1 Anilina

2 Acetanilid

3 Mrówczan etylu

4 Kwas mrówkowy

5 Nitrobenzen

6 *m*-Dinitrobenzen

7 *p*-Nitroacetanilid

8 *p*-Bromoacetanilid

9 Fenol

10 *o*-Nitrofenol

11 *p*-Nitrofenol

12 Kwas antranilowy

13 Kwas *o*-chlorobenzoesowy

14 Jodobenzen

15 Kwas cynamonowy

16 Aldehyd benzoesowy

17 *m*-Nitroanilina

18 *p*-Metyloacetofenon

19 Kwas *p*-toluilowy

20 Kwas salicylowy

21 Kwas acetylosalicylowy

22 Toluen

23 *p*-Jodonitrobenzen

24 *p*-Nitroanilina

25 Octan etylu

26 Etanol

Anilina

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

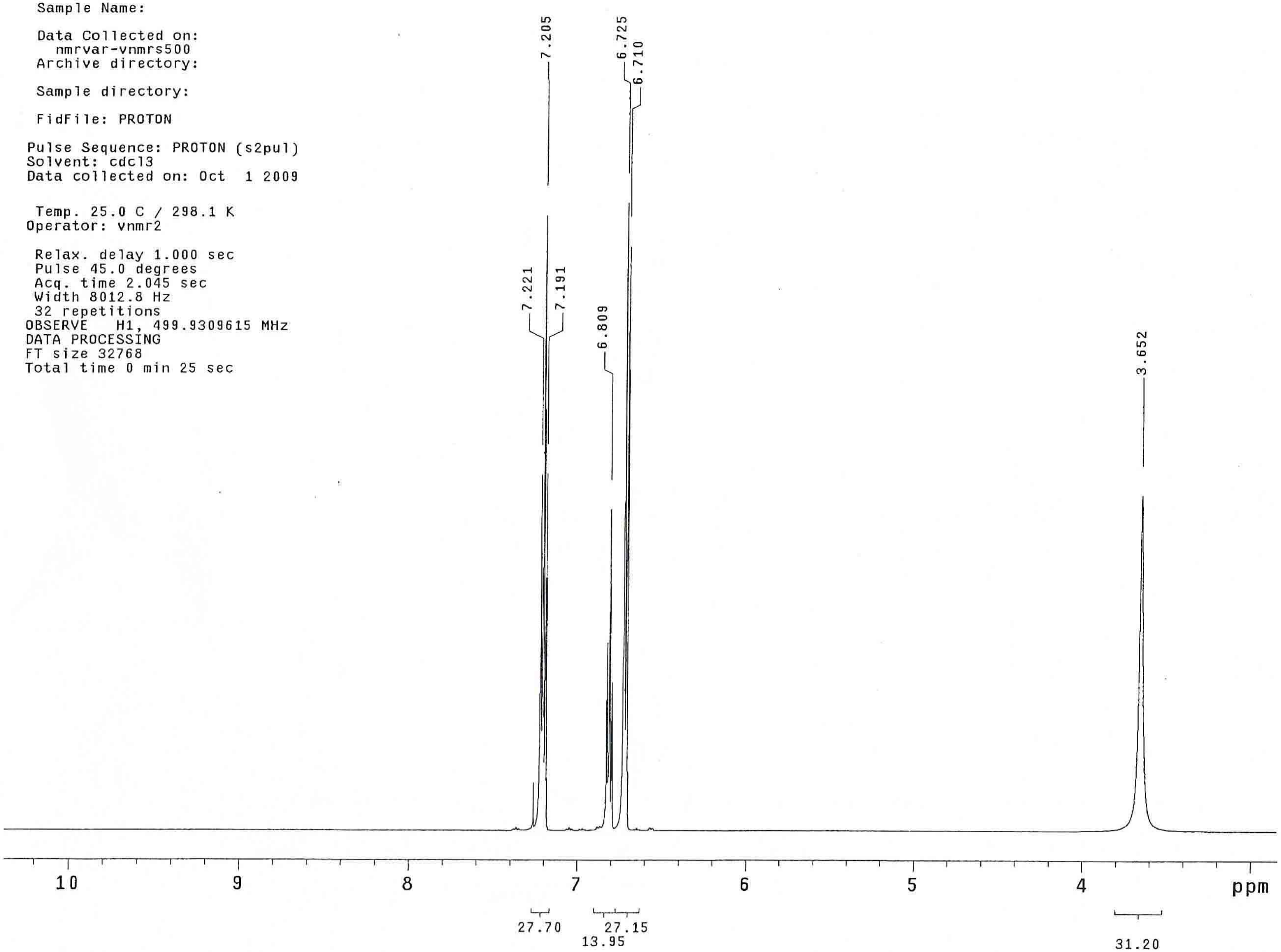
Sample directory:

FidFile: PROTON

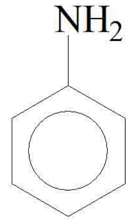
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 1 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

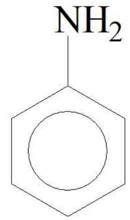
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

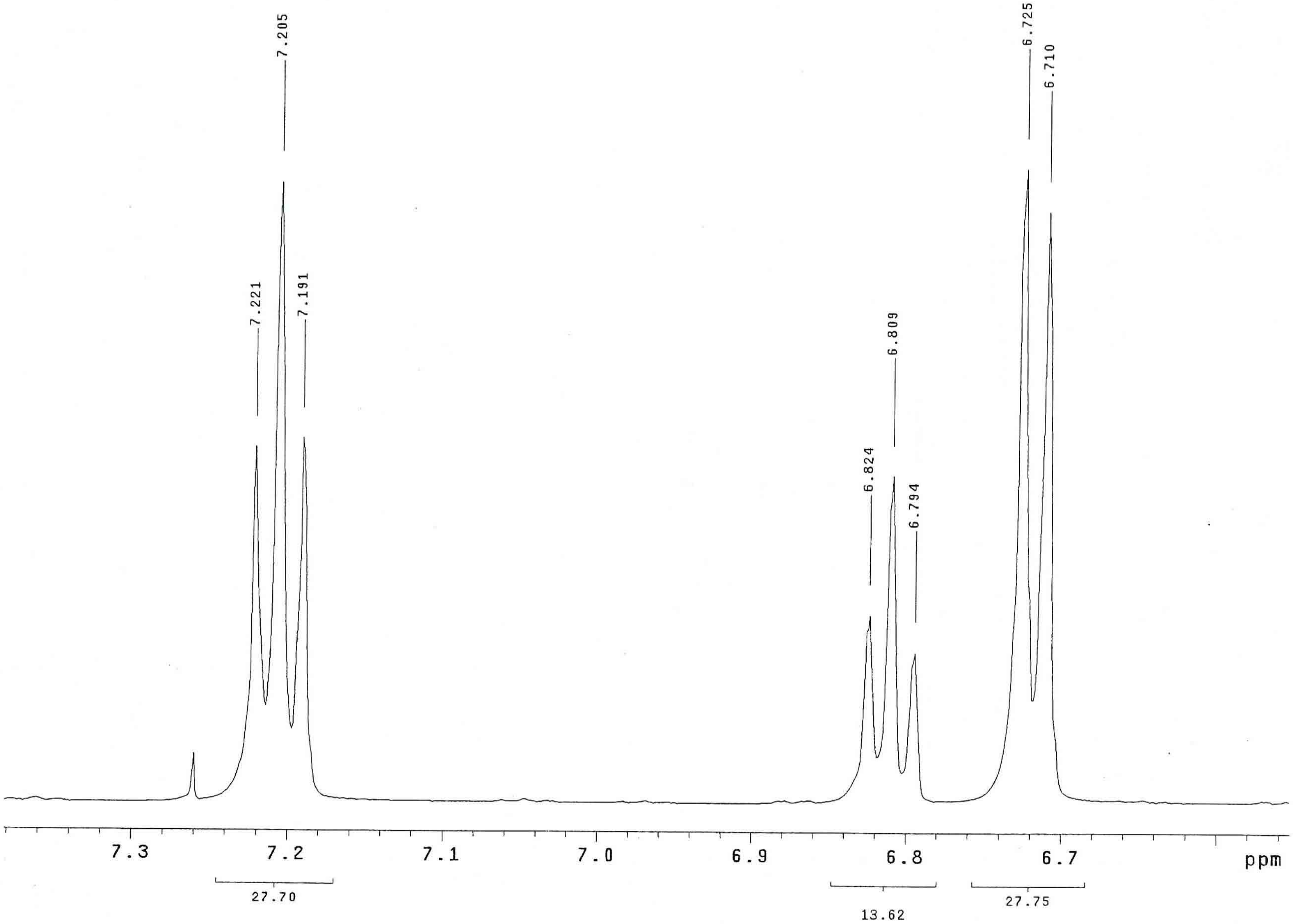


1



1


NH2

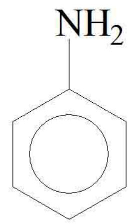

7.205
7.221
7.191
6.809
6.824
6.794
6.725
6.710
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
27.70
13.62
27.75

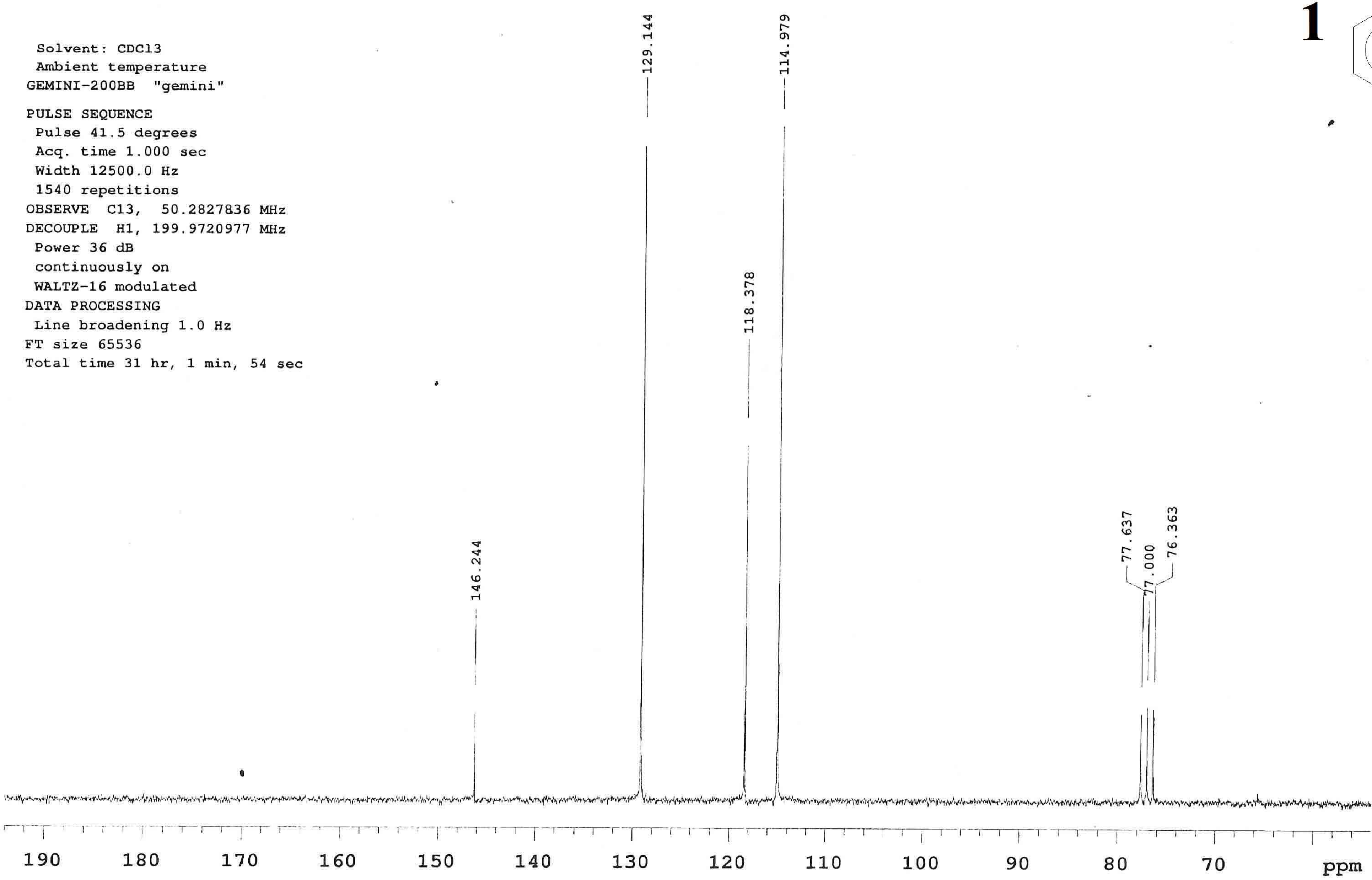
Anilina

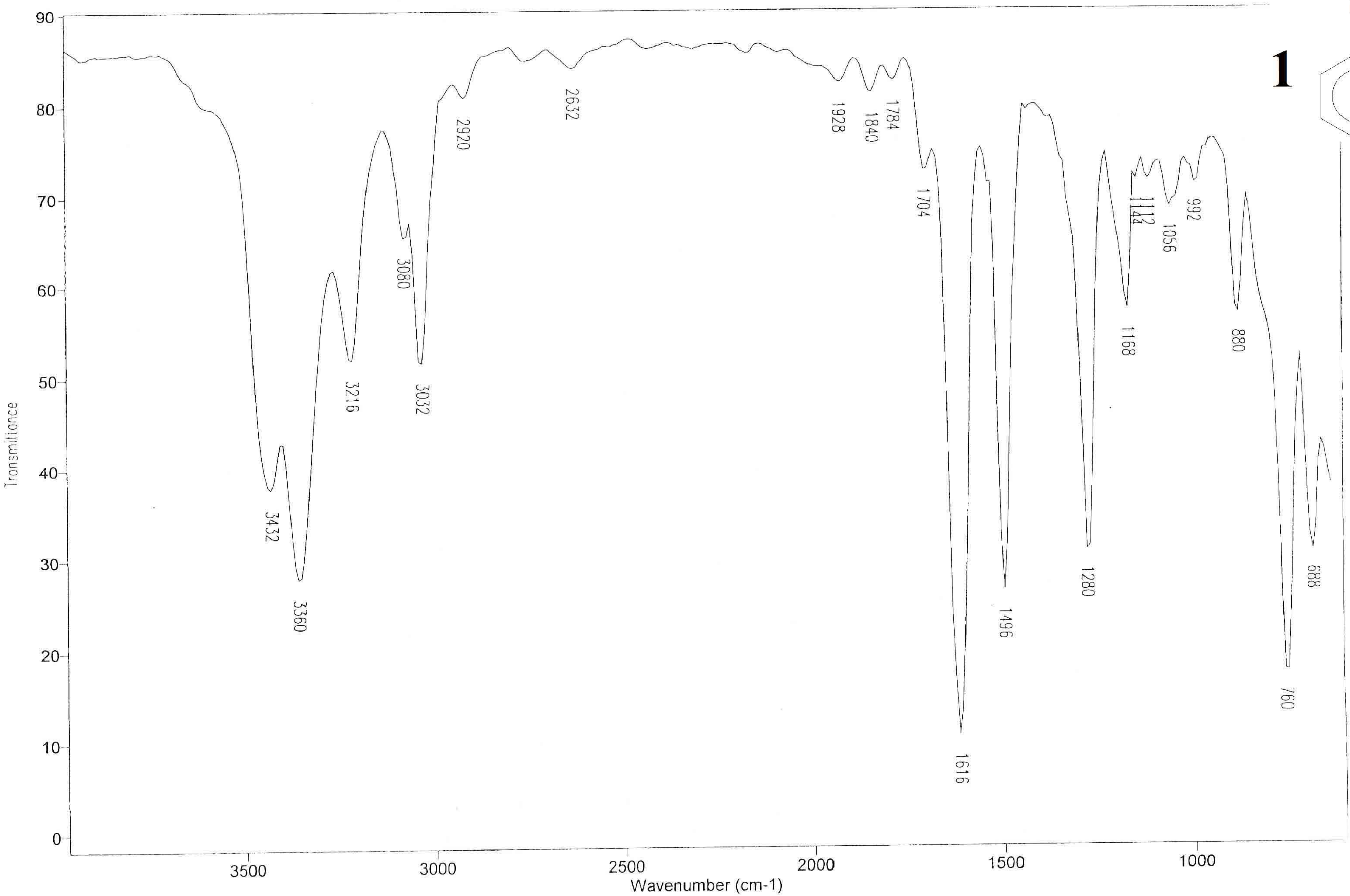
Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1540 repetitions
OBSERVE C13, 50.2827836 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

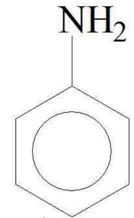
1



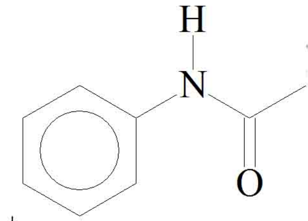


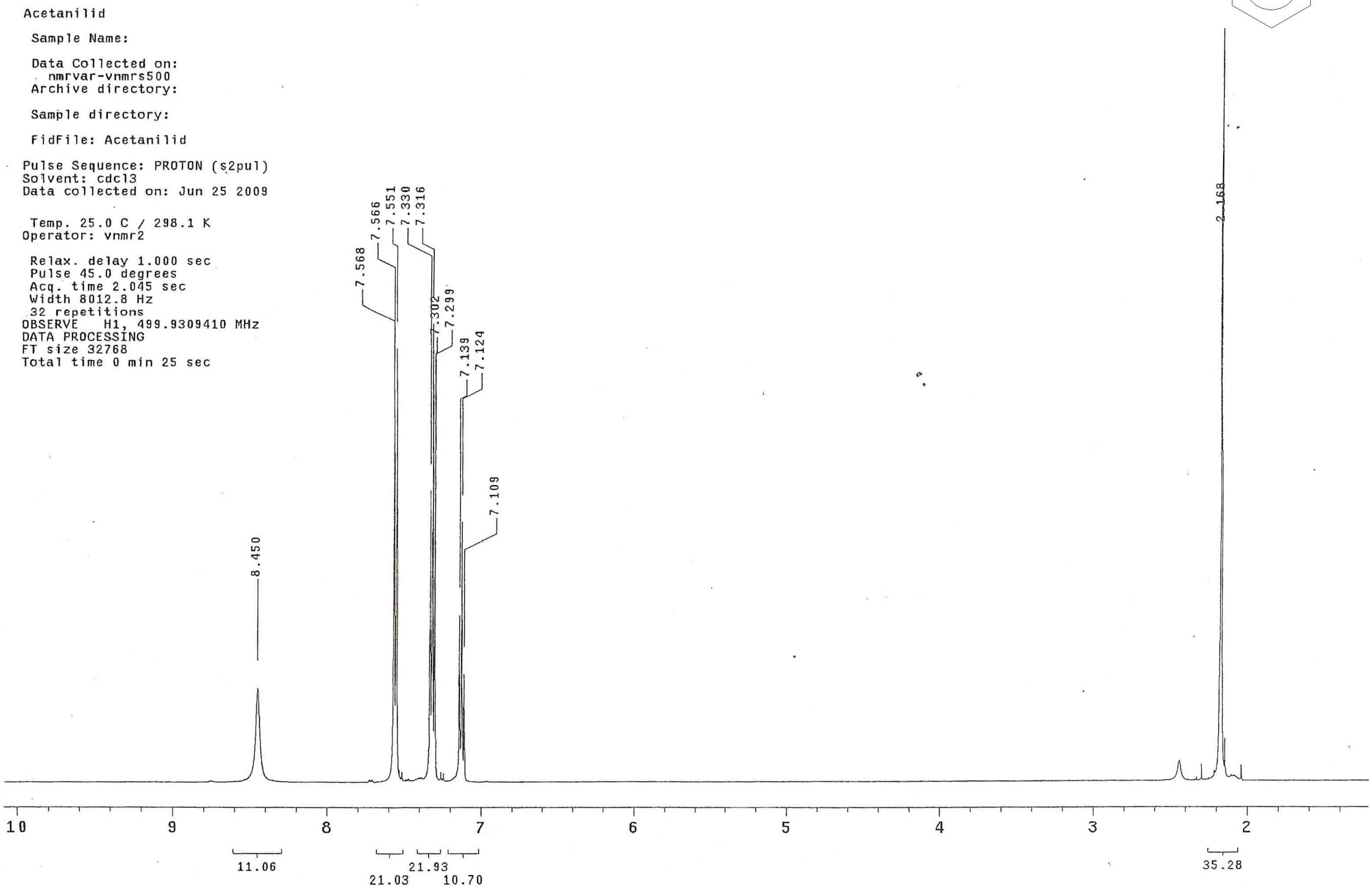

90
80
70
60
50
40
30
20
10
0
Transmittance
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
3432
3360
3216
3080
3032
2920
2632
1928
1840
1784
1704
1616
1496
1280
1168
1112
1144
1056
992
880
760
688

1


NH2

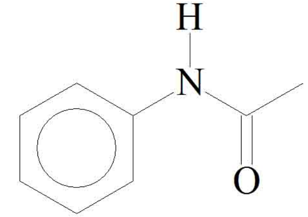
2

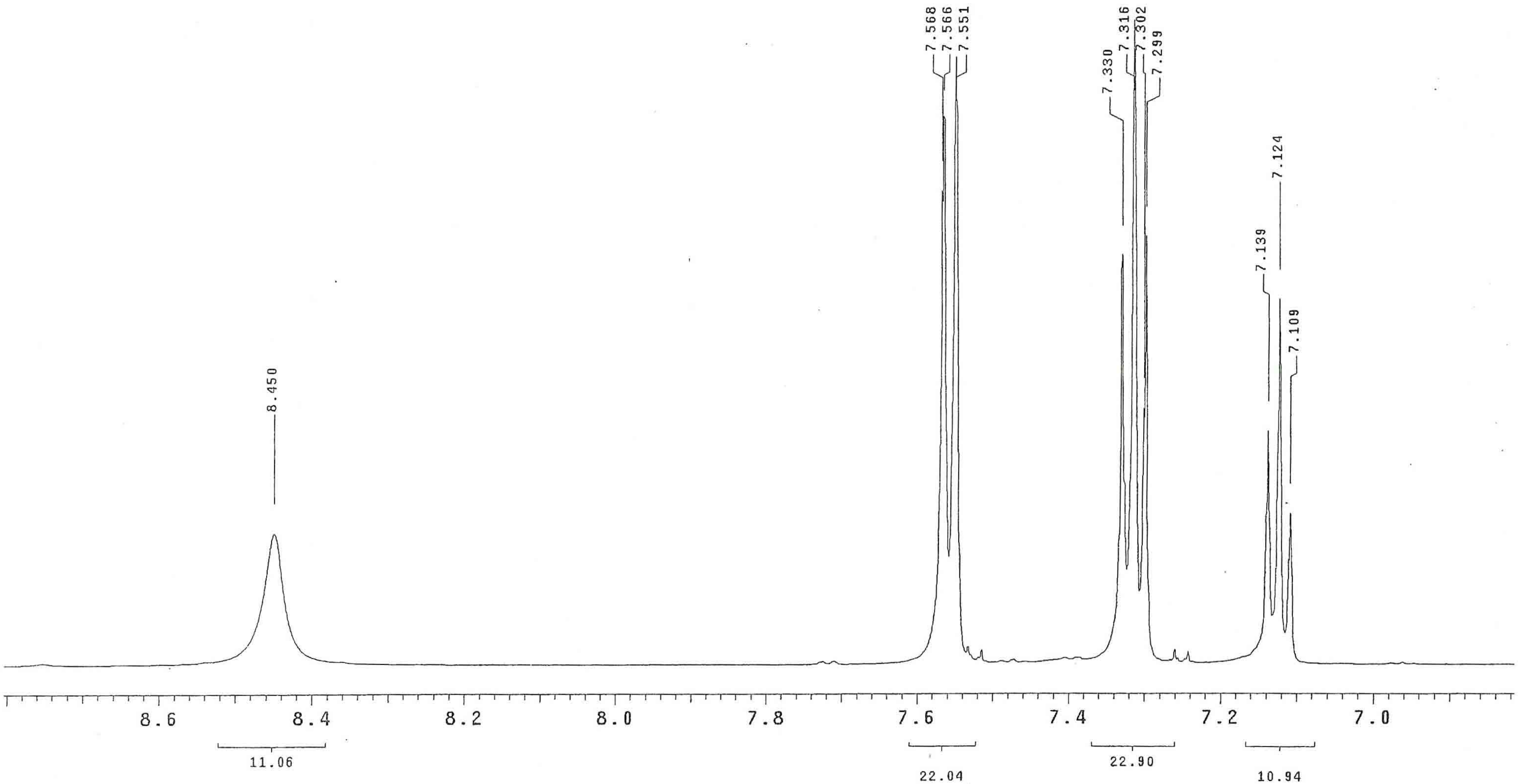




Acetanilid
Sample Name:
Data Collected on:
nmrvar-vnmrs500
Archive directory:
Sample directory:
FidFile: Acetanilid
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 25 2009
Temp. 25.0 C / 298.1 K
Operator: vnmr2
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309410 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
8.450
7.568
7.566
7.551
7.330
7.316
7.302
7.299
7.139
7.124
7.109
2.168
10
9
8
7
6
5
4
3
2
11.06
21.03
21.93
10.70
35.28

2


H
N
O

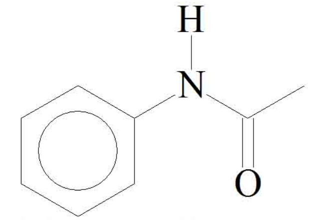

8.450
7.568
7.566
7.551
7.330
7.316
7.302
7.299
7.139
7.124
7.109
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
11.06
22.04
22.90
10.94

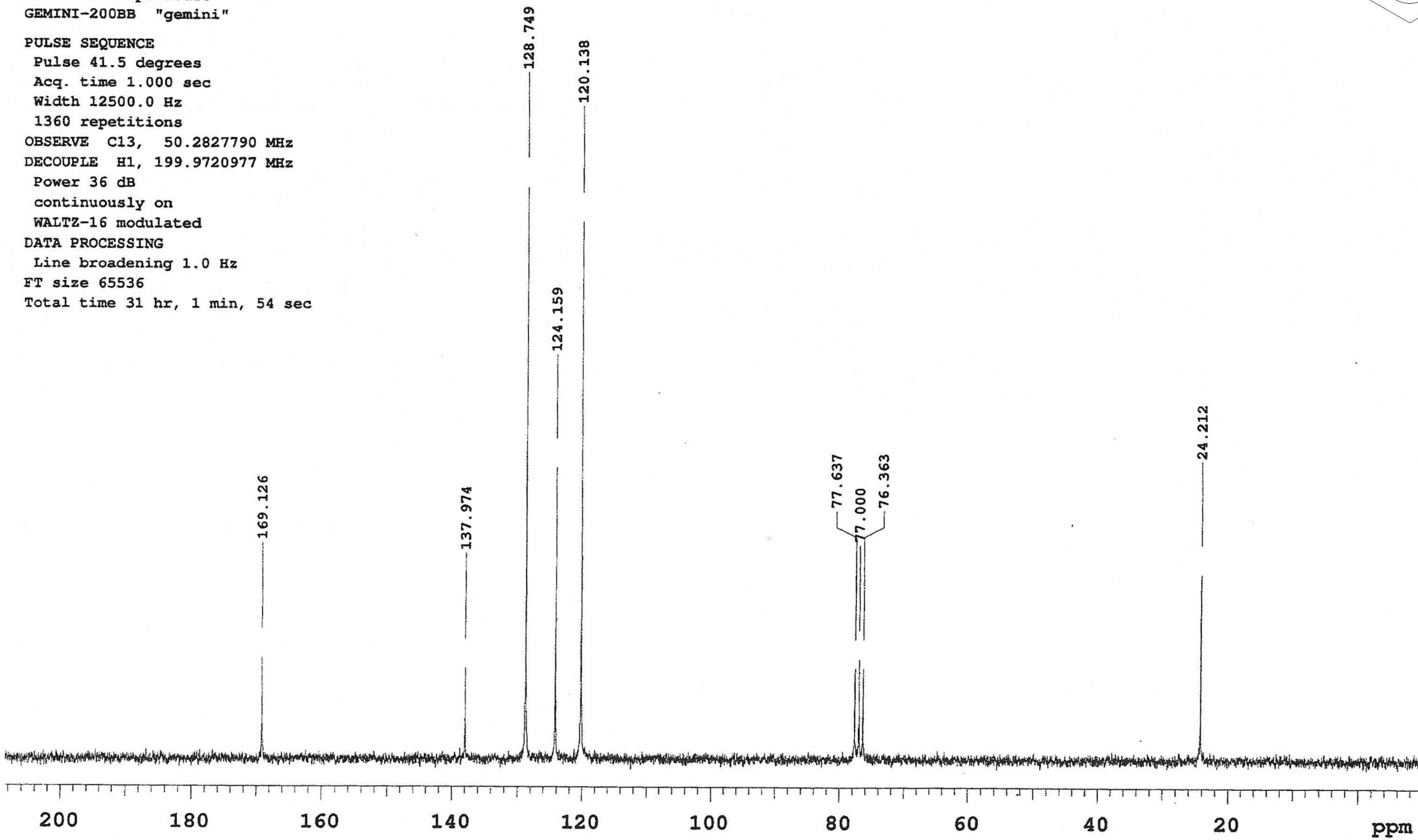
Acetanilid

Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

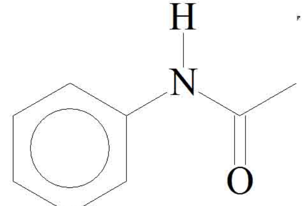
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1360 repetitions
OBSERVE C13, 50.2827790 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

2

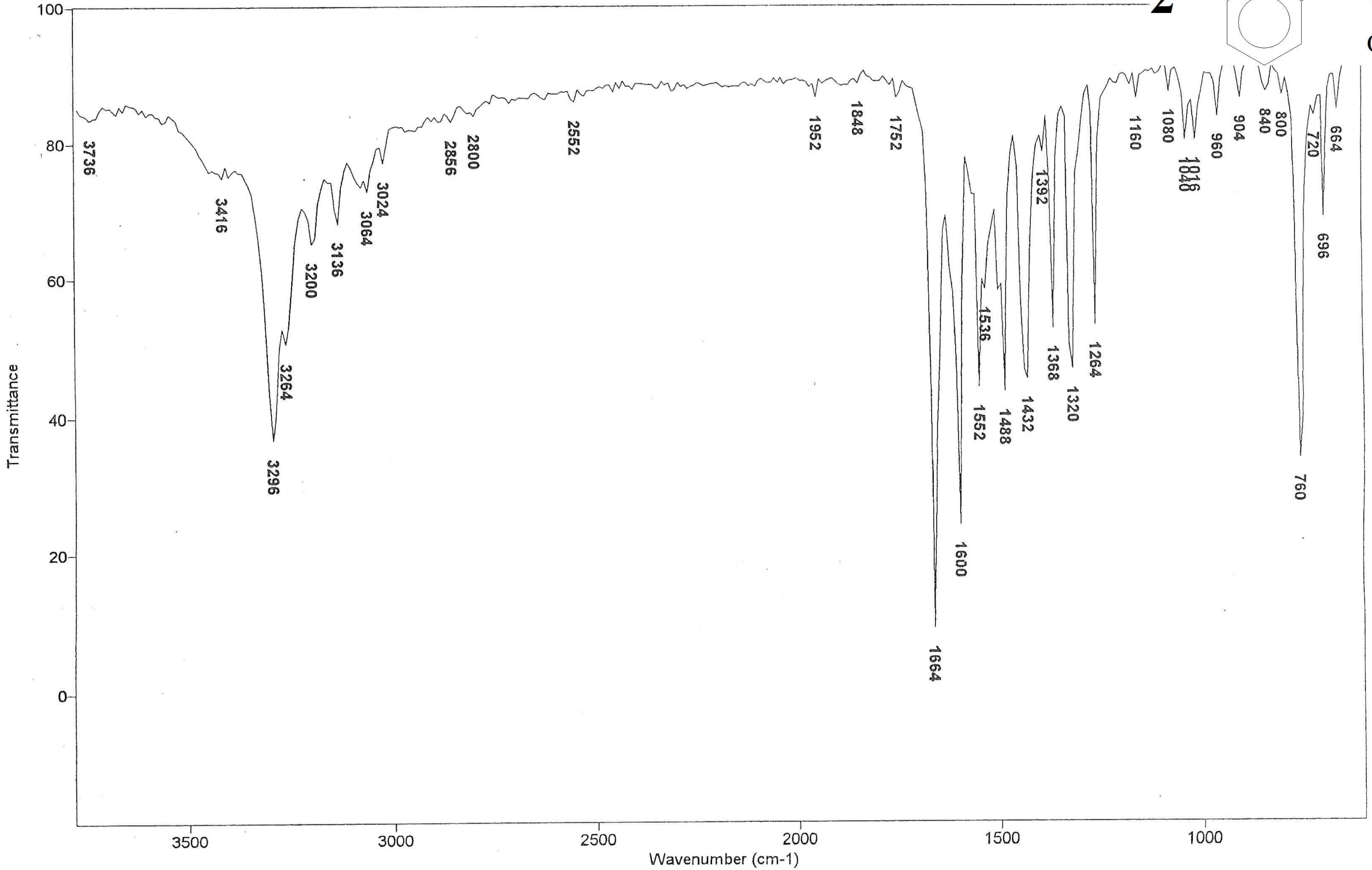




2

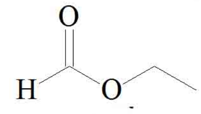


H
N
O

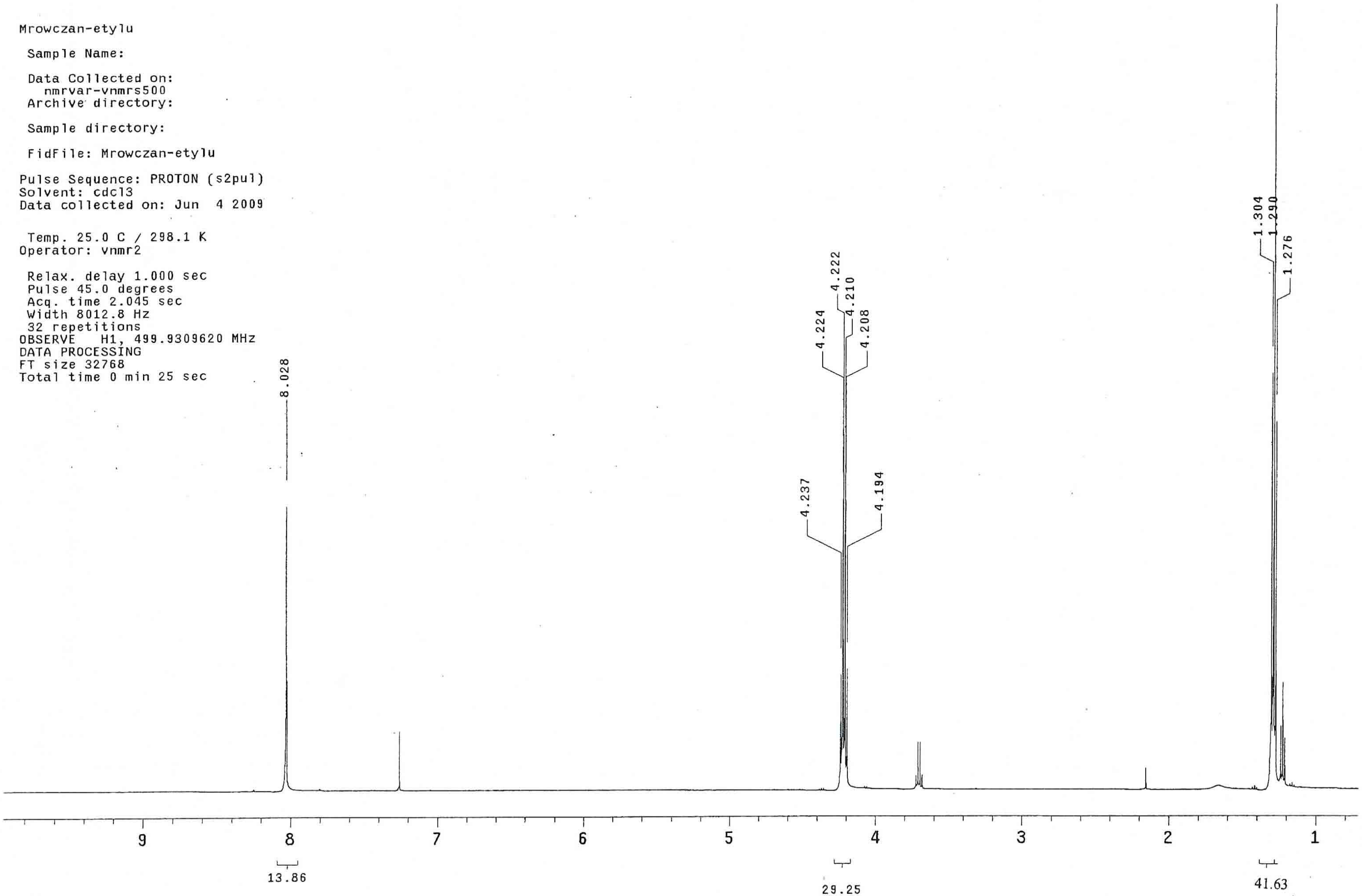


Transmittance
Wavenumber (cm-1)
100
80
60
40
20
0
3500
3000
2500
2000
1500
1000
3736
3416
3296
3264
3200
3136
3064
3024
2856
2800
2552
1952
1848
1752
1664
1600
1552
1536
1488
1432
1392
1368
1320
1264
1160
1080
1048
1016
960
904
840
800
760
720
696
664

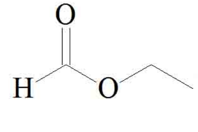
3

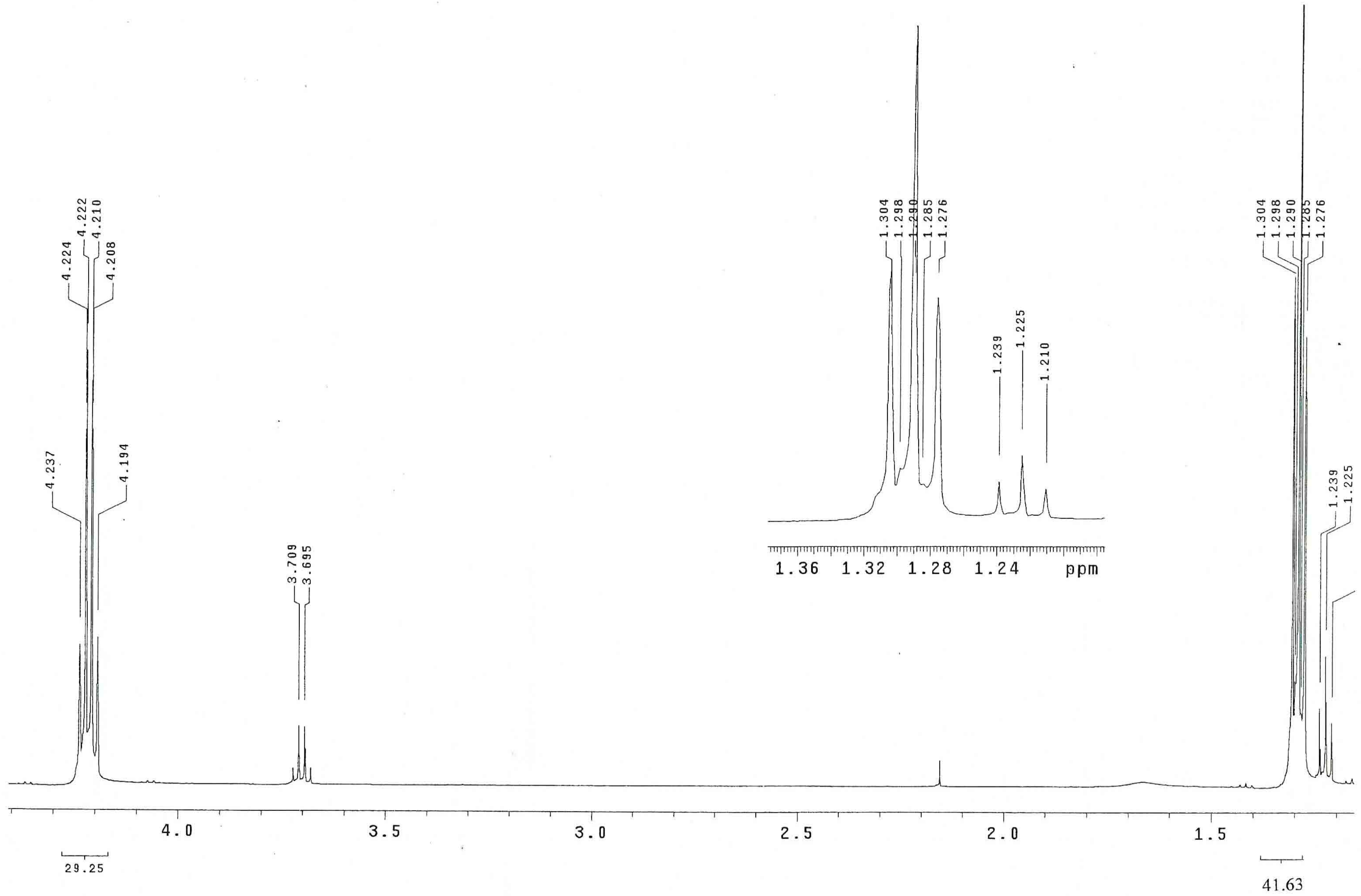



```
Mrowczan-etylu

 Sample Name:

 Data Collected on:
   nmrvar-vnmrs500
 Archive directory:

 Sample directory:

 FidFile: Mrowczan-etylu

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun  4 2009

 Temp. 25.0 C / 298.1 K
Operator: vnmr2

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.045 sec
 Width 8012.8 Hz
 32 repetitions
OBSERVE   H1, 499.9309620 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
```



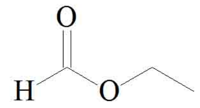
3




4.237
4.224
4.222
4.210
4.208
4.194
3.709
3.695
1.304
1.298
1.290
1.285
1.276
1.239
1.225
1.210
1.36 1.32 1.28 1.24 ppm
4.0
3.5
3.0
2.5
2.0
1.5
29.25
41.63

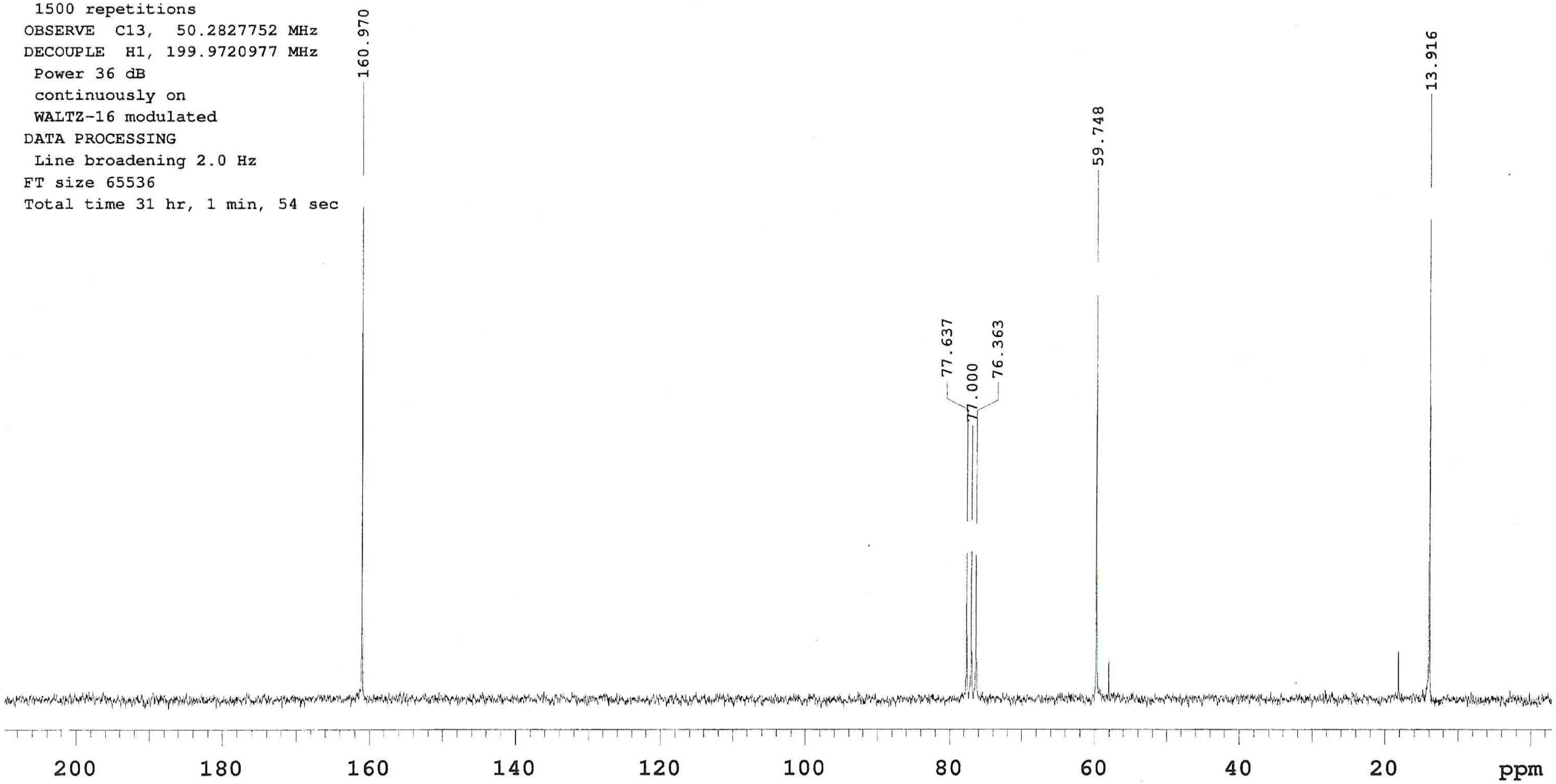
Mrowczan_etylu

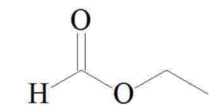
3



Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827752 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

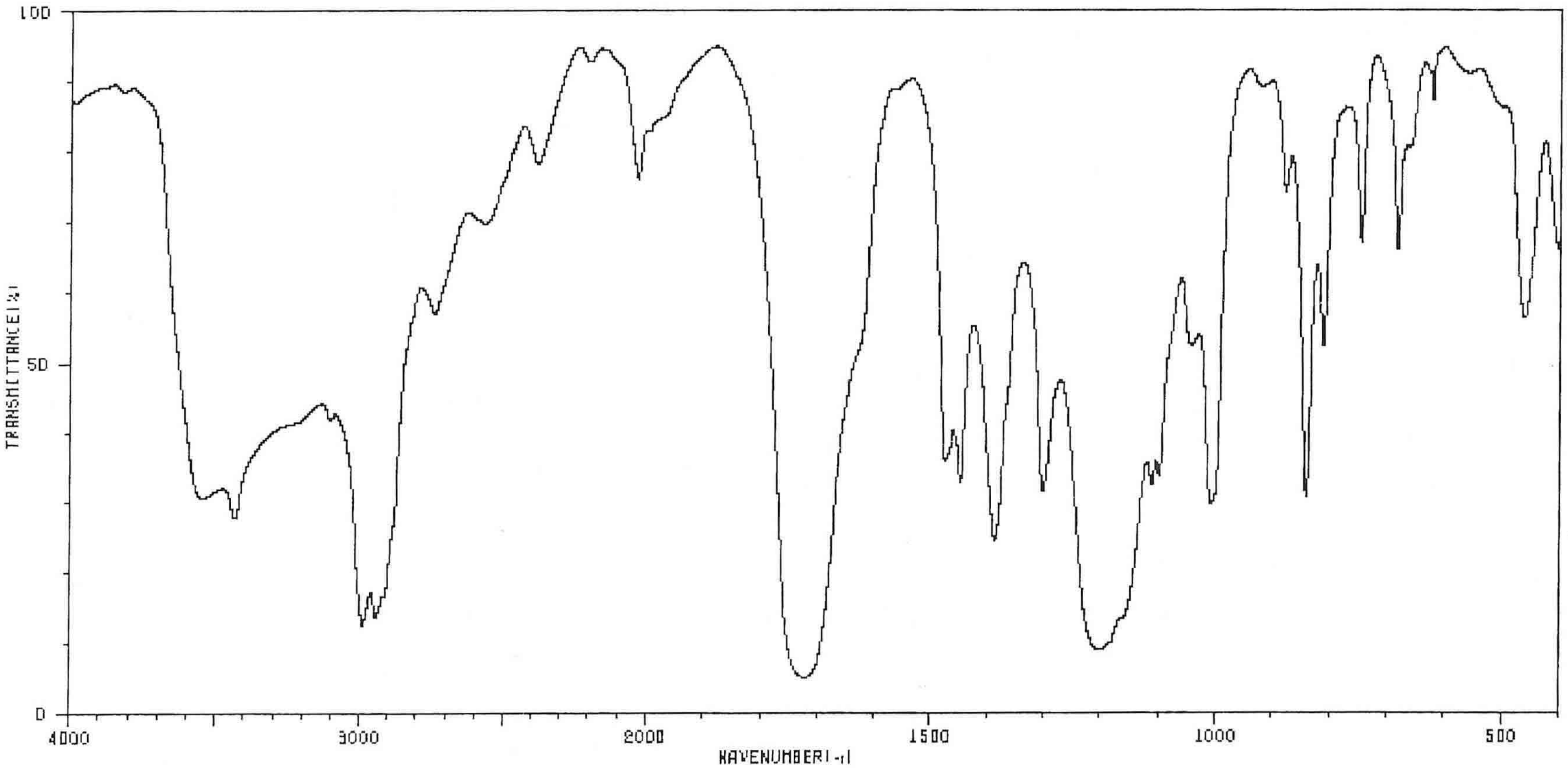


3 

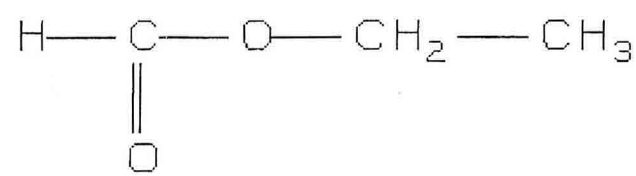
HIT-NO=1311	SCORE= ( )	SDBS-NO=1216	IR-NIDA-09170 : LIQUID FILM

ETHYL FORMATE

$C_3H_6O_2$



3646	29	2030	72	1206	8	880	70	462	63
3432	26	1726	4	1200	8	842	29		
2967	12	1721	4	1113	31	813	50		
2943	13	1477	34	1100	32	748	64		
2739	55	1449	31	1043	50	684	64		
2567	66	1388	29	1010	28	668	77		
2383	74	1303	30	920	86	623	84		



Źródło: ***https://sdbs.db.aist.go.jp***

4 HCOOH

Kwas-mrowkowy

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

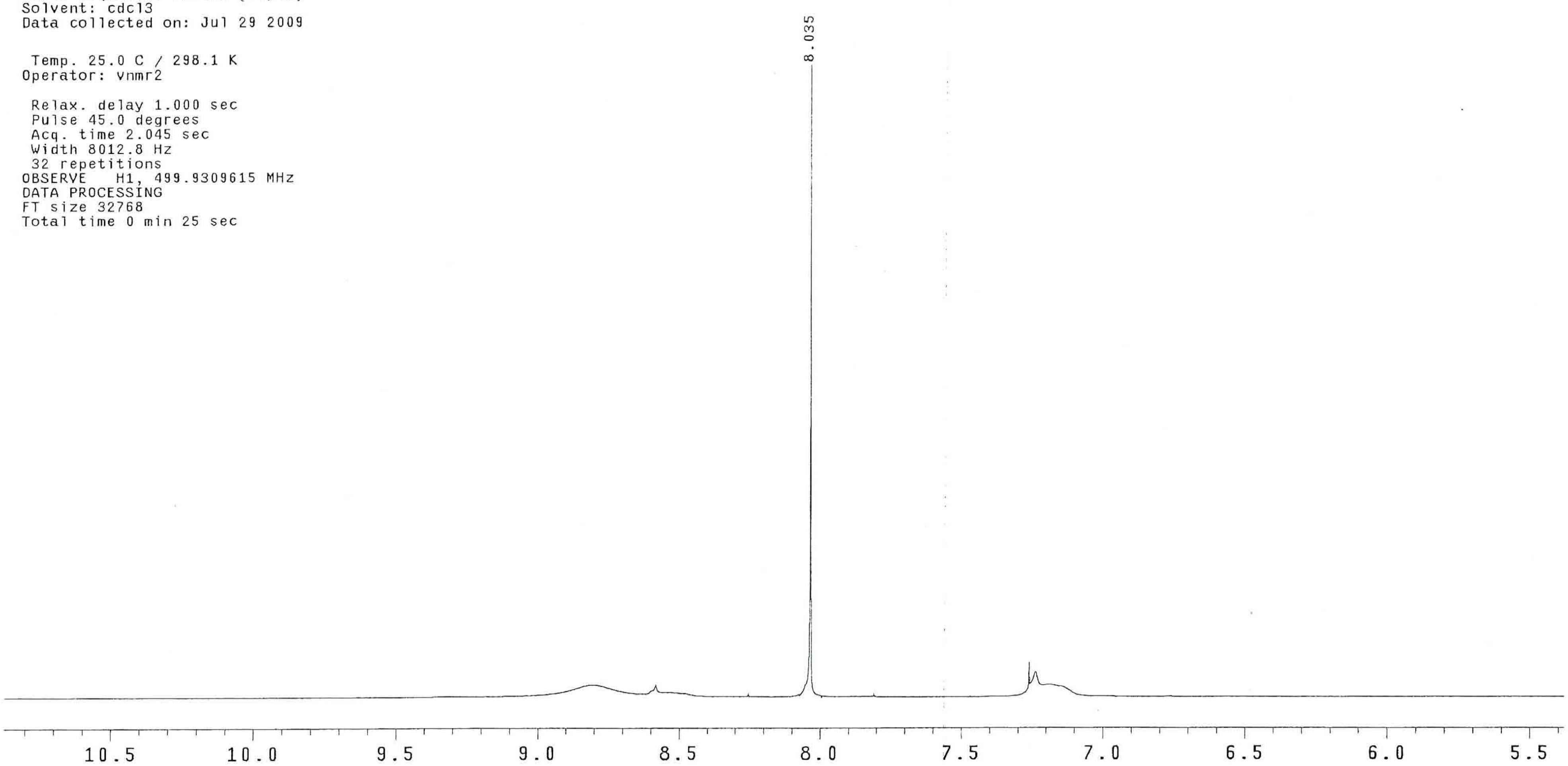
Sample directory:

FidFile: Kwas-mrowkowy

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 29 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

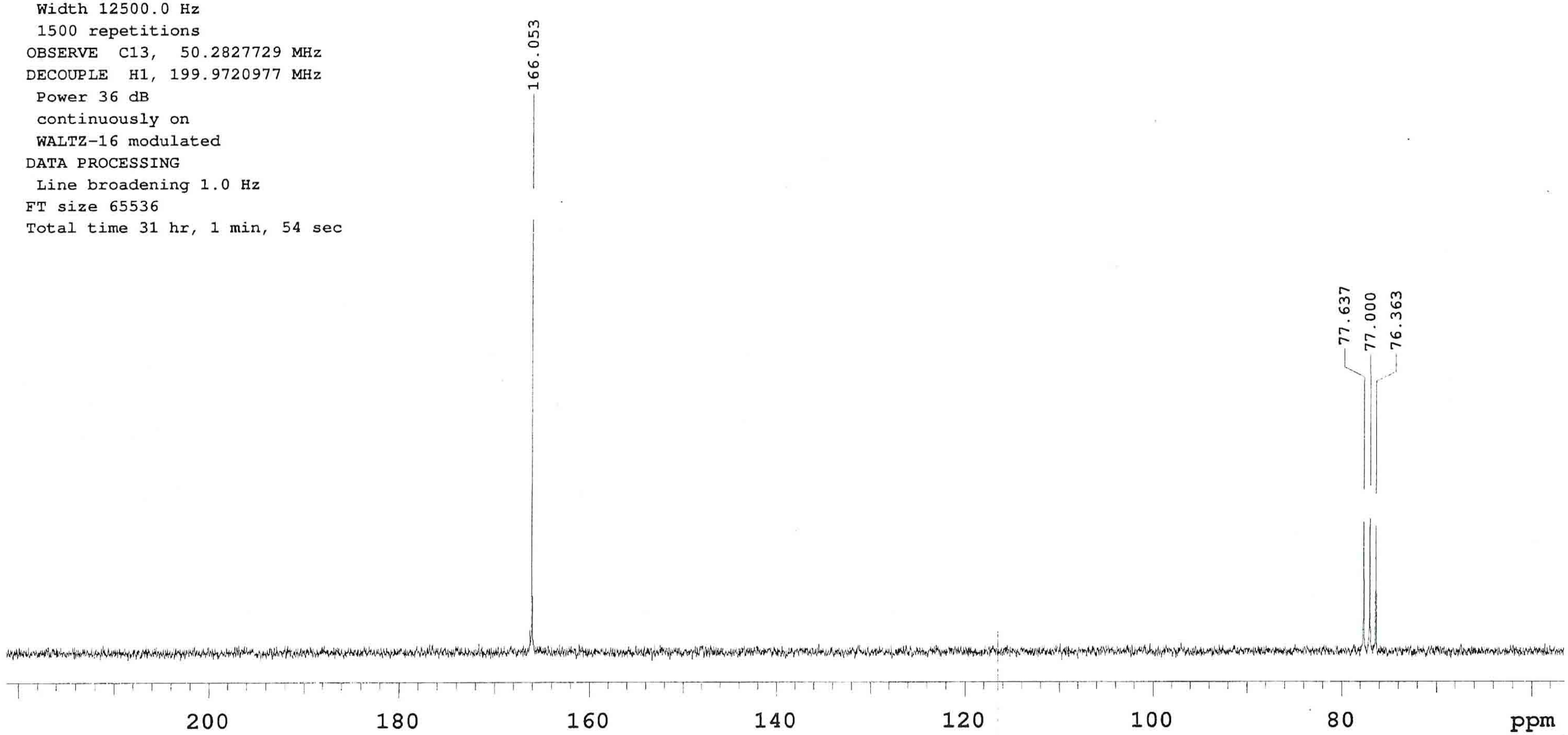


4 HCOOH

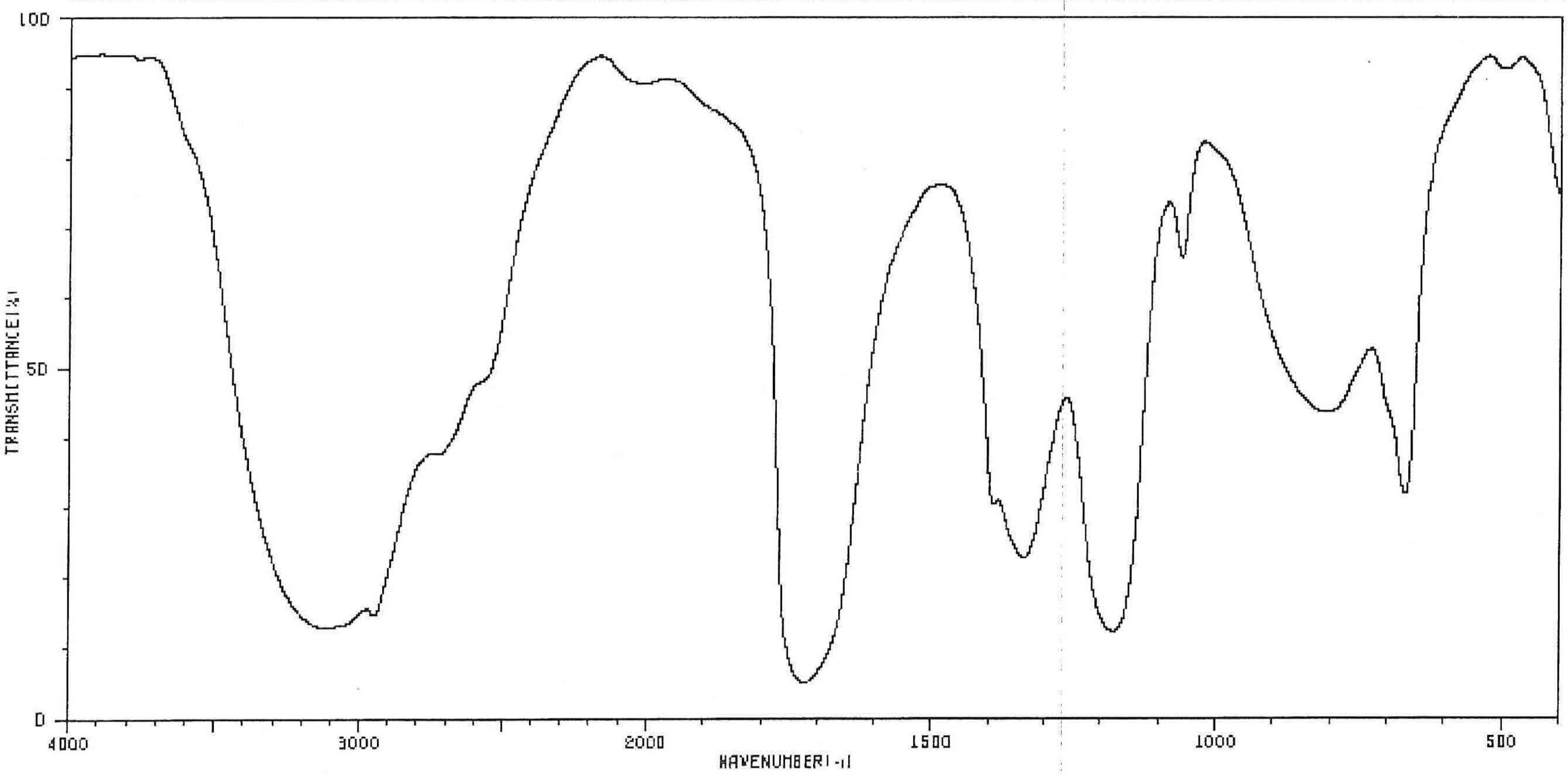
Kwas_mrowkowy

Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827729 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

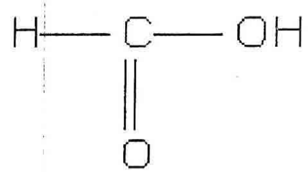


HIT-NO=4173	SCORE= ( )	SDBS-NO=10523	IR-NIDA-60826 : LIQUID FILM
FORMIC ACID			
CH_2O_2			



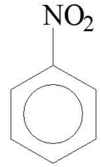
1727	4
1722	4
1338	21
1180	11
1062	64
671	30

Źródło: ***https://sdbs.db.aist.go.jp***

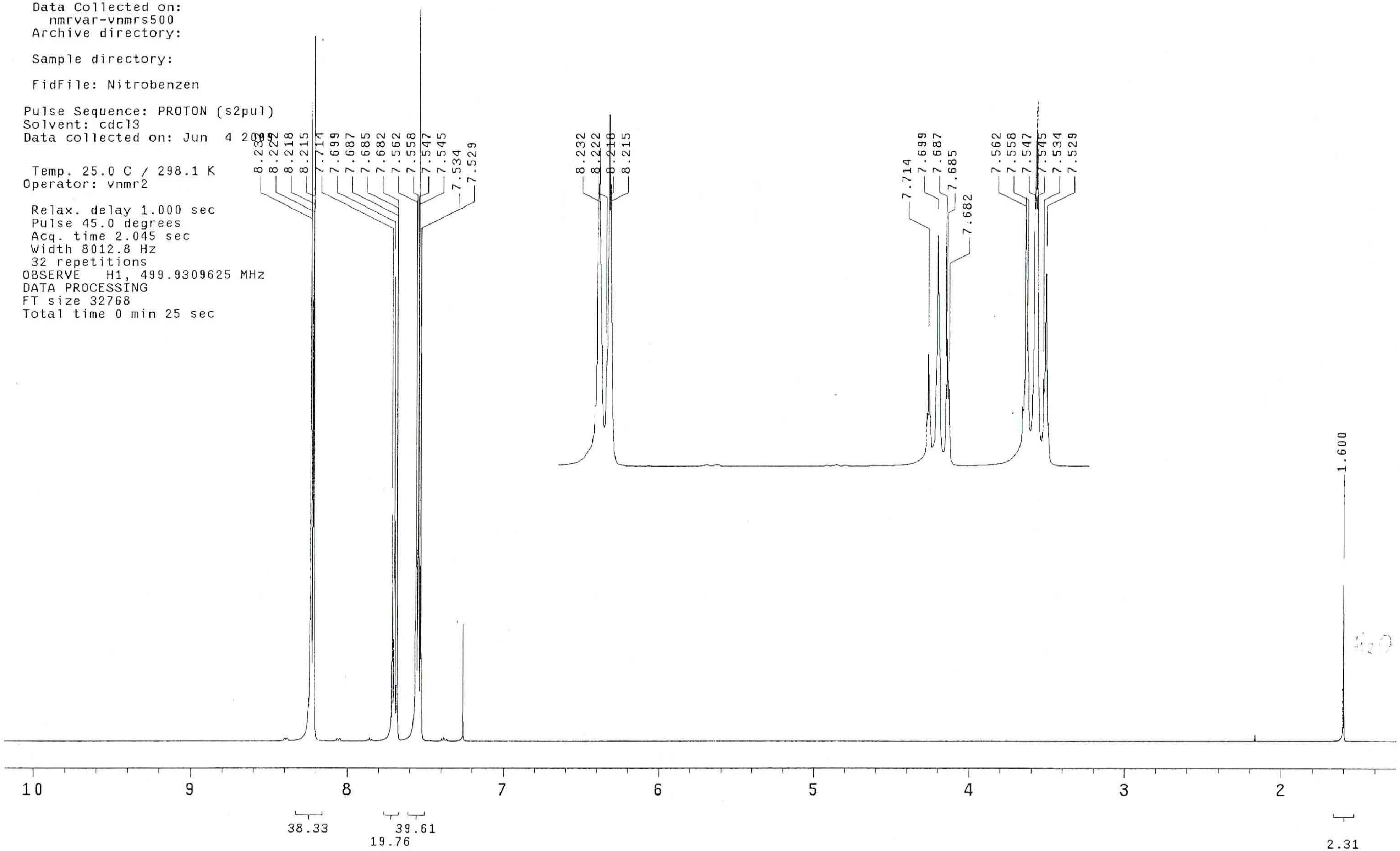


Nitrobenzen

5

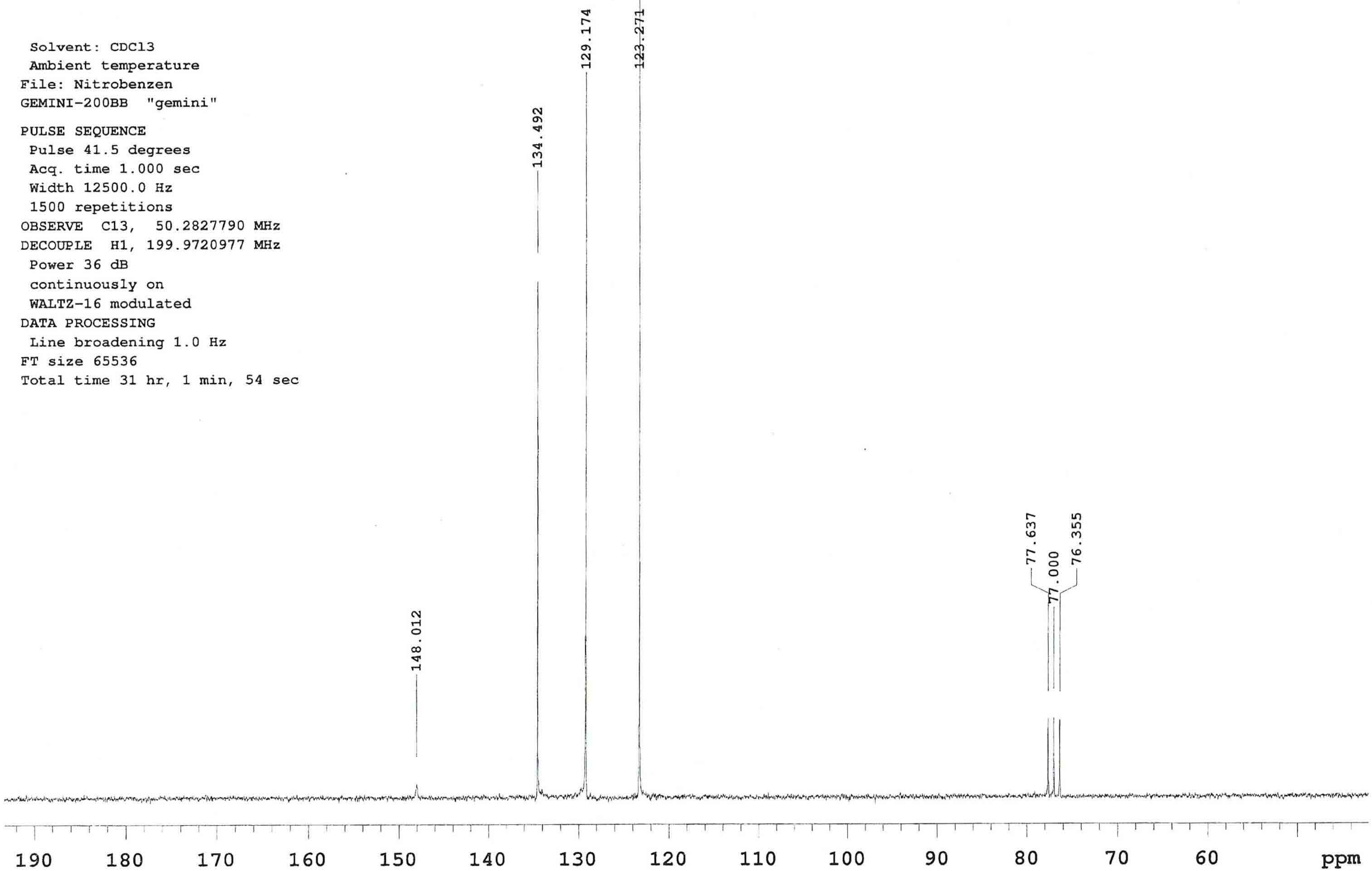



```
STANDARD PROTON PARAMETERS

 Sample Name:

 Data Collected on:
   nmrvar-vnmrs500
 Archive directory:

 Sample directory:

 FidFile: Nitrobenzen

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun  4 2009

 Temp. 25.0 C / 298.1 K
Operator: vnmr2

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.045 sec
 Width 8012.8 Hz
 32 repetitions
OBSERVE   H1, 499.9309625 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
```

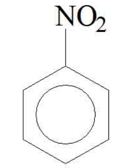


Nitrobenzen

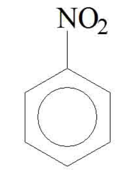
Solvent: CDCl3
Ambient temperature
File: Nitrobenzen
GEMINI-200BB "gemini"
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827790 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

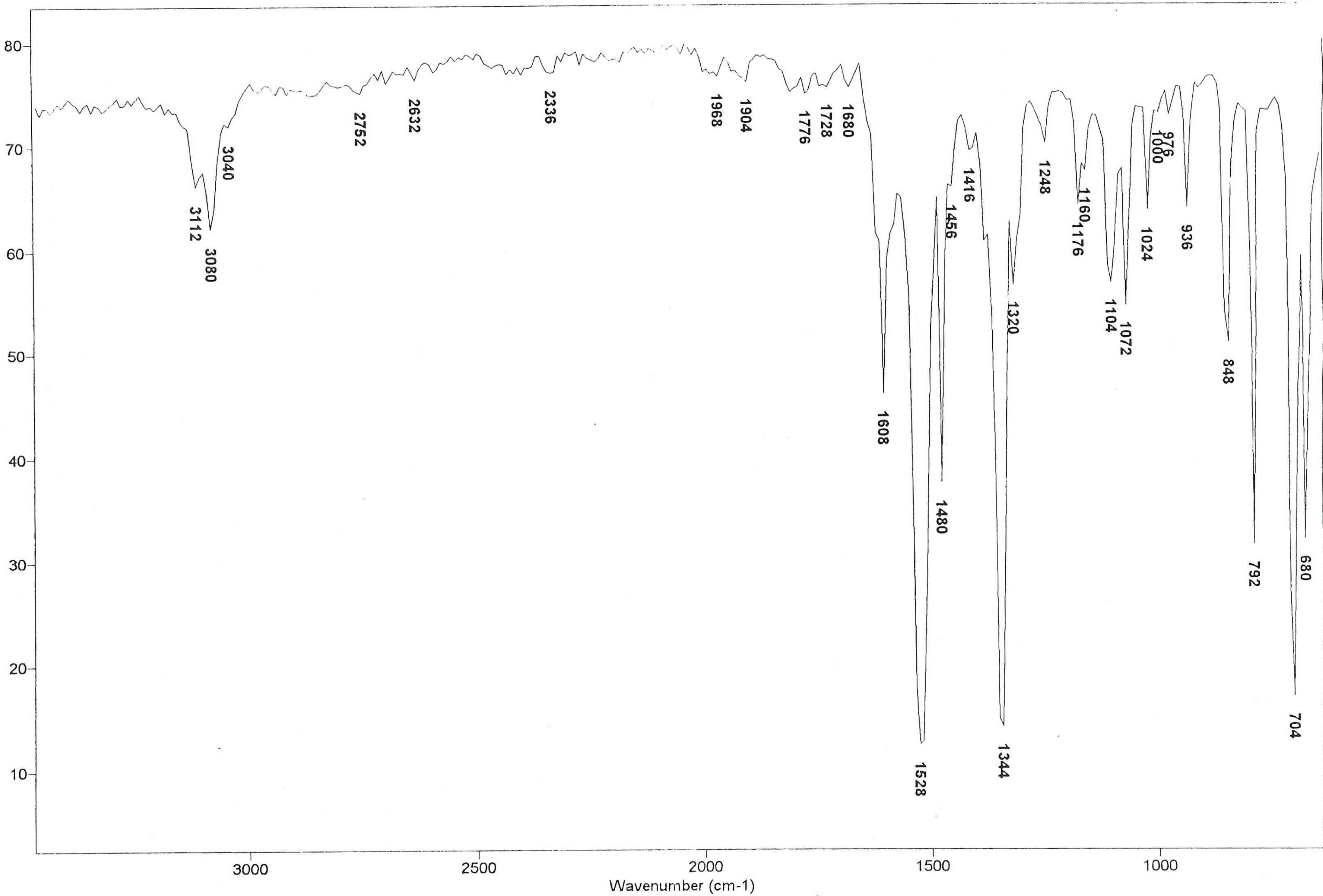


5

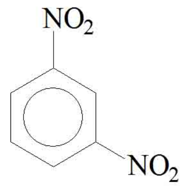


5


NO2


80
70
60
50
40
30
20
10
3000
2500
2000
1500
1000
Wavenumber (cm-1)
3112
3080
3040
2752
2632
2336
1968
1904
1776
1728
1680
1608
1528
1480
1456
1416
1344
1320
1248
1176
1160
1104
1072
1024
1000
976
936
848
792
704
680

6



m-Dinitrobenzen

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

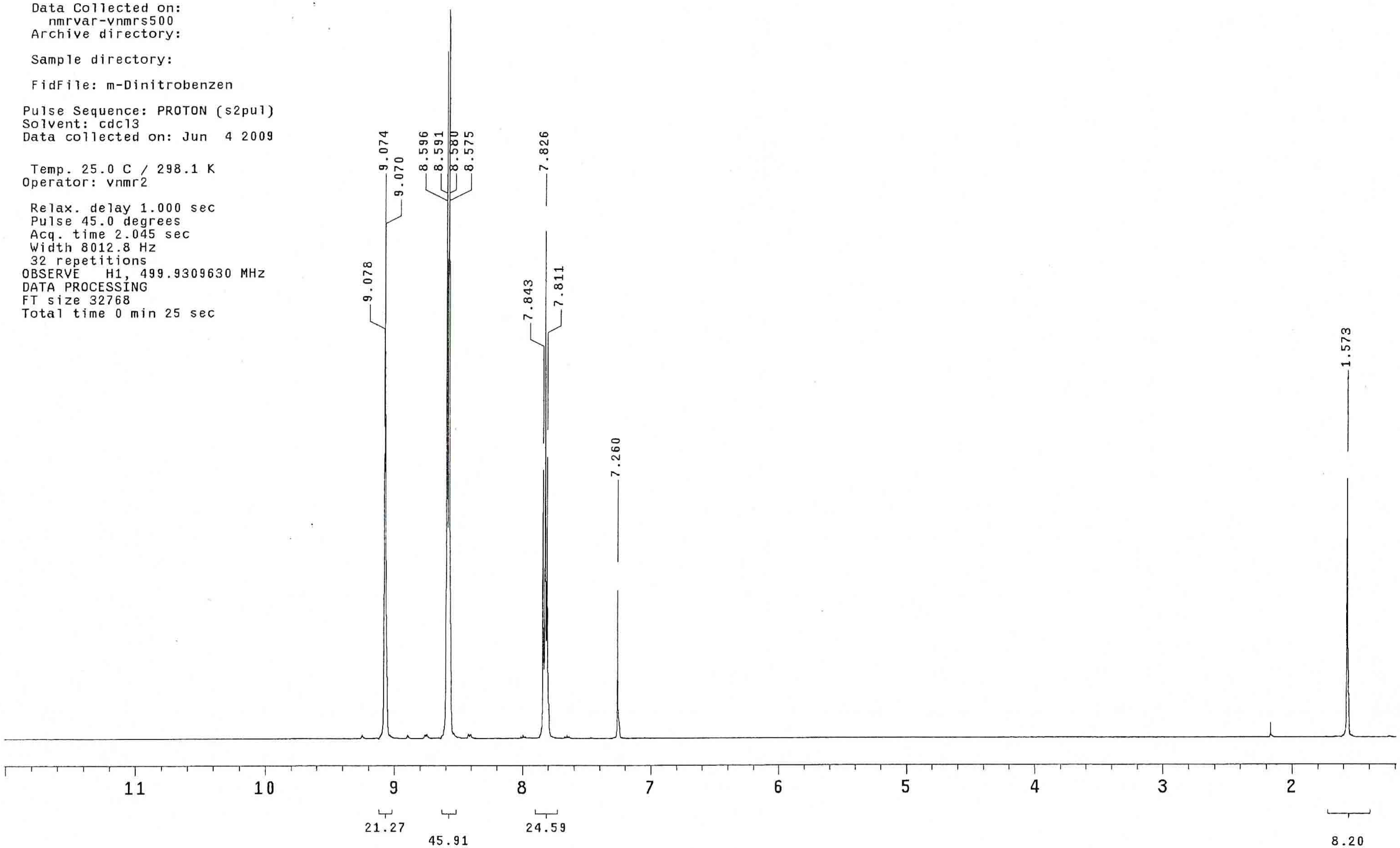
Sample directory:

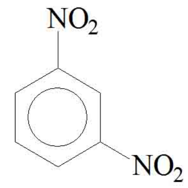
FidFile: m-Dinitrobenzen

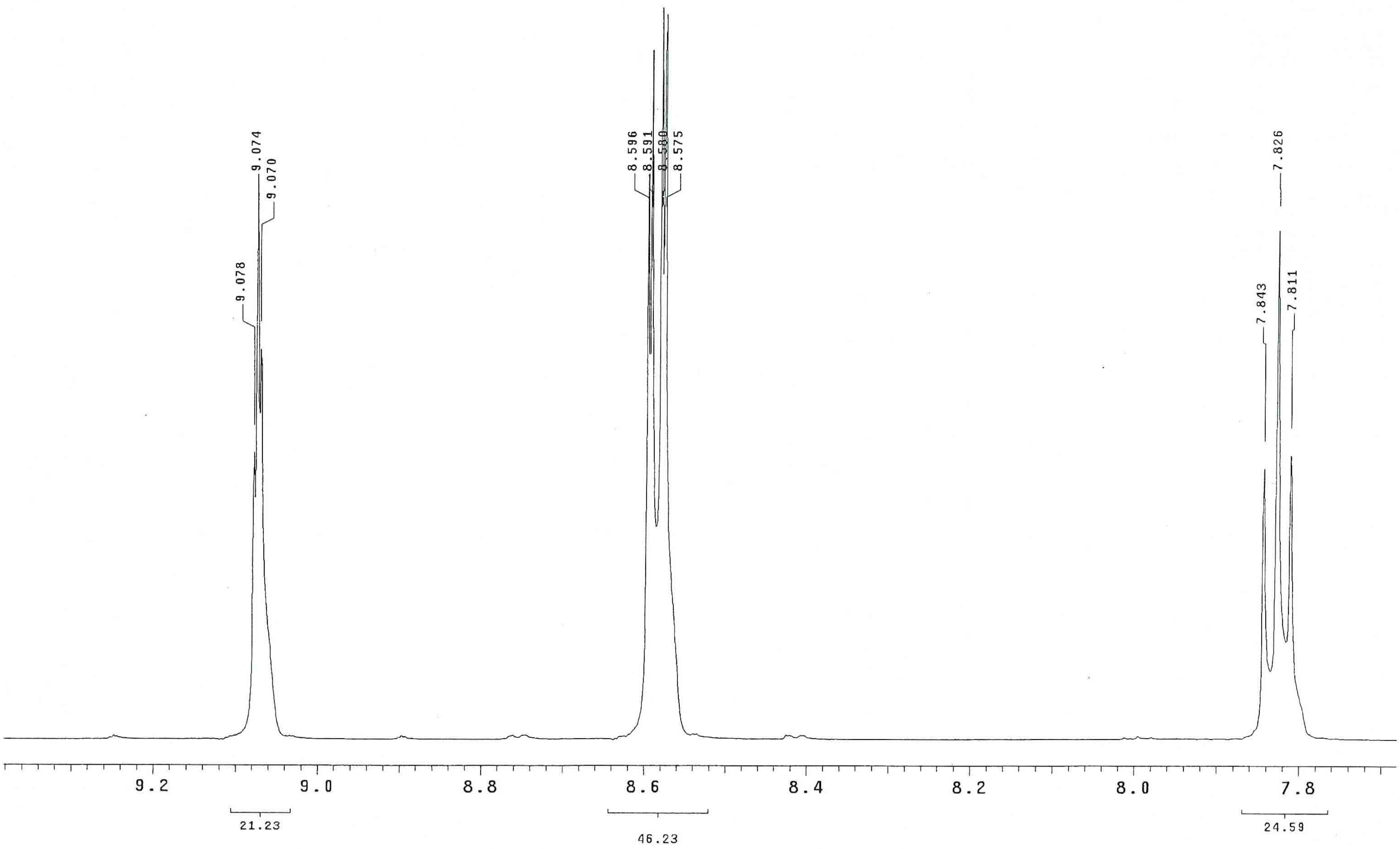
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 4 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309630 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

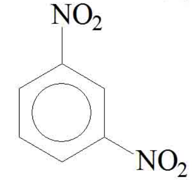


6 
NO2
NO2


9.078
9.074
9.070
8.596
8.591
8.580
8.575
7.843
7.826
7.811
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
21.23
46.23
24.59

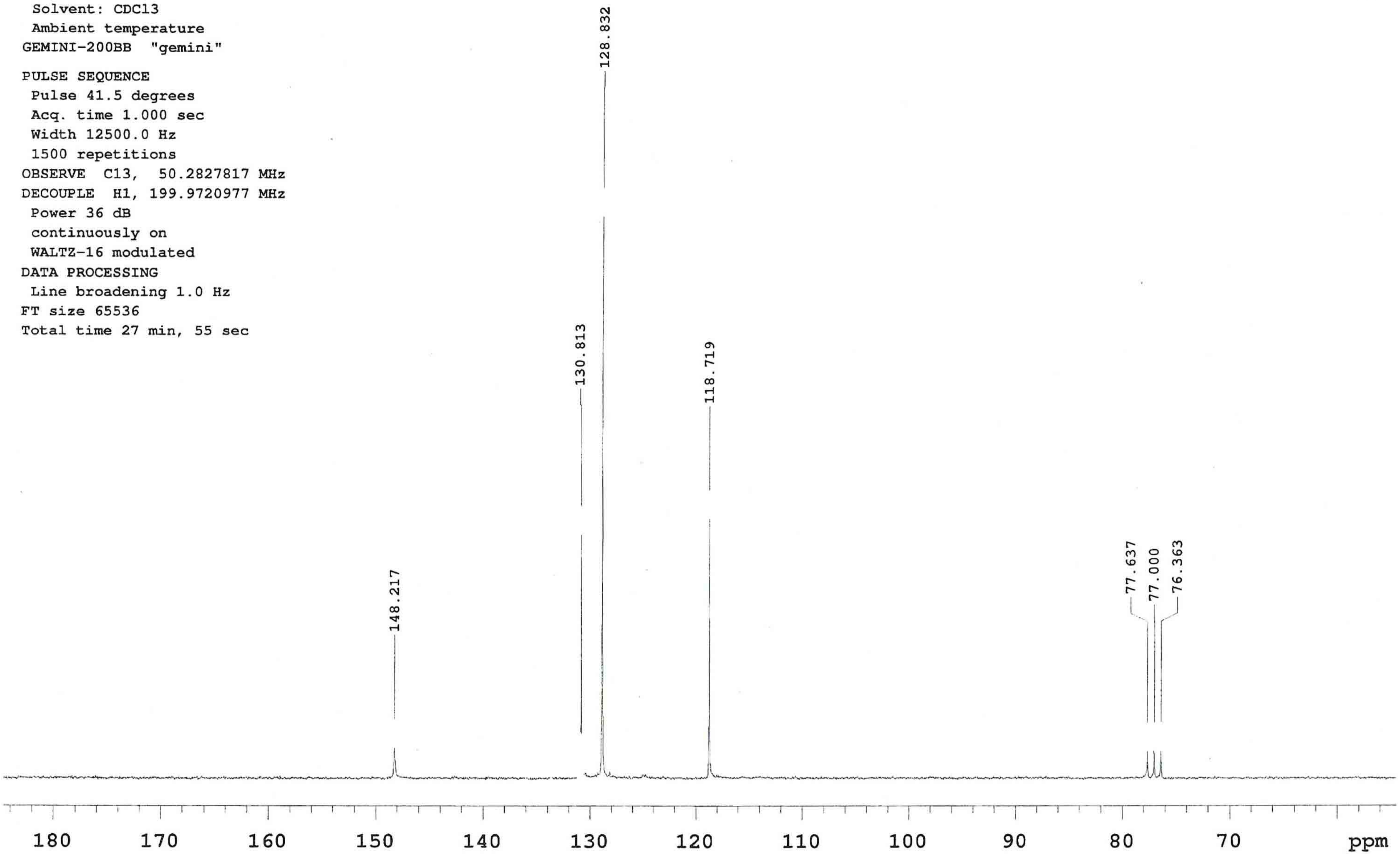
m-Dinitrobenzen

6

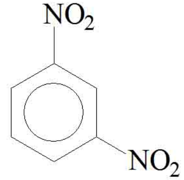


Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

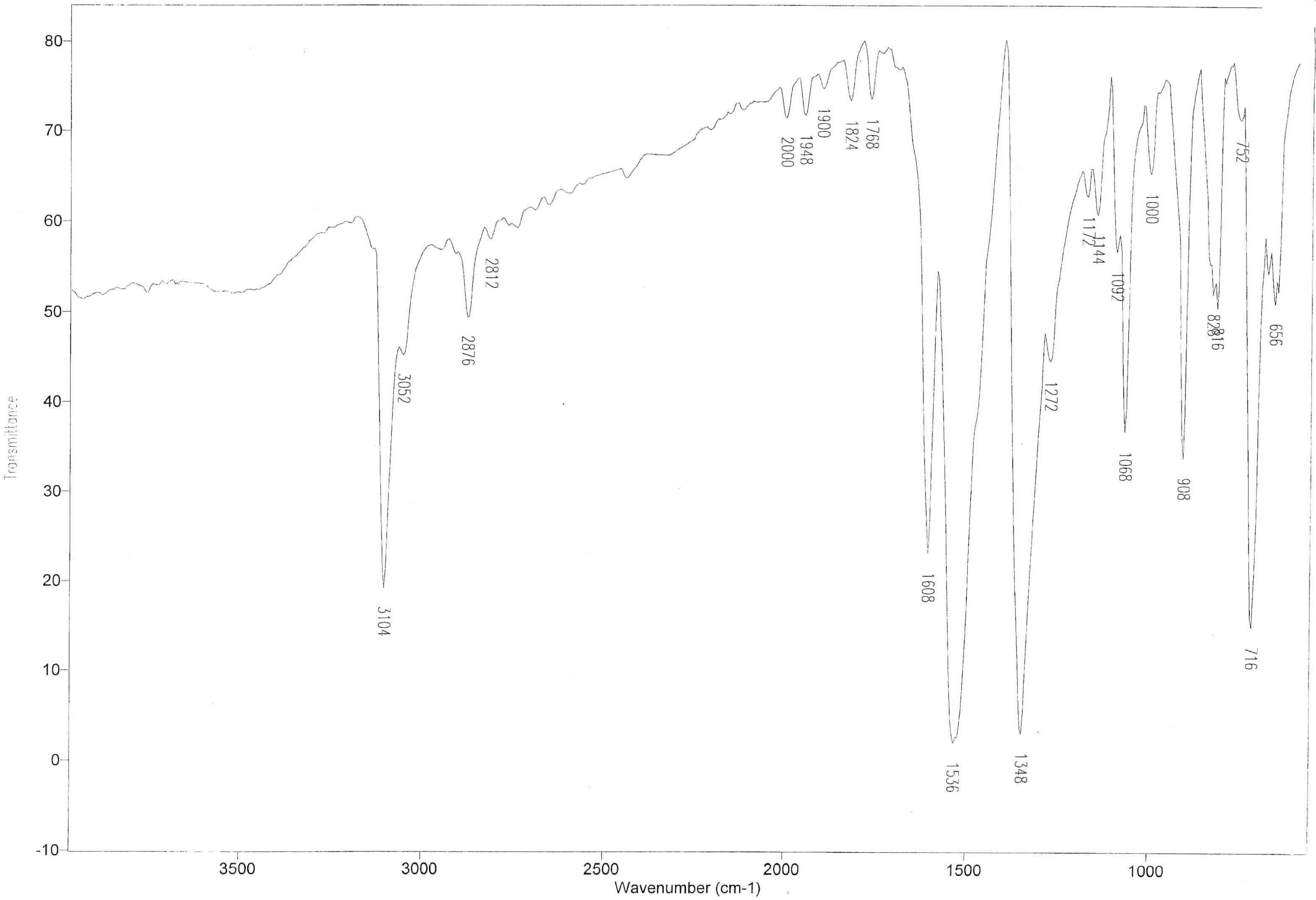
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827817 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 27 min, 55 sec



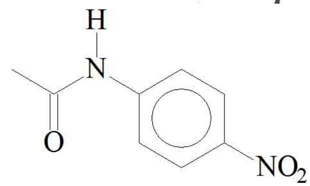
6



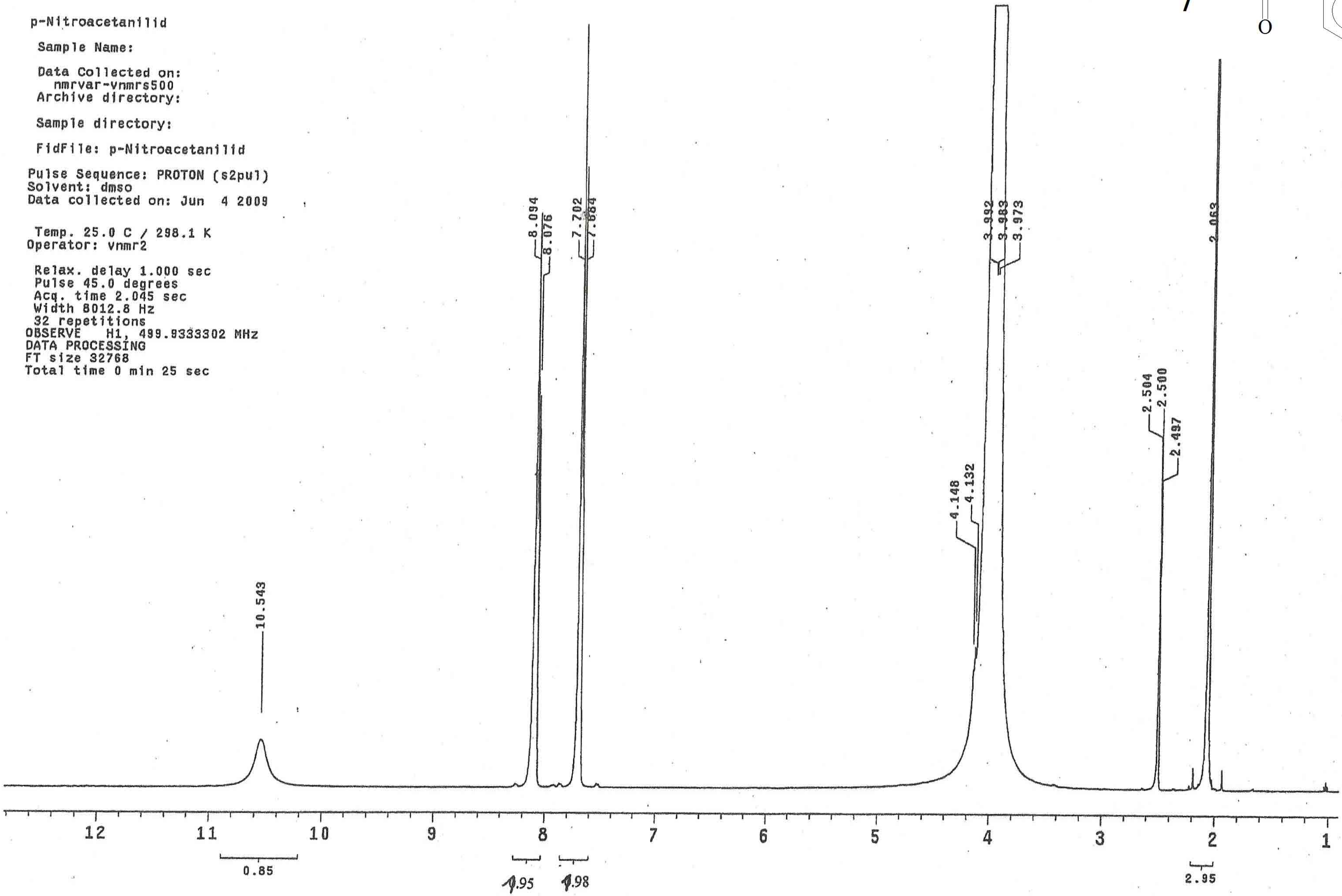
NO_2
NO_2



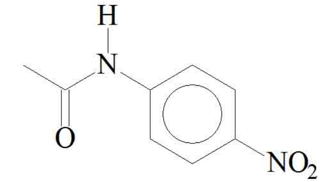
Transmittance
Wavenumber (cm-1)
80
70
60
50
40
30
20
10
0
-10
3500
3000
2500
2000
1500
1000
3104
3052
2876
2812
2000
1948
1900
1824
1768
1608
1536
1348
1272
1172
1144
1092
1068
1000
908
828
816
752
716
656

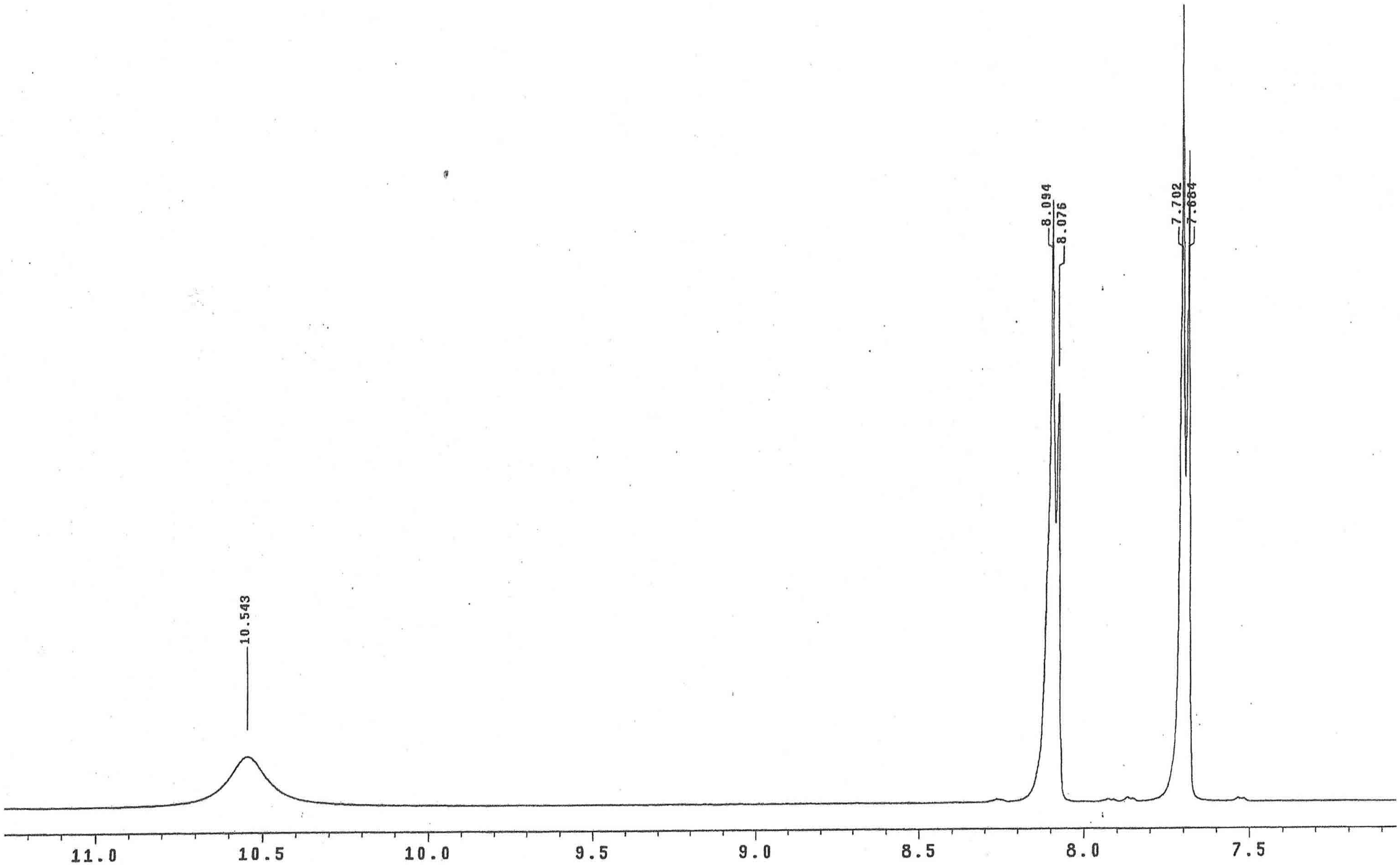
7 

H
N
O
NO2

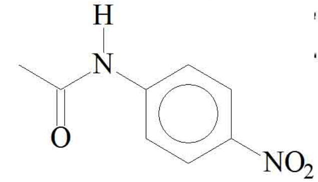


p-Nitroacetanilid
Sample Name:
Data Collected on:
nmrvar-vnmrs500
Archive directory:
Sample directory:
FidFile: p-Nitroacetanilid
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jun 4 2009
Temp. 25.0 C / 298.1 K
Operator: vnmr2
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9333302 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
10.543
8.094
8.076
7.702
7.684
4.148
4.132
3.992
3.983
3.973
2.504
2.500
2.497
2.063
12
11
10
9
8
7
6
5
4
3
2
1
0.85
1.95
1.98
2.95

7 



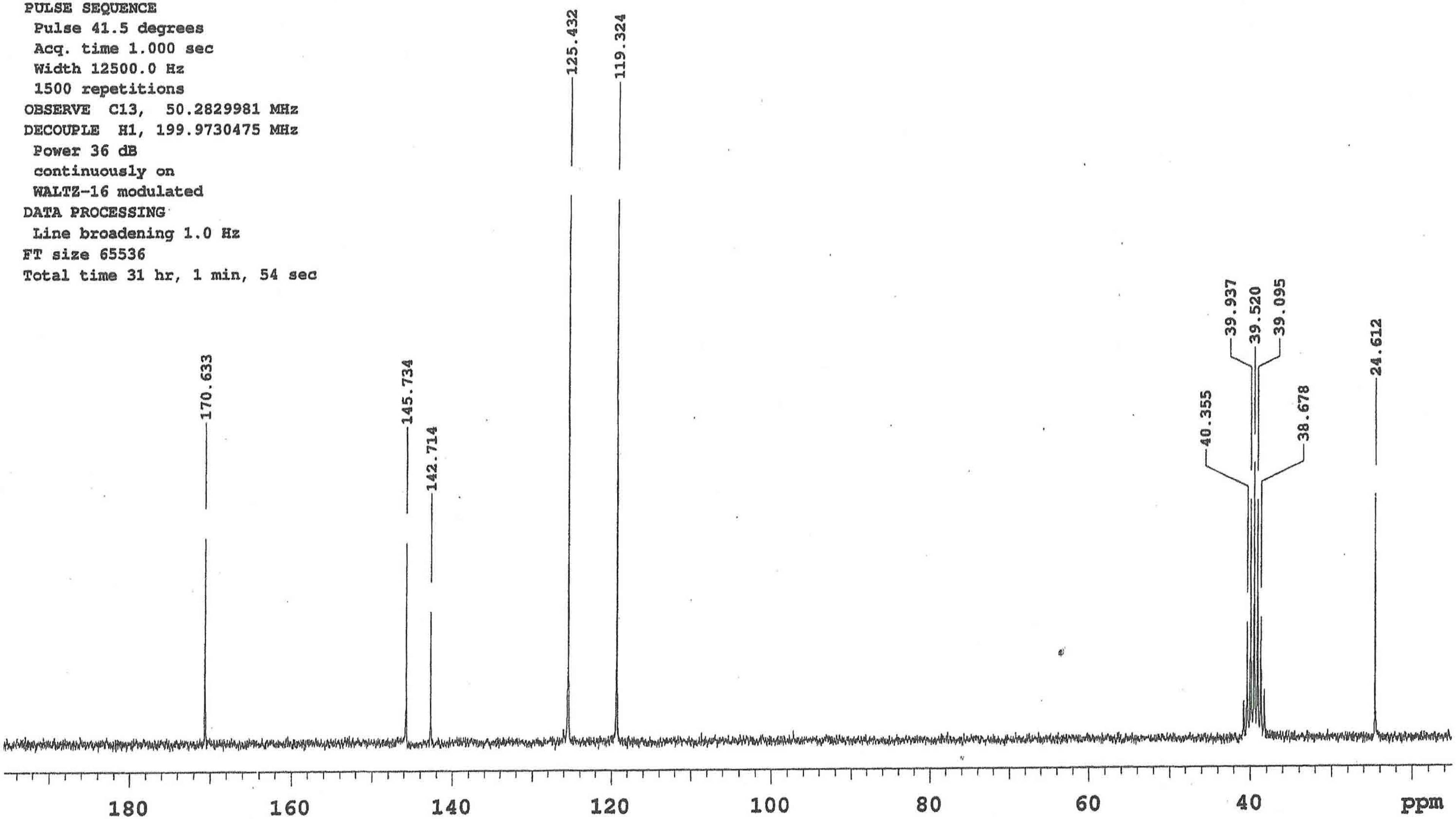
7



p-Nitroacetanilid

Solvent: DMSO
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2829981 MHz
DECOUPLE H1, 199.9730475 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec



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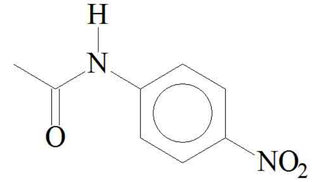
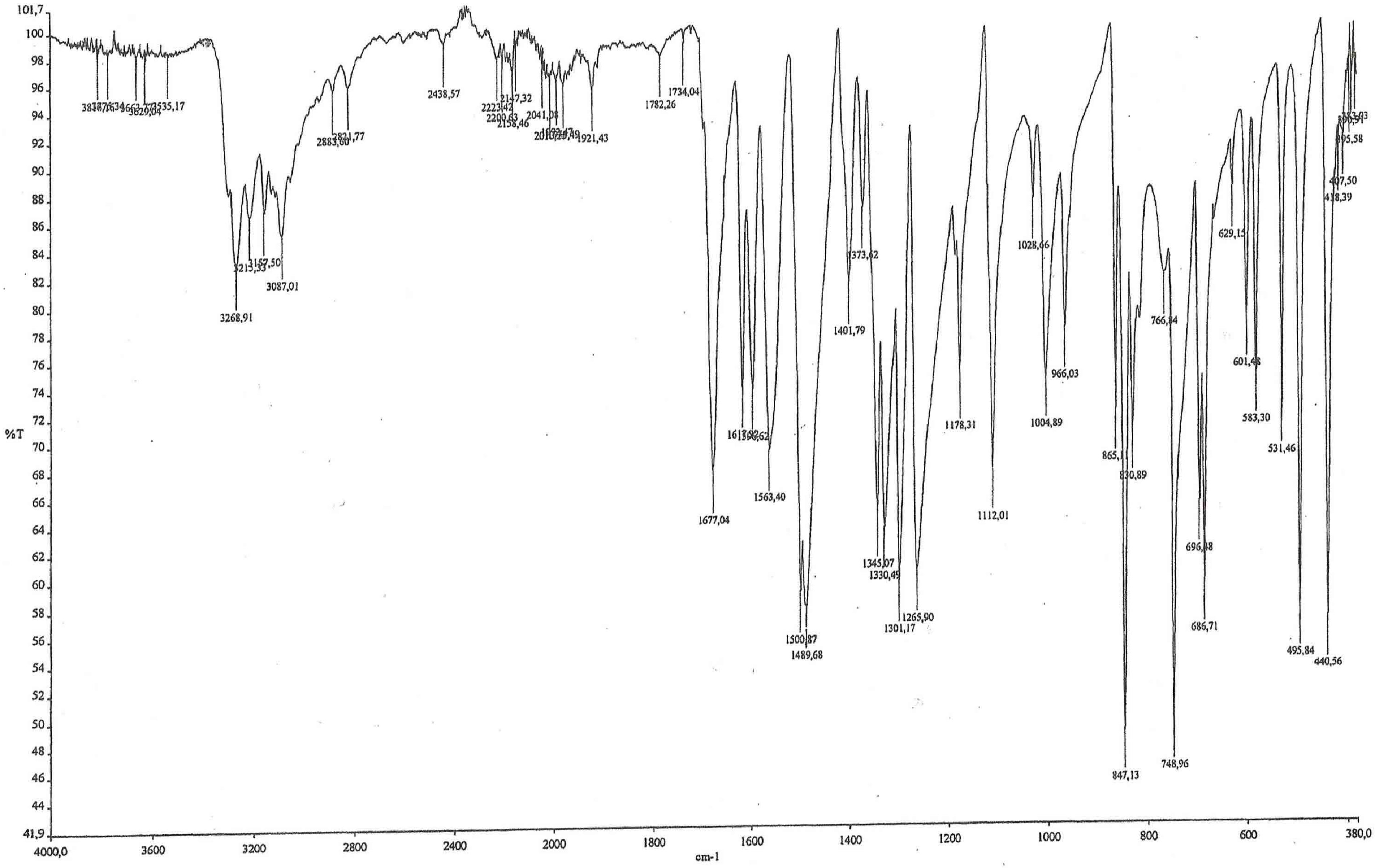
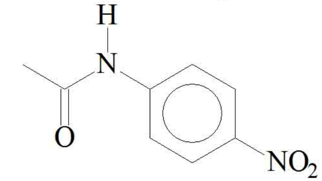


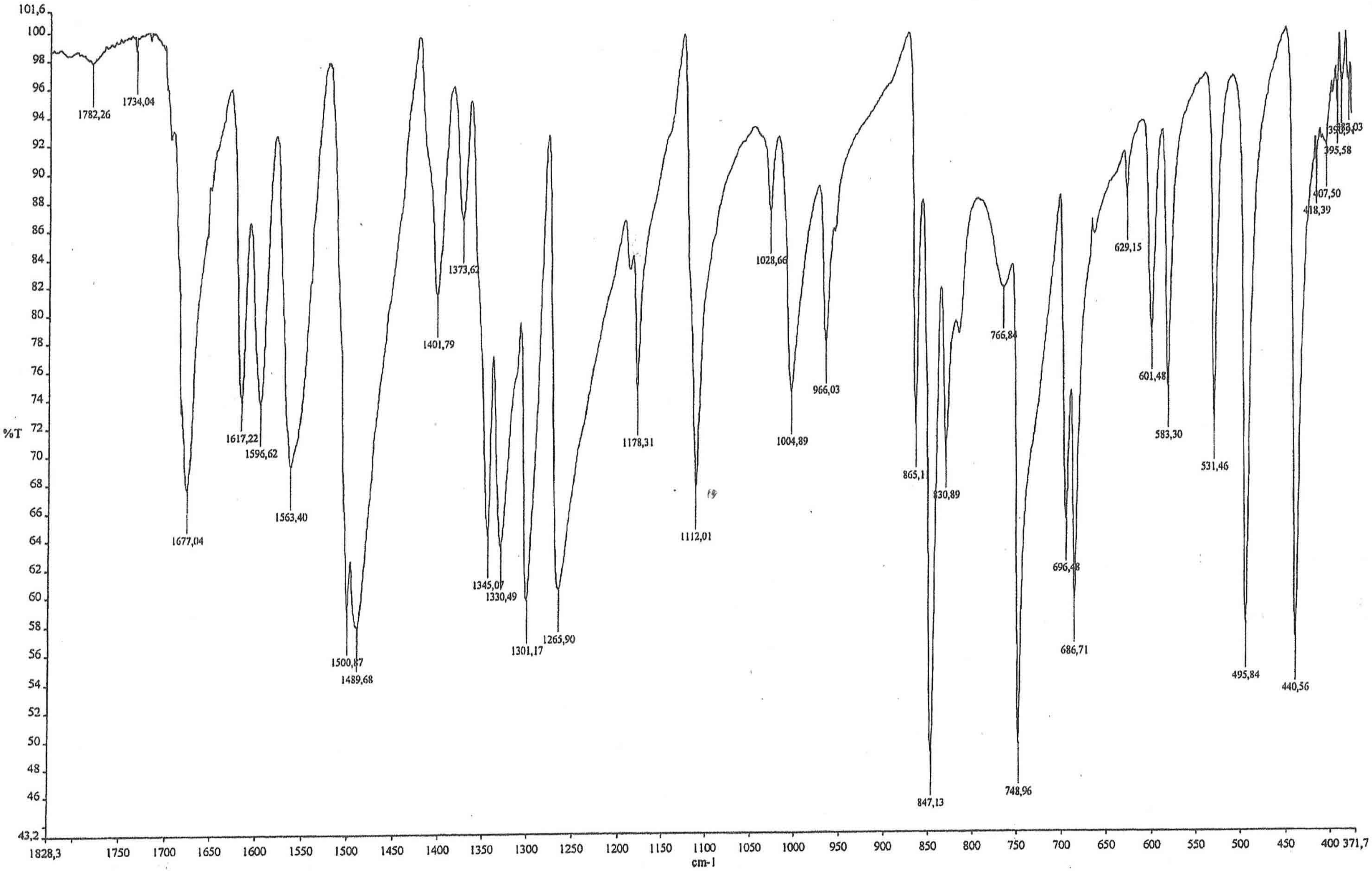
p-Nitroacetanilid (ATR)

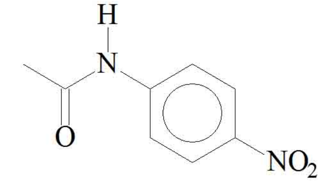


p-Nitroacetanilid (ATR)

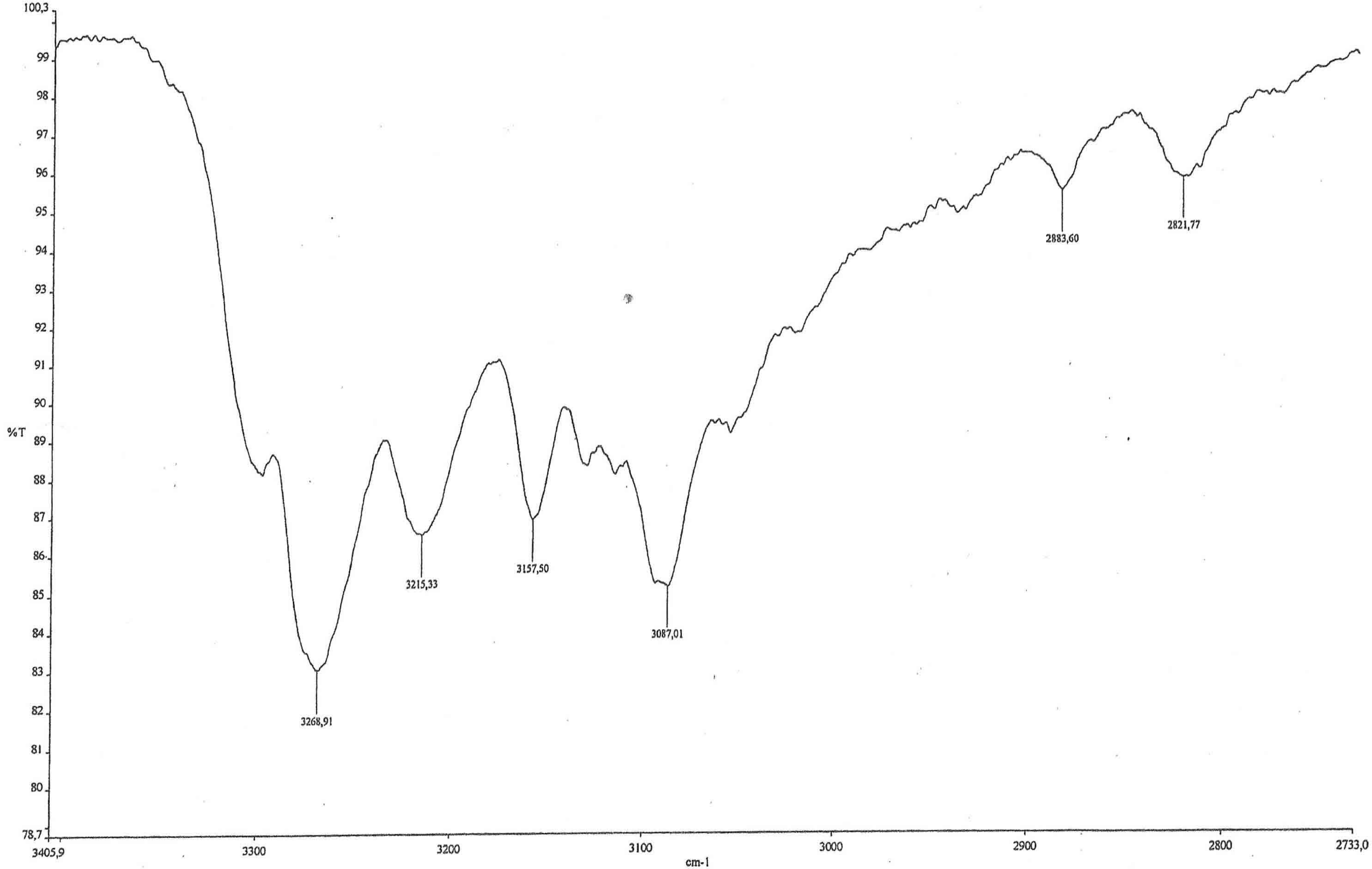
7





7 

p-Nitroacetanilid (ATR)



p-Bromoacetanilid

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

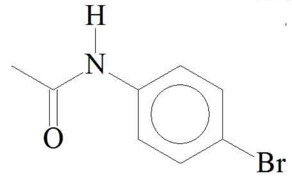
FidFile: p-Bromoacetanilid

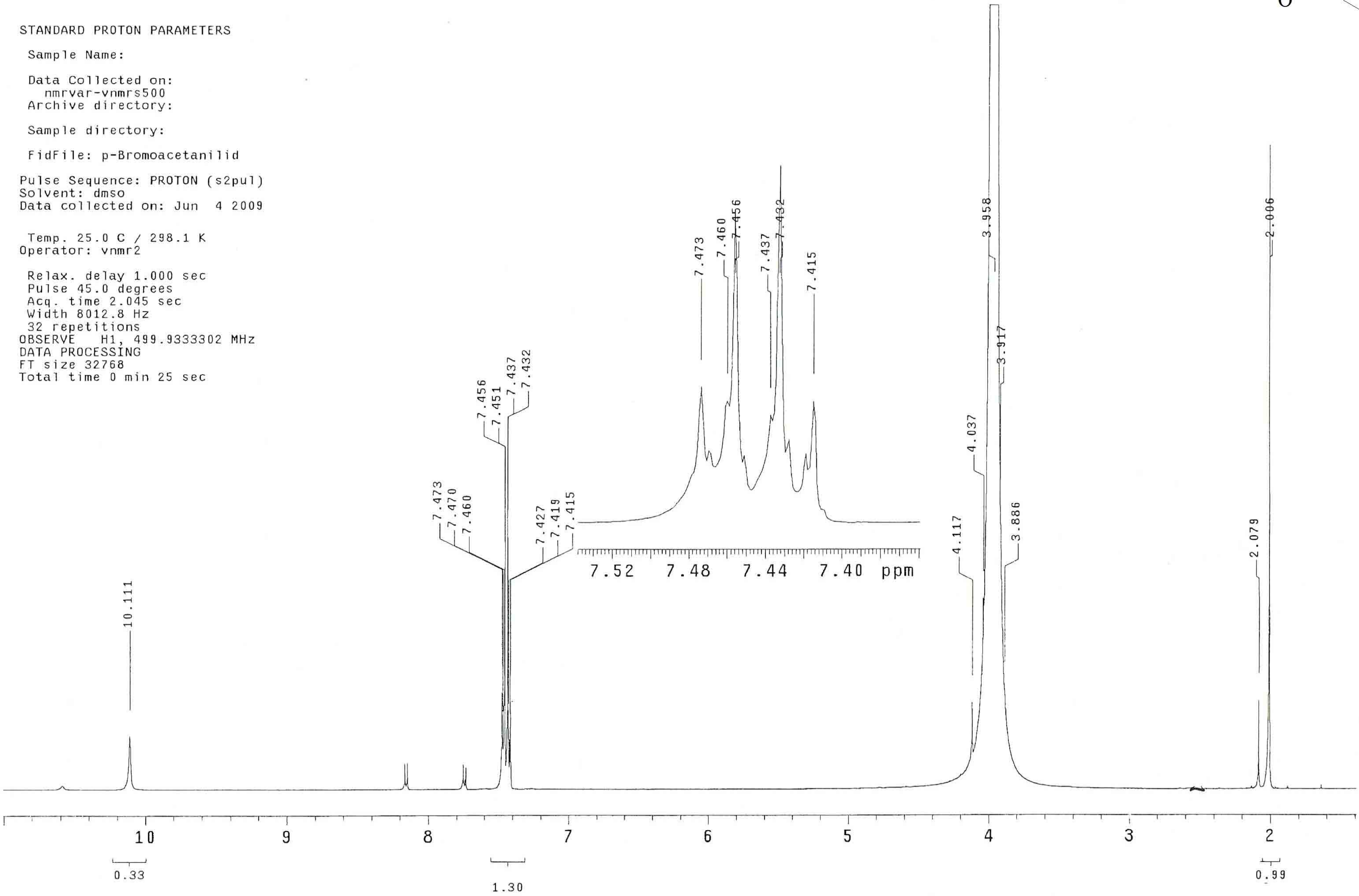
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jun 4 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9333302 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

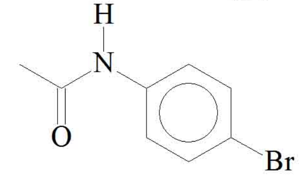
8





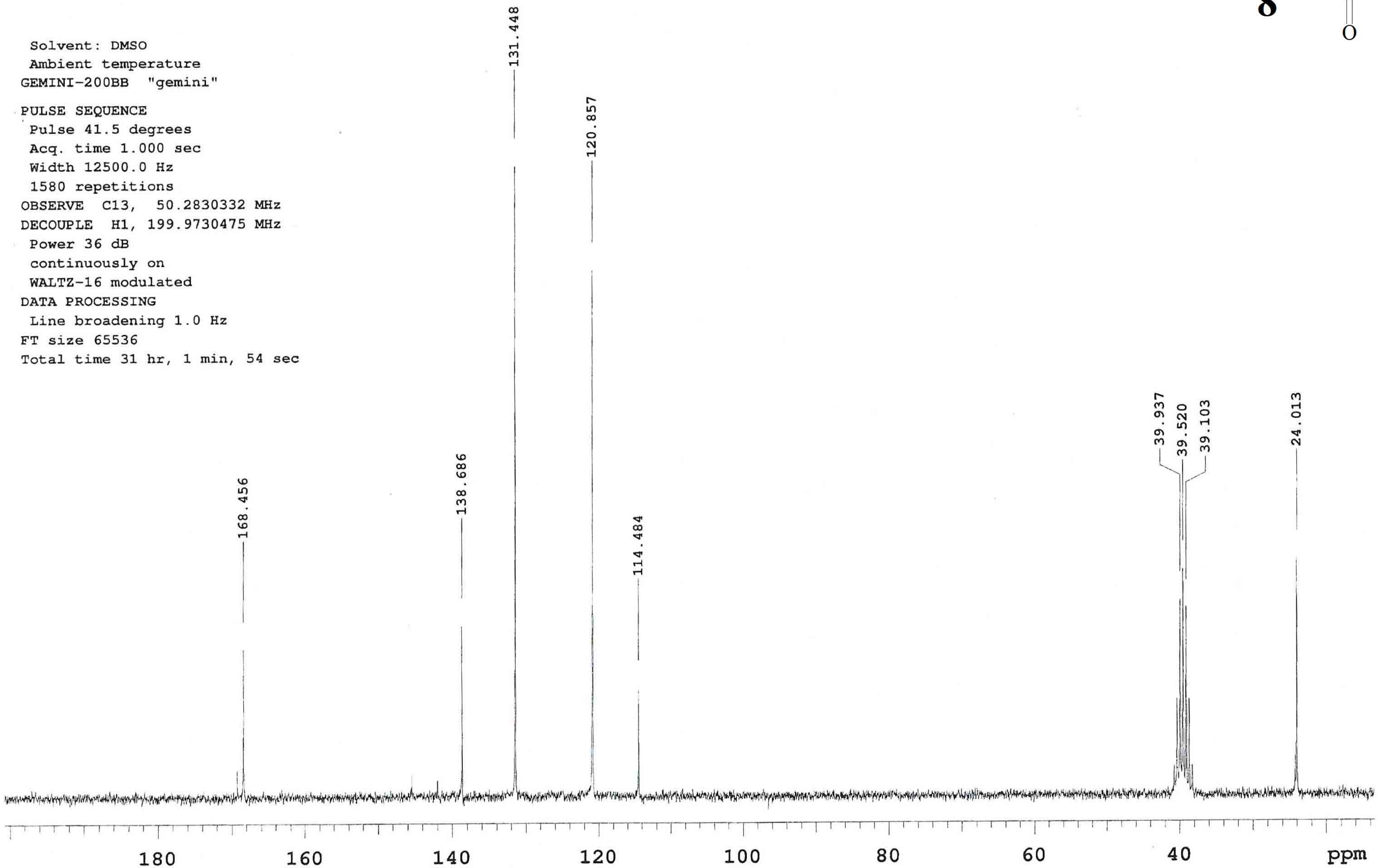
p-Bromoacetanilid

8

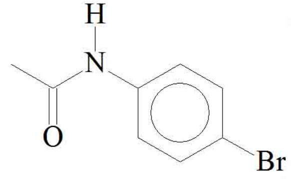


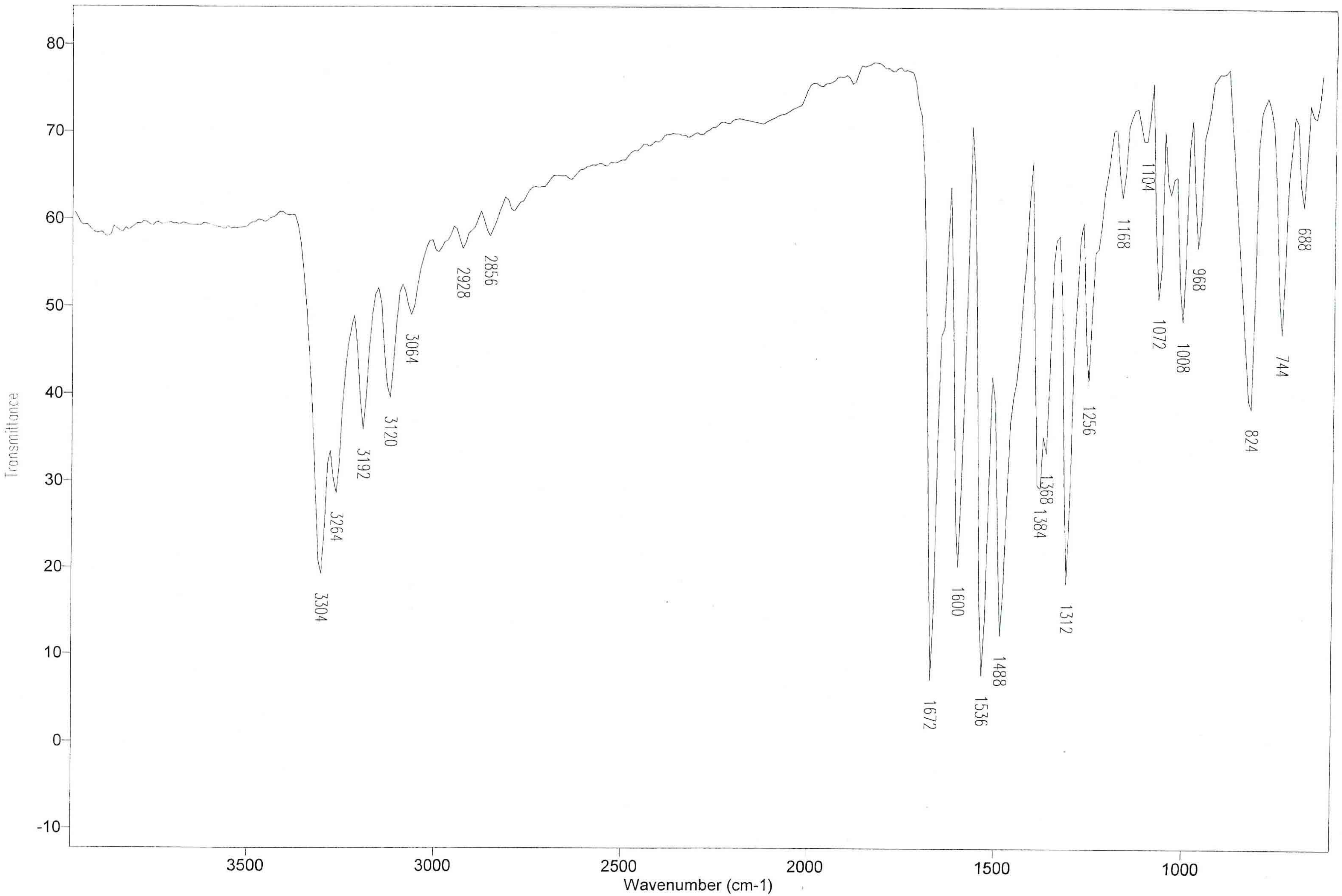
Solvent: DMSO
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1580 repetitions
OBSERVE C13, 50.2830332 MHz
DECOUPLE H1, 199.9730475 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

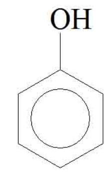


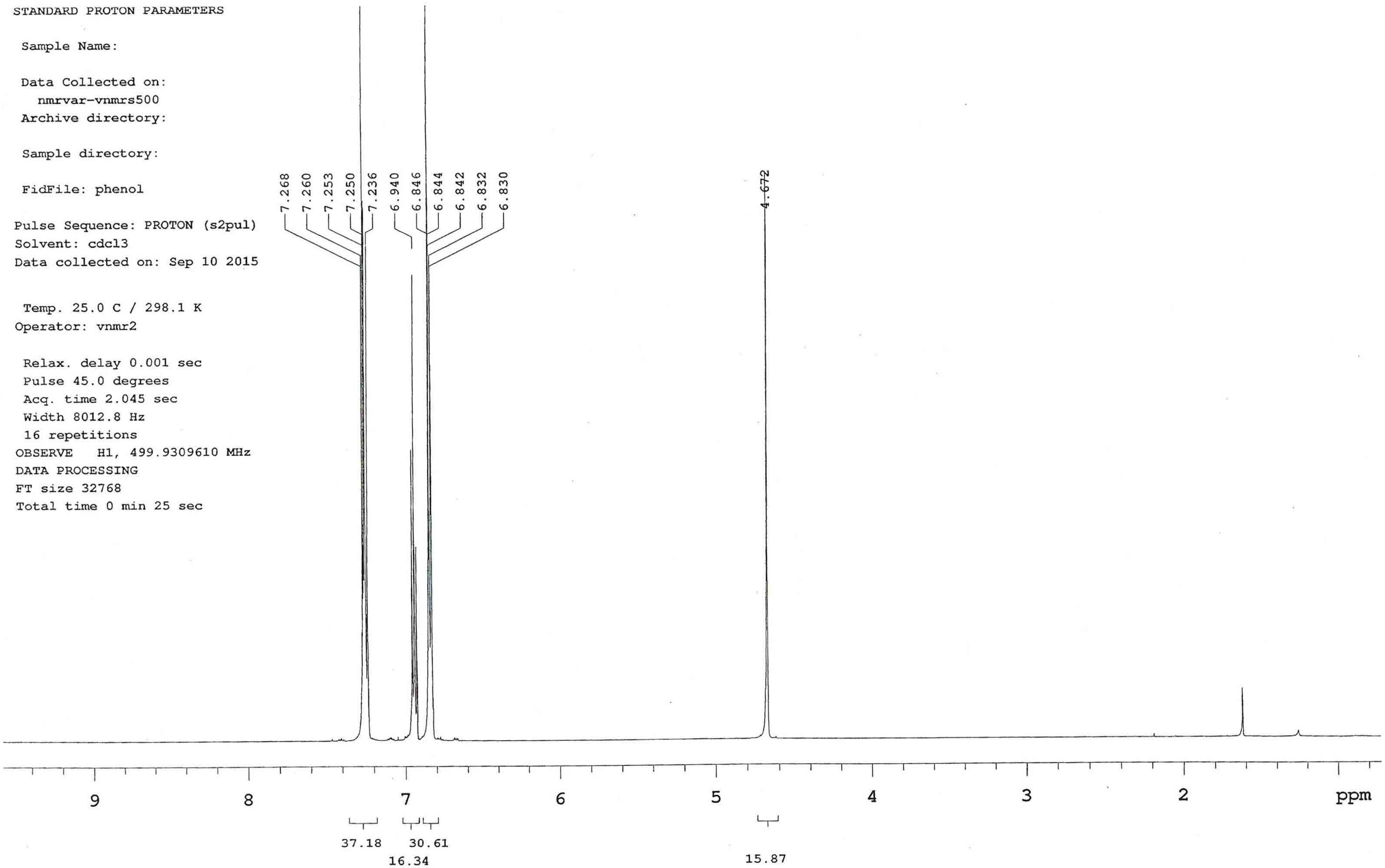
8



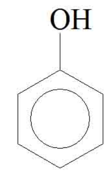

Transmittance
80
70
60
50
40
30
20
10
0
-10
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
3304
3264
3192
3120
3064
2928
2856
1672
1600
1536
1488
1384
1368
1312
1256
1168
1104
1072
1008
968
824
744
688

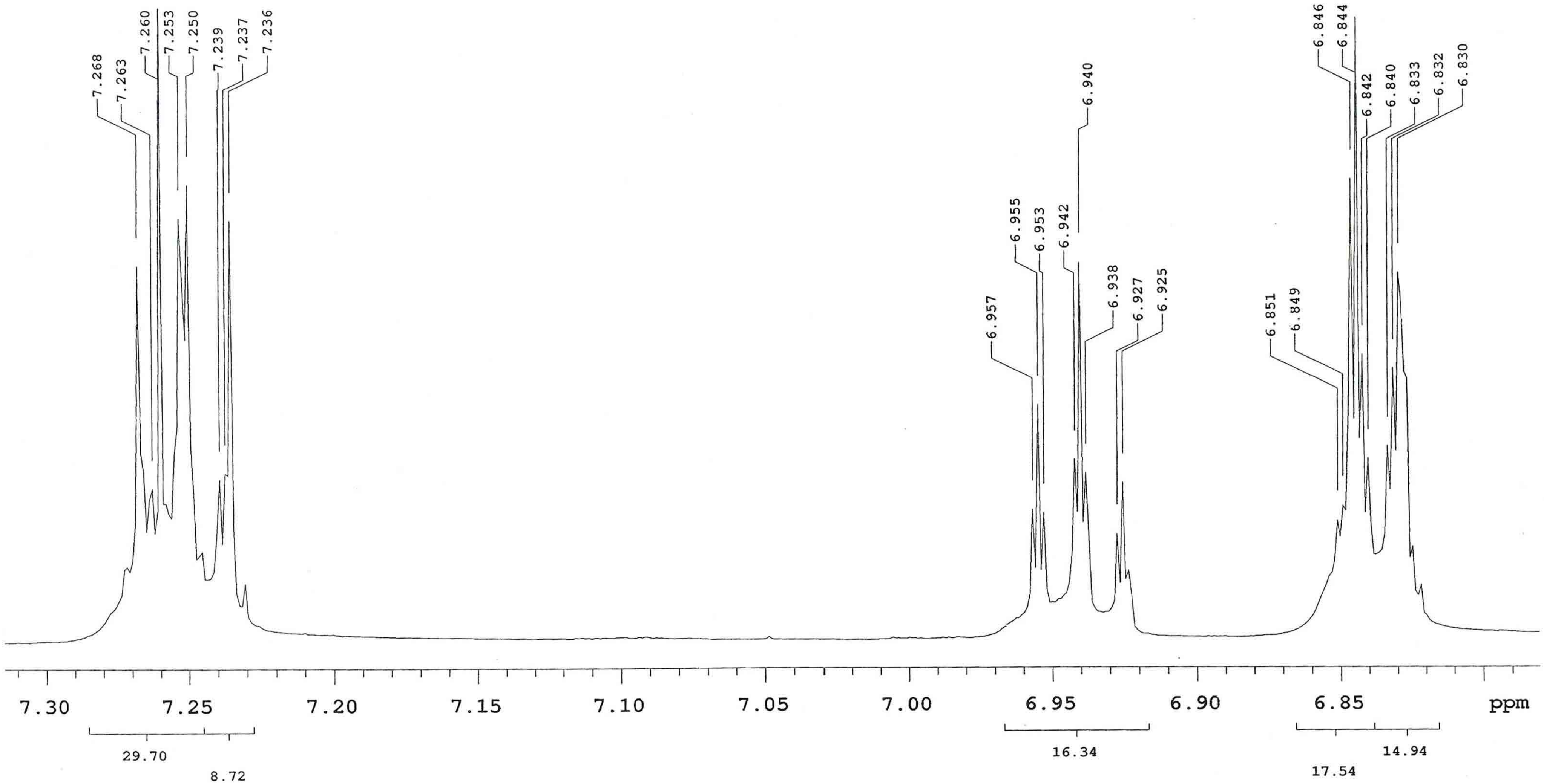
9


OH

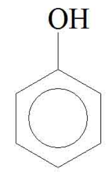

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
nmrvar-vnmrs500
Archive directory:
Sample directory:
FidFile: phenol
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 10 2015
Temp. 25.0 C / 298.1 K
Operator: vnmr2
Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309610 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
7.268
7.260
7.253
7.250
7.236
6.940
6.846
6.844
6.842
6.832
6.830
4.672
9
8
7
6
5
4
3
2
ppm
37.18
16.34
30.61
15.87

9


OH


7.268
7.263
7.260
7.253
7.250
7.239
7.237
7.236
6.957
6.955
6.953
6.942
6.940
6.938
6.927
6.925
6.851
6.849
6.846
6.844
6.842
6.840
6.833
6.832
6.830
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
ppm
29.70
8.72
16.34
17.54
14.94

9



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

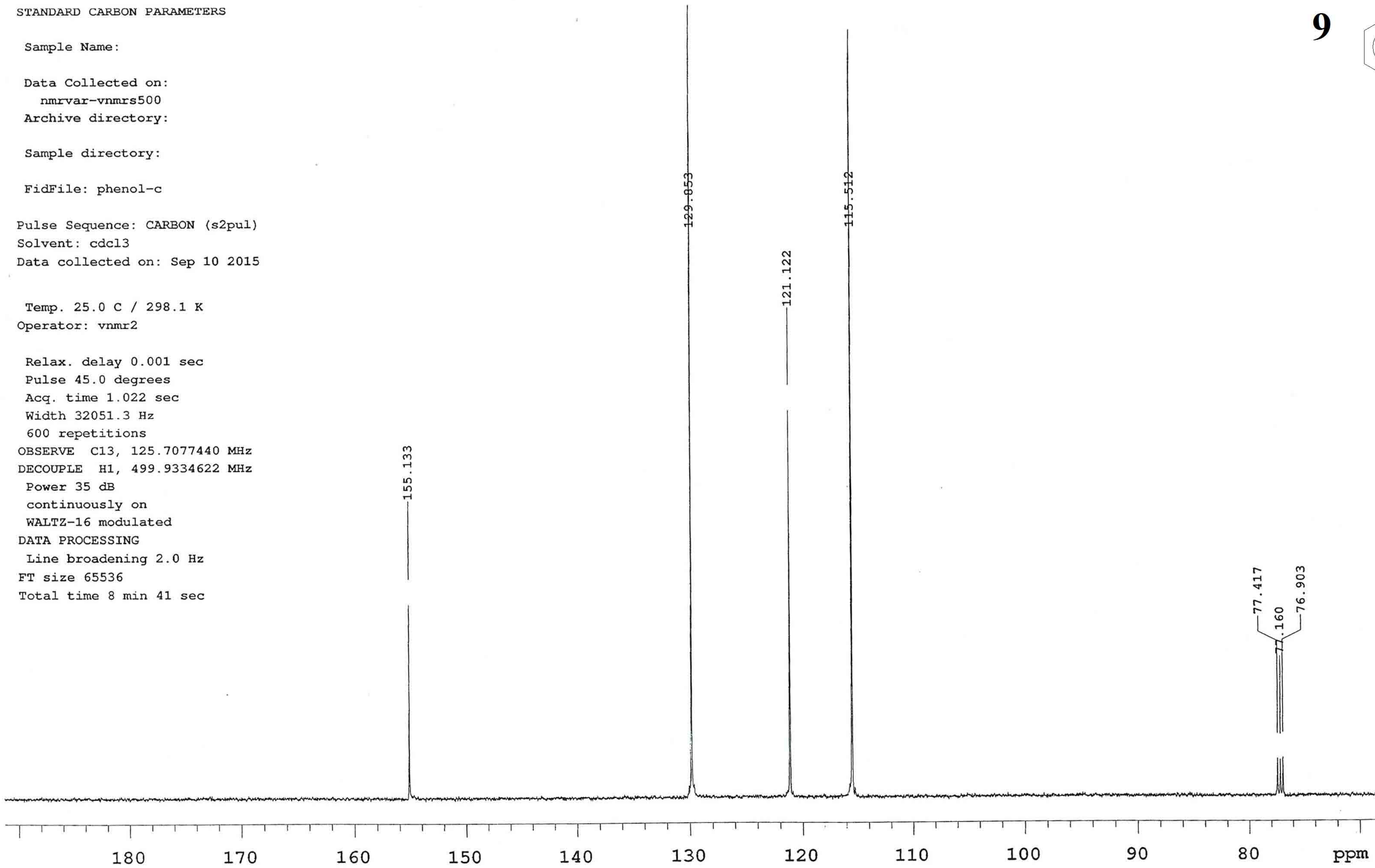
Sample directory:

FidFile: phenol-c

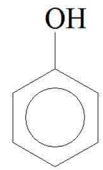
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 10 2015

Temp. 25.0 C / 298.1 K
Operator: vnmr2

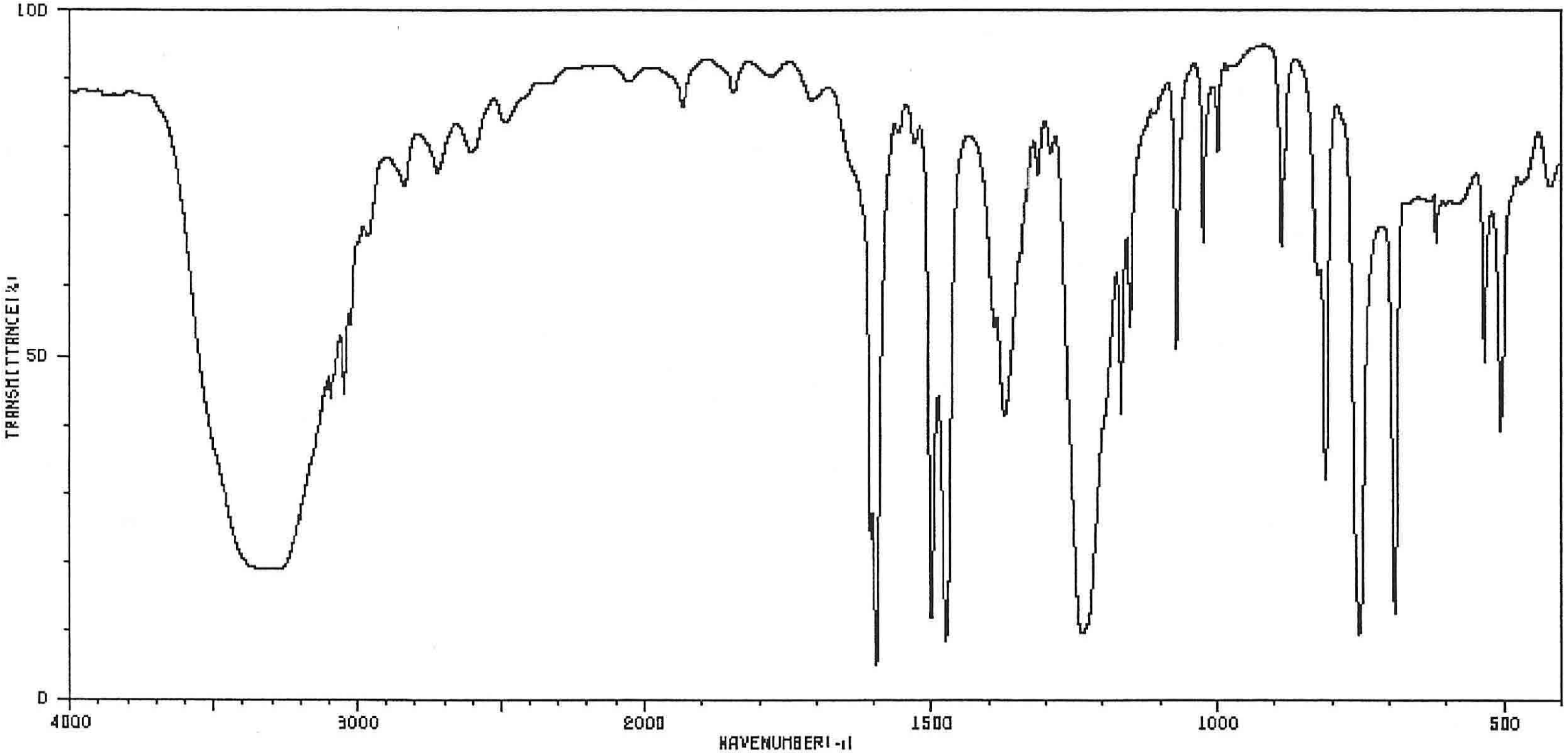
Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
600 repetitions
OBSERVE C13, 125.7077440 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

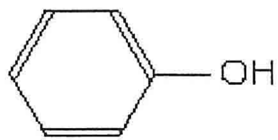


9

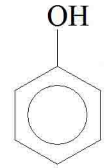


HIT-NO=1030	SCORE= ( )	SDBS-NO=554	IR-NIDA-65045 : KBR DISC
PHENOL			
C_6H_6O			

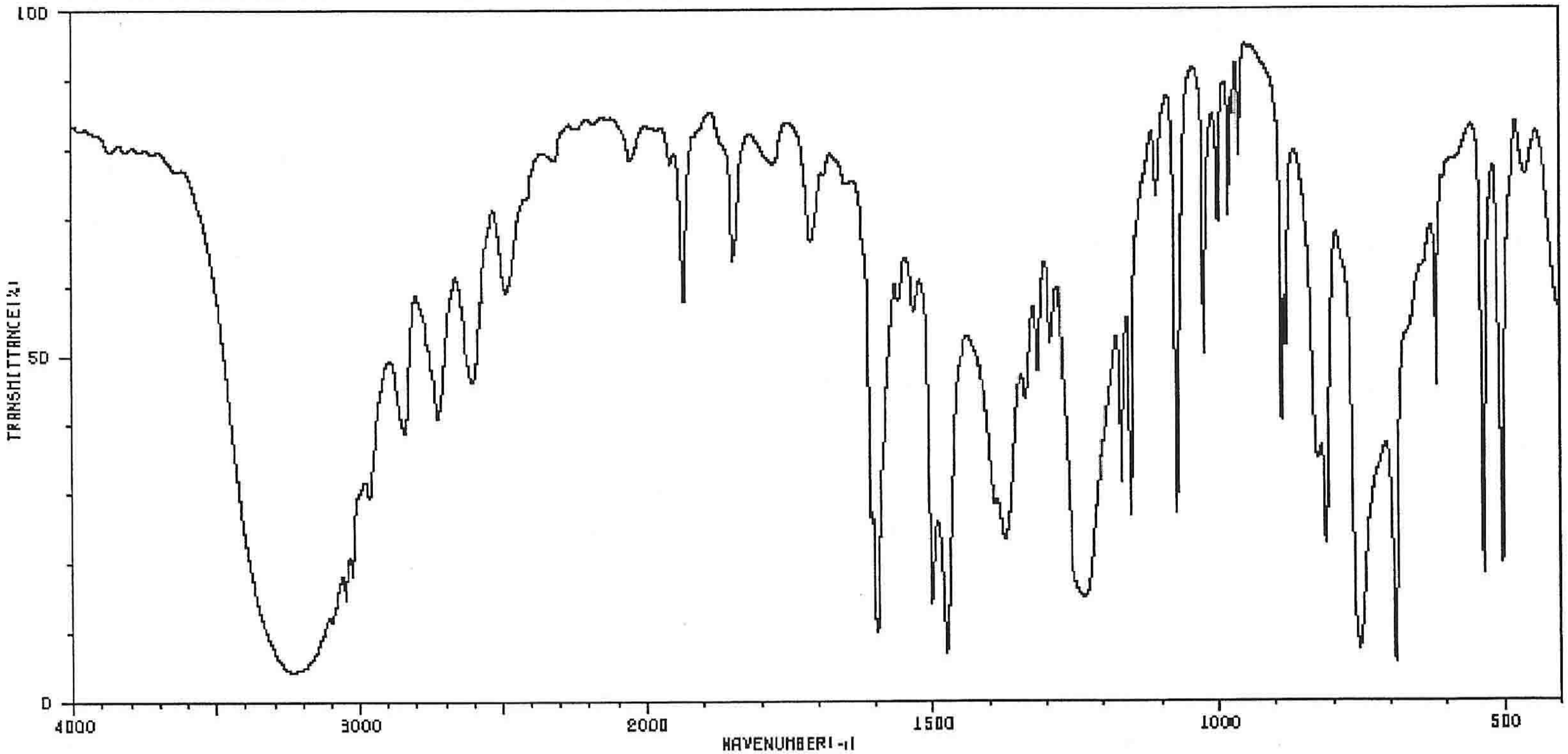


3093	42	2606	77	1631	77	1236	9	826	68	
3047	43	2487	81	1500	11	1168	41	812	31	
3023	52	1934	81	1475	8	1153	52	753	9	
2963	64	1846	84	1391	62	1072	49	690	12	
2847	72	1606	22	1373	39	1024	64	618	64	
2837	72	1598	4	1315	72	999	77	535	47	
2723	74	1567	78	1293	77	888	64	507	38	

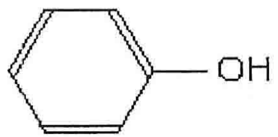
Źródło: ***https://sdbs.db.aist.go.jp***

9 

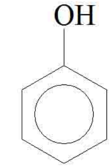
HIT-NO=1060	SCORE= ( )	SDBS-NO=554	IR-NIDA-29806 : LIQUID FILM
PHENOL			
C_6H_6O			



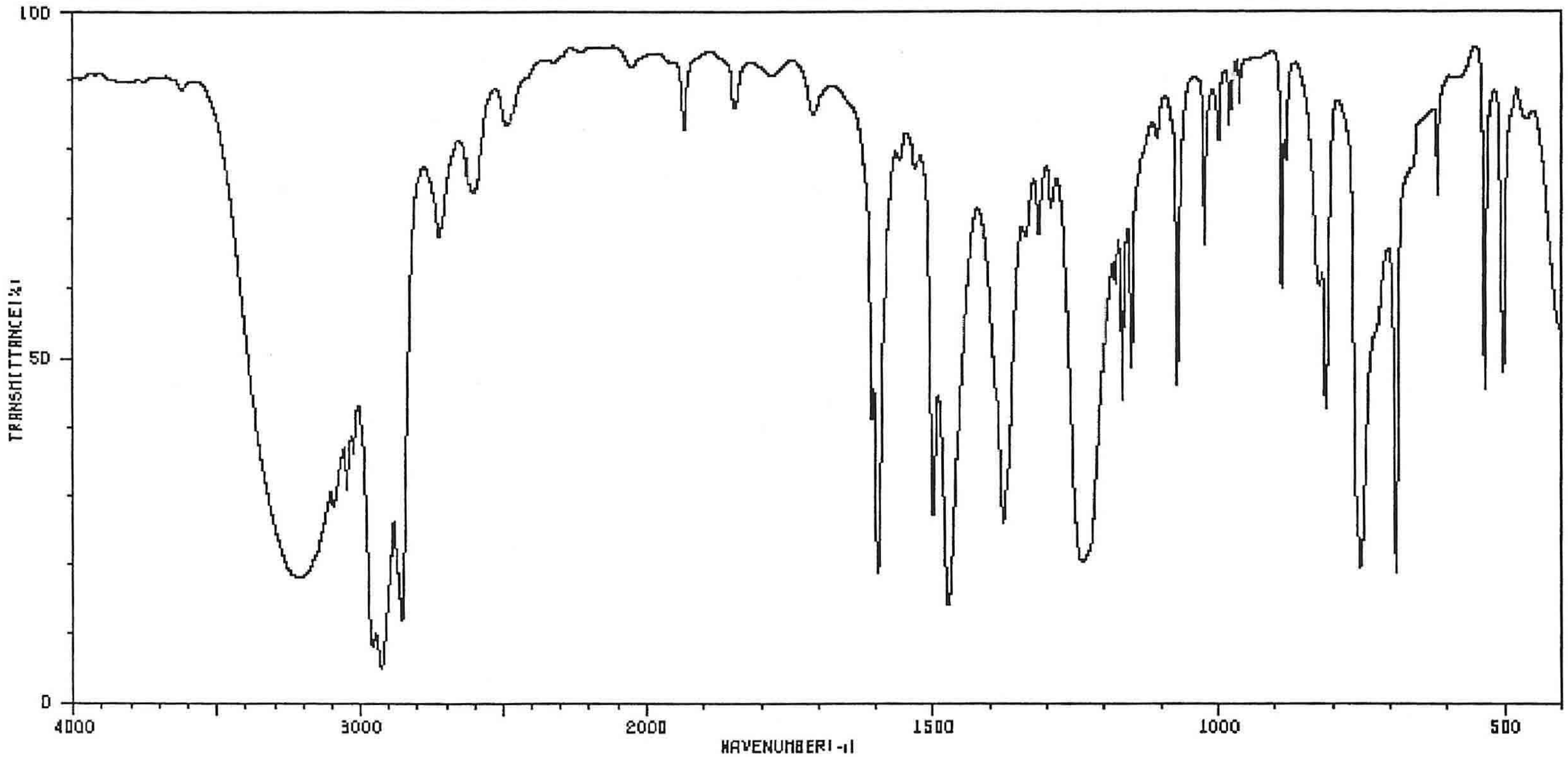
3229	4	2484	58	1632	66	1234	16	626	36
3048	15	1933	57	1501	14	1169	31	812	23
3025	18	1847	62	1474	7	1153	26	754	8
2962	29	1711	64	1372	23	1072	27	691	6
2837	38	1606	26	1336	43	1024	49	617	44
2723	41	1598	10	1315	47	889	41	535	18
2699	46	1569	67	1293	60	881	60	602	20



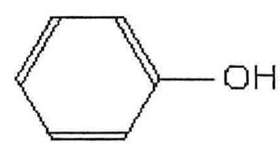
Źródło: ***https://sdbs.db.aist.go.jp***

9 

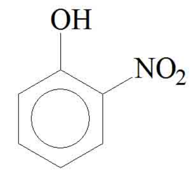
HIT-NO=418	SCORE= ( )	SDBS-NO=554	IR-NIDA-24091 : NUJOL MULL
PHENOL			
C_6H_6O			



3226	17	2926	4	1600	26	1181	68	823	68
3215	17	2855	11	1474	13	1168	42	812	41
3205	17	2723	64	1376	24	1153	46	753	18
3094	26	2602	70	1337	66	1072	44	690	18
3047	29	1606	39	1315	66	1024	64	617	70
3023	35	1598	17	1294	88	888	57	535	43
2966	7	1632	74	1238	19	881	77	503	46



Źródło: ***https://sdbs.db.aist.go.jp***

10 

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

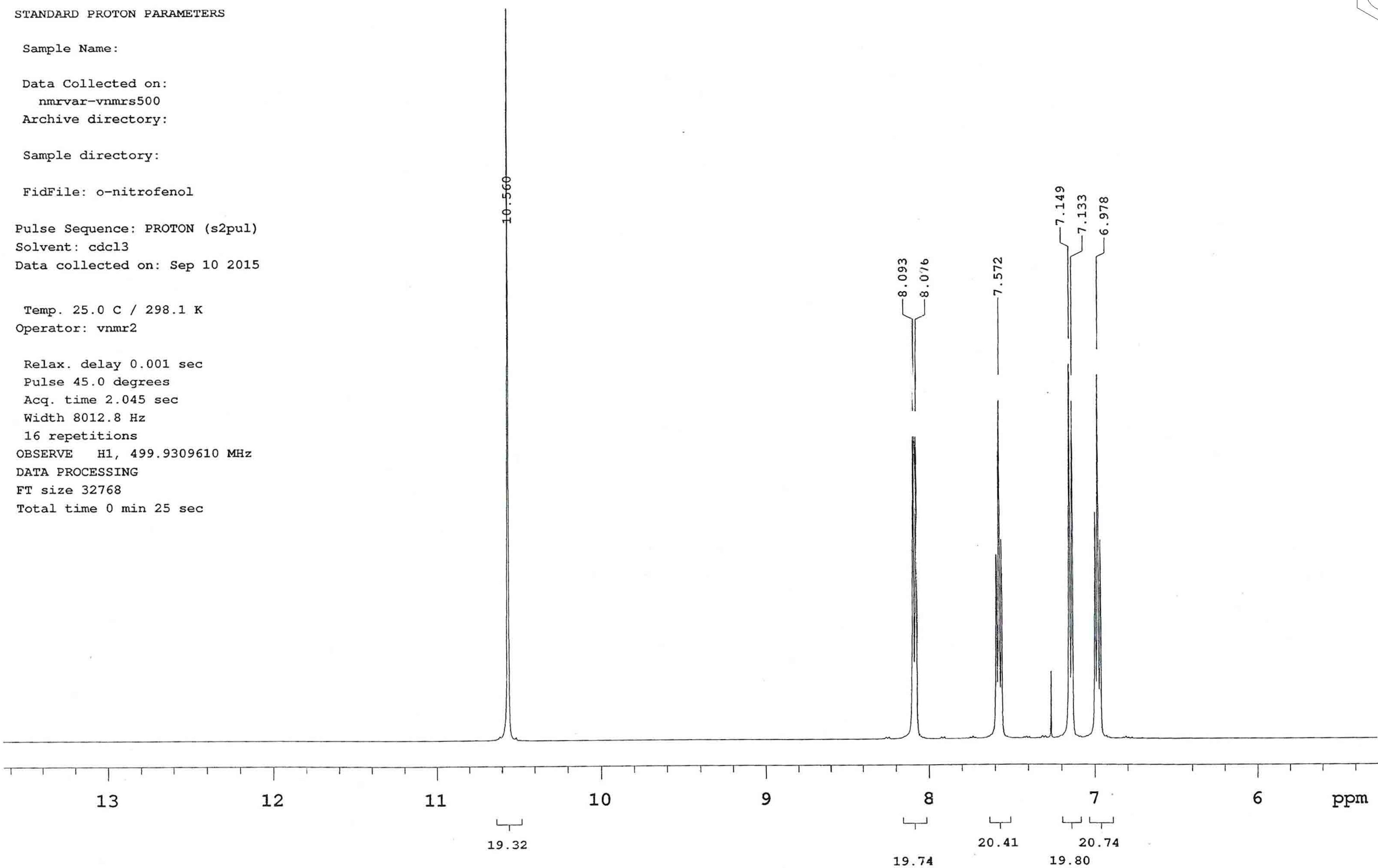
Sample directory:

FidFile: o-nitrofenol

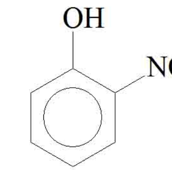
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 10 2015

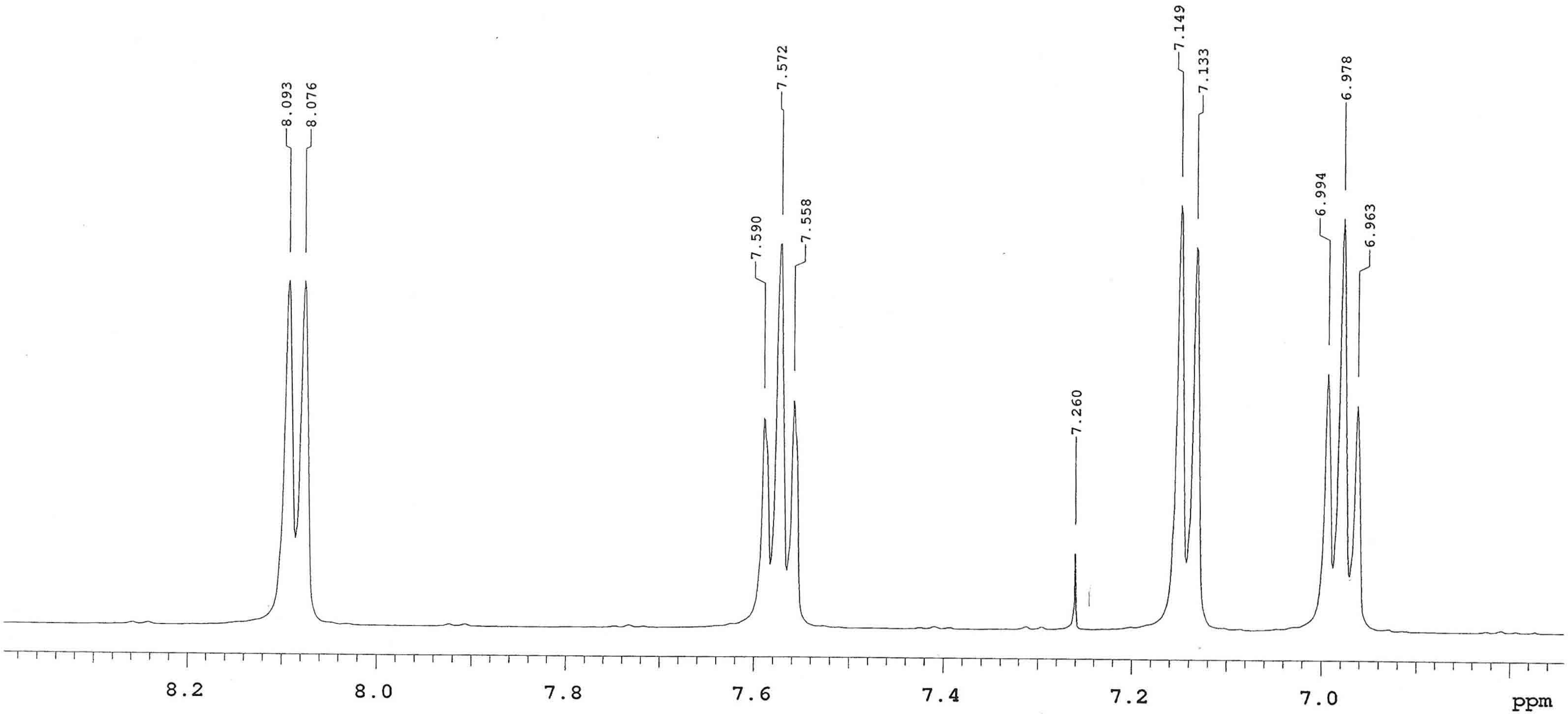
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309610 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

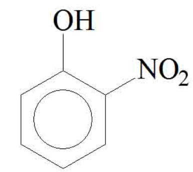


10


OH
NO2


8.093
8.076
7.590
7.572
7.558
7.260
7.149
7.133
6.994
6.978
6.963
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm

10



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

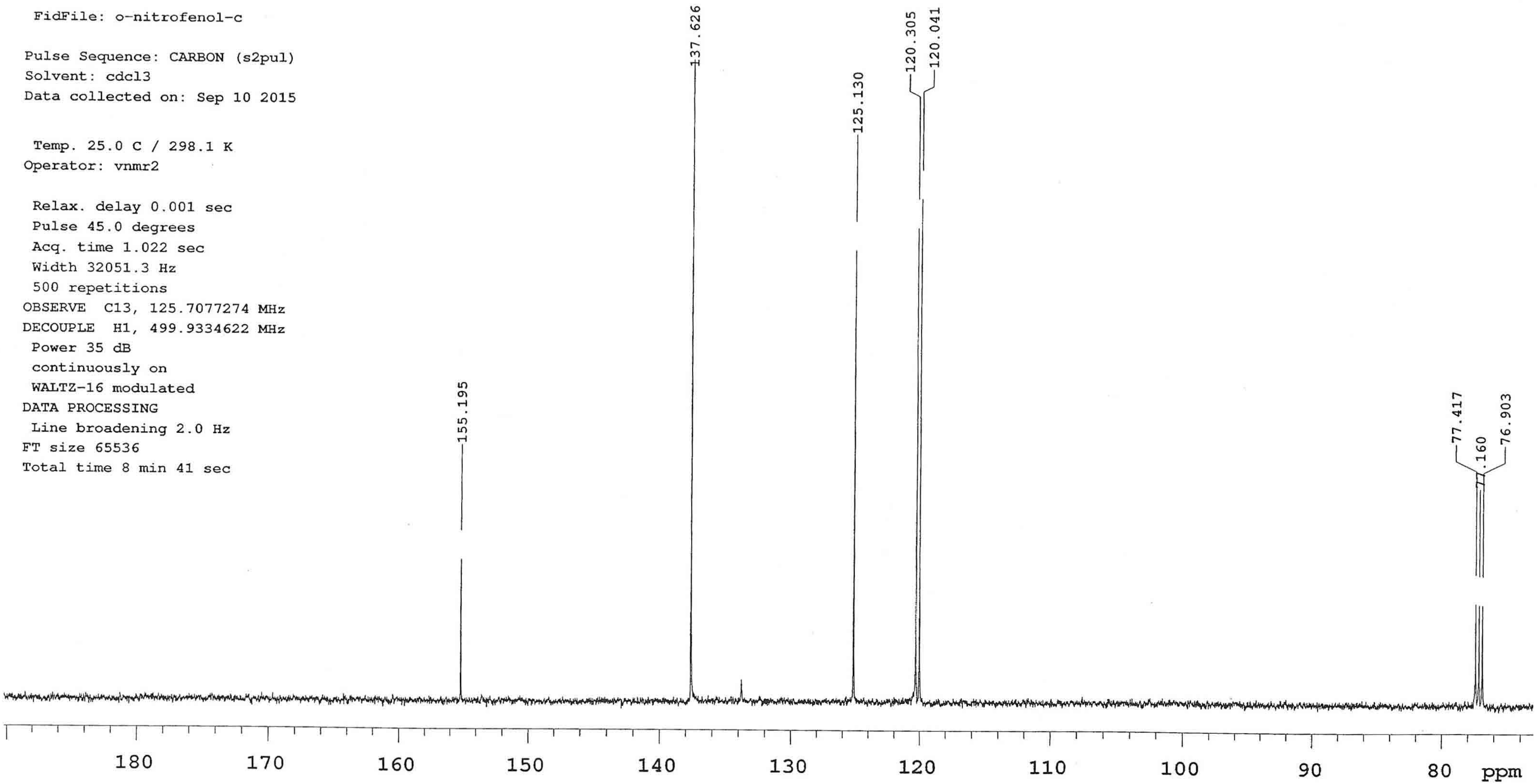
Sample directory:

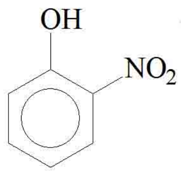
FidFile: o-nitrofenol-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 10 2015

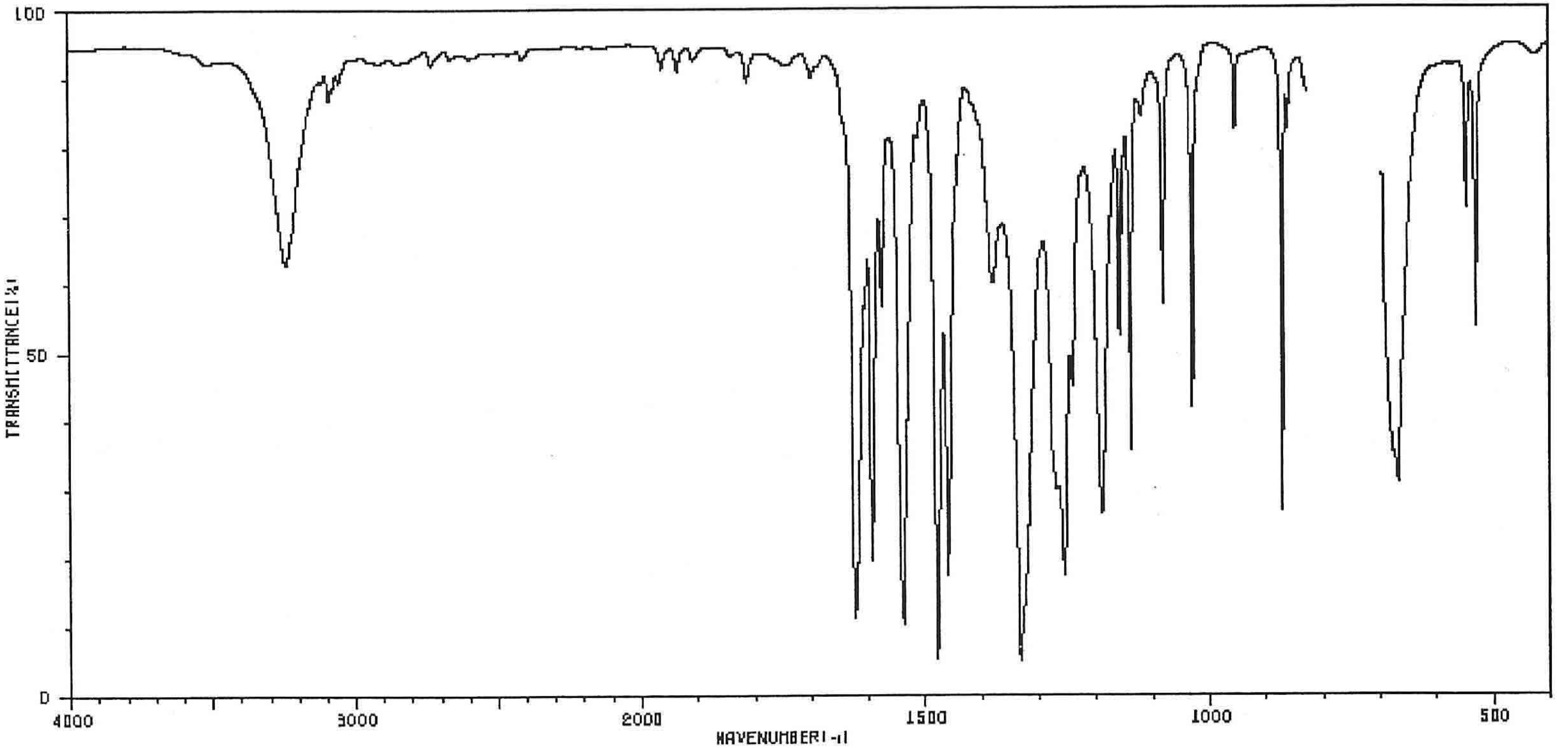
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
500 repetitions
OBSERVE C13, 125.7077274 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

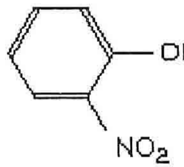


10 

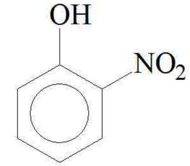
HIT-NO=1240	SCORE= ( )	SDBS-NO=2650	IR-NIDA-06902 : CCL4 SOLUTION
O-NITROPHENOL			
$C_6H_5NO_3$			



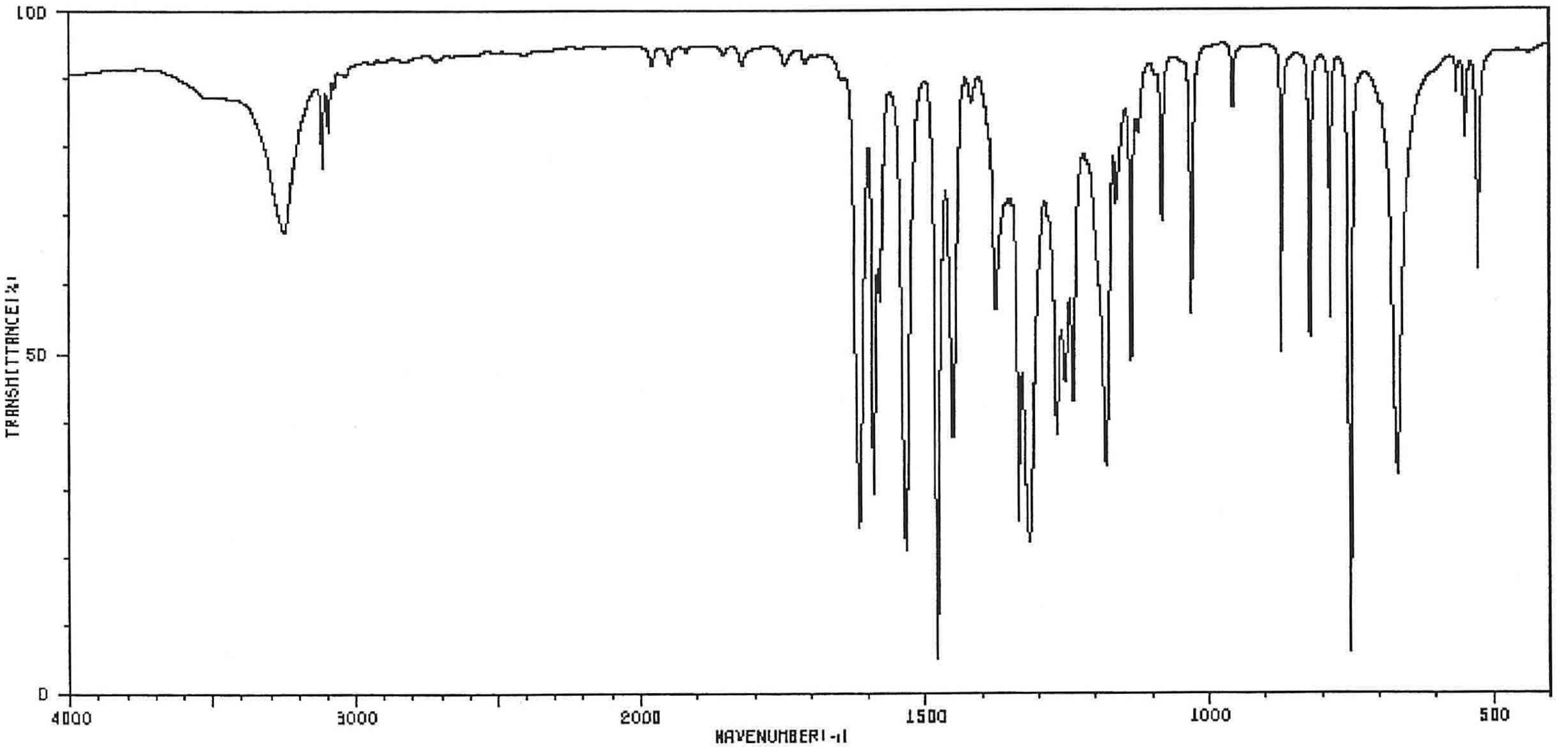
3241	60	1593	18	1268	28	1081	66	630	62
3089	84	1575	55	1256	16	1030	39		
3076	84	1538	9	1241	43	954	79		
3052	86	1479	6	1190	26	870	26		
1810	86	1460	16	1158	50	860	79		
1623	10	1379	58	1139	34	667	29		
1606	63	1333	4	1119	81	646	68		

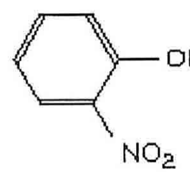


Źródło: ***https://sdbs.db.aist.go.jp***

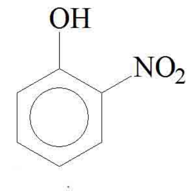
10 

HIT-NO=2103	SCORE= ( )	SDBS-NO=2650	IR-NIDA-08574 : KBR DISC
O-NITROPHENOL			
$C_6H_5NO_3$			

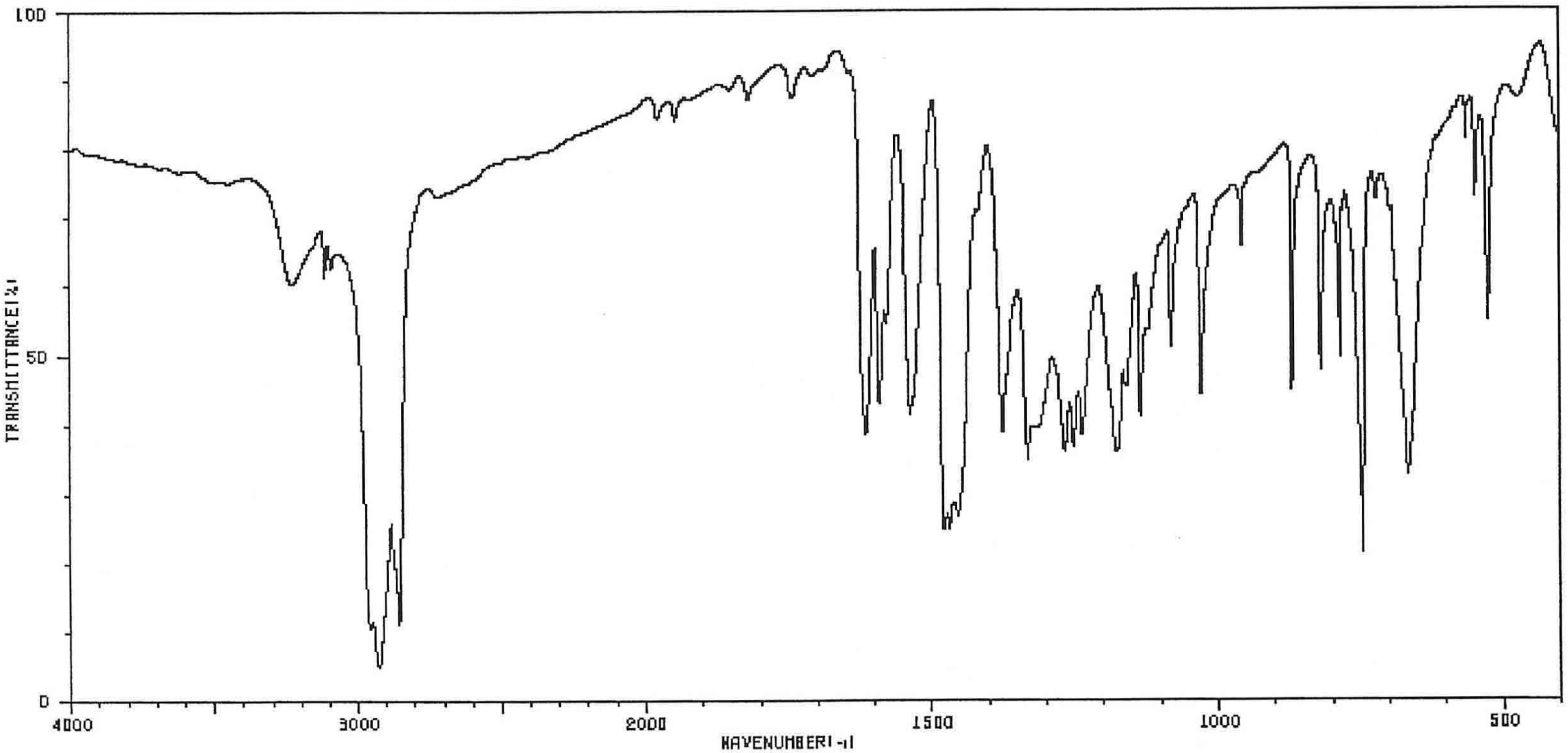


3249	64	1633	20	1267	36	1082	66	667	30	
3116	74	1479	4	1254	44	1030	53	565	84	
3095	79	1451	56	1239	41	957	81	549	79	
3074	84	1418	84	1181	32	871	47	526	60	
1615	23	1376	53	1164	68	821	50			
1590	28	1335	25	1136	47	785	59			
1579	66	1317	21	1123	79	760	6			

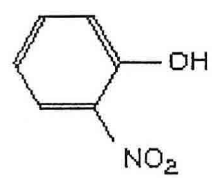
Źródło: *https://sdbs.db.aist.go.jp*

10 

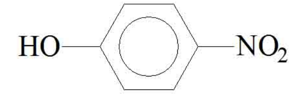
HIT-NO=1421	SCORE= ( )	SDBS-NO=2650	IR-NIDA-64741 : NUJOL MULL
O-NITROPHENOL			
$C_6H_5NO_3$			



3226	68	1691	41	1376	37	1176	34	870	43
3114	58	1578	52	1332	33	1160	43	820	46
3091	60	1538	39	1322	38	1135	39	765	47
2966	10	1478	29	1316	37	1122	62	760	68
2925	4	1468	23	1268	34	1081	49	746	20
2854	10	1459	27	1253	35	1029	42	667	31
1616	37	1463	26	1238	37	967	62	626	52



Źródło: ***https://sdbs.db.aist.go.jp***

11 

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

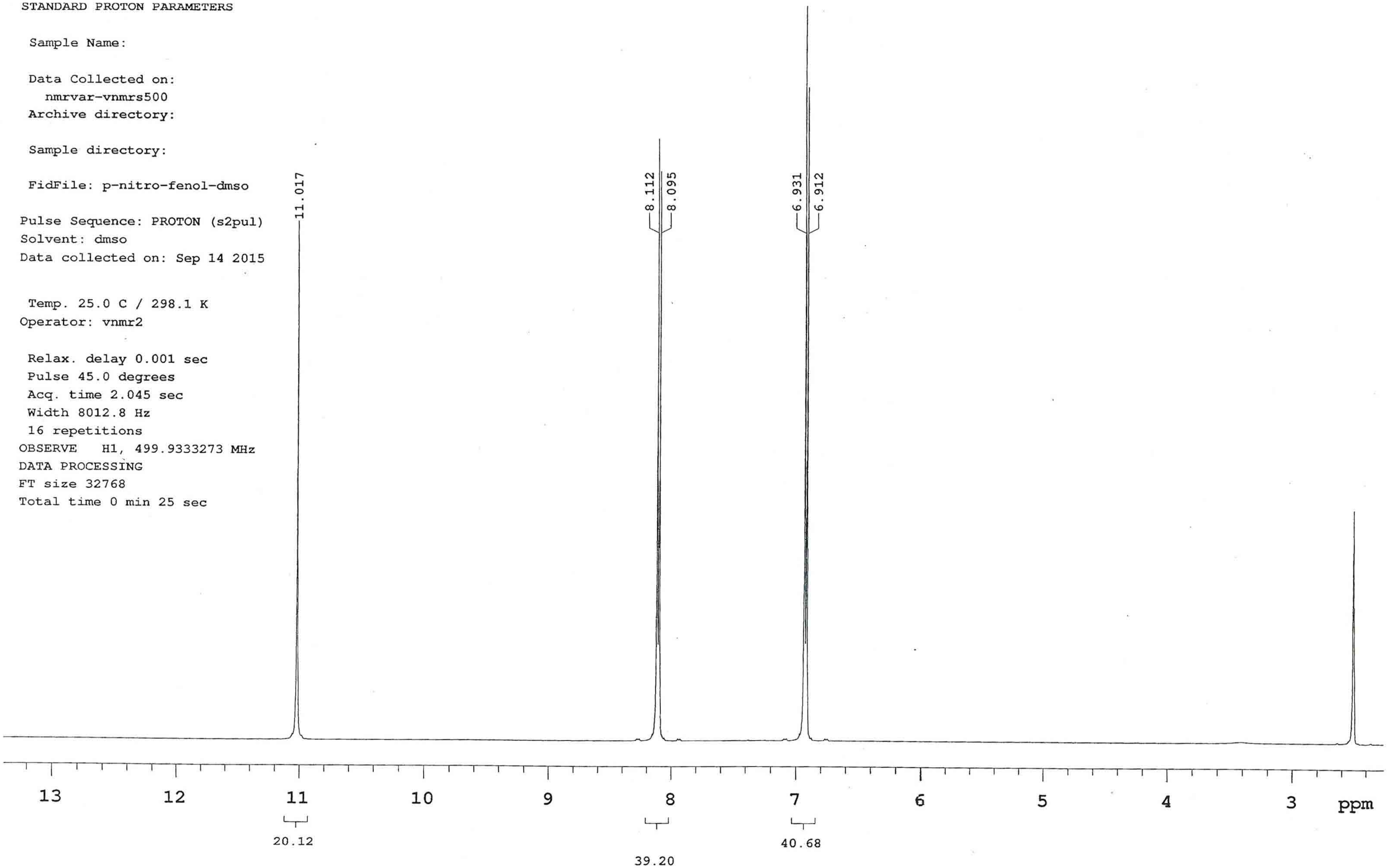
Sample directory:

FidFile: p-nitro-fenol-dmso

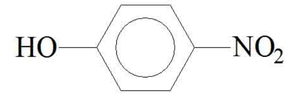
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Sep 14 2015

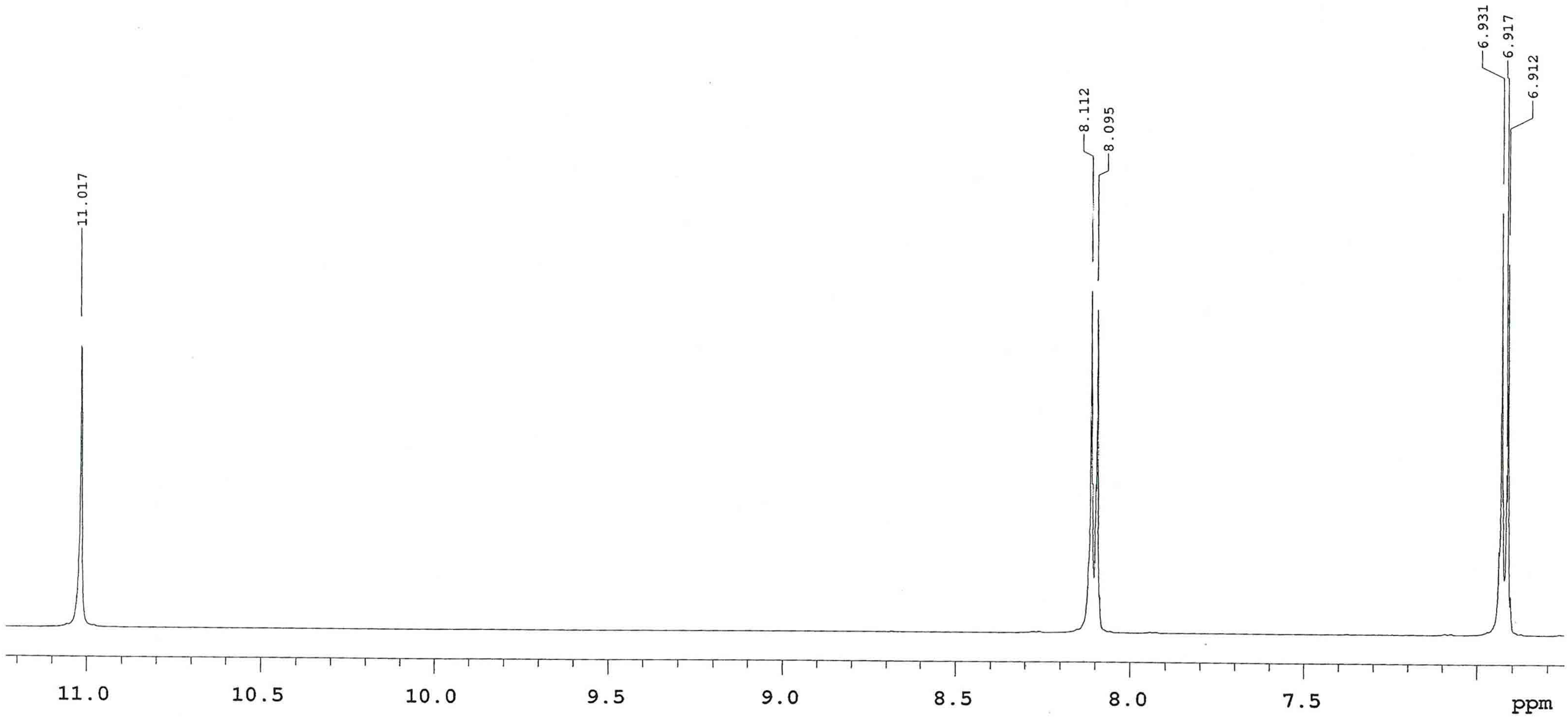
Temp. 25.0 C / 298.1 K
Operator: vnmr2

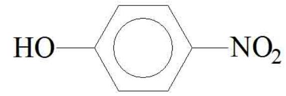
Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9333273 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



11


HO
NO2


11.017
8.112
8.095
6.931
6.917
6.912
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
ppm

11 

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

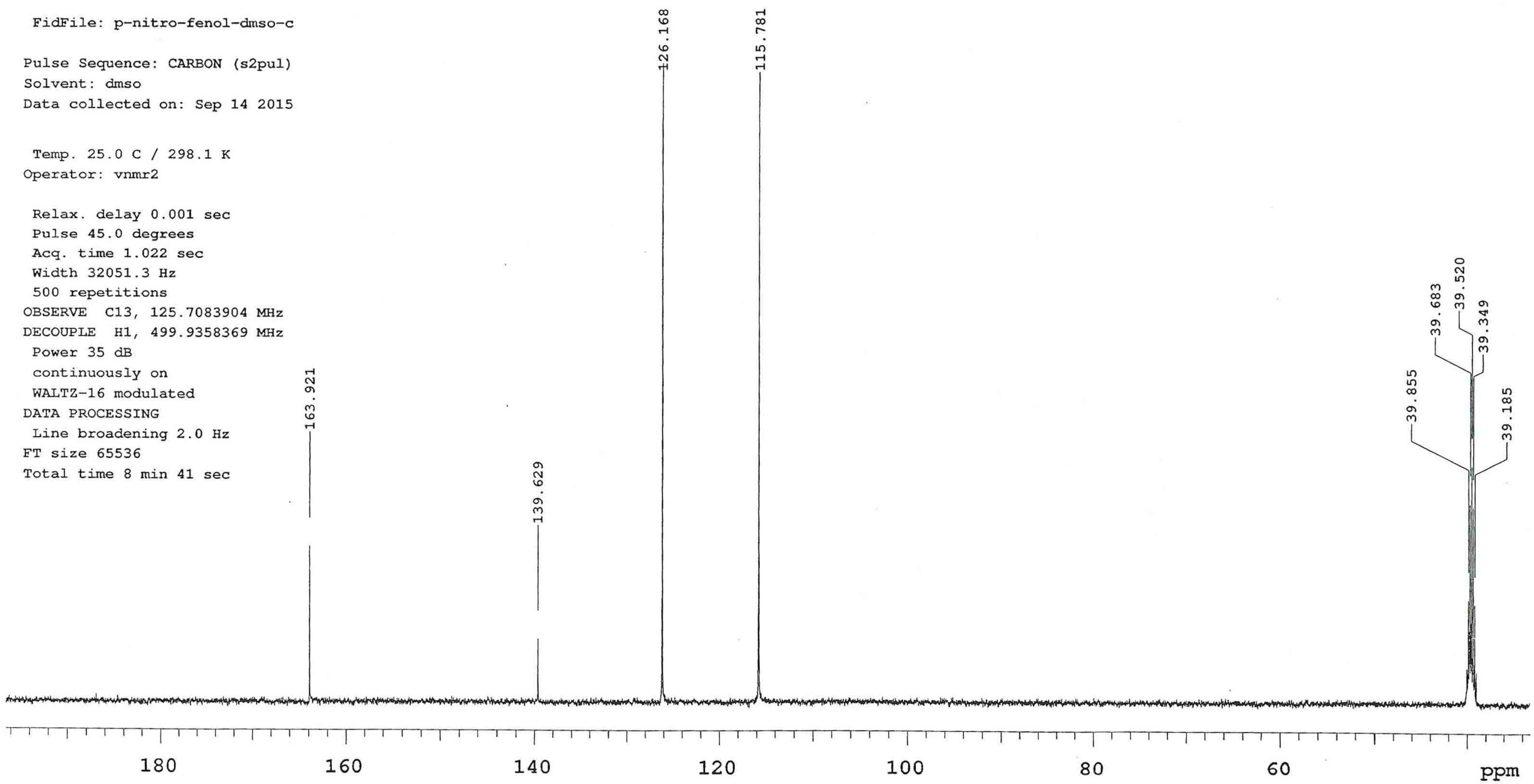
Sample directory:

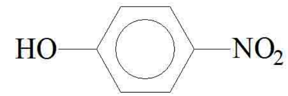
FidFile: p-nitro-fenol-dmso-c

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Sep 14 2015

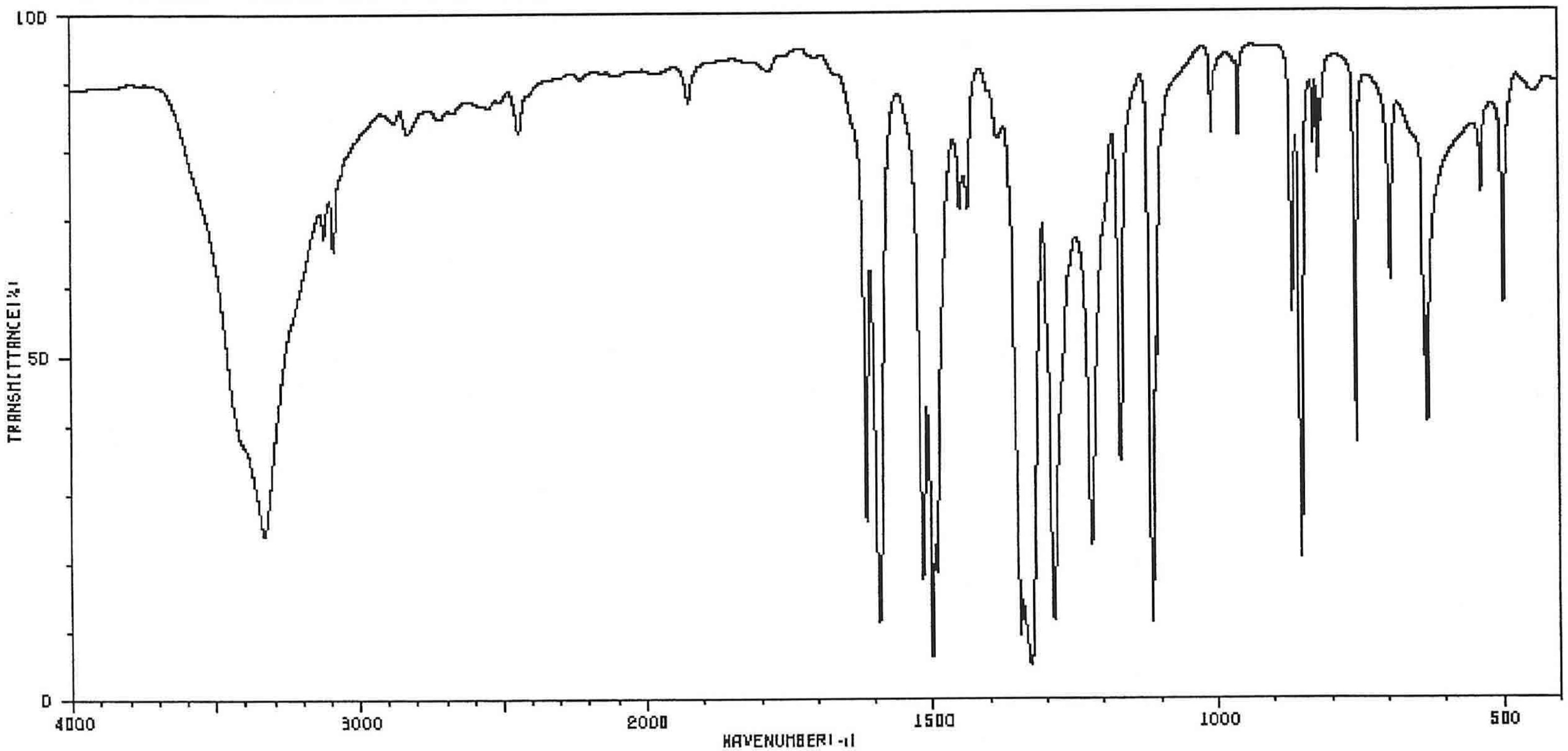
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
500 repetitions
OBSERVE C13, 125.7083904 MHz
DECOUPLE H1, 499.9358369 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

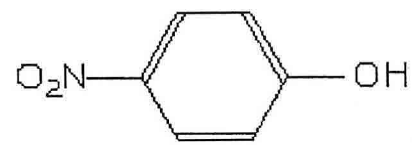


11 

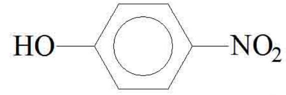
HIT-NO=2127	SCORE= ( )	SDBS-NO=2681	IR-NIDA-00444 : KBR DISC
P-NITROPHENOL			
$C_6H_5NO_3$			



3331	23	1923	84	1437	68	1114	10	821	74
3121	64	1614	25	1383	79	1105	49	815	81
3086	82	1592	10	1346	9	1009	79	755	37
2876	81	1516	17	1328	4	961	79	696	68
2826	79	1500	6	1288	11	867	53	631	38
2722	81	1492	17	1220	21	852	20	537	70
2439	79	1461	68	1169	33	829	77	498	66



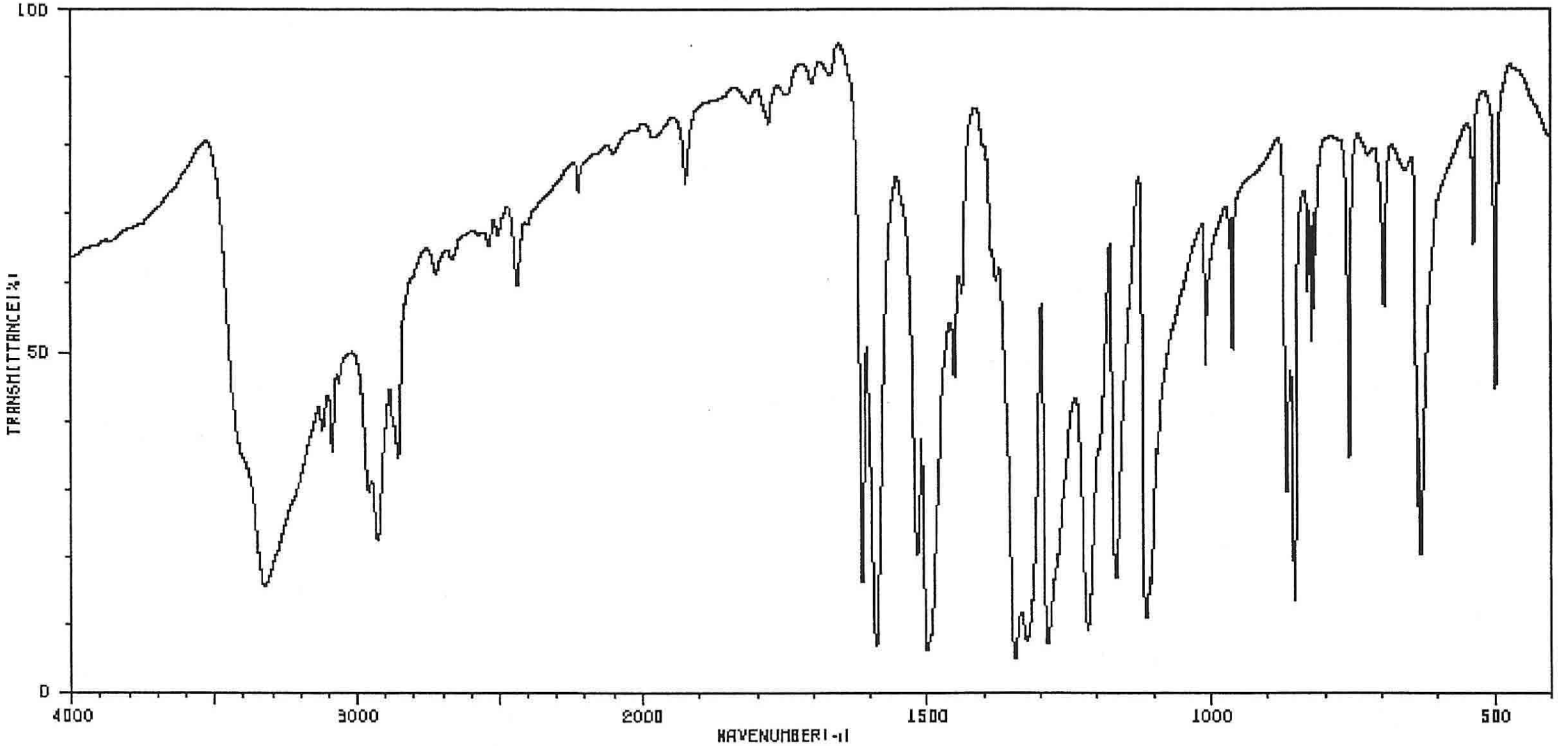
Źródło: ***https://sdbs.db.aist.go.jp***



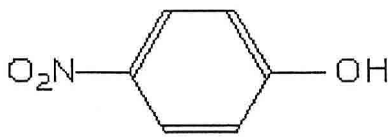
HIT-NO=1443	SCORE= ( )	SDBS-NO=2681	IR-NIDA-22769 : NUJOL MULL

P-NITROPHENOL

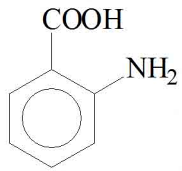
$C_6H_5NO_3$



3324	16	2866	33	1461	44	1167	16	829	67
3122	37	2720	58	1438	57	1113	10	821	50
3085	34	2438	58	1378	58	1104	15	756	34
3061	43	1614	16	1346	4	1008	47	696	66
2957	29	1589	6	1324	7	961	49	636	26
2926	21	1518	20	1288	7	866	28	631	20
2871	38	1500	6	1217	8	863	19	498	43



Źródło: https://sdbs.db.aist.go.jp

12 

Kwas-antranilowy

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

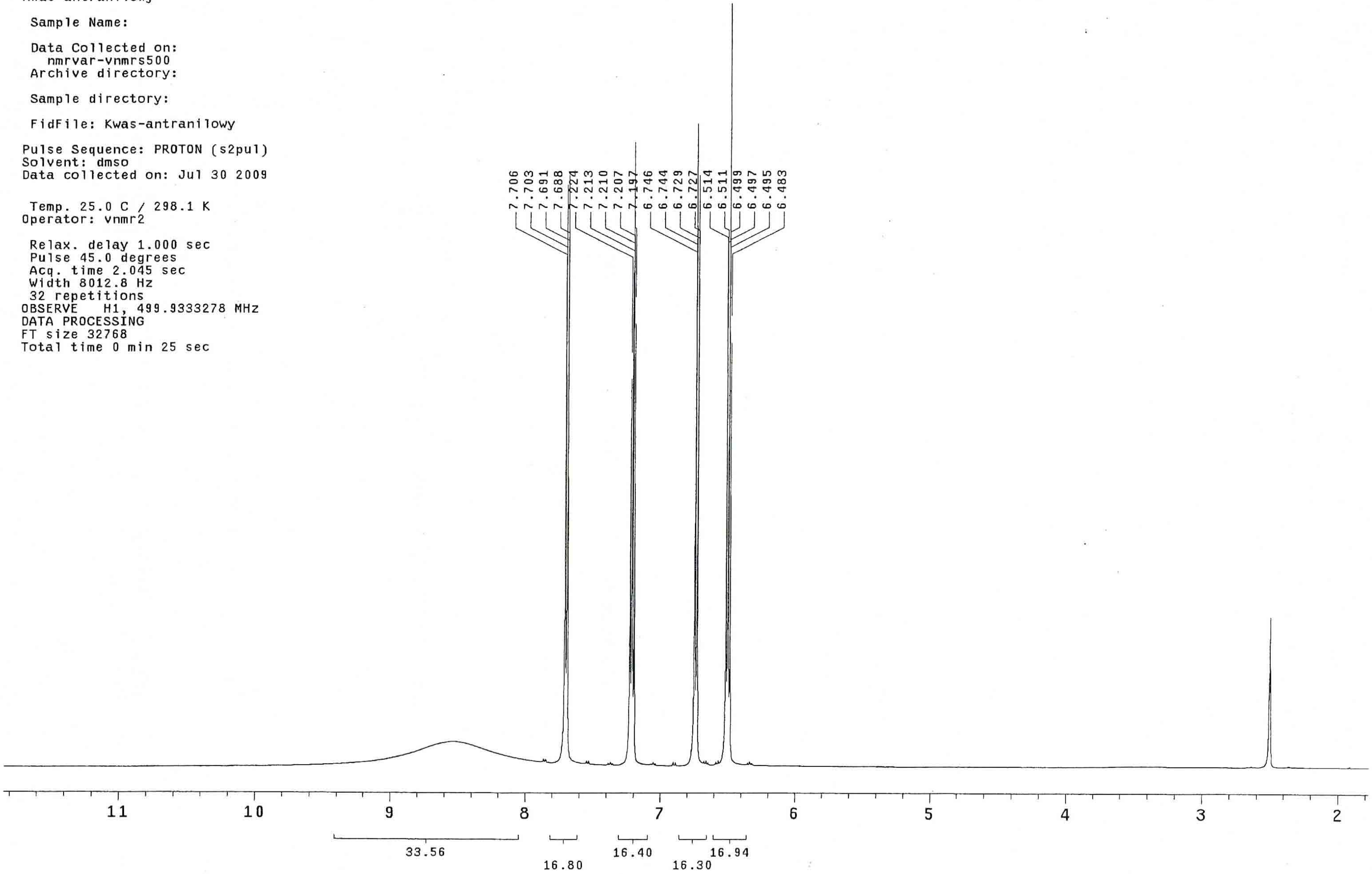
Sample directory:

FidFile: Kwas-antranilowy

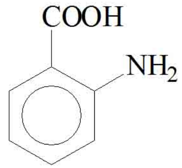
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jul 30 2009

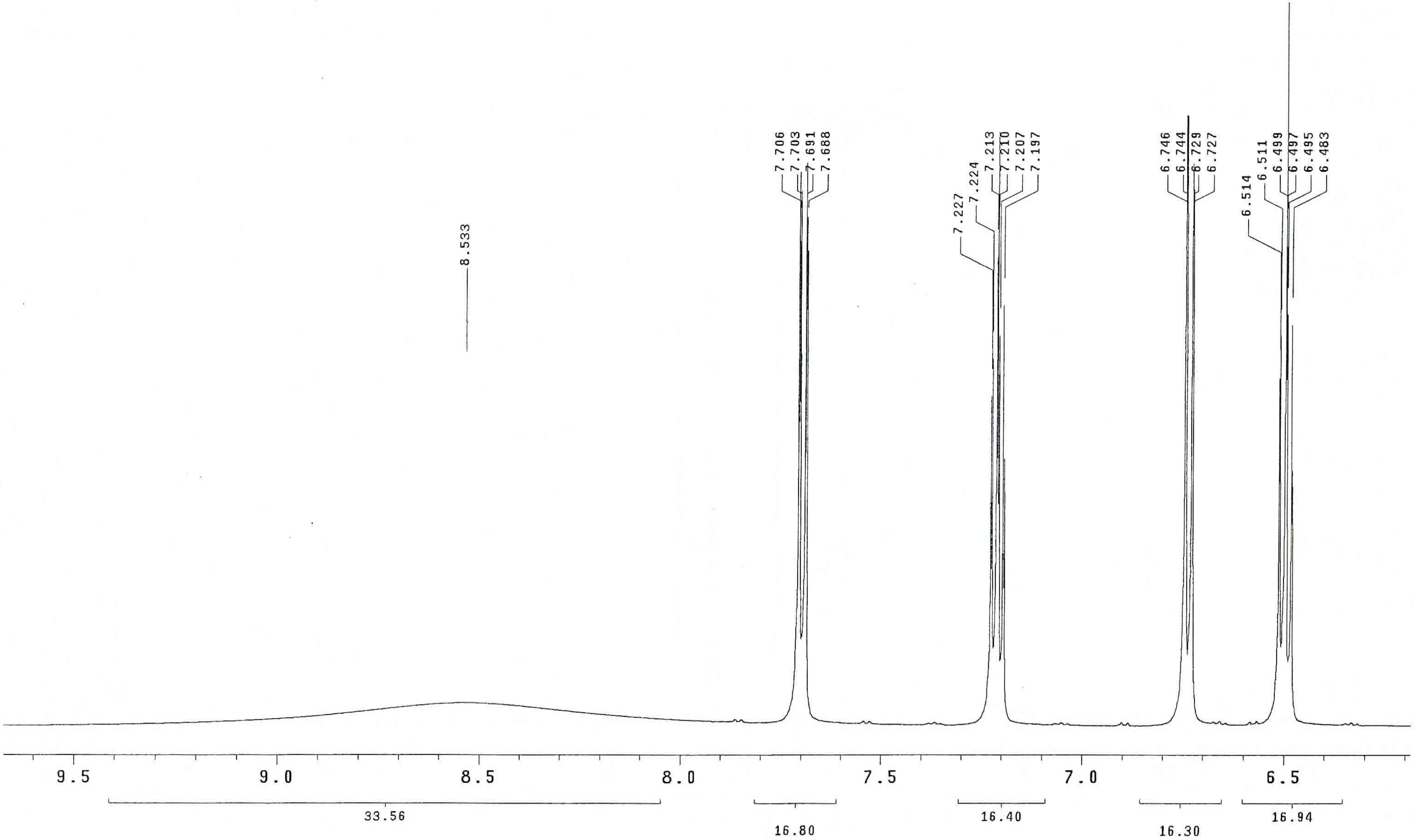
Temp. 25.0 C / 298.1 K
Operator: vnmr2

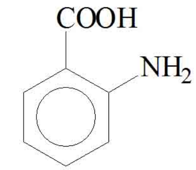
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9333278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



12


COOH
NH_2

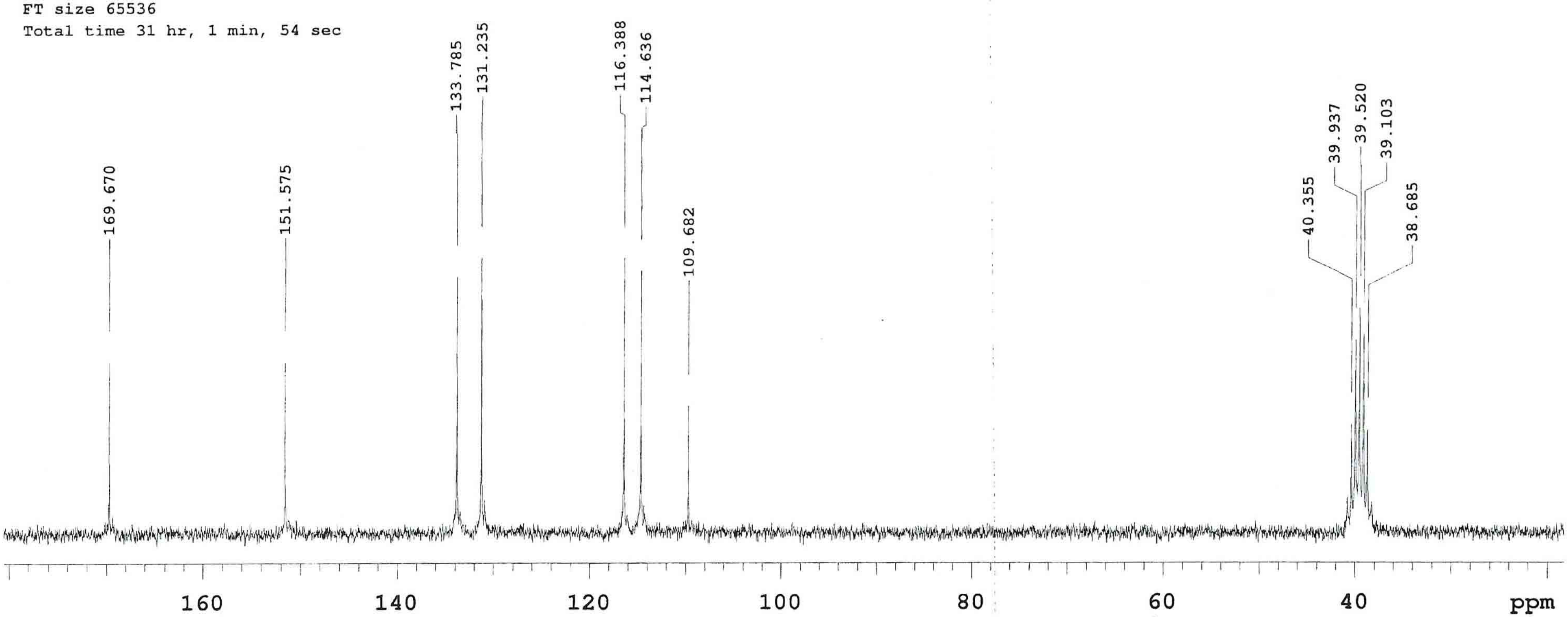

8.533
7.706
7.703
7.691
7.688
7.227
7.224
7.213
7.210
7.207
7.197
6.746
6.744
6.729
6.727
6.514
6.511
6.499
6.497
6.495
6.483
9.5
9.0
8.5
8.0
7.5
7.0
6.5
33.56
16.80
16.40
16.30
16.94

12 

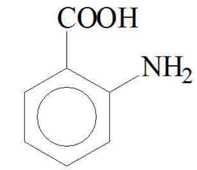
Kwas-antranilowy

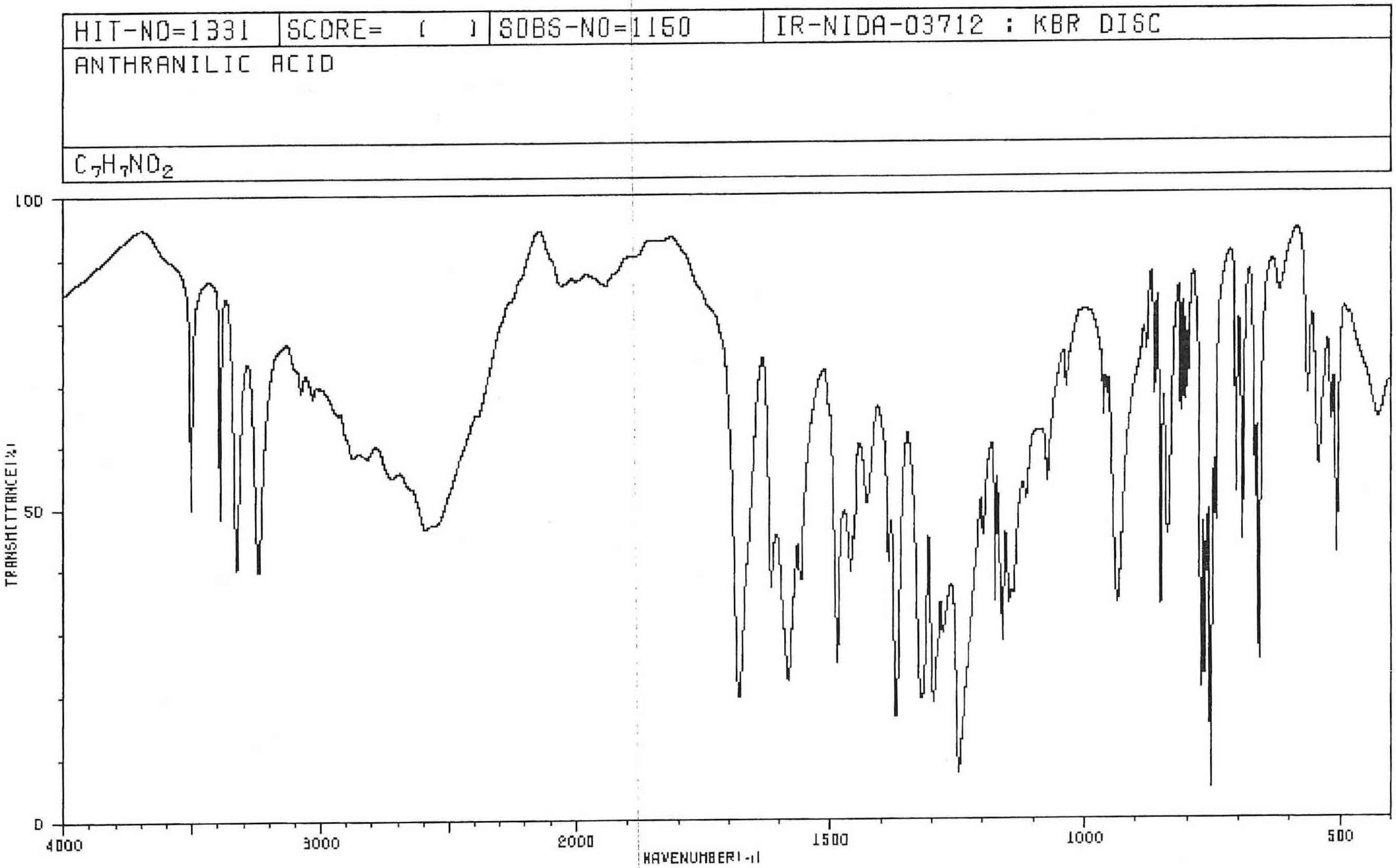
Solvent: DMSO
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2830302 MHz
DECOUPLE H1, 199.9730475 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

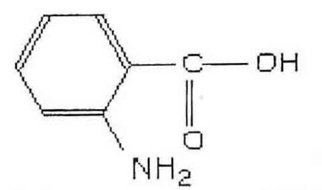


12

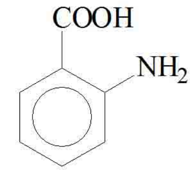




3602	47	1616	36	1371	16	1161	26	766	21
3390	46	1583	21	1321	18	1149	33	755	4
3324	38	1557	36	1298	17	1140	34	744	44
3240	37	1486	29	1279	28	936	33	692	42
2586	44	1460	37	1248	7	851	32	667	49
2565	44	1454	42	1199	43	837	43	660	23
1679	18	1386	38	1176	33	772	20	607	41



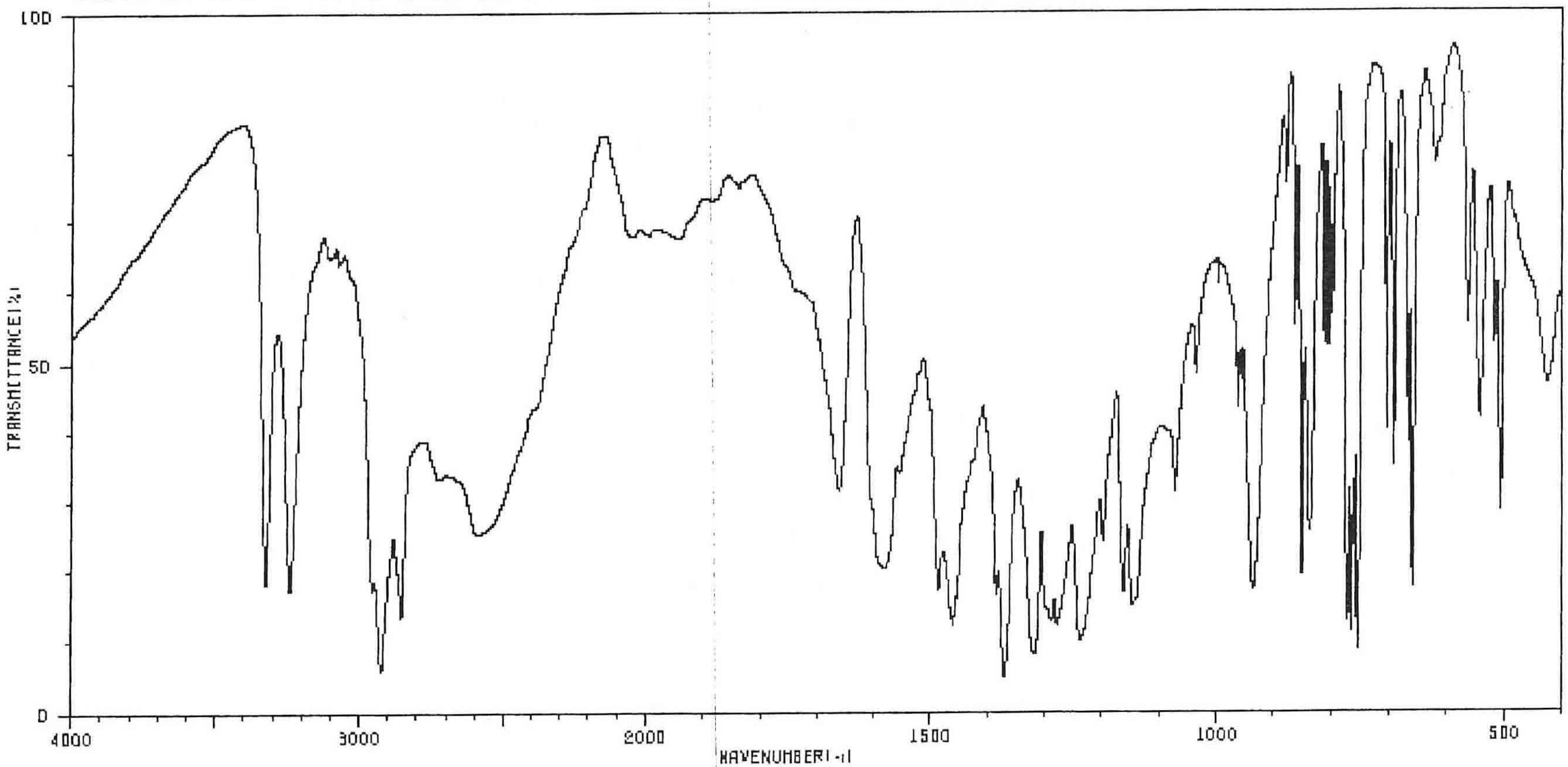
Źródło: ***https://sdbs.db.aist.go.jp***

12 

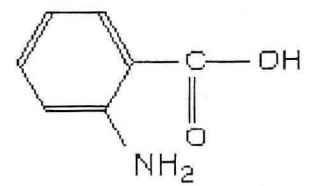
HIT-NO=705	SCORE= ( )	SDBS-NO=1150	IR-NIDA-67175 : NUJOL MULL

ANTHRANILIC ACID

$C_7H_7NO_2$

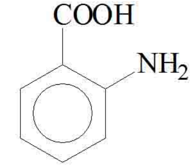


3324	17	1662	30	1319	7	1148	14	754	8
3239	16	1580	19	1297	13	1073	30	705	38
2955	16	1488	16	1290	12	935	16	693	33
2923	6	1460	11	1280	11	861	18	667	36
2869	18	1454	15	1239	9	838	24	660	16
2854	12	1385	15	1199	23	772	12	542	39
2690	23	1371	4	1162	16	766	10	507	27

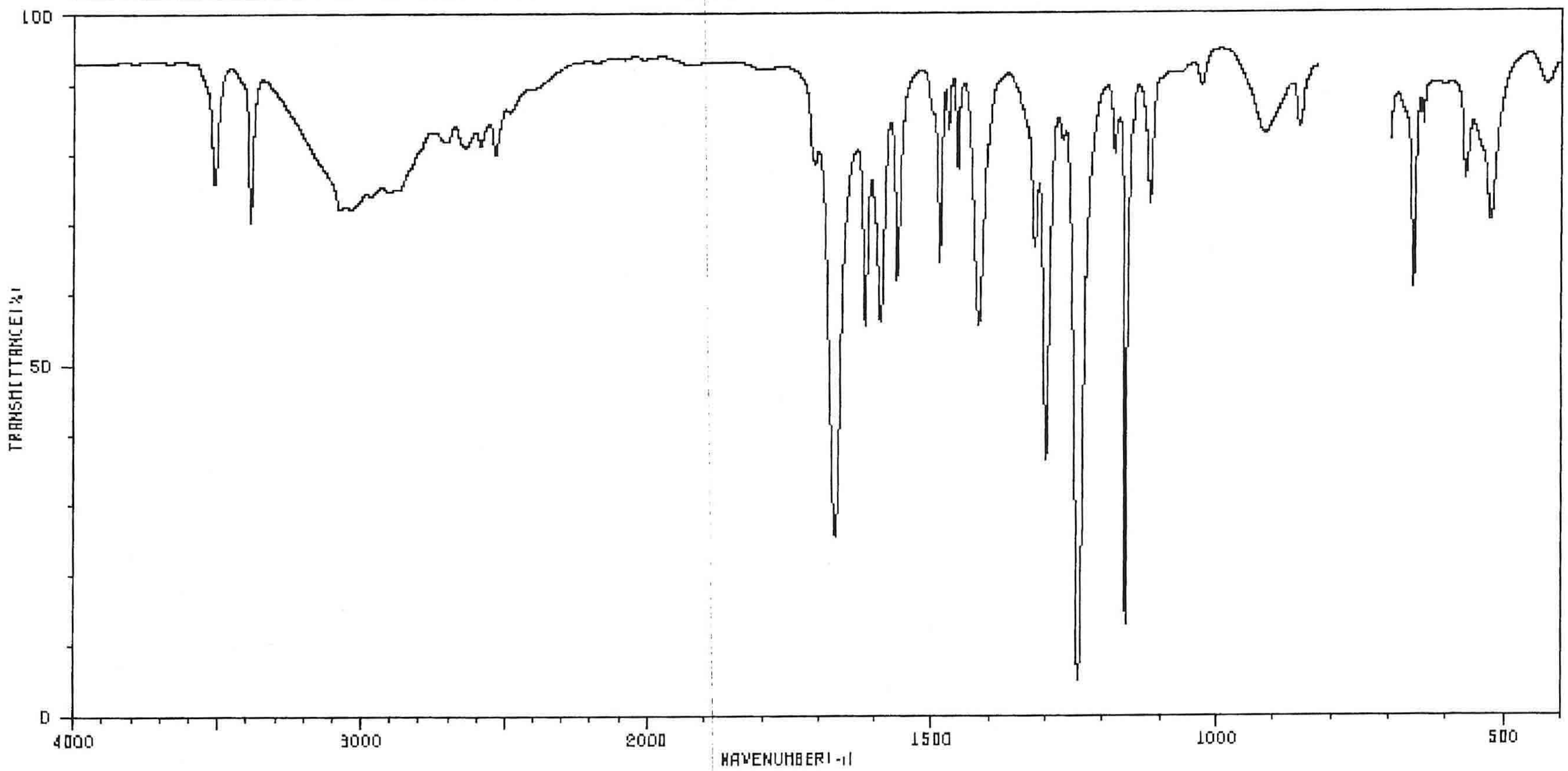


Źródło: https://sdbs.db.aist.go.jp

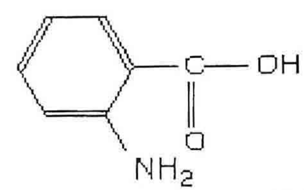
12



HIT-NO=803	SCORE= ( )	SDBS-NO=1150	IR-NIDA-06180 : CCL4 SOLUTION
ANTHRANILIC ACID			
$C_7H_7NO_2$			

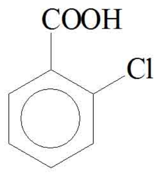


3612	72	1707	77	1466	74	1162	12	668	74
3387	68	1671	24	1418	53	1118	70	524	68
3037	70	1617	55	1320	64	1027	86	426	66
2707	79	1591	63	1300	34	916	79		
2642	77	1561	58	1272	79	855	81		
2587	79	1488	62	1244	4	658	58		
2536	77	1471	81	1181	77	641	81		



Źródło: ***https://sdbs.db.aist.go.jp***

13



Kwas_o-chlorobenzoesowy

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

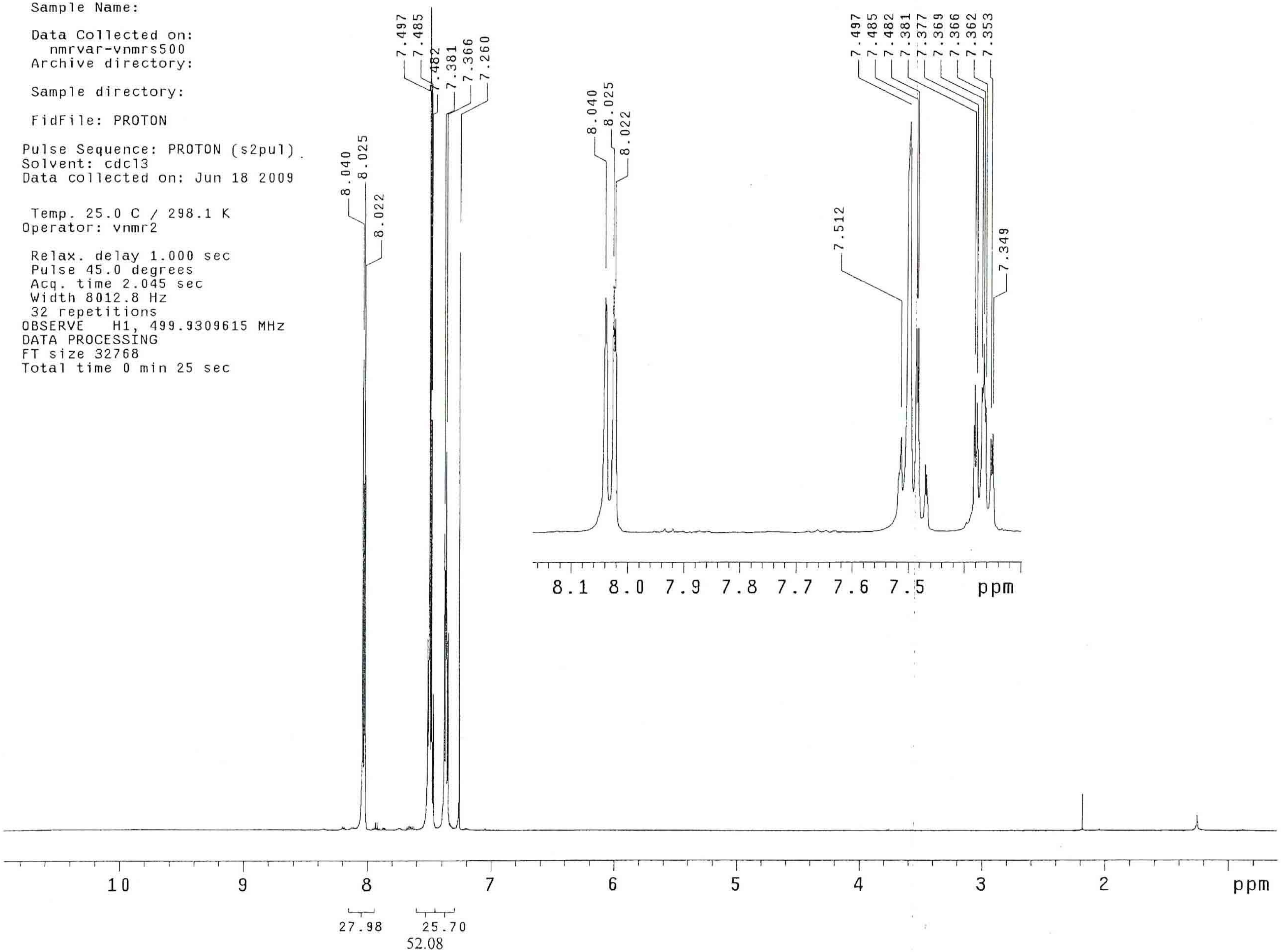
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 18 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

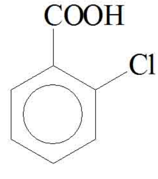


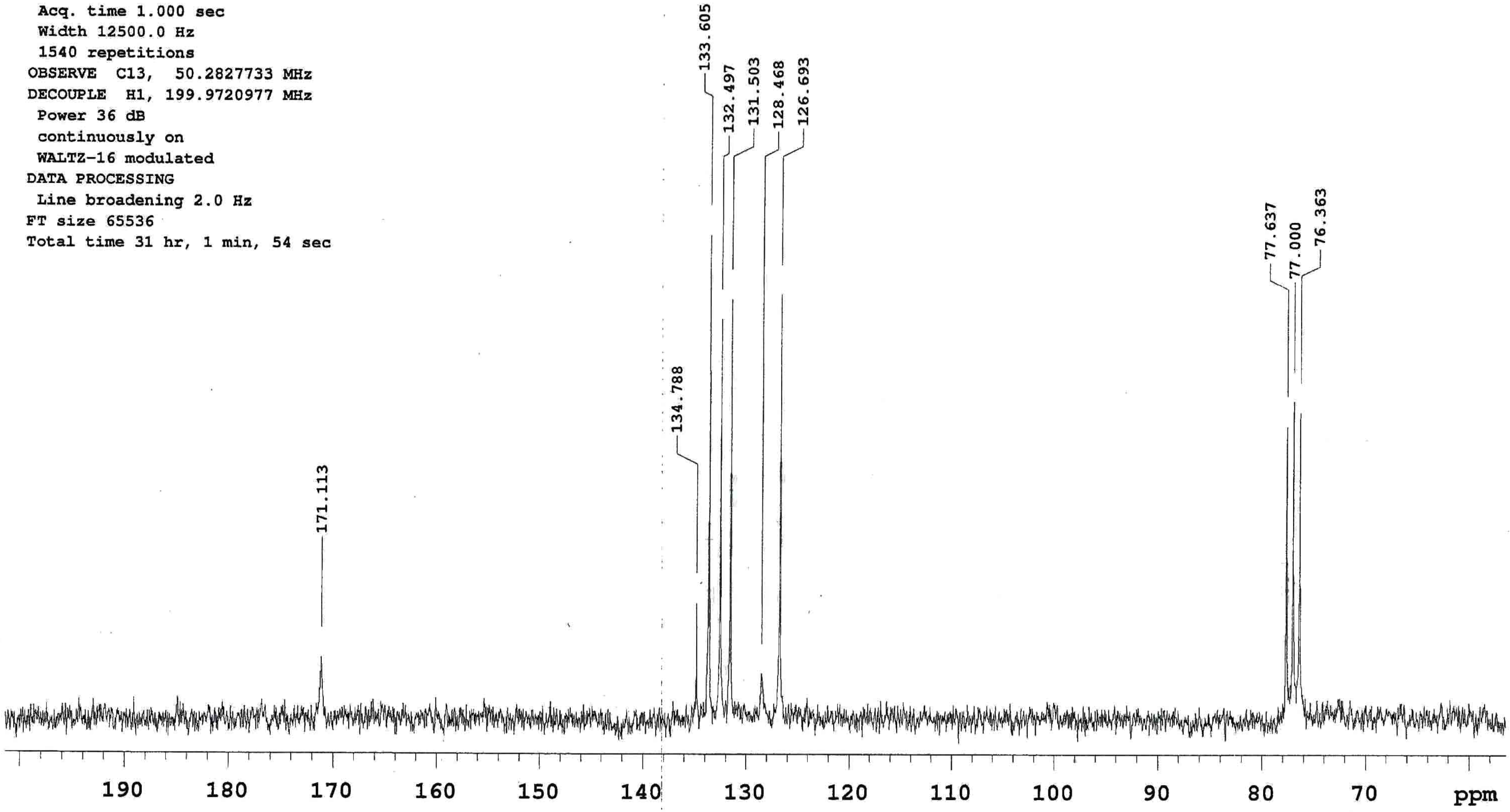
Kwas_o-chlorobenzoesowy

Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

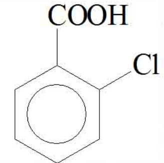
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1540 repetitions
OBSERVE C13, 50.2827733 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

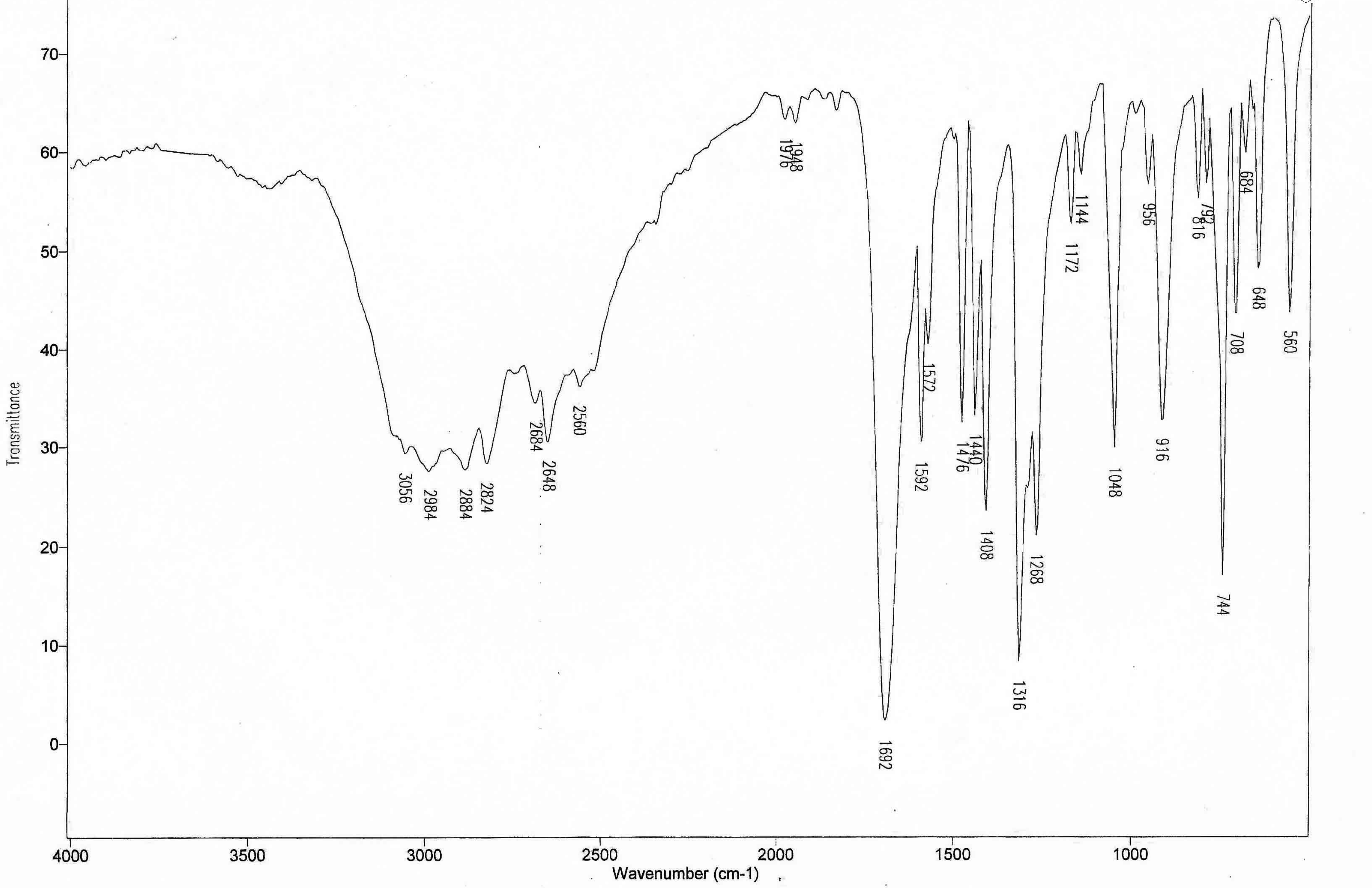
13





13


COOH
Cl


Transmittance
Wavenumber (cm-1)
4000
3500
3000
2500
2000
1500
1000
70
60
50
40
30
20
10
0
3056
2984
2884
2824
2684
2648
2560
1976
1948
1692
1592
1572
1476
1440
1408
1316
1268
1172
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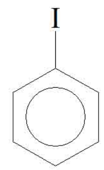
1048
956
916
816
792
744
708
684
648
560

14



Jodobenzen

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

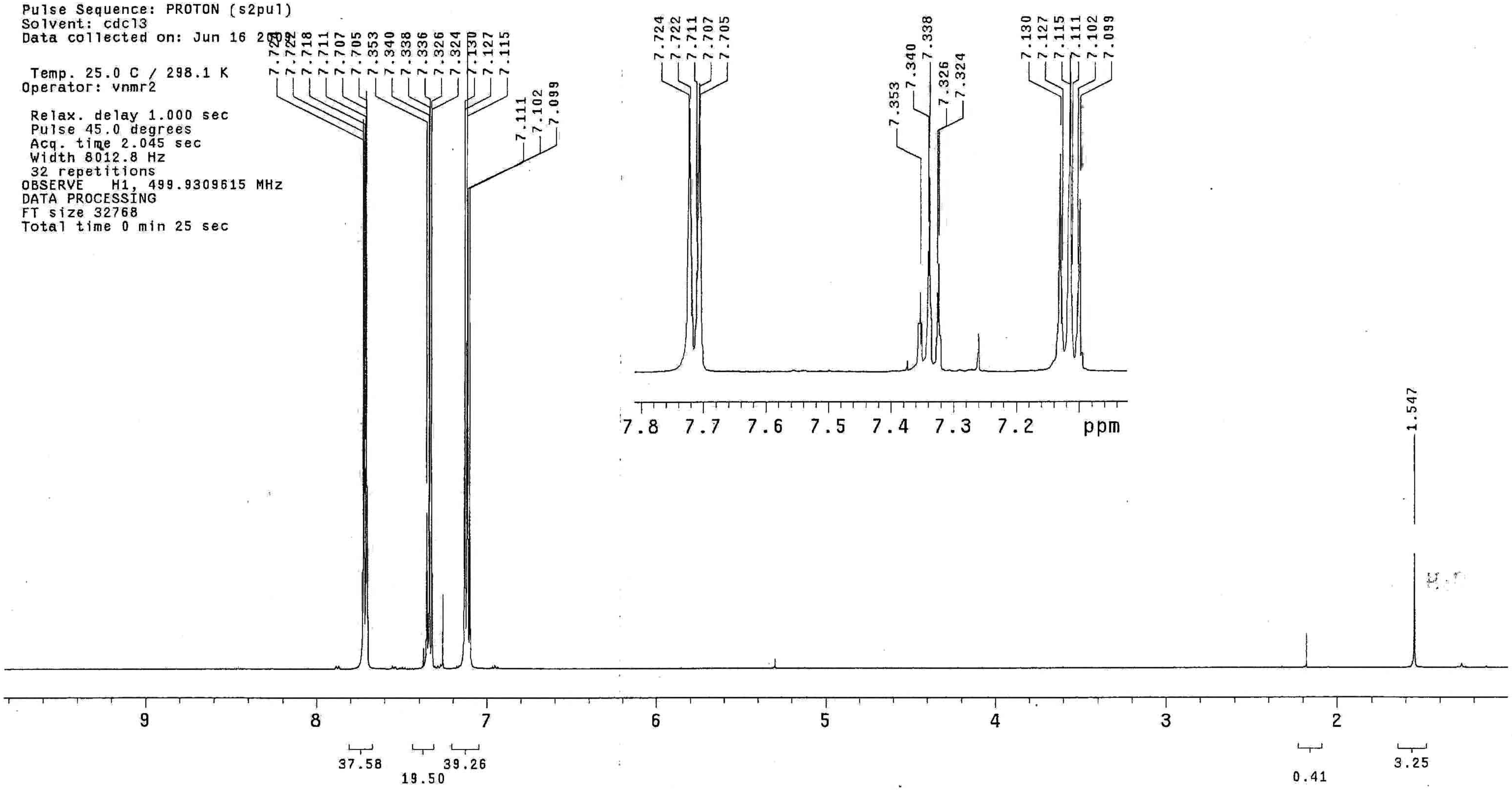
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 16 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

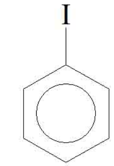


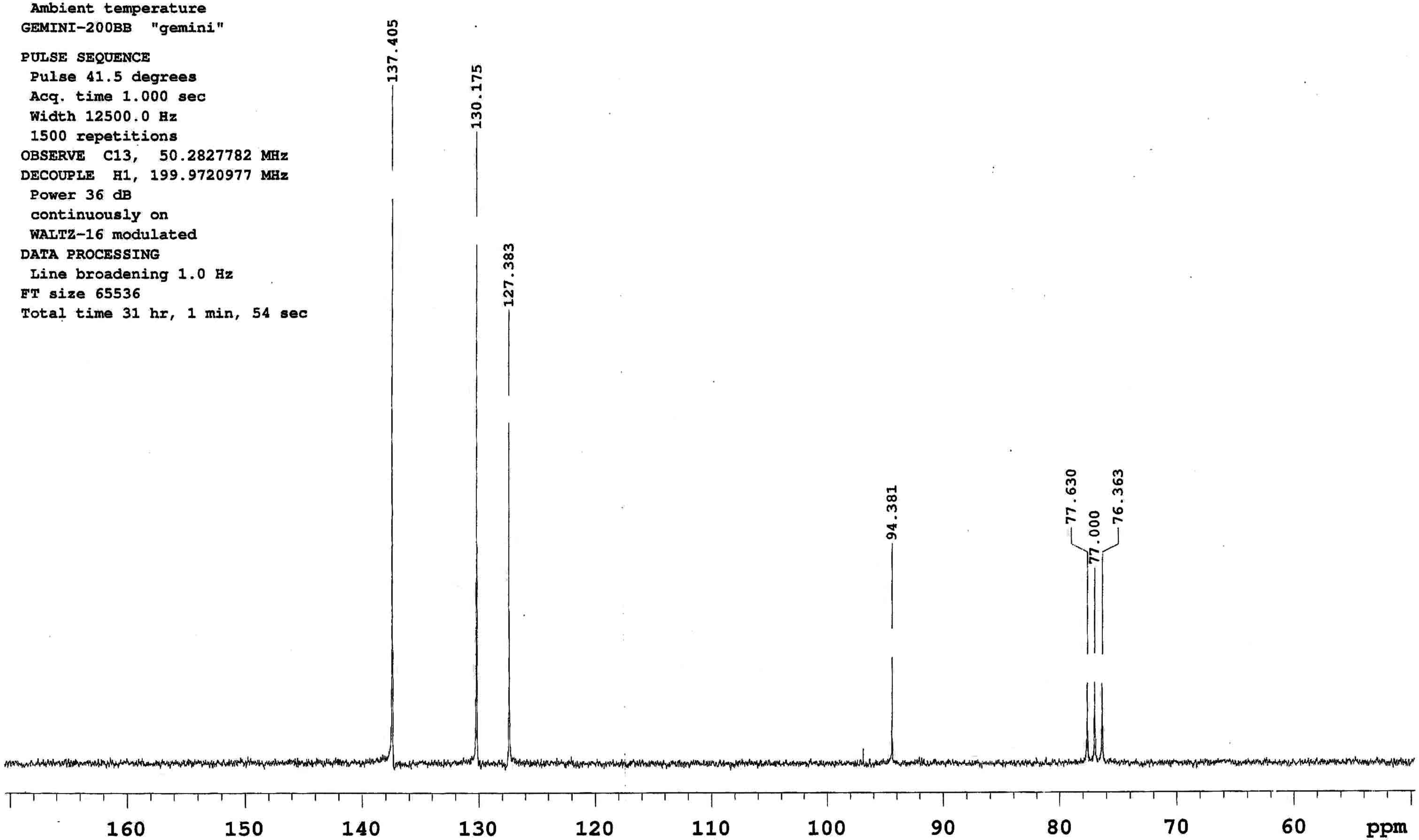
Jodobenzen

Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

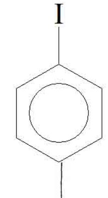
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827782 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

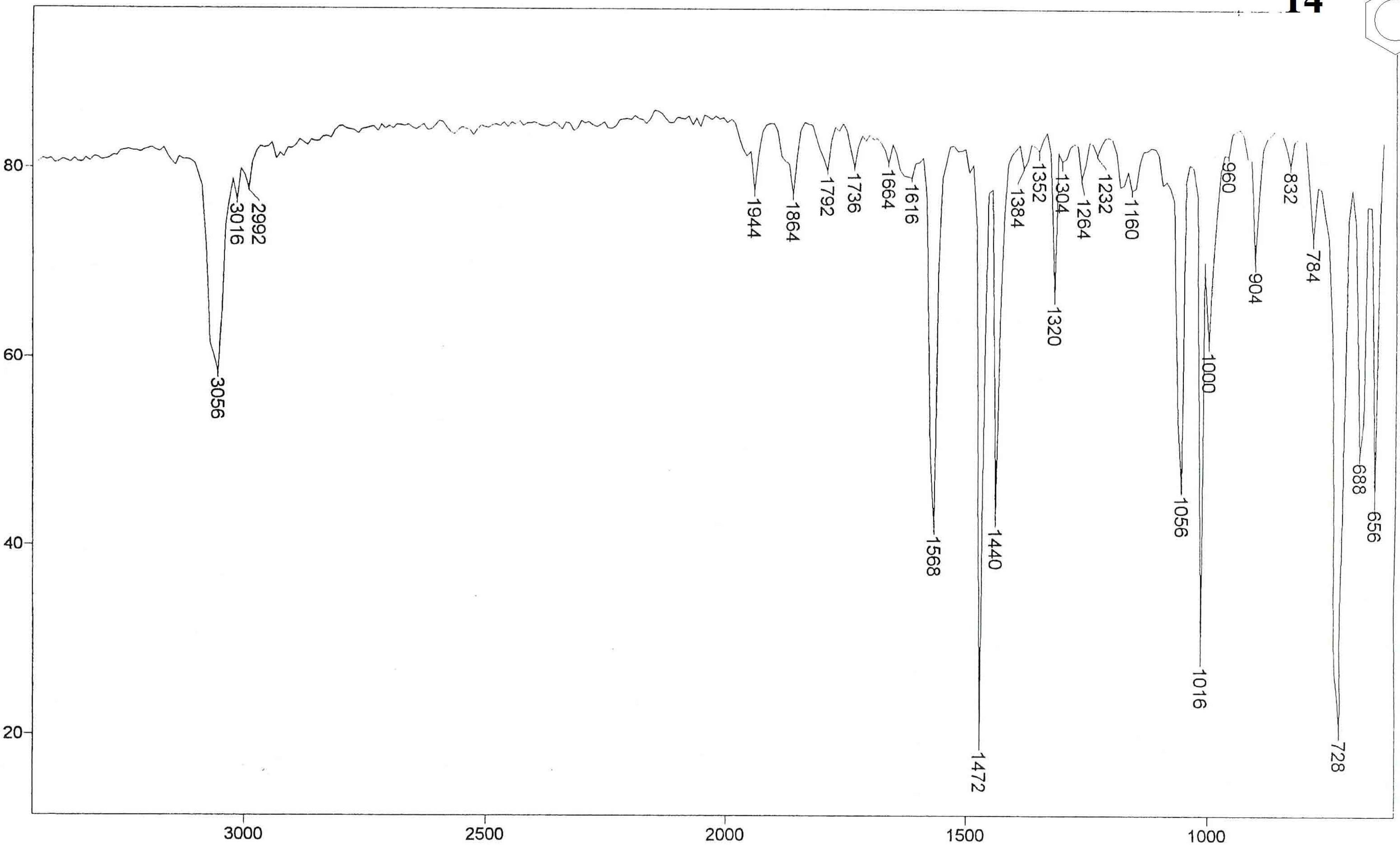
14





14



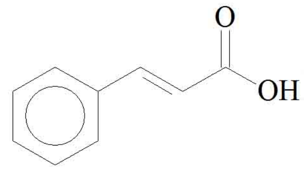


Transmittance / Wavenumber (cm-1)

File # 5 = [redacted]

Paged X-Zoom SCROLL

99-02-24 12:26 Res=4.000000

15 

Kwas-cynamonowy

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

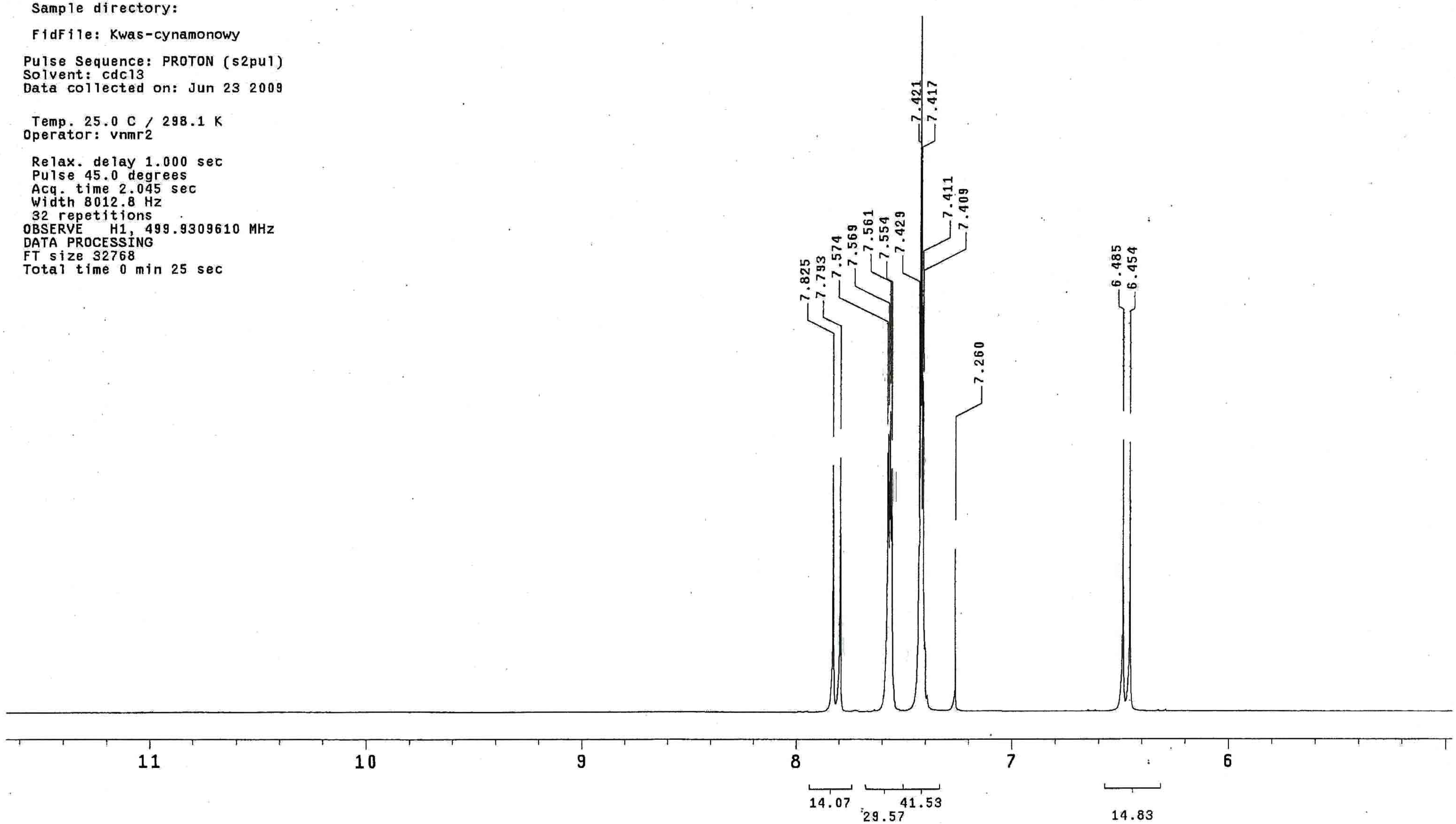
Sample directory:

FidFile: Kwas-cynamonowy

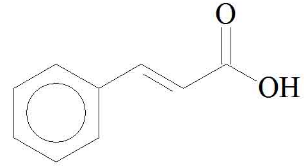
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

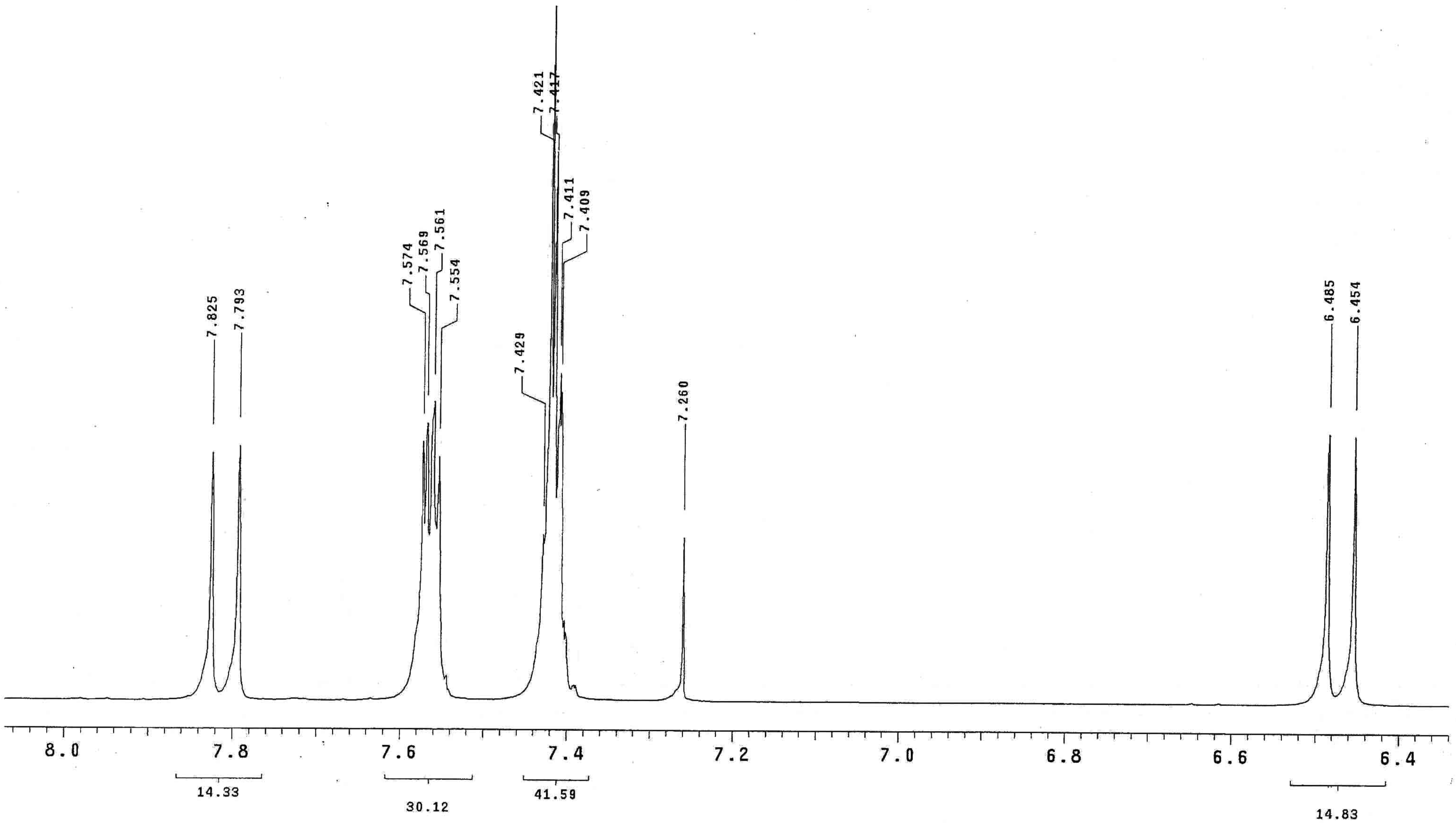
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309610 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



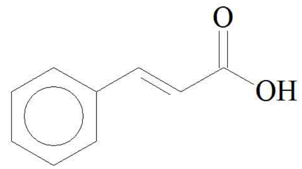
15



O
OH



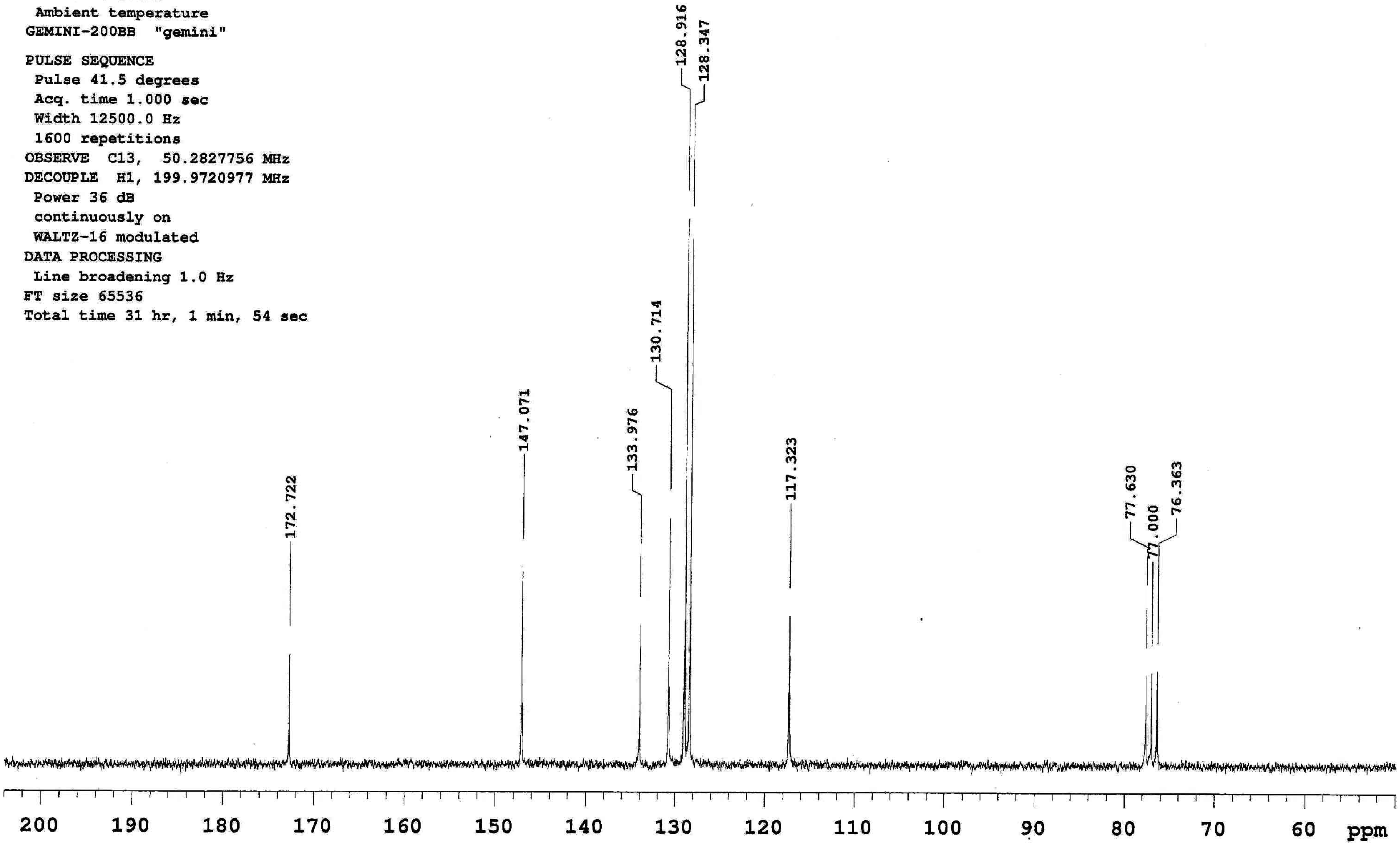
7.825
7.793
7.574
7.569
7.561
7.554
7.429
7.421
7.417
7.411
7.409
7.260
6.485
6.454
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
14.33
30.12
41.59
14.83

15 

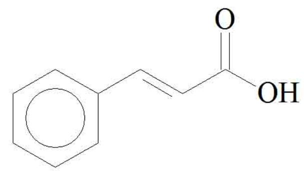
Kwas-cynamonowy

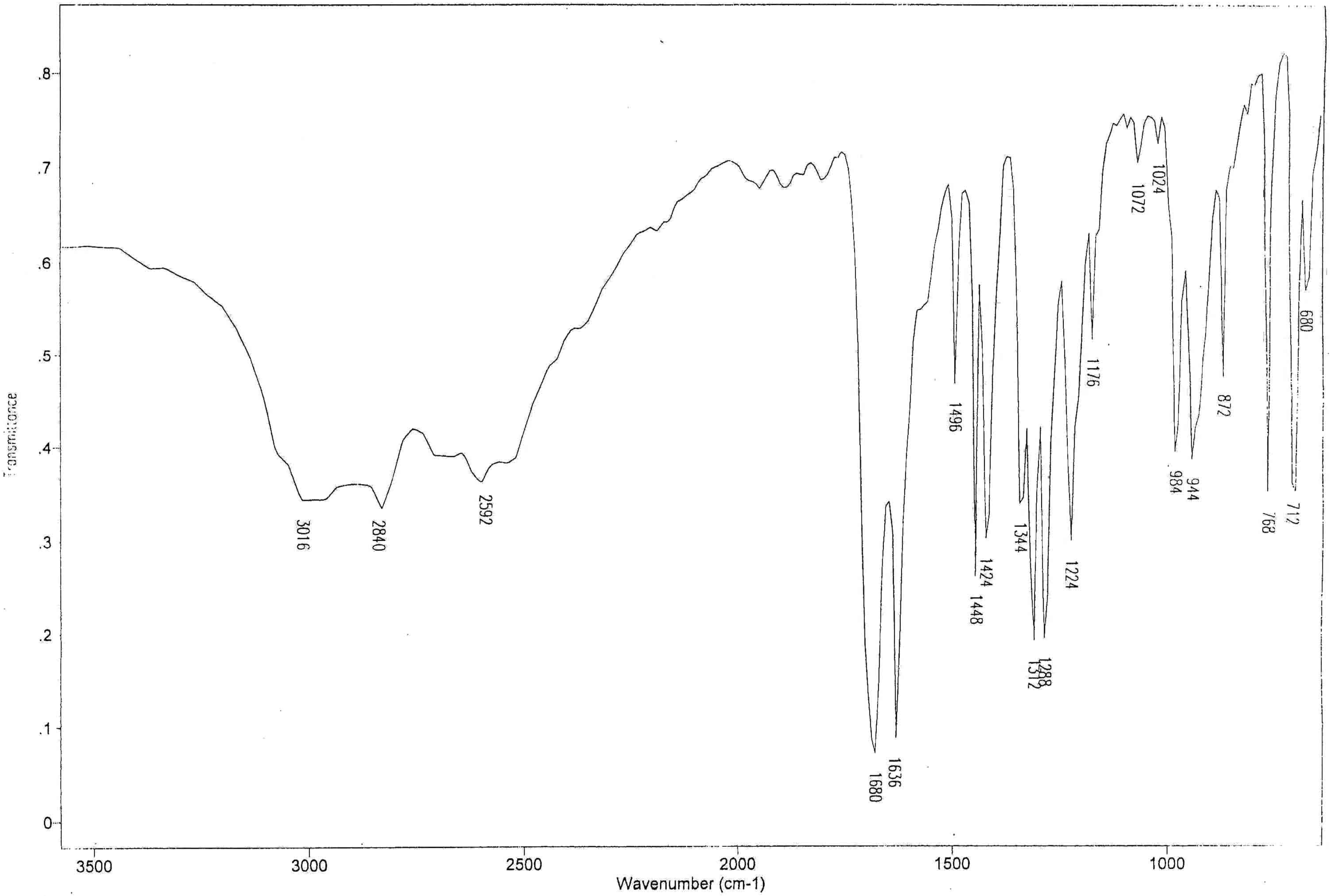
Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

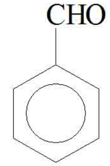
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1600 repetitions
OBSERVE C13, 50.2827756 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec



15


O
OH

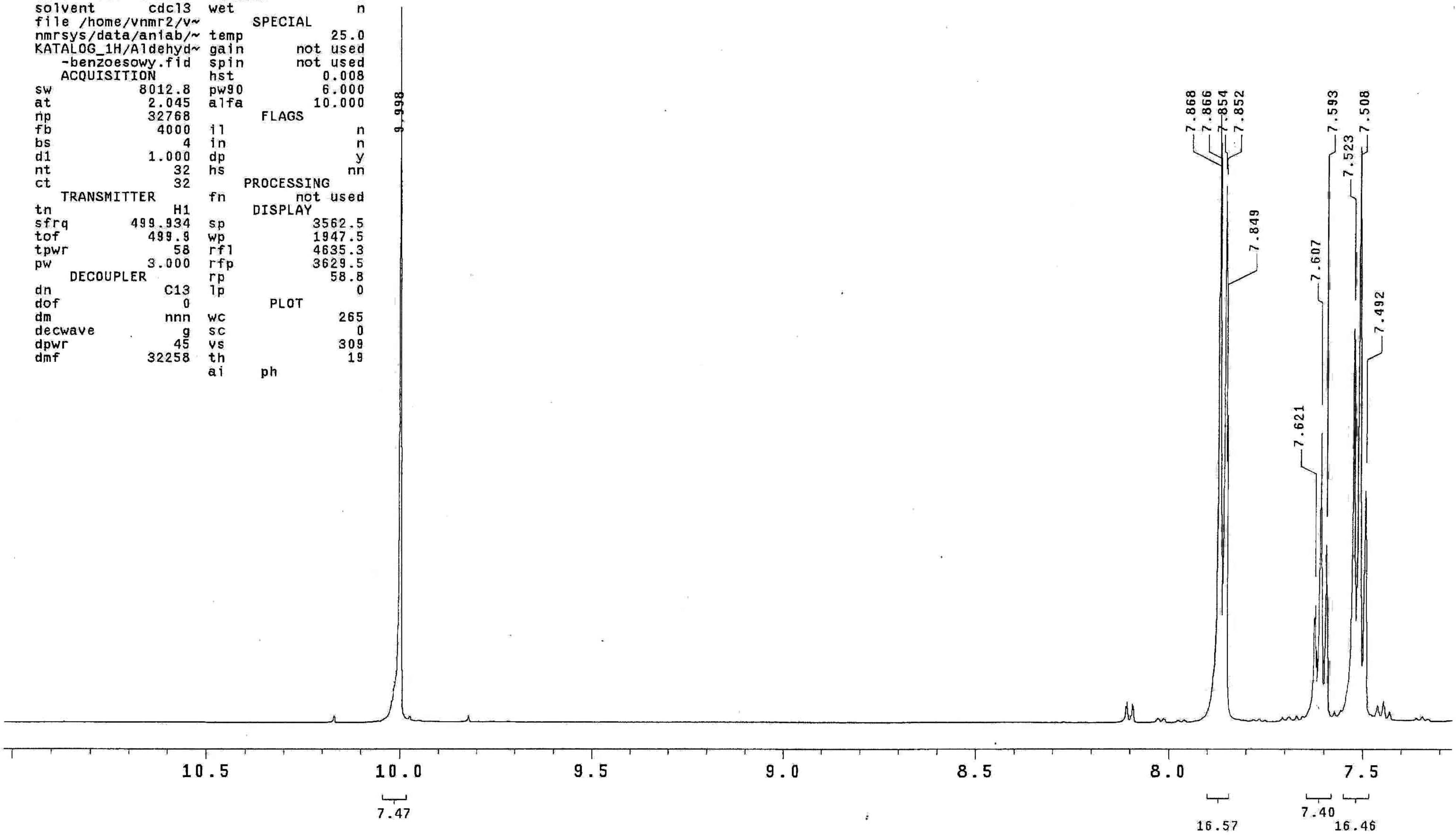

Transmittance
Wavenumber (cm-1)
.8
.7
.6
.5
.4
.3
.2
.1
0
3500
3000
2500
2000
1500
1000
3016
2840
2592
1680
1636
1496
1448
1424
1344
1312
1288
1224
1176
1072
1024
984
944
872
768
712
680

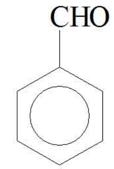
16 

Aldehyd-benzoesowy

exp1 PROTON

```
      SAMPLE               PRESATURATION
date    Oct  1 2009  satmode             n
solvent       cdcl3  wet                 n
file /home/vnmr2/v~       SPECIAL
nmrsys/data/aniab/~  temp             25.0
KATALOG_1H/Aldehyd~  gain         not used
  -benzoesowy.fid    spin         not used
   ACQUISITION       hst             0.008
sw           8012.8  pw90            6.000
at            2.045  alfa           10.000
np            32768         FLAGS
fb             4000  il                  n
bs                4  in                  n
d1            1.000  dp                  y
nt               32  hs                 nn
ct               32       PROCESSING
   TRANSMITTER       fn           not used
tn               H1         DISPLAY
sfrq        499.934  sp             3562.5
tof           499.9  wp             1947.5
tpwr             58  rfl            4635.3
pw            3.000  rfp            3629.5
   DECOUPLER         rp               58.8
dn              C13  lp                  0
dof               0           PLOT
dm              nnn  wc                265
decwave           g  sc                  0
dpwr             45  vs                309
dmf           32258  th                 19
                     ai     ph
```

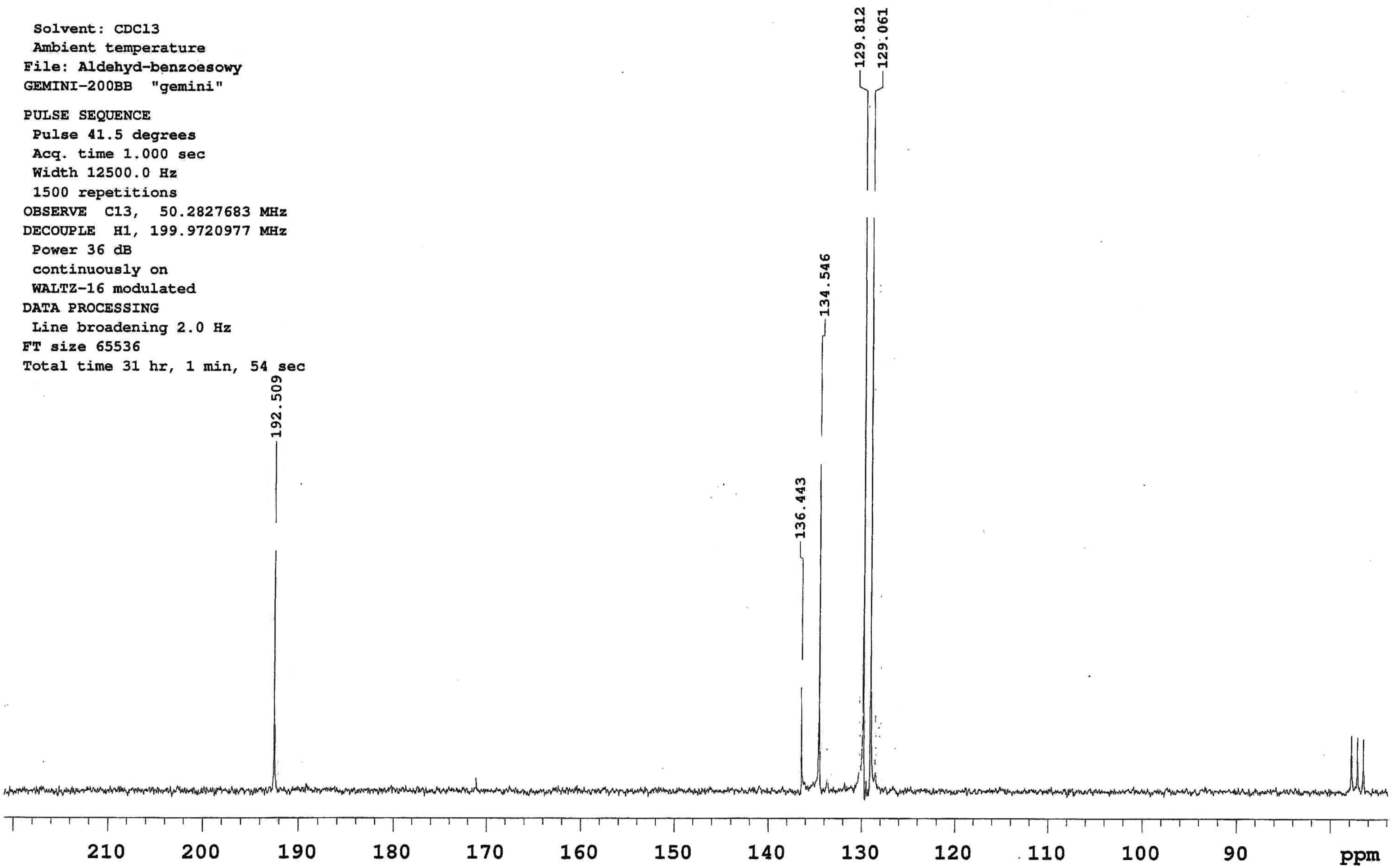


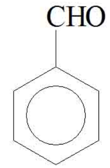
16 

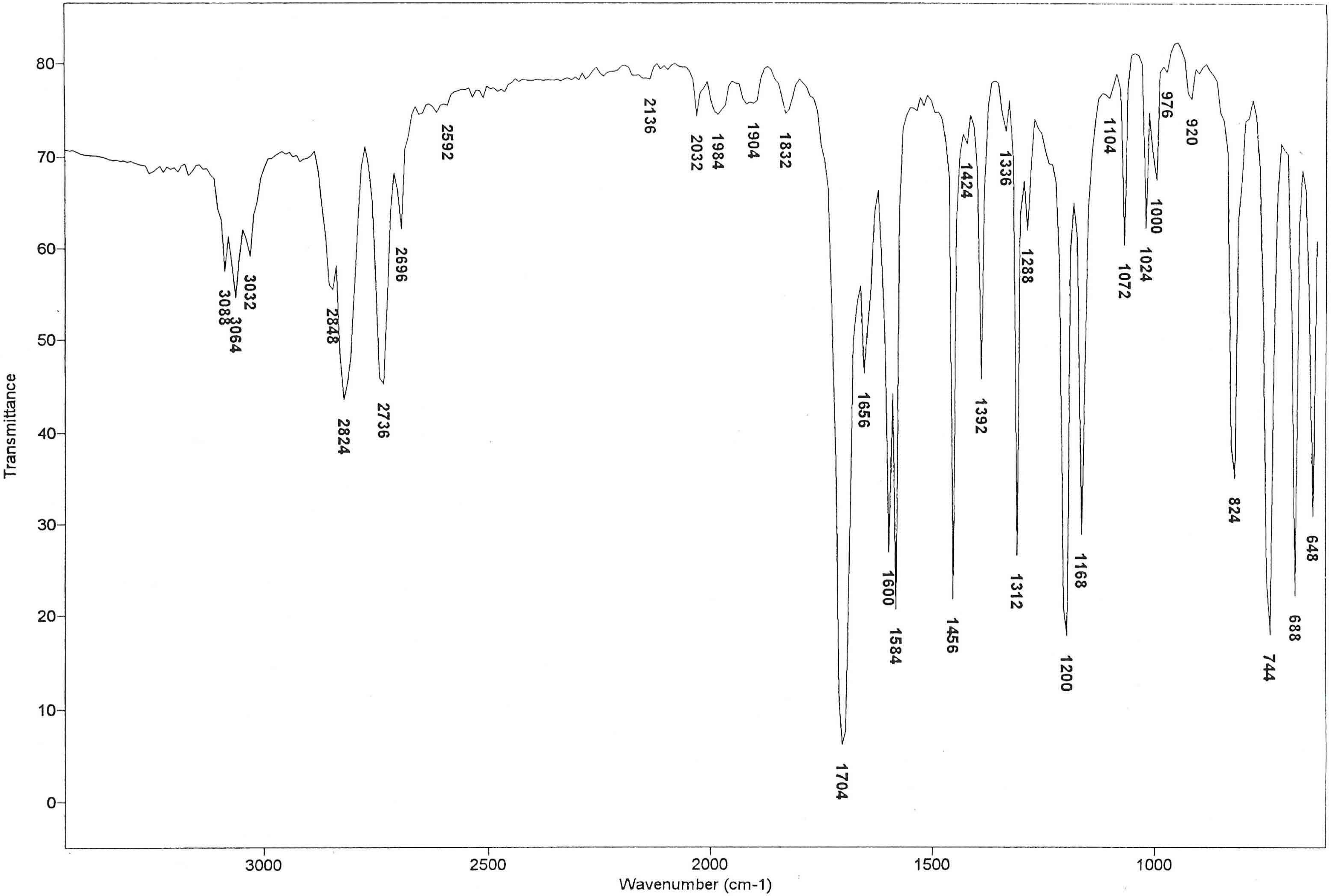
Aldehyd-benzoesowy

Solvent: CDC13
Ambient temperature
File: Aldehyd-benzoesowy
GEMINI-200BB "gemini"

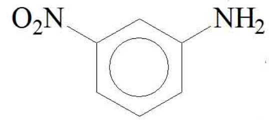
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827683 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec



16 
CHO


Transmittance
Wavenumber (cm-1)
80
70
60
50
40
30
20
10
0
3000
2500
2000
1500
1000
3088
3064
3032
2848
2824
2736
2696
2592
2136
2032
1984
1904
1832
1704
1656
1600
1584
1456
1424
1392
1336
1312
1288
1200
1168
1104
1072
1024
1000
976
920
824
744
688
648

17



m-Nitroanilina

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

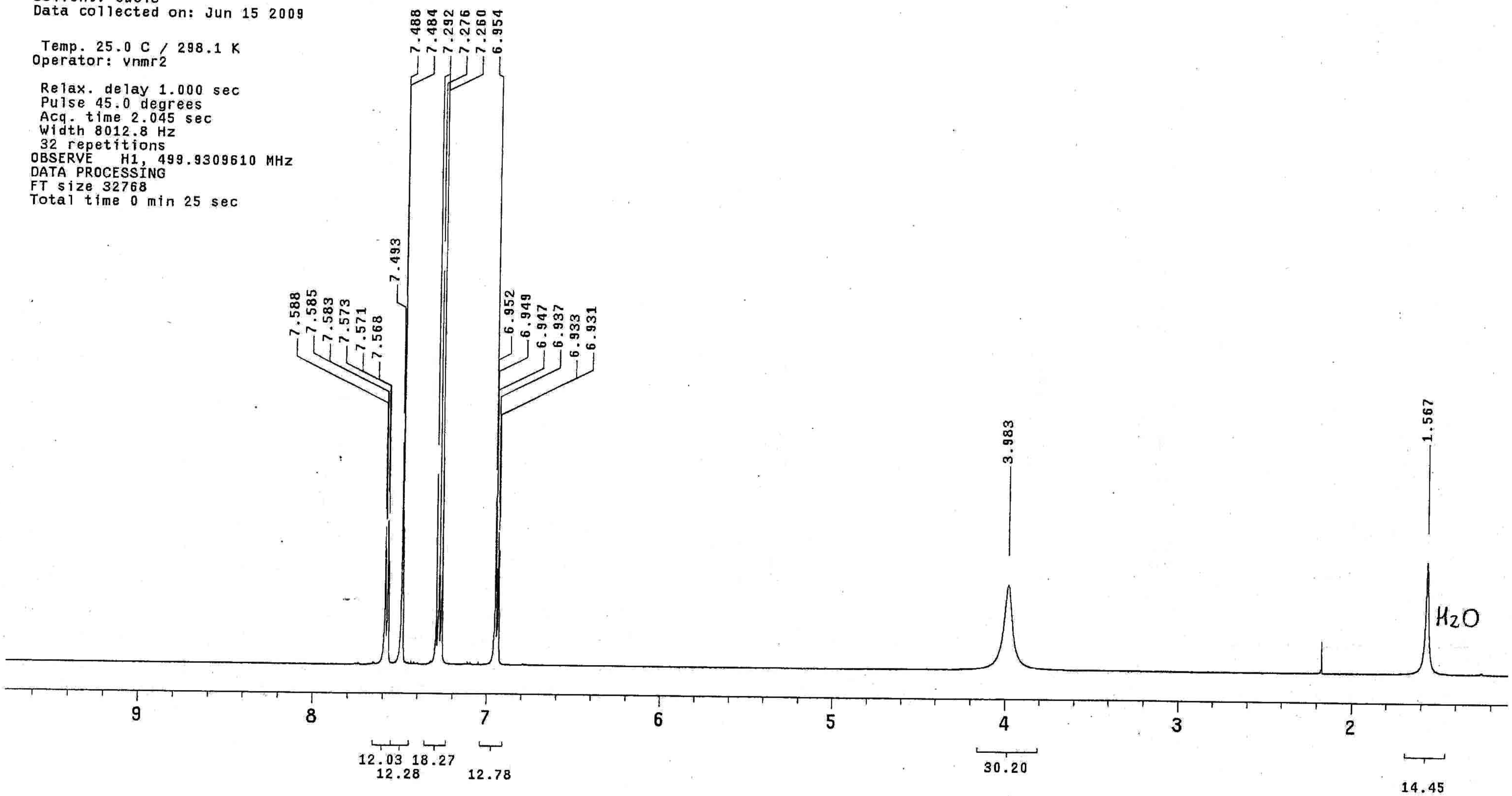
Sample directory:

FidFile: m-Nitroanilina

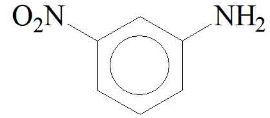
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 15 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

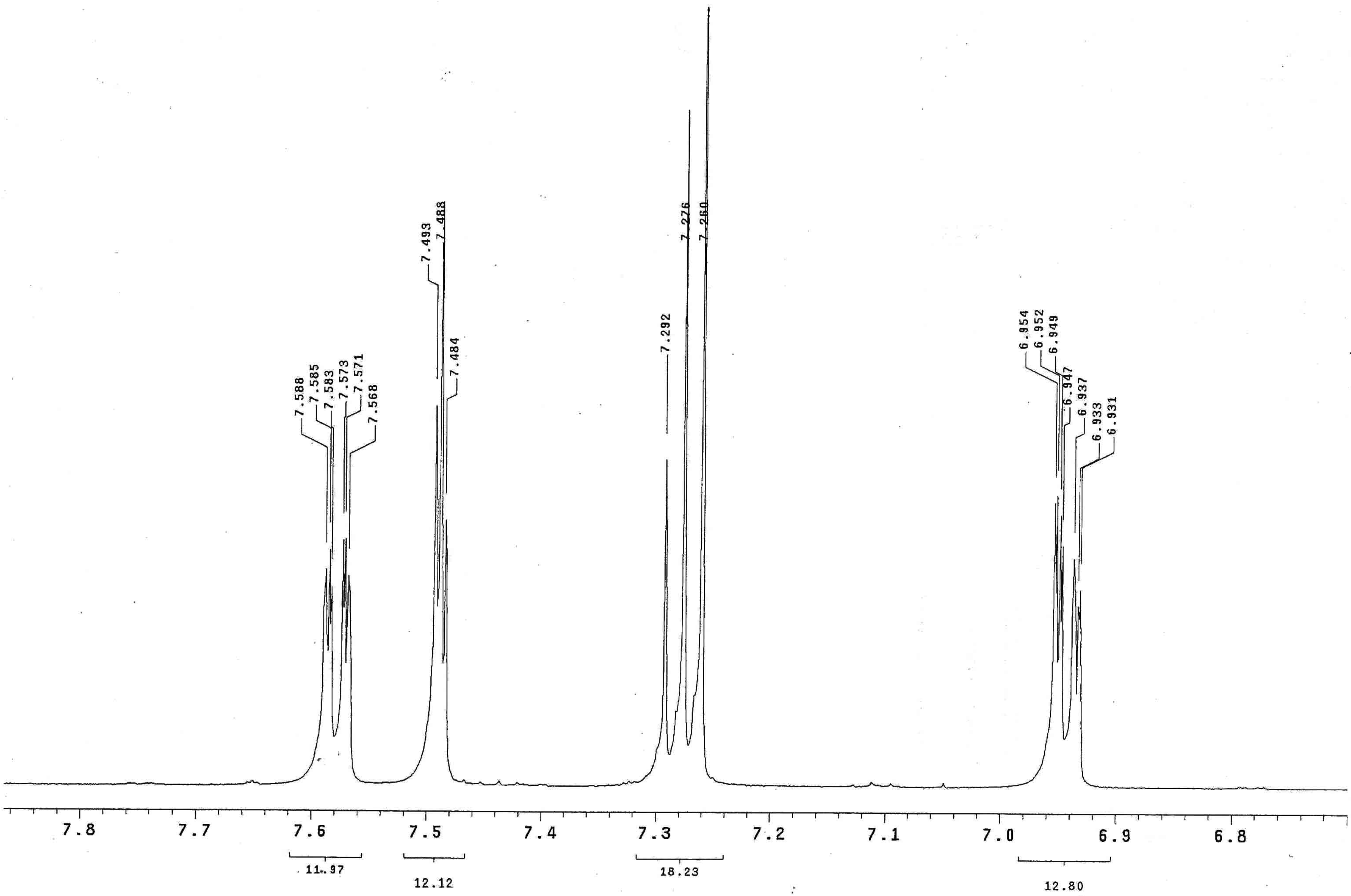
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309610 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



17



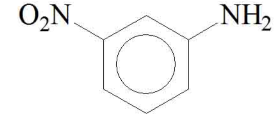
O_2N
NH_2



7.588
7.585
7.583
7.573
7.571
7.568
7.493
7.488
7.484
7.292
7.276
7.260
6.954
6.952
6.949
6.947
6.937
6.933
6.931
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
11.97
12.12
18.23
12.80

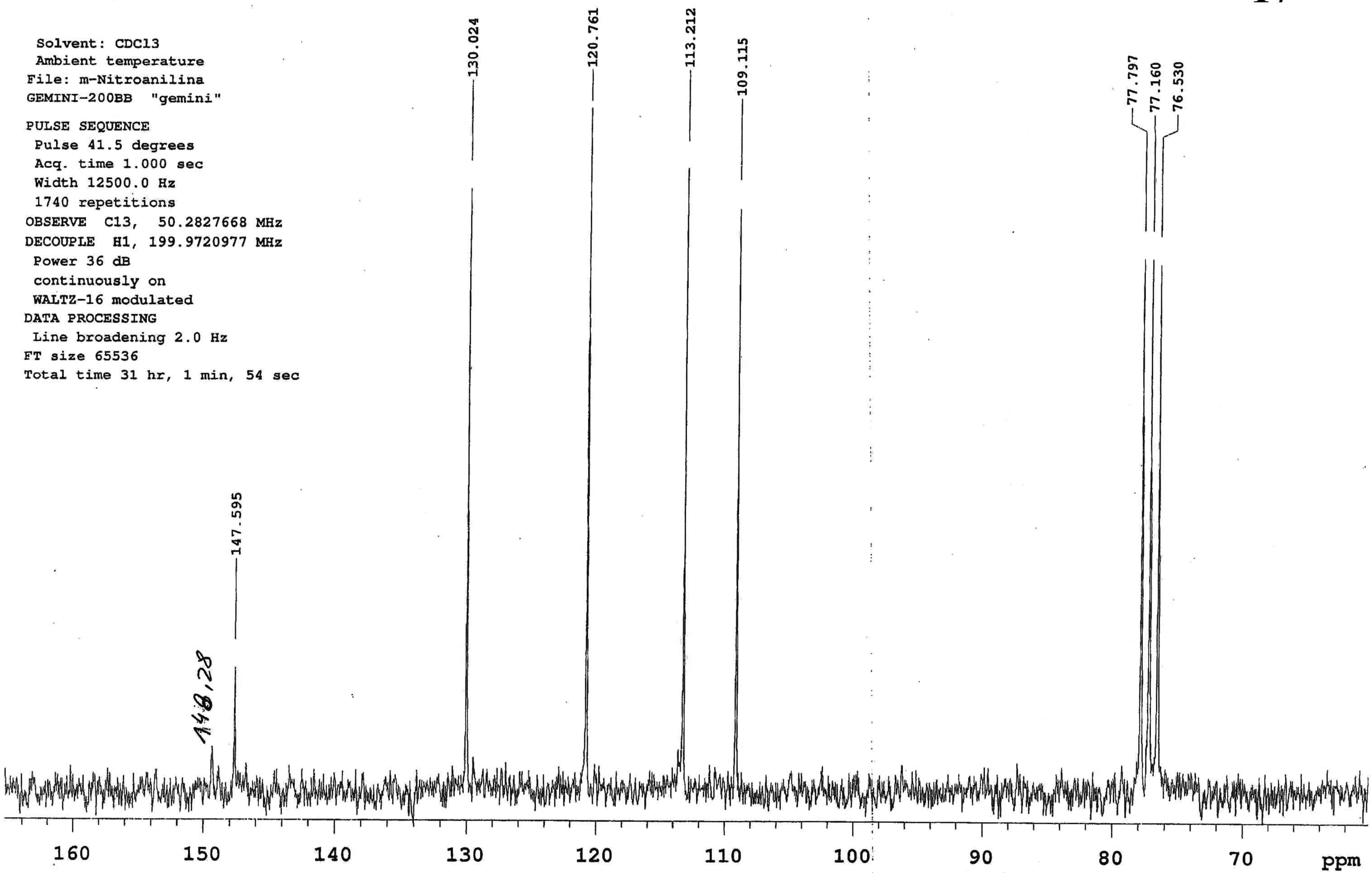
m-Nitroanilina

17

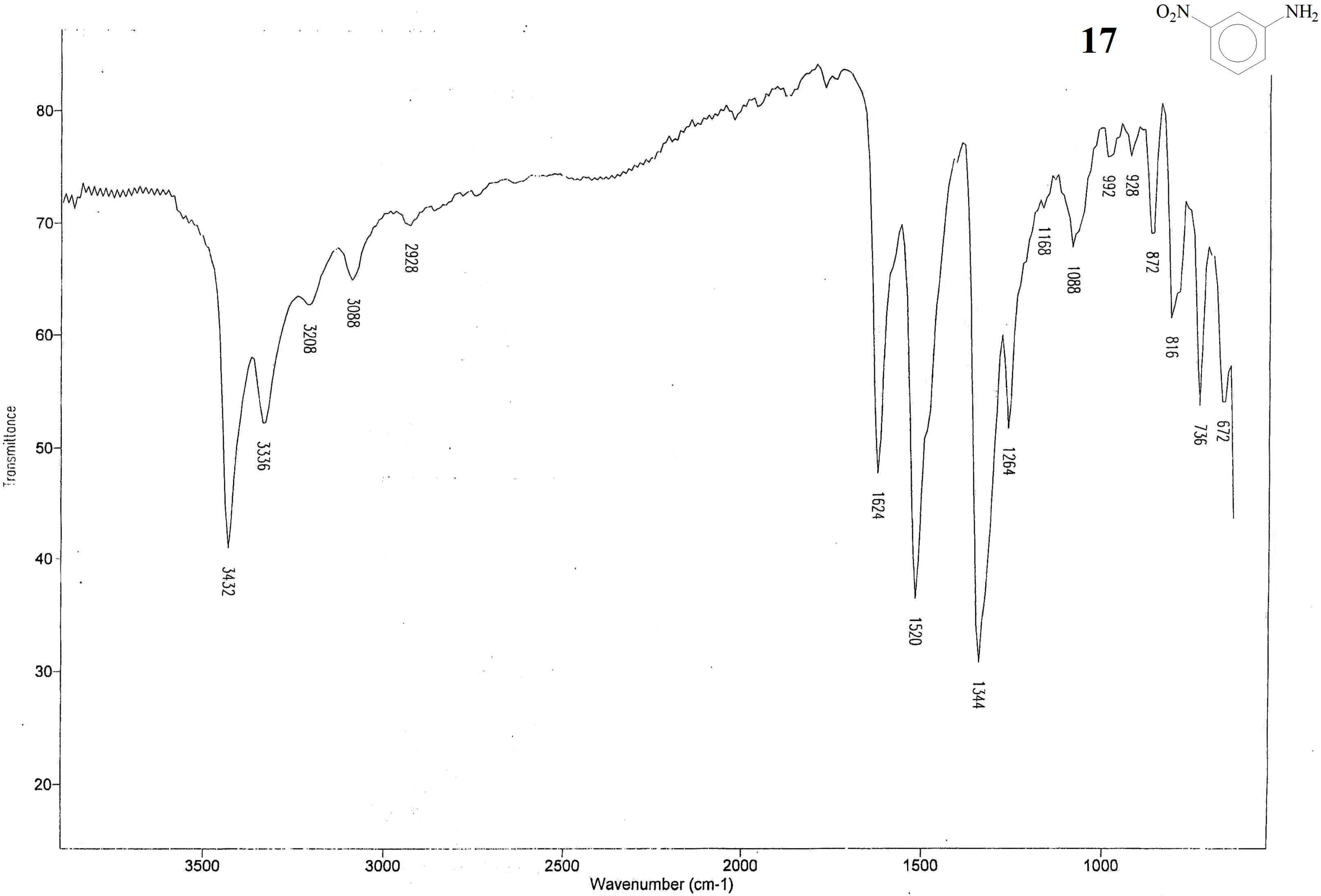


Solvent: CDCl3
Ambient temperature
File: m-Nitroanilina
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1740 repetitions
OBSERVE C13, 50.2827668 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

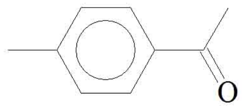


17



O_2N
NH_2
Transmittance
80
70
60
50
40
30
20
3432
3336
3208
3088
2928
1624
1520
1344
1264
1168
1088
992
928
872
816
736
672
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

18



p-Metyloacetofenon

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

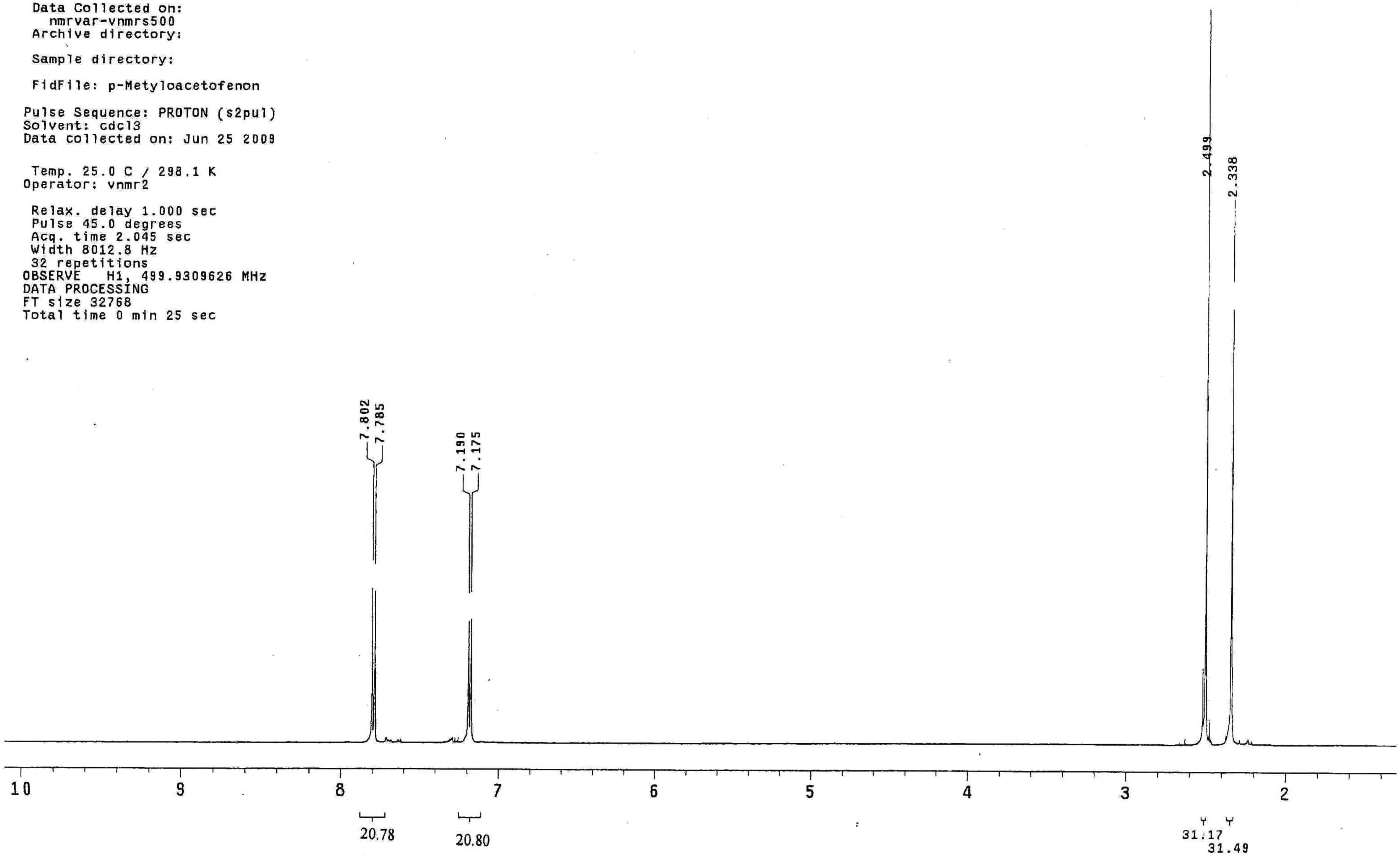
Sample directory:

FidFile: p-Metyloacetofenon

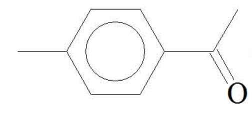
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 25 2009

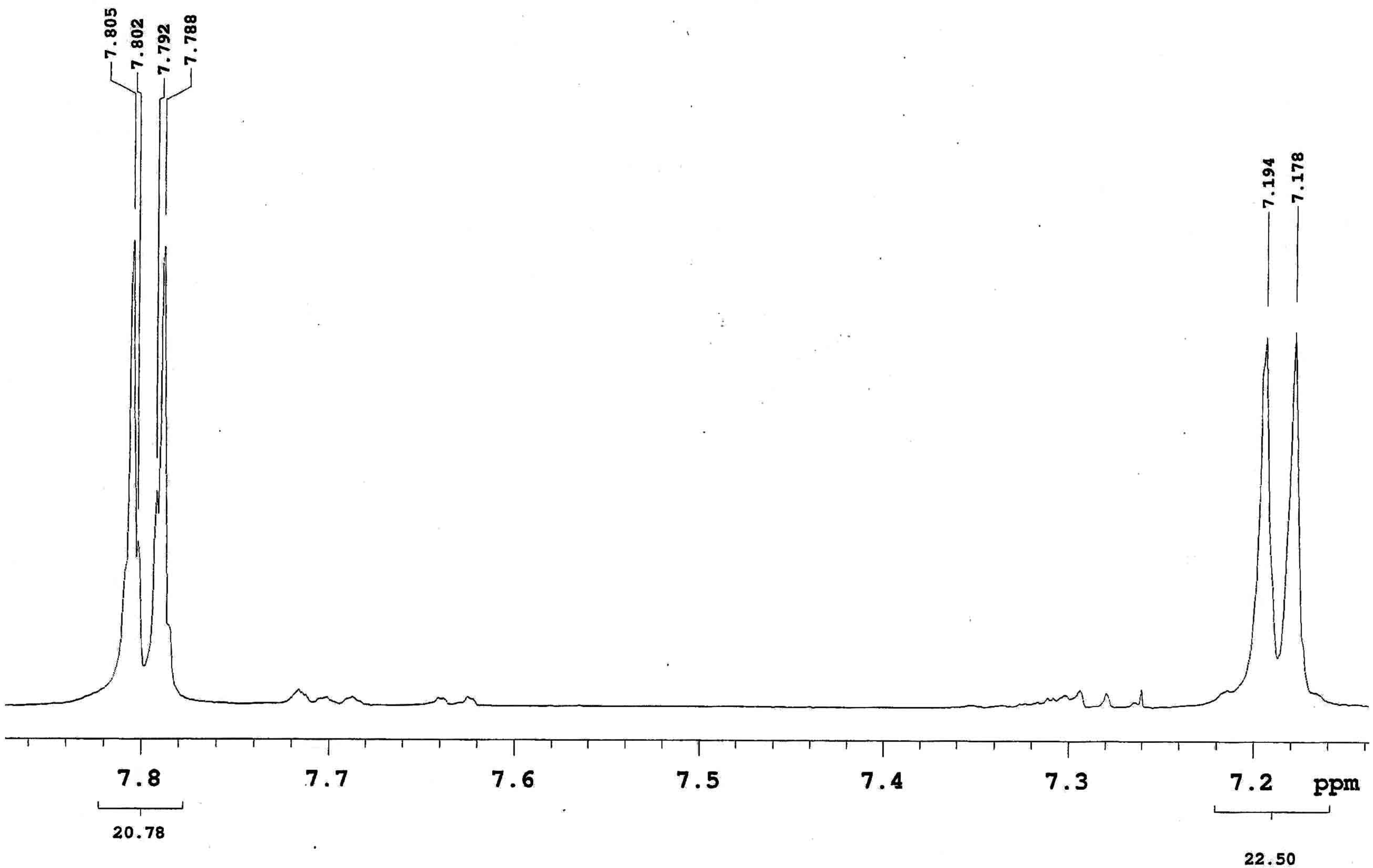
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309626 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



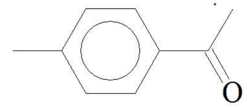
18


O


7.805
7.802
7.792
7.788
7.194
7.178
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
20.78
22.50

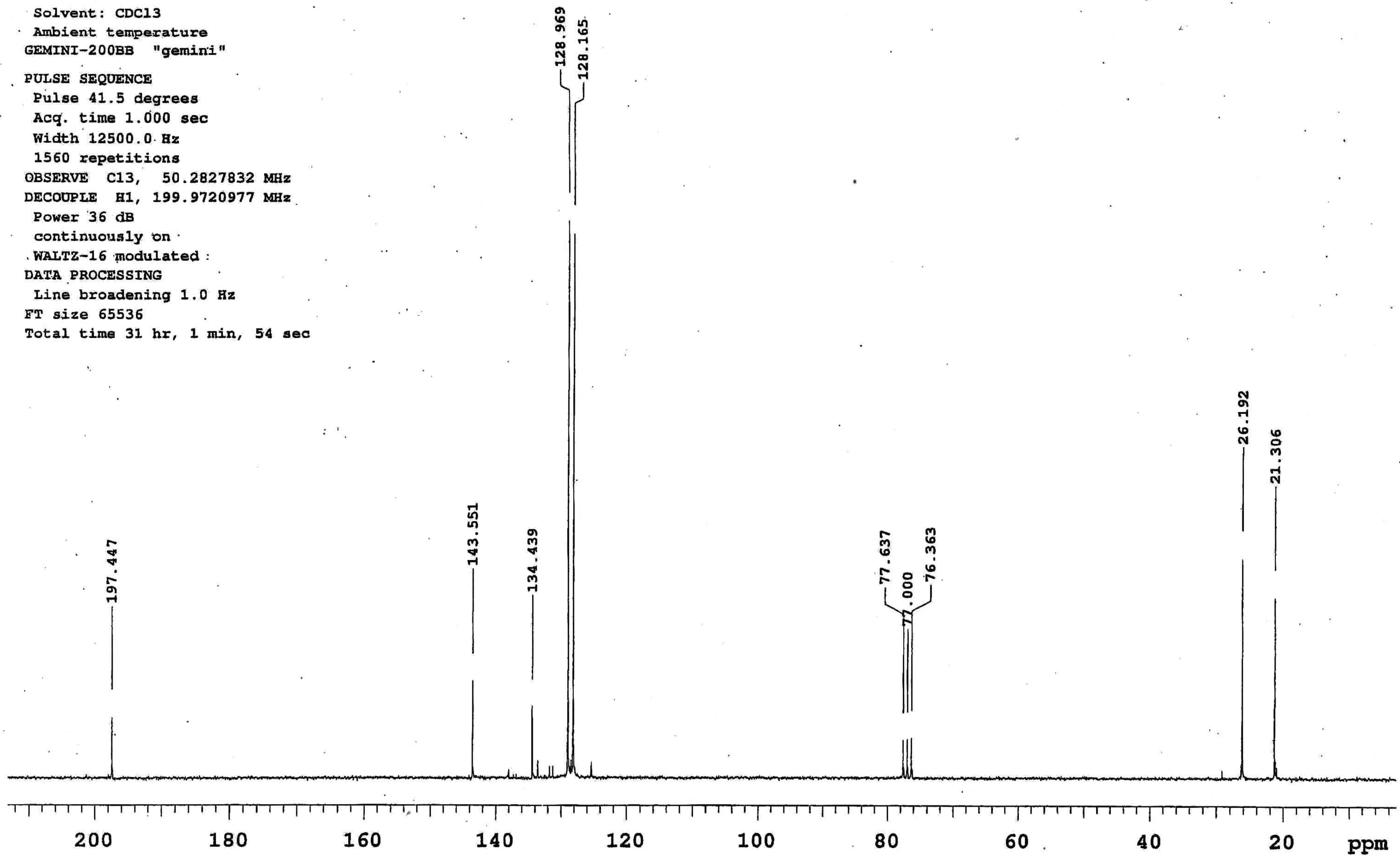
p-Metyloacetofenon

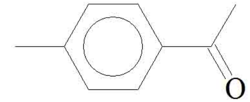
18

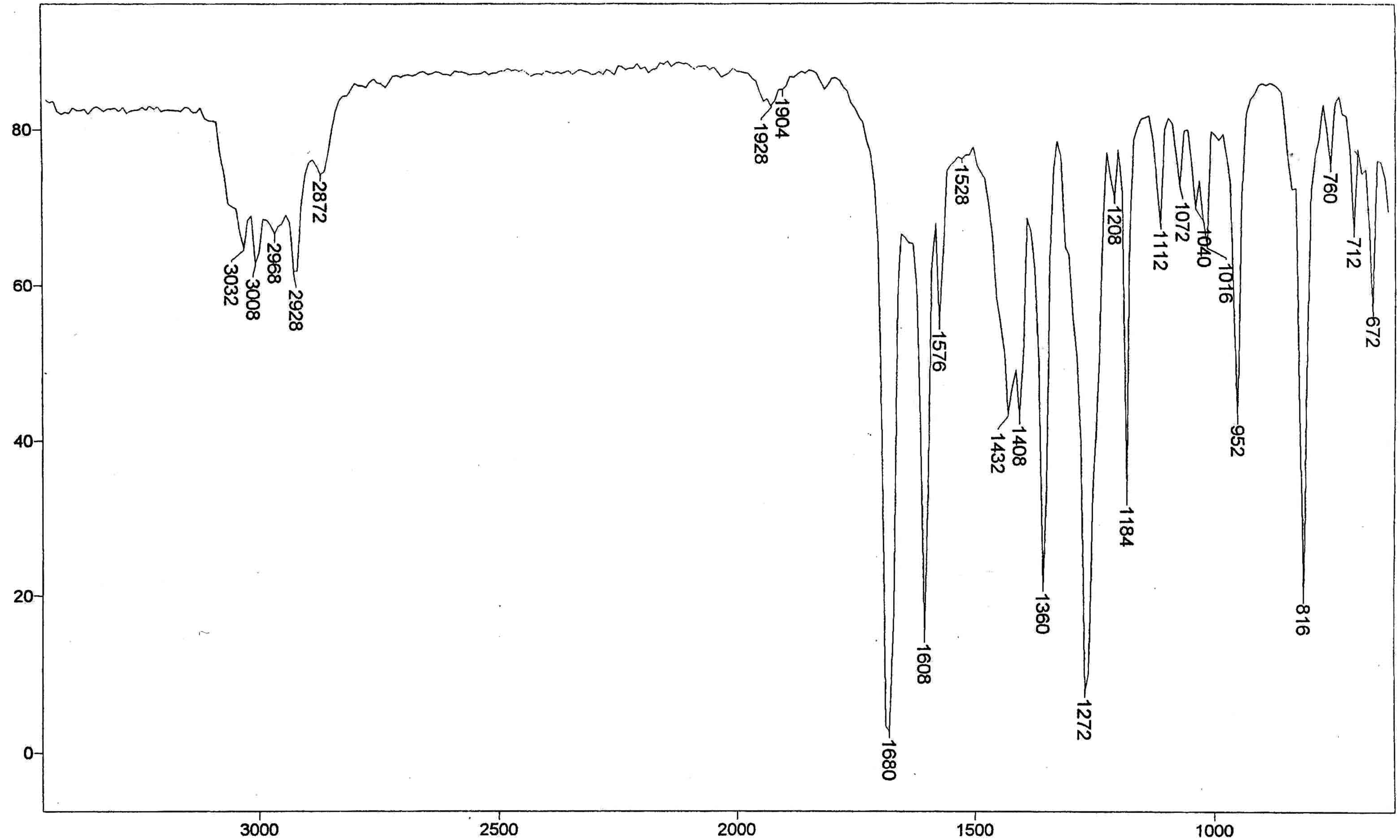


Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1560 repetitions
OBSERVE C13, 50.2827832 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec



18 

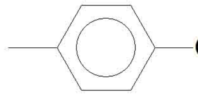


Transmittance / Wavenumber (cm-1)

File # 1 = [redacted]

Paged X-Zoom SCROLL

99-03-08 11:08 Res=4.000000

19 

Kwas_p-toluilowy

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

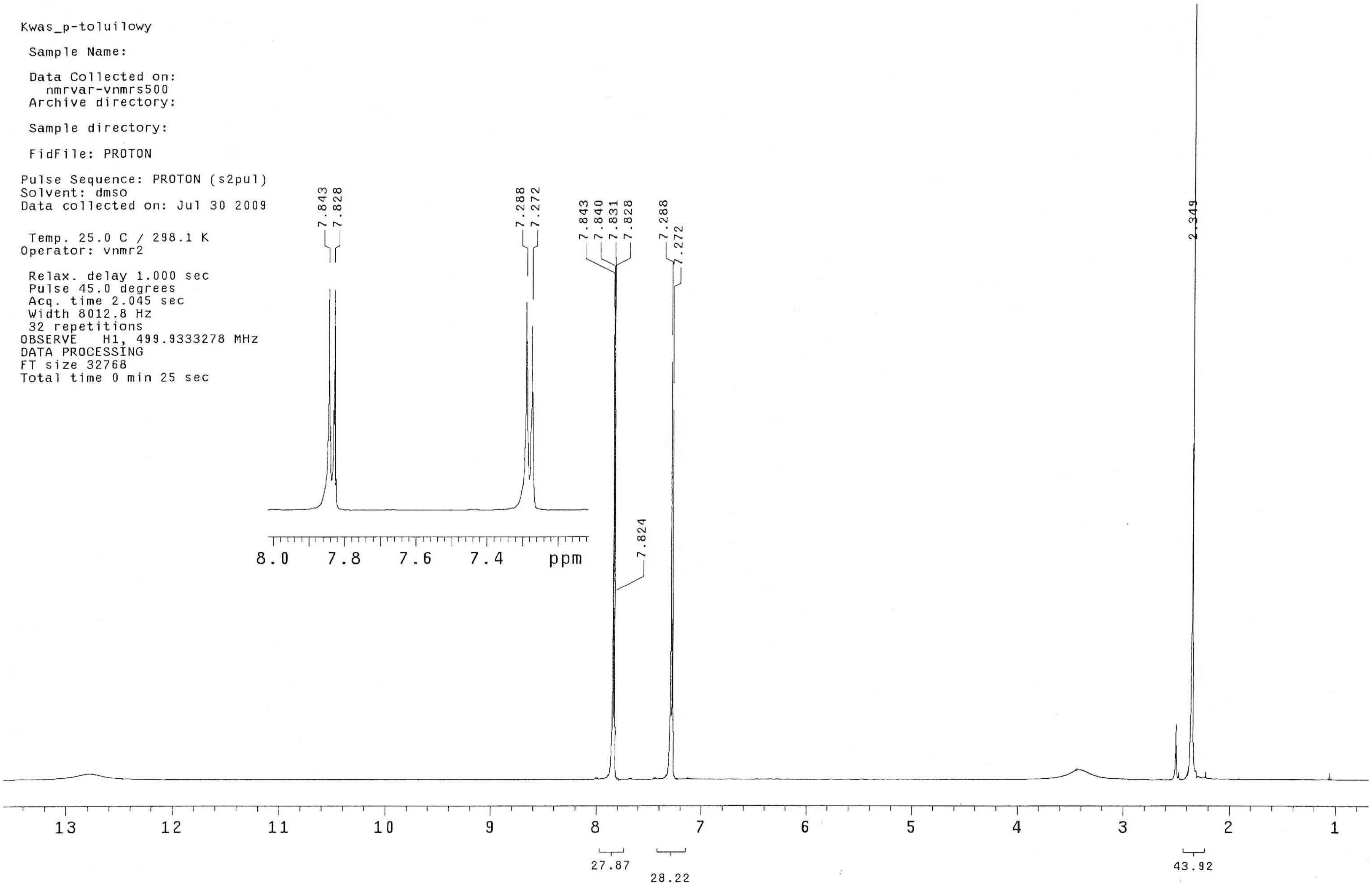
Sample directory:

FidFile: PROTON

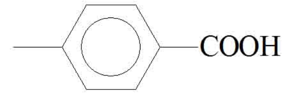
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jul 30 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9333278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

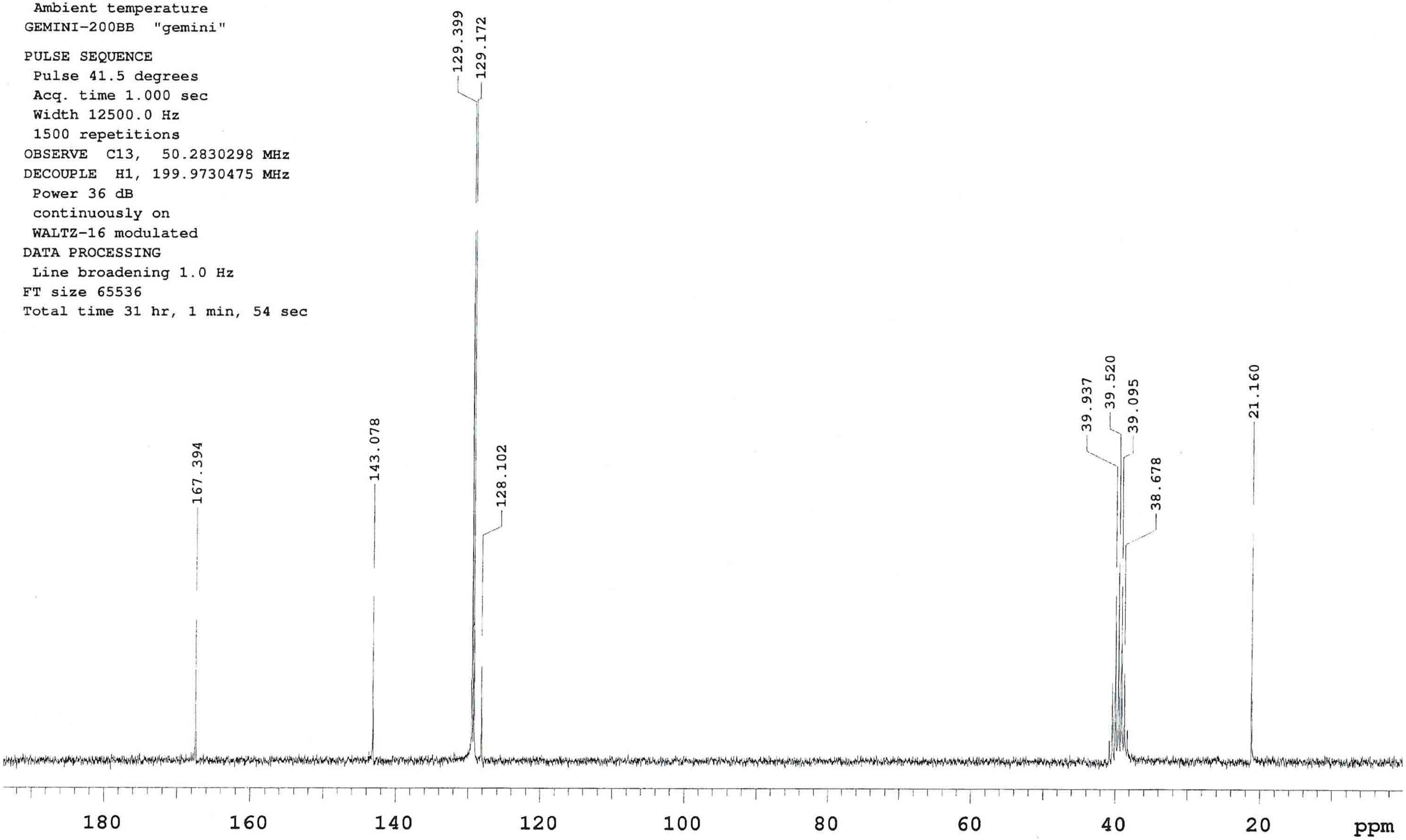


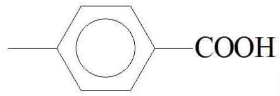
Kwas_p-toluilowy

19 

Solvent: DMSO
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2830298 MHz
DECOUPLE H1, 199.9730475 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

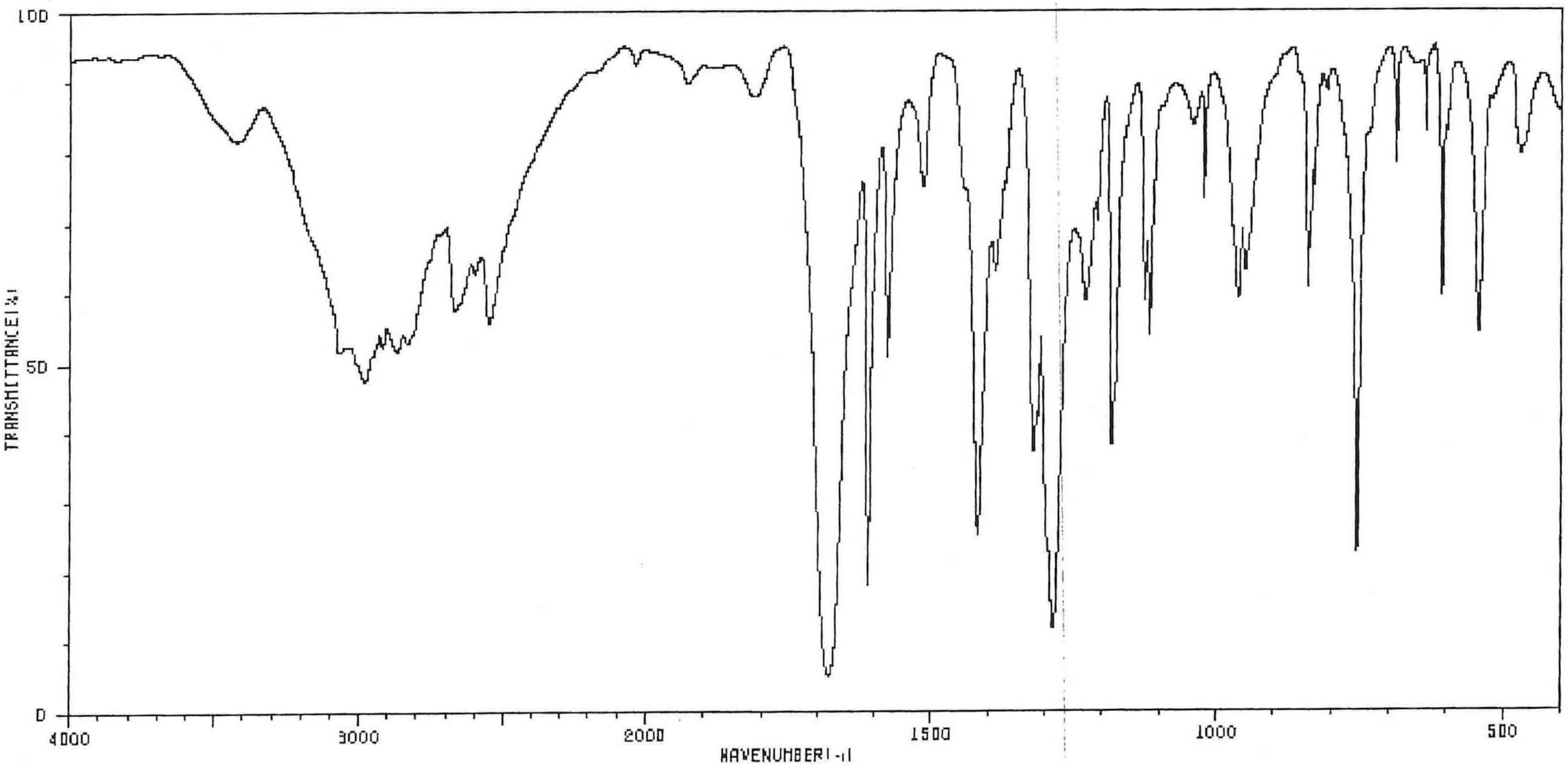


19 

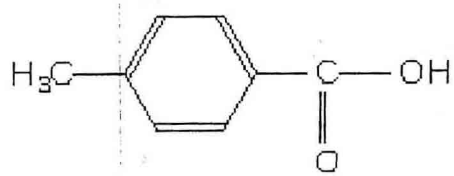
HIT-NO=1468	SCORE= ( )	SDBS-NO=1448	IR-NIDA-21206 : KBR DISC

P-TOLUIC ACID

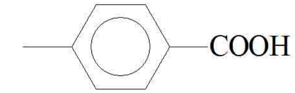
$C_8H_8O_2$



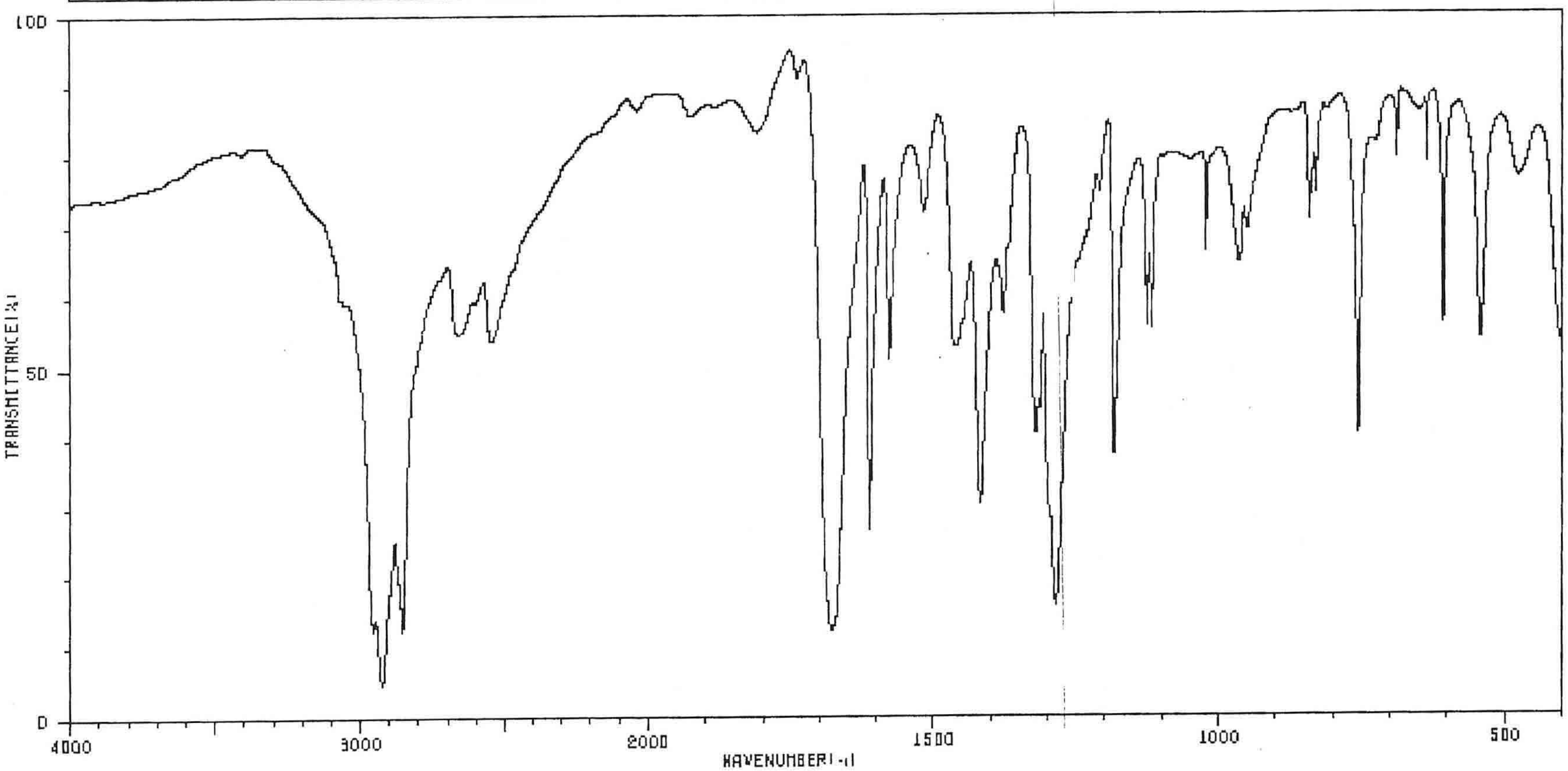
3420	79	2649	69	1322	36	1041	81	767	21
2978	46	1680	4	1287	11	1023	70	689	74
2919	50	1613	17	1231	57	962	57	636	79
2869	60	1577	49	1210	68	960	60	609	67
2833	50	1515	72	1185	36	841	58	601	79
2670	55	1420	24	1126	57	830	72	543	52
2698	60	1388	60	1118	62	808	84	472	77



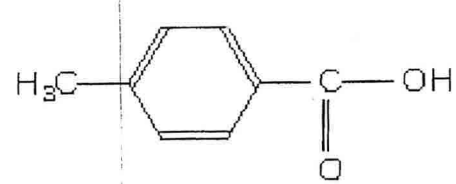
Źródło: ***https://sdbs.db.aist.go.jp***

19 

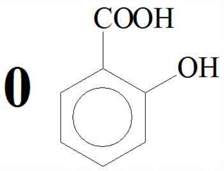
HIT-NO=836	SCORE= ( )	SDBS-NO=1448	IR-NIDA-63770 : NUJOL MULL
P-TOLUIC ACID			
$C_8H_8O_2$			



2964	12	1928	81	1461	62	1186	36	830	72
2925	4	1921	81	1419	29	1126	53	757	39
2854	12	1809	81	1378	55	1118	59	689	77
2669	63	1678	12	1322	39	1023	64	636	77
2659	53	1612	26	1314	43	963	62	608	55
2543	52	1577	49	1267	15	950	68	543	52
2038	84	1617	70	1210	72	841	68	476	74



Źródło: ***https://sdbs.db.aist.go.jp***

20 

STANDARD PROTON PARAMETERS

Sample Name: KWas salicylony

Data Collected on:
nmrvar-vnmrs500
Archive directory:

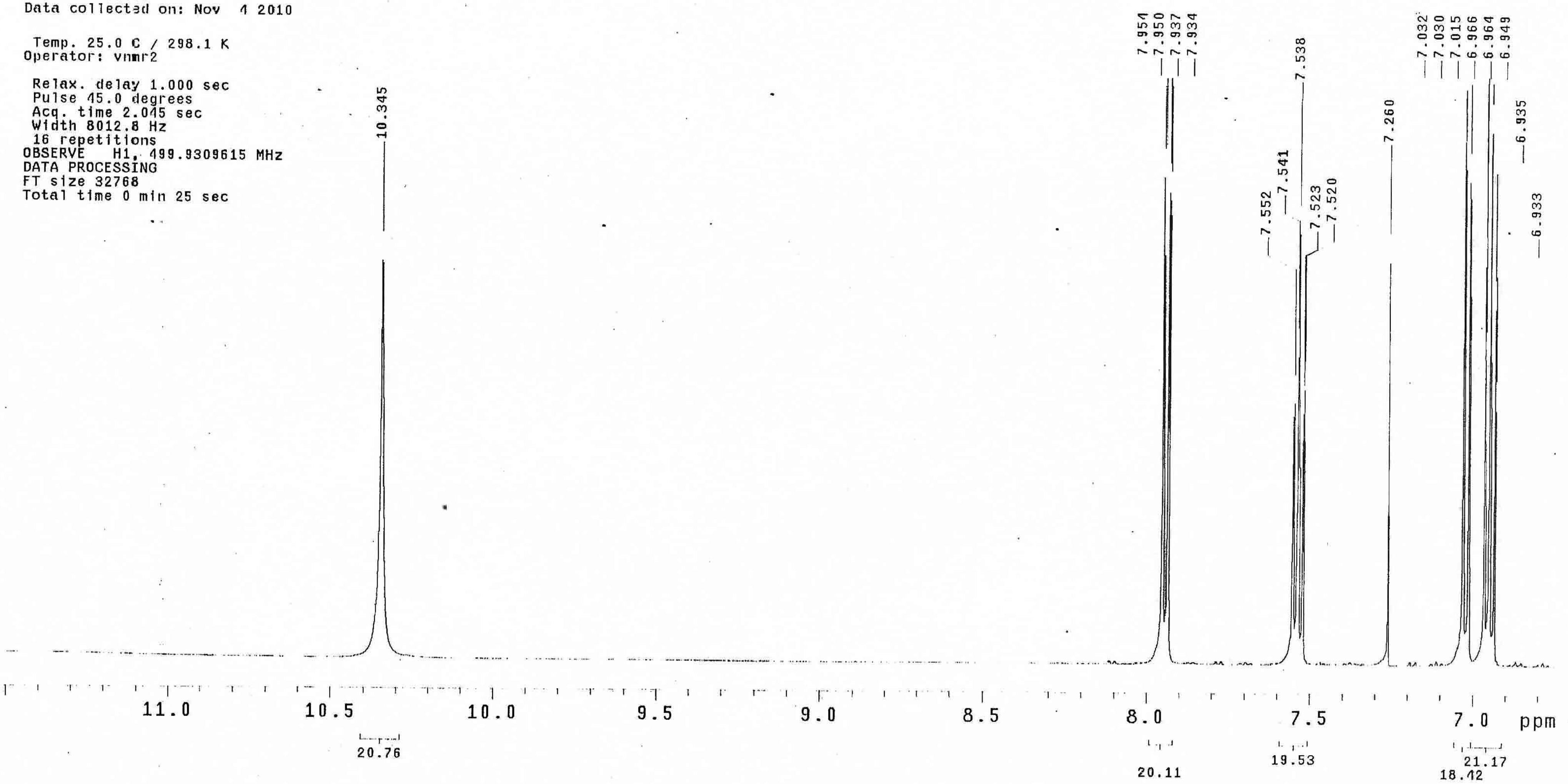
Sample directory:

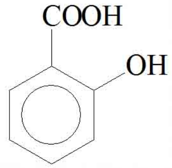
FidFile: PROTON

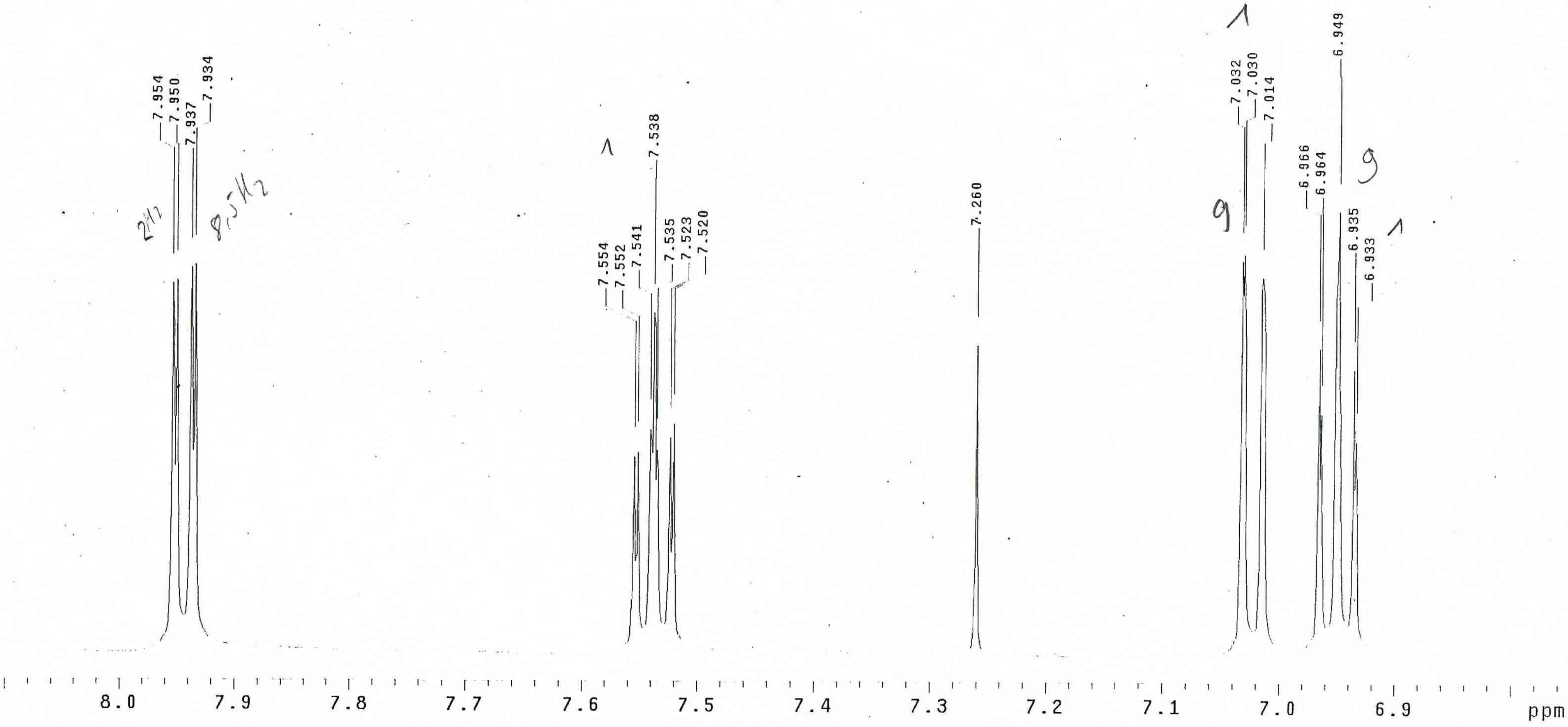
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 4 2010

Temp. 25.0 C / 298.1 K
Operator: vnmr2

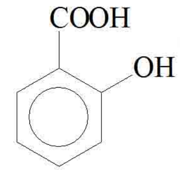
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



20 
COOH
OH


7.954
7.950
7.937
7.934
2Hz
8.5Hz
1
7.554
7.552
7.541
7.538
7.535
7.523
7.520
7.260
1
7.032
7.030
7.014
9
6.966
6.964
6.949
9
6.935
6.933
1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm

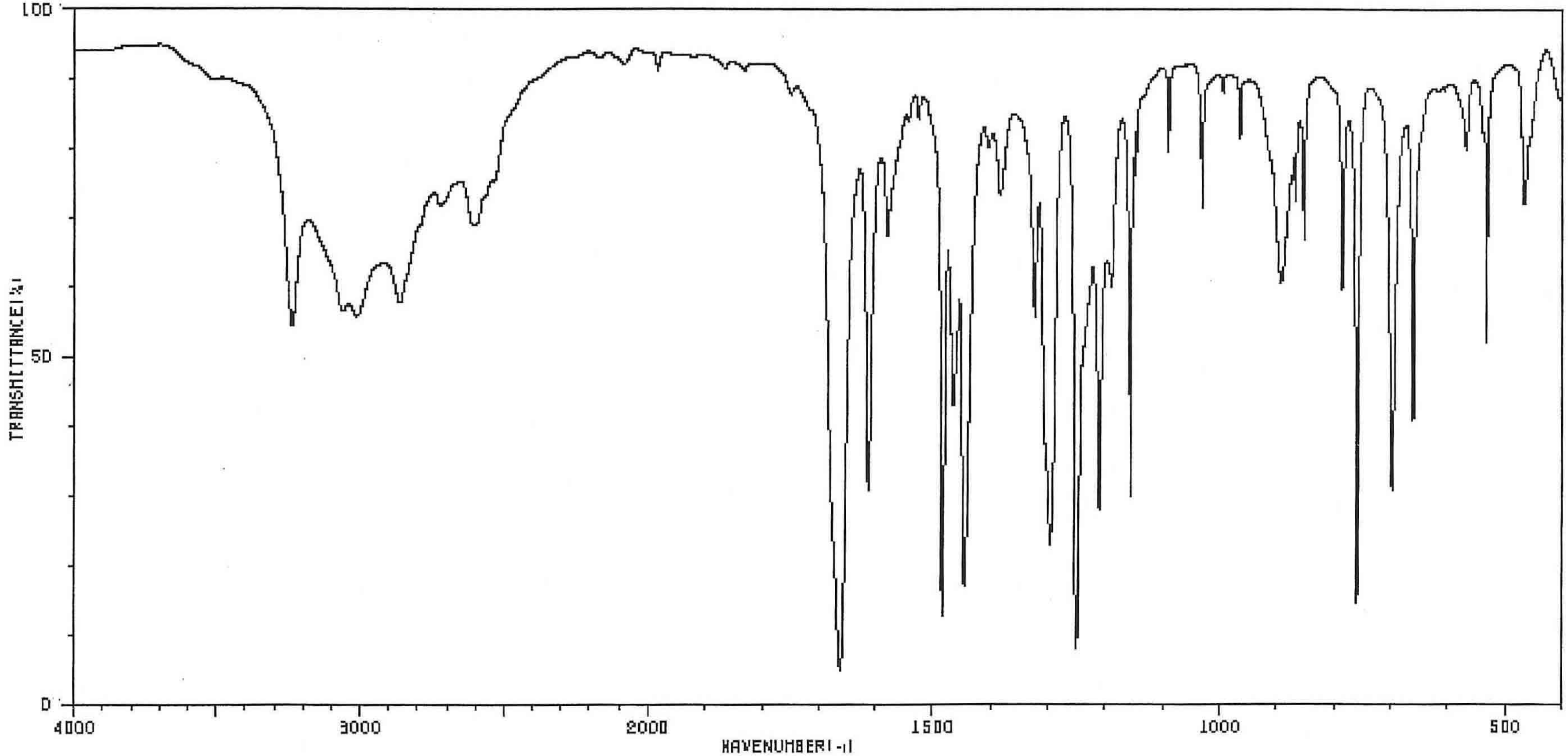
20



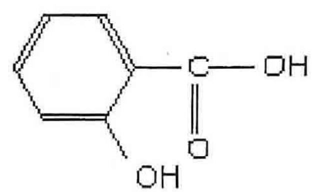
HIT-NO=1330	SCORE= ( )	SDBS-NO=1149	IR-NIDA-08453 : KBR DISC

SALICYLIC ACID

$C_7H_6O_3$

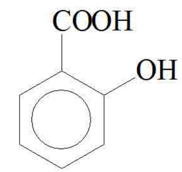


3240	62	1680	64	1326	63	1161	72	786	67
3013	53	1527	81	1297	21	1091	77	760	13
2864	55	1484	12	1251	7	1032	68	699	29
2724	70	1467	41	1239	49	966	79	661	38
2605	66	1447	16	1212	26	893	58	569	77
1862	4	1405	77	1190	58	868	70	533	50
1613	29	1386	70	1157	28	863	64	467	70

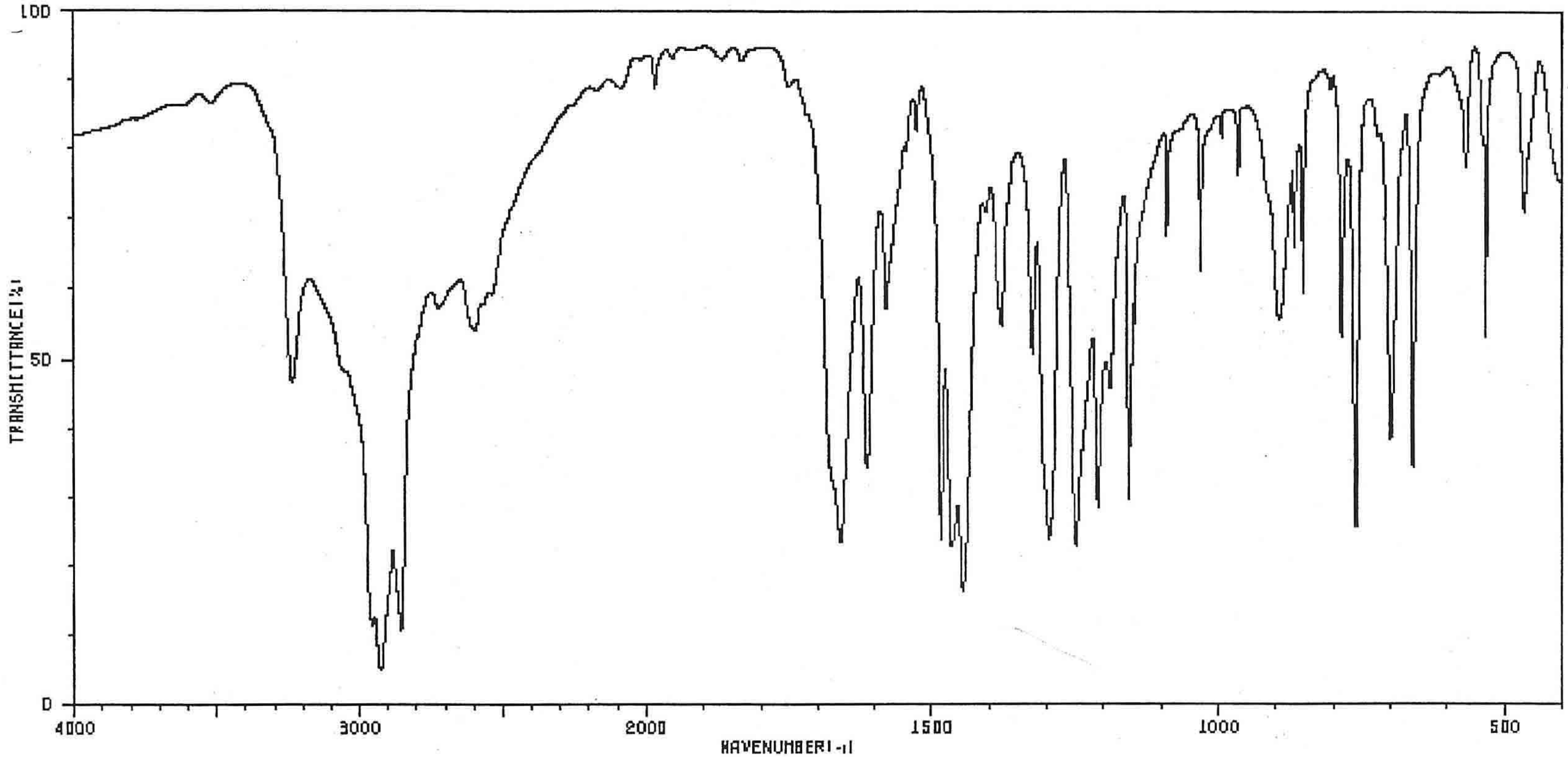


Źródło: ***https://sdbs.db.aist.go.jp***

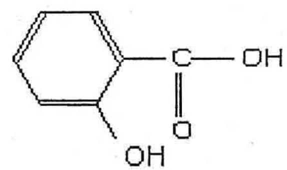
20



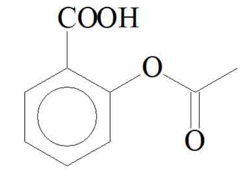
HIT-NO=704	SCORE= ( )	SDBS-NO=1149	IR-NIDA-63703 : NUJOL MULL
SALICYLIC ACID			
$C_7H_6O_3$			

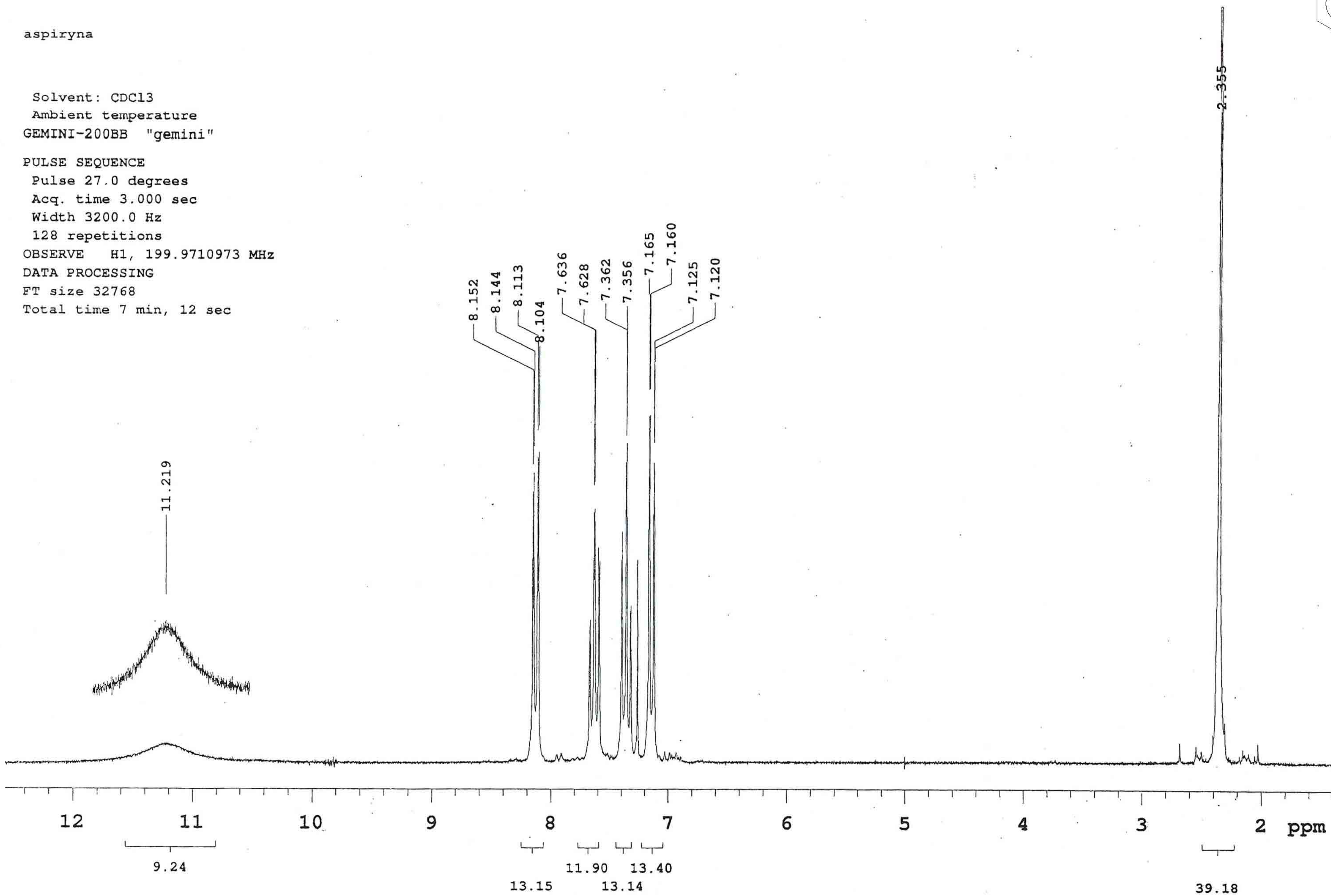


3236	44	1613	39	1326	49	1090	64	776	77
2953	10	1580	55	1297	22	1032	60	760	24
2925	4	1484	22	1249	21	965	74	699	37
2864	10	1466	21	1211	26	894	59	661	33
2721	55	1445	15	1189	43	868	64	568	74
2594	52	1405	68	1157	28	853	57	533	50
1660	22	1379	59	1146	63	786	50	467	68



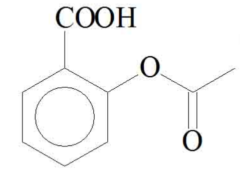
Źródło: ***https://sdbs.db.aist.go.jp***

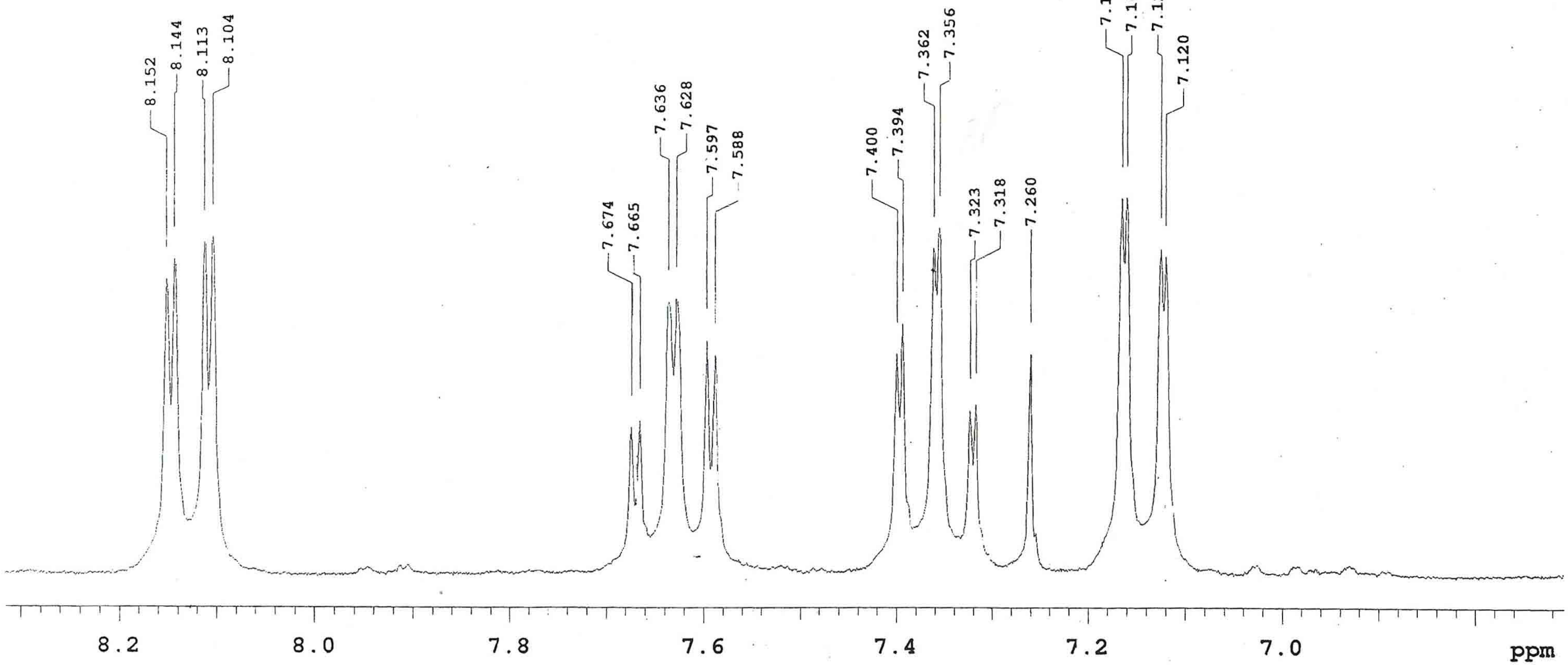
21 

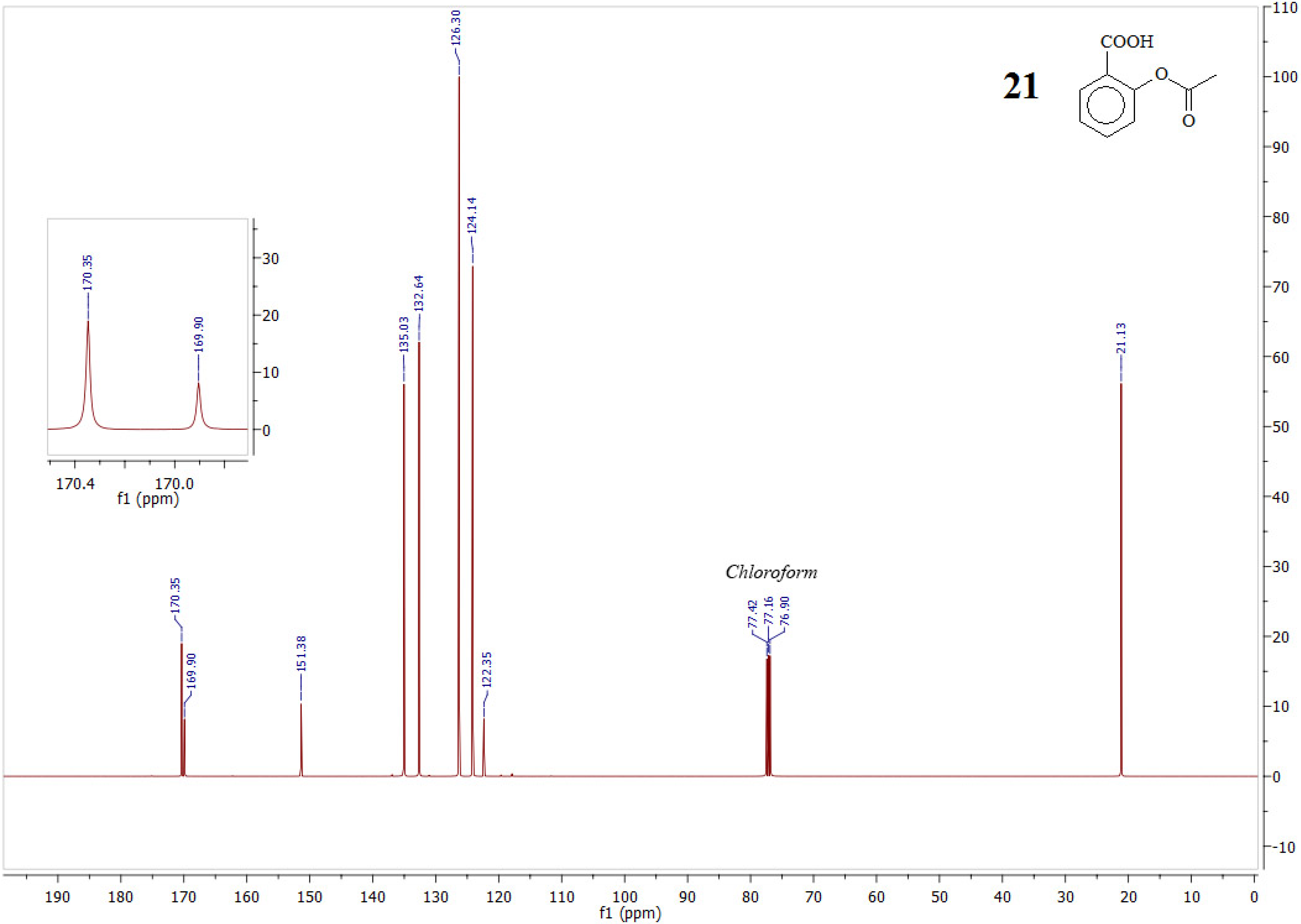


aspiryna
Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"
PULSE SEQUENCE
Pulse 27.0 degrees
Acq. time 3.000 sec
Width 3200.0 Hz
128 repetitions
OBSERVE H1, 199.9710973 MHz
DATA PROCESSING
FT size 32768
Total time 7 min, 12 sec
11.219
8.152
8.144
8.113
8.104
7.636
7.628
7.362
7.356
7.165
7.160
7.125
7.120
2.355
12
11
10
9
8
7
6
5
4
3
2 ppm
9.24
13.15
11.90
13.14
13.40
39.18

21

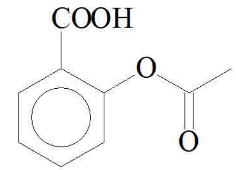

COOH
O
O


8.152
8.144
8.113
8.104
7.674
7.665
7.636
7.628
7.597
7.588
7.400
7.394
7.362
7.356
7.323
7.318
7.260
7.165
7.160
7.125
7.120
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm



21
COOH
O
O
170.35
169.90
170.4
170.0
f1 (ppm)
151.38
135.03
132.64
126.30
124.14
122.35
Chloroform
77.42
77.16
76.90
21.13
f1 (ppm)

21

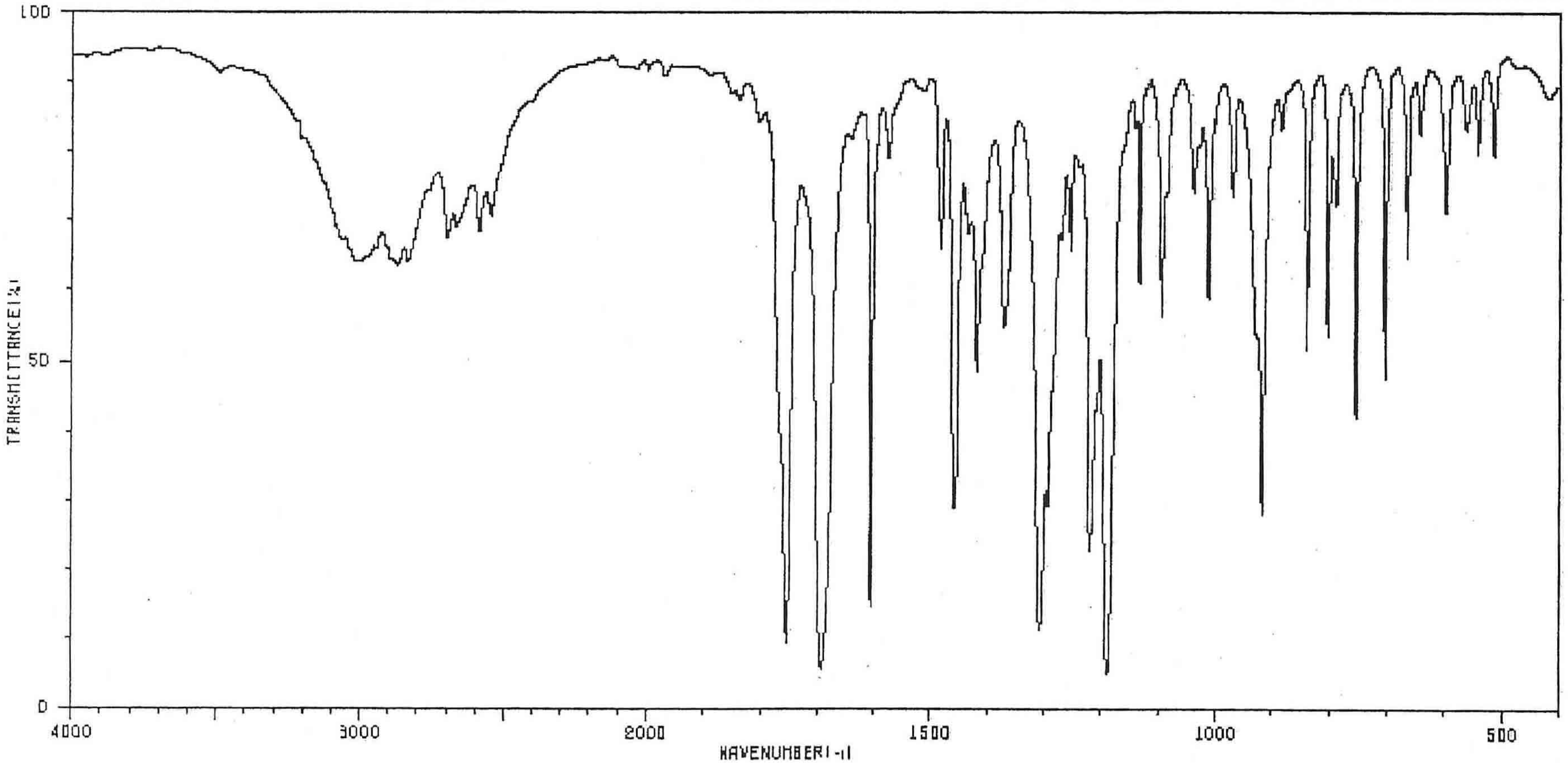


HIT-NO=1022	SCORE= ( )	SDBS-NO=532	IR-NIDA-63853 : KBR DISC

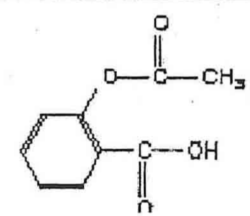
O-ACETOXYBENZOIC ACID

aspiryna

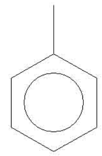
$C_9H_8O_4$



3006	62	2689	66	1436	66	1222	21	918	26
2983	62	2548	68	1420	47	1190	4	841	50
2891	62	1754	9	1372	53	1136	58	805	52
2872	62	1693	5	1308	10	1096	66	756	41
2834	62	1606	14	1295	28	1014	57	706	46
2701	66	1483	64	1272	64	971	70	667	62
2670	66	1469	27	1257	64	928	52	600	68



Źródło: ***https://sdbs.db.aist.go.jp***

22 

Toluen

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

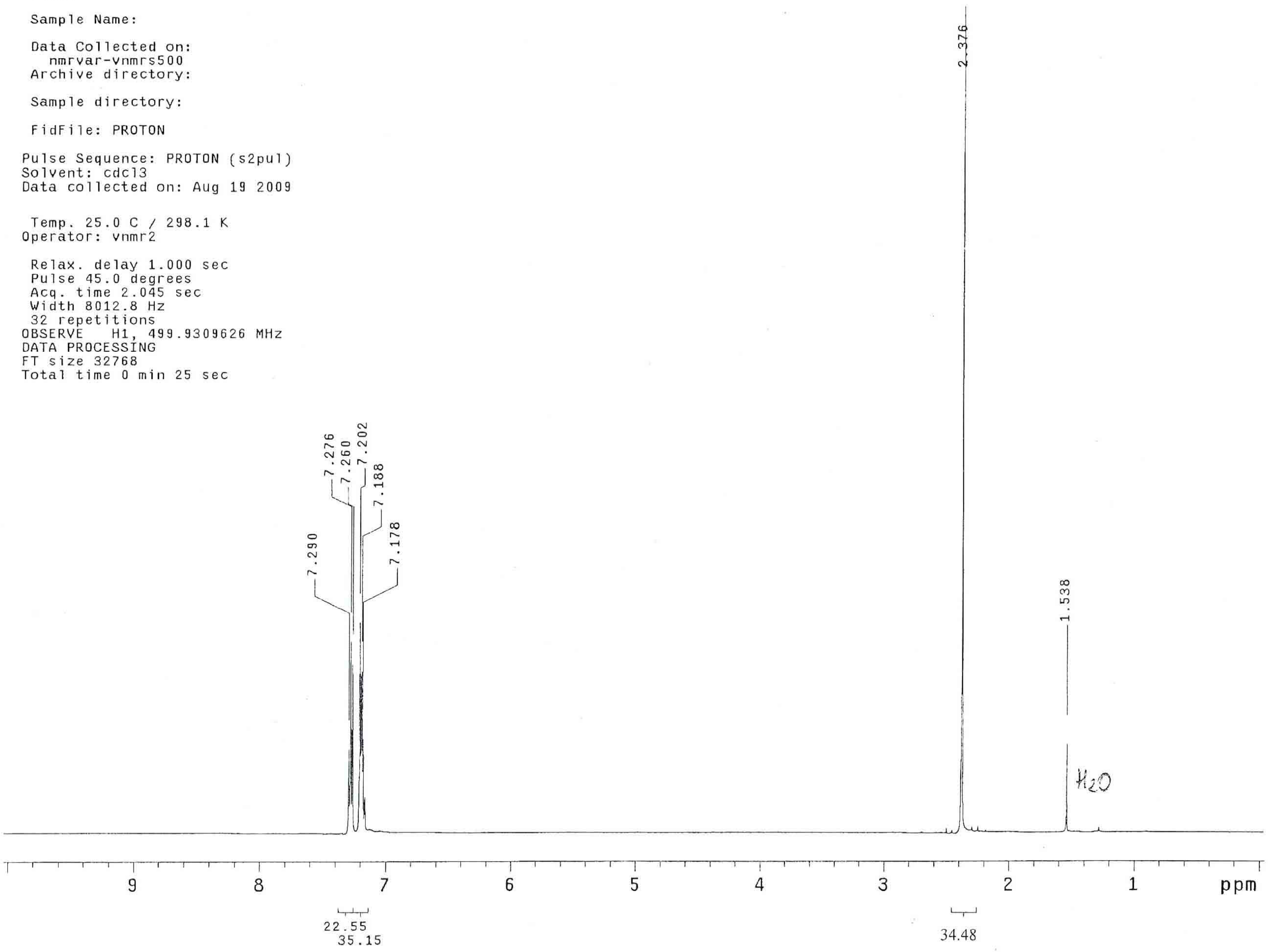
Sample directory:

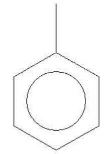
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 19 2009

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9309626 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

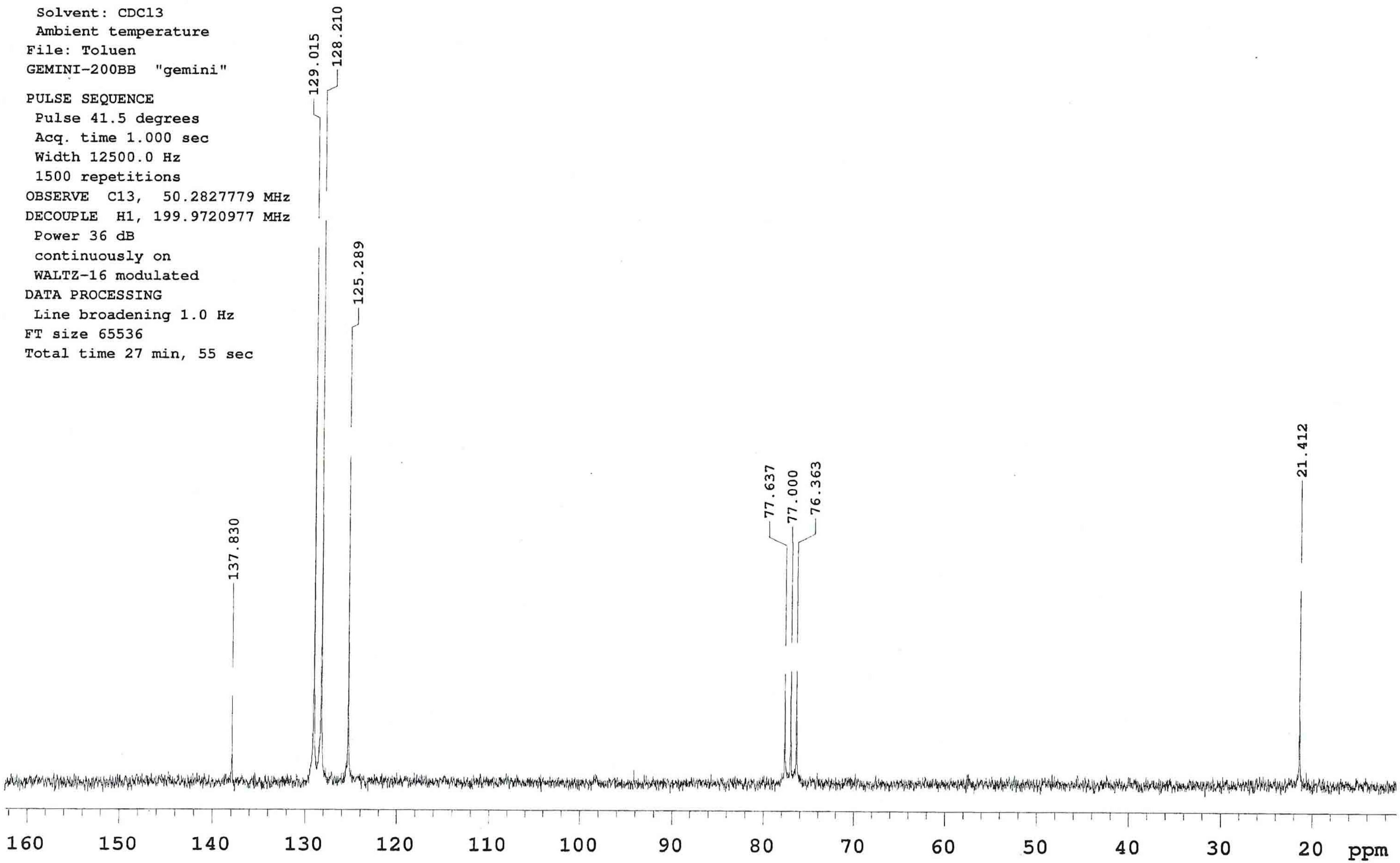


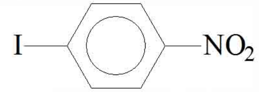
22 

Toluen

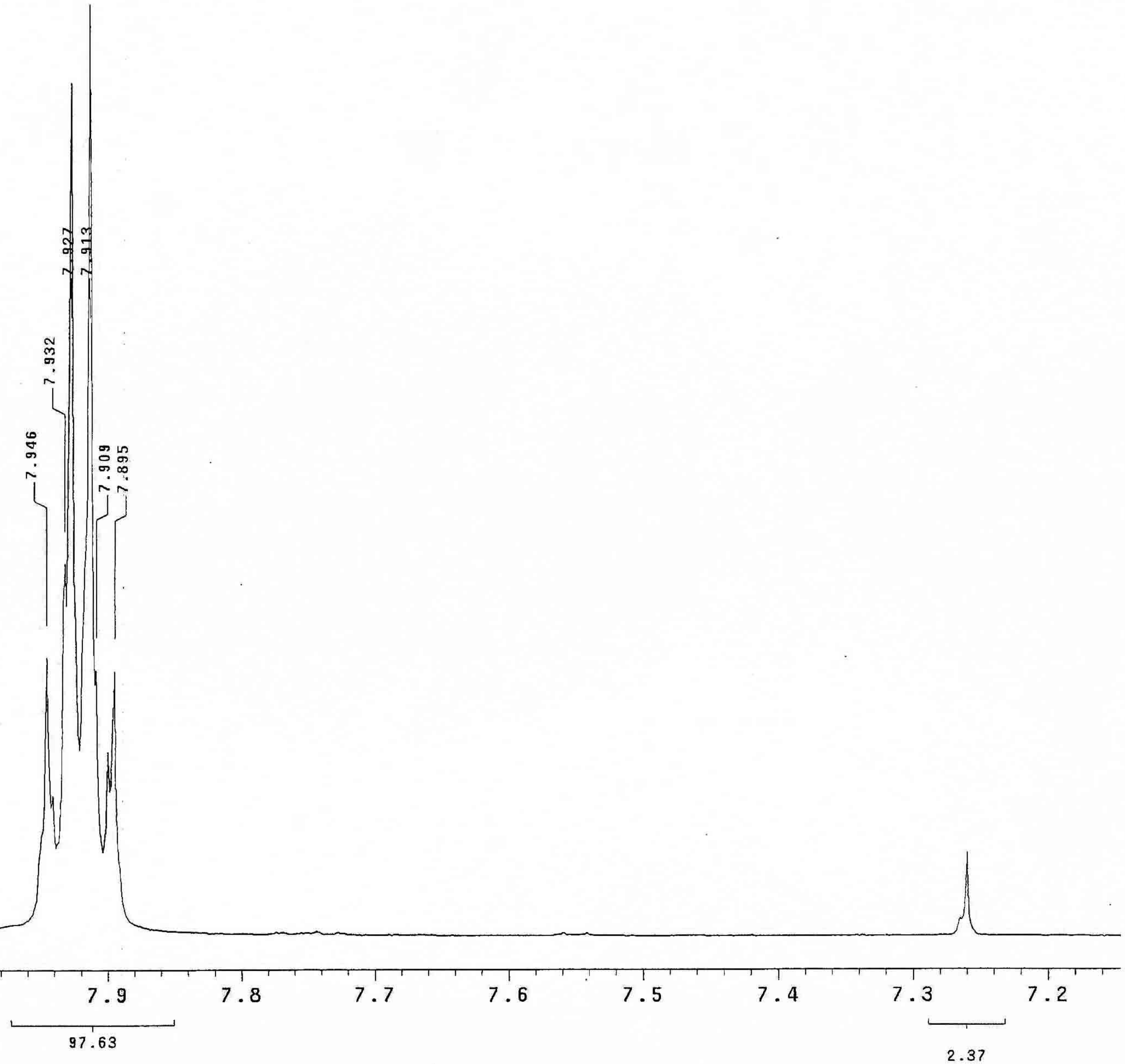
Solvent: CDCl3
Ambient temperature
File: Toluen
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1500 repetitions
OBSERVE C13, 50.2827779 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 27 min, 55 sec



23 


```
p-Jodonitrobenzen

 Sample Name:

 Data Collected on:
   nmrvar-vnmrs500
 Archive directory:

 Sample directory:

 FidFile: p-Jodonitrobenzen

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2009

 Temp. 25.0 C / 298.1 K
Operator: vnmr2

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.045 sec
 Width 8012.8 Hz
 32 repetitions
OBSERVE   H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
```

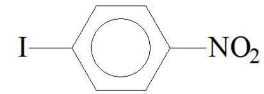


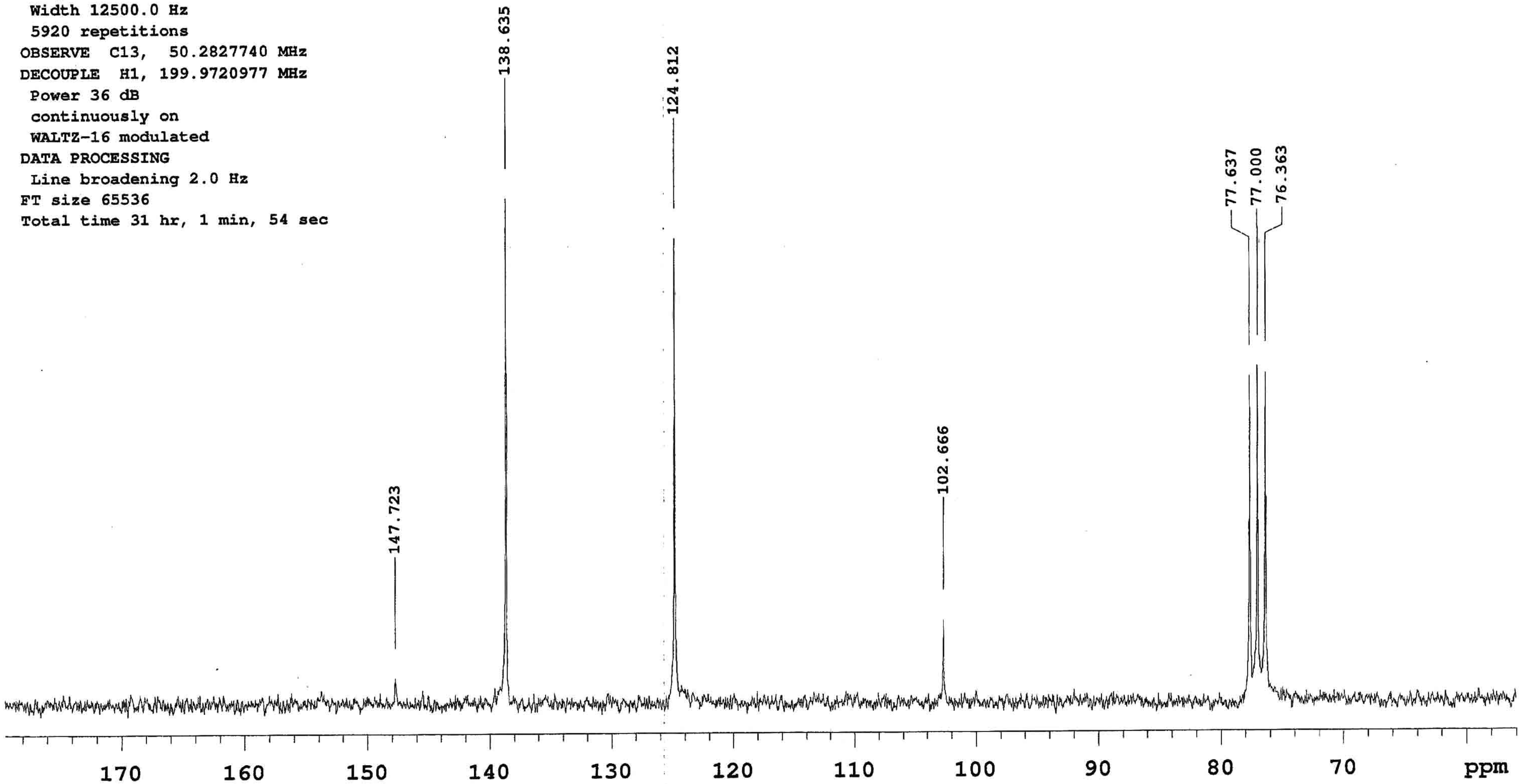
p-Jodonitrobenzen

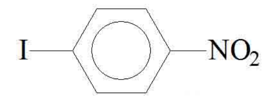
Solvent: CDCl3
Ambient temperature
GEMINI-200BB "gemini"

PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
5920 repetitions
OBSERVE C13, 50.2827740 MHz
DECOUPLE H1, 199.9720977 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

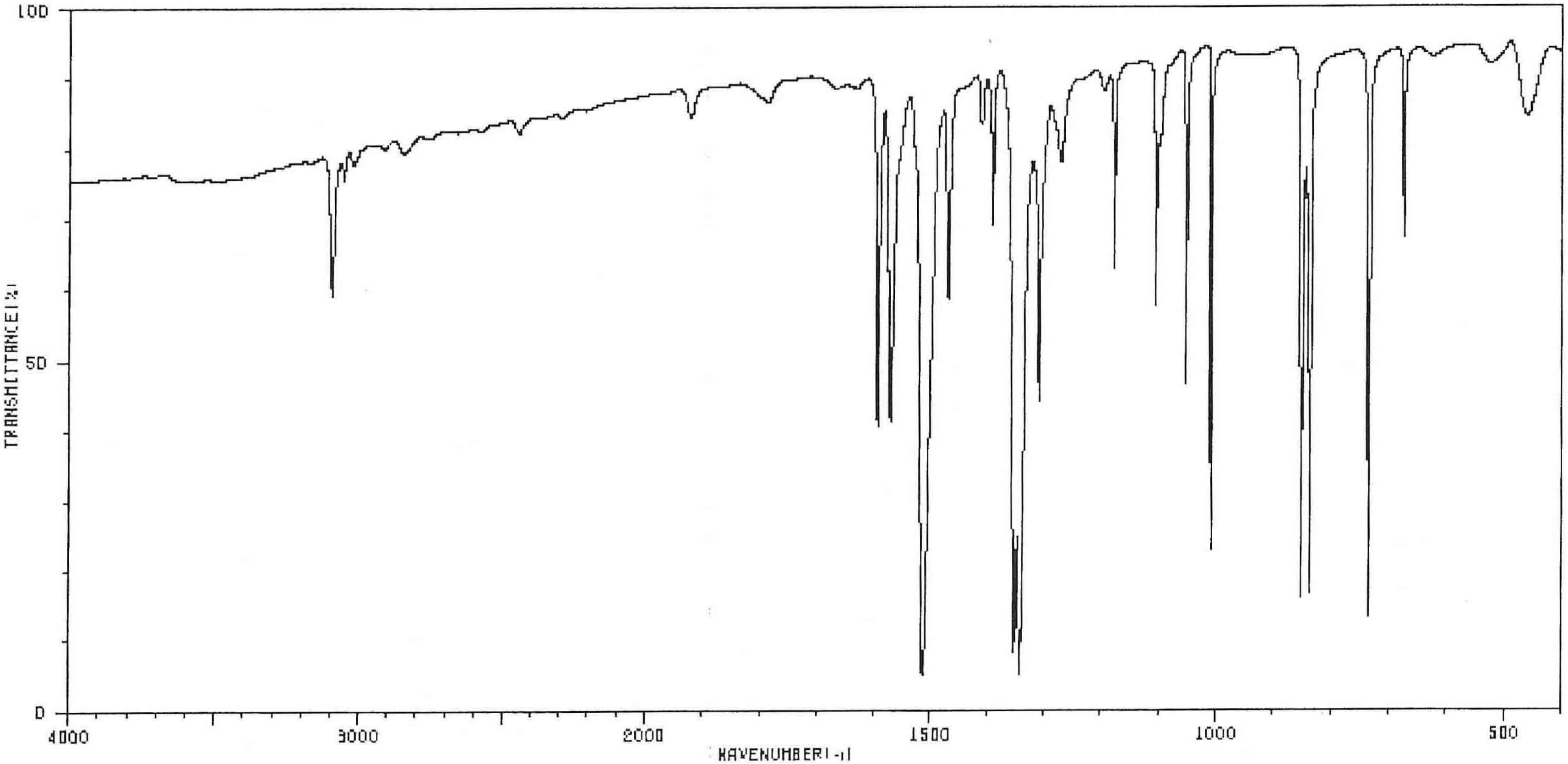
23



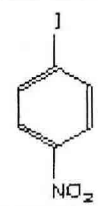


23 

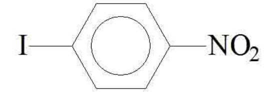
HIT-NO=1307	SCORE= ( )	SDBS-NO=1116	IR-NIDA-04086 : KBR DISC
P-IODONITROBENZENE			
$C_6H_4INO_2$			



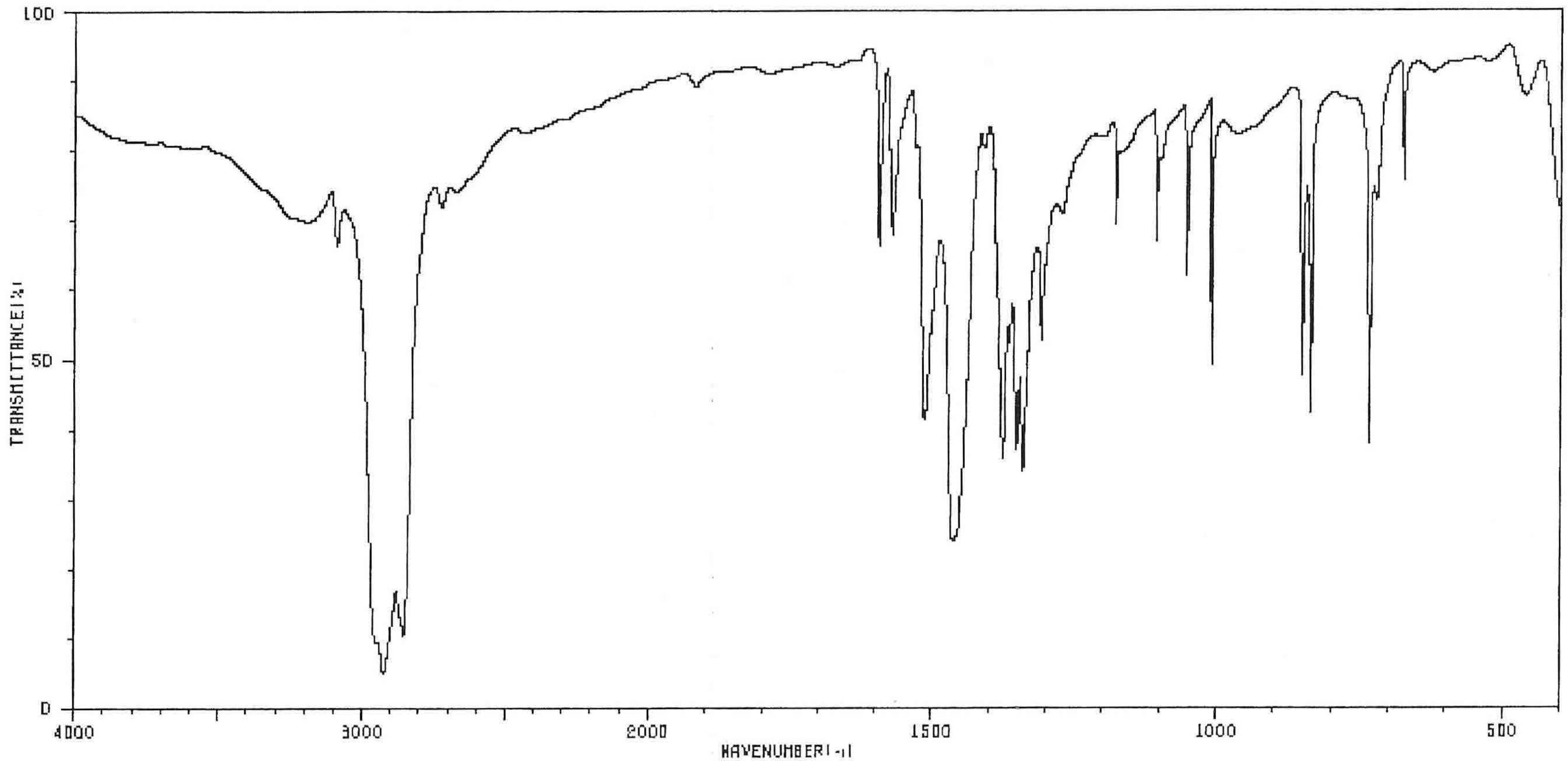
3093	67	1596	38	1343	4	1063	44	461	81
3054	72	1572	39	1310	42	1010	21		
3018	74	1515	4	1273	74	853	15		
2843	77	1470	57	1198	84	844	70		
2445	79	1411	81	1179	60	837	15		
1921	81	1392	66	1107	55	736	12		
1787	84	1363	7	1099	77	676	64		



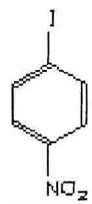
Źródło: ***https://sdbs.db.aist.go.jp***

23 

HIT-NO=682	SCORE= ( )	SDBS-NO=1116	IR-NIDA-10092 : NUJOL MULL
P-IODONITROBENZENE			
$C_6H_4INO_2$			

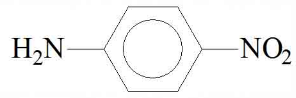


3091	64	1672	66	1342	32	1098	77	676	72
2952	8	1514	39	1310	50	1053	60	462	84
2924	4	1463	25	1273	88	1010	47		
2866	10	1411	77	1179	66	863	46		
2723	68	1377	34	1171	77	837	41		
1921	86	1368	50	1166	77	735	36		
1695	64	1363	36	1107	64	723	70		

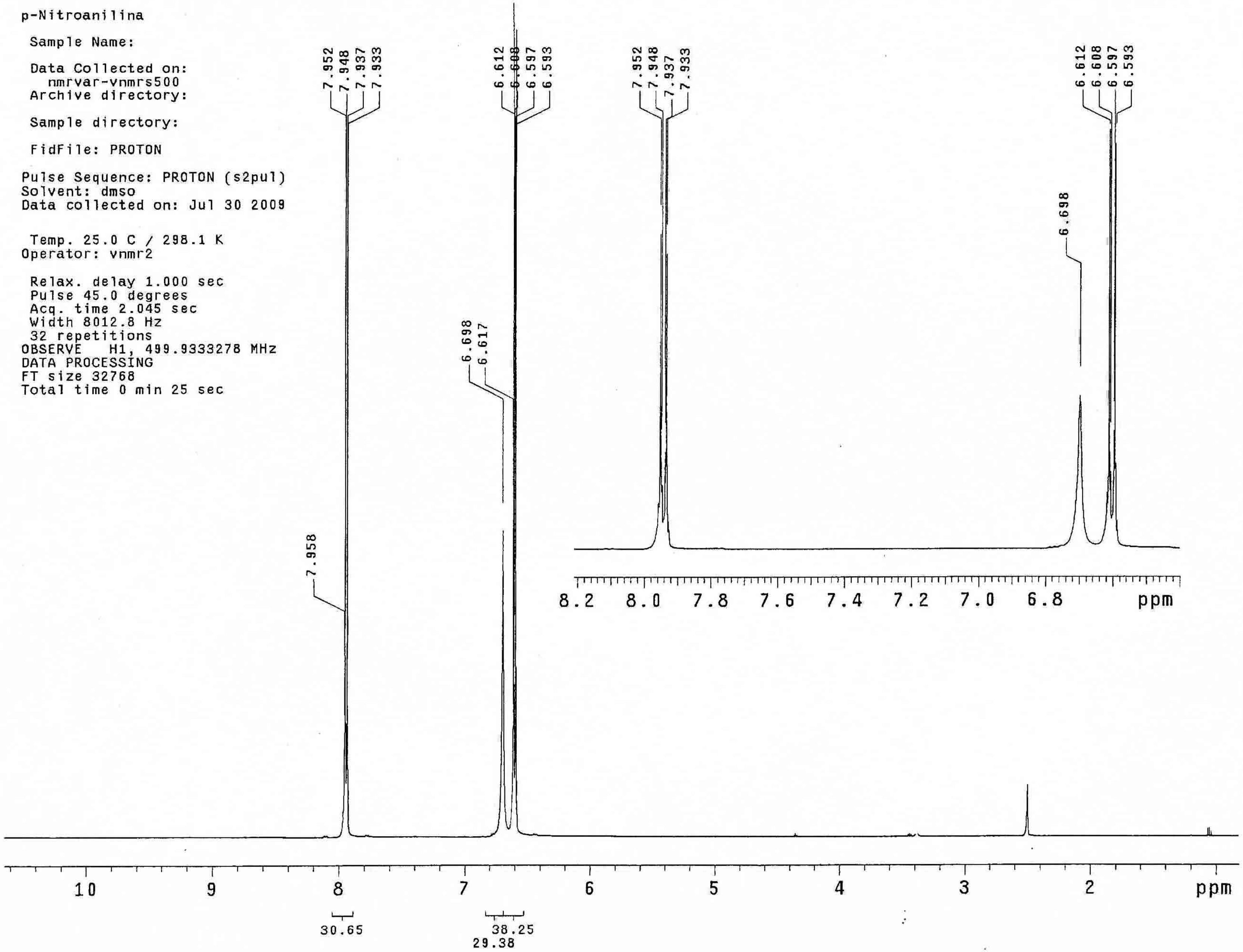


Źródło: ***https://sdbs.db.aist.go.jp***

24



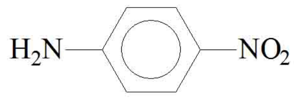
H_2N
NO_2



p-Nitroanilina
Sample Name:
Data Collected on:
nmrvar-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jul 30 2009
Temp. 25.0 C / 298.1 K
Operator: vnmr2
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.9333278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
7.952
7.948
7.937
7.933
6.612
6.608
6.597
6.593
6.698
6.617
7.958
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 ppm
10 9 8 7 6 5 4 3 2 ppm
30.65
38.25
29.38

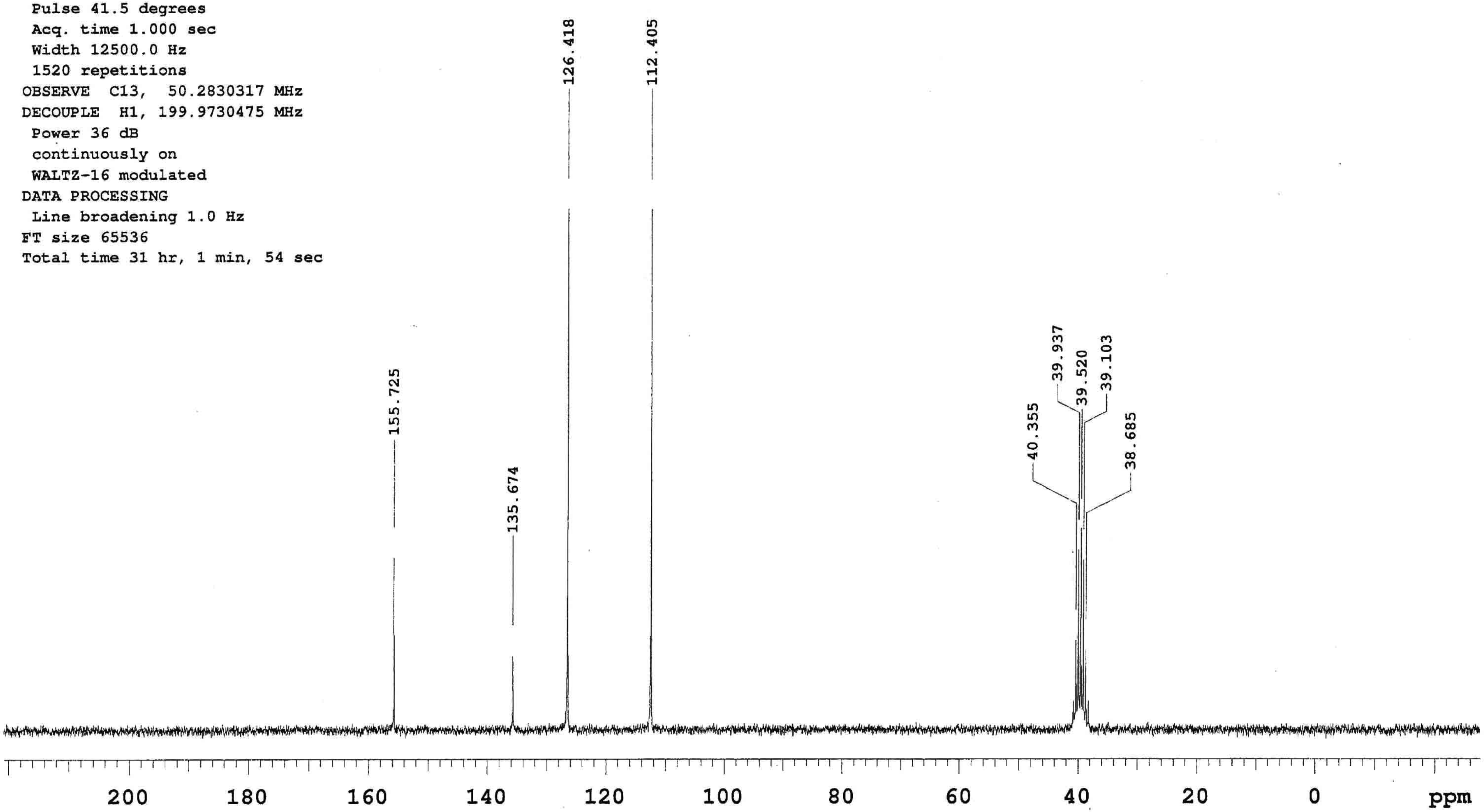
p-Nitroanilina

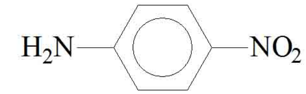
24

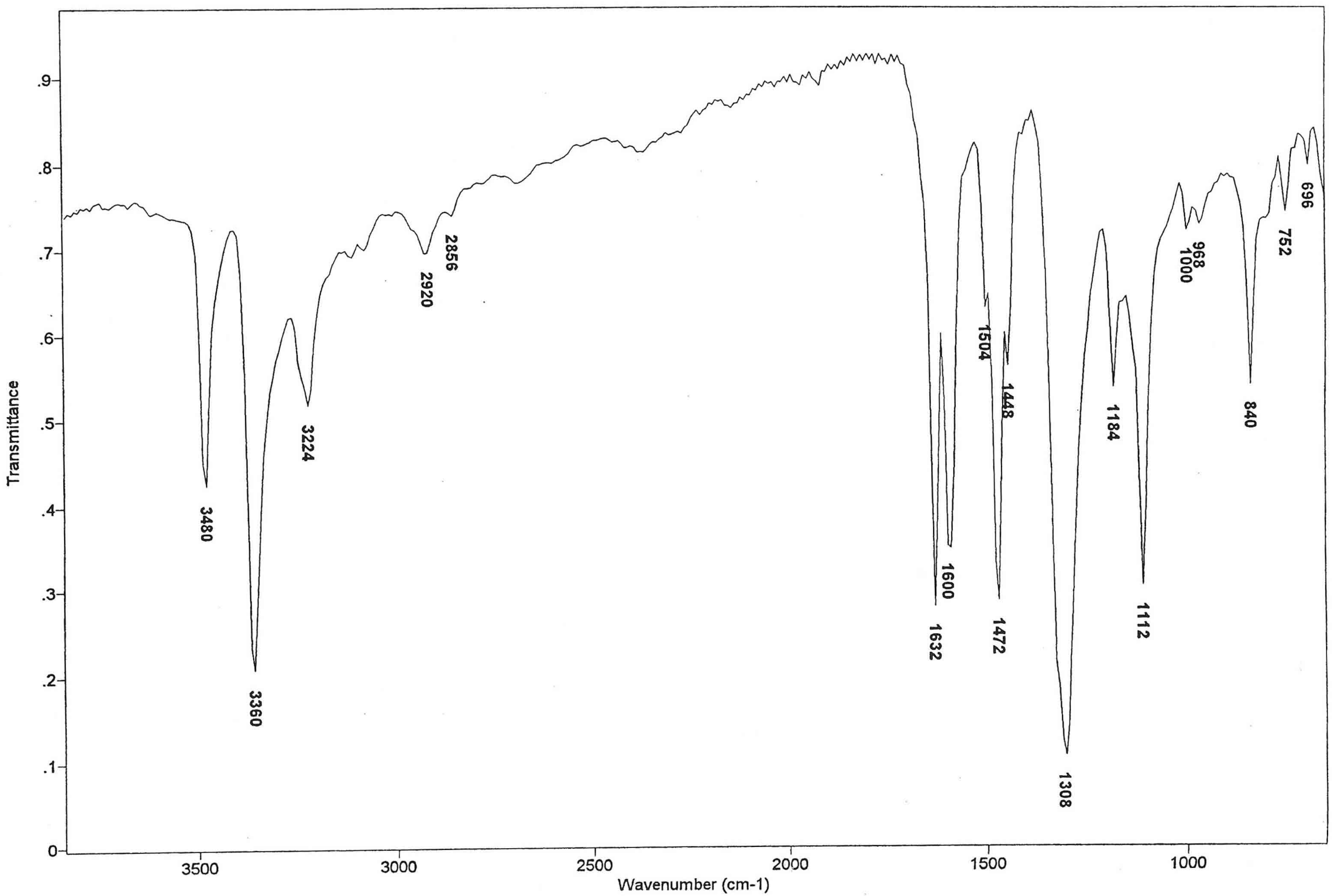


Solvent: DMSO
Ambient temperature
GEMINI-200BB "gemini"

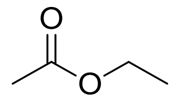
PULSE SEQUENCE
Pulse 41.5 degrees
Acq. time 1.000 sec
Width 12500.0 Hz
1520 repetitions
OBSERVE C13, 50.2830317 MHz
DECOUPLE H1, 199.9730475 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 1 min, 54 sec

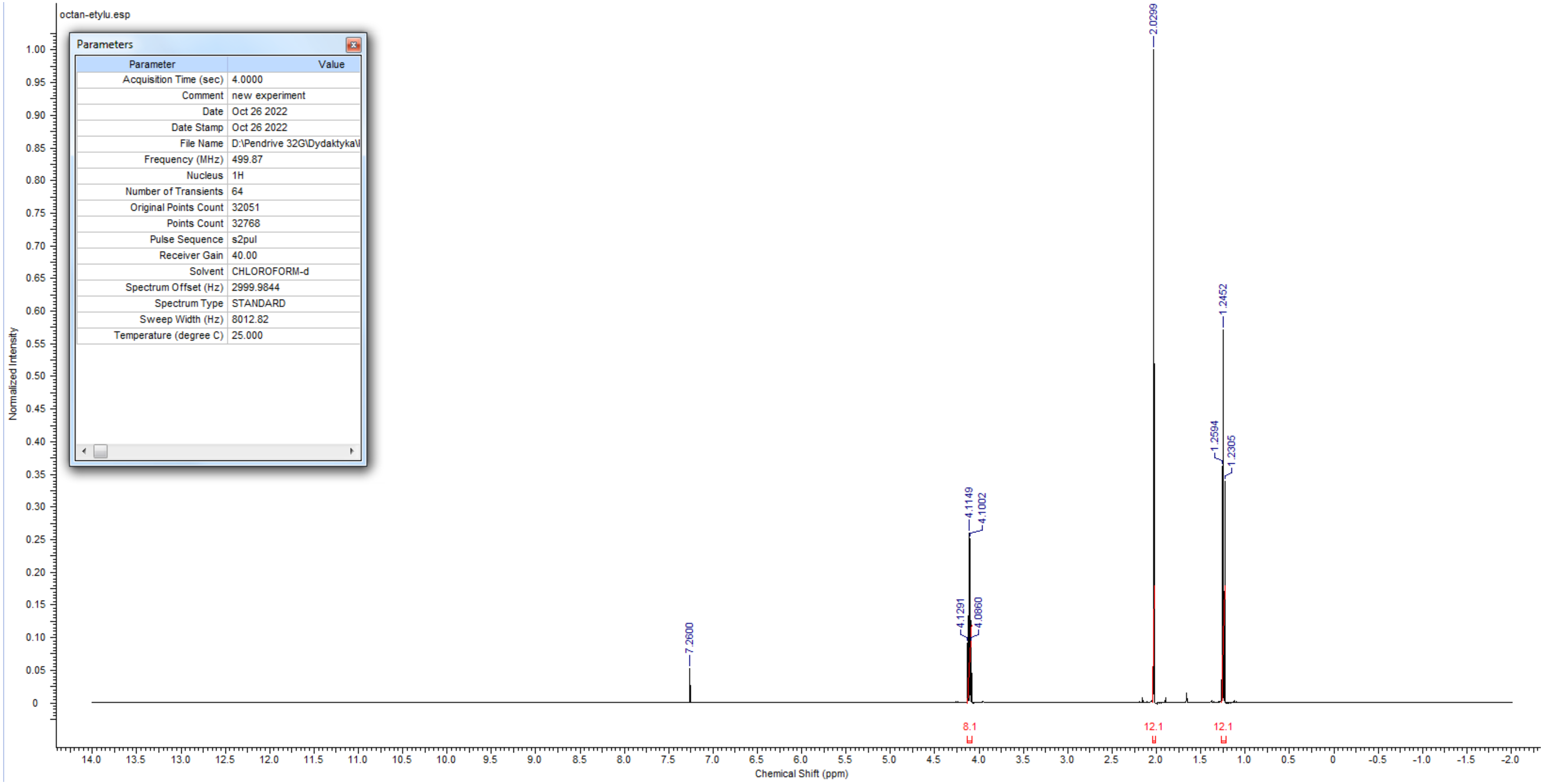


24 
H2N
NO2

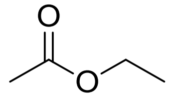

Transmittance
Wavenumber (cm-1)
3480
3360
3224
2920
2856
1632
1600
1504
1472
1448
1308
1184
1112
1000
968
840
752
696

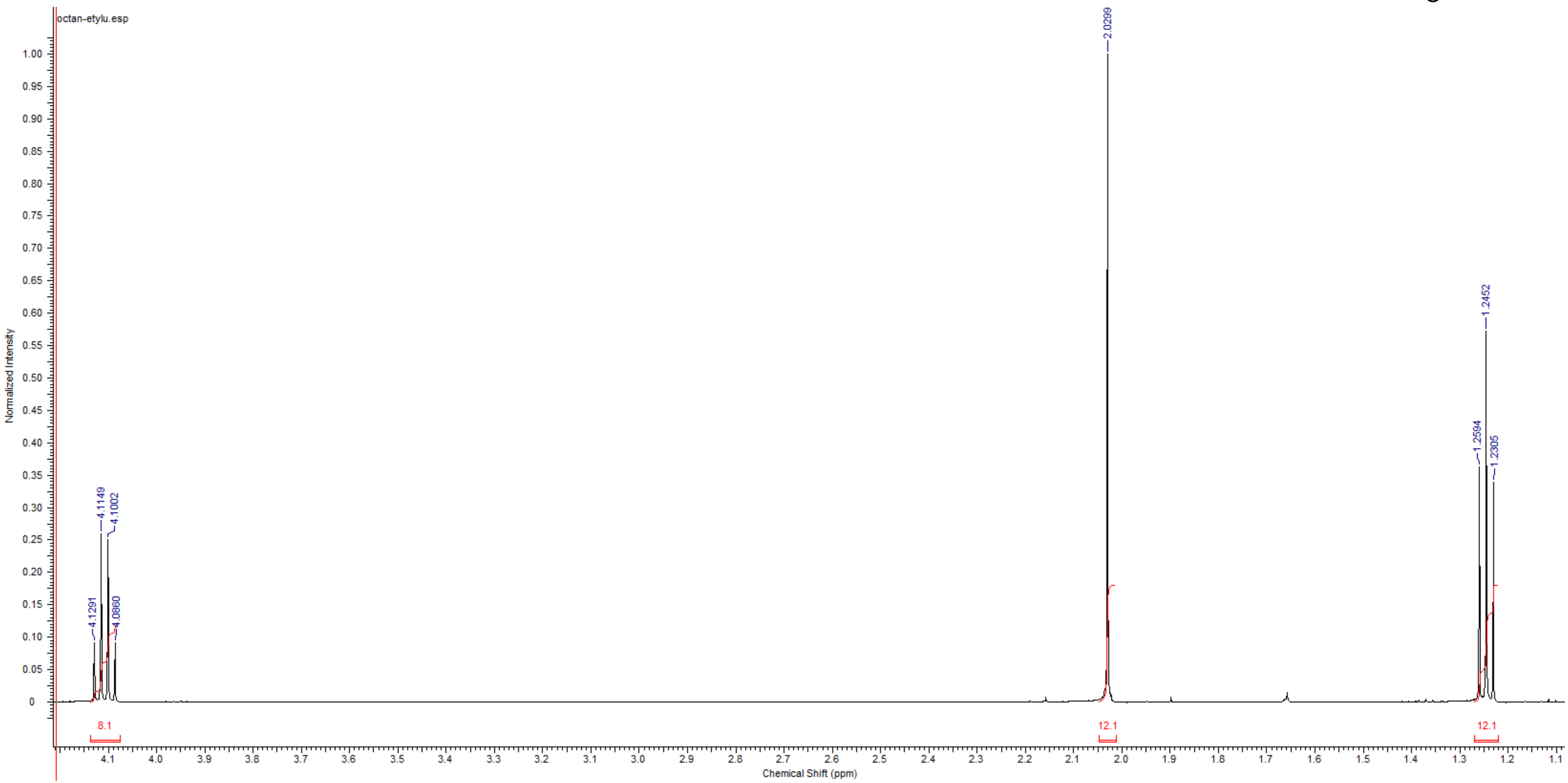
25



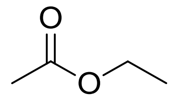

octan-etylu.esp
Parameters
Parameter | Value
Acquisition Time (sec) | 4.0000
Comment | new experiment
Date | Oct 26 2022
Date Stamp | Oct 26 2022
File Name | D:\Pendrive 32G\Dydaktyka\
Frequency (MHz) | 499.87
Nucleus | 1H
Number of Transients | 64
Original Points Count | 32051
Points Count | 32768
Pulse Sequence | s2pul
Receiver Gain | 40.00
Solvent | CHLOROFORM-d
Spectrum Offset (Hz) | 2999.9844
Spectrum Type | STANDARD
Sweep Width (Hz) | 8012.82
Temperature (degree C) | 25.000
Normalized Intensity
Chemical Shift (ppm)
7.2600
4.1291
4.1149
4.1002
4.0860
2.0299
1.2594
1.2452
1.2305
8.1
12.1
12.1

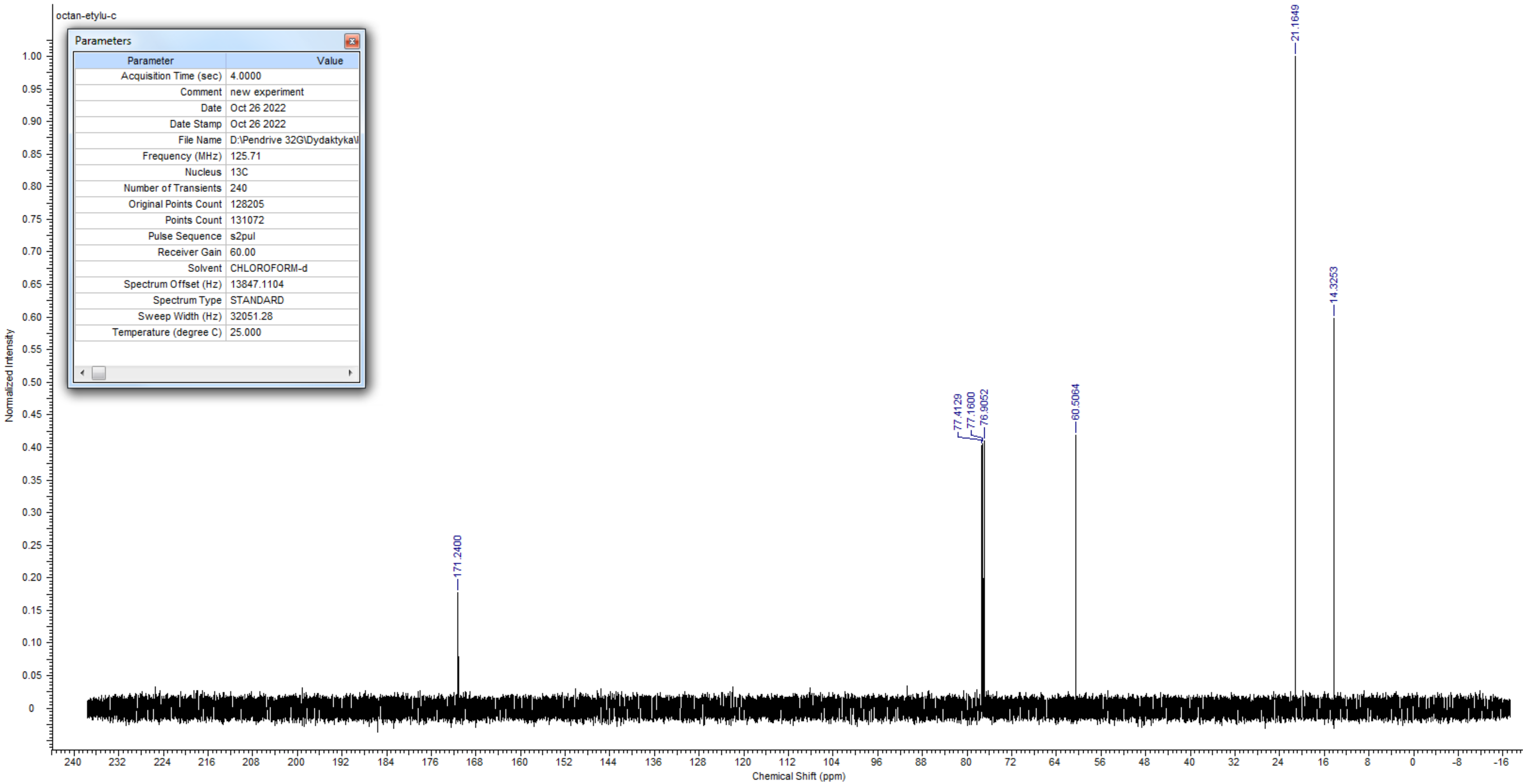
25




octan-etylu.esp
2.0299
1.2452
1.2594
1.2305
4.1149
4.1002
4.1291
4.0860
8.1
12.1
12.1
Normalized Intensity
Chemical Shift (ppm)

25

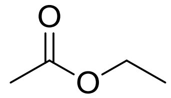


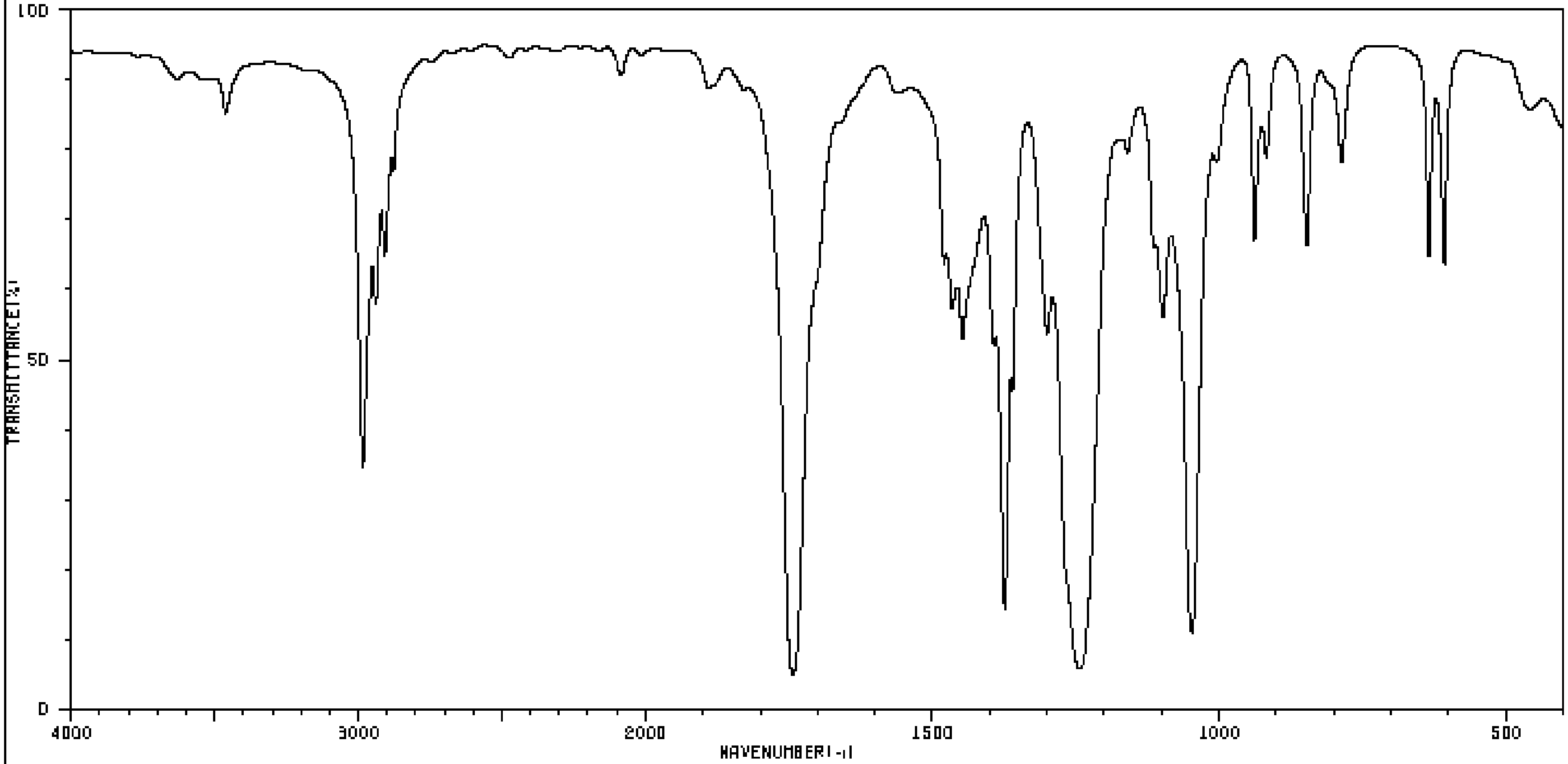


octan-etylu-c
Parameters
Parameter | Value
Acquisition Time (sec) | 4.0000
Comment | new experiment
Date | Oct 26 2022
Date Stamp | Oct 26 2022
File Name | D:\Pendrive 32G\Dydaktyka\
Frequency (MHz) | 125.71
Nucleus | 13C
Number of Transients | 240
Original Points Count | 128205
Points Count | 131072
Pulse Sequence | s2pul
Receiver Gain | 60.00
Solvent | CHLOROFORM-d
Spectrum Offset (Hz) | 13847.1104
Spectrum Type | STANDARD
Sweep Width (Hz) | 32051.28
Temperature (degree C) | 25.000
171.2400
77.4129
77.1600
76.9052
60.5064
21.1649
14.3253
Normalized Intensity
Chemical Shift (ppm)

HIT-NO=1229	SCORE= ( )	SDBS-NO=889	IR-NIDA-01804 : LIQUID FILM
ETHYL ACETATE			
$C_4H_8O_2$			

25

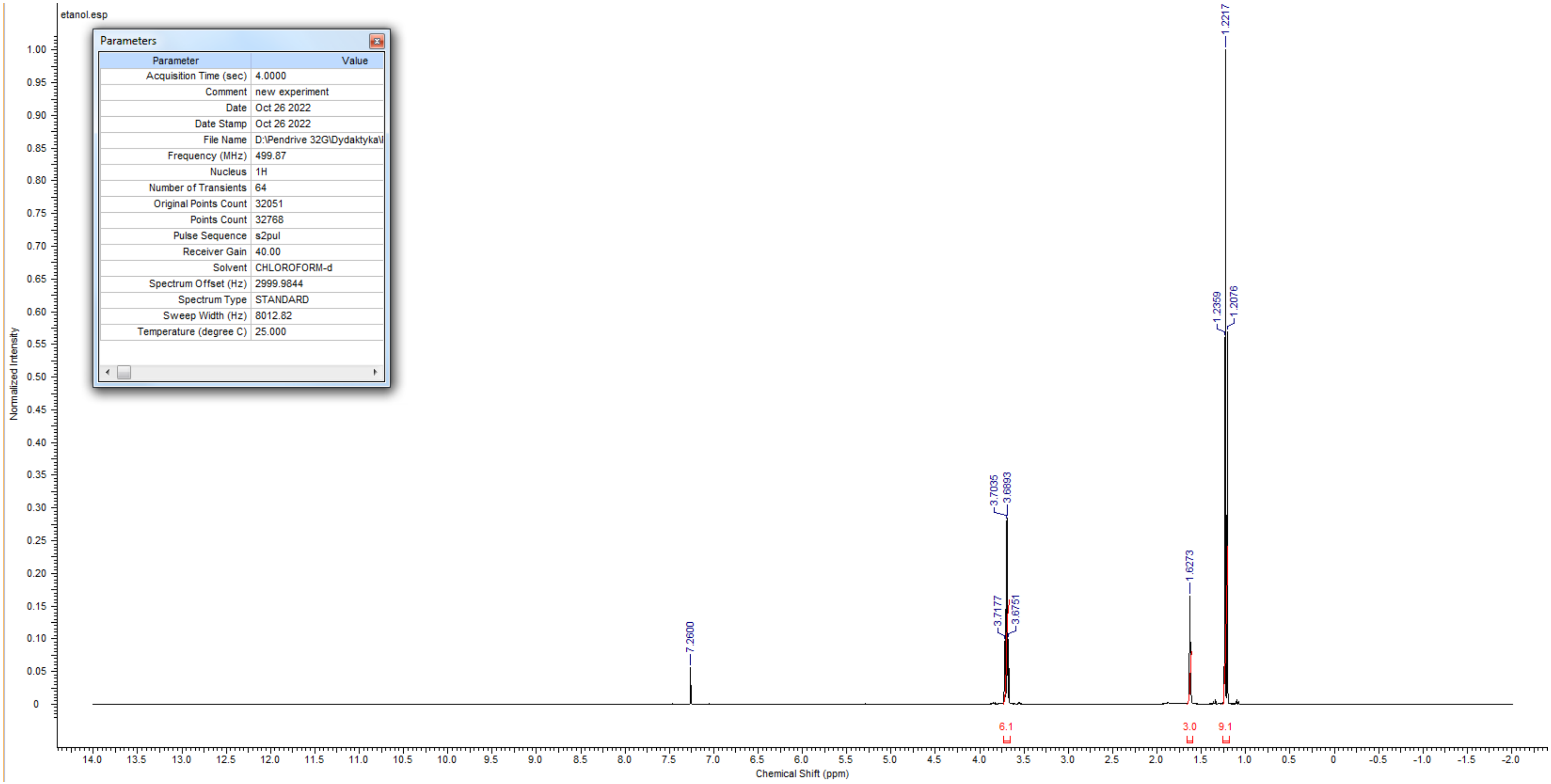




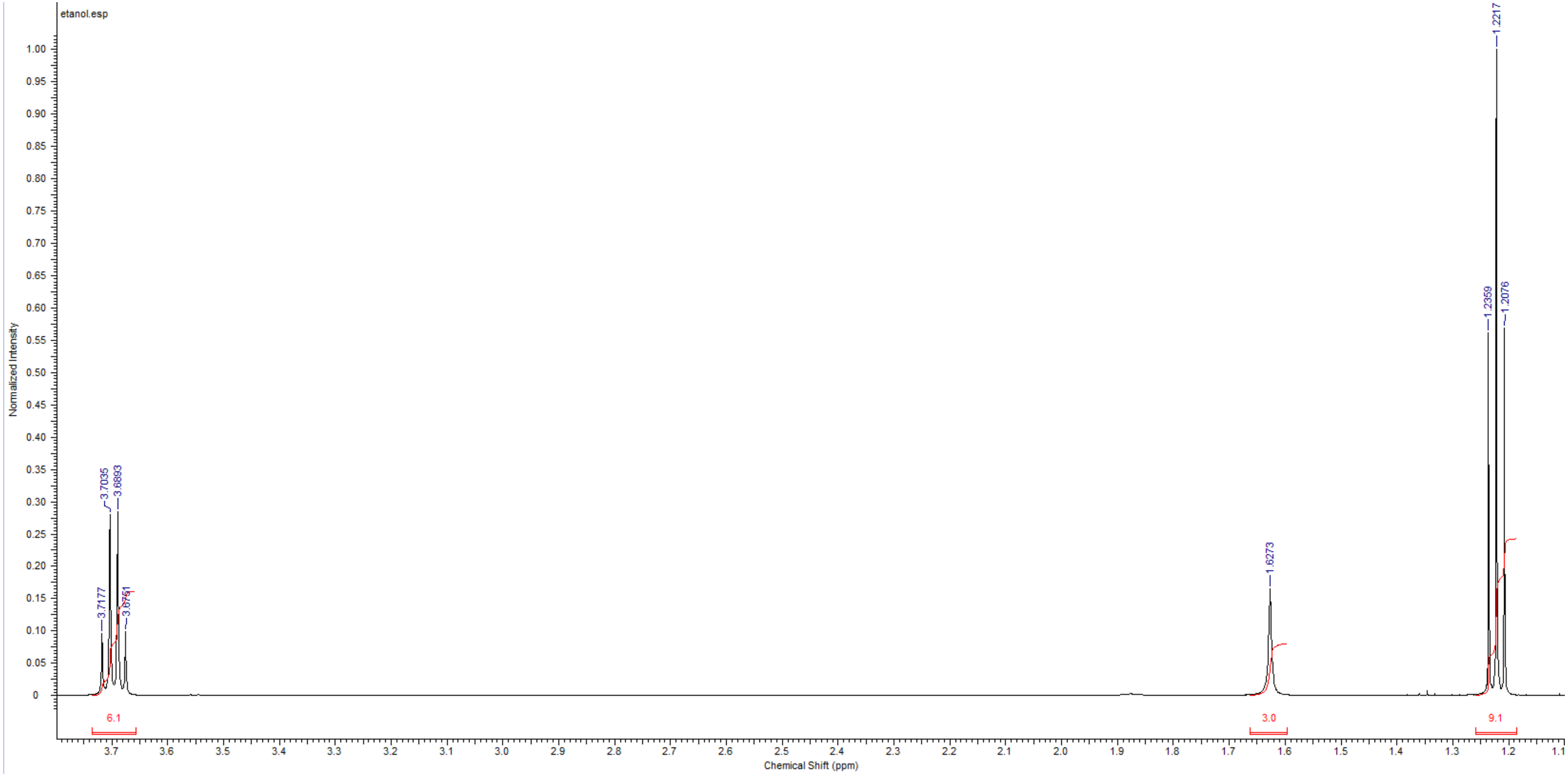
3462	81	1480	60	1243	6	847	64
2983	33	1466	55	1160	77	786	74
2940	55	1448	50	1111	84	634	62
2908	62	1393	60	1098	63	608	60
2877	74	1374	13	1048	10	457	81
1889	86	1360	45	939	84		
1743	4	1301	62	917	77		

$CH_3-\underset{\displaystyle O}{\underset{\|}{C}}-O-CH_2-CH_3$

26 C_2H_5OH

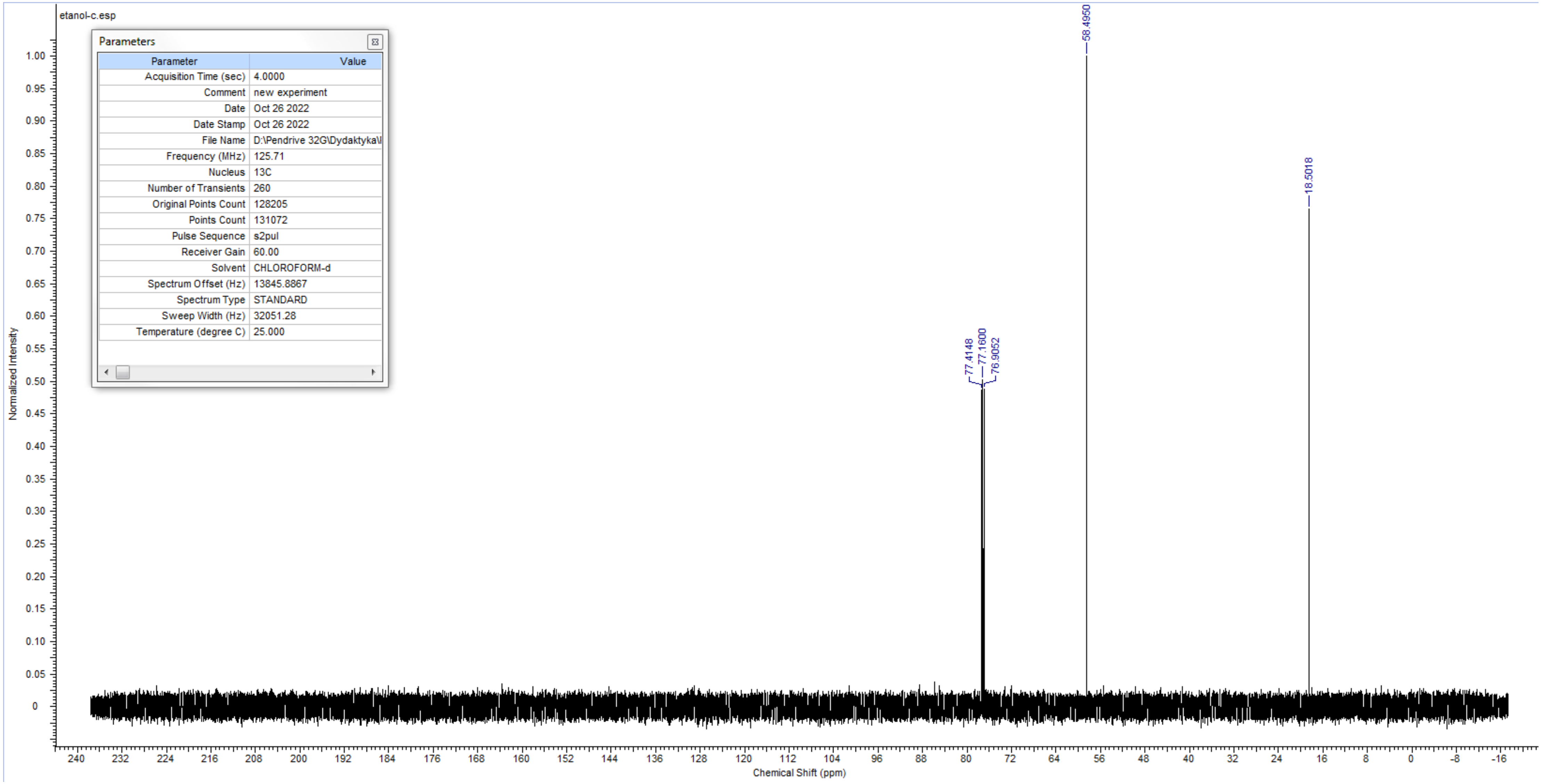

etanol.esp
Parameters
Parameter | Value
Acquisition Time (sec) | 4.0000
Comment | new experiment
Date | Oct 26 2022
Date Stamp | Oct 26 2022
File Name | D:\Pendrive 32G\Dydaktyka\
Frequency (MHz) | 499.87
Nucleus | 1H
Number of Transients | 64
Original Points Count | 32051
Points Count | 32768
Pulse Sequence | s2pul
Receiver Gain | 40.00
Solvent | CHLOROFORM-d
Spectrum Offset (Hz) | 2999.9844
Spectrum Type | STANDARD
Sweep Width (Hz) | 8012.82
Temperature (degree C) | 25.000
7.2600
3.7177
3.7035
3.6893
3.6751
1.6273
1.2359
1.2217
1.2076
6.1
3.0
9.1
Normalized Intensity
Chemical Shift (ppm)

26 C_2H_5OH



etanol.esp
Normalized Intensity
Chemical Shift (ppm)
3.7177
3.7035
3.6893
3.6751
1.6273
1.2359
1.2217
1.2076
6.1
3.0
9.1

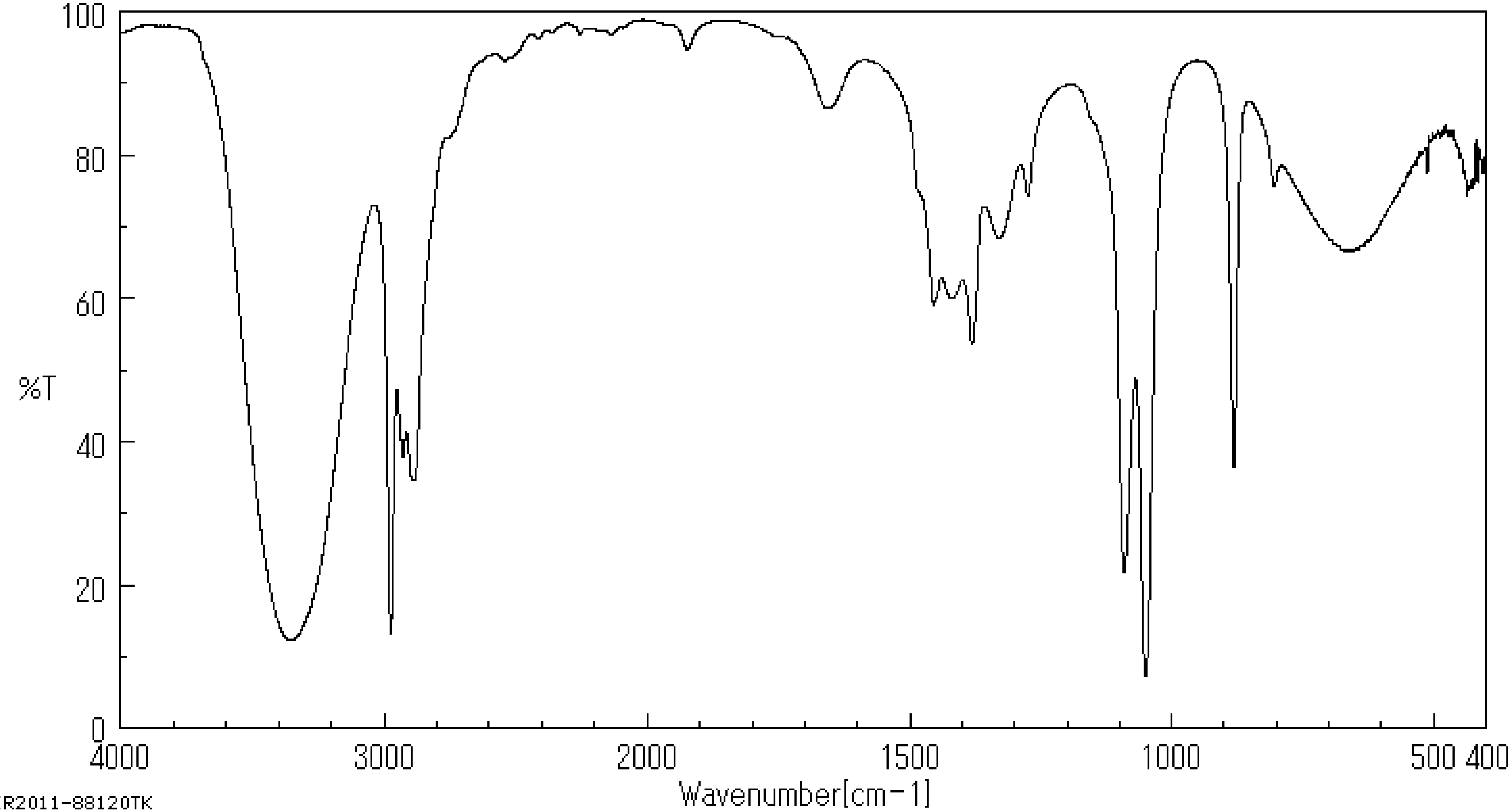
26 C_2H_5OH



Parameters

Parameter	Value
Acquisition Time (sec)	4.0000
Comment	new experiment
Date	Oct 26 2022
Date Stamp	Oct 26 2022
File Name	D:\Pendrive 32G\Dydaktyka\
Frequency (MHz)	125.71
Nucleus	13C
Number of Transients	260
Original Points Count	128205
Points Count	131072
Pulse Sequence	s2pul
Receiver Gain	60.00
Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	13845.8867
Spectrum Type	STANDARD
Sweep Width (Hz)	32051.28
Temperature (degree C)	25.000

26 C_2H_5OH



IR2011-88120TK

Wave number (cm^{-1}) and Transmittance (T%)

3358	12	1381	54	881	37
2974	13	1330	68	669	67
2927	38	1274	74		
2887	35	1090	22		
1455	59	1050	7		