Supplementary Material

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

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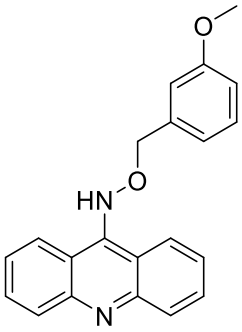
General Procedures

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 ^{1}H 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 ^{1}H) multinuclear FT-NMR. Infrared spectra were collected using a Thermo Scientific iD_5 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).

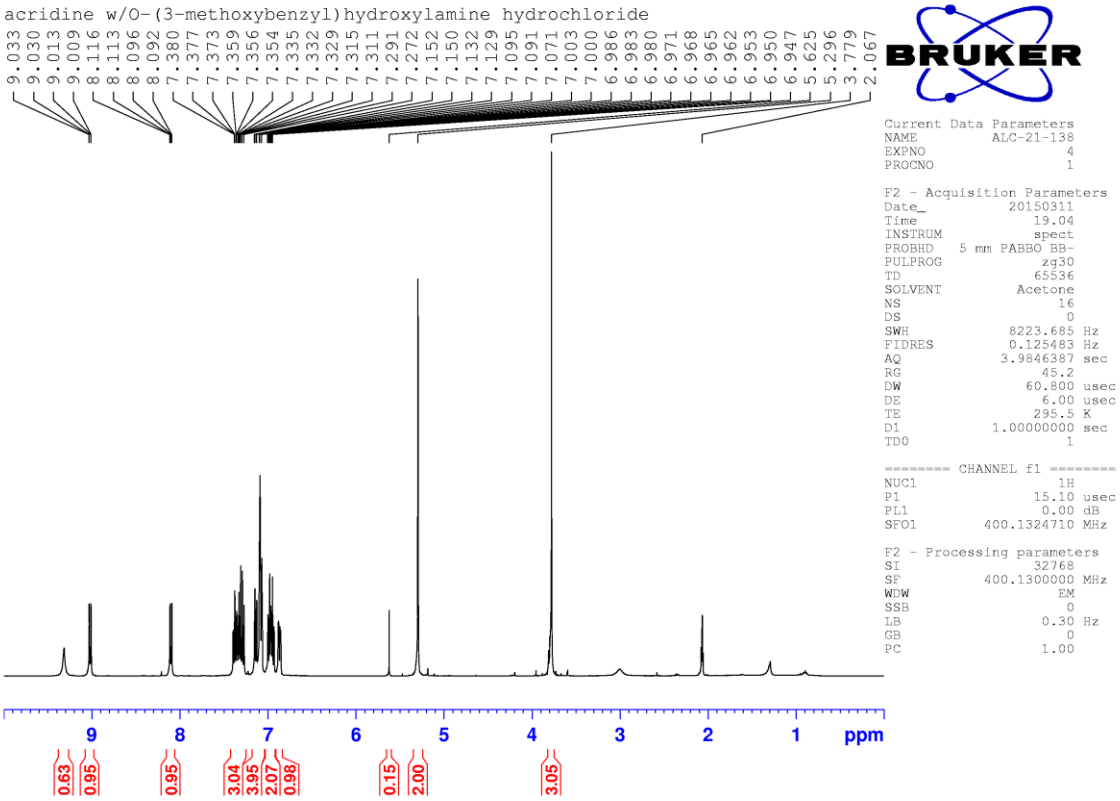
General procedure for preparation of O-benzyl-N-(9'-acridinyl)-hydroxylamines (6a-l)

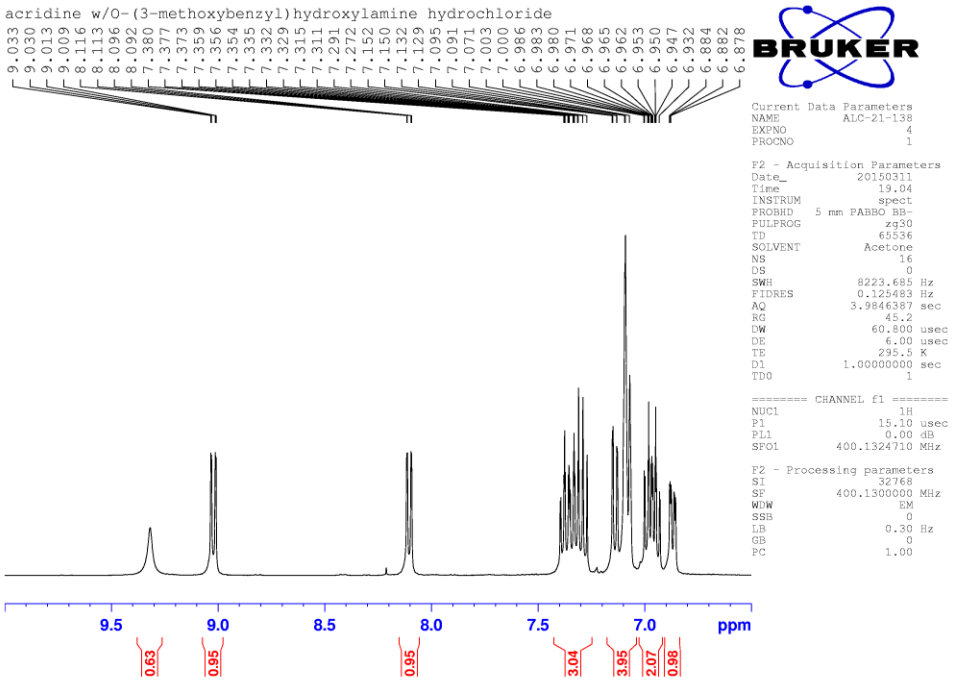
The appropriate salt, **4a-l**, (7.02×10^{-4} mol) was treated with commercially available 9-chloroacridine (**5**) (4.68×10^{-4} mol). The reaction was carried out in molten phenol using 3.0 grams of phenol per gram of 9-chloroacridine (**5**). The reaction was heated between 80-100 °C for a period 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, CH_2Cl_2:Et_2O 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%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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.





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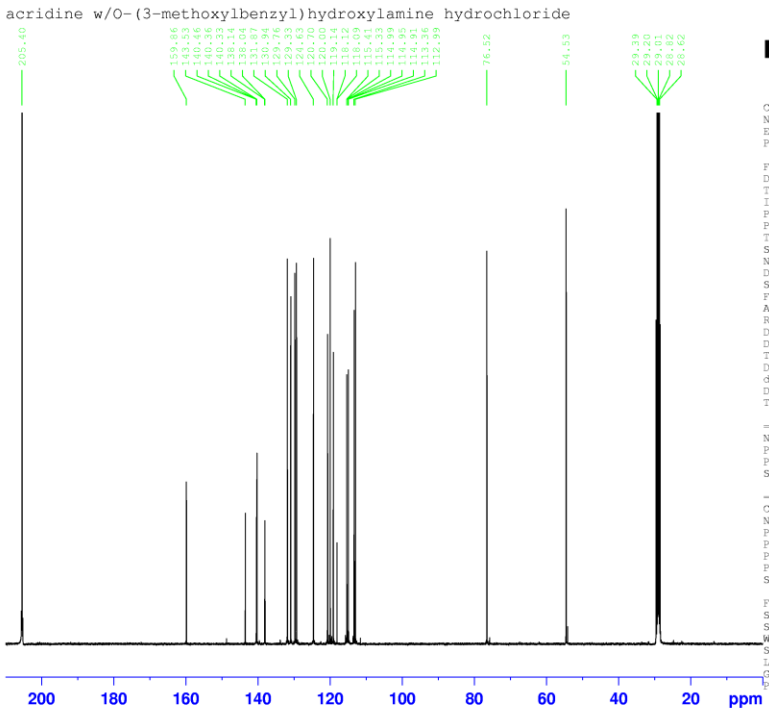

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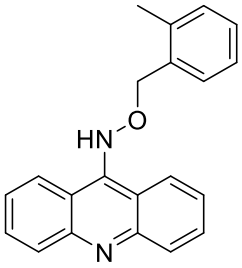
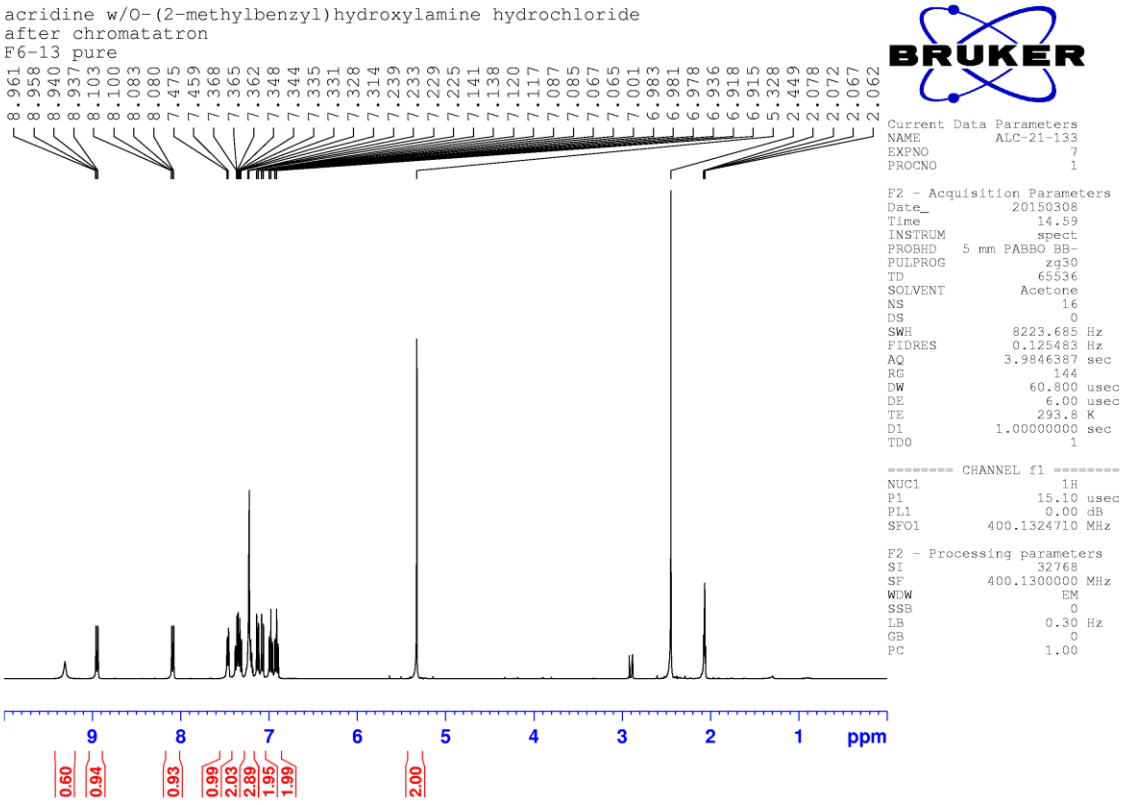
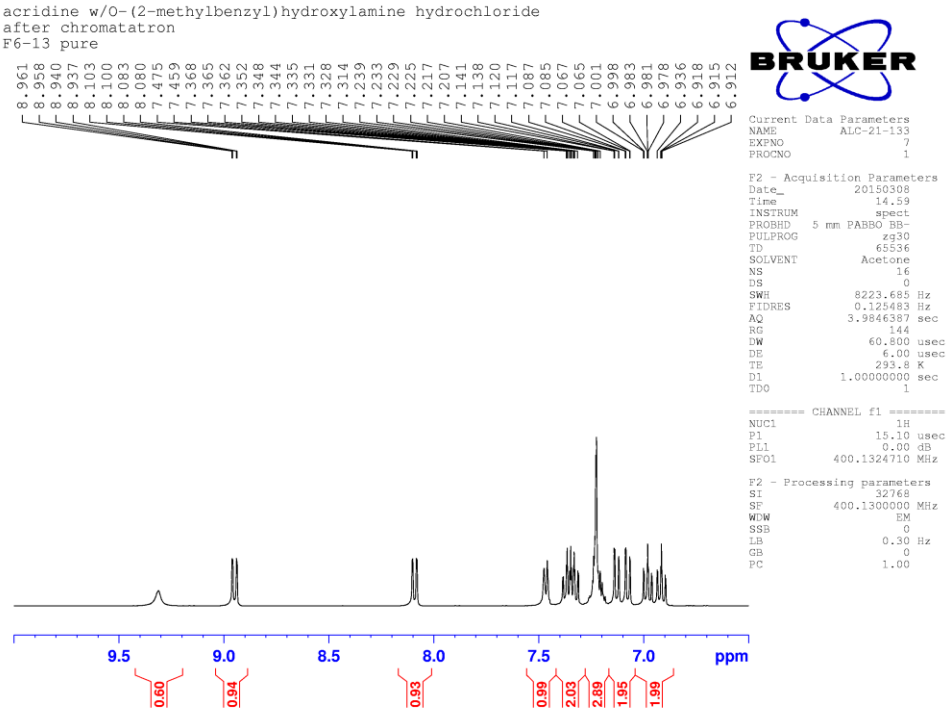


O-(2-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6c

Yield: 49%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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 ($C_{21}H_{19}N_2O$). ΔT_m = 15.5°C. MTT IC_{50} = 17.7±0.2μM





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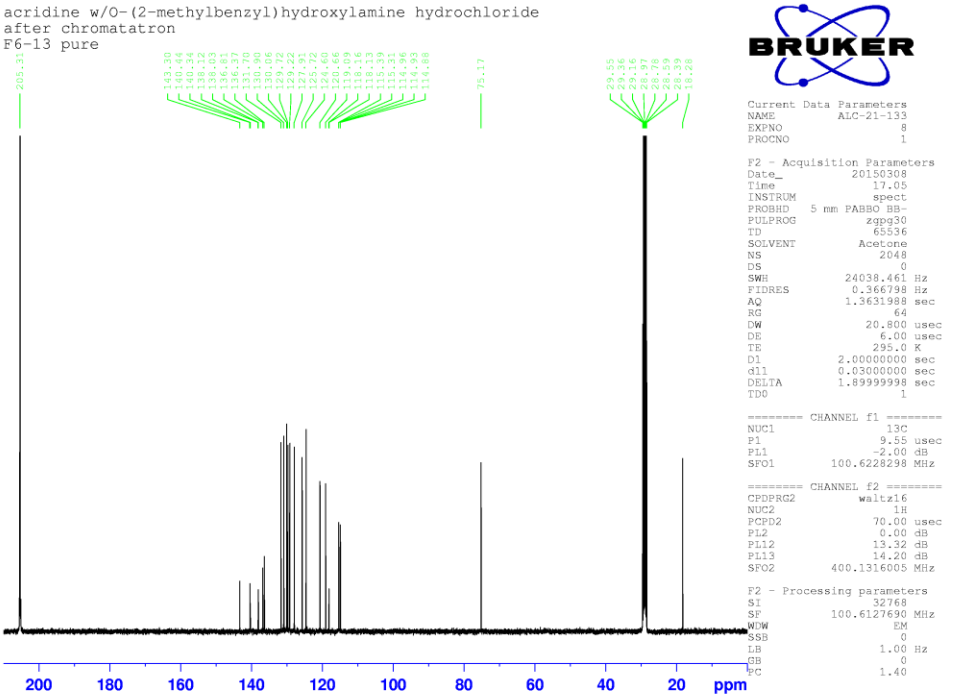

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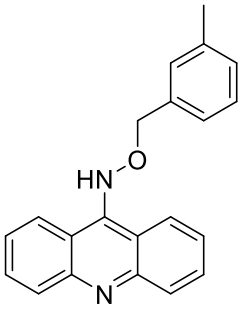
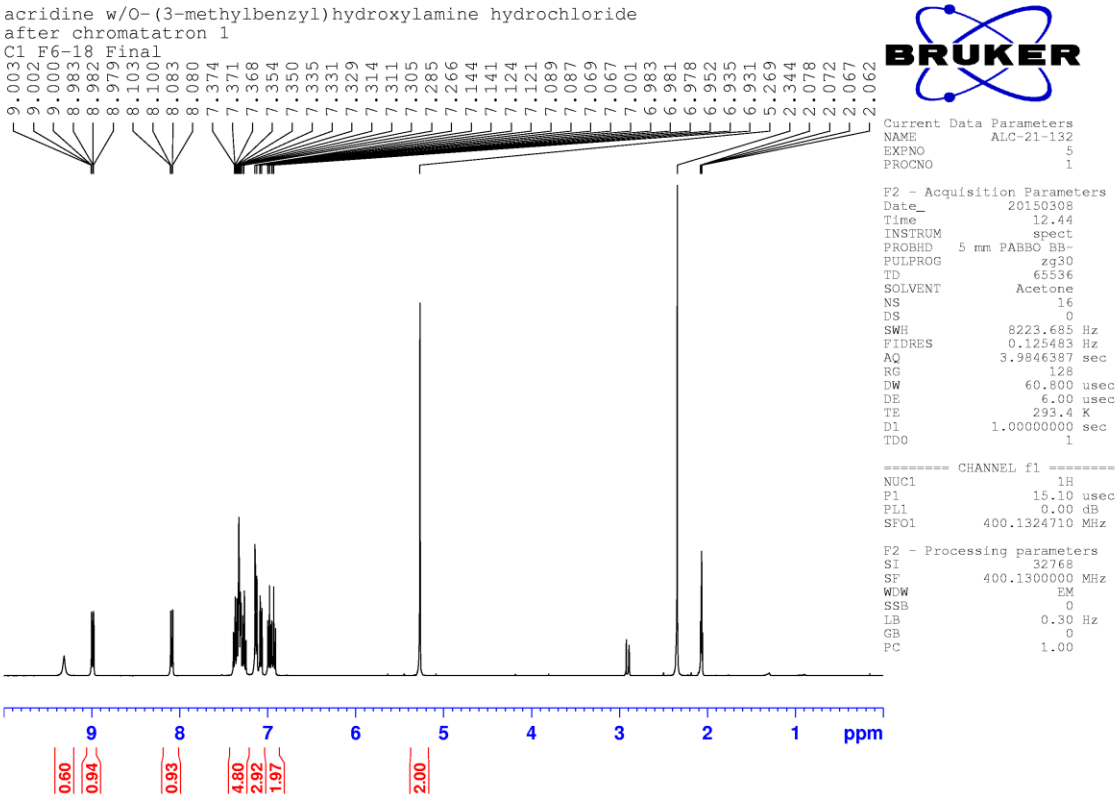
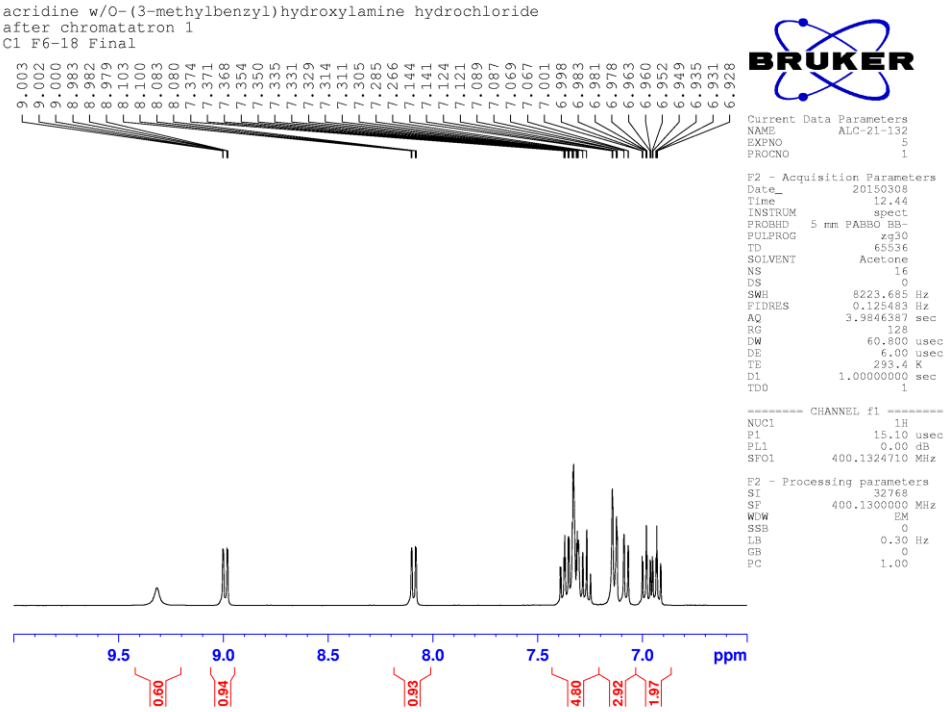
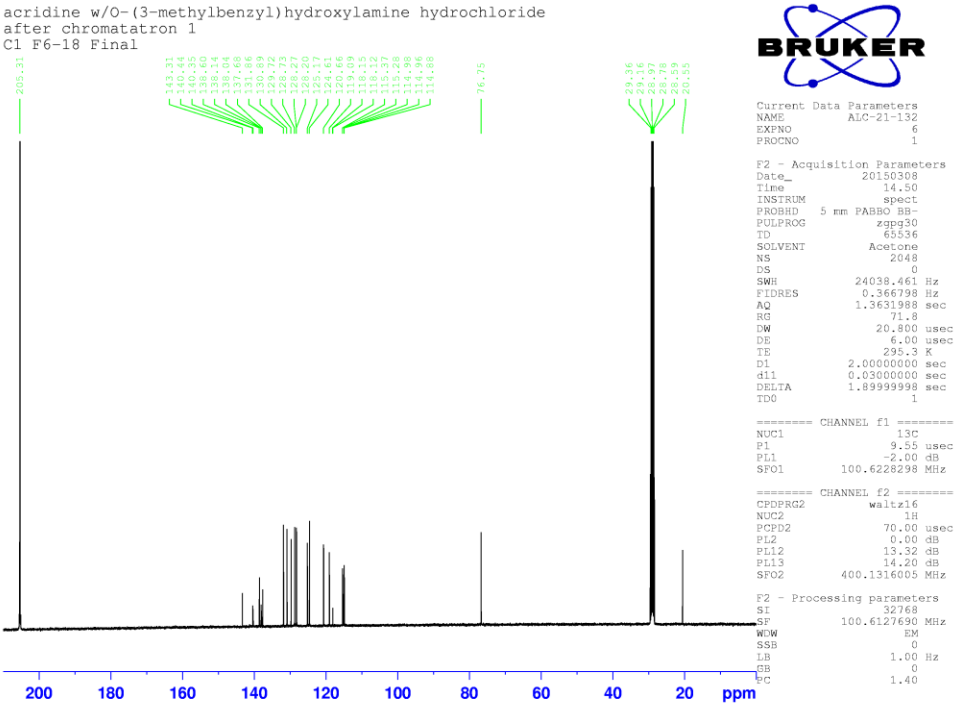


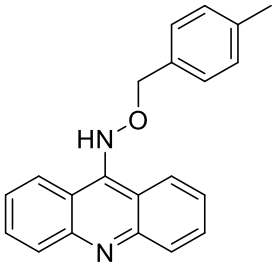
O-(3-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6d

Yield: 71%. ^{1}H 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 ($C_{21}H_{19}N_2O$). ΔT_m = 19.0°C. MTT IC_{50} = 20.7±0.5μM



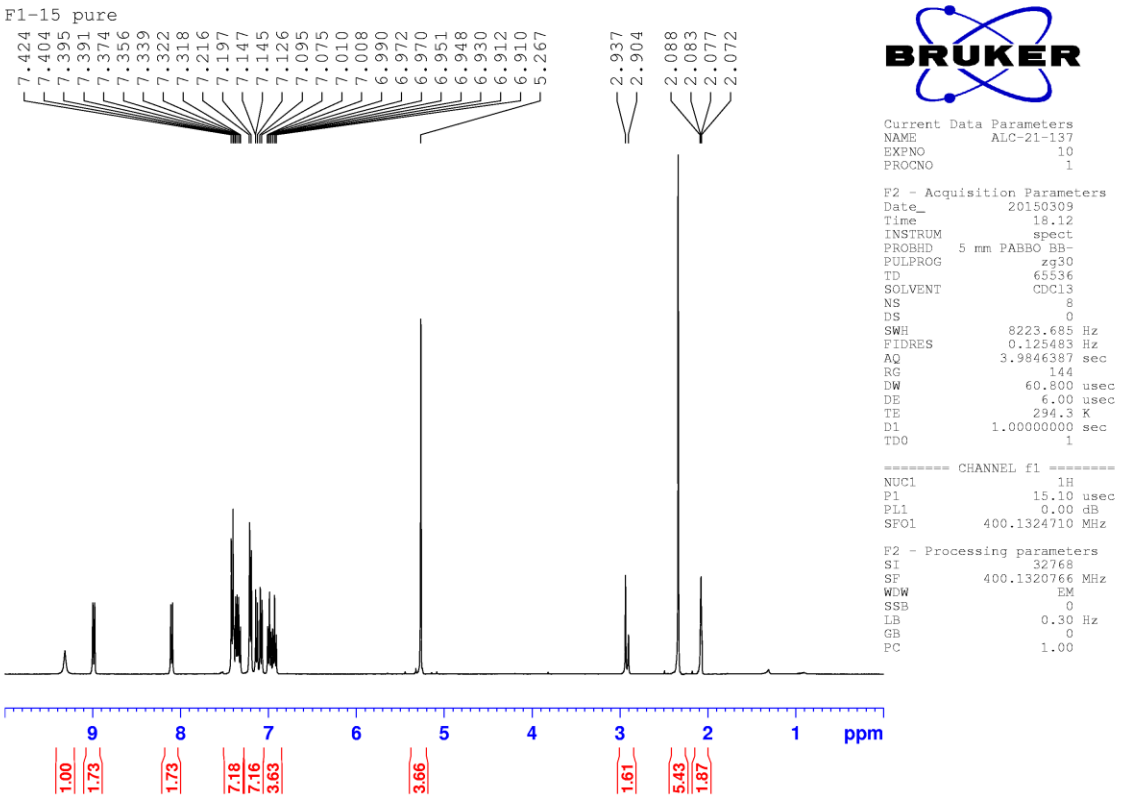






O-(4-methylbenzyl)-N-(9'-acridinyl)-hydroxylamine, 6e

Yield: 40%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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 ($C_{21}H_{19}N_2O$). ΔT_m = 19.0°C. MTT IC_{50} = 22.2±1.7μM.



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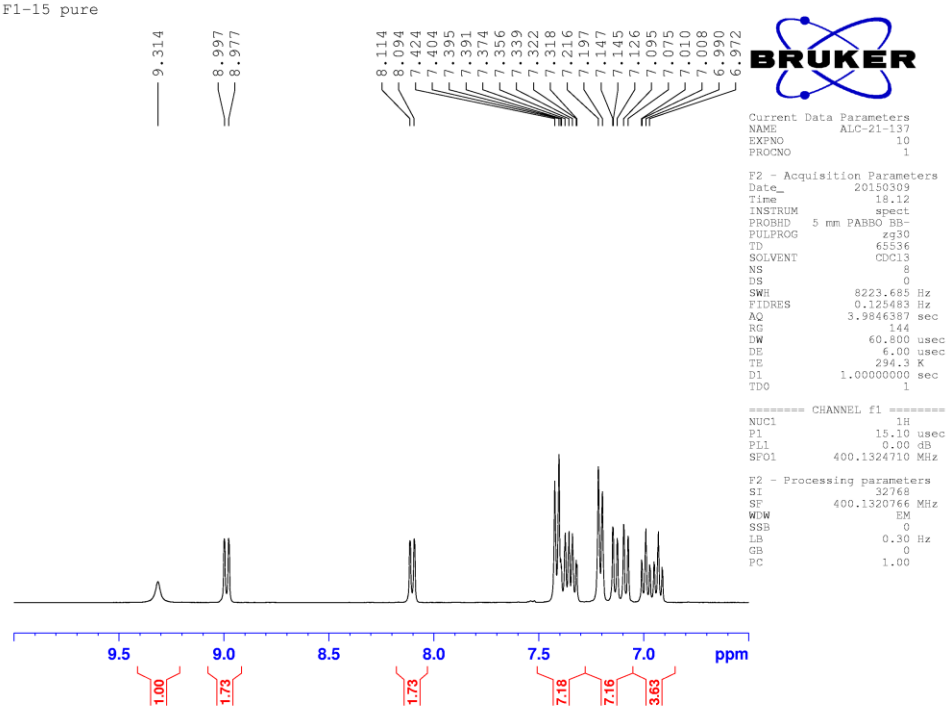

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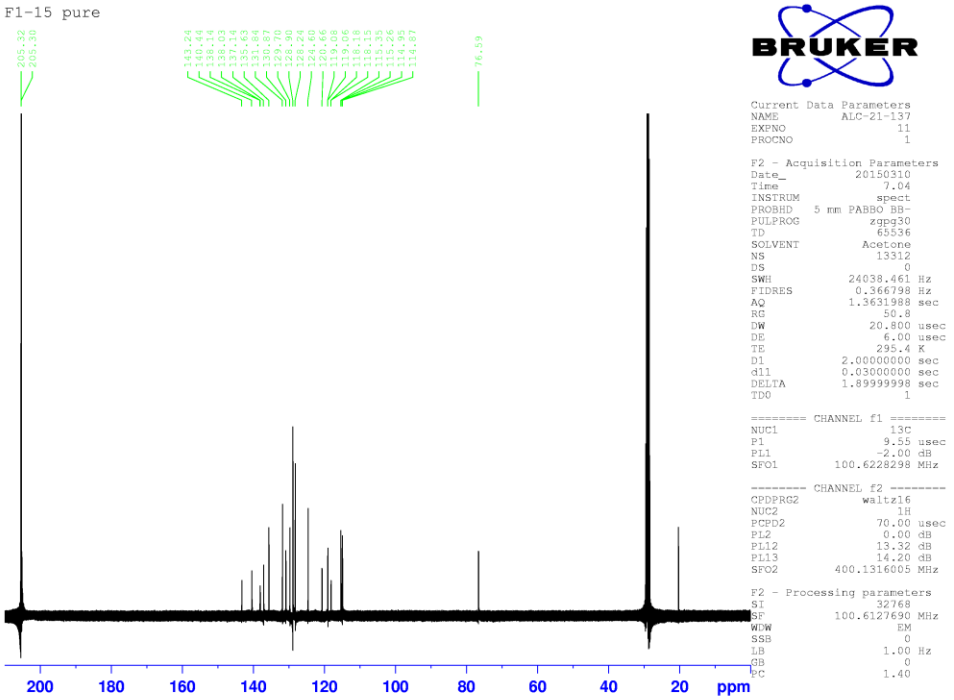

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FIDRES 0.366798 Hz
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RG 50.8
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DE 6.00 usec
TE 295.4 K
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d11 0.03000000 sec
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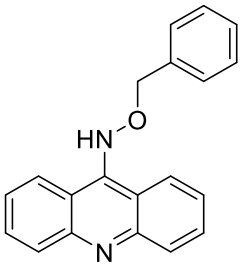
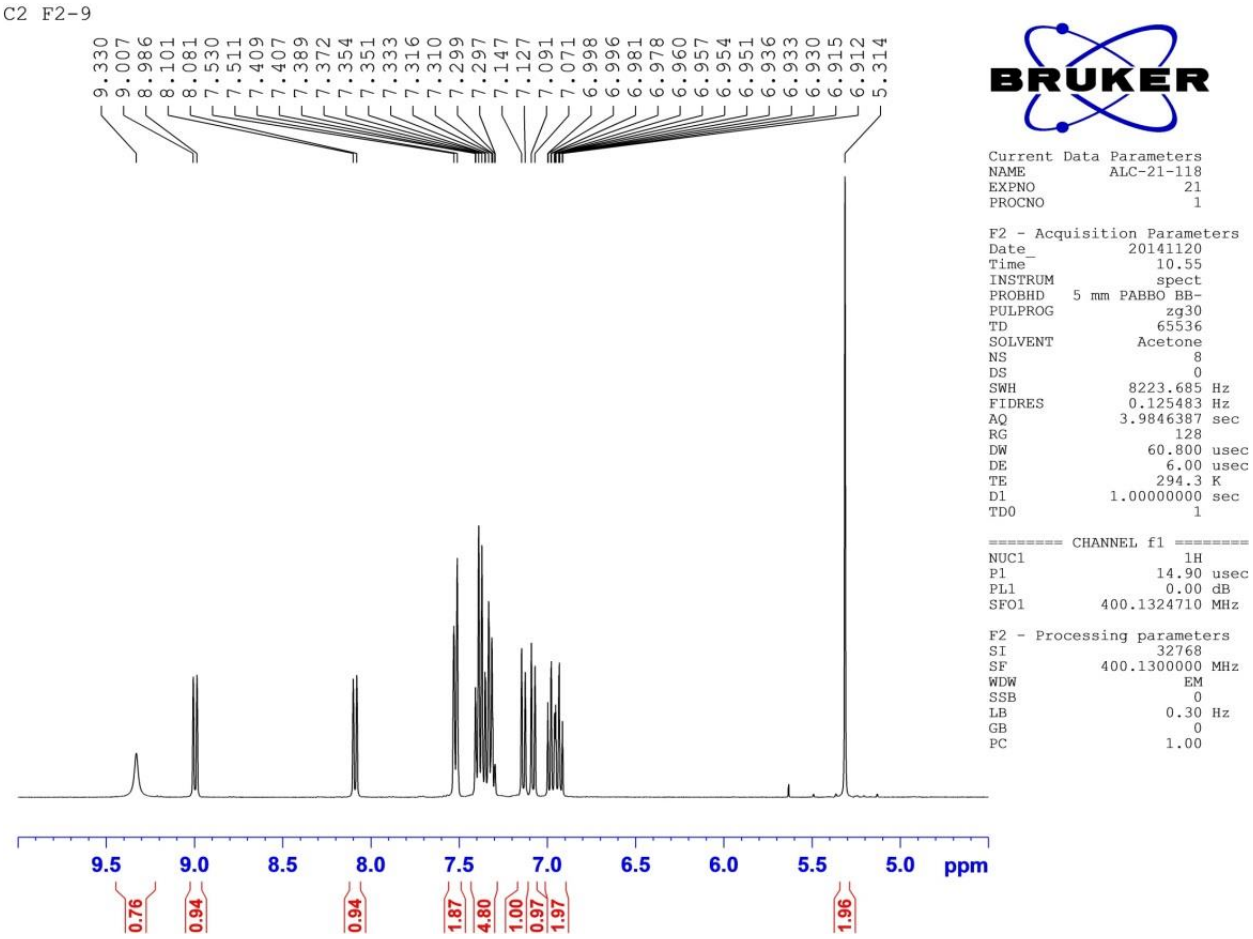


O-benzyl-N-(9'-acridinyl)-hydroxylamine, 6f

Yield: 16%. ^{1}H 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 ($C_{20}H_{17}N_2O$). UV λ_{max}: 259 nm, A_{259} = 0.36471. ΔT_m = 6.6°C. MTT IC_{50} = 33.2±0.6μM.

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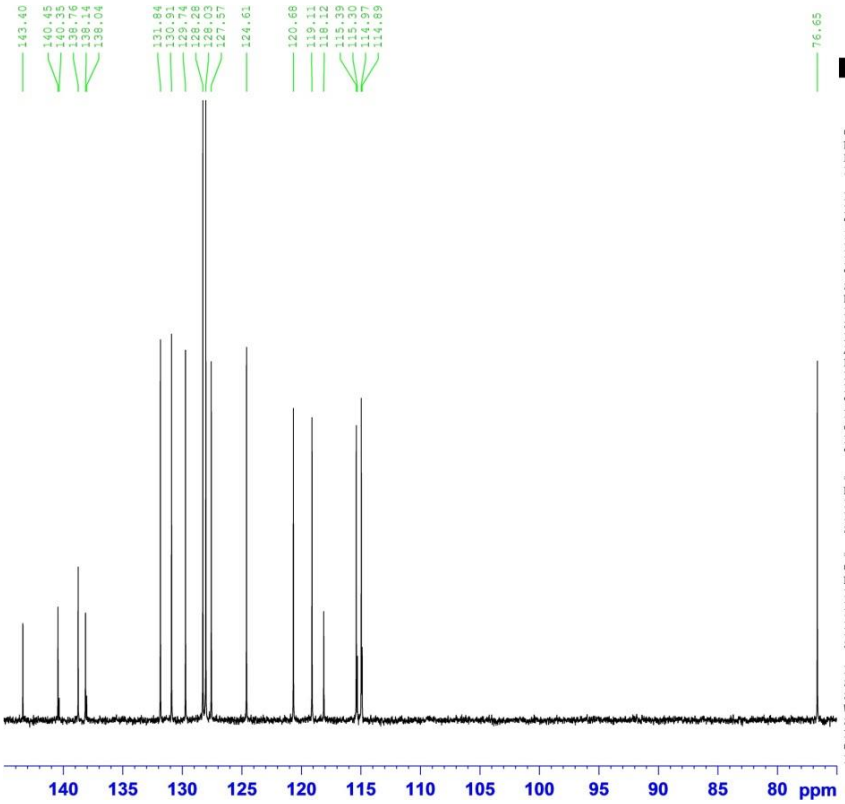


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FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                   64
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DE                 6.00 usec
TE                296.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

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P1                  9.55 usec
PL1                -2.00 dB
SFO1         100.6228298 MHz

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NUC2                 1H
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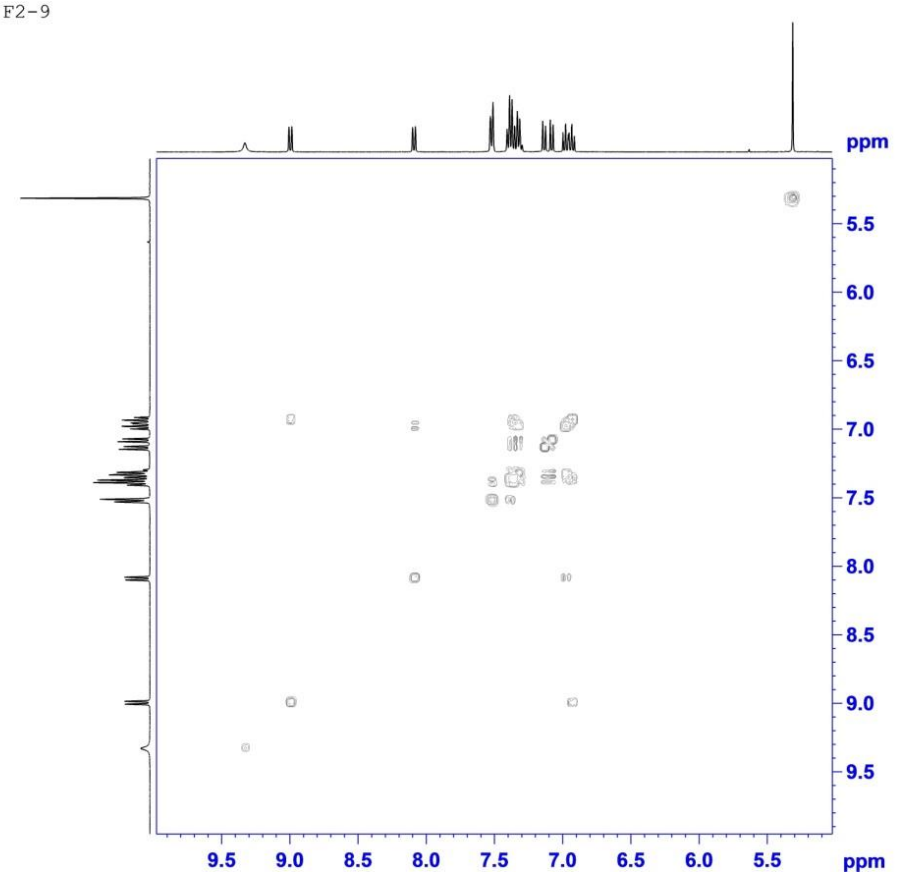


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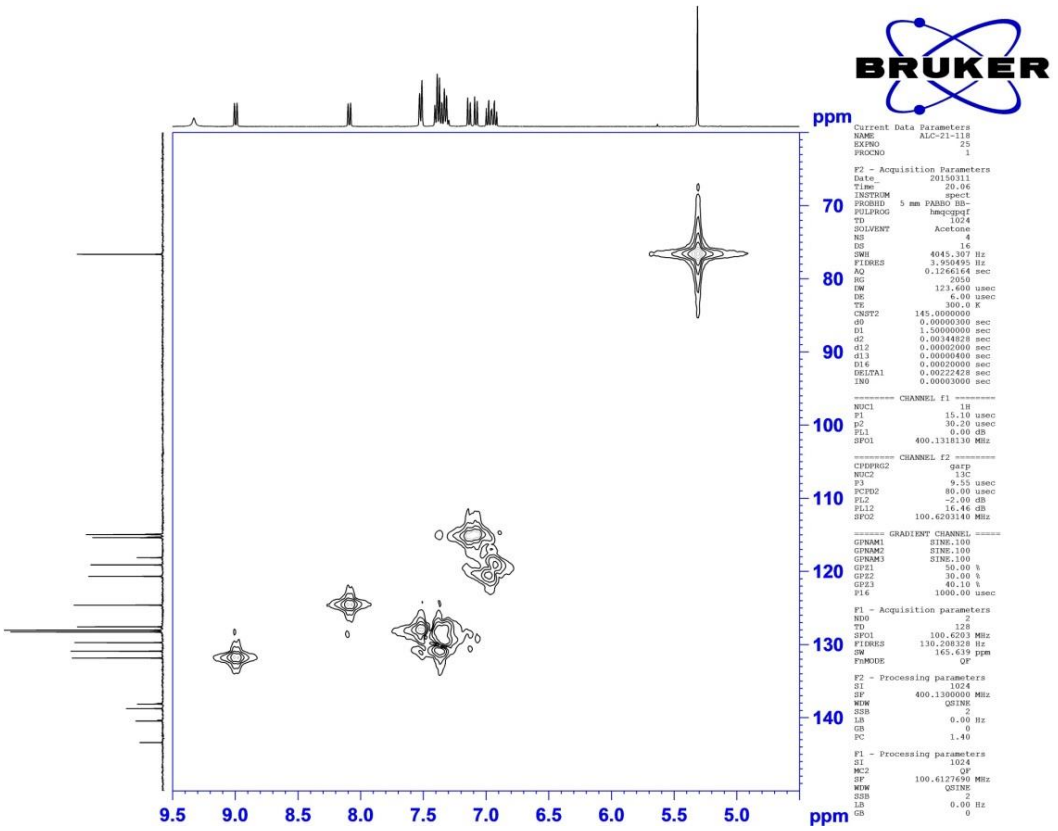
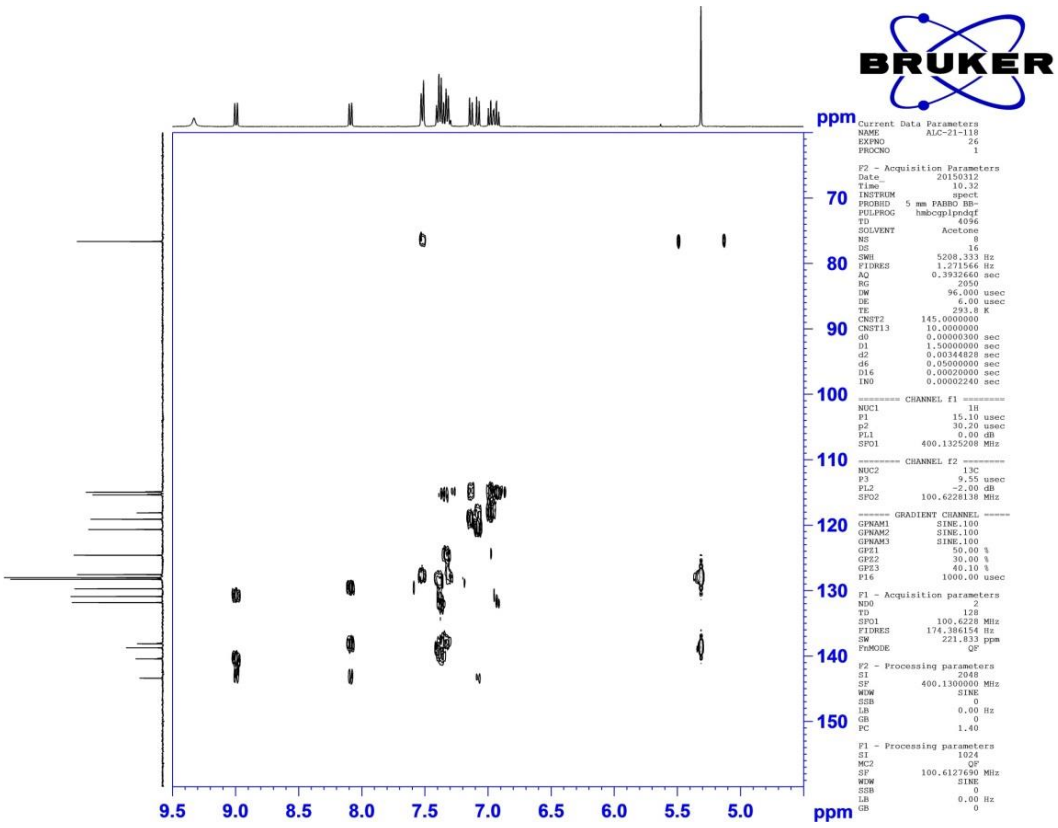
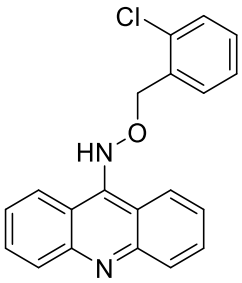
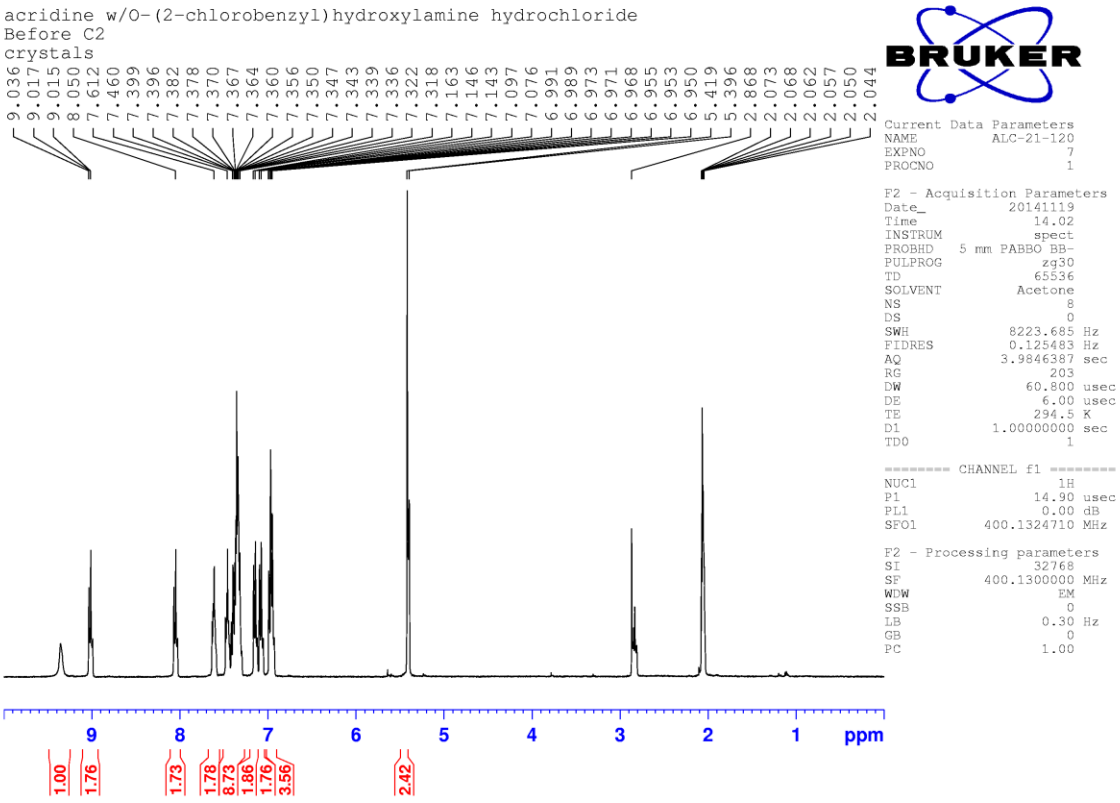


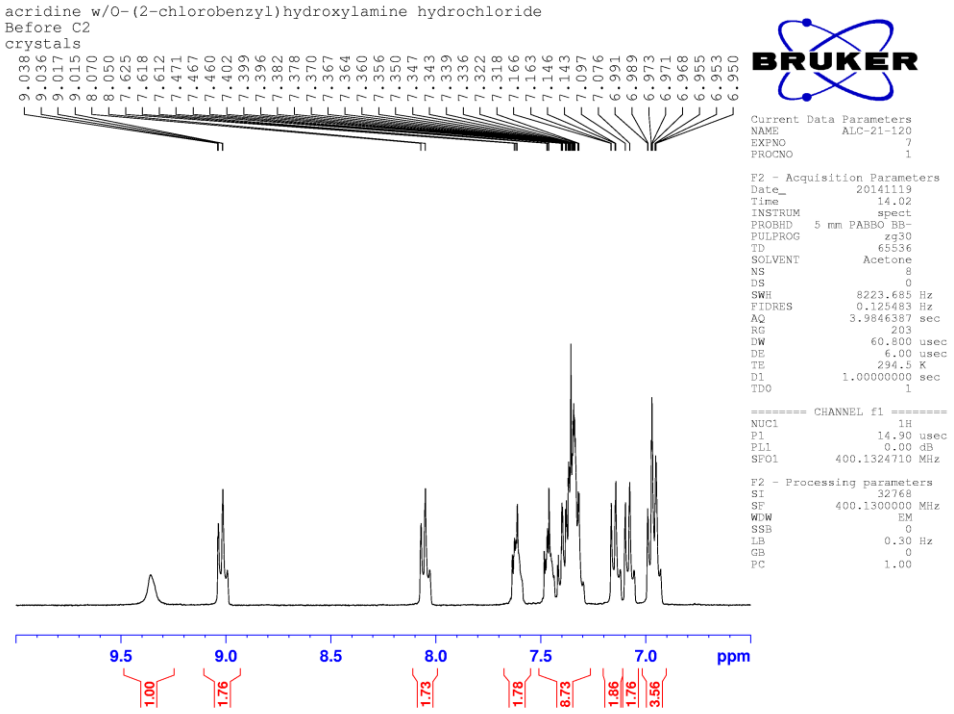


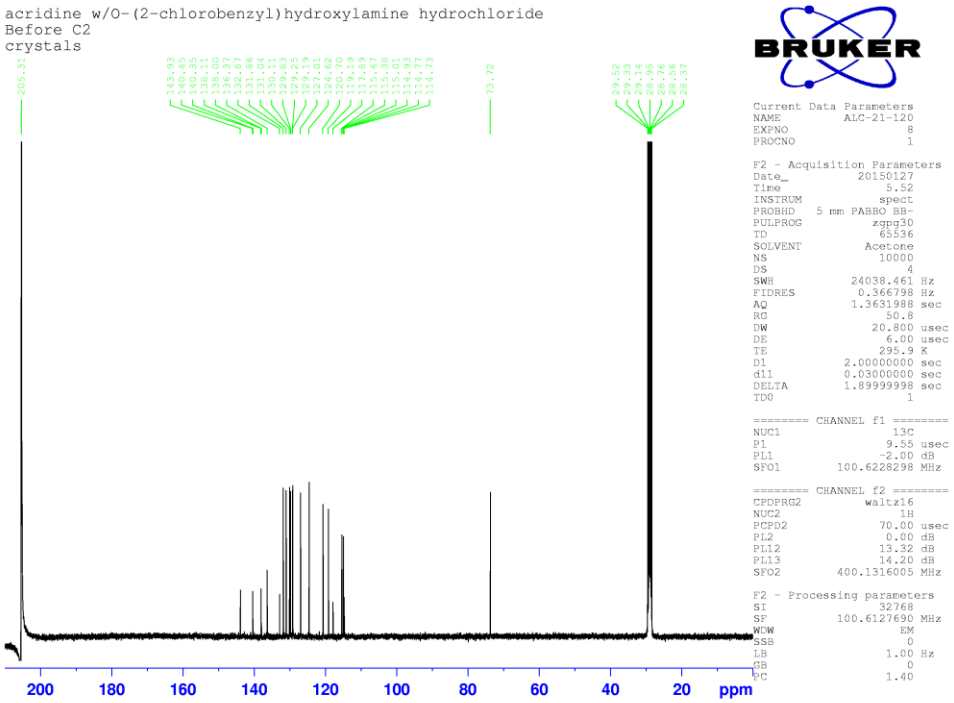


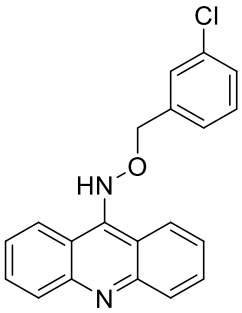
O-(2-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6g

Yield: 15%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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 ($C_{20}H_{16}N_2OCl$). ΔT_m = 18.2°C. MTT IC_{50} = 17.4±0.2μM.



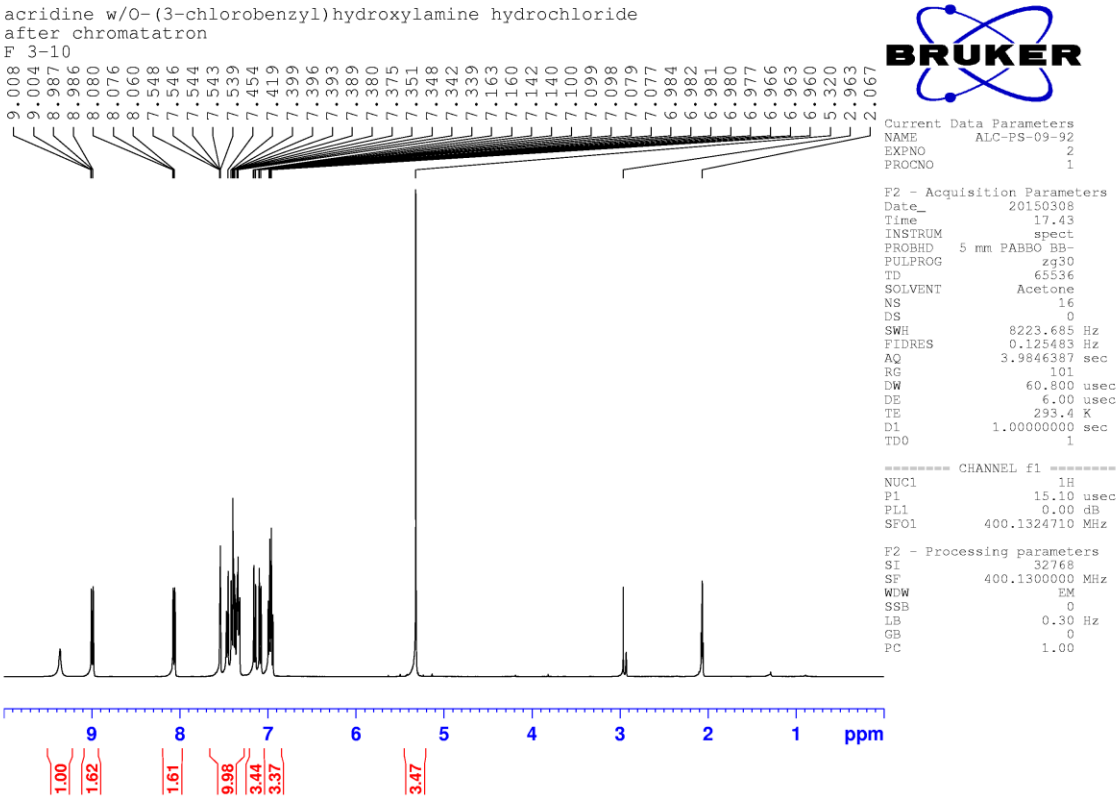


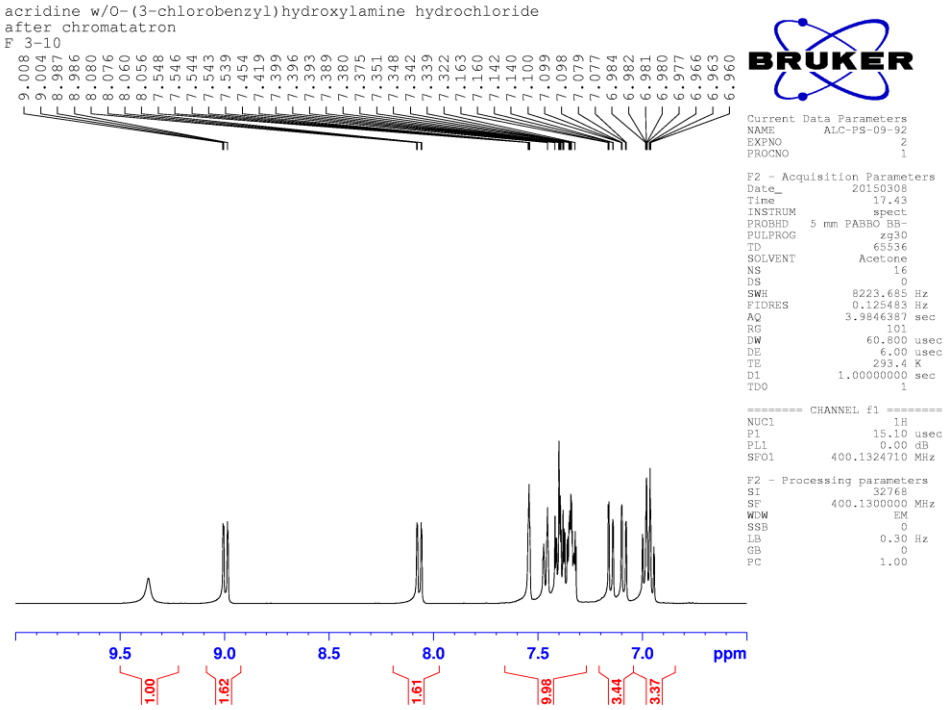


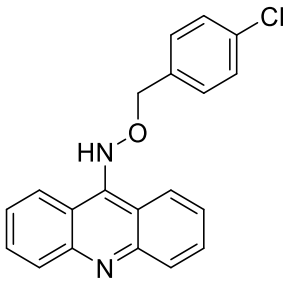


O-(3-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6h

Yield: 46%. ^{1}HNMR (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}CNMR (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 ($C_{20}H_{16}N_2OCl$). ΔT_m = 18.5°C. MTT IC_{50} = 18.0±0.2μM

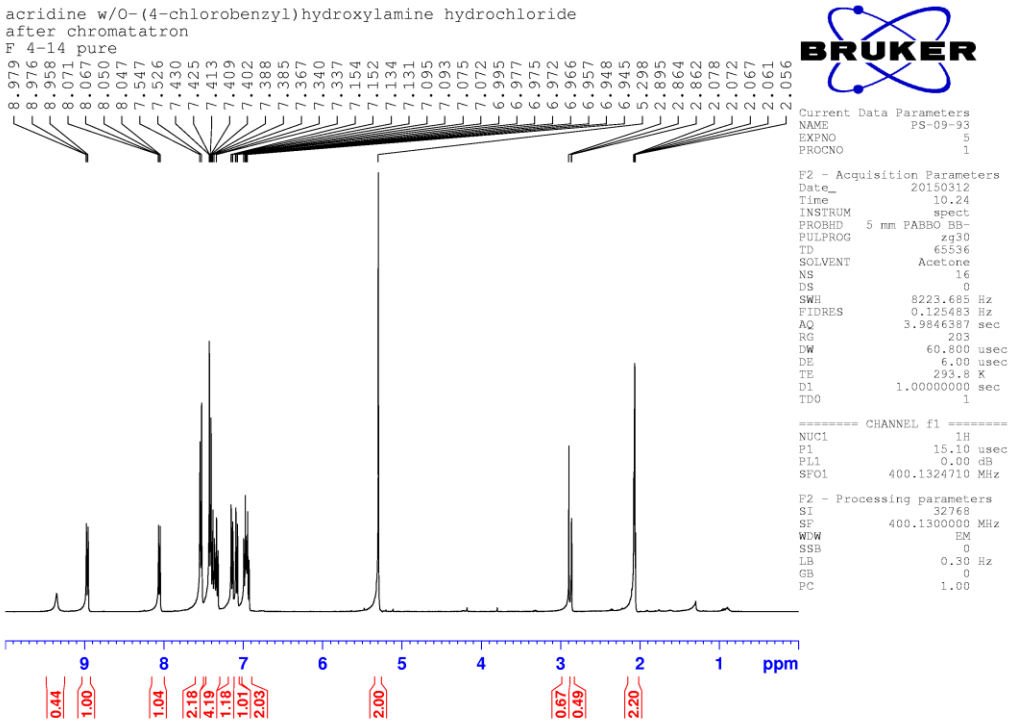


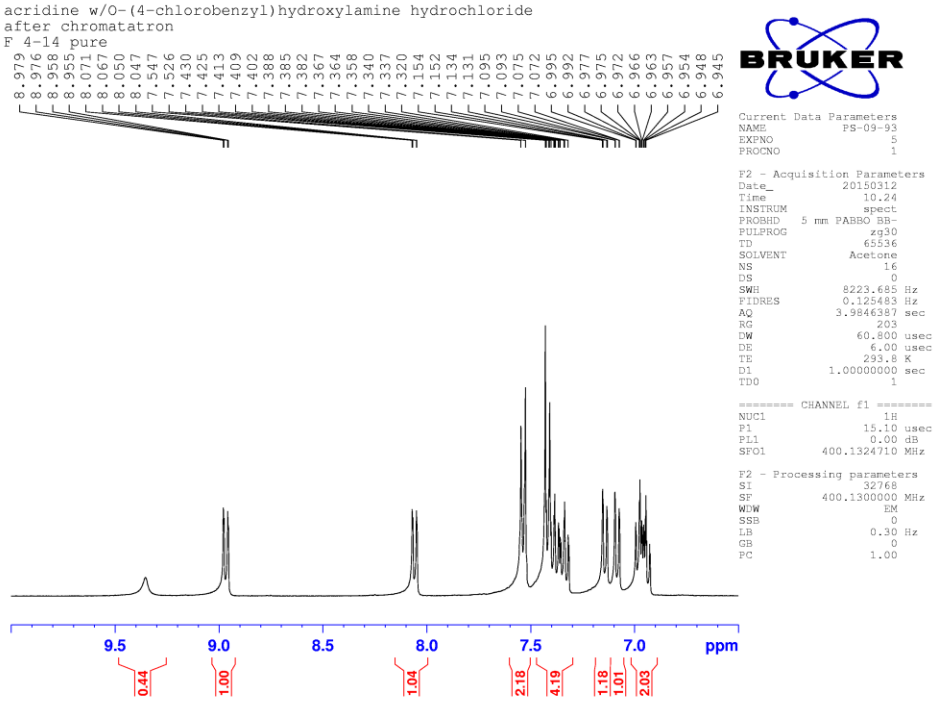




O-(4-chlorobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6i

Yield: 30%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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 ($C_{20}H_{16}N_2OCl$). ΔT_m = 20.2°C. MTT IC_{50} = 17.0±0.4μM.



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EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
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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                  1.00000000 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
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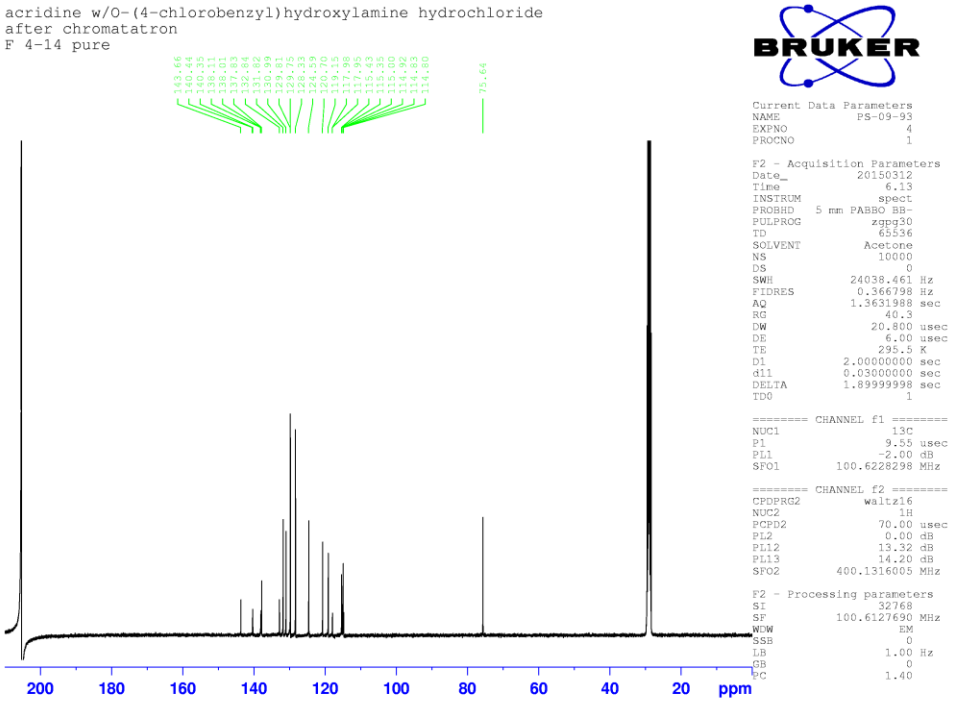


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Current Data Parameters
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EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
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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                  2.00000000 sec
d11                 0.03000000 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
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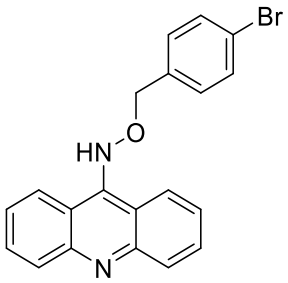
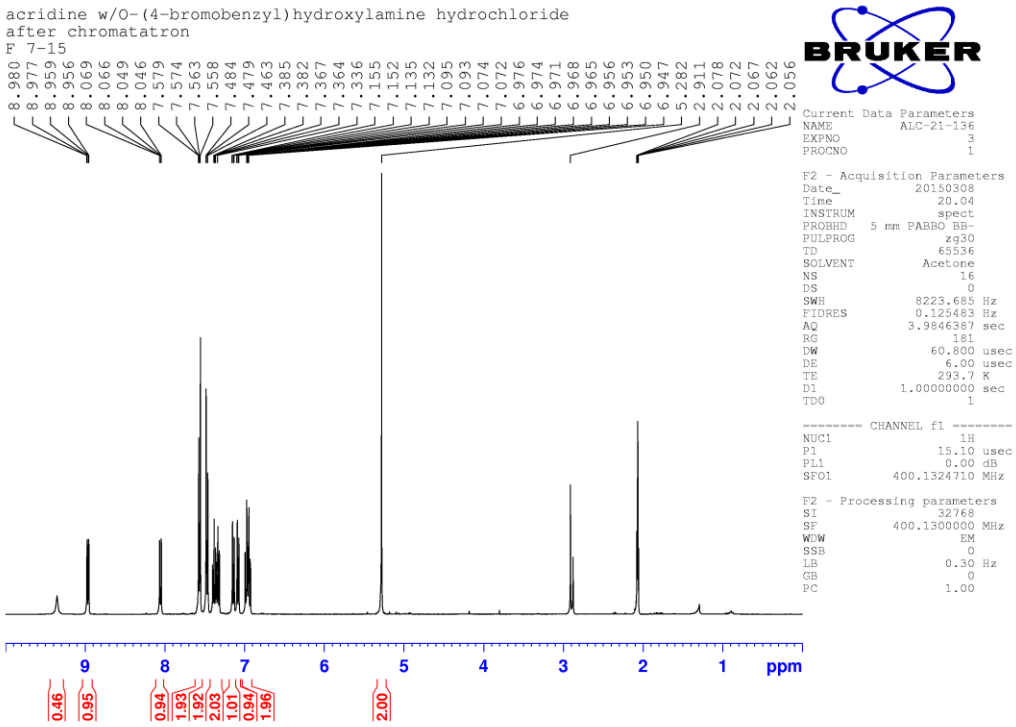
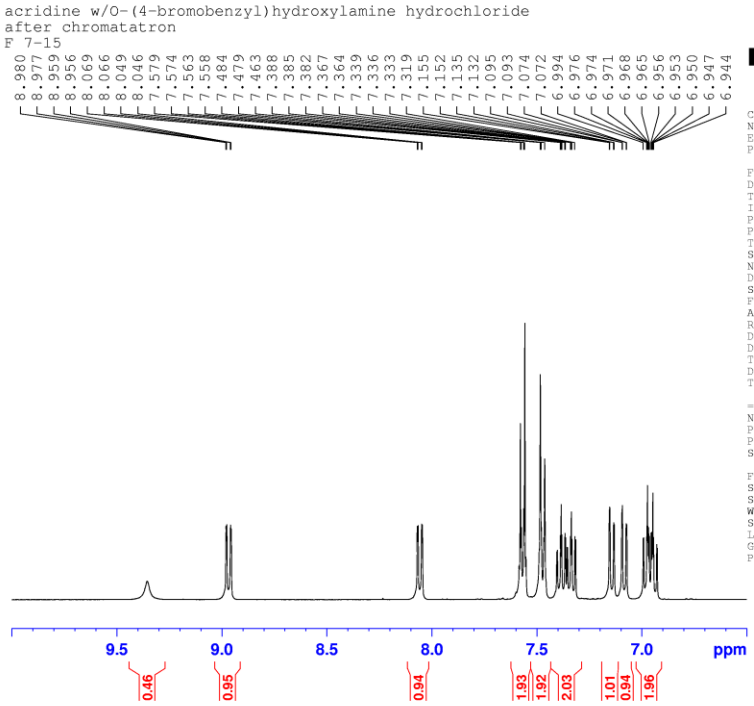
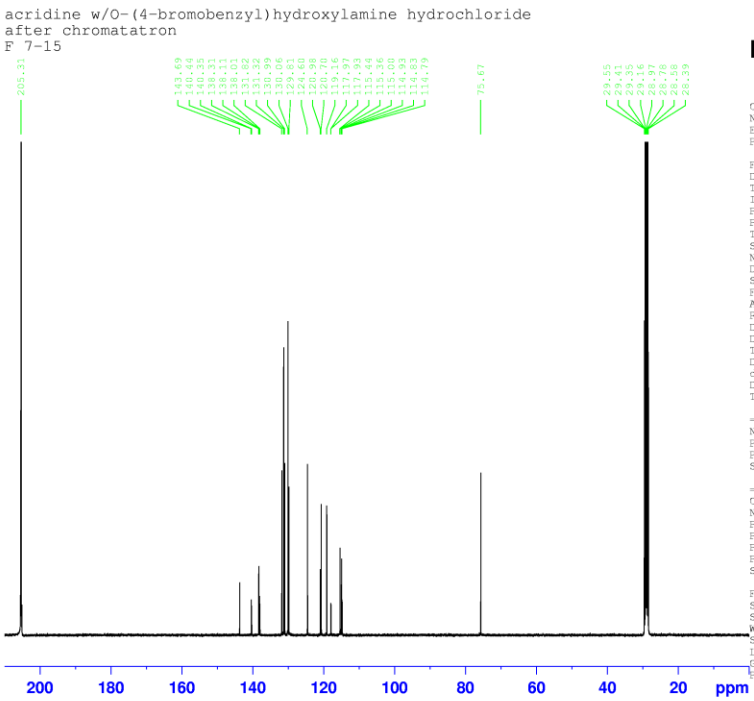


O-(4-bromobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6j

Yield: 51%. ^{1}HNMR (acetone-d_6) 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). ^{13}CNMR (acetone-d_6) 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 ($C_{20}H_{16}N_2OBr$). ΔT_m = 18.1°C. MTT IC_{50} = 18.5±4.3μM







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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
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Time 7.38
INSTRUM spect
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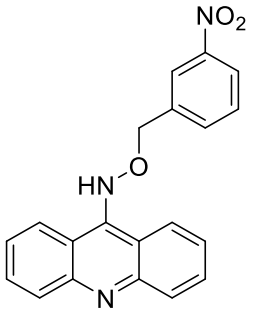
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 12000
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

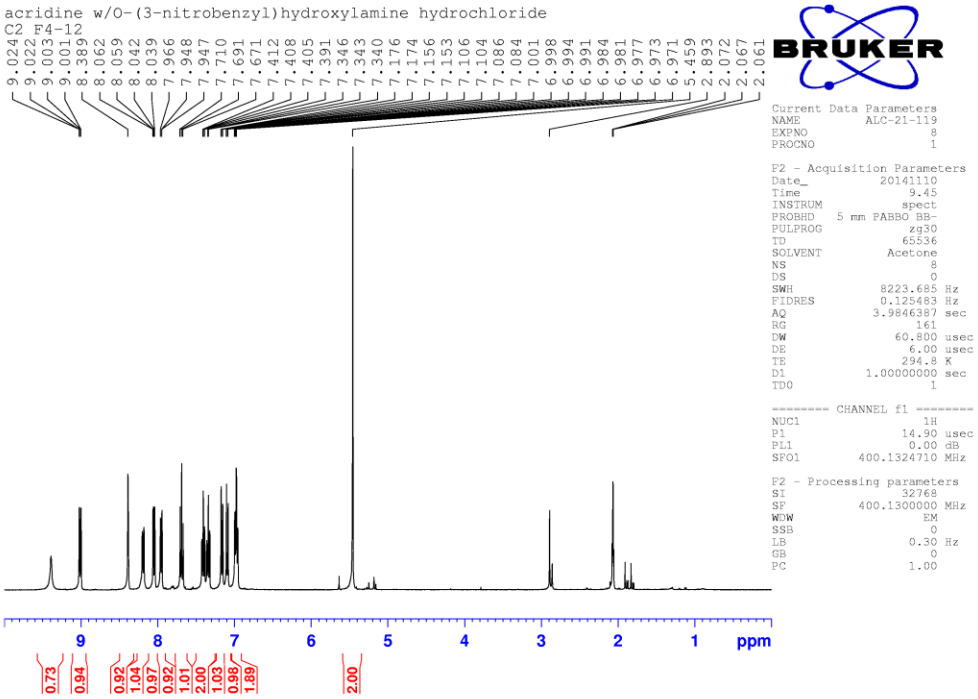
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 13.32 dB
PL13 14.20 dB
SFO2 400.1316005 MHz

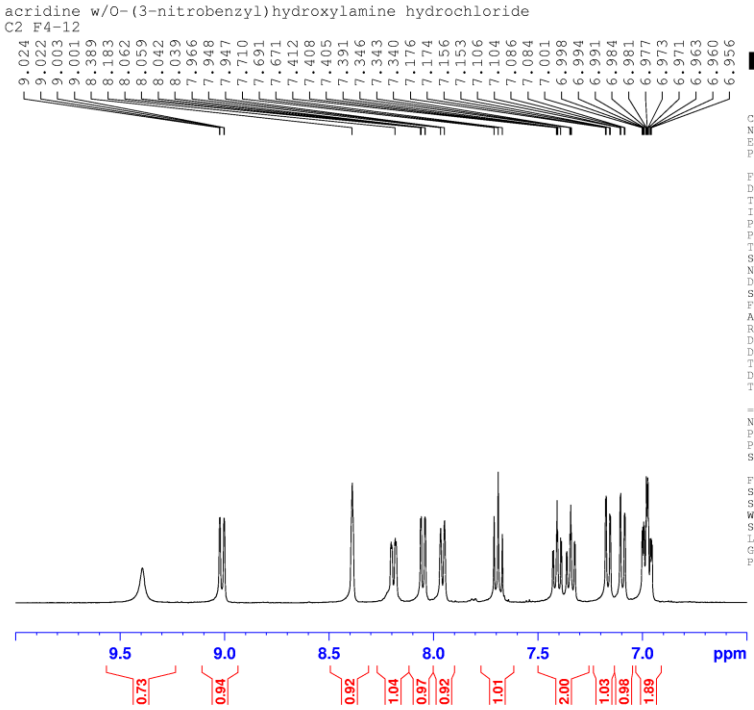
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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

Yield: 41%. ^{1}HNMR (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}CNMR (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 ($C_{20}H_{16}N_3O_3$).. ΔT_m = 15.1°C. MTT IC_{50} = 31.8±0.1μM





BRUKER

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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            1.00000000 sec
TD0                    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
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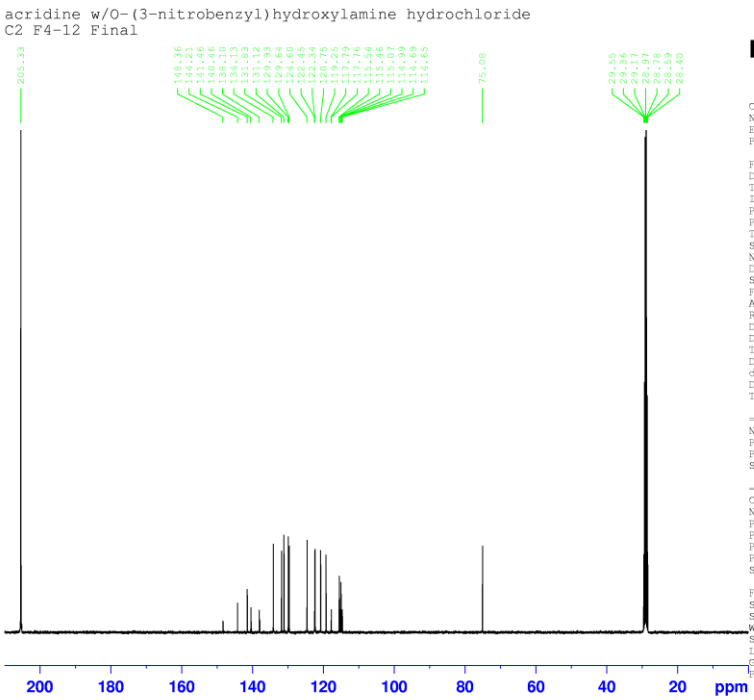

BRUKER

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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            2.00000000 sec
d11           0.03000000 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
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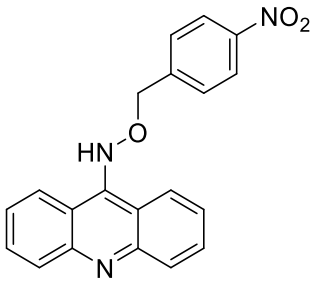
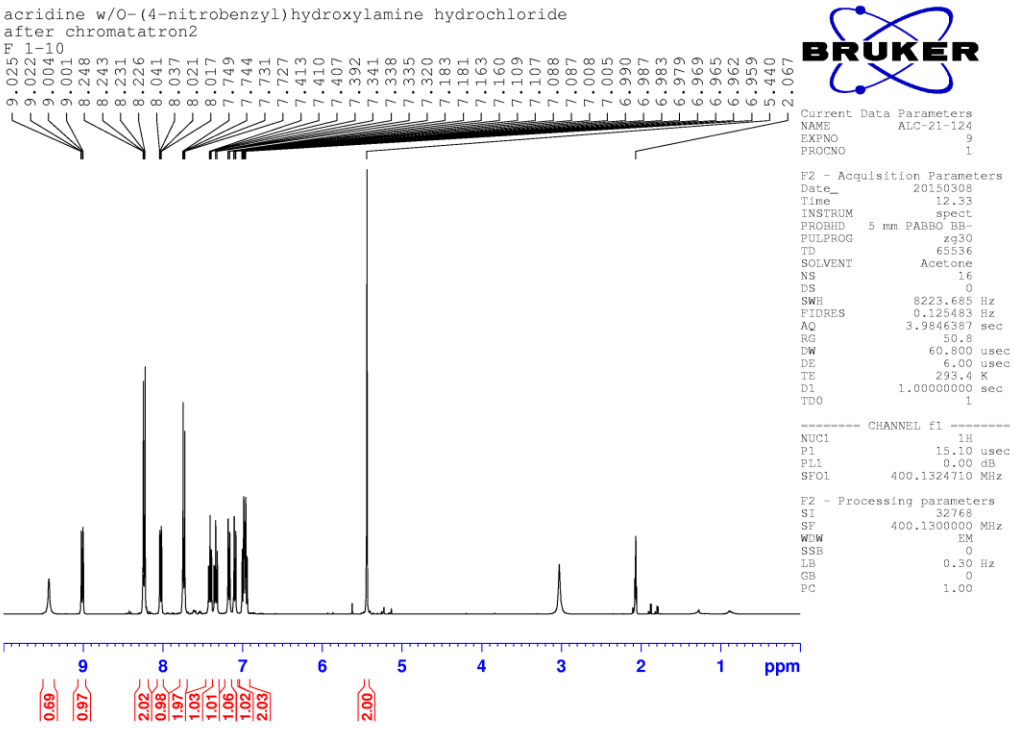
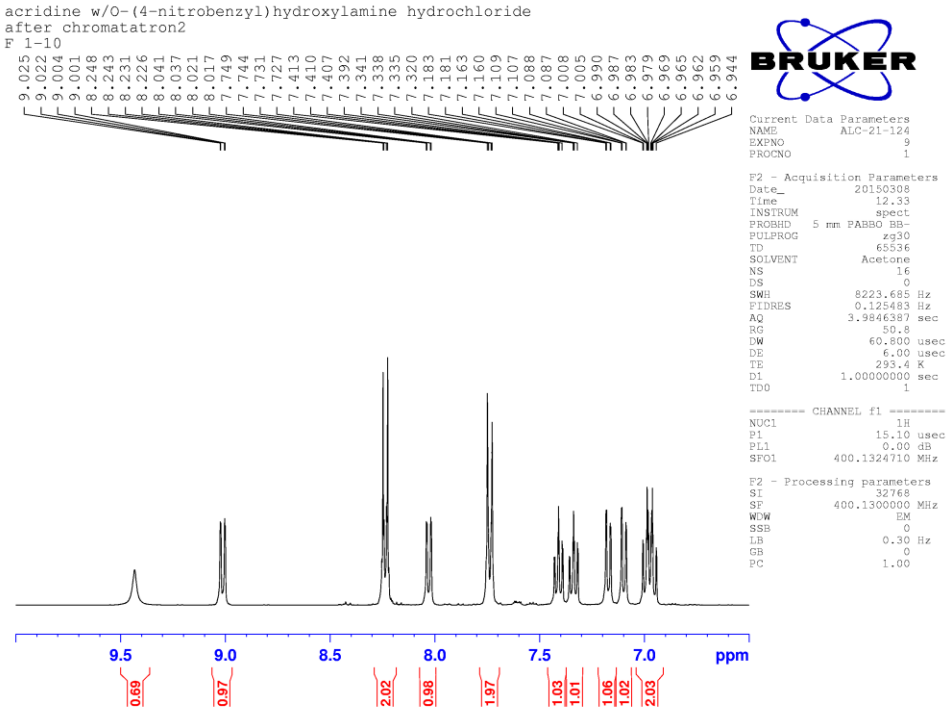


O-(4-nitrobenzyl)-N-(9'-acridinyl)-hydroxylamine, 6l

Yield: 38%. ^{1}HNMR (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}CNMR (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 ($C_{20}H_{16}N_3O_3$). MTT IC_{50} = 30.3±1.4μM





BRUKER

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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
DW               60.800 usec
DE                6.00 usec
TE               293.4 K
D1            1.00000000 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
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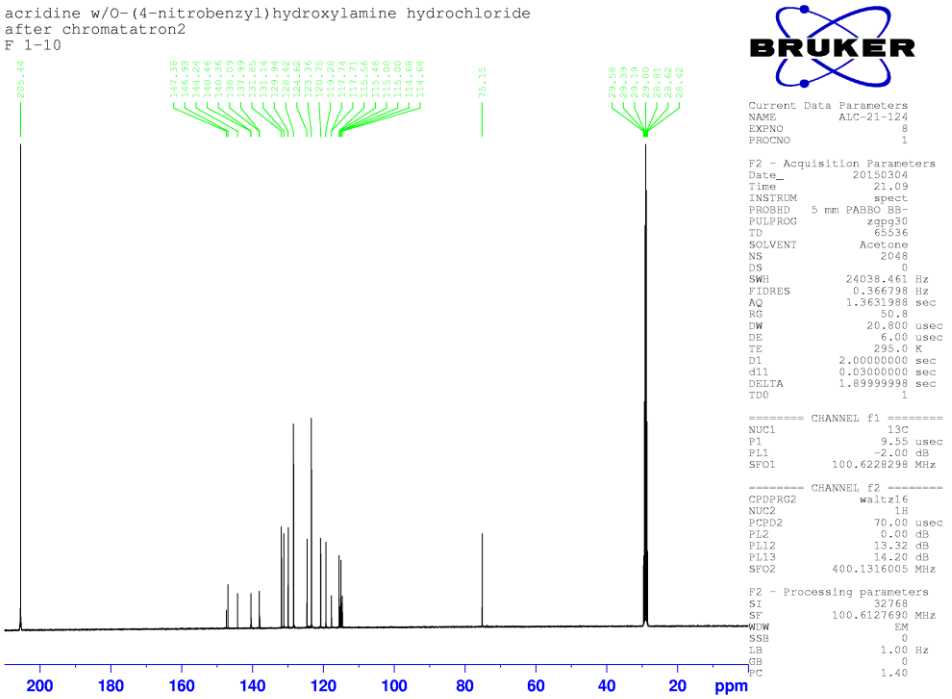

BRUKER

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

F2 - Acquisition Parameters
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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
DW               20.800 usec
DE                6.00 usec
TE               295.0 K
D1            2.00000000 sec
d11           0.03000000 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
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