

Supplementary Material

O-Benzyl-N-(9'-acridinyl)hydroxylamines

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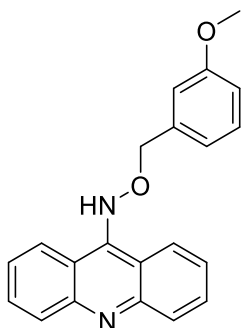
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General Procedures

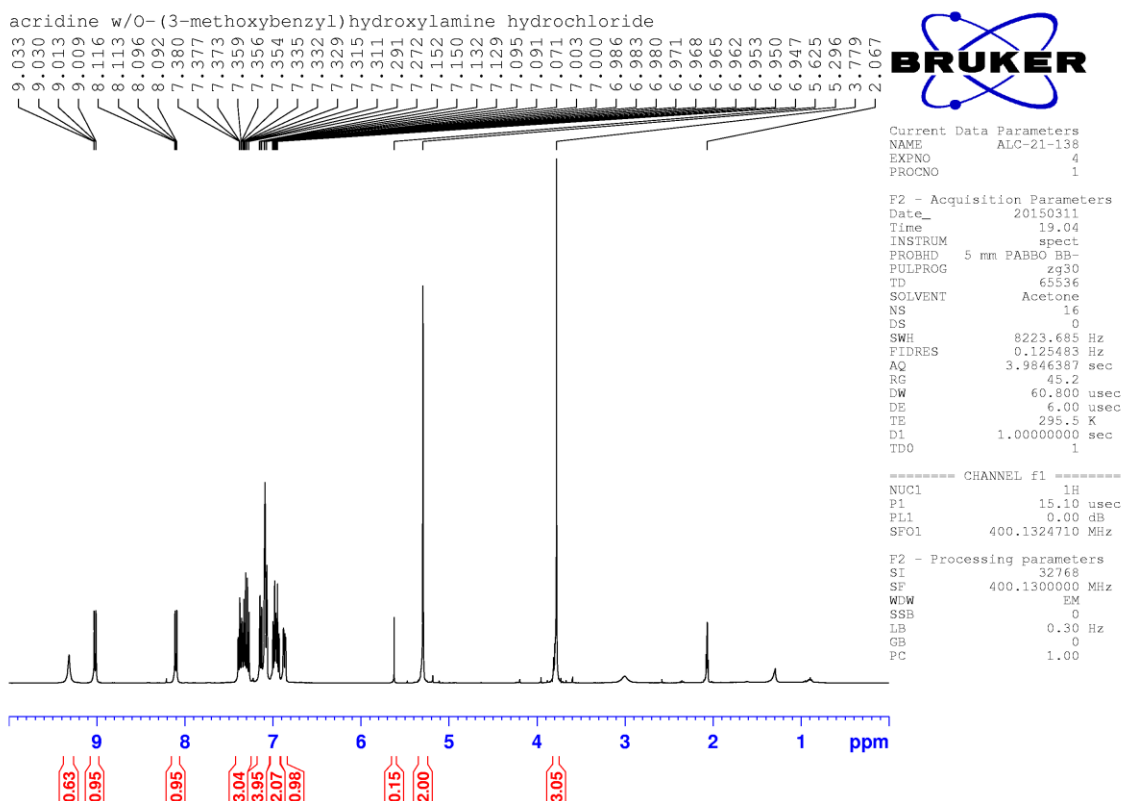
Benzyl chloride, substituted benzyl chlorides, N-hydroxyphthalimide, 9-chloroacridine (**5**) and other reagents were obtained commercially from Sigma Aldrich, and were used after a determination of purity via ^1H NMR spectroscopy. Compounds **3** and **4** were prepared using the method of Bonaccorsi and Giorgi (ref. 9). All solvents used were dried prior to use and their purity verified via spectroscopic methods. Hydrogen chloride gas was generated as needed through the addition of concentrated sulfuric acid to sodium chloride. Radial chromatography was performed using a Harrison Associates Chromatotron[®] on 2mm-thick silica gel plates containing fluorescent indicator that were pre-cleaned with methanol and stored at elevated temperatures prior to use. NMR spectra were obtained on a Bruker Avance II (400 MHz for ^1H) multinuclear FT-NMR. Infrared spectra were collected using a Thermo Scientific iD₅ ATR ZnSe cell. All UV-visible data were measured using an Agilent UV-visible diode-array spectrophotometer with a Peltier-temperature controller. MTT assay data were collected using published procedures (ref. 15).

General procedure for preparation of O-benzyl-N-(9'-acridinyl)-hydroxylamines (**6a-l**)

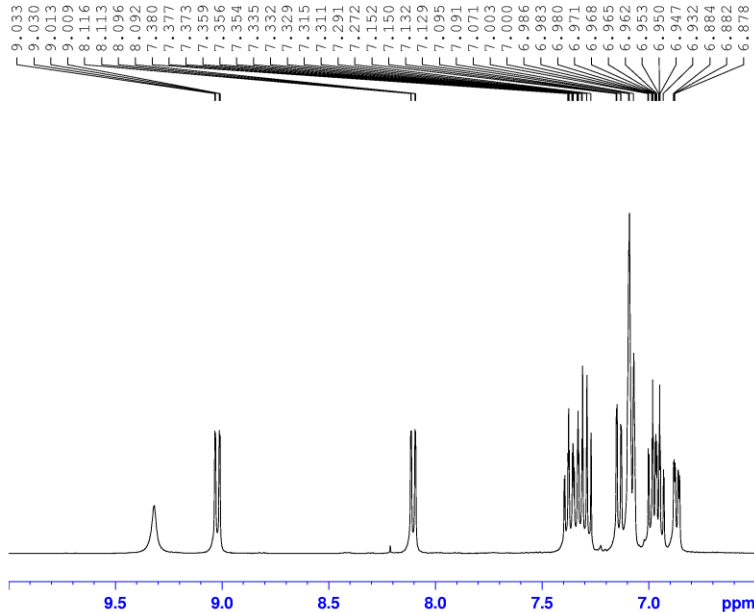
The appropriate salt, **4a-l**, (7.02×10^{-4} mol) was treated with commercially available 9-chloroacridine (**5**) (4.68×10^{-4} mol). The reaction was carried out in molten phenol using 3.0 grams of phenol per gram of 9-chloroacridine (**5**). The reaction was heated between 80-100 °C for a period of 6-8 hours, then cooled to room temperature and dissolved in CH_2Cl_2 . The resulting orange or red organic solution was washed repeatedly with 0.25 M NaOH until greater than a 1:1 molar ratio of hydroxide to phenol was used. The organic phase was then washed with water (once) and brine (once). The organic layer was dried over anhydrous sodium sulfate, gravity filtered, and concentrated to a final volume of approximately 1 mL. This sample was then transferred to the top of a 5-cm column of silica gel constructed from a 10-mL syringe barrel and eluted with ethyl acetate. The orange filtrate was collected, concentrated to a final volume of 0.5-1.0 mL, and subjected to radial chromatography (2mm plate, silica gel, $\text{CH}_2\text{Cl}_2:\text{Et}_2\text{O}$ 100:0 to 90:10 gradient elution). Compounds **6a-l** were obtained in pure form by evaporation of the solvent from the bands that eluted.


O-(3-methoxybenzyl)-N-(9'-acridinyl)-hydroxylamine, 6a

Yield: 64%. ¹HNMR (acetone-d₆) δ, in ppm: 9.32 (s, 1H); 9.03 (d, 1H); 8.10 (d, 1H); 7.34 (m, 3H); 7.13 (m, 4H); 6.97 (m, 2H); 6.88 (m, 1H); 5.30 (s, 2H); 3.78 (s, 3H). ¹³CNMR (acetone-d₆) δ, in ppm: 159.9; 143.5; 140.5; 140.4; 140.3; 138.1; 138.0; 131.9; 130.9; 129.8; 129.3; 124.6; 120.7; 120.0; 119.1; 118.1; 118.1; 115.4; 115.3; 115.0; 115.0; 114.9; 113.4; 113.0; 76.5; 54.5. IR (ATR-ZnSe) in cm⁻¹: 747.39; 964.12; 1157.11; 1265.46; 1474.23; 1598.05; 1614.45. ΔT_m = 9.1°C.



acridine w/O-(3-methoxybenzyl)hydroxylamine hydrochloride



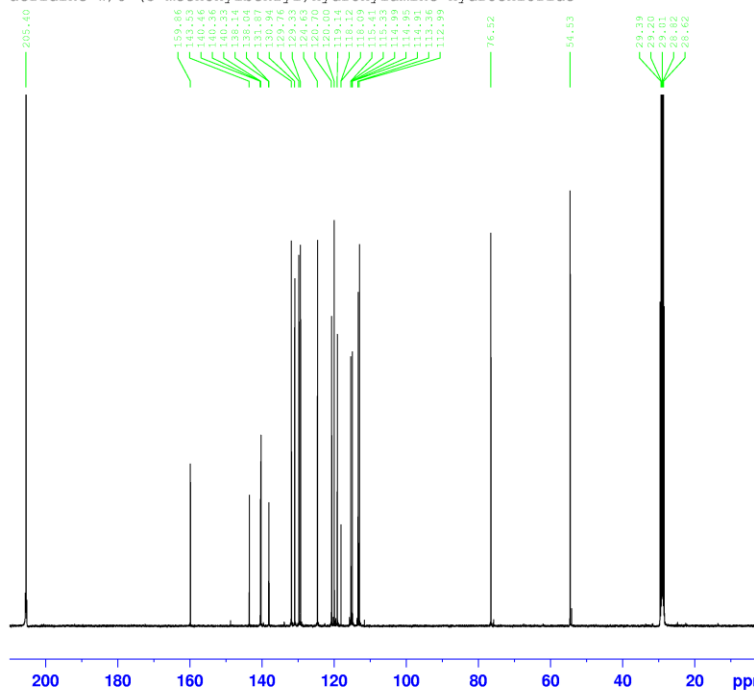
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acridine w/O-(3-methoxybenzyl)hydroxylamine hydrochloride



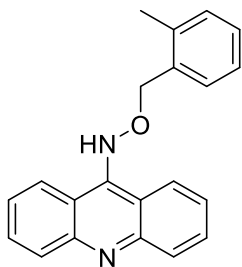
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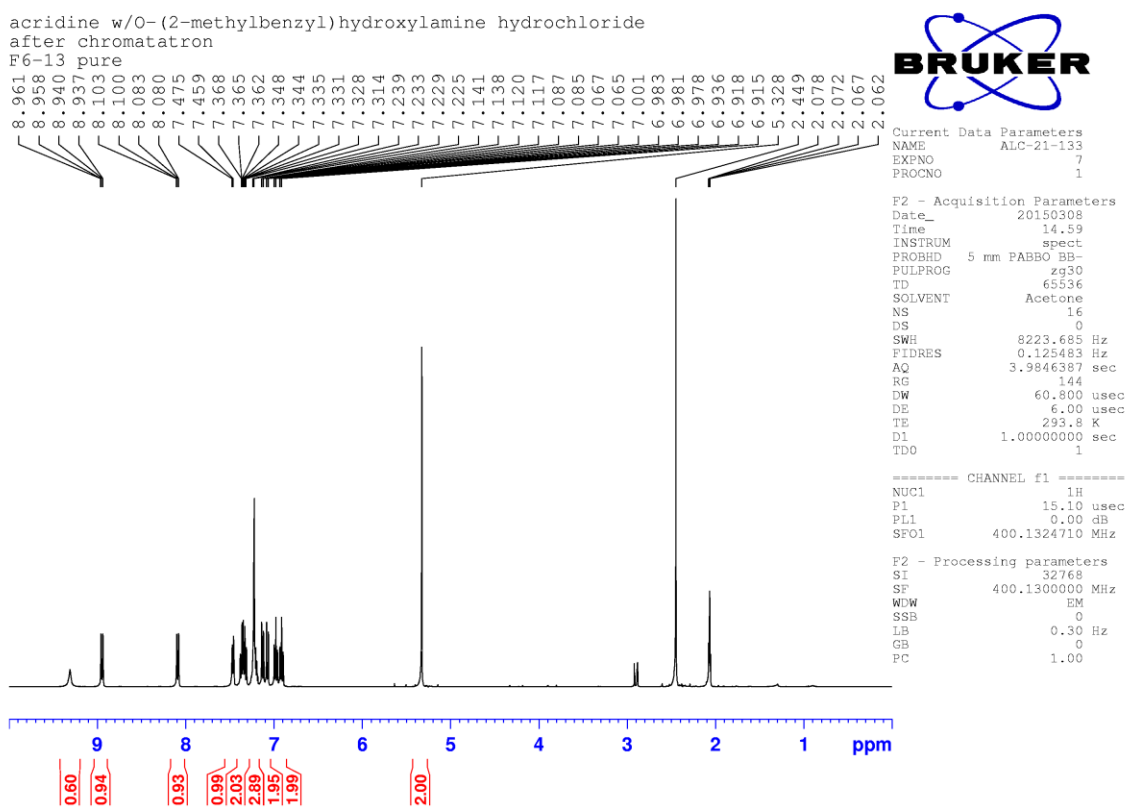
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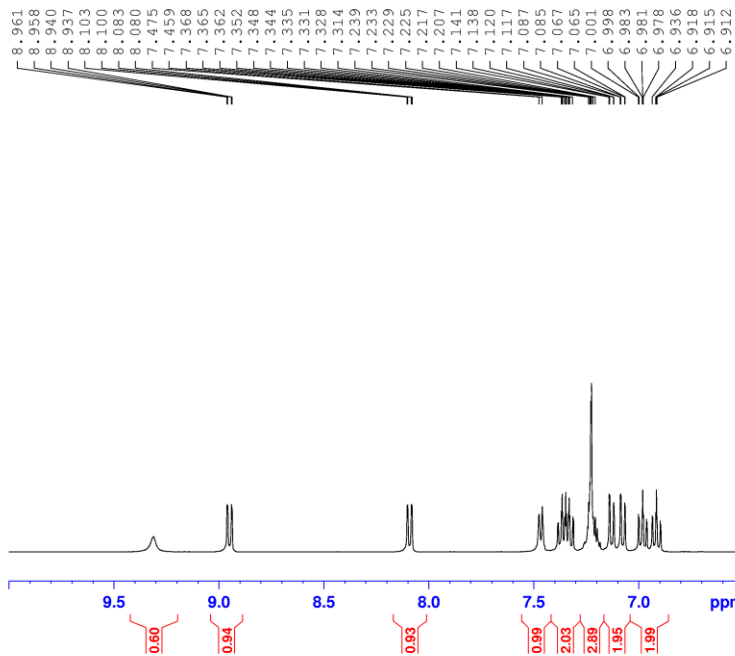


O-(2-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6c

Yield: 49%. ¹HNMR (acetone-d₆) δ, in ppm: 9.31 (s, 1H); 8.95 (m, 1H); 8.09 (d, 1H); 7.47 (d, 1H); 7.34 (m, 2H); 7.23 (m, 3H); 7.12 (m, 2H); 6.98 (m, 2H); 5.33 (s, 2H); 2.45 (s, 3H). ¹³CNMR (acetone-d₆) δ, in ppm: 143.3; 140.4; 140.3; 138.1; 138.0; 136.8; 136.4; 131.7; 130.9; 130.0; 129.7; 129.2; 127.9; 125.7; 124.6; 120.6; 119.1; 118.2; 118.1; 115.4; 115.3; 115.0; 114.9; 114.9; 75.2. IR (ATR-ZnSe) in cm⁻¹: 1473. HRMS: M-1, 315.1496 (C₂₁H₁₉N₂O). ΔT_m = 15.5°C. MTT IC₅₀ = 17.7±0.2μM



acridine w/O-(2-methylbenzyl)hydroxylamine hydrochloride
after chromatatron
F6-13 pure



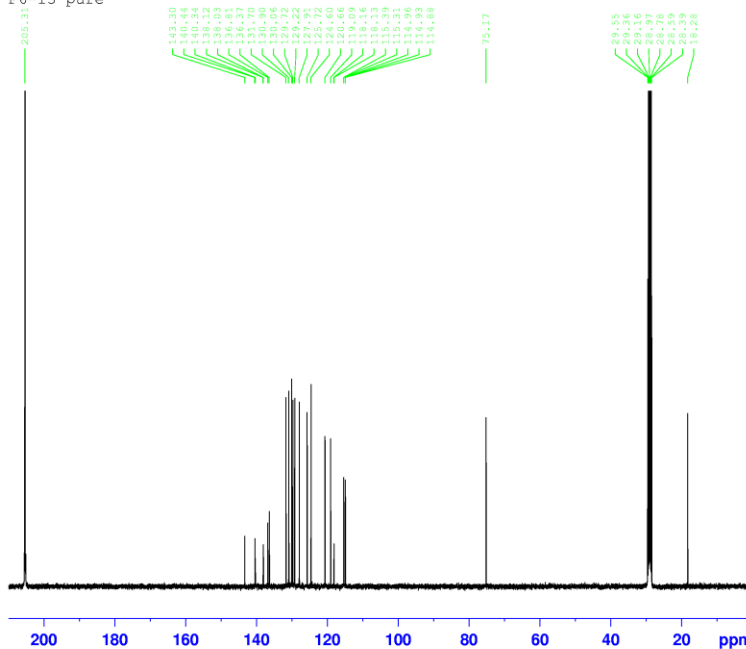
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acridine w/O-(2-methylbenzyl)hydroxylamine hydrochloride
after chromatatron
F6-13 pure



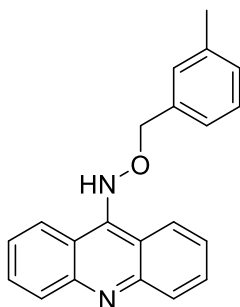
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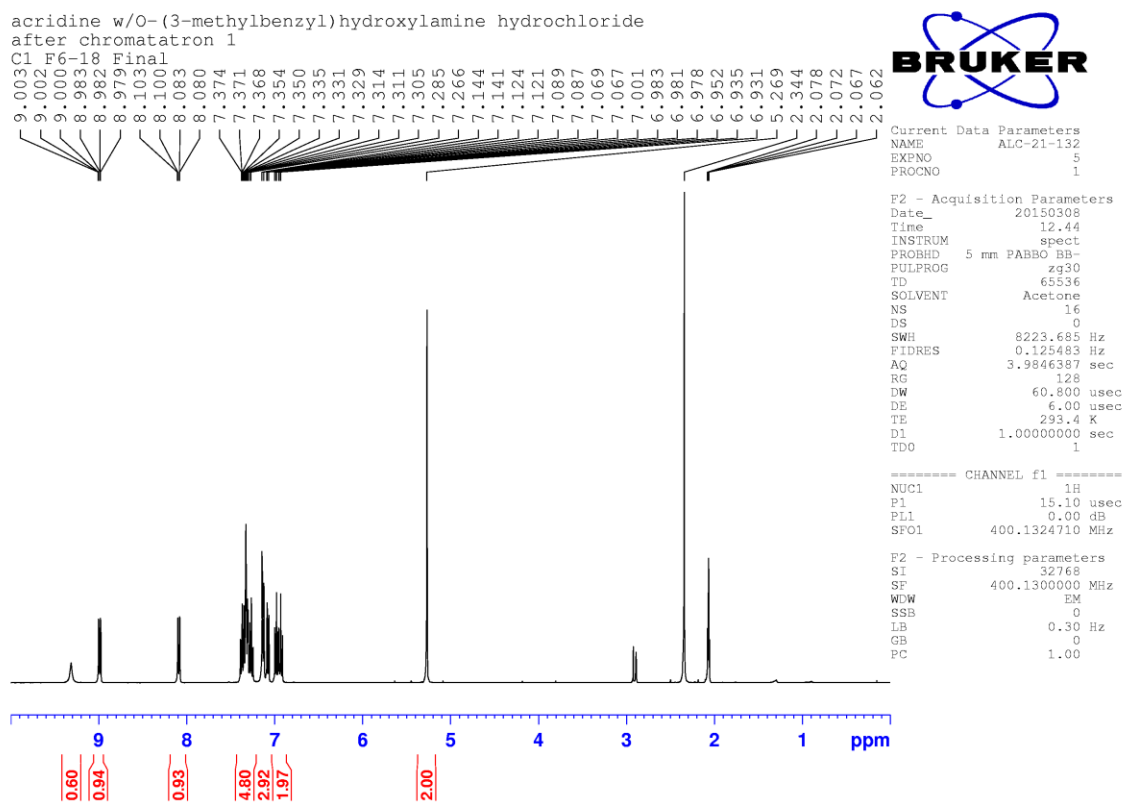
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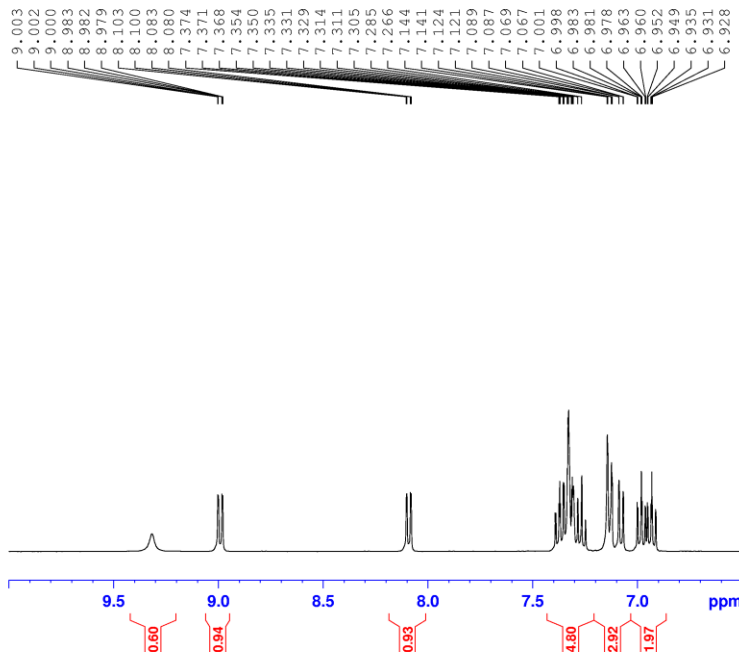


O-(3-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6d

Yield: 71%. ^1H NMR (acetone- d_6) δ , in ppm: 9.31 (s, 1H); 8.99 (d, 1H); 8.09 (d, 1H); 7.33 (m, 5H); 7.10 (m, 3H); 6.98 (m, 2H); 5.27 (s, 2H); 2.34 (s, 3H). ^{13}C NMR (acetone- d_6) δ , in ppm: 143.3; 140.4; 140.4; 138.6; 138.1; 138.0; 137.7; 131.9; 130.9; 129.7; 128.7; 128.3; 128.2; 125.2; 124.6; 120.7; 119.1; 118.2; 118.1; 115.4; 115.3, 114.98, 115.0; 114.9; 76.8. IR (ATR-ZnSe) in cm^{-1} : 745; 770; 964, 1156; 1472; 1486; 1598; 1614. HRMS: M-1, 315.1477 ($\text{C}_{21}\text{H}_{19}\text{N}_2\text{O}$). $\Delta T_m = 19.0^\circ\text{C}$. MTT $\text{IC}_{50} = 20.7 \pm 0.5 \mu\text{M}$



acridine w/O-(3-methylbenzyl)hydroxylamine hydrochloride
after chromatatron 1
C1 F6-18 Final



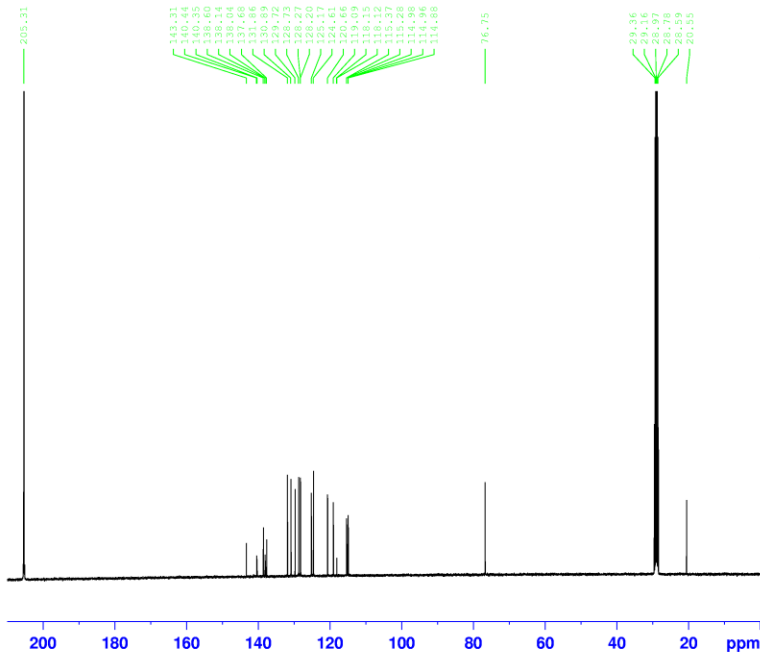
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TE 293.4 K
D1 1.00000000 sec
TD0 1

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acridine w/O-(3-methylbenzyl)hydroxylamine hydrochloride
after chromatatron 1
C1 F6-18 Final



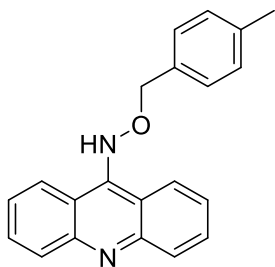
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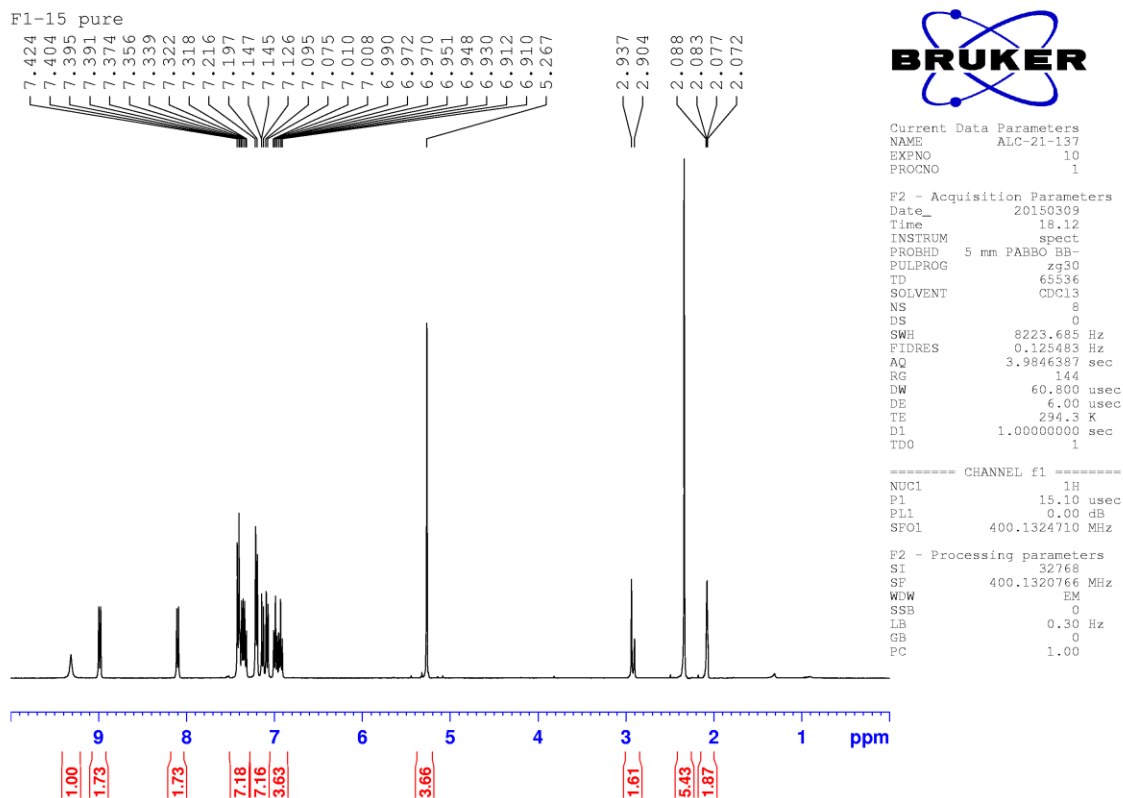
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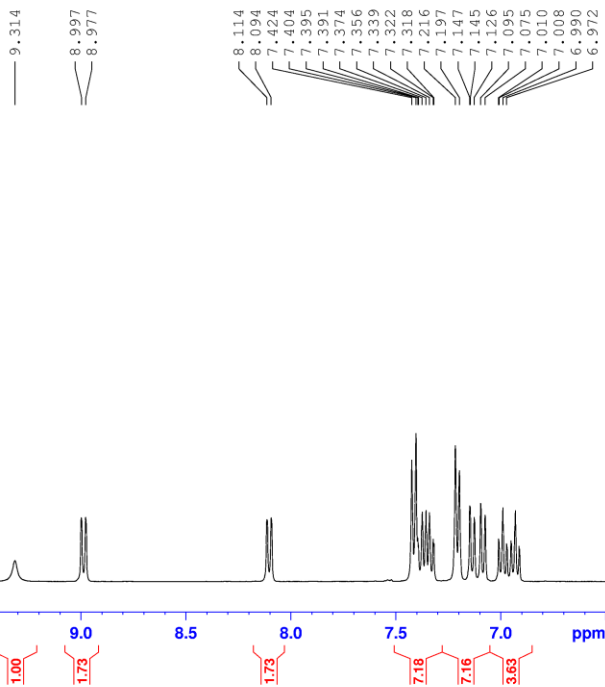


O-(4-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6e

Yield: 40%. ¹HNMR (acetone-d₆) δ, in ppm: 9.31 (s, 1H); 8.98 (m, 1H); 8.11 (m, 1H); 7.37 (m, 4H); 7.14 (m, 4H); 6.96 (m, 2H); 5.27 (s, 2H); 2.33 (s, 3H). ¹³CNMR (acetone-d₆) δ, in ppm: 143.2; 140.4; 138.1; 138.0; 137.1; 135.6; 131.8; 130.9; 129.7; 128.9; 128.2; 124.6; 120.7; 119.1; 119.1; 118.2; 115.4; 115.3; 115.0; 114.9; 76.6. IR (ATR-ZnSe) in cm⁻¹: 746, 965, 1157, 1472. HRMS: M-1, 315.1490 (C₂₁H₁₉N₂O). ΔT_m = 19.0°C. MTT IC₅₀ = 22.2±1.7 μM.



F1-15 pure



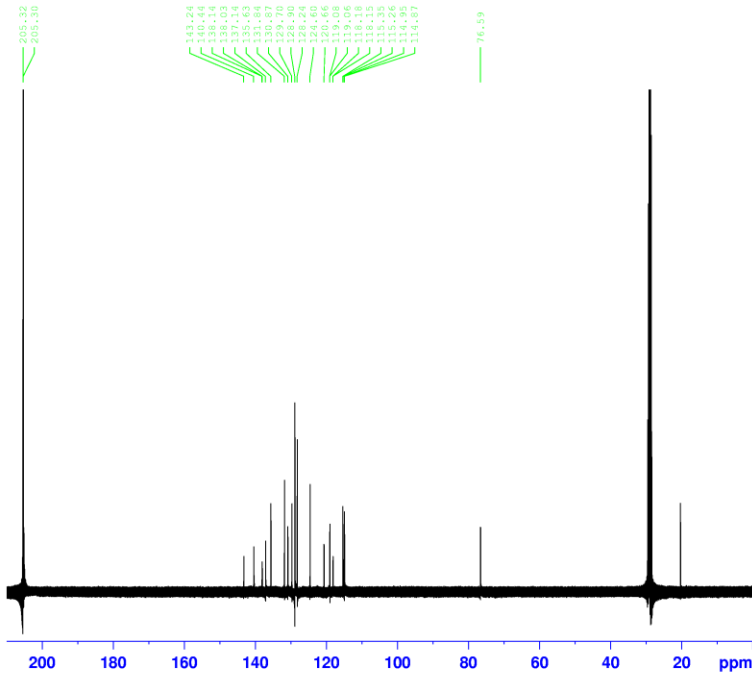
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 TDO 1

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F1-15 pure



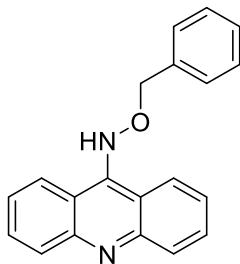
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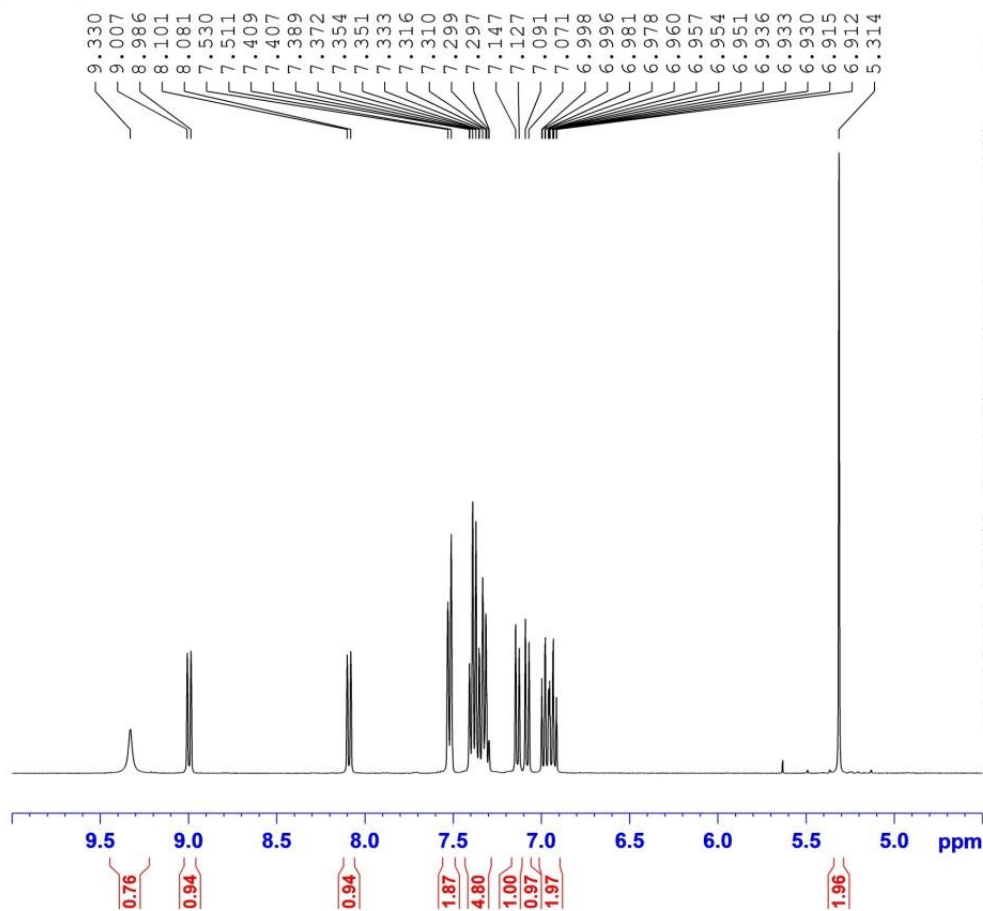
O-benzyl-N-(9'-acridinyl)-hydroxylamine, **6f**

Yield: 16%. ^1H NMR (acetone- d_6) δ , in ppm: 9.33 (s, 1H); 9.00 (m, 1H); 8.09 (m, 1H); 7.54 (m, 2H); 7.35 (m, 5H); 7.14 (m, 1H); 7.08 (m, 2H); 6.95 (m, 2H); 5.31 (s, 2H).

^{13}C NMR (acetone- d_6) δ , in ppm: 143.40; 140.45; 138.76; 138.14; 131.84; 130.91; 129.74; 128.28; 128.03; 127.57; 124.61; 120.68; 119.11; 118.12; 115.39; 115.30; 114.97; 114.89; 76.65. IR (ATR-ZnSe) in cm^{-1} : 1473.

HRMS: M-1, 301.1341 ($\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}$). UV λ_{max} : 259 nm, $A_{259} = 0.36471$. $\Delta T_m = 6.6^\circ\text{C}$. MTT $\text{IC}_{50} = 33.2 \pm 0.6 \mu\text{M}$.

C2 F2-9



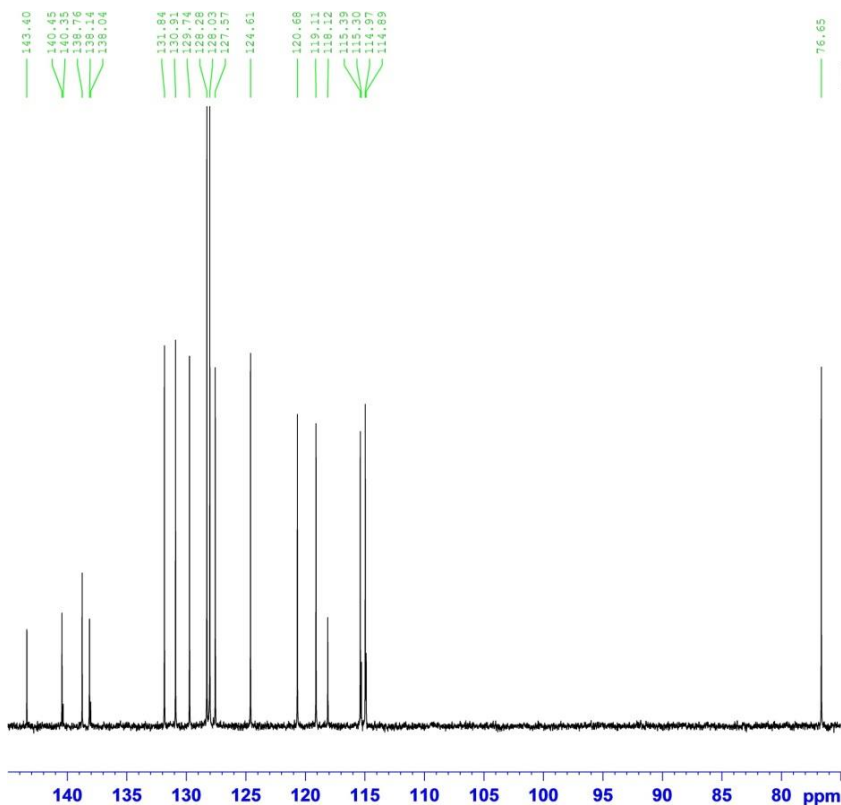
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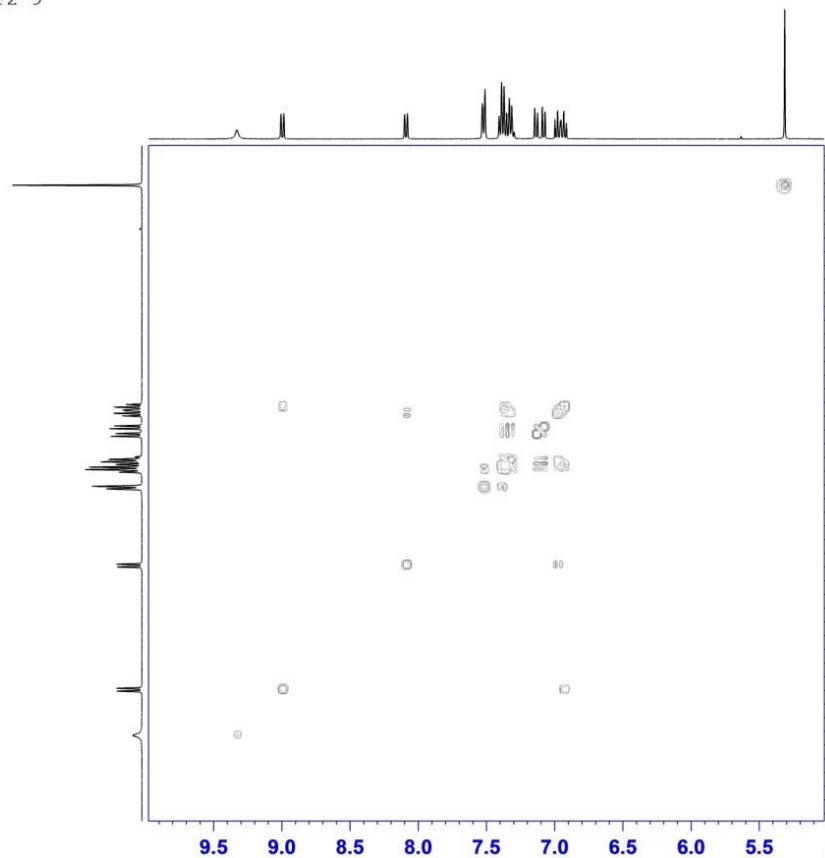
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FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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PL1 -2.00 dB
SFO1 100.6228298 Mhz

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C2 F2-9



Current Data Parameters
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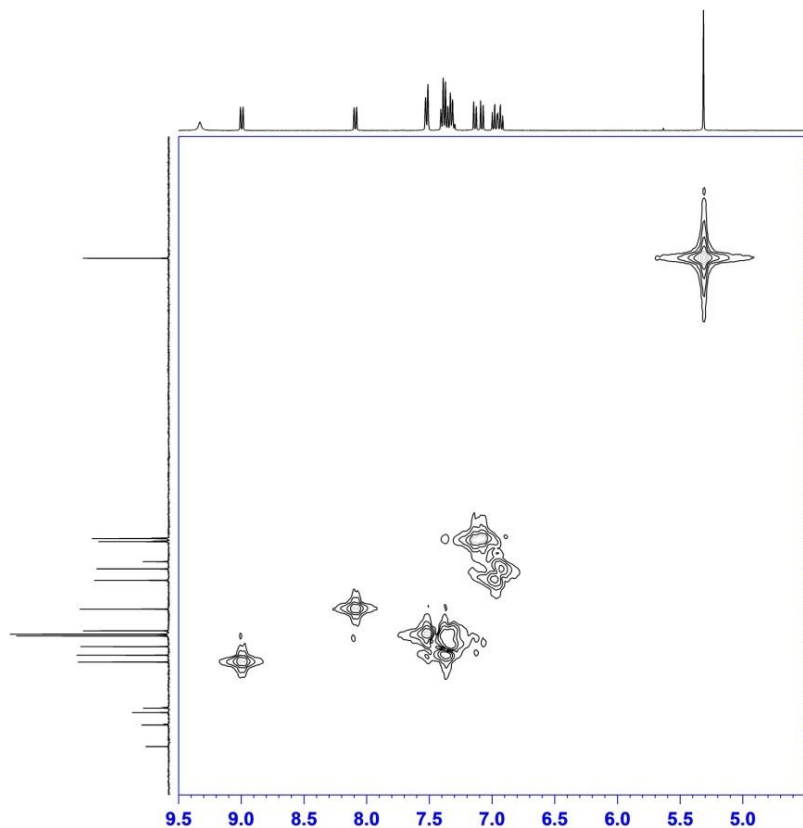
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MC2 QF
SF 400.1301112 Mhz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0



Current Data Parameters
 NAME AIC-21-118
 EXPNO 25
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150311
 Time 20.06
 INSTRUM spect
 PROBRD 5 mm F400 DD-
 PULPROG hmcpsppmgf
 TD 1024
 SOLVENT Acetone
 NS 4
 DS 16
 SWH 4045.307 Hz
 FIDRES 3.904490 Hz
 AQ 0.1246164 sec
 RG 2050
 LW 123.600 usec
 DE 4.00 usec
 TE 300.2 K
 CMT2 145.000000
 d0 0.0000000 sec
 d1 1.5000000 sec
 d2 0.0034428 sec
 d12 0.0000200 sec
 d13 0.0000400 sec
 d14 0.0002000 sec
 DELTA1 0.0027428 sec
 INO 0.0000300 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 15.10 usec
 P2 30.20 usec
 PL1 0.00 dB
 SFO1 400.1318130 MHz

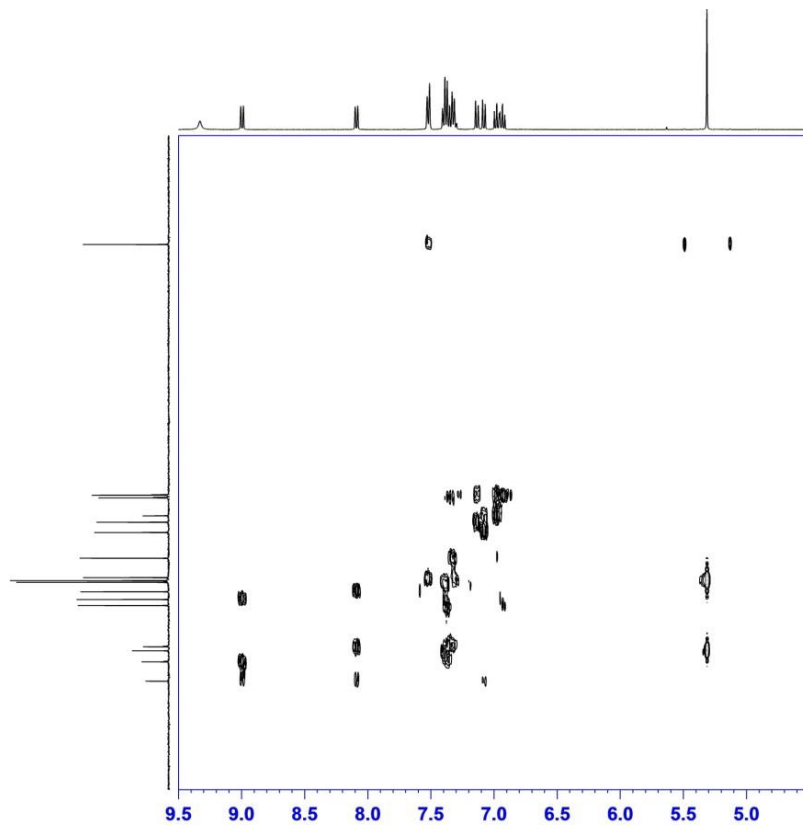
----- CHANNEL f2 -----
 CPDPRG2 gssp
 NUC2 13C
 P3 9.55 usec
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 16.48 dB
 SFO2 100.6203140 MHz

----- GRADIENT CHANNEL -----
 GPRAM1 SINE:100
 STIM:100
 GPRAM2 SINE:100
 STIM:100
 GPRAM3 SINE:100
 STIM:100
 GFZ1 50.00 %
 GFZ2 30.00 %
 GFZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 MD 2
 TD 128
 SFO1 100.6203 MHz
 FIDRES 130.238328 Hz
 SW 165.639 ppm
 FWHM 0.0

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 0
 SF 100.6127690 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0



Current Data Parameters
 NAME AIC-21-118
 EXPNO 26
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150312
 Time 10.32
 INSTRUM spect
 PROBRD 5 mm F400 DD-
 PULPROG hmcpsppmgf
 TD 1024
 SOLVENT Acetone
 NS 8
 DS 16
 SWH 5208.333 Hz
 FIDRES 1.271546 Hz
 AQ 0.3932660 sec
 RG 2050
 LW 96.000 usec
 DE 6.00 usec
 TE 293.8 K
 CMT2 145.000000
 CMT13 10.000000
 d0 0.0000000 sec
 d1 1.5000000 sec
 d2 0.0034428 sec
 d5 0.0000000 sec
 d16 0.0002000 sec
 INO 0.0000240 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 15.10 usec
 P2 30.20 usec
 PL1 0.00 dB
 SFO1 400.1322028 MHz

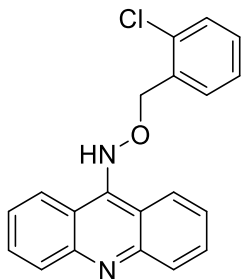
----- CHANNEL f2 -----
 NUC2 13C
 P3 9.55 usec
 PL2 -2.00 dB
 SFO2 100.6228139 MHz

----- GRADIENT CHANNEL -----
 GPRAM1 SINE:100
 STIM:100
 GPRAM2 SINE:100
 STIM:100
 GPRAM3 SINE:100
 STIM:100
 GFZ1 50.00 %
 GFZ2 30.00 %
 GFZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 MD 2
 TD 128
 SFO1 100.6228 MHz
 FIDRES 174.366154 Hz
 SW 221.833 ppm
 FWHM 0.0

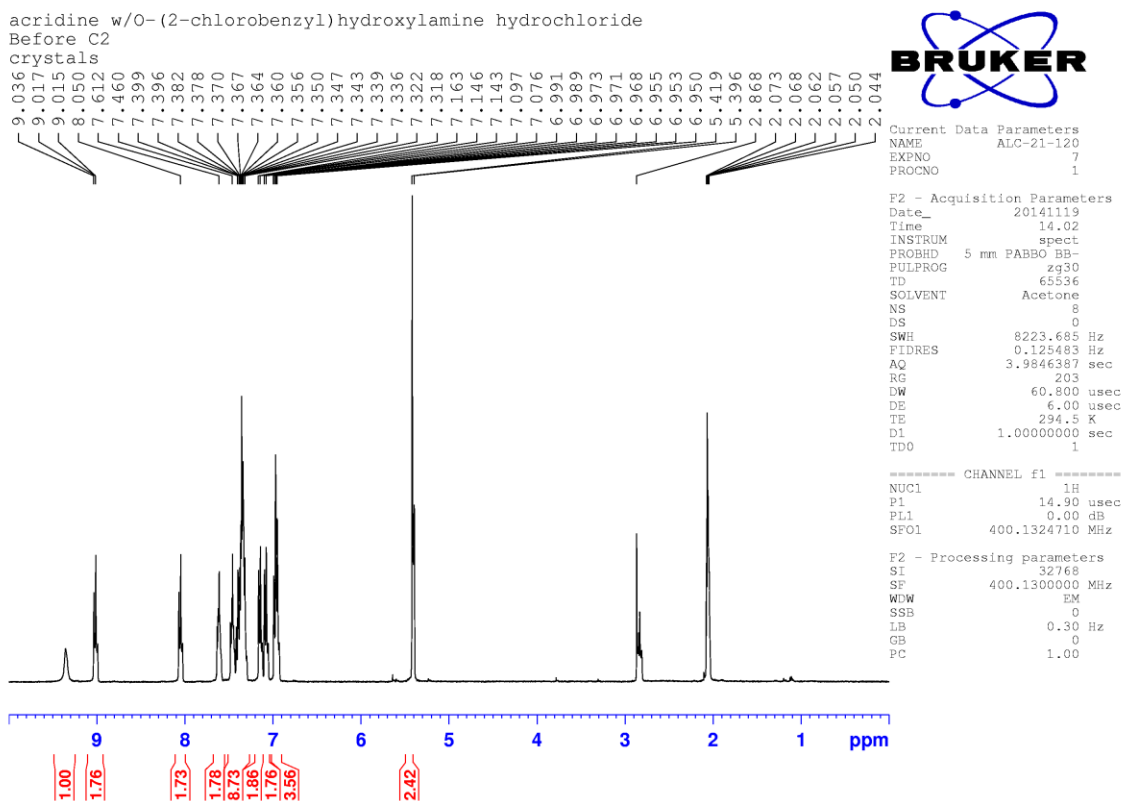
F2 - Processing parameters
 SI 2048
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 0
 SF 100.6127690 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

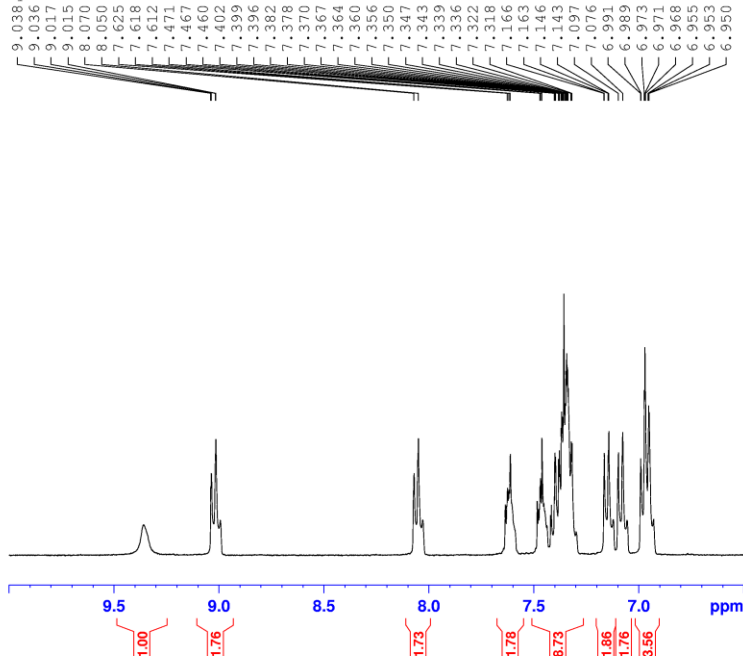


O-(2-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6g

Yield: 15%. ¹HNMR (acetone-d₆) δ, in ppm: 9.37 (s, 1H); 9.02 (m, 2H); 8.05 (m, 2H); 7.61 (m, 2H); 7.36 (m, 8H); 7.15 (m, 2H); 7.09 (m, 1H); 6.97 (m, 3H); 5.05 (s, 2H). ¹³CNMR (acetone-d₆) δ, in ppm: 143.9; 140.4; 140.4; 138.1; 138.0; 136.4; 132.9; 131.9; 131.0; 130.1; 129.8; 129.2; 129.2; 127.0; 124.6; 120.7; 119.2; 117.9; 115.5; 115.4; 115.0; 114.9; 114.8; 73.7. IR (ATR-ZnSe) in cm⁻¹: 746 1474. HRMS: M-1, 335.0952 (C₂₀H₁₆N₂OCl). ΔT_m = 18.2°C. MTT IC₅₀ = 17.4±0.2μM.



acridine w/O-(2-chlorobenzyl)hydroxylamine hydrochloride
Before C2
crystals



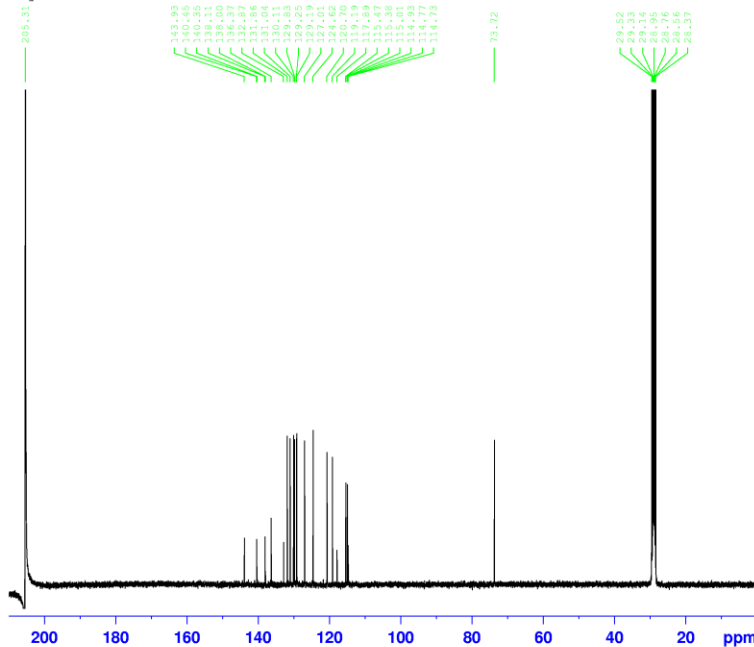
Current Data Parameters
NAME ALC-21-120
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141119
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125683 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TDO

===== CHANNEL f1 =====
NUC1 1H
P1 14.90 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

acridine w/O-(2-chlorobenzyl)hydroxylamine hydrochloride
Before C2
crystals



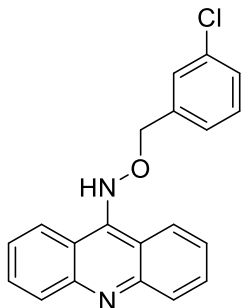
Current Data Parameters
NAME ALC-21-120
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150127
Time 5.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 10000
DS 4
SWH 24038.461 Hz
FIDRES 0.1366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO

===== CHANNEL f1 =====
NUC1 13C
P1 9.55 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

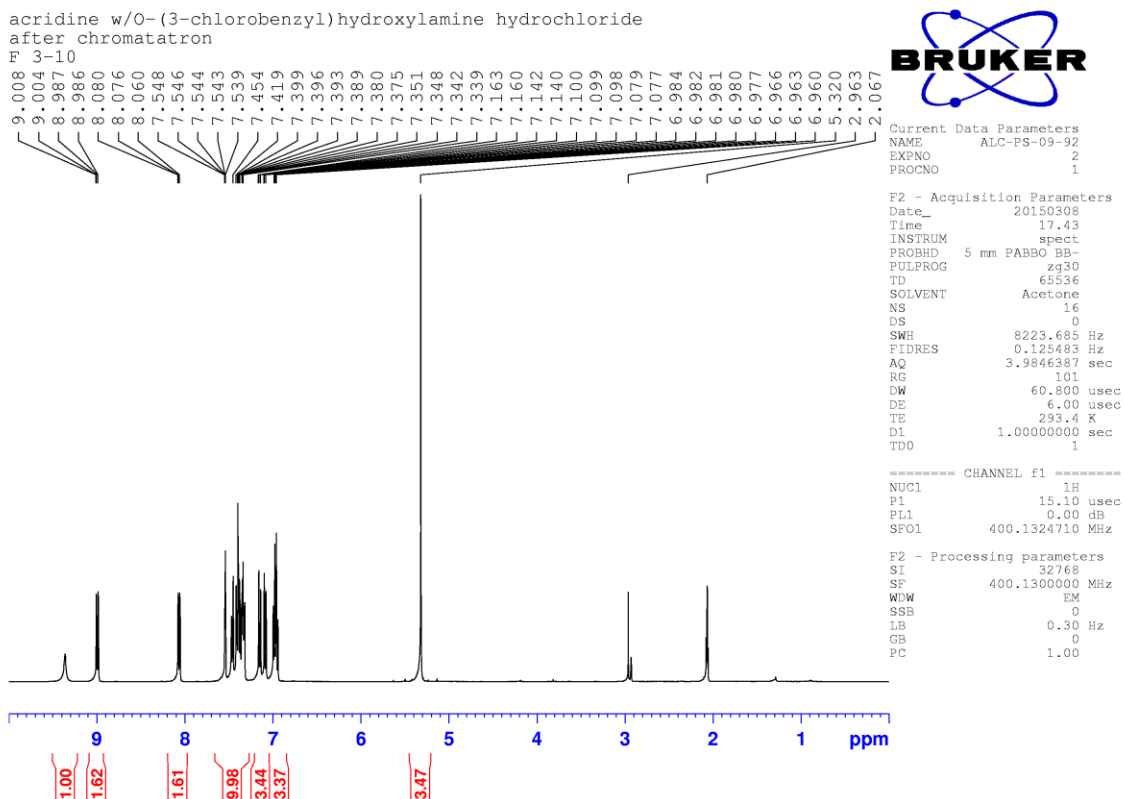
===== CHANNEL f2 =====
CPCPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

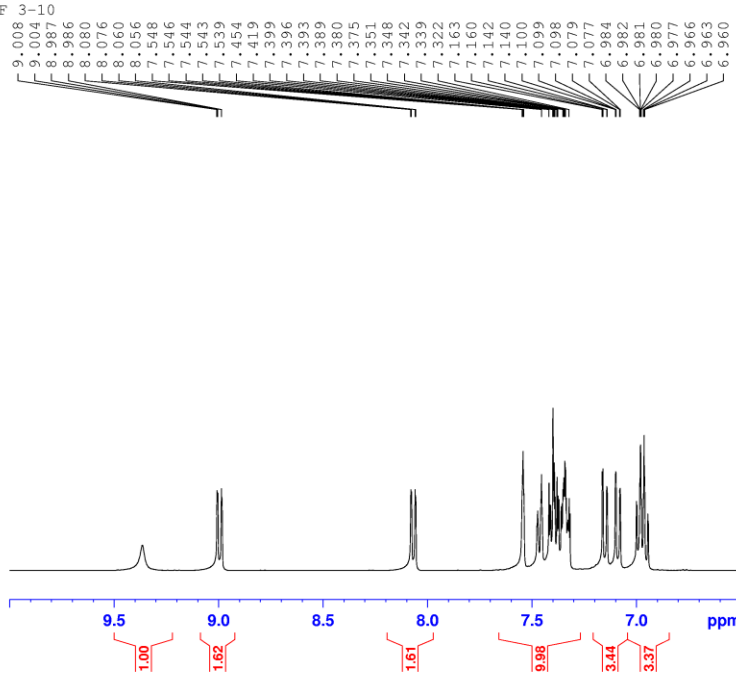


O-(3-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6h

Yield: 46%. ^1H NMR (acetone- d_6) δ , in ppm: 9.37 (s, 1H); 9.00 (m, 1H); 8.08 (m, 1H); 7.40 (m, 6H); 7.10 (m, 2H); 6.98 (m, 2H); 5.32 (s, 2H). ^{13}C NMR (acetone- d_6) δ , in ppm: 143.8; 141.5; 140.4; 140.4; 138.1; 138.0; 133.6; 131.8; 131.0; 130.0; 129.8; 127.8; 127.5; 126.3; 124.6; 120.7; 119.2; 117.9; 117.9; 115.5; 115.4; 115.04; 115.0; 114.8; 114.8; 75.6. IR (ATR-ZnSe) in cm^{-1} : 747, 1474. HRMS: M-1, 335.0948 ($\text{C}_{20}\text{H}_{16}\text{N}_2\text{OCl}$). $\Delta T_m = 18.5^\circ\text{C}$. MTT $\text{IC}_{50} = 18.0 \pm 0.2 \mu\text{M}$



acridine w/O-(3-chlorobenzyl)hydroxylamine hydrochloride
after chromatatron
F 3-10

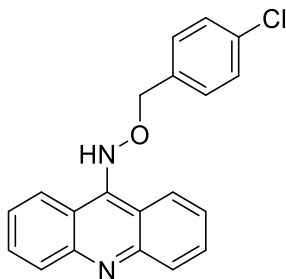


Current Data Parameters
NAME ALC-PS-09-92
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150308
Time 17.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWE 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TDO 1

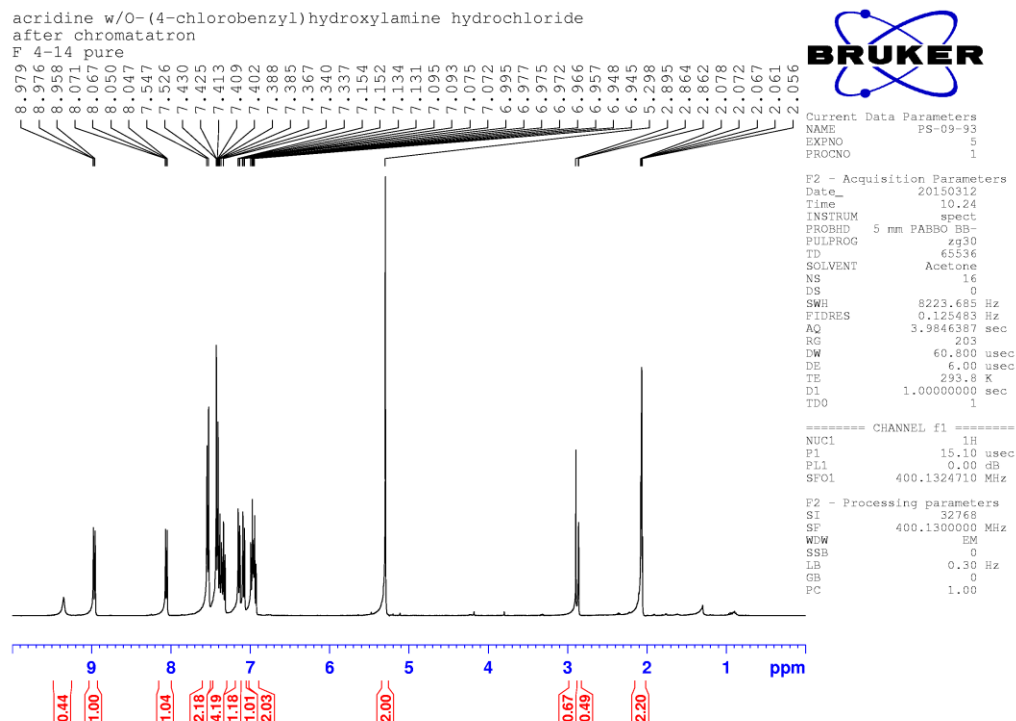
===== CHANNEL f1 =====
NUC1 1H
P1 15.10 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



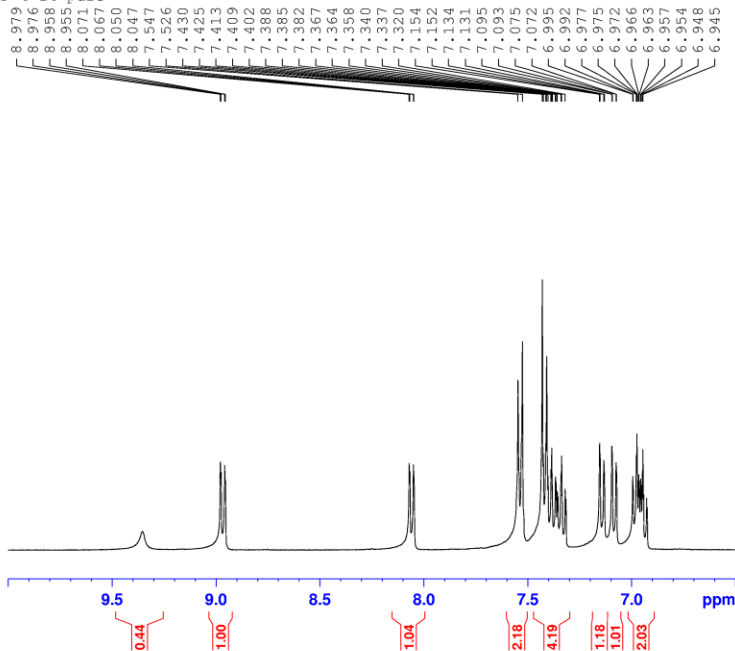
O-(4-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6i

Yield: 30%. ¹HNMR (acetone-d₆) δ, in ppm: 9.34 (s, 1H); 8.98 (m, 1H); 8.06 (m, 1H); 7.54 (m, 2H); 7.40 (m, 4H); 7.14 (m, 1H); 7.08 (m, 1H); 6.97 (m, 2H); 5.30 (s, 2H). ¹³CNMR (acetone-d₆) δ, in ppm: 143.7; 140.4; 140.4; 138.1; 138.0; 137.8; 132.8; 131.8; 131.0; 129.8; 129.8; 128.3; 124.6; 120.7; 119.2; 118.0; 118.0; 115.4; 115.4; 115.0; 114.9; 114.8; 114.8; 75.6. IR (ATR-ZnSe) in cm⁻¹: 747; 964; 1473; 1489; 1598. HRMS: M-1, 335.0951 (C₂₀H₁₆N₂OCl). ΔT_m = 20.2°C. MTT IC₅₀ = 17.0±0.4 μM.



acridine w/O-(4-chlorobenzyl)hydroxylamine hydrochloride
after chromatatron

F 4-14 pure



Current Data Parameters
NAME PS-09-93
EXPNO 5
PROCNO 1

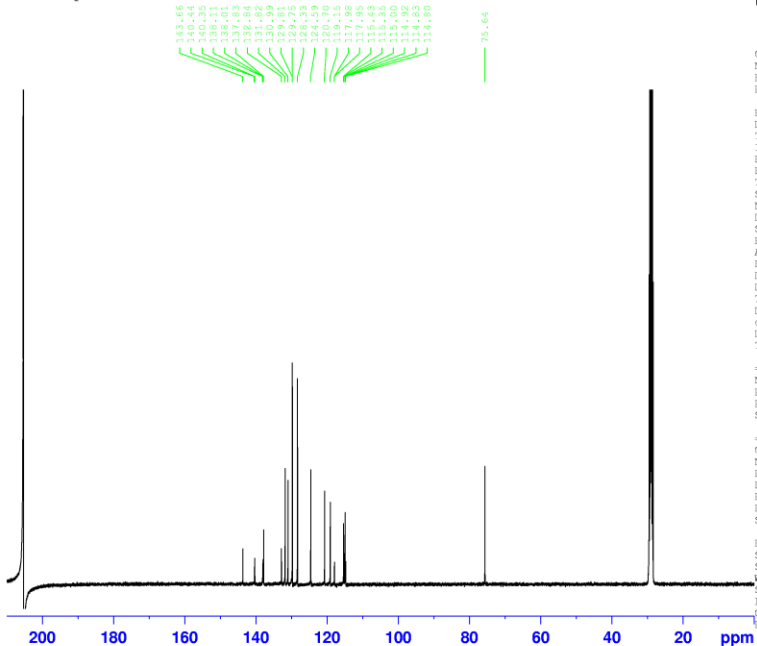
F2 - Acquisition Parameters
Date_ 20150312
Time 10.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 293.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.10 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

acridine w/O-(4-chlorobenzyl)hydroxylamine hydrochloride
after chromatatron

F 4-14 pure



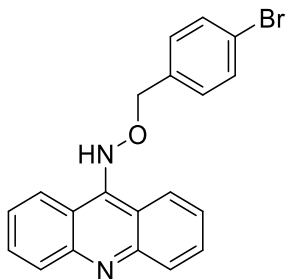
Current Data Parameters
NAME PS-09-93
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150312
Time 6.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 10000
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.55 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

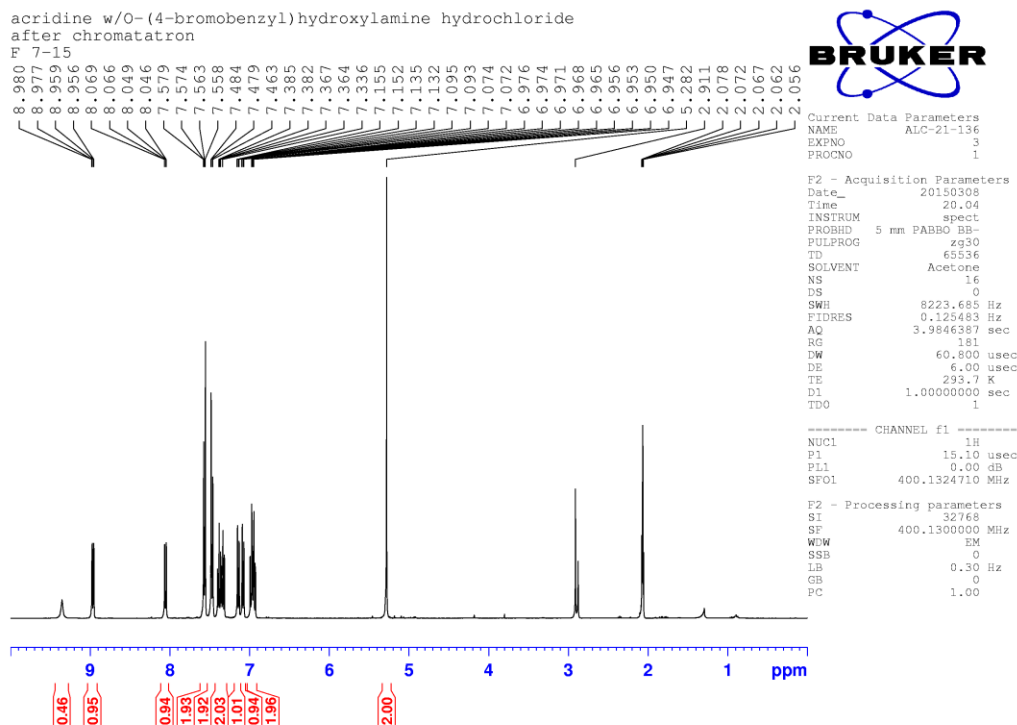
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

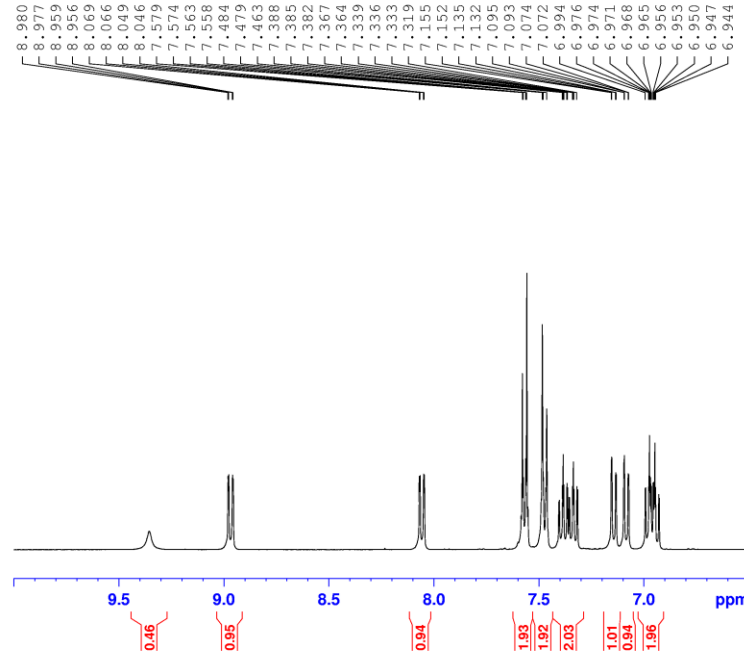


O-(4-bromobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6j

Yield: 51%. ¹HNMR (acetone-d₆) δ, in ppm: 9.34 (s, 1H); 8.97 (m, 1H); 8.06 (m, 1H); 7.57 (m, 2H); 7.48 (m, 2H); 7.37 (m, 2H); 7.14 (m, 1H); 7.08 (m, 1H); 6.96 (m, 2H); 5.28 (s, 2H). ¹³CNMR (acetone-d₆) δ, in ppm: 143.7; 140.4; 140.4; 138.3; 138.1; 138.0; 131.8; 131.3; 131.0; 130.1; 129.8; 124.6; 121.0; 120.7; 119.2; 118.0; 117.9; 115.4; 115.4; 115.0; 114.9; 114.8; 114.8; 75.7 ppm. IR (ATR ZnSe) in cm⁻¹: 747; 964; 1008; 1473; 1486. HRMS: M-1, 379.0421 (C₂₀H₁₆N₂OBr). ΔT_m = 18.1°C. MTT IC₅₀ = 18.5±4.3 μM



acridine w/O-(4-bromobenzyl)hydroxylamine hydrochloride
after chromatatron
F 7-15



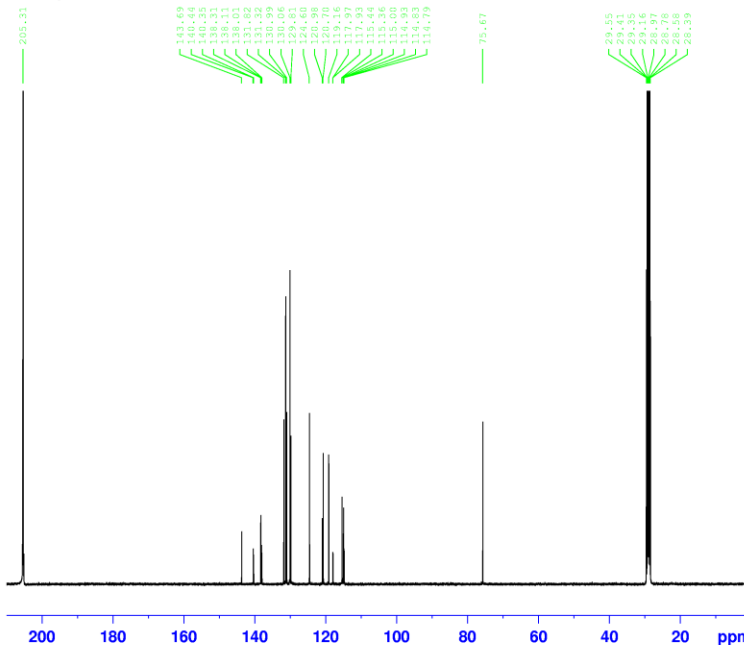
Current Data Parameters
NAME ALC-21-136
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150308
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.10 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

acridine w/O-(4-bromobenzyl)hydroxylamine hydrochloride
after chromatatron
F 7-15



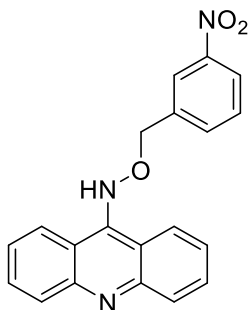
Current Data Parameters
NAME ALC-21-136
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time 7.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 12000
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.55 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

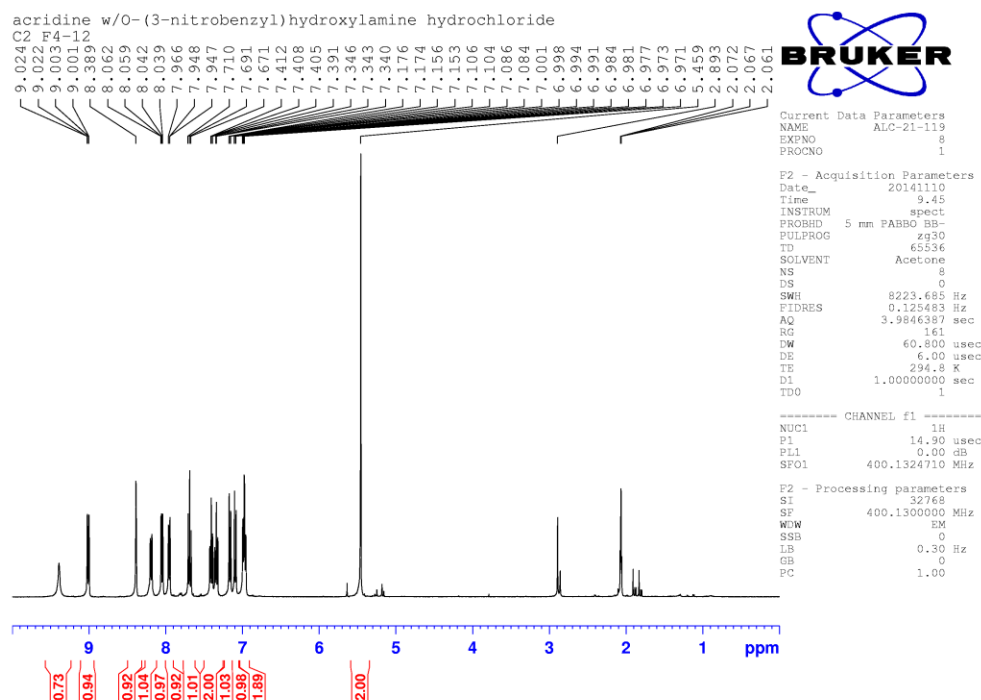


O-(3-nitrobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6k

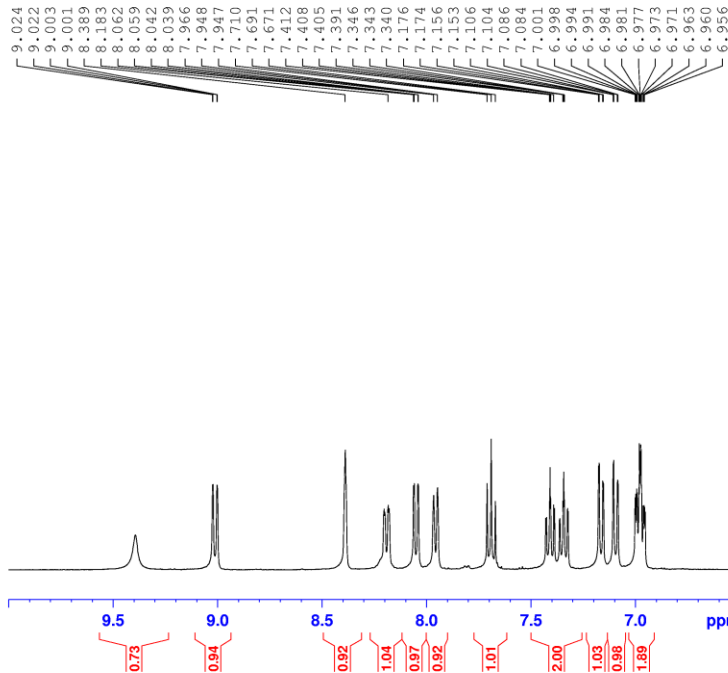
Yield: 41%. ^1H NMR (acetone- d_6) δ , in ppm: 9.40 (s, 1H); 9.01 (s, 1H); 8.39 (s, 1H); 8.18 (m, 1H); 8.05 (m, 1H); 7.95 (m, 1H); 7.69 (m, 1H); 7.39 (m, 2H); 7.16 (m, 1H); 7.10 (m, 1H); 6.98 (m, 2H); 5.46 (s, 2H).

^{13}C NMR (acetone- d_6) δ , in ppm: 148.36; 144.21; 141.46; 140.46; 138.10; 134.13; 131.83; 131.12; 129.93; 129.64; 124.60; 122.45; 122.34; 120.75; 119.25; 117.79; 117.76; 115.54; 115.46; 115.07; 114.99; 114.69; 114.65; 75.08. IR (ATR ZnSe) in cm^{-1} : 963; 1346; 1473; 1524; 1615. HRMS: M-1, 346.1194

($\text{C}_{20}\text{H}_{16}\text{N}_3\text{O}_3$).. $\Delta T_m = 15.1^\circ\text{C}$. MTT $\text{IC}_{50} = 31.8 \pm 0.1 \mu\text{M}$



acridine w/O-(3-nitrobenzyl)hydroxylamine hydrochloride
C2 F4-12



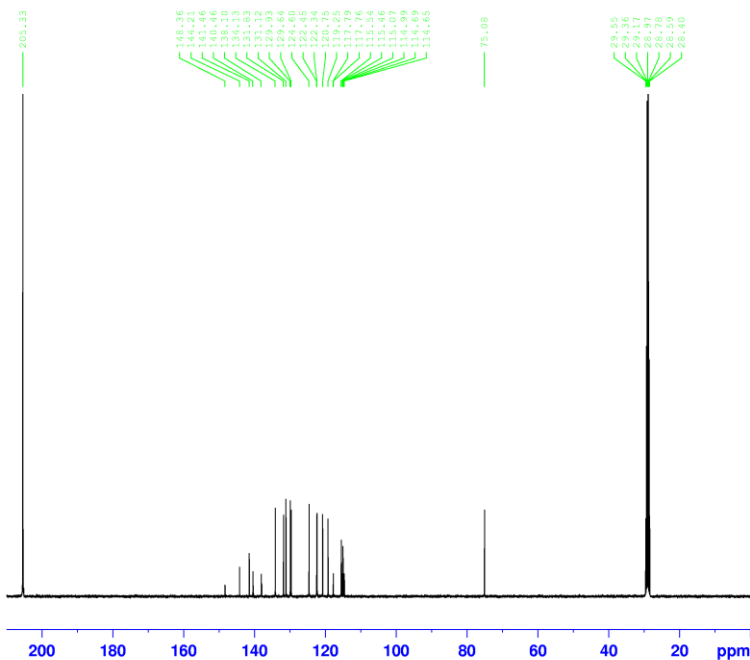
Current Data Parameters
NAME ALC-21-119
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141110
Time 9.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.90 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

acridine w/O-(3-nitrobenzyl)hydroxylamine hydrochloride
C2 F4-12 Final



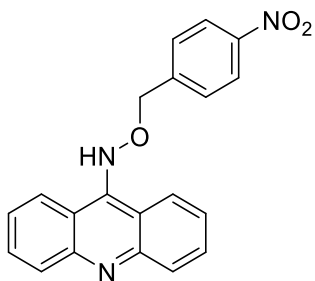
Current Data Parameters
NAME ALC-21-119
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150126
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 71.8
DW 20.800 usec
DE 6.00 usec
TE 296.6 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.55 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

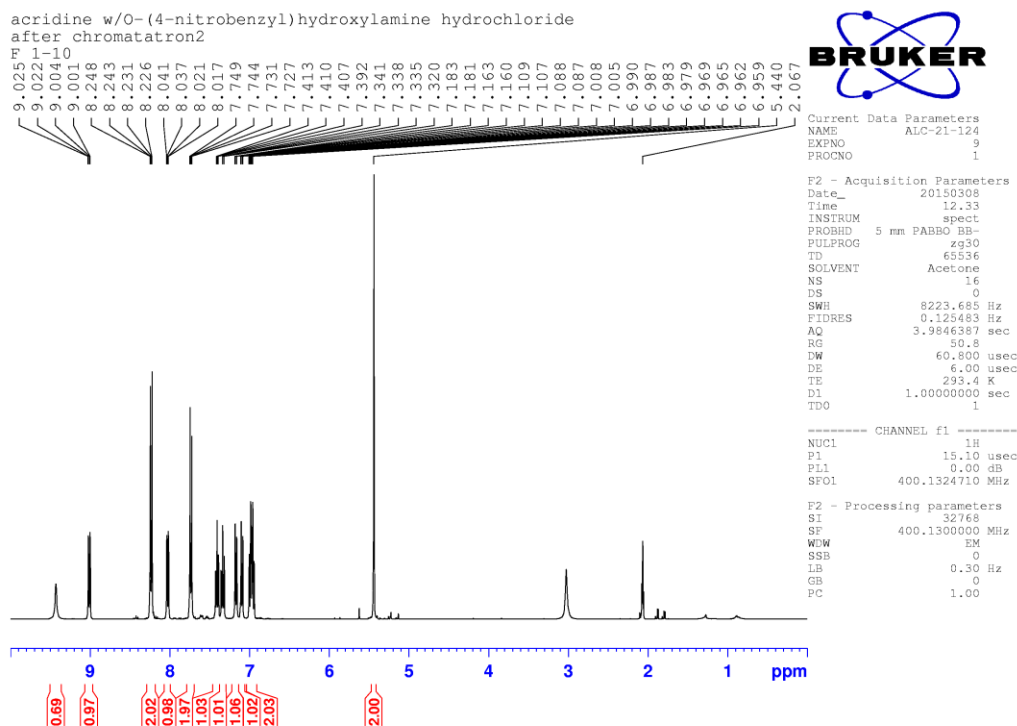
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

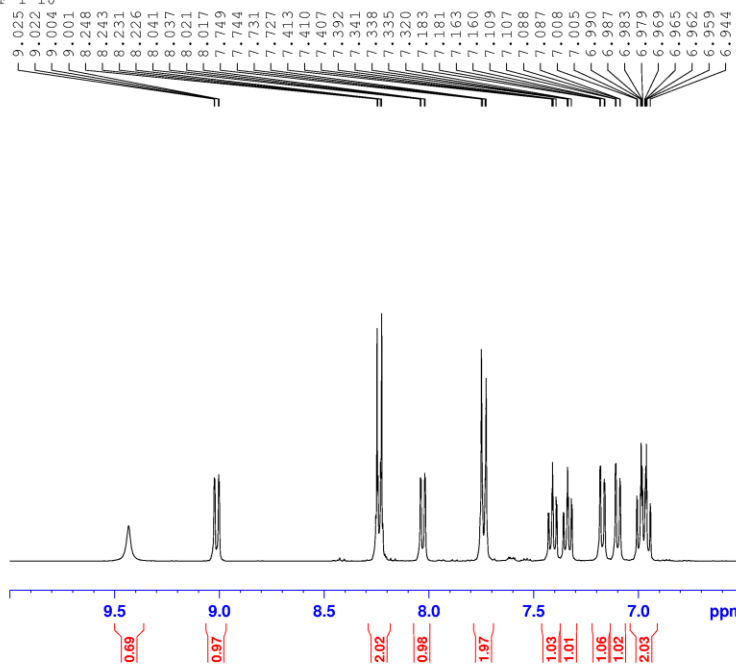


O-(4-nitrobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6l

Yield: 38%. ^1H NMR (acetone- d_6) δ , in ppm: 9.43 (s, 1H); 9.01 (m, 1H); 8.24 (m, 2H); 8.03 (m, 1H); 7.74 (m, 2H); 7.41 (m, 1H); 7.34 (m, 1H); 7.17 (m, 1H); 7.10 (m, 1H); 6.98 (m, 2H); 5.44 (s, 2H). ^{13}C NMR (acetone- d_6) δ , in ppm: 147.4; 146.9; 144.2; 140.5; 140.4; 138.1; 138.0; 131.8; 131.1; 129.9; 128.4; 123.4; 120.8; 119.3; 117.7; 117.7; 115.6; 115.5; 115.1; 115.0; 114.7; 114.6; 75.1. IR (ATR ZnSe) in cm^{-1} : 748; 1342; 1474; 1518. HRMS: M-1, 346.1172 ($\text{C}_{20}\text{H}_{16}\text{N}_3\text{O}_3$). MTT IC_{50} = $30.3 \pm 1.4 \mu\text{M}$



acridine w/O-(4-nitrobenzyl)hydroxylamine hydrochloride
after chromatatron2
F 1-10



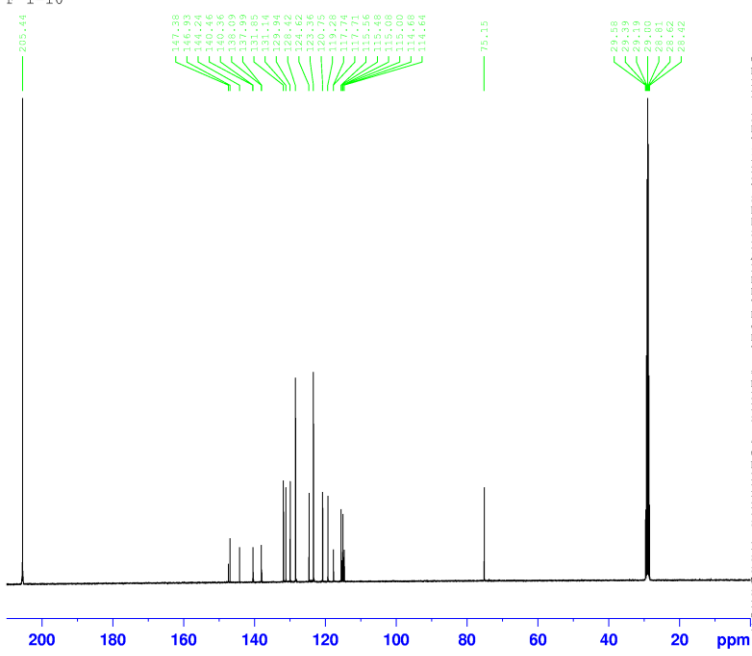
Current Data Parameters
NAME ALC-21-124
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150308
Time 12.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 50.8
LW 60.800 usec
DE 6.00 usec
TE 293.4 K
DI 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 15.10 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

acridine w/O-(4-nitrobenzyl)hydroxylamine hydrochloride
after chromatatron2
F 1-10



Current Data Parameters
NAME ALC-21-124
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150304
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
LW 20.800 usec
DE 6.00 usec
TE 295.0 K
DI 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.55 usec
PL1 2.00 dB
SFO1 100.6228298 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40