

SUPPORTING INFORMATION

Chiral bicyclic skeleton-tethered bipyridine–Zn(OTf)₂ complex as Lewis acid: Enantioselective Friedel–Crafts alkylation of indoles with nitroalkenes

Kesa Venkatanna, Santhakumar Yeswanth Kumar, Muthupandi Karthick, Ramanathan
Padmanaban, Chinnasamy Ramaraj Ramanathan*

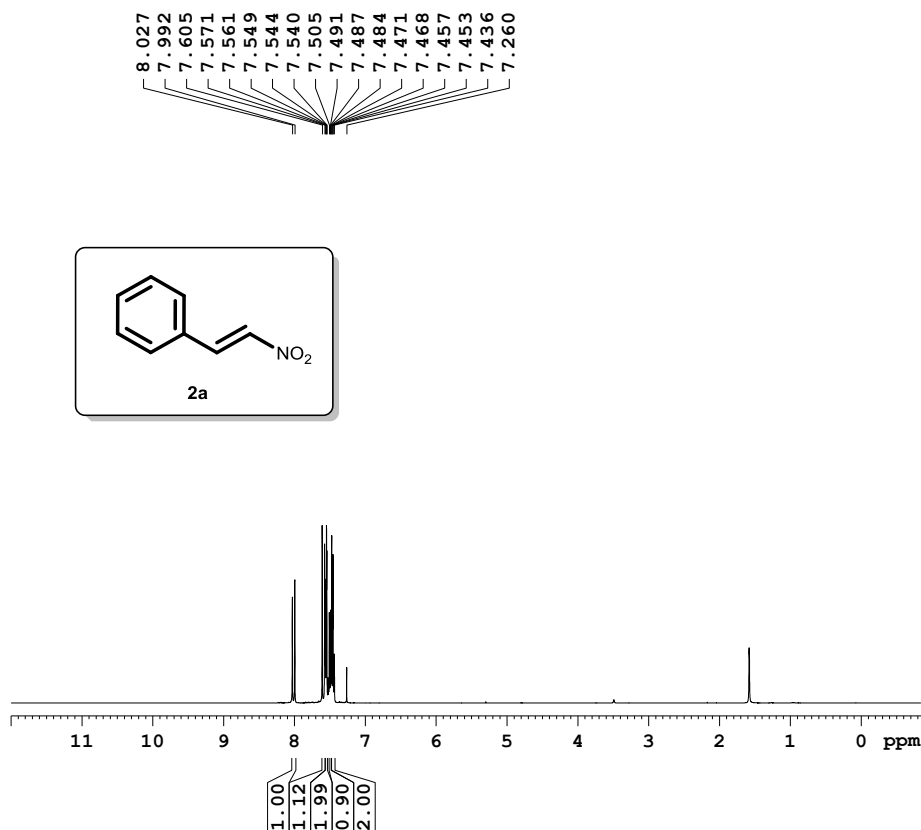
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Data:

S. No.	Details	Page No.
1.	Copies of ^1H NMR spectra of compounds, 2a-2q	S4 – S12
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**1. Copies of ^1H NMR spectra of
compounds, 2a-2q**

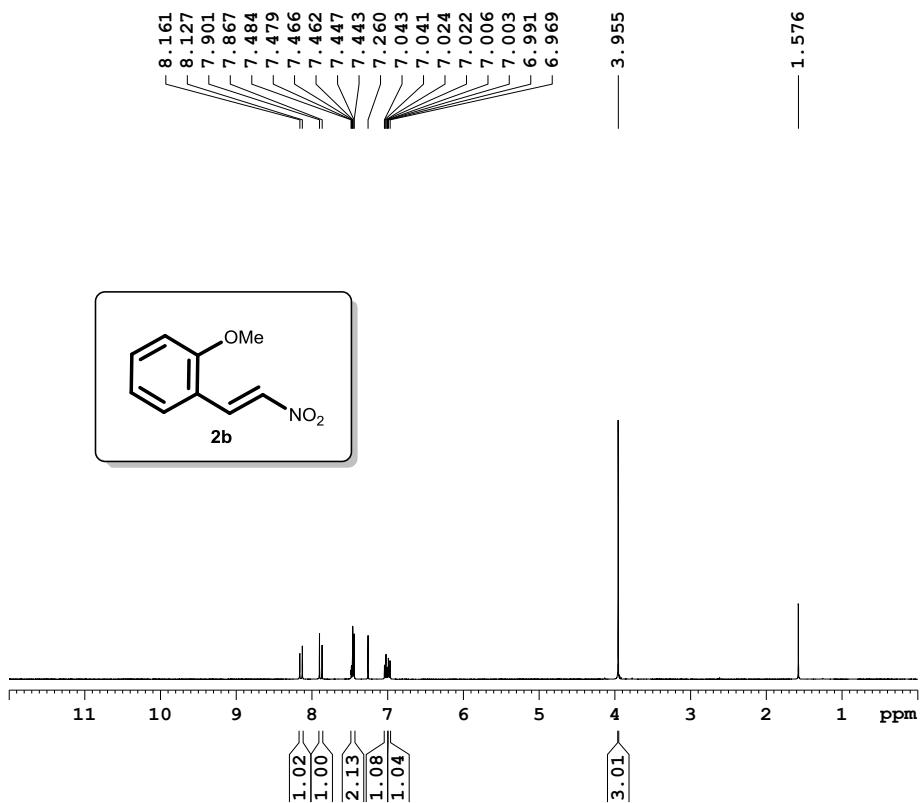


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 NS 16
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 FIDRES 0.125483 Hz
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 RG 228
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 DE 6.00 usec
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 TD0 1

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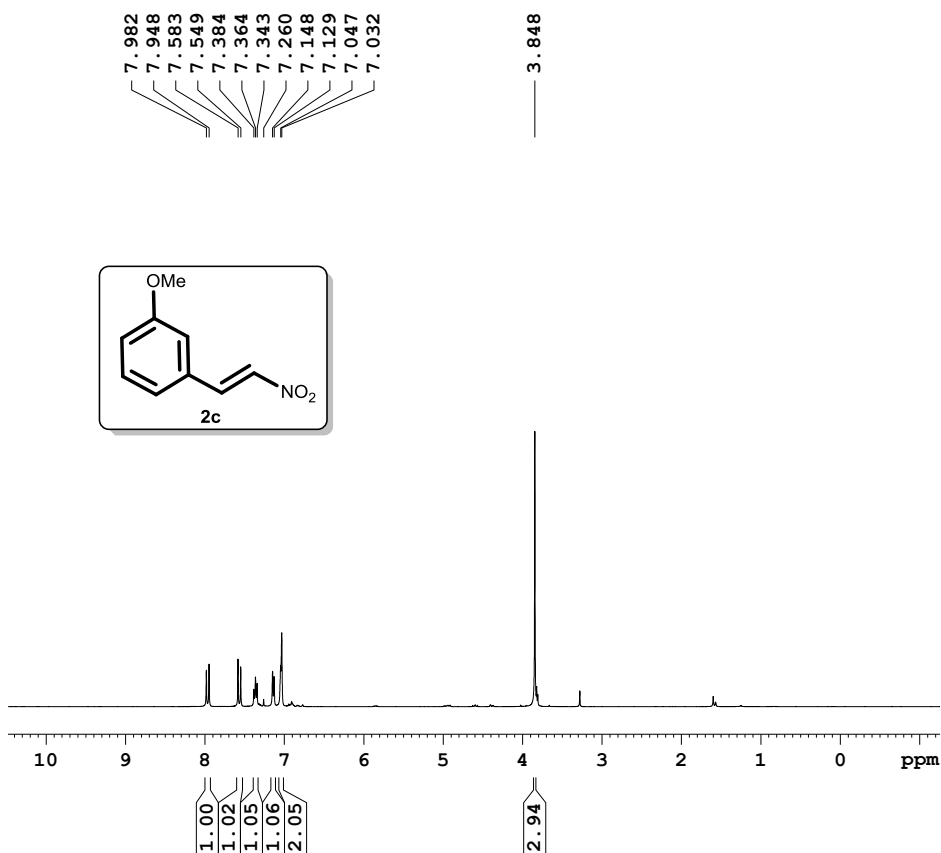


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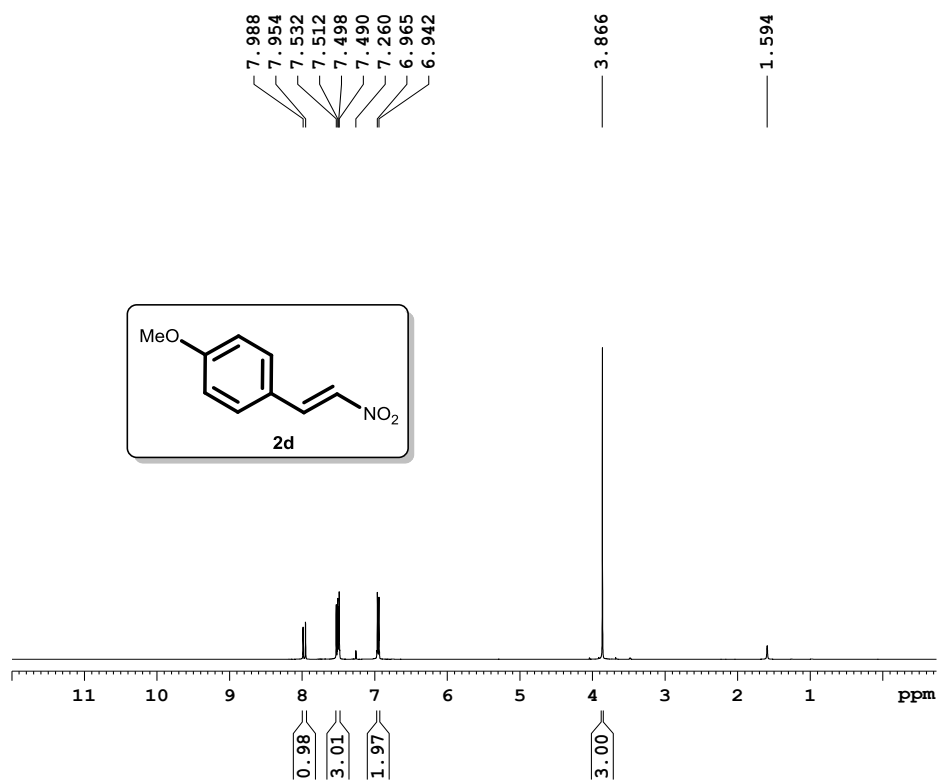


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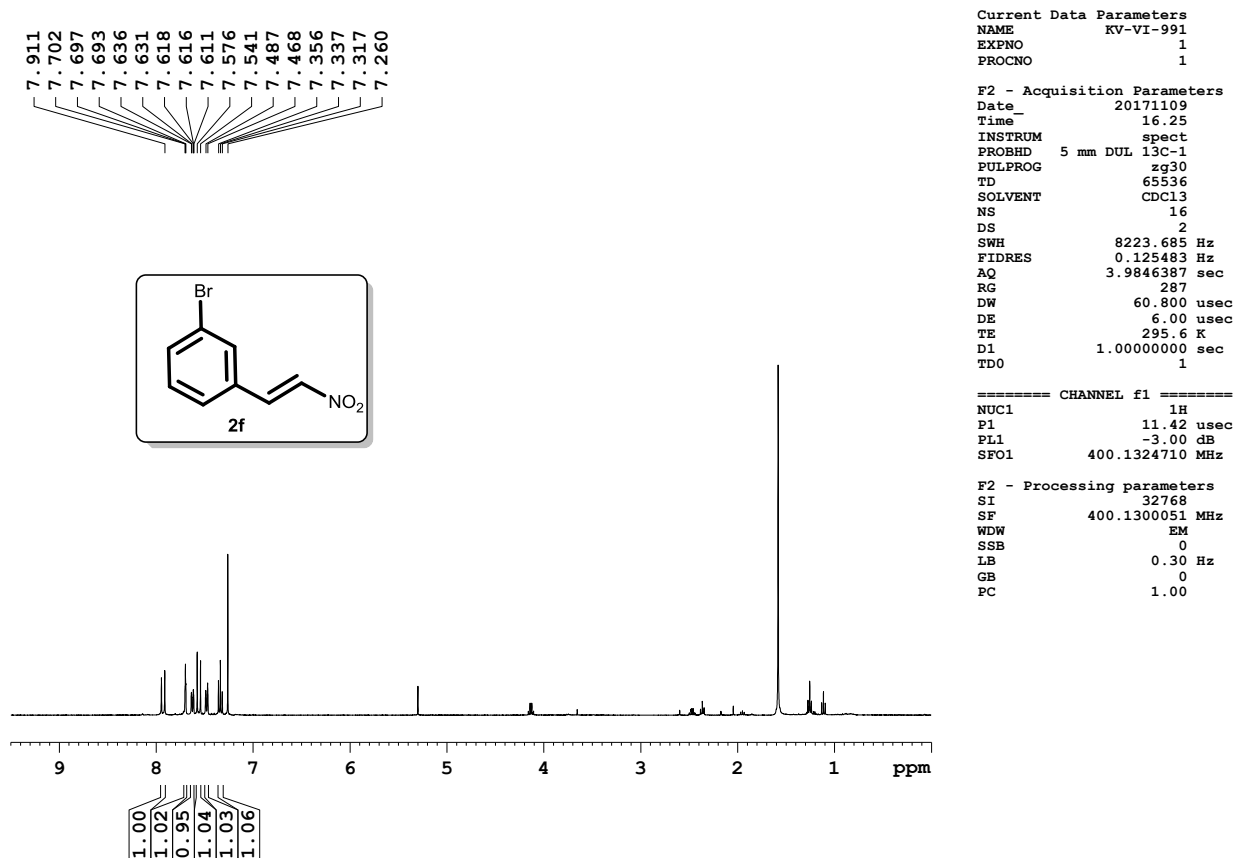
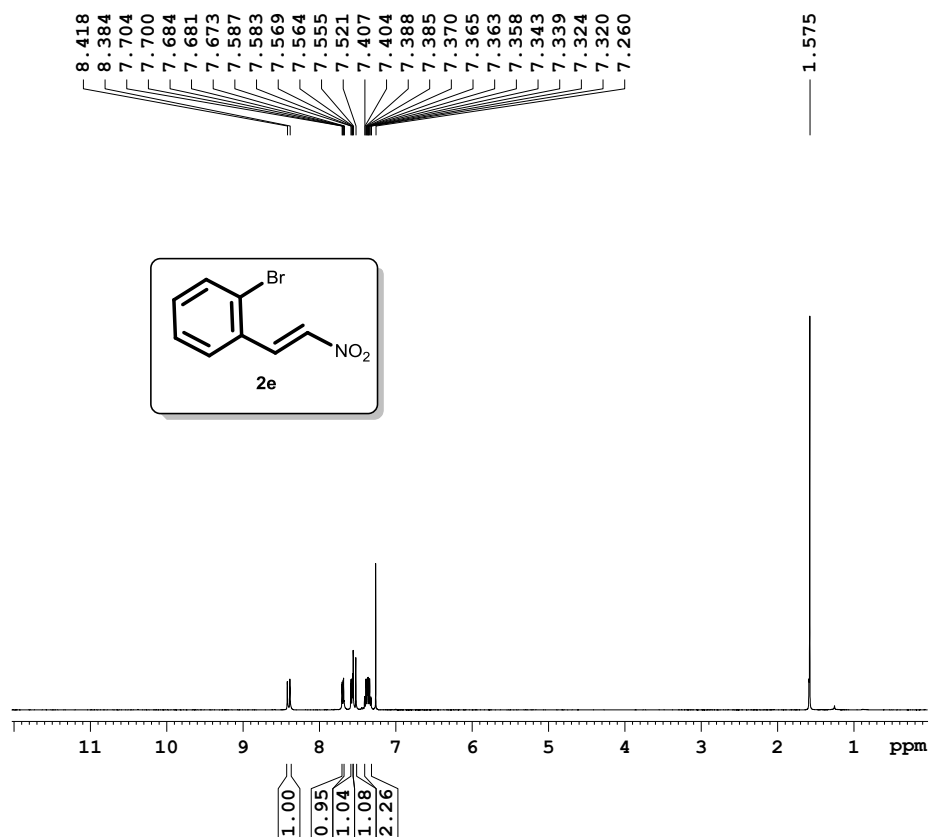


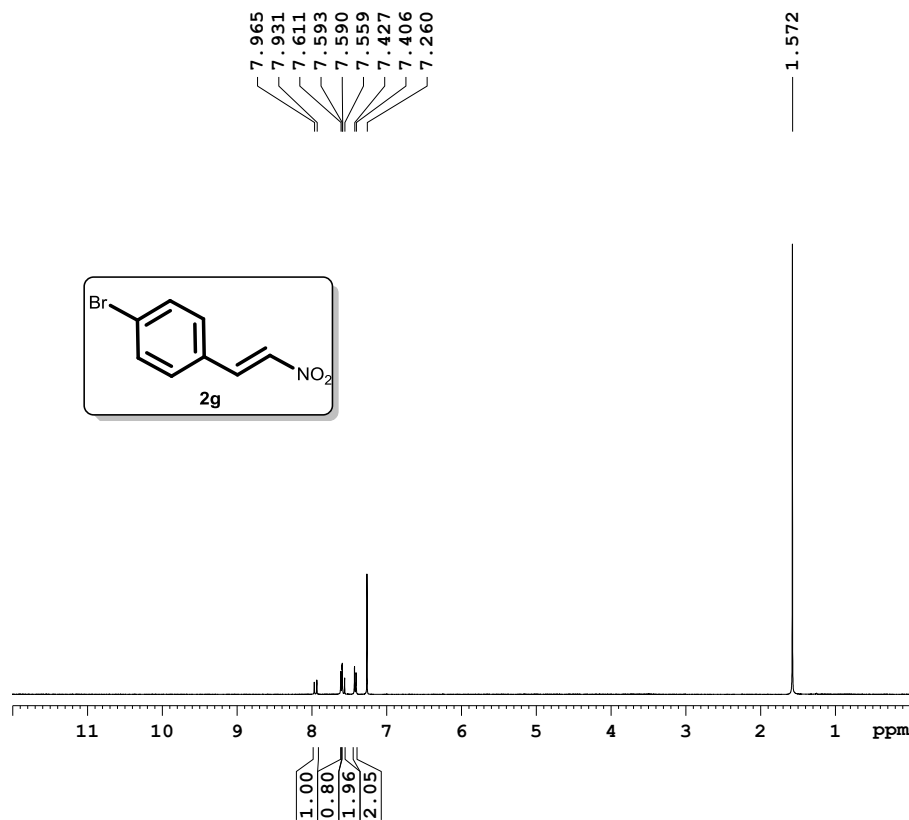
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TE 298.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
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P1 11.42 usec
PL1 -3.00 dB
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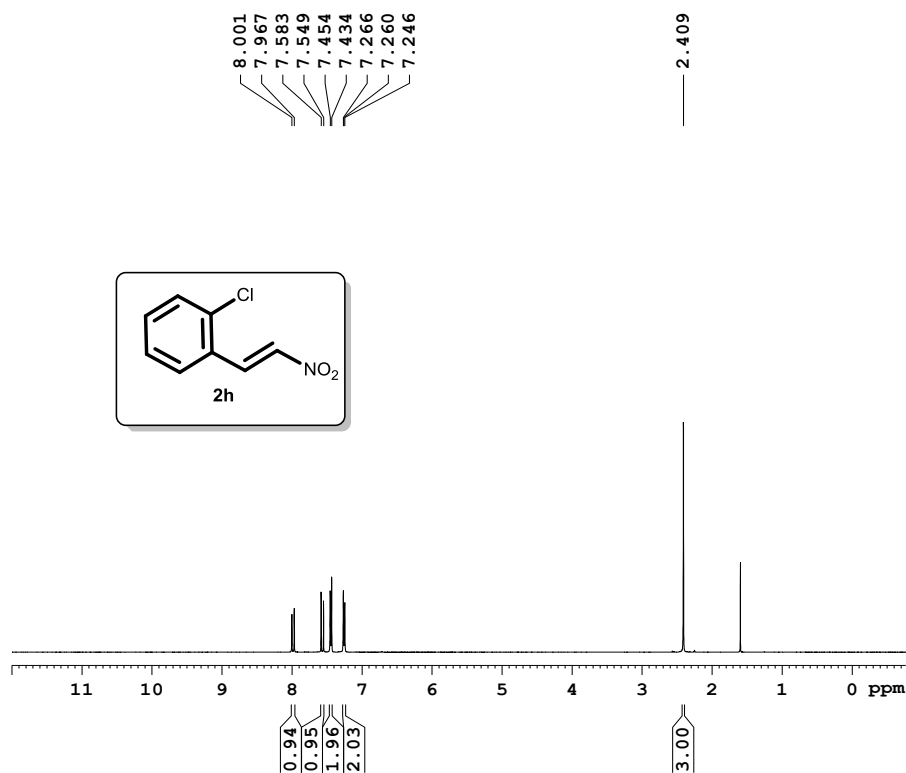


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AQ 3.9846387 sec
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DE 6.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

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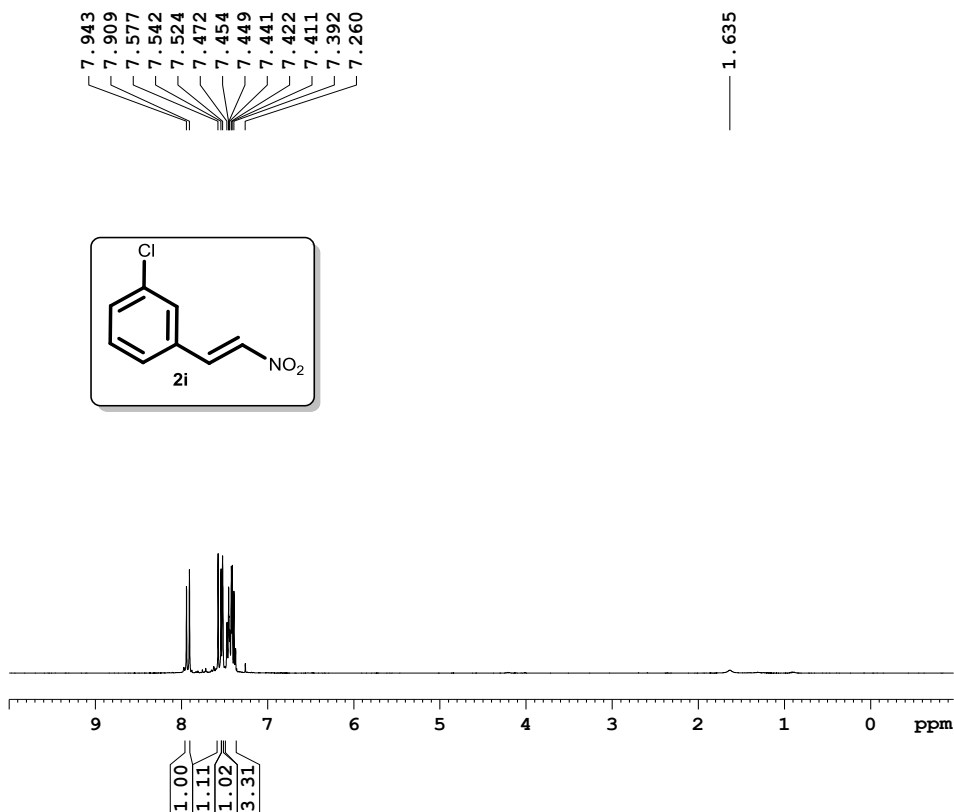


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SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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SF 400.1300051 MHz
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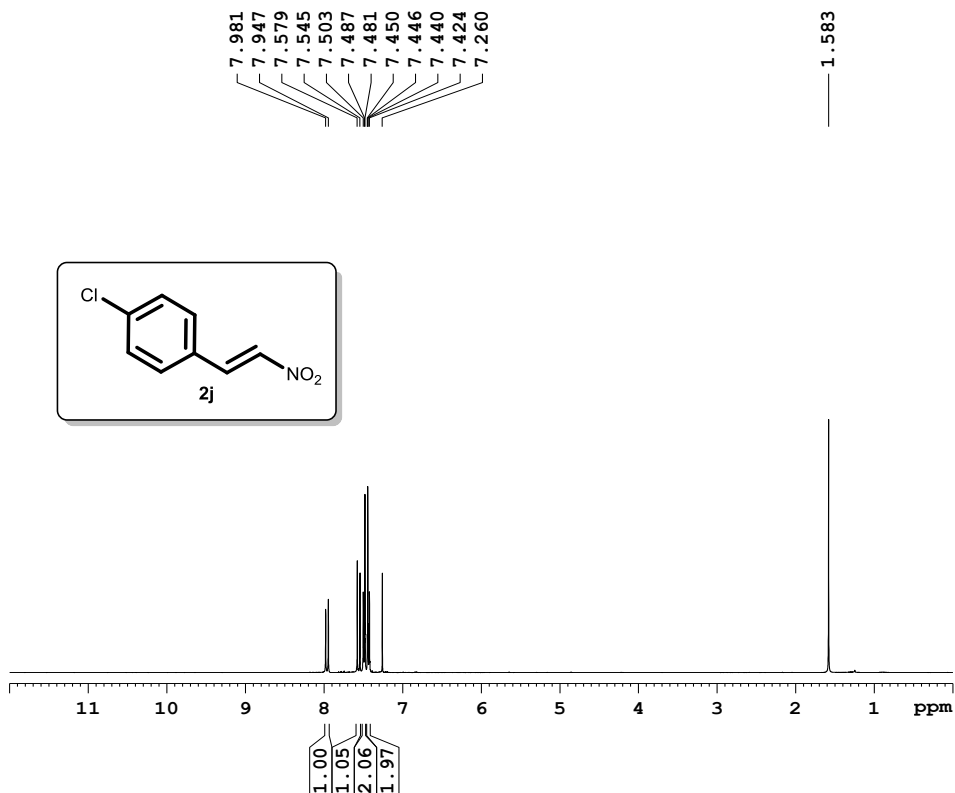
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TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         287
DW         60.800 usec
DE         6.00 usec
TE         295.6 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.35 usec
PL1        -1.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
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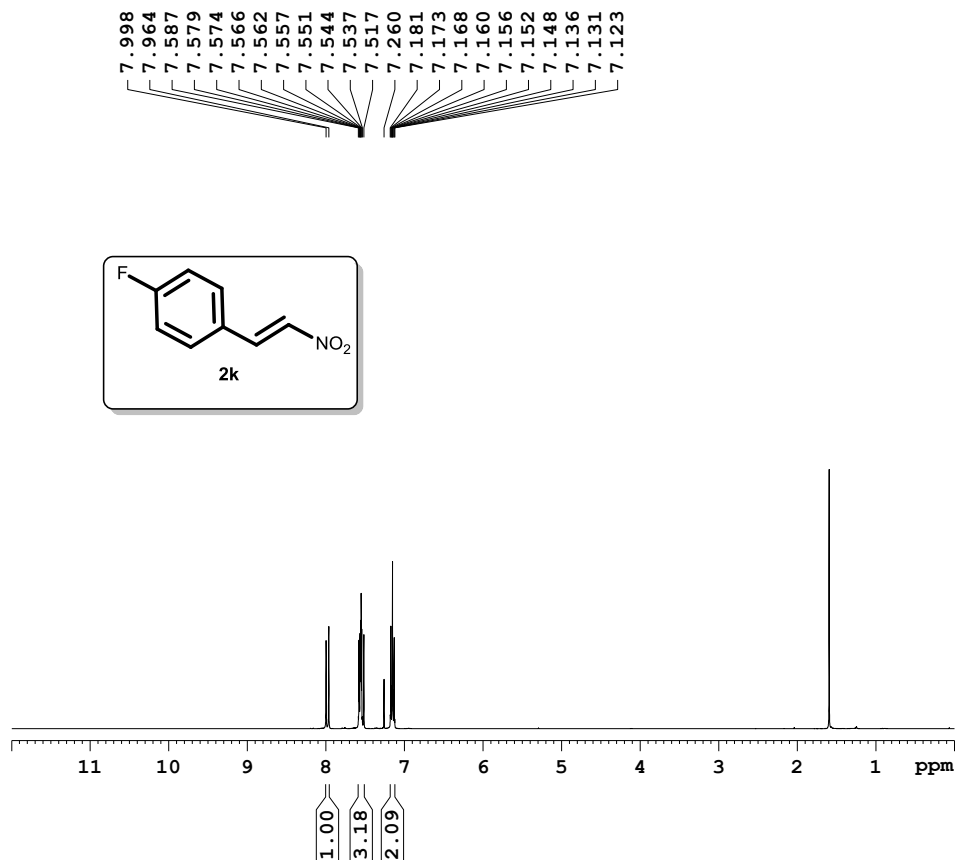
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SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         287
DW         60.800 usec
DE         6.00 usec
TE         293.5 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         11.42 usec
PL1        -3.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
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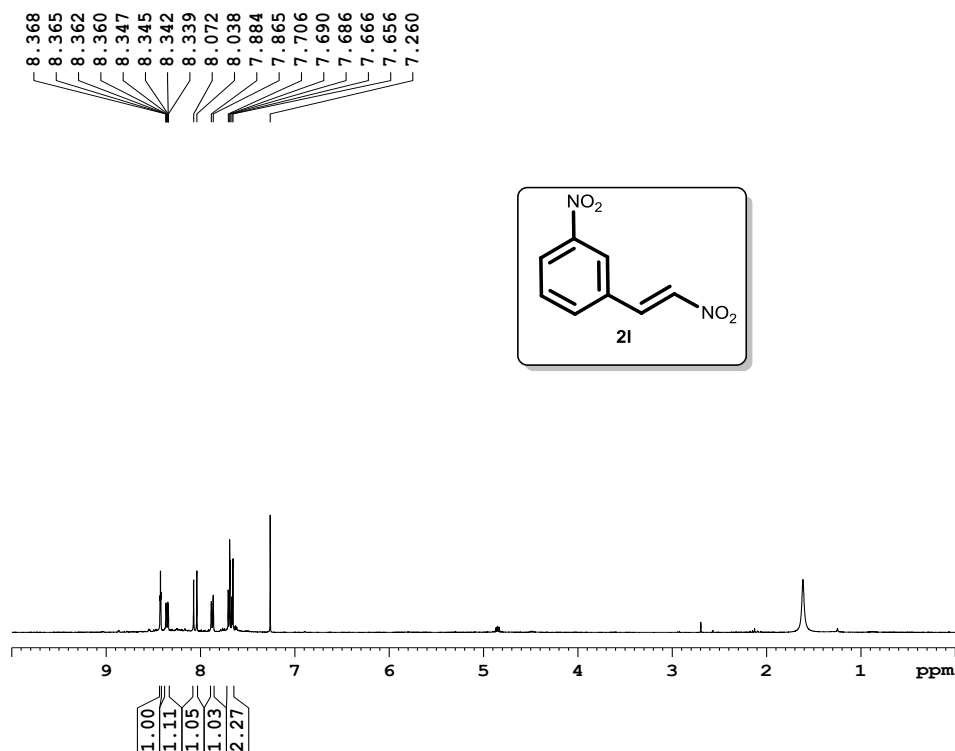



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EXPNO 1
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SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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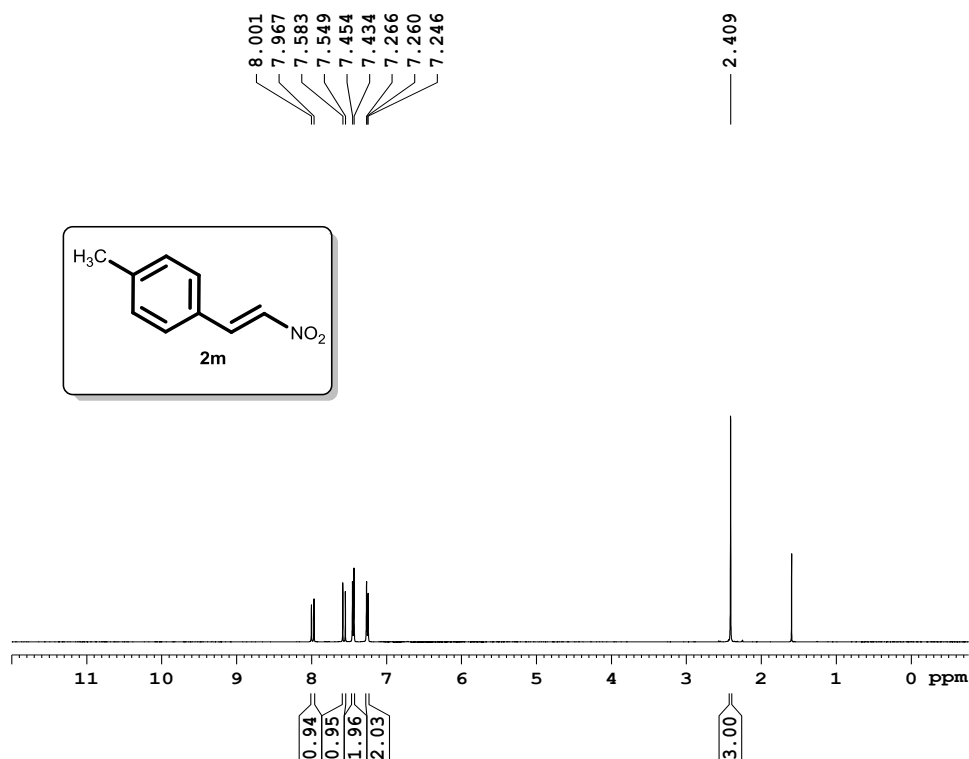


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RG 256
DW 60.800 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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SF 400.1300051 MHz
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PC 1.00

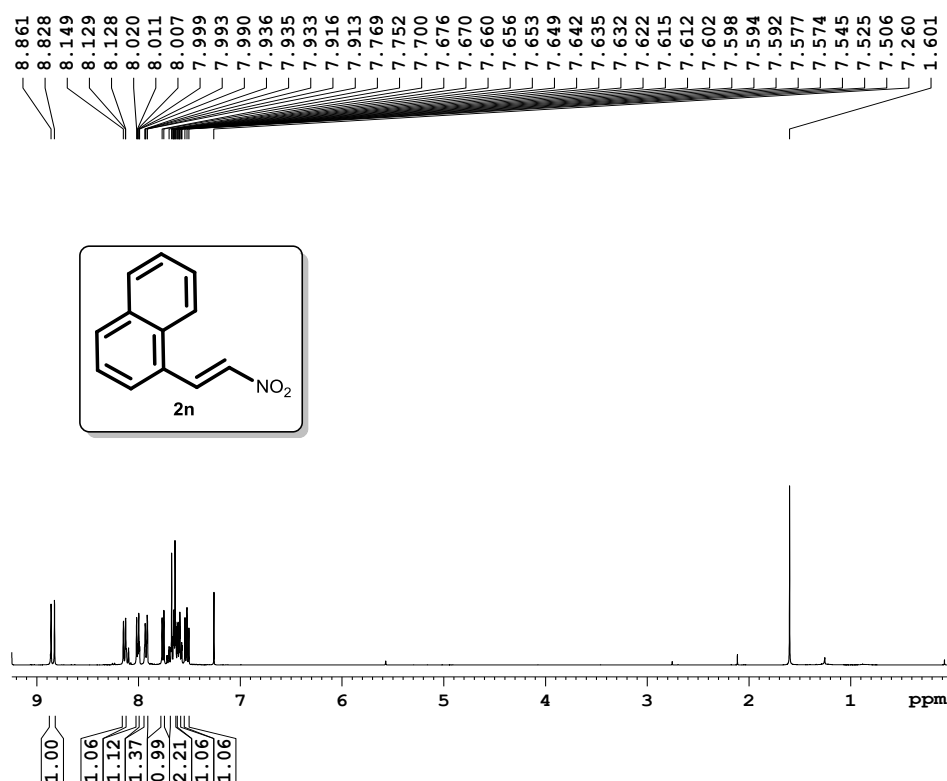


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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
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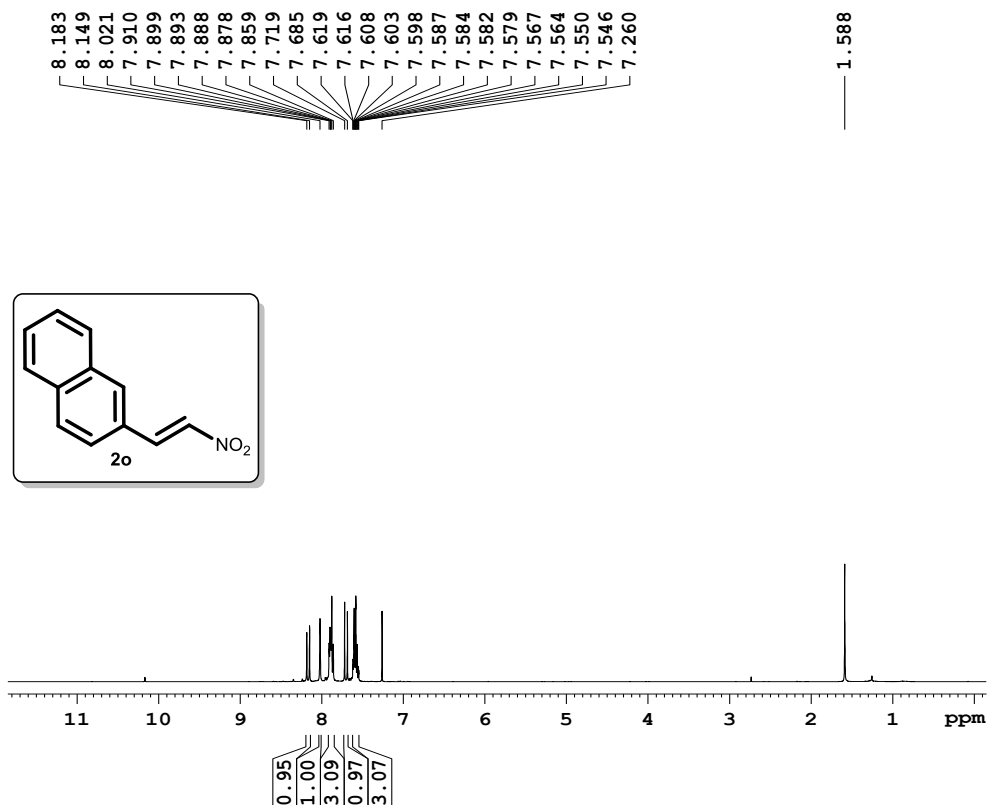


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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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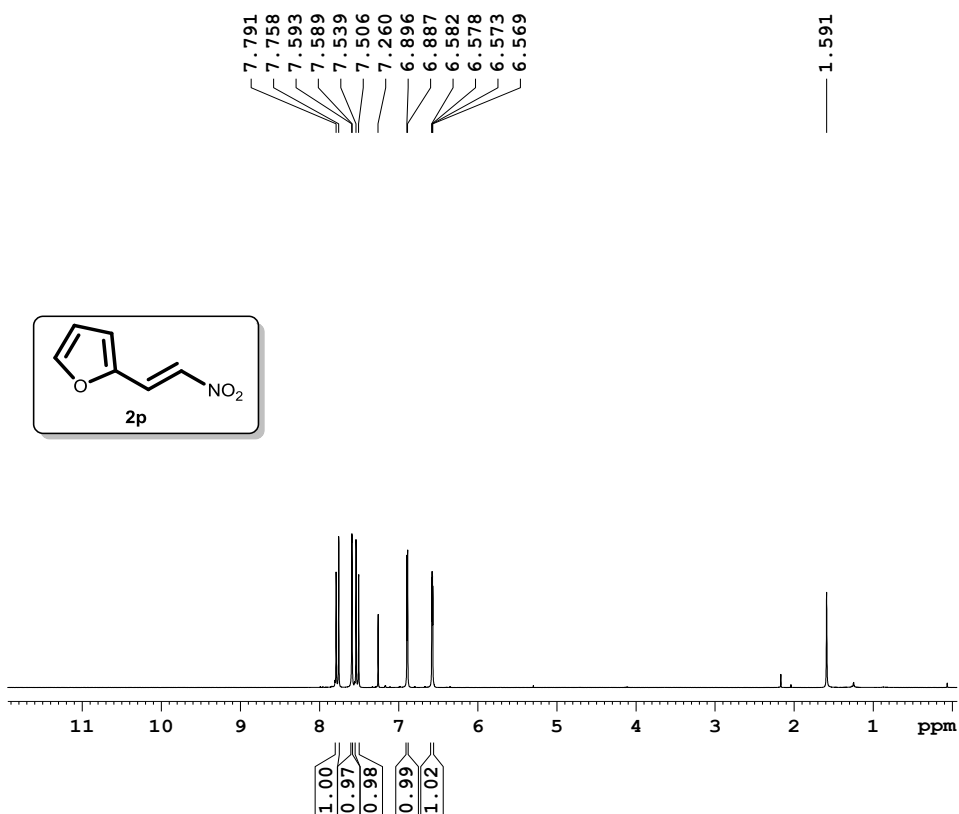
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PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         228
DW         60.800 usec
DE         6.00 usec
TE         293.4 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         11.42 usec
PL1        -3.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
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SF         400.1300051 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

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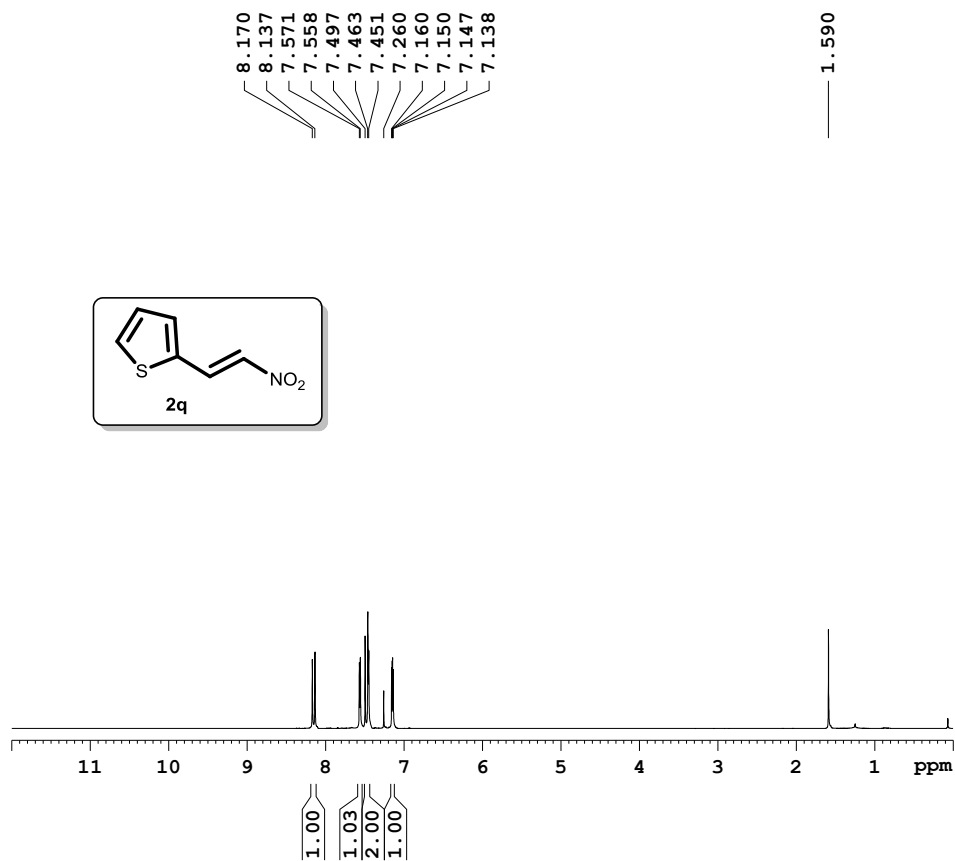
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TD         65536
SOLVENT   CDC13
NS         16
DS         2
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FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         228
DW         60.800 usec
DE         6.00 usec
TE         293.3 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         11.42 usec
PL1        -3.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI         32768
SF         400.1300051 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

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Current Data Parameters
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PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
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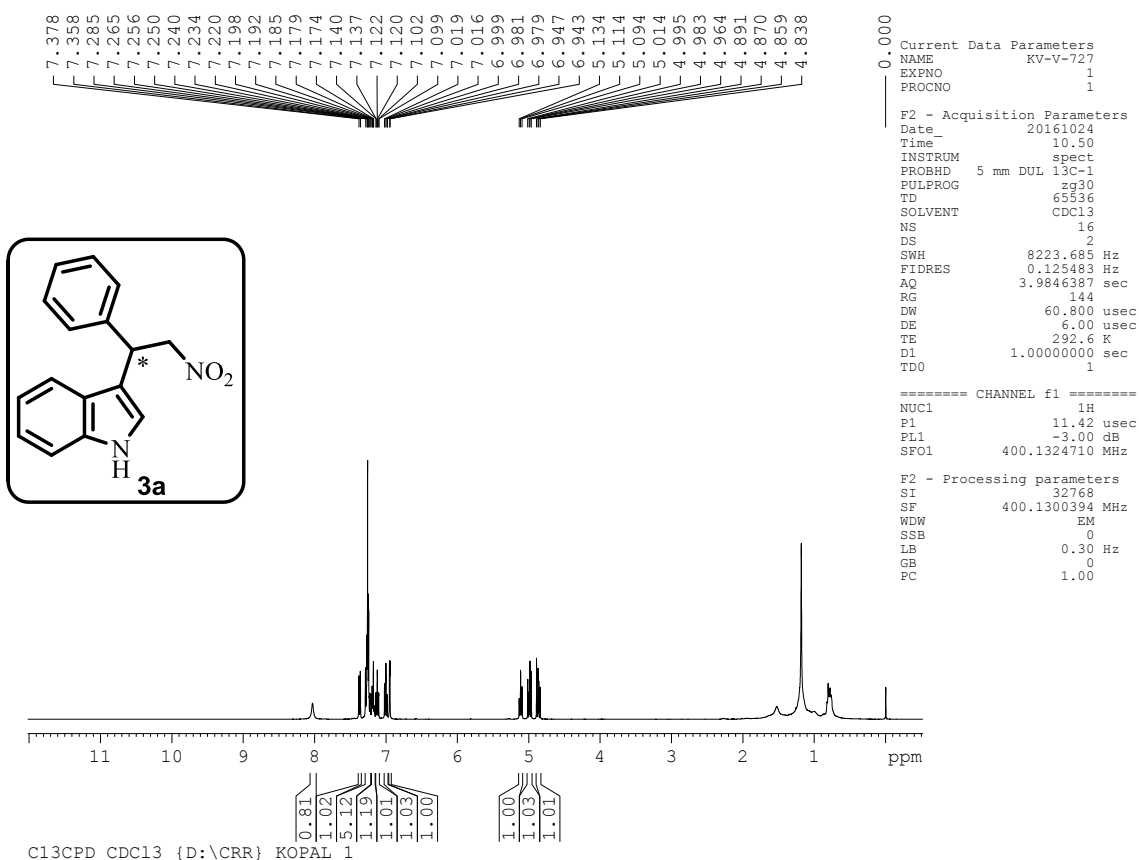
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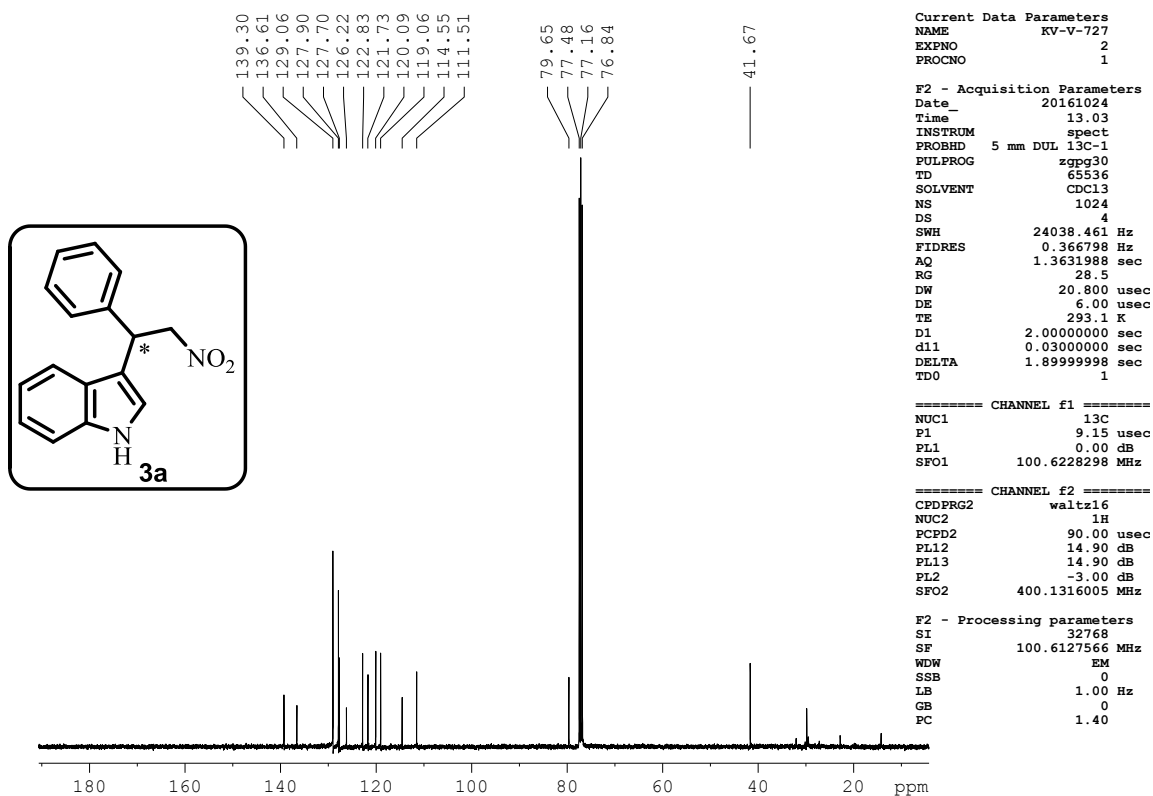
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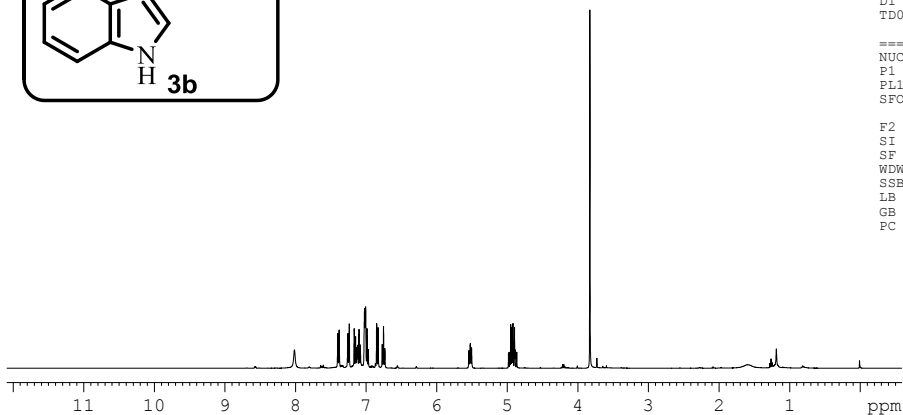
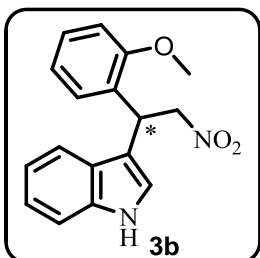
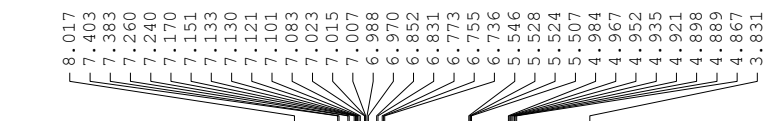
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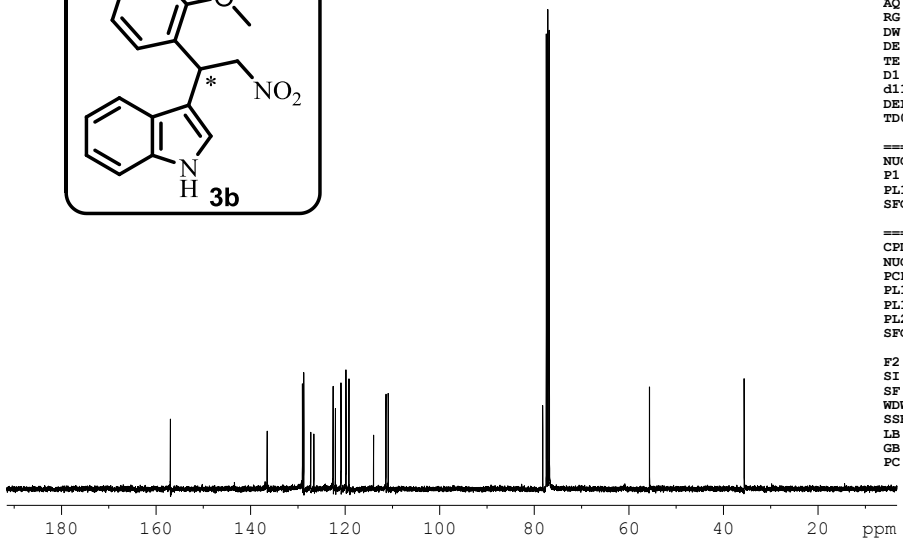
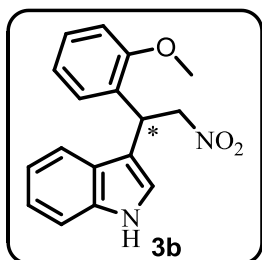
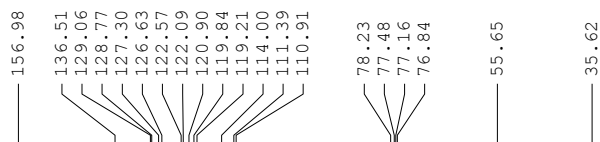
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SOLVENT CDC13
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DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300409 MHz
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LB 0.30 Hz
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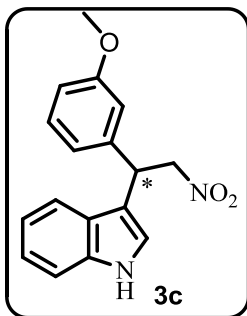
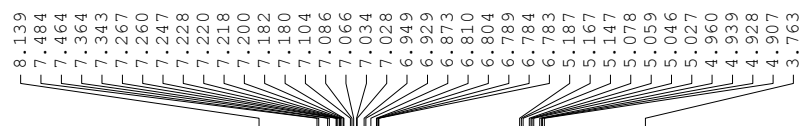
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SOLVENT CDC13
NS 512
DS 4
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FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

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PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
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PC 1.40

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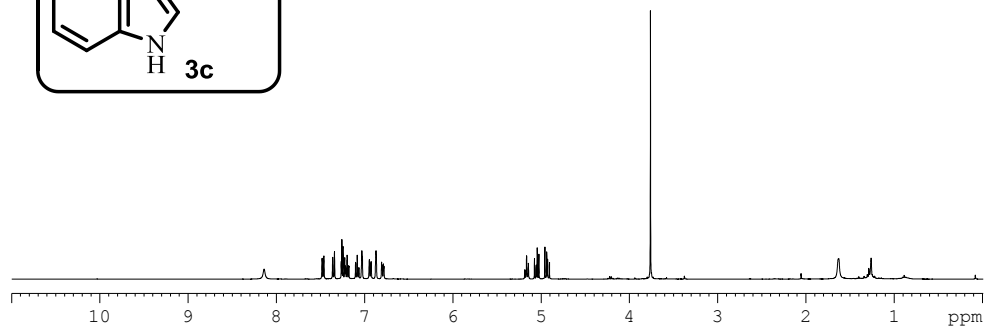


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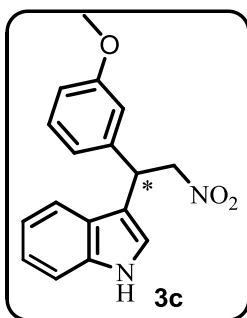
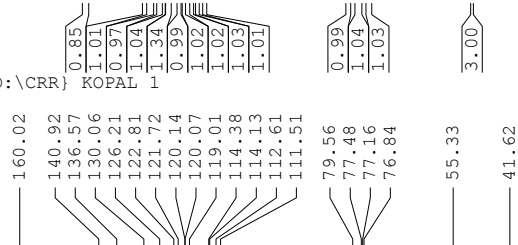
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SOLVENT CDCl3
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DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 290.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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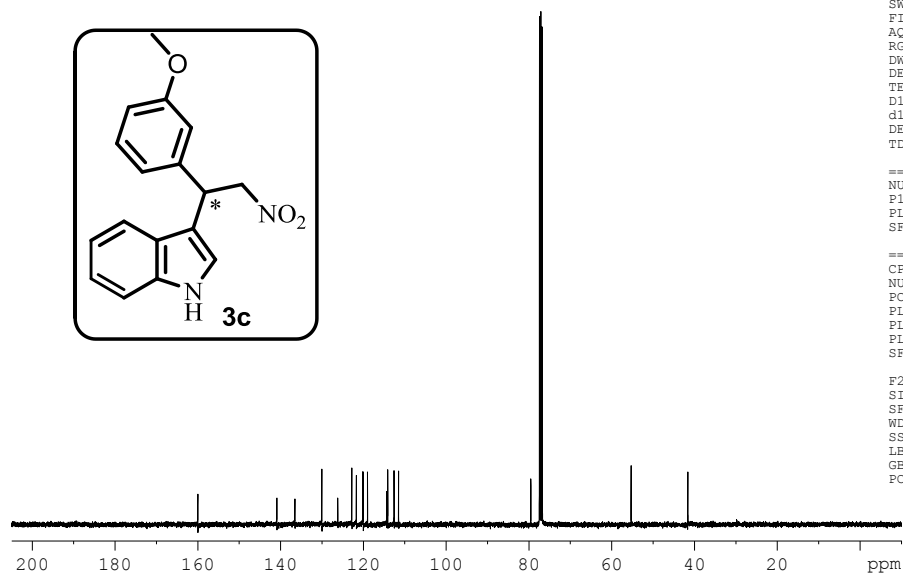
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 290.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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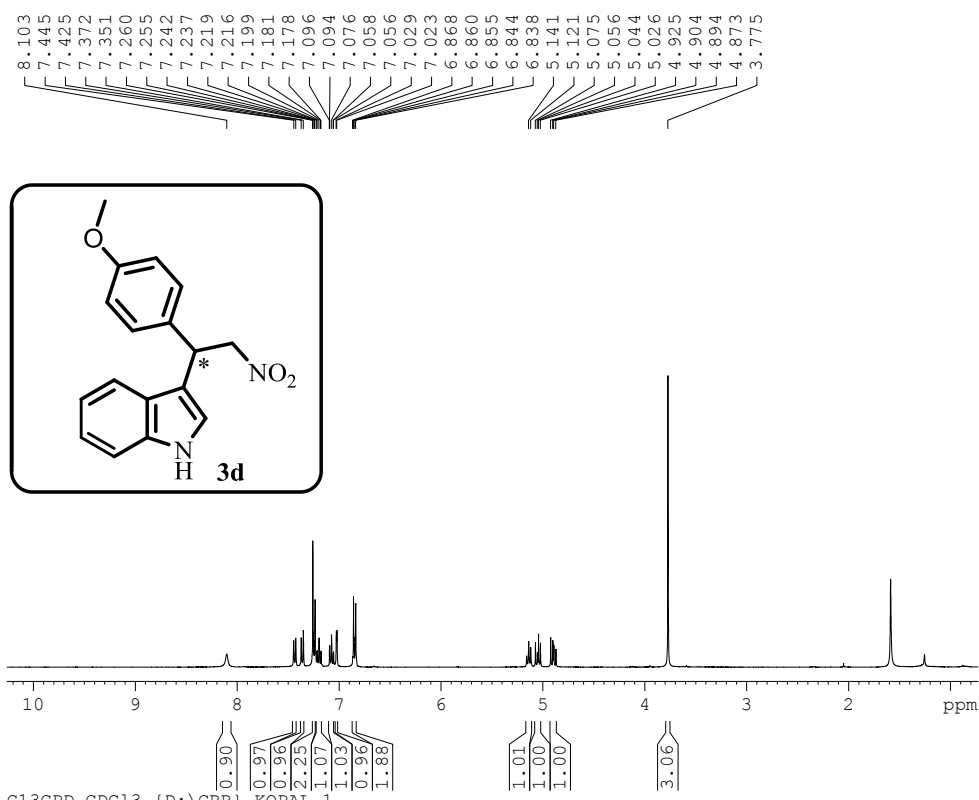
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NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127577 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



PROTON CDC13 {D:\CRR} KOPAL 1



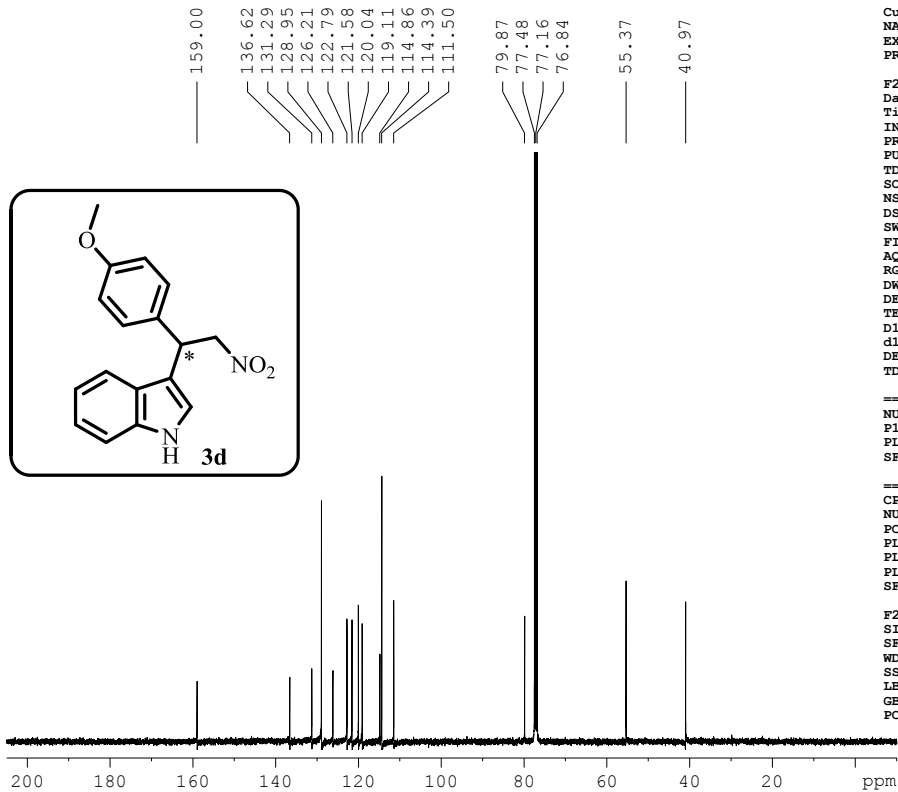
Current Data Parameters
NAME KV-V-862
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170508
Time 11.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 291.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-862
EXPNO 3
PROCNO 1

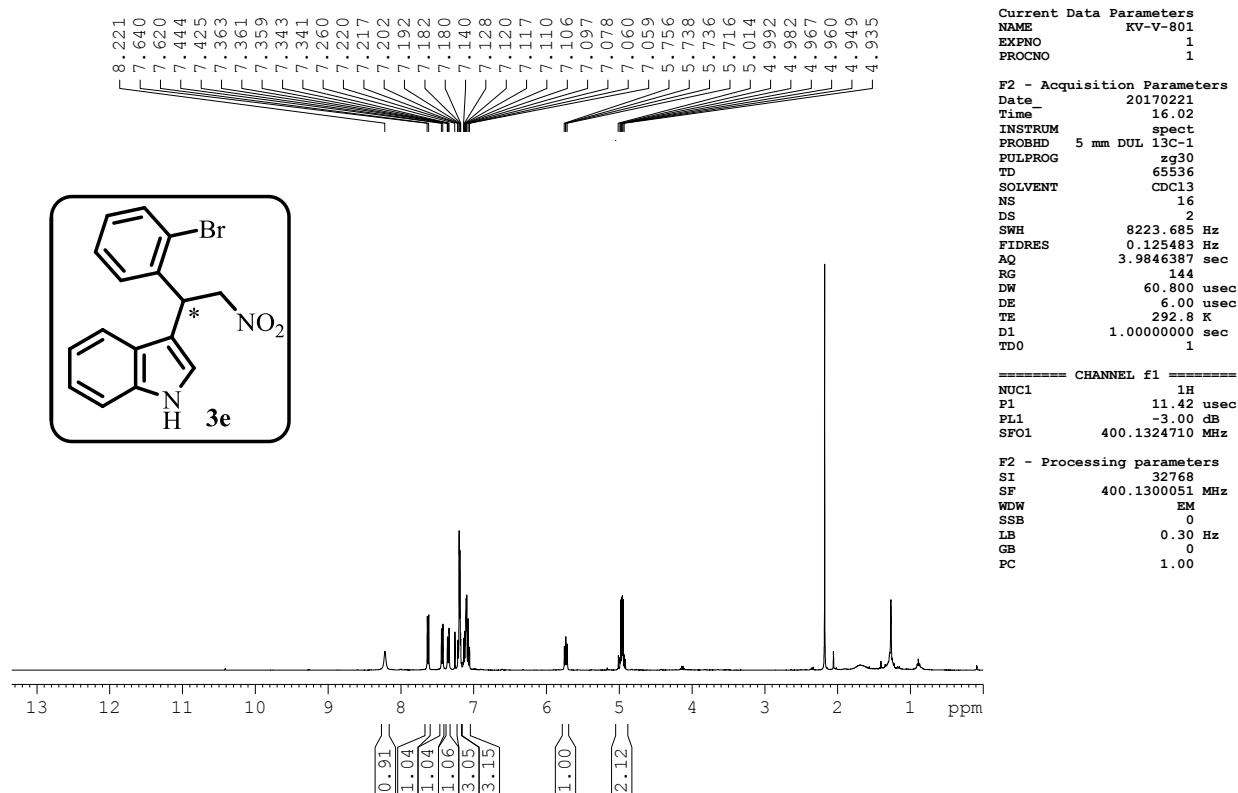
F2 - Acquisition Parameters
Date_ 20170508
Time 13.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

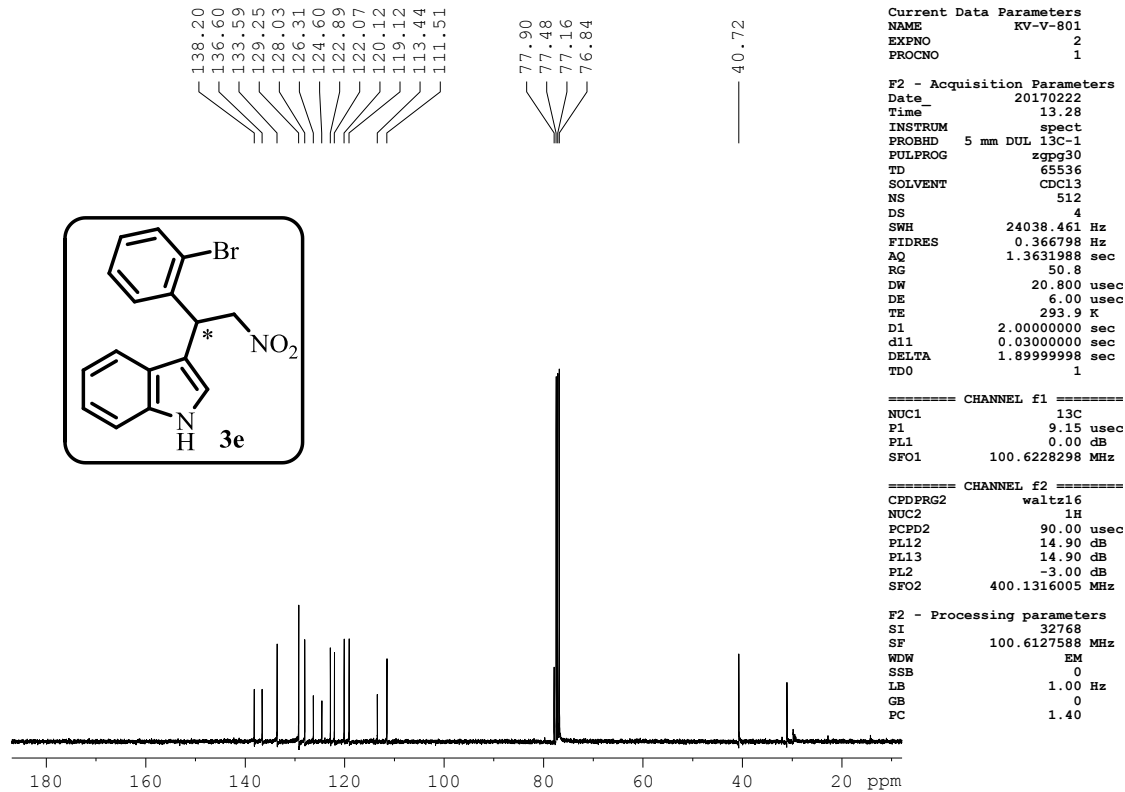
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

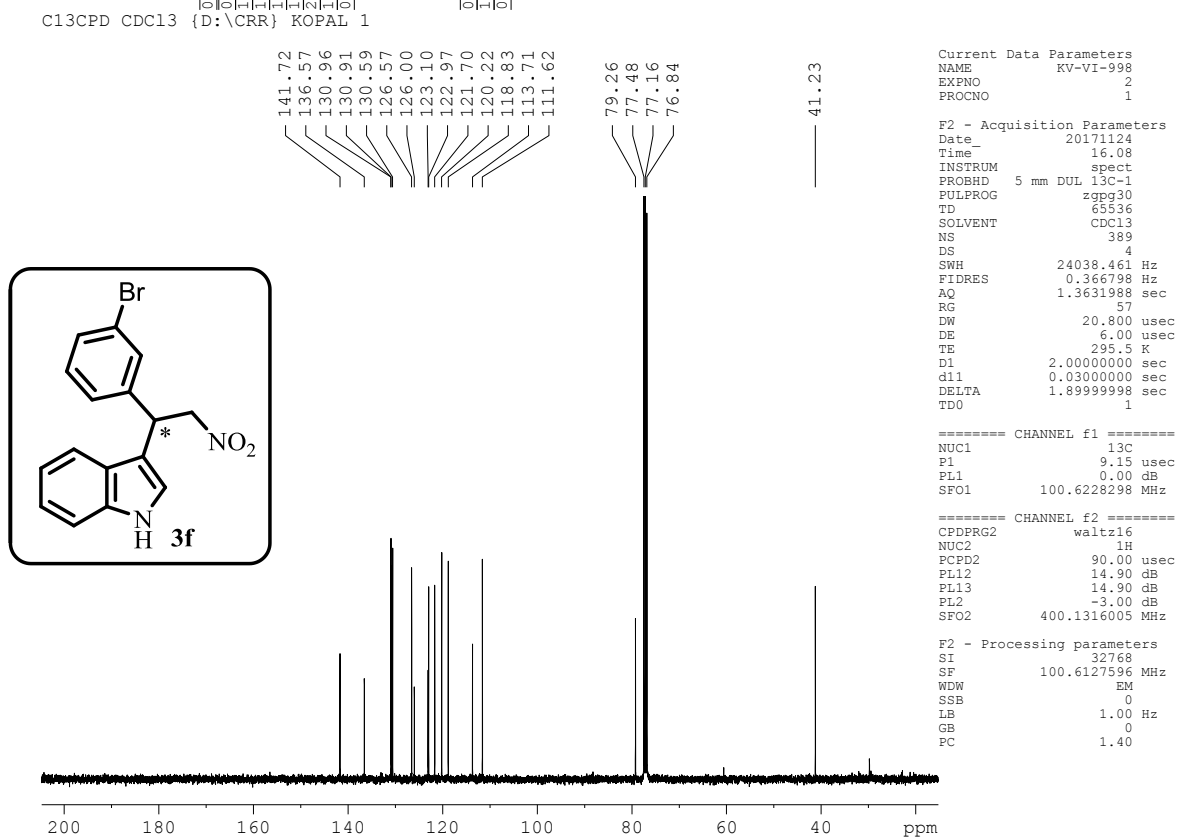
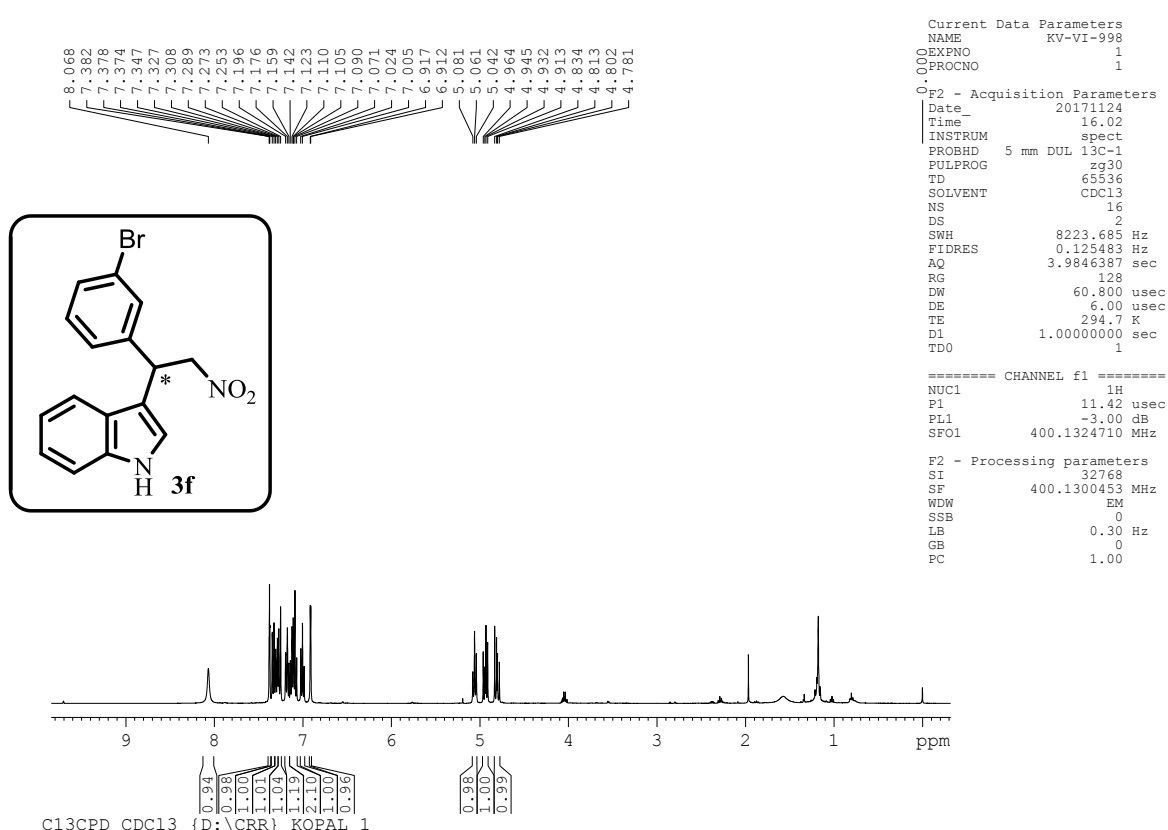
PROTON CDC13 {D:\CRR} KOPAL 1



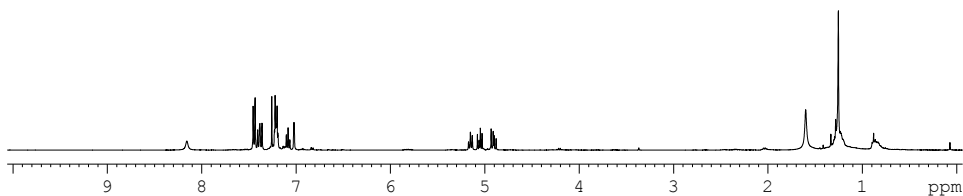
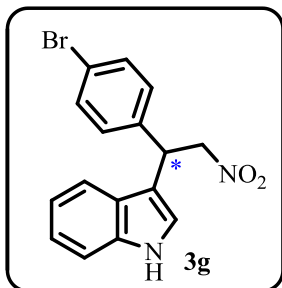
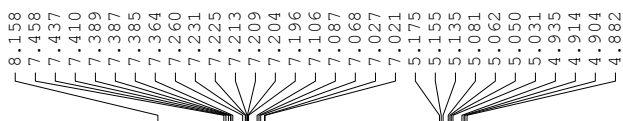
C13CPD CDC13 {D:\CRR} KOPAL 1



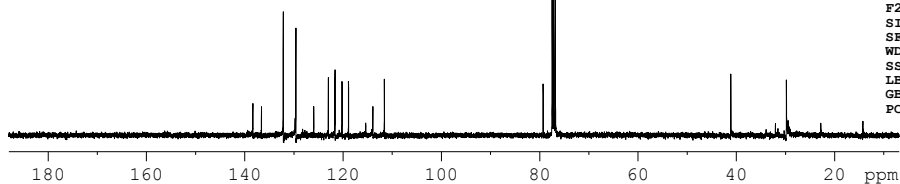
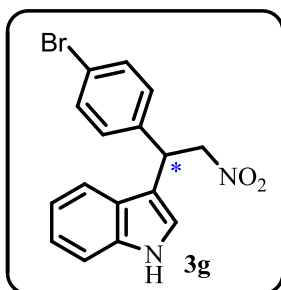
PROTON CDC13 {D:\CRR} KOPAL 1



PROTON CDCl3 {D:\CRR} KOPAL 1



C13CPD CDCl3 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-821
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170313
Time 12.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME KV-V-821
EXPNO 2
PROCNO 1

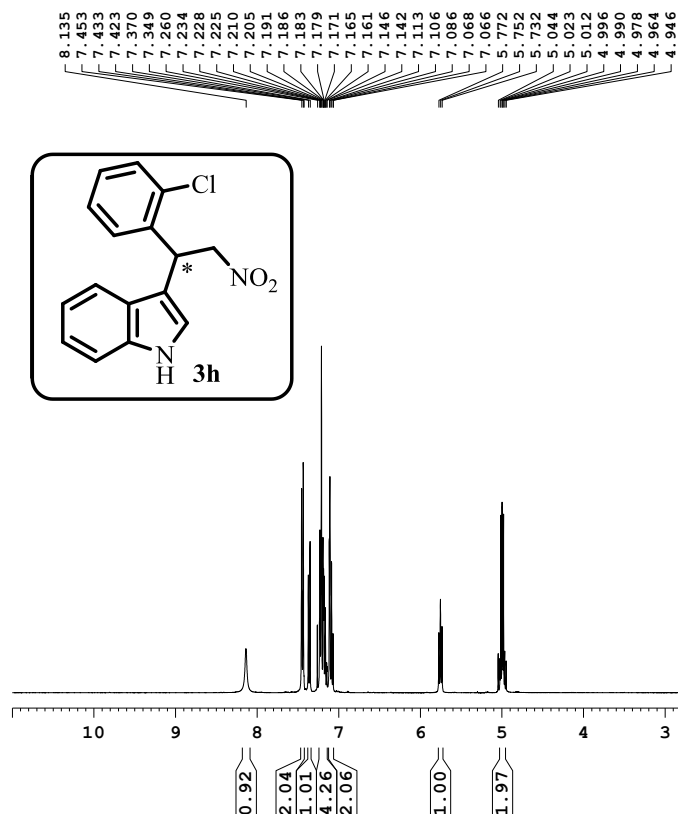
F2 - Acquisition Parameters
Date_ 20170313
Time 13.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32
DW 20.800 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1



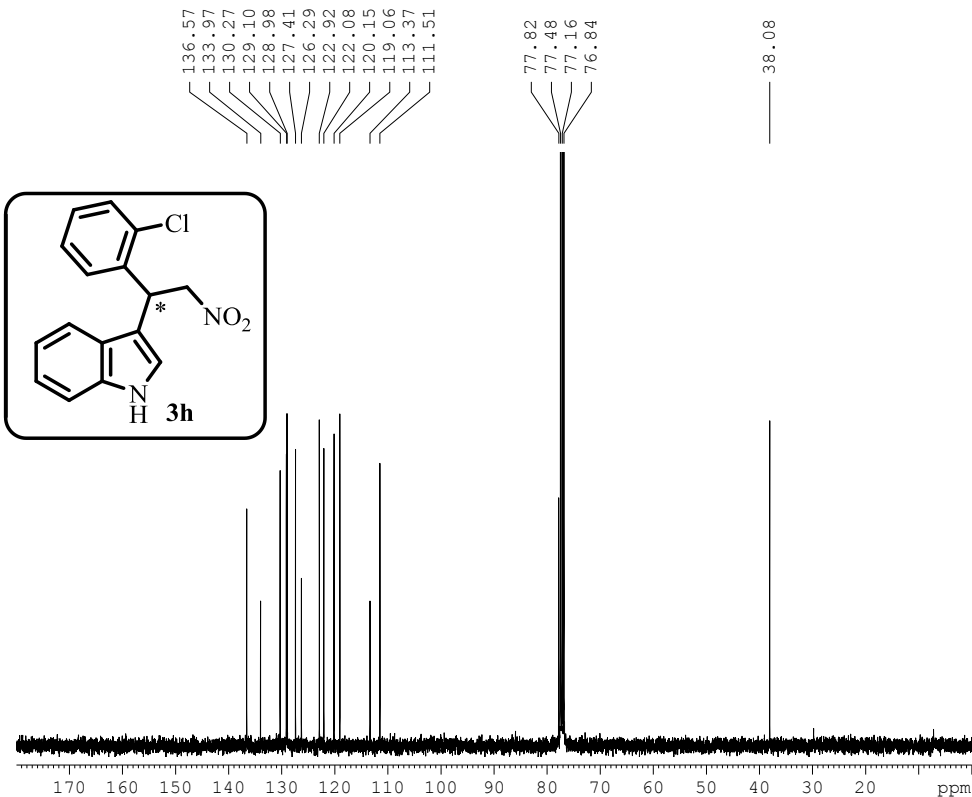
Current Data Parameters
NAME KV-VI-925
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170828
Time 12.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846397 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-VI-925
EXPNO 2
PROCNO 1

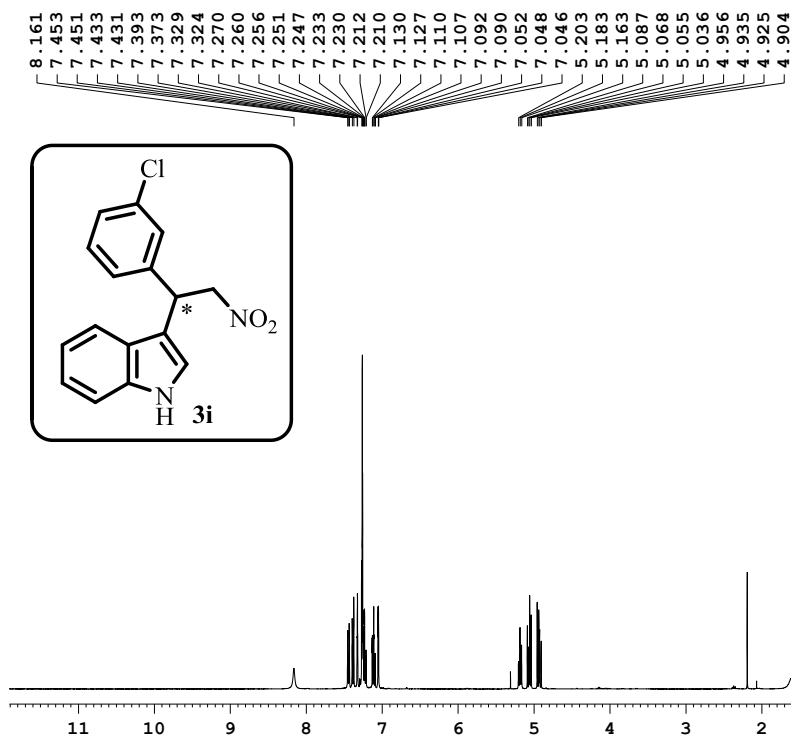
F2 - Acquisition Parameters
Date_ 20170830
Time 12.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127578 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1



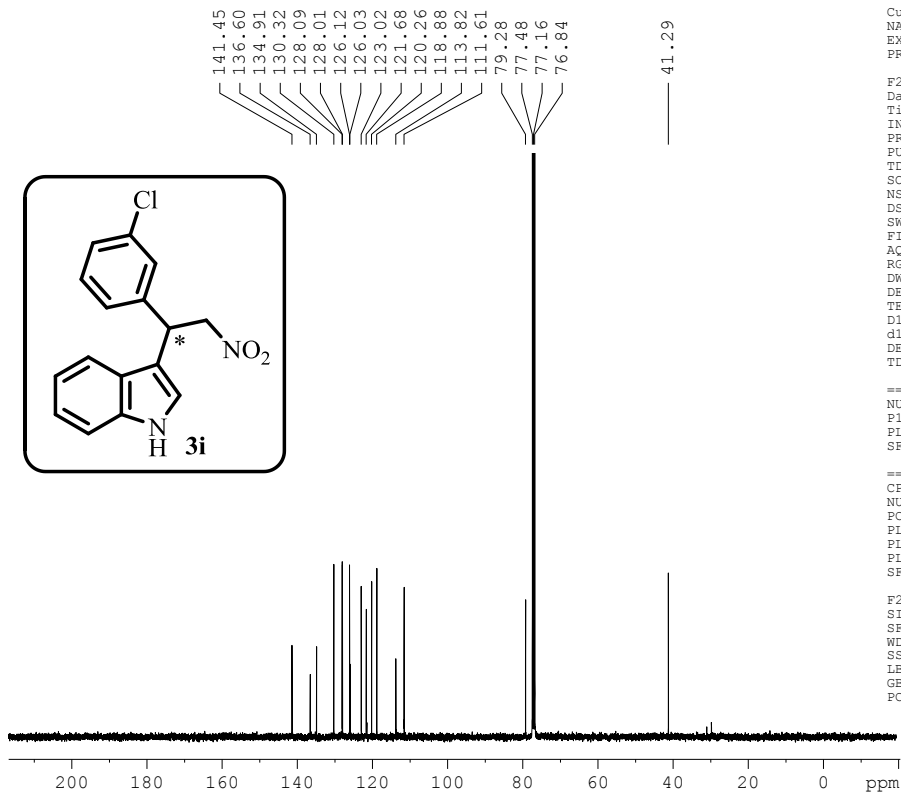
Current Data Parameters
NAME KV-V-868
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170713
Time 11.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846397 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-868
EXPNO 6
PROCNO 1

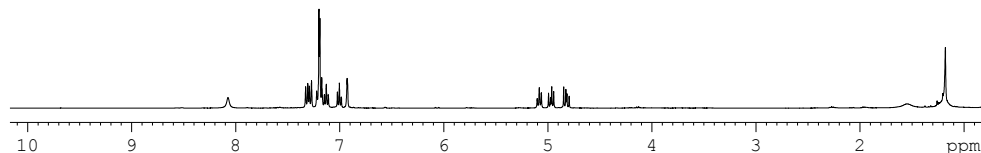
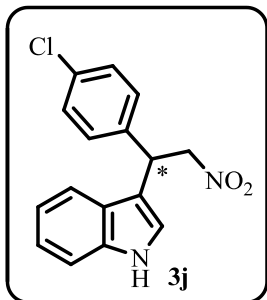
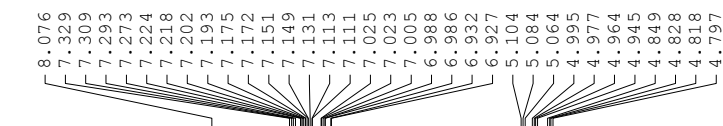
F2 - Acquisition Parameters
Date_ 20170717
Time 13.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

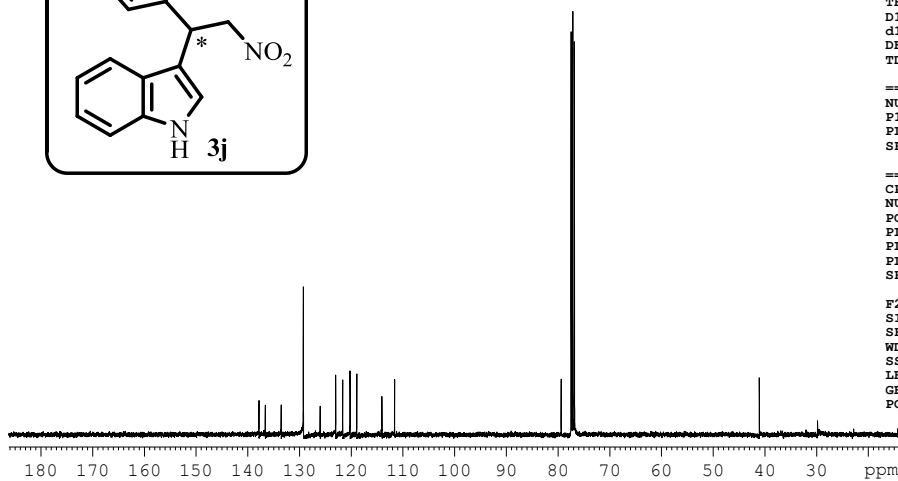
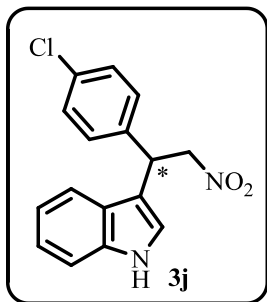
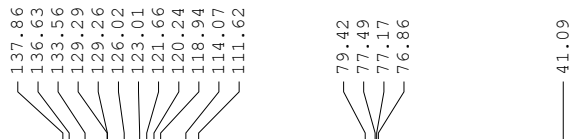
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127566 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1



C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-798
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170221
Time 15.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300389 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME KV-V-798
EXPNO 2
PROCNO 1

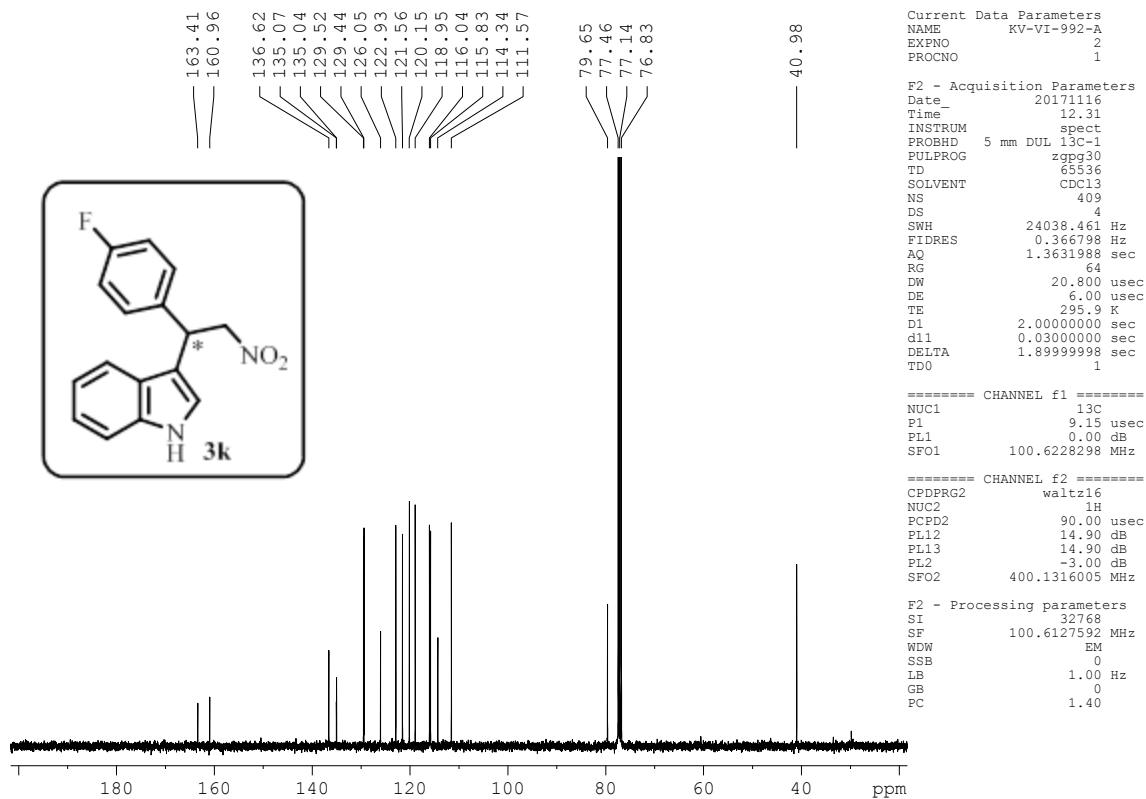
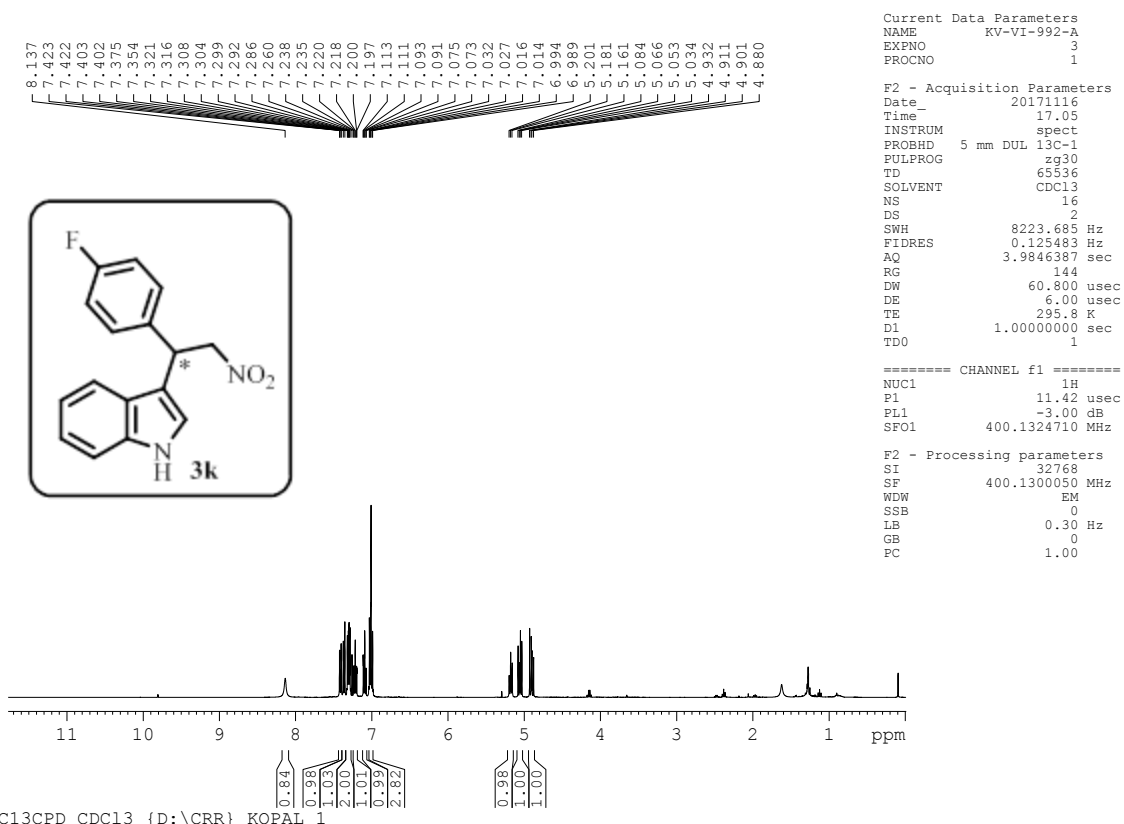
F2 - Acquisition Parameters
Date_ 20170223
Time 14.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 293.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

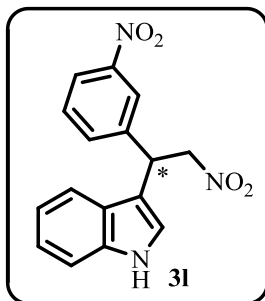
F2 - Processing parameters
SI 32768
SF 100.6127556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1



PROTON CDC13 {D:\CRR} KOPAL 1

8.294
8.211
8.206
8.201
8.135
8.133
8.130
8.127
8.114
8.112
8.109
8.107
7.719
7.699
7.522
7.502
7.482
7.400
7.397
7.395
7.393
7.382
7.380
7.377
7.374
7.260
7.245
7.242
7.227
7.225
7.222
7.206
7.204
7.114
7.112
7.097
7.094
7.093
7.083
7.082
7.077
7.075
5.322
5.302
5.282
5.136
5.119
5.104
5.087
5.024
5.002

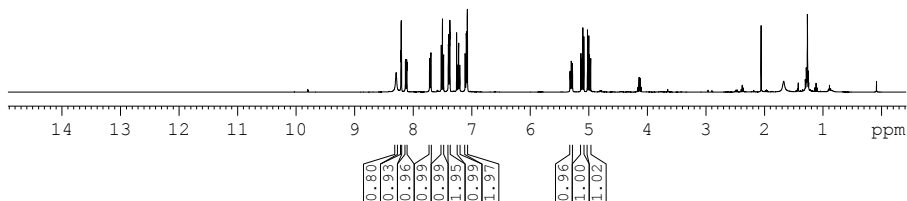


Current Data Parameters
NAME KV-VI-996
EXPNO 1
PROCNO 1

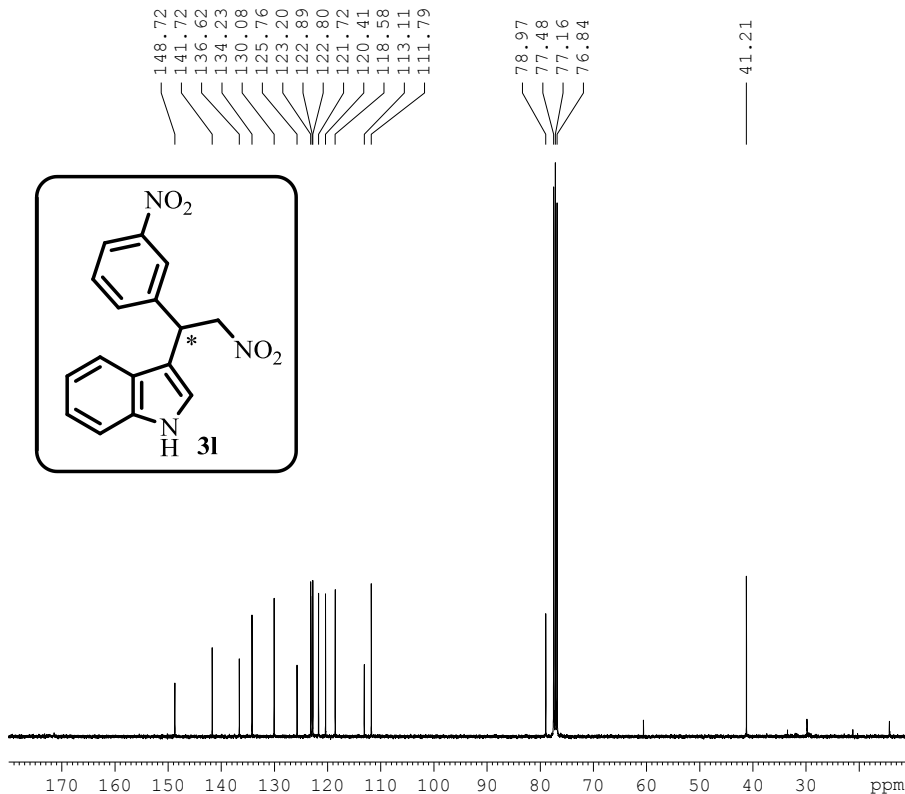
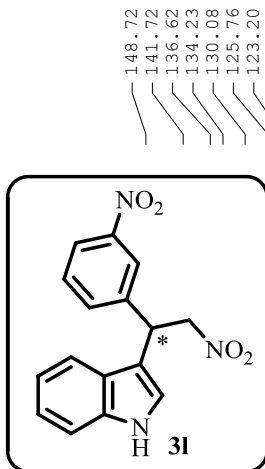
F2 - Acquisition Parameters
Date_ 20171122
Time 17.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-VI-996
EXPNO 2
PROCNO 1

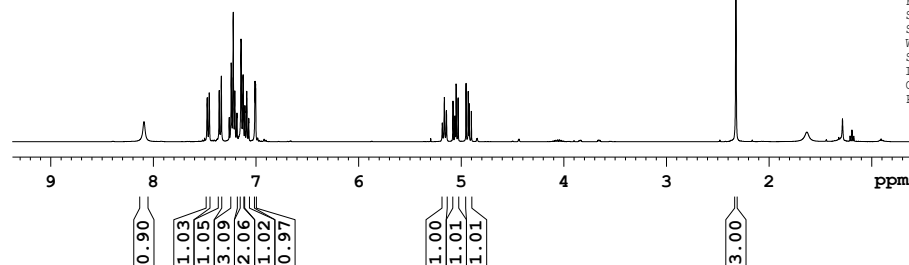
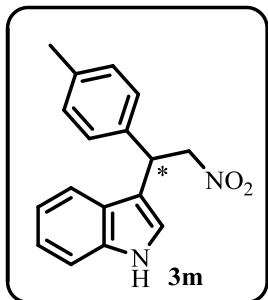
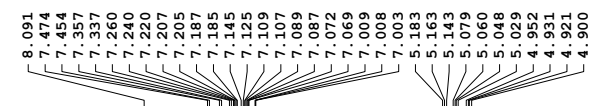
F2 - Acquisition Parameters
Date_ 20171122
Time 19.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.899999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

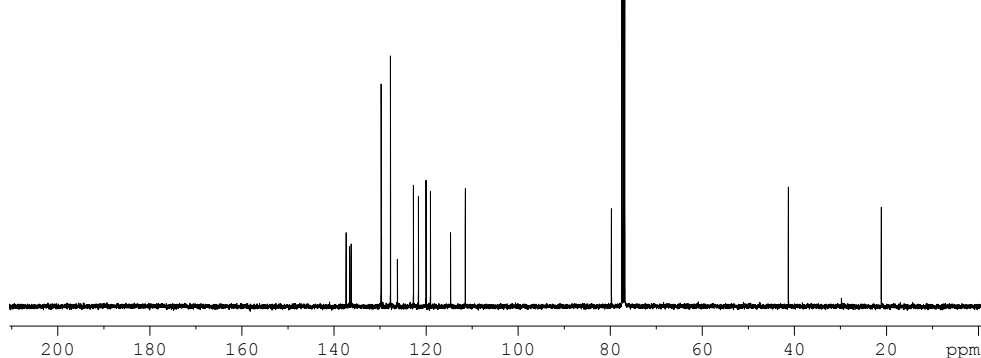
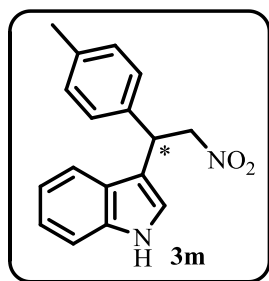
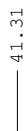
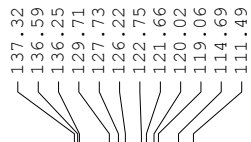
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127584 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDCl3 {D:\CRR} KOPAL 1



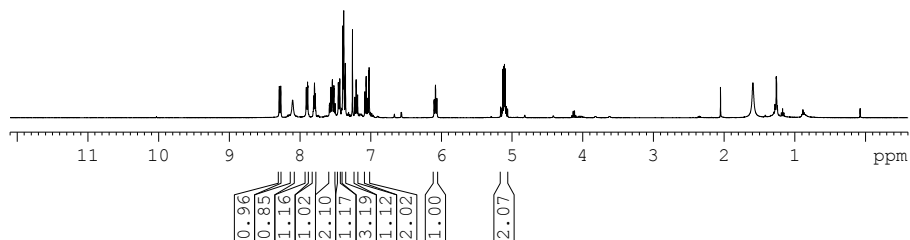
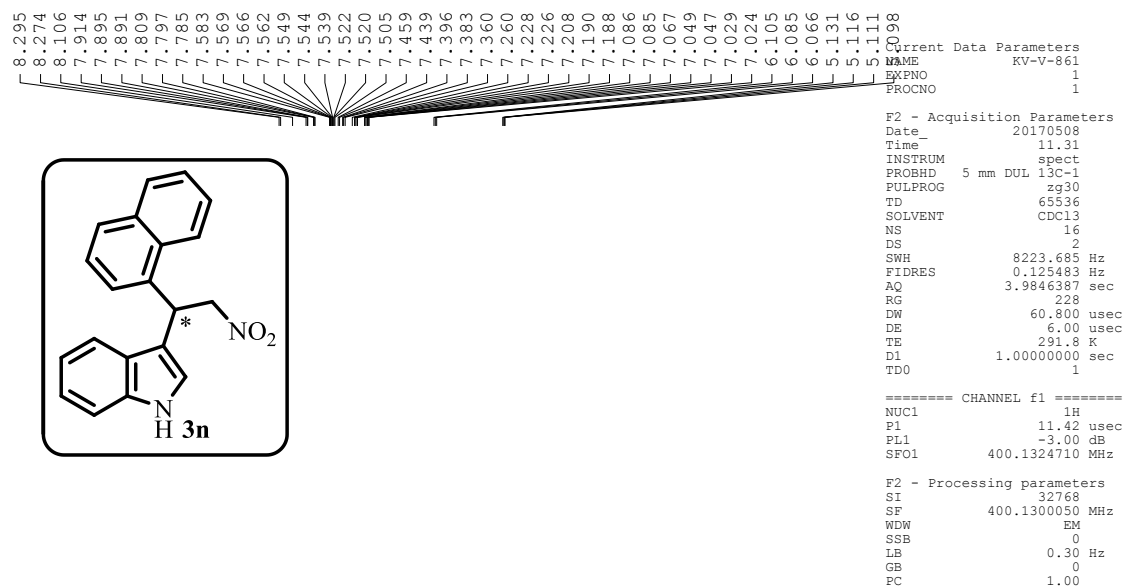
C13CPD CDCl3 {D:\CRR} KOPAL 1



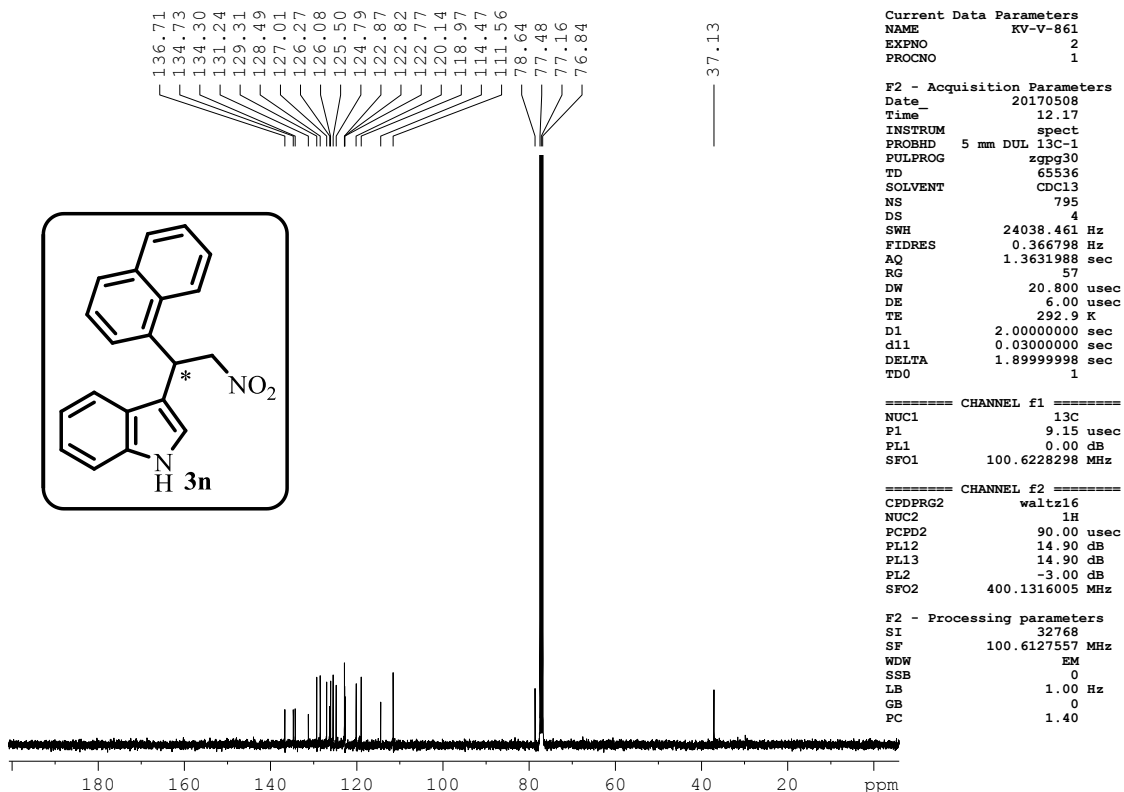
Current Data Parameters
NAME KV-VI-923
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170828
Time 12.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846397 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME KV-VI-923
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170830
Time 16.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 423
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 293.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127593 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1

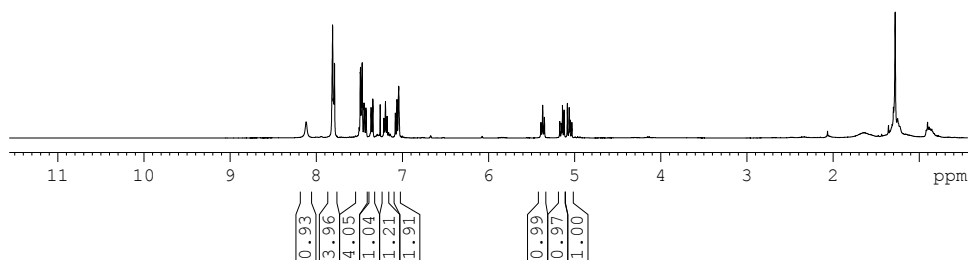
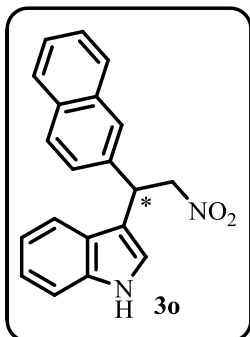


C13CPD CDC13 {D:\CRR} KOPAL 1



PROTON CDC13 {D:\CRR} KOPAL 1

8.120 7.812 7.803 7.798 7.790 7.492 7.489 7.479 7.469 7.447 7.443 7.426 7.422 7.366 7.346 7.260 7.218 7.216 7.199 7.181 7.085 7.065 7.047 7.045 5.391 5.372 5.352 5.173 5.155 5.142 5.123 5.085 5.064 5.054 5.033



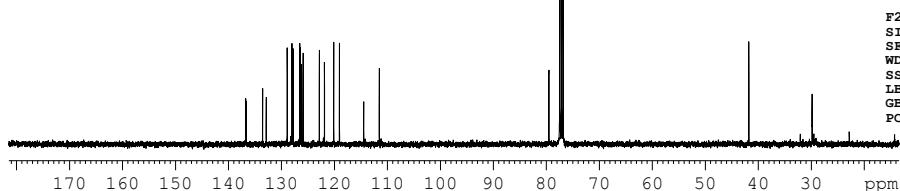
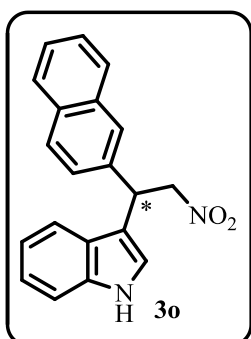
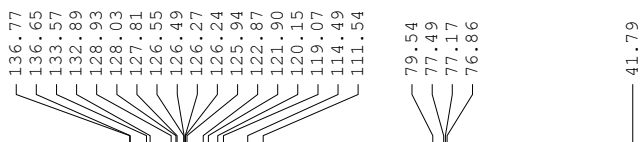
Current Data Parameters
NAME KV-V-795
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170603
Time 15.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-795
EXPNO 4
PROCNO 1

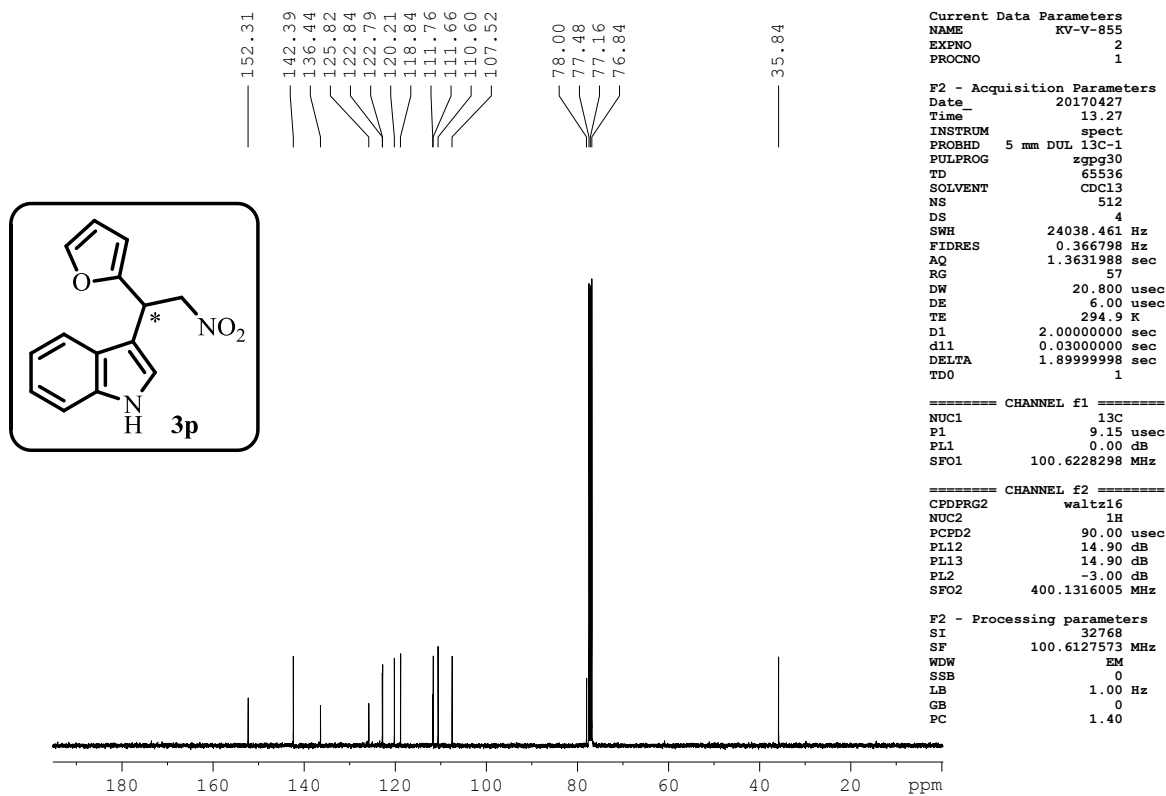
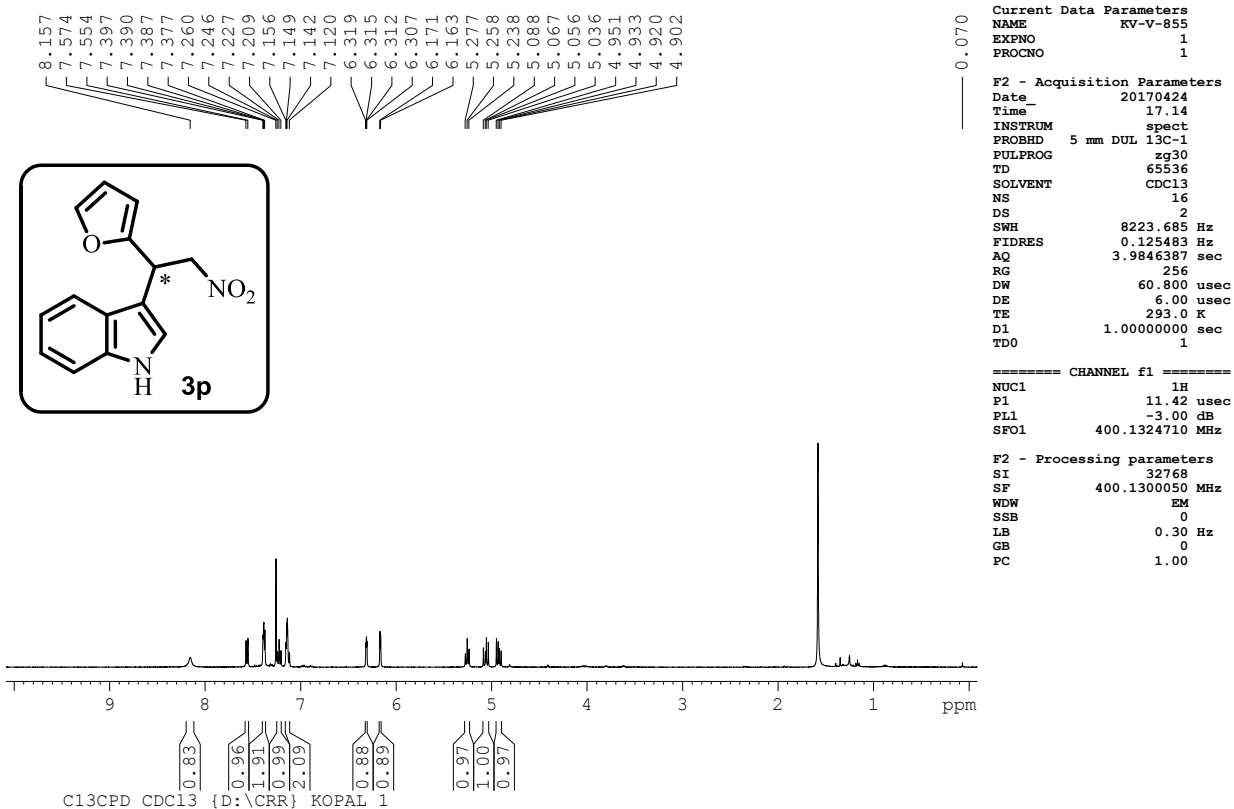
F2 - Acquisition Parameters
Date_ 20170603
Time 17.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 596
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

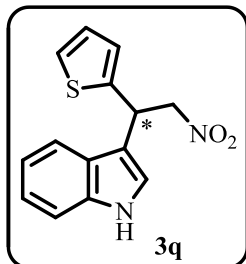
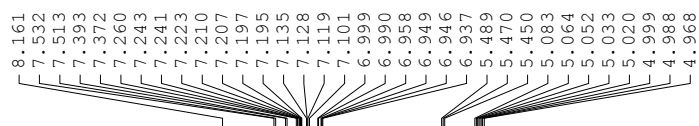
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127557 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\CRR} KOPAL 1



PROTON CDC13 {D:\CRR} KOPAL 1

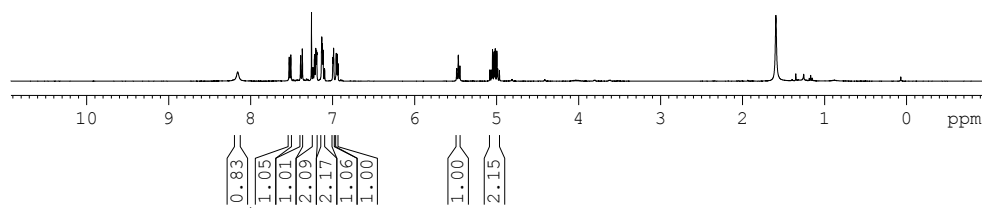


Current Data Parameters
NAME KV-V-856
EXPNO 1
PROCNO 1

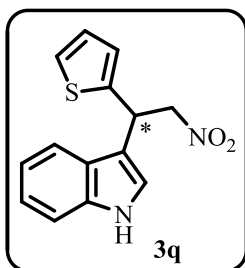
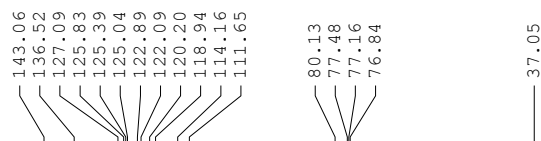
F2 - Acquisition Parameters
Date_ 20170424
Time 17.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 292.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



C13CPD CDC13 {D:\CRR} KOPAL 1



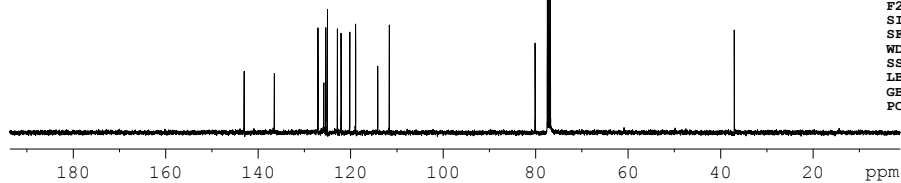
Current Data Parameters
NAME KV-V-856
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170503
Time 21.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 293.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

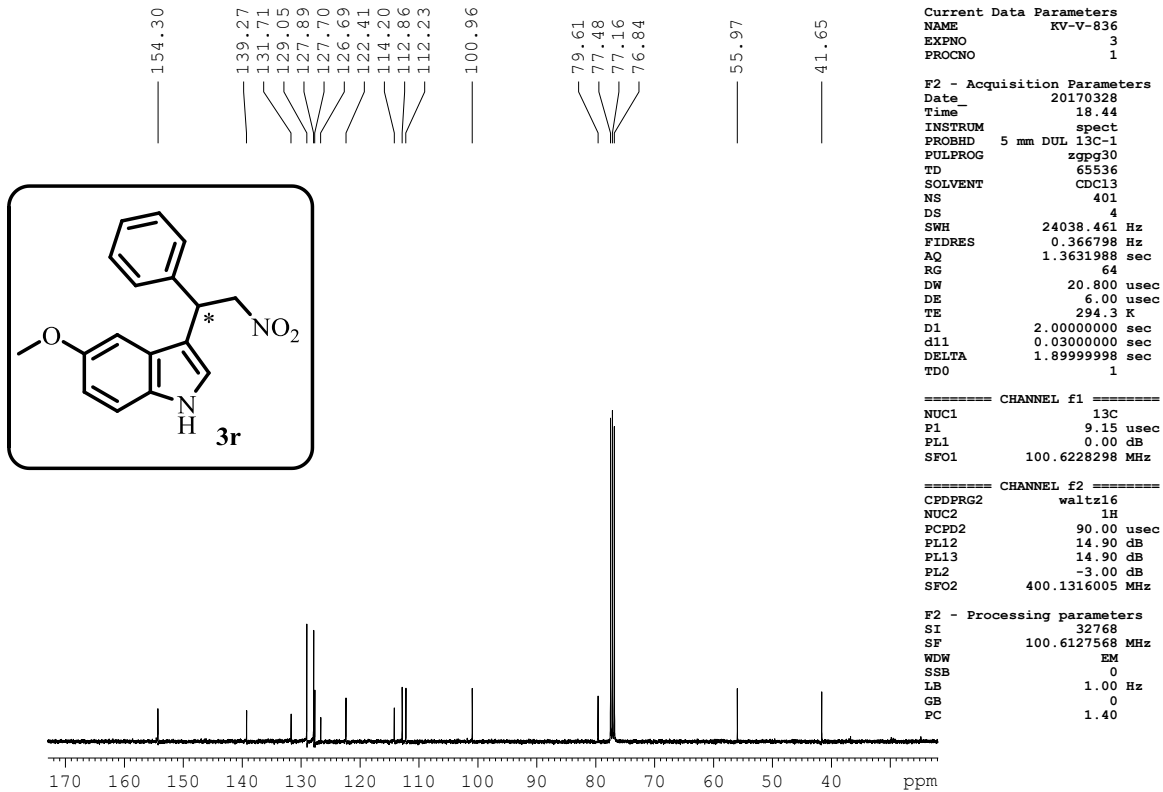
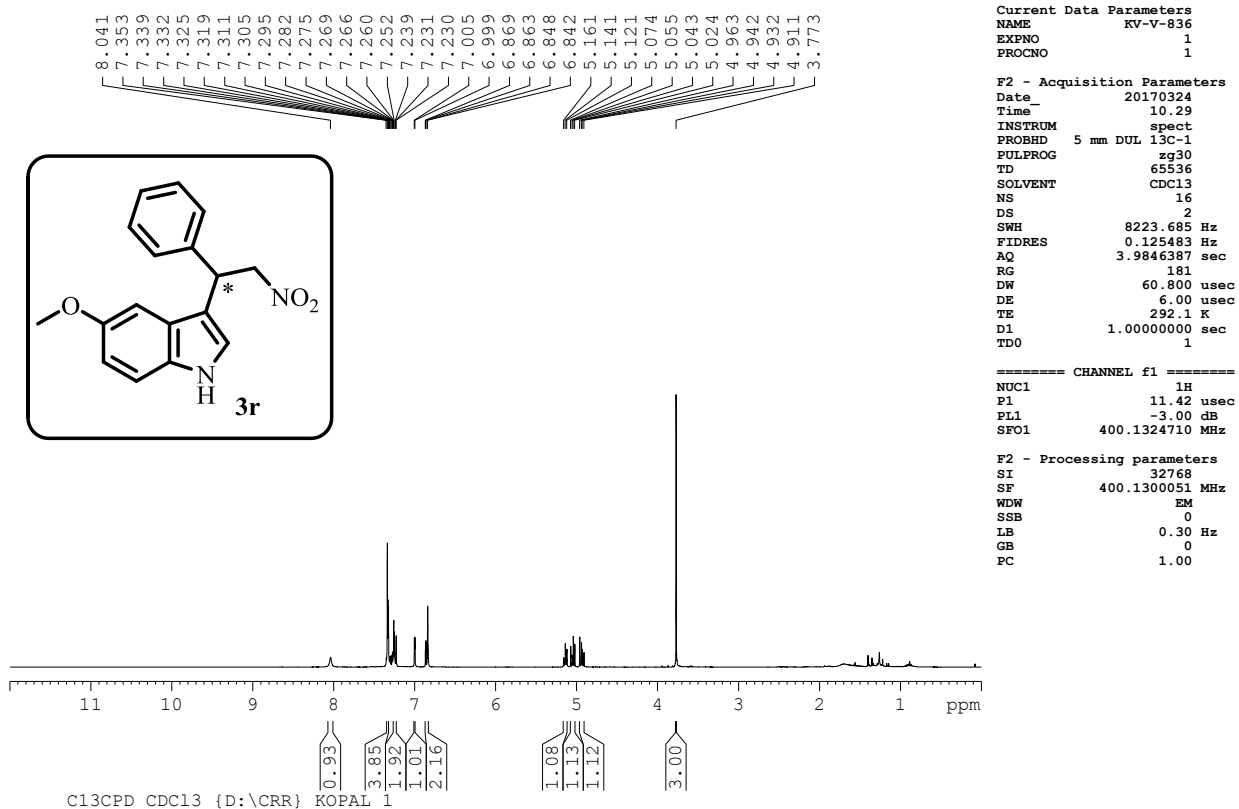
===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

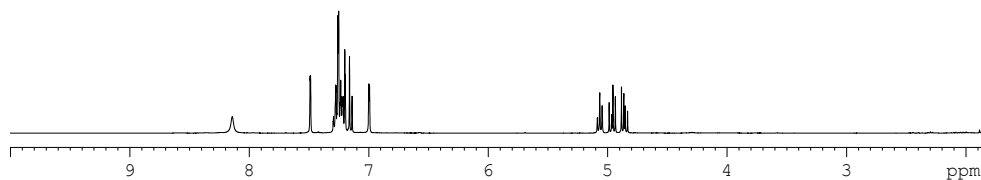
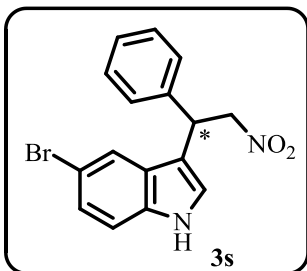
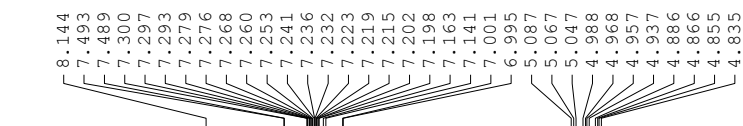
F2 - Processing parameters
SI 32768
SF 100.6127590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



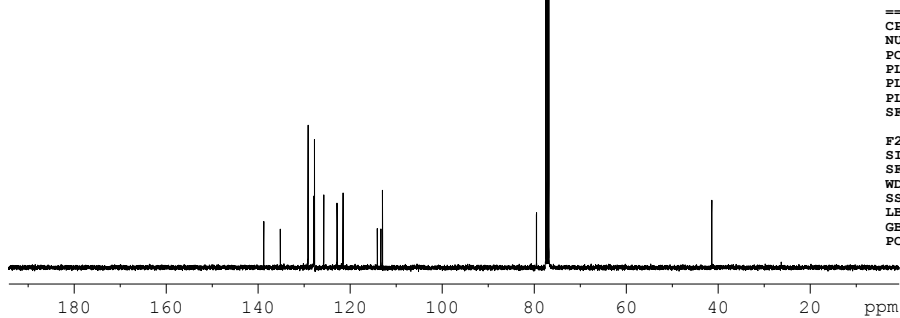
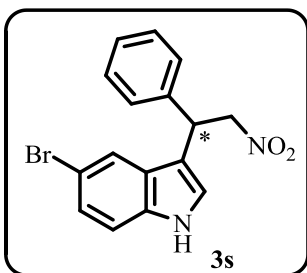
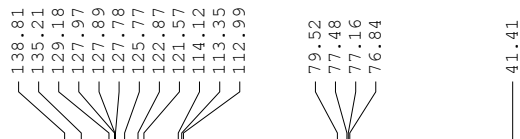
PROTON CDC13 {D:\CRR} KOPAL 1



PROTON CDC13 {D:\CRR} KOPAL 1



C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME KV-V-857
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170428
Time 9.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300281 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME KV-V-857
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170428
Time 10.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 276
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 294.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

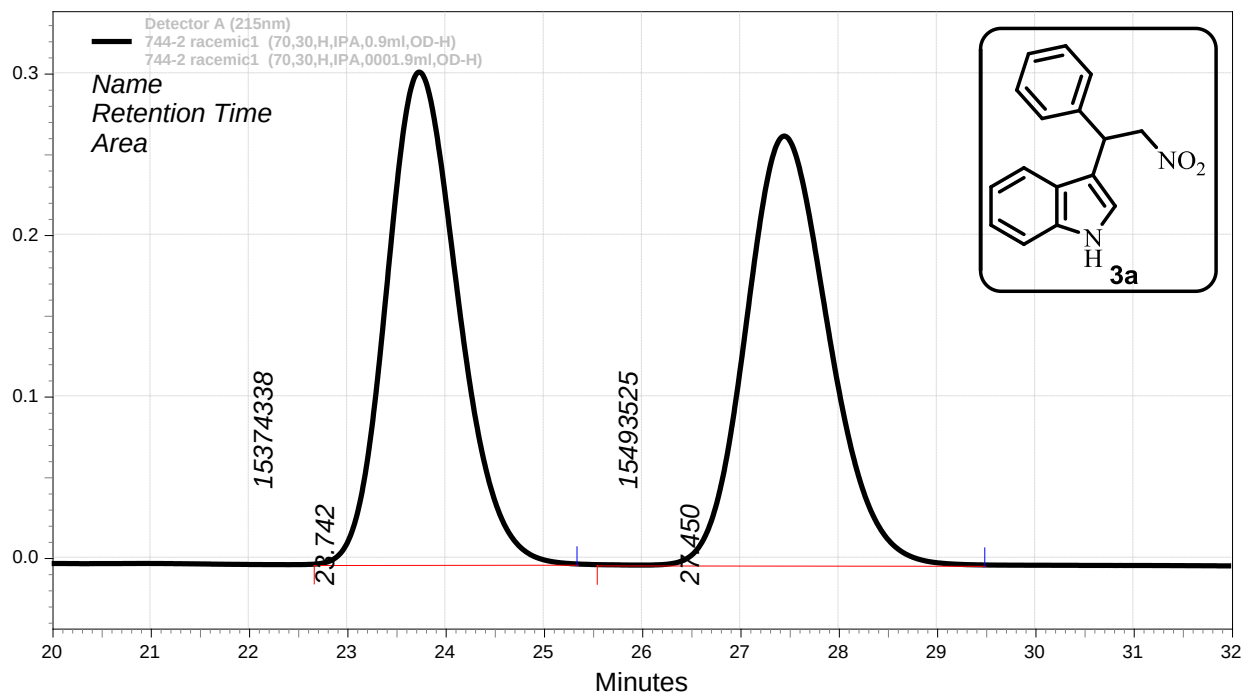
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3. HPLC chromatogram of compounds,
3a-3s

HPLC chromatogram of 3a

Data Graph



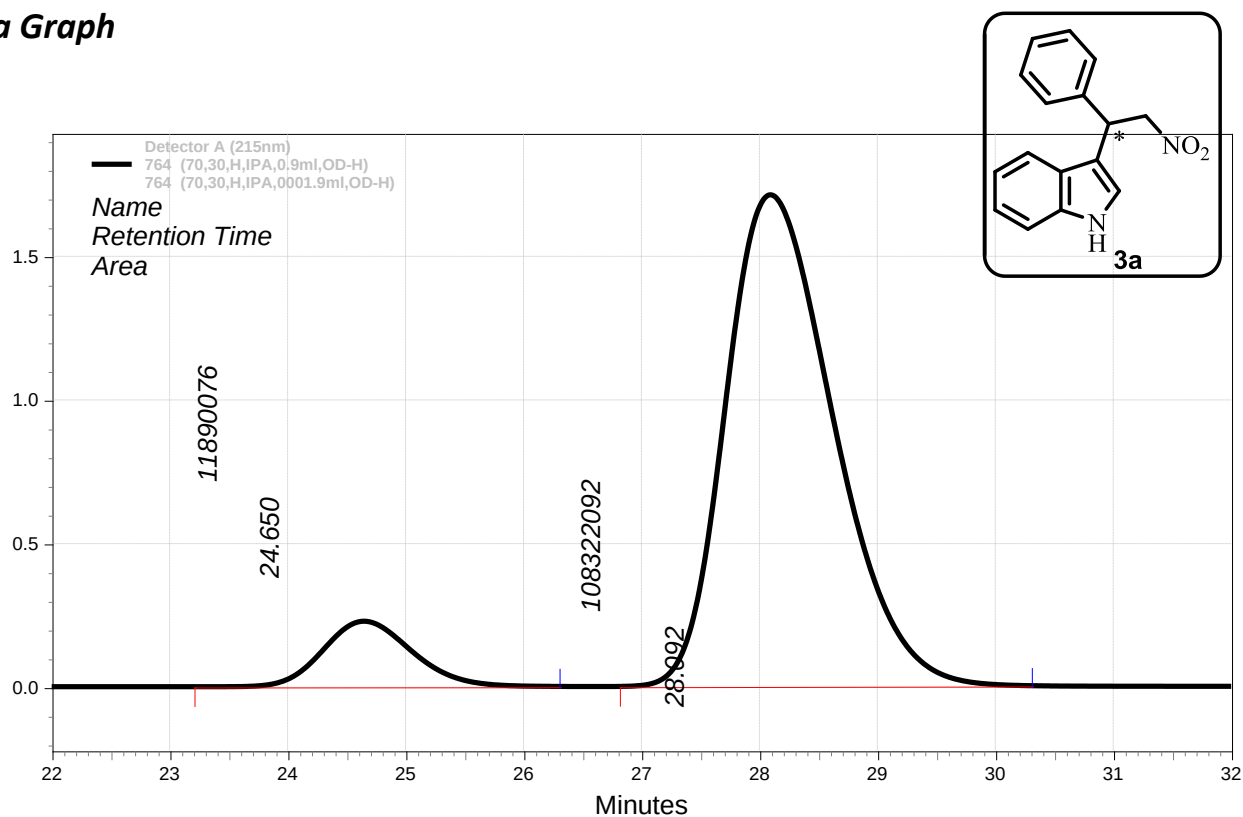
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.742	15374338	304685		49.81	MM
2		27.450	15493525	265447		50.19	MM

Totals			30867863	570132		100.00	
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Data Graph



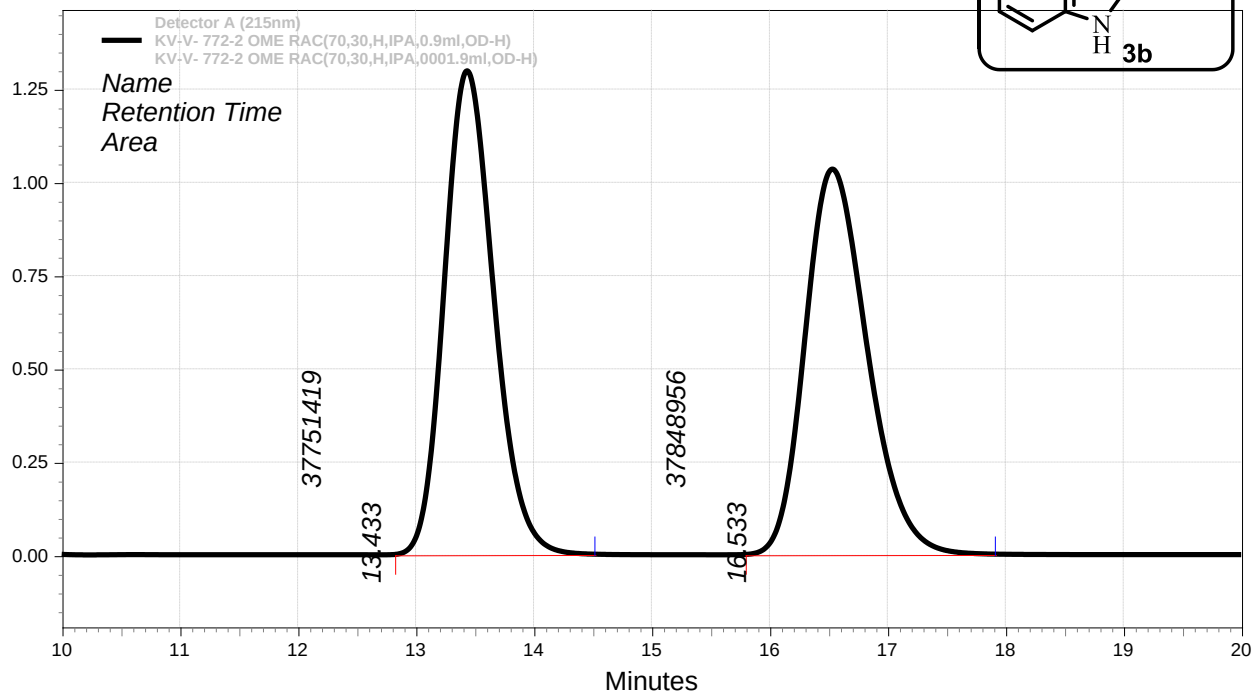
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		24.650	11890076	227370		9.89	MM
2		28.092	108322092	1709995		90.11	MM
Totals			120212168	1937365		100.00	

HPLC chromatogram of 3b

Data Graph

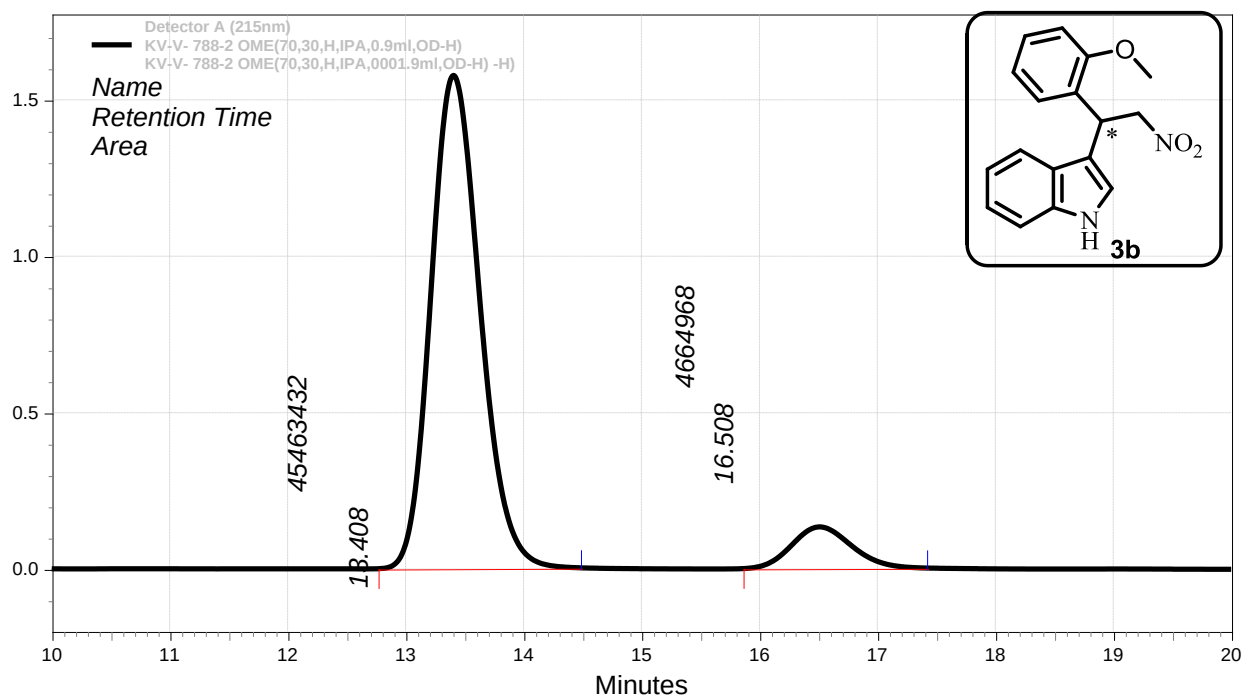


Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		13.433	37751419	1296054		49.94	MM
2		16.533	37848956	1032740		50.06	MM
Totals			75600375	2328794		100.00	

Data Graph



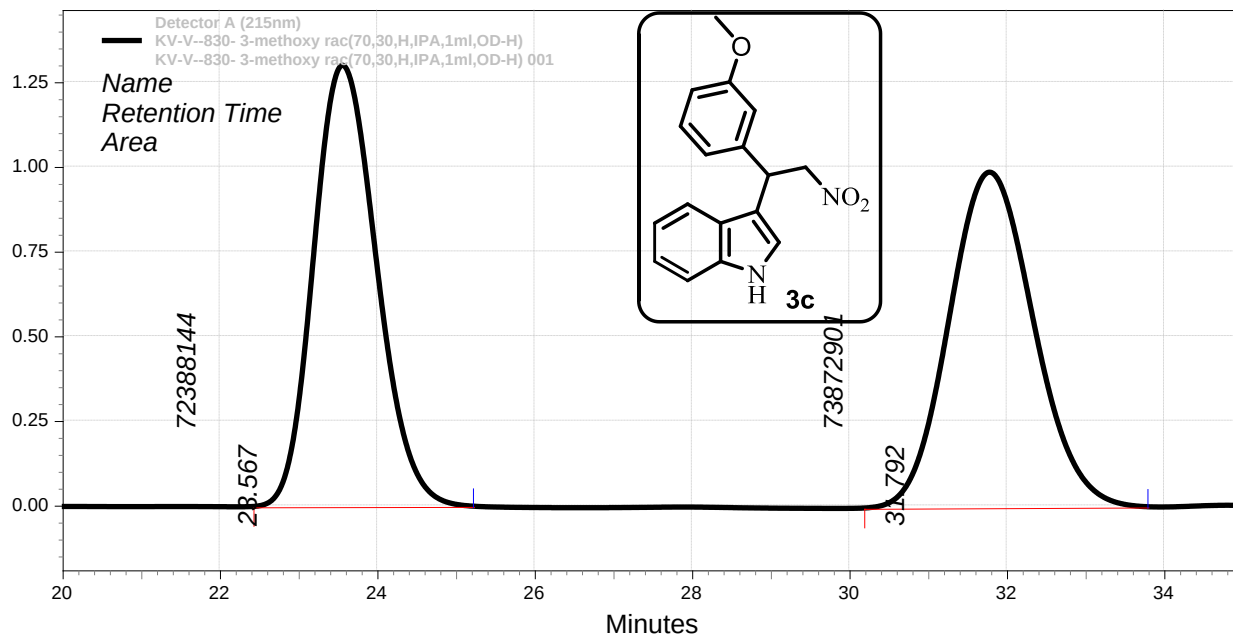
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		13.408	45463432	1575641		90.69	MM
2		16.508	4664968	132522		9.31	MM
Totals			50128400	1708163		100.00	

HPLC chromatogram of 3c

Data Graph

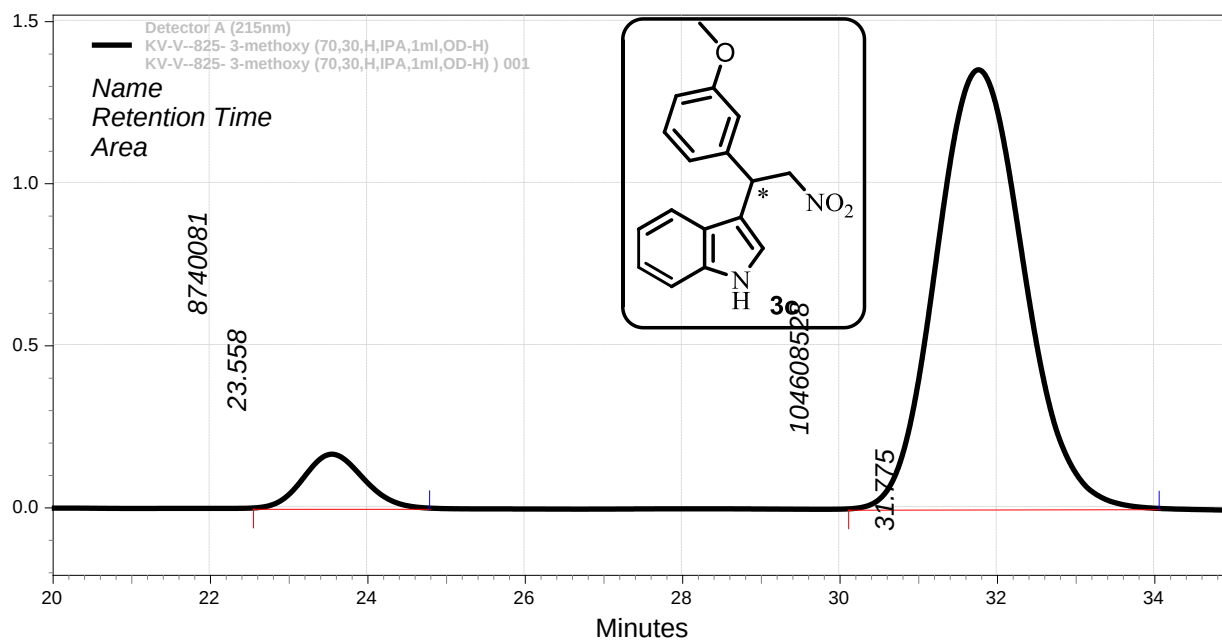


Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.567	72388144	1302427		49.49	MM
2		31.792	73872901	989913		50.51	MM
Totals			146261045	2292340		100.00	

Data Graph



Run Report

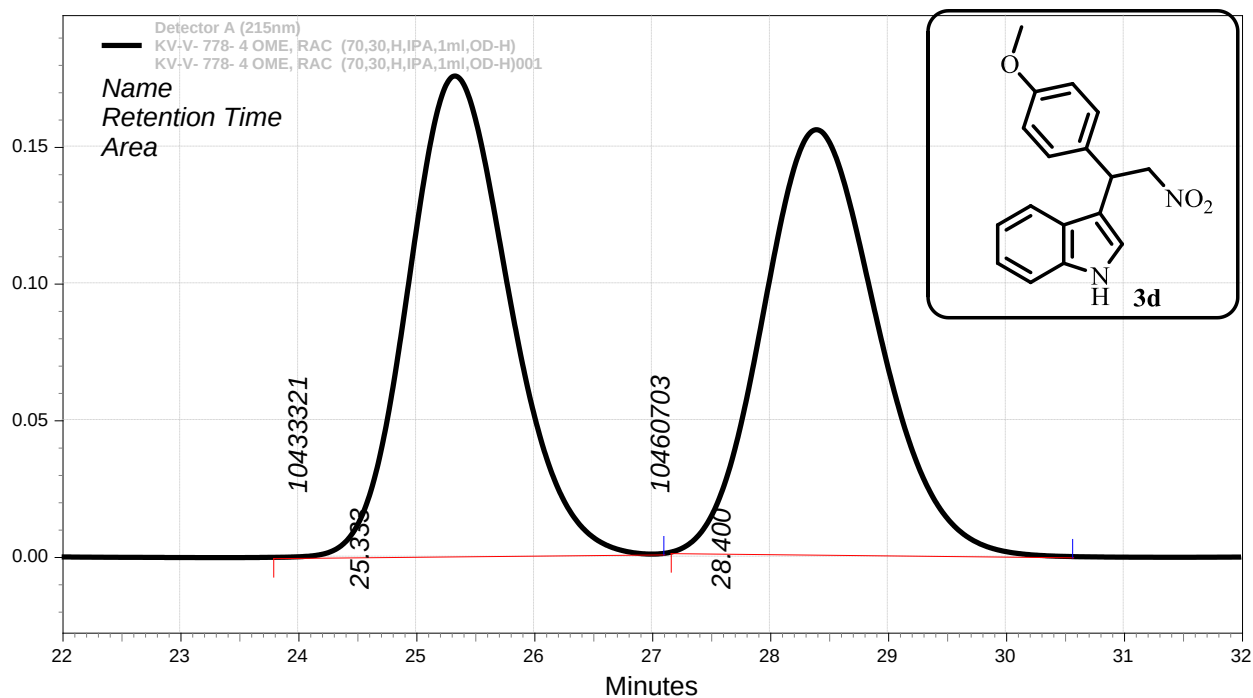
Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.558	8740081	166035		7.71	MM
2		31.775	104608528	1353930		92.29	MM

Totals			113348609	1519965		100.00	
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HPLC chromatogram of 3d

Data Graph



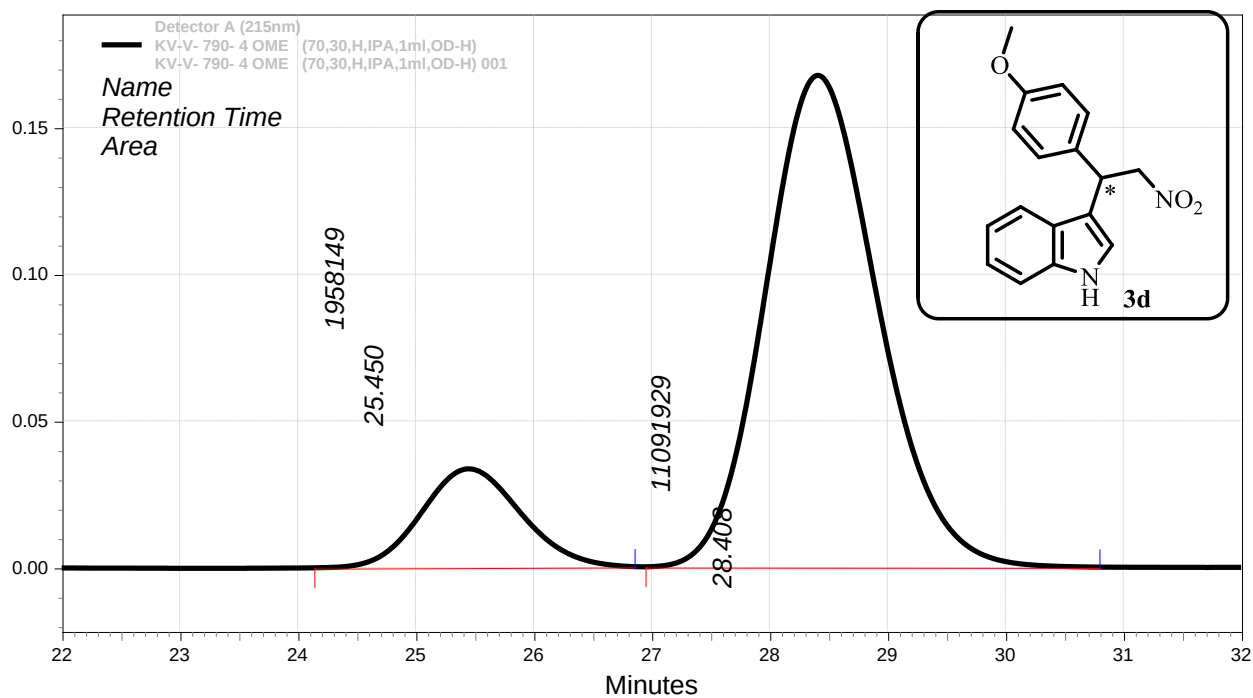
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		25.333	10433321	175432		49.93	MM
2		28.400	10460703	155170		50.07	MM

Totals			20894024	330602		100.00	
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Data Graph



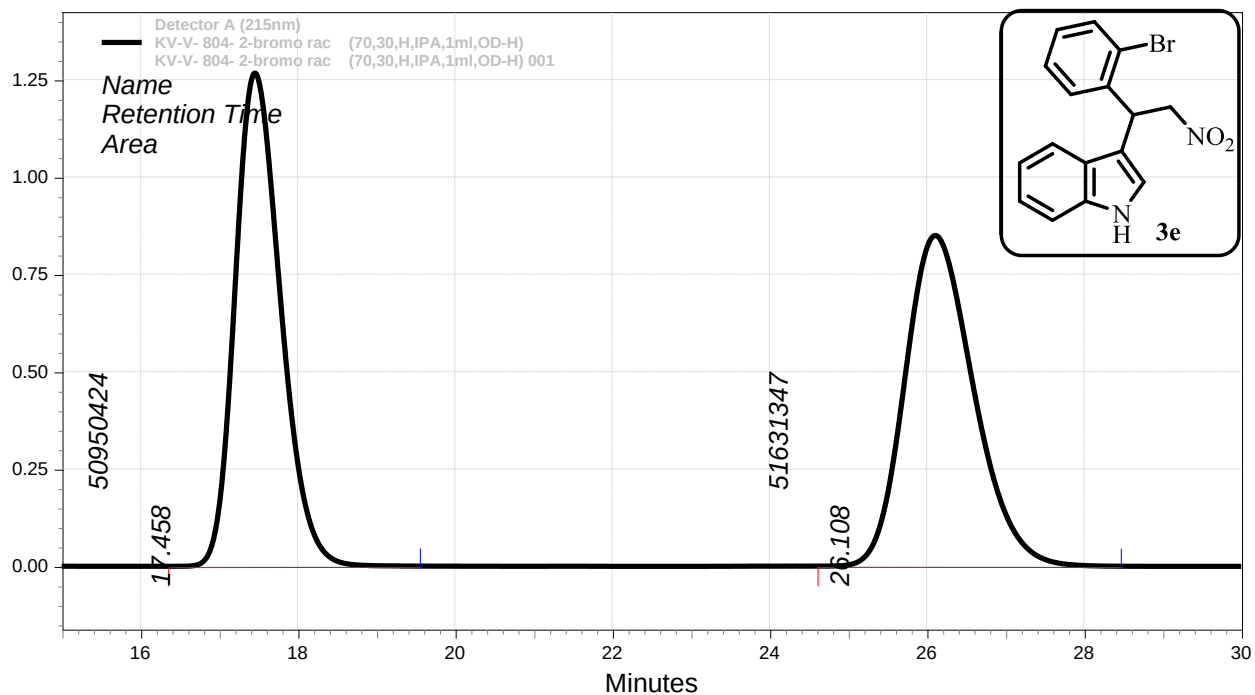
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		25.450	1958149	33525		15.00	MM
2		28.408	11091929	167495		85.00	MM
Totals			13050078	201020		100.00	

HPLC chromatogram of 3e

Data Graph



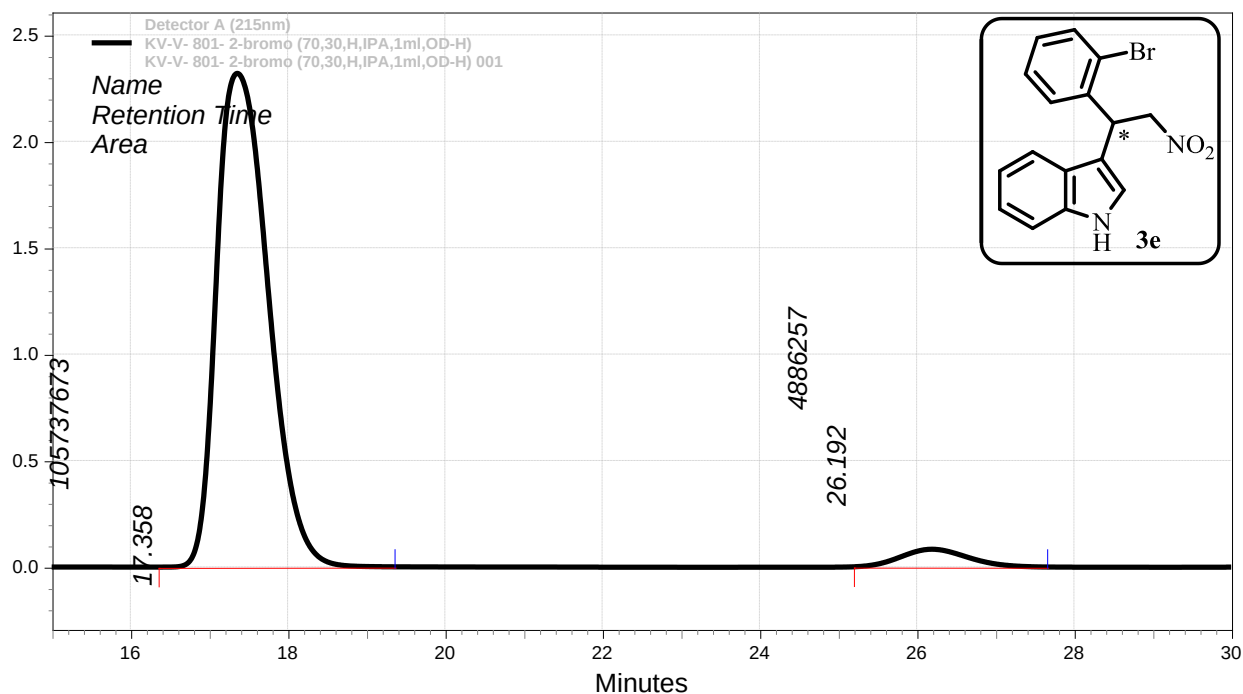
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent
1		17.458	50950424	1266967		49.67
2		26.108	51631347	849369		50.33

Totals			102581771	2116336		100.00
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Data Graph



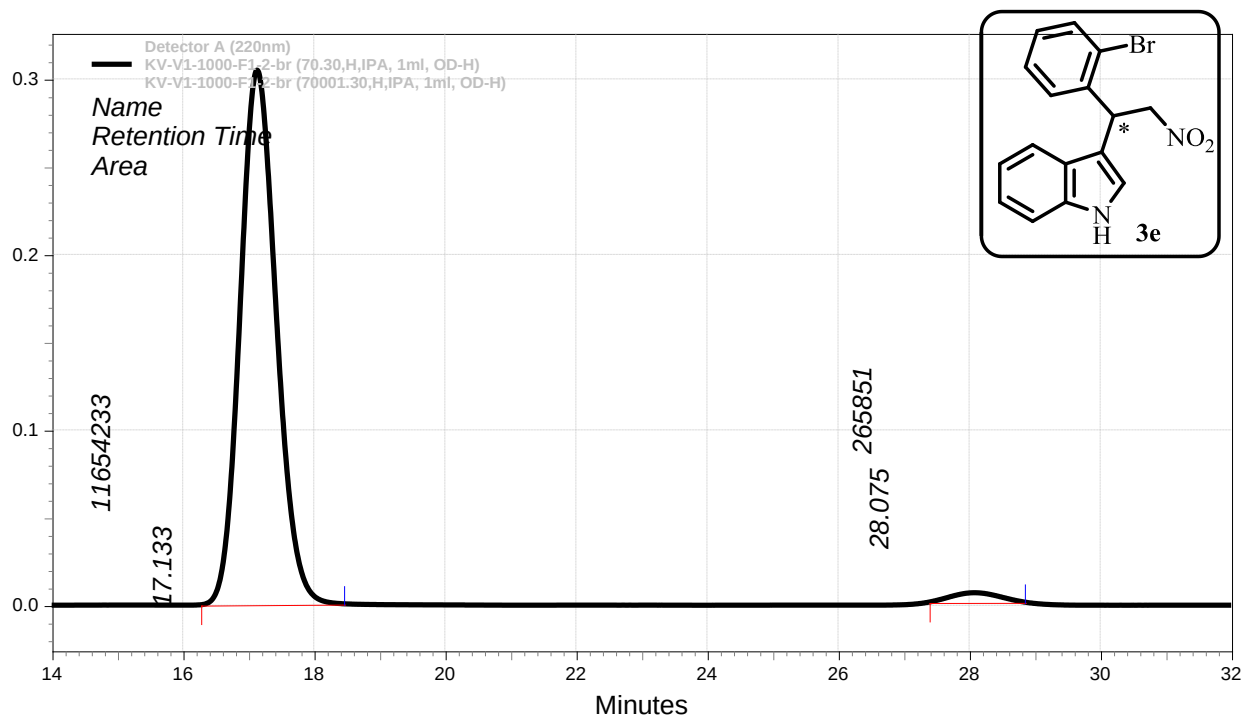
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.358	105737673	2319452		95.58	MM
2		26.192	4886257	82789		4.42	MM
Totals			110623930	2402241		100.00	

HPLC chromatogram of 3e (Gram scale reaction)

Data Graph



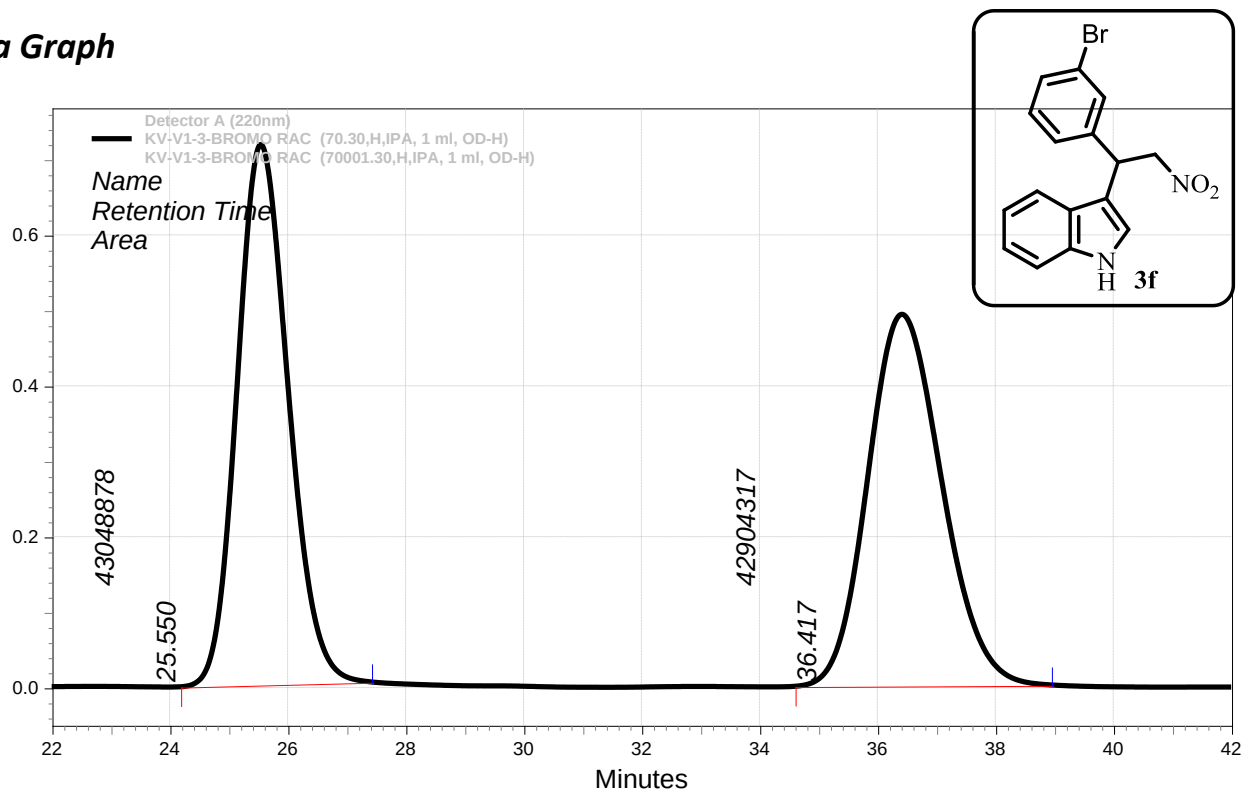
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.133	11654233	304521		97.77	MM
2		28.075	265851	5333		2.23	MM
Totals			11920084	309854		100.00	

HPLC chromatogram of 3f

Data Graph

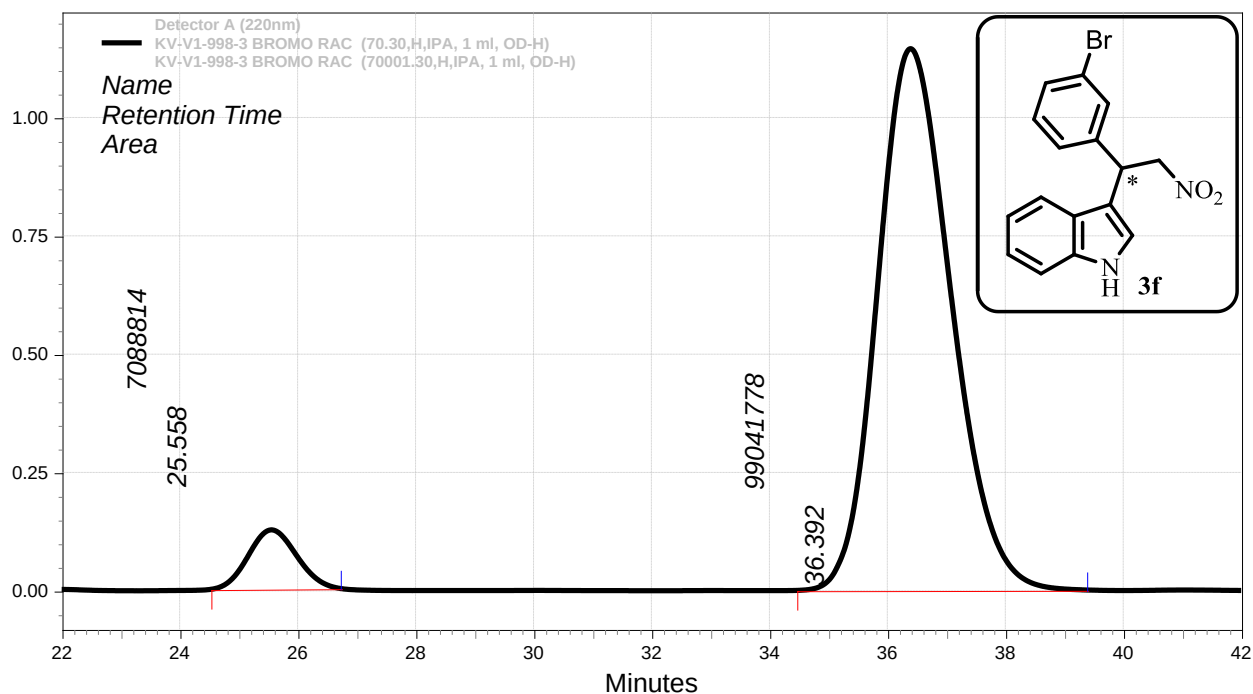


Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		25.550	43048878	715912		50.08	MM
2		36.417	42904317	492289		49.92	MM
Totals			85953195	1208201		100.00	

Data Graph



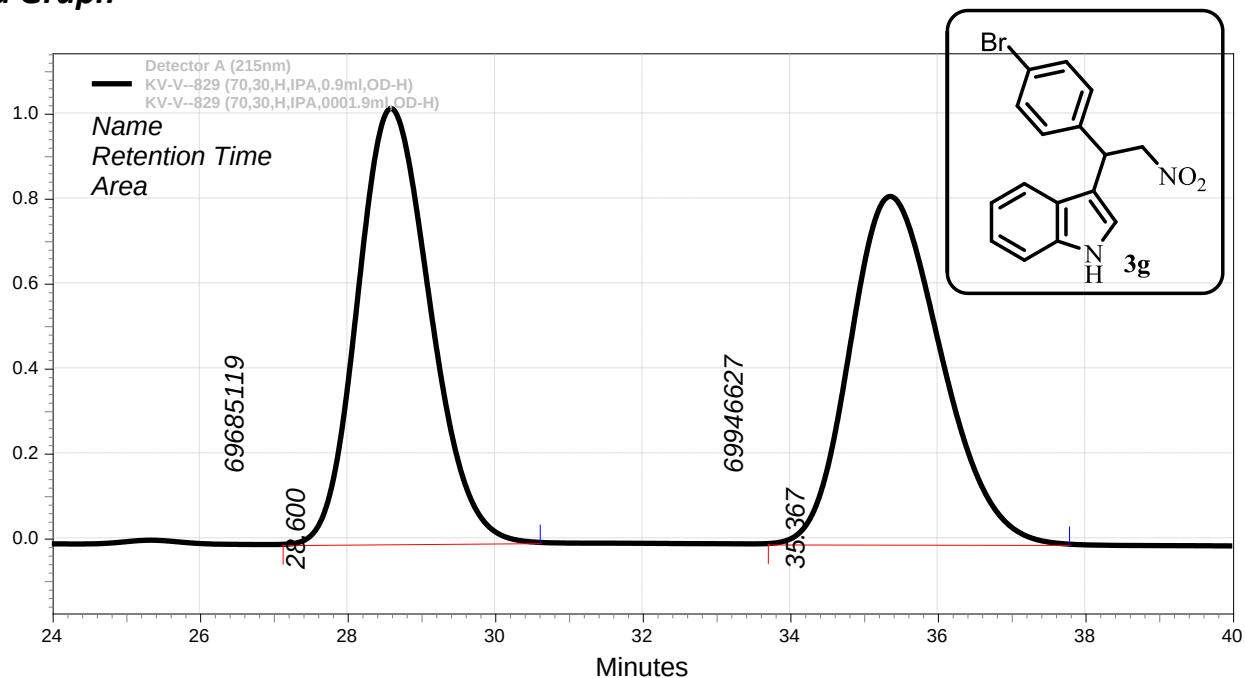
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		25.558	7088814	124734		6.68	MM
2		36.392	99041778	1144285		93.32	MM
Totals			106130592	1269019		100.00	

HPLC chromatogram of 3g

Data Graph



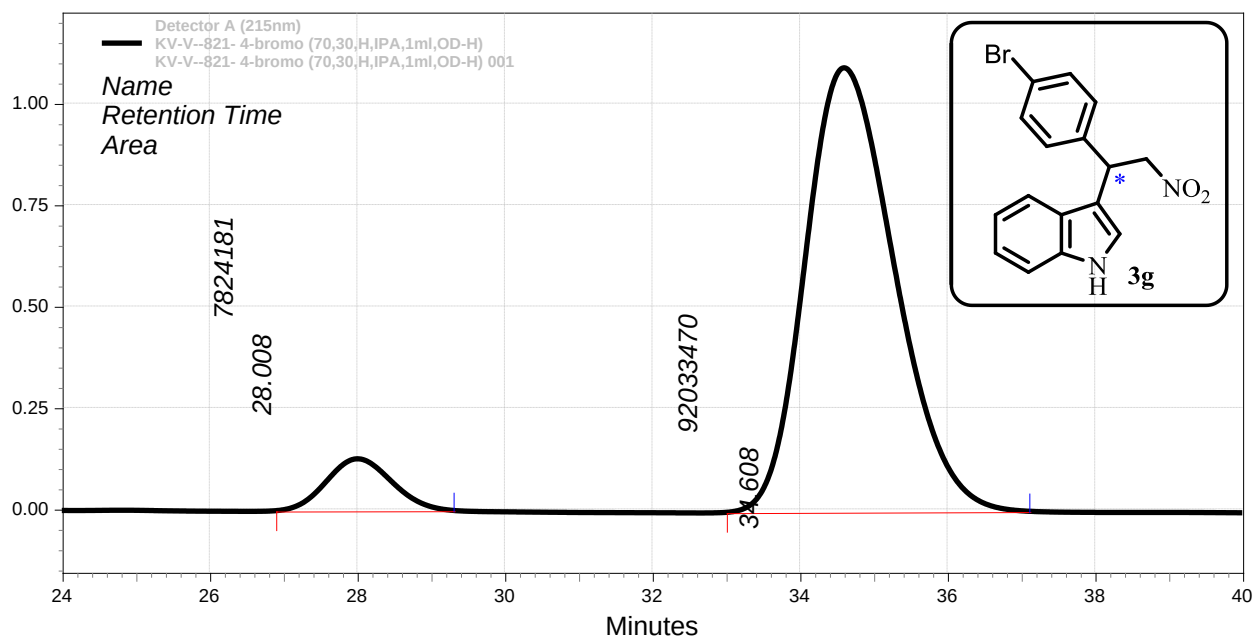
Run Report

Detector A (215nm)

PK #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		28.600	69685119	1023855		49.91	MM
2		35.367	69946627	817482		50.09	MM

Totals			139631746	1841337		100.00	
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Data Graph



Run Report

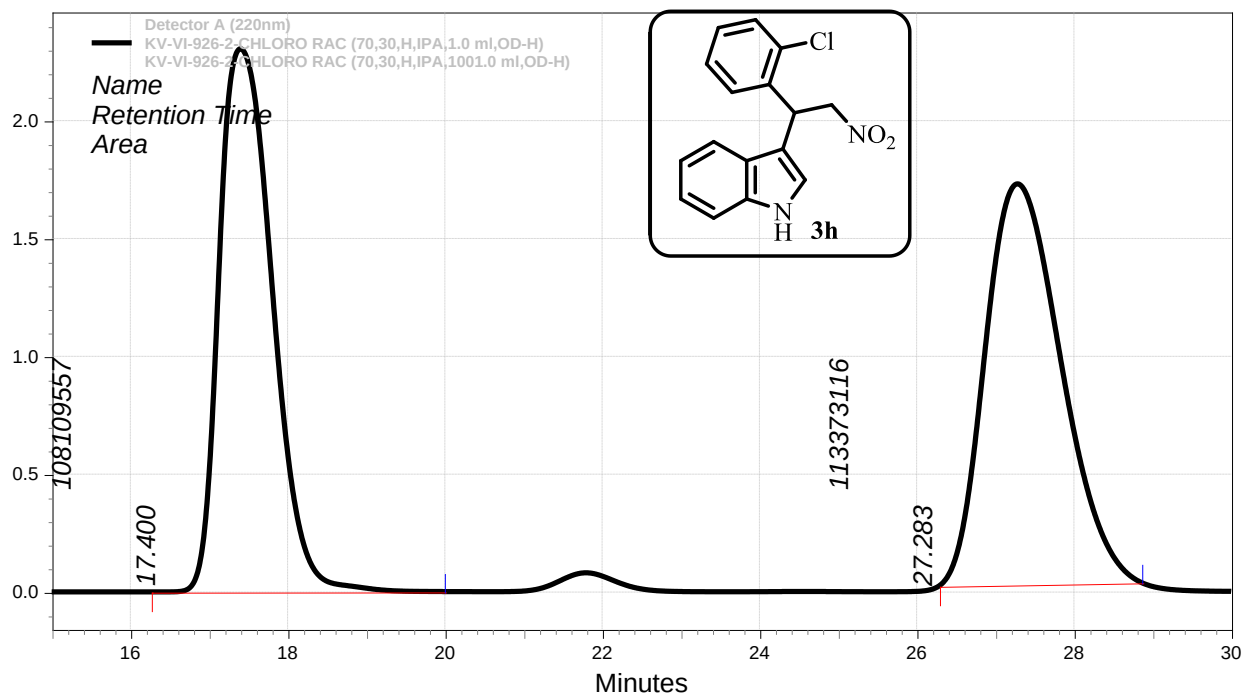
Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		28.008	7824181	127636		7.84	MM
2		34.608	92033470	1094653		92.16	MM

Totals			99857651	1222289		100.00	
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HPLC chromatogram of 3h

Data Graph



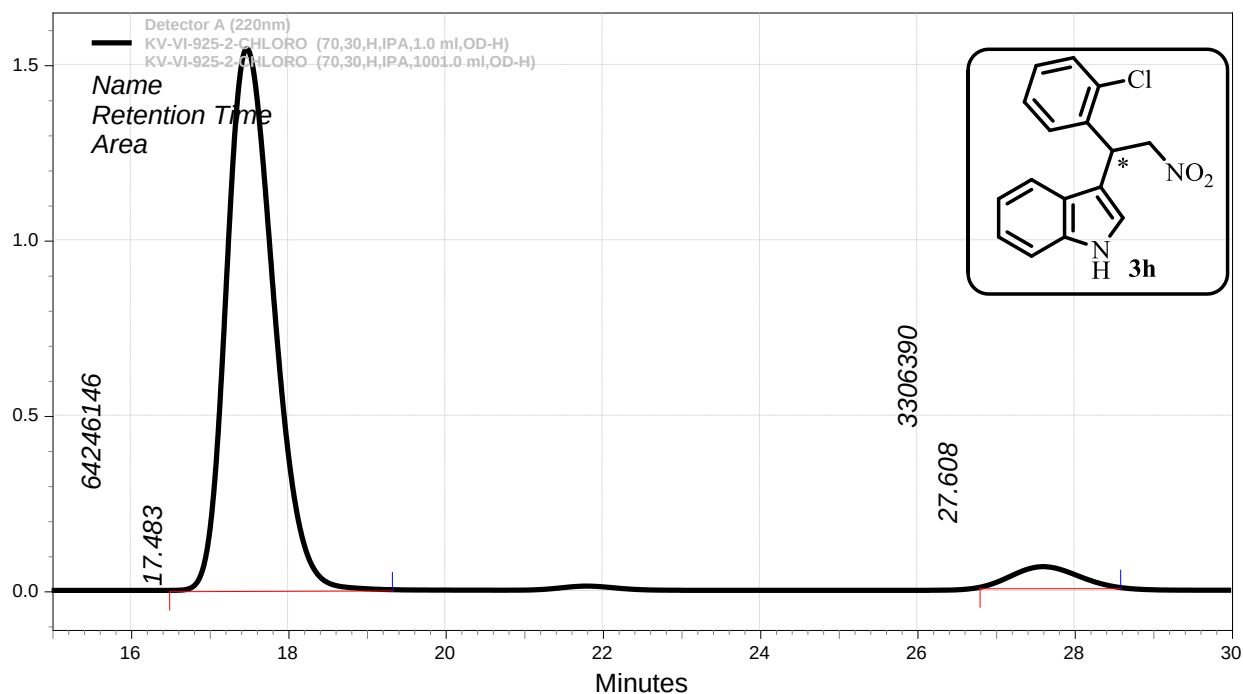
Run Report

Detector A (220nm)

PK #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.400	108109557	2303986		48.81	MM
2		27.283	113373116	1700283		51.19	MM

Totals			221482673	4004269		100.00	
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Data Graph



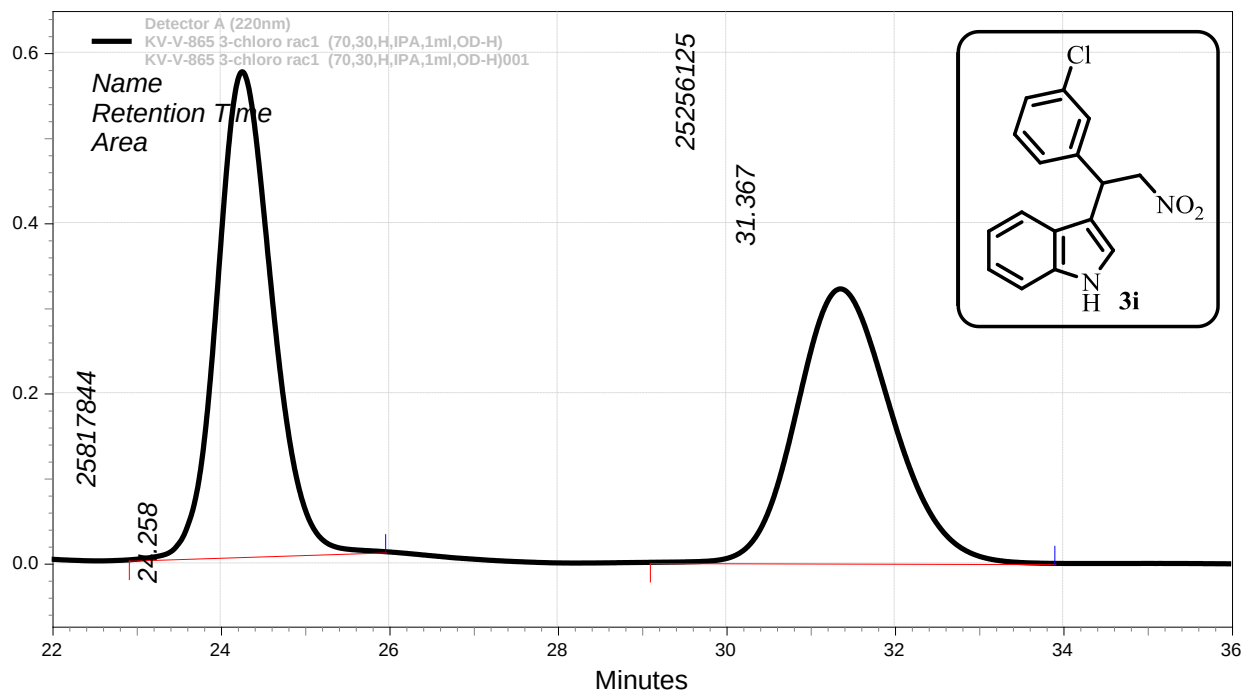
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.483	64246146	1543635		95.11	MM
2		27.608	3306390	59164		4.89	MM
Totals			67552536	1602799		100.00	

HPLC chromatogram of 3i

Data Graph



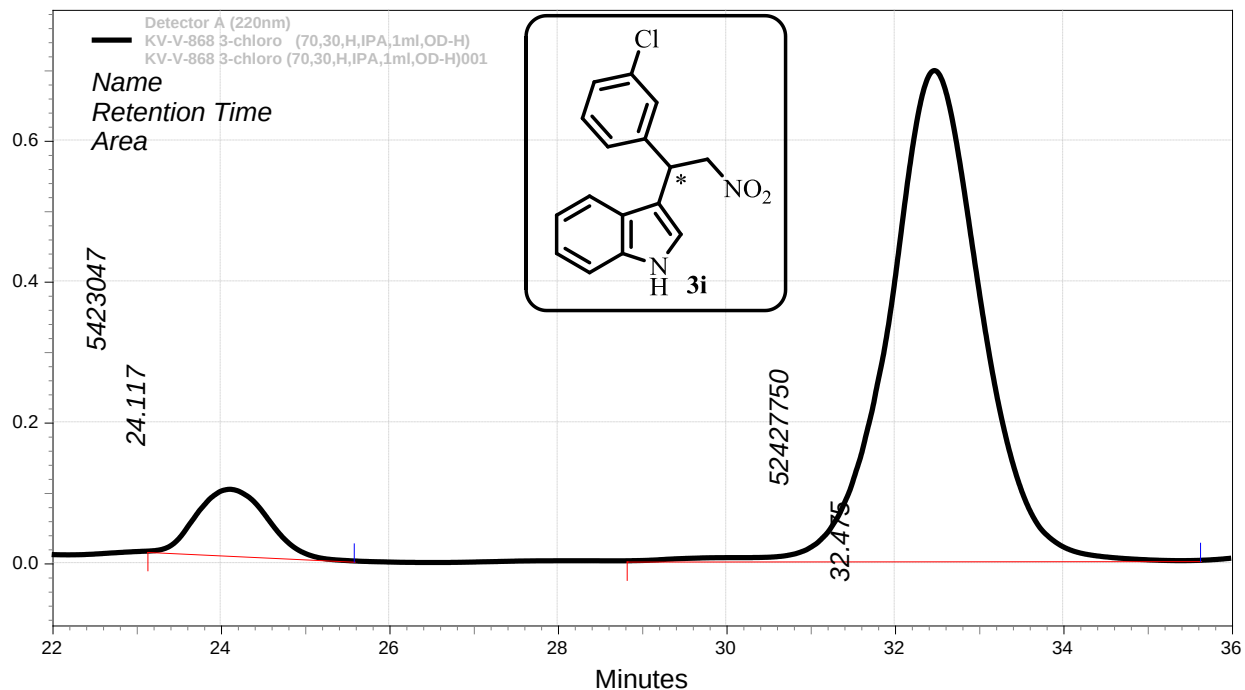
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		24.258	25817844	569362		50.55	MM
2		31.367	25256125	321903		49.45	MM

Totals			51073969	891265		100.00	
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Data Graph



Run Report

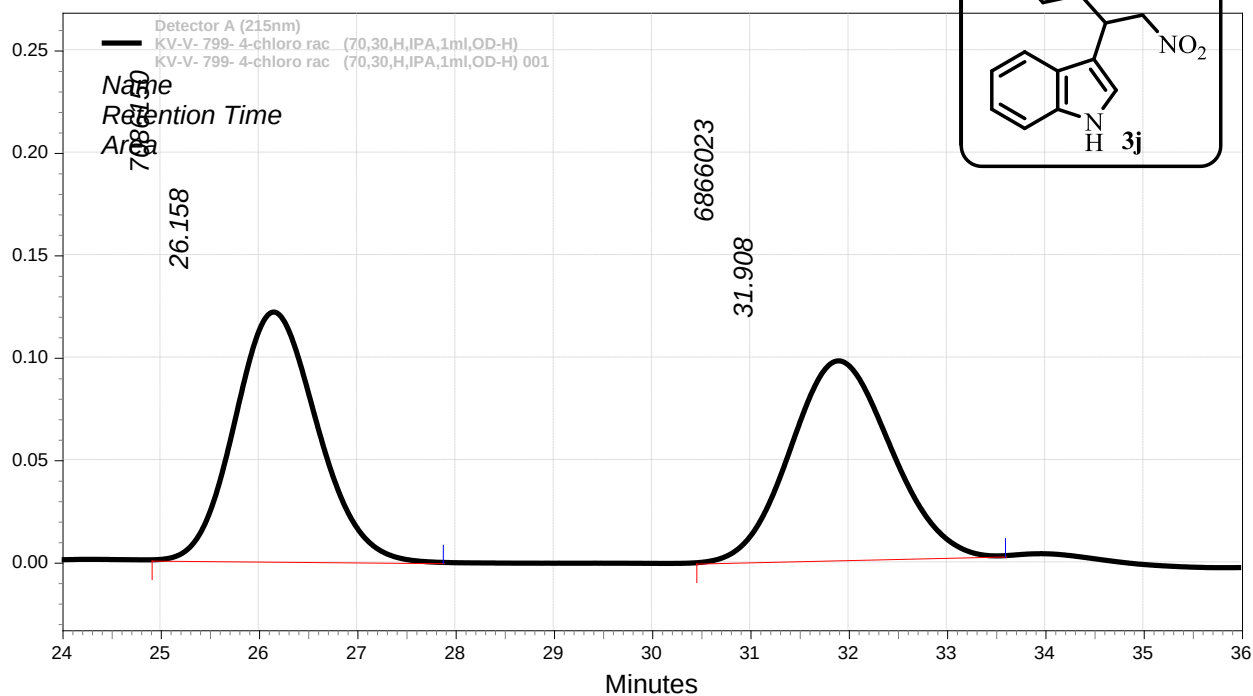
Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		24.117	5423047	93401		9.37	MM
2		32.475	52427750	695635		90.63	MM

Totals			57850797	789036		100.00	
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HPLC chromatogram of 3j

Data Graph

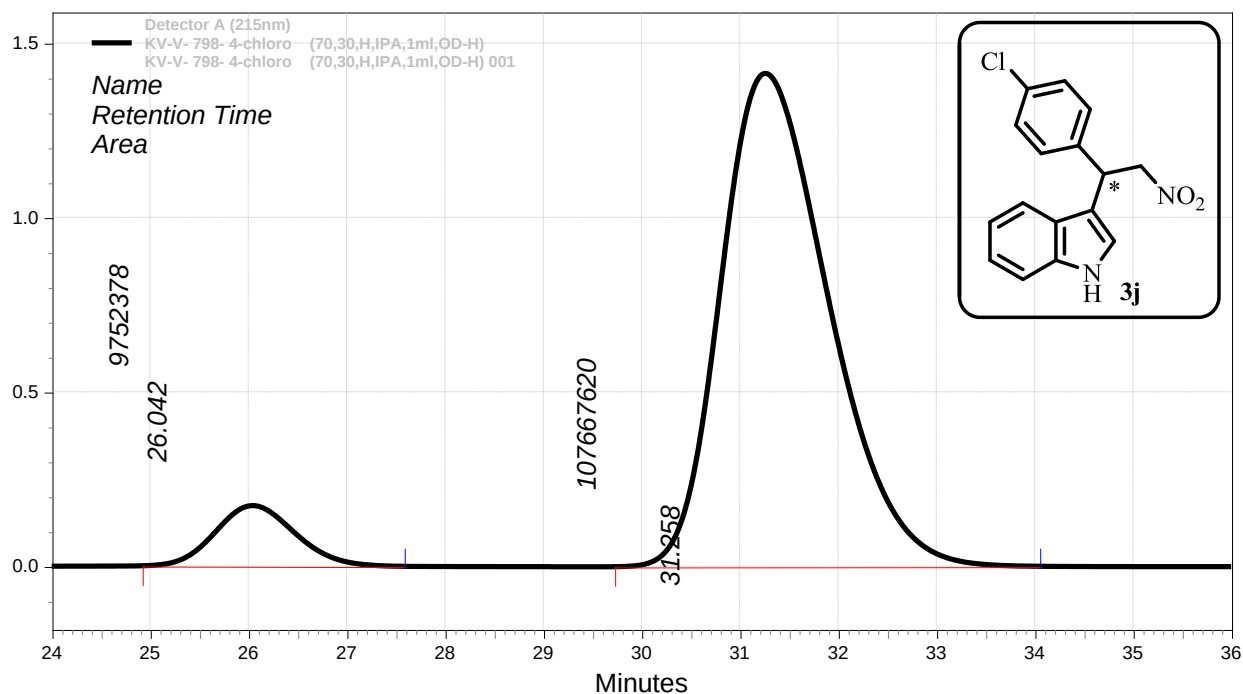


Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		26.158	7086150	121478		50.79	MM
2		31.908	6866023	96960		49.21	MM
Totals			13952173	218438		100.00	

Data Graph



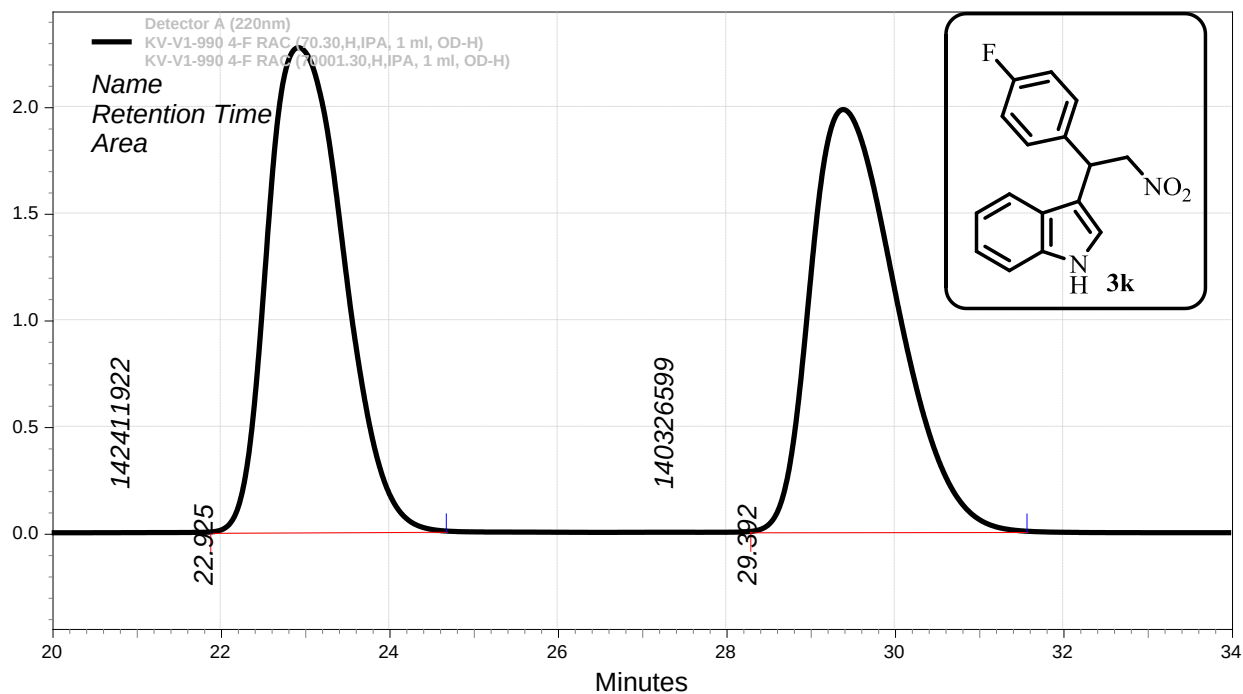
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		26.042	9752378	173109		8.31	MM
2		31.258	107667620	1413574		91.69	MM
Totals			117419998	1586683		100.00	

HPLC chromatogram of 3k

Data Graph



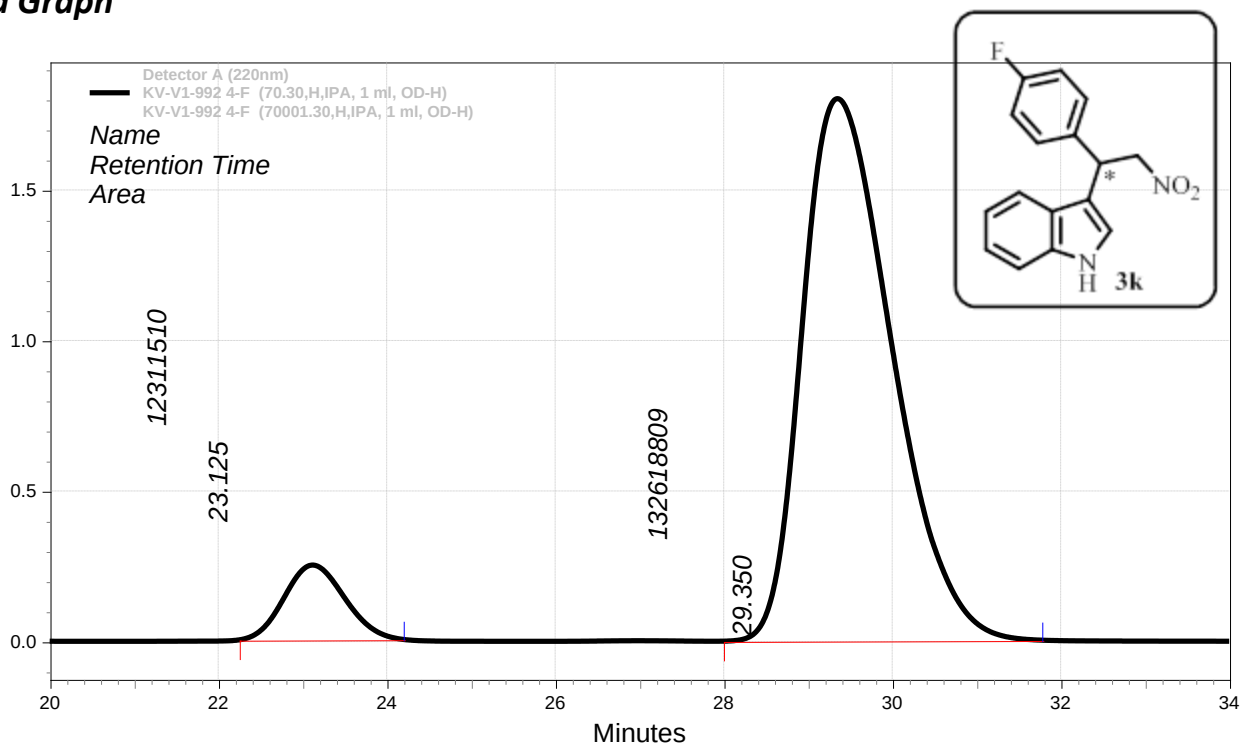
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		22.925	142411922	2268586		50.37	MM
2		29.392	140326599	1977432		49.63	MM

Totals			282738521	4246018		100.00	
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Data Graph



Run Report

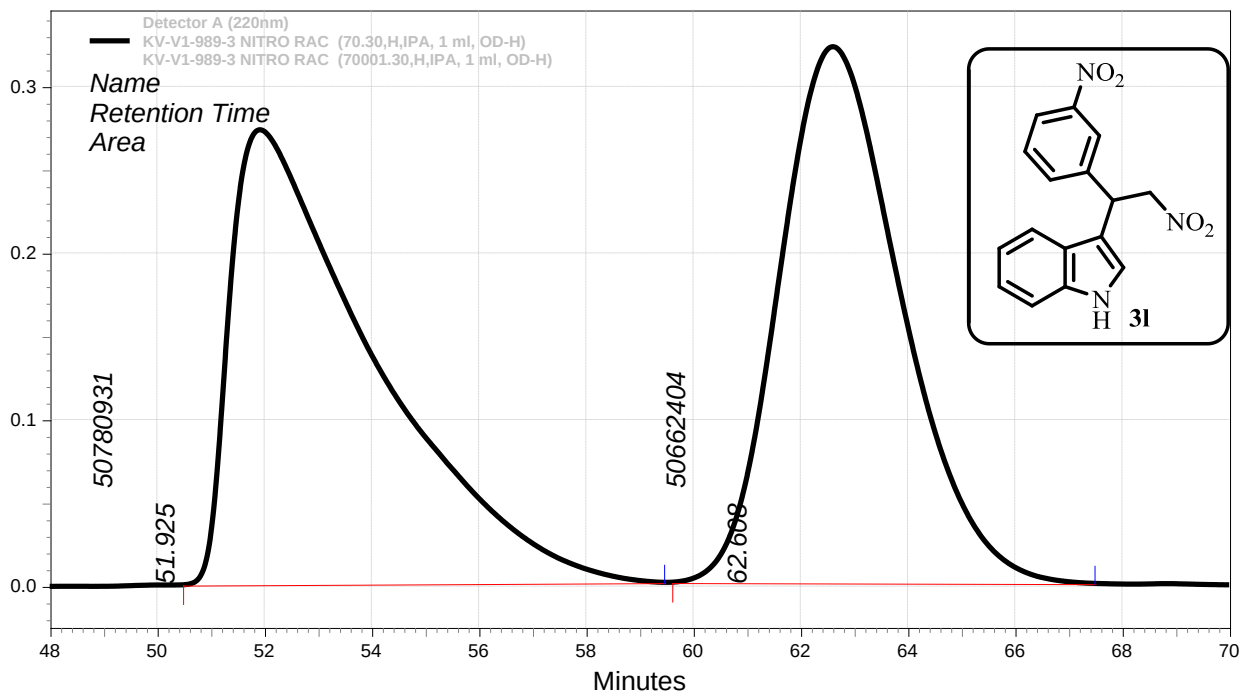
Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.125	12311510	247683		8.49	MM
2		29.350	132618809	1801035		91.51	MM

Totals			144930319	2048718		100.00	
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HPLC chromatogram of 3l

Data Graph



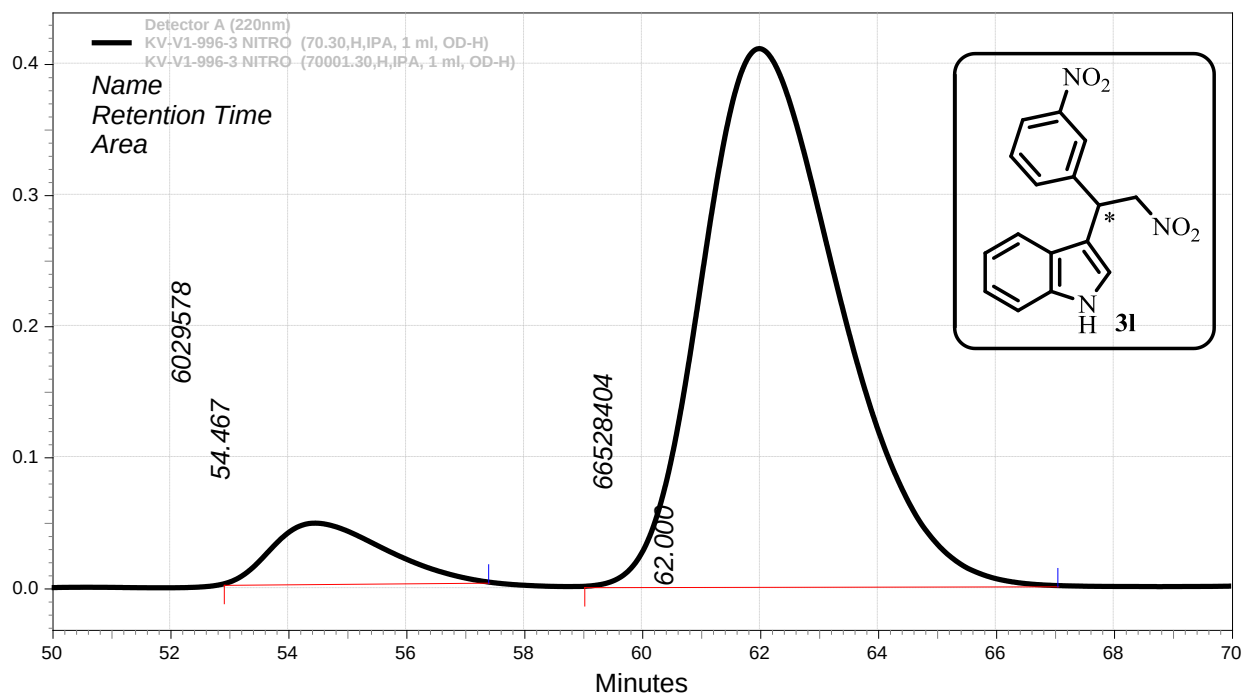
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		51.925	50780931	272925		50.06	MM
2		62.608	50662404	321747		49.94	MM

Totals			101443335	594672		100.00	
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Data Graph



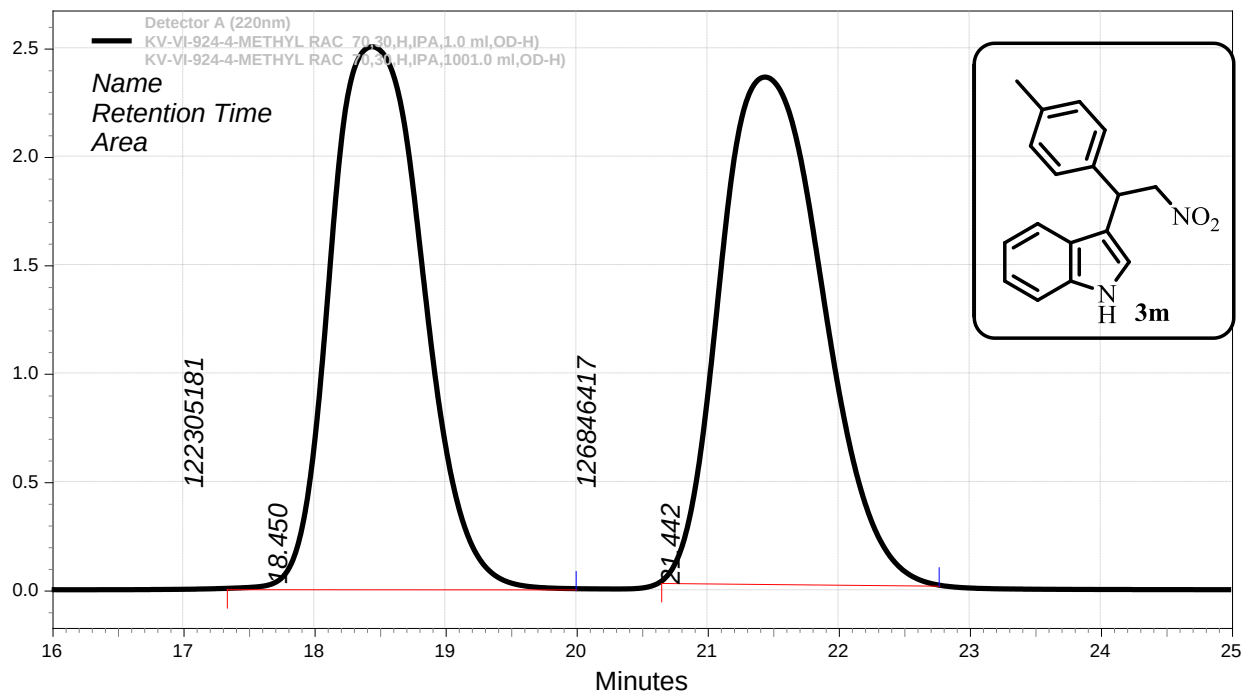
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		54.467	6029578	45836		8.31	MM
2		62.000	66528404	409924		91.69	MM
Totals			72557982	455760		100.00	

HPLC chromatogram of 3m

Data Graph



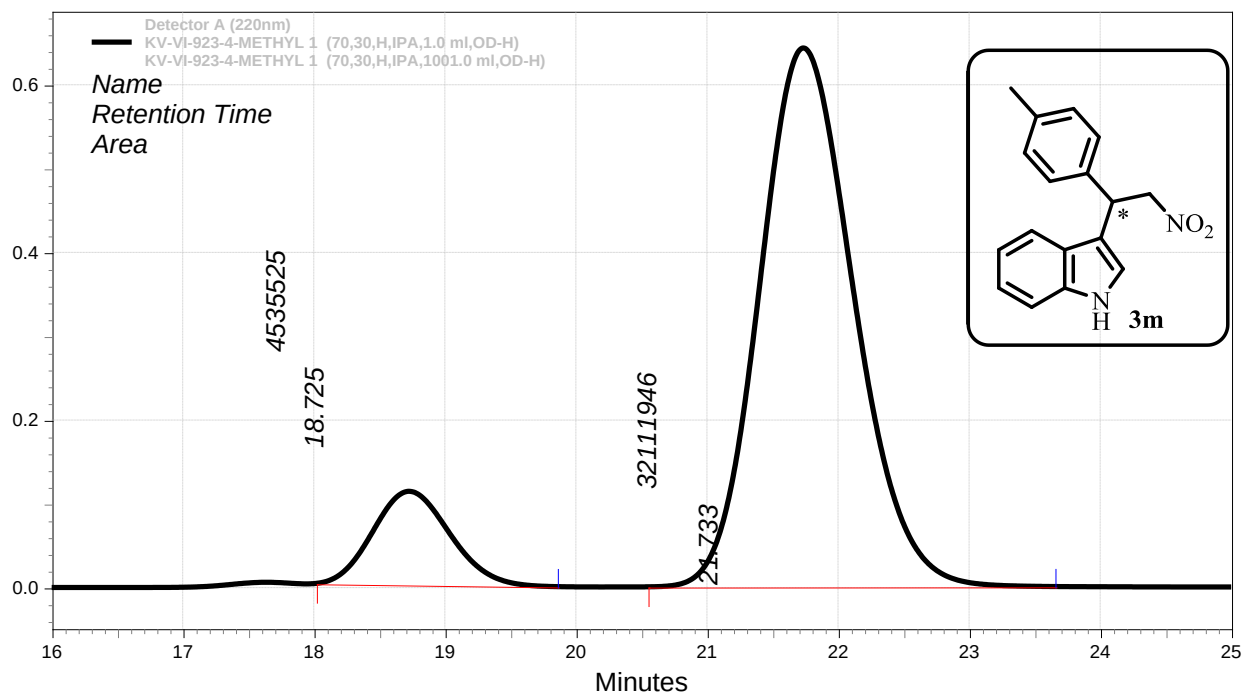
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		18.450	122305181	2498915		49.09	MM
2		21.442	126846417	2334296		50.91	MM

Totals			249151598	4833211		100.00	
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Data Graph



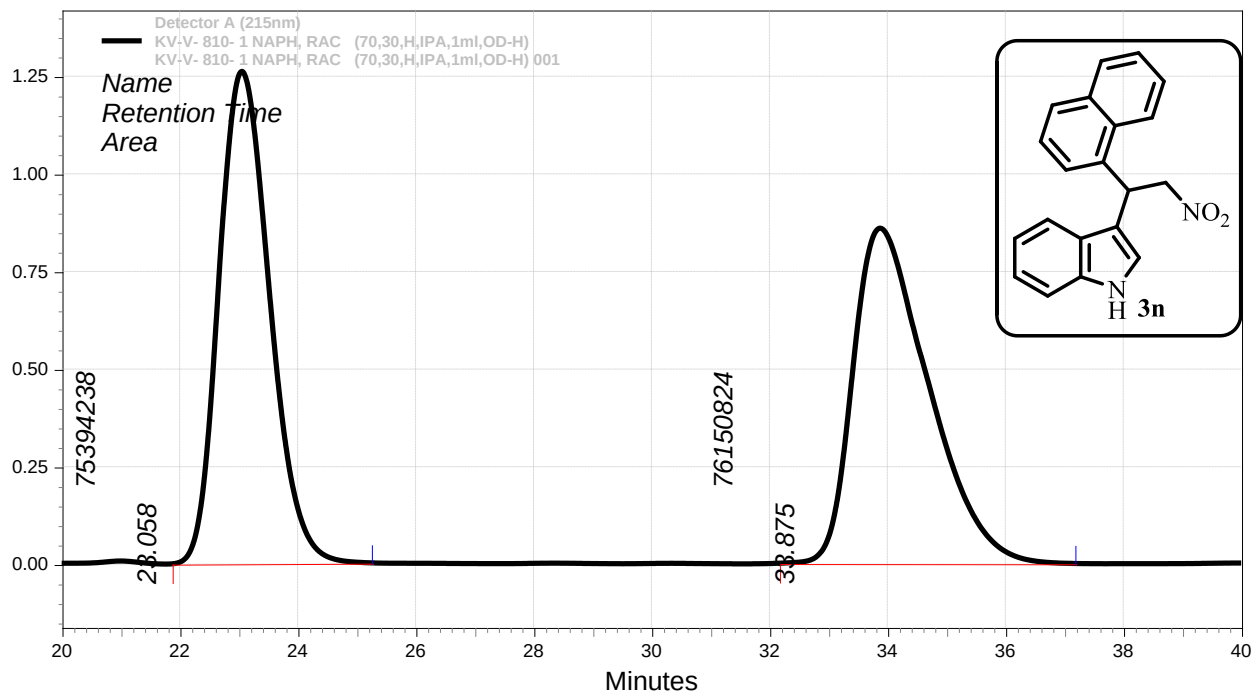
Run Report

Detector A (220nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		18.725	4535525	111354		12.38	MM
2		21.733	32111946	642779		87.62	MM
Totals			36647471	754133		100.00	

HPLC chromatogram of 3n

Data Graph



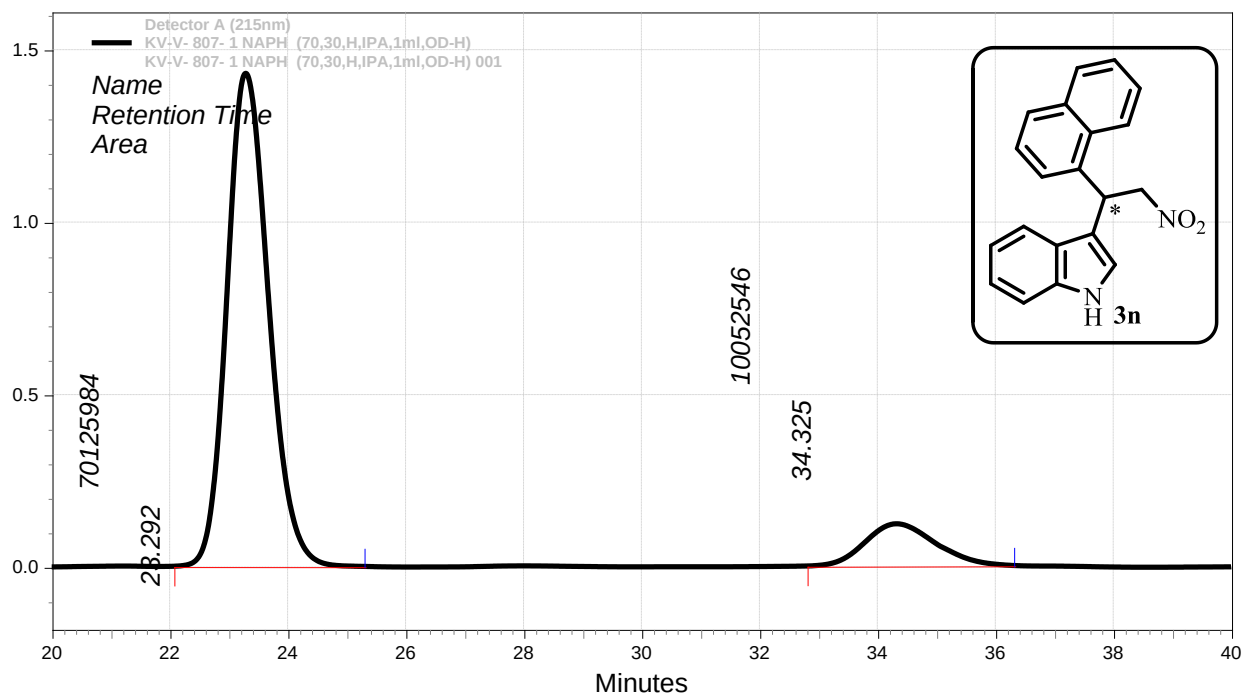
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.058	75394238	1260431		49.75	MM
2		33.875	76150824	858235		50.25	MM

Totals			151545062	2118666		100.00	
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Data Graph



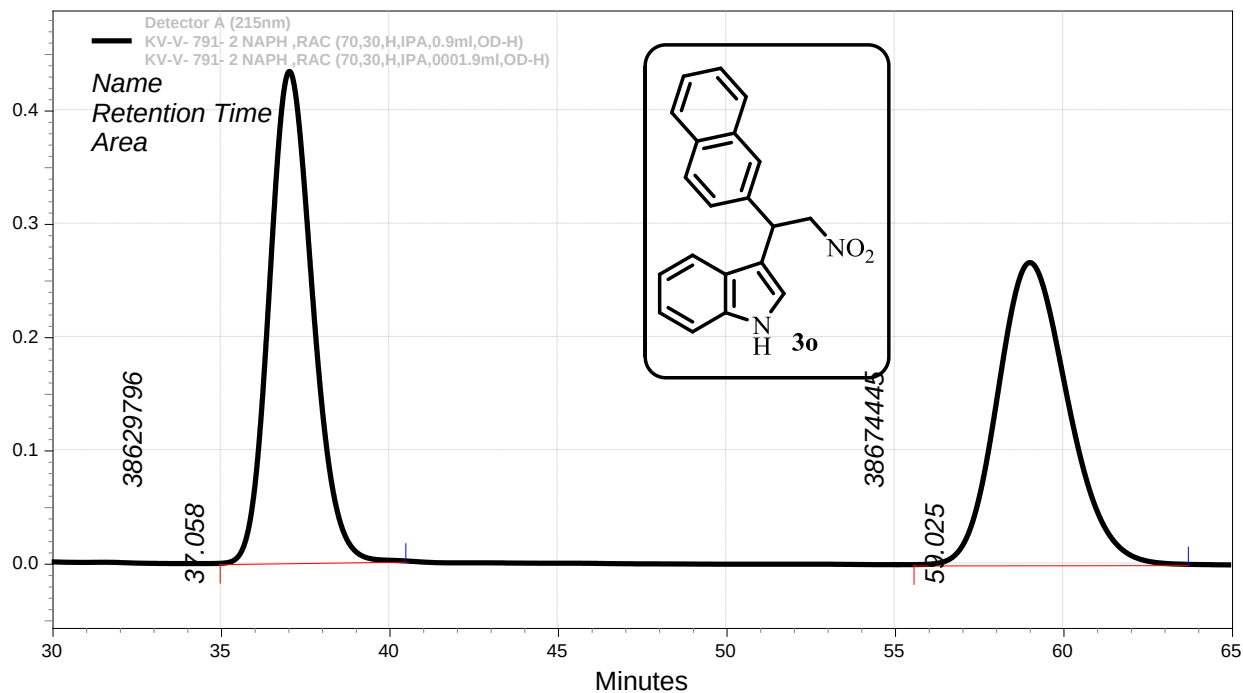
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		23.292	70125984	1429080		87.46	MM
2		34.325	10052546	121711		12.54	MM
Totals			80178530	1550791		100.00	

HPLC chromatogram of 3o

Data Graph



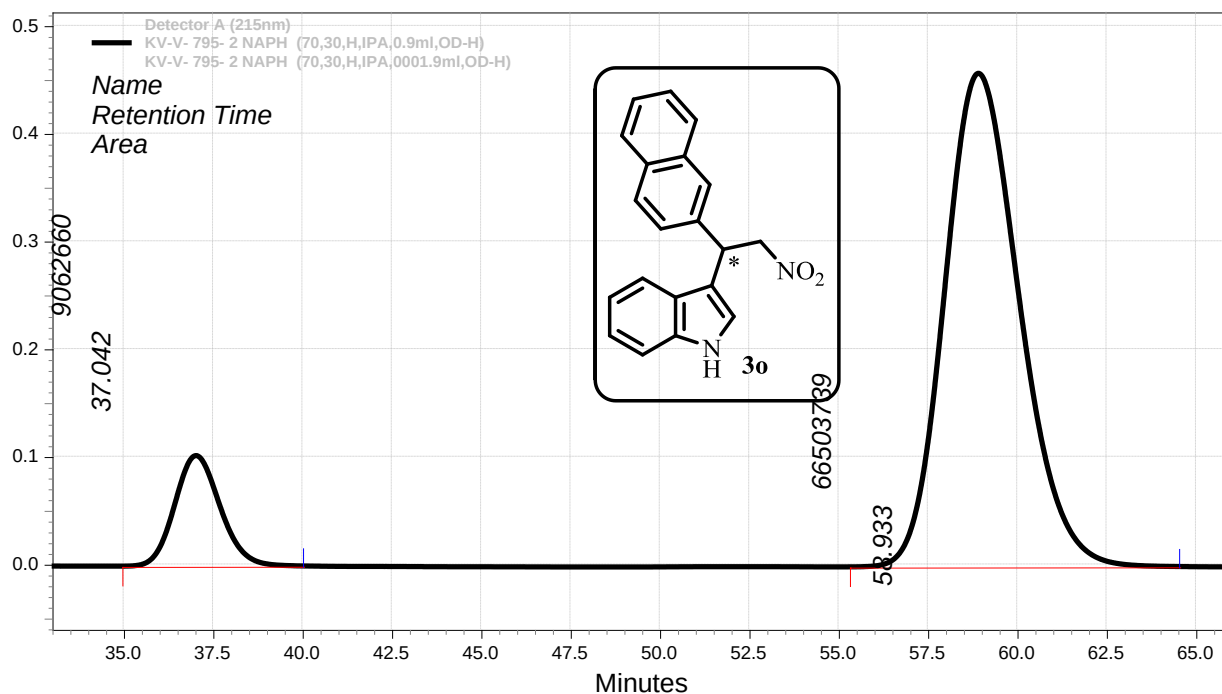
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		37.058	38629796	433422		49.97	MM
2		59.025	38674445	266509		50.03	MM

Totals			77304241	699931		100.00	
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Data Graph

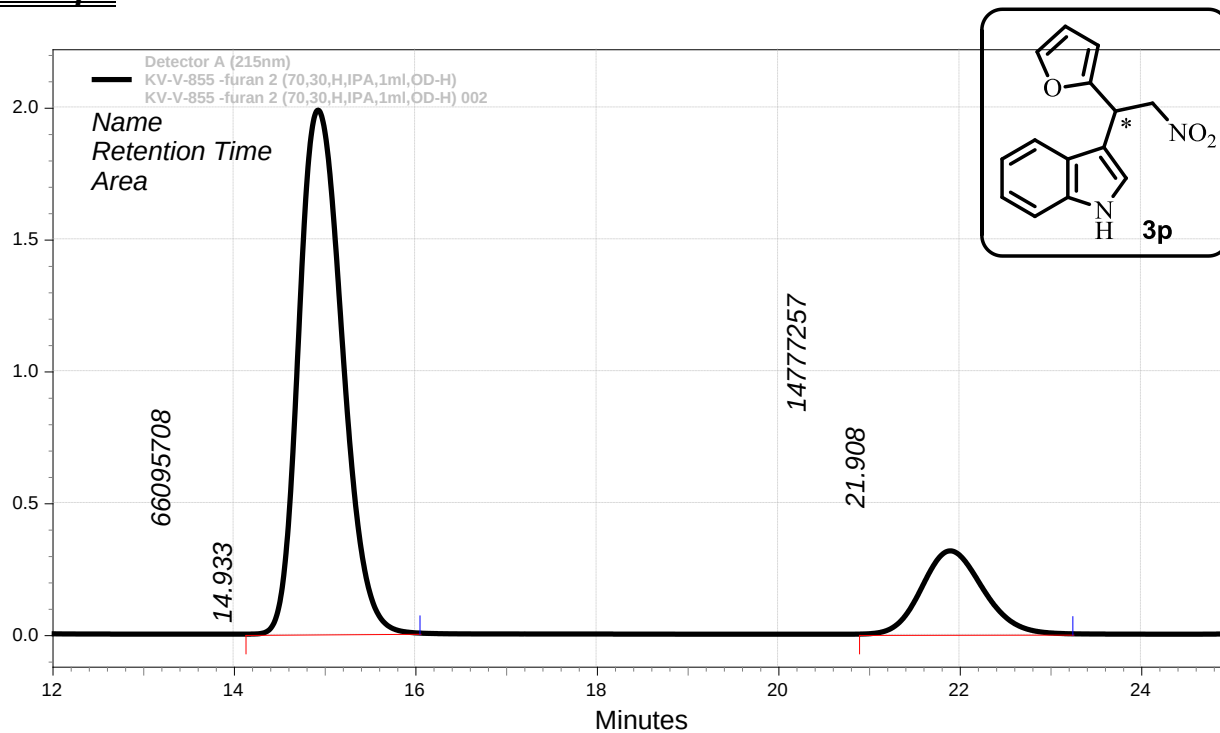


Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		37.042	9062660	102566		11.99	MM
2		58.933	66503739	458084		88.01	MM
Totals			75566399	560650		100.00	

Data Graph



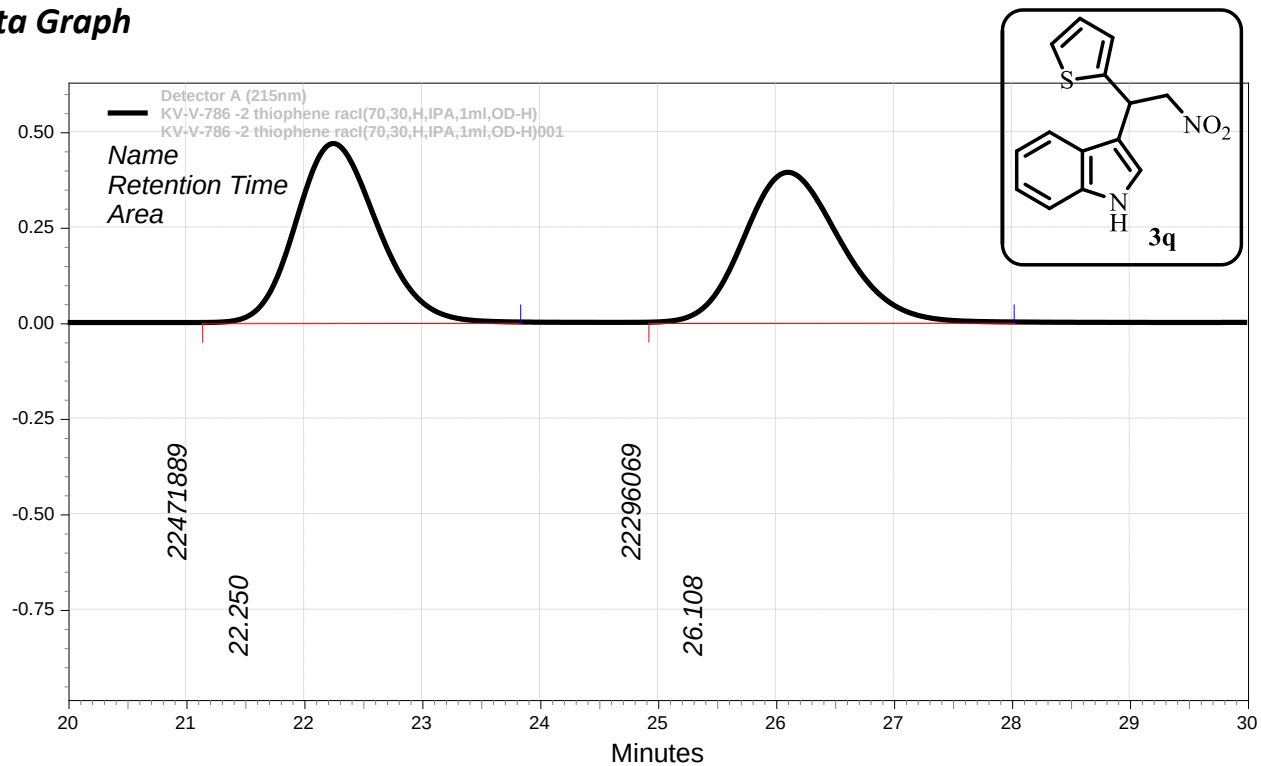
Run Report

Detector A (215nm)

<u>Pk #</u>	<u>Name</u>	<u>Retention Time</u>	<u>Area</u>	<u>Height</u>	<u>Units</u>	<u>Area Percent</u>	<u>Integration Codes</u>
<u>1</u>		<u>14.933</u>	<u>66095708</u>	<u>1984981</u>		<u>81.73</u>	<u>MM</u>
<u>2</u>		<u>21.908</u>	<u>14777257</u>	<u>315032</u>		<u>18.27</u>	<u>MM</u>
<u>Totals</u>			<u>80872965</u>	<u>2300013</u>		<u>100.00</u>	

HPLC chromatogram of 3q

Data Graph



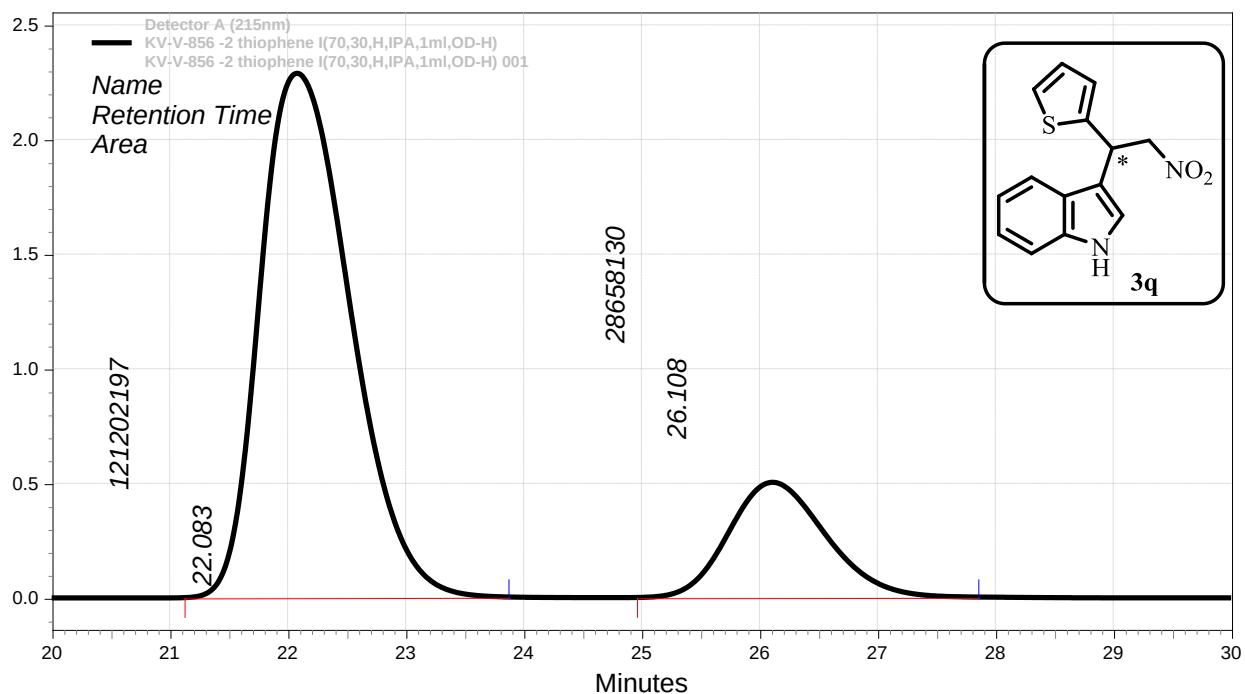
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		22.250	22471889	467786		50.20	MM
2		26.108	22296069	392018		49.80	MM

Totals			44767958	859804		100.00	
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Data Graph



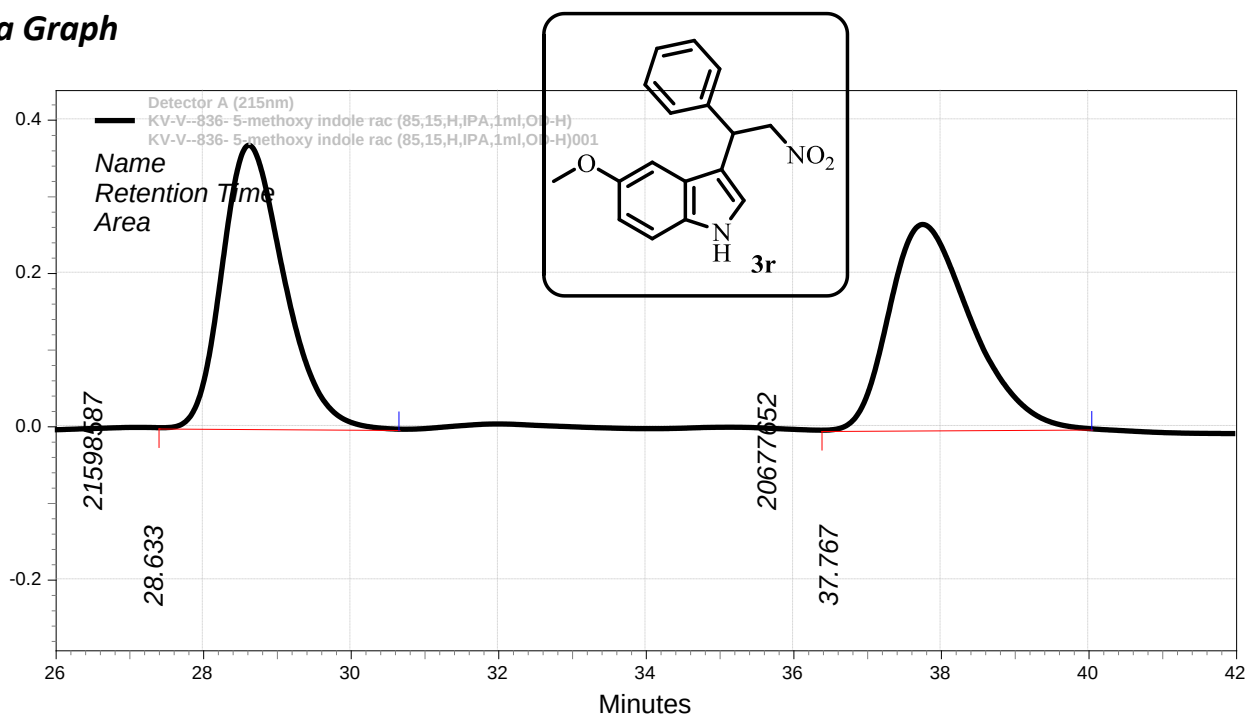
Run Report

Detector A (215nm)

<u>Pk #</u>	<u>Name</u>	<u>Retention Time</u>	<u>Area</u>	<u>Height</u>	<u>Units</u>	<u>Area Percent</u>	<u>Integration Codes</u>
<u>1</u>		<u>22.083</u>	<u>121202197</u>	<u>2285854</u>		<u>80.88</u>	<u>MM</u>
<u>2</u>		<u>26.108</u>	<u>28658130</u>	<u>501563</u>		<u>19.12</u>	<u>MM</u>
<u>Totals</u>			<u>149860327</u>	<u>2787417</u>		<u>100.00</u>	

HPLC chromatogram of 3r

Data Graph

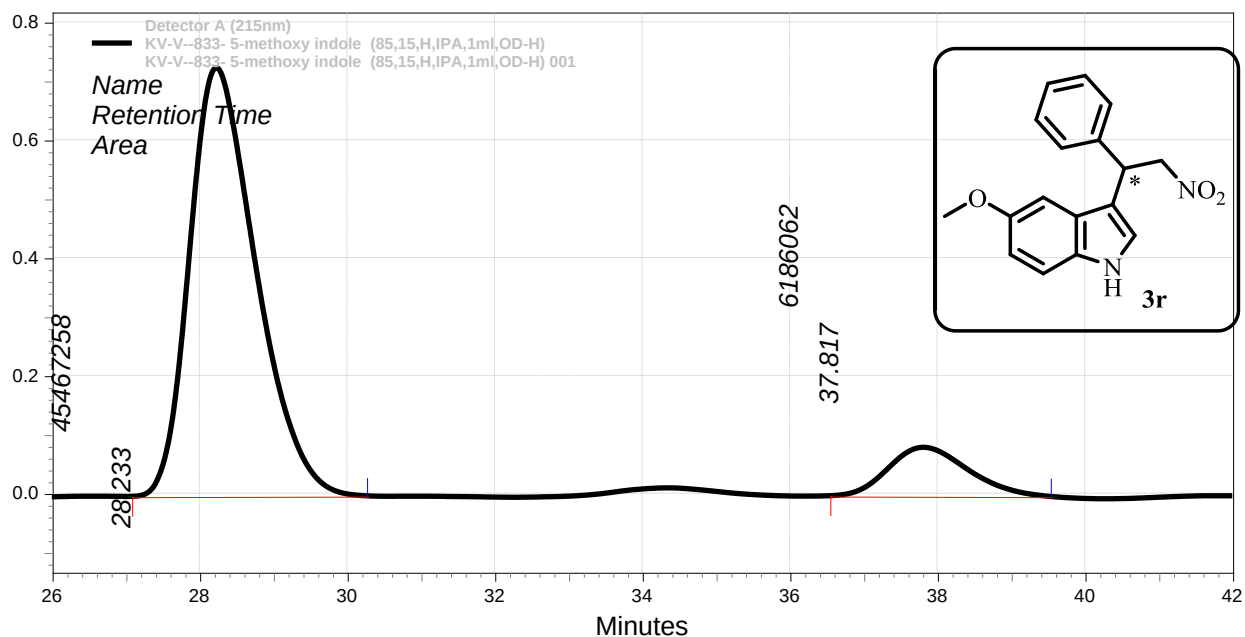


Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		28.633	21598587	369081		51.09	MM
2		37.767	20677652	267605		48.91	MM
Totals			42276239	636686		100.00	

Data Graph



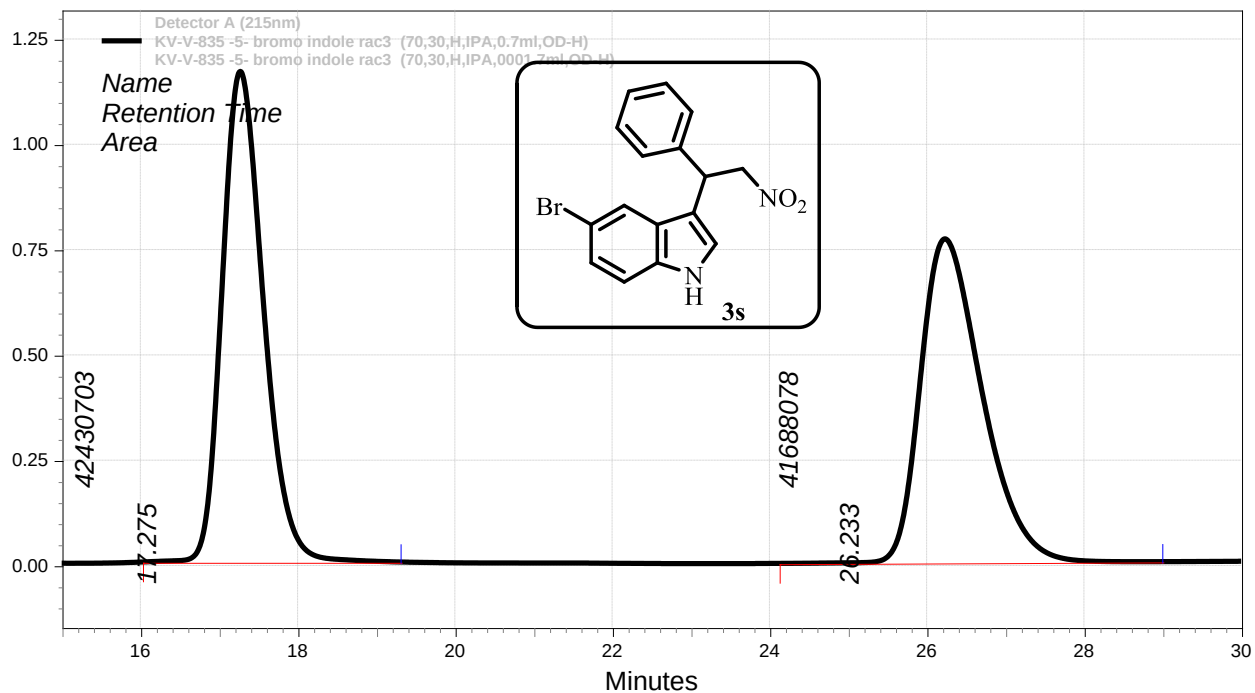
Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		28.233	45467258	727072		88.02	MM
2		37.817	6186062	82632		11.98	MM
Totals			51653320	809704		100.00	

HPLC chromatogram of 3s

Data Graph



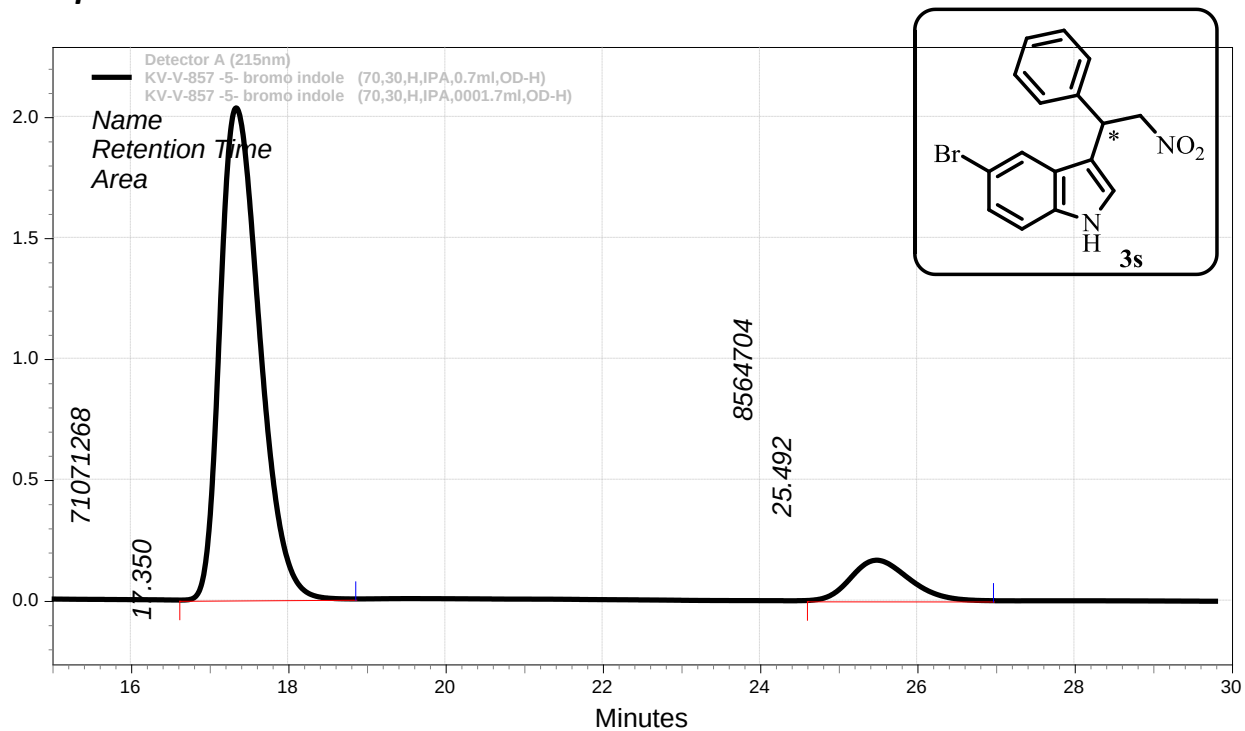
Run Report

Detector A (215nm)

PK #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.275	42430703	1164735		50.44	MM
2		26.233	41688078	768726		49.56	MM

Totals			84118781	1933461		100.00	
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Data Graph



Run Report

Detector A (215nm)

Pk #	Name	Retention Time	Area	Height	Units	Area Percent	Integration Codes
1		17.350	71071268	2033264		89.25	MM
2		25.492	8564704	166981		10.75	MM
Totals			79635972	2200245		100.00	

Comparison of observed and reported optical rotations for 3a-3s

S. No	Compound	Reported $[\alpha]_D^{20}$	Observed $[\alpha]_D^{20}$	Reported		Observed	
				Retention time t_R	ee (%)	Retention time t_R	ee (%)
1	3a^a	$[\alpha]_D^{20} = -23.9$	$[\alpha]_D^{28} = -15.0$	$t_{\text{minor}} = 19.2$ min $t_{\text{major}} = 23.7$ min 1.0 ml/min	96%ee	$t_{\text{minor}} = 24.6$ min $t_{\text{major}} = 28.0$ min, 0.9 ml/min	80%ee
2	3b^a	$[\alpha]_D^{20} = -47.8$	$[\alpha]_D^{26} = -28.6$	$t_{\text{major}} = 16.1$ min $t_{\text{minor}} = 18.0$ min, 0.8 ml/min	95%ee	$t_{\text{major}} = 13.4$ min $t_{\text{minor}} = 16.5$ min, 0.9 ml/min	81%ee
3	3c^a	$[\alpha]_D^{20} = -16.4$	$[\alpha]_D^{32} = -10.0$	$t_{\text{minor}} = 49.5$ min, $t_{\text{major}} = 70.6$ min, 0.5 ml/min	97%ee	$t_{\text{minor}} = 23.5$ min, $t_{\text{major}} = 31.7$ min, 1.0 ml/min	84%ee
4	3d^a	$[\alpha]_D^{20} = -28.2$	$[\alpha]_D^{26} = -11.2$	$t_{\text{minor}} = 31.0$ min $t_{\text{major}} = 35.7$ min, 0.8 ml/min	95%ee	$t_{\text{minor}} = 25.4$ min $t_{\text{major}} = 28.4$ min, 1.0 ml/min	70%ee
5	3e^a		$[\alpha]_D^{28} = -79.9$			$t_{\text{major}} = 17.3$ min, $t_{\text{minor}} = 26.1$ min	91%ee
6	3f^a	$[\alpha]_D^{20} = -16.0$	$[\alpha]_D^{30} = -13.1$	$t_{\text{minor}} = 21.4$ min $t_{\text{major}} = 30.3$ min, 1.0 ml/min	95%ee	$t_{\text{minor}} = 25.5$ min $t_{\text{major}} = 36.3$ min, 1.0 ml/min	83%ee
7	3g^a	$[\alpha]_D^{20} = +1.8$	$[\alpha]_D^{25} = +0.9$	$t_{\text{minor}} = 23.3$ min $t_{\text{major}} = 30.5$ min, 1.0 ml/min	95%ee	$t_{\text{minor}} = 28.0$ min $t_{\text{major}} = 34.6$ min, 1.0 ml/min	84%ee
8	3h^a	$[\alpha]_D^{20} = -50.0$	$[\alpha]_D^{25} = -58.4$	$t_{\text{major}} = 14.3$ min $t_{\text{minor}} = 22.7$ min, 1.0 ml/min	72%ee	$t_{\text{major}} = 17.5$ min $t_{\text{minor}} = 27.6$ min, 1.0 ml/min	90%ee
9	3i^b	$[\alpha]_D^{20} = -18.1$	$[\alpha]_D^{31} = -14.2$	$t_{\text{minor}} = 21.7$ min $t_{\text{major}} = 19.6$ min, 1.0 ml/min	92%ee	$t_{\text{minor}} = 24.1$ min, $t_{\text{major}} = 32.4$ min, 1.0 ml/min	81%ee
10	3j^a	$[\alpha]_D^{20} = -7.1$	$[\alpha]_D^{30} = -5.4$	$t_{\text{minor}} = 22.2$ min $t_{\text{major}} = 28.5$ min, 1.0 ml/min	95%ee	$t_{\text{minor}} = 26.0$ min $t_{\text{major}} = 31.2$ min 1.0 ml/min	83%ee
11	3k^a	$[\alpha]_D^{20} = -35.0$	$[\alpha]_D^{30} = -19.3$	$t_{\text{minor}} = 19.5$ min, $t_{\text{major}} = 25.1$ min,	95%ee	$t_{\text{minor}} = 23.1$ min, $t_{\text{major}} = 29.7$ min,	83%ee

				1.0 ml/min		1.0 ml/min	
12	3l^a	$[\alpha]_D^{20} = -14.8$	$[\alpha]_D^{30} = -8.3$	$t_{\text{minor}} = 36.3 \text{ min},$ $t_{\text{major}} = 50.1 \text{ min}$	94%ee	$t_{\text{minor}} = 54.5 \text{ min},$ $t_{\text{major}} = 62.0 \text{ min},$ 1.0 ml/min	83%ee
13	3m^a	$[\alpha]_D^{20} = -13.3$	$[\alpha]_D^{26} = -8.0$	$t_{\text{minor}} = 15.6 \text{ min},$ $t_{\text{major}} = 18.8 \text{ min}$	93%ee	$t_{\text{minor}} = 18.7 \text{ min},$ $t_{\text{major}} = 21.7 \text{ min},$ 1.0 ml/min	85%ee
14	3n^a	$[\alpha]_D^{20} = -25.8$	$[\alpha]_D^{25} = -13.7$	$t_{\text{major}} = 31.1 \text{ min}$ $t_{\text{minor}} = 39.7 \text{ min},$ 0.8 ml/min	94%ee	$t_{\text{major}} = 23.2 \text{ min}$ $t_{\text{minor}} = 34.3 \text{ min},$ 1.0 ml/min	75%ee
15	3o^a	$[\alpha]_D^{20} = -3.5$	$[\alpha]_D^{30} = -2.1$	$t_{\text{minor}} = 48.8 \text{ min}$ $t_{\text{major}} = 61.3 \text{ min},$ 0.8 ml/min	95%ee	$t_{\text{minor}} = 37.0 \text{ min}$ $t_{\text{major}} = 58.9 \text{ min},$ 0.9 ml/min	76%ee
16	3p^a	$[\alpha]_D^{20} = +38.2$	$[\alpha]_D^{32} = +10.0$	$t_{\text{major}} = 18.6 \text{ min},$ $t_{\text{minor}} = 26.1 \text{ min},$ 0.8 ml/min	95%ee	$t_{\text{major}} = 14.9 \text{ min},$ $t_{\text{minor}} = 21.9 \text{ min},$ 1.0 ml/min	63%ee
17	3q^a	$[\alpha]_D^{30} = -25.3$	$[\alpha]_D^{25} = -32.0$	$t_{\text{major}} = 27.3 \text{ min},$ $t_{\text{minor}} = 31.7 \text{ min},$ 0.8 ml/min	92%ee	$t_{\text{major}} = 22.0 \text{ min},$ $t_{\text{minor}} = 26.1 \text{ min},$ 1.0 ml/min	61%ee
18	3r^a	$[\alpha]_D^{30} = +30.2$	$[\alpha]_D^{30} = +15.7$	$t_{\text{major}} = 16.6 \text{ min}$ $t_{\text{minor}} = 19.6 \text{ min},$ 0.8 ml/min	96%ee	$t_{\text{major}} = 28.2 \text{ min}$ $t_{\text{minor}} = 37.8 \text{ min},$ 1.0 ml/min	76%ee
19	3s^a	$[\alpha]_D^{30} = +41.0$	$[\alpha]_D^{31} = +18.4$	$t_{\text{major}} = 15.7 \text{ min},$ $t_{\text{minor}} = 20.4 \text{ min},$ 0.8 ml/min	93%ee	$t_{\text{major}} = 17.3 \text{ min},$ $t_{\text{minor}} = 25.4 \text{ min},$ 0.7 ml/min	78%ee
^a HPLC (Daicel Chiralcel OD-H, hexane/2-propanol = 70:30, ^b HPLC (Daicel Chiralpak AD-H, hexane/2-propanol = 90:10							

Optimized coordinates and Energies of **CRCB TETHERED BIPYRIDINE-Zn- β -NITROSTYRENE COMPLEX I** are given below (in Hartrees):

Sum of electronic and zero-point Energies	=	-2842.571443
Sum of electronic and thermal Energies	=	-2842.515336
Sum of electronic and thermal Enthalpies	=	-2842.514391
Sum of electronic and thermal Free Energies	=	-2842.671105

C	-0.67822200	-3.72332000	-0.57301400
C	-2.66316100	-2.49196900	-0.15419200
C	-3.44265400	-3.61333000	-0.43264900
C	-2.81453800	-4.81068700	-0.80748200
C	-1.43380000	-4.86999400	-0.87565900
H	-4.52190300	-3.55352900	-0.37591000
H	-3.41031800	-5.68670700	-1.04449500
H	-0.94354800	-5.78857100	-1.17359400
N	-1.31152700	-2.55200800	-0.24321100
C	-5.06319200	-0.99897400	-1.51406700
C	-3.77837800	-0.34902700	-1.04987700
C	-5.62944800	-0.35252000	0.76932300
C	-6.08217800	-0.96569700	-0.54489000
C	-4.11089700	1.04445900	-0.53562500
C	-5.08396800	1.03279800	0.47776000
H	-6.41074400	-0.34357500	1.53031100
H	-3.00916800	-0.32924000	-1.82665500
C	-4.41239700	-1.21265800	1.26781100
H	-4.75800600	-2.24698900	1.37777900
C	-3.25312600	-1.14568400	0.21843300
H	-2.44812400	-0.54643800	0.64665500
C	-4.00380100	-0.77813800	2.67615700
O	-4.78118900	-0.33749800	3.49729800
O	-2.69170500	-0.97330400	2.90133000
C	-2.15128900	-0.50799300	4.16461700
H	-1.14327300	-0.17264200	3.91290200
H	-2.74664200	0.34308700	4.50164000
C	-2.15075500	-1.62267700	5.19820400
C	-3.48326600	2.23121700	-0.90092400
C	-3.85931200	3.42398000	-0.27191700
C	-4.84322300	3.41770400	0.71872600
C	-5.45520300	2.21920500	1.10440600
H	-2.69071900	2.23042200	-1.64371700
H	-3.36722600	4.35219000	-0.54523600
H	-5.12690600	4.34741800	1.20378400
H	-6.20380800	2.20921500	1.89178500
C	-7.58496400	-2.04531800	-2.09161300
C	-7.34248200	-1.48185700	-0.83244000
C	-5.29631200	-1.59291200	-2.75202300
C	-6.55841900	-2.13013200	-3.03360600
H	-8.56943000	-2.44072500	-2.32512900
H	-8.13354900	-1.43977700	-0.08790800

H	-4.50484100	-1.63352500	-3.49632200
H	-6.74736700	-2.58545300	-4.00165700
H	-3.17299600	-1.92847900	5.43687800
H	-1.59684000	-2.49421100	4.83603500
H	-1.67414200	-1.27345500	6.12032100
C	0.78589500	-3.70370400	-0.59299100
C	2.74294700	-2.36438500	-0.50596900
C	3.54880900	-3.49266300	-0.64281300
C	2.94720400	-4.75588100	-0.74963900
C	1.56775400	-4.86448700	-0.72874500
H	4.62691300	-3.39428500	-0.64768400
H	3.56236700	-5.64537900	-0.84390100
H	1.09858900	-5.83801700	-0.79803900
N	1.39289300	-2.48069400	-0.46678800
C	4.99335600	-1.42751000	1.45560700
C	3.71506900	-0.66707200	1.16214100
C	5.67186500	-0.00472500	-0.40899400
C	6.04984900	-1.07591000	0.59594300
C	4.02690500	0.81738800	1.19483400
C	5.09498300	1.17592000	0.35685300
H	6.49802900	0.28271700	-1.06065500
H	2.89940000	-0.93112600	1.84082600
C	4.50310600	-0.60999800	-1.26608900
H	4.88173600	-1.52017900	-1.74568900
C	3.29335100	-0.96246900	-0.33860900
H	2.48344100	-0.26939700	-0.57181900
C	4.14490500	0.32421400	-2.42221800
O	4.92724000	1.09786000	-2.93362500
O	2.87271300	0.15087400	-2.82384200
C	2.37040600	1.03570500	-3.85840900
H	1.31515900	1.16115000	-3.60894800
H	2.88303600	1.99578300	-3.77016800
C	2.57115500	0.42880000	-5.23775700
C	3.33150400	1.78896300	1.90932000
C	3.73265900	3.12570800	1.80883100
C	4.81625900	3.47896900	1.00230200
C	5.49352600	2.50580200	0.25903800
H	2.47412700	1.51086500	2.51620600
H	3.19541000	3.89267300	2.35854300
H	5.12008800	4.51929100	0.93125700
H	6.31237600	2.78365800	-0.39846100
C	7.46926400	-2.68957100	1.69326400
C	7.28231200	-1.71484300	0.70490800
C	5.18328500	-2.39004100	2.44333100
C	6.43097200	-3.01301500	2.56824900
H	8.43260900	-3.18235200	1.78938800
H	8.09600400	-1.45109300	0.03378900
H	4.36954300	-2.65260300	3.11484100
H	6.58683700	-3.75917600	3.34223000
H	3.63602800	0.32634100	-5.46317600
H	2.09853900	-0.55582500	-5.30627200

H	2.12164000	1.07749000	-5.99705100
Zn	0.02241200	-0.95696500	-0.09250900
O	-0.17061600	0.51780800	1.26877800
O	0.19272900	0.87399400	-0.92986000
N	-0.01375500	1.43139200	0.27970600
C	-0.10583900	2.74592100	0.48805900
H	-0.32288600	2.97932100	1.52299900
C	0.05360900	3.70782000	-0.49308600
H	0.31816800	3.36075200	-1.48628200
C	-0.08803300	5.12681000	-0.29891300
C	0.18733600	6.00600500	-1.37863300
C	-0.49504400	5.72849700	0.92189400
C	0.07598300	7.38470100	-1.24628400
H	0.49908600	5.57980000	-2.32927100
C	-0.60110000	7.10821100	1.04847300
H	-0.73794500	5.10325300	1.77624000
C	-0.31713600	7.95388500	-0.03030200
H	0.29876700	8.02320100	-2.09769500
H	-0.91475700	7.53205900	1.99951400
H	-0.40460000	9.03118300	0.07417300