Electronic Supplementary Material (ESI) for Chemical Communications

Synthesis of Arylketones by Ruthenium-Catalyzed Cross- Coupling of Aldehydes with Arylboronic Acids

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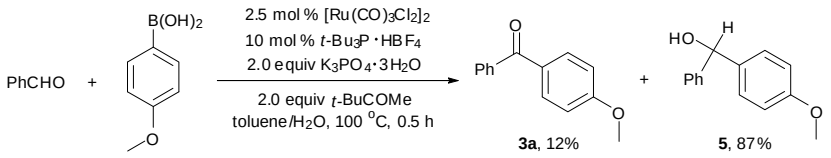
General Information

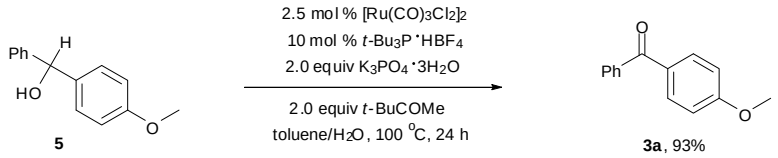
All manipulations were carried out under Argon atmosphere. $[Ru(CO)_3Cl_2]_2$ was purchased form Sigam-Aldrich, tri-tert-butylphosphonium tetrafluoroborate was purchesed from J&K. Column chromatography was generally performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions. The ^1H NMR (400MHz) and ^{13}C NMR (100MHz or 75MHz) data were recorded on Varian 400M or Varian 300M spectrometers using $CDCl_3$ as solvent at room temperature. The chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. ^1H NMR spectra was recorded with tetramethylsilane (δ= 0.00 ppm) as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference. NMR, IR, MS were performed by the State-authorized Analytical Center in Soochow University.

General procedures for products

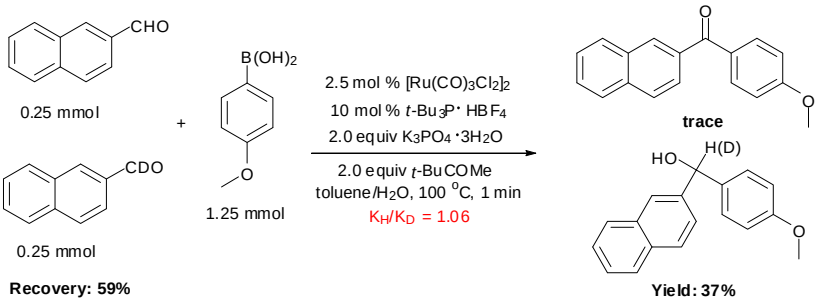
Aldehyde (0.5 mmol, 1 equiv), arylboronic (1.25 mmol, 2.5 equiv), tri-*tert*-butylphosphonium tetrafluoroborate (0.05 mmol, 10 mol %), $[Ru(CO)_3Cl_2]_2$ (0.0125 mmol, 2.5 mol %) and $K_3PO_4{\cdot}3H_2O$ (1.0 mmol, 2.0 equiv) were added to an schlenck tube. Toluene (2.0 mL), pinacolone (1.0 mmol, 2.0 equiv) and water (0.2 mL) were added via syringe. The septum-sealed tube was evacuated and refilled with Ar thrice. The reaction mixture was heated in an oil bath at 100 ^oC for 24 h. After cooling down the reaction mixture to ambient temperature, it was extracted with dichloromethane (2 × 25 mL) and washed with water (2 × 30 mL). The dichloromethane layer was separated and dried over $MgSO_4$. After evaporation of the solvent, the residue was purified by flash column chromatography to give the desired arylketone.


PhCHO
B(OH)2
2.5 mol % [Ru(CO)3Cl2]2
10 mol % t-Bu3P·HBF4
2.0 equiv K3PO4·3H2O
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 0.5 h
3a, 12%
5, 87%

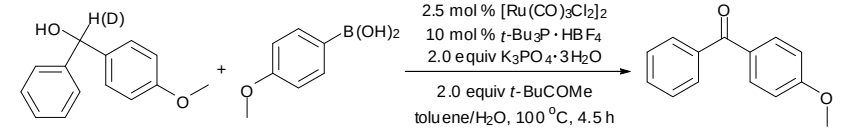
(1)


5
2.5 mol % [Ru(CO)3Cl2]2
10 mol % t-Bu3P·HBF4
2.0 equiv K3PO4·3H2O
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 24 h
3a, 93%

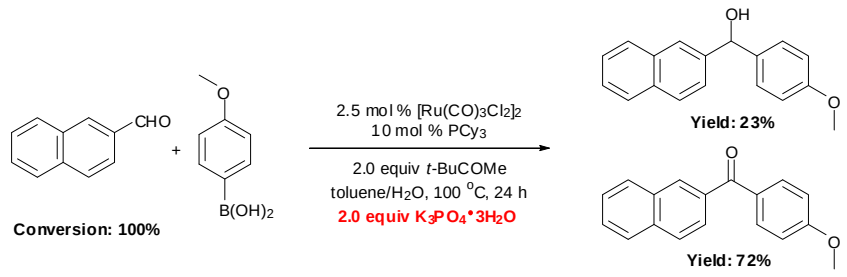
(2)


0.25 mmol
CDO
0.25 mmol
B(OH)2
1.25 mmol
2.5 mol % [Ru(CO)3Cl2]2
10 mol % t-Bu3P·HBF4
2.0 equiv K3PO4·3H2O
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 1 min
KH/KD = 1.06
trace
H(D)
Recovery: 59%
Yield: 37%

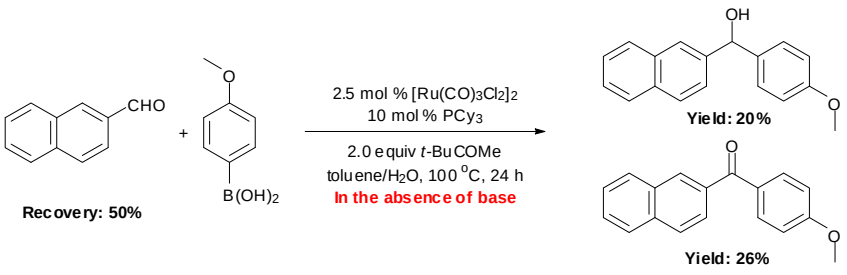
(3)


H(D)
0.25mmol 5 and 0.25mmol D-5
B(OH)2
1.25 mmol
2.5 mol % [Ru(CO)3Cl2]2
10 mol % t-Bu3P·HBF4
2.0 equiv K3PO4·3H2O
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 4.5 h
KH/KD = 3.13
Recovery of mixture of 5 and D-5: 18%
Yield: 78%

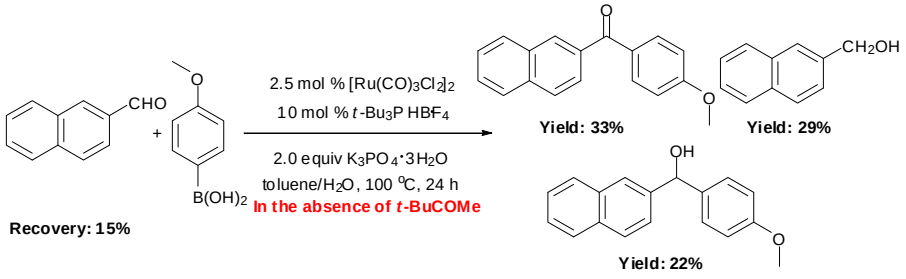
(4)


CHO
B(OH)2
2.5 mol % [Ru(CO)3Cl2]2
10 mol % PCy3
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 24 h
2.0 equiv K3PO4·3H2O
Conversion: 100%
Yield: 23%
Yield: 72%

(5)

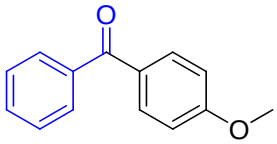

CHO
B(OH)2
2.5 mol % [Ru(CO)3Cl2]2
10 mol % PCy3
2.0 equiv t-BuCOMe
toluene/H2O, 100 °C, 24 h
In the absence of base
Recovery: 50%
Yield: 20%
Yield: 26%

(6)

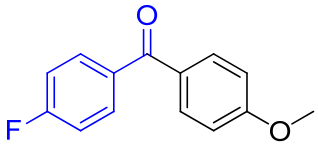

CHO
B(OH)2
2.5 mol % [Ru(CO)3Cl2]2
10 mol % t-Bu3P·HBF4
2.0 equiv K3PO4·3H2O
toluene/H2O, 100 °C, 24 h
In the absence of t-BuCOMe
Recovery: 15%
Yield: 33%
CH2OH
Yield: 29%
Yield: 22%

(7)

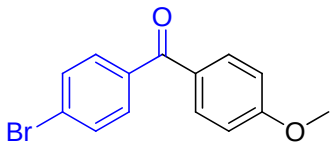
Compound characterizations:



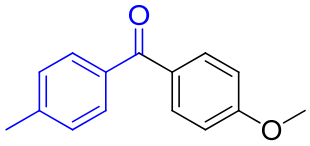
(4-methoxyphenyl)(phenyl)methanone (3a) [1]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.83 (d, J = 8.8 Hz, 2H), 7.75 (d, J = 7.5 Hz, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.5 Hz, 2H), 6.96 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.5, 163.1, 138.2, 132.5, 131.8, 130.0, 129.6, 128.1, 113.5, 55.4; MS ($C_{14}H_{12}O_2$): 212; IR (KBr, cm^{-1}): ν 1650.



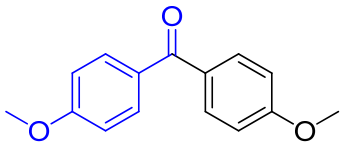
(4-fluorophenyl)(4-methoxyphenyl)methanone (3b) [2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.81-7.77 (m, 4H), 7.16-7.12 (m, 2H), 6.96 (d, J=8.8, 2H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 194.0, 166.2, 163.7, 163.1, 134.3, 134.3, 132.3, 132.2, 132.1, 129.8, 115.3, 115.1 113.5, 55.4; MS ($C_{14}H_{11}FO_2$): 230; IR (KBr, cm^{-1}): ν 1641.



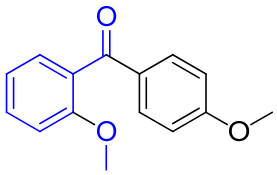
(4-bromophenyl)(4-methoxyphenyl)methanone (3c) [1]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.79 (d, J=8.5, 1H), 7.62 (s, 1H), 6.96 (d, J=8.5, 1H), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 194.3, 163.3, 136.9, 132.4, 131.4, 131.2, 129.6, 126.8, 113.6, 55.5; MS ($C_{14}H_{11}BrO_2$): 290, 294; IR (KBr, cm^{-1}): ν 1639.



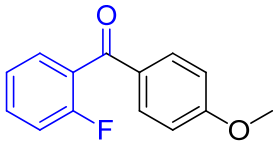
(4-methoxyphenyl)(p-tolyl)methanone (3d) [1]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.83 (d, J=8.8, 2H), 7.70 (d, J=8.0, 2H), 7.29 (d, J=8.0, 2H), 6.97 (d, J=8.8, 2H), 3.89 (s, 3H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.2, 162.9, 142.5, 135.4, 132.3, 130.3, 129.9, 128.8, 113.4, 55.4, 21.5; MS ($C_{15}H_{12}O_2$): 226; IR (KBr, cm^{-1}): ν 1645.



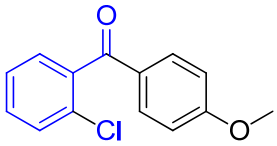
bis(4-methoxyphenyl)methanone (3e) [1]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.78 (d, J=8.9, 4H), 6.96 (d, J=8.9, 4H), 3.87 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 194.4, 162.7, 132.1, 130.6, 113.4, 55.4; MS ($C_{15}H_{14}O_3$): 242; IR (KBr, cm^{-1}): ν 1635.



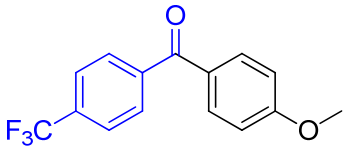
(2-methoxyphenyl)(4-methoxyphenyl)methanone (3f) [1]. ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.81 (d, J=8.9, 2H), 7.46-7.42 (m, 1H), 7.32-7.30 (m, 1H), 7.04-6.97 (m, 2H), 6.90 (d, J=8.9, 2H), 3.85 (s, 3H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$, 100MHz): δ = 195.0, 163.4, 156.8, 132.1, 131.3, 130.5, 129.1, 129.0, 120.3, 113.4, 111.2, 55.5, 55.3; MS ($C_{15}H_{14}O_3$): 242; IR (KBr, cm^{-1}): ν 1655.



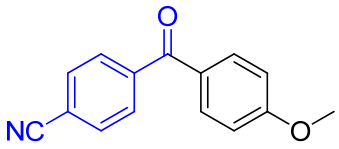
(2-fluorophenyl)(4-methoxyphenyl)methanone (3g)[3]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.83 (d, J=8.8, 2H), 7.53 – 7.46 (m, 2H), 7.25 (t, J=7.6, 1H), 7.14 (t, J=9.0, 1H), 6.94 (d, J=8.8, 2H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 191.9, 163.9, 161.3, 158.0, 132.5, 132.4, 132.2, 130.4, 130.35, 130.1, 127.5, 127.3, 124.2, 124.1, 116.2, 115.9, 113.7, 55.5; MS ($C_{14}H_{11}FO_2$): 230; IR (KBr, cm^{-1}): ν 1655.



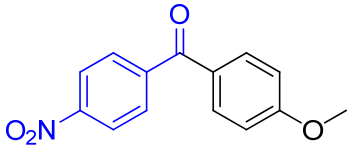
(2-chlorophenyl)(4-methoxyphenyl)methanone (3h)[4]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.80 (d, J=8.8, 2H), 7.72 (s, 1H), 7.61 (d, J=7.7, 1H), 7.54-7.50 (m, 1H), 7.40 (t, J=7.7, 1H), 6.97 (d, J=8.8, 2H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 193.9, 163.4, 139.9, 134.3, 132.5, 131.7, 129.5, 129.4, 127.7, 113.6, 55.5; MS ($C_{14}H_{11}ClO_2$): 246, 248; IR (KBr, cm^{-1}): ν 1650.



(4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methanone (3i)[1]**.** ^{1}HNMR ($CDCl_3$, 300 MHz): δ = 7.85-7.81 (m, 4H), 7.74 (d, J=8.1, 2H), 6.98 (d, J=8.8, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 75MHz): δ = 194.2 163.7, 141.4, 133.4, 132.9, 132.6, 129.7, 129.25, 125.5, 125.2, 125.16, 121.9, 113.7, 55.5; MS ($C_{15}H_{11}F_3O_2$): 280; IR (KBr, cm^{-1}): ν 1641.

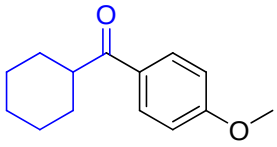


4-(4-methoxybenzoyl)benzonitrile (3j)[5]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.84-7.77 (m, 6H), 6.99 (d, J=8.8, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz):δ = 193.7, 163.8, 142.0, 132.6, 132.1, 129.9, 128.9, 118.1, 115.1, 113.9, 55.57; MS ($C_{15}H_{11}NO_2$): 237; IR (KBr, cm^{-1}): ν 2232, 1642.

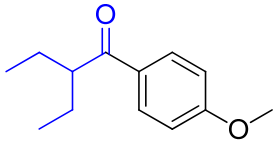


(4-methoxyphenyl)(4-nitrophenyl)methanone (3k)[1]**.** ^{1}HNMR ($CDCl_3$, 400MHz): δ = 8.33 (d, J=8.3, 2H), 7.88 (d, J=8.3, 2H), 7.81 (d, J=8.5, 2H), 7.00 (d, J=8.5, 2H), 3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 193.4, 163.9, 149.4, 143.7,

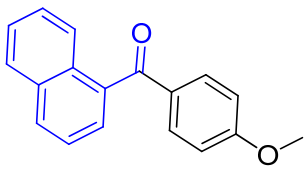
132.6, 130.3, 128.8, 123.4, 113.9, 55.6; MS ($C_{14}H_{11}NO_4$): 257; IR (KBr, cm^{-1}): ν 1641.



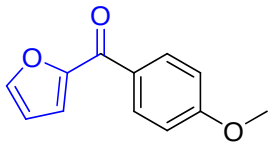
cyclohexyl(4-methoxyphenyl)methanone (3l) [6]. ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.94 (d, J=8.8, 2H), 6.93 (d, J=8.8, 2H), 3.86 (s, 3H), 3.28 – 3.16 (m, 1H), 1.90 – 1.81 (m, 4H), 1.73 (d, J=12.3, 1H), 1.56 – 1.20 (m, 5H).; ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 202.4, 163.1, 130.4, 129.2, 113.6, 55.4, 45.2, 29.5, 25.9, 25.85; MS ($C_{14}H_{18}O_2$): 218; IR (KBr, cm^{-1}): ν 2927, 2852, 1660.



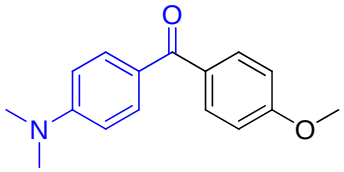
2-ethyl-1-(4-methoxyphenyl)butan-1-one (3m) [7]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.97 (d, *J*=8.1, 2H), 6.94 (d, *J*=8.1, 2H), 3.85 (s, 3H), 3.30-3.23 (m, 1H), 1.83 – 1.71 (m, 2H), 1.78-1.52 (m, 2H), 0.86 (t, *J*=7.6, 6H).^{13}C NMR ($CDCl_3$, 100 MHz):δ = 200.8, 163.2, 130.7, 130.2, 113.5, 55.2, 48.5, 24.9, 11.8; MS ($C_{15}H_{11}NO_2$): 206; IR (KBr, cm^{-1}): ν 2964,2934,2876,1672.



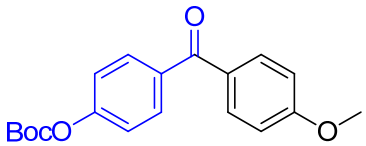
(4-methoxyphenyl)(naphthalen-1-yl)methanone (3n)[8]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.99 (t, J=8.2, 2H), 7.91 (d, J=8.0, 1H), 7.85 (d, J=8.2, 2H), 7.57 – 7.44 (m, 4H), 6.92 (d, J=8.6, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 196.5, 163.6, 136.8, 133.5, 132.6, 130.9, 130.7, 130.5, 128.2, 126.9, 126.7, 126.2, 125.5, 124.3, 113.5, 55.3; MS ($C_{18}H_{14}O_2$): 262; IR (KBr, cm^{-1}): ν 1651.



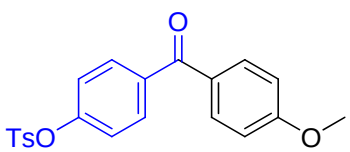
furan-2-yl(4-methoxyphenyl)methanone (3o) [9]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 8.03 (d, J=8.9, 2H), 7.68 (d, J=0.7, 1H), 7.22 (d, J=3.5, 1H), 6.98 (d, J=8.9, 2H), 6.59-6.57 (m, 1H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 181.0, 163.2, 152.5, 146.5, 131.6, 129.7, 119.6, 113.6, 112.0, 55.4; MS ($C_{12}H_{10}O_3$): 202; IR (KBr, cm^{-1}): ν 2924, 1633.



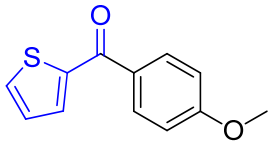
(4-(dimethylamino)phenyl)(4-methoxyphenyl)methanone (3p)[10]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.77-7.74 (m, 4H), 6.93 (d, J=8.8, 2H), 6.65 (d, J=8.8, 2H), 3.84 (s, 3H), 3.02 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 193.9, 162.0, 152.8, 132.3, 131.7, 131.4, 124.9, 113.1, 110.3, 55.2, 39.8; MS ($C_{16}H_{17}NO_2$): 255; IR (KBr, cm^{-1}): ν 1630.



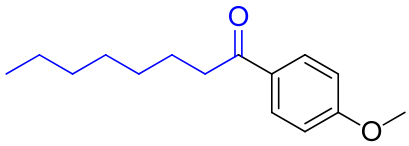
3'-methyl-2'-(1H-pyrazol-1-yl)biphenyl-4-carbaldehyde (3q). ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.81 (d, J=3.8, 2H), 7.79 (d, J=3.5, 2H), 7.29 (d, J=8.6, 2H), 6.95 (d, J=8.8, 2H), 3.86 (s, 3H), 1.58 (s, 9H).; ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 194.1, 163.1, 153.6, 151.1, 135.4, 132.3, 131.1, 129.8, 120.9, 113.4, 83.9, 55.3, 27.5; HRMS: Anal. Calcd. For $C_{19}H_{20}O_5$: 328.1311, Found: 328.1301; IR (KBr, cm^{-1}): ν 1757, 1655.



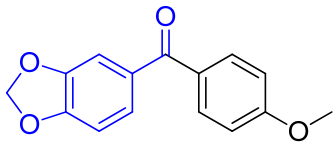
4-(4-methoxybenzoyl)phenyl 4-methylbenzenesulfonate (3r). ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.81 – 7.68 (m, 6H), 7.34 (d, J=8.1, 2H), 7.11 (d, J=8.6, 2H), 6.96 (d, J=8.8, 2H), 3.88 (s, 3H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ= 193.8, 163.5, 151.9, 145.6, 136.7, 132.3, 131.9, 131.2, 129.8, 129.3, 128.3, 122.0, 113.5, 55.4, 21.6; HRMS: Anal. Calcd. For $C_{21}H_{18}O_5S$: 382.0875, Found: 382.0873; IR (KBr, cm^{-1}): ν 1651.



(4-methoxyphenyl)(thiophen-2-yl)methanone (3s)[11]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.89 (d, *J*=8.9, 2H), 7.67 (d, *J*=4.9, 1H), 7.63 (d, *J*=4.1, 1H), 7.20 – 7.09 (m, 1H), 6.97 (d, *J*=8.9, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 186.7, 162.9, 143.6, 133.9, 133.3, 131.4, 130.4, 127.7, 113.5, 55.4; MS ($C_{12}H_{10}O_2S$): 218; IR (KBr, cm^{-1}): ν 1629.

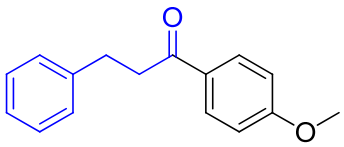


1-(4-methoxyphenyl)octan-1-one (3t)[12]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.94 (d, J=8.9, 2H), 6.92 (d, J=8.9, 2H), 3.85 (s, 3H), 2.90 (t, J=7.5, 2H), 1.76 – 1.67 (m, 2H), 1.39 – 1.25 (m, 8H), 0.88 (t, J=6.6, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 199.1, 163.2, 130.2, 130.1, 113.5, 55.3, 38.2, 31.6, 29.3, 29.1, 24.5, 22.6, 14.0; MS ($C_{15}H_{22}O_2$): 234; IR (KBr, cm^{-1}): ν 2934, 2582, 1670.

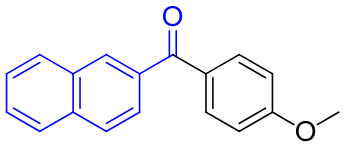


benzo[d][1,3]dioxol-5-yl(4-methoxyphenyl)methanone (3u)[13]**.** ^{1}H NMR ($CDCl_3$, 300MHz): δ = 7.81 – 7.74 (m, 2H), 7.36 – 7.28 (m, 2H), 6.95 (d, J=8.8, 2H), 6.85 (d, J=7.9, 1H), 6.04 (s, 2H), 3.87 (s, 3H): ^{13}C NMR ($CDCl_3$, 75 MHz)**:** δ = 193.9, 162.8, 151.0, 147.7, 132.3, 132.1, 130.4, 126.1, 113.4, 109.8, 107.5, 101.7, 55.4; MS

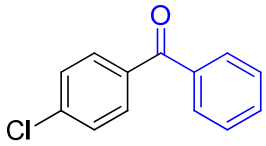
($C_{15}H_{12}O_4$): 256; IR (KBr, cm^{-1}): ν 1632.



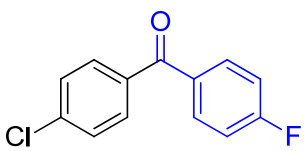
1-(4-methoxyphenyl)-3-phenylpropan-1-one (3v)[1]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.92 (d, J=8.9, 2H), 7.31 – 7.15 (m, 5H), 6.89 (d, J=8.9, 2H), 3.82 (s, 3H), 3.22 (t, J=8.0, 2H), 3.04 (t, J=8.0, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 197.6, 163.3, 141.3, 130.2, 129.7, 128.4, 128.3, 125.9, 113.6, 55.3, 40.0, 30.2; MS ($C_{16}H_{16}O_2$): 240; IR (KBr, cm^{-1}): ν 3061, 3026, 2934, 1670.



(4-methoxyphenyl)(naphthalen-2-yl)methanone (3w)[8]**.** ^{1}H NMR ($CDCl_3$, 400MHz):δ = 8.23 (s, 1H), 7.98 – 7.85 (m, 6H), 7.57 (dt, J=14.9, 7.0, 2H), 6.99 (d, J=7.6, 2H), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.2, 163.0, 135.2, 134.8, 132.4, 132.0, 130.9, 130.1, 129.0, 128.0, 127.8, 127.6, 126.5, 125.6, 113.4, 55.3; MS ($C_{18}H_{14}O_2$): 262; IR (KBr, cm^{-1}): ν 1637.

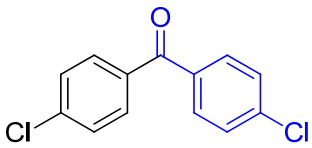


(4-chlorophenyl)(phenyl)methanone (4a) [14]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.78-7.75 (m, 4H), 7.60 (t, J=7.4, 1H), 7.51-7.45 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.5, 138.9, 137.2, 135.8, 132.7, 131.5, 129.9, 128.1, 128.4; MS ($C_{13}H_9ClO$): 216, 218; IR (KBr, cm^{-1}): ν 1652.

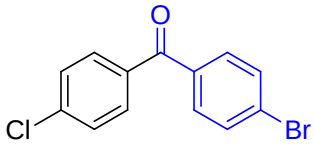


(4-chlorophenyl)(4-fluorophenyl)methanone (4b)[15]**.** ^{1}H NMR ($CDCl_3$,

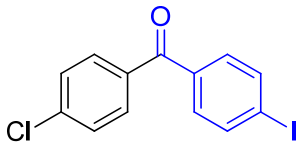
400MHz): δ = 7.83-7.80 (m, 2H), 7.73 (d, J=8.4, 2H), 7.47 (d, J=8.4, 2H), 7.19-7.14 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 193.9, 166.7, 164.1, 138.9, 135.7, 133.4, 133.4, 132.5, 132.4, 131.2, 128.6, 115.6, 115.4; MS ($C_{13}H_8FClO$): 234, 236; IR (KBr, cm^{-1}): ν 1650.



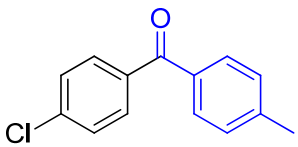
bis(4-chlorophenyl)methanone (4c) [16]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.73 (d, J=8.6, 4H), 7.47 (d, J=8.6, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 194.2, 139.1, 135.4, 131.3, 128.7; MS ($C_{13}H_8Cl_2O$): 250, 252; IR (KBr, cm^{-1}): ν 1655.



(4-bromophenyl)(4-chlorophenyl)methanone (4d)[17]**.** ^{1}H NMR($CDCl_3$, 400MHz): δ = 7.72 (d, J=8.4, 2H), 7.64 (m, 4H), 7.46 (d, J=8.4, 2H); ^{13}C NMR($CDCl_3$, 100 MHz): δ = 194.3, 139.1, 135.9, 135.3, 131.7, 131.3, 131.3, 128.7, 127.7; MS ($C_{13}H_8BrClO$): 294, 296, 297; IR (KBr, cm^{-1}): ν 1645.

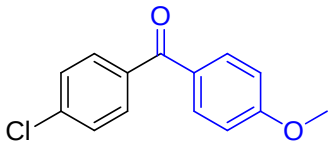


(4-chlorophenyl)(4-iodophenyl)methanone (4e)[18]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ = 7.85 (d, J=8.1, 2H), 7.72 (d, J=8.3, 2H), 7.51 – 7.44 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz):δ = 194.6, 139.1, 137.6, 136.4, 135.3, 131.3, 131.2, 128.7, 100.4; MS ($C_{13}H_8ClIO_3$): 342, 344; IR (KBr, cm^{-1}): ν 1644.

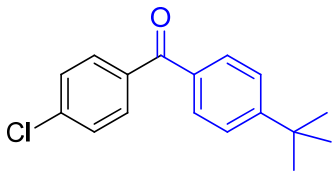


(4-chlorophenyl)(p-tolyl)methanone (4f) [11]**.** ^{1}H NMR ($CDCl_3$, 400MHz): δ =

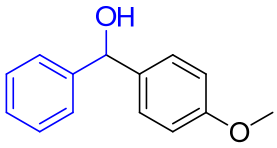
7.72 (d, J=8.6, 2H), 7.68 (d, J=8.0, 2H), 7.44 (d, J=8.6, 2H), 7.28 (d, J=8.0, 2H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.1, 143.4, 138.5, 136.1, 134.4, 131.3, 130.1, 129.0, 128.5, 21.6; MS ($C_{14}H_{11}ClO$): 230, 232; IR (KBr, cm^{-1}): ν 1644.



(4-chlorophenyl)(4-methoxyphenyl)methanone (4g) [1]**.** ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.80 (d, J=8.6, 2H), 7.71 (d, J=8.3, 2H), 7.45 (d, J=8.3, 2H), 6.97 (d, J=8.6, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.0, 163.2, 138.1, 136.4, 132.3, 131.0, 129.6, 128.3, 113.5, 55.4; MS ($C_{14}H_{11}ClO_2$): 246, 248; IR (KBr, cm^{-1}): ν 1638.



(4-(tert-butyl)phenyl)(4-chlorophenyl)methanone (4h) [19]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.76-7.72 (m, 4H), 7.50 (d, J=8.4, 2H), 7.44 (d, J=8.4, 2H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 195.1, 156.4, 138.5, 136.1, 134.4, 131.3, 130.0, 128.5, 125.3, 35.1, 31.1; MS ($C_{17}H_{17}ClO$): 272, 274; IR (KBr, cm^{-1}): ν 1652.



(4-methoxyphenyl)(phenyl)methanol (5)[20]**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.28 (m, 4H), 7.23 (d, J = 8.3 Hz, 3H), 6.82 (d, J = 8.3 Hz, 2H), 5.72 (s, 1H), 3.74 (s, 3H), 2.42 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.8, 143.9, 136.1, 128.3, 127.8, 127.2, 126.3, 113.7, 75.5, 55.1; MS ($C_{14}H_{14}O_2$): 214; IR (KBr, cm^{-1}): ν 3404.

References:

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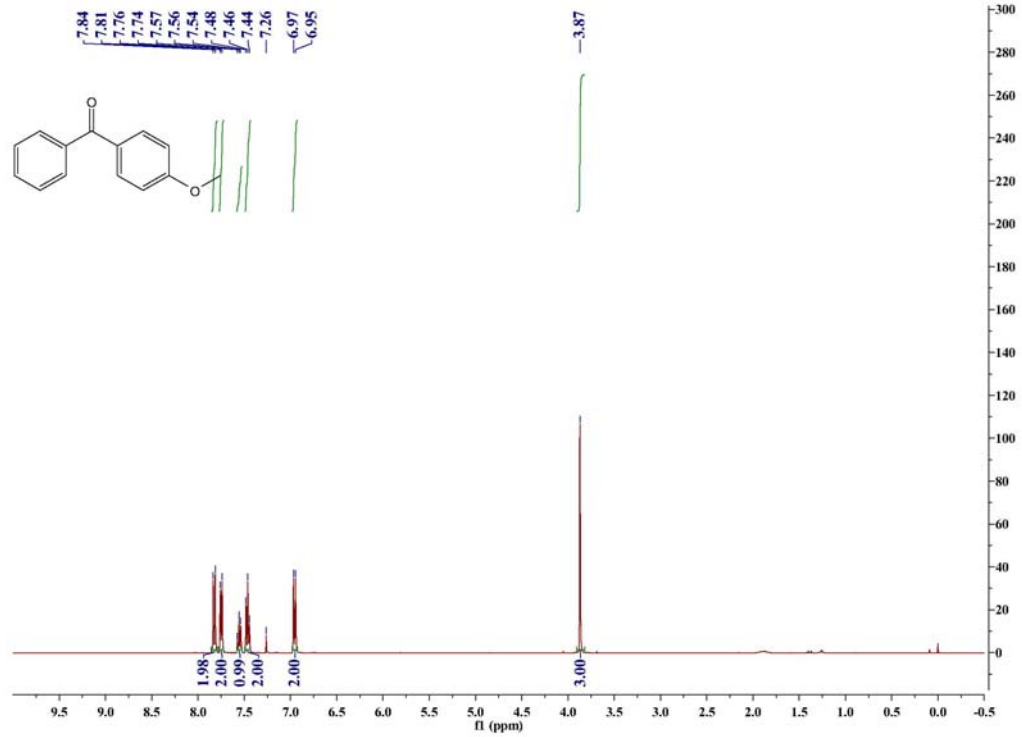
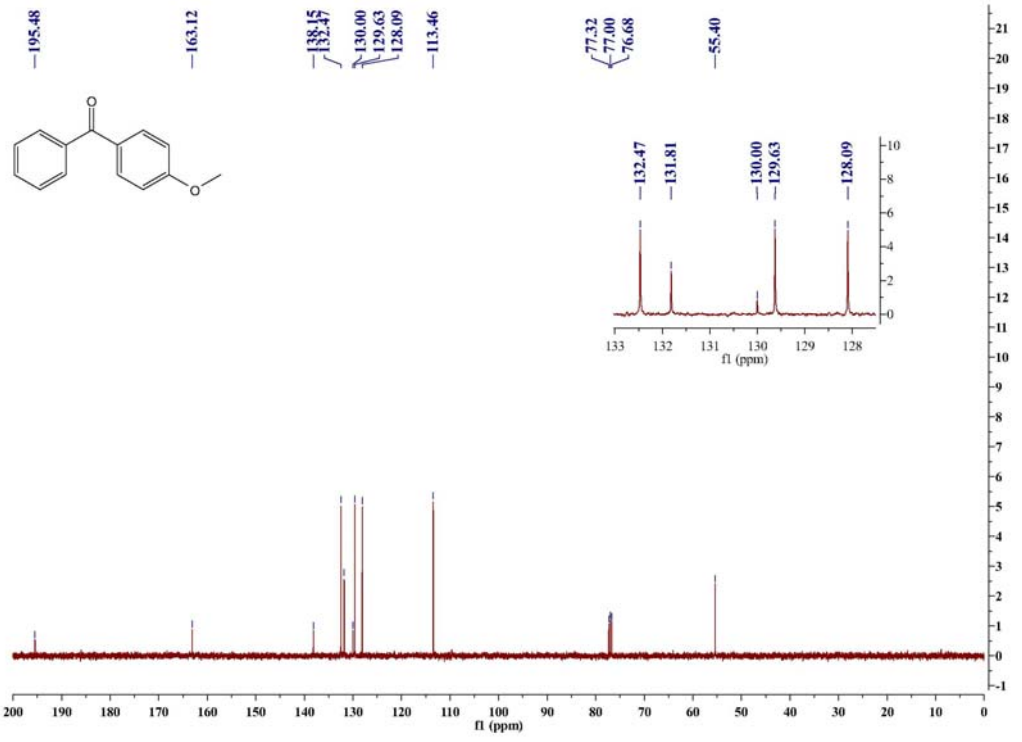
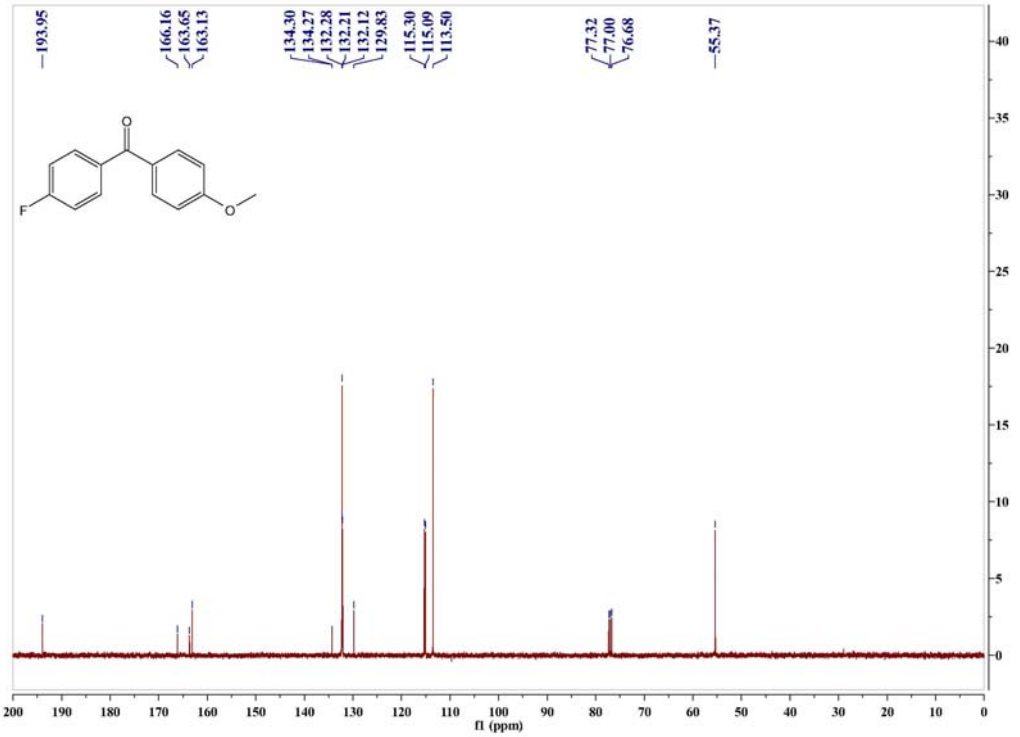
Spectroscopic Data for Products:

3a





3b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132.28
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77.32
77.00
76.68
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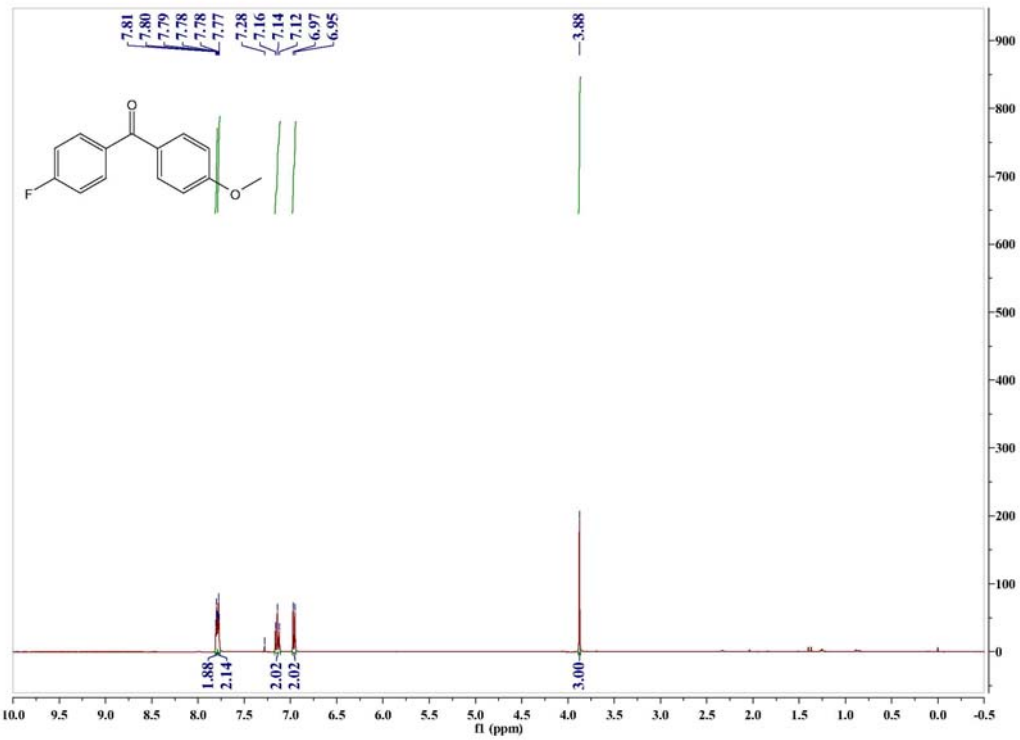
F
O
O
f1 (ppm)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7.16
7.14
7.12
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F
O
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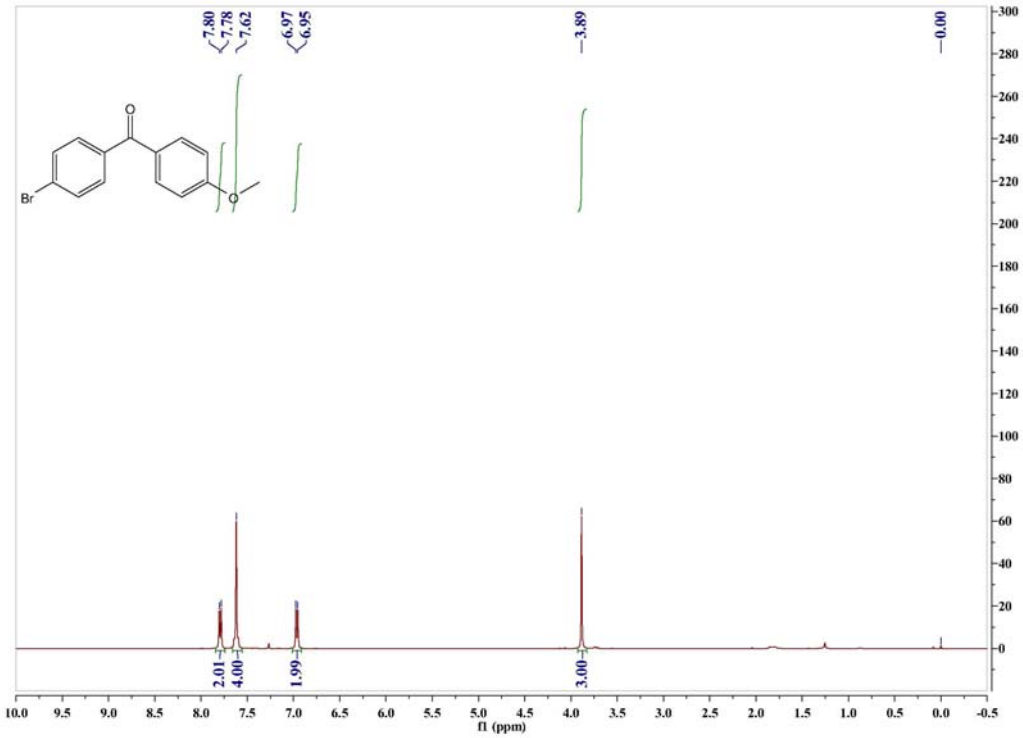
1.88
2.14
2.02
2.02
3.00
f1 (ppm)

3c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Br
O
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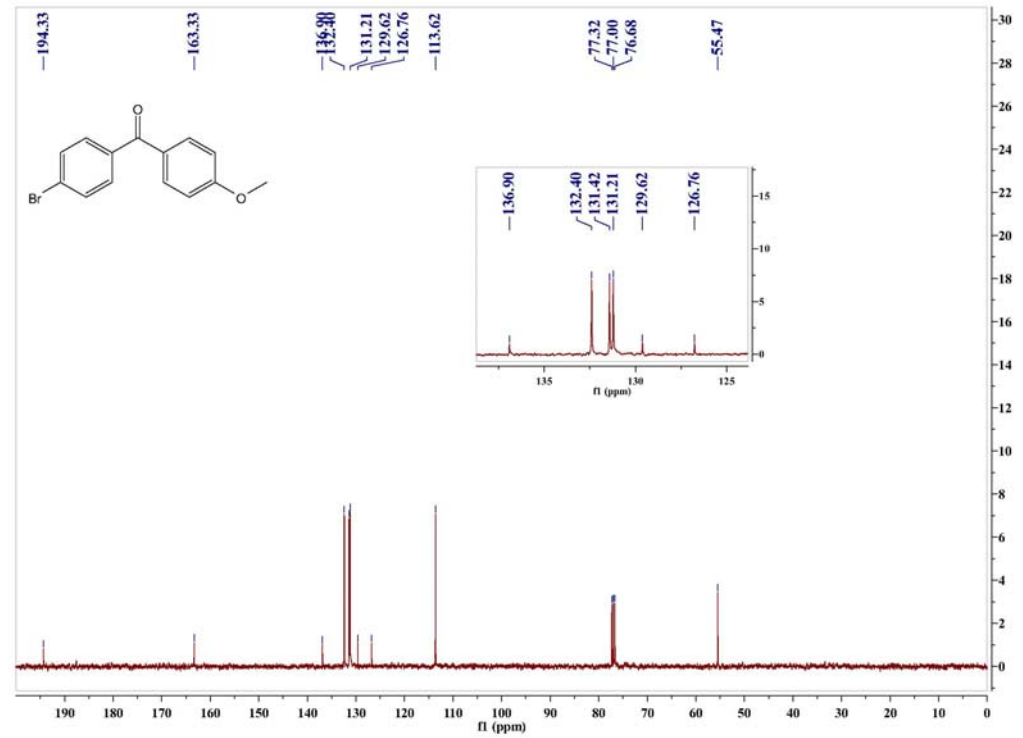
3.00
f1 (ppm)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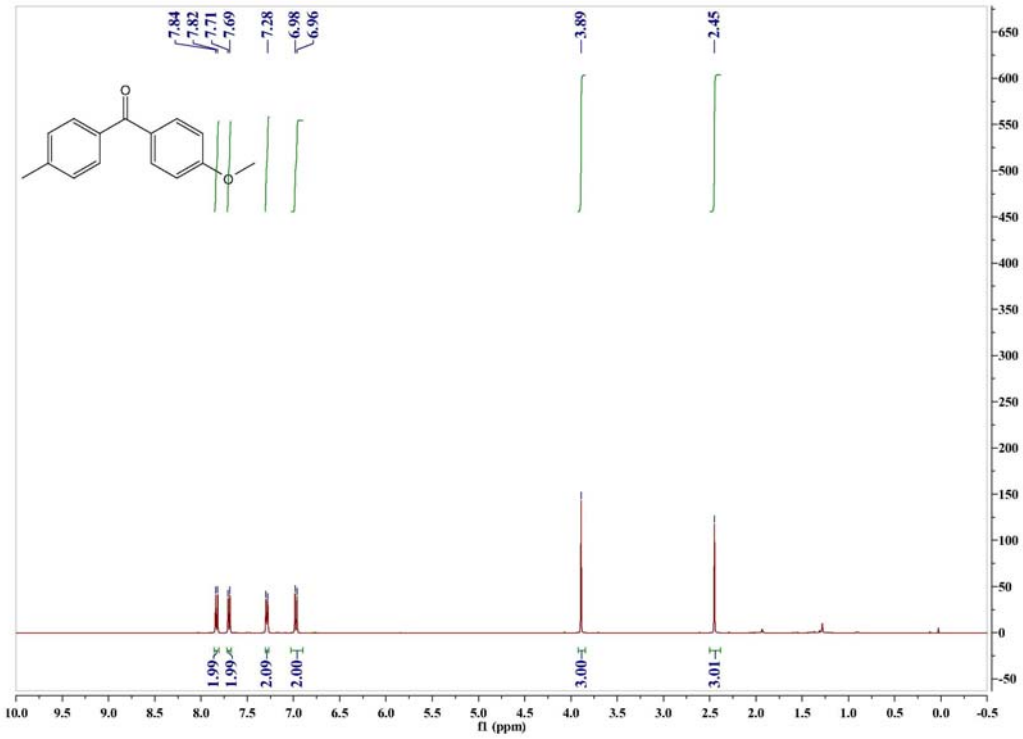
O
f1 (ppm)

3d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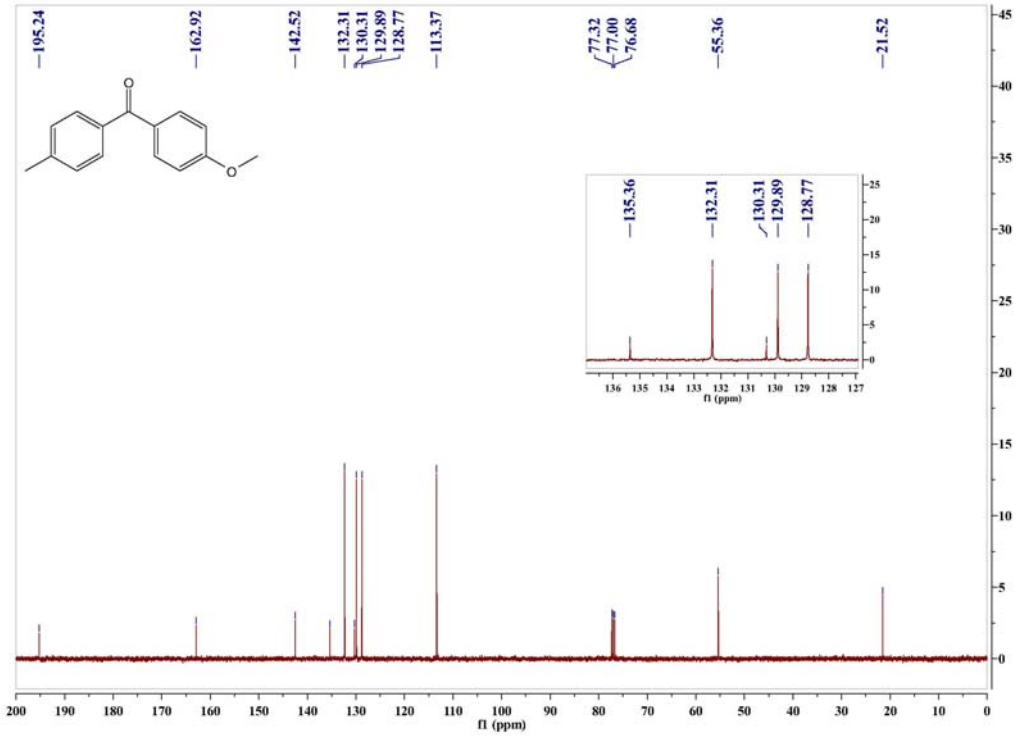
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130.31
129.89
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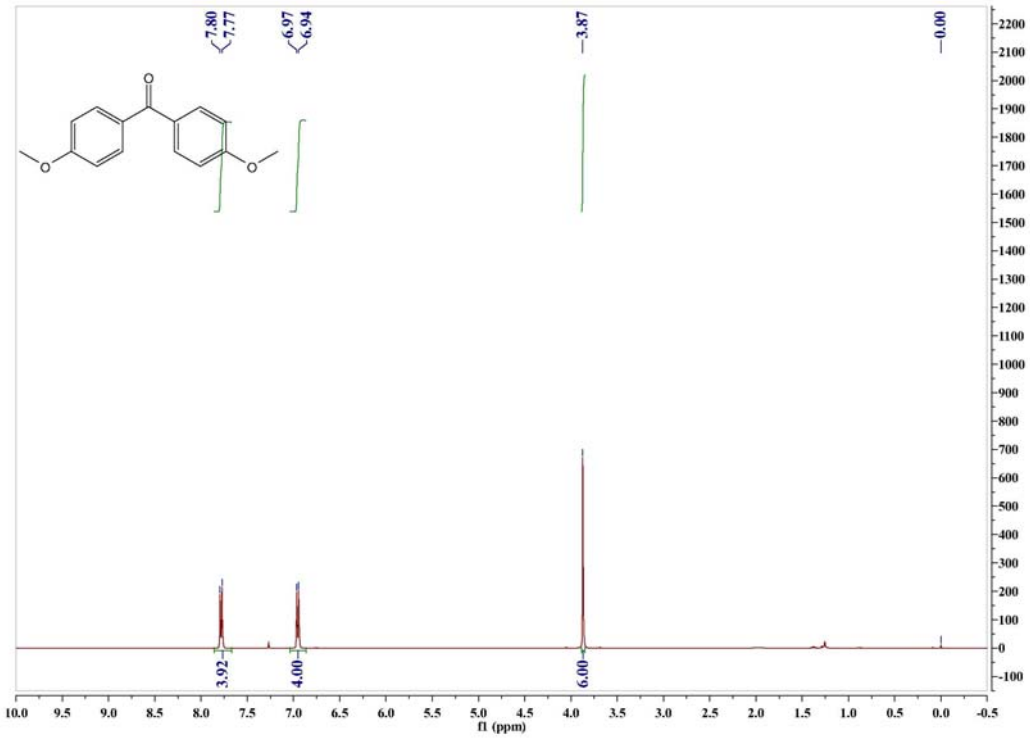
f1 (ppm)

3e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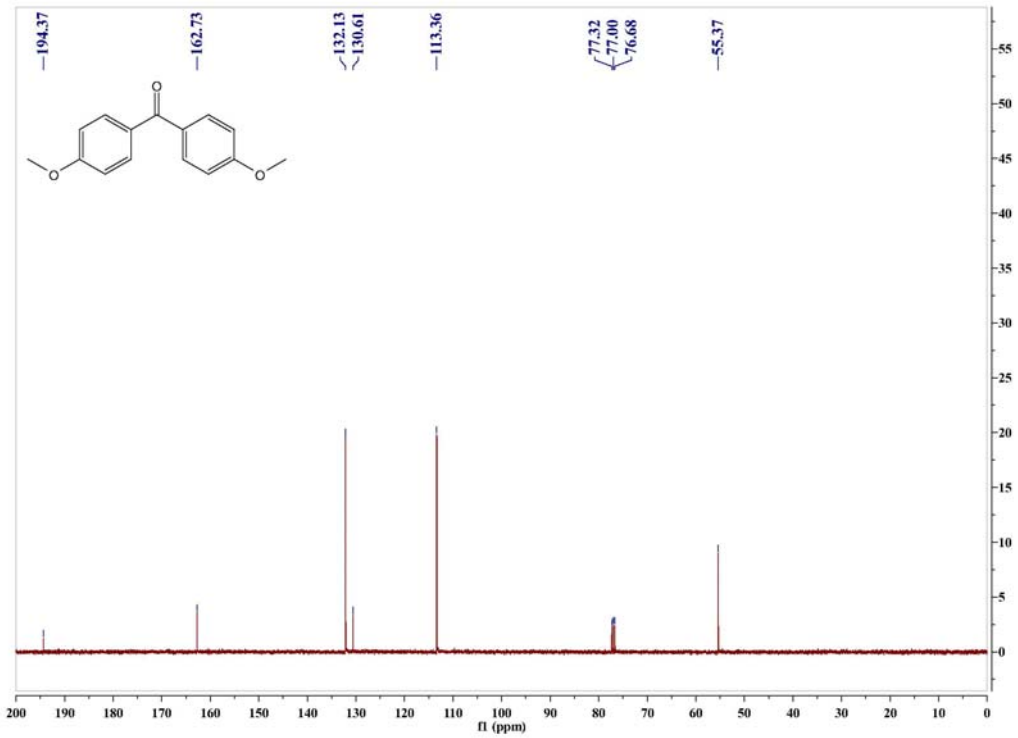
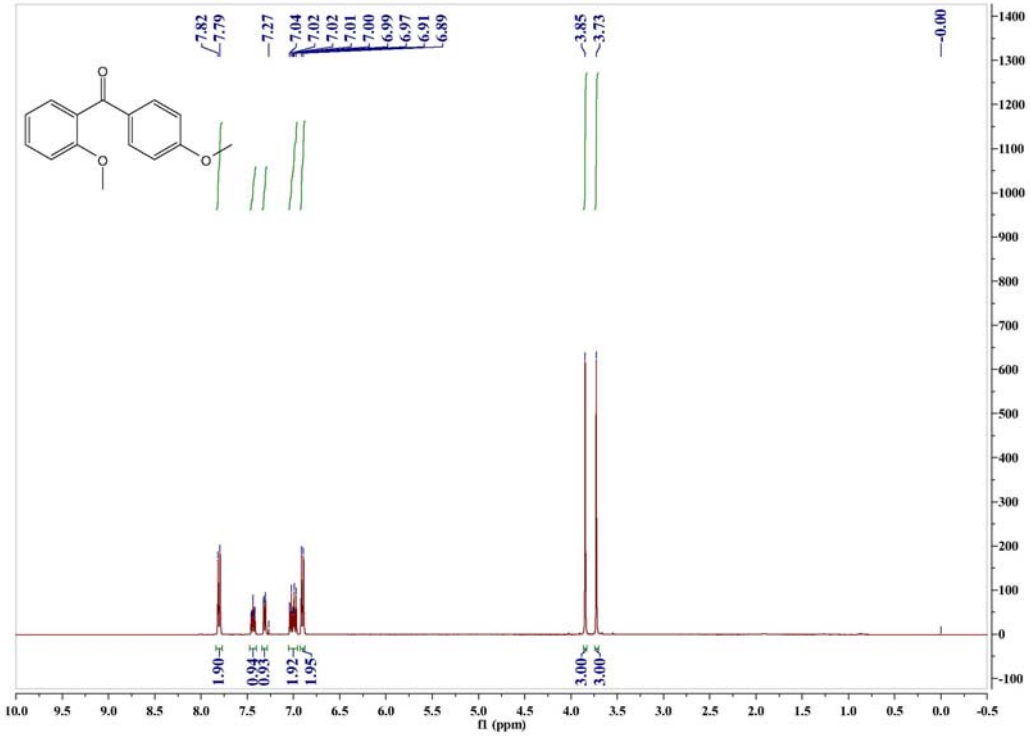
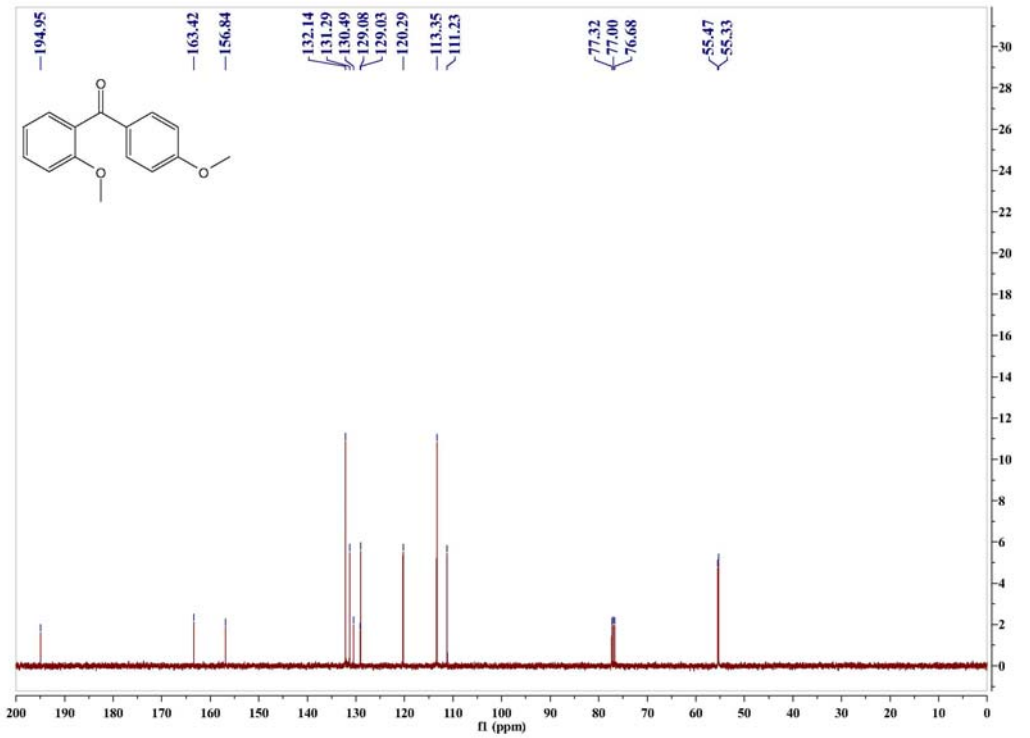
4.00
6.00
f1 (ppm)

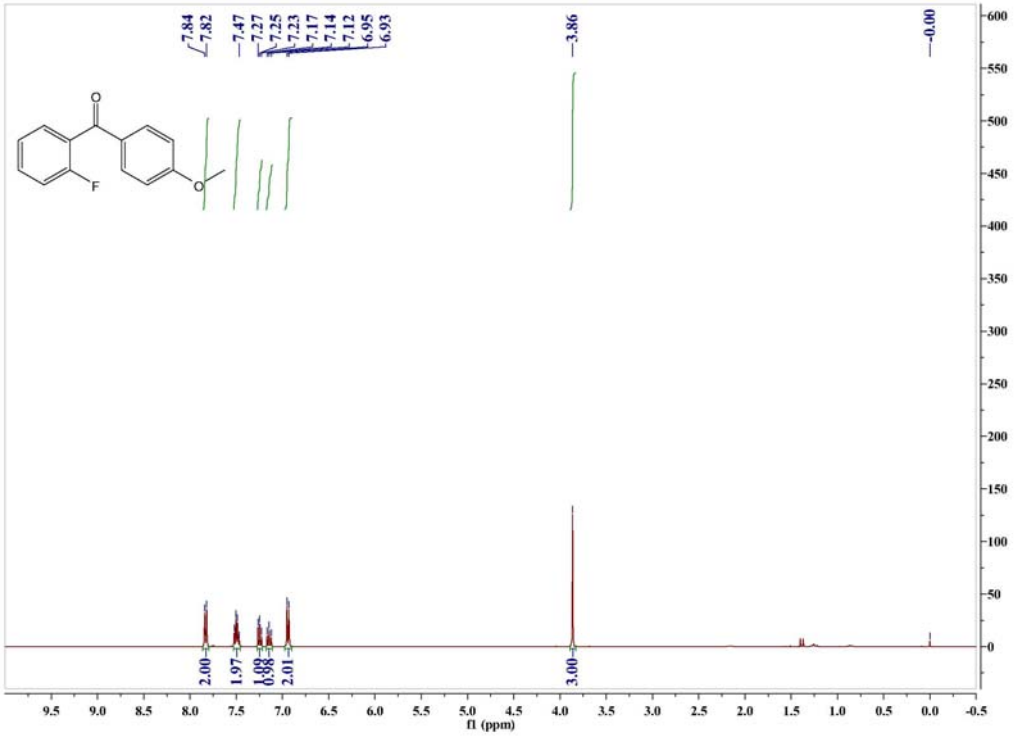

194.37
162.73
132.13
130.61
113.36
77.32
77.00
76.68
55.37
f1 (ppm)

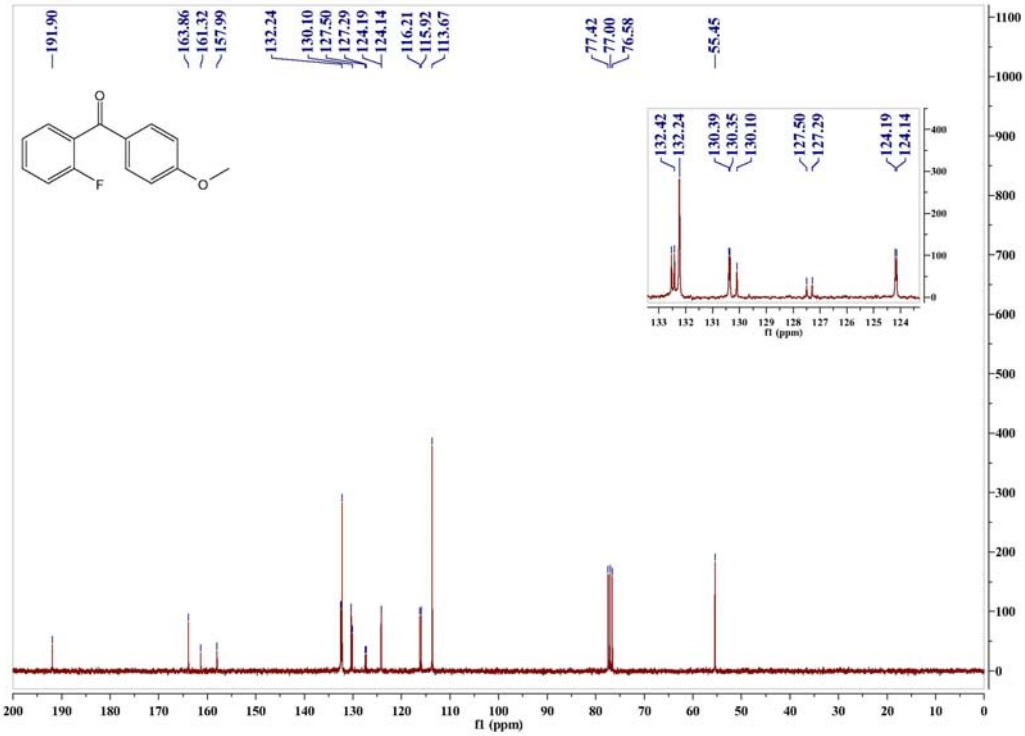
3f


7.82
7.79
7.27
7.04
7.02
7.02
7.01
7.00
6.99
6.97
6.91
6.89
3.85
3.73
0.00
1.90
0.94
0.93
1.92
1.95
3.00
3.00
f1 (ppm)

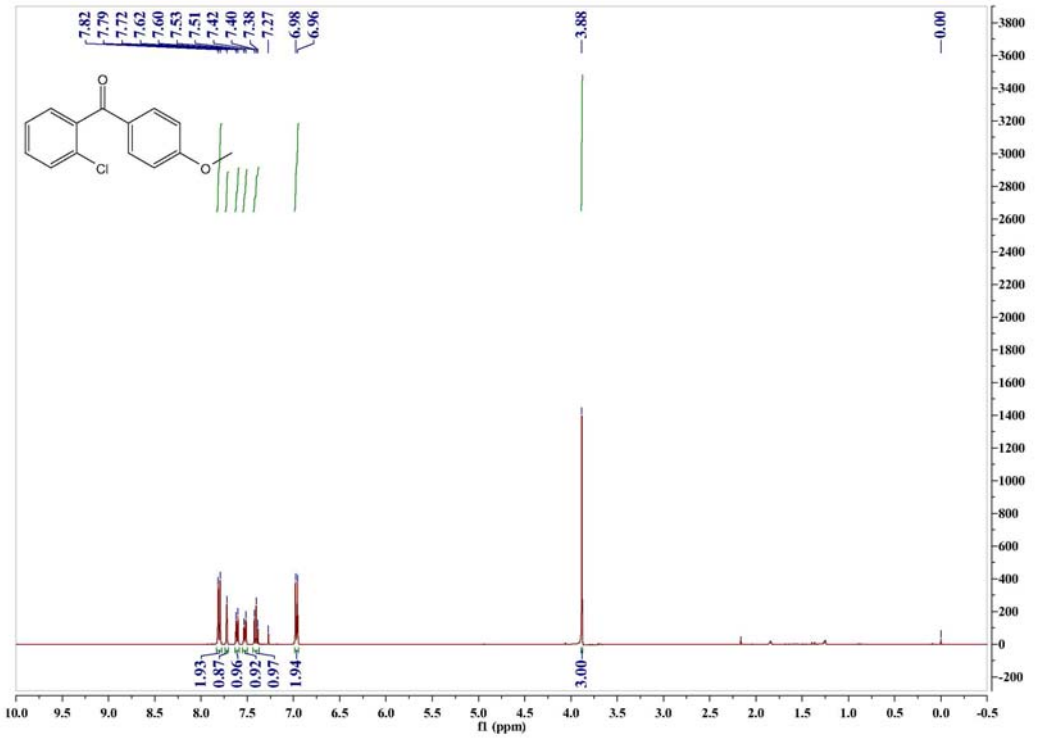

194.95
163.42
156.84
132.14
131.29
130.49
129.08
129.03
120.29
113.35
111.23
77.32
77.00
76.68
55.47
55.33
f1 (ppm)

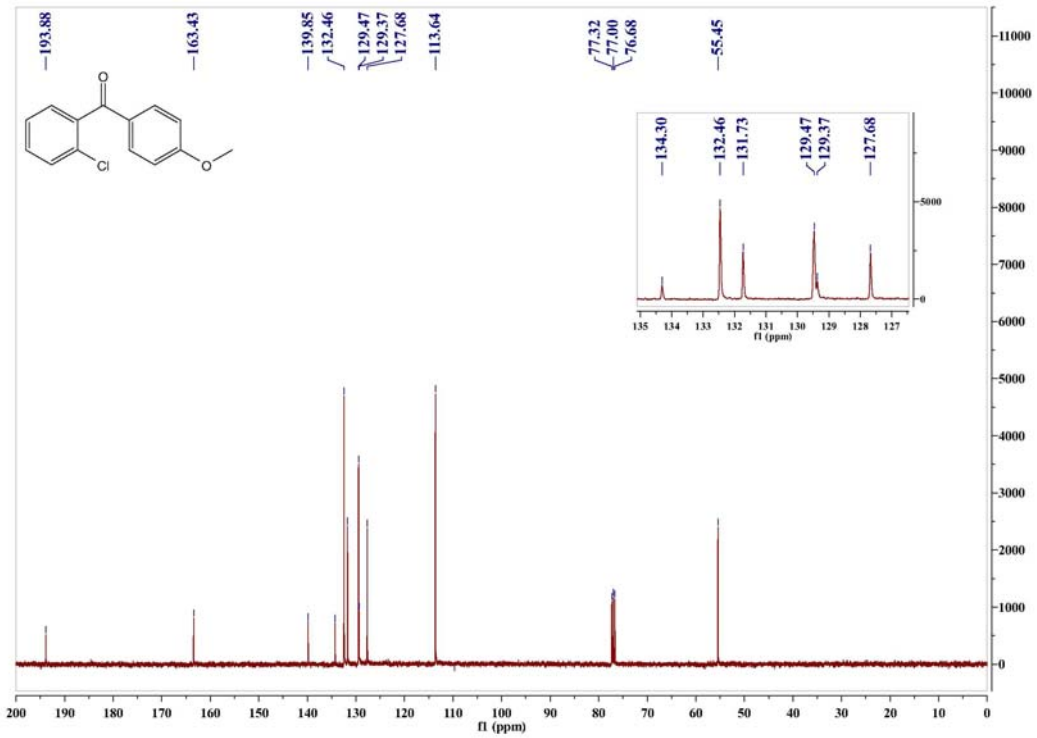
3g


7.84
7.82
7.47
7.27
7.25
7.23
7.17
7.14
7.12
6.95
6.93
3.86
0.00
2.00
1.97
1.08
0.98
2.01
3.00
f1 (ppm)

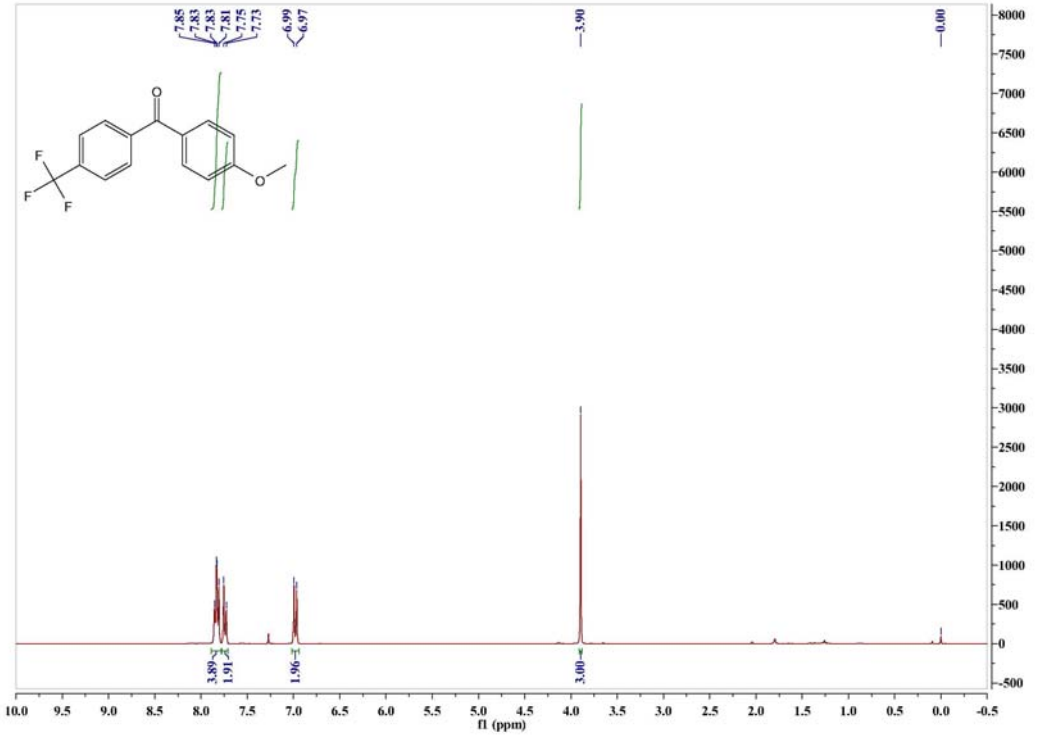

191.90
163.86
161.32
157.99
132.24
130.10
127.50
127.29
124.19
124.14
116.21
115.92
113.67
77.42
77.00
76.58
55.45
132.42
132.24
130.39
130.35
130.10
127.50
127.29
124.19
124.14
f1 (ppm)

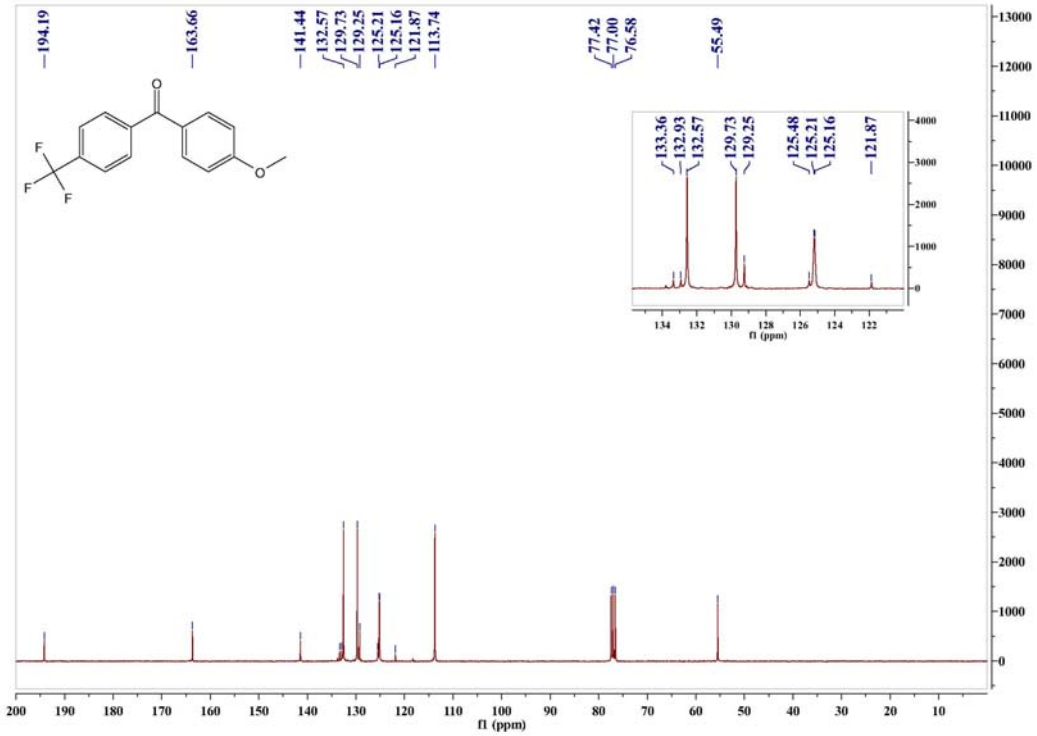
3h


7.82
7.79
7.72
7.62
7.60
7.53
7.51
7.42
7.40
7.38
7.27
6.98
6.96
3.88
0.00
Cl
O
1.93
0.87
0.96
0.92
0.97
1.94
3.00
f1 (ppm)

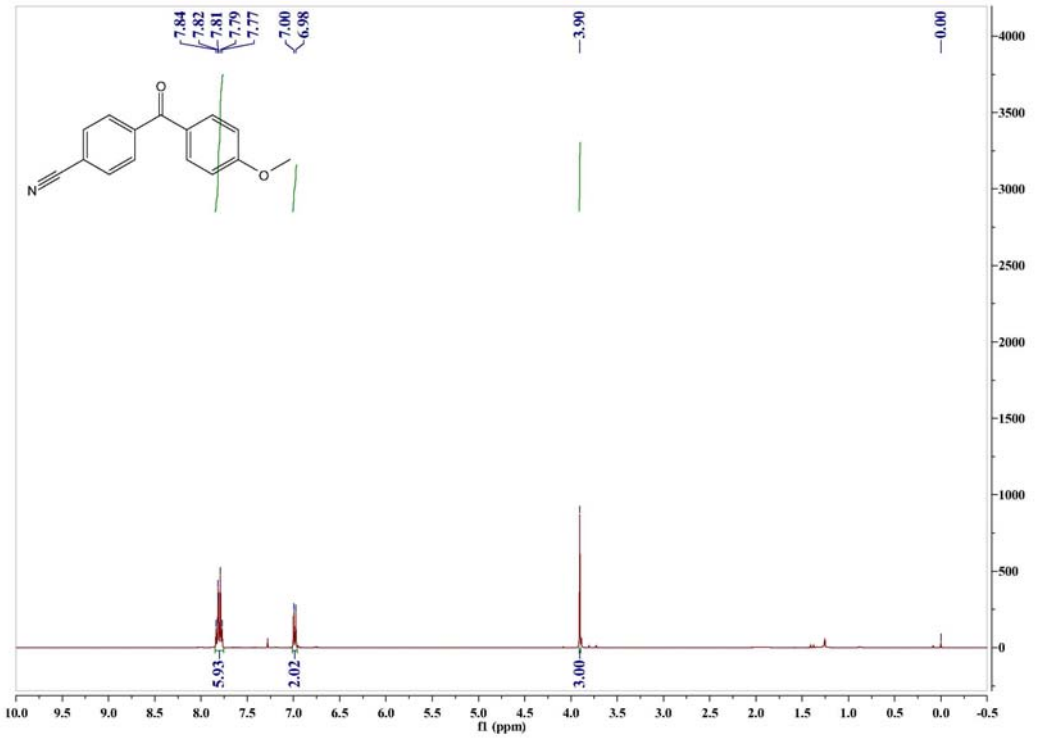

193.88
163.43
139.85
132.46
129.47
129.37
127.68
113.64
77.32
77.00
76.68
55.45
134.30
132.46
131.73
129.47
129.37
127.68
Cl
O
f1 (ppm)

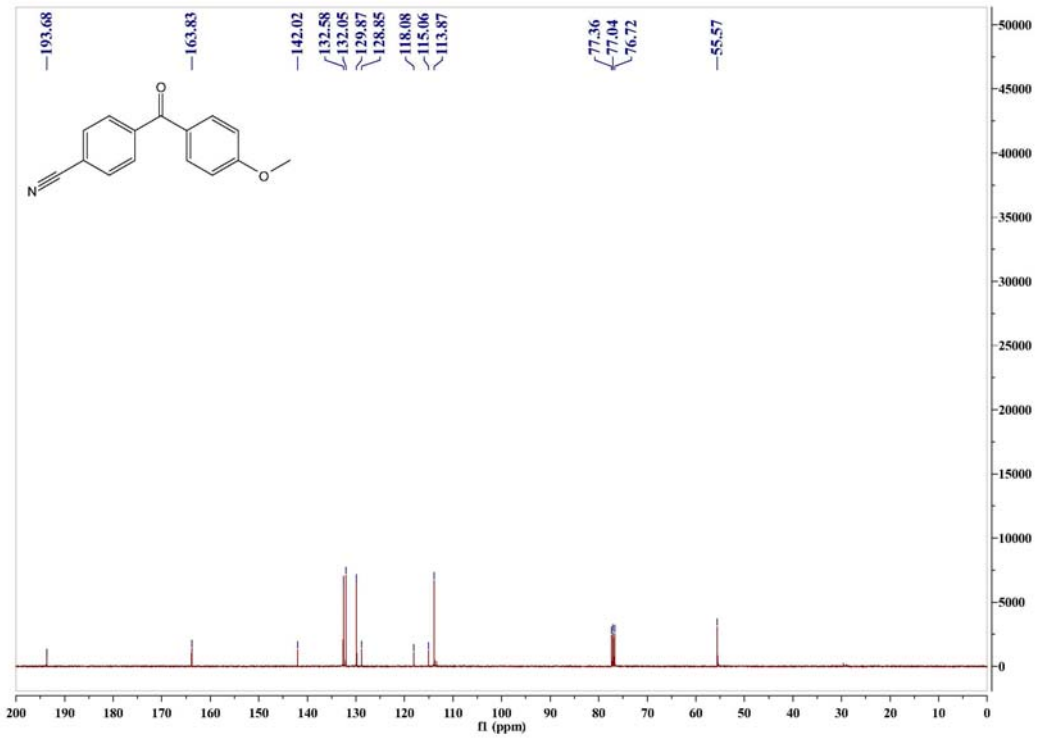
3i


7.85
7.83
7.83
7.81
7.75
7.73
6.99
6.97
3.90
0.00
3.89
1.91
1.96
3.00
f1 (ppm)

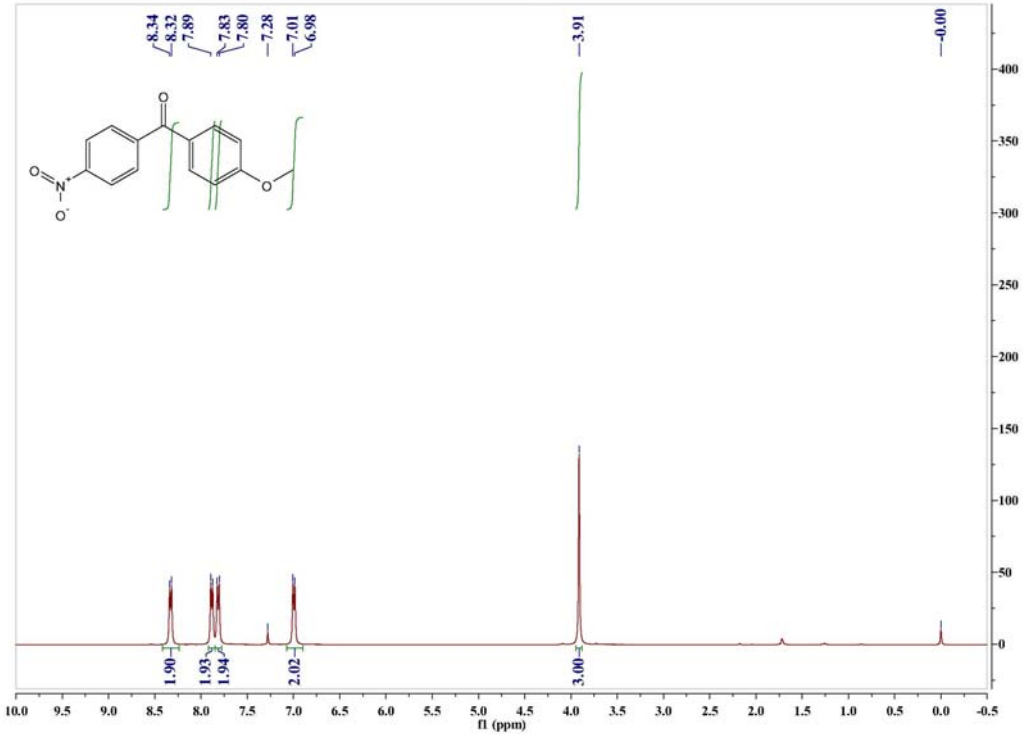

194.19
163.66
141.44
132.57
129.73
129.25
125.21
125.16
121.87
113.74
77.42
77.00
76.58
55.49
133.36
132.93
132.57
129.73
129.25
125.48
125.21
125.16
121.87
f1 (ppm)

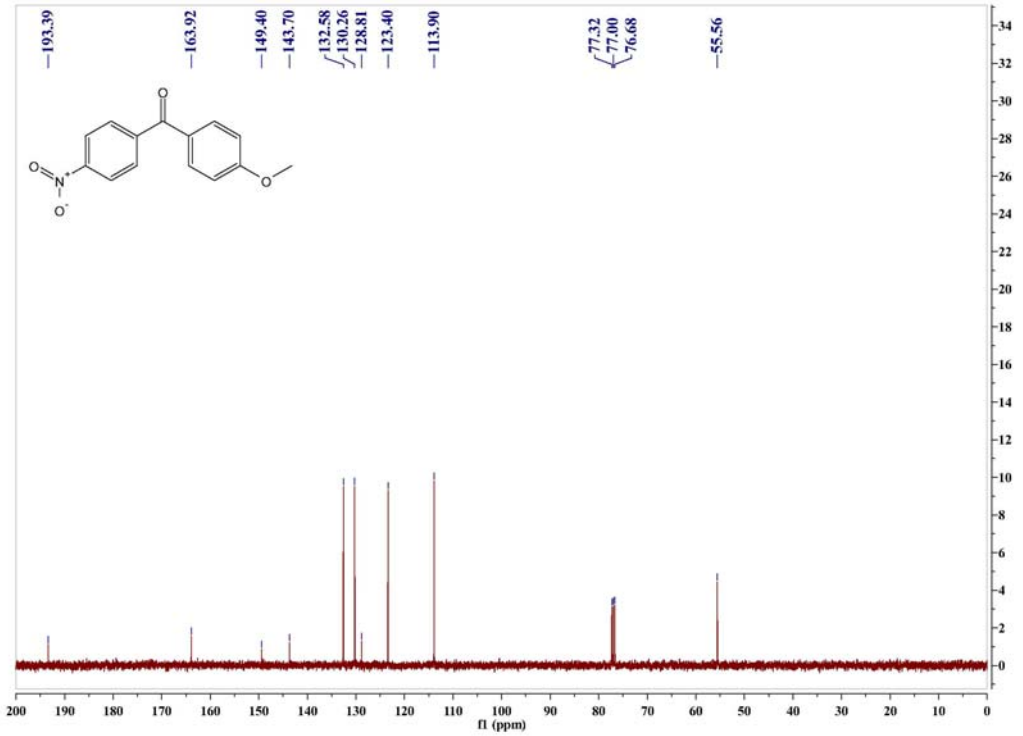
3j


7.84
7.82
7.81
7.79
7.77
7.00
6.98
3.90
0.00
5.93
2.02
3.00
f1 (ppm)

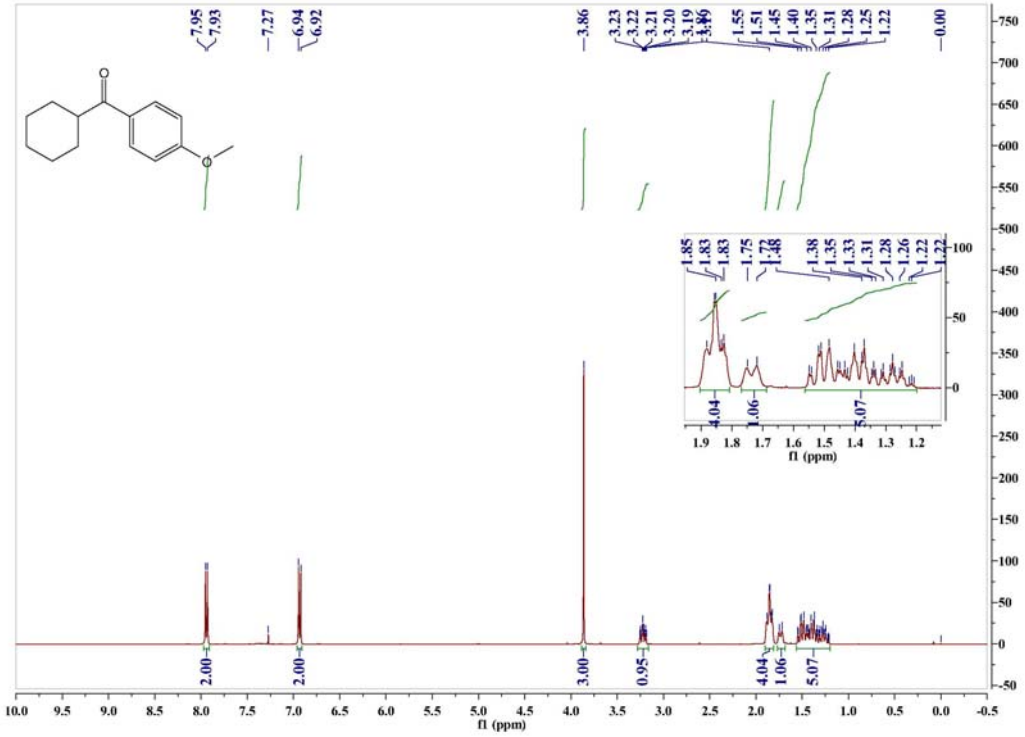

193.68
163.83
142.02
132.58
132.05
129.87
128.85
118.08
115.06
113.87
77.36
77.04
76.72
55.57
f1 (ppm)

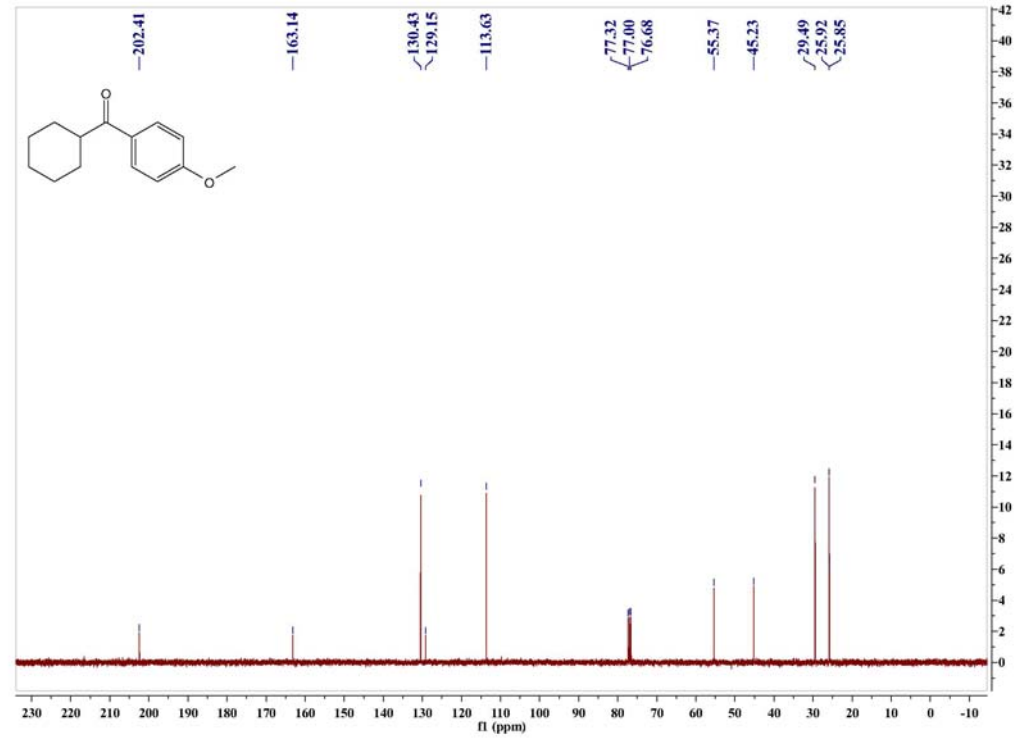
3k


8.34
8.32
7.89
7.83
7.80
7.28
7.01
6.98
3.91
0.00
1.90
1.93
1.94
2.02
3.00
f1 (ppm)

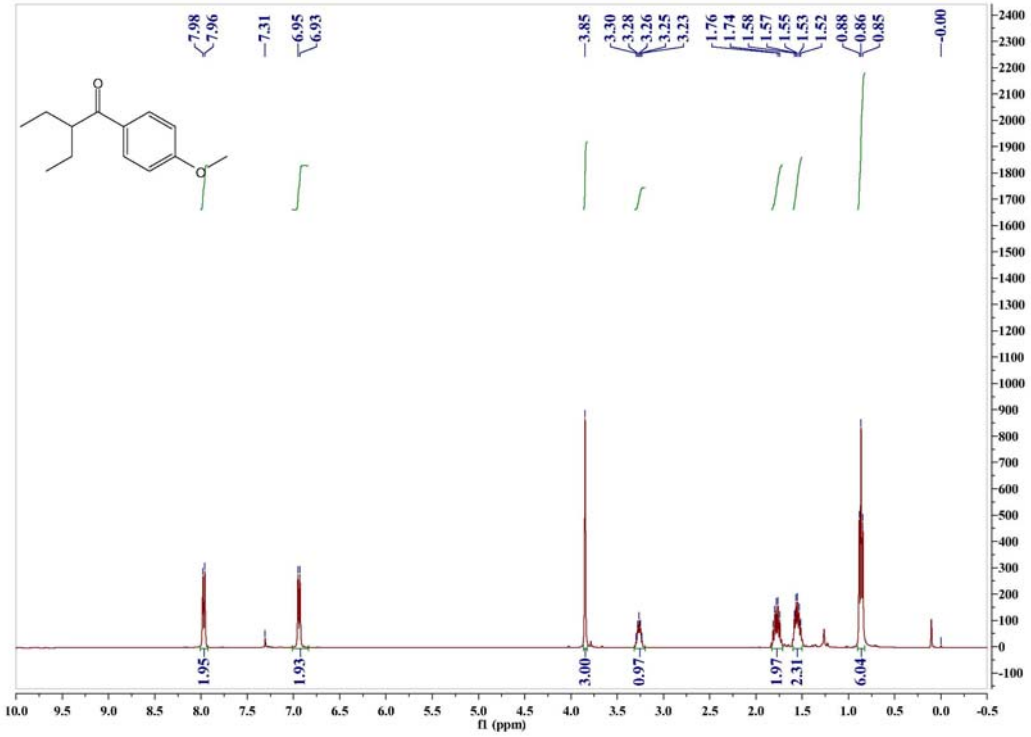

193.39
163.92
149.40
143.70
132.58
130.26
128.81
123.40
113.90
77.32
77.00
76.68
55.56
f1 (ppm)

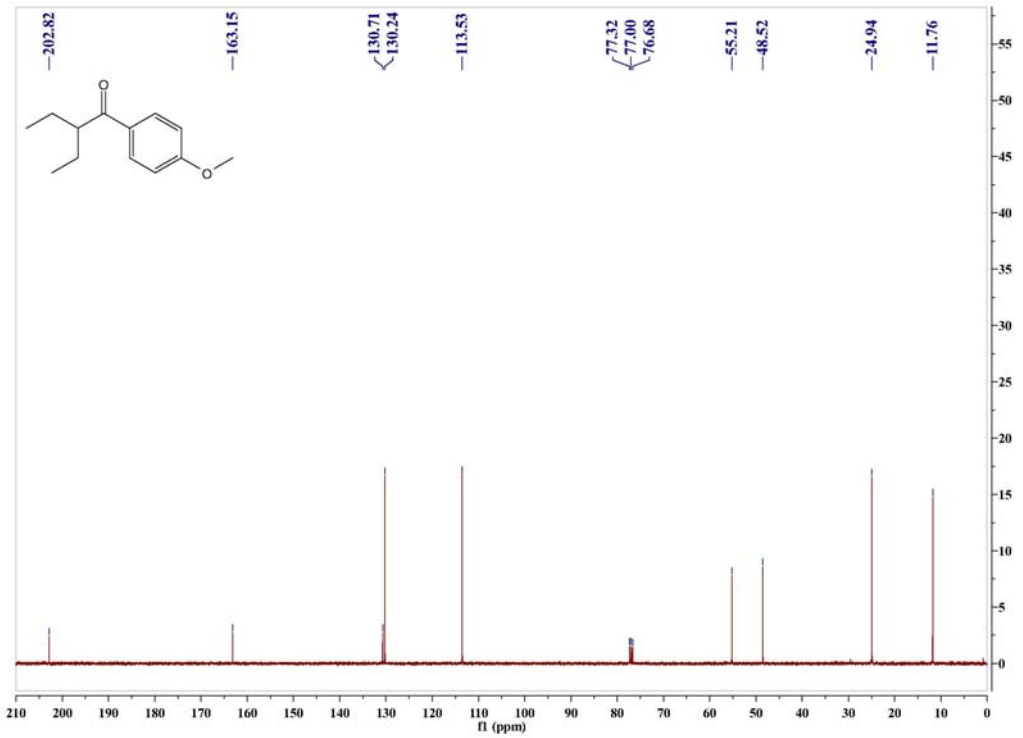
3l


7.95
7.93
7.27
6.94
6.92
3.86
3.23
3.22
3.21
3.20
3.19
1.55
1.51
1.45
1.40
1.35
1.31
1.28
1.25
1.22
0.00
1.85
1.83
1.83
1.75
1.72
1.48
1.38
1.35
1.33
1.31
1.28
1.26
1.22
1.22
4.04
1.06
5.07
f1 (ppm)
2.00
2.00
3.00
0.95
4.04
1.06
5.07
f1 (ppm)

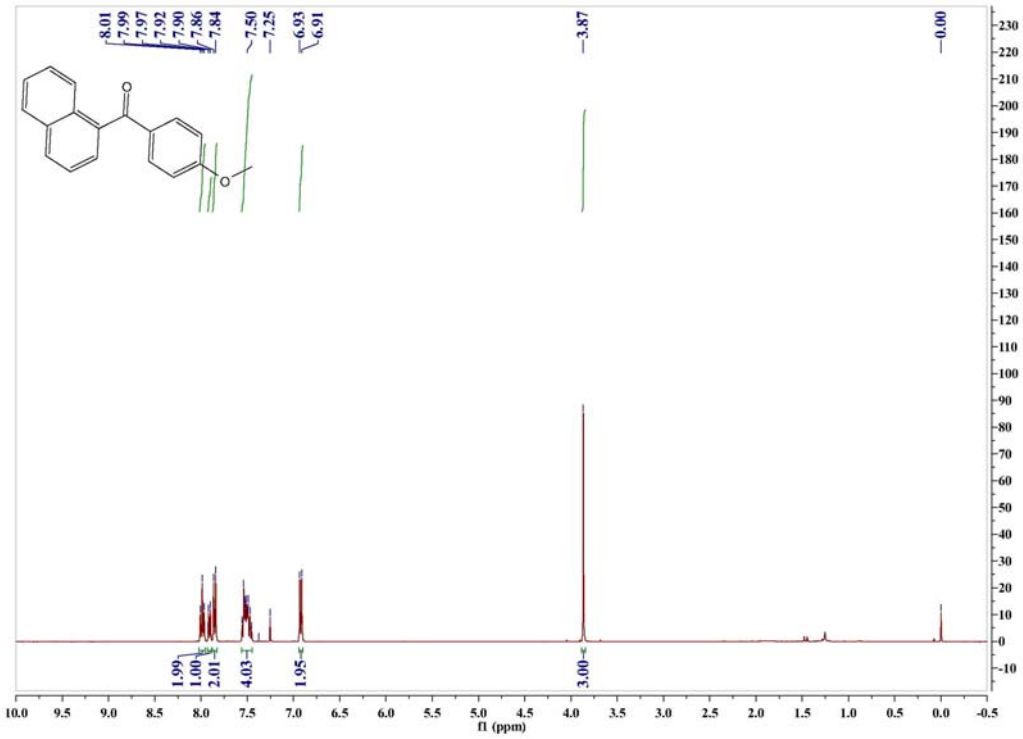

202.41
163.14
130.43
129.15
113.63
77.32
77.00
76.68
55.37
45.23
29.49
25.92
25.85
f1 (ppm)

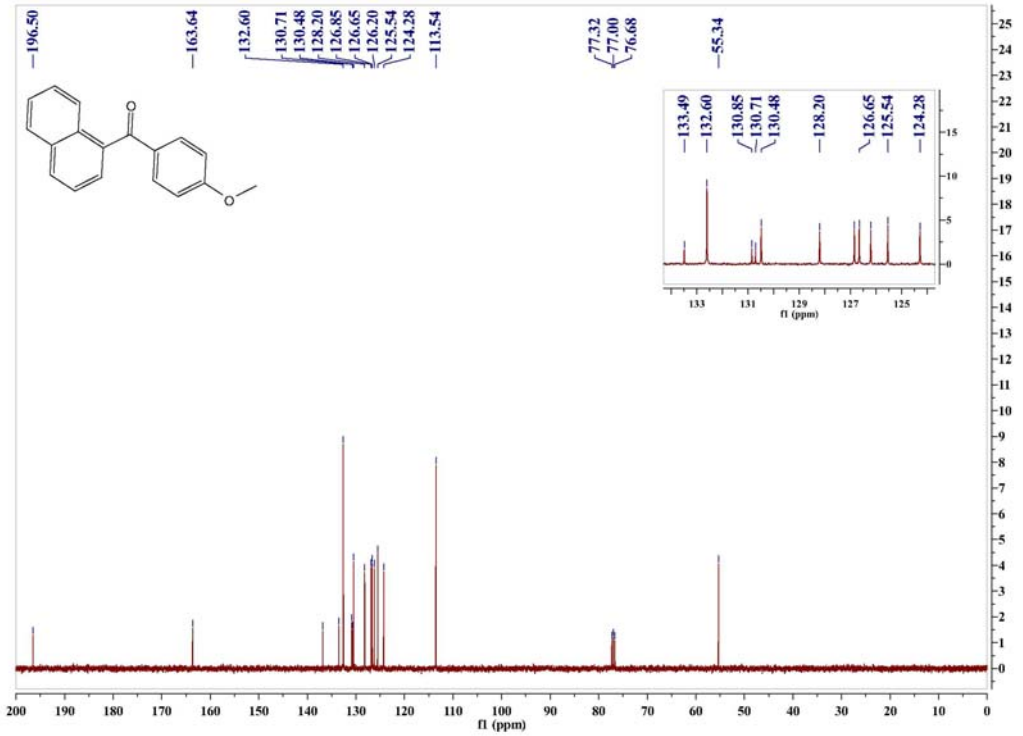
3m


7.98
7.96
7.31
6.95
6.93
3.85
3.30
3.28
3.26
3.25
3.23
1.76
1.74
1.58
1.57
1.55
1.53
1.52
0.88
0.86
0.85
0.00
1.95
1.93
3.00
0.97
1.97
2.31
6.04
f1 (ppm)

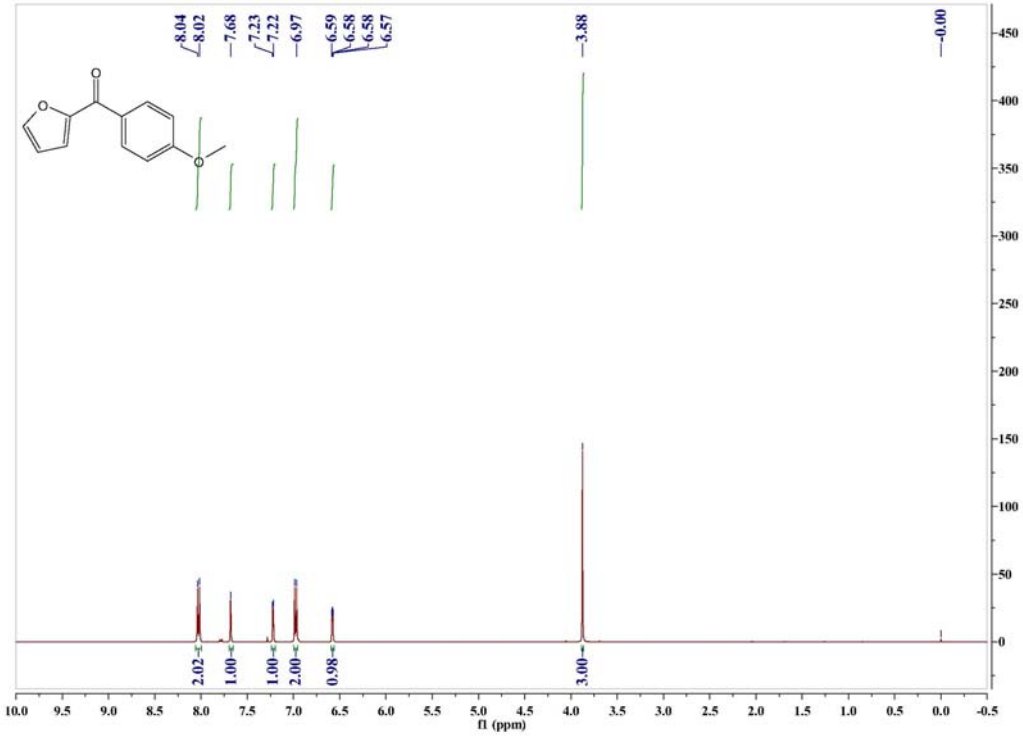

202.82
163.15
130.71
130.24
113.53
77.32
77.00
76.68
55.21
48.52
24.94
11.76
f1 (ppm)

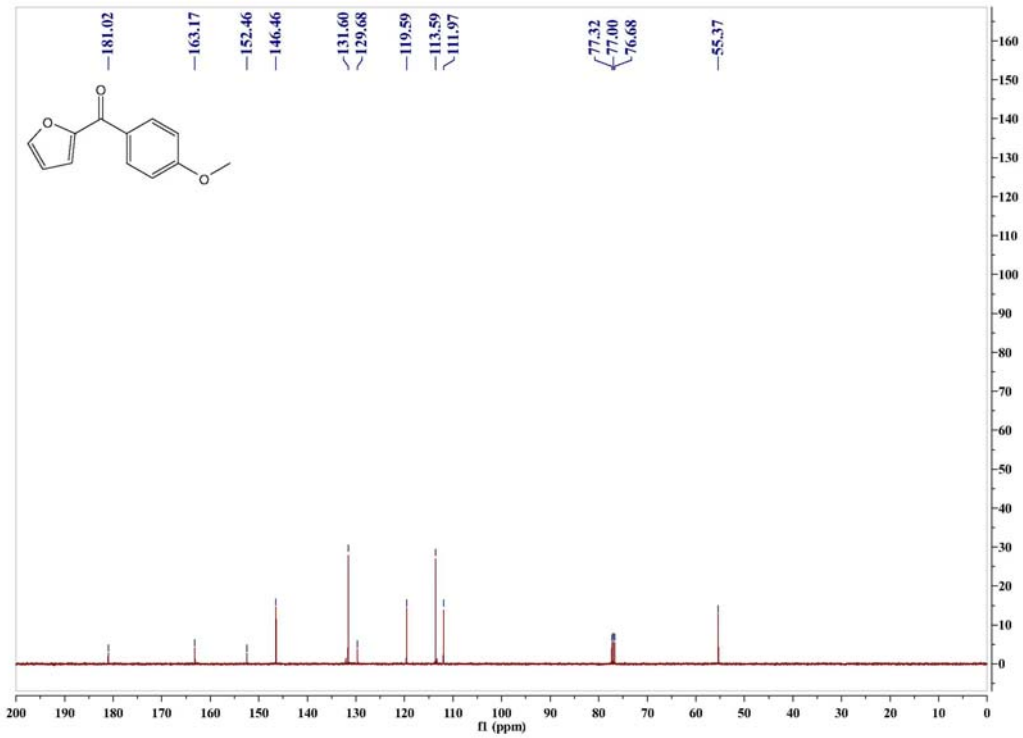
3n


8.01
7.99
7.97
7.92
7.90
7.86
7.84
7.50
7.25
6.93
6.91
3.87
0.00
1.99
1.00
2.01
4.03
1.95
3.00
f1 (ppm)

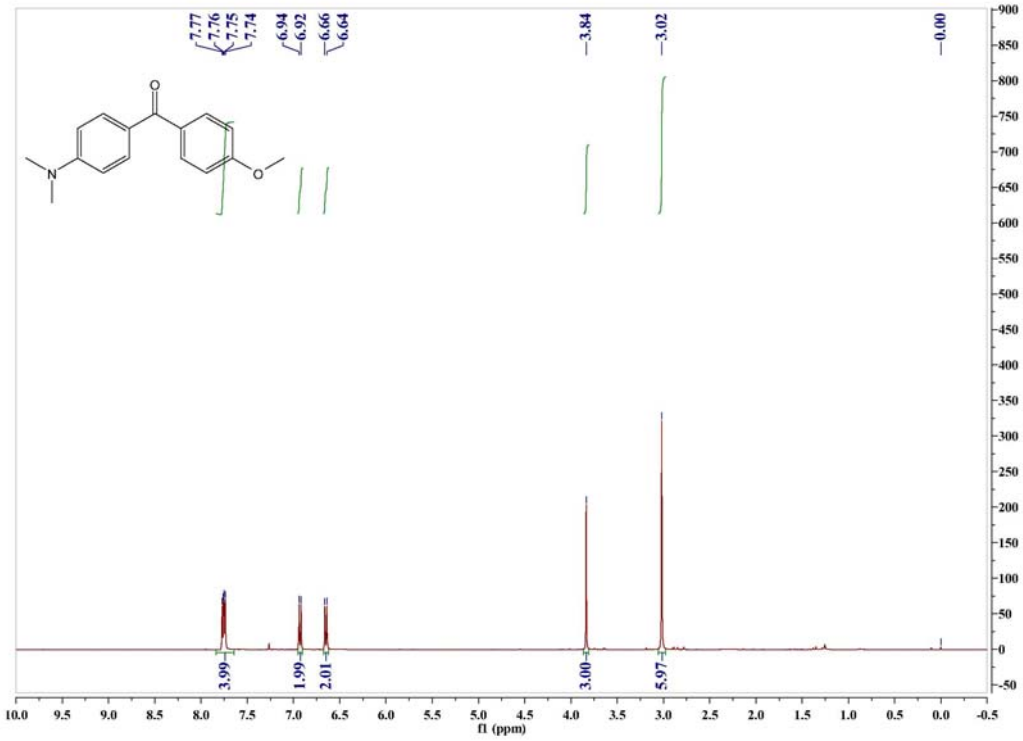

196.50
163.64
132.60
130.71
130.48
128.20
126.85
126.65
126.20
125.54
124.28
113.54
77.32
77.00
76.68
55.34
133.49
132.60
130.85
130.71
130.48
128.20
126.65
125.54
124.28
f1 (ppm)

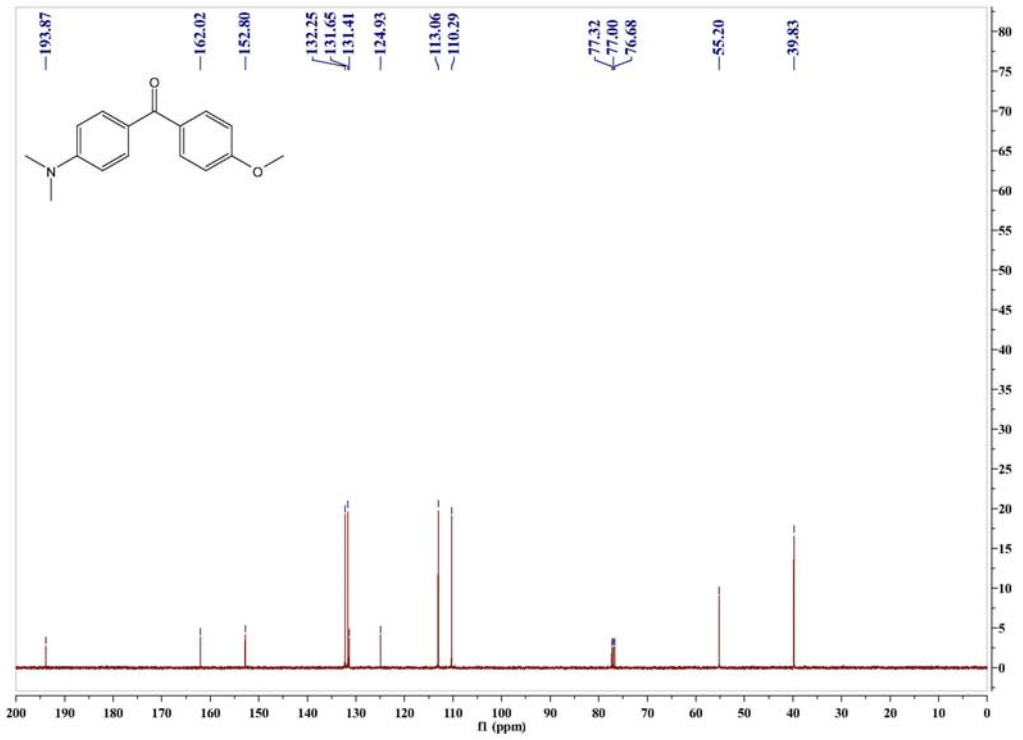
3o


8.04
8.02
7.68
7.23
7.22
6.97
6.59
6.58
6.58
6.57
3.88
-0.00
2.02
1.00
1.00
2.00
0.98
3.00
f1 (ppm)

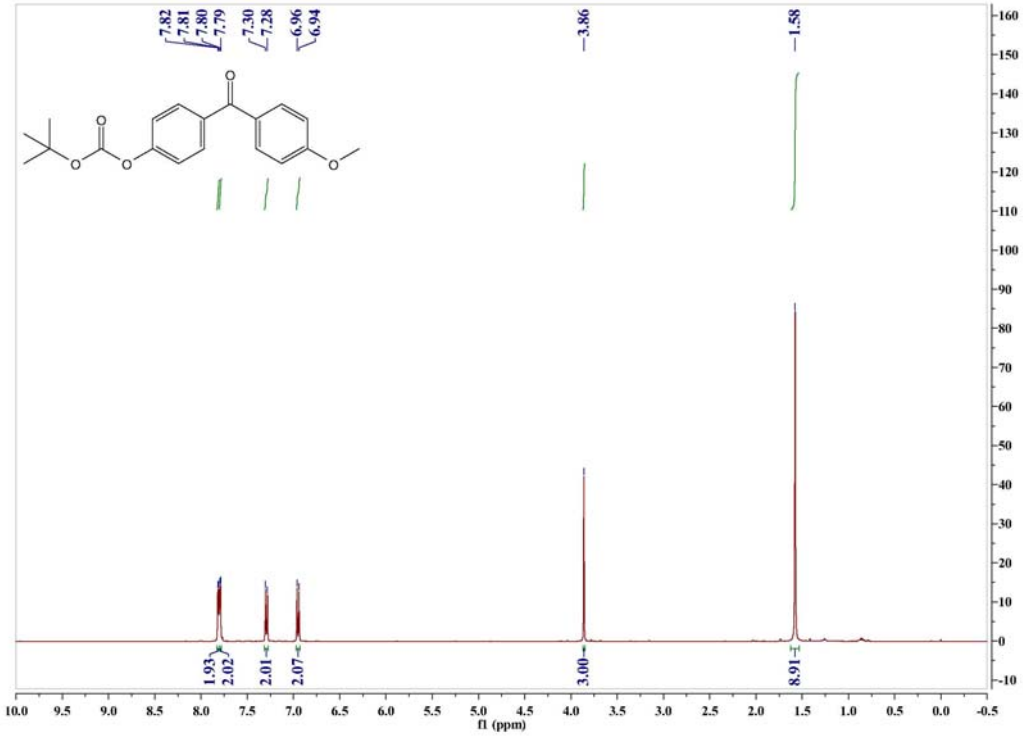

181.02
163.17
152.46
146.46
131.60
129.68
119.59
113.59
111.97
77.32
77.00
76.68
55.37
f1 (ppm)

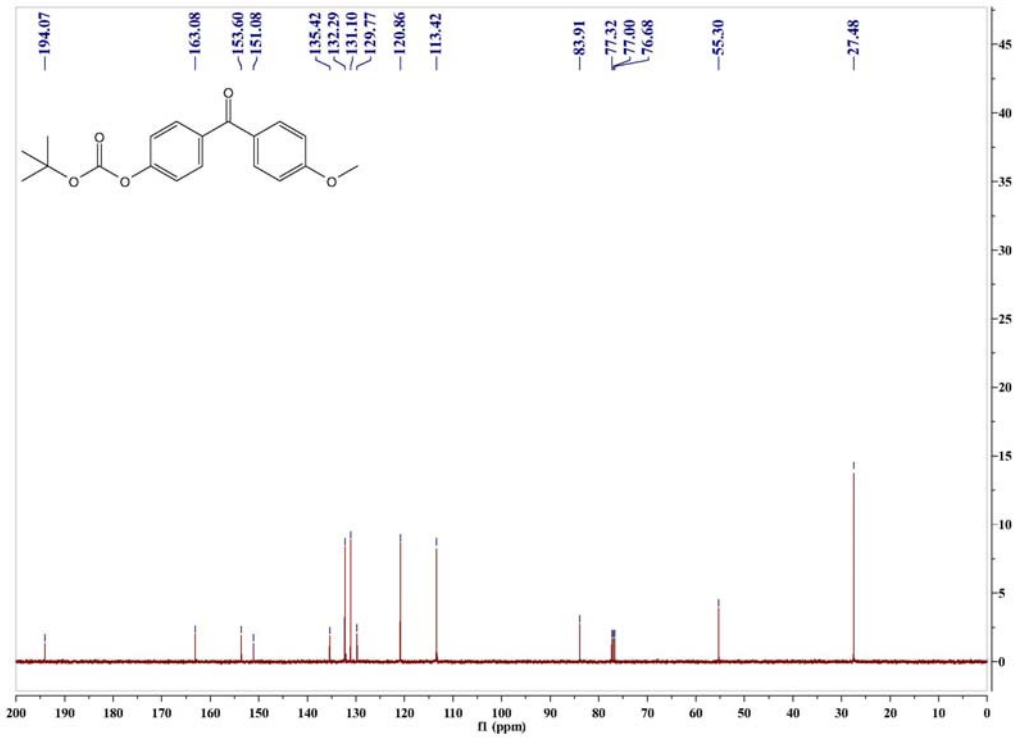
3p


7.77
7.76
7.75
7.74
6.94
6.92
6.66
6.64
3.84
3.02
0.00
3.99
1.99
2.01
3.00
5.97
f1 (ppm)

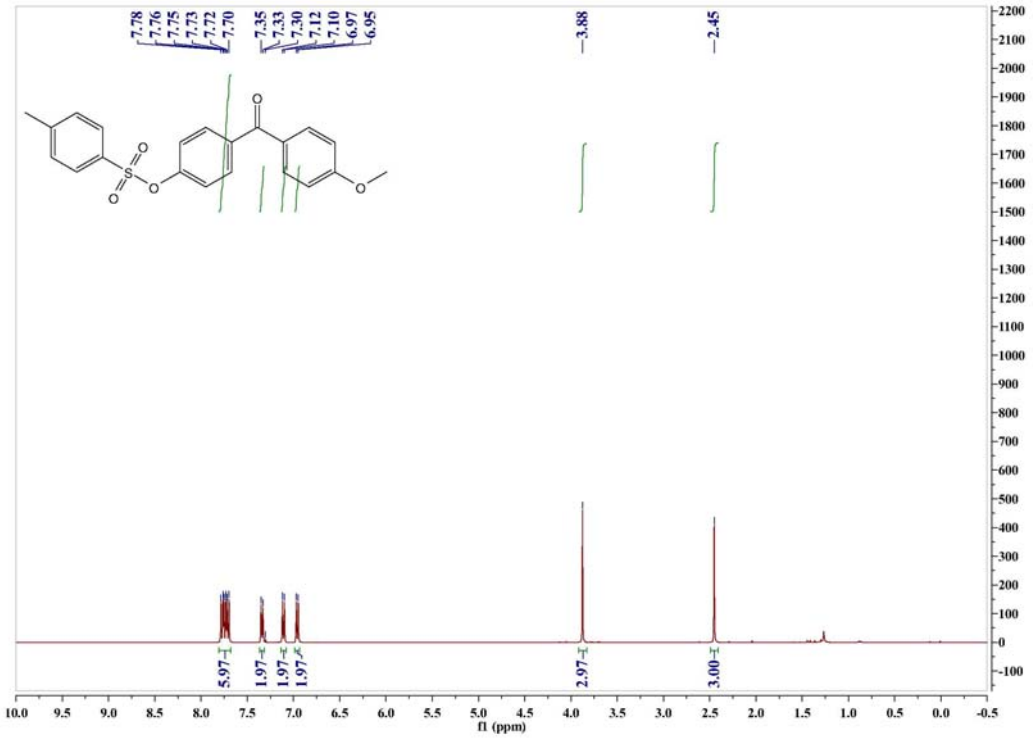

193.87
162.02
152.80
132.25
131.65
131.41
124.93
113.06
110.29
77.32
77.00
76.68
55.20
39.83
f1 (ppm)

3q


7.82
7.81
7.80
7.79
7.30
7.28
6.96
6.94
3.86
1.58
1.93
2.02
2.01
2.07
3.00
8.91
f1 (ppm)


194.07
163.08
153.60
151.08
135.42
132.29
131.10
129.77
120.86
113.42
83.91
77.32
77.00
76.68
55.30
27.48
f1 (ppm)

3r


7.78
7.76
7.75
7.73
7.72
7.70
7.35
7.33
7.30
7.12
7.10
6.97
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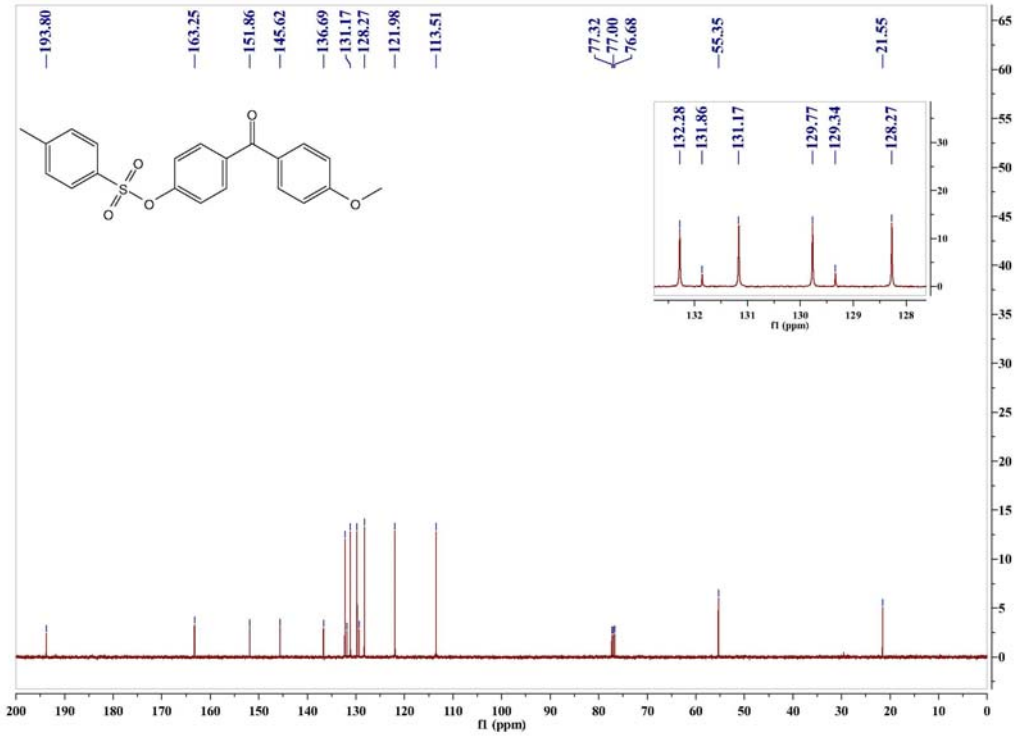
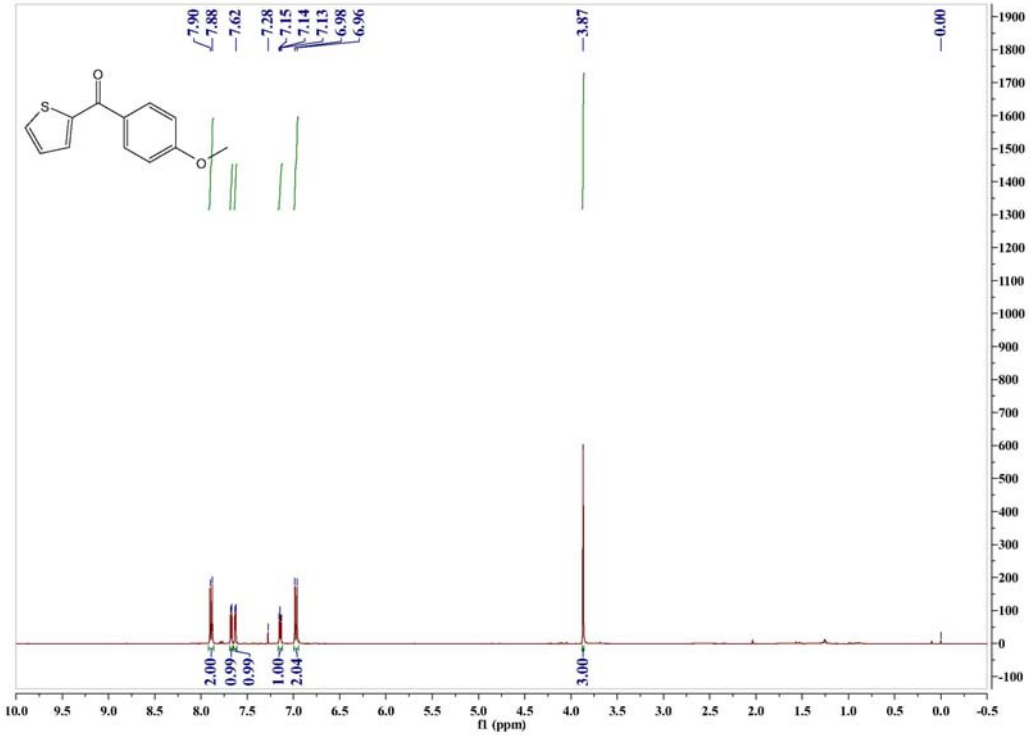
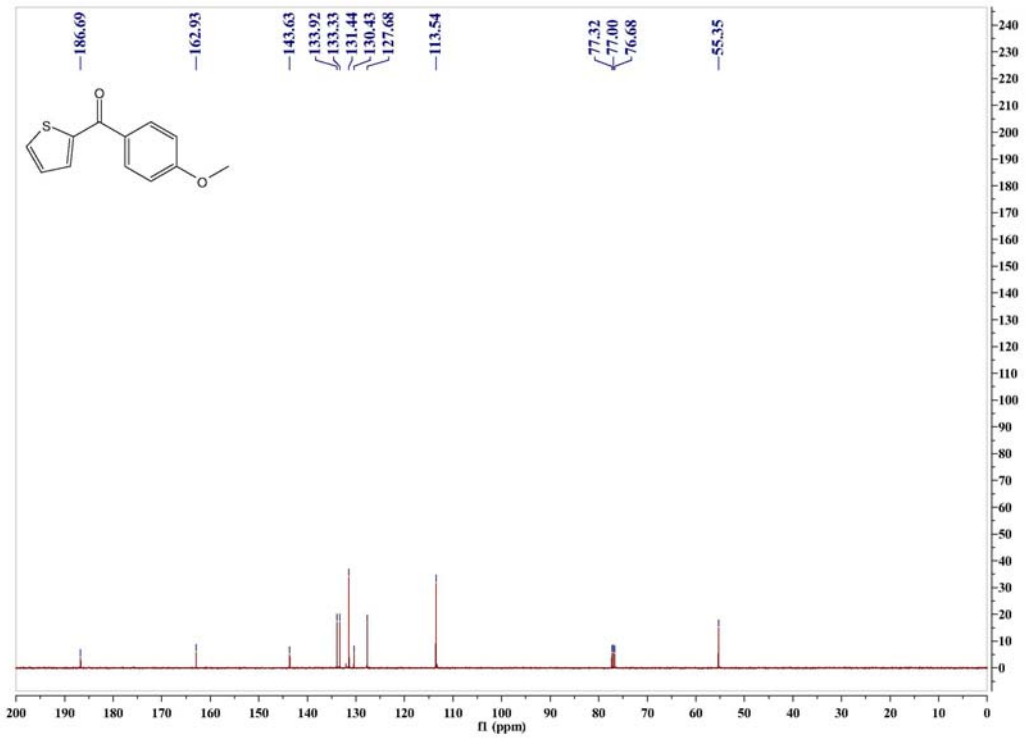
1.97
1.97
1.97
2.97
3.00
f1 (ppm)

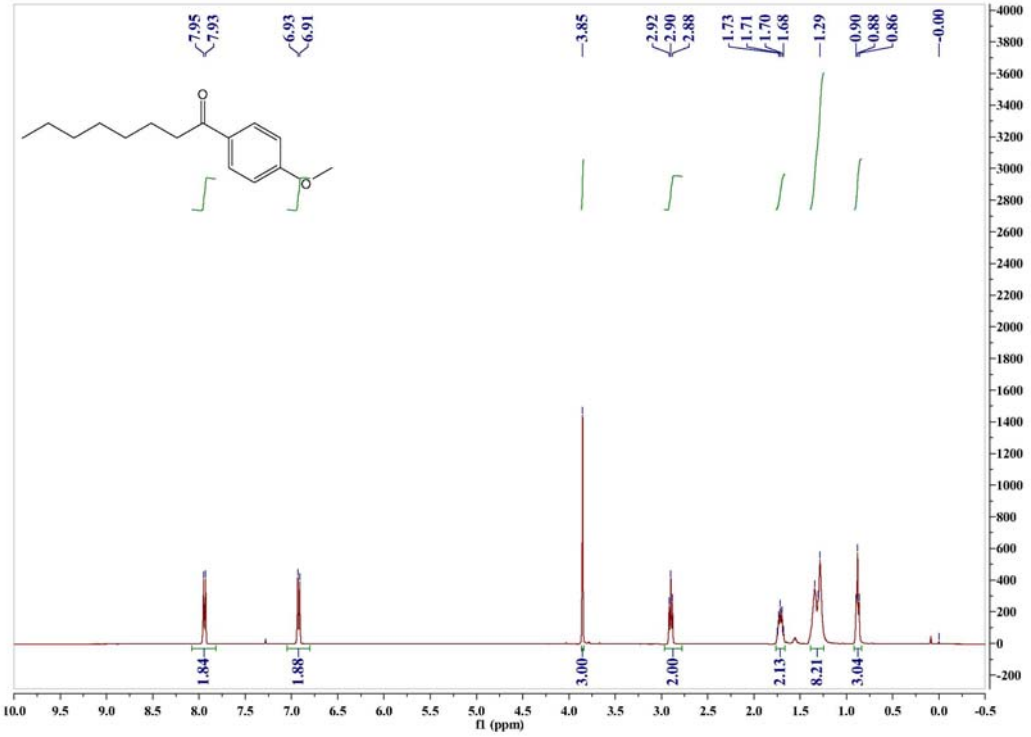

193.80
163.25
151.86
145.62
136.69
131.17
128.27
121.98
113.51
77.32
77.00
76.68
55.35
21.55
132.28
131.86
131.17
129.77
129.34
128.27
f1 (ppm)

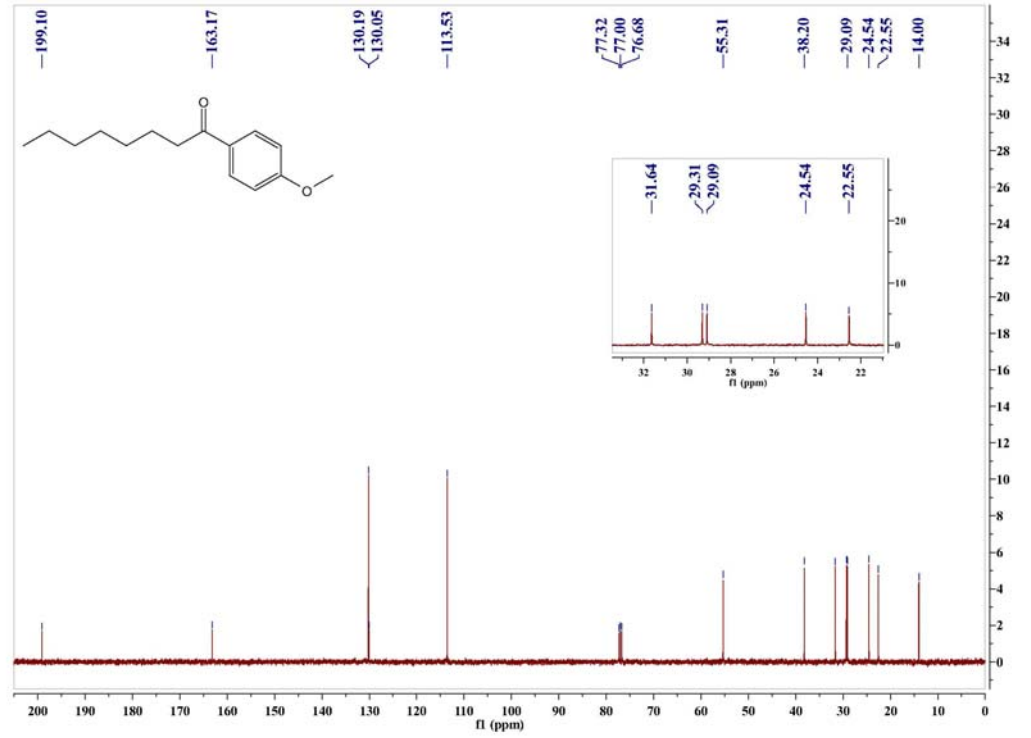
3s


7.90
7.88
7.62
7.28
7.15
7.14
7.13
6.98
6.96
3.87
0.00
2.00
0.99
0.99
1.00
2.04
3.00
f1 (ppm)

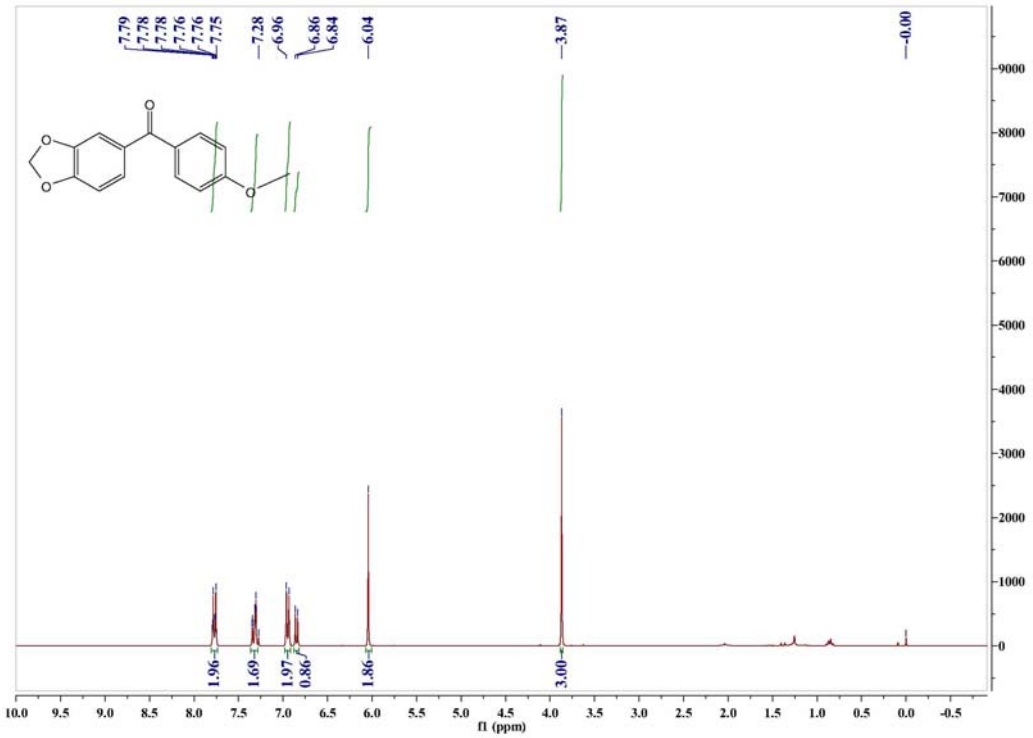

186.69
162.93
143.63
133.92
133.33
131.44
130.43
127.68
113.54
77.32
77.00
76.68
55.35
f1 (ppm)

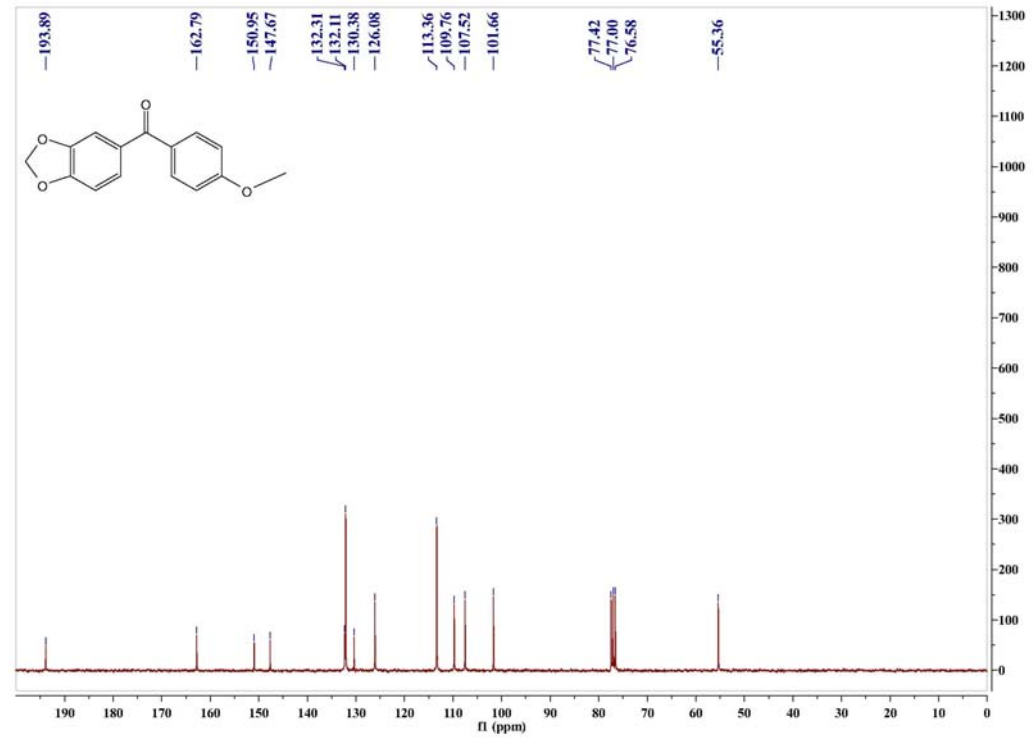
3t


7.95
7.93
6.93
6.91
3.85
2.92
2.90
2.88
1.73
1.71
1.70
1.68
1.29
0.90
0.88
0.86
0.00
1.84
1.88
3.00
2.00
2.13
8.21
3.04
f1 (ppm)

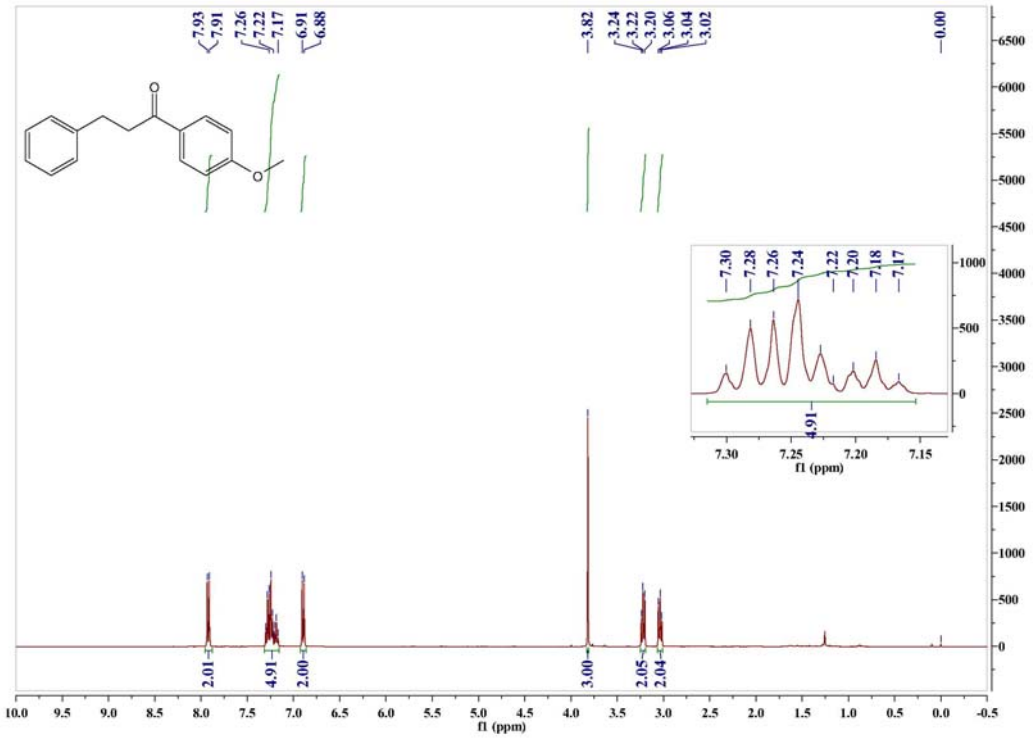

199.10
163.17
130.19
130.05
113.53
77.32
77.00
76.68
55.31
38.20
29.09
24.54
22.55
14.00
31.64
29.31
29.09
24.54
22.55
f1 (ppm)

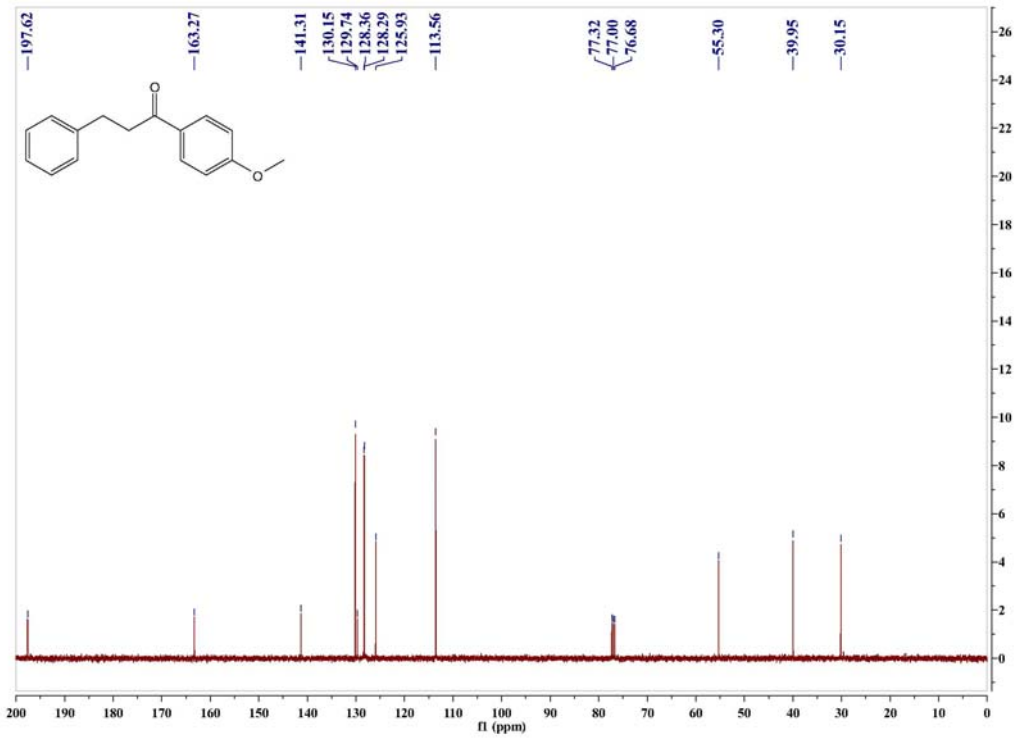
3u


7.79
7.78
7.78
7.76
7.76
7.75
7.28
6.96
6.86
6.84
6.04
3.87
0.00
1.96
1.69
1.97
0.86
1.86
3.00
f1 (ppm)

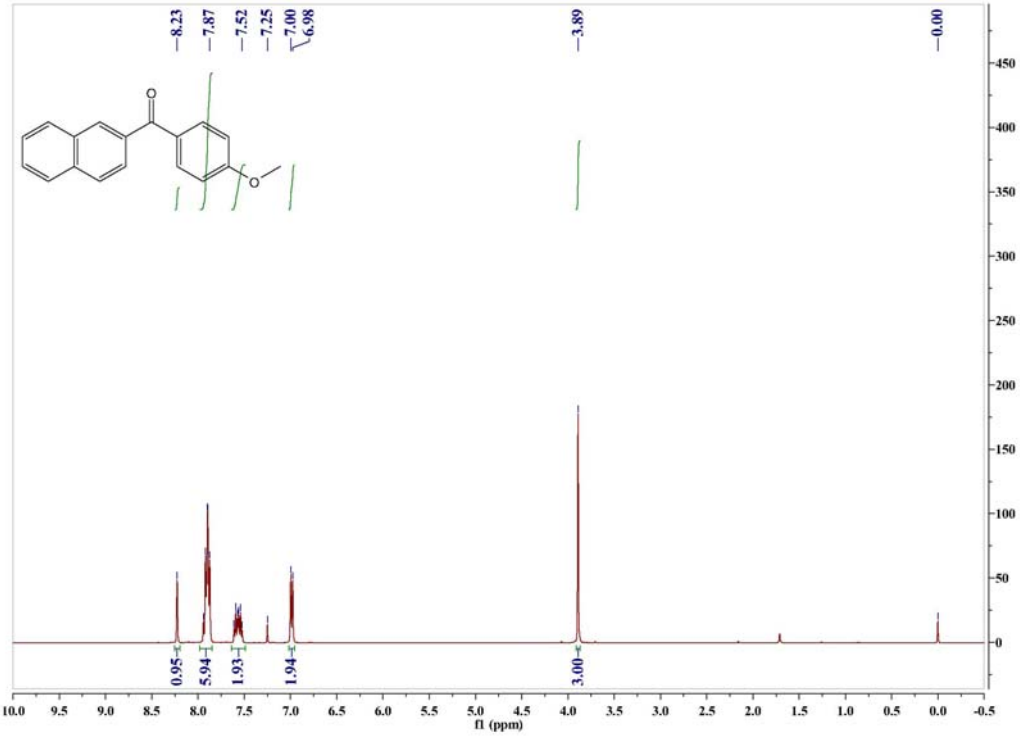

193.89
162.79
150.95
147.67
132.31
132.11
130.38
126.08
113.36
109.76
107.52
101.66
77.42
77.00
76.58
55.36
f1 (ppm)

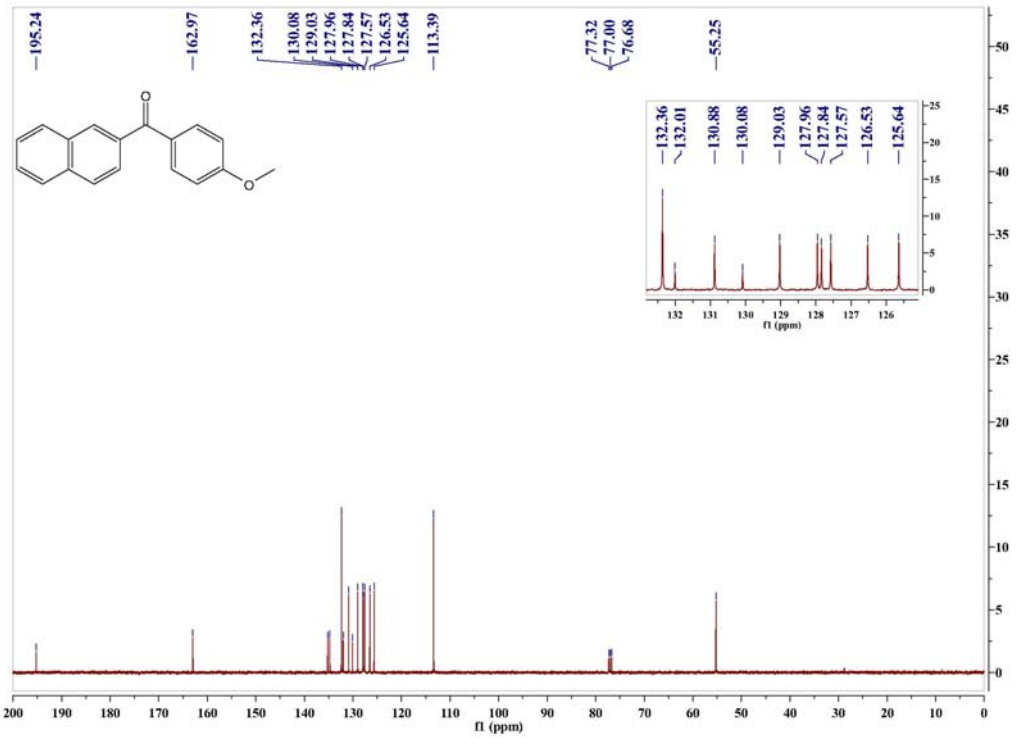
3v


7.93
7.91
7.26
7.22
7.17
6.91
6.88
3.82
3.24
3.22
3.20
3.06
3.04
3.02
0.00
7.30
7.28
7.26
7.24
7.22
7.20
7.18
7.17
4.91
2.01
4.91
2.00
3.00
2.05
2.04
f1 (ppm)

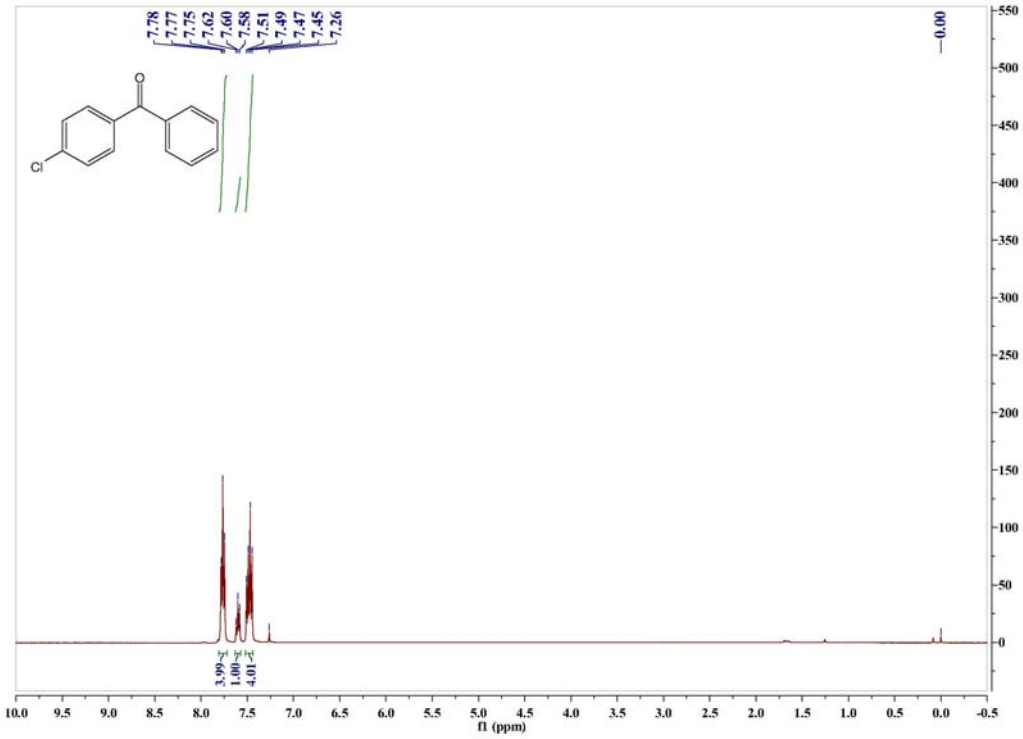

197.62
163.27
141.31
130.15
129.74
128.36
128.29
125.93
113.56
77.32
77.00
76.68
55.30
39.95
30.15
f1 (ppm)

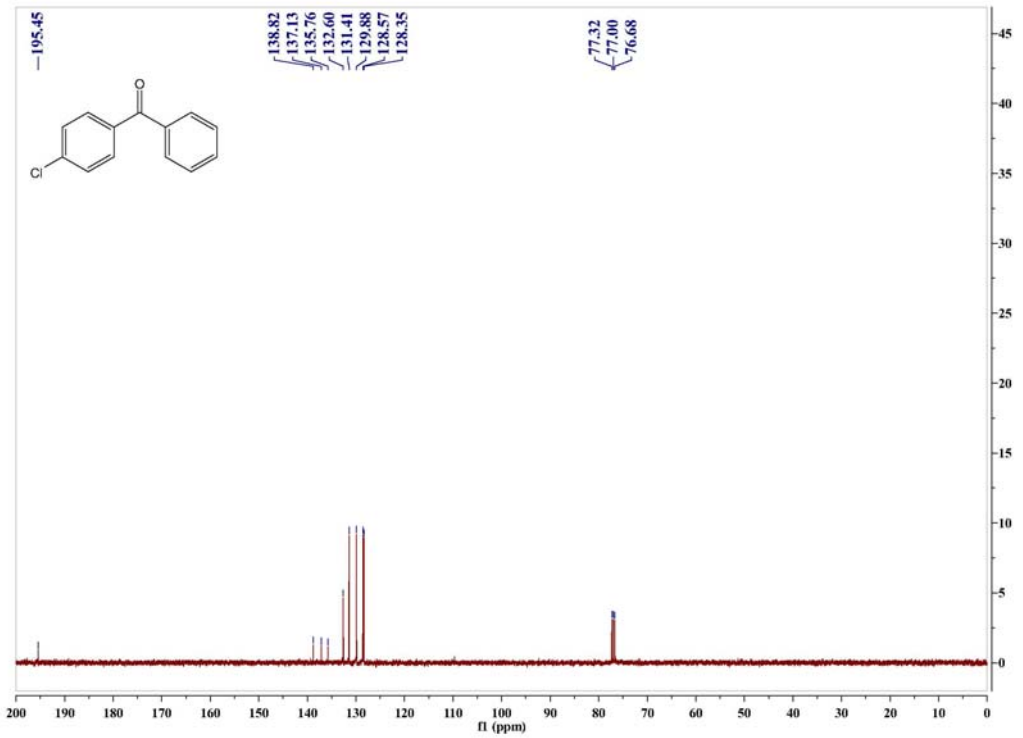
3w


8.23
7.87
7.52
7.25
7.00
6.98
3.89
0.00
0.95
5.94
1.93
1.94
3.00
f1 (ppm)

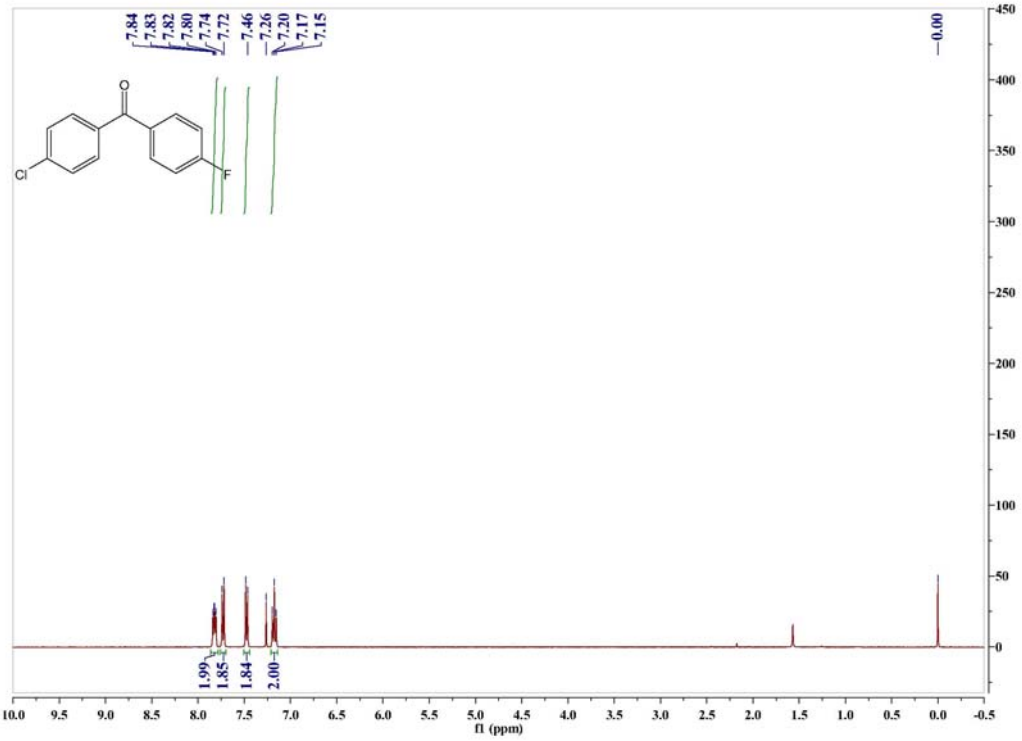

195.24
162.97
132.36
130.08
129.03
127.96
127.84
127.57
126.53
125.64
113.39
77.32
77.00
76.68
55.25
132.36
132.01
130.88
130.08
129.03
127.96
127.84
127.57
126.53
125.64
f1 (ppm)

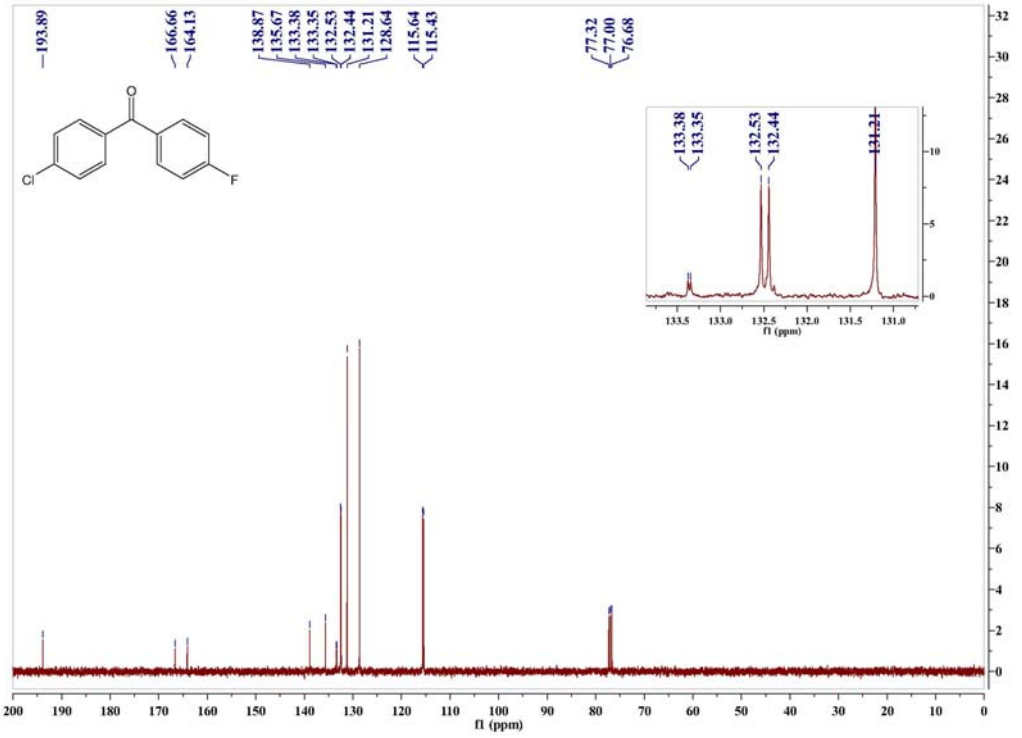
4a


7.78
7.77
7.75
7.62
7.60
7.58
7.51
7.49
7.47
7.45
7.26
0.00
3.99
1.00
4.01
f1 (ppm)

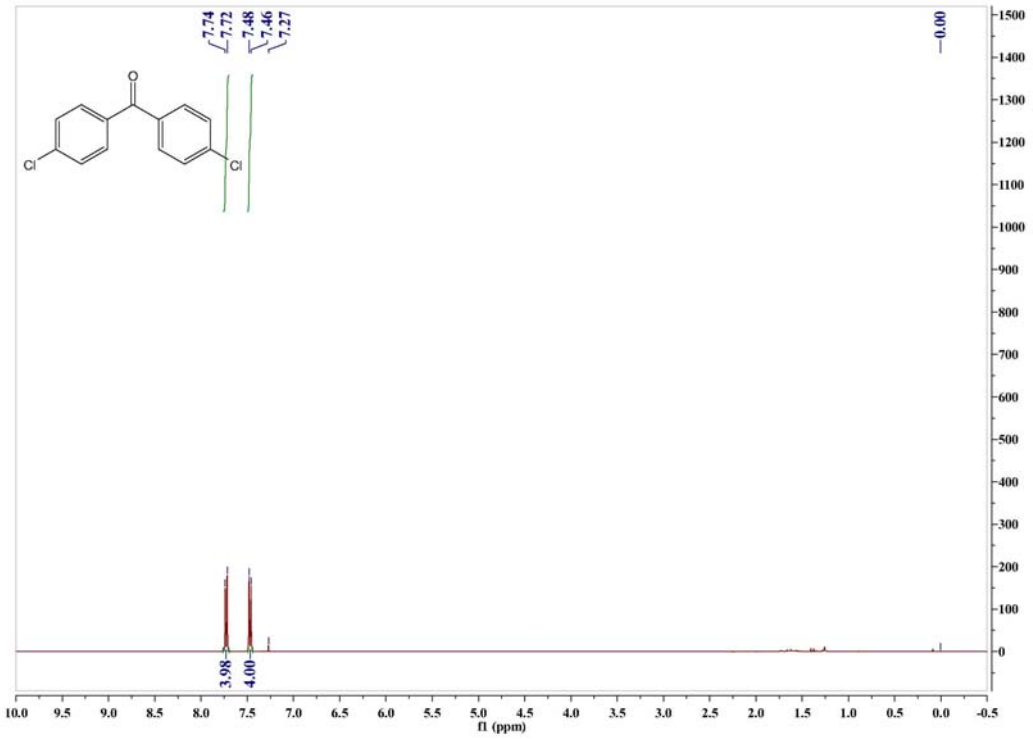

195.45
138.82
137.13
135.76
132.60
131.41
129.88
128.57
128.35
77.32
77.00
76.68
f1 (ppm)

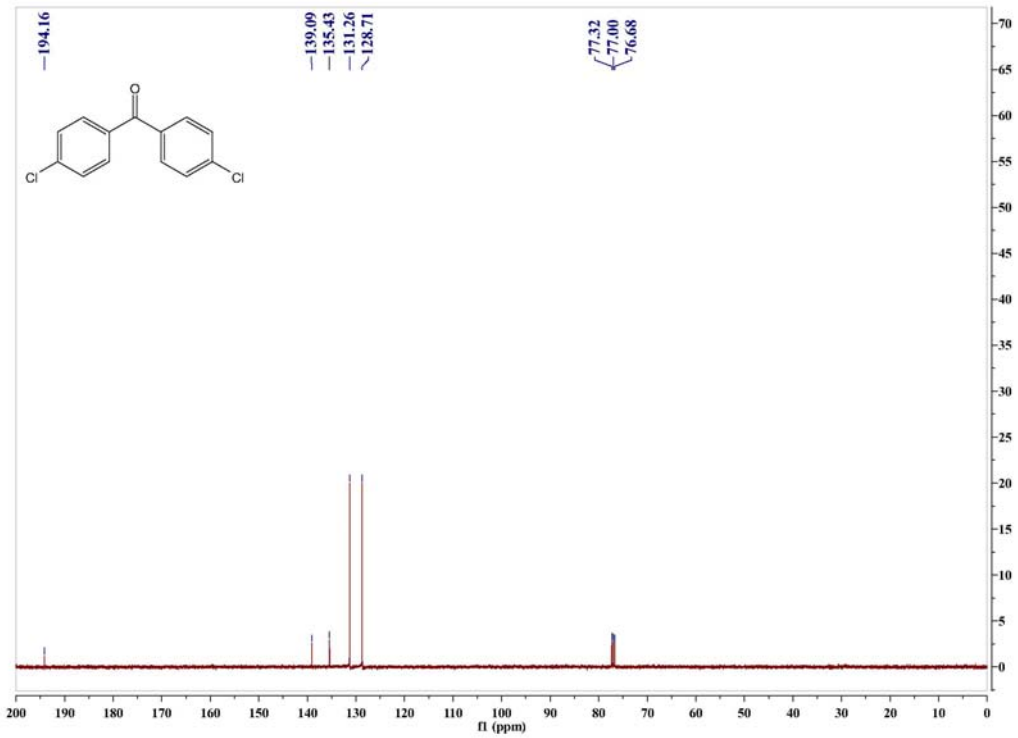
4b


7.84
7.83
7.82
7.80
7.74
7.72
7.46
7.26
7.20
7.17
7.15
0.00
Cl
F
O
1.99
1.85
1.84
2.00
f1 (ppm)

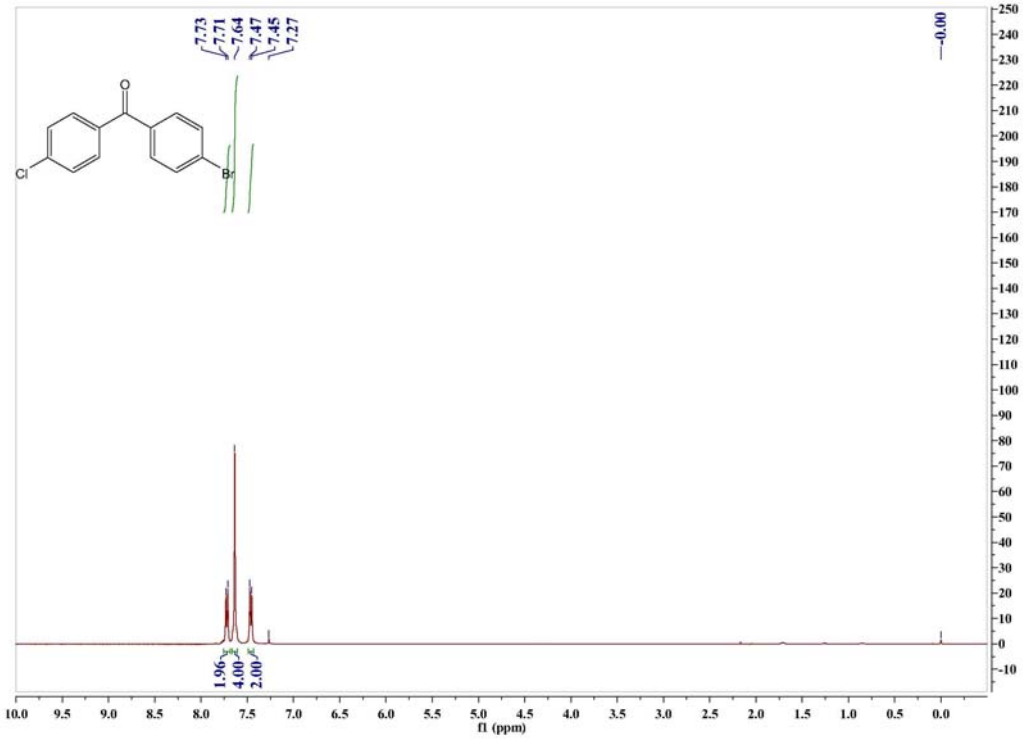

193.89
166.66
164.13
138.87
135.67
133.38
133.35
132.53
132.44
131.21
128.64
115.64
115.43
77.32
77.00
76.68
133.38
133.35
132.53
132.44
131.21
Cl
F
O
f1 (ppm)

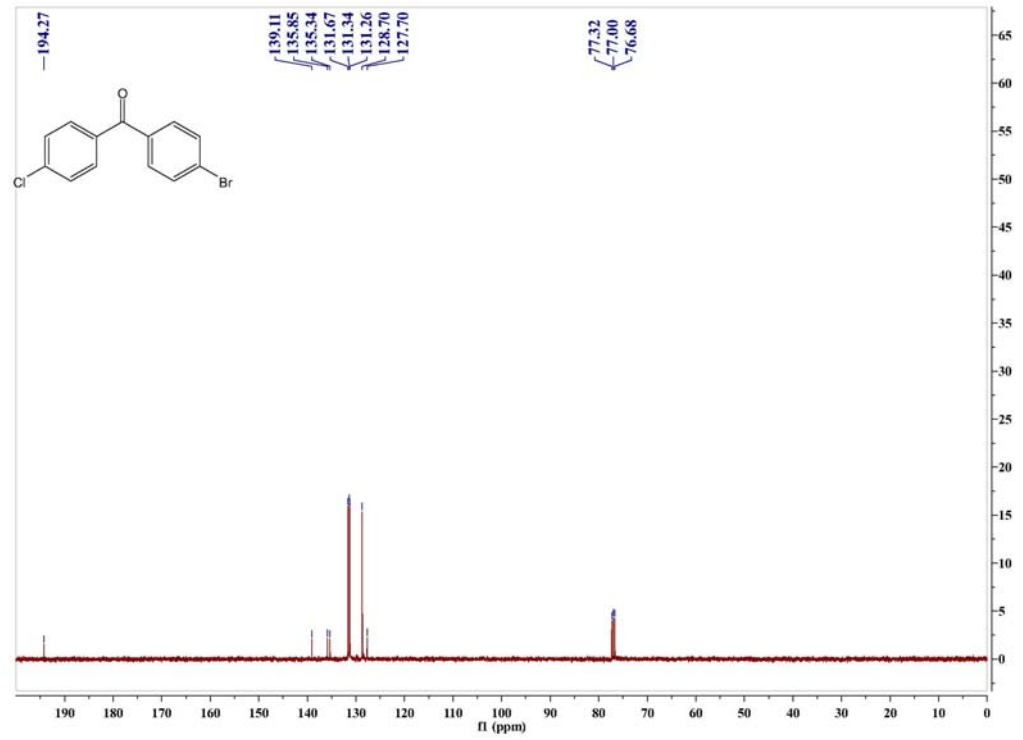
4c


7.74
7.72
7.48
7.46
7.27
0.00
O
Cl
Cl
3.98
4.00
f1 (ppm)

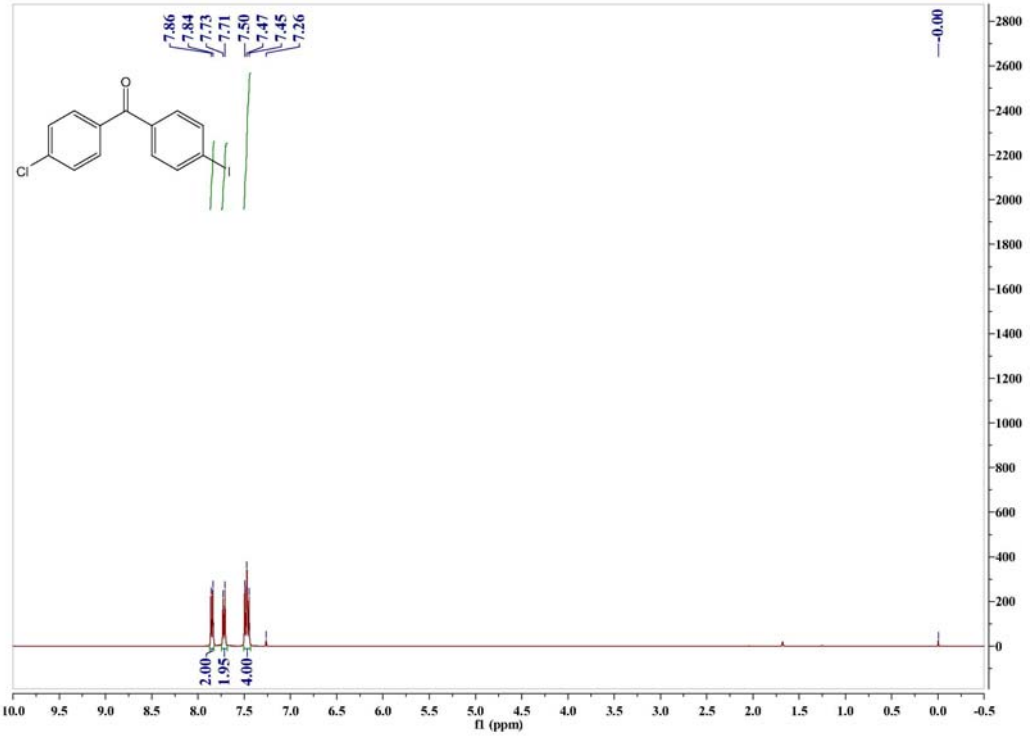

194.16
139.09
135.43
131.26
128.71
77.32
77.00
76.68
O
Cl
Cl
f1 (ppm)

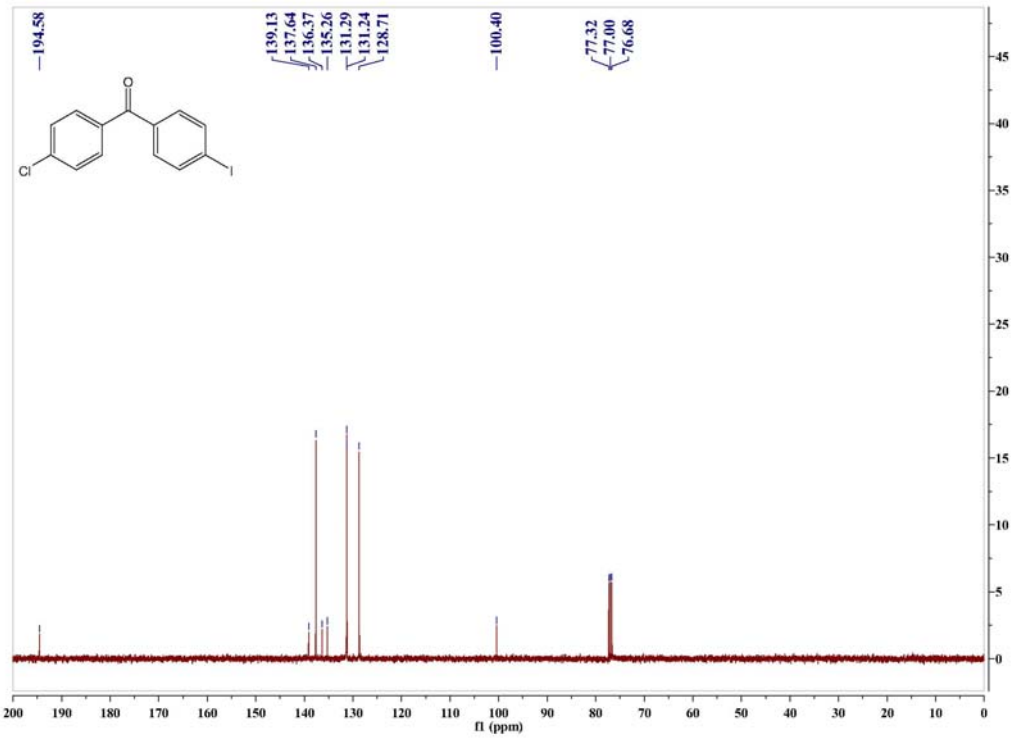
4d


7.73
7.71
7.64
7.47
7.45
7.27
-0.00
O
Cl
Br
1.96
4.00
2.00
f1 (ppm)

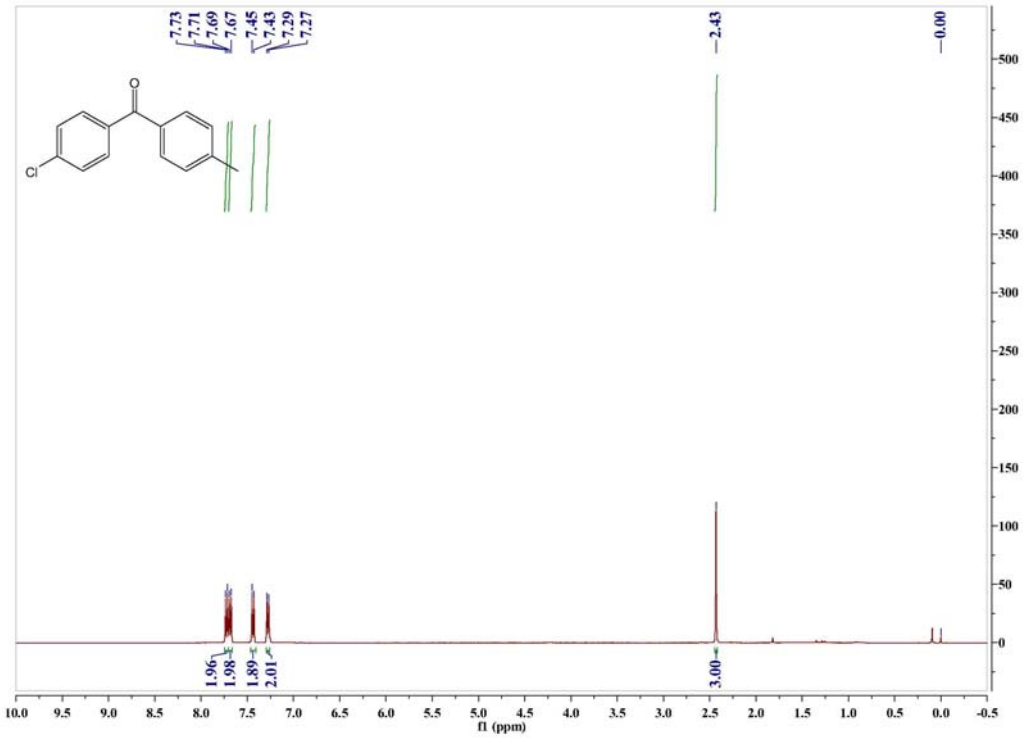

194.27
139.11
135.85
135.34
131.67
131.34
131.26
128.70
127.70
77.32
77.00
76.68
O
Cl
Br
f1 (ppm)

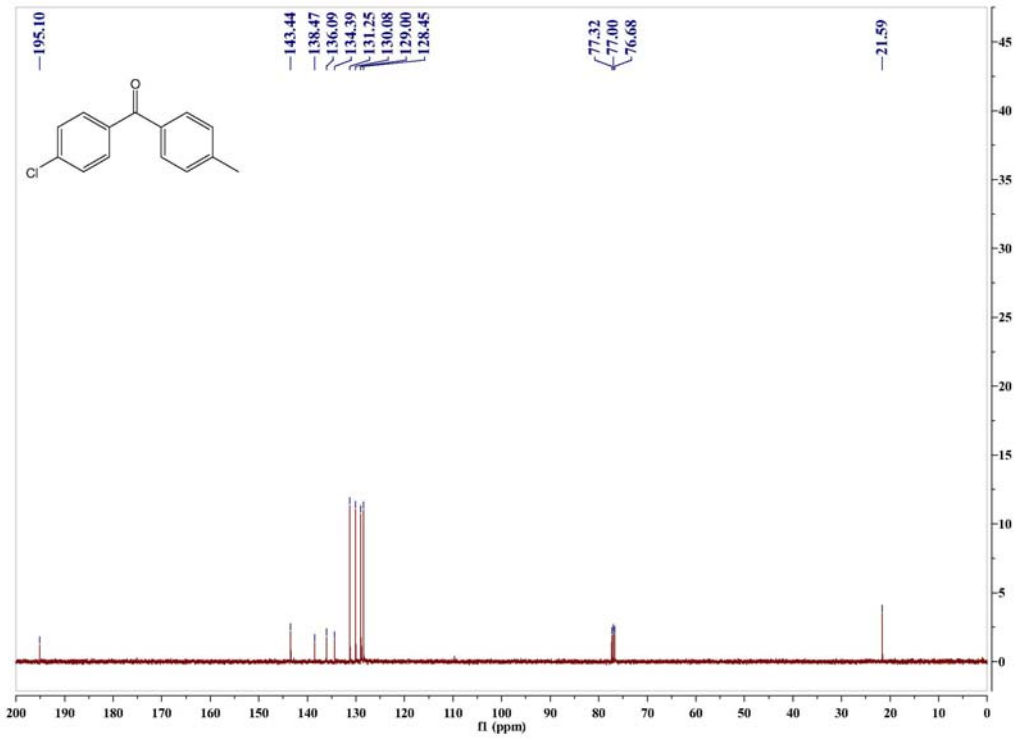
4e


7.86
7.84
7.73
7.71
7.50
7.47
7.45
7.26
-0.00
O
Cl
I
2.00
1.95
4.00
f1 (ppm)

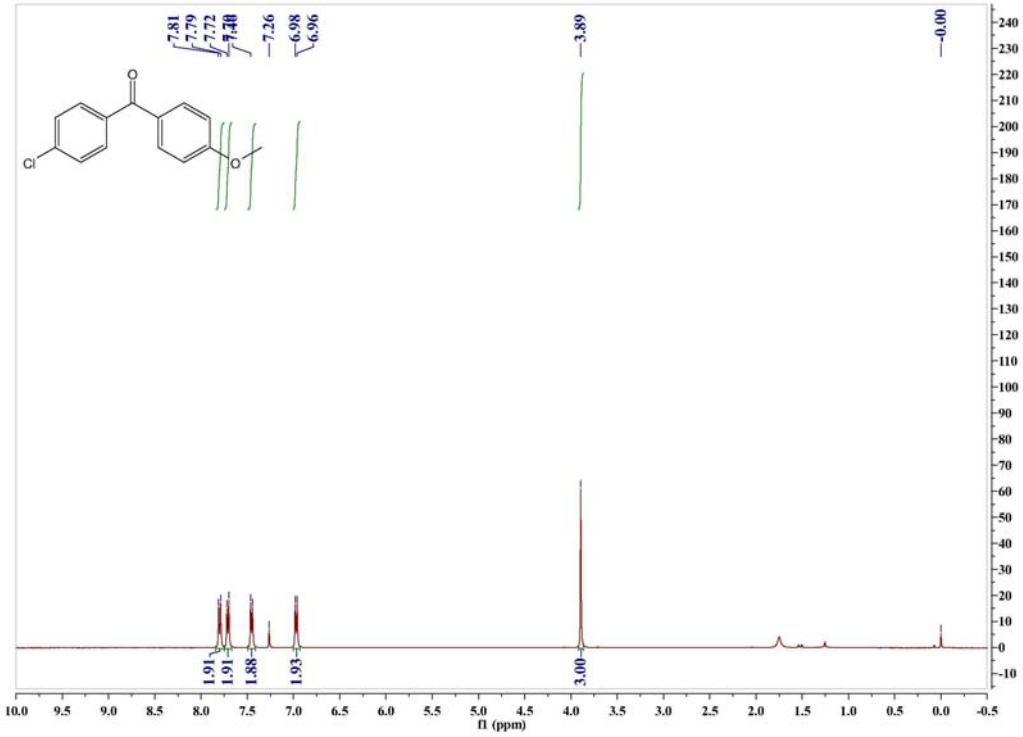

194.58
139.13
137.64
136.37
135.26
131.29
131.24
128.71
100.40
77.32
77.00
76.68
O
Cl
I
f1 (ppm)

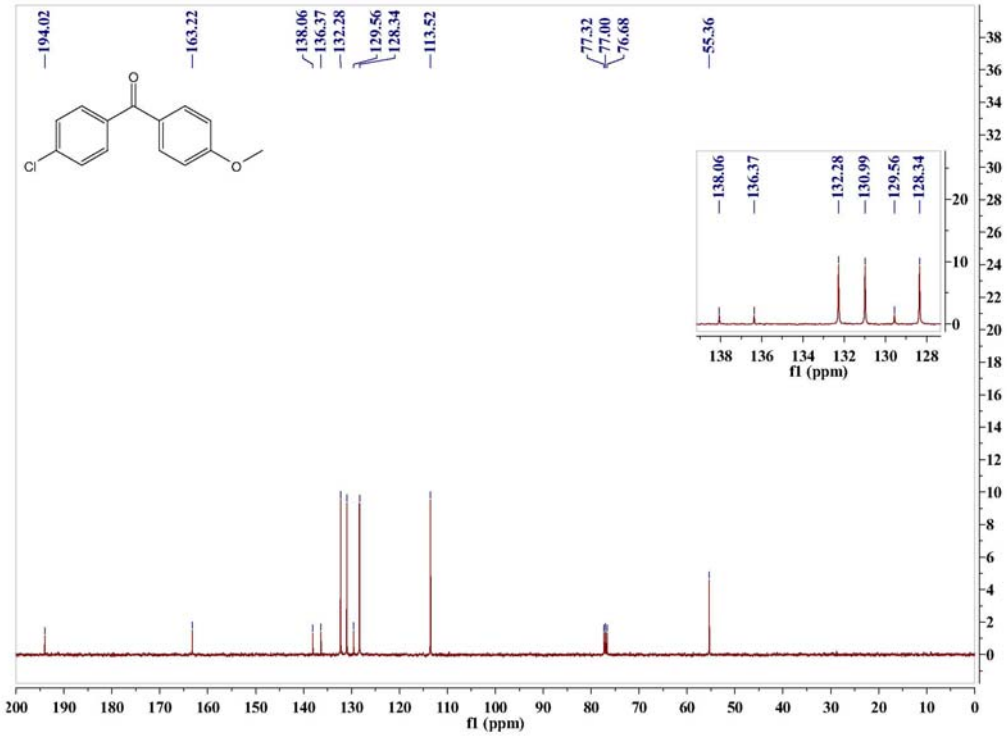
4f


7.73
7.71
7.69
7.67
7.45
7.43
7.29
7.27
2.43
0.00
Cl
O
1.96
1.98
1.89
2.01
3.00
f1 (ppm)

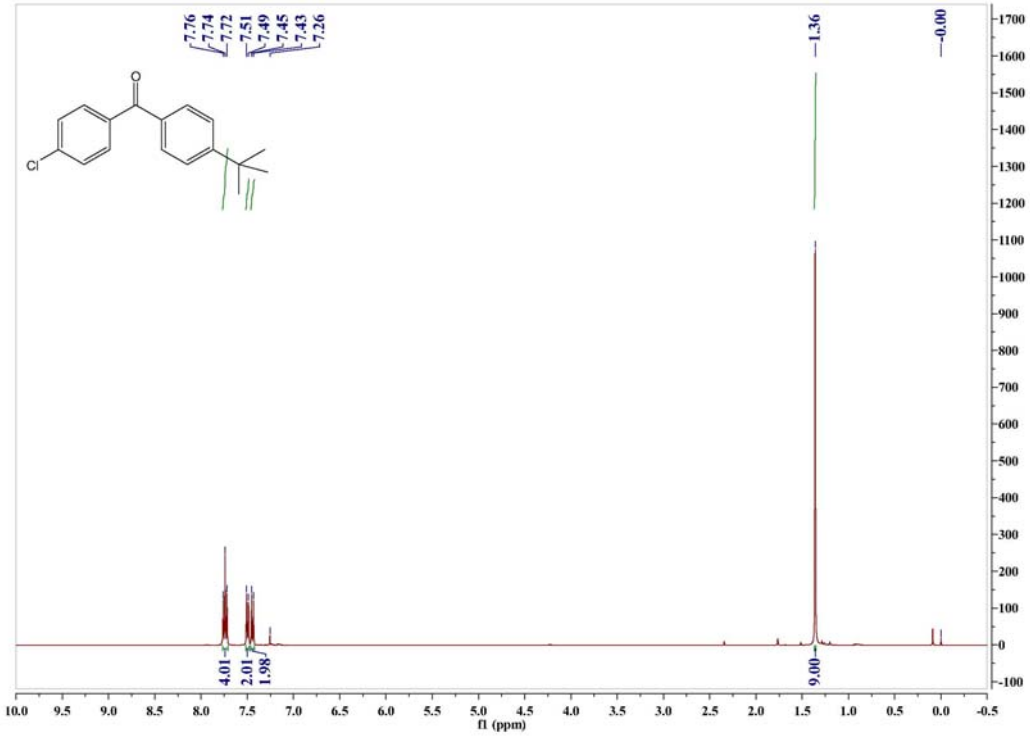

195.10
143.44
138.47
136.09
134.39
131.25
130.08
129.00
128.45
77.32
77.00
76.68
21.59
Cl
O
f1 (ppm)

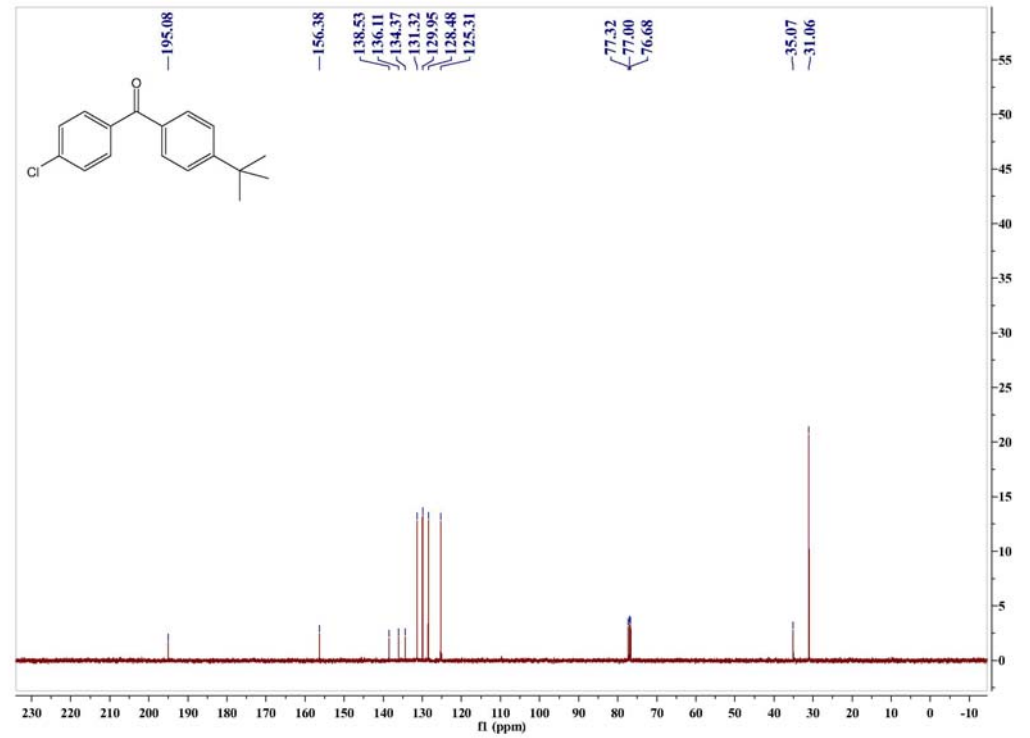
4g


7.81
7.79
7.72
7.26
6.98
6.96
3.89
0.00
Cl
O
O
1.91
1.91
1.88
1.93
3.00
f1 (ppm)

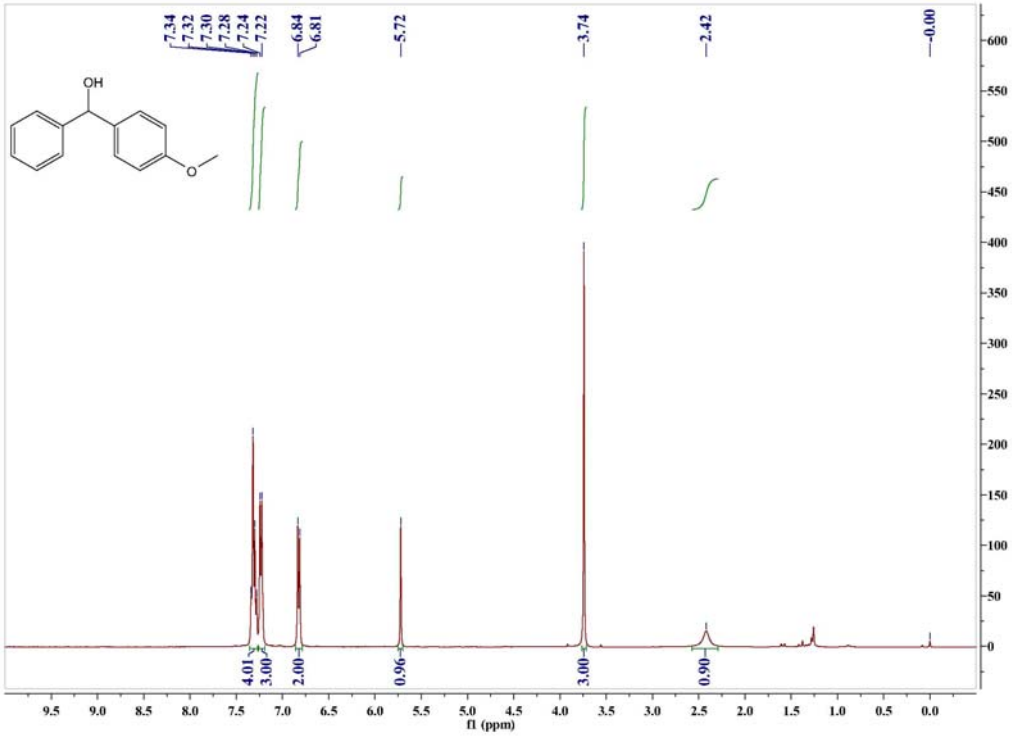

194.02
163.22
138.06
136.37
132.28
129.56
128.34
113.52
77.32
77.00
76.68
55.36
Cl
O
O
f1 (ppm)

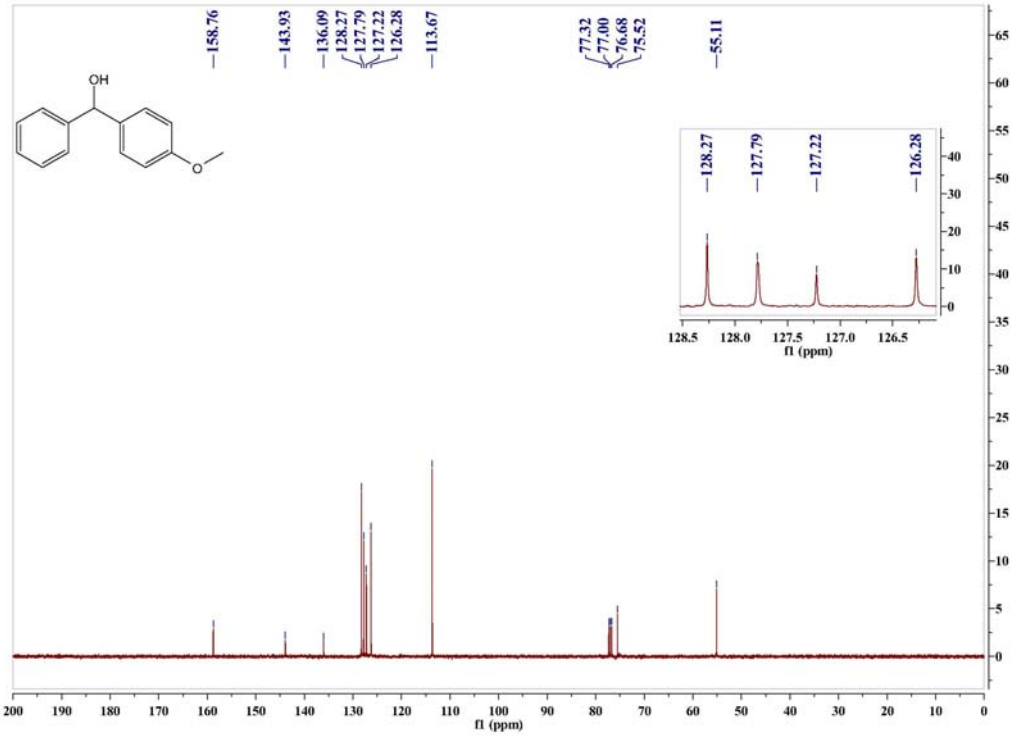
4h


7.76
7.74
7.72
7.51
7.49
7.45
7.43
7.26
1.36
0.00
Cl
O
4.01
2.01
1.98
9.00
f1 (ppm)


195.08
156.38
138.53
136.11
134.37
131.32
129.95
128.48
125.31
77.32
77.00
76.68
35.07
31.06
Cl
O
f1 (ppm)

5


7.34
7.32
7.30
7.28
7.24
7.22
6.84
6.81
5.72
3.74
2.42
0.00
OH
O
4.01
3.00
2.00
0.96
3.00
0.90
f1 (ppm)


158.76
143.93
136.09
128.27
127.79
127.22
126.28
113.67
77.32
77.00
76.68
75.52
55.11
OH
O
f1 (ppm)