Electronic supplementary information

Heterogeneous O–arylation of nitroarenes with substituted phenols over copper immobilized mesoporous silica catalyst#

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#All authors have equal contribution.

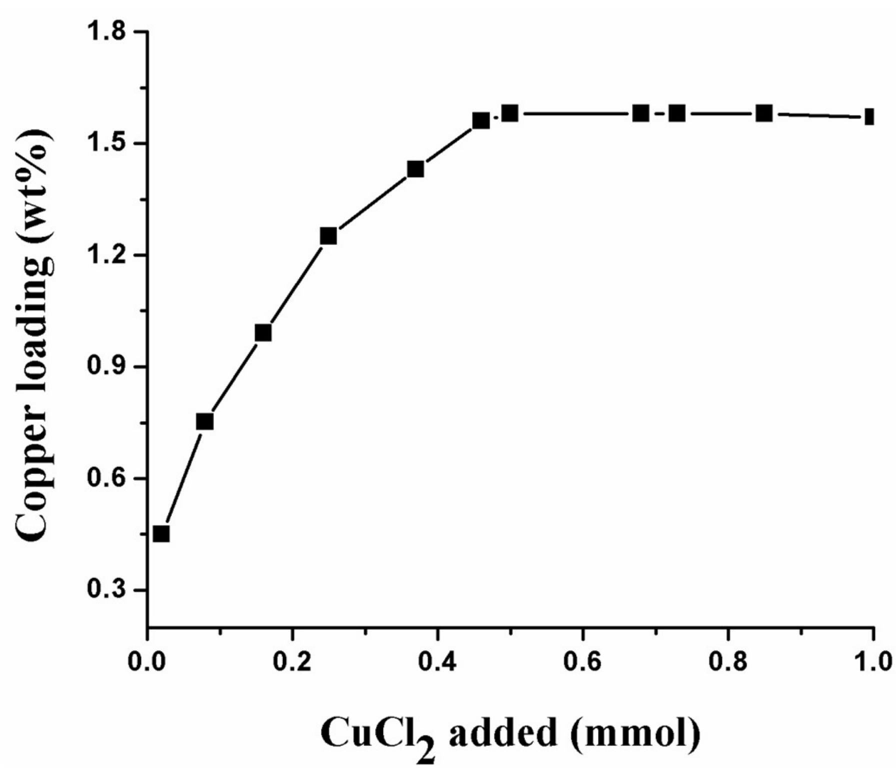


Fig. S1 Plot for optimal copper loading

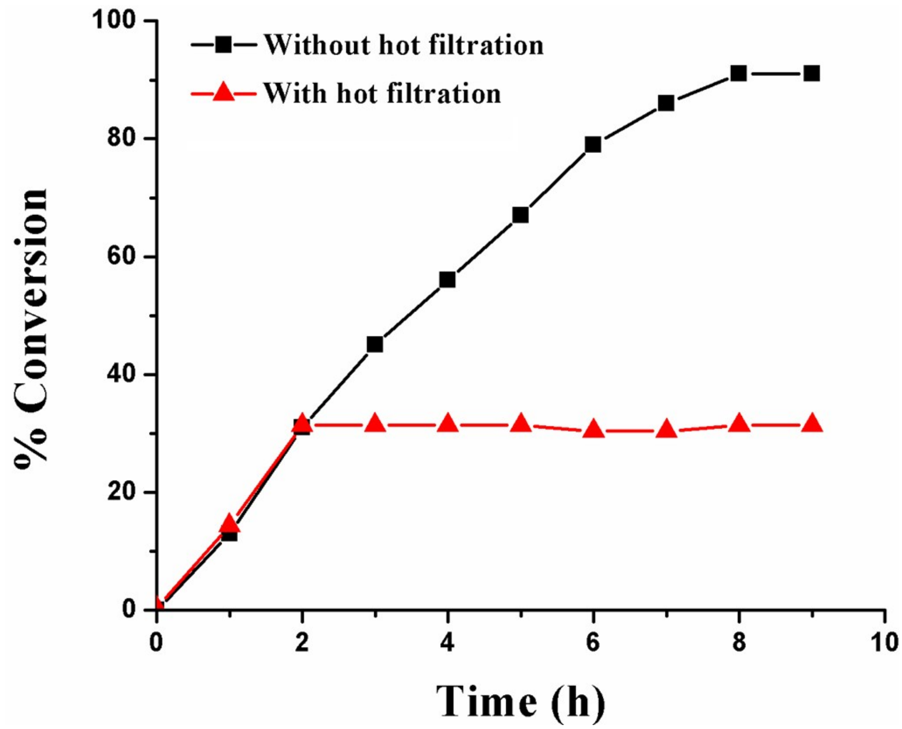


Fig. S2 Plot showing hot filtration test for O–arylation reaction of phenol with *p*-nitrobenzaldehyde

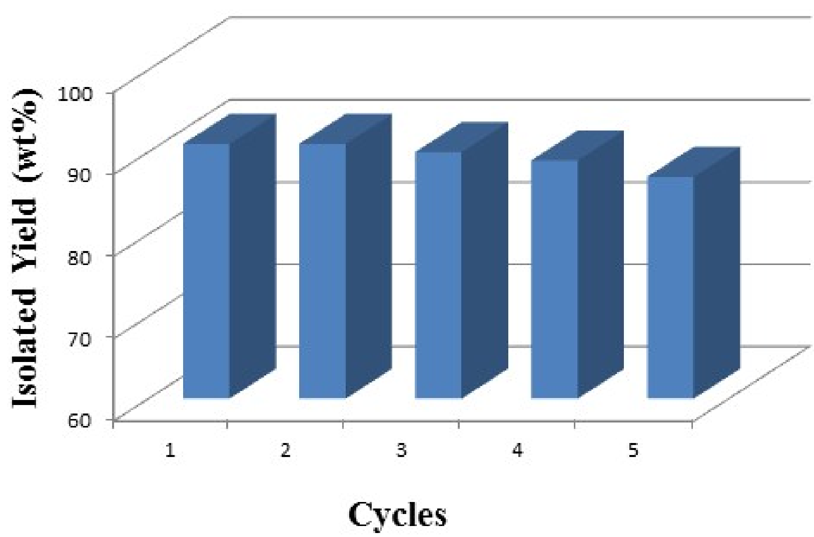


Fig. S3 Bar diagram showing recyclability of the catalyst for O–arylation of phenol

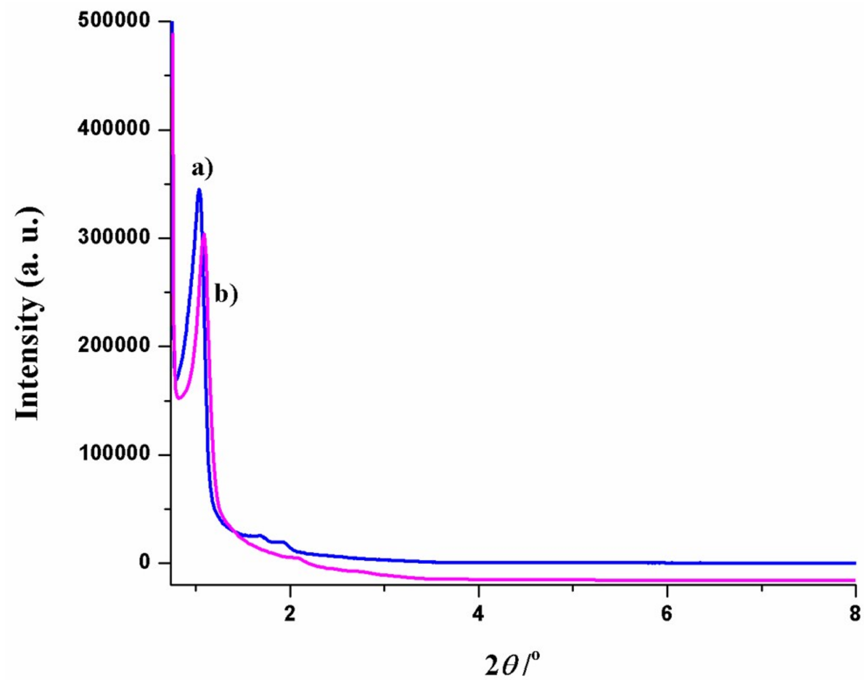


Fig. S4 PXRD patterns of (a) pristine S@Cu and (b) recovered S@Cu

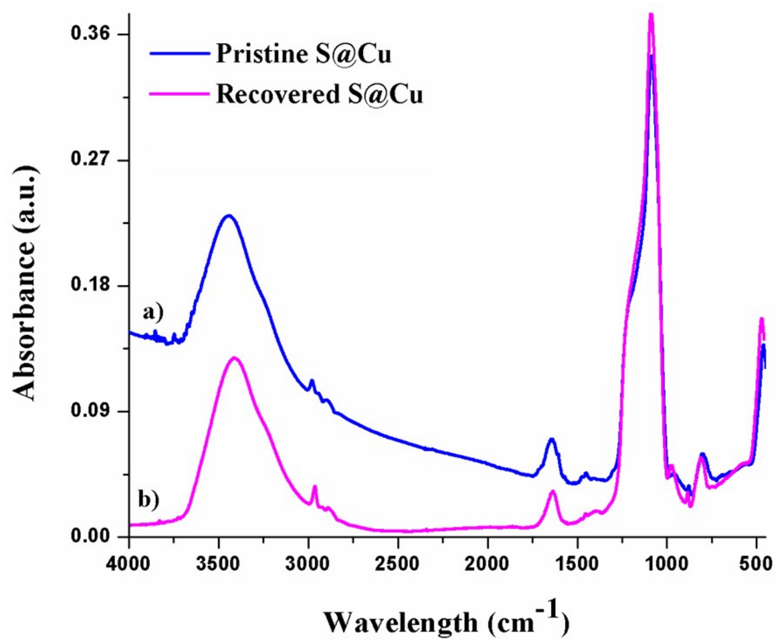


Fig. S5 FTIR spectra of (a) pristine S@Cu and (b) recovered S@Cu

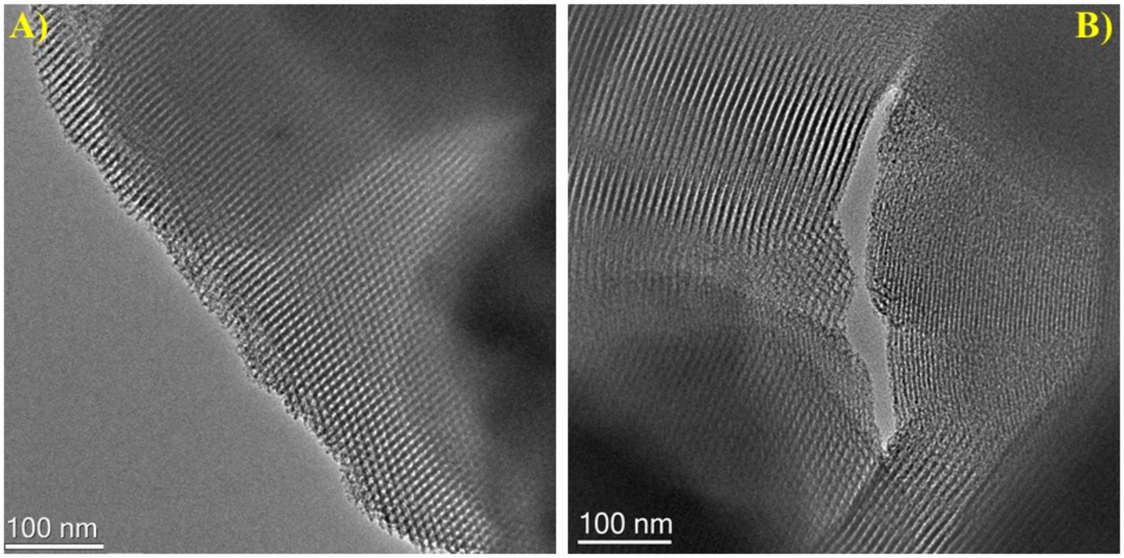


Fig. S6 TEM images of (a) pristine S@Cu and (b) recovered S@Cu

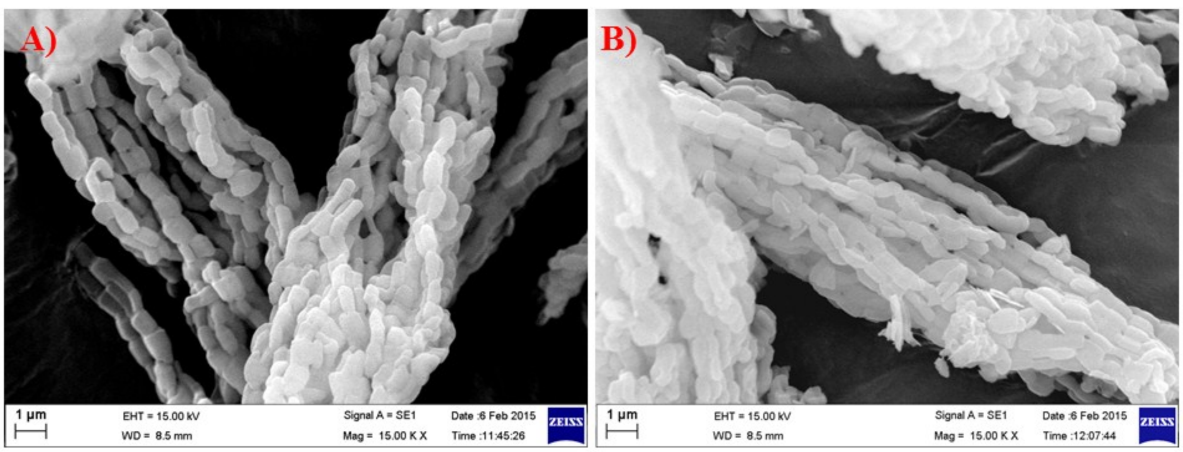
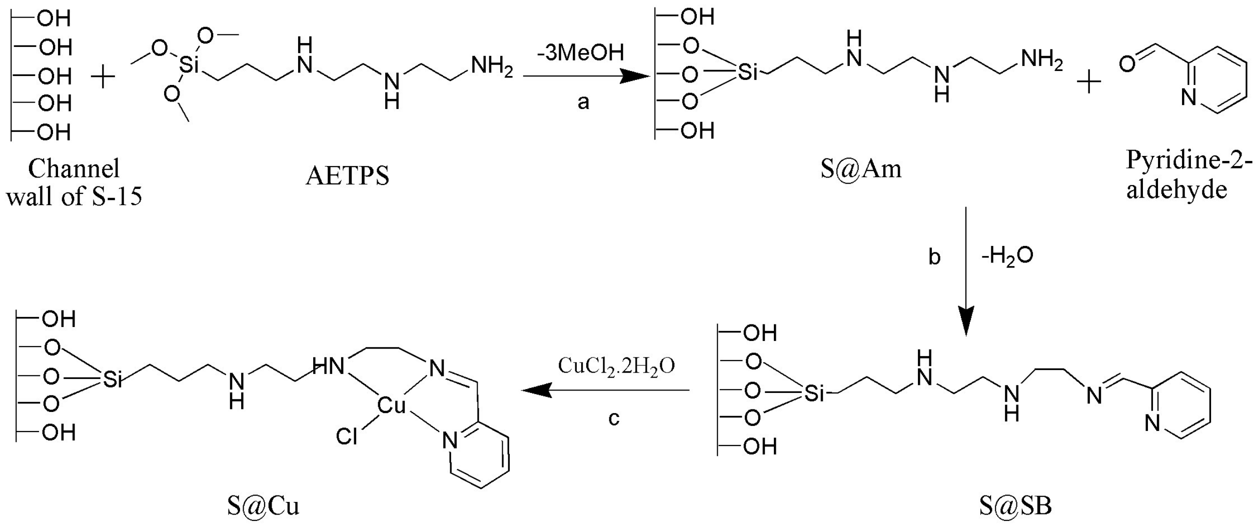
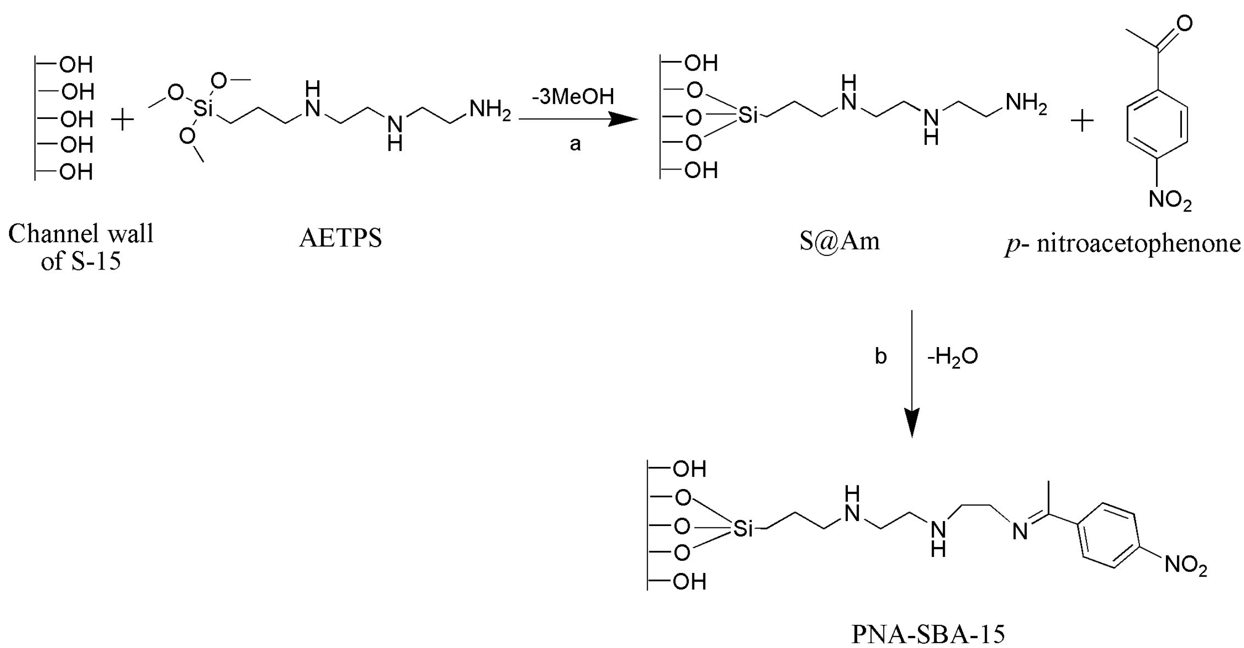


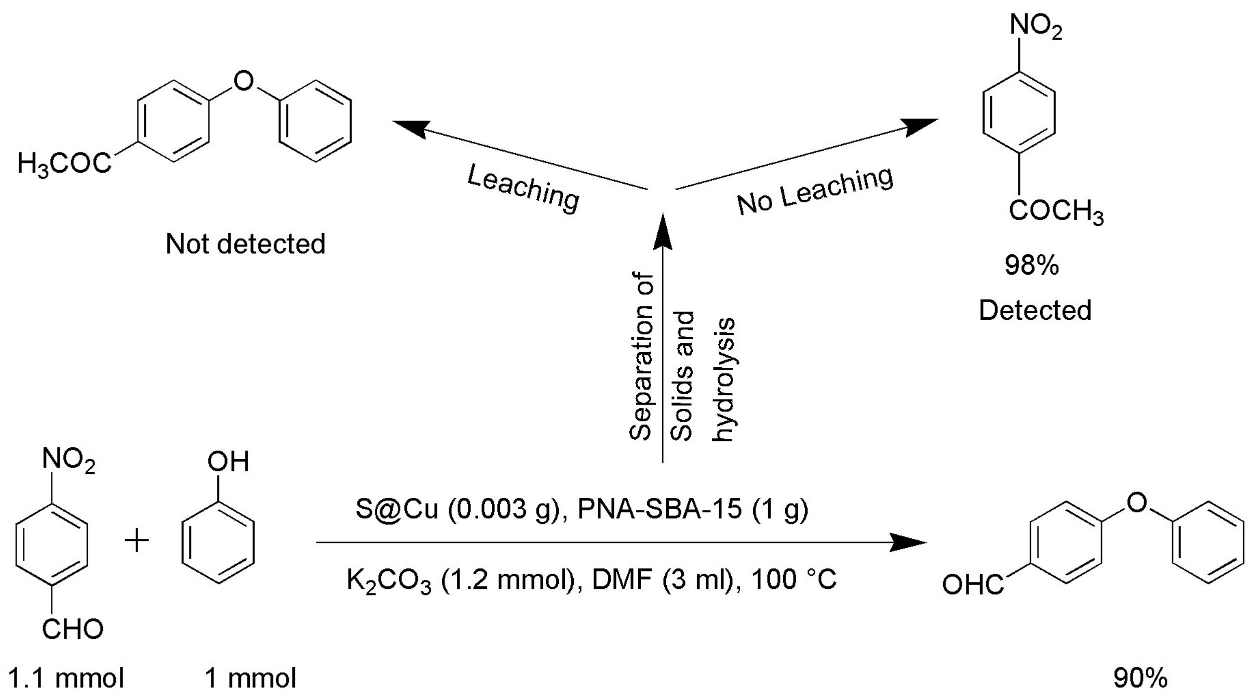
Fig. S7 SEM images of (a) pristine S@Cu and (b) recovered S@Cu



Scheme S1 (a) Modification of S–15 channel wall: AETPS/toluene, (b) condensation with pyridine-2-aldehyde in methanol, (c) metal complex formation: $CuCl_2{\cdot}2H_2O$/methanol/reflux.



Scheme S2 (a) Organic modification of SBA–15: AETPS/toluene, (b) anchoring of *p*–nitroacetophenone onto SBA–15 (in methanol)

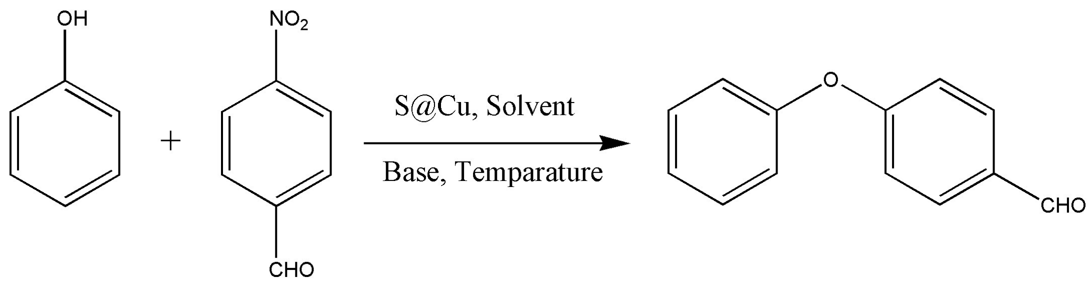


Scheme S3 Three-phase test for O–arylation reaction

Table S1 N_2 adsorption characteristics of supports and catalysis at 77 K: specific surface area, S_{BET} ($m^2\ g^{-1}$); pore volume ($cm^3\ g^{-1}$); half pore width, D_{NLDFT} (Å)

Materials	S_{BET}	Pore volume	D_{NLDFT}
SBA–15	1431	1.62	31
S@Am	750	1.02	24
S@Cu	312	0.39	22

Table S2 Optimization of reaction conditions[a]



Entry	Catalyst	Base	Solvent	Yield[b] (%)
1	–	K_2CO_3	DMF	–
2	S@Cu	K_2CO_3	DMF	**91**
3	S@Cu	K_2CO_3	DMSO	87
4	S@Cu	K_2CO_3	Toluene	15
5	S@Cu	K_2CO_3	Acetonitrile	31
6	S@Cu	K_2CO_3	Methanol	58
7	S@Cu	K_2CO_3	Ethyleneglycol	64
8	S@Cu	K_2CO_3	Dioxane	62
9	S@Cu	KOH	DMF	55
10	S@Cu	Na_2CO_3	DMF	62
11	S@Cu	Cs_2CO_3	DMF	90
12	S@Cu	CH_3COONa	DMF	–
13	S@Cu	tBuOK	DMF	21
14	S@Cu	DABCO	DMF	–
15[c]	S@Cu	K_2CO_3	DMF	58[d]
16[e]	S@Cu	K_2CO_3	DMF	79
17	S@Am+ $CuCl_2{\cdot}2H_2O$	K_2CO_3	DMF	25
18	S@SB+ $CuCl_2{\cdot}2H_2O$	K_2CO_3	DMF	29
19	$CuCl_2{\cdot}2H_2O$	K_2CO_3	DMF	73

[a] Reaction condition: *p*–nitrobenzaldehyde (1.1 mmol), phenol (1.0 mmol), base (1.2 mmol), catalyst (0.025 mol%), solvent (3 mL) at 100 °C for 8 h.

[b] Isolated yield.

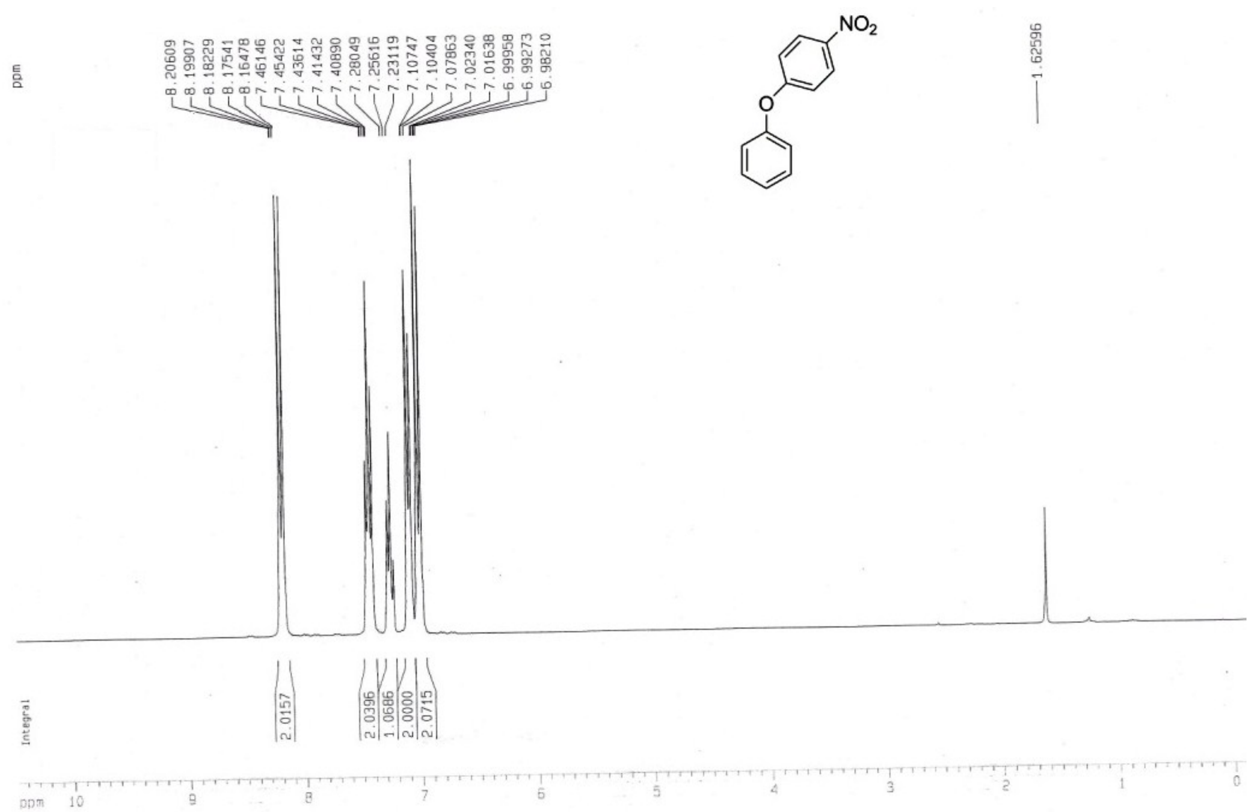
[c] temperature was 60 °C.

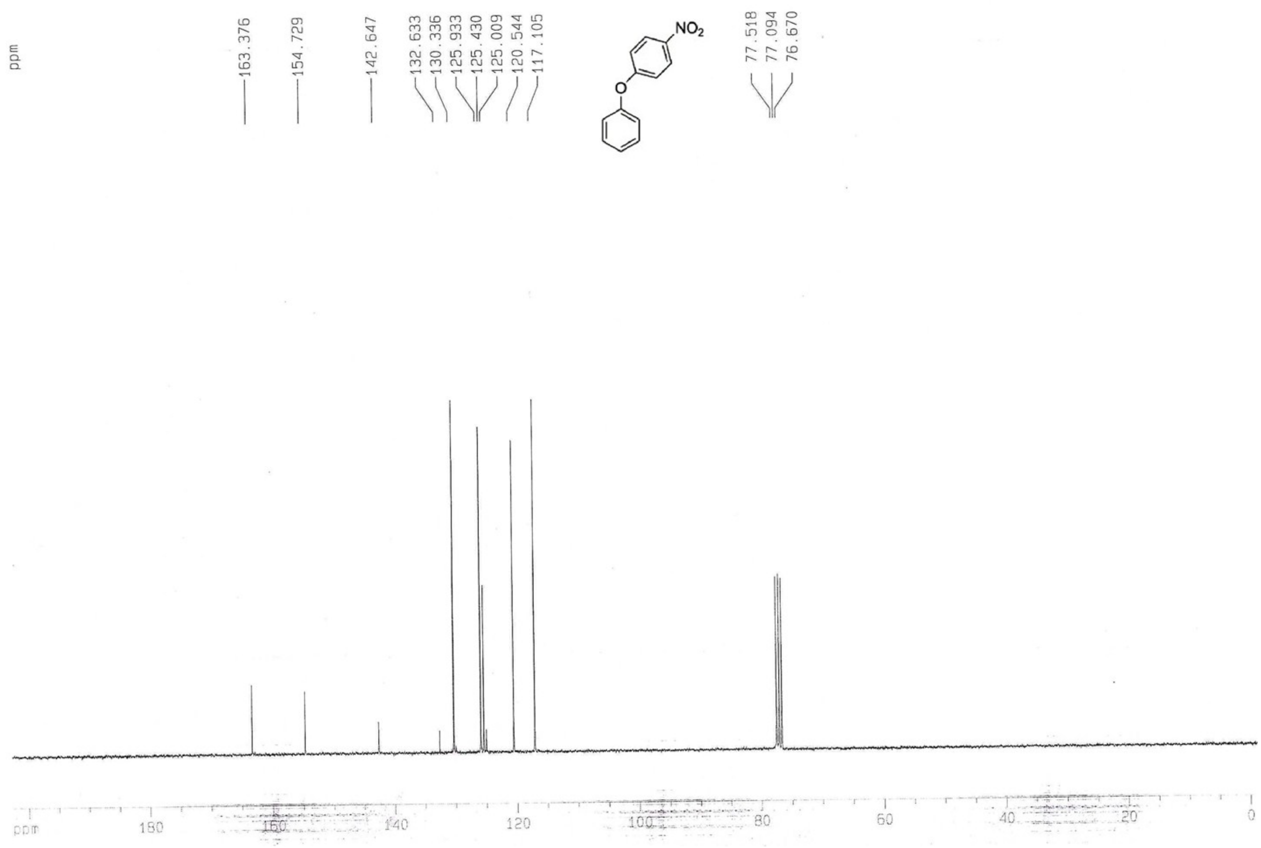
[d] Isolated yield at 20 h.

[e] temperature was 120 °C at 8 h**.**

Characterization of products

1a; δ_H (300 MHz, $CDCl_3$, ppm) 6.98–7.11 (m, 4H), 7.23–7.28 (m, 1H), 7.41–7.46 (m, 2H), 8.16–8.20 (m, 2H); δ_C (75 MHz; $CDCl_3$) 117.11, 120.54, 125.43, 125.93, 130.34, 132.63, 142.65, 154.73, 163.38; *m/z* 216.0592 [$(M+H)^+$, 100%]; Elemental analysis (found: C, 66.93; H, 4.24; N, 6.49. for $C_{12}H_9NO_3$ requires: C, 66.97; H, 4.22; N, 6.51%).

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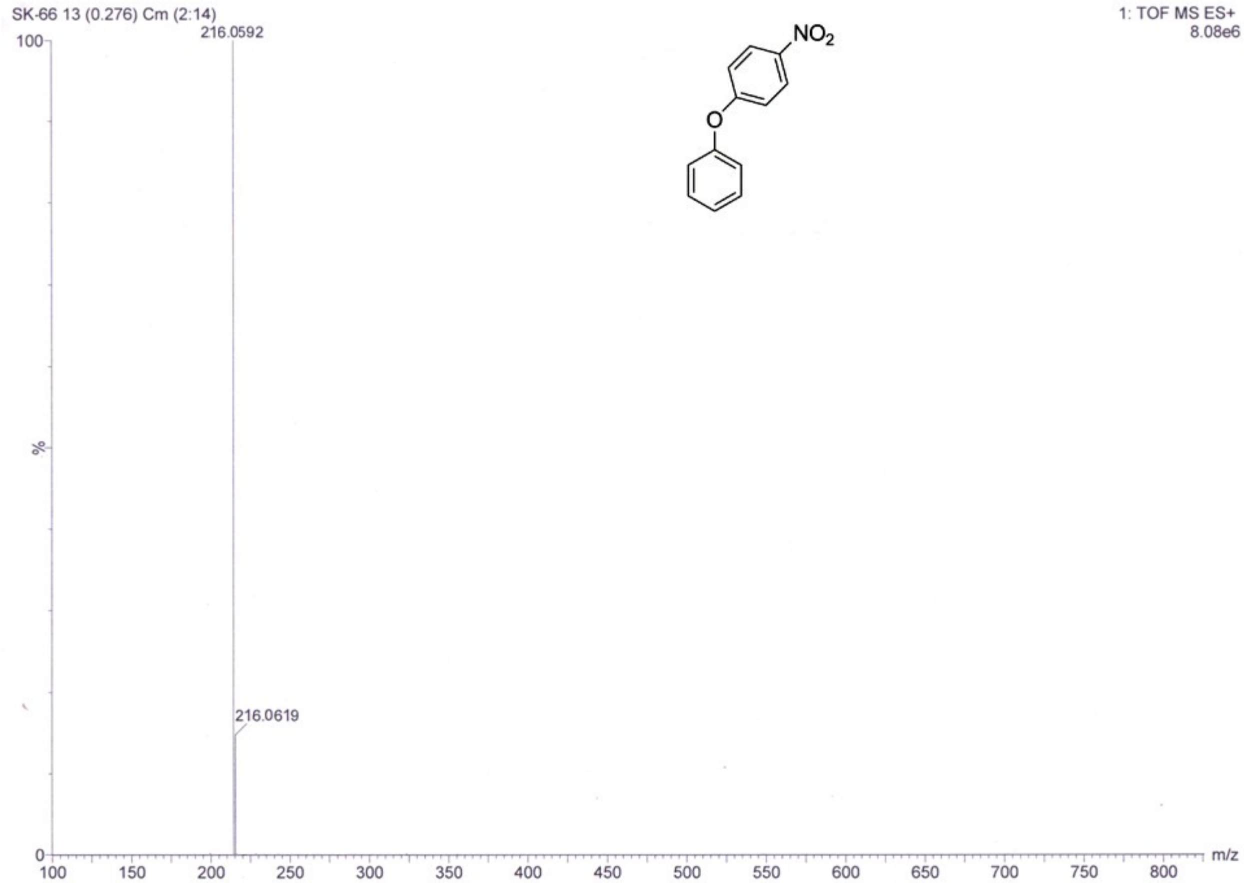
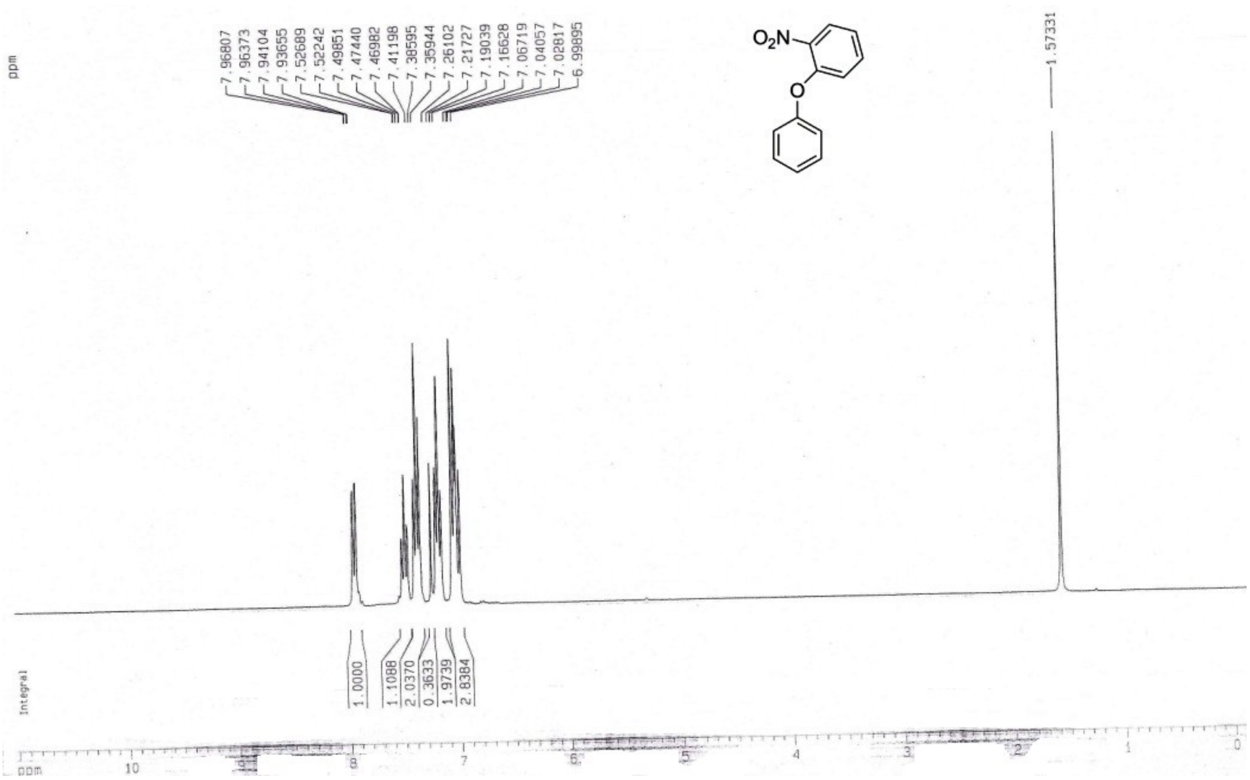
80
60
40
20
0



1b; δ_H (300 MHz, $CDCl_3$, ppm) 6.99–7.07 (m, 3H), 7.17–7.22 (m, 2H), 7.39 (t, J = 7.9 Hz, 2H), 7.47–7.53 (m, 1H), 7.94–7.97 (m, 1H); δ_C (75 MHz; $CDCl_3$) 117.11, 120.54, 125.43, 125.93, 130.34, 132.63, 142.65, 154.73, 163.38; Elemental analysis (found: C, 66.98; H, 4.24; N, 6.52. for $C_{12}H_9NO_3$ requires: C, 66.97; H, 4.22; N, 6.51%).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7.38595
7.35944
7.26102
7.21727
7.19039
7.16628
7.06719
7.04057
7.02817
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Integral
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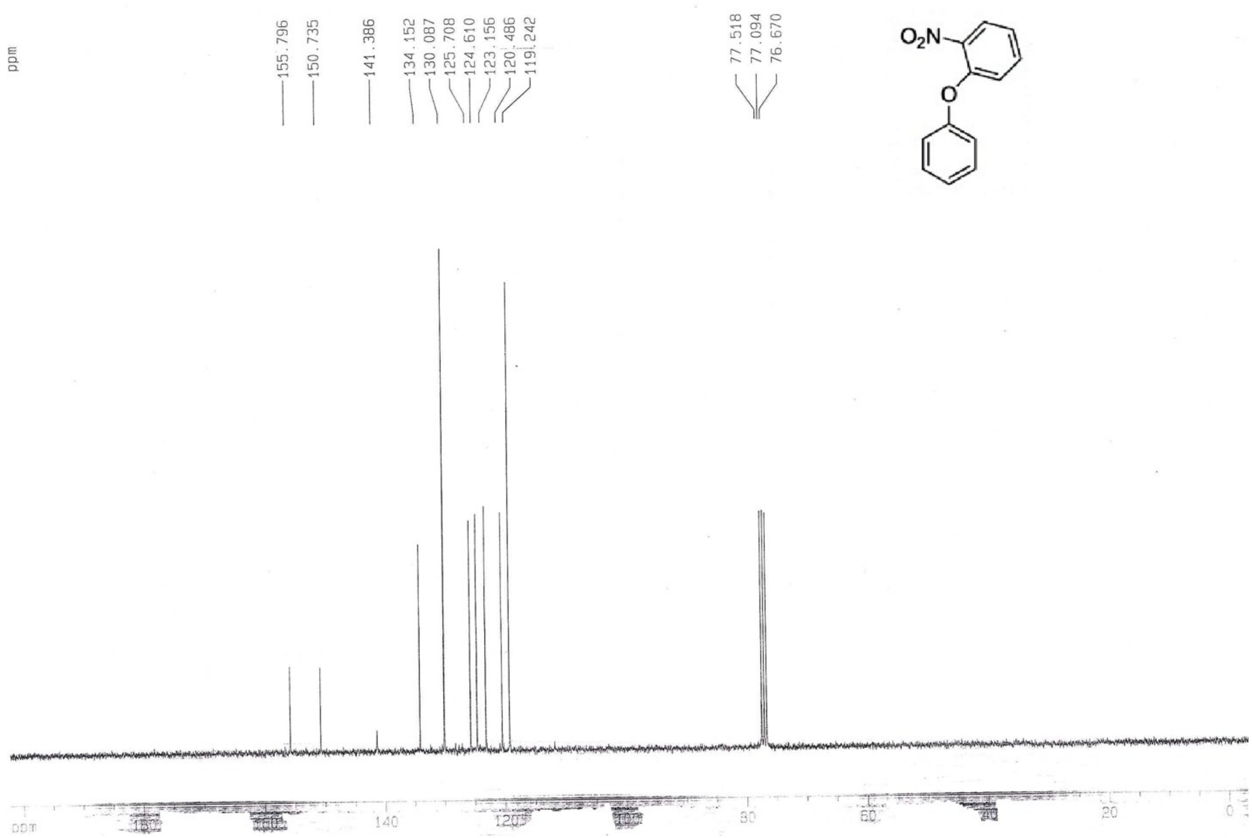
ppm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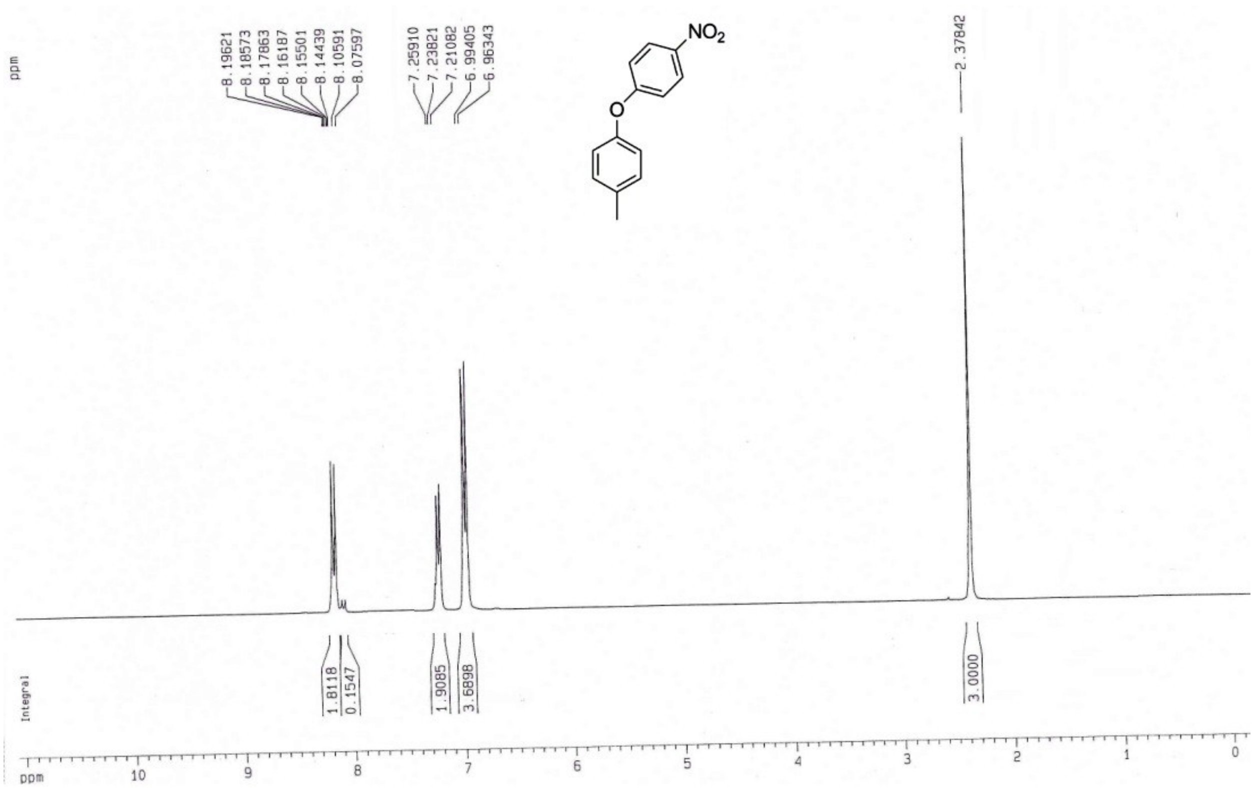
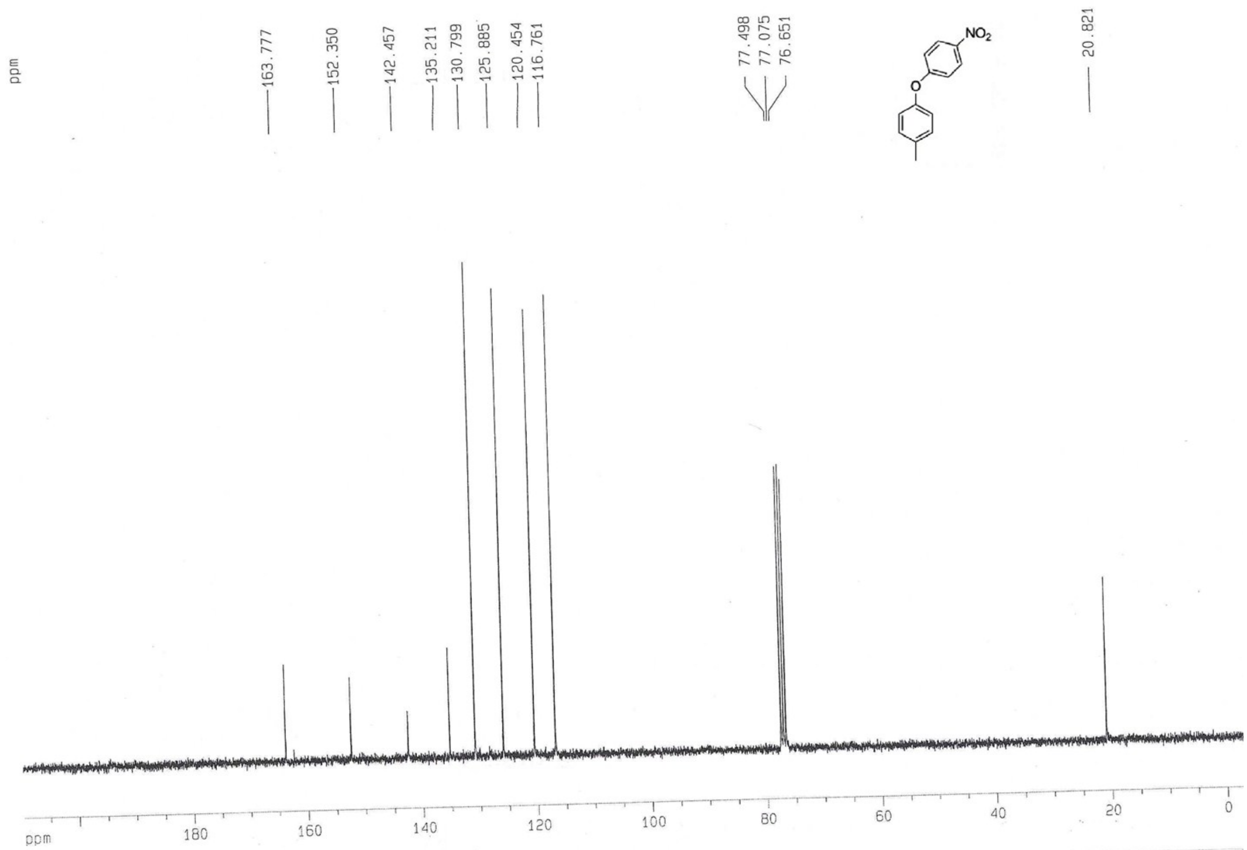
124.610
123.156
120.486
119.242
77.518
77.094
76.670
O_2N
O
ppm
140
80
60
20

1c; δ_H (300 MHz, $CDCl_3$, ppm) 2.38 (s, 3H), 6.98 (d, J = 9.2 Hz, 4H), 7.22 (d, J = 8.2 Hz, 2H), 8.16–8.19 (m, 2H); δ_C (75 MHz; $CDCl_3$) 20.82, 116.76, 120.45, 125.89, 125.93, 130.79, 135.21, 142.46, 152.35, 163.78; *m/z* 230.0736 [$(M+H)^+$, 100%]; Elemental analysis (found: C, 68.13; H, 4.86; N, 6.12. for $C_{13}H_{11}NO_3$ requires: C, 68.11; H, 4.84; N, 6.11%).





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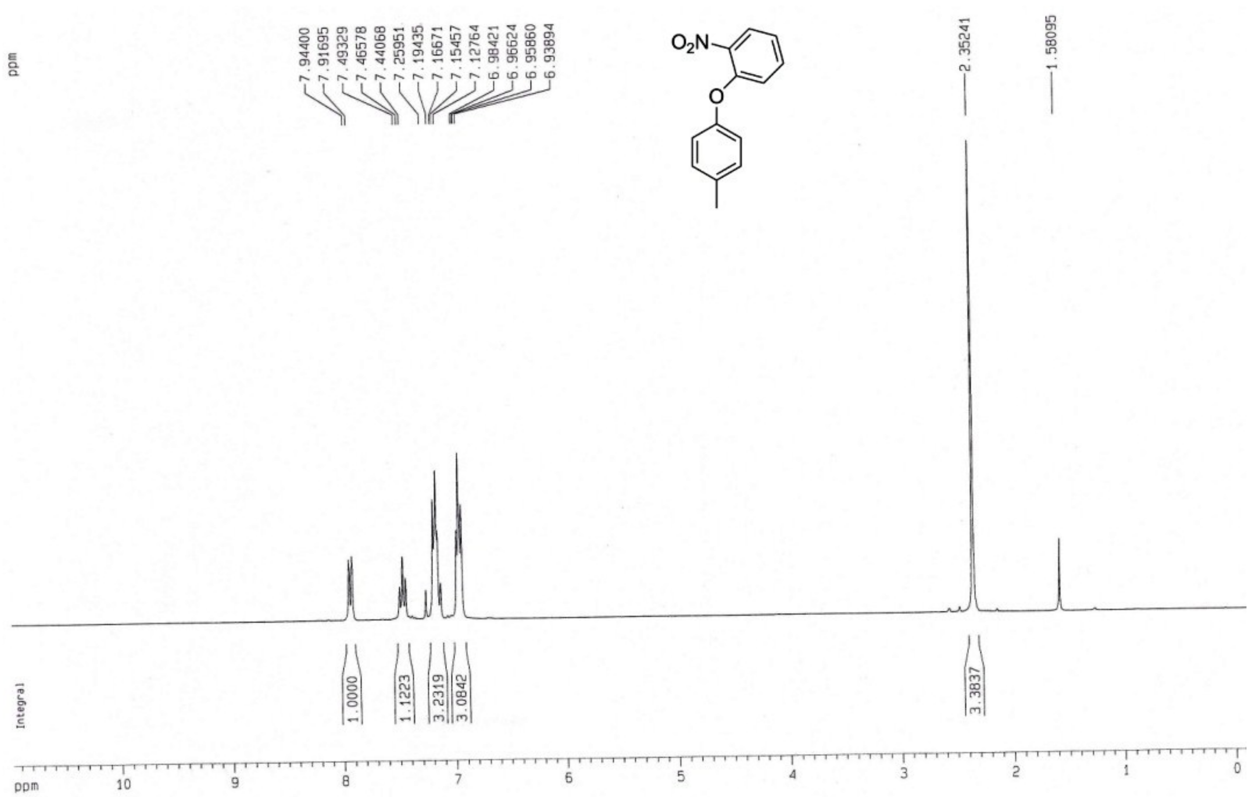
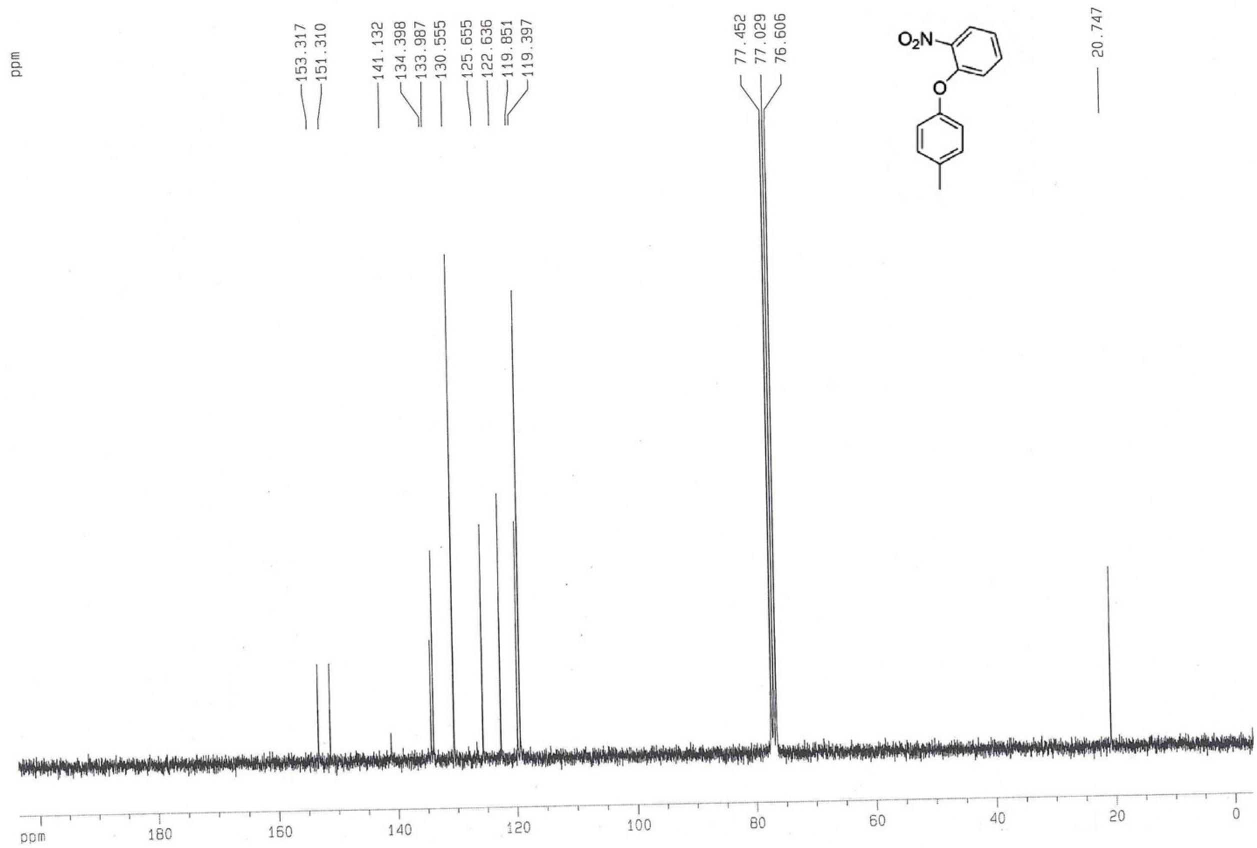
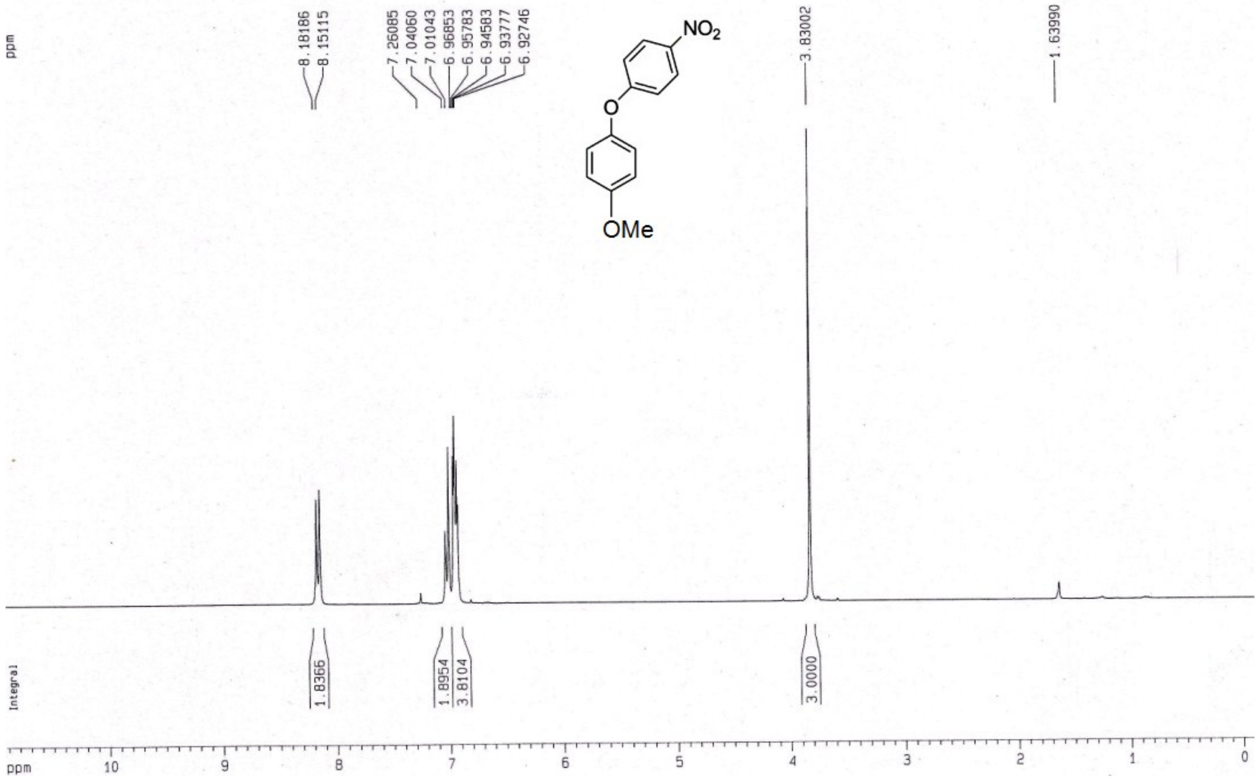
142.457
135.211
130.799
125.885
120.454
116.761
77.498
77.075
76.651
20.821
NO_2
O
ppm
180
160
140
120
100
80
60
40
20
0

1d; δ_H (300 MHz, $CDCl_3$, ppm) 2.35 (s, 3H), 6.94–6.98 (m, 3H), 7.13–7.19 (m, 3H), 7.47 (m, 1H), 7.93 (d, J = 8.3 Hz, 1H); δ_C (75 MHz; $CDCl_3$) 20.75, 119.39, 119.85, 122.64, 125.66, 130.56, 133.99, 134.39, 141.13, 151.31, 153.32; Elemental analysis (found: C, 68.15; H, 4.85; N, 6.14. for $C_{13}H_{11}NO_3$ requires: C, 68.11; H, 4.84; N, 6.11%).





1e; δ_H (300 MHz, $CDCl_3$, ppm) 3.83 (s, 3H), 6.93–7.03 (m, 6H), 8.17 (d, *J* = 9.2 Hz, 2H); δ_C (75 MHz; $CDCl_3$) 55.67, 115.31, 116.38, 121.83, 125.89, 142.34, 147.86, 157.19, 164.17; *m/z* 246.0634 [$(M+H)^+$, 100%]; Elemental analysis (found: C, 63.69; H, 4.54; N, 5.73. for $C_{13}H_{11}NO_4$ requires: C, 63.67; H, 4.52; N, 5.71%).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6.93777
6.92746
NO2
O
OMe
3.83002
1.63990
Integral
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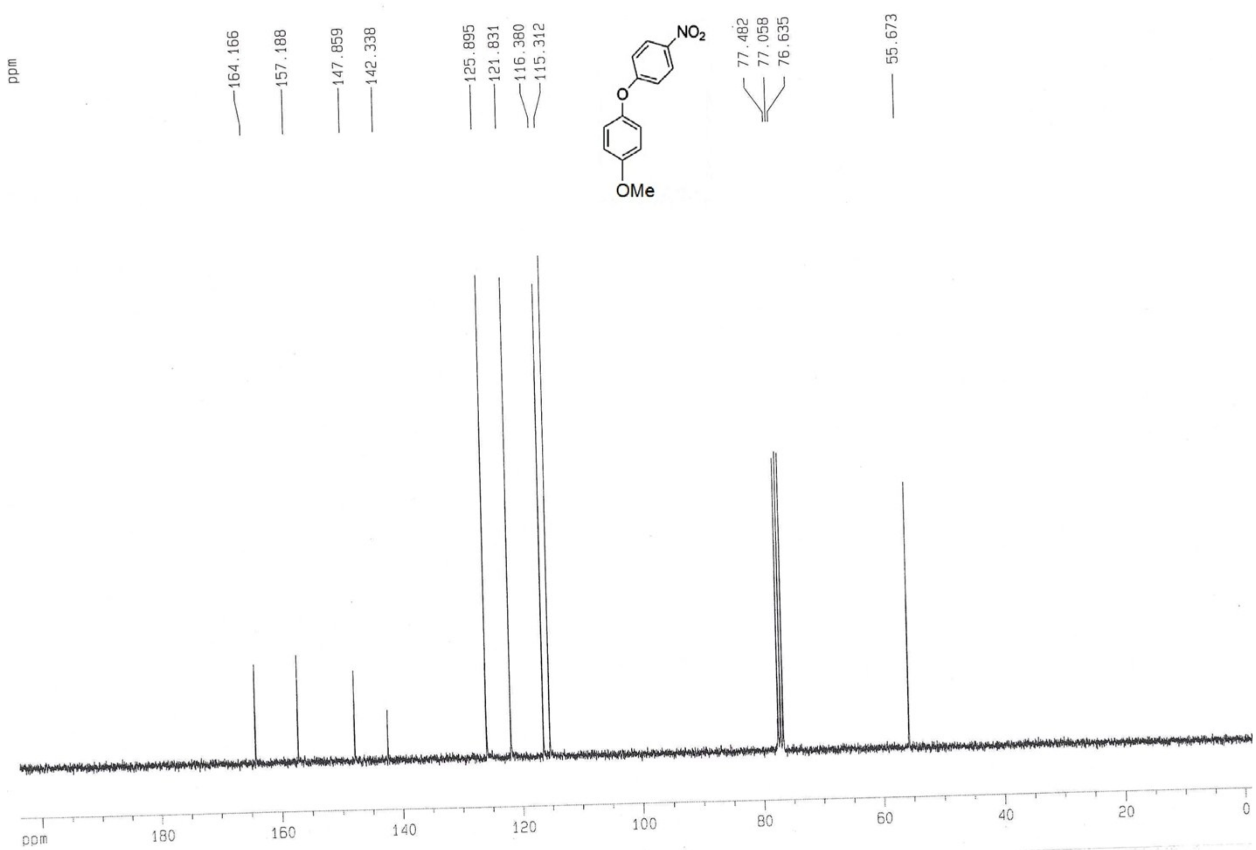
1.8954
3.8104
3.0000
ppm
10
9
8
7
6
5
4
3
2
1
0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115.312
NO2
OMe
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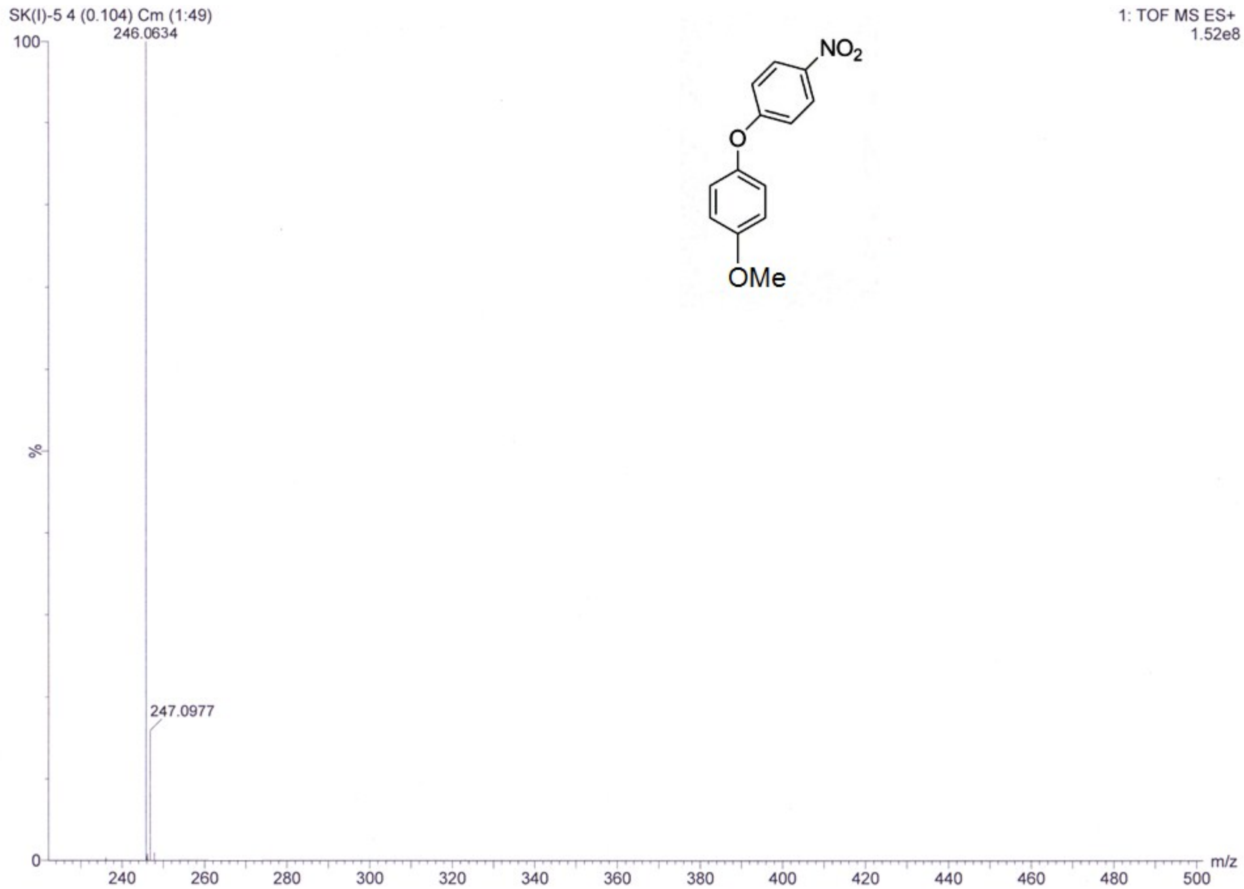
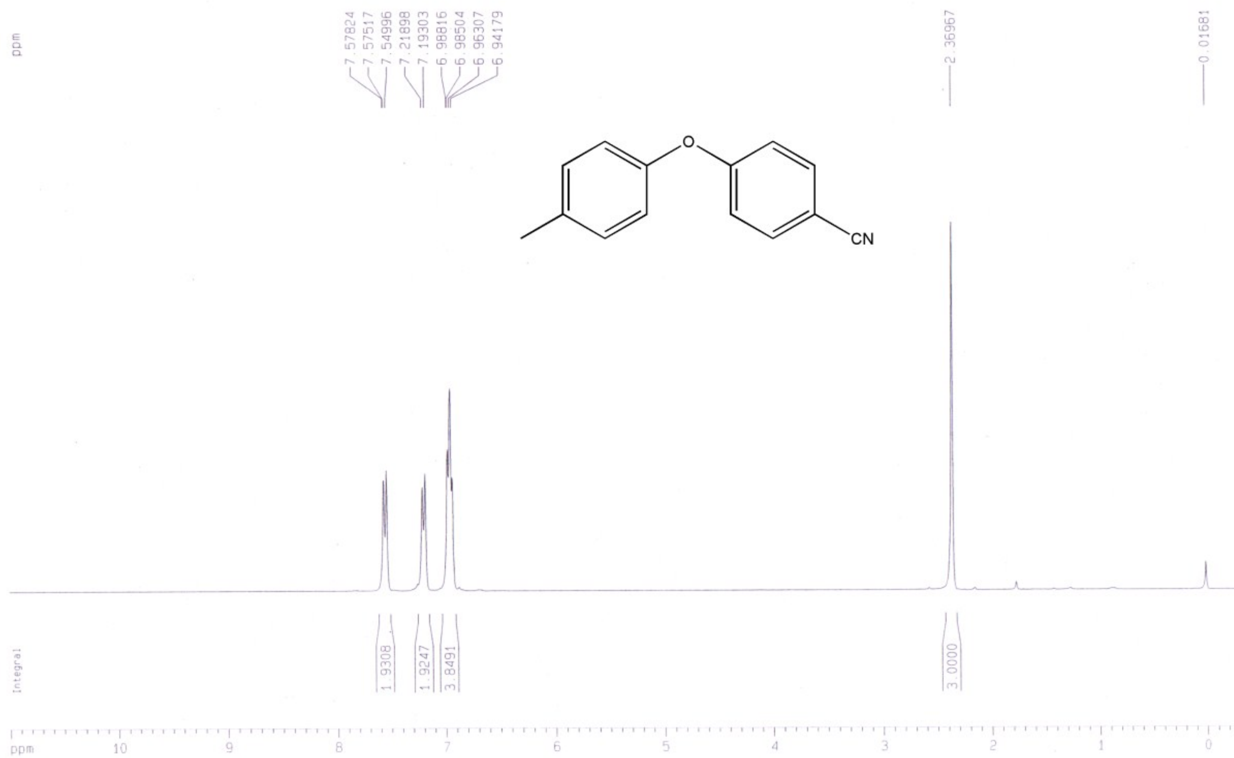
76.635
55.673
ppm
180
160
140
120
100
80
60
40
20
0



1f; δ_H (300 MHz; $CDCl_3$) 2.37 (3H, s), 6.99-6.94 (4H, m), 7.21 (2H, d, J = 7.8 Hz), 7.56 (2H, d, J = 8.4 Hz); δ_C (75 MHz; $CDCl_3$) 20.83, 105.49, 117.59, 117.91, 118.90, 120.39, 129.94, 134.08, 134.92, 152.42, 162.07; *m/z* 210.0896 [$(M+H)^+$, 100%]; Elemental analysis (found: C 80.36, H 5.30, N 6.69; for $C_{14}H_{12}O_2$ requires: C 80.34, H 5.37, N 6.63%).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CN
Integral
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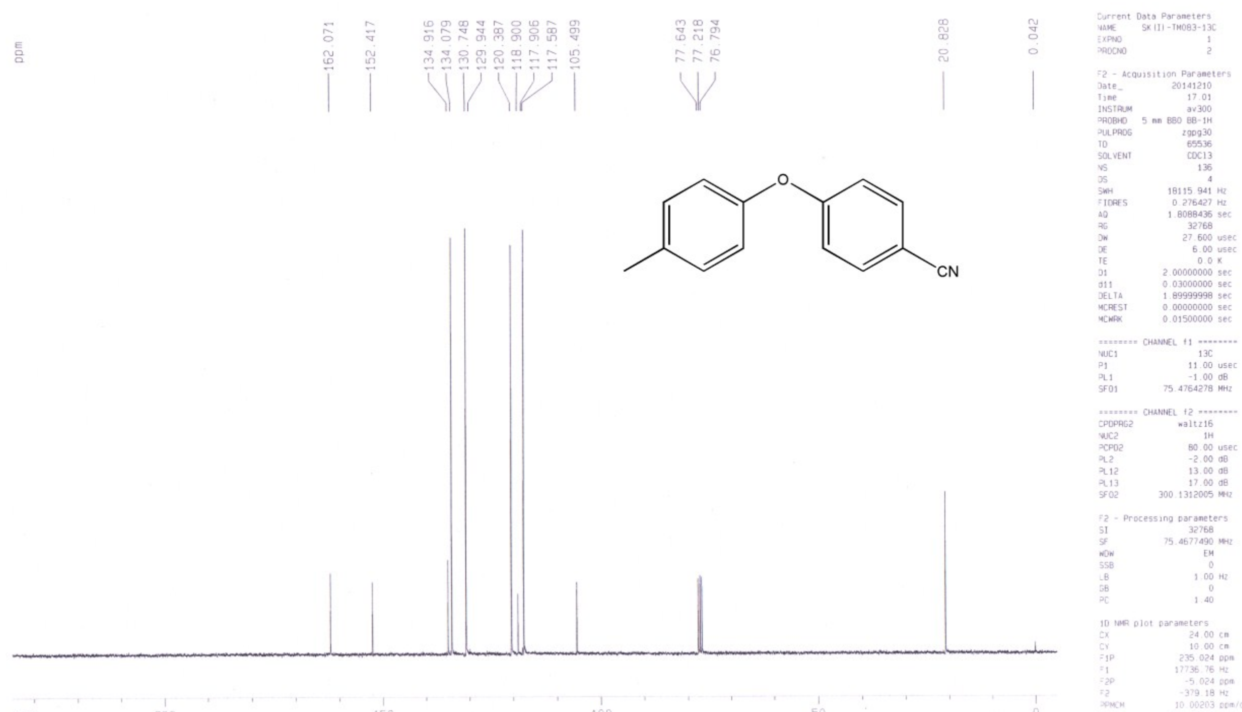
ppm 10 9 8 7 6 5 4 3 2 1 0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76.794
20.828
0.042
CN
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PROCNO 2
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FIDRES 0.276427 Hz
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DW 27.600 usec
DE 6.00 usec
TE 0.0 K
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d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4764278 MHz
======== CHANNEL f2 ========
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PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
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SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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CY 10.00 cm
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F2P -5.024 ppm
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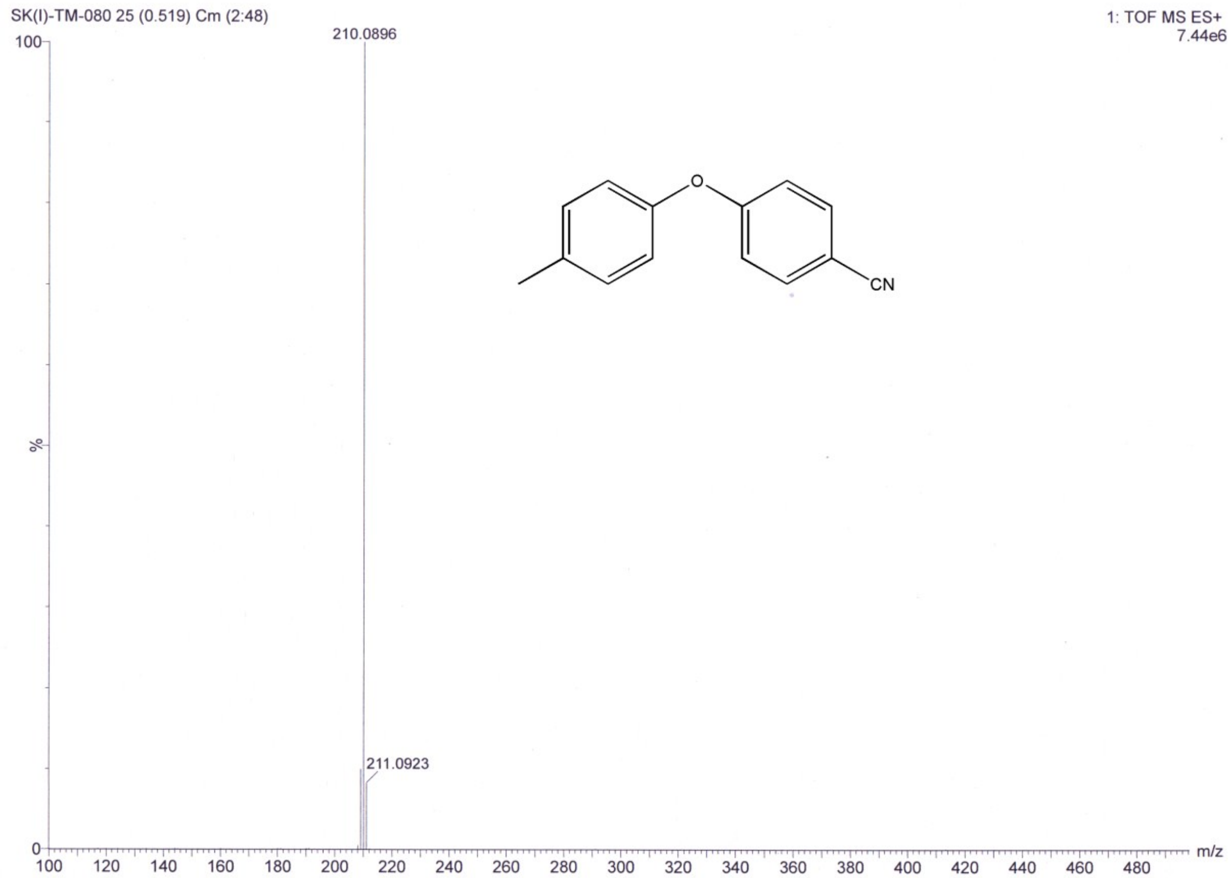
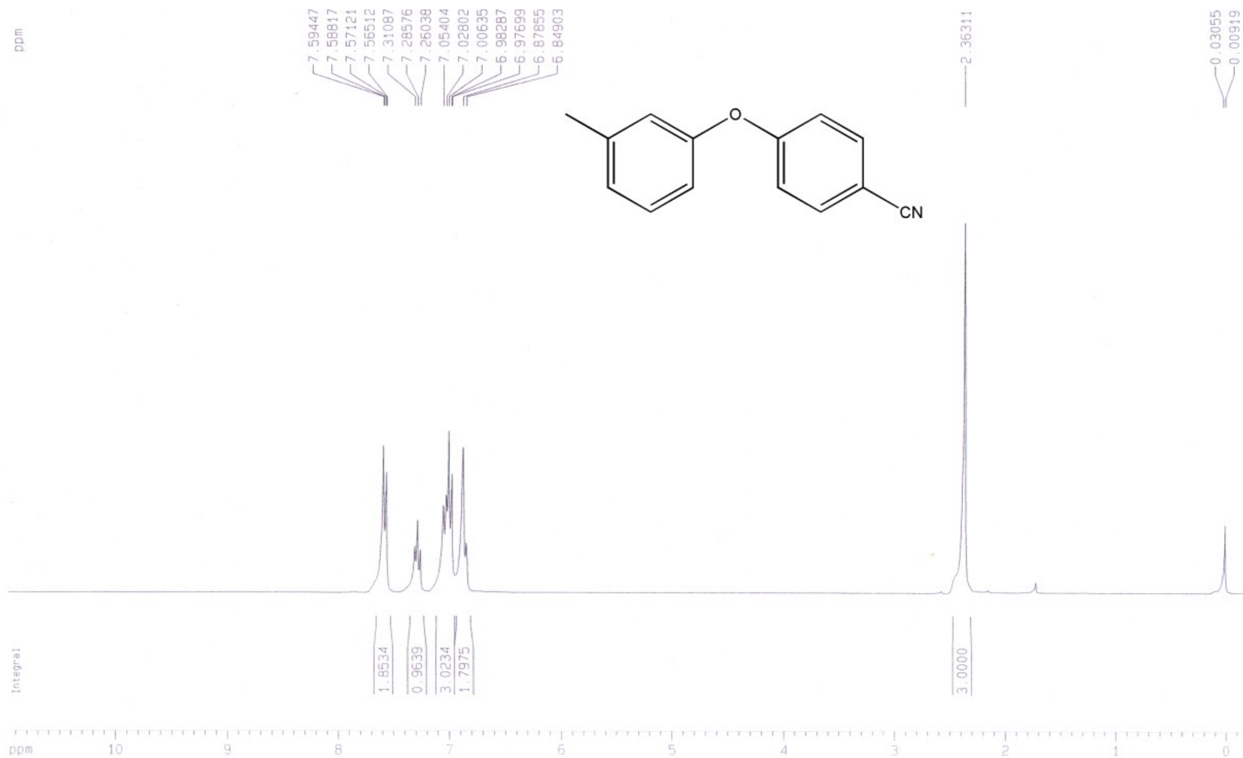
HZCM 754.83099 Hz/cm



1g; δ_H (300 MHz; $CDCl_3$) 2.36 (3H, s), 6.85-7.05 (5H, m), 7.29 (1H, t, J = 7.6 Hz), 7.57-7.59 (2H, m); δ_C (75 MHz; $CDCl_3$) 21.37, 105.68, 117.34, 117.90, 118.89, 121.04, 125.97, 129.95, 134.10, 140.57, 154.78, 161.79; Elemental analysis (found: C 80.36, H 5.30, N 6.69; for $C_{14}H_{12}O_2$ requires: C 80.32, H 5.28, N 6.62%).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7.28576
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7.05404
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7.00635
6.98287
6.97699
6.87855
6.84903
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0.00919
ppm
Integral
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9
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7
6
5
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3
2
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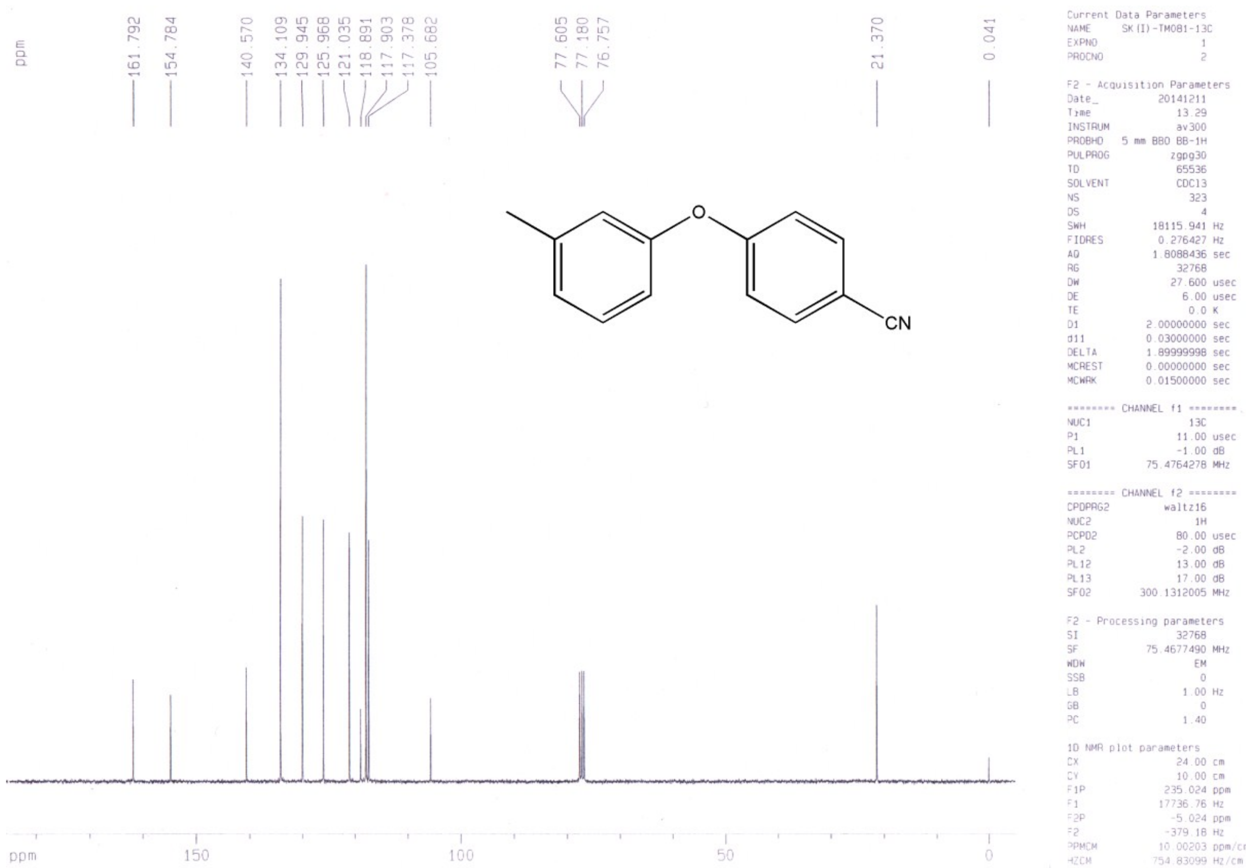
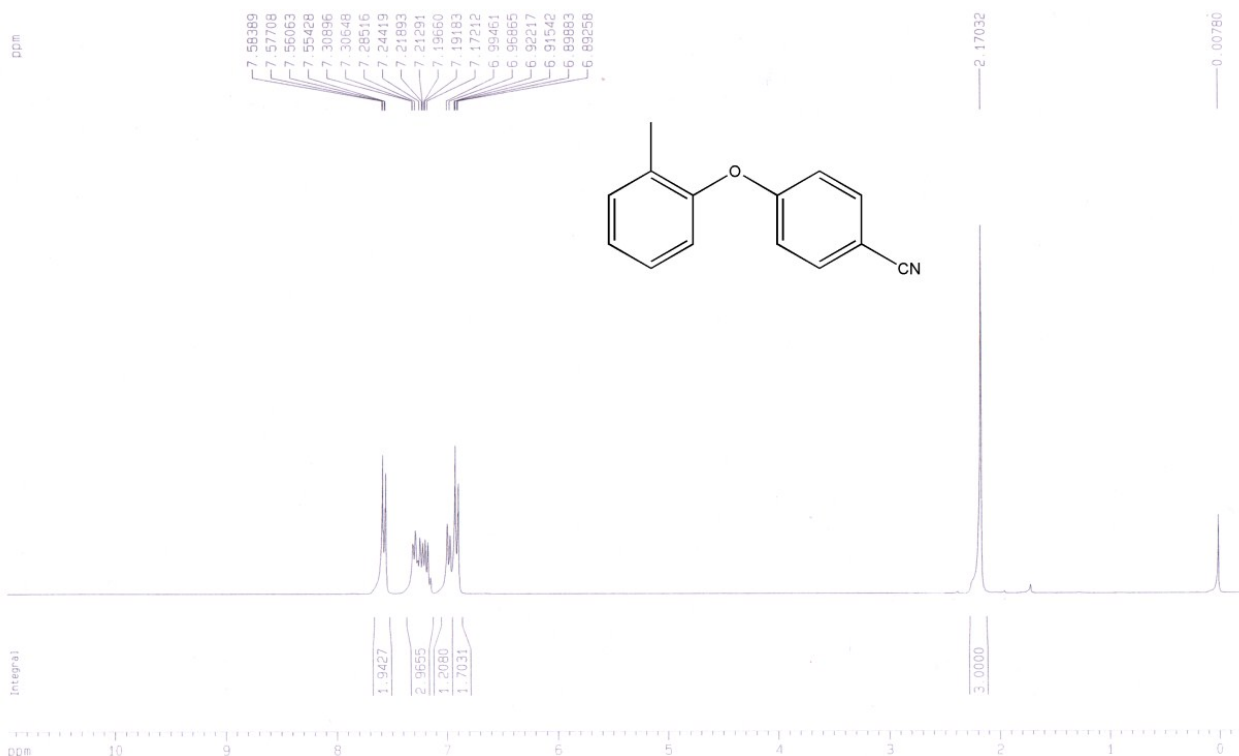


1h; δ_H (300 MHz; $CDCl_3$) 2.17 (3H, s), 6.89-6.99 (3H, m), 7.17-7.30 (3H, m), 7.57 (2H, dd, J = 1.9 and J = 6.8 Hz); δ_C (75 MHz; $CDCl_3$) 16.02, 105.29, 116.80, 118.94, 121.10, 125.73, 127.68, 130.55, 131.95, 134.19, 134.58, 152.43, 161.76; Elemental analysis (found: C 80.36, H 5.30, N 6.69; for $C_{14}H_{12}O_2$ requires: C 80.39, H 5.34, N 6.72%).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7.19660
7.19183
7.17212
6.99461
6.96865
6.92217
6.91542
6.89883
6.89258
2.17032
0.00780
CN
O
Integral
1.9427
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1.2080
1.7031
3.0000
ppm
10
9
8
7
6
5
4
3
2
1
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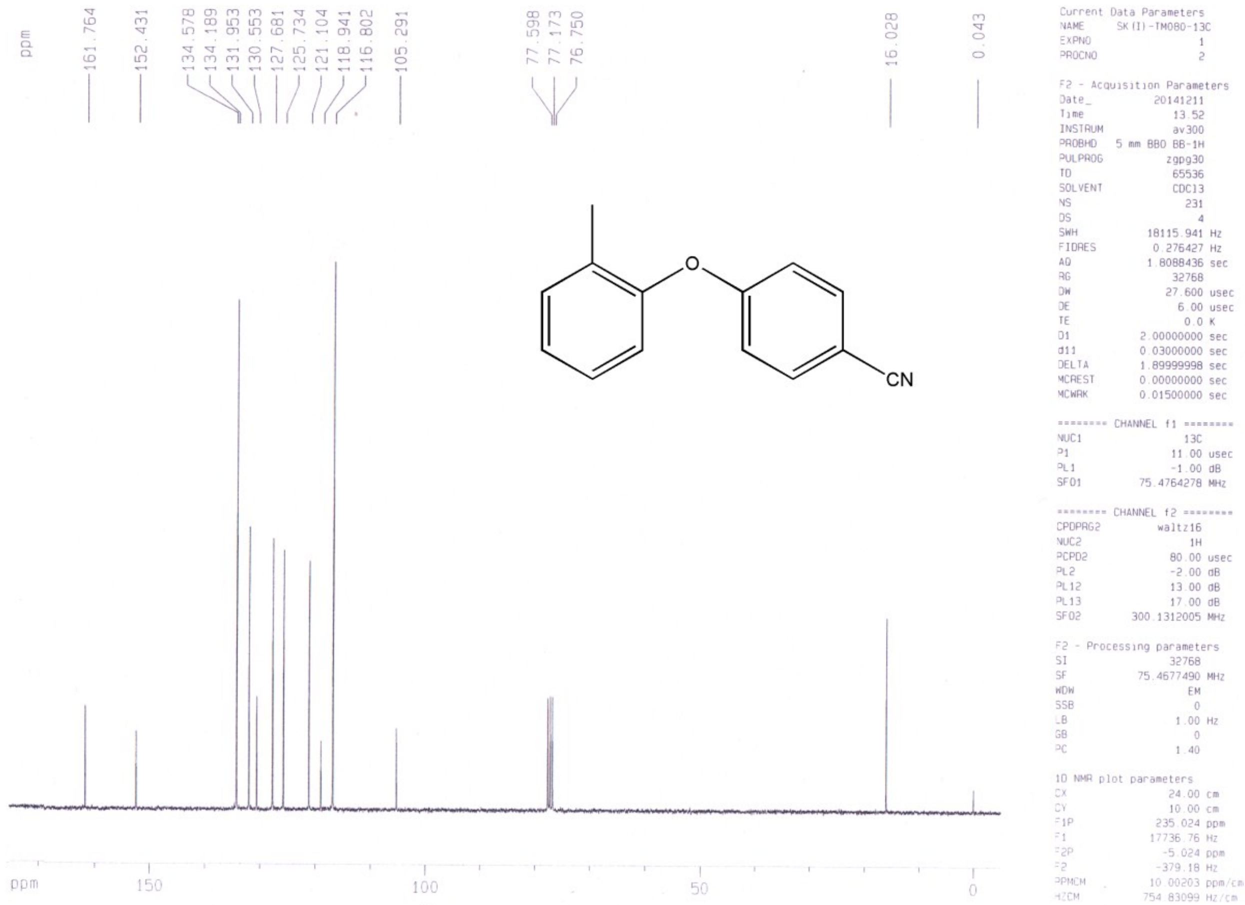
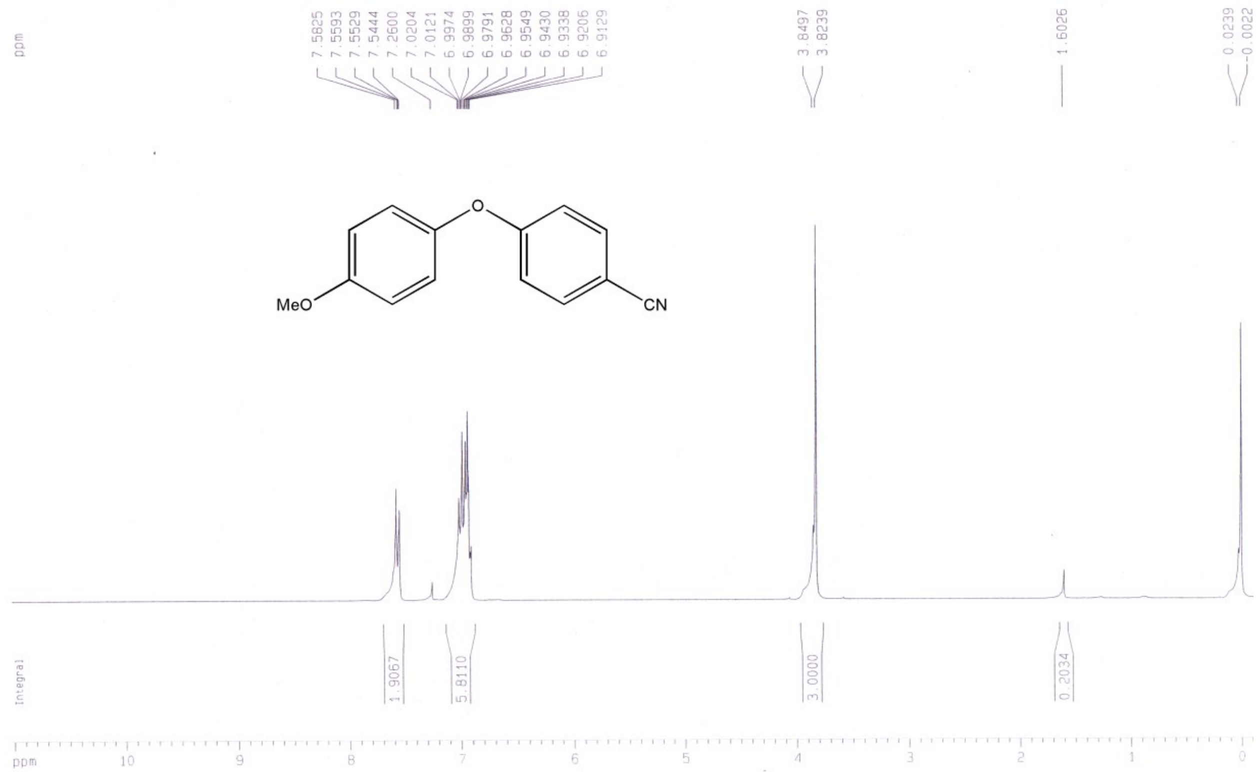


1i; δ_H (300 MHz; $CDCl_3$) 3.83-3.85 (3H, m), 6.91-7.02 (6H, m), 7.54-7.58 (2H, m); δ_C (75 MHz; $CDCl_3$) 55.67, 105.29, 115.25, 117.15, 118.94, 121.80, 134.07, 147.89, 157.03, 162.51; *m/z* 226.0869 [$(M+H)^+$, 100%]; Elemental analysis (found: C 74.65, H 4.92, N 6.22; for $C_{14}H_{12}O_2$ requires: C 74.62, H 4.97, N 6.20%).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7.2600
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7.0121
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6.9899
6.9791
6.9628
6.9549
6.9430
6.9338
6.9206
6.9129
3.8497
3.8239
1.6026
0.0239
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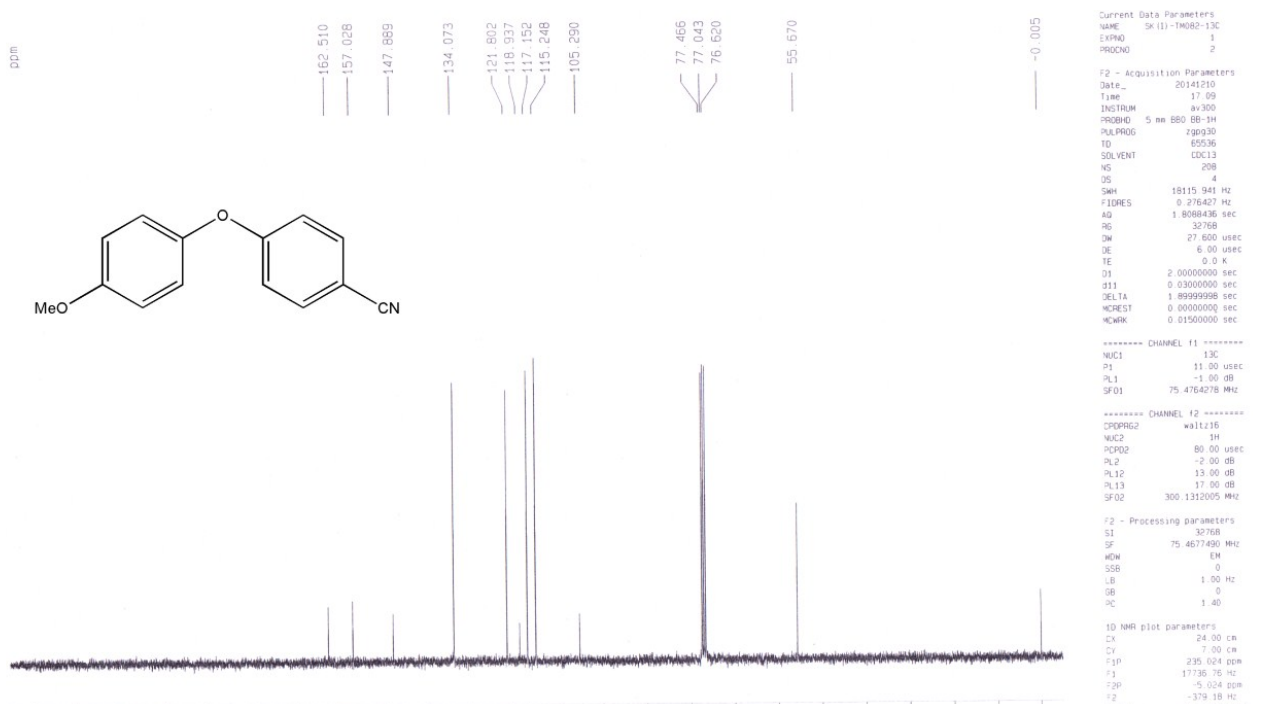
MeO
O
CN
Integral
1.9067
5.8110
3.0000
0.2034
ppm 10 9 8 7 6 5 4 3 2 1 0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157.028
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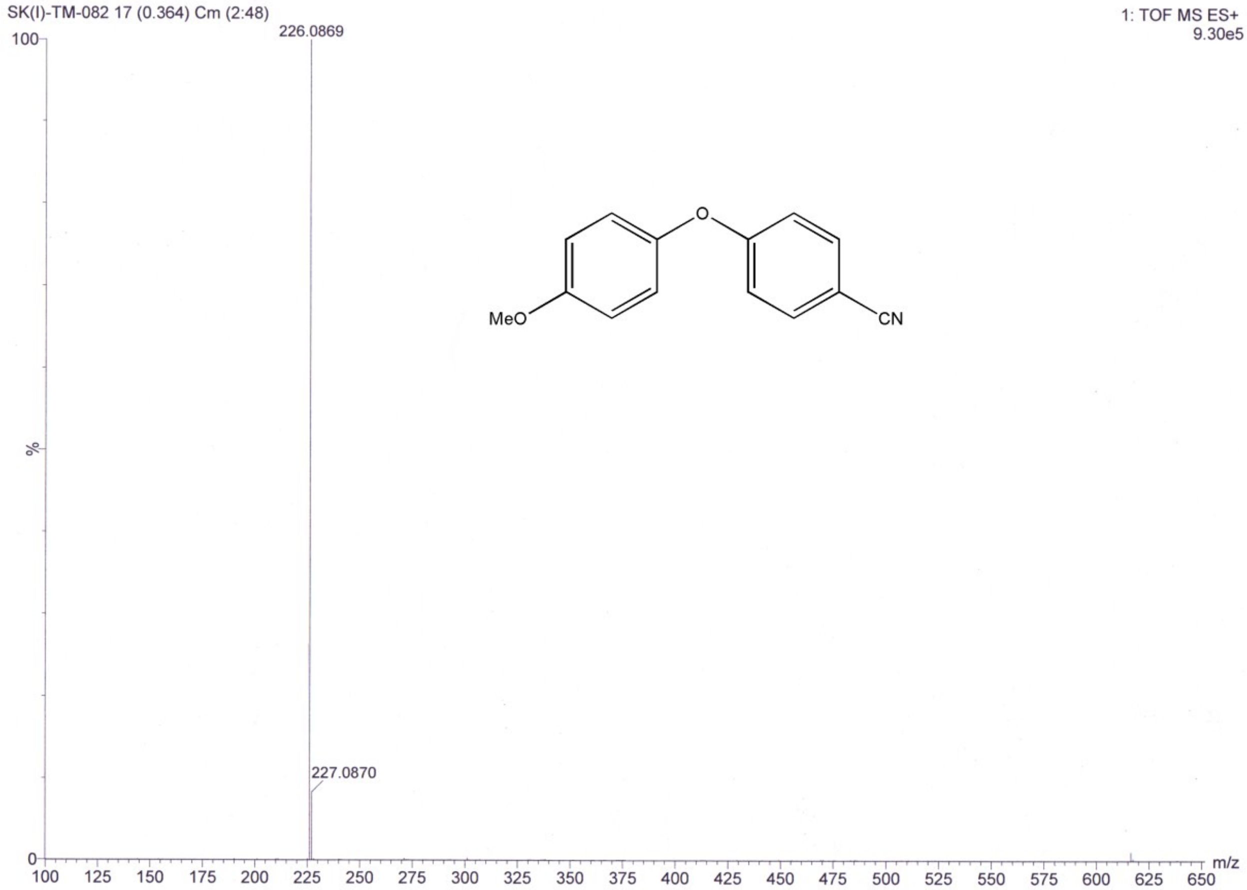
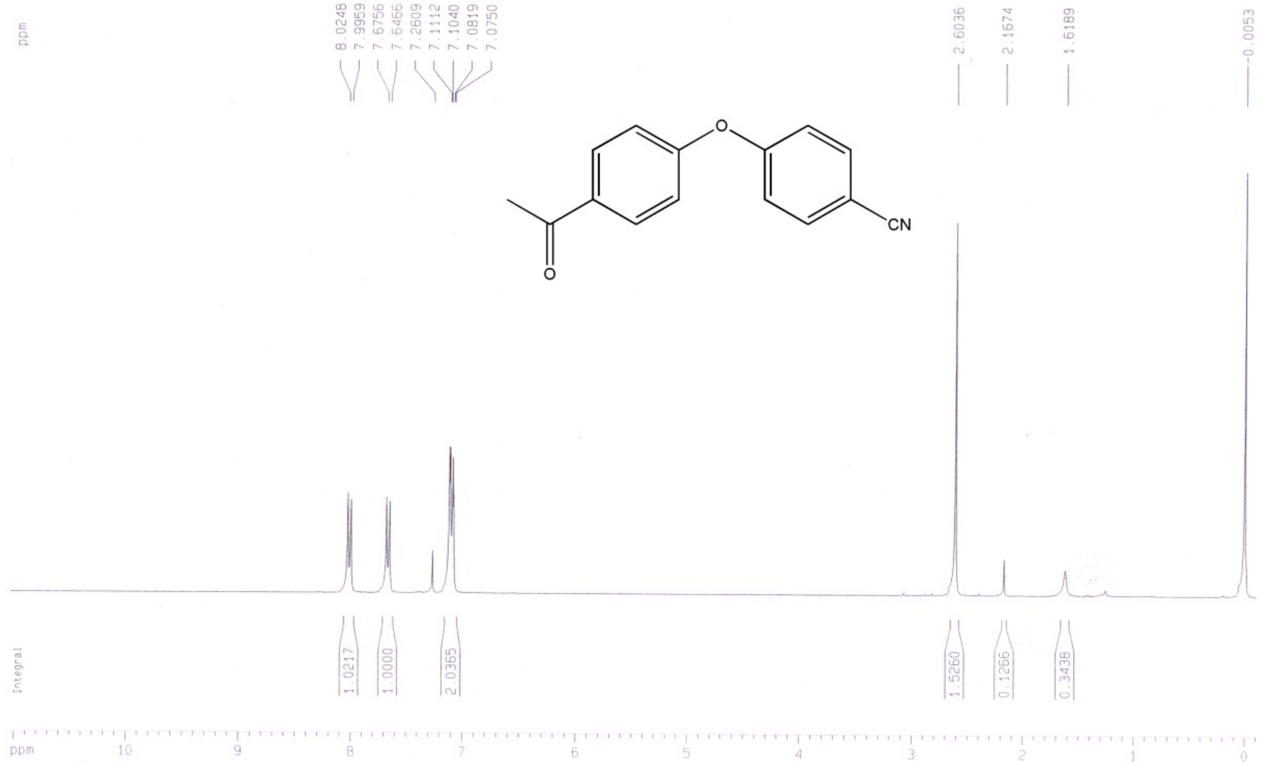
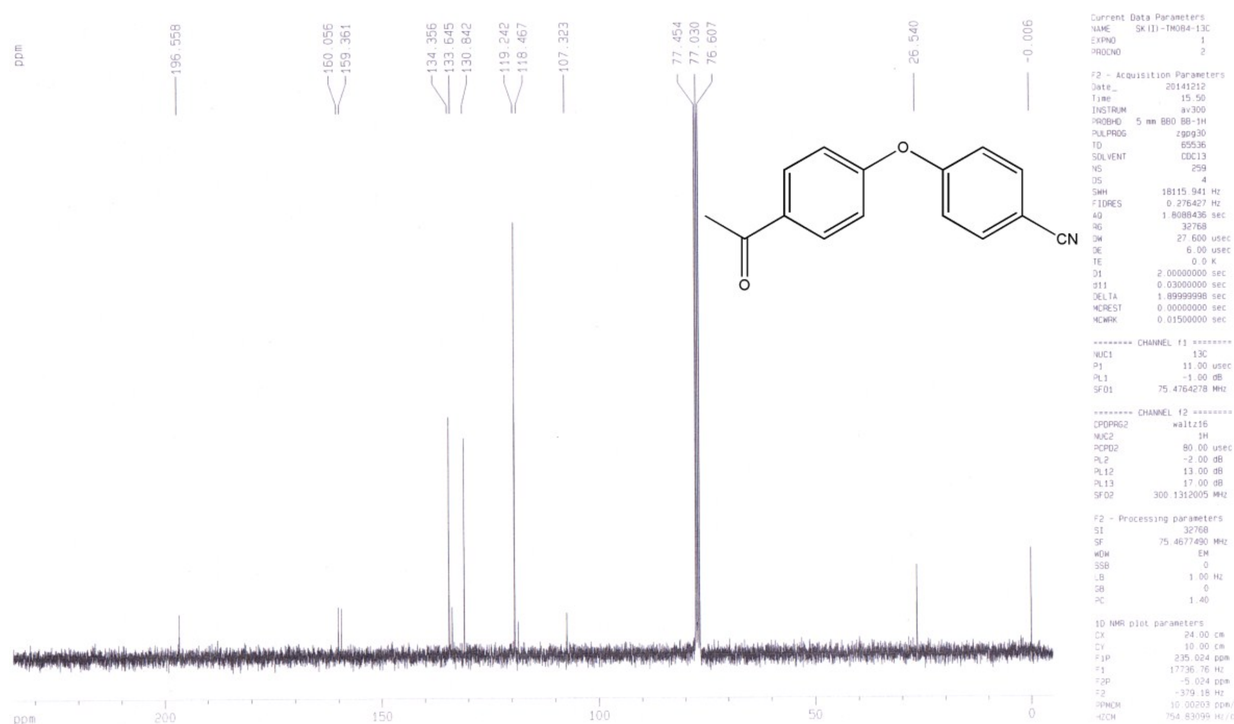
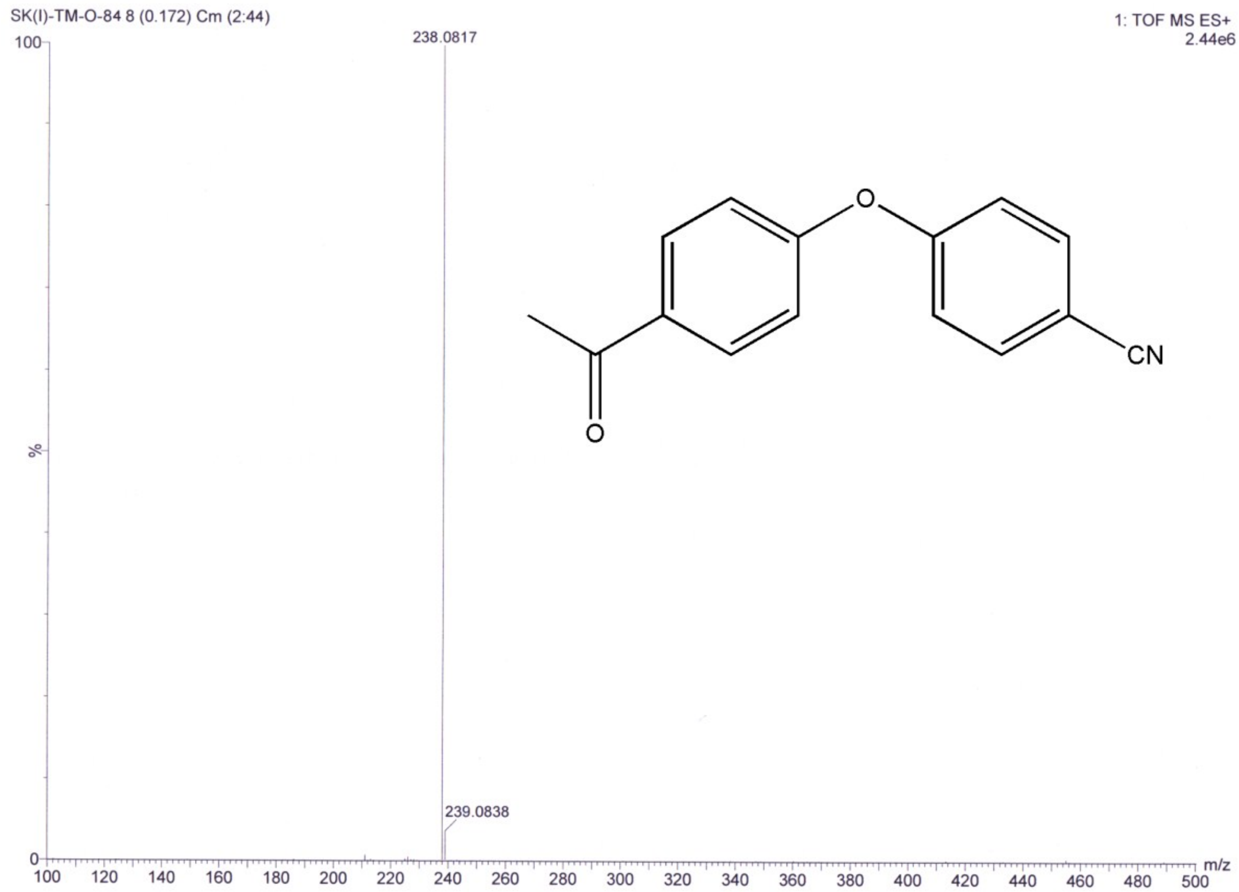
134.073
121.802
118.937
117.152
115.248
105.290
77.466
77.043
76.620
55.670
-0.005
MeO
O
CN
ppm 200 150 100 50 0
Current Data Parameters
NAME SK(1)-TM082-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20141210
Time 17.09
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 208
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 32768
DW 27.600 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4764278 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 7.00 cm
F1P 235.024 ppm
F1 17736.76 Hz
F2P -5.024 ppm
F2 -379.18 Hz
PPMCM 10.00203 ppm/cm
HZCM 754.83099 Hz/cm



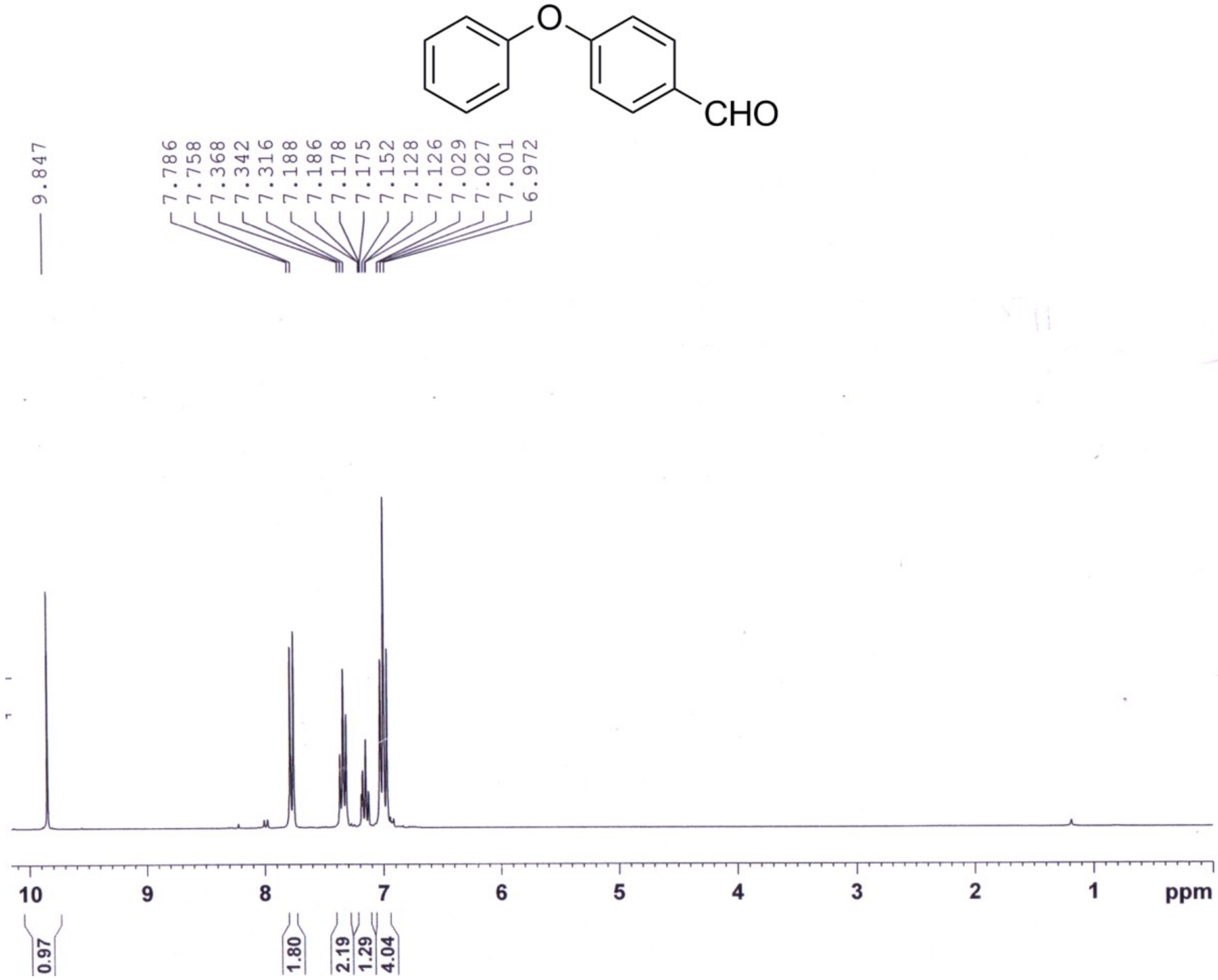
1j; δ_H (300 MHz; $CDCl_3$) 2.60 (3H, s), 6.99-6.94 (4H, m), 7.09 (4H, dd, J = 2.1 and J = 8.7 Hz), 7.66 (2H, d, J = 8.7 Hz), 8.01 (2H, d, J = 8.7 Hz); δ_C (75 MHz; $CDCl_3$) 26.54, 107.32, 118.47, 119.24, 130.84, 133.65, 134.36, 159.36, 160.06, 196.57; *m/z* 238.0817 [$(M+H)^+$, 100%]; Elemental analysis (found: C 75.94, H 4.67, N 5.90; for $C_{14}H_{12}O_2$ requires: C 75.98, H 4.69, N 5.93%).

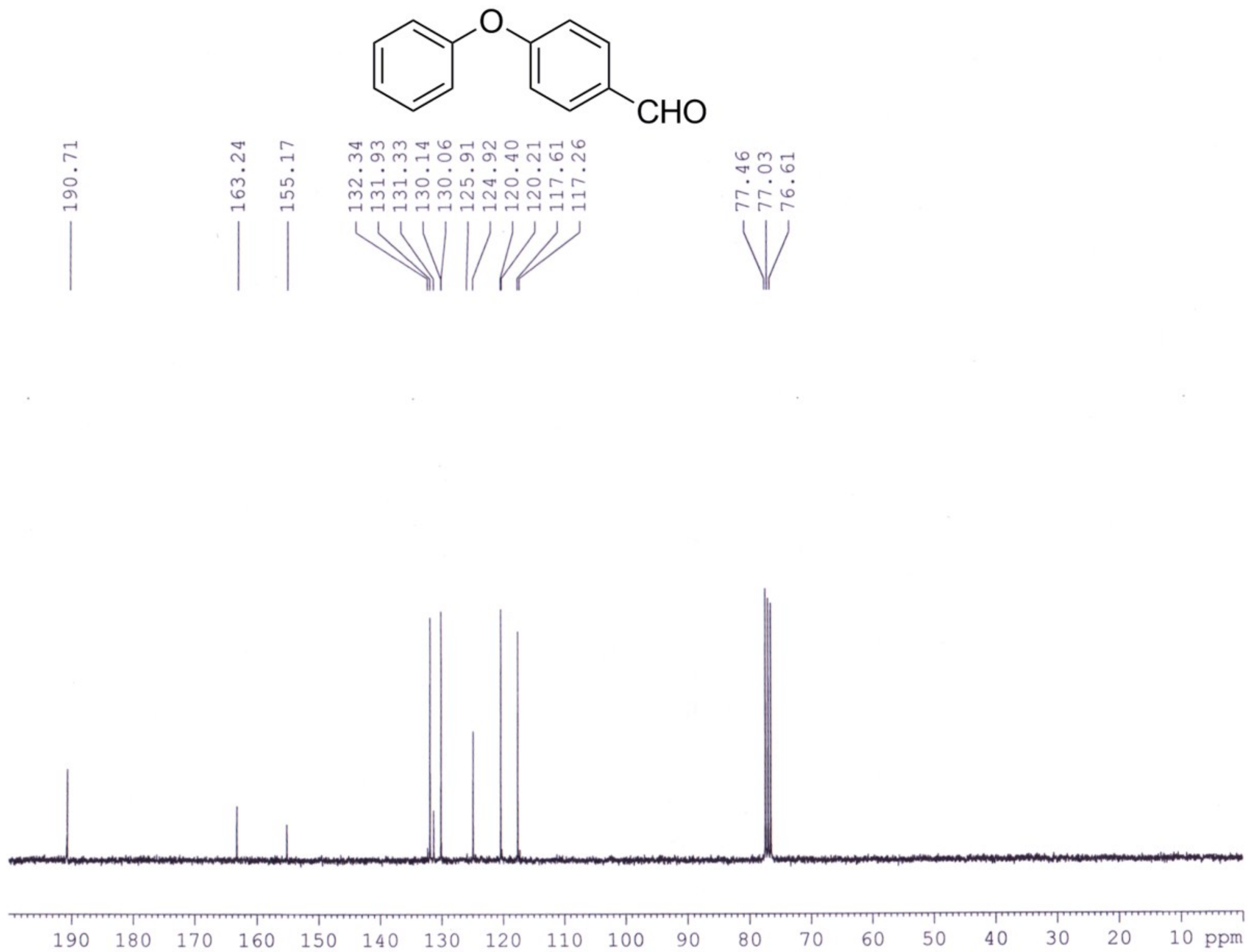

ppm
8.0248
7.9959
7.6756
7.6466
7.2609
7.1112
7.1040
7.0819
7.0750
2.6036
2.1674
1.6189
-0.0053
CN
O
Integral
1.0217
1.0000
2.0365
1.5260
0.1266
0.3438
ppm
10
9
8
7
6
5
4
3
2
1
0

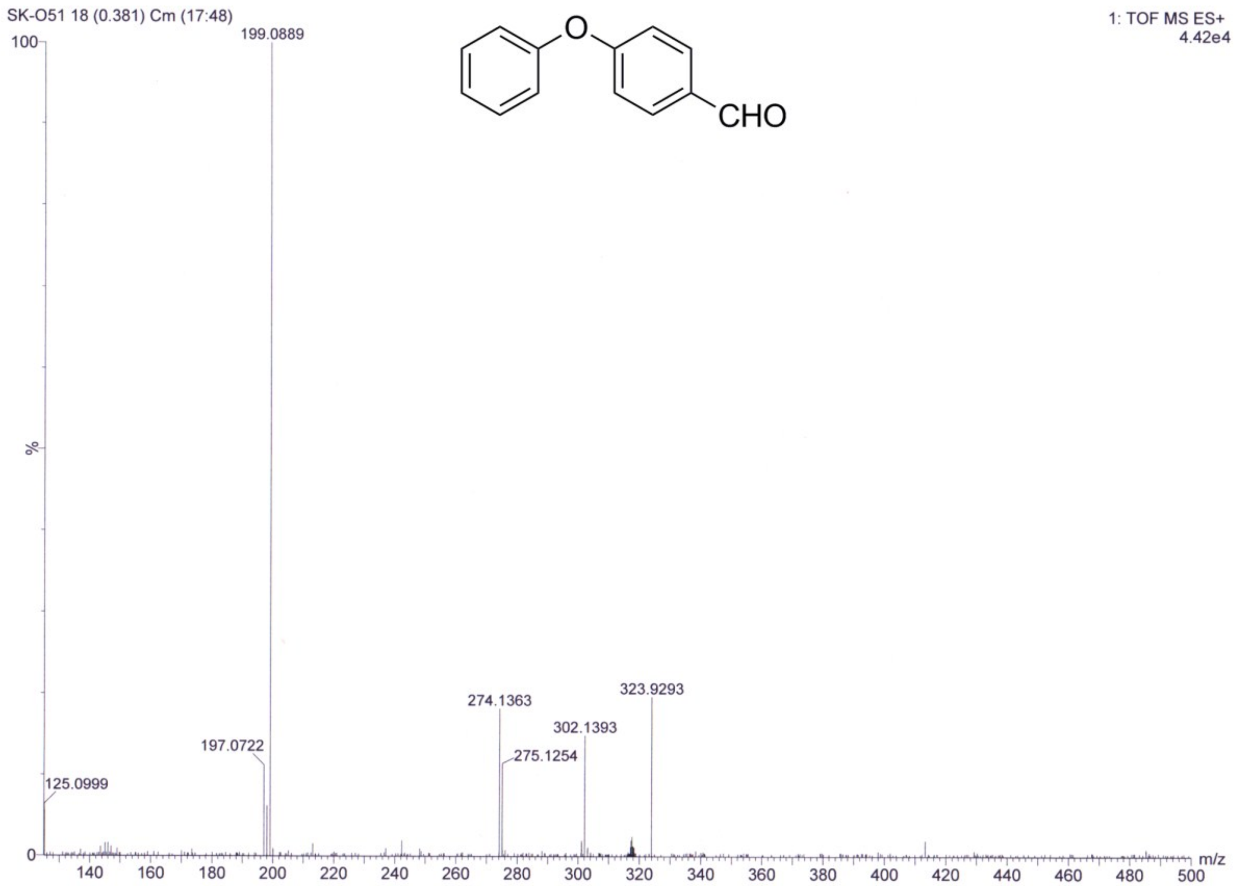

ppm
196.558
160.056
159.361
134.356
133.645
130.842
119.242
118.467
107.323
77.454
77.030
76.607
26.540
-0.006
O
CN
Current Data Parameters
NAME SK(I)-TM084-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20141212
Time 15.50
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 259
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 32768
DW 27.600 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4764278 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 10.00 cm
F1P 235.024 ppm
F1 17736.76 Hz
F2P -5.024 ppm
F2 -379.18 Hz
PPMCM 10.00203 ppm/cm
HZCM 754.83099 Hz/cm
ppm
200
150
100
50
0



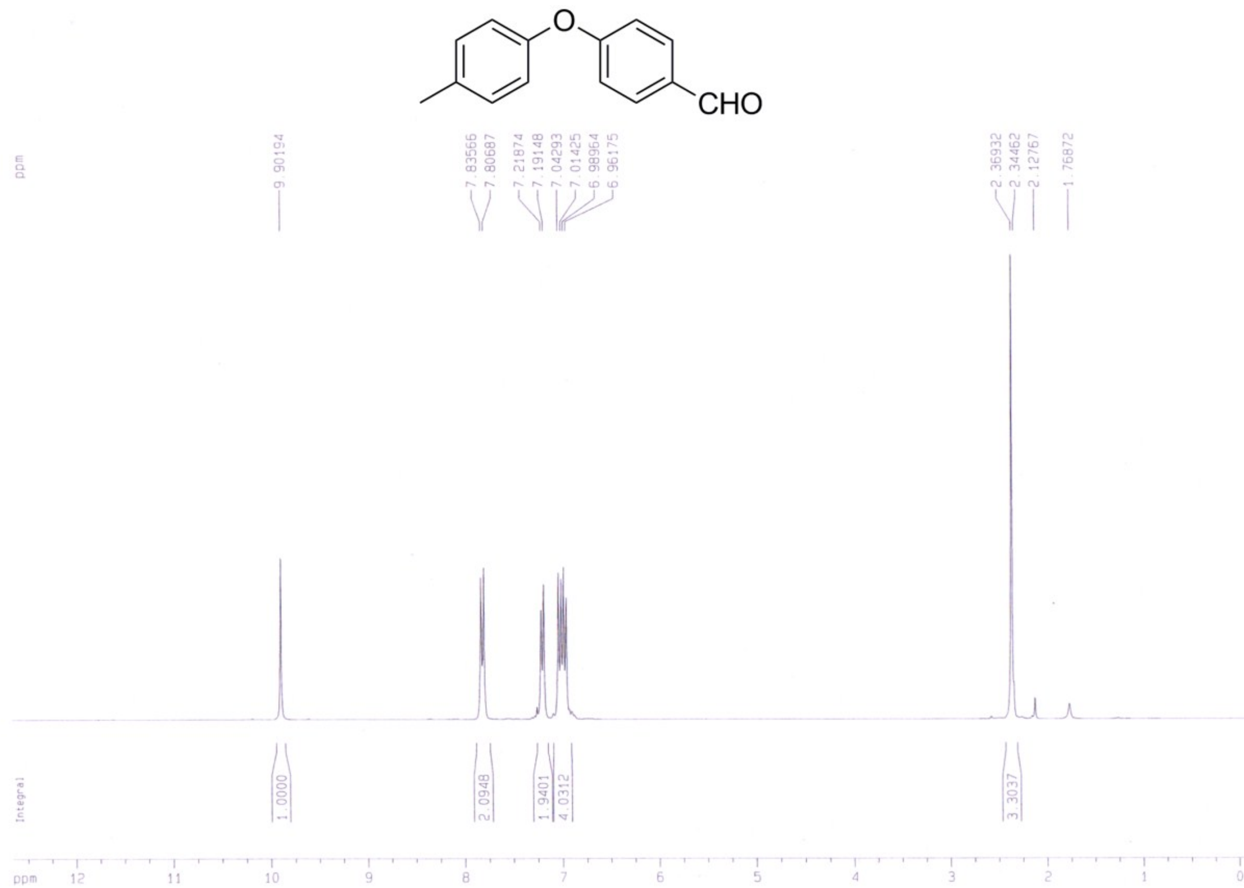
1k; δ_H (300 MHz; $CDCl_3$) 6.97-7.03 (4H, m), 7.13-7.19 (1H, m), 7.34 (2H, t, J = 7.8 Hz), 7.77 (2H, d, J = 8.4 Hz), 9.85 (1H, s); δ_C (75 MHz; $CDCl_3$) 117.61, 120.40, 125.91, 130.14, 131.33, 131.93, 132.34, 155.17, 163.24, 190.71; *m/z* 199.0889 [$(M+H)^+$, 100%]; Yield ca. 93% based on amine; Elemental analysis (found: C 78.79, H 5.10; for $C_{13}H_{10}O_2$ requires: C 78.77, H 5.09%).

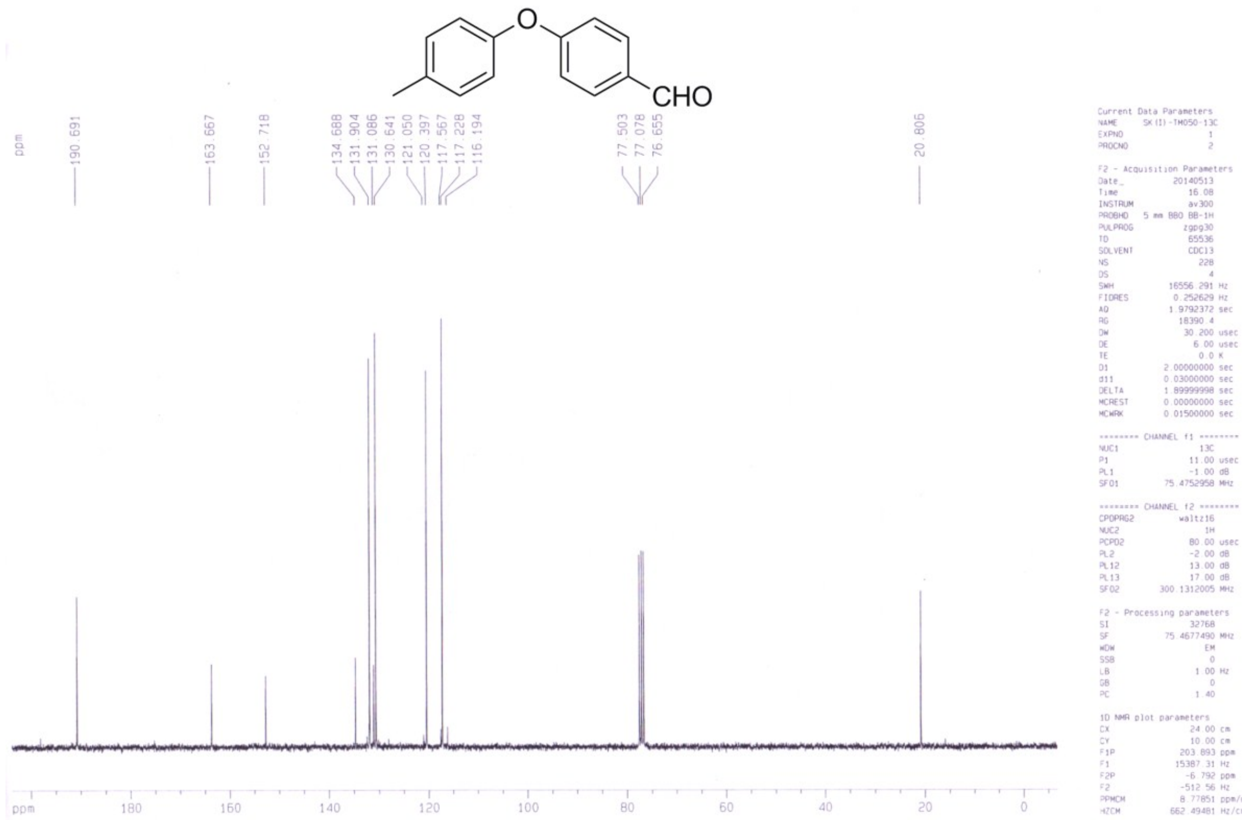


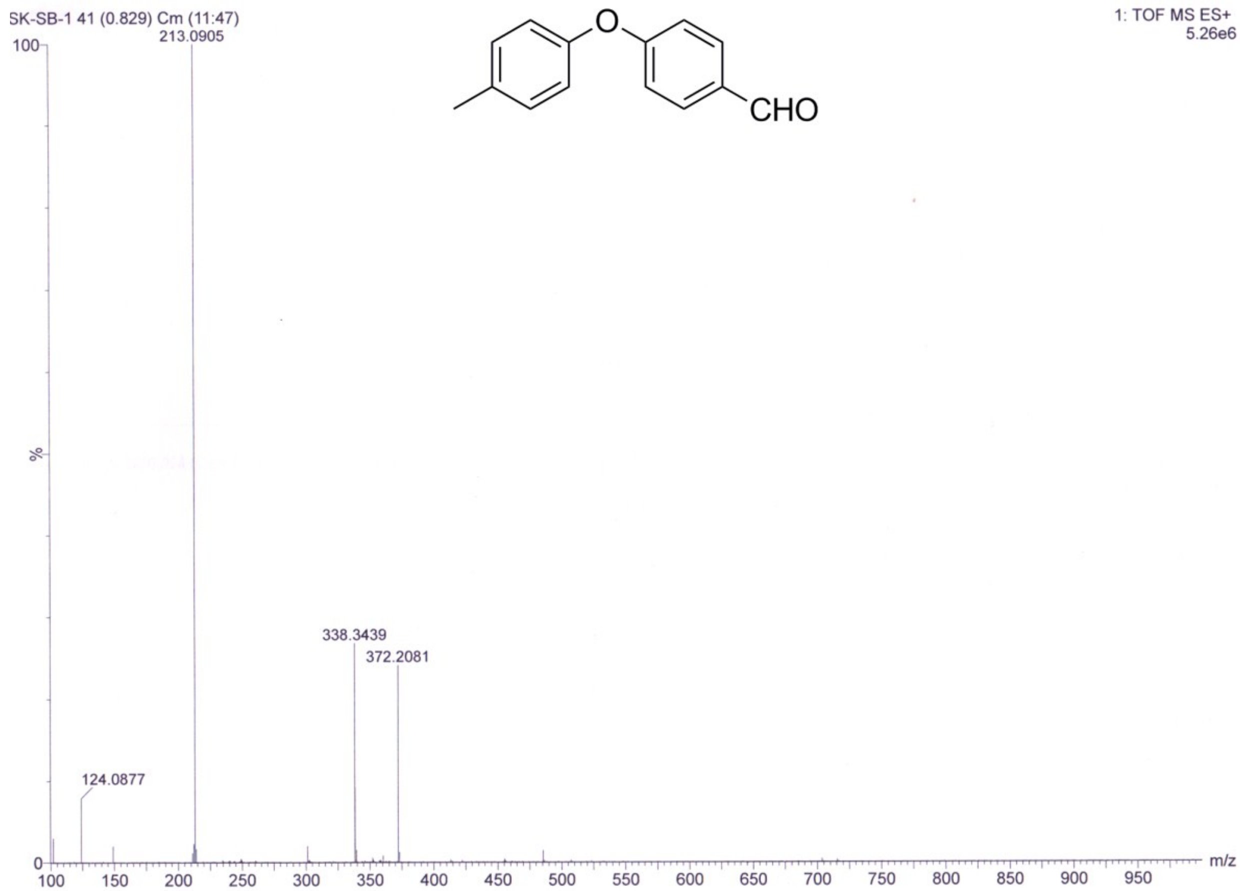

CHO
190.71
163.24
155.17
132.34
131.93
131.33
130.14
130.06
125.91
124.92
120.40
120.21
117.61
117.26
77.46
77.03
76.61
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



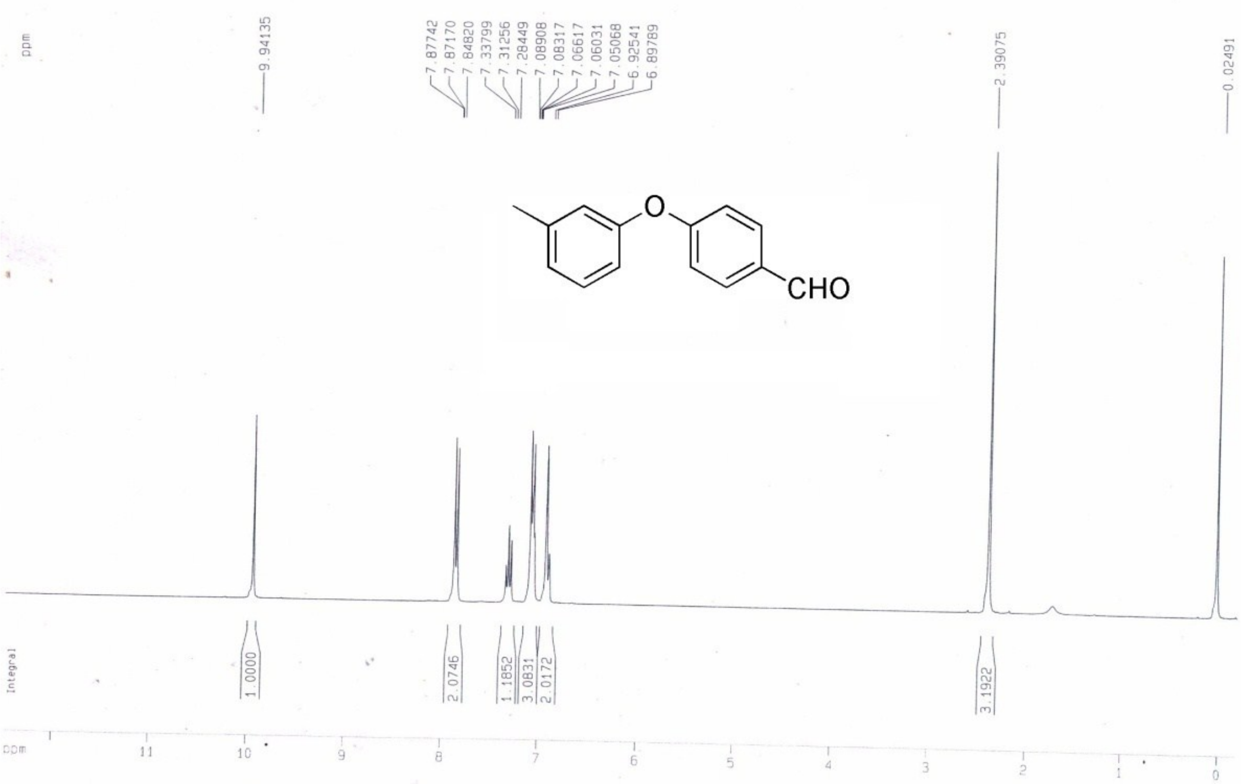
1l; δ_H (300 MHz; $CDCl_3$) 2.37 (3H, s), 6.96-7.04 (4H, m), 7.21 (2H, d, J = 8.2 Hz), 7.82 (2H, d, J = 8.6 Hz), 9.90 (1H, s); δ_C (75 MHz; $CDCl_3$) 20.81, 116.19, 117.23, 117.57, 120.39, 121.05, 130.64, 131.09, 131.90, 134.69, 152.72, 163.67, 190.69; *m/z* 213.0905 [$(M+H)^+$, 100%]; Elemental analysis (found: C 79.25, H 5.72; for $C_{14}H_{12}O_2$ requires: C 79.22, H 5.70%).

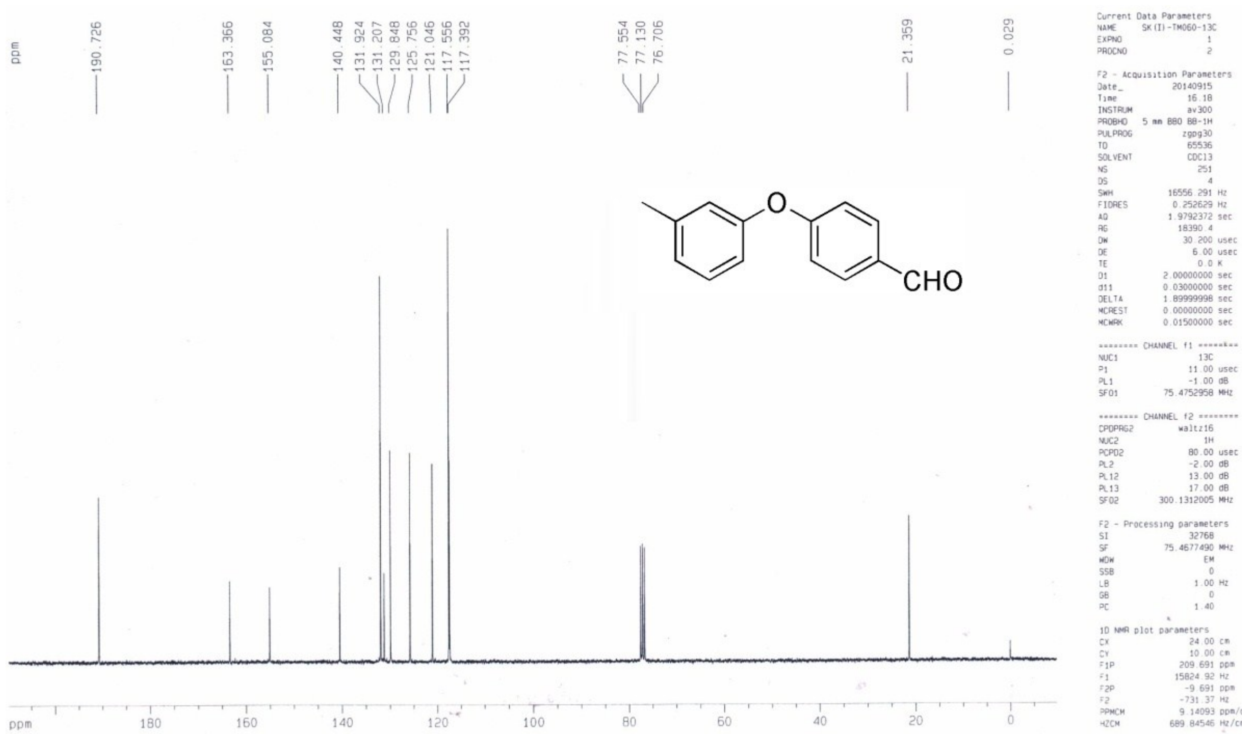

CHO
ppm
9.90194
7.83566
7.80687
7.21874
7.19148
7.04293
7.01425
6.98964
6.96175
2.36932
2.34462
2.12767
1.76872
Integral
1.0000
2.0948
1.9401
4.0312
3.3037
ppm 12 11 10 9 8 7 6 5 4 3 2 1 0



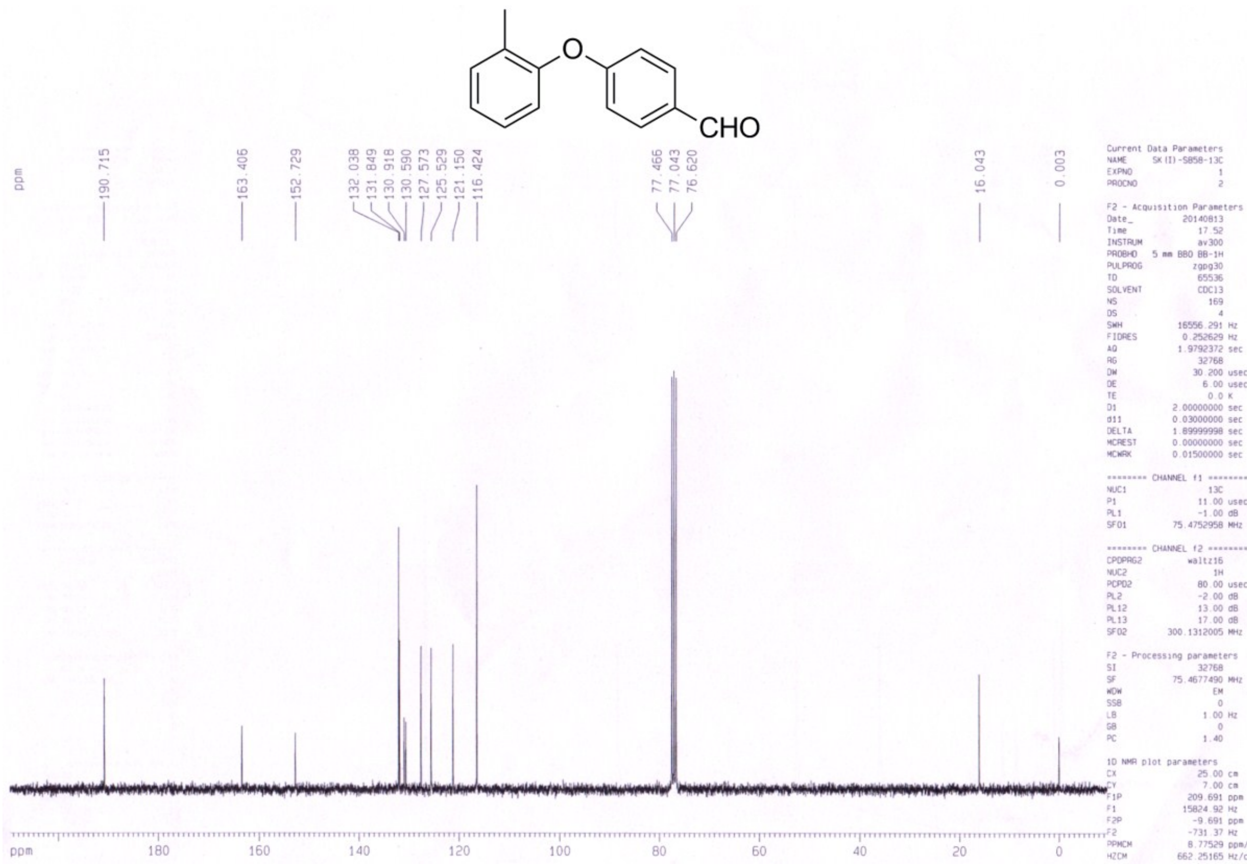


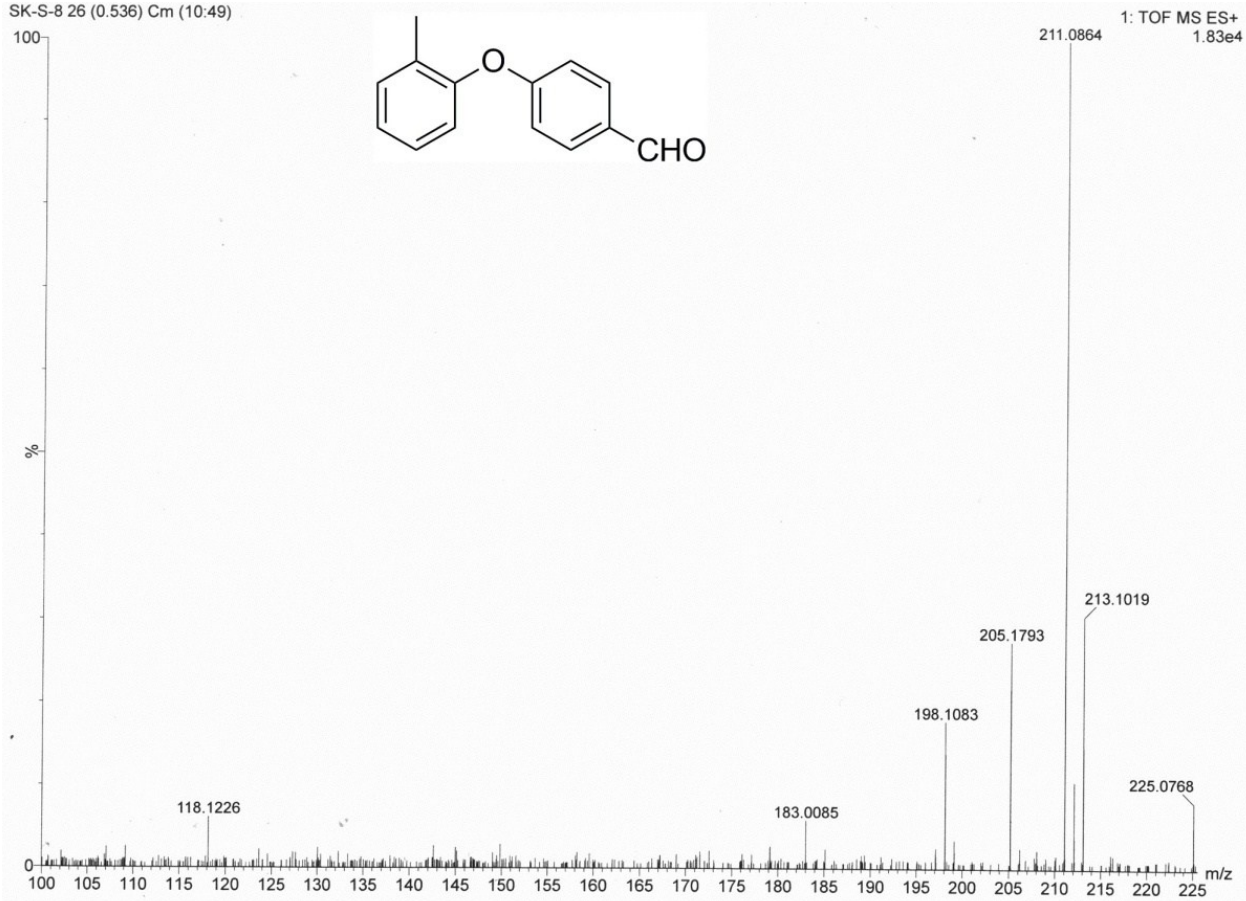
1m; δ_H (300 MHz; $CDCl_3$, TMS) 2.39 (3H, s), 6.91 (2H, d, *J* = 8.3 Hz), 7.05-7.09 (3H, m), 7.31 (1H, t, *J* = 7.6 Hz), 7.85-7.88 (2H, m), 9.94 (1H, s); δ_C (75 MHz; $CDCl_3$, TMS) 21.36, 117.39, 117.56, 121.05, 125.76, 129.85, 131.21, 131.92, 140.45, 155.08, 163.37, 190.73; Elemental analysis (found: C 79.24, H 5.71; for $C_{14}H_{12}O_2$ requires: C 79.22, H 5.70%).


ppm
9.94135
7.87742
7.87170
7.84820
7.33799
7.31256
7.28449
7.08908
7.08317
7.06617
7.06031
7.05068
6.92541
6.89789
2.39075
0.02491
O
CHO
Integral
1.0000
2.0746
1.1852
3.0831
2.0172
3.1922
ppm
11
10
9
8
7
6
5
4
3
2
1
0

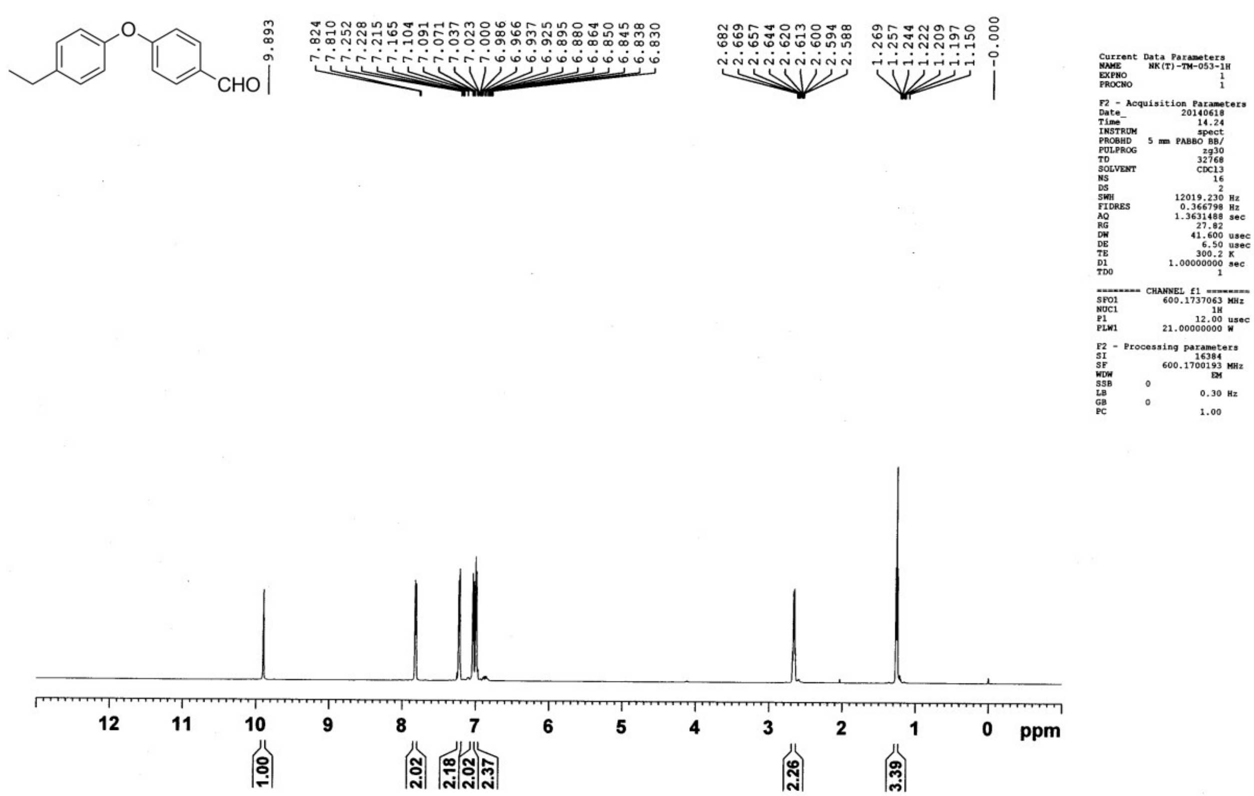

ppm
190.726
163.366
155.084
140.448
131.924
131.207
129.848
125.756
121.046
117.556
117.392
77.554
77.130
76.706
21.359
0.029
O
CHO
ppm
180
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME SK(I)-TM060-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20140915
Time 16.18
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 251
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 10.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84546 Hz/cm

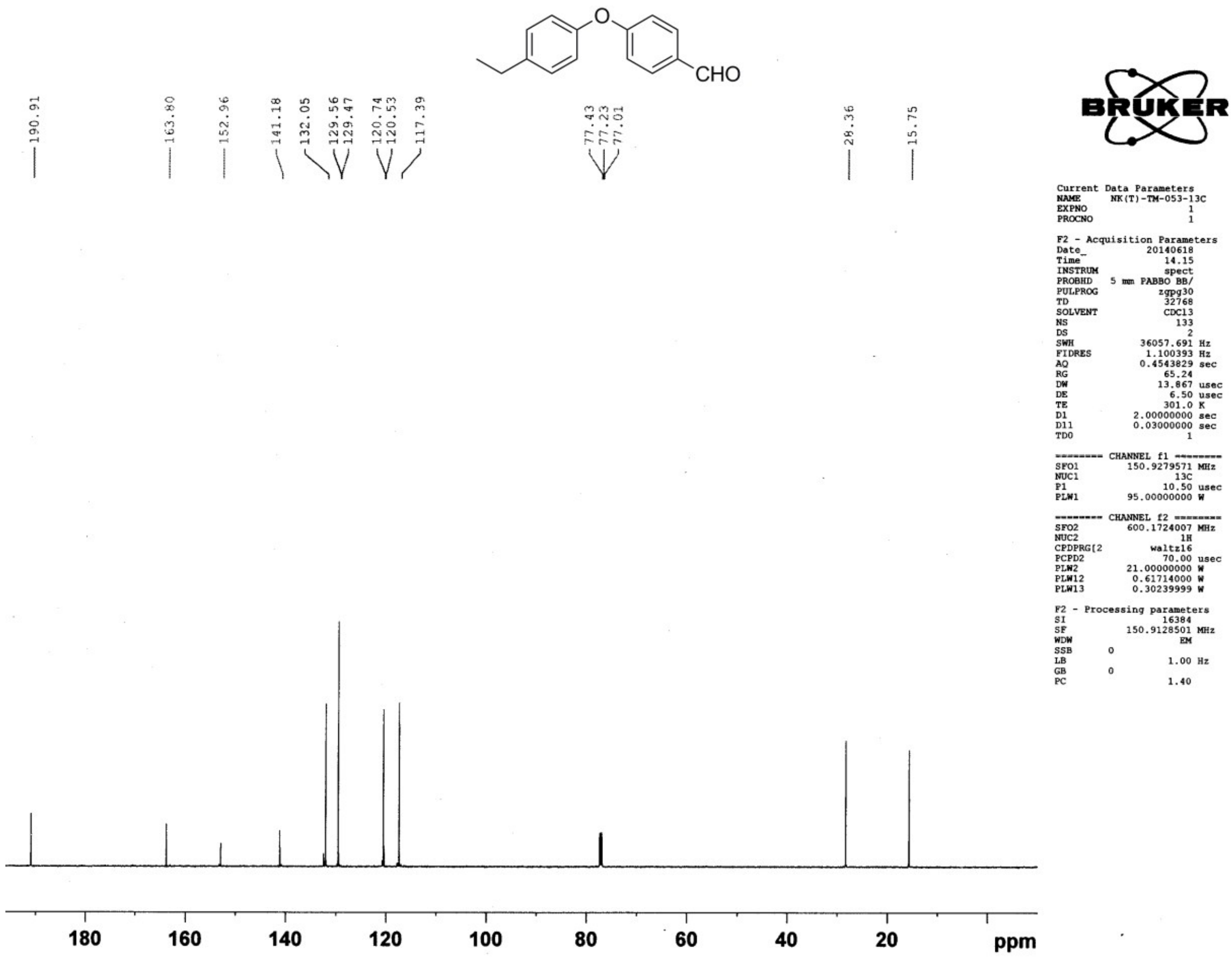
1n; δ_H (300 MHz; $CDCl_3$, TMS) 2.19 (3H, s), 6.95-7.02 (3H, m), 7.17-7.31 (3H, m), 7.83 (2H, d, J = 8.7 Hz), 9.91 (1H, s); δ_C (75 MHz; $CDCl_3$, TMS) 16.04, 116.42, 121.15, 125.53, 127.57, 130.59, 130.92, 131.85, 132.04, 152.73, 163.41, 190.72; m/z 213.1019 [$(M+H)^+$, 30%]; Elemental analysis (found: C 79.23, H 5.69; for $C_{14}H_{12}O_2$ requires: C 79.22, H 5.70%).





1o; δ_H (600 MHz; $CDCl_3$, TMS) 1.15-1.27 (3H, m), 2.59-2.68 (2H, m), 6.93-7.10 (4H, m), 7.22-7.23 (2H, m), 7.82 (2H, d, J = 8.4 Hz), 9.89 (1H, s); δ_C (150 MHz; $CDCl_3$, TMS) 15.75, 28.36, 117.39, 120.53, 129.56, 132.05, 141.28, 152.96, 163.80, 190.91; *m/z* 227.0817 [$(M+H)^+$, 100%]; Elemental analysis (found: C 79.60, H 6.22; for $C_{15}H_{14}O_2$ requires: C 79.62, H 6.24%).




CHO
190.91
163.80
152.96
141.18
132.05
129.56
129.47
120.74
120.53
117.39
77.43
77.23
77.01
28.36
15.75
BRUKER
Current Data Parameters
NAME NK(T)-TM-053-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140618
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 133
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 301.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W
======== CHANNEL f2 ========
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W
F2 - Processing parameters
SI 16384
SF 150.9128501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
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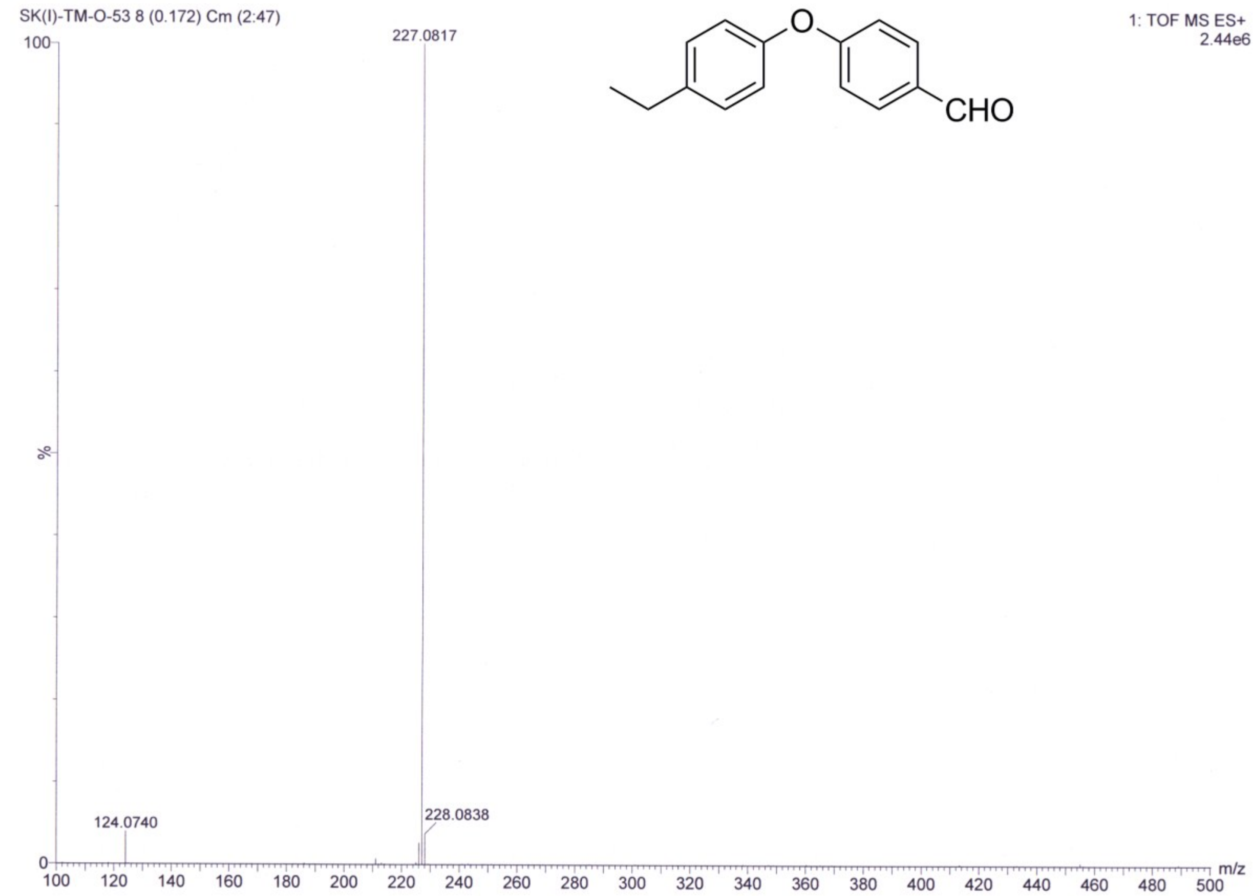
80
60
40
20
ppm


SK(I)-TM-O-53 8 (0.172) Cm (2:47)
1: TOF MS ES+
2.44e6
CHO
O
227.0817
228.0838
124.0740
100
%
0
m/z
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500