

Supporting Information
for
Simple synthesis of pyrrolo[3,2-e]indole-1-carbonitriles

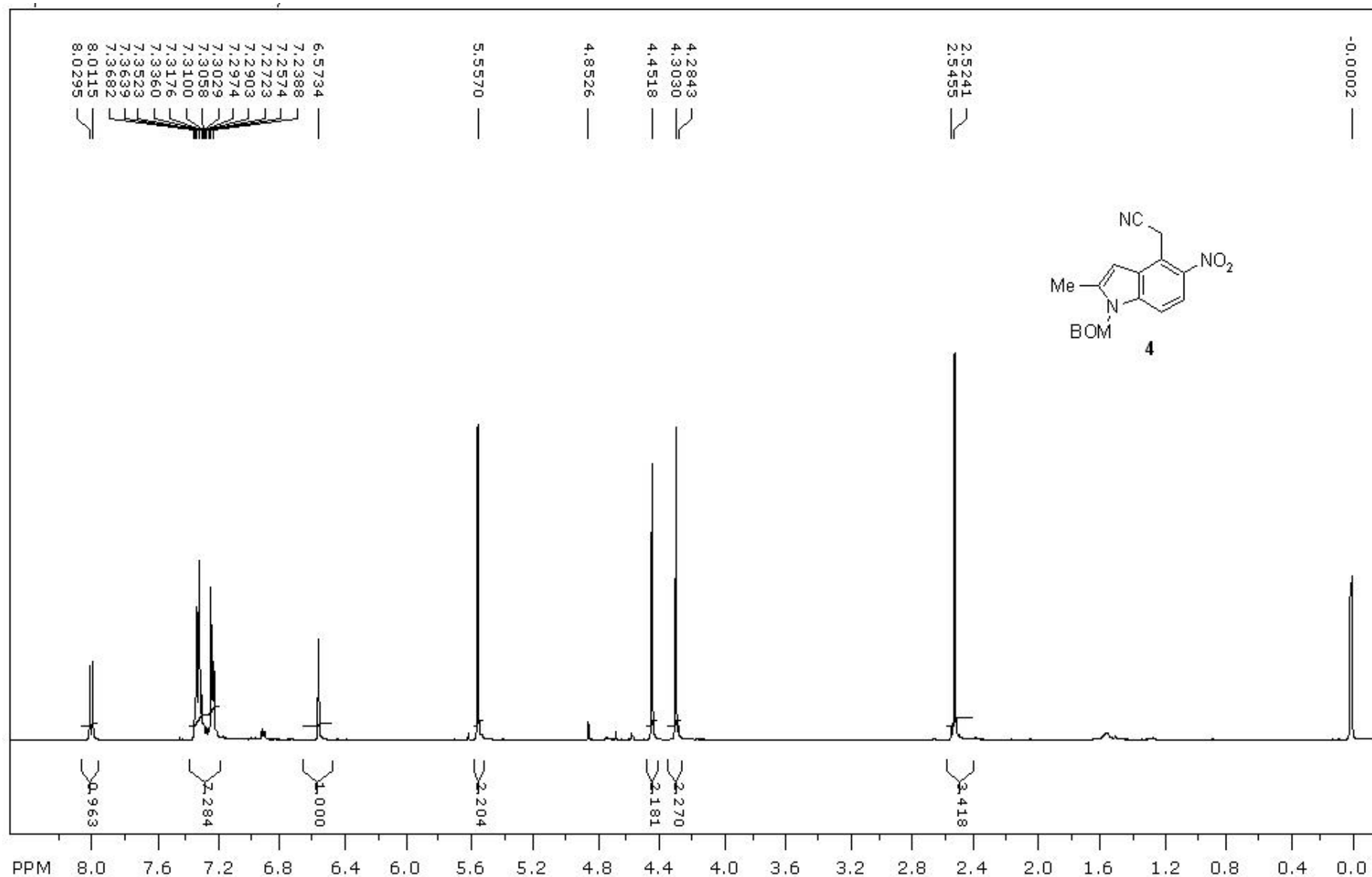
Adam Trawczyński^{1,2}, Robert Bujok¹, Zbigniew Wróbel¹, Krzysztof Wojciechowski¹

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E-mail: Krzysztof Wojciechowski - krzysztof.wojciechowski@icho.edu.pl

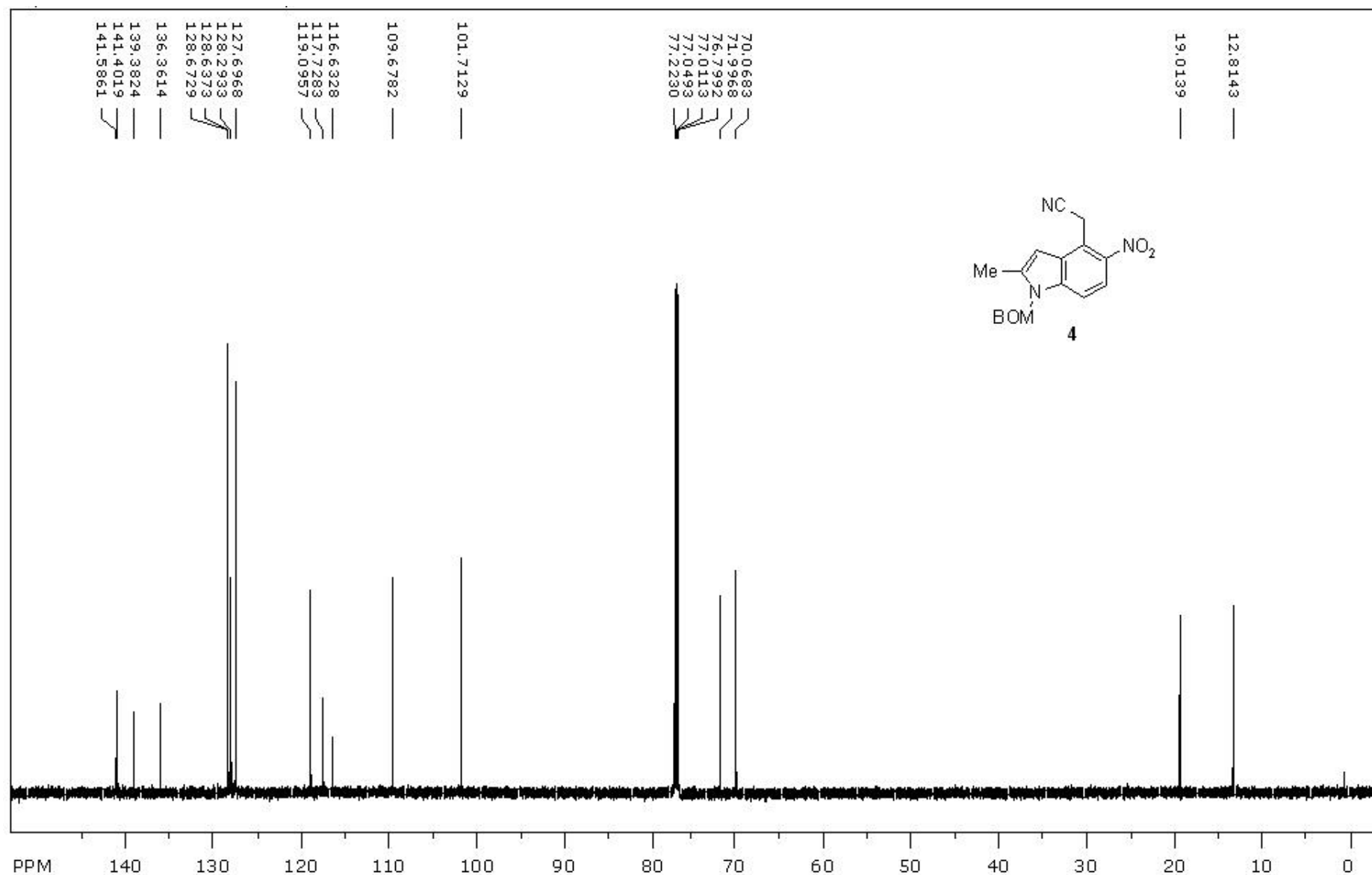
*Corresponding author

¹H and ¹³C NMR, IR and mass spectra for compounds 4, 5a–g, 6a–g, 8a, 8d, 9a and 10a



file: ...LEVAR500\ATIN-9\ATIN-9-H1.fid\fid block # 1 expt: "s2pul"
 transmitter freq.: 499.833542 MHz
 time domain size: 32768 points
 width: 5506.61 Hz = 11.0169 ppm = 0.168048 Hz/pt
 number of scans: 32

freq. of 0 ppm: 499.831293 MHz
 processed size: 32768 complex points
 LB: 1.061 GF: 0.0000
 Hz/cm: 174.554 ppm/cm: 0.34922

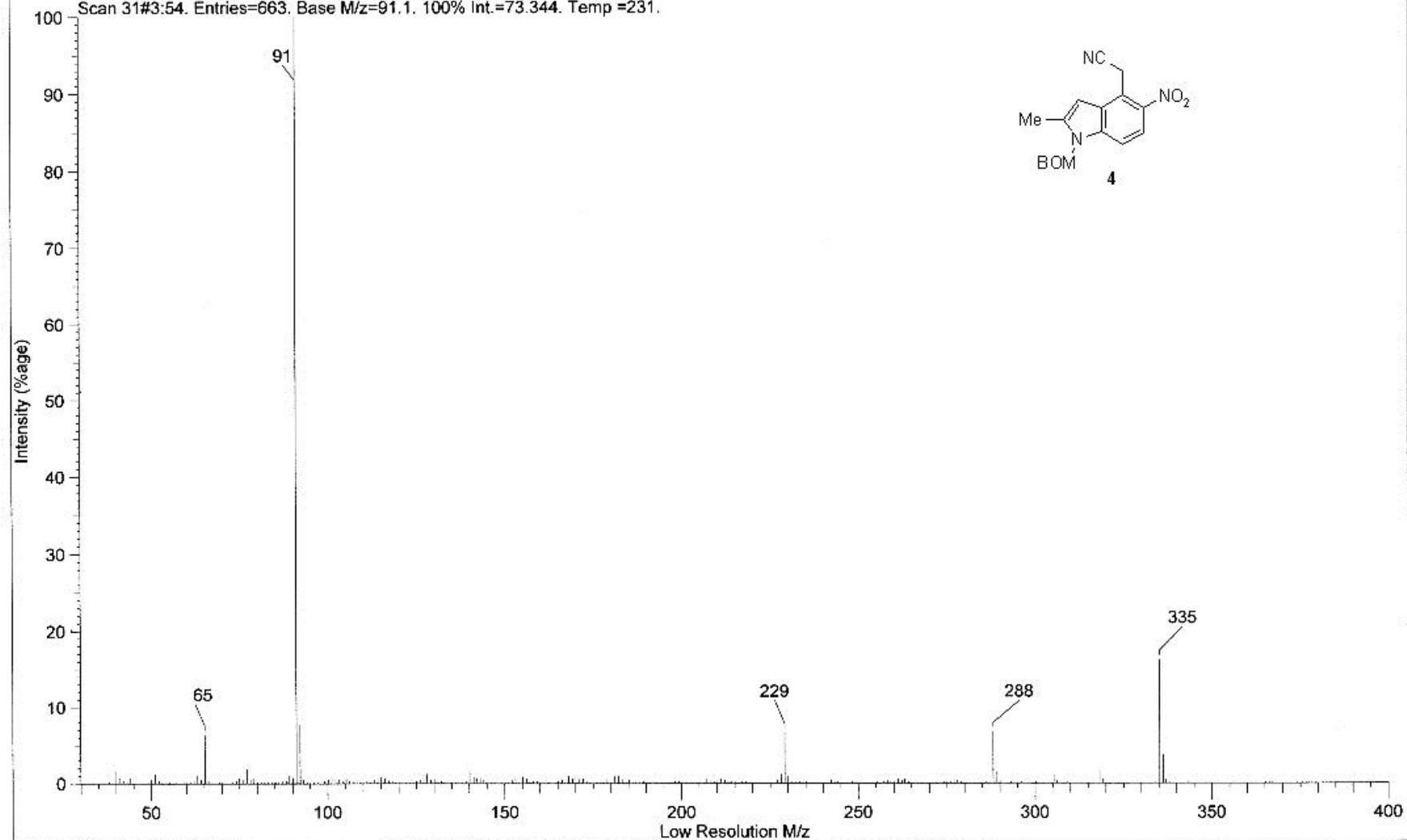


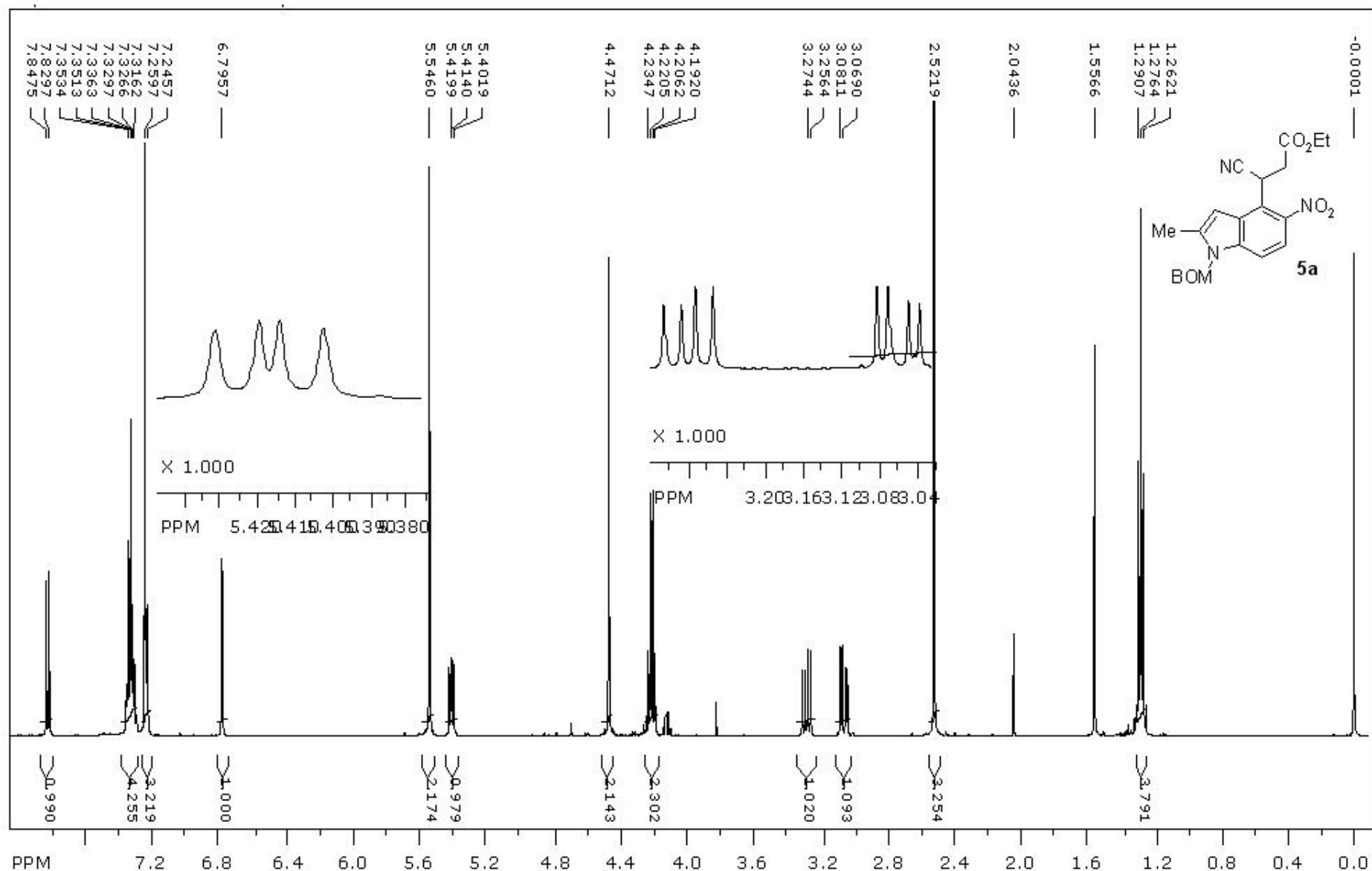
file: ...LOINDOLE\ATIN-5\ATIN-5-C13.fid\fid block # 1 expt: "s2pul"
 transmitter freq.: 150.845241 MHz
 time domain size: 90910 points
 width: 37878.79 Hz = 251.1103 ppm = 0.416663 Hz/pt
 number of scans: 1088

freq. of 0 ppm: 150.828649 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 950.009 ppm/cm: 6.29791

File Name : E:\Inne\PW_Warszawa\af1066.ms2
Creation Date/Time : 11-04-07 at 13:17:22
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [II32/99D9]
File Title : ATIN-5 (EI 70 eV 33-1000)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

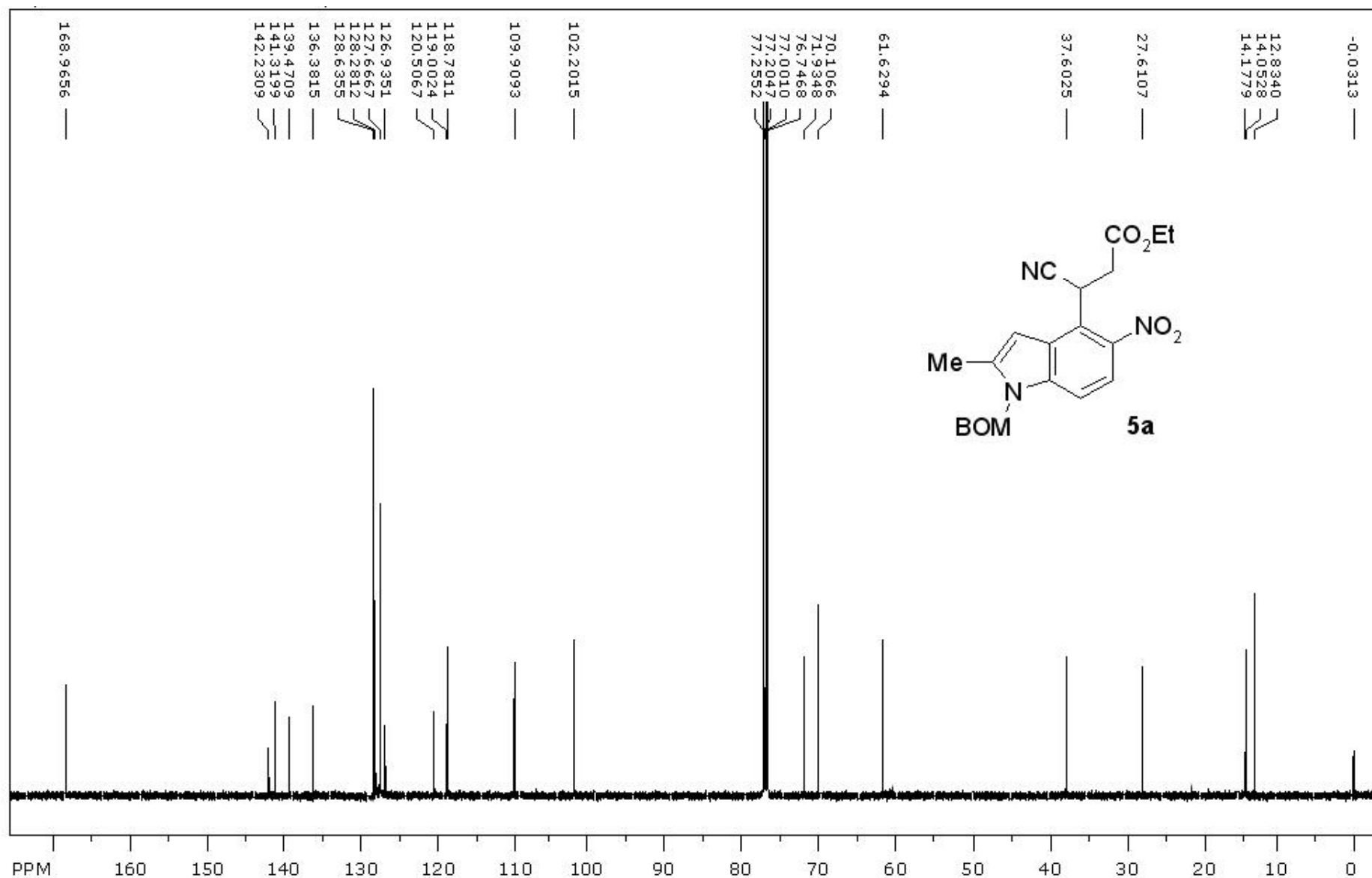
SCAN GRAPH, Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 31#3:54. Entries=663. Base M/z=91.1. 100% Int.=73.344. Temp =231.





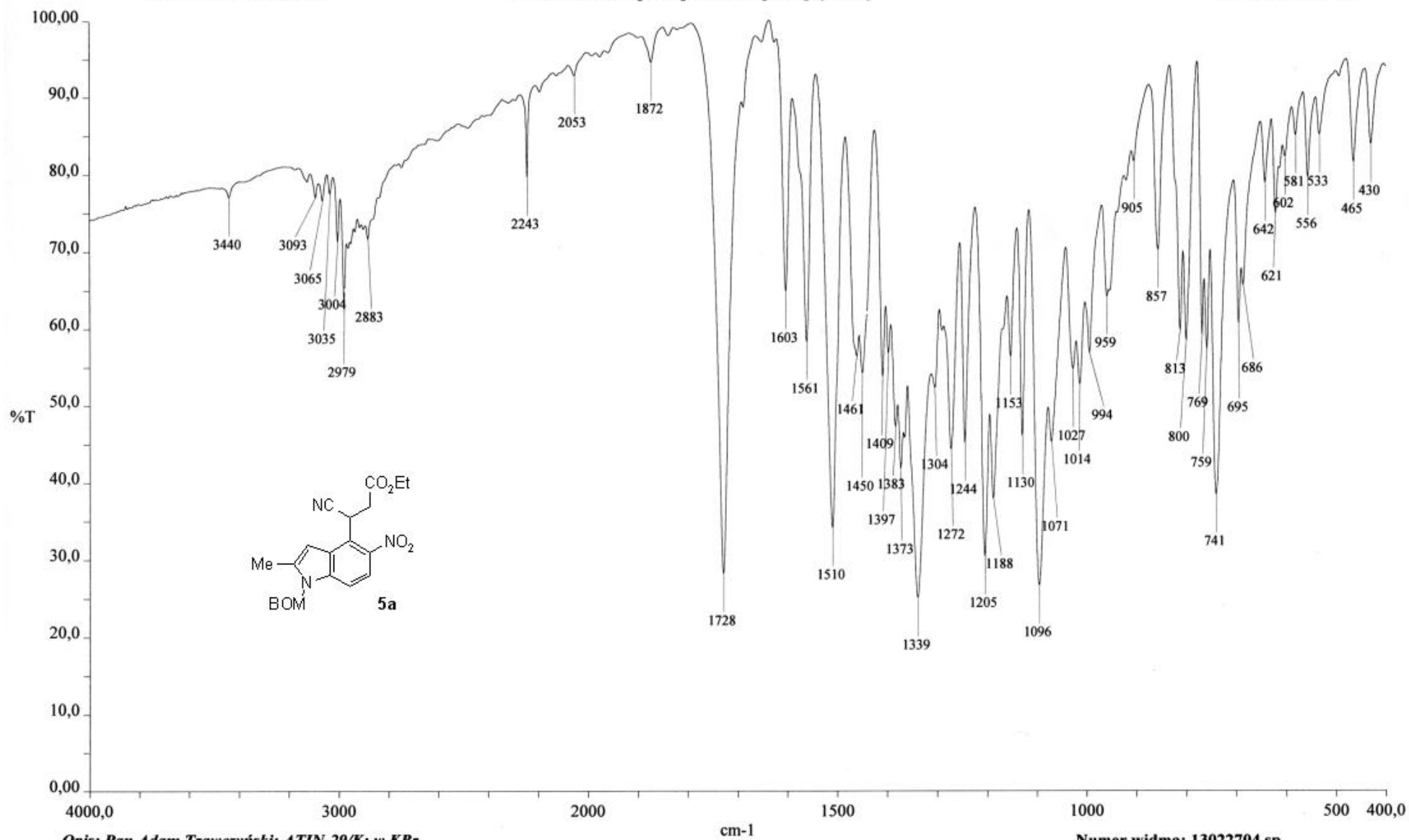
file: ...OLE\ATIN-29_K\ATIN-29_K-H1.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 499.835542 MHz
 time domain size: 65536 points
 width: 9541.98 Hz = 19.0902 ppm = 0.145599 Hz/pt
 number of scans: 32

freq. of 0 ppm: 499.831293 MHz
 processed size: 65536 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 163.386 ppm/cm: 0.32688



file: ...DOLE\ATIN-10K\ATIN-10K-C13.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 125.696504 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9894 ppm = 0.400001 Hz/pt
 number of scans: 2128

freq. of 0 ppm: 125.682680 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 904.602 ppm/cm: 7.19671



Opis: Pan Adam Trawczyński; ATIN-29/K; w KBr

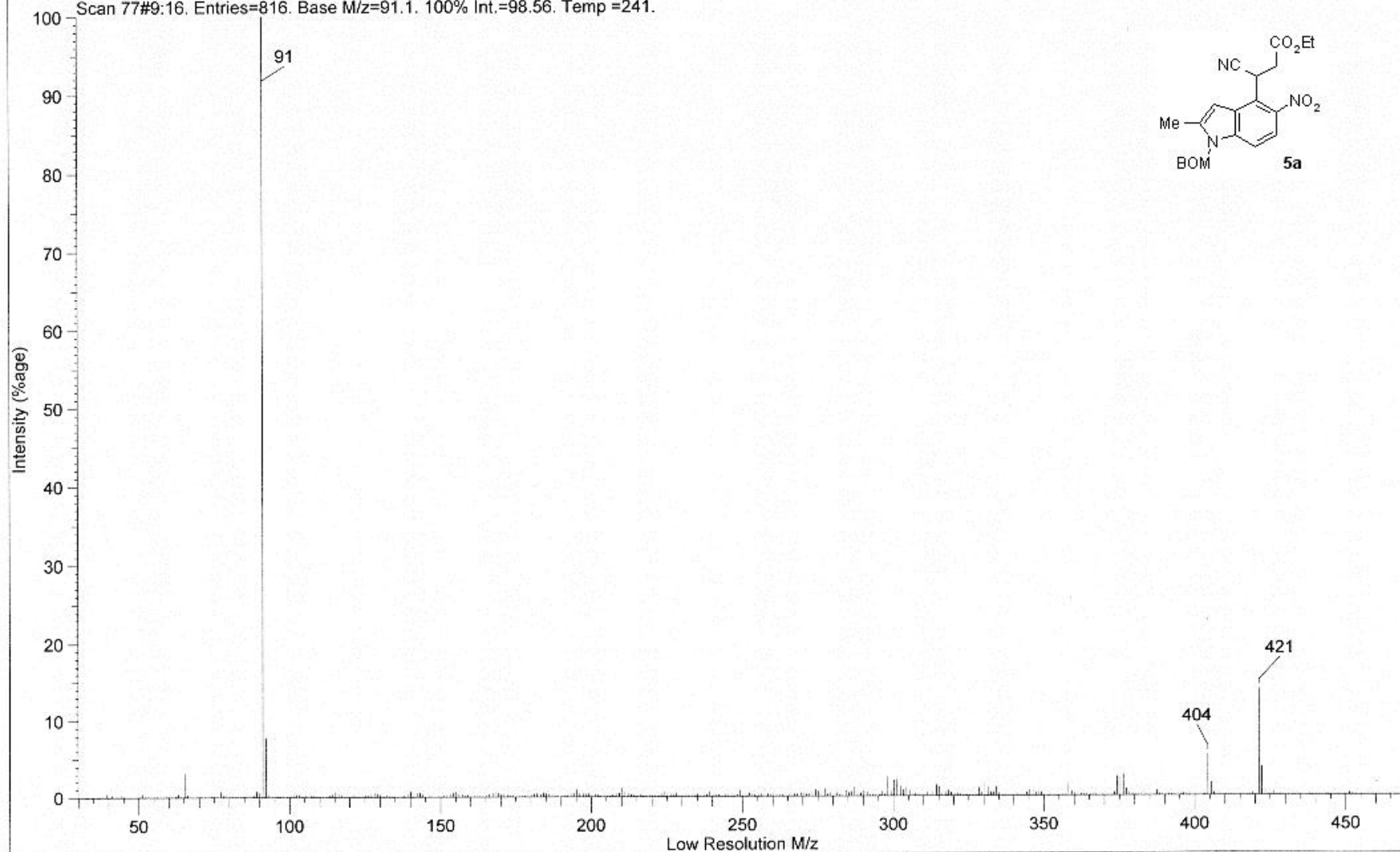
Uwagi:

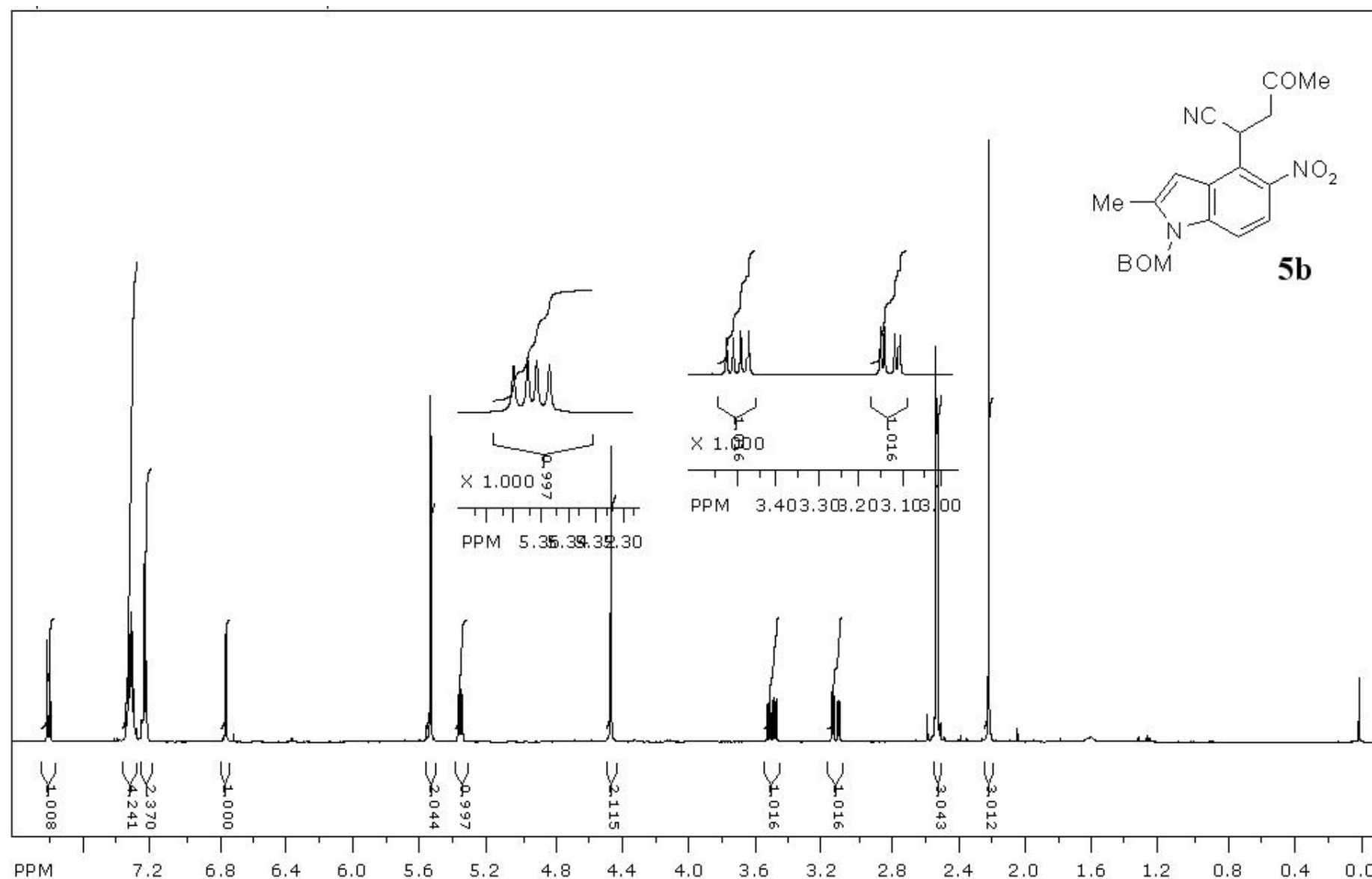
Numer widma: 13022704.sp

Operator: Alicja Dzedzic

File Name : E:\ChO\Z07_EG\at1755.ms2
Creation Date/Time : 11-06-13 at 14:48:00
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-10/K (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

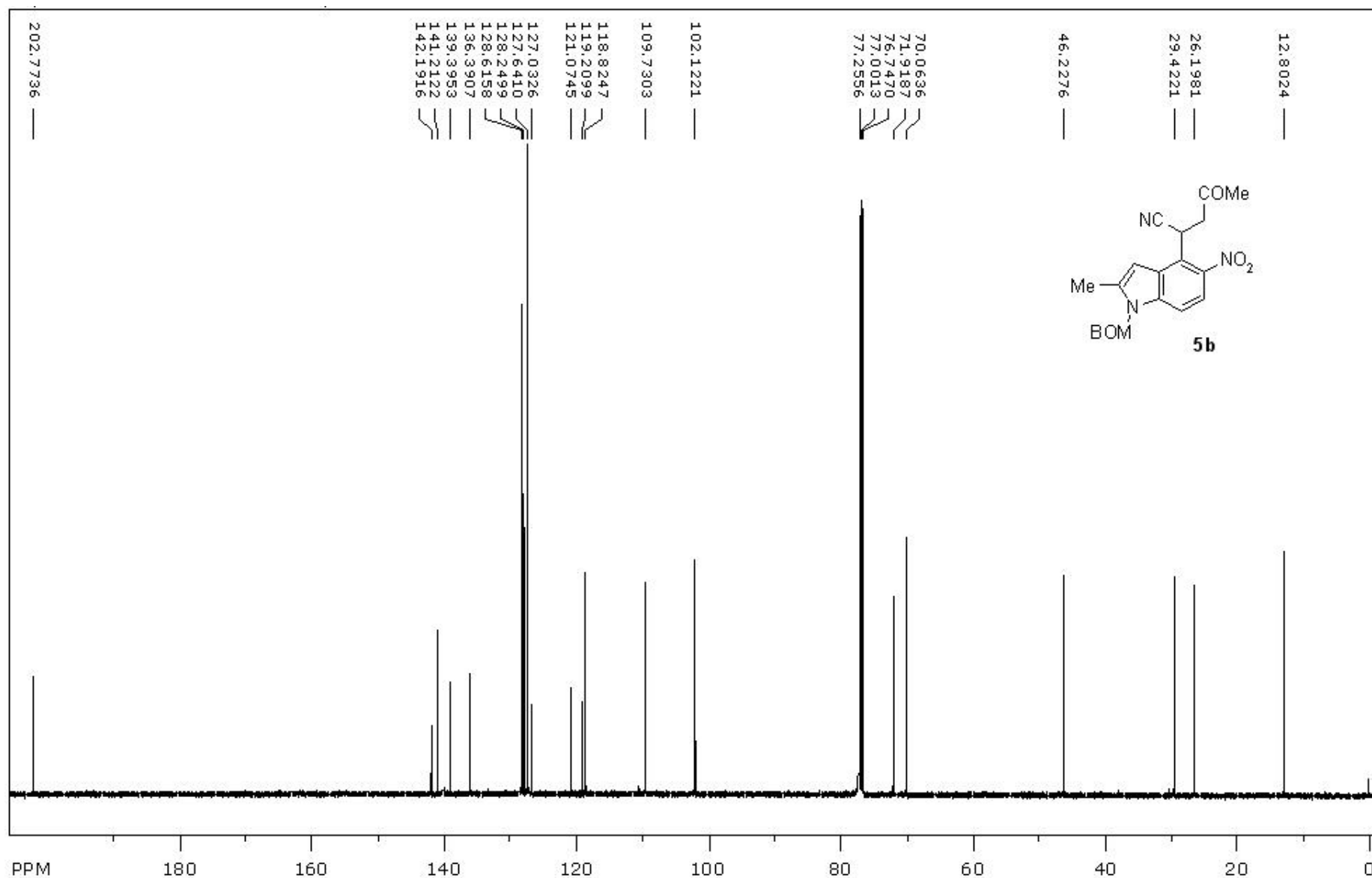
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 77#9:16. Entries=816. Base M/z=91.1. 100% Int.=98.56. Temp =241.





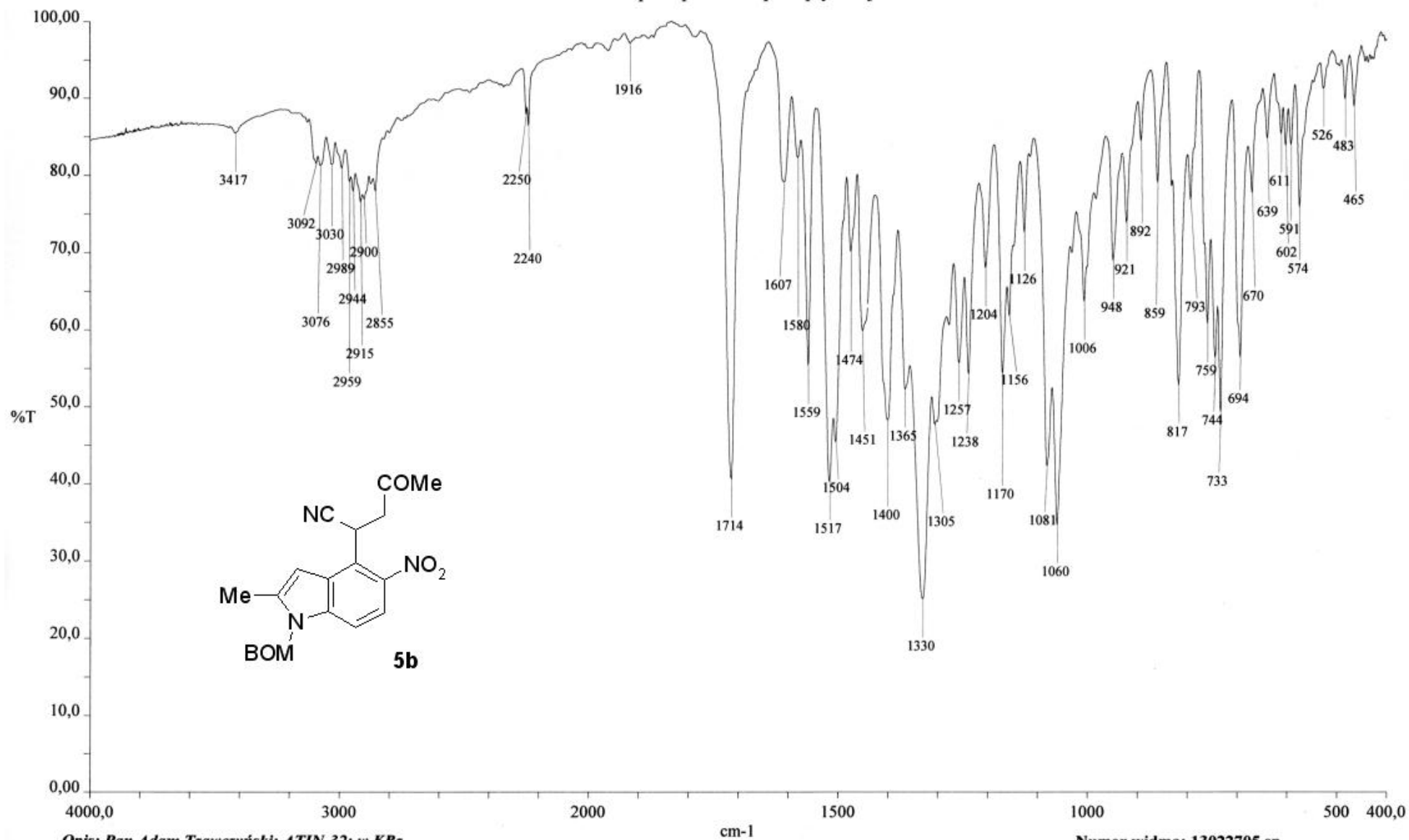
file: ...OINDOLE\ATIN-32\ATIN-32-H1.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 499.834042 MHz
 time domain size: 127118 points
 width: 10593.22 Hz = 21.1935 ppm = 0.083334 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.831293 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 163.911 ppm/cm: 0.32793



file: ...INDOLE\ATIN-32\ATIN-32-C13.fid\fid block #1 expt: "s2pul"
 transmitter freq.: 125.696504 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9894 ppm = 0.400001 Hz/pt
 number of scans: 2320

freq. of 0 ppm: 125.682683 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 1047.919 ppm/cm: 8.33690



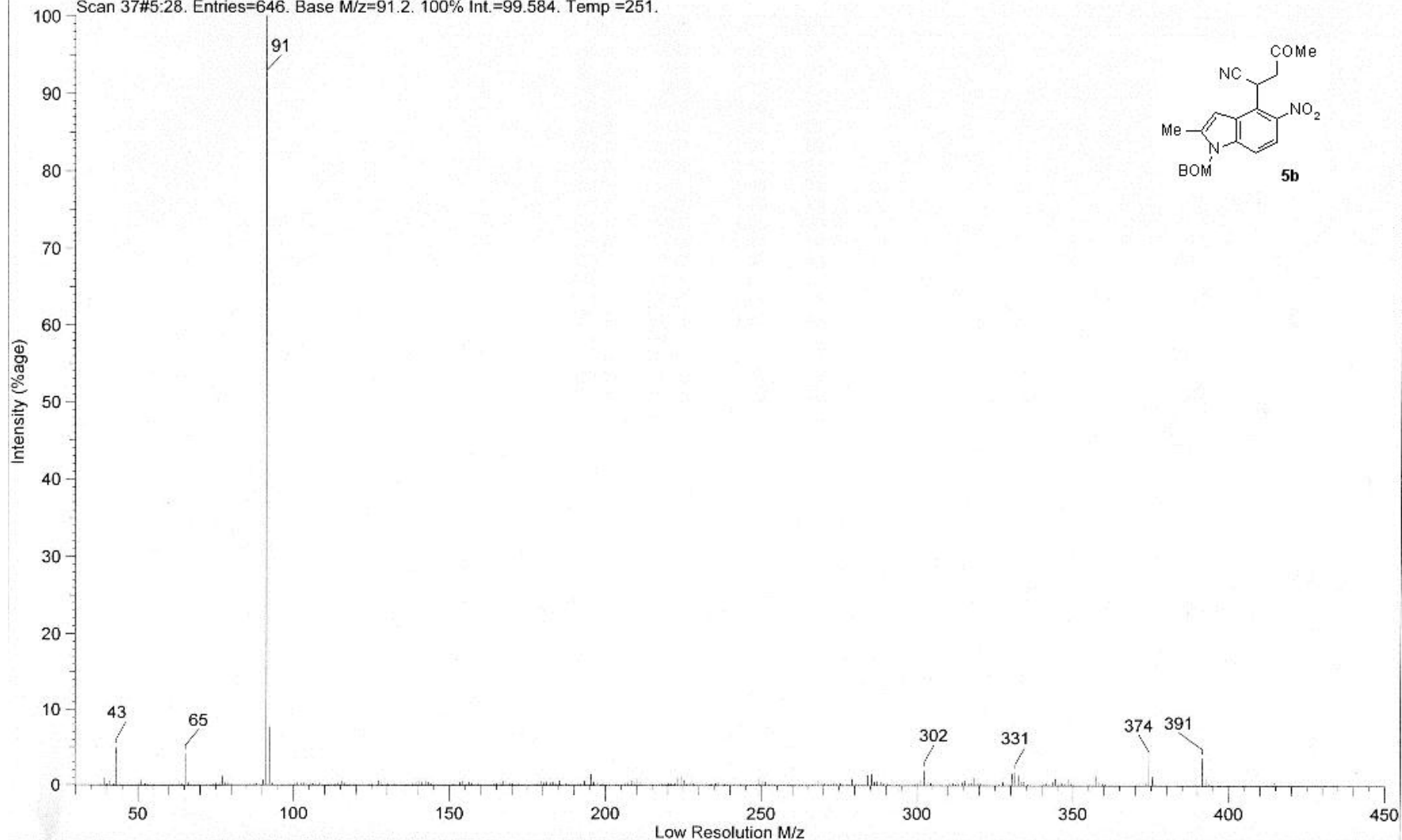
Opis: Pan Adam Trawczyński; ATIN-32; w KBr

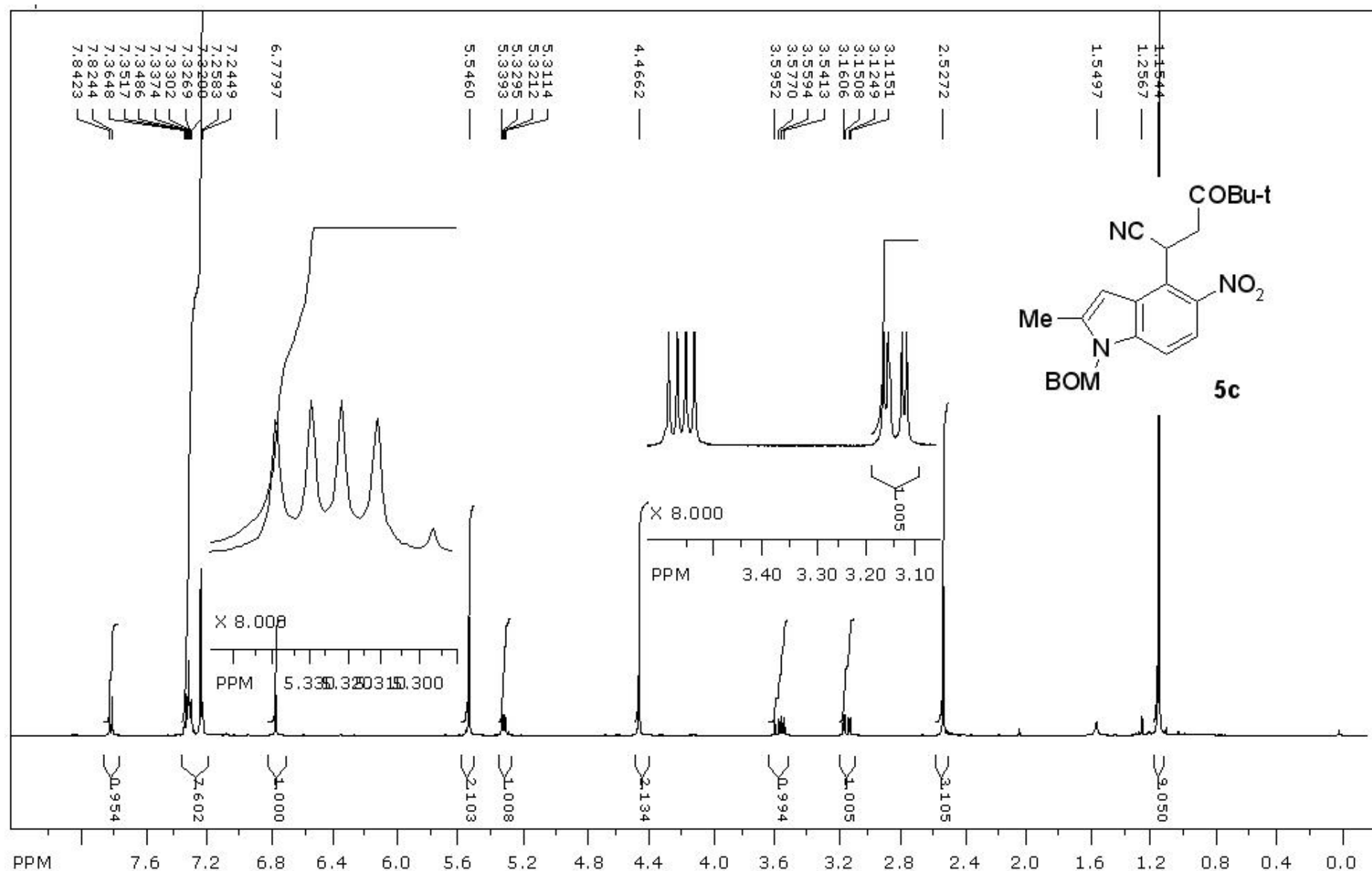
Uwagi:

Numer widma: 13022705.sp
Operator: Alicja Dziezic

File Name : E:\ChO\Z07_EG\at2985.ms2
Creation Date/Time : 11-10-10 at 14:16:27
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [II32/99D9]
File Title : ATIN-32 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

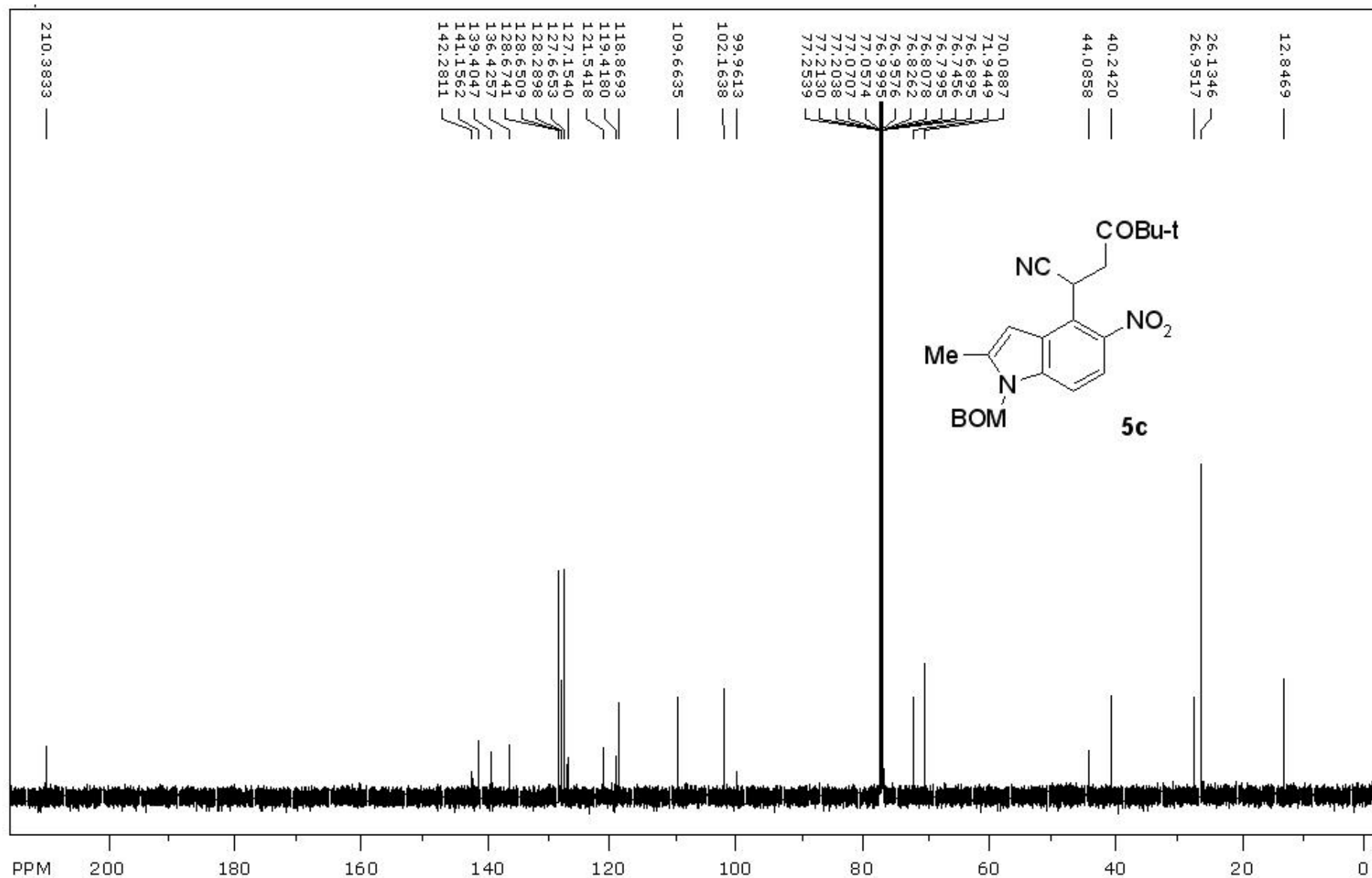
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 37#5:28. Entries=646. Base M/z=91.2. 100% Int.=99.584. Temp =251.





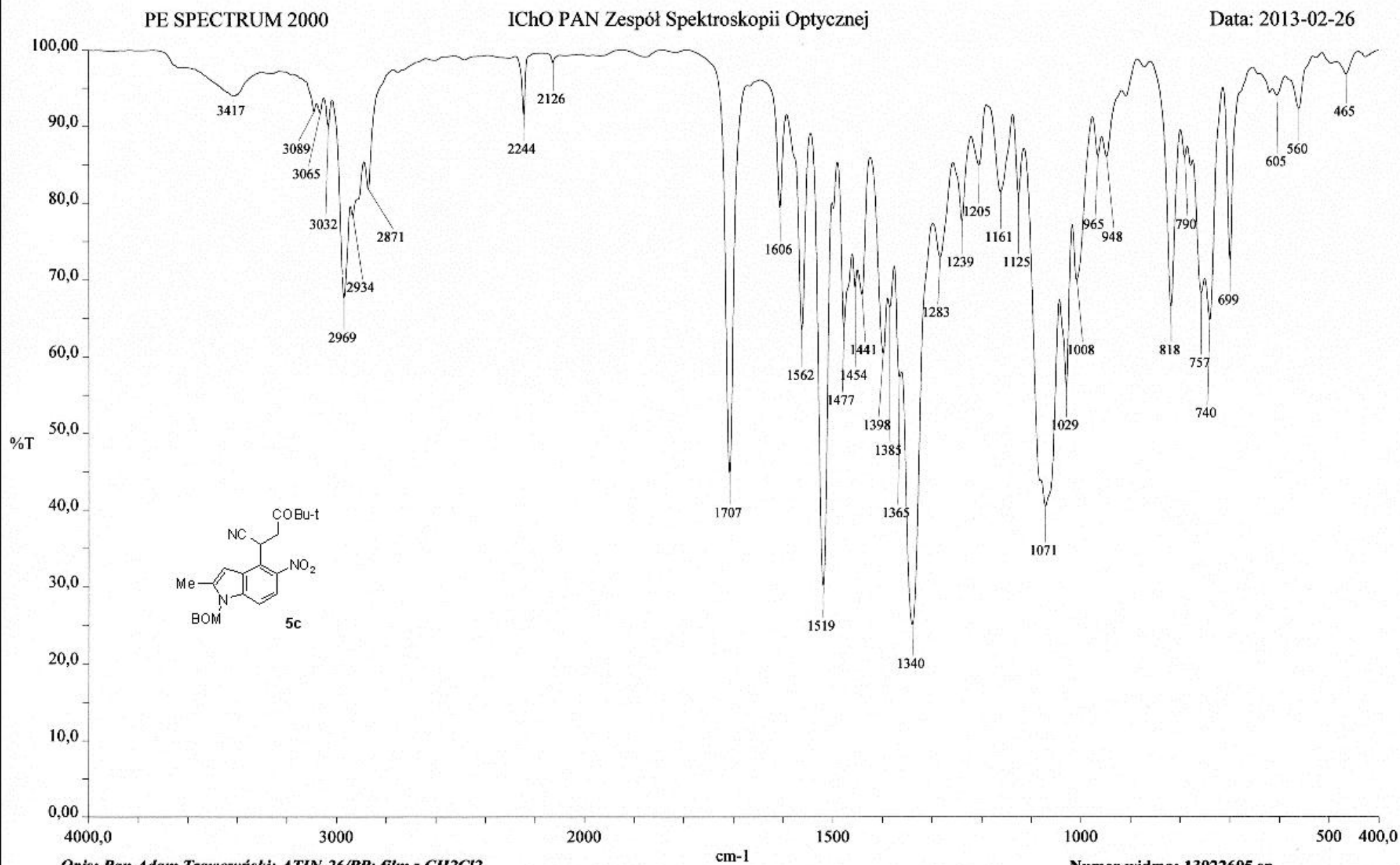
file: ... \NMR\PIROLOINDOLE\ATIN-26-PP\1\fid expt: <zg>
 transmitter freq.: 500.133089 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.130025 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 173.339 ppm/cm: 0.34659



file: ...\\NMR\\PIROLOINDOLE\\ATIN-26-PP\\2\\fid expt: <zgpg>
 transmitter freq.: 125.770364 MHz
 time domain size: 65536 points
 width: 32679.74 Hz = 259.8366 ppm = 0.498653 Hz/pt
 number of scans: 1271

freq. of 0 ppm: 125.757794 MHz
 processed size: 262144 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 1101.020 ppm/cm: 8.75421



Opis: Pan Adam Trawczyński; ATIN-26/PP; film z CH₂Cl₂

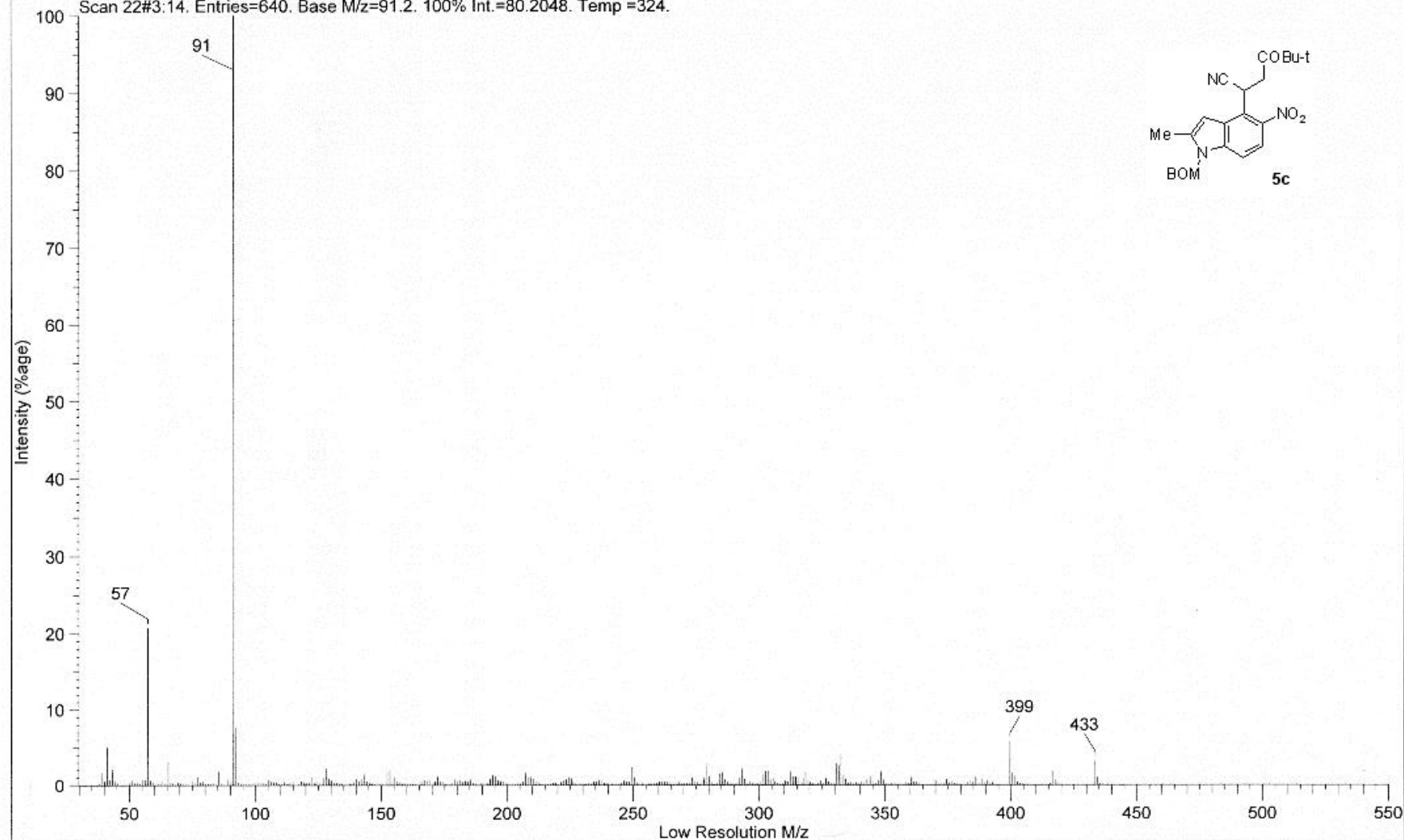
Uwagi:

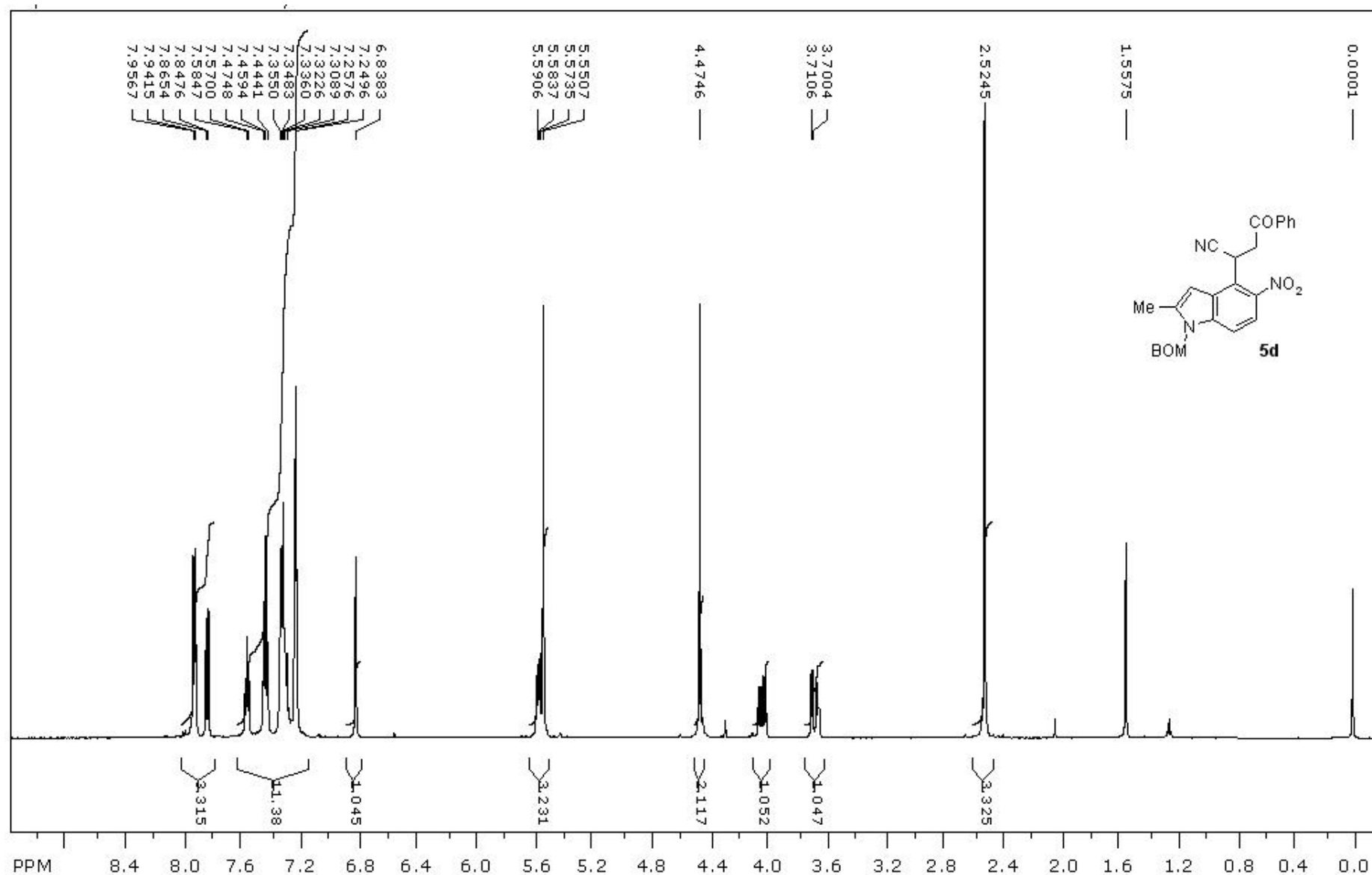
Numer widma: 13022605.sp

Operator: Alicja Dziedzic

File Name : E:\ChO\Z07_EG\at2505.ms2
Creation Date/Time : 11-09-09 at 14:36:54
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-26 (EI 70 eV 33-800)
Operator : Małgorzata Grela
Instrument : AMD 604
Notes : A. Trawczyński

SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 22#3:14. Entries=640. Base M/z=91.2. 100% Int.=80.2048. Temp =324.





file: ...OINDOLE\ATIN-67\ATIN-67-H1.fid\fid block#1 expt: "s2pul"
 transmitter freq.: 499.834317 MHz
 time domain size: 121528 points
 width: 12135.92 Hz = 24.2799 ppm = 0.099861 Hz/pt
 number of scans: 16

freq. of 0 ppm: 499.831294 MHz
 processed size: 262144 complex points
 LB: 1.500 GF: 0.0000
 Hz/cm: 187.512 ppm/cm: 0.37515

A. Trawczynski
zesp7/Var500/ATIN_23/ATIN_23-C13

Sample Name:
ATIN_23
Data Collected on:
Varian-NMR-vnmrs500
Archive directory:

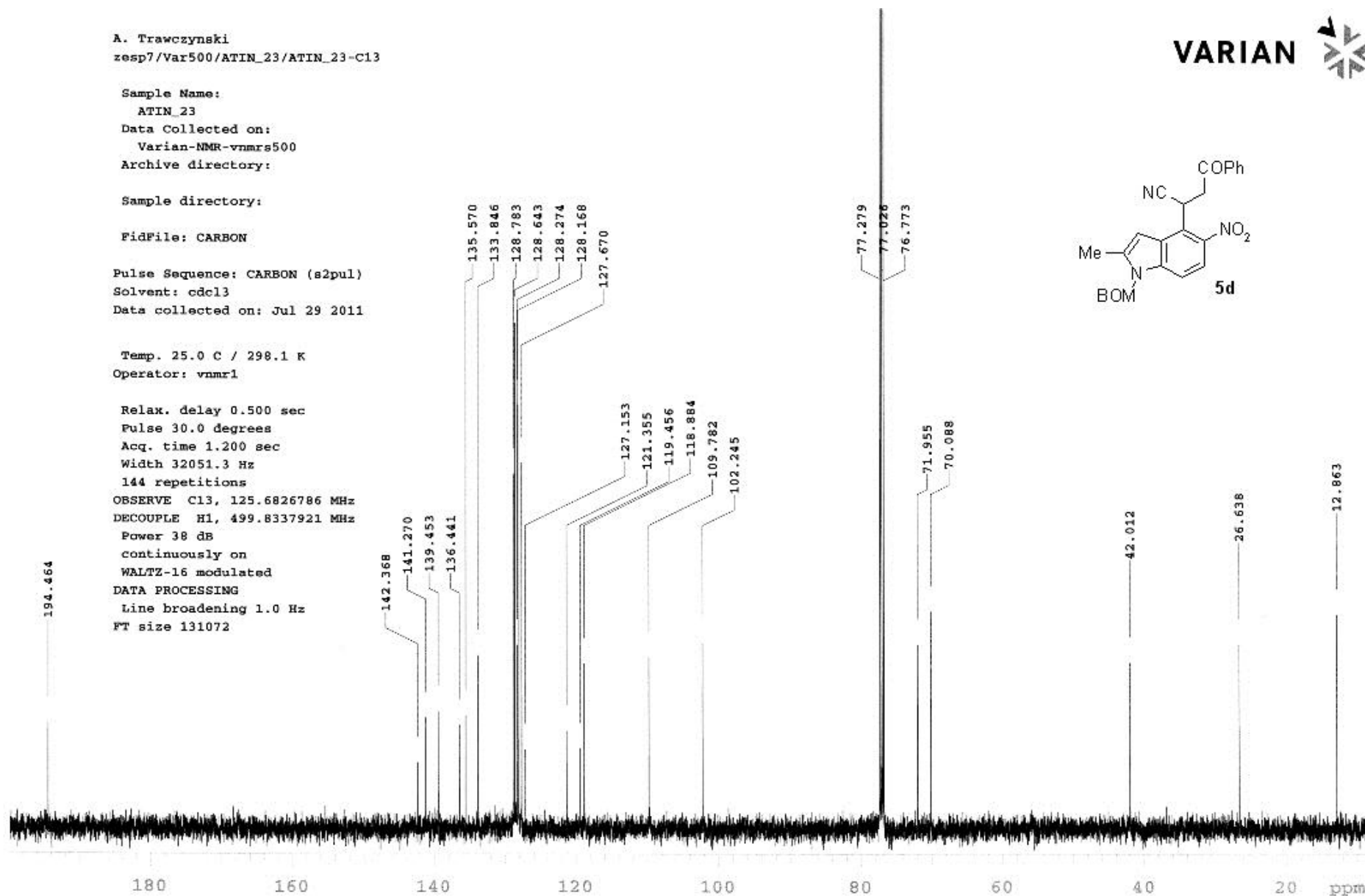
Sample directory:

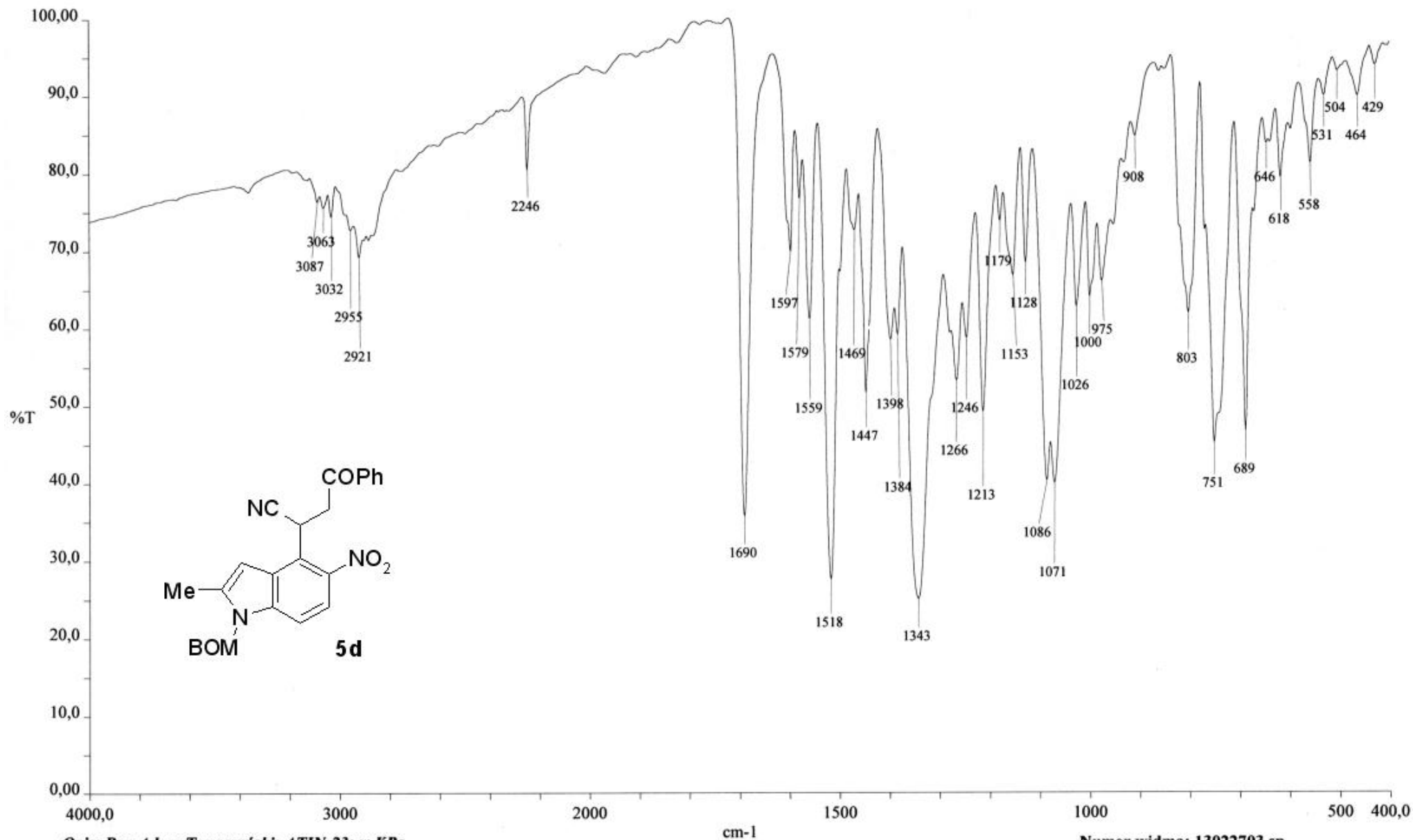
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 29 2011

Temp. 25.0 C / 298.1 K
Operator: vnmr1

Relax. delay 0.500 sec
Pulse 30.0 degrees
Acq. time 1.200 sec
Width 32051.3 Hz
144 repetitions
OBSERVE C13, 125.6826786 MHz
DECOUPLE H1, 499.8337921 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072





Opis: Pan Adam Trawczyński; ATIN-23; w KBr

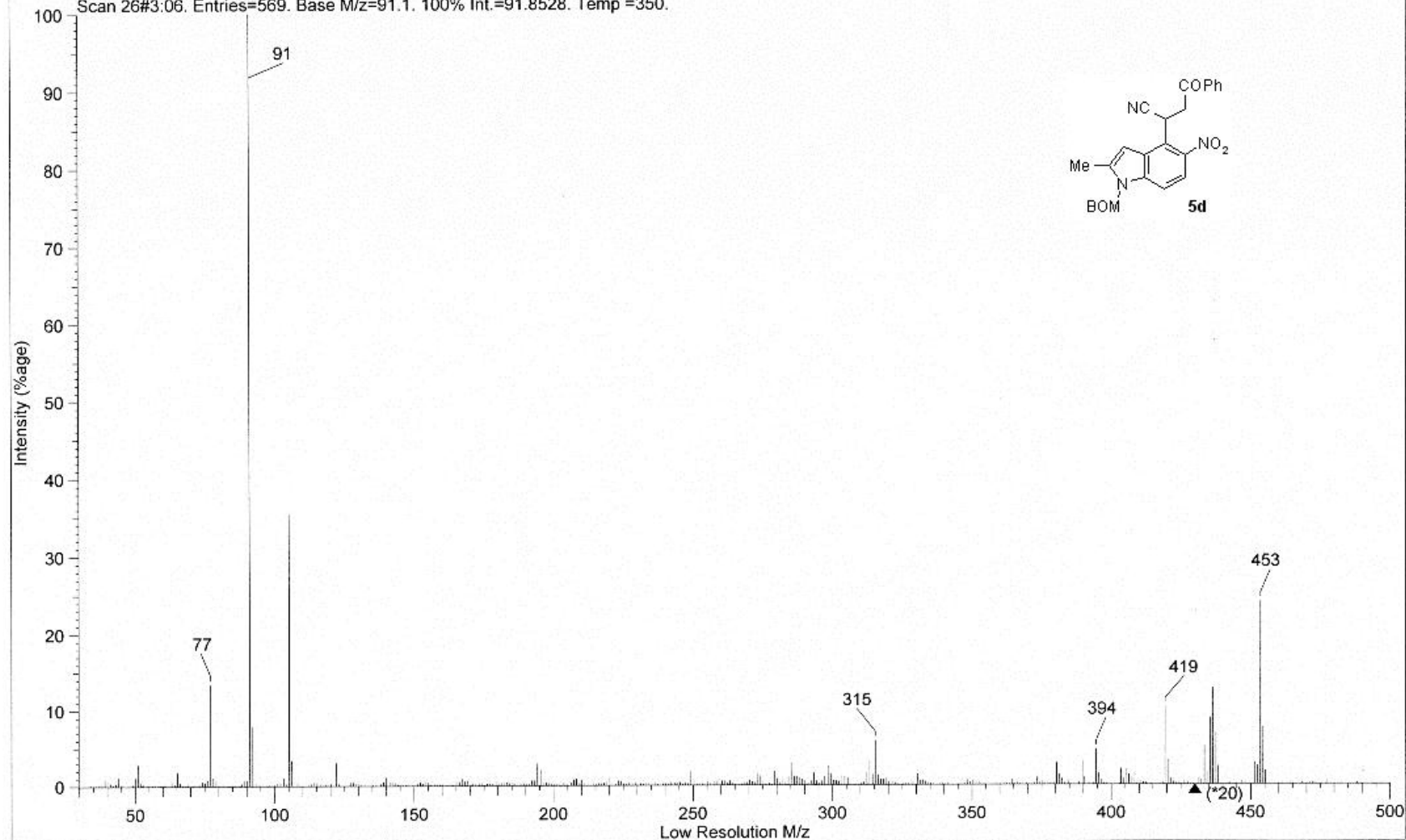
Uwagi:

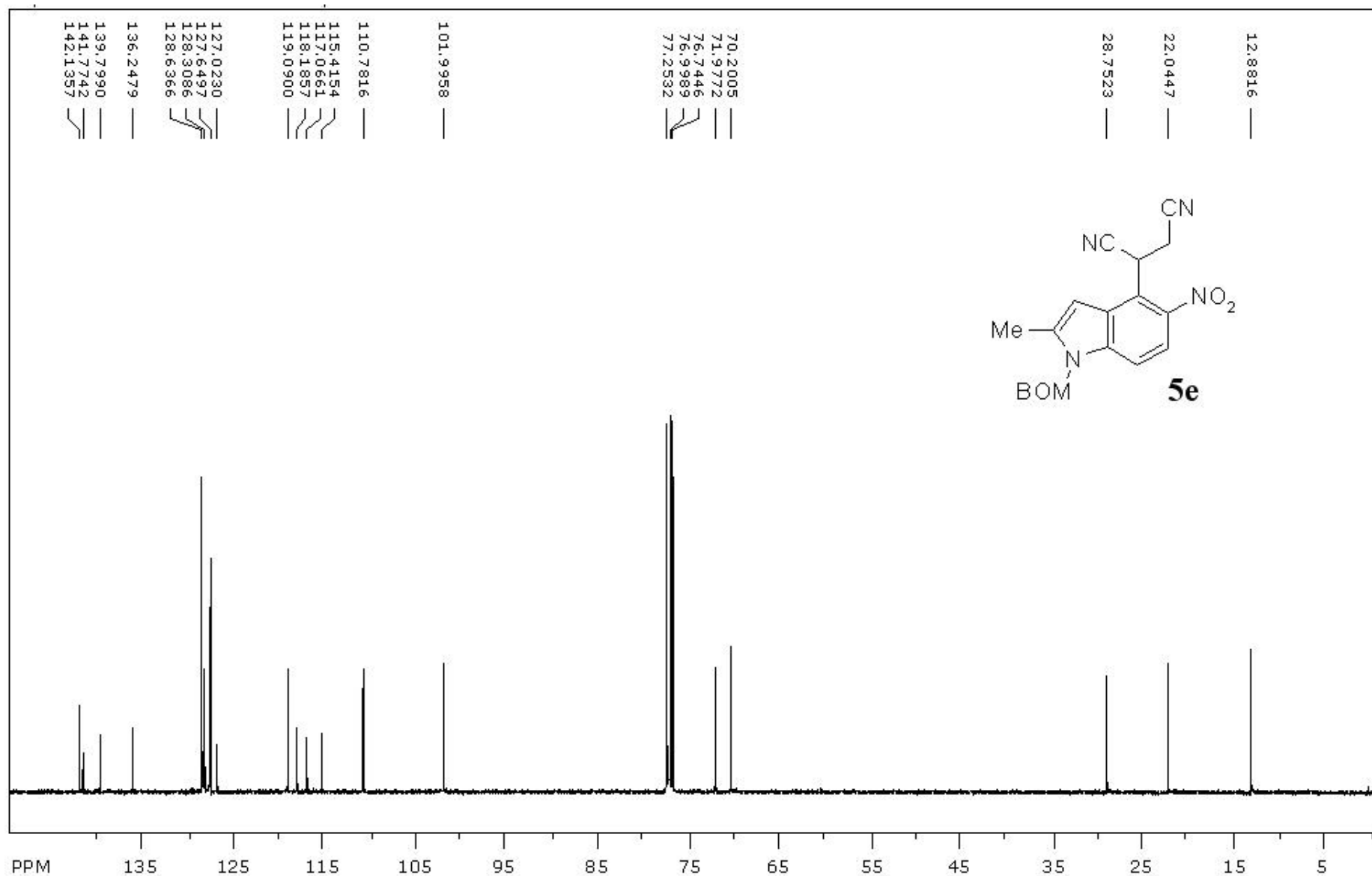
Numer widma: 13022703.sp

Operator: Alicja Dziedzic

File Name : E:\ChO\Z07_EG\at2209.ms2
Creation Date/Time : 11-08-01 at 16:50:08
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPec II system [I132/99D9]
File Title : ATIN-23 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

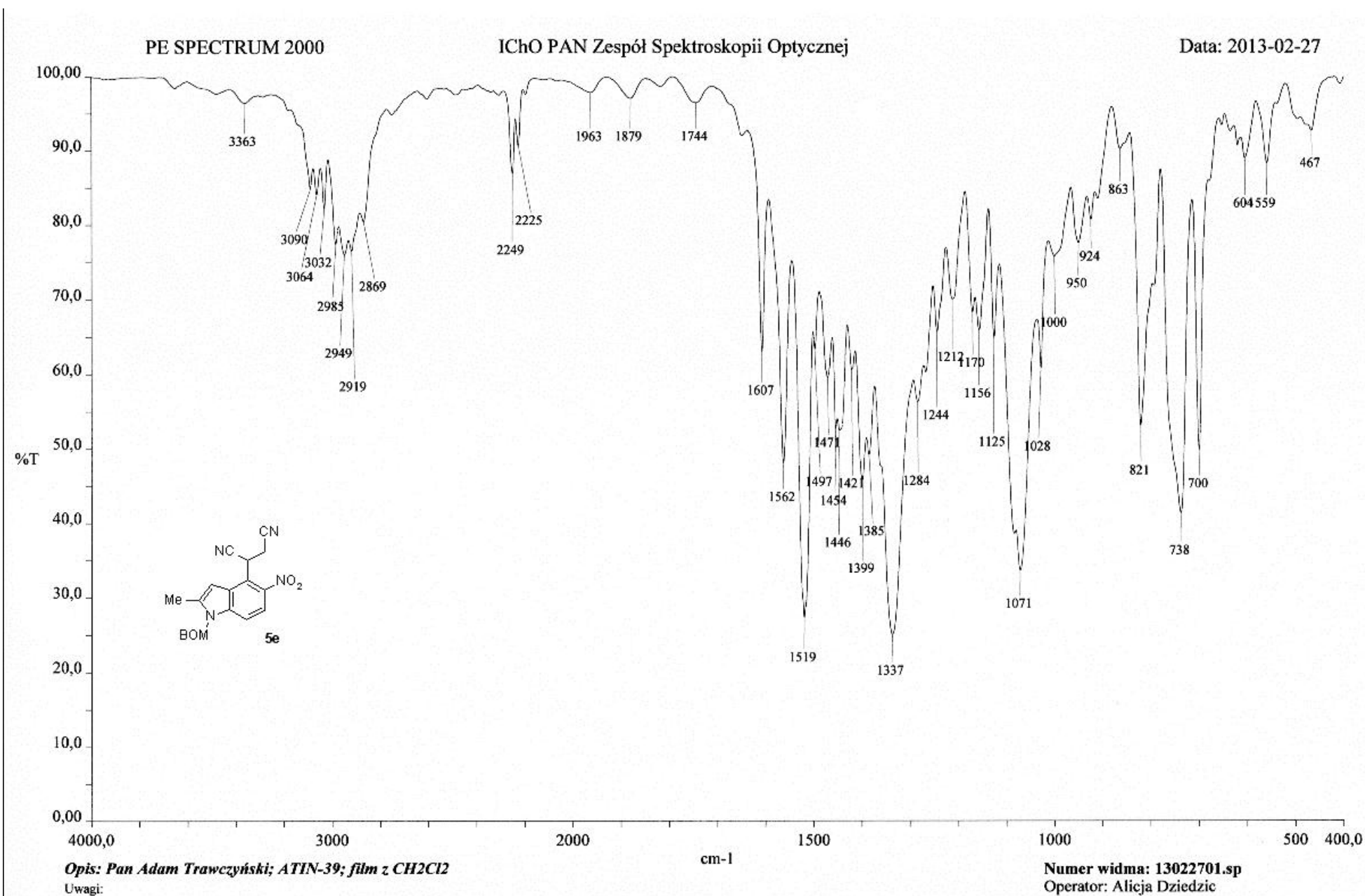
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 26#3:06. Entries=569. Base M/z=91.1. 100% Int.=91.8528. Temp =350.





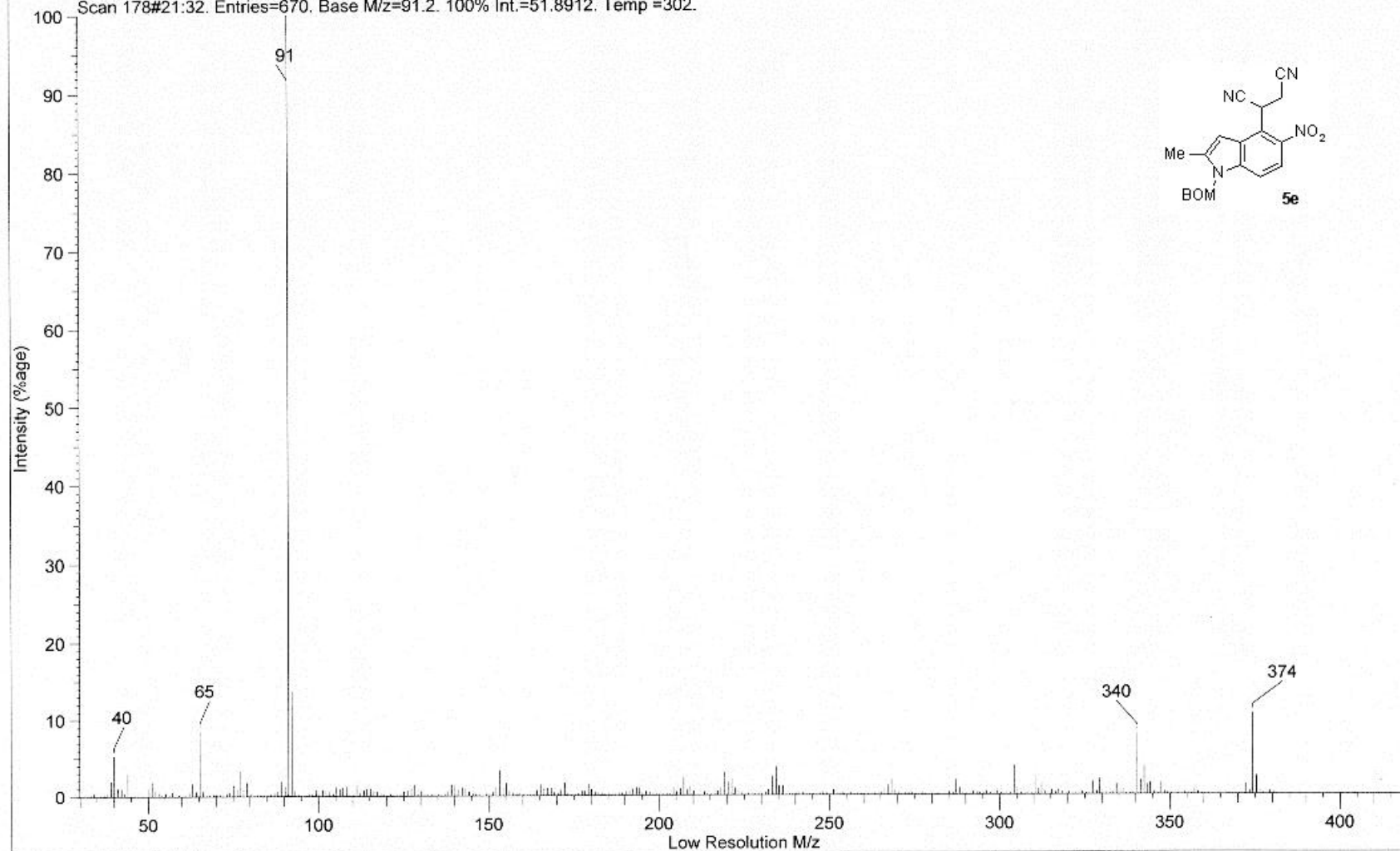
file: ...INDOLE\ATIN-39\ATIN-39-C13.fid\fid block # 1 expt: "s2pul"
 transmitter freq.: 125.696504 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9894 ppm = 0.400001 Hz/pt
 number of scans: 1344

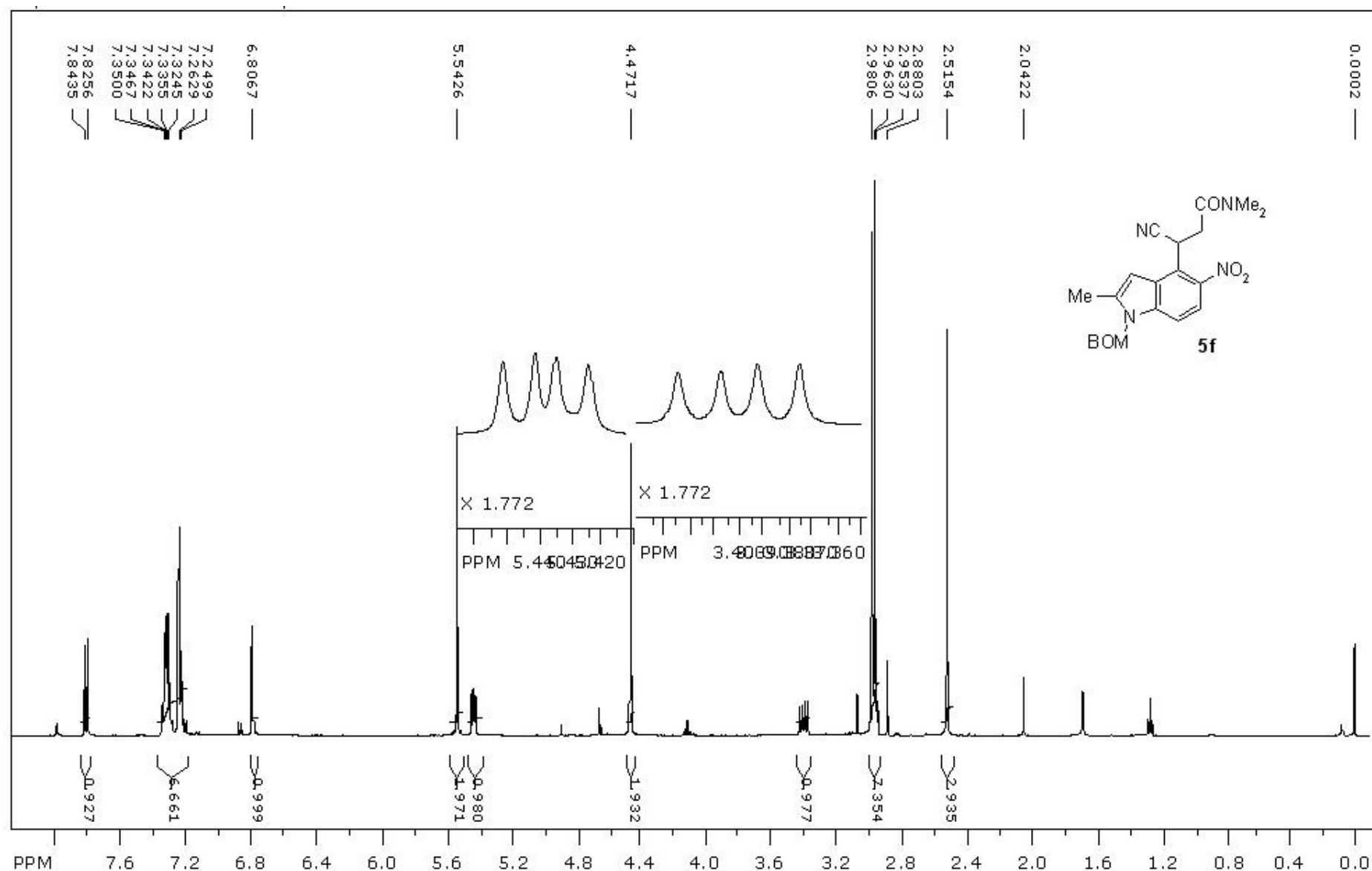
freq. of 0 ppm: 125.682684 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 759.865 ppm/cm: 6.04524



File Name : E:\ChO\Z07_EG\at2986.ms2
Creation Date/Time : 11-10-10 at 13:10:43
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-39 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

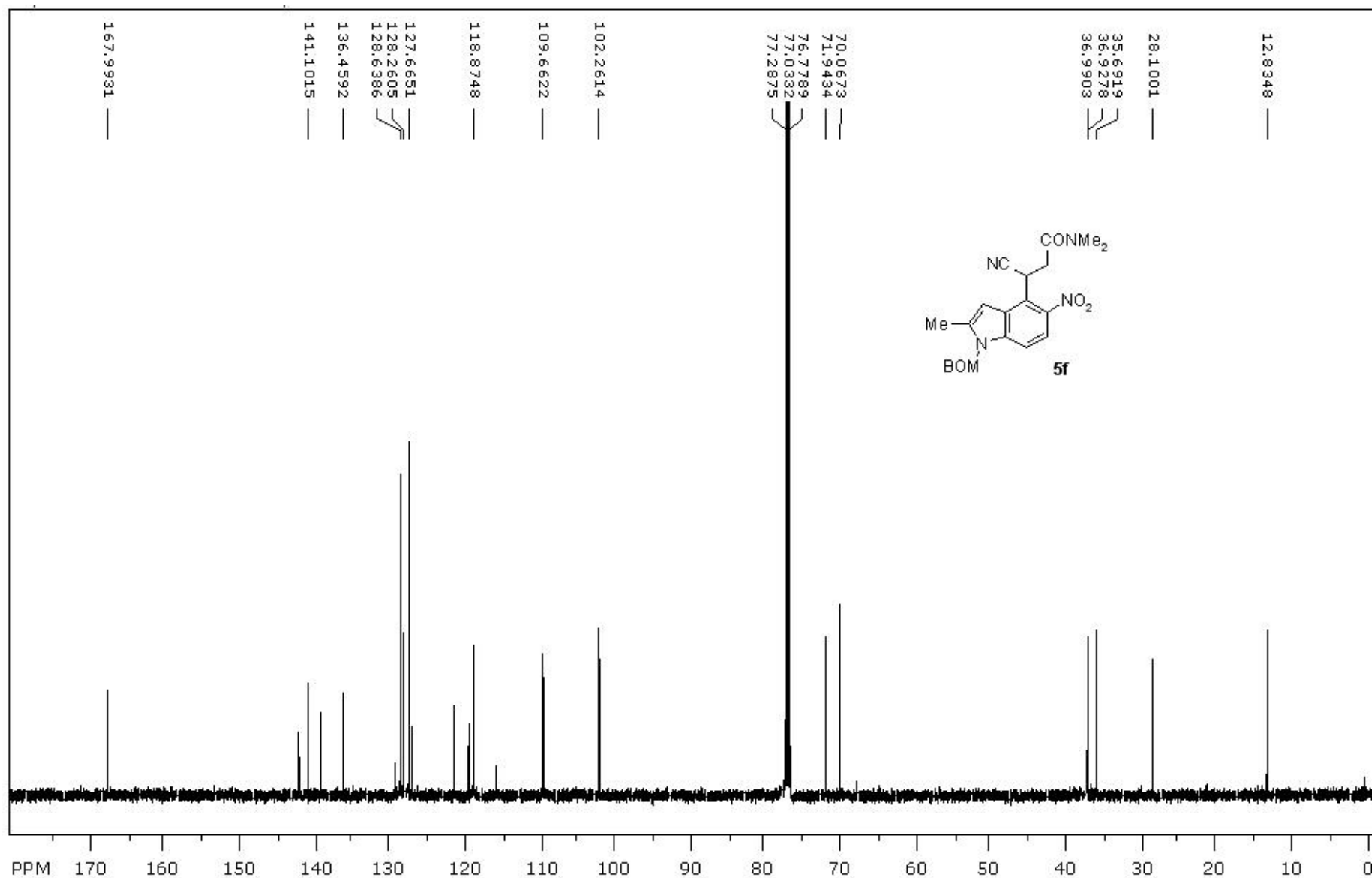
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 178#21:32. Entries=670. Base M/z=91.2. 100% Int.=51.8912. Temp =302.





file: ...OINDOLE\ATIN-55\ATIN-55-H1.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 499.834042 MHz
 time domain size: 131072 points
 width: 10504.20 Hz = 21.0154 ppm = 0.080141 Hz/pt
 number of scans: 28

freq. of 0 ppm: 499.831291 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 168.114 ppm/cm: 0.33634



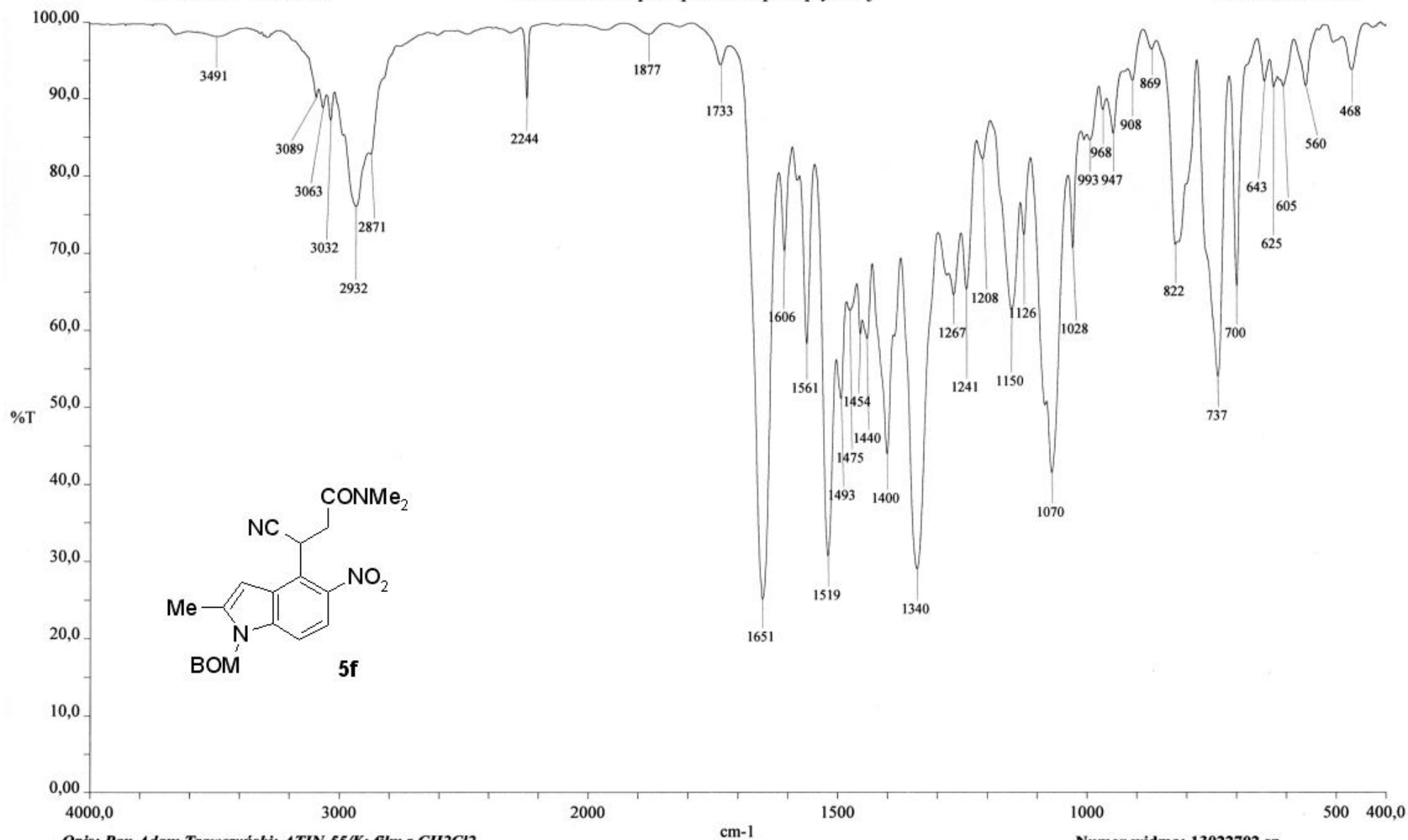
file: ...INDOLE\ATIN-55\ATIN-55-C13.fid\fid block # 1 expt: "s2pul"
 transmitter freq.: 125.696504 MHz
 time domain size: 90910 points
 width: 37878.79 Hz = 301.3512 ppm = 0.416663 Hz/pt
 number of scans: 368

freq. of 0 ppm: 125.682679 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 921.501 ppm/cm: 7.33116

PE SPECTRUM 2000

IChO PAN Zespół Spektroskopii Optycznej

Data: 2013-02-27

Opis: Pan Adam Trawczyński; ATIN-55/K; film z CH₂Cl₂

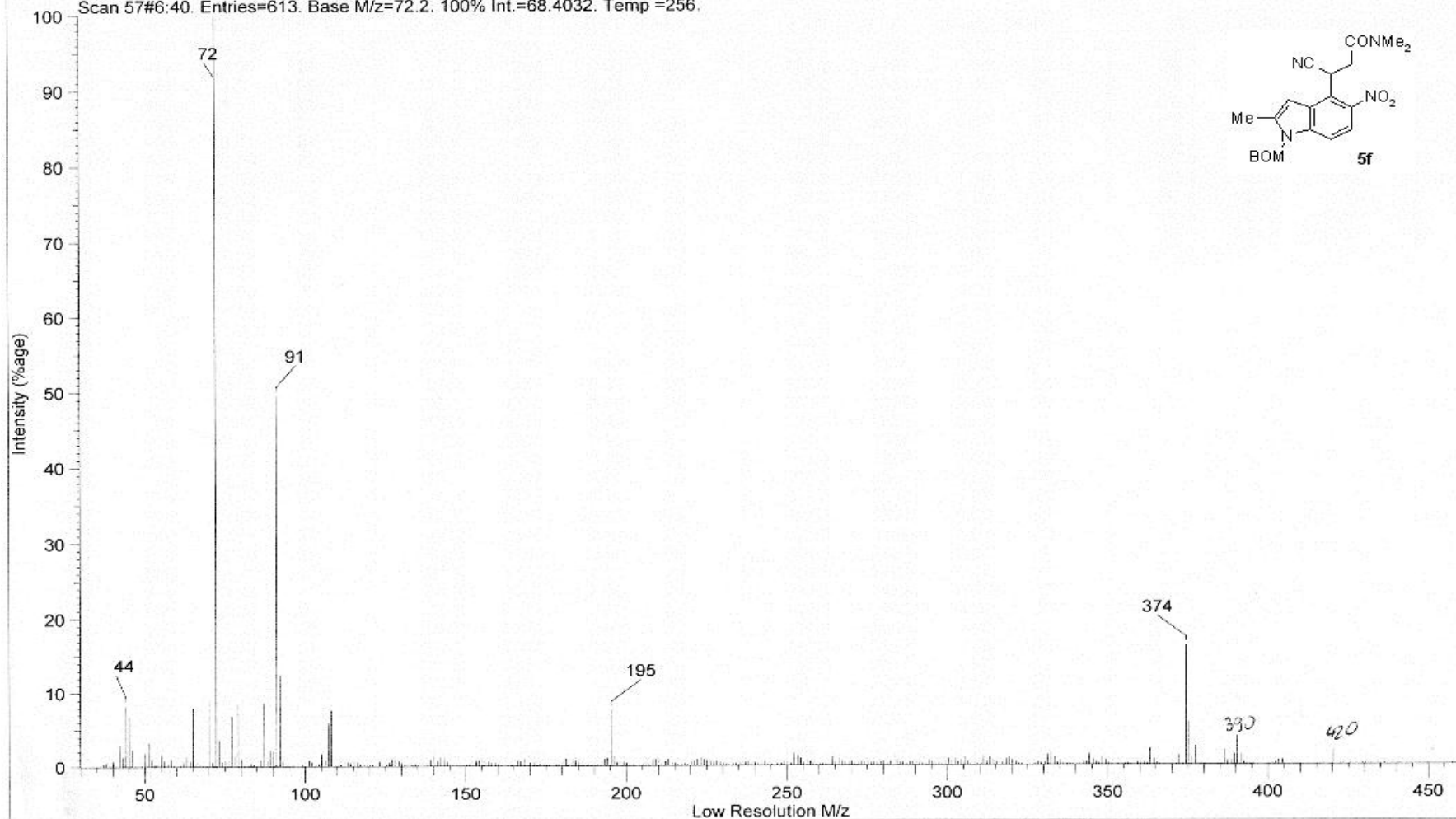
Uwagi:

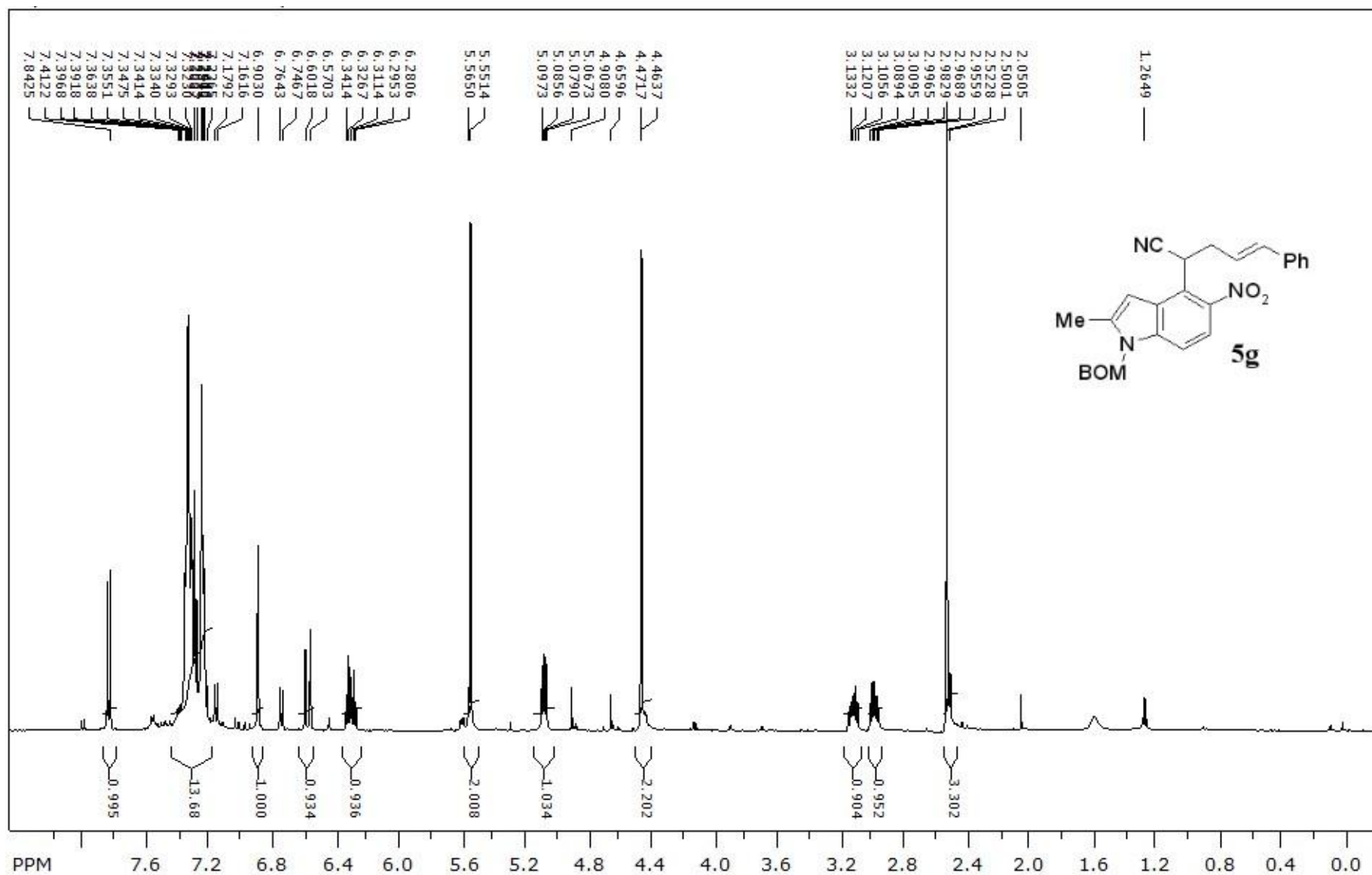
Numer widma: 13022702.sp

Operator: Alicja Dziedzic

File Name : E:\ChO\Z07_EG\at3540.ms2
 Creation Date/Time : 11-12-07 at 10:13:45
 File Type : Lo-Res Data - Ctd (Magnet)
 File Source : Acquired on MASPEC II system [II32/99D9]
 File Title : ATIN-55 (EI 70 eV 33-800)
 Operator : Marian Olejnik
 Instrument : AMD 604
 Notes : A. Trawczyński

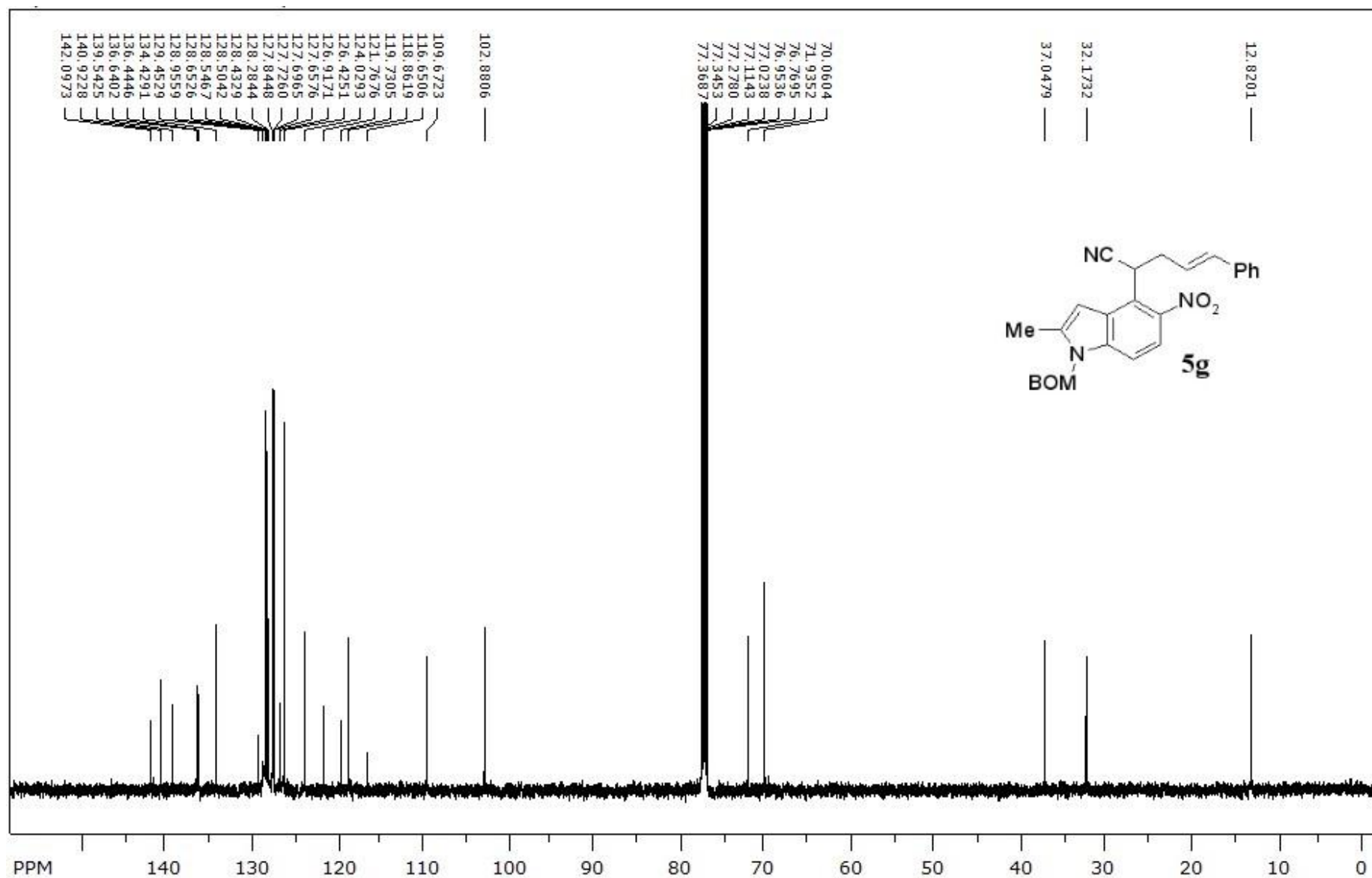
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
 Scan 57#6:40. Entries=613. Base M/z=72.2. 100% Int.=68.4032. Temp =256.





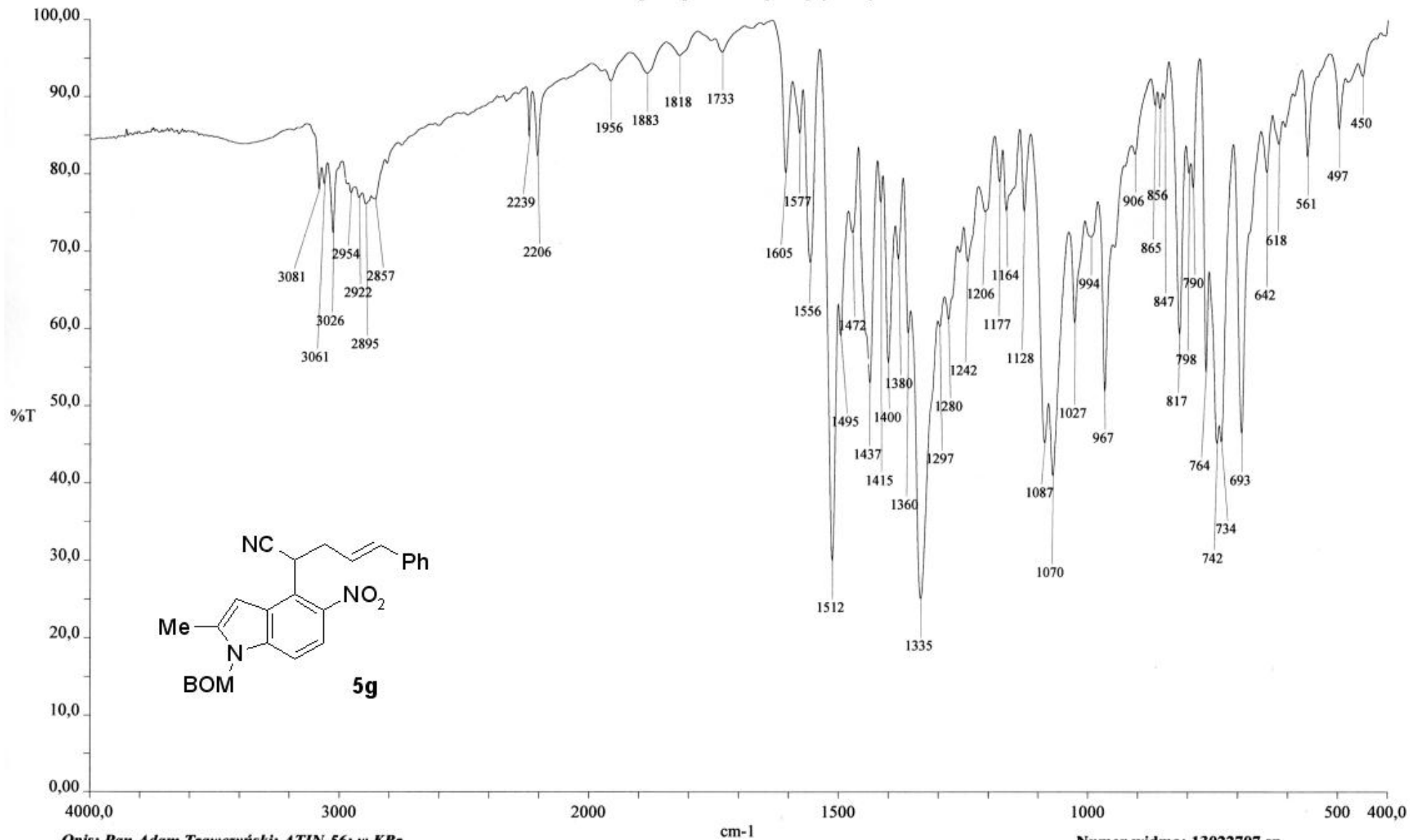
file: ...OINDOLE\ATIN-56\ATIN-56-H1.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 499.834042 MHz
 time domain size: 131072 points
 width: 10504.20 Hz = 21.0154 ppm = 0.080141 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.831293 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 173.462 ppm/cm: 0.34704



file: ...INDOLE\ATIN-56\ATIN-56-C13.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 125.696504 MHz
 time domain size: 90910 points
 width: 37878.79 Hz = 301.3512 ppm = 0.416663 Hz/pt
 number of scans: 448

freq. of 0 ppm: 125.682679 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 808.304 ppm/cm: 6.43060



Opis: Pan Adam Trawczyński; ATIN-56; w KBr

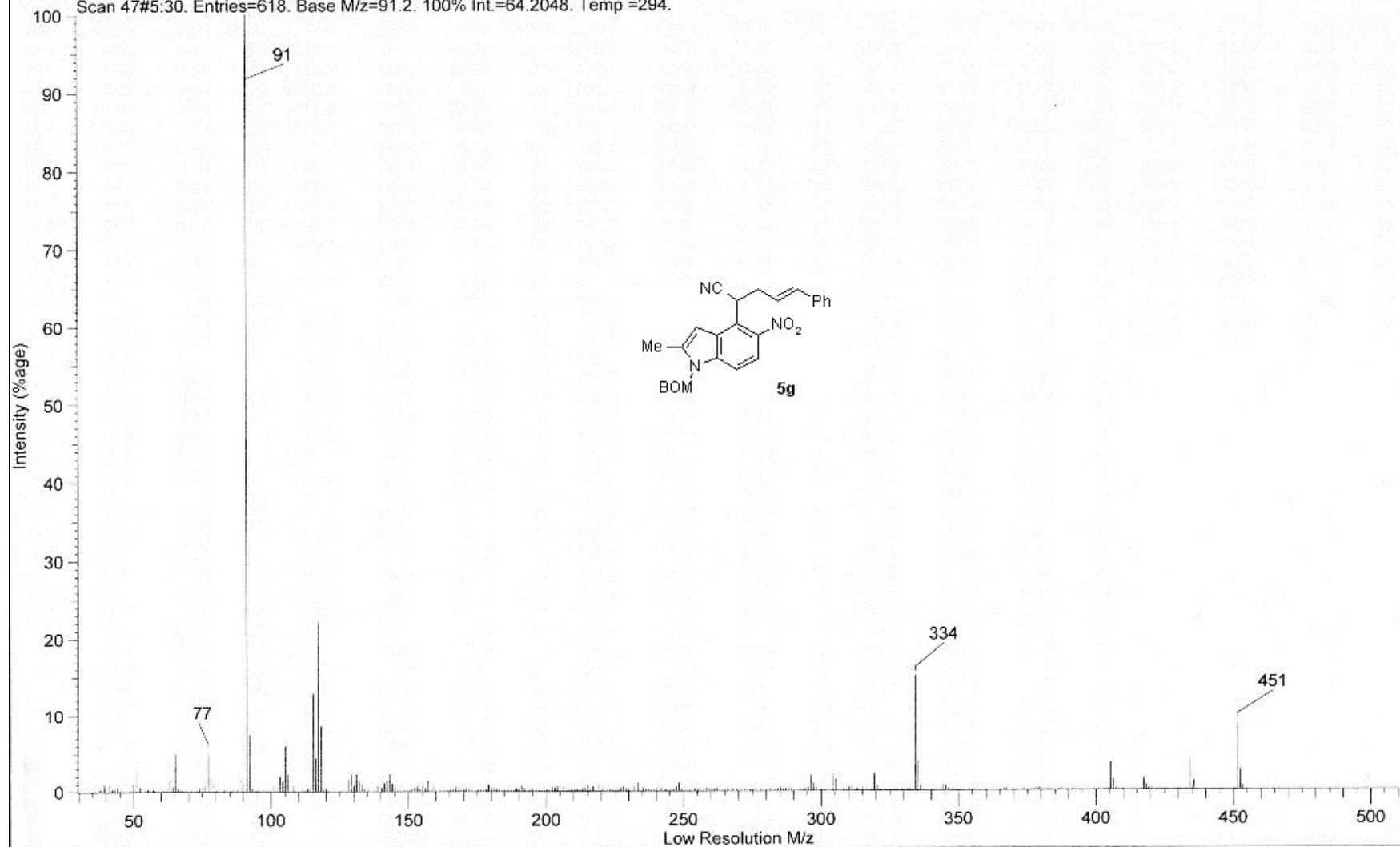
Uwagi:

Numer widma: 13022707.sp
Operator: Alicja Dzedzic

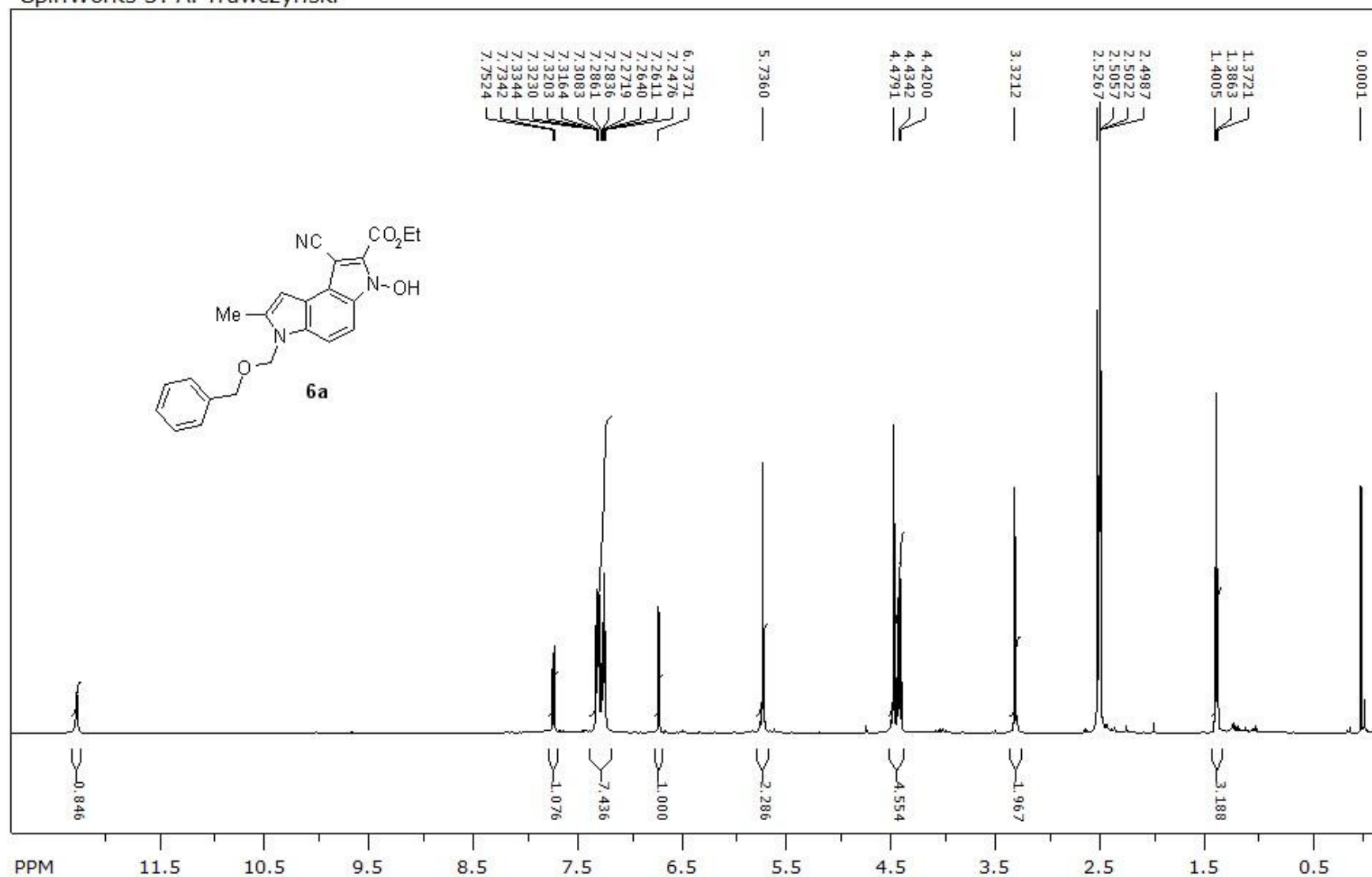
File Name : E:\ChO\Z07_EG\at3622.ms2
Creation Date/Time : 11-12-07 at 12:35:27
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-56 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.

Scan 47#5:30. Entries=618. Base M/z=91.2. 100% Int.=64.2048. Temp.=294.

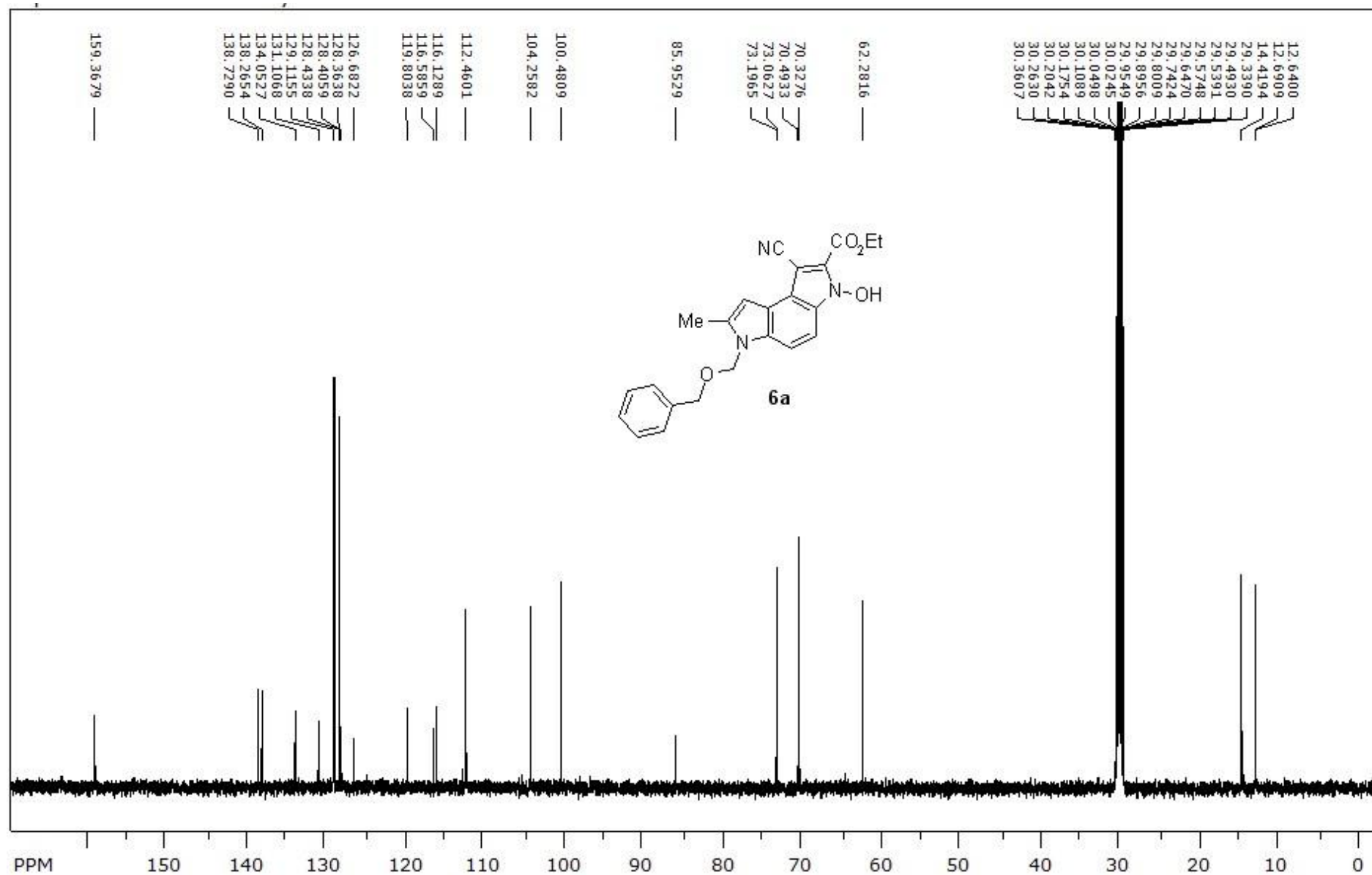


SpinWorks 3: A. Trawczynski



file: ...NDOLE\ATIN-8-3\ATIN-8-3-H1.fid\fid_block# 1 expt: "s2pul"
 transmitter freq.: 499.836166 MHz
 time domain size: 131072 points
 width: 10245.90 Hz = 20.4985 ppm = 0.078170 Hz/pt
 number of scans: 36

freq. of 0 ppm: 499.833658 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 262.413 ppm/cm: 0.52500



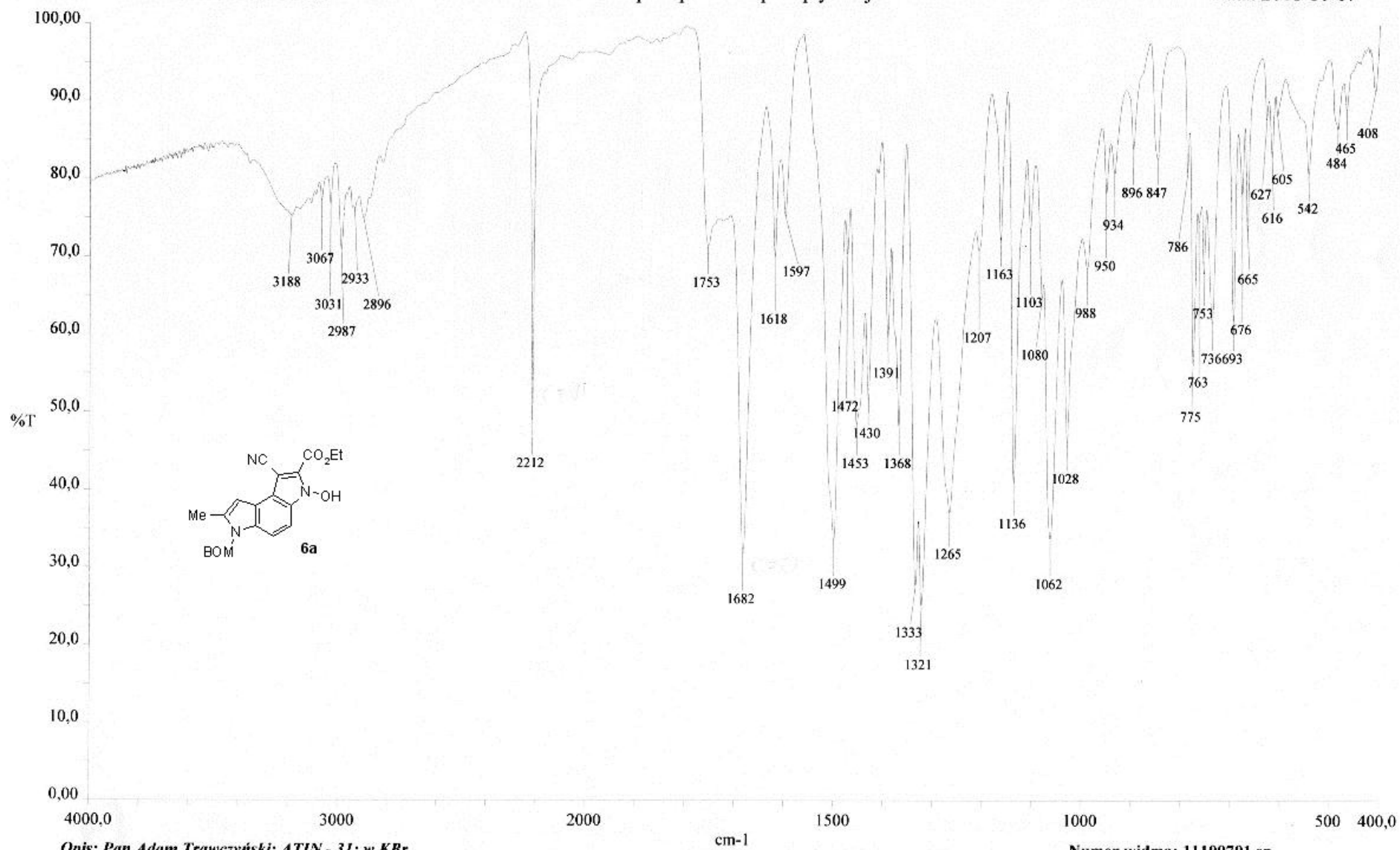
file: ...INDOLE\ATIN-31\ATIN-31-C13.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 125.697156 MHz
 time domain size: 90910 points
 width: 37878.79 Hz = 301.3496 ppm = 0.416663 Hz/pt
 number of scans: 400

freq. of 0 ppm: 125.683223 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 866.999 ppm/cm: 6.89752

PE SPECTRUM 2000

IChO PAN Zespół Spektroskopii Optycznej

Data: 2011-10-07



Opis: Pan Adam Trawczyński; ATIN - 31; w KBr

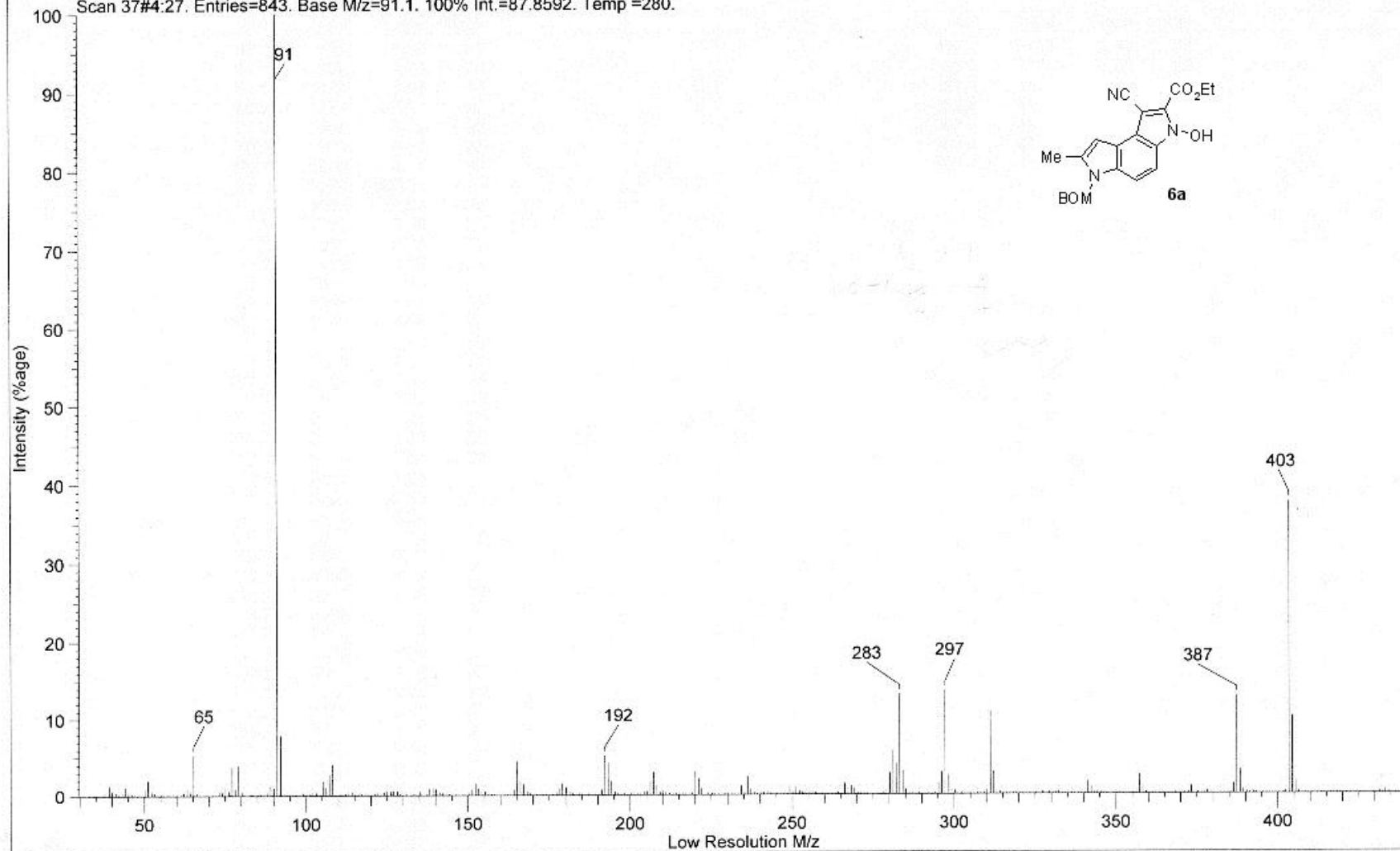
Uwagi:

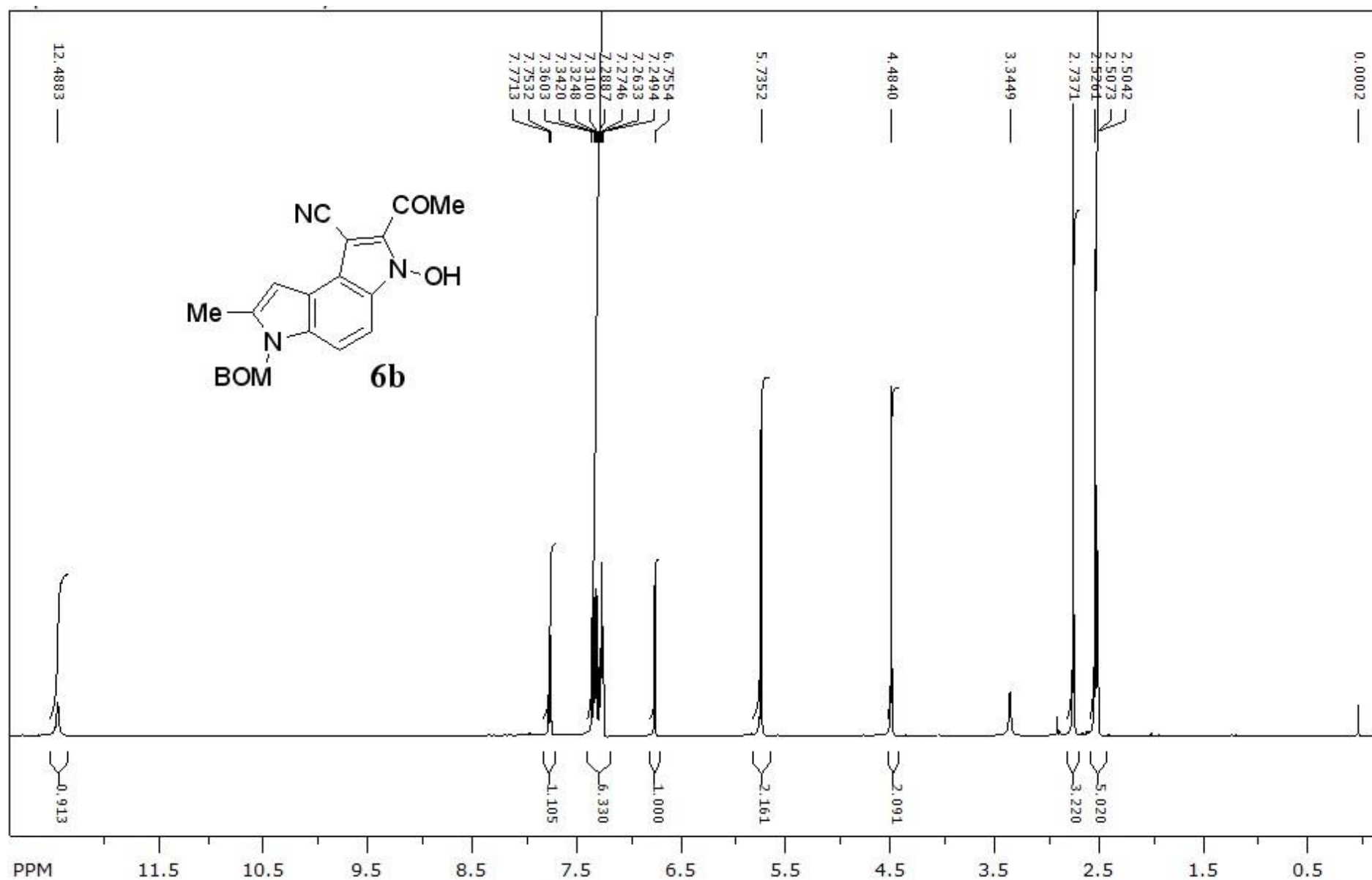
Numer widma: 11100701.sp

Operator: Alicja Dziedzic

File Name : E:\ChOI\Z07_EG\at1155.ms2
Creation Date/Time : 11-04-18 at 10:25:23
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-8-3 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

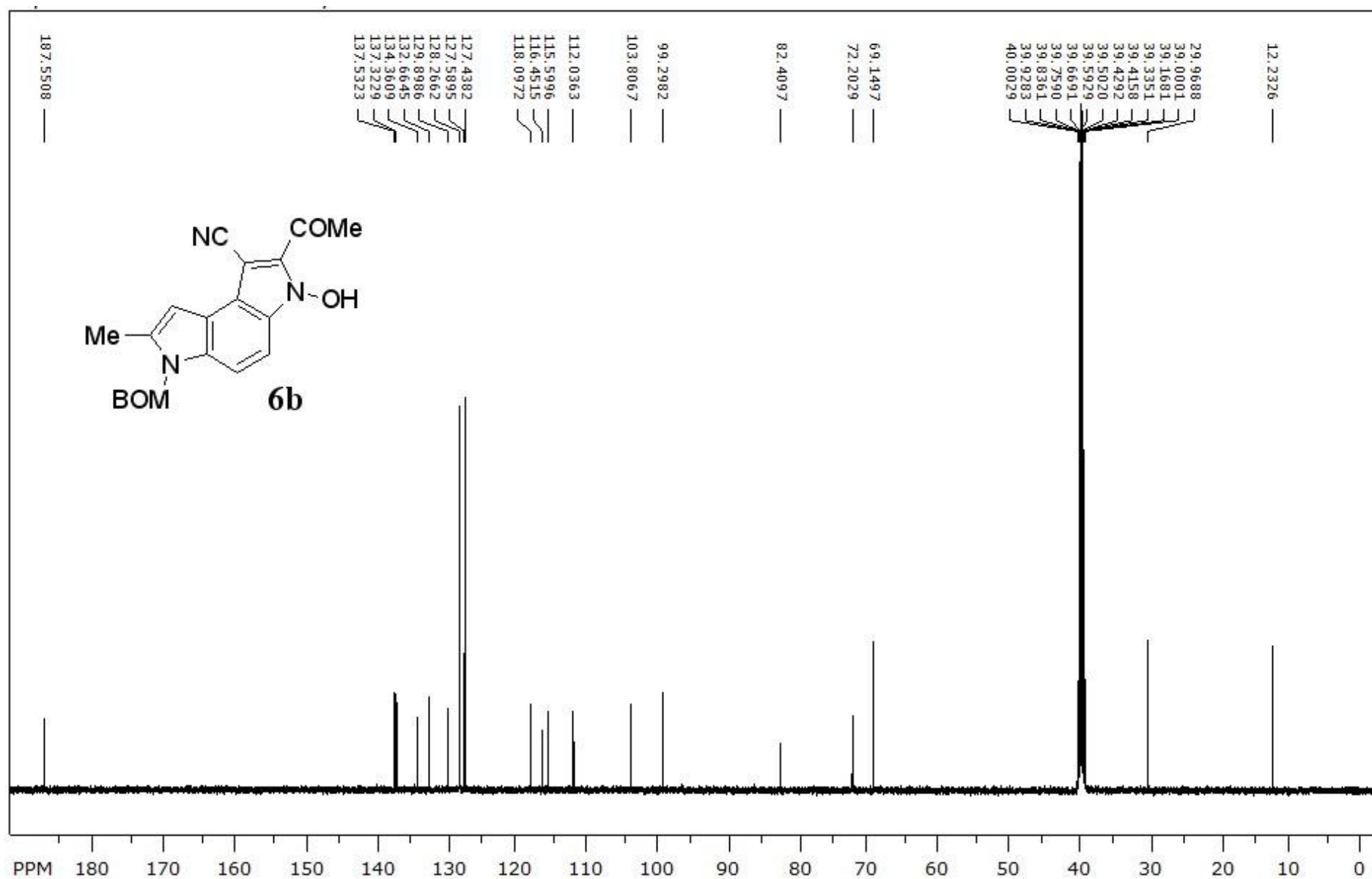
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 37#4:27. Entries=843. Base M/z=91.1. 100% Int.=87.8592. Temp =280.





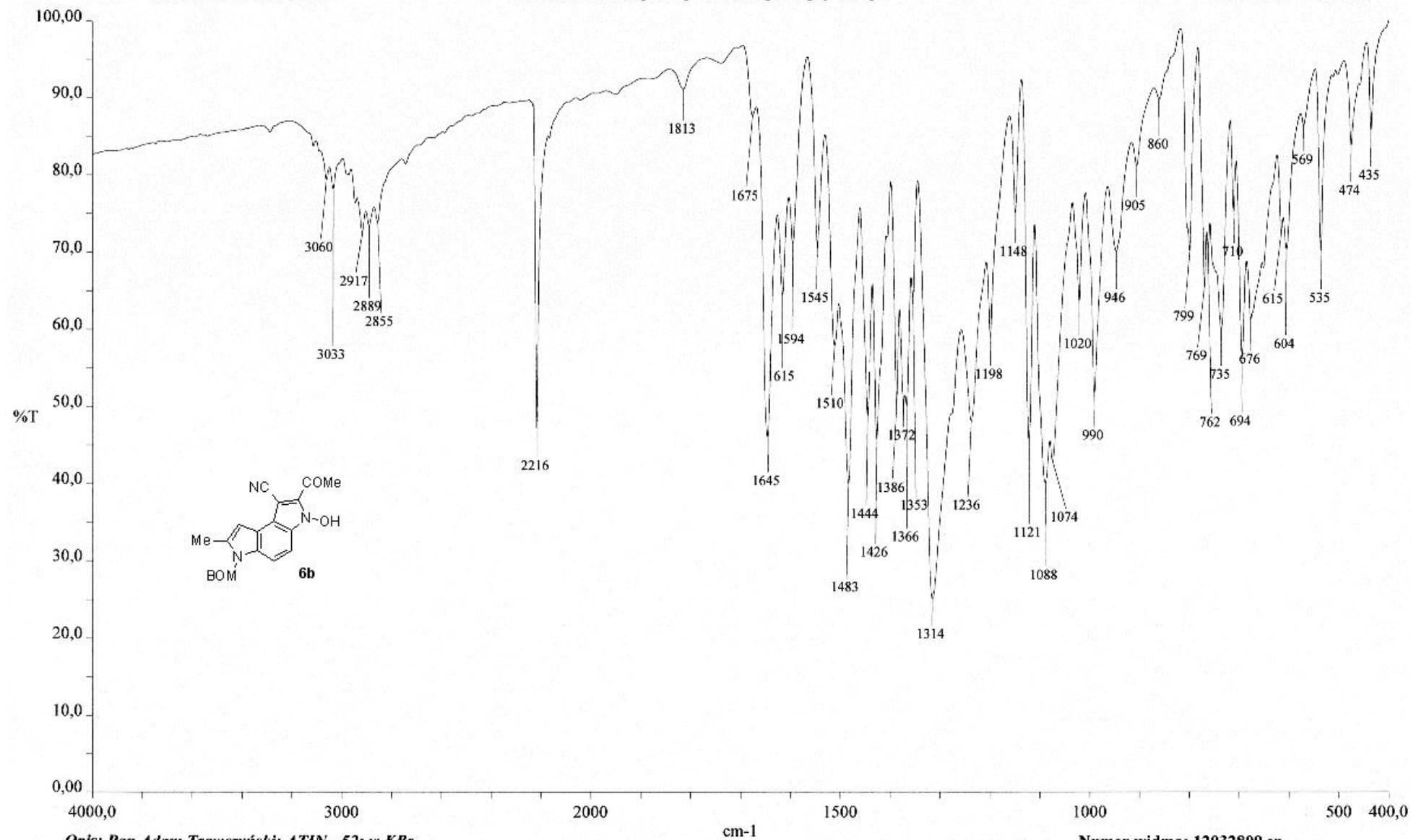
file: ...OINDOLE\ATIN-52\ATIN-52-H1.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 499.836466 MHz
 time domain size: 127118 points
 width: 10593.22 Hz = 21.1934 ppm = 0.083334 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.833657 MHz
 processed size: 131072 complex points
 LB: 1.061 GF: 0.0000
 Hz/cm: 262.867 ppm/cm: 0.52591



file: ...INDOLE\ATIN-52\ATIN-52-C13.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 125.697101 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9882 ppm = 0.400001 Hz/pt
 number of scans: 528

freq. of 0 ppm: 125.683336 MHz
 processed size: 131072 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 980.787 ppm/cm: 7.80278



Opis: Pan Adam Trawczyński; ATIN - 52; w KBr

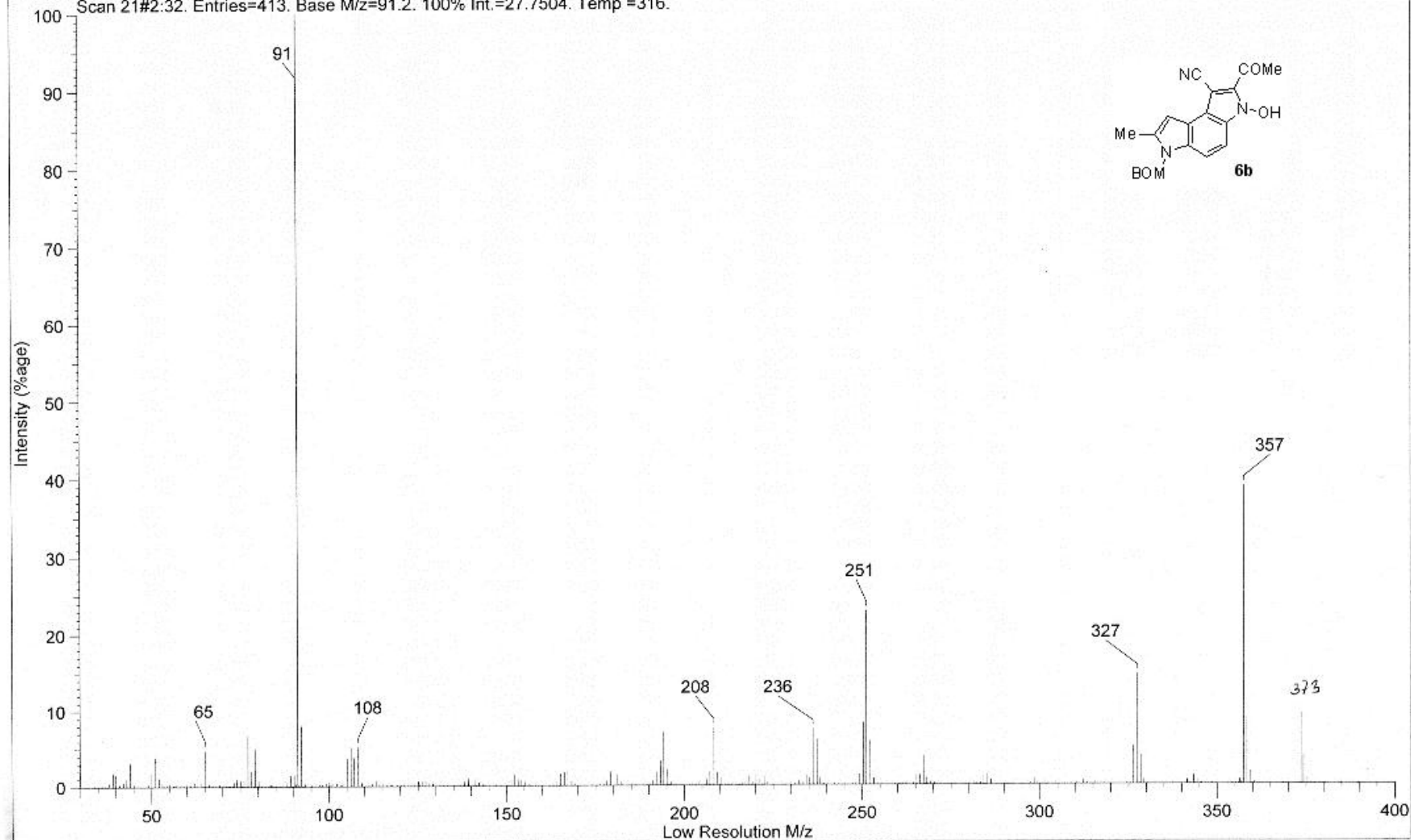
Uwagi:

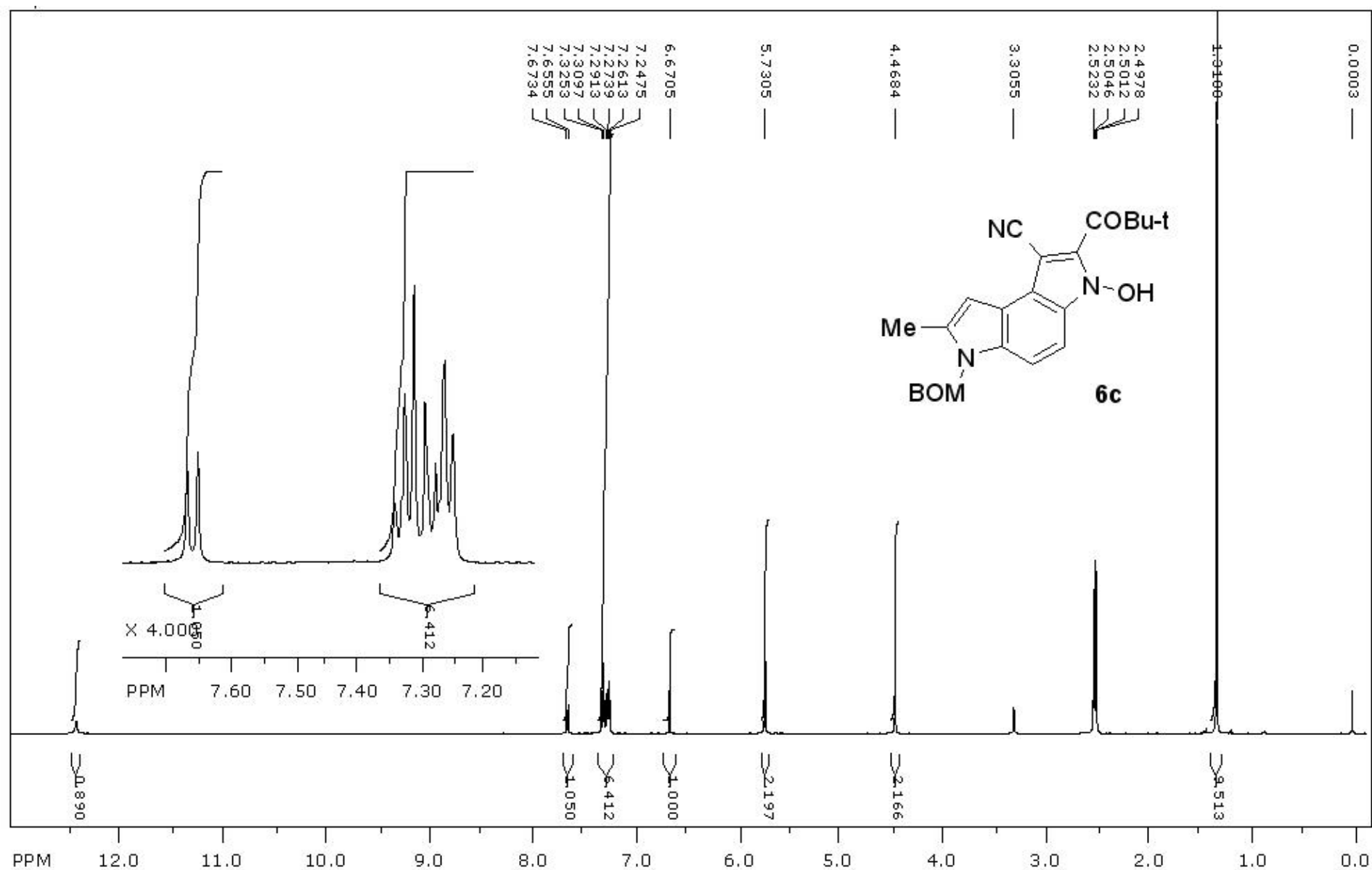
Numer widma: 12032809.sp

Operator: Alicja Dziezic

File Name : E:\ChO\Z07_EG\at3475.ms2
Creation Date/Time : 11-11-28 at 12:54:06
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [1132/99D9]
File Title : ATIN-52 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

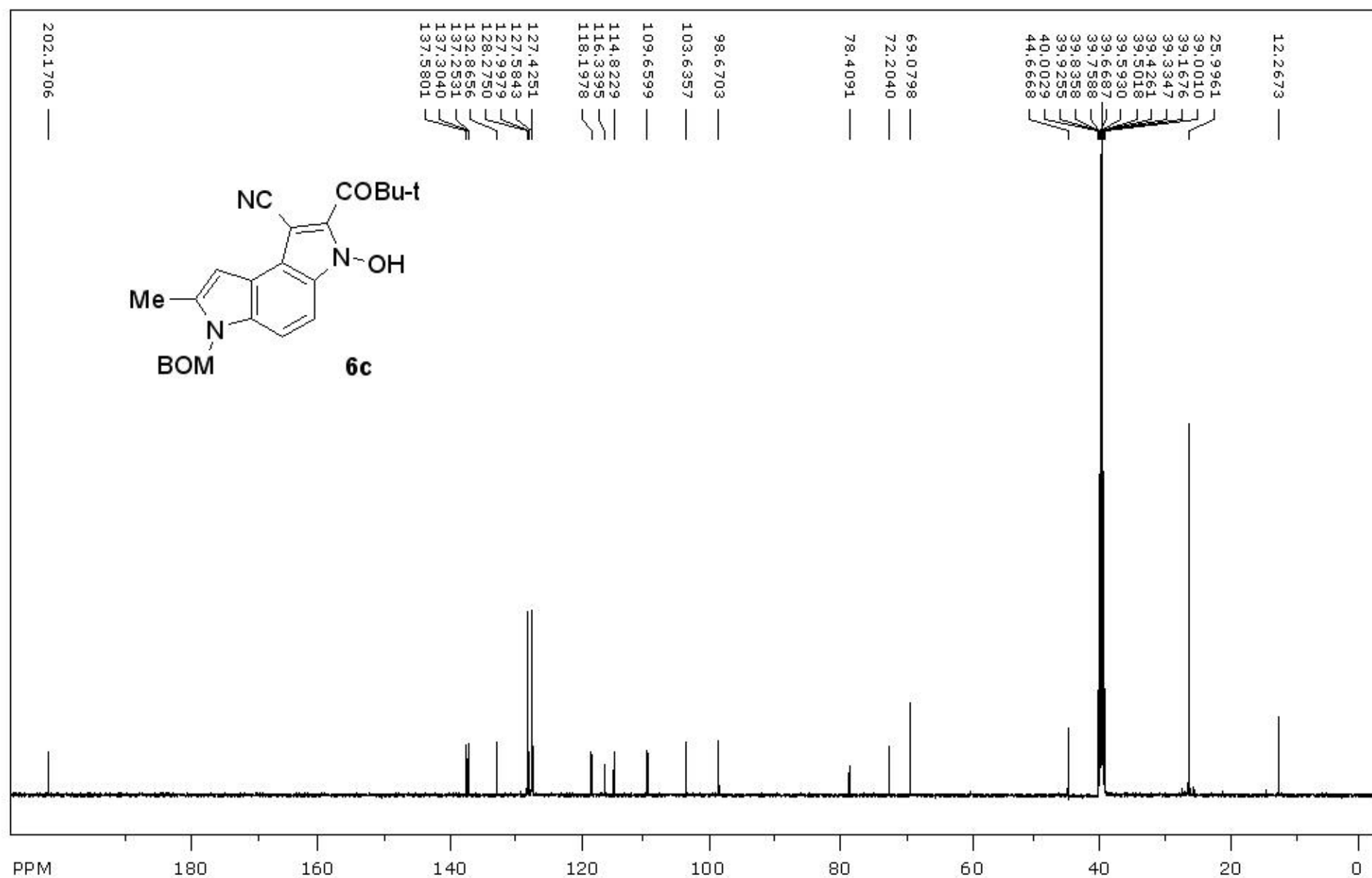
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 21#2:32. Entries=413. Base M/z=91.2. 100% Int.=27.7504. Temp =316.





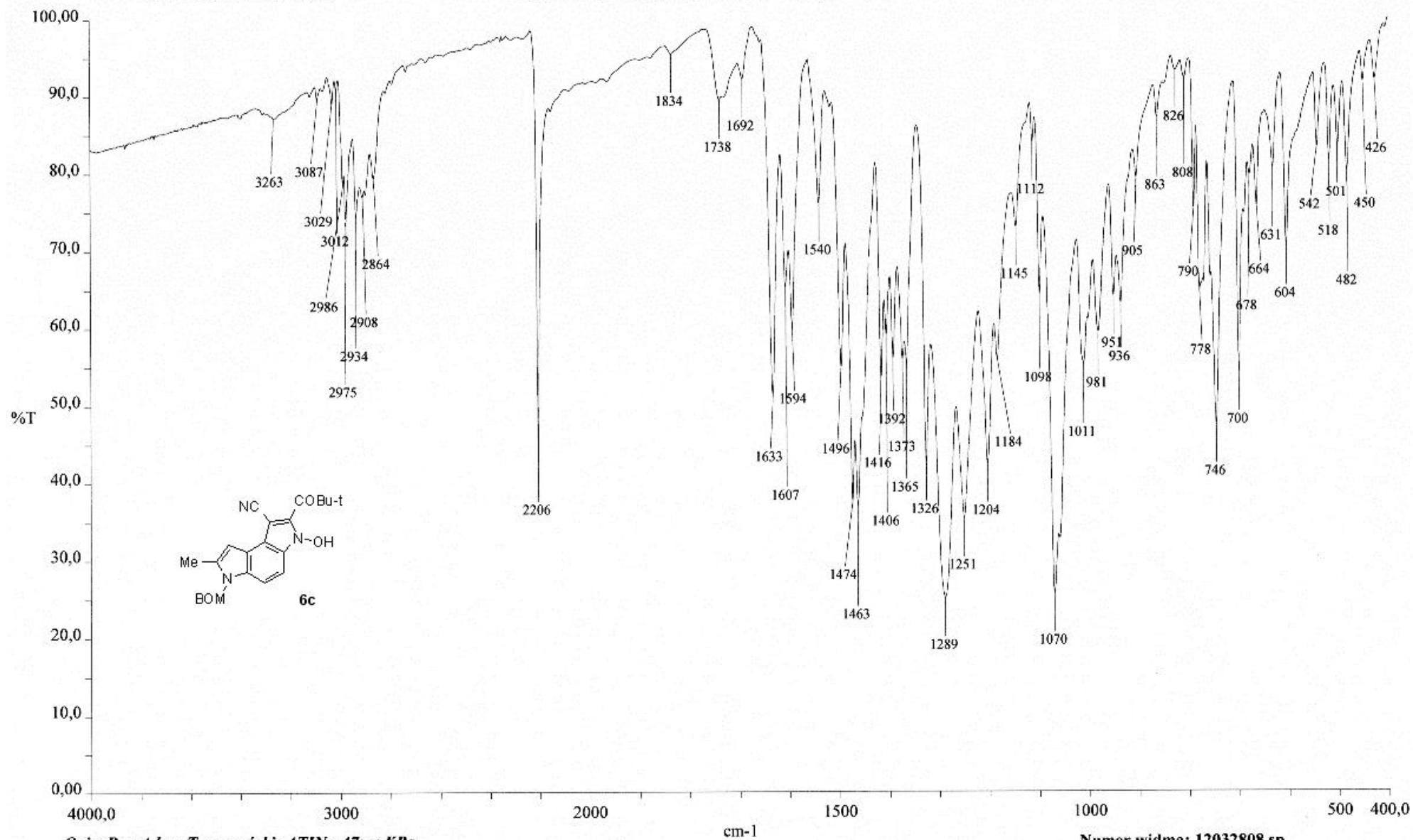
file: ...A\NMR\PIROLOINDOLE\ATIN-47-W\1\fid expt: <zg>
 transmitter freq.: 500.133089 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.130004 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 265.268 ppm/cm: 0.53039



file: ...INDOLE\ATIN-47\ATIN-47-C13.fid\fid block #1 expt: "s2pul"
 transmitter freq.: 125.697101 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9882 ppm = 0.400001 Hz/pt
 number of scans: 1248

freq. of 0 ppm: 125.683334 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 1063.528 ppm/cm: 8.46104



Opis: Pan Adam Trawczyński: ATIN - 47; w KBr

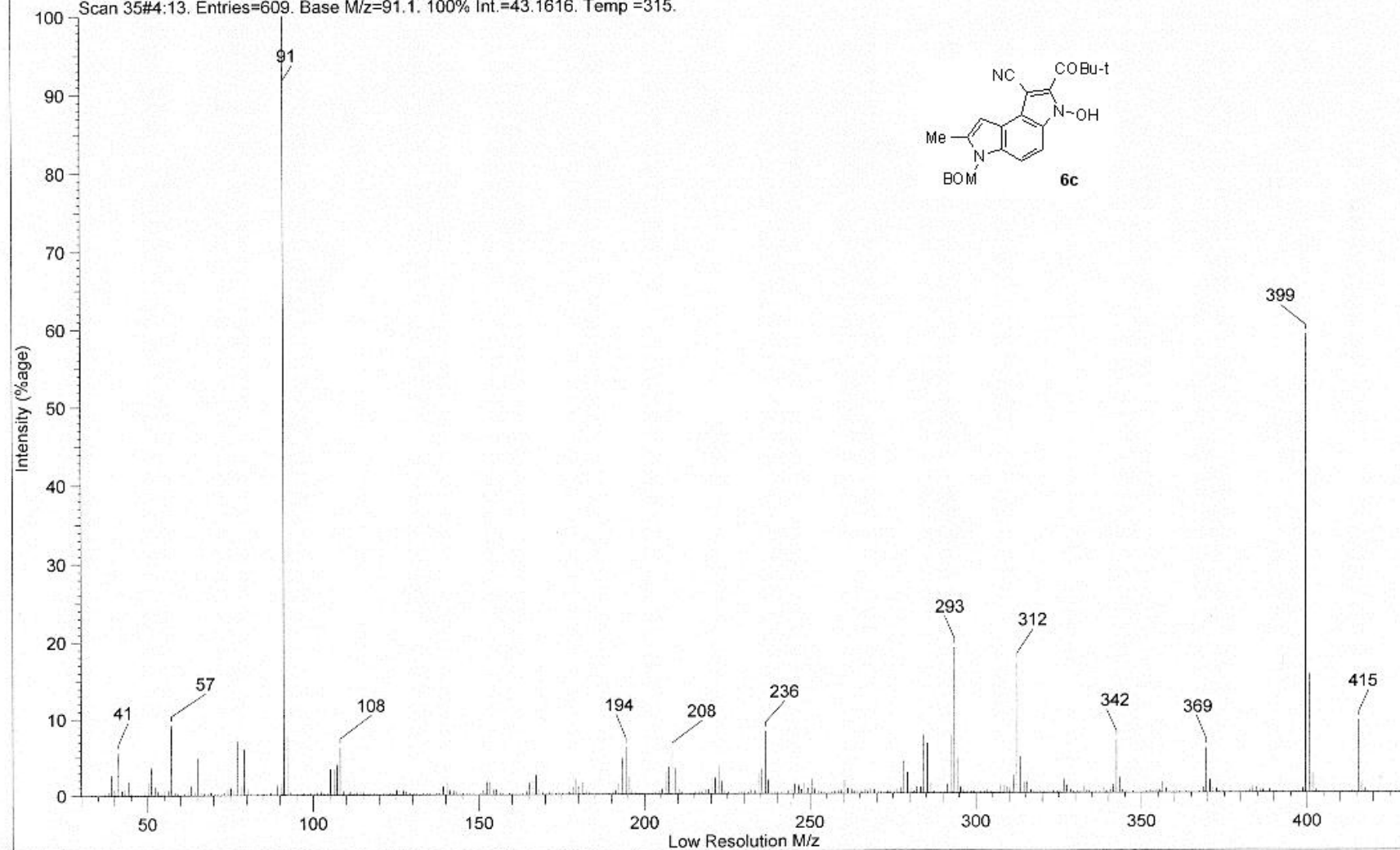
Uwagi:

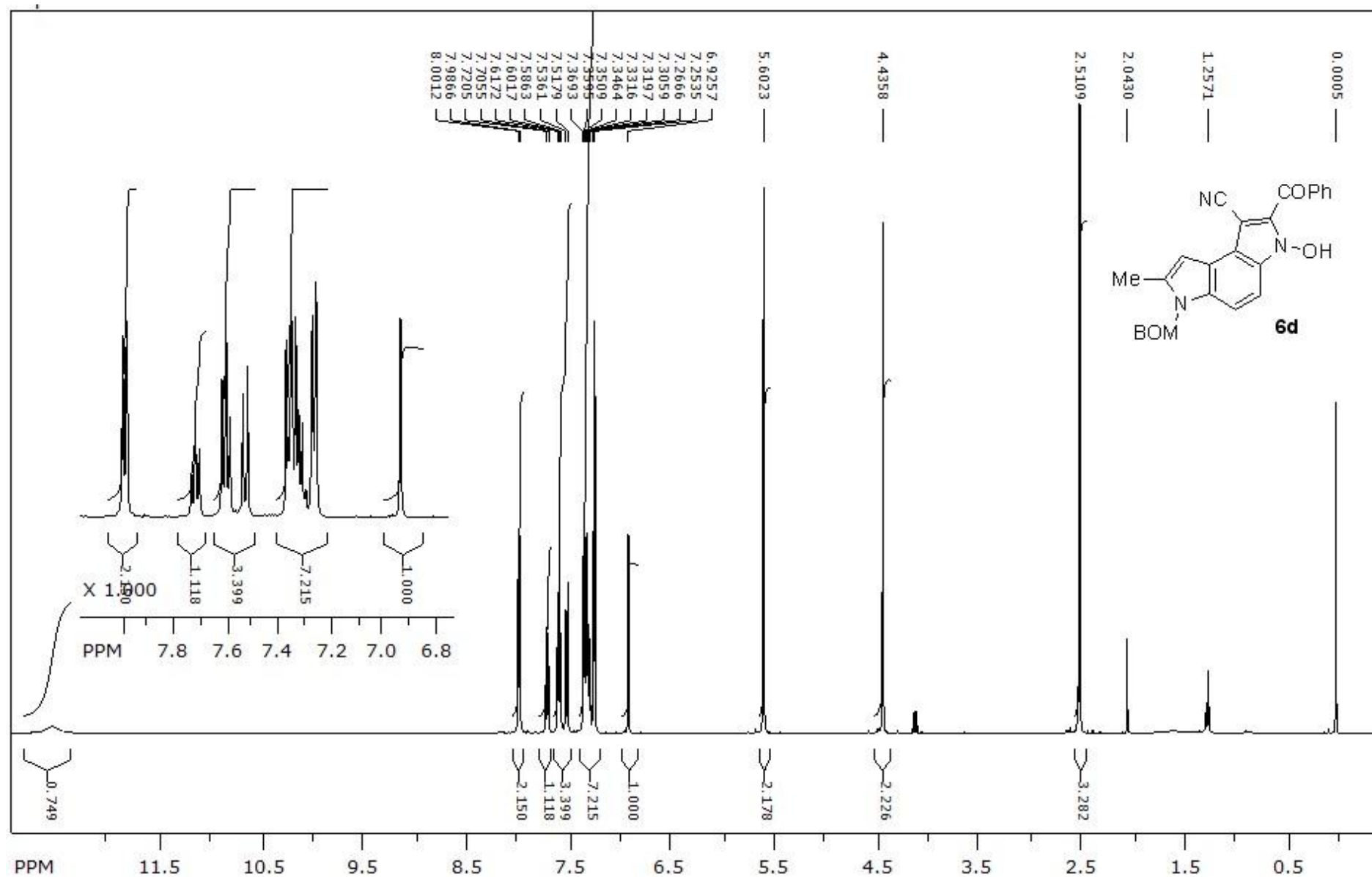
Numer widma: 12032808.sp

Operator: Alicja Dziedzic

File Name : E:\ChO\Z07_EG\at3209.ms2
Creation Date/Time : 11-10-27 at 15:09:09
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-47 (EI 70 eV 33-800)
Operator : Marian Olejnik
Instrument : AMD 604
Notes : A. Trawczyński

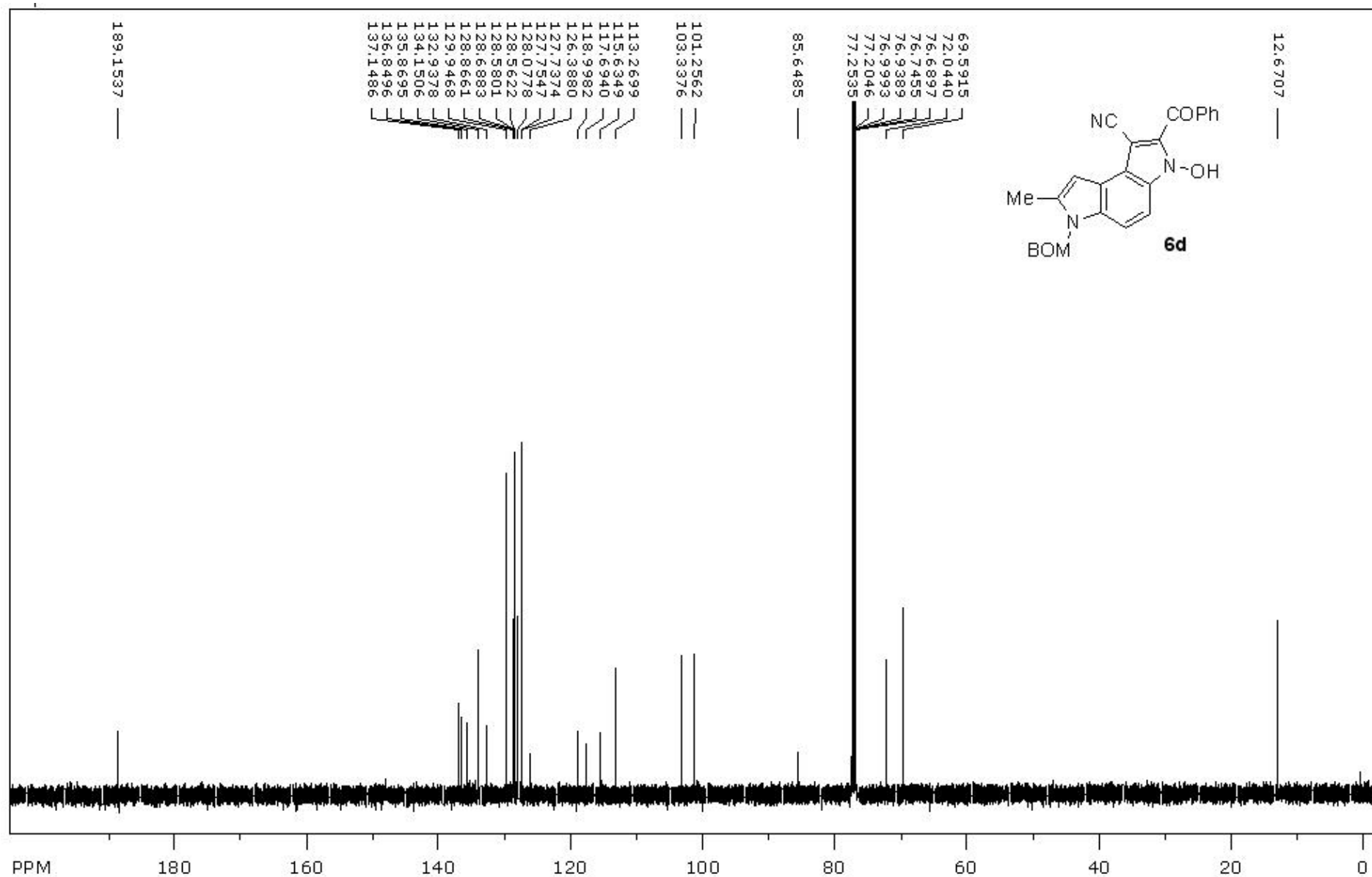
SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 35#4:13. Entries=609. Base M/z=91.1. 100% Int.=43.1616. Temp =315.





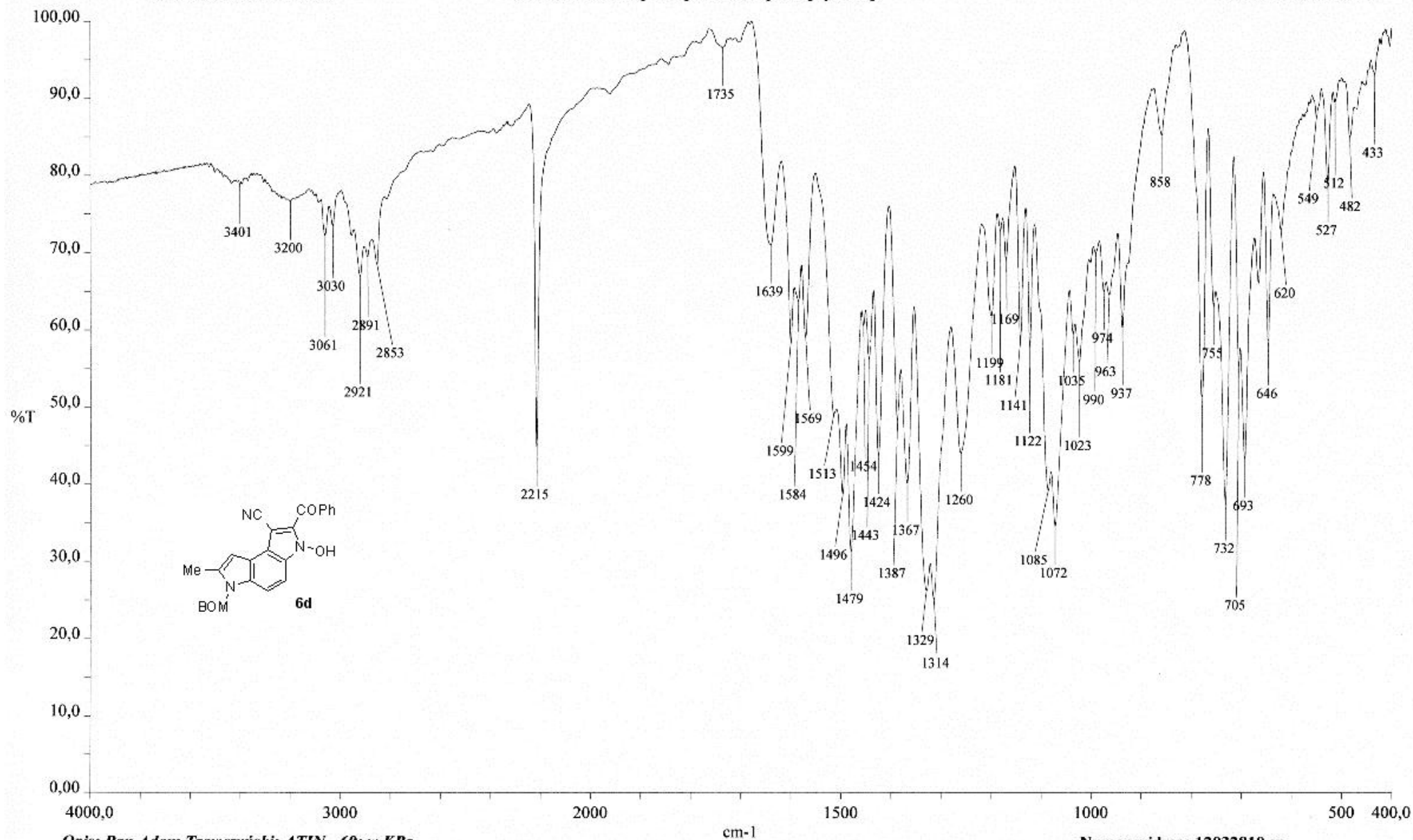
file: D:\NMR\PIROLOINDOLE\ATIN-69\1\fid expt: <zg>
 transmitter freq.: 500.133089 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.130017 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 267.326 ppm/cm: 0.53451



file: ...MIA\NMR\PIROLOINDOLE\ATIN-69\2\fid_expt: <zgpg>
 transmitter freq.: 125.770364 MHz
 time domain size: 65536 points
 width: 32679.74 Hz = 259.8366 ppm = 0.498653 Hz/pt
 number of scans: 840

freq. of 0 ppm: 125.757795 MHz
 processed size: 262144 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 1048.935 ppm/cm: 8.34008



Opis: Pan Adam Trawczyński; ATIN - 69; w KBr

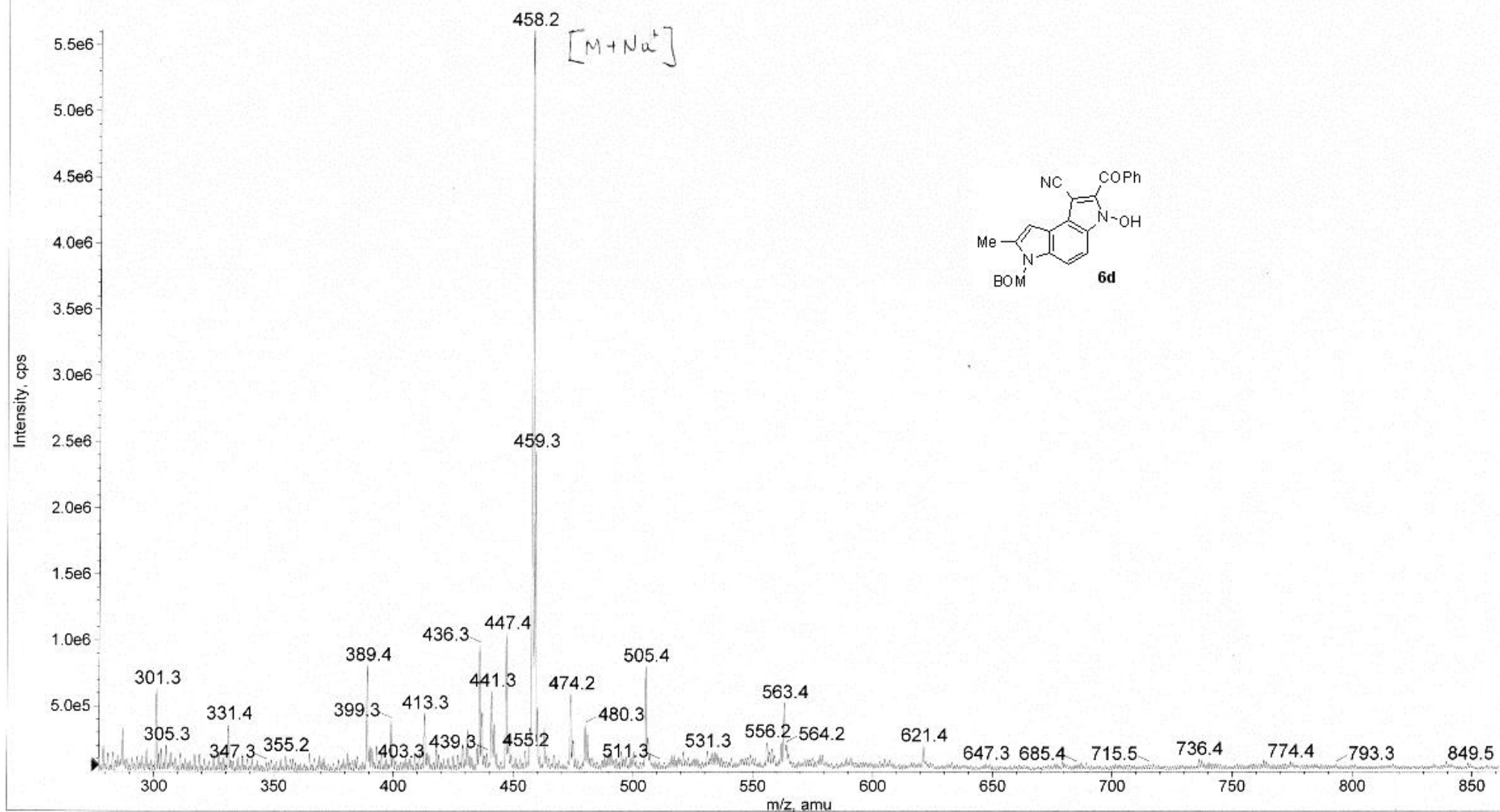
Uwagi:

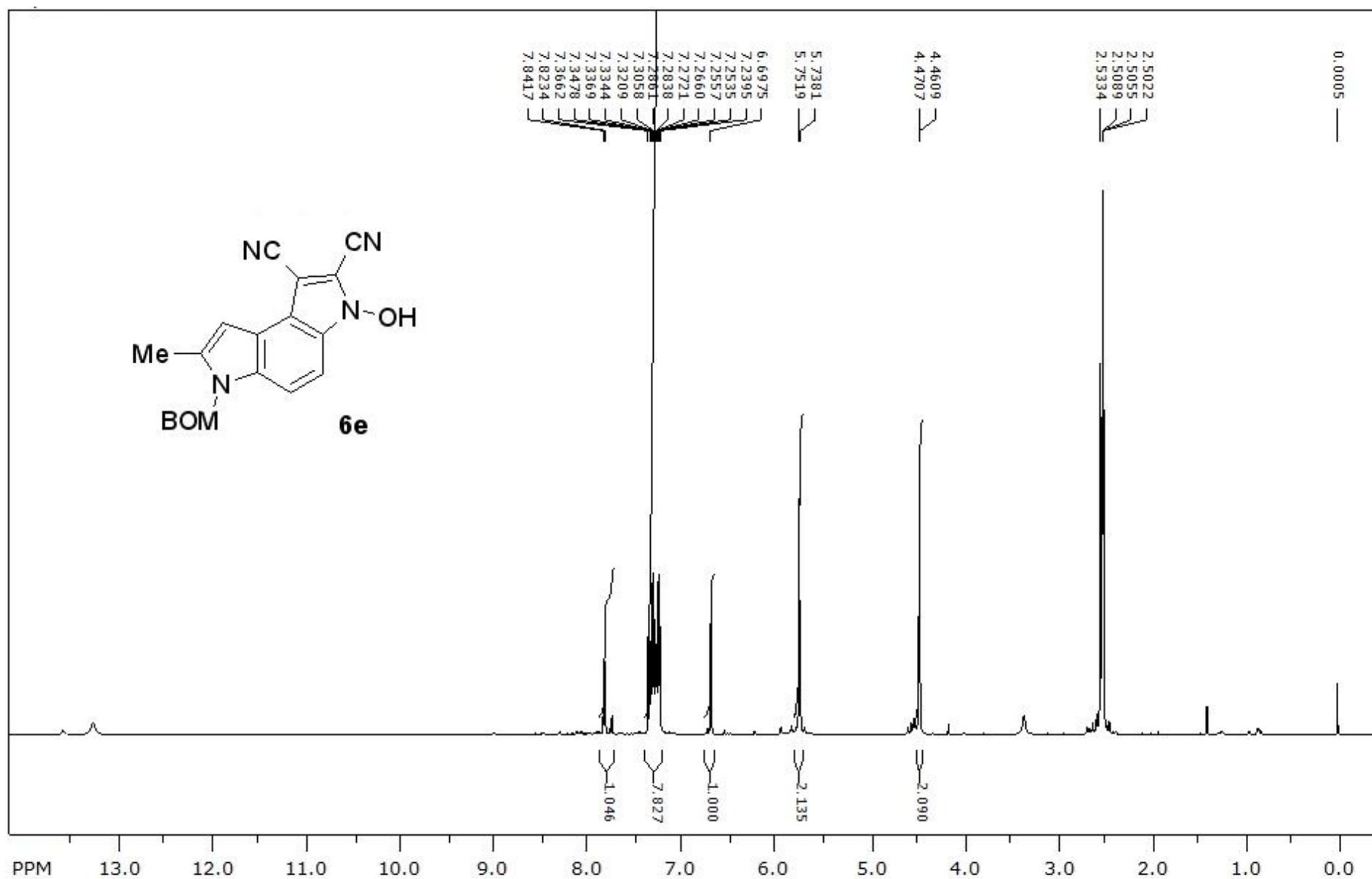
Numer widma: 12032810.sp

Operator: Alicja Dziedzic

■ +Q1: 0.033 to 1.170 min from Sample 1 (ATIN-69) of at858.wiff (Turbo Spray)

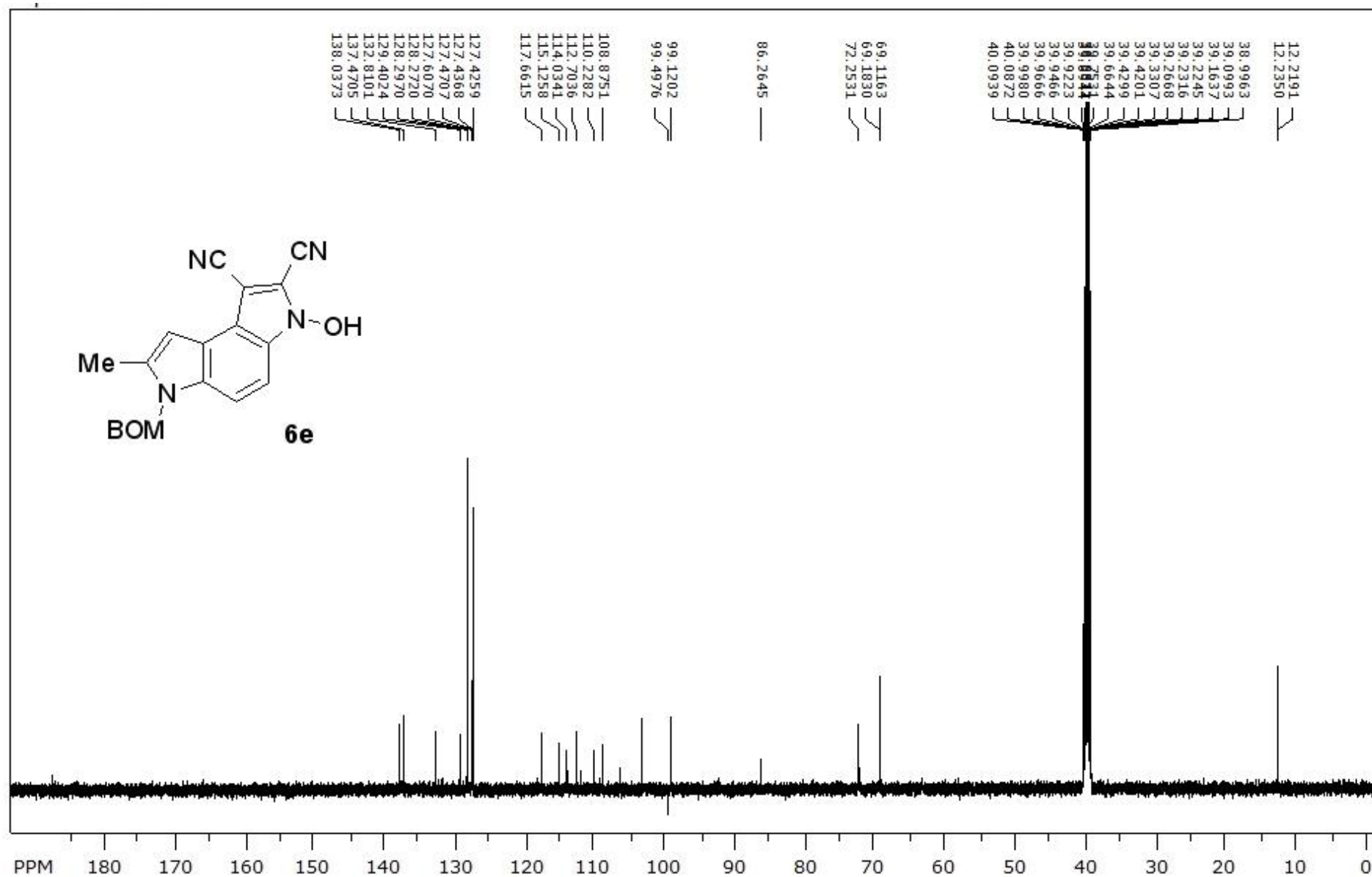
Max. 5.6e6 cps





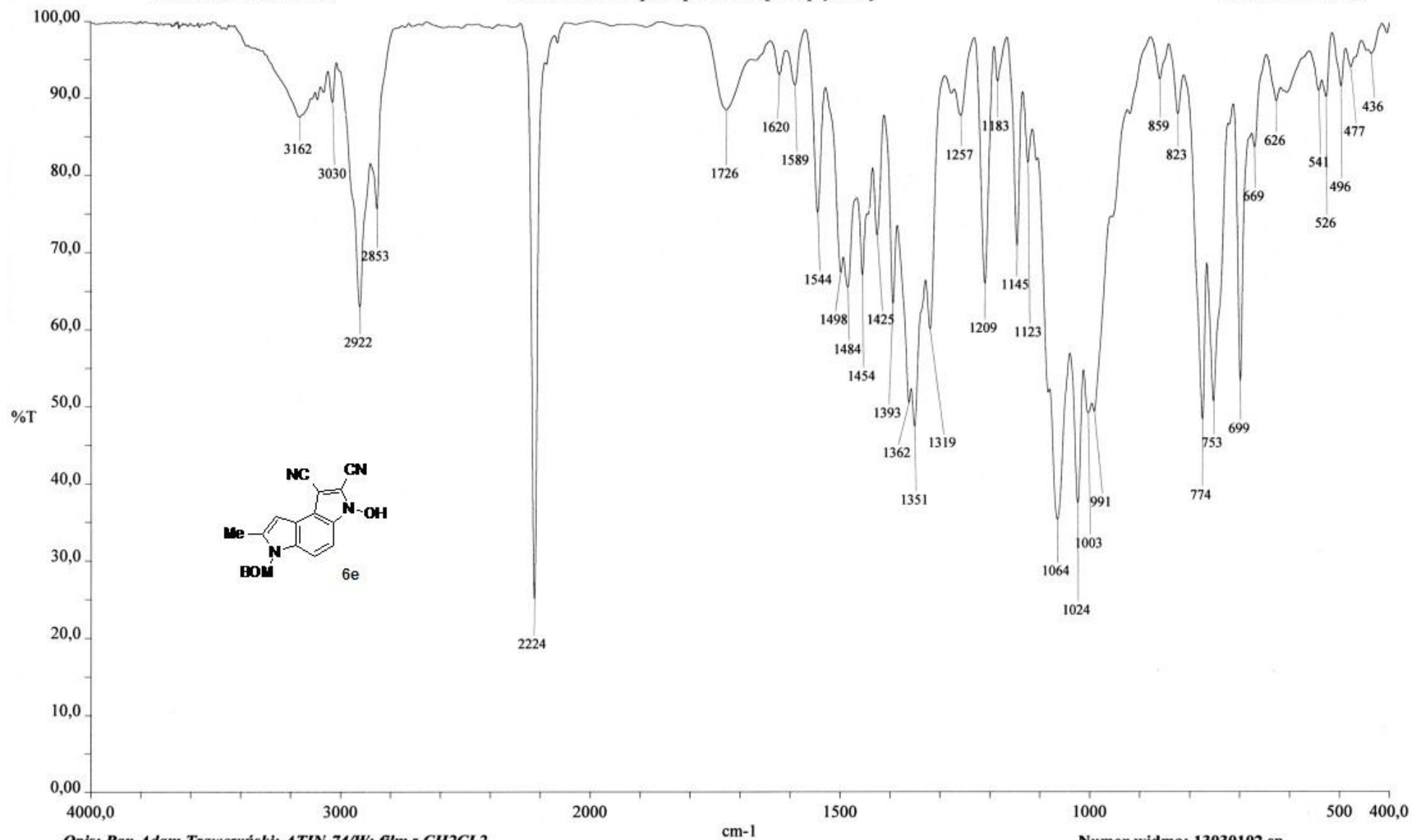
file: D:\NMR\PIROLOINDOLE\ATIN-74\1\fid expt: <zg>
 transmitter freq.: 500.133089 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.130003 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 292.674 ppm/cm: 0.58519



file: D:\NMR\PIROLOINDOLE\ATIN-74\2\fid exp: <zgpg>
 transmitter freq.: 125.770364 MHz
 time domain size: 65536 points
 width: 32679.74 Hz = 259.8366 ppm = 0.498653 Hz/pt
 number of scans: 1880

freq. of 0 ppm: 125.757852 MHz
 processed size: 262144 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 984.463 ppm/cm: 7.82747



Opis: Pan Adam Trawczyński; ATIN-74/W; film z CH₂CL₂

Uwagi:

Numer widma: 13030102.sp

Operator: Alicja Dziezic

15.425

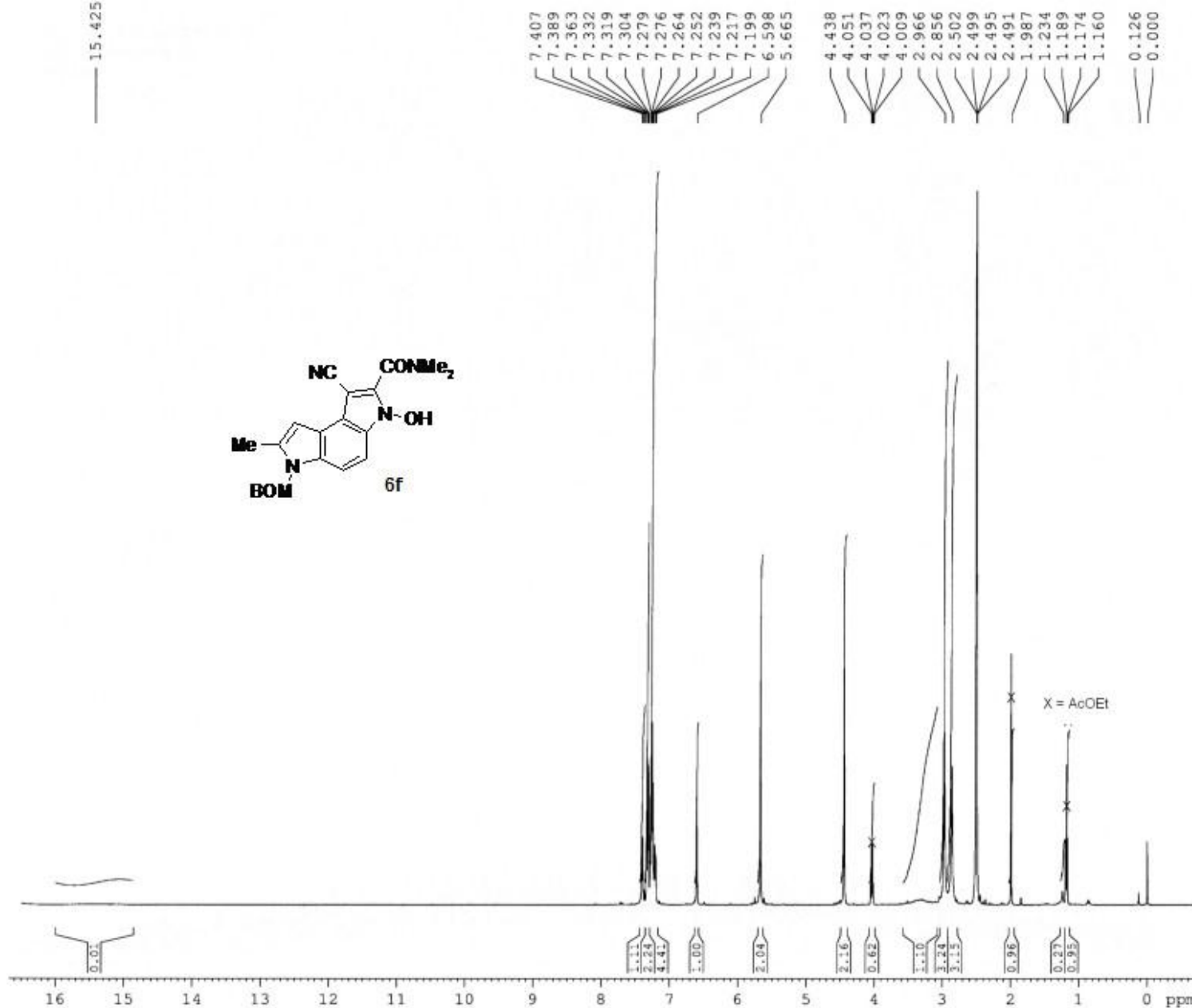


Current Data Parameters
NAME ATIN-57-K
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130301
Time 9.16
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 228.1
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.20 usec
PL1 5.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300049 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME ATIN-57-K
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130301
 Time 9.29
 INSTRUM DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 160
 DS 4
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027508 sec
 RG 32768
 DW 15.300 usec
 DE 7.10 usec
 TE 303.0 K
 DI 1.00000000 sec
 d11 0.03000000 sec
 DELTA 0.89999998 sec
 TD0 1

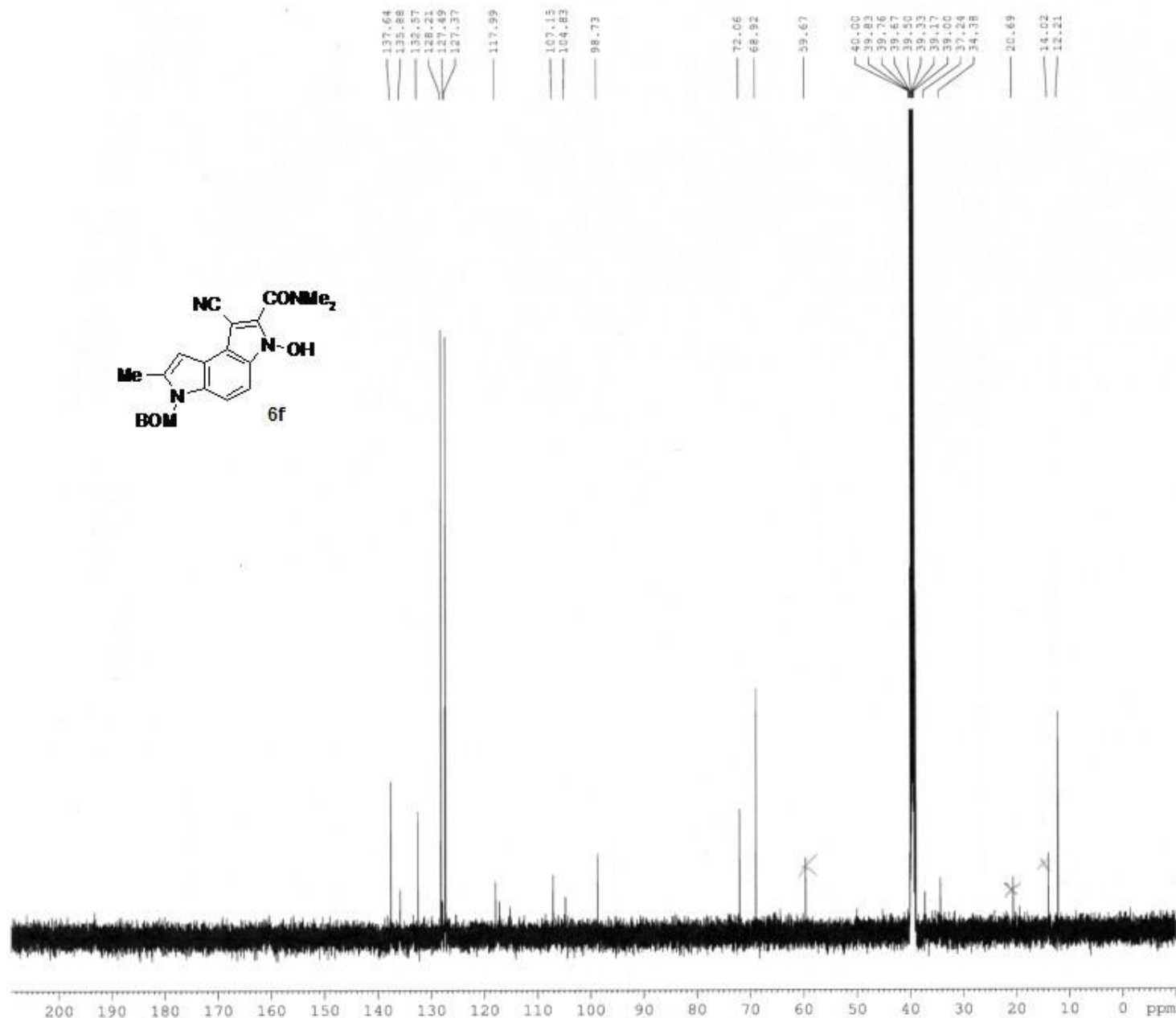
===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -3.00 dB
 SFO1 125.7703643 MHz

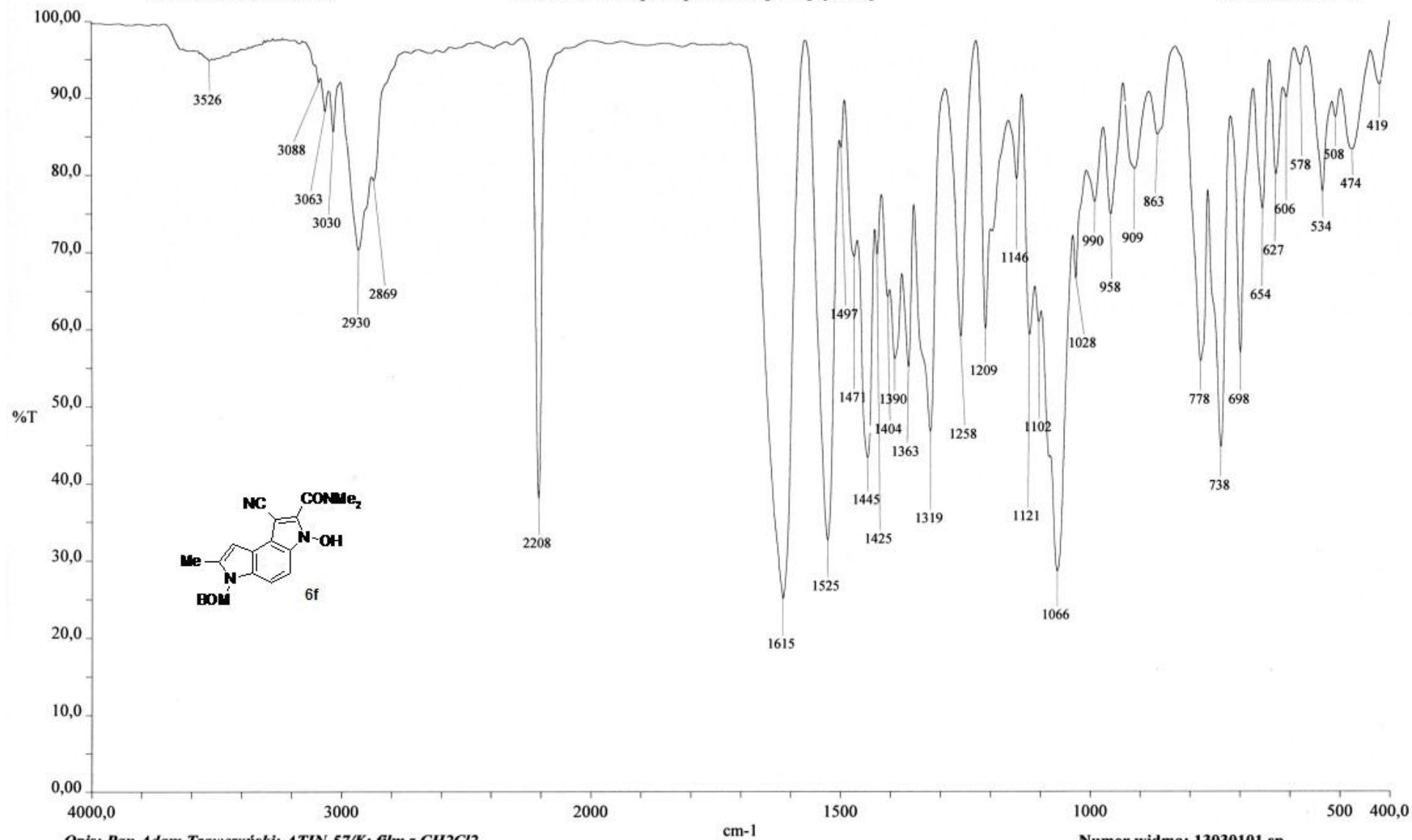
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 98.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 32.00 dB
 SFO2 500.1320005 MHz

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.132 MHz
 FIDRES 7.812500 Hz
 SW 1.999 ppm
 FMODE QF

F2 - Processing parameters
 SI 262144
 SF 125.7578564 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.30 Hz
 GB 0.1





Opis: Pan Adam Trawczyński; ATIN-57/K; film z CH₂Cl₂

Uwagi:

Numer widma: 13030101.sp

Operator: Alicja Dziejczak

A. Trawczynski

ATIN-57/K

z07_at0626 35 (2.775) Cm (35:36)

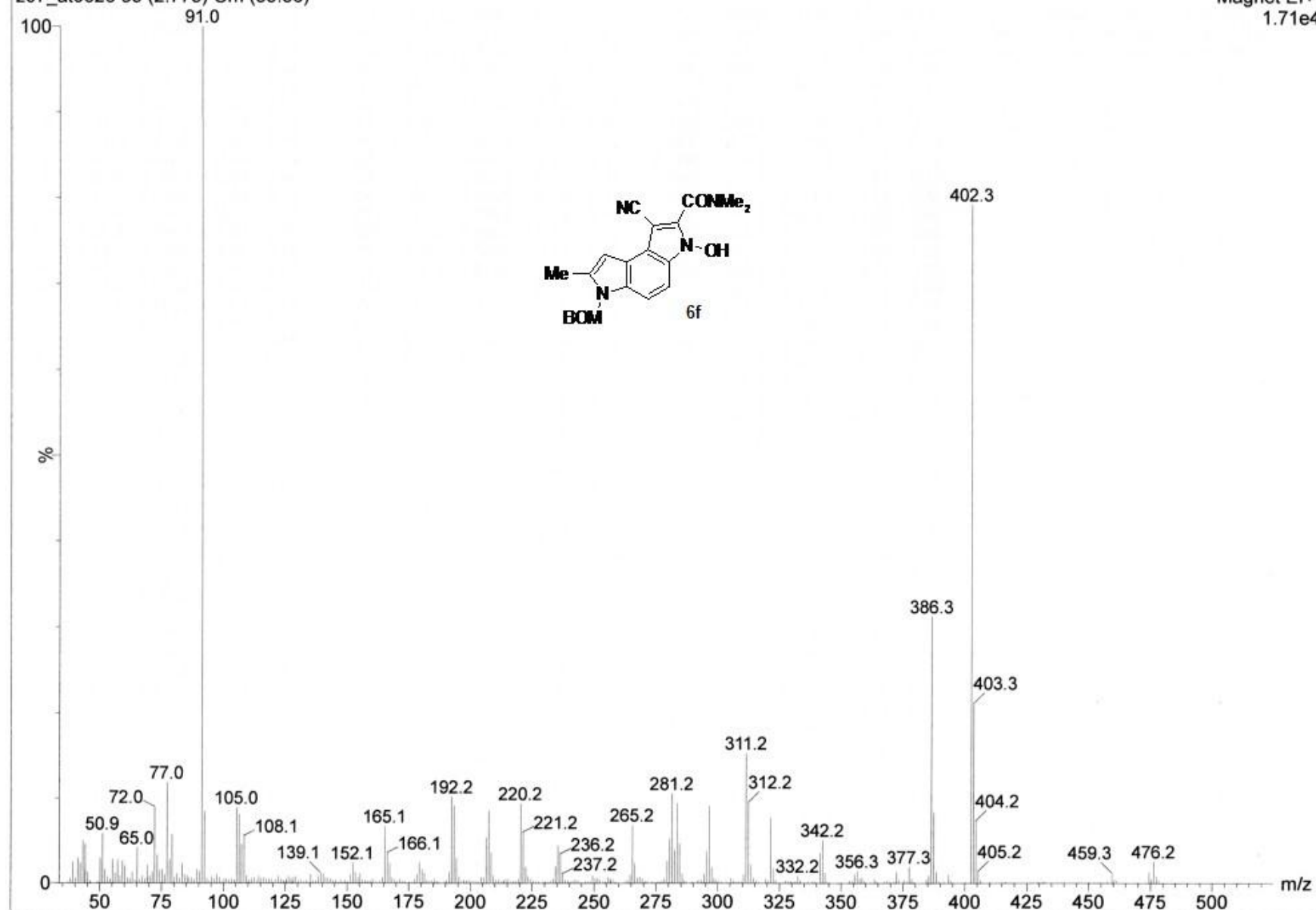
AUTOSPEC

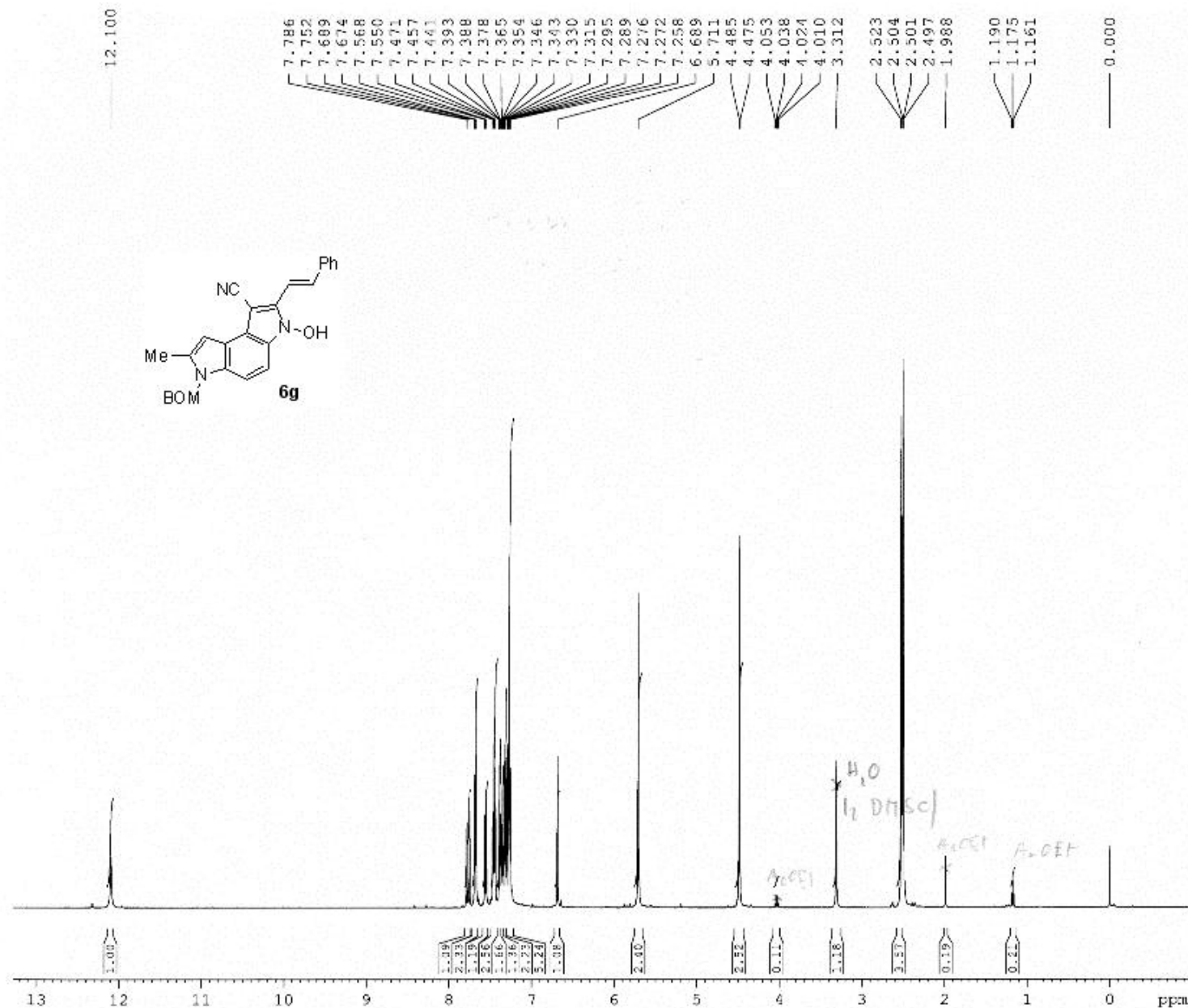
28-Feb-2013 16:02:48

operator: Marian Olejnik

Magnet EI+

1.71e4



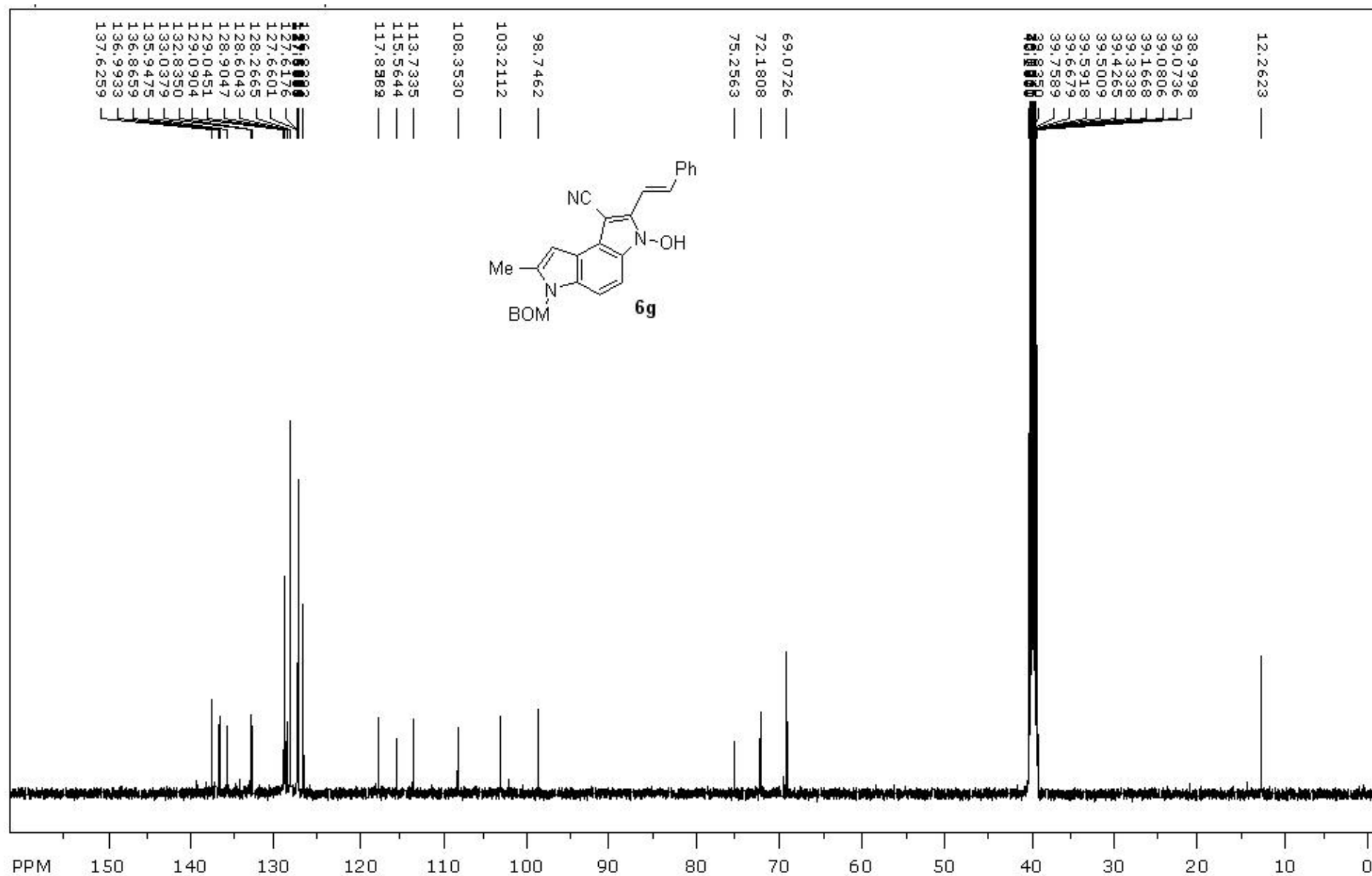


Current Data Parameters
NAME ATIN-59-K
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130226
Time 9.17
INSTRUM DRX
PROBHD 5 mm TBI 1H/13
PULPROG zg
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DW 48.400 usec
DE 6.78 usec
TE 303.0 K
D1 1.00000000 sec
TDC 1

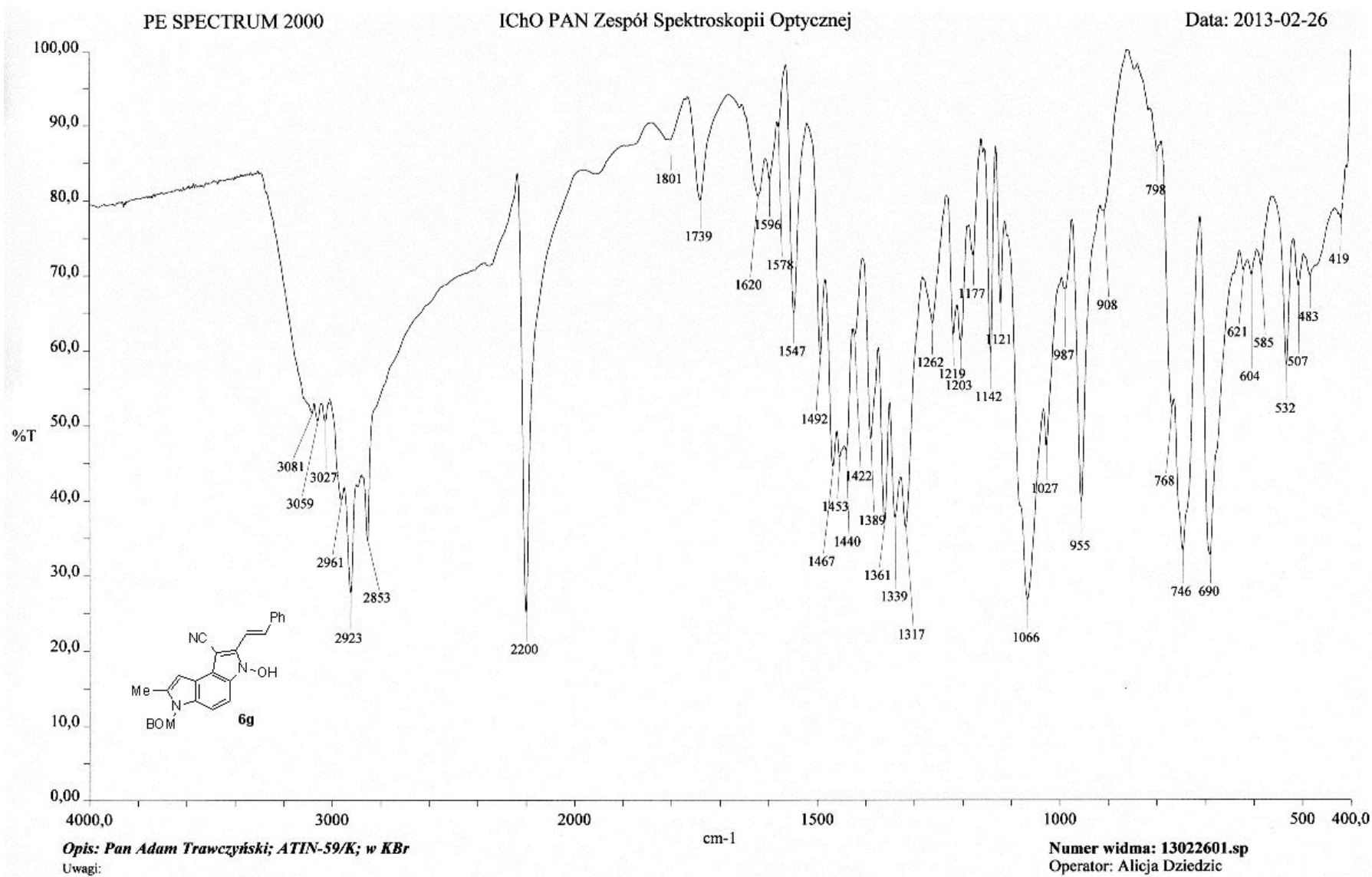
----- CHANNEL f1 -----
NUC1 1H
P1 2.50 usec
PL1 0.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300050 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



file: ...DOLE\ATIN-592\ATIN-592-C13.fid\fid block# 1 expt: "s2pul"
 transmitter freq.: 125.697101 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9882 ppm = 0.400001 Hz/pt
 number of scans: 3072

freq. of 0 ppm: 125.683336 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 823.010 ppm/cm: 6.54757



ATIN - 59/K

SYNAPT G2S HDMS

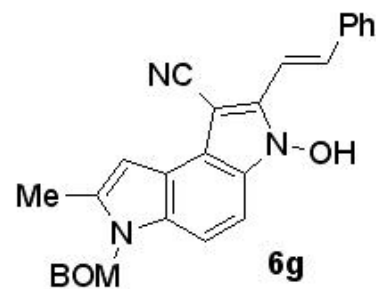
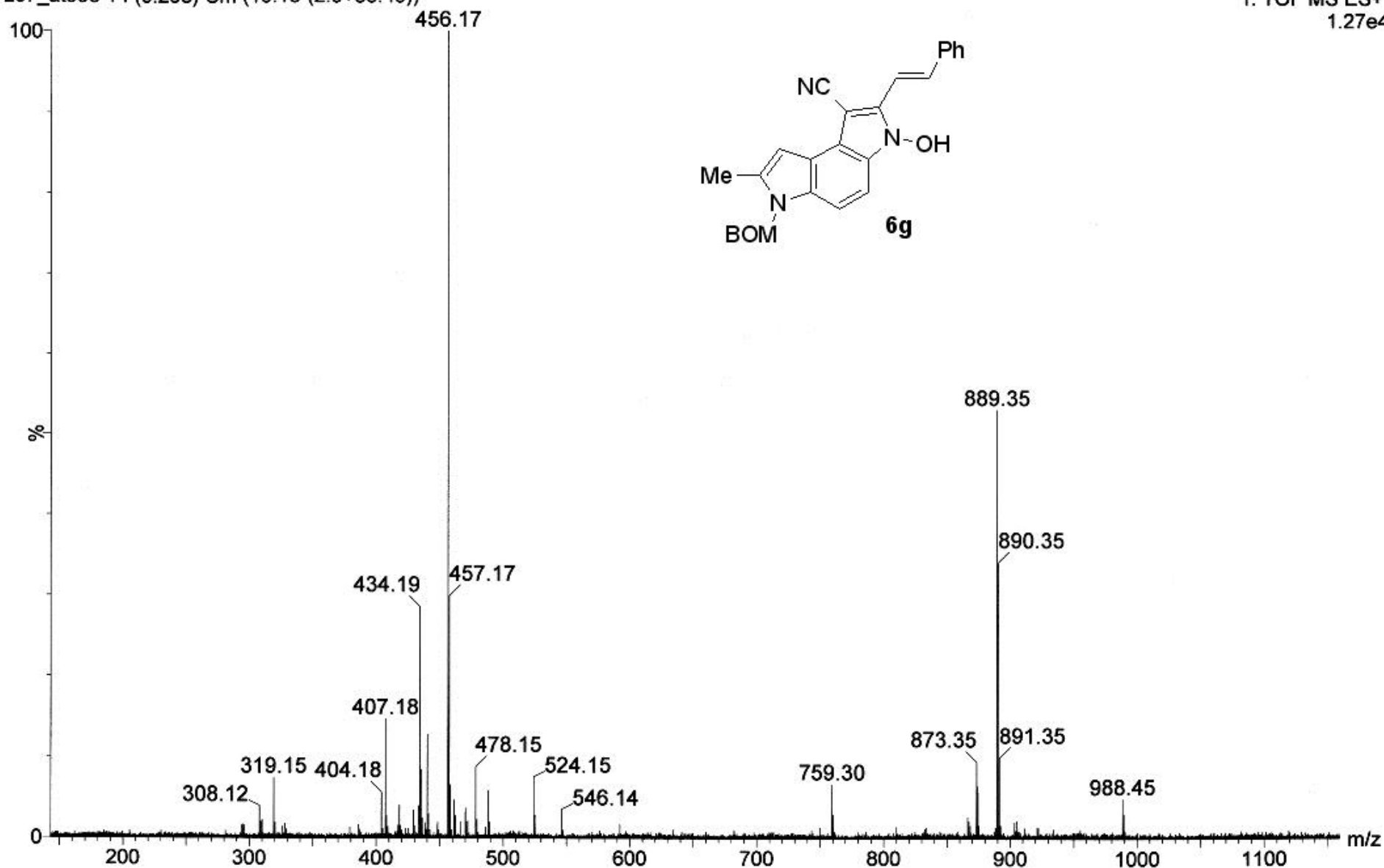
27-Feb-2013

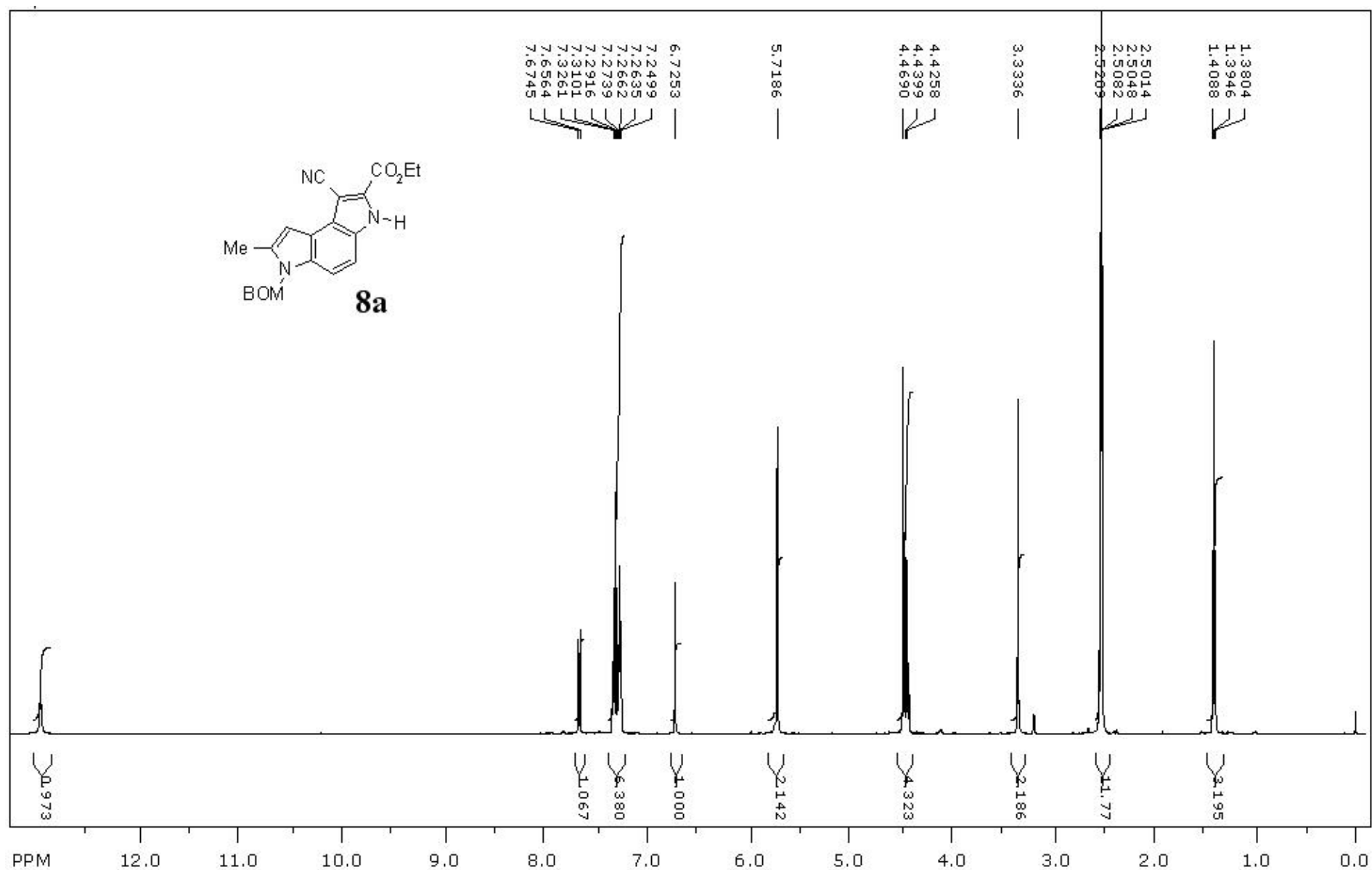
13:29:31

1: TOF MS ES+

1.27e4

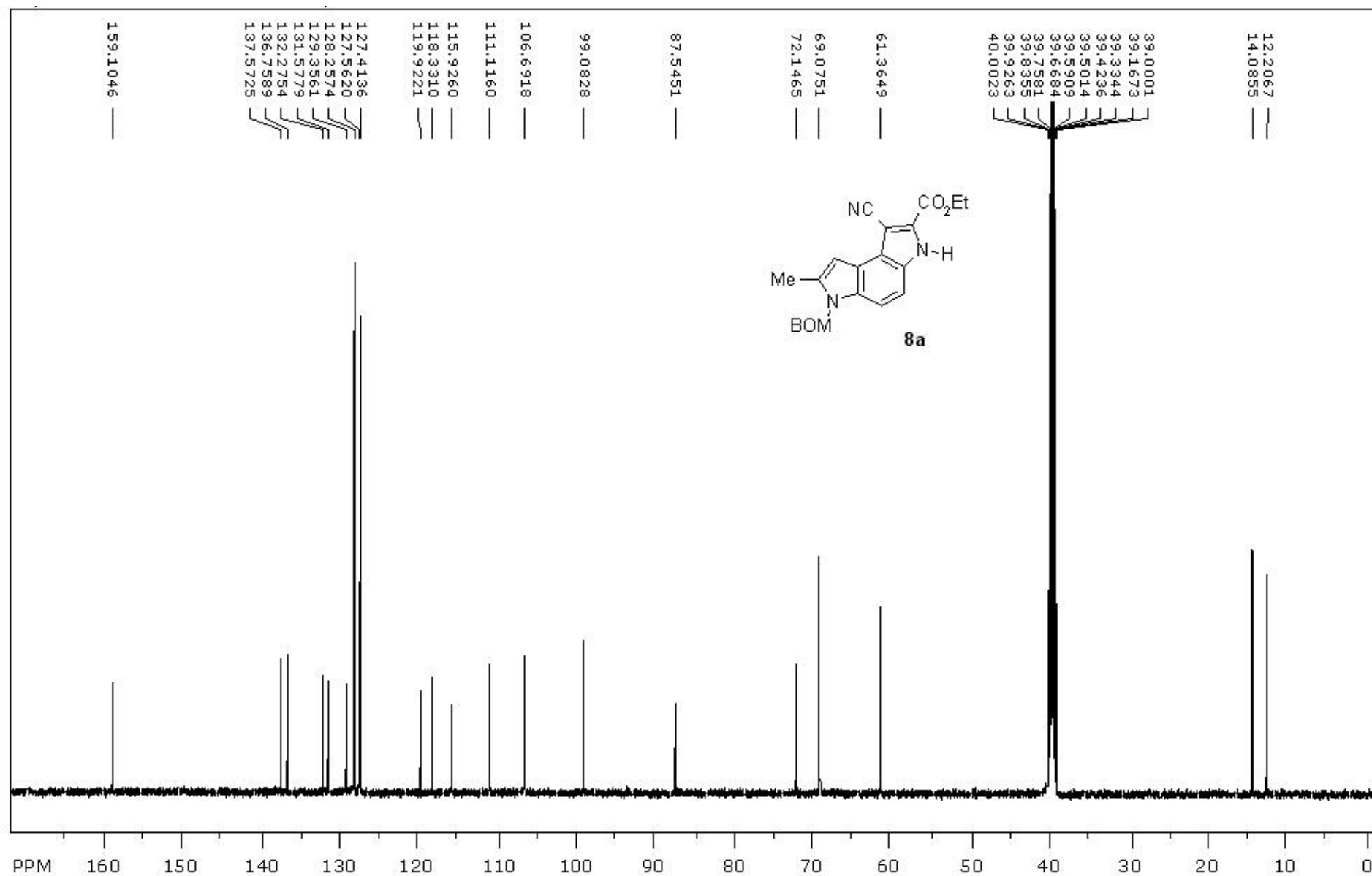
z07_at595 14 (0.293) Cm (10:18-(2:9+38:49))





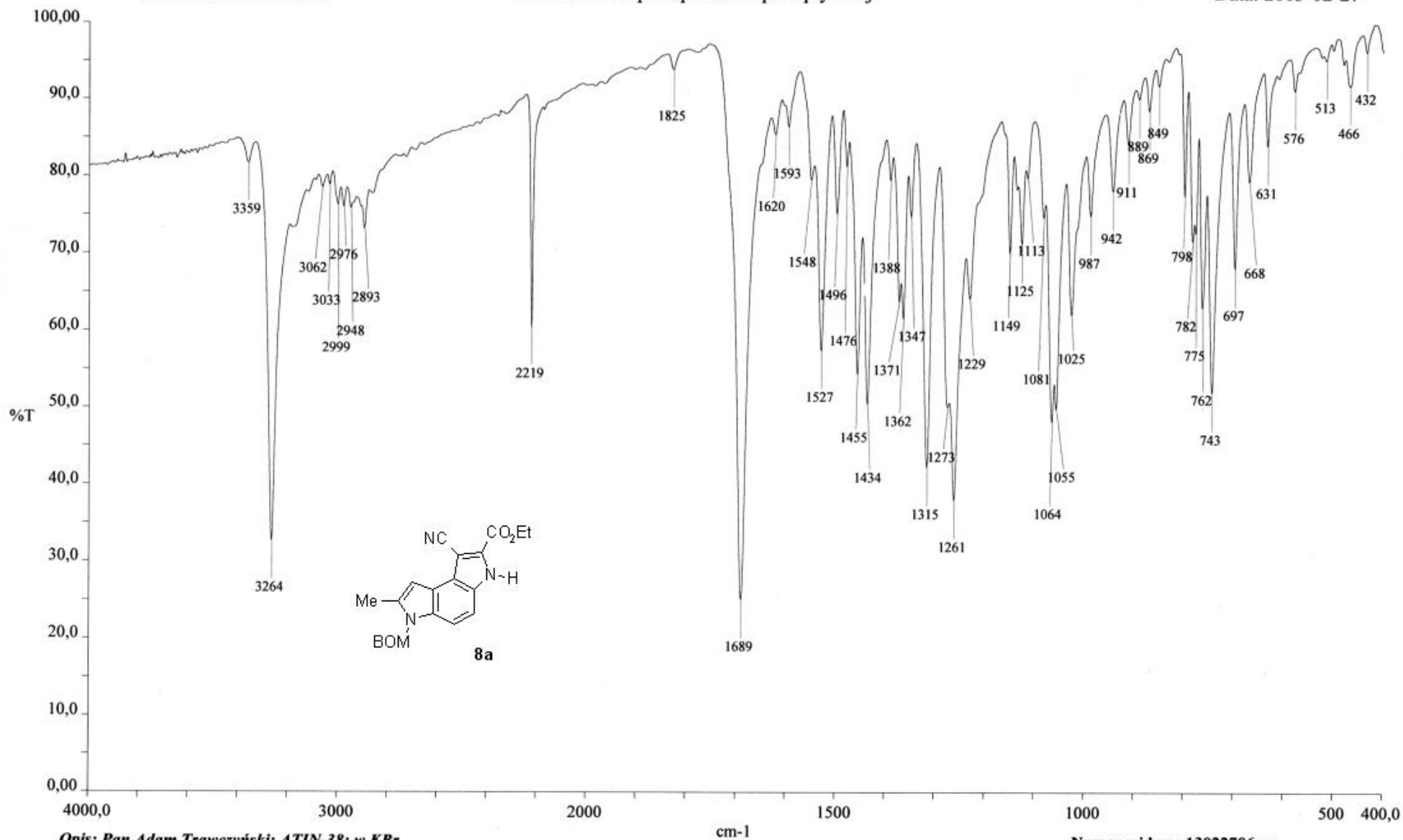
file: ...MIA\NMR\PIROLOINDOLE\ATIN-79\1\fid_expt: <zg>
 transmitter freq.: 500.133089 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.130003 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 268.289 ppm/cm: 0.53643



file: ...INDOLE\ATIN-38\ATIN-38-C13.fid\fid block # 1 expt: "s2pul"
 transmitter freq.: 125.697101 MHz
 time domain size: 80128 points
 width: 32051.28 Hz = 254.9882 ppm = 0.400001 Hz/pt
 number of scans: 1152

freq. of 0 ppm: 125.683335 MHz
 processed size: 131072 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 875.513 ppm/cm: 6.96526



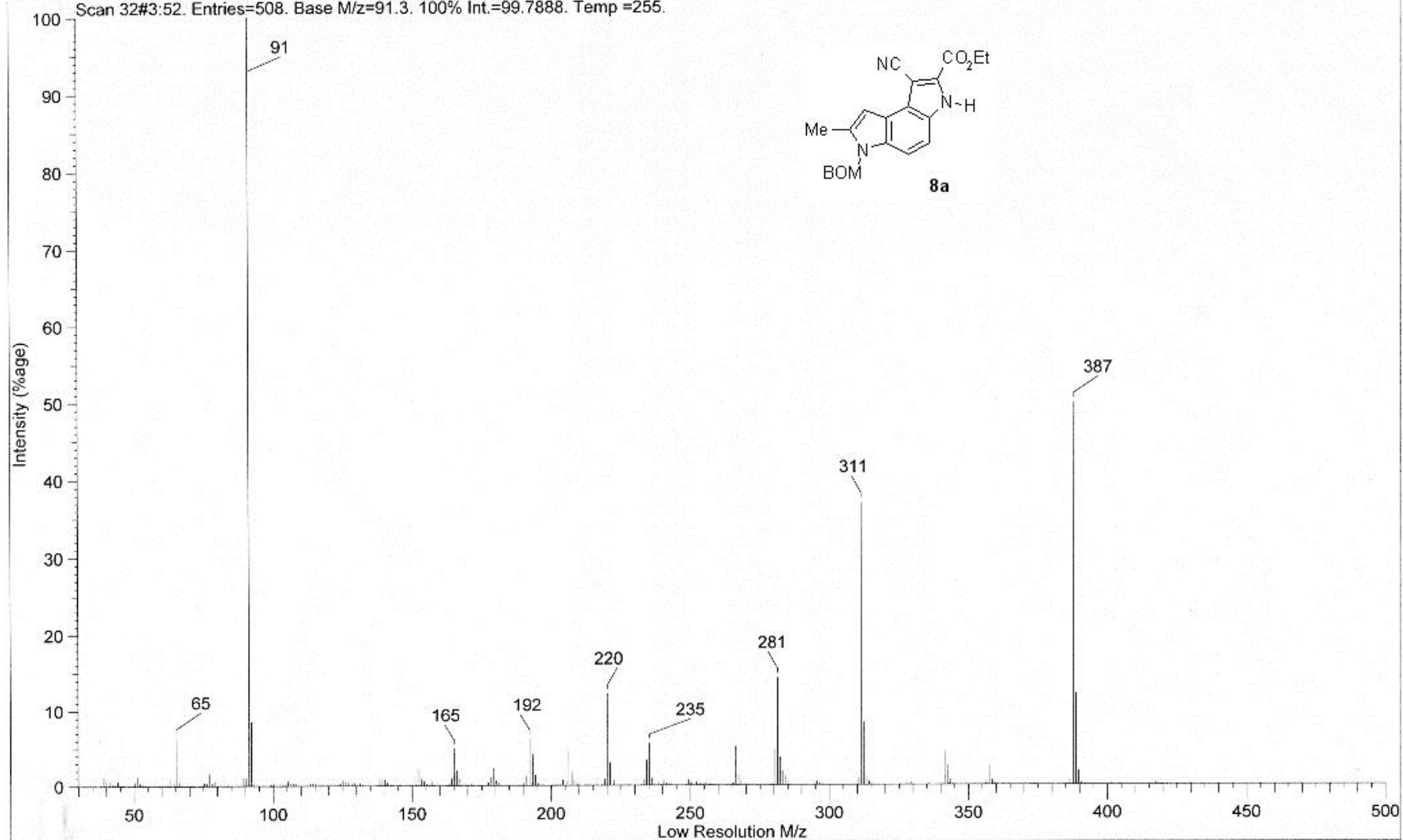
Opis: Pan Adam Trawczyński; ATIN-38; w KBr

Uwagi:

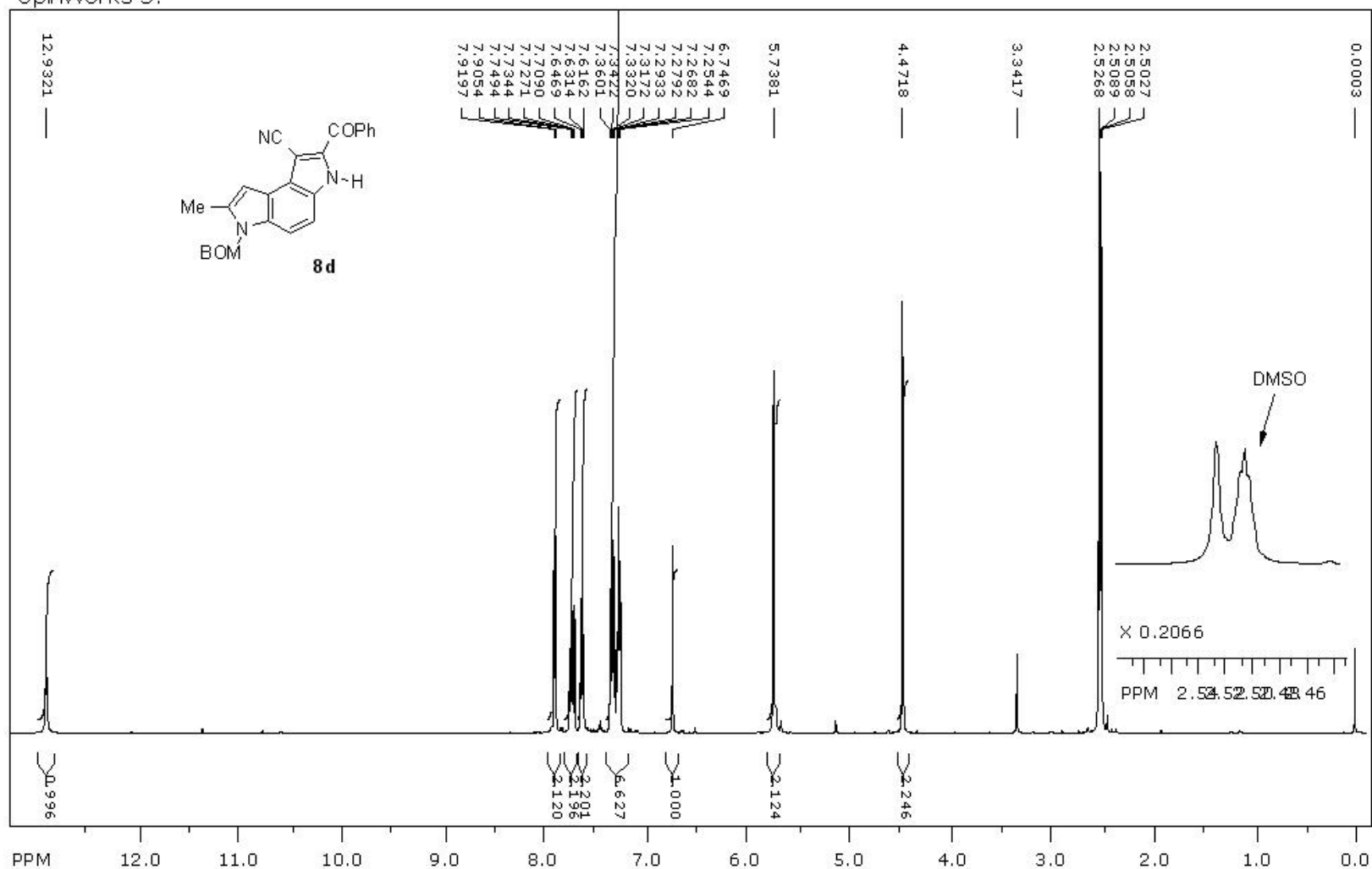
Numer widma: 13022706.sp
Operator: Alicja Dziezic

File Name : E:\CHO\Z07_EG\at2928.ms2
Creation Date/Time : 11-10-05 at 10:55:28
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [I132/99D9]
File Title : ATIN-38 (EI 70 eV 33-800)
Operator : Małgorzata Grela
Instrument : AMD 604
Notes : A. Trawczyński

SCAN GRAPH. Flagging=Nominal M/z. Highlighting=Base Peak.
Scan 32#3:52. Entries=508. Base M/z=91.3. 100% Int.=99.7888. Temp =255.

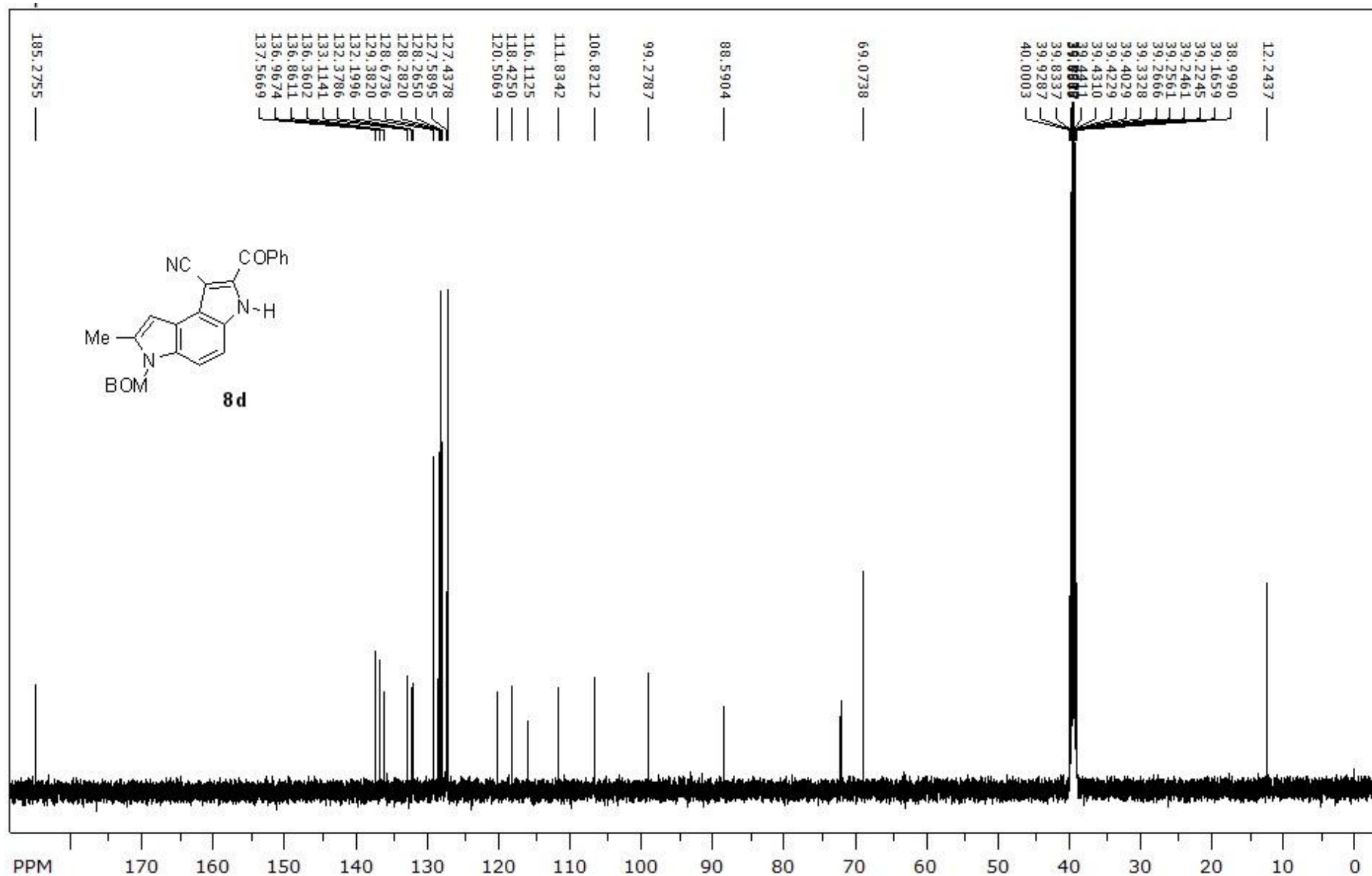


SpinWorks 3:



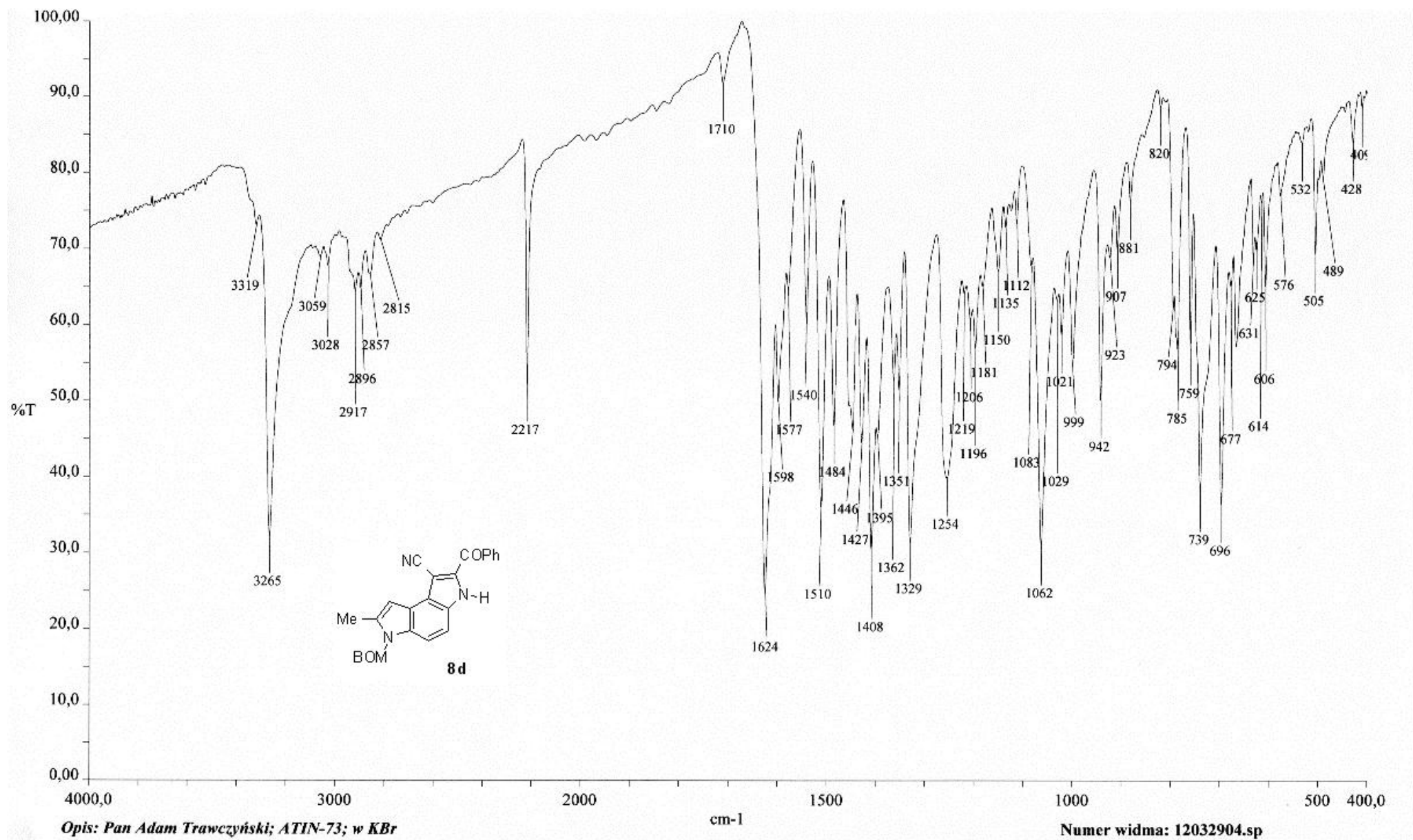
```
file: ...MIA\NMR\PIROLOINDOLE\ATIN-73\1\fid exp: <zg>
transmitter freq: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 32
```

freq. of 0 ppm: 500.130003 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 268.469 ppm/cm: 0.53680

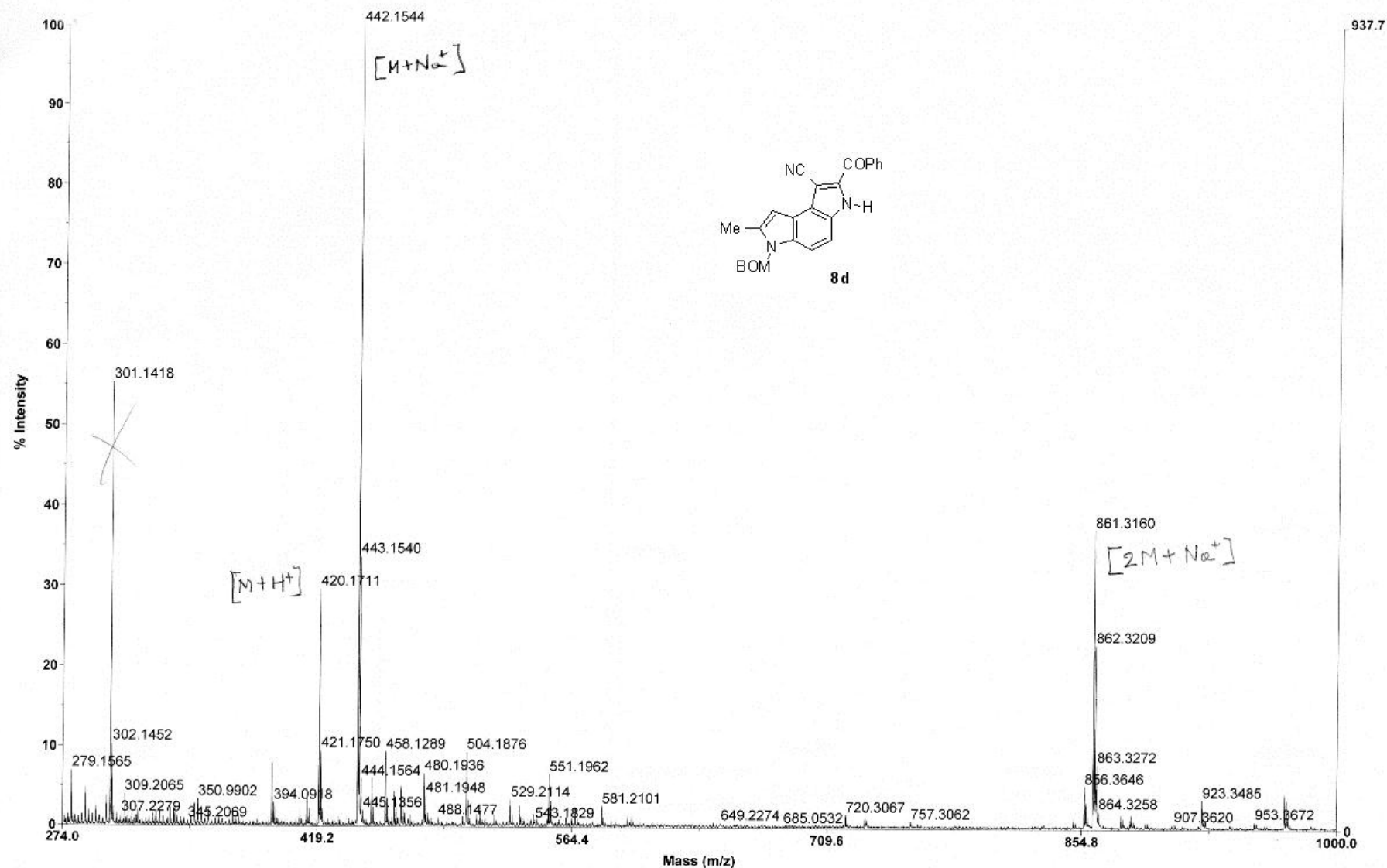


file: D:\NMR\PIROLOINDOLE\ATIN-73\2\fid expt: <zpgg>
 transmitter freq.: 125.770364 MHz
 time domain size: 65536 points
 width: 32679.74 Hz = 259.8366 ppm = 0.498653 Hz/pt
 number of scans: 1151

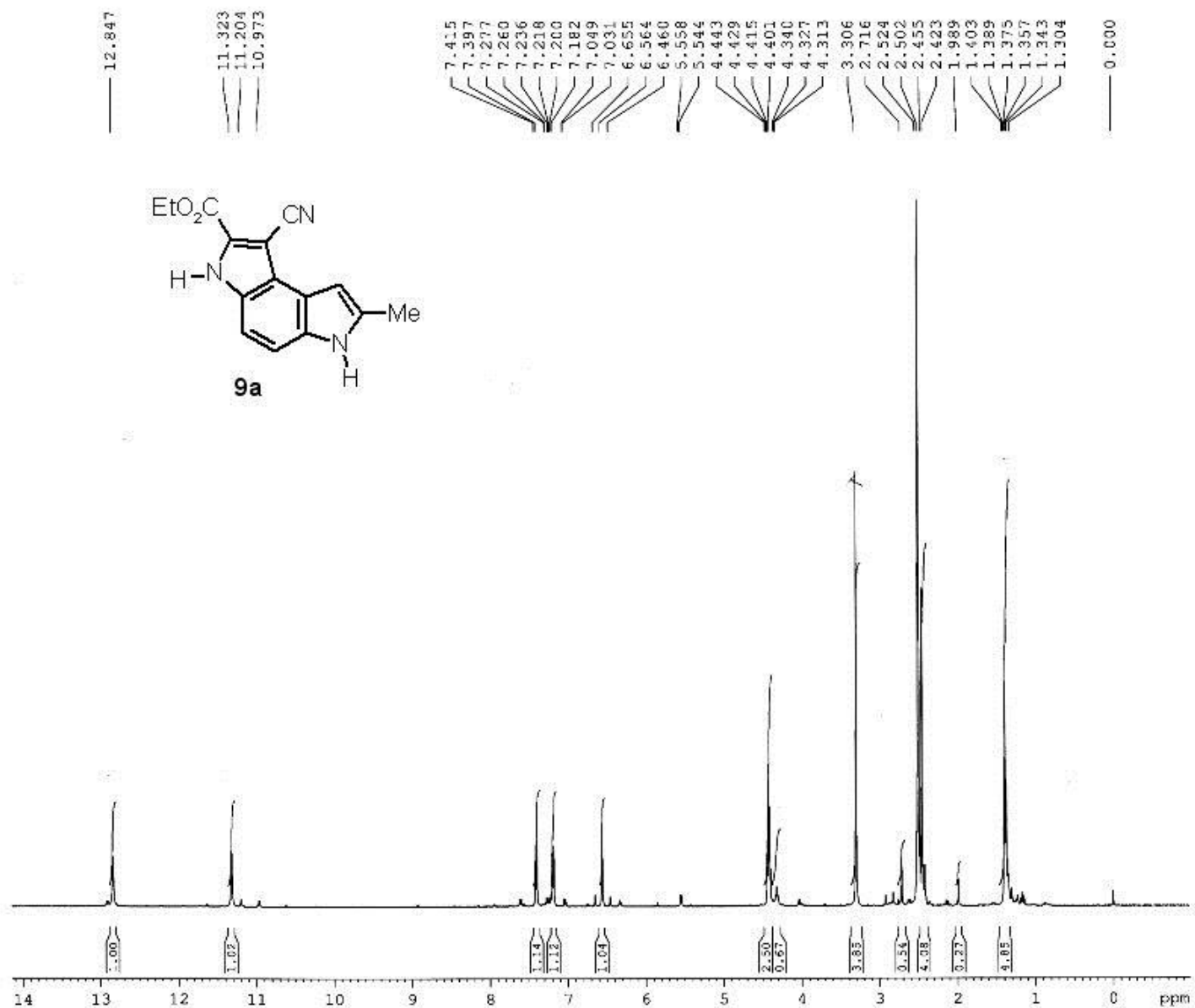
freq. of 0 ppm: 125.757852 MHz
 processed size: 262144 complex points
 LB: 0.500 GF: 0.0000
 Hz/cm: 965.743 ppm/cm: 7.67862



Mariner Spec /1:9 (T /0.00:0.43) ASC MC[BP = 442.1, 938]



Mariner - Magda Kania - A. Trawczynski - ATIN-73 (MeOH, jony dodatnie)
 Z:\AT869001.dat
 Acquired: Mar 19 10:24:00 2012



Current Data Parameters
 NAME IND-363-B
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130412
 Time 11.51
 INSTRUM DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 287.4
 DW 48.400 usec
 DE 6.78 usec
 TE 303.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 8.20 usec
 PL1 5.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME IND-363-B
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130412
 Time 11.59
 INSTRUM DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 1555
 DS 4
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027508 sec
 RG 32768
 DW 15.300 usec
 DE 7.10 usec
 TE 303.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 DELTA 0.89999998 sec
 TD0 1

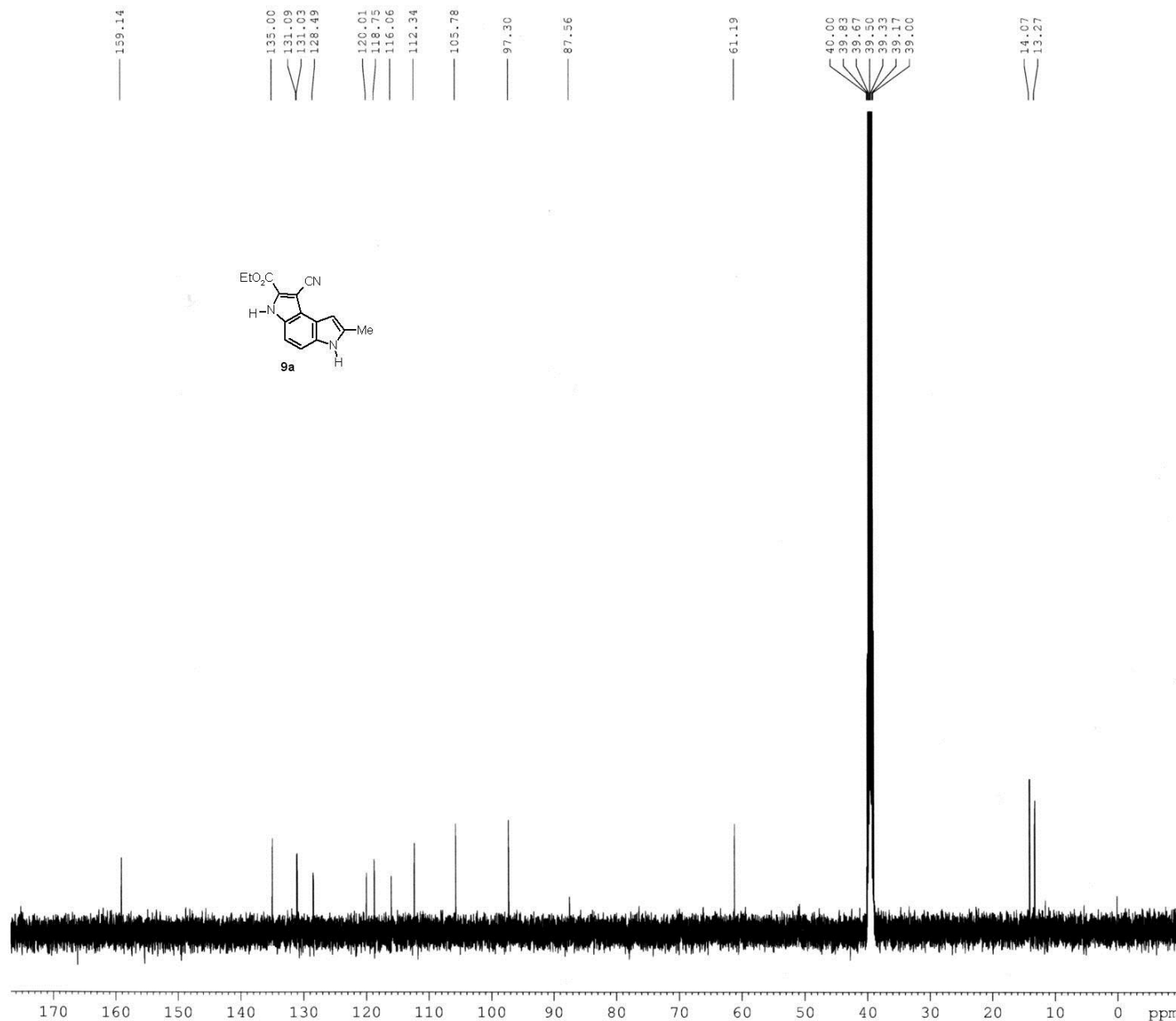
===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -3.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 98.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 32.00 dB
 SFO2 500.1320005 MHz

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.132 MHz
 FIDRES 7.812500 Hz
 SW 1.999 ppm
 FnMODE QF

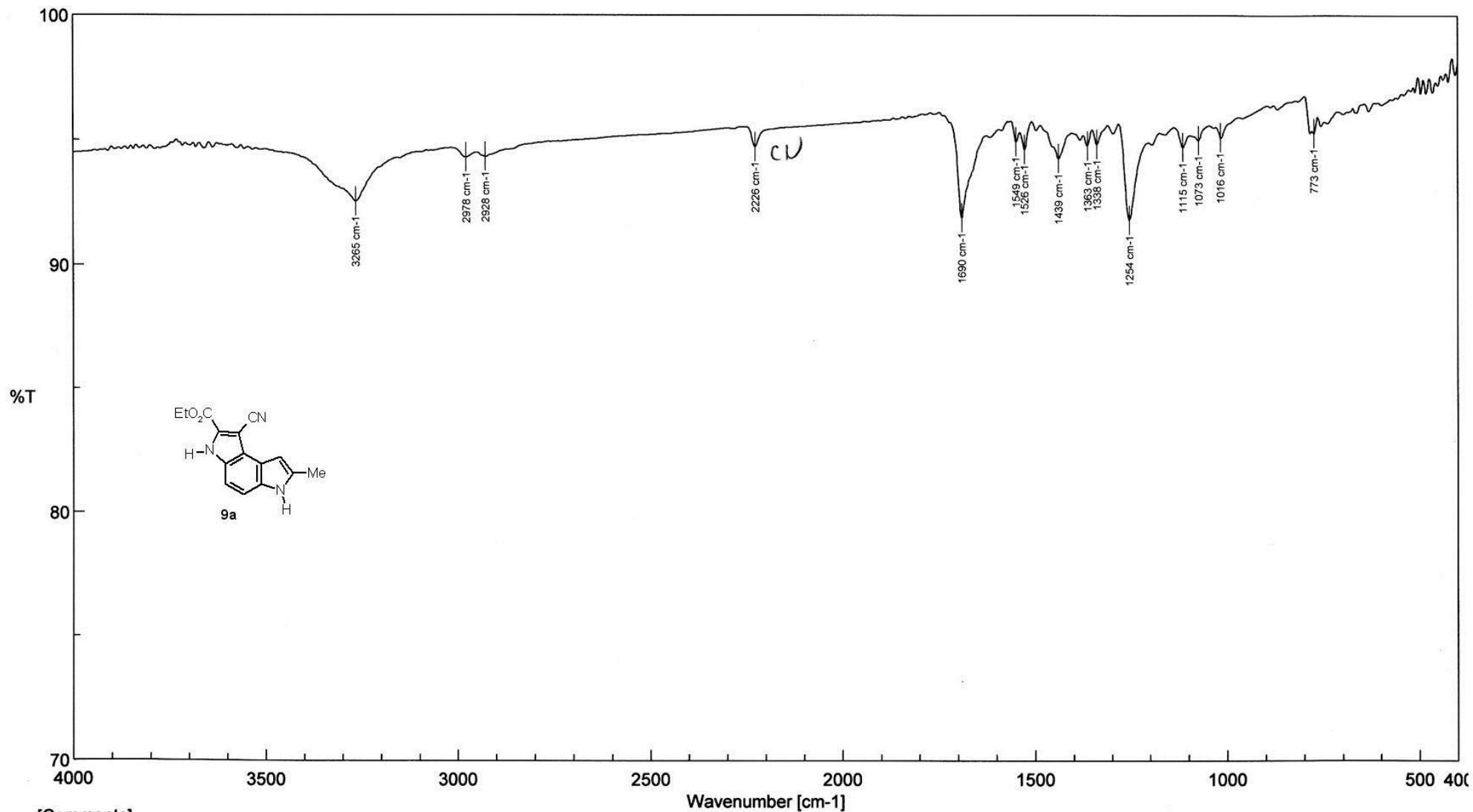
F2 - Processing parameters
 SI 262144
 SF 125.7578564 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.30 Hz
 GB 0.1



JASCO FT/IR-6200

ICHO PAN Pracownia Spektroskopii Optycznej



[Comments]

Sample name IND-363/B; film z CH₂Cl₂
 Comment Pan Robert Bujok
 User Alicja
 Division Pracownia Spektroskopii Optycznej
 Company IChO PAN

13041204.jws

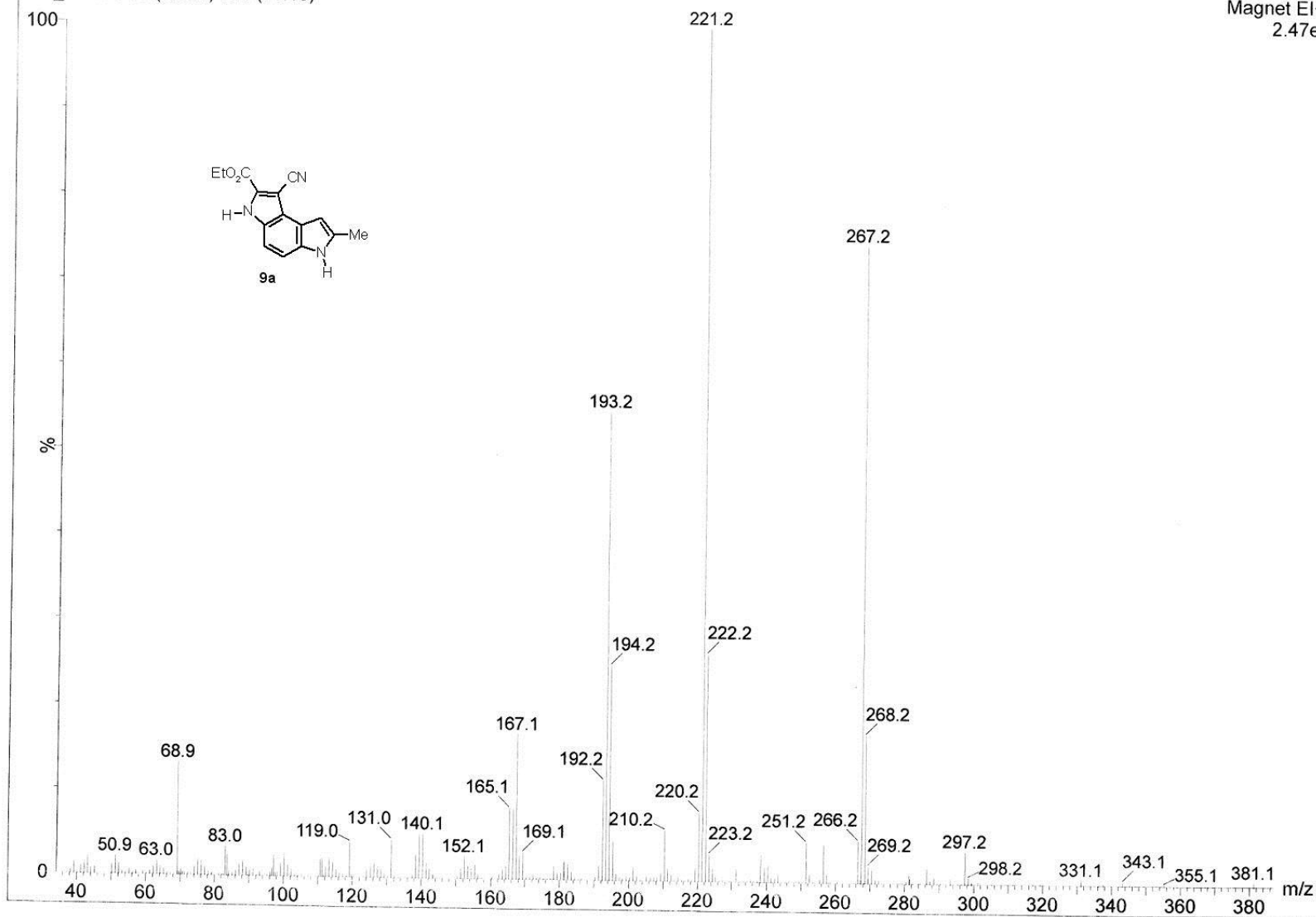
R. Bujok
IND-363/B

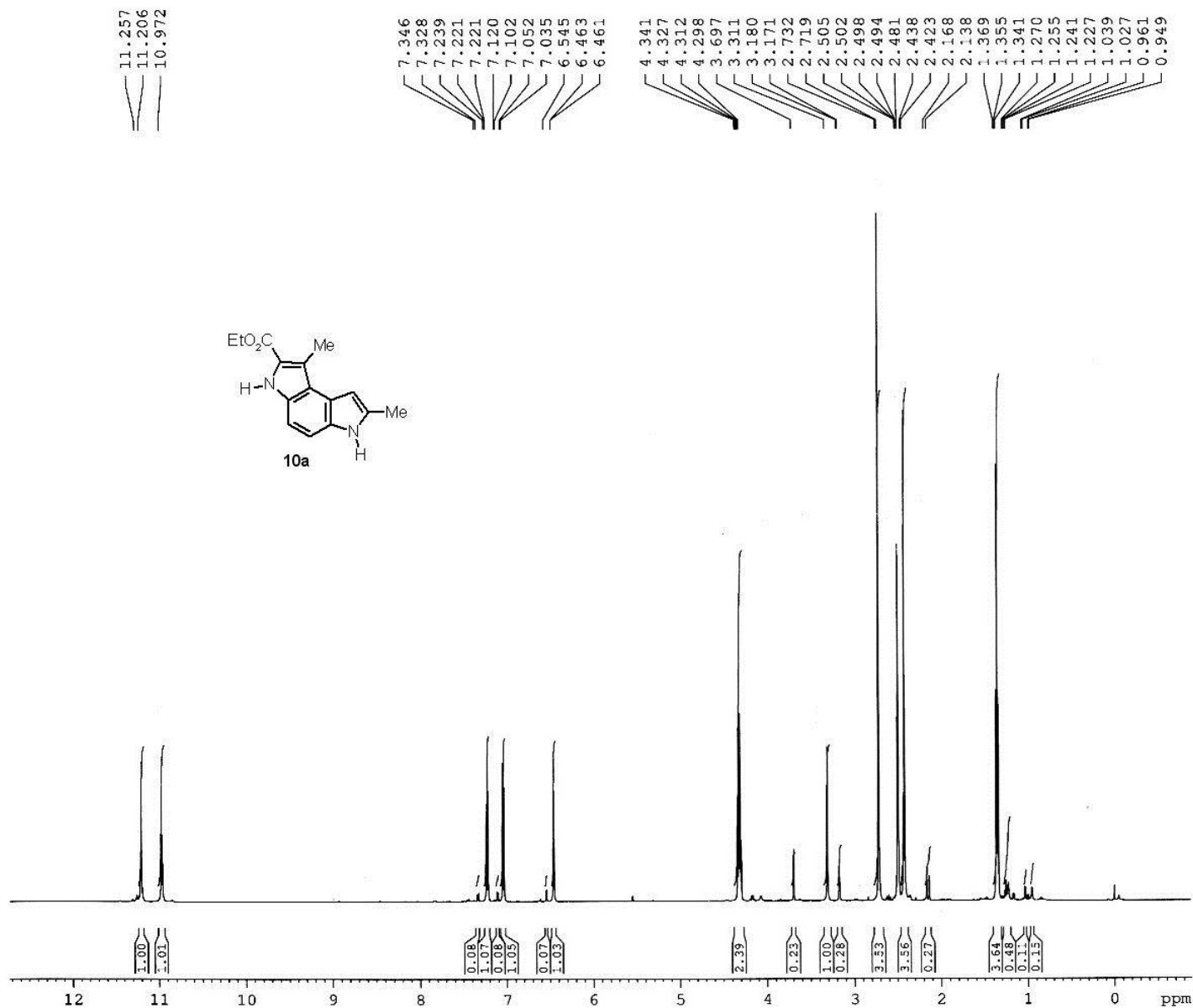
AUTOSPEC

12-Apr-2013 12:34:28
operator: Malgorzata Grela

z07_rb1153 12 (0.951) Cm (11:13)

Magnet EI+
2.47e4





Current Data Parameters
 NAME IND-361-K
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130411
 Time 8.59
 INSTRUM DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 161.3
 DW 48.400 usec
 DE 6.78 usec
 TE 303.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 8.20 usec
 PL1 5.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300065 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME IND-361-K
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130411
 Time_ 9.22
 INSTRUM DRX
 PROBHD 5 mm TBI 1H/13
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 1125
 DS 4
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027508 sec
 RG 32768
 DW 15.300 usec
 DE 7.10 usec
 TE 303.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 DELTA 0.89999998 sec
 TD0 1

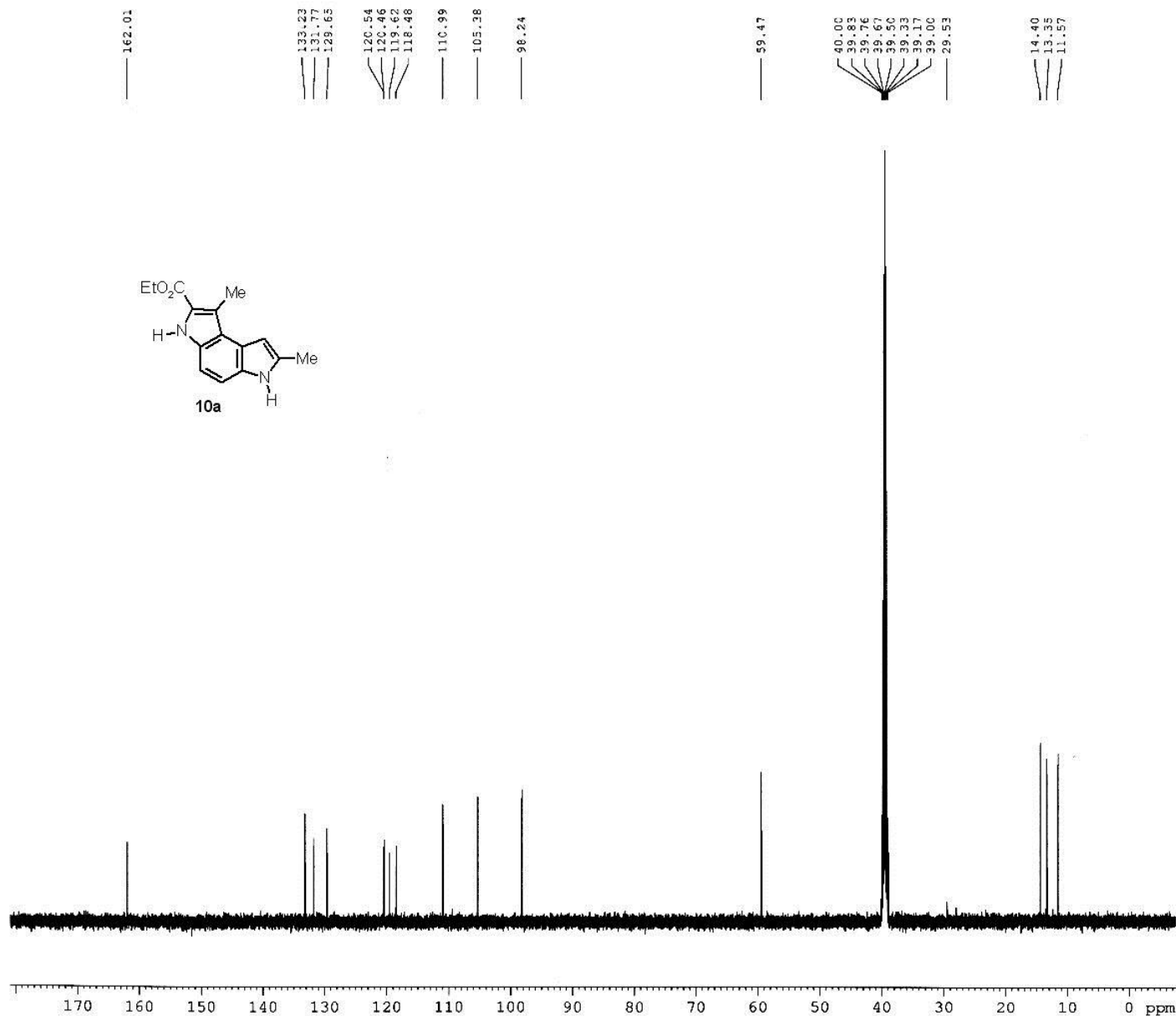
===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -3.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P1 98.00 usec
 PL2 3.00 dB
 PL12 23.00 dB
 PL13 32.00 dB
 SFO2 500.1320005 MHz

F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.132 MHz
 FIDRES 7.812500 Hz
 SW 1.999 ppm
 F1MODE QF

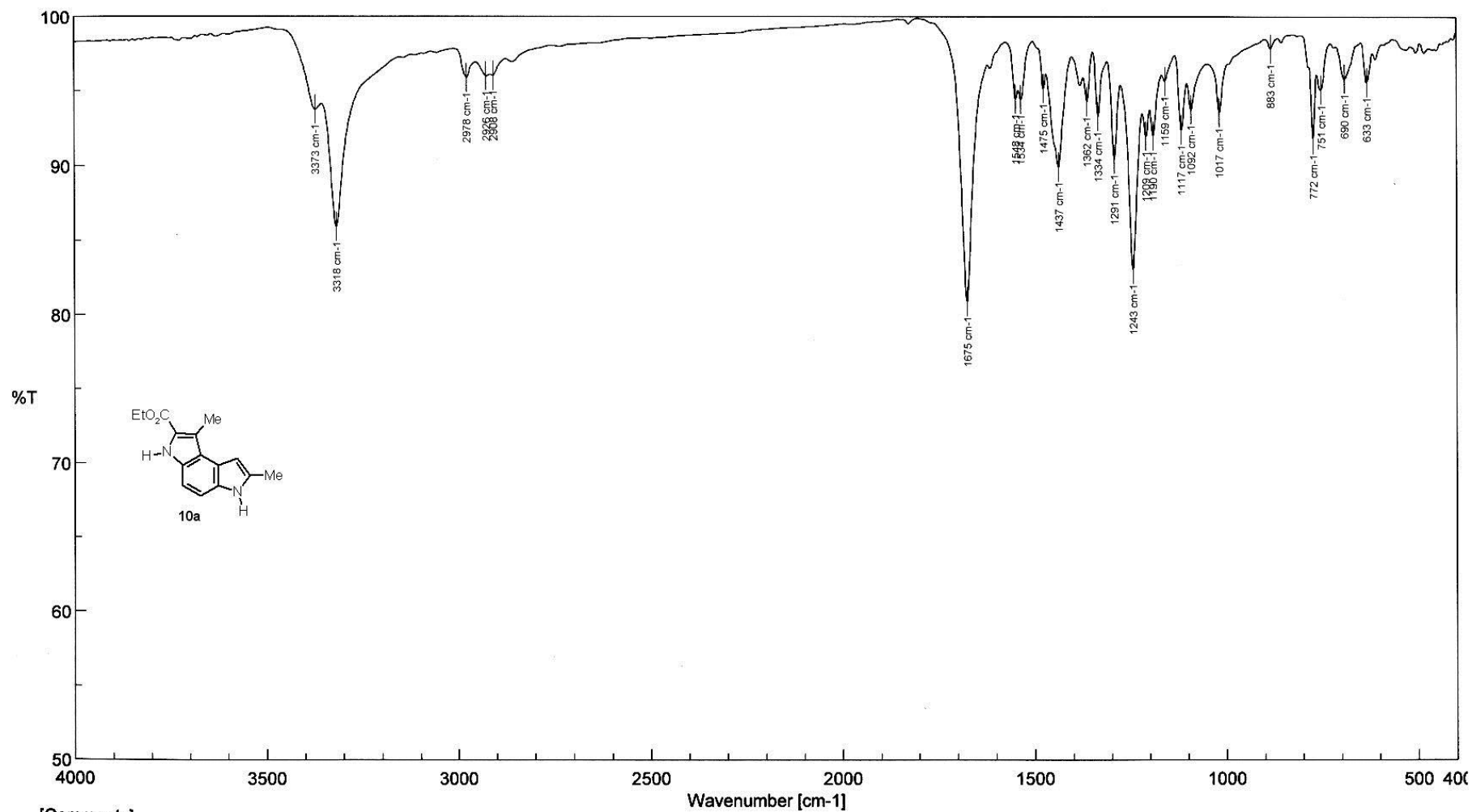
F2 - Processing parameters
 SI 262144
 SF 125.7578561 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.30 Hz
 GB 0.1



JASCO FT/IR-6200

IChO PAN Pracownia Spektroskopii Optycznej



[Comments]

Sample name IND-361/K; w KBr
 Comment Pan Robert Bujok
 User Alicja
 Division Pracownia Spektroskopii Optycznej
 Company IChO PAN

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