Supplementary Information

N-Propyl Benzoguanamine Sulfonic acid supported on magnetic Fe_3O_4 nanoparticles: A novel and efficient magnetically heterogeneous catalyst for the synthesis of 1, 8-dioxo-decahydroacridine derivatives

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General experimental procedure:

All chemicals were purchased from Merck or Fluka and were used without further purification. The melting points were uncorrected and measured using capillary tubes on an electrothermal digital apparatus. IR spectra were recorded on a Shimadzo (FT)-IR 300 spectrophotometer in KBr. ^{1}H-NMR 500 MHz and ^{13}C-NMR spectra were obtained on Brucker 125 MHz spectrometers in $CDCl_3$ or DMSO-d_6 as the solvent with TMS as an internal standard. The progress of the reaction was monitored by TLC (thin-layer chromatography) using n–hexane/EtOAc as an eluent. Nanoparticles were characterized using a X-Pert Pro MPD X-ray diffraction (XRD) diffractometer (Cu-K_α, k = 0.154056 nm) over the range 2θ = 10–80 using 0.04^0 as the step length. The scanning electron microscope measurement was carried out on a Hitachi S-4700 field emission-scanning electron microscope (FE-SEM). TEM analysis of the catalyst was recorded using Zeiss-EM10C transmission electron microscope.The thermogravimetric analysis (TGA) curves were recorded using Diamond TGA/DTA SII Perkin Elmer Company. The magnetization was measured at room temperature using a vibrating sample magnetometer (Model 7300 VSM system, Lake Shore Cryotronic, Inc., Westerville, OH, USA). Incuctively coupled mass spectroscopy (ICP-MS) was also done in order to confirm the iron loading ICP-MS (Model Elan 6000 DRC). The iron content in the catalyst supernatant was estimated by atomic absorption spectroscopy (AAS) on a Model novAA-400p atomic absorption spectrometer.

General procedure for preparation of MNPs-N-Propyl-Benzoguanamine-SO_3H

Fe_3O_4 MNPs were prepared by chemical co-precipitation of Fe^{3+} and Fe^{2+} ions as described in the literature. The Fe_3O_4 coated with SiO_2 was prepared through a modified sol–gel method.

Chloropropyl-modified silica-coated MNPs were prepared according to a reported procedure. To a magnetically stirred mixture of the prepared Fe_3O_4/SiO_2-Chloropropyl (1 g) was added benzoguanamine (10 mmol, 1.87 g) and triethylamine (10 mmol, 1.39 ml) in dried toluene (50 mL) and the mixture was sonicated for 2 h under N_2 atmosphere, then stirred for 48 h under reflux conditions. The obtained solid was magnetically collected from the solution and washed with water/ethanol (20:10 mL) for three times and dried in vacuum for 5 h. To a mixture of benzoguanamine-modified silica-coated Fe_3O_4 MNPs (1 g) in dried $CHCl_3$ (3 mL), chlorosulfonic acid ($ClSO_3H$, 1 mL) was added dropwise at 0 ^{0}C over 2 h and then the mixture was filtered and washed with ethanol (5 mL) and dried at room temperature to afford the title compound.

General procedure for synthesis of 1, 8-dioxo-decahydroacridin derivatives

To a mixture of dimedone (2 mmol), aromatic benzaldehyde (1 mmol) and ammonium acetate or aniline (1.2 mmol) was added MNPs-N-Propyl-Benzoguanamine-SO_3H (6 mg) in 2 mL aqueous ethanol [V (ethanol): V (H_2O) = 3 : 1] as the solvent and the reaction mixture stirred magnetically under reflux (100 ^{0}C) conditions. The progress of the reaction was followed by thin layer chromatography (TLC). After the completion of the reaction, mixture was added 0.5 mL water and stirred for a moment. Then, the reaction mixture was cooled to room temperature and the catalyst was easily separated by an external magnet. The solvent was evaporated to afford the crude solid. Finally, the resulting solid was filtered, then washed with 30% aqueous ethanol without further purification and dried in an oven at 60 °C. The pure 1, 8-dioxo-decahydroacridin derivatives were obtained in excellent yields.

Spectral data for selected of 1, 8-dioxo-decahydroacridin derivatives:

3,3,6,6-tetramethyl-9-phenyl-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 1, Table 2): White solid; m.p: 288–290 ^{0}C; Yield 93%; IR (KBr, cm^{-1}) v_{max}; 1591 (C=O), 2879-2961 (CH_3 str.), 3068 (NH); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ ppm:1.11 (s, 6H, $2CH_3$), 1.24 (s, 6H, $2CH_3$), 2.30-2.49 (m, 8H, $4CH_2$), 7.10-7.29 (m, 5H, Ar-H), 11.91 (s,1H, NH); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ ppm: 27.4, 29.6, 31.4, 32.7, 46.4, 47.0, 115.6, 125.8, 126.7, 128.2, 138.0, 189.4, 190.5.

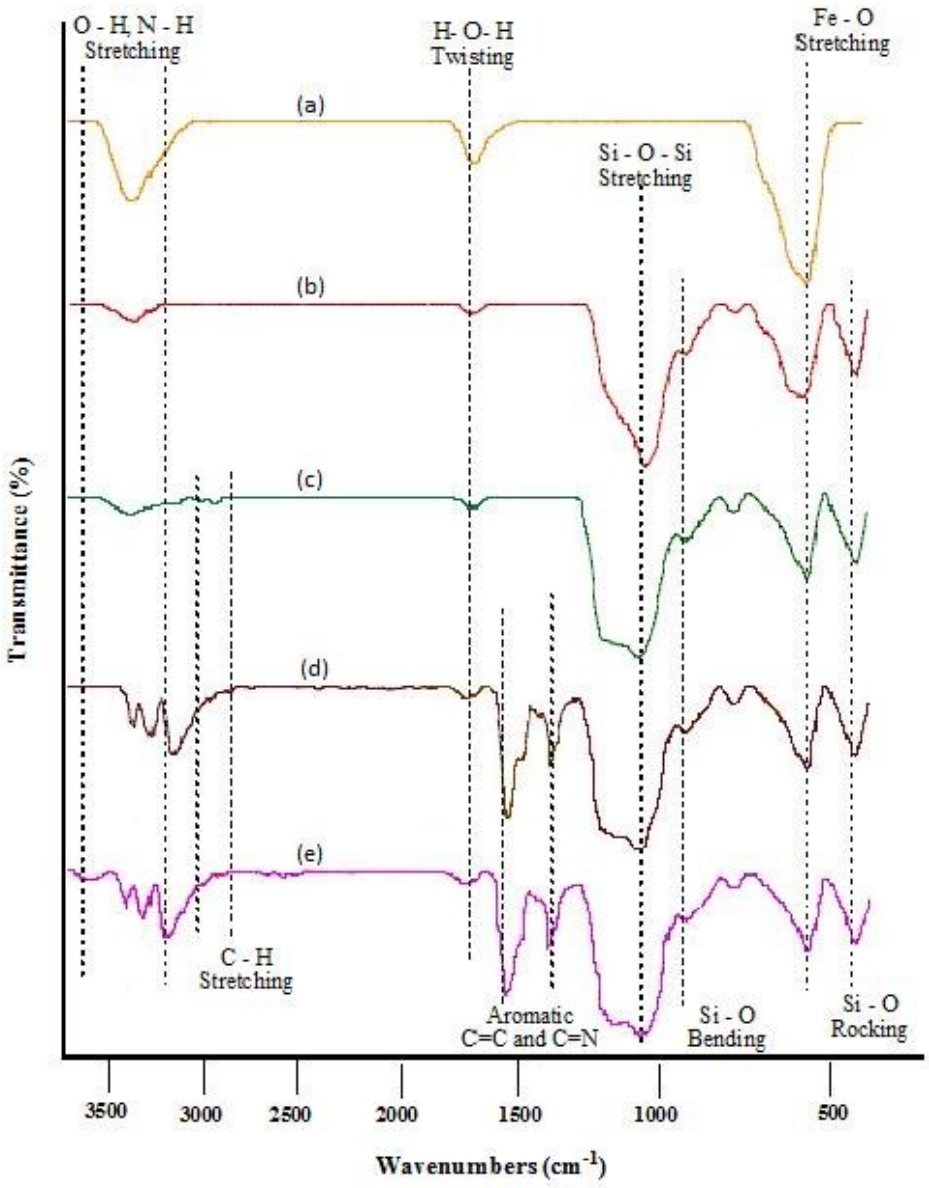
3,3,6,6-tetramethyl-9-(p-tolyl)-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 2, Table 2): White solid; m.p: 279–281 ^{0}C; Yield 85%; IR (KBr, cm^{-1}) v_{max}; 1596 (C=O), 2878-2961 (CH_3 str.), 3021 (NH); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ ppm: 1.11 (s, 6H, $2CH_3$), 1.24 (s, 6H, $2CH_3$), 2.31 (s, 3H, CH_3), 2.32-2.49 (m, 8H, $4CH_2$), 5.52 (s, 1H, CH), 6.99-7.09 (dd, 4H, Ar-H, J= 7.7 Hz), 11.93 (s, 1H, NH); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ ppm: 20.7, 20.9, 27.2, 27.3, 29.1, 29.4, 31.2, 31.3, 32.0, 32.3, 40.7, 46.3, 46.9, 50.6, 115.5, 115.6, 126.5, 128.1, 128.6, 128.8, 134.8, 135.1, 135.5, 141.1, 161.9, 189.2, 190.2, 196.2.

9-(3-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 6, Table 2): Yellow solid; m.p: 308–310 ^{0}C; Yield 89%; IR (KBr, cm^{-1}) v_{max}; 1617 (C=O), 2878-2928 (CH_3 str.), 3282 (NH), 3447 (OH); ^{1}H-NMR (DMSO-d_6, 500 MHz) δ ppm: 0.87 (s, 6H, $2CH_3$), 0.99 (s, 6H, $2CH_3$), 1.97-2.00 (d, 2H, CH_2, J= 16.1 Hz), 2.14-2.17 (d, 2H, CH_2, J= 16.1 Hz), 2.28-2.31 (d, 2H, CH_2, J= 17.0 Hz), 2.41-2.44 (d, 2H, CH_2, J= 17.0 Hz), 4.73 (s, 1H, CH), 6.39-6.42 (d, 1H, Ar-H, J= 11.0 Hz), 6.55-6.57 (d, 1H, Ar-H, J= 7.65 Hz), 6.61 (s, 1H, Ar-H), 6.89-6.92 (t, Ar-H, J= 7.5 Hz), 9.03 (s, 1H, NH), 9.23 (s, 1H, OH); ^{13}C-NMR (DMSO-d_6, 125 MHz) δ ppm: 26.5, 26.6, 27.9, 28.8, 31.9, 32.2, 32.6, 40.0, 46.6, 50.1, 50.3, 111.5, 112.5, 114.5, 114.7, 118.4, 128.7, 148.5, 149.3, 156.7, 157.1, 162.9, 194.5, 196.1.

3,3,6,6-tetramethyl-9-(2-nitrophenyl)-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 7, Table 2): Yellow solid; m.p: 297–299 ^{0}C; Yield 92%; IR (KBr, cm^{-1}) v_{max}; 1343 and 1520 (NO_2), 1723 (C=O), 2900-2955 (CH_3 str.), 3381 (NH); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ ppm: 1.02 (s, 6H, $2CH_3$), 1.15 (s, 6H, $2CH_3$), 2.20-2.51 (m, 8H, $4CH_2$), 6.04 (s, 1H, CH), 7.24-7.55 (m, 4H, Ar-H), 11.6 (s, 1H, NH); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ ppm: 28.1, 28.5, 30.0, 31.9, 46.2, 46.8, 114.6, 124.3, 127.2, 129.6, 131.3, 132.1, 149.7, 189.4, 190.4.

9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 8, Table 2): White solid; m.p: 298–301 ^{0}C; Yield 91%; IR (KBr, cm^{-1}) v_{max}; 673-885 (Cl), 1590 (C=O), 2881-3005 (CH_3 str.), 3049 (NH); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ ppm: 1.09 (s, 6H, 2CH3), 1.21 (s, 6H, 2CH3), 2.29-2.47 (m, 8H, 4CH2), 5.47 (s, 1H, CH), 7.00-7.02 (d, 2H, Ar-H, J= 8.0 Hz), 7.21-7.23 (d, 2H, Ar-H, J= 8.0 Hz), 11.87 (s, 1H, NH); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ ppm: 27.2, 27.4, 29.2, 29.5, 31.3, 31.4, 32.1, 32.4, 40.8, 46.4, 47.0, 50.6, 115.2, 115.3, 128.1, 128.3, 129.7, 131.5, 131.9, 136.7, 142.6, 162.4, 189.3, 190.5, 196.2.

3,3,6,6-tetramethyl-9,10-diphenyl-3,4,6,7,9,10-hexahydroacridine-1,8(2H,5H)-dione (Entry 1, Table 3): White solid; m.p: 253–255 ^{0}C; Yield 95%; IR (KBr, cm^{-1}) v_{max}; 1595 (C=O), 2873-2962 (CH_3 str.); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ ppm: 1.10 (s, 6H, $2CH_3$), 1.24 (s, 6H, $2CH_3$), 2.30-2.48 (m, 8H, $4CH_2$), 5.55 (s, 1H, CH), 7.09-7.28 (m, 10H, 2 Ar-H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ ppm: 27.3, 29.5, 31.3, 32.7, 46.4, 47.0, 115.5, 125.7, 126.7, 128.1, 138.0, 189.3, 190.4.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Twisting
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(b)
(c)
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(e)
C - H
Stretching
Aromatic
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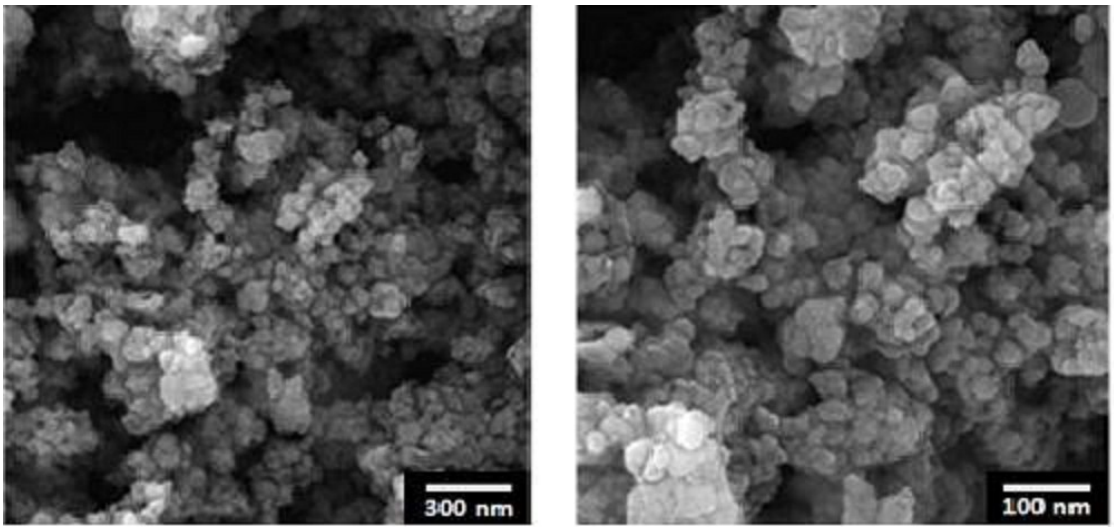
FIGURE 1



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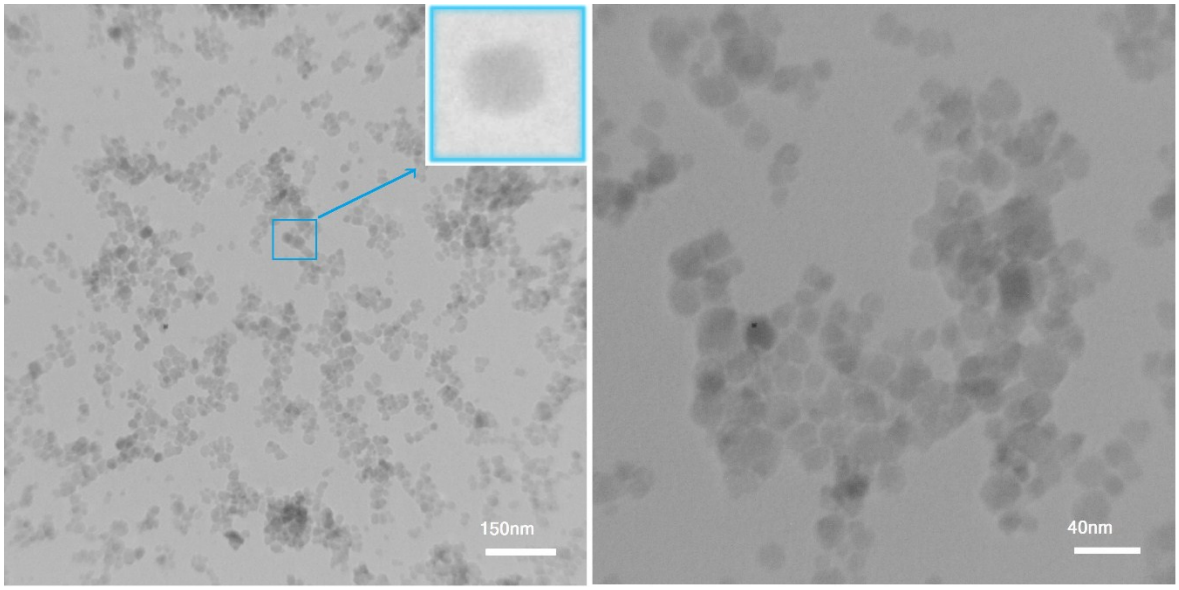

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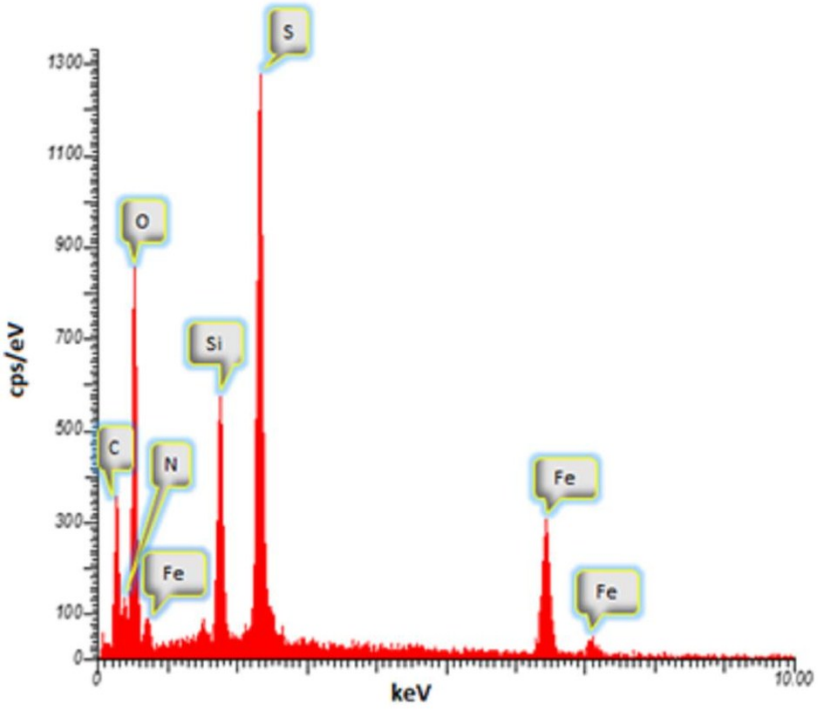

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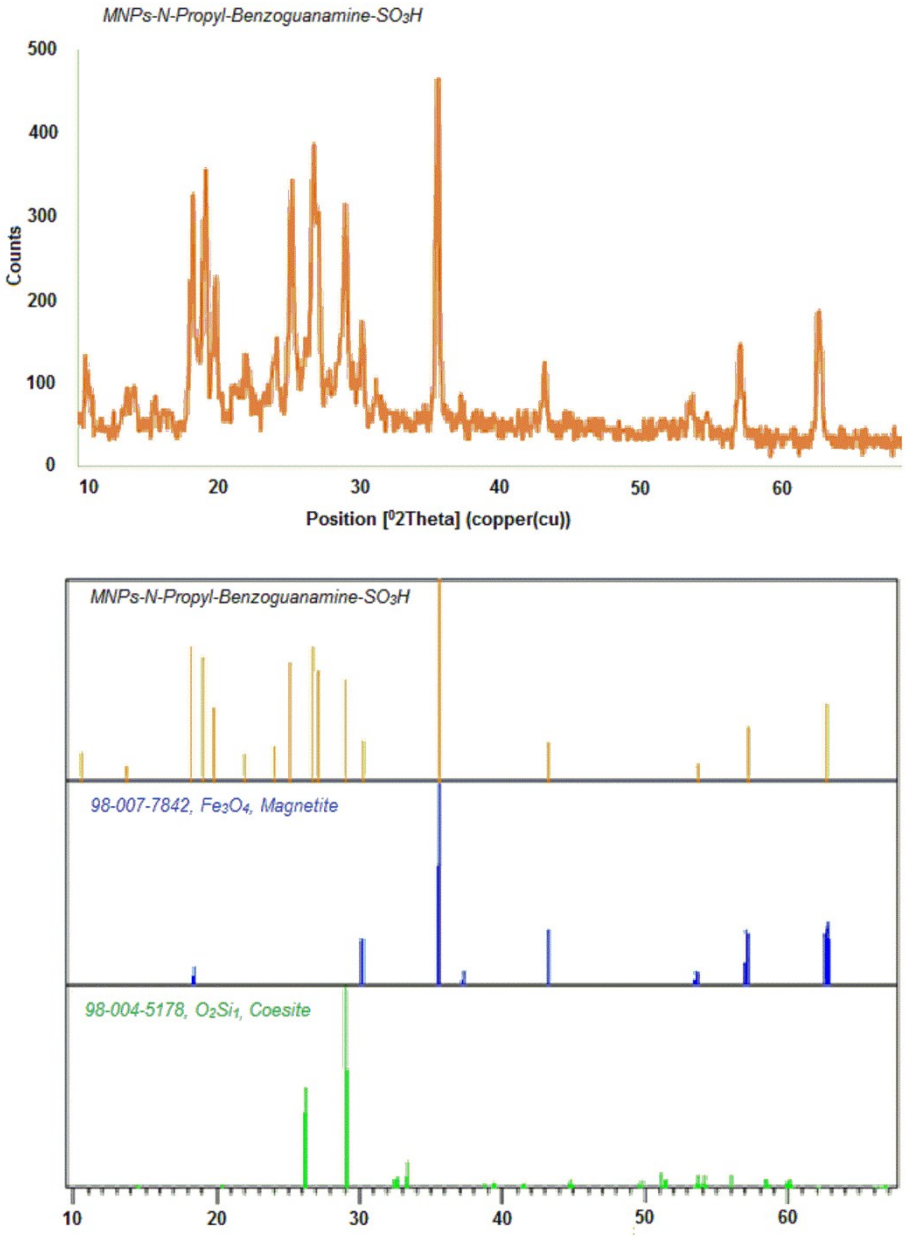
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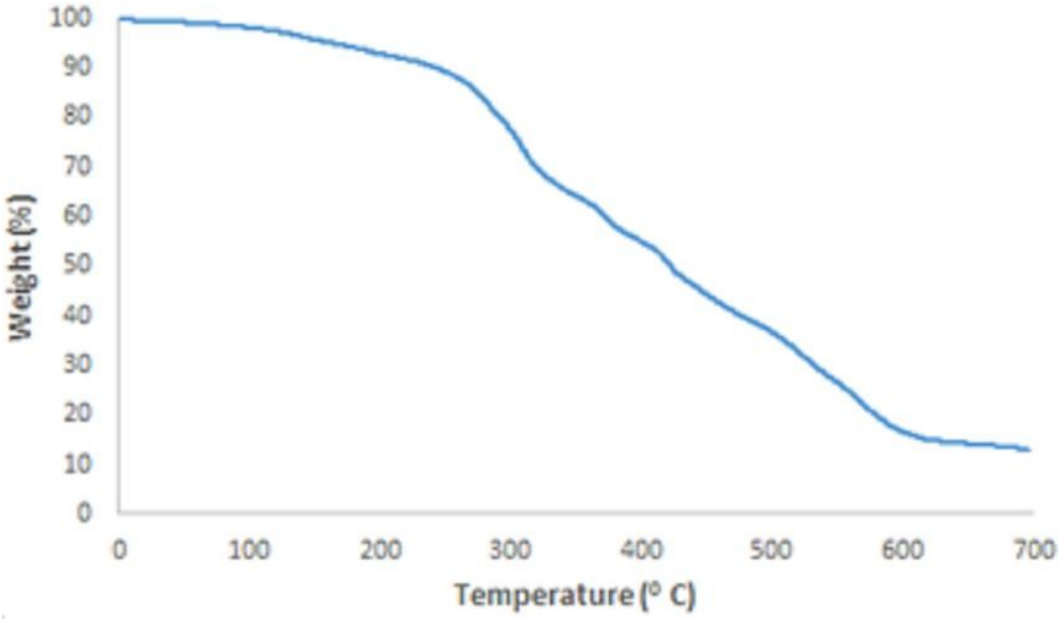

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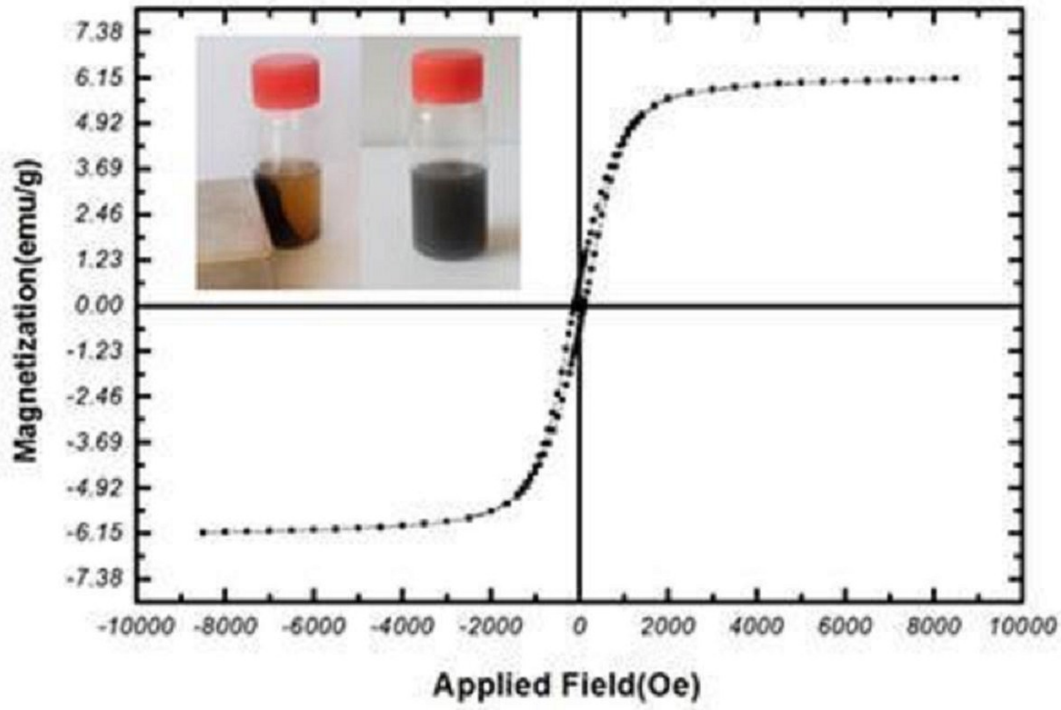

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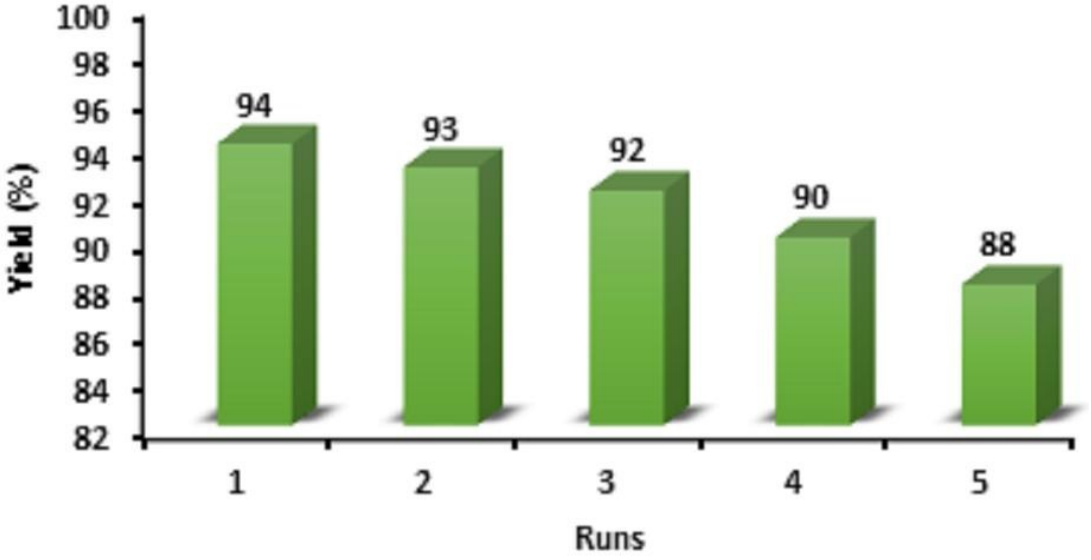

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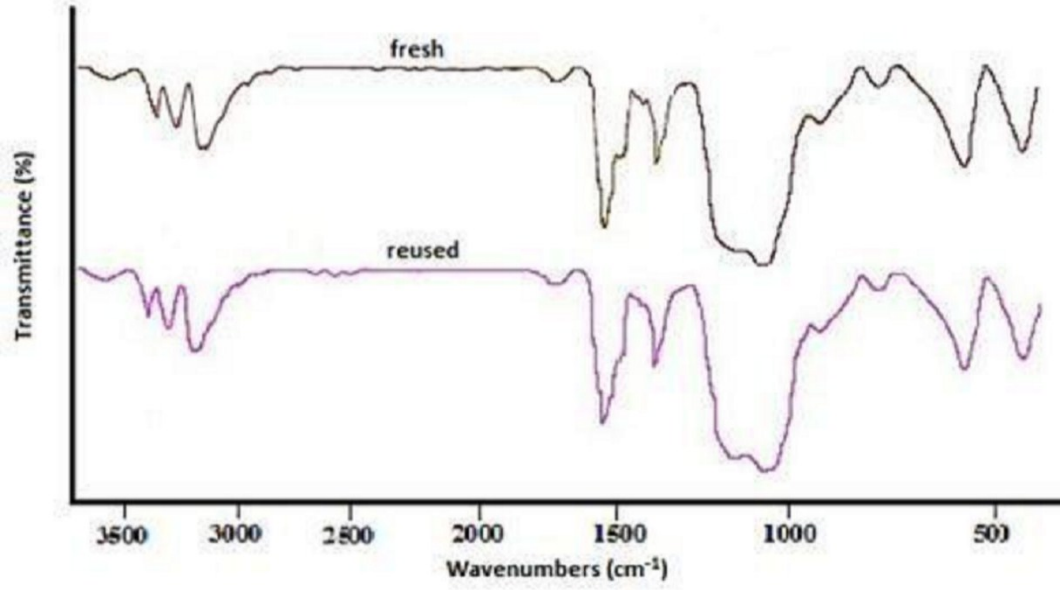

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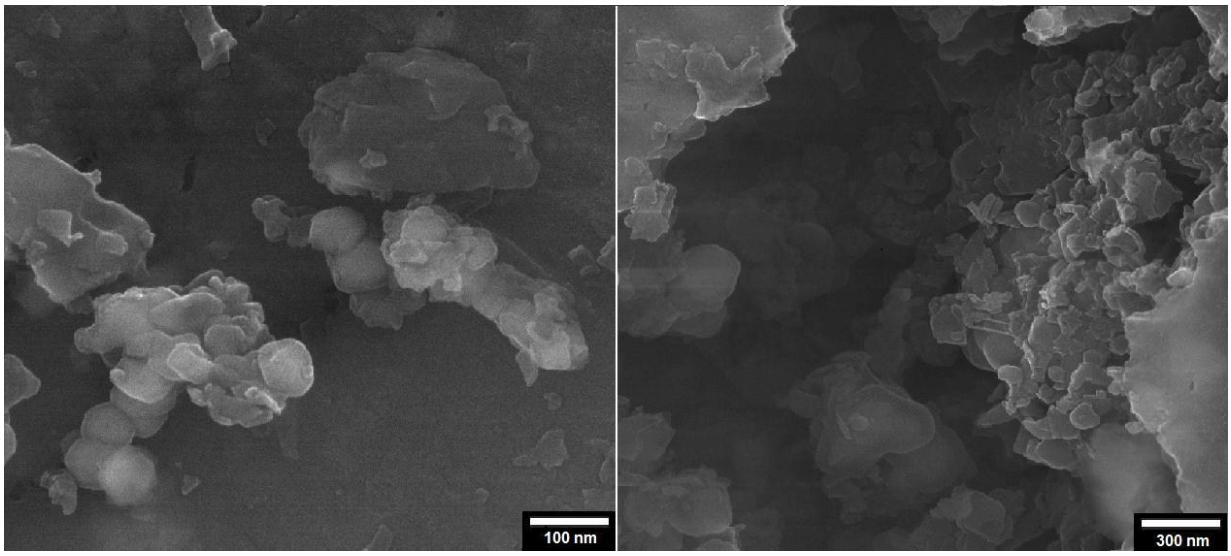

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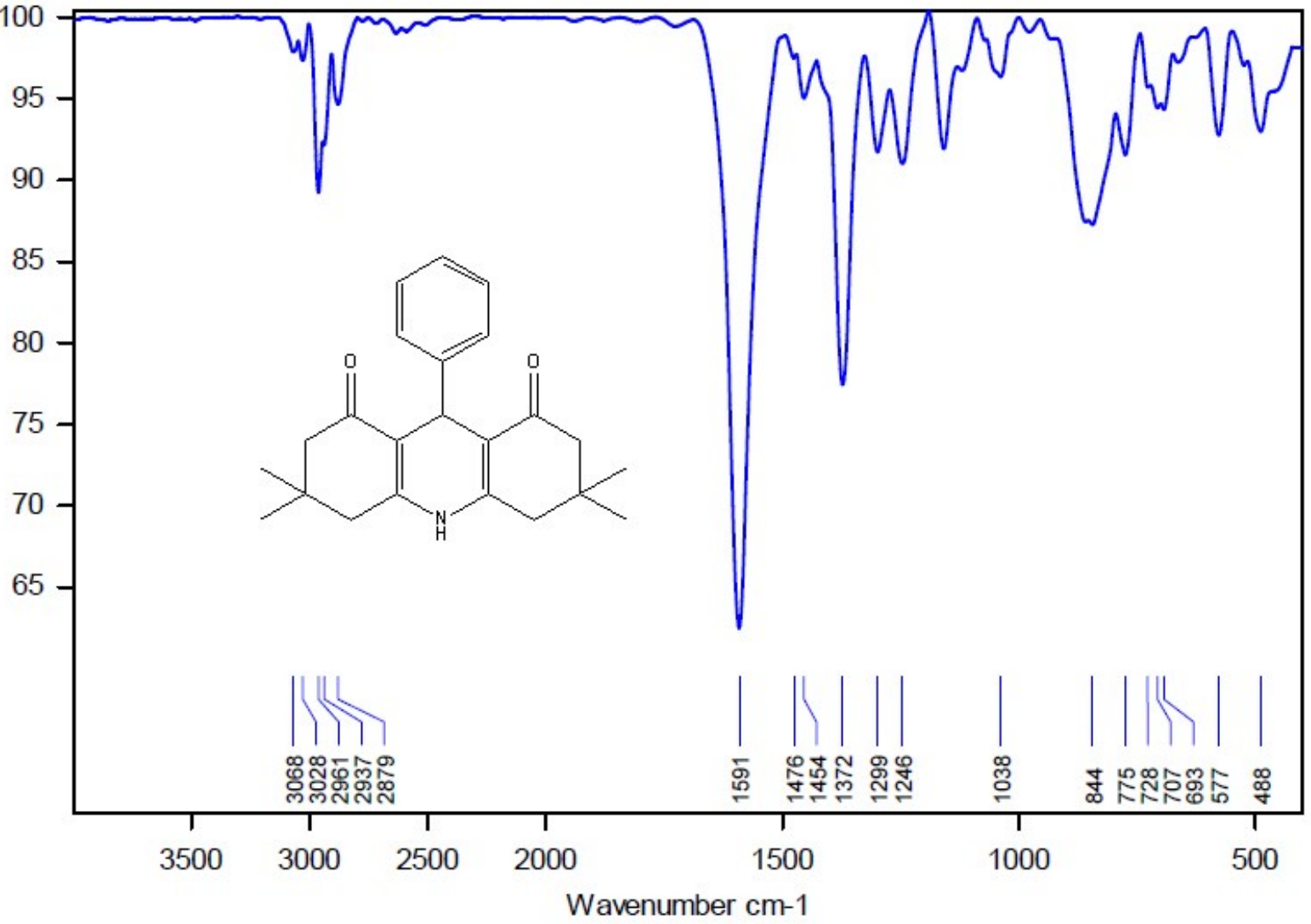
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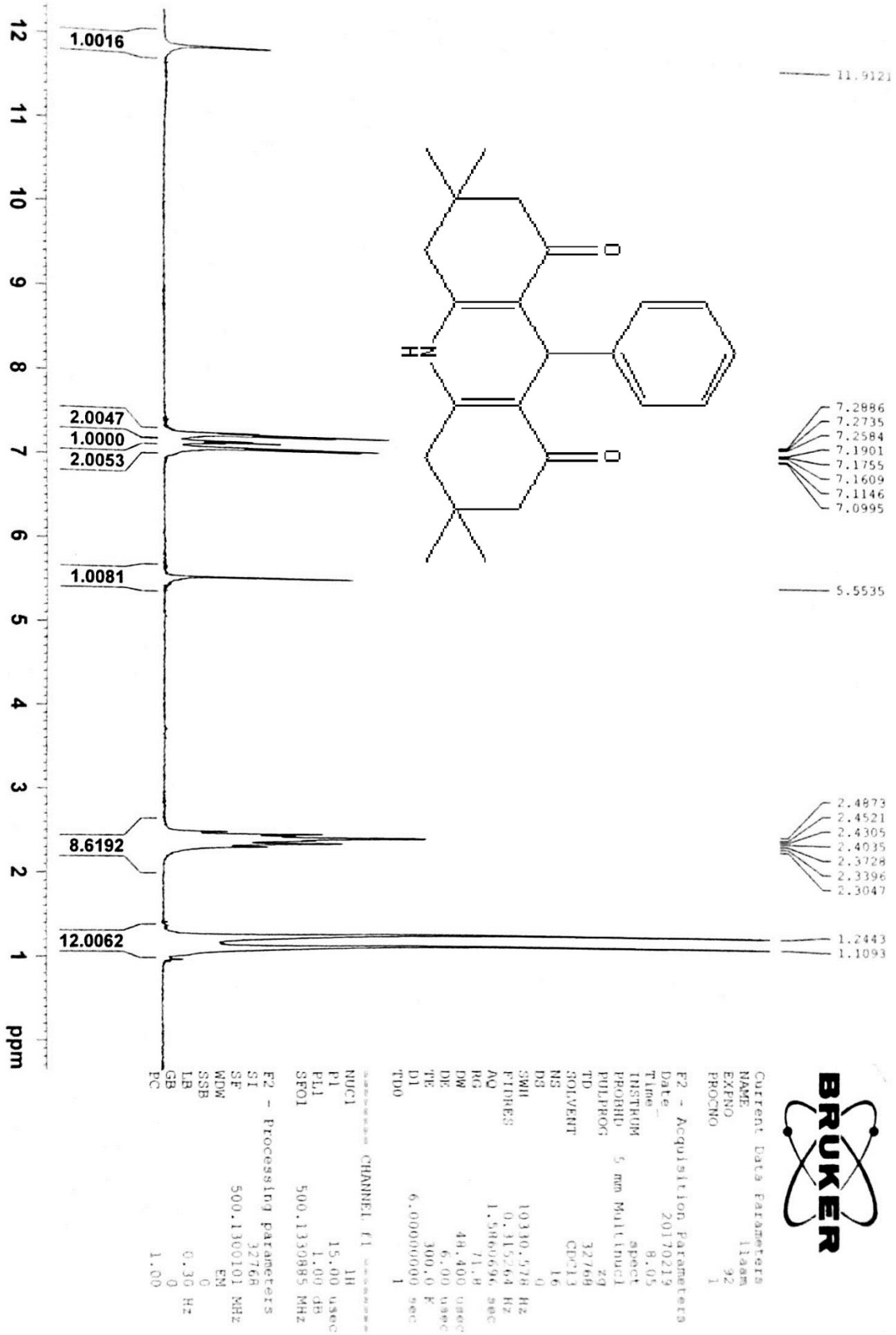
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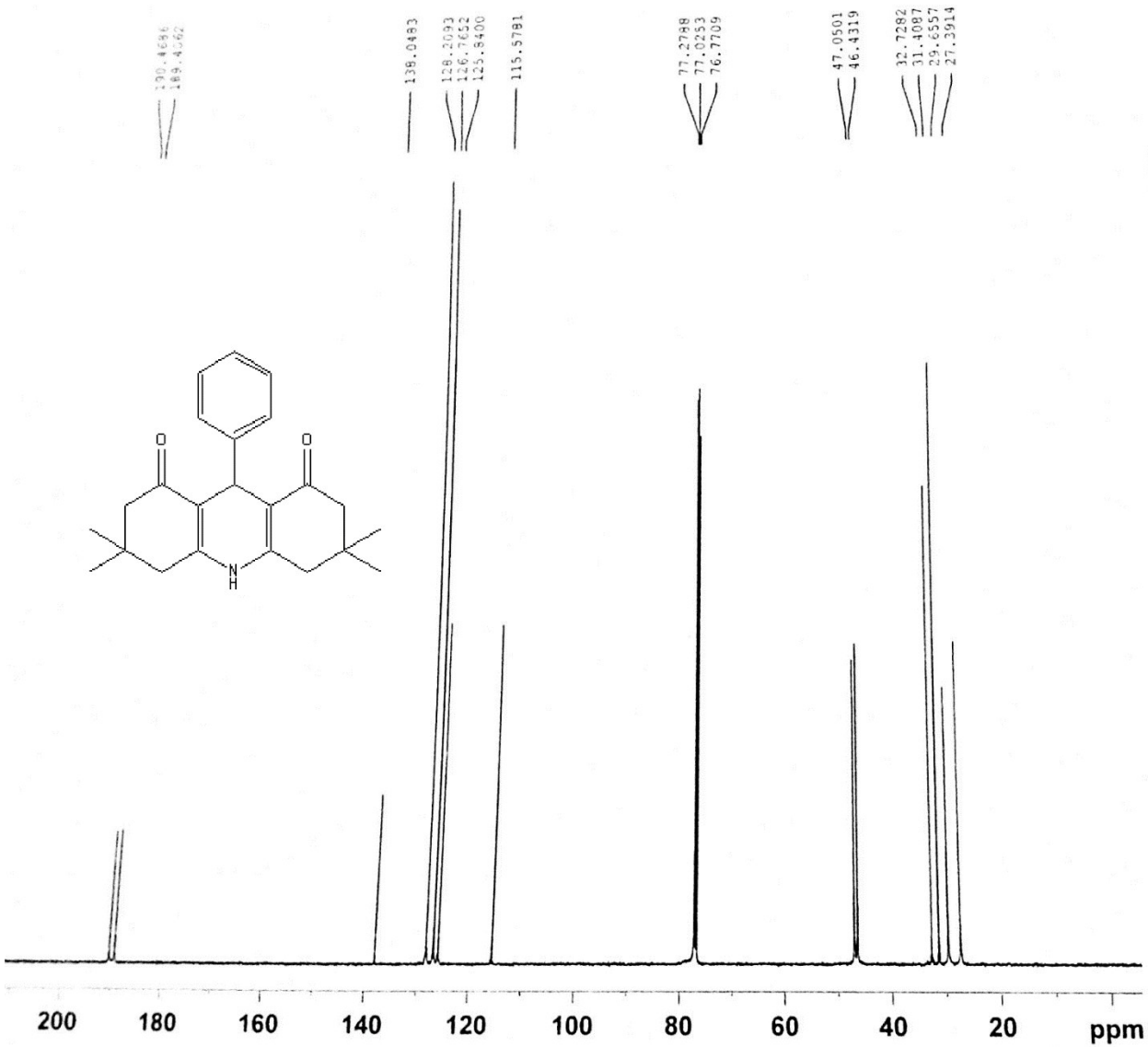

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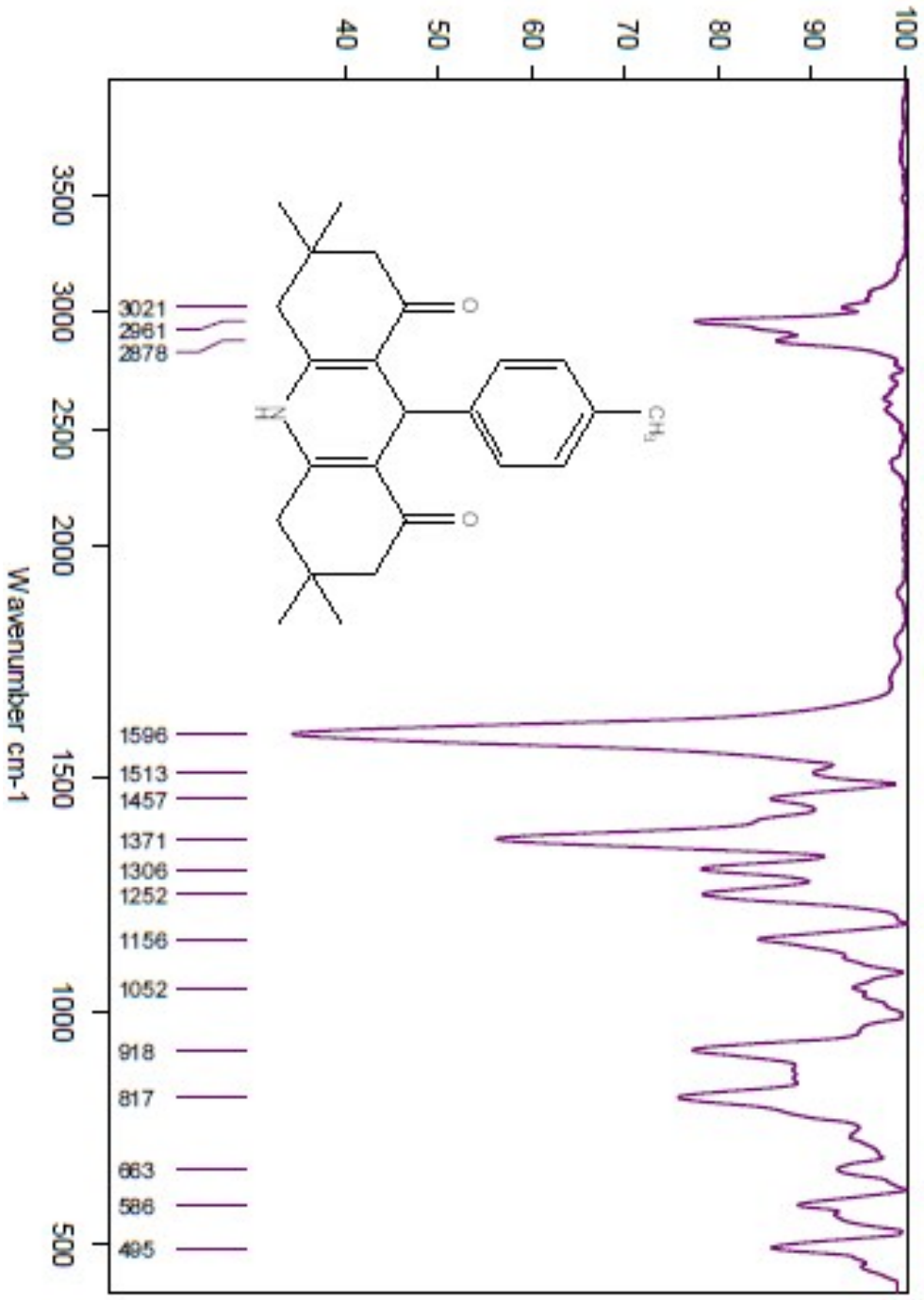
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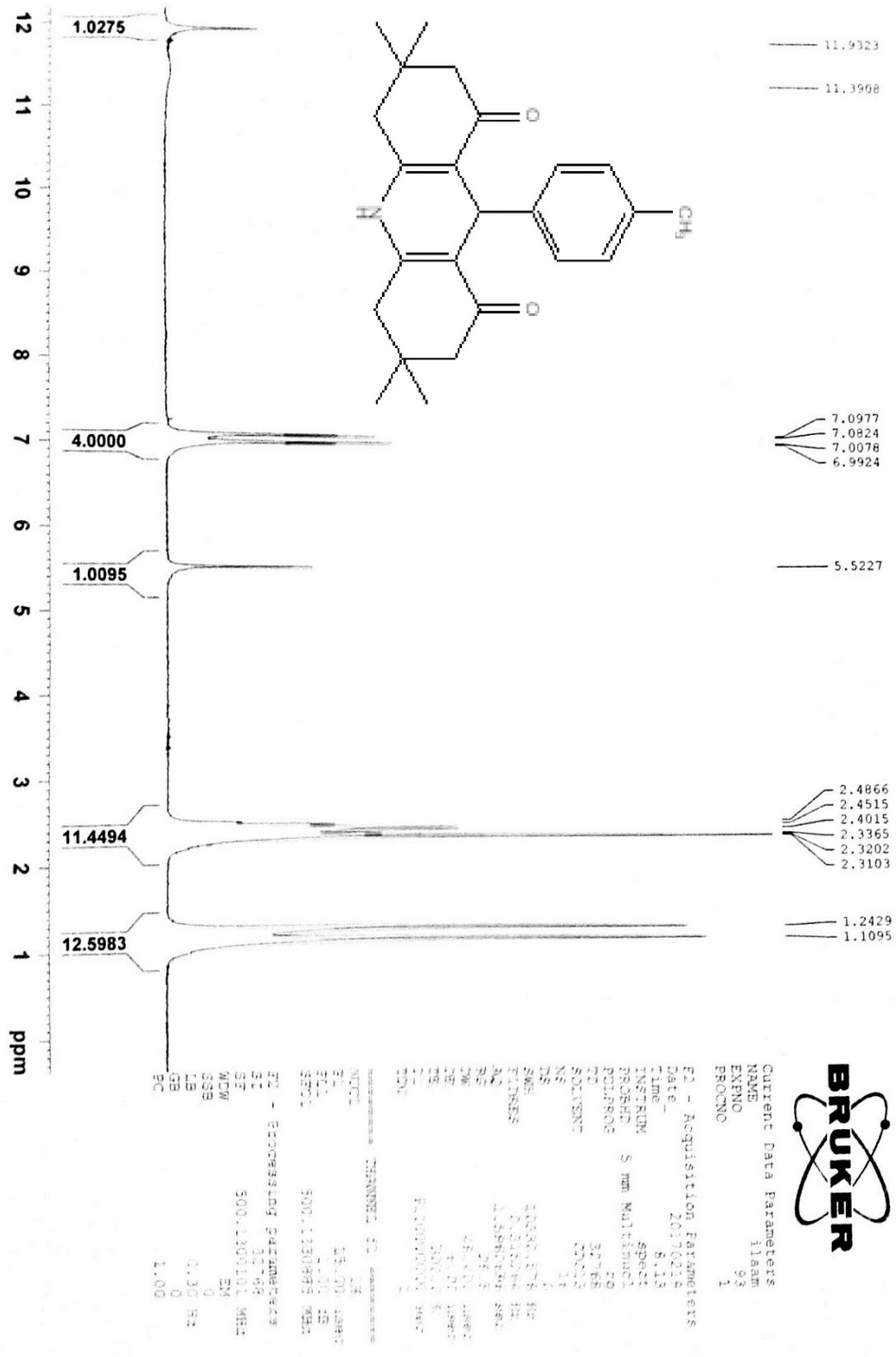
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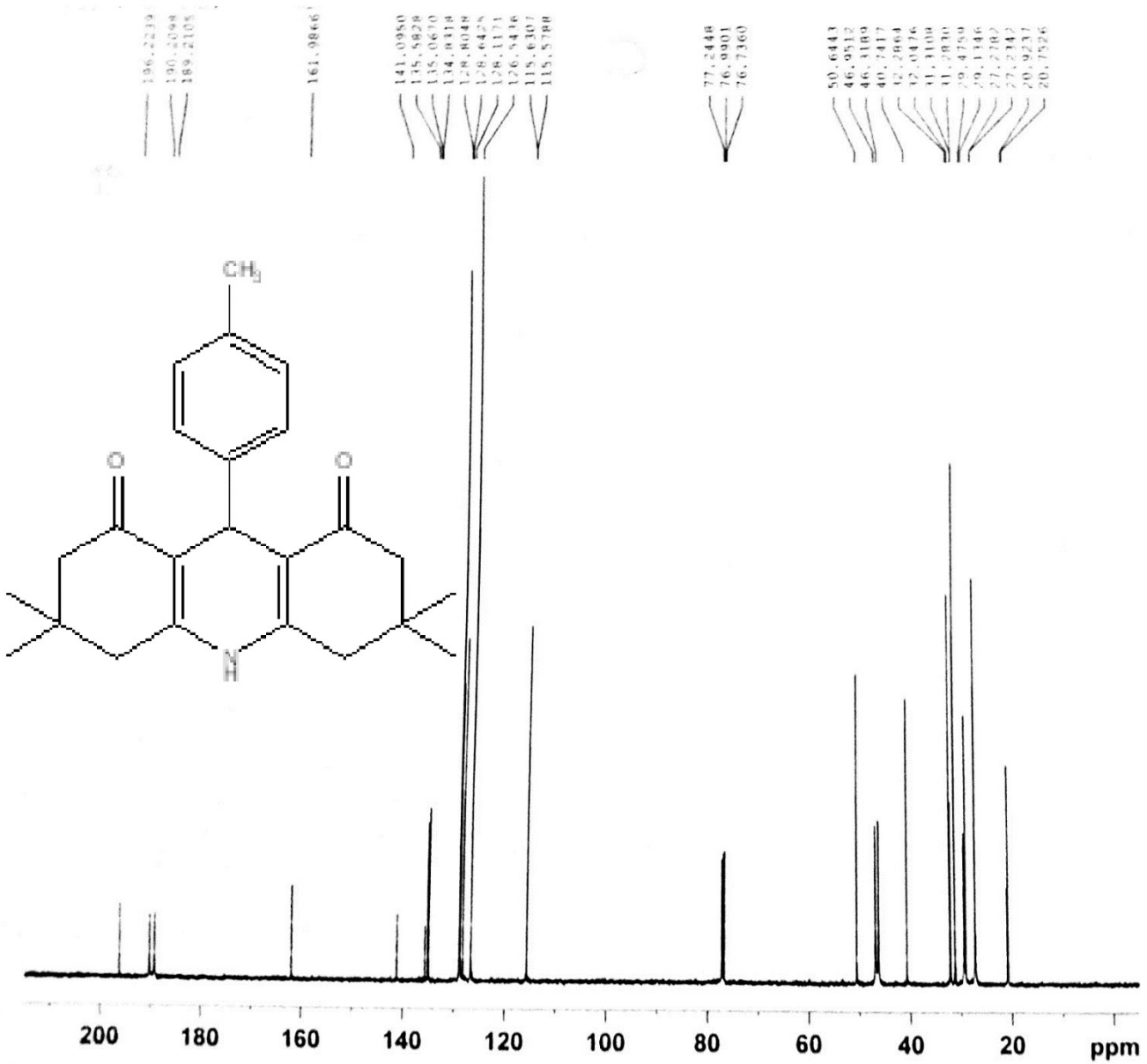

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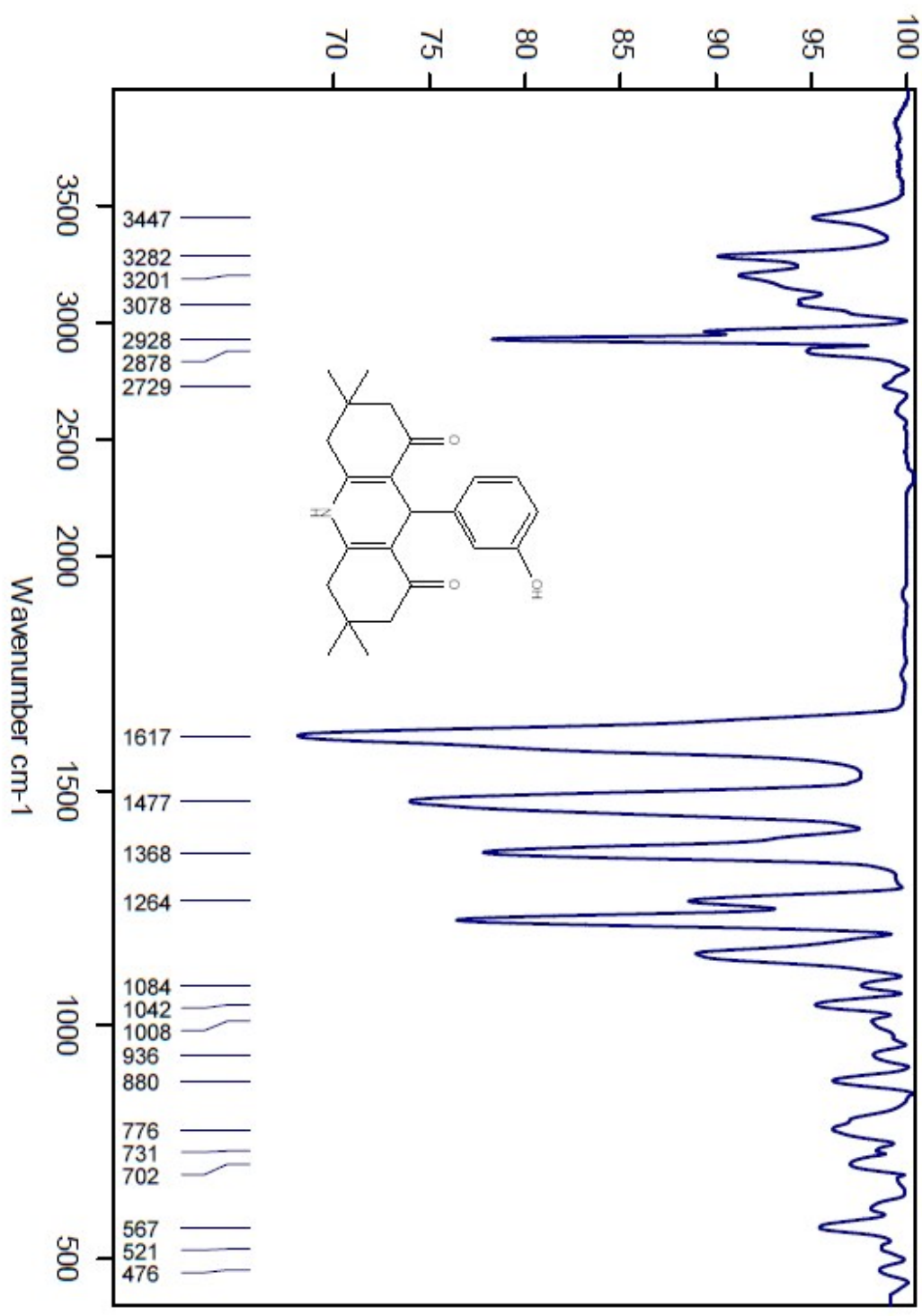
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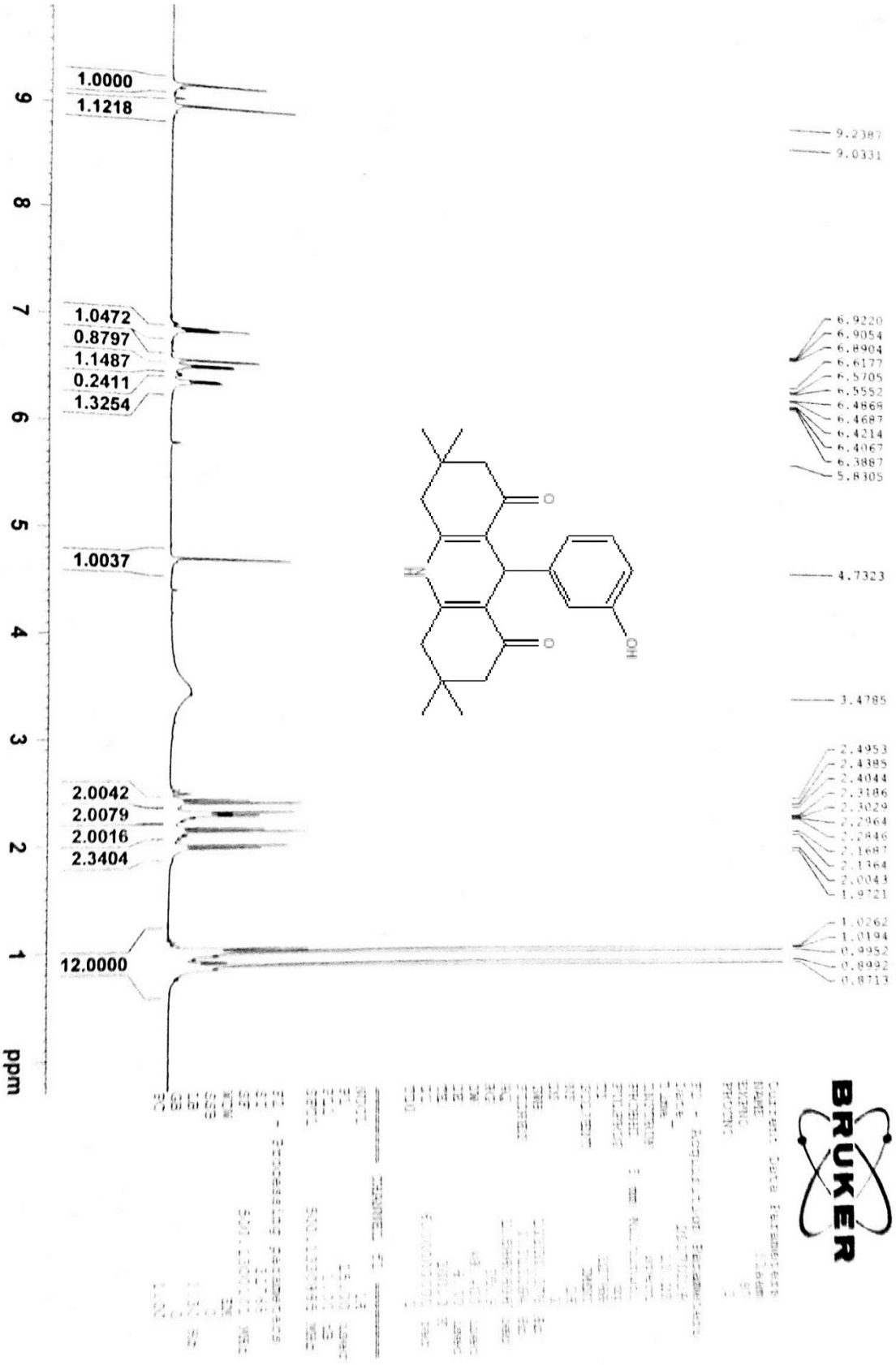
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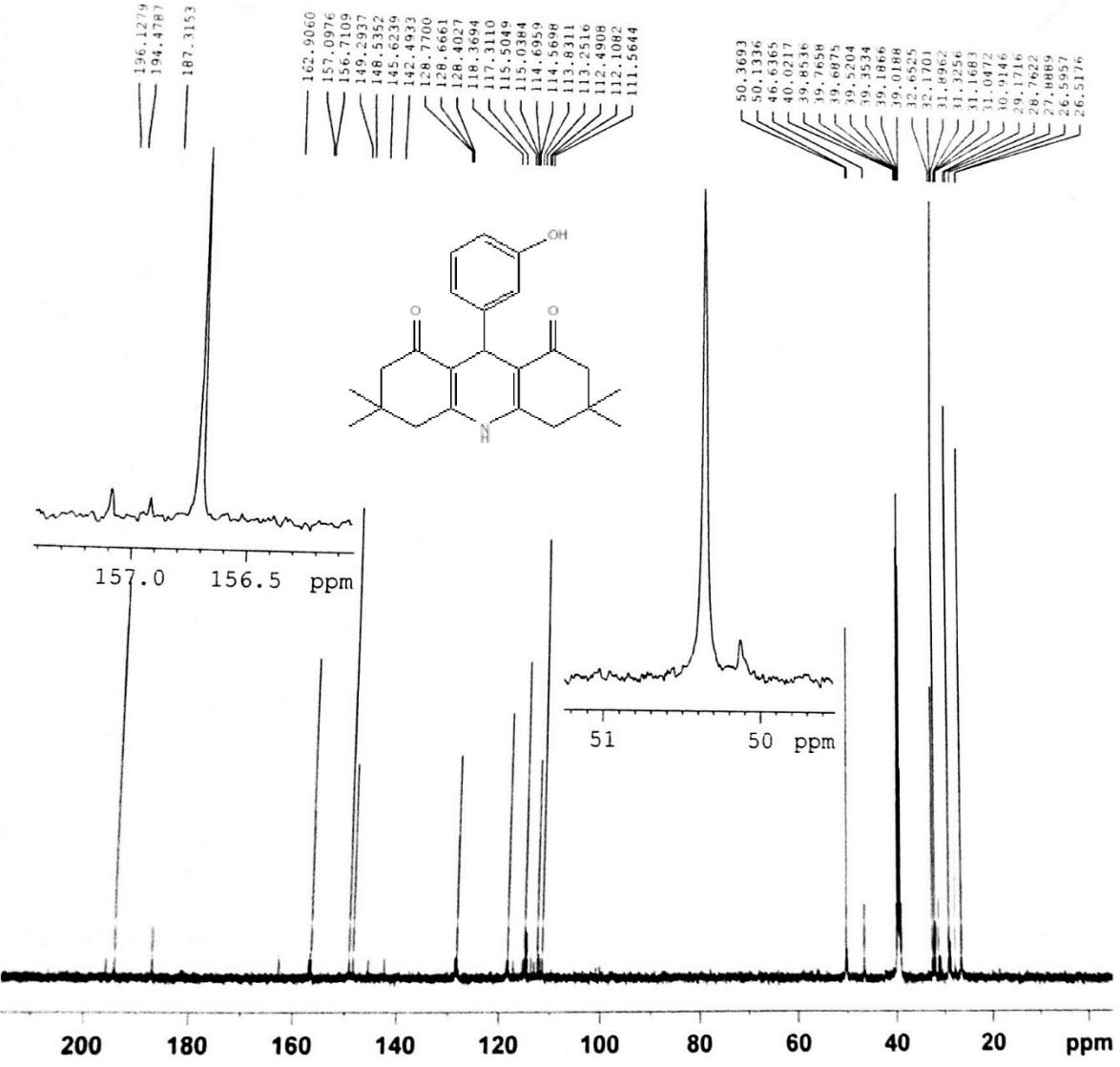
OH
BRUKER



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Current Data Parameters

NAME	ilaam
EXPNO	103
PROCNO	1

F2 - Acquisition Parameters

Date_	20170312
Time	7.09
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zgpg
TD	65536
SOLVENT	DMSO
NS	160
DS	0
SWH	31446.541 Hz
FIDRES	0.479836 Hz
AQ	1.0420883 sec
RG	2298.8
DW	15.900 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

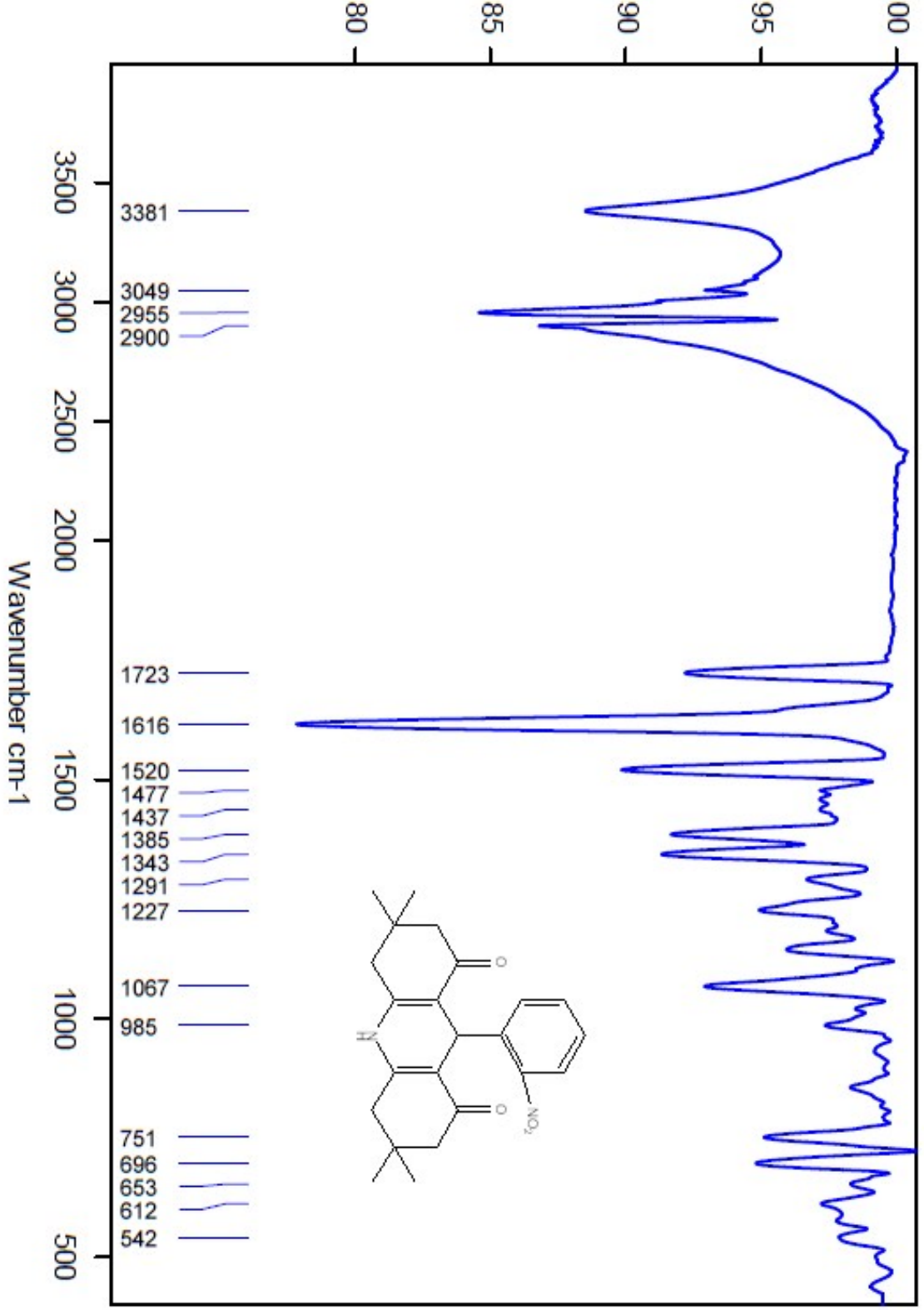
NUC1	13C
P1	10.00 usec
PL1	3.00 dB
SFO1	125.7716224 MHz

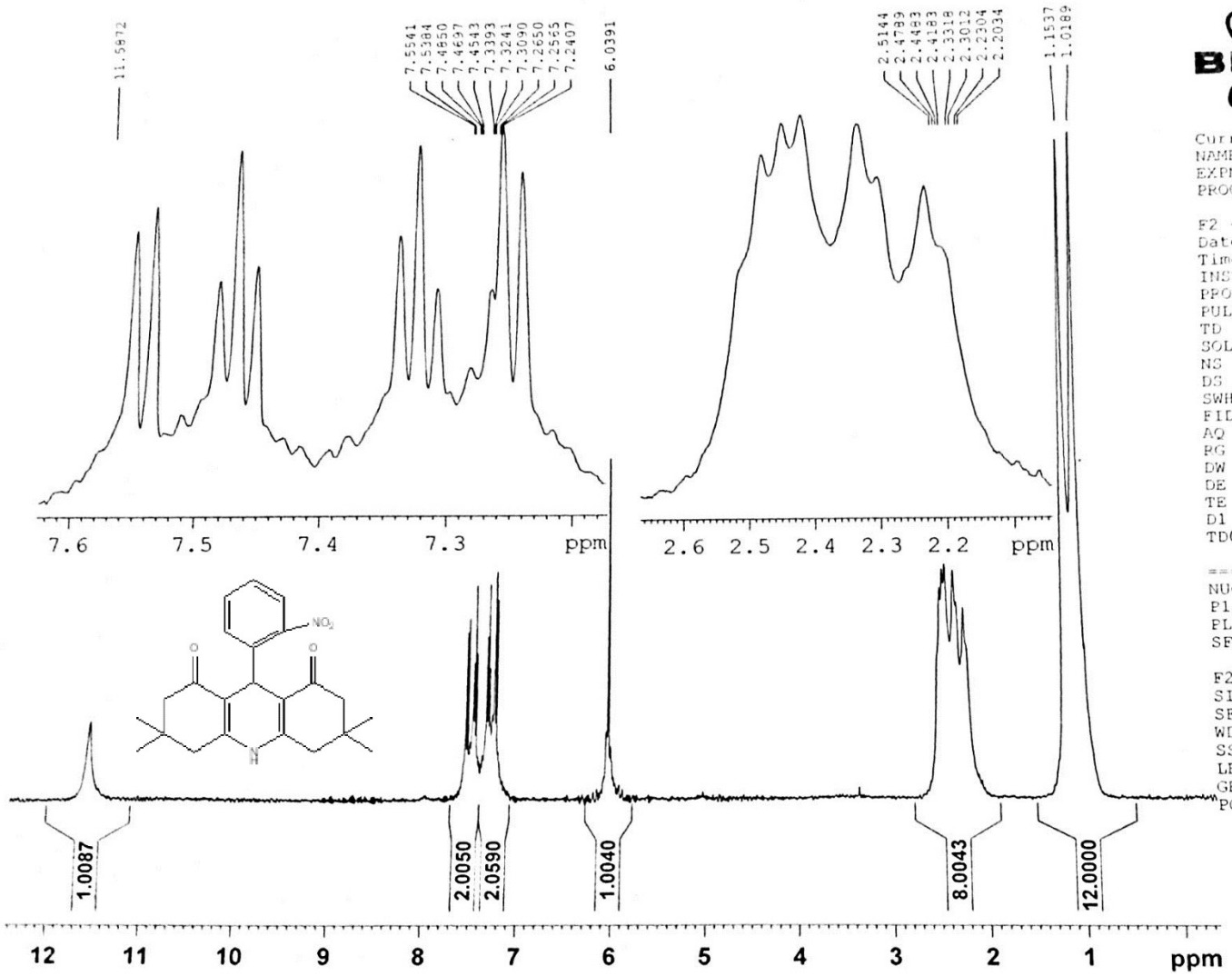
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	20.00 dB
PL13	20.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7578407 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00


3381
3049
2955
2900
1723
1616
1520
1477
1437
1385
1343
1291
1227
1067
985
751
696
653
612
542
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
80
85
90
95
00
O
N
H
O
NO2



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Current Data Parameters

NAME	ilaam
EXPNO	94
PROCNO	1

F2 - Acquisition Parameters

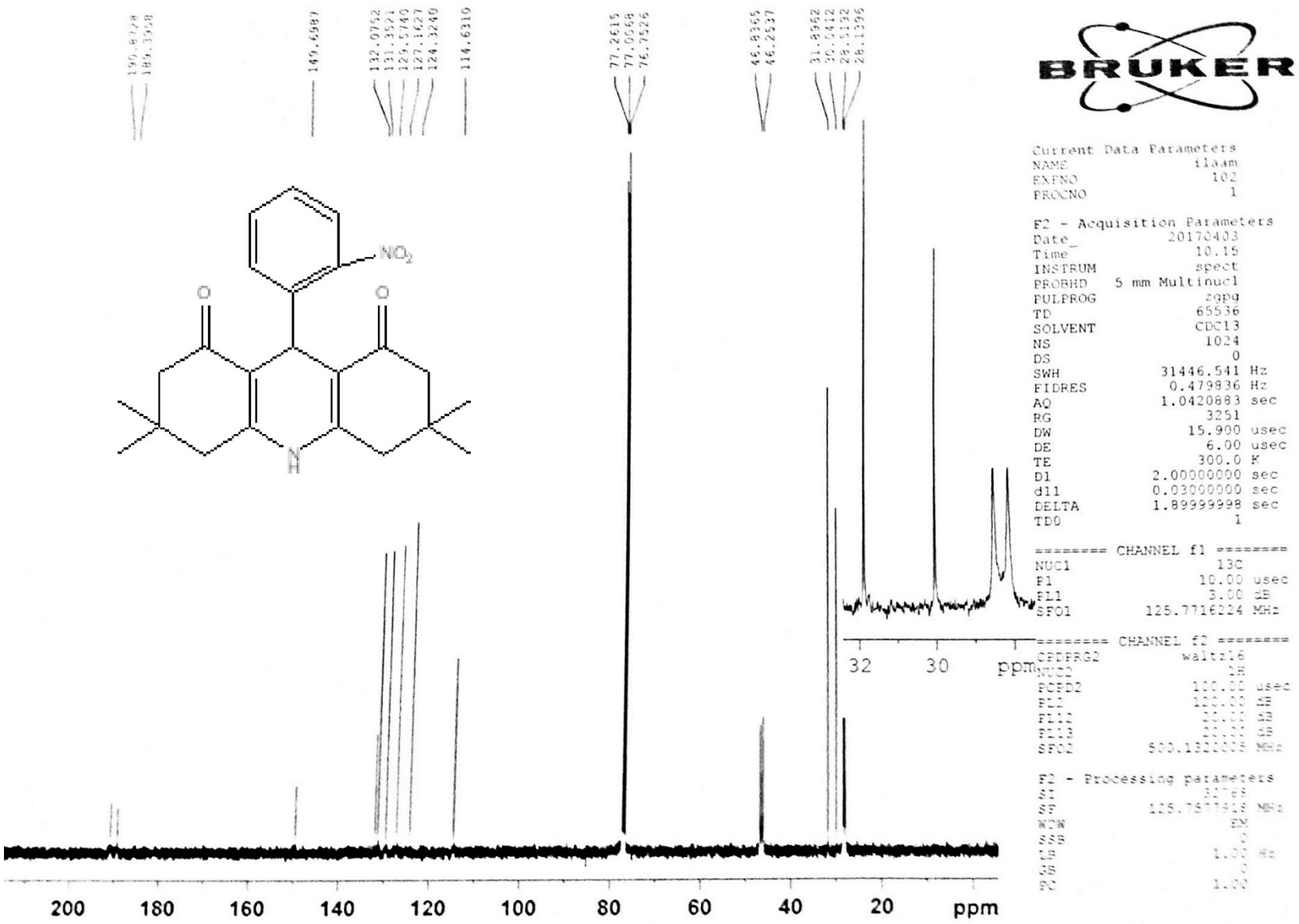
Date_	20170219
Time	8.21
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.315264 Hz
AQ	1.5860696 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	300.0 K
D1	6.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	15.00 usec
PL1	1.00 dB
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	32768
SF	500.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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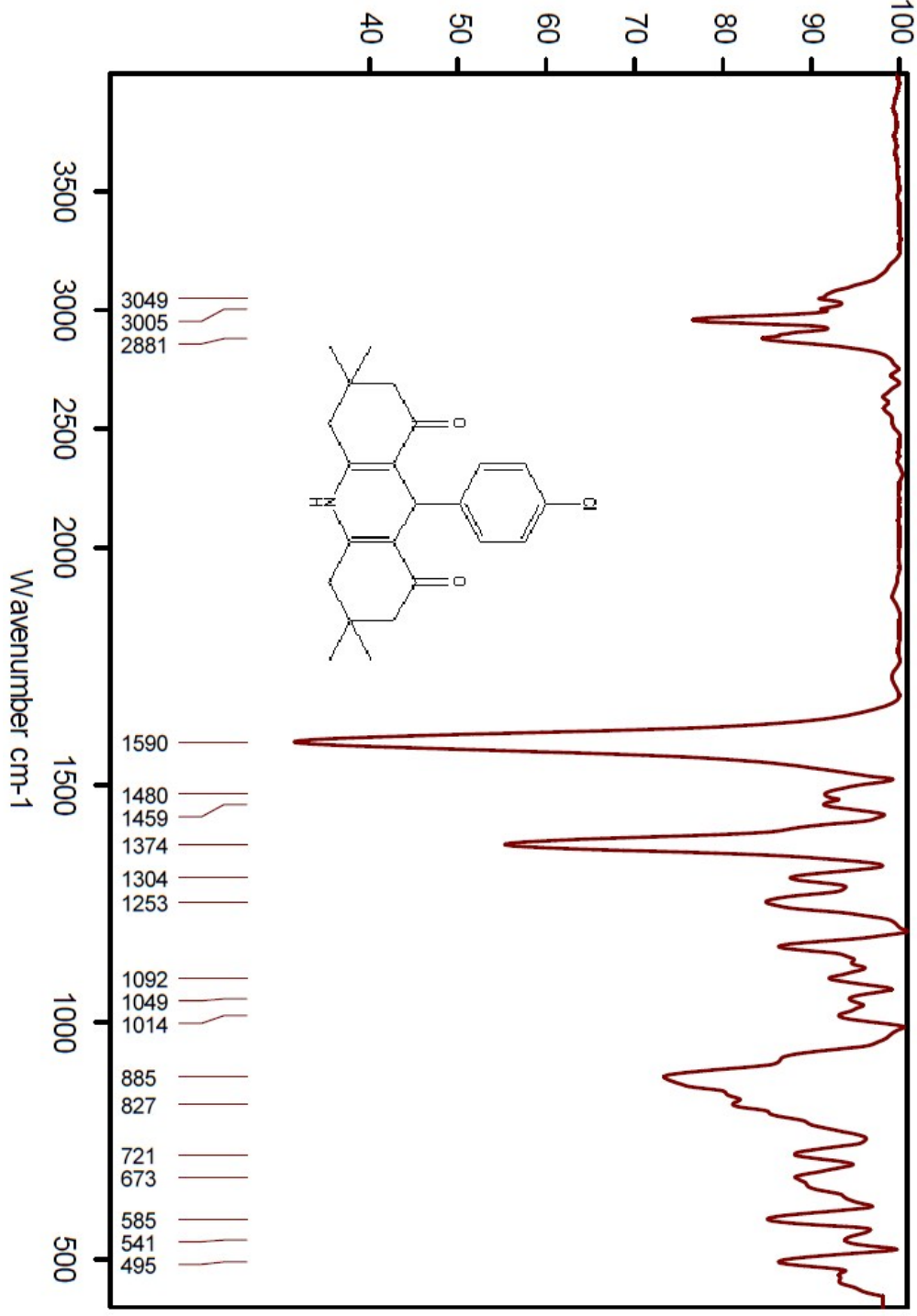
Current Data Parameters
NAME ilaam
EXPNO 102
PROCNO 1

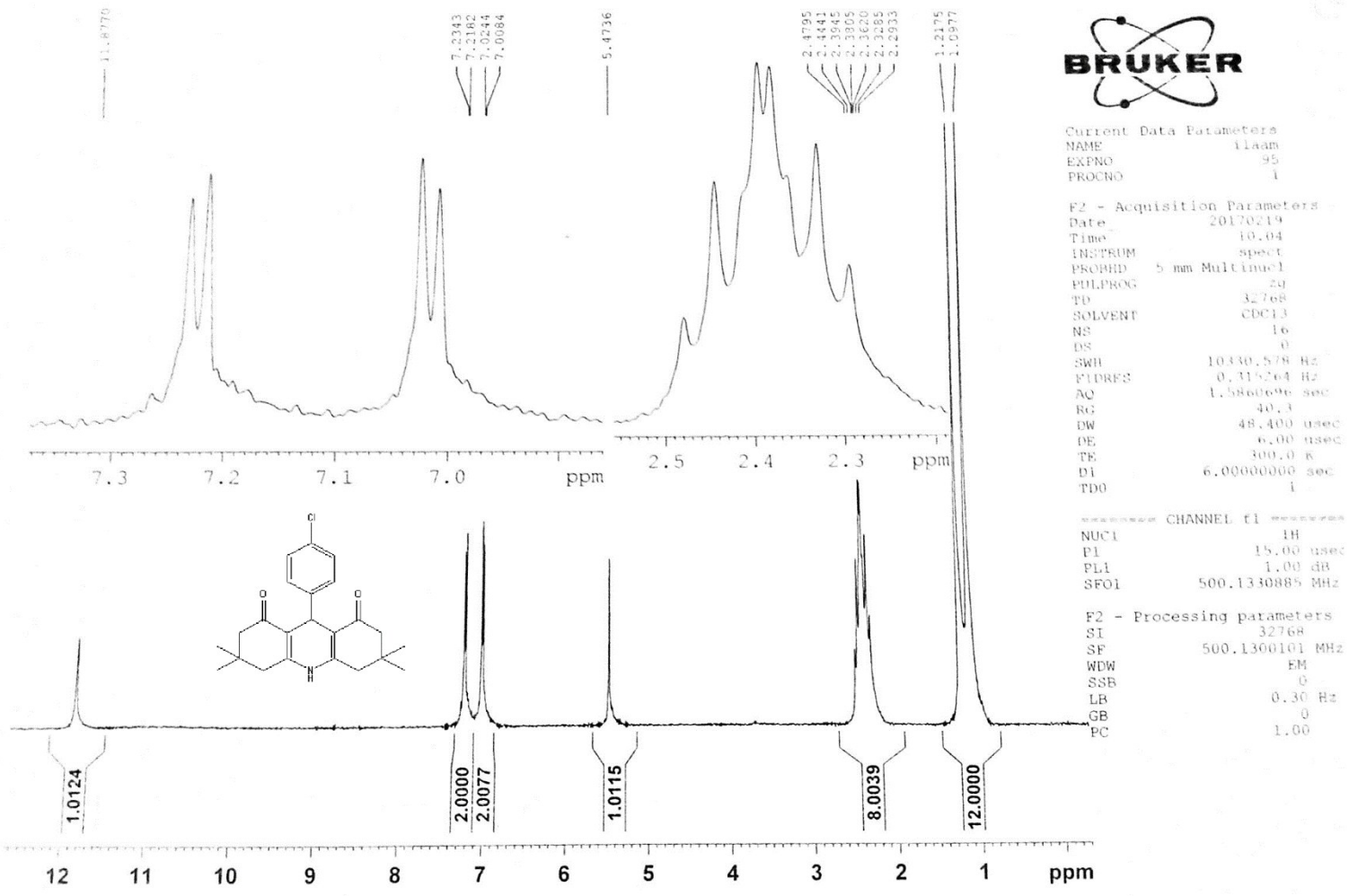
F2 - Acquisition Parameters
Date_ 20170403
Time 10.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1024
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420683 sec
RG 3251
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.00 dB
SFO1 125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577918 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


40
50
60
70
80
90
100
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3049
3005
2881
1590
1480
1459
1374
1304
1253
1092
1049
1014
885
827
721
673
585
541
495
O
HN
Cl
O



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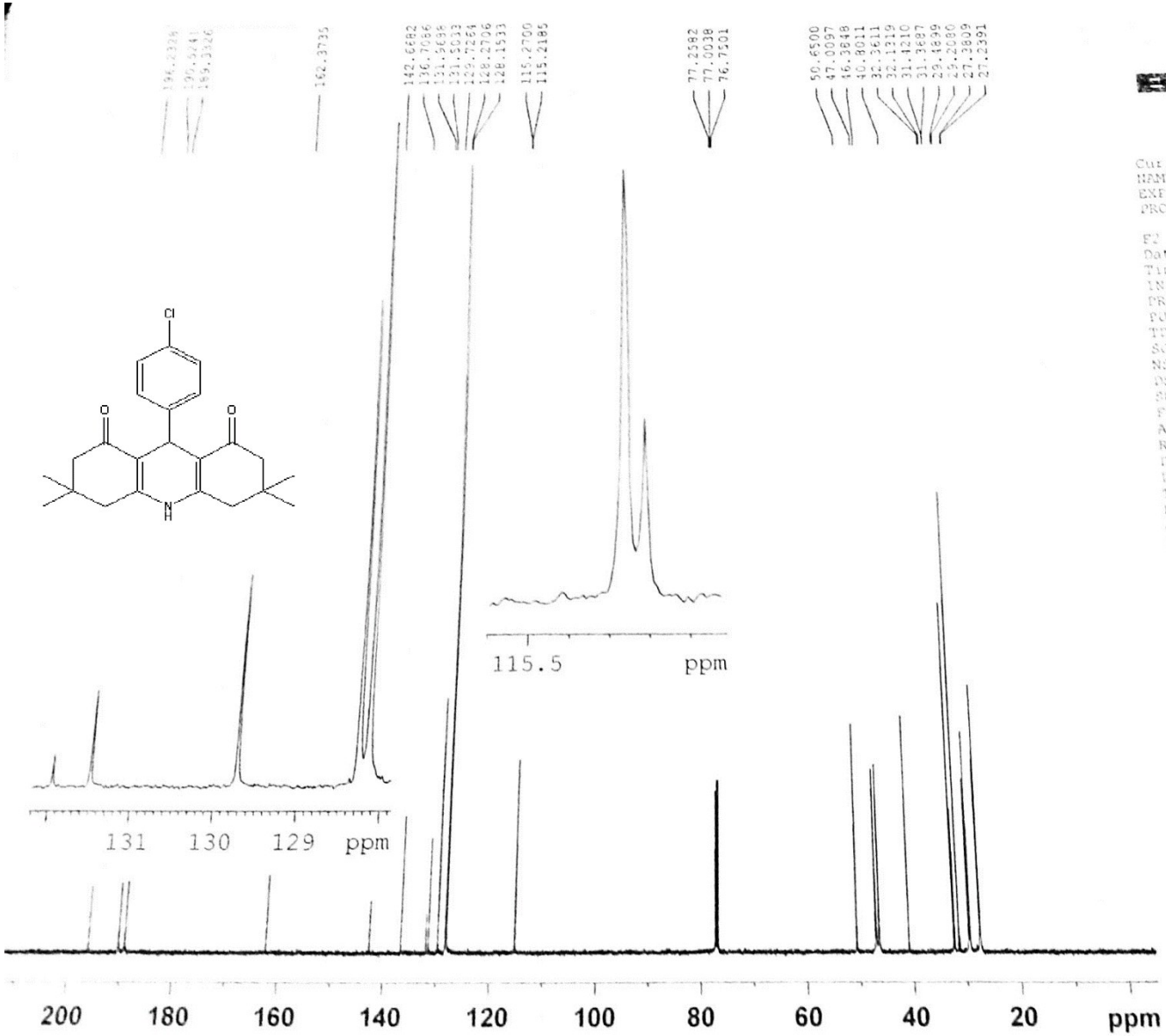
Current Data Parameters
NAME tlaam
EXPNO 95
PROCNO 1

F2 - Acquisition Parameters
Date 20170219
Time 10.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 40.3
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 1.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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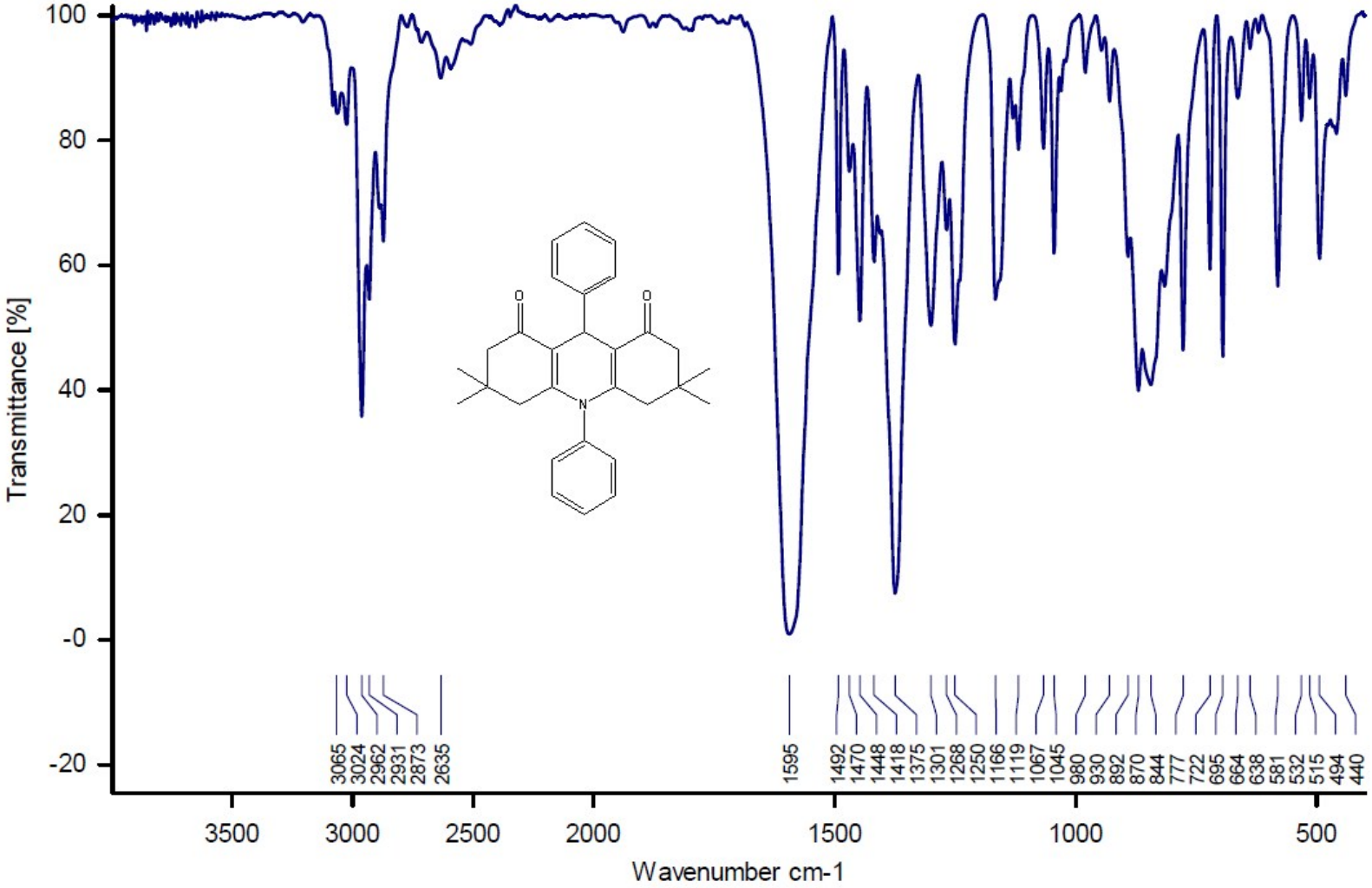
Current Data Parameters
NAME ilaam
EXPNO 105
PROCNO 1

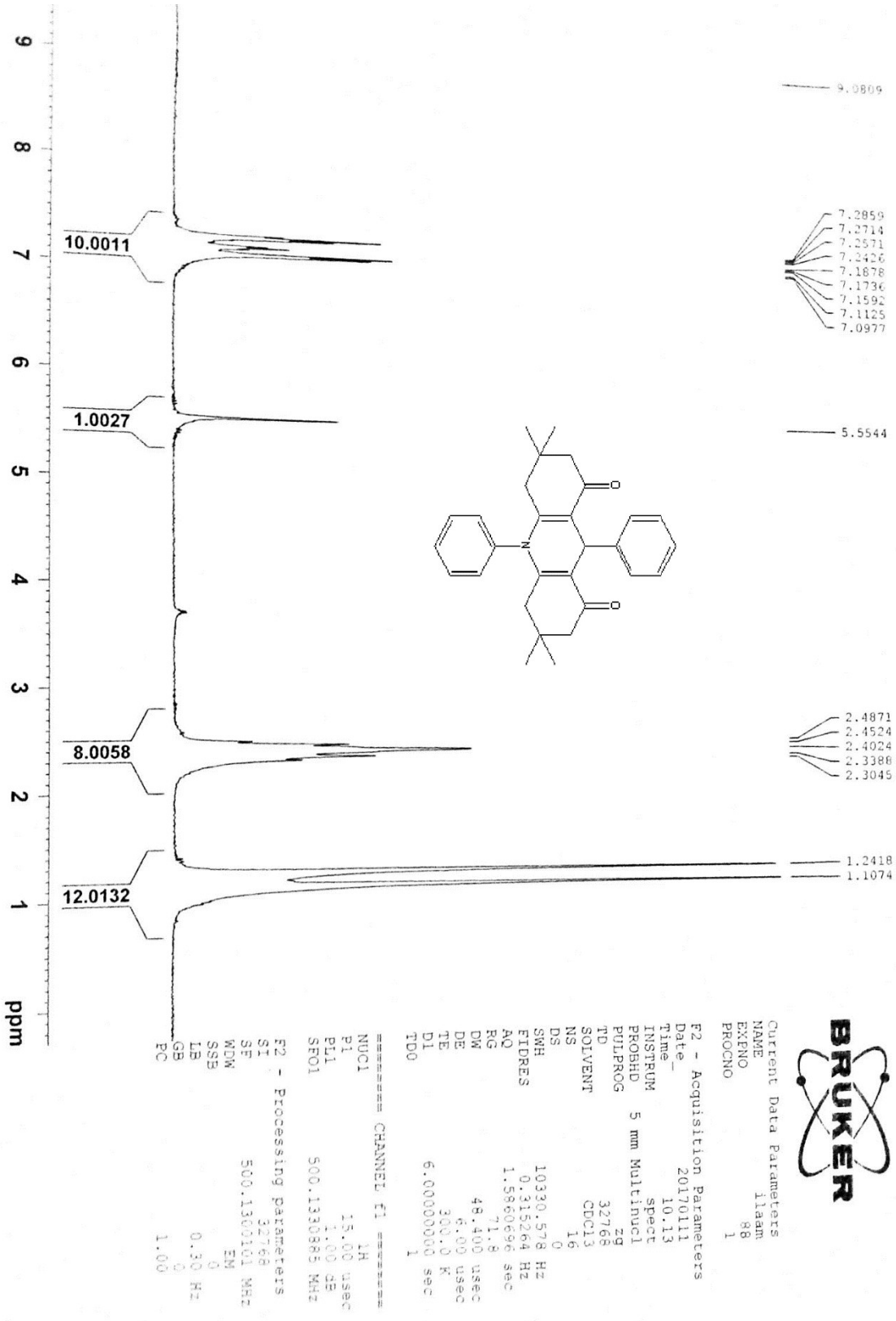
F2 - Acquisition Parameters
Date_ 20170312
Time 7.54
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 425
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420853 sec
RG 7298.2
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

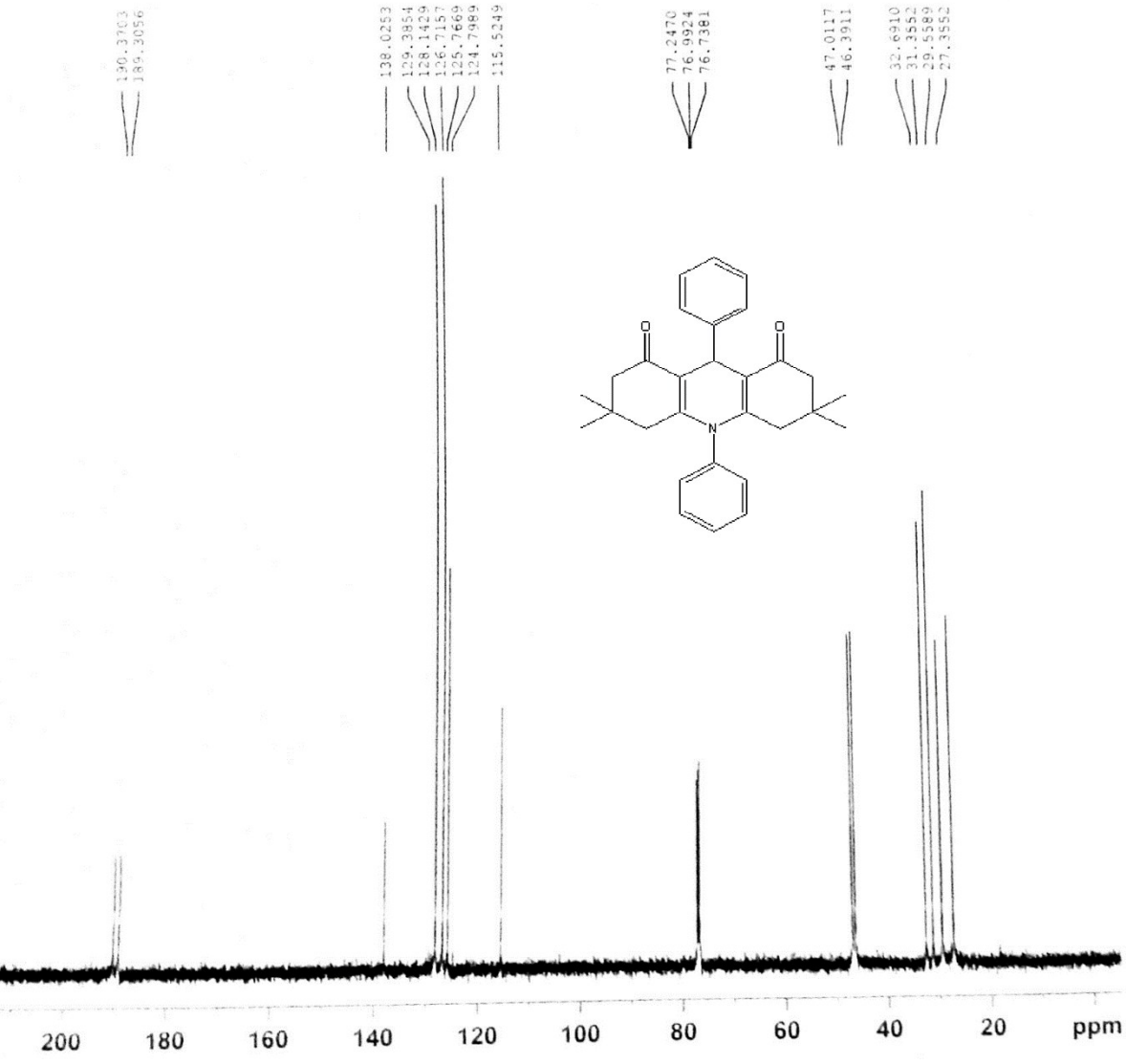
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.00 dB
SFO1 125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577968 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


100
80
60
40
20
-0
-20
Transmittance [%]
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3065
3024
2962
2931
2873
2635
1595
1492
1470
1448
1418
1375
1301
1268
1250
1166
1119
1067
1045
980
930
892
870
844
777
722
695
664
638
581
532
515
494
440
O
O
N


9.0809
7.2859
7.2714
7.2571
7.2426
7.1878
7.1736
7.1592
7.1125
7.0977
5.5544
2.4871
2.4524
2.4024
2.3388
2.3045
1.2418
1.1074
10.0011
1.0027
8.0058
12.0132
ppm
Current Data Parameters
NAME ilaam
EXPNO 88
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170111
Time_ 10.13
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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```
Current Data Parameters
NAME                  ilaam
EXPNO                    89
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170219
Time                   7.24
INSTRUM               spect
PROBHD    5 mm Multinucl
PULPROG               zgpg
TD                   65536
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              31446.541 Hz
FIDRES           0.479836 Hz
AQ               1.0420883 sec
RG                    6502
DW                  15.900 usec
DE                   6.00 usec
TE                  300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PL1                   3.00 dB
SFO1          125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                  120.00 dB
PL12                  20.00 dB
PL13                  22.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                     32768
SF            125.7571486 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.00
```