

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

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Ref. No.: O200700175

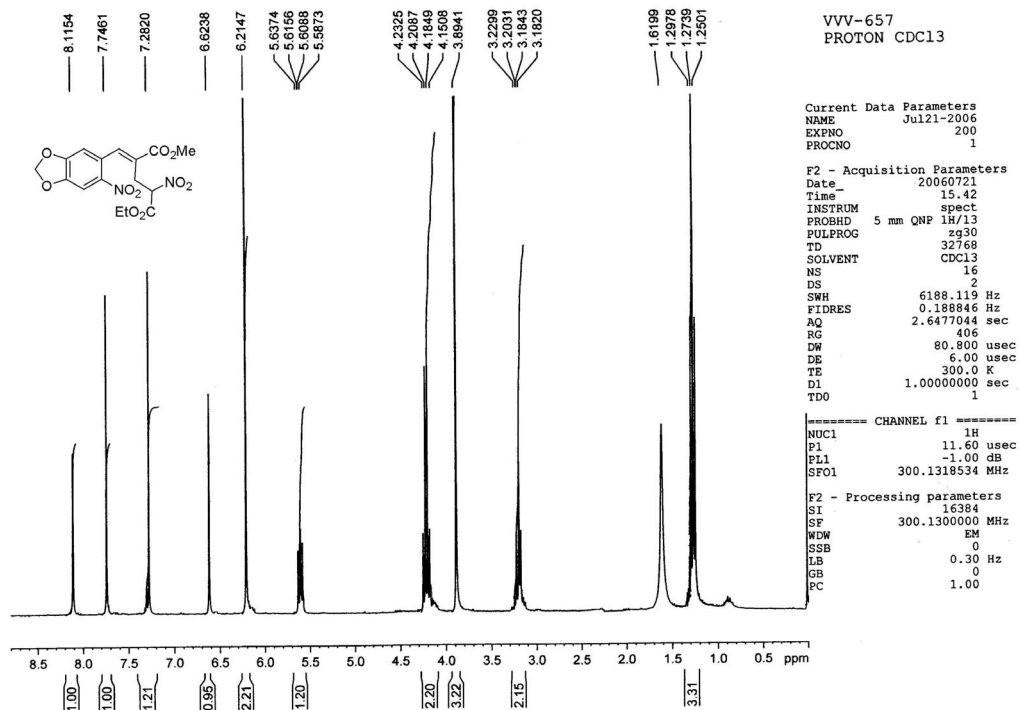


Fig.-1: ^1H NMR spectrum of compound 7c

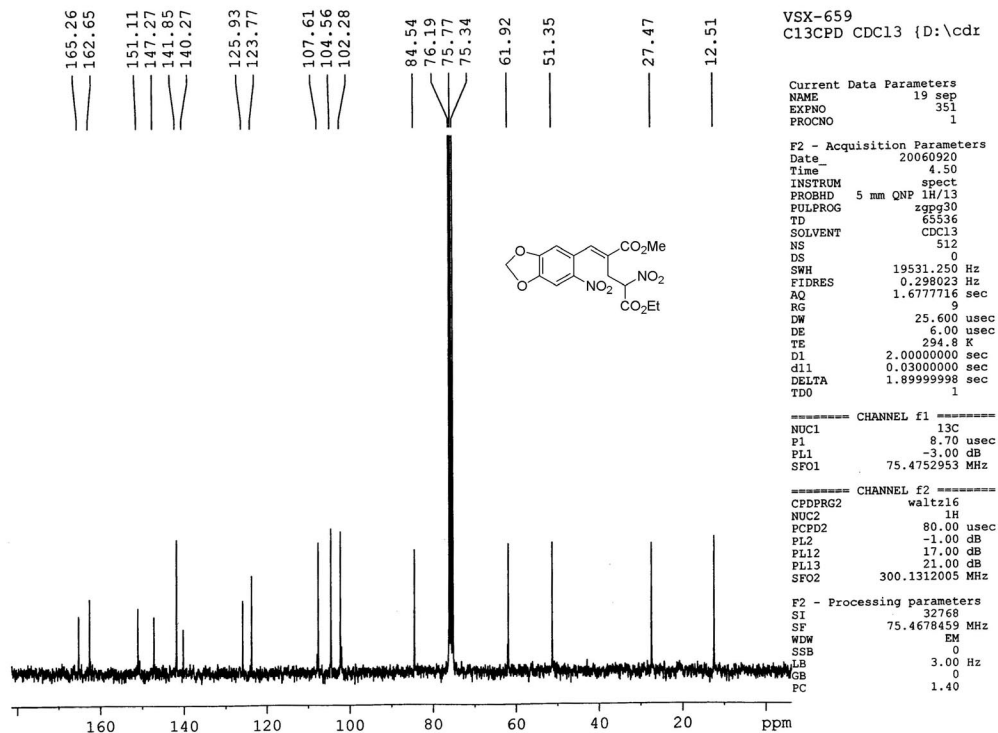


Fig.-2: ^{13}C NMR spectrum of compound 7c

[Mass Spectrum]
 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 %

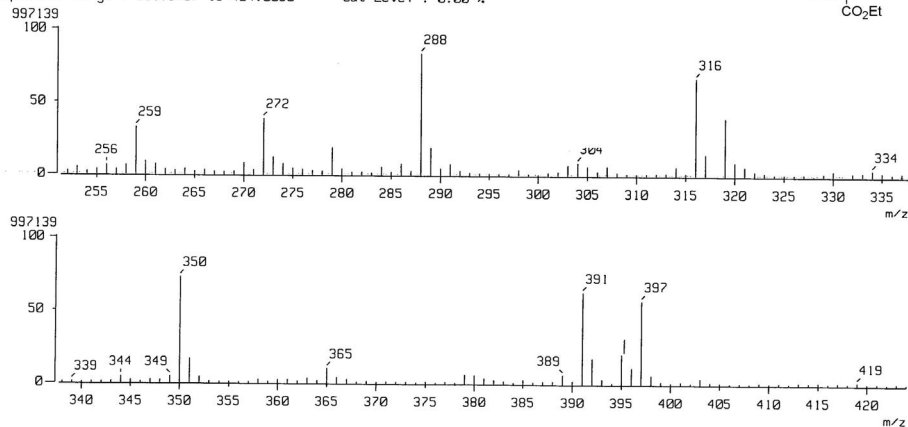
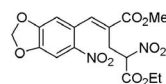


Fig.-3: Mass spectrum of compound 7c

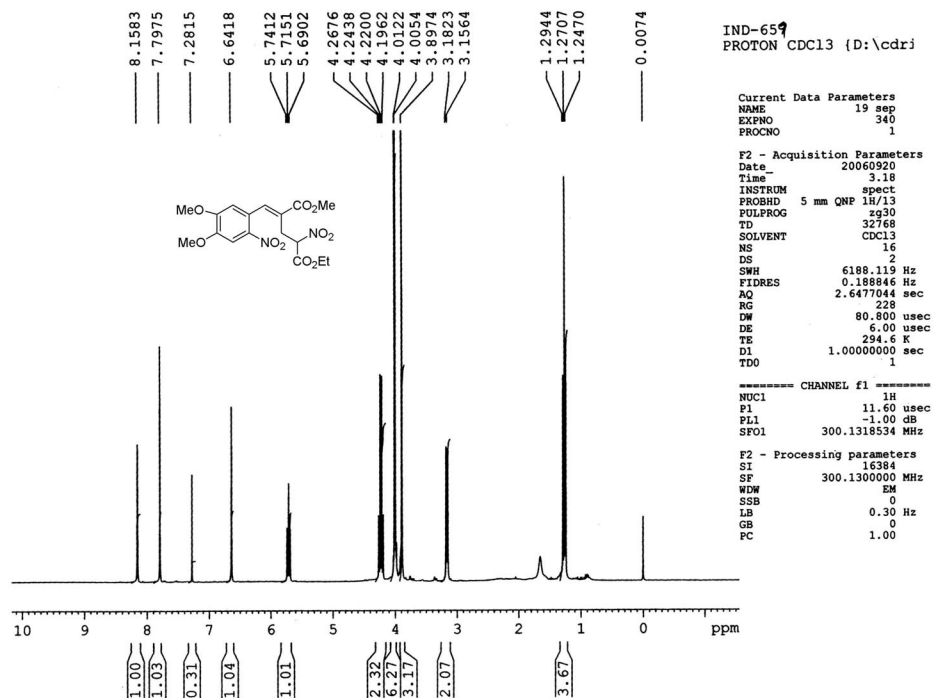


Fig.-4: ¹H NMR spectrum of compound 7d

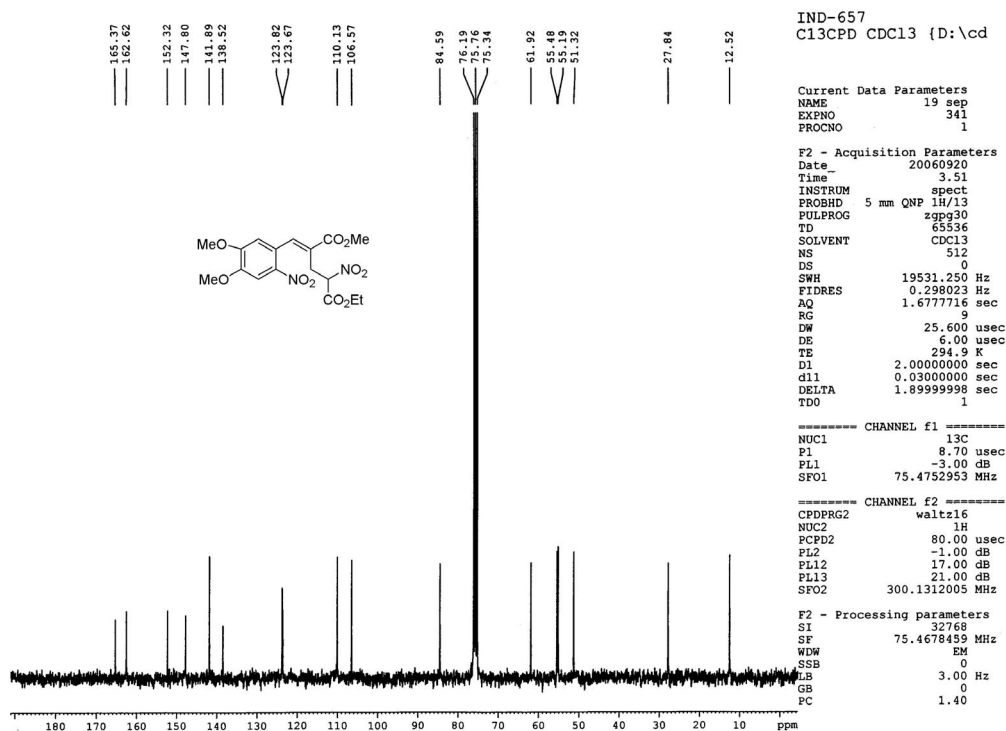


Fig.-5: ^{13}C NMR spectrum of compound 7d

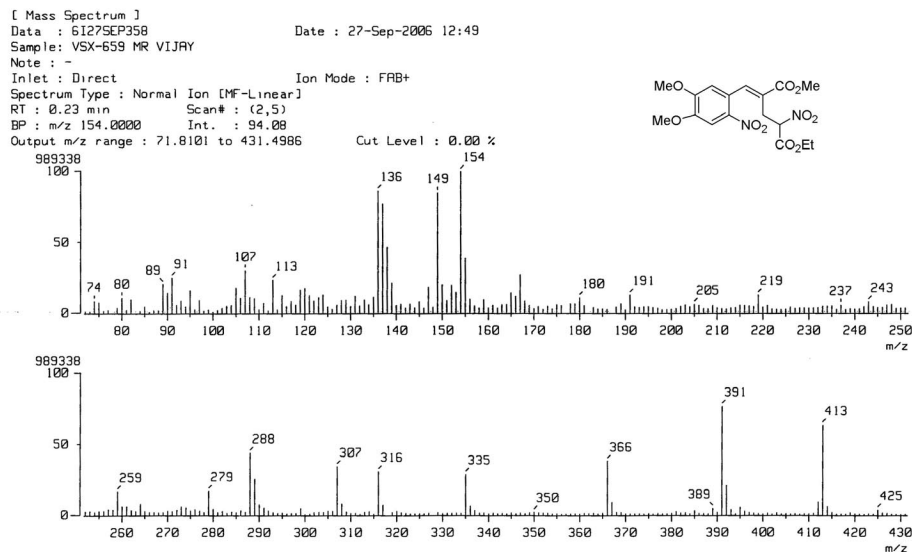


Fig.-6: Mass spectrum of compound 7d

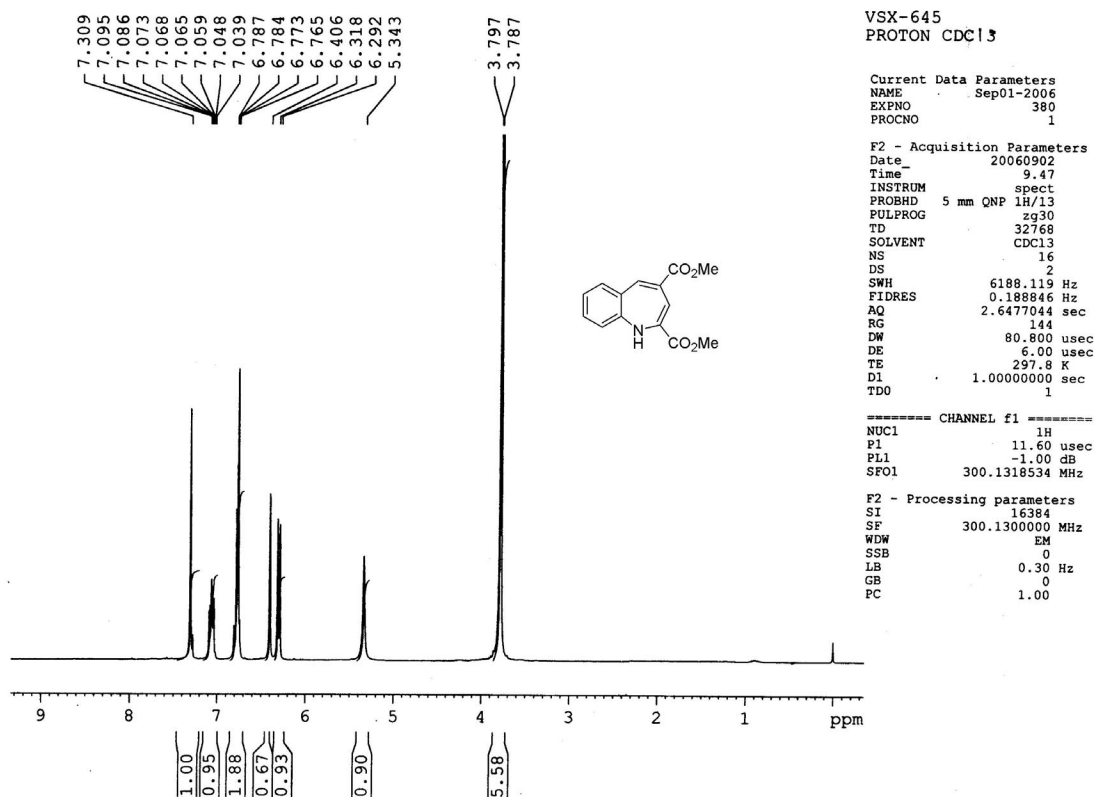


Fig.-16: ¹H NMR spectrum of compound 10a

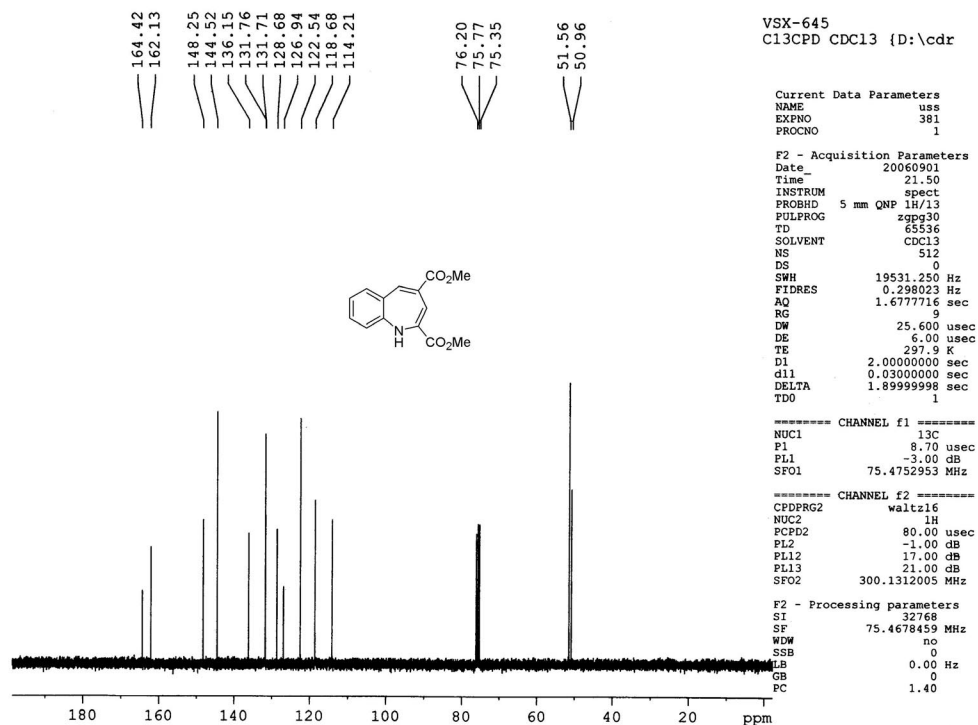


Fig.-17: ¹³C NMR spectrum of compound 10a

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: A:31
 6110JUL24707100246_120446 #31-102 RT: 0.30-1.00 AV: 72 SB: 2 0.00, 0.00 NL: 2.29E7
 T: + c ESI Full ms [50.00-500.00]

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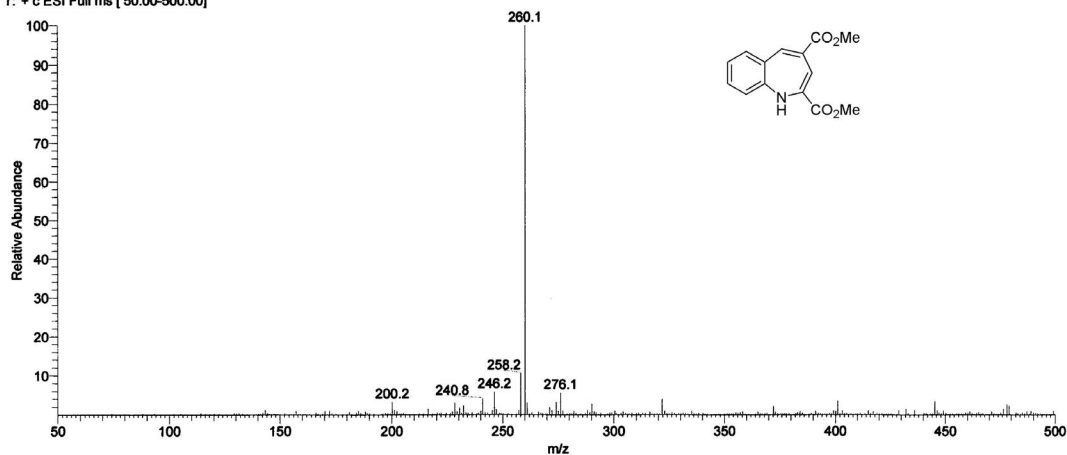


Fig.-18: Mass spectrum of compound 10a

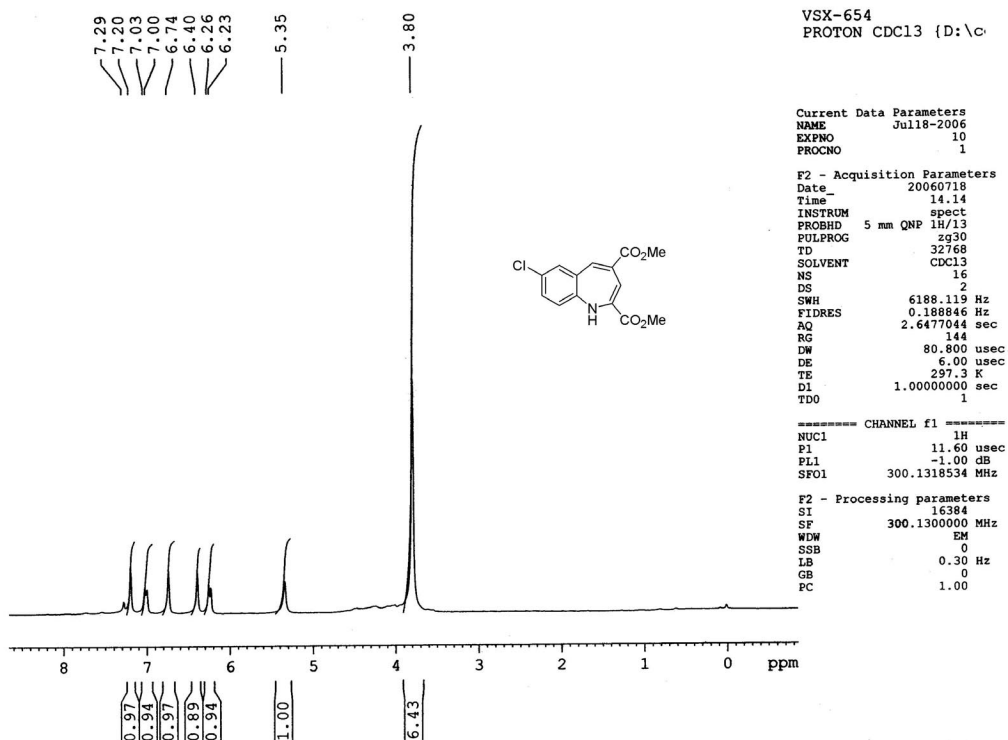


Fig.-19: ¹H NMR spectrum of compound 10b

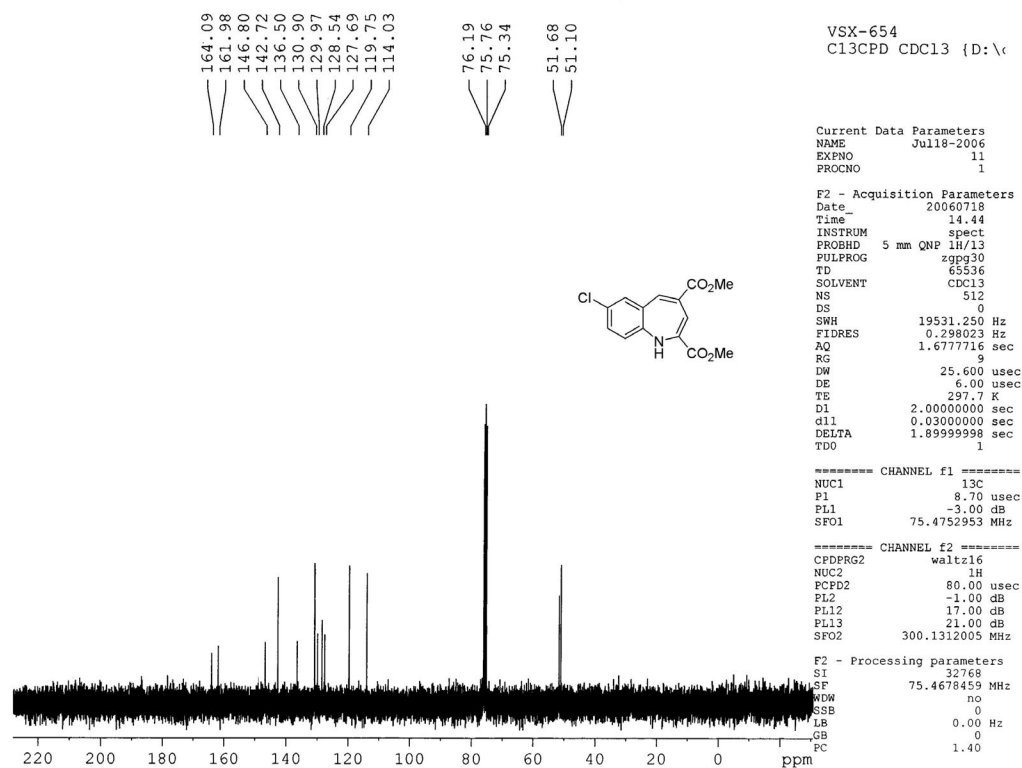


Fig.-20: ^{13}C NMR spectrum of compound 10b

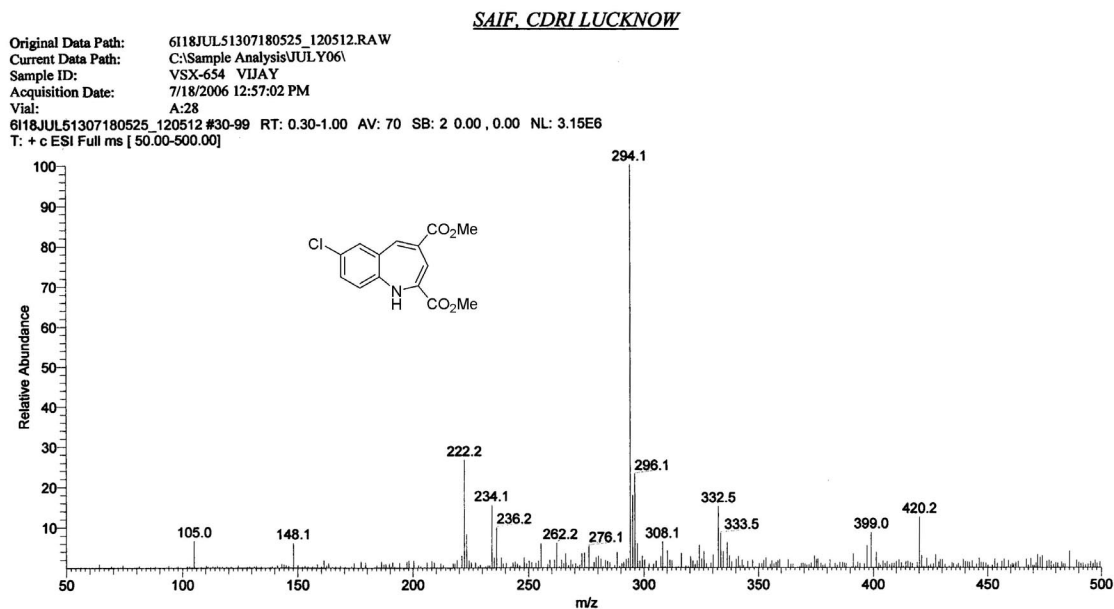


Fig.-21: Mass spectrum of compound 10b

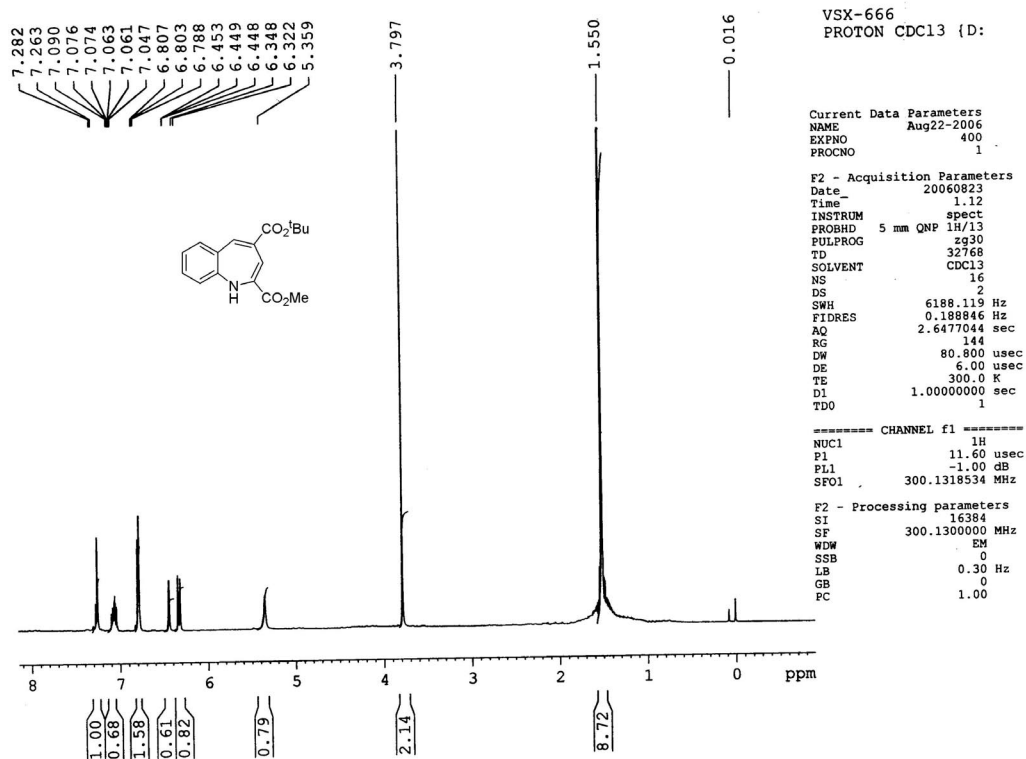


Fig.-25: ^1H NMR spectrum of compound 12a

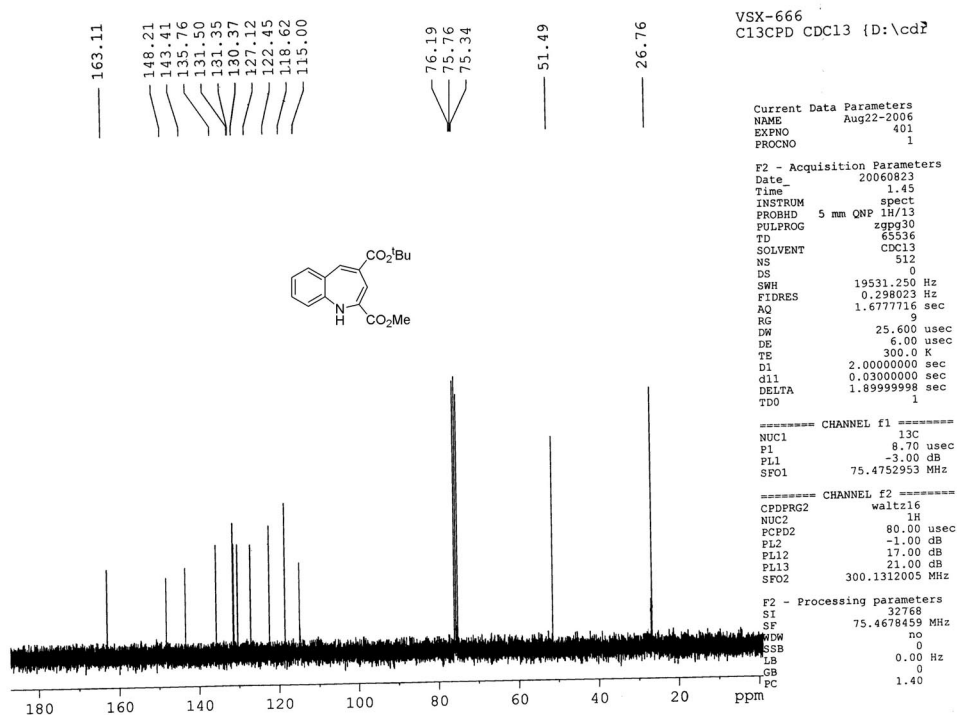


Fig.-26: ^{13}C NMR spectrum of compound 12a

Original Data Path: 6127JUL82507270830_122314.RAW
 Current Data Path: C:\Sample Analysis\JULY06\
 Sample ID: VSX-666 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]

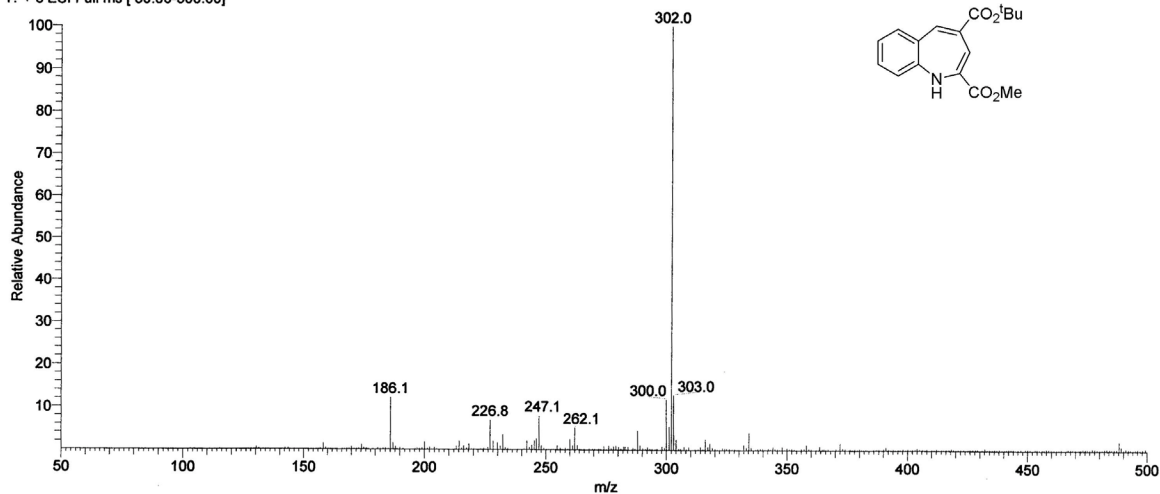
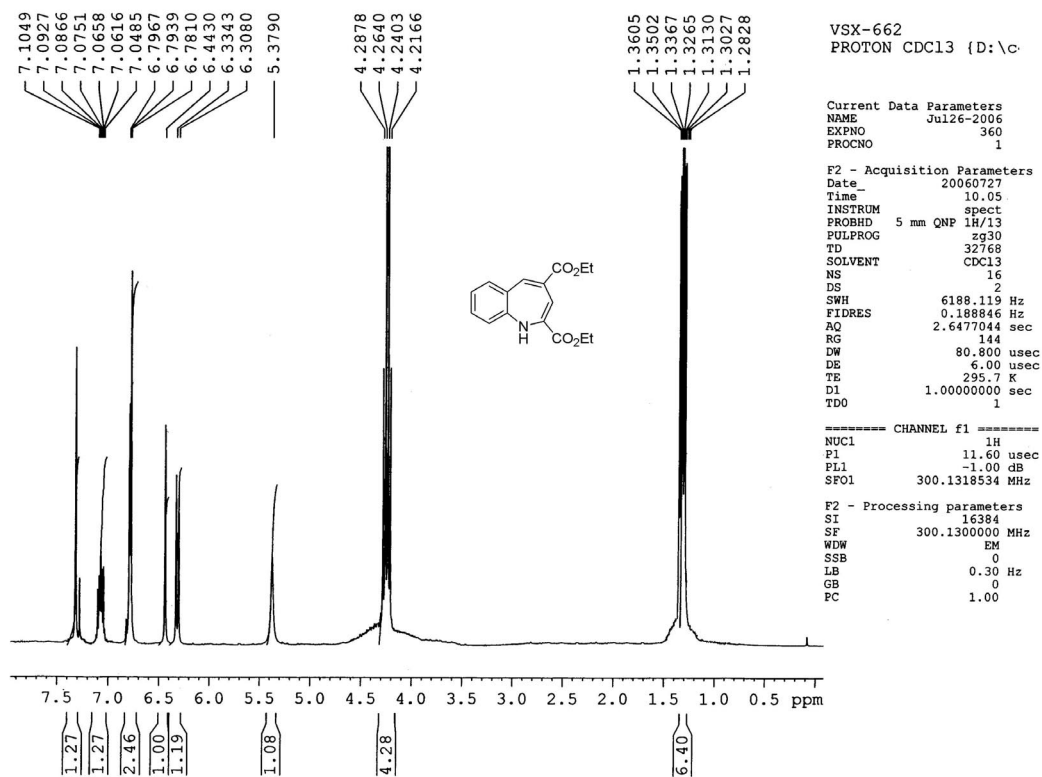


Fig.-27: Mass spectrum of compound 12a

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

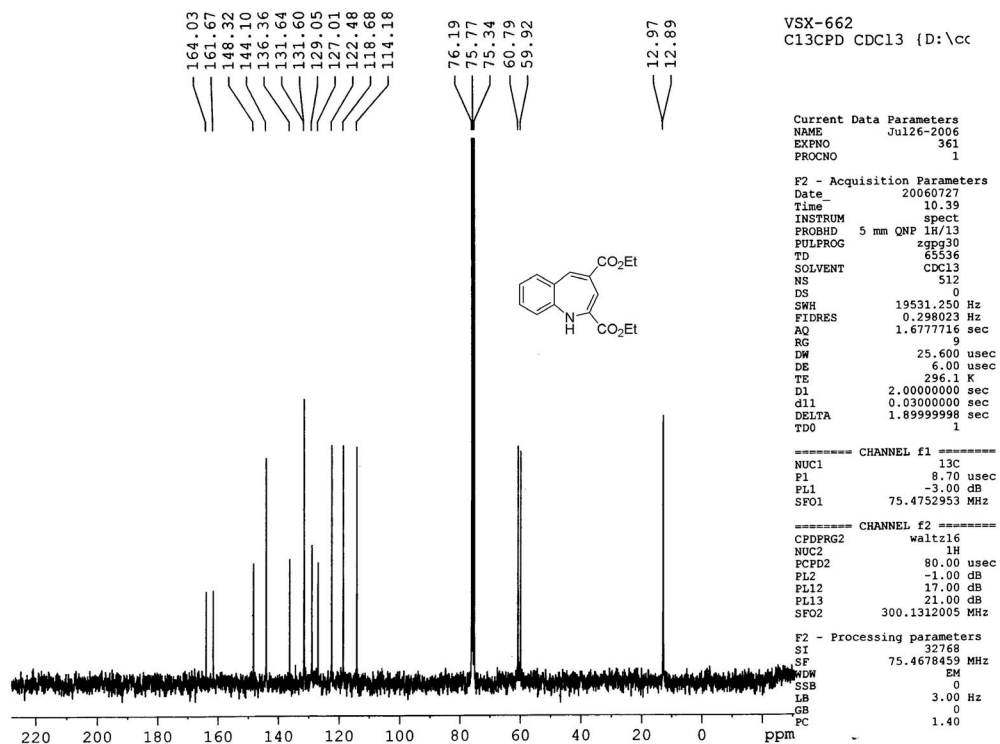


Fig.-23: ^{13}C NMR spectrum of compound **13a**

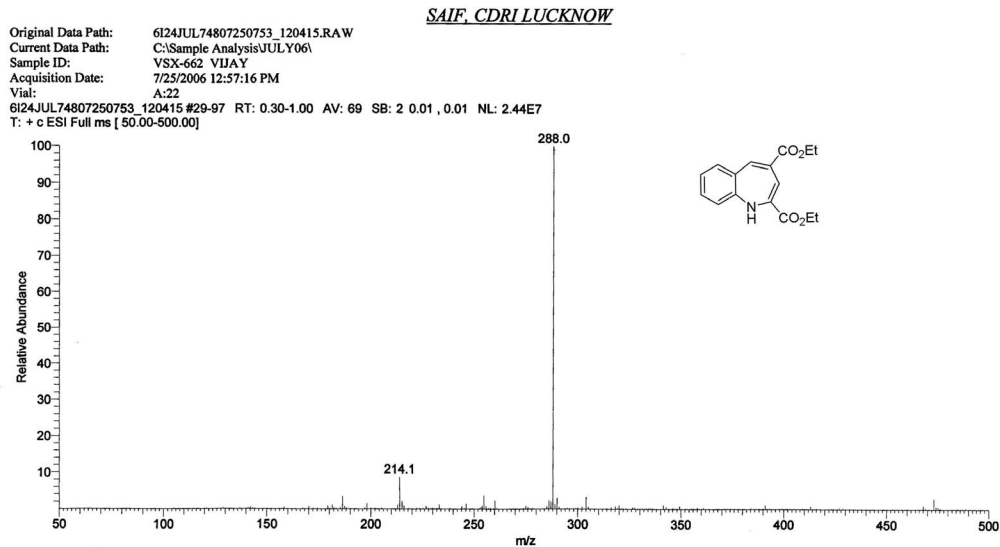


Fig.-24: Mass spectrum of compound **13a**

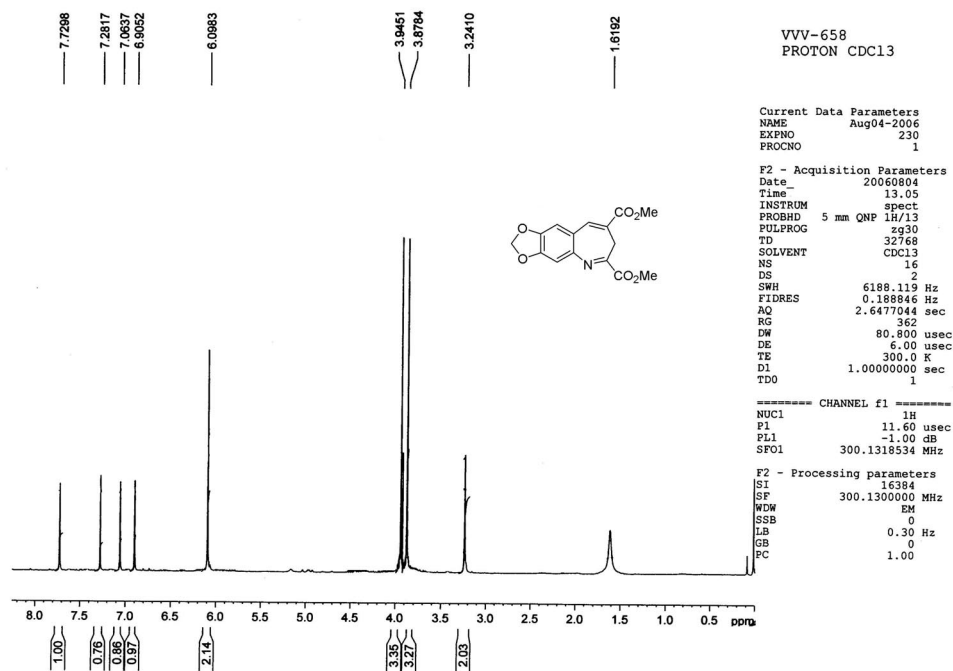


Fig.-28: ^1H NMR spectrum of compound 14c

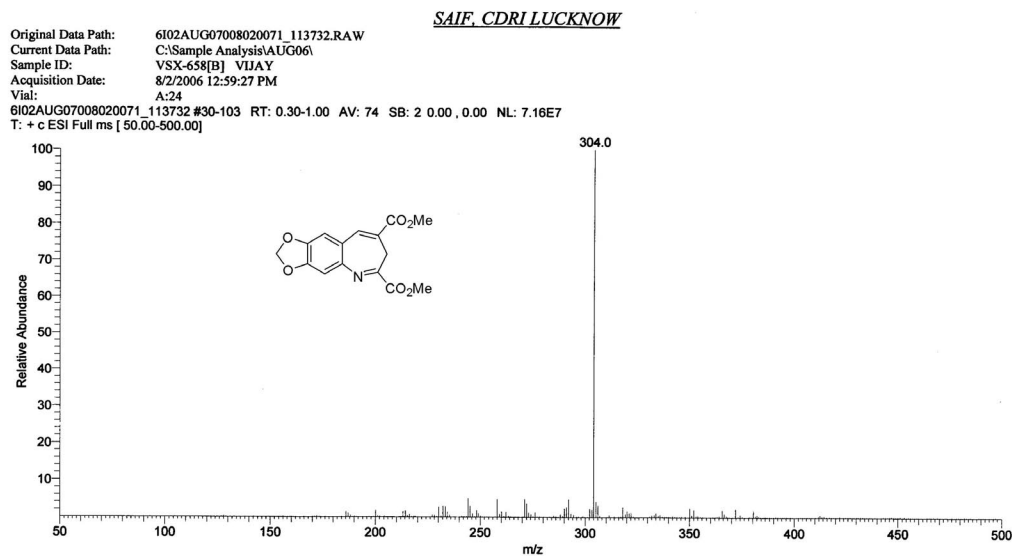


Fig.-29: Mass spectrum of compound 14c

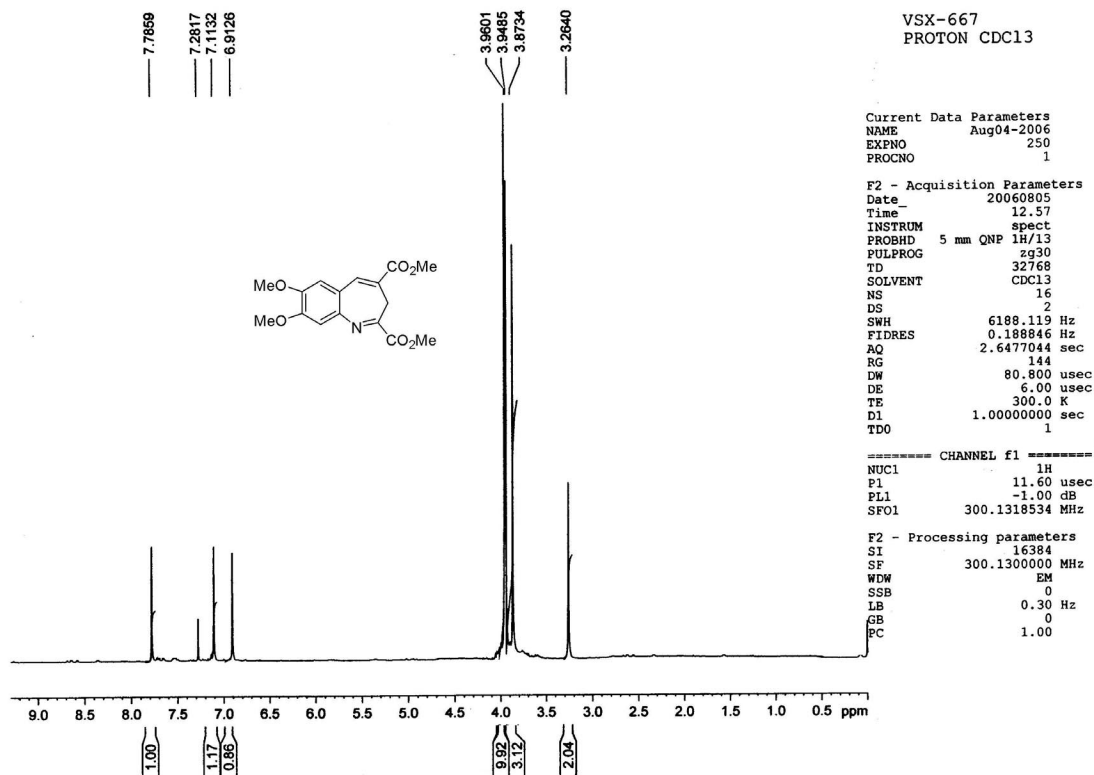


Fig.-30: ^1H NMR spectrum of compound **14d**

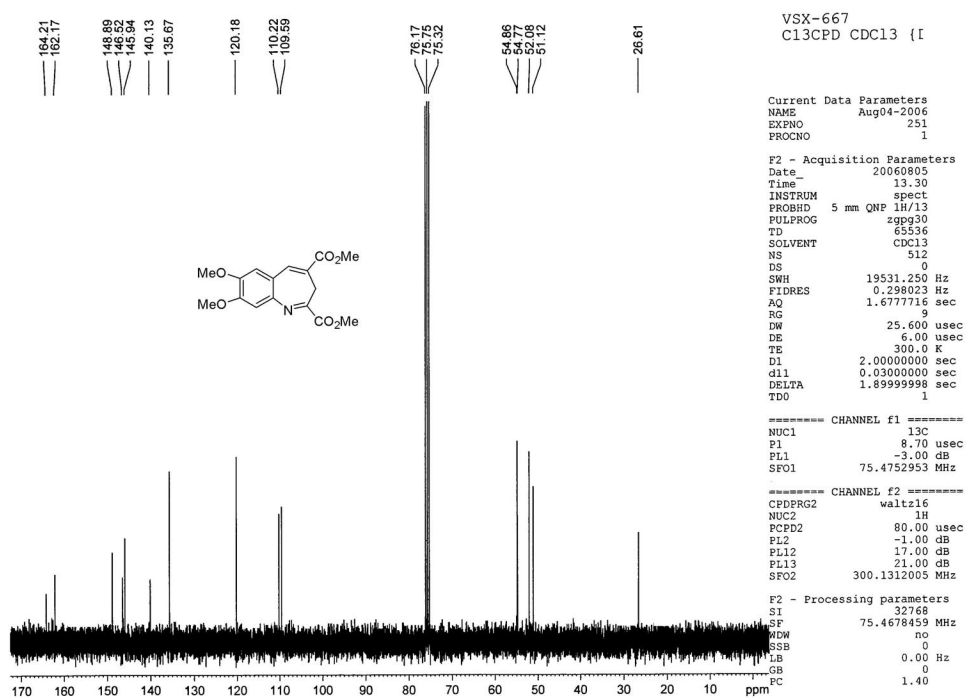


Fig.-31: ^{13}C NMR spectrum of compound **14d**

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
 6101AUG02108010021_112134 #27-97 RT: 0.30-1.00 AV: 71 SB: 2 0.01, 0.01 NL: 9.19E7
 T: + c ESI Full ms [50.00-500.00]

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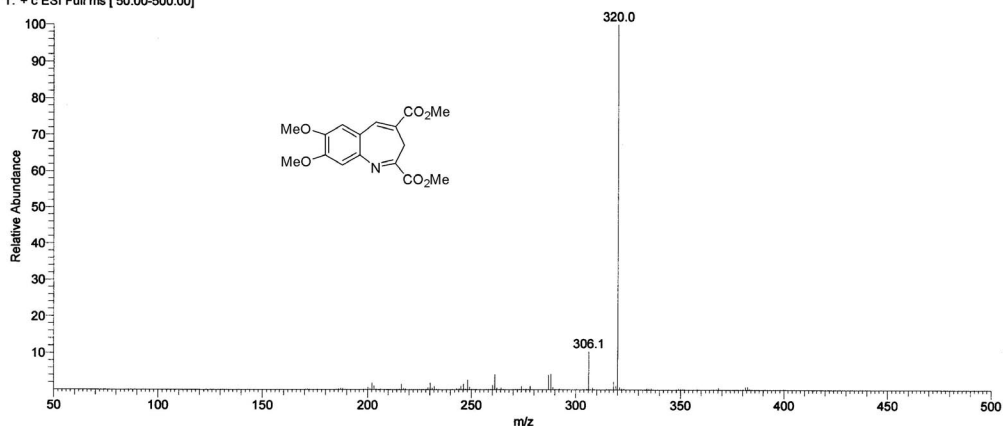


Fig.-32: Mass spectrum of compound 14d

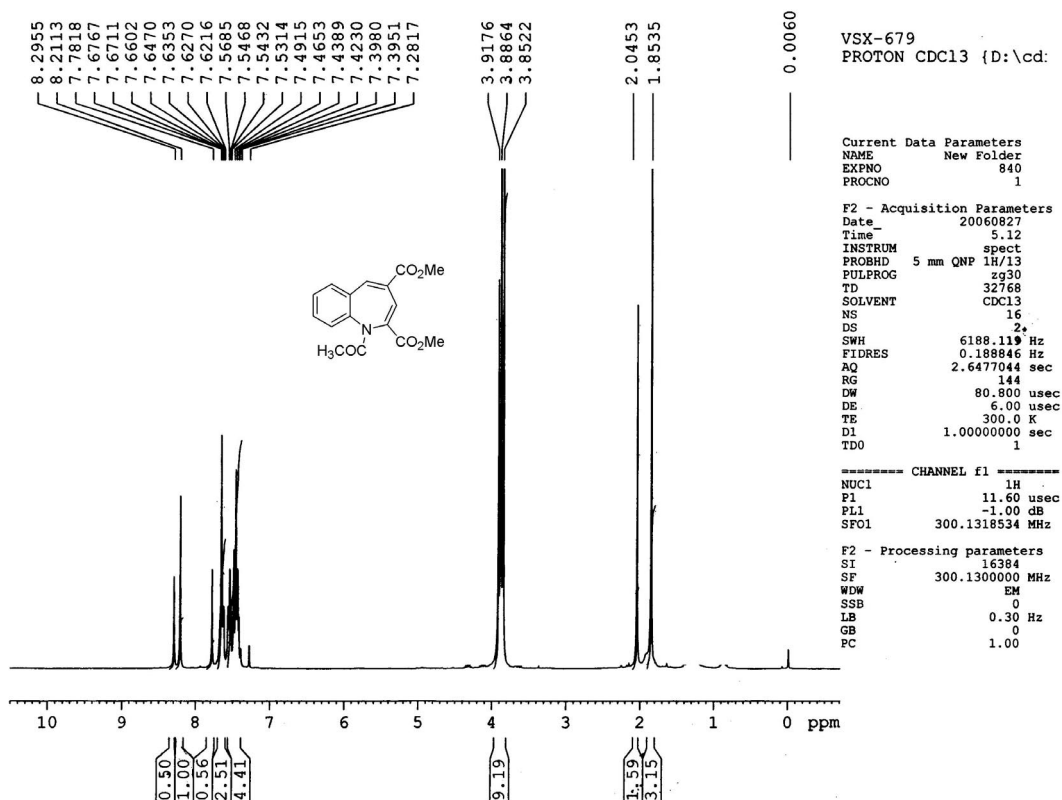


Fig.-41: ¹H NMR spectrum of compound 15

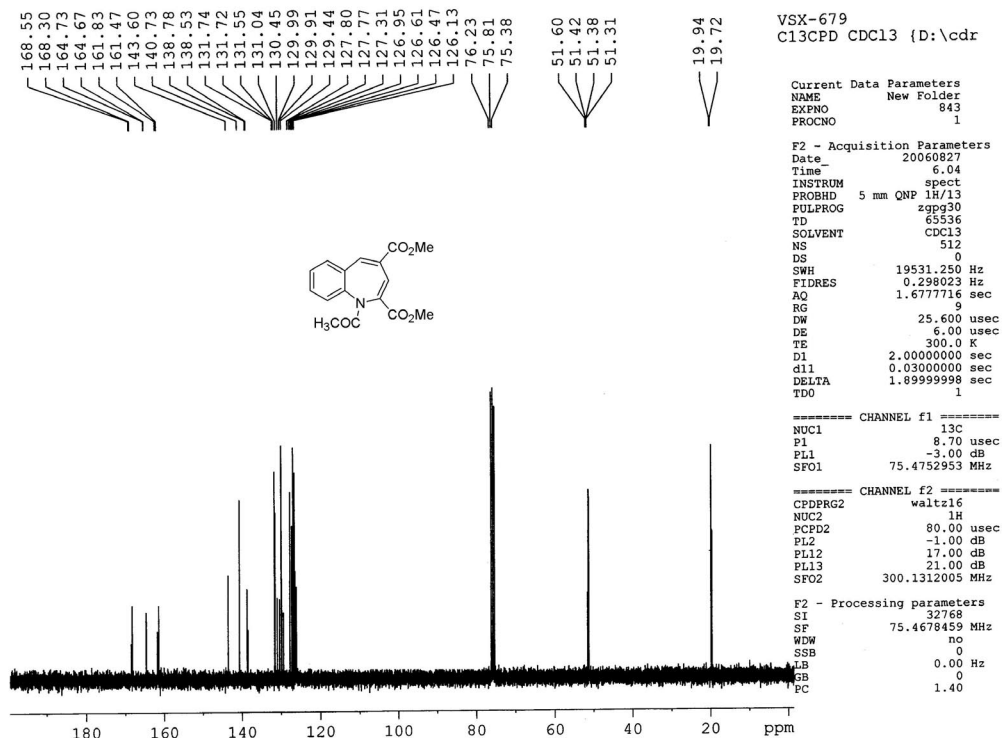


Fig.-42: ¹³C NMR spectrum of compound 15

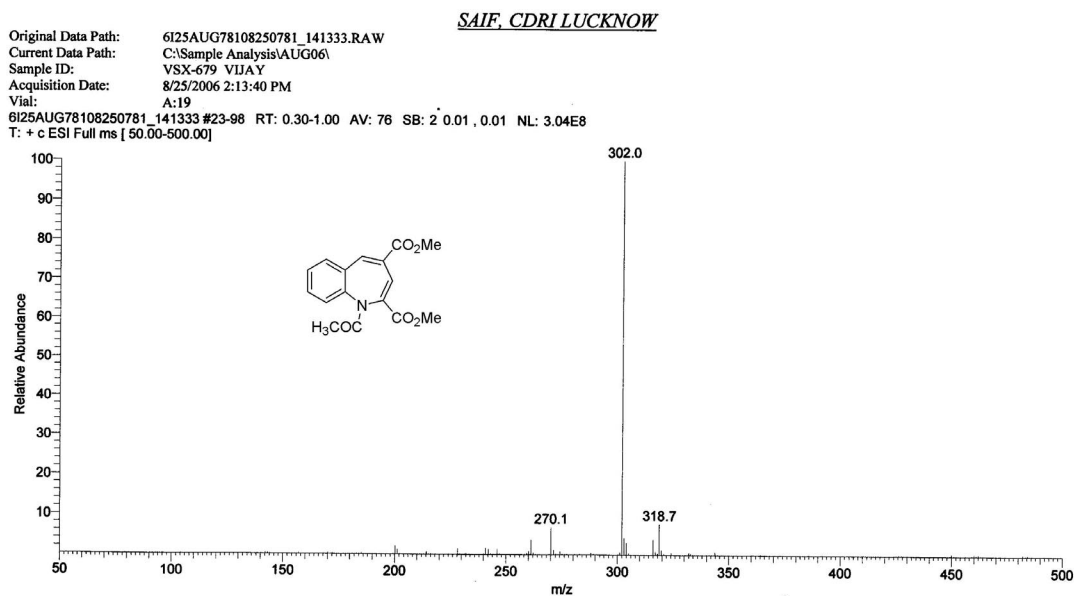


Fig.-43: Mass spectrum of compound 15

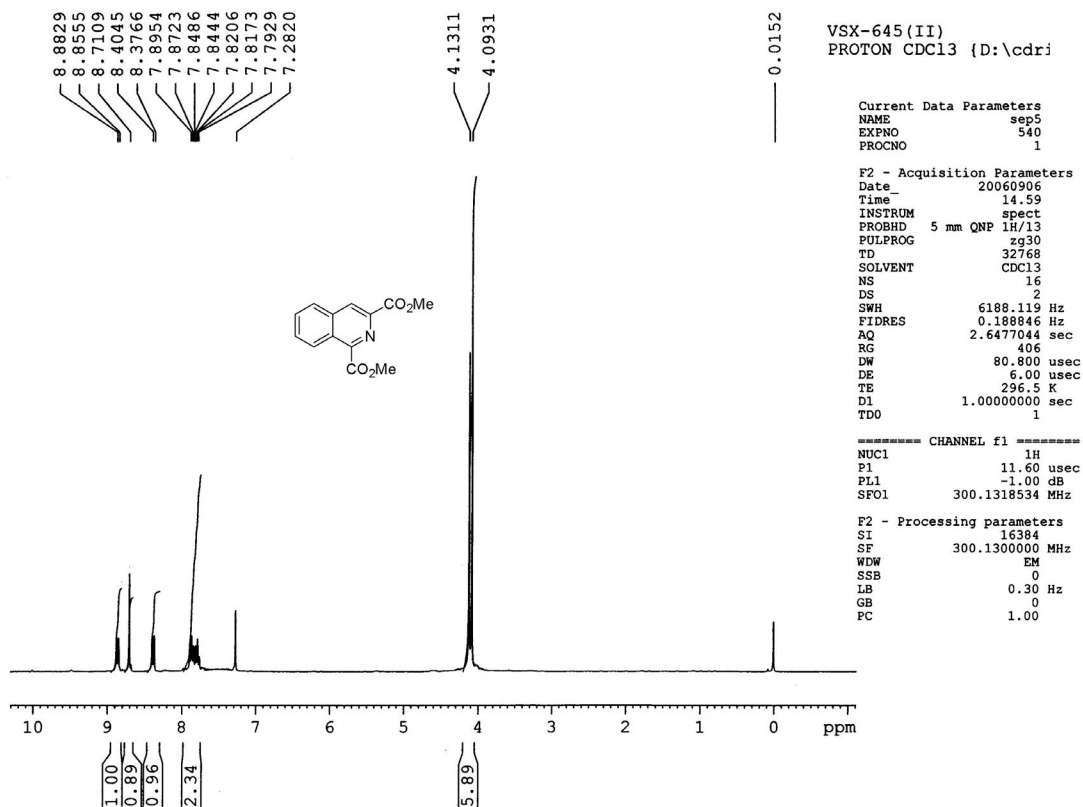


Fig.-44: ¹H NMR spectrum of compound 17a

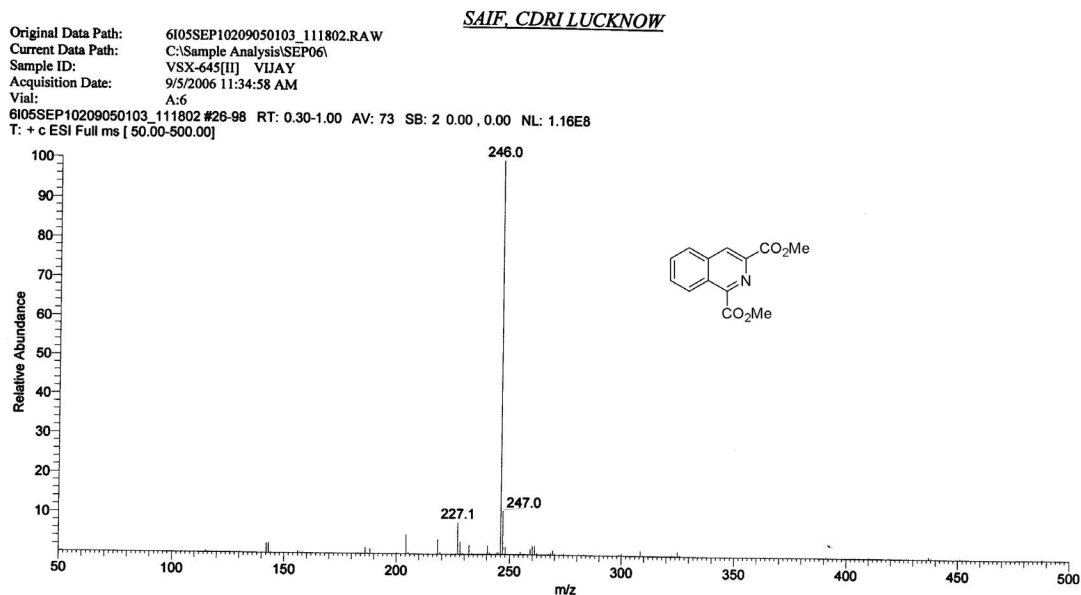


Fig.-45: Mass spectrum of compound 17a

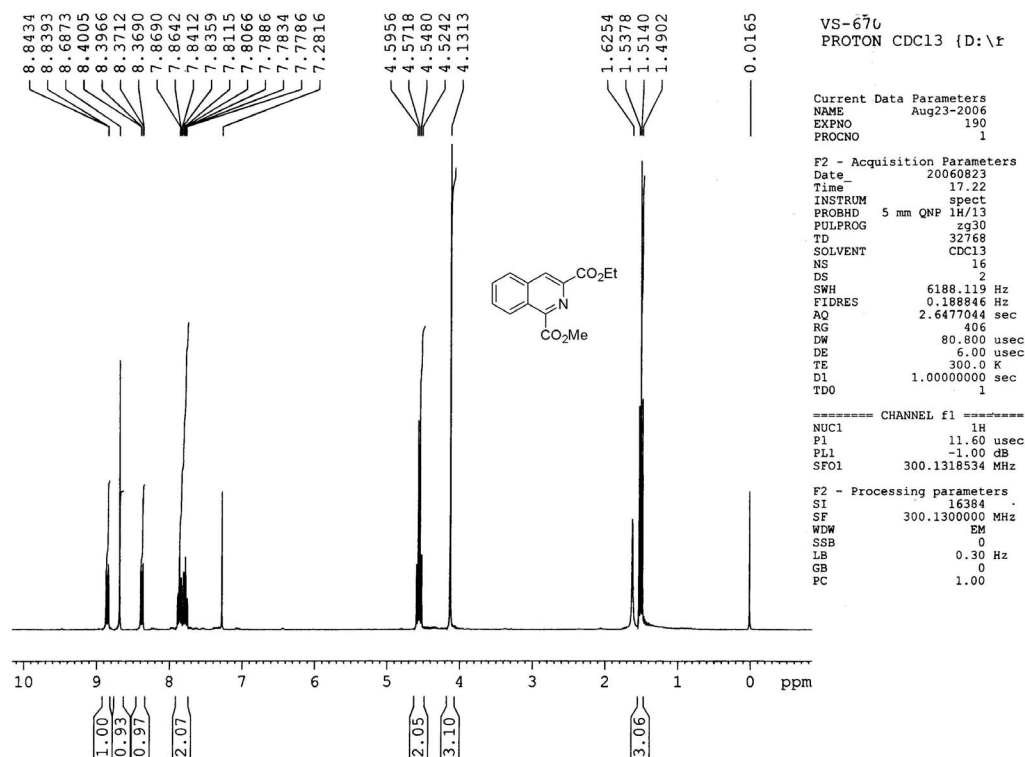


Fig.-46: ^1H NMR spectrum of compound 18a

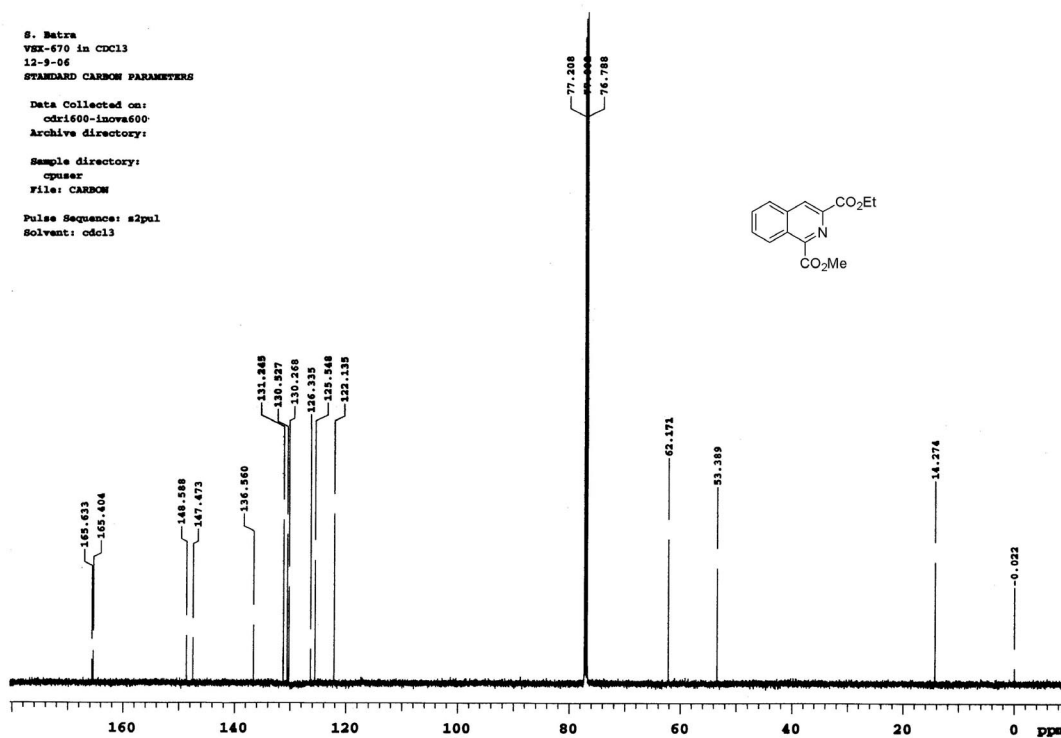


Fig.-47: ^{13}C NMR spectrum of compound 18a

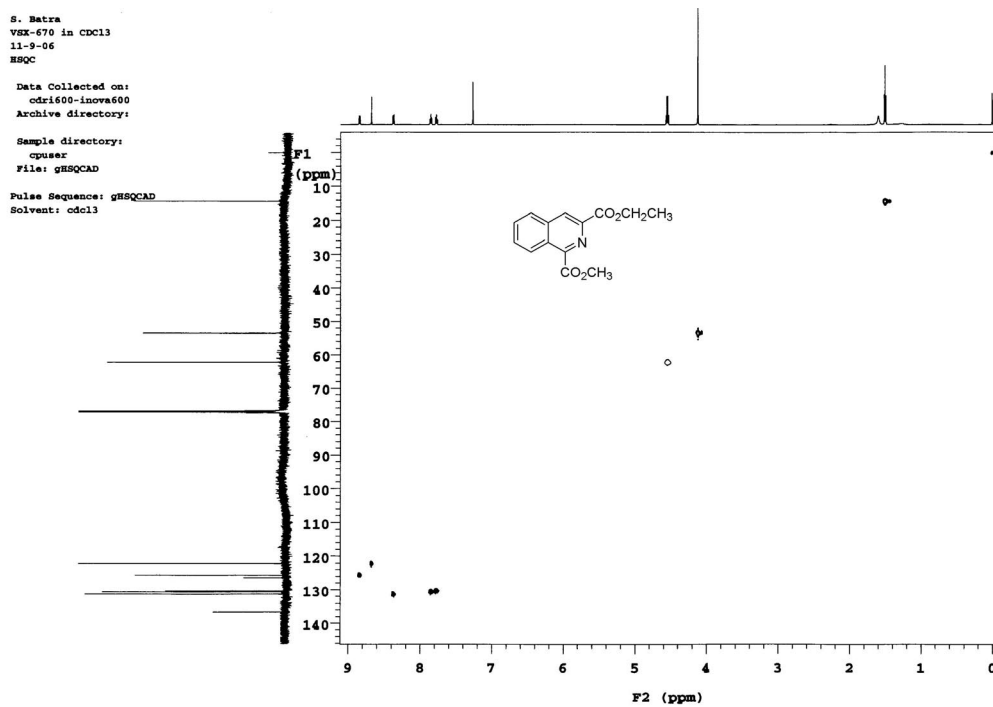


Fig.-48: HSQC spectrum of compound **18a**

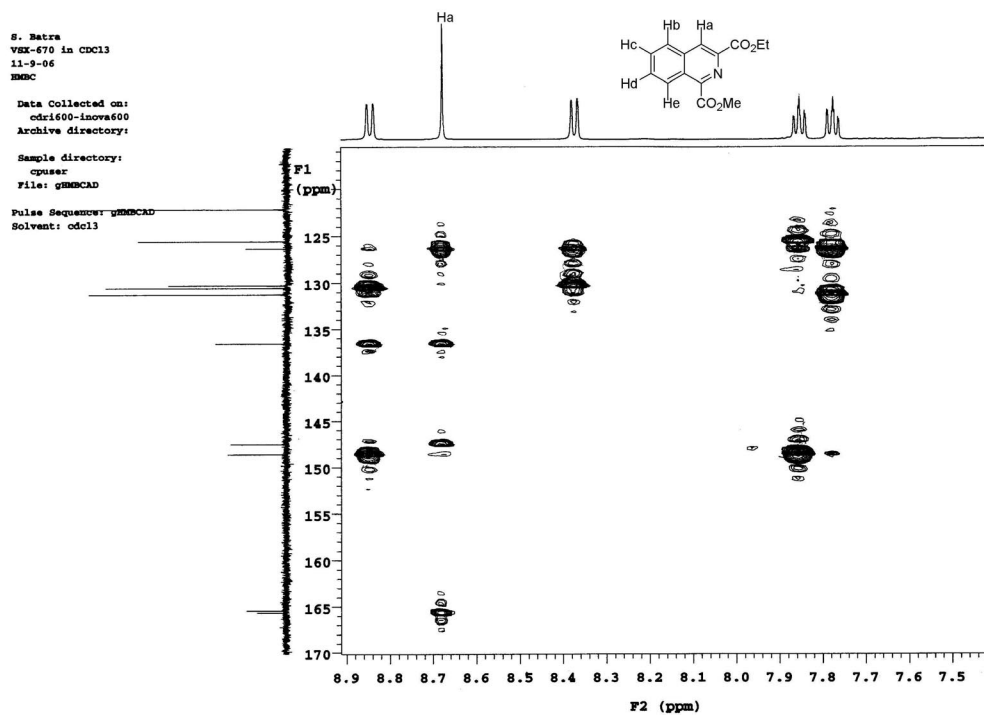


Fig.-49: HMBC spectrum (expanded) of compound **18a**

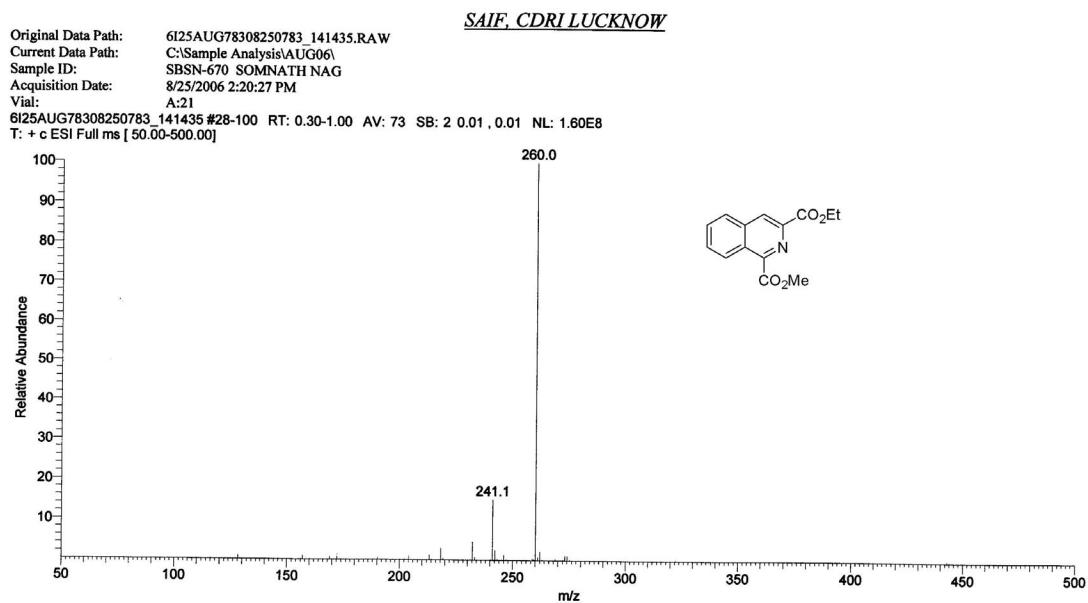


Fig.-50: Mass spectrum of compound **18a**

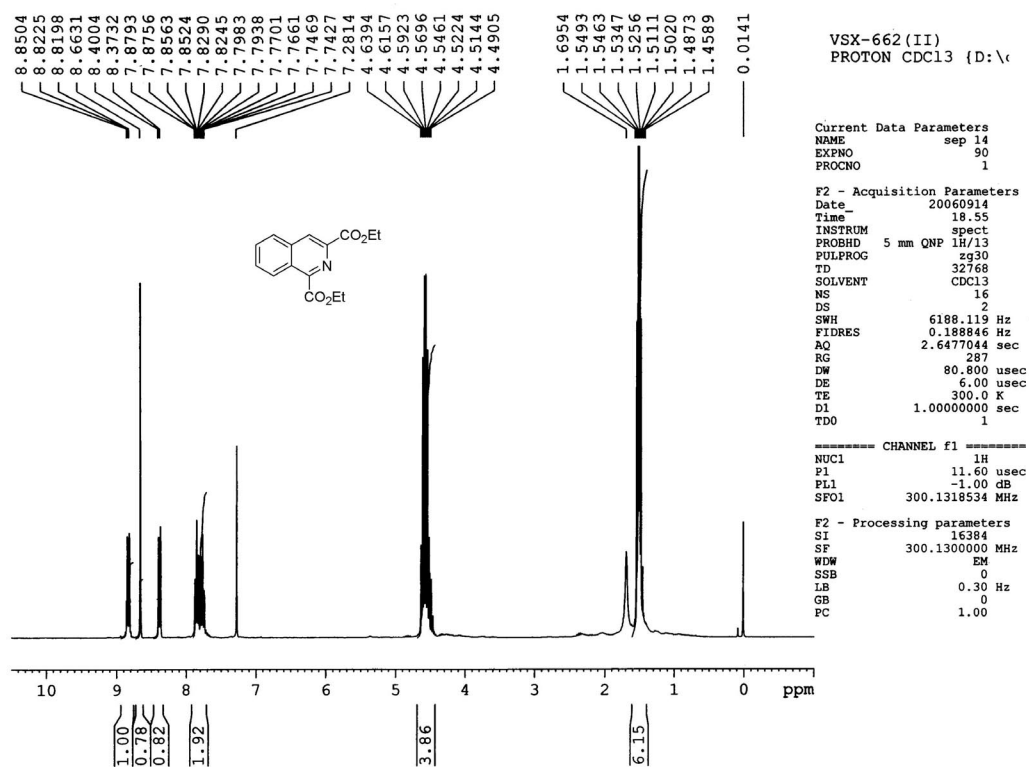


Fig.-51: ¹H NMR spectrum of compound **19a**.

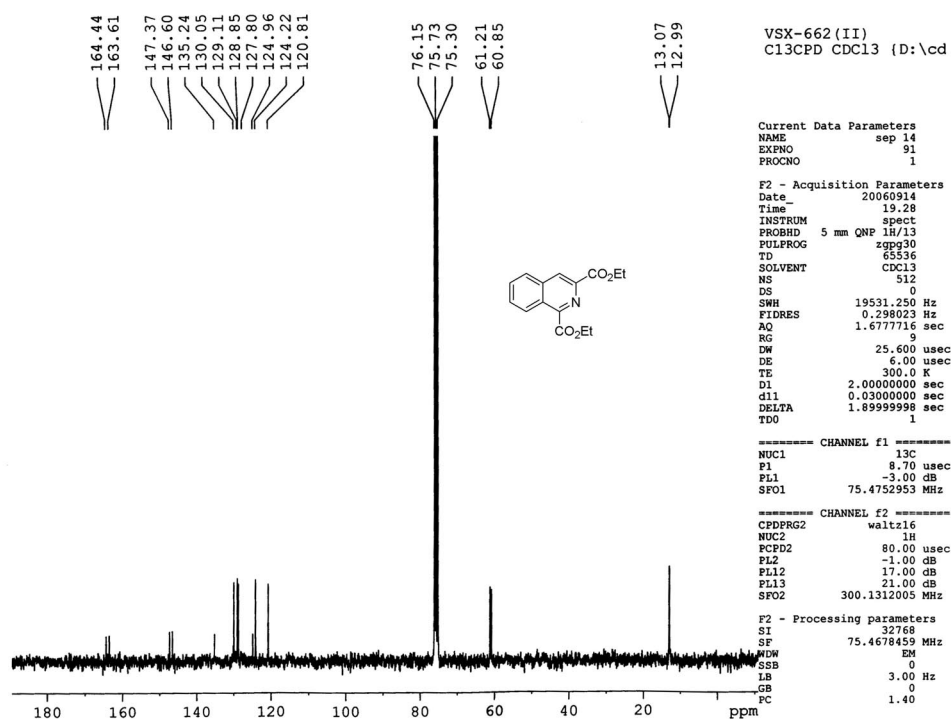


Fig.-52: ^{13}C NMR spectrum of compound **19a**

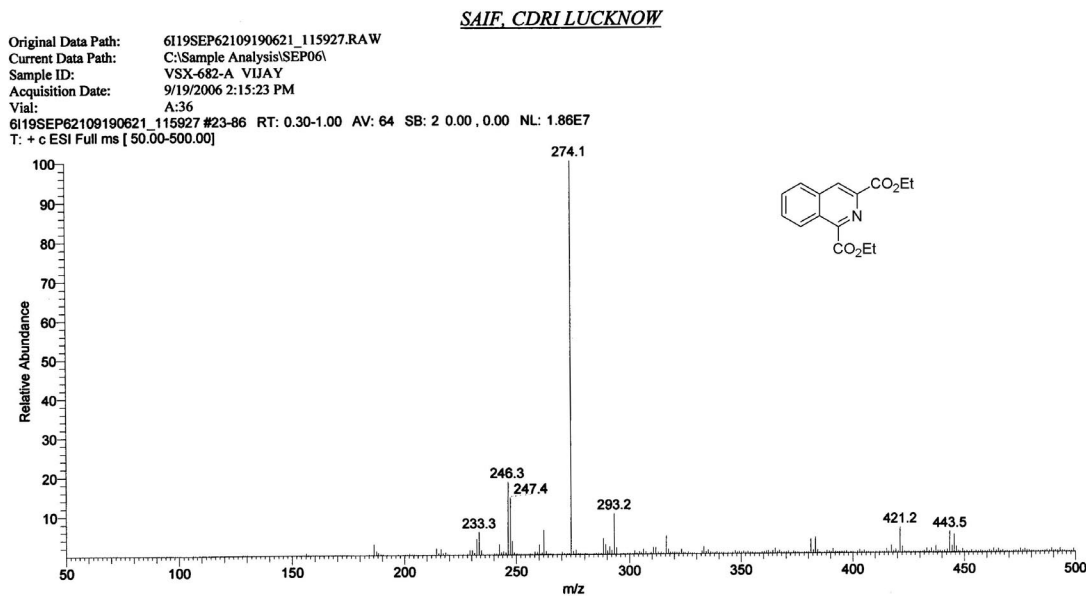


Fig.-53: Mass spectrum of compound **19a**

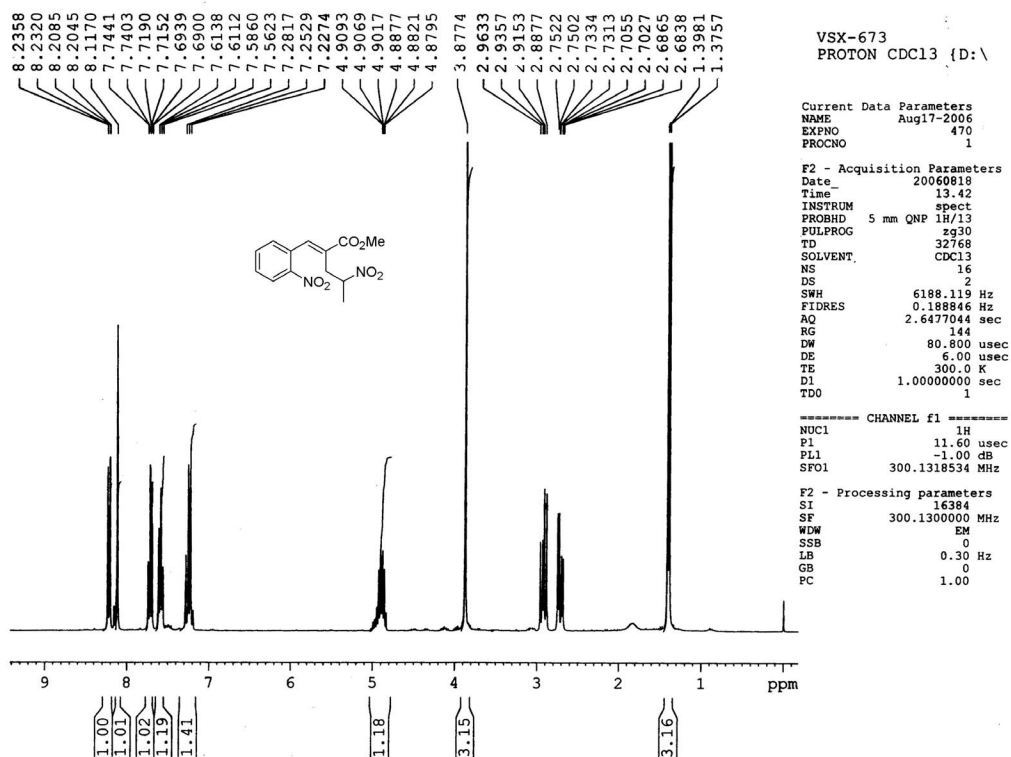


Fig-7: ^1H NMR spectrum of compound 21a

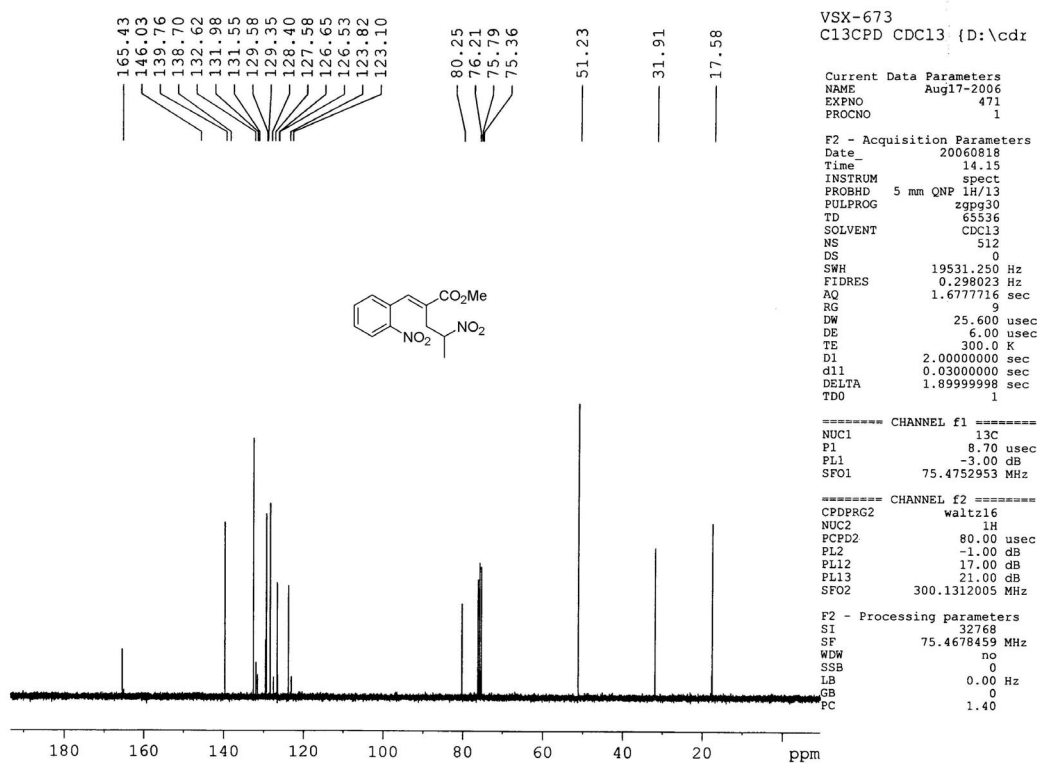


Fig-8: ^{13}C NMR spectrum of compound 21a

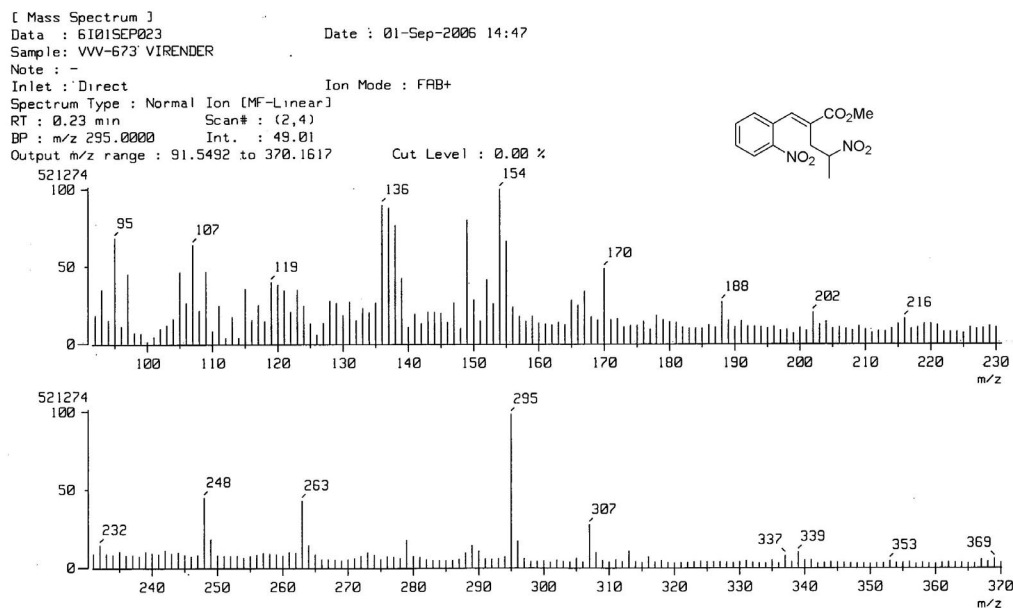


Fig.-9: Mass spectrum of compound 21a

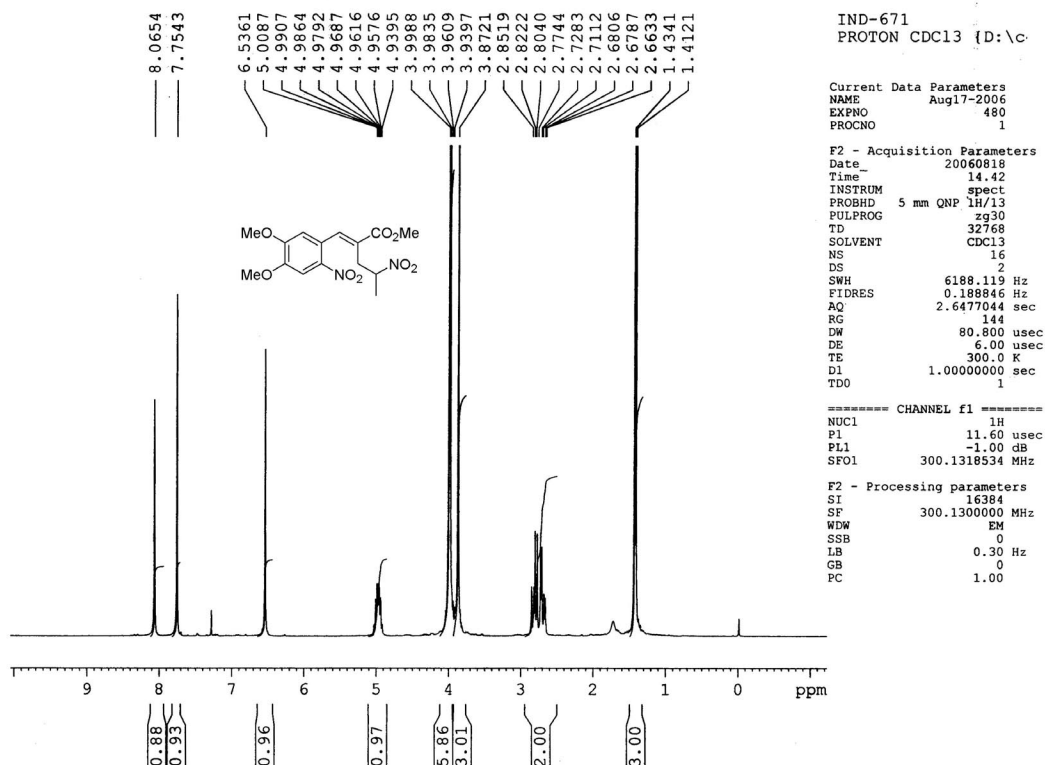


Fig.-10: ¹H NMR spectrum of compound 21d

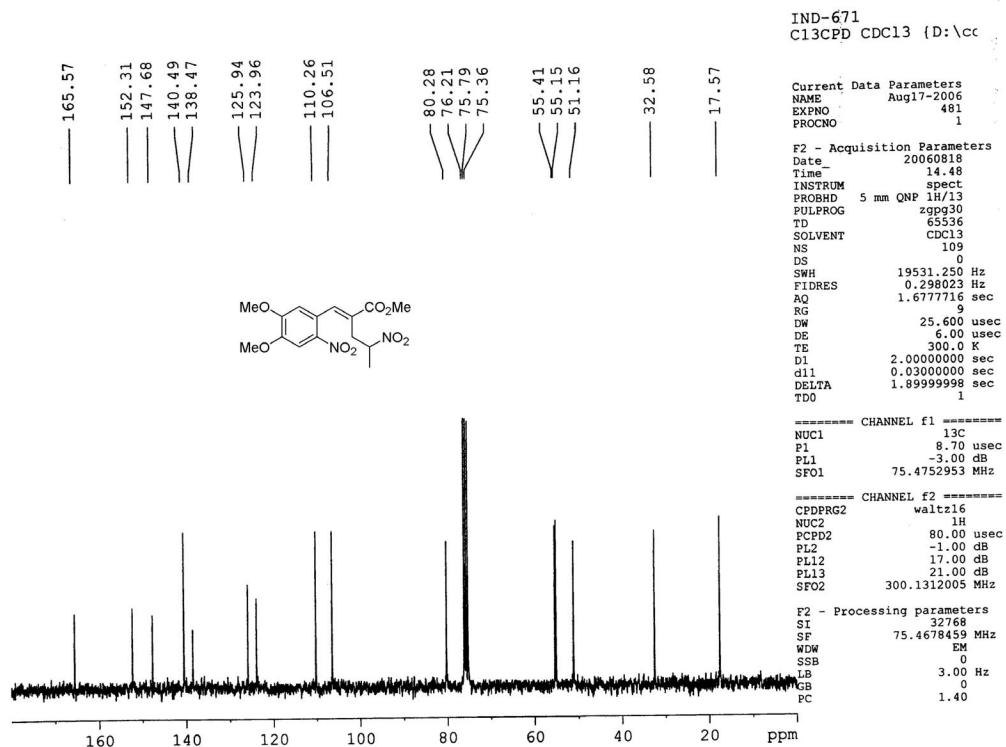


Fig.-11: ¹³C NMR spectrum of compound 21d

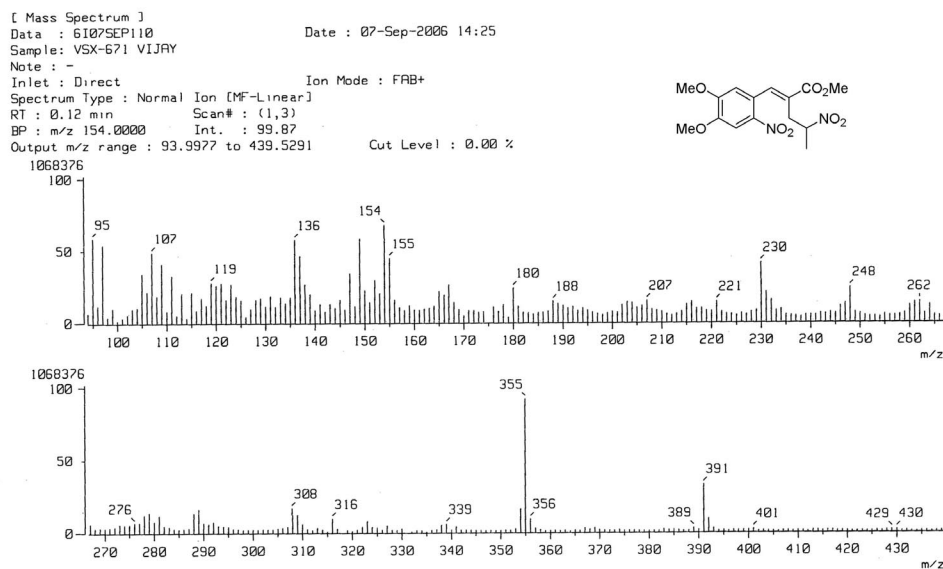


Fig.-12: Mass spectrum of compound 21d

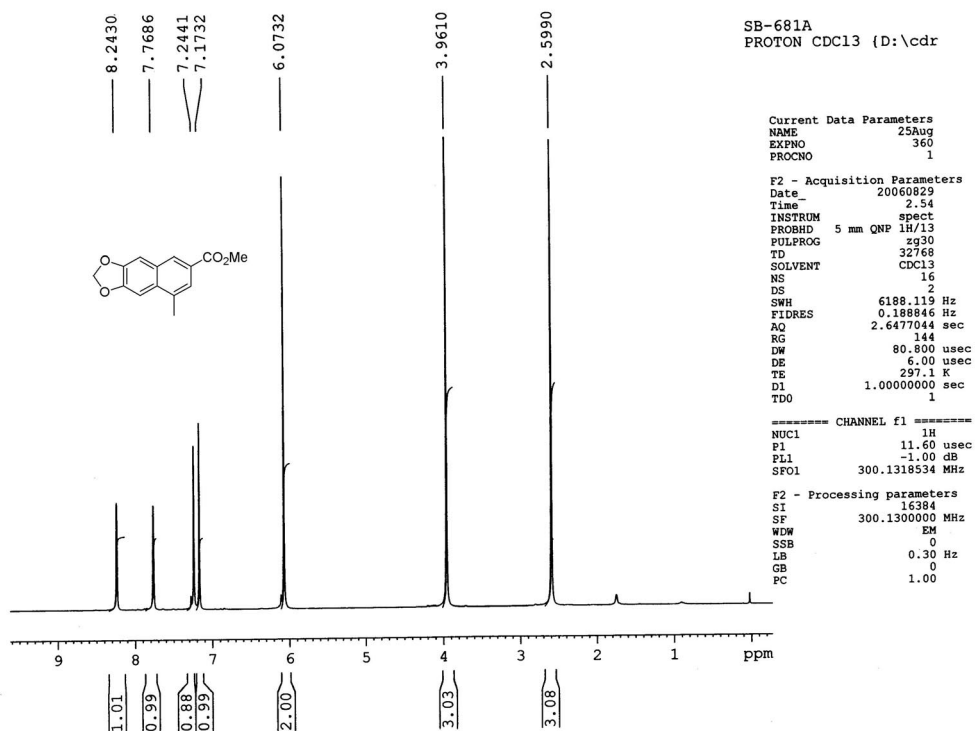


Fig.-13: ^1H NMR spectrum of compound **23c**

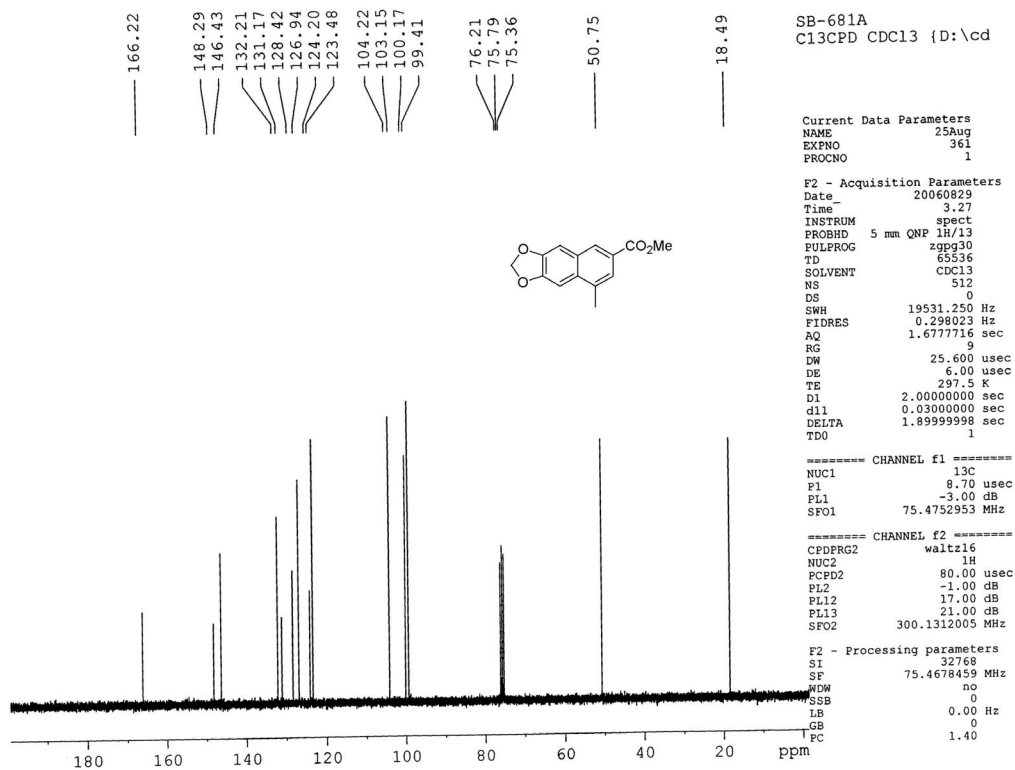


Fig.-14: ^{13}C NMR spectrum of compound **23c**

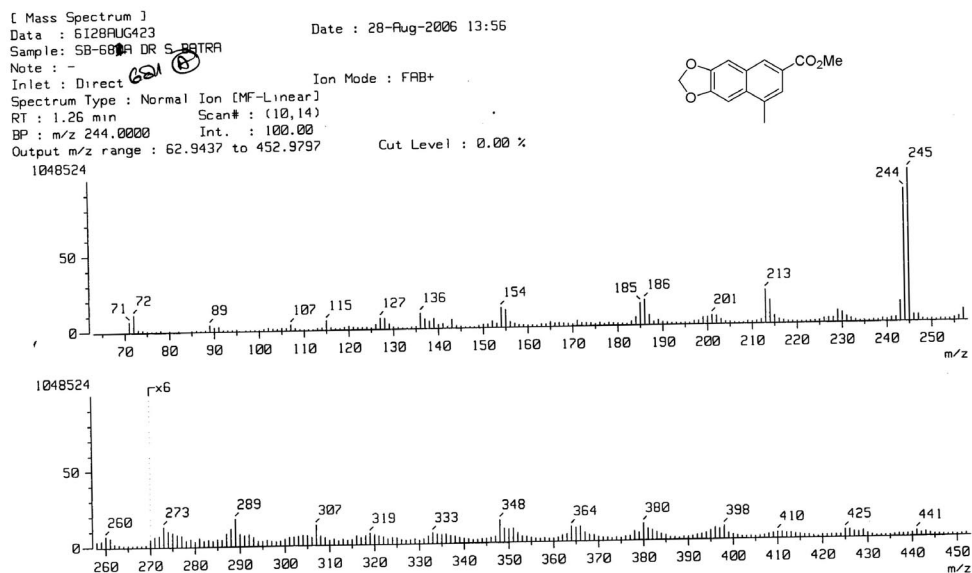


Fig.-15: Mass spectrum of compound 23c

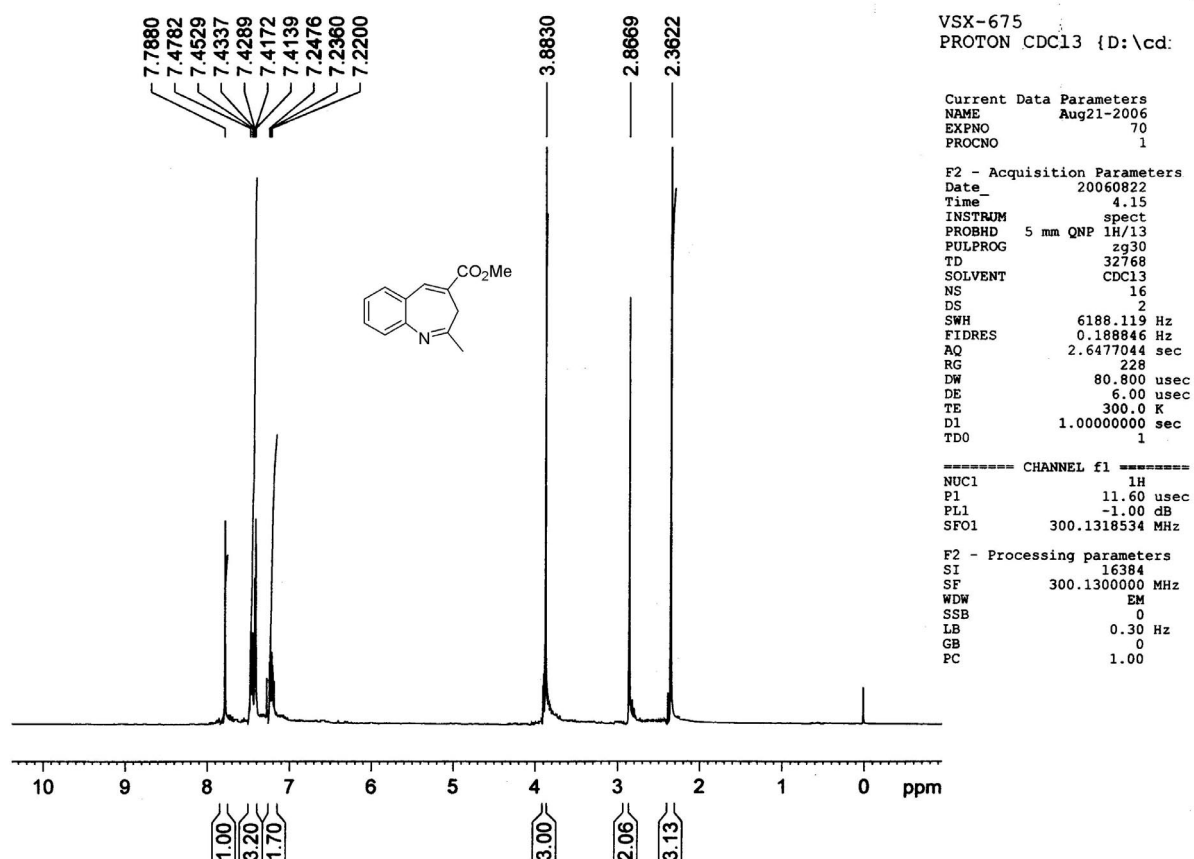


Fig.-33: ¹H NMR spectrum of compound 25a

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 Data Path: C:\Sample Analysis\AUG06\
 ID: VSX-675 VIJAY
 ion Date: 8/24/2006 2:43:05 PM
 A:11

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372108240723_120029 #29-101 RT: 0.30-1.00 AV: 73 SB: 2 0.00, 0.00 NL: 4.21E7
 SI Full ms [50.00-500.00]

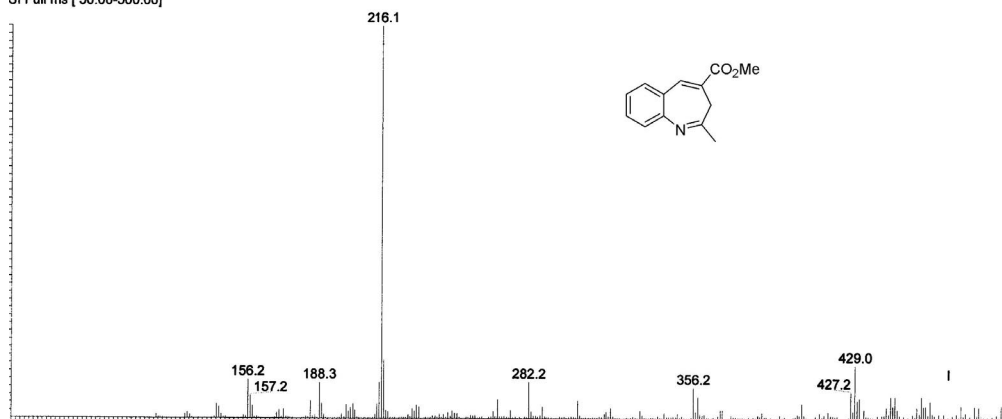


Fig.-34: Mass spectrum of compound **25a**

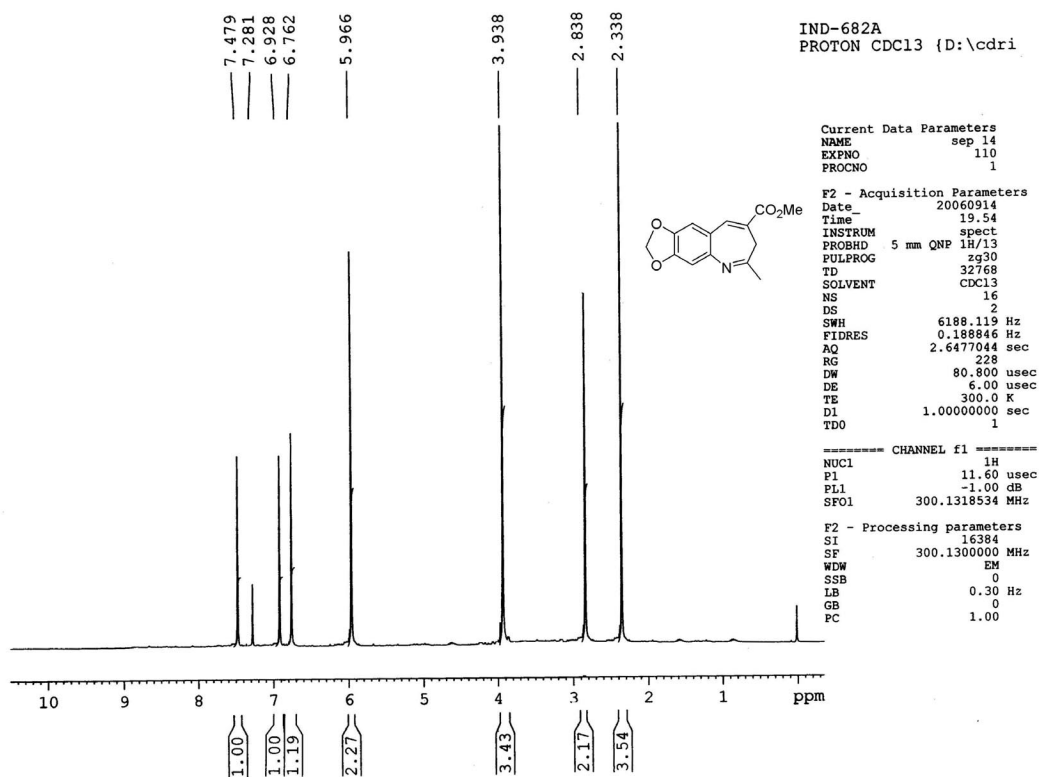


Fig.-35: ^1H NMR spectrum of compound **25c**

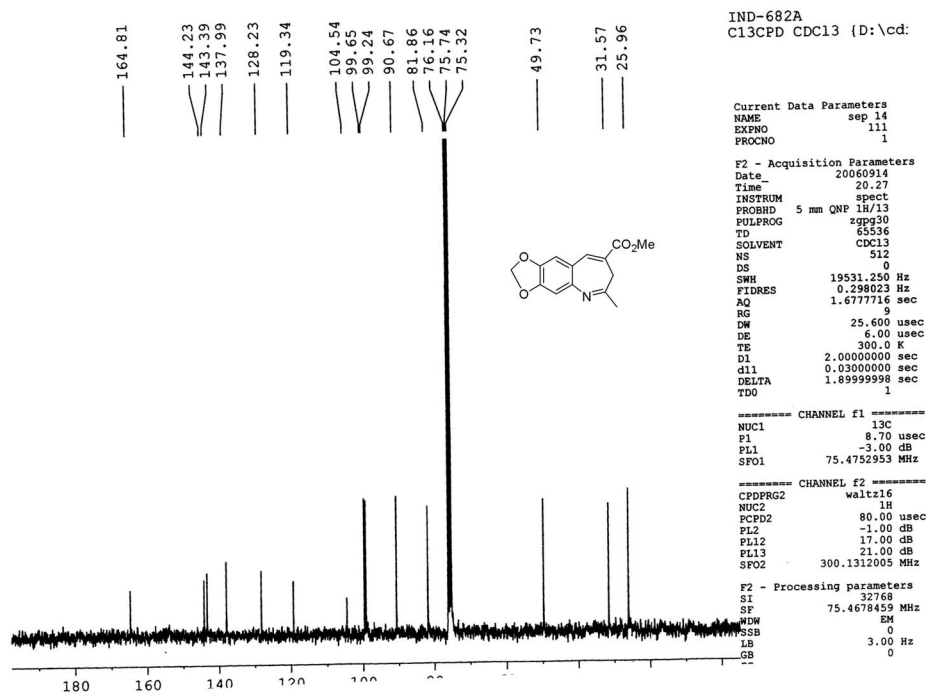


Fig.-36: ^{13}C NMR spectrum of compound **25c**

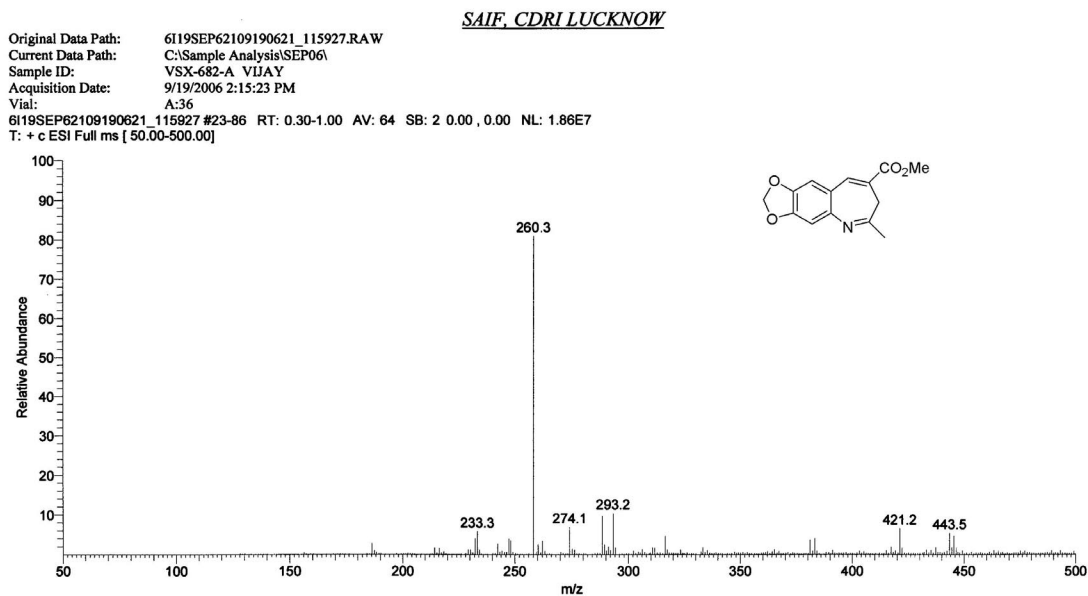


Fig.-37: Mass spectrum of compound **25c**

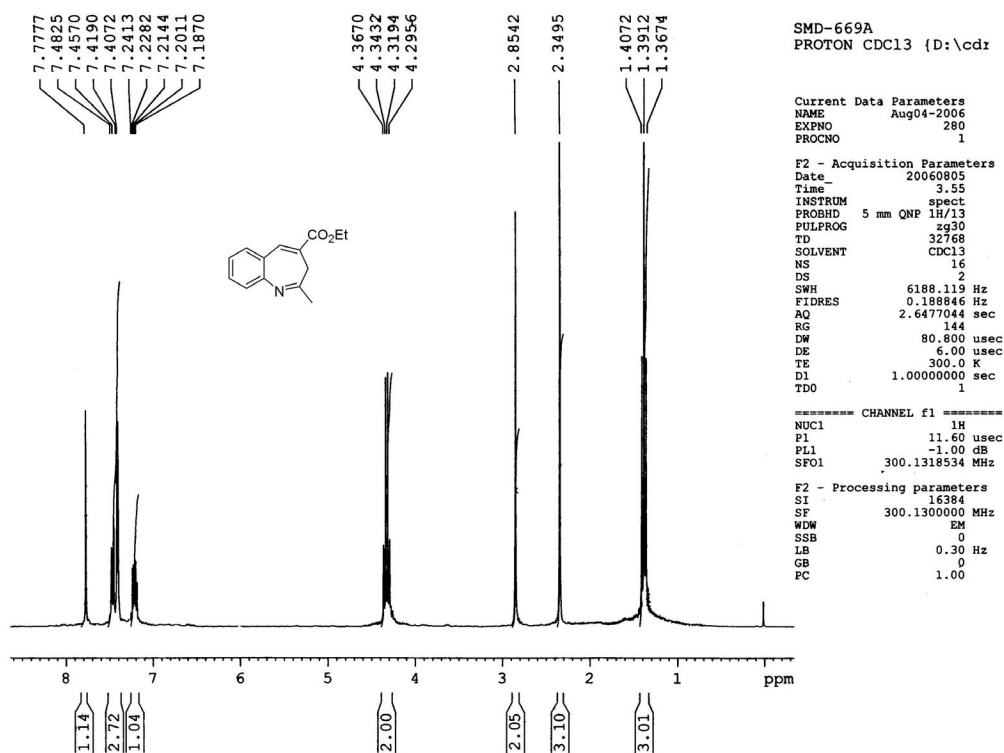


Fig.-37: ^1H NMR spectrum of compound **26a**

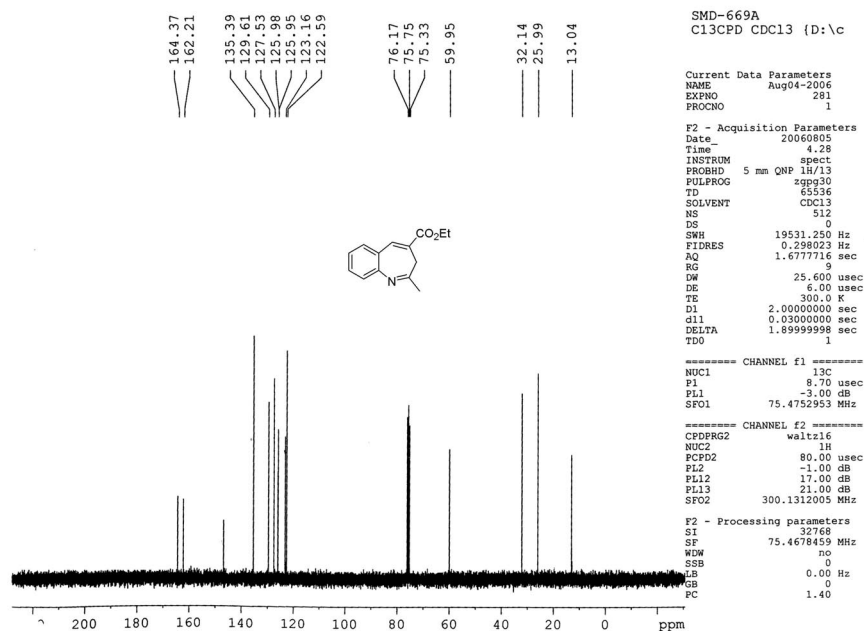


Fig.-39: ^{13}C NMR spectrum of compound **26a**

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 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]

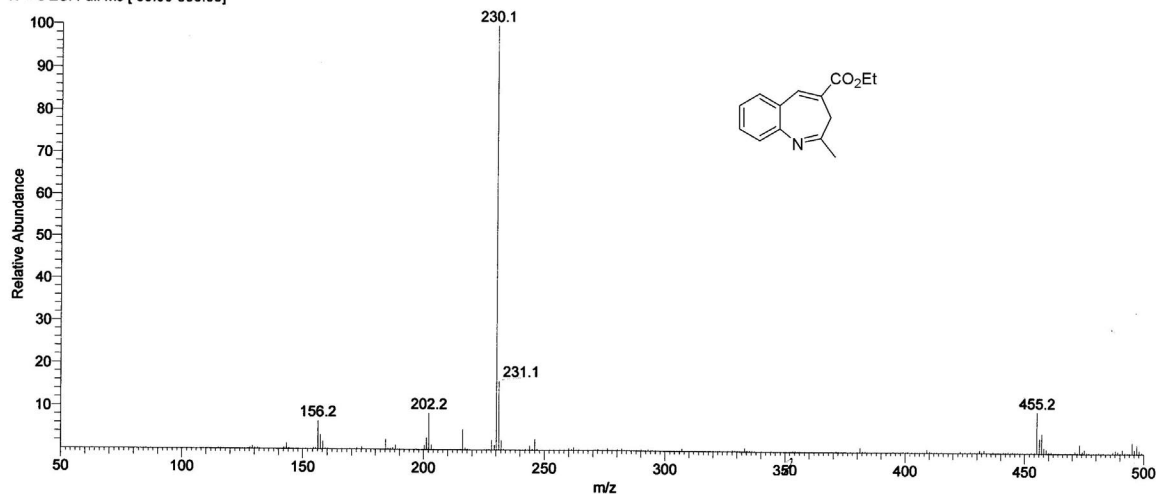
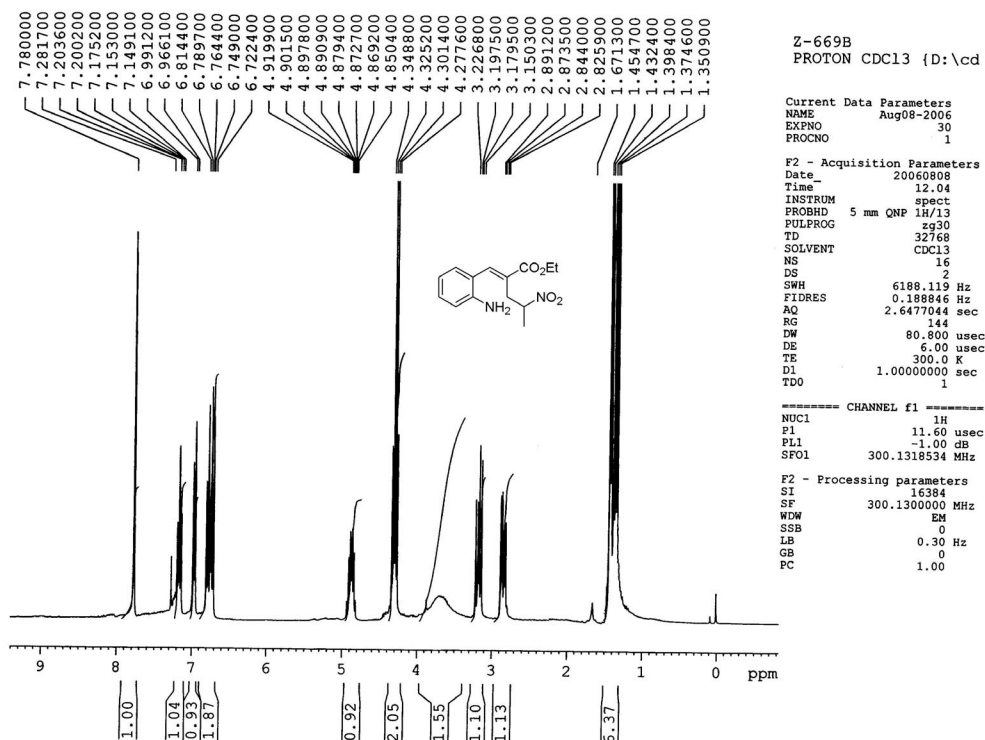


Fig.-40: Mass spectrum of compound 26a

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

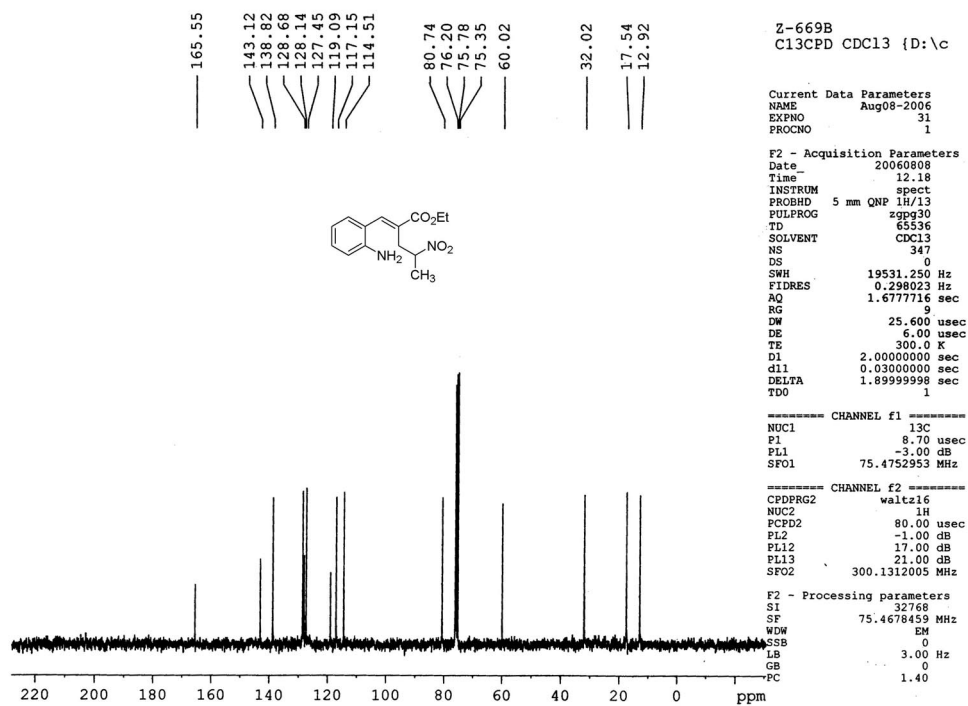


Fig.-55: ^{13}C NMR spectrum of compound 27a.

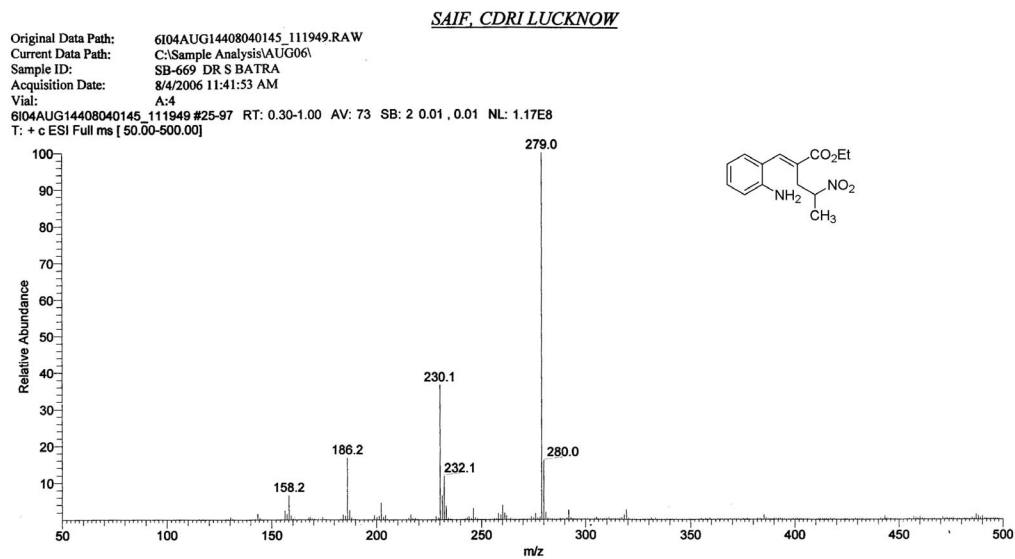


Fig.-56: Mass spectrum of compound 27a.