Electronic Supplementary Information

Metal Free Visible Light Driven Oxidation of Alcohols to Carbonyls Using 3, 6-Di(pyridin-2-yl)-1,2,4,5-tetrazine (pytz)as Catalyst

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1. General Information

All solvents and commercially available reagents were purchased from commercial sources and used directly. Thin layer chromatography (TLC) was performed on EMD precoated plates (silica gel 60 F254, Art 5715) and visualized by fluorescence quenching under UV light. Column chromatography was performed on Silica Gel (60– 120 Mesh). The synthesis of 3,6-di(pyridin-2-yl)-1,2,4,5-*s*-tetrazine (**pytz**) and 3,6-diphenyl-1,2,4,5-tetrazine (**phtz**) were carried out following the method reported earlier.[1] A Xenon lamp with a power of 300 W equipped with a cut-off filter (λ> 420 nm) was used as a visible light source. The reaction was carried out in a 100 mL double walled quartz beaker flask having water inlet and outlet to maintain the room temperature of the reaction vessel.^{1}H NMR spectra were recorded using 300, 400MHz NMR spectrometers. All ^{1}Hdata were reported in parts per million (ppm) relative totetramethylsilane (δ_H = 0) in thedeuterated solvents. All GC analyses were performed on a GC systemwith an FID detector using a J & W HP−5 column (30 m, 0.32 mm internal diameter) and n-decaneas the internal standard. Melting points were determined in open capillaries andare uncorrected.

2. Experimental

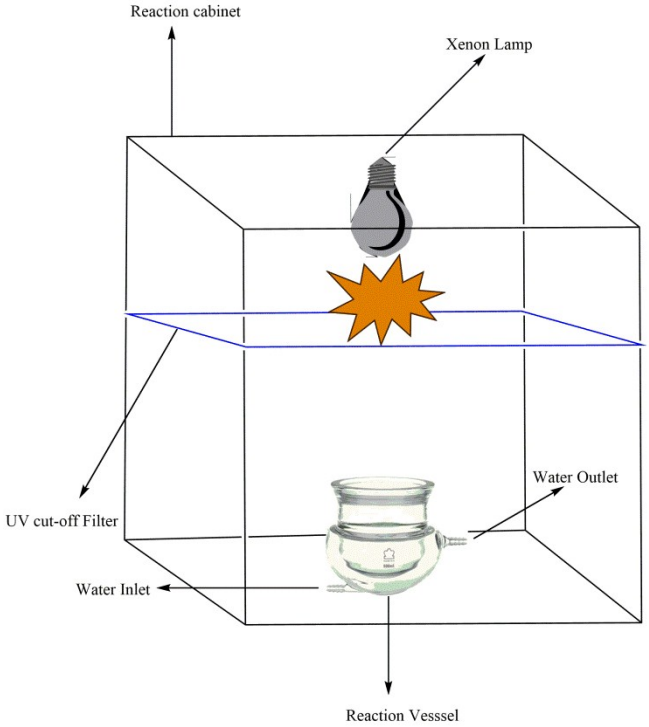
General Procedure for the Alcohol Oxidation

Method A: Alcohol(2mmol) was taken in a 100 mL double-walled quartzbeaker having water inlet and outlet to maintain the temperature of thereaction vessel in acetonitrile (5 mL). 3,6-di(pyridin-2-yl)-1,2,4,5-*s*-tetrazine (pytz, 23.6 mg, 5 mol%) is added to the reaction mixture and the beaker was exposed to visiblelight under stirring condition and was allowed to proceed for 10−12 h at room temperature.The progress of the reaction was monitored by TLC or gas chromatography.When the reaction reached completion, or no further conversion was observed by gas chromatography, solvent was evaporatedat reduced pressure and the product was dissolved in minimumvolume of hexane.The reaction mixture was eluted through a plug of silica using hexane affording the corresponding product. Reported yields are the average of at least three runs.

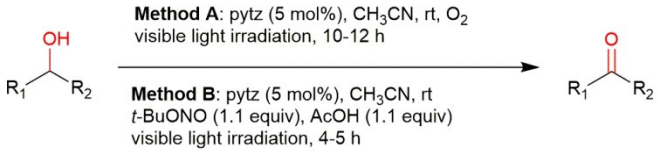
Method B: Alcohol(2mmol), *tert*-butylnitrite(2.2mmol, 230mg),acetic acid (2.2 mmol, 130 mg),and 3,6-di(pyridin-2-yl)-1,2,4,5-*s*-tetrazine (pytz, 23.6 mg, 5 mol%) were taken in a 100 mL double-walled quartz beaker having water inlet and outlet to maintain the temperature of the

reaction vessel in acetonitrile (5 mL).The reaction mixture was exposed to visible light under stirring condition and the reaction was allowed to proceed for 4−5 h at room temperature.The progress of the reaction was monitored by TLC or gas chromatography. When the reaction reached completion, or no further conversion was observed by gas chromatography, solvent was evaporated at reduced pressure and the product was dissolved in minimum volume of hexane. The solution was washed with water (2 × 5 mL) and the hexane layer was dried over anhydrous Na_2SO_4. The reaction mixture was then eluted through a plug of silica using hexane affording the corresponding product.Reported yields are the average of at least three runs.

Gram-scale Oxidation of Alcohol: Benzyl alcohol (20 mmol, 2.16 g),*tert*-butyl nitrite (21 mmol, 2.17 g) and acetic acid (21 mmol, 1.26 g) were taken in a 100 mL double-walled quartzbeaker having water inlet and outlet to maintain the temperature of thereaction vessel in acetonitrile (50 mL). 3,6-di(pyridin-2-yl)-1,2,4,5-*s*-tetrazine (pytz, 0.47g, 5 mol%) is added to the reaction mixture and the beaker was exposed to visible light under stirring condition and was allowed to proceed for 7 h at room temperature. The progress of the reaction was monitored by TLC or gas chromatography.When the reaction reached completion, or no further conversion was observed by gas chromatography, solvent was evaporated at reduced pressure and the product was dissolved in minimum volume of hexane.The reaction mixture was eluted through a plug of silica using hexane affording the benzaldehyde; yield: 2.06 g (97%).



Scheme S1 Schematic Diagram of Reaction Set-UP



Scheme S2 Oxidation of Alcohols to Carbonyls

3. Analytical Data for Aldehydes and Ketones

Benzaldehyde (Scheme 4, Entry 2a)[2]: colorless liquid (method A: 90 mg, 85%; method B: 97 mg, 92%).^{1}HNMR (400 MHz, $CDCl_3$) δ_H 9.987 (s, 1H), 8.109 (d, 1H, *J* =7.6 Hz), 7.858 (d, 1H, *J* = 7.2 Hz), 7.588 (dd, 2H, *J* = 7.2 & 8.4 Hz), 7.496-7.424 (m, 2H).

3-Nitrobenzaldehyde(Scheme 4, Entry 2b)[3]: off White solid (method A: 116 mg, 77% ; method B: 126 mg, 84%), mp 107 ºC.^{1}HNMR (400 MHz, $CDCl_3$) δ_H 10.157 (s, 1H), 8.724-8.272 (m, 2H), 7.725 (t, 1H, *J* = 7.6, 8.0 Hz).

4-Hydroxybenzaldehyde(Scheme 4, Entry 2c)[4]: Off white solid (method A: 89 mg, 73% ; method B: 97 mg, 80%), mp 115 ºC.^{1}HNMR (400 MHz, $CDCl_3$) δ_H 9.837 (s, 1H), 7.827 (d, 3H, *J* = 6.4 Hz), 7.015 (d, 2H, *J* = 4.4 Hz).

4-(Dimethylamino)benzaldehyde(Scheme 4, Entry 2d)[5]: White solid (method A: 111 mg, 75% ; method B: 128 mg, 86%),mp 74 ºC.^{1}HNMR (400 MHz,$CDCl_3$) δ_H 9.715 (s, 1H), 7.712(s, 2H, *J* = 8.4 Hz), 6.671 (d, 2H), 3.052 (s, 6H).

4-Bromobenzaldehyde (Scheme 4, Entry 2e)[2]: Off white solid (method A: 131 mg, 72% ; method B: 144 mg, 79%), mp55 ºC.^{1}HNMR (500 MHz, $CDCl_3$) δ_H 9.953 (s, 1H), 7.937-7.507 (m, 4H).

Anthracene-9-carbaldehyde (Scheme 4, Entry 2f)[6]: Off White solid (method A: 162 mg, 79% ; method B: 181 mg, 88%), mp 107 ºC.^{1}HNMR (400 MHz, $CDCl_3$) δ_H 11.411 (s, 1H), 8.9 (d, 2H, *J* = 8.4 Hz), 8.528 (s, 1H), 7.95 (d, 2H, *J* = 8.4 Hz), 7.640-7.474 (m, 4H).

Nicotinaldehyde(Scheme 4, Entry 2g)[7]: color less liquid (method A: 72 mg, 68% ; method B: 81 mg, 76%).^{1}HNMR (400 MHz, $CDCl_3$) δ_H 9.882 (s, 1H), 8.829 (s, 1H), 8.583 (s, 1H), 7.931 (d, 1H, *J* = 7.2 Hz), 7.265 (s, 1H).

Thiophene-2-carbaldehyde (Scheme 4, Entry 2h)[8]:colorless liquid (method A: 79 mg, 71% ; method B: 90 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 9.927 (s, 1H), 7.786 (dd, 2H, *J* = 2.4, 7.6, 4.4 Hz), 7.185 (d, 1H, *J* = 3.6 Hz).

(Z)-3,7-Dimethylocta-2,6-dienal(Scheme 4, Entry 2i)[9]: colorless liquid (method A: 98 mg, 65% ; method B: 109 mg, 72%), ^{1}H NMR (400 MHz, $CDCl_3$) δ_H 9.934 (dd, 1H, *J*= 7.6, 7.2

Hz), 5.874 (d, 1H, *J*= 7.2 Hz), 5.087 (t, 1H, *J* = 6.8, 5.2 Hz), 2.594 (t, 1H, J= 6.8, 7.2 Hz), 2.227 (s, 2H), 2.175 (s, 2H), 1.986 (s, 2H), 1.677(s, 3H), 1.600(d, 3H, *J*= 6.8 Hz).

4-Hydroxy-3-methoxybenzaldehyde(Scheme 4, Entry 2j)[10]: white solid (method A: 120 mg, 79% ; method B: 130 mg, 86%), ^{1}H NMR (300MHz, $CDCl_3$) δ_H 9.706 (s, 1H), 7.338-7.310 (m, 2H), 6.94 (dd, 1H, *J* = 3.3, 1.8 Hz).

Acetophenone (Scheme 5, Entry 4a) [2]: colorless oil (method A: 105 mg, 88%; method B: 108 mg, 90%).^{1}HNMR (400 MHz, $CDCl_3$) δ_H 7.932 (d, 2H, *J* = 7.6 Hz), 7.547-7.408 (m, 3H), 2.563 (s, 3H).

1-(3-Bromophenyl)ethanone(Scheme 5, Entry 4b)[11]: white solid (method A: 149 mg, 76% ; method B: 157 mg, 80%).^{1}H NMR (400MHz, $CDCl_3$) δ_H 8.033 (s, 1H), 7.840 (d, 1H, *J* = 7.6 Hz), 7.638 (d, 1H, *J* = 7.6 Hz),7.316(t, 1H, *J* = 7.6, 8 Hz), 2.569 (s, 3H).

1-p-Tolylethanone (Scheme 5, Entry 4c)[12]:White solid (method A: 108 mg, 81% ; method B: 115 mg, 86%).^{1}H NMR (400 MHz, $CDCl_3$) δ_H 7.787 (s, 2H), 7.164 (s, 2H), 2.472 (s, 3H), 2.166 (s, 2H).

1-(3-Nitrophenyl)ethanone (Scheme 5, Entry 4d): Brown solid (method A: 132 mg, 80% ; method B: 143 mg, 87%),mp 77ºC.^{1}HNMR (400 MHz, $CDCl_3$) δ_H 8.718 (s, 1H), 8.382 (d, 1H, *J* = 7.6 Hz), 8.265 (d, 1H, *J* = 7.6 Hz), 7.675 (t, 1H, *J* = 7.6 Hz).

Benzophenone(Scheme 5, Entry 4e)[13]: white solid (method A: 134 mg, 74% ; method B: 149 mg, 82%), mp 47-49 ºC.^{1}H NMR (300MHz, $CDCl_3$) δ_H 7.736 (d, 4H, *J* =8.1 Hz,), 7.543-7.491 (m, 2H), 7.434-7.382 (m, 4H.

1-(Anthracen-9-yl)ethanone (Scheme 5, Entry 4f)[14]: Yellow solid (method A: 160 mg, 73% ; method B: 176 mg, 80%). mp76 ºC. ^{1}HNMR (400 MHz, $CDCl_3$) δ_H 8.427 (s, 1H), 7.981 (d, 2H, *J* = 8 Hz), 7.823 (d, 2H, *J* = 8.4 Hz), 7.504-7.432 (m, 4H), 2.785 (s, 3H).

10,10a-Dihydroanthracen-9(8aH)-one(Scheme 5, Entry 4g): Yellow solid (method A: 156 mg, 80% ; method B: 170 mg, 87%). ^{1}H NMR (400MHz, $CDCl_3$) δ_H 8.308 (d, 2H, *J* = 7.6 Hz), 7.543 (t, 2H, *J* = 7.6, 7.2 Hz), 7.415 (t, 4H, *J* = 7.6 Hz), 3.845 (s, 3H).

1-(Thiophen-3-yl)ethanone(Scheme 5, Entry 4h):colorless liquid (method A: 82 mg, 65% ; method B: 89 mg, 71%),mp58-62 ºC.^{1}HNMR (400 MHz, $CDCl_3$) δ_H 8.043 (s, 1H), 7.526 (d, 1H, J = 4.8 Hz), 7.302 (dd, 1H, J = 2.4, 2.8 Hz).

Cyclohexanone(Scheme 5, Entry 4i)[13]: Colorless liquid (method A: 70 mg, 72% ; method B: 77 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) 2.337 (t, 3H, J = 6.4 Hz), 1.868-1.282 (m, 7H).

4. Reference

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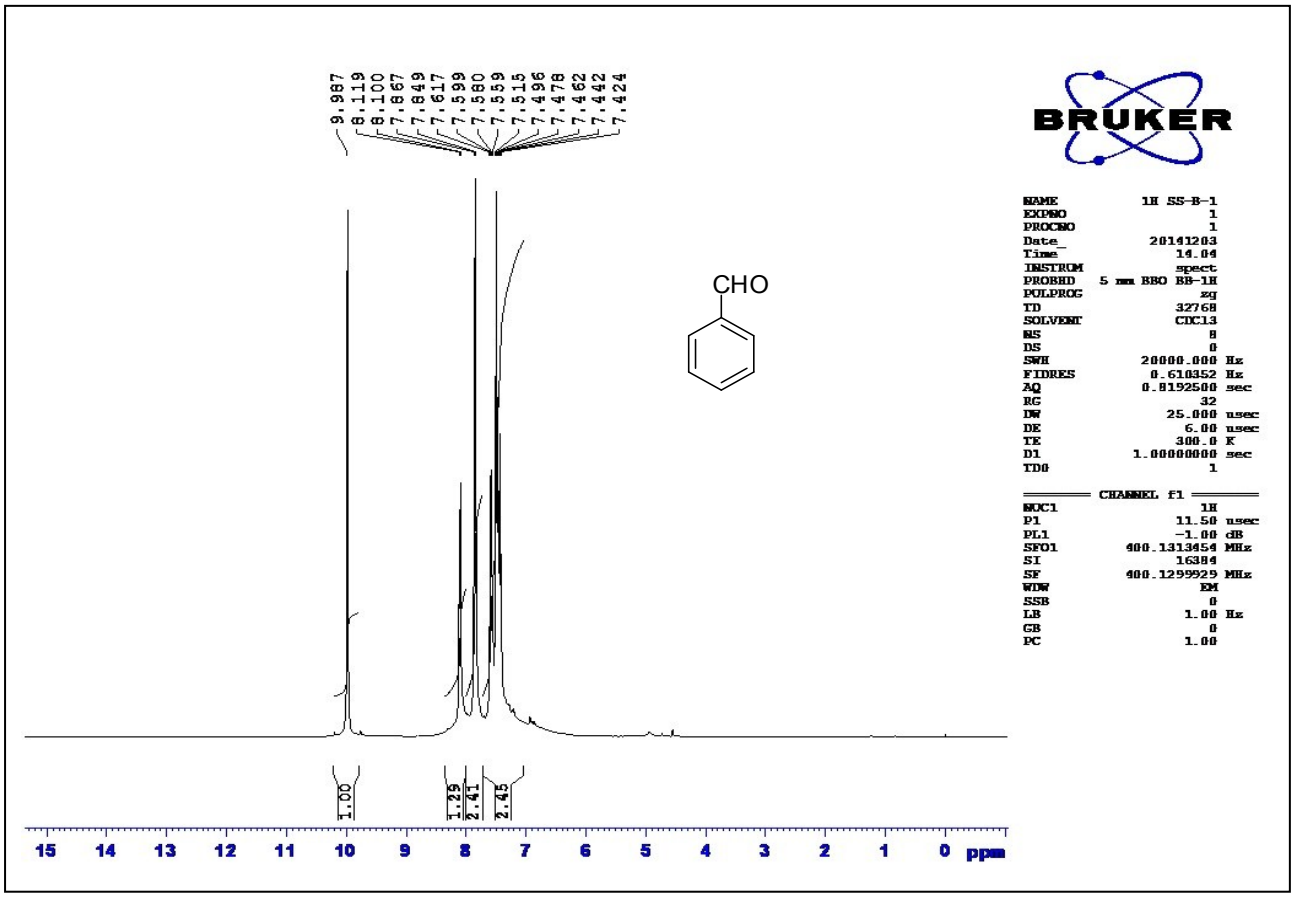
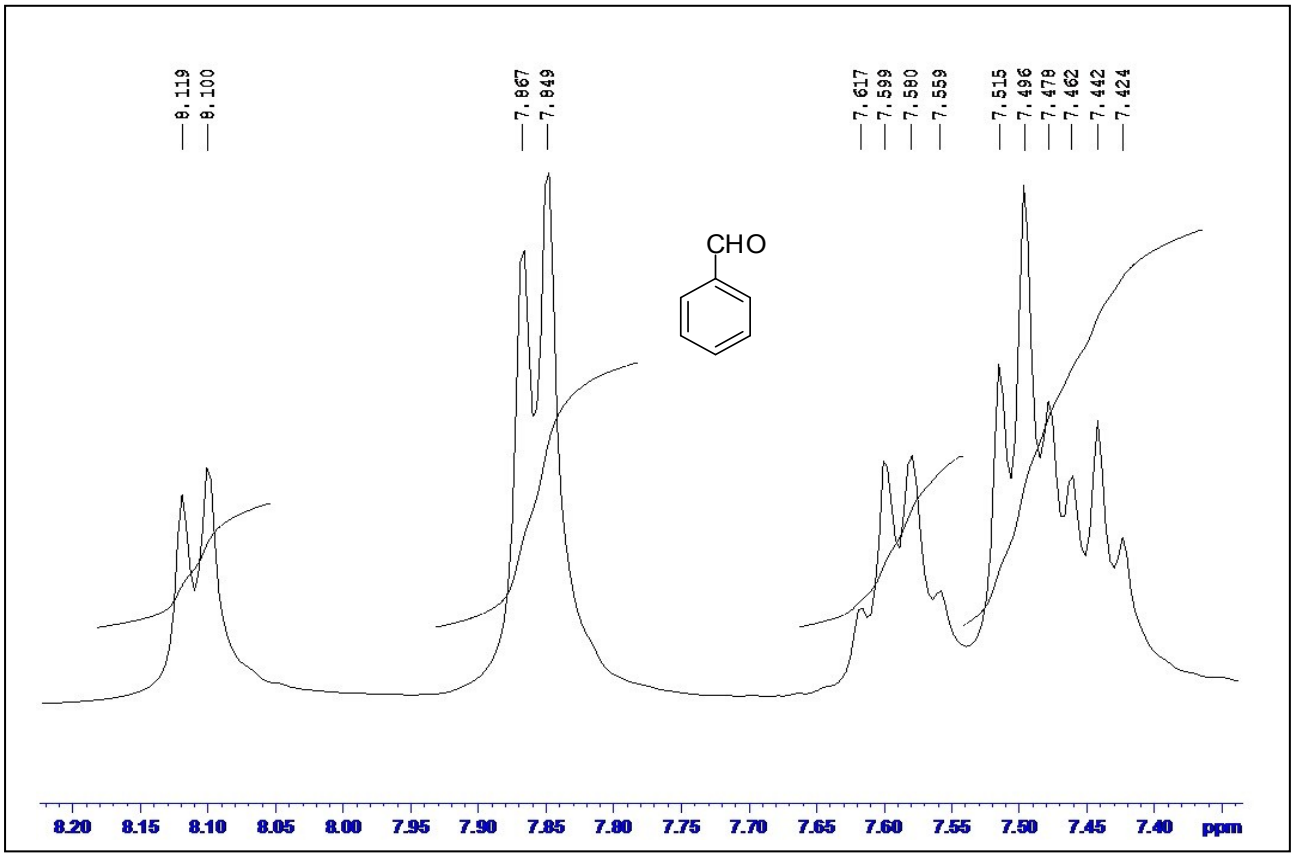
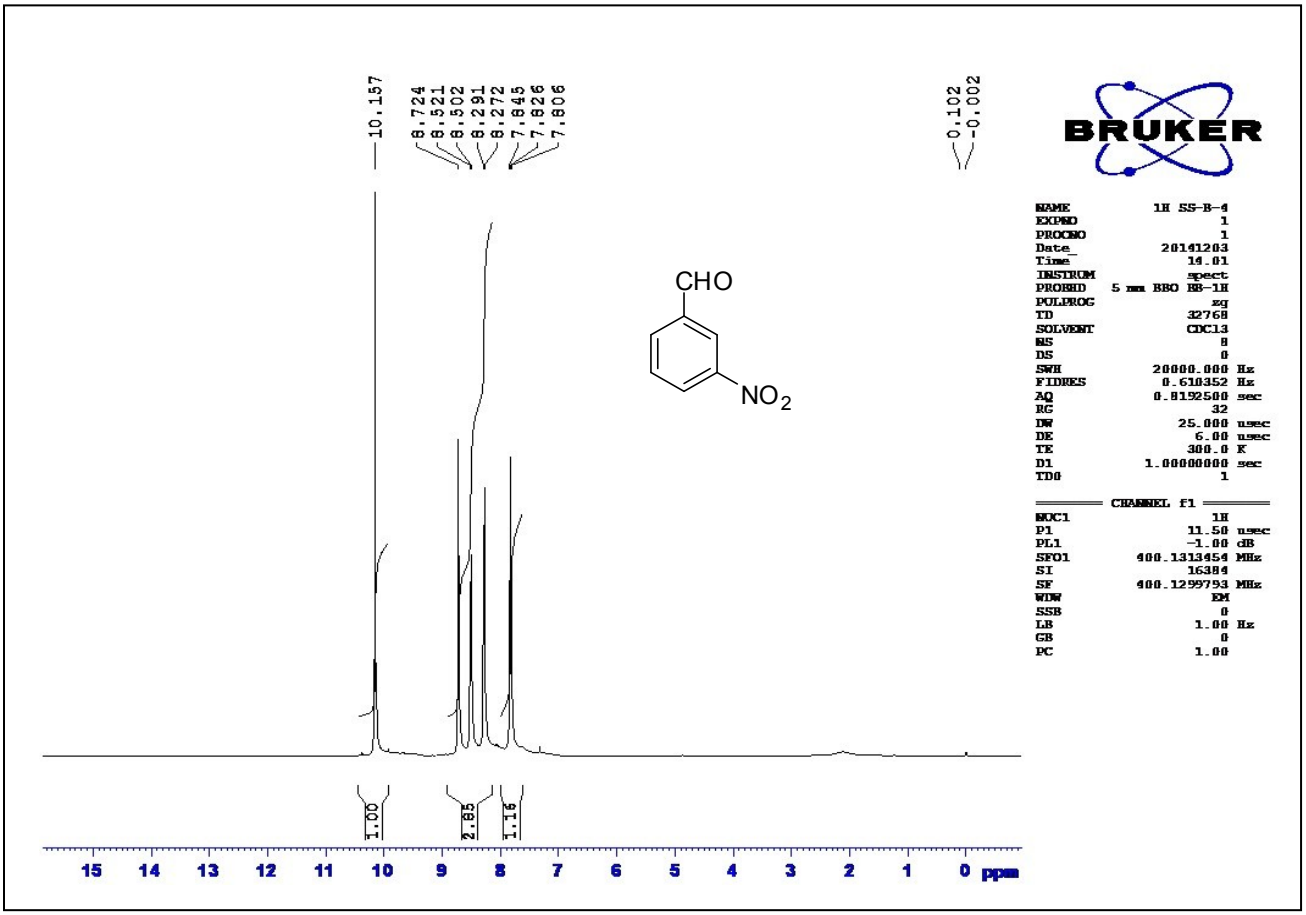
5.[1]H NMR Spectra



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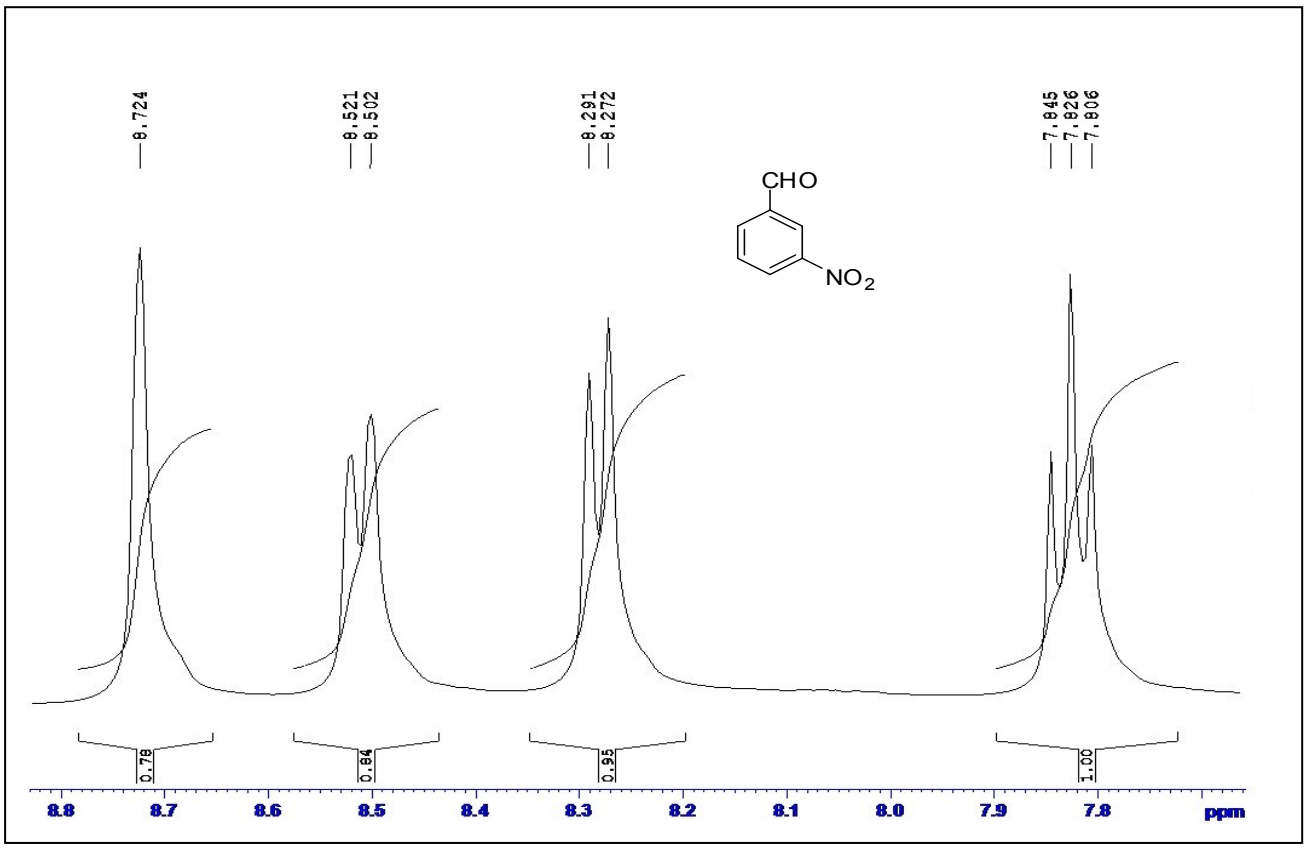
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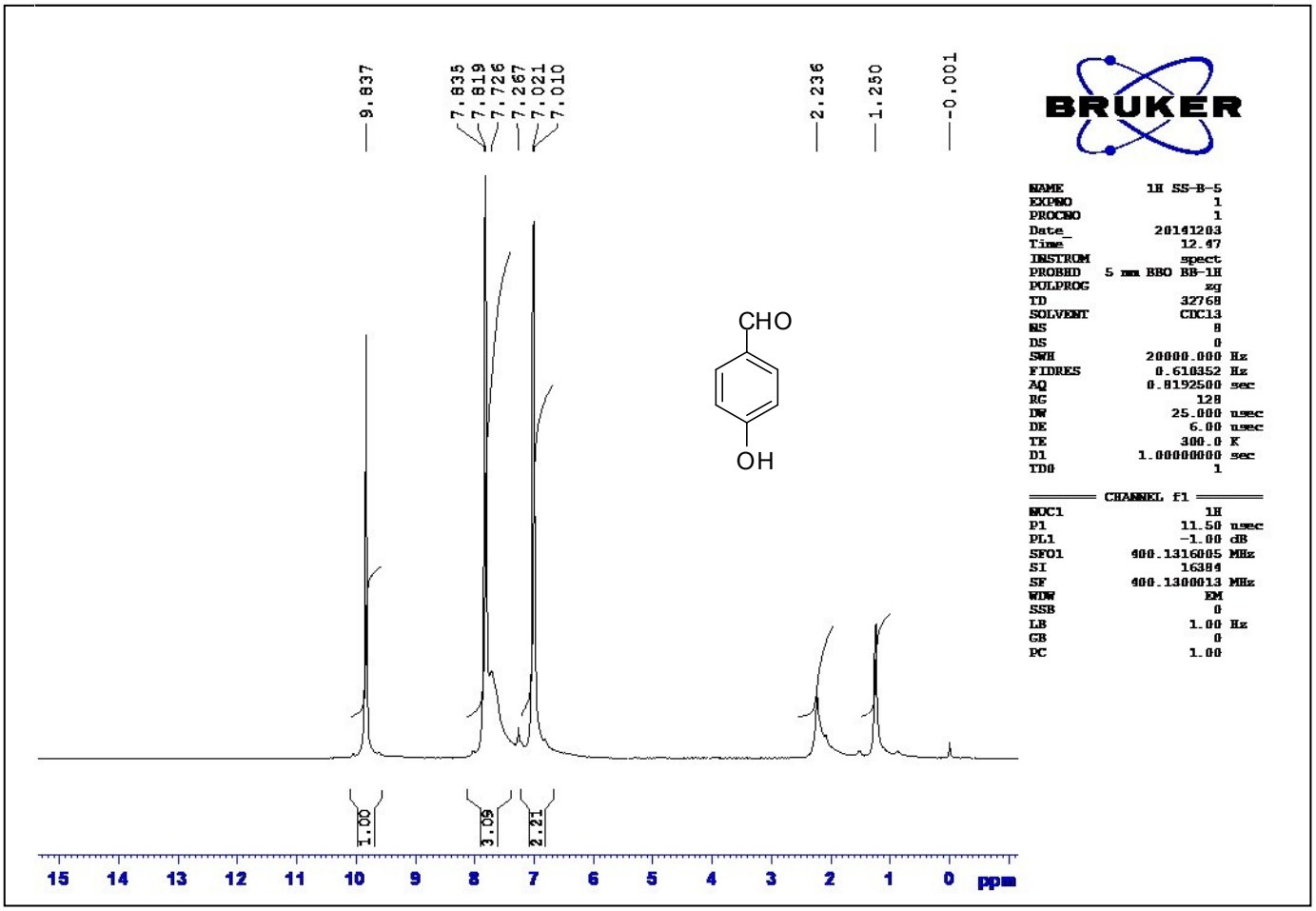
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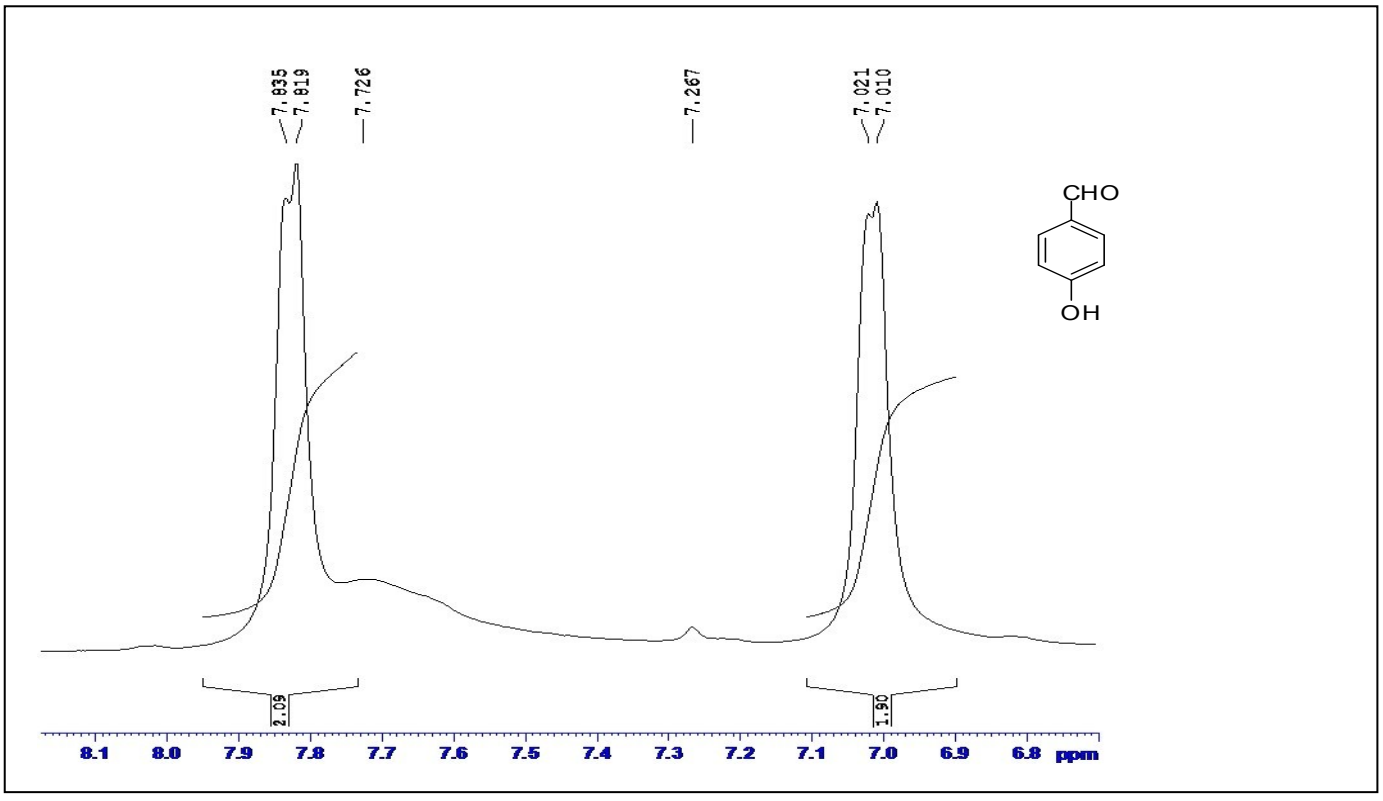
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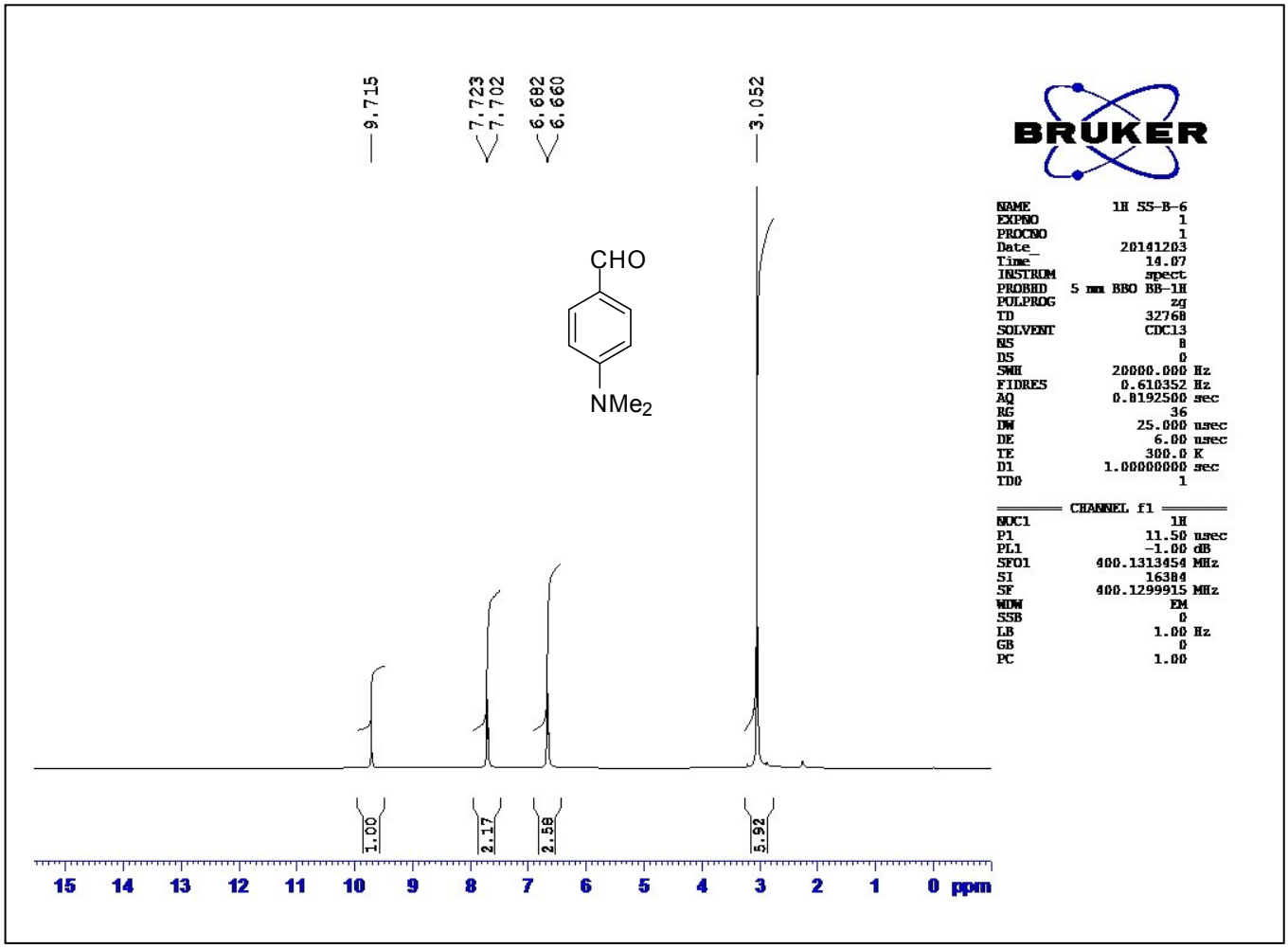
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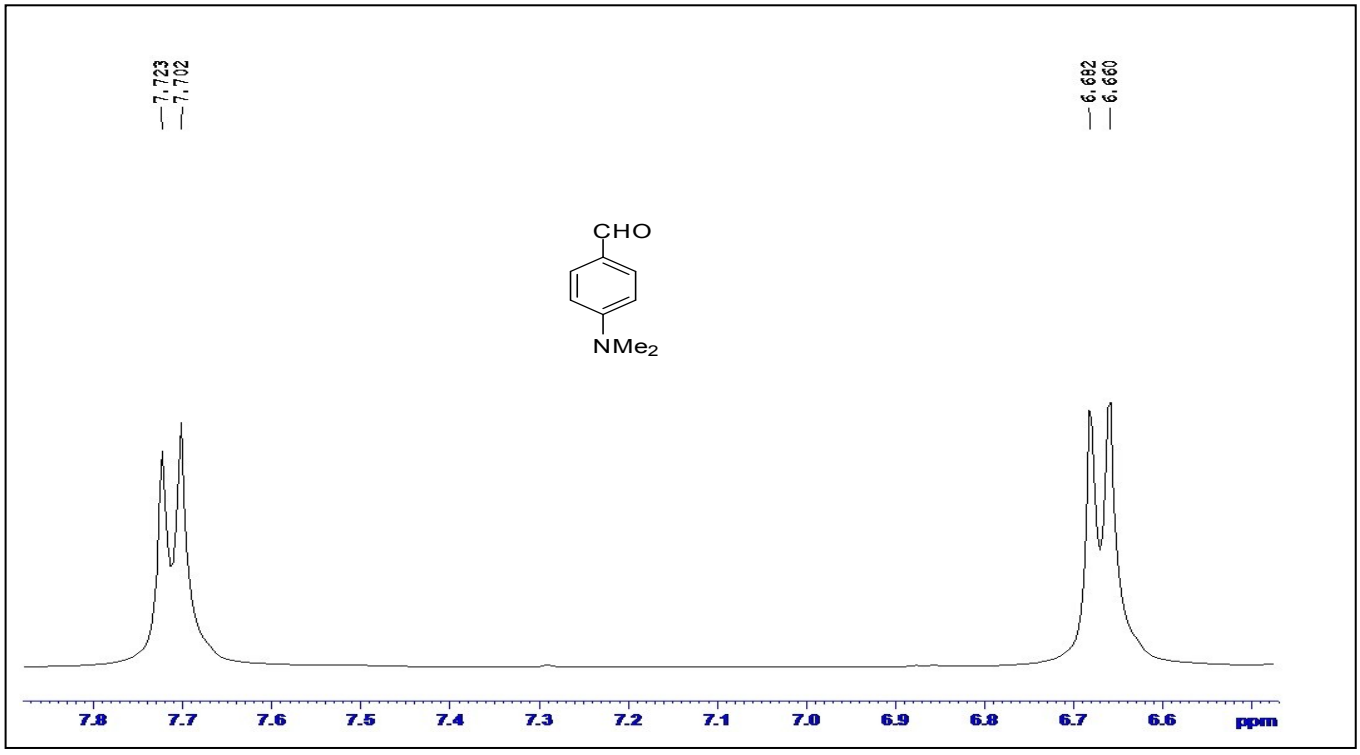
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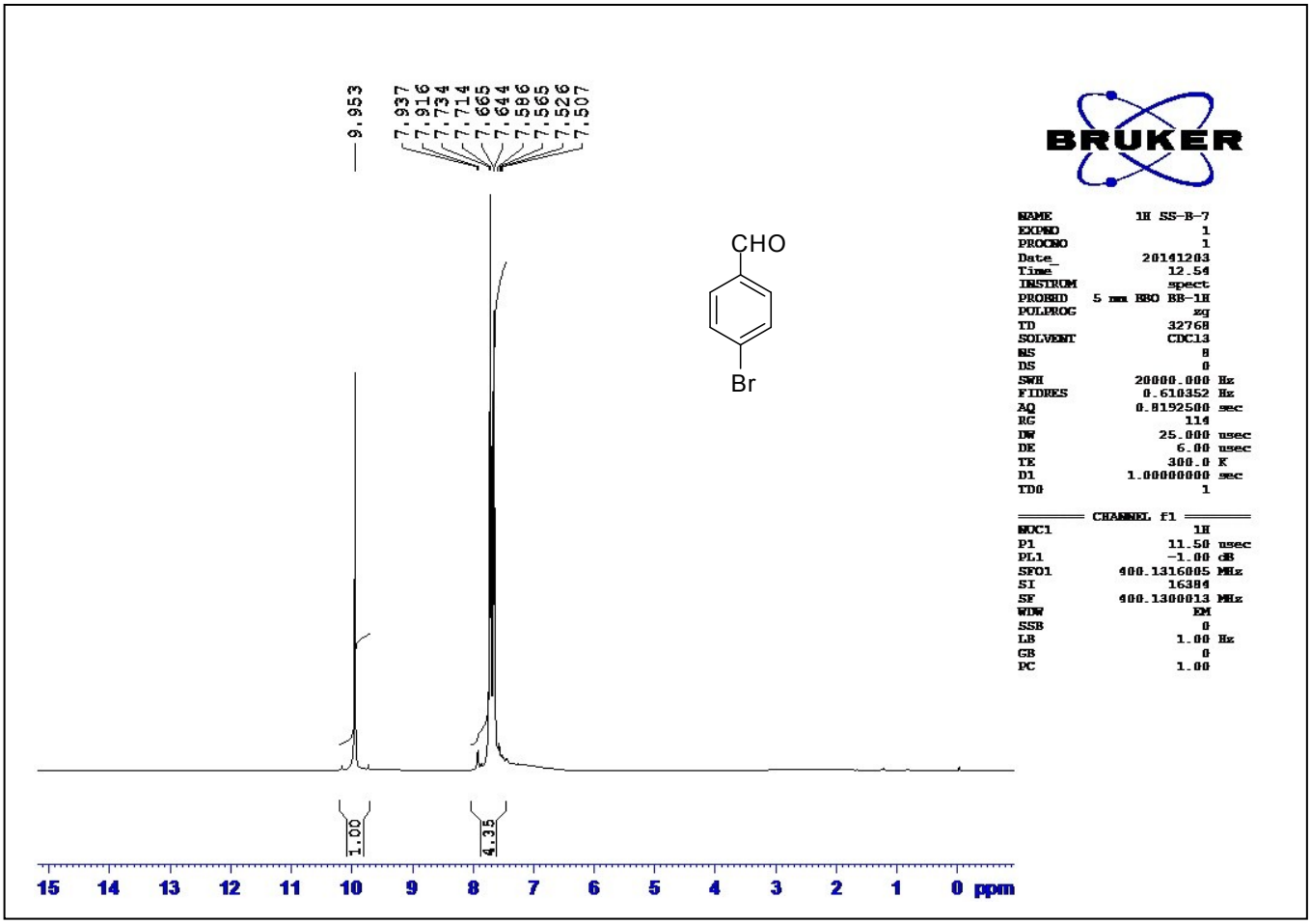
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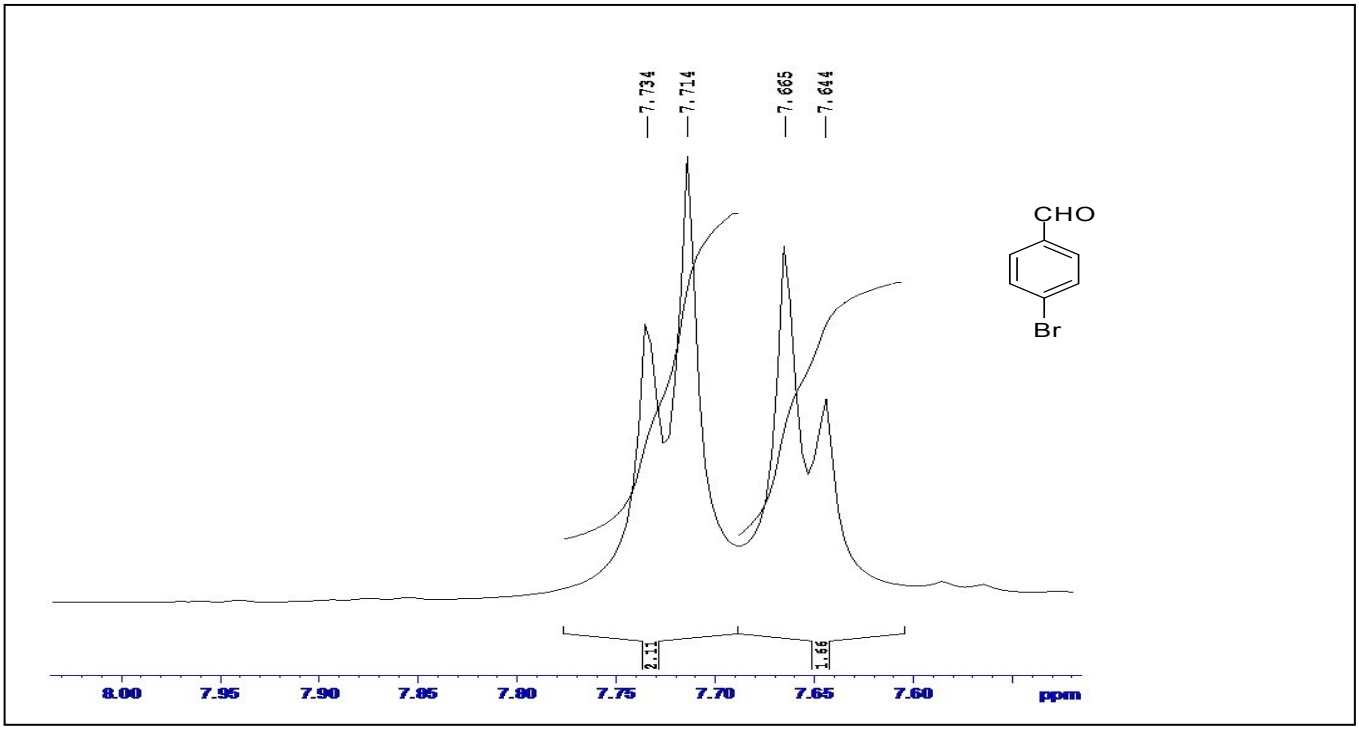
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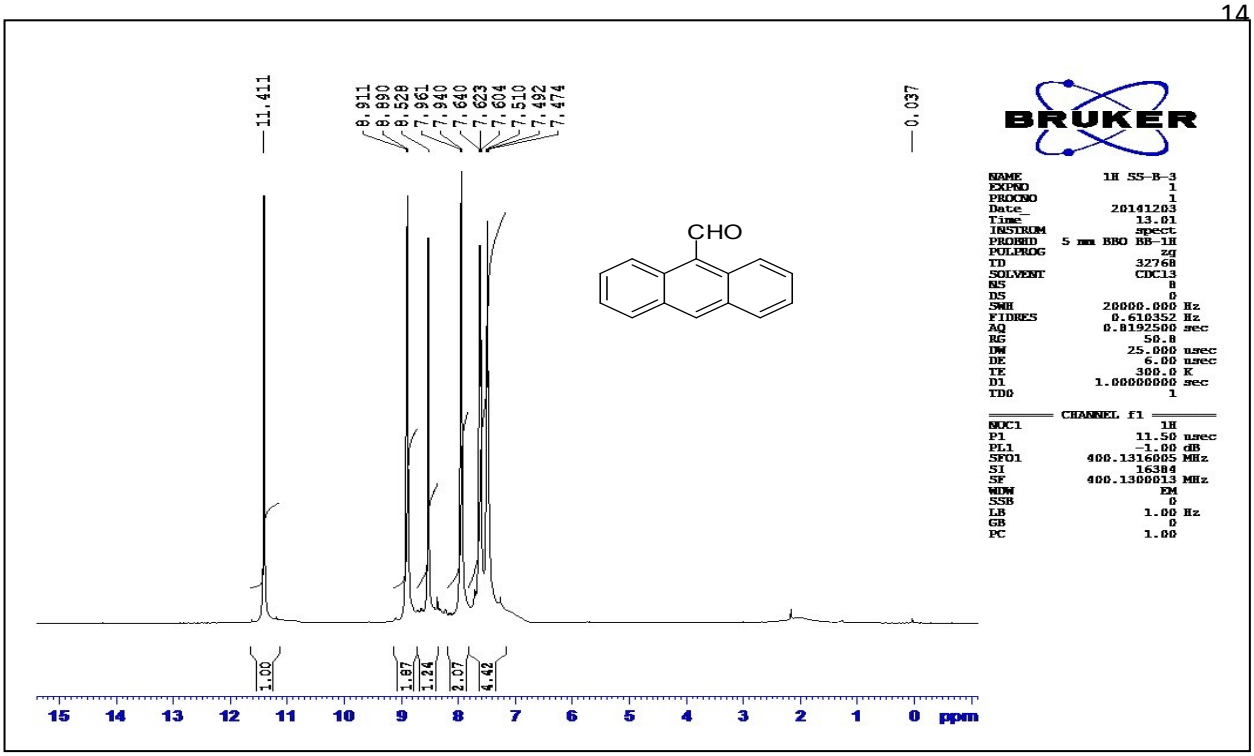
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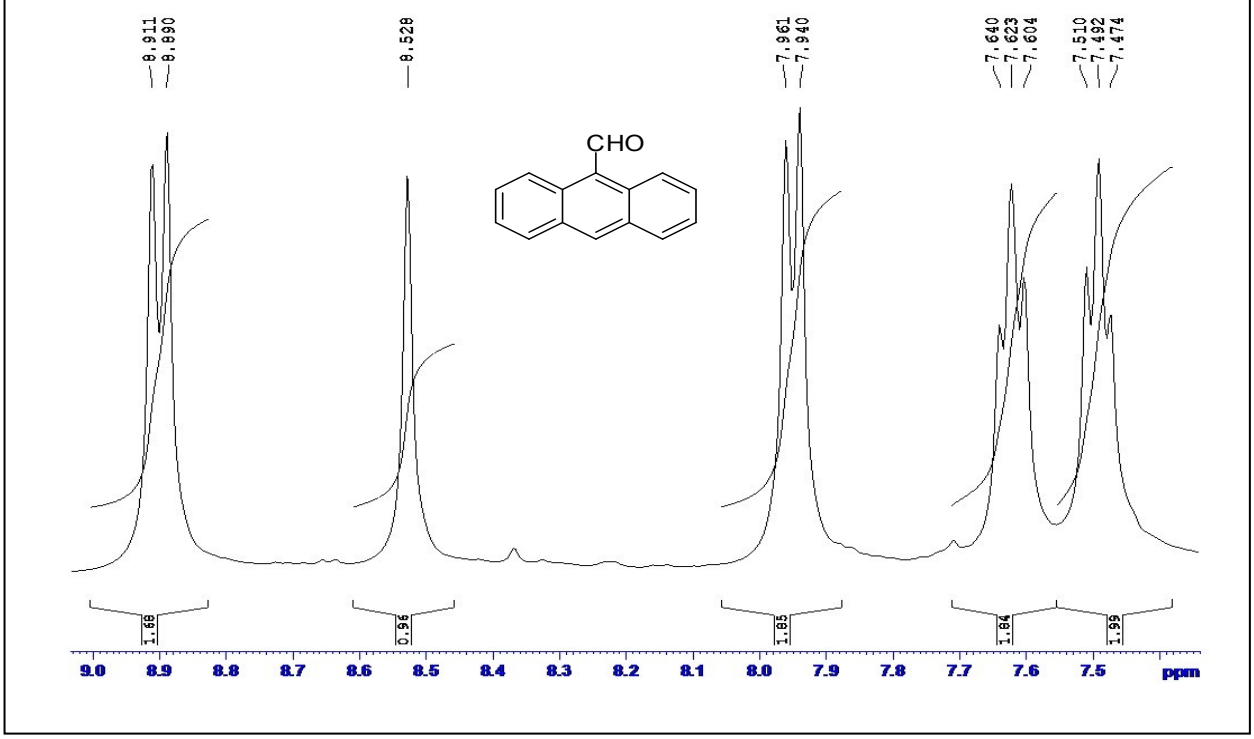
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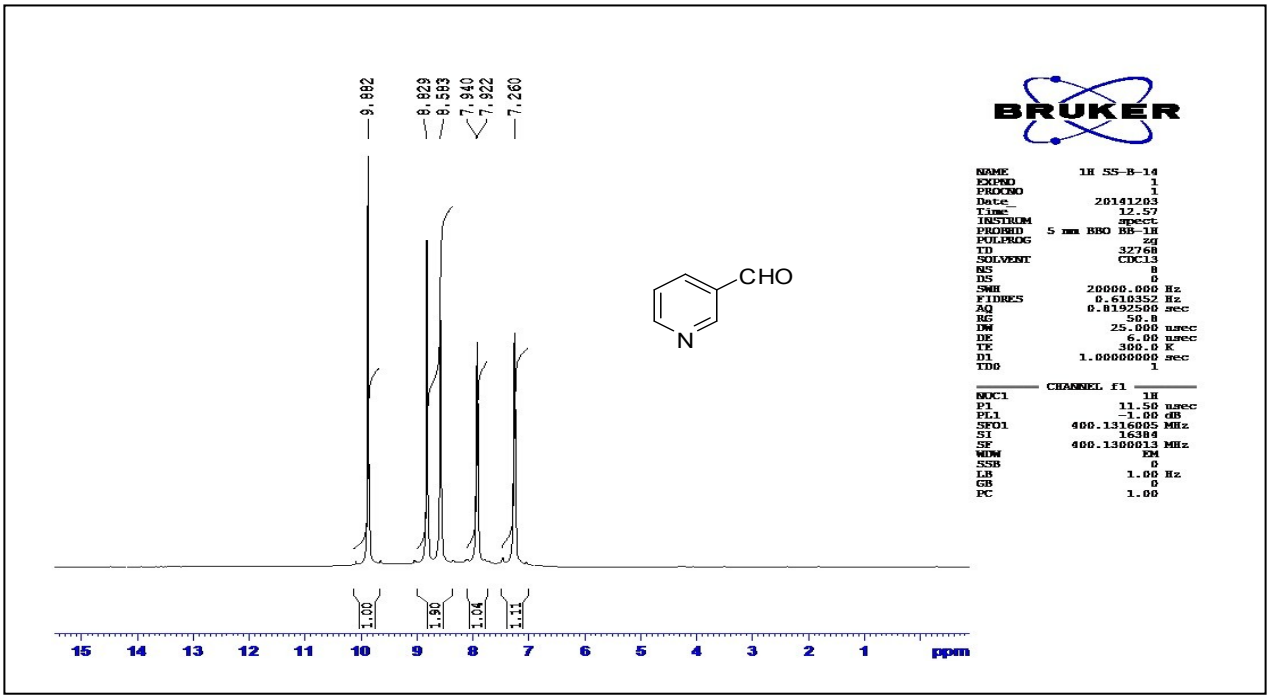
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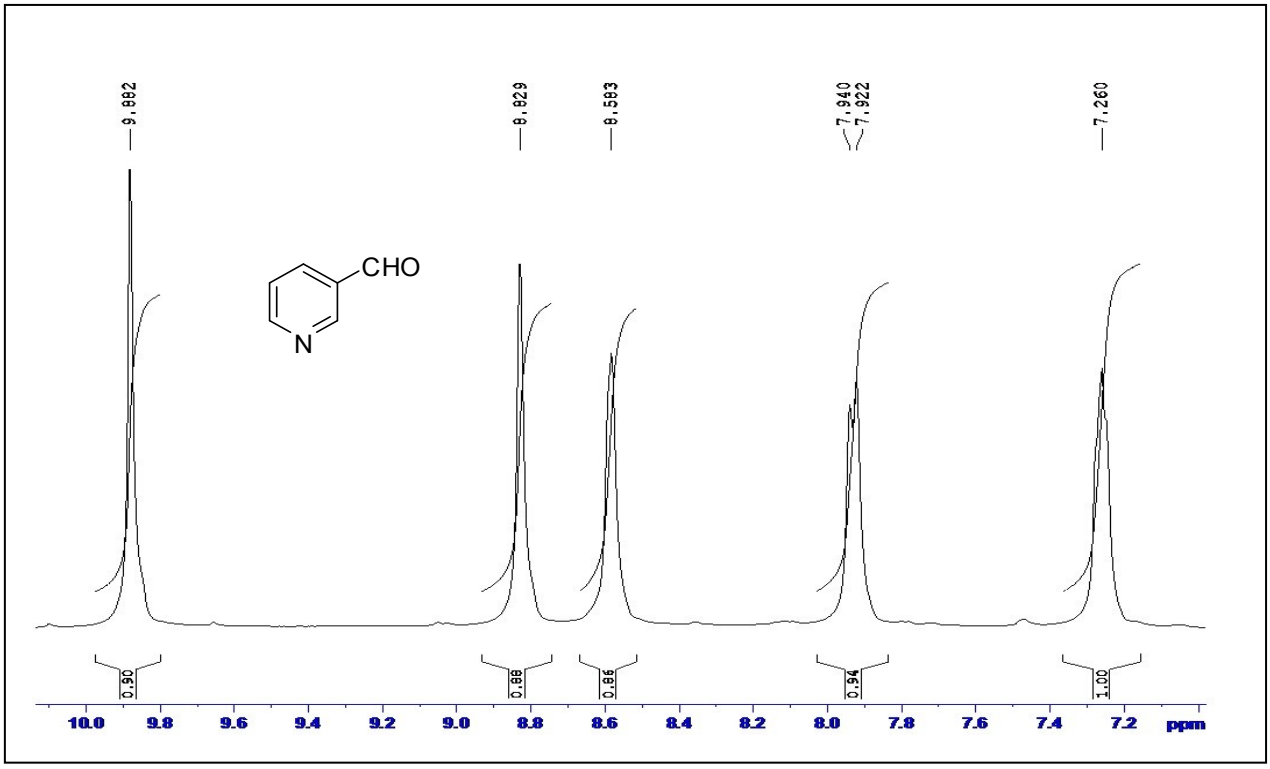
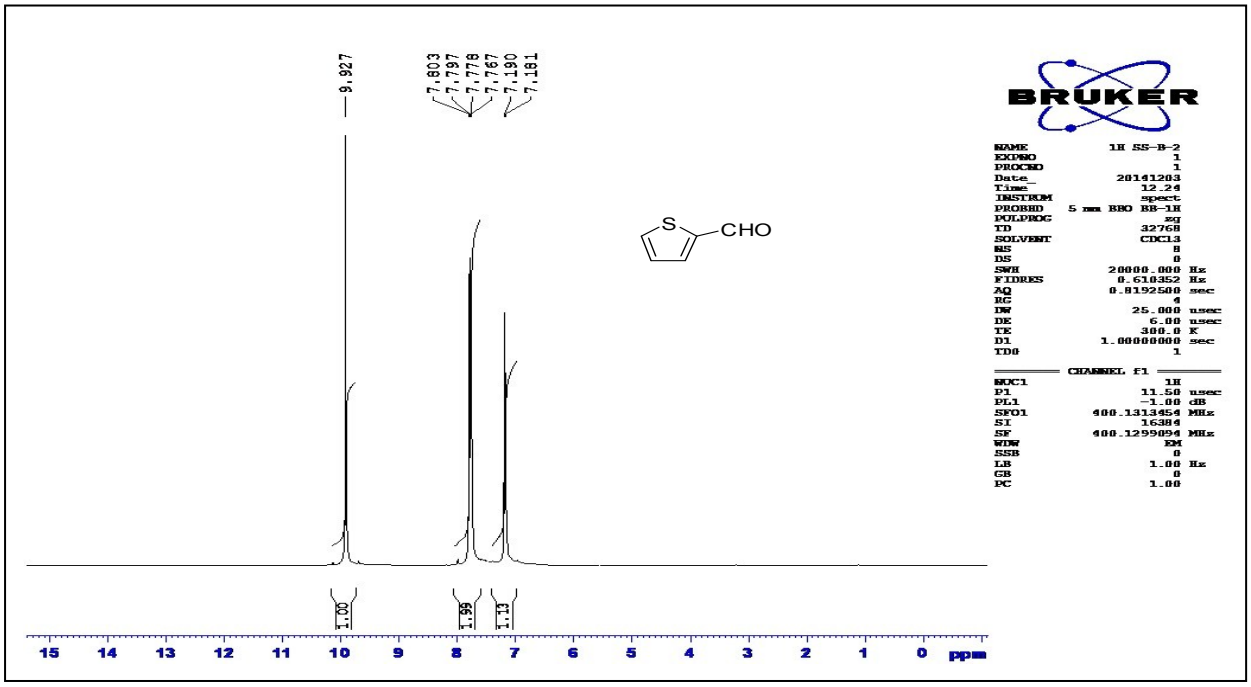
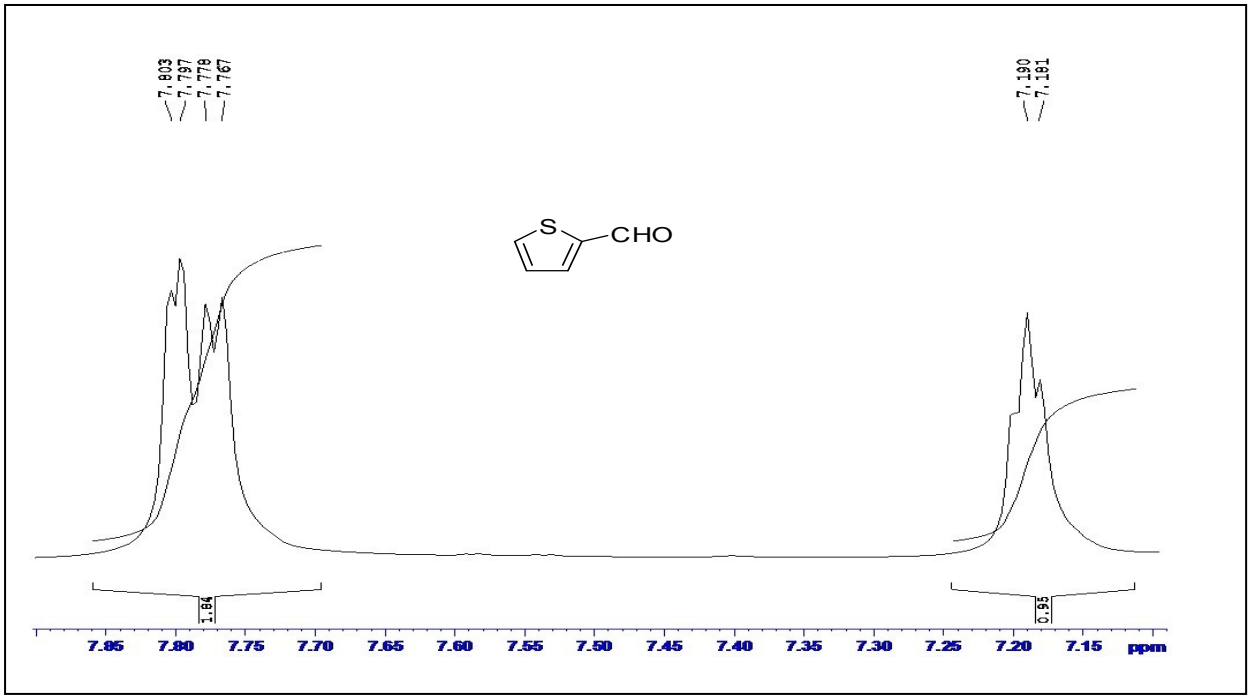
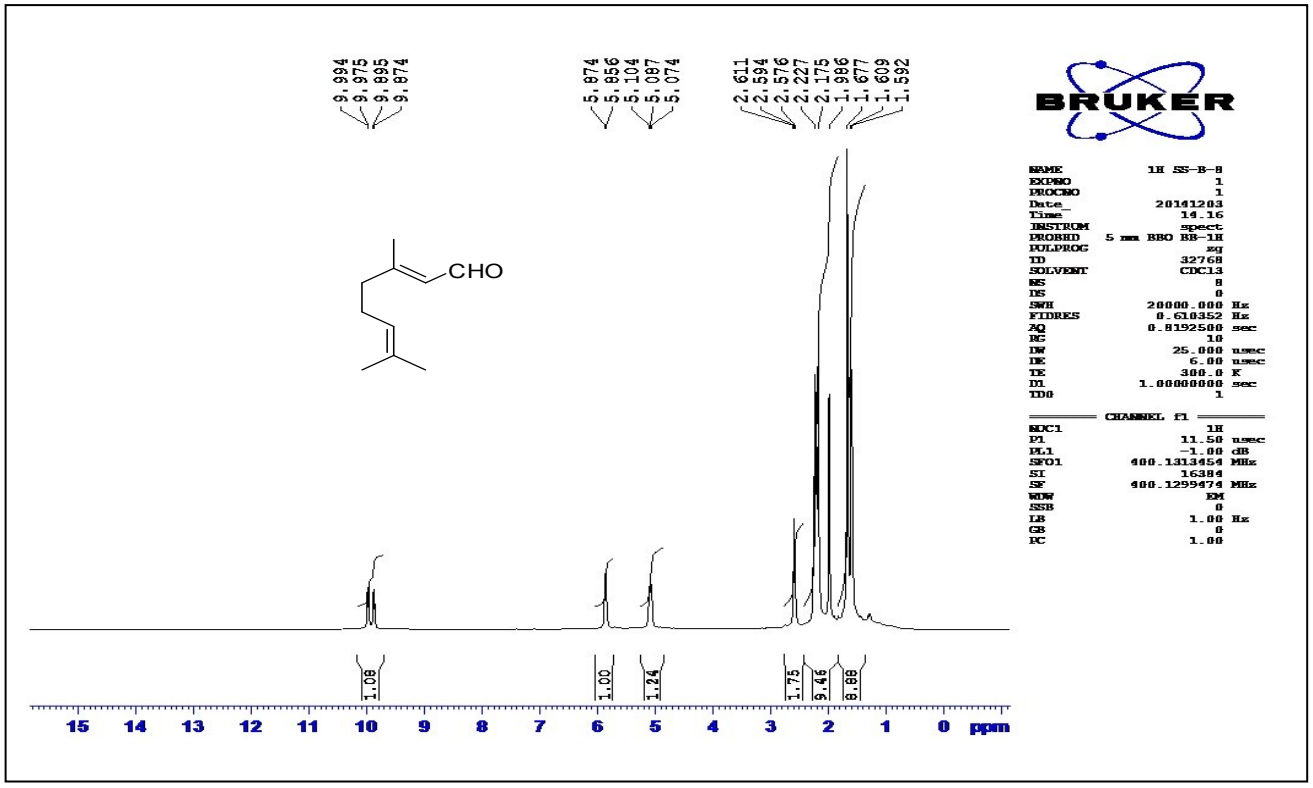
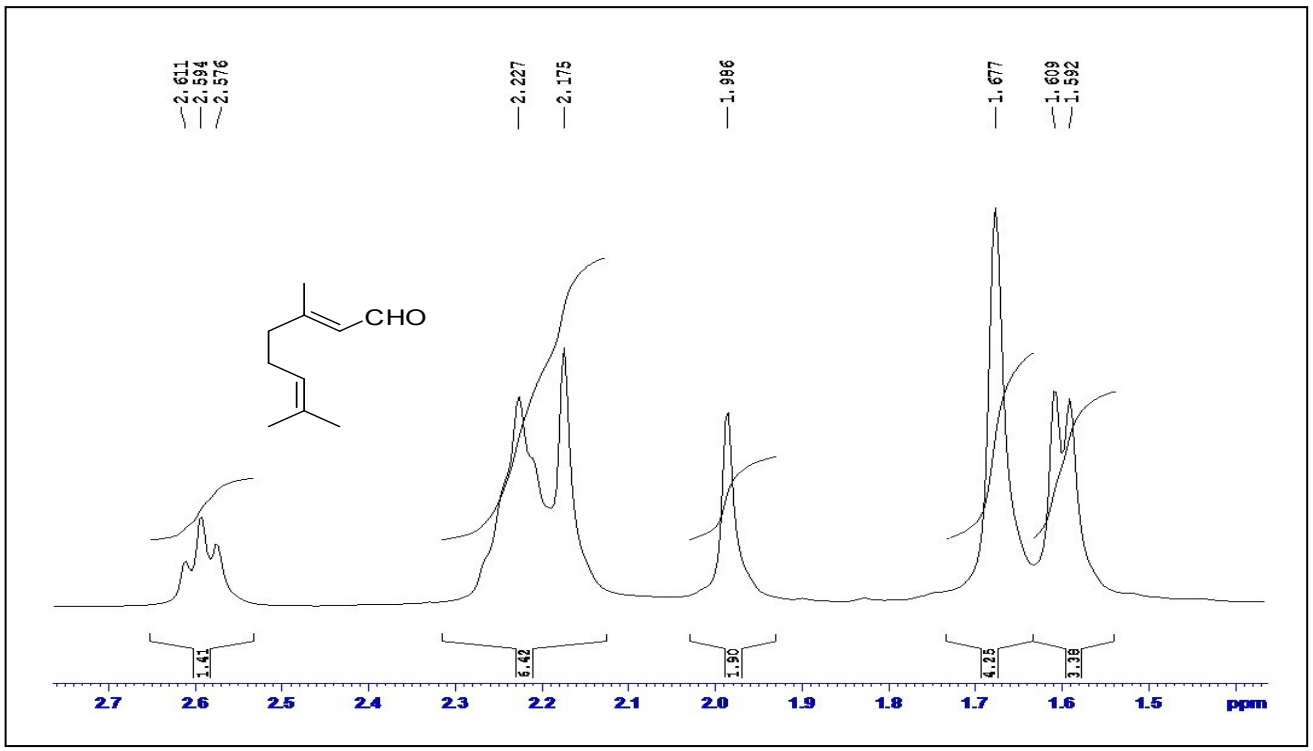
1.00
1.90
1.04
1.11
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
BRUKER
NAME 1H SS-B-14
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 50.8
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1316005 MHz
SI 16384
SF 400.1300013 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

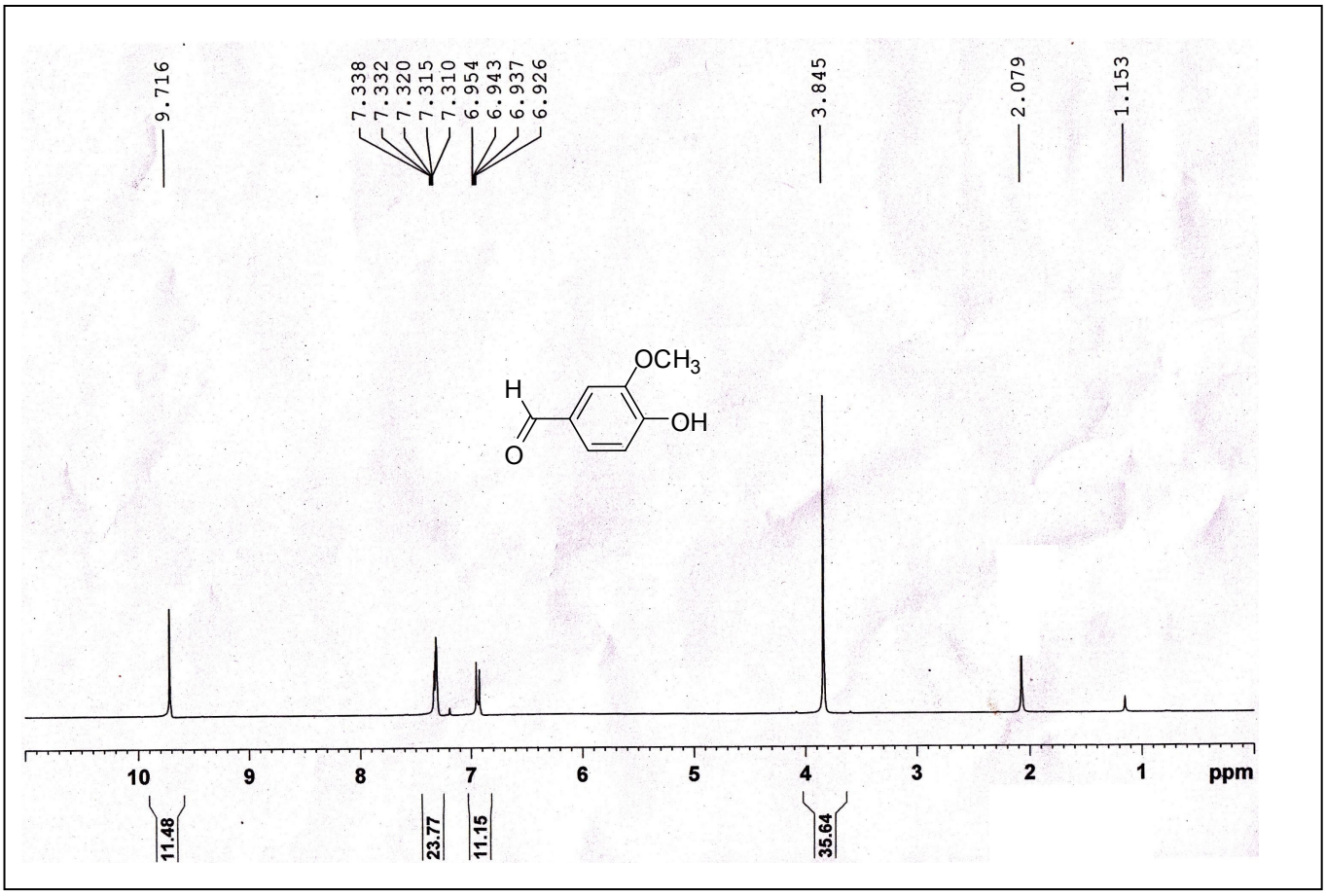

9.882
8.829
8.583
7.940
7.922
7.260
CHO
N
0.90
0.88
0.86
0.94
1.00
10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 ppm

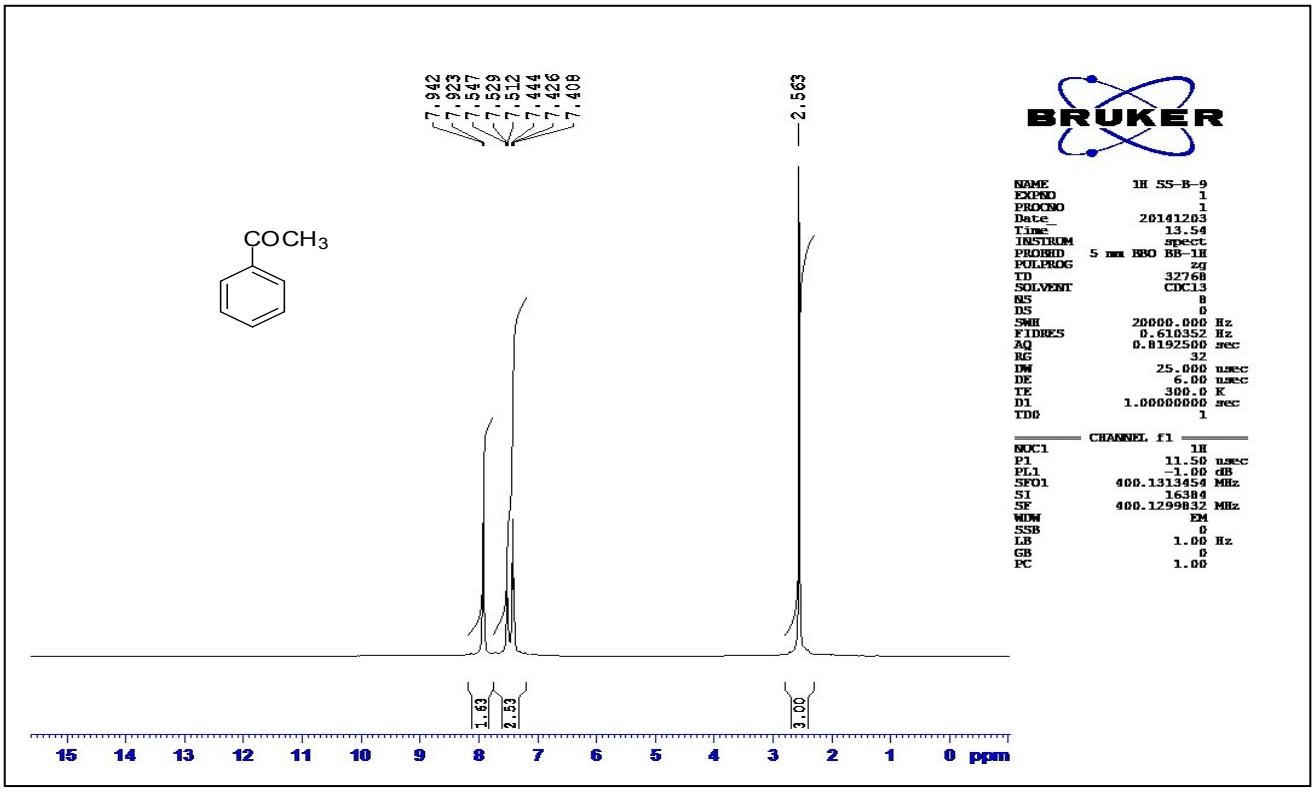

9.927
7.803
7.797
7.778
7.767
7.190
7.181
S
CHO
1.00
1.99
1.13
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
NAME 1H SS-B-2
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 4
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299894 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

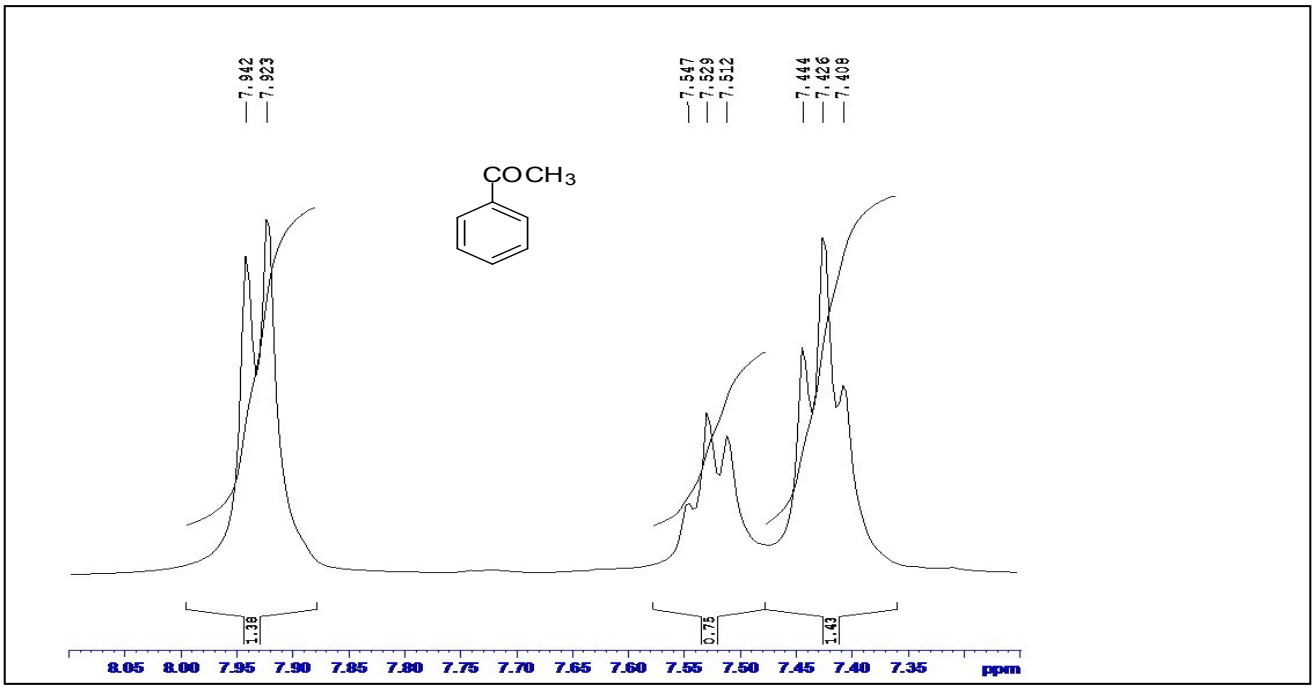

7.803
7.797
7.778
7.767
7.190
7.181
S
CHO
1.84
0.95
7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 ppm

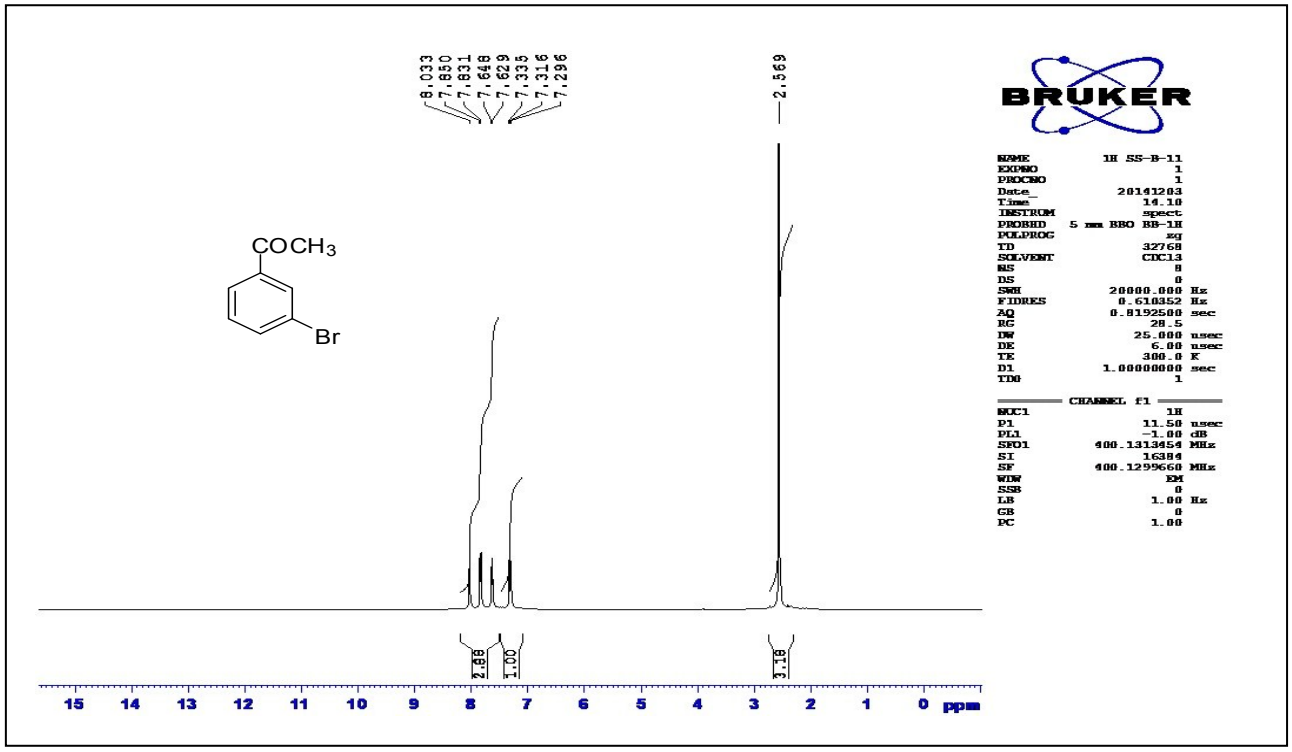

9.994
9.975
9.895
9.874
5.874
5.856
5.104
5.087
5.074
2.611
2.594
2.576
2.227
2.175
1.986
1.677
1.609
1.592
CHO
1.08
1.00
1.24
1.75
9.46
8.88
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
NAME 1H SS-B-8
EXPNO 1
PROCNO 1
Date_ 20141203
Time 14.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 10
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299474 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

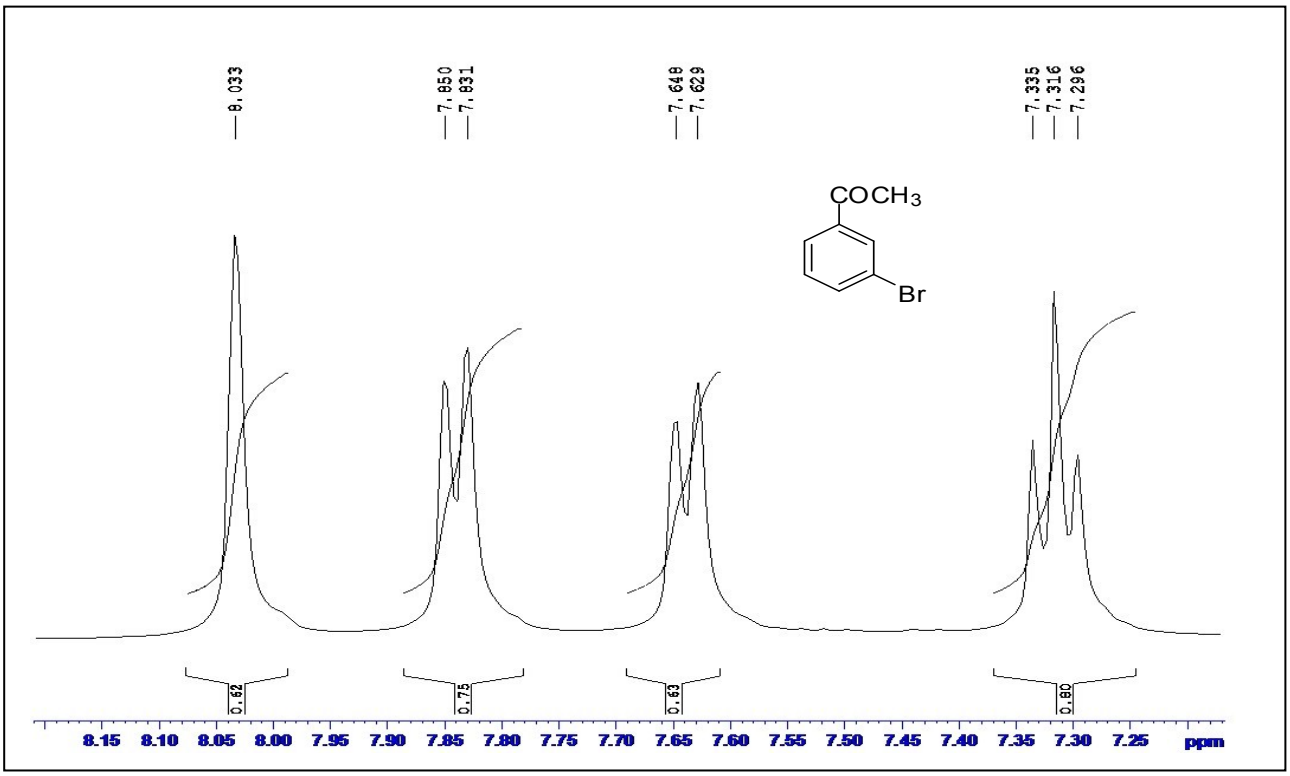

2.611
2.594
2.576
2.227
2.175
1.986
1.677
1.609
1.592
CHO
1.41
6.42
1.90
4.25
3.38
2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 ppm

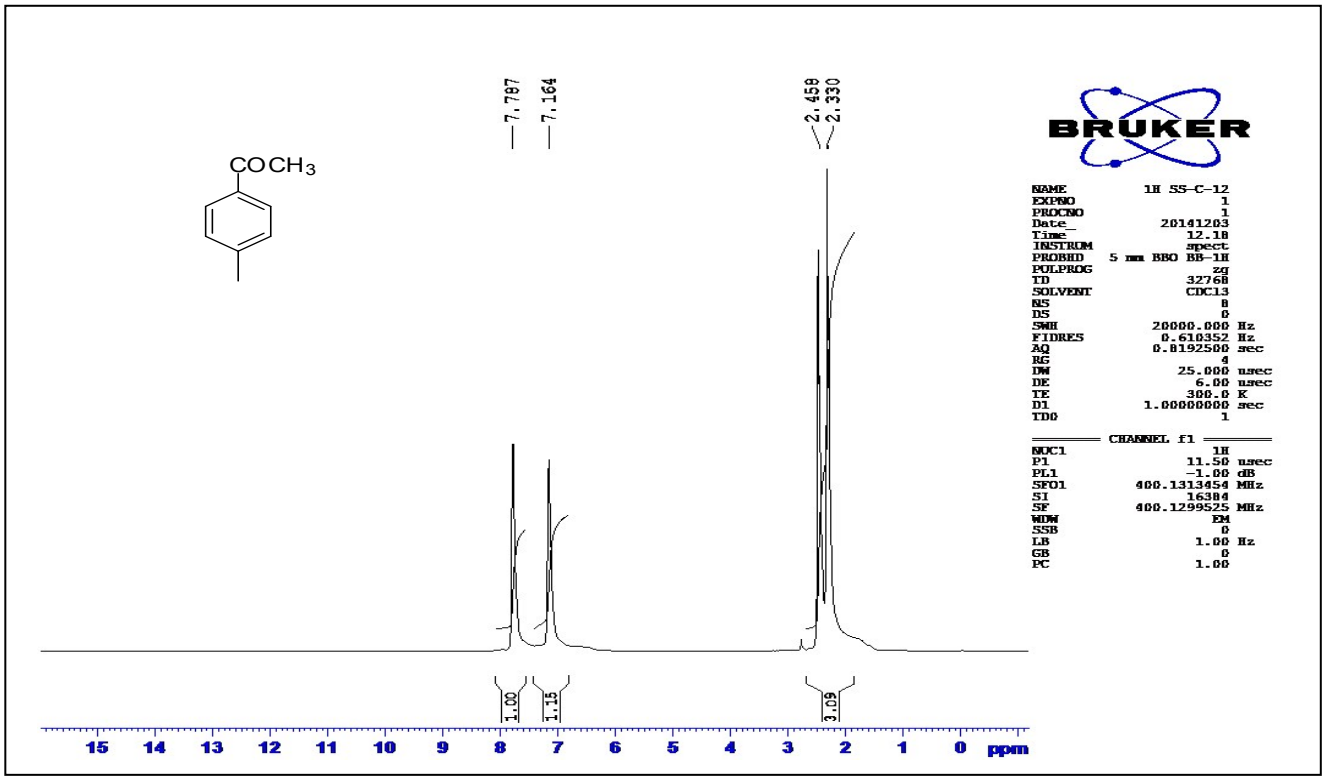

9.716
7.338
7.332
7.320
7.315
7.310
6.954
6.943
6.937
6.926
3.845
2.079
1.153
OCH3
H
O
OH
10
9
8
7
6
5
4
3
2
1
ppm
11.48
23.77
11.15
35.64

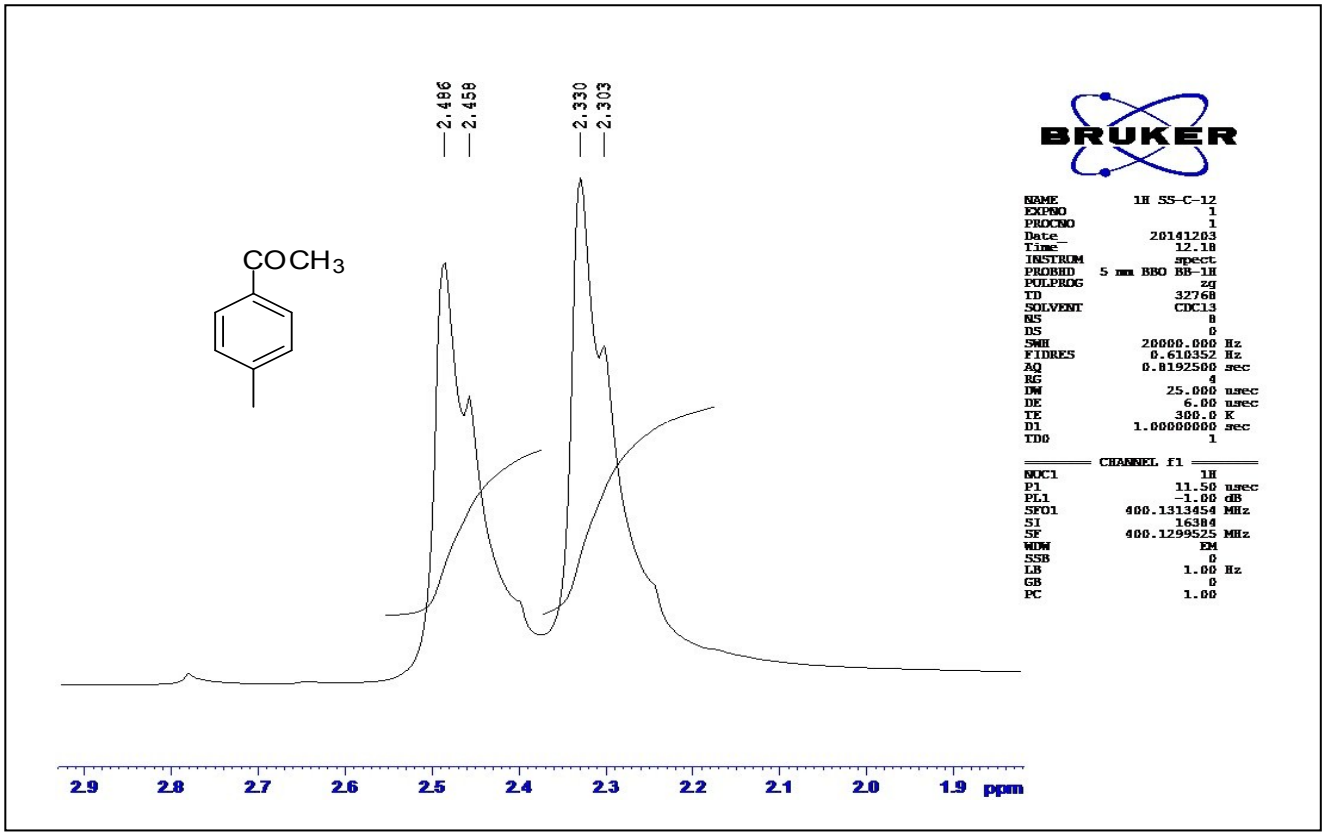

7.942
7.923
7.547
7.529
7.512
7.444
7.426
7.408
2.563
COCH3
BRUKER
NAME 1H SS-B-9
EXPNO 1
PROCNO 1
Date_ 20141203
Time 13.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 32
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299832 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1.63
2.53
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

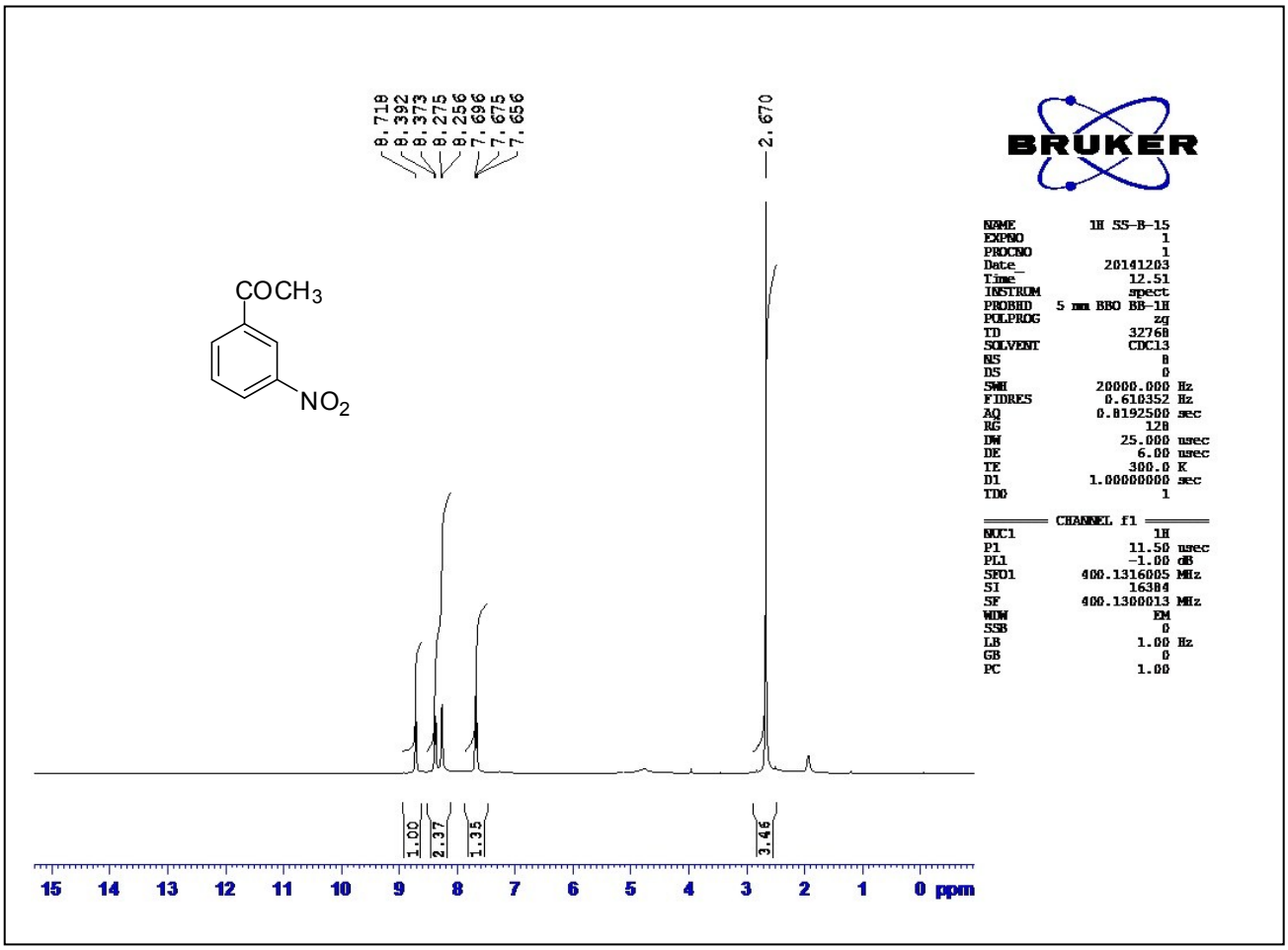

7.942
7.923
7.547
7.529
7.512
7.444
7.426
7.408
COCH3
1.38
0.75
1.43
8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 ppm

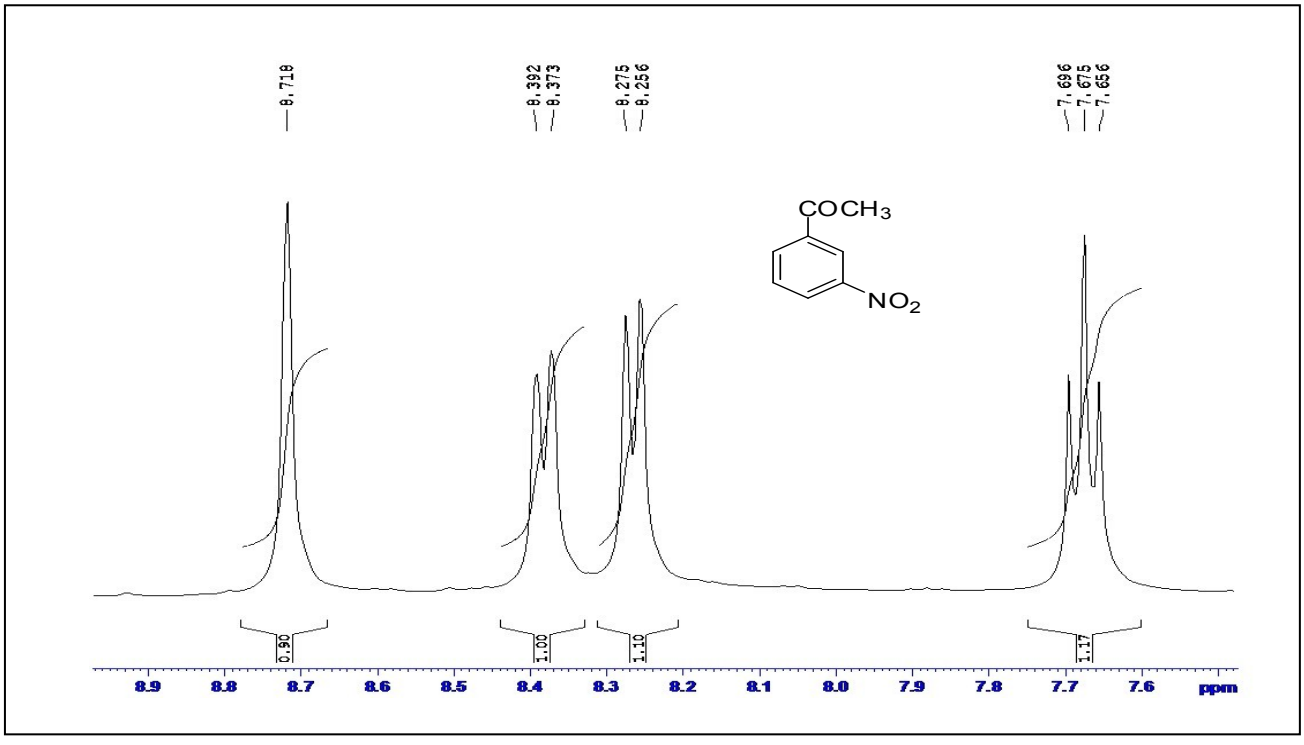

8.033
7.850
7.831
7.648
7.629
7.335
7.316
7.296
2.569
COCH3
Br
BRUKER
NAME 1H SS-B-11
EXPNO 1
PROCNO 1
Date_ 20141203
Time 14.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 28.5
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313854 MHz
SI 16384
SF 400.1299660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
2.88
1.00
3.18
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

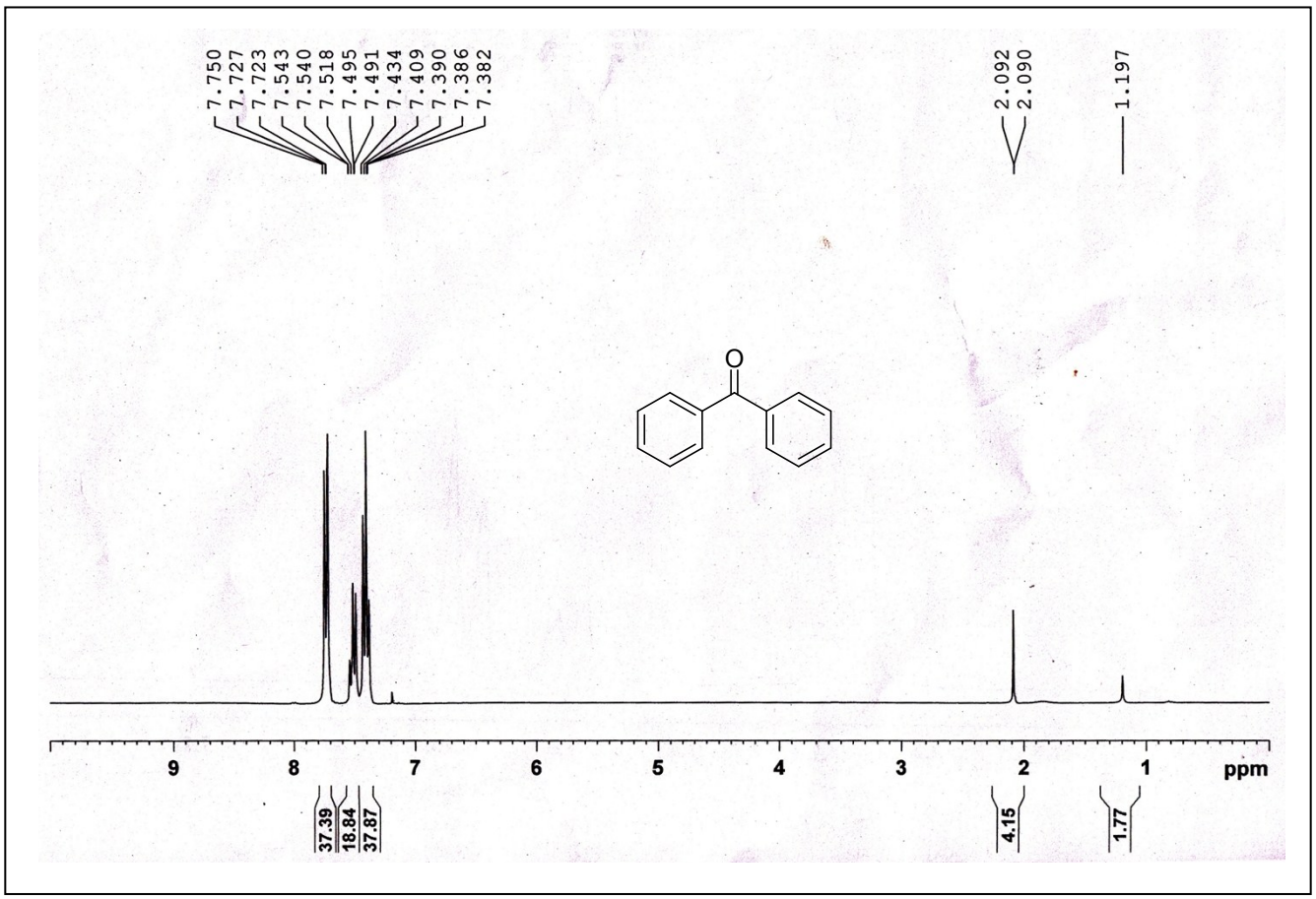

8.033
7.850
7.831
7.648
7.629
7.335
7.316
7.296
COCH3
Br
0.62
0.75
0.63
0.80
8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 ppm

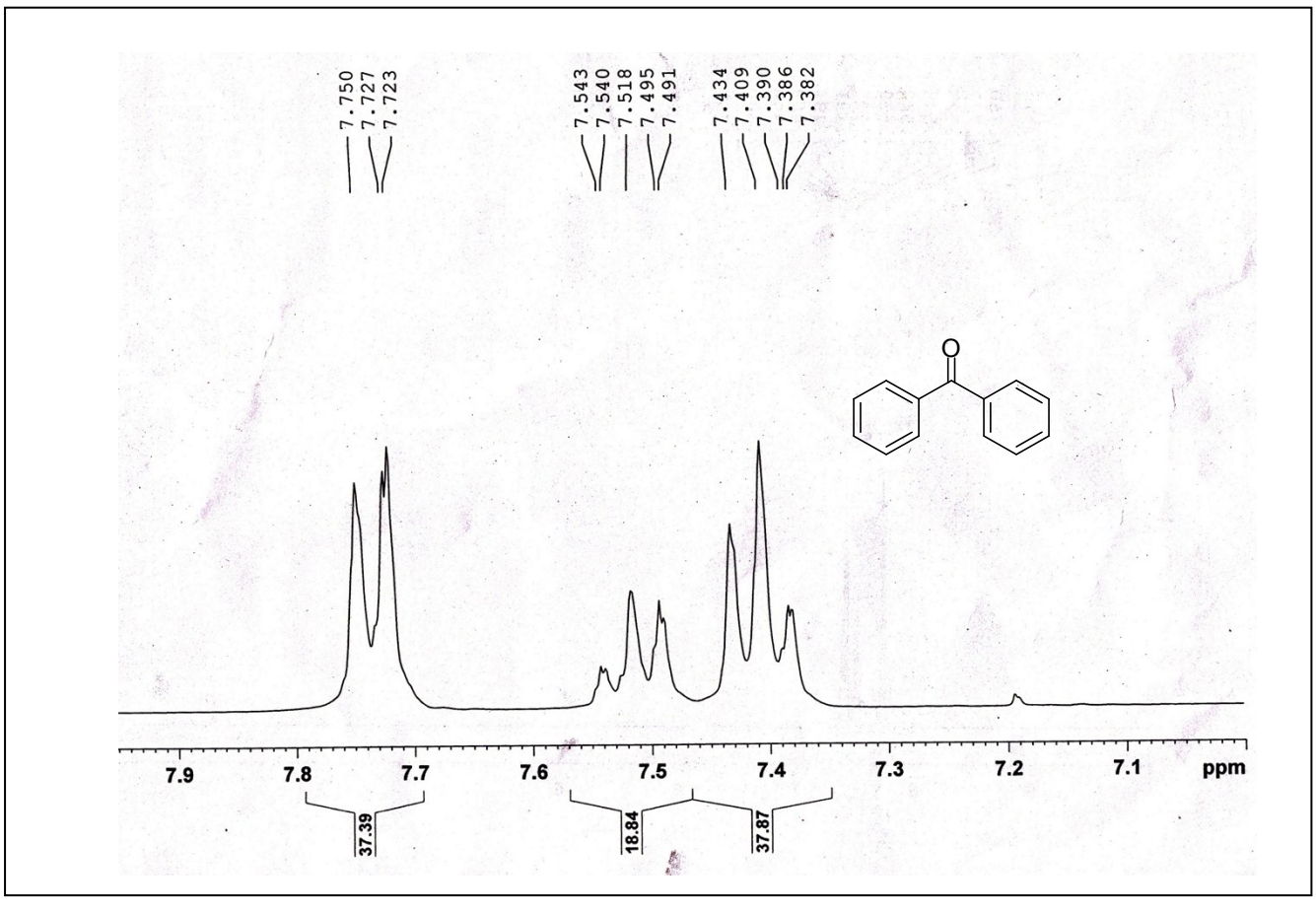

COCH3
7.787
7.164
2.458
2.330
1.00
1.15
3.09
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
NAME 1H SS-C-12
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 4
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299525 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

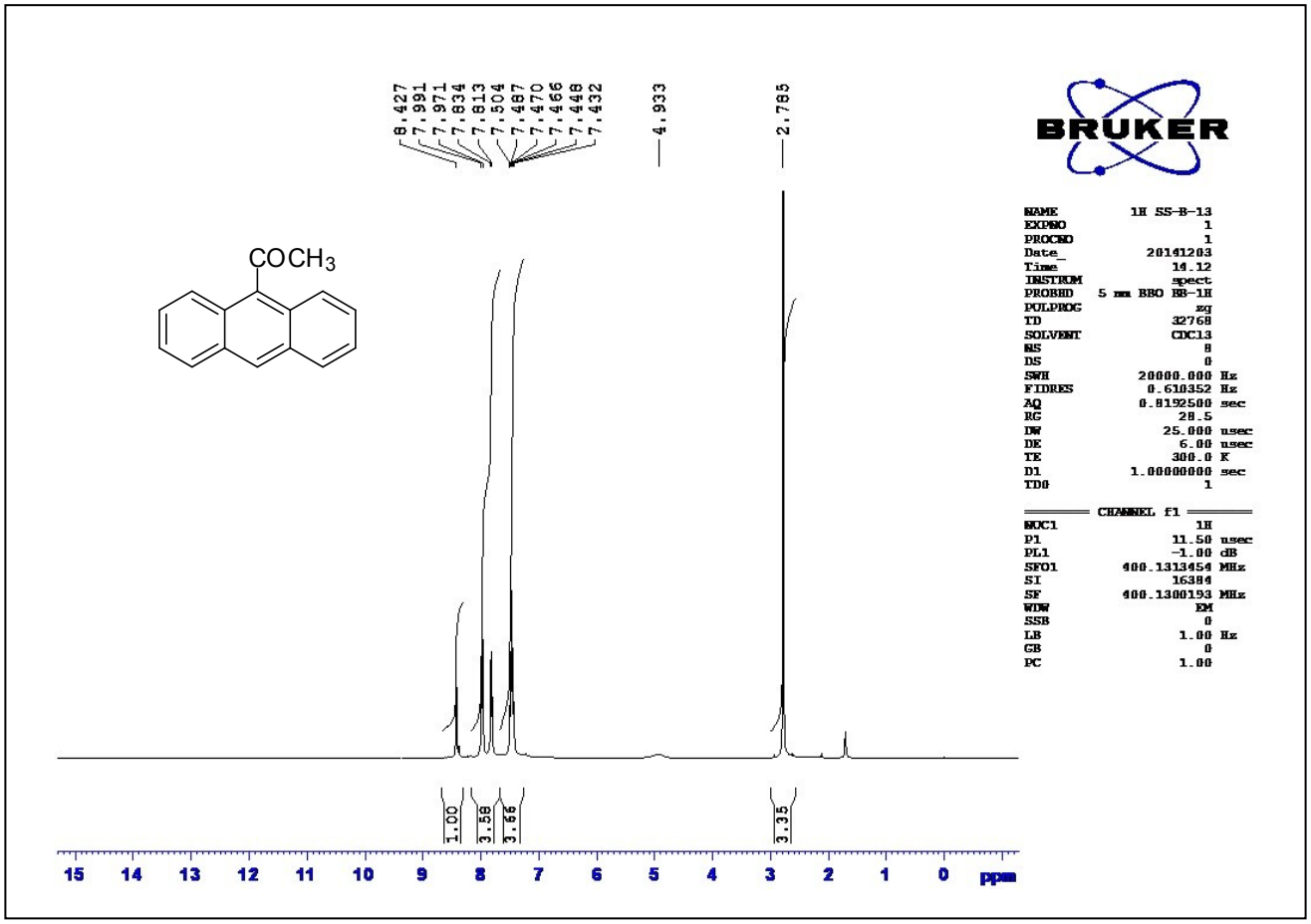

COCH3
2.486
2.458
2.330
2.303
2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 ppm
BRUKER
NAME 1H SS-C-12
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 4
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299525 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

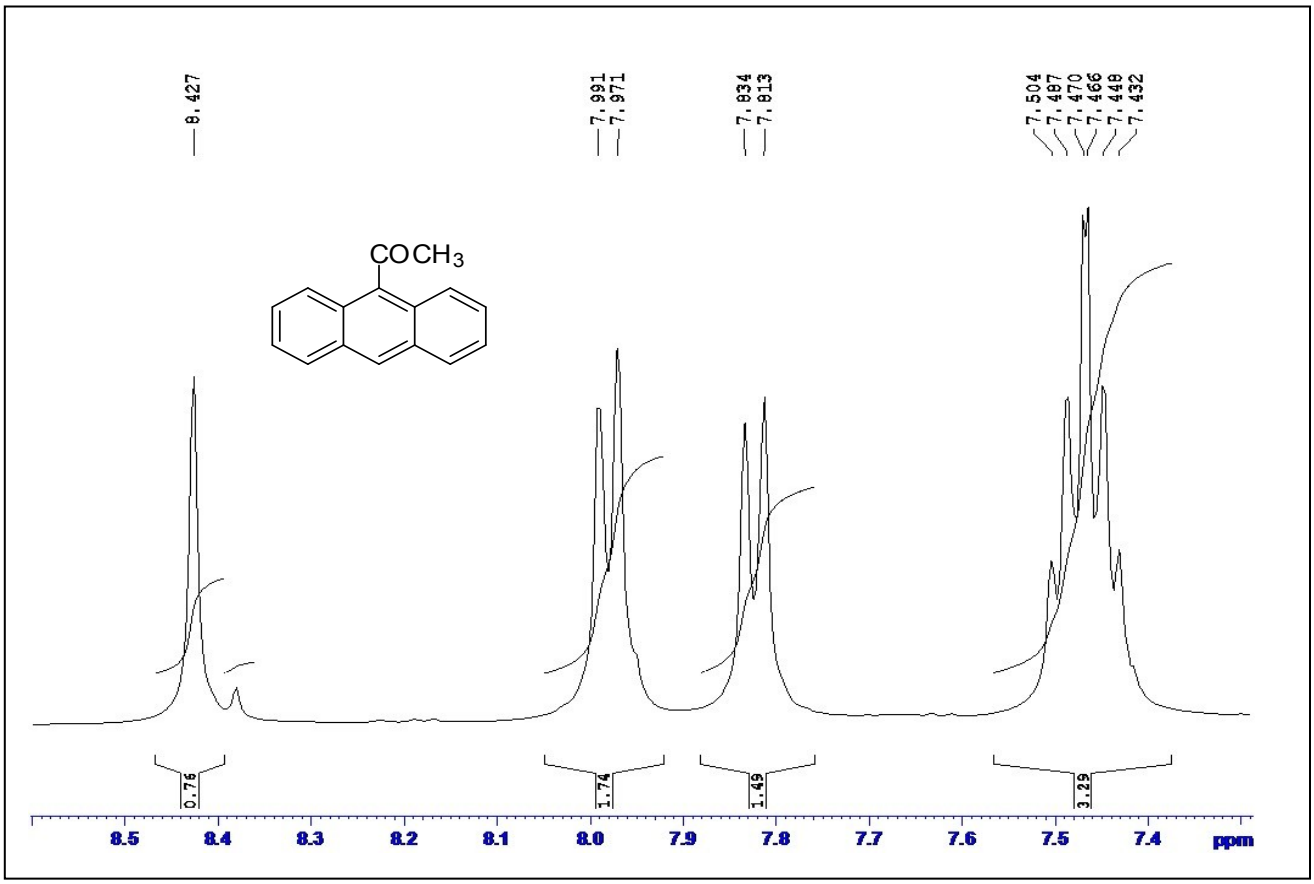

8.718
8.392
8.373
8.275
8.256
7.696
7.675
7.656
2.670
COCH3
NO2
BRUKER
NAME 1H SS-B-15
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 128
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1316005 MHz
SI 16384
SF 400.1300013 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1.00
2.37
1.35
3.46
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

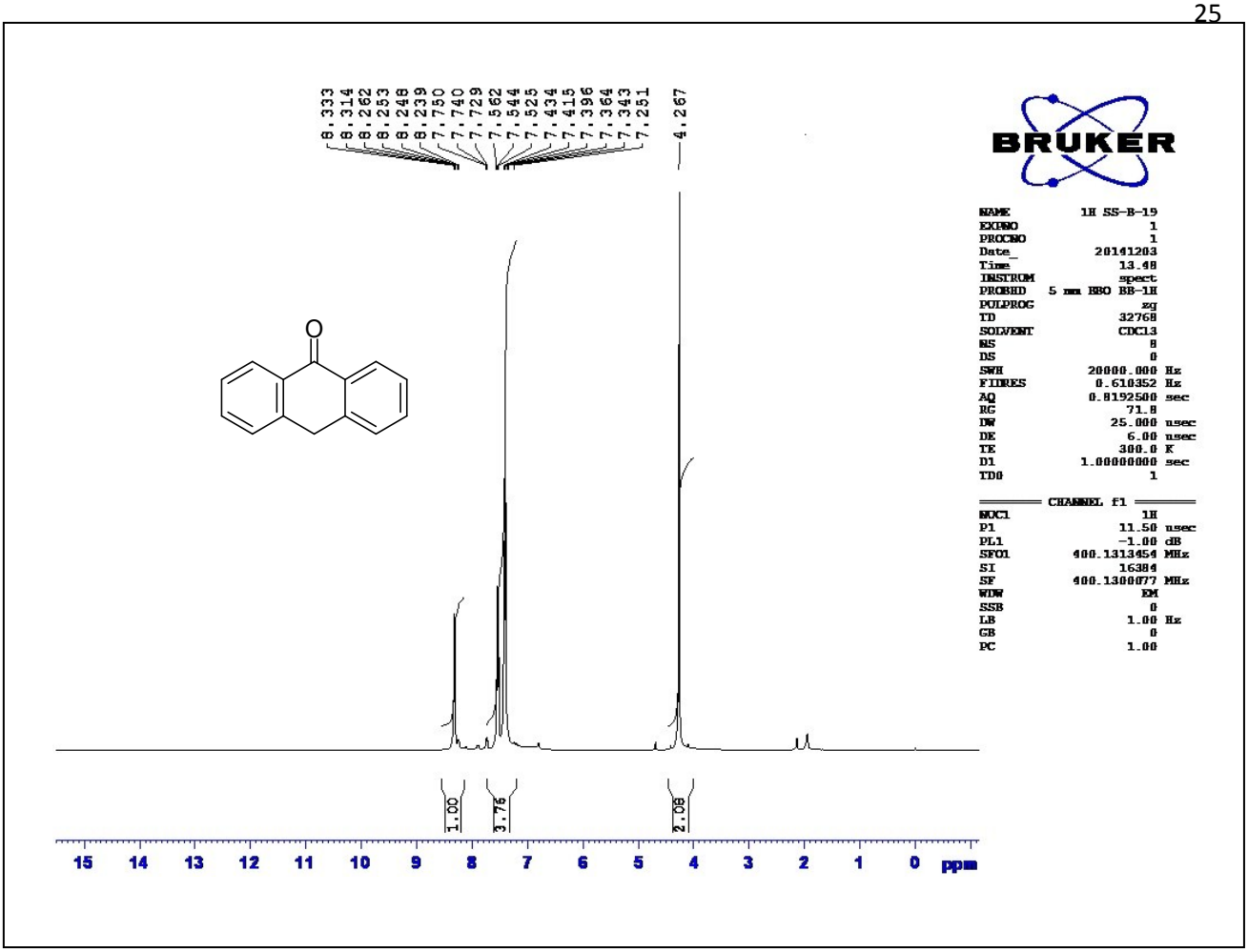

8.718
8.392
8.373
8.275
8.256
7.696
7.675
7.656
COCH3
NO2
0.90
1.00
1.10
1.17
8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 ppm

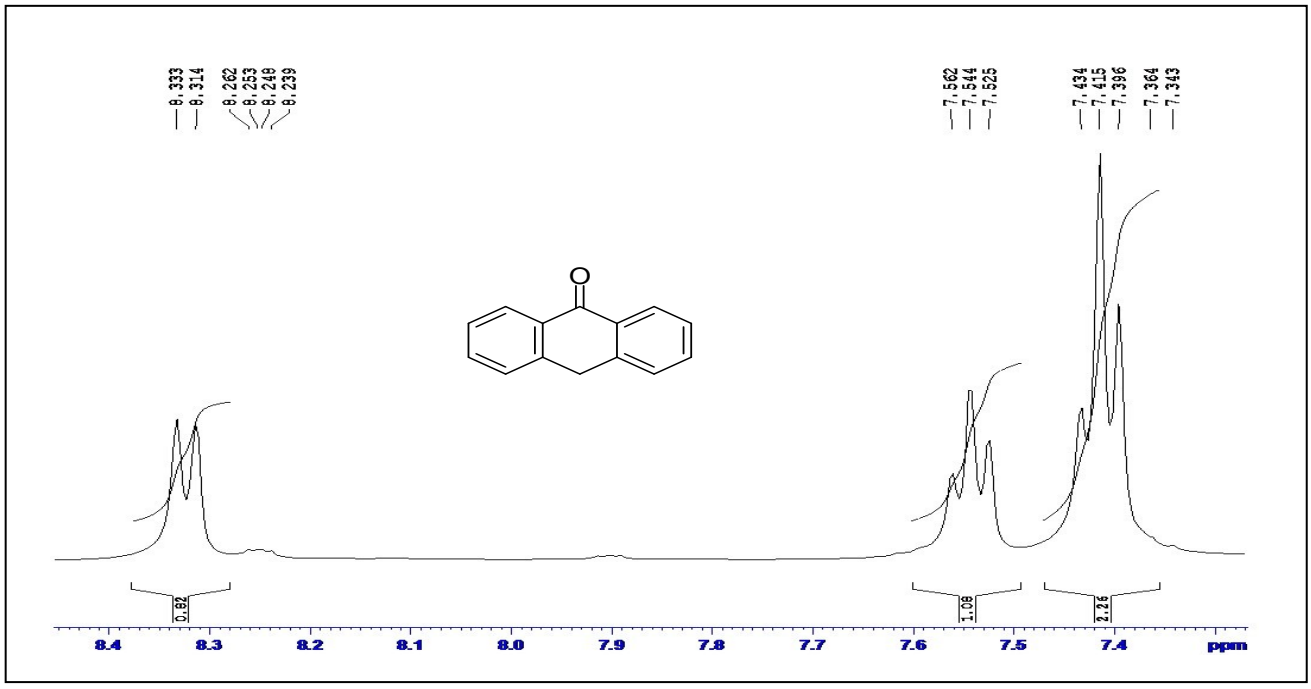

7.750
7.727
7.723
7.543
7.540
7.518
7.495
7.491
7.434
7.409
7.390
7.386
7.382
2.092
2.090
1.197
O
9
8
7
6
5
4
3
2
1
ppm
37.39
18.84
37.87
4.15
1.77

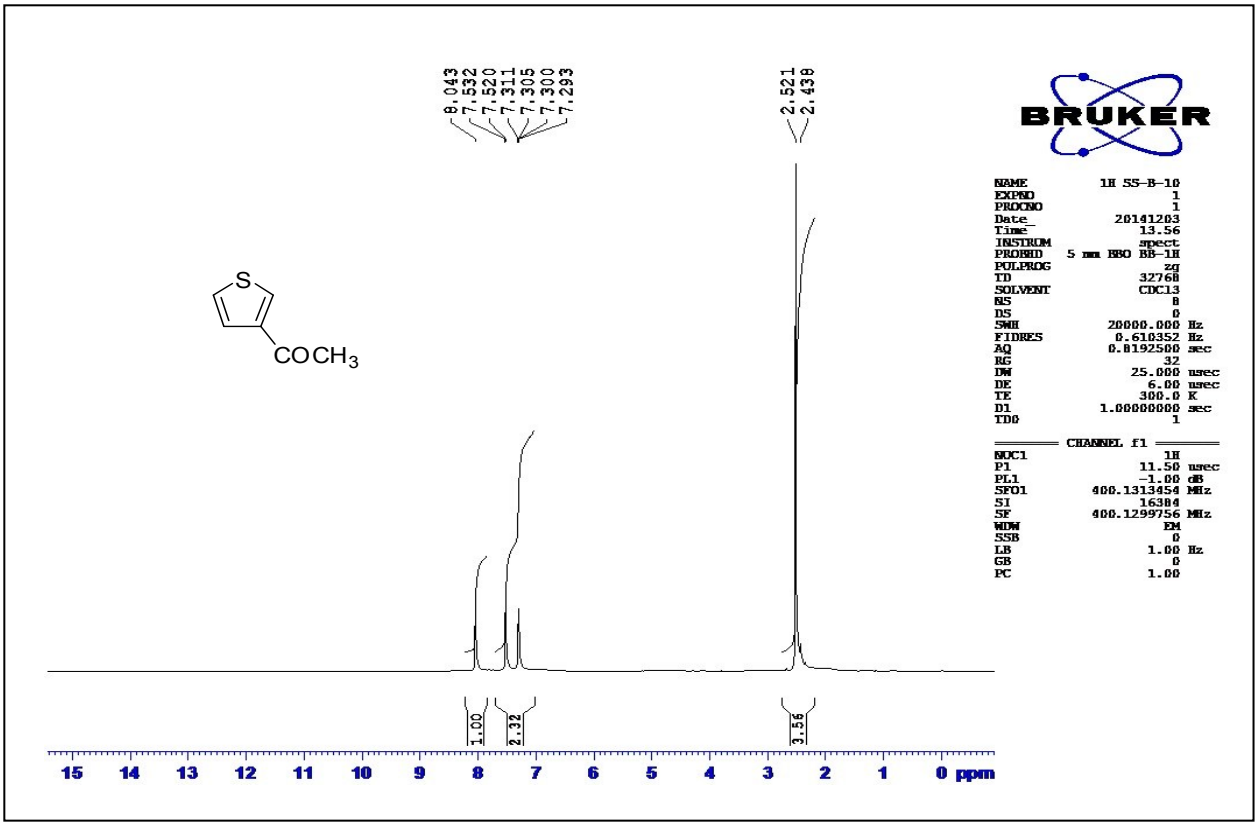

7.750
7.727
7.723
7.543
7.540
7.518
7.495
7.491
7.434
7.409
7.390
7.386
7.382
O
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
37.39
18.84
37.87

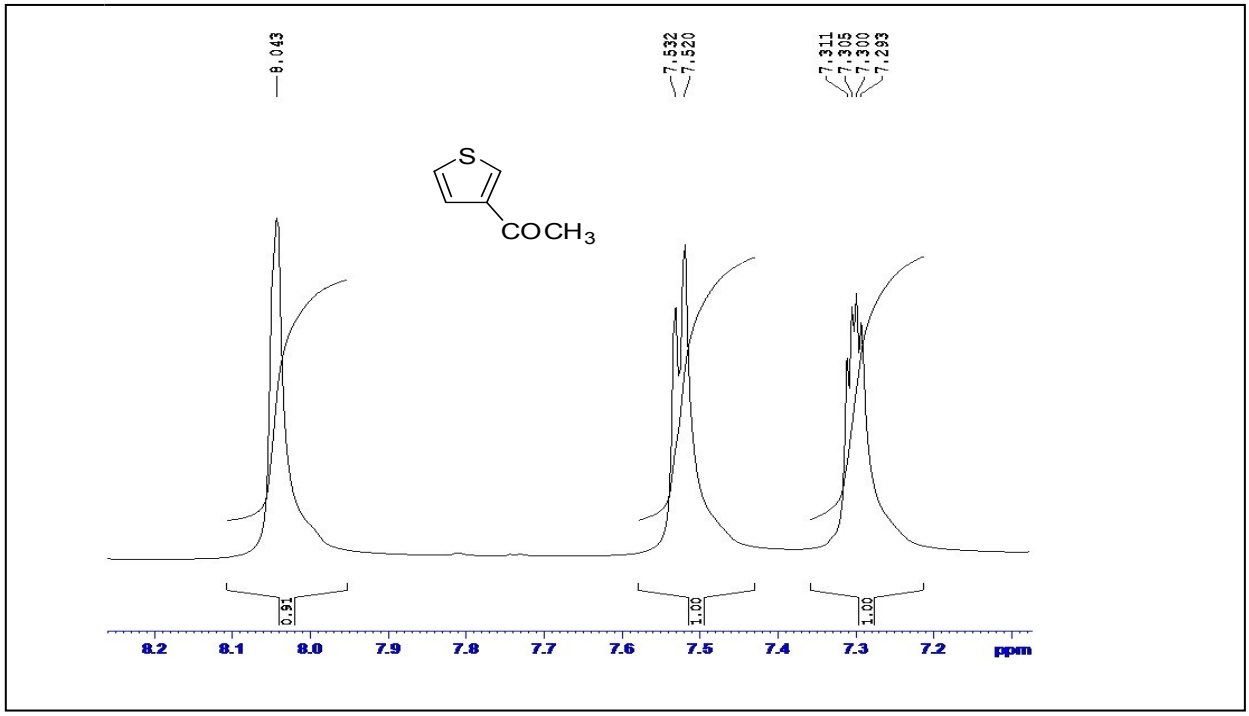

8.427
7.991
7.971
7.834
7.813
7.504
7.487
7.470
7.466
7.448
7.432
4.933
2.785
COCH3
BRUKER
NAME 1H SS-B-13
EXPNO 1
PROCNO 1
Date_ 20141203
Time 14.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 28.5
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1300193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1.00
3.58
3.66
3.35
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

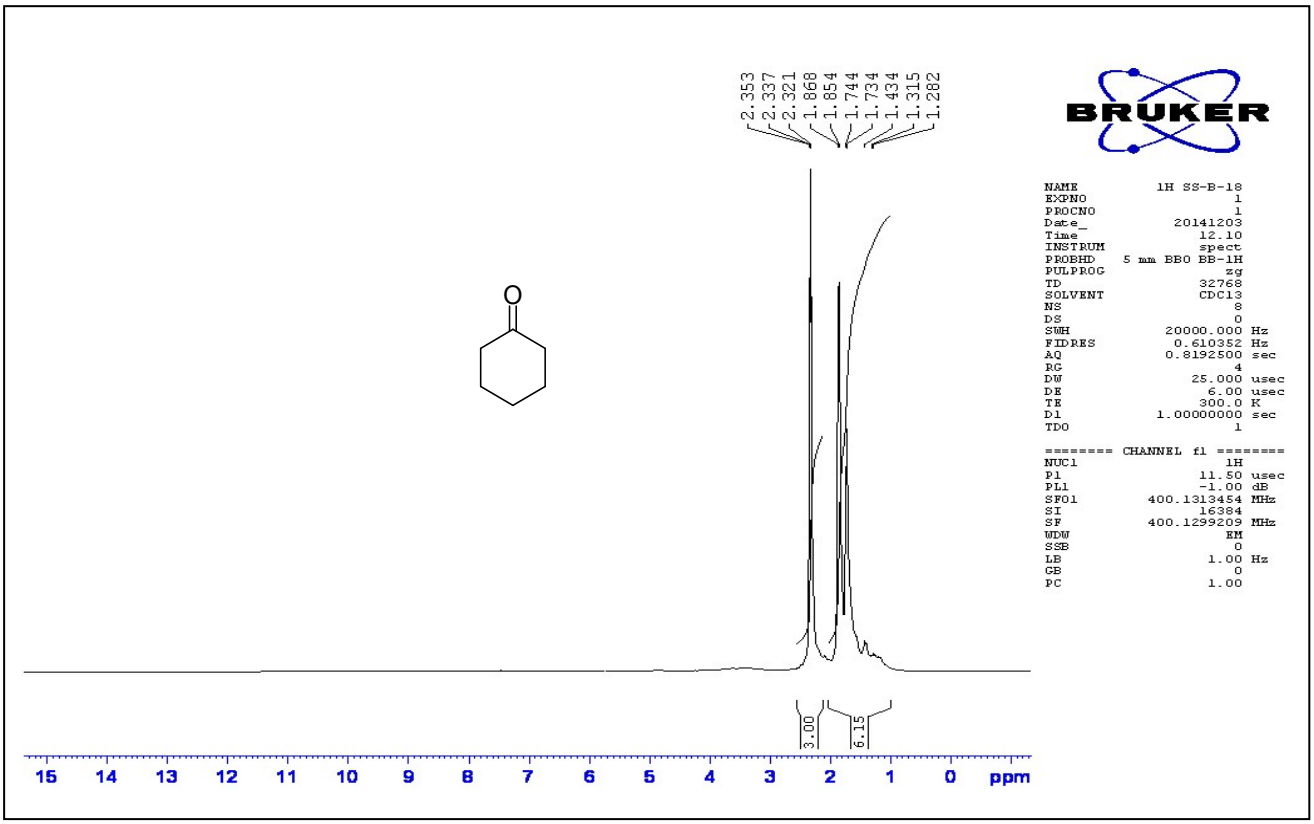

8.427
7.991
7.971
7.834
7.813
7.504
7.487
7.470
7.466
7.448
7.432
COCH3
0.76
1.74
1.49
3.29
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm

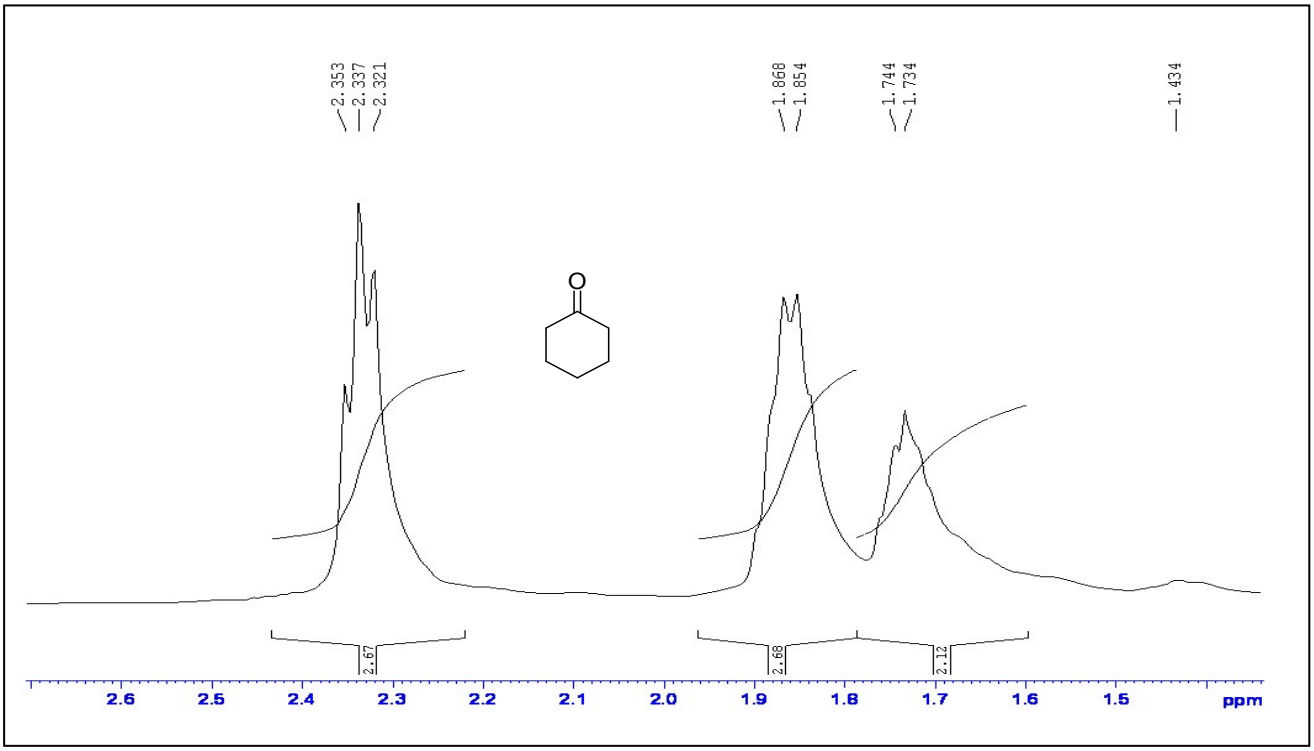

8.333
8.314
8.262
8.253
8.248
8.239
7.750
7.740
7.729
7.562
7.544
7.525
7.434
7.415
7.396
7.364
7.343
7.251
4.267
O
1.00
3.76
2.08
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
NAME 1H SS-B-19
EXPNO 1
PROCNO 1
Date_ 20141203
Time 13.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 71.8
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


8.333
8.314
8.262
8.253
8.248
8.239
7.562
7.544
7.525
7.434
7.415
7.396
7.364
7.343
O
0.92
1.08
2.26
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm


8.043
7.532
7.520
7.311
7.305
7.300
7.293
2.521
2.438
S
COCH3
BRUKER
NAME 1H SS-B-10
EXPNO 1
PROCNO 1
Date_ 20141203
Time 13.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 32
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299756 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1.00
2.32
3.56
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm


8.043
7.532
7.520
7.311
7.305
7.300
7.293
S
COCH3
0.91
1.00
1.00
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm


2.353
2.337
2.321
1.868
1.854
1.744
1.734
1.434
1.315
1.282
O
3.00
6.15
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
NAME 1H SS-B-18
EXPNO 1
PROCNO 1
Date_ 20141203
Time 12.10
INSTRUM spect
PROBHD 5 mm BB0 BB-1H
PULPROG sg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 4
DW 25.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
SFO1 400.1313454 MHz
SI 16384
SF 400.1299209 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


2.353
2.337
2.321
1.868
1.854
1.744
1.734
1.434
O
2.67
2.68
2.12
2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 ppm