

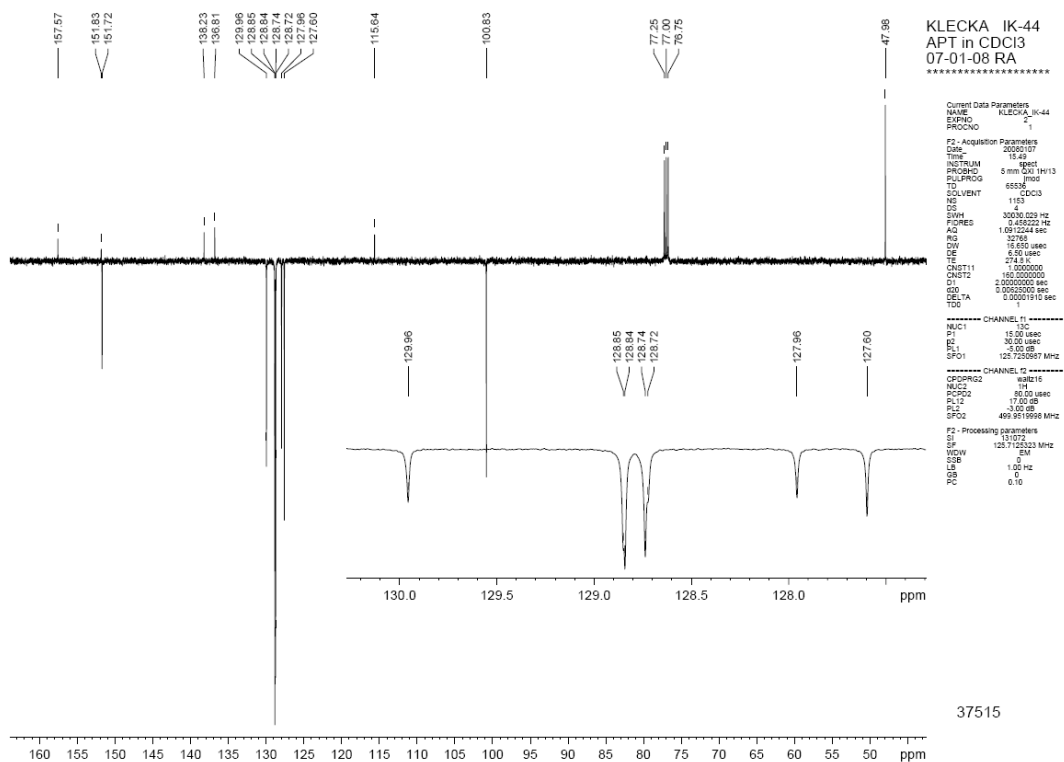
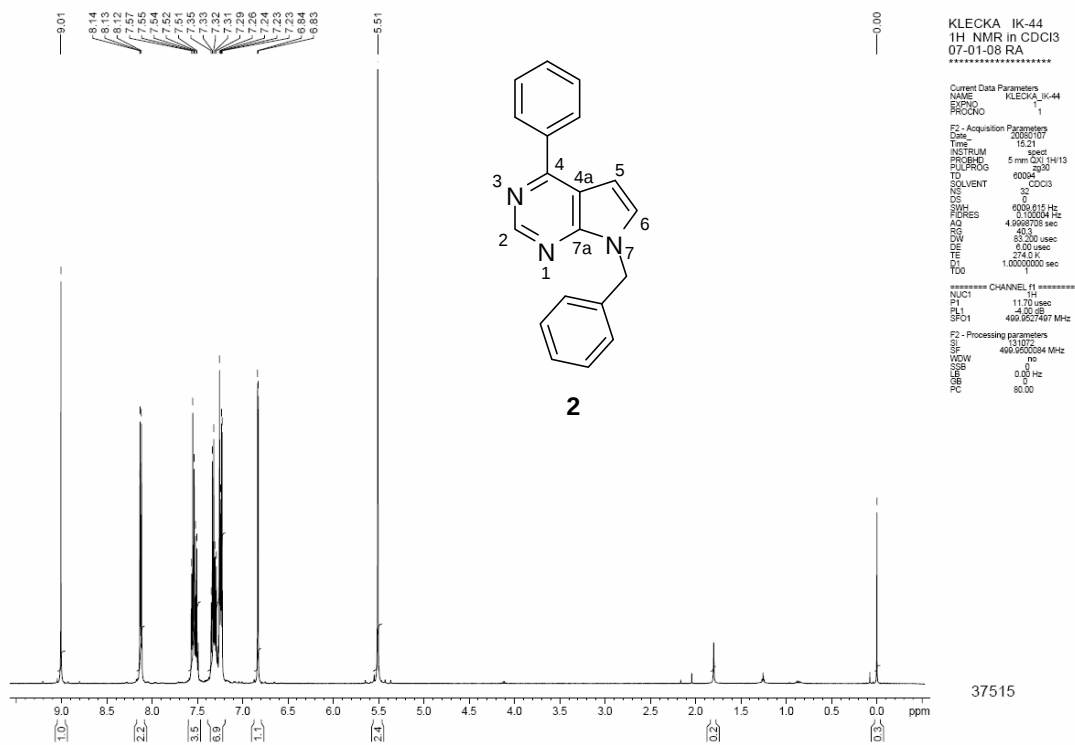
Supporting Information II

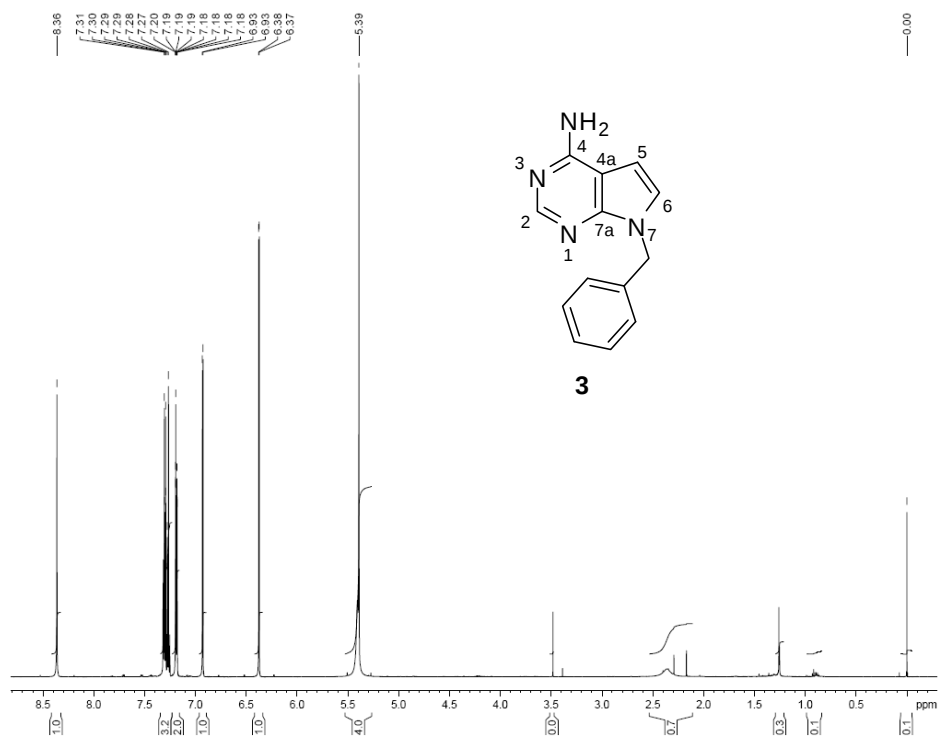
Direct C-H Borylation and C-H Arylation of Pyrrolo[2,3-d]pyrimidines: Synthesis of 6,8-Disubstituted 7-deazapurines.

Martin Klečka, Radek Pohl, Blanka Klepetářová, and Michal Hocek*

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1. Copies of NMR spectra	S2
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KLECKA IK-129
1H NMR in CDCl₃
12-08-08 RA

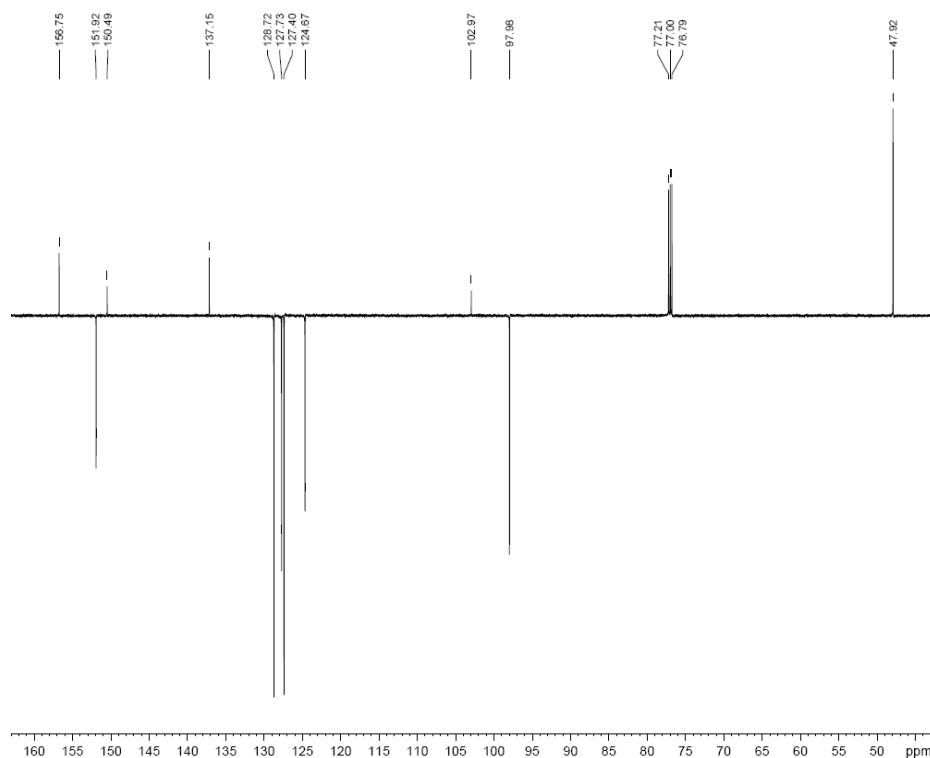
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PROCNO 1

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INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 72114
SOLVENT CDCl₃
NS 8
DS 0
SWH 7211.539 Hz
FIDRES 0.100002 Hz
AQ 4.9999542 sec
RG 22.6
DW 69.333 usec
DE 20.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 8.10 dB
SFO1 600.1353007 MHz

F2 - Processing parameters
SI 131072
SF 600.1300688 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 40.00

38811



KLECKA IK-129
APT in CDCl₃
12-08-08 RA

Current Data Parameters
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EXPNO 2
PROCNO 1

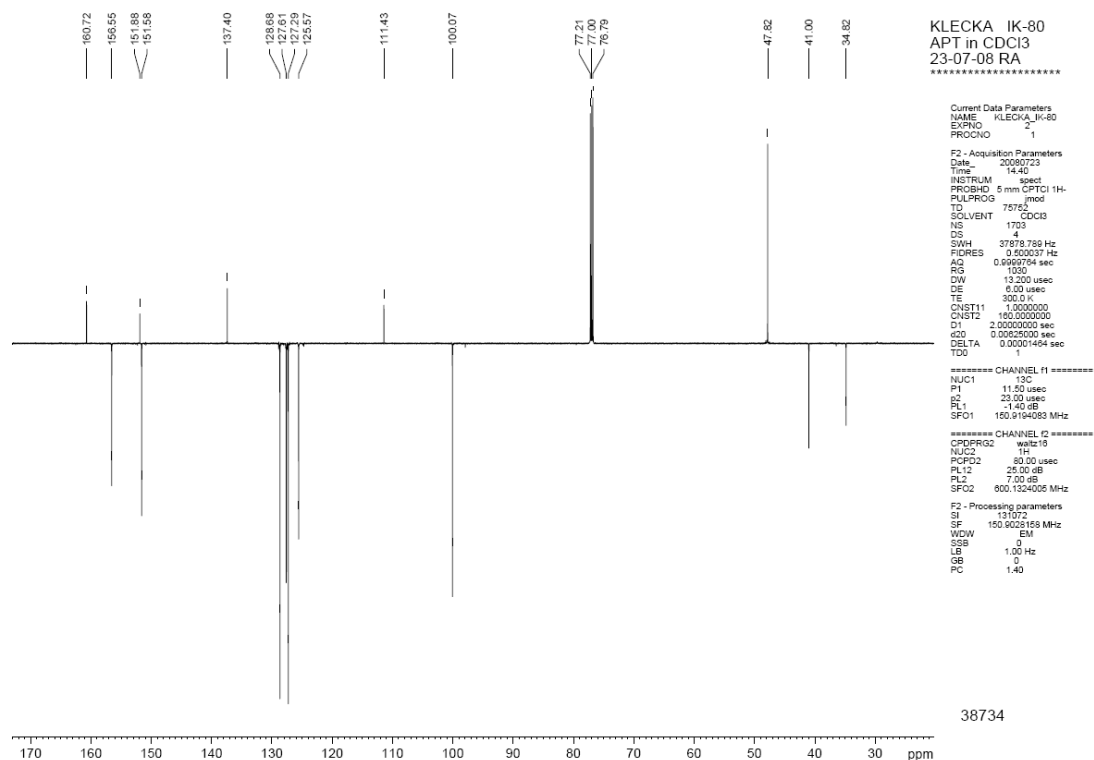
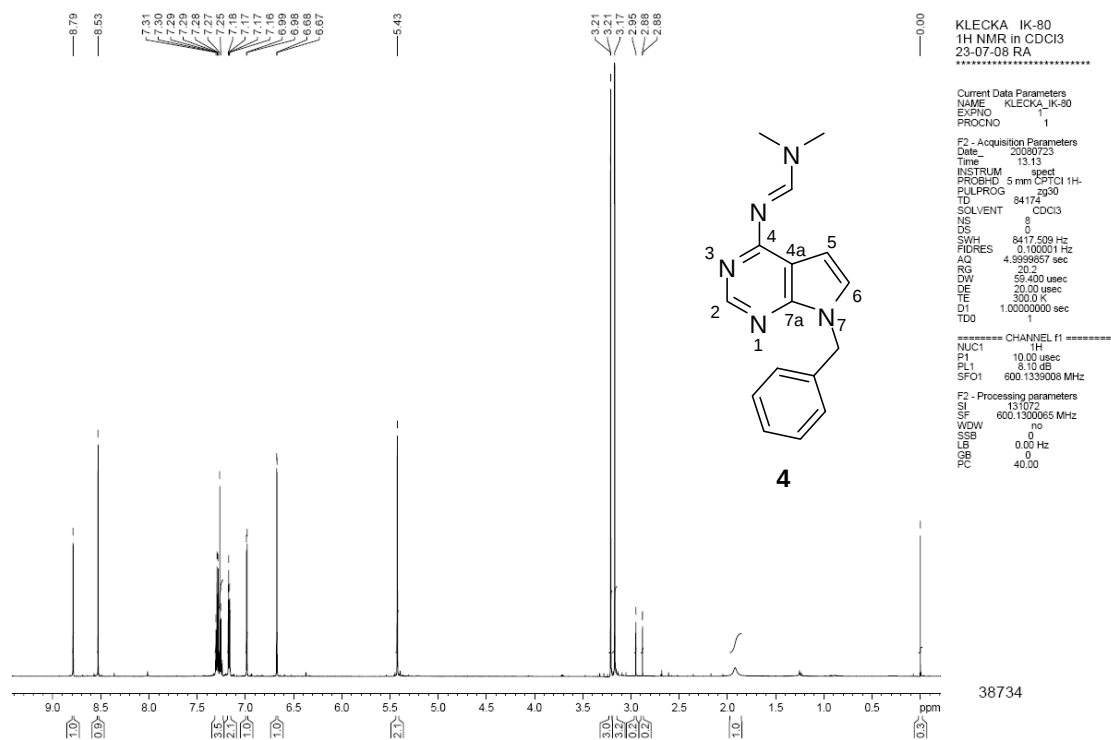
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Time 7.18
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG gmod
TD 75762
SOLVENT CDCl₃
NS 104
DS 4
SWH 37879.788 Hz
FIDRES 0.500037 Hz
AQ 0.6999254 sec
RG 812
DW 13.200 usec
DE 6.00 usec
TE 300.0 K
CNST11 1.0000000
CNST2 160.0000000
D1 2.00000000 sec
DELTA 0.00625000 sec
TD0 1

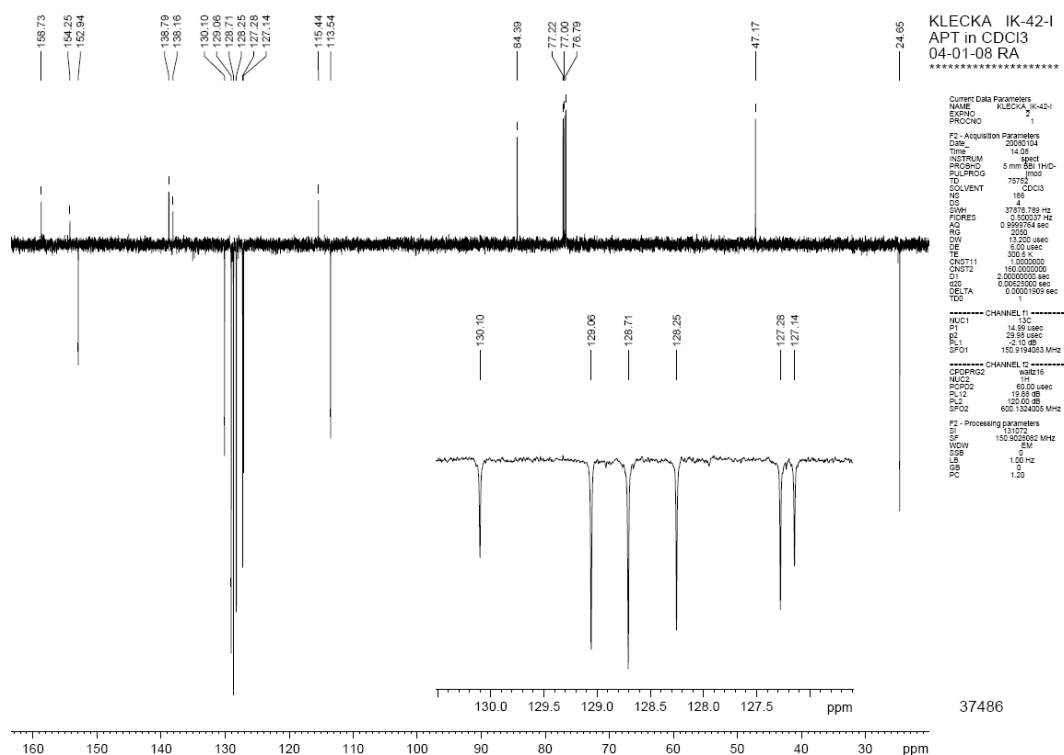
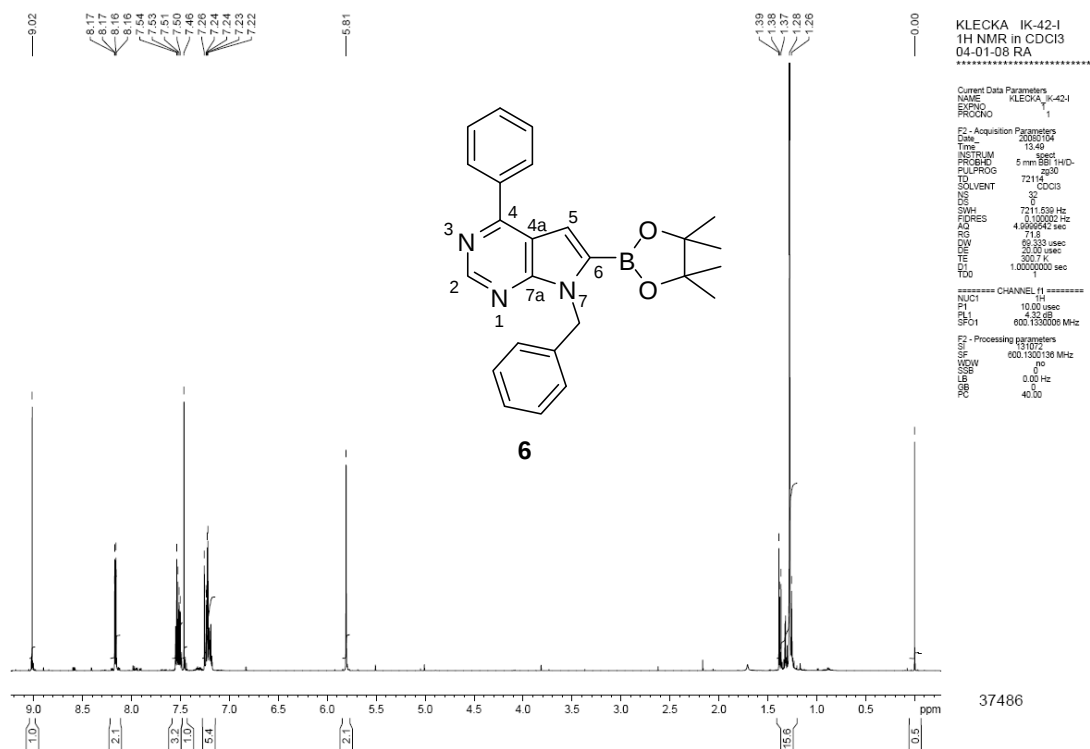
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P1 11.50 usec
P2 23.00 usec
PL1 -1.40 dB
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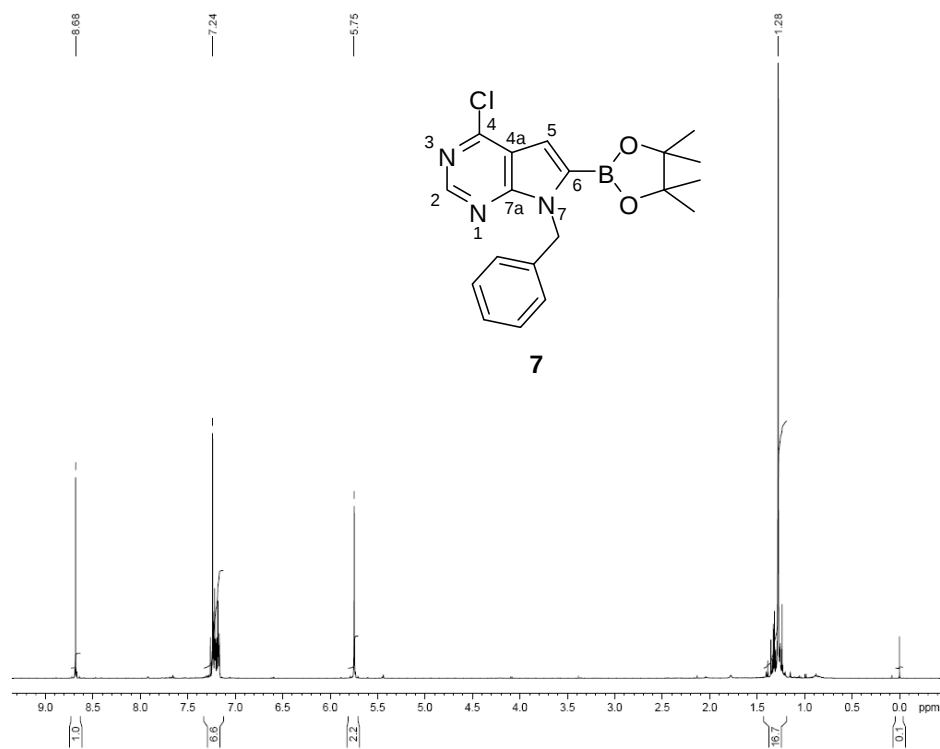
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 25.00 dB
PL2 7.00 dB
SFO2 600.1324005 MHz

F2 - Processing parameters
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SF 150.9026182 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

38811



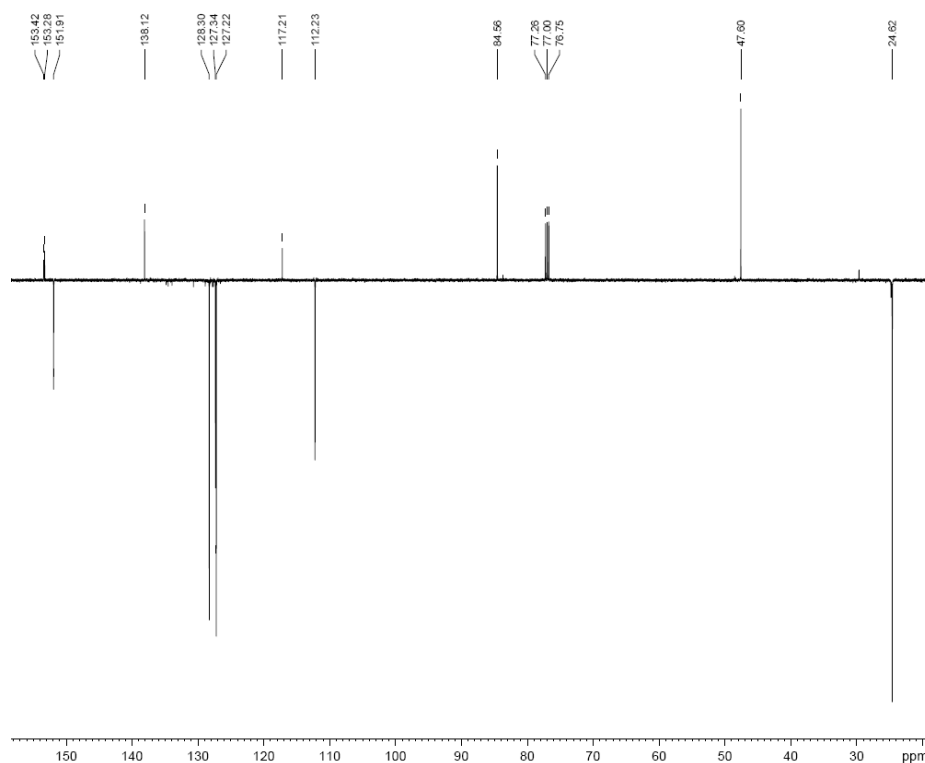




KLECKA IK-91
1H NMR in CDCl₃
09-04-08 RA

Current Data Parameters
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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080409
Time 15.43
INSTRUM spect
PROBHD 5 mm TBO BB-1H
PULPROG zg30
TD 69960
SOLVENT CDCl₃
NS 32
DS 0
SWH 6996.299 Hz
FIDRES 0.100004 Hz
AQ 4.9998579 sec
RG 322
DW 71.487 usec
DE 20.00 usec
TE 297.4 K
D1 0.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.68 usec
PL1 -2.00 dB
SFO1 499.8426992 MHz
F2 - Processing parameters
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SF 499.840078 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

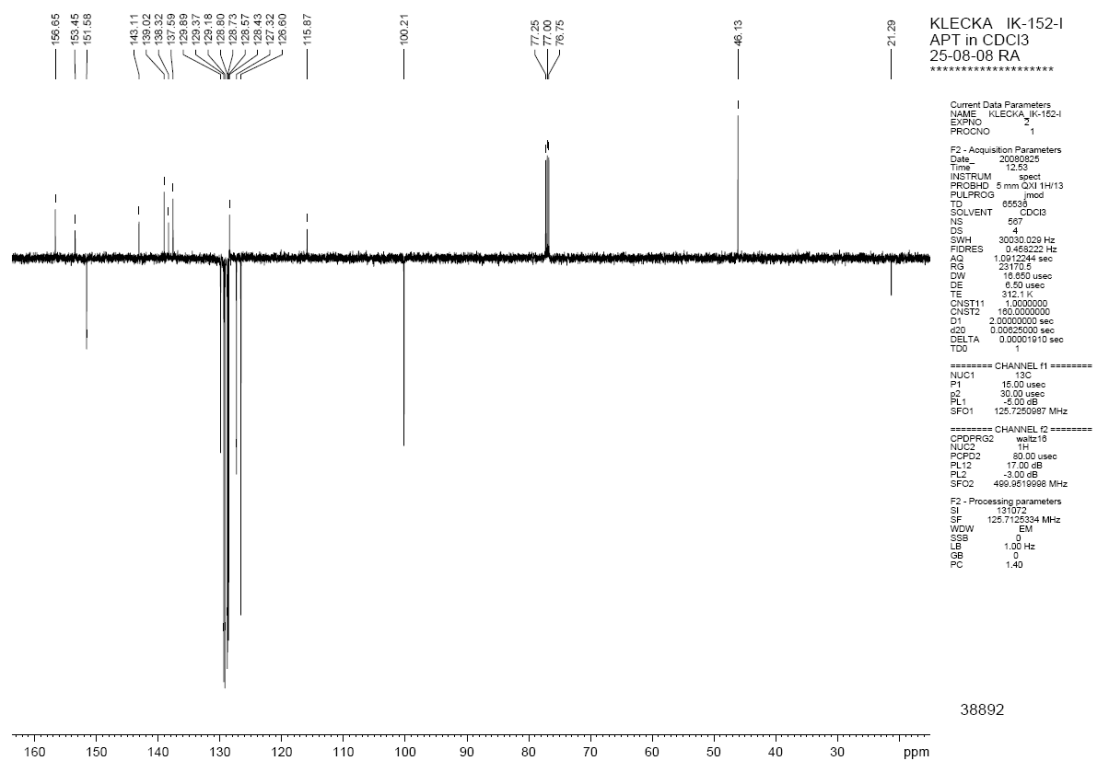
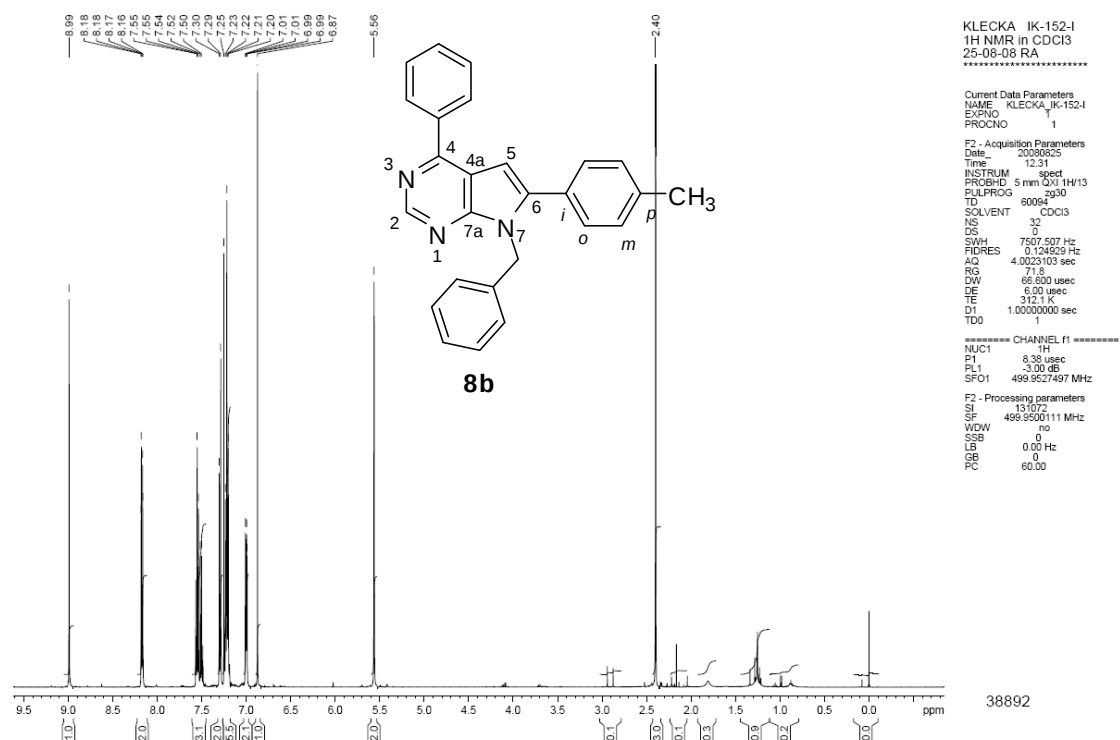
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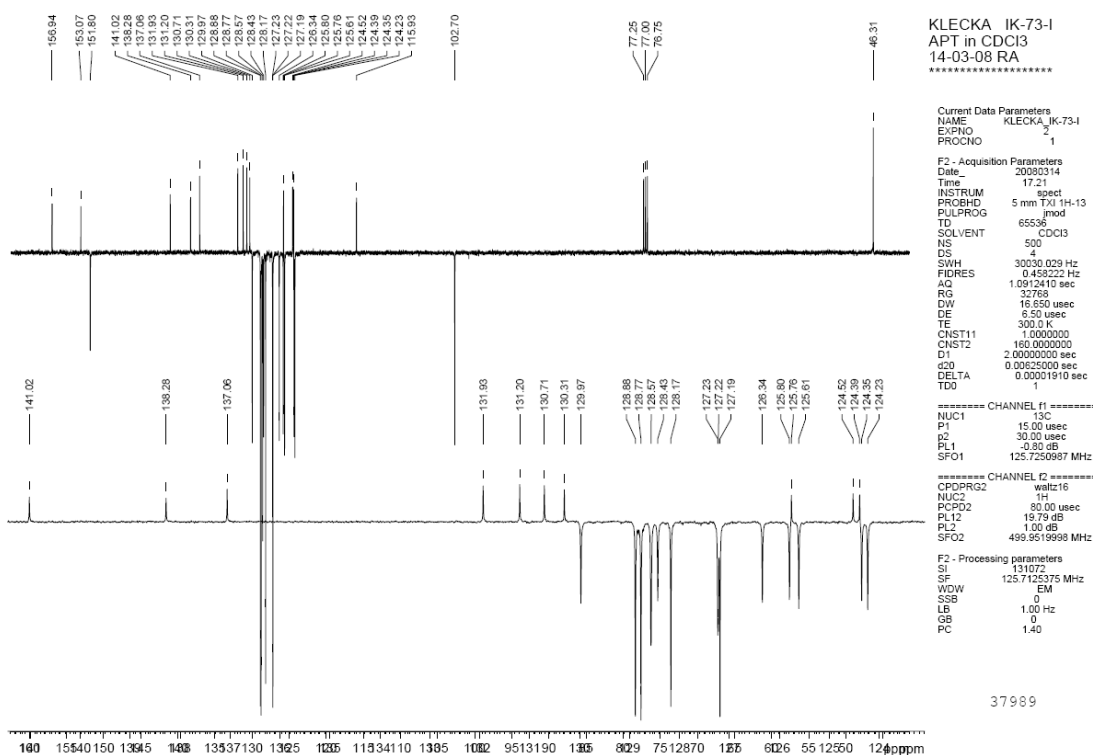
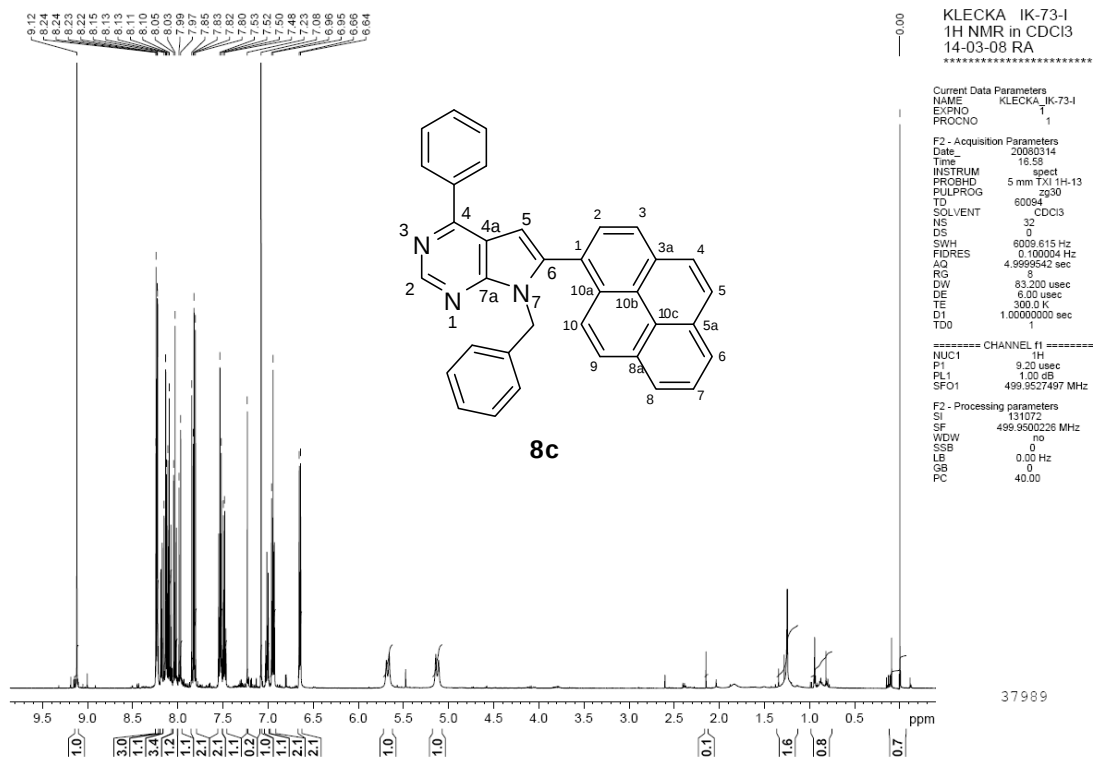


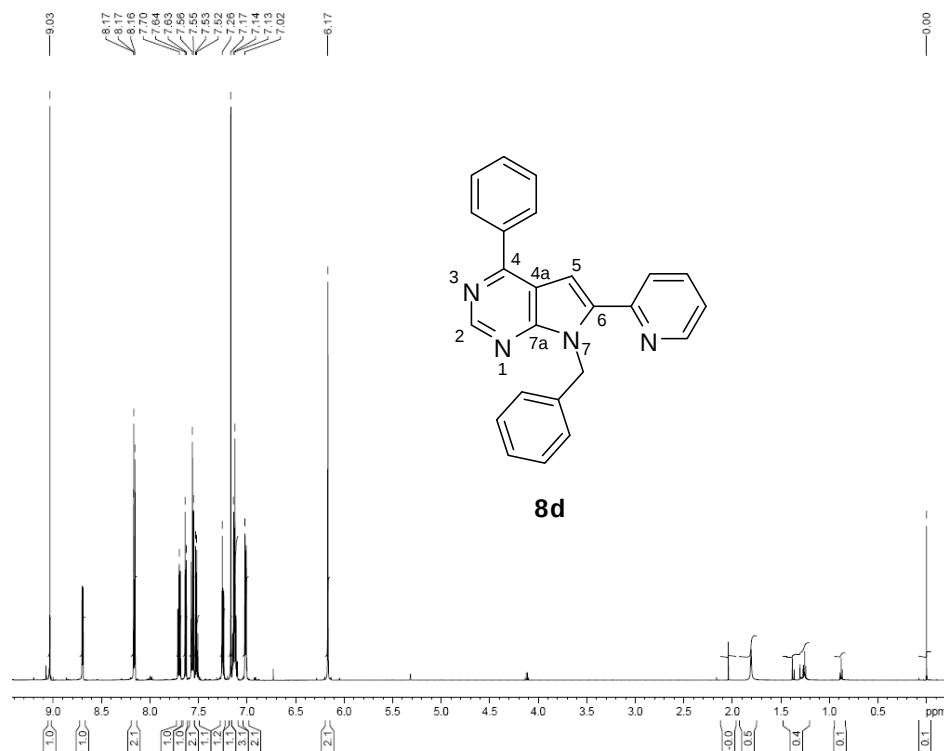
KLECKA IK-91
APT in CDCl₃
09-04-08 RA

Current Data Parameters
NAME KLECKA IK-91
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080409
Time 15.56
INSTRUM spect
PROBHD 5 mm TBO BB-1H
PULPROG zg30
TD 69960
SOLVENT CDCl₃
NS 32
DS 4
SWH 20761.904 Hz
FIDRES 0.464131 Hz
AQ 1.1010548 sec
RG 322
DW 16.800 usec
DE 20.00 usec
TE 297.2 K
CNST1 1.0000000
CNST2 160.0000000
D1 2.00000000 sec
d20 0.00825000 sec
DELTA 0.00001019 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 16.00 usec
PL2 -3.30 dB
SFO1 125.6674385 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.71 dB
PL2 -2.00 dB
SFO2 499.8419994 MHz
F2 - Processing parameters
SI 131072
SF 125.6648744 MHz
WDW EM
SSB 0
LB 0.70 Hz
GB 0
PC 1.20

38213







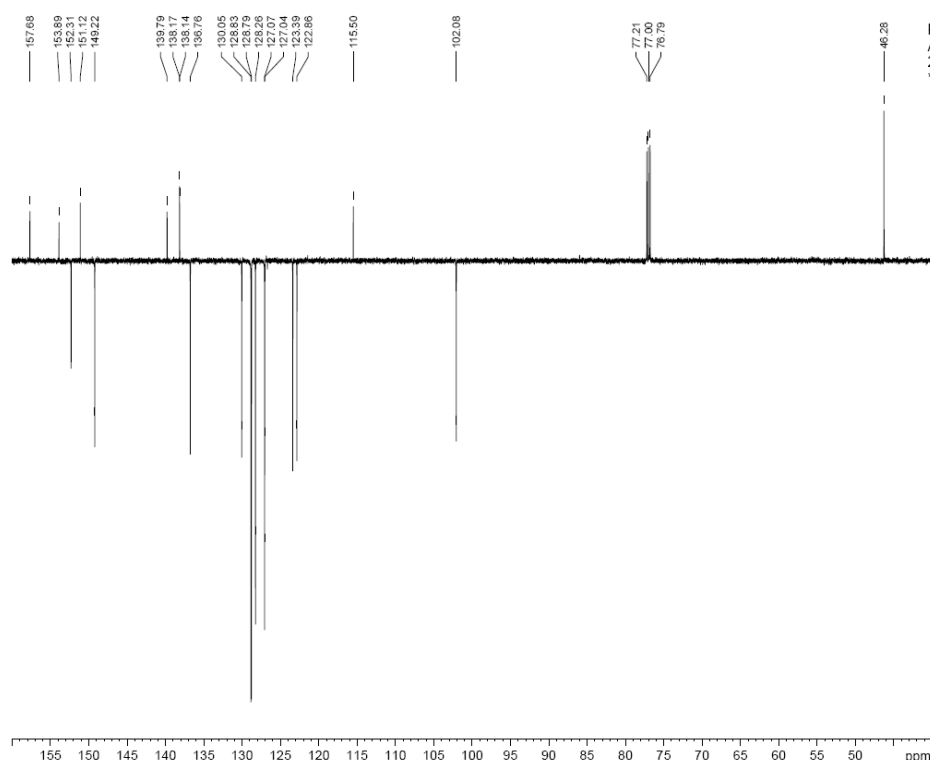
KLECKA IK-109-I
1H NMR in CDCl₃
23-07-08 RA

Current Data Parameters
NAME KLECKA_IK-109-I
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080723
Time 11.22
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 84174
SOLVENT CDCl₃
NS 8
DS 4
SWH 8417.509 Hz
FIDRES 0.100001 Hz
AQ 4.999667 sec
RG 20.2
DW 59.400 usec
DE 20.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 8.10 dB
SFO1 600.1339008 MHz

F2 - Processing parameters
SI 131072
SF 600.1300122 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
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KLECKA IK-109-I
13C NMR in CDCl₃
23-07-08 RA

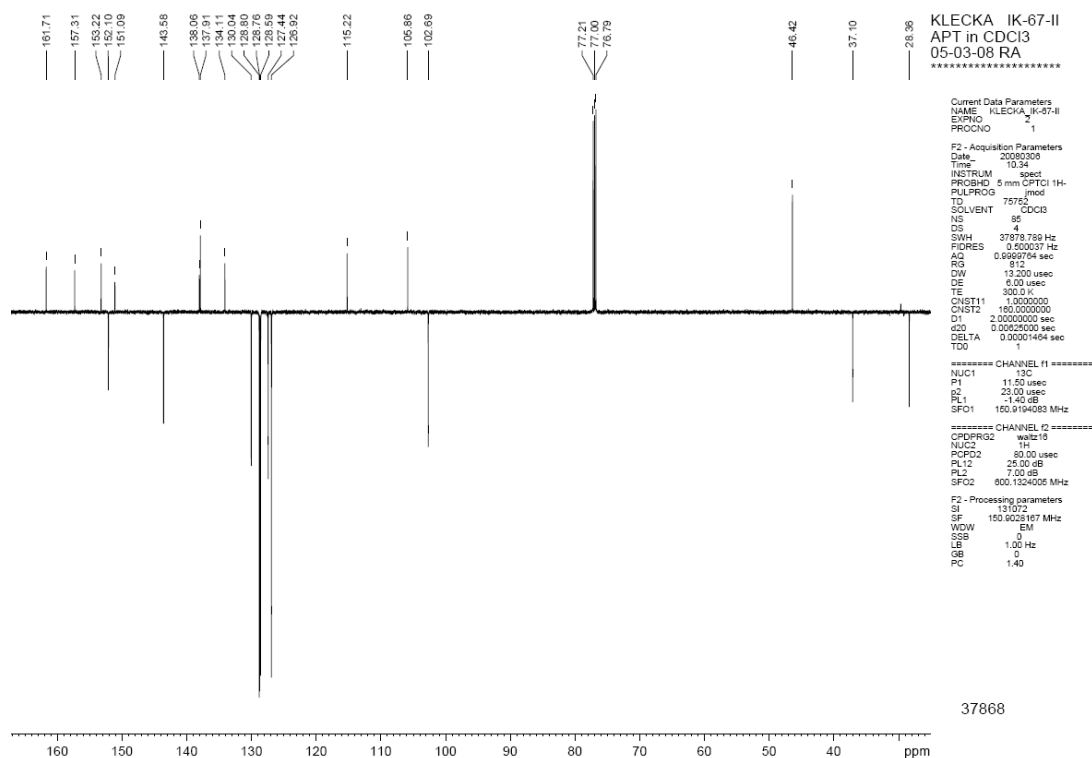
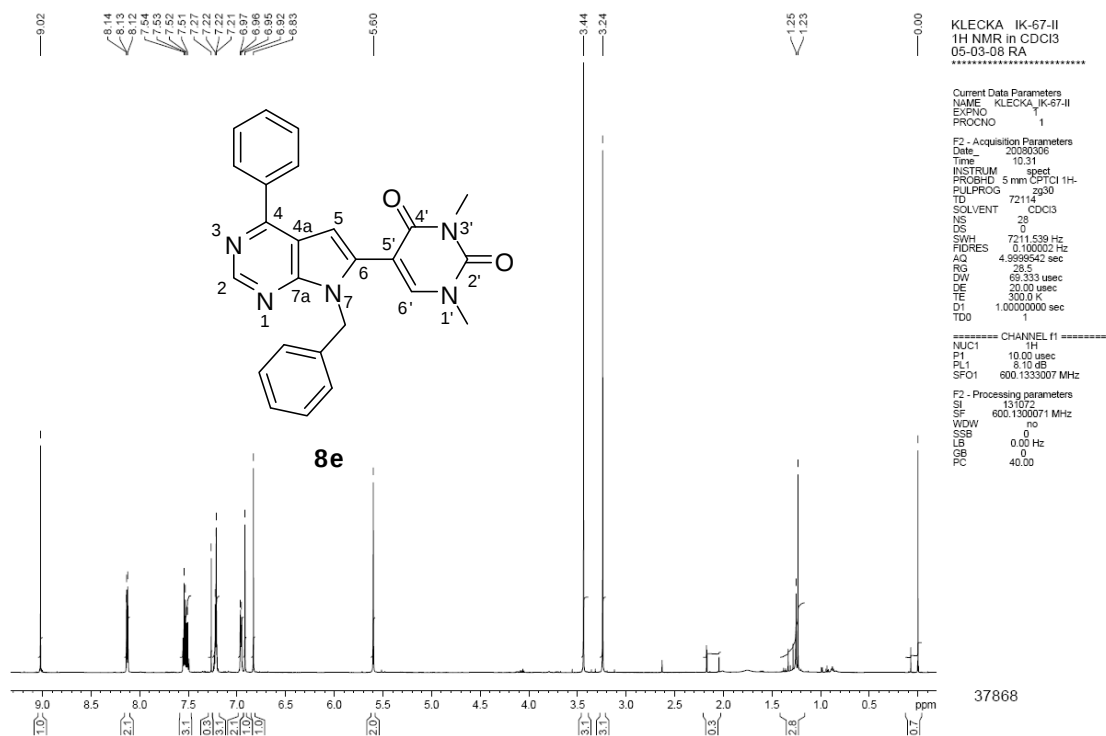
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EXPNO 1
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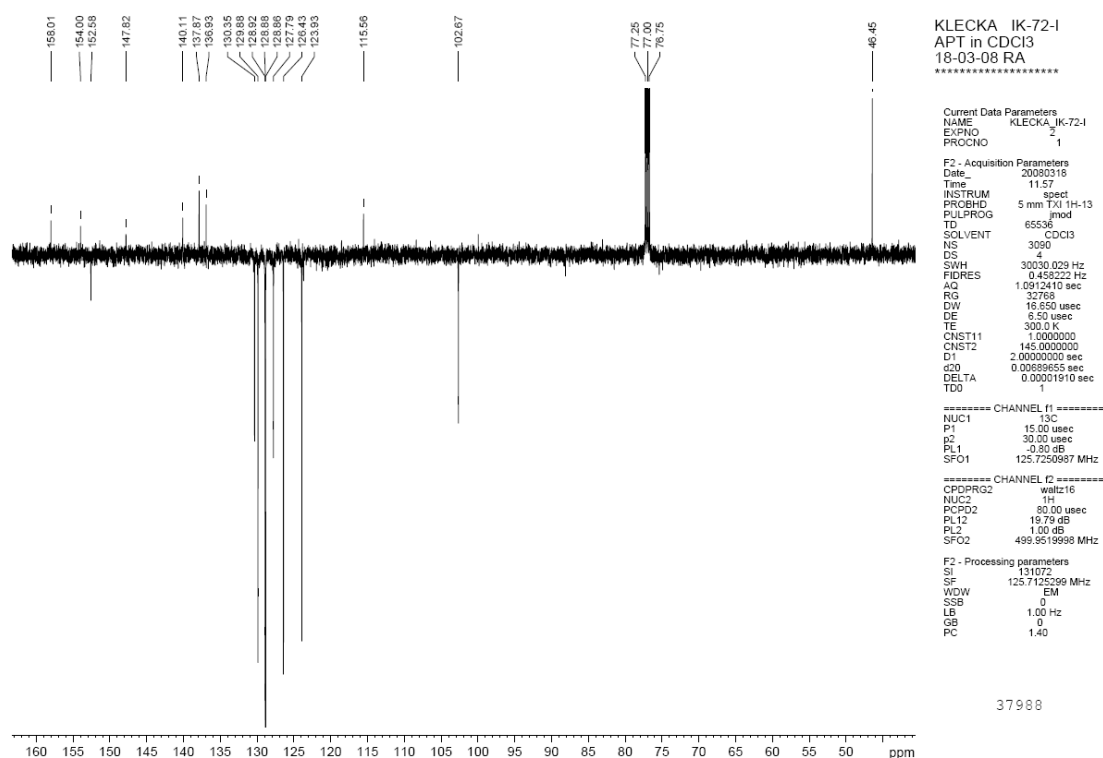
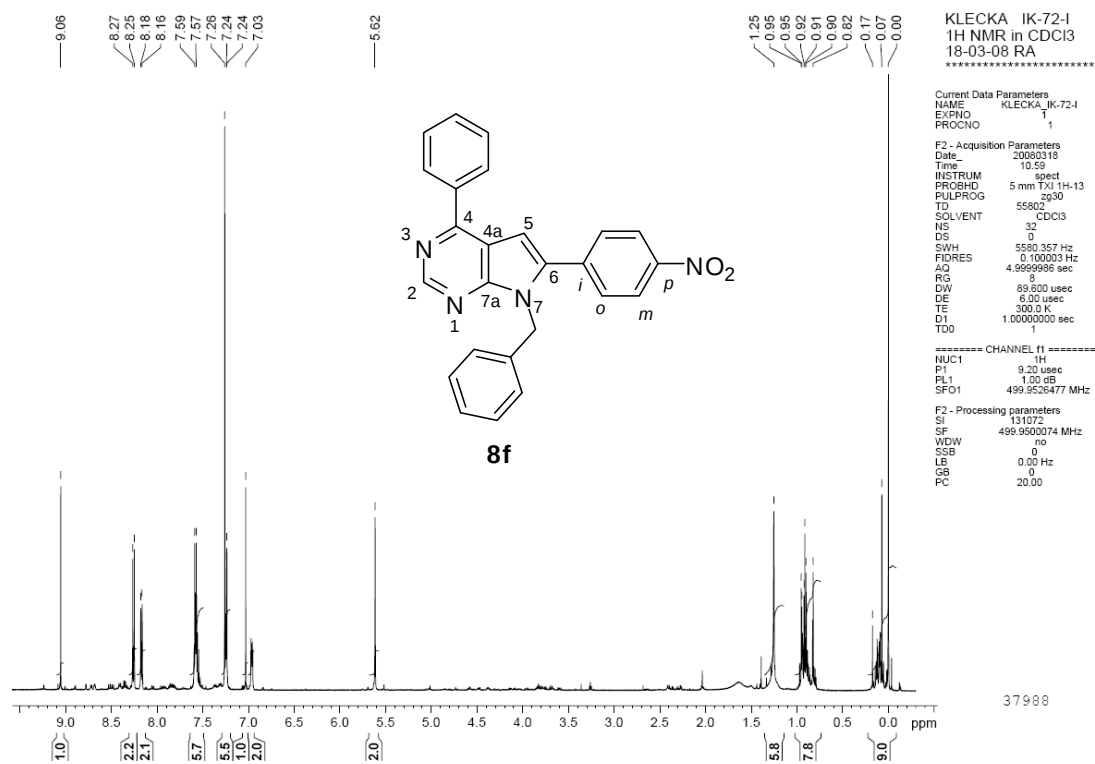
F2 - Acquisition Parameters
Date_ 20080723
Time 11.23
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 75762
SOLVENT CDCl₃
NS 15
DS 4
SWH 37878.788 Hz
FIDRES 0.600037 Hz
AQ 0.9999704 sec
RG 915
DW 13.200 usec
DE 6.00 usec
TE 300.0 K
CNST11 1.0000000
CNST12 160.0000000
D1 2.0000000 sec
d20 0.0000000 sec
DELTA 0.00001464 sec
TD0 1

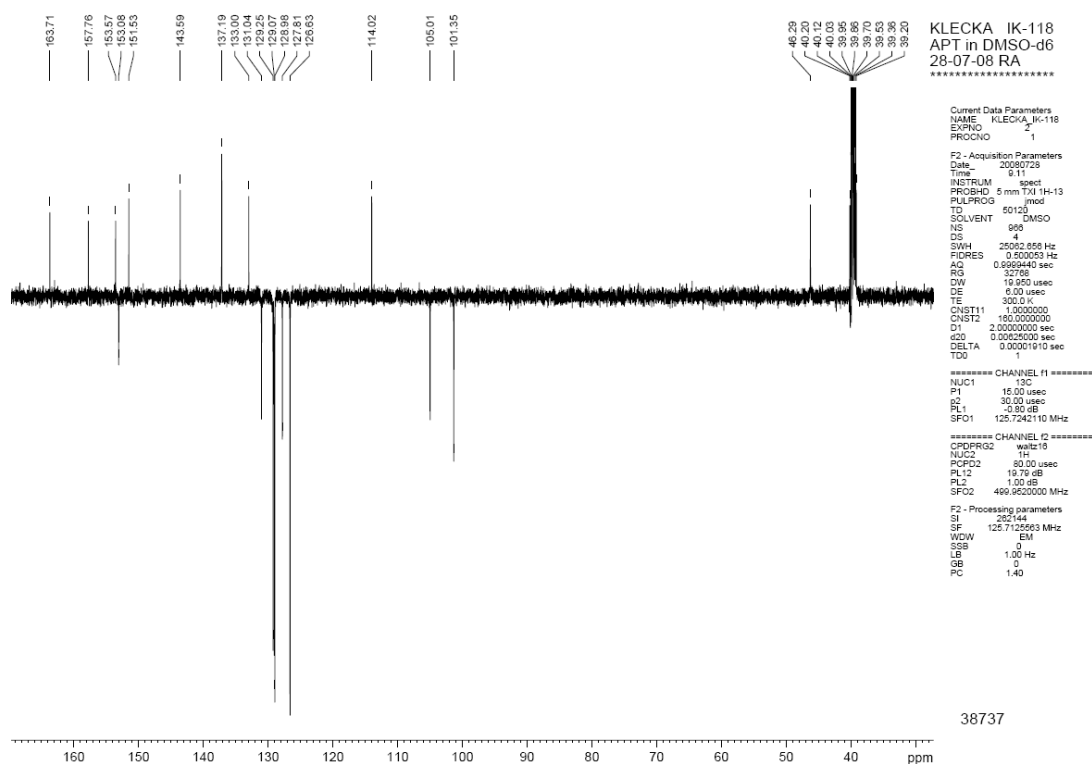
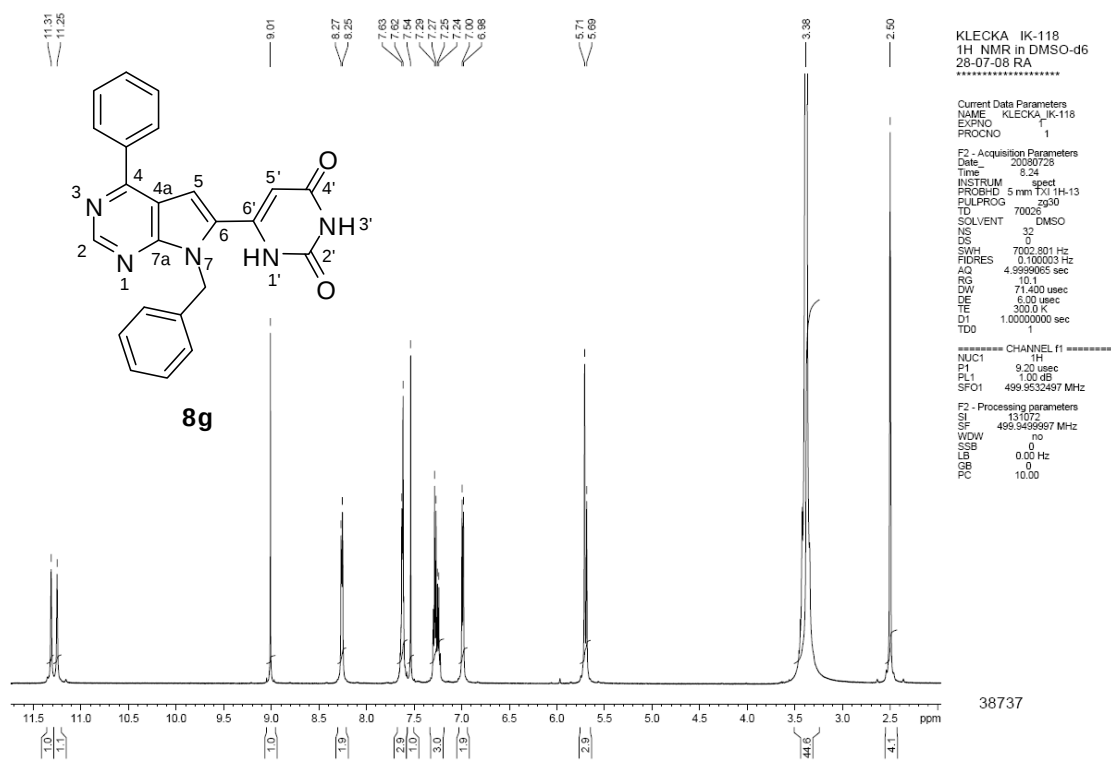
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NUC1 13C
P1 11.50 usec
PL1 25.00 dB
SFO1 100.6194063 MHz

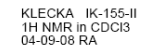
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 80.00 usec
PL2 25.00 dB
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 131072
SF 100.6025183 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



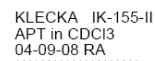






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EXPNO     1
PROCNO    1
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Date_      20080908
Time       14.13
INSTRUM    spect
PROBHD     5 mm QNP 1H/13
PULPROG    zg30
RG          8016
SOLVENT    CDCl3
NS          32
DS          2
SWH         801.820 kHz
FIDRES     0.100003 Hz
AQ          4.8699123 sec
RG          226.1
DW          6.2040000 sec
DE          6.0000000 sec
TE          312.1 K
TD0         1.00000000 sec
===== CHANNEL f1 =====
NUC1       1H
P1         8.38 usec
PL1        -3.00 db
SFO1       499.9537496 MHz

F2 - Processing parameters
SI          131072
SF          499.9500059 MHz
WDW         no
SSB         0
GB          0.00 Hz
LB          0
GB          0
GB          60.00
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EXPNO 1
PROCNO 1

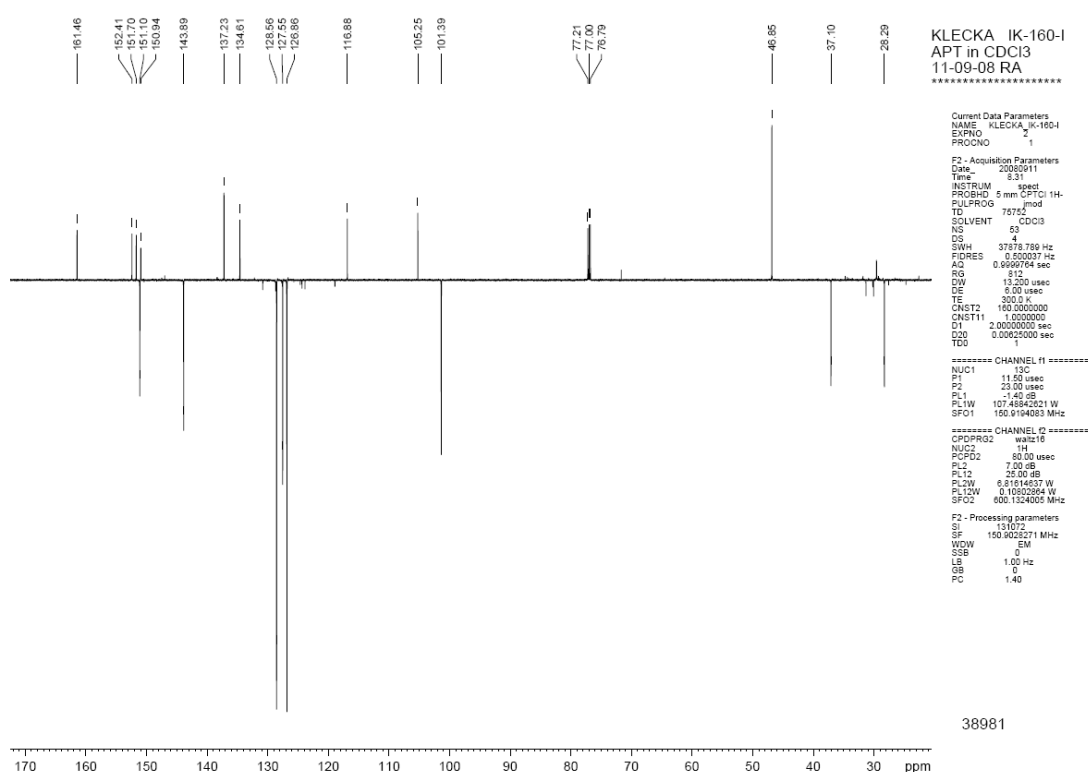
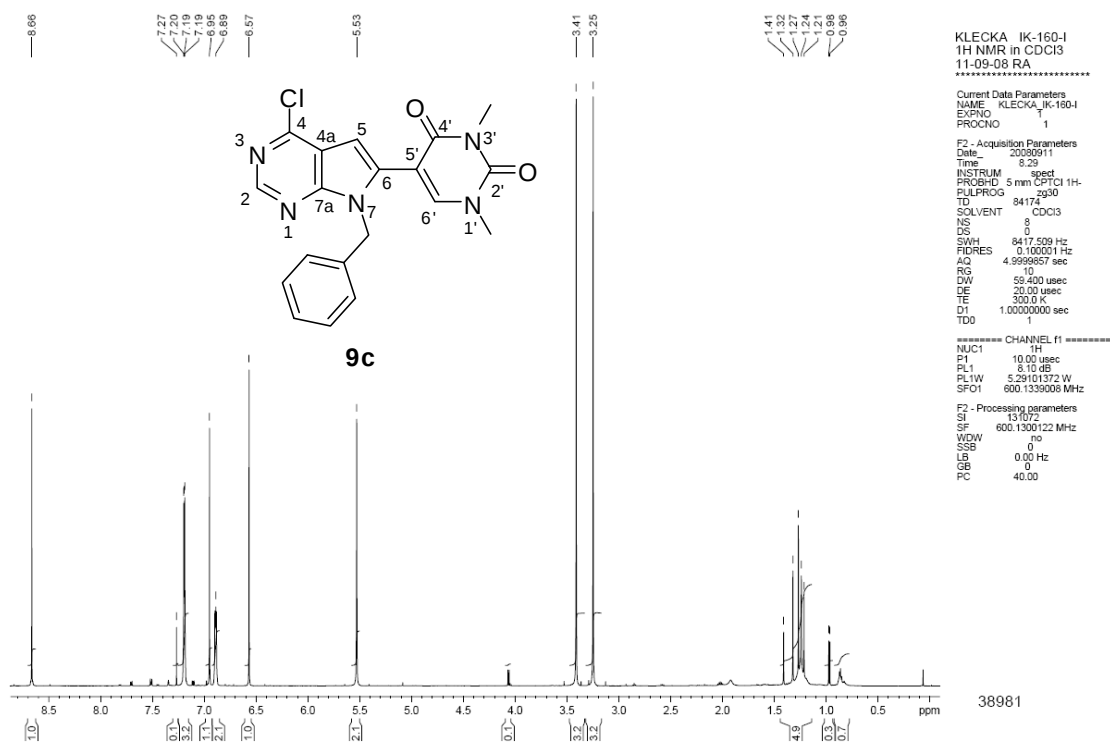
F2 - Acquisition Parameters
Time 20090804
Date_ 15 12 2009
INSTRUM spect
PROBHD 5mm QNP 1H/13
PULPROG zgpg30
PCPDPRG2 6554
SOLVENT CDCl3
NS 1791
DS 4
SWH 30330.029 Hz
FIDRES 15.150 Hz
AQ 1.0017244 sec
RG 312.5
AQ 16.880 sec
TE 300.2 K
DE 6.50 uV
TE 300.2 K
NS111 1.0000000
SFO1 100.6261300 MHz
SFO2 125.7603500 MHz
T1 2.00000000 sec
T1RHO 0.00000000 sec
DELTA 0.00001910 sec
TDO 1

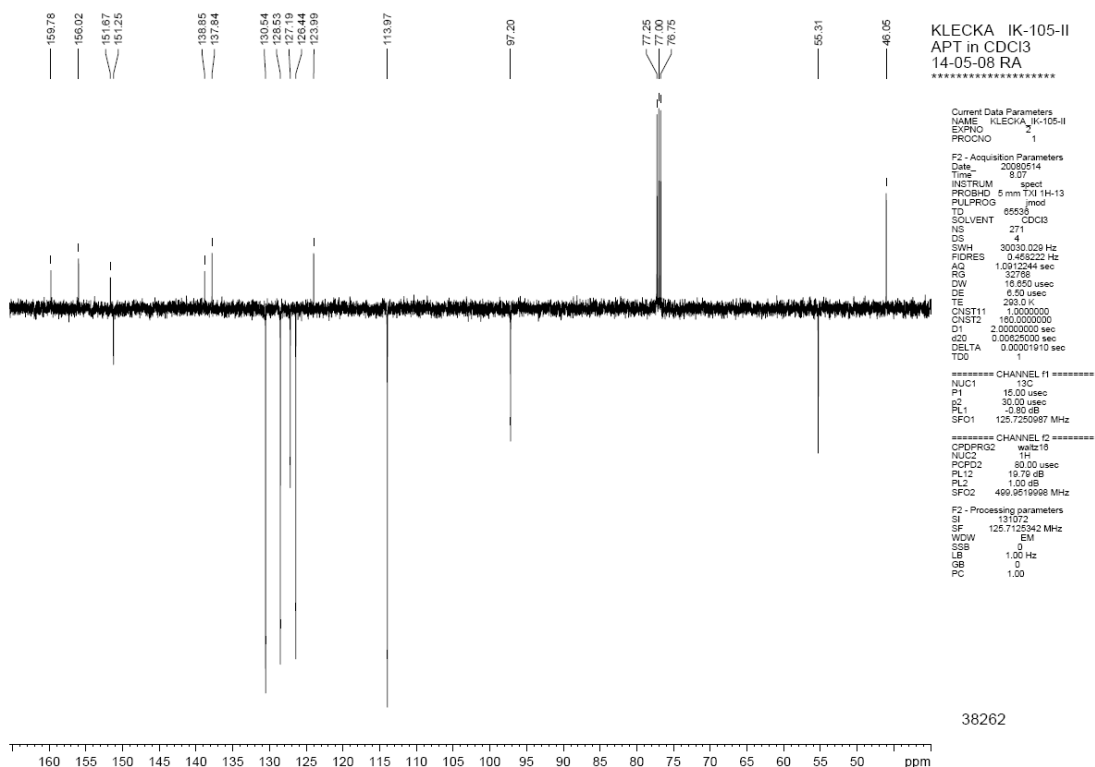
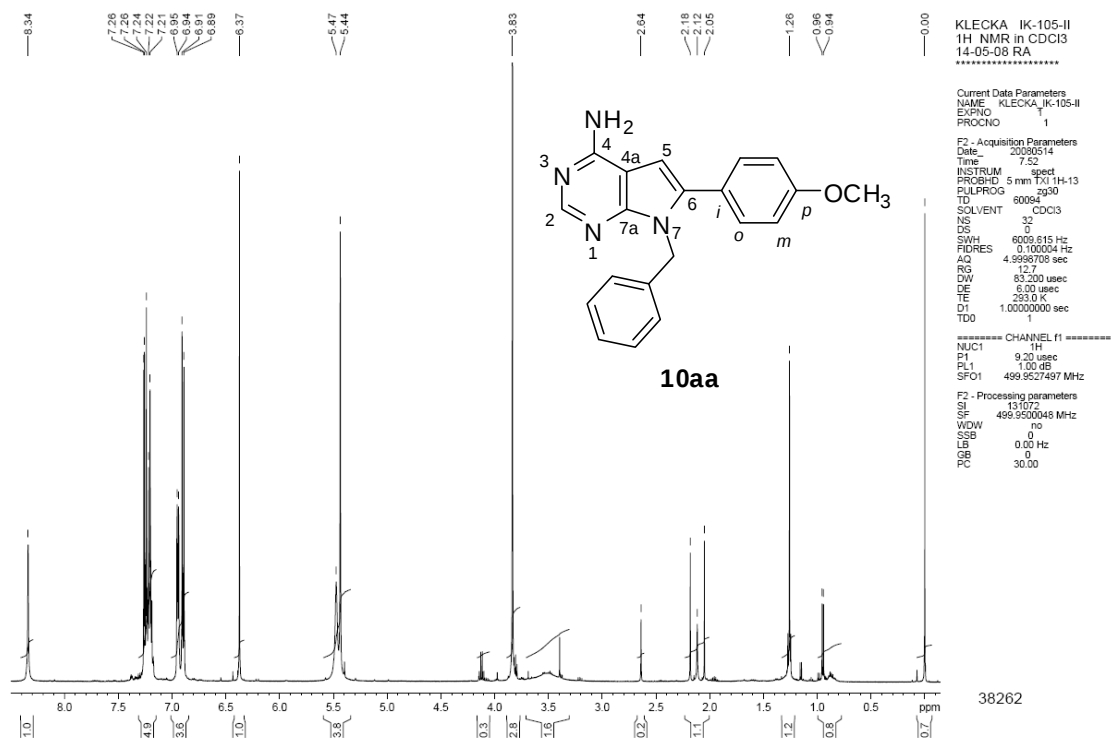
===== CHANNEL f1 =====
NUC1 13C
P1 16.00 uV
PC 32.00 dB
PL1 -6.00 dB
SFO1 125.7250987 MHz

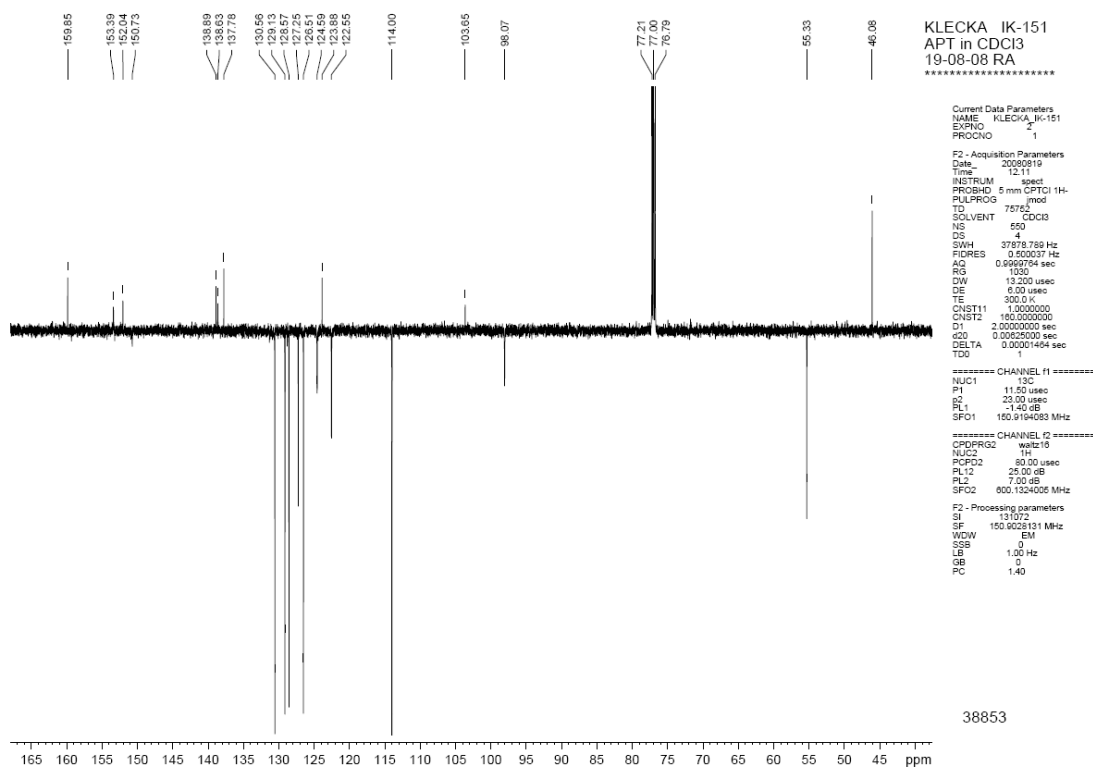
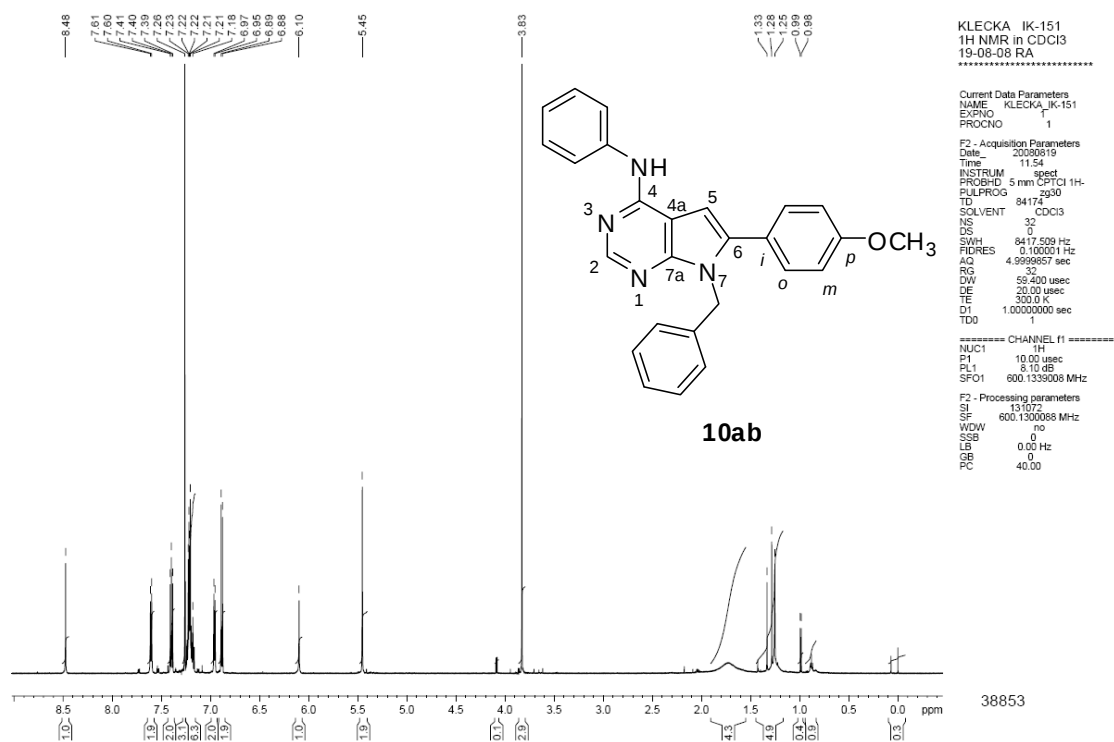
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NUC2 1H
P2 16.00 uV
PC 32.00 dB
PL2 17.00 dB
SFO2 499.9519688 MHz

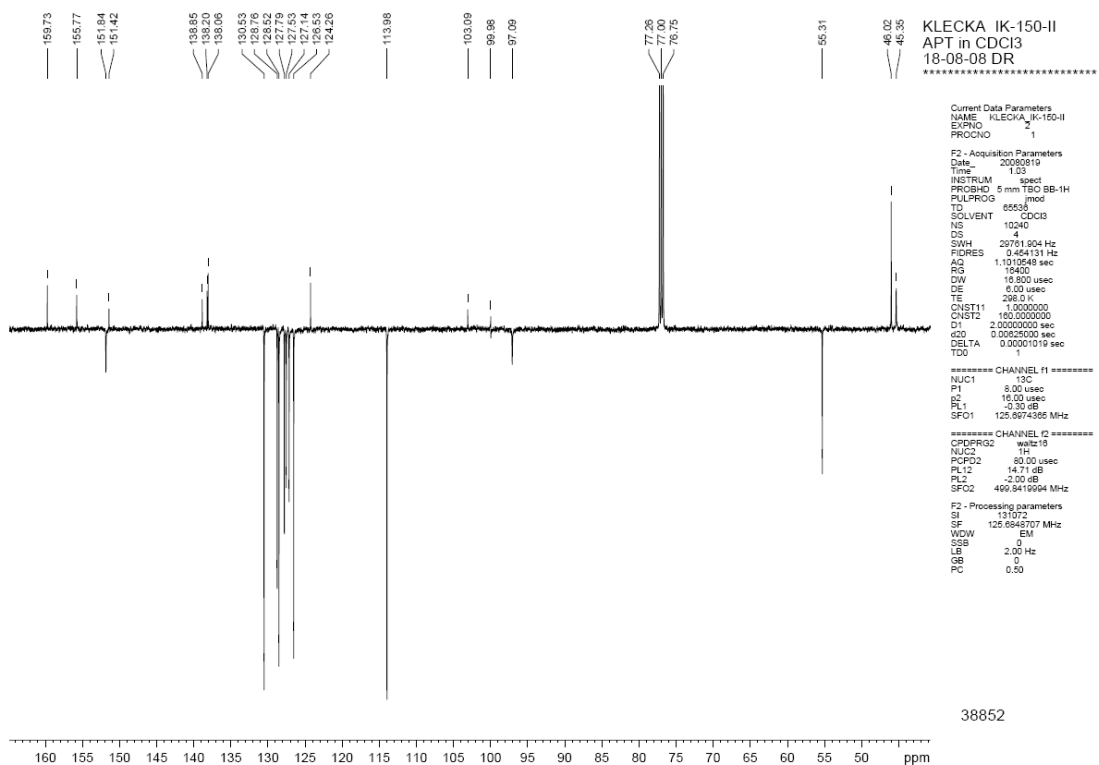
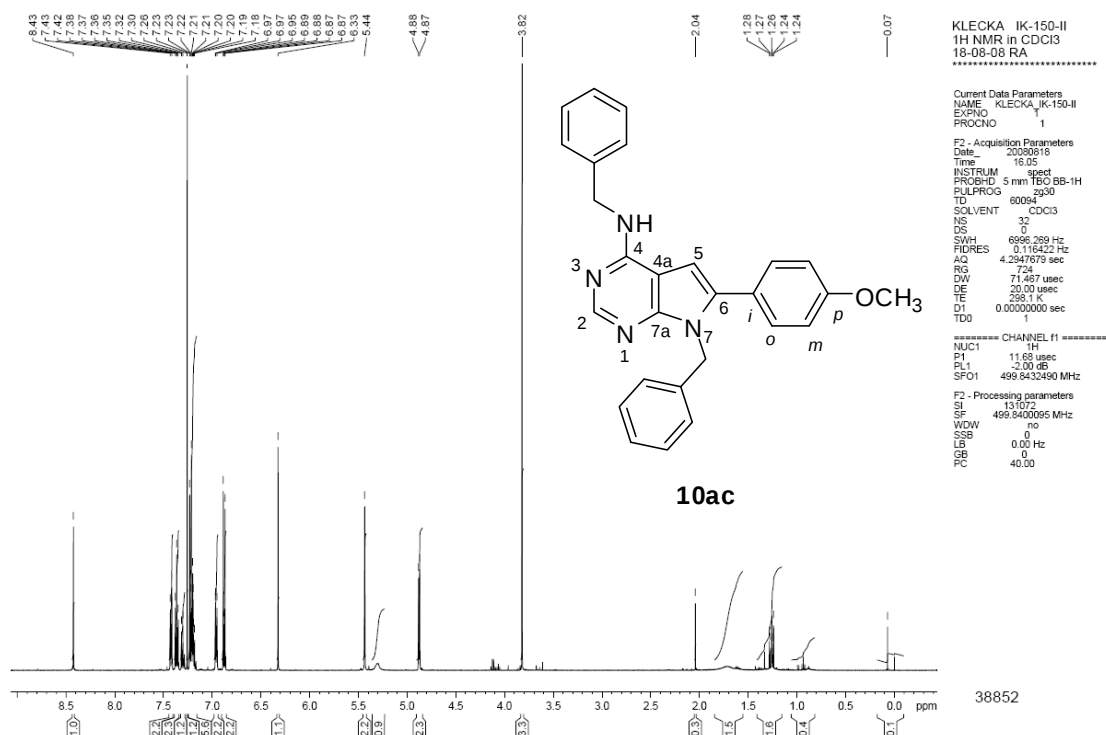
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SSB 0
LB 1.000 Hz
GB 0
PC 1.40

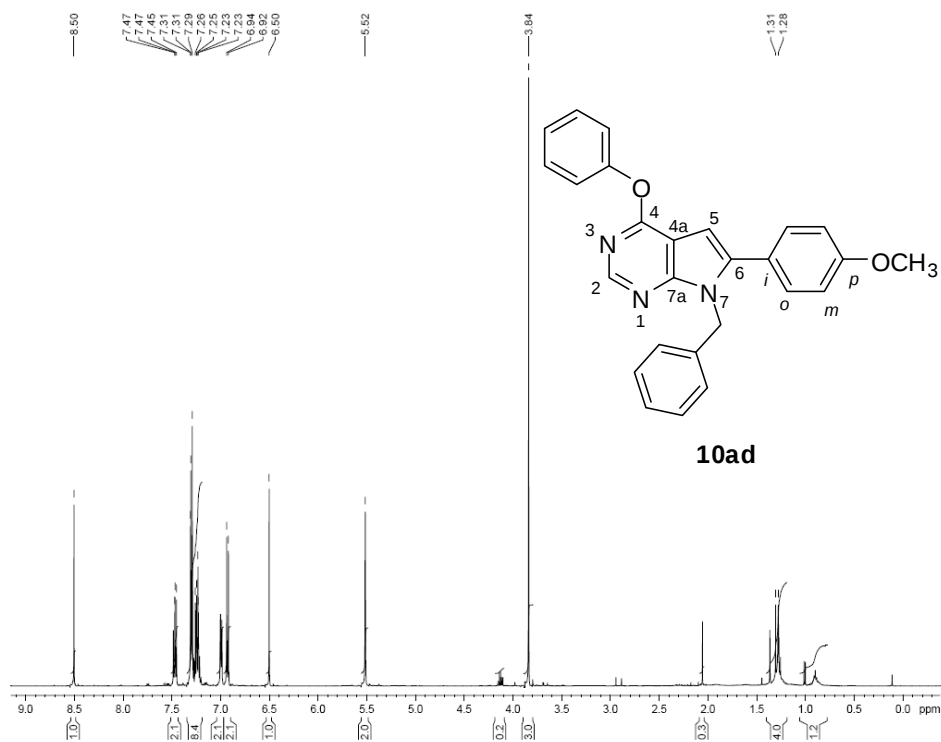
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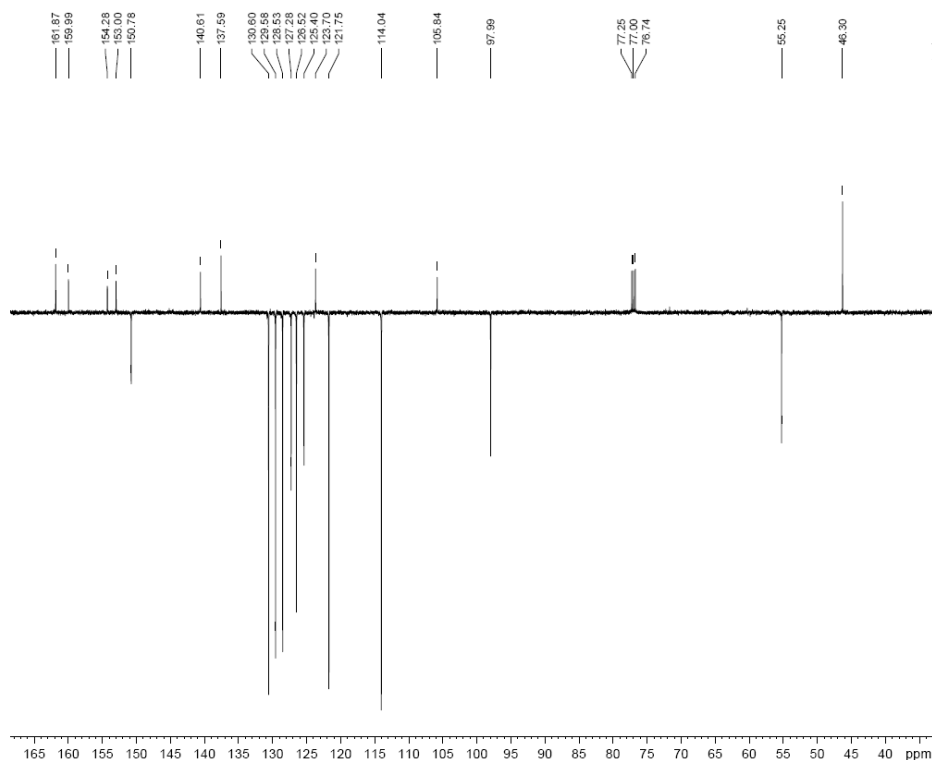




KLECKA IK-153-I
1H NMR in CDCl₃
25-08-08 RA

Current Data Parameters
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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080825
Time 11.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 60000
SOLVENT CDCl₃
NS 0
DS 0
SWH 7507.507 Hz
FIDRES 0.124629 Hz
AQ 4.0023103 sec
RG 32
DQ 62.600 usec
DE 6.00 usec
TE 312.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.38 usec
PL1 3.00 dB
SFO1 499.9527497 MHz
F2 - Processing parameters
SI 131072
SF 499.9500072 MHz
WDW 0
SSB 0
LB 0.00 Hz
GB 0
PC 40.00



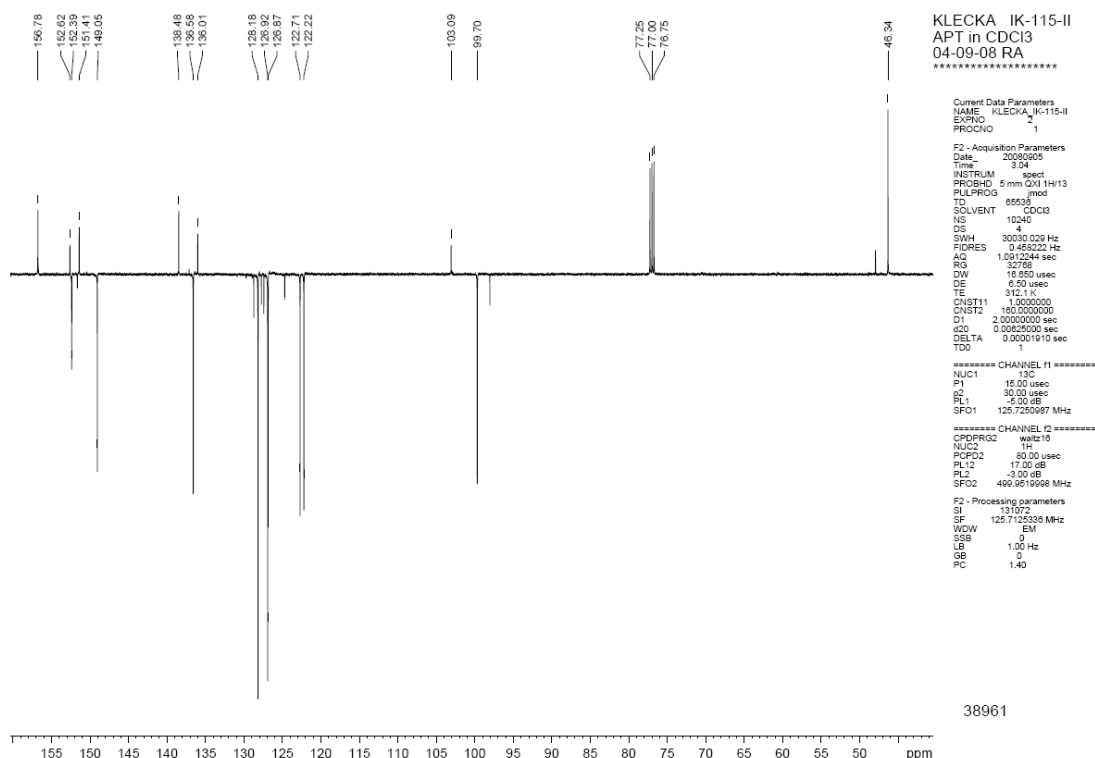
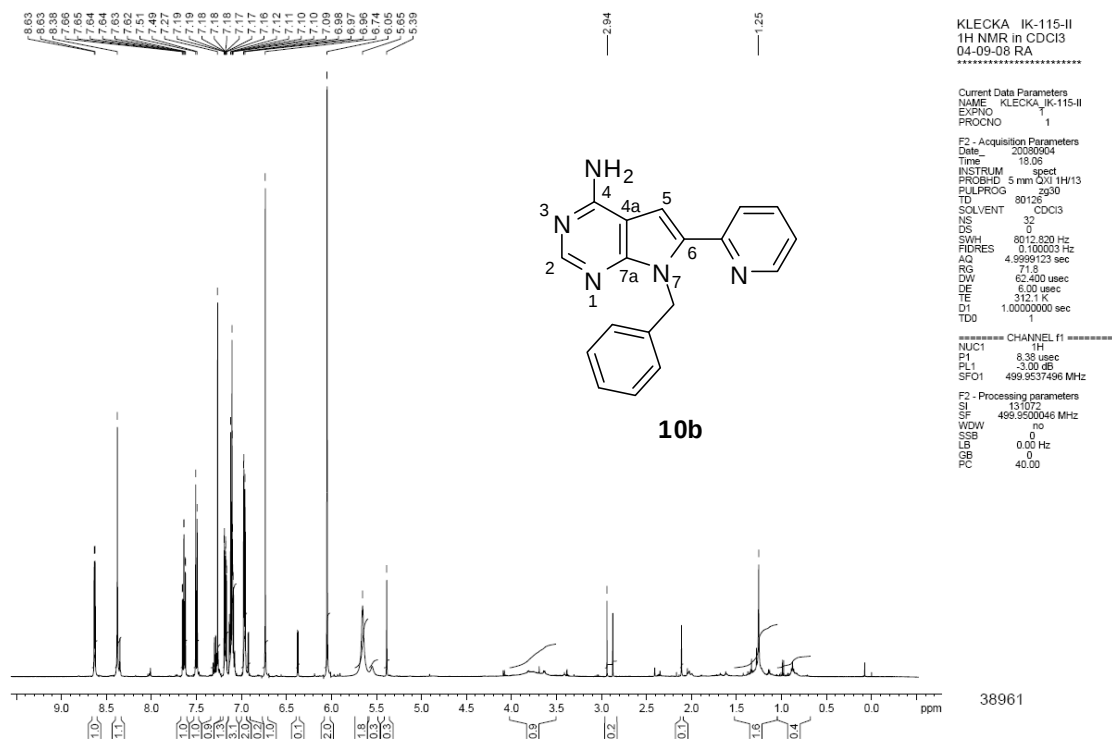
KLECKA IK-153-I
APT in CDCl₃
25-08-08 RA

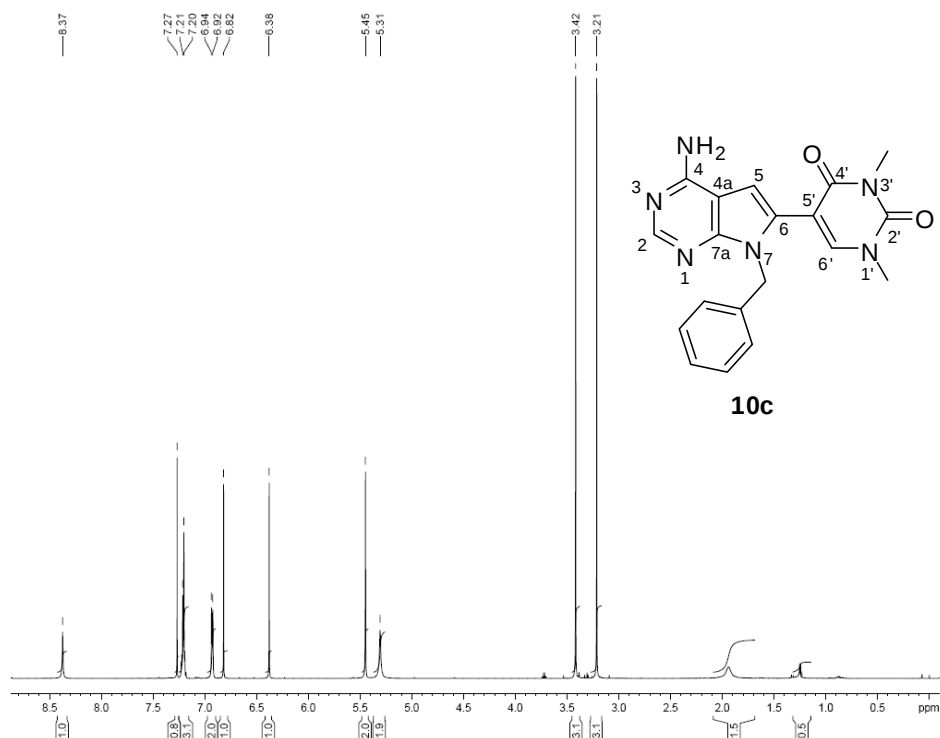
Current Data Parameters
NAME KLECKA IK-153-I
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080825
Time 11.43
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG jmod
TD 6553
SOLVENT CDCl₃
NS 638
DS 4
SWH 30030.029 Hz
FIDRES 0.466222 Hz
AQ 1.0912244 sec
RG 23170.5
DQ 12.650 usec
DE 6.50 usec
TE 312.1 K
CNST11 1.0000000
CNST12 100.0000000
D1 2.0000000 sec
d0 0.00625000 sec
DELTA 0.0001610 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 16.00 usec
PL 30.00 dB
SFO1 125.7250987 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.00 dB
PL2 3.00 dB
SFO2 499.9519998 MHz

F2 - Processing parameters
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SF 125.712564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

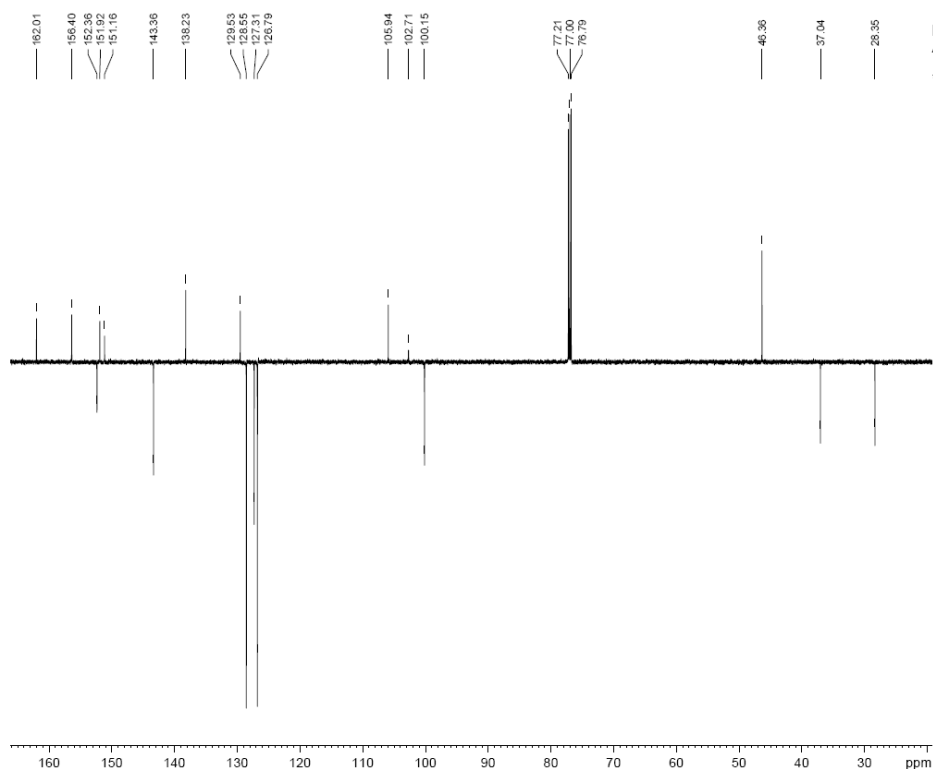




KLECKA IK-159-III
1H NMR in CDCl₃
11-09-08 RA

Current Data Parameters
NAME KLECKA IK-159-III
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080911
Time 7.48
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 84174
SOLVENT CDCl₃
NS 8
DS 0
SWH 8417.509 Hz
FIDRES 0.100001 Hz
AQ 4.999957 sec
RG 32
RG 59.400 usec
DE 20.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 ¹H
P1 10.00 usec
PL1 8.10 dB
PL1W 5.29101372 W
SFO1 600.1330008 MHz
F2 - Processing Parameters
SI 131072
SF 600.1300124 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 40.00

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KLECKA IK-159-III
APT in CDCl₃
11-09-08 RA

Current Data Parameters
NAME KLECKA IK-159-III
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080911
Time 7.53
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 76755
SOLVENT CDCl₃
NS 140
DS 4
SWH 37878.786 Hz
FIDRES 0.050037 Hz
AQ 0.9999764 sec
RG 812
RG 13.200 usec
DE 6.00 usec
TE 300.0 K
CNST2 160.0000000
CHET11 1.0000000
D1 2.00000000 sec
D20 0.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 ¹³C
P1 11.50 usec
PL1 23.00 usec
PL1 23.40 dB
PL1W 107.48842621 W
SFO1 160.9194083 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 12.00 dB
PL2 20.00 dB
PL2W 6.81614457 W
PL2W 0.10512664 W
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 131072
SF 160.9028171 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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