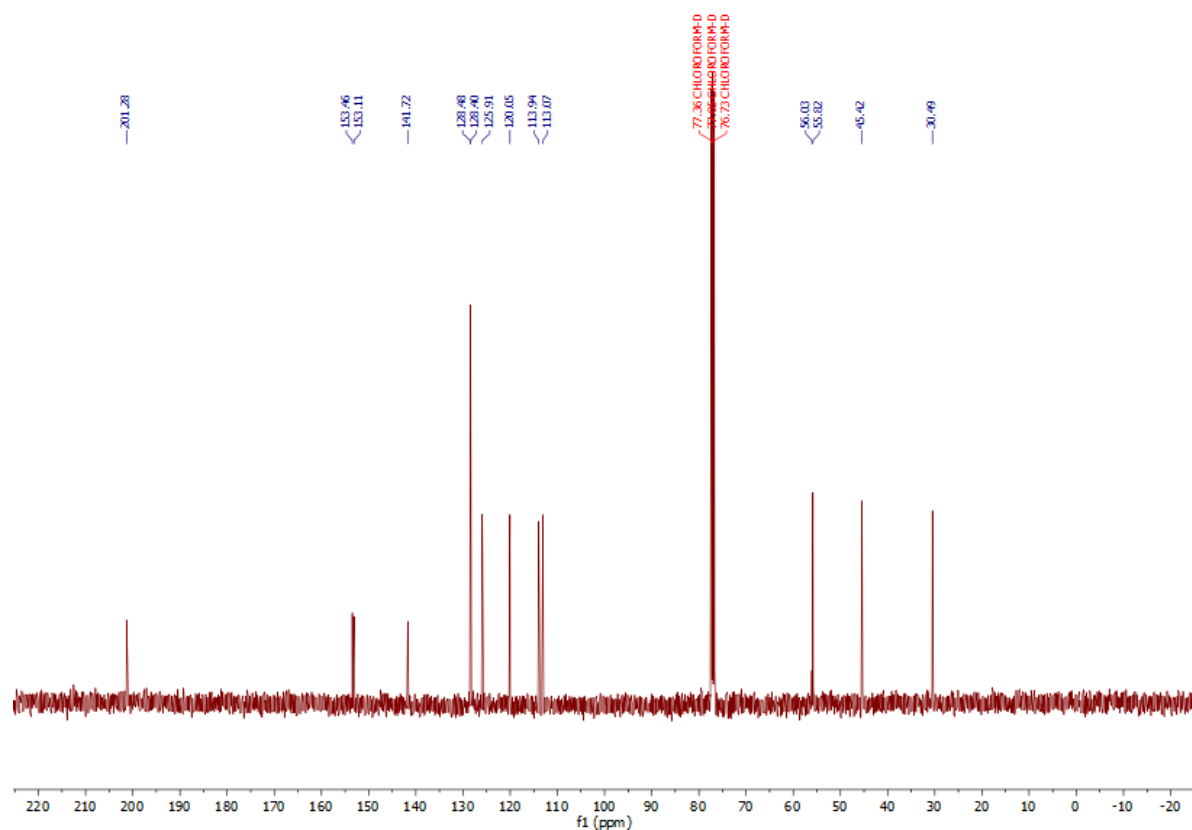
¹³C NMR of 1-(4-(benzyloxy)phenyl)-3-phenylpropan-1-one (2i):



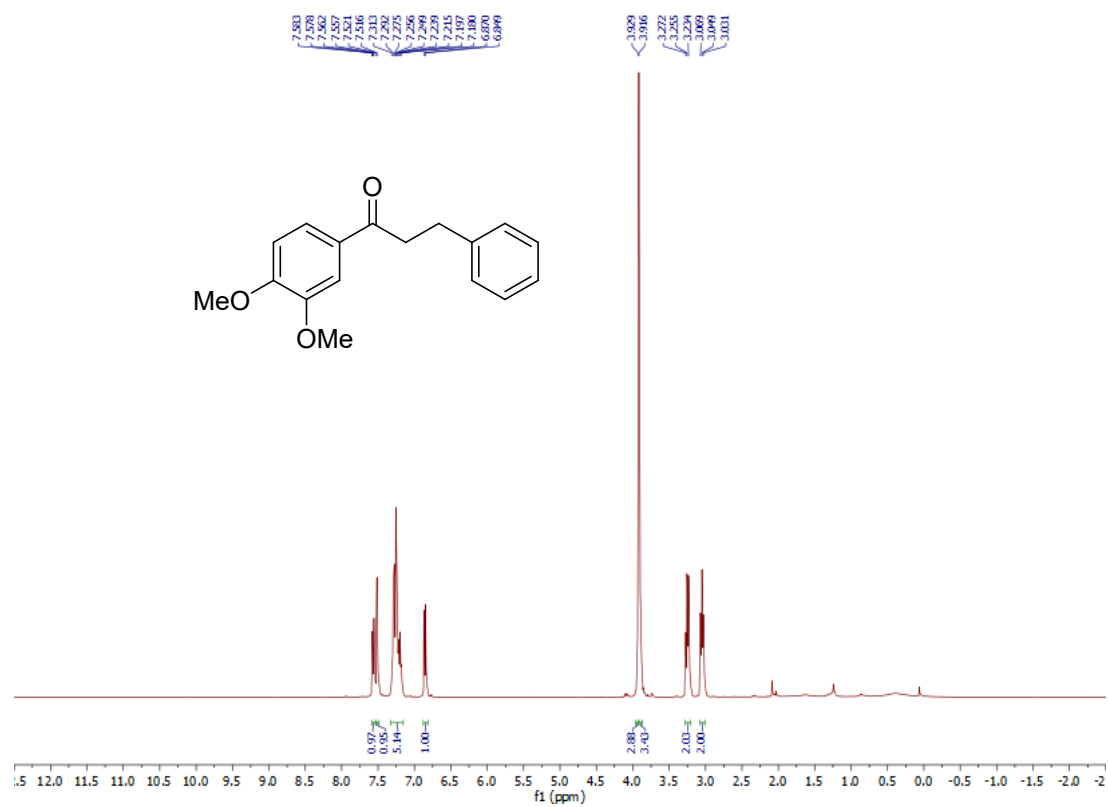
¹H NMR of 1-(2, 5-dimethoxyphenyl)-3-phenylpropane-1-one (2j):



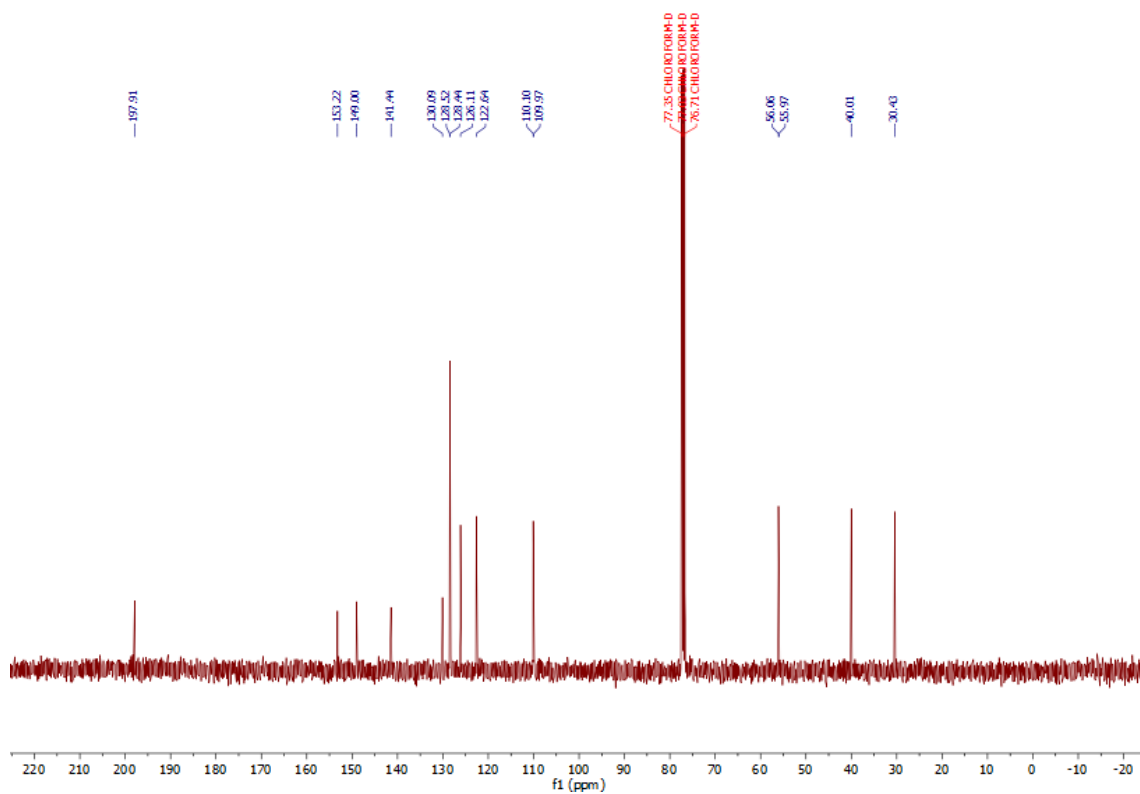
¹³C NMR of 1-(2, 5-dimethoxyphenyl)-3-phenylpropane-1-one (2j):



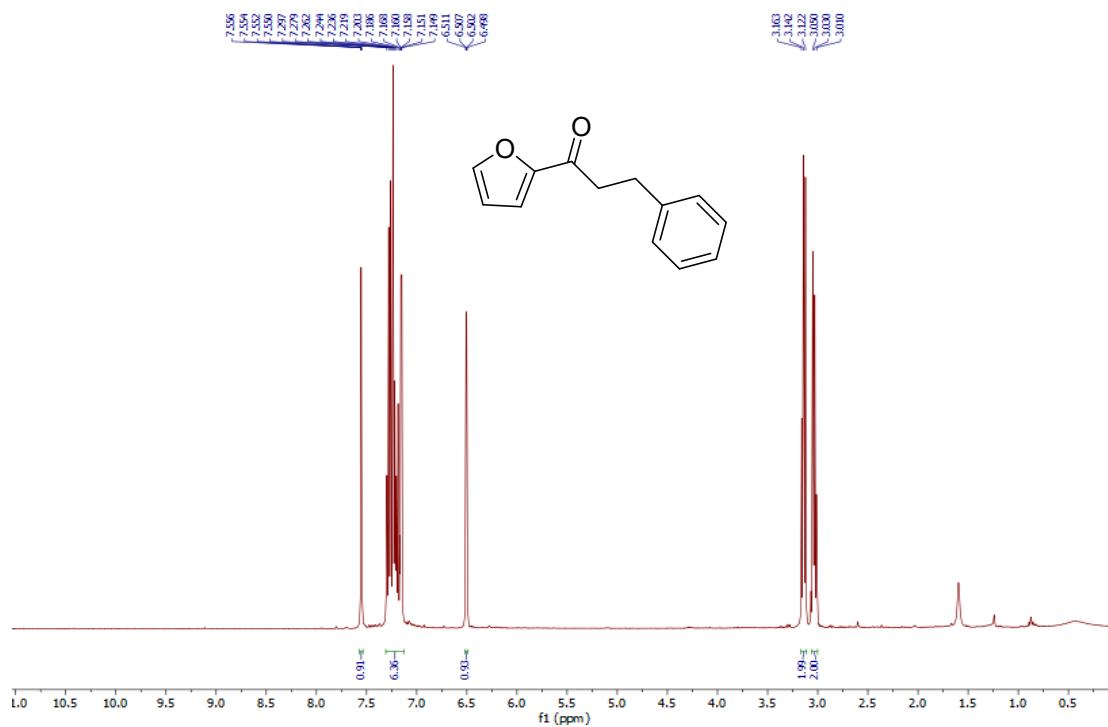
¹H NMR of 1-(3, 4-dimethoxyphenyl)-3-phenylpropane-1-one (2k):



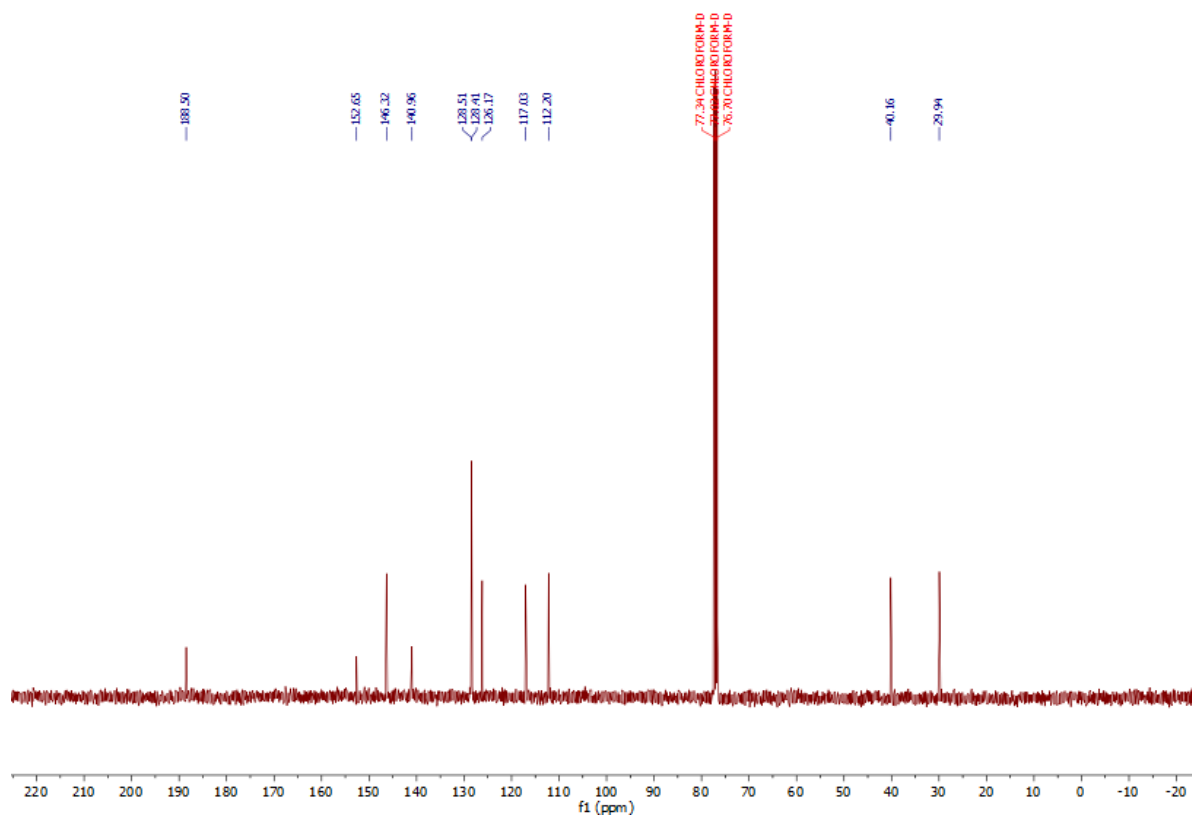
¹³C NMR of 1-(3, 4-dimethoxyphenyl)-3-phenylpropane-1-one (2k):



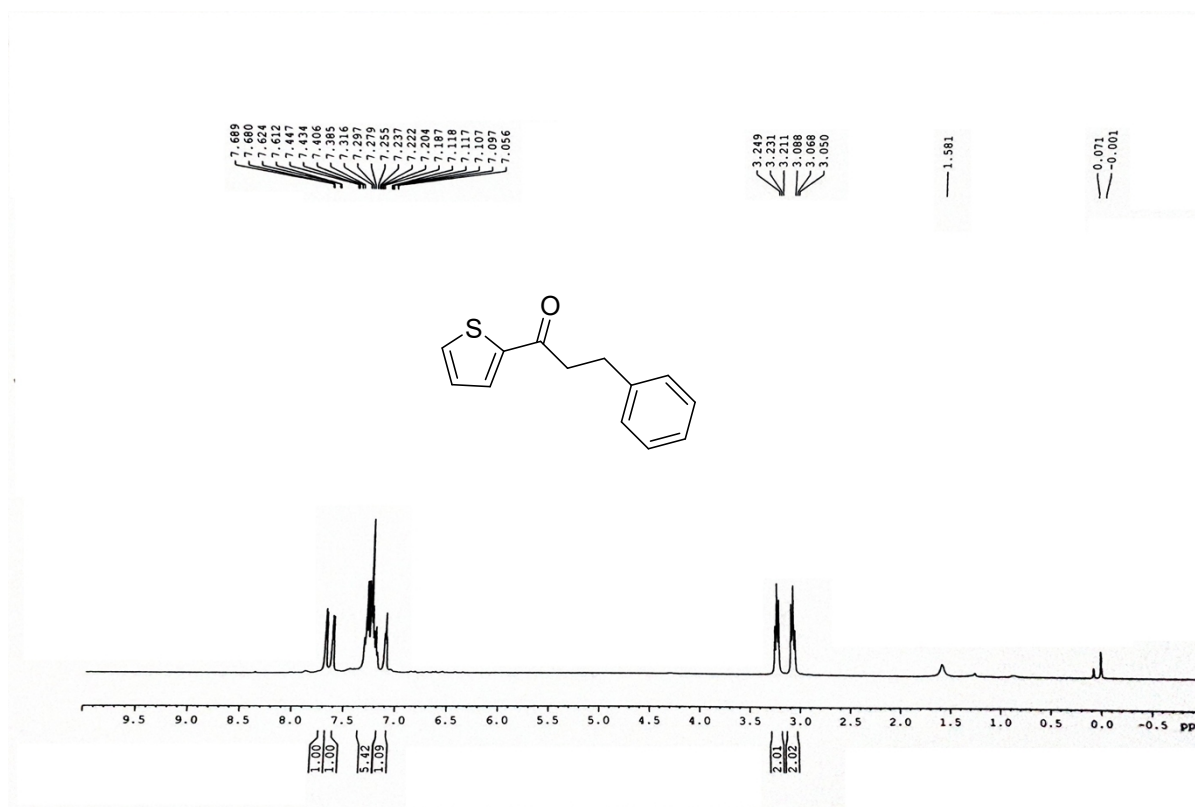
¹H NMR of 1-(furan-2-yl)-3-phenylpropan-1-one (2l):



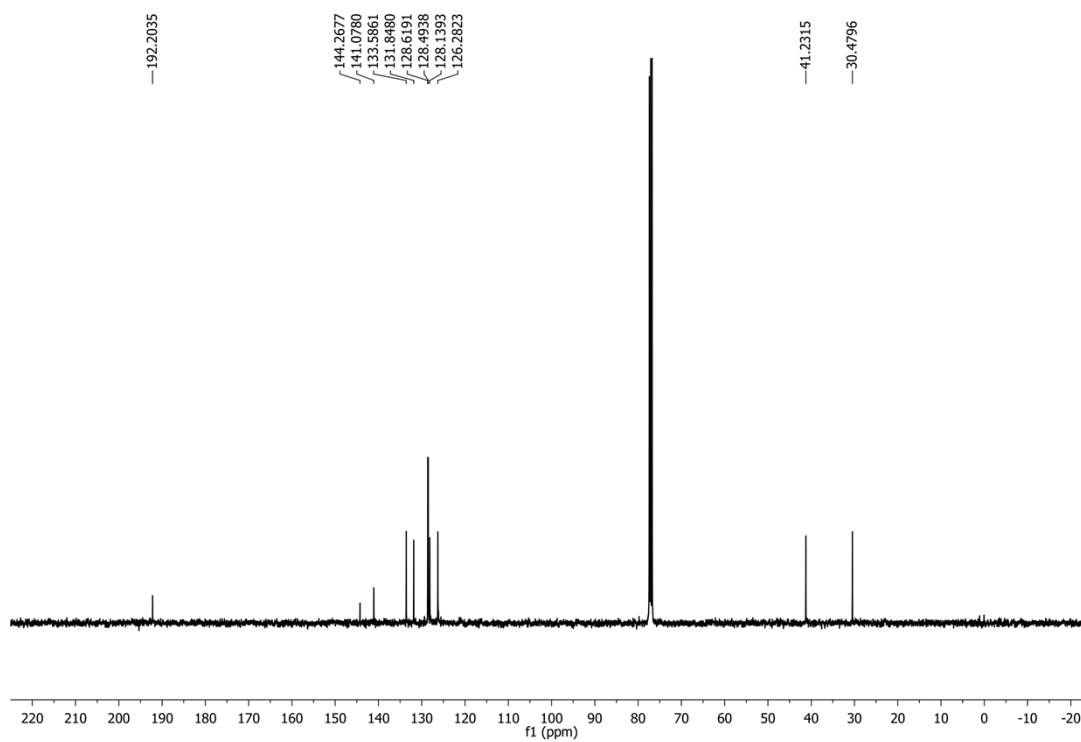
¹³C NMR of 1-(furan-2-yl)-3-phenylpropan-1-one (2l):



¹H NMR of 3-phenyl-1-(thiophen-2-yl) propane-1-one (2m):



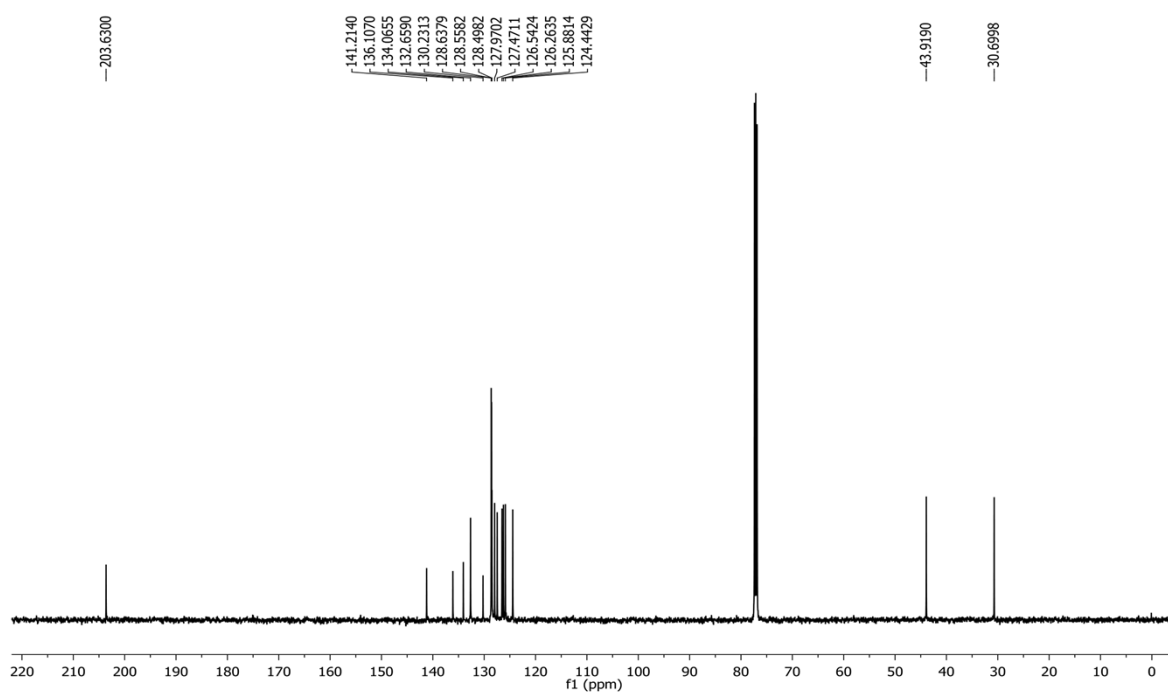
¹³C NMR of 3-phenyl-1-(thiophen-2-yl) propane-1-one (2m):



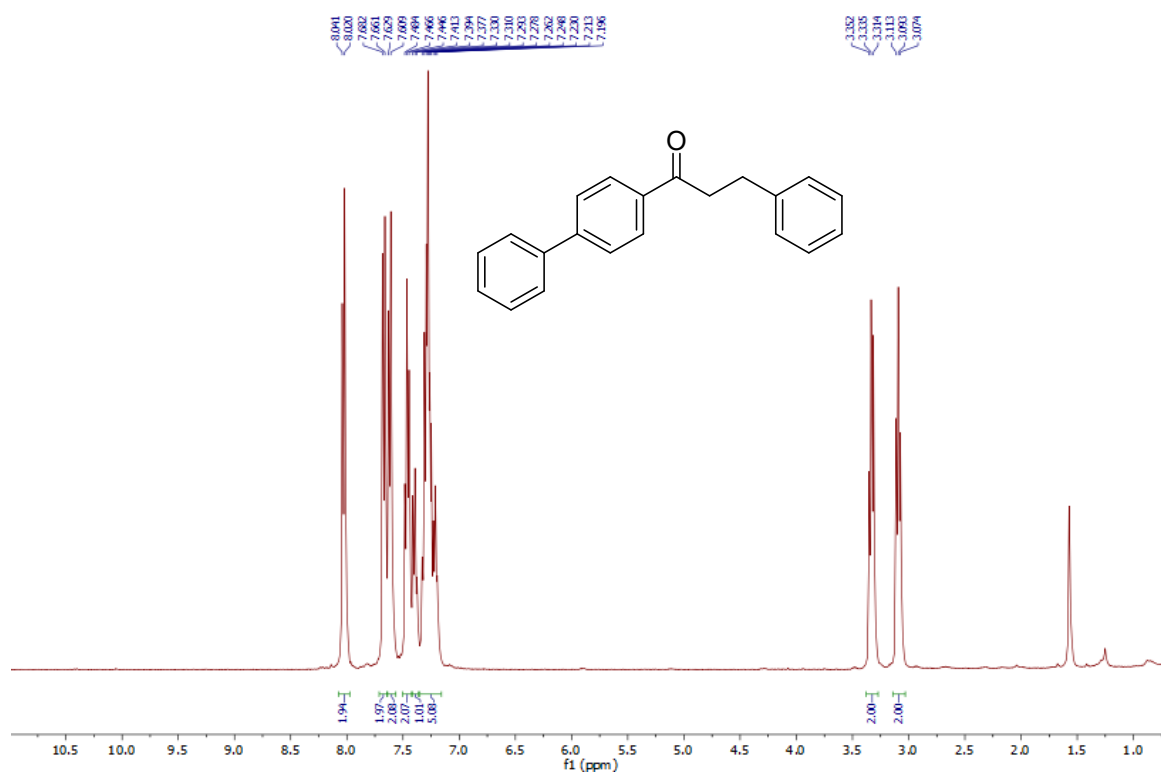
¹H NMR of 1-(naphthalene-1-yl)-3-phenylpropan-1-one (2n):



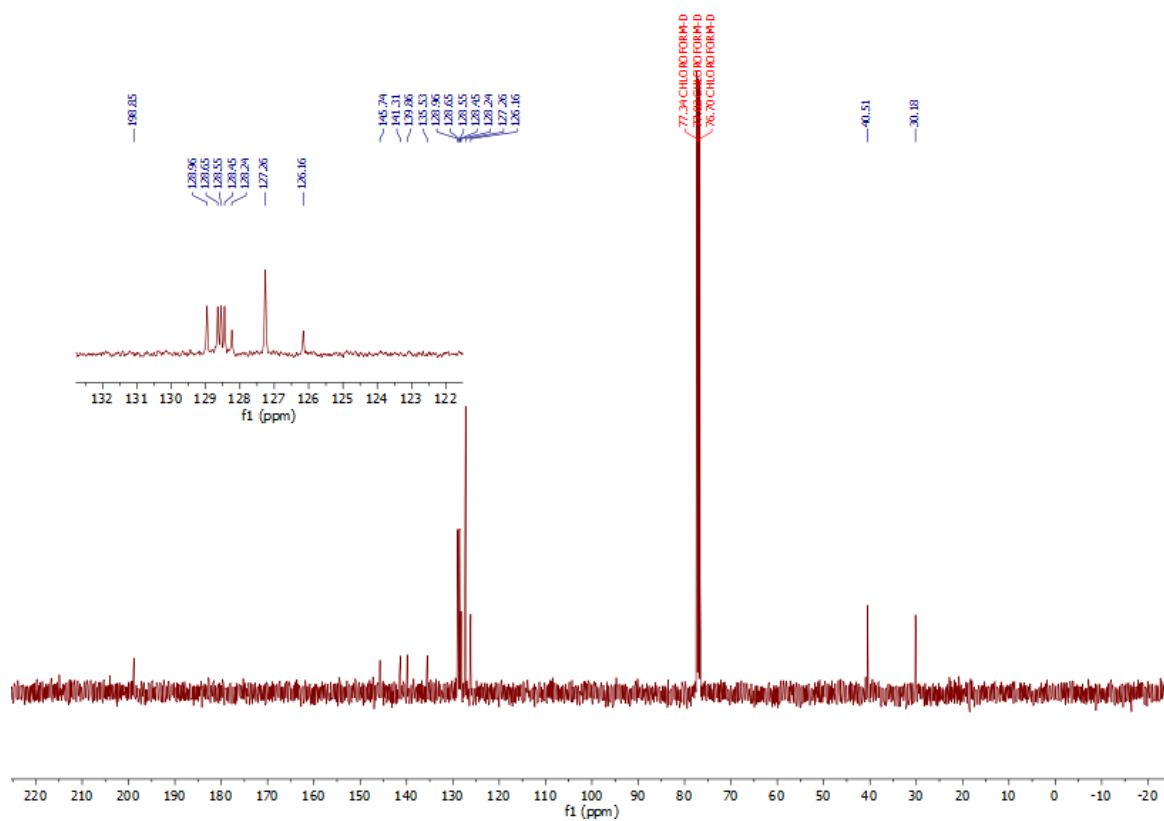
¹³C NMR of 1-(naphthalene-1-yl)-3-phenylpropan-1-one (2n):



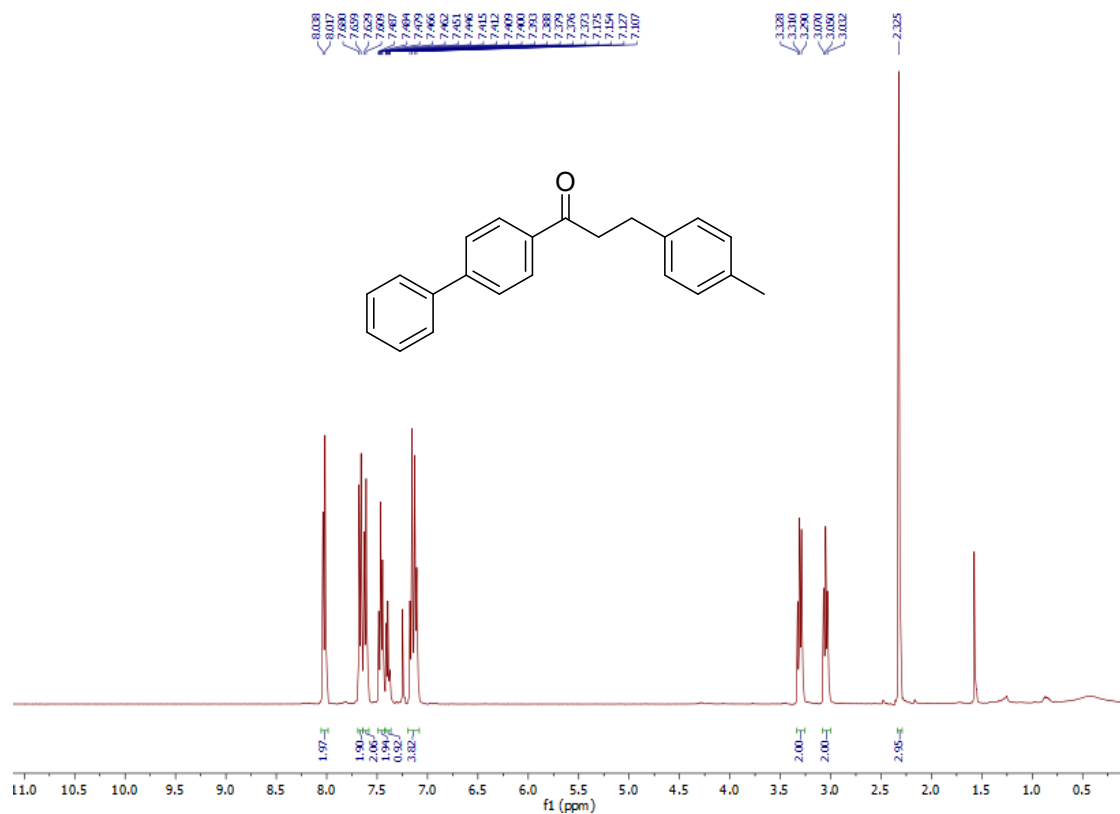
¹H NMR of 1-([1, 1'-biphenyl]-4-yl)-3-phenylpropan-1-one (2o):



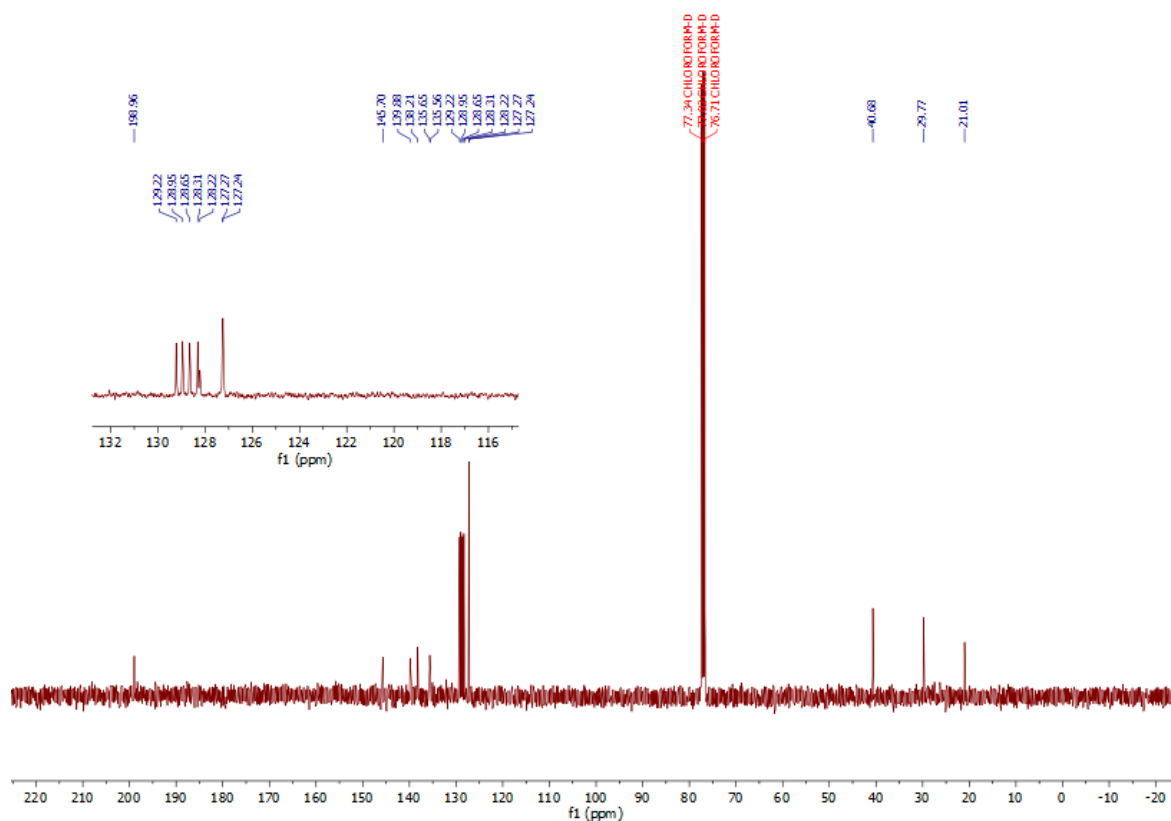
¹³C NMR of 1-([1, 1'-biphenyl]-4-yl)-3-phenylpropan-1-one (2o):



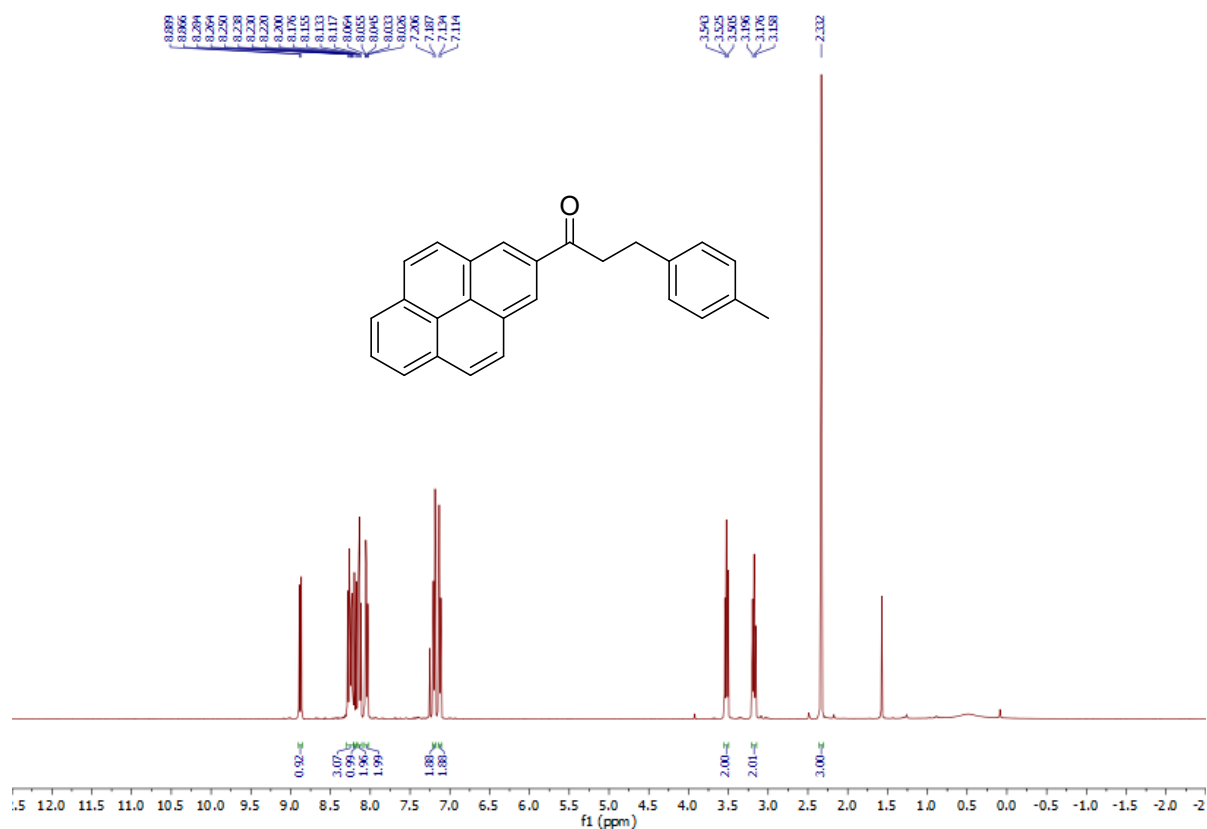
¹H NMR of 1-([1, 1'-biphenyl]-4-yl)-3-(*p*-tolyl) propan-1-one (2q):



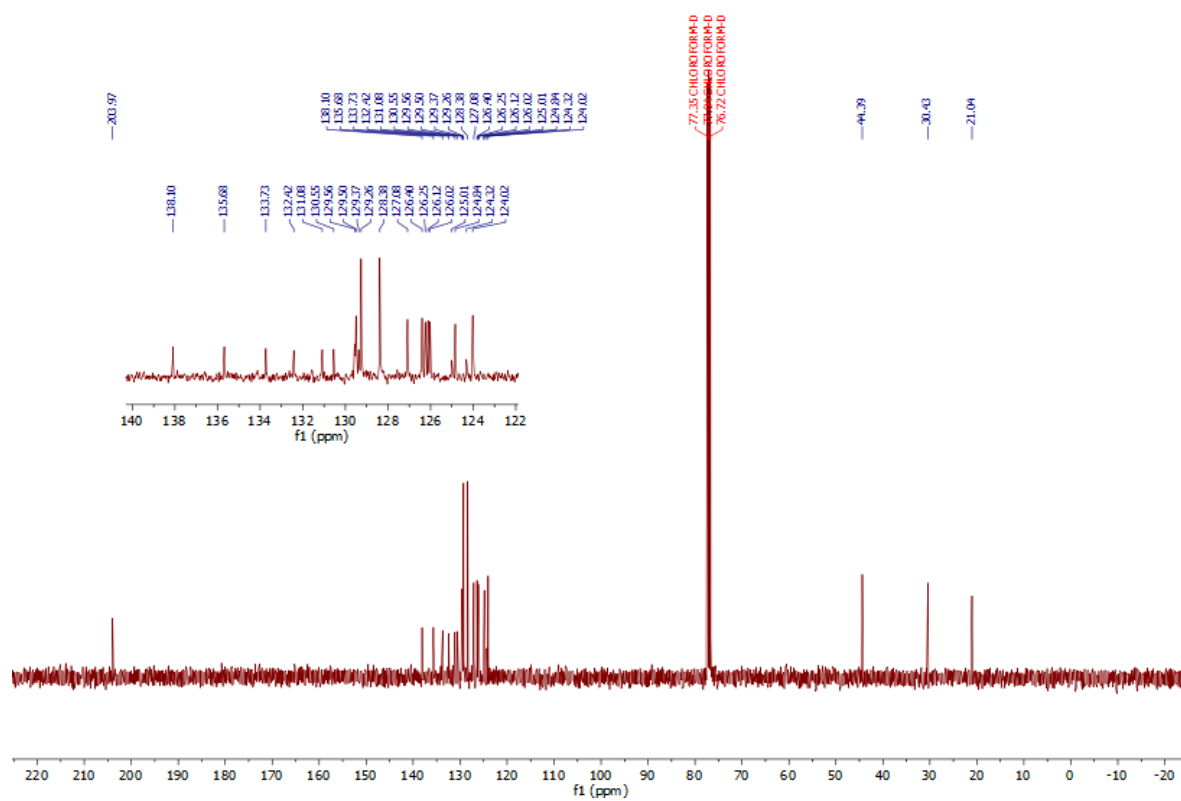
¹³C NMR of 1-([1, 1'-biphenyl]-4-yl)-3-(*p*-tolyl) propan-1-one (2q):



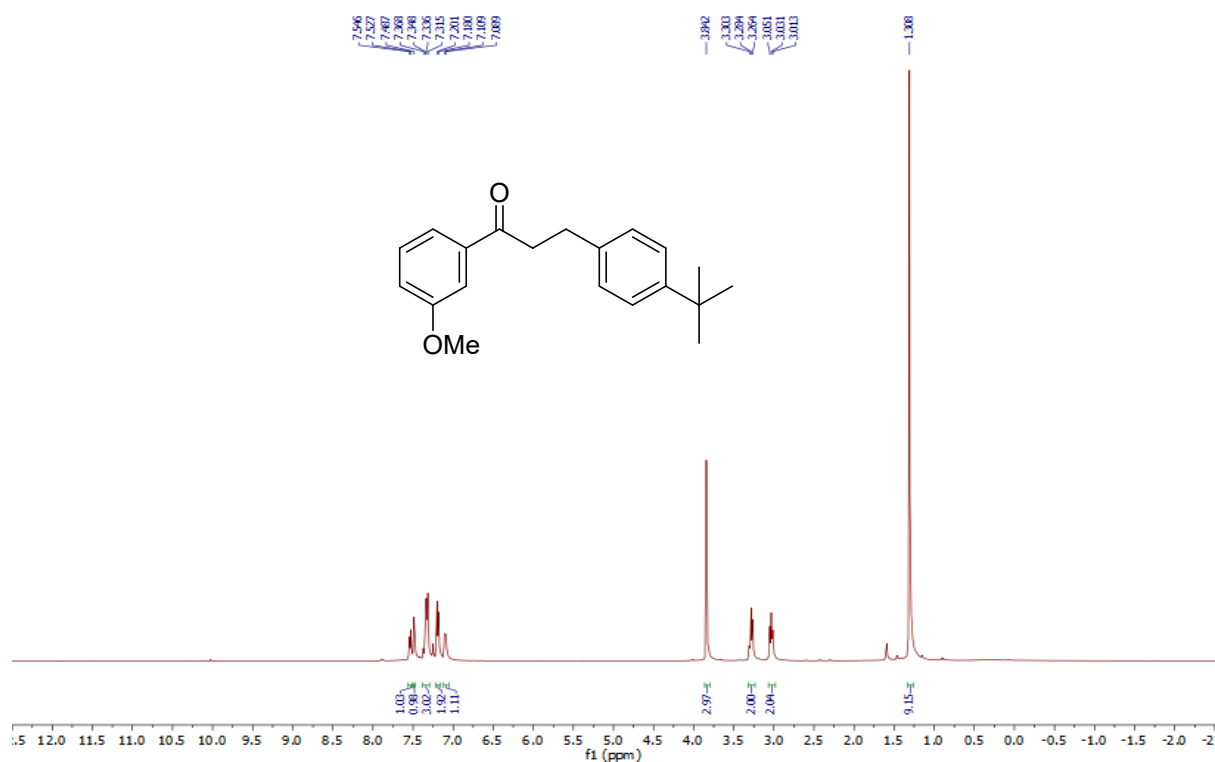
¹H NMR of 1-(pyren-2-yl)-3-(*p*-tolyl) propan-1-one (2r):



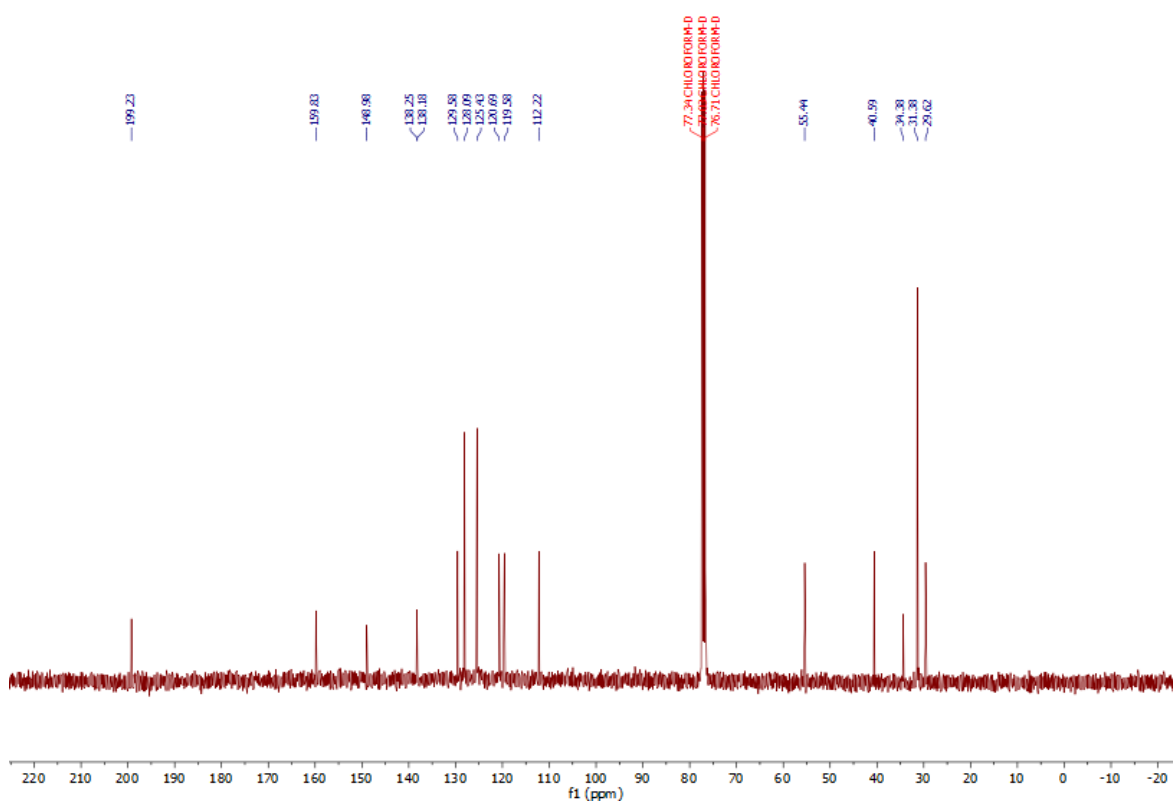
¹³C NMR of 1-(pyren-2-yl)-3-(*p*-tolyl) propan-1-one (2r):



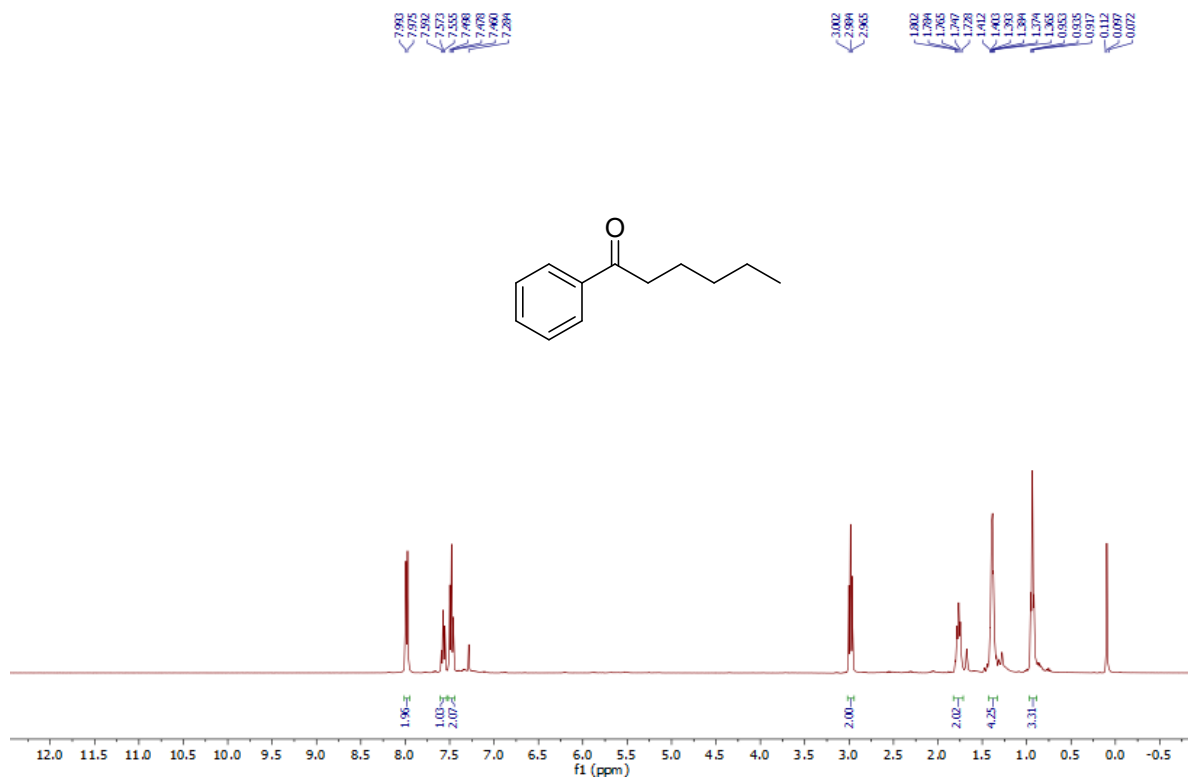
¹H NMR of 3-(4-(tert-butyl) phenyl)-1-(3-methoxyphenyl) propan-1-one (2t):



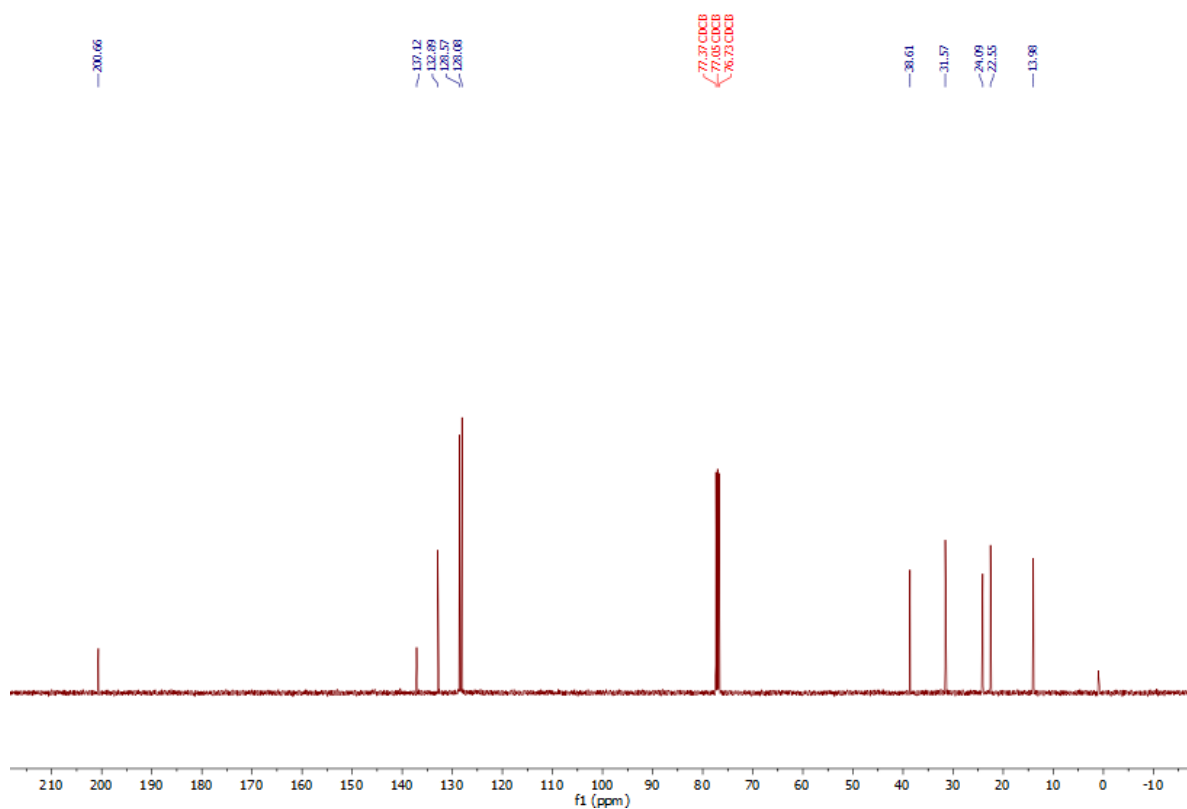
¹³C NMR of 3-(4-(tert-butyl) phenyl)-1-(3-methoxyphenyl) propan-1-one (2t):



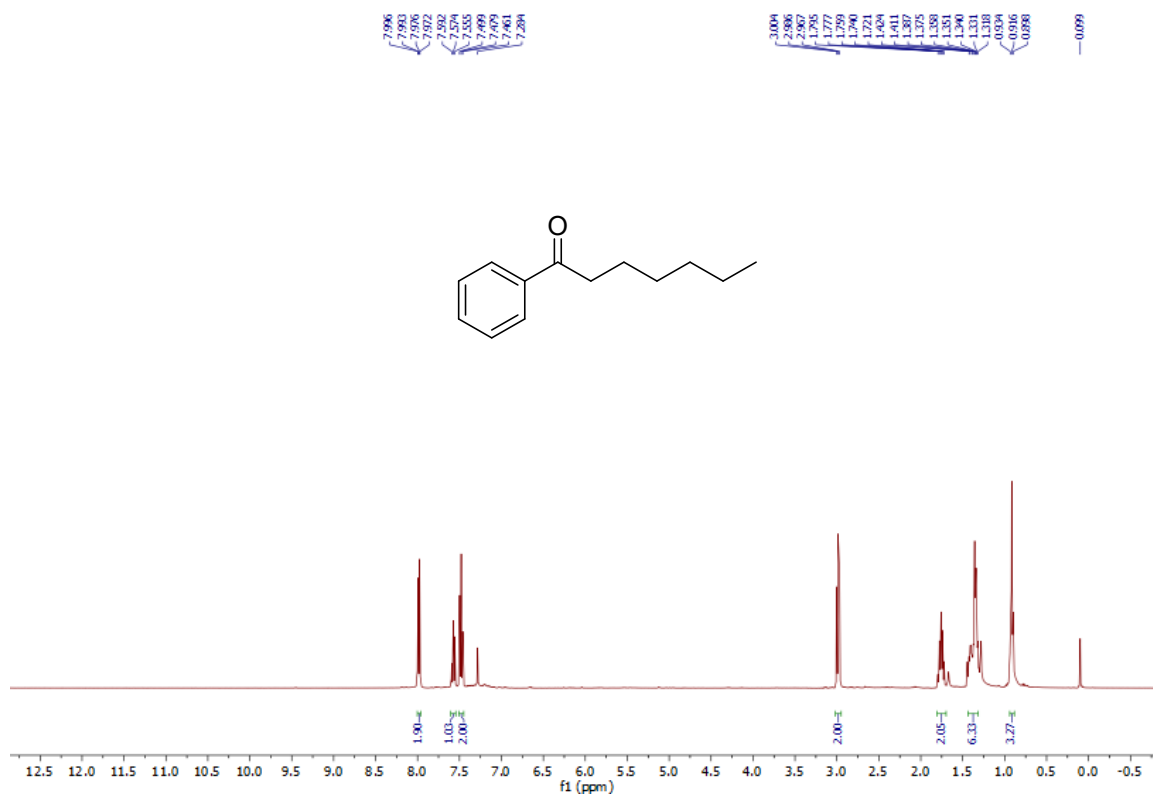
¹H NMR of 1-phenylhexan-1-one (2u):



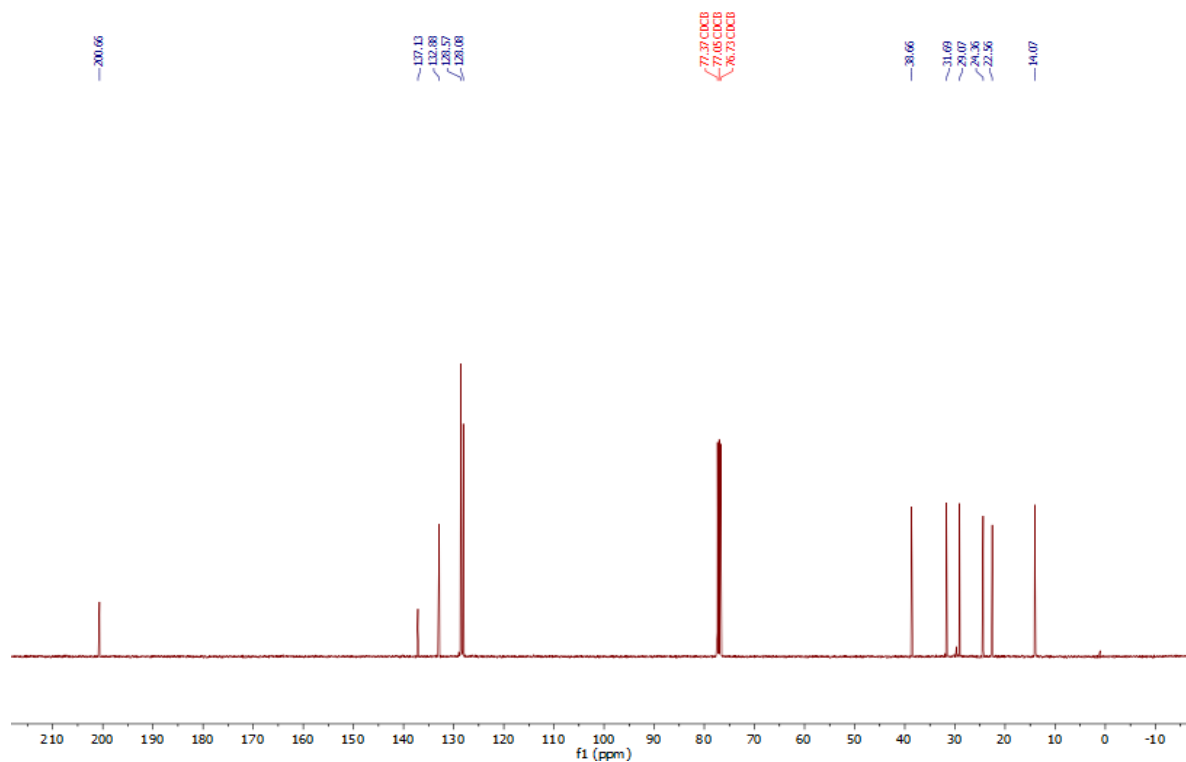
¹³C NMR of 1-phenylhexan-1-one (2u):



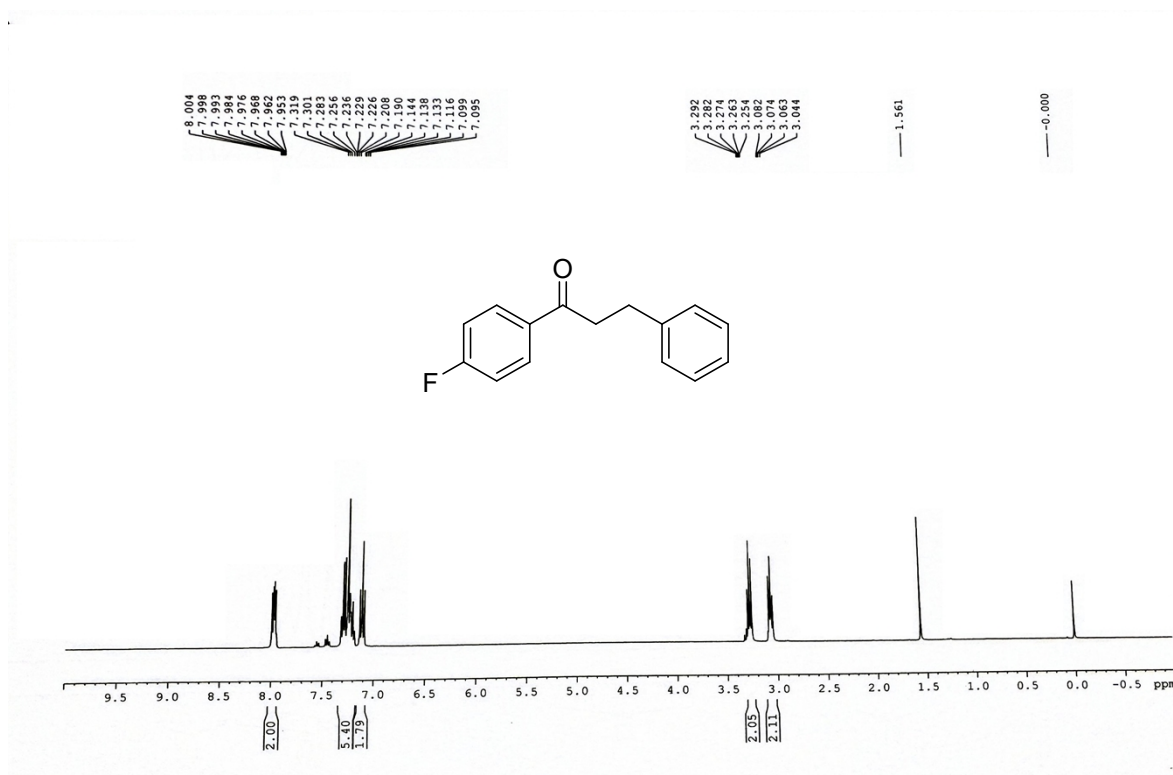
¹H NMR of 1-phenylheptan-1-one (2v):



¹³C NMR of 1-phenylheptan-1-one (2v):



^1H NMR of 1-(4-fluorophenyl)-3-phenylpropane-1-one (2w):



^{13}C NMR of 1-(4-fluorophenyl)-3-phenylpropane-1-one (2w):

