

Supporting Information

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Quinolone Alkaloids Along with Other Constituents from Zanthoxylum rhetsa and their Chemotaxonomic Significance

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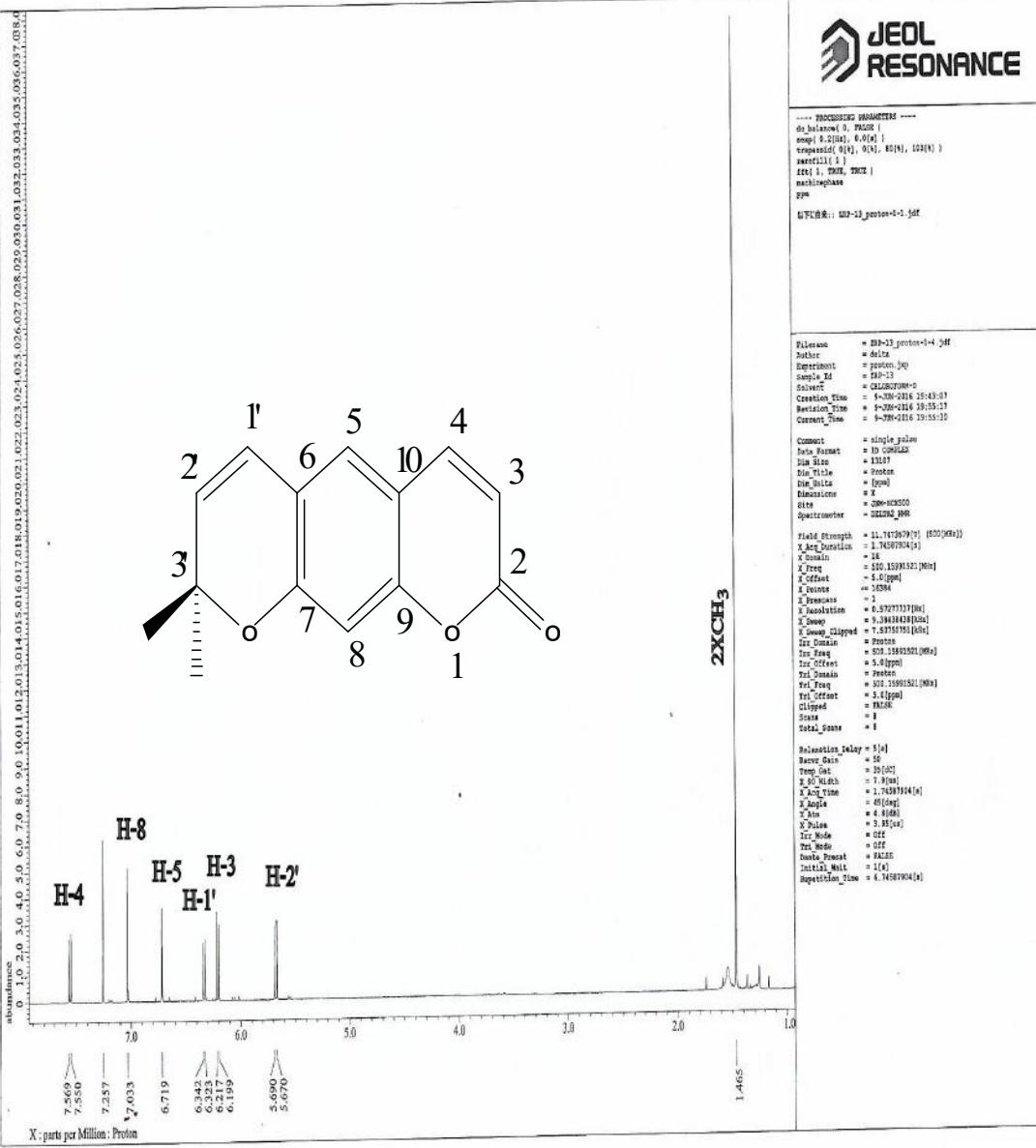
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Bangladesh*

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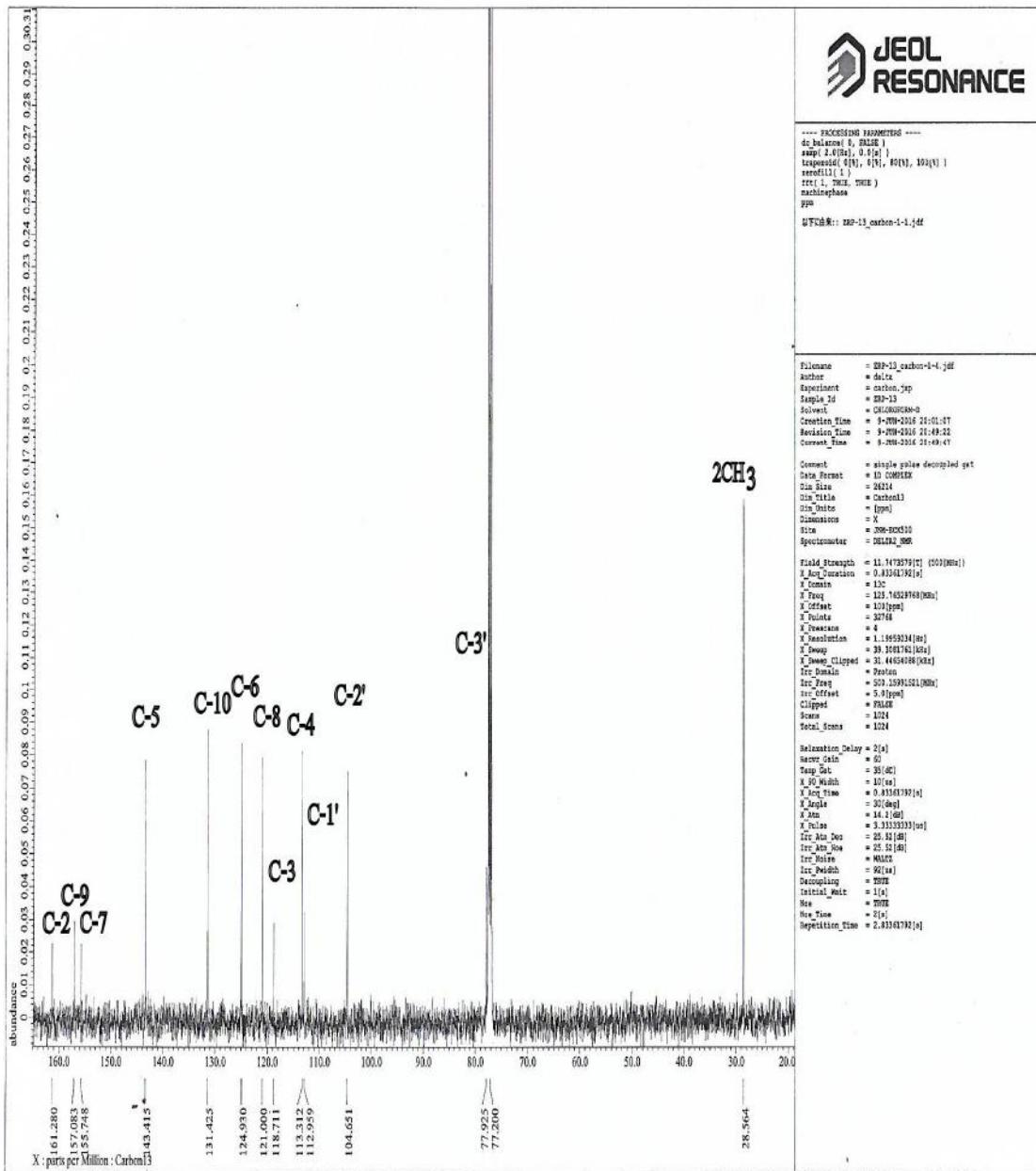
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S1: ^1H NMR (500 MHz, CDCl_3) Spectrum of Compound **1**(Xanthyletin).



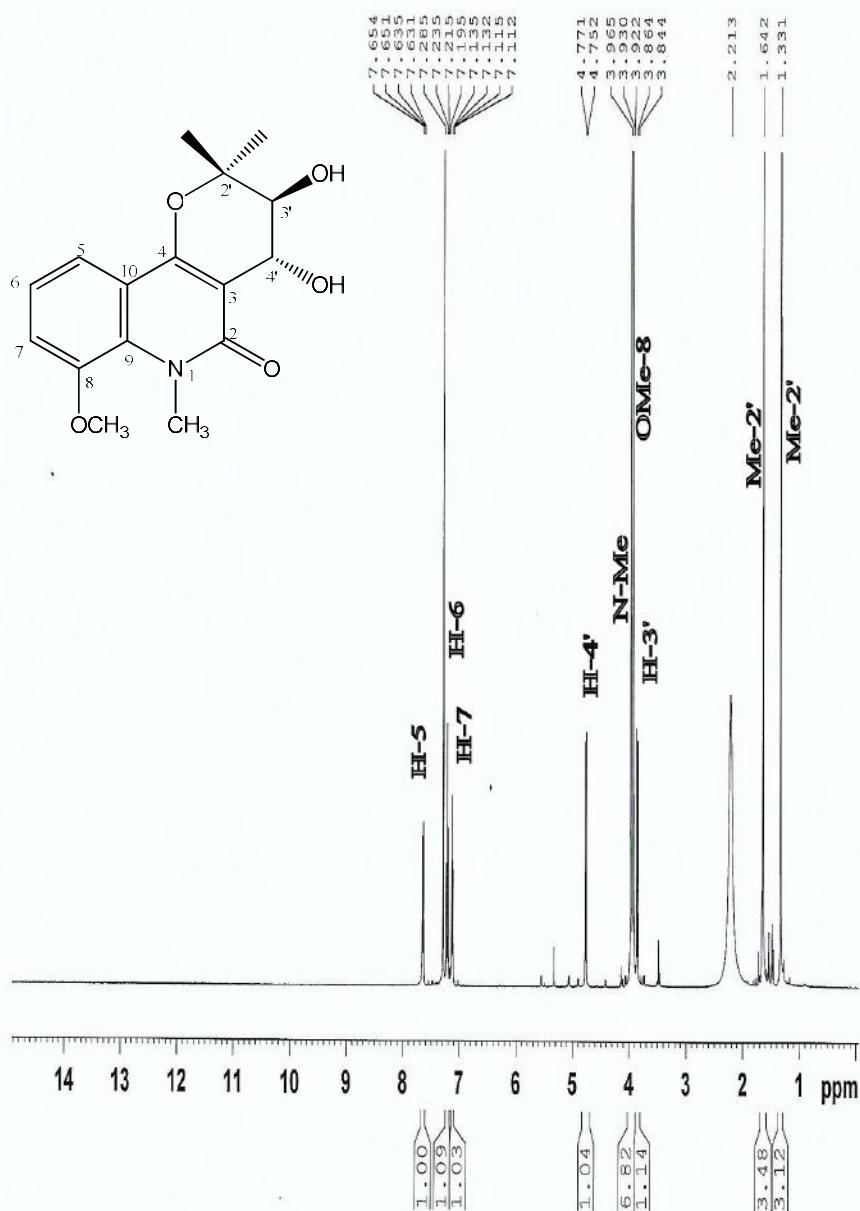
S2: ^{13}C NMR spectrum (150 MHz, CDCl_3) of Compound 1(Xanthyletin).

Xanthyletin (I): white crystals; $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 7.56 (1H, d, $J= 9.5$ Hz, H-4), 7.03 (1H, s, H-5), 6.72 (1H, s, H-8), 6.33 (1H, d, $J= 10.0$ Hz, H-4'), 6.21 (1H, d, $J= 9.5$ Hz, H-3), 5.68 (1H, d, $J= 10$ Hz, H-3'), 1.47 (6H, s, 2 x Me, H-5', 6').

Wazed Miah Science Research Center (WMSRC)

Jahangirnagar University

Sample: DU_ZRP_12

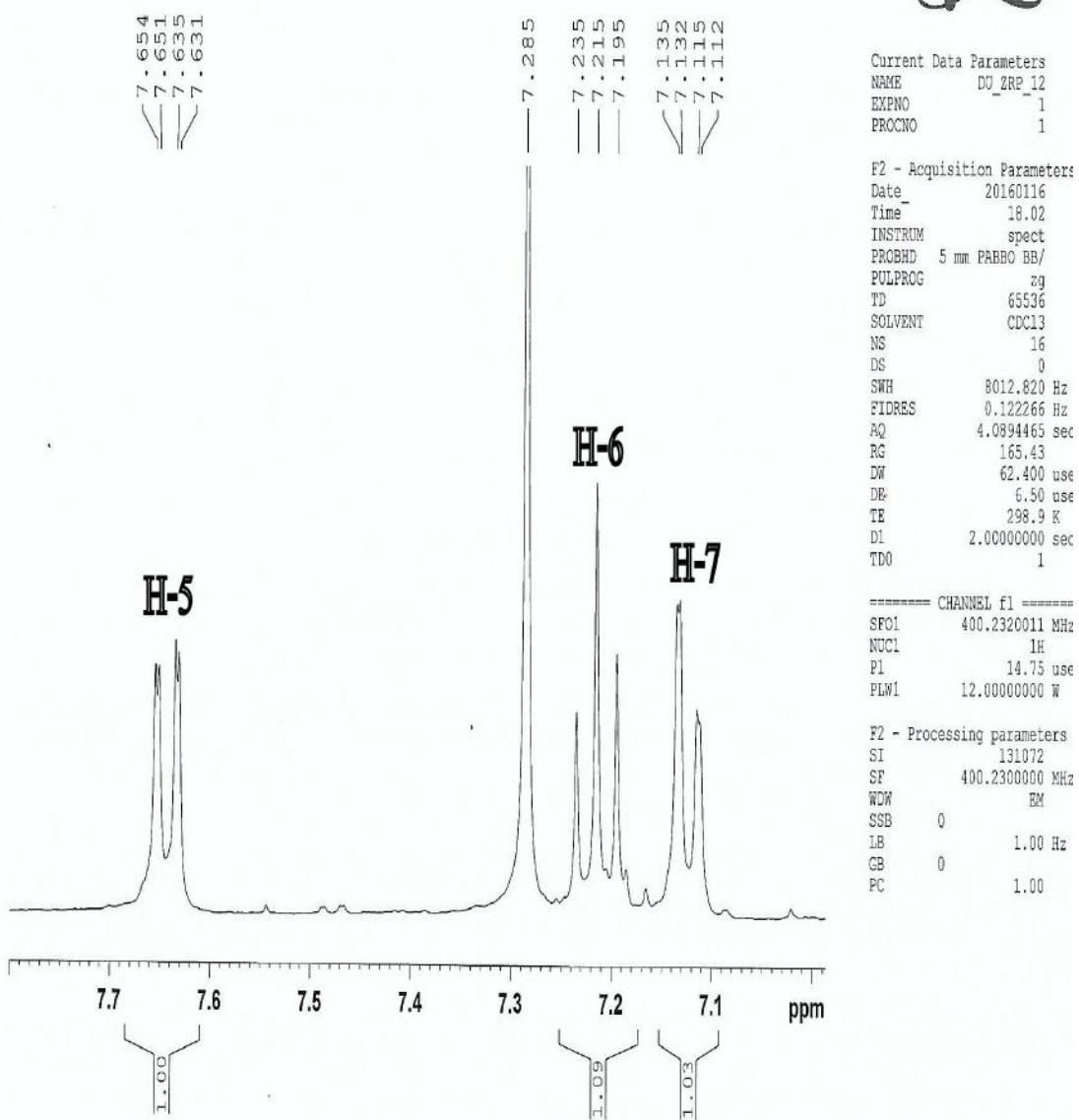


S3: ^1H NMR (400 MHz, CDCl_3) Spectrum of Compound 2 (Zanthodioline)

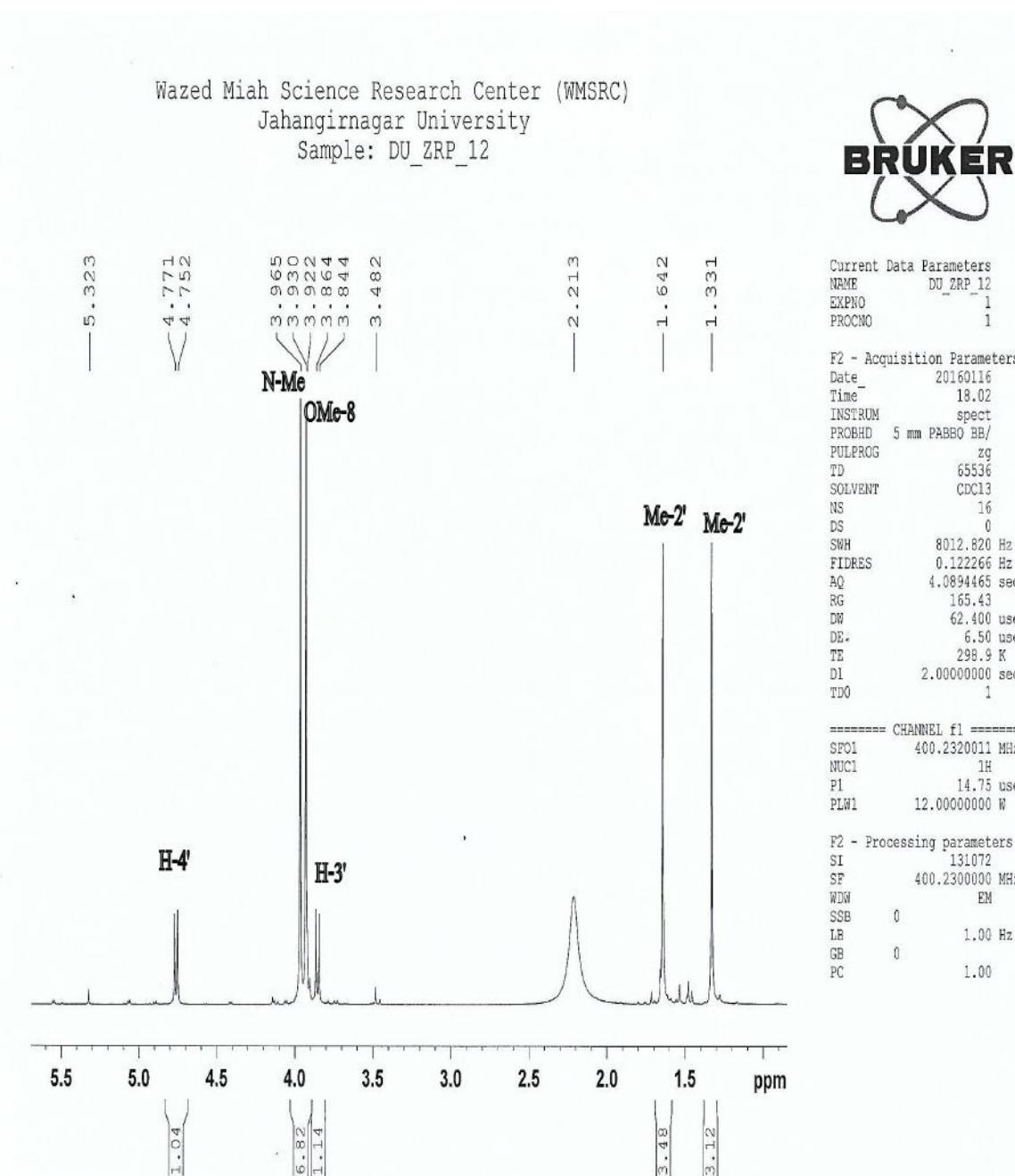
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Jahangirnagar University

Sample: DU_ZRP_12



S4 : Partially expanded ^1H NMR spectrum (400 MHz, CDCl_3) of Compound 2



S5 : Partially expanded ^1H NMR (400 MHz, CDCl_3) Spectrum of Compound 2
(Zanthodioline)

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 Jahangirnagar University
 Sample: DU_ZRP12



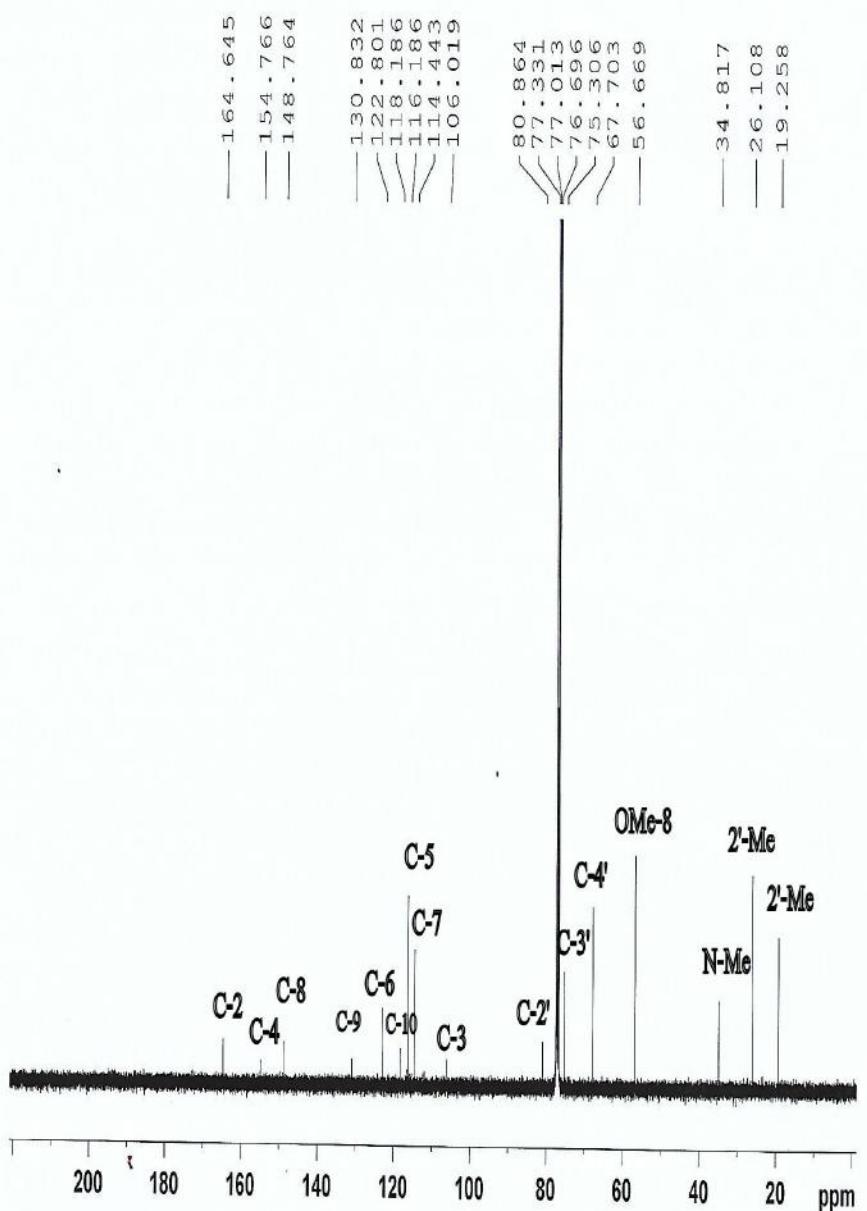
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 PROCNO 1

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 SOLVENT CDCl3
 NS 4096
 DS 0
 SWH 25252.525 Hz
 FIDRES 0.048165 Hz
 AQ 10.3809023 se
 RG 208.5
 DW 19.800 us
 DE 6.50 us
 TE 300.2 K
 D1 1.0000000 se
 D11 0.03000000 se
 TDO 1

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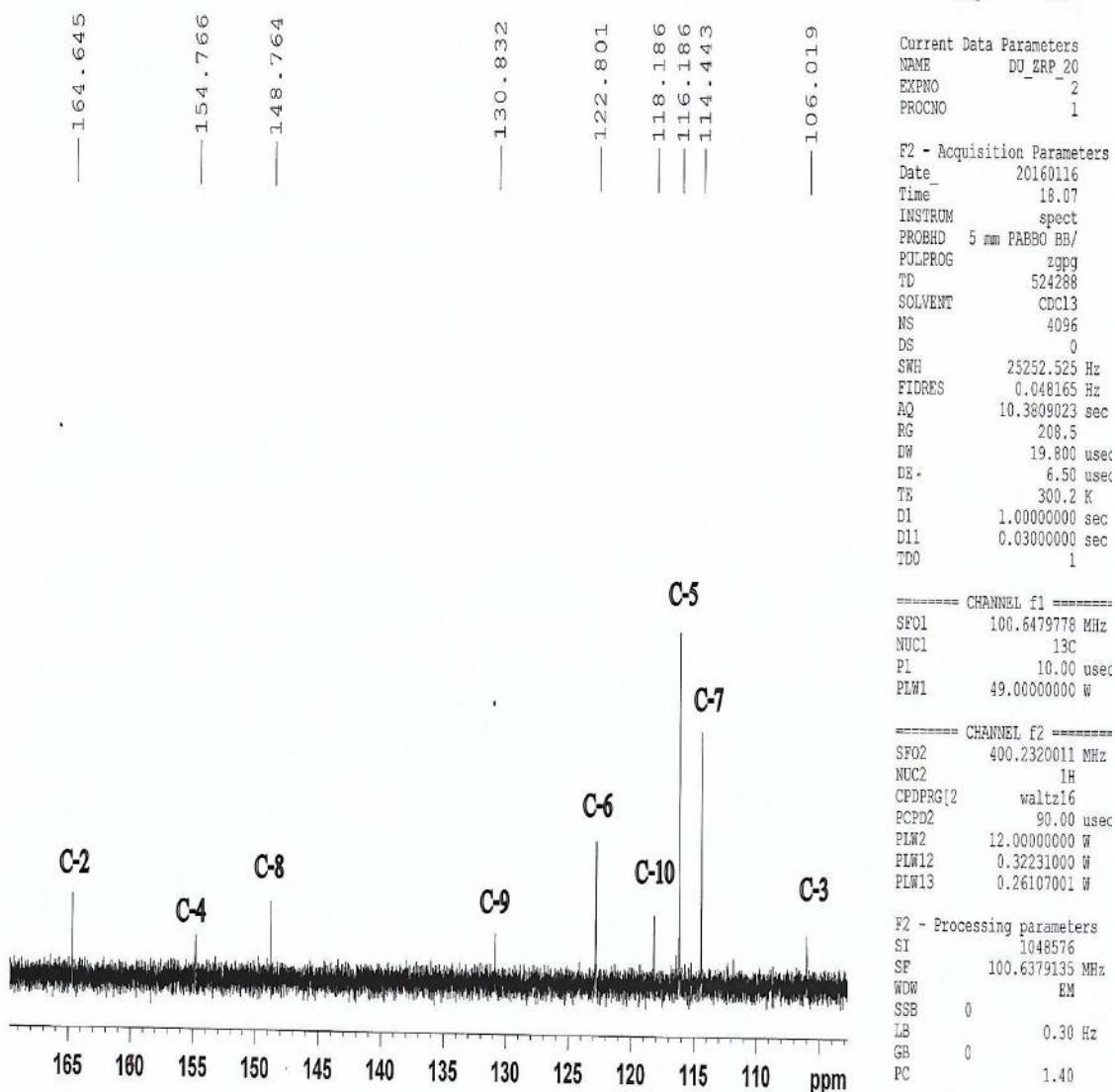
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 PLW13 0.26107001 W

F2 - Processing parameters
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 SSB 0
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 GB 0
 PC 1.40



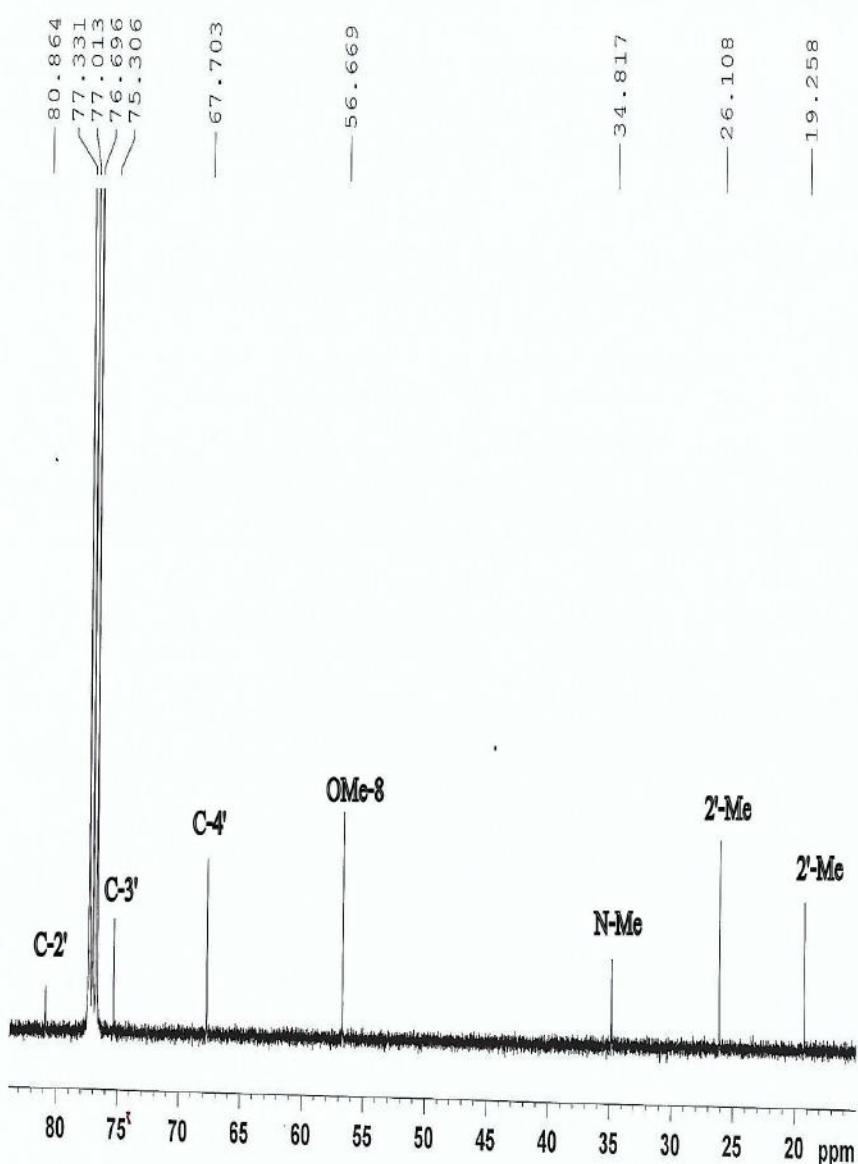
S6: ^{13}C NMR spectrum (100 MHz, CDCl_3) of Compound 2 (Zanthodioline)

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 Sample: DU_ZRP_12



S7 : Partially expanded ¹³C NMR spectrum (100 MHz, CDCl₃) of Compound 2
 (Zanthodioline)

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 Jahangirnagar University
 Sample: DU_ZRP12



Current Data Parameters
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 PROCN0 1

F2 - Acquisition Parameters
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 PULPROG zgpg
 TD 524288
 SOLVENT CDCl3
 NS 4096
 DS 0
 SWH 25252.525 Hz
 FIDRES 0.048165 Hz
 AQ 10.3809023 s
 RG 208.5
 DW 19.800 us
 DE 6.50 us
 TE 300.2 K
 D1 1.0000000 s
 D11 0.03000000 s
 TDO 1

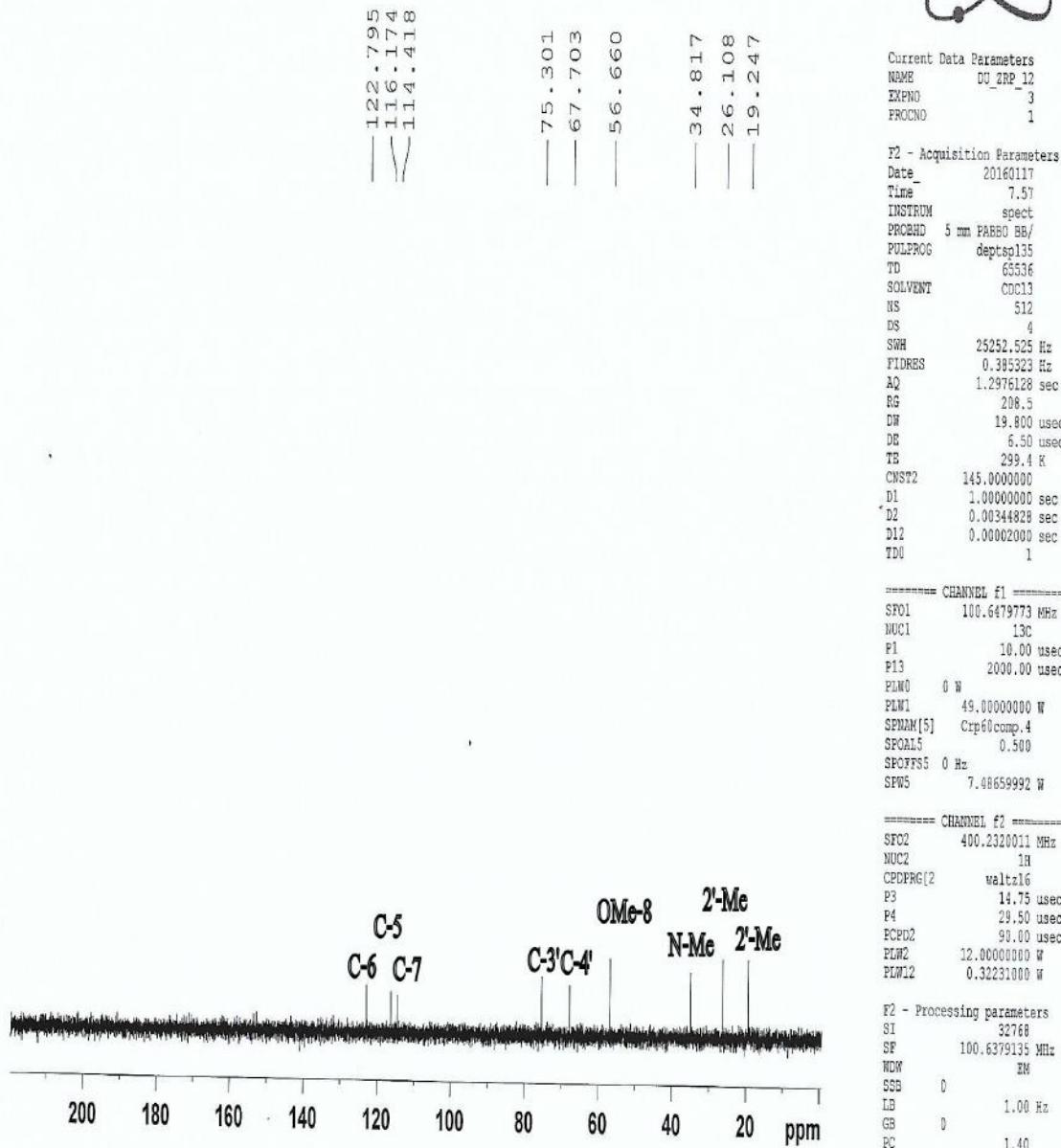
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 NUC2 1H
 CPDPRG[2] waltz16
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 PLW12 0.32231000 W
 PLW13 0.26107001 W

F2 - Processing parameters
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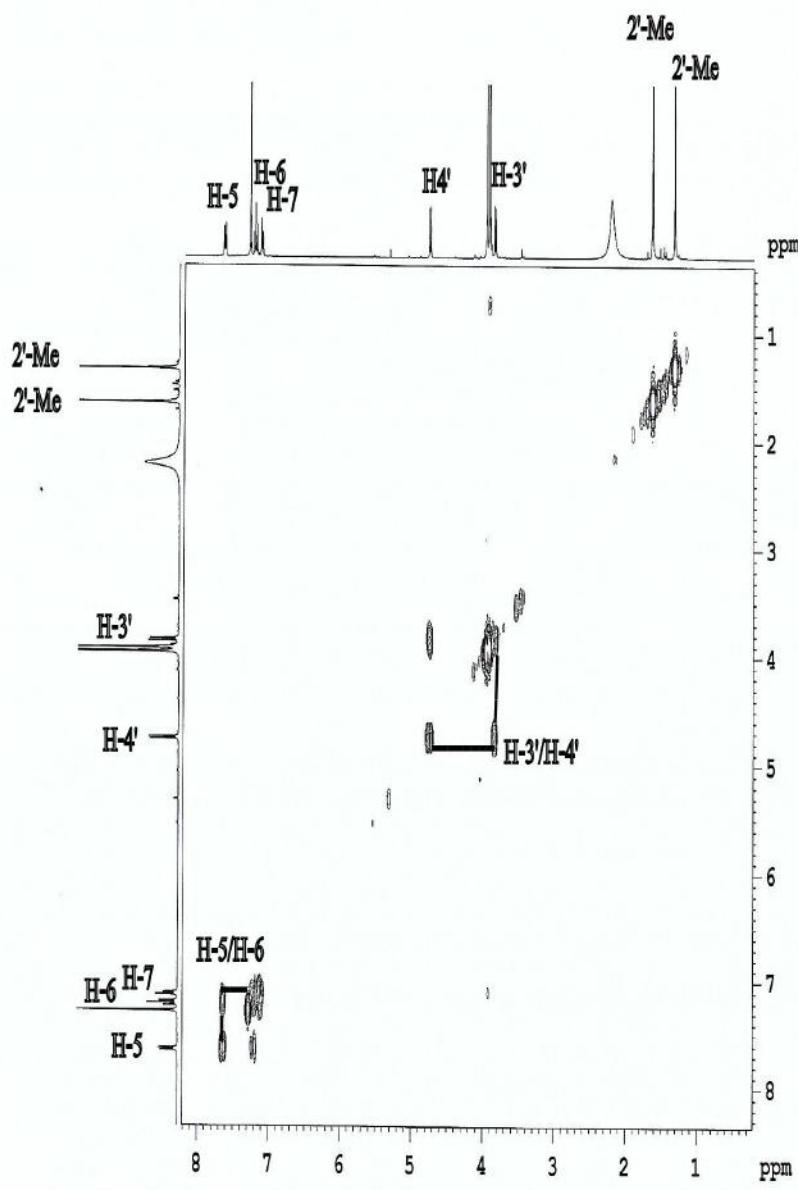
S8 : Partially expanded ^{13}C NMR spectrum (100 MHz, CDCl_3) of Compound 2
 (Zanthodioline)

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 Sample: DU_ZRP_12, dept-135



S9: DEPT-135 spectrum of Compound 2 (Zanthodioline)

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 Jahangirnagar University
 Sample: DU_ZRP_12, cosy



Current Data Parameters
 NAME DU_ZRP_12
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 PROCNO 1
 F2 - Acquisition Parameters
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 DS 4
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 FIDRES 3.912510 Hz
 AQ 0.1277952 sec
 RG 208.5
 DW 62.400 usec
 DE 6.50 usec
 TE 288.9 K
 D0 0.0000300 sec
 D1 1.0000000 sec
 D13 0.00003400 sec
 D16 0.00020000 sec
 ERO 0.00012400 sec

===== CHANNEL f1 =====
 SF01 400.2320011 MHz
 NUC1 1H
 P0 14.75 usec
 P1 14.75 usec
 PLW1 12.0000000 W

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 GP21 10.00 %
 P16 1000.00 usec

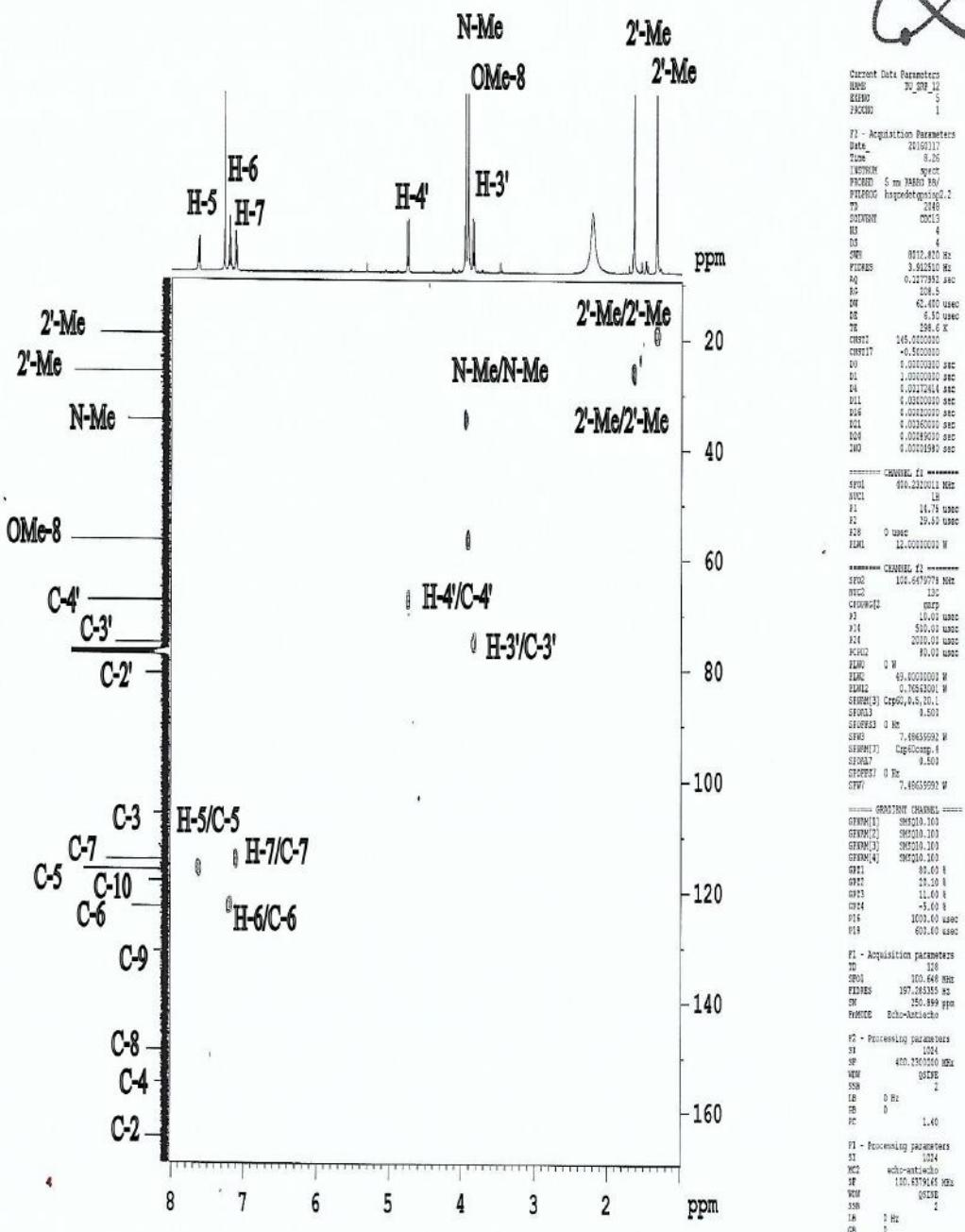
F1 - Acquisition parameters
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 FIDRES 62.600159 Hz
 SW 20.020 ppm
 Envelope QF

F2 - Processing parameters
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 SF 400.2300010 MHz
 WIDN QSTIME
 SSB 0
 LB 0 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
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 MC2 QF
 SF 400.2300011 MHz
 MWL QSTIME
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 LB 0 Hz
 GB 0

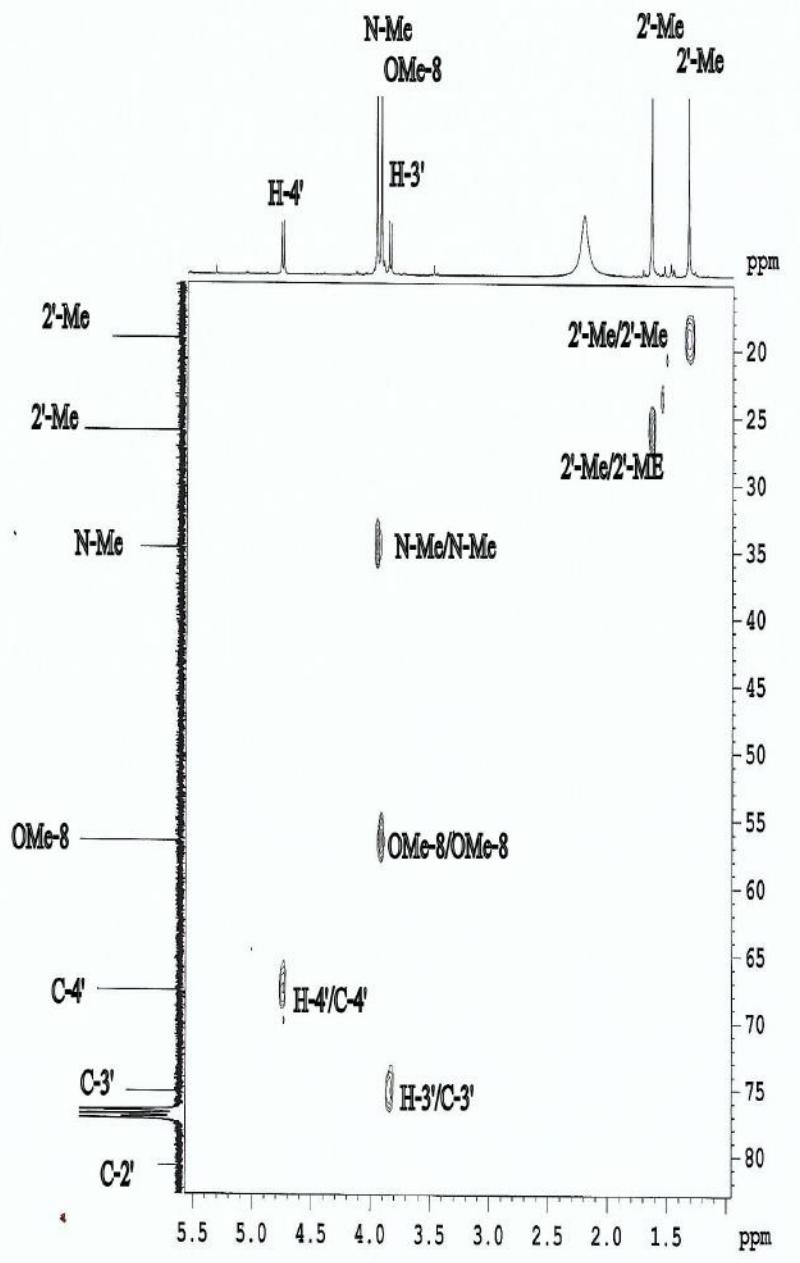
S10: COSY-NMR spectrum (400 MHz, CDCl_3) of Compound 2 (Zanthodioline)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRP_12, hsqc



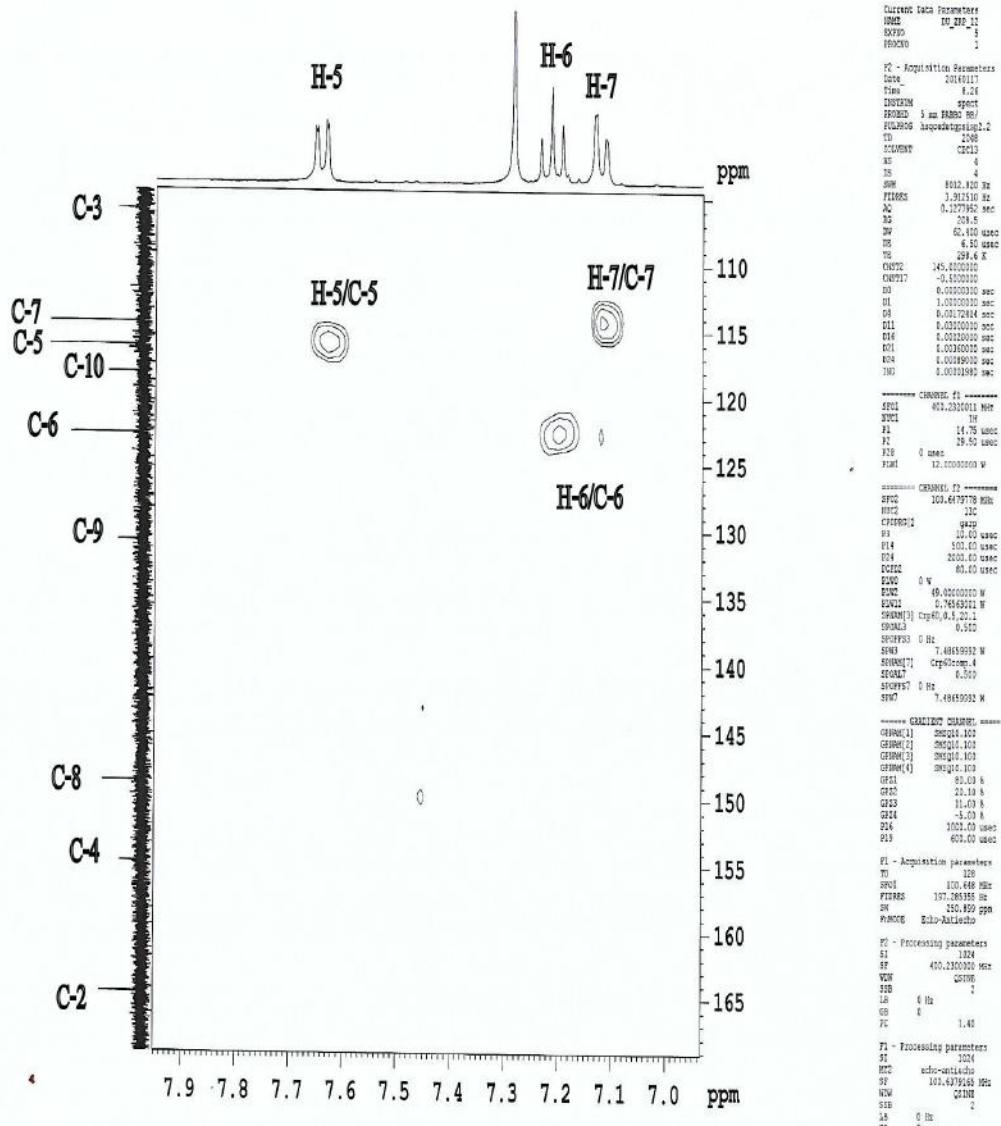
S11 : HSQC- NMR spectrum (400 MHz, CDCl₃) of Compound 2 (Zanthodioline)

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 Jahangirnagar University
 Sample: DU_ZRP_12, hsqc



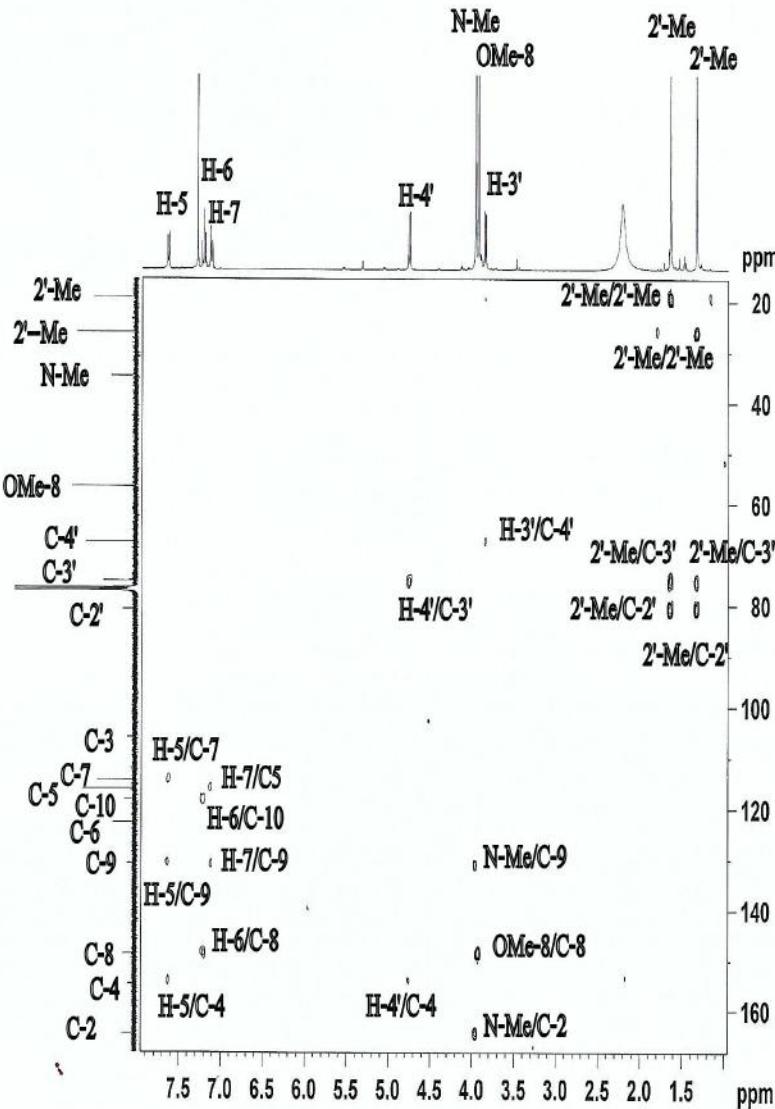
S12: Partially expanded HSQC- NMR spectrum (400 MHz, CDCl_3) of Compound 2
 (Zanthodioline)

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Jahangirnagar University
Sample: DU_ZRP_12, hsqc



S13: Partially expanded HSQC-NMR spectrum (400 MHz, CDCl₃) of Compound 2
(Zanthodioline)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRP_12, hmbc



Current Data Parameters
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 PROBOD: 1

P2 - Acquisition Parameters
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 TD: 2048
 SOLVENT: CDCl3
 NS: 4
 DS: 4
 SWH: 8012.82 Hz
 FIDRES: 3.91510 Hz
 AQ: 0.1277952 sec
 RG: 208.5
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 299.0 K
 CNST12: 145.0000000
 CNST13: 10.0000000
 DD: 0.00000300 sec
 D1: 1.00000000 sec
 D2: 0.00244823 sec
 D6: 0.05000000 sec
 D16: 0.00020001 sec
 IN0: 0.00001398 sec

===== CHANNEL f1 =====
 SF01: 400.2320011 MHz
 NUC1: 1H
 F1: 16.75 usec
 P1: 29.50 usec
 PLW1: 12.00000000 W

===== CHANNEL f2 =====
 SF02: 100.6479773 MHz
 NUC2: 13C
 F2: 10.00 usec
 PLW2: 49.00000000 W

===== GRADIENT CHANNEL =====
 GRDM1[1]: SWS210.100
 GRDM1[2]: SWS210.100
 GRDM1[3]: SWS210.100
 GP1: 50.00 %
 GP2: 30.00 %
 GP3: 40.10 %
 PL1: 1000.00 usec

P1 - Acquisition parameters
 TD: 128
 SF01: 100.648 MHz
 FIDRES: 197.285355 Hz
 SW: 250.899 ppm
 ENDS: 0

P2 - Processing parameters
 SI: 2048
 SF: 400.2300000 MHz
 NW: 512
 SSB: 0
 LR: 0 Hz
 GB: 0
 PC: 1.40

P1 - Processing parameters
 SI: 1024
 MC2: 0
 SF: 100.6379135 MHz
 NW: 512
 SSB: 0
 LR: 0 Hz
 GB: 0

S14: HMBC- NMR spectrum (400 MHz, CDCl_3) of Compound 2 (Zanthodioline)

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 Jahangirnagar University
 Sample: DU_ZRP_12, hmbc



Current Data Parameters

NAME DU_ZRP_12

EXPRO 6

PR0M0 1

P2 - Acquisition Parameters

Date 20140217

Time 8.38

INSTRUM spect

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FULPROG hmbo1g1p1d1f

TD 2048

SOLVENT CDCl3

NS 4

DS 4

SWH 8012.820 Hz

FINRES 3.91210 Hz

AQ 0.1277362 sec

RG 208.8

DW 62.400 used

DE 6.50 used

TE 299.8 K

CNST2 145.0000000

CNST13 10.0000000

DO 0.0000030 sec

D1 0.0001628 sec

D6 0.0500000 sec

D18 0.0002000 sec

IR0 0.00001390 sec

----- CHANNEL f1 -----

SF01 400.2320011 Hz

MNU1 1H

P1 14.75 usec

P2 79.50 usec

DDW1 12.0000000 W

----- CHANNEL f2 -----

SF02 100.6471713 MHz

MNU2 13C

T2 10.00 usec

P1M2 49.0000000 W

----- GRADIENT CHANNEL -----

GR0M1[1] SMC10.100

GR0M1[2] SMC10.100

GR0M1[3] SMC10.100

GR21 50.00 %

GR22 30.00 %

GR23 40.10 %

P16 1000.00 usec

----- P1 - Acquisition parameters -----

TD 128

SF01 100.648 MHz

FINRES 197.28535 Hz

SW 256.899 ppm

PR0M0 QF

----- P2 - Processing parameters -----

SI 1024

N1 400.2300000 Hz

SF QF

SW 100.6379135 MHz

WDW SINE

SSB 0 Hz

LB 0 Hz

GS 0

TC 1.40

----- P1 - Processing parameters -----

SI 1024

N1 QF

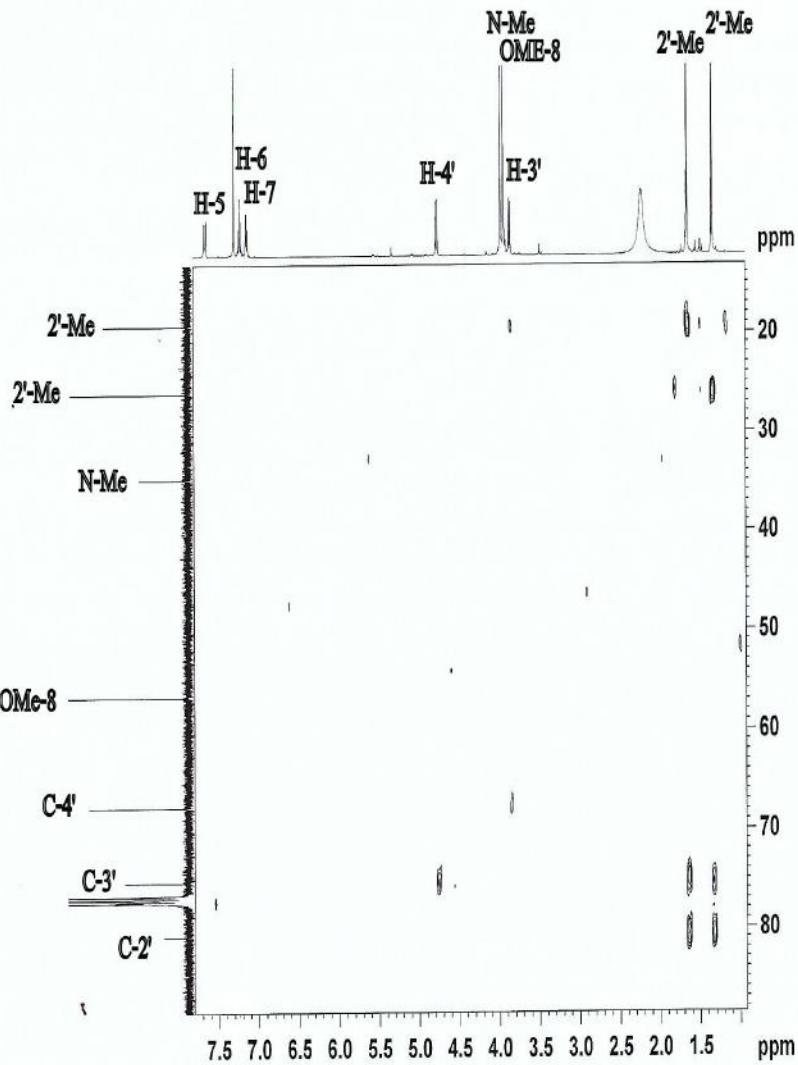
SF 100.6379135 MHz

WDW SINE

SSB 0 Hz

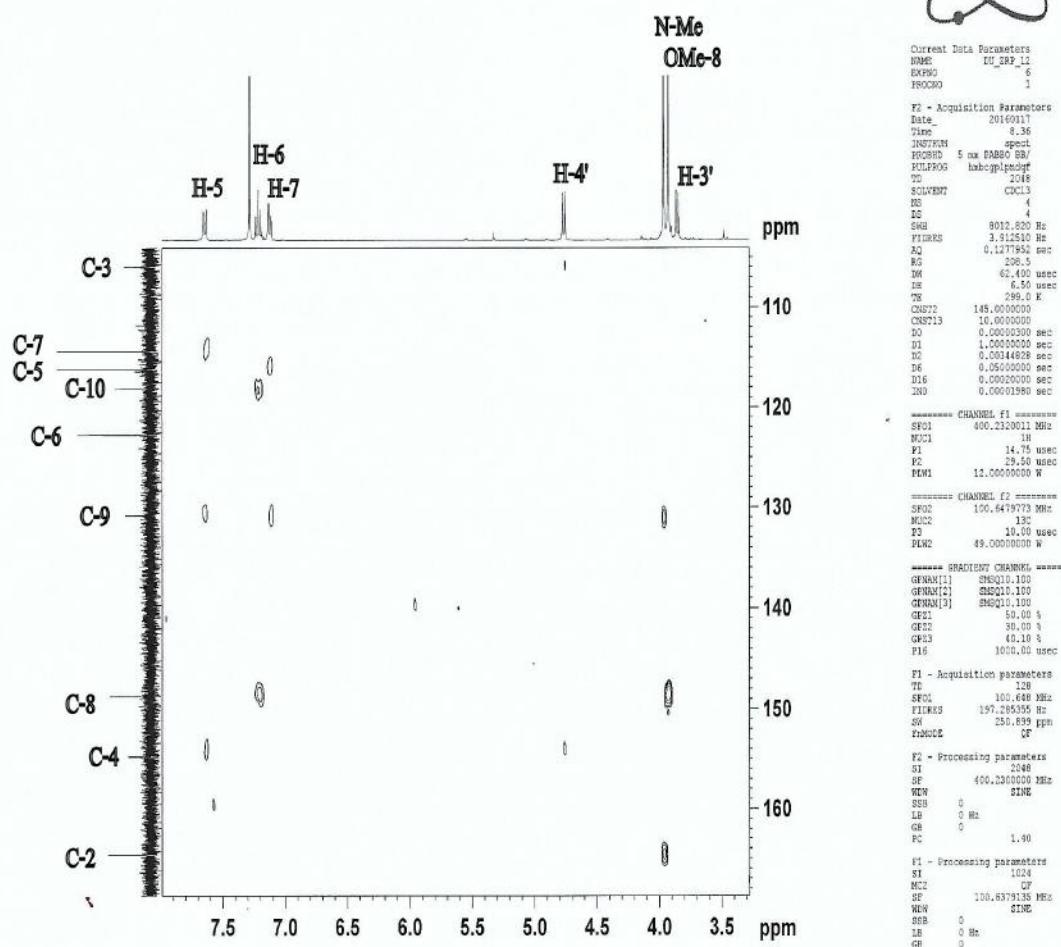
LB 0 Hz

GS 0



S15 : Partially expanded HMBC- NMR spectrum (400 MHz, CDCl₃) of Compound 2 (Zanthodioline)

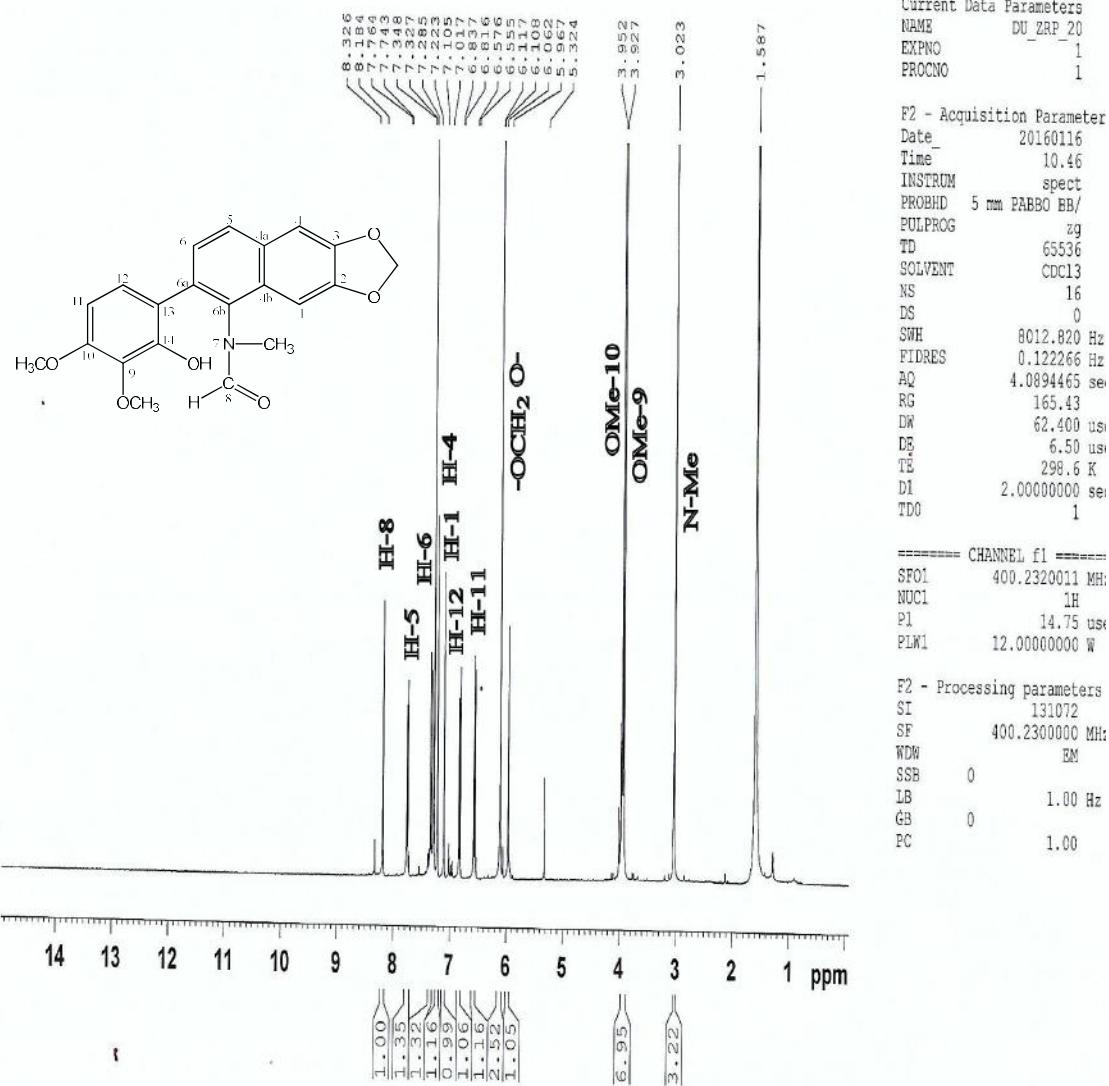
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 Jahangirnagar University
 Sample: DU_ZRP_12, hmbc



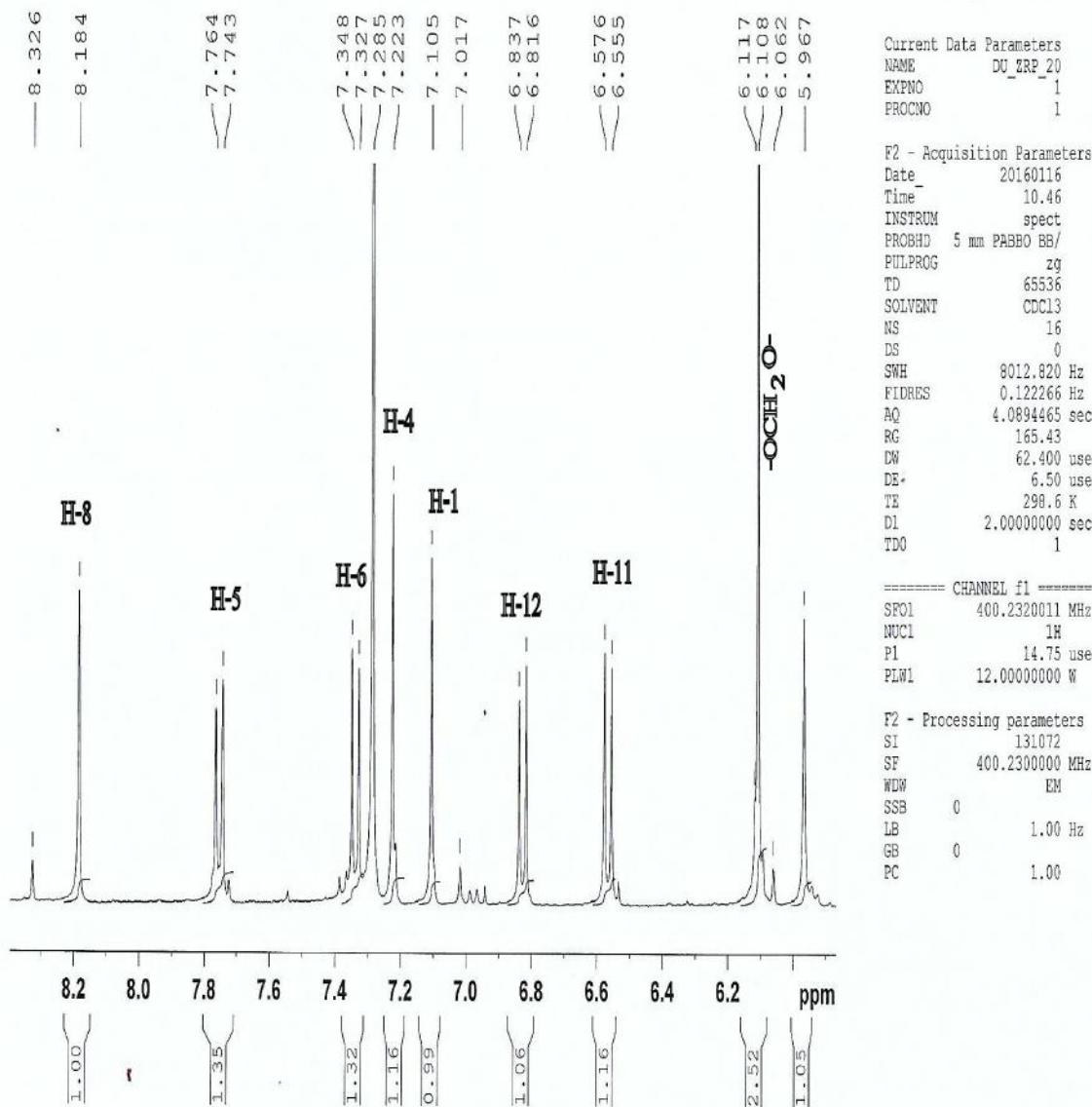
S16: Partially expanded HMBC- NMR spectrum (400 MHz, CDCl₃) of Compound 2 (Zanthodioline).

Zanthodioline (2): white crystals; ¹H-NMR (500 MHz, CDCl₃): δ 7.64 (dd, J= 8.0, 1.2 Hz, H-5), 7.22 (1H, t, J= 8.0 Hz, H-6), 7.12 (1H, dd, J= 8.0, 1.2 Hz, H-7), 4.76 (1H, d, J= 8 Hz, H-4'), 3.97 (3H, s, N-Me), 3.93 (3H, s, OMe-8), 3.84 (1H, d, J= 8 Hz, H-3'), 1.64 (3H s, H-2' Me), 1.33 (3H, s, H-2' Me). ¹³C-NMR (125 MHz, CDCl₃): δ 164.6 (C-2), 154.8 (C-4), 148.8 (C-8), 130.8 (C-9), 122.8 (C-6), 118.2 (C-10), 116.2 (C-5), 114.4 (C-7), 106.0 (C-3), 80.9 (C-2'), 75.3 (C-3'), 67.7 (C-4'), 56.7 (OMe-8), 34.8 (N-Me), 26.1 (C-2' Me), 19.3 (C-2' Me).

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 Jahangirnagar University
 Sample: DU_ZRP_20

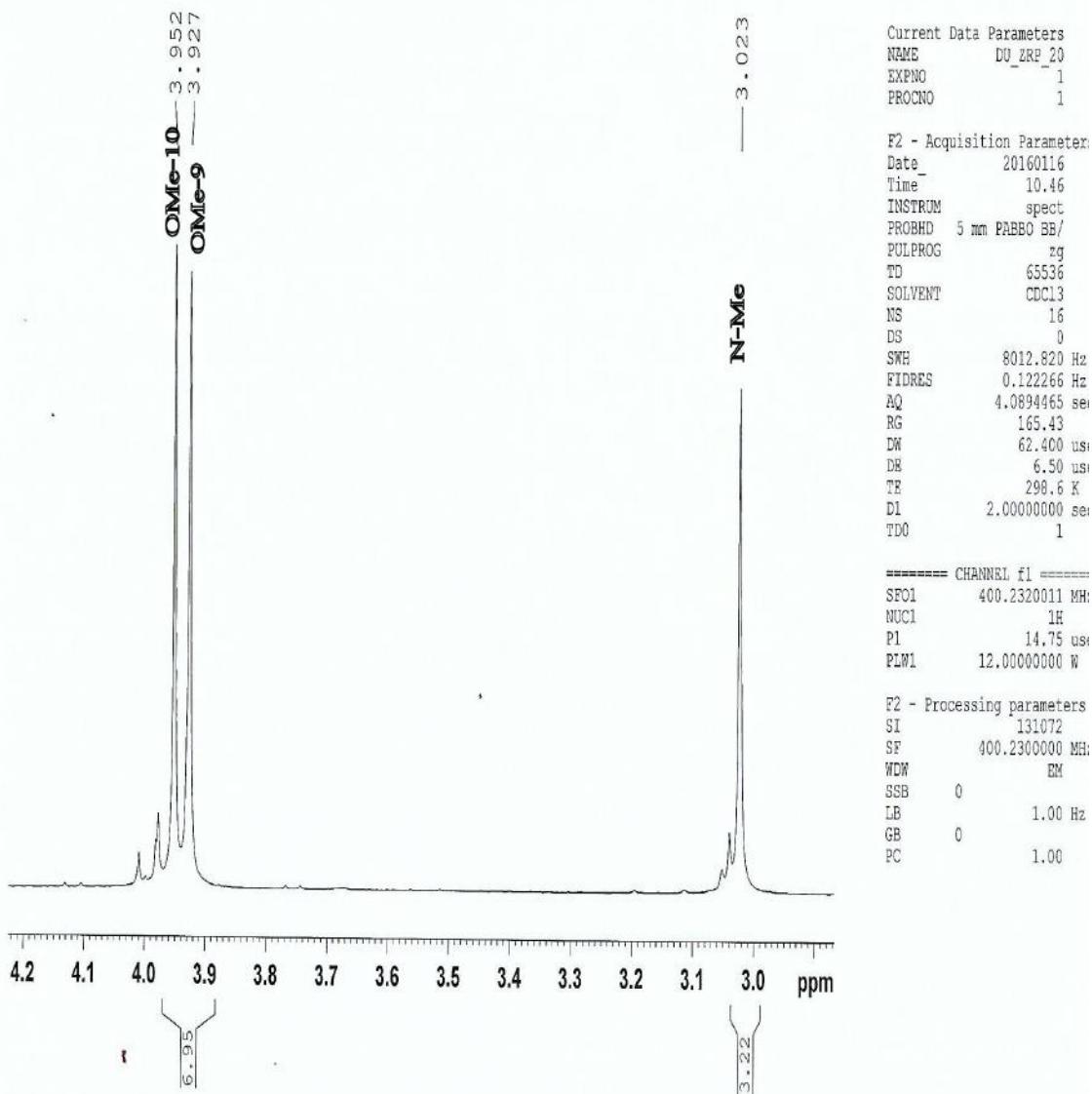


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 Jahangirnagar University
 Sample: DU_ZRP_20



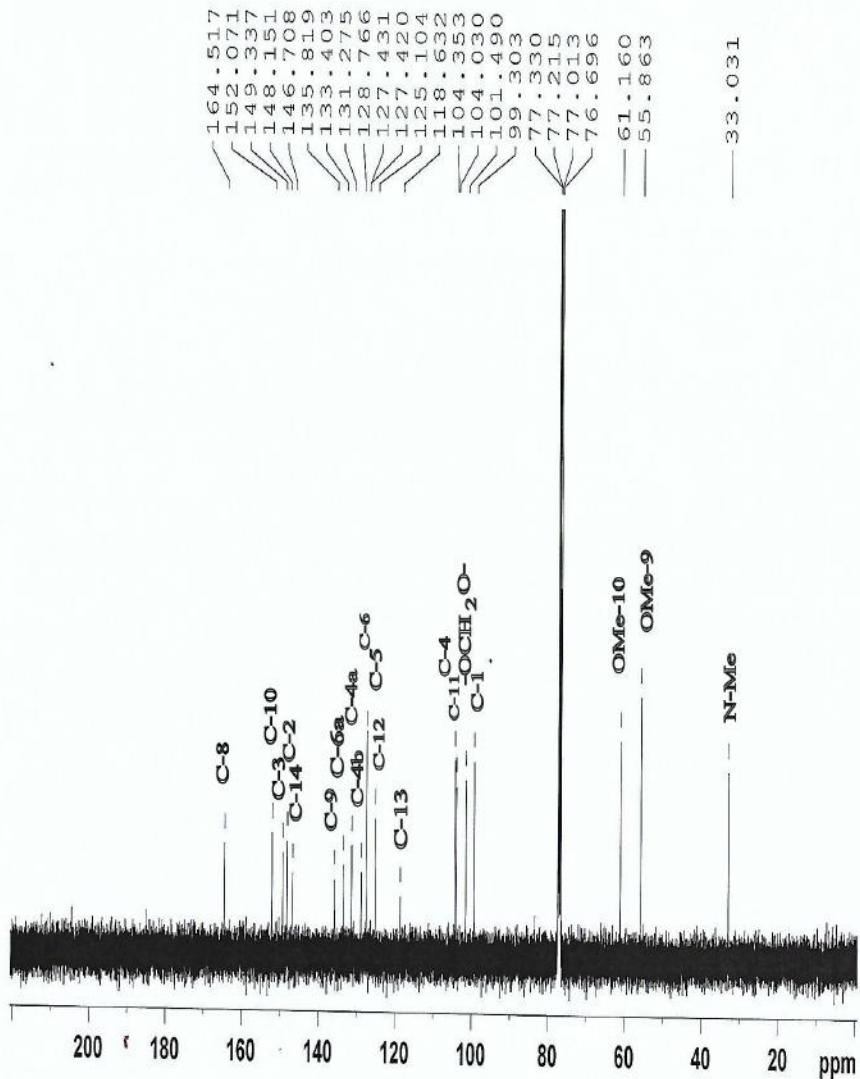
S18 : Partially expanded ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 3 (Arnottianamide).

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 Sample: DU_ZRP_20



S19 : Partially expanded ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 3 (Arnotianamide).

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 Jahangirnagar University
 Sample: DU_ZRP_20



Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameter
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 FIDRES 0.048165 Hz
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 DE 6.50 us
 TE 300.7 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TDO 1

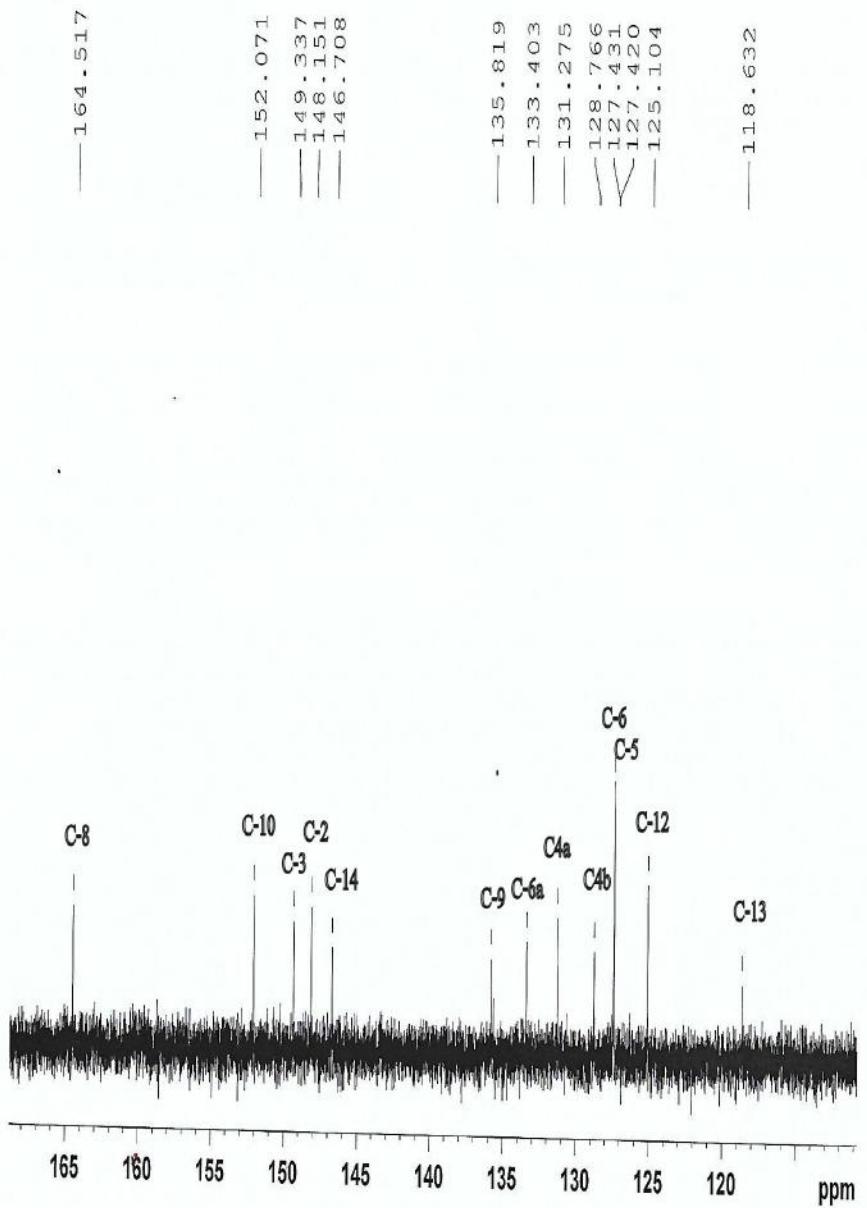
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 NUC1 13C
 P1 10.00 us
 PLW1 49.00000000 W

===== CHANNEL f2 =====
 SP02 400.2320011 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 us
 PLW2 12.00000000 W
 PLW12 0.32231000 W
 PLW13 0.26107001 W

F2 - Processing parameters
 SI 1048576
 SP 100.6379135 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.40

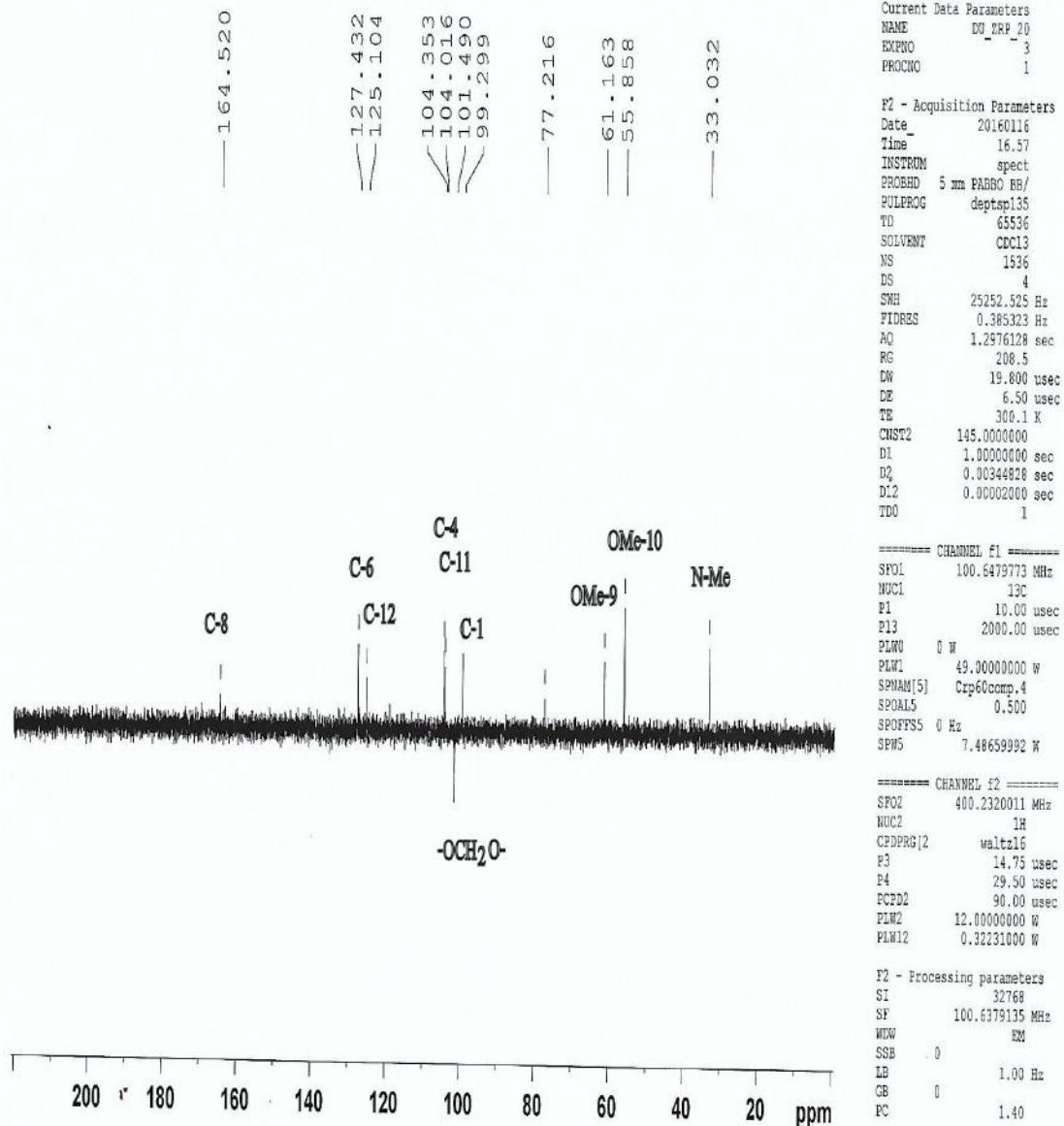
S20 : ^{13}C NMR spectrum (100 MHz, CDCl_3) of Compound 3 (Arnottianamide).

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 Sample: DU_ZRP_20



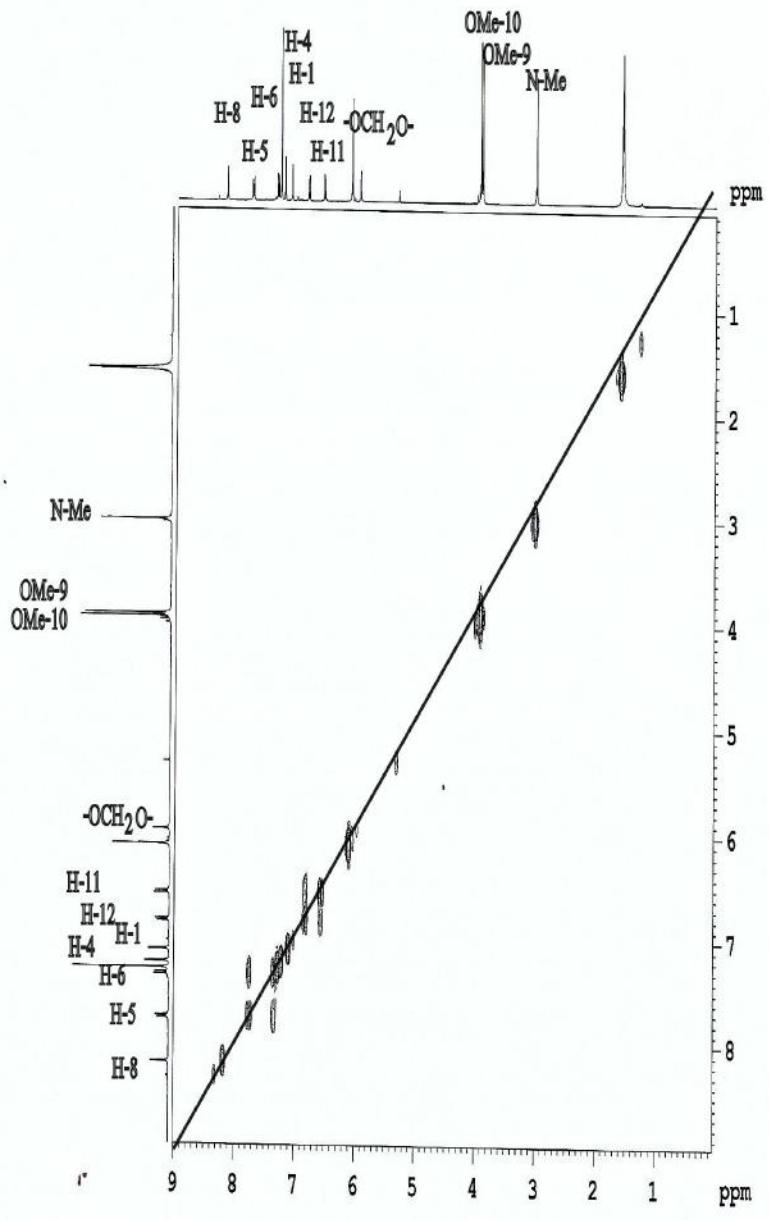
S21: Partially expanded ¹³C NMR spectrum (100 MHz, CDCl₃) of Compound 3 (Arnottianamide).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRP_20, dept-135



S22 : DEPT-135 NMR spectrum (100 MHz, CDCl₃) of Compound 3 (Arnottianamide).

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 Jahangirnagar University
 Sample: DU_ZRP_20, cosy



Current Data Parameters
 NNAME DU_ZRP_20
 EXPNO 4
 PROBNO 1

F2 - Acquisition Parameters
 Date 20160116
 Time 17.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG cosypprf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 3.912510 Hz
 AQ 0.1277952 sec
 RG 208.5
 TM 62.400 usec
 DE 6.50 usec
 TB 299.6 K
 DQ 0.0000300 sec
 D1 1.0000000 sec
 D13 0.0000400 sec
 D16 0.0002000 sec
 TIN 0.00012480 sec

===== CHANNEL f1 =====
 SF01 400.2320011 MHz
 NUC1 1H
 R0 14.75 usec
 F1 14.75 usec
 PL01 12.0000000 W

===== GRADIENT CHANNEL =====
 GRADIM[1] SMSQ10.100
 GZ1 10.00 %
 P16 1000.00 usec

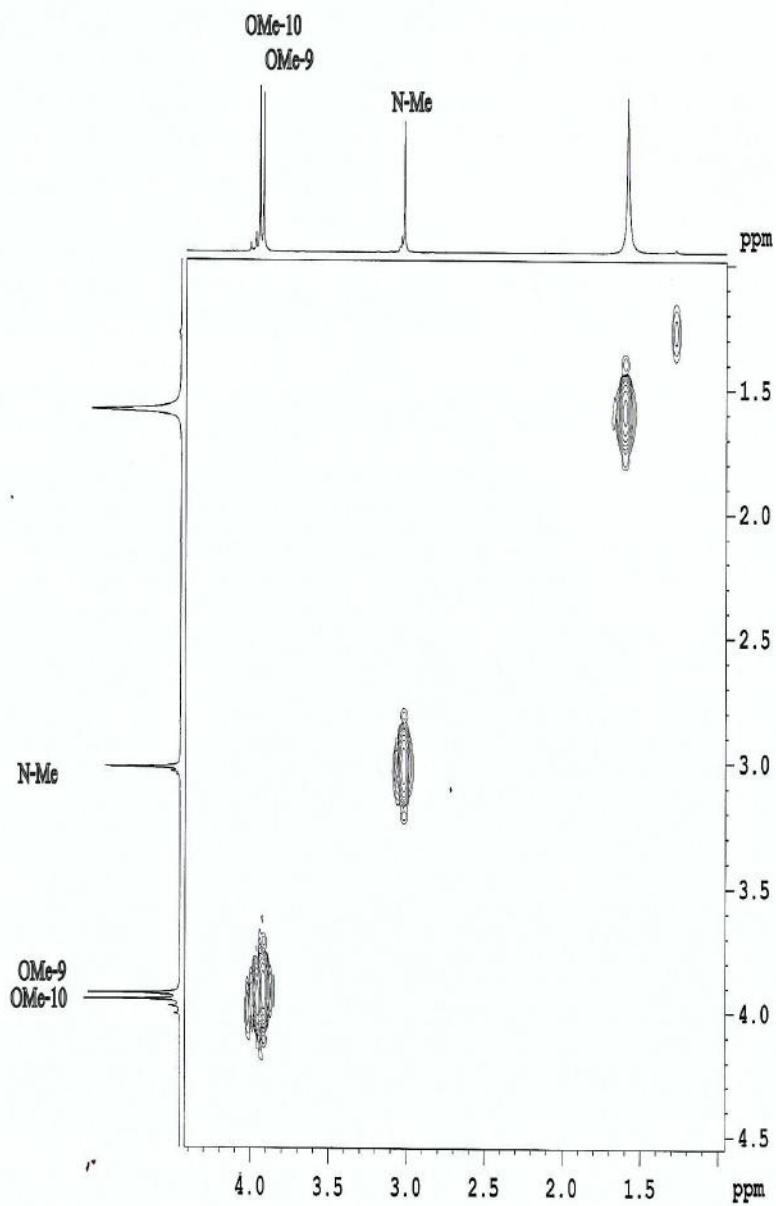
F1 - Acquisition parameters
 TD 118
 SF01 400.232 MHz
 FIDRES 62.600159 Hz
 SW 20.020 ppm
 FMODE QF

F2 - Processing parameters
 SI 2048
 SF 400.2300000 MHz
 WM QSINE
 SSB 0
 LB 0 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.2300000 MHz
 WM QSINE
 SSB 0
 LB 0 Hz
 GB 0

S23: COSY-NMR spectrum (400 MHz, CDCl_3) of Compound 3 (Arnottianamide).

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 Jahangirnagar University
 Sample: DU_ZRP_20, cosy



Current Data Parameters
 NAME DU_ZRP_20
 EXPNO 4
 PROBNO 1

F1 - Acquisition Parameters
 Date 20160116
 Time 17:14
 INSTRUM spect
 PROBHD 5 mm BBBO BB/
 PULPROG cosyppf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 3.91251 Hz
 AQ 0.1277952 sec
 RG 208.5
 DW 62.400 usec
 DE 6.50 usec
 TZ 299.5 K
 DO 0.0000030 sec
 D1 1.0000001 sec
 DL3 0.00000401 sec
 DL6 0.00020000 sec
 IN0 0.00012480 sec

===== CHANNEL f1 =====
 SF01 400.2320011 MHz
 NUC1 1H
 PD 14.75 usec
 PL 14.75 usec
 PLW1 12.0000000 W

===== GRADIENT CHANNEL =====
 GRADM[1] SWSQ10.100
 GPR1 10.00 %
 PL6 1000.00 usec

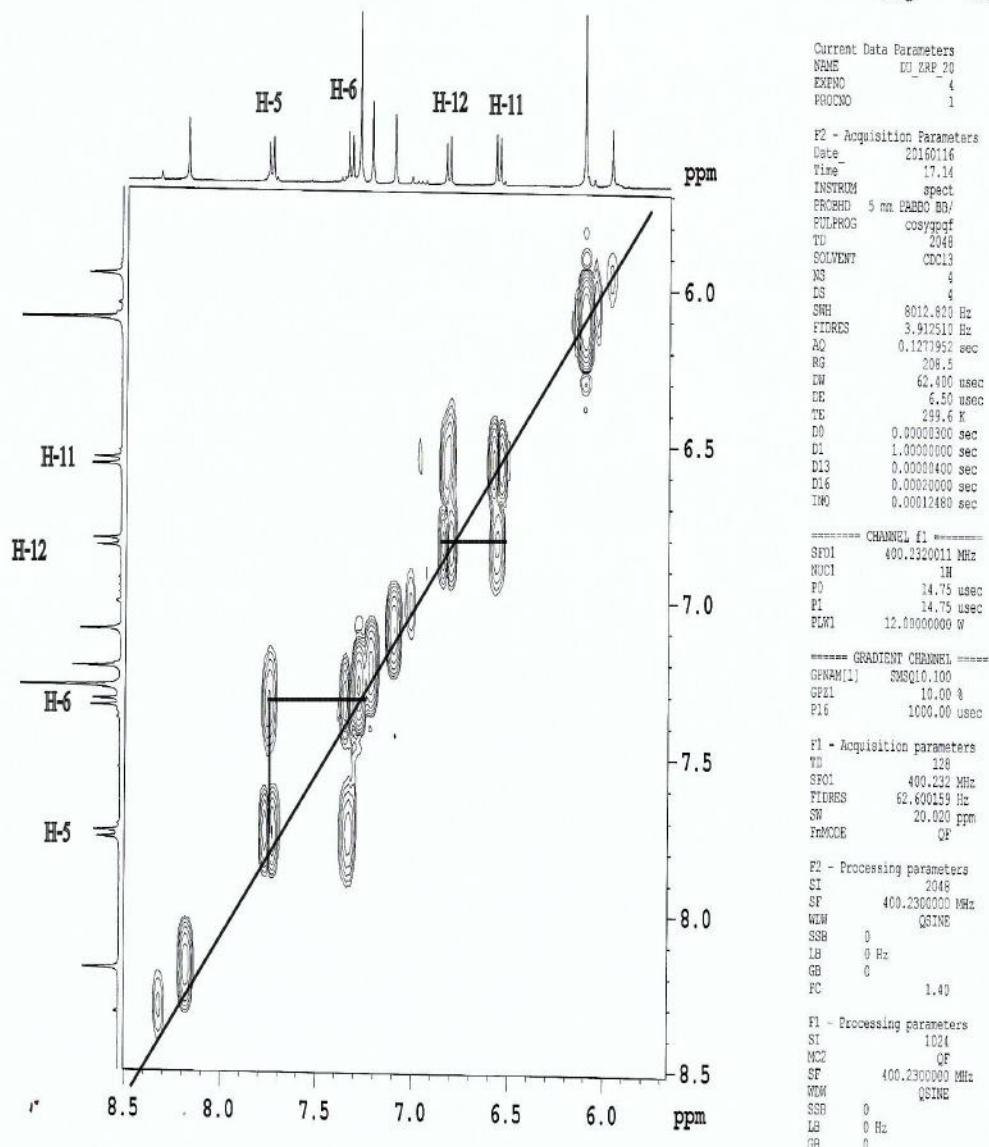
F1 - Acquisition parameters
 TD 128
 SF01 400.232 MHz
 FIDRES 62.600159 Hz
 SW 20.020 ppm
 PmMode QF

F2 - Processing parameters
 SI 2048
 SF 400.2300000 MHz
 MW 0 QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 0 QF
 SF 400.2300000 MHz
 MW 0 QSINE
 SSB 0
 LB 0 Hz
 GB 0

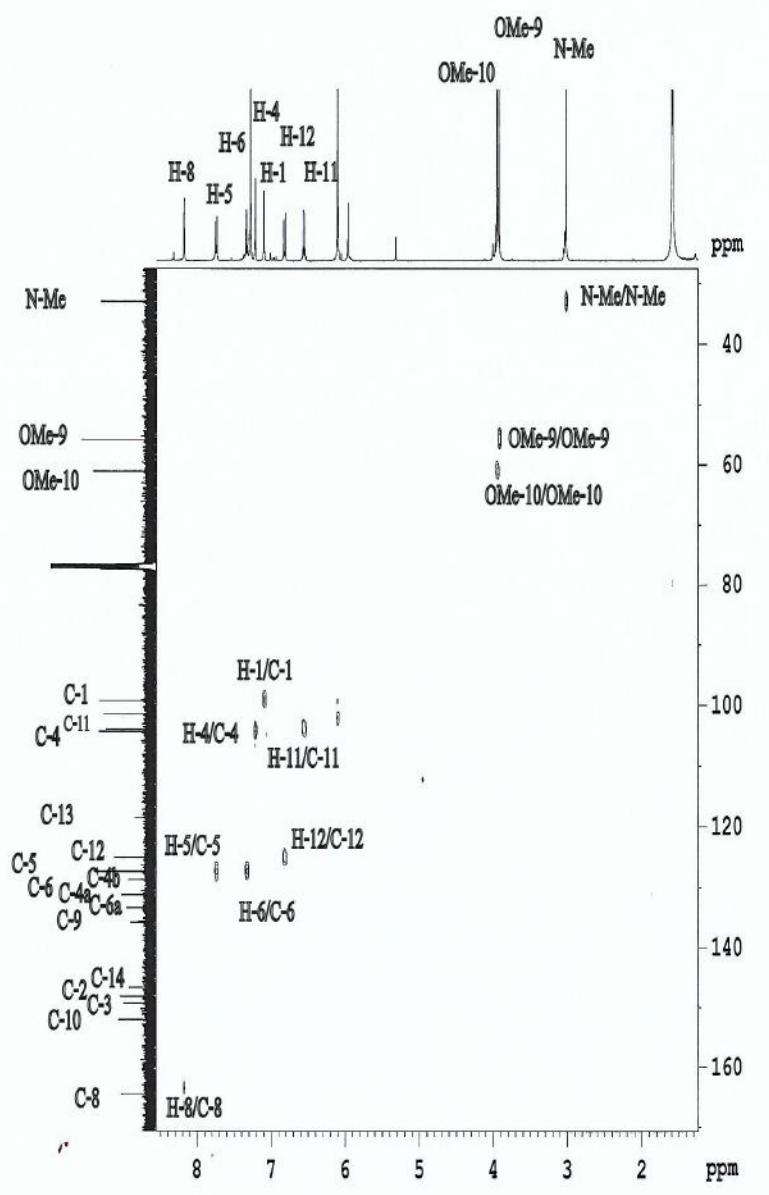
S24 : Partially expanded COSY- NMR spectrum (400 MHz, CDCl₃) of Compound 3 (Arnottianamide).

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 Sample: DU_ZRP_20, cosy



S25 : Partially expanded COSY- NMR spectrum (400 MHz, CDCl₃) of Compound **3** (Arnottianamide).

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 Sample: DU_ZRP_20, hsqc



Current Data Parameters
 NAME: DU_ZRP_20
 EXPNO: 5
 PROBID: 1

 P2 - Acquisition Parameters
 Date: 20160116
 TIME: 17:24
 DURATION: 1000.000000
 SOLVENT: CDCl_3
 T1: 30.00
 SOLVENT: CDCl_3
 NS: 4
 SW1: 8001.420 Hz
 FIDRES: 3.93210 Hz
 AQ: 0.127352 sec
 RG: 100.5
 TM: 6.50 sec
 TB: 6.50 sec
 T2: 799.1 K
 CRUSH: 148.000000
 CRUSH17: -0.5400000
 DW: 0.01000000 sec
 DR: 1.00000000 sec
 D1: 1.007700 sec
 D1B: 0.01000000 sec
 D1E: 0.01000000 sec
 D2A: 0.01360000 sec
 D2B: 0.01190000 sec
 D2C: 0.01100000 sec

 CHANNEL 1 -----
 FID1: 410.232011 MHz
 JRES1: 18 Hz
 F1: 18.75 ussec
 F2: 25.30 ussec
 ZSYN: 0 ussec
 P1M: 11.01000000 W

 CHANNEL 2 -----
 FID2: 100.449778 MHz
 JRES2: 18 Hz
 CYCLES2: 1
 P2: 10.00 ussec
 F1A: 500.00 ussec
 F2A: 2000.00 ussec
 P1B: 60.00 ussec
 P1M: 0 V
 P1G: 49.00100000 W
 P1G2: 0.76582501 W
 SWRFL1: Cpmg,0.5,31.1
 SWRFL2: 0.500
 SWPFG1: 0 Hz
 SWPFG2: 7.44651920 Hz
 SWPFT1: Cpmg,10ms,8
 SWPFT2: 0.500
 SWPFT3: 0 Hz
 T: 7.44659992 Hz

 GRADIENT CHIMES -----
 GRADIN[1]: 0.0020,100
 GRADIN[2]: 0.0010,100
 GRADIN[3]: 0.0020,100
 GRADIN[4]: 0.0010,100
 GRIN: 80.00 Hz
 GRIN2: 50.10 Hz
 GRIN3: 11.00 Hz
 GRIN4: -5.00 Hz
 P1G: 1001.00 ussec
 P1G2: 601.00 ussec

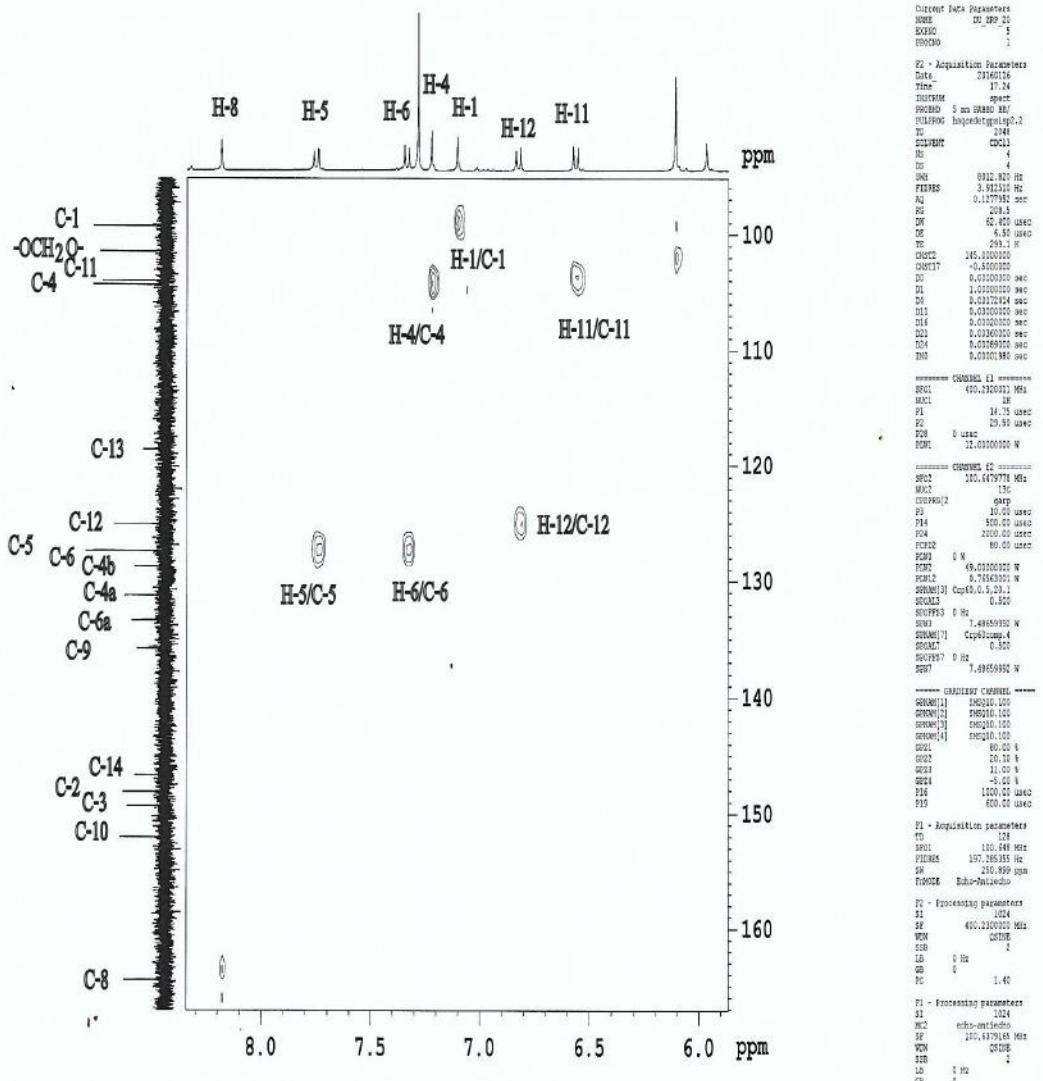
 F1 - Acquisition parameters
 TD: 128
 SCAL: 301.448 MHz
 FIDRES: 137.394000 Hz
 SW: 150.489 MHz
 T90WSE: Edge-Matched

 F1 - Processing parameters
 ST: 32768
 SF: 401.12000000 MHz
 NW: 1000000
 SSB: 2
 1B: 0 Hz
 GZ: 0
 PG: 1.00

 F1 - Processing parameters
 ST: 1024
 NC: 1024-antialiased
 SF: 151.637500 MHz
 NW: 204800
 SSB: 1
 1B: 0 Hz
 GZ: 0

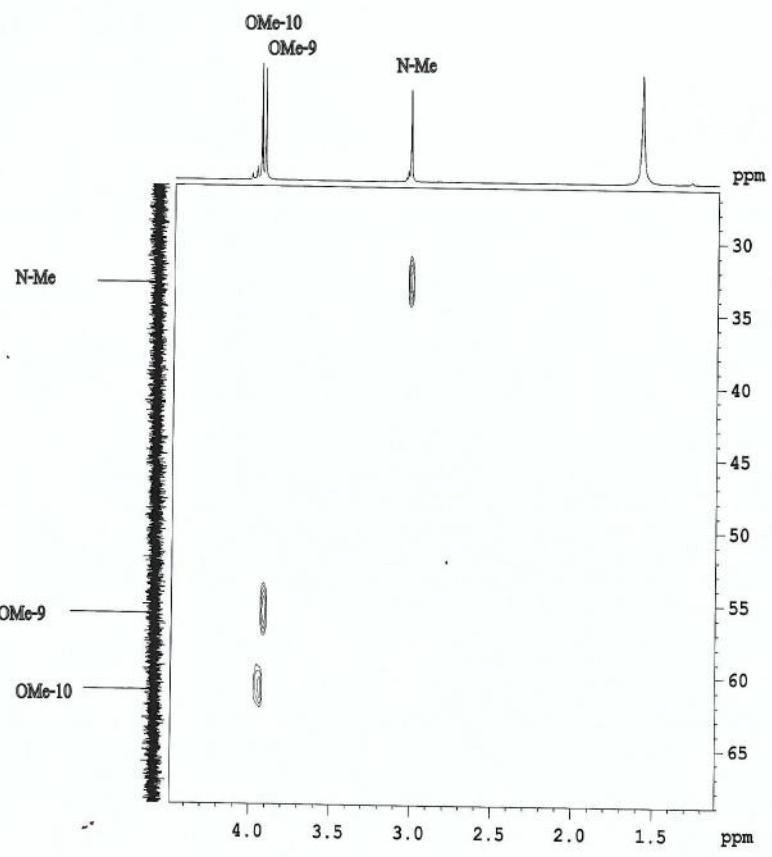
S26 : HSQC- NMR spectrum (400 MHz, CDCl_3) of Compound 3 (Arnottianamide).

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 Jahangirnagar University
 Sample: DU_ZRP_20, hsqc



S27 : Partially expanded HSQC- NMR spectrum (400 MHz, CDCl₃) of Compound 3 (Arnottianamide).

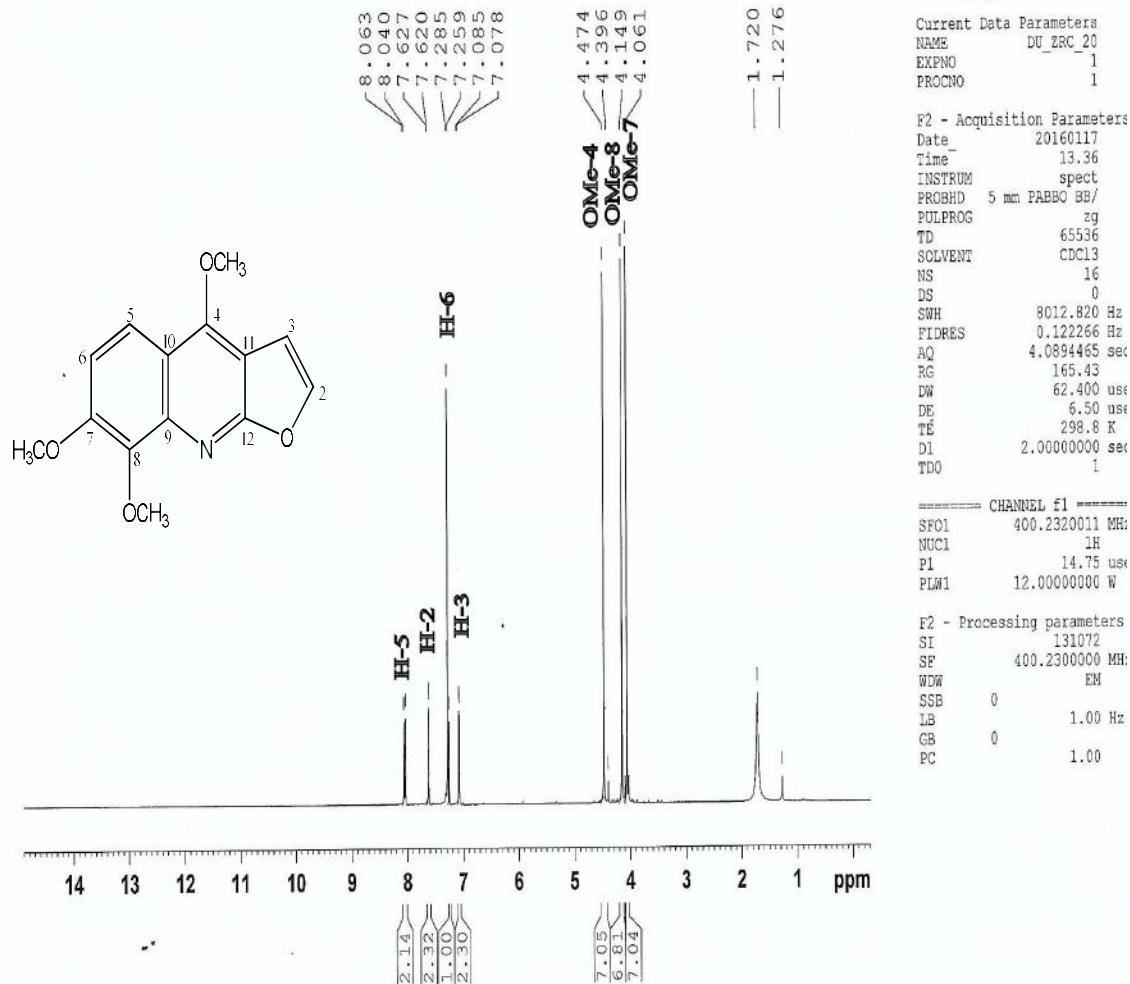
Wazed Miah Science Research Center (WMSRC)
Jahangirnagar University
Sample: DU_ZRP_20, hsqc



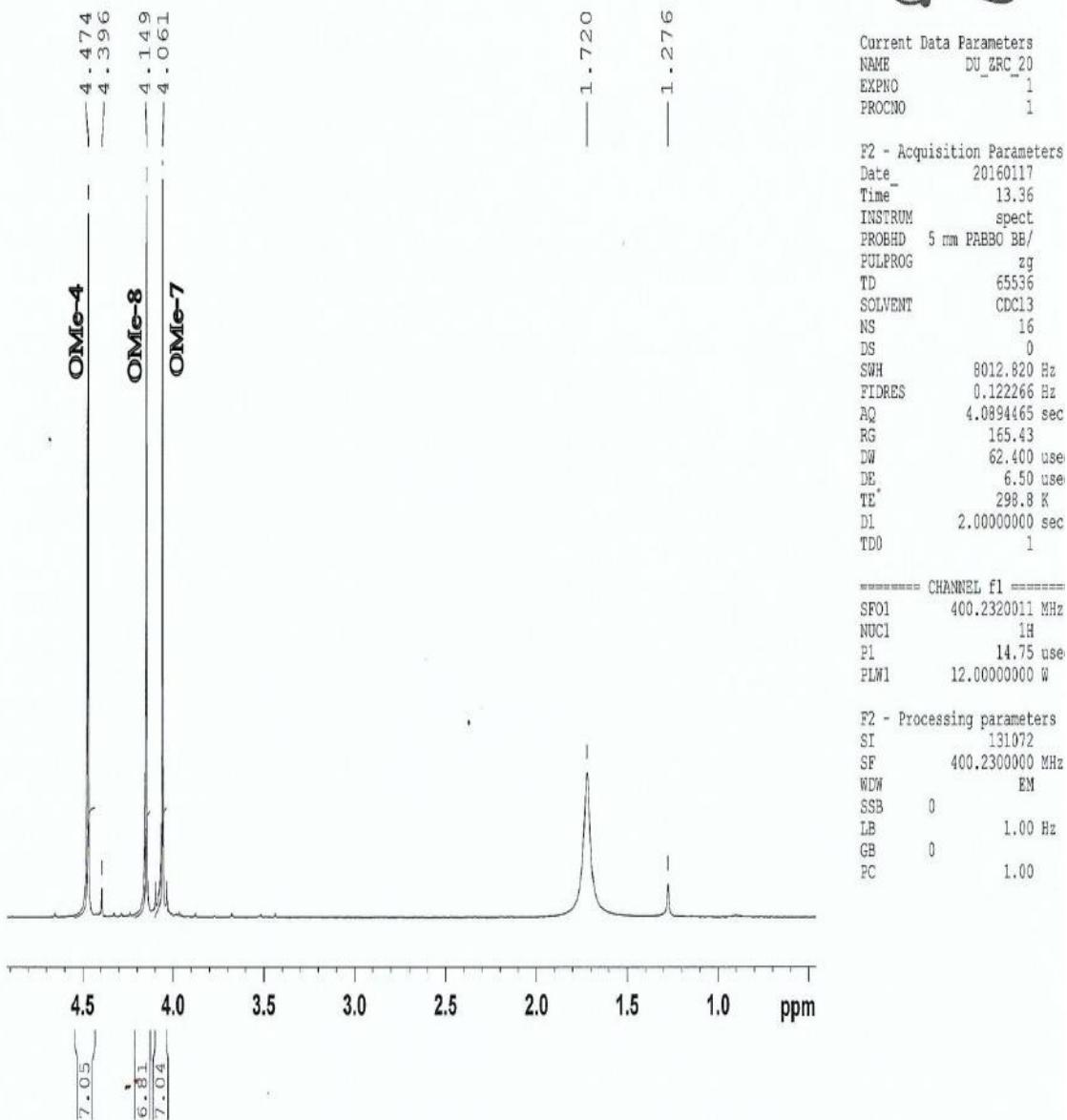
S28: Partially expanded HSQC- NMR spectrum (400 MHz, CDCl₃) of Compound 3
(Arnottianamide).

Arnottianamide (3): white amorphous; ¹H-NMR (500 MHz, CDCl₃): δ 8.18 (1H, s, H-8), 7.75 (1H, d, J= 8.4 Hz, H-5), 7.33 (1H, d, J= 8.4 Hz, H-6), 7.22 (1H, s, H-4), 7.11 (1H, s, H-1), 6.83 (1H, d, J= 8.4 Hz, H-12), 6.57 (1H, d, J= 8.4 Hz, H-11), 6.11 (2H, s, OCH₂O), 3.95 (3H, s, OMe-10), 3.93 (3H, s, OMe-9), 3.02 (3H, s, N-Me). ¹³C-NMR (125 MHz, CDCl₃): δ 164.5 (C-8), 152.1 (C-10), 149.3 (C-3), 148.2 (C-2), 146.7 (C-14), 135.8 (C-6b, 9), 133.4 (C-6a), 131.3 (C-4a), 128.8 (C-4b), 127.4 (C-5, 6), 125.1 (C-12), 118.6 (C-13), 104.4 (C-4), 104.0 (C-11), 101.5 (OCH₂O), 99.3 (C-1), 61.2 (OMe-10), 55.9 (OMe-9), 33.0 (N-Me).

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 Jahangirnagar University
 Sample: DU_ZRC_20

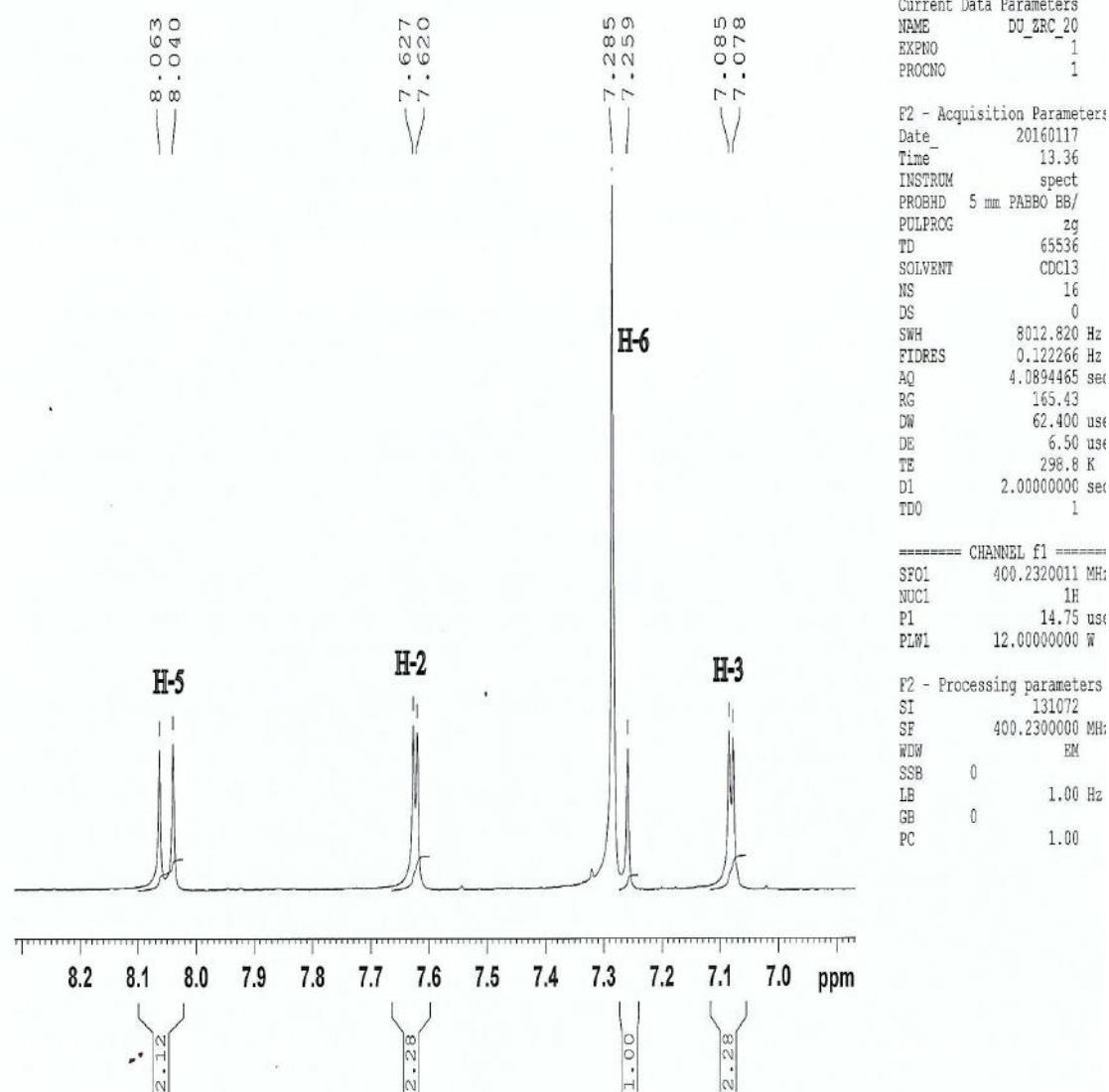


Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_20



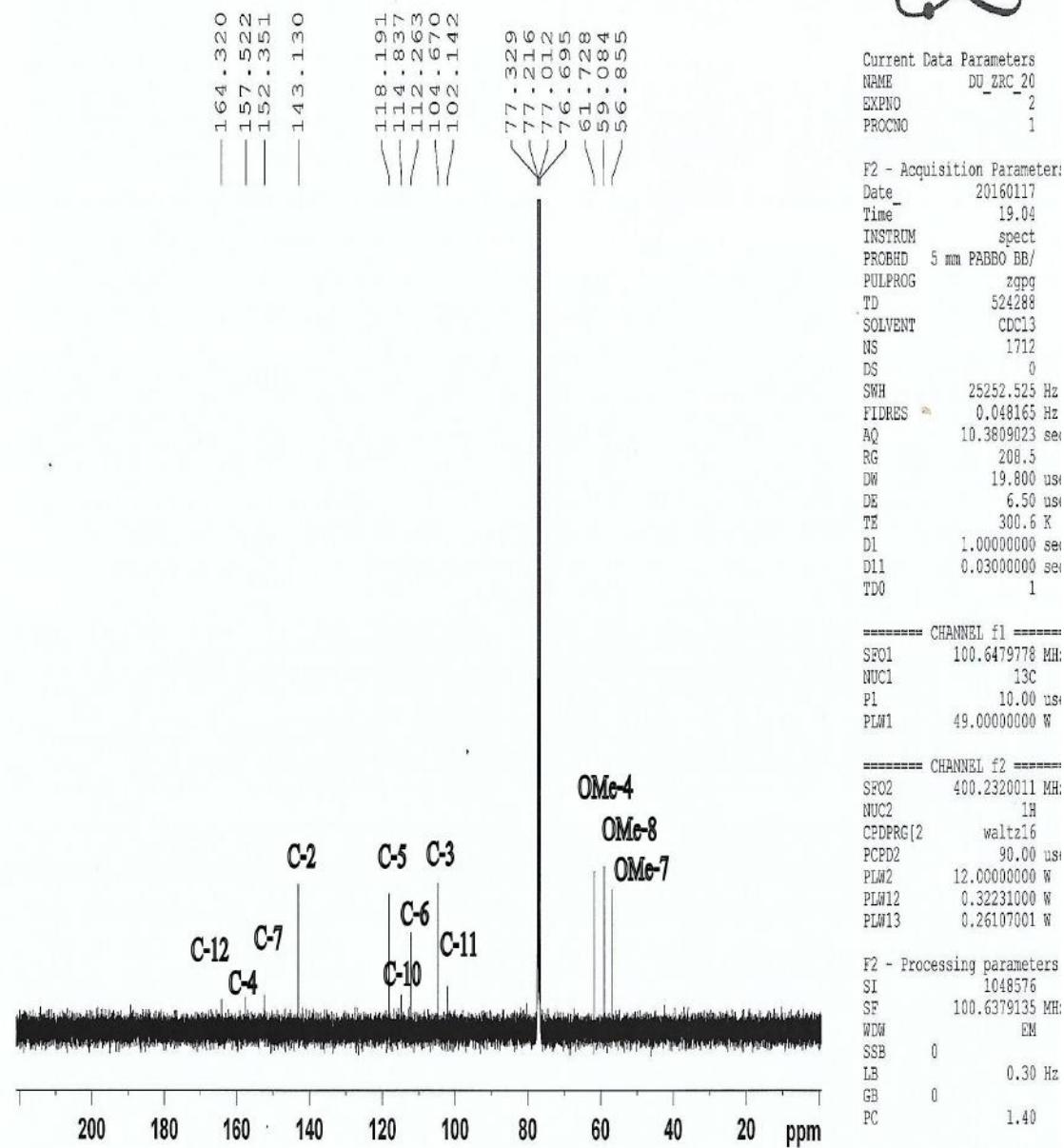
S30: Partially expanded ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_20

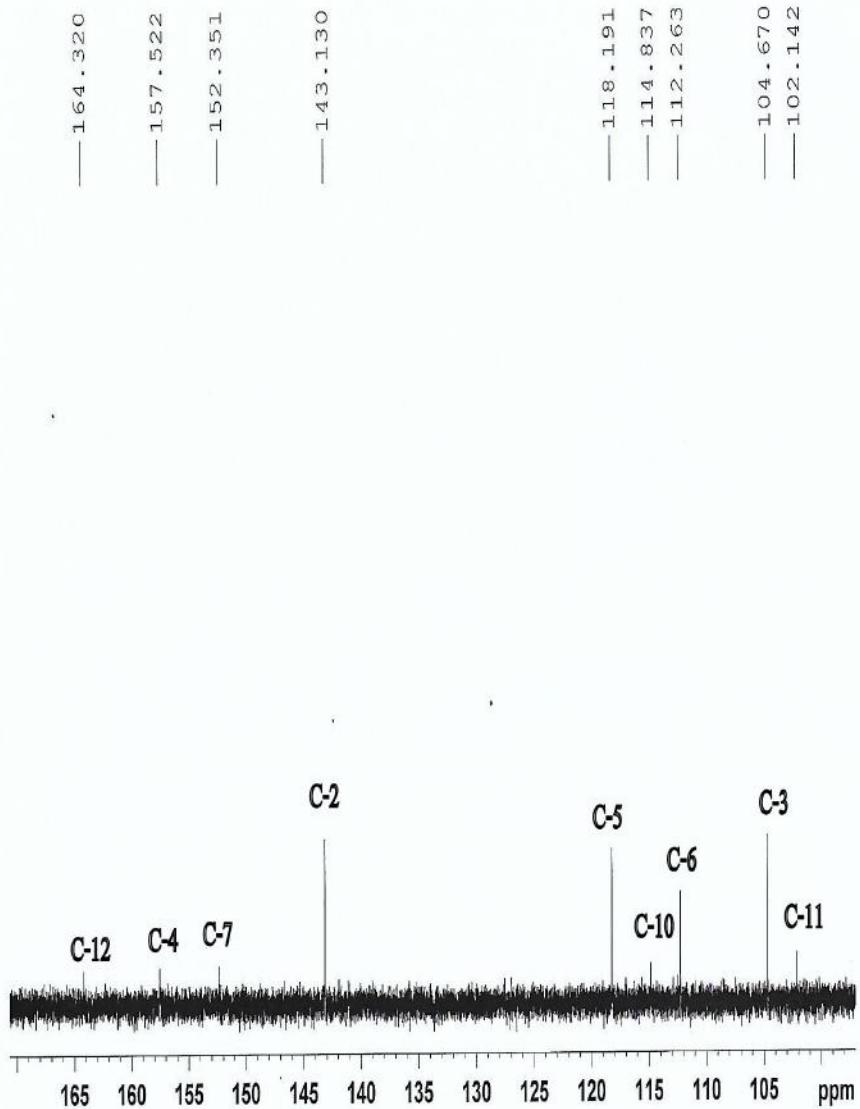


S31: Partially expanded ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_20

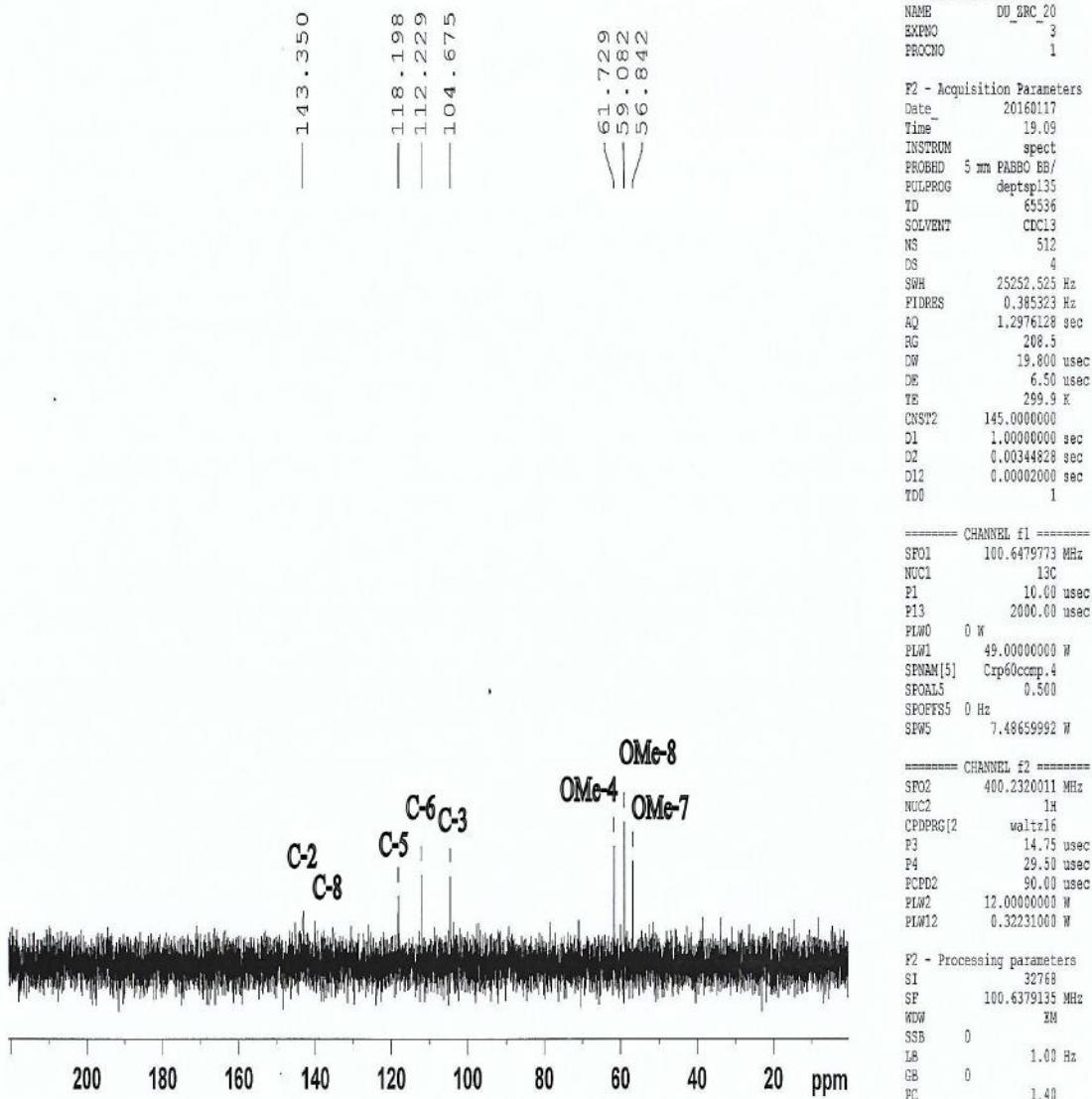


Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_20



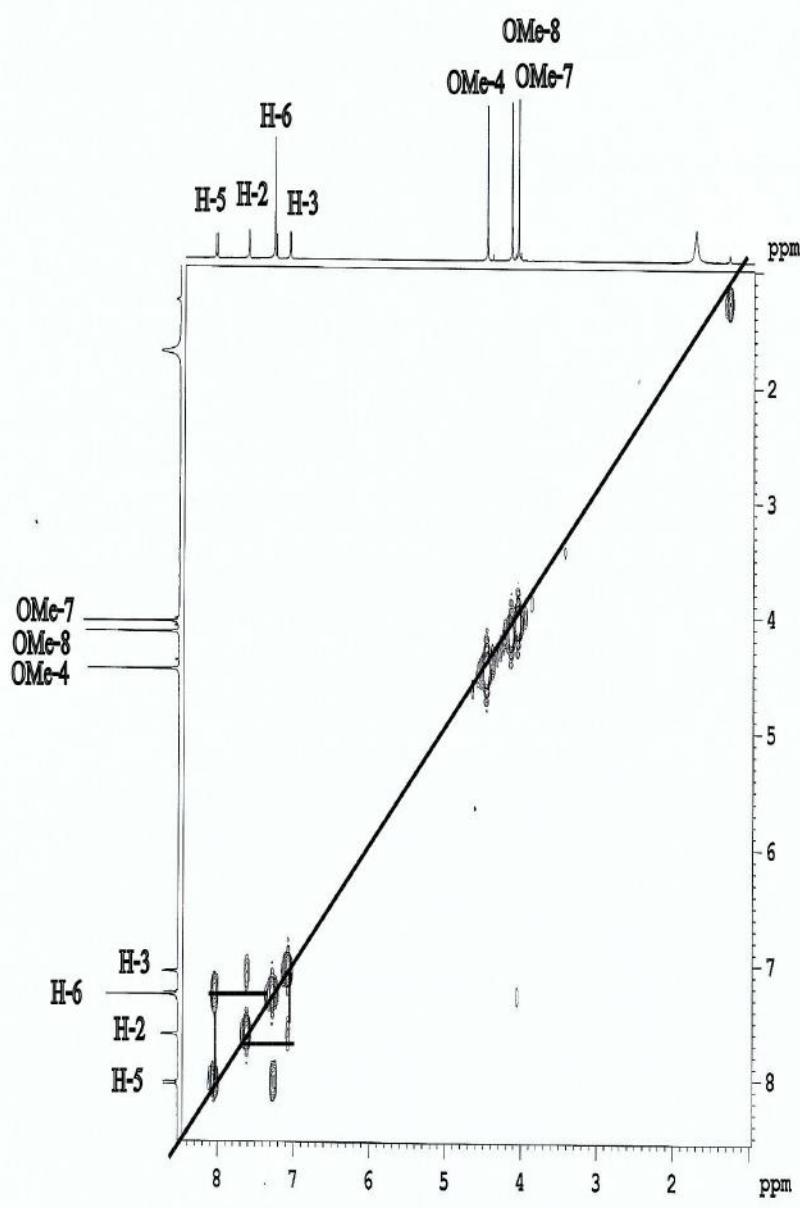
S33: Partially expanded ¹³C NMR (100 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, dept-135



S34 : DEPT-135 NMR (100 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, cosy



Current Data Parameters
 NAME DU_ZRC_20
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160117
 Time 19:25
 INSTRUM spect
 PROBHD 5 mm PARBO BB/
 PULPROG cosyqf1
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 3.91250 Hz
 AQ 0.1277952 sec
 RG 208.5
 IM 62,400 usec
 D8 6.50 usec
 T8 299.6 K
 D0 0.0000300 sec
 D1 1.0000000 sec
 D13 0.0000400 sec
 D16 0.0002000 sec
 J3Q 0.00012480 sec

===== CHANNEL f1 =====
 SP01 400.2320011 MHz
 NUC1 1H
 F0 14.75 usec
 P1 14.75 usec
 PL01 12.0000000 W

===== GRADIENT CHANNEL =====
 GPRGM[1] SNSQ10.100
 GPR1 10.00 %
 P1F 1000.00 usec

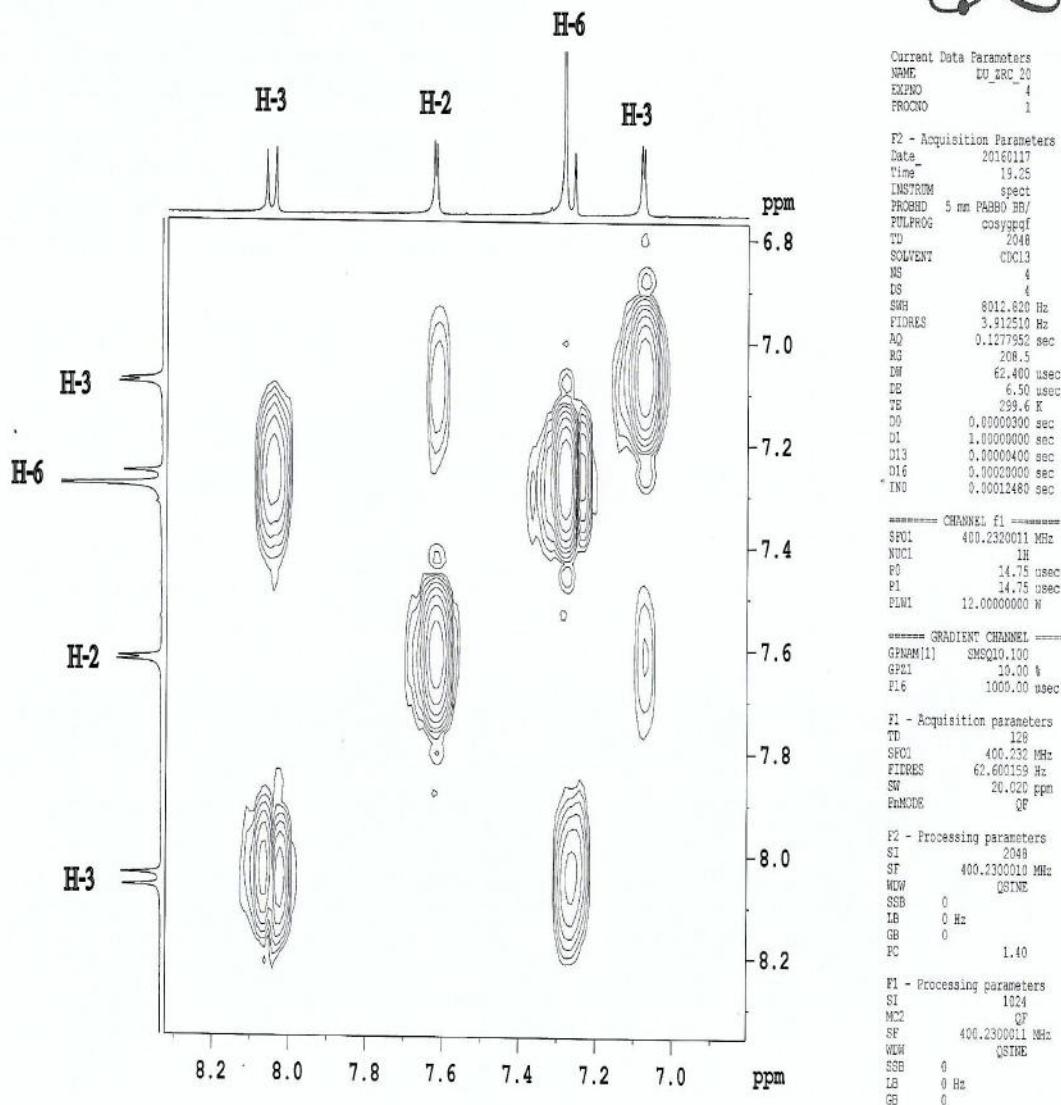
F1 - Acquisition parameters
 TD 128
 SP01 400.232 MHz
 FIDRES 62.600159 Hz
 SW 20.020 ppm
 PRMDE QF

F2 - Processing parameters
 SI 2048
 SF 400.2300011 MHz
 MW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

T1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.2300011 MHz
 MW QSINE
 SSB 0
 LB 0 Hz
 GB 0

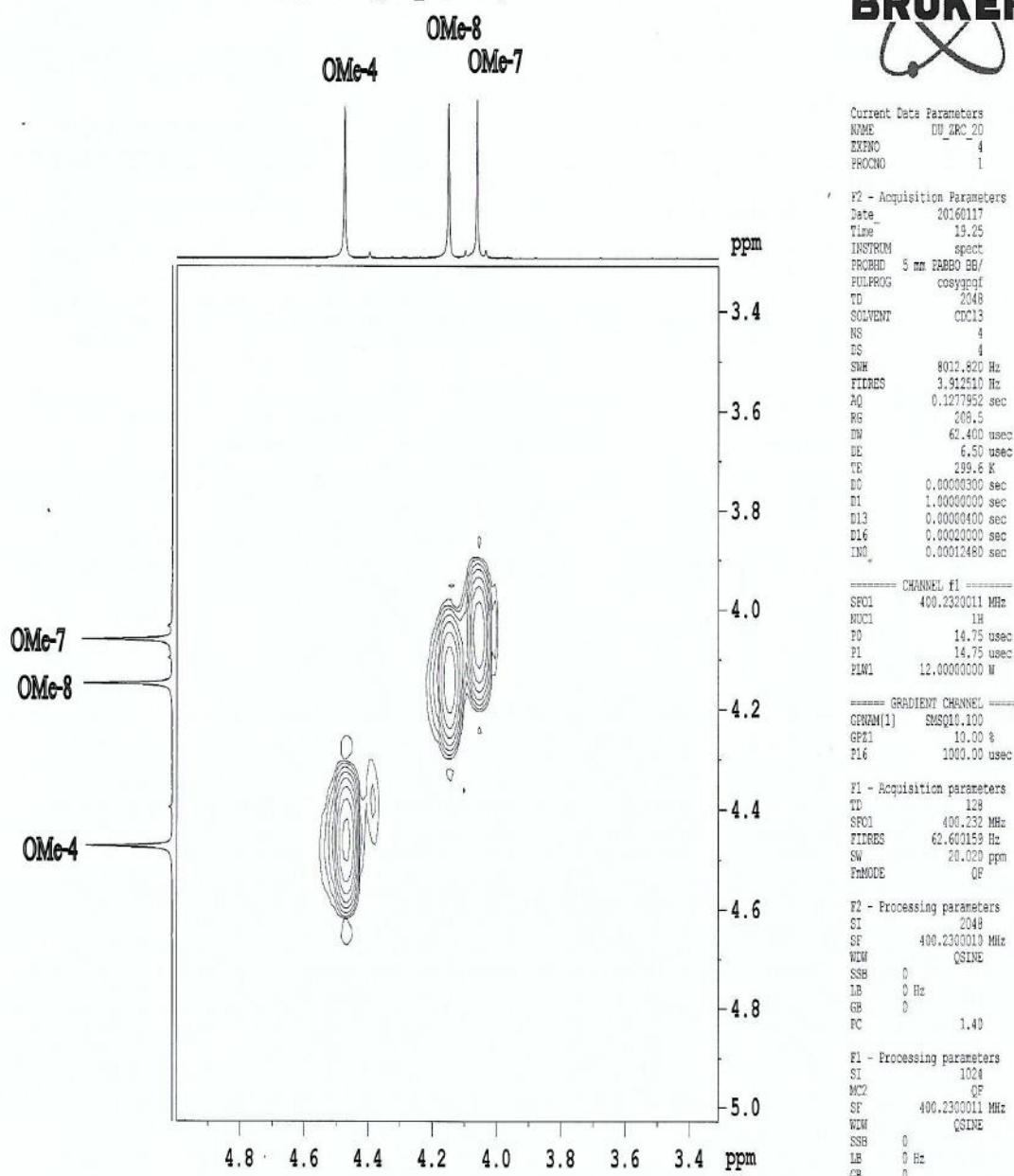
S35 : COSY-NMR (400 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, cosy



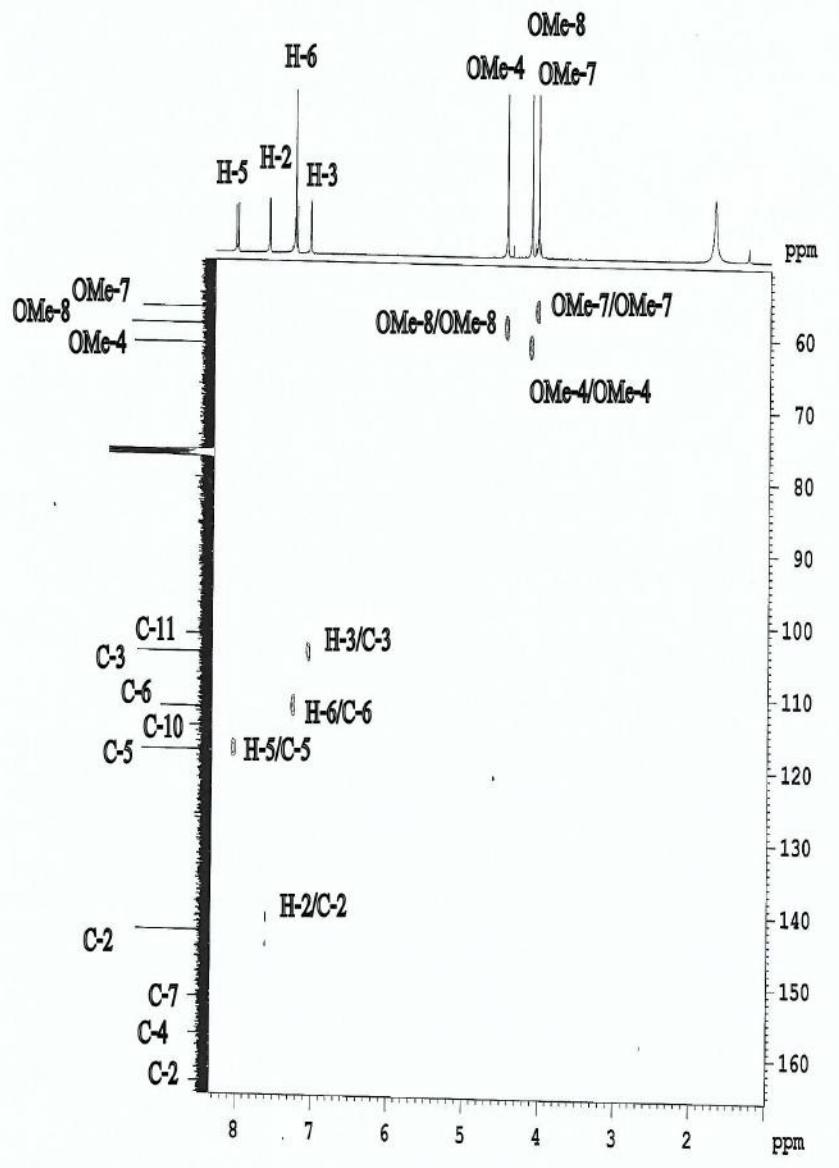
S36 : Partially expanded COSY-NMR (400 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, cosy



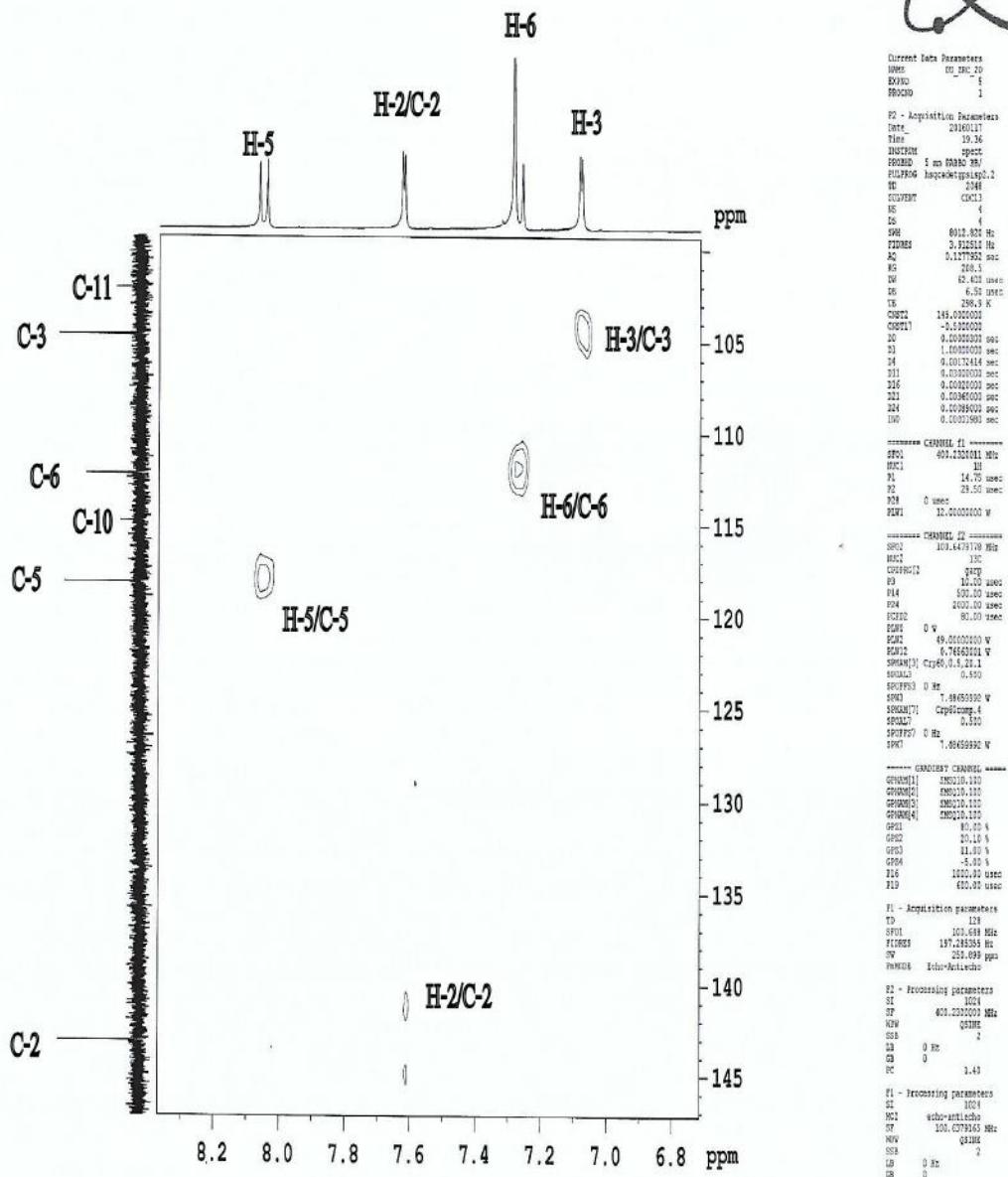
S37 : Partially expanded COSY-NMR (400 MHz, CDCl₃) spectrum of Compound 4
 (Skimmianine)

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 Jahangirnagar University
 Sample: DU_ZRC_20, hsqc



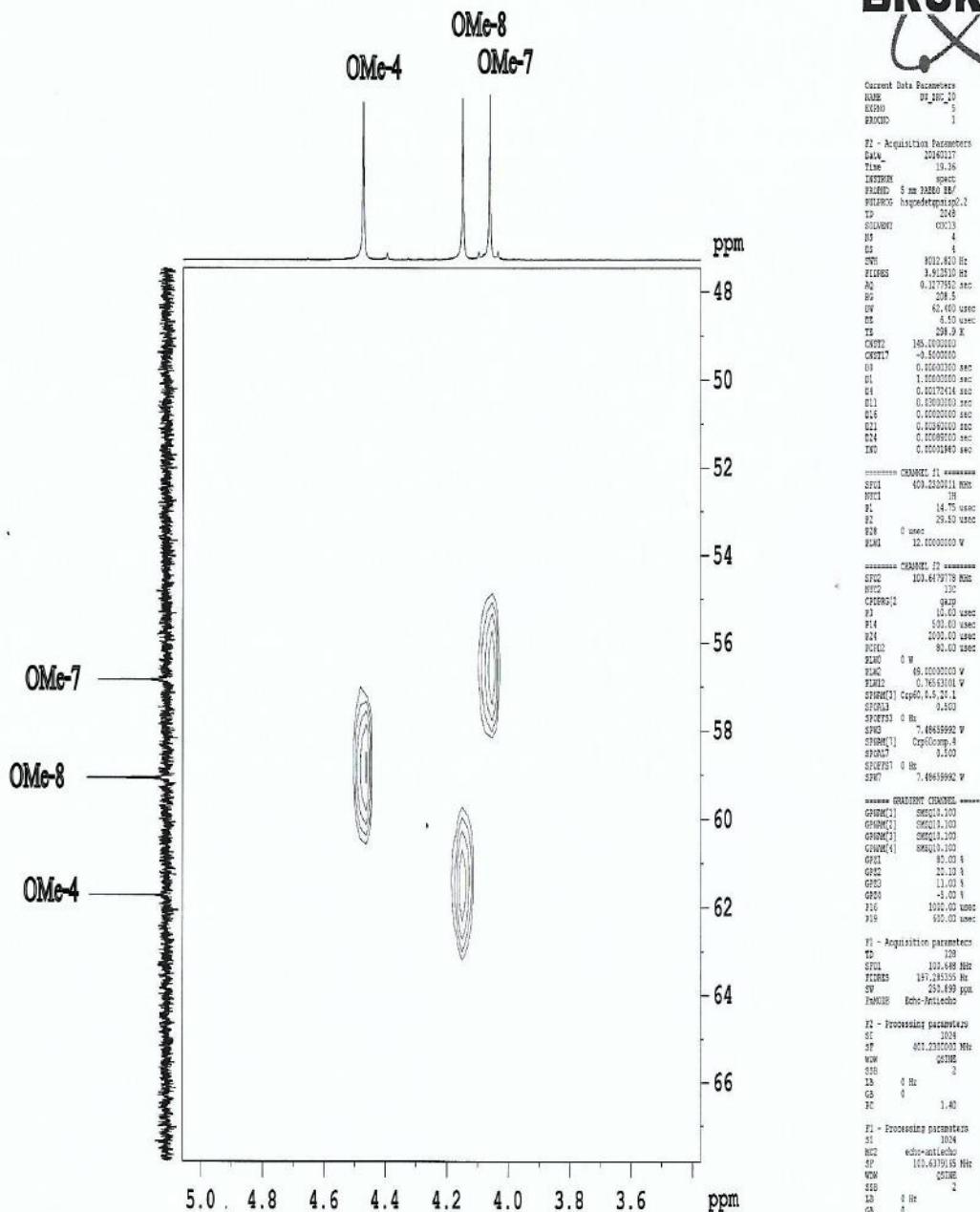
S38: HSQC-NMR (400 MHz, CDCl_3) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, hsqc



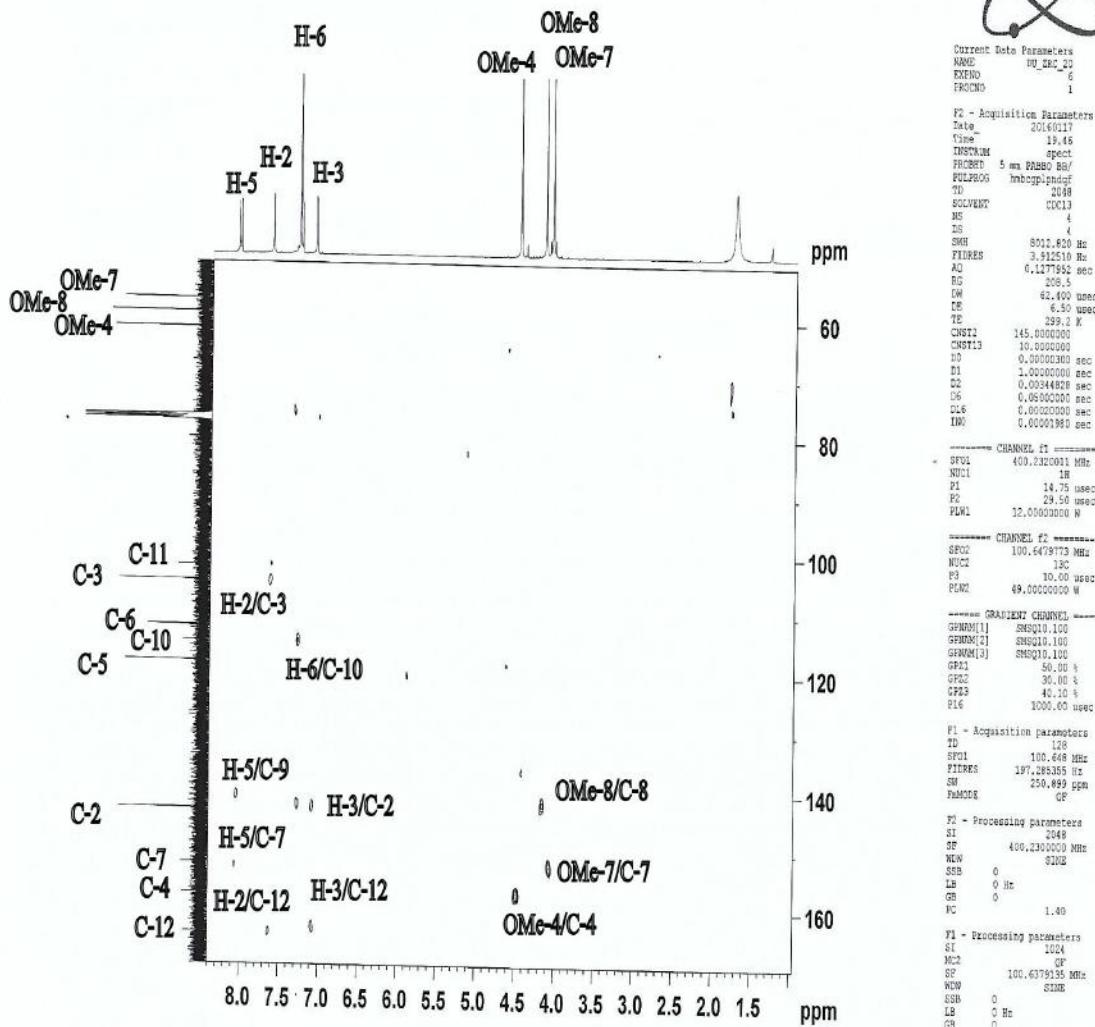
S39: Partially expanded HSQC-NMR (400 MHz, CDCl₃) spectrum of Compound 4 (Skimmianine).

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 Jahangirnagar University
 Sample: DU_ZRC_20, hsqc



S40: Partially expanded HSQC-NMR (400 MHz, CDCl_3) spectrum of Compound 4 (Skimmianine)

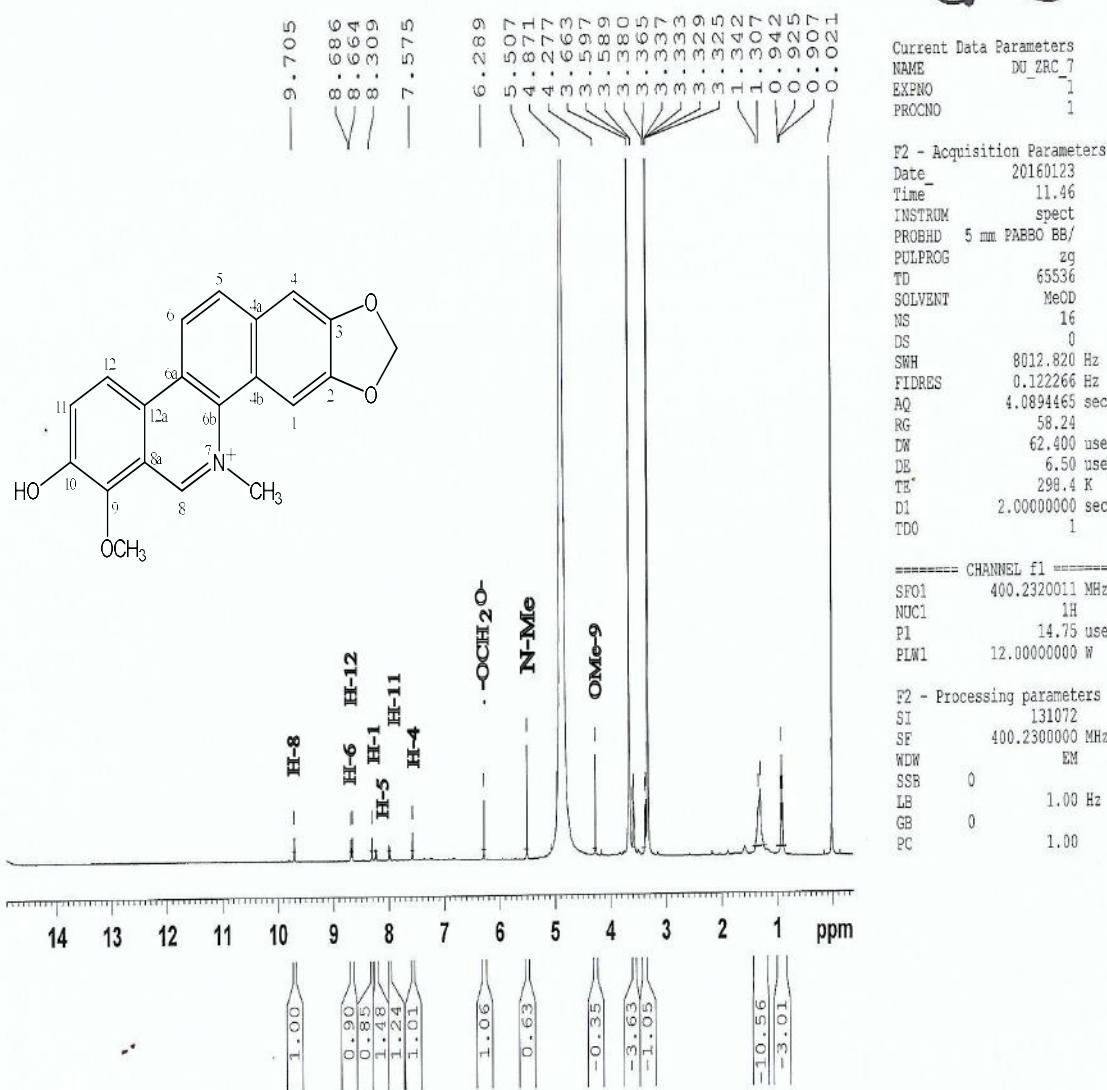
Wazed Miah Science Research Center (WMSRC)
Jahangirnagar University
Sample: DU_ZRC_20, hmbc



S41: HMBC-NMR (400 MHz, CDCl_3) spectrum of Compound 4 (Skimmianine)

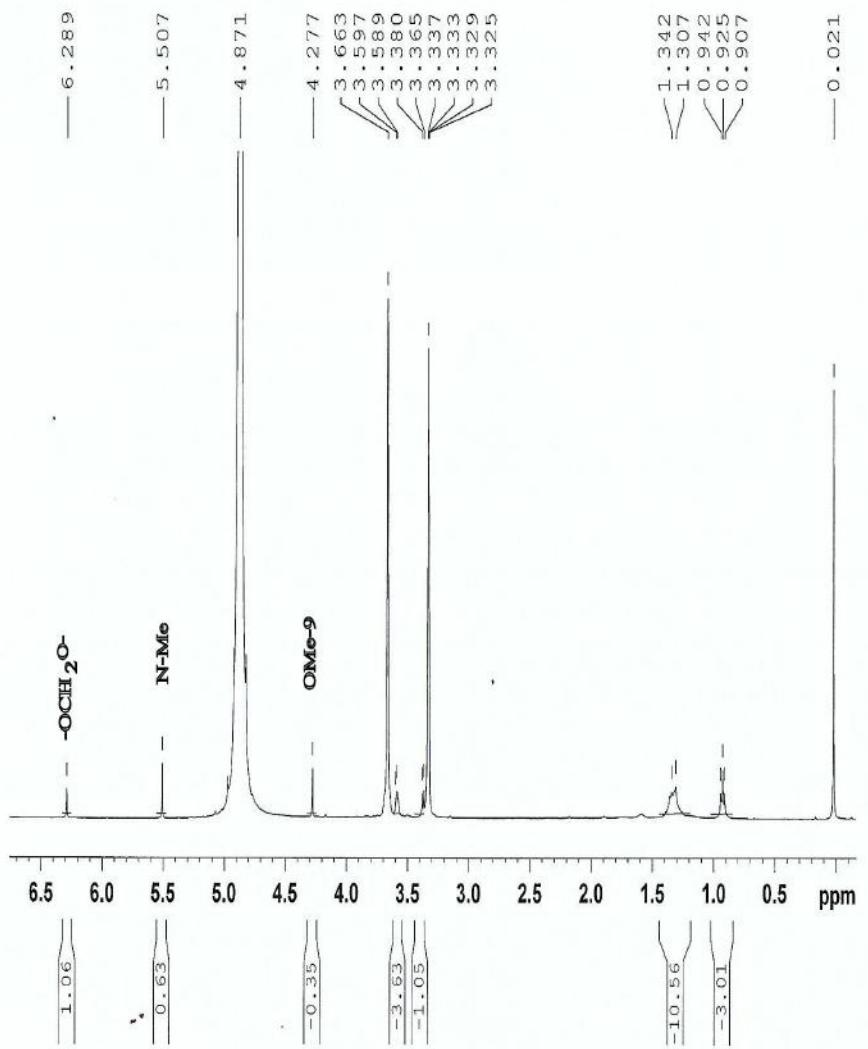
Skimmianine (**4**): colourless crystals; ^1H -NMR (500 MHz, CDCl_3): δ 8.05 (1H, d, $J= 9.2$ Hz, H-5), 7.62 (1H, d, $J= 2.8$ Hz, H-2), 7.27 (1H, d, $J= 9.2$ Hz, H-6), 7.08 (1H, d, $J= 2.8$ Hz, H-3), 4.47 (3H, s, OMe-4), 4.15 (3H, s, OMe-8), 4.06 (3H, s, OMe-7). ^{13}C -NMR (125 MHz, CDCl_3): δ 164.3 (C-12), 157.5 (C-4), 152.4 (C-7), 143.1 (C-2), 142.0 (C-8), 141.5 (C-9), 118.2 (C-5), 114.8 (C-10), 112.3 (C-6), 104.7 (C-3), 102.1 (C-11), 61.7 (OMe-8), 59.1 (OMe-4), 56.9 (OMe-7).

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 Sample: DU_ZRC_7



S42 : $^1\text{H-NMR}$ spectrum (400 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) of Compound 5 (Fagaridine).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_7



Current Data Parameters
 NAME DU_ZRC_7
 EXPNO 1
 PROCNO 1

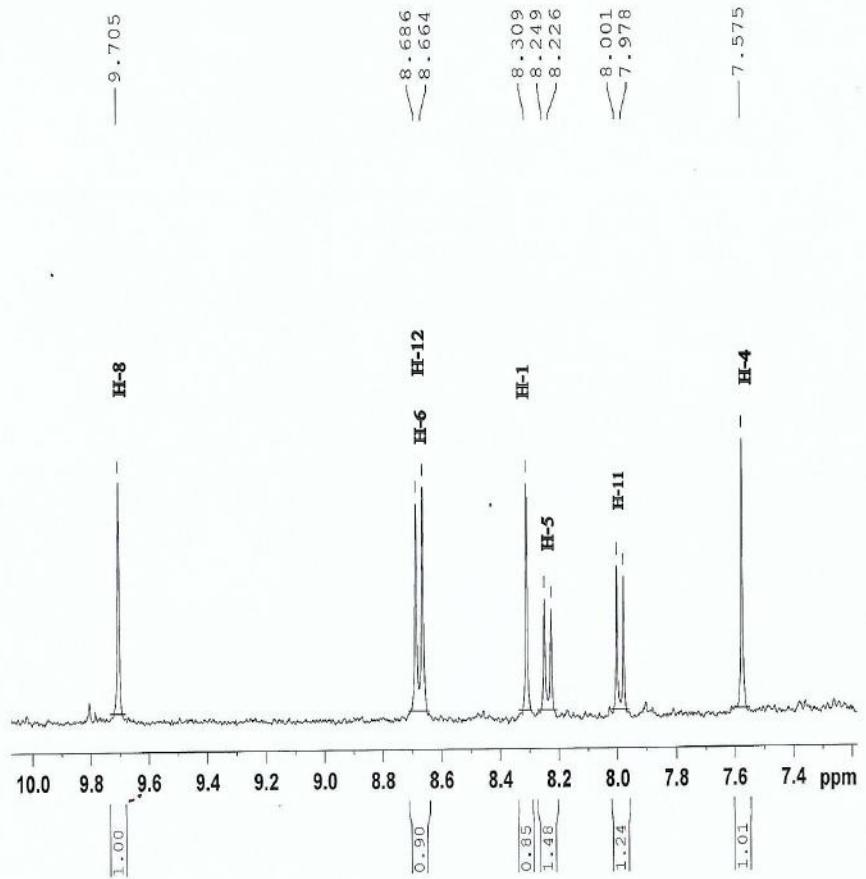
F2 - Acquisition Parameters
 Date 20160123
 Time 11.46
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0834465 sec
 RG 58.24
 DW 62.400 usec
 DE 6.50 usec
 TE 298.4 K
 D1 2.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.2320011 MHz
 NUC1 1H
 PI 14.75 usec
 PLM1 12.00000000 W

F2 - Processing parameters
 SI 131072
 SF 400.2300000 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

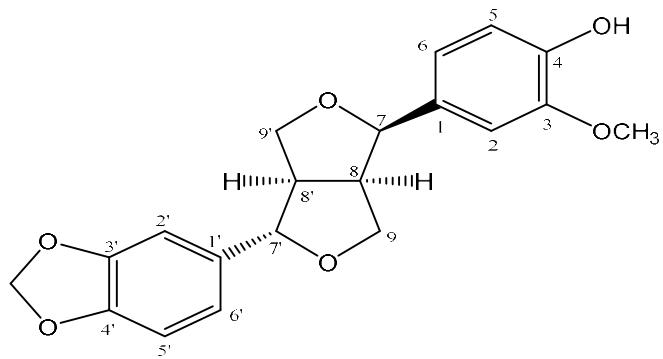
S43 : Expansion of ¹H-NMR spectrum (400 MHz, CDCl₃+CD₃OD) of Compound 5 (Fagaridine).

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 Jahangirnagar University
 Sample: DU_ZRC_7

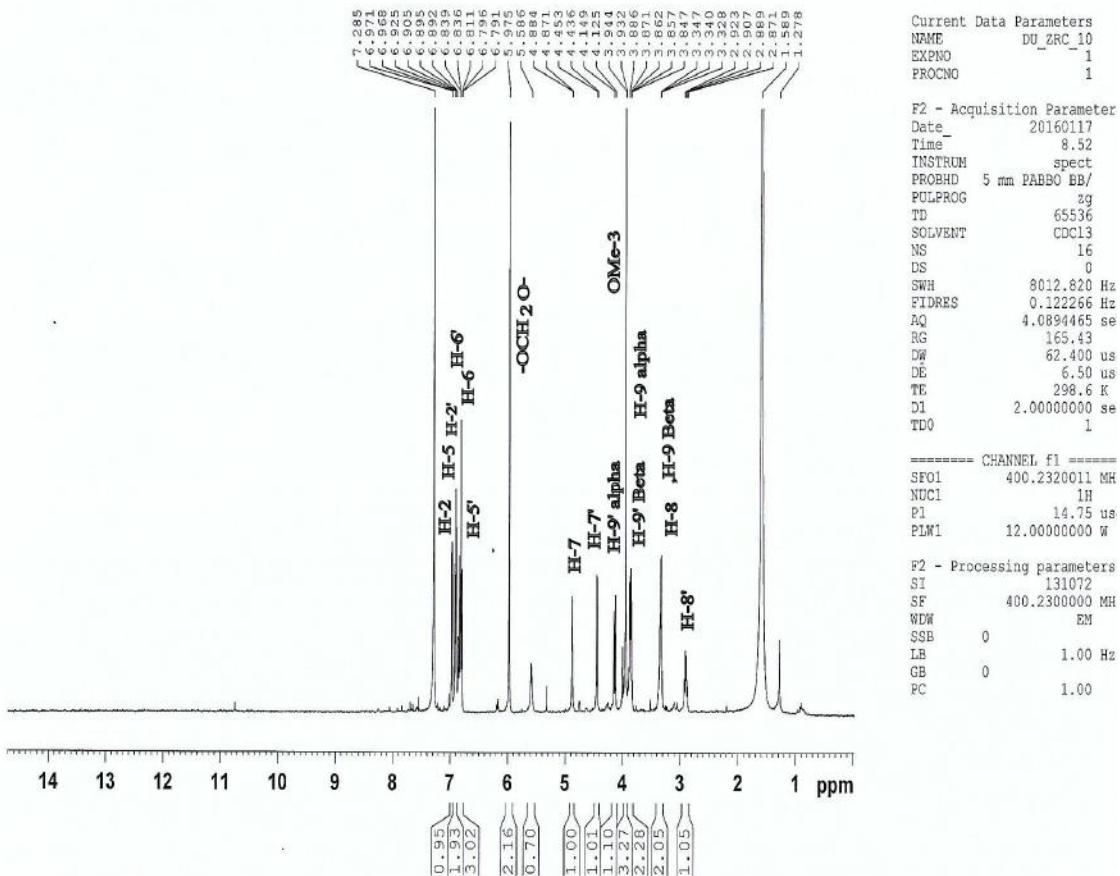


S44 : Expansion of ^1H -NMR spectrum (400 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) of Compound 5 (Fagaridine).

Fagaridine (5): light yellow powder; ^1H -NMR (500 MHz, CDCl_3): δ 9.71 (1H, s, H-8), 8.67 (1H, d, $J= 8.8$ Hz, H-12), 8.31 (1H, s, H-1), 8.24 (1H, d, $J= 9.2$ Hz, H-5), 7.99 (1H, d, $J= 9.2$ Hz, H-11), 7.57 (1H, s, H-4), 7.54 (1H, d, $J= 8.8$ Hz, H-6), 6.23 (2H, s, OCH_2O), 5.50 (3H, s, N-Me), 4.28 (3H, s, OMe-9).



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Jahangirnagar University
Sample: DU_ZRC_10



S45: ¹H-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilol).

Wazed Miah Science Research Center (WMSRC)
Jahangirnagar University
Sample: DU_ZRC_10

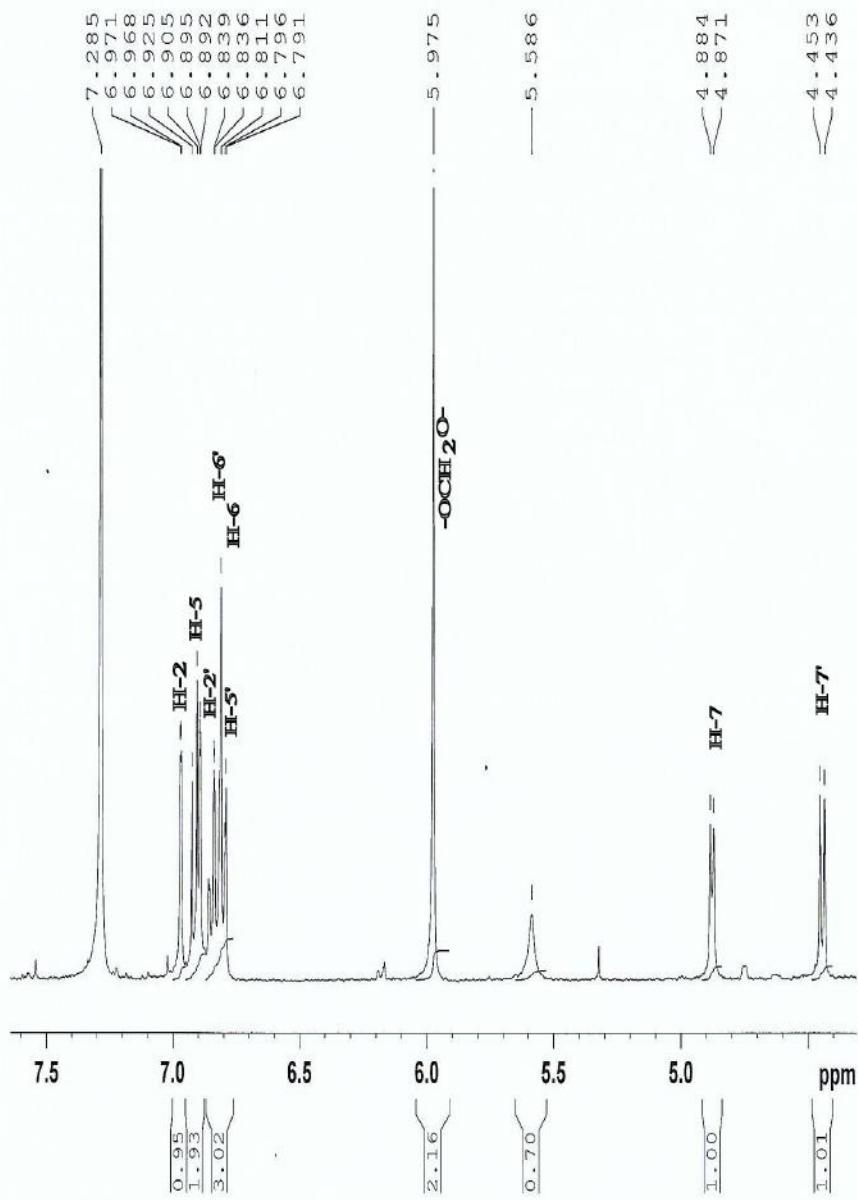


Current Data Parameters
NAME DU_ZRC_10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160117
Time 8.52
INSTRUM spect
PROBHD 5 mm PABEO BB/
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 se
RG 165.43
DW 62.400 us
DE 6.50 us
TE 298.6 K
D1 2.0000000 se
TDO 1

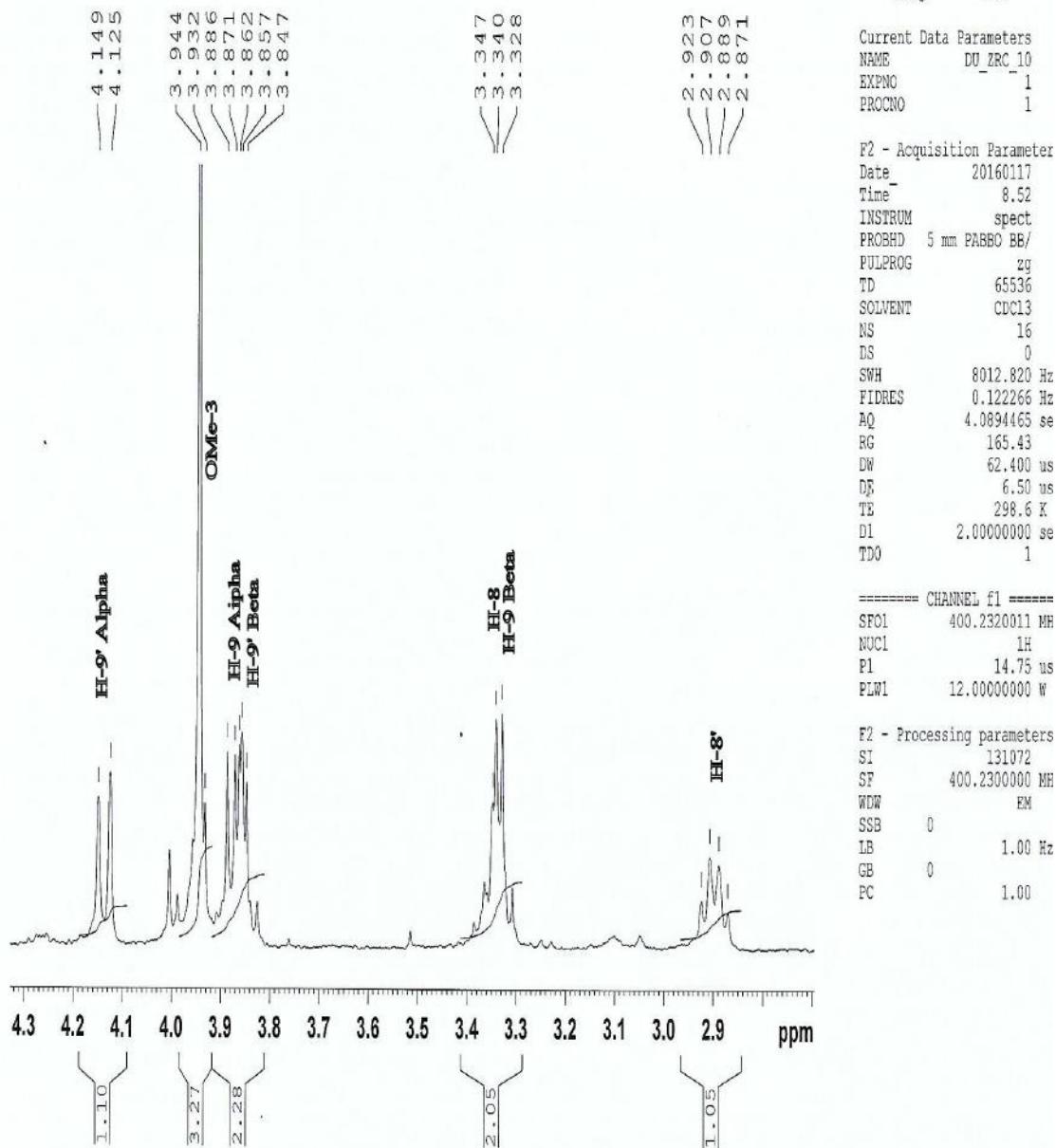
===== CHANNEL f1 =====
SF01 400.2320011 MHz
NUC1 1H
P1 14.75 us
PLW1 12.0000000 W

F2 - Processing parameters
SI 131072
SF 400.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



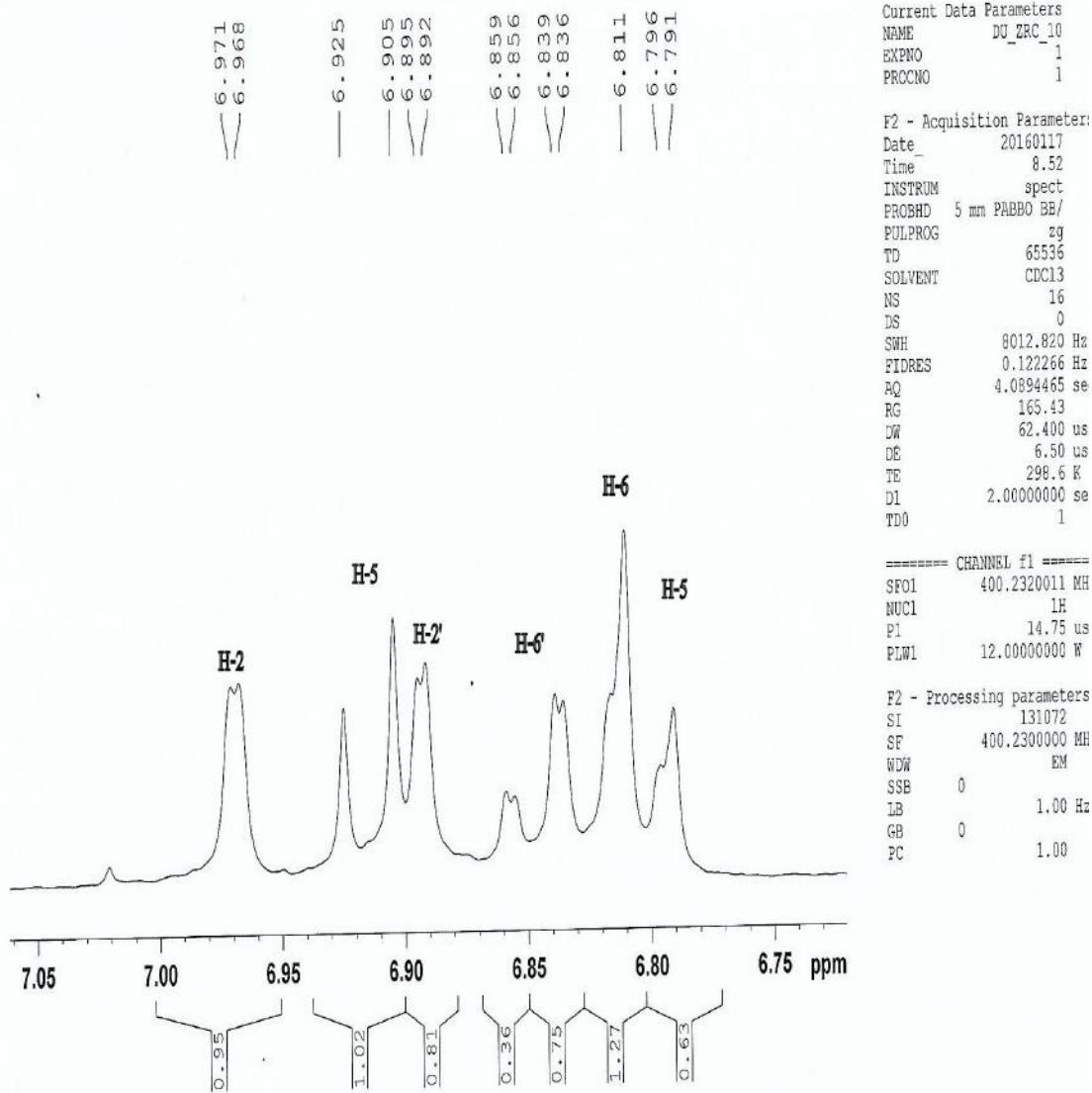
S46 : Partially expanded ^1H -NMR spectrum(400 MHz, CDCl_3) of Compound 6 (Pluviatilol)

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 Jahangirnagar University
 Sample: DU_ZRC_10



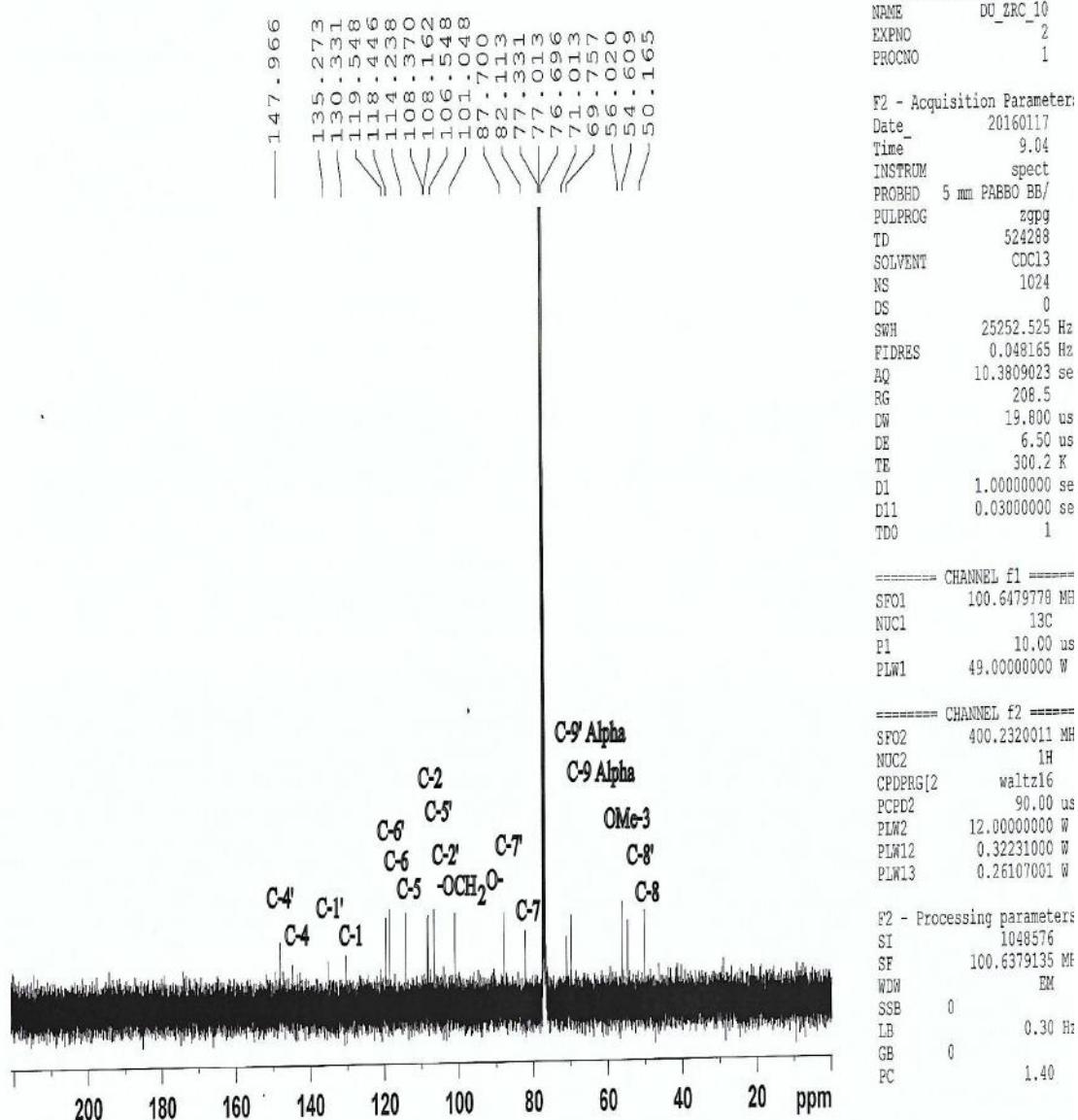
S47: Partially expanded ¹H-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilo).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10



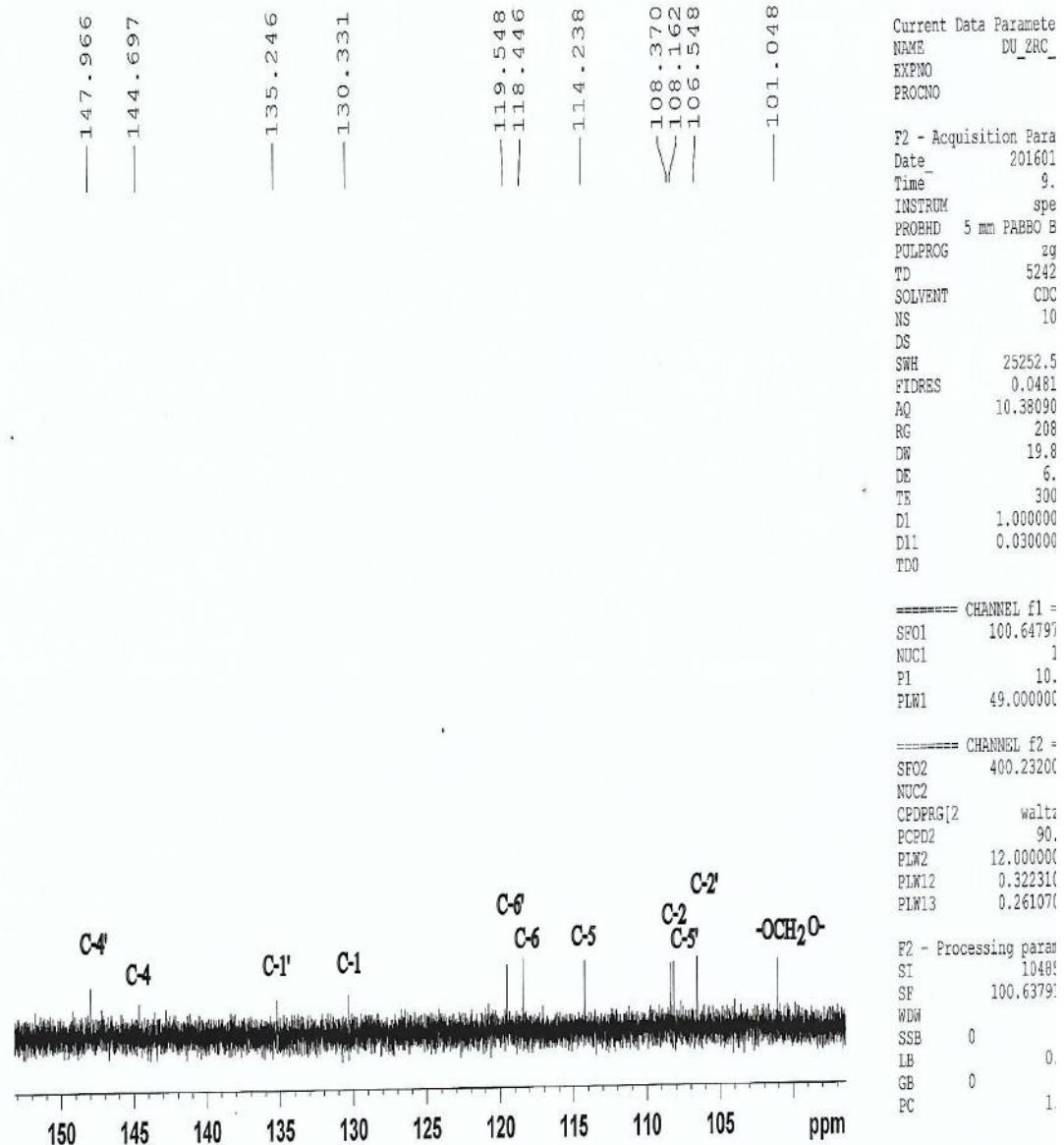
S48: Partially expanded ¹H-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilol).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10



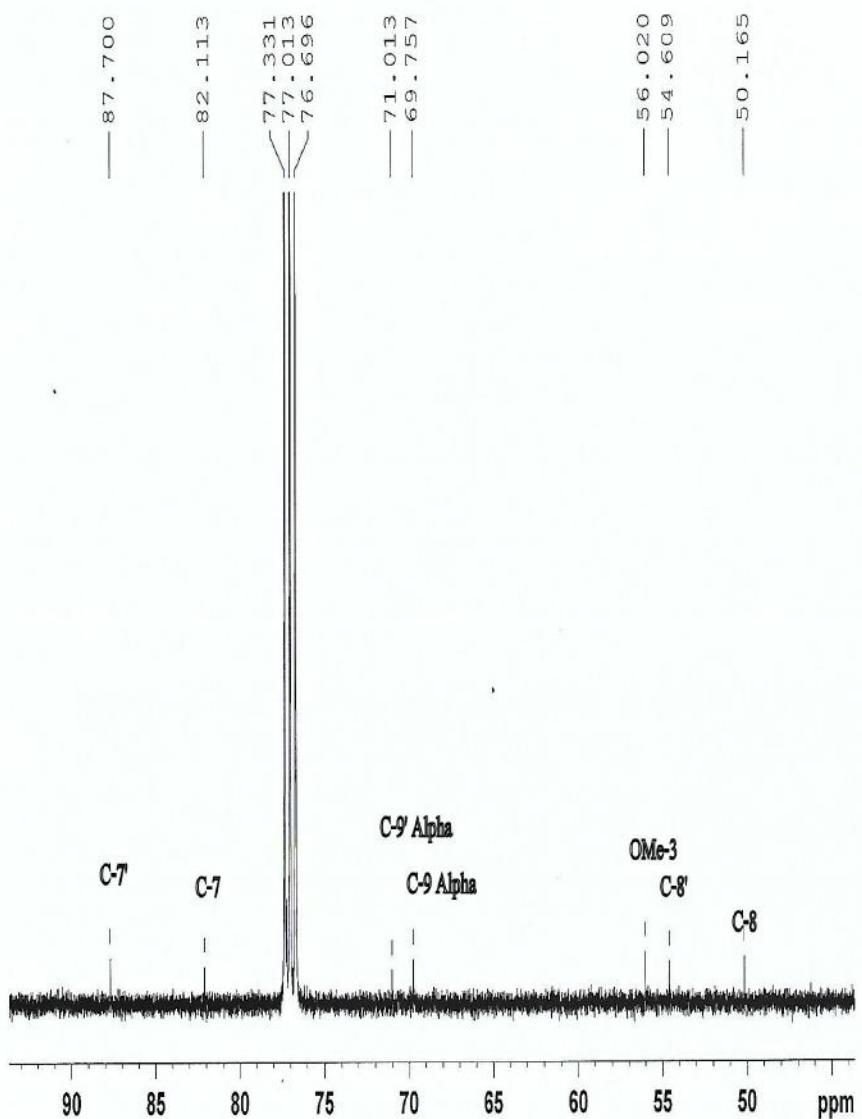
S49 : ¹³C NMR spectrum (100 MHz, CDCl₃) of Compound 6 (Pluviatilol).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10



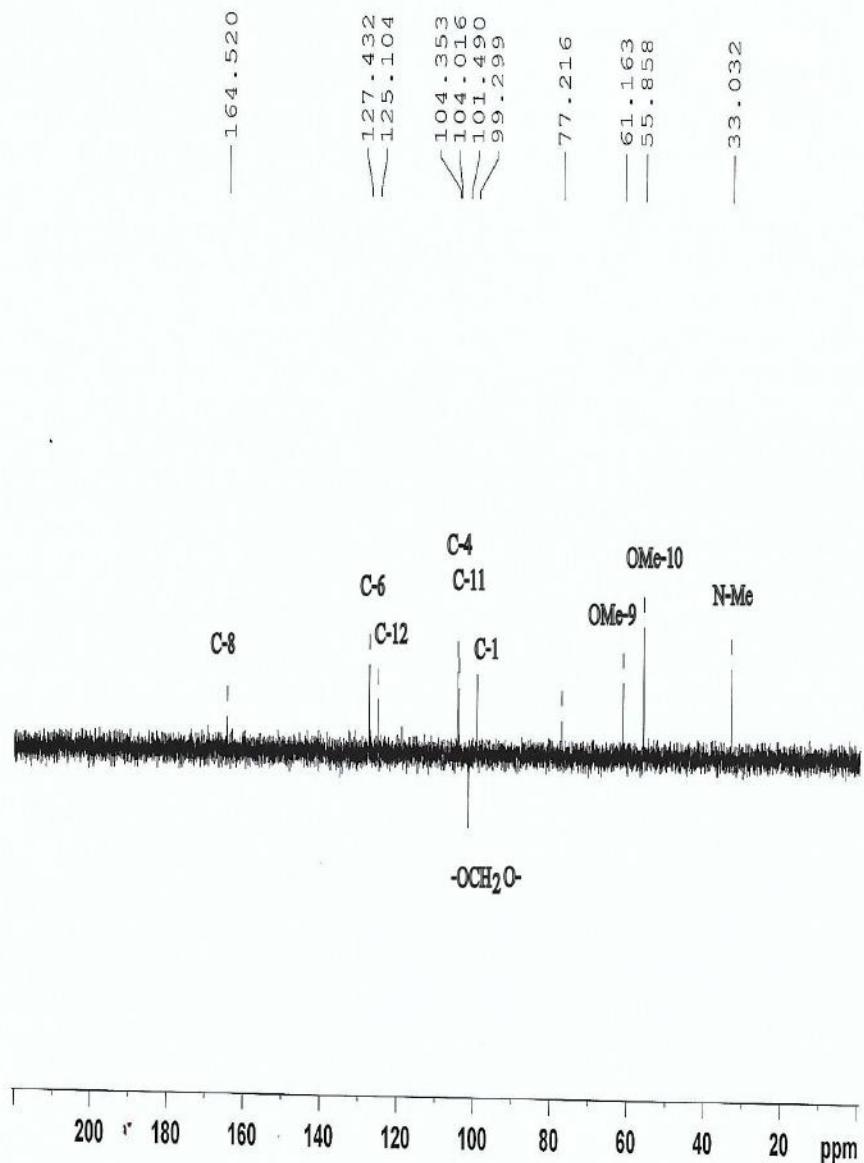
S50: Partially expanded ^{13}C -NMR spectrum (100 MHz, CDCl_3) of Compound 6 (Pluviatilol)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10



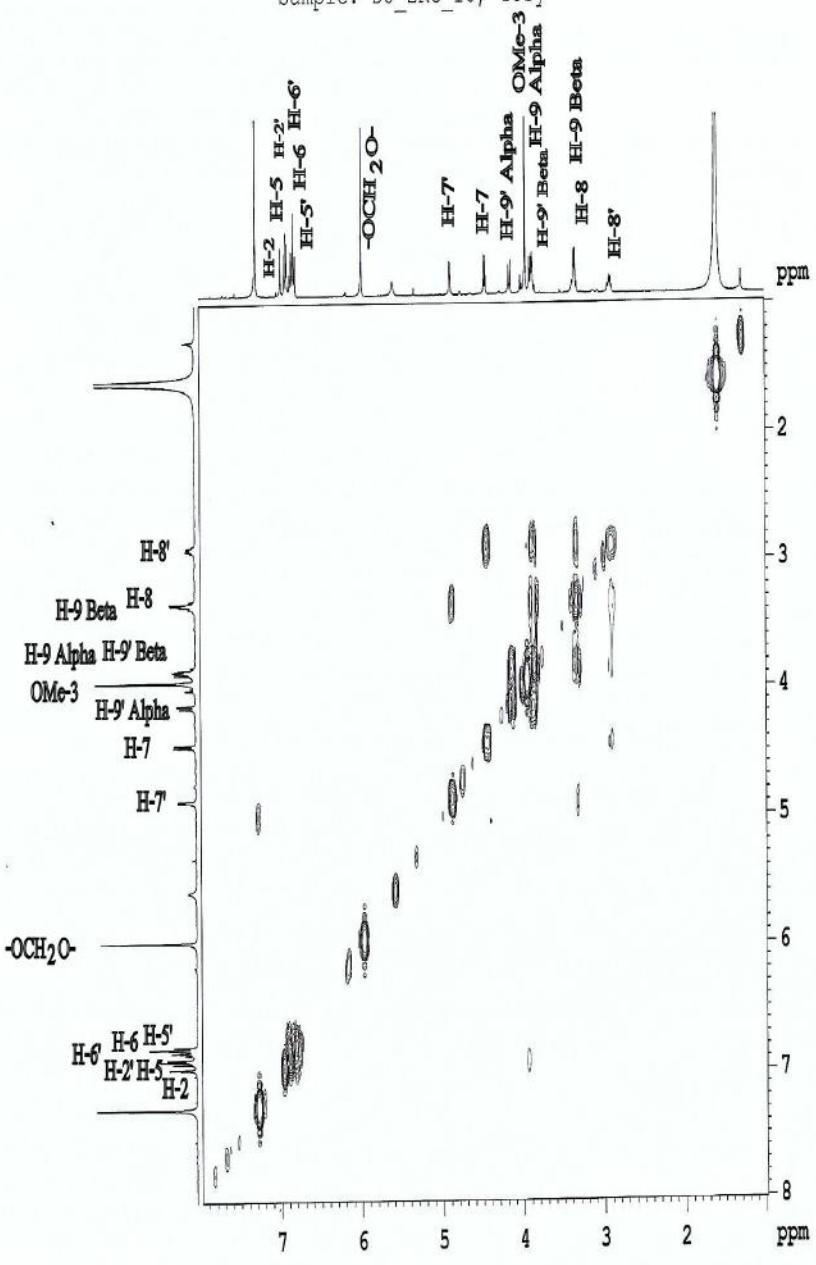
S51: Partially expanded ¹³C-NMR spectrum (100 MHz, CDCl₃) of Compound 6 (Pluviatilol)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRP_20, dept-135



S52: DEPT-135 NMR spectrum (100 MHz, CDCl₃) of Compound 6 (Pluviatilol).

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 Jahangirnagar University
 Sample: DU_ZRC_10, cosy



Current Data Parameters
 NAME DU_ZRC_10
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160117
 Time 12:52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG cosyppgf
 T1 2048
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 8012.820 Hz
 FIDRES 3.91250 Hz
 AQ 0.1277352 sec
 RG 208.5
 DW 62.400 usec
 DE 6.50 usec
 TR 239.2 K
 D1 0.00000300 sec
 D11 1.0000000 sec
 D13 0.00000400 sec
 D15 0.0002000 sec
 D16 0.00012480 sec
 INC 0.00012480 sec

===== CHANNEL f1 =====
 SFO1 400.2320011 MHz
 NUC1 1H
 F0 14.75 usec
 P1 14.75 usec
 PL1 12.0000000 W

===== GRADIENT CHANNEL =====
 GRADNM[1] SWSQ10.100
 GPF1 10.00 %
 PL1 1000.00 usec

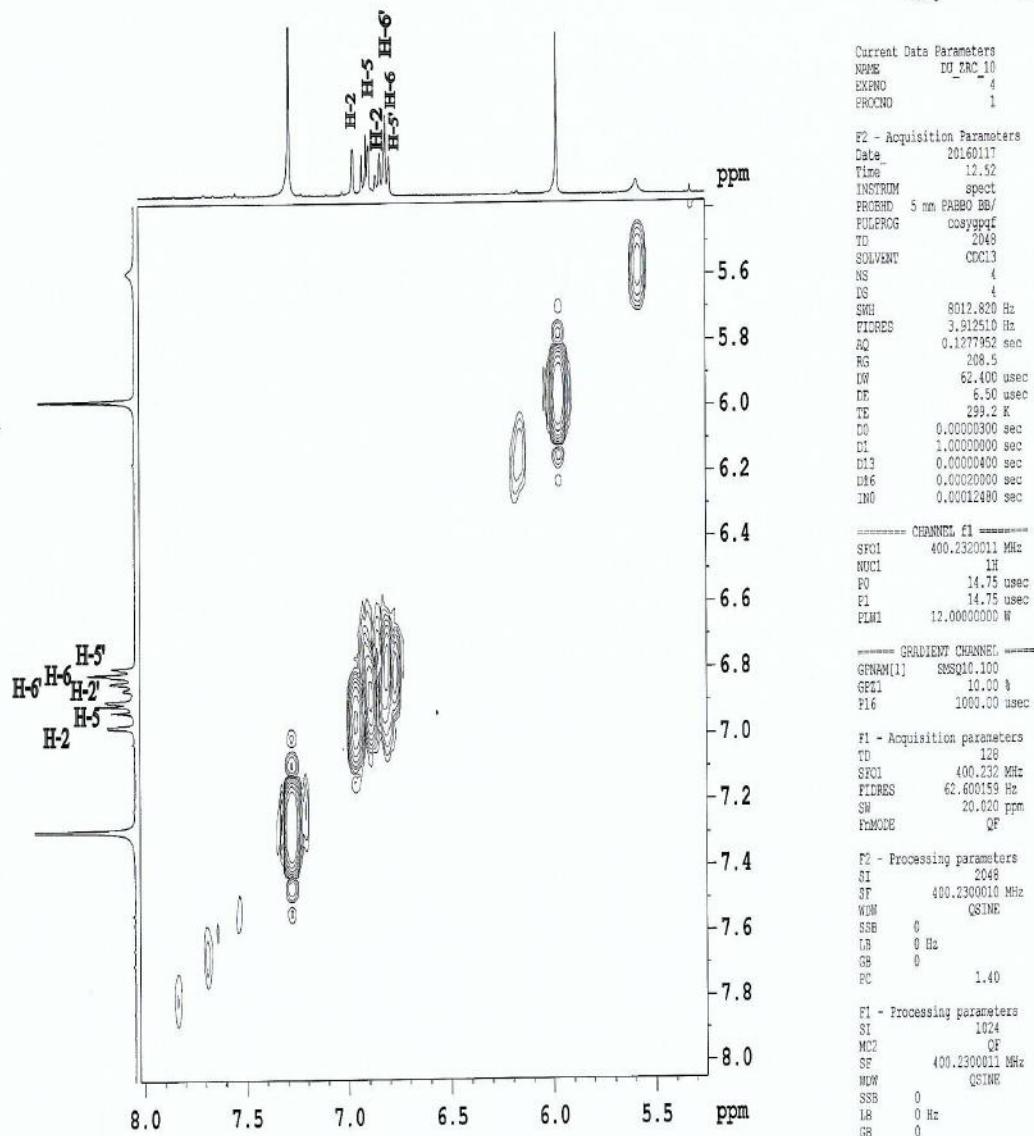
F1 - Acquisition parameters
 TD 128
 SFO1 400.232 MHz
 FIDRES 62.600159 Hz
 SW 20.020 ppm
 RENOME QF

F2 - Processing parameters
 SI 2048
 SF 400.2300010 MHz
 WM QSIMB
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.2300011 MHz
 WM QSIMB
 SSB 0
 LB 0 Hz
 GB 0

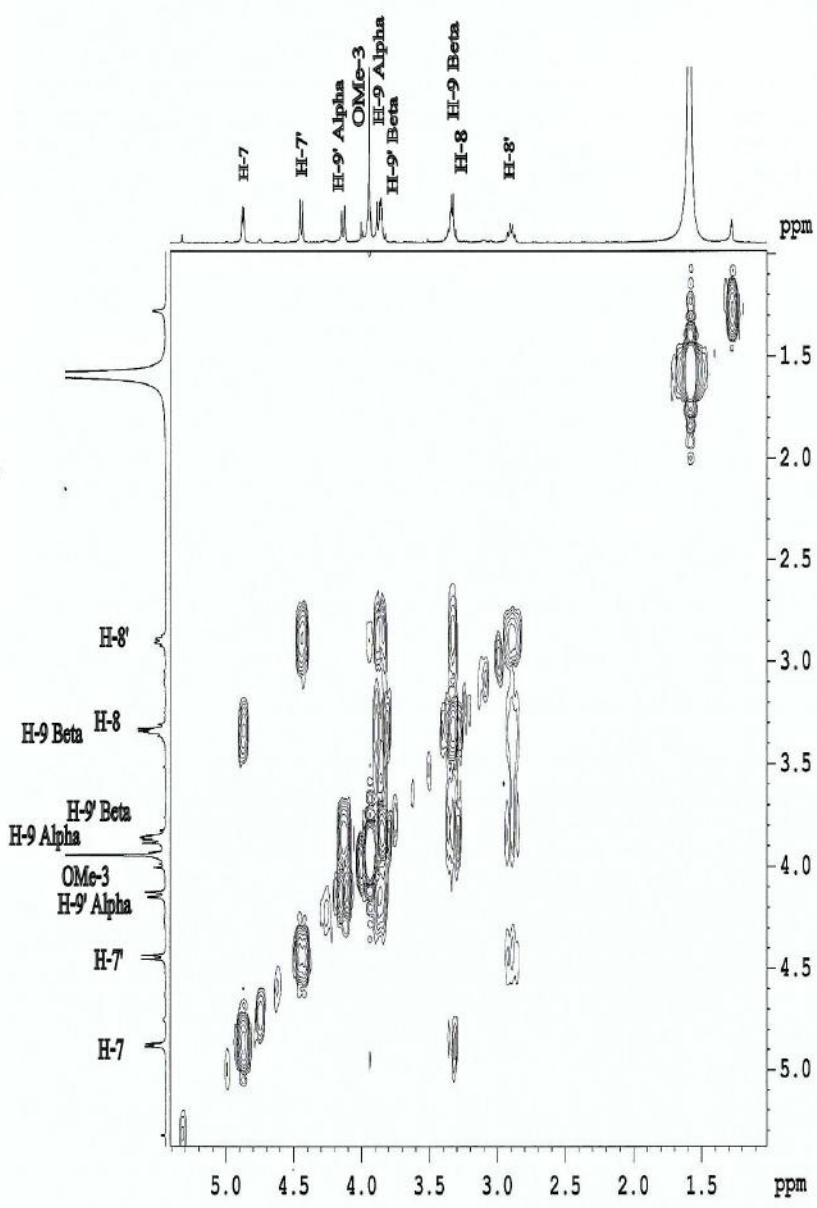
S53: COSY-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilol).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10, cosy



S54 : Partially expanded COSY-NMR spectrum (400 MHz, CDCl₃) of Compound **6**
 (Pluviatilol)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10, cosy



Current Data Parameters
 NAME DU_ZRC_10
 EXENO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160117
 Time 12.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG cosyngf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 8012.420 Hz
 FIDRES 3.912510 Hz
 AQ 0.1277952 sec
 RG 209.5
 DW 62.400 usec
 DE 6.50 usec
 TB 299.2 K
 D0 0.00000300 sec
 D1 1.0000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 TIN 0.00012480 sec

===== CHANNEL F1 =====
 SP01 400.2320011 MHz
 NUC1 1H
 F0 14.75 usec
 P1 14.75 usec
 PLW1 12.00000000 W

===== GRADIENT CHANNEL =====
 GRADNM[1] SMSQ10.100
 G281 10.00 %
 P16 1000.00 usec

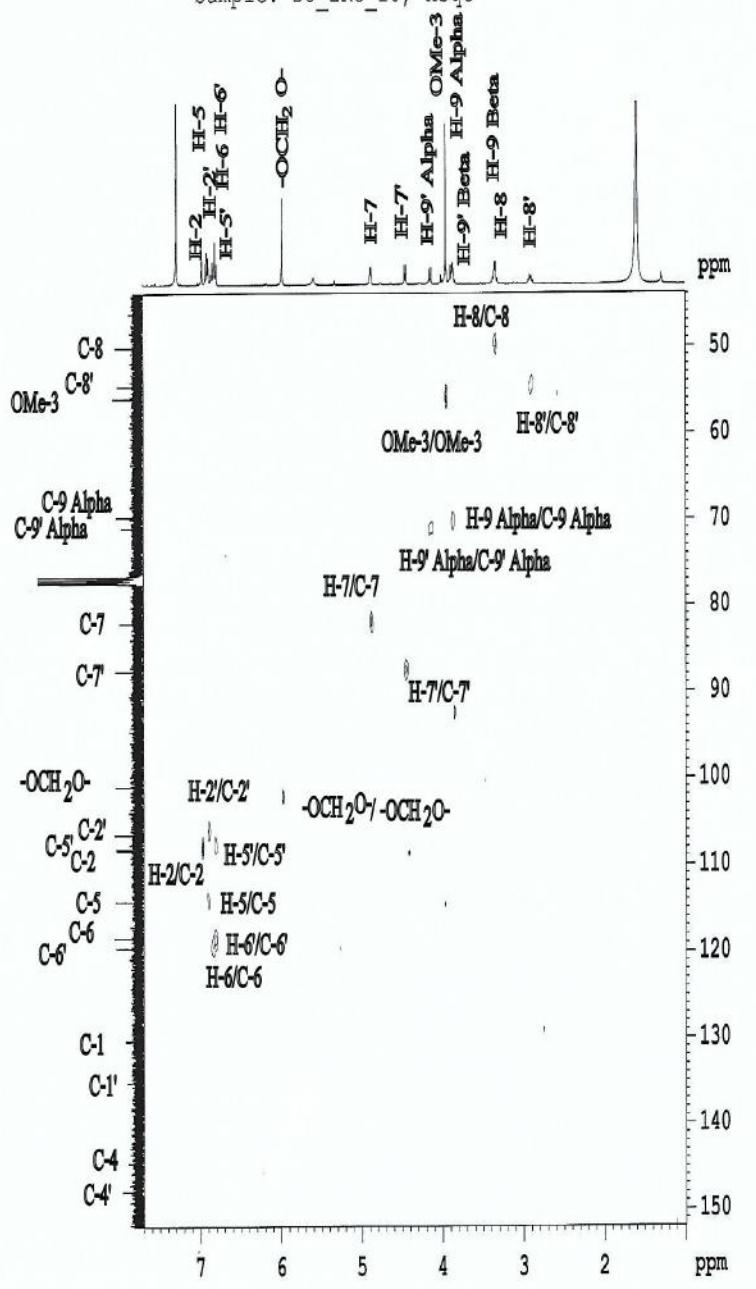
F1 - Acquisition parameters
 TD 128
 SP01 400.232 MHz
 FIDRES 62.600159 Hz
 SW 20.020 ppm
 FMODE QF

F2 - Processing parameters
 SI 2048
 SF 400.2300010 MHz
 NW 0 QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MD2 0 QF
 SF 400.2300011 MHz
 NW 0 QSINE
 SSB 0
 LB 0 Hz
 GB 0

S55 : Partially expanded COSY-NMR spectrum (400 MHz, CDCl_3) of Compound **6** (Pluviatilol)

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_10, hsqc



Current Data Parameters

DIM3 1024

SW1 13.18

SW2 8.97

PW1 5 ms JMMB Ad

PW1PR 5 ms JMMB Ad

TD 2048

SOLVENT CDCl₃

NS 4

DS 0

TB 811.2 Hz

TE 3.01210 Hz

TEPR 0.33333 sec

TEPPR 204.3

TEP 63.402 uses

TEW 6.50 uses

TB 254.3 K

CSEN1 145.000000

CSEN17 -4.000000

TDZ 1.000000 sec

TDZP 2.000000 sec

TDZT 0.2017314 sec

TDZL 0.0303300 sec

TDZB 0.0030300 sec

TDZC 0.0036300 sec

TDZD 0.0039300 sec

TDZG 0.0003190 sec

===== CHANNEL 1 =====

SW1 811.232011 MHz

SW2 13.18

PI 14.75 uses

PS 23.51 uses

PSB 12.0000000 N

===== CHANNEL 2 =====

SW1 110.417974 MHz

SW2 13.18

QCPMG12 interp

PI 16.21 uses

PIA 500.00 uses

PS 2100.00 uses

PSB 60.00 uses

PSW 0 N

PW1 49.0000000 N

PW2 0.76563551 N

SWW(1) Cgpp,0.1,1,1

SWW(2) 0.500

SWW(3) 0 Hz

SWW(4) T,1.015952 N

SWW(5) Cgpp,0.1,1

SWW(6) 0.500

SWW(7) 0 Hz

SWW(8) T,1.015952 N

===== GRADIENT GRAPHS =====

GRADIENT1 185.201,100

GRADIENT2 295.00,100

GRADIENT3 295.00,100

GRADIENT4 295.00,100

GR1 69.00 s

GR2 23.10 s

GR3 11.00 s

GR4 -3.00 s

PI 100.00 uses

PIB 601.00 uses

PII - Acquisition parameters

TD 128

SW1 101.648 MHz

SW2 137.261553 Hz

SP 250.093 ppm

VOLUME Echo-Rotatable

PL - Processing parameters

S1 1024

S2 400.2301000 MHz

SW 0.51038

SSB 2

LB 1 Hz

GB 1

TC 1.41

PL - Processing parameters

S1 1024

S2 echo-antisymmetric

SW 100.879145 MHz

SP 250.093 ppm

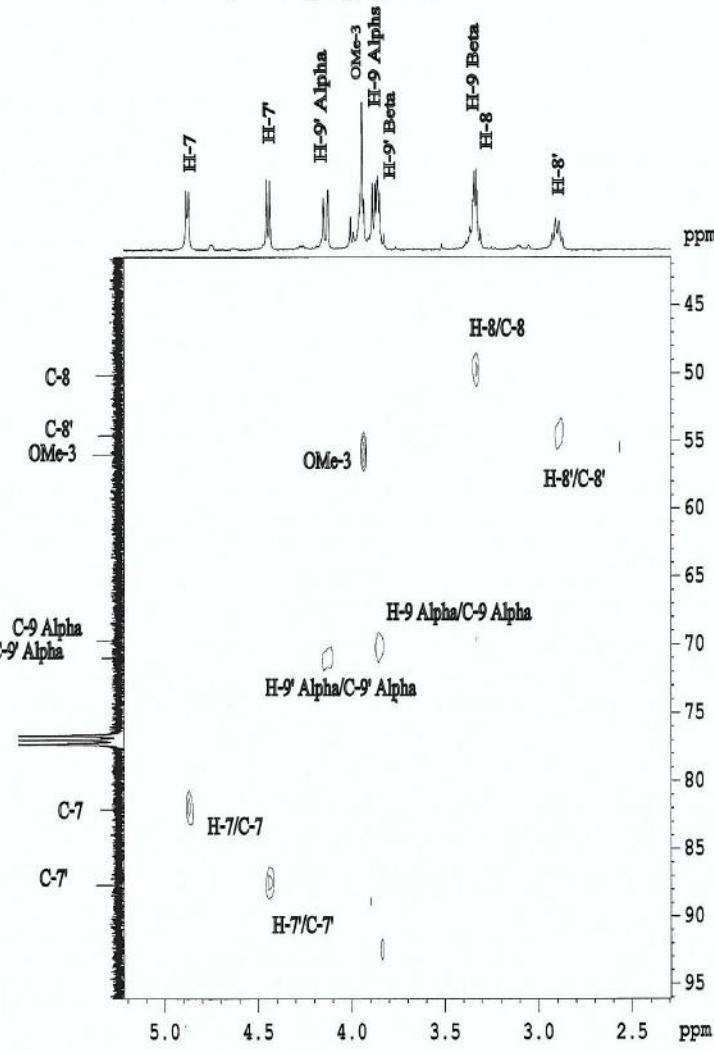
SSB 2

LB 1 Hz

GB 1

S56: HSQC-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilol).

Wazed Miah Science Research Center (WMSRC)
Jahangirnagar University
Sample: DU_ZRC_10, hsqc

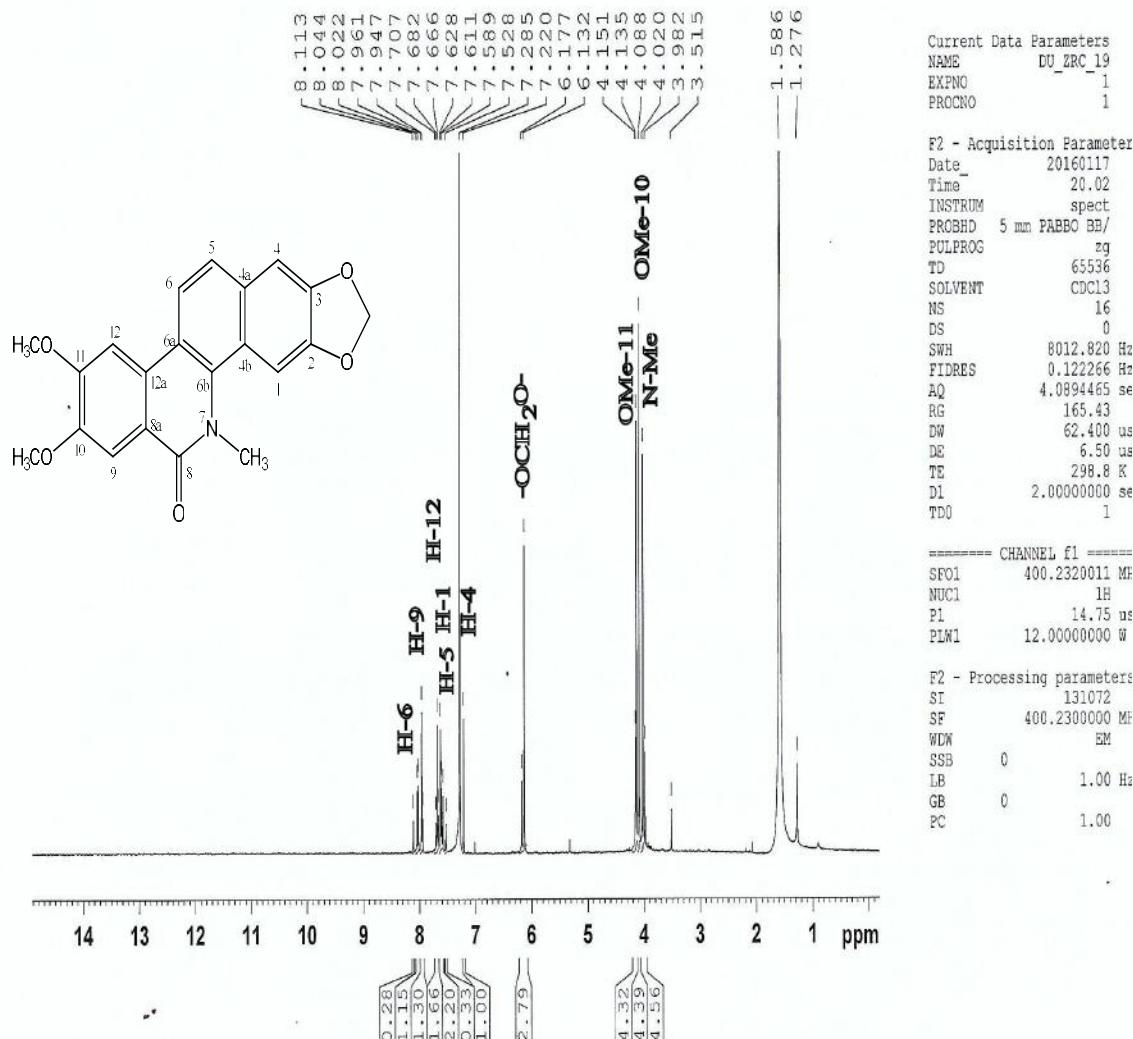


Current Data Parameters
Date: 20160117
Time: 13:12
Pulse: 90°
PR180: 5 ms DARE 8°
PR180S: 5 ms DARE 8°
TD: 32768
SW: 12500 Hz
NS: 4
DS: 4
SF: 32768 Hz
ETR200: 3.000000 Hz
DQ: 0.1273952 sec
RG: 250.1
DW: 62.500 usec
ZX: 8.00 usec
TZ: 250.0 sec
ETR222: 145.000000 Hz
C9D17: -0.5000000 sec
D9: 0.3000000 sec
D1: 1.0000000 sec
D11: 0.2500000 sec
D16: 0.3000000 sec
D17: 0.2000000 sec
D18: 0.2500000 sec
D2: 0.2000000 sec
DW: 12.5000000 sec
==== CHANNEL F1 =====
SP1: 400.2220001 MHz
TP1: 1H
F1: 14.50 usec
SI: 20,500 sec
SF1: 0 usec
SW1: 12.5000000 sec
==== CHANNEL F2 =====
SP2: 103.487978 MHz
TP2: 1H
CPB2: 90°
R2: 15.05 usec
SI2: 10,000 sec
SF2: 30.03 usec
PCP2: 90.03 usec
PL2: 0 sec
DW2: 10.0000000 sec
F1M2: 0.3653401 sec
SPHOM2: Crp40,5,5,26.1
SIHOM2: 0 sec
SPHOM3: 7.4665992 sec
SIHOM4: Crp40,5,5,26.1
SIHOM5: 0 sec
SIHOM6: 7.4665992 sec
SIHOM7: Crp40,5,5,26.1
SIHOM8: 0 sec
==== GRADIENT CHANNEL =====
GPRMC1: SMC01,100
GPRMC2: SMC01,100
GPRMC3: SMC01,100
GPRMC4: SMC01,100
GPRMC5: SMC01,100
GPRMC6: SMC01,100
GPRMC7: SMC01,100
GPRMC8: SMC01,100
F1: 100.00 usec
SI: 100.00 usec
DW: 100.00 usec
==== Acquisition parameters =====
P1: 228
SP1: 103.487978 MHz
PR180: 137.245535 Hz
DW: 253.8499999 Hz
PW180D: Echo-Planar
==== Processing parameters =====
A1: 4042
SF: 400.2200000 MHz
V1: 100.0000000 MHz
C1: 2
T0: 1 sec
GB: 4
TC: 1.45
F1: Processing parameters
A1: 4042
SF: 400.2200000 MHz
V1: 100.0000000 MHz
C1: 2
T0: 1 sec
L0: 1 Hz
G0: 1

S57: Partially expanded HSQC-NMR spectrum (400 MHz, CDCl₃) of Compound 6 (Pluviatilol)

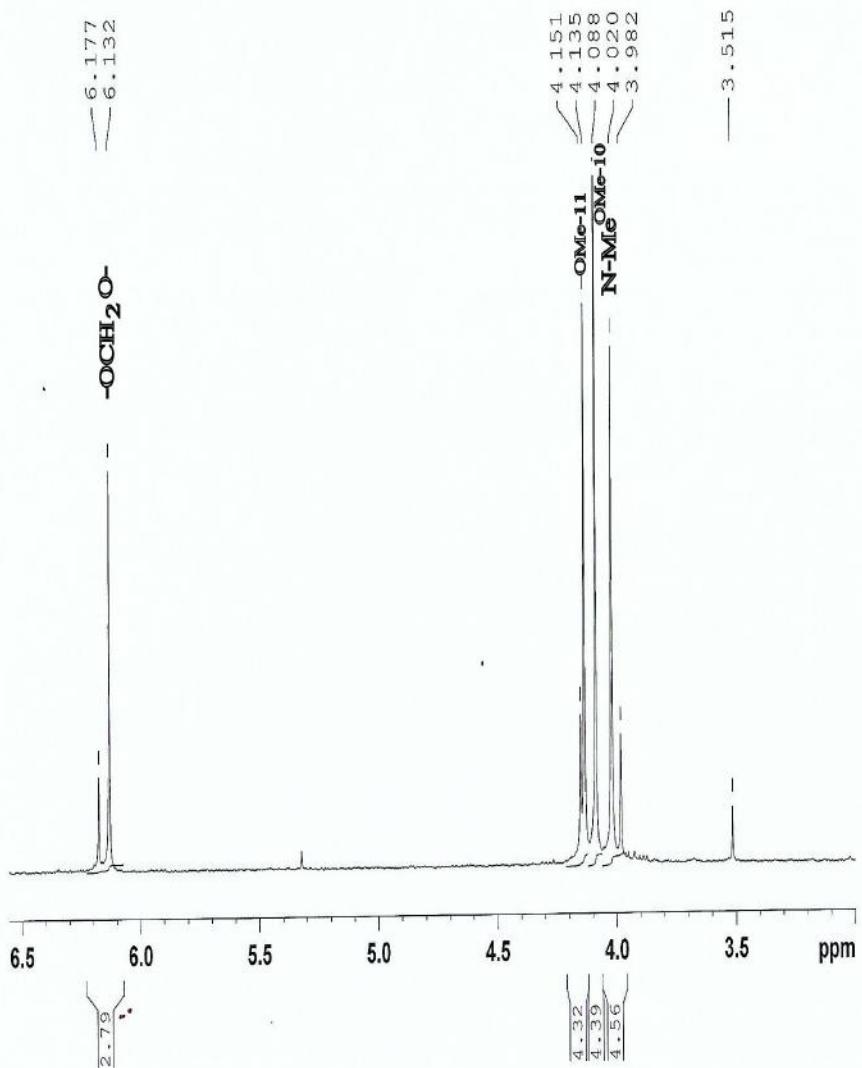
Pluviatilol (6): white crystals; ¹H-NMR (500 MHz, CDCl₃): δ 6.97 (1H,d, J= 1.2 Hz, H-2), 6.92 (1H, d, J= 8.0 Hz, H-5), 6.89 (1H, d, J= 1.2 Hz, H-2'), 6.85 (1H, dd, J= 8.0, 1.2 Hz, H-6'), 6.81 (1H, dd, J= 8.0, 2.0 Hz, H-6), 6.80 (1H, d, J= 8.0 Hz, H-5'), 5.98 (2H, s, OCH₂O), 4.87 (1H, d, J= 5.2 Hz, H-7), 4.44 (1H, d, J= 6.8 Hz, H-7'), 4.13 (1H, d, J= 9.6 Hz, H-9'a), 3.93 (3H, s, OMe-3), 3.87 (1H, dd, J= 9.6, 6.0 Hz, H-9α), 3.86 (1H, m, H-9'β), 3.34 (1H, m, H-8), 3.34 (1H, m, H-9β), 2.89 (1H, dd, J= 7.2, 6.4 Hz, H-8'). ¹³C-NMR (125 MHz, CDCl₃): δ 148.0* (C-4'), 147.2* (C-3'), 145.9* (C-3), 144.7* (C-4), 130.3 (C-1), 119.5 (C-6'), 118.4 (C-6), 114.2 (C-5), 108.4 (C-2), 108.2 (C-5'), 106.5 (C-2'), 101.0 (OCH₂O), 87.7 (C-7'), 82.1 (C-7), 71.0 (C-9'), 69.8 (C-9), 56.0 (OMe-3), 54.6 (C-8'), 50.2 (C-8).

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 Sample: DU_ZRC_19



S58: ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 7 (Oxynitidine).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_19



Current Data Parameters
 NAME DU_ZRC_19
 EXPNO 1
 PROCN 1

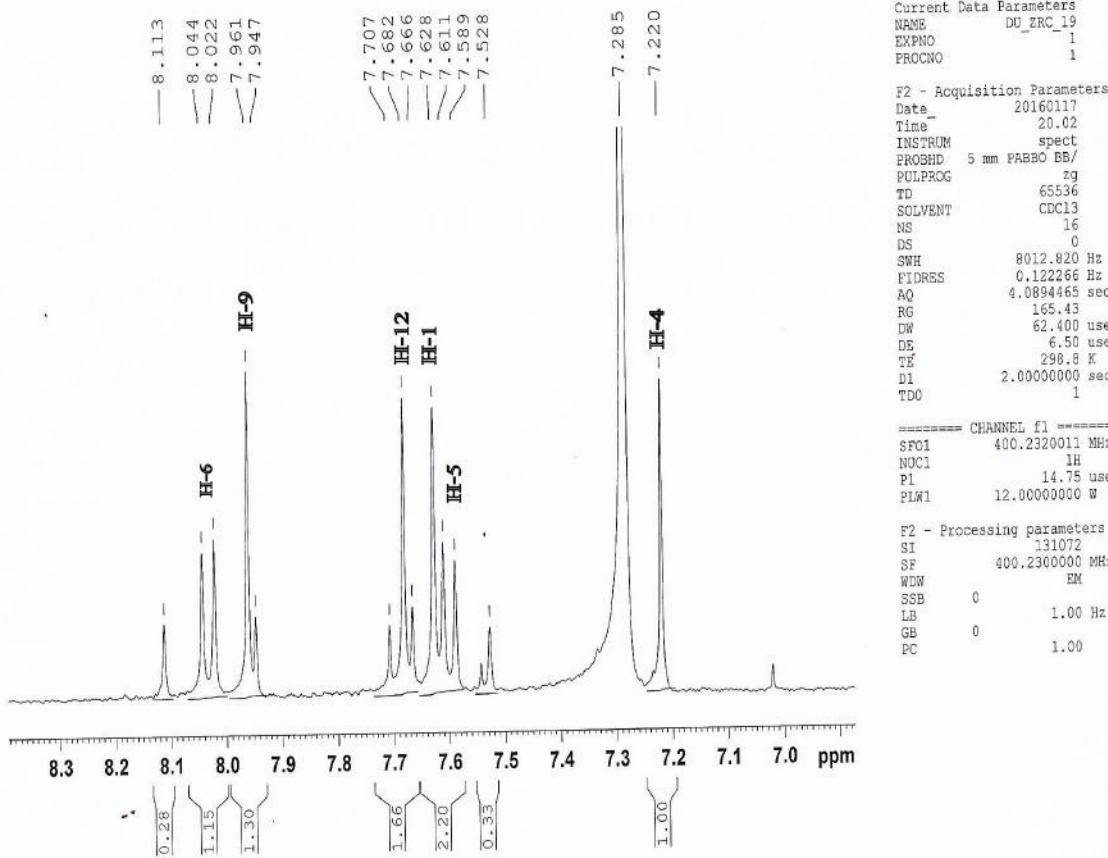
F2 - Acquisition Parameters
 Date 20160117
 Time 20.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 165.43
 DW 62.400 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 400.2320011 MHz
 NUCL 1H
 PI 14.75 usec
 PLW1 12.0000000 W

F2 - Processing parameters
 SI 131072
 SF 400.2300000 MHz
 WDW EM
 SSB 0 1.00 Hz
 LB 0
 GB 0 1.00
 PC

S59: Expansion of ^1H NMR (400 MHz, CDCl_3) spectrum of Compound 7 (Oxynitidine).

Wazed Miah Science Research Center (WMSRC)
 Jahangirnagar University
 Sample: DU_ZRC_19



S60: Expansion of ¹H NMR (400 MHz, CDCl₃) spectrum of Compound 7 (Oxynitidine).

Oxynitidine (**7**): white amorphous; ¹H-NMR (500 MHz, CDCl₃): δ 8.02 (1H, d, *J*= 8.8 Hz, H-6), 7.96 (1H, s, H-9), 7.68 (1H, s, H-12), 7.63 (1H, s, H-1), 7.60 (1H, d, *J*= 8.8 Hz, H-5), 7.22 (1H, s, H-4), 6.13 (2H, s, OCH₂O), 4.14 (3H, s, OMe-11), 4.08 (3H, s, OMe-11), 4.02 (3H, s, N-Me).

