Isolation and Characterization of Trinuclear Cobalt Complex Containing Trigonal Prismatic Cobalt in Secondary Alcohol Aerobic Oxidation

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SUPPORTING INFORMATION

Table of contents

X-Ray crystallographic analysis

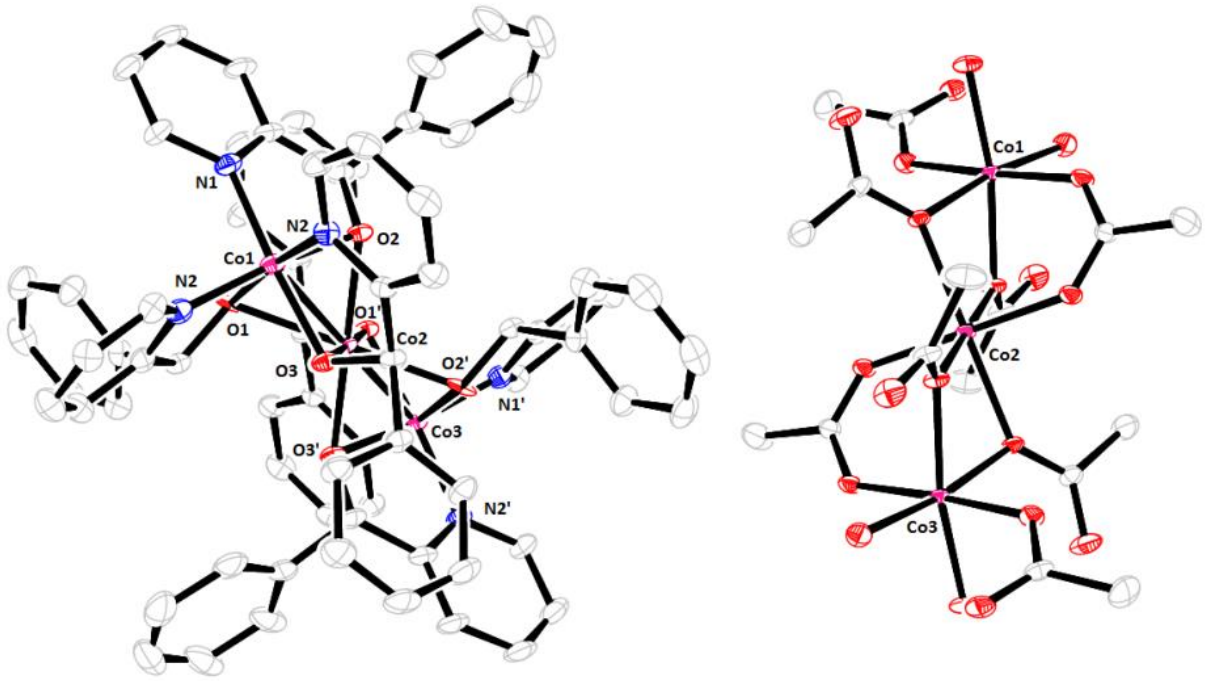


Figure 1. ORTEP diagram of Cobalt trinuclear complex **A**. H atoms omitted for clarity. Relevant bond lengths [Å] and angles [°]: Co1-Co2 2.6351(8), Co1–N1 1.921(7), Co1–N2 1.927(6), Co1–N3 1.930(4), Co1–O1 1.881(3), Co1-O2 1.883(3), Co1-O3 1.871(3), Co3-O4 2.102(2), Co3-O5 2.167(3);N1-Co1-N2 99.0(2), N1-Co1-N3 98.4(2), N1-Co1-O1 86.0(2), N1-Co1-O2 171.2(2), N1-Co1-O3 87.4(2) CCDC No-781092.

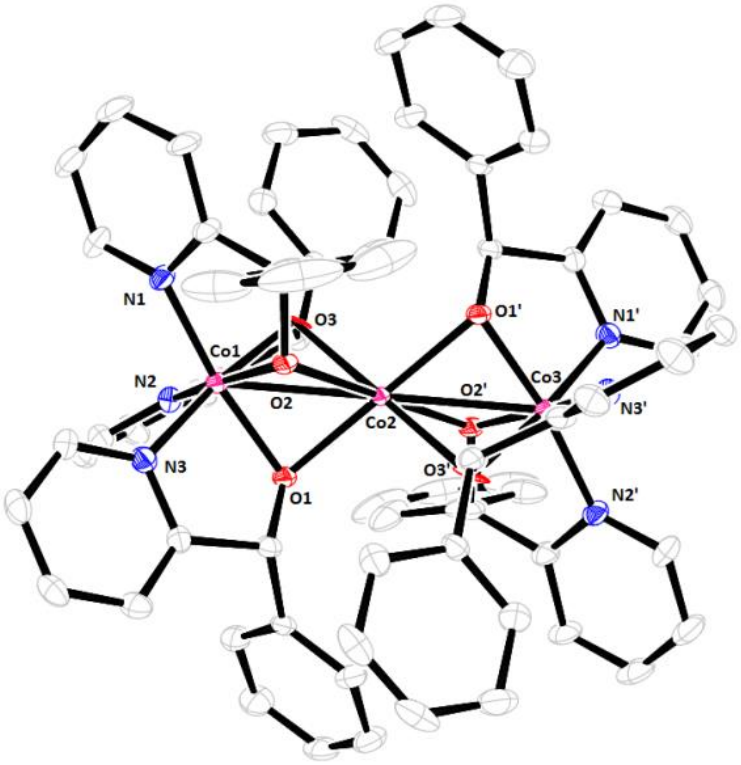


Figure 2. ORTEP diagram of Cobalt trinuclear complex **B**. Thermal ellipsoids are set at 30% probability and H atoms and Acetic acid molecule have been omitted for clarity. Relevant bond lengths [Å] and angles [º]: Co1-Co2 2.6351(8), Co1–N1 1.929(7), Co1–N2 1.920(6), Co1–N3 1.920(4), Co1–O1 1.885(3), Co1-O2 1.882(5), Co1-O3 1.879(4);N1-Co1-N2 98.9(2), N1-Co1-N3 97.8(2), N1-Co1-O1 85.2(2), N1-Co1-O2 170.3(2), N1-Co1-O3 90.4(2).

Table S1: Crystal data and refinement details for **1** and **2**.*

Complex	**A**	**B**
empirical formula	$C_{44}H_{55}Co_3N_3O_{17}$	$C_{76}H_{78}Co_3N_6O_{15}$
formula weight	1074.70	1492.23
crystal system	triclinic	monoclinic
space group	P -1	C2/c
a [Å]	12.6137(7)	29.163(2)
b [Å]	13.1611(7)	17.1312(12)

c [Å]	17.9352(10)	18.0064(13)
α/°	91.643(2)	90.00
β/°	108.545(2)	122.096(2)
γ/°	118.316(2)	90.00
Unit cell volume/Å3	2426.88	7621
Temperature/K	173(2)	293(2)
Measurement reflections used	4323	8234
Measurement theta min	2.6	2.3
Measurement theta max	25.2	23.0
Crystal colour	pink	black

*Supplementary crystallographic data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif: CCDC-781092 (**1**), CCDC-789671(**2**).

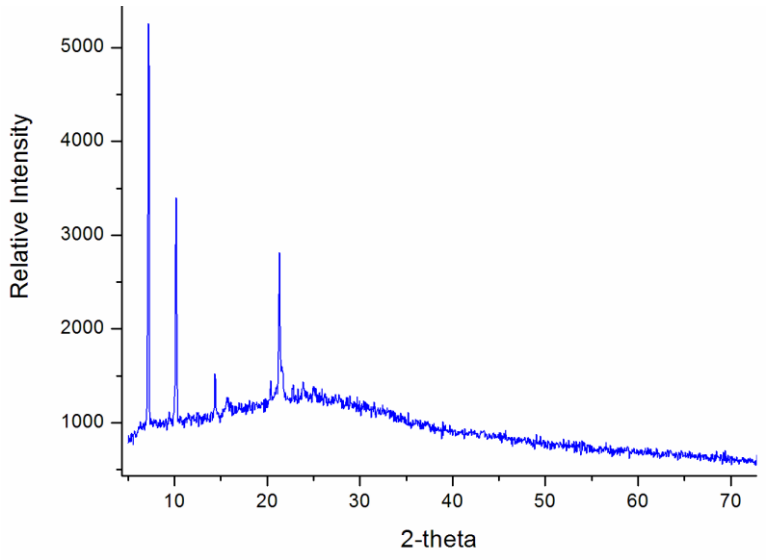
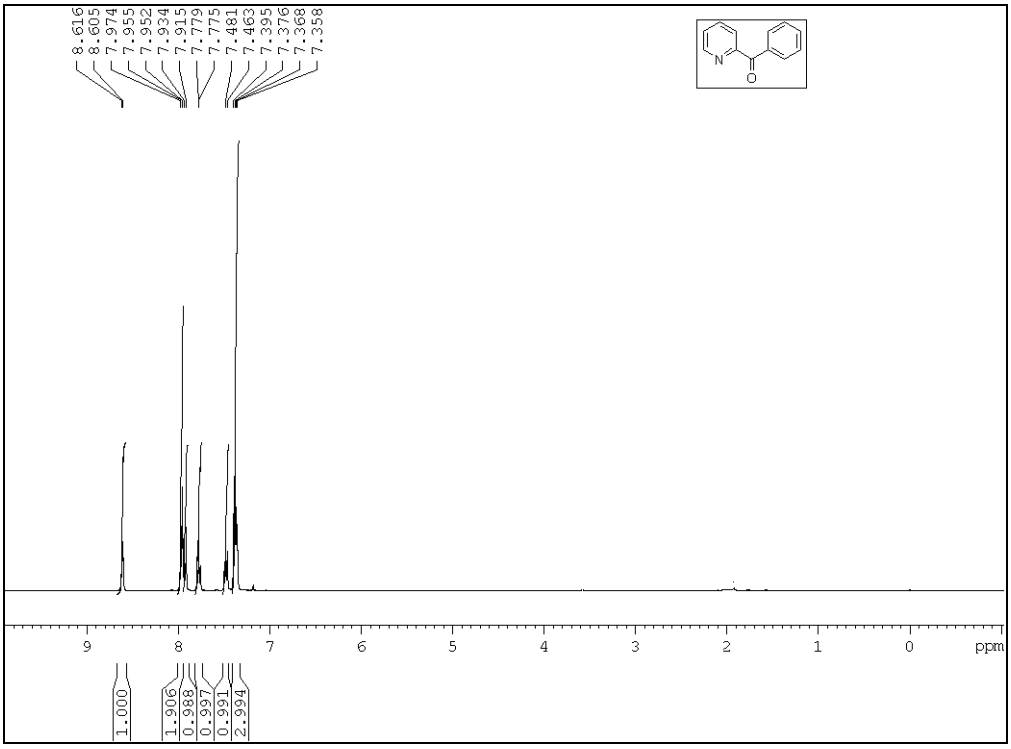
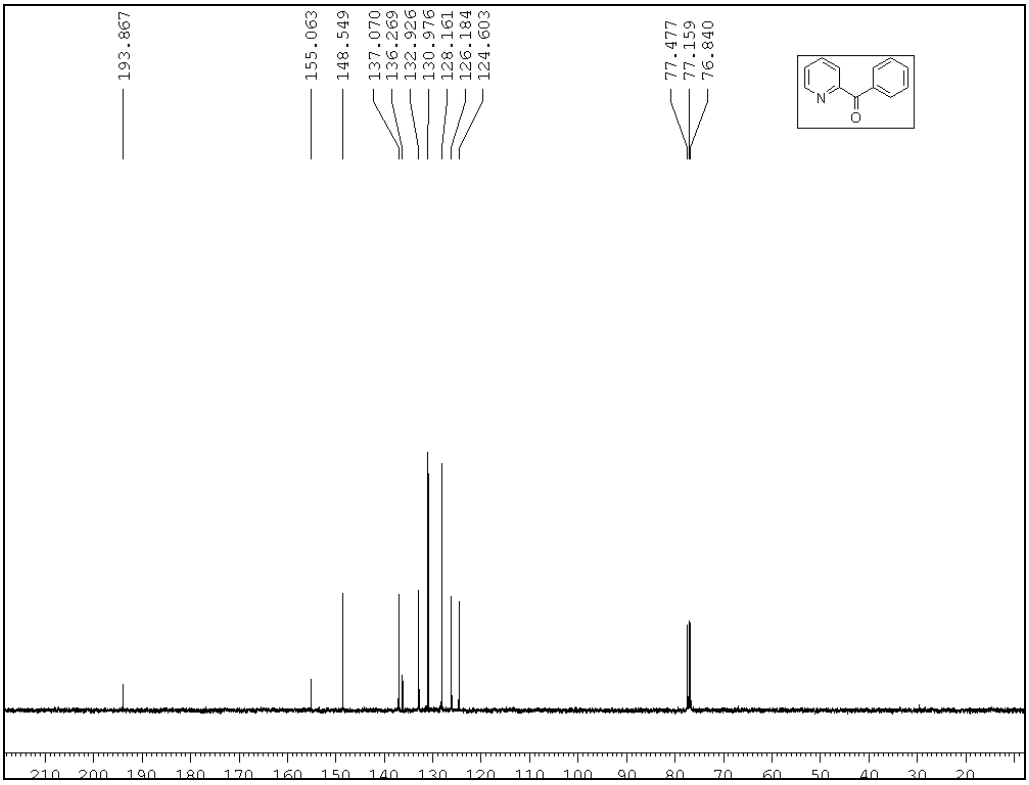


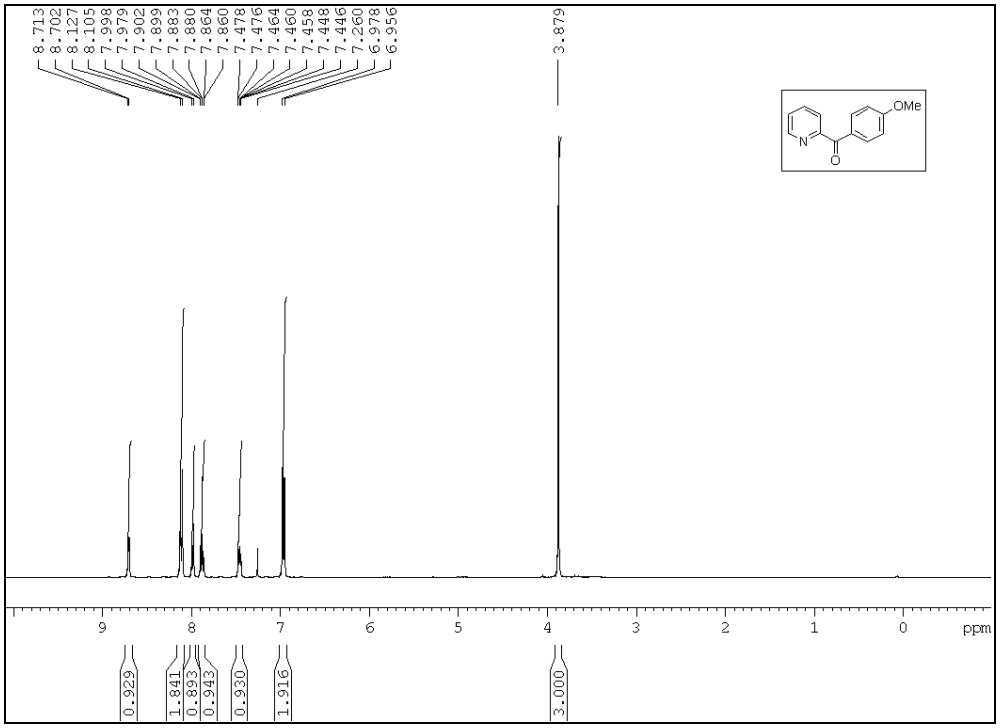
Figure 3. Powder XRD spectrum of reecovered residue



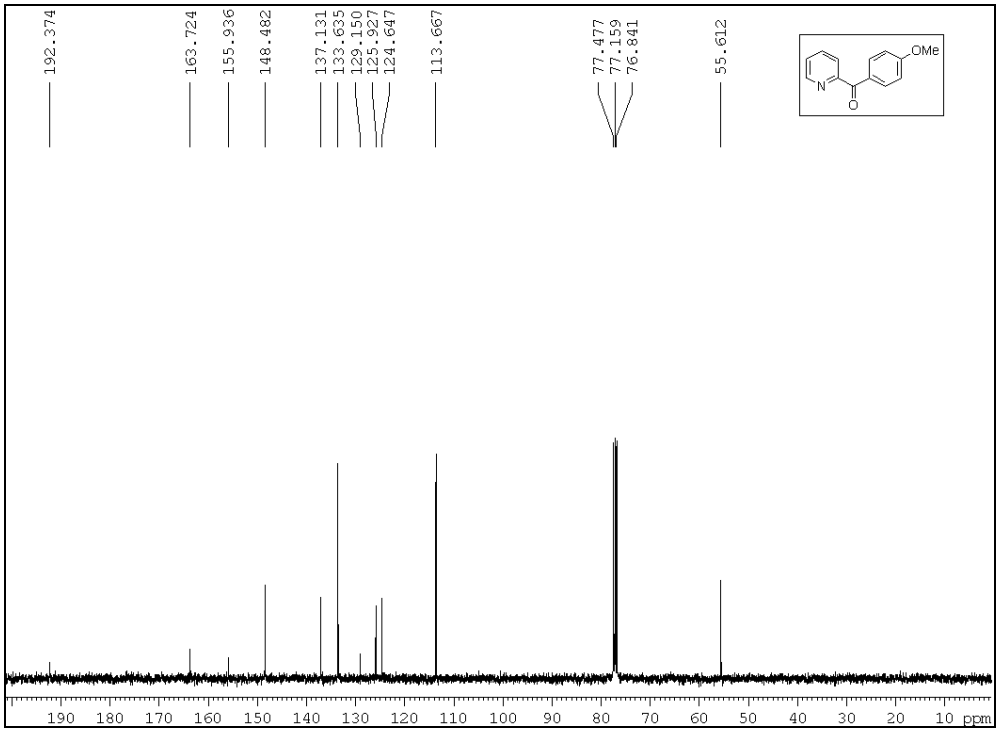
400 MHz ^{1}H NMR of phenyl(pyridin-2-yl)methanone in $CDCl_3$



100 MHz ^{13}C NMR of phenyl(pyridin-2-yl)methanone in $CDCl_3$



400 MHz ^{1}H NMR of (4-Methoxyphenyl) (pyridin-2-yl)methanone in $CDCl_3$



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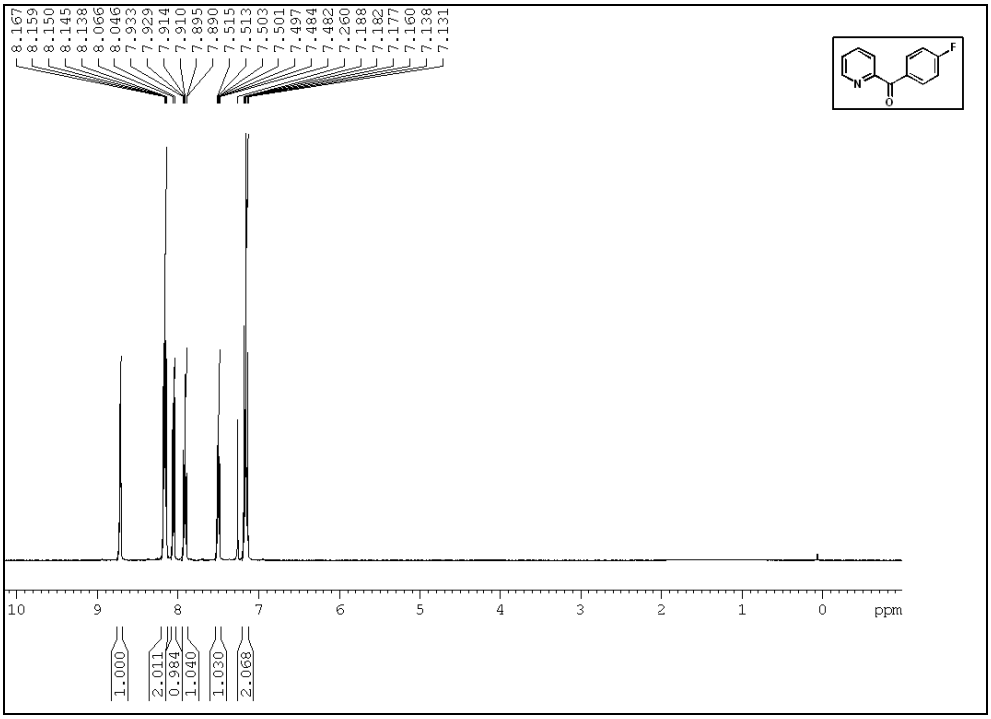
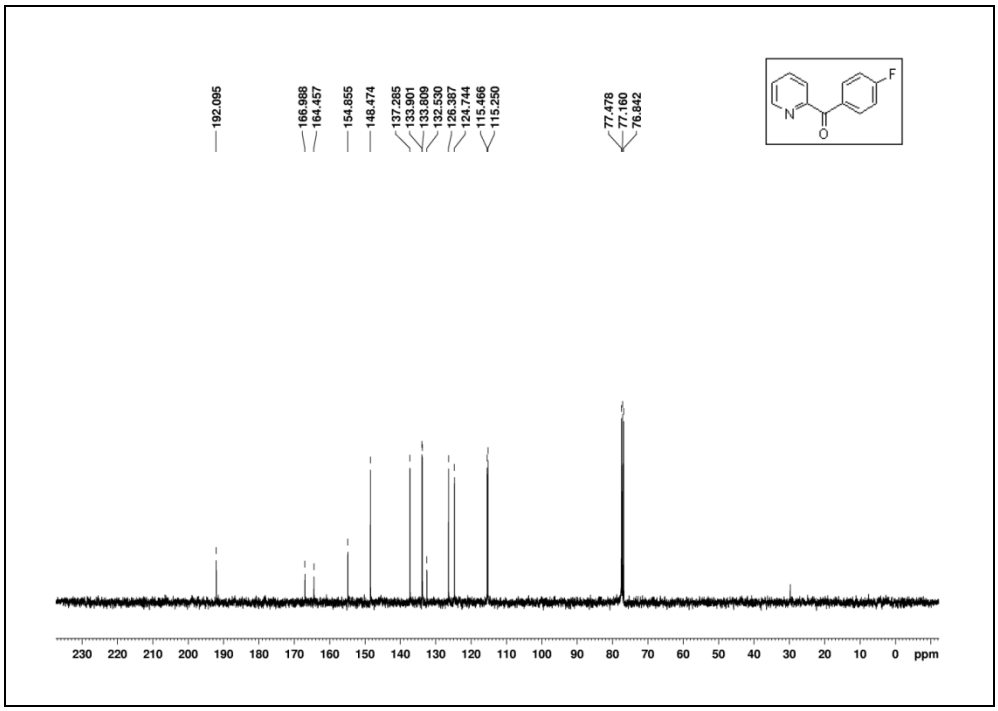


400 MHz ^{1}H NMR of (4-fluorophenyl)(pyridin-2-yl)methanone in $CDCl_3$



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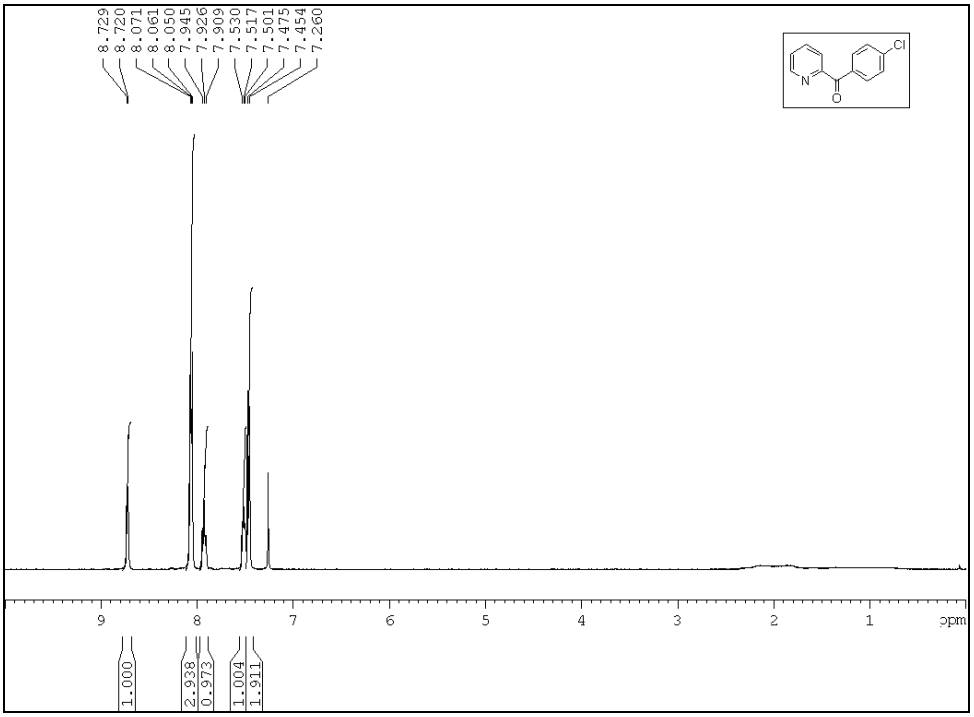
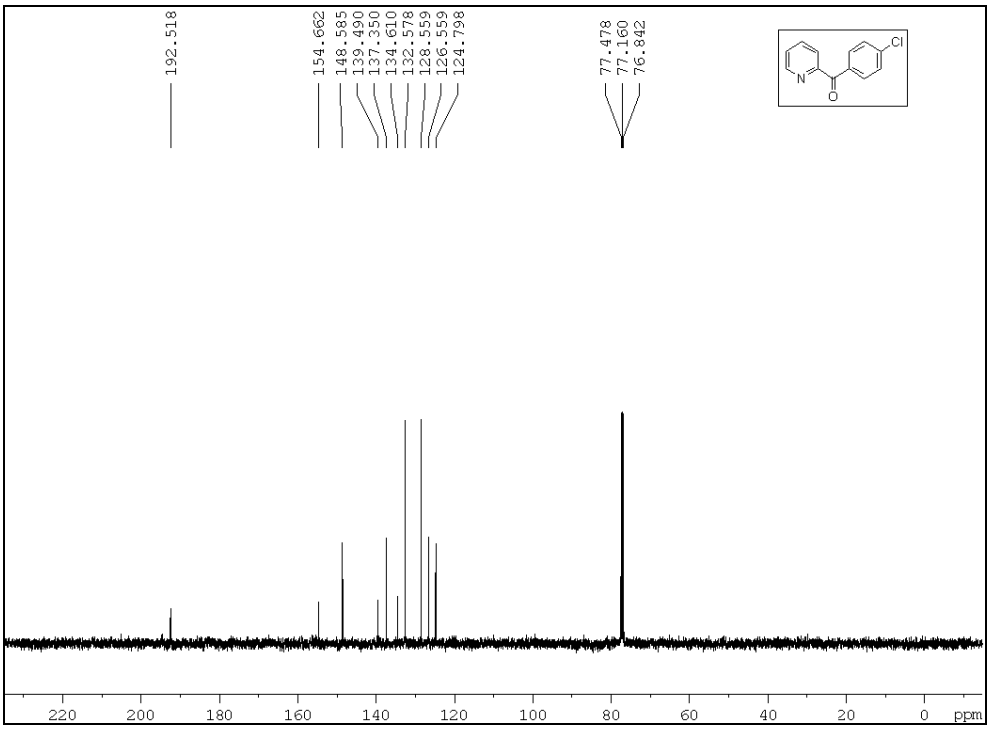


400 MHz ^{1}H NMR of (4-chlorophenyl)(pyridin-2-yl)methanone in $CDCl_3$



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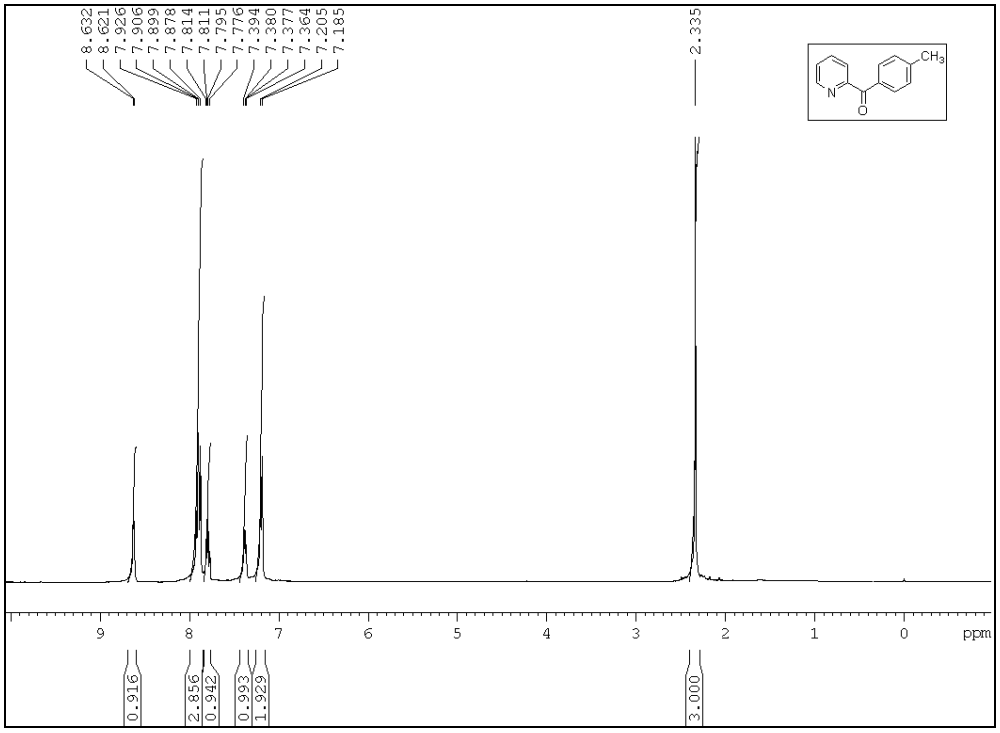
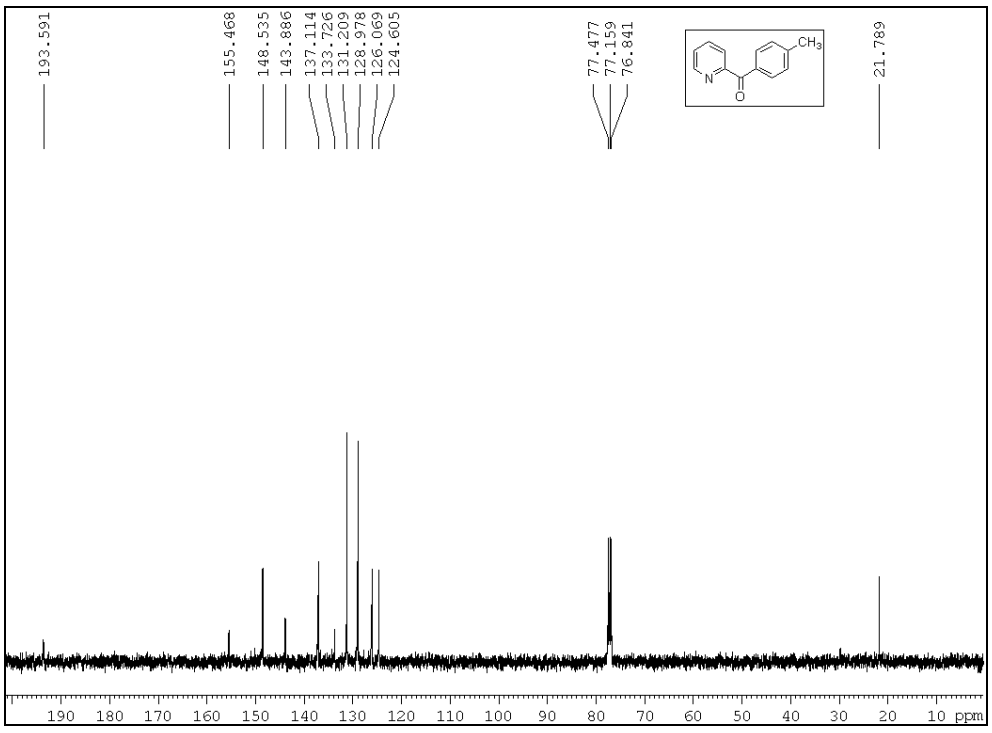


400 MHz ^{1}H NMR of pyridin-2-yl(p-tolyl)methanone in $CDCl_3$



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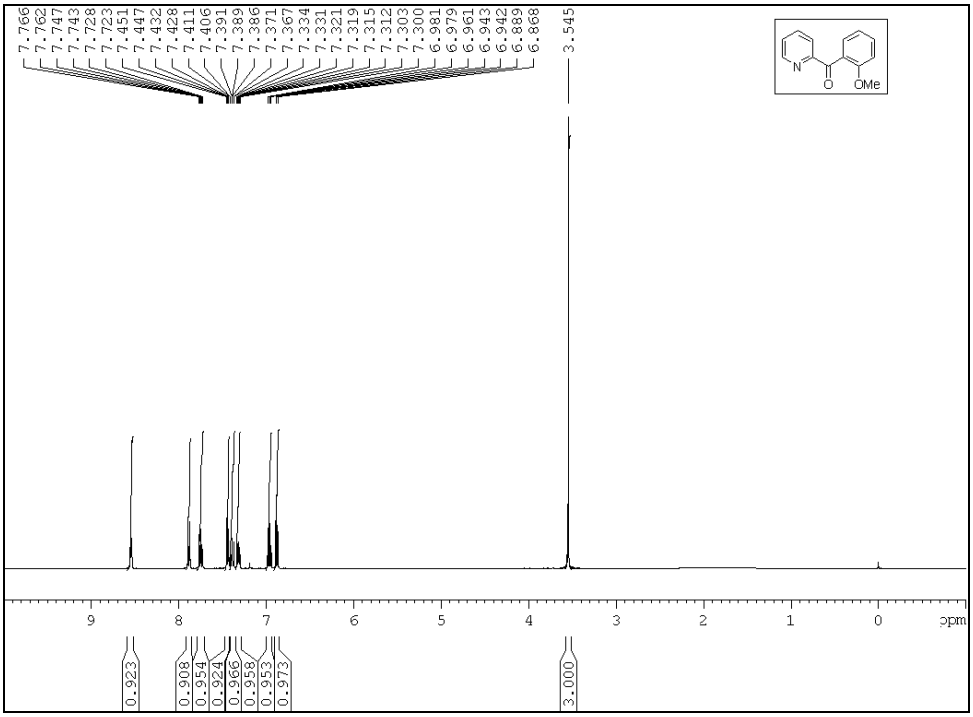
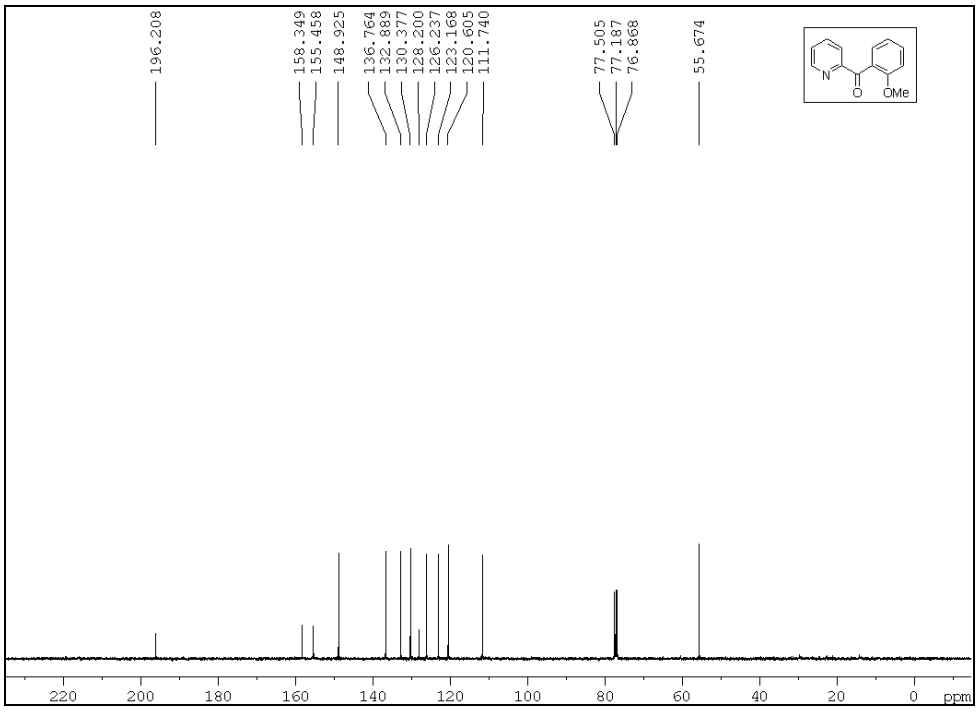
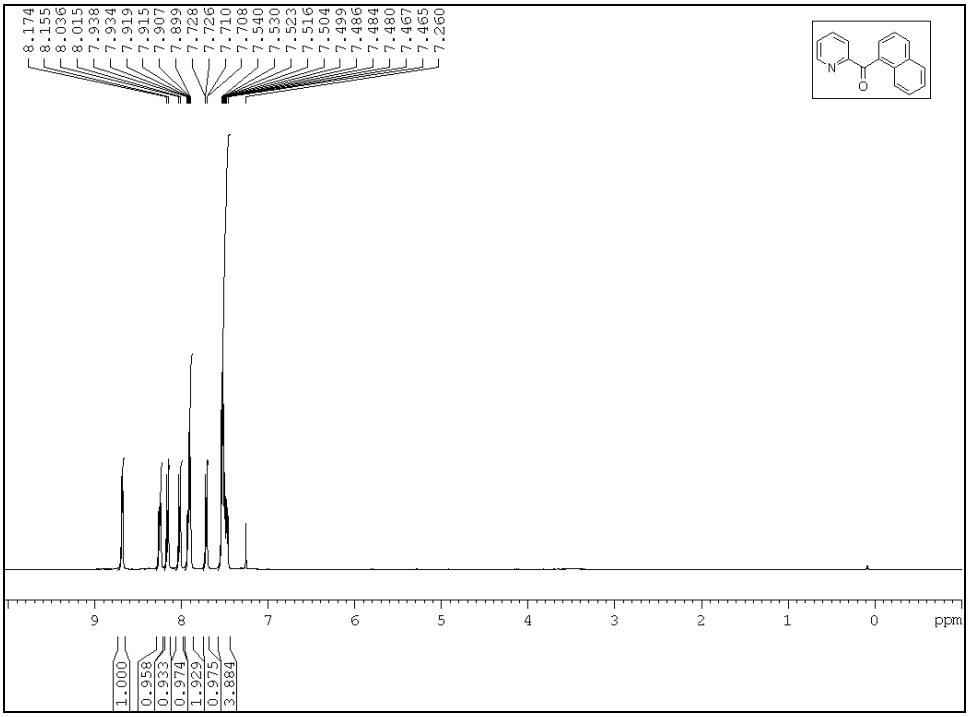


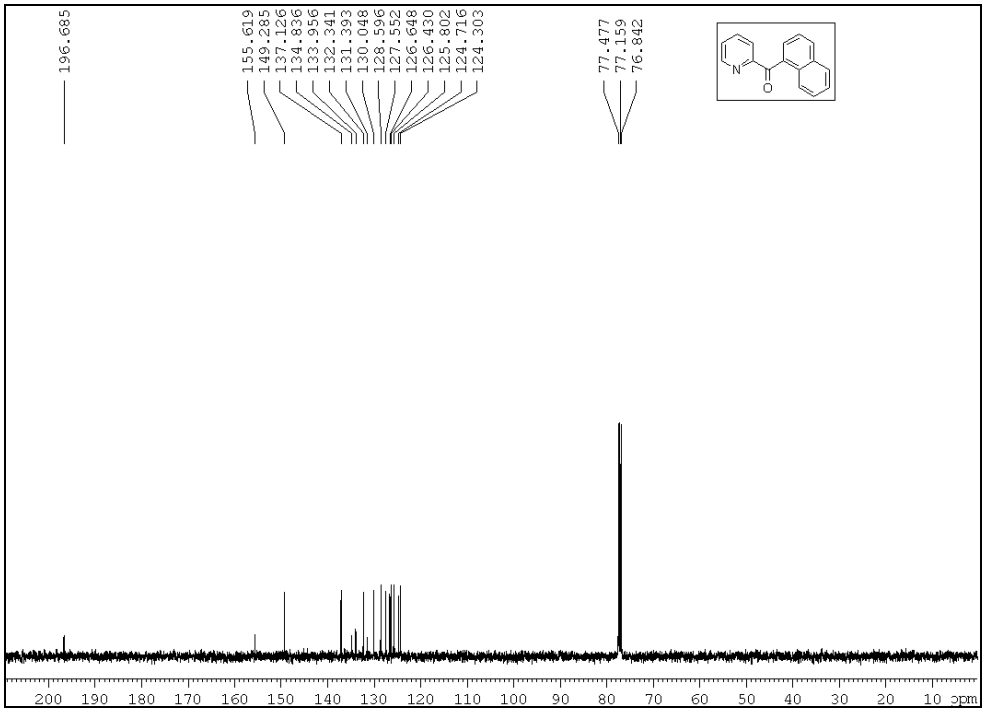
400 MHz ^{1}H NMR of (2-methoxyphenyl)(pyridin-2-yl)methanone in $CDCl_3$



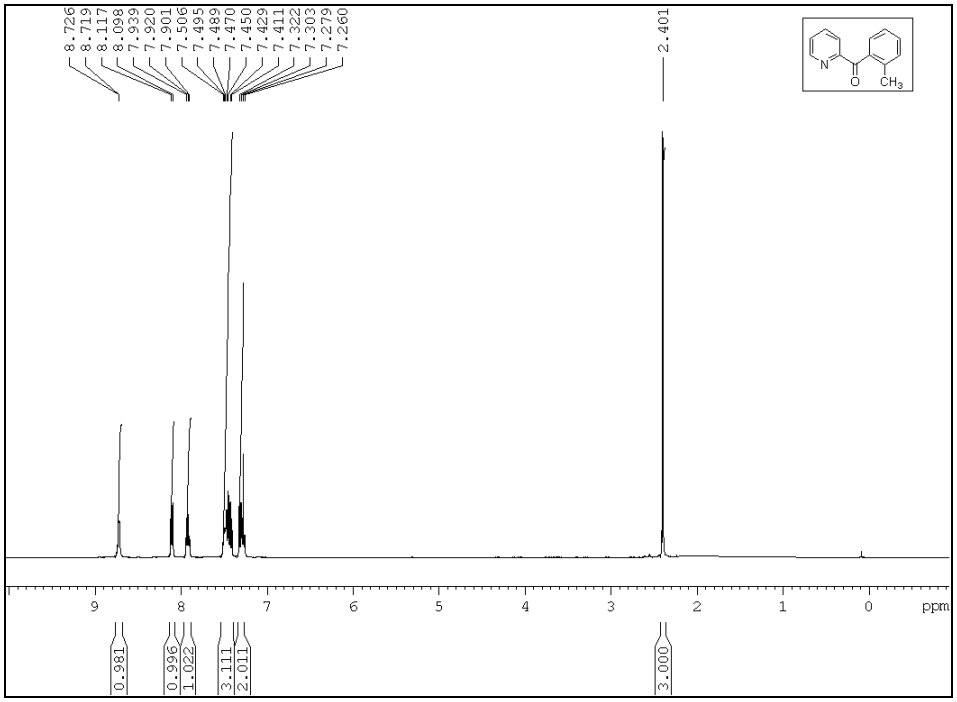
100 MHz ^{13}C NMR of (2-methoxyphenyl)(pyridin-2-yl)methanone in $CDCl_3$



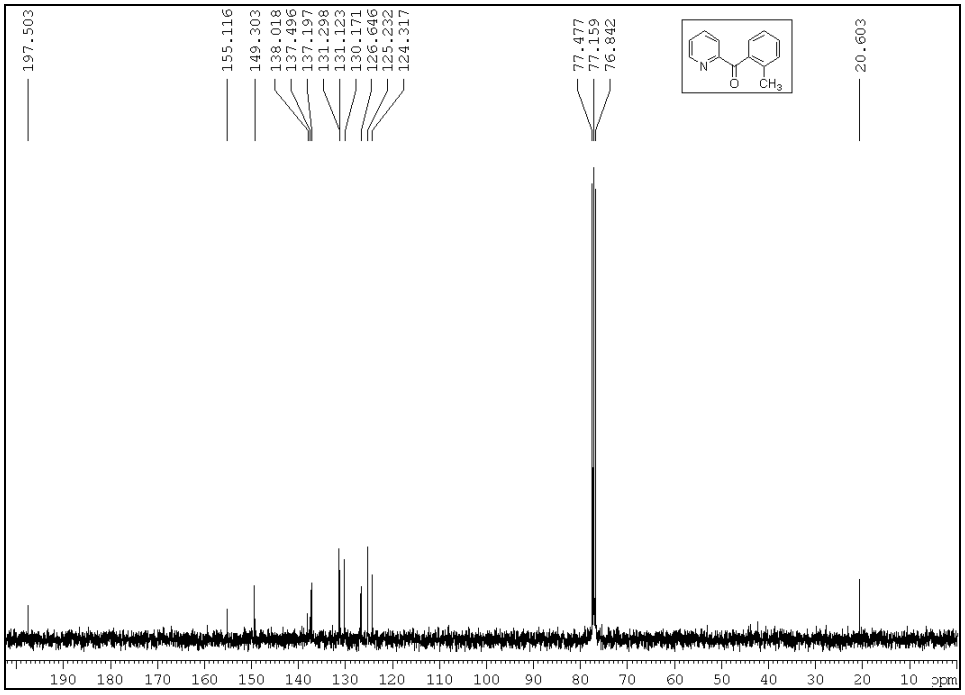
400 MHz ^{1}H NMR of naphthalen-1-yl(pyridin-2-yl)methanone in $CDCl_3$



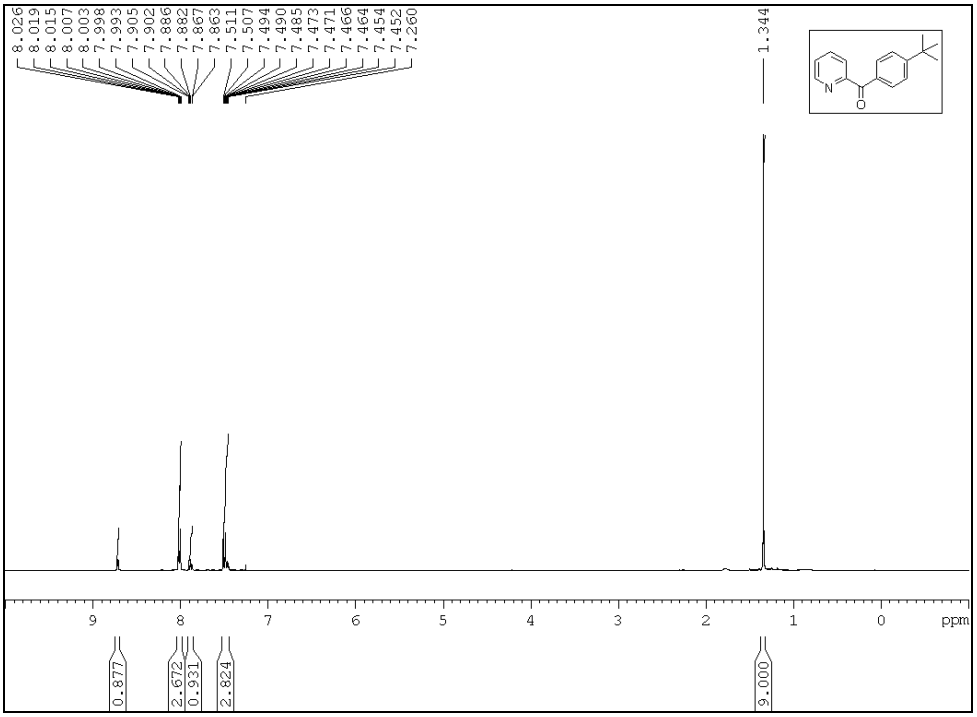
100 MHz ^{13}C NMR of naphthalen-1-yl(pyridin-2-yl)methanone in $CDCl_3$



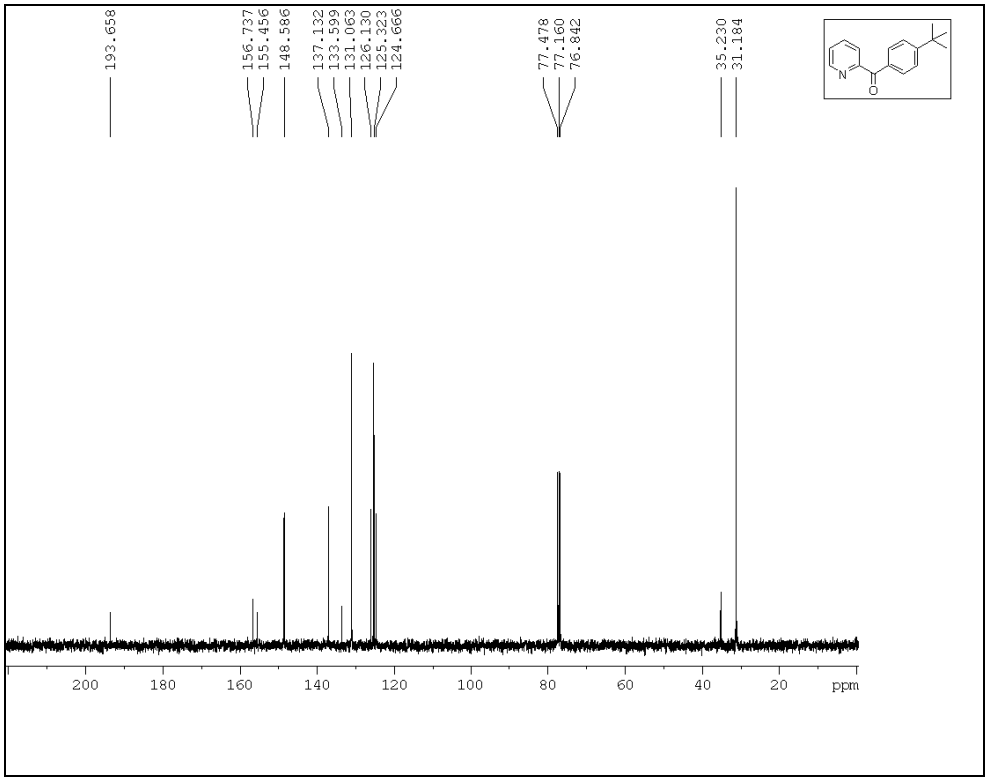
400 MHz ^{1}H NMR of pyridin-2-yl(o-tolyl)methanone in $CDCl_3$



100 MHz ^{13}C NMR of pyridin-2-yl(o-tolyl)methanone in $CDCl_3$



400 MHz ^{1}H NMR of (4-tert-butylphenyl)(pyridin-2-yl)methanone in $CDCl_3$



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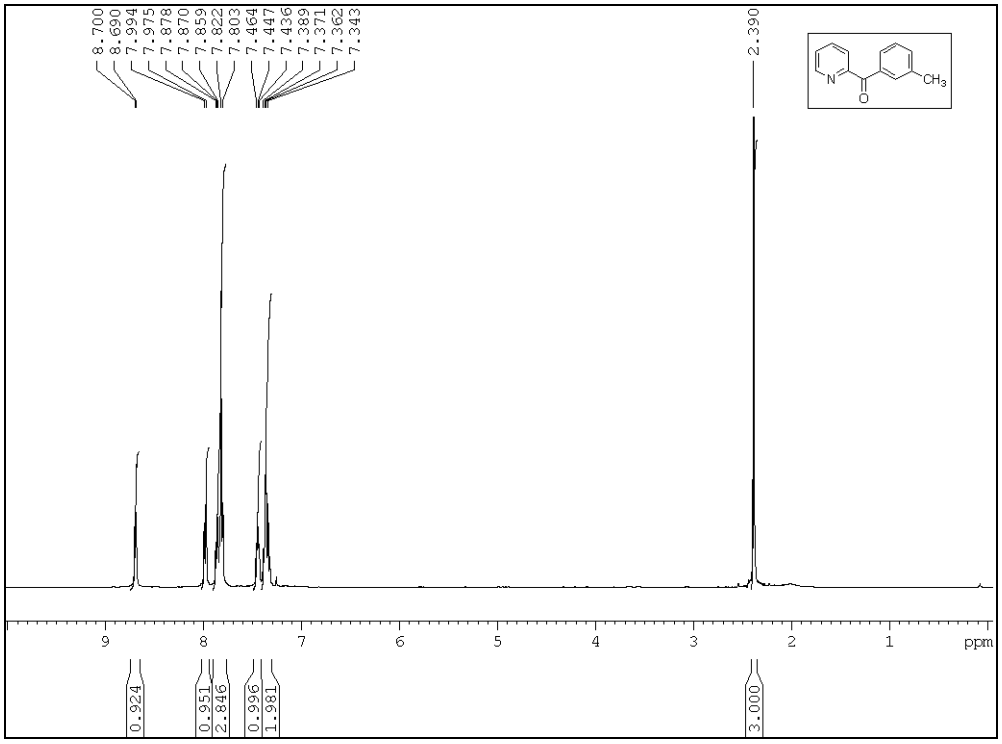
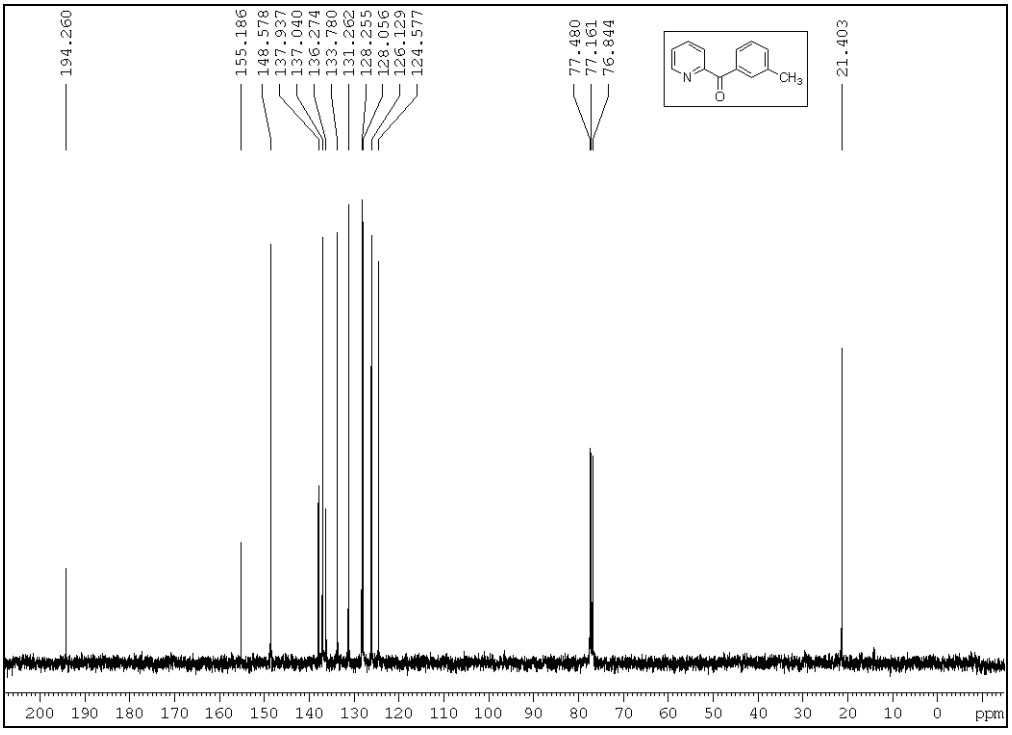


400 MHz ^{1}H NMR of pyridin-2-yl(m-tolyl)methanone in $CDCl_3$



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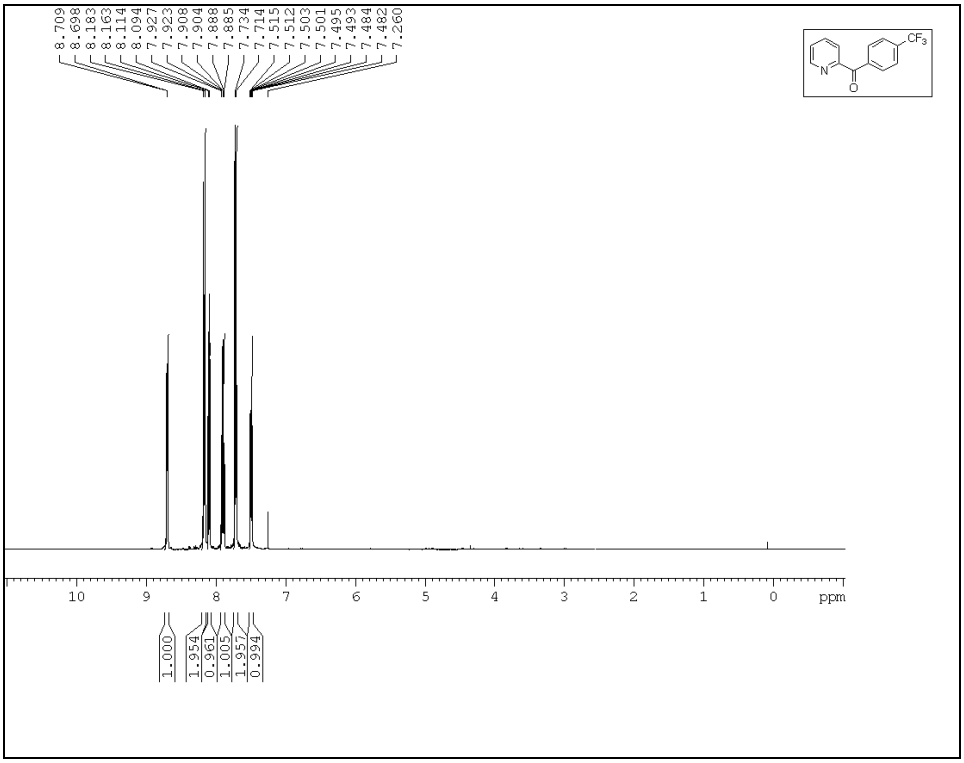
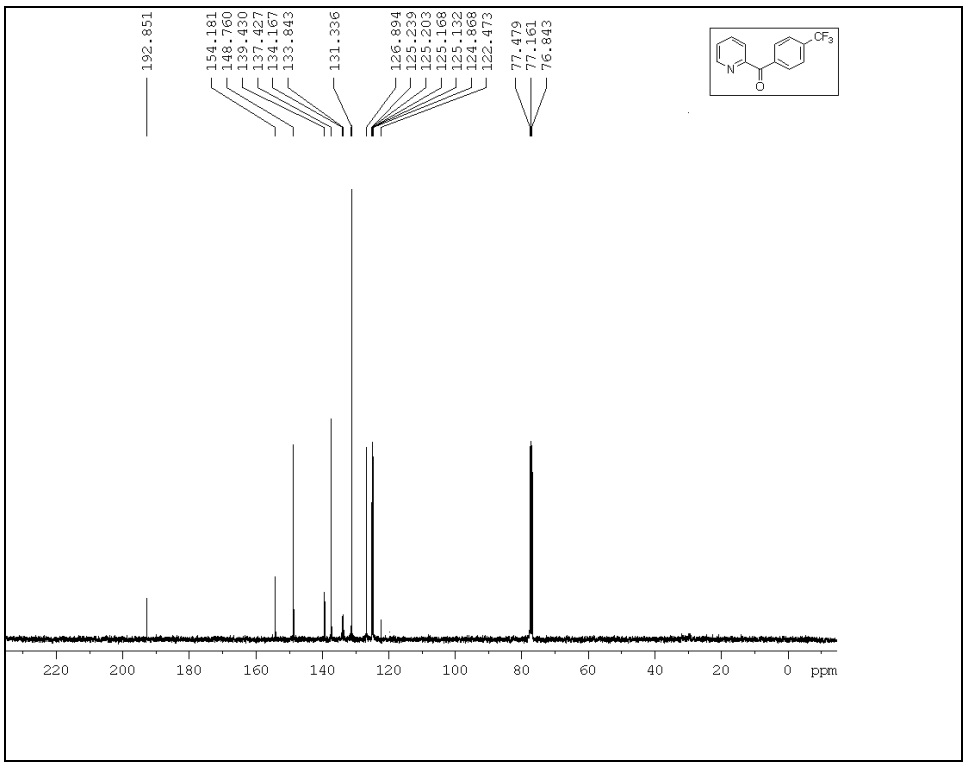
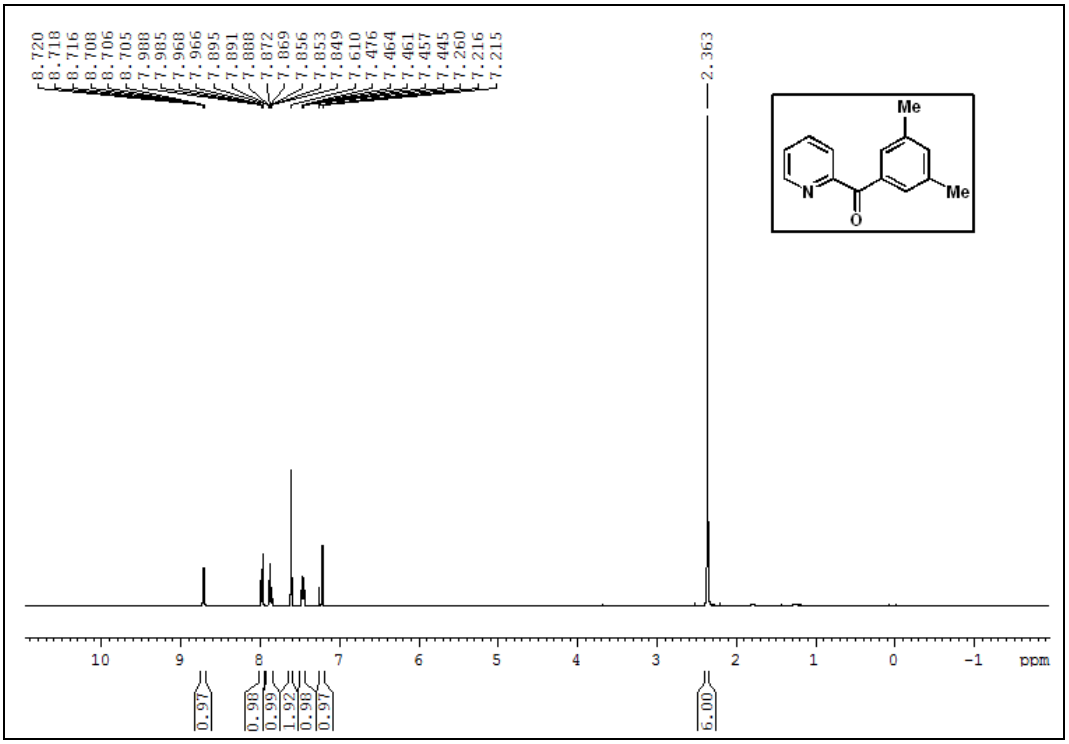


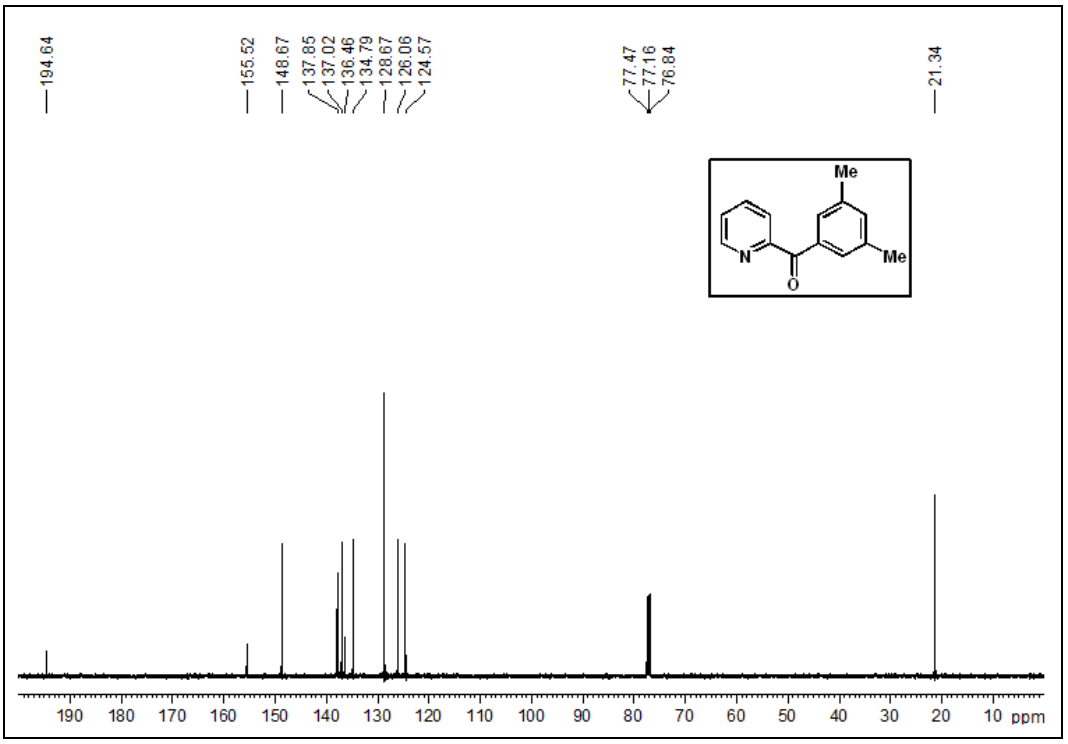
400 MHz ^{1}H NMR of pyridin-2-yl(4-(trifluoromethyl)phenyl)methanone in $CDCl_3$



100 MHz ^{13}C NMR of pyridin-2-yl(4-(trifluoromethyl)phenyl)methanone in $CDCl_3$



400 MHz ^{1}H NMR of (3,5-dimethylphenyl)(pyridin-2-yl)methanone in $CDCl_3$



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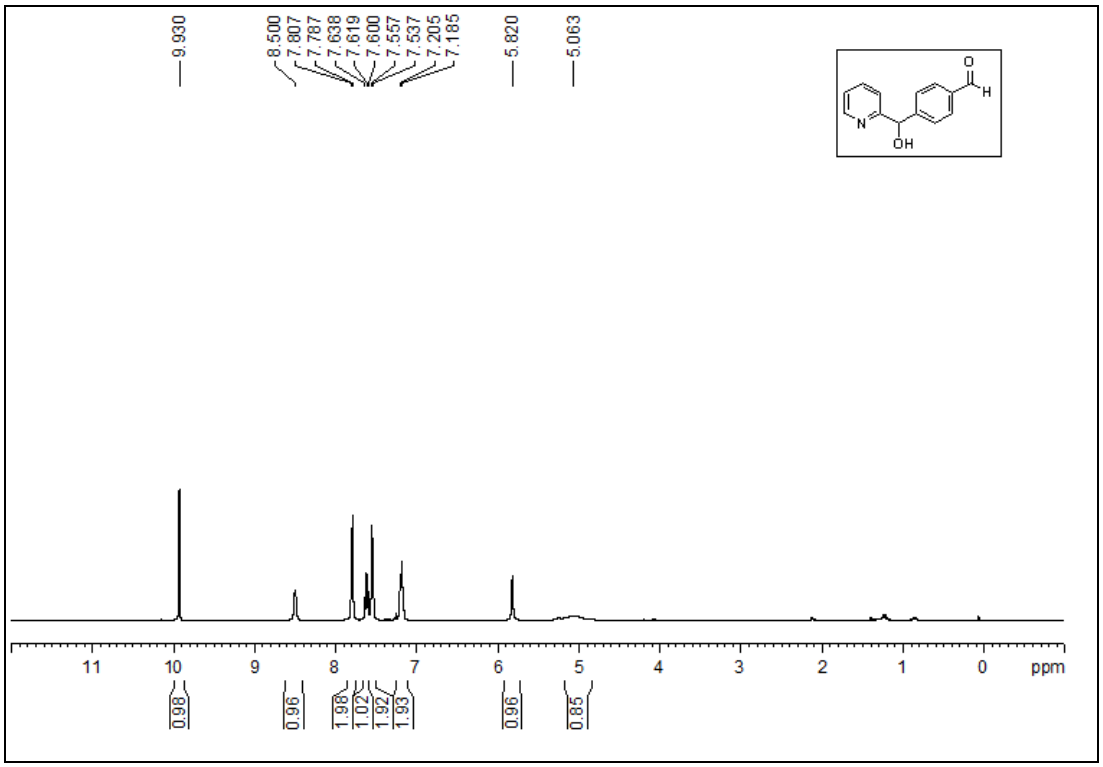
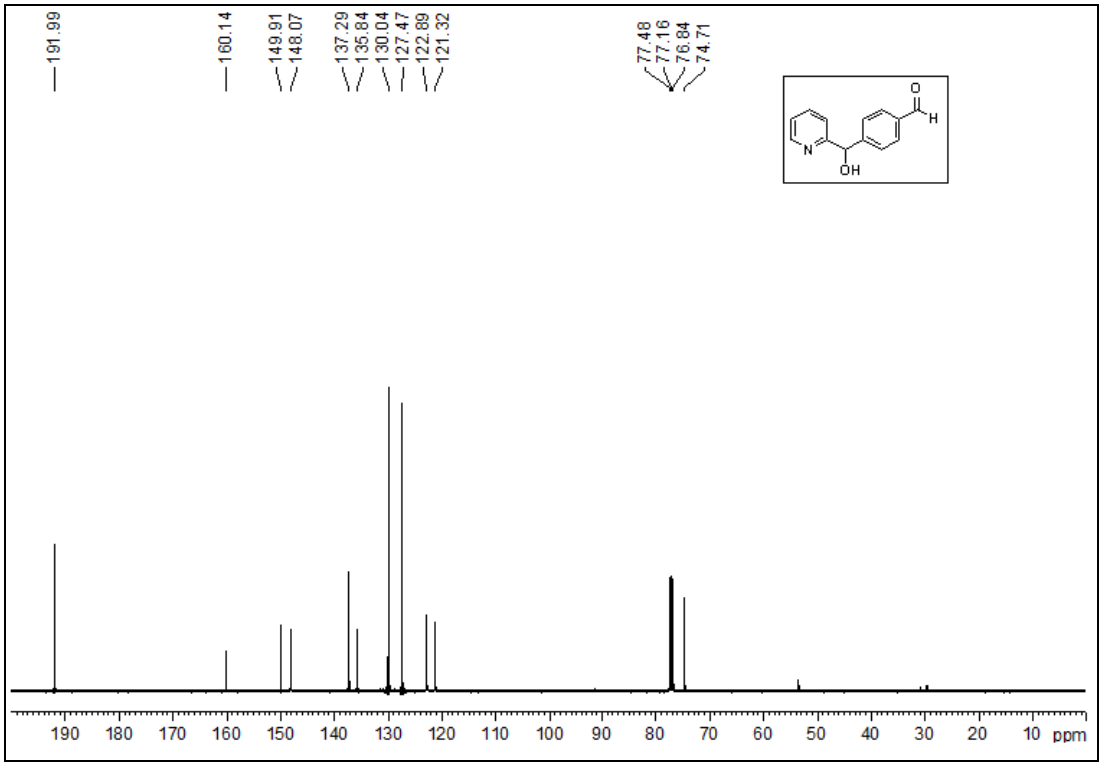


400 MHz ^{1}H NMR of 4-(hydroxy(pyridin-2-yl)methyl)benzaldehyde in $CDCl_3$



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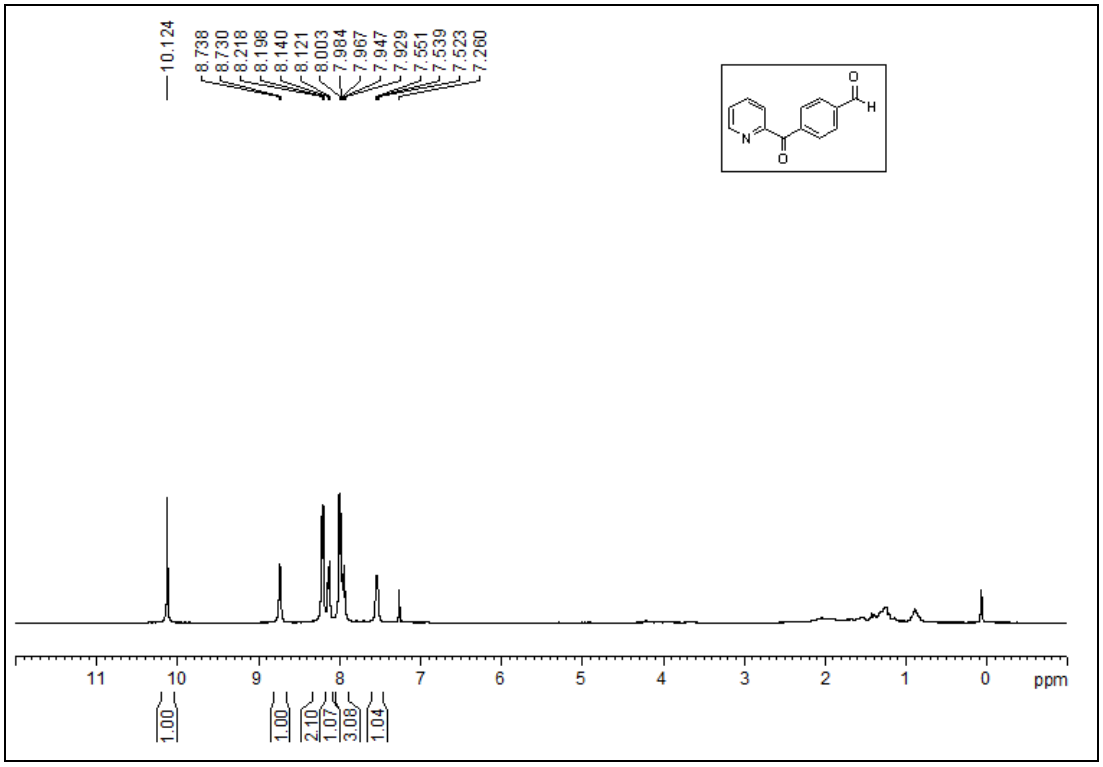
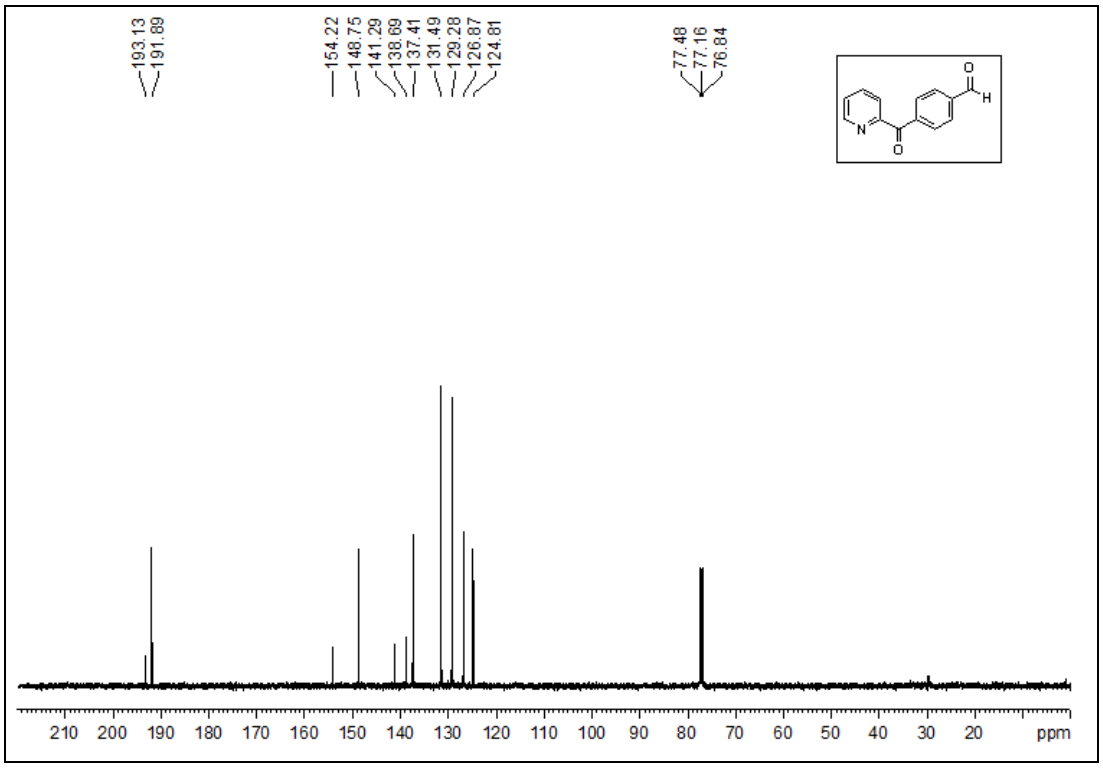


400 MHz ^{1}H NMR of 4-picolinoylbenzaldehyde in $CDCl_3$



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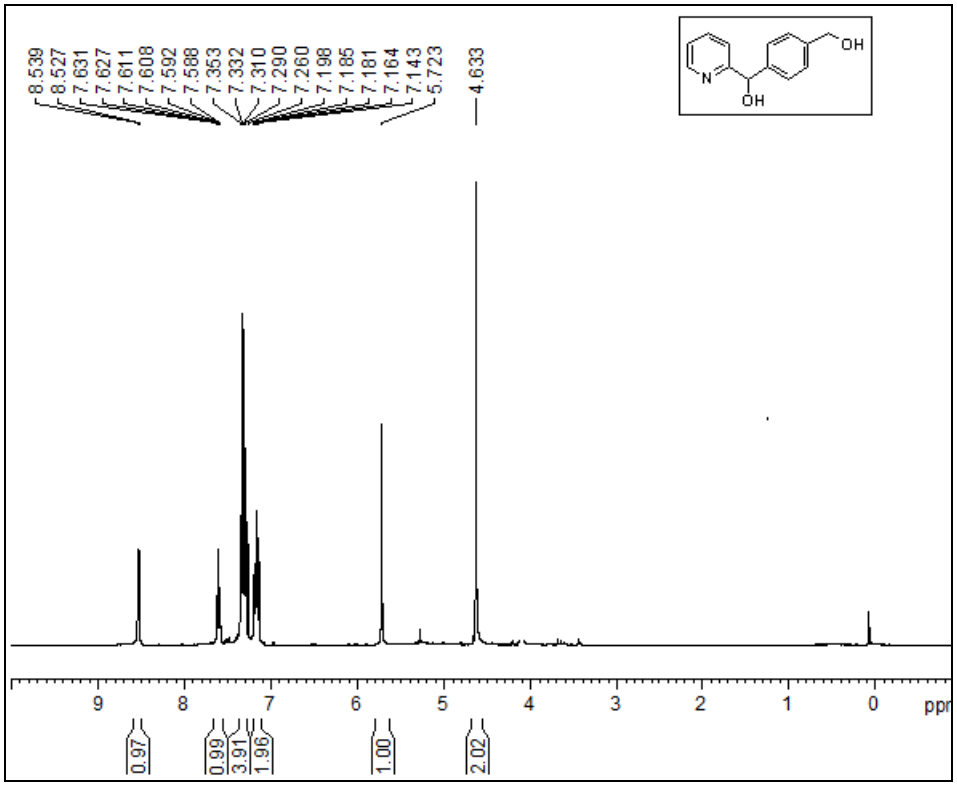
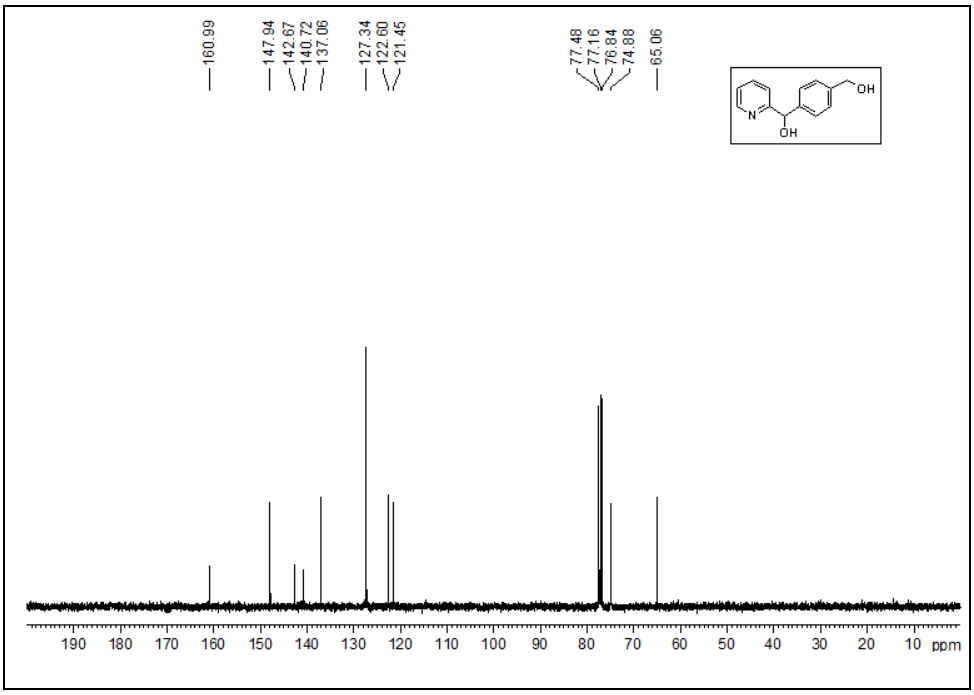


400 MHz ^{1}H NMR of (4-(hydroxymethyl)phenyl)(pyridin-2-yl)methanol in $CDCl_3$



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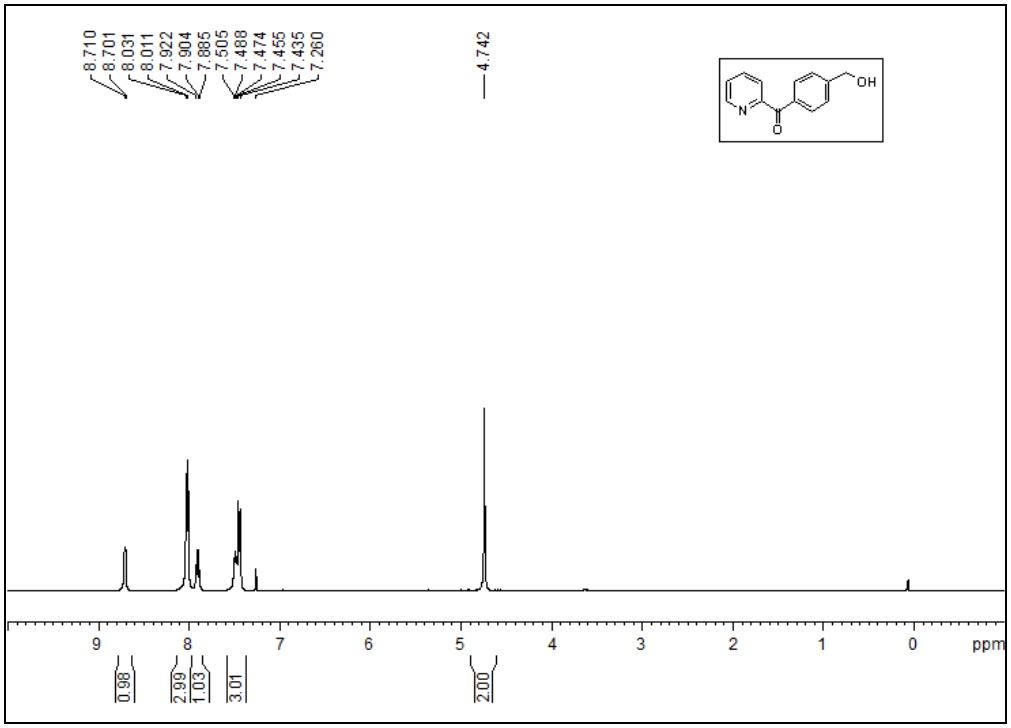

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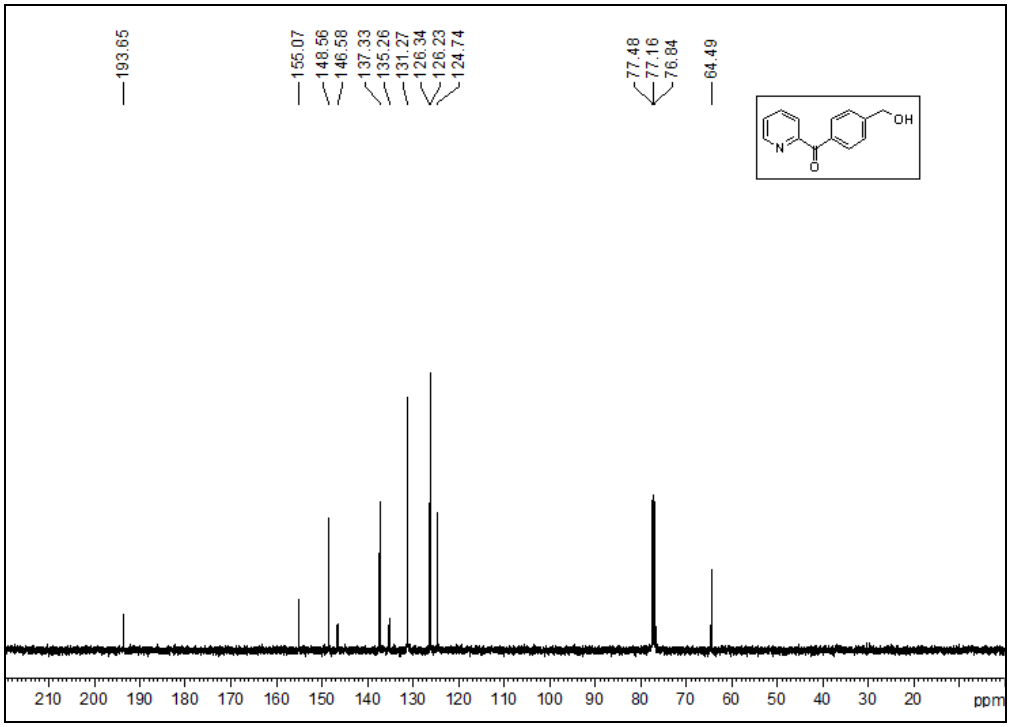

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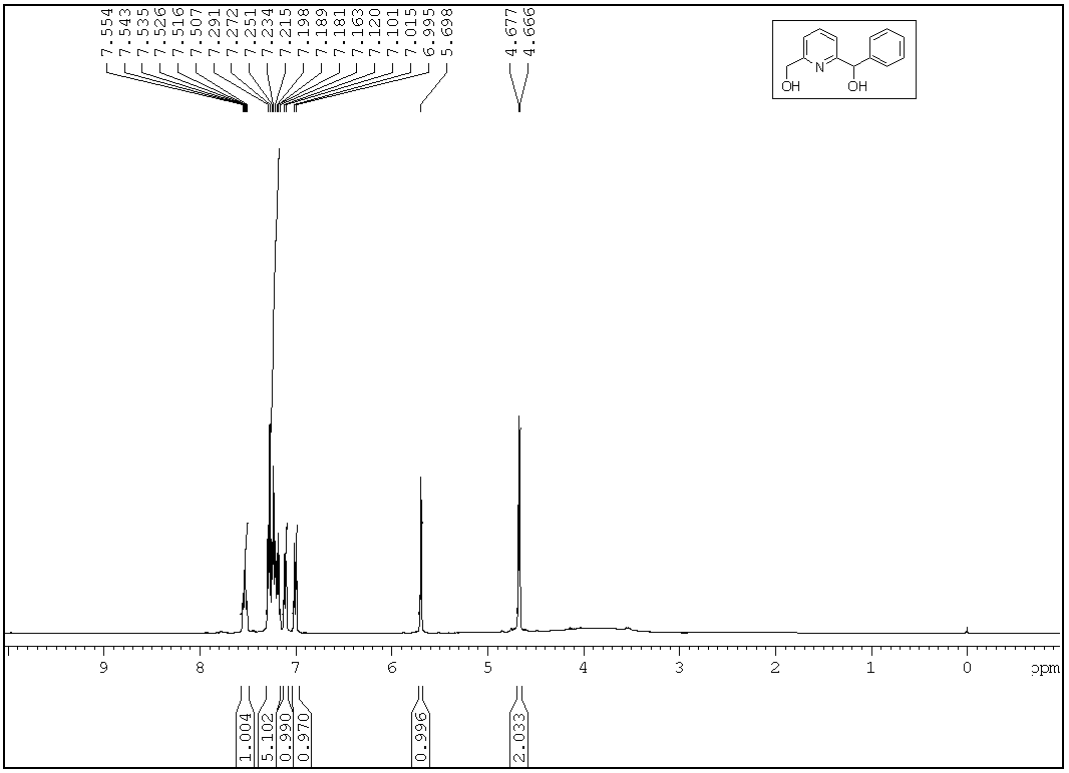
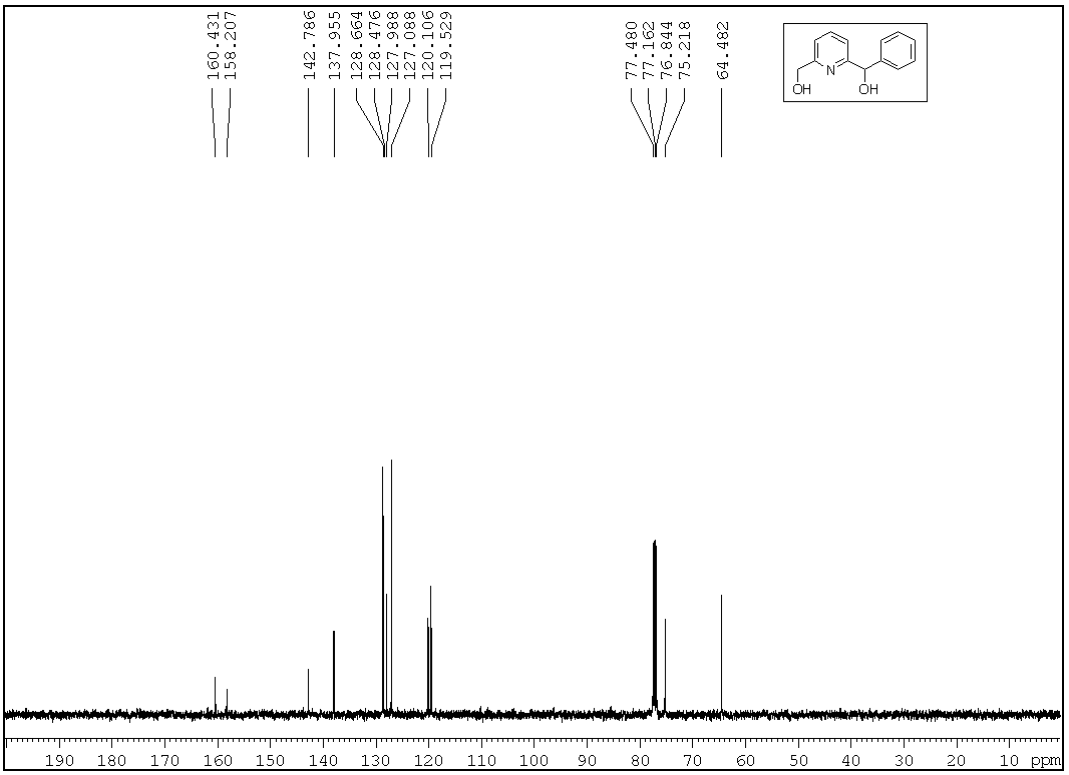
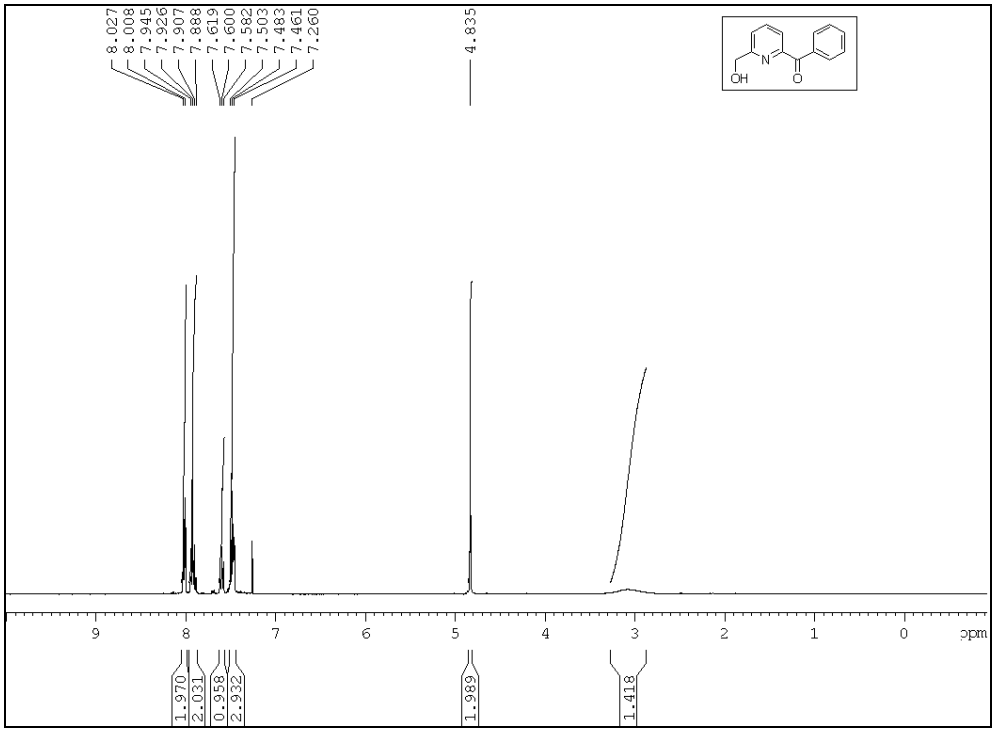


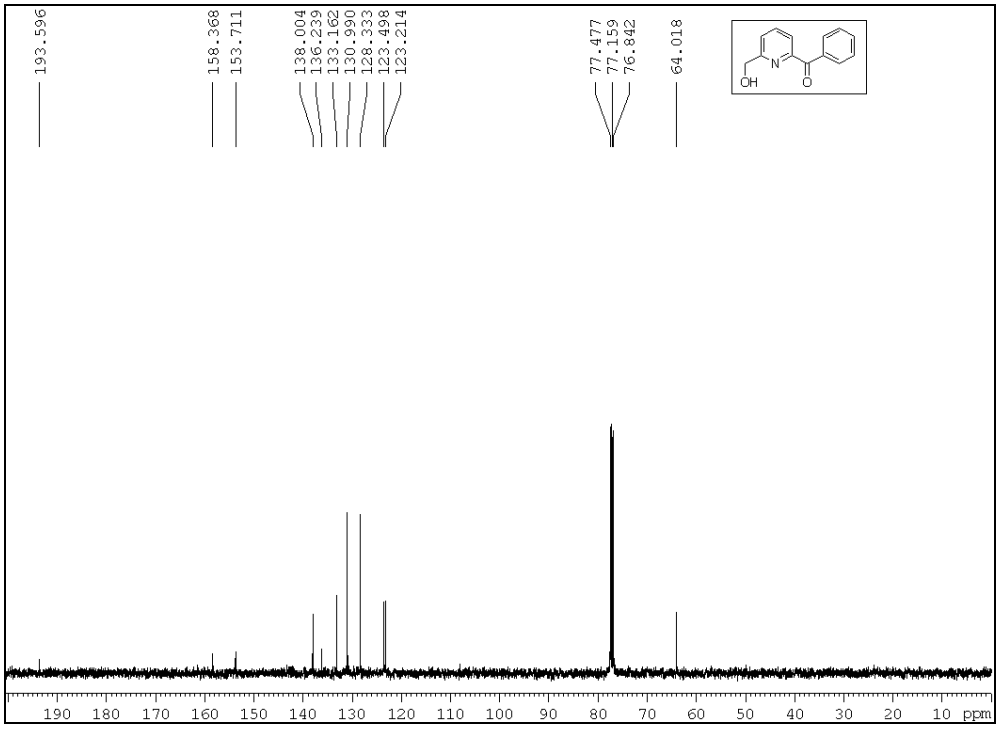
100 MHz ^{13}C NMR of 6-(hydroxymethyl)pyridin-2-yl)(phenyl)methanol in $CDCl_3$



100 MHz ^{13}C NMR of 6-(hydroxymethyl)pyridin-2-yl)(phenyl)methanol in $CDCl_3$



400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(phenyl)methanone in $CDCl_3$



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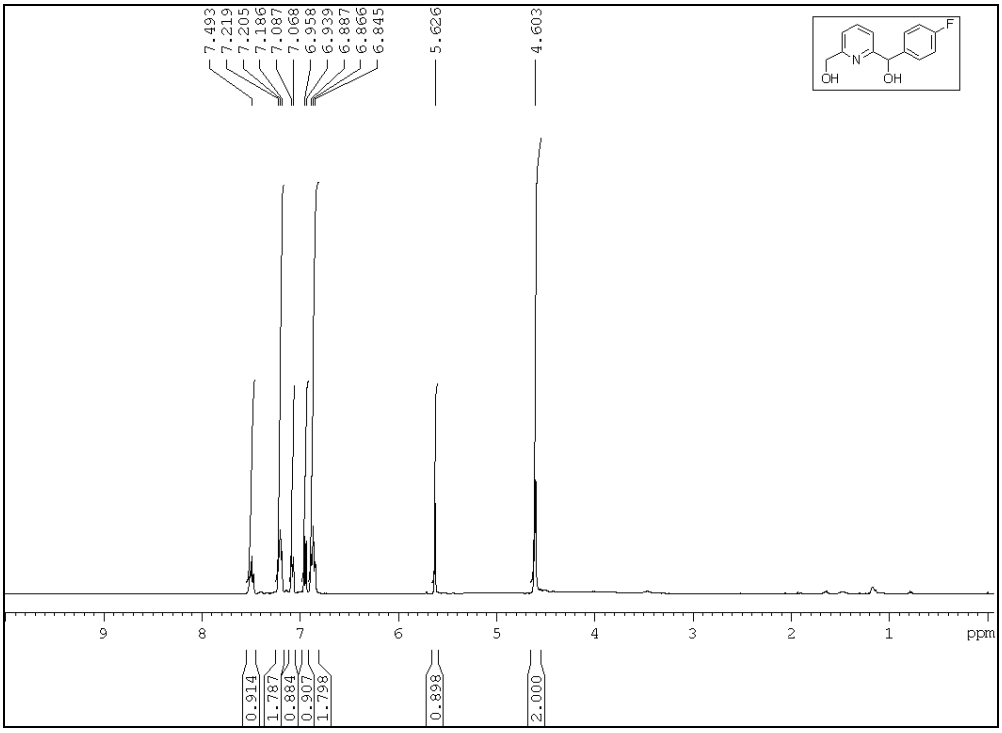
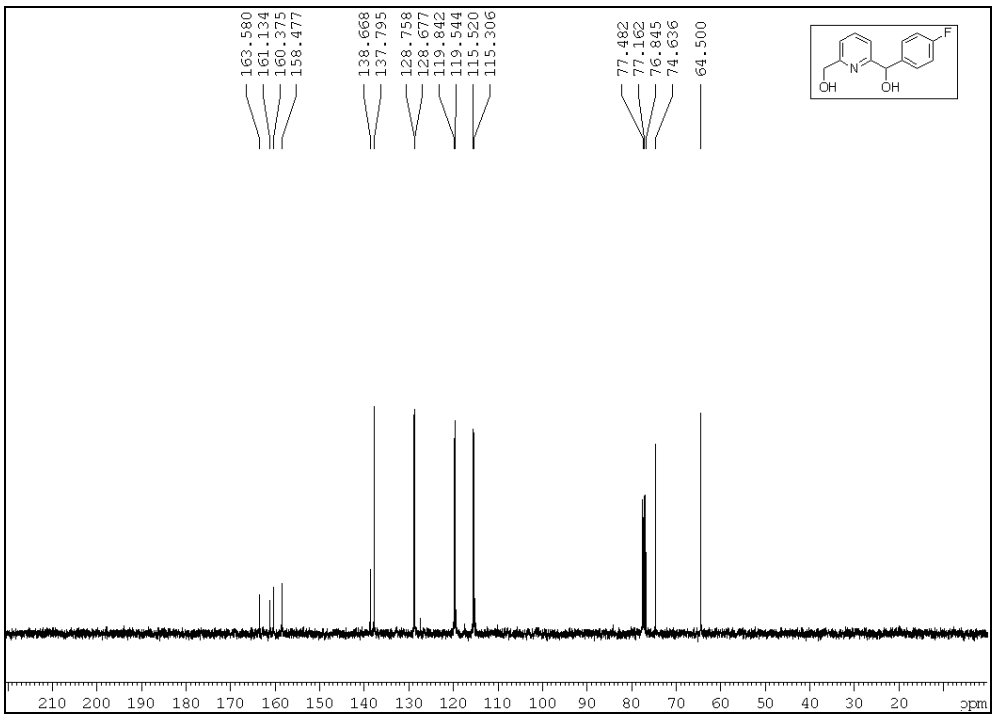


400 MHz ^{1}H NMR of (4-fluorophenyl)(6-(hydroxymethyl)pyridin-2-yl)methanol in $CDCl_3$



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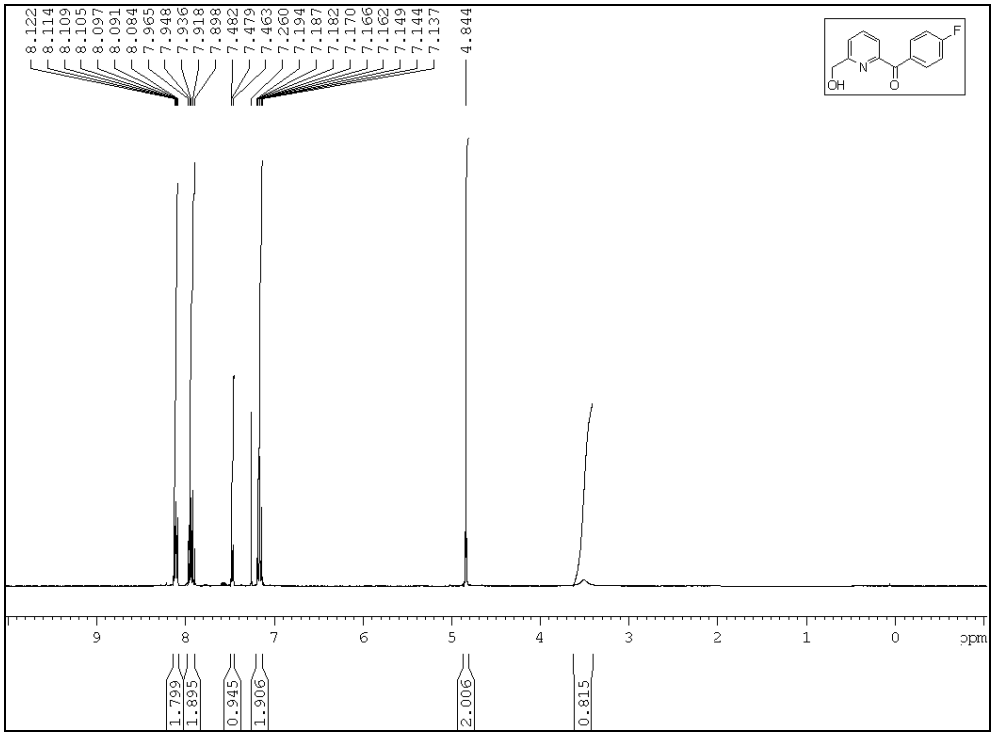

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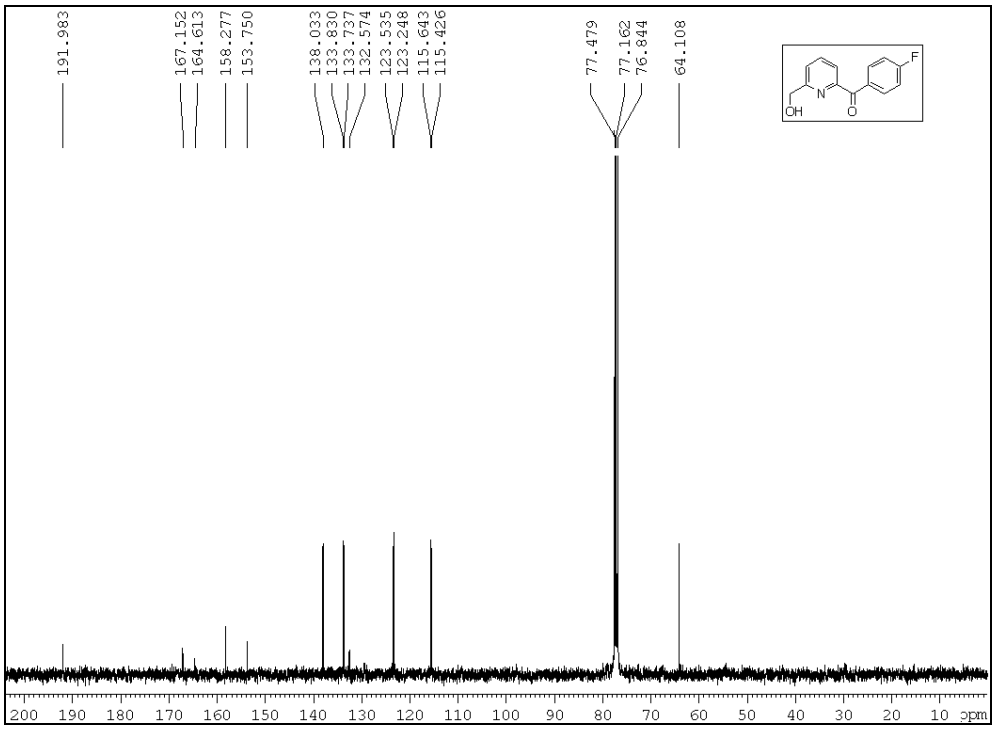

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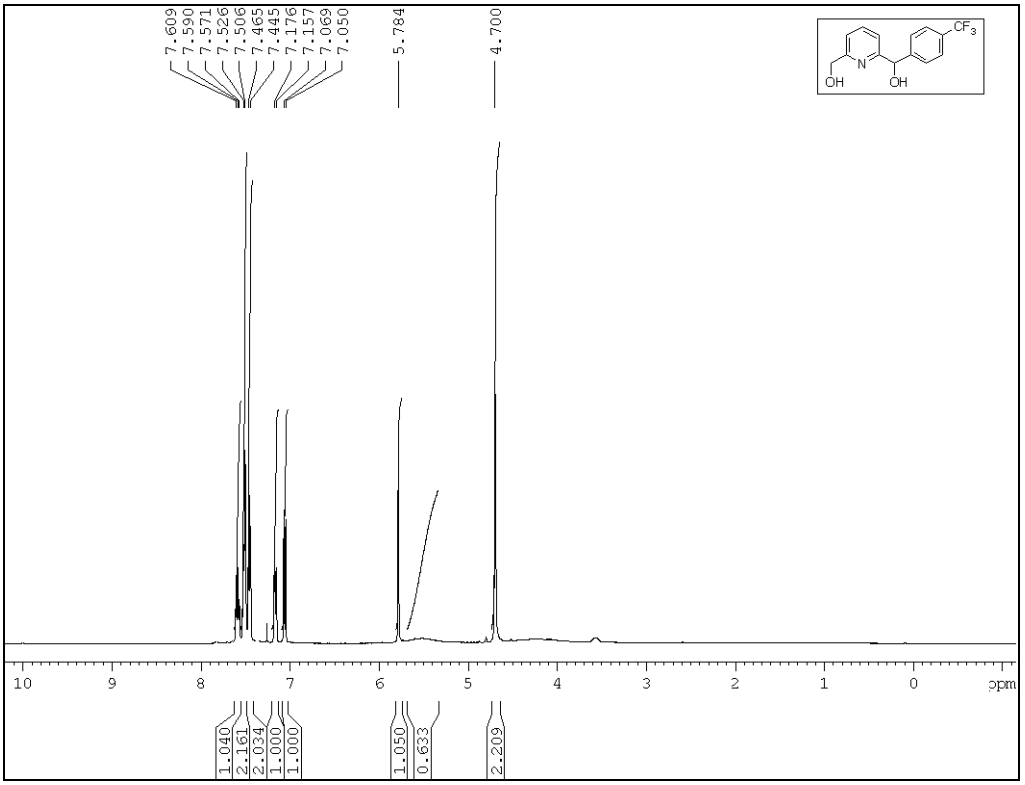
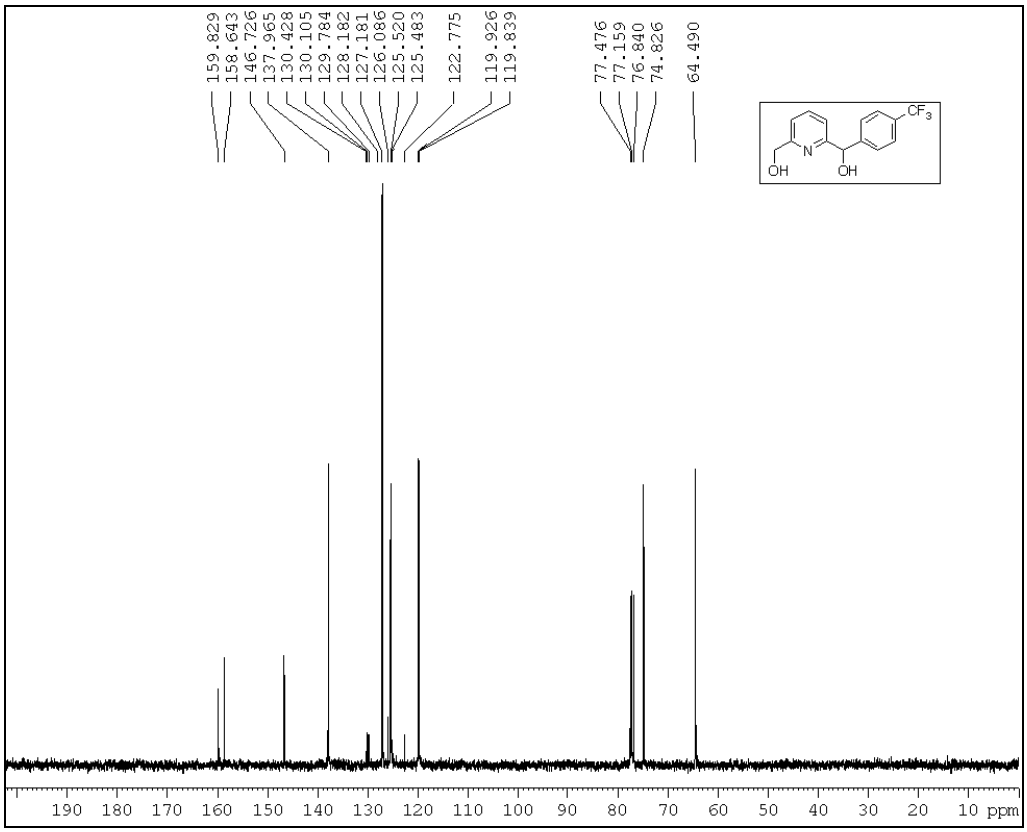
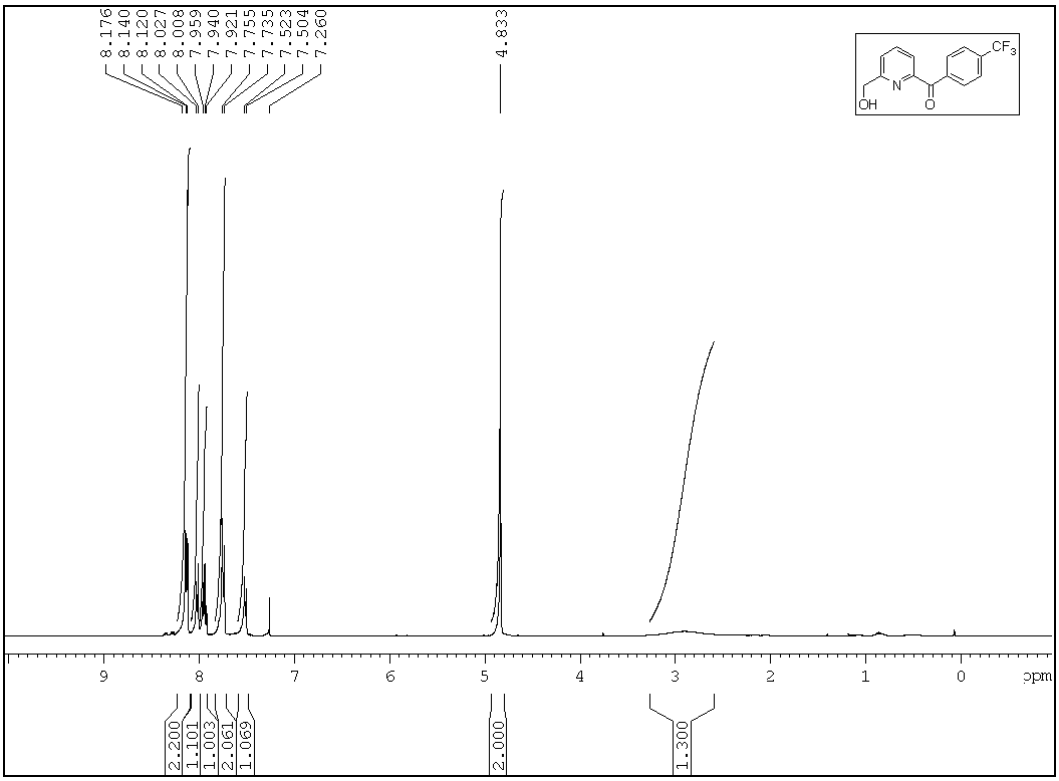


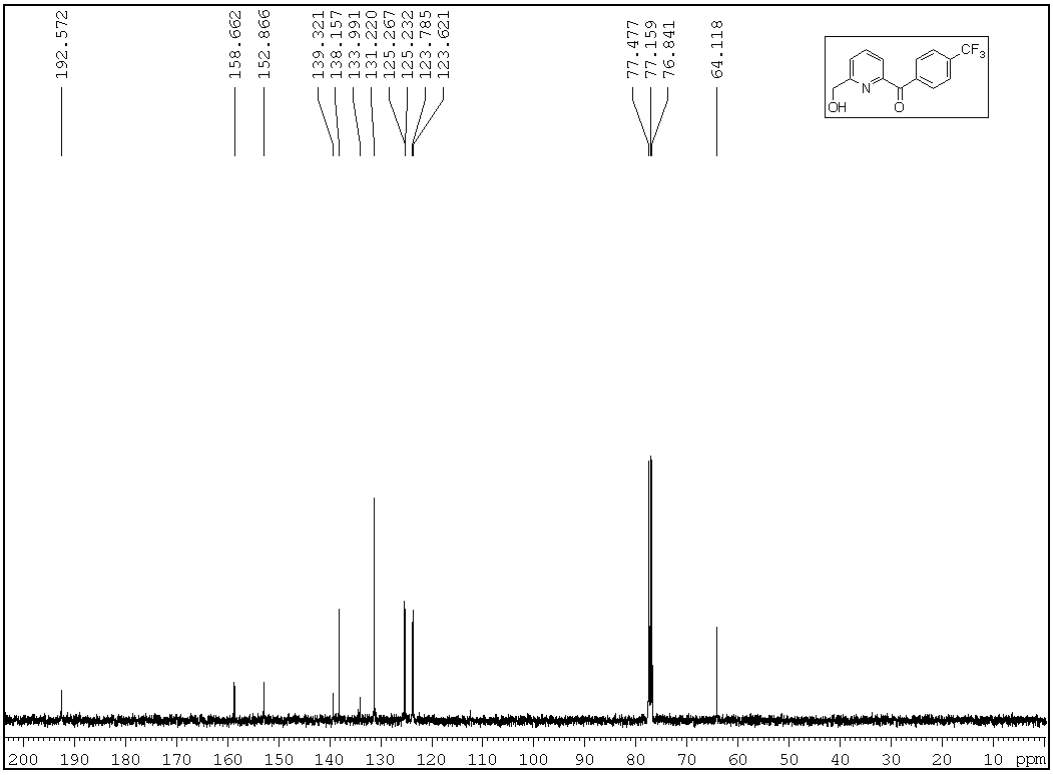
400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-(trifluoromethyl)phenyl)methanol in $CDCl_3$



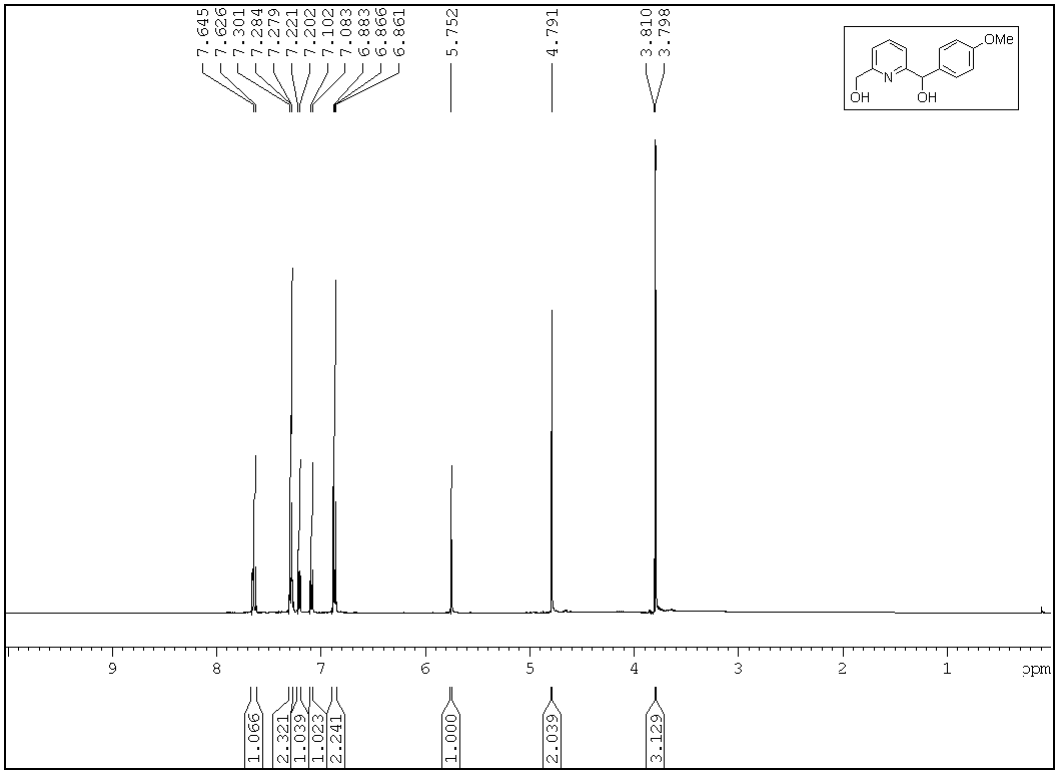
100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-(trifluoromethyl)phenyl)methanol in $CDCl_3$



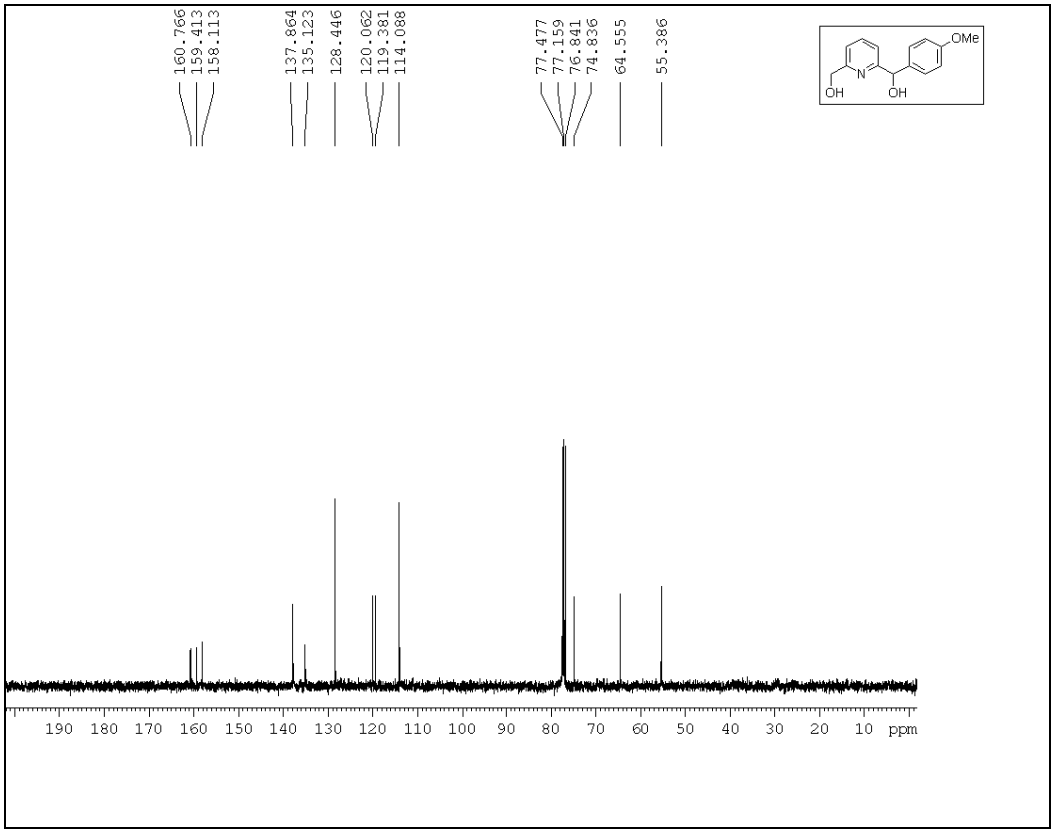
400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-(trifluoromethyl)phenyl)methanone in $CDCl_3$



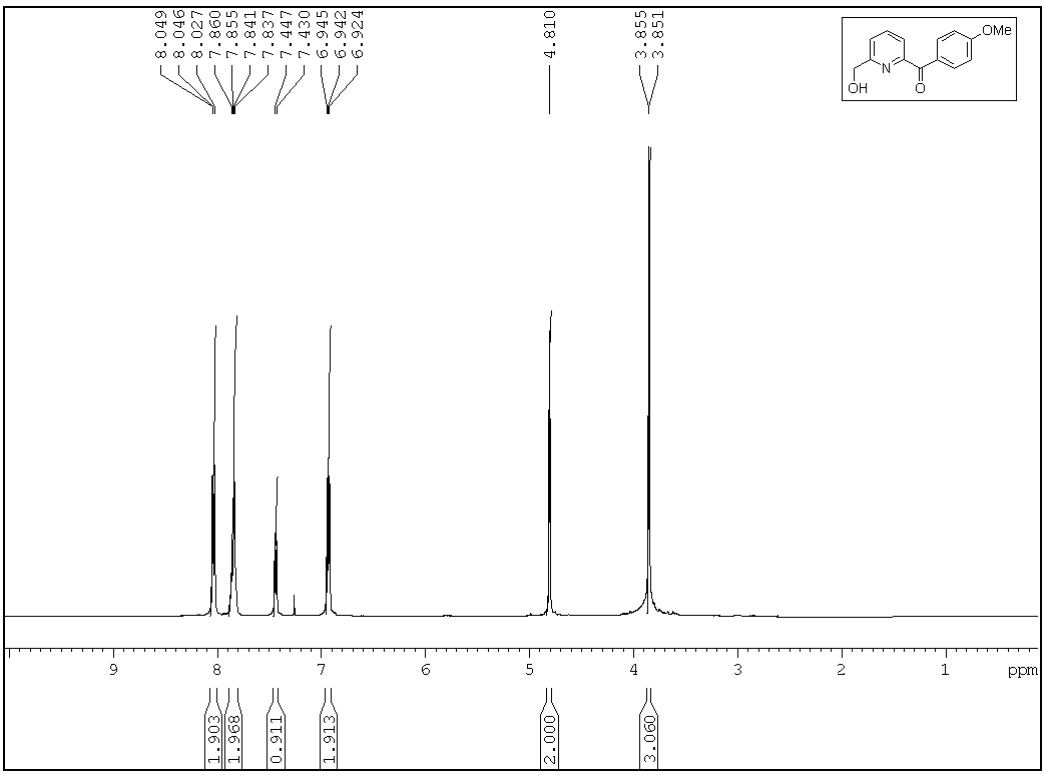
100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-(trifluoromethyl)phenyl)methanone in $CDCl_3$



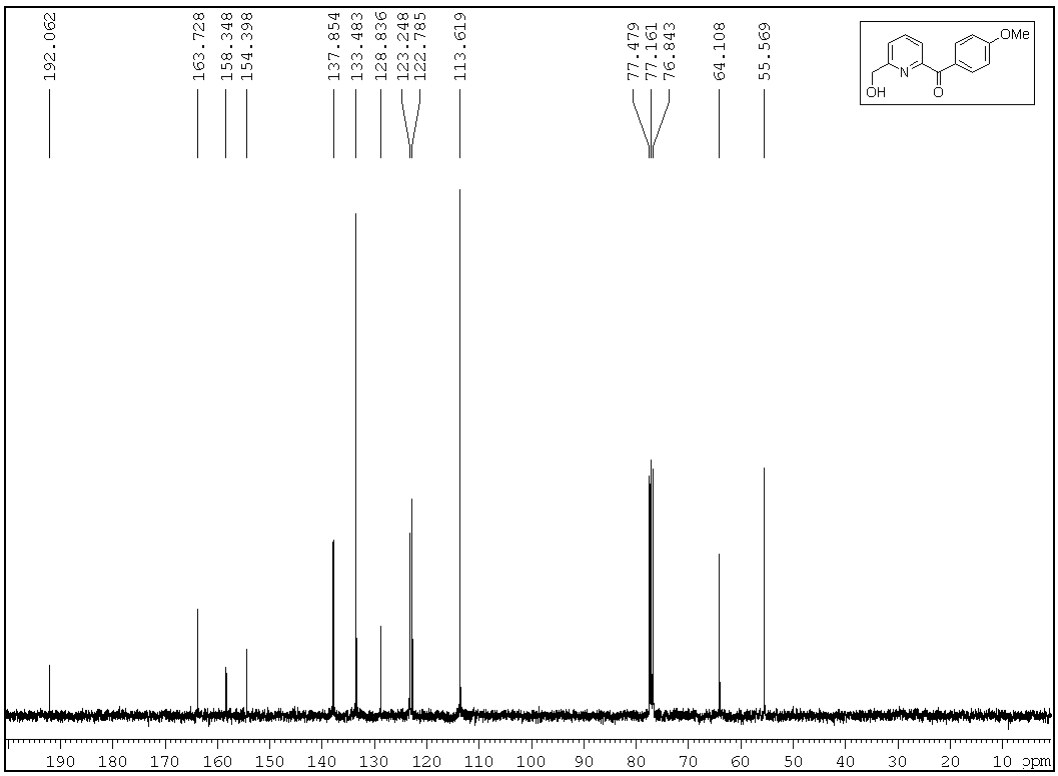
400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-methoxyphenyl)methanol in $CDCl_3$



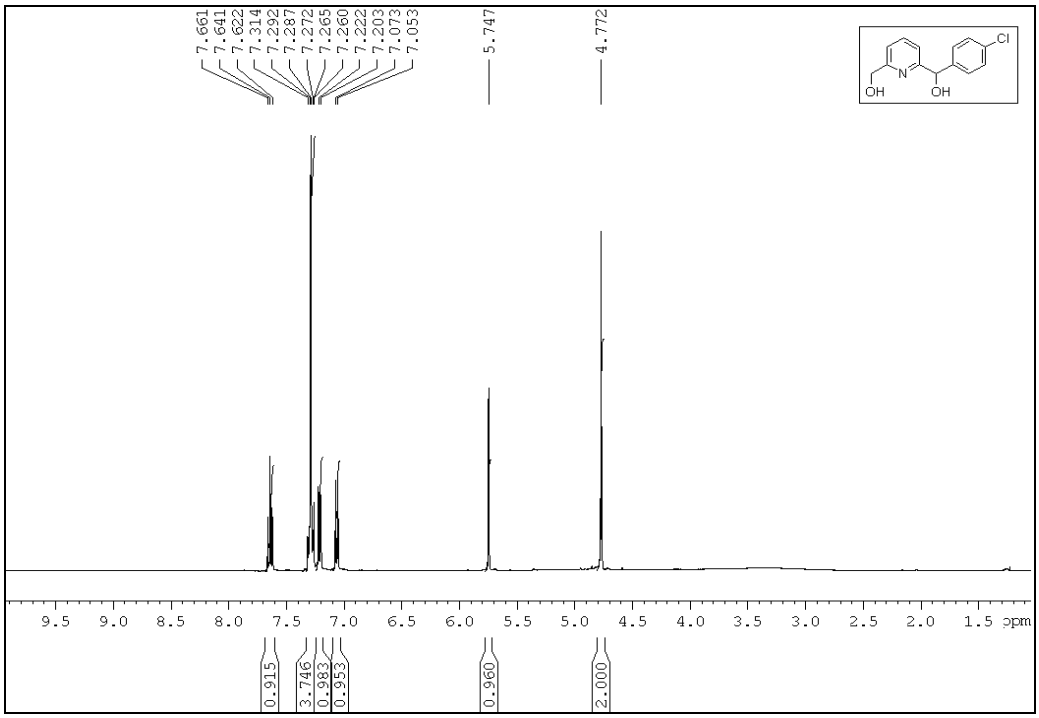
100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-methoxyphenyl)methanol in $CDCl_3$



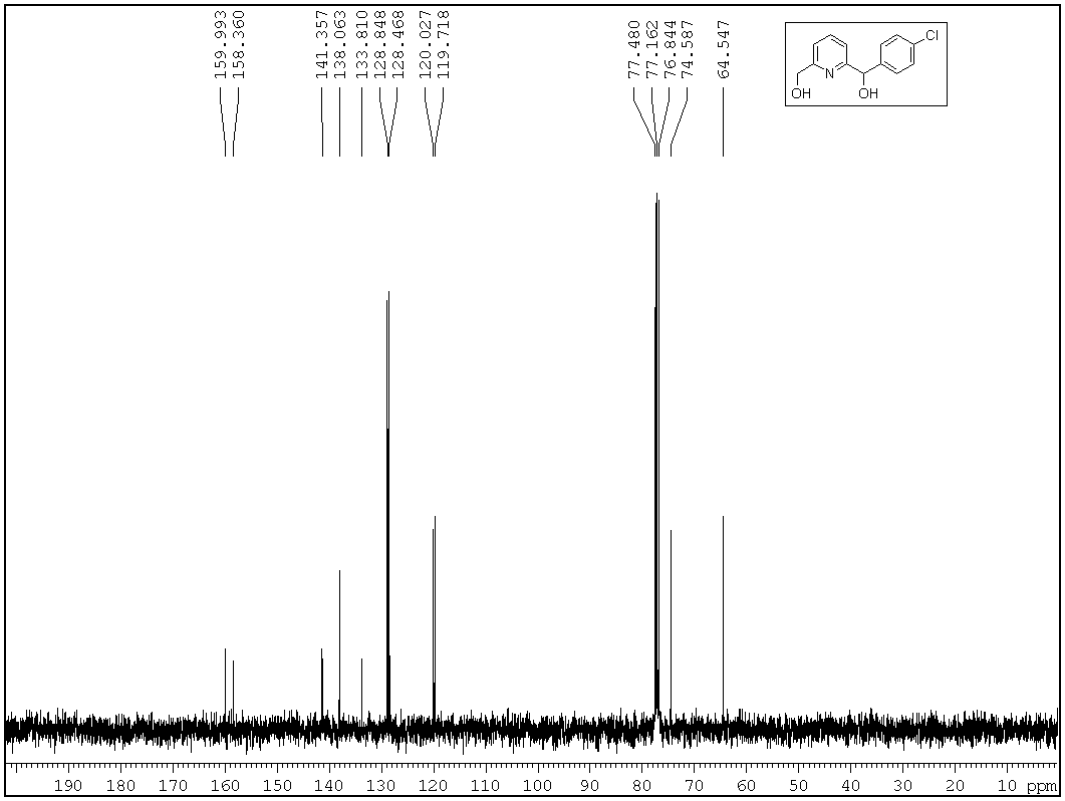
400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-methoxyphenyl)methanone in $CDCl_3$



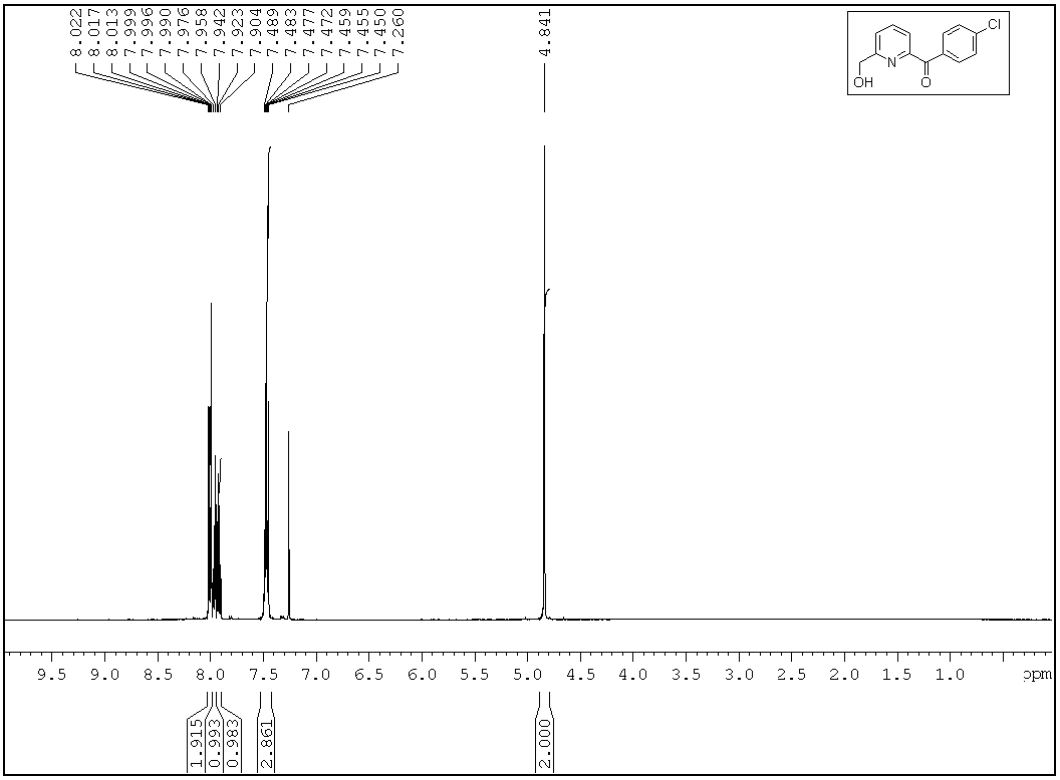
100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(4-methoxyphenyl)methanone in $CDCl_3$



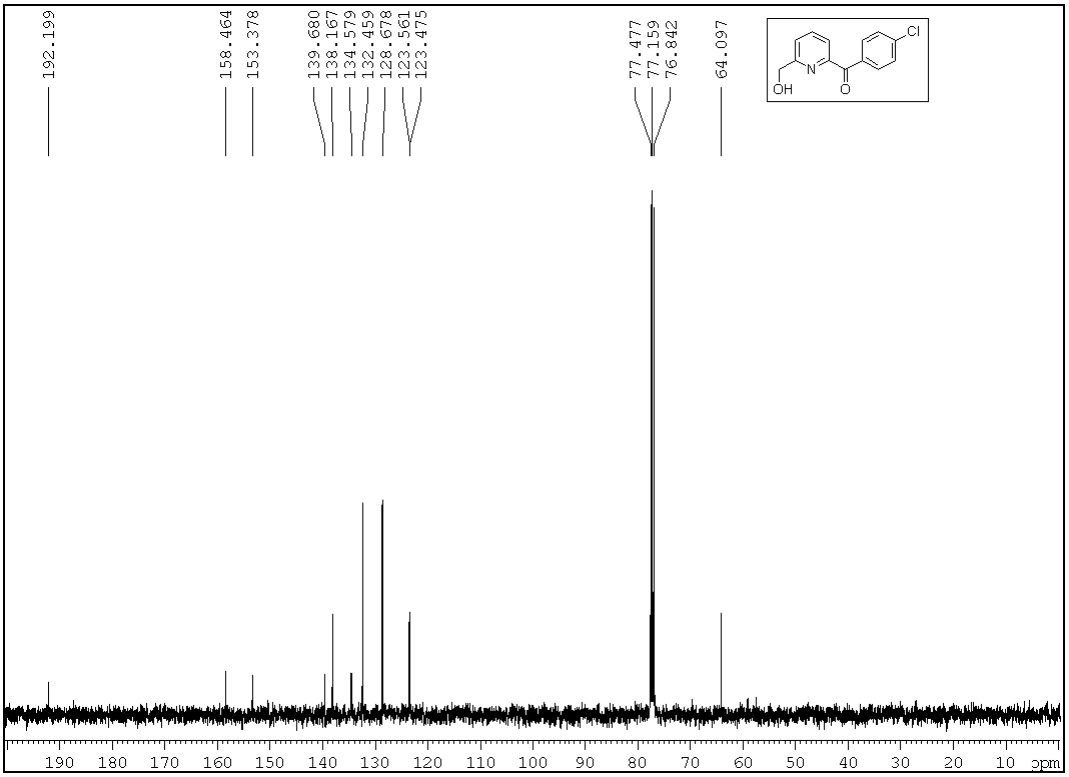
400 MHz ^{1}H NMR of (4-chlorophenyl)(6-(hydroxymethyl)pyridin-2-yl)methanol in $CDCl_3$



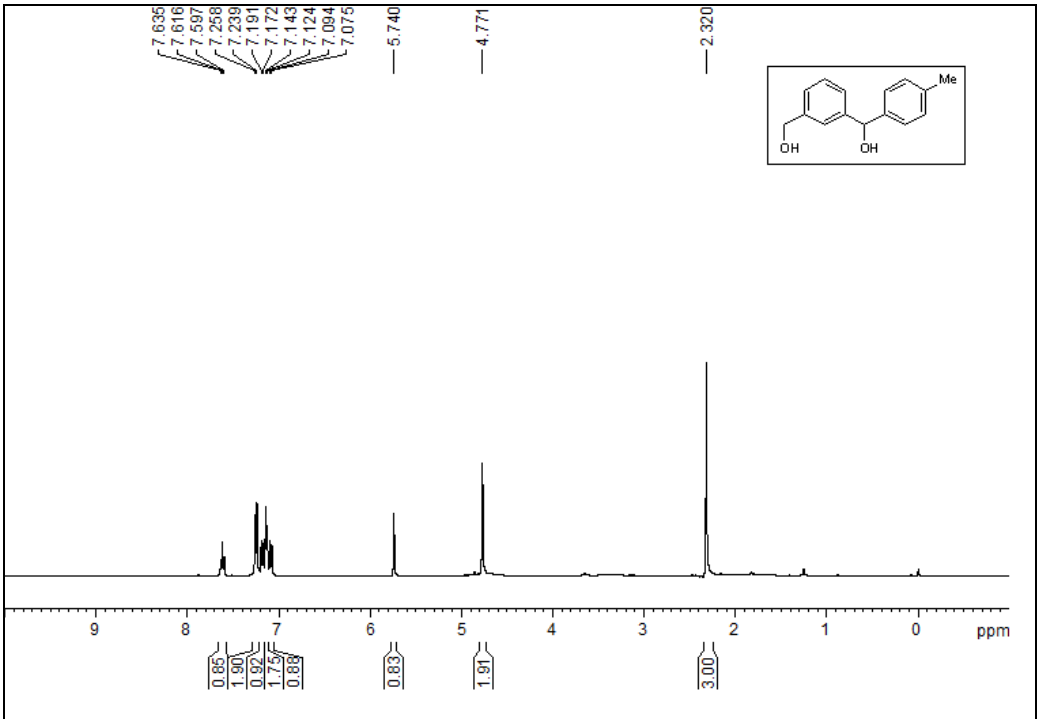
100 MHz ^{13}C NMR of (4-chlorophenyl)(6-(hydroxymethyl)pyridin-2-yl)methanol in $CDCl_3$



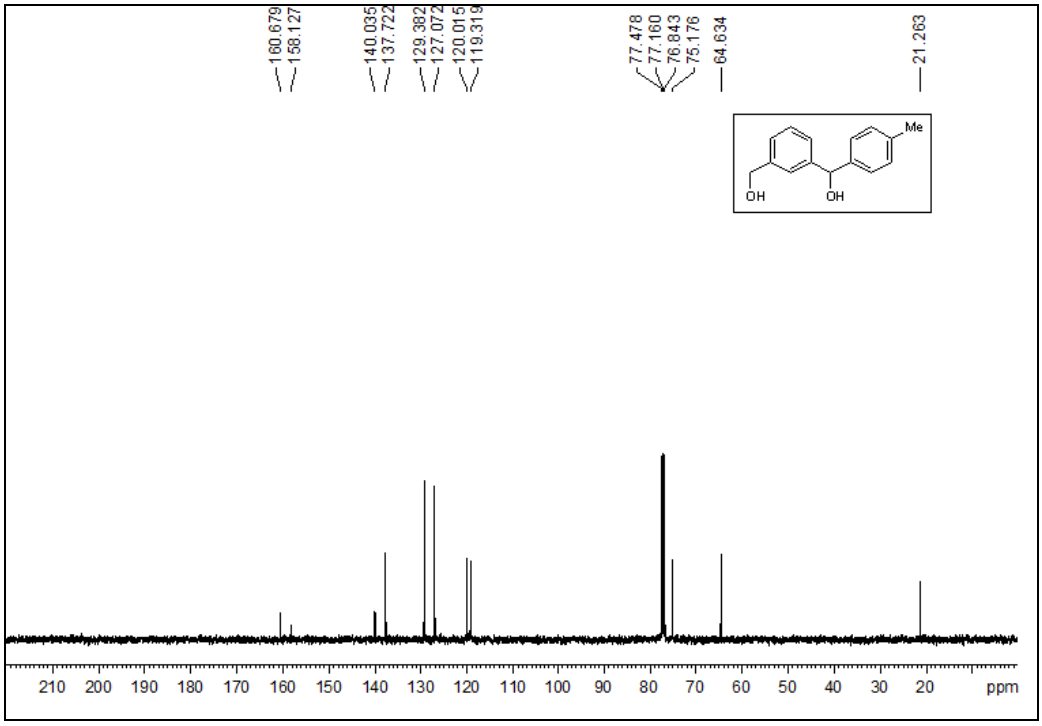
400 MHz ^{1}H NMR of (4-chlorophenyl)(6-(hydroxymethyl)pyridin-2-yl)methanone in $CDCl_3$



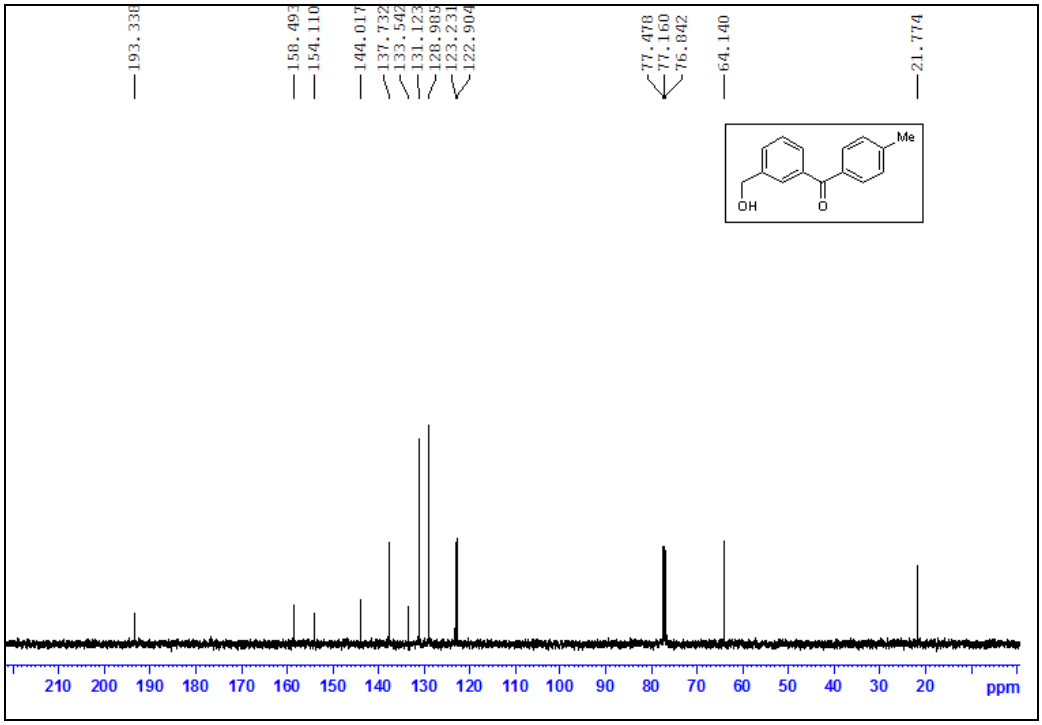
100 MHz ^{13}C NMR of (4-chlorophenyl)(6-(hydroxymethyl)pyridin-2-yl)methanone in $CDCl_3$



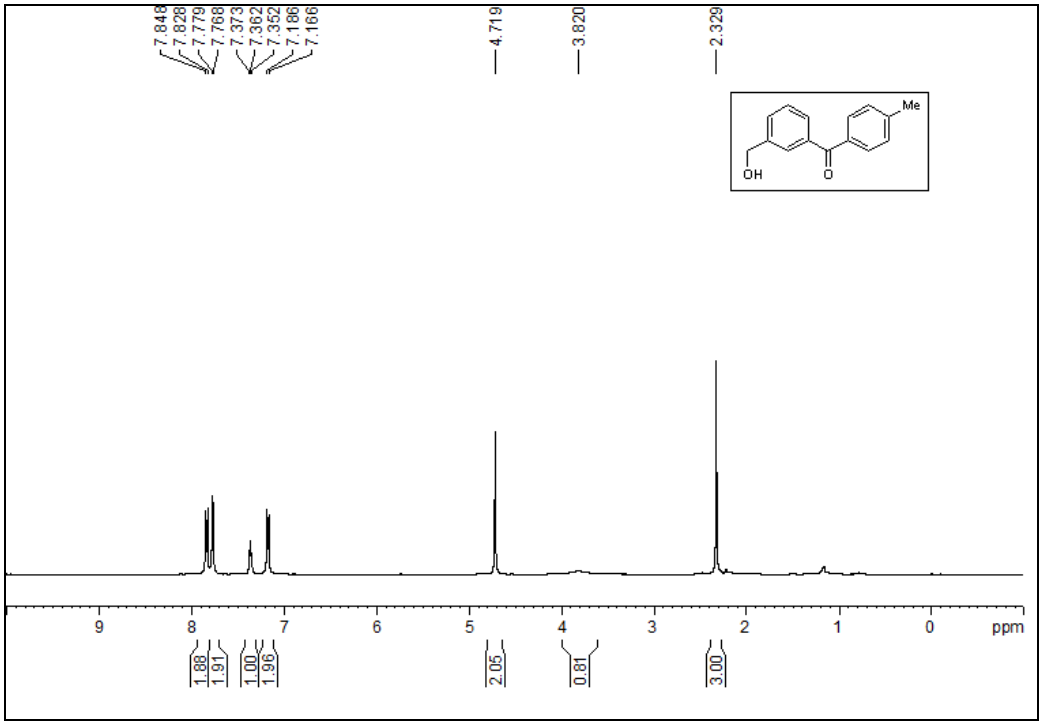
400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(p-tolyl)methanol in $CDCl_3$



100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(p-tolyl)methanol in $CDCl_3$



400 MHz ^{1}H NMR of (6-(hydroxymethyl)pyridin-2-yl)(p-tolyl)methanone in $CDCl_3$



100 MHz ^{13}C NMR of (6-(hydroxymethyl)pyridin-2-yl)(p-tolyl)methanone in $CDCl_3$

Crystals Data

Crystal A

Empirical formula	: C44 H55 Co3 N3 O17
Formula weight	: 1074.70
Temperature	: 173(2) K
Wavelength	: 0.71073 A
Crystal system, space group	: Triclinic, P-1
Unit cell dimensions	: a = 12.6137(7) A α = 91.643(2) deg. b = 13.1611(7) A β = 108.545(2) deg. c = 17.9352(10) A γ = 118.316(2) deg.
Volume	: 2426.9(2) A^3
Z, Calculated density	: 2, 1.471 Mg/m^3
Absorption coefficient	:1.086 mm^-1
F(000)	: 1114
Crystal size	: 0.42 x 0.38 x 0.10 mm
Theta range for data collection	: 1.80 to 28.36 deg.
Limiting indices	: -12<=h<=16, -16<=k<=16, -22<=l<=23
Reflections collected / unique	: 29310 / 10143 [R(int) = 0.0349]
Completeness to theta	: 25.00 96.5 %
Absorption correction	: Semi-empirical from equivalents
Max. and min. transmission	: 0.932 and 0.612
Refinement method	: Full-matrix least-squares on F^2
Data / restraints / parameters	: 10143 / 0 / 640
Goodness-of-fit on F^2	: 1.044
Final R indices [I>2sigma(I)]	: R1 = 0.0567, wR2 = 0.1631
R indices (all data)	: R1 = 0.0802, wR2 = 0.1837
Largest diff. peak and hole	: 2.412 and -0.831 e.A^-3

Bond lengths	**angstroms**
C(1)-N(1)	1.354(6)
C(1)-C(2)	1.358(7)
C(1)-H(1)	0.9500
C(2)-C(3)	1.385(9)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(8)
C(3)-H(3)	0.9500
C(4)-C(5)	1.397(6)
C(4)-H(4)	0.9500
C(5)-N(1)	1.357(6)
C(5)-C(6)	1.488(7)
C(6)-O(1)	1.429(5)
C(6)-C(7)	1.512(7)
C(6)-H(6)	1.0000
C(7)-C(12)	1.375(9)
C(7)-C(8)	1.396(9)
C(8)-C(9)	1.344(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.342(15)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(16)
C(10)-H(10)	0.9500
C(11)-C(12)	1.404(12)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-N(2)	1.323(6)
C(13)-C(14)	1.371(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.377(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.378(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.376(7)

Bond lengths	angstroms
C(16)-H(16)	0.9500
C(17)-N(2)	1.360(6)
C(17)-C(18)	1.519(6)
C(18)-O(2)	1.427(5)
C(18)-C(19)	1.513(6)
C(18)-H(18)	1.0000
C(19)-C(24)	1.376(7)
C(19)-C(20)	1.382(6)
C(20)-C(21)	1.395(8)
C(20)-H(20)	0.9500
C(21)-C(22)	1.354(9)
C(21)-H(21)	0.9500
C(22)-C(23)	1.354(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.400(7)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-N(3)	1.343(6)
C(25)-C(26)	1.375(7)
C(25)-H(25)	0.9500
C(26)-C(27)	1.363(8)
C(26)-H(26)	0.9500
C(27)-C(28)	1.373(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.398(7)
C(28)-H(28)	0.9500
C(29)-N(3)	1.338(6)
C(29)-C(30)	1.512(6)
C(30)-O(3)	1.382(5)
C(30)-C(31)	1.507(6)
C(30)-H(30)	1.0000
C(31)-C(32)	1.379(7)
C(31)-C(36)	1.386(7)

Bond lengths	angstroms
C(32)-C(33)	1.388(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.376(9)
C(33)-H(33)	0.9500
C(34)-C(35)	1.354(9)
C(34)-H(34)	0.9500
C(35)-C(36)	1.376(8)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-O(11)	1.235(6)
C(37)-O(4)	1.294(5)
C(37)-C(38)	1.504(7)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-O(12)	1.238(5)
C(39)-O(5)	1.278(5)
C(39)-C(40)	1.507(7)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-O(7)	1.251(5)
C(41)-O(6)	1.259(5)
C(41)-C(42)	1.516(7)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-O(13)	1.243(6)
C(43)-O(8)	1.279(5)
C(43)-C(44)	1.496(7)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800

Bond lengths	**angstroms**
N(1)-Co(1)	1.921(4)
N(2)-Co(1)	1.927(4)
N(3)-Co(1)	1.931(4)
O(1)-Co(1)	1.881(3)
O(1)-Co(2)	2.110(3)
O(2)-Co(1)	1.883(3)
O(2)-Co(2)	2.062(3)
O(3)-Co(1)	1.871(2)
O(3)-Co(2)	2.162(3)
O(4)-Co(4)	2.090(3)
O(4)-Co(3)	2.102(3)
O(5)-Co(4)	2.142(3)
O(5)-Co(3)	2.167(3)
O(6)-Co(3)	2.062(3)
O(7)-Co(4)	2.047(3)
O(8)-Co(4)	2.097(3)
O(8)-H(8A)	0.8400
O(9)-Co(4)	2.141(3)
O(9)-H(9A)	0.94(7)
O(9)-H(9B)	0.95(7)
O(10)-Co(4)	2.080(3)
O(10)-H(10A)	0.79(7)
O(10)-H(10B)	0.85(7)
Co(1)-Co(2)	2.6195(6)
Co(2)-O(2)#1	2.062(3)
Co(2)-O(1)#1	2.110(3)
Co(2)-O(3)#1	2.162(3)
Co(2)-Co(1)#1	2.6195(6)
Co(3)-O(6)#2	2.062(3)
Co(3)-O(4)#2	2.102(3)
Co(3)-O(5)#2	2.167(3)

Bond Angles	**(degrees)v**
N(1)-C(1)-C(2)	122.2(5)
N(1)-C(1)-H(1)	118.9
C(2)-C(1)-H(1)	118.9
C(1)-C(2)-C(3)	119.1(5)
C(1)-C(2)-H(2)	120.5
C(3)-C(2)-H(2)	120.5
C(4)-C(3)-C(2)	119.6(5)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-C(5)	119.2(5)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N(1)-C(5)-C(4)	120.2(5)
N(1)-C(5)-C(6)	116.1(4)
C(4)-C(5)-C(6)	123.6(5)
O(1)-C(6)-C(5)	110.4(4)
O(1)-C(6)-C(7)	107.5(4)
C(5)-C(6)-C(7)	114.2(4)
O(1)-C(6)-H(6)	108.2
C(5)-C(6)-H(6)	108.2
C(7)-C(6)-H(6)	108.2
C(12)-C(7)-C(8)	119.4(6)
C(12)-C(7)-C(6)	119.3(6)
C(8)-C(7)-C(6)	121.2(5)
C(9)-C(8)-C(7)	119.8(8)
C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	122.1(9)
C(10)-C(9)-H(9)	118.9
C(8)-C(9)-H(9)	118.9
C(9)-C(10)-C(11)	120.2(8)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	118.7(9)

Bond lengths	**angstroms**
C(10)-C(11)-H(11)	120.7
C(12)-C(11)-H(11)	120.7
C(7)-C(12)-C(11)	119.7(9)
C(7)-C(12)-H(12)	120.1
C(11)-C(12)-H(12)	120.1
N(2)-C(13)-C(14)	122.1(5)
N(2)-C(13)-H(13)	118.9
C(14)-C(13)-H(13)	118.9
C(13)-C(14)-C(15)	119.7(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	118.6(4)
C(14)-C(15)-H(15)	120.7
C(16)-C(15)-H(15)	120.7
C(17)-C(16)-C(15)	119.3(5)
C(17)-C(16)-H(16)	120.4
C(15)-C(16)-H(16)	120.4
N(2)-C(17)-C(16)	121.4(4)
N(2)-C(17)-C(18)	114.6(4)
C(16)-C(17)-C(18)	123.9(4)
O(2)-C(18)-C(19)	107.1(3)
O(2)-C(18)-C(17)	109.3(3)
C(19)-C(18)-C(17)	114.7(3)
O(2)-C(18)-H(18)	108.5
C(19)-C(18)-H(18)	108.5
C(17)-C(18)-H(18)	108.5
C(24)-C(19)-C(20)	119.9(4)
C(24)-C(19)-C(18)	120.1(4)
C(20)-C(19)-C(18)	119.7(4)
C(19)-C(20)-C(21)	119.6(5)
C(19)-C(20)-H(20)	120.2
C(21)-C(20)-H(20)	120.2

Bond Angles	**(degrees)v**
C(22)-C(21)-C(20)	119.9(5)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(21)-C(22)-C(23)	121.3(5)
C(21)-C(22)-H(22)	119.3
C(23)-C(22)-H(22)	119.3
C(22)-C(23)-C(24)	119.9(5)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(19)-C(24)-C(23)	119.5(5)
C(19)-C(24)-H(24)	120.3
C(23)-C(24)-H(24)	120.3
N(3)-C(25)-C(26)	122.1(5)
N(3)-C(25)-H(25)	119.0
C(26)-C(25)-H(25)	119.0
C(27)-C(26)-C(25)	118.4(5)
C(27)-C(26)-H(26)	120.8
C(25)-C(26)-H(26)	120.8
C(26)-C(27)-C(28)	120.8(5)
C(26)-C(27)-H(27)	119.6
C(28)-C(27)-H(27)	119.6
C(27)-C(28)-C(29)	118.2(5)
C(27)-C(28)-H(28)	120.9
C(29)-C(28)-H(28)	120.9
N(3)-C(29)-C(28)	121.0(4)
N(3)-C(29)-C(30)	116.9(4)
C(28)-C(29)-C(30)	122.0(4)
O(3)-C(30)-C(31)	107.8(3)
O(3)-C(30)-C(29)	106.6(3)
C(31)-C(30)-C(29)	113.8(4)
O(3)-C(30)-H(30)	109.5
C(31)-C(30)-H(30)	109.5
C(29)-C(30)-H(30)	109.5

Bond Angles	(degrees)v
C(32)-C(31)-C(36)	119.0(4)
C(32)-C(31)-C(30)	121.7(4)
C(36)-C(31)-C(30)	119.2(4)
C(31)-C(32)-C(33)	120.5(5)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(34)-C(33)-C(32)	119.3(5)
C(34)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
C(35)-C(34)-C(33)	120.4(5)
C(35)-C(34)-H(34)	119.8
C(33)-C(34)-H(34)	119.8
C(34)-C(35)-C(36)	120.8(5)
C(34)-C(35)-H(35)	119.6
C(36)-C(35)-H(35)	119.6
C(35)-C(36)-C(31)	119.9(5)
C(35)-C(36)-H(36)	120.0
C(31)-C(36)-H(36)	120.0
O(11)-C(37)-O(4)	123.1(4)
O(11)-C(37)-C(38)	120.0(4)
O(4)-C(37)-C(38)	116.9(4)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
O(12)-C(39)-O(5)	123.6(4)
O(12)-C(39)-C(40)	117.5(4)
O(5)-C(39)-C(40)	118.9(4)
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5

Bond Angles	(degrees)v
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(7)-C(41)-O(6)	125.4(4)
O(7)-C(41)-C(42)	117.0(4)
O(6)-C(41)-C(42)	117.7(4)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
O(13)-C(43)-O(8)	123.7(4)
O(13)-C(43)-C(44)	119.4(4)
O(8)-C(43)-C(44)	116.9(4)
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(1)-N(1)-C(5)	119.6(4)
C(1)-N(1)-Co(1)	128.2(4)
C(5)-N(1)-Co(1)	111.4(3)
C(13)-N(2)-C(17)	118.9(4)
C(13)-N(2)-Co(1)	128.0(3)
C(17)-N(2)-Co(1)	113.1(3)
C(29)-N(3)-C(25)	119.5(4)
C(29)-N(3)-Co(1)	111.9(3)
C(25)-N(3)-Co(1)	128.2(3)
C(6)-O(1)-Co(1)	112.1(3)
C(6)-O(1)-Co(2)	115.5(3)
Co(1)-O(1)-Co(2)	81.82(11)

Bond Angles	**(degrees)v**
C(18)-O(2)-Co(1)	113.3(2)
C(18)-O(2)-Co(2)	117.2(3)
Co(1)-O(2)-Co(2)	83.08(11)
C(30)-O(3)-Co(1)	116.5(2)
C(30)-O(3)-Co(2)	111.4(2)
Co(1)-O(3)-Co(2)	80.66(11)
C(37)-O(4)-Co(4)	122.7(3)
C(37)-O(4)-Co(3)	136.7(3)
Co(4)-O(4)-Co(3)	99.88(11)
C(39)-O(5)-Co(4)	125.4(3)
C(39)-O(5)-Co(3)	136.9(3)
Co(4)-O(5)-Co(3)	96.27(11)
C(41)-O(6)-Co(3)	131.2(3)
C(41)-O(7)-Co(4)	130.6(3)
C(43)-O(8)-Co(4)	129.4(3)
C(43)-O(8)-H(8A)	109.5
Co(4)-O(8)-H(8A)	120.0
Co(4)-O(9)-H(9A)	102(4)
Co(4)-O(9)-H(9B)	97(4)
H(9A)-O(9)-H(9B)	110(5)
Co(4)-O(10)-H(10A)	99(5)
Co(4)-O(10)-H(10B)	122(4)
H(10A)-O(10)-H(10B)	110(6)
O(3)-Co(1)-O(1)	87.84(13)
O(3)-Co(1)-O(2)	88.04(13)
O(1)-Co(1)-O(2)	86.37(13)
O(3)-Co(1)-N(1)	87.38(14)
O(1)-Co(1)-N(1)	85.95(15)
O(2)-Co(1)-N(1)	171.20(15)
O(3)-Co(1)-N(2)	173.37(15)
O(1)-Co(1)-N(2)	90.75(15)
O(2)-Co(1)-N(2)	85.40(14)

Bond Angles	**(degrees)v**
N(1)-Co(1)-N(2)	98.99(16)
O(3)-Co(1)-N(3)	83.28(15)
O(1)-Co(1)-N(3)	169.88(14)
O(2)-Co(1)-N(3)	88.47(15)
N(1)-Co(1)-N(3)	98.45(17)
N(2)-Co(1)-N(3)	97.52(16)
O(3)-Co(1)-Co(2)	54.51(11)
O(1)-Co(1)-Co(2)	52.88(9)
O(2)-Co(1)-Co(2)	51.39(9)
N(1)-Co(1)-Co(2)	120.05(12)
N(2)-Co(1)-Co(2)	119.88(11)
N(3)-Co(1)-Co(2)	117.39(11)
O(2)-Co(2)-O(2)	180.00(17)
O(2)-Co(2)-O(1)	76.25(11)
O(2)-Co(2)-O(1)	103.75(11)
O(2)-Co(2)-O(1)	103.75(11)
O(2)-Co(2)-O(1)	76.25(11)
O(1)-Co(2)-O(1)	179.999(1)
O(2)-Co(2)-O(3)	76.25(11)
O(2-Co(2)-O(3)	103.75(11)
O(1)-Co(2)-O(3)	75.08(11)
O(1)-Co(2)-O(3)	104.92(11)
O(2)-Co(2)-O(3)	103.75(11)
O(2)-Co(2)-O(3)	76.25(11)
O(1)-Co(2)-O(3)	104.92(11)
O(1)-Co(2)-O(3)	75.08(11)
O(3)-Co(2)-O(3)	179.999(1)
O(2)-Co(2)-Co(1)	45.52(8)
O(2)-Co(2)-Co(1)	134.48(8)
O(1)-Co(2)-Co(1)	45.31(8)
O(1)-Co(2)-Co(1)	134.69(8)
O(3)-Co(2)-Co(1)	44.83(7)
O(3)-Co(2)-Co(1)	135.17(7)

Bond Angles	**(degrees)v**
O(2)-Co(2)-Co(1)	134.48(8)
O(2)-Co(2)-Co(1)	45.52(8)
O(1)-Co(2)-Co(1)	134.69(8)
O(1)-Co(2)-Co(1)	45.31(8)
O(3)-Co(2)-Co(1)	135.17(7)
O(3)-Co(2)-Co(1)	44.83(7)
Co(1)-Co(2)-Co(1)	180.00(3)
O(6)-Co(3)-O(6)	180.000(2)
O(6)-Co(3)-O(4)	91.05(12)
O(6)-Co(3)-O(4)	88.95(12)
O(6)-Co(3)-O(4)	88.95(12)
O(6)-Co(3)-O(4)	91.05(12)
O(4)-Co(3)-O(4)	180.00(15)
O(6)-Co(3)-O(5)	88.48(11)
O(6)-Co(3)-O(5)	91.52(11)
O(4)-Co(3)-O(5)	76.93(10)
O(4)-Co(3)-O(5)	103.07(10)
O(6)-Co(3)-O(5)	91.52(11)
O(6)-Co(3)-O(5)	88.48(11)
O(4)-Co(3)-O(5)	103.07(10)
O(4)-Co(3)-O(5)	76.93(11)
O(5)-Co(3)-O(5)	180.000(2)
O(7)-Co(4)-O(10)	91.26(13)
O(7)-Co(4)-O(4)	92.57(12)
O(10)-Co(4)-O(4)	168.25(14)
O(7)-Co(4)-O(8)	175.89(12)
O(10)-Co(4)-O(8)	87.32(13)
O(4)-Co(4)-O(8)	89.57(12)
O(7)-Co(4)-O(9)	88.83(13)
O(10)-Co(4)-O(9)	96.42(15)
O(4)-Co(4)-O(9)	94.76(13)
O(8)-Co(4)-O(9)	87.49(13)
O(7)-Co(4)-O(5)	89.56(12)

Bond Angles	**(degrees)v**
O(10)-Co(4)-O(5)	91.18(13)
O(4)-Co(4)-O(5)	77.75(11)
O(8)-Co(4)-O(5)	94.33(11)
O(9)-Co(4)-O(5)	172.26(12)

Crystal B

Empirical formula	: C76 H78 Co3 N6 O15
Formula weight	: 1492.23
Temperature	: 293(2) K
Wavelength	: 0.71073 A
Crystal system, space group	: Monoclinic, C2/c
Unit cell dimensions	: a = 29.163(2) A α = 90 deg. b = 17.1312(12) A β = 122.096(2) deg. c = 18.0064(13) A γ = 90 deg.
Volume	: 7621.0(9) A^3
Z, Calculated density	: 4, 1.301 Mg/m^3
Absorption coefficient	: 0.712 mm^-1
F(000)	: 3108
Crystal size	: 0.30 x 0.20 x 0.20 mm
Theta range for data collection	:1.45 to 23.35 deg.
Limiting indices	: -32<=h<=32, -19<=k<=15, -20<=l<=13
Reflections collected / unique	: 21884 / 5519 [R(int) = 0.0401]
Completeness to theta	: 23.35 99.6 %
Absorption correction	: Semi-empirical from equivalents
Max. and min. transmission	: 0.841 and 0.753
Refinement method	: Full-matrix least-squares on F^2
Data / restraints / parameters	: 5519 / 138 / 478
Goodness-of-fit on F^2	: 1.144
Final R indices [I>2sigma(I)]	: R1 = 0.0757, wR2 = 0.2214
R indices (all data)	: R1 = 0.1067, wR2 = 0.2544
Extinction coefficient	: 0.0051(5)
Largest diff. peak and hole	: 1.287 and -0.777 e.A^-3

Bond lengths	**angstroms**
C(1)-O(1)	1.428(7)
C(1)-C(2)	1.500(9)
C(1)-C(7)	1.516(9)
C(1)-H(1)	0.9800
C(2)-N(1)	1.332(8)
C(2)-C(3)	1.377(9)
C(3)-C(4)	1.367(11)
C(3)-H(3)	0.9300
C(4)-C(5)	1.370(12)
C(4)-H(4)	0.9300
C(5)-C(6)	1.367(10)
C(5)-H(5)	0.9300
C(6)-N(1)	1.353(9)
C(6)-H(6)	0.9300
C(7)-C(12)	1.358(10)
C(7)-C(8)	1.382(10)
C(8)-C(9)	1.362(13)
C(8)-H(8)	0.9300
C(9)-C(10)	1.314(16)
C(9)-H(9)	0.9300
C(10)-C(11)	1.418(16)
C(10)-H(10)	0.9300
C(11)-C(12)	1.372(12)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-N(2)	1.343(9)
C(13)-C(14)	1.392(11)
C(13)-H(13)	0.9300
C(14)-C(15)	1.350(12)
C(14)-H(14)	0.9300
C(15)-C(16)	1.368(12)
C(15)-H(15)	0.9300
C(16)-C(17)	1.379(9)
C(16)-H(16)	0.9300

Bond lengths	**angstroms**
C(17)-N(2)	1.342(8)
C(17)-C(18)	1.502(9)
C(18)-O(2)	1.416(7)
C(18)-C(19)	1.521(9)
C(18)-H(18)	0.9800
C(19)-C(20)	1.350(11)
C(19)-C(24)	1.372(11)
C(20)-C(21)	1.412(12)
C(20)-H(20)	0.9300
C(21)-C(22)	1.356(18)
C(21)-H(21)	0.9300
C(22)-C(23)	1.324(18)
C(22)-H(22)	0.9300
C(23)-C(24)	1.387(14)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-N(3)	1.334(8)
C(25)-C(26)	1.370(10)
C(25)-H(25)	0.9300
C(26)-C(27)	1.360(13)
C(26)-H(26)	0.9300
C(27)-C(28)	1.385(12)
C(27)-H(27)	0.9300
C(28)-C(29)	1.382(10)
C(28)-H(28)	0.9300
C(29)-N(3)	1.350(8)
C(29)-C(30)	1.508(8)
C(30)-C(31)	1.4137
C(30)-O(3)	1.415(6)
C(30)-C(31')	1.5506
C(30)-H(30)	0.9800
C(31)-C(36)	1.3900

Bond lengths	**angstroms**
C(31)-C(32)	1.3902
C(32)-C(33)	1.3900
C(32)-H(32)	0.9300
C(33)-C(34)	1.3900
C(33)-H(33)	0.9300
C(34)-C(35)	1.3900
C(34)-H(34)	0.9300
C(35)-C(36)	1.3899
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(31')-C(36')	1.3900
C(31')-C(32')	1.3901
C(32')-C(33')	1.3900
C(32')-H(32')	0.9300
C(33')-C(34')	1.3899
C(33')-H(33')	0.9300
C(34')-C(35')	1.3901
C(34')-H(34')	0.9300
C(35')-C(36')	1.3900
C(35')-H(35')	0.9300
C(36')-H(36')	0.9300
C(37)-O(6)	1.23(2)
C(37)-O(5)	1.26(2)
C(37)-C(38)	1.484(16)
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
N(1)-Co(1)	1.929(5)
N(2)-Co(1)	1.920(5)
N(3)-Co(1)	1.920(5)
O(1)-Co(1)	1.885(4)
O(1)-Co(2)	2.091(4)
O(2)-Co(1)	1.883(4)

Bond lengths	**angstroms**
O(2)-Co(2)	2.082(4)
O(3)-Co(1)	1.880(4)
O(3)-Co(2)	2.078(4)
O(5)-H(5A)	0.8200
Co(1)-Co(2)	2.6350(8)
Co(2)-O(3)	2.078(4)
Co(2)-O(2)	2.082(4)
Co(2)-O(1)	2.091(4)
Co(2)-Co(1)	2.6350(8)
O(8)-O(8)	1.58(9)

Bond Angles	**(degrees)v**
O(1)-C(1)-C(2)	109.3(5)
O(1)-C(1)-C(7)	108.8(5)
C(2)-C(1)-C(7)	114.0(5)
O(1)-C(1)-H(1)	108.2
C(2)-C(1)-H(1)	108.2
C(7)-C(1)-H(1)	108.2
N(1)-C(2)-C(3)	120.8(6)
N(1)-C(2)-C(1)	116.6(5)
C(3)-C(2)-C(1)	122.4(6)
C(4)-C(3)-C(2)	120.0(7)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	118.8(7)
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-H(4)	120.6
C(6)-C(5)-C(4)	119.8(7)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1

Bond Angles	**(degrees)v**
N(1)-C(6)-C(5)	120.9(7)
N(1)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(12)-C(7)-C(8)	119.8(7)
C(12)-C(7)-C(1)	121.3(6)
C(8)-C(7)-C(1)	118.9(7)
C(9)-C(8)-C(7)	119.6(10)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	121.4(10)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.3
C(9)-C(10)-C(11)	120.6(9)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	117.8(10)
C(12)-C(11)-H(11)	121.1
C(10)-C(11)-H(11)	121.1
C(7)-C(12)-C(11)	120.8(9)
C(7)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
N(2)-C(13)-C(14)	120.3(7)
N(2)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.2(7)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(14)-C(15)-C(16)	119.2(7)
C(14)-C(15)-H(15)	120.4
C(16)-C(15)-H(15)	120.4
C(15)-C(16)-C(17)	119.7(7)
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1

Bond Angles	**(degrees)v**
N(2)-C(17)-C(16)	121.0(6)
N(2)-C(17)-C(18)	115.8(5)
C(16)-C(17)-C(18)	123.2(6)
O(2)-C(18)-C(17)	109.7(5)
O(2)-C(18)-C(19)	107.9(5)
C(17)-C(18)-C(19)	113.5(5)
O(2)-C(18)-H(18)	108.6
C(17)-C(18)-H(18)	108.6
C(19)-C(18)-H(18)	108.6
C(20)-C(19)-C(24)	119.6(7)
C(20)-C(19)-C(18)	120.1(7)
C(24)-C(19)-C(18)	120.0(7)
C(19)-C(20)-C(21)	119.8(10)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(22)-C(21)-C(20)	119.2(11)
C(22)-C(21)-H(21)	120.4
C(20)-C(21)-H(21)	120.4
C(23)-C(22)-C(21)	120.9(10)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	120.8(11)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(19)-C(24)-C(23)	119.7(10)
C(19)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
N(3)-C(25)-C(26)	122.8(7)
N(3)-C(25)-H(25)	118.6
C(26)-C(25)-H(25)	118.6
C(27)-C(26)-C(25)	117.9(7)
C(27)-C(26)-H(26)	121.1
C(25)-C(26)-H(26)	121.1

Bond Angles	**(degrees)v**
C(26)-C(27)-C(28)	120.9(7)
C(26)-C(27)-H(27)	119.5
C(28)-C(27)-H(27)	119.5
C(29)-C(28)-C(27)	118.1(8)
C(29)-C(28)-H(28)	121.0
C(27)-C(28)-H(28)	121.0
N(3)-C(29)-C(28)	120.9(7)
N(3)-C(29)-C(30)	115.9(5)
C(28)-C(29)-C(30)	123.2(6)
C(31)-C(30)-O(3)	114.4(2)
C(31)-C(30)-C(29)	115.8(3)
O(3)-C(30)-C(29)	109.0(4)
C(31)-C(30)-C(31')	20.9
O(3)-C(30)-C(31')	103.1(3)
C(29)-C(30)-C(31')	106.5(3)
C(31)-C(30)-H(30)	105.5
O(3)-C(30)-H(30)	105.5
C(29)-C(30)-H(30)	105.5
C(31')-C(30)-H(30)	126.4
C(36)-C(31)-C(32)	120.0
C(36)-C(31)-C(30)	121.2
C(32)-C(31)-C(30)	118.8
C(33)-C(32)-C(31)	120.0
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(32)-C(33)-C(34)	120.0
C(32)-C(33)-H(33)	120.0
C(34)-C(33)-H(33)	120.0
C(33)-C(34)-C(35)	120.0
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(36)-C(35)-C(34)	120.0
C(36)-C(35)-H(35)	120.0

Bond Angles	**(degrees)v**
C(34)-C(35)-H(35)	120.0
C(35)-C(36)-C(31)	120.0
C(35)-C(36)-H(36)	120.0
C(31)-C(36)-H(36)	120.0
C(36')-C(31')-C(32')	120.0
C(36')-C(31')-C(30)	109.9
C(32')-C(31')-C(30)	129.5
C(33')-C(32')-C(31')	120.0
C(33')-C(32')-H(32')	120.0
C(31')-C(32')-H(32')	120.0
C(34')-C(33')-C(32')	120.0
C(34')-C(33')-H(33')	120.0
C(32')-C(33')-H(33')	120.0
C(33')-C(34')-C(35')	120.0
C(33')-C(34')-H(34')	120.0
C(35')-C(34')-H(34')	120.0
C(36')-C(35')-C(34')	120.0
C(36')-C(35')-H(35')	120.0
C(34')-C(35')-H(35')	120.0
C(35')-C(36')-C(31')	120.0
C(35')-C(36')-H(36')	120.0
C(31')-C(36')-H(36')	120.0
O(6)-C(37)-O(5)	125(2)
O(6)-C(37)-C(38)	111(2)
O(5)-C(37)-C(38)	124(2)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(2)-N(1)-C(6)	119.7(5)
C(2)-N(1)-Co(1)	112.0(4)

Bond Angles	**(degrees)v**
C(6)-N(1)-Co(1)	127.8(5)
C(17)-N(2)-C(13)	119.6(6)
C(17)-N(2)-Co(1)	112.8(4)
C(13)-N(2)-Co(1)	127.6(5)
C(25)-N(3)-C(29)	119.3(6)
C(25)-N(3)-Co(1)	128.1(5)
C(29)-N(3)-Co(1)	112.4(4)
C(1)-O(1)-Co(1)	112.4(3)
C(1)-O(1)-Co(2)	114.1(3)
Co(1)-O(1)-Co(2)	82.85(15)
C(18)-O(2)-Co(1)	113.4(4)
C(18)-O(2)-Co(2)	118.4(4)
Co(1)-O(2)-Co(2)	83.14(14)
C(30)-O(3)-Co(1)	114.2(3)
C(30)-O(3)-Co(2)	116.9(3)
Co(1)-O(3)-Co(2)	83.32(15)
C(37)-O(5)-H(5A)	109.5
O(3)-Co(1)-O(2)	85.00(17)
O(3)-Co(1)-O(1)	85.99(17)
O(2)-Co(1)-O(1)	85.99(17)
O(3)-Co(1)-N(2)	170.0(2)
O(2)-Co(1)-N(2)	85.28(19)
O(1)-Co(1)-N(2)	91.0(2)
O(3)-Co(1)-N(3)	85.0(2)
O(2)-Co(1)-N(3)	90.31(19)
O(1)-Co(1)-N(3)	170.6(2)
N(2)-Co(1)-N(3)	97.4(2)
O(3)-Co(1)-N(1)	90.3(2)
O(2)-Co(1)-N(1)	170.3(2)
O(1)-Co(1)-N(1)	85.17(19)
N(2)-Co(1)-N(1)	98.9(2)
N(3)-Co(1)-N(1)	97.8(2)
O(3)-Co(1)-Co(2)	51.57(12)

Bond Angles	**(degrees)v**
O(2)-Co(1)-Co(2)	51.67(12)
O(1)-Co(1)-Co(2)	51.92(12)
N(2)-Co(1)-Co(2)	119.60(16)
N(3)-Co(1)-Co(2)	119.40(16)
N(1)-Co(1)-Co(2)	119.04(16)
O(3)-Co(2)-O(3)	179.999(1)
O(3)-Co(2)-O(2)	75.32(15)
O(3)-Co(2)-O(2)	104.68(15)
O(3)-Co(2)-O(2)	104.68(15)
O(3)-Co(2)-O(2)	75.32(15)
O(2)-Co(2)-O(2)	180.00(16)
O(3)-Co(2)-O(1)	103.97(16)
O(3)-Co(2)-O(1)	76.03(16)
O(2)-Co(2)-O(1)	103.97(15)
O(2)-Co(2)-O(1)	76.03(15)
O(3)-Co(2)-O(1)	76.03(16)
O(3)-Co(2)-O(1)	103.97(16)
O(2)-Co(2)-O(1)	76.03(15)
O(2)-Co(2)-O(1)	103.97(15)
O(1)-Co(2)-O(1)	180.000(1)
O(3)-Co(2)-Co(1)	45.11(11)
O(3)-Co(2)-Co(1)	134.89(11)
O(2)-Co(2)-Co(1)	45.19(10)
O(2)-Co(2)-Co(1)	134.81(10)
O(1)-Co(2)-Co(1)	134.77(11)
O(1)-Co(2)-Co(1)	45.23(11)
O(3)-Co(2)-Co(1)	134.89(11)
O(3)-Co(2)-Co(1)	45.11(11)
O(2)-Co(2)-Co(1)	134.81(10)
O(2)-Co(2)-Co(1)	45.19(10)
O(1)-Co(2)-Co(1)	45.23(11)
O(1)-Co(2)-Co(1)	134.77(11)
Co(1)-Co(2)-Co(1)	180.0