Electronic Supplementary Material (ESI) for RSC Advances

Zinc triflate catalyzed regioselective synthesis of pyrrolo[2,3-*c*]carbazoles via heteroannulation

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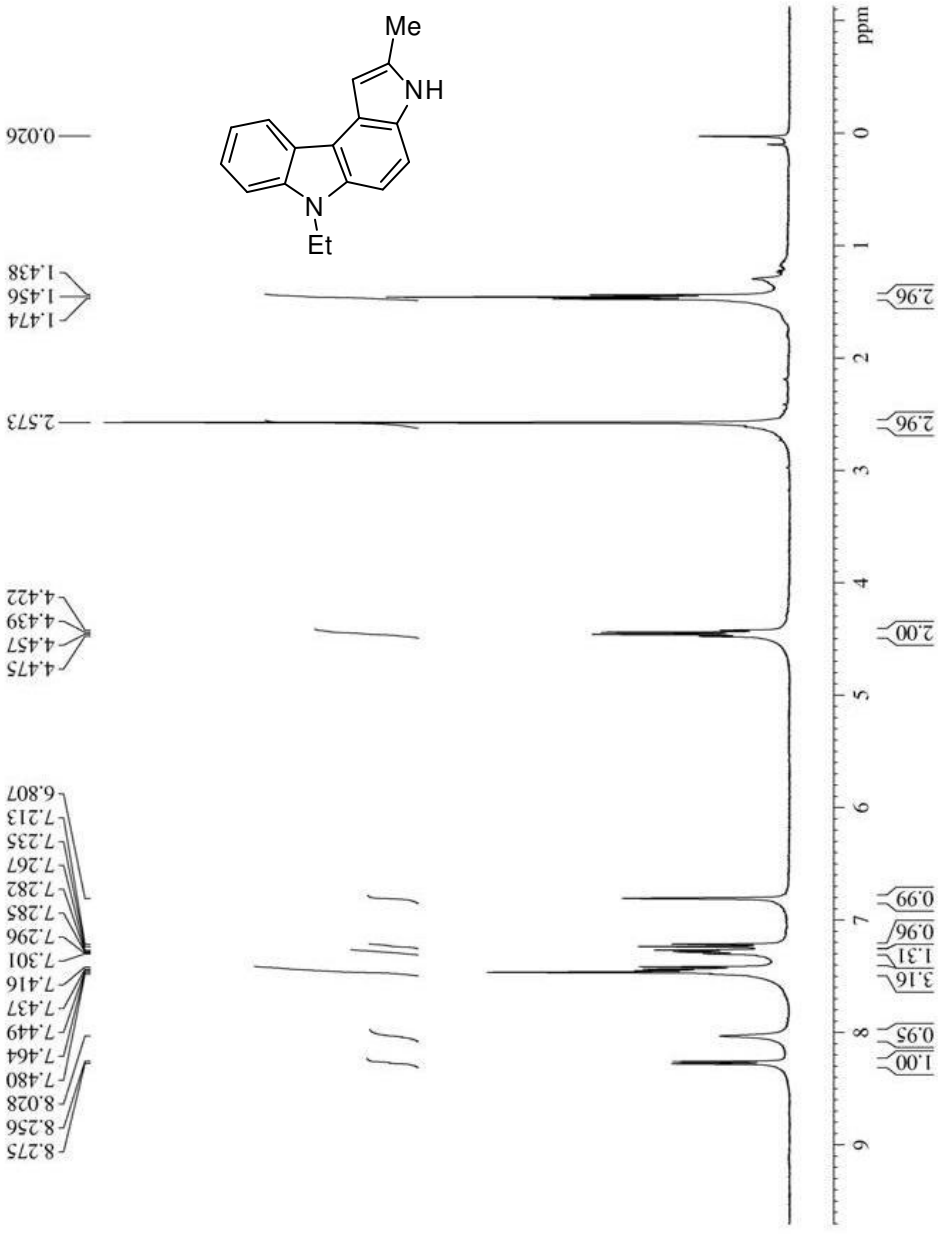
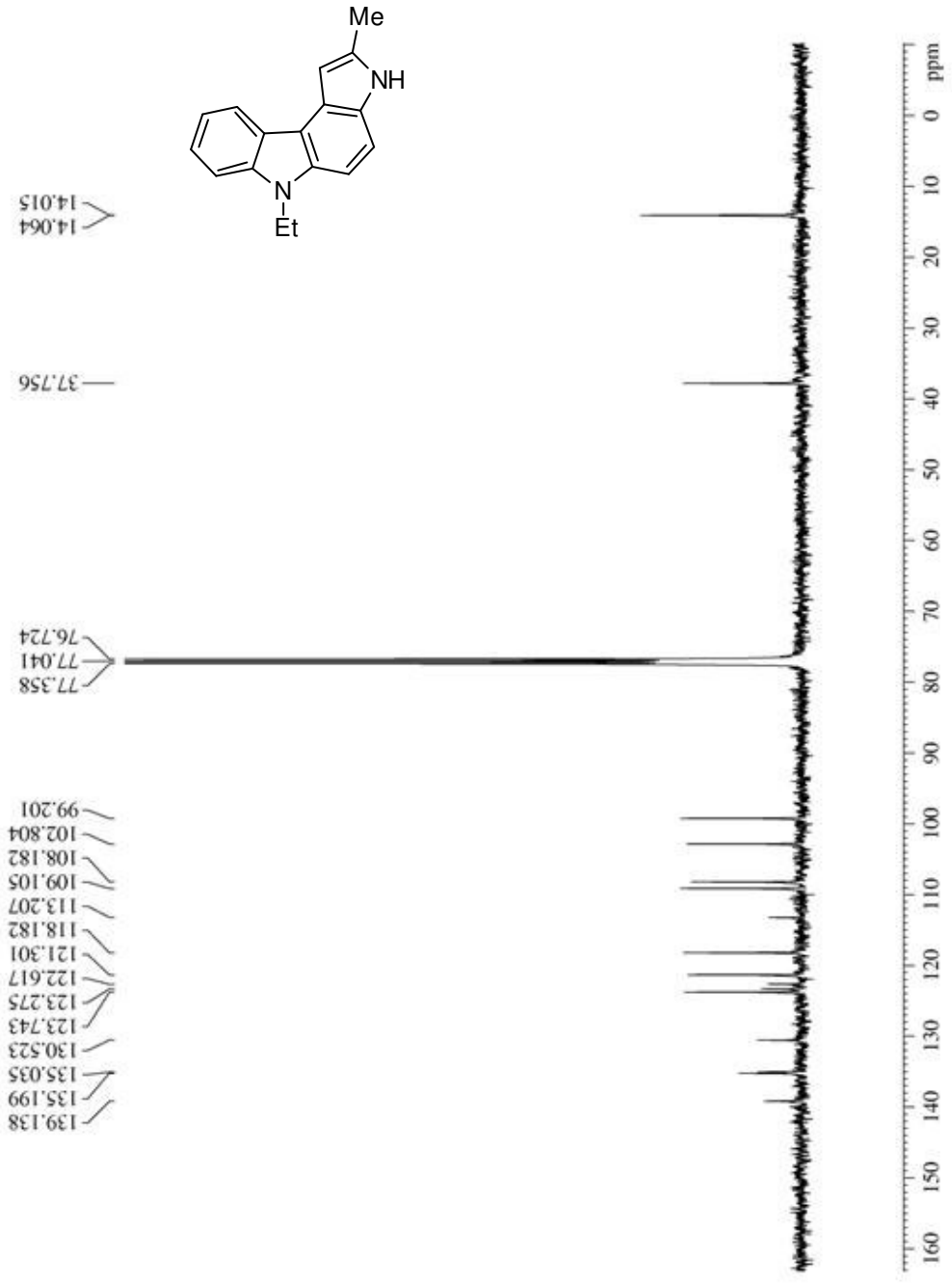
Analytical Data

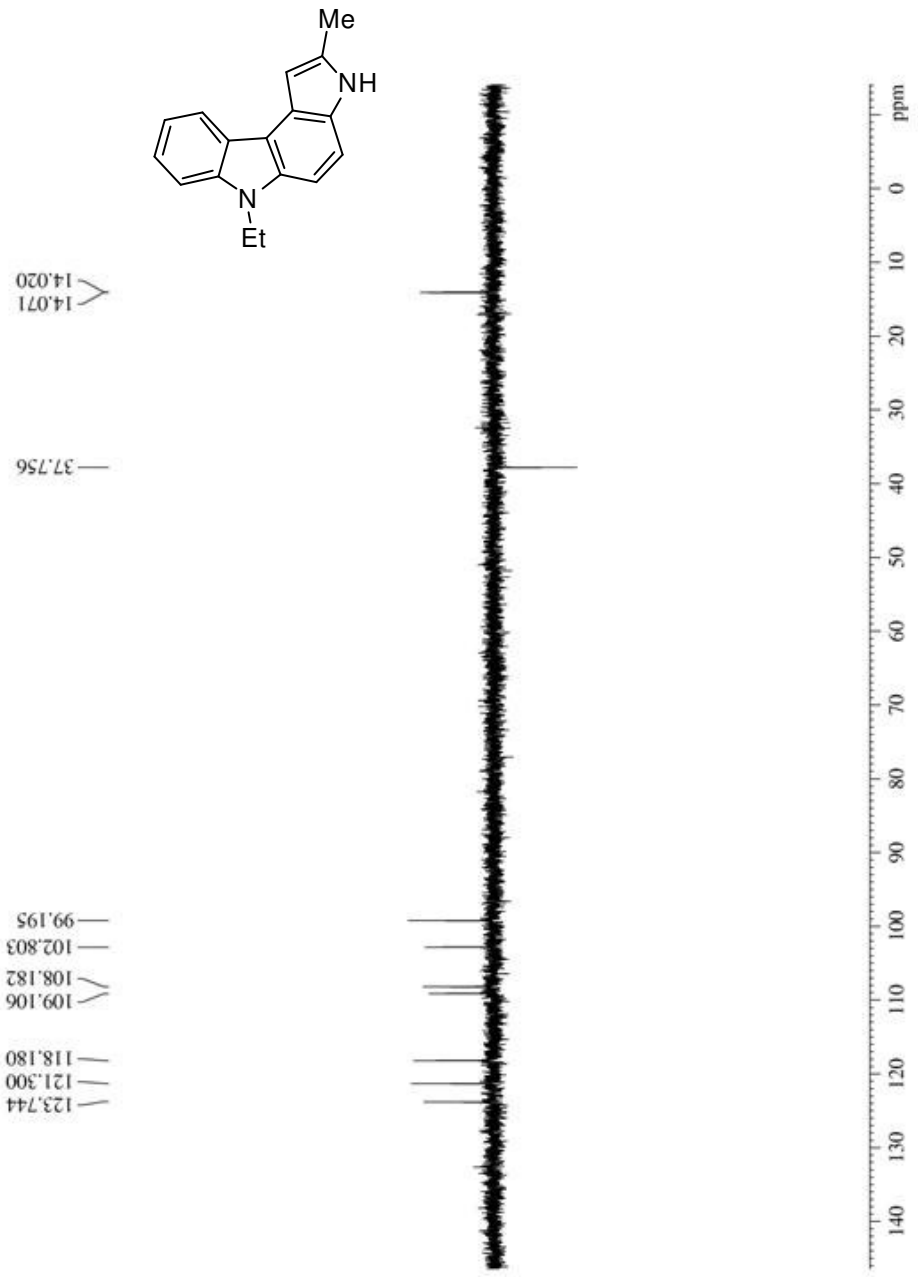
^{1}H NMR of 6-Ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3a):



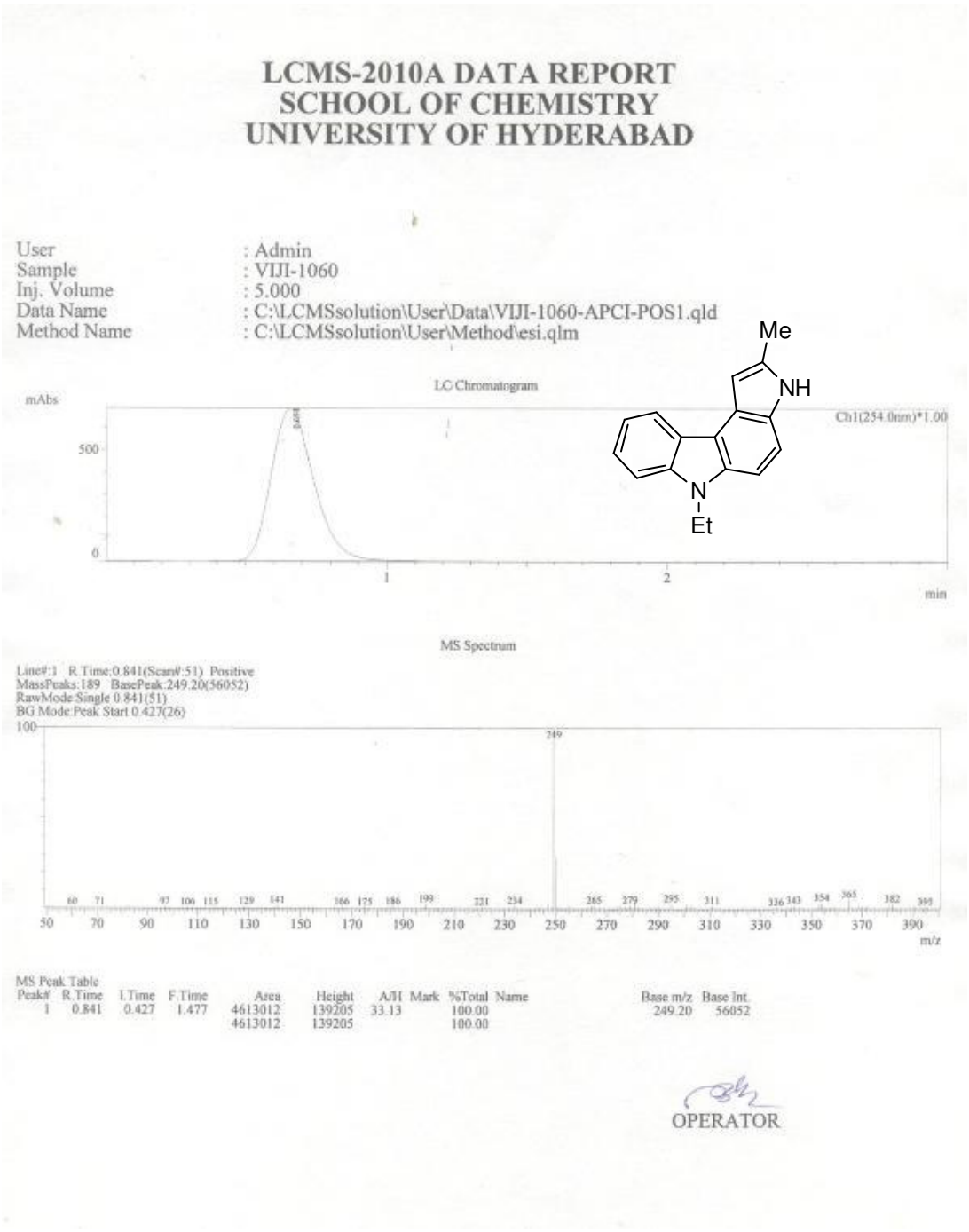
^{13}C NMR of 6-Ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3a):



DEPT of 6-Ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3a):



LC-MS of 6-Ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3a):



LCMS-2010A DATA REPORT
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User : Admin
Sample : VIJI-1060
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\VIJI-1060-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram

MS Spectrum

Line#:1 R.Time:0.841(Scan#:51) Positive
MassPeaks:189 BasePeak:249.20(56052)
RawMode:Single 0.841(51)
BG Mode:Peak Start 0.427(26)

MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.841	0.427	1.477	4613012	139205	33.13		100.00		249.20	56052
				4613012	139205			100.00			

OPERATOR

Elemental Analysis of 6-Ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3a):

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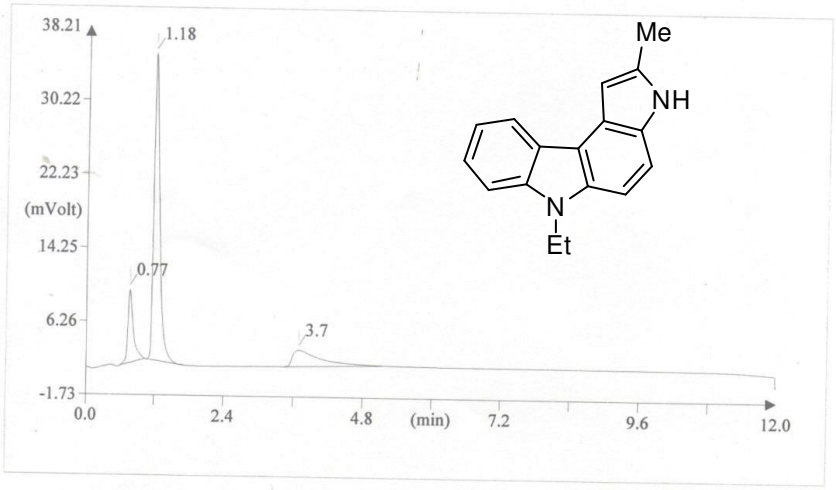
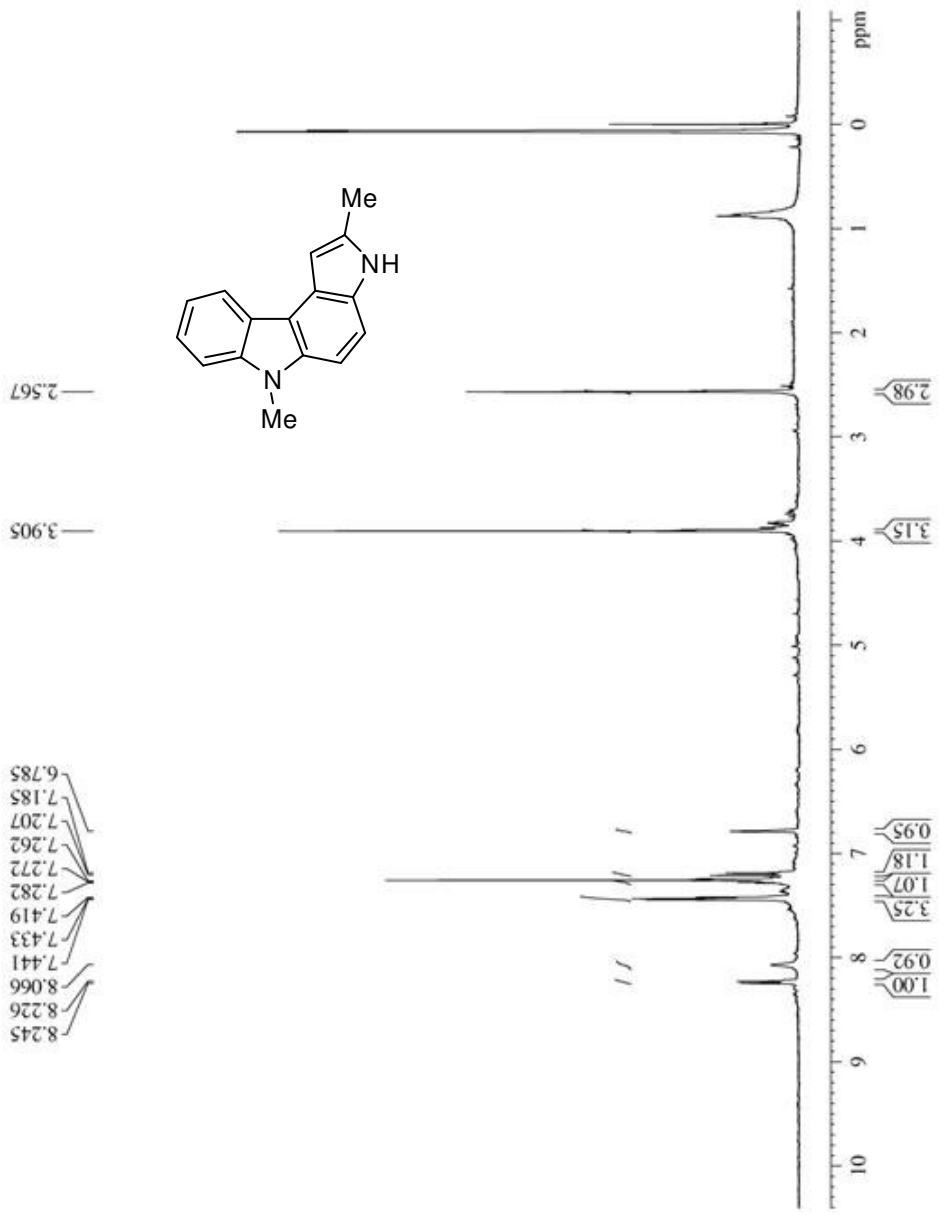
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1074 (# 67)
Analysis type:	UnkNown
Chromatogram filename:	UNK-17102011-17.dat
Sample weight:	.982

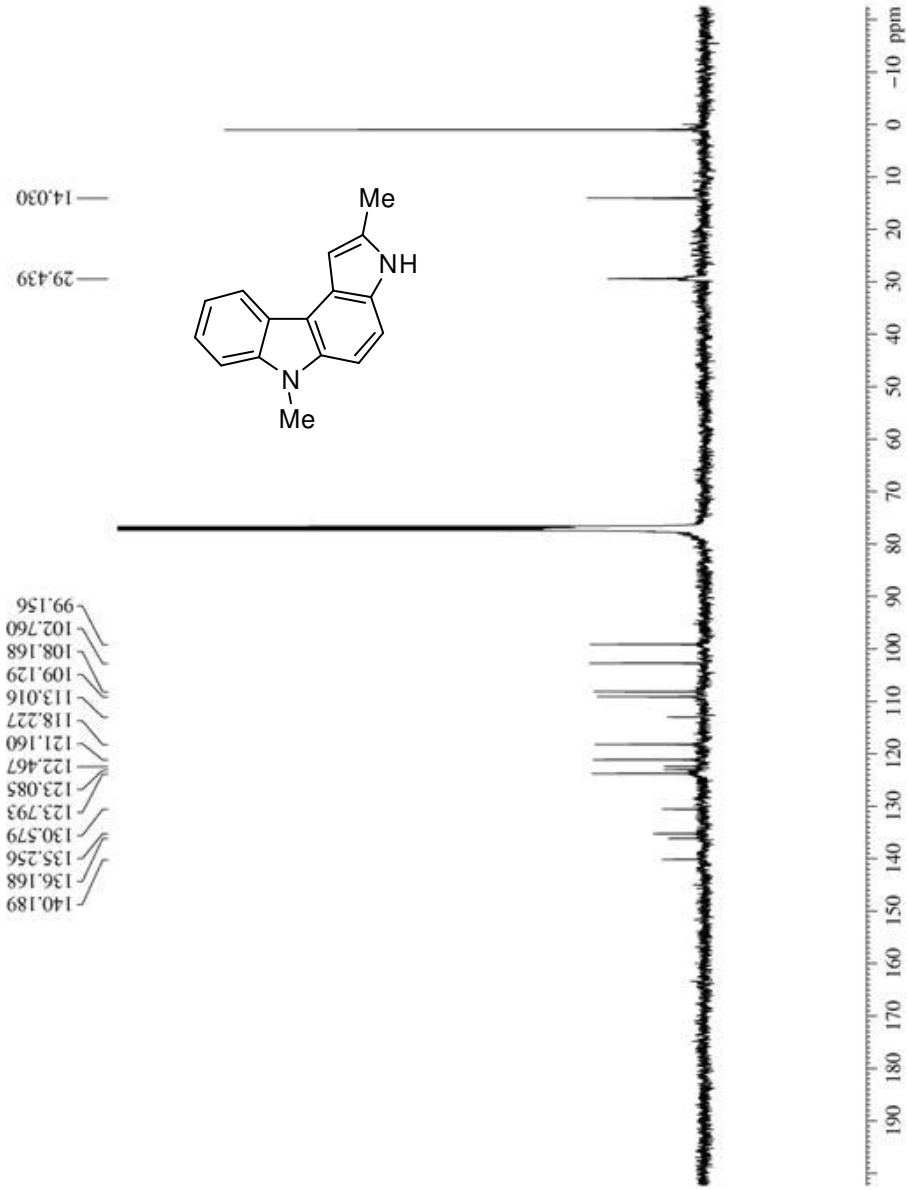


Element Name	Element %	Ret. Time
Nitrogen	11. 15	0. 77
Carbon	82. 36	1. 18
Hydrogen	6. 55	3. 70

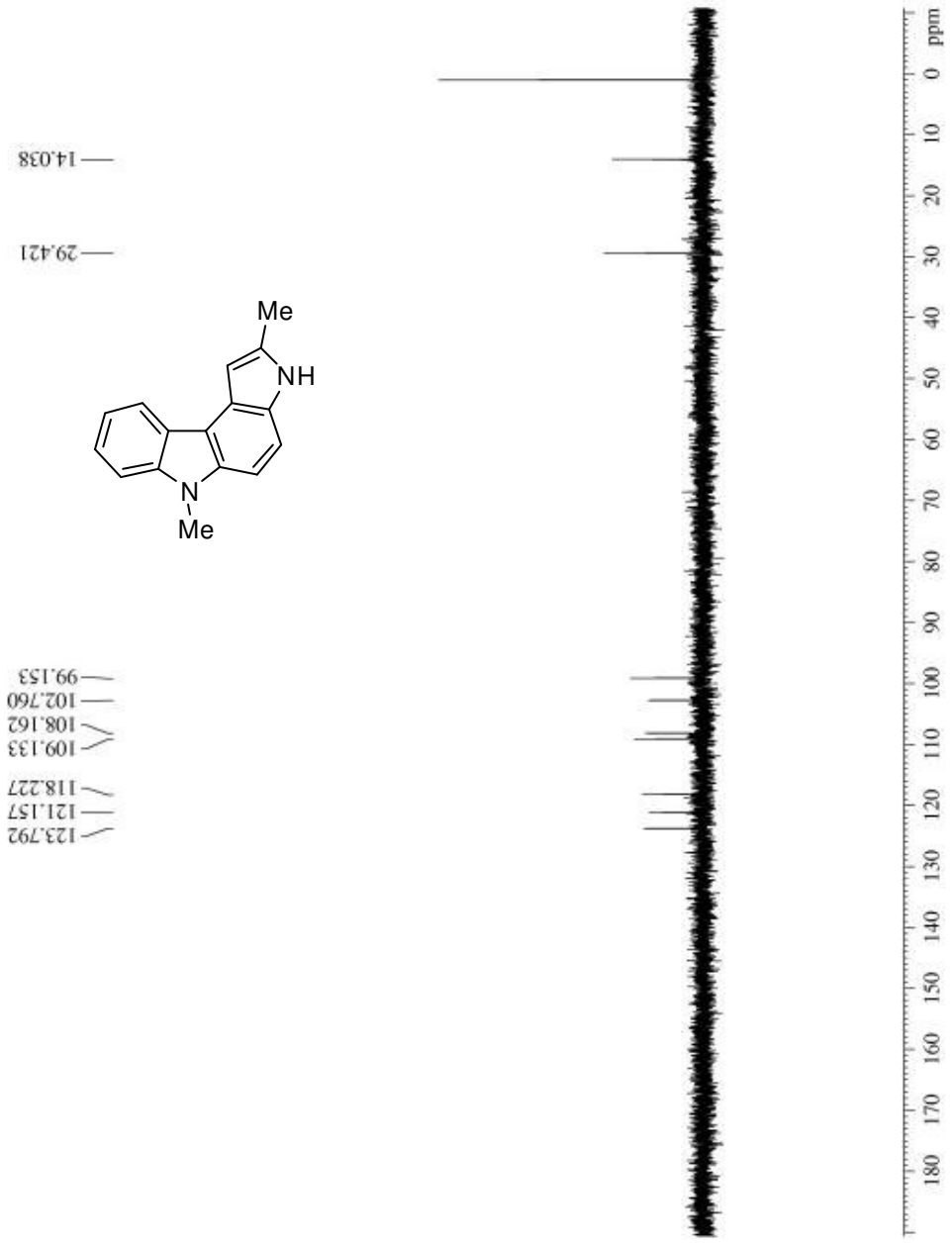
^{1}H NMR of 2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3b)



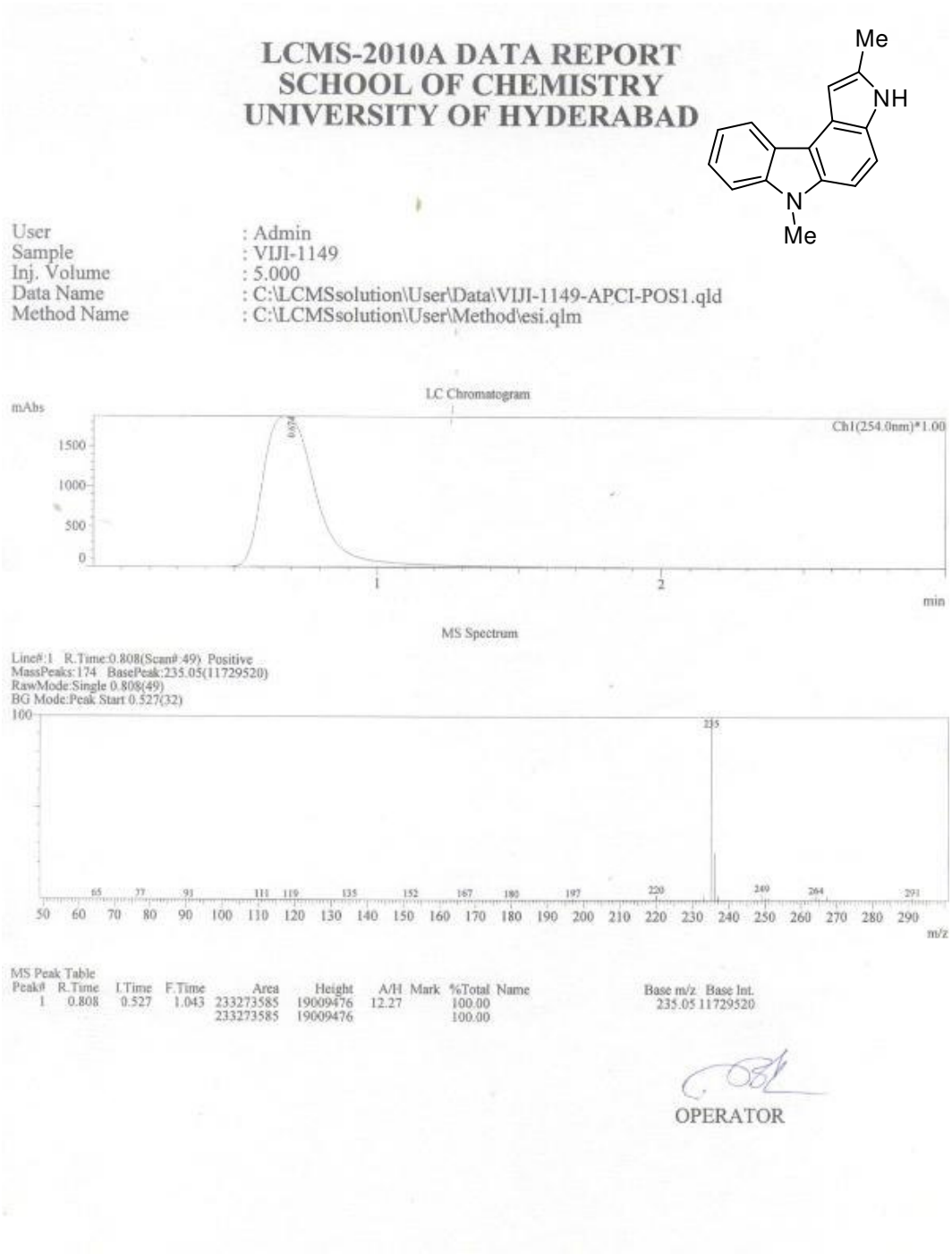
^{13}C NMR of 2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3b)



DEPT of 2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3b)



LC-MS of 2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3b)



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Elemental Analysis of 2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3b)

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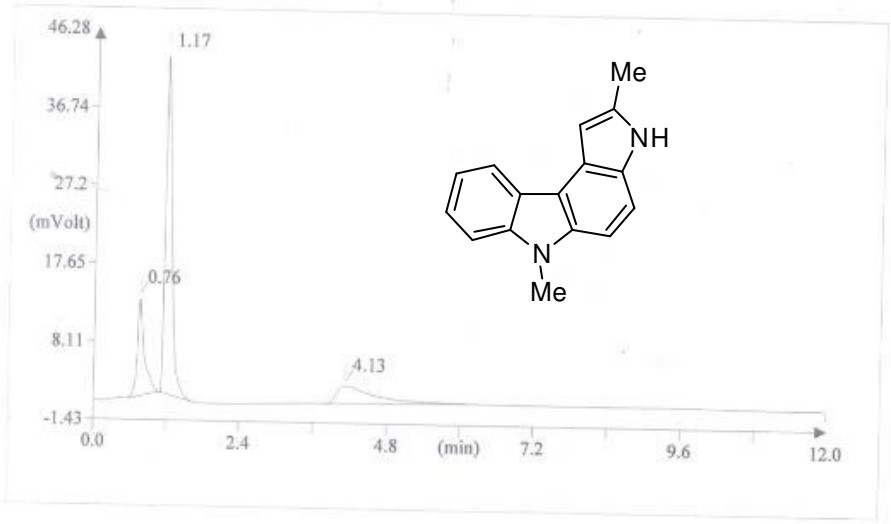
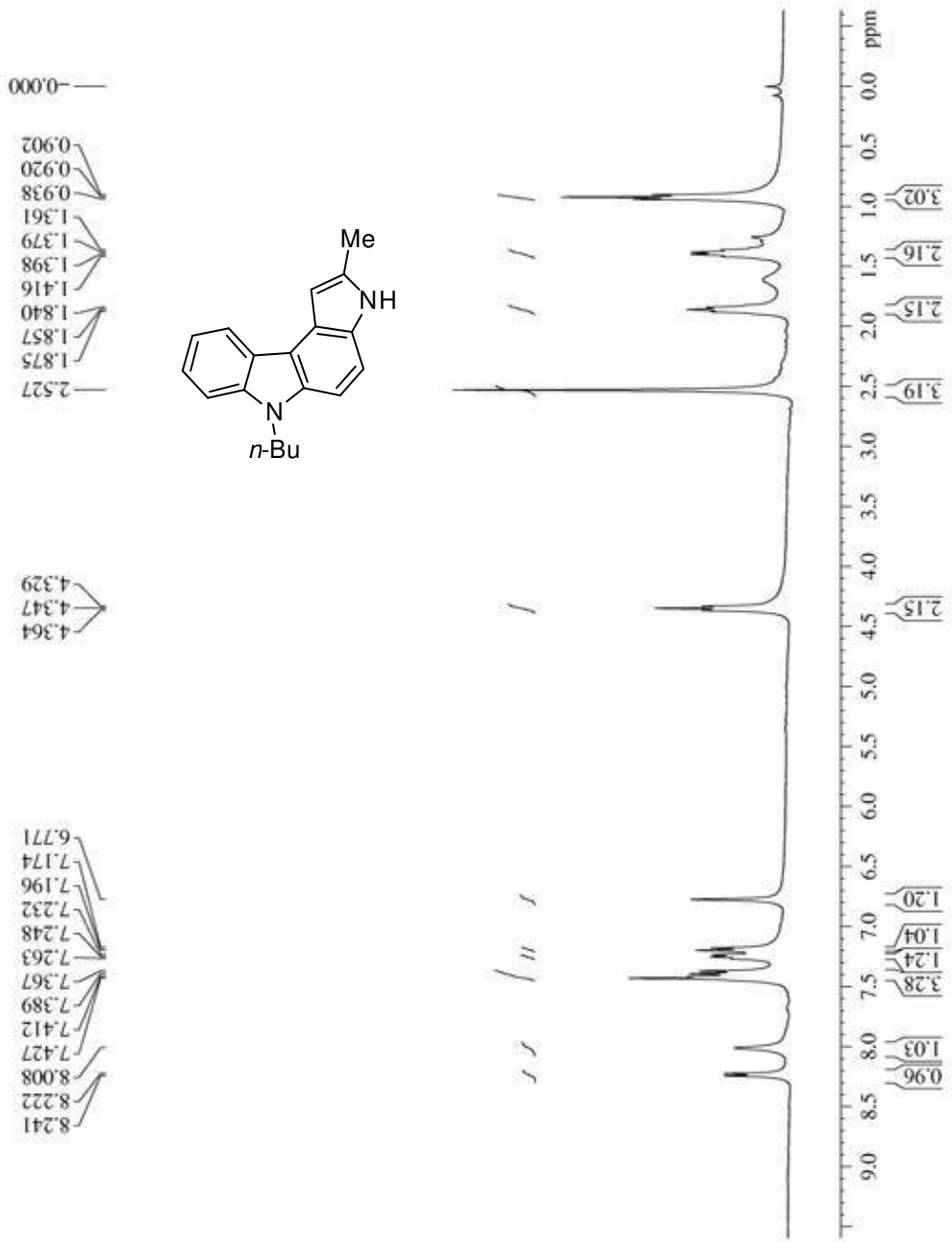
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1149 (# 15)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-15.dat
Sample weight:	1.132

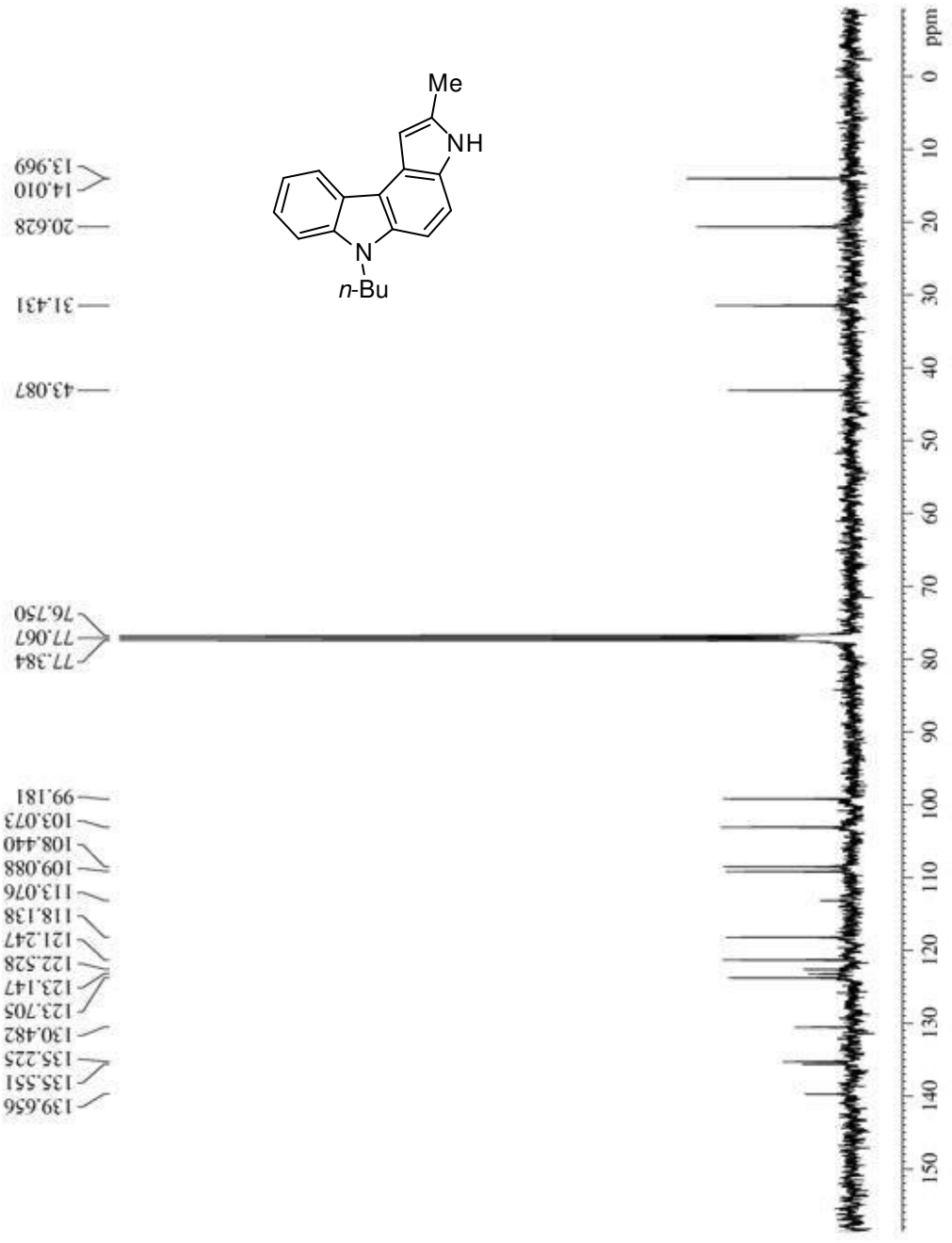


Element Name	Element %	Ret. Time
Nitrogen	11. 78	0. 76
Carbon	81. 92	1. 17
Hydrogen	6. 12	4. 13

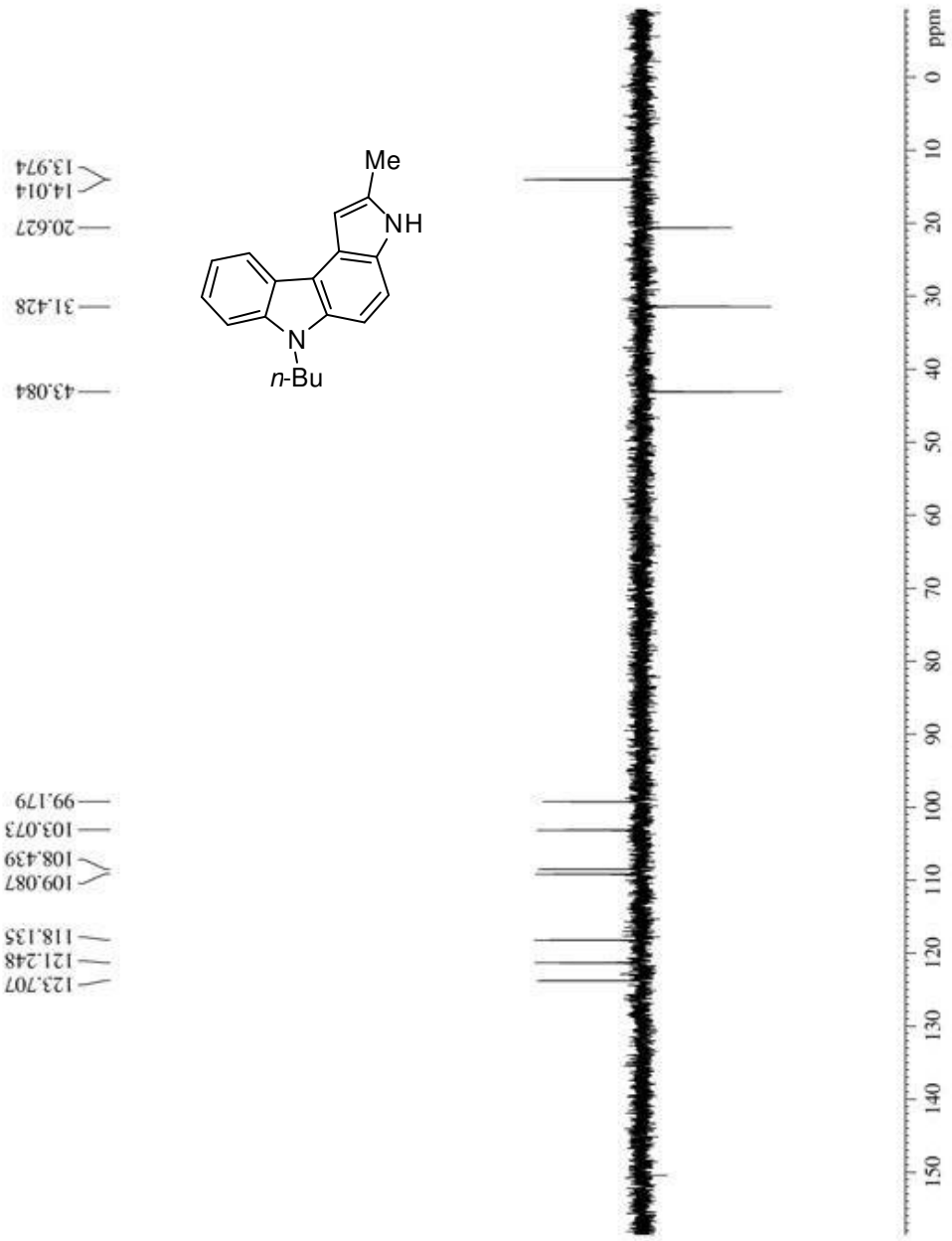
^{1}H NMR of 6-Butyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3c)



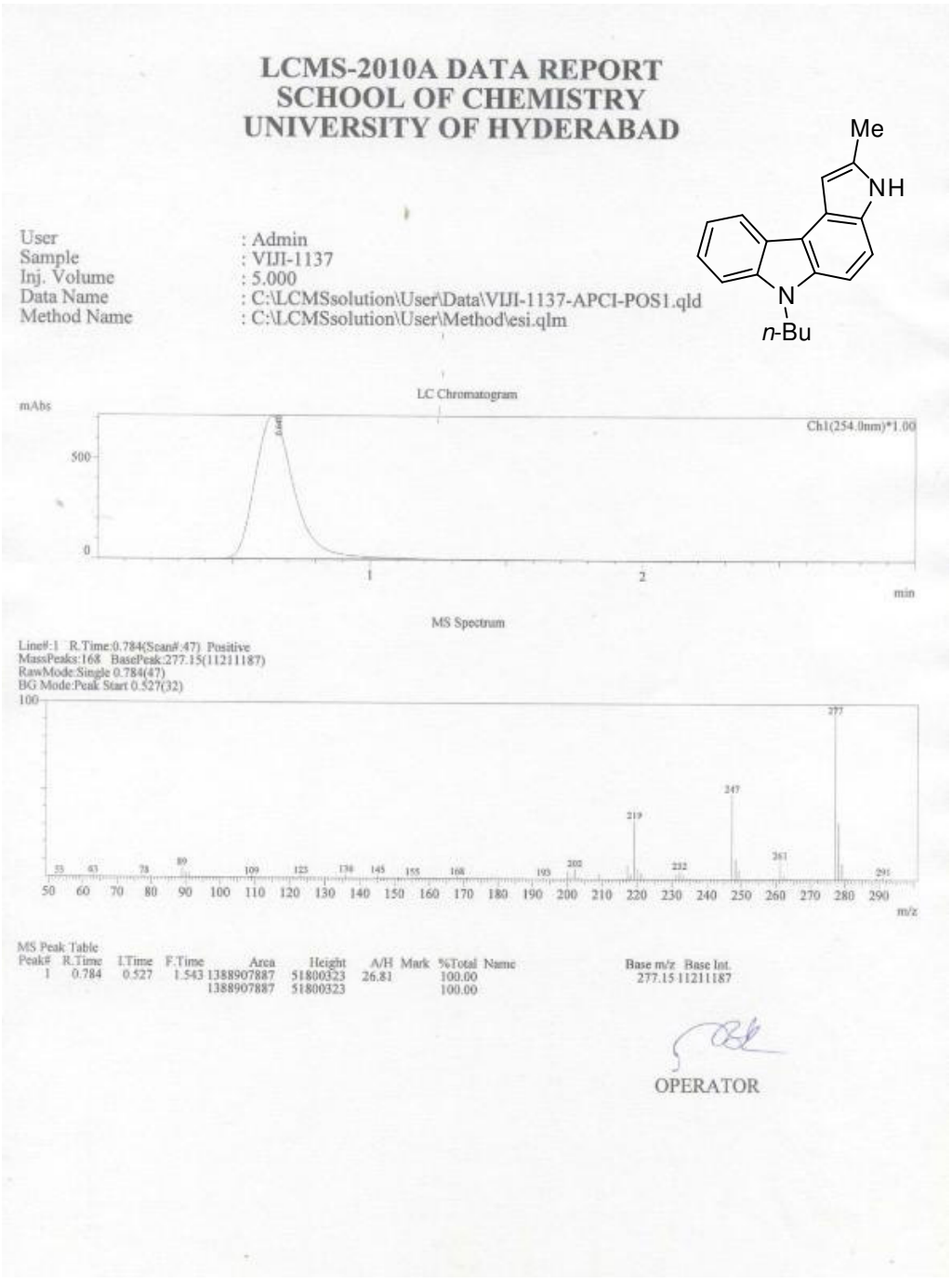
^{13}C NMR of 6-Butyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3c)



DEPT of 6-Butyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3c)



LC-MS of 6-Butyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3c)



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Elemental Analysis of 6-Butyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3c)

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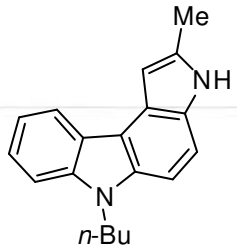
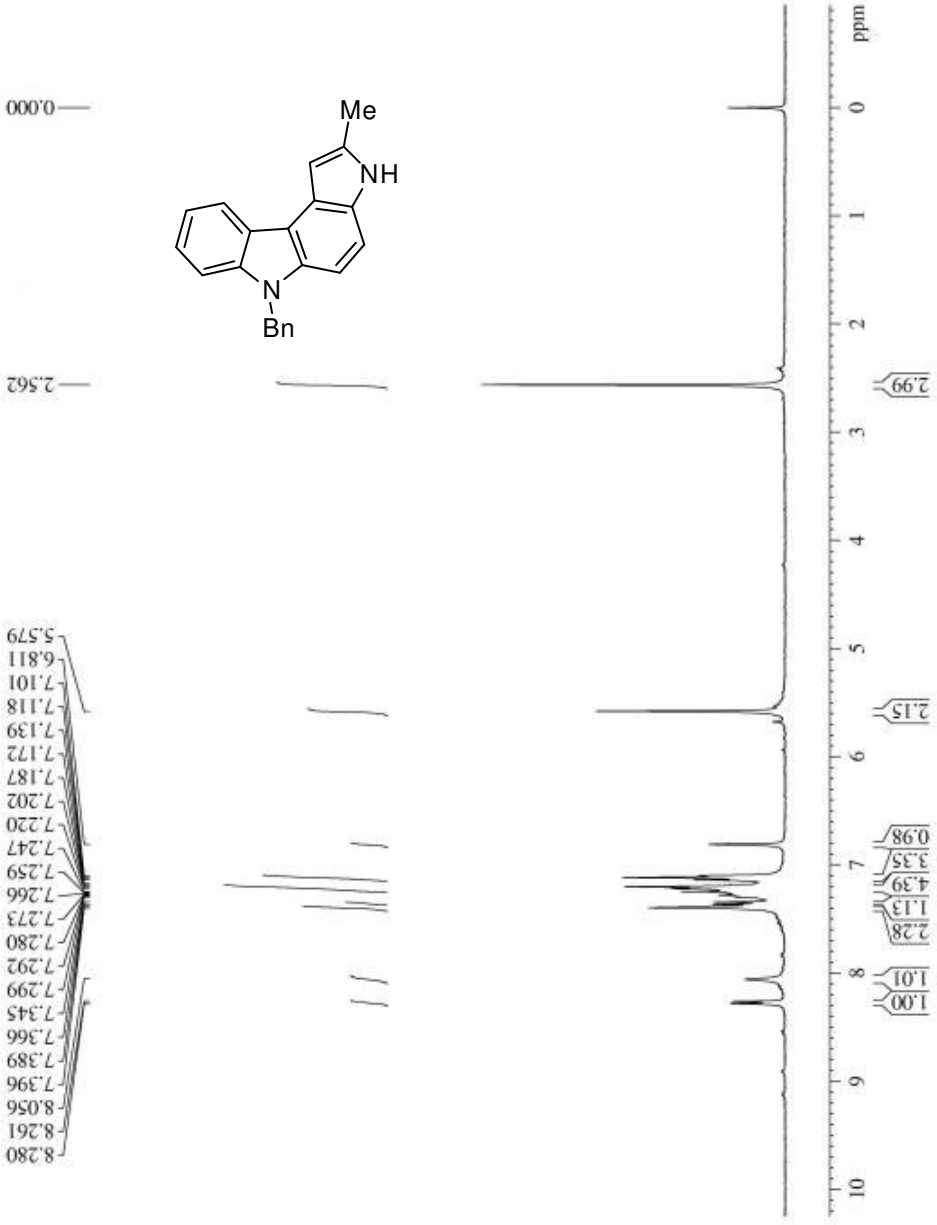
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1137 (# 14)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-14.dat
Sample weight:	1.129

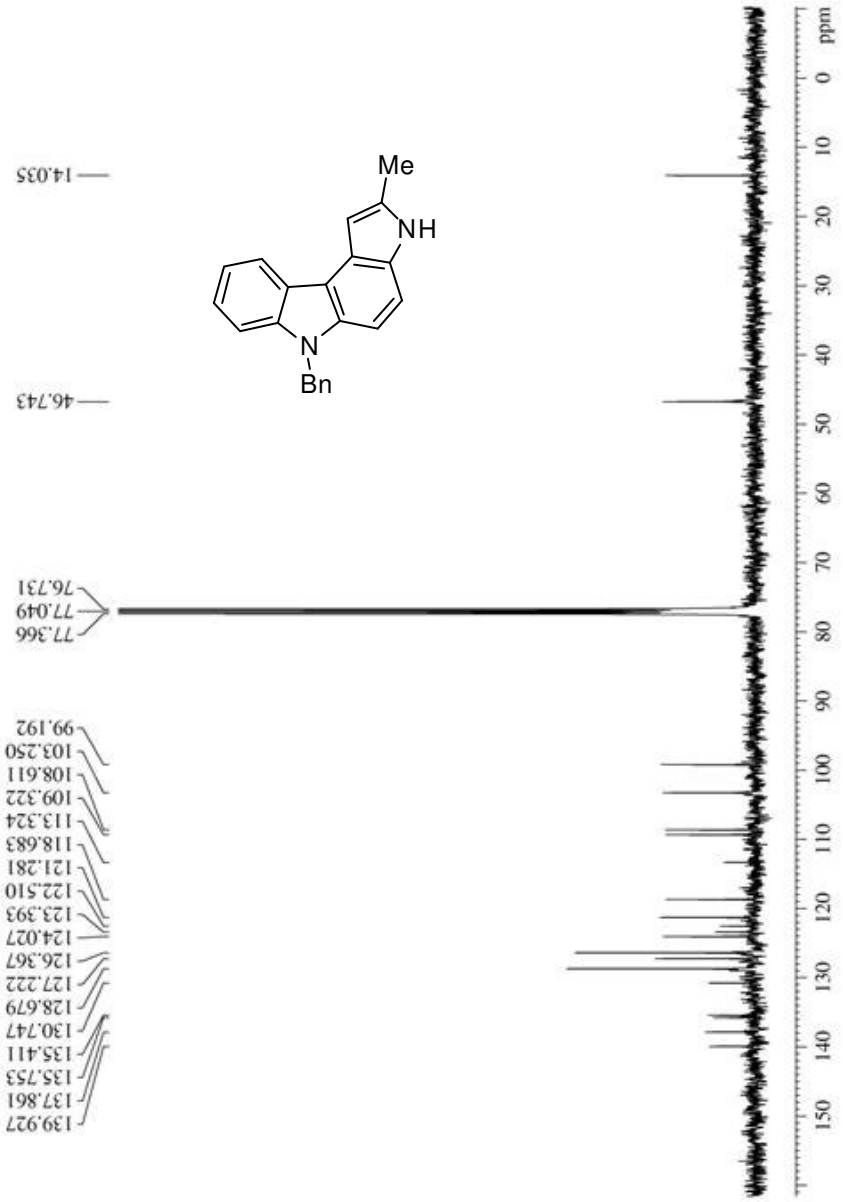


Element Name	Element %	Ret. Time
Nitrogen	10. 25	0. 88
Carbon	82. 45	1. 38
Hydrogen	7. 23	4. 67

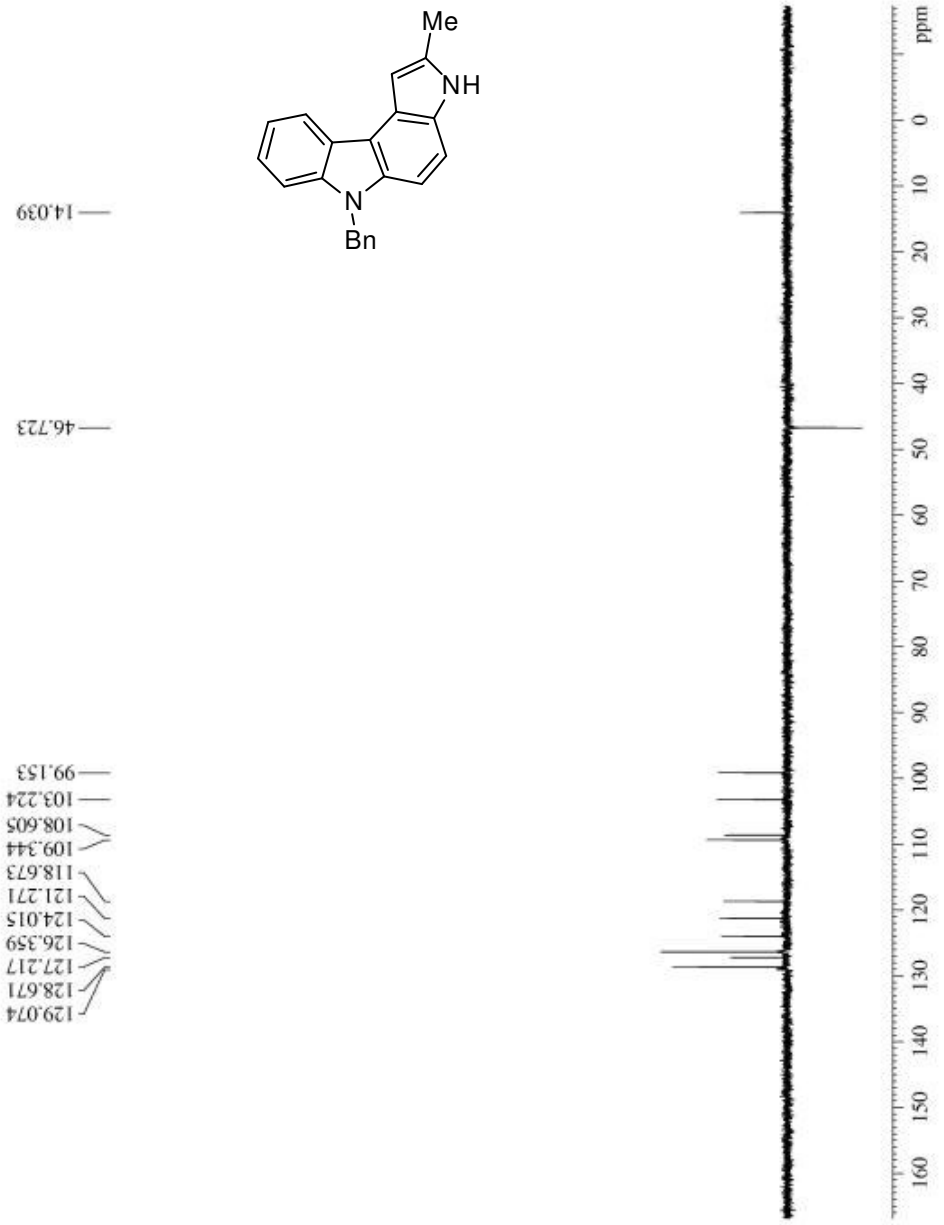
^{1}H NMR of 6-Benzyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3d)



^{13}C NMR of 6-Benzyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3d)



DEPT of 6-Benzyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3d)



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LC-MS of 6-benzyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3d)

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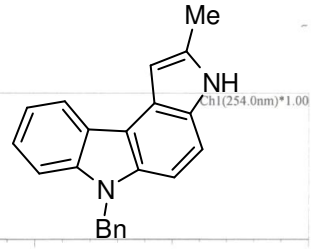
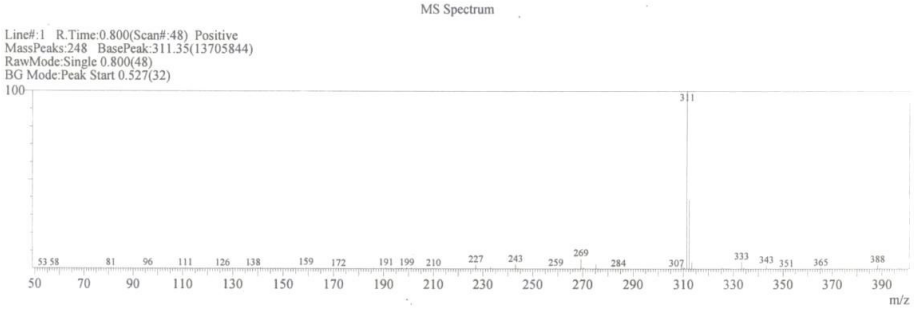
User	: Admin
Sample	: VIJI-1119
Inj. Volume	: 5.000
Data Name	: C:\LCMSsolution\User\Data\VIJI-1119-APCI-POS1.qld
Method Name	: C:\LCMSsolution\User\Method\esi.qlm





MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.800	0.527	1.143	557798340	29755190	18.74		100.00		311.35	13705844
				557798340	29755190			100.00			

OPERATOR

Electronic Supplementary Material (ESI) for RSC Advances

Elemental Analysis of 6-benzyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3d)

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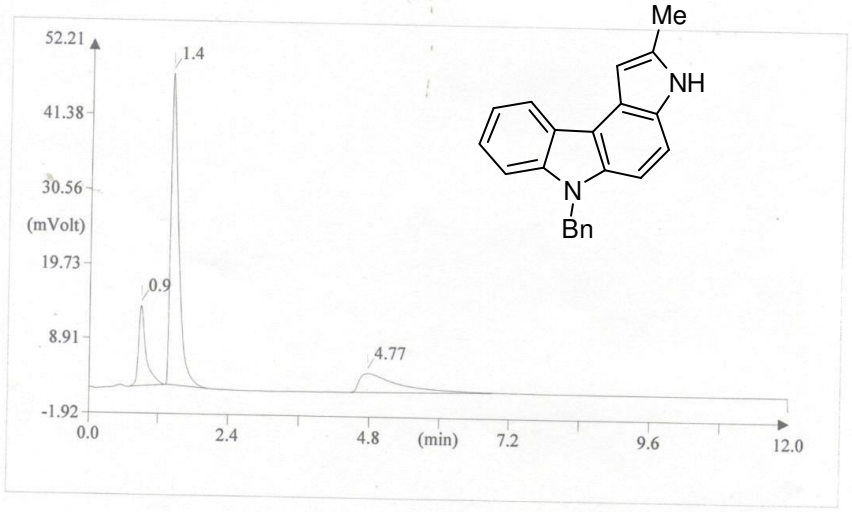
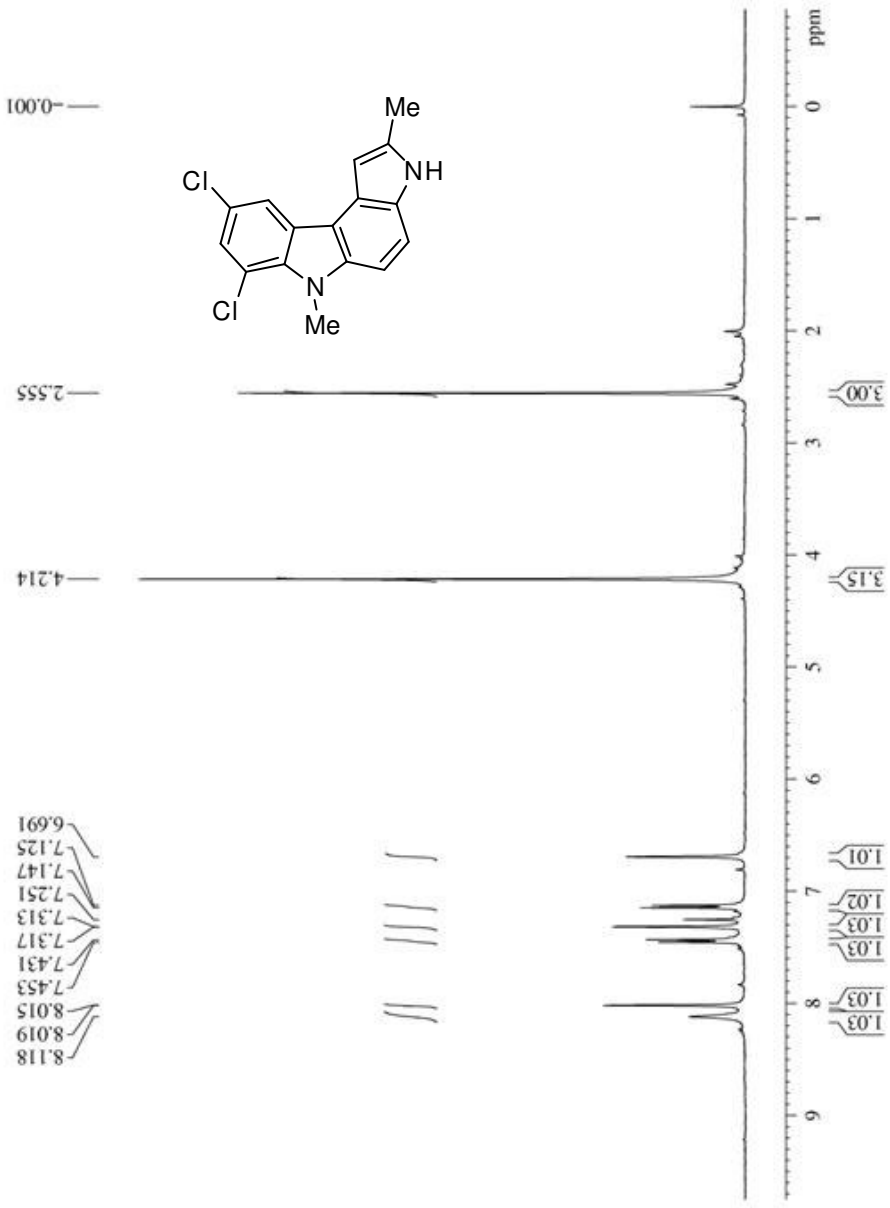
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1119 (# 68)
Analysis type:	UnkNown
Chromatogram filename:	UNK-17102011-18.dat
Sample weight:	1.006

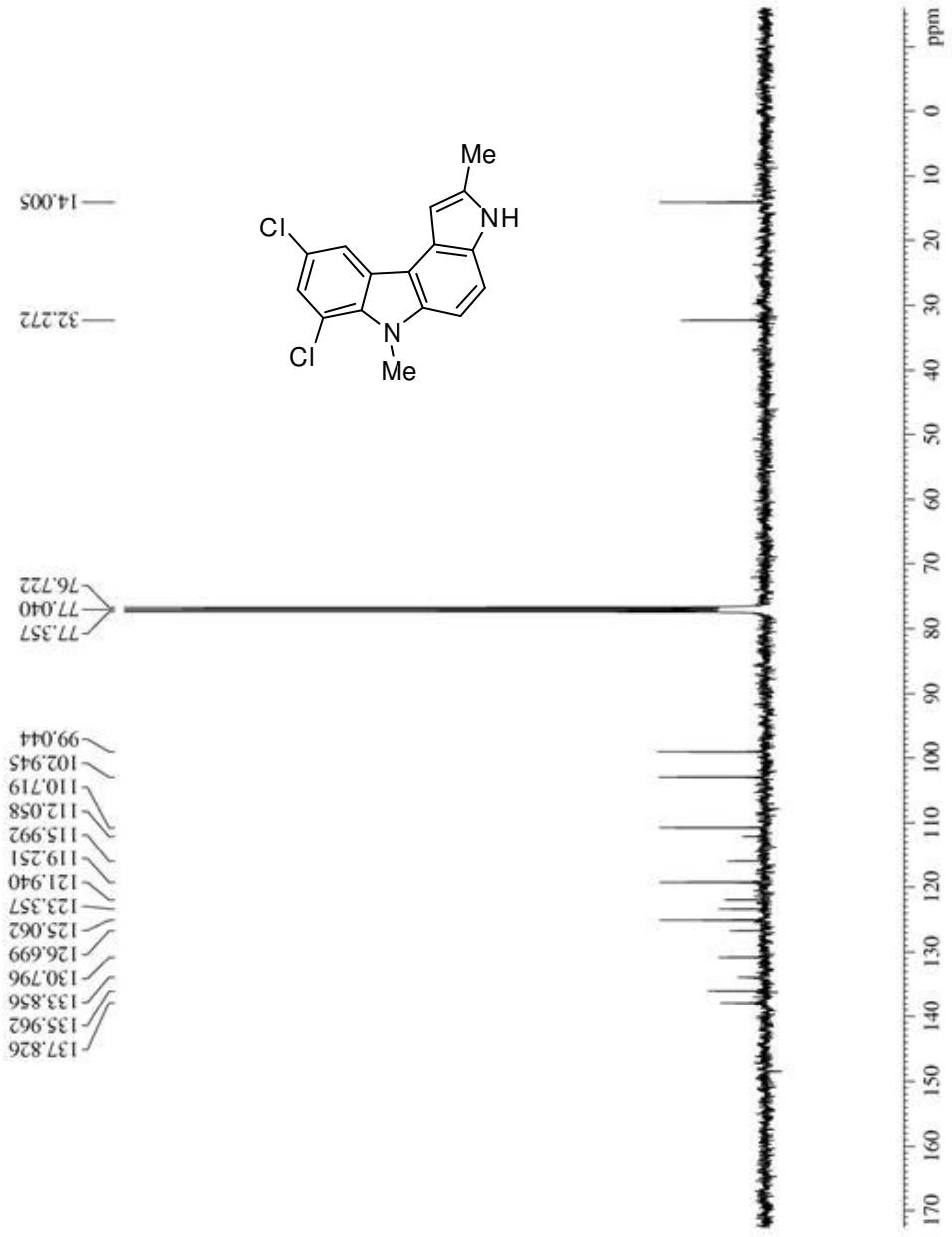


Element Name	Element %	Ret. Time
Nitrogen	9. 12	0. 90
Carbon	84. 91	1. 40
Hydrogen	5. 79	4. 77

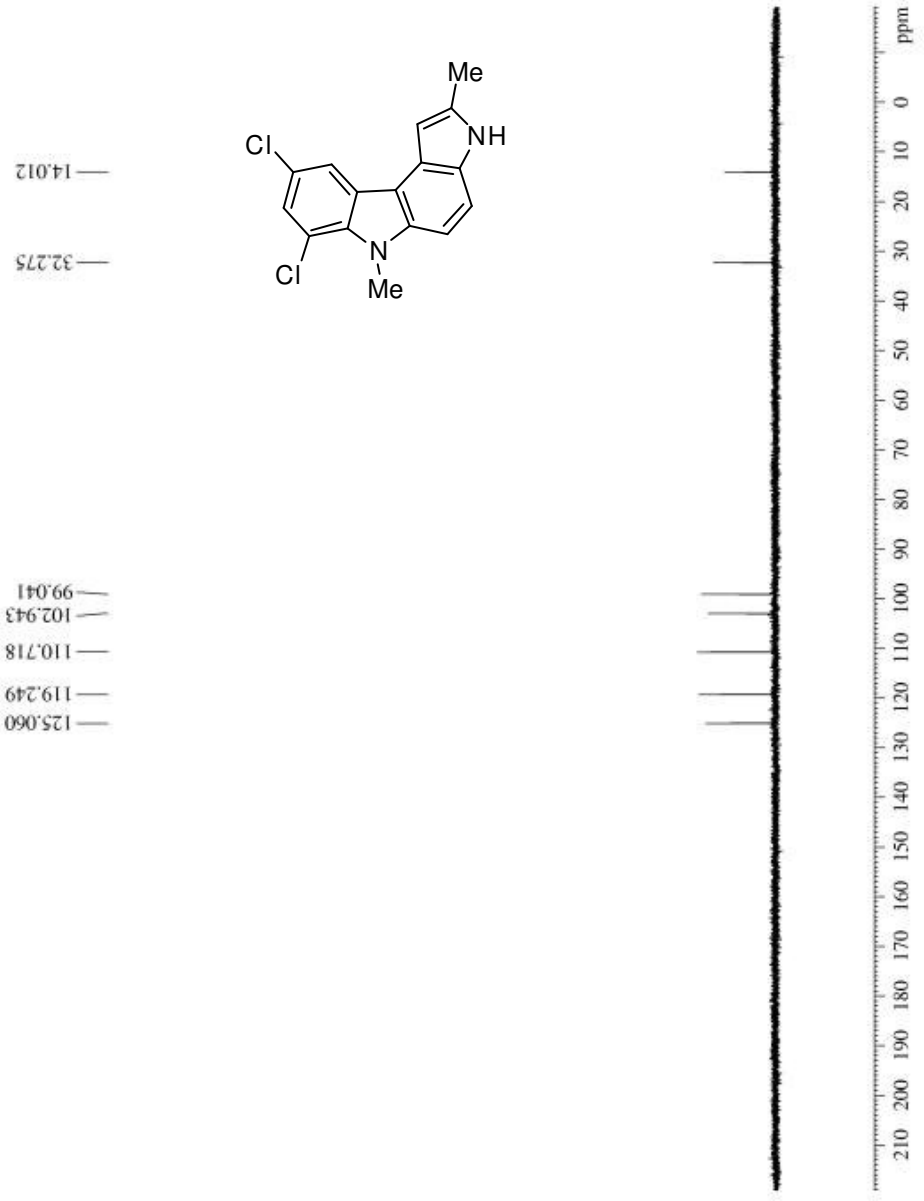
^{1}H NMR of 7,9-Dichloro-2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3e)



^{13}C NMR of 7,9-Dichloro-2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3e)



DEPT of 7,9-Dichloro-2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3e)



LC-MS Spectra of 7,9-Dichloro-2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3e)

LCMS-2010A DATA REPORT
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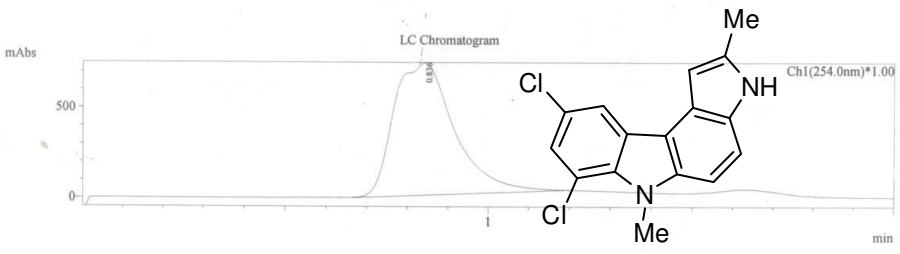
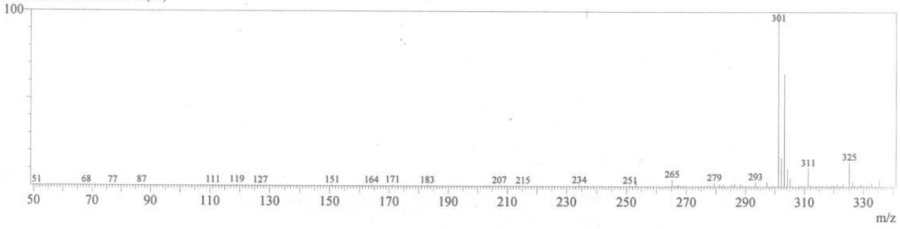
User : Admin
Sample : VIJI1121
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\VIJI1121-ESI-NEG1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm



MS Spectrum

Line#:1 R.Time:0.877(Scan#:53) Negative
MassPeaks:145 BasePeak:301.10(548969)
RawMode:Single 0.877(53)
BG Mode:Peak Start 0.710(43)



MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.877	0.710	1.193	47627177	3731805	12.76		100.00		301.10	548969
				47627177	3731805			100.00			

OPERATOR

Elemental Analysis Spectra of 7,9-Dichloro-2,6-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3e)

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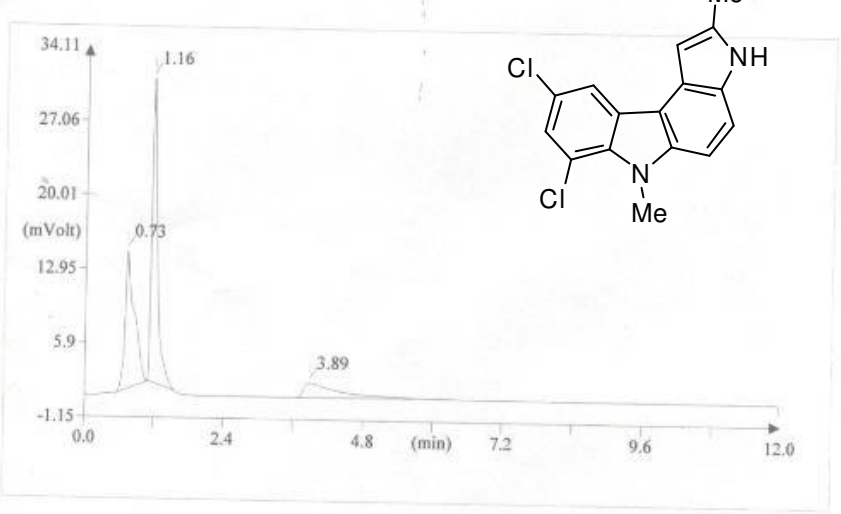
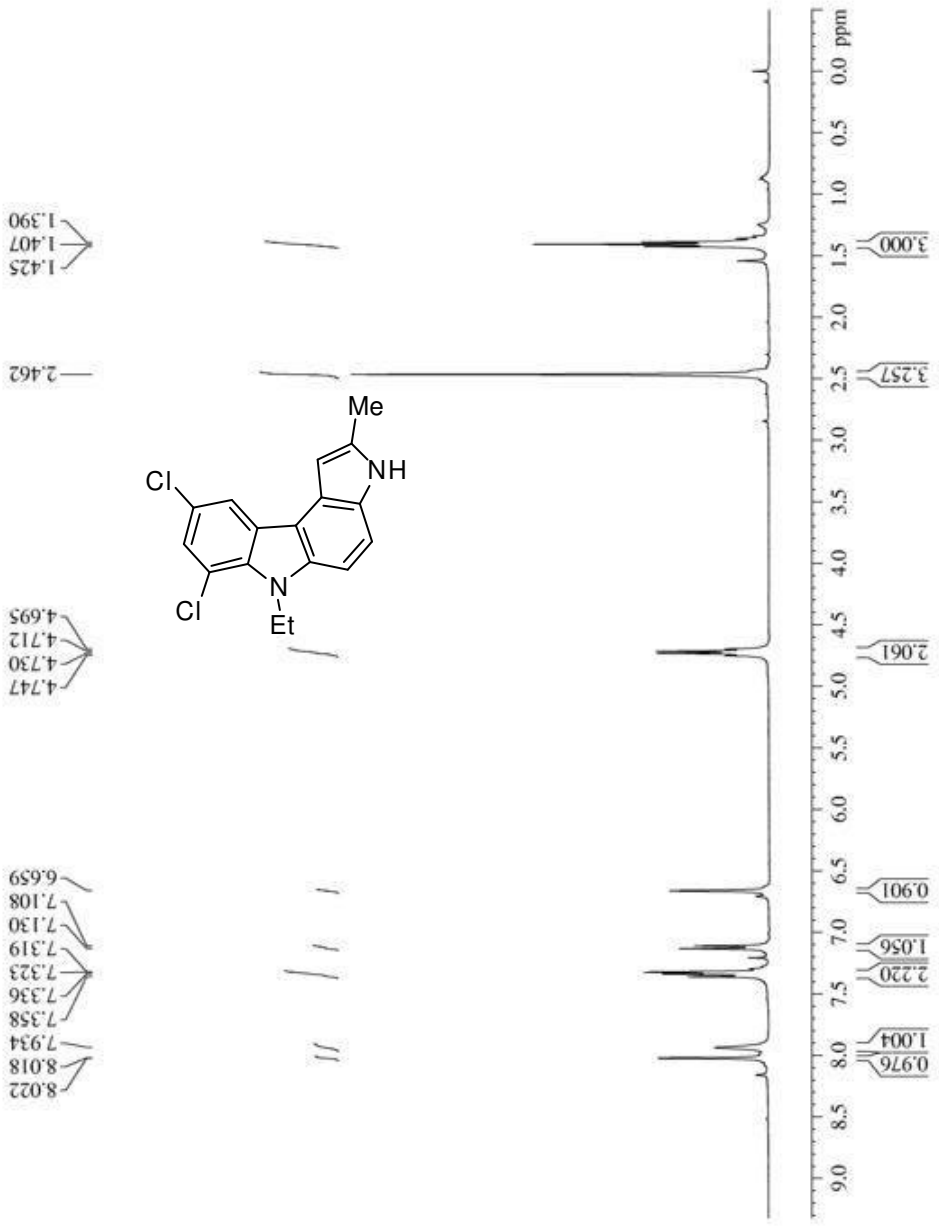
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1121 (# 65)
Analysis type:	UnkNown
Chromatogram filename:	UNK-17102011-15.dat
Sample weight:	1.113

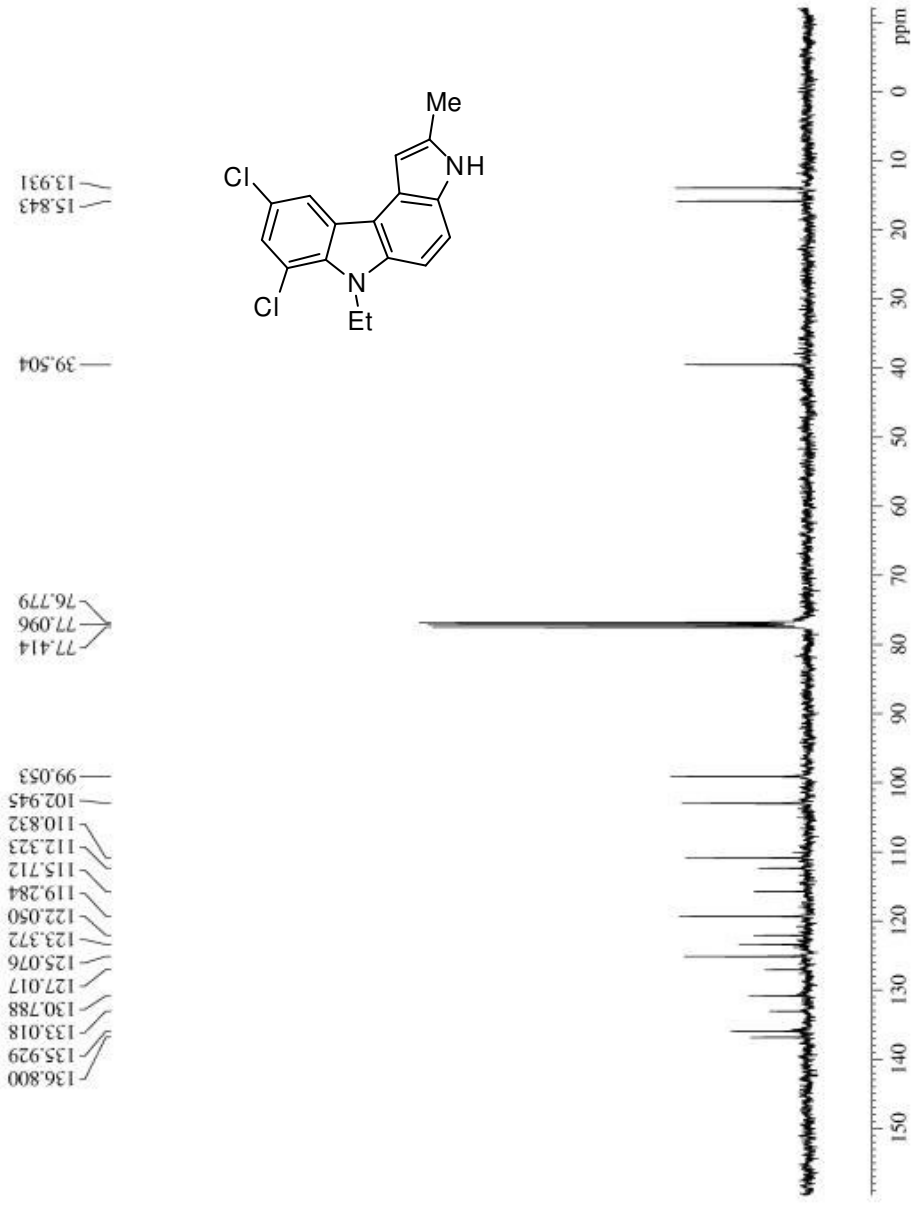


Element Name	Element %	Ret. Time
Nitrogen	9. 15	0. 73
Carbon	63. 45	1. 16
Hydrogen	3. 91	3. 89

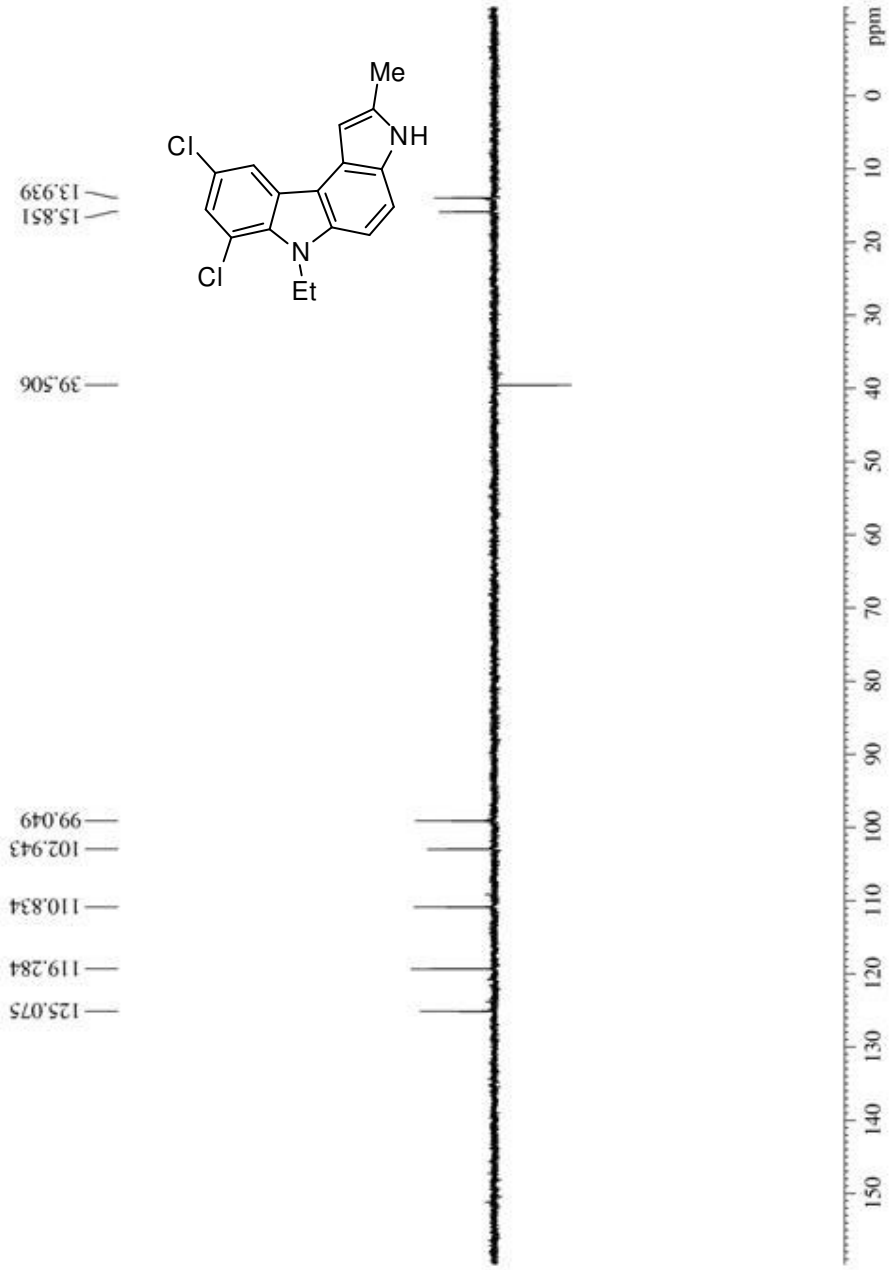
^{1}H NMR of 7,9-Dichloro-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3f)



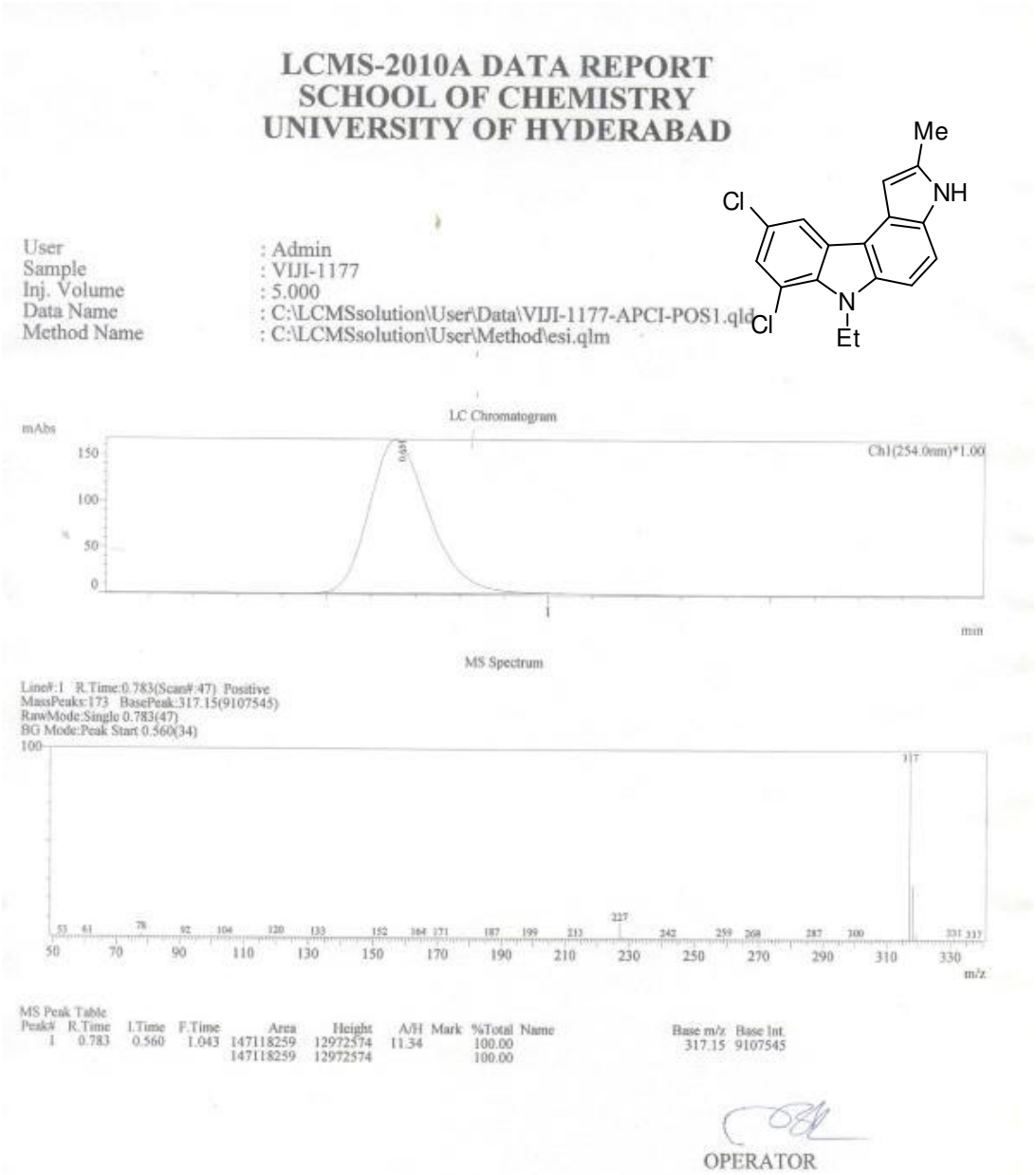
^{13}C NMR of 7,9-Dichloro-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3f)



DEPT of 7,9-Dichloro-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3f)



LC-MS of 7,9-Dichloro-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3f)



Elemental Analysis of 7,9-Dichloro-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3f)

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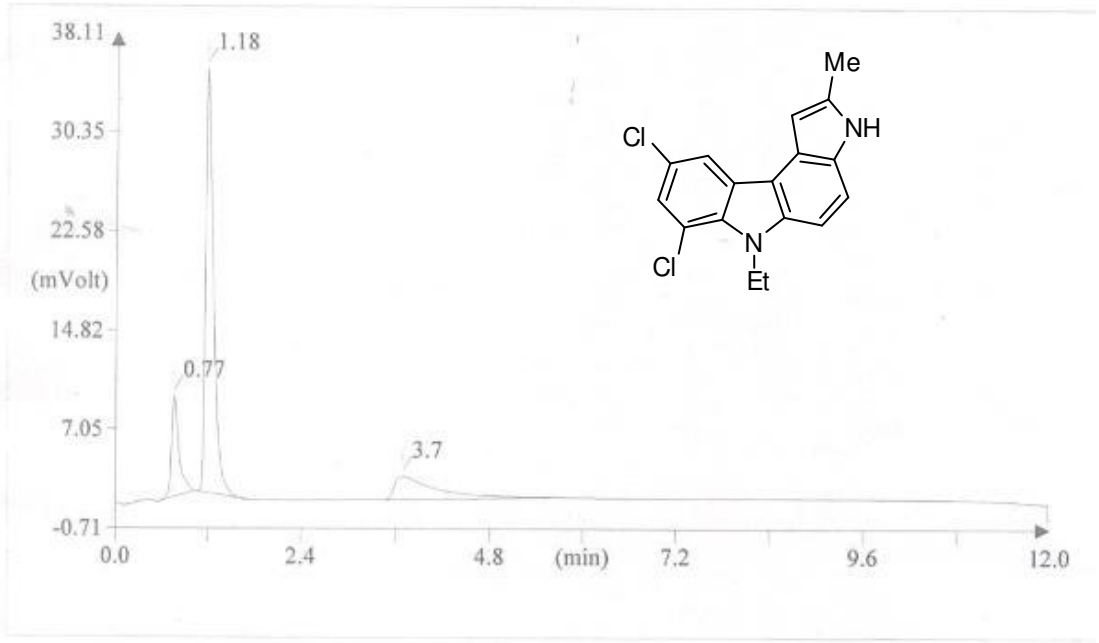
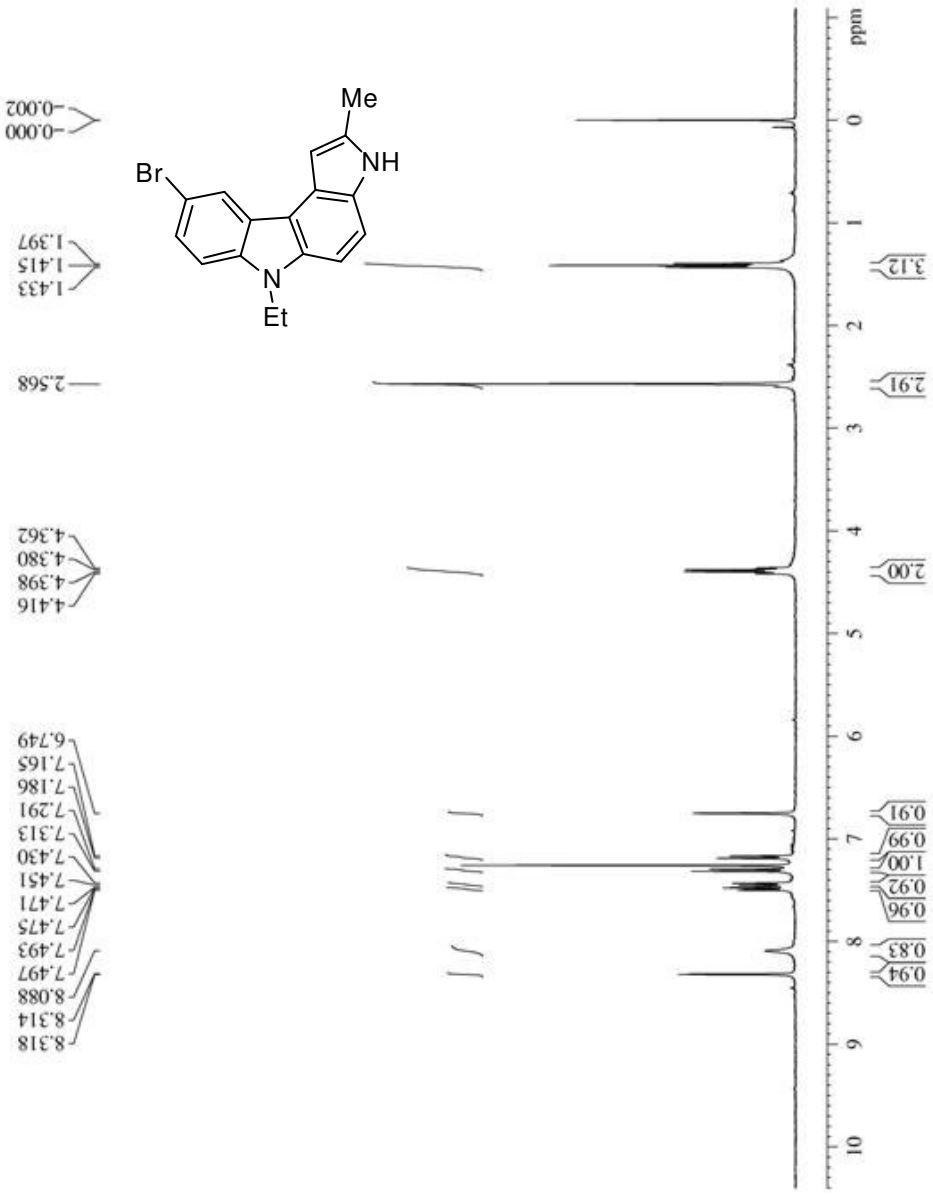
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1177 (# 1)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-1.dat
Sample weight:	1.127

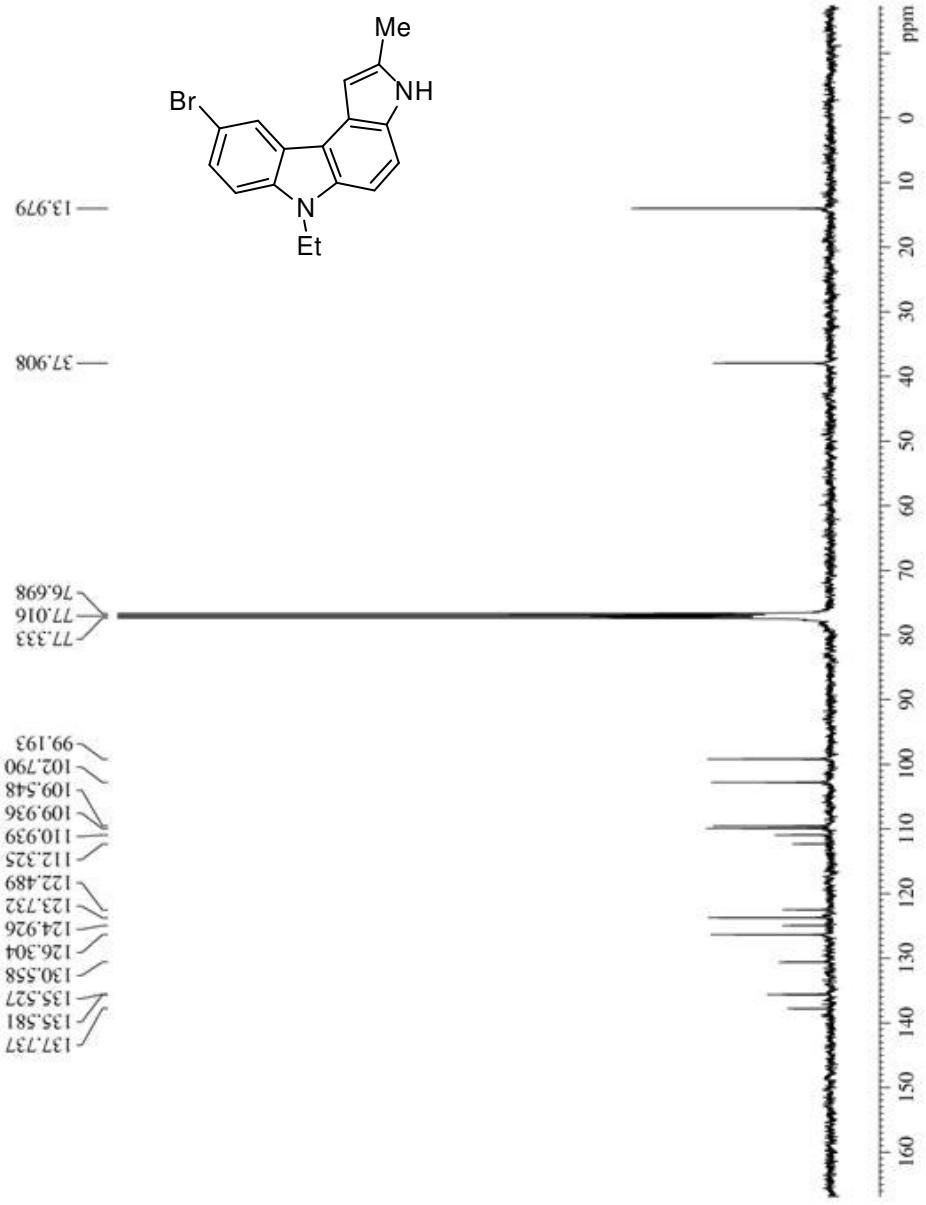


Element Name	Element %	Ret. Time
Nitrogen	8. 96	0. 77
Carbon	64. 21	1. 18
Hydrogen	4. 51	3. 70

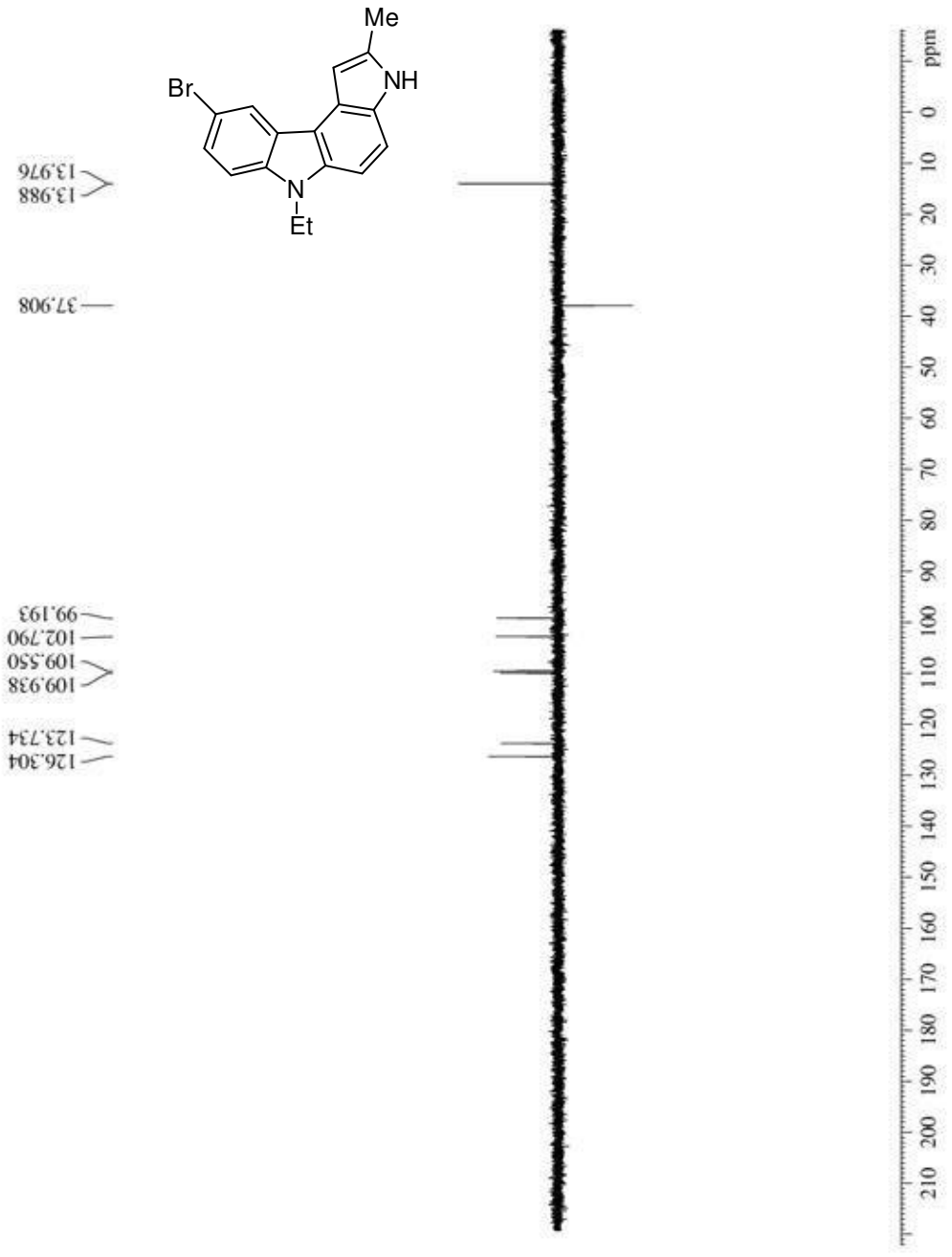
^{1}H NMR of 9-Bromo-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3g)



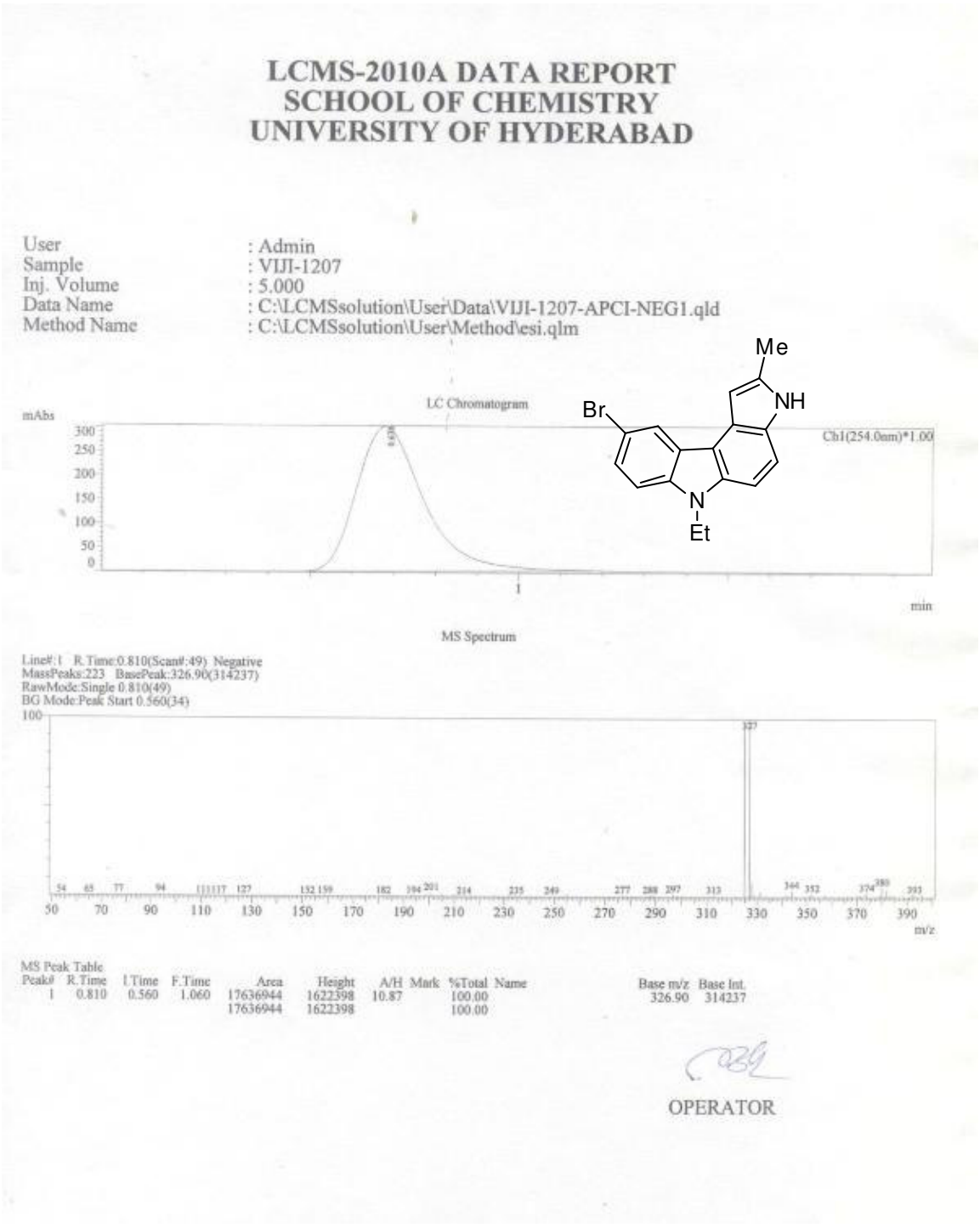
^{13}C NMR of 9-Bromo-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3g)



DEPT of 9-Bromo-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3g)



LC-MS of 9-Bromo-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3g)



Elemental Analysis of 9-Bromo-6-ethyl-2-methyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3g)

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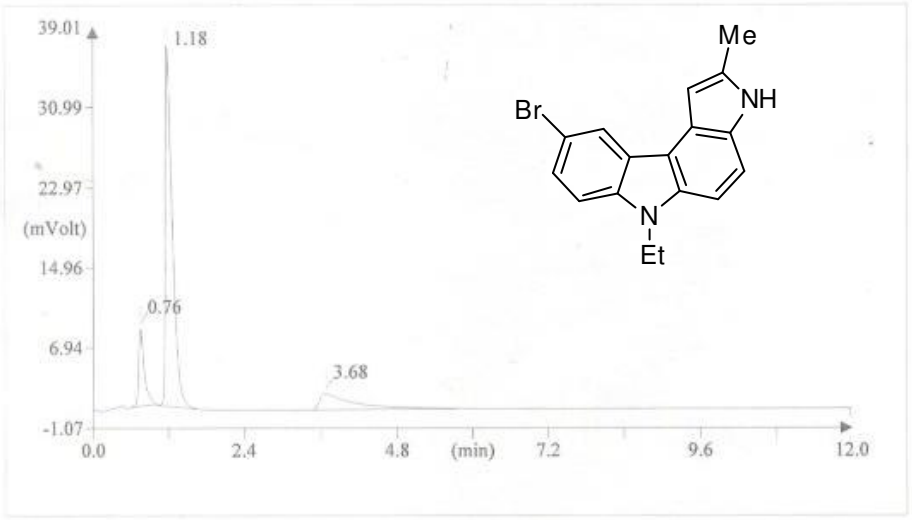
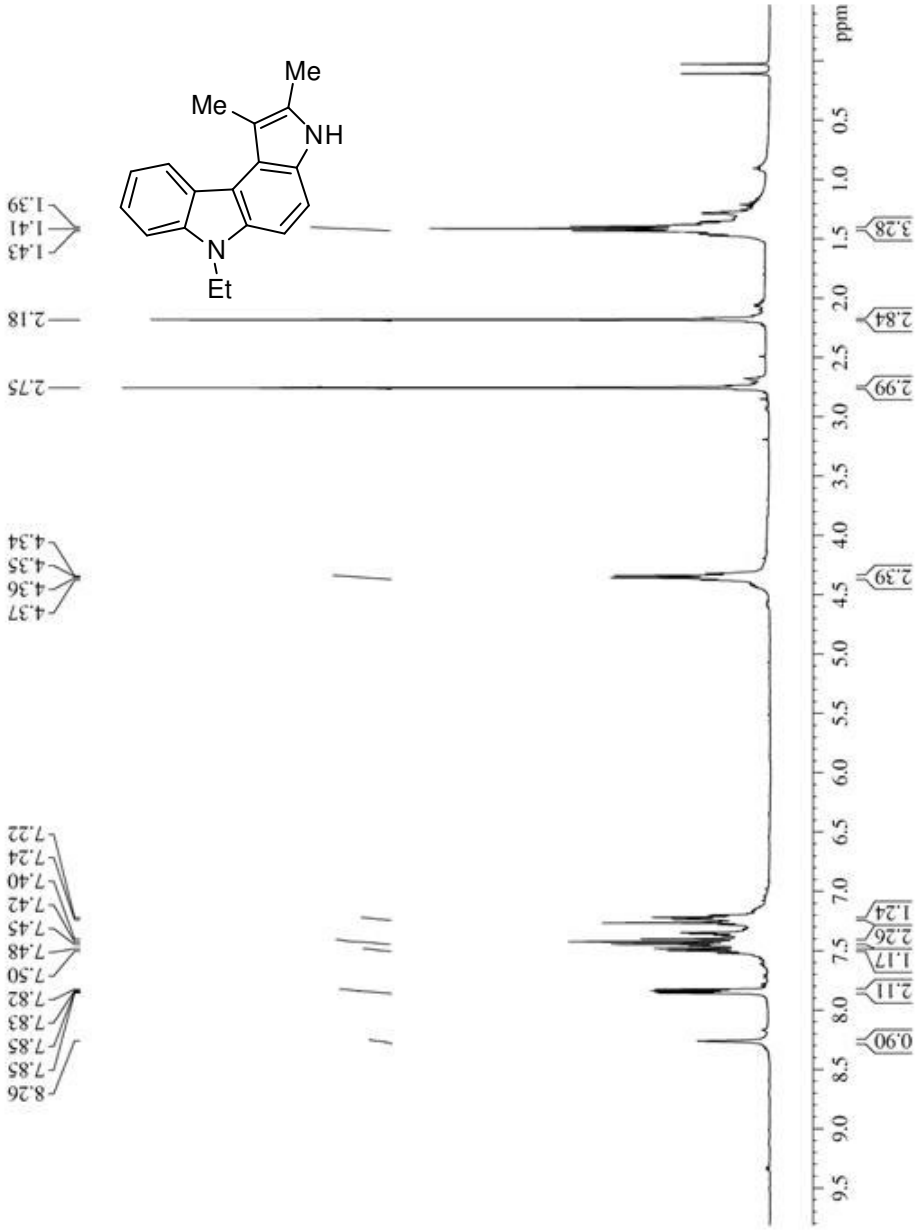
UNIVERSITY OF HYDERABAD

Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1207 (# 6)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-6.dat
Sample weight:	1.136

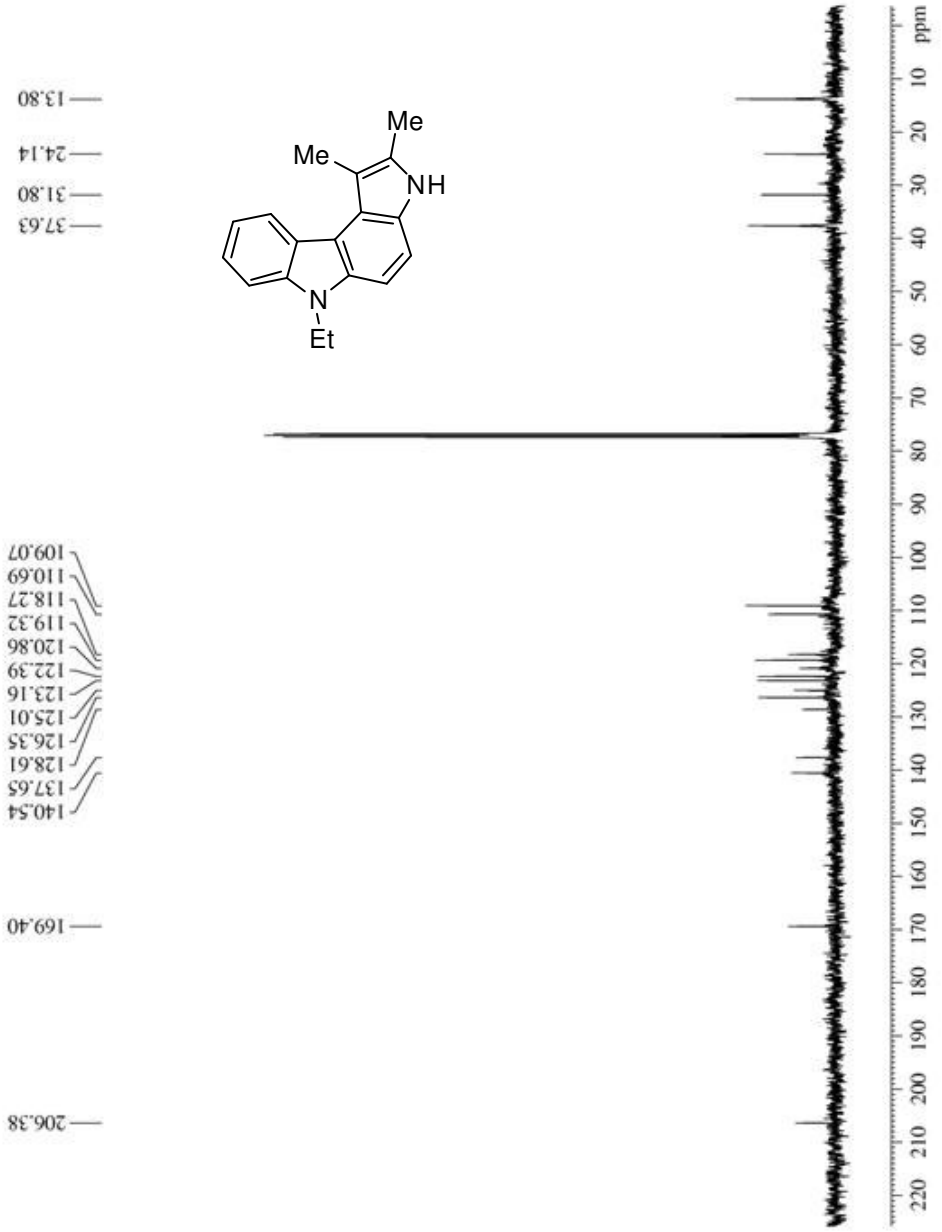


Element Name	Element %	Ret. Time
Nitrogen	8. 45	0. 76
Carbon	62. 21	1. 18
Hydrogen	4. 71	3. 68

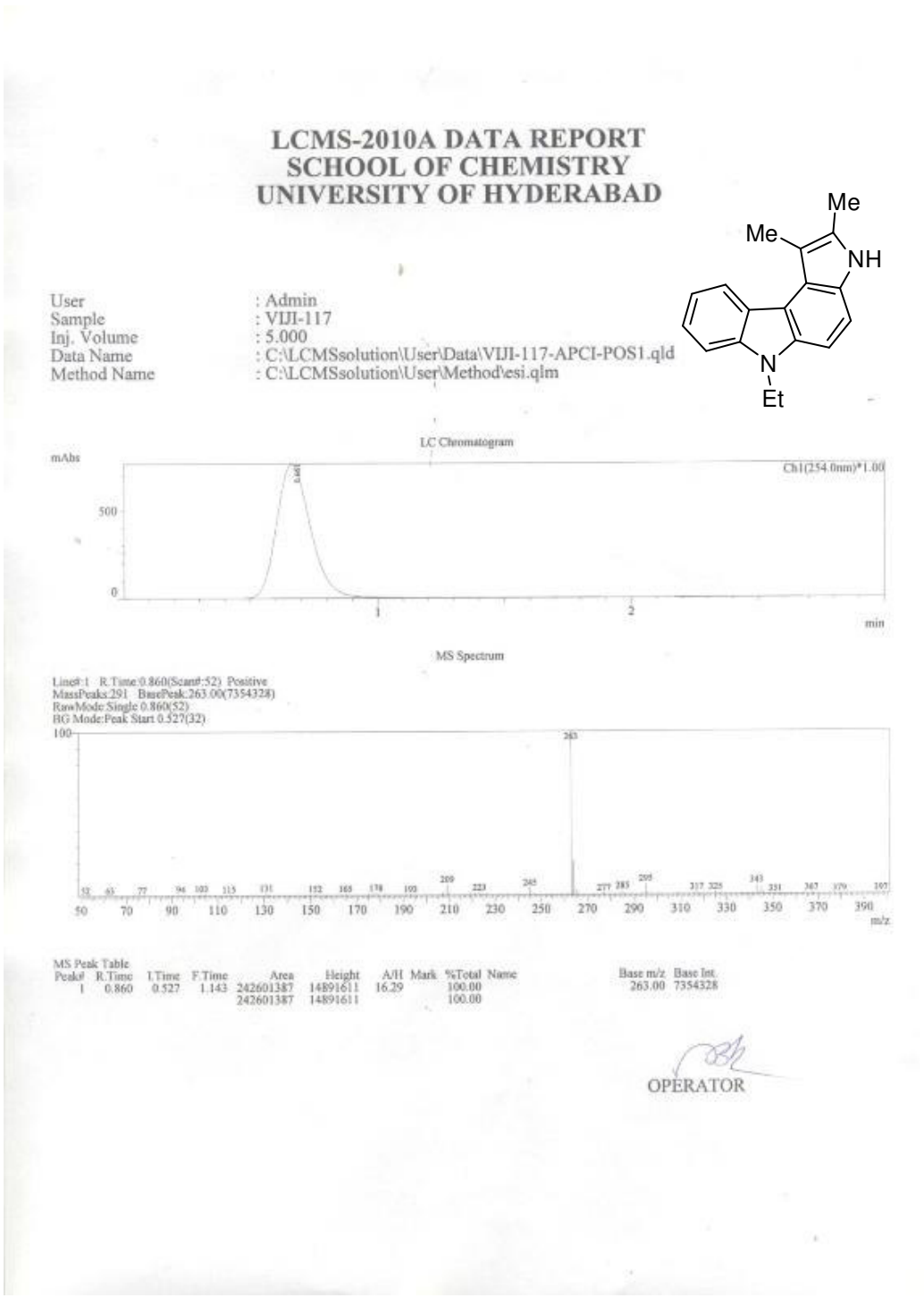
^{1}H NMR of 6-Ethyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3h)



^{13}C NMR of 6-Ethyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3h)



LC-MS of 6-Ethyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3h)



Elemental Analaysis of 6-Ethyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3h)

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
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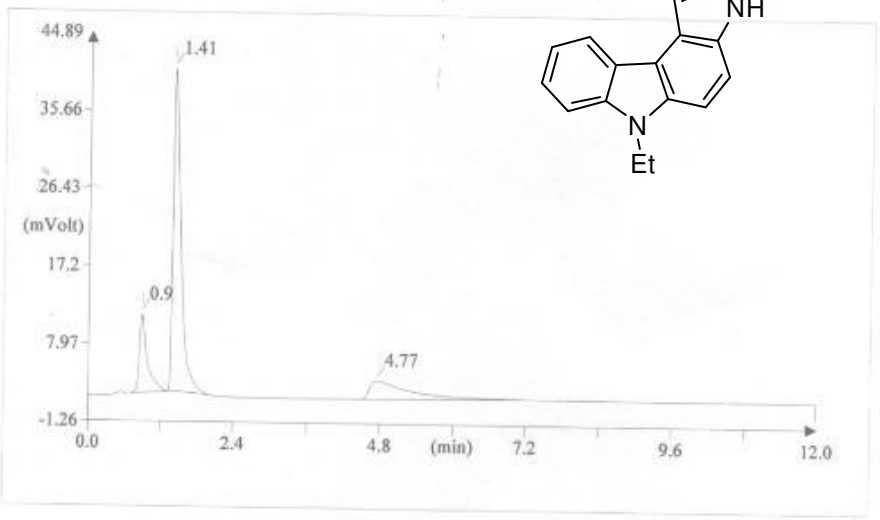
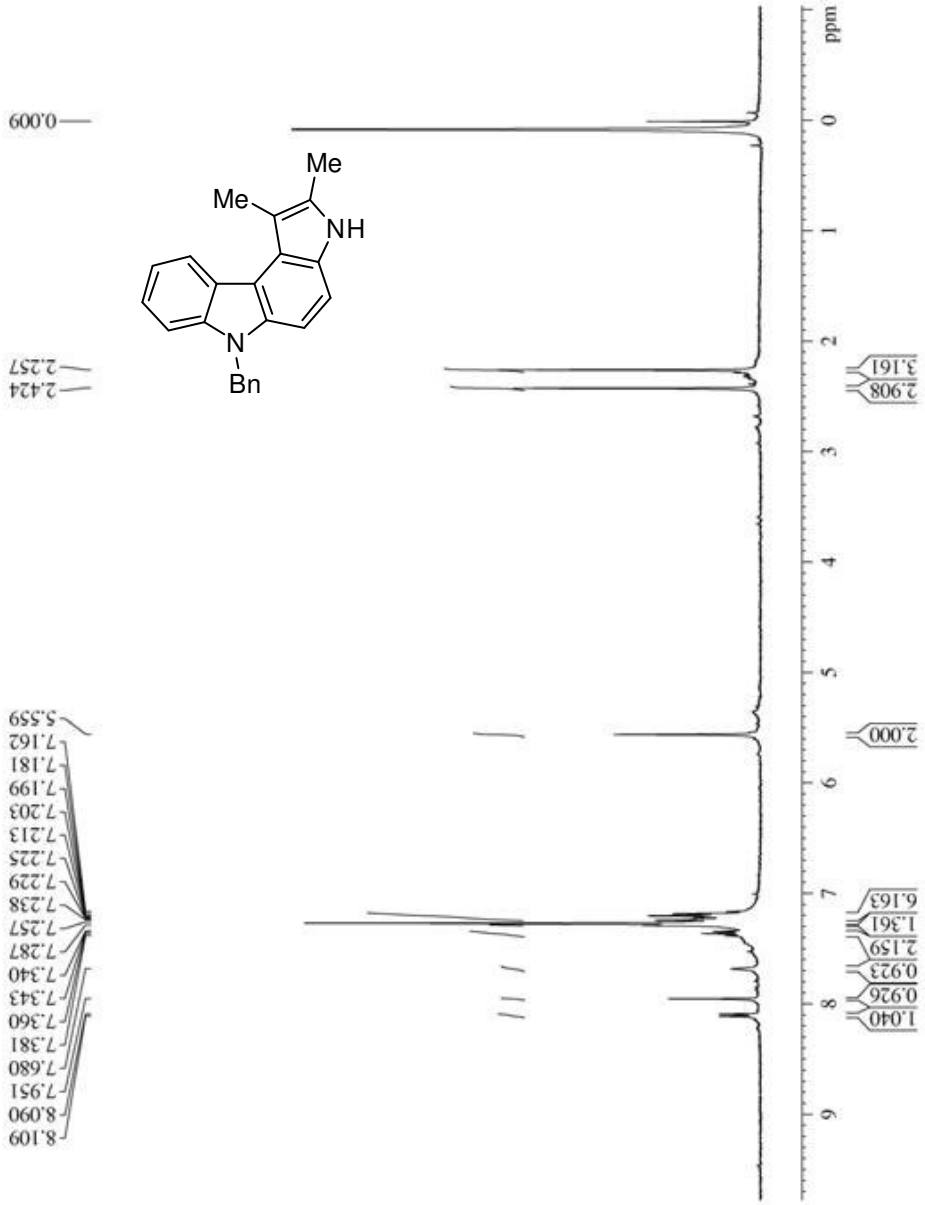
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-117 (# 66)
Analysis type:	UnkNown
Chromatogram filename:	UNK-17102011-16.dat
Sample weight:	.991

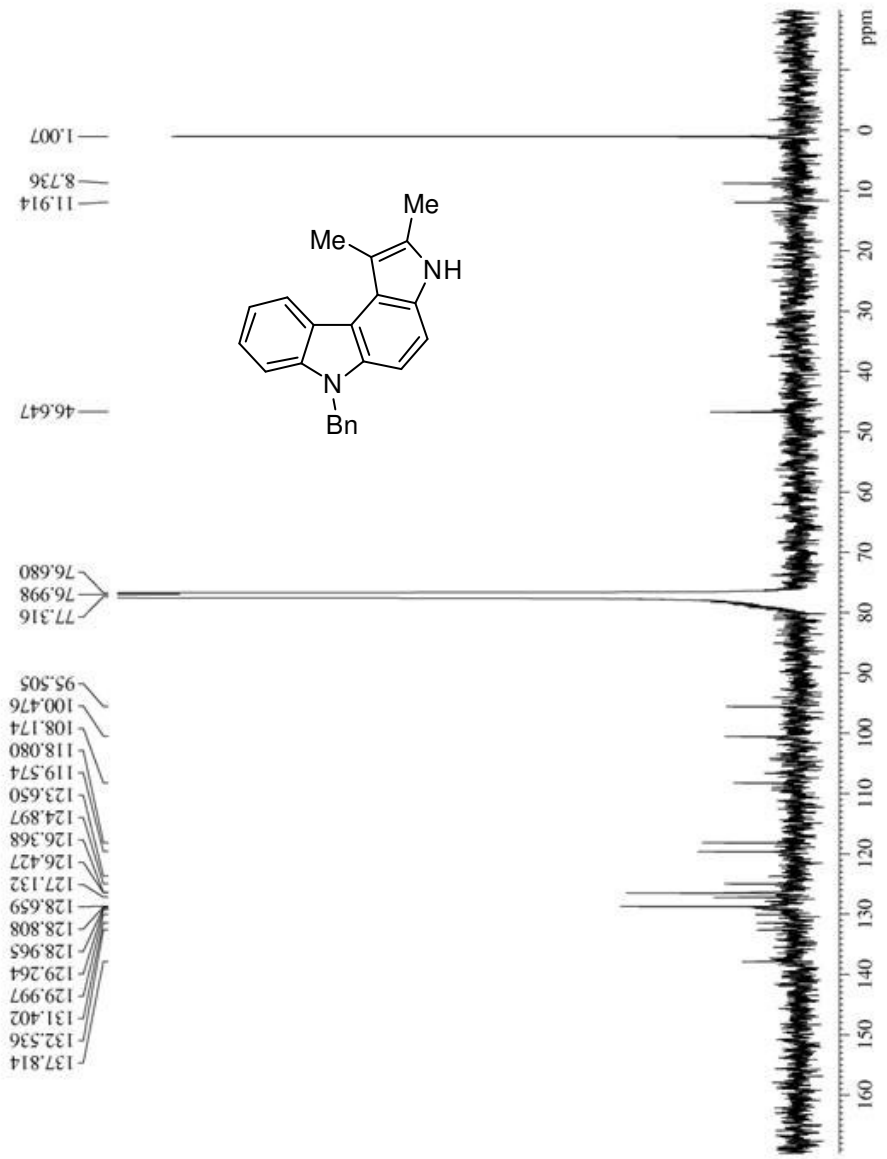


Element Name	Element %	Ret. Time
Nitrogen	10. 58	0. 90
Carbon	82. 25	1. 41
Hydrogen	6. 98	4. 77

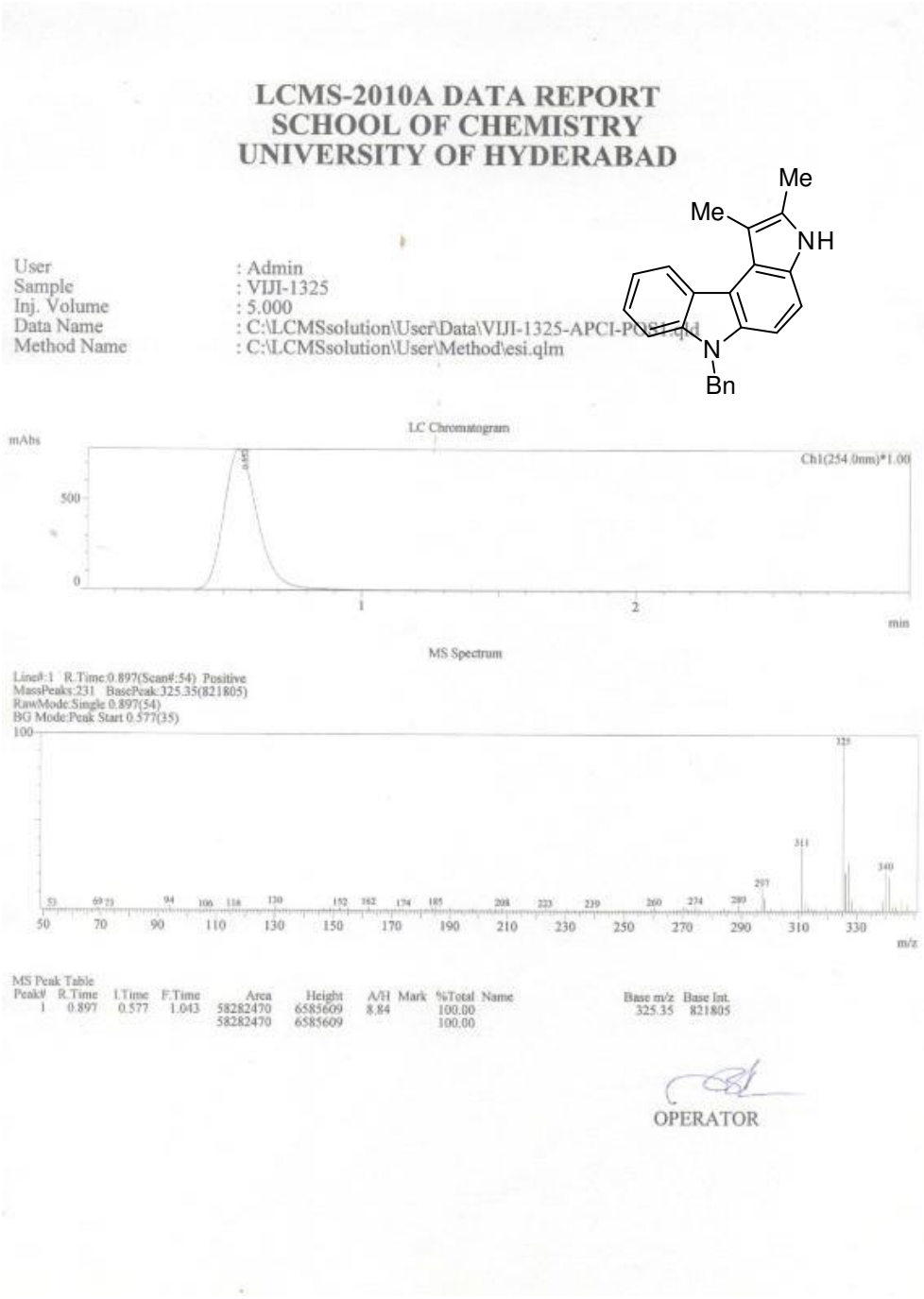
^{1}H NMR of 6-Benzyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3i)



^{13}C NMR of 6-Benzyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3i)



LC-MS of 6-Benzyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3i)



Elemental Analysis of 6-Benzyl-1,2-dimethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3i)

FLASH EA 1112 SERIES CHN REPORT
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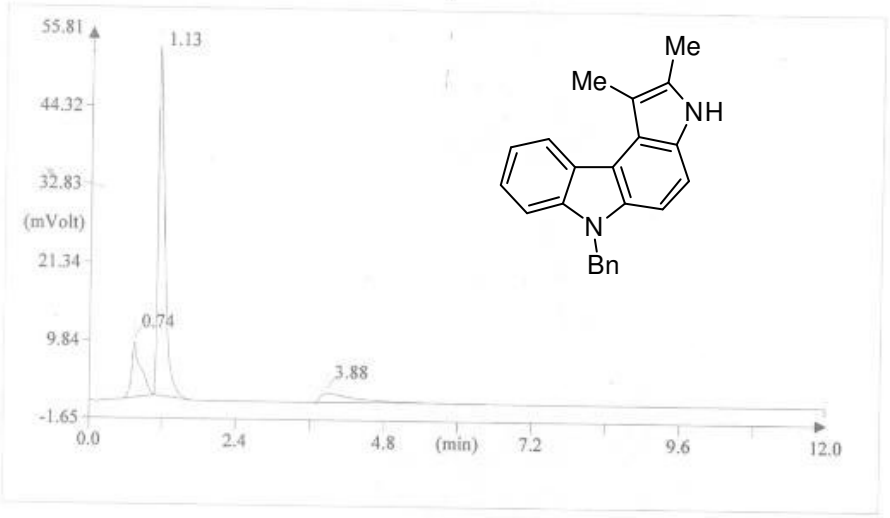
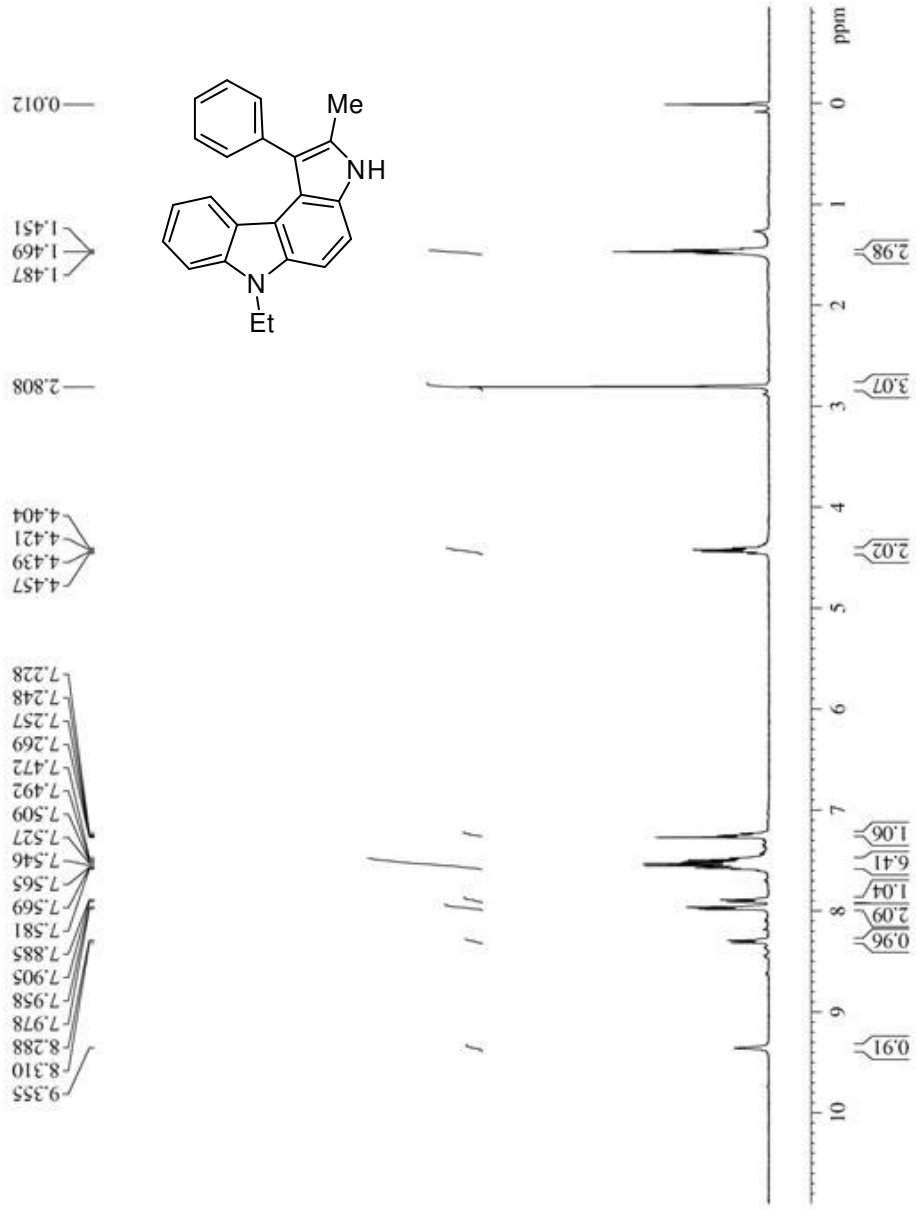
UNIVERSITY OF HYDERABAD

Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1325 (# 8)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-8.dat
Sample weight:	1.246

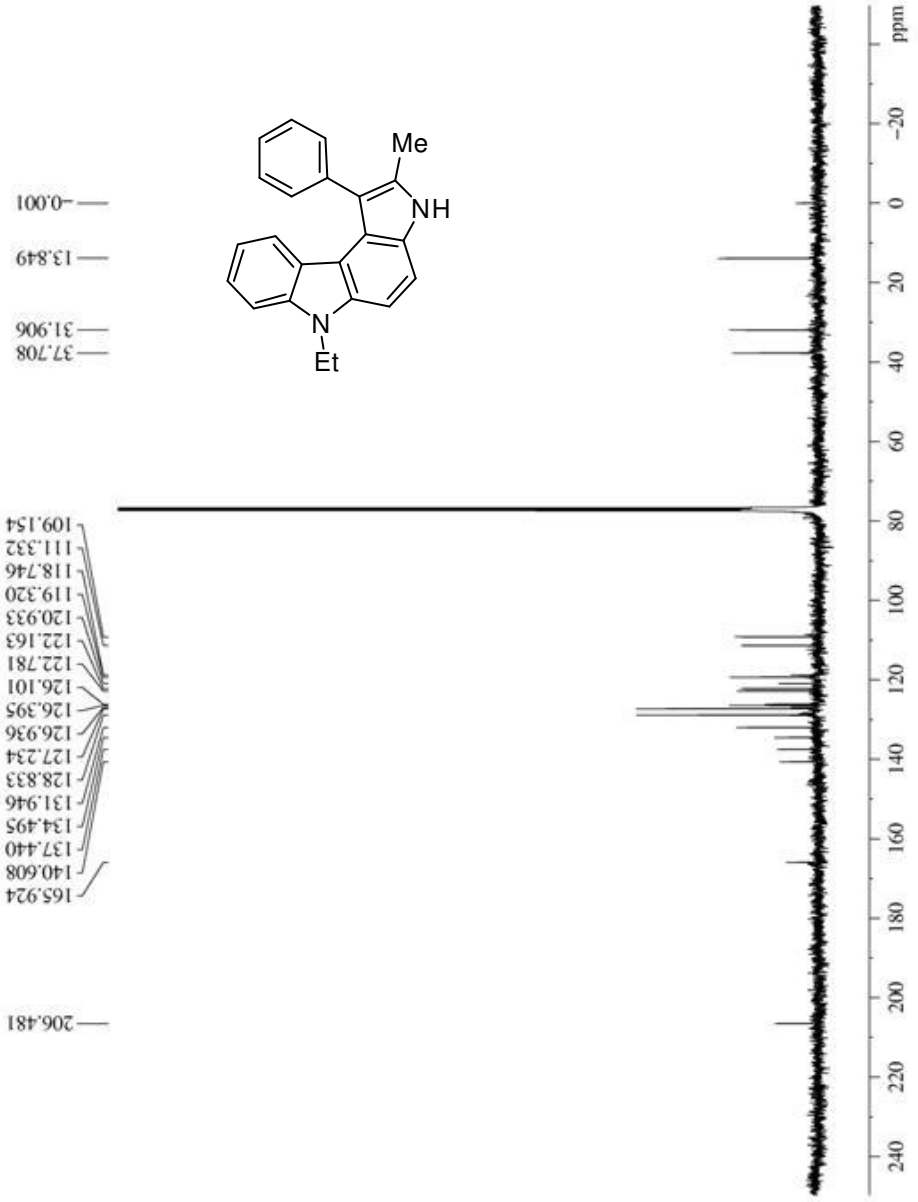


Element Name	Element %	Ret. Time
Nitrogen	8. 56	0. 74
Carbon	85. 02	1. 13
Hydrogen	6. 28	3. 88

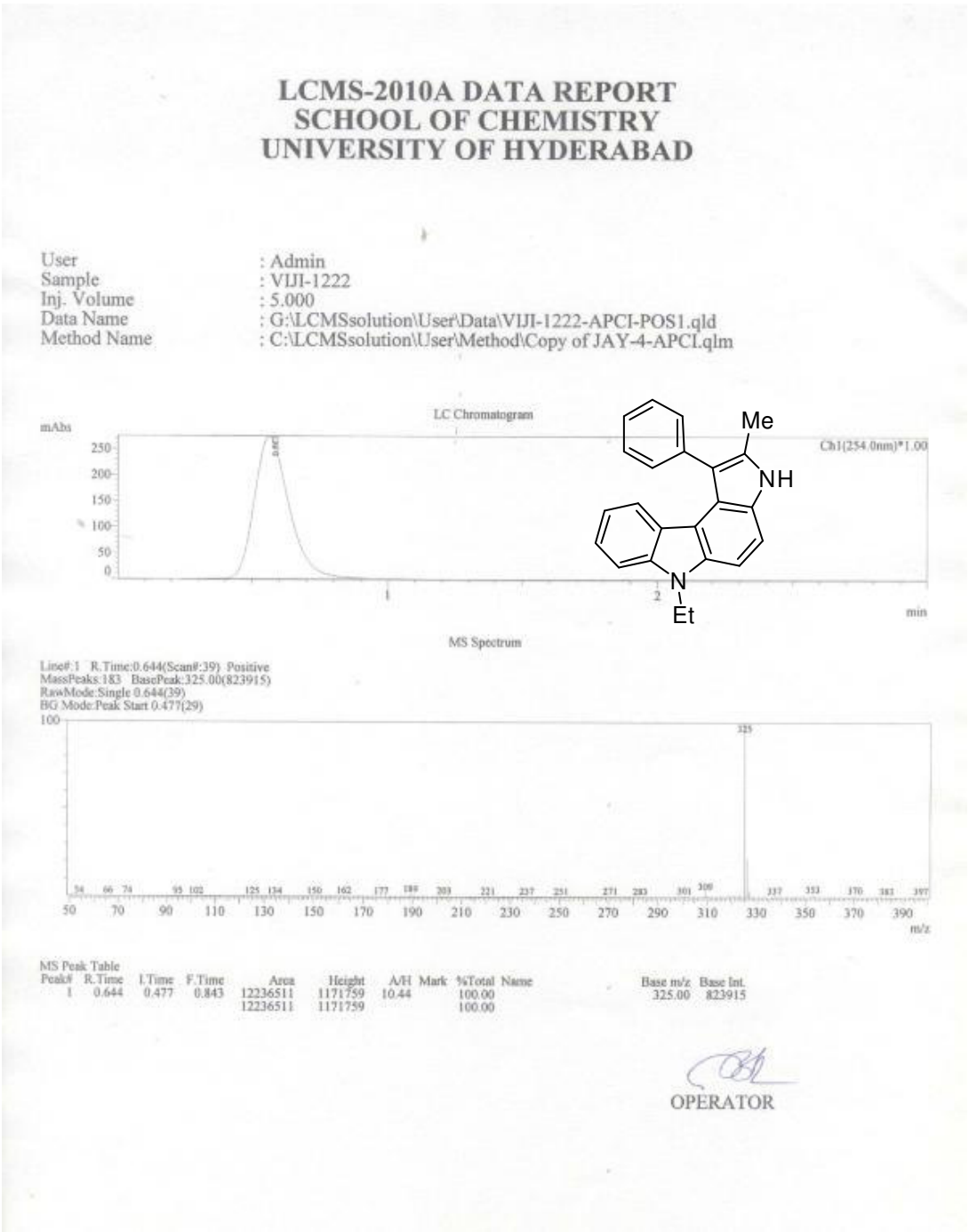
^{1}H NMR of 6-Ethyl-2-methyl-1-phenyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3j)



^{13}C NMR of 6-Ethyl-2-methyl-1-phenyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3j)



LC-MS of 6-Ethyl-2-methyl-1-phenyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3j)



LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : VIJI-1222
Inj. Volume : 5.000
Data Name : G:\LCMSsolution\User\Data\VIJI-1222-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\Copy of JAY-4-APCI.qlm

LC Chromatogram

mAbs

Ch1(254.0nm)*1.00

min

MS Spectrum

Line#:1 R.Time:0.644(Scan#:39) Positive
MassPeaks:183 BasePeak:325.00(823915)
RawMode:Single 0.644(39)
BG Mode:Peak Start 0.477(29)

m/z

MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.644	0.477	0.843	12236511	1171759	10.44		100.00		325.00	823915
				12236511	1171759			100.00			

OPERATOR

Elemental Analysis of 6-Ethyl-2-methyl-1-phenyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3j)

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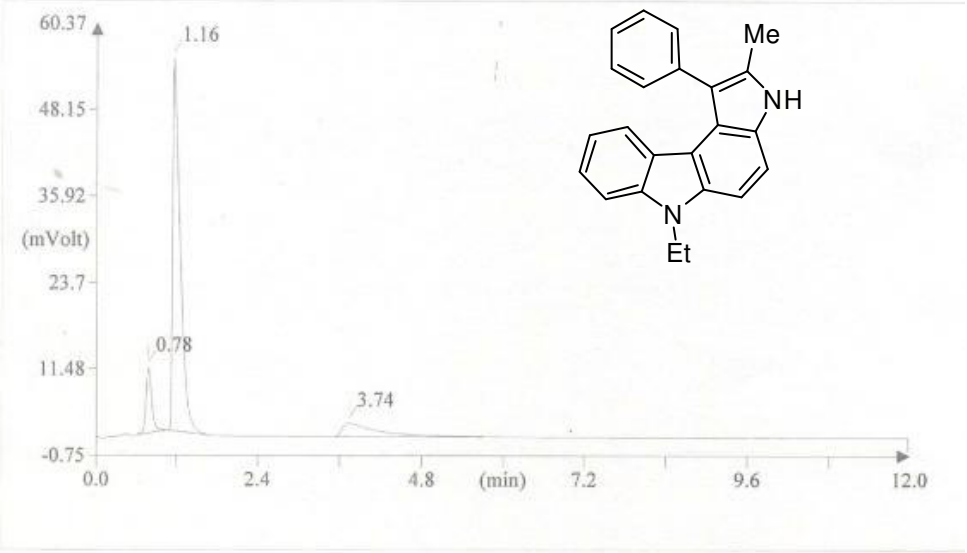
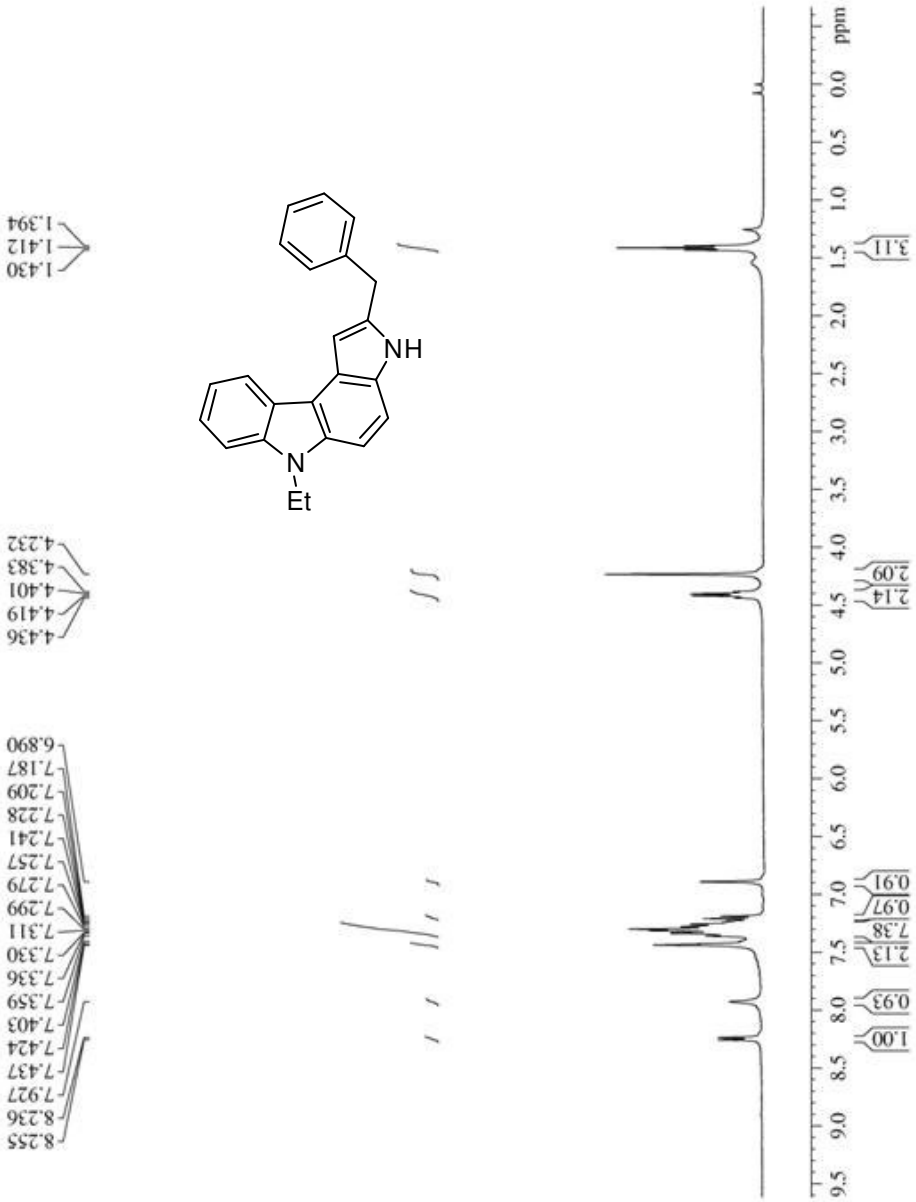
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1222 (# 5)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-5.dat
Sample weight:	1.263

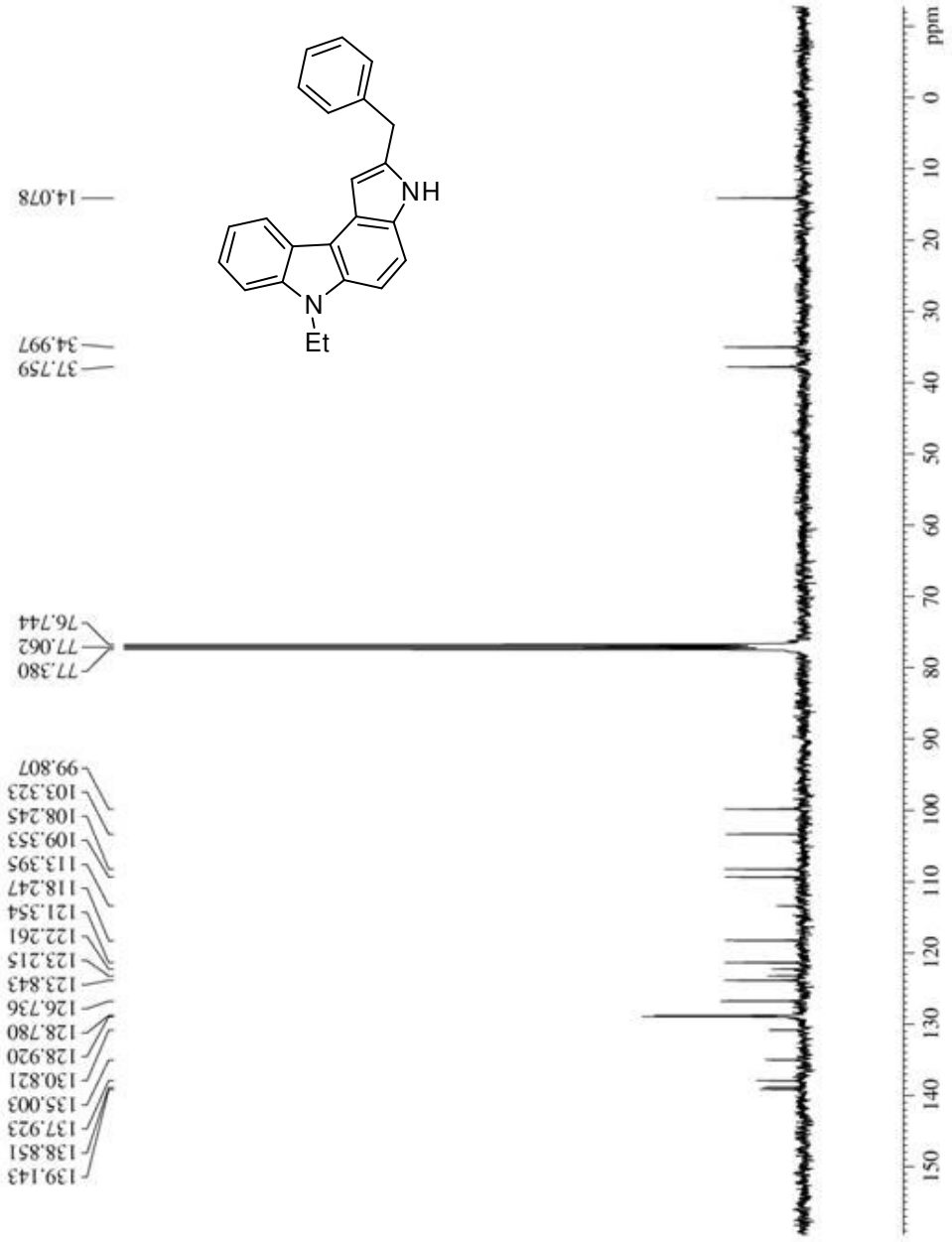


Element Name	Element %	Ret. Time
Nitrogen	8. 81	0. 78
Carbon	85. 26	1. 16
Hydrogen	6. 15	3. 74

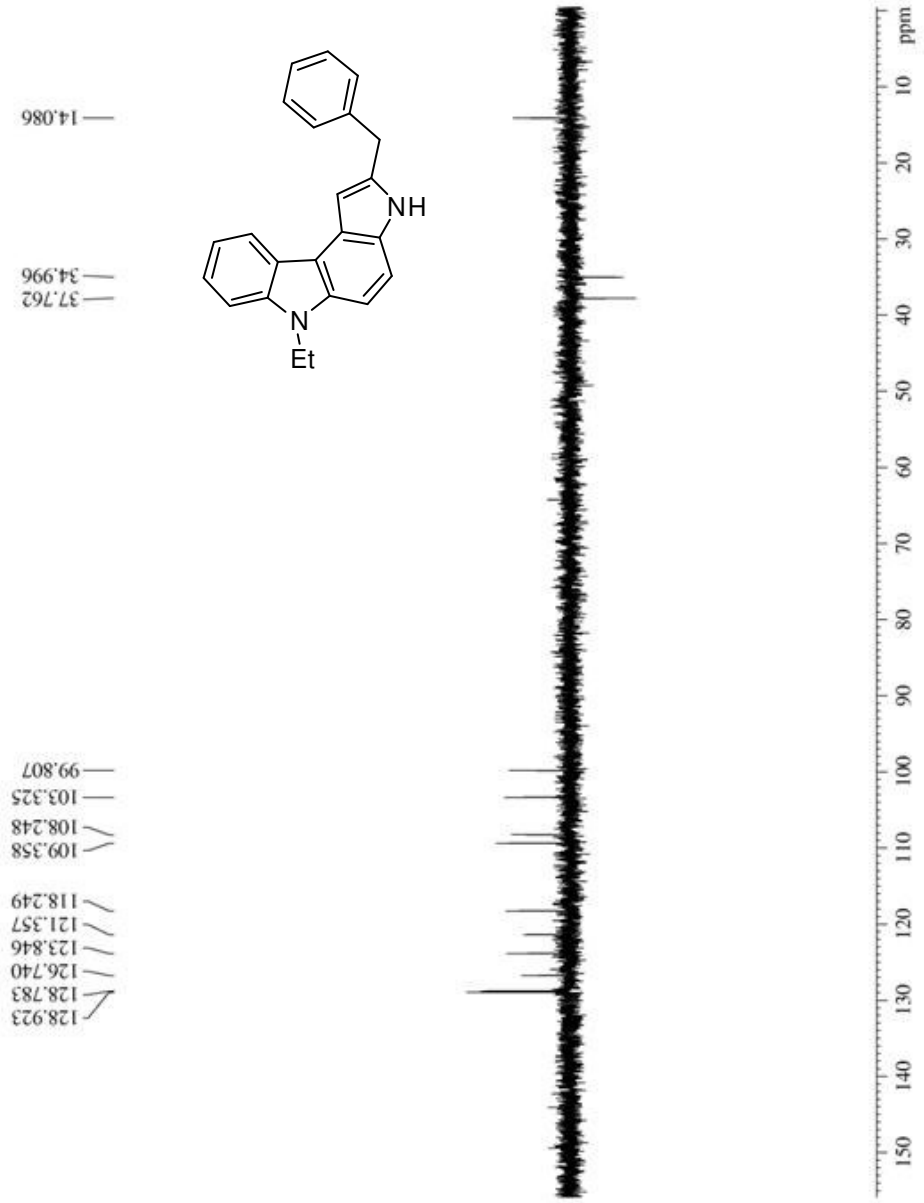
^{1}H NMR of 2-Benzyl-6-ethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3k)



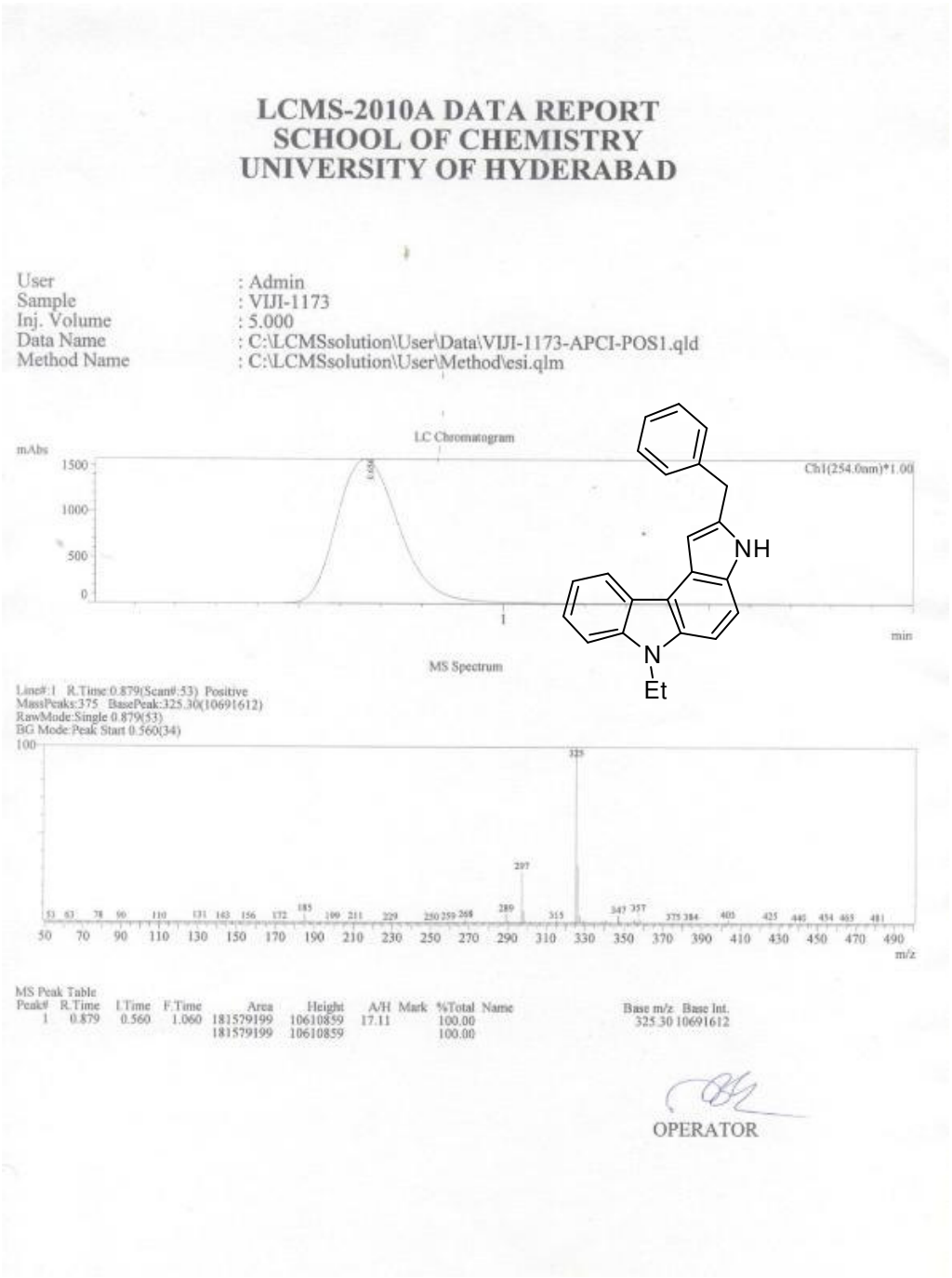
^{13}C NMR of 2-Benzyl-6-ethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3k)



DEPT of 2-Benzyl-6-ethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3k)



LC-MS of 2-Benzyl-6-ethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3k)



Electronic Supplementary Material (ESI) for RSC Advances

Elemental Analysis of 2-Benzyl-6-ethyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3k)

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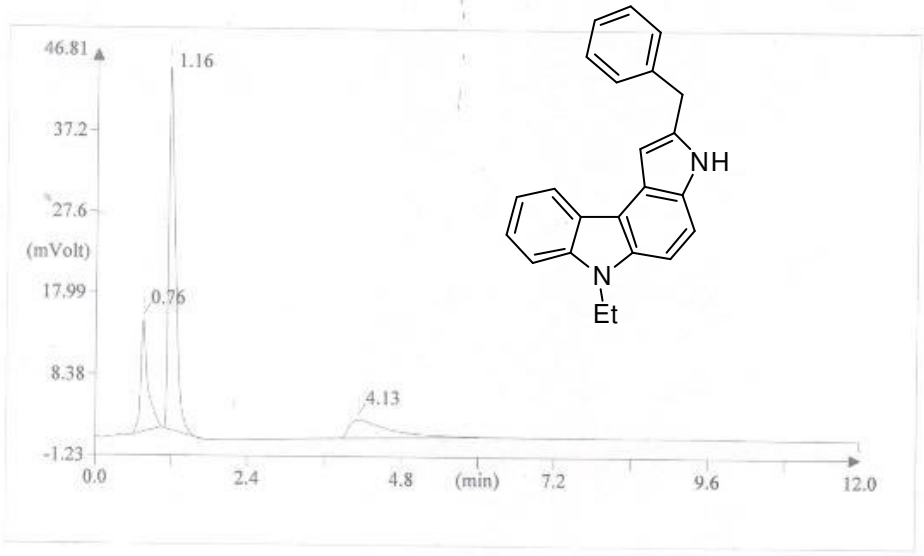
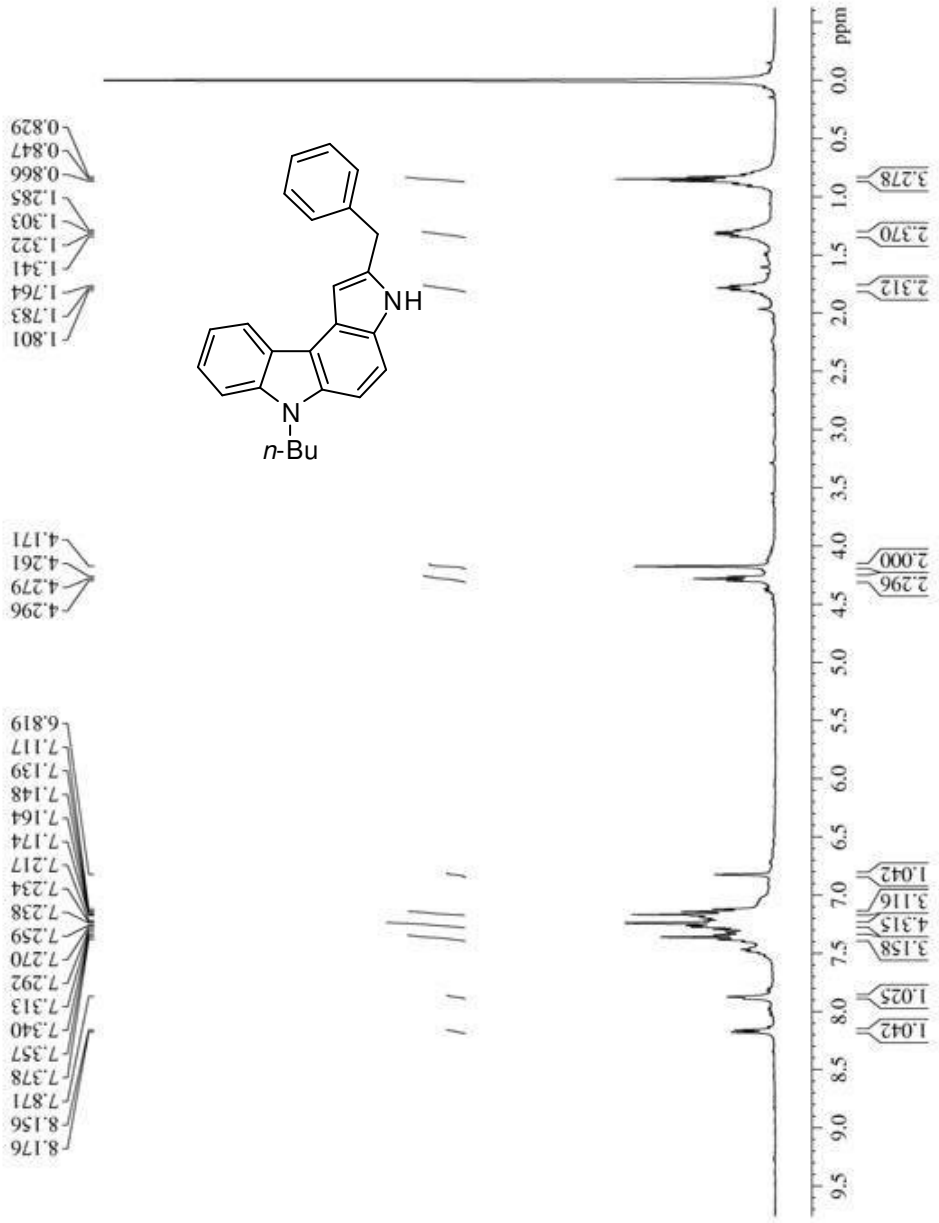
UNIVERSITY OF HYDERABAD

Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1173 (# 17)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-17.dat
Sample weight:	1.119

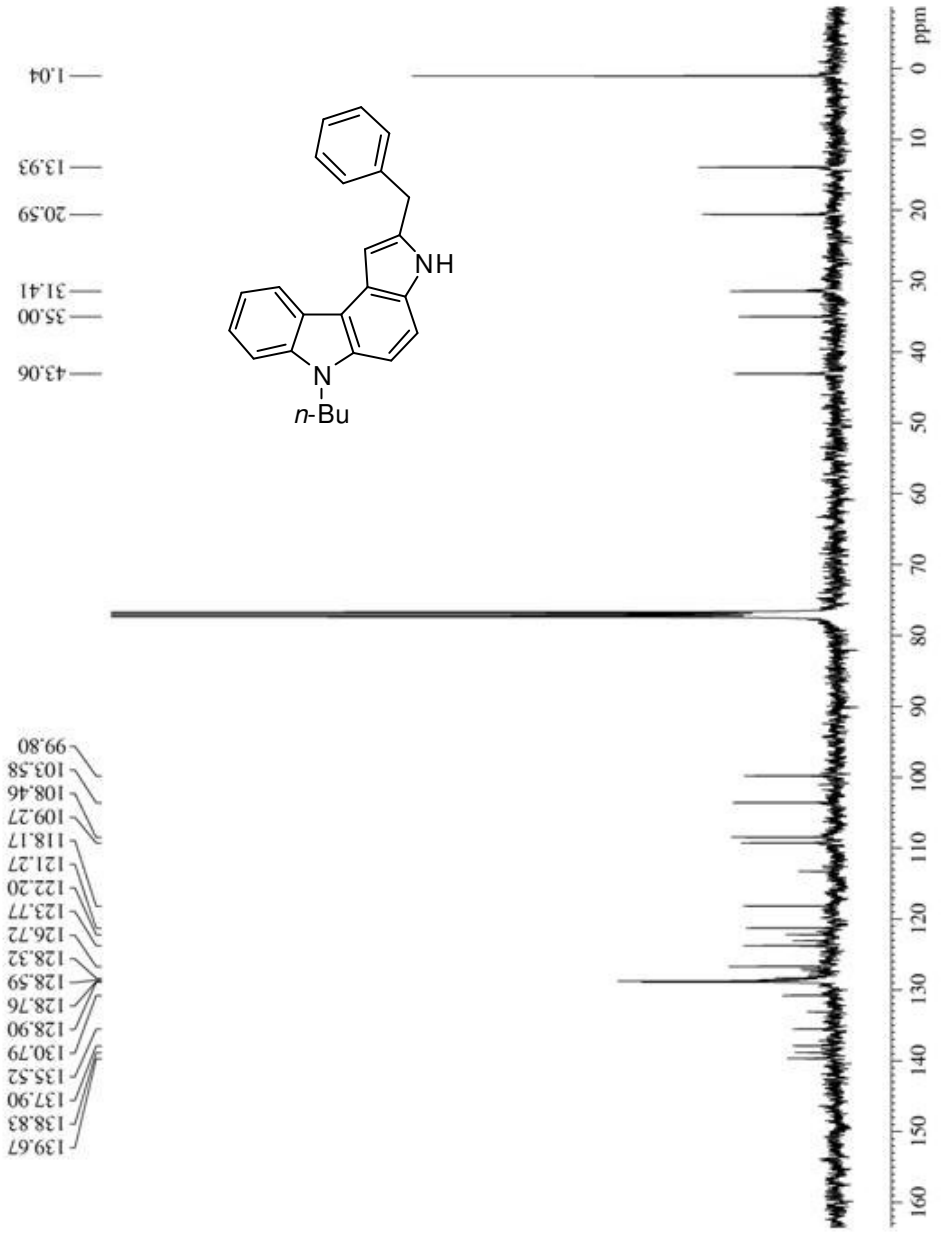


Element Name	Element %	Ret. Time
Nitrogen	8. 71	0. 76
Carbon	85. 26	1. 16
Hydrogen	6. 15	4. 13

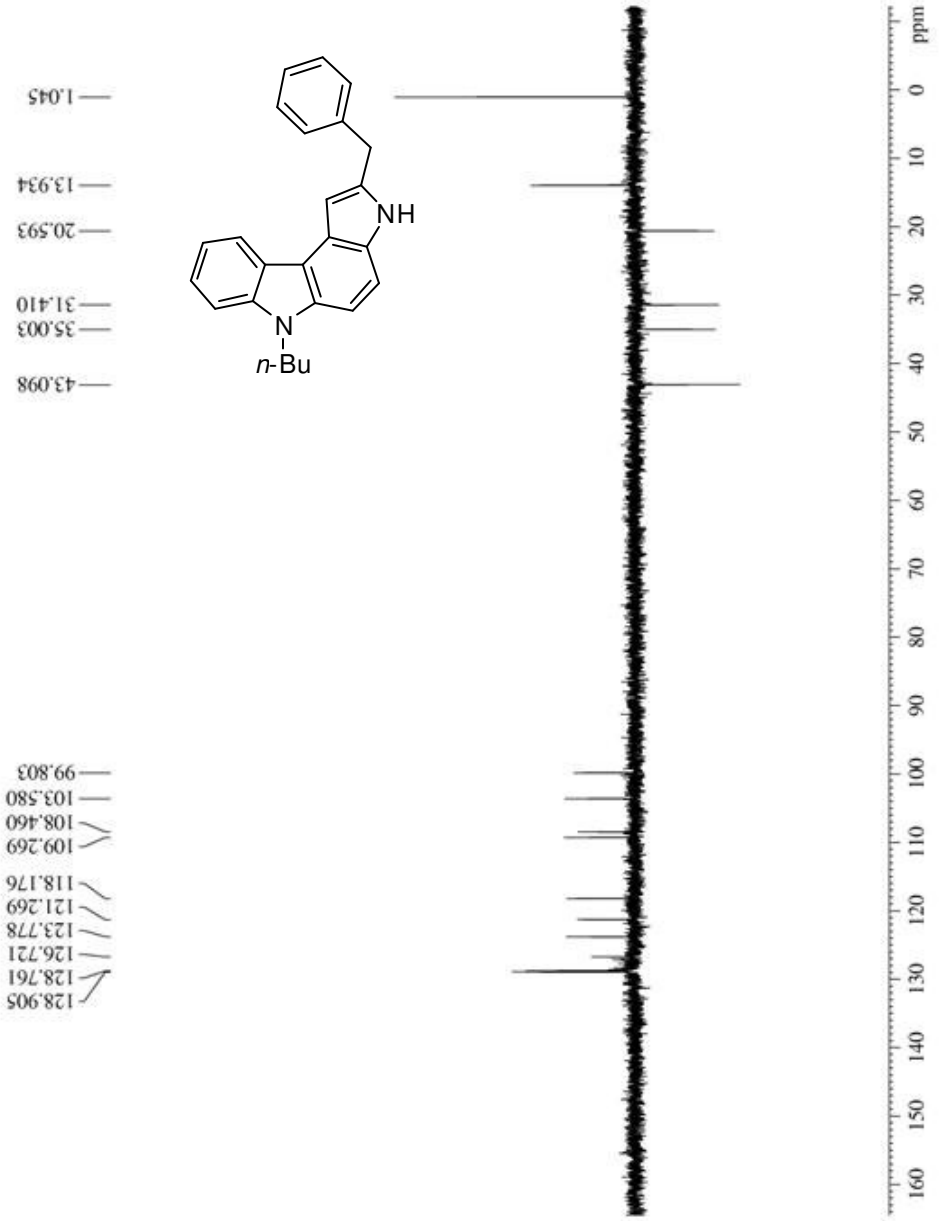
^{1}H NMR of 2-Benzyl-6-butyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3l)



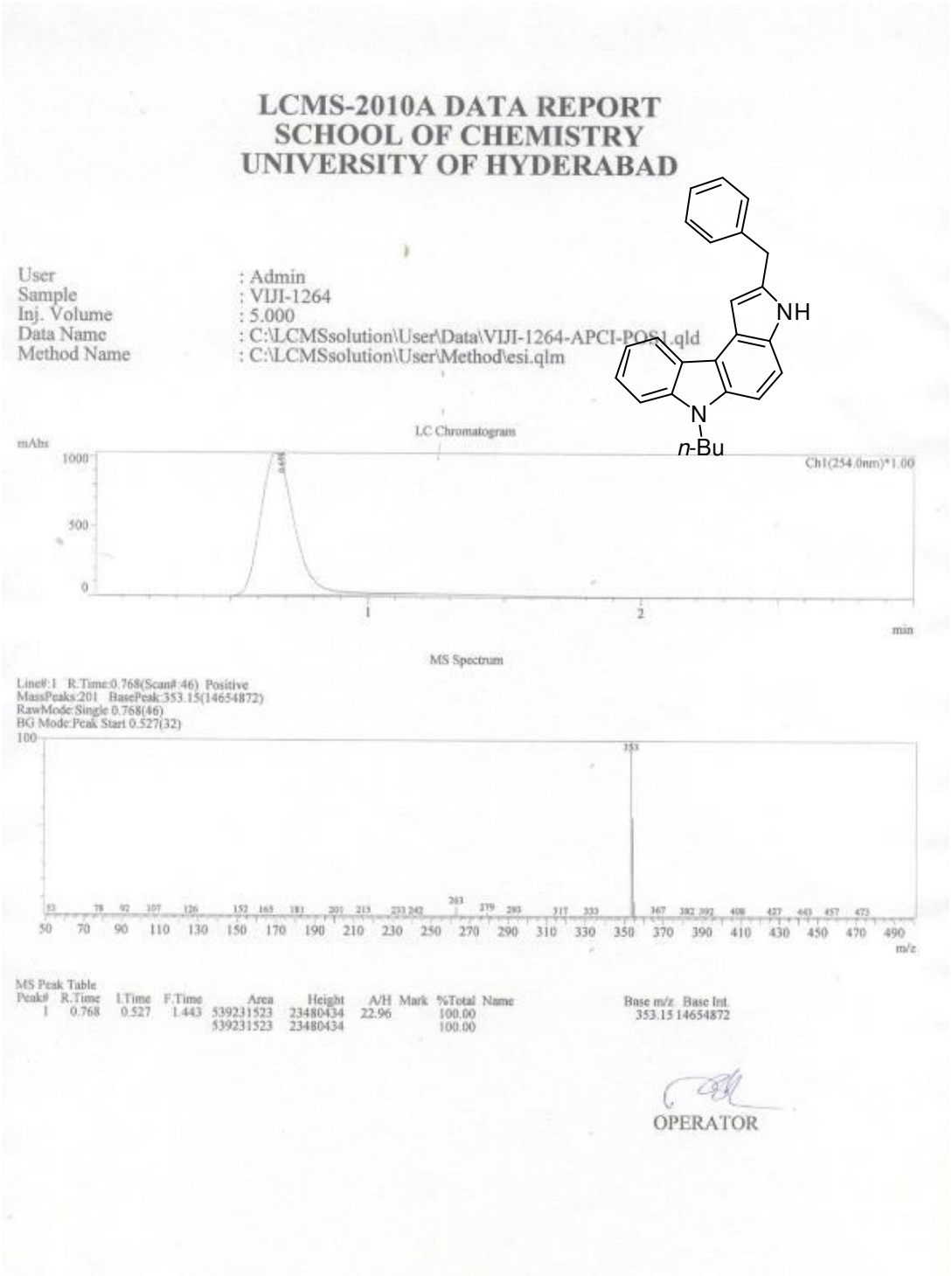
^{13}C NMR of 2-Benzyl-6-butyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3l)



DEPT of 2-Benzyl-6-butyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3l)



LC-MS of 2-Benzyl-6-butyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3l)



Electronic Supplementary Material (ESI) for RSC Advances

Elememntal Analysis of 2-Benzyl-6-butyl-3,6-dihydropyrrolo[2,3-*c*]carbazole (3l)

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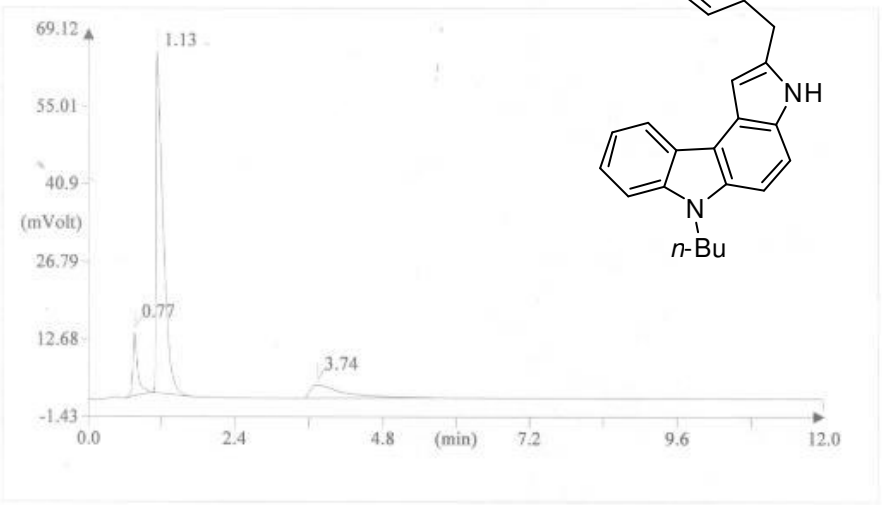
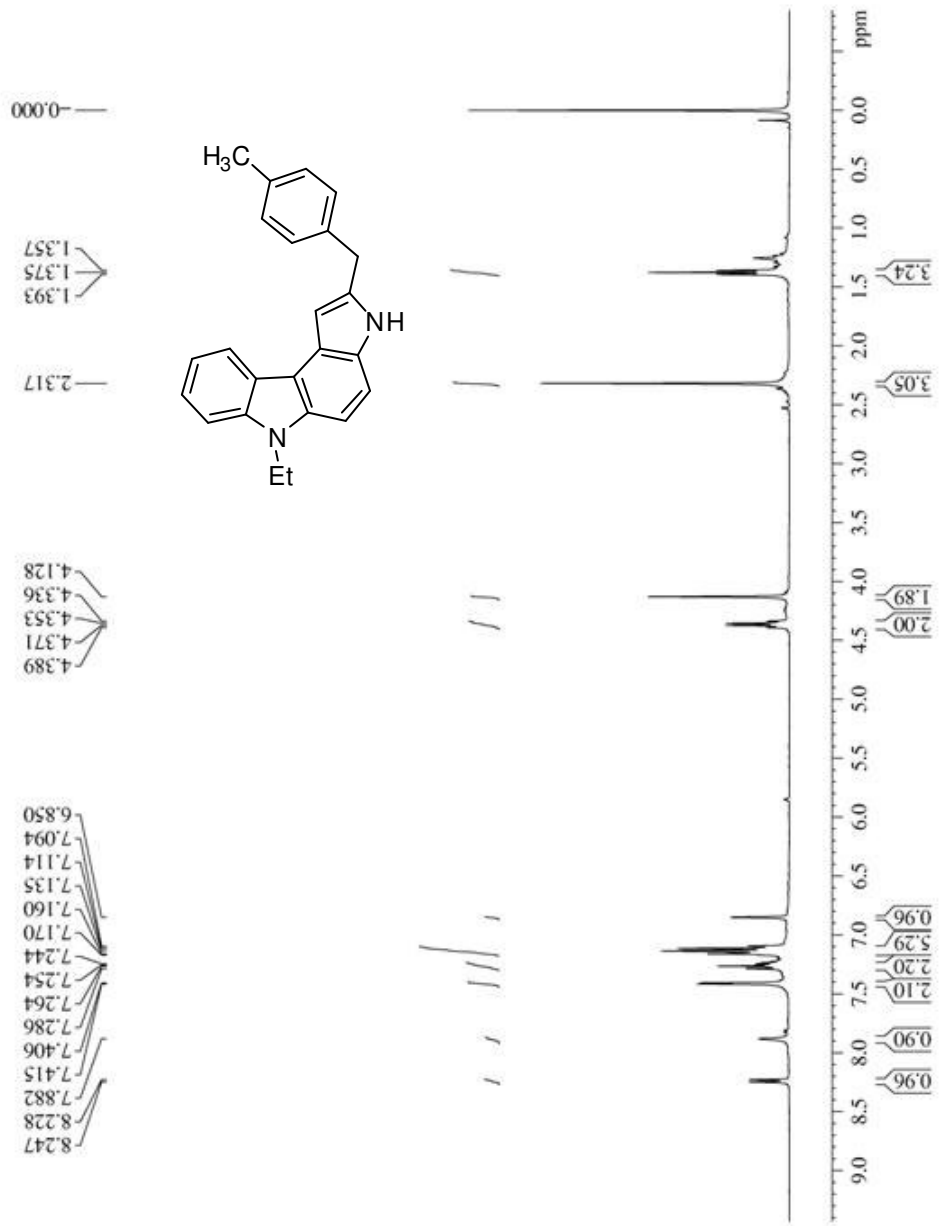
Method filename:	C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1264 (# 4)
Analysis type:	UnkNown
Chromatogram filename:	UNK-26072012-4.dat
Sample weight:	1.315

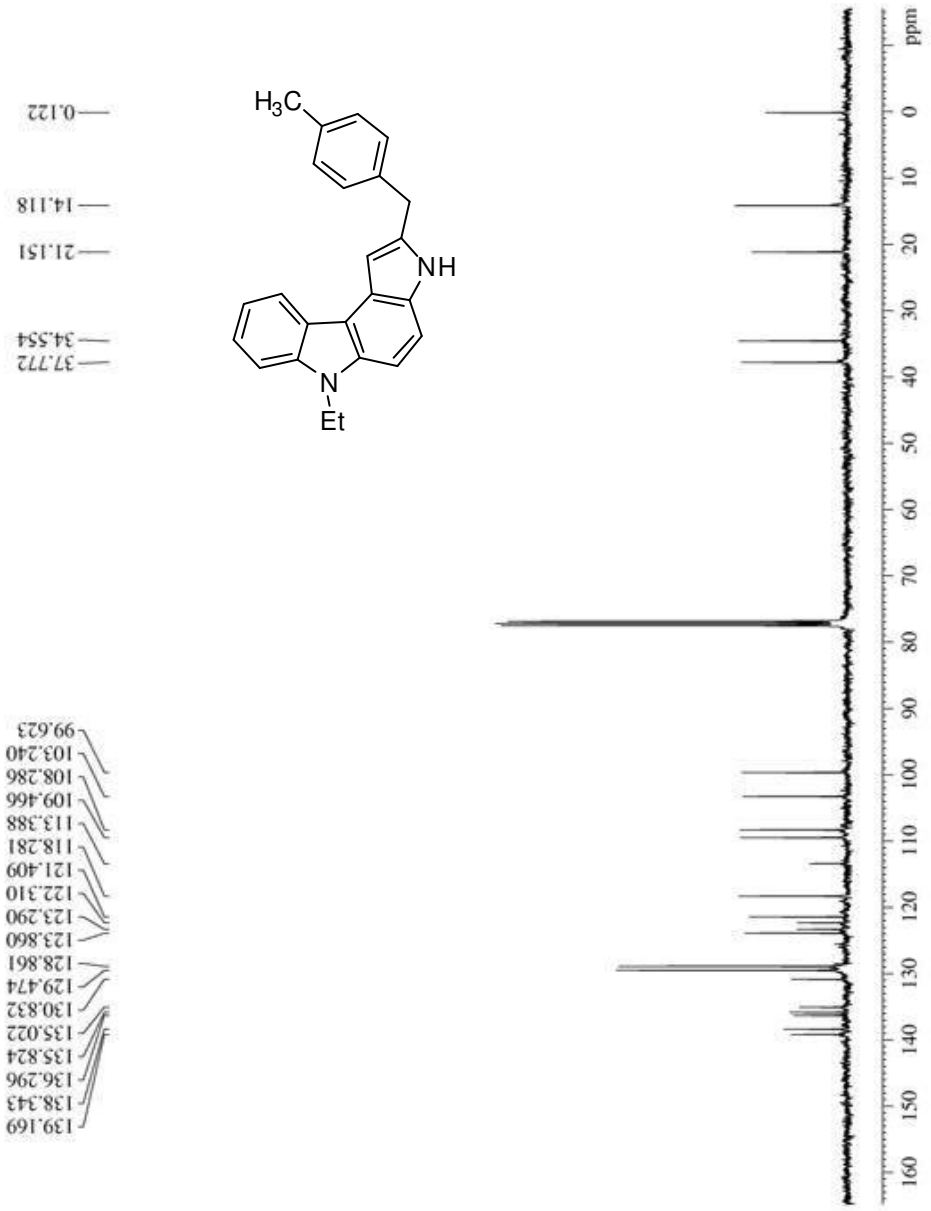


Element Name	Element %	Ret. Time
Nitrogen	7. 76	0. 77
Carbon	85. 21	1. 13
Hydrogen	6. 83	3. 74

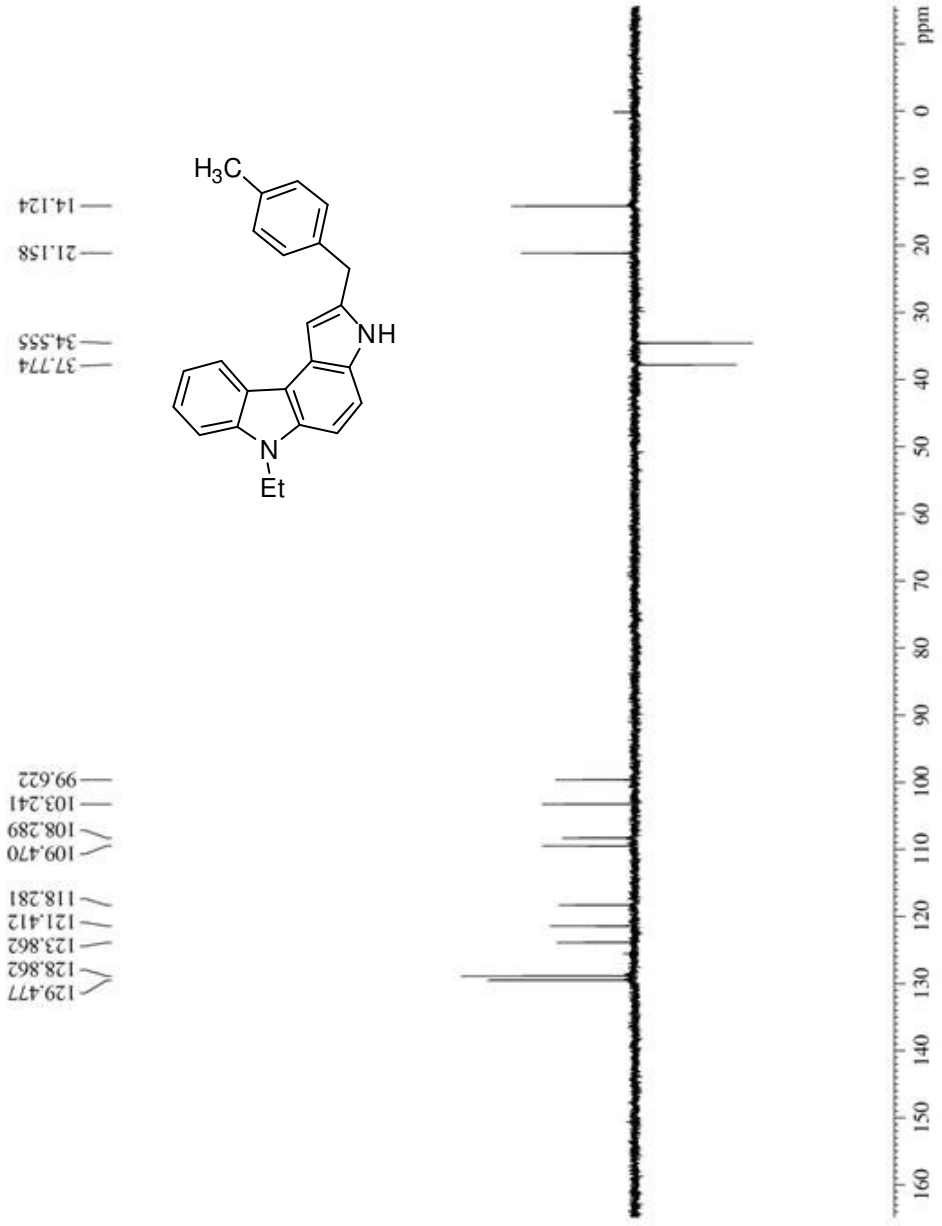
^{1}H NMR of 6-Ethyl-2-(4-methylbenzyl)-3,6-dihydropyrrolo[2,3-*c*]carbazole (3m)



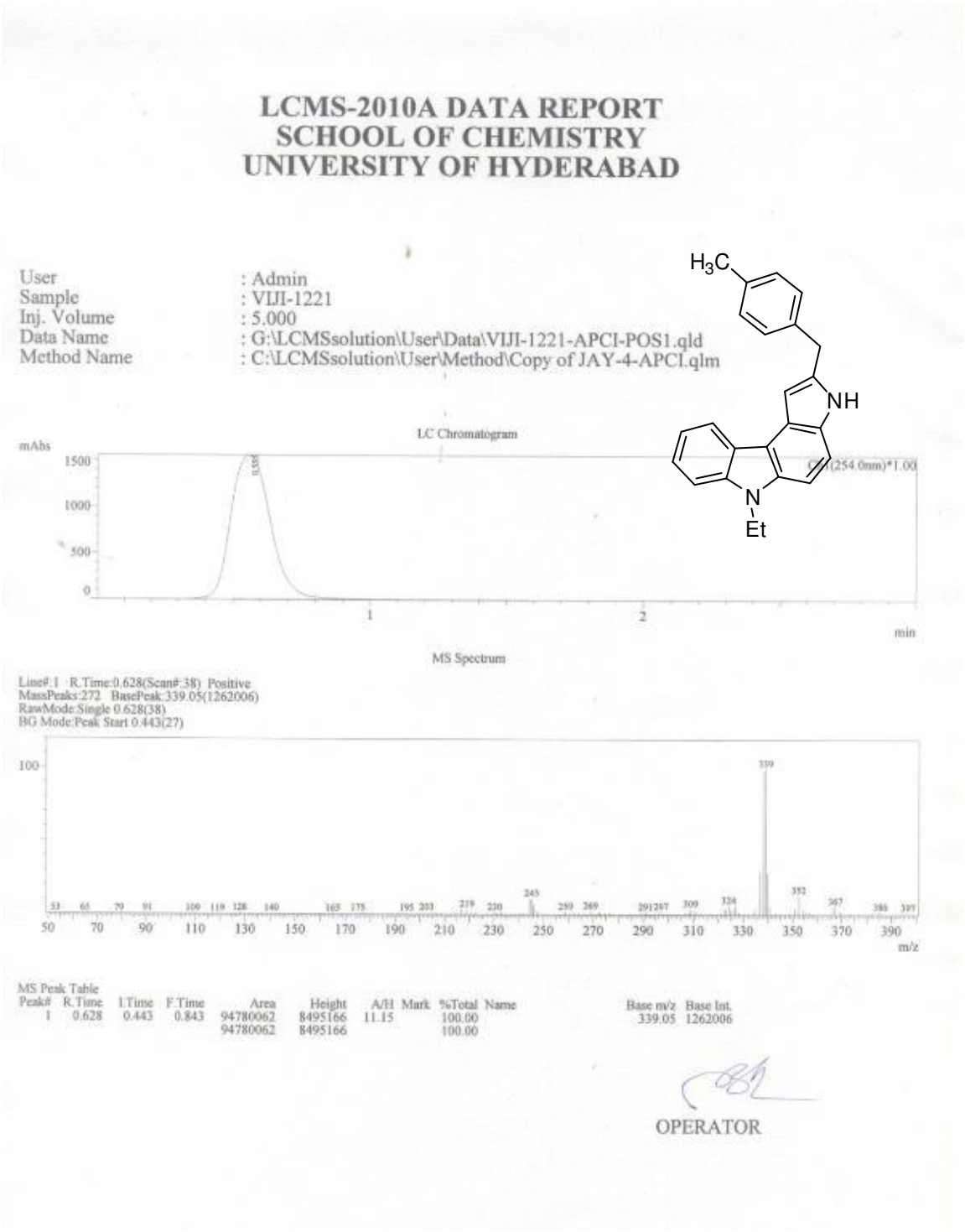
^{13}C NMR of 6-Ethyl-2-(4-methylbenzyl)-3,6-dihydropyrrolo[2,3-*c*]carbazole (3m)



DEPT of 6-Ethyl-2-(4-methylbenzyl)-3,6-dihydropyrrolo[2,3-*c*]carbazole (3m)



LC-MS of 6-Ethyl-2-(4-methylbenzyl)-3,6-dihydropyrrolo[2,3-*c*]carbazole (3m)



LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : VIJI-1221
Inj. Volume : 5.000
Data Name : G:\LCMSsolution\User\Data\VIJI-1221-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\Copy of JAY-4-APCI.qlm

LC Chromatogram

MS Spectrum

Line#:1 R.Time:0.628(Scan#:38) Positive
MassPeaks:272 BasePeak:339.05(1262006)
RawMode:Single 0.628(38)
BG Mode:Peak Start 0.443(27)

MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.628	0.443	0.843	94780062	8495166	11.15		100.00		339.05	1262006
				94780062	8495166			100.00			

OPERATOR

Elemental Analysis of 6-Ethyl-2-(4-methylbenzyl)-3,6-dihydropyrrolo[2,3-*c*]carbazole (3m)

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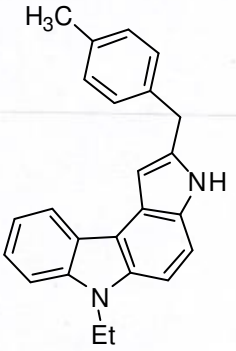
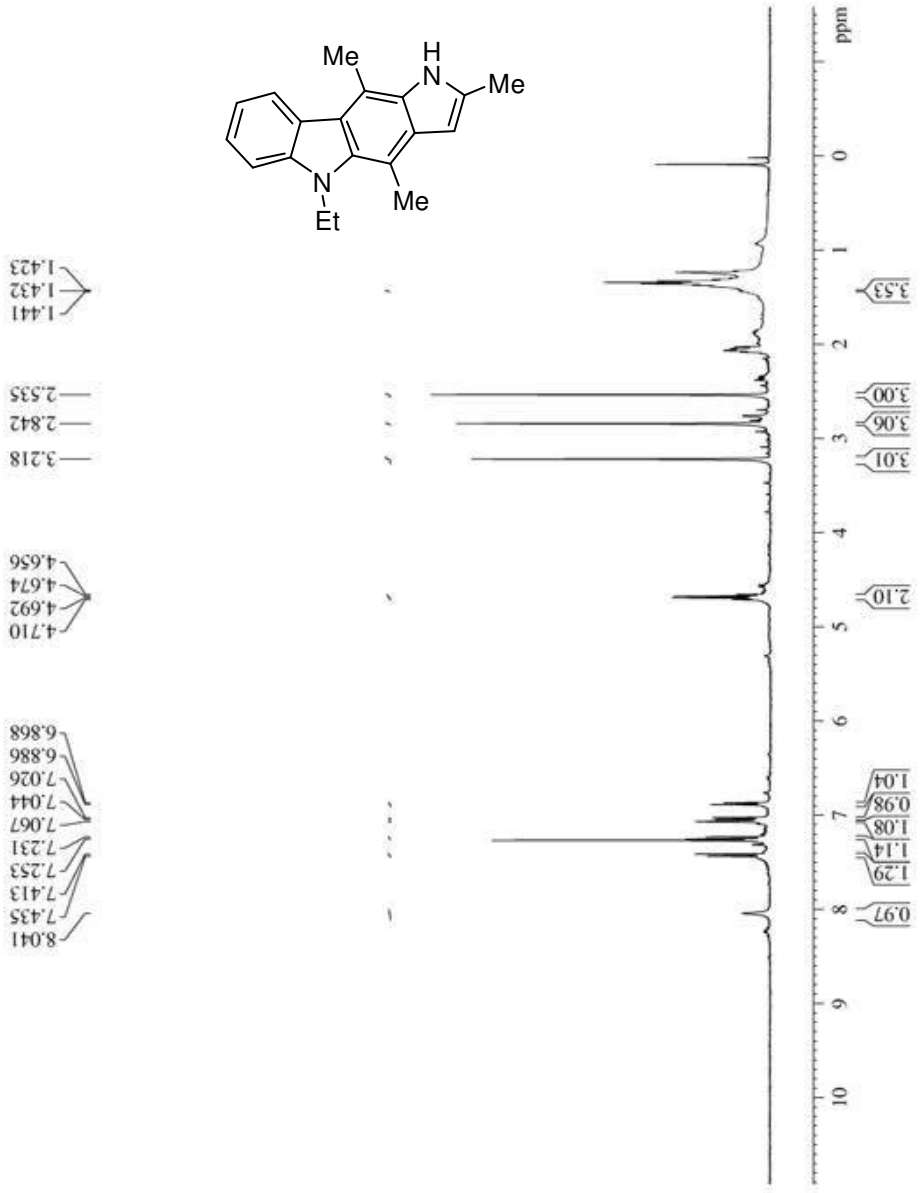
Method filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: VIJI-1221 (# 7)
Analysis type: UnkNown
Chromatogram filename: UNK-11072012-7.dat
Sample weight: 1.237

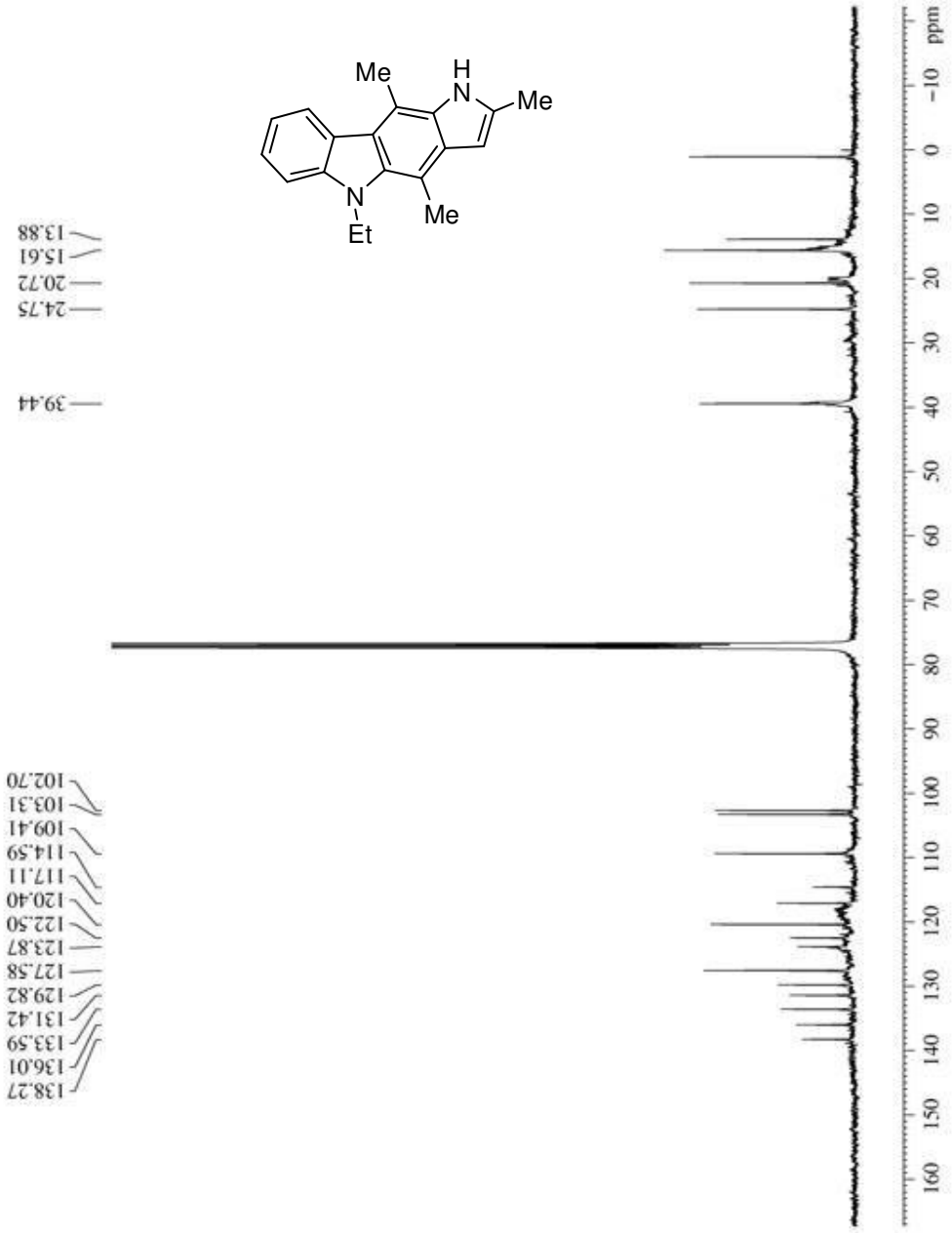


Element Name	Element %	Ret. Time
Nitrogen	8. 21	0. 87
Carbon	85. 31	1. 35
Hydrogen	6. 45	4. 68

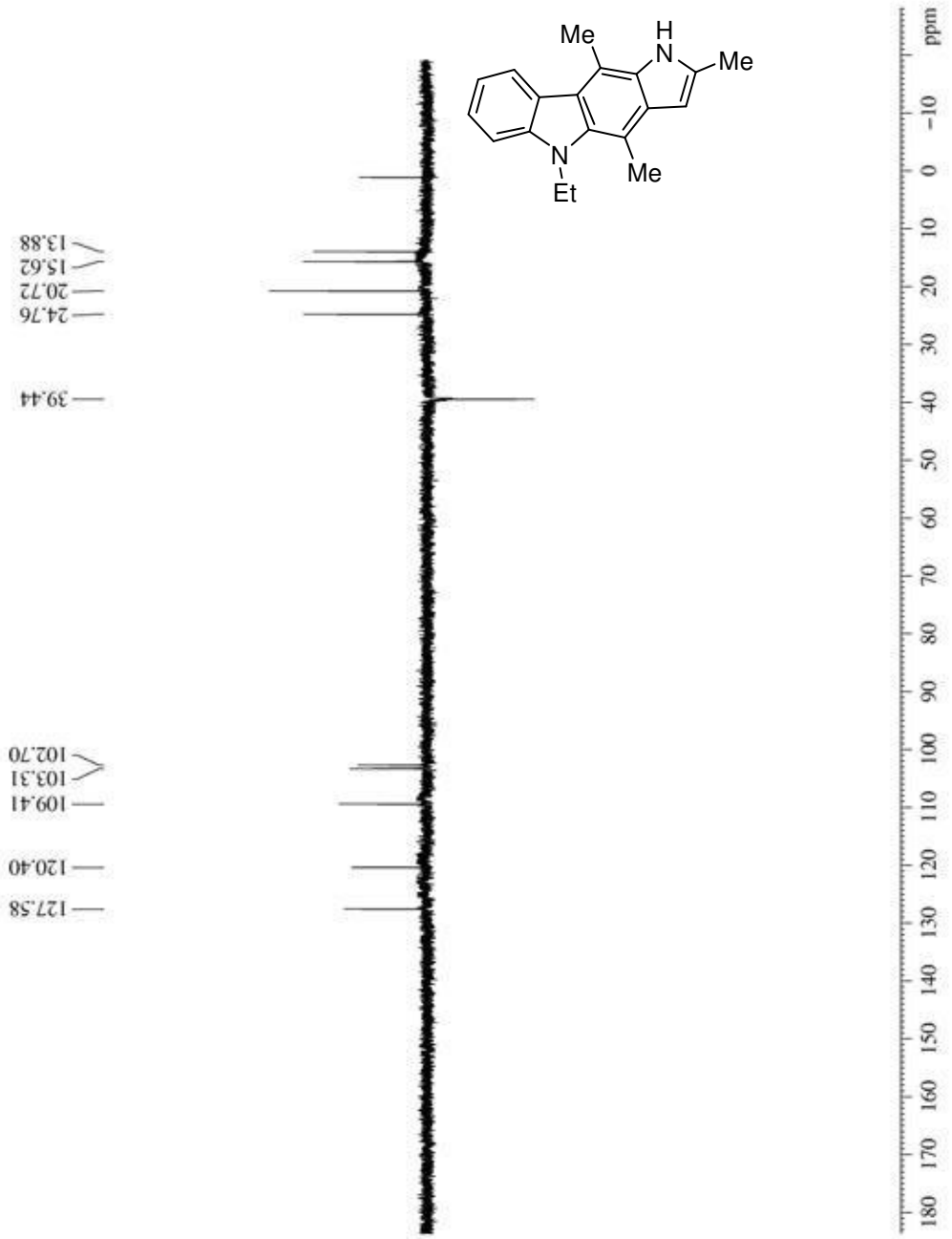
^{1}H NMR of 5-ethyl-2,4,10-trimethyl-1,5-dihydropyrrolo[3,2-*b*]carbazole (3n)



^{13}C NMR of 5-ethyl-2,4,10-trimethyl-1,5-dihydropyrrolo[3,2-*b*]carbazole (3n)

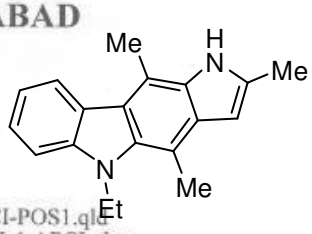


DEPT of 5-ethyl-2,4,10-trimethyl-1,5-dihydropyrrolo[3,2-*b*]carbazole (3n)



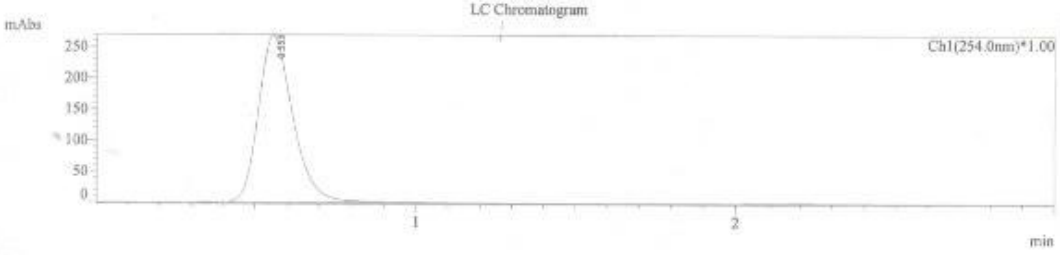
LC-MS of 5-ethyl-2,4,10-trimethyl-1,5-dihydropyrrolo[3,2-*b*]carbazole (3n)

LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD



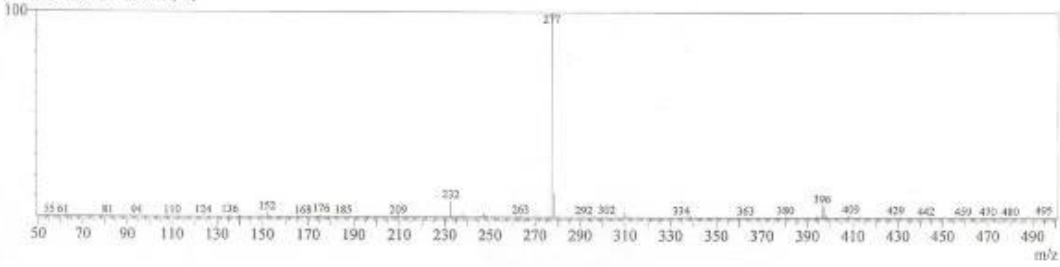
User : Admin
Sample : VIJI-1178
Inj. Volume : 5.000
Data Name : G:\LCMSsolution\User\Data\VIJI-1178-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\Copy of JAY-4-APCI.qlm

LC Chromatogram



MS Spectrum

Line#:1 R.Time:0.648(Scan#:39) Positive
MassPeaks:378 BasePeak:277.30(6550609)
RawMode:Single 0.648(39)
BG Mode:Peak Start 0.427(26)



MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.648	0.427	0.843	124712044	12321967	10.12		100.00		277.30	6550609
				124712044	12321967			100.00			

OPERATOR

Elemental Analysis of 5-ethyl-2,4,10-trimethyl-1,5-dihydropyrrolo[3,2-*b*]carbazole (3n)

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
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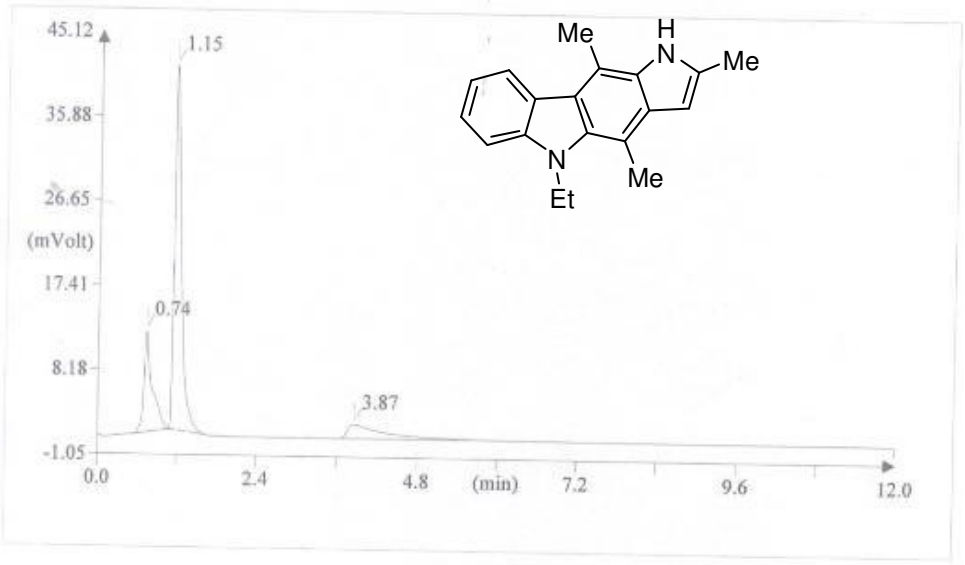
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	VIJI-1178 (# 13)
Analysis type:	UnkNown
Chromatogram filename:	UNK-11072012-13.dat
Sample weight:	1.106



Element Name	Element %	Ret. Time
Nitrogen	10. 21	0. 74
Carbon	82. 68	1. 15
Hydrogen	7. 21	3. 87