

Efficient synthesis of pyrene-1-carbothioamides and carboxamides. Tunable solid-state fluorescence of pyrene-1-carboxamides

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Supplementary Information

(S1) Fluorescence measurements

(S2) CIE chromacity coordinates for compounds **2a-d,h,k-m**.

(S3) X-ray diffraction analysis of *N*-tert-butylpyrene-1-carboxamide **2c**

(S4) IR, ¹H and ¹³C NMR spectra of the synthesized compounds

(S1) Fluorescence measurements:

Corrected fluorescence spectra were obtained on a Fluorolog FL3-221 spectrofluorometer from Horriba Jobin-Yvon, including an integration sphere accessory which allows to record excitation and emission spectra and to determine absolute quantum yield values in the powder state.

Fluorescence decay curves recorded by the time-correlated single-photon counting (TCSPC) method were obtained with femtosecond laser excitation using a Spectra-Physics set-up composed of a Titanium Sapphire laser (Tsunami, Spectra-Physics) pumped by a doubled YAG laser (Millennia, Spectra-Physics), which itself was pumped by two laser diode arrays. Light pulses at 740 nm were selected by optoacoustic crystals at a repetition rate of 4 MHz and then doubled at 370 nm by non-linear crystals. Fluorescence photons were detected through a monochromator by means of a Hamamatsu MCP R3809U photomultiplier connected to a constant-fraction discriminator. The time-to-amplitude converter was purchased from Tennelec. The instrumental response function was recorded before each decay measurement. The fluorescence data were analyzed using the Globals software package developed at the Laboratory for Fluorescence Dynamics at the University of Illinois at Urbana-Champaign, which includes reconvolution analysis and the global non-linear least-squares minimization method.

Fluorescence decay curves recorded using the laser flash photolysis spectrometer were obtained using an Edinburgh instrument LP920, with an NdYAG laser (Continuum) and a tripling crystal used to reach 355nm excitation. The Levenberg-Marquardt algorithm was used for non-linear least square fit (tail fit) as implemented in the L900 software (Edinburgh instrument). The weighted residuals were calculated in order to estimate the quality of the fit.

(S2) CIE chromacity coordinates for compounds 2a-d,h,j-l.

Table 2. CIE chromacity coordinates for compounds **2a-d,h,j-l**.

Compound	x	y
2a	0,1851	0,1663
2b	0,2321	0,4442
2c	0,1535	0,1556
2d	0,1665	0,1832
2h	0,1968	0,296
2j	0,1609	0,2637

2k	0,1736	0,154
2l	0,4056	0,4896

(S3) X-ray diffraction analysis of *N*-tert-butylpyrene-1-carboxamide **2c**

CCDC deposition number 1006140

Crystals suitable for X-ray analysis were obtained after a long standing (2-3 weeks) in a concentrated solution in DMSO in an open tube at room temperature. The crystals were colorless prisms.

Data for the crystal of **2c** were collected on an Agilent Supernova 4 circle diffractometer system equipped with a copper and molybdenum microsource and an Atlas CCD detector. The data were collected using copper radiation with CrysAlis171[i] software and integrated with CrysAlisPRO [ii] software. Data were corrected for absorption effects using the multi-scan method (SCALE3 ABSPACK[i]).

The structure was solved by direct methods using SXELXS[vi] and refined by full-matrix least squares procedure with SHELXL[vi] within the OLEX2[vii] graphical interface. Figures were produced using Ortep3v2[viii] and Mercury_3.3[ix] software.

All H atoms were visible in the residual density map, but were added geometrically and refined in riding approximation. The position of the H atom involved in the hydrogen bond was refined with restraint applied to the N – H distance as suggested by SHELXL[vi] for 100K.

The quantitative descriptors of the data processing and structure refinement for all compounds are presented in Table .

Identification code	2c
Empirical formula	C ₂₁ H ₁₉ NO
Formula weight	301.37
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	13.5079(4)
b/Å	11.1040(4)

c/Å	10.4205(3)
α /°	90
β /°	97.455(3)
γ /°	90
Volume/Å ³	1549.78(8)
Z	4
ρ calc/mg/mm ³	1.292
μ /mm ⁻¹	0.614
F(000)	640
Crystal size/mm ³	0.3×0.12×0.02
	CuK α
Radiation Å	(λ = 1.54184)
2 Θ range for data collection	7.962° to 153.866°
	-17 ≤ h ≤ 16,
	-13 ≤ k ≤ 13,
Index ranges	-12 ≤ l ≤ 8
Reflections collected	7469
Independent reflections	3213
Rint	0.0204
Rsigma	0.0316
Data/restraints	
/parameters	3213/1/214
Goodness-of-fit on F ²	1.042
	R1 = 0.0418,
Final R indexes [$I \geq 2\sigma(I)$]	wR2 = 0.1136
Final R indexes	R1 = 0.0492,
[all data]	wR2 = 0.1212
Largest diff. peak/hole / e	
Å ⁻³	0.264/-0.188

REFERENCES

[i] CrysAlisPro, Agilent Technologies, Version 1.171.36.20 (release 01-02-2013
CrysAlis171.NET)

[ii] CrysAlisRED, Agilent Technologies, Version 1.171.36.20 (release 01-02-2013
CrysAlis171.NET)

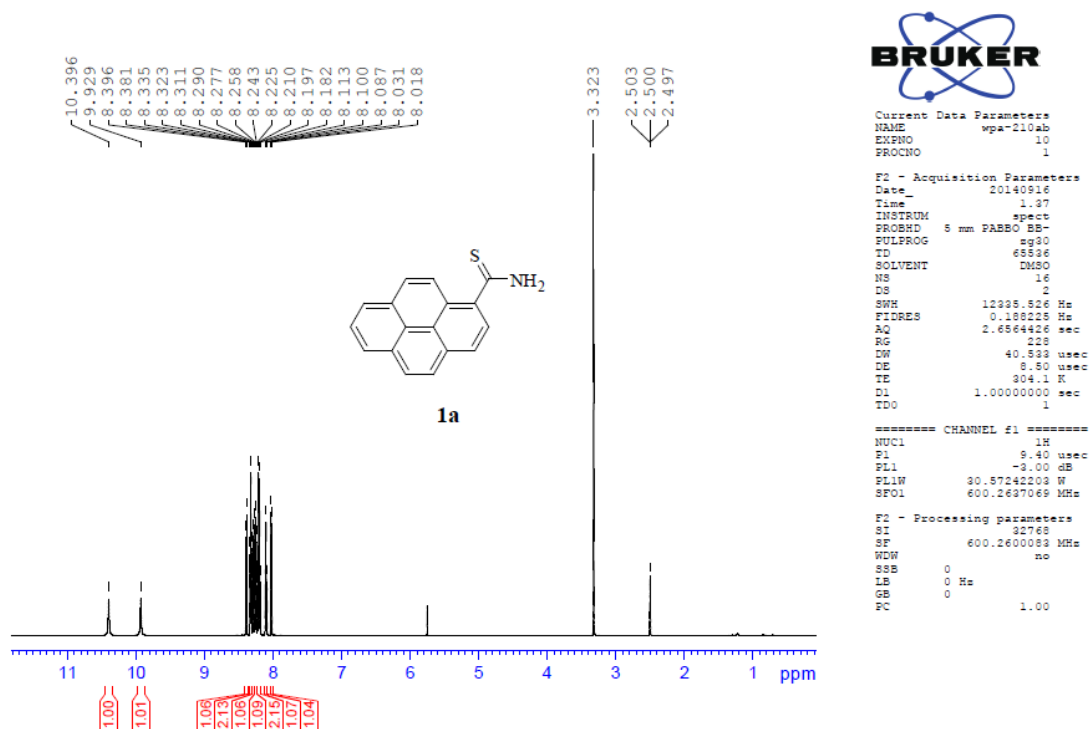
[vi] SHELX: G. Sheldrick, A short history of SHELX, Acta Crystallographica Section A, 64
(2008) 112-122.

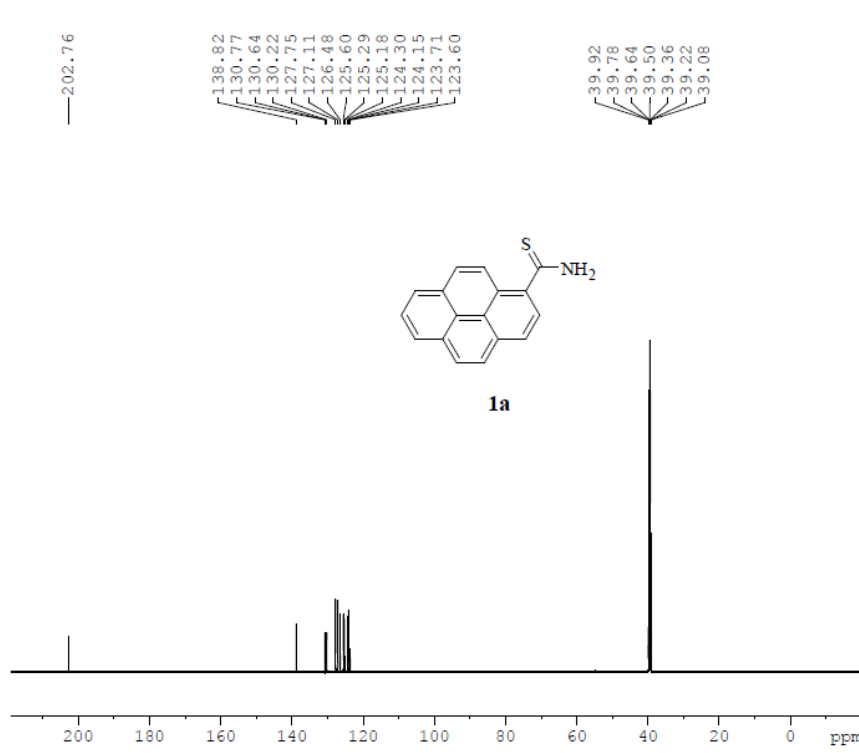
[vii] OLEX2: O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann,
OLEX2: a complete structure solution, refinement and analysis program, Journal of Applied
Crystallography, 42 (2009) 339-341.

[viii] ORTEP: L. J. Farrugia, *J. Appl. Cryst.* (2012), **45**, 849-854

[ix] MERCURY: C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R.
Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.*, 39, 453-457, **2006**.

(S4) IR, ¹H and ¹³C NMR spectra of the synthesized compounds





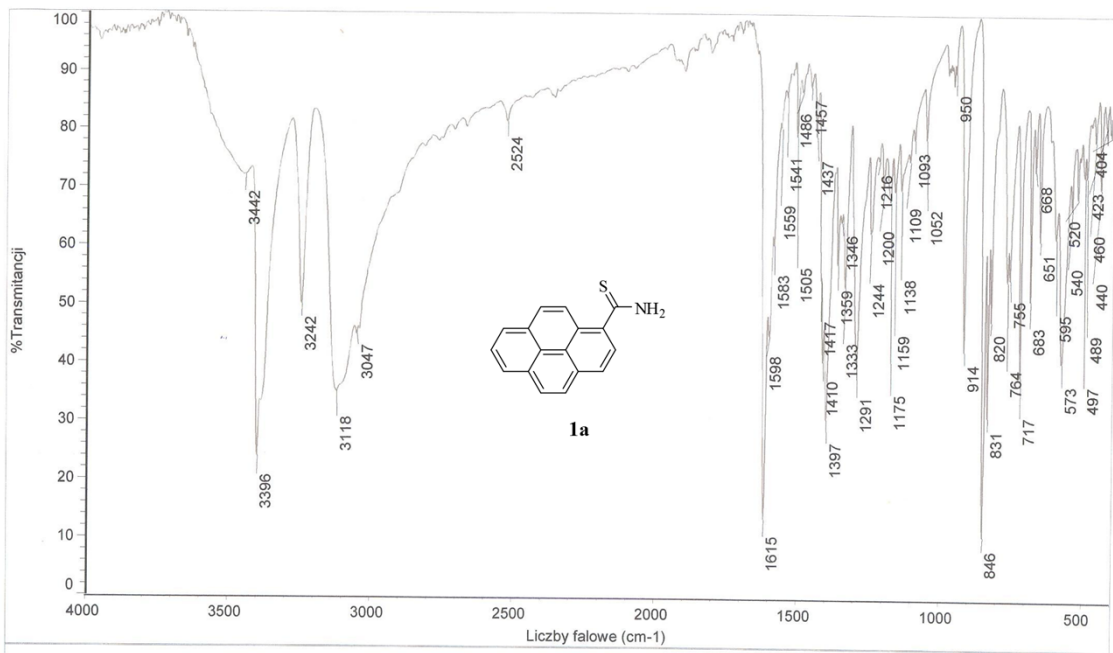
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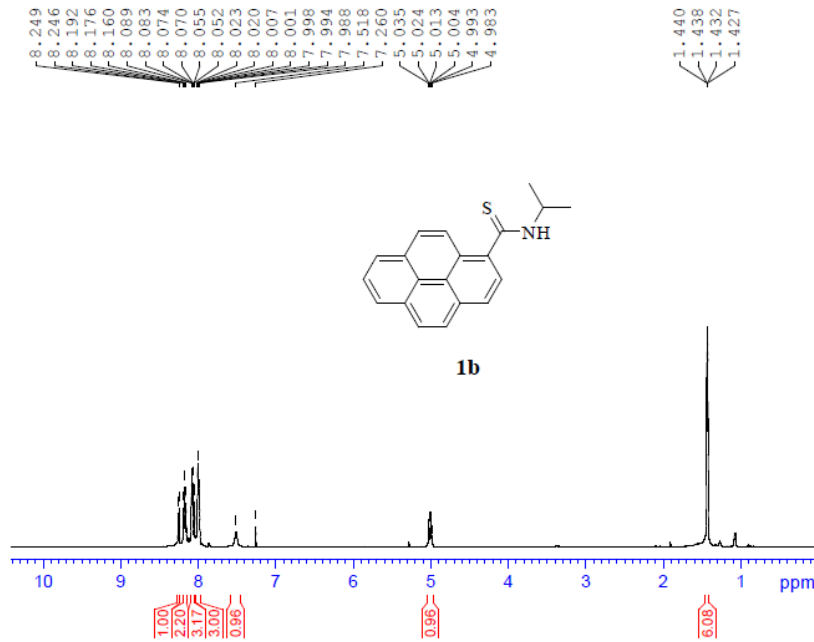
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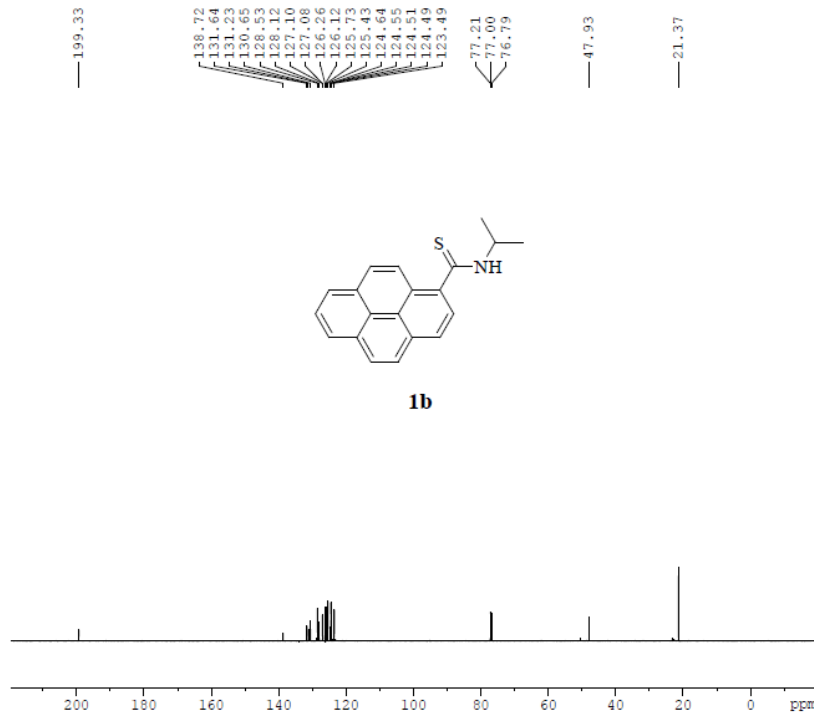


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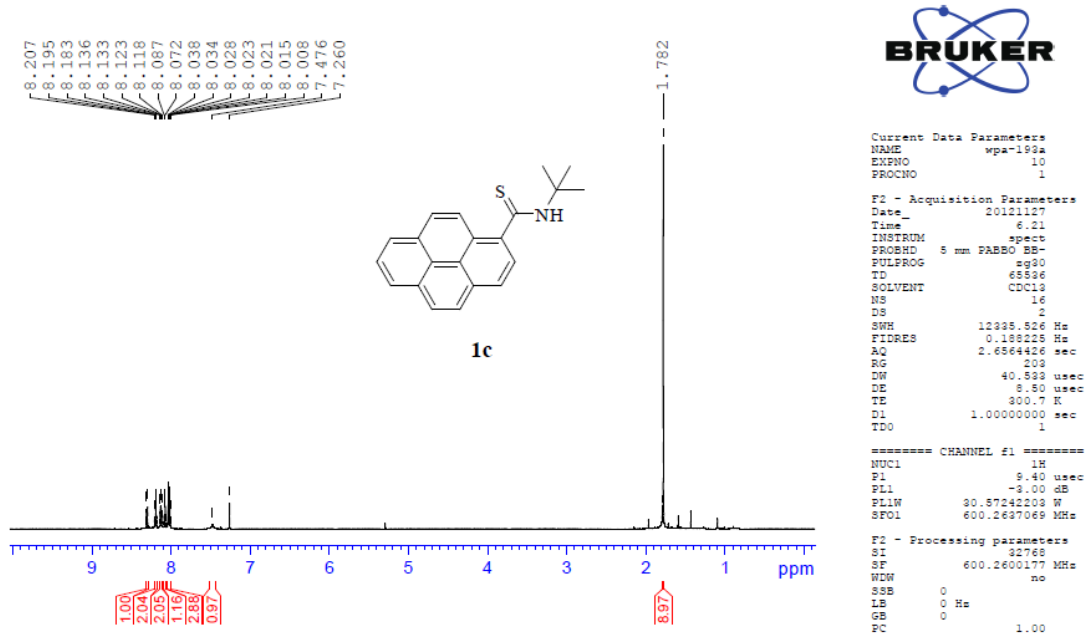
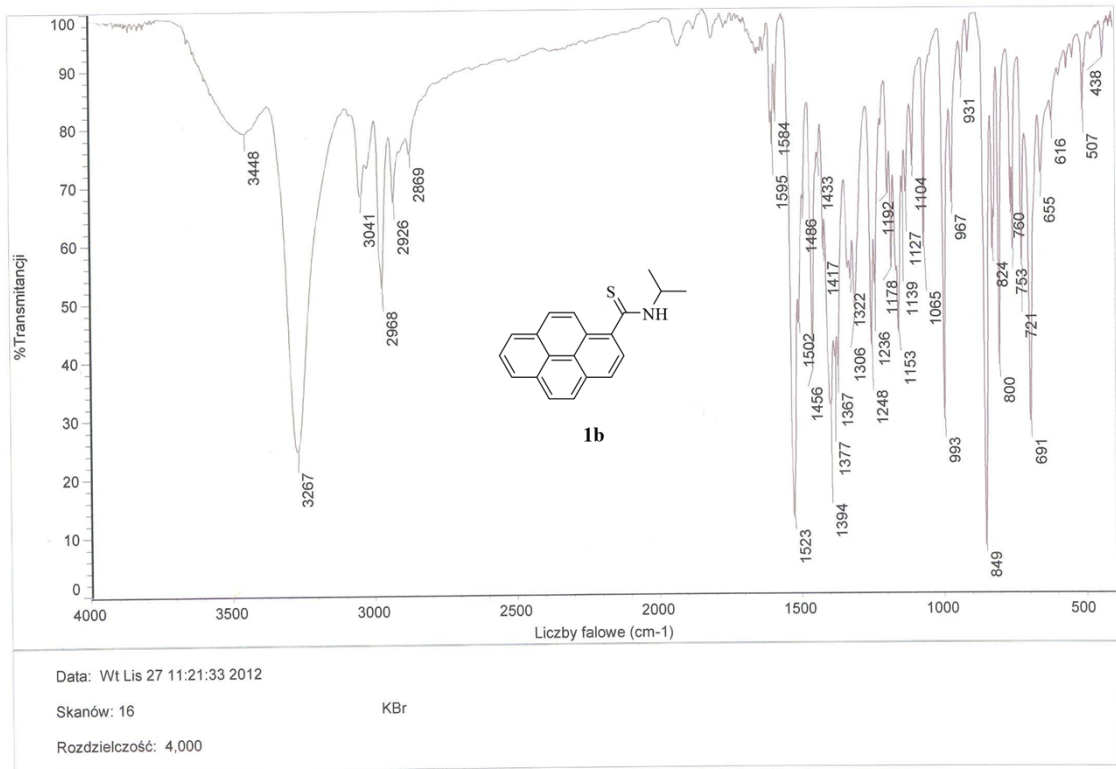
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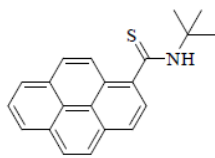
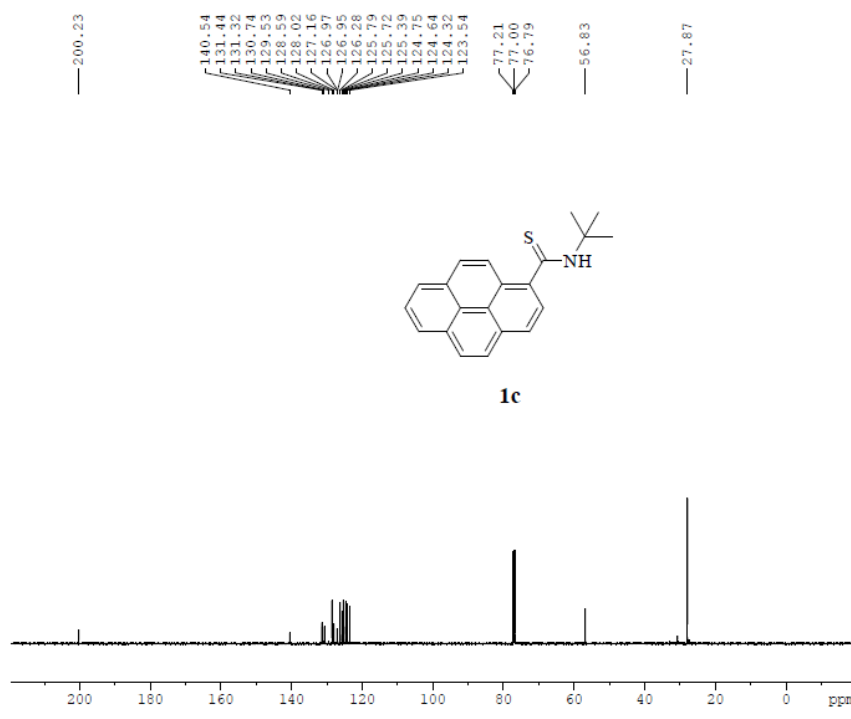
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PL1W 0.24284597 W
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1c



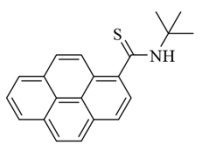
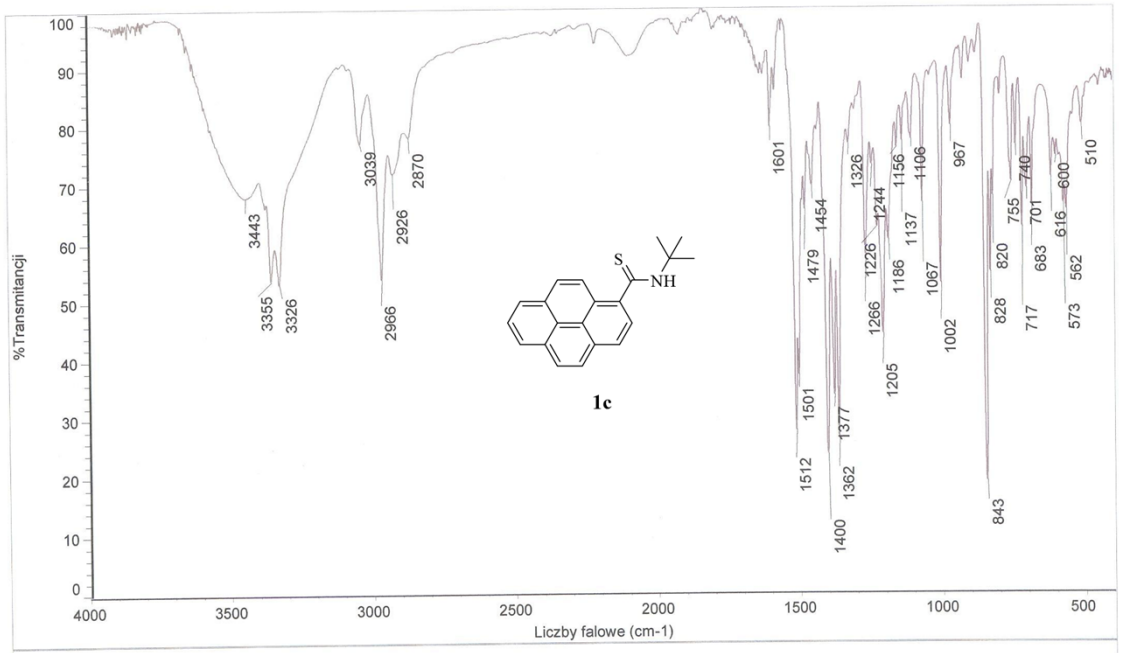
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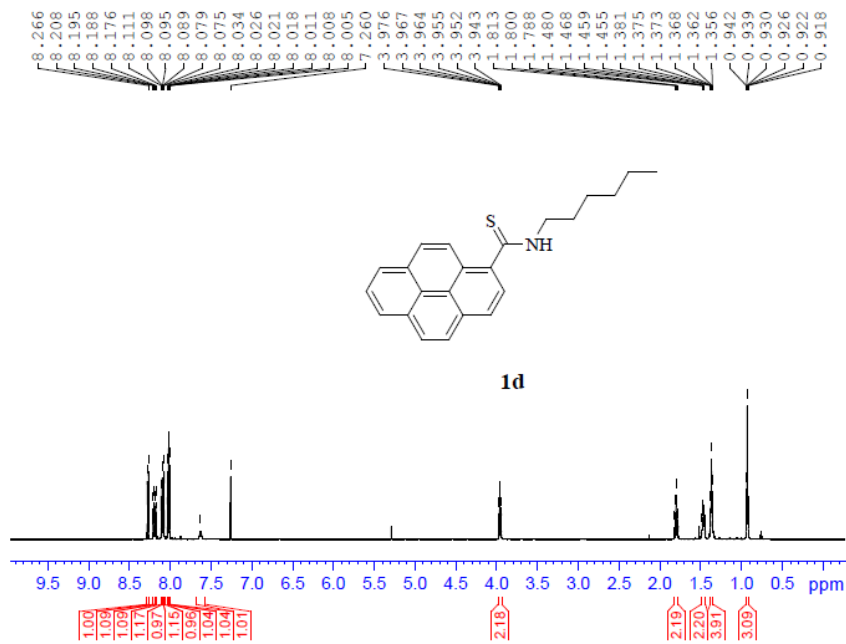
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1c

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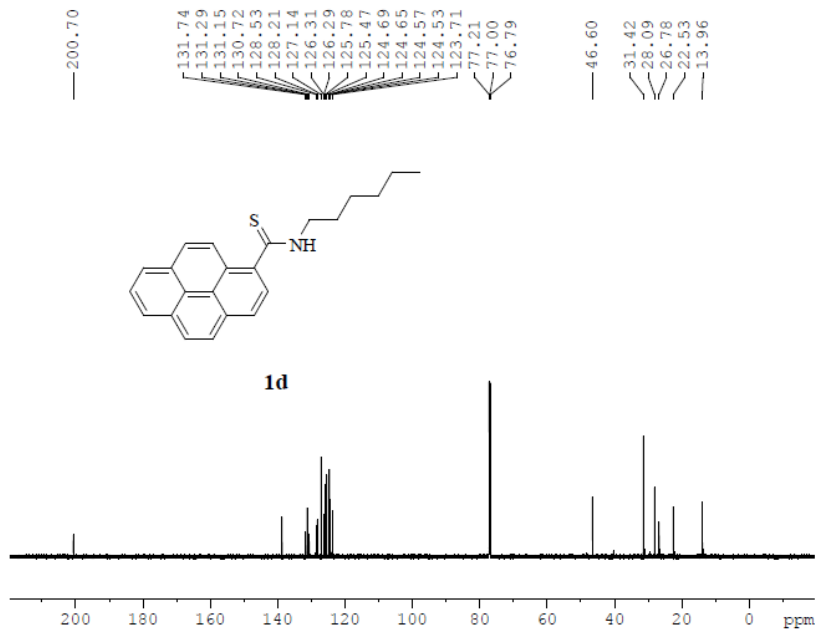


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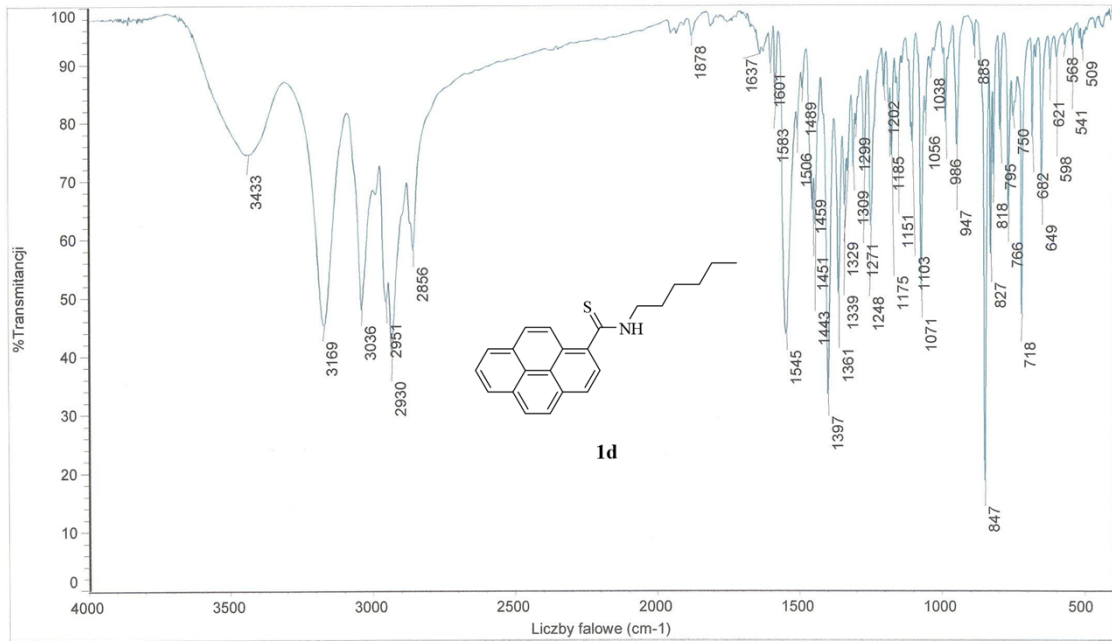
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 AQ 0.9088159 sec
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 PL13 18.00 dB
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 PL13W 0.24284837 W
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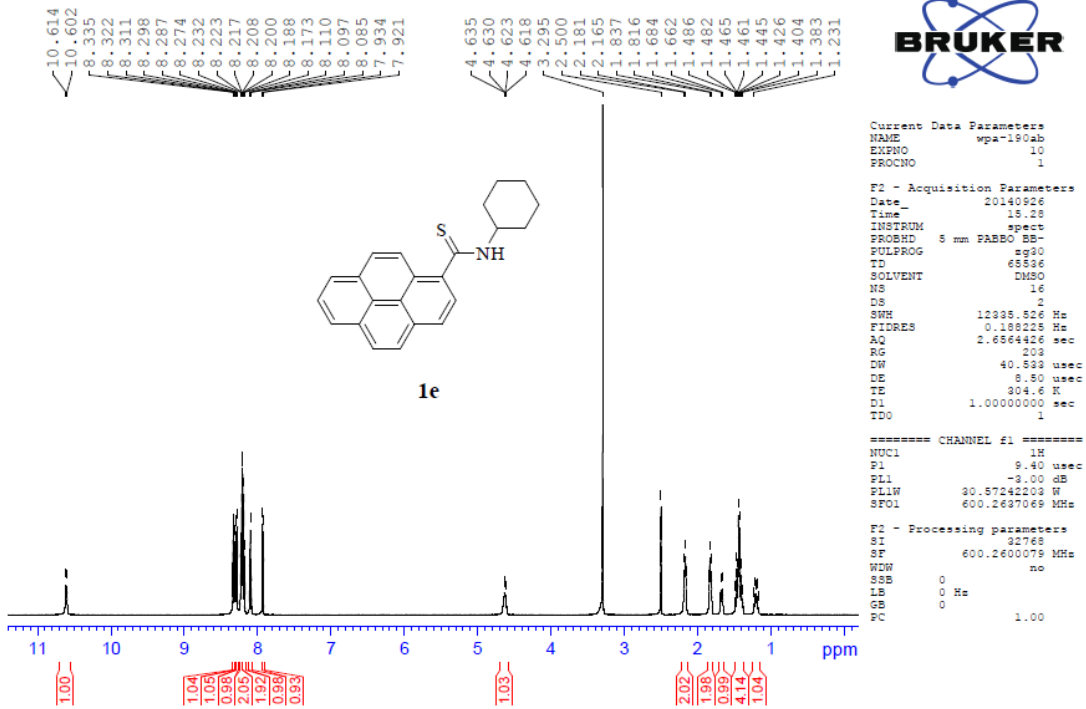


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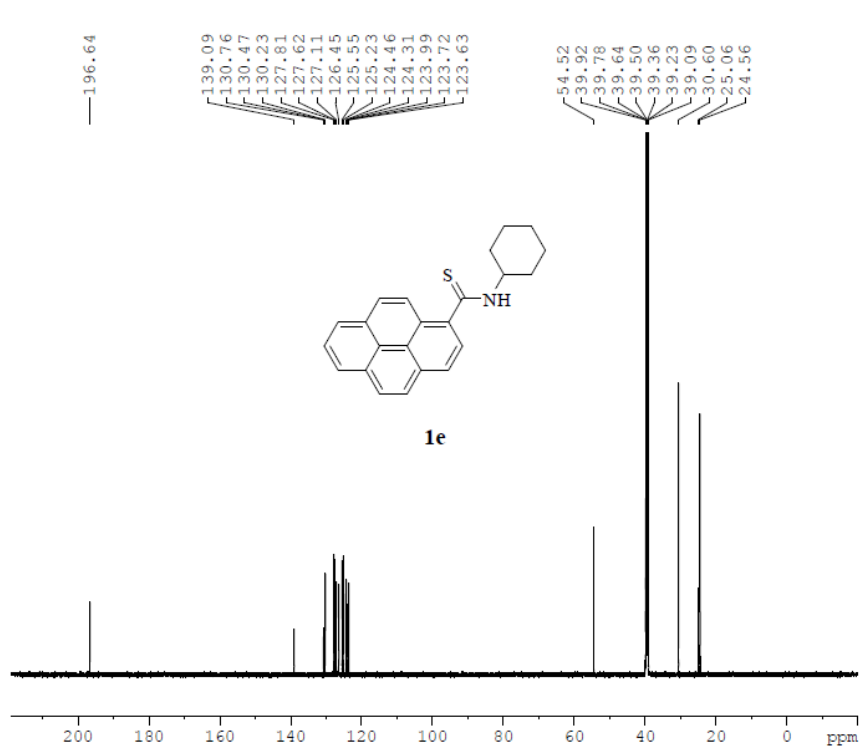
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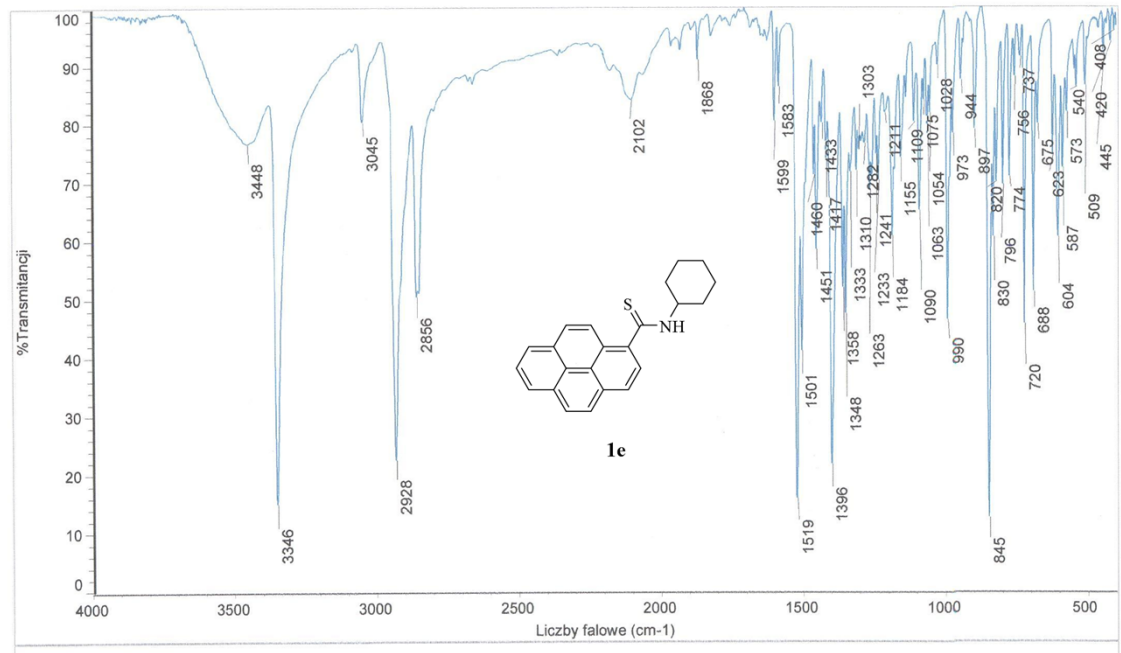
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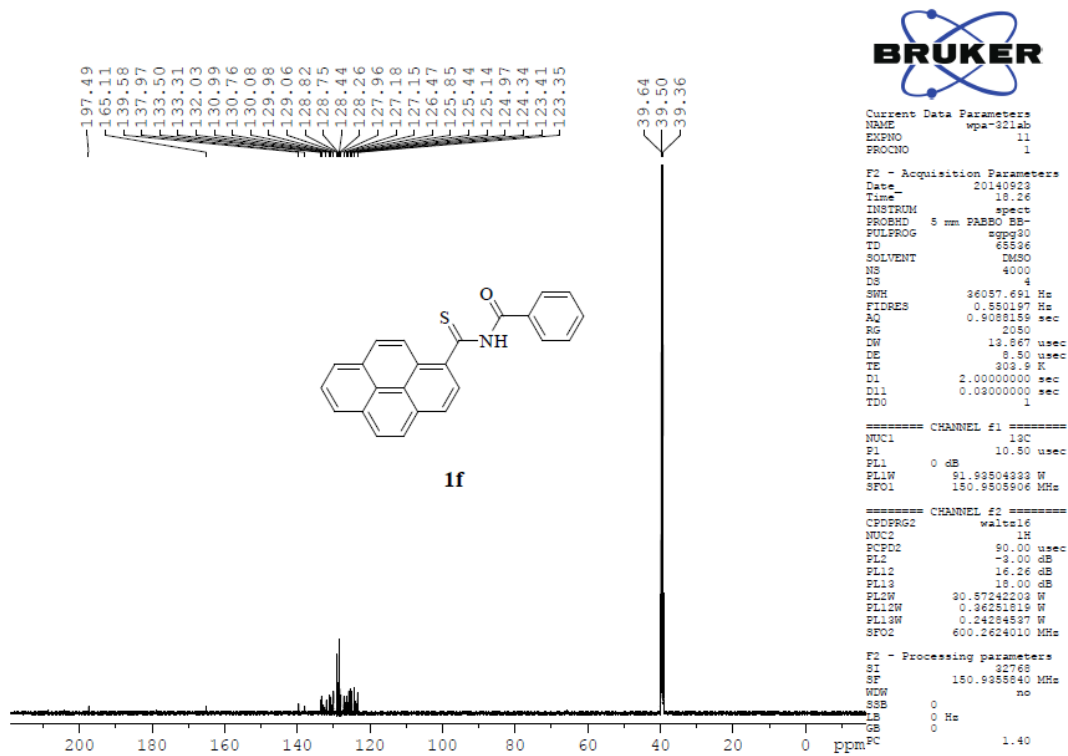
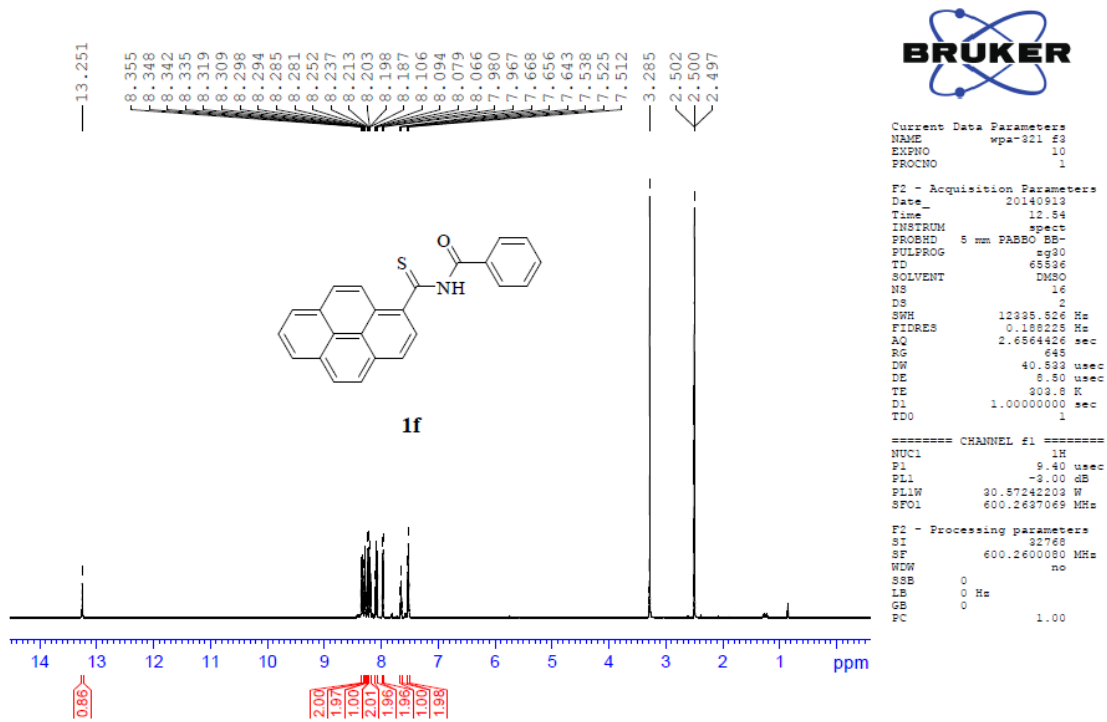
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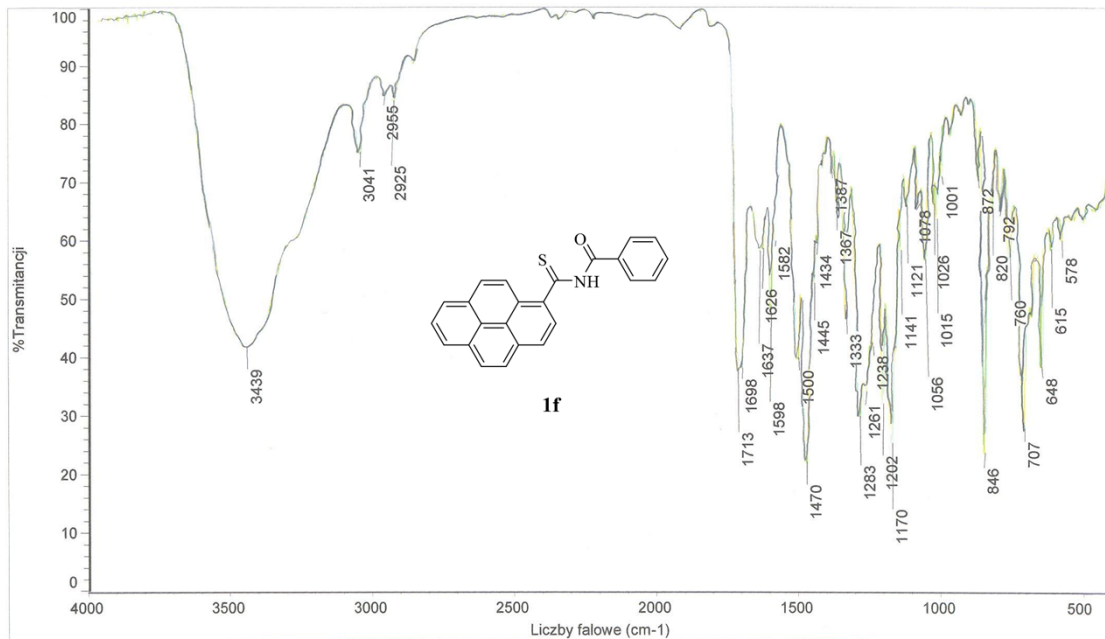
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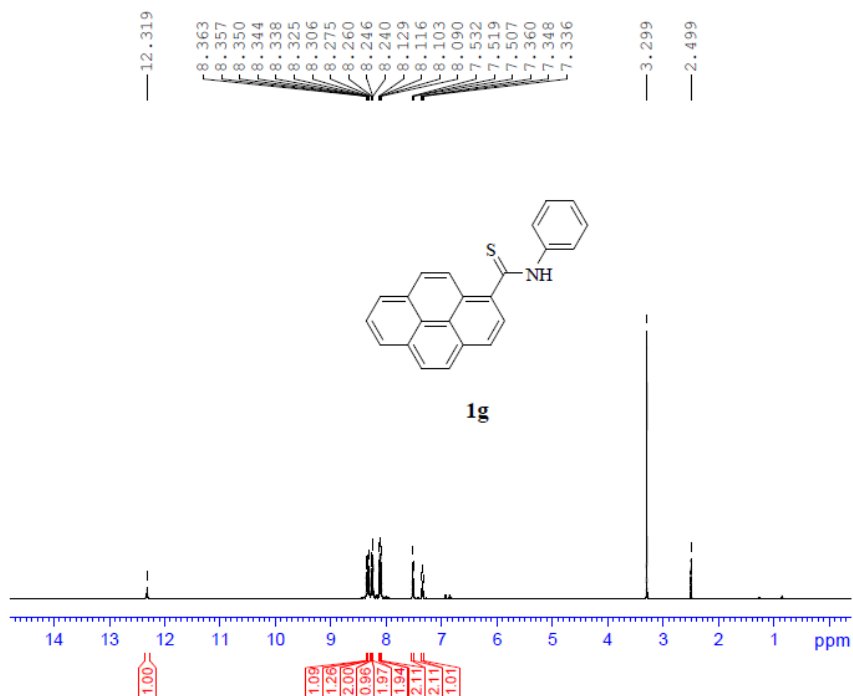


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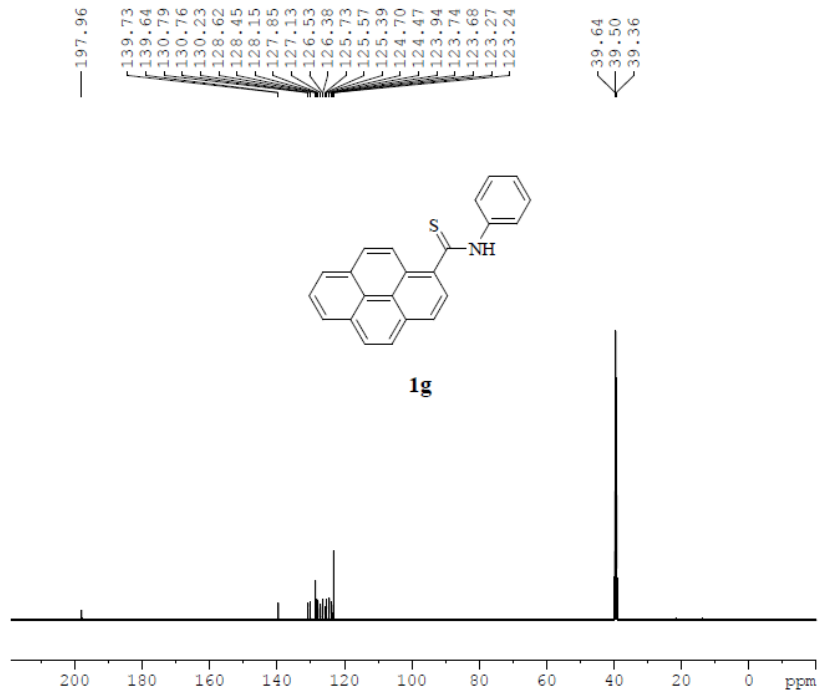
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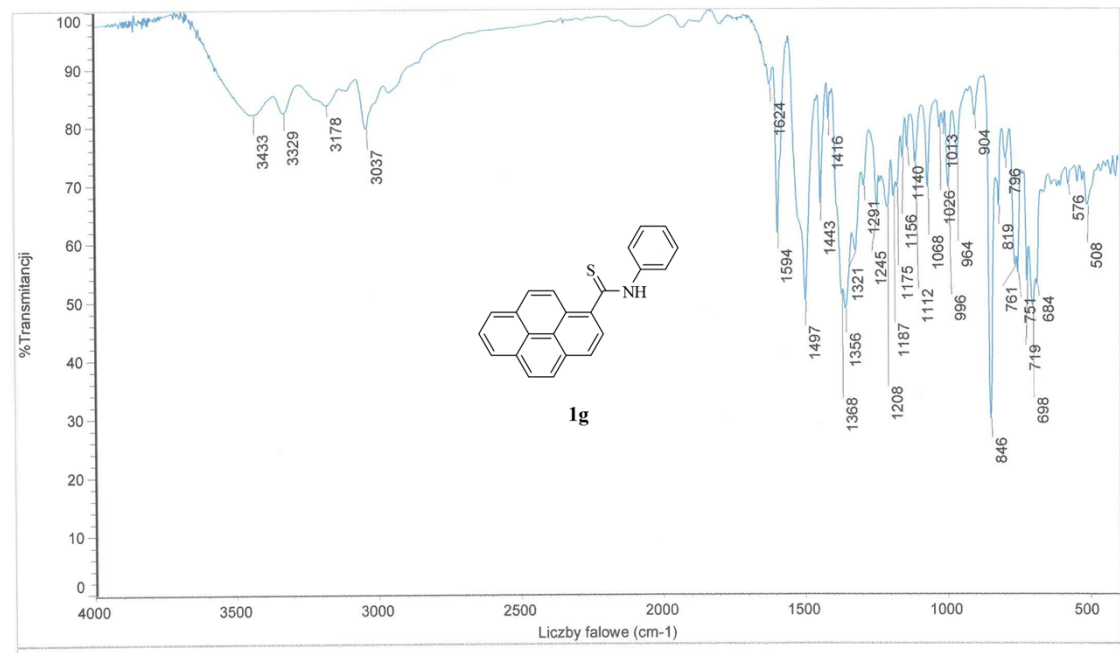
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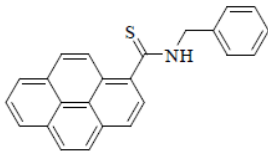
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Skanów: 16

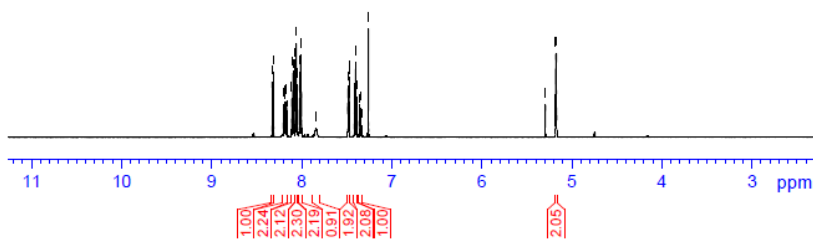
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Rozdzielczość: 4,000

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1h



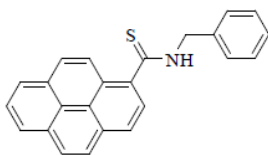
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DW 40.533 usec
DE 8.50 usec
TE 300.8 K
D1 1.00000000 sec
TDO 1

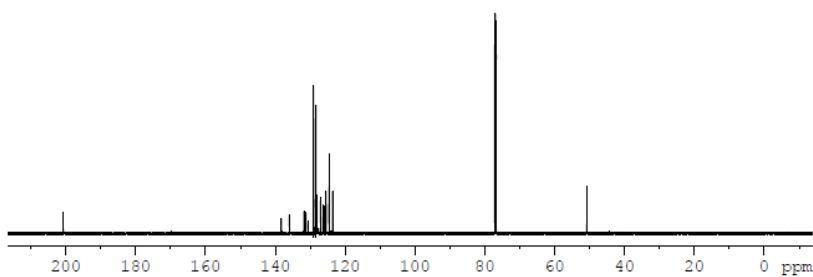
===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 -2.00 dB
PL1W 30.57242203 W
SF01 600.2637069 MHz

F2 - Processing parameters
SI 32768
SF 600.2600173 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

200.81
138.34
136.04
131.88
131.28
130.68
129.06
128.86
128.63
128.44
128.32
128.32
128.28
127.63
127.13
126.43
126.34
125.83
125.53
124.71
124.68
124.53
123.66
77.21
77.00
76.79
50.81



1h



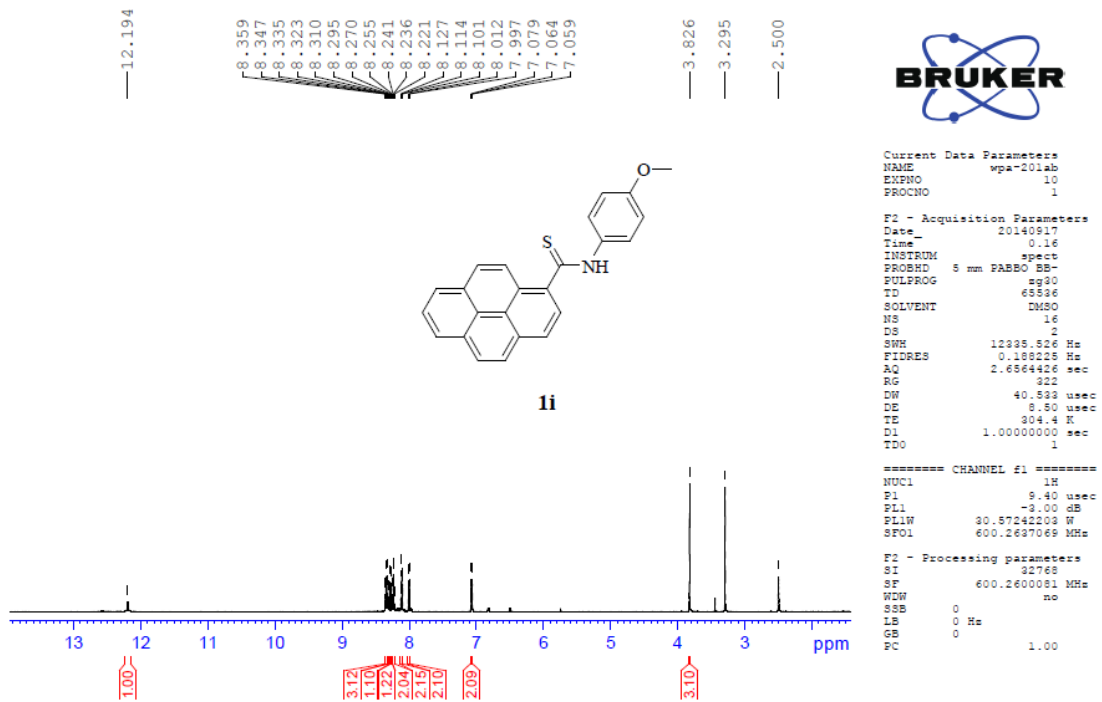
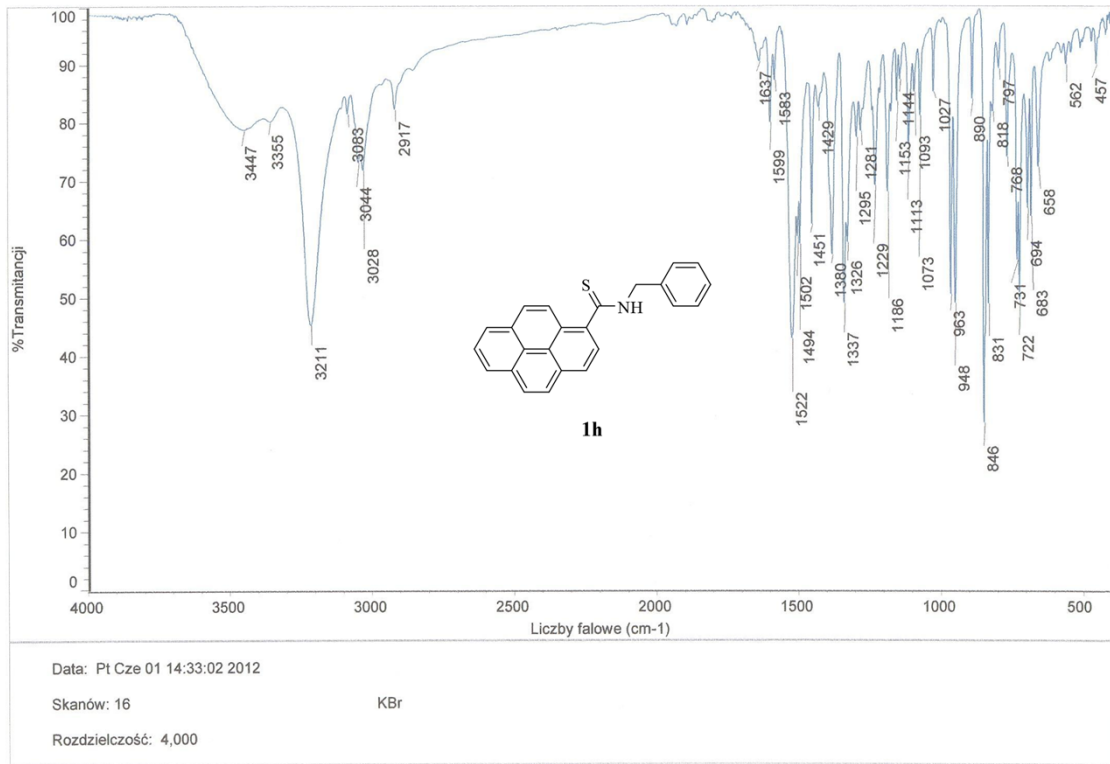
Current Data Parameters
NAME wpa-200a
EXPNO 11
PROCNO 1

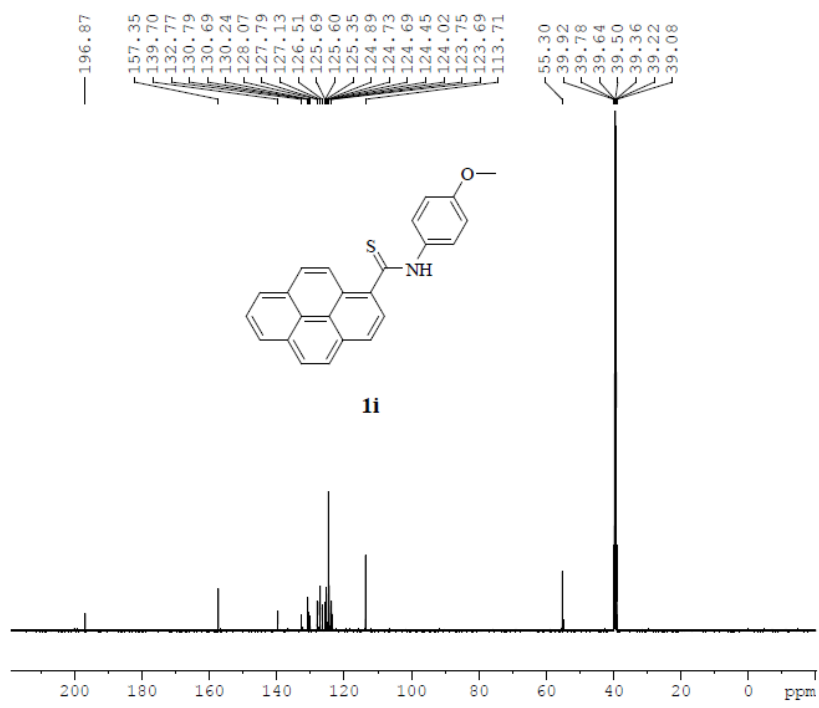
F2 - Acquisition Parameters
Date_ 20121122
Time 6.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2500
DS 4
SWH 36057.691 Hz
FIDRES 0.580197 Hz
AQ 0.9080159 sec
RG 2050
DW 13.867 usec
DE 8.50 usec
TE 300.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL1W 51.93504233 W
SF01 150.9505906 MHz

===== CHANNEL f2 =====
CDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.26 dB
PL13 18.00 dB
PL2W 30.57242203 W
PL12W 0.34251819 W
PL13W 0.34251819 W
SF02 600.2624010 MHz

F2 - Processing parameters
SI 32768
SF 150.9355007 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40





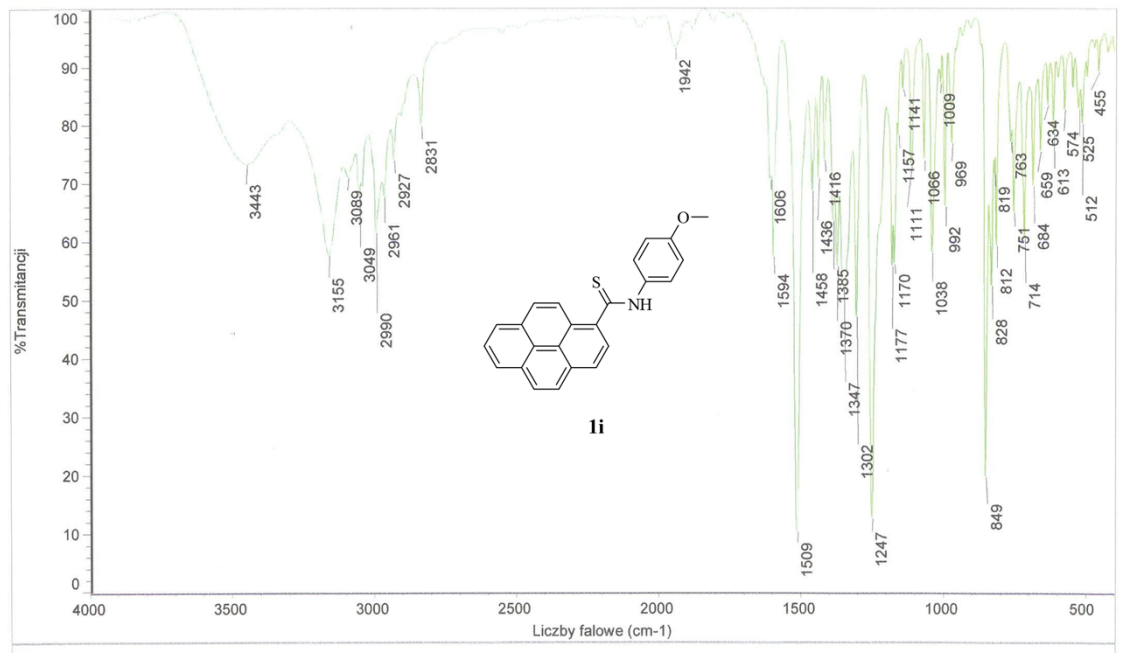
Current Data Parameters
 NAME mpa-201ab
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140817
 Time 8.26
 INSTRUM spect
 PROBHD 5 mm F4BBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9088159 sec
 RG 2050
 SFO 200.130 MHz
 DE 13.867 usec
 TE 8.50 usec
 TB 304.1 K
 FI 2.0000000 sec
 DL1 0.0300000 sec
 TDO 1

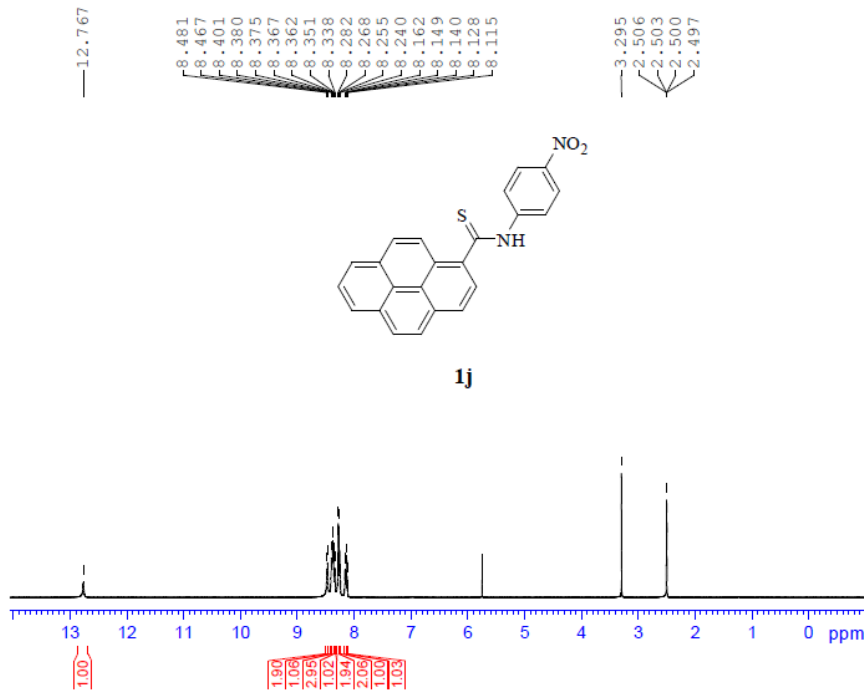
==== CHANNEL f1 =====
 NUCL1 13C
 P1 10.50 usec
 PL1 0 dB
 PL1W 91.93504833 W
 SFO1 150.9355806 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.000 dB
 PL2W 16.00000000 W
 PL3 18.000 dB
 PL3W 30.57242203 W
 PL12W 0.36251319 W
 PL13W 0.24284537 W
 SFO2 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.9355806 MHz
 WDW no
 SSB no
 GB 0
 PC 1.40



Data: Wt Cze 05 12:00:25 2012
 Skanów: 16
 Rozdzielczość: 4,000
 KBr

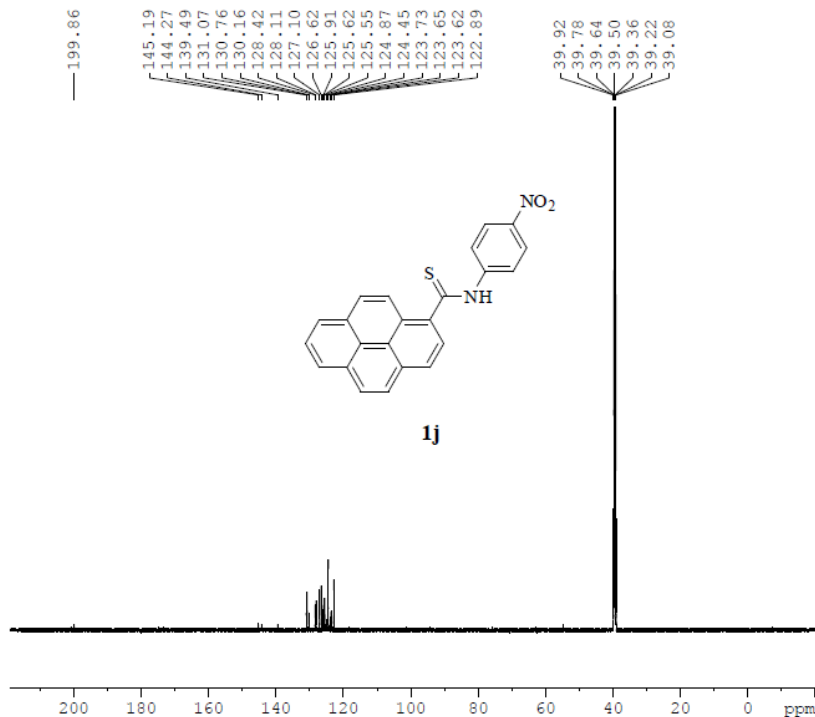


Current Data Parameters
 NAME wpa-320a
 EXPMO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140913
 Time 9.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 FIDRES 0.158235 Hz
 AQ 2.6564426 sec
 RG 456
 DW 40.523 usec
 DE 8.50 usec
 TE 303.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUCL1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.57242209 W
 SFO1 600.2637069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.2600084 MHz
 WDW no
 SSB no
 LB 0 Hz
 GB 0
 PC 1.00



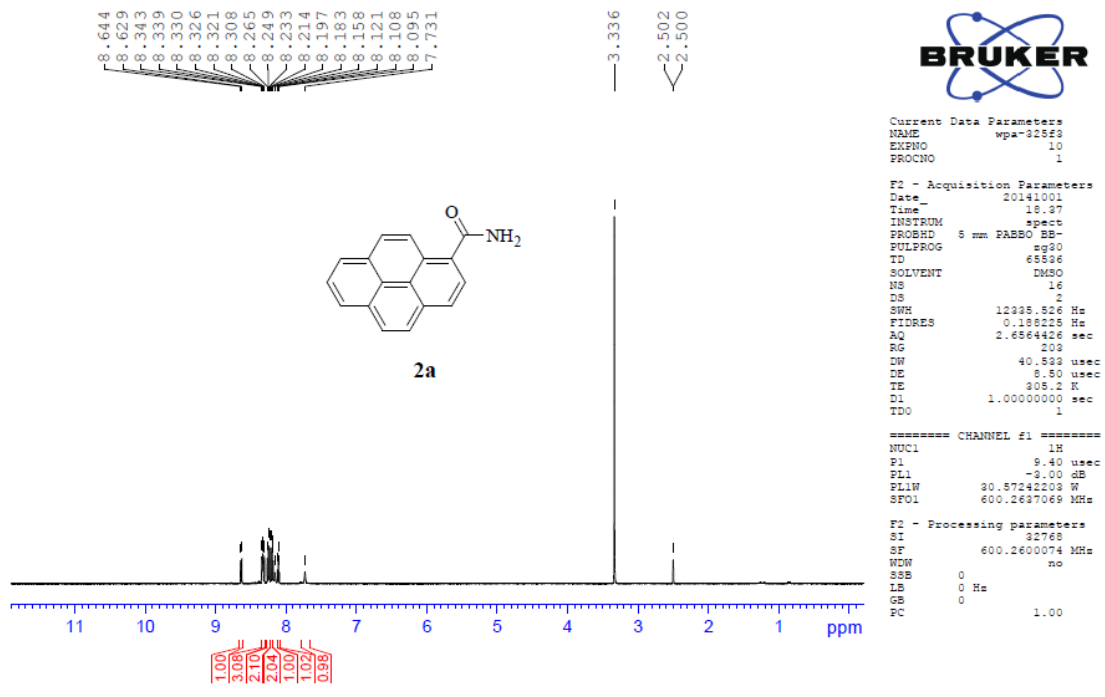
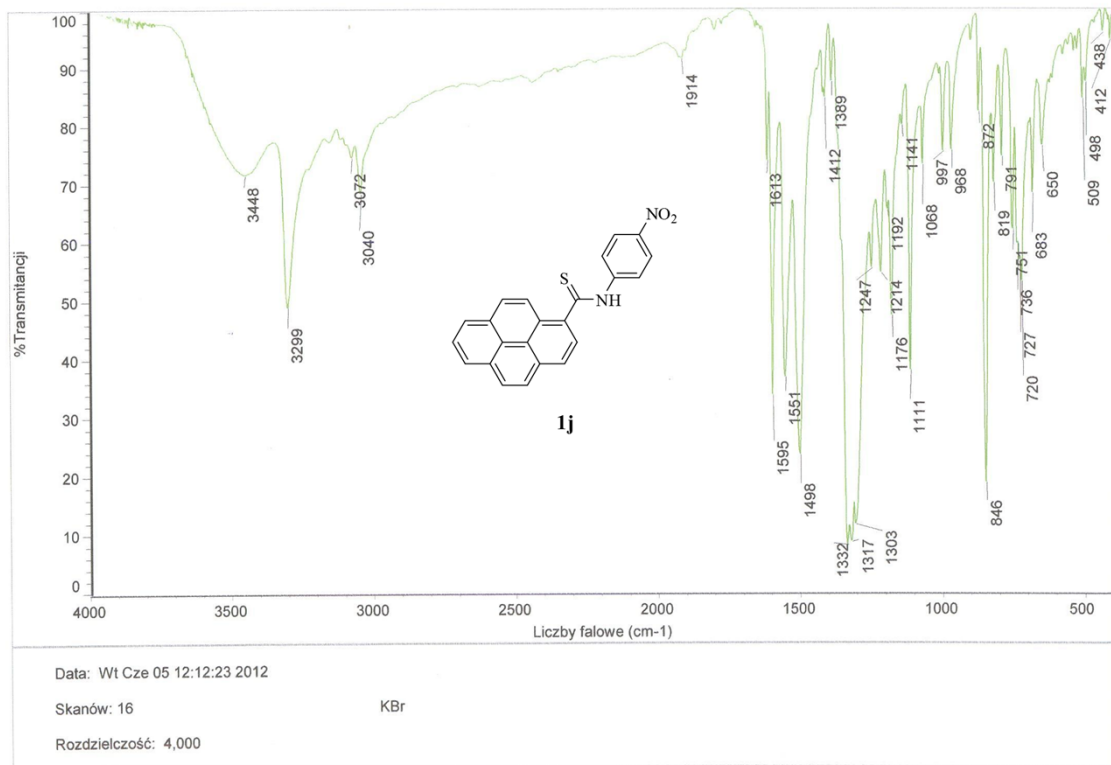
Current Data Parameters
 NAME wpa-320a
 EXPMO 11
 PROCNO 1

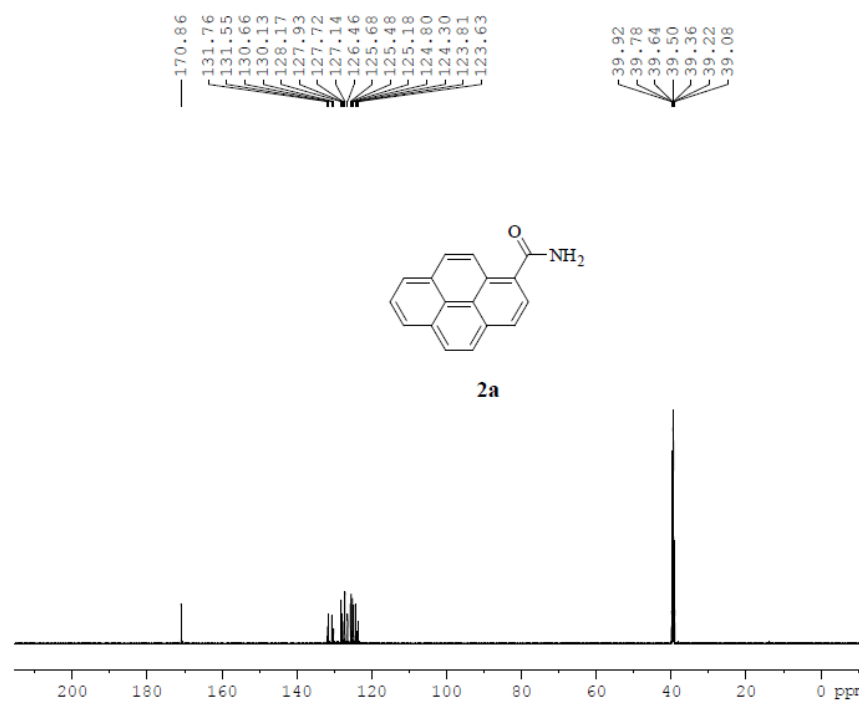
F2 - Acquisition Parameters
 Date_ 20140913
 Time 12.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 36057.693 Hz
 FIDRES 0.550197 Hz
 AQ 0.9088159 sec
 RG 2080
 DW 19.887 usec
 DE 8.50 usec
 TE 304.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUCL1 13C
 P1 10.90 usec
 PL1 0 dB
 PL1W 91.98504333 W
 SFO1 150.9505906 MHz

===== CHANNEL f2 =====
 CQCPFG2 waltz16
 NUCL2 1H
 PCPD2 90.00 usec
 PL2 -3.00 dB
 PL12 16.26 dB
 PL13 16.00 dB
 PL2W 30.57242209 W
 FLL2W 0.36251819 W
 FLL3W 0.24284597 W
 SFO2 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.9355947 MHz
 WDW no
 SSB no
 LB 0 Hz
 GB 0
 PC 1.40





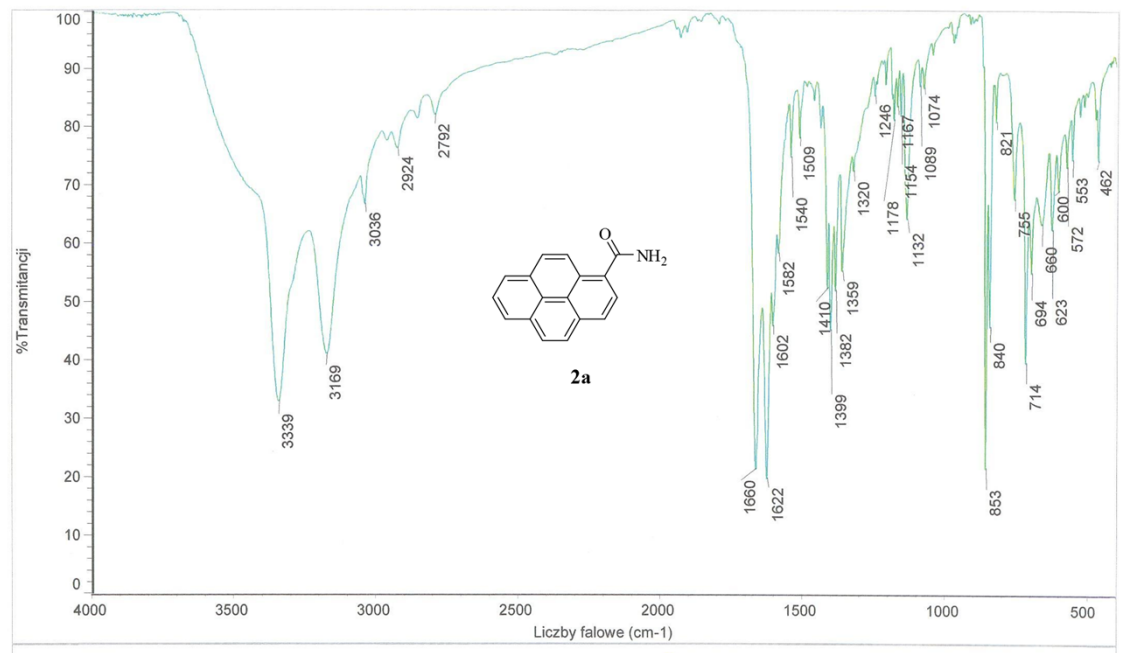
Current Data Parameters
NAME wpa-225f3
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141001
Time 21.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT H₂O
NS 4000
DS 4
SWH 9687.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DM 13.867 usec
DE 8.50 usec
TE 304.4 K
D1 2.00000000 sec
D11 0.09000000 sec
TD0 1

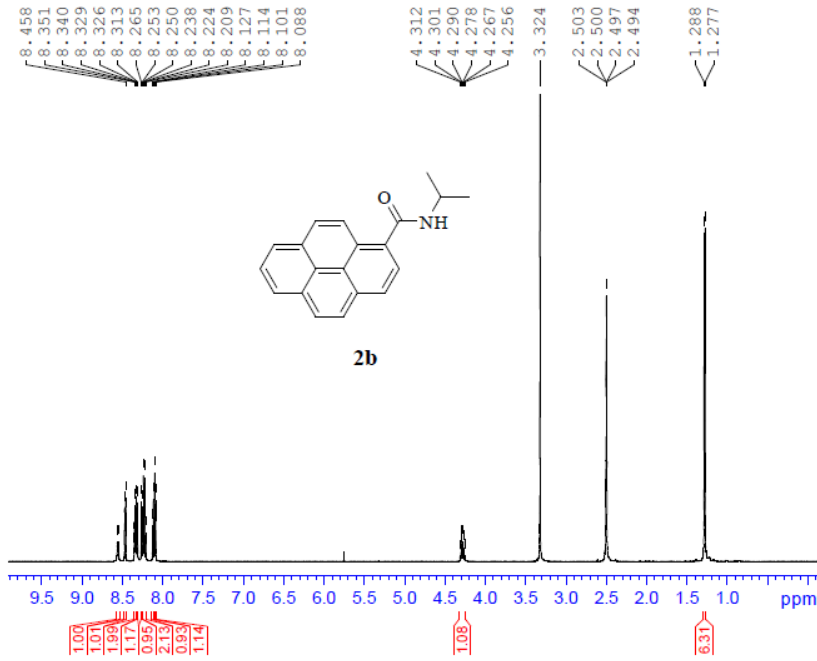
==== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL1W 91.98504333 W
SFO1 100.6264010 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 16.26 dB
PL13 16.26 dB
PL14 16.26 dB
PL1W 30.57242303 W
SFO2 400.1420010 MHz
PL12W 0.3628181818 W
PL13W 0.24284597 W
SFO2 600.2624010 MHz

F2 - Processing parameters
SI 32768
SF 150.9955789 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
WB 0
W 1.40



Data: Czw Paź 02 12:23:20 2014
Skanów: 16 KBr
Rozdzielczość: 4,000



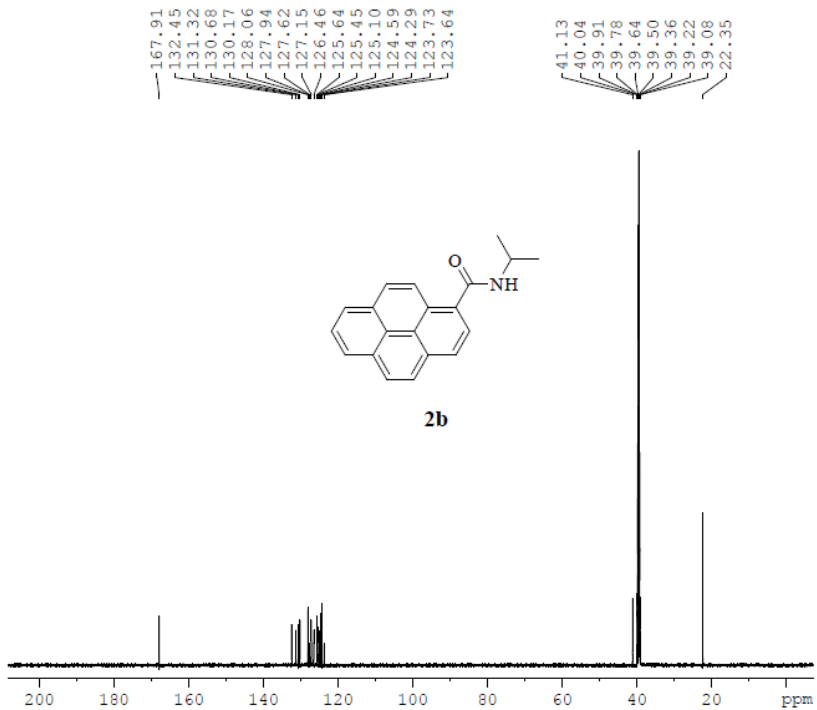
```

Current Data Parameters
NAME      wpa-211
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20121130
Time     20.54
INSTRUM  spect
PROBHD   5 mm FAPBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        2
SMH       123395.526 Hz
FIDRES   0.188225 Hz
AQ        2.6564426 sec
RG        203
SW        40.532 usec
DE        8.50 usec
TE        300.2 K
D1        1.00000000 sec
TD0       1

===== CHANNEL #1 =====
NUC1      1H
P1        9.40 usec
PL1       -3.00 dB
PL1W     30.57242203 W
SFO1     600.2637069 MHz

F2 - Processing parameters
SI        32768
SF        600.2600075 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0
PC        1.00
  
```



```

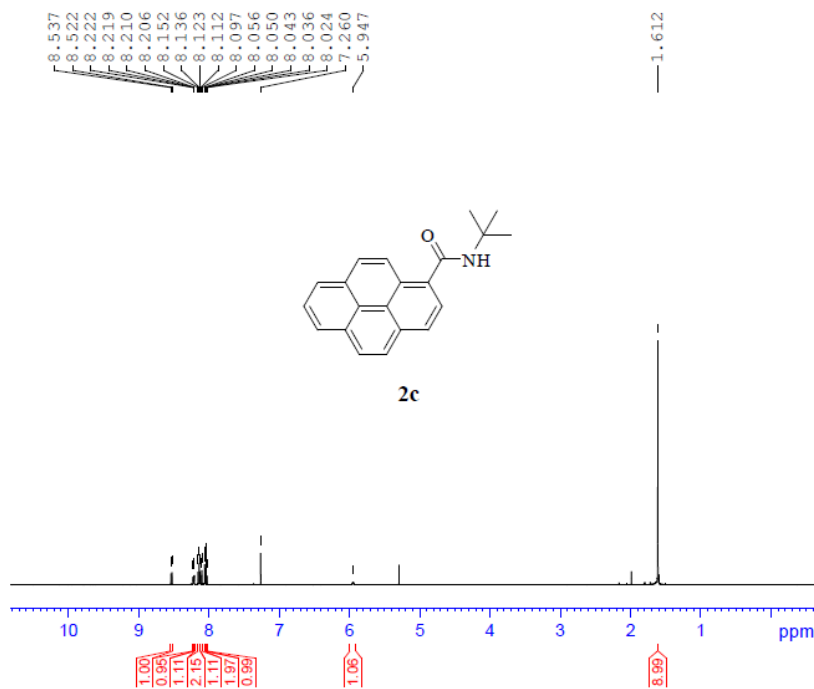
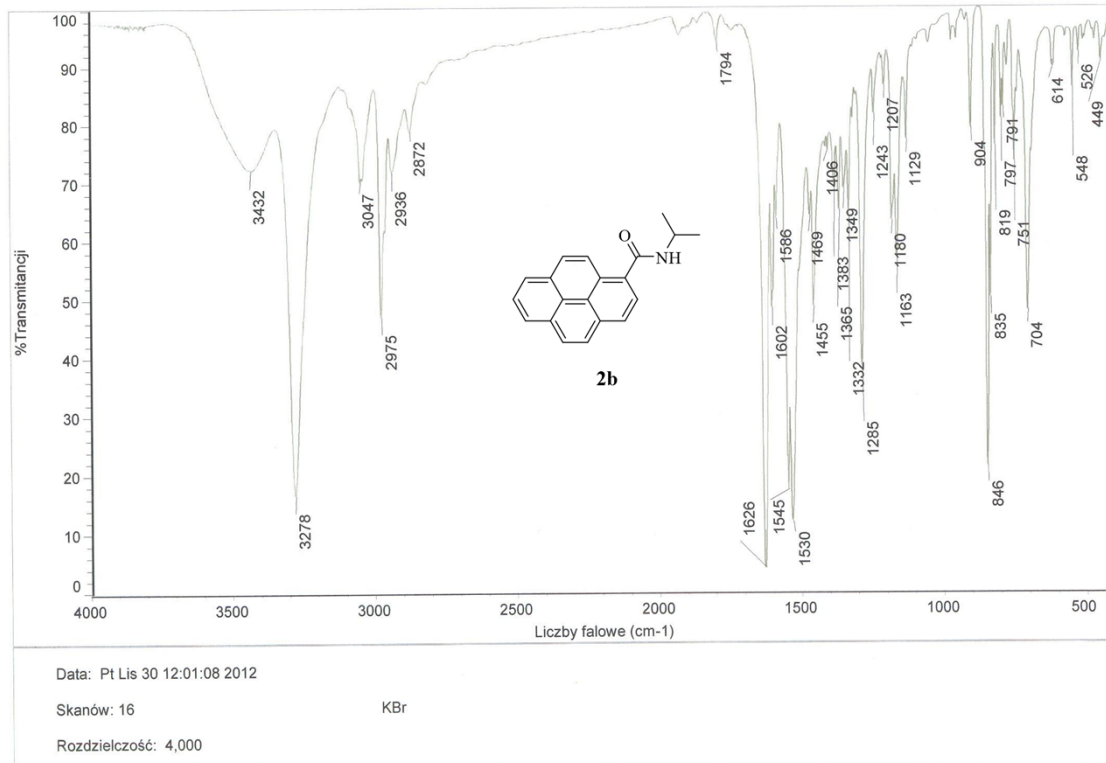
Current Data Parameters
NAME      wpa-211
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20121130
Time     22.96
INSTRUM  spect
PROBHD   5 mm FAPBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        2048
DS        4
SMH       36087.681 Hz
FIDRES   0.550197 Hz
AQ        0.9088159 sec
RG        2050
SW        13.867 usec
DE        8.50 usec
TE        302.0 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL #1 =====
NUC1      13C
P1        10.50 usec
PL1       0 dB
PL1W     91.93504333 W
SFO1     150.9355906 MHz

===== CHANNEL #2 =====
CFPRG2   waltz16
NUC2      1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     16.26 dB
PL13     15.00 dB
PL2W     30.57242203 W
PL12W    0.36251819 W
PL13W    0.24284897 W
SFO2     600.2624010 MHz

F2 - Processing parameters
SI        32768
SF        150.9355796 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0
PC        1.40
  
```



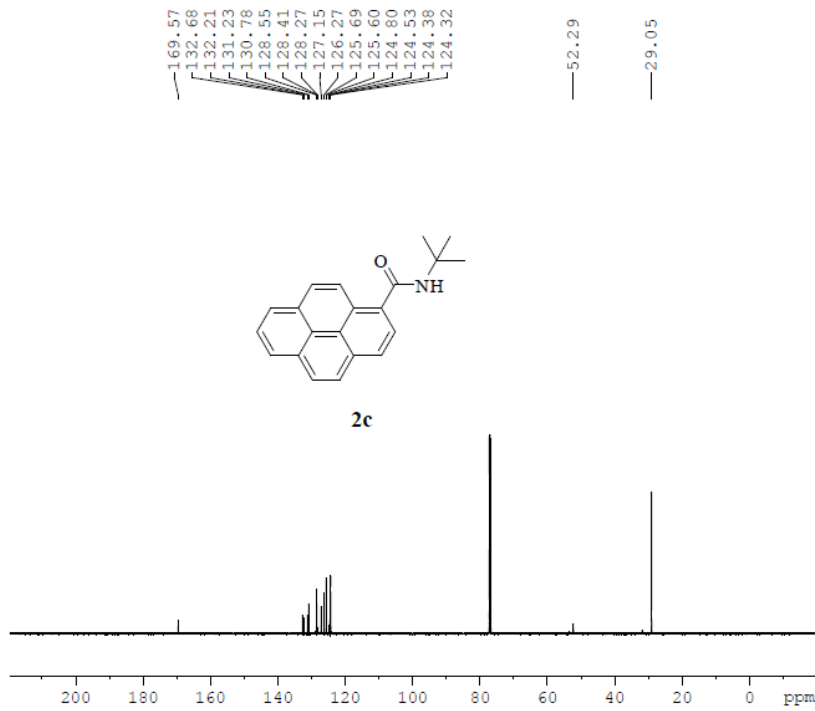
```

Current Data Parameters
NAME      wpa-199a
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20121125
Time      6.29
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        12335.526 Hz
FIDRES     0.188225 Hz
AQ         2.6564126 sec
RG         257
EM         40.523 usec
DE         8.50 usec
TE         301.9 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.40 usec
PL1        -9.00 dB
PL1W       30.57242203 W
SFO1       600.2637069 MHz

F2 - Processing parameters
SI         32765
SF         600.2600173 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         1.00
  
```



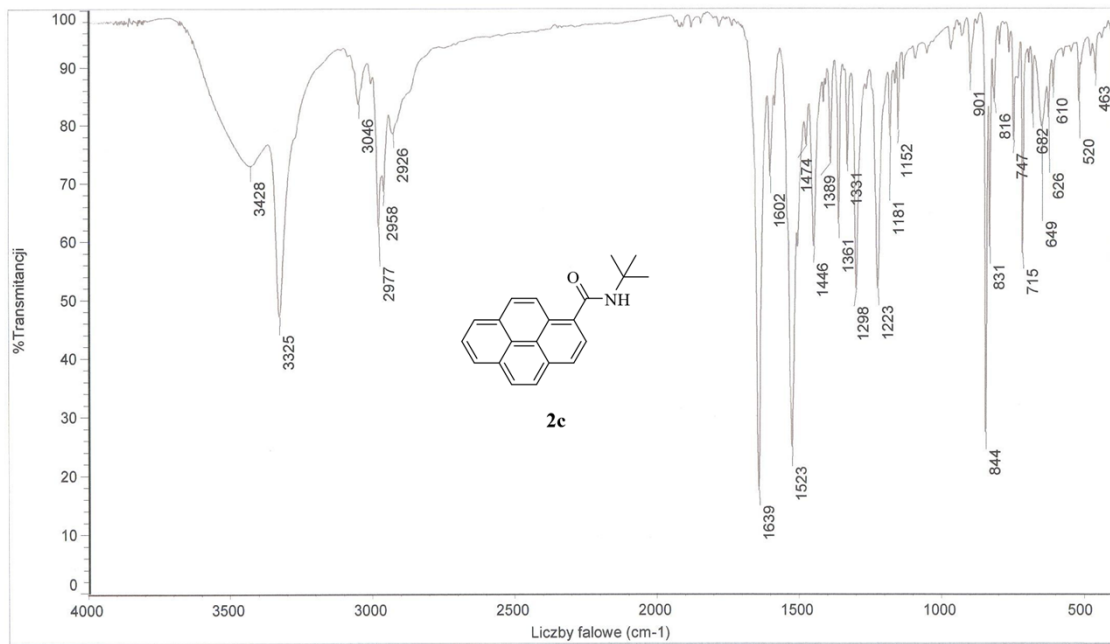
Current Data Parameters
NAME wpa-199a
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121125
Time_ 9.48
INSTRUM spect
PROBHD 5 mm F400 BBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 36087.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 3280
DW 13.867 usec
DE 8.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL12 91.92504333 W
SFO1 150.9858906 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 19.00 dB
PL12 16.36 dB
PL13 18.00 dB
PL14 18.00 dB
PL2W 30.57242203 W
PL2W 0.26255819 W
PL13W 0.24284897 W
SFO2 600.2624010 MHz

F2 - Processing parameters
SI 32768
SF 150.9854970 MHz
WDW no
SSB no
GB 0 Hz
PC 1.40



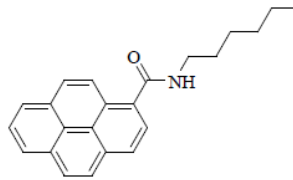
Data: Pon Lis 26 14:35:35 2012

Skanów: 16

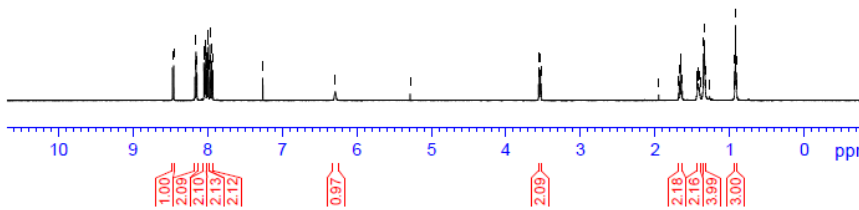
KBr

Rozdzielczość: 4,000

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8.040
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8.026
8.011
8.008
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7.995
7.986
7.969
7.956
7.945
7.930
7.920
7.260
6.288
5.284
3.561
3.549
3.539
3.527
1.952
1.684
1.672
1.660
1.648
1.635
1.432
1.429
1.420
1.407
1.395
1.359
1.349
1.343
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1.337
1.333
1.325
1.325
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0.928
0.921
0.909



2d



Current Data Parameters
NAME wpa-197a
EXPNO 11
PROCNO 1

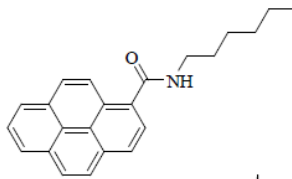
F2 - Acquisition Parameters
Date_ 20121029
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12395.826 Hz
FIDRES 0.188229 Hz
AQ 2.6564426 sec
RG 123
DW 40.593 usec
DE 8.50 usec
TE 299.9 K
D1 1.00000000 sec
TDO

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 -3.00 dB
PL1W 30.57242203 W
SFO1 600.2637069 MHz

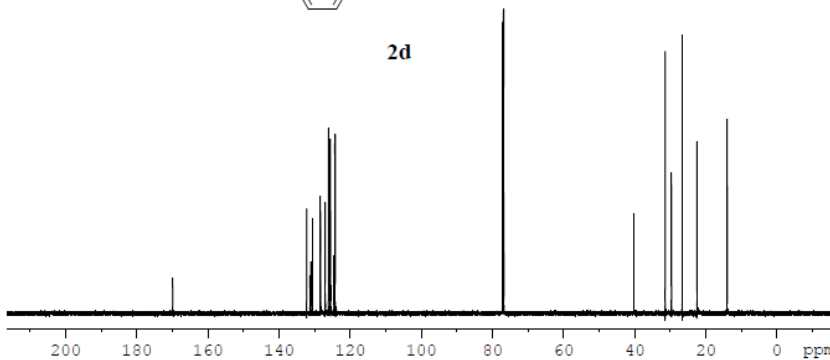
F2 - Processing parameters
SI 32768
SF 600.2600174 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
FC 1.00



169.92
132.24
131.36
131.07
130.63
128.41
128.38
128.34
126.99
126.17
125.64
125.55
124.60
124.36
124.32
124.15
77.21
77.00
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40.27
31.49
29.68
26.70
22.55
13.99



2d



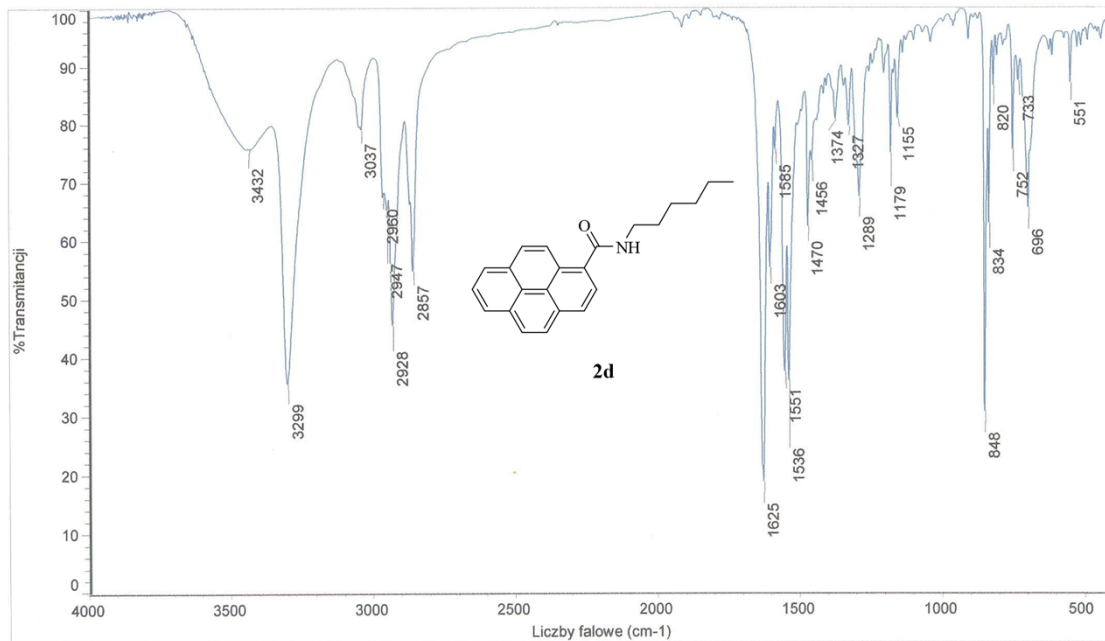
Current Data Parameters
NAME wpa-197a
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121029
Time 19.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 96057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2080
DW 19.987 usec
DE 8.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.02000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL1W 91.93504333 W
SFO1 150.98505906 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 16.26 dB
PL13 18.00 dB
PL2W 30.57242203 W
PL12W 0.26251915 W
PL13W 0.24284537 W
SFO2 600.2624010 MHz

F2 - Processing parameters
SI 32768
SF 150.9850591 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
FC 1.40

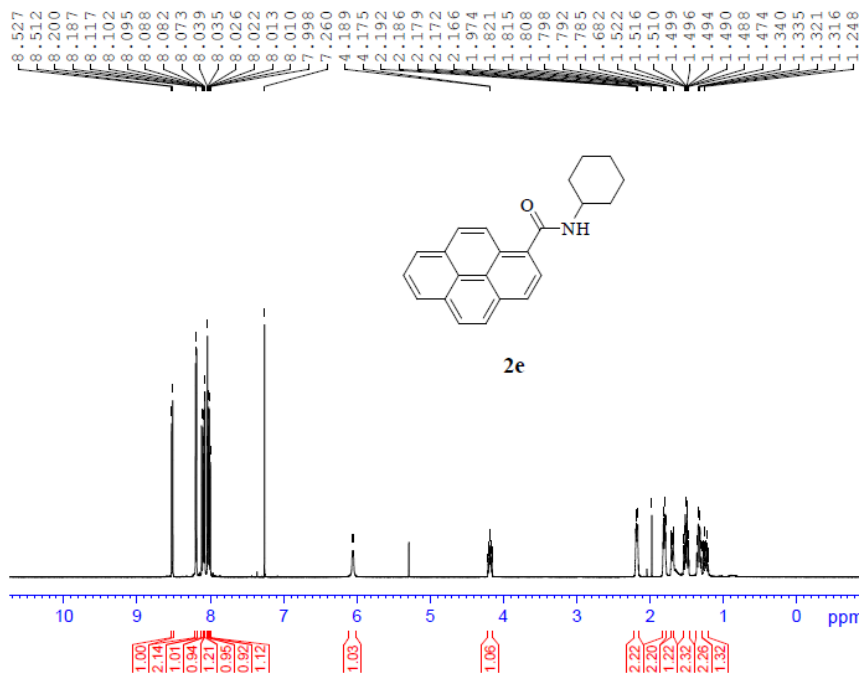


Data: Pt Cze 01 15:07:12 2012

Skanów: 16

KBr

Rozdzielczość: 4,000



Current Data Parameters
 NAME wpa-196
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121025
 Time 2.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 DE 12335.526 Hz
 SWH 0.188225 Hz
 FIDRES 2.6564426 sec
 AQ 228
 RG 40.532 usec
 DE 8.50 usec
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -9.00 dB
 PL1W 30.57242203 W
 SFO1 600.2607069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.260074 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



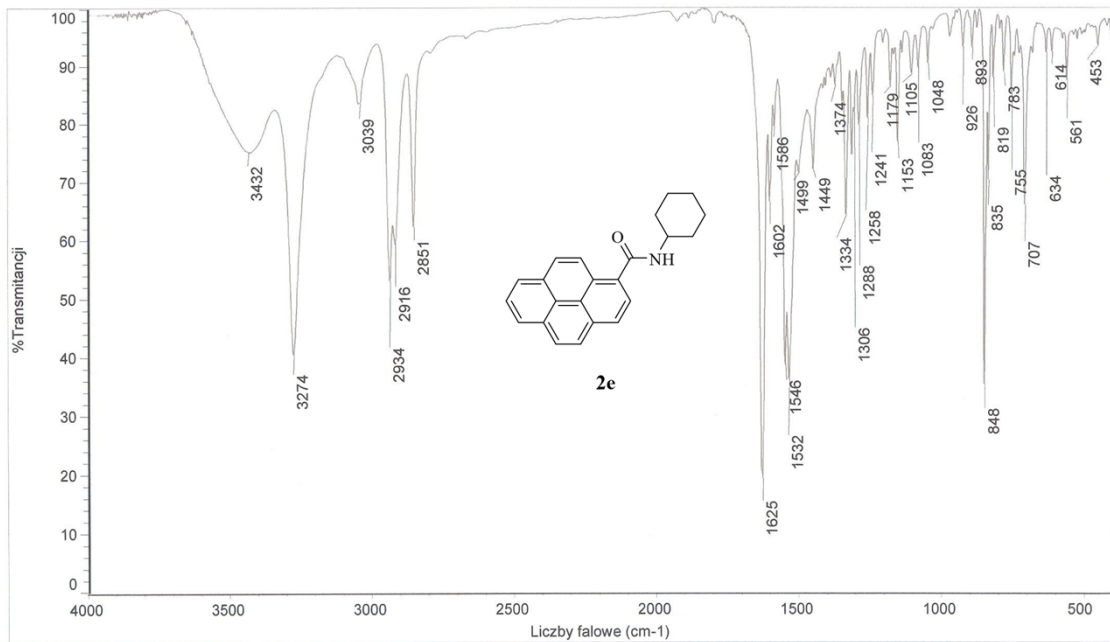
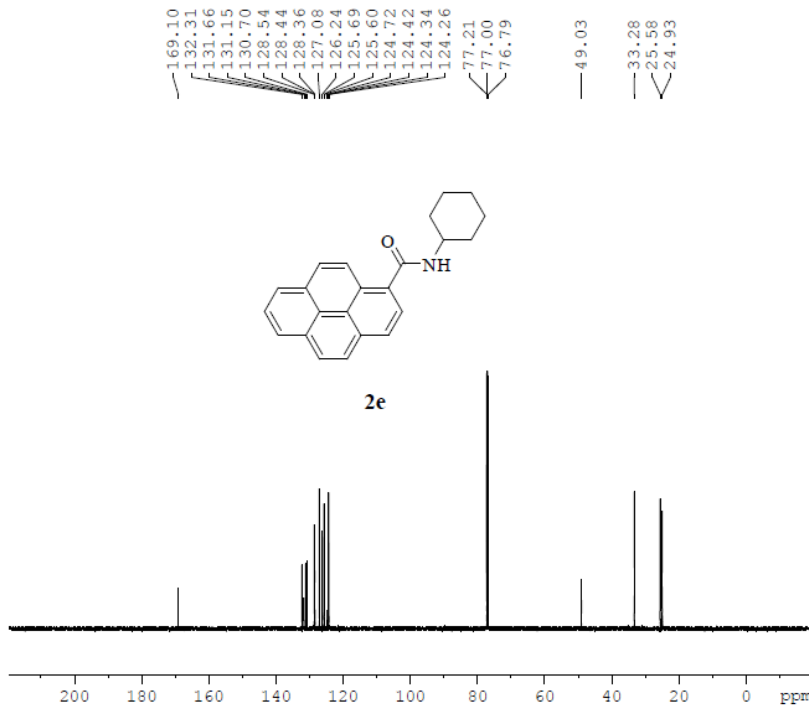
Current Data Parameters
NAME wpa-196
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121025
Time 4.26
INSTRUM spect
PROBHD 5 mm PABBO BBI
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088189 sec
RG 2050
LW 13.867 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL1W 31.93504323 W
SFO1 150.9058906 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 19.00 dB
PL12 16.26 dB
PL13 18.00 dB
PL2W 30.57442203 W
PL1W 0.36231816 W
PL13W 0.24284537 W
SFO2 600.1324010 MHz

F2 - Processing parameters
SI 32768
SF 150.9054970 MHz
WDW no
SSB no
LB 0 Hz
GB 0
FB 1.40

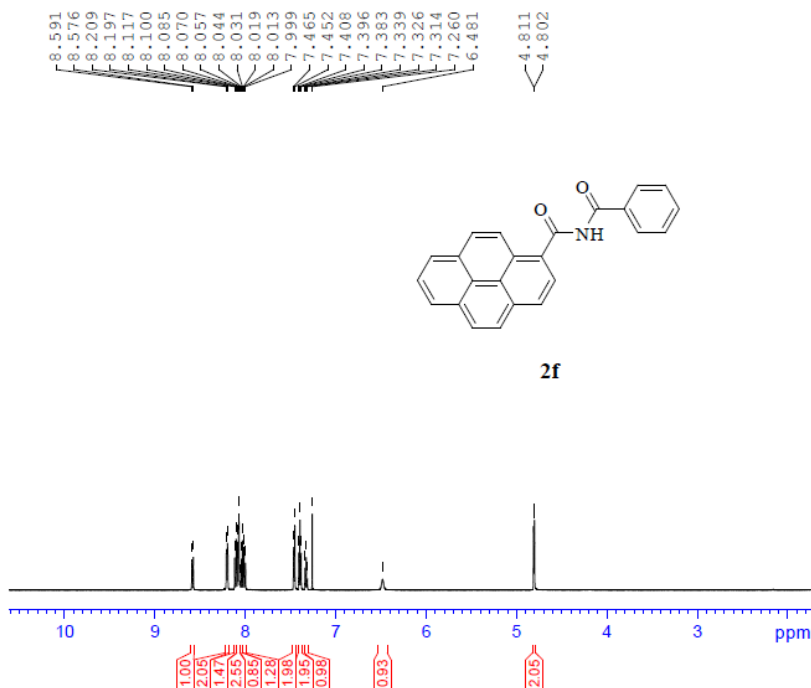


Data: Wt Lis 20 14:48:49 2012

Skanów: 16

KBr

Rozdzielczość: 4,000



```

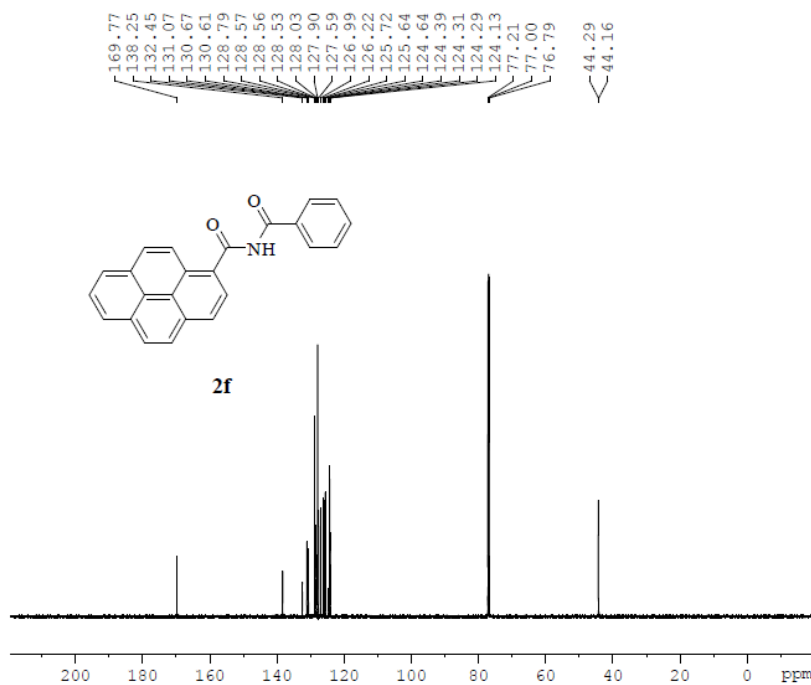
Current Data Parameters
NAME      wpa-202c
EXNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_    20130215
Time     10.56
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      12335.526 Hz
FIDRES   0.188225 Hz
AQ       2.6564426 sec
RG       322
DW       40.538 usec
DE       8.50 usec
TE       302.0 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       9.40 usec
PL1     -3.00 dB
PL1W    30.57242203 W
SFO1    600.2607069 MHz

F2 - Processing parameters
SI       32768
SF       600.2600171 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       1.00

```



```

Current Data Parameters
NAME      wpa-202b
EXNO     11
PROCNO    1

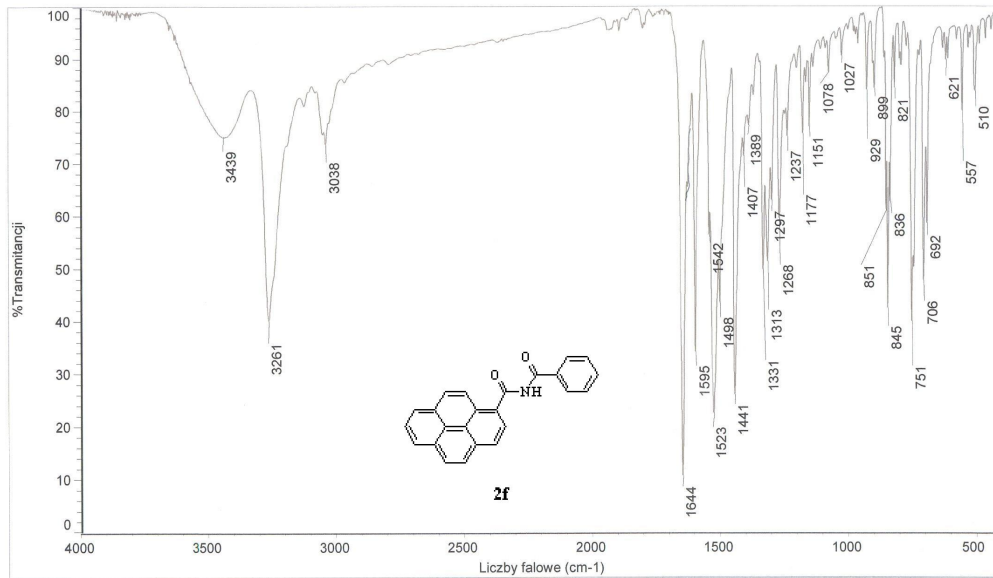
F2 - Acquisition Parameters
Date_    20130213
Time     22.56
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2500
DS       4
SWH      36087.691 Hz
FIDRES   0.550197 Hz
AQ       0.9088159 sec
RG       2080
DW       19.867 usec
DE       8.50 usec
TE       302.2 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     13C
P1       10.50 usec
PL1      0 dB
PL1W    91.93504333 W
SFO1    150.9850906 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2     -3.00 dB
PL12    16.26 dB
PL13    18.00 dB
PL2W    30.57242203 W
PL12W   0.24284837 W
PL13W   0.24284837 W
SFO2    600.2624010 MHz

F2 - Processing parameters
SI       32768
SF       150.985040 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       1.40

```

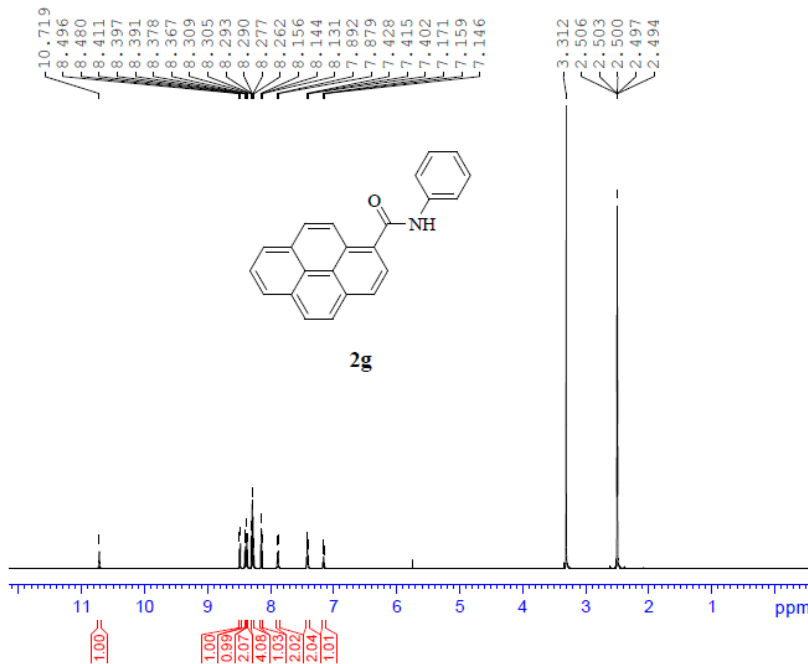


Data: Pon Lis 26 14:46:28 2012

Skanów: 16

KBr

Rozdzielczość: 4,000

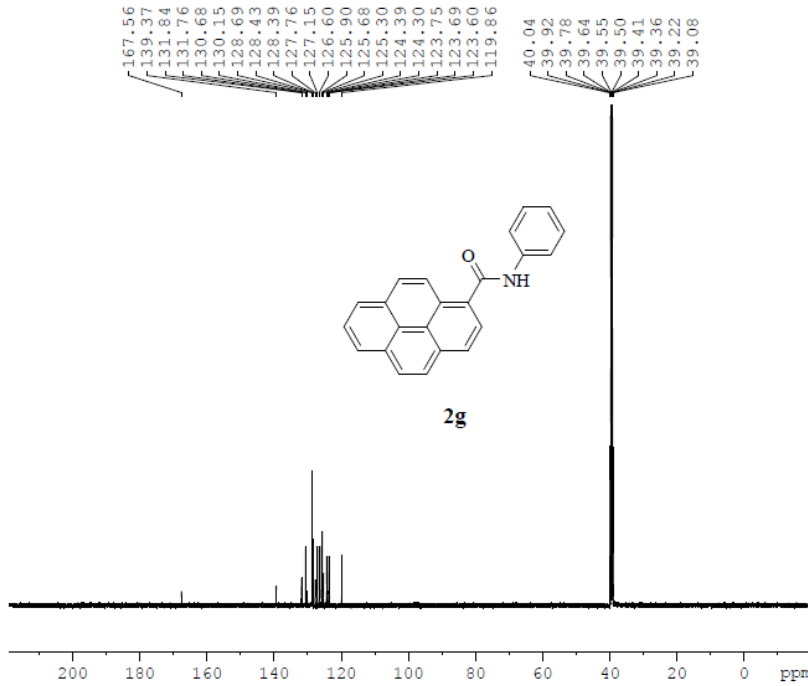


Current Data Parameters
 NAME wpa-198a
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121125
 Time 2.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.158225 Hz
 AQ 2.6564426 sec
 RG 287
 DW 40.533 usec
 DE 8.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.57242209 W
 SFO1 600.2637069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.2600079 MHz
 WHW no
 SSE 0
 LB 0 Hz
 GB 0
 PC 1.00



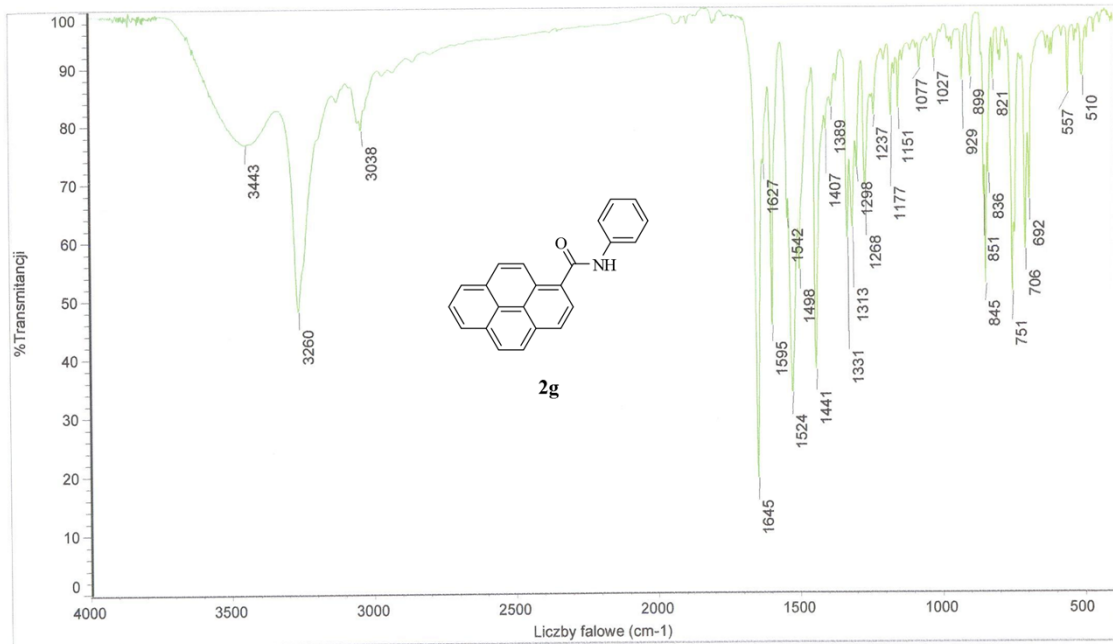
Current Data Parameters
NAME wpa-198a
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121125
Time 6.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.5088159 sec
RG 2080
LW 19.867 usec
TE 302.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO

==== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL1W 91.93504323 W
SFO1 100.62846010 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 16.26 dB
PL13 18.00 dB
PL1W 30.57241003 W
PL12W 0.36251819 W
PL13W 0.24284527 W
SFO2 600.2624010 MHz

F2 - Processing parameters
SI 32768
SF 100.62846010 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.40

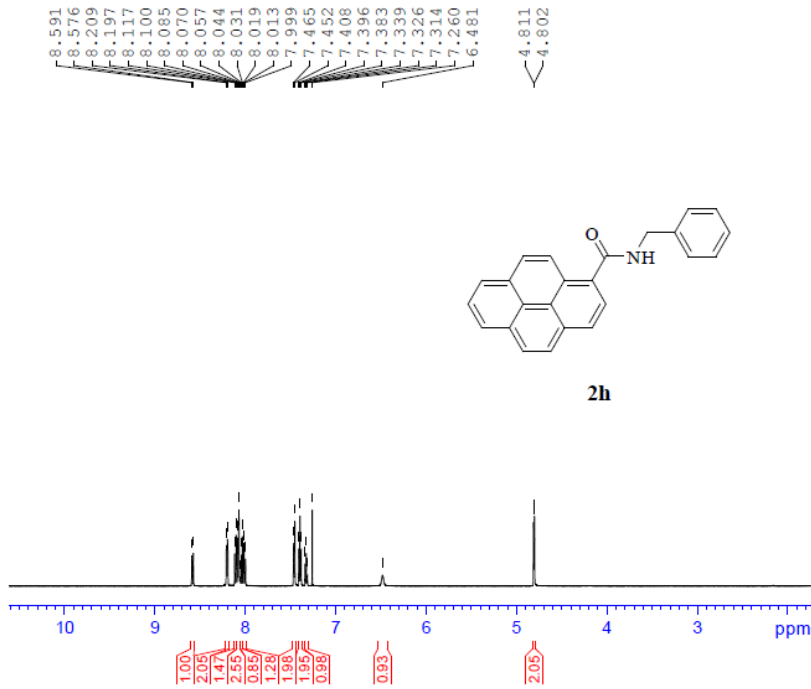


Data: Pon Cze 04 11:50:15 2012

Skanów: 16

KBr

Rozdzielczość: 4,000

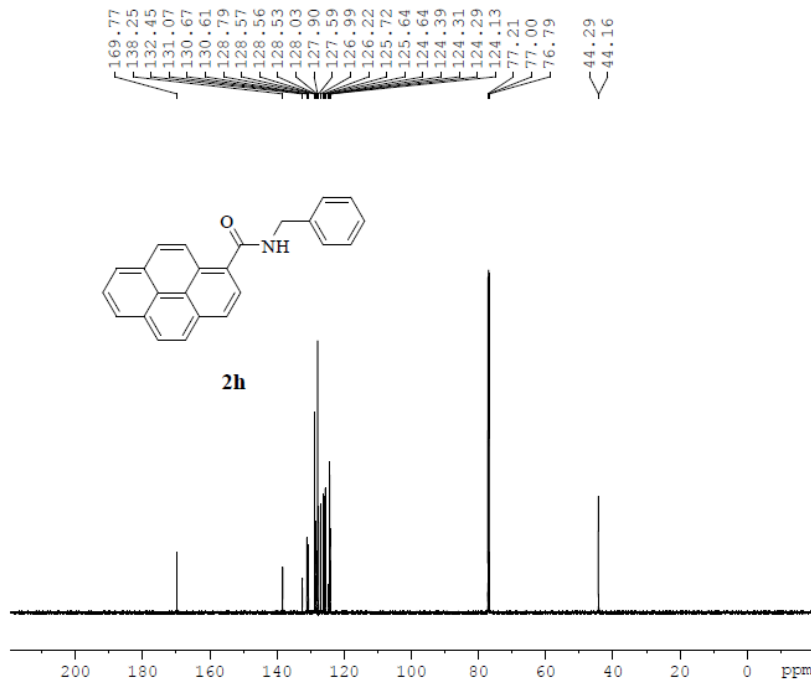


Current Data Parameters
 NAME wpa-202c
 EXPRNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130215
 Time 10.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.188225 Hz
 AQ 2.6564426 sec
 RG 322
 DW 40.538 usec
 DE 8.50 usec
 TE 302.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.57242203 W
 SFO1 600.2607069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.260711 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



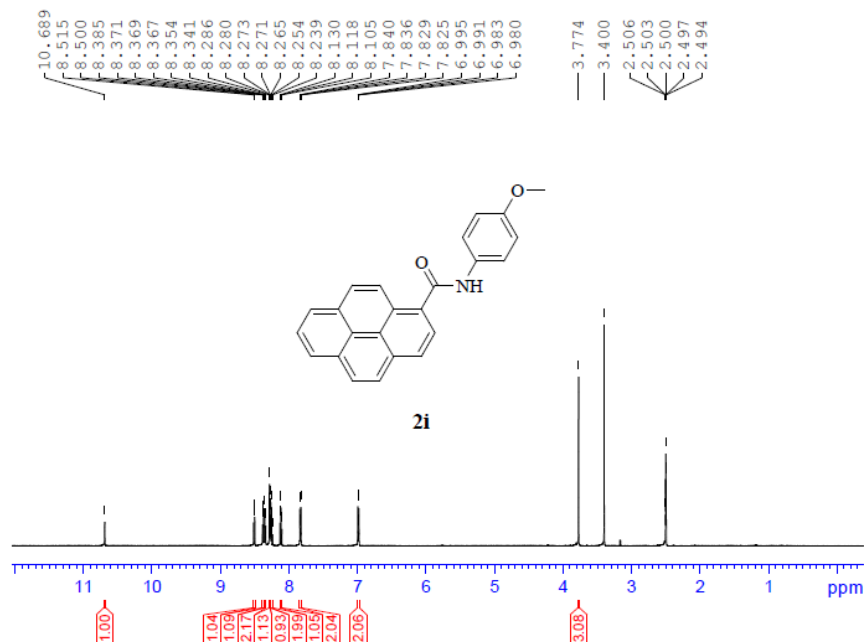
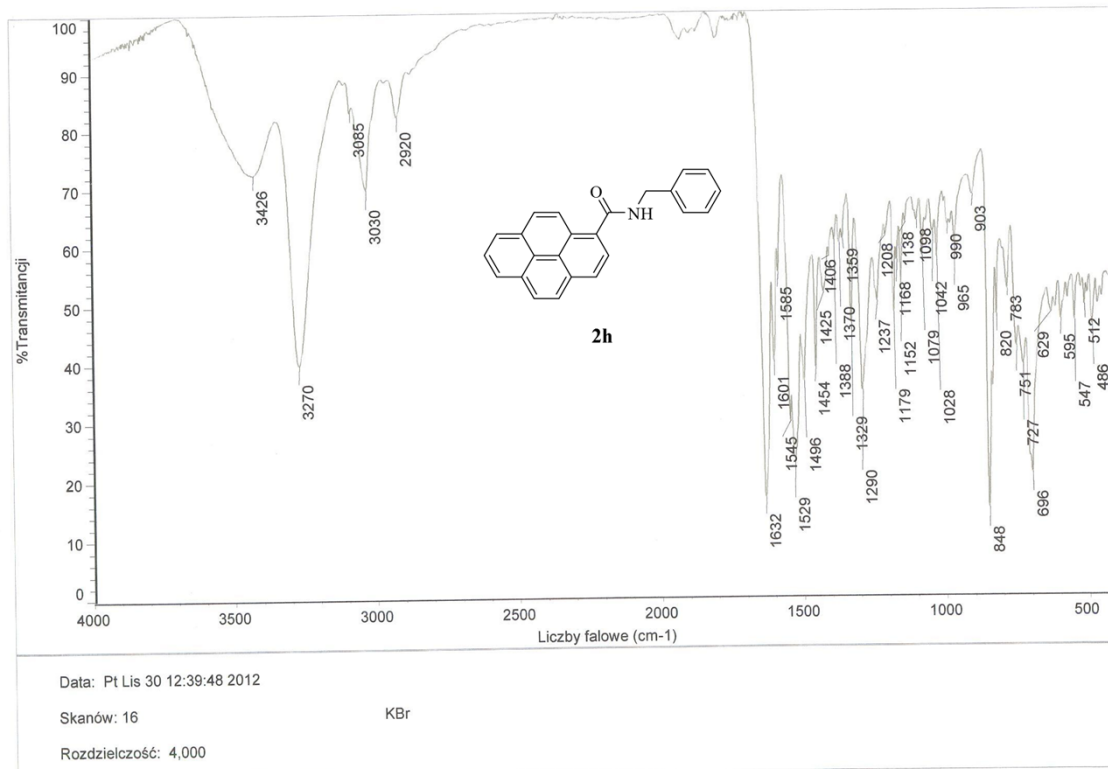
Current Data Parameters
 NAME wpa-202b
 EXPRNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130213
 Time 22.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2500
 DS 4
 SWH 36087.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9085159 sec
 RG 2080
 DW 19.867 usec
 DE 8.50 usec
 TE 302.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0 dB
 PL1W 91.93504333 W
 SFO1 101.6253750 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.00 dB
 PL12 16.26 dB
 PL13 18.00 dB
 PL2W 30.57242203 W
 PL12W 0.24284837 W
 PL13W 0.24284837 W
 SFO2 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.935040 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40



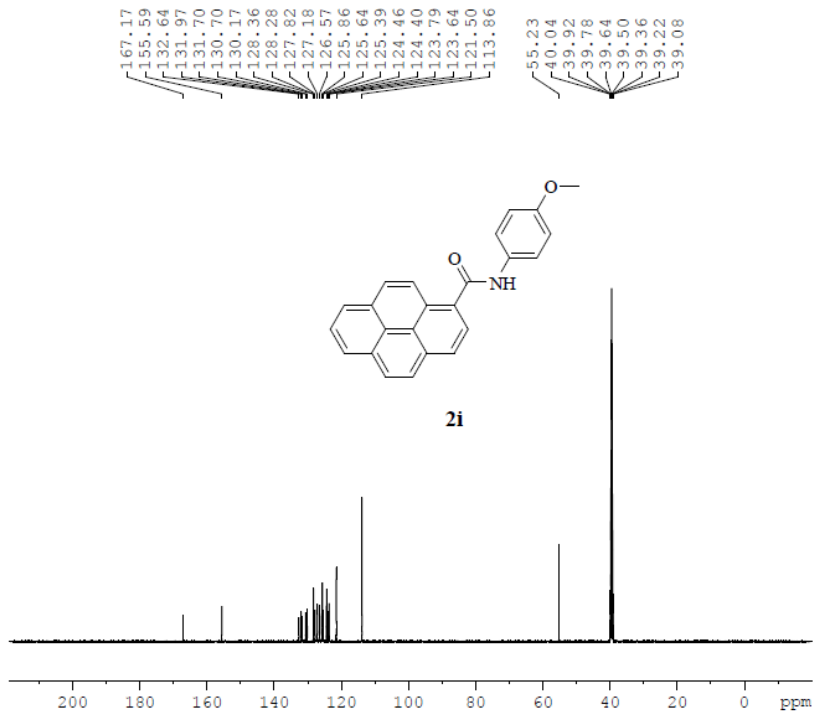
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Current Data Parameters
NAME      wpa-27053
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20120916
Time     20.53
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      12398.526 Hz
FIDRES   0.188223 Hz
AQ       2.654442 sec
RG       162
DW       40.533 usec
DE       8.50 usec
TE       301.3 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       9.40 usec
PL1     -2.00 dB
PL1W    30.57242203 W
SFO1     600.2637069 MHz

F2 - Processing parameters
SI       32768
SF       600.2600078 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       1.00
  
```

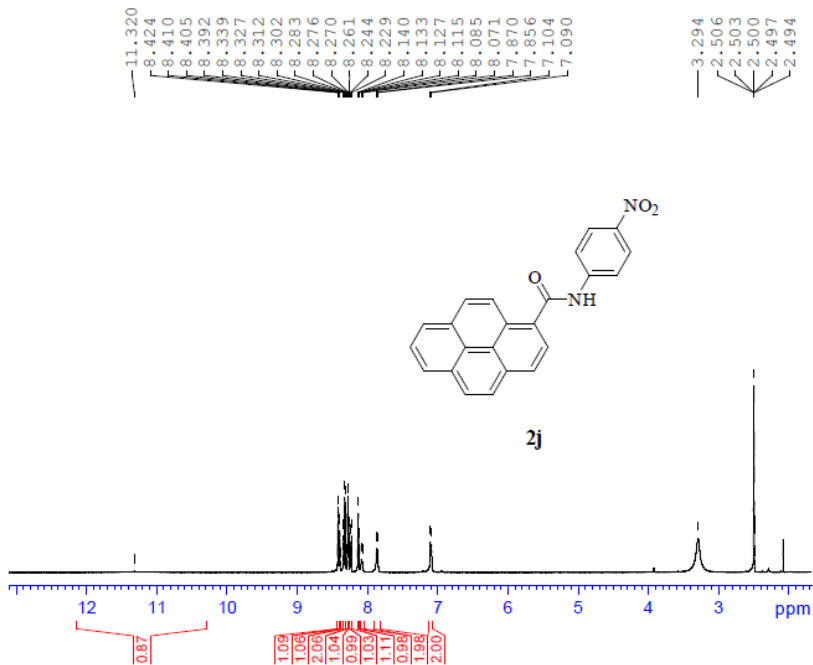
Current Data Parameters
 NAME wpa-27323
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120216
 Time_ 23.23
 INSTRUM spect
 PROBHD 5 mm FABS0 ES-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 3000
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9085159 sec
 RG 2050
 DW 13.967 usec
 DE 8.50 usec
 TE 303.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0 dB
 PL1W 91.92504223 W
 SF01 150.9505906 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.00 dB
 PL12 14.24 dB
 PL13 18.00 dB
 PL2W 30.57242203 W
 PL12W 0.24384937 W
 SF02 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.955763 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

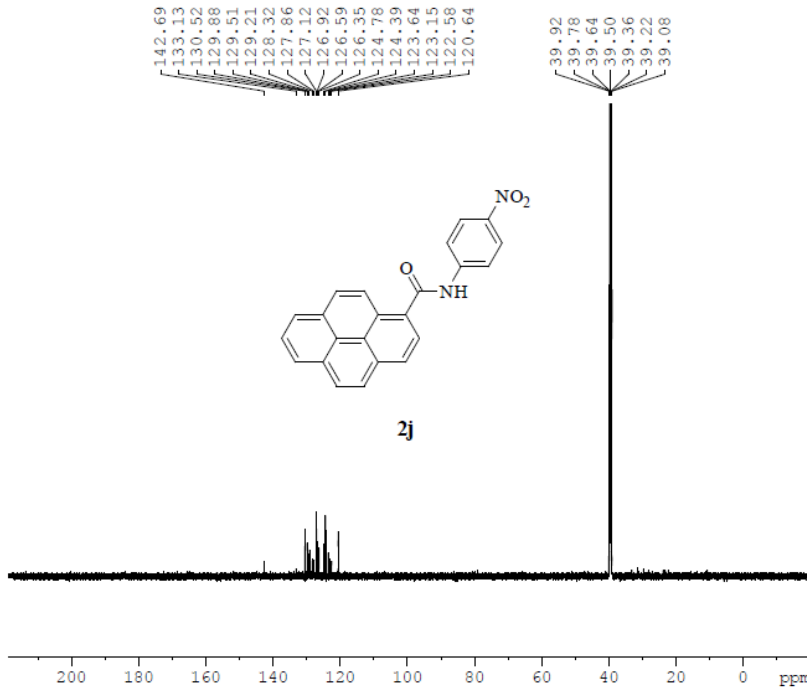


Current Data Parameters
 NAME wpa-322
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140918
 Time_ 18.47
 INSTRUM spect
 PROBHD 5 mm FABS0 ES-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.188225 Hz
 AQ 2.6564426 sec
 RG 406
 DW 40.593 usec
 DE 8.50 usec
 TE 304.1 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.57242203 W
 SF01 600.2687069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.260082 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



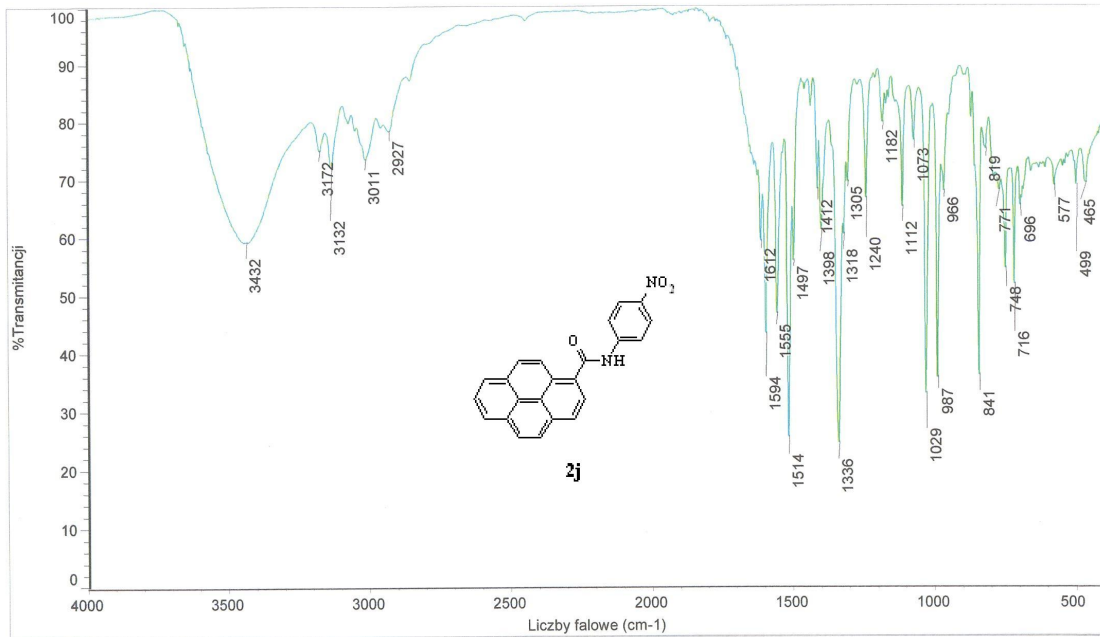
Current Data Parameters
NAME mpa-322
EXPNO 1
PROCNO 1

PC - Acquisition Parameters
Date_ 20140918
Time_ 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 6000
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 8.50 usec
TE 304.6 K
D1 2.0000000 sec
D11 0.02000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 0 dB
PL12 10.00 dB
SFO1 101.625375 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 10.00 dB
PL13 18.00 dB
PL14 18.00 dB
PL15 18.00 dB
PL16 18.00 dB
SFO2 400.146201 MHz

F2 - Processing parameters
SI 32768
SF 150.9058033 MHz
WDW no
SSB no
GB 0
PC 1.40

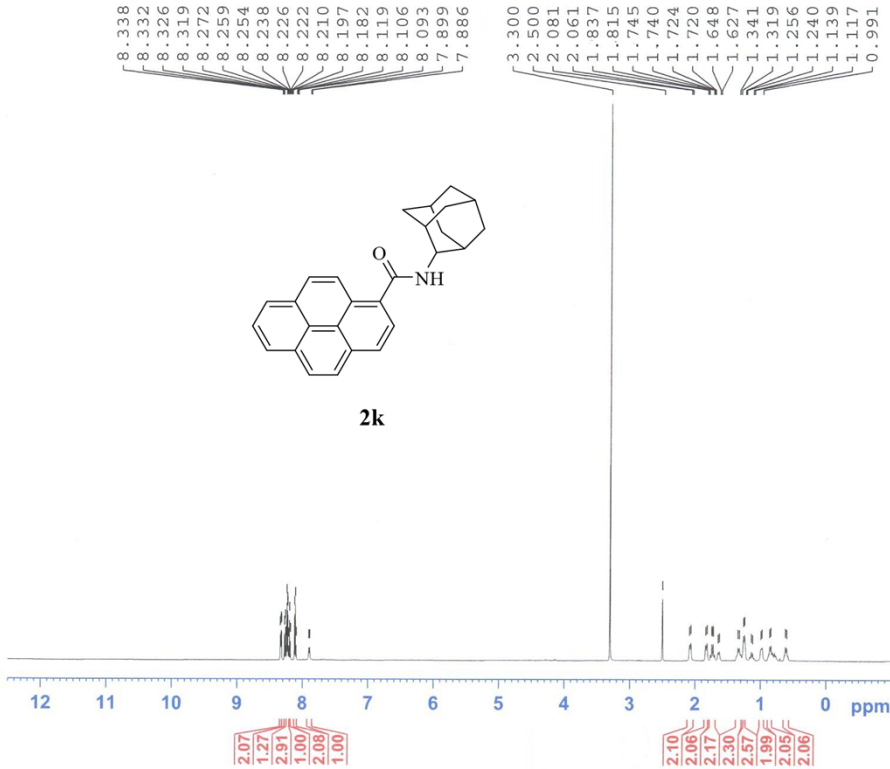


Data: Pt Wrz 26 12:47:20 2014

Skanów: 16

KBr

Rozdzielczość: 4,000

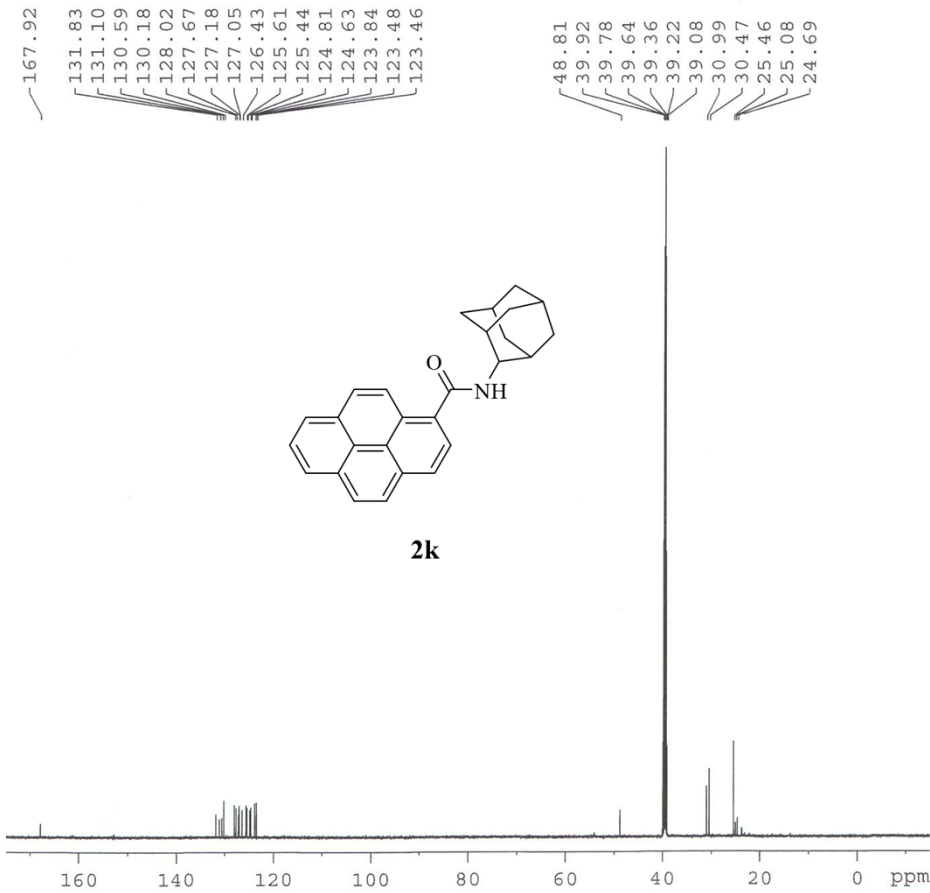


Current Data Parameters
 NAME wpa-238k2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141002
 Time 19.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.188225 Hz
 AQ 2.6564426 sec
 RG 228
 DW 40.533 usec
 DE 8.50 usec
 TE 305.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.57242203 W
 SFO1 600.2637069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.2600078 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



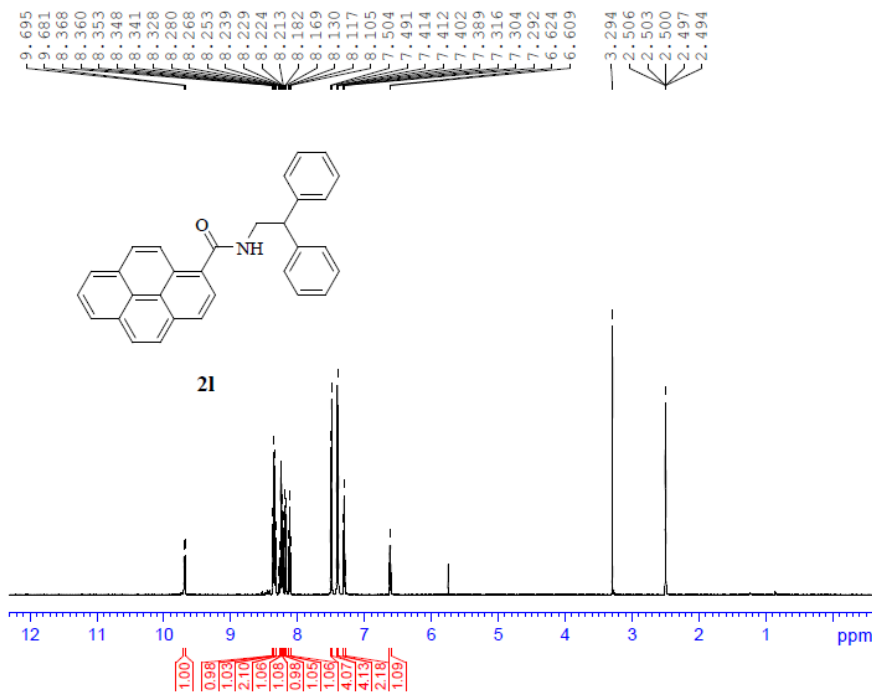
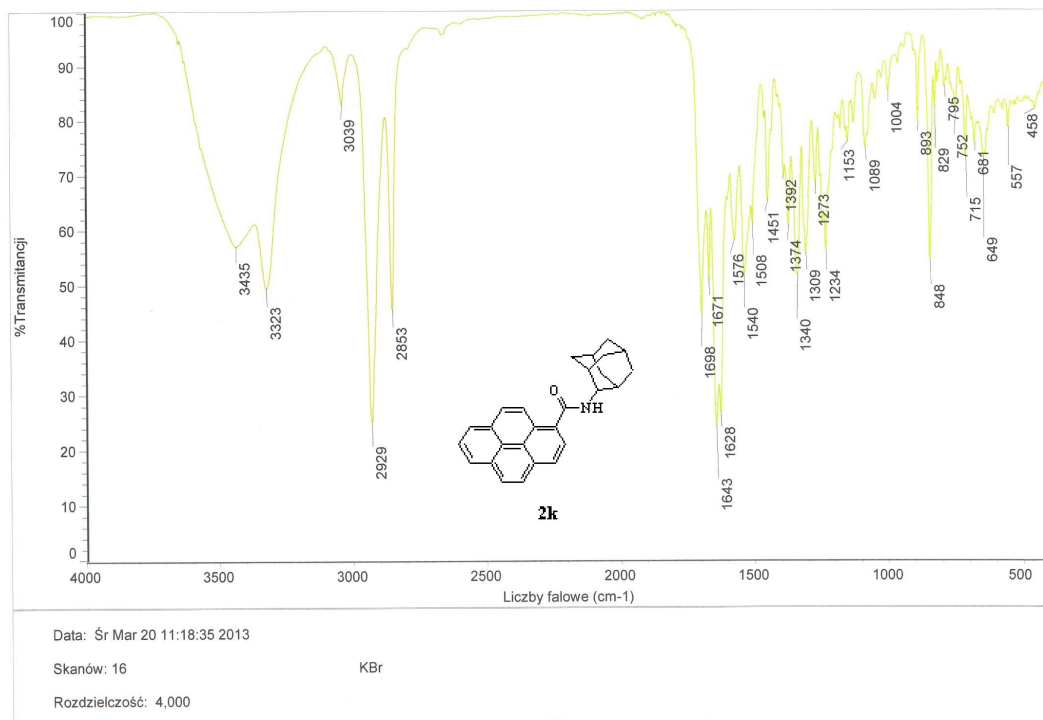
Current Data Parameters
 NAME wpa-238k2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141002
 Time 19.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9088159 sec
 RG 2050
 DW 13.867 usec
 DE 8.50 usec
 TE 304.7 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0 dB
 PL1W 91.93504333 W
 SFO1 150.9505906 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.00 dB
 PL12 16.26 dB
 PL13 18.00 dB
 PL2W 30.57242203 W
 PL12W 0.36251819 W
 PL13W 0.24284537 W
 SFO2 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.9355828 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

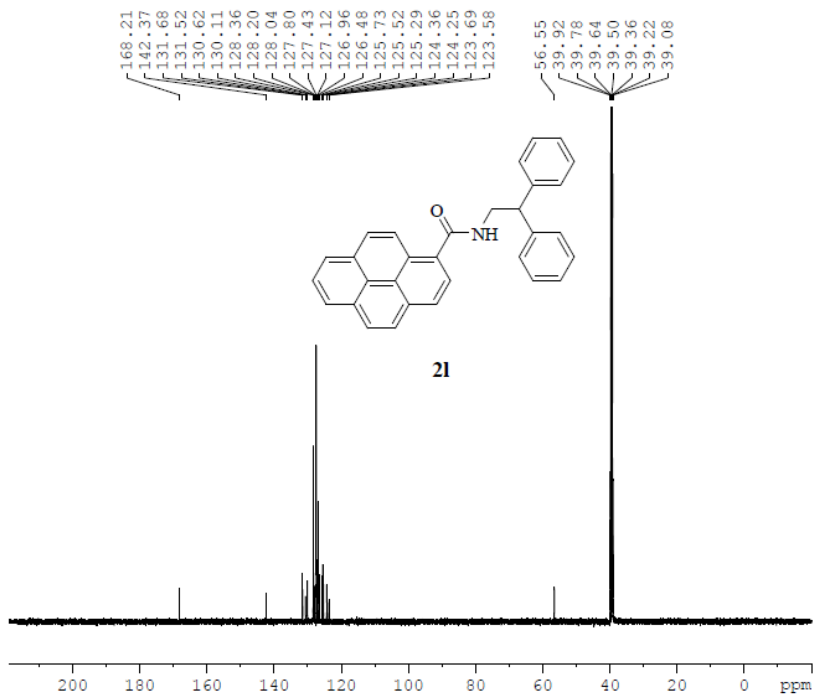


Current Data Parameters
 NAME wpa-253a
 EXNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140414
 Time_ 18.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65524
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10295.806 Hz
 FIDRES 0.188225 Hz
 AQ 2.6564426 sec
 RG 406
 DW 40.533 usec
 DE 8.50 usec
 TE 302.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 30.5724203 W
 SFO1 400.2637069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.260075 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 F0 1.00



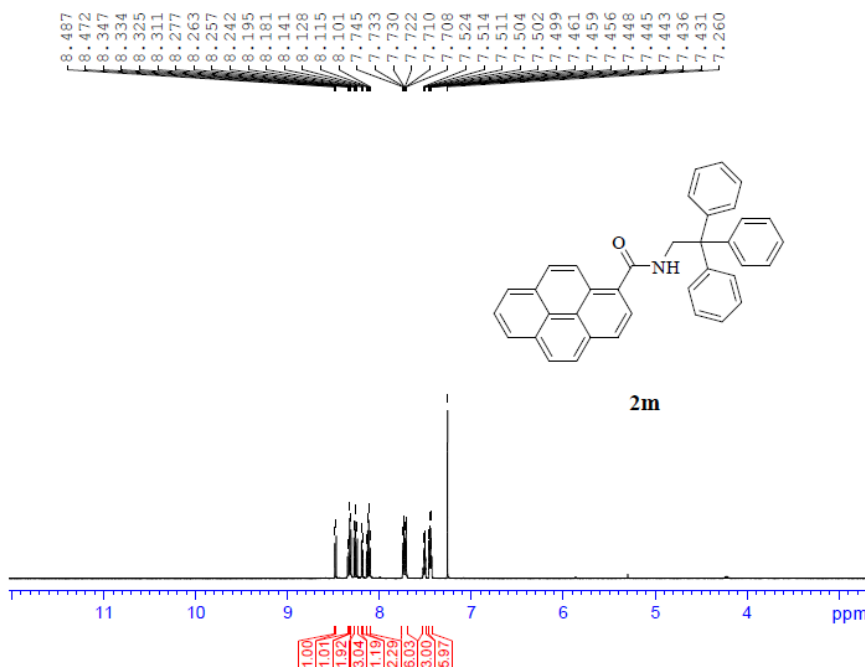
Current Data Parameters
 NAME wpa-259a
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140414
 Time 19.97
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.908199 sec
 RG 2080
 DW 13.867 usec
 DE 8.50 usec
 TE 303.0 K
 DL 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 0 dB
 PL1W 51.93504933 W
 SFO1 150.9505906 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.00 dB
 PL12 16.26 dB
 PL13 18.00 dB
 PLW 30.57242203 W
 PL1W 0.34251819 W
 PL1W 0.24234537 W
 SFO2 600.2624010 MHz

F2 - Processing parameters
 SI 32768
 SF 150.9355829 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

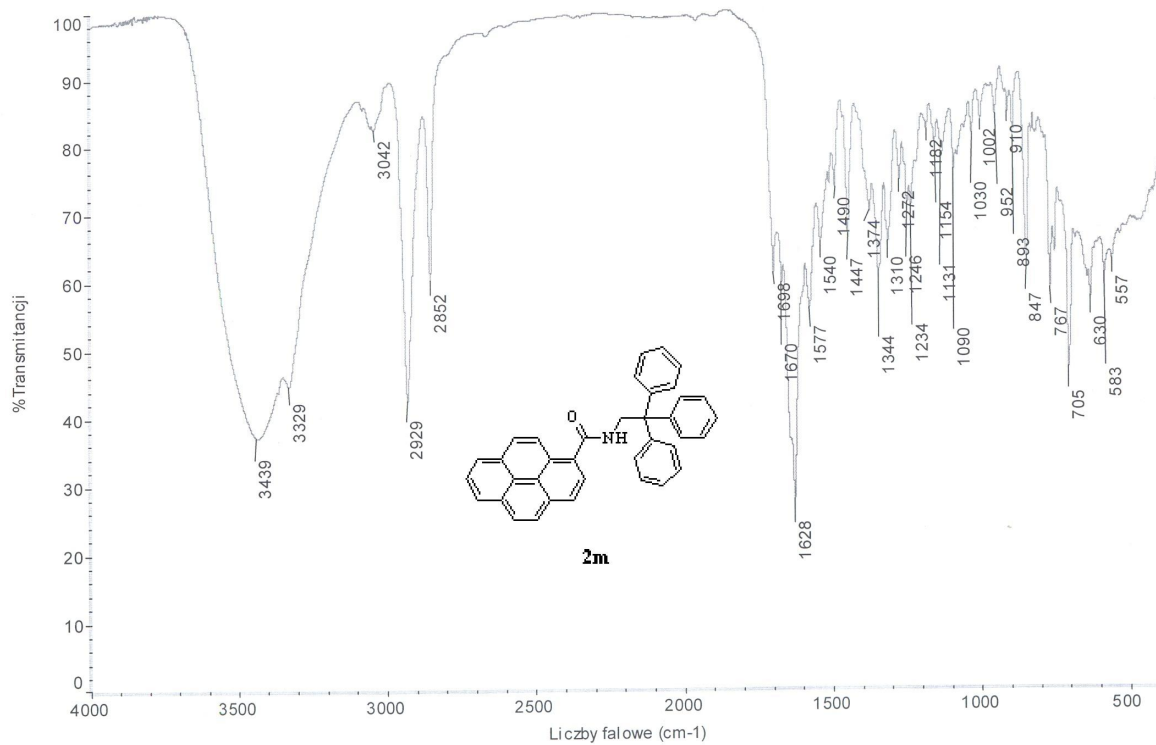


Current Data Parameters
 NAME wpa-267a
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140113
 Time 13.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 12225.526 Hz
 FIDRES 0.188223 Hz
 AQ 2.6564426 sec
 RG 512
 DW 40.533 usec
 DE 8.50 usec
 TE 303.0 K
 DL 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 -3.00 dB
 PL1W 20.57242203 W
 SFO1 600.2637069 MHz

F2 - Processing parameters
 SI 32768
 SF 600.2600174 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



10.02.2014

KBr