

SUPPORTING INFORMATION

Title: Synthesis of Substituted 1*H*- and 3*H*-1-Benzazepines and Rearrangement of Alkyl 1*H*-1-Benzazepine-2-carboxylates into Isoquinolines

Author(s): Vijay Singh, Sanjay Batra*

Ref. No.: O200700175

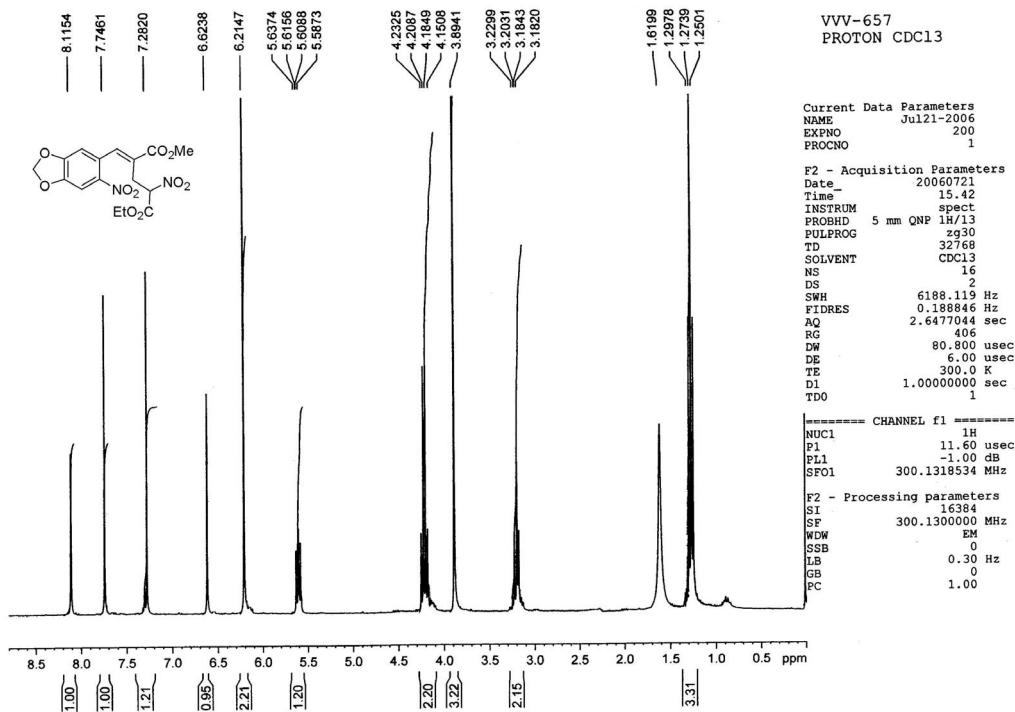


Fig.-1: ^1H NMR spectrum of compound 7c

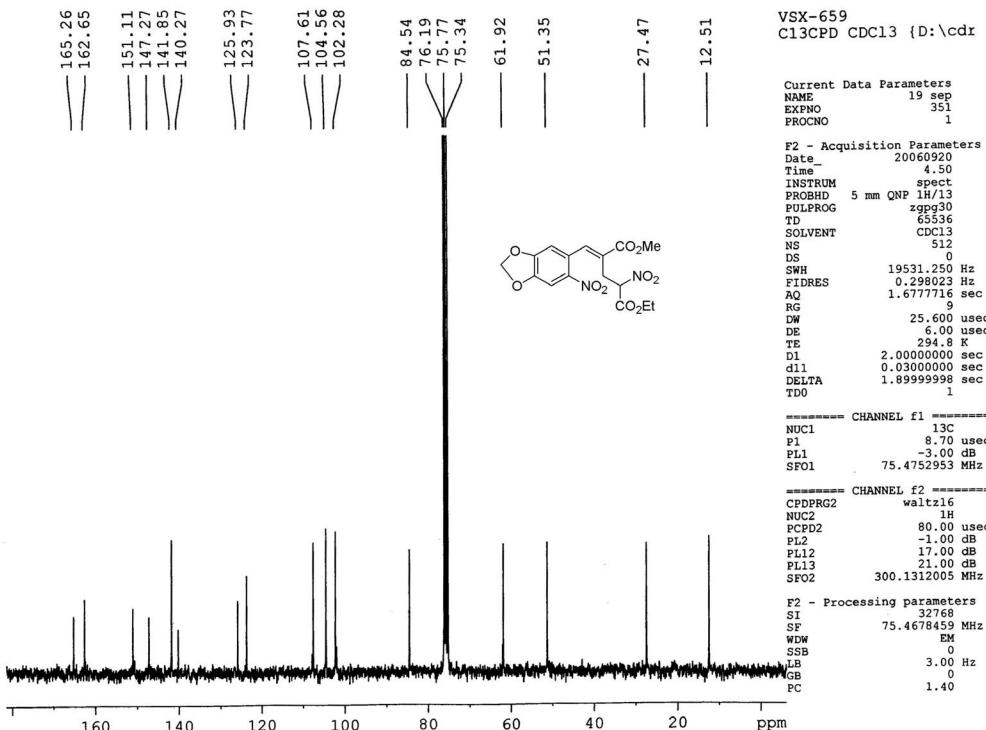


Fig.-2: ^{13}C NMR spectrum of compound 7c

[Mass Spectrum]
 Data : 6127SEP359 Date : 27-Sep-2006 13:41
 Sample: SB-657 DR S BATRA
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.35 min Scan# : (2,6)
 BP : m/z 149.0000 Int. : 94.28
 Output m/z range : 251.3457 to 424.0090 Cut Level : 0.00 %

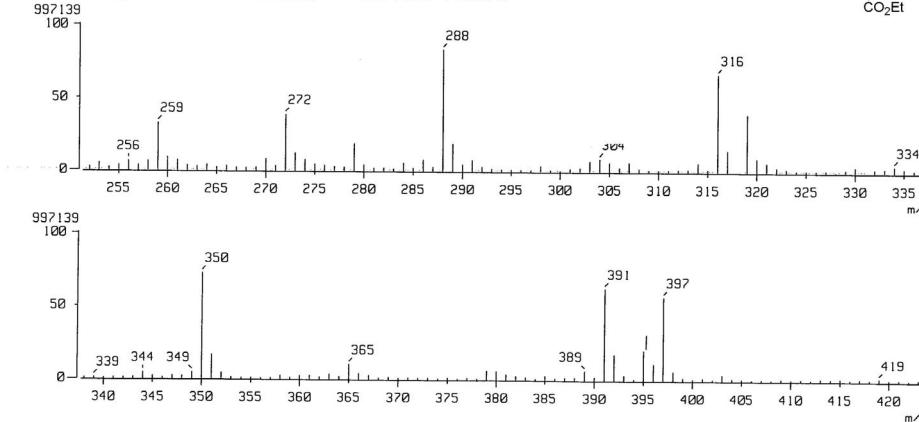
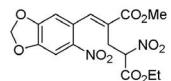


Fig.-3: Mass spectrum of compound 7c

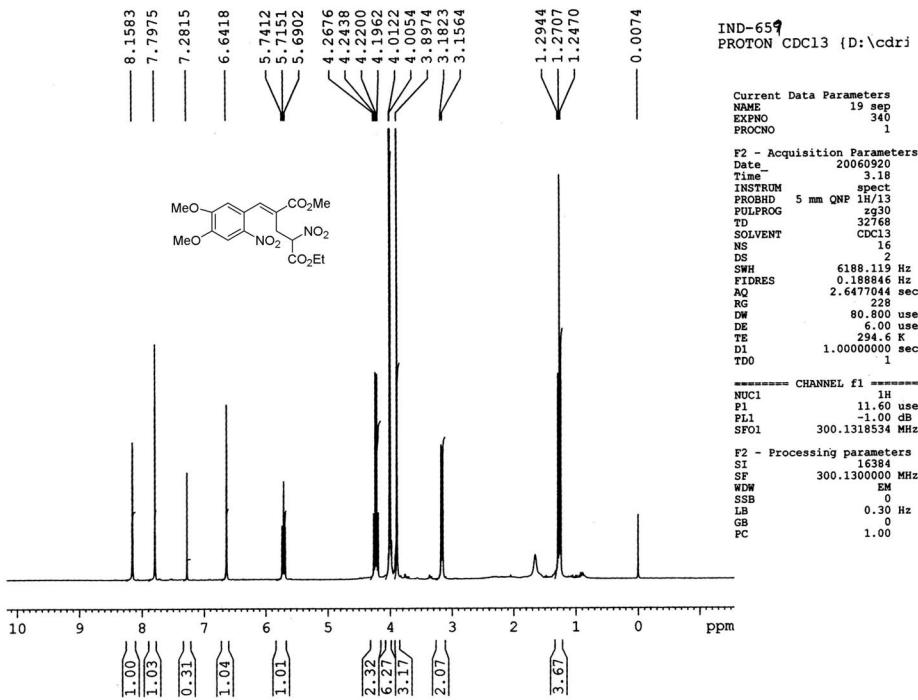


Fig.-4: ^1H NMR spectrum of compound 7d

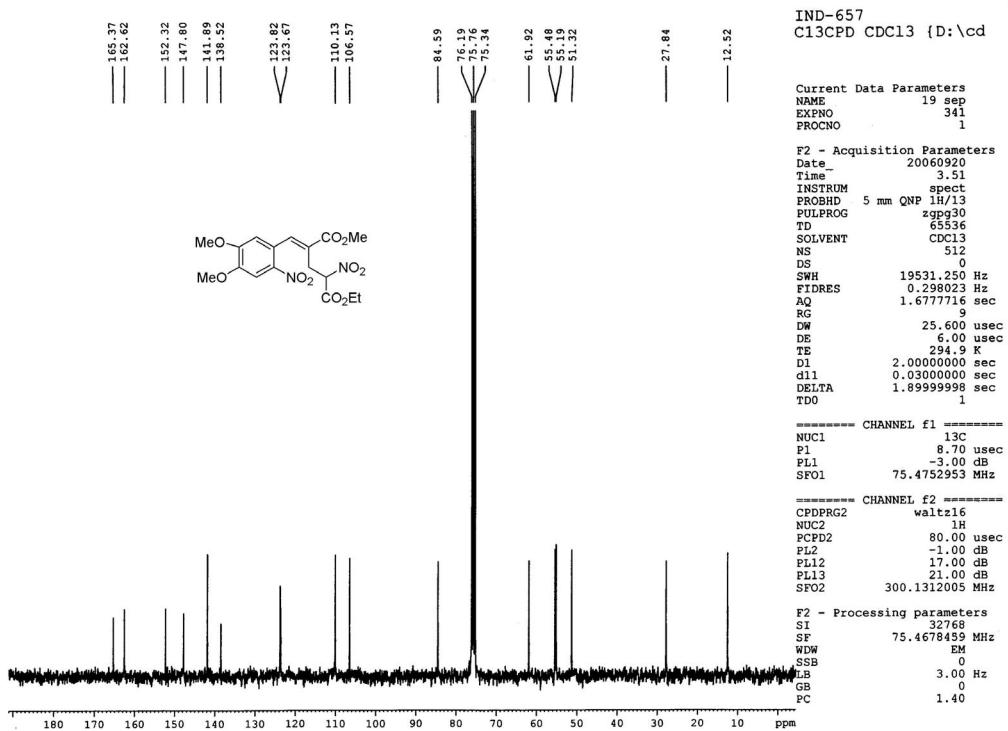


Fig.-5: ¹³C NMR spectrum of compound 7d

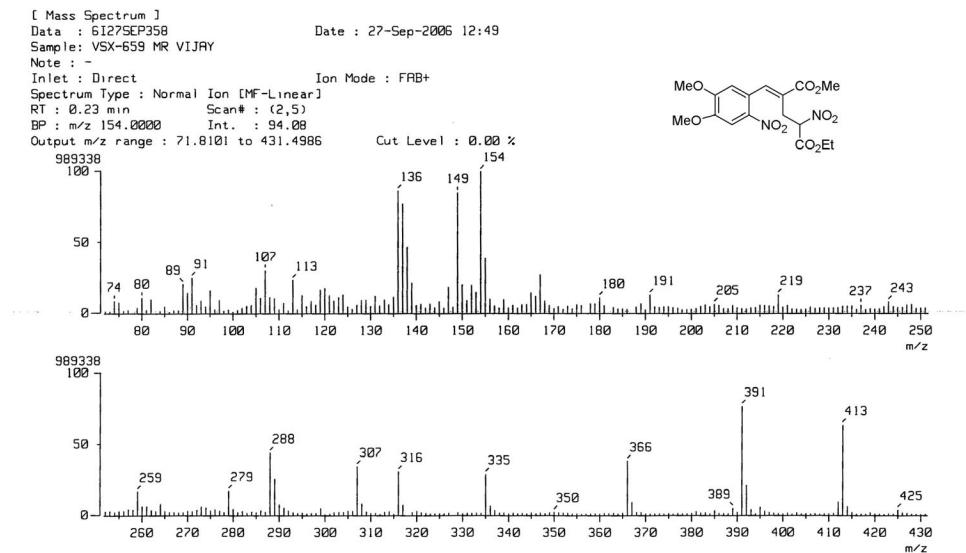


Fig.-6: Mass spectrum of compound 7d

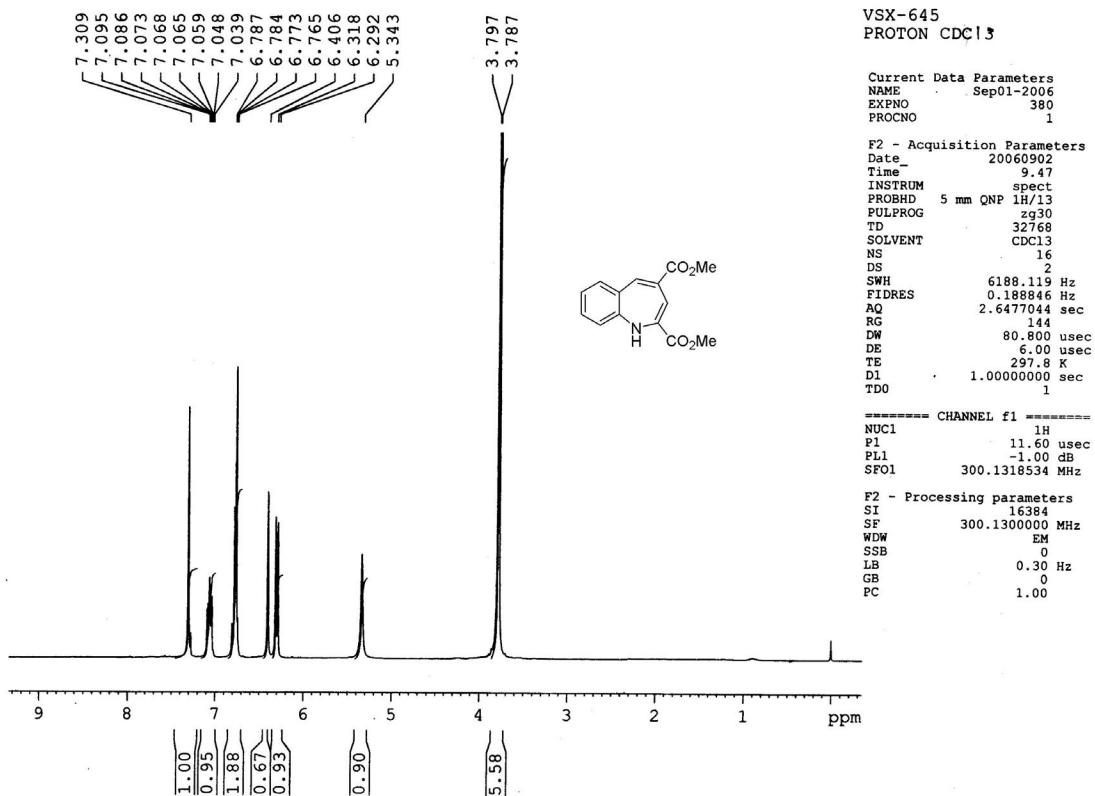


Fig.-16: ¹H NMR spectrum of compound 10a

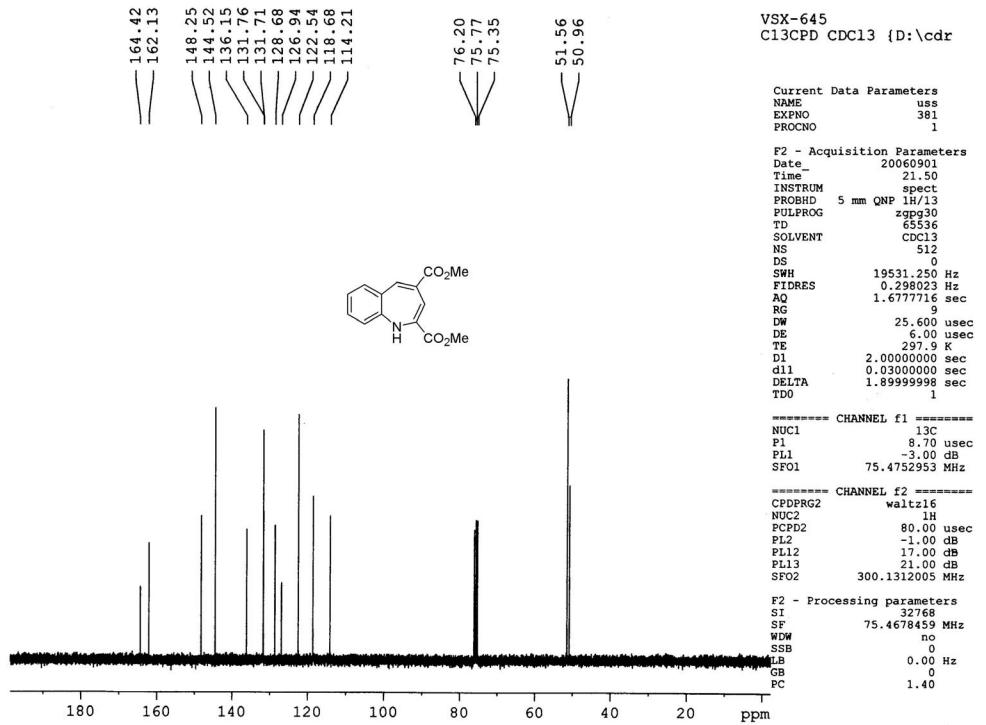


Fig.-17: ¹³C NMR spectrum of compound 10a

SAIF, CDRI LUCKNOW

Original Data Path: 6110JUL24707100246_120446.RAW
 Current Data Path: C:\Sample Analysis\JULY06\
 Sample ID: VSX-645 VIJAY
 Acquisition Date: 7/10/2006 1:22:32 PM
 Vial: A31
 T: + c ESI Full ms [50.00-500.00]

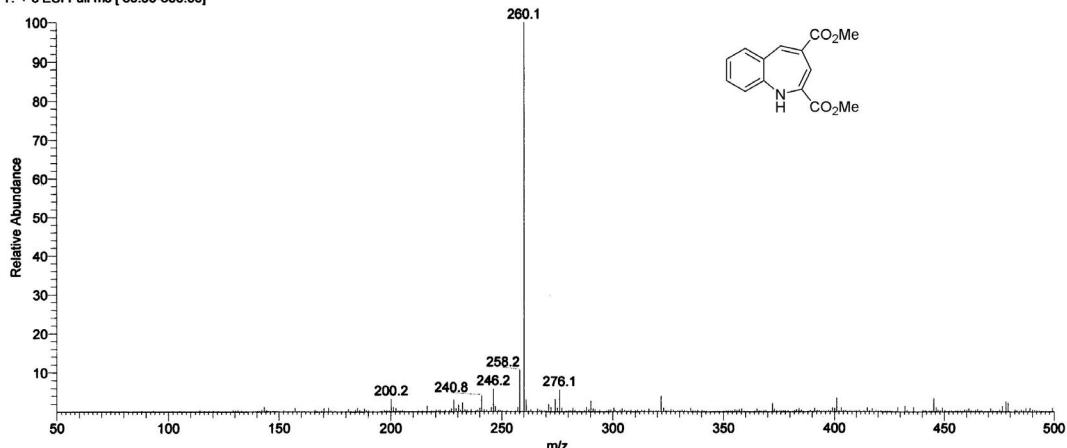


Fig.-18: Mass spectrum of compound 10a

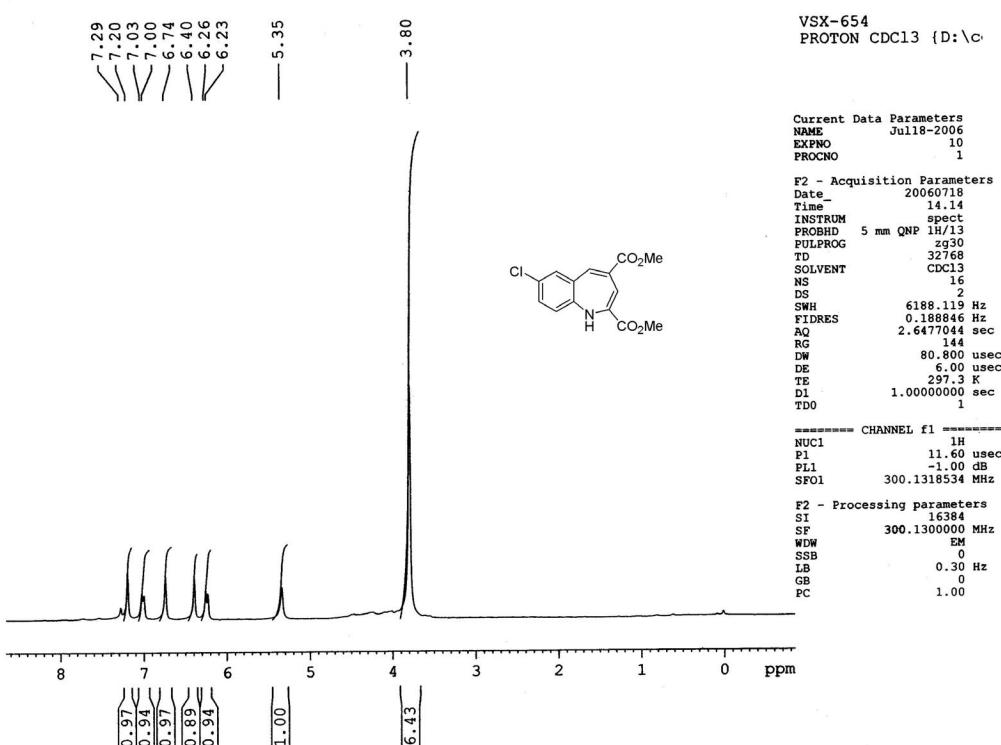


Fig.-19: ^1H NMR spectrum of compound 10b

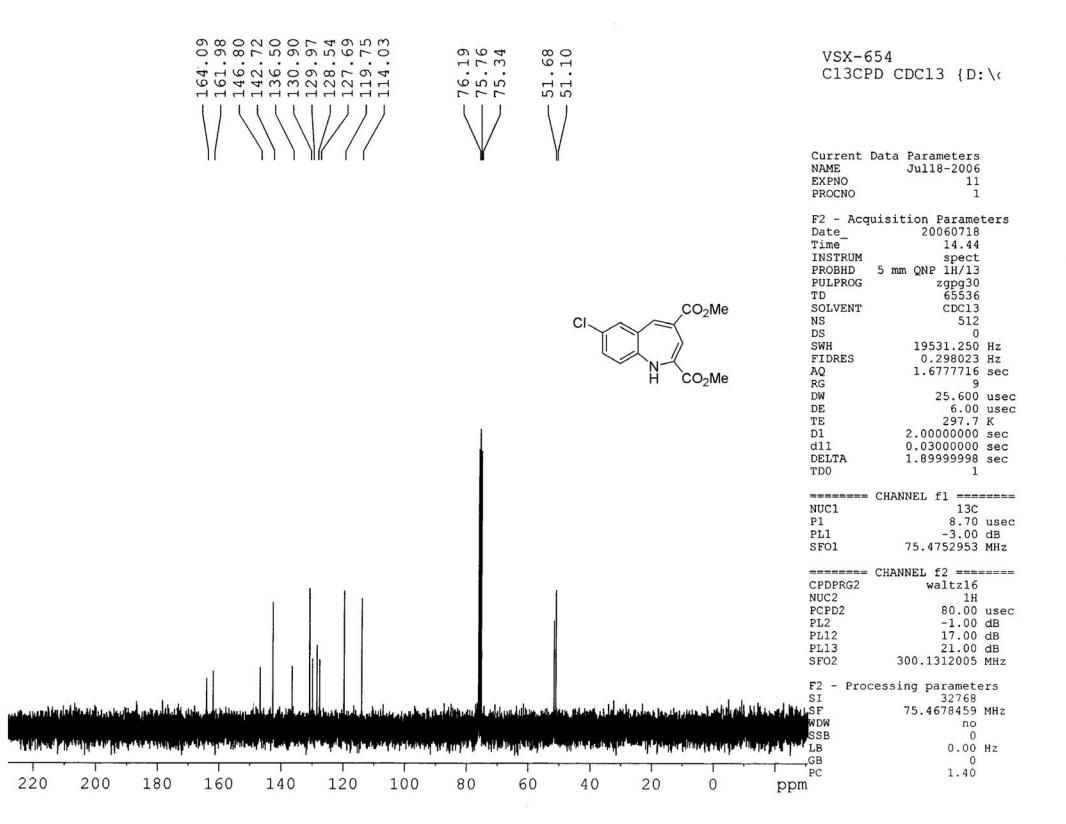


Fig.-20: ¹³C NMR spectrum of compound 10b

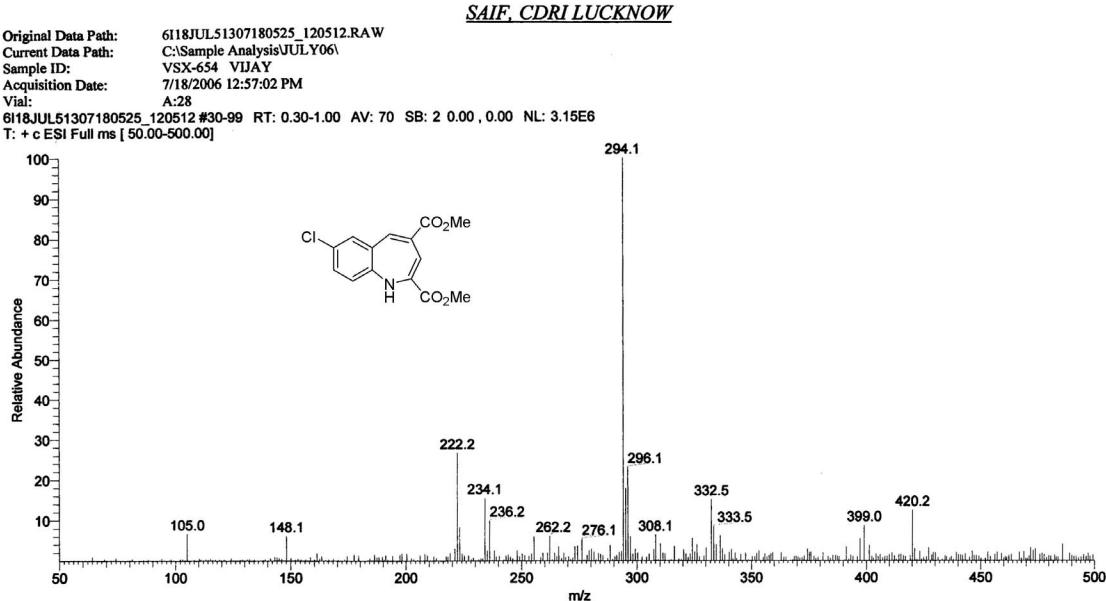


Fig.-21: Mass spectrum of compound 10b

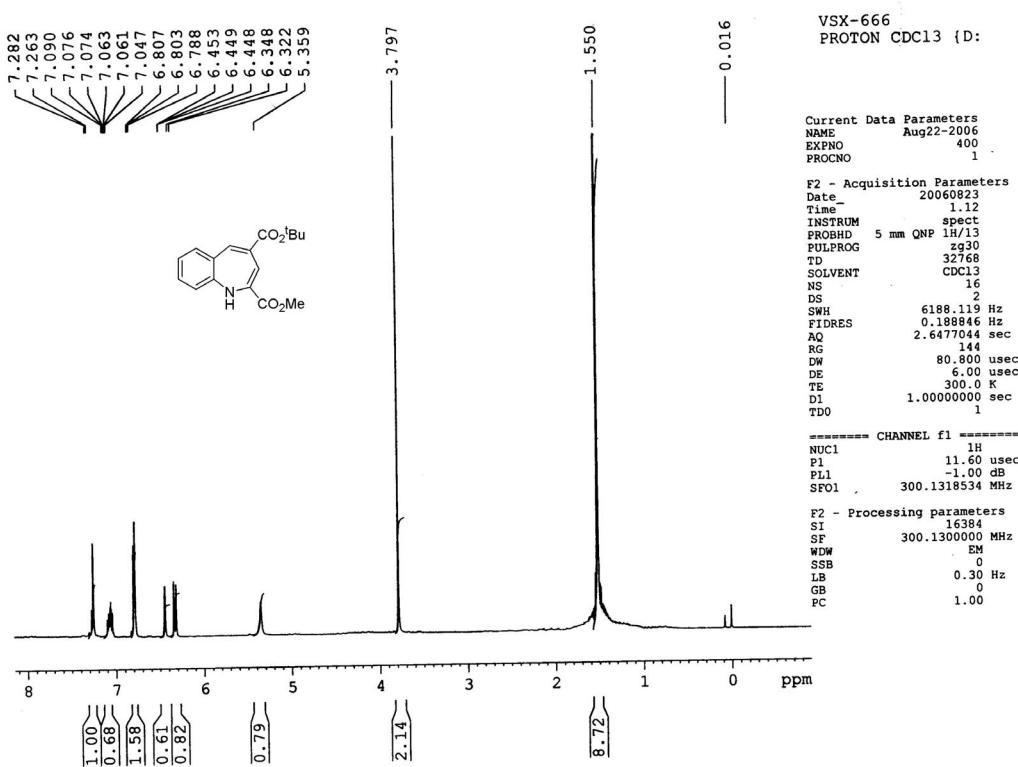


Fig.-25: ¹H NMR spectrum of compound 12a

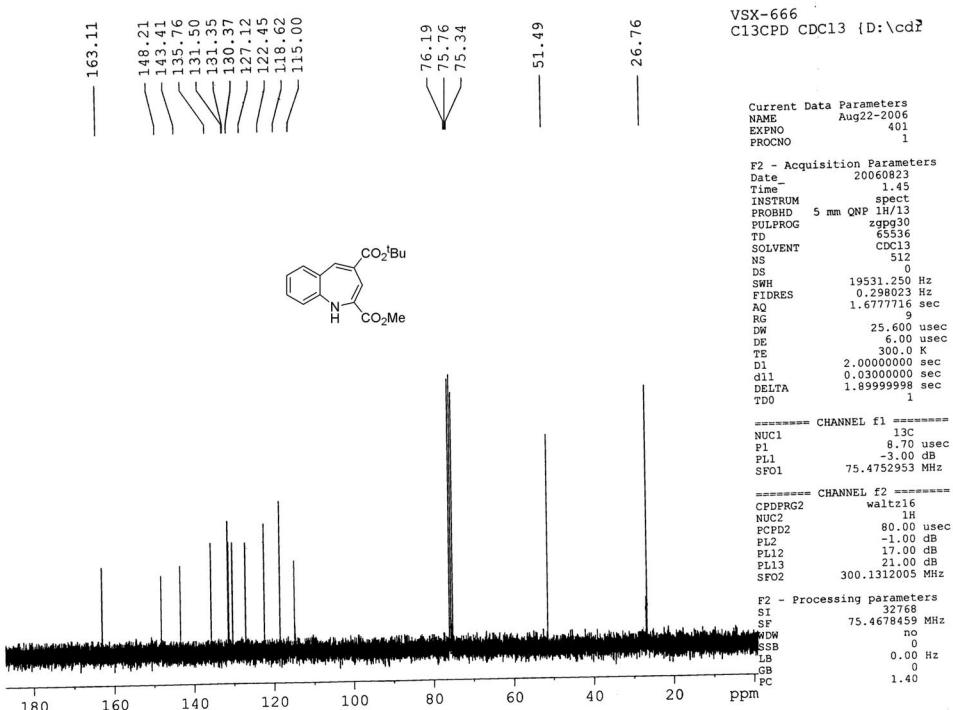


Fig.-26: ¹³C NMR spectrum of compound 12a

SAIF, CDRI LUCKNOW

Original Data Path: 6127JUL82507270830_122314.RAW
 Current Data Path: C:\Sample Analysis\JULY06
 Sample ID: VSX-662 VIJAY
 Acquisition Date: 7/27/2006 1:20:30 PM
 Vial: A:25
 6127JUL82507270830_122314 #28-97 RT: 0.30-1.00 AV: 70 SB: 2 0.00 , 0.00 NL: 3.60E7
 T: + c ESI Full ms [50.00-500.00]

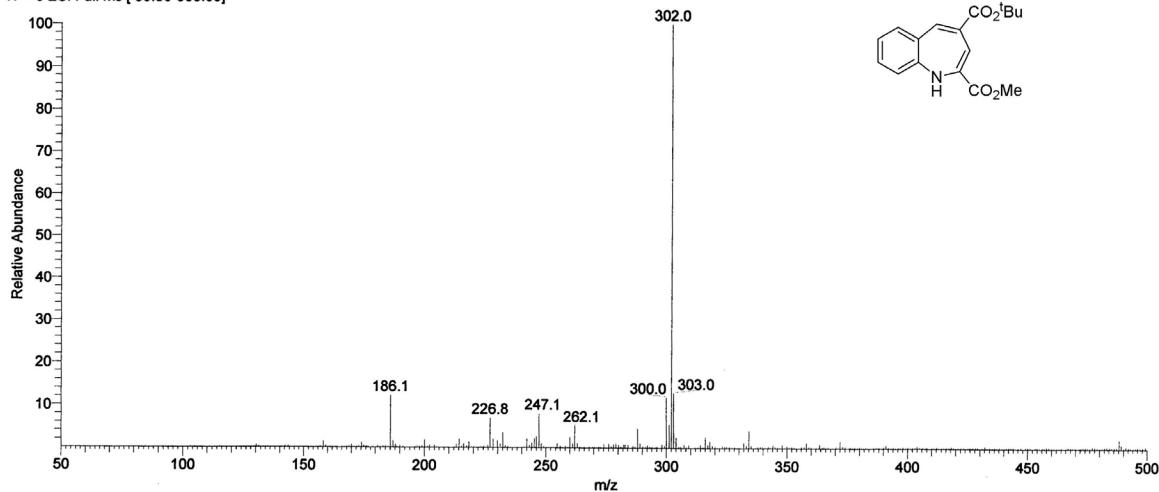


Fig.-27: Mass spectrum of compound 12a

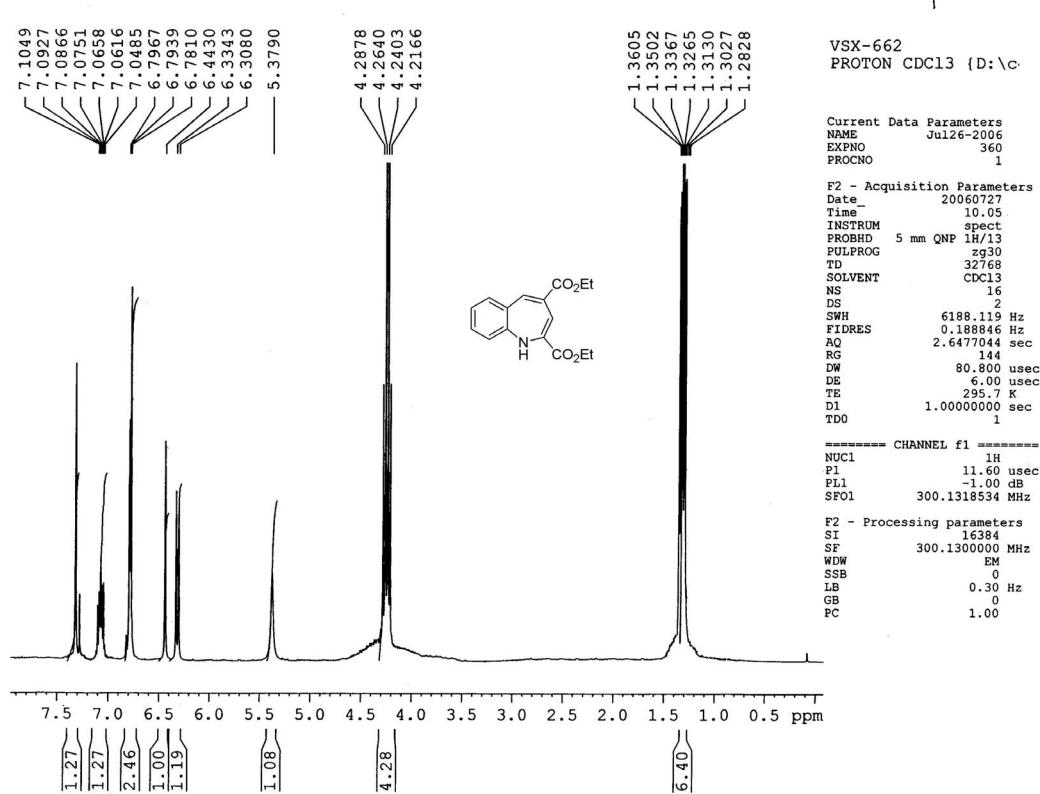


Fig.-22: ^1H NMR spectrum of compound 13a

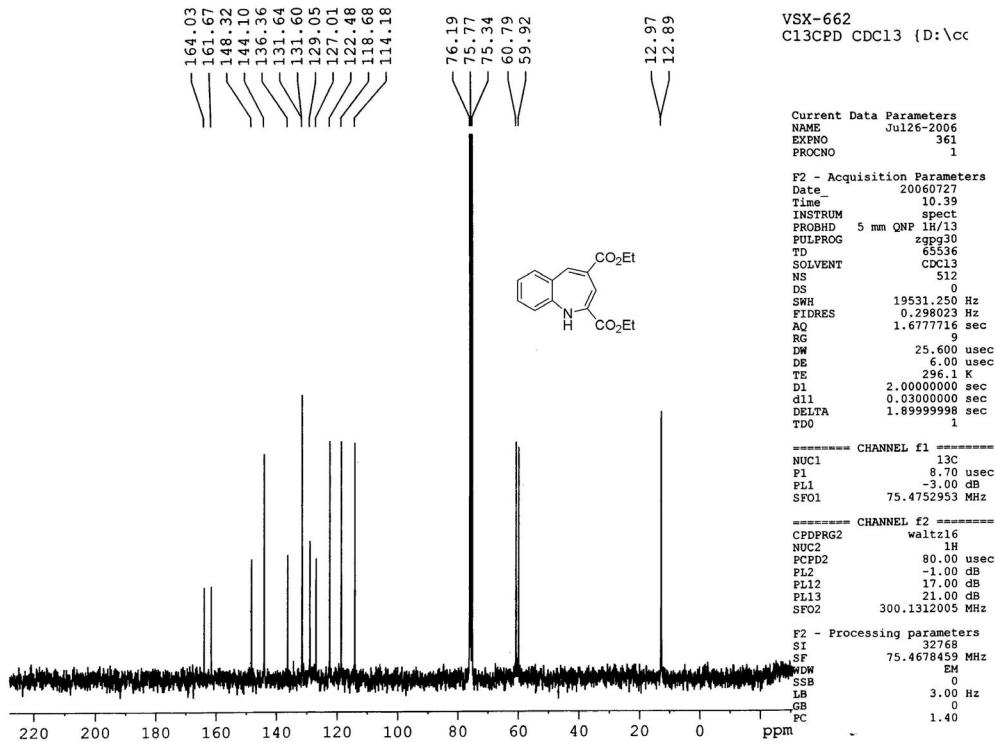


Fig.-23: ^{13}C NMR spectrum of compound 13a

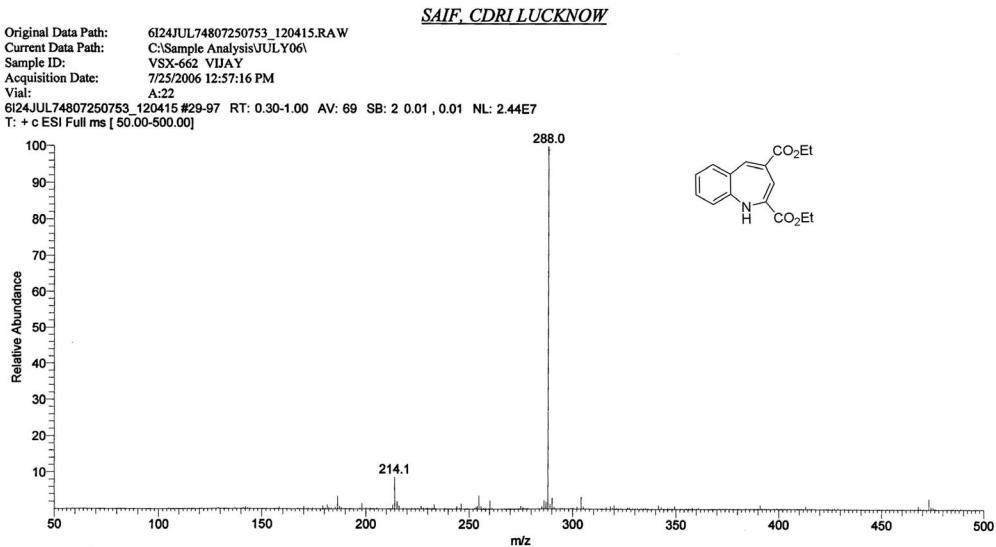


Fig.-24: Mass spectrum of compound 13a

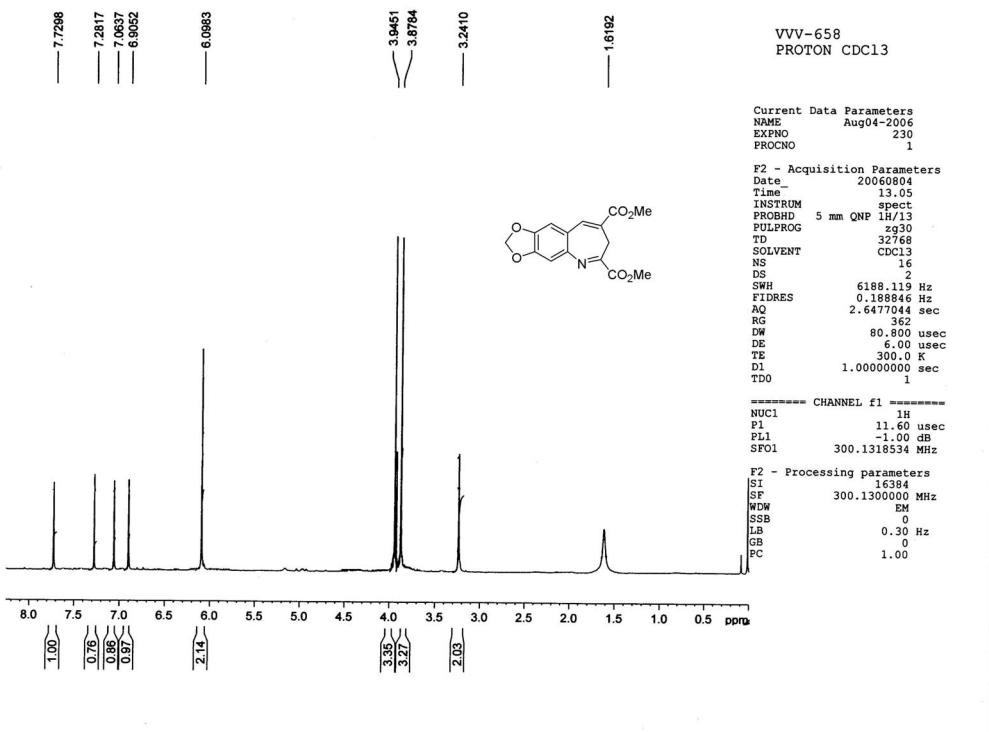


Fig.-28: ^1H NMR spectrum of compound 14c

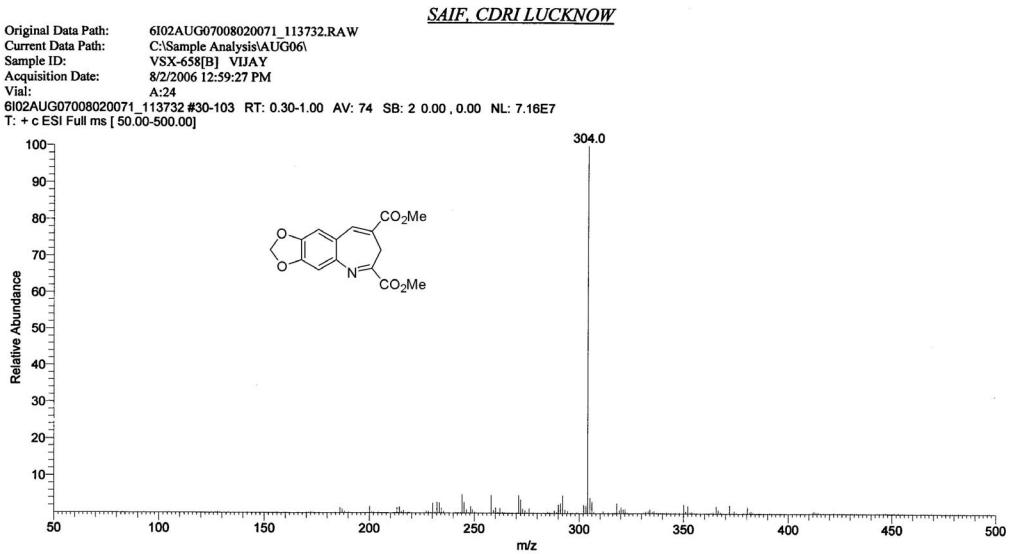


Fig.-29: Mass spectrum of compound 14c

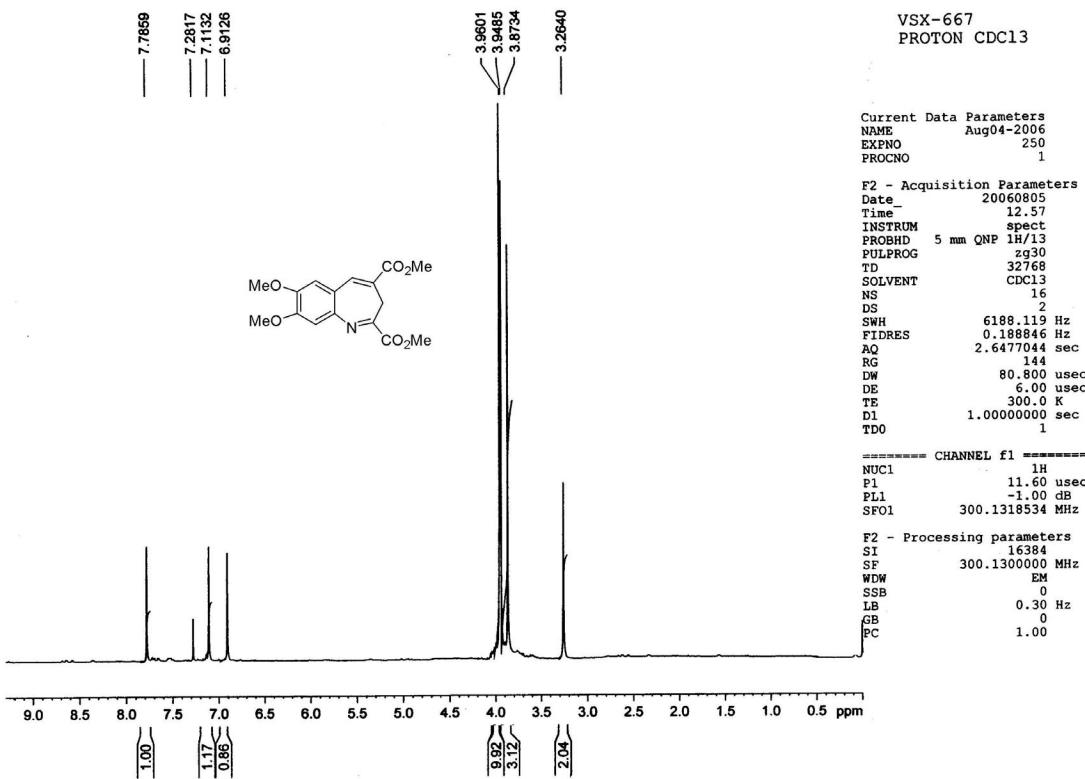


Fig.-30: ^1H NMR spectrum of compound 14d

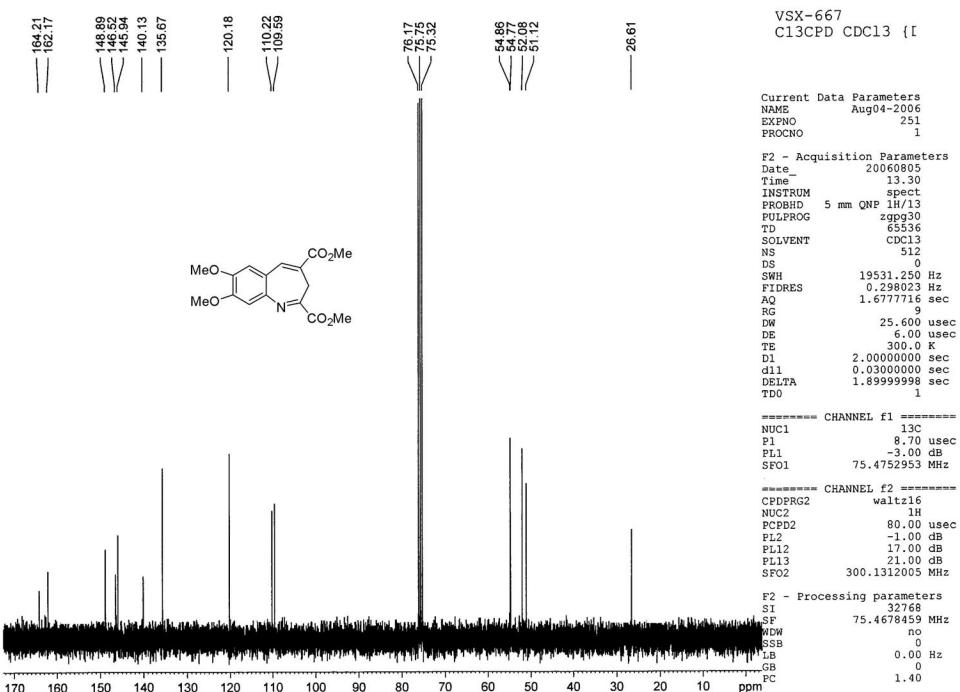


Fig.-31: ^{13}C NMR spectrum of compound 14d

SAIF, CDRI LUCKNOW

Original Data Path: 6101AUG02108010021_112134.RAW
 Current Data Path: C:\Sample Analysis\AUG06\
 Sample ID: VSX-667 VIJAY
 Acquisition Date: 8/1/2006 12:25:09 PM
 Vial: A:20
 T: + c ESI Full ms [50.00-500.00]

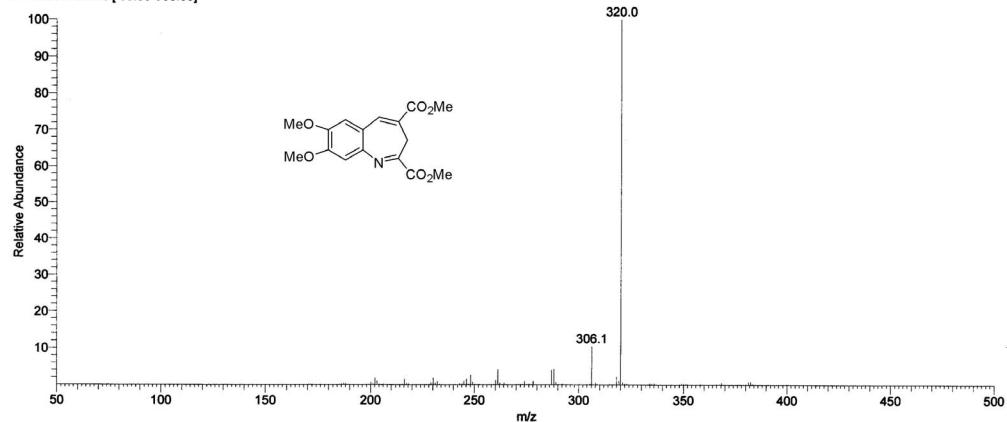


Fig.-32: Mass spectrum of compound 14d

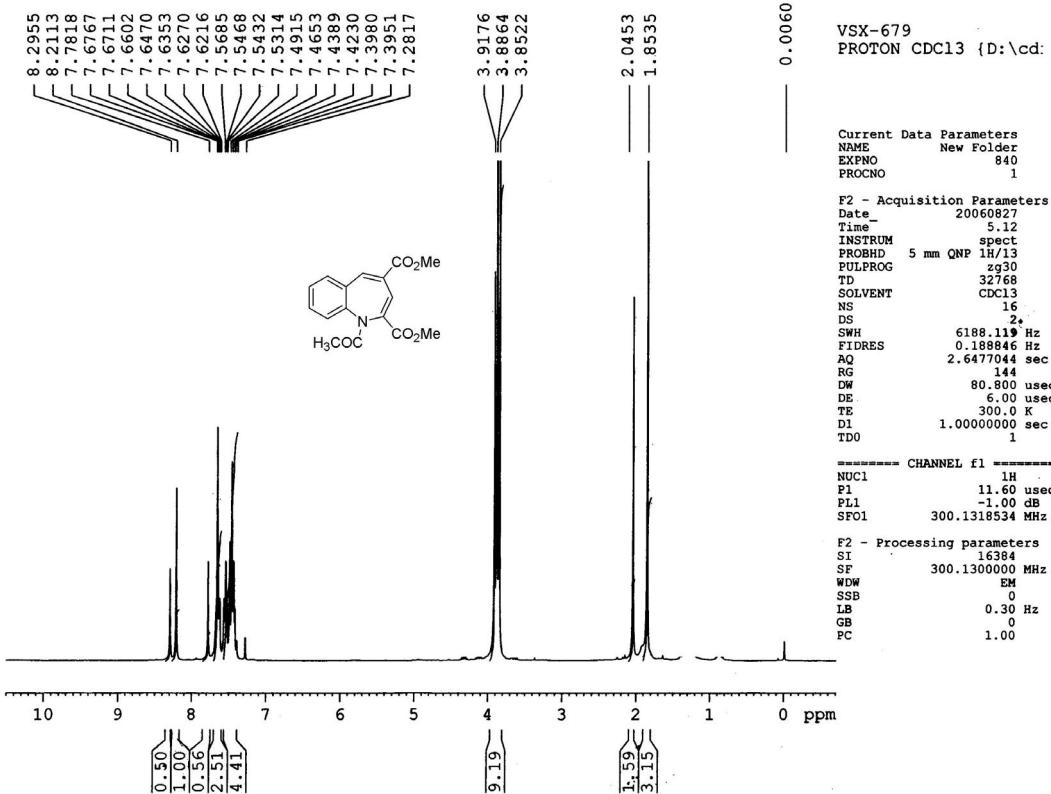


Fig.-41: ¹H NMR spectrum of compound 15

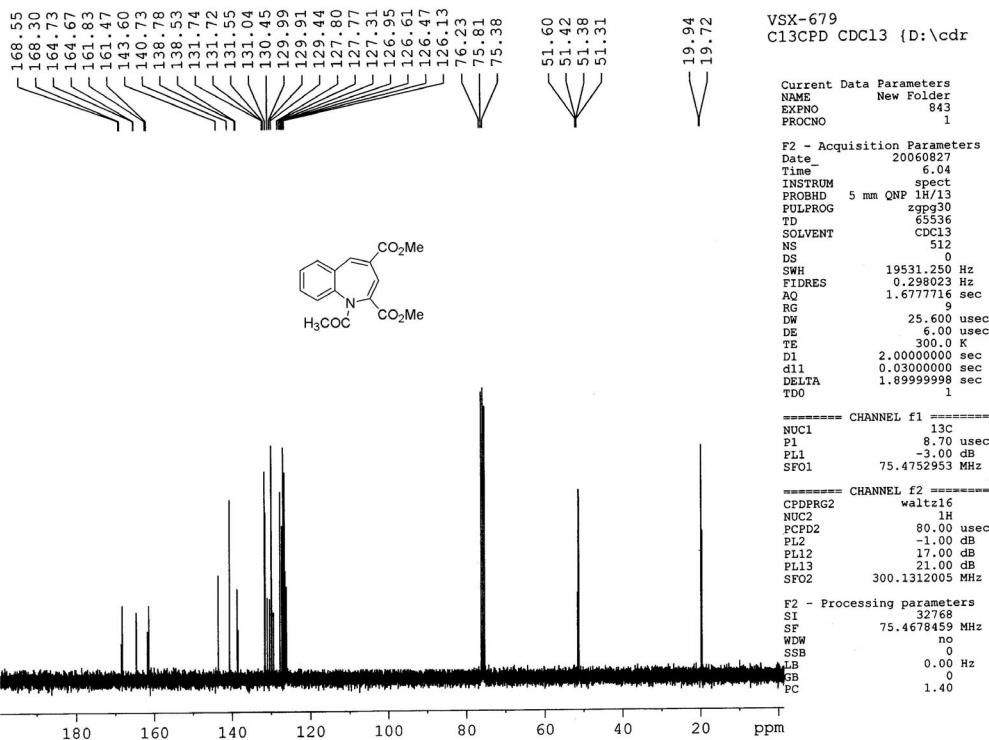


Fig.-42: ^{13}C NMR spectrum of compound 15

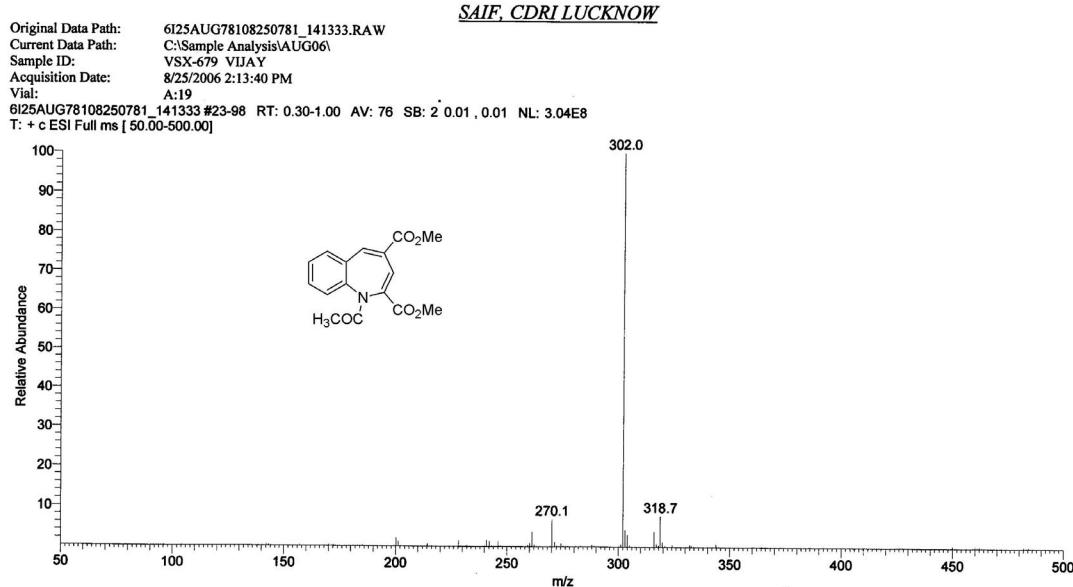


Fig.-43: Mass spectrum of compound 15

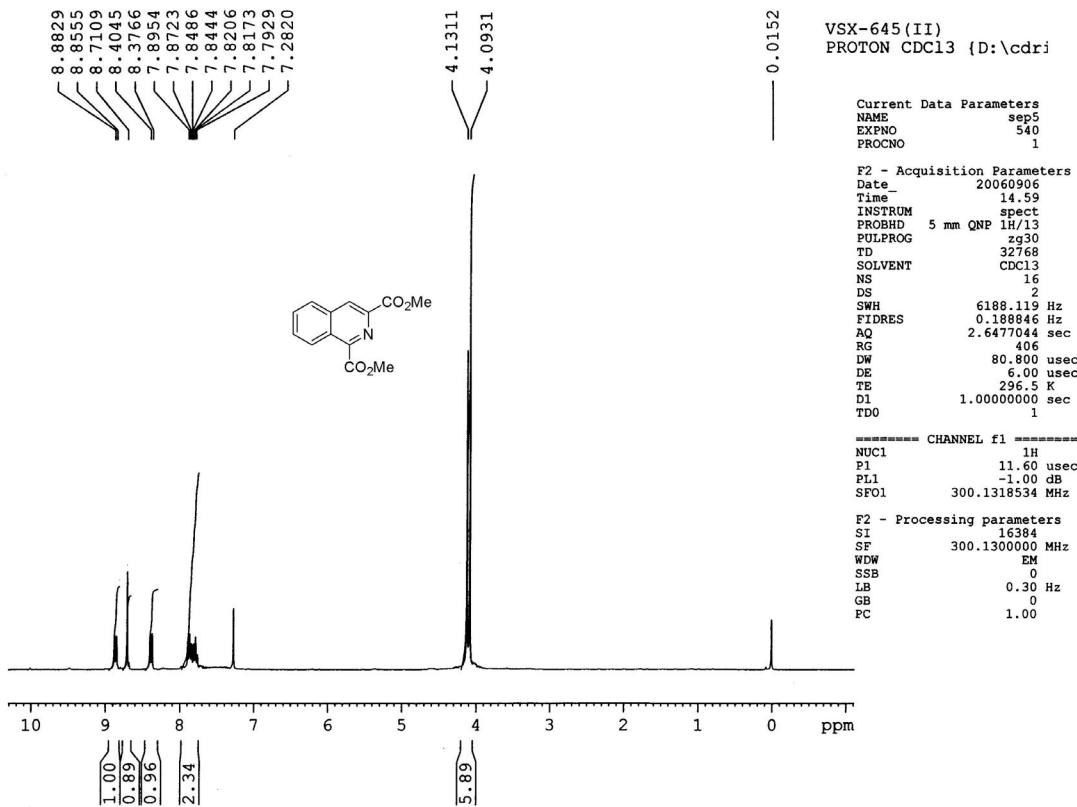


Fig.-44: ¹H NMR spectrum of compound 17a

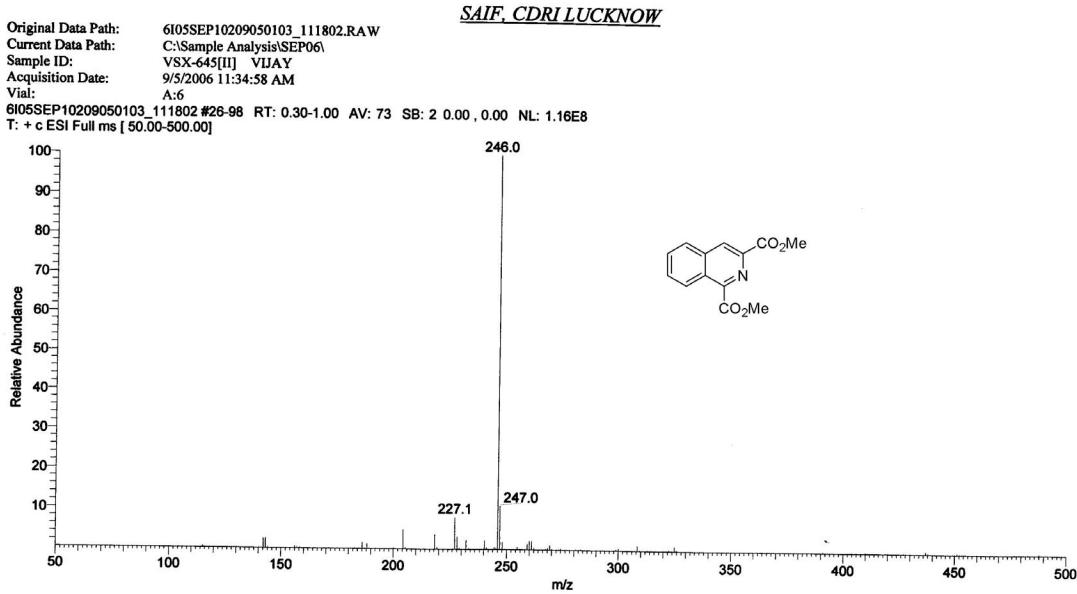


Fig.-45: Mass spectrum of compound 17a

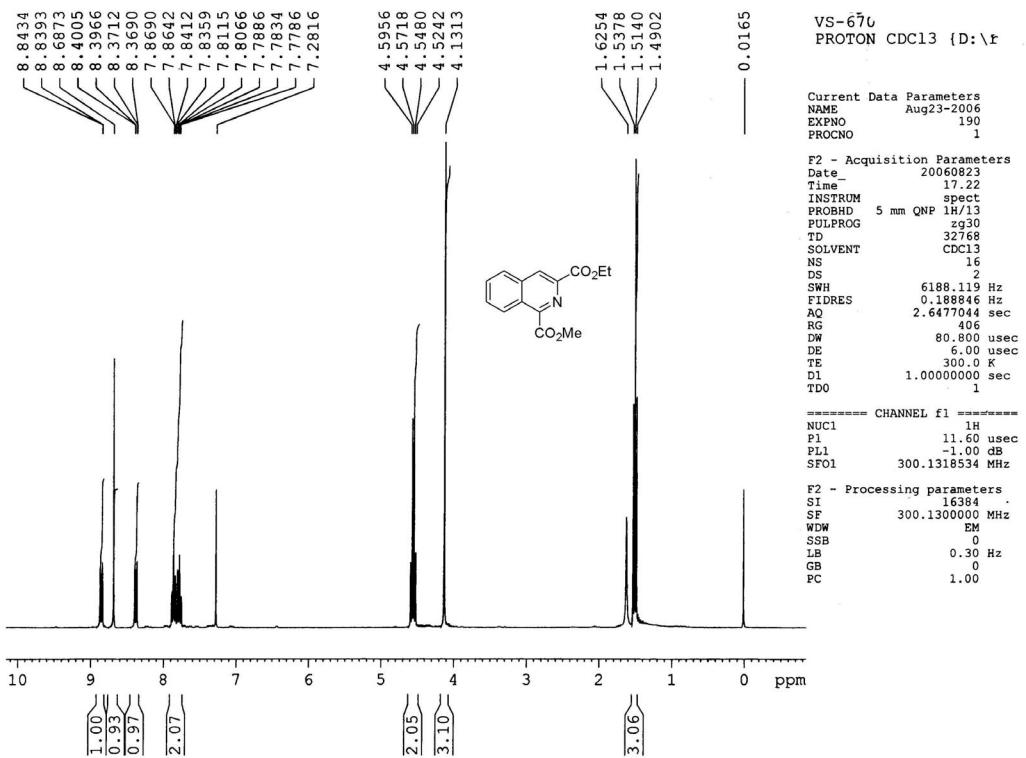


Fig.-46: ¹H NMR spectrum of compound 18a

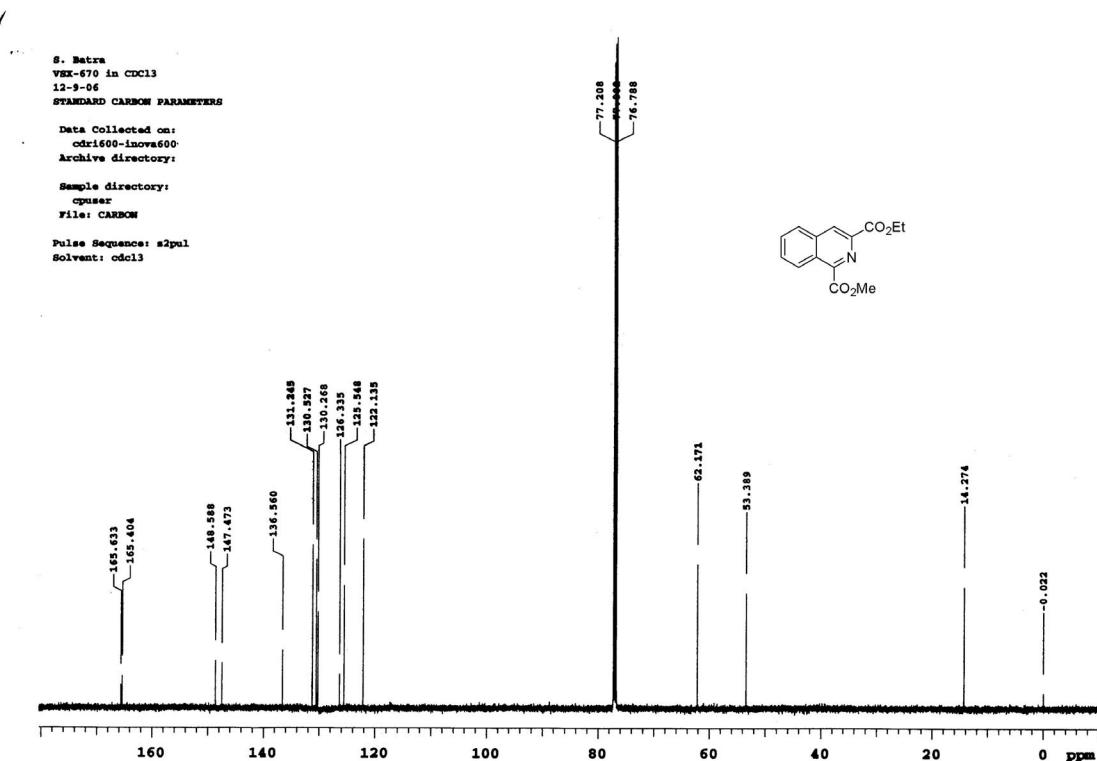


Fig.-47: ¹³C NMR spectrum of compound 18a

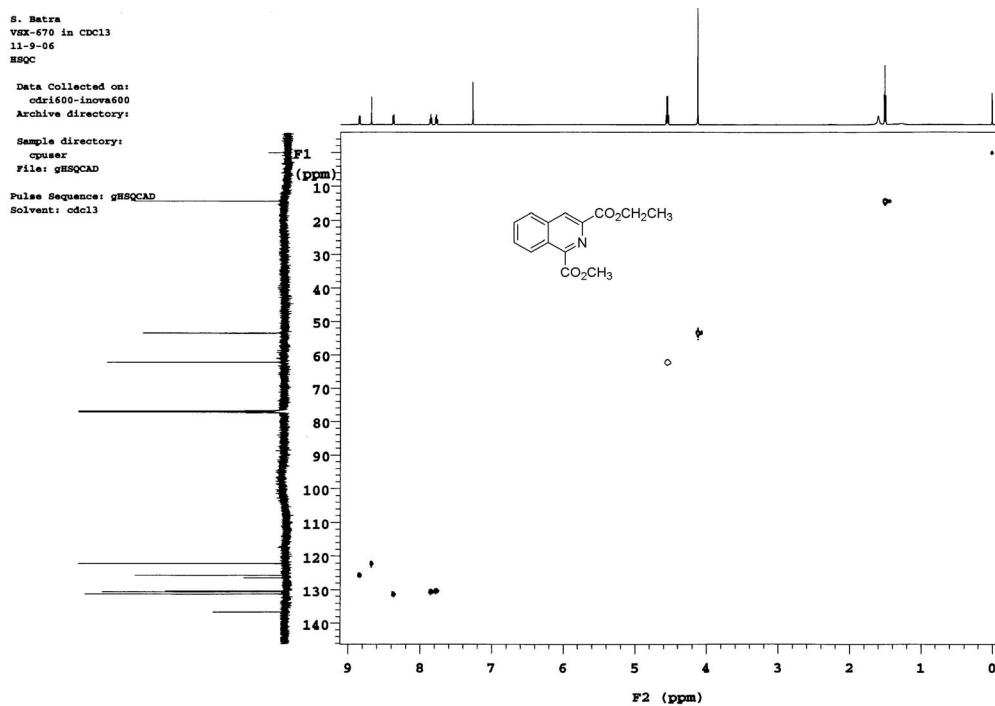


Fig.-48: HSQC spectrum of compound 18a

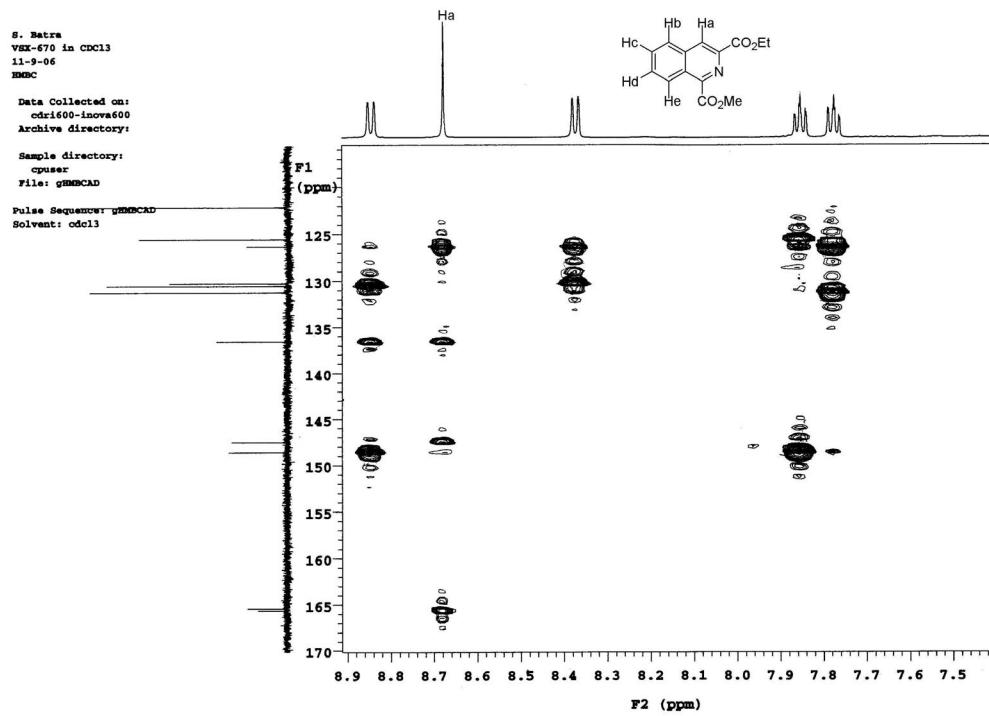


Fig.-49: HMBC spectrum (expanded) of compound 18a

SAIF, CDRI LUCKNOW

Original Data Path: 6125AUG78308250783_141435.RAW
 Current Data Path: C:\Sample Analysis\AUG06\
 Sample ID: SBSN-670 SOMNATH NAG
 Acquisition Date: 8/25/2006 2:20:27 PM
 Vial: A:21
 6125AUG78308250783_141435 #28-100 RT: 0.30-1.00 AV: 73 SB: 2 0.01 , 0.01 NL: 1.60E8
 T: + c ESI Full ms [50.00-500.00]

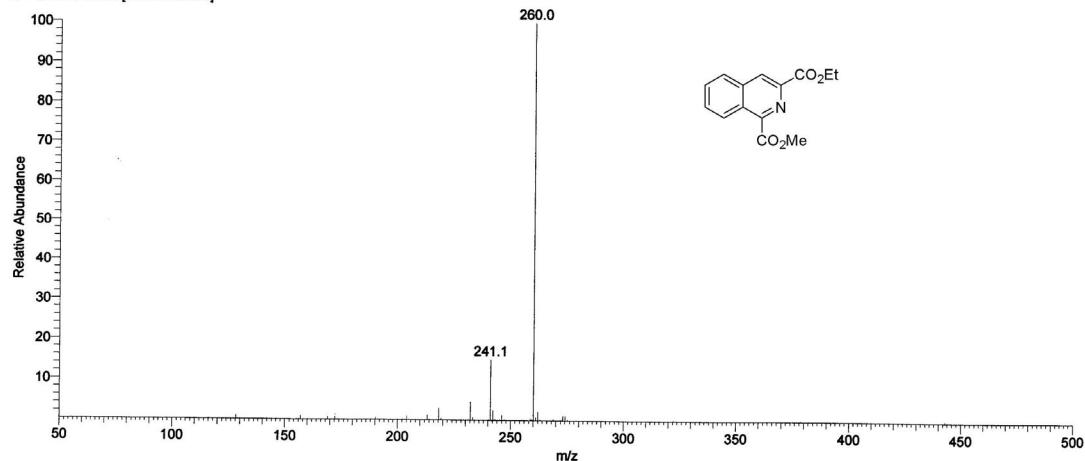


Fig.-50: Mass spectrum of compound 18a

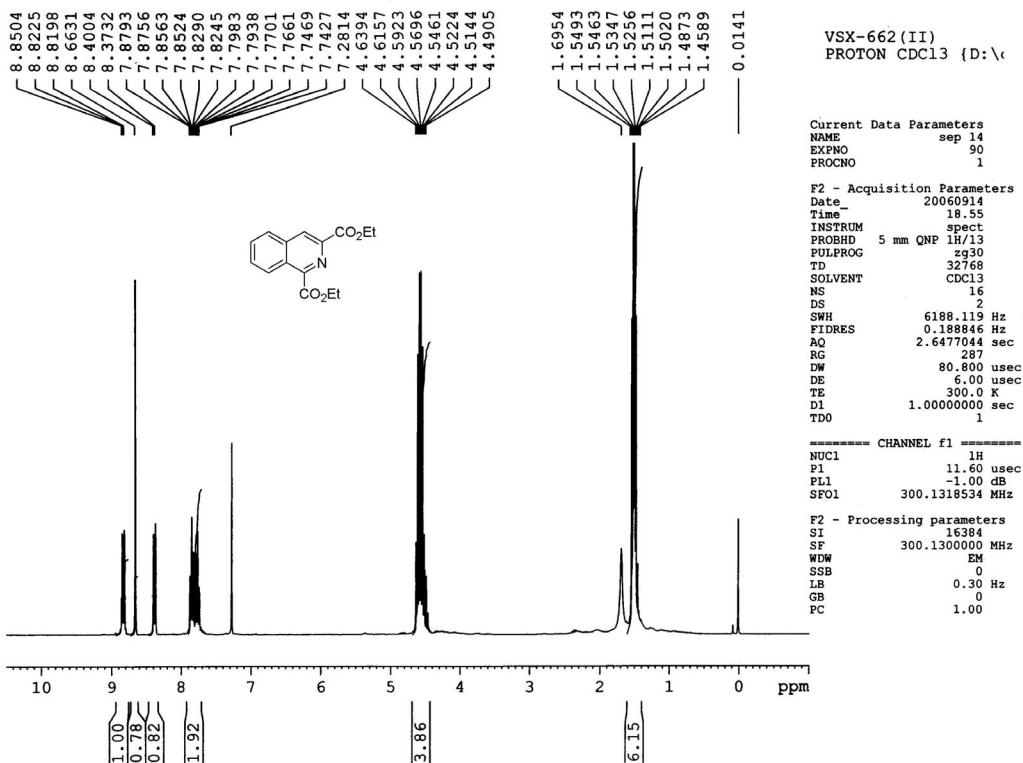


Fig.-51: ^1H NMR spectrum of compound 19a.

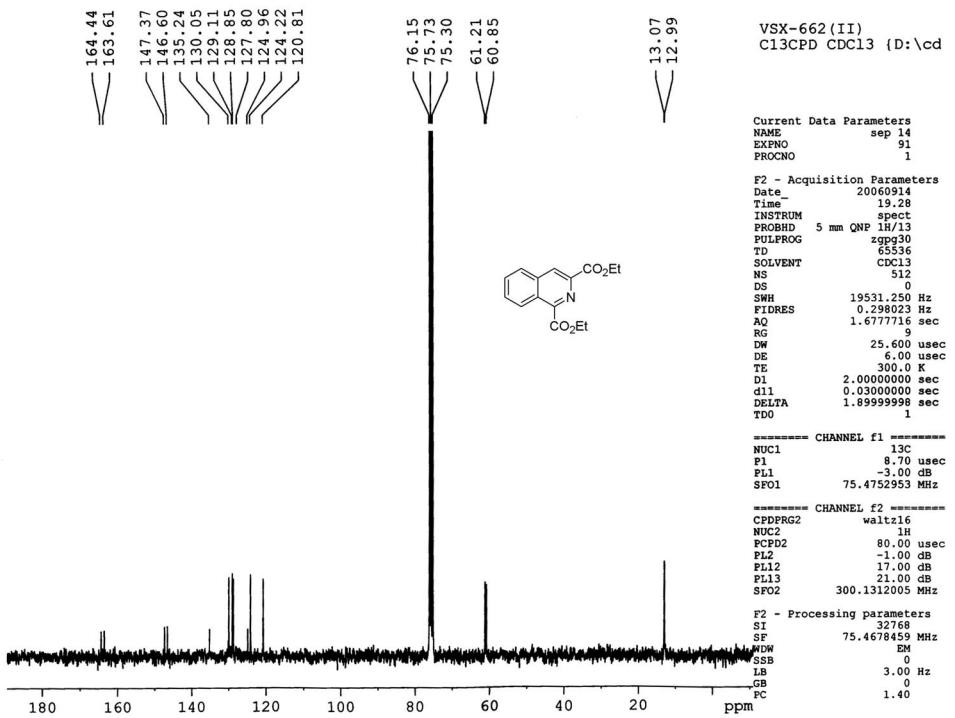


Fig.-52: ¹³C NMR spectrum of compound 19a

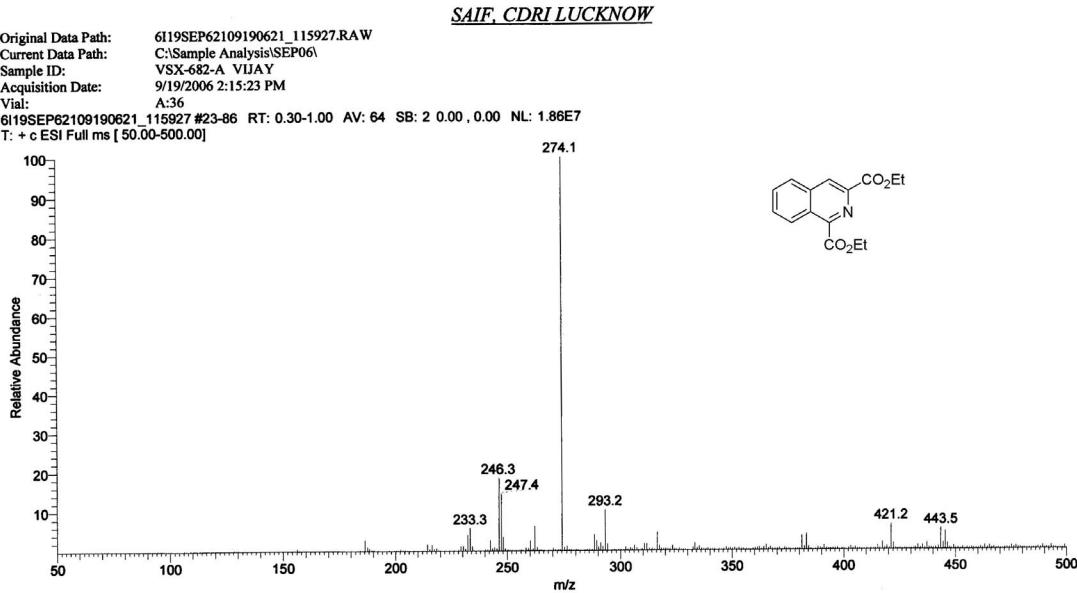


Fig.-53: Mass spectrum of compound 19a

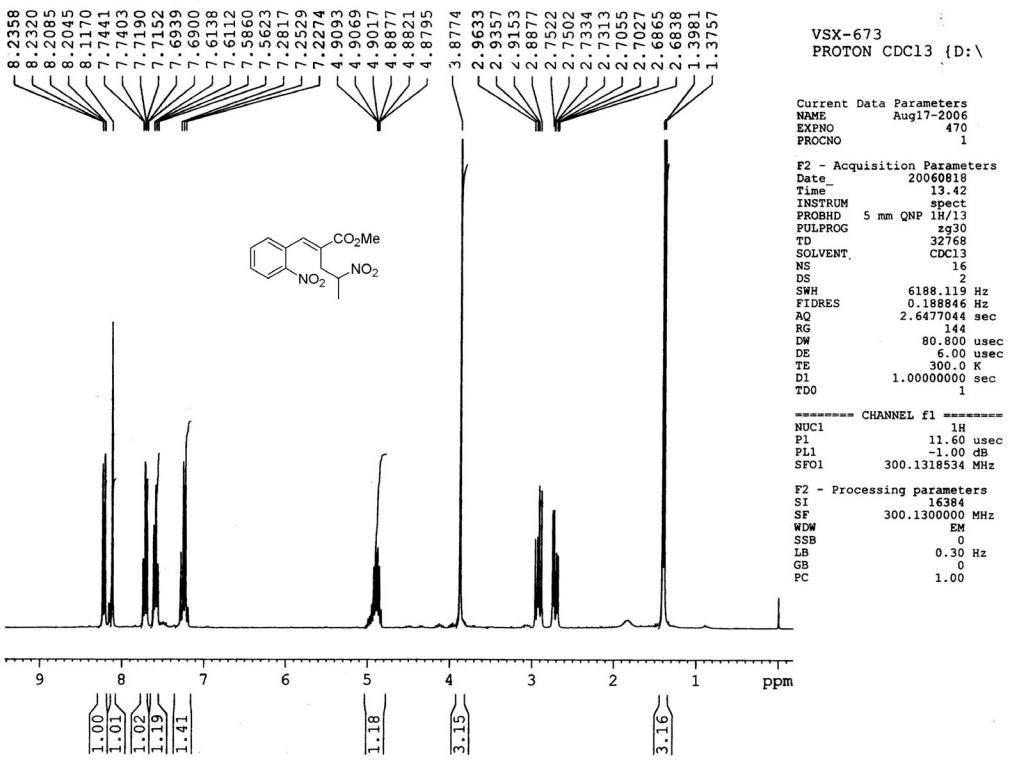


Fig.-7: ^1H NMR spectrum of compound 21a

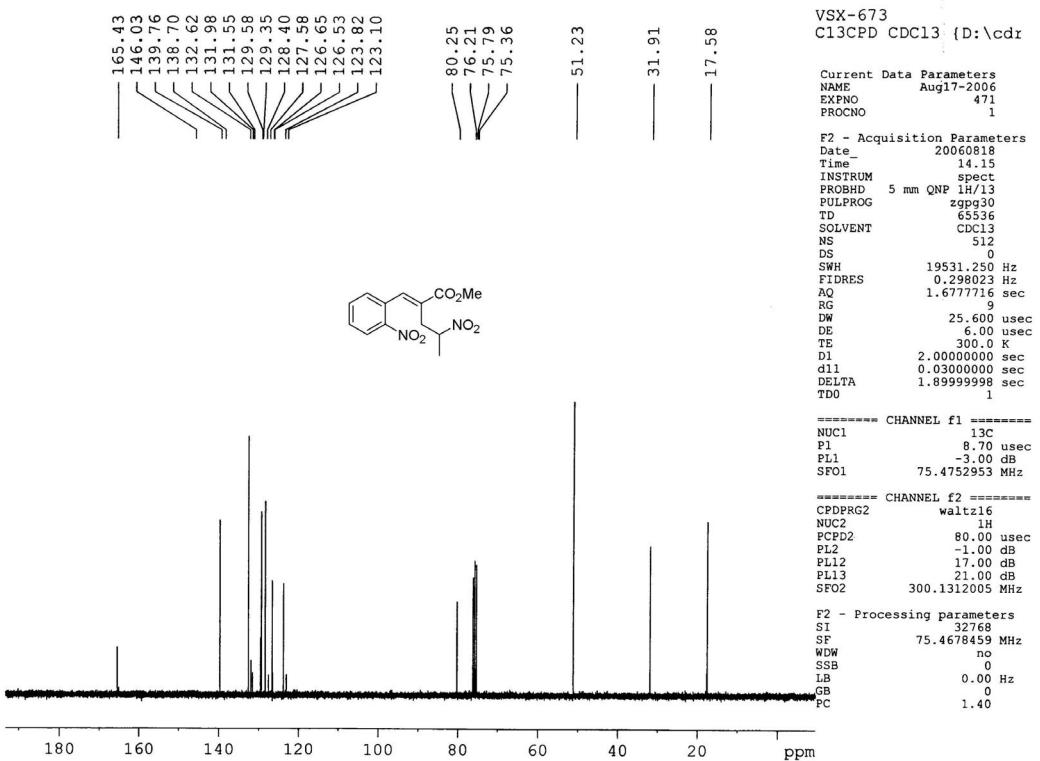


Fig.-8: ^1H NMR spectrum of compound 21a

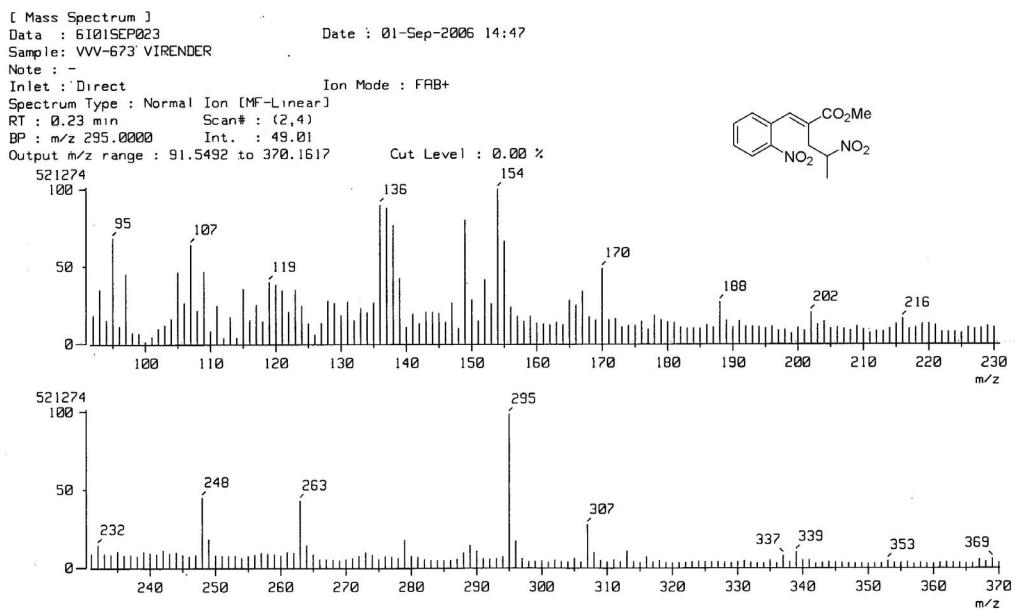


Fig.-9: Mass spectrum of compound 21a

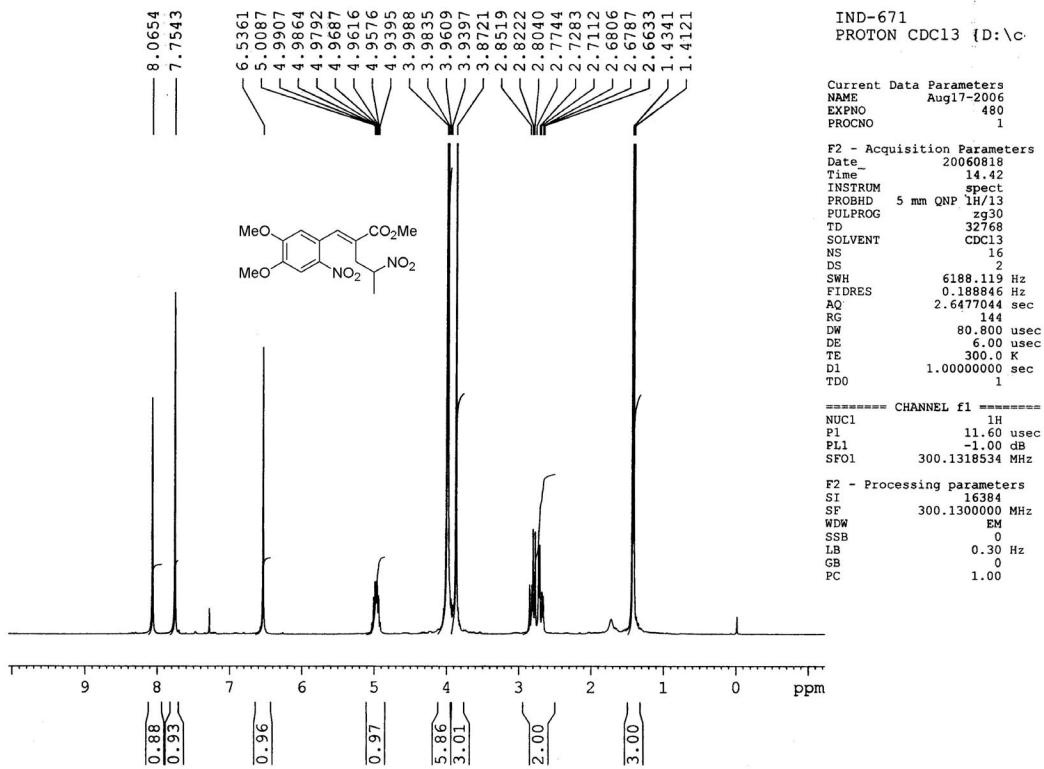


Fig.-10: ¹H NMR spectrum of compound 21d

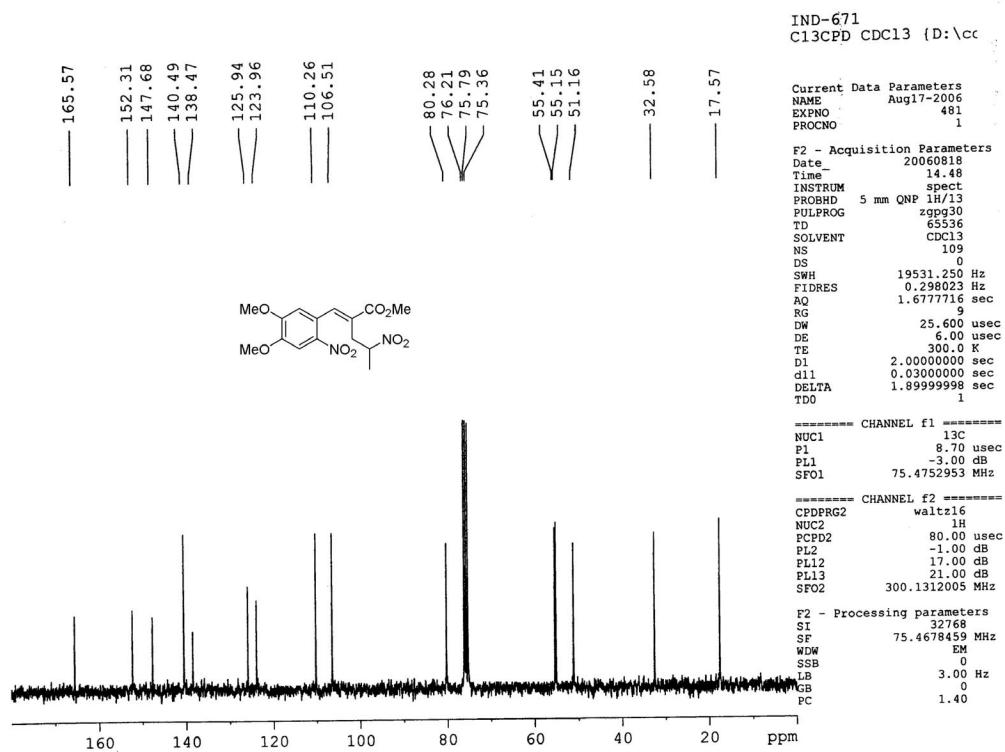


Fig.-11: ^{13}C NMR spectrum of compound 21d

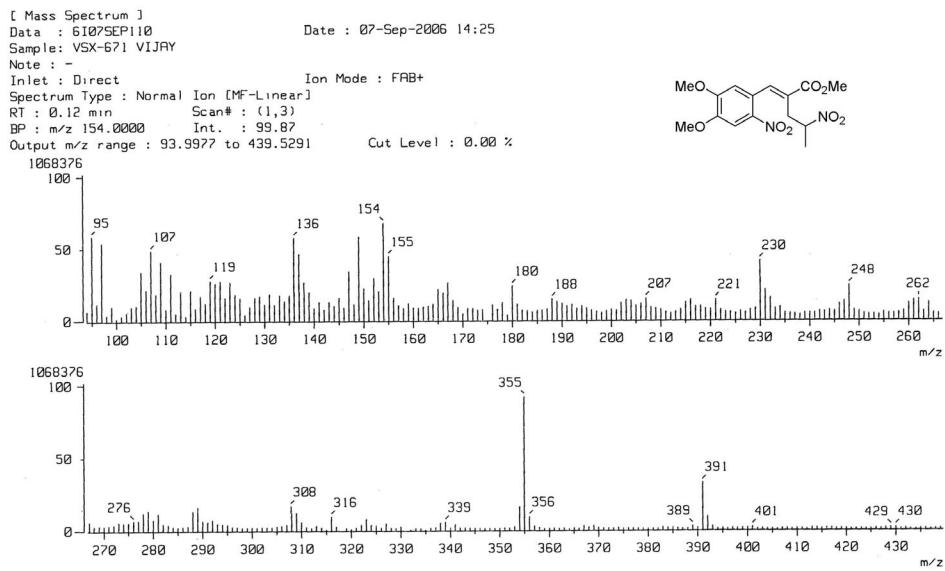


Fig.-12: Mass spectrum of compound 21d

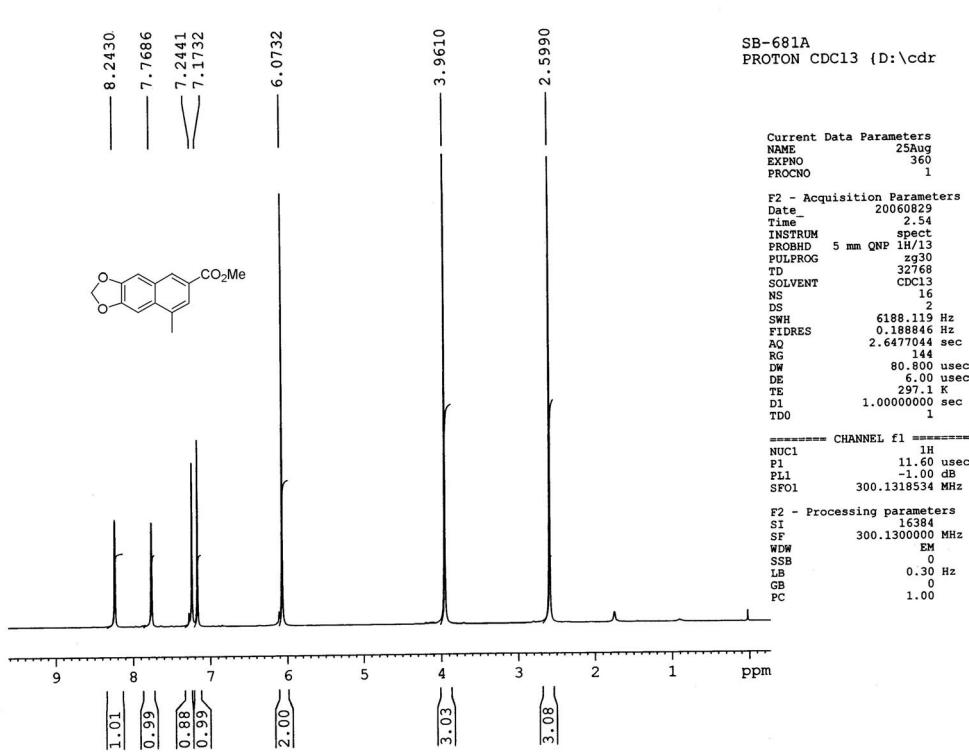


Fig.-13: ¹H NMR spectrum of compound 23c

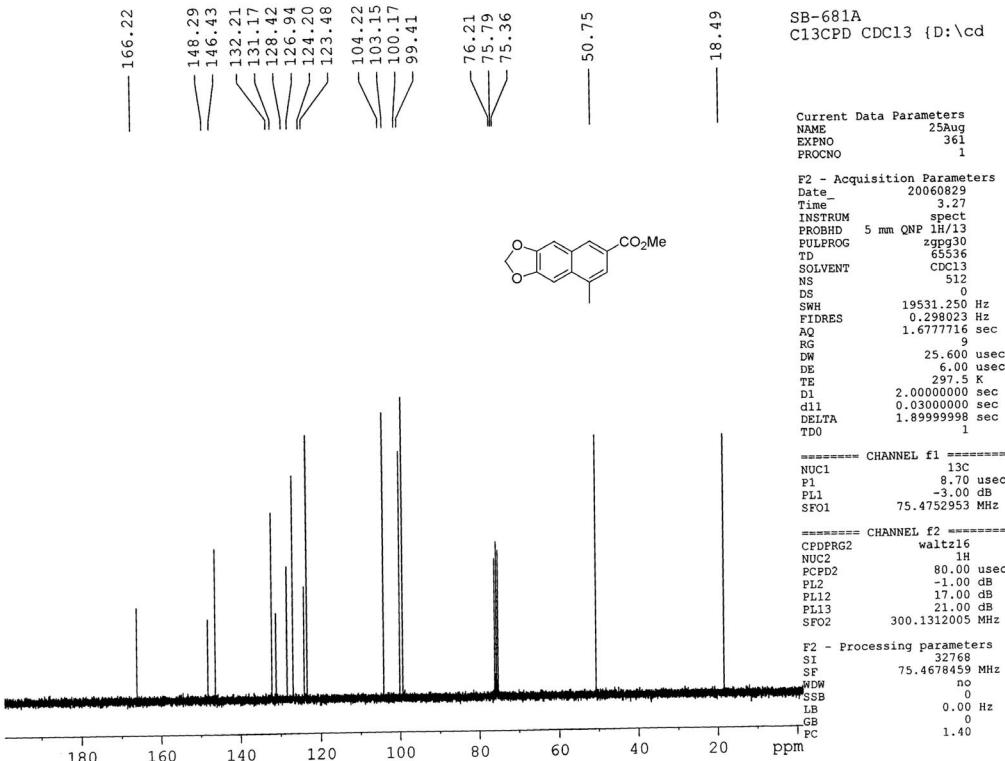


Fig.-14: ¹³C NMR spectrum of compound 23c

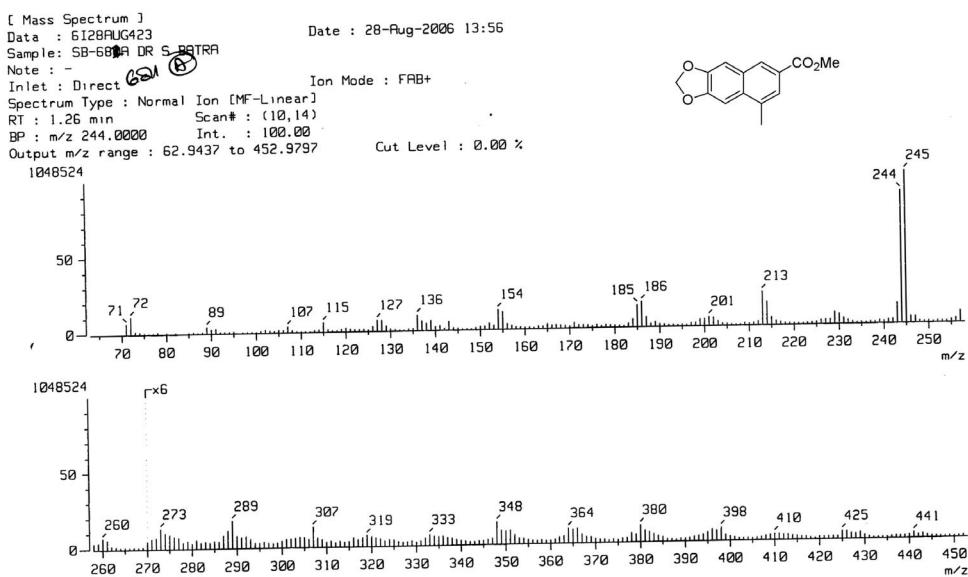


Fig.-15: Mass spectrum of compound 23c

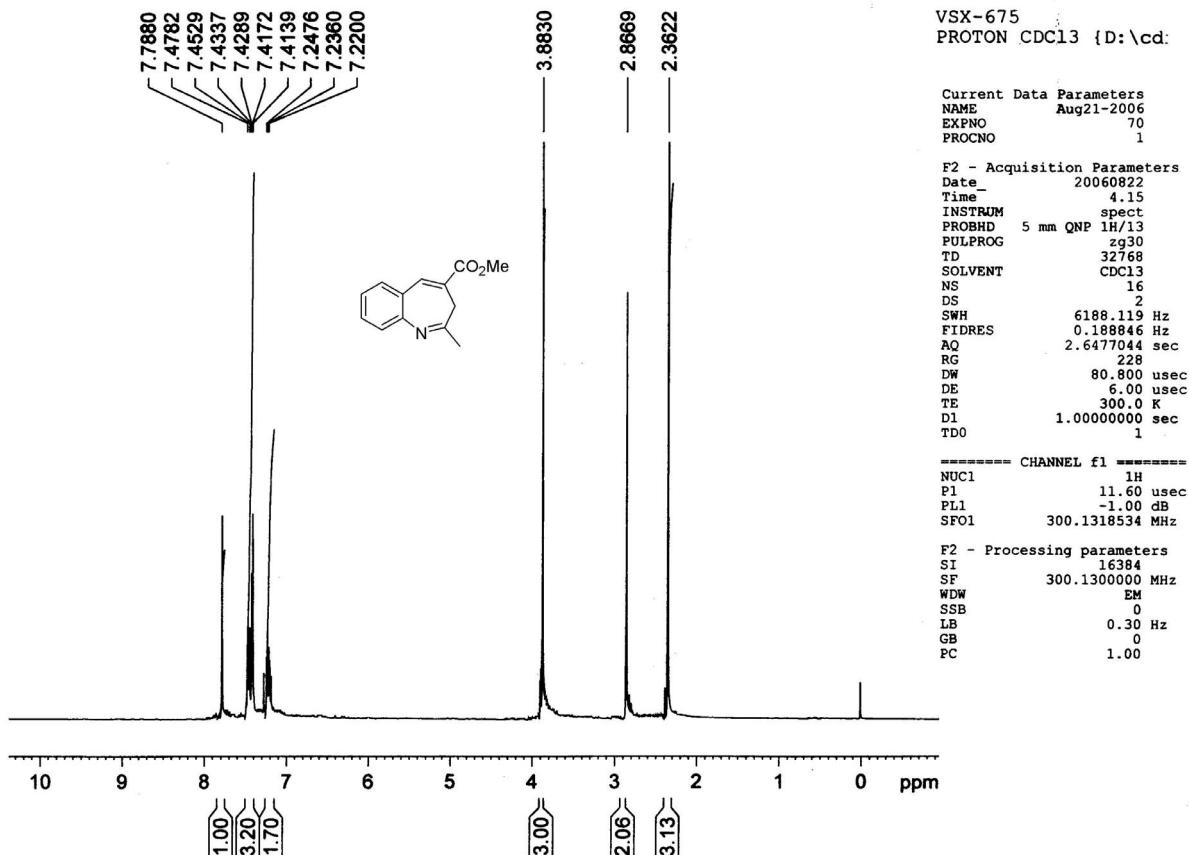


Fig.-33: ¹H NMR spectrum of compound 25a

SAIF, CDRI LUCKNOW

Data Path: G:\24AUG72108240723_120029.RAW
 Data Path: C:\Sample Analysis\AU\G06\
 ID: VSX-675 VIJAY
 ion Date: 8/24/2006 2:43:05 PM
 A:11
 372108240723_120029 #29-101 RT: 0.30-1.00 AV: 73 SB: 2.000, 0.00 NL: 4.21E7
 SI Full ms [50.00-500.00]

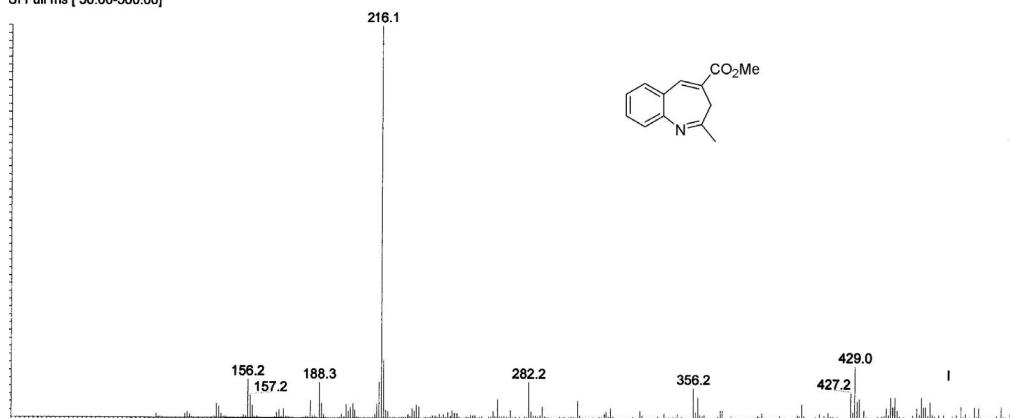


Fig.-34: Mass spectrum of compound 25a

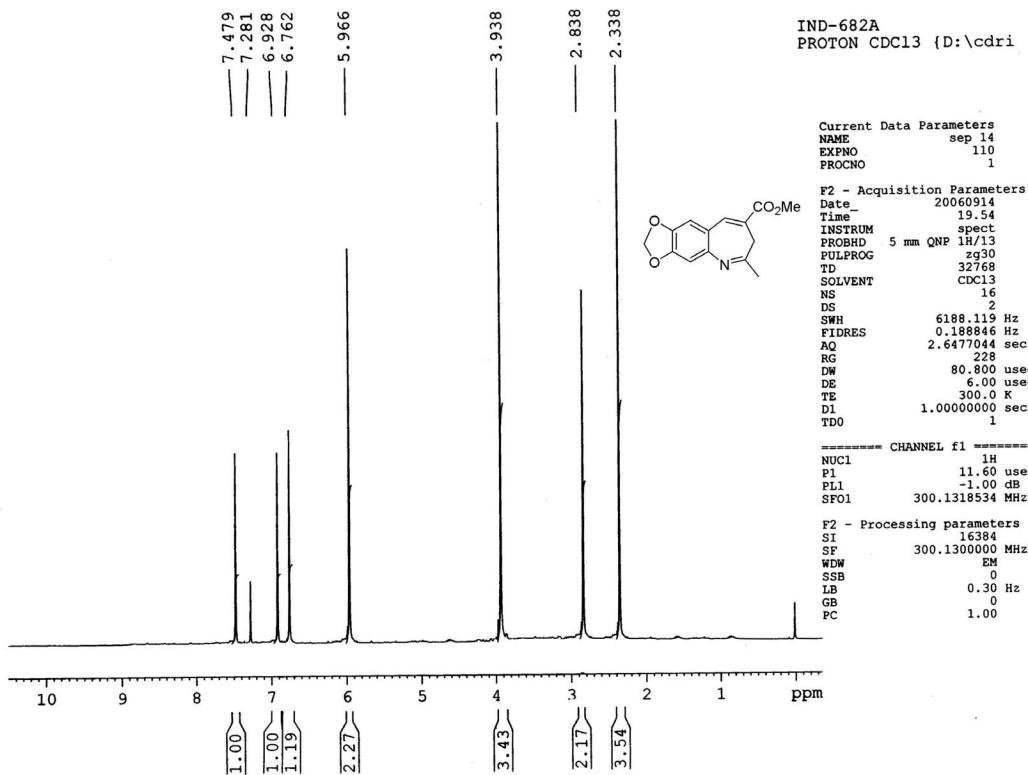


Fig.-35: ^1H NMR spectrum of compound 25c

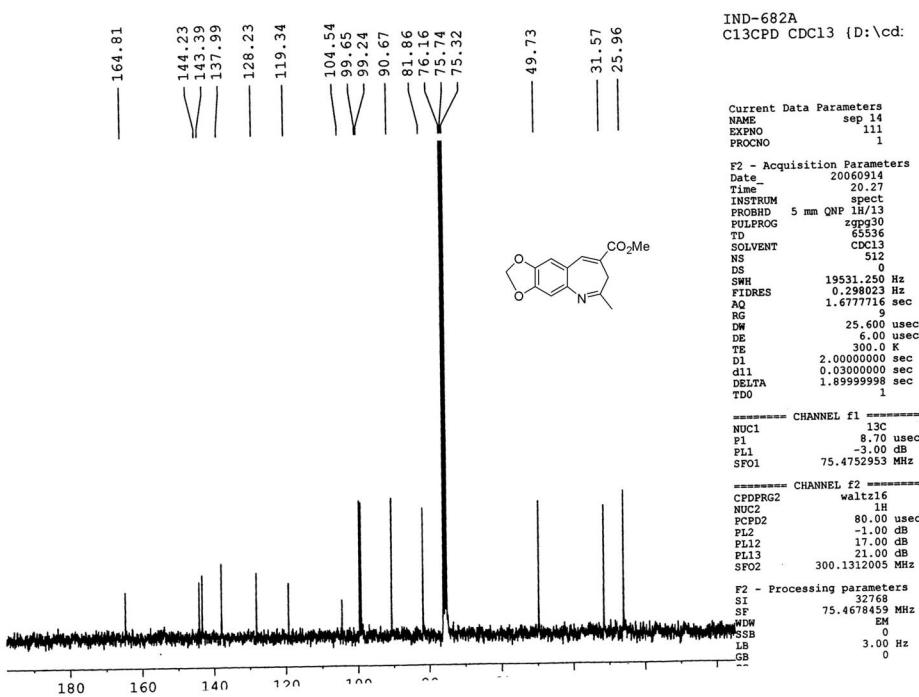


Fig.-36: ^{13}C NMR spectrum of compound 25c

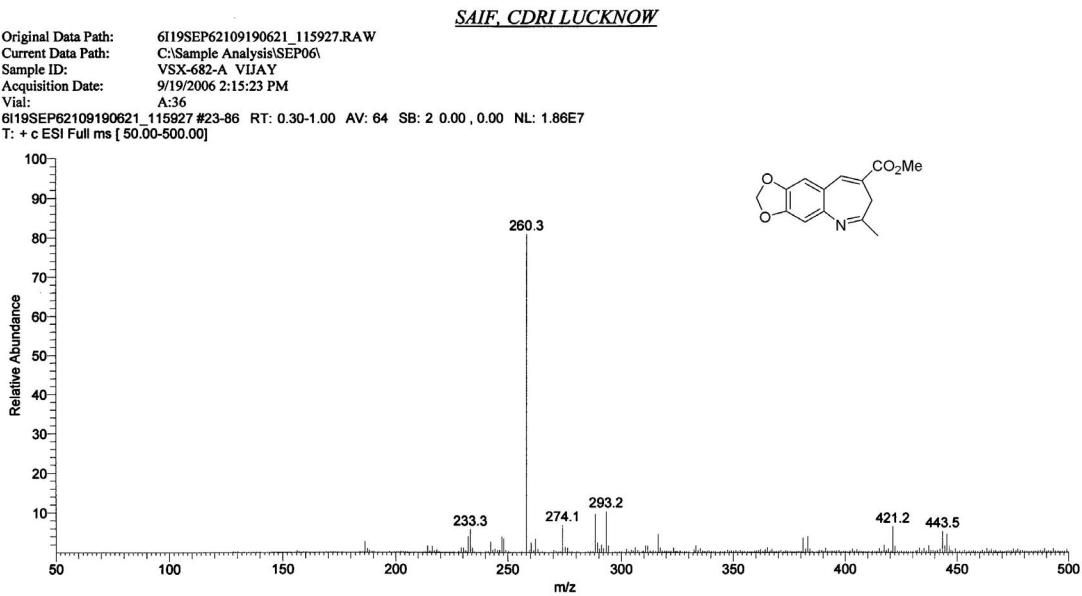


Fig.-37: Mass spectrum of compound 25c

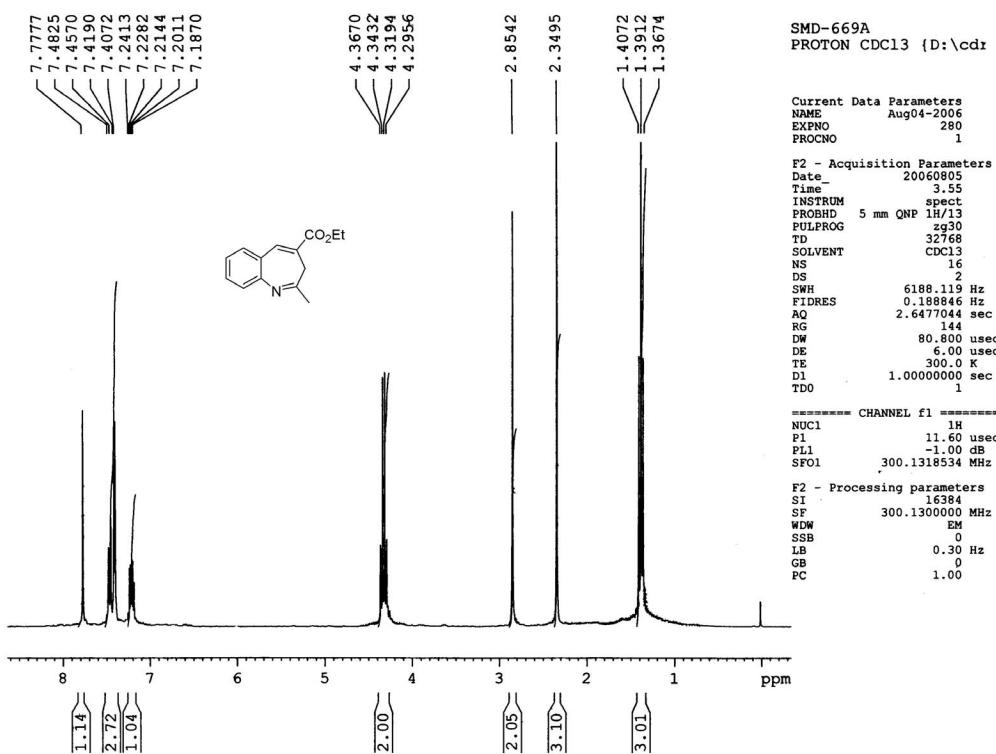


Fig.-37: ^1H NMR spectrum of compound 26a

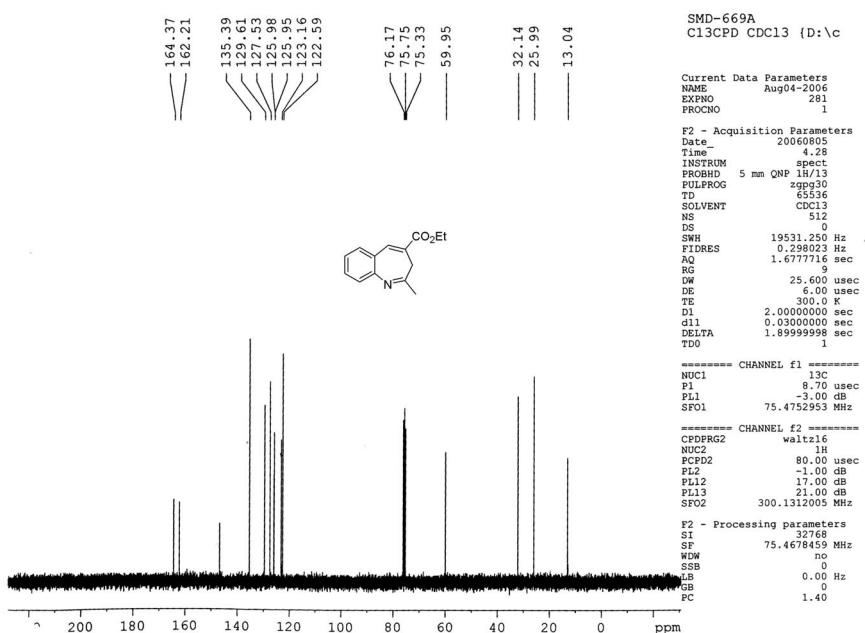


Fig.-39: ^{13}C NMR spectrum of compound 26a

SAIF, CDRI LUCKNOW

Original Data Path: 6I04AUG16508040167_113549.RAW
 Current Data Path: C:\Sample Analysis\AUG06\
 Sample ID: VSX-669 VIJAY
 Acquisition Date: 8/4/2006 12:53:37 PM
 Vial: A:26
 6I04AUG16508040167_113549 #28-100 RT: 0.30-1.00 AV: 73 SB: 2 0.01 , 0.01 NL: 9.74E7
 T: + c ESI Full ms [50.00-500.00]

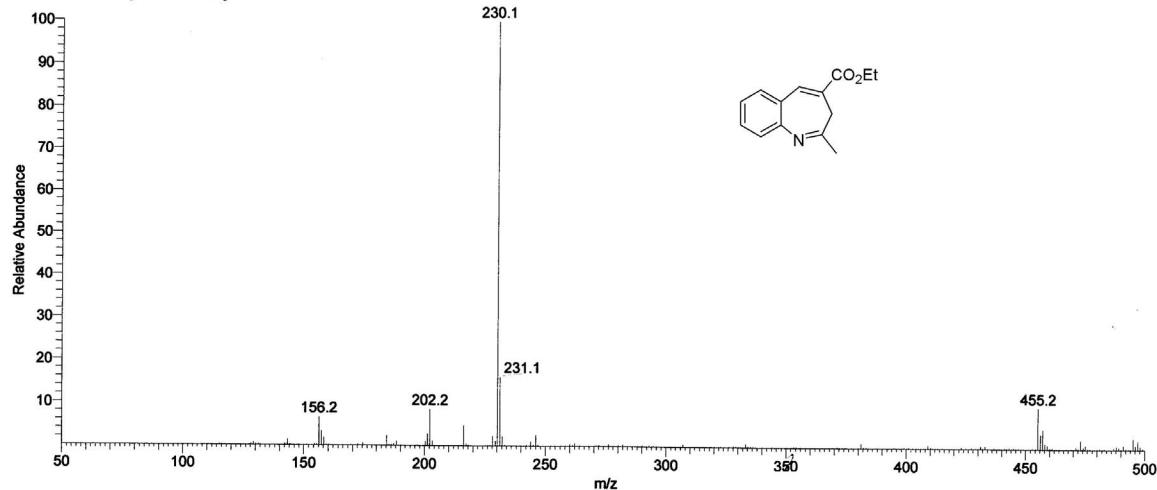


Fig.-40: Mass spectrum of compound 26a

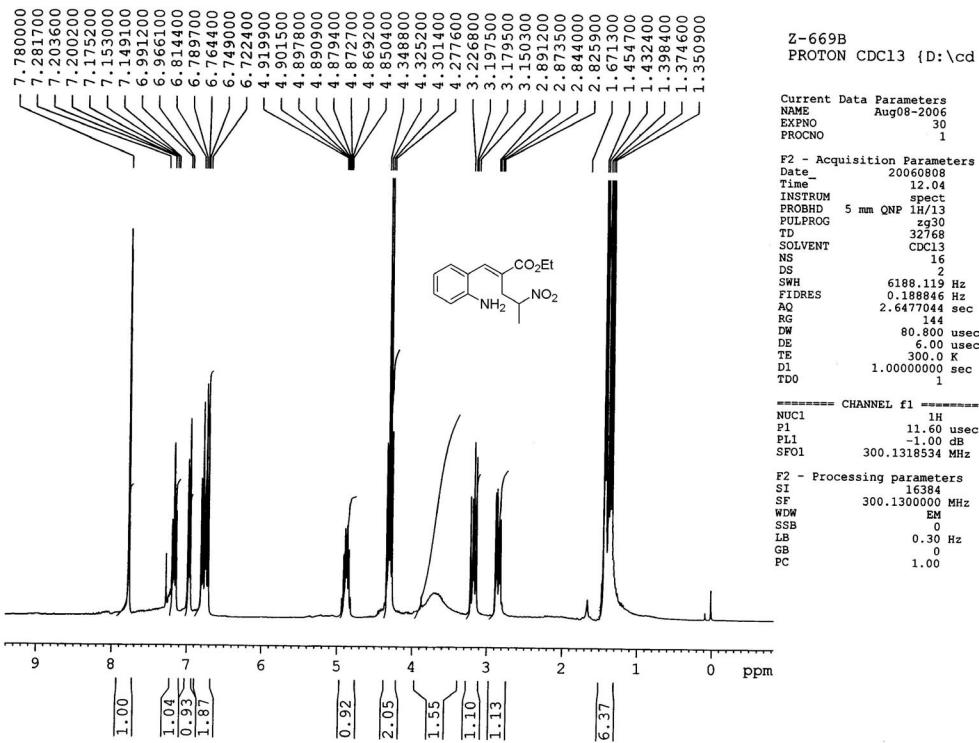


Fig.-54: ^1H NMR spectrum of compound 27a.

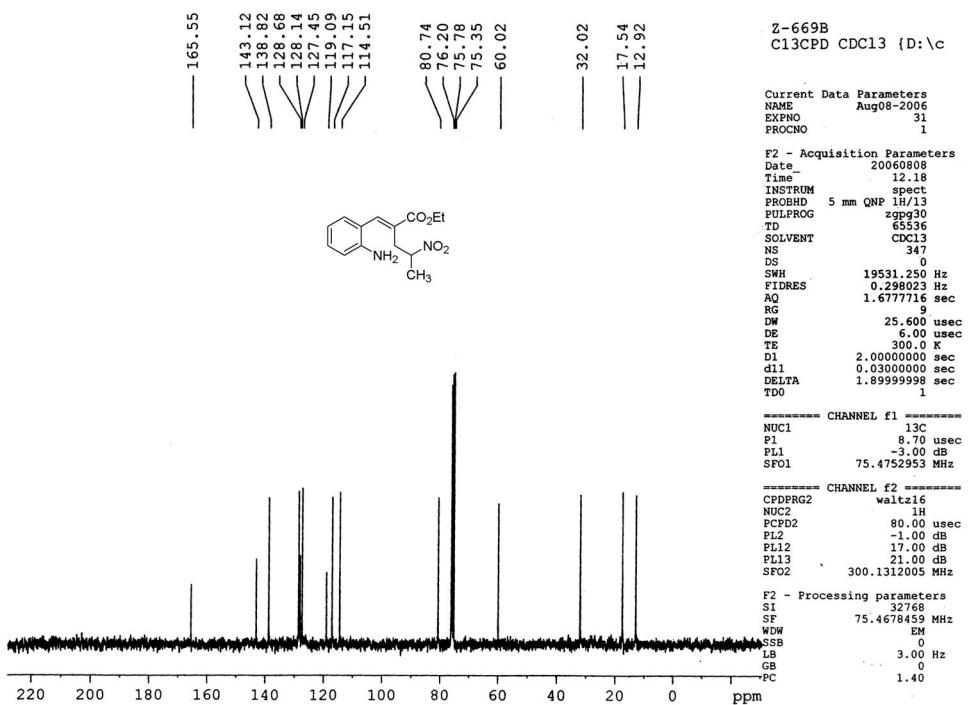


Fig.-55: ¹³C NMR spectrum of compound 27a.

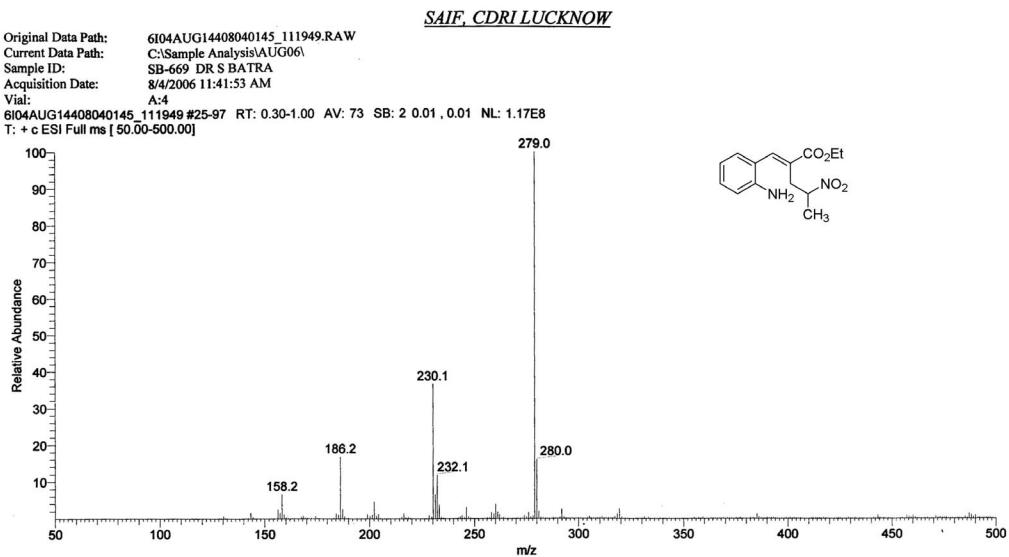


Fig.-56: Mass spectrum of compound 27a.