

Supplementary Information

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Supplement: DMFDMA catalyzed synthesis of 2-((Dimethylamino)methylene)-3,4-dihydro-9-arylacridin-1(2H)-ones and their derivatives: *in-vitro* antifungal, antibacterial and antioxidant evaluations

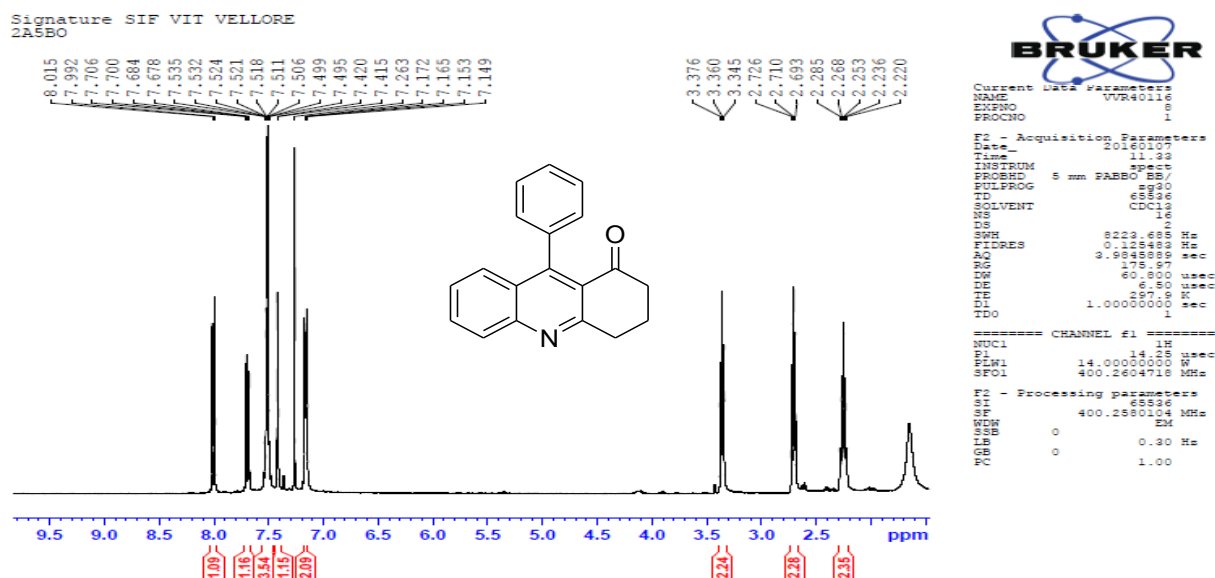


Figure 1: ¹H NMR spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

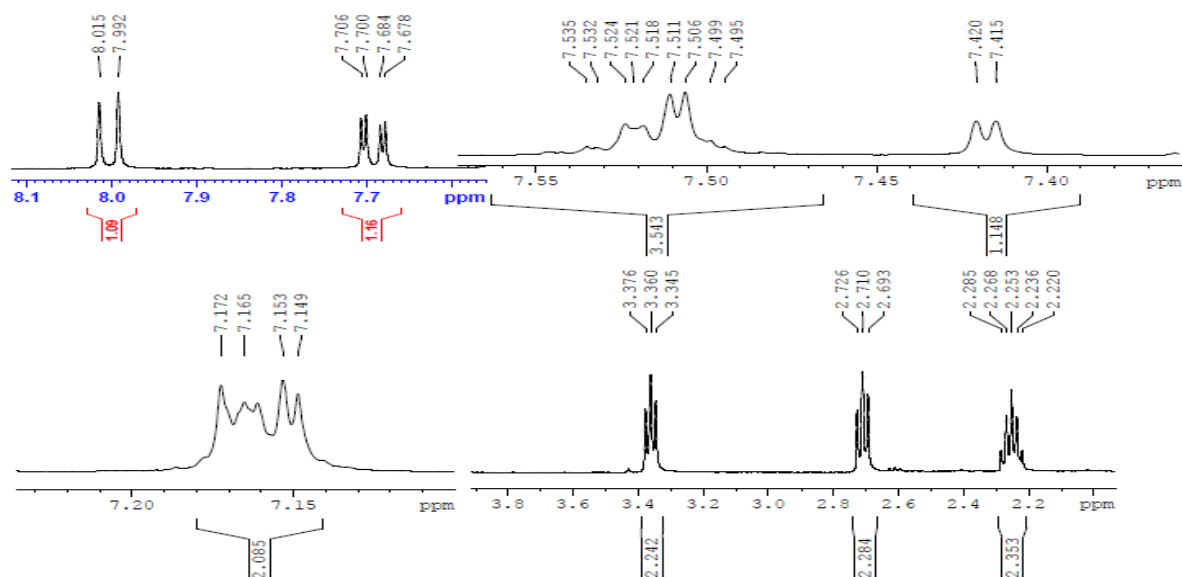


Figure 2: Enlarged ^1H NMR spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

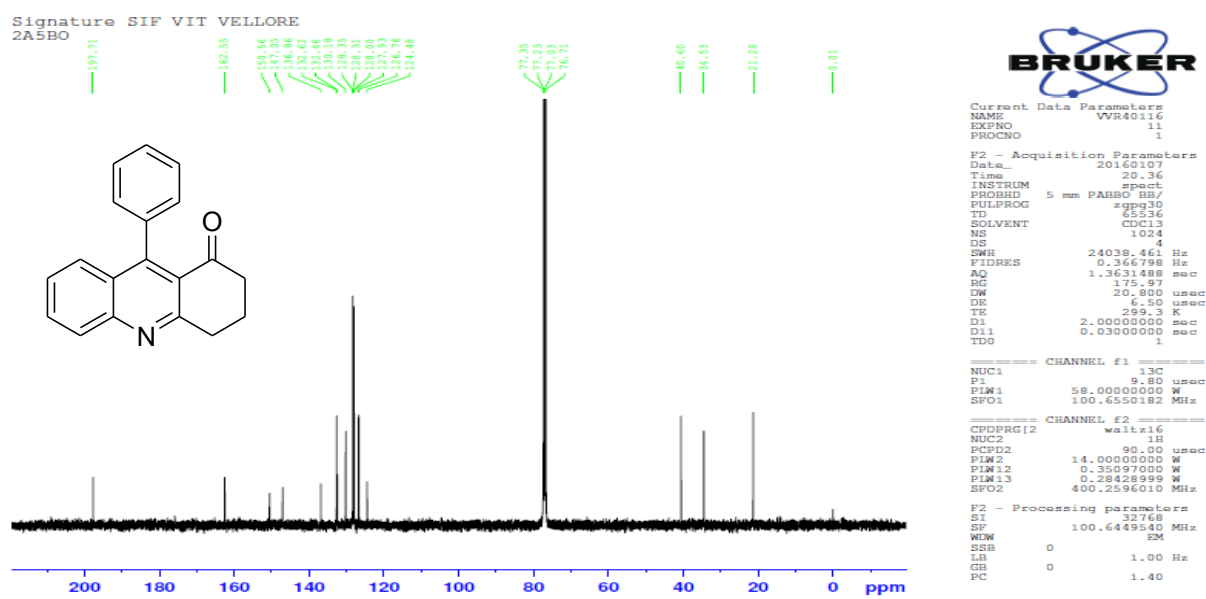


Figure 3: ^{13}C NMR spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

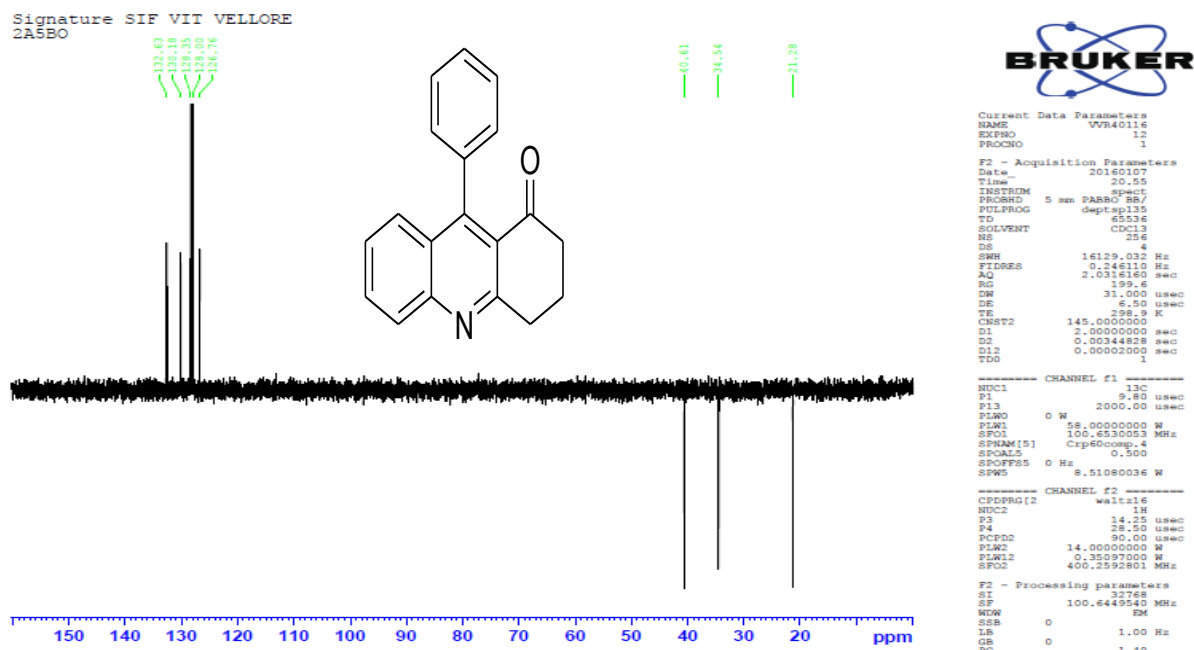


Figure 4: DEPT 135 spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

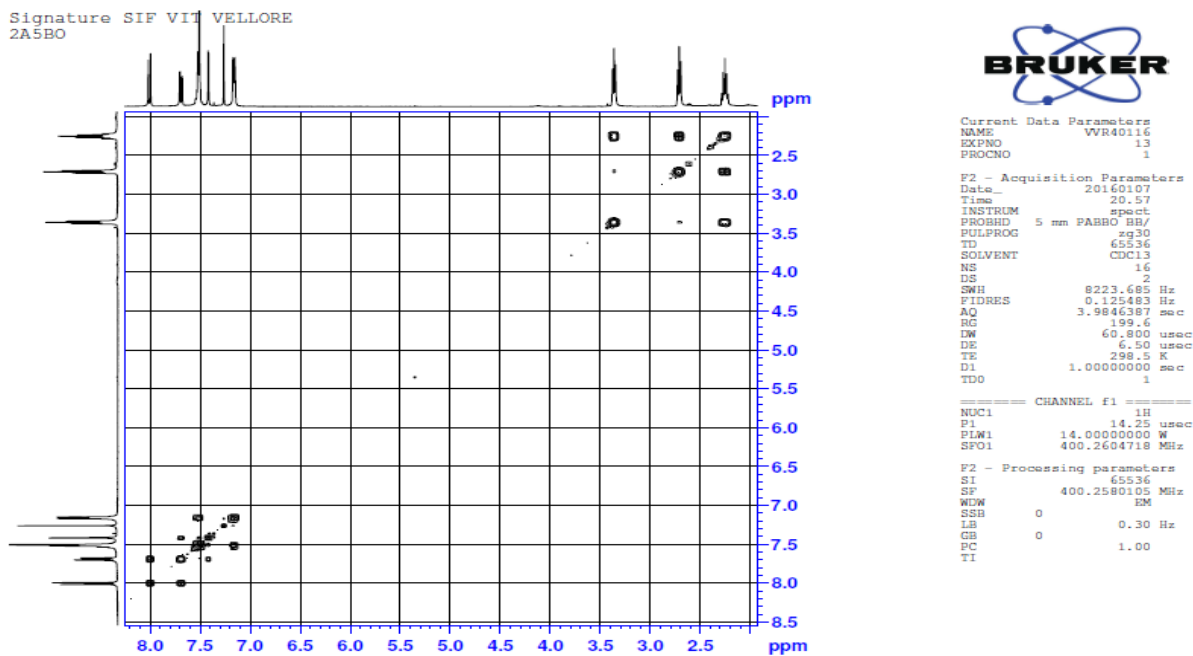
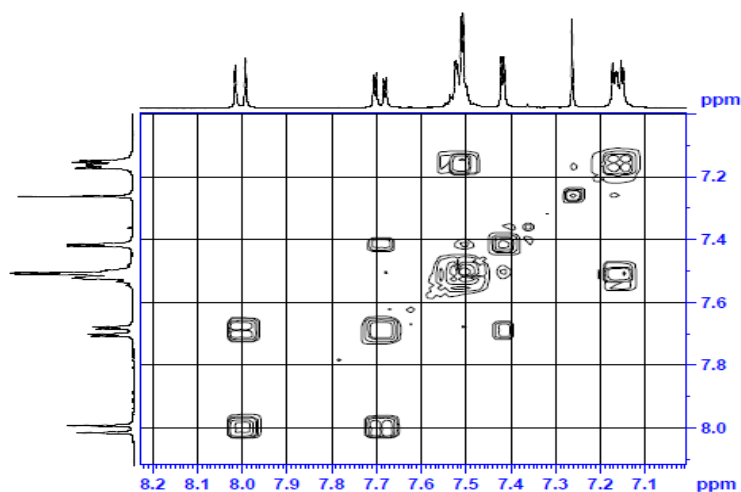


Figure 5: H-H COSY spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

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2A5BO



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Current Data Parameters
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PROCNO    1

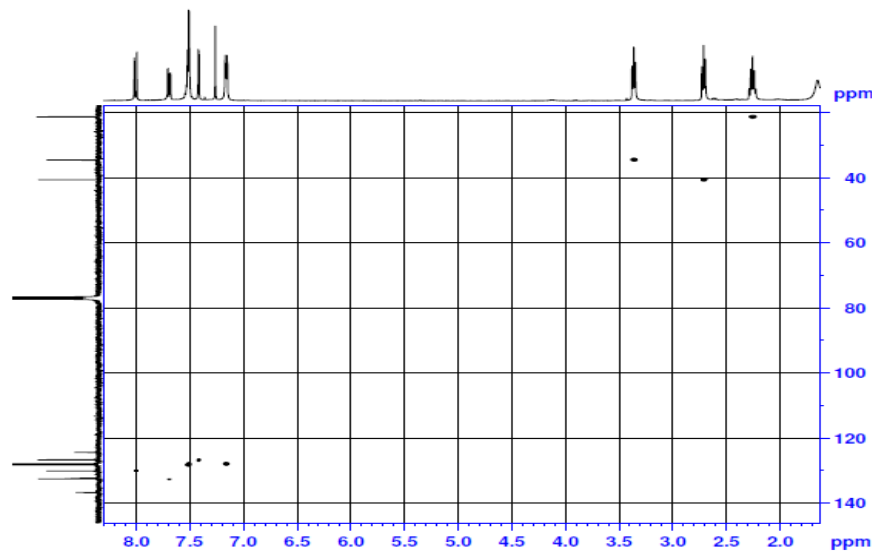
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DS         2
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FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         178.97
DW         60.800 usec
DE         6.50 usec
TE         297.5 K
D1         1.00000000 sec
TD0        1

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PLW1       14.00000000 W
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F2 - Processing parameters
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SF         400.2580104 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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Figure 6: Enlarged H-H COSY spectrum of 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

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Current Data Parameters
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PROCNO    1

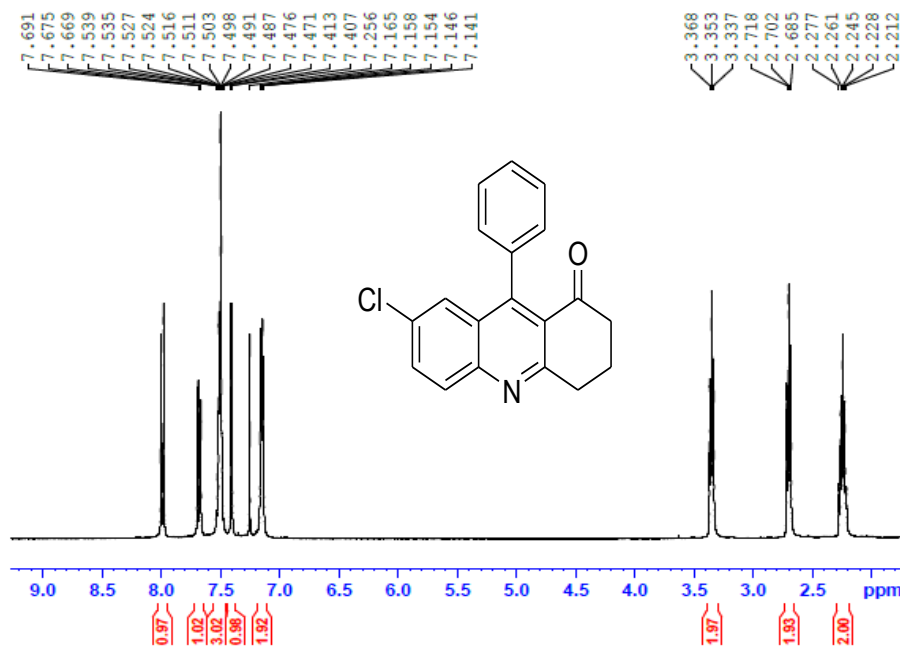
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SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         178.97
DW         60.800 usec
DE         6.50 usec
TE         298.5 K
D1         1.00000000 sec
TD0        1

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PLW1       14.00000000 W
SFO1       400.2604718 MHz

F2 - Processing parameters
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SF         400.2580105 MHz
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LB         0.30 Hz
GB         0
PC         1.00
TI
  
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Figure 7: HSQC of spectrum 3,4-dihydro-9-phenylacridin-1(2H)-one (2a):

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2A5CO



Current Data Parameters
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EXPNO 9
PROCNO 1

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SOLVENT CDCl3
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FIDRES 0.123483 Hz
AQ 3.984589 sec
RG 142.72
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TE 297.9 K
D1 1.00000000 sec
TD0 1

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SFO1 400.2604718 MHz

F2 - Processing parameters
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SF 400.2580133 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

Figure 8: ^1H NMR spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

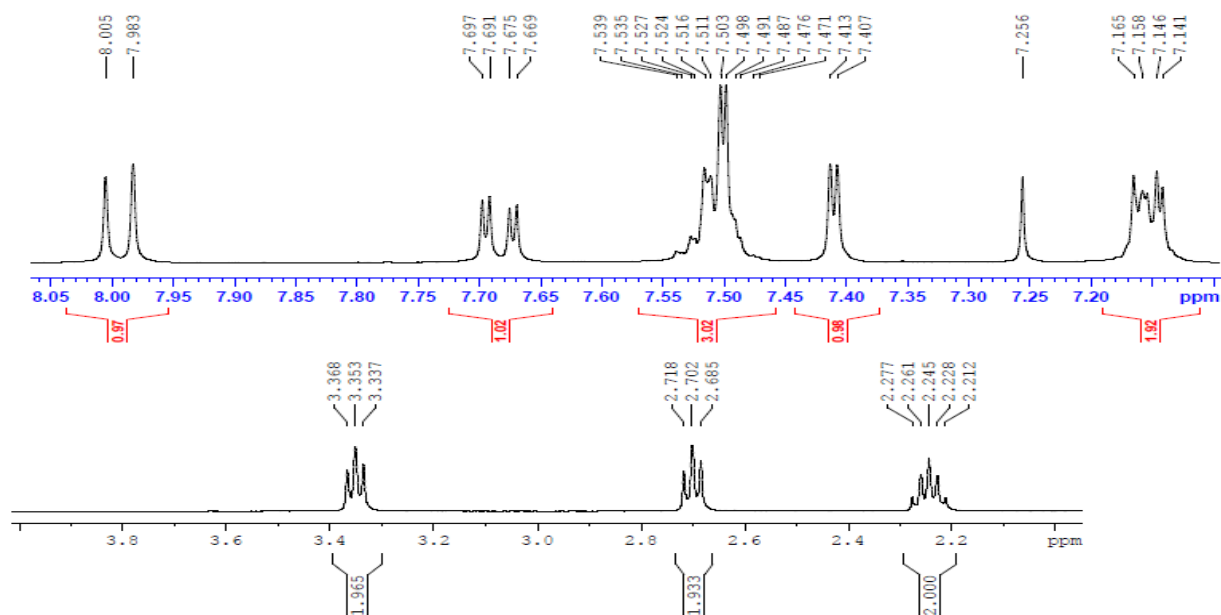


Figure 9: Enlarged ^1H NMR spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

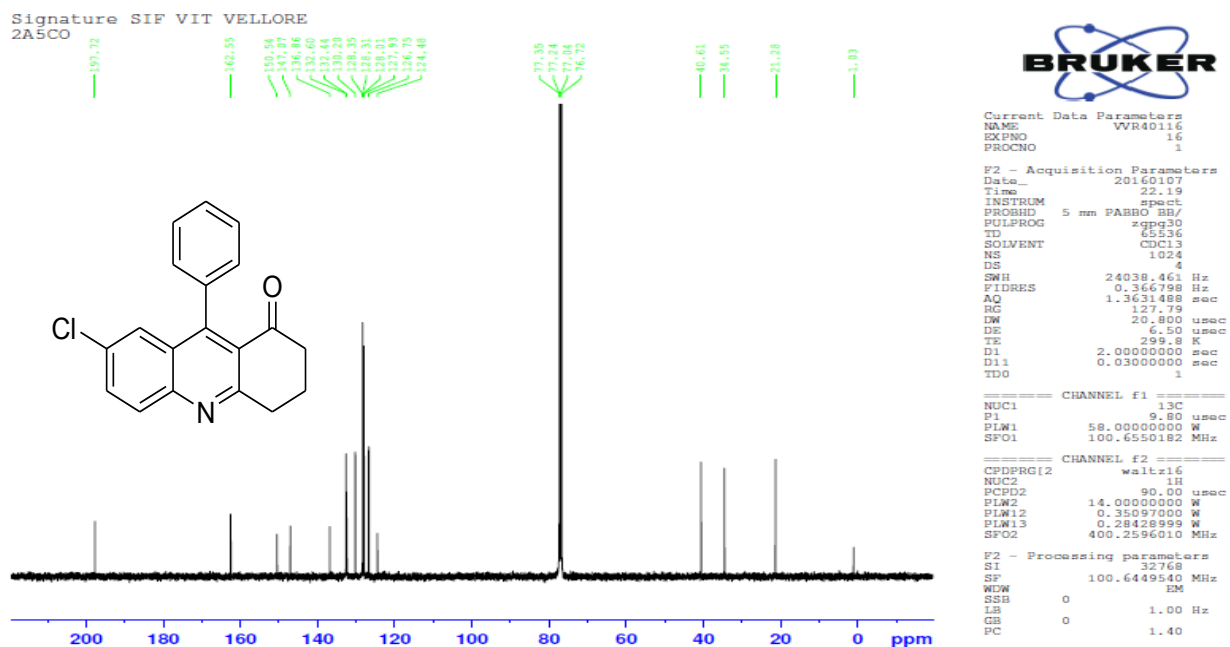
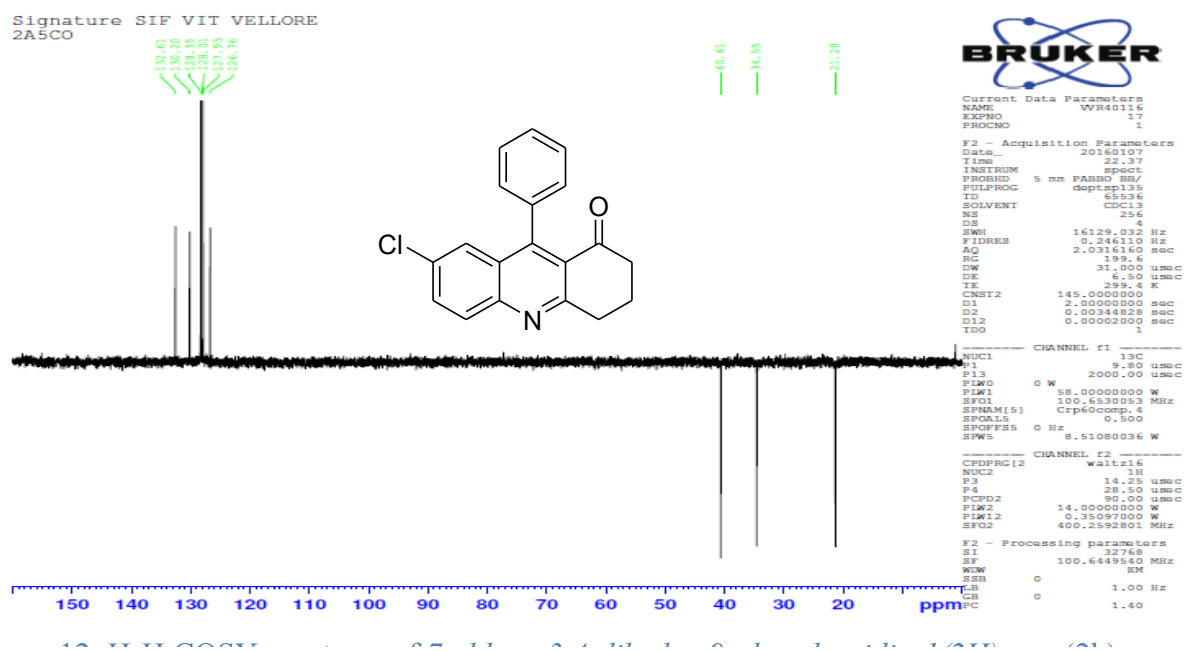
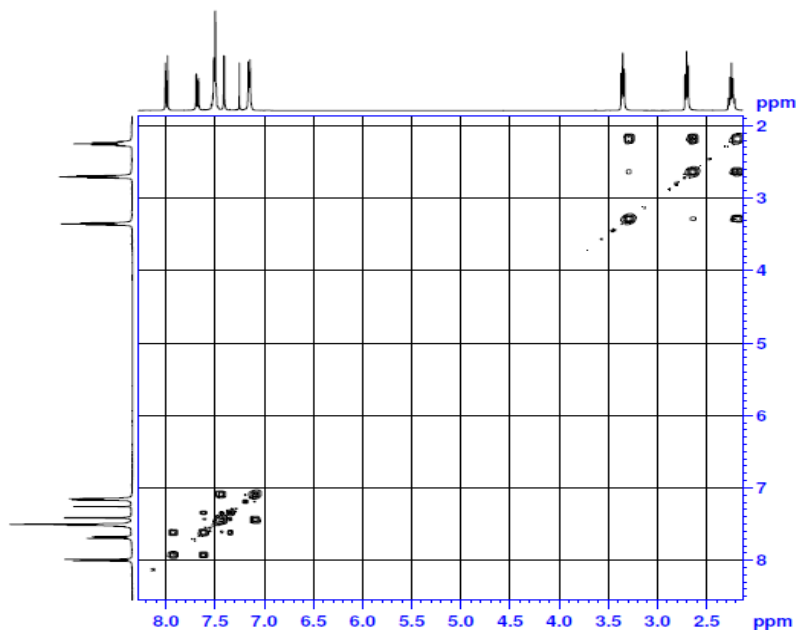
Figure 10: ^{13}C NMR spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

Figure 11: DEPT 135 spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

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Current Data Parameters
NAME VVR40116
EXPNO 9
PROCNO 1

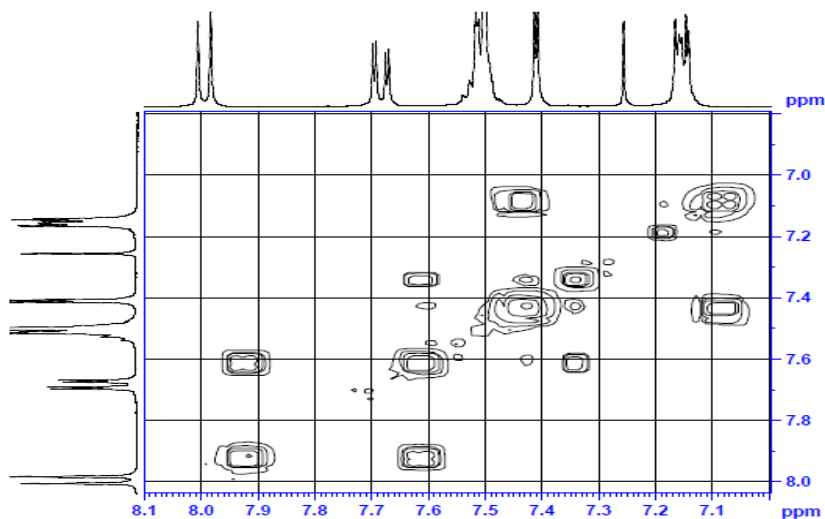
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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 12: H-H COSY spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

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Current Data Parameters
NAME VVR40116
EXPNO 9
PROCNO 1

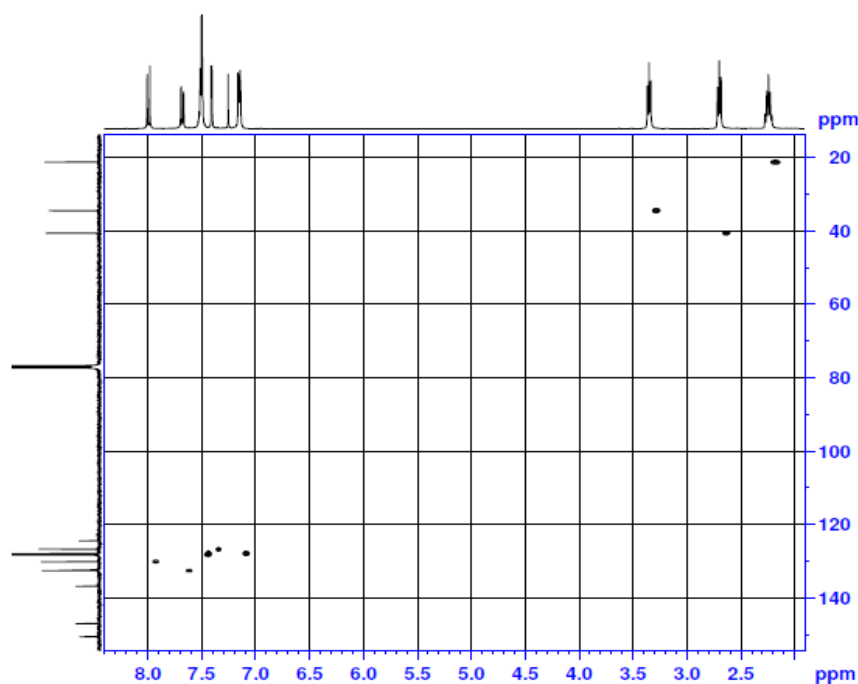
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 13: Enlarged H-H COSY spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

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2A5CO



Current Data Parameters
NAME VWR40116
EXPNO 9
PROCNO 1

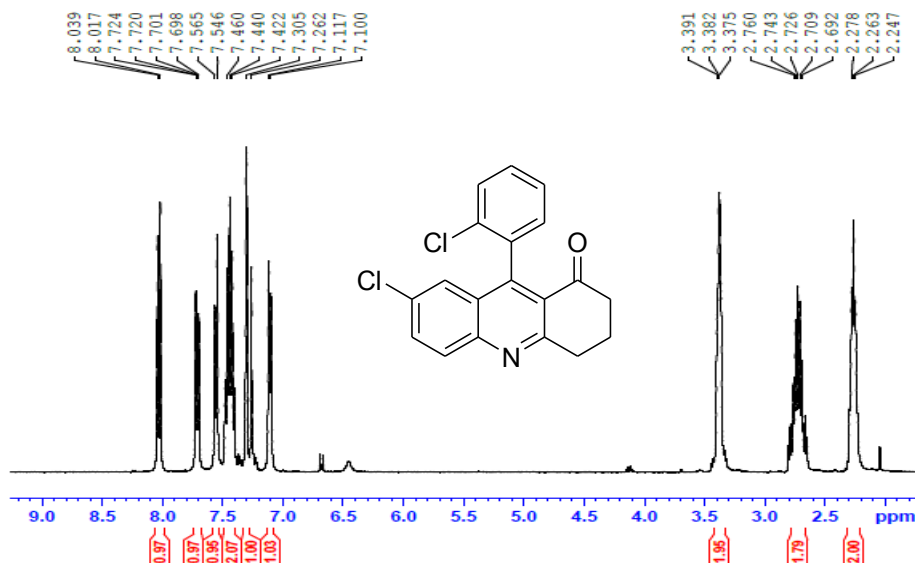
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 14: HSQC spectrum of 7-chloro-3,4-dihydro-9-phenylacridin-1(2H)-one (2b):

Signature SIF VIT VELLORE
2ACLLO



Current Data Parameters
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EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 175.97
DW 60.800 usec
DE 6.50 usec
TE 301.3 K
D1 1.00000000 sec
TDO 1

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P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580133 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

Figure 15: ¹H NMR spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c):

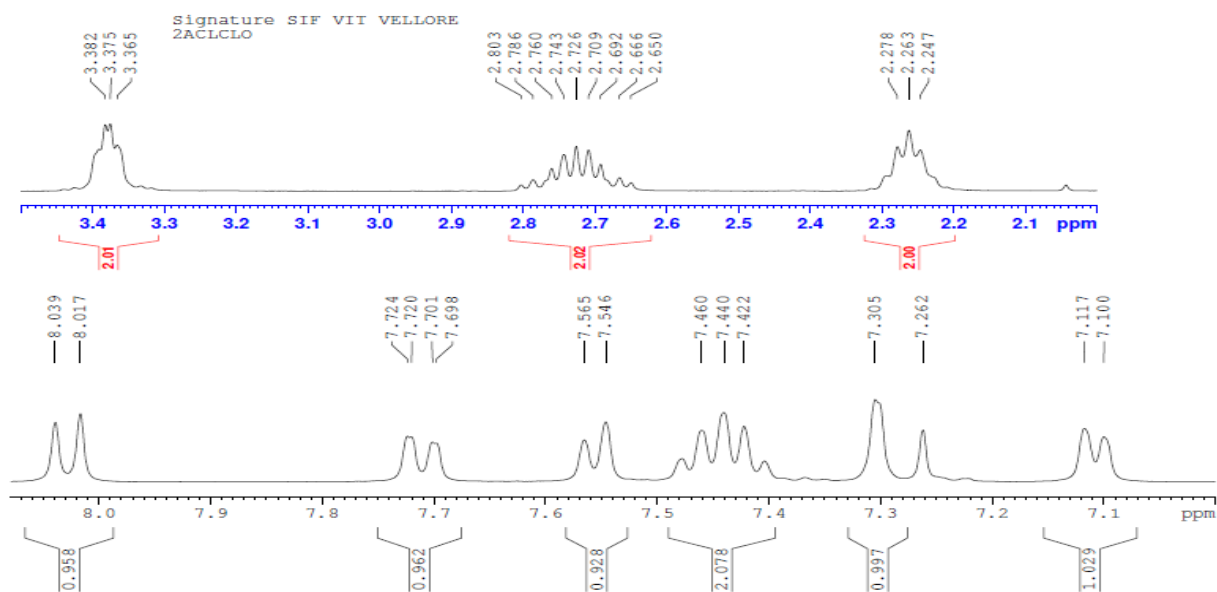


Figure 16: Enlarged ¹H NMR spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c):

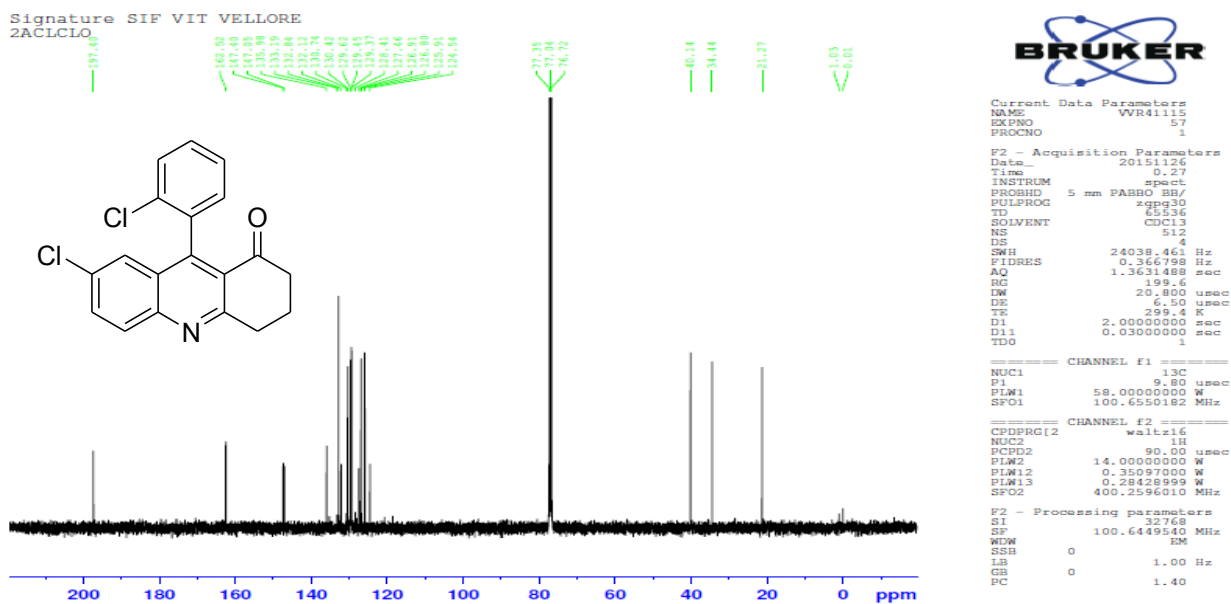
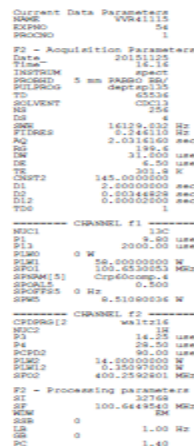


Figure 17: ¹³C NMR spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c) :



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2ACLCLO

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PROCNO 1

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PULPROG zgpg30
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FIDRES 1.835644 Hz
AQ 0.273365 sec
RG 112.69
SW 133.00 Hz
DE 35.40 Hz
TE 301.2 K
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D1 1.91395 sec
D11 0.0300000 sec
D13 0.0300000 sec
D15 0.0000400 sec
D16 0.0002000 sec
D19 0.0002600 sec

CHANNEL F1
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P2 14.25 sec
P17 2500.00 sec
P18 14.0000000 sec
P19 4.20539999 sec
SFO1 400.253005 MHz

GRADIENT CHANNEL
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GPI1 16.00 s
P16 1000.00 sec

F1 - Acquisition parameters
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FIDRES 1.835644 Hz
SW 133.00 Hz
PULPROG zgpg30

F2 - Processing parameters
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GB 0
WDW 0
SSB 0 Hz
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 0
SF 400.258011 MHz
WDW 0
SSB 0
LB 0 Hz
GB 0

Figure 19: H-H COSY spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c):

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2ACLCLO

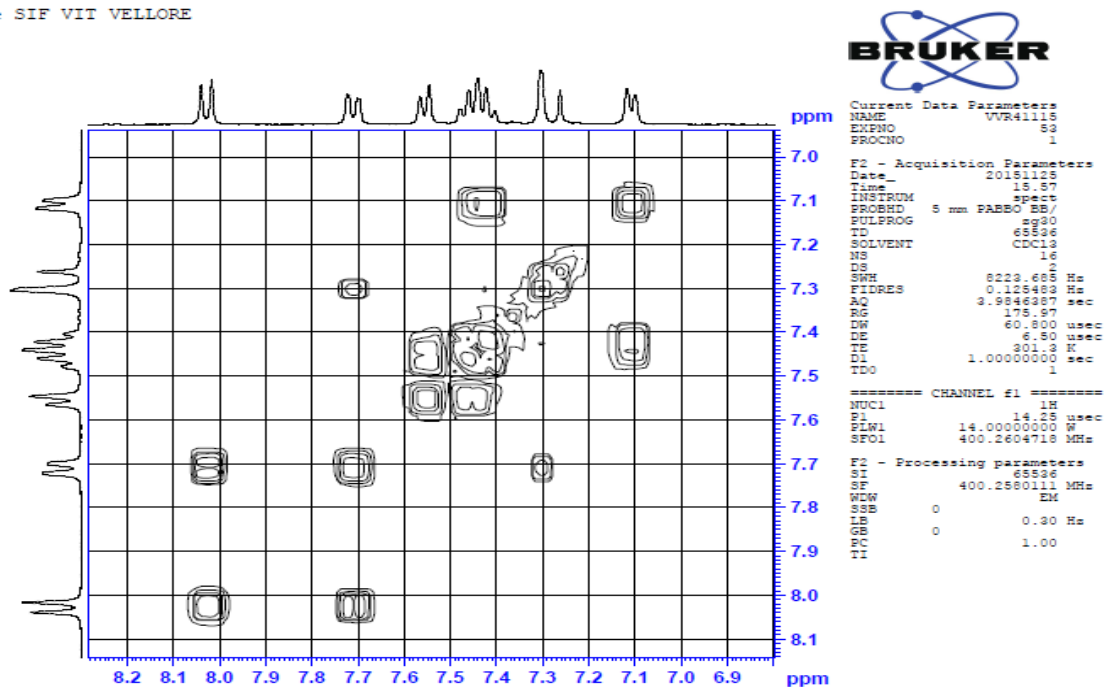


Figure 20: Enlarged H-H COSY spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c):

Signature SIF VIT VELLORE
2ACLCLO

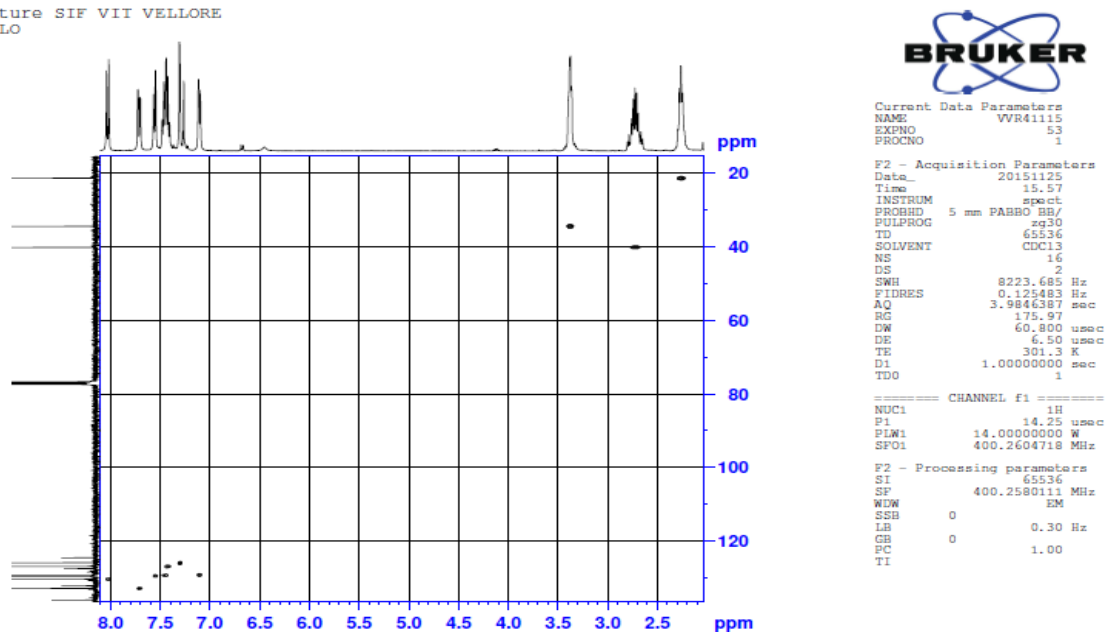


Figure 21: Enlarged HSQC spectrum of 7-chloro-9-(2-chlorophenyl)-3,4-dihydroacridin-1(2H)-one (2c):

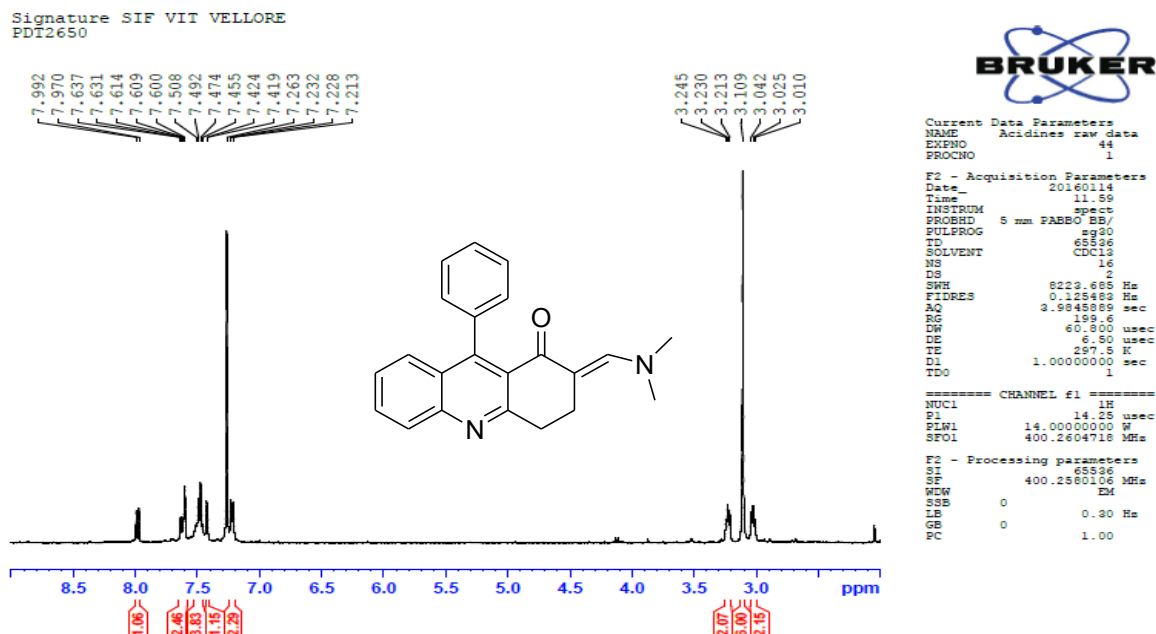


Figure 22: ^1H NMR spectrum of (E)-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3a):

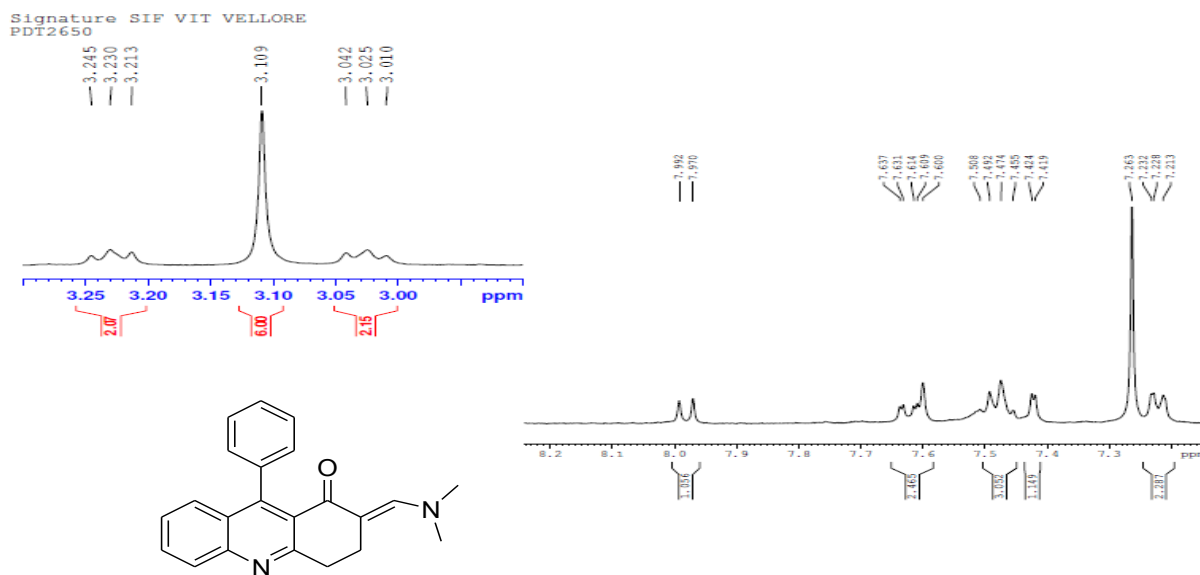


Figure 23: Enlarged ^1H NMR spectrum of (E)-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3a):

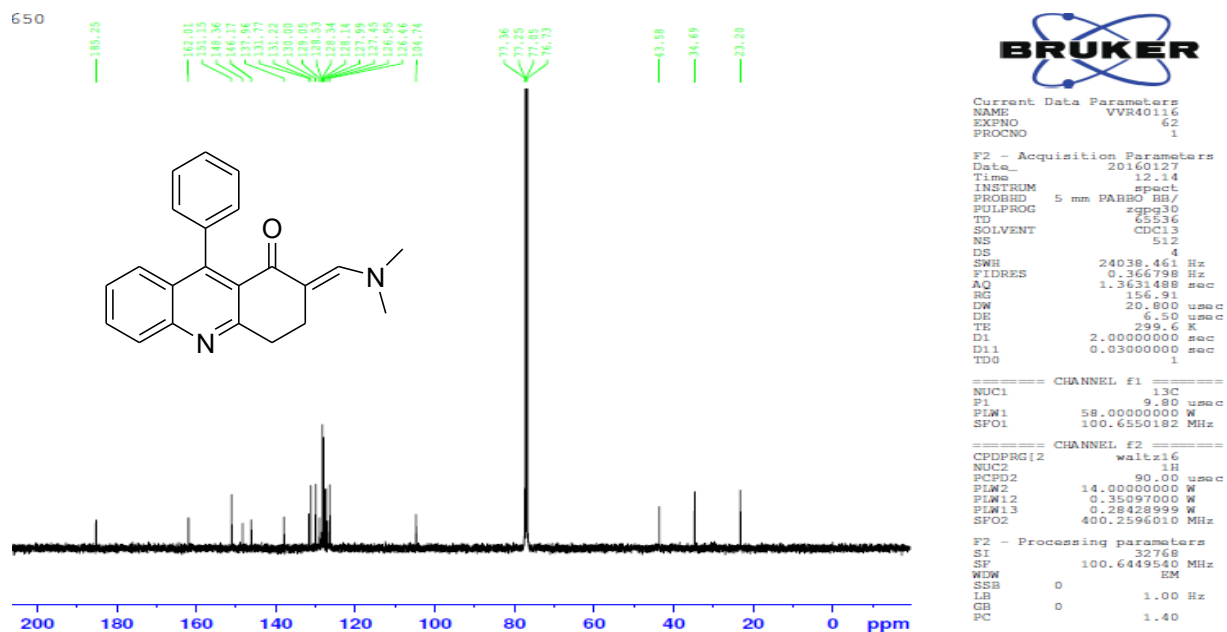


Figure 24: ^{13}C NMR spectrum of (*E*)-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2*H*)-one (3a):

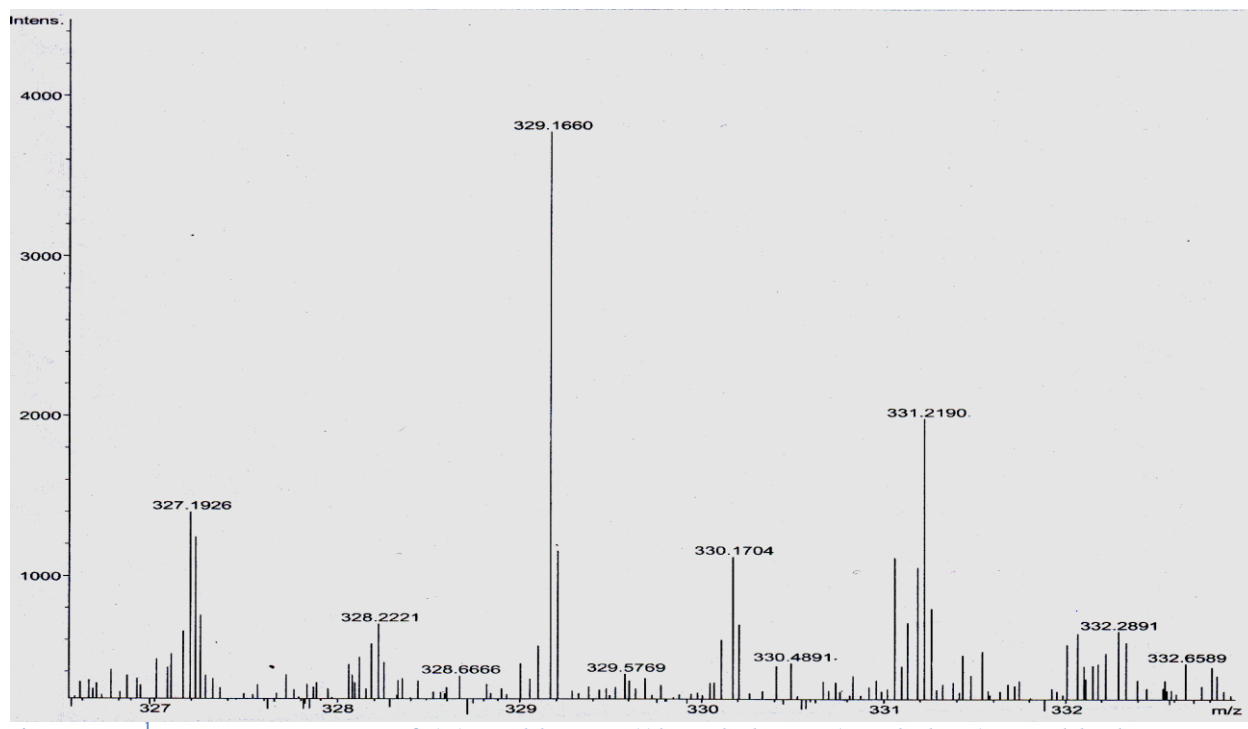


Figure 25: HRMS of (*E*)-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2*H*)-one (3a):

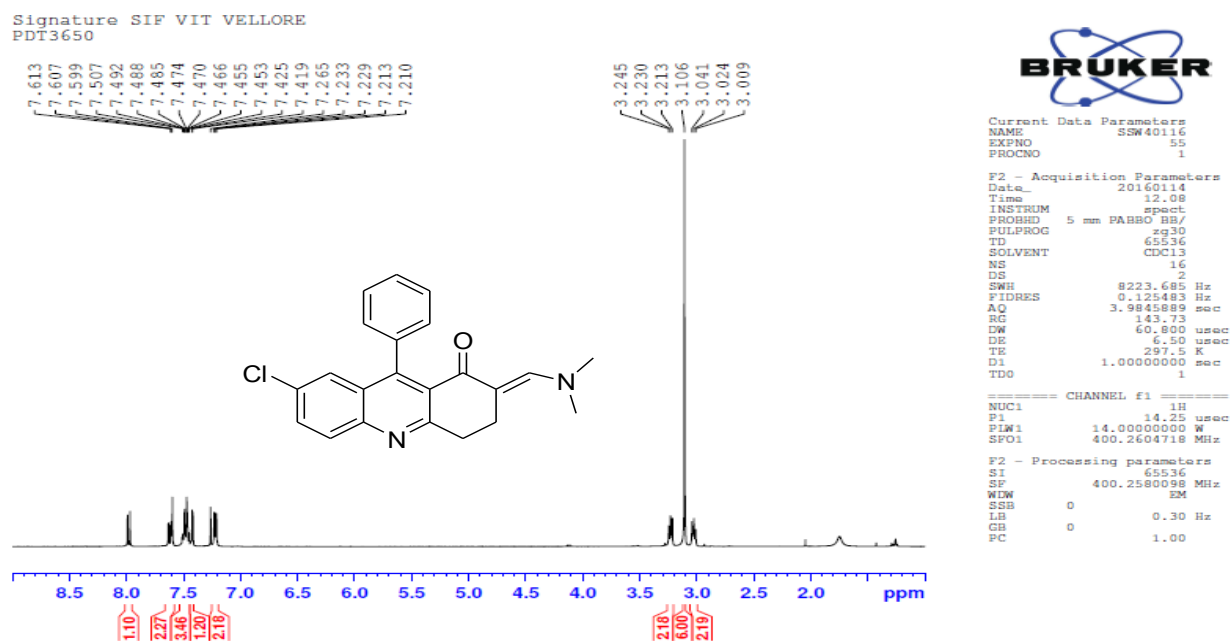


Figure 26: ^1H NMR spectrum of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

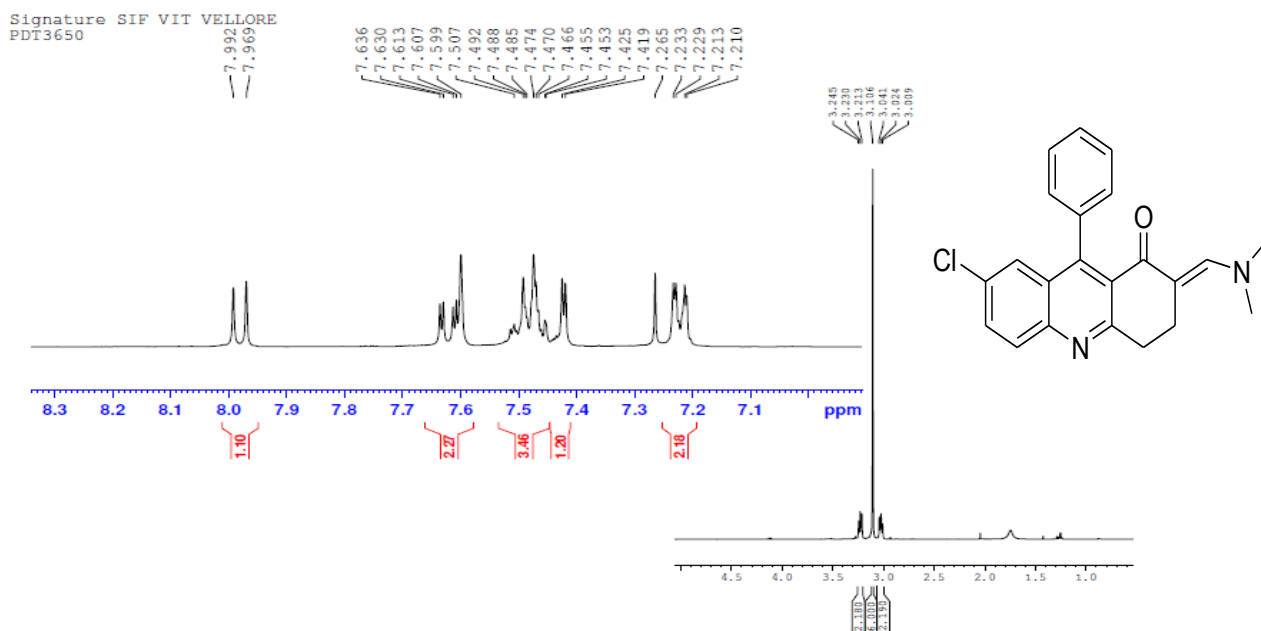


Figure 27: Enlarged ^1H NMR spectrum of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

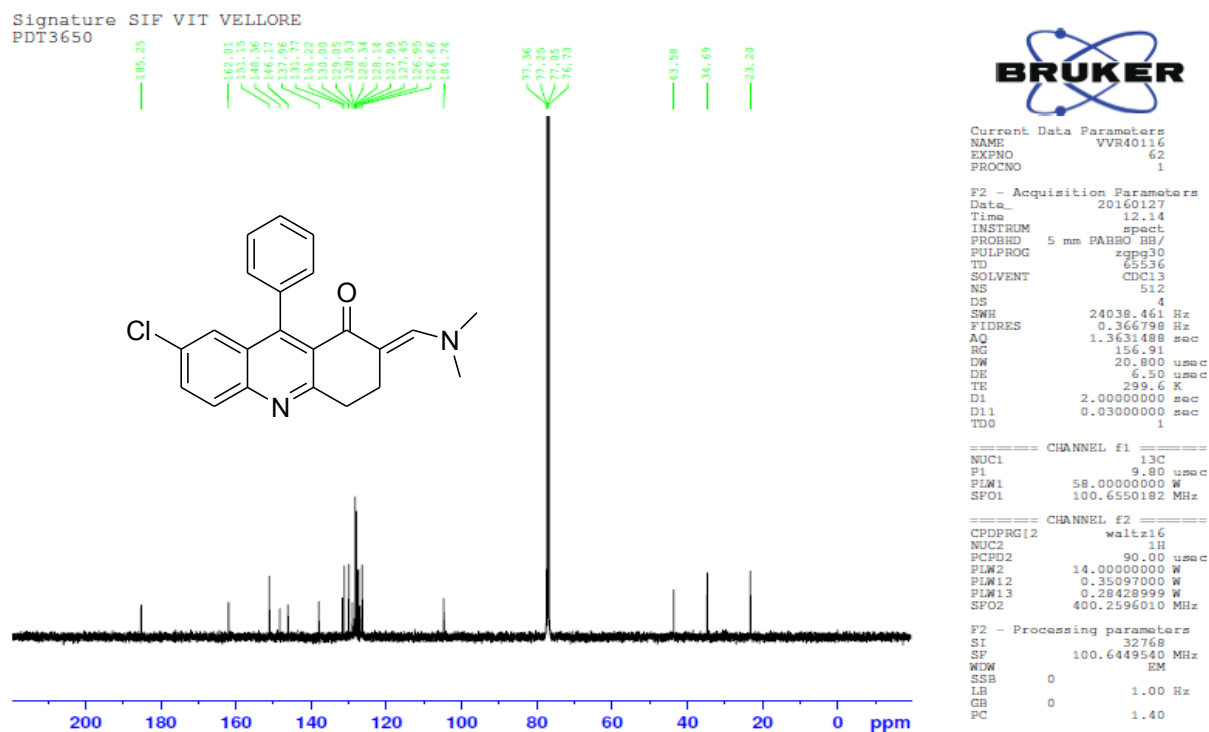
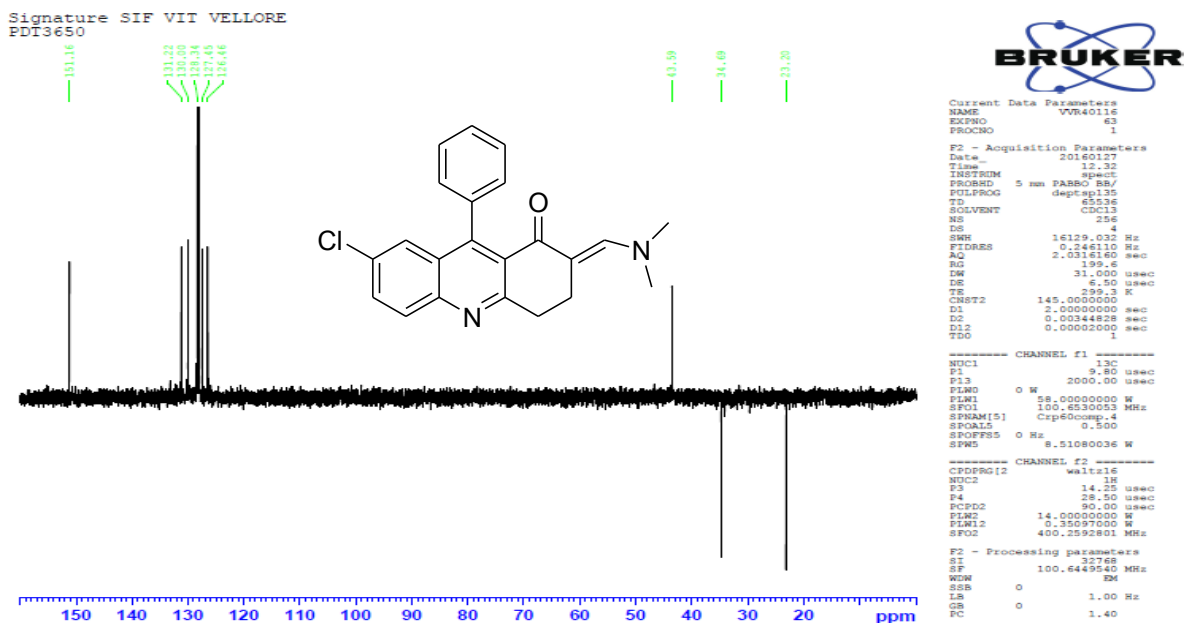
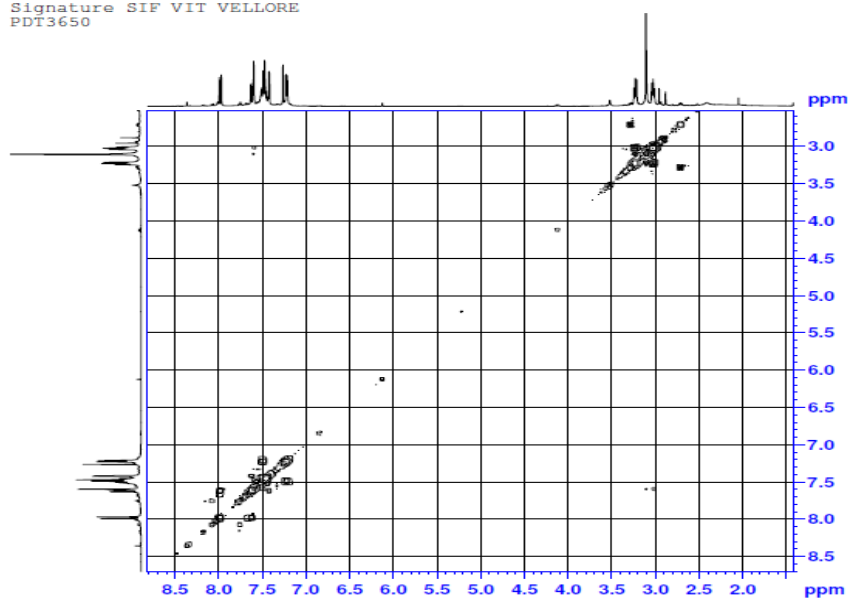
Figure 28: ^{13}C NMR spectrum of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

Figure 29: DEPT-135 spectrum of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

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PDT3650



Current Data Parameters
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EXPNO 61
PROCNO 1

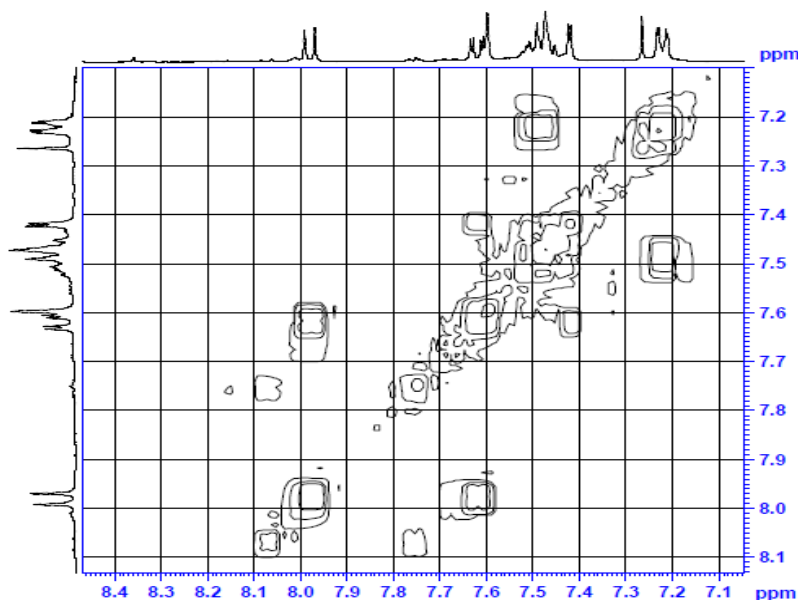
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SOLVENT CDCl3
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DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580095 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00
TI

Figure 30: H-H COSY spectrum of (*E*)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

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PDT3650



Current Data Parameters
NAME VVR40116
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 143.73
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
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SF 400.2580095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TI

Figure 31: Enlarged H-H COSY spectrum of (*E*)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

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PDT3650

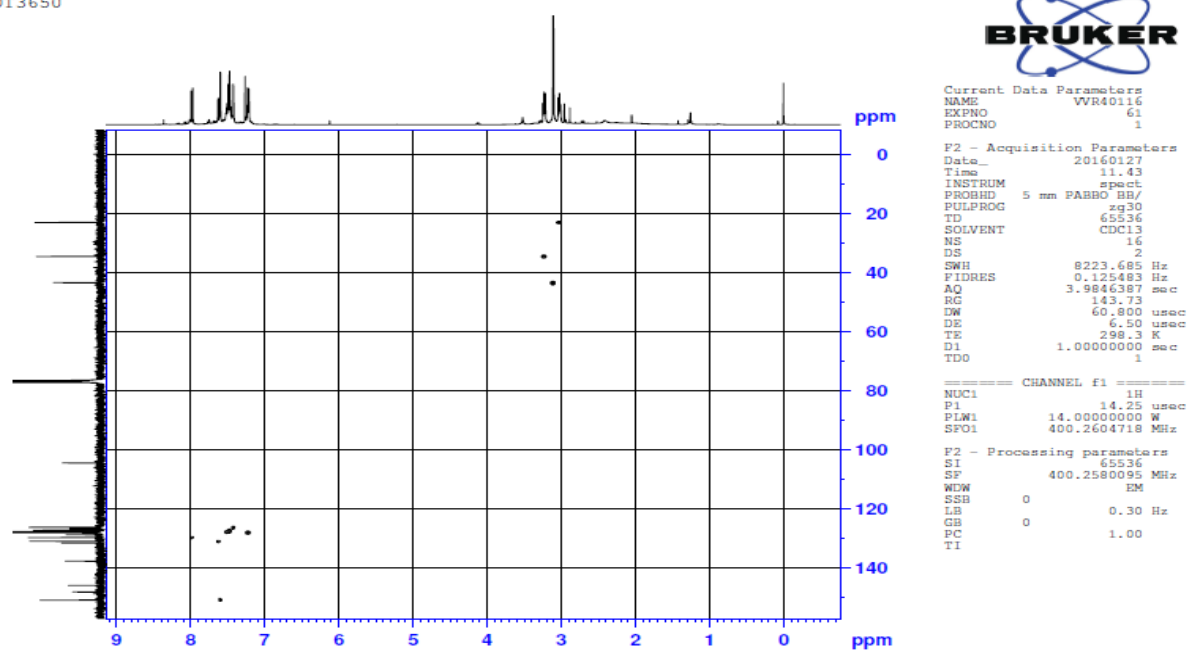


Figure 32: HSQC spectrum of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one (3b):

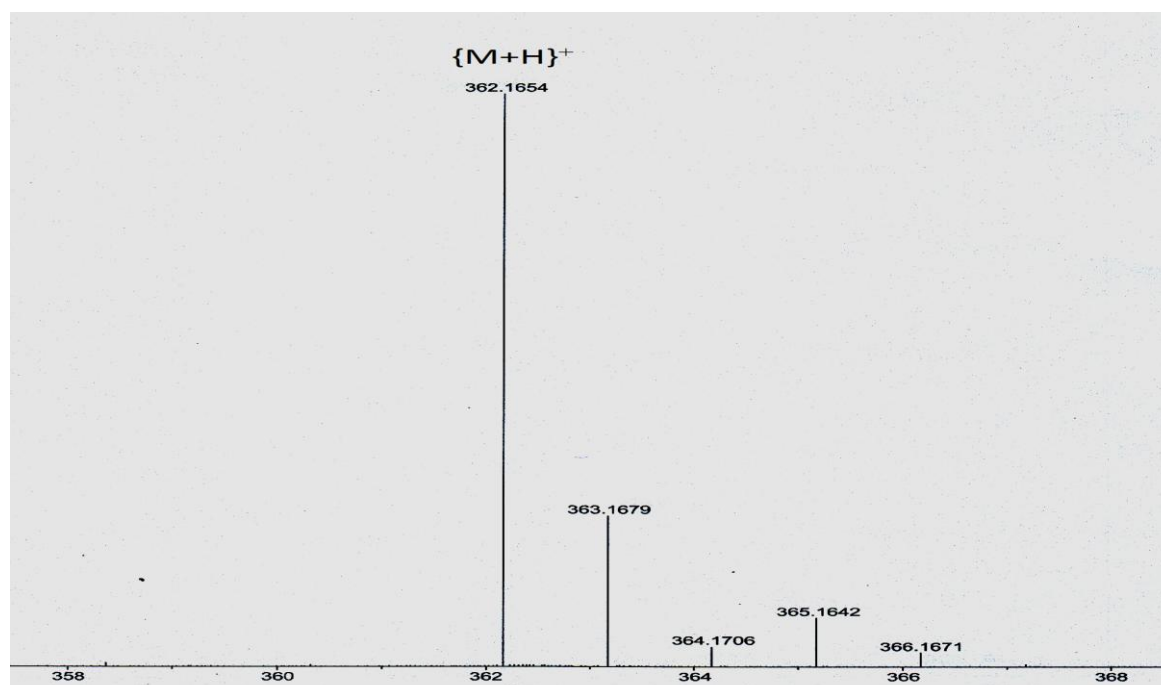


Figure 33: HRMS of (E)-7-chloro-2-((dimethylamino)methylene)-3,4-dihydro-9-phenylacridin-1(2H)-one(3b):

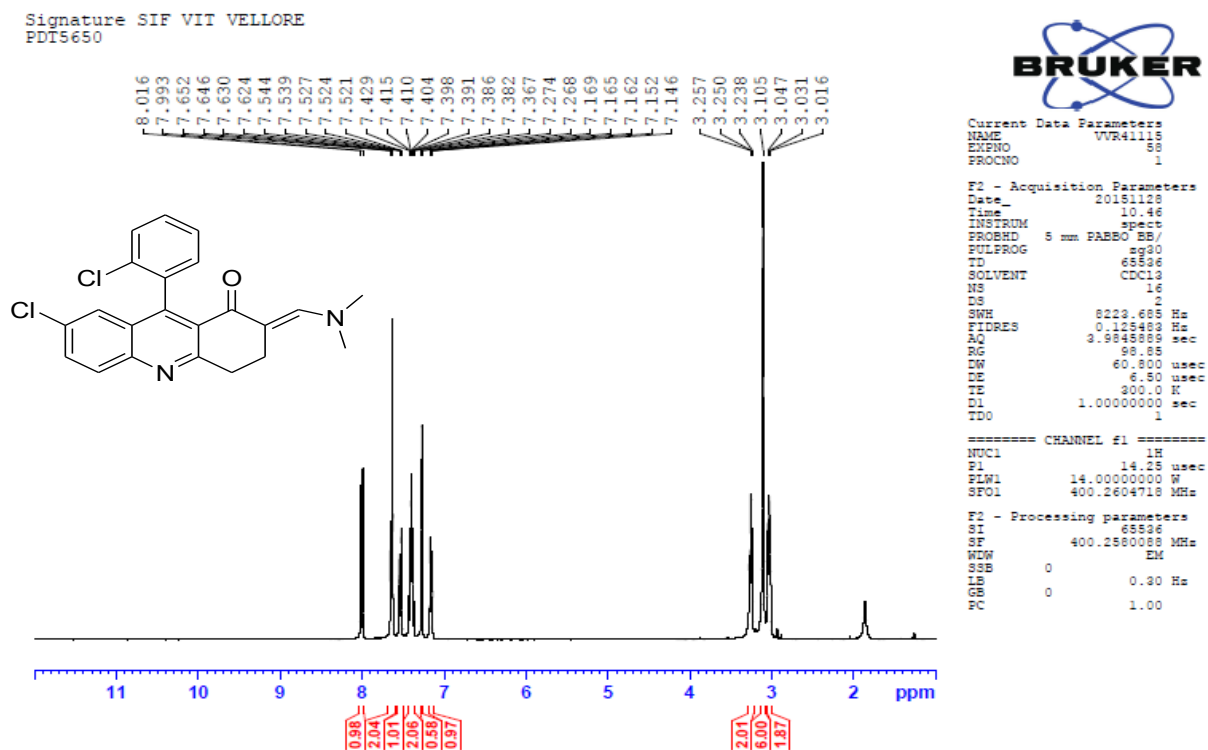


Figure 34: ^1H NMR spectrum of (E)-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

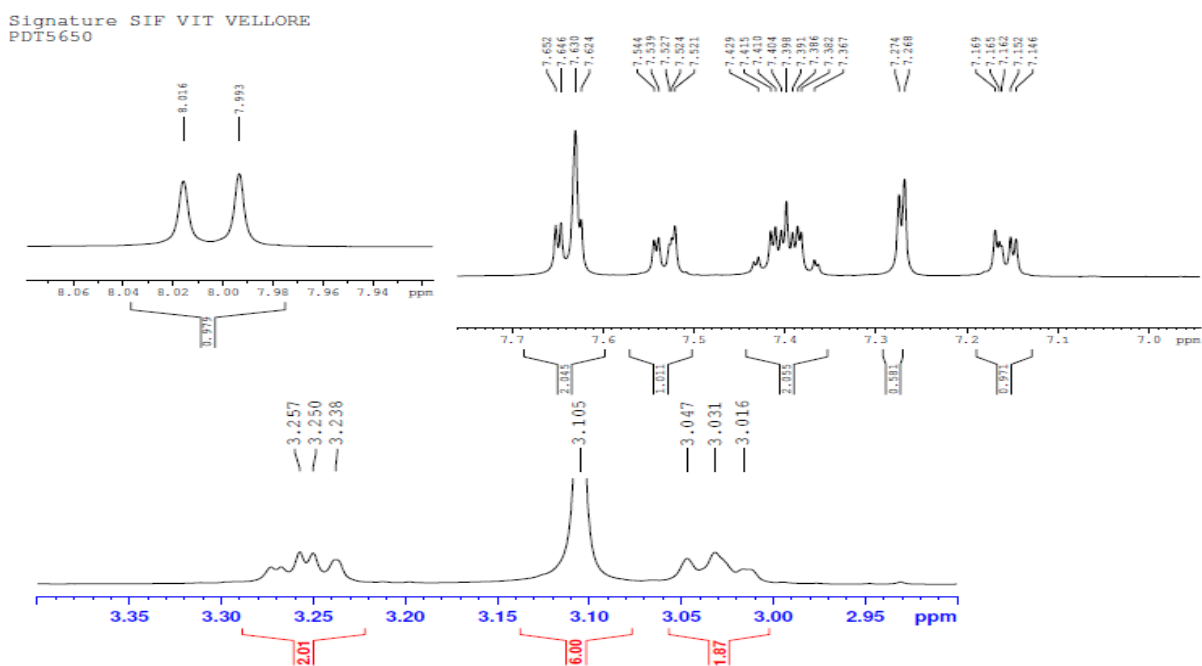
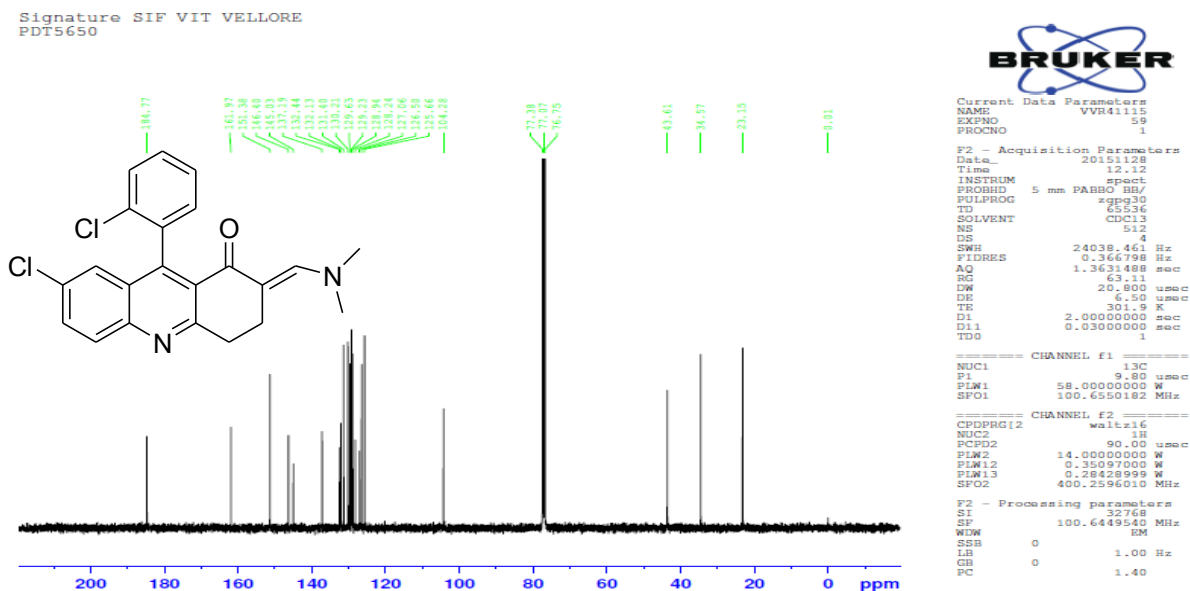


Figure 35: Enlarged ^1H NMR spectrum of (E)-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

Figure 36: ^{13}C NMR spectrum of *(E)*-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):Figure 37: DEPT-135 spectrum of *(E)*-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

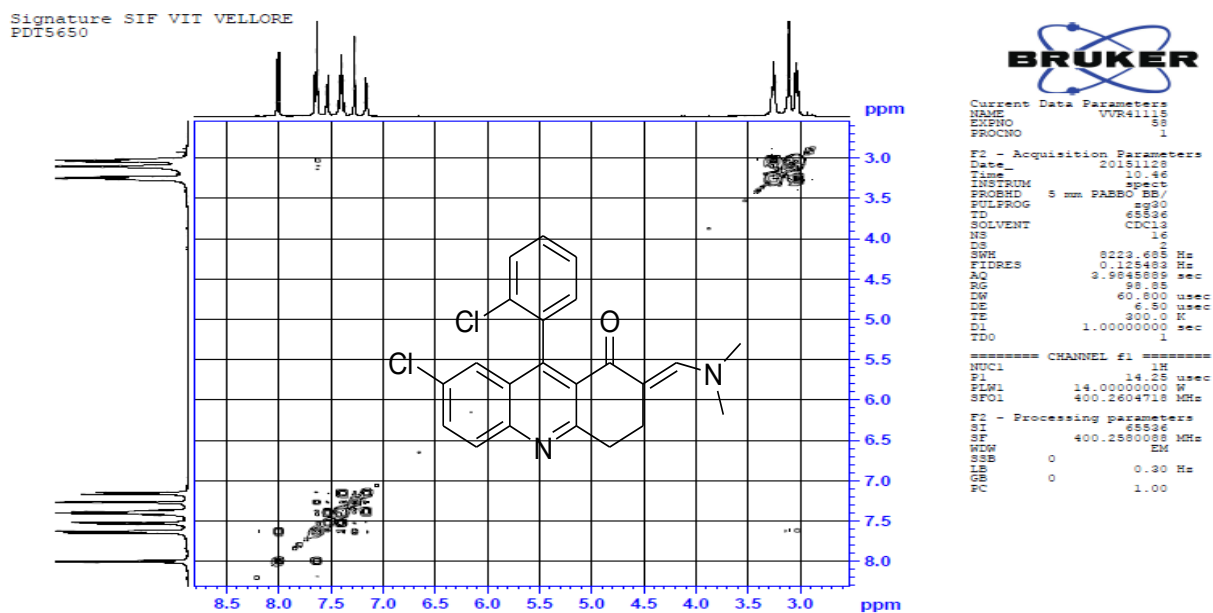


Figure 38: H-H COSY spectrum of (E)-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

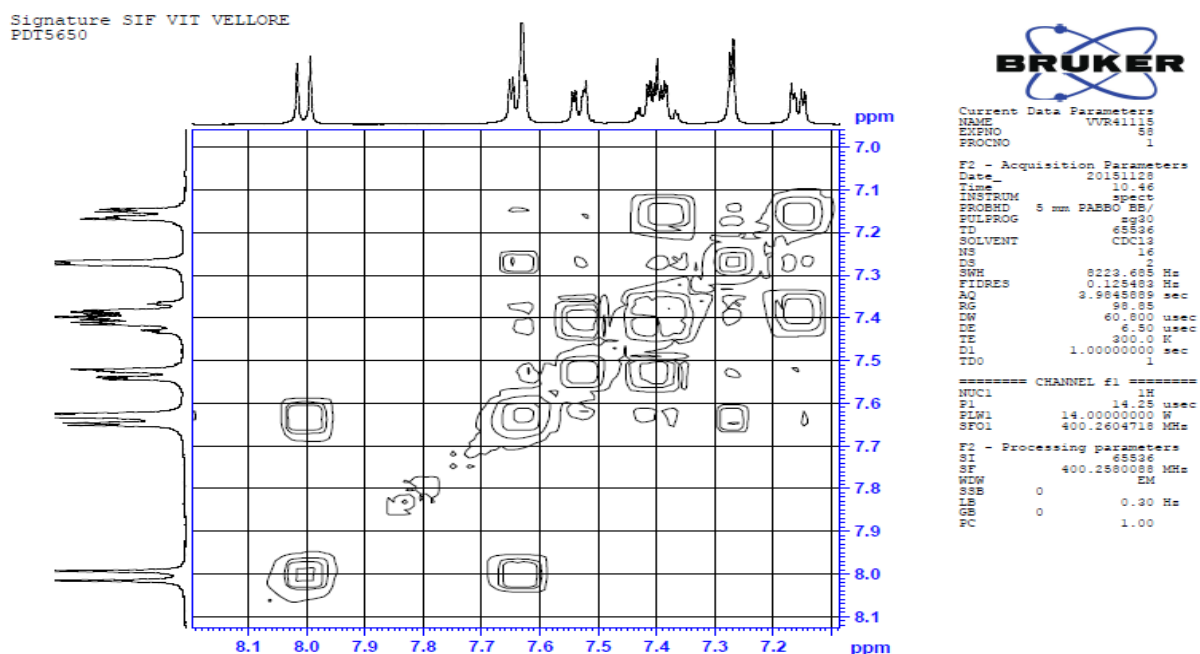


Figure 39: Enlarged H-H COSY spectrum of (E)-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

Signature SIF VIT VELLORE
PDS650

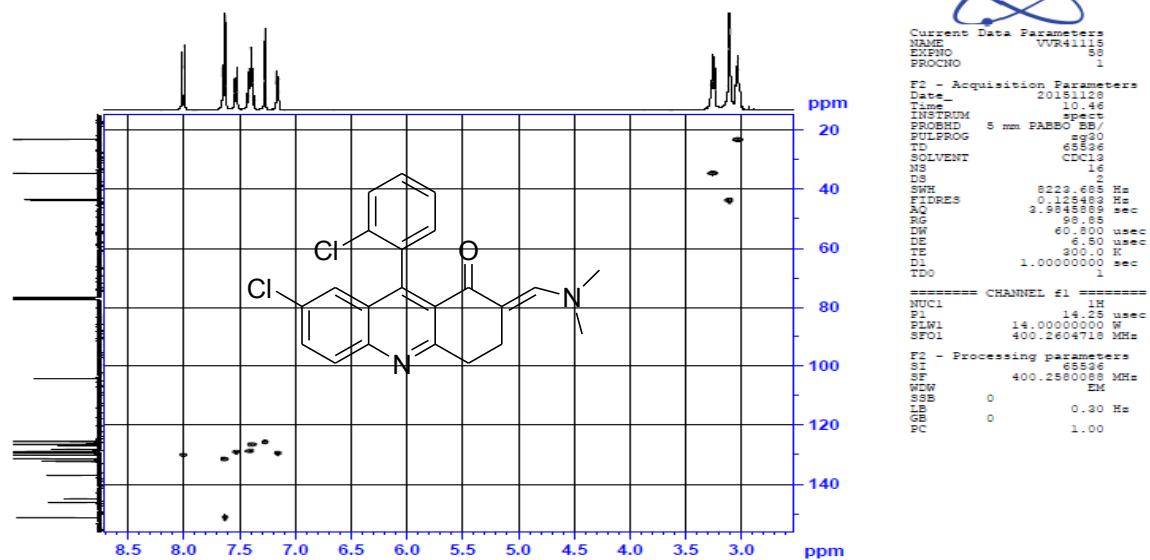


Figure 40: HSQC spectrum of *(E)*-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one (3c):

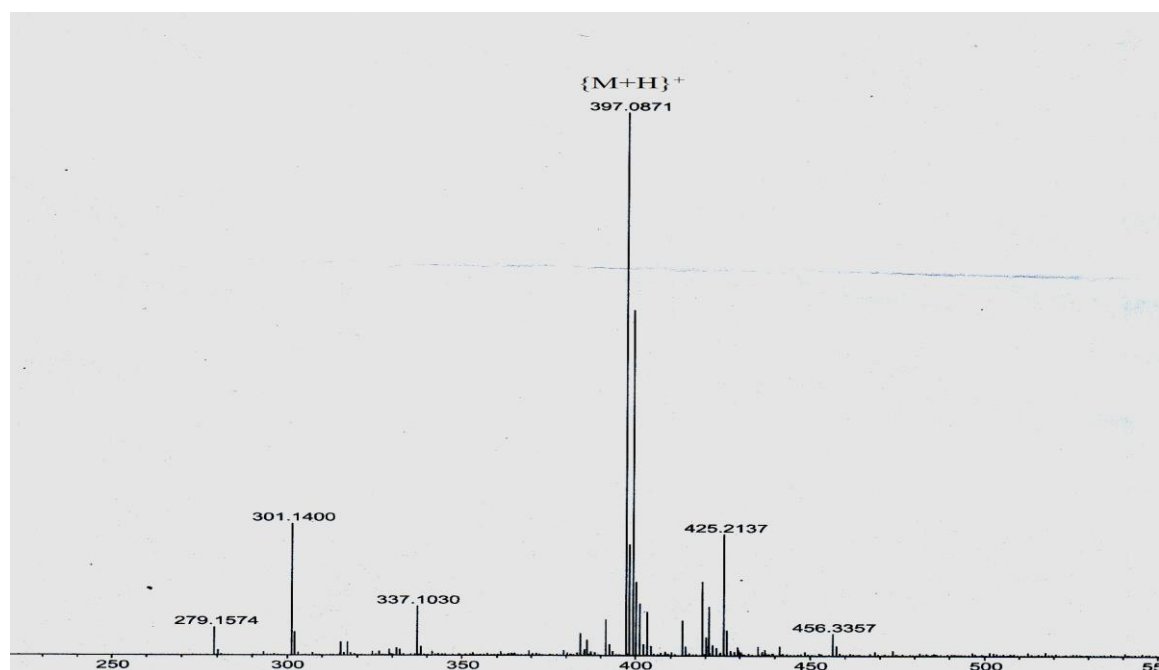


Figure 41: HRMS of *(E)*-7-chloro-9-(2-chlorophenyl)-2-((dimethylamino)methylene)-3,4-dihydroacridin-1(2H)-one(3c):

Signature SIF VIT VELLORE
265H

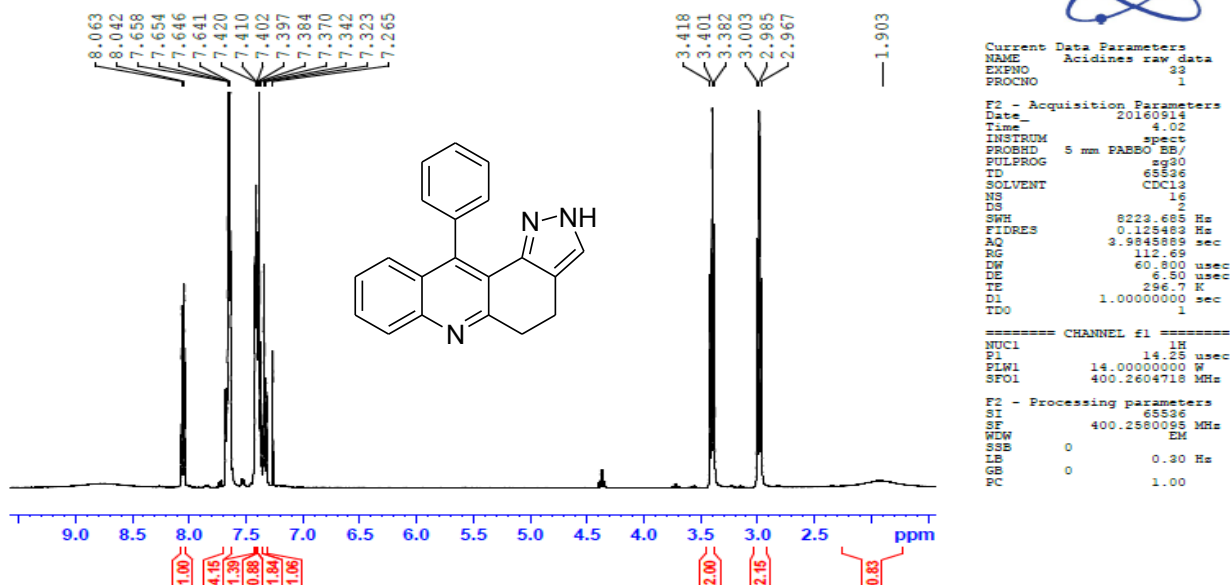


Figure 42: ^1H NMR spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

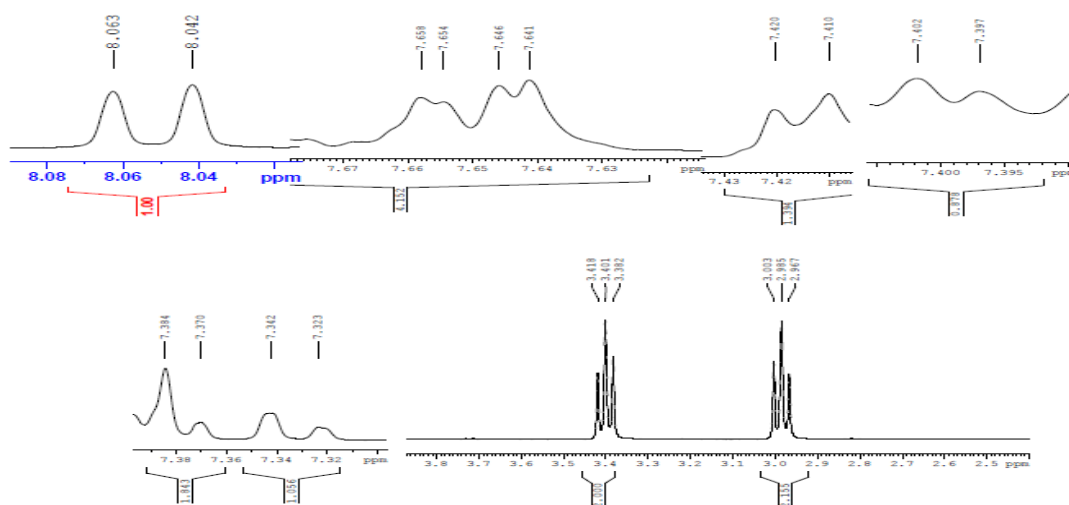
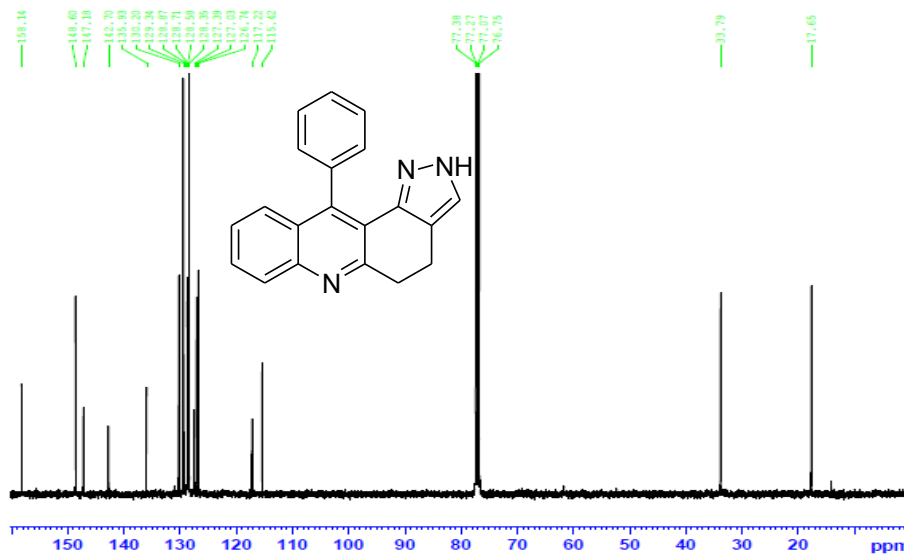


Figure 43: Enlarged ^1H NMR spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]Acridine (4a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME Dr.VVR120516
EXPNO 230
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160910
Time 19:22
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.40 Hz
FIDRES 0.3667888 Hz
AQ 1.3631488 sec
RG 127.76
DW 20.000 usec
DE 6.500 usec
TE 298.2 K
D1 2.00000000 sec
D2 0.03000000 sec
D3 0.03000000 sec

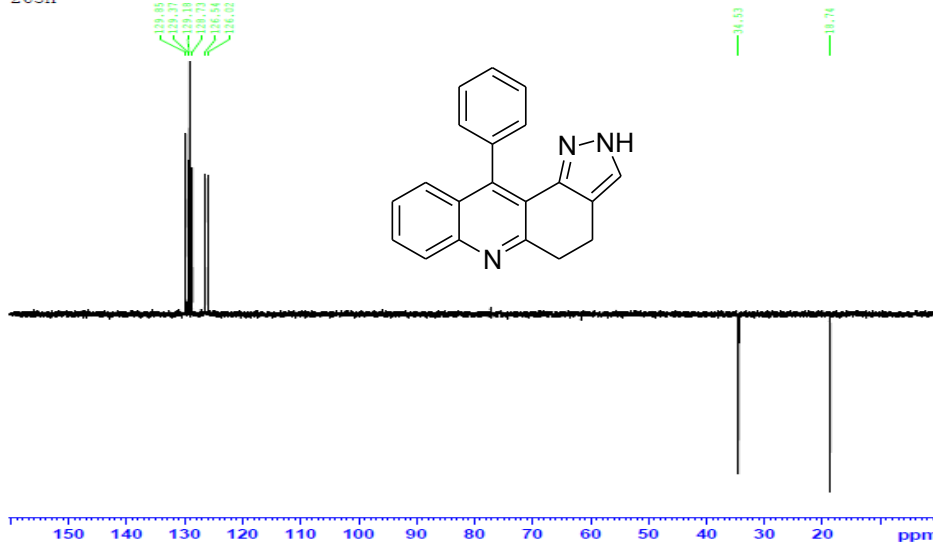
===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 58.00000000 W
SFO1 100.6261192 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 14.00000000 W
PLM2 0.35097000 W
PLM3 0.3543899 W
SFO2 400.2536010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 44: ^{13}C NMR spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

Signature SIF VIT VELLORE
265H



Current Data Parameters
NAME VIT 100 Aug 2016 omoroda
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160914
Time 4:41
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg135
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 16129.033 Hz
FIDRES 0.245110 Hz
AQ 2.0316160 sec
RG 199.5
DW 31.000 usec
DE 6.500 usec
TE 297.2 K
D1 145.0000000 sec
D2 2.00000000 sec
D3 0.0344828 sec
D12 0.00000000 sec
D13 0.00000000 sec
D14 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 58.00000000 W
PLM1 0.35097000 W
SFO1 100.6261192 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 14.00000000 W
PLM2 0.35097000 W
PLM3 0.3543899 W
SFO2 400.2536010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 45: DEPT-135 spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

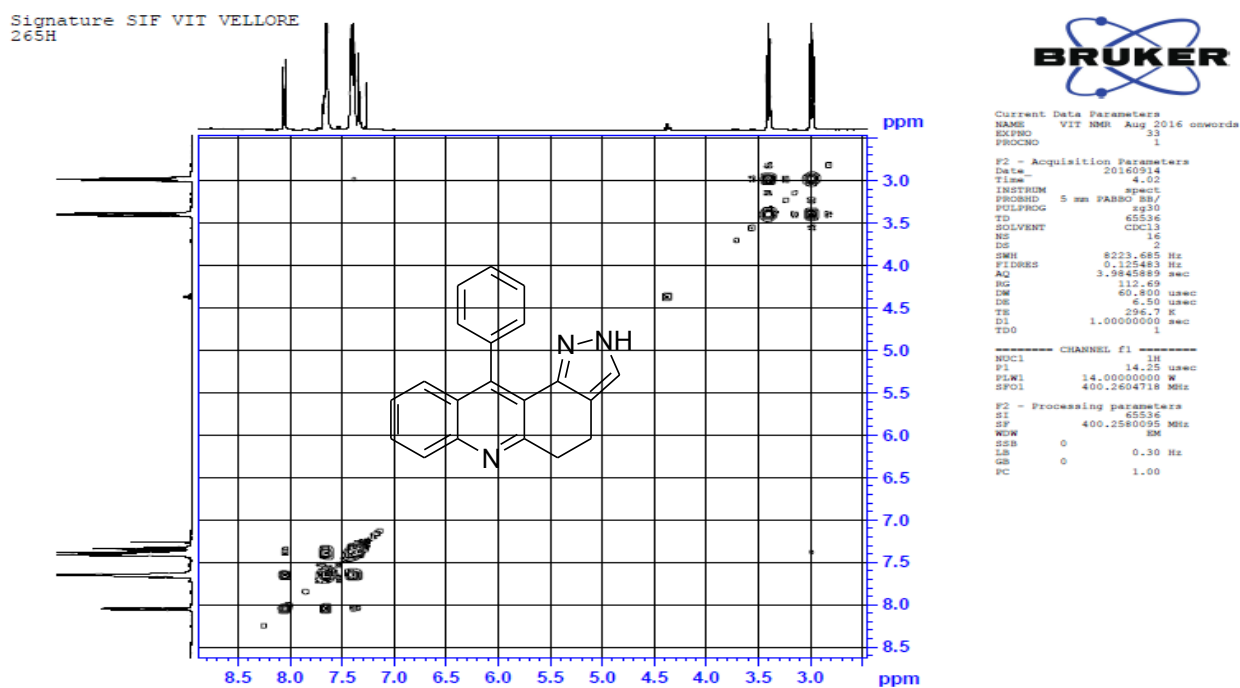


Figure 46: H-H COSY spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

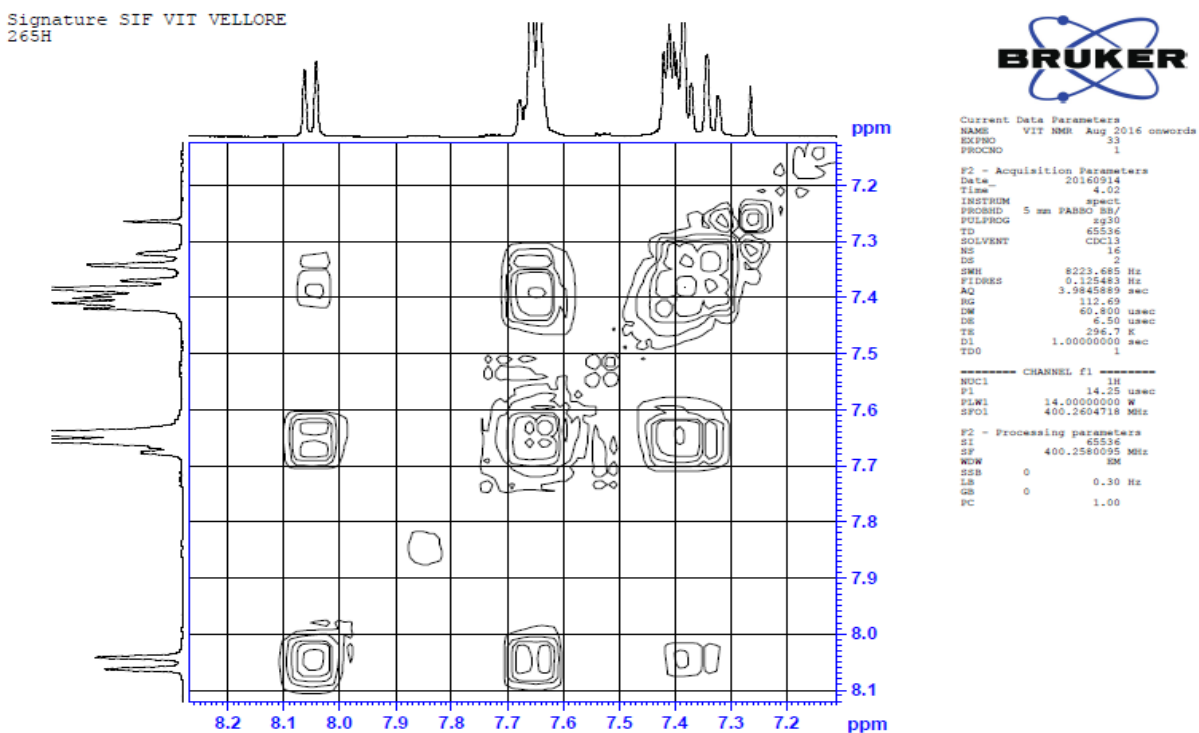
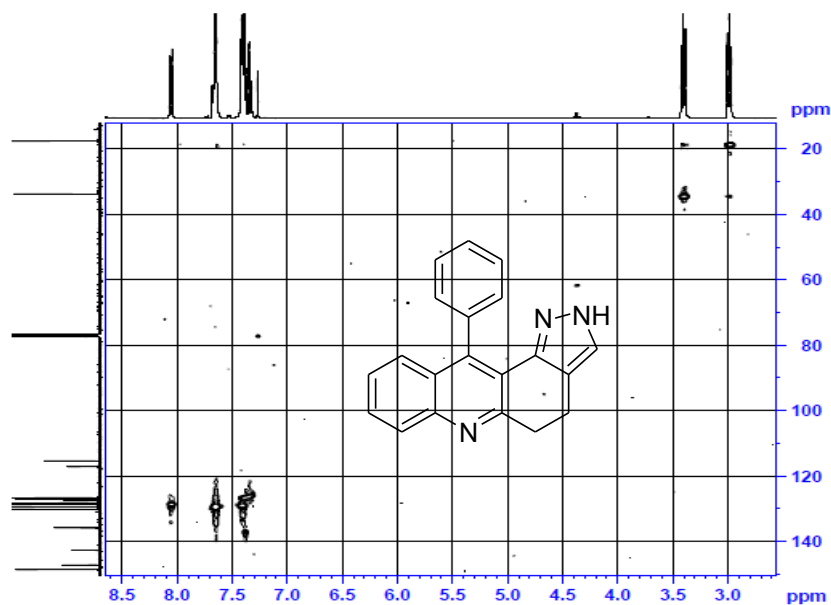


Figure 47: Enlarged H-H COSY spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

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265H



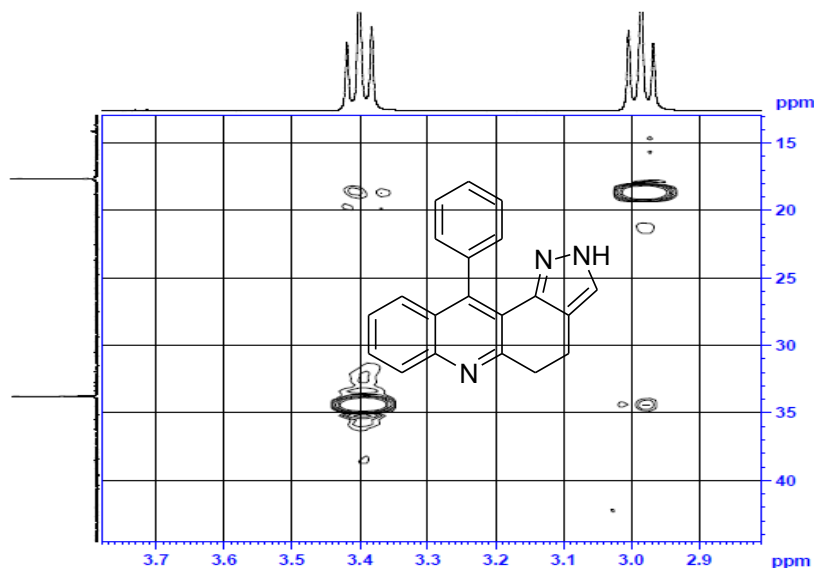
Current Data Parameters
NAME VIT NMR Aug 2016 onwards
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160914
Time 4.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 112.69
DM 60.800 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz
F2 - Processing parameters
SI 65536
SF 400.2580095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 48: HSQC spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

Signature SIF VIT VELLORE
265H



Current Data Parameters
NAME VIT NMR Aug 2016 onwards
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160914
Time 4.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 112.69
DM 60.800 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz
F2 - Processing parameters
SI 65536
SF 400.2580095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 49: Enlarged HSQC spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

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265H

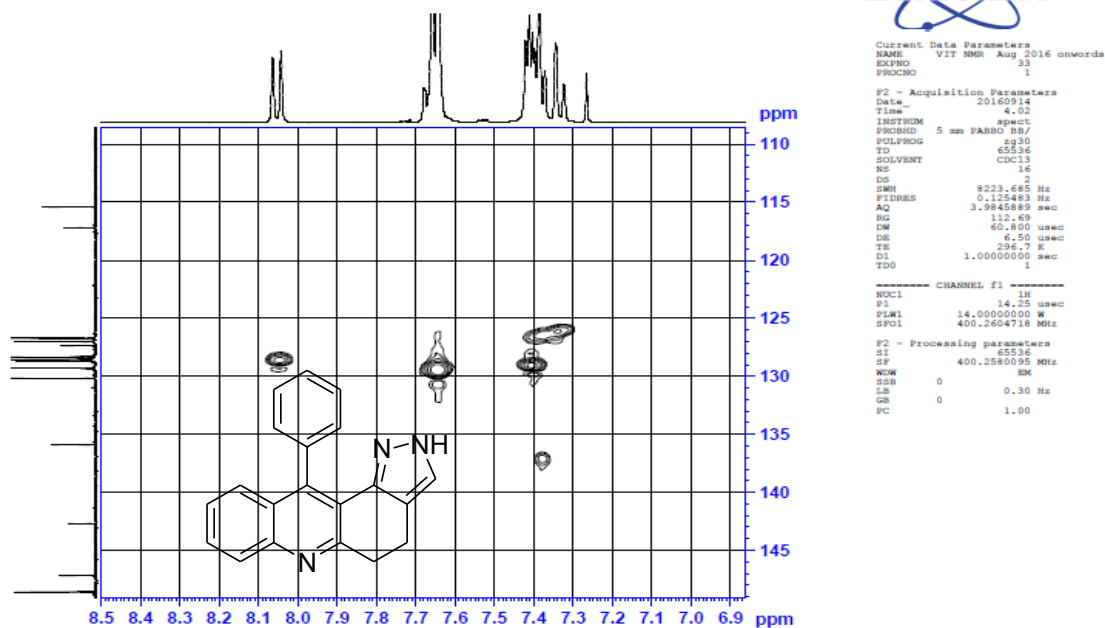


Figure 50: Enlarged HSQC spectrum of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

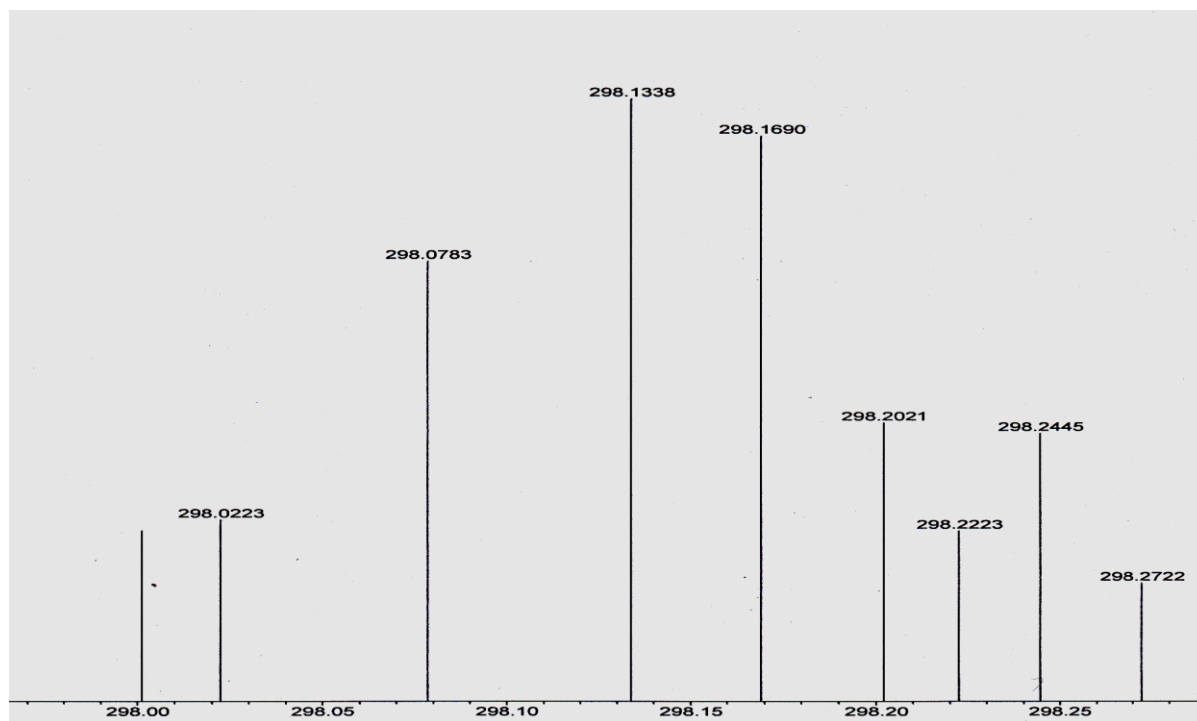


Figure 51: HRMS of 4,5-dihydro-11-phenyl-2H-pyrazolo[3,4-a]acridine (4a):

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5650HYD

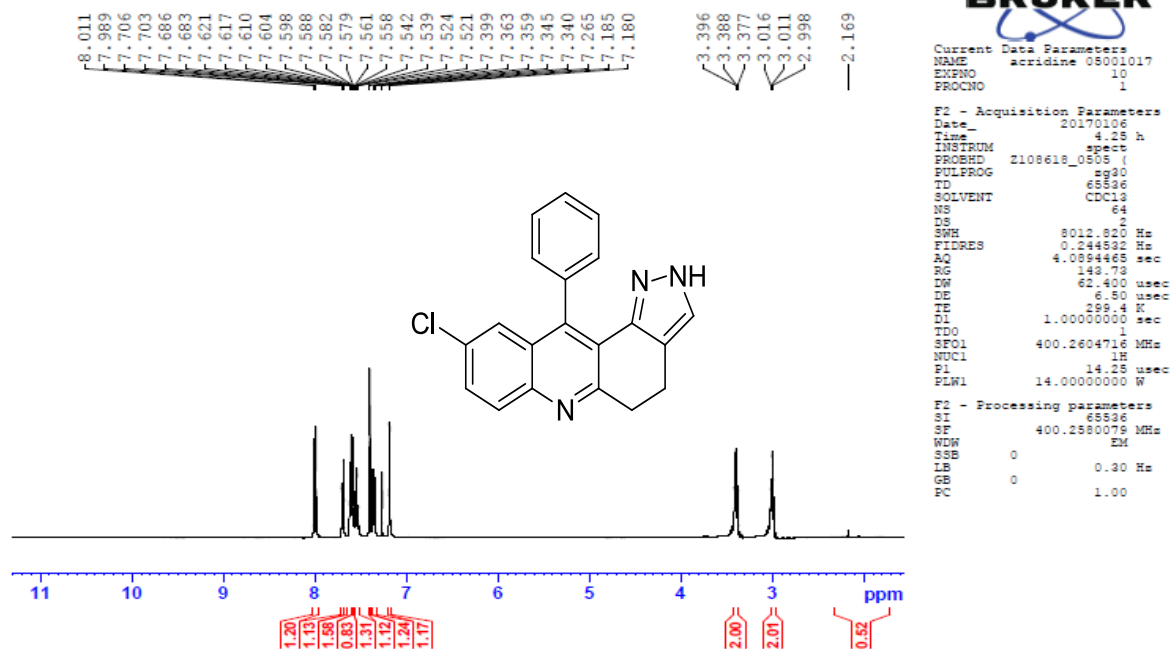


Figure 52: ^1H NMR spectrum of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

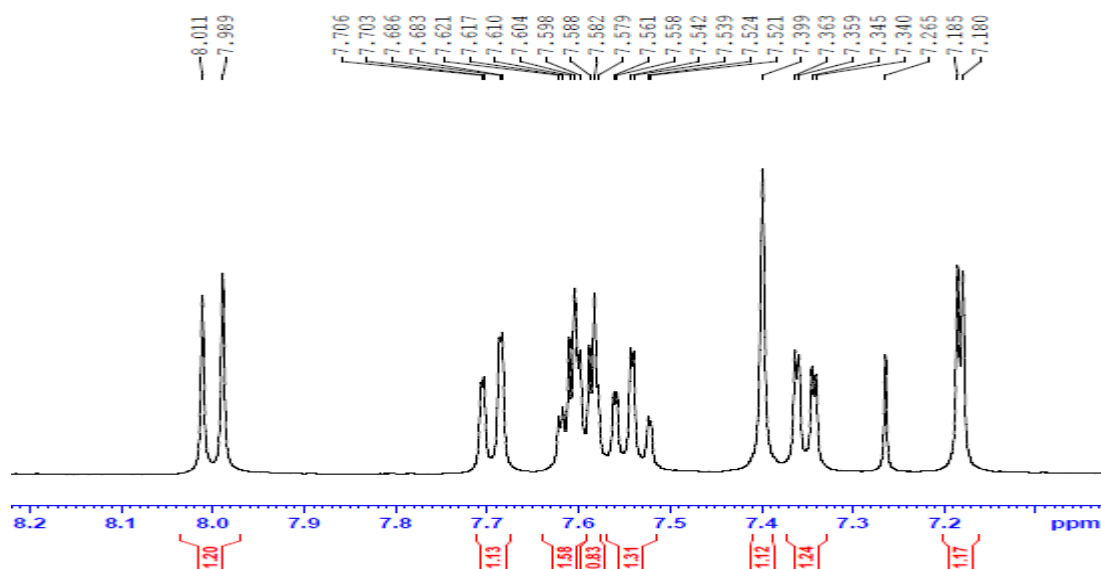


Figure 53: Enlarged ^1H NMR spectrum of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

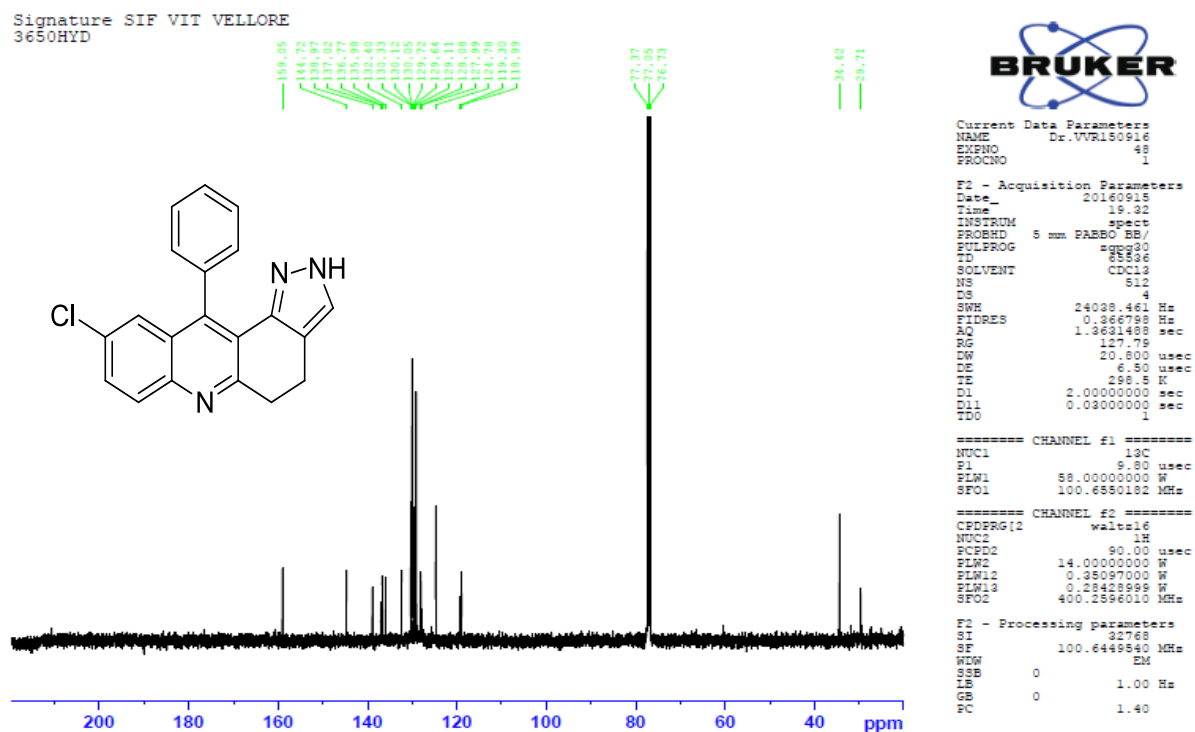
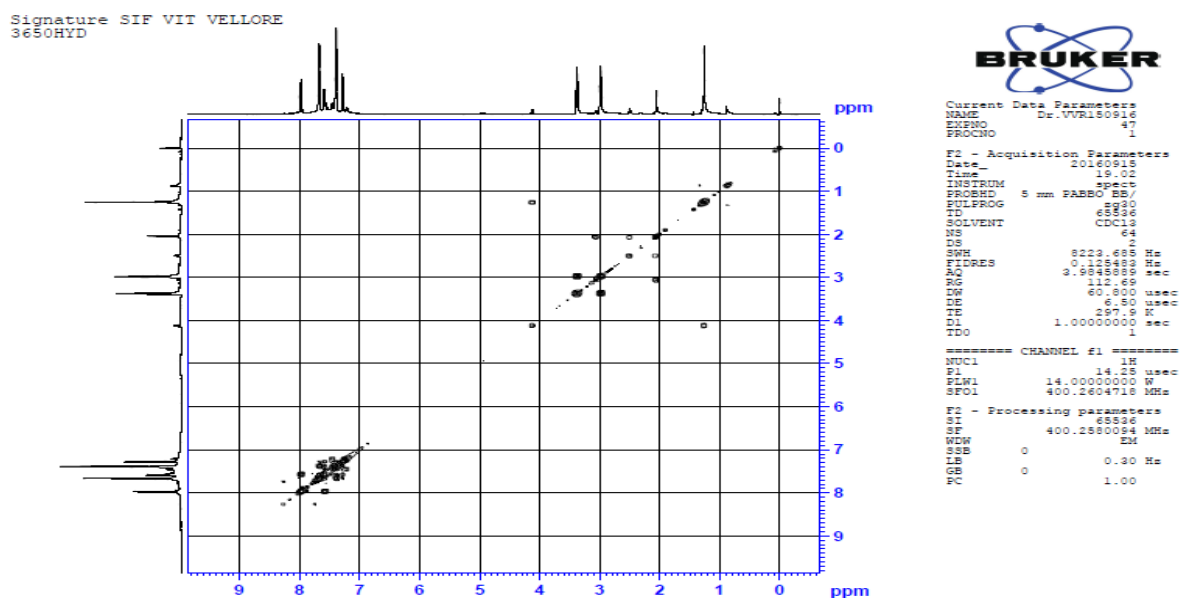
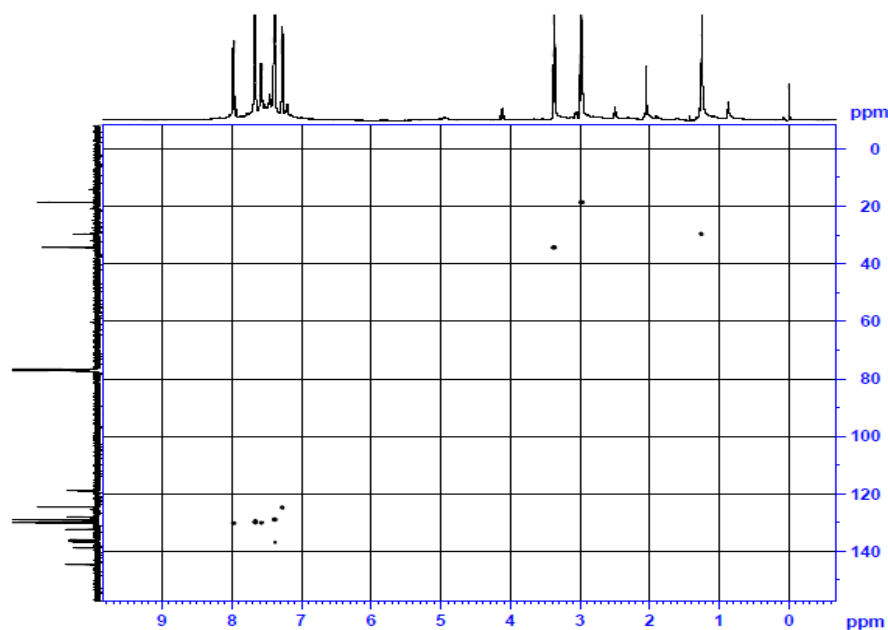
Figure 54: ^{13}C NMR spectrum of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

Figure 55: H-H COSY spectrum of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

Signature SIF VIT VELLORE
3650HYD



Current Data Parameters
NAME Dr.VVR150916
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160916
Time 19.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.688 Hz
FIDRES 0.125492 Hz
AQ 3.9845889 sec
RG 112.69
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 56: HSQC spectrum of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

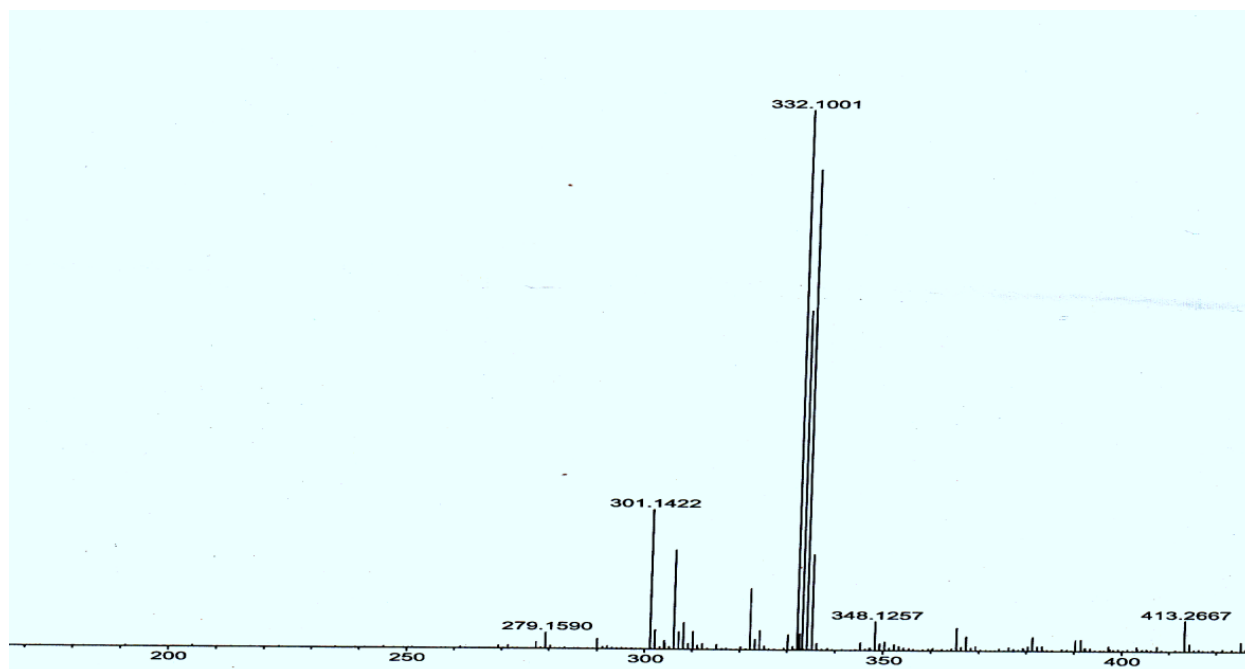


Figure 57: HRMS of 9-chloro-4,5-dihydro-11-phenyl-1H-pyrazolo[3,4-a]acridine (4b):

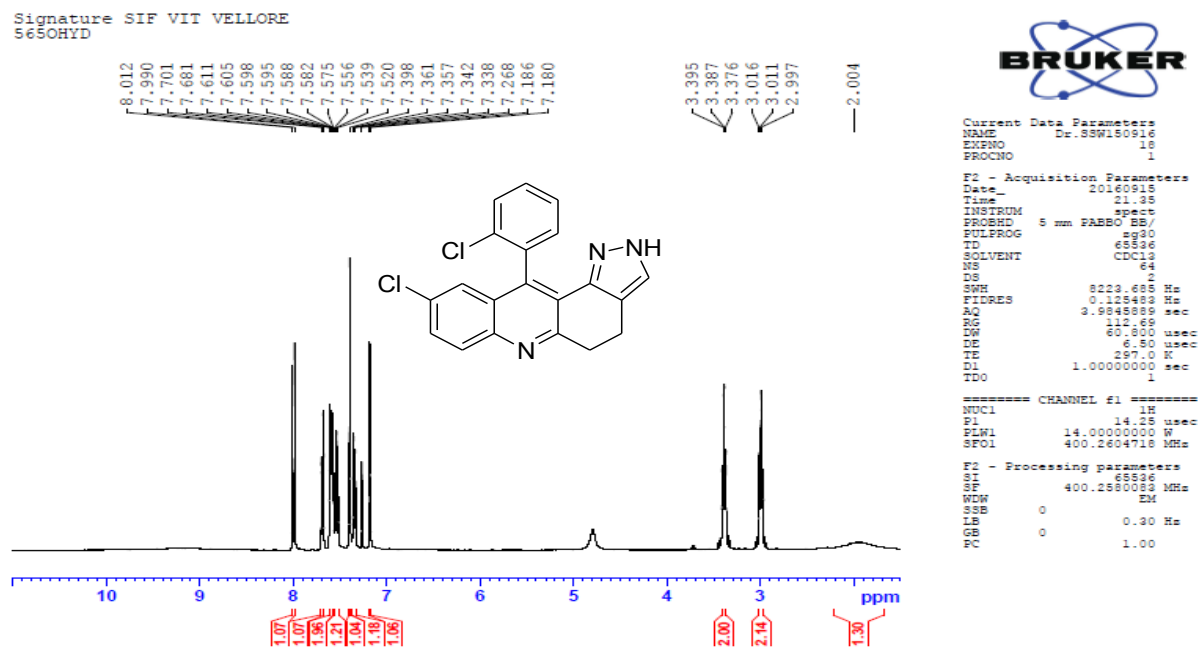


Figure 58: ^1H NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1H-pyrazolo[3,4-a]acridine (4c):

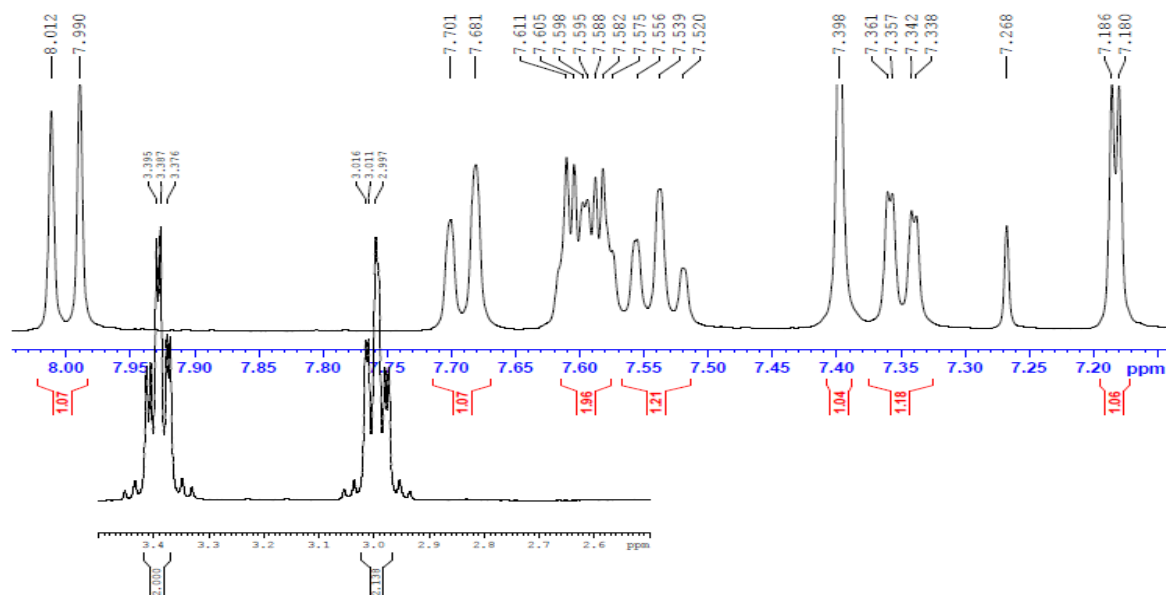


Figure 59: Enlarged ^1H NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1H-pyrazolo[3,4-a]acridine (4c):

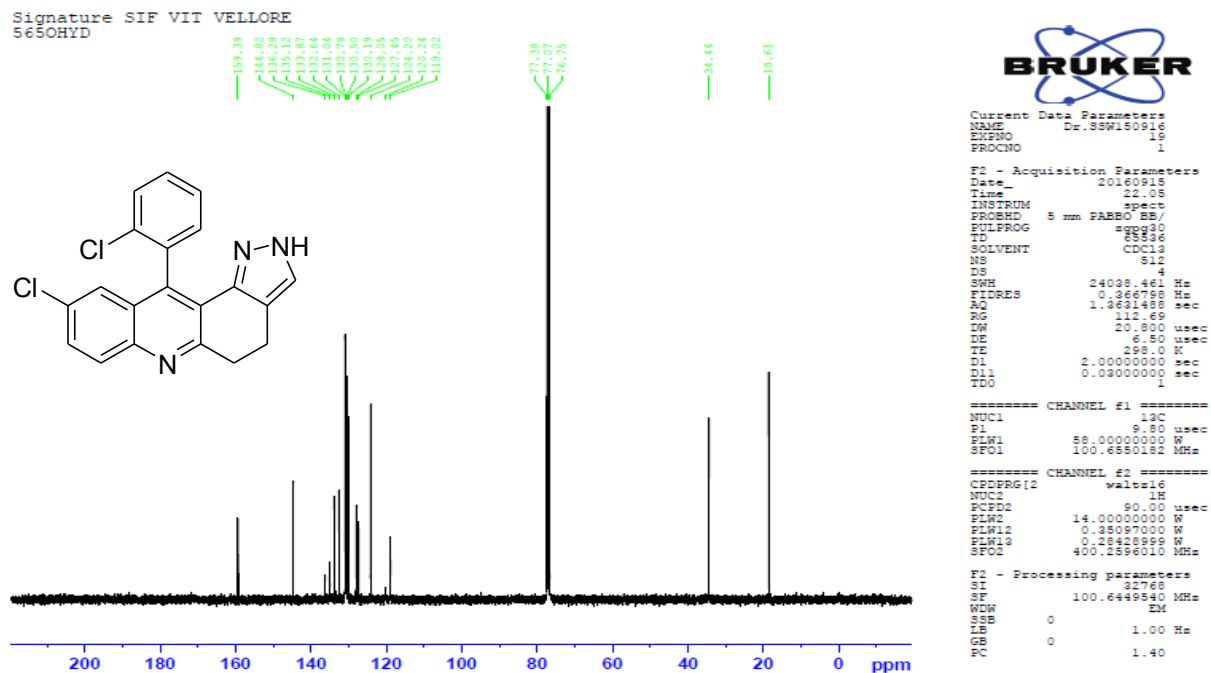
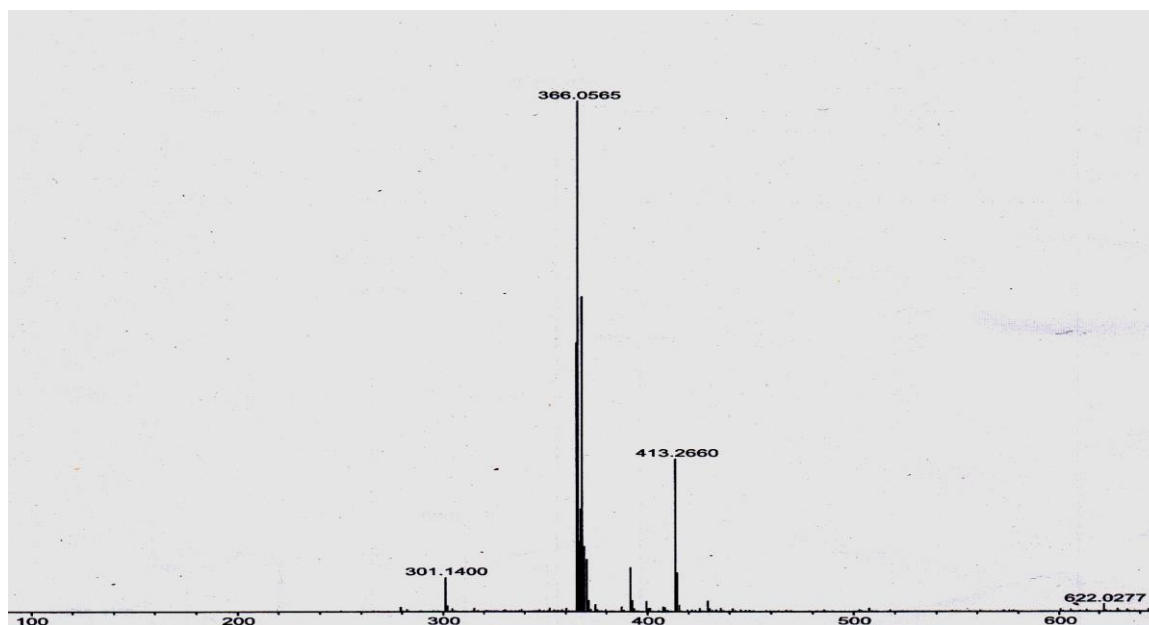
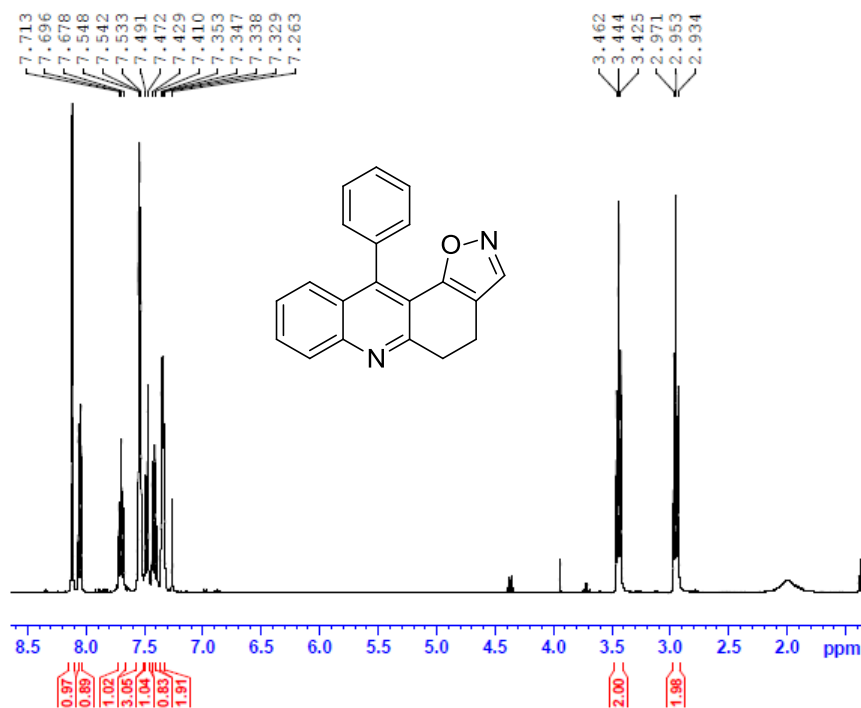
Figure 60: ^{13}C NMR of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1H-pyrazolo[3,4-a]acridine (4c):

Figure 61: HRMS of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1H-pyrazolo[3,4-a]acridine (4c):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME 37
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160914
Time 4.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 95.85
DQ 60.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.28 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580105 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00

Figure 62: ^1H NMR spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

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265N

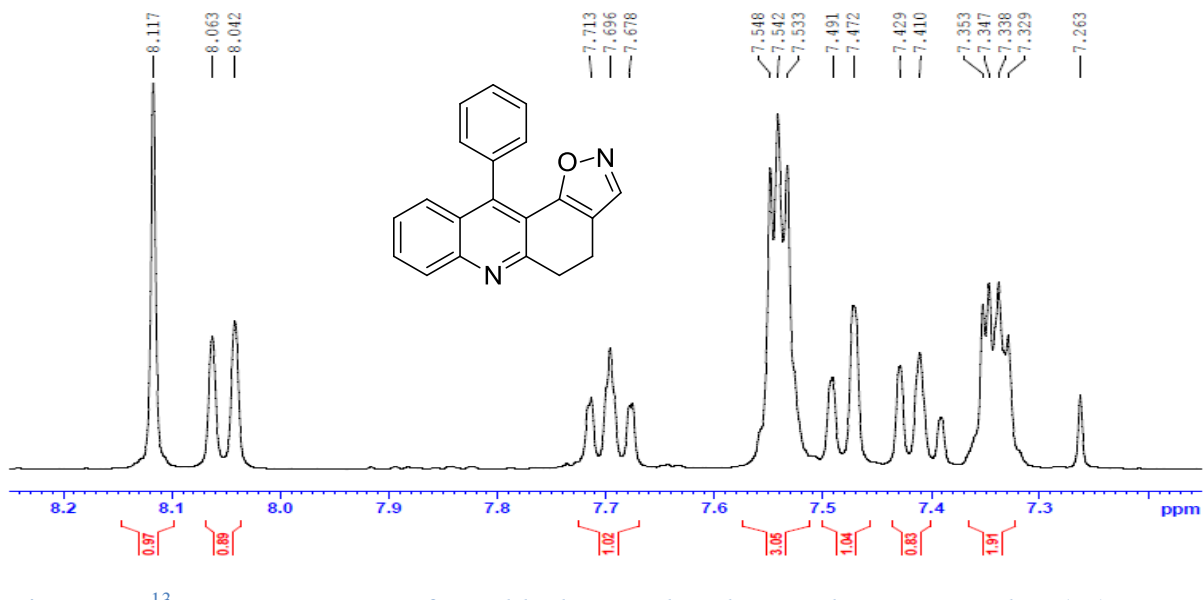
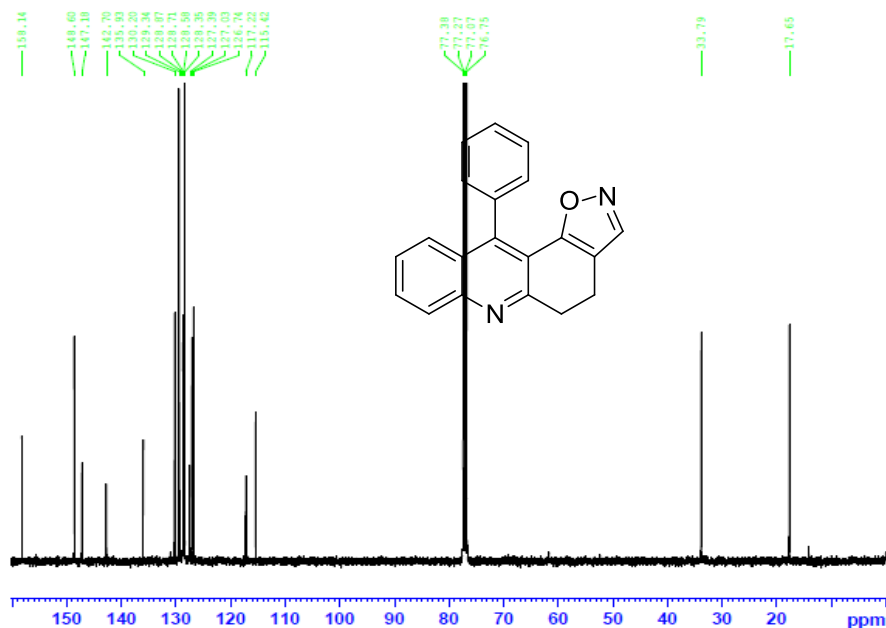


Figure 63: Enlarged ^1H NMR spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME Dr.VVR120916
EXPNO 2
PROCNO 1

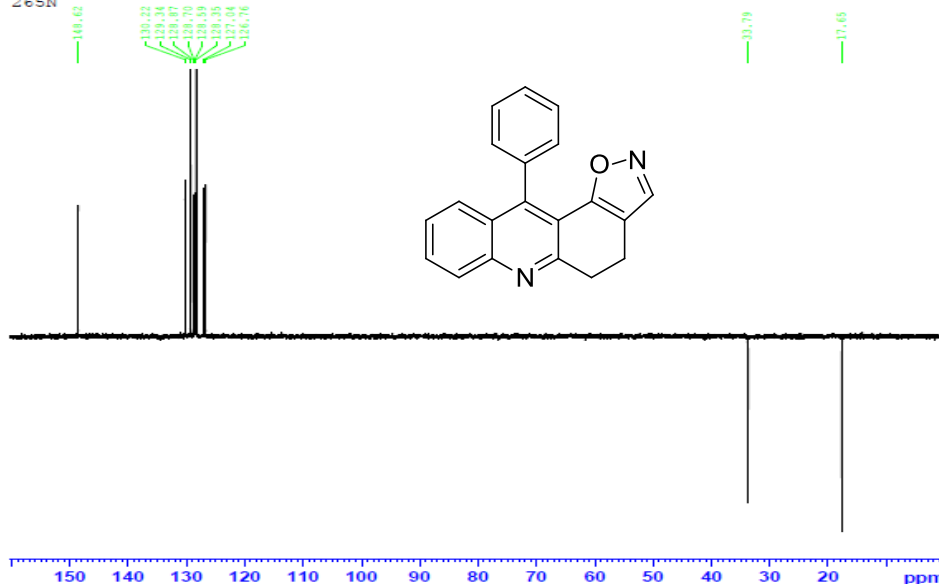
F2 - Acquisition Parameters
Date_ 20160812
Time 19.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 612
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.861188 sec
RG 127.79
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO

===== CHANNEL #1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz
===== CHANNEL #2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
P4 28.50 usec
PLW2 14.00000000 W
PLW12 0.38097000 W
PLW13 0.28428999 W
SFO2 400.255010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 64: ^{13}C NMR spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME VIT NMR Aug 2016 onwards
EXPNO 41
PROCNO 1

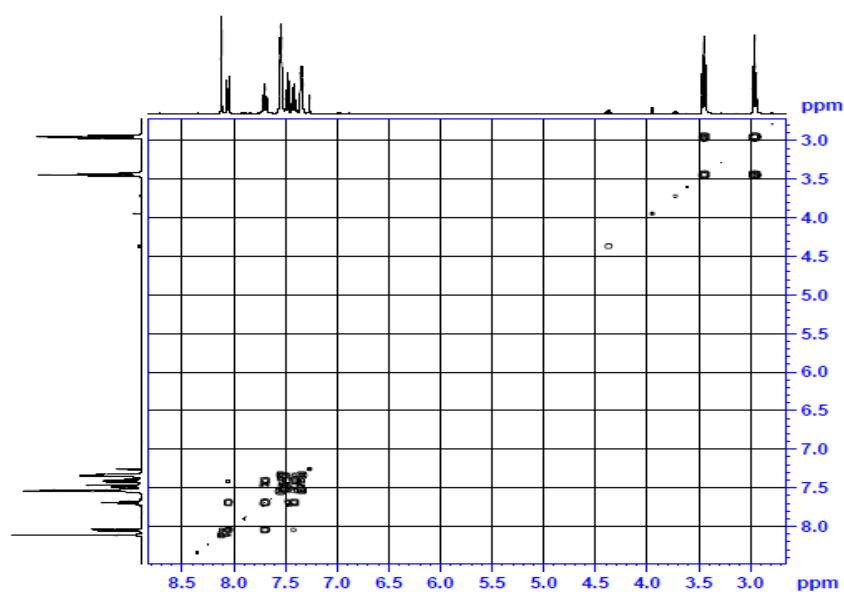
F2 - Acquisition Parameters
Date_ 20160914
Time 5.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 297.3 K
CPDPRG2 waltz16
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz
SFOAL5 Cmp60comp 4
SFOAL5 0.500
SFOAL5 8.51080036 W

===== CHANNEL #1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz
===== CHANNEL #2 =====
CPDPRG2 waltz16
NUC2 1H
P2 14.25 usec
P4 28.50 usec
PCPD2 80.00 usec
PLW2 14.00000000 W
PLW12 0.38097000 W
PLW13 0.28428999 W
SFO2 400.255010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 65: DEPT-135 spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME VVR40916
EXPNO 38
PROCNO 1

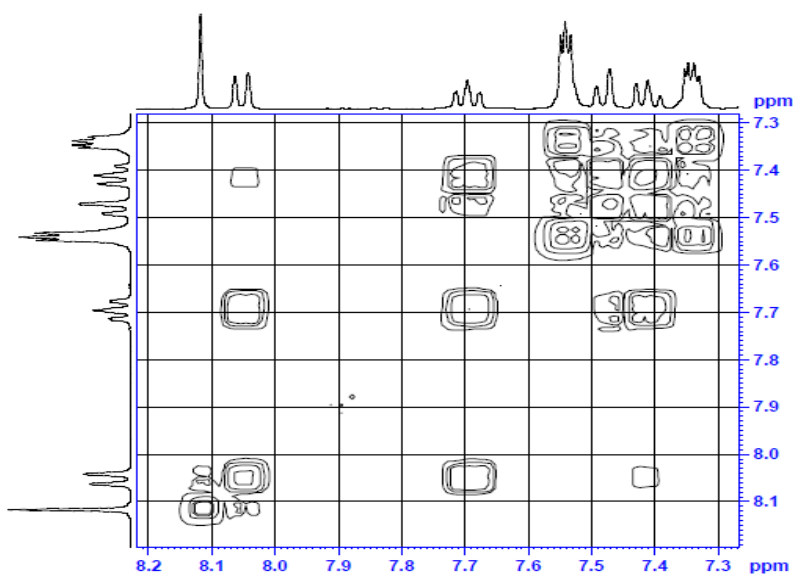
F2 - Acquisition Parameters
Date_ 20160914
Time 4.48
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1.6
DS
SWH 8223.688 Hz
FIDRES 0.123483 Hz
AQ 3.934637 sec
RG 99.66
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SFO2 400.2580105 MHz
WDW EM
SSB 0
GB 0
PC 0.30 Hz
PR 1.00

Figure 66: H-H COSY spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME VVR40916
EXPNO 38
PROCNO 1

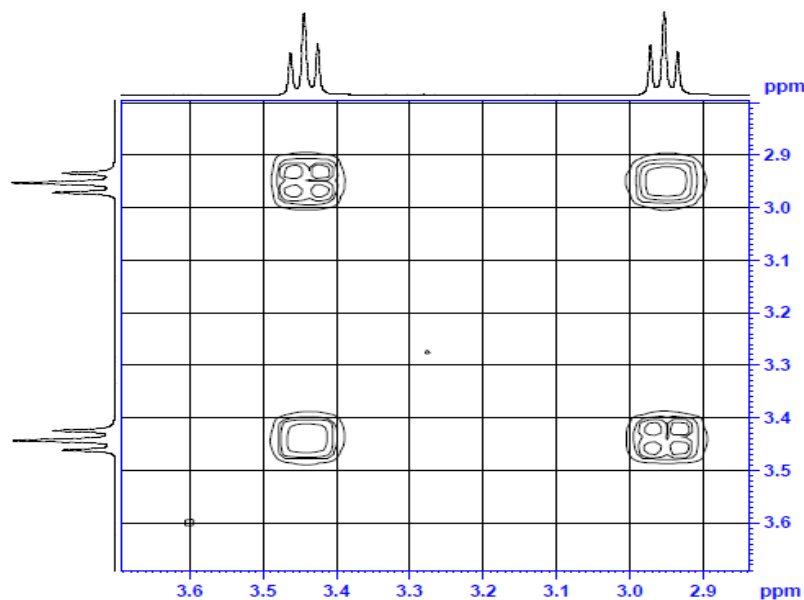
F2 - Acquisition Parameters
Date_ 20160914
Time 4.48
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1.6
DS
SWH 8223.688 Hz
FIDRES 0.123483 Hz
AQ 3.934637 sec
RG 99.66
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SFO2 400.2580105 MHz
WDW EM
SSB 0
GB 0
PC 0.30 Hz
PR 1.00

Figure 67: Enlarged H-H COSY spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]Acridine (5a):

Signature SIF VIT VELLORE
265N



Current Data Parameters
NAME VVR40916
EXPNO 2
PROCNO 1

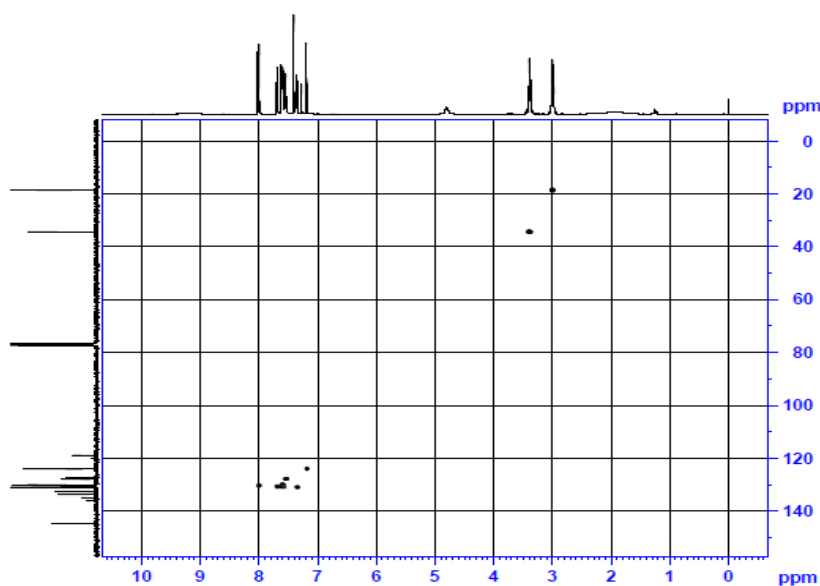
F2 - Acquisition Parameters
Date_ 20160916
Time 4.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.688 Hz
FIDRES 0.123483 Hz
AQ 3.984687 sec
RG 98.88
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PLW1 14.00000000 W
SF01 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00
FI

Figure 68: Enlarged H-H COSY spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]Acridine (5a):

Signature SIF VIT VELLORE
565OHYD



Current Data Parameters
NAME Dr.SSW180916
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160916
Time 21.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.688 Hz
FIDRES 0.123483 Hz
AQ 3.984687 sec
RG 112.65
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PLW1 14.00000000 W
SF01 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00
FI

Figure 69: HSQC spectrum of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

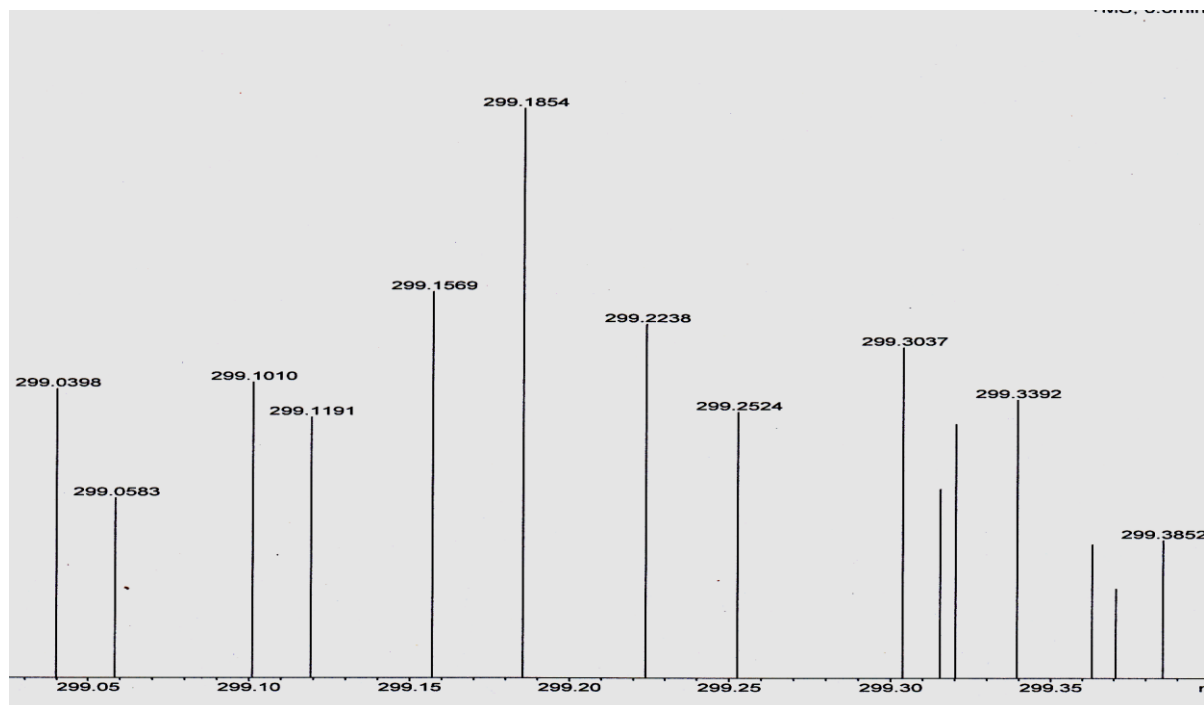


Figure 70: HRMS of 4,5-dihydro-11-phenylisoxazolo[5,4-a]acridine (5a):

Signature SIF VIT VELLORE
365ONO

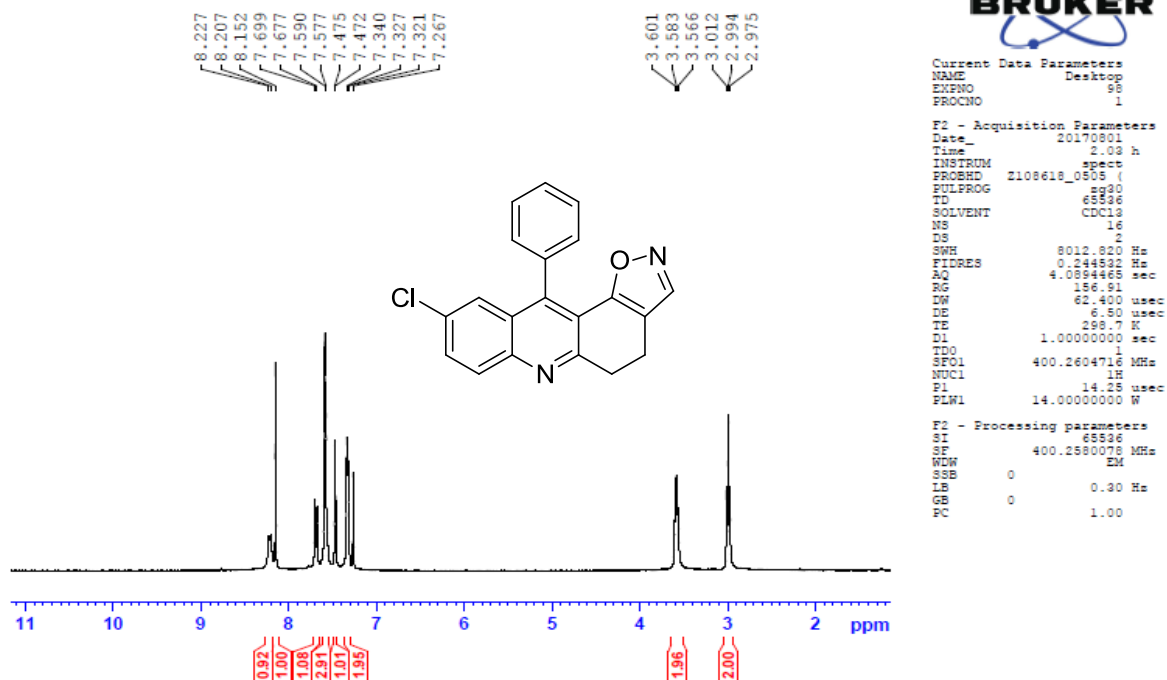
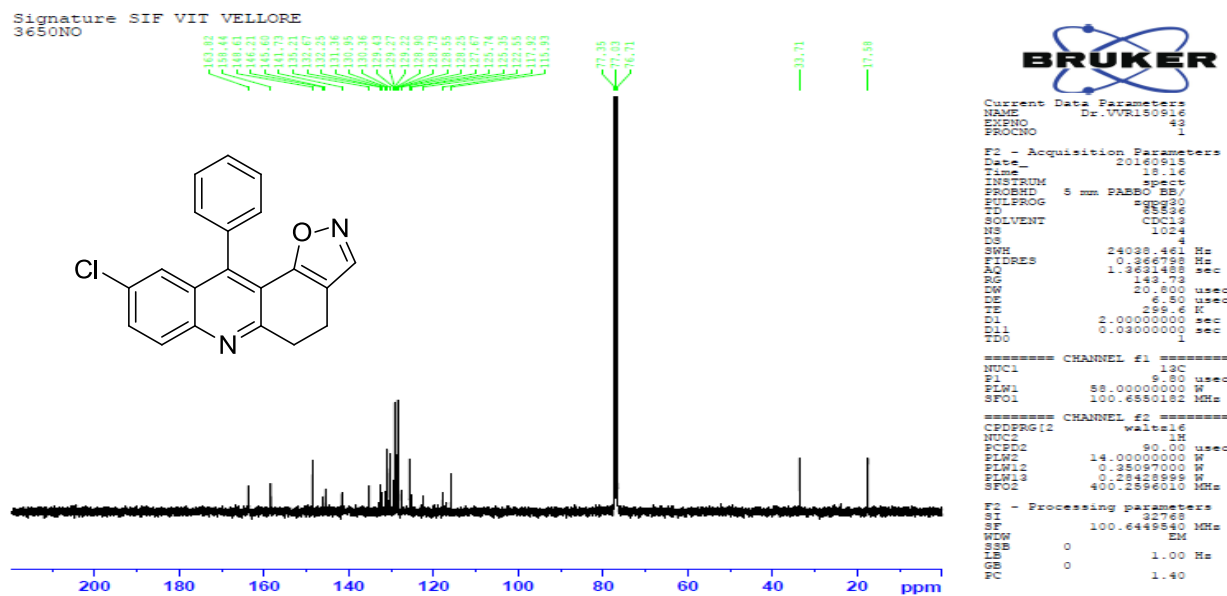
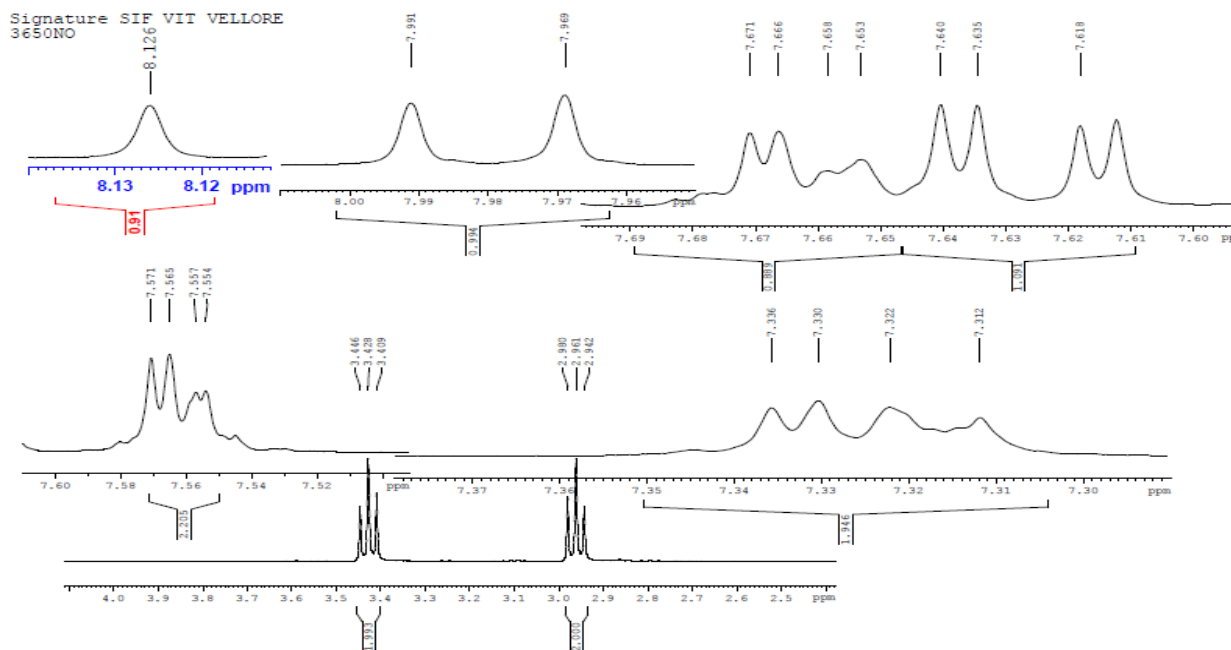


Figure 71: ^1H NMR spectrum of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):



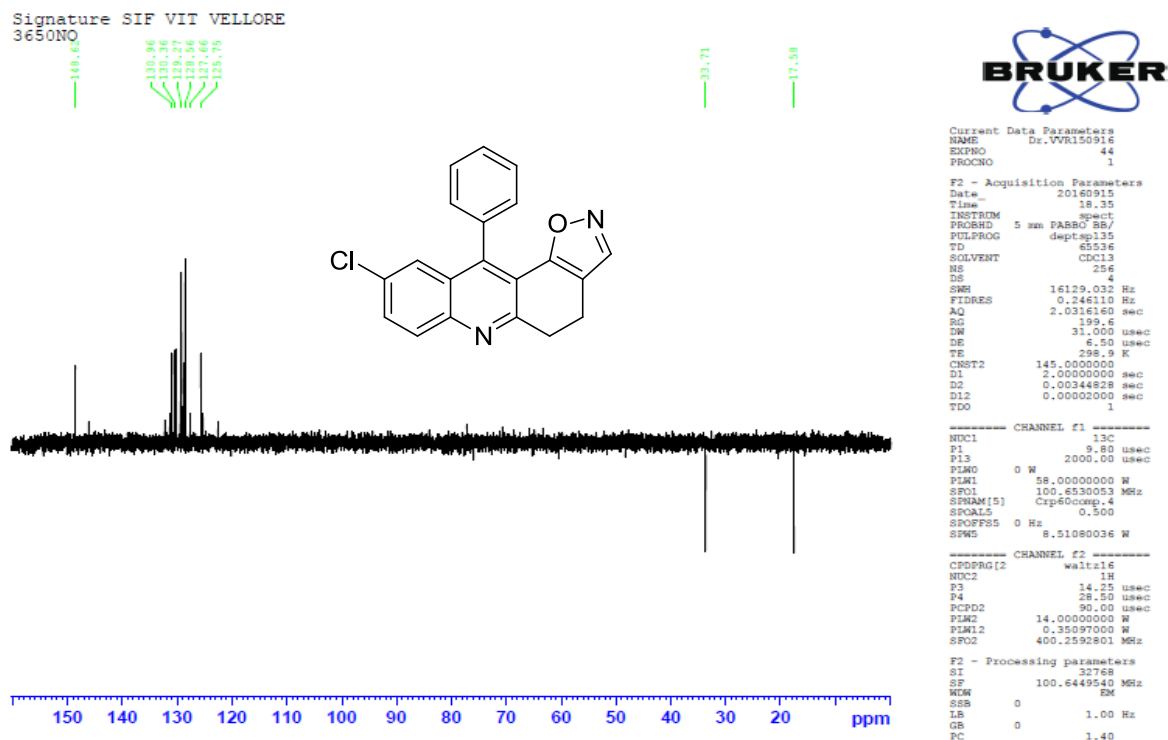


Figure 74: DEPT-135 spectrum of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):

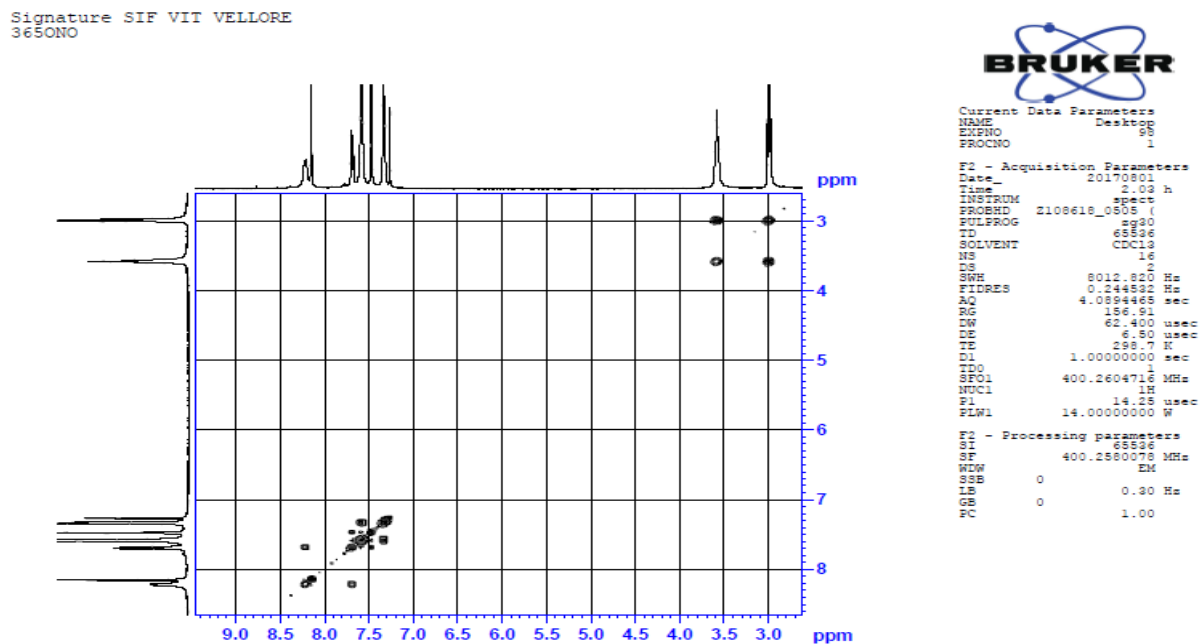


Figure 75: Enlarged H-H COSY spectrum of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):

Signature SIF VIT VELLORE
3650NO

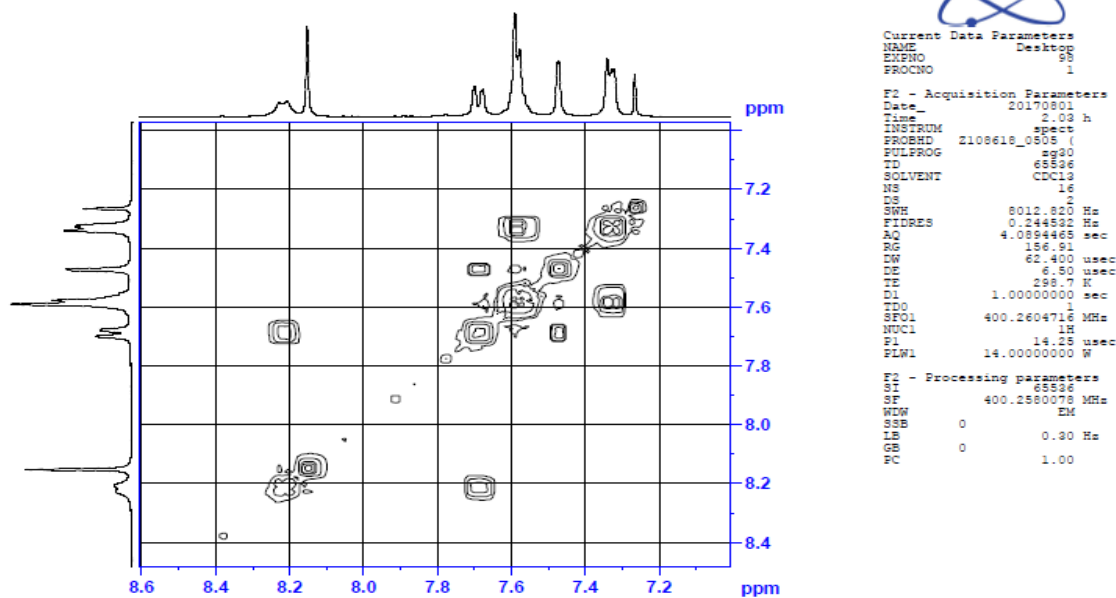


Figure 76: Enlarged H-H COSY spectrum of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):

Signature SIF VIT VELLORE
3650NO

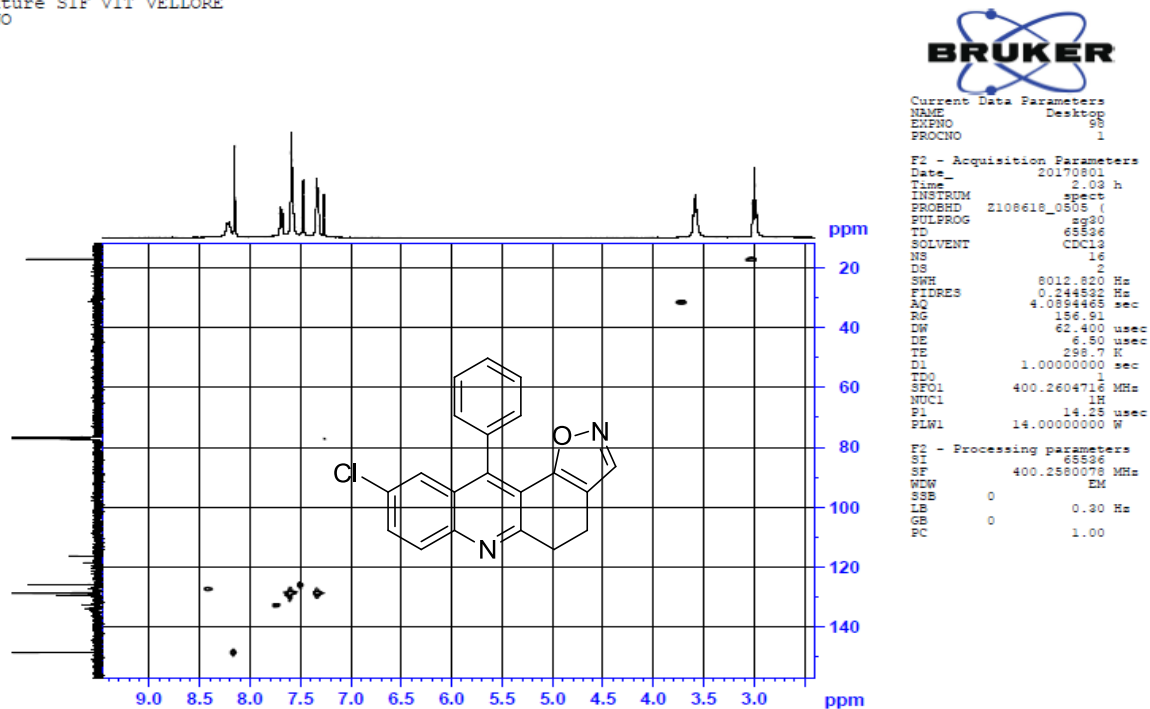


Figure 77: HSQC spectrum of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):

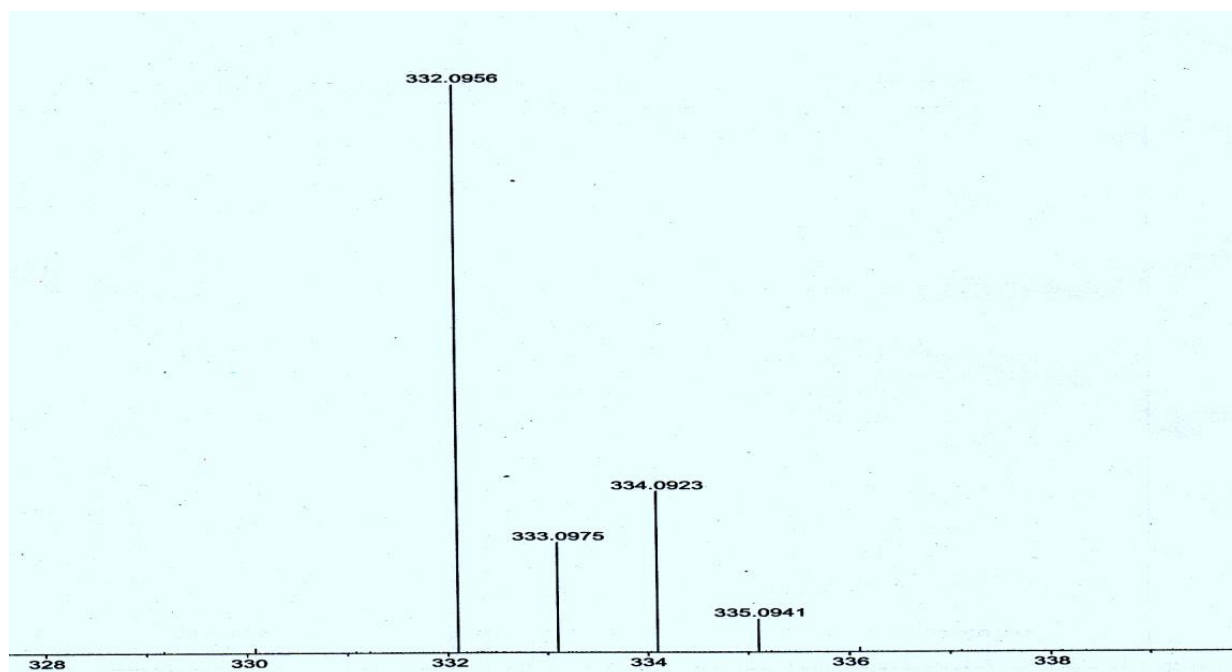
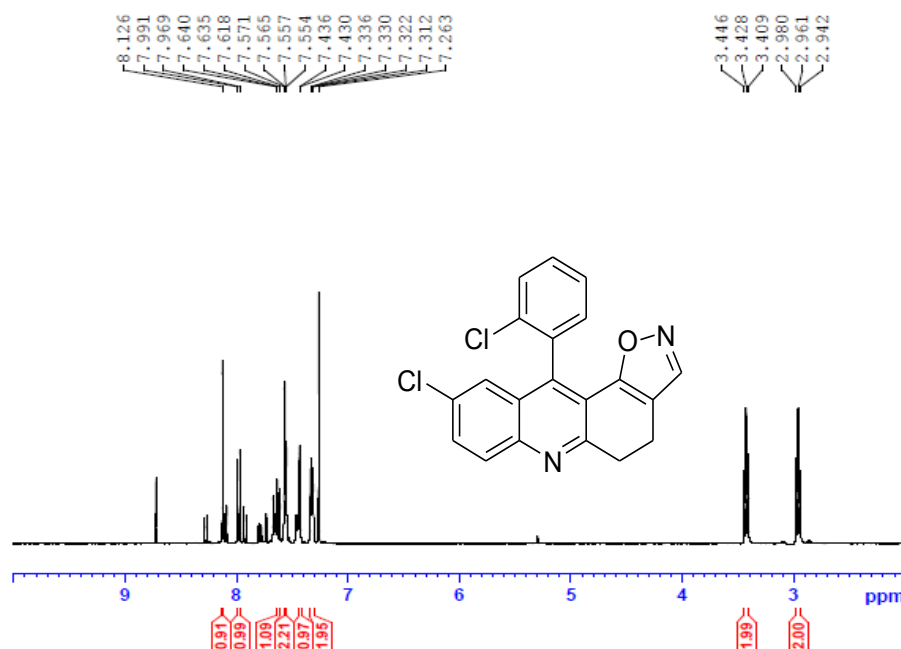


Figure 78: HRMS of 9-chloro-4,5-dihydro-11-phenylisoxazolo[3,4-a]acridine (5b):

Signature SIF VIT VELLORE
3650NO



BRUKER

Current Data Parameters
NAME Dr.VVR150916
EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160915
Time 17.17
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8229.685 Hz
FIDRES 0.125489 Hz
AQ 3.9845889 sec
RG 199.6
DW 60.800 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580103 MHz
WDW EM
SBB 0
GB 0.30 Hz
PC 1.00

Figure 79: ^1H NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydroisoxazolo[5,4-a]acridine (5c):

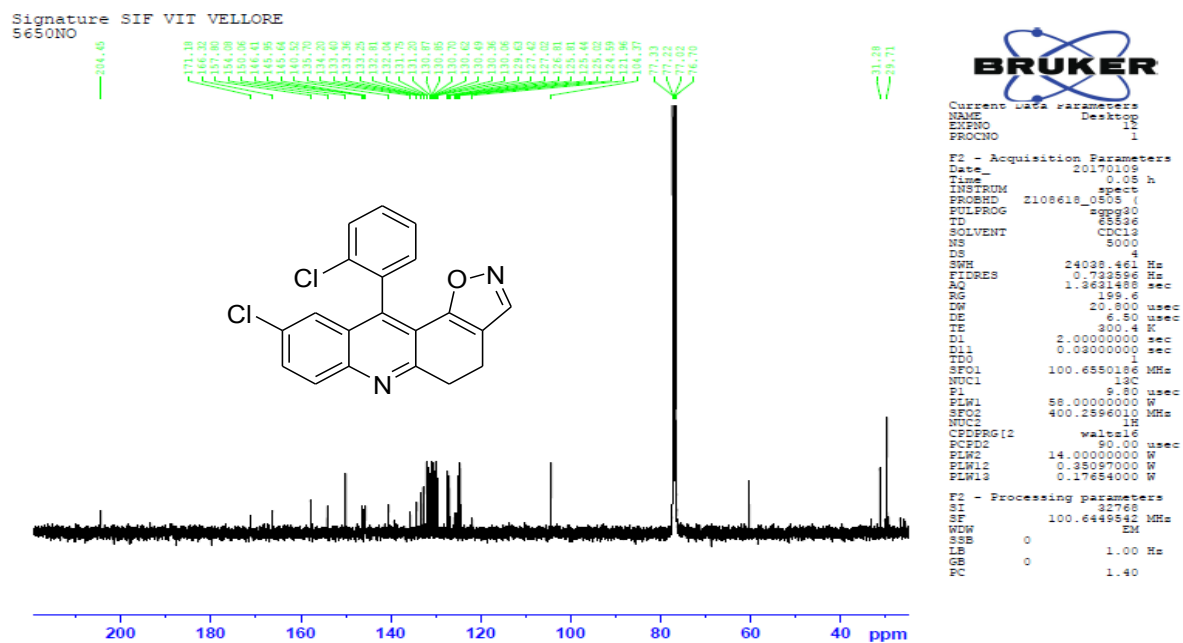


Figure 80: ^{13}C NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydroisoxazolo[5,4-a]acridine (5c)

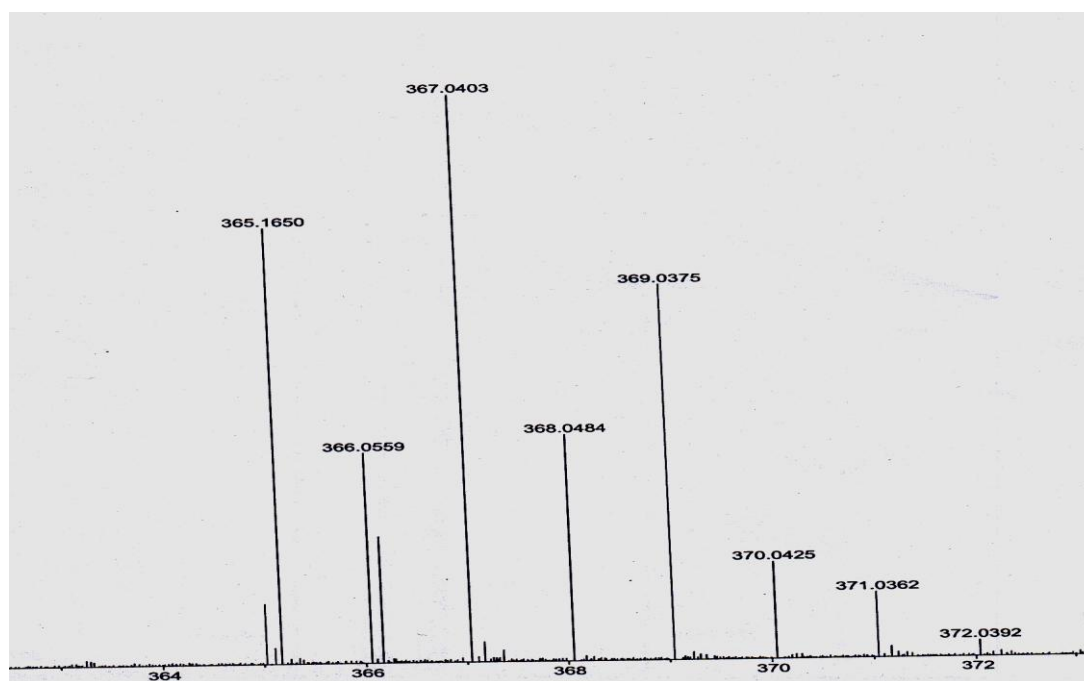
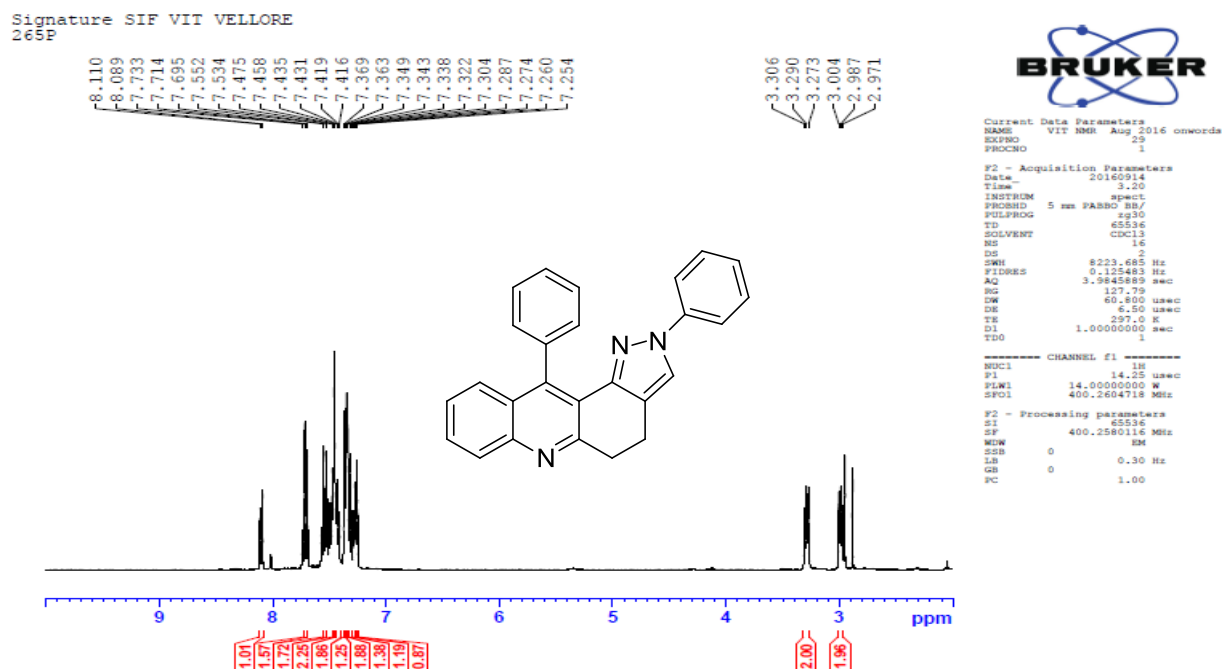
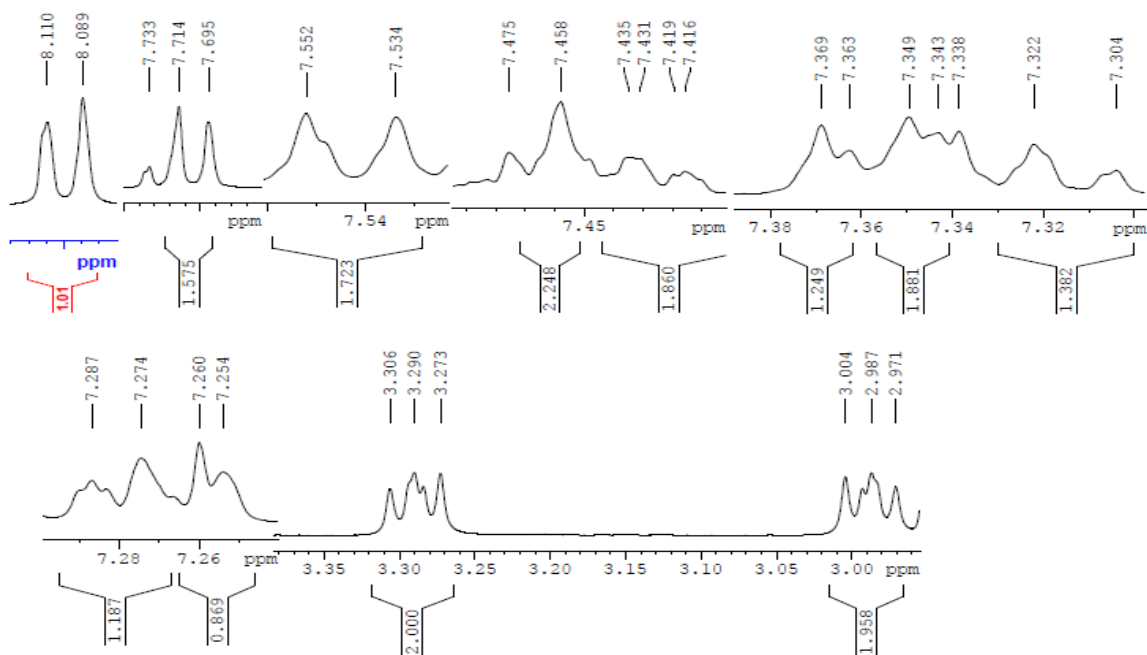


Figure 81: HRMS of 9-chloro-11-(2-chlorophenyl)-4,5-dihydroisoxazolo[5,4-a]acridine (5c):

Figure 82: ^1H NMR spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):Figure 83: Enlarged ^1H NMR spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

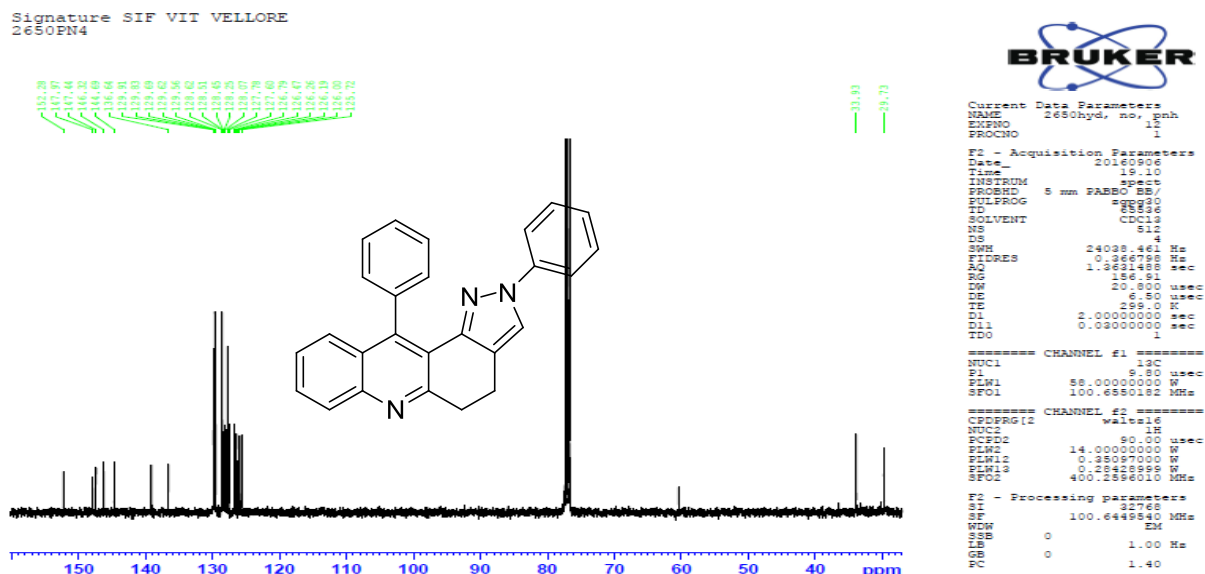
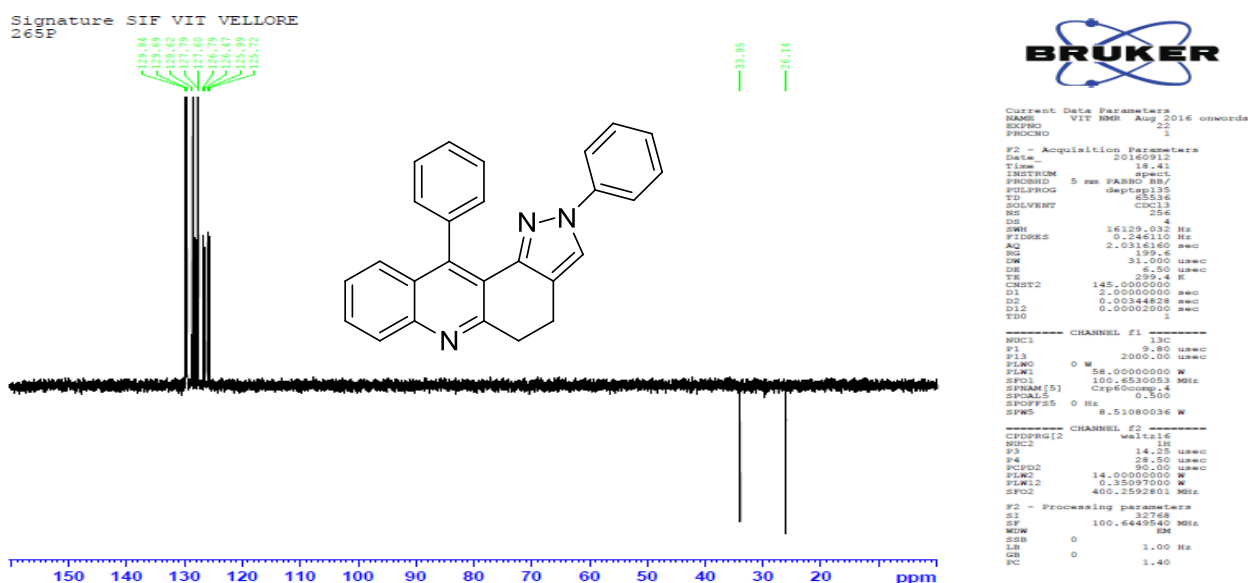
Figure 84: ^{13}C NMR spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

Figure 85: DEPT-135 spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

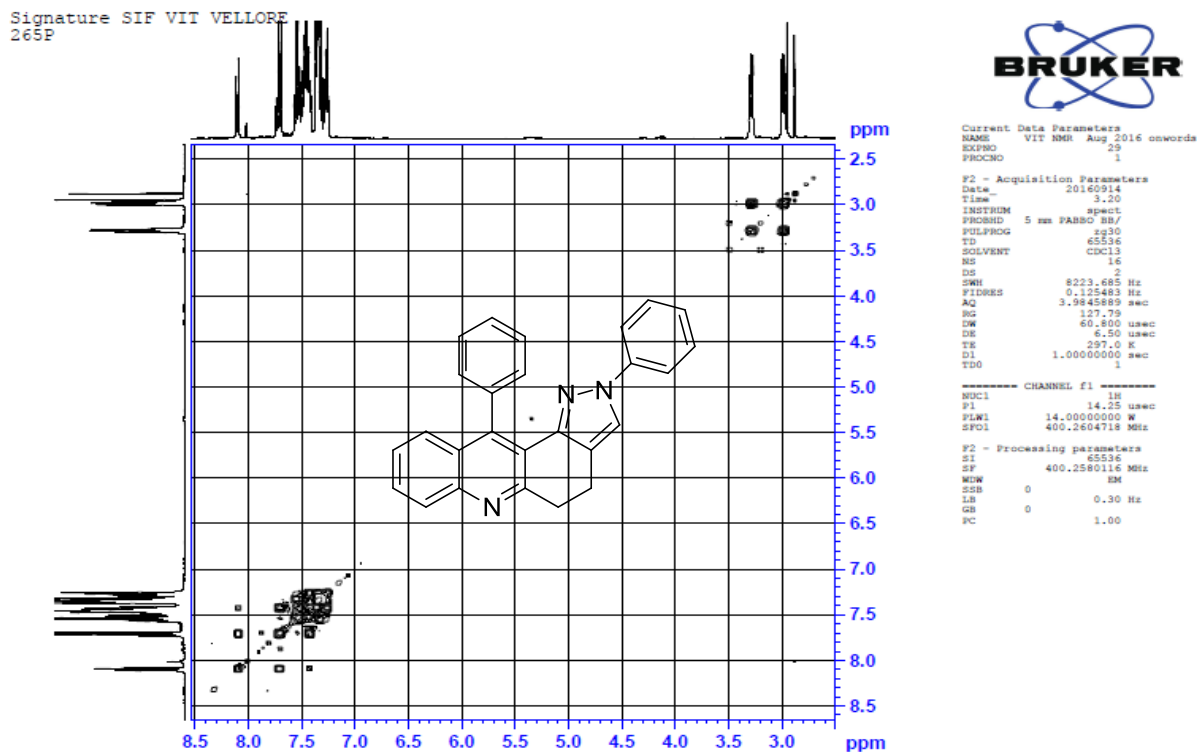


Figure 86: H-H COSY spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

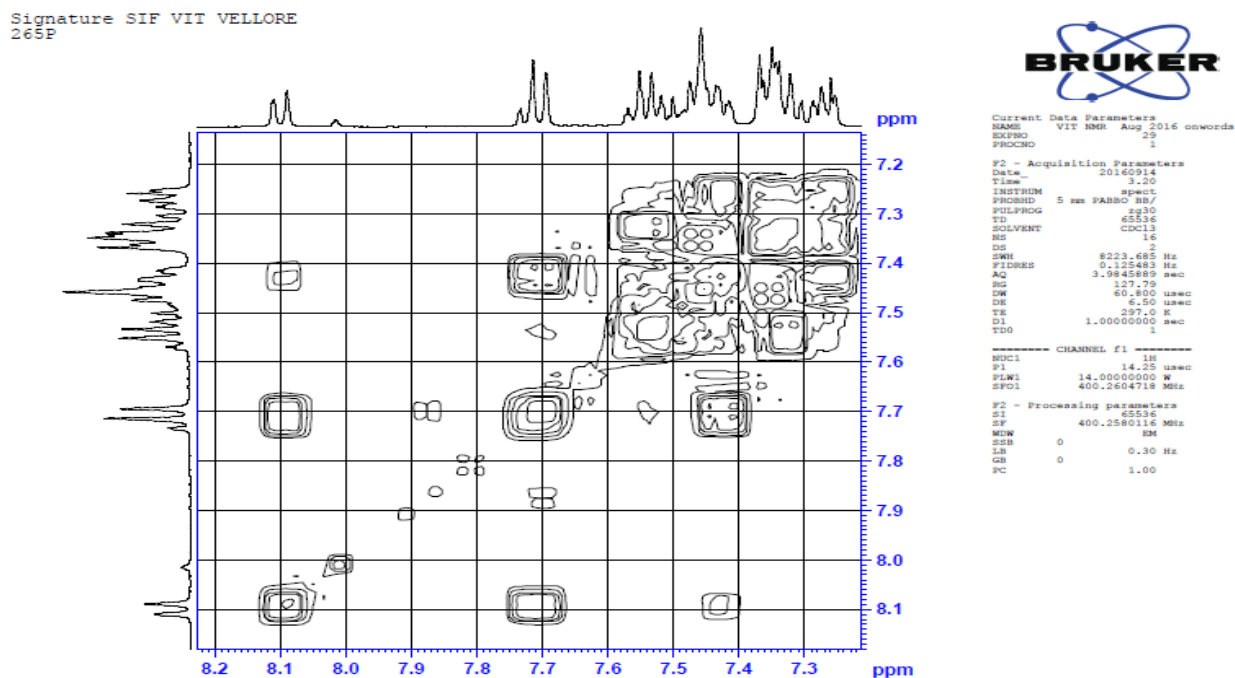


Figure 87: Enlarged H-H COSY spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

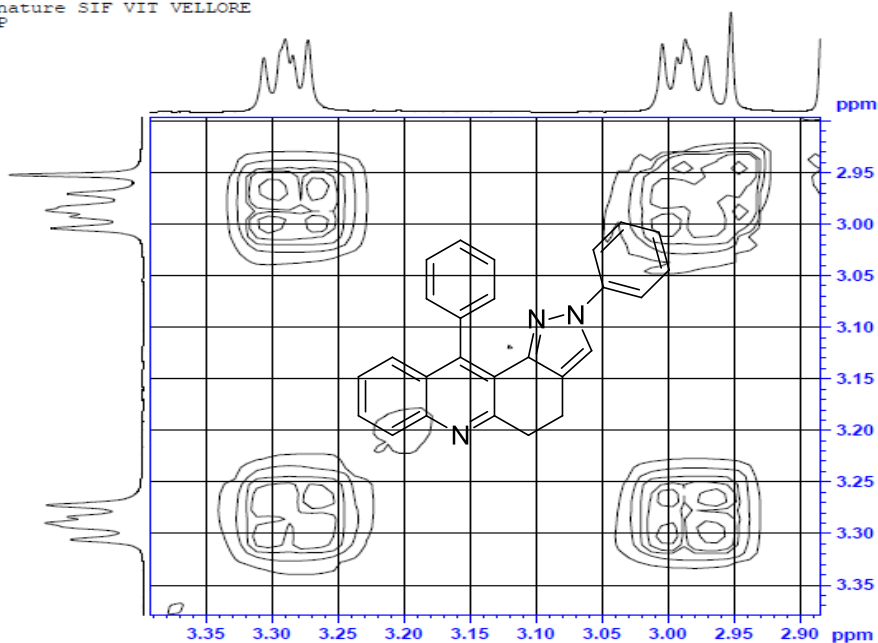
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265PCurrent Data Parameters
NAME VIT NMR Aug 2016 onwards
EXPNO 29
PROCNO 1F2 - Acquisition Parameters
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Time_ 3.20
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 127.79
DM 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.0000000 sec
TDO 1----- CHANNEL f1 -----
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHzF2 - Processing parameters
SI 65536
SF 400.2580116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 88: Enlarged H-H COSY spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

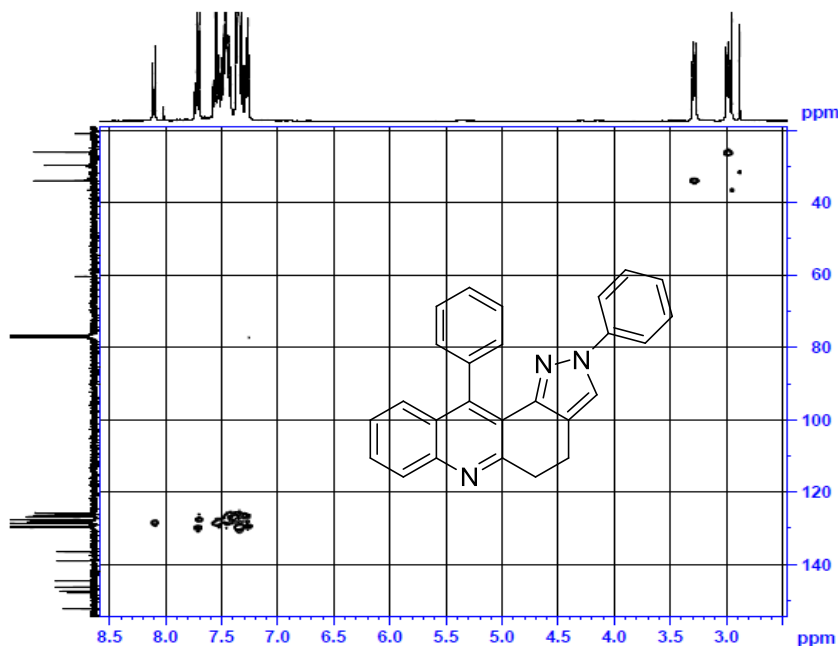
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EXPNO 29
PROCNO 1F2 - Acquisition Parameters
Date_ 20160914
Time_ 3.20
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PROBHD 5 mm PARBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 127.79
DM 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.0000000 sec
TDO 1----- CHANNEL f1 -----
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHzF2 - Processing parameters
SI 65536
SF 400.2580116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 89: HSQC spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

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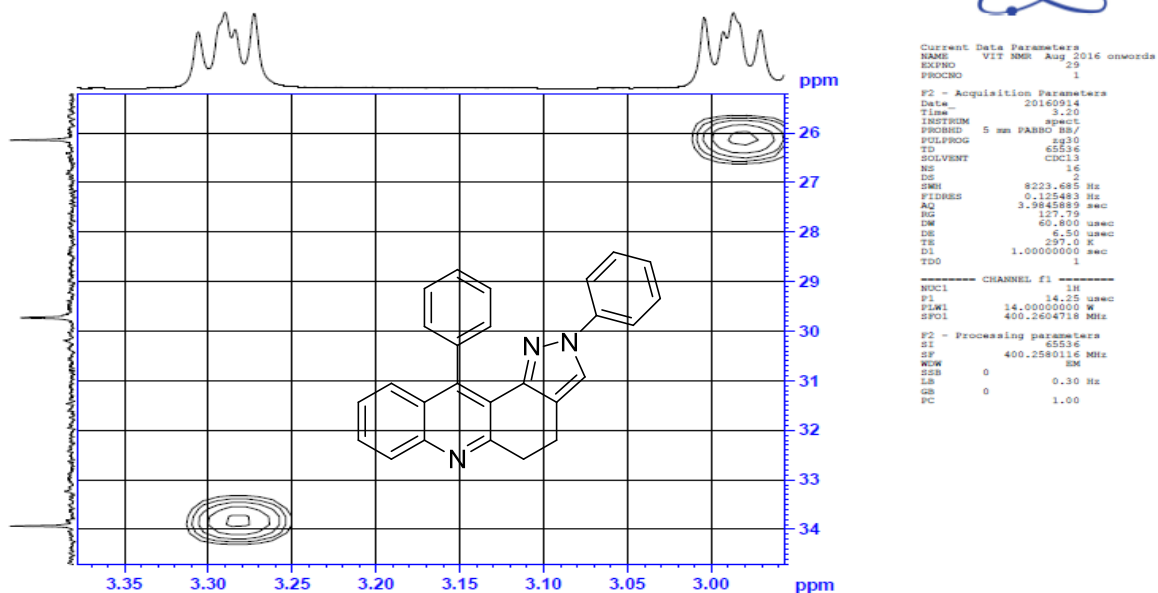


Figure 90: Enlarged HSQC spectrum of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

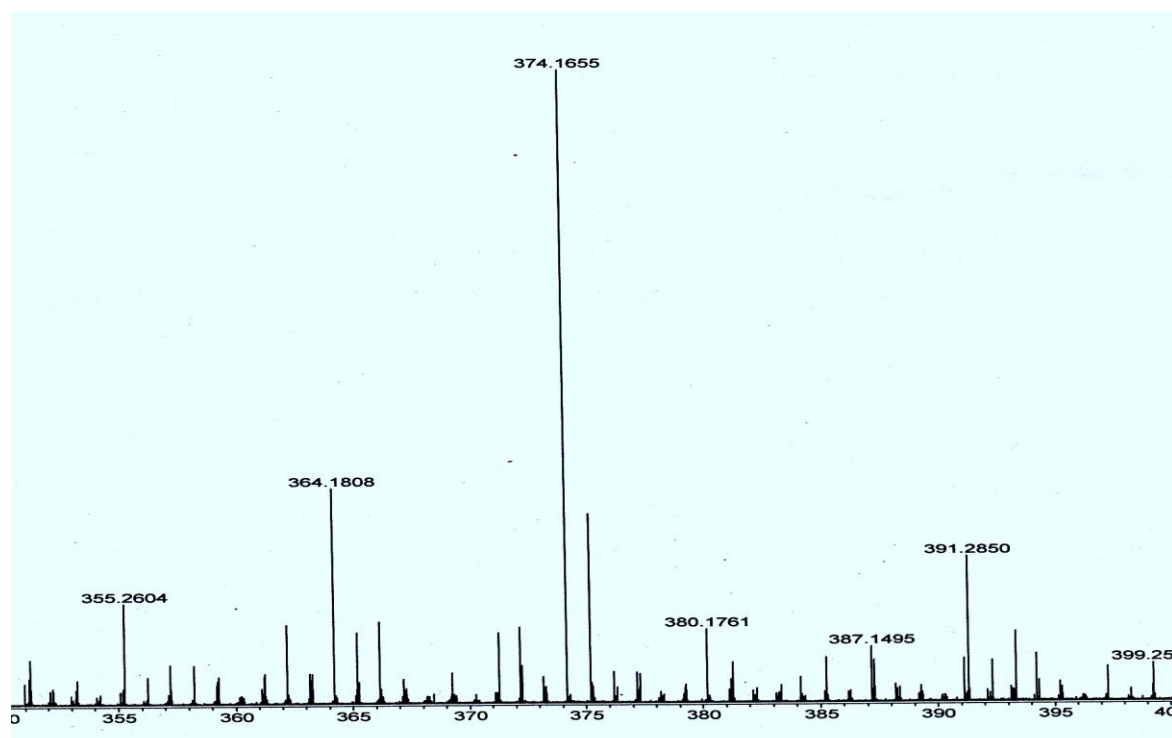
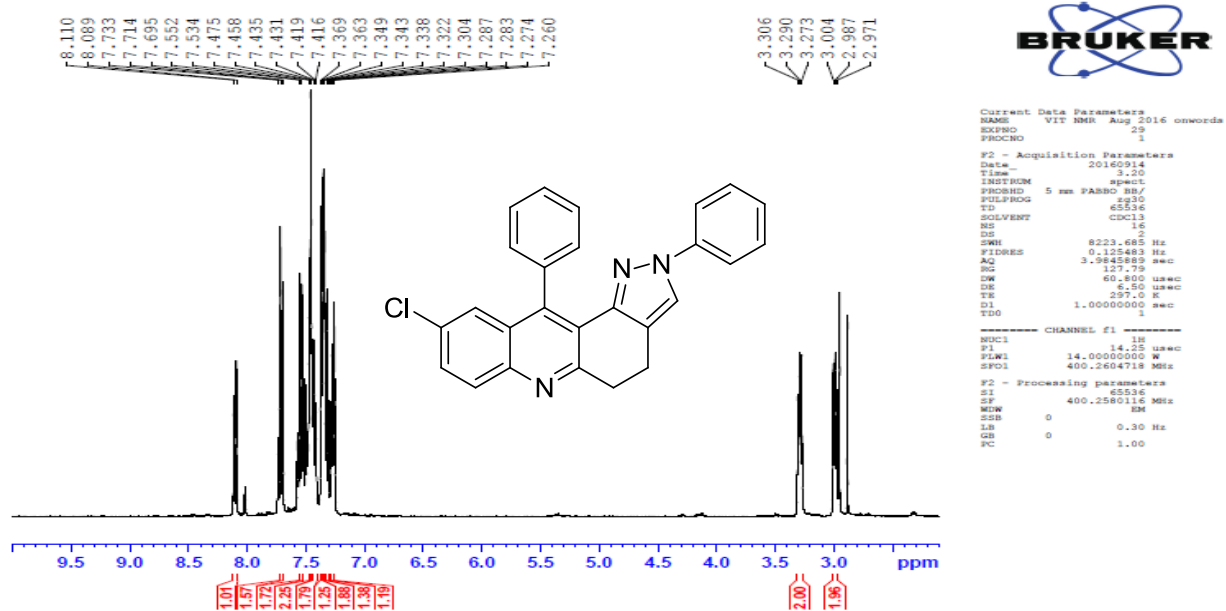
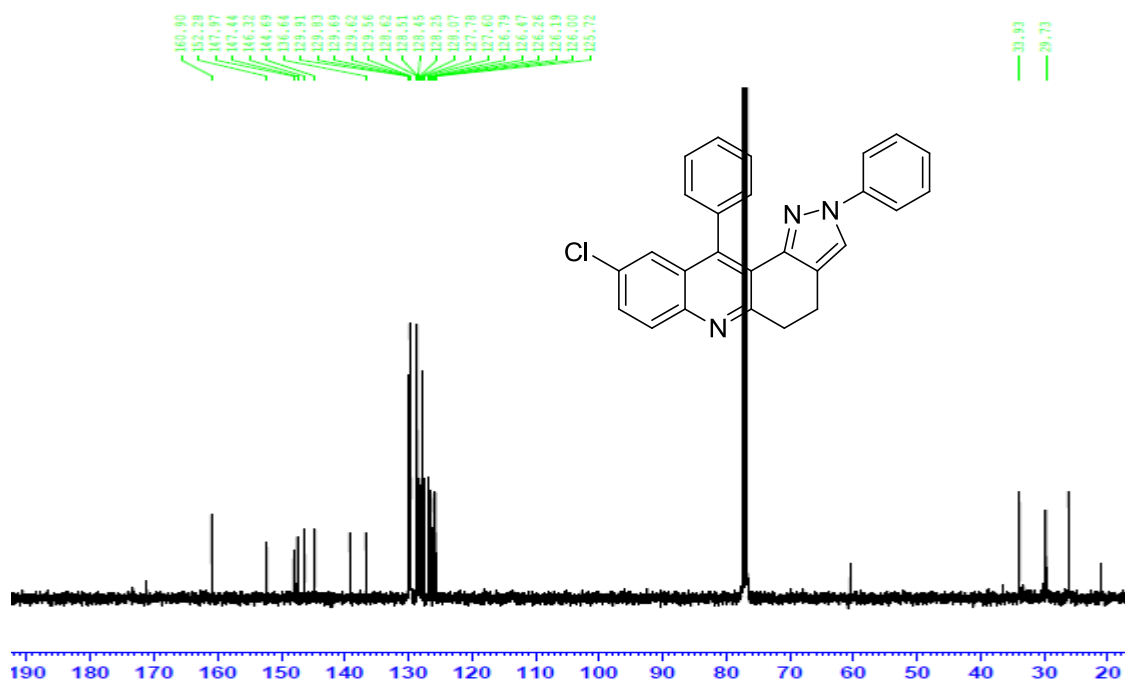


Figure 91: HRMS of 4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6a):

Figure 92: ¹H NMR spectrum of 9-chloro-4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6b):Figure 93: ¹³C NMR spectrum of 9-chloro-4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6b):

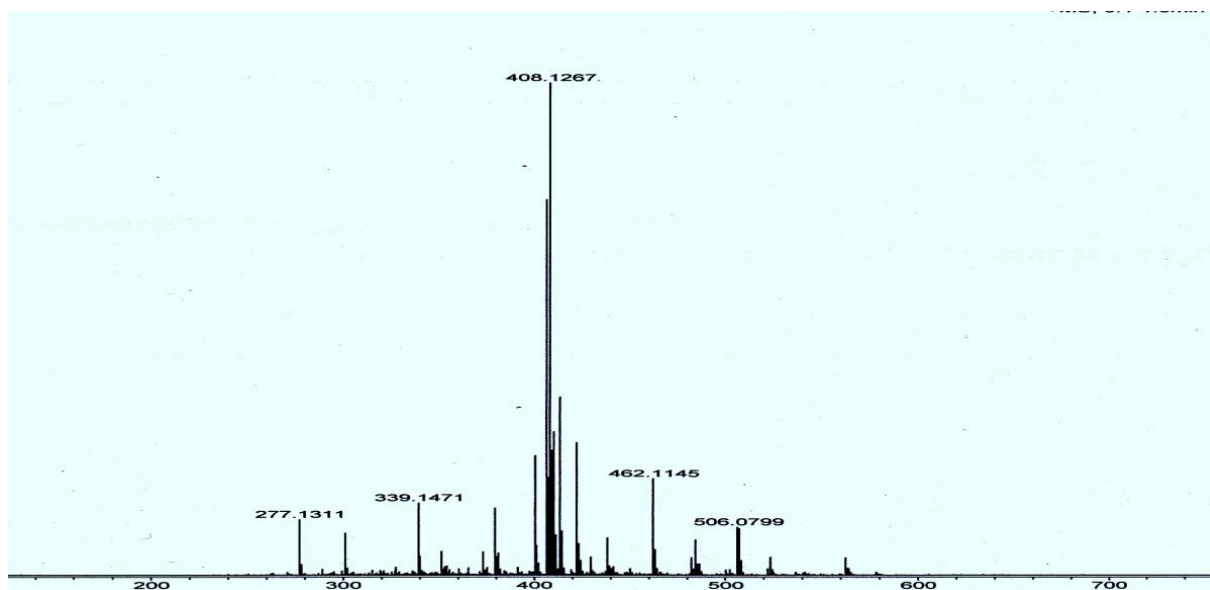


Figure 94: HRMS of 9-chloro-4,5-dihydro-1,11-diphenyl-1H-pyrazolo[3,4-a]acridine (6b):

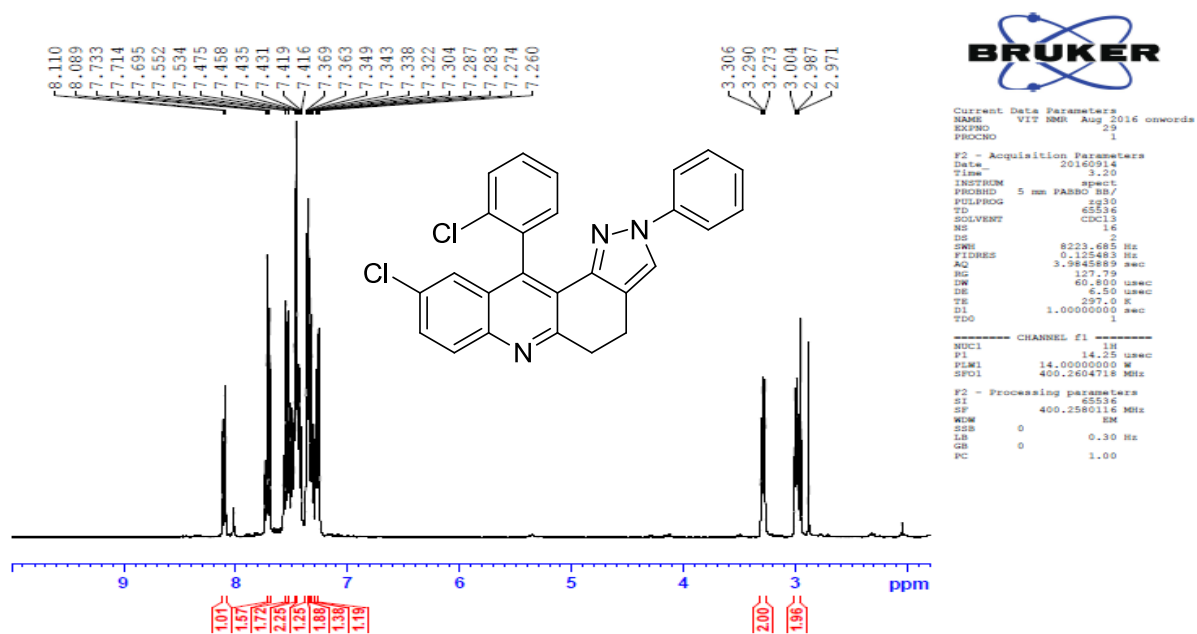


Figure 95: ¹H NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1-phenyl-1H-pyrazolo[3,4-a]acridine (6c):

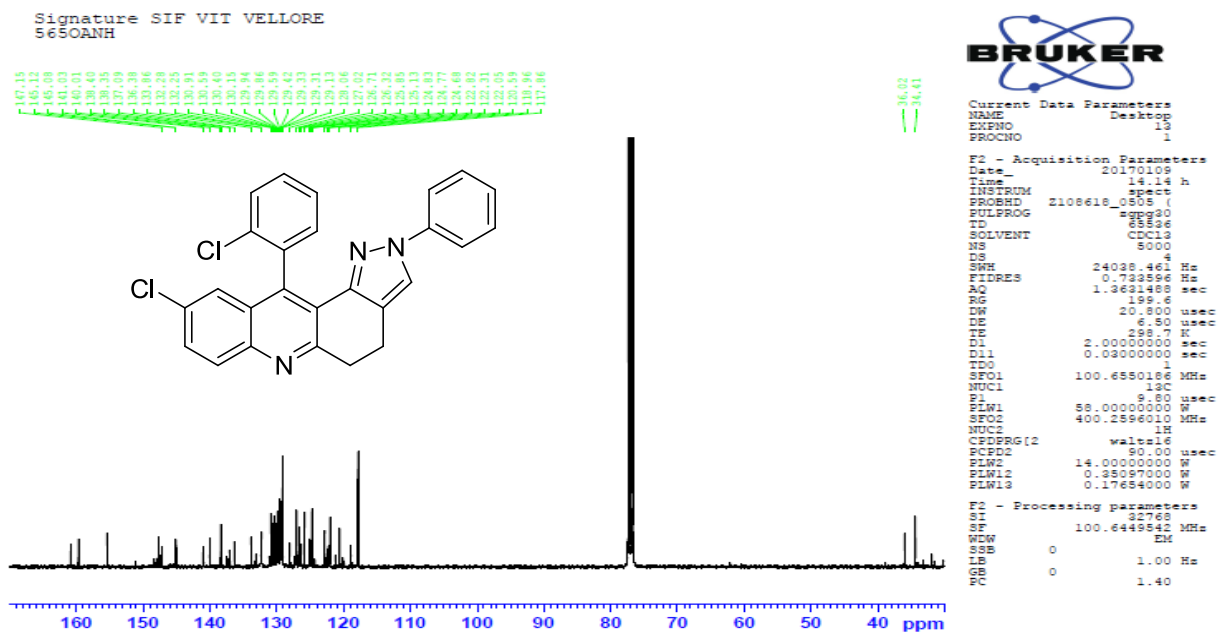


Figure 96: ^{13}C NMR spectrum of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1-phenyl-1H-pyrazolo[3,4-a]acridine (6c):

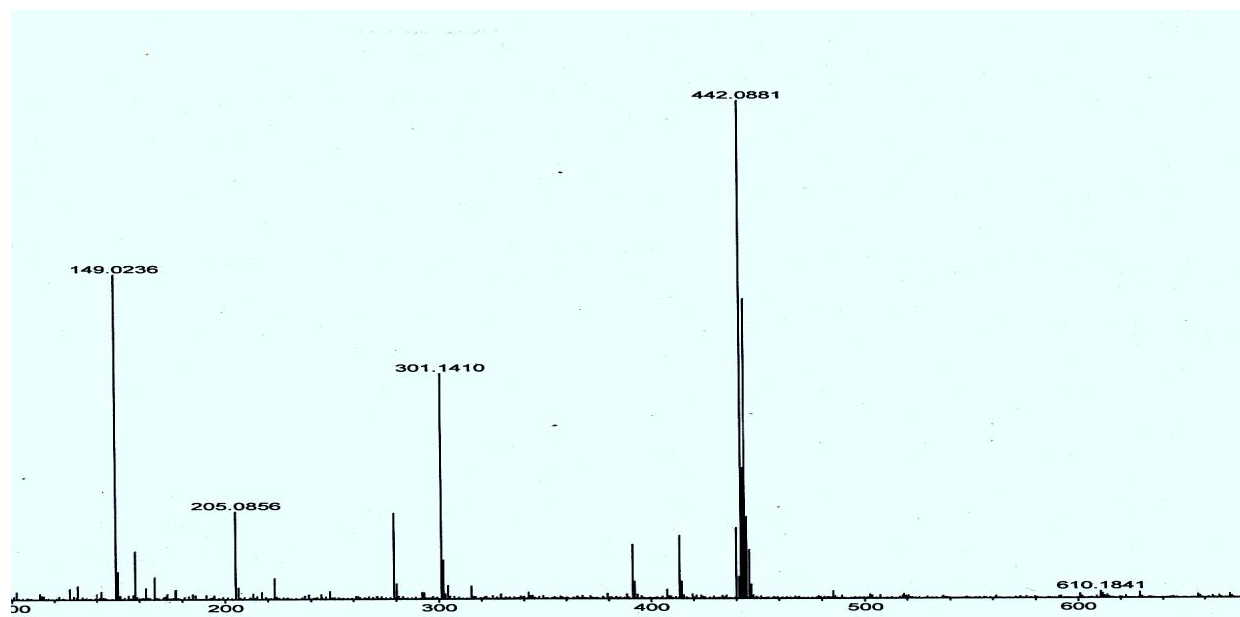


Figure 97: HRMS of 9-chloro-11-(2-chlorophenyl)-4,5-dihydro-1-phenyl-1H-pyrazolo[3,4-a]acridine (6c):