

Supplementary Material

Synthesis of novel benzimidazole-diindolylmethane hybrid compounds within the green chemistry context

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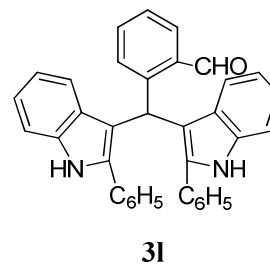
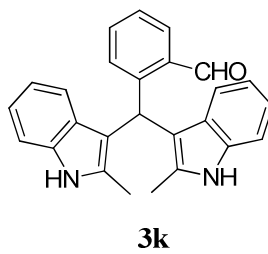
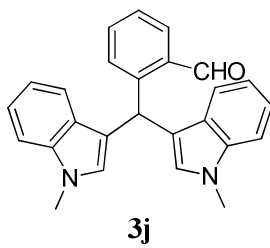
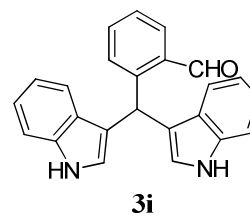
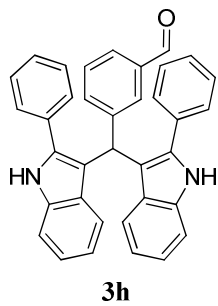
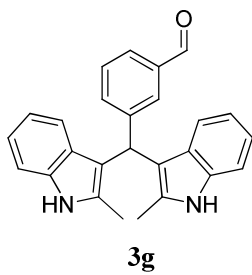
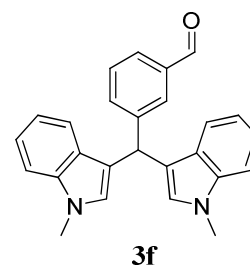
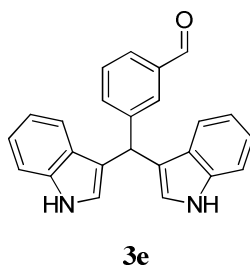
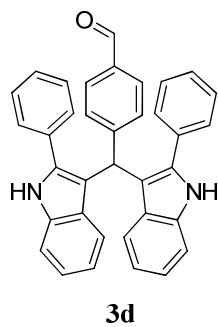
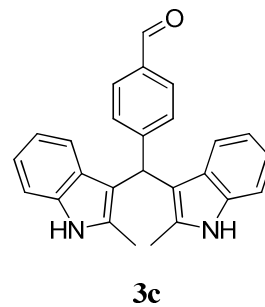
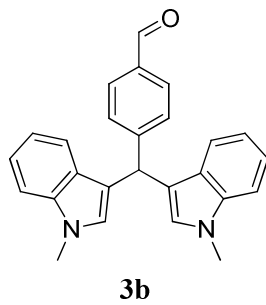
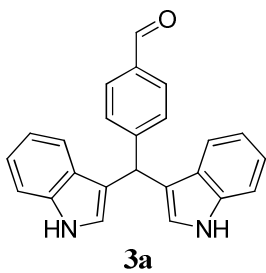
^b*Instituto de Química-Universidad Nacional Autónoma de México, Ciudad Universitaria, Circuito Exterior, México D.F., C.P. 04510.*

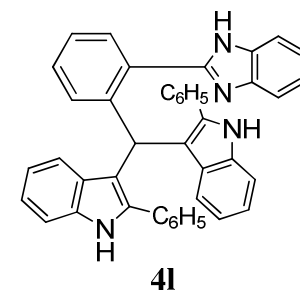
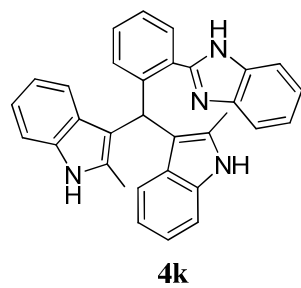
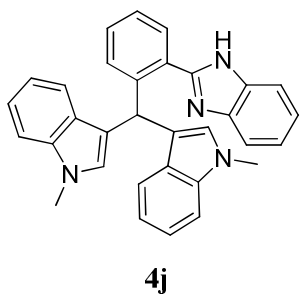
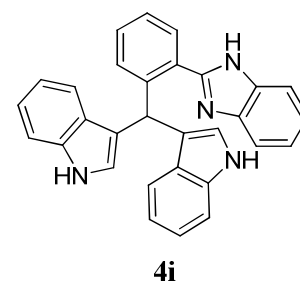
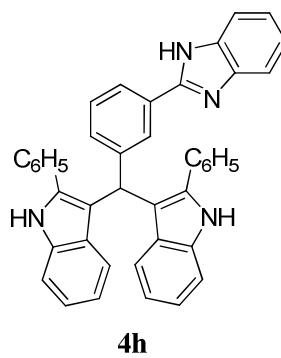
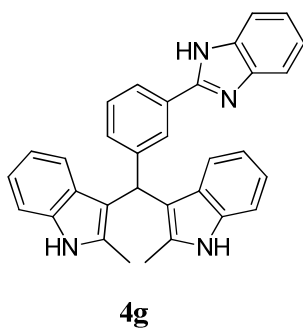
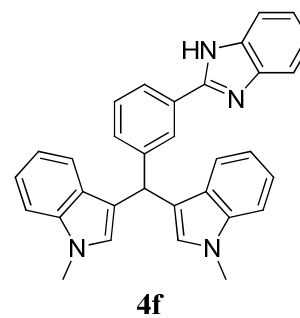
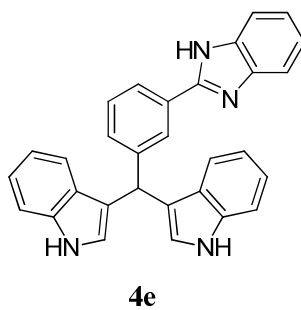
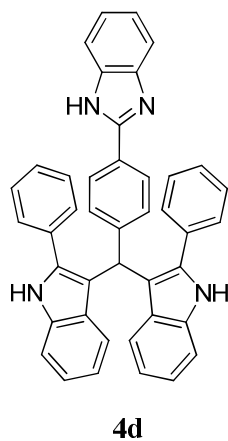
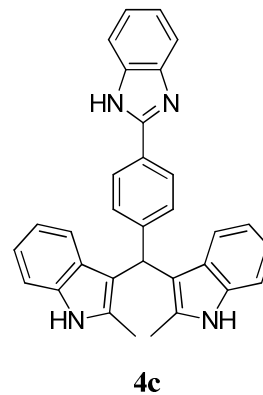
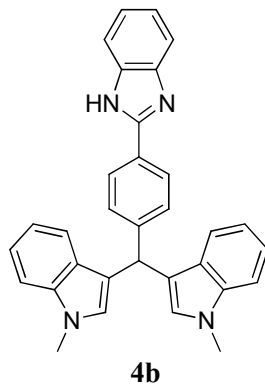
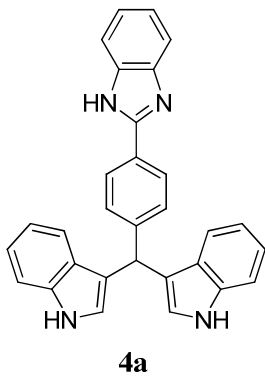
^c*Departamento de Alimentos y Biotecnología, Facultad de Química, Edificio E, UNAM, Av. Universidad 3000, C.U., Coyoacán, México, D.F., 04510, México.*

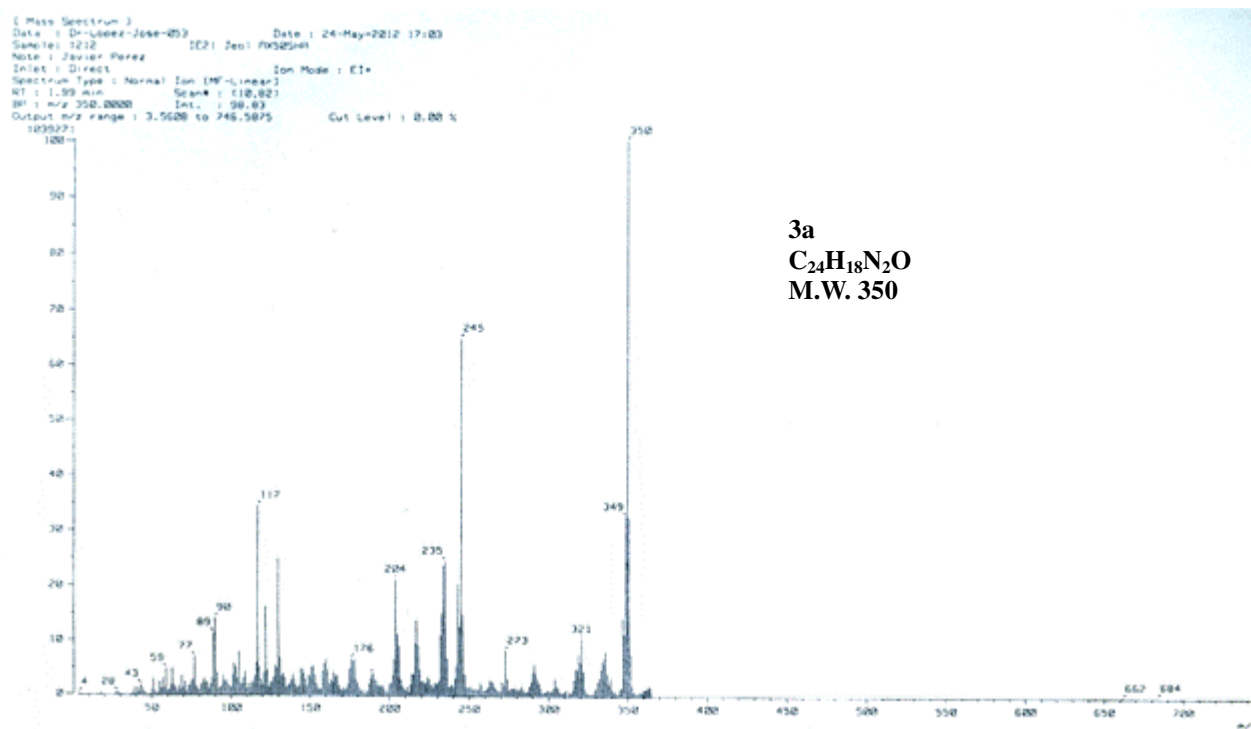
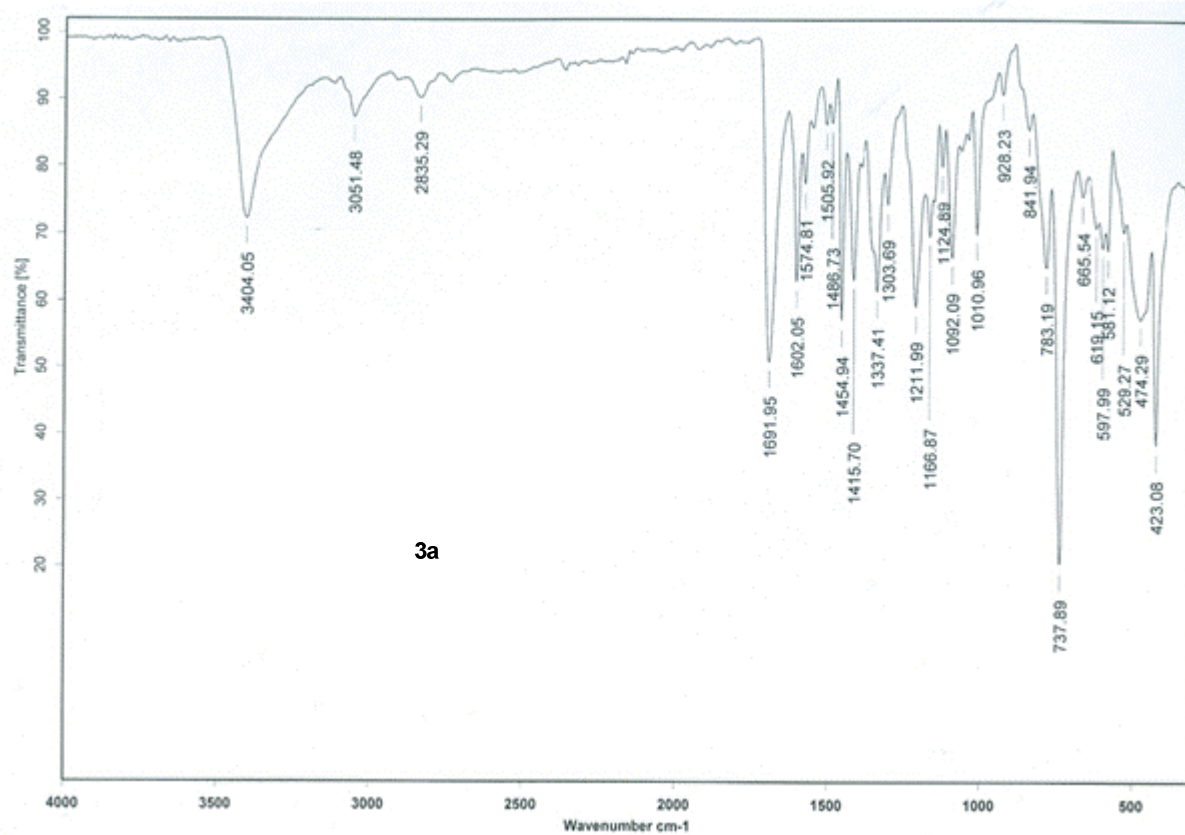
E-mail: penieres@unam.mx

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IR, MS, ¹ H NMR, ¹³ C NMR Spectra	S4





IR, MS, ^1H NMR, ^{13}C NMR Spectra

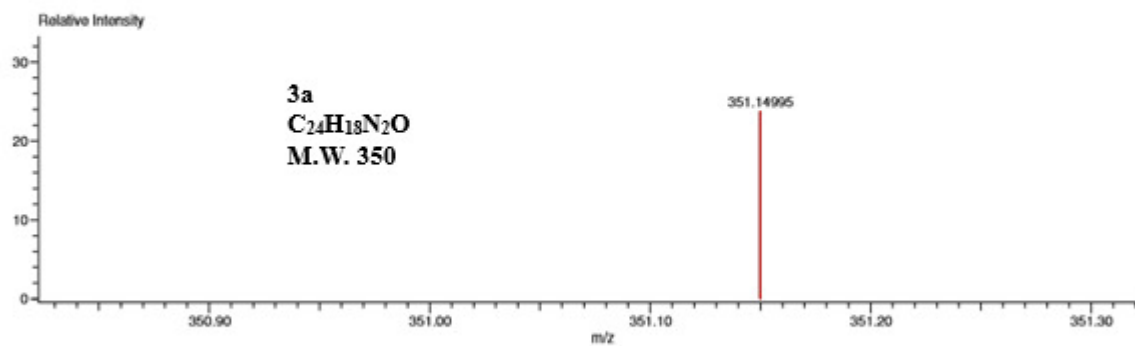
3a
 $\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}$
M.W. 350

Data:2580 indol.p
 Sample Name:Dr Alvarez Cocilio Operador: Carmen Garcia/ Javier Perez
 Description:
 Ionization Mode:ESI+
 History:Detomine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1]) 0.6...

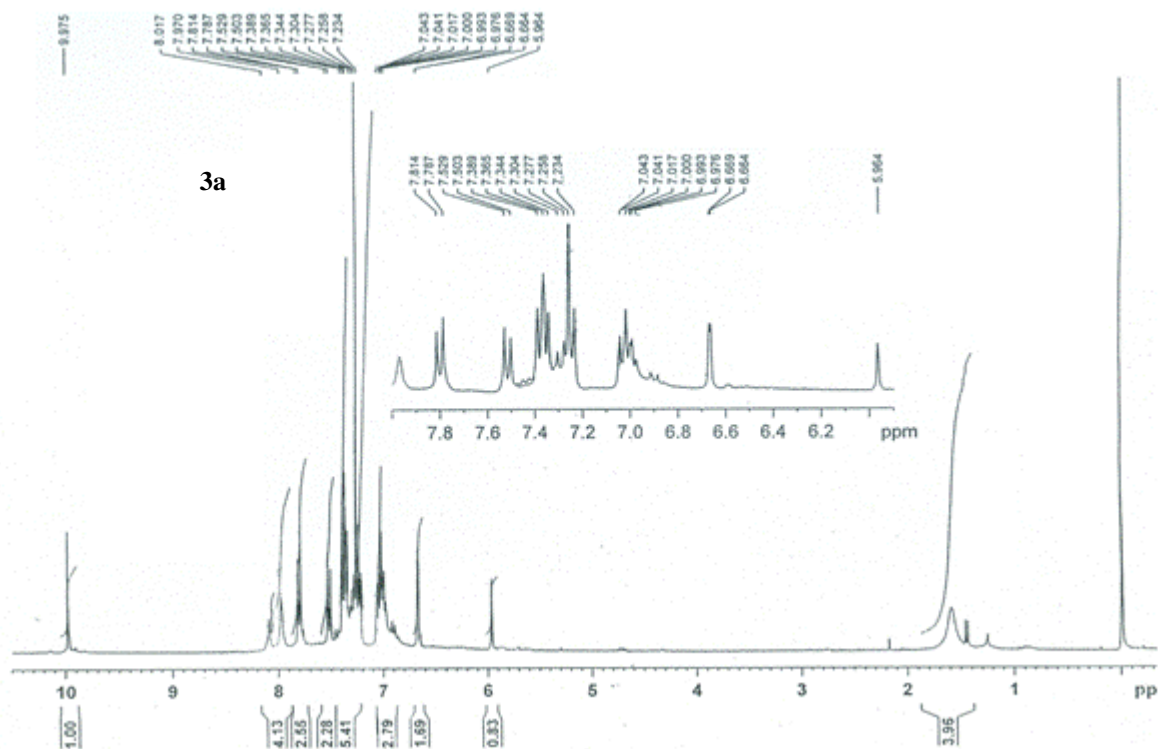
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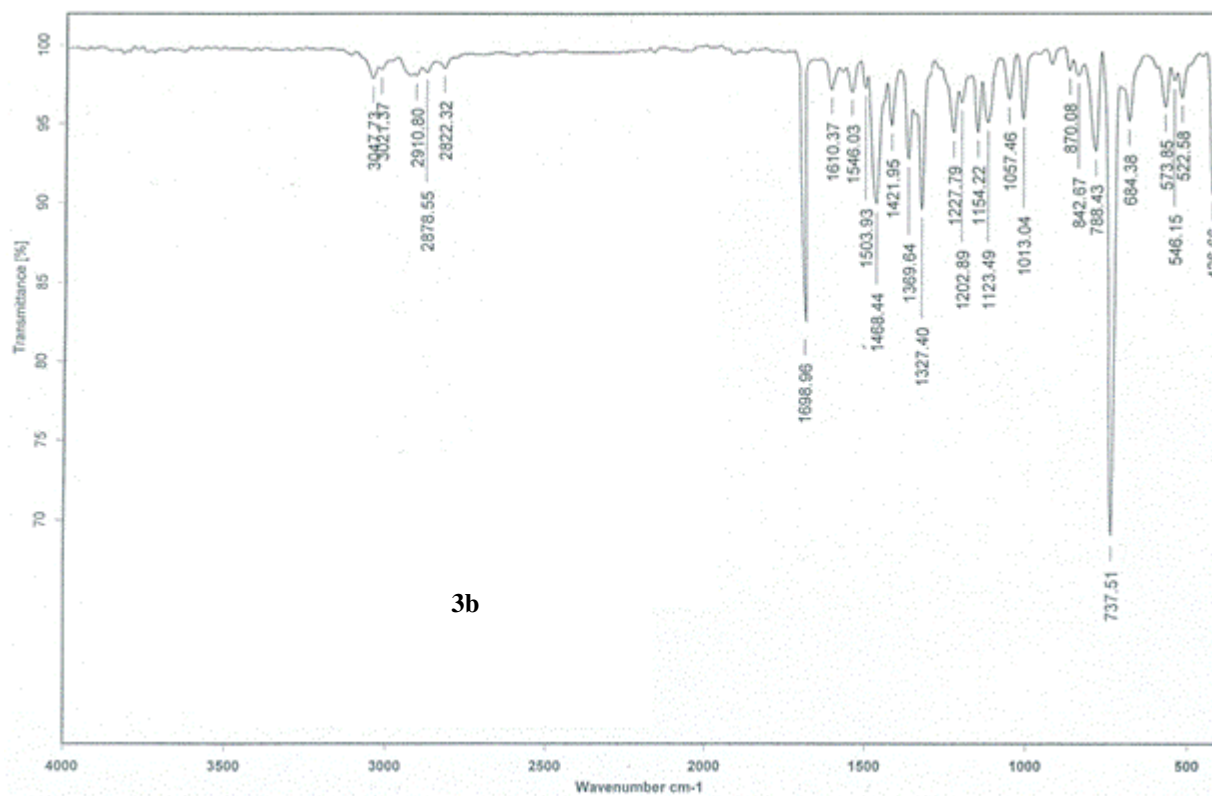
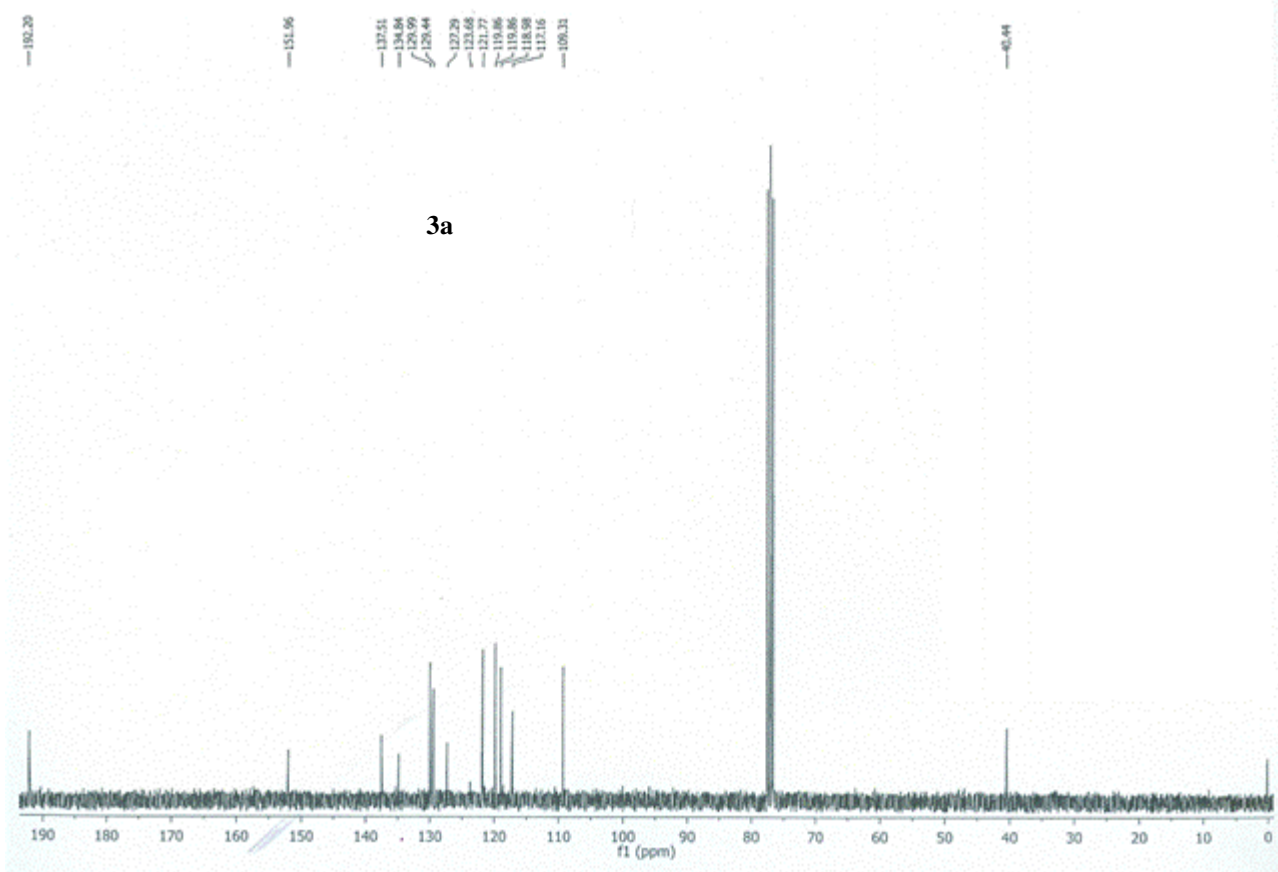
Charge number:1
 Element:¹²C:0 .. 56, ¹H:0 .. 120, ¹⁴N:0 .. 2, ¹⁶O:0 .. 1
 Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

Unsaturation Number:0.0 .. 30.0 (Fraction:Both)

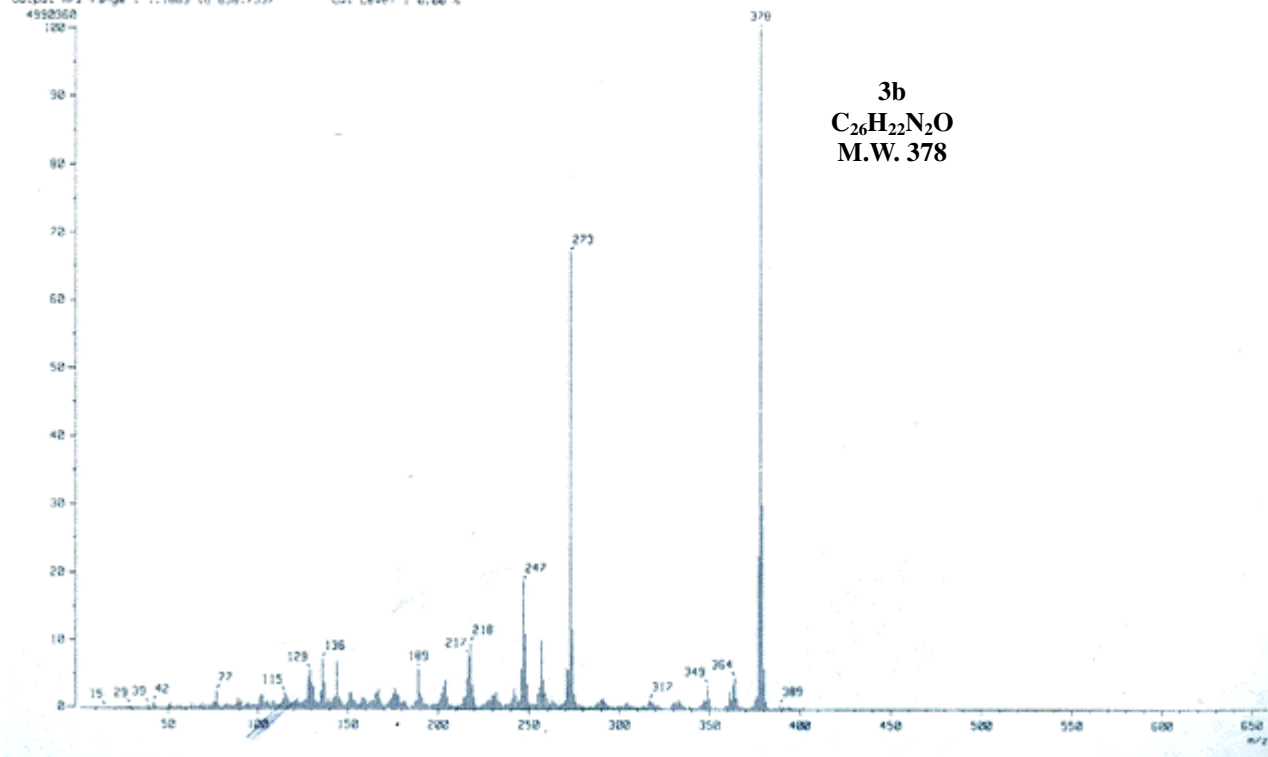


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14995	11159.75	351.14974	0.21	0.61	$^{12}C_{24}^{1}H_{18}^{14}N_2^{16}O_1$	16.5





[Mass Spectrum]
 Date : Dr-Lopez-Jose-055 Date : 24-May-2012 17:32
 Sample: 1222 IET1 Jeol RK5254R
 Note : Javier Perez
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 2.03 min Scan : [37,37]
 BP : m/z 378.0000 Int. : 474.55
 Output m/z range : 1.1869 to 658.7537 Cut Level : 0.00 %



3b
 $C_{26}H_{22}N_2O$
 M.W. 378

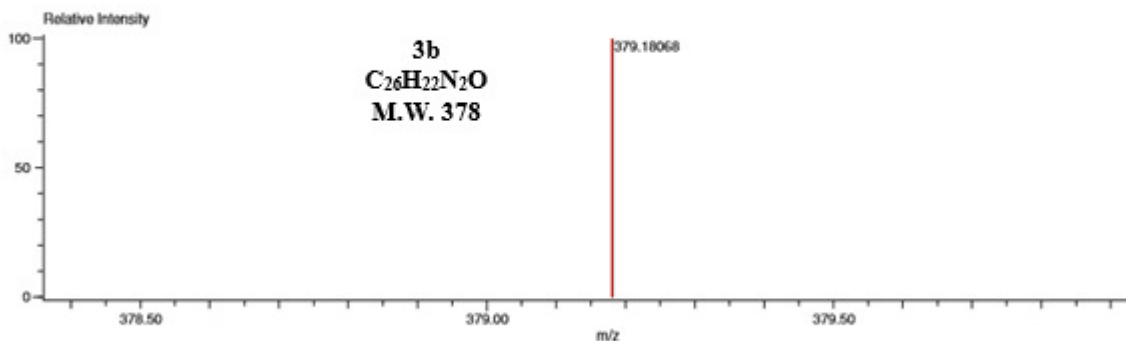
Data:2579 1-Me-p
 Sample Name:Dr Alvarez Cocilio Operator: Carmen Garcia/ Javier Perez
 Description:
 Ionization Mode:ESI-
 History:Dotormine m/z[Peak Detect[Controid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.7...

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 Operator:AccuTOF
 Mass Calibration data:Cal_Peg_600
 Created:9/3/2015 3:16:29 PM
 Created by:AccuTOF

Charge number:1
 Element: $^{12}C:0 .. 56, ^1H:0 .. 120, ^{14}N:0 .. 2, ^{16}O:0 .. 1$

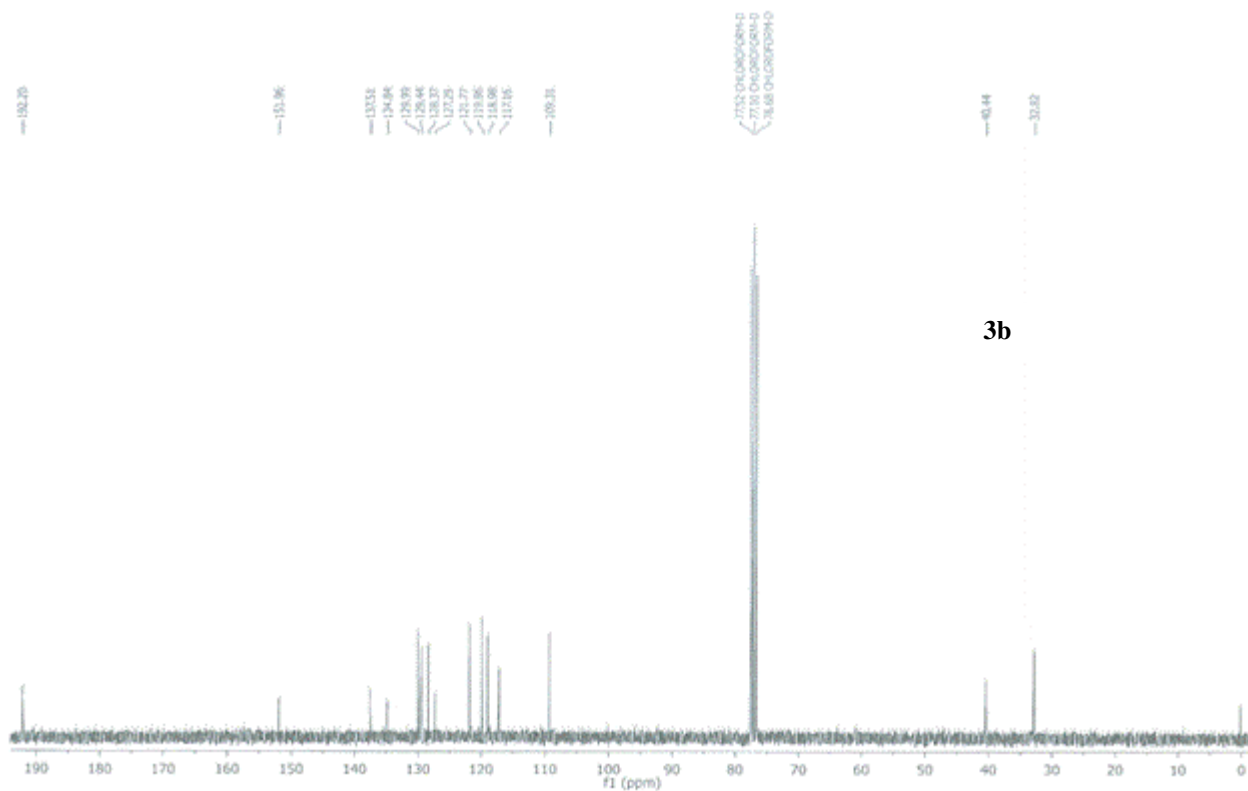
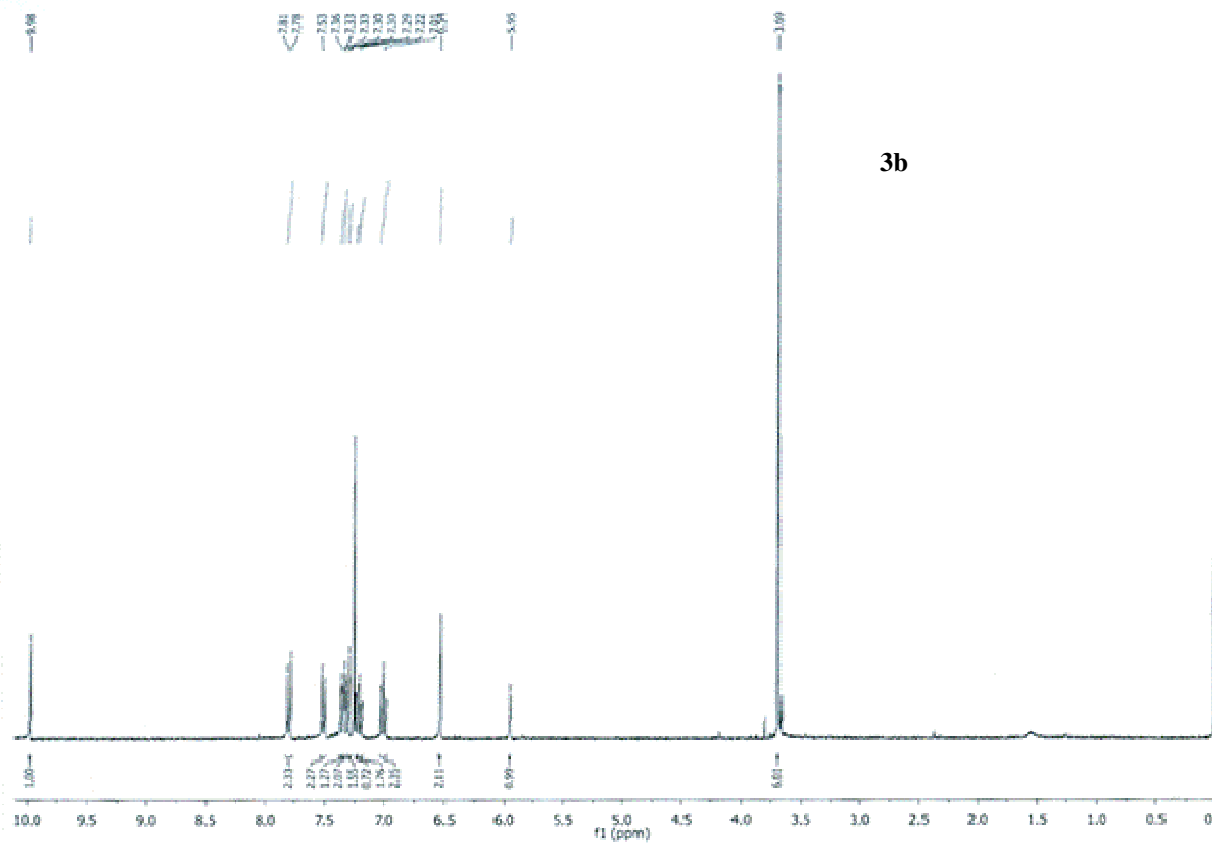
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

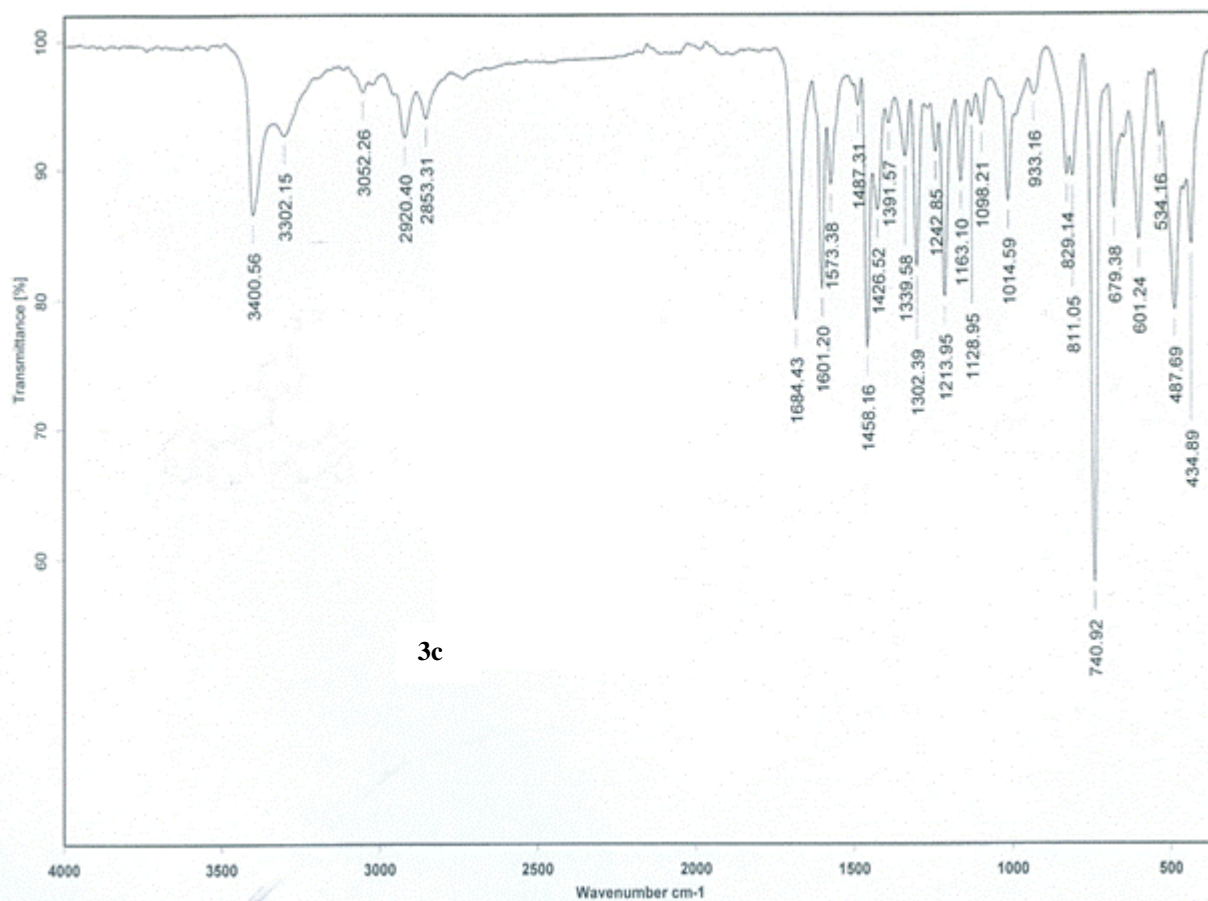
Unsaturation Number:0.0 .. 30.0 (Fraction:Both)



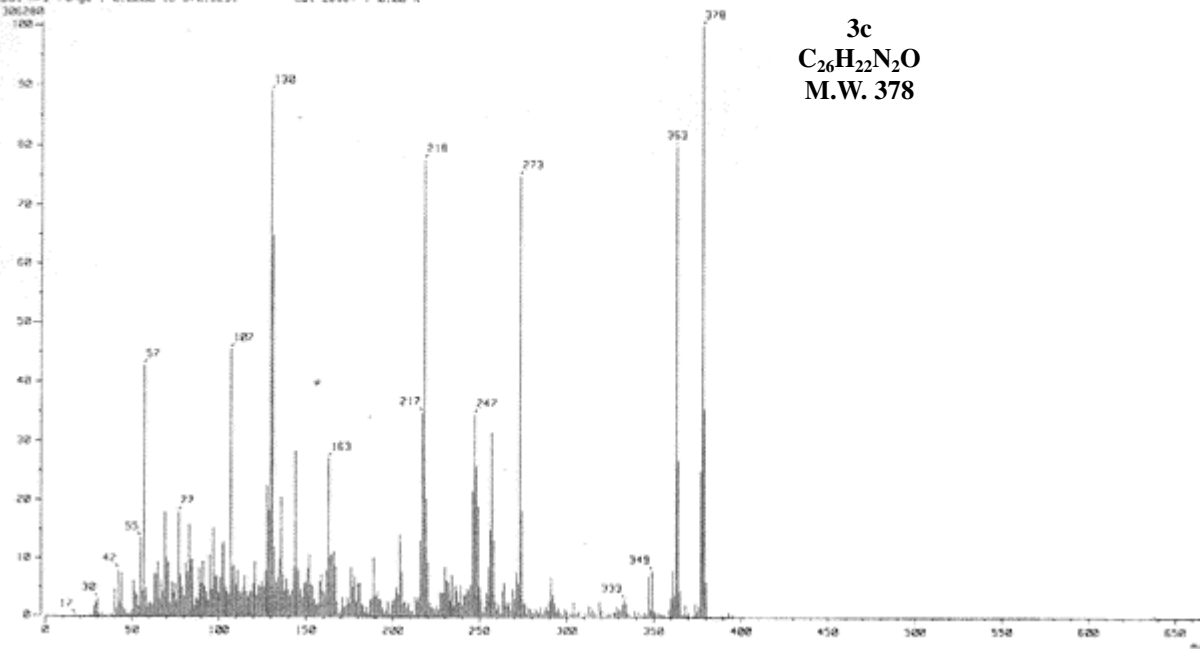
3b
 $C_{26}H_{22}N_2O$
 M.W. 378

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18068	13748.00	379.18104	-0.36	-0.95	$^{12}C_{26}^{1}H_{22}^{14}N_2^{16}O_1$	16.5





[Mass Spectrum]
 Date : 17-Apr-2012 19:25
 Sample: 502 IC19 Jeol RMU205M
 Note : Javier Perez
 Inlet : Direct Ion Mode : E1+
 Spectrum Type : Normal Ion (M-Linear)
 RT : 1.43 min Scan# : 133,55
 BP : m/z 378.20000 Int. : 29,04
 Output m/z range : 0.0000 to 678.6233 Cut Level : 0.20 %
 300280



Data:2581 2-Me-p
 Sample Name:Dr Alvarez Cocilio Operador: Carmen Garcia/ Javier Perez
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1]] 0.3...

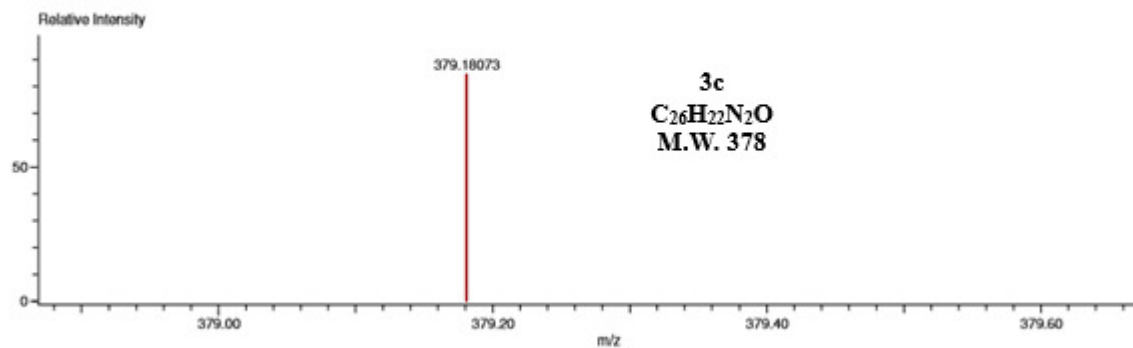
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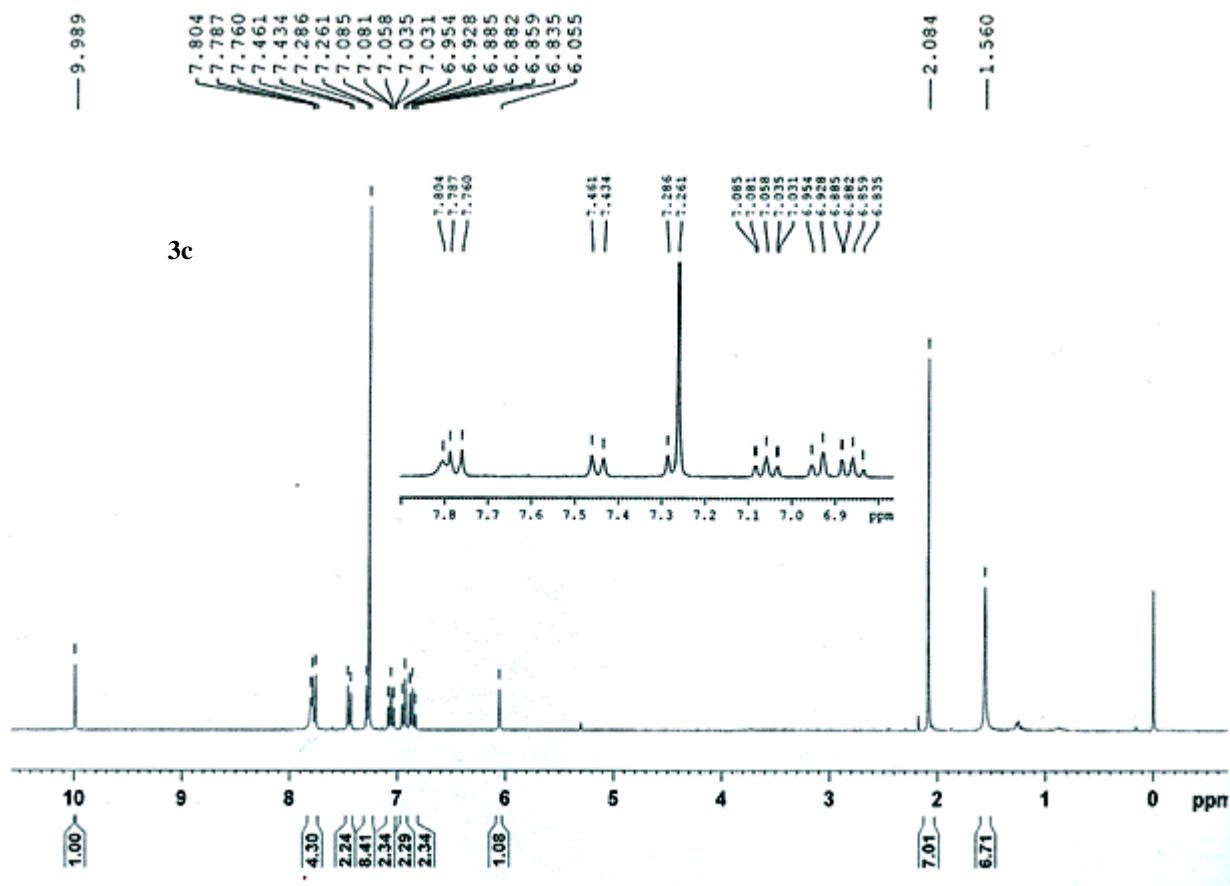
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

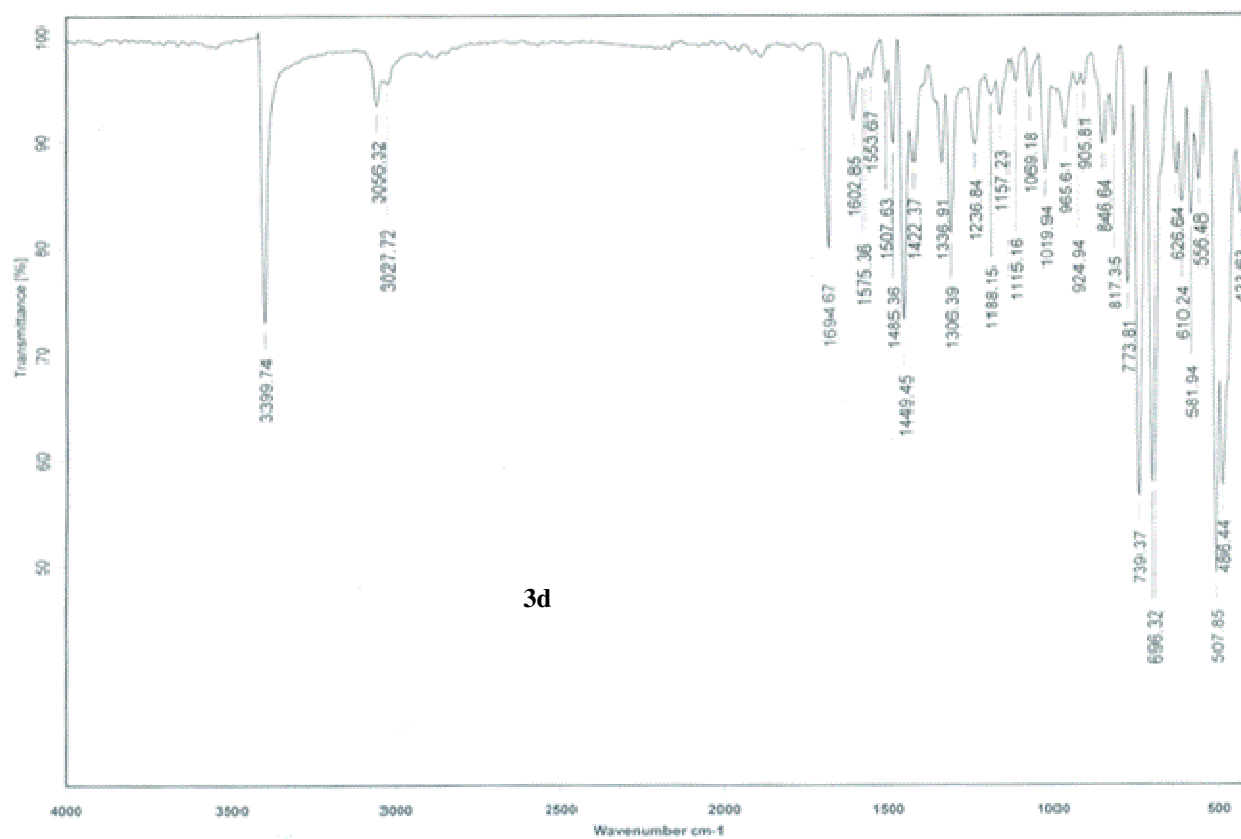
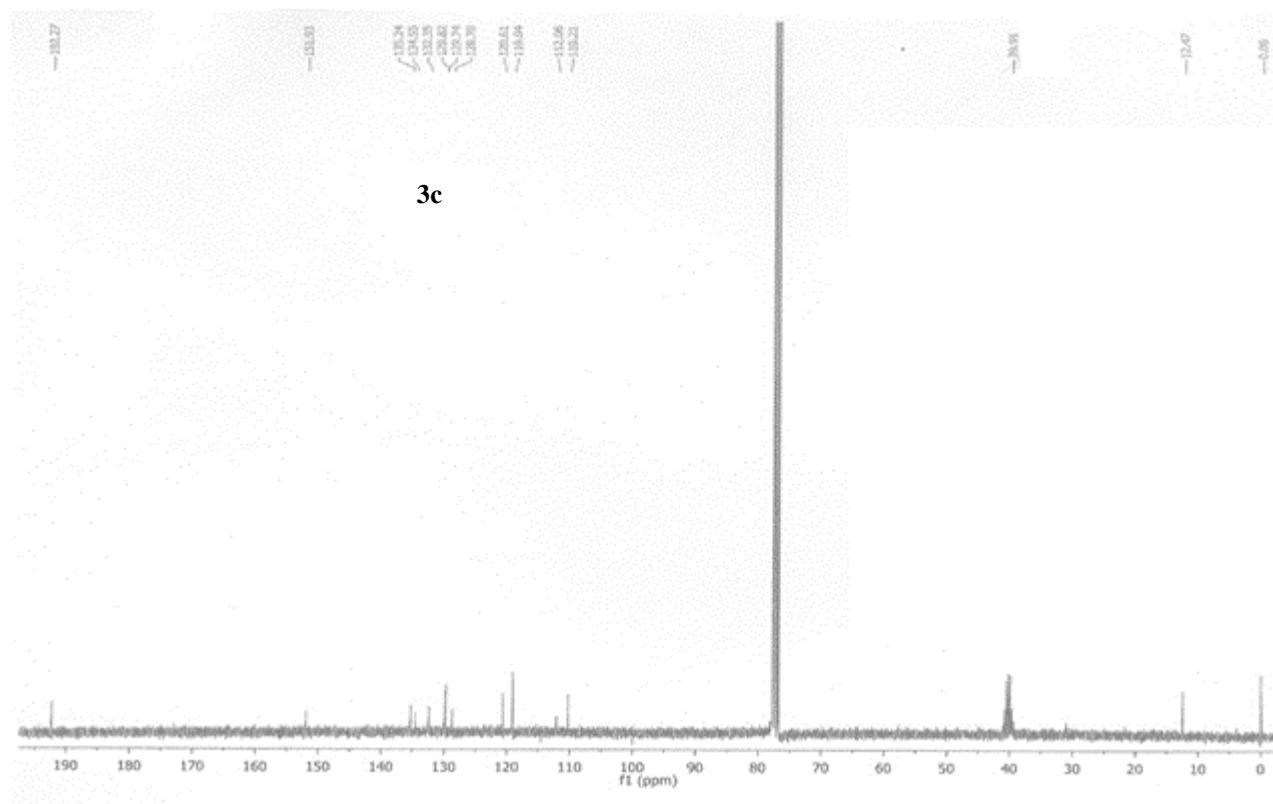
Unsaturation Number:0.0 .. 30.0 (Fraction:Both)

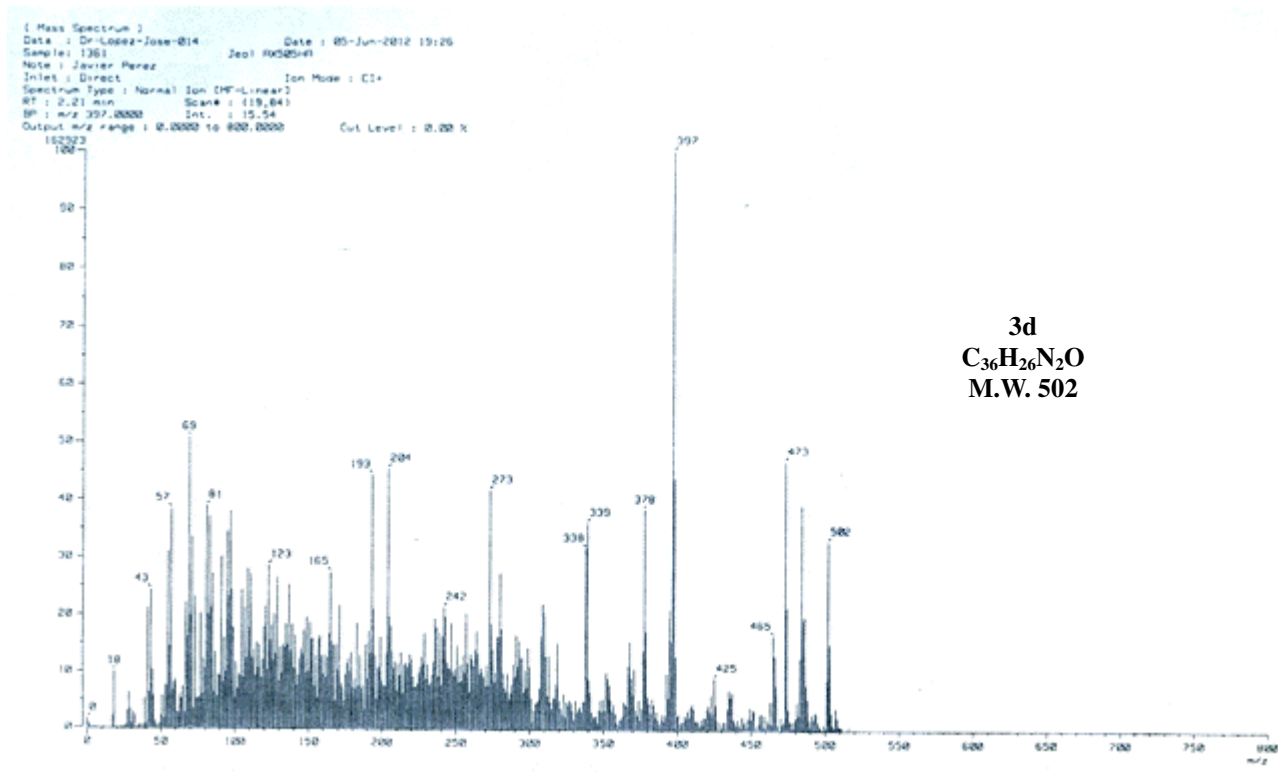
Element:¹²C:0 .. 56, ¹H:0 .. 120, ¹⁴N:0 .. 2, ¹⁶O:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18073	20083.50	379.18104	-0.31	-0.81	$^{12}C_{26}^{1}H_{22}^{14}N_2^{16}O_1$	16.5



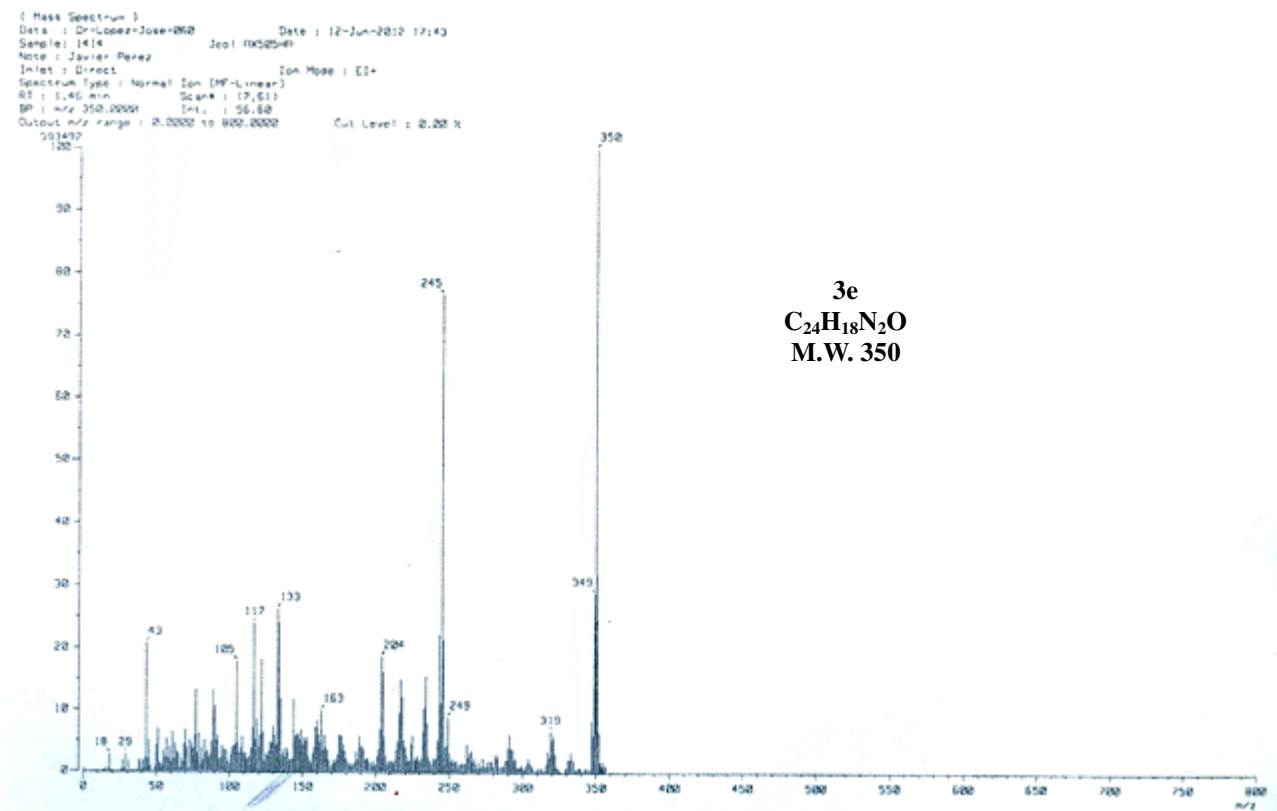
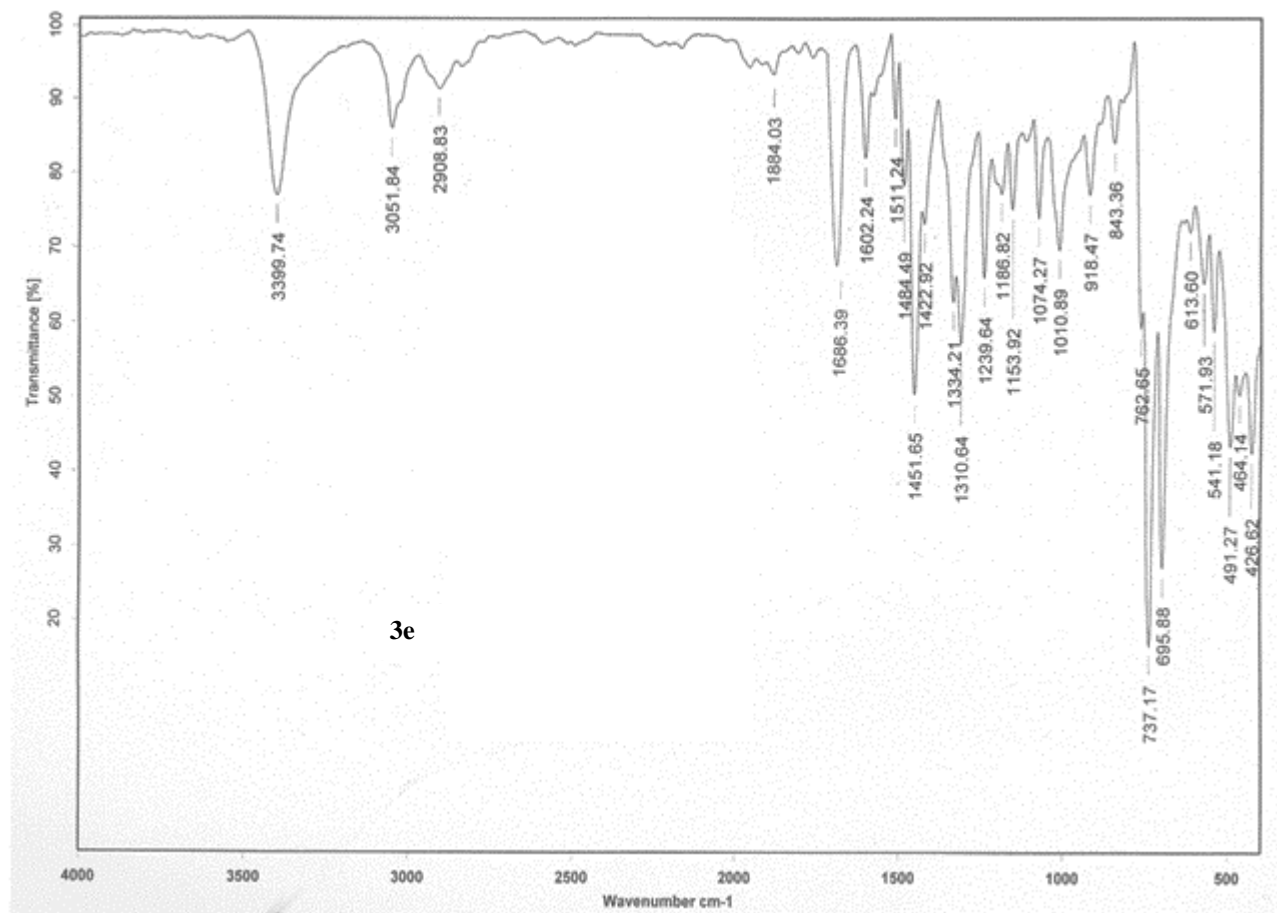




Data : Dr Cecilio-Alvarez059 Date : 02-Sep-2015 11:20
 Instrument : MStation
 Sample : 2582 2-ph-p
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 0.75 min Scan# : (6,7)
 Elements : C 40/0, H 49/0, N 3/0, O 2/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : -0.5 - 45.0

3d
 $C_{36}H_{26}N_2O$
 M.W. 502

Observed m/z	Int%	Estimated m/z	Err [ppm / mmu] U.S.	C	H	N	O
502.2049	25.03	502.2045	+0.8 / +0.4	36	26	2	1

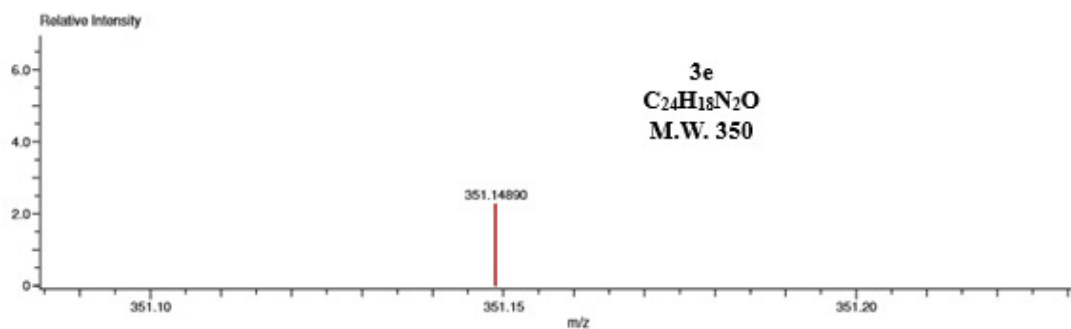


Data:3010 Indol.m
 Sample Name:Dr Alvarez Cocilio/ Operador: Carmen Garcia-Javier Perez
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 1.1...

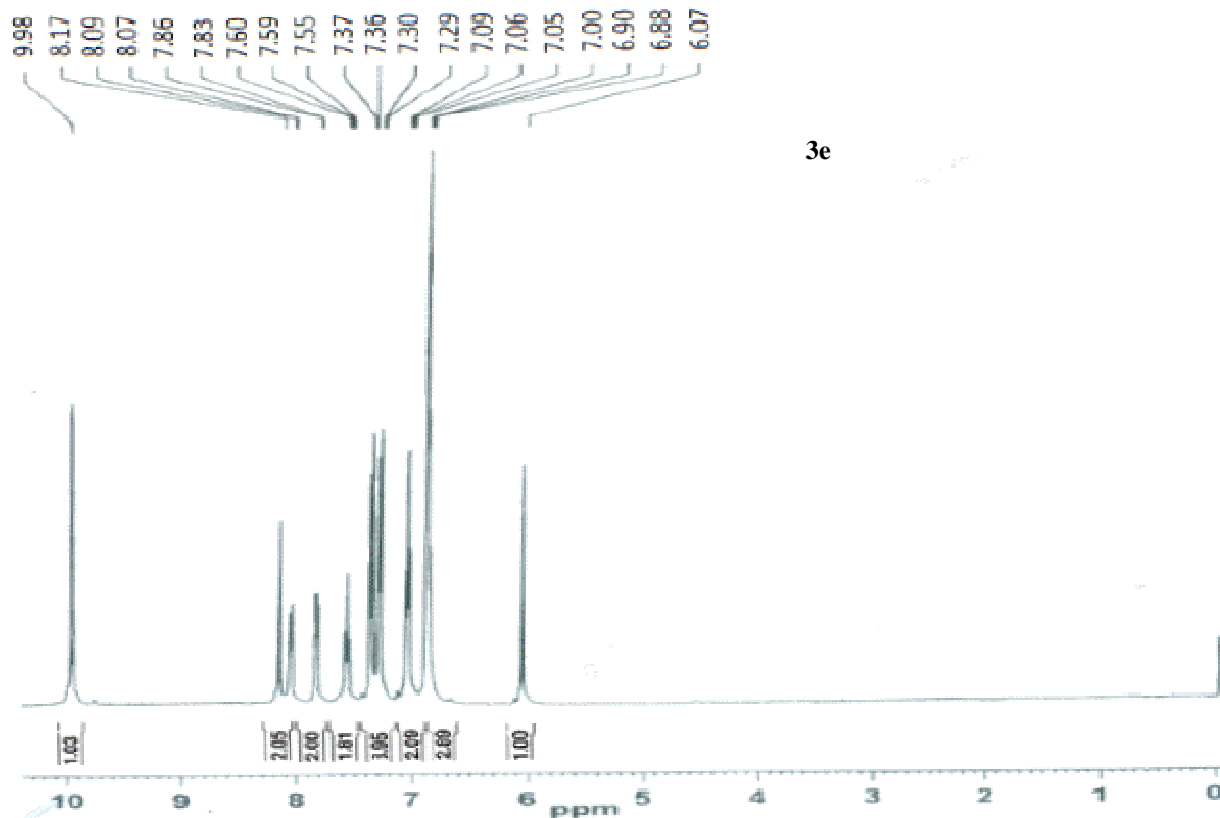
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 Mass Calibration data:Cal_Peg_600
 Created:9/30/2015 12:15:17 PM
 Created by:AccuTOF

Charge number:1
 Element:¹²C:0 .. 56, ¹H:0 .. 120, ¹⁴N:0 .. 2, ¹⁶O:0 .. 3
 Tolerance:3.00(mmu)

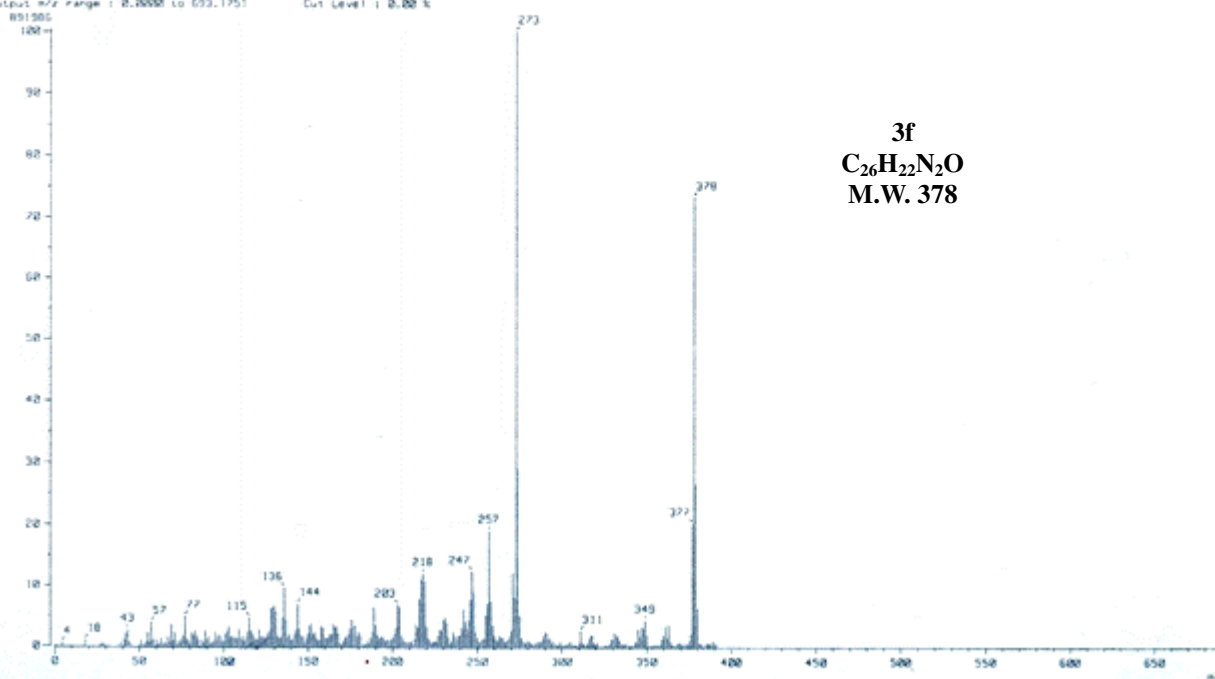
Unsaturation Number:2.0 .. 20.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14890	1386.79	351.14974	-0.84	-2.38	$^{12}C_{24}^{1}H_{18}^{14}N_2^{16}O_1$	16.5



[Mass Spectrum]
 Date : Dr-Lopez-Jose-204 Date : 24-May-2012 17:18
 Sample : 1213 IEP1 Joel RAS200m
 Note : Javier Perez
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion (PS-Linear)
 RT : 1.40 min Scan# : 16,821
 BP : m/z 273,2000 Int. : 84.58
 Output m/z range : 0.20000 to 653.1751 Cut Level : 0.00 k

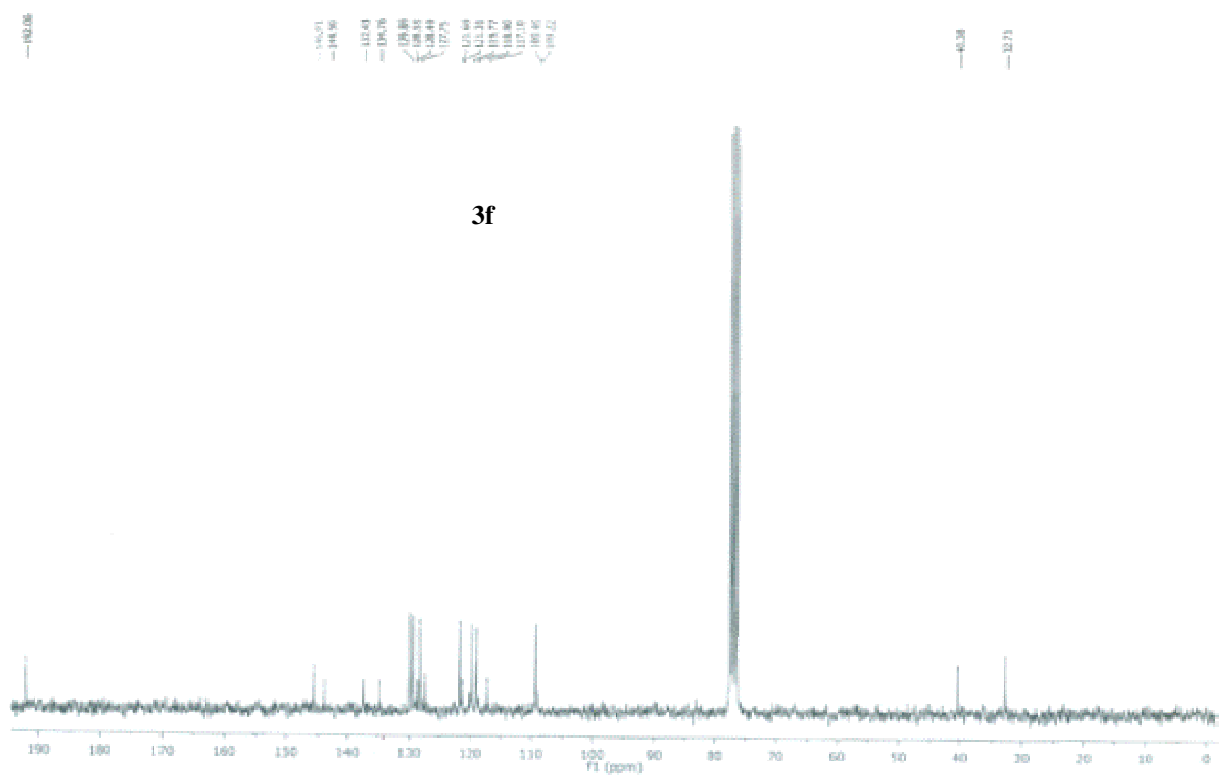
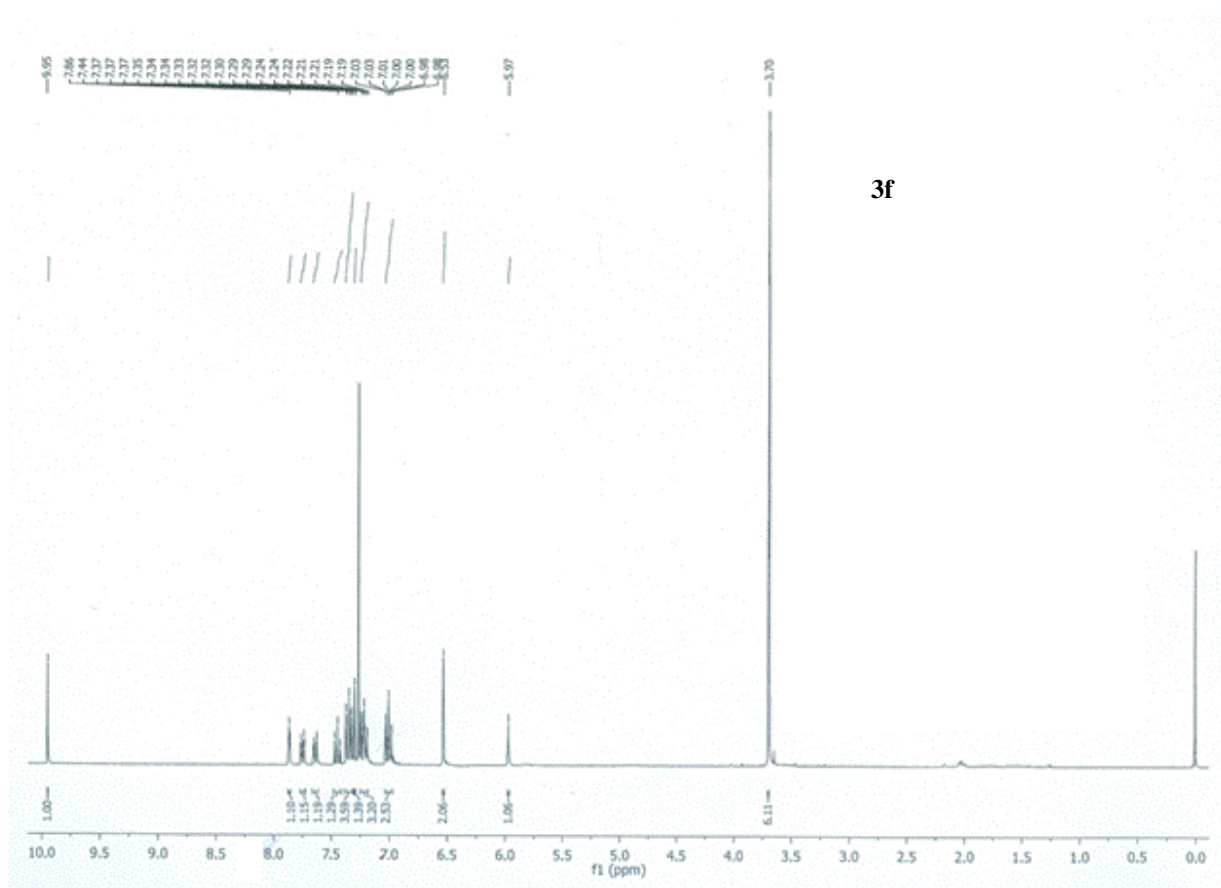


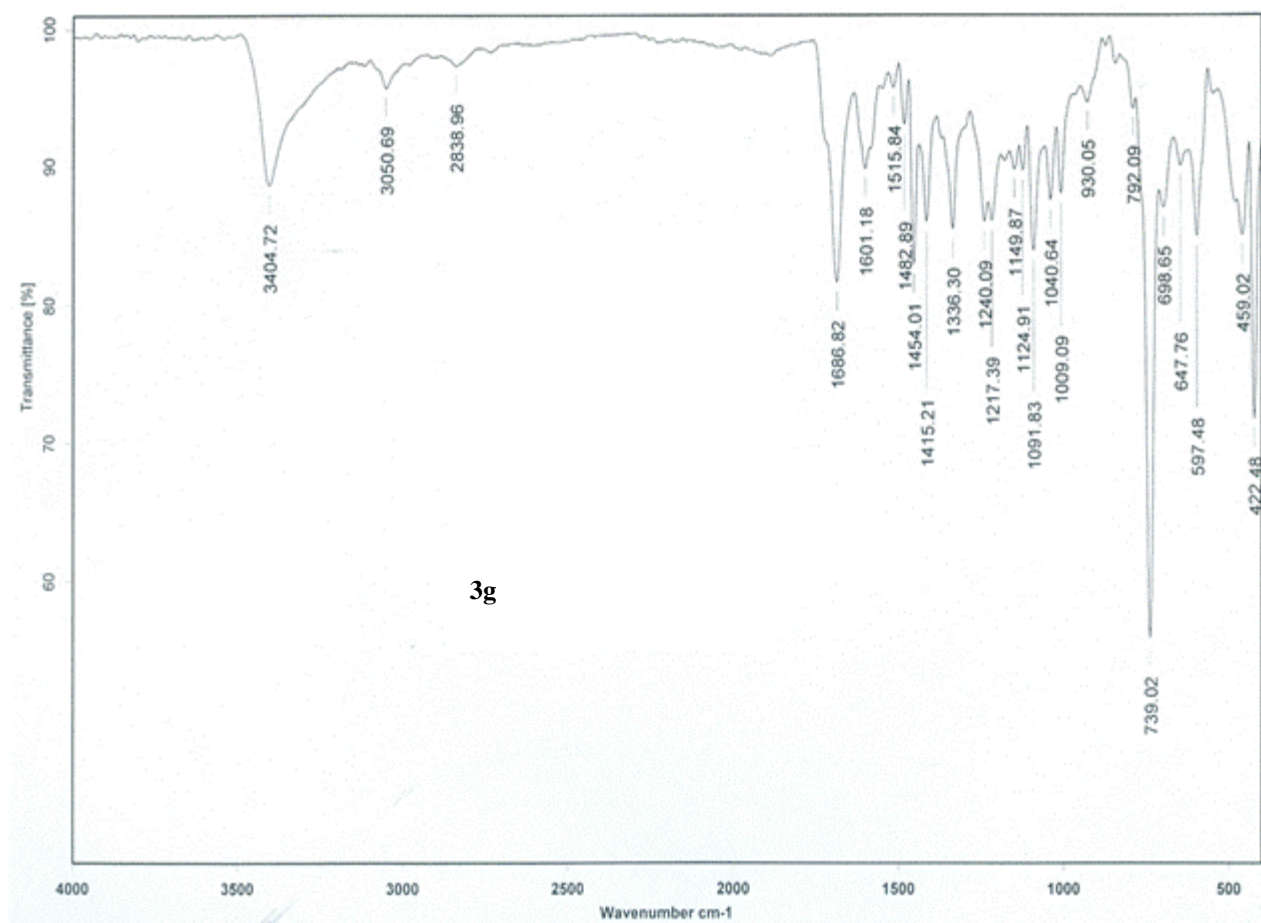
3f
 $C_{26}H_{22}N_2O$
 M.W. 378

Data : Dr Cecilio Alvarez033 Date : 06-Oct-2015 12:27
 Instrument : MStation
 Sample : 3011 1-Me-m
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 0.00 min Scan# : (1,4)
 Elements : C 30/0, H 49/0, N 3/0, O 2/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : -0.5 - 23.0

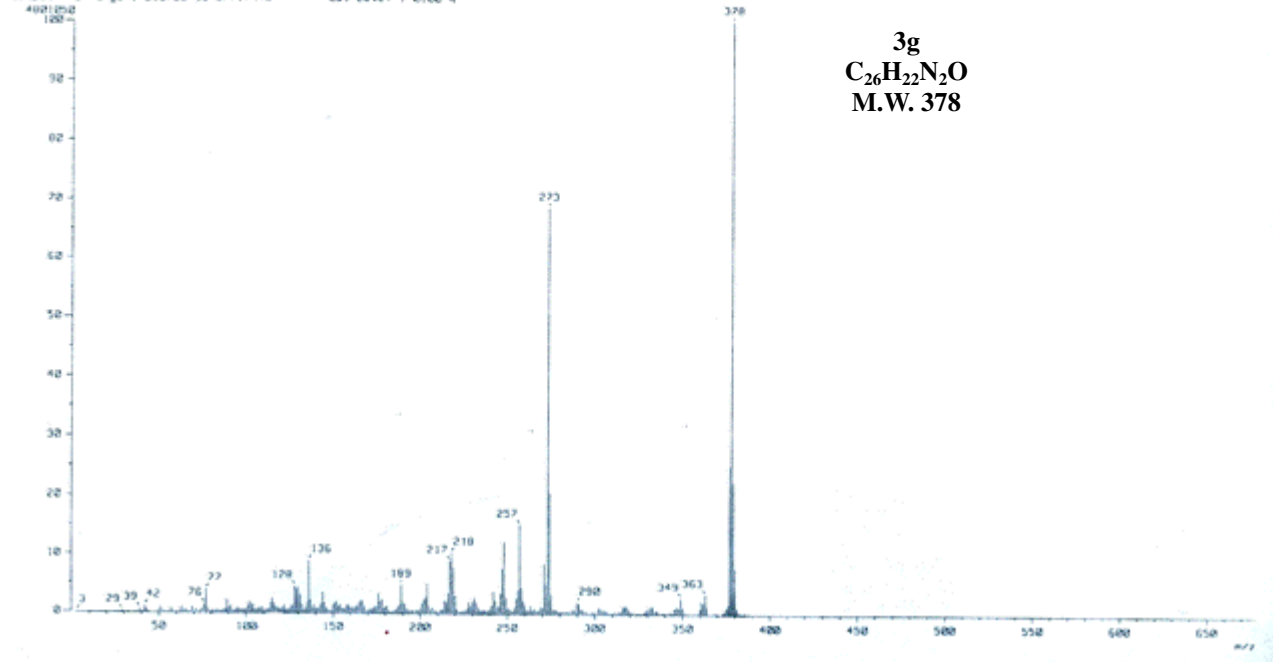
3f
 $C_{26}H_{22}N_2O$
 M.W. 378

Observed m/z	Int%	Estimated m/z	Err [ppm / mmu] U.S.	C	H	N	O
378.1729	43.23	378.1732	-0.8 / -0.3 17.0	26	22	2	1





(Mass Spectrum)
 Data : Dr.Lopez-Jose-013 Date : 05-Jun-2012 15:17
 Sample : 1362 Zeol F050041
 Note : Javier Perez
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion (MS-Linear)
 RT : 1.68 min Scan# : (34,45)
 BP : m/z 370.0000 Int. : 457.66
 Output m/z range : 2.3739 to 677.7440 Cut Level : 0.00 %

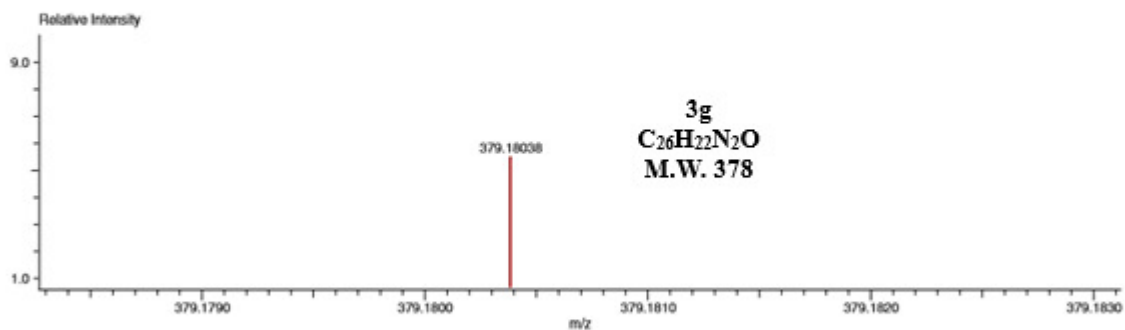


Data:2013 2-Me-m
 Sample Name:Dr Alvarez Cecilio/ Operator: Carmen Garcia-Javier Perez
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%],Average[MS[1]] 0.4...

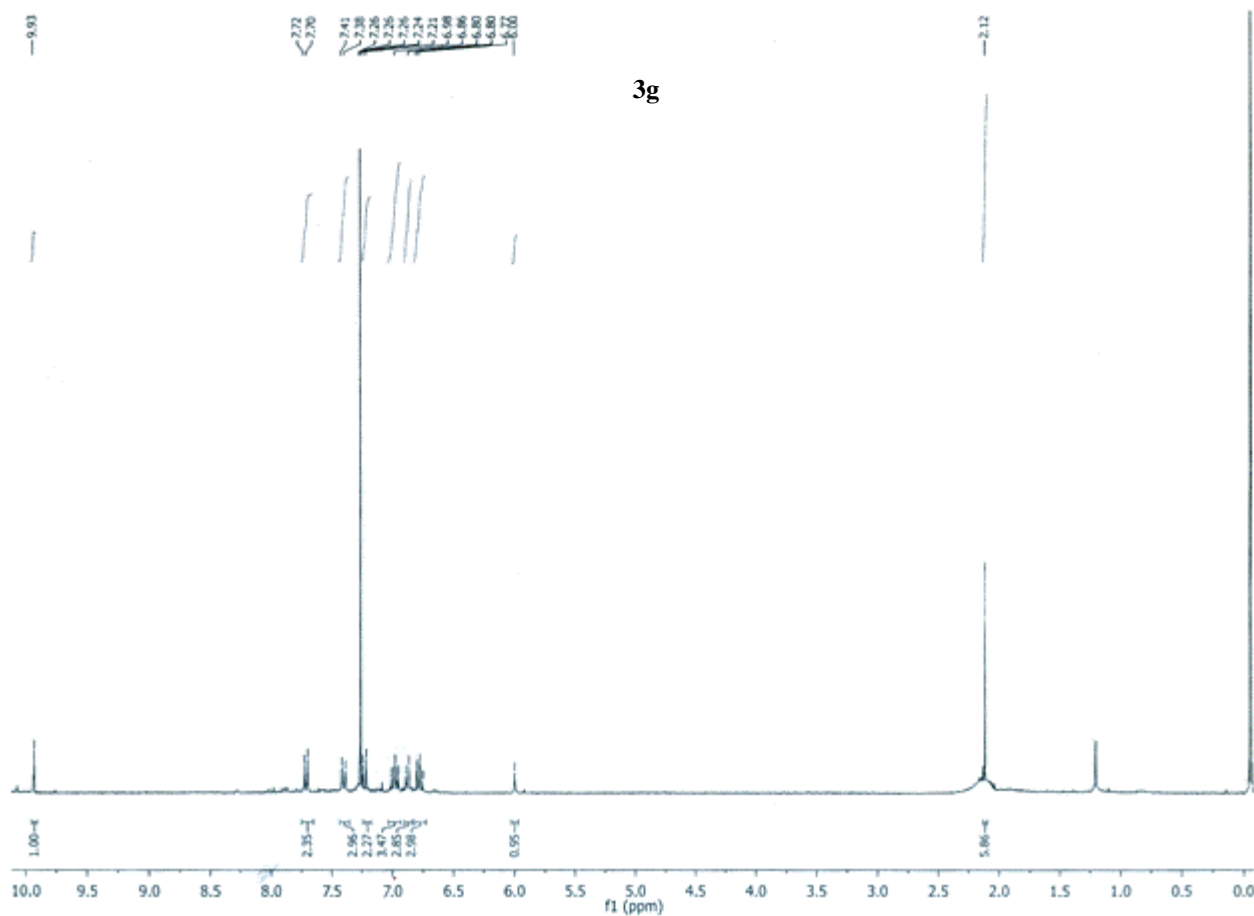
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 Created by:AccuTOF

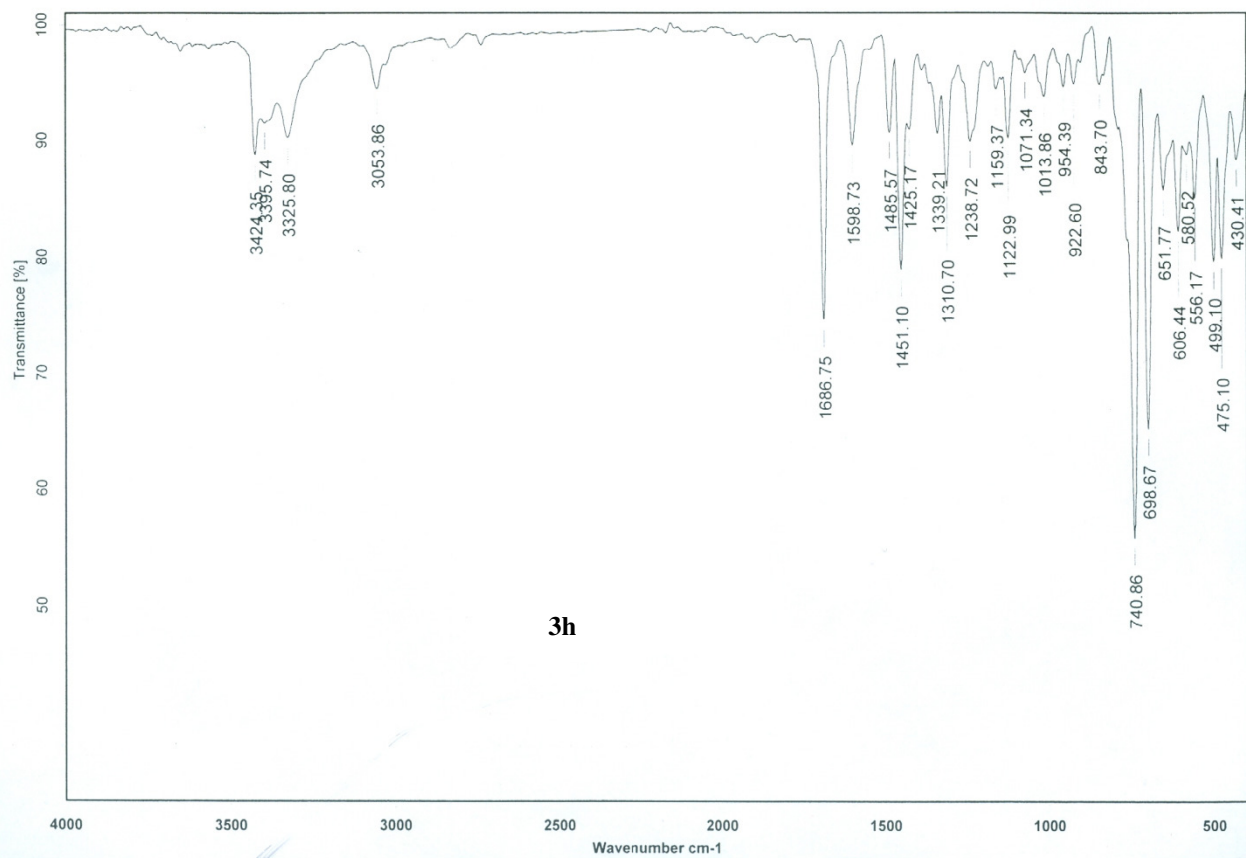
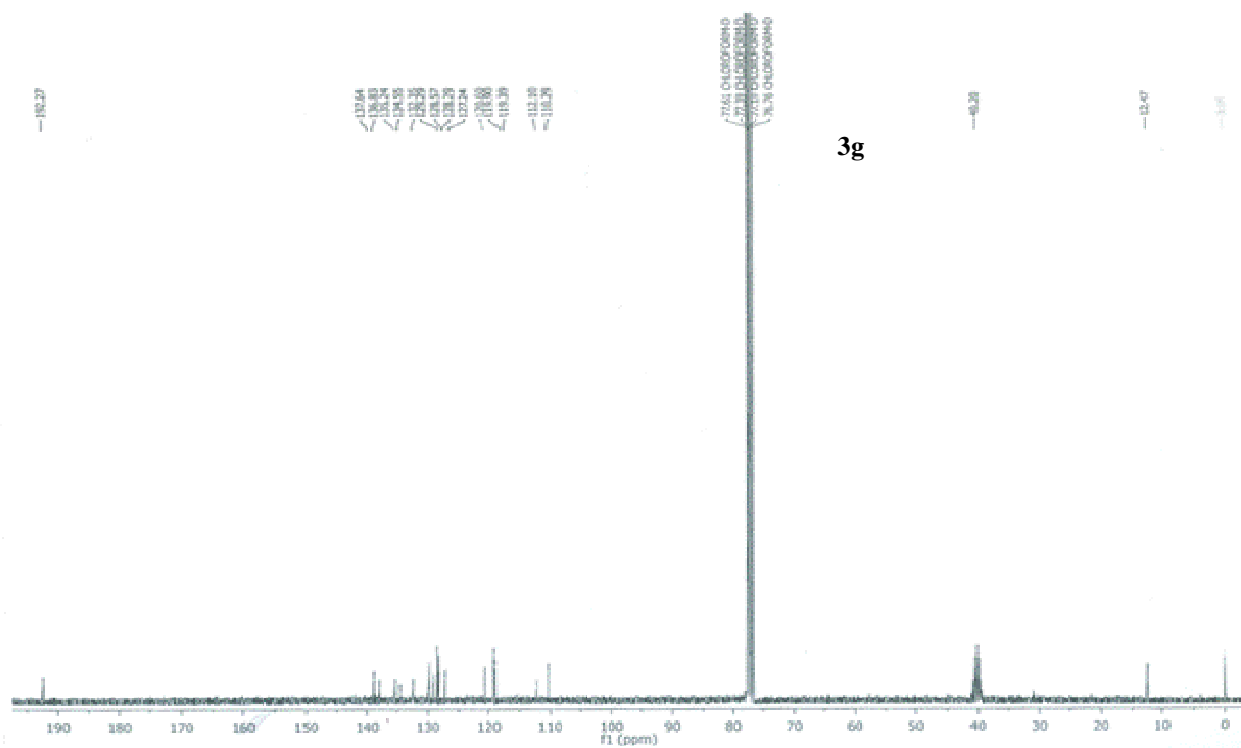
Charge number:1
 Element:¹²C:0 .. 56, ¹H:0 .. 120, ¹⁴N:0 .. 2, ¹⁶O:0 .. 3
 Tolerance:3.00(mmu)

Unsaturation Number:2.0 .. 20.0 (Fraction:Both)

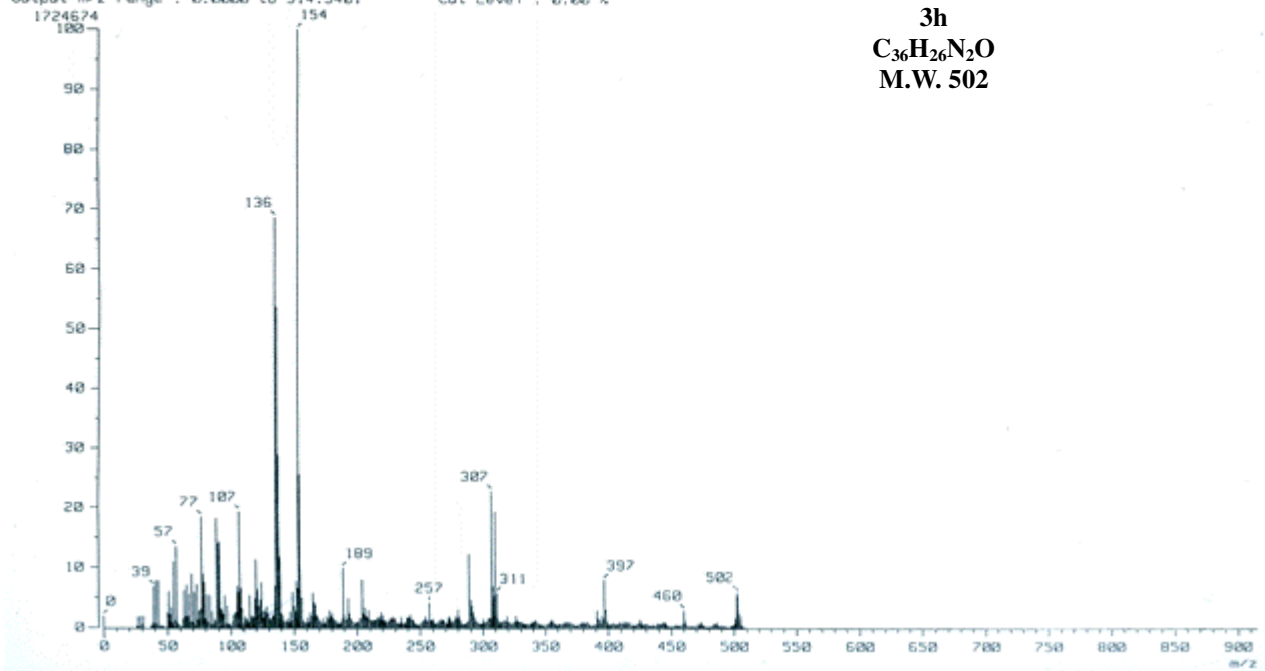


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18038	1642.76	379.18104	-0.65	-1.73	¹³ C ₂₆ ¹ H ₂₂ ¹⁴ N ₂ ¹⁶ O ₁	16.5





[Mass Spectrum]
 Data : Dr-Jose-Lopez-858 Date : 07-Aug-2012 10:33
 Sample: 1778
 Note : Luis-Velasco
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion (MF-Linear)
 RT : 3.09 min Scan# : (5,17)
 BP : m/z 154.0000 Int. : 164.48
 Output m/z range : 0.0000 to 914.5481 Cut Level : 0.00 %



3h
 $C_{36}H_{26}N_2O$
 M.W. 502

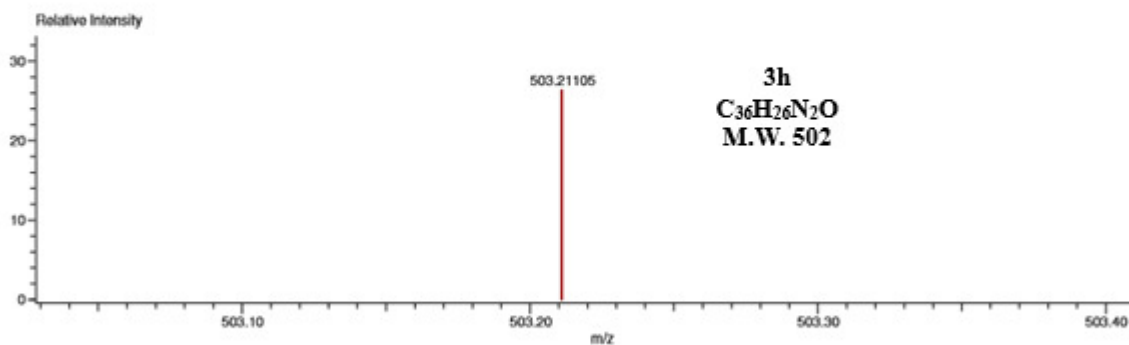
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 Sample Name:
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.3...

Acquired:3/31/2016 5:33:57 PM
 Operator:AccuTOF
 Mass Calibration data:PEG600
 Created:4/11/2016 6:08:30 PM
 Created by:AccuTOF

Charge number:1
 Element:¹²C:0 .. 100, ¹H:0 .. 100, ¹⁴N:0 .. 3, ¹⁶O:0 .. 3

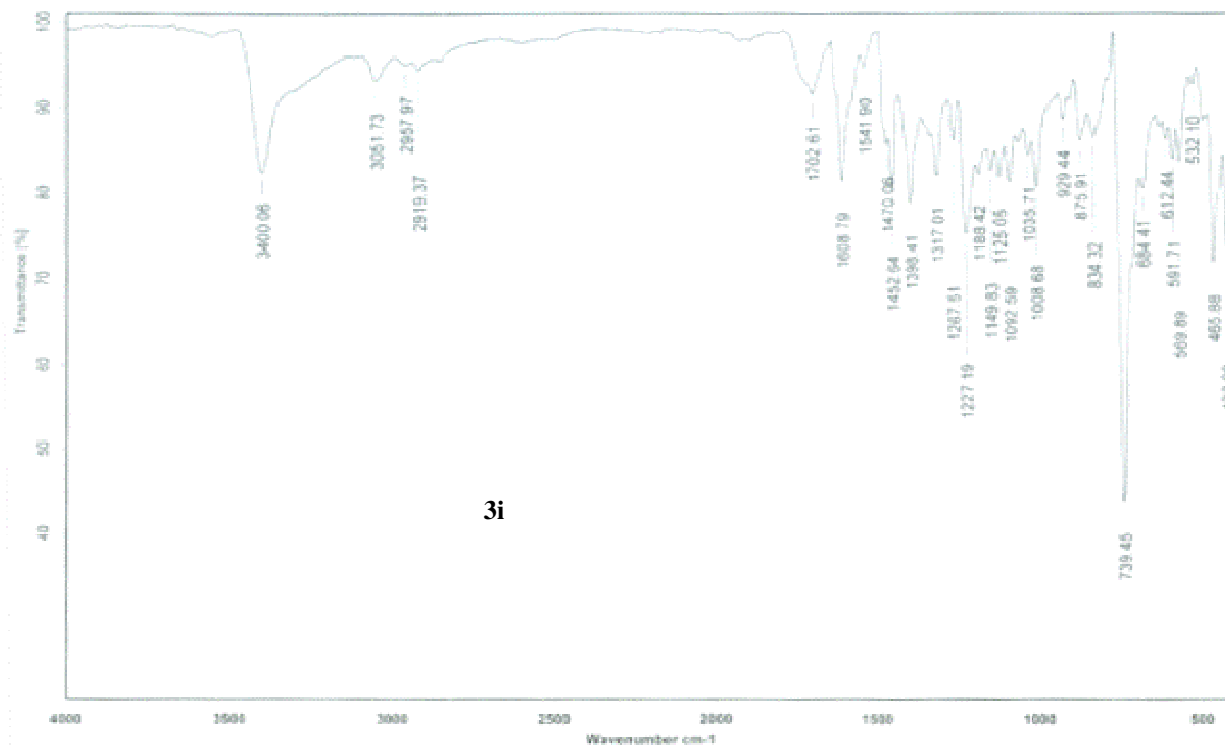
Tolerance:3.00(mmu)

Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



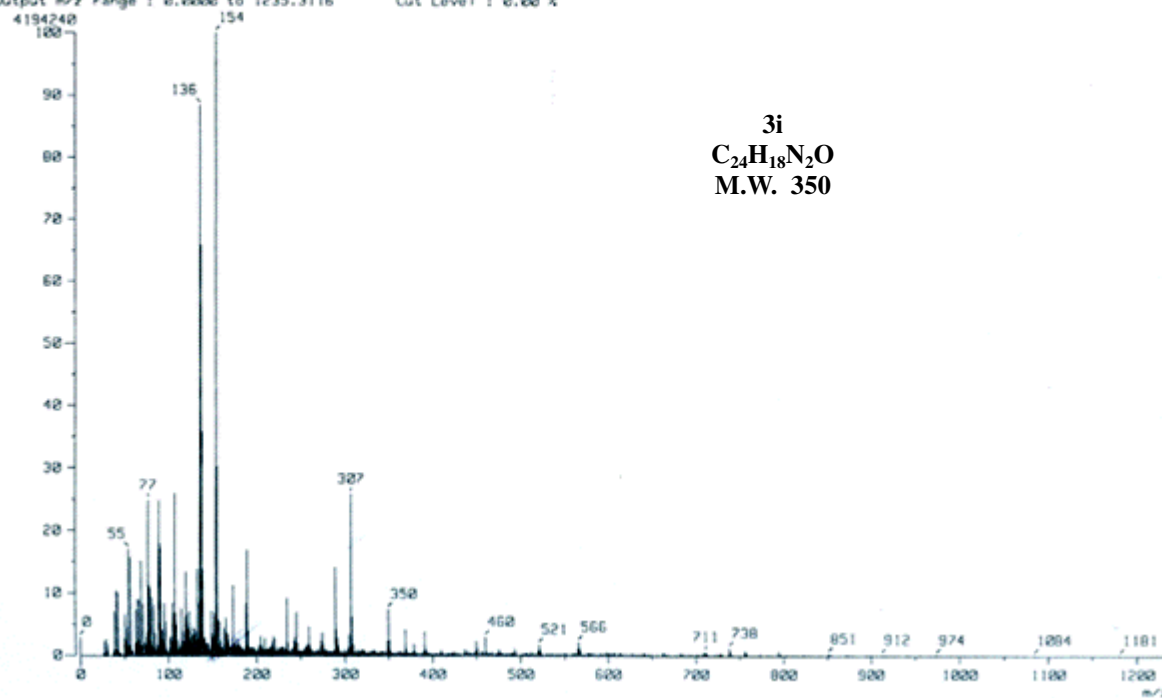
3h
 $C_{36}H_{26}N_2O$
 M.W. 502

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21105	2115.38	503.21234	-1.28	-2.55	$^{12}C_{36}^{1}H_{26}^{14}N_2^{16}O_1$	24.5



3i

Sample: 61
 Note: Luis-Velasco
 Inlet: Direct Ion Mode: FRB+
 Spectrum Type: Normal Ion (MF-Linear)
 RT: 1.24 min Scan#: (3,8)
 BP: m/z 154.0000 Int.: 399.99
 Output m/z range: 0.0000 to 1235.3116 Cut Level: 0.00 %



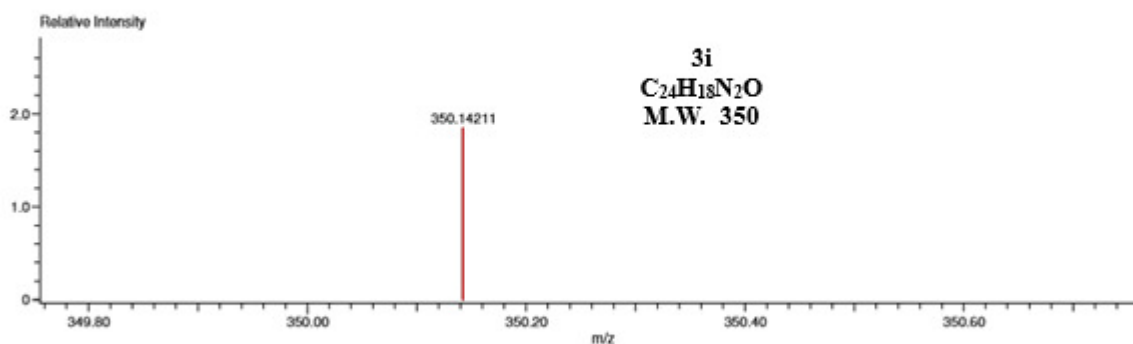
3i
 $C_{24}H_{18}N_2O$
 M.W. 350

Data: CAT 10
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect [Centroid, 30, Area], Correct Base [5.0%], Correct Base [5.0%], Average [MS [1] 0.7...

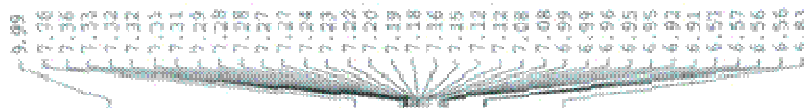
Acquired: 3/31/2016 5:41:52 PM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 6:29:41 PM
 Created by: AccuTOF

Charge number: 1
 Element: ¹²C: 0 .. 100, ¹H: 0 .. 100, ¹⁴N: 0 .. 3, ¹⁶O: 0 .. 3
 Tolerance: 3.00 (mmu)

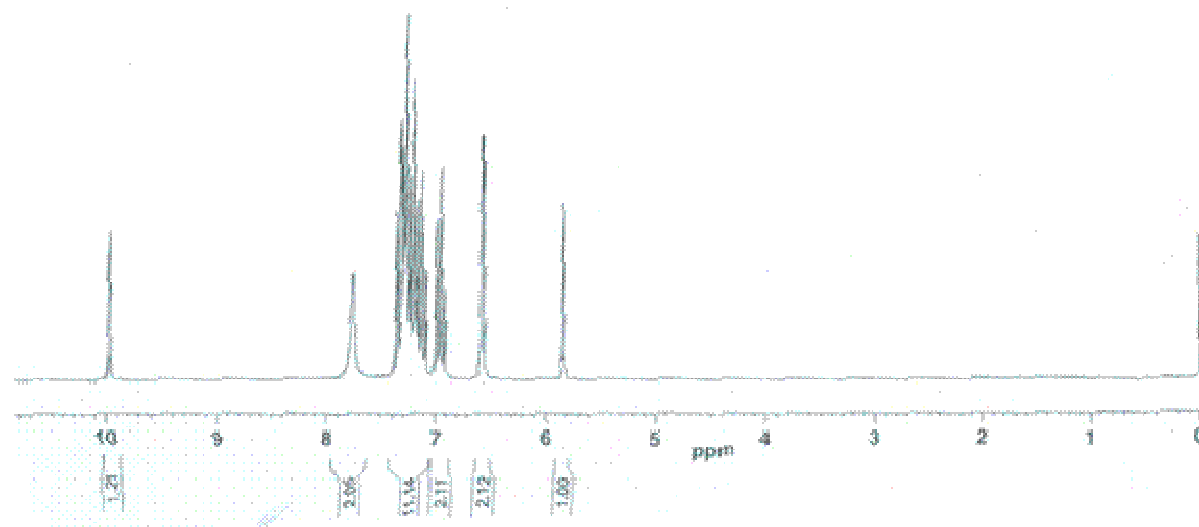
Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

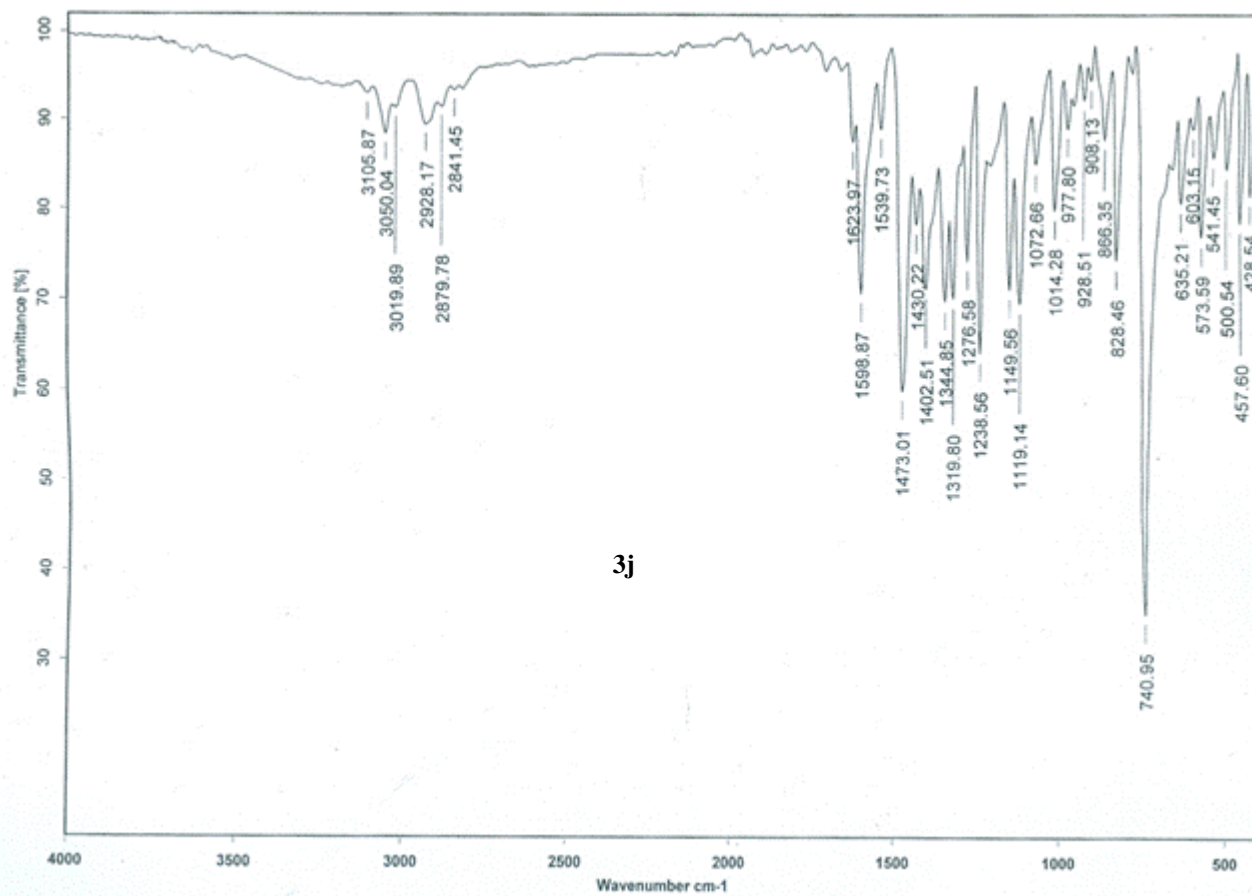
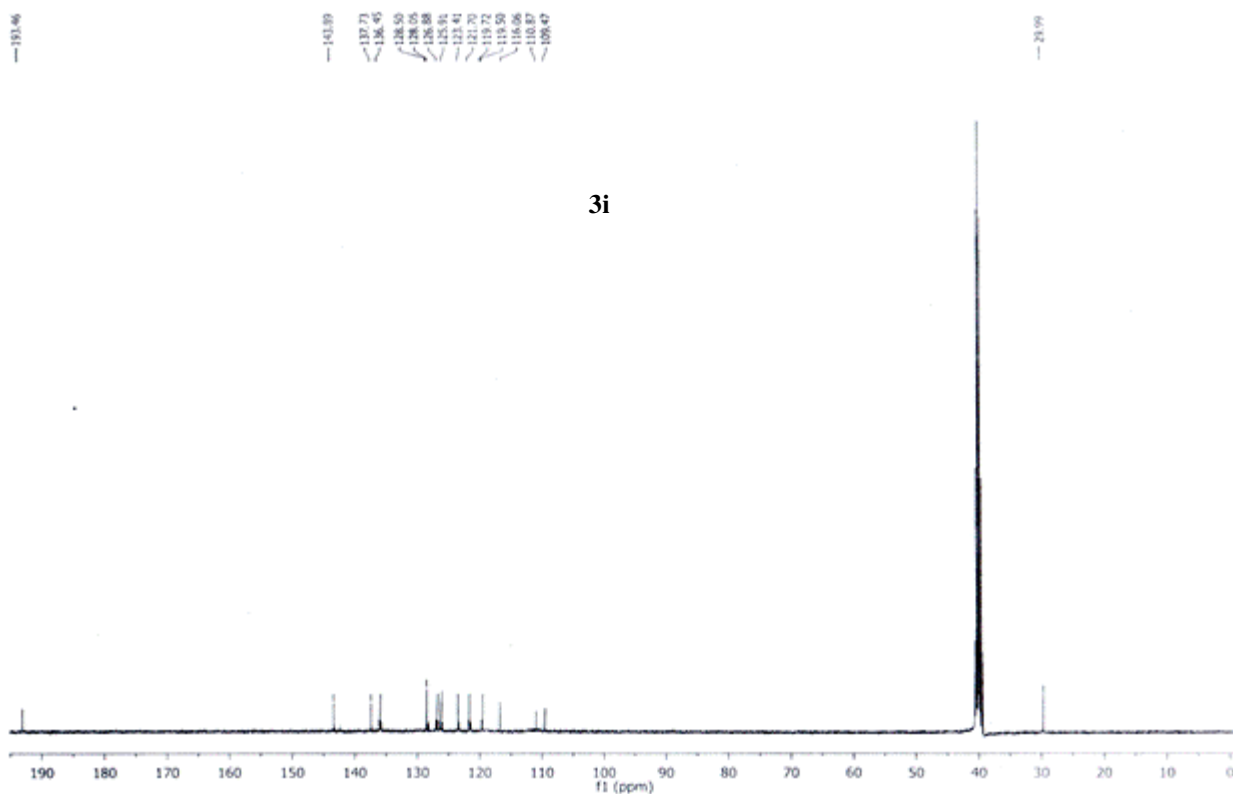


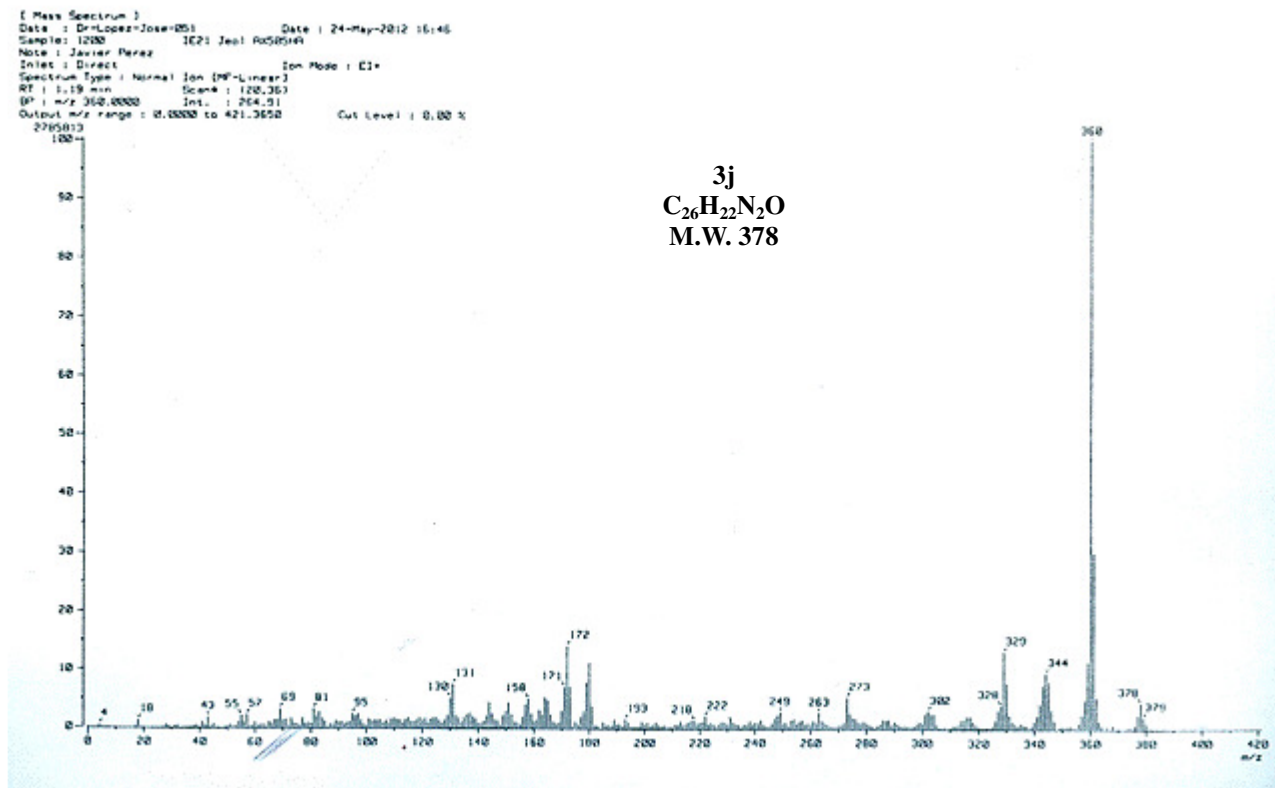
Mass	Intensity	Calc. Mass	Mass Difference (mnu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
350.14211	2134.88	350.14191	0.19	0.55	¹² C ₂₄ ¹ H ₁₈ ¹⁴ N ₂ ¹⁶ O ₁	17.0



3i







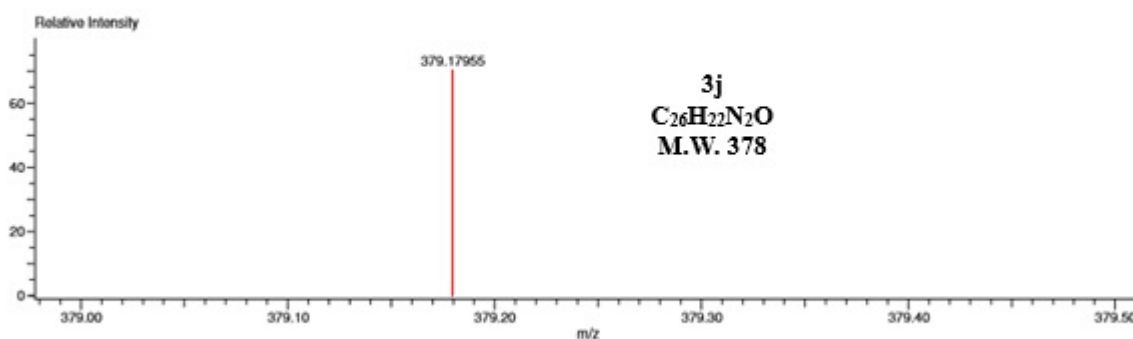
Data:CAT 9
 Sample Name:
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%],Average[MS[1] 0.2...]

Acquired:3/31/2016 5:36:53 PM
 Operator:AccuTOF
 Mass Calibration data:PEG600
 Created:4/11/2016 6:17:51 PM
 Created by:AccuTOF

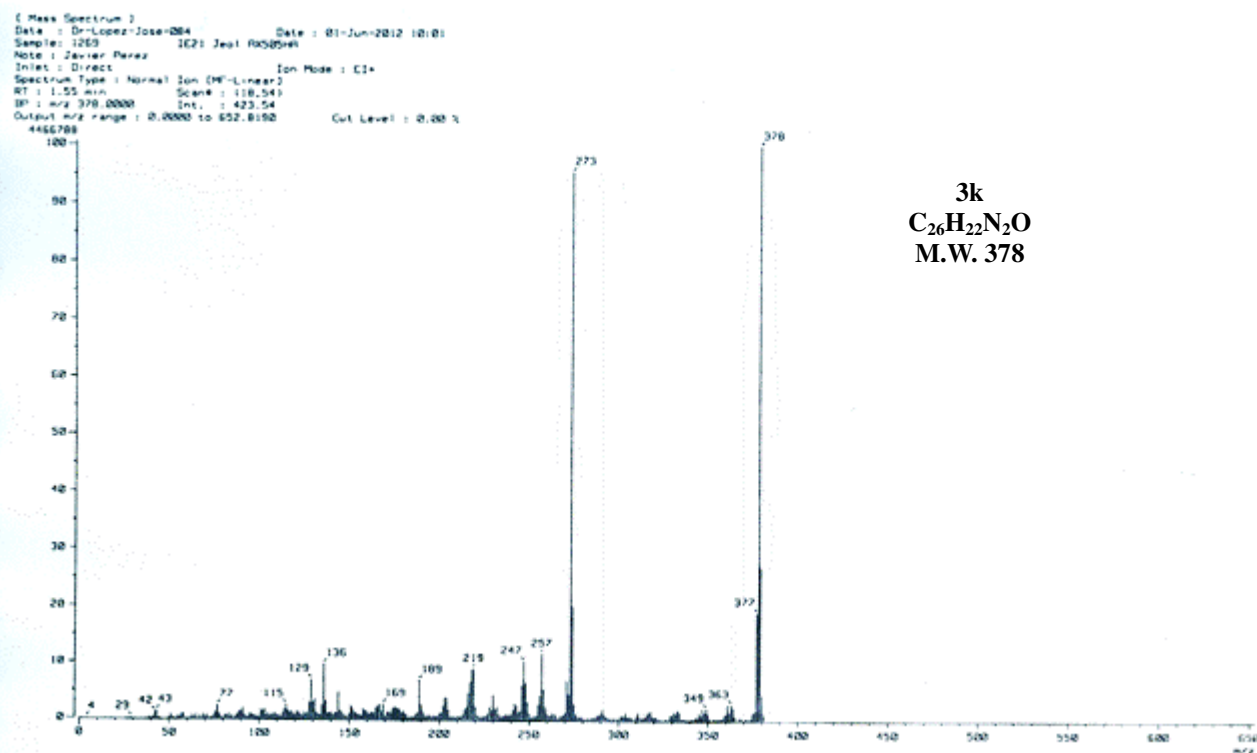
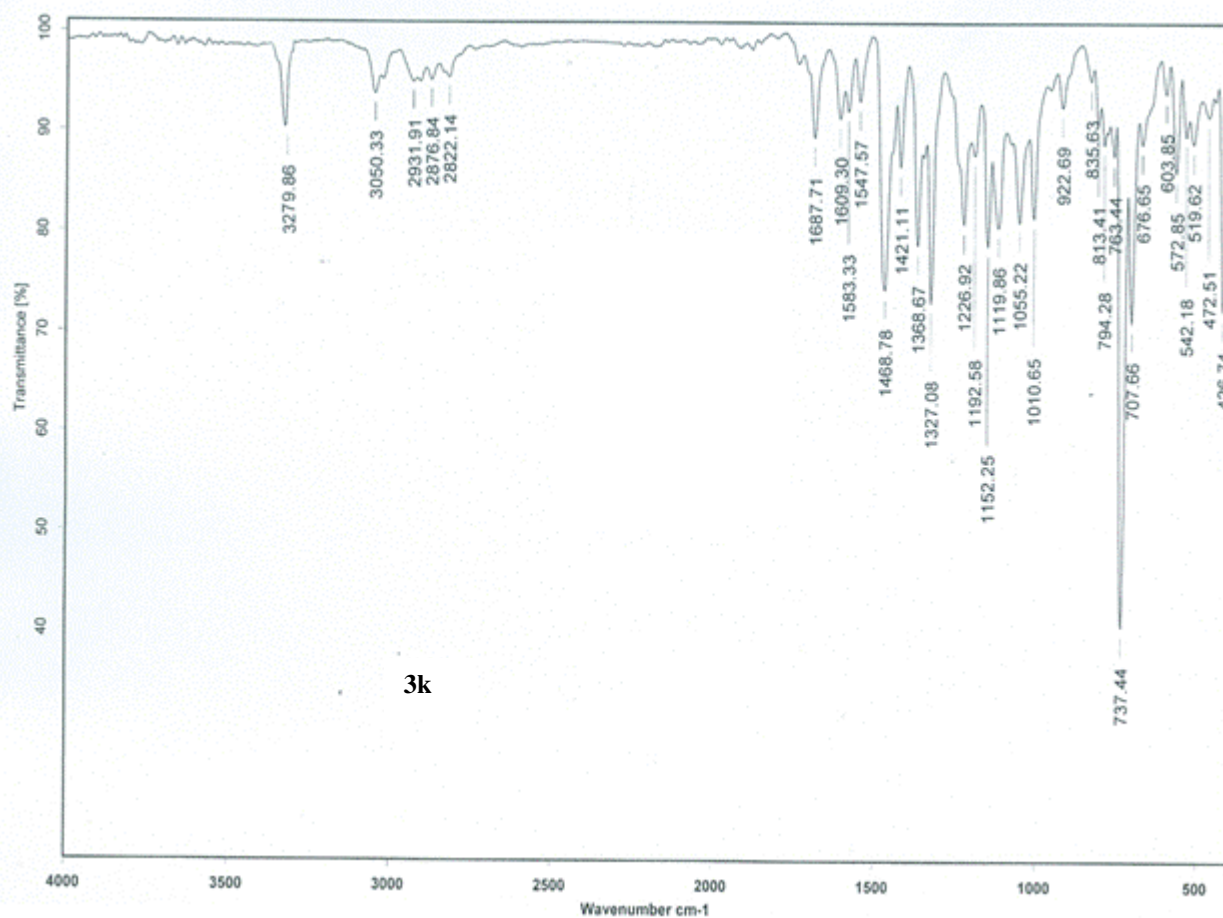
Charge number:1
 Element:¹²C:0 .. 100, ¹H:0 .. 100, ¹⁴N:0 .. 3, ¹⁶O:0 .. 3

Tolerance:3.00(mmu)

Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.17955	5429.27	379.18104	-1.49	-3.93	$^{12}C_{26}^{1}H_{22}^{14}N_2^{16}O_1$	16.5



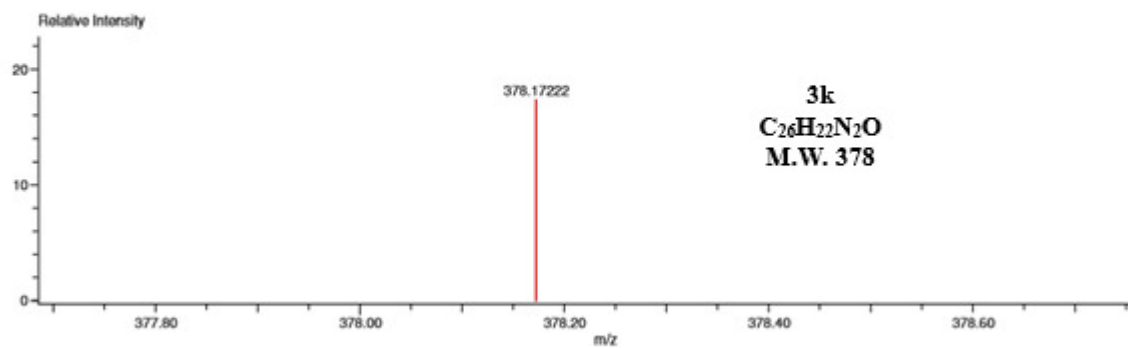
Data: CAT 11
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect [Centroid, 30, Area], Correct Base [5.0%], Correct Base [5.0%], Average [MS [1] 0.8...

Acquired: 3/31/2016 5:44:43 PM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 6:33:44 PM
 Created by: AccuTOF

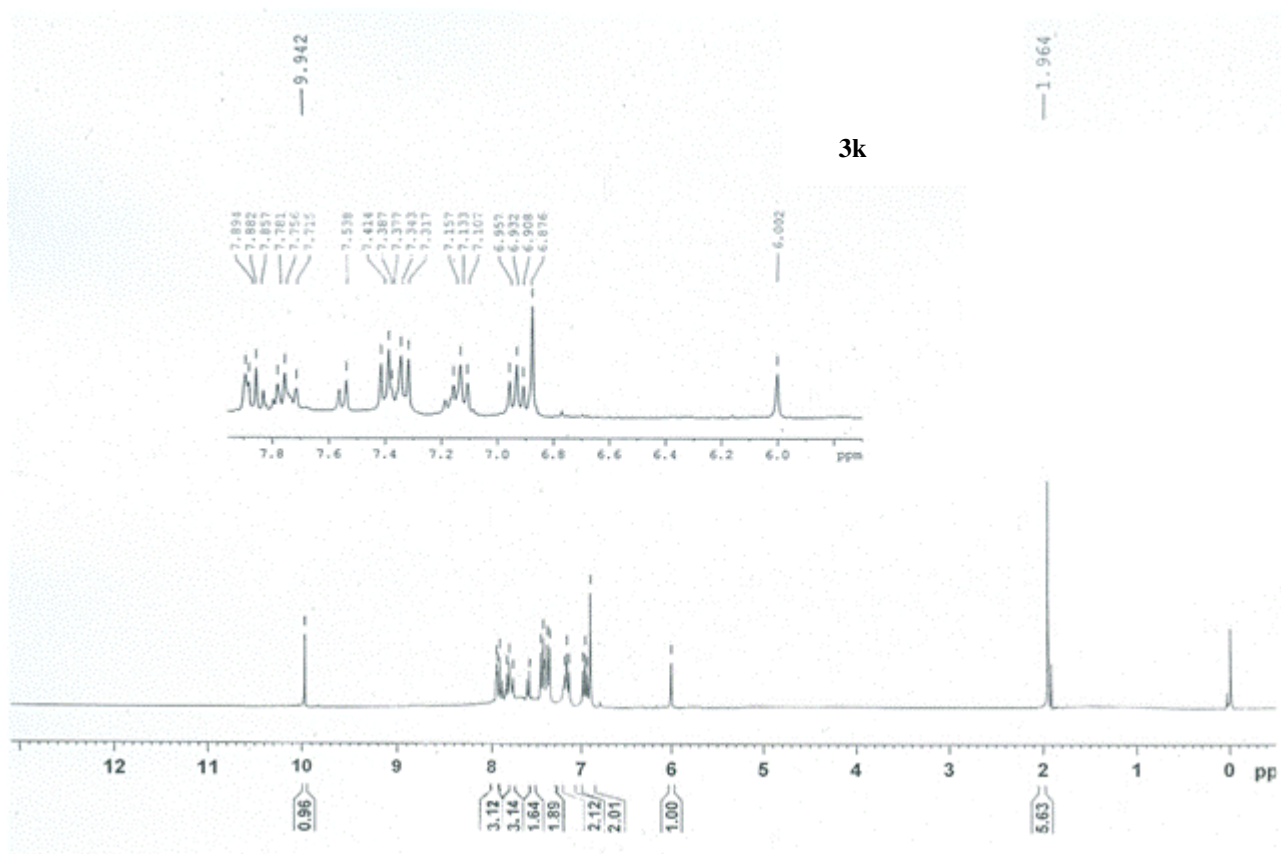
Charge number: 1
 Element: ^{12}C : 0 .. 100, ^1H : 0 .. 100, ^{14}N : 0 .. 3, ^{16}O : 0 .. 3

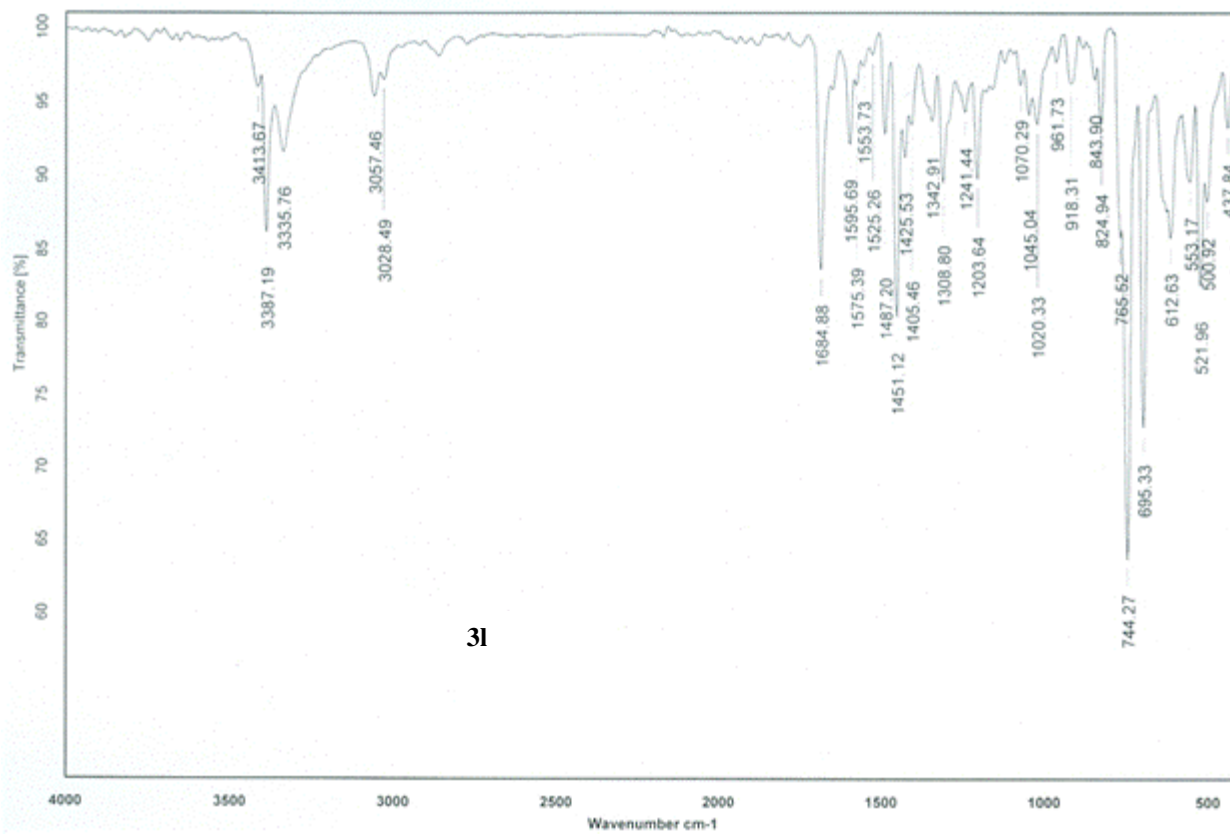
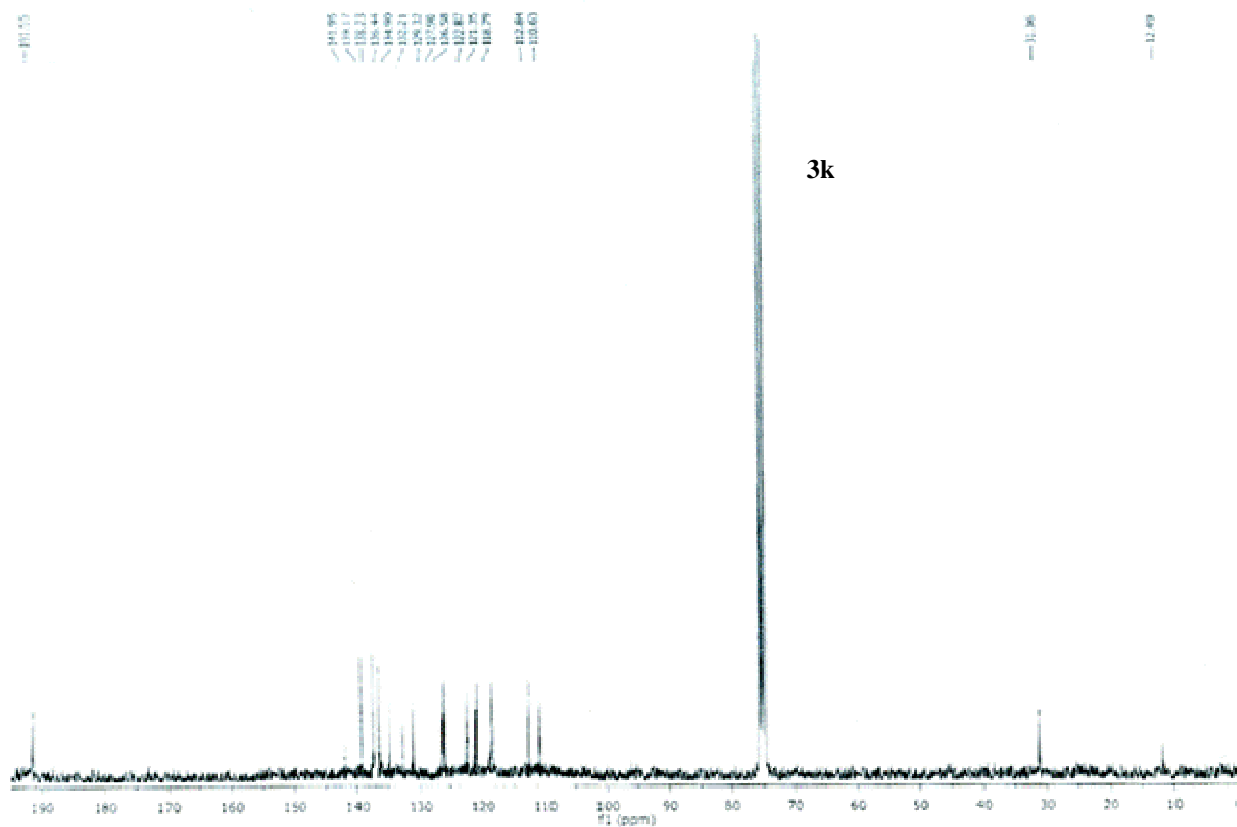
Tolerance: 3.00 (mmu)

Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

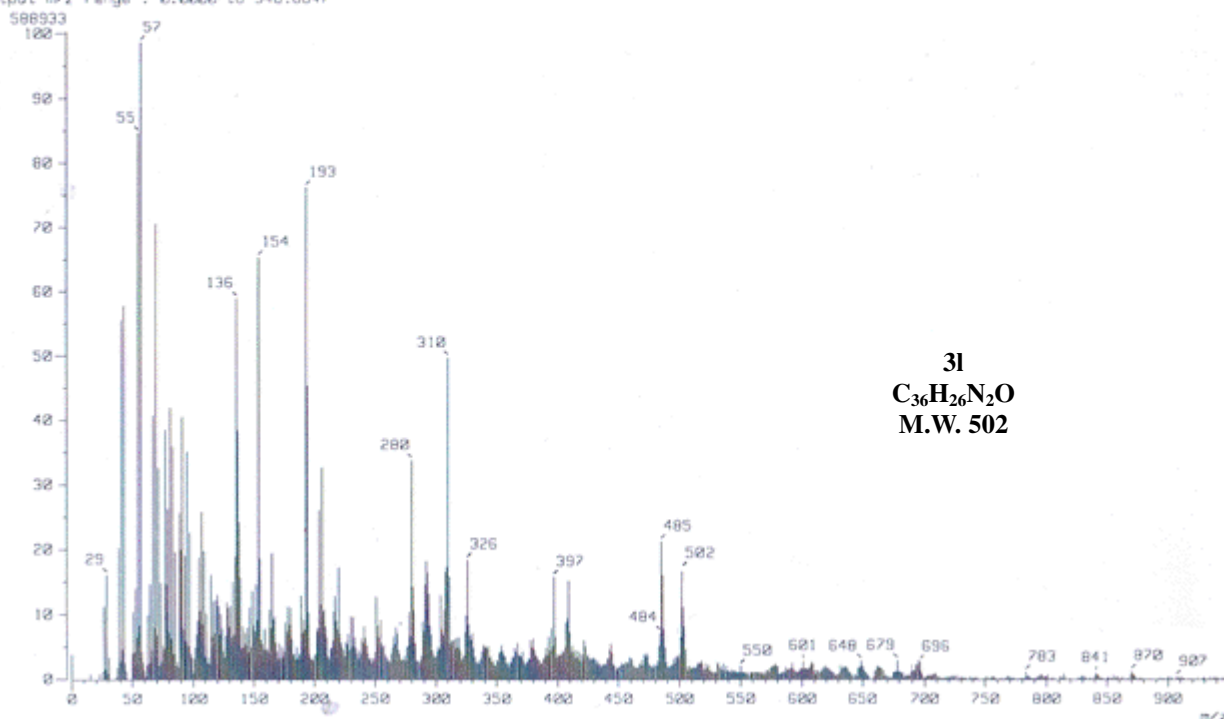


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
378.17222	13695.63	378.17321	-0.99	-2.62	$^{12}\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}$	17.0





[Mass Spectrum]
 Inlet : Direct Ion Mode : FRB+
 Spectrum Type : Normal Ion (MF-Linear)
 RT : 2.47 min Scan# : (2,16)
 BP : m/z 679.0000 Int. : 56.00
 Output m/z range : 0.0000 to 948.6647



31
 $C_{36}H_{26}N_2O$
 M.W. 502

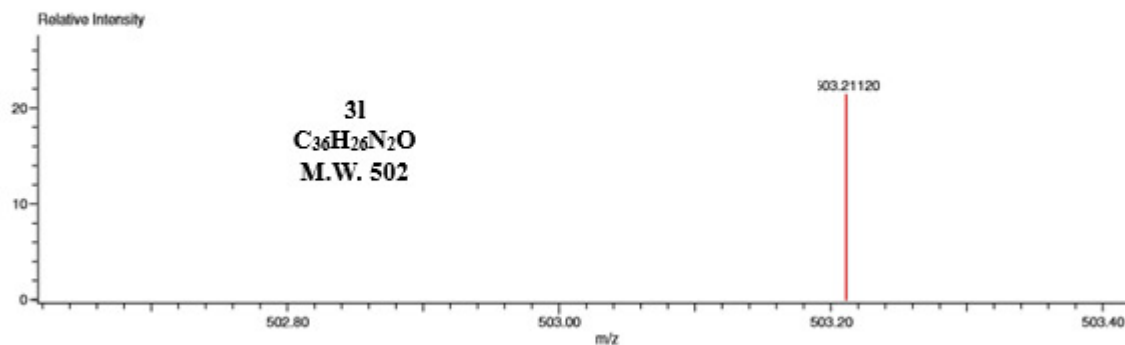
Data:CAT 12
 Sample Name:
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%];Average[MS[1] 0.7...

Acquired:3/31/2016 5:47:18 PM
 Operator:AccuTOF
 Mass Calibration data:PEG600
 Created:4/11/2016 6:35:57 PM
 Created by:AccuTOF

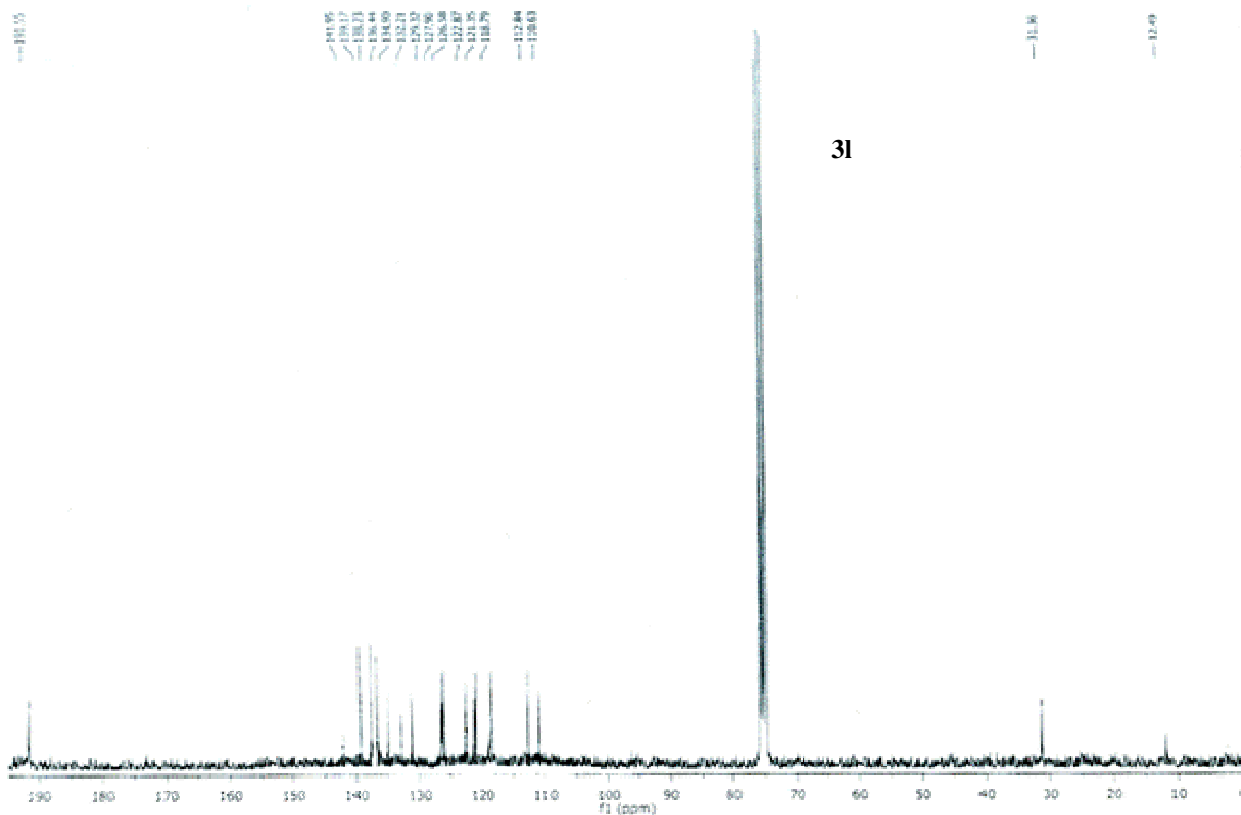
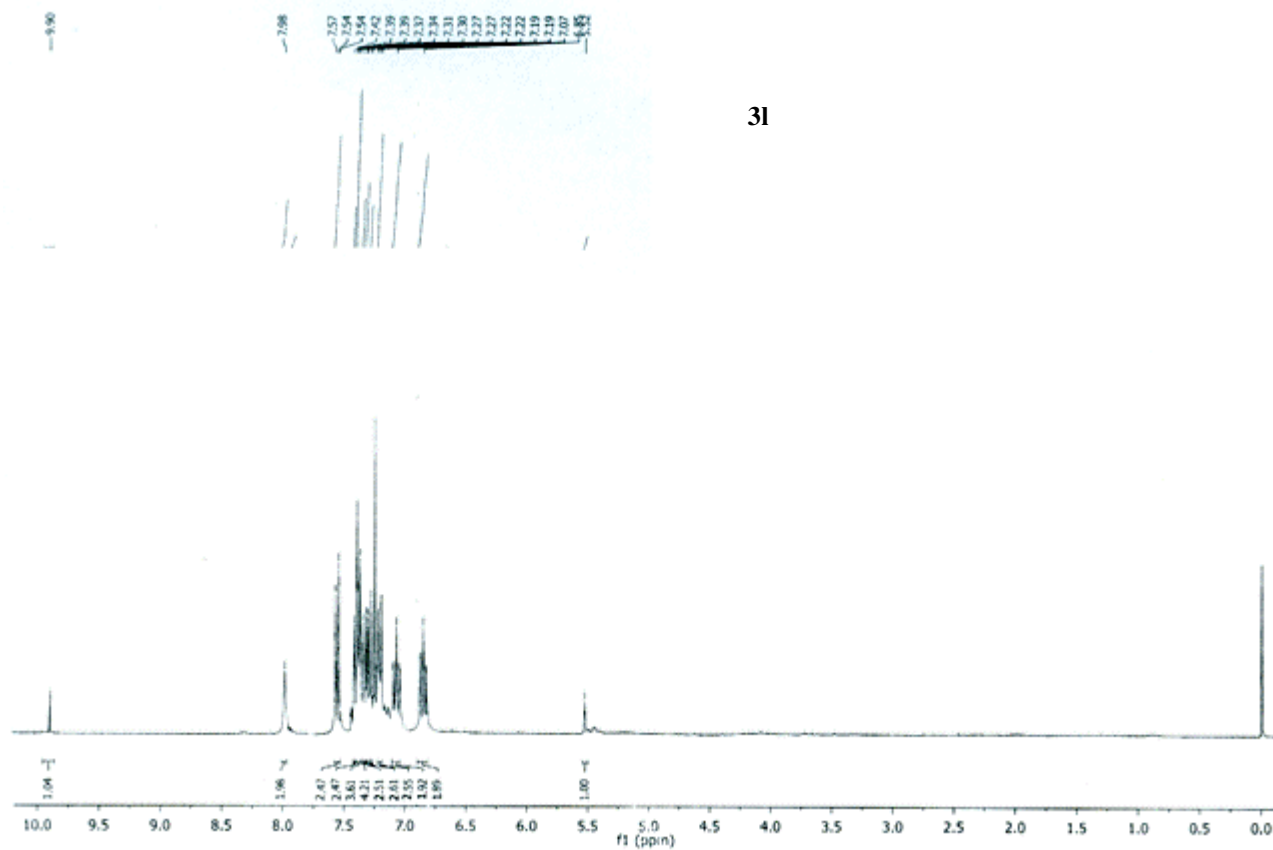
Charge number:1
 Element: $^{12}C:0..100$, $^1H:0..100$, $^{14}N:0..3$, $^{16}O:0..3$

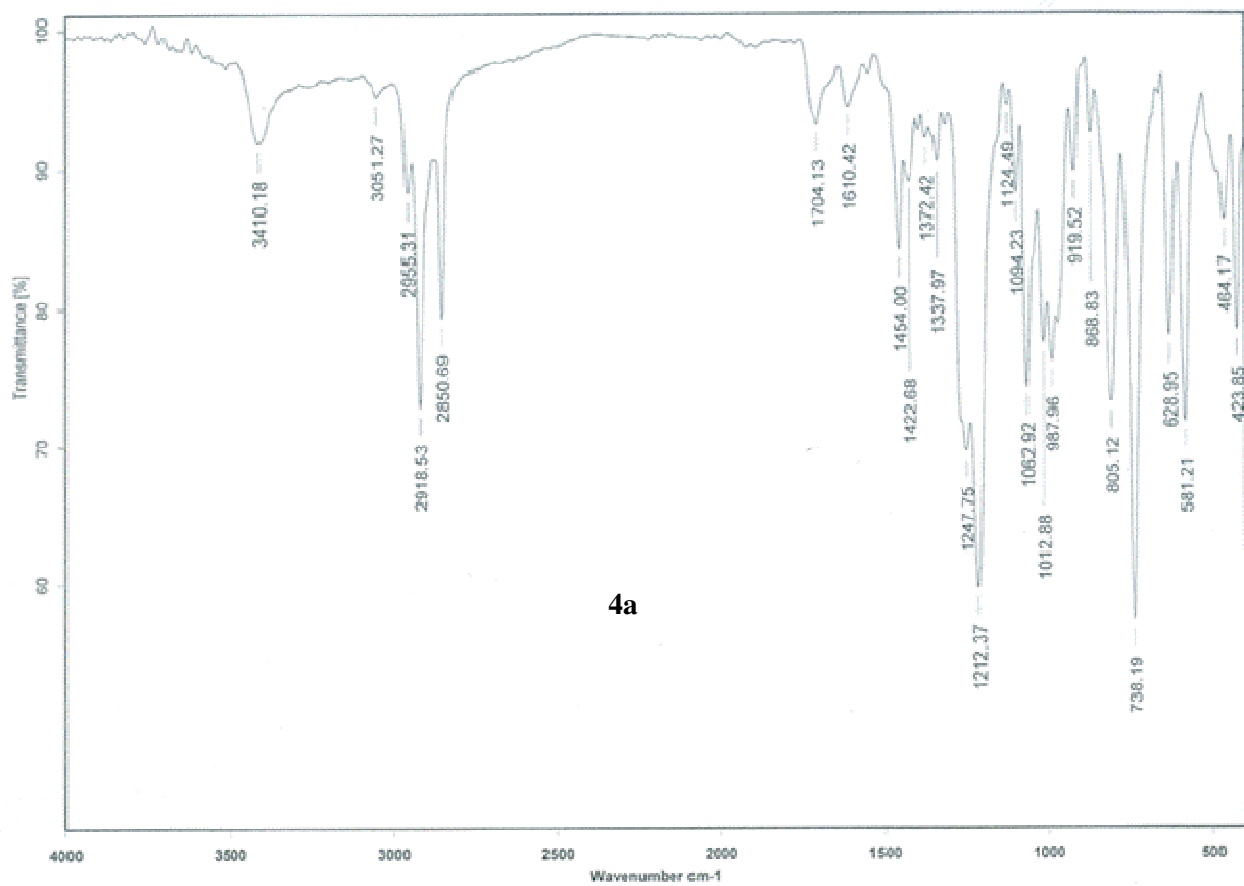
Tolerance:3.00(mmu)

Unsaturation Number:0.0 .. 32.0 (Fraction:Both)

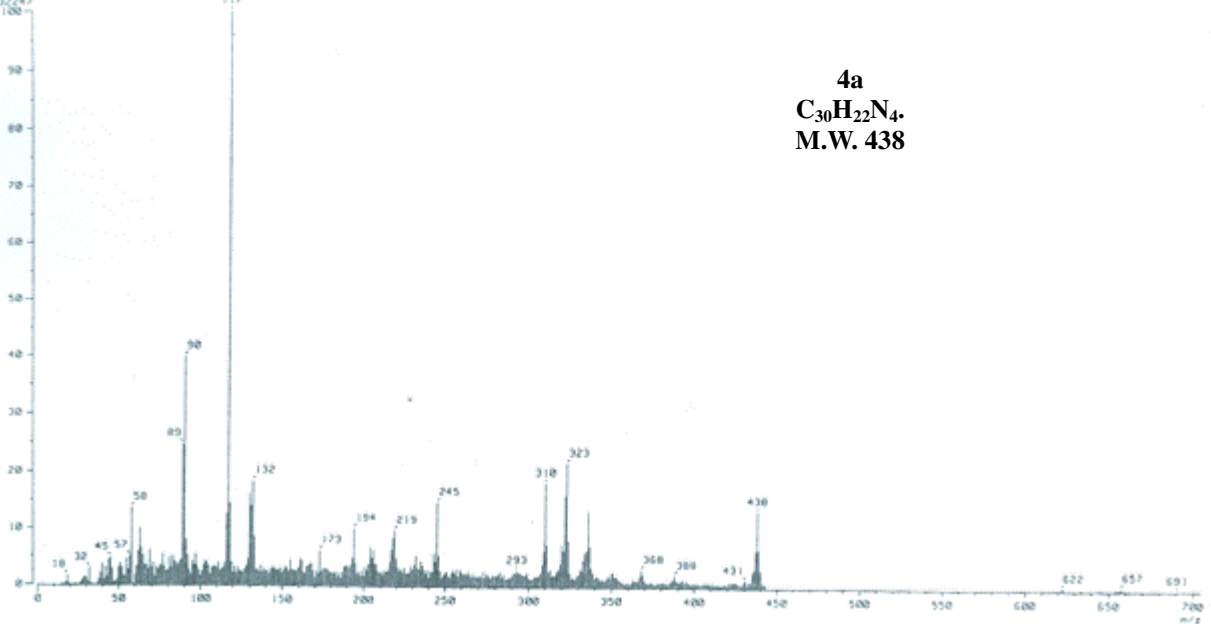


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21120	6693.89	503.21234	-1.13	-2.25	$^{12}C_{36}^{1}H_{27}^{14}N_2^{16}O_1$	24.5





[Mass Spectrum]
Date : Dr-Lopez-Jose-024 Date : 21-Sep-201
Sample: 225 I(27 Zeal 4050544)
Note : Javier Perez
Inlet : Direct Ion Mode : E1+
Spectrum Type : Normal Ion (HF-linear)
RT : 1.50 min Scan# : (10,60)
BP : m/z 117.0000 Int. : 231.96
Output m/z range : 0.0000 to 705.0445
Cut Level
2432247 117



Data: CAT 14
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 2.6...

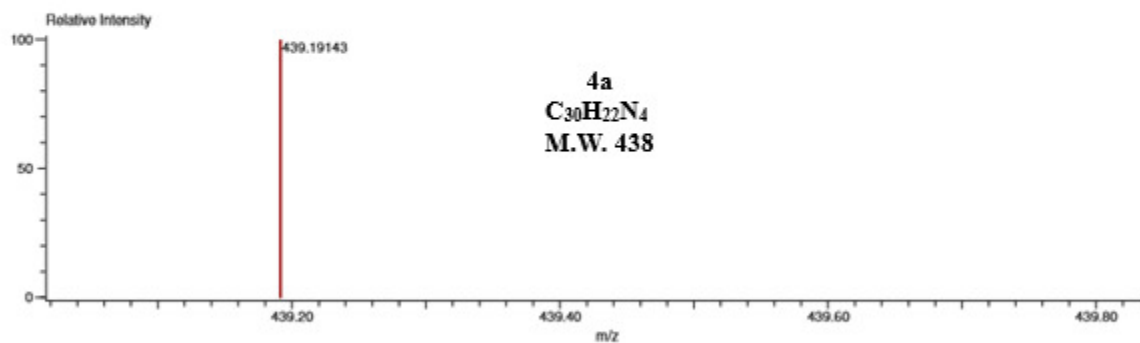
Acquired: 3/31/2016 5:49:59 PM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 6:40:29 PM
 Created by: AccuTOF

Charge number: 1

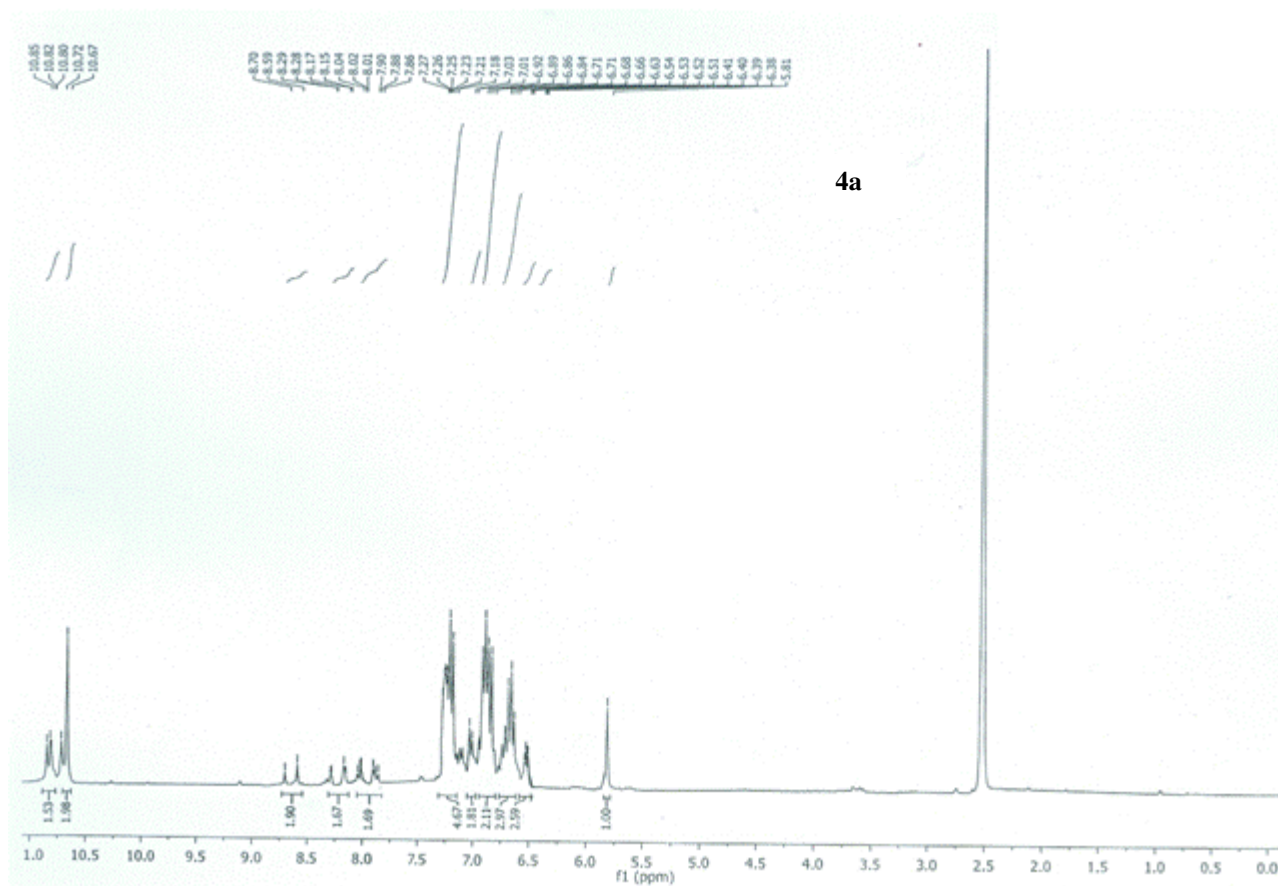
Tolerance: 3.00 (mmu)

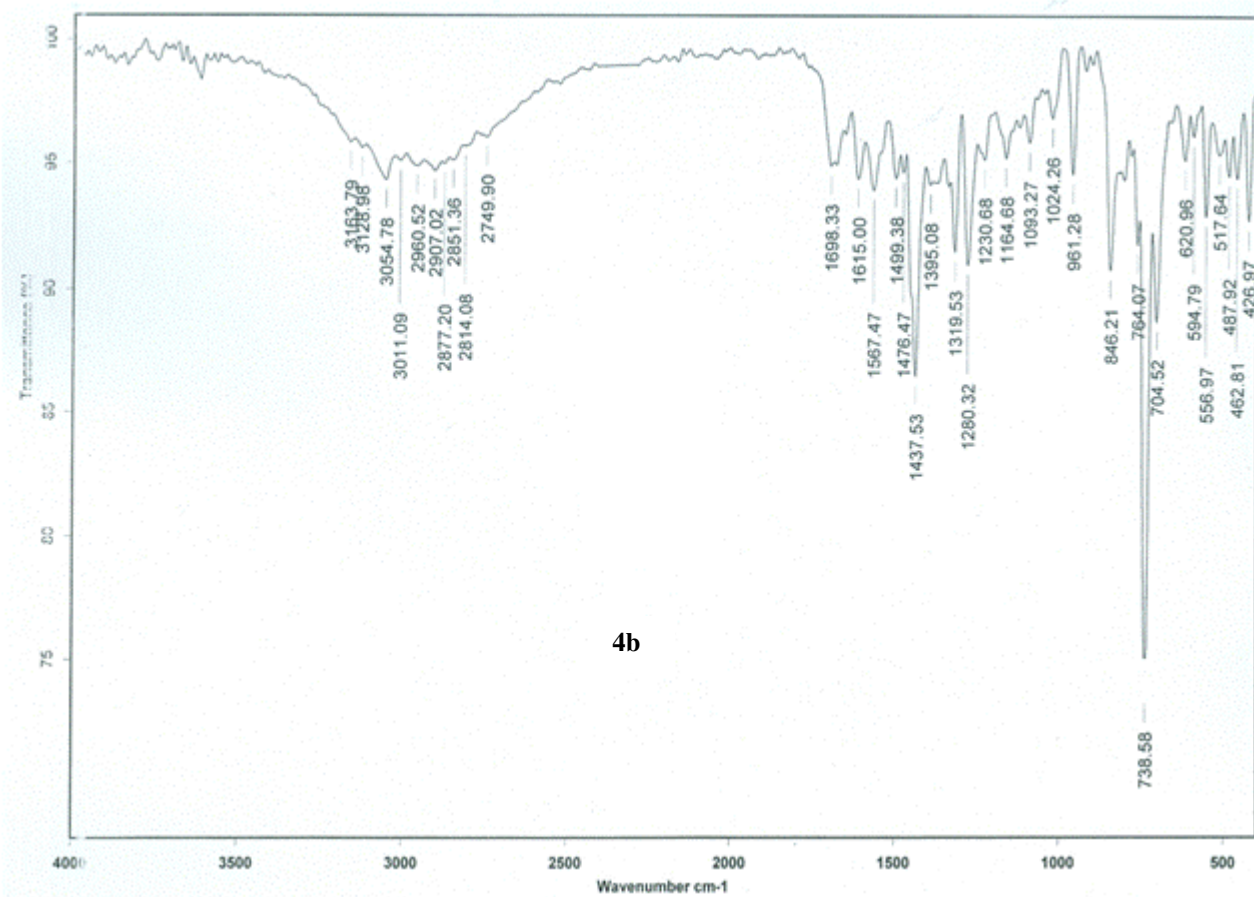
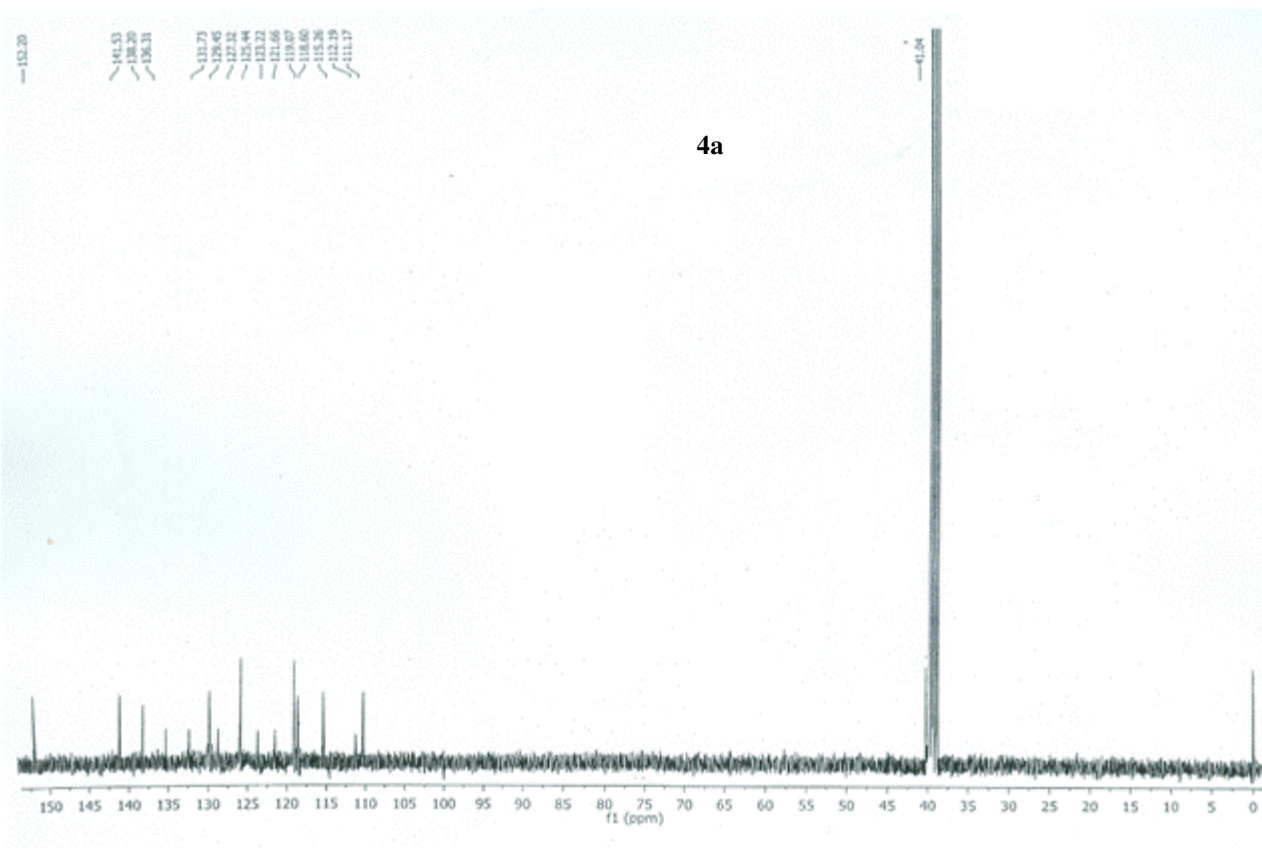
saturation Number: 0.0 .. 32.0 (Fraction: Both)

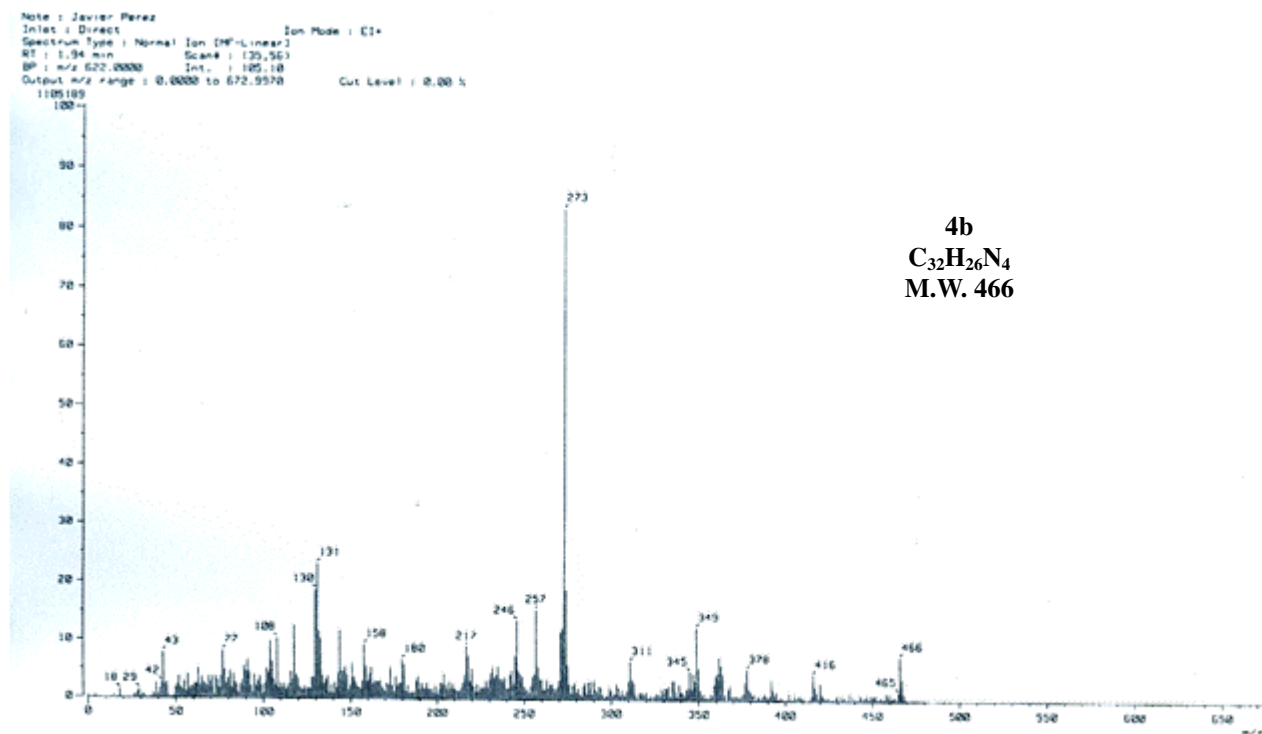
Element: ¹³C: 0 .. 100, ¹H: 0 .. 100, ¹⁴N: 2 .. 5



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	¹² C ₃₀ ¹ H ₂₂ ¹⁴ N ₄	21.5



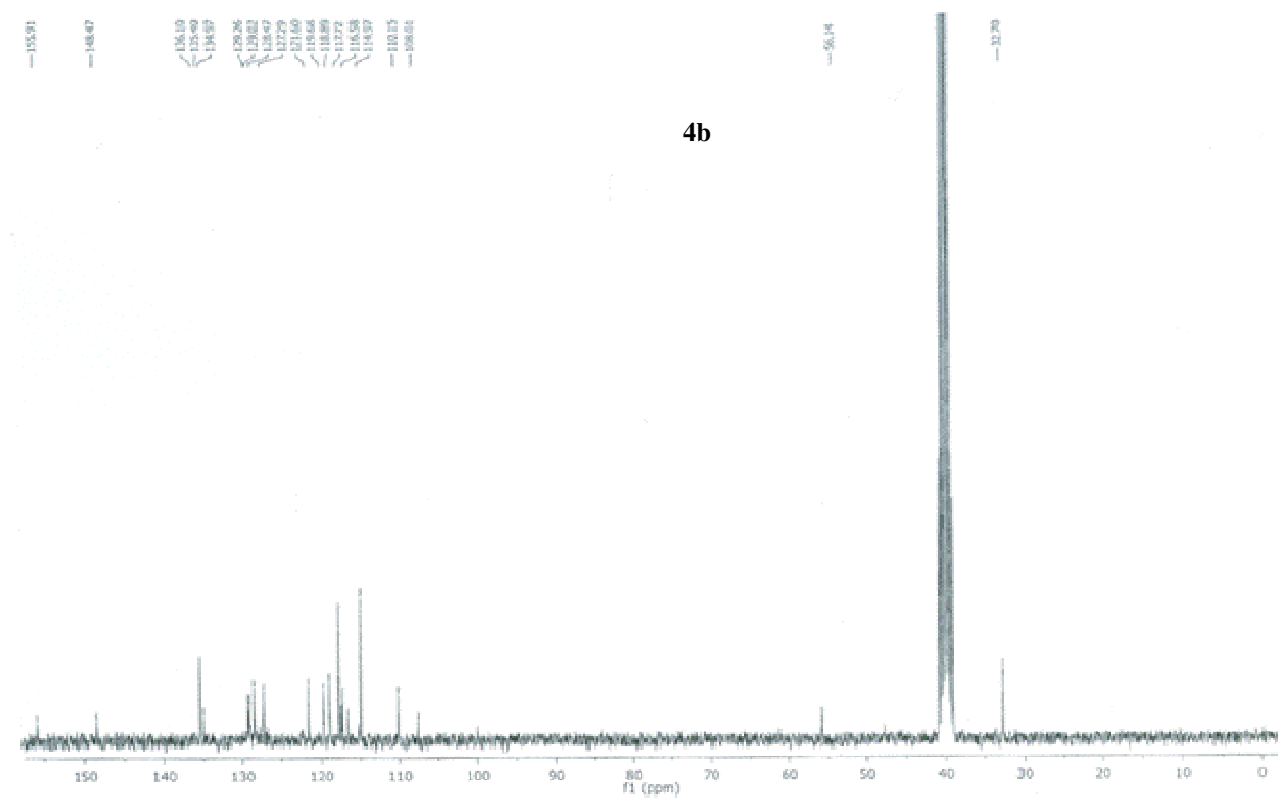
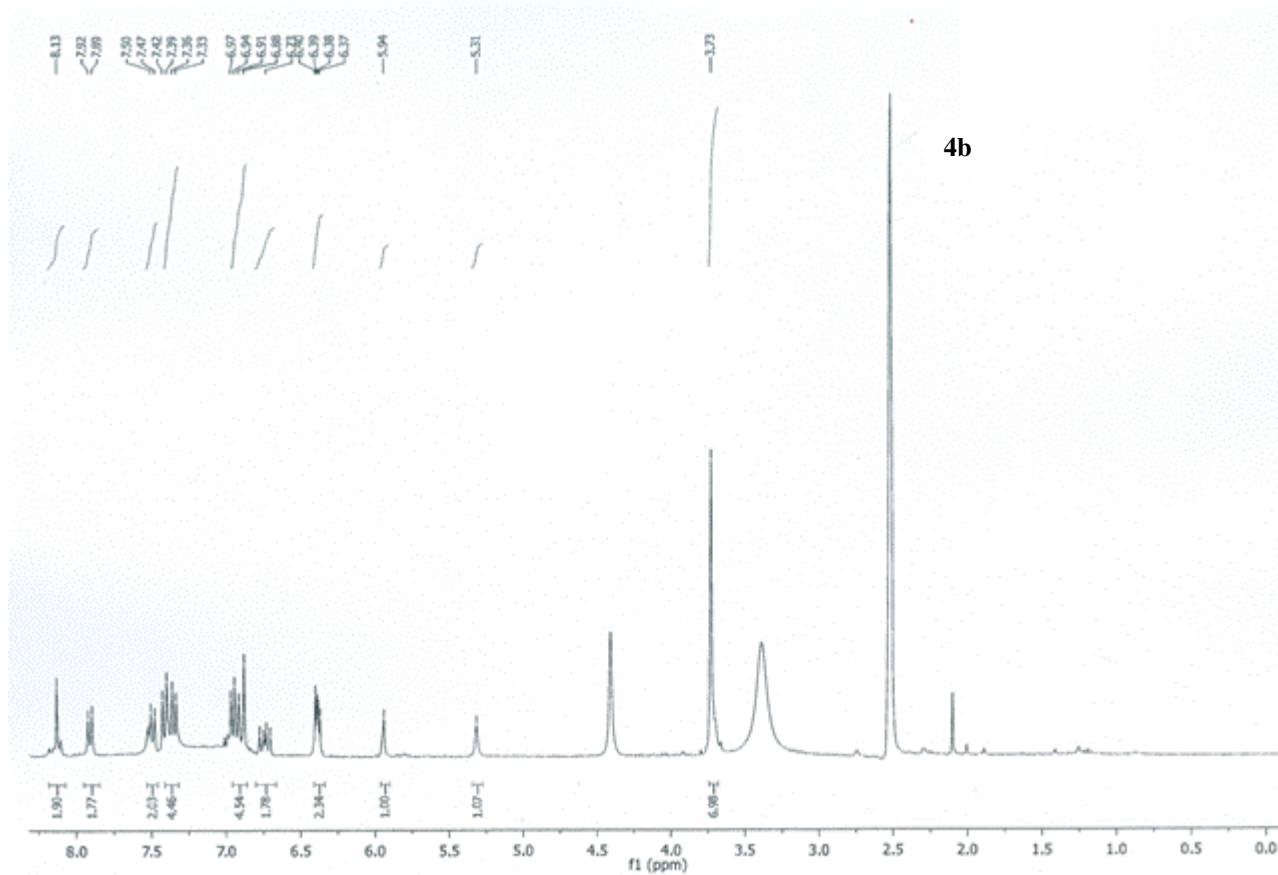


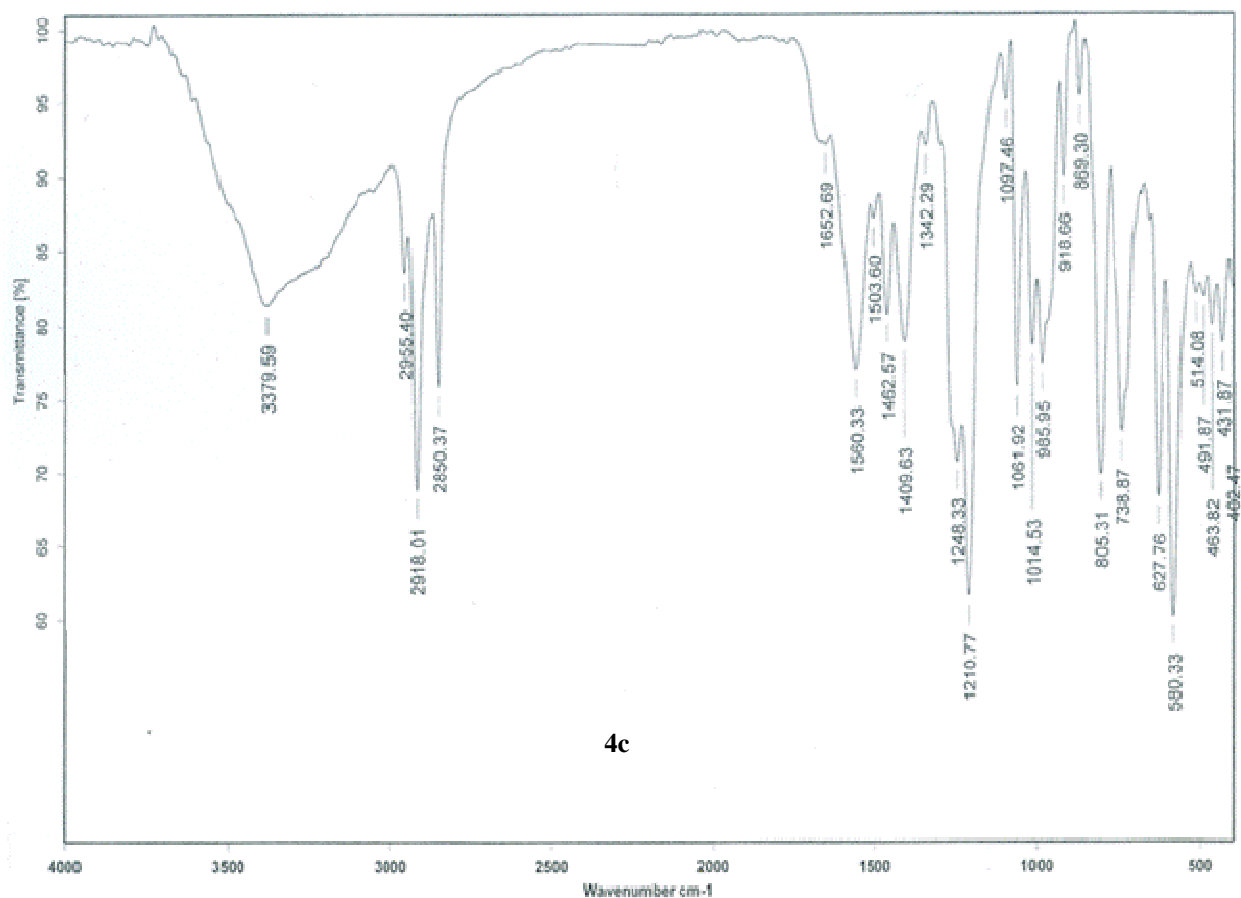


Data : Dr Ceilio Alvarez2029 Date : 29-Oct-2015 17:00
 Instrument : MStation
 Sample : 3275 1-Me-bz-p
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 3.59 min Scan# : (26,48)
 Elements : C 34/0, H 49/0, N 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : -0.5 - 34.0

4b
 $C_{32}H_{26}N_4$
 M.W. 466

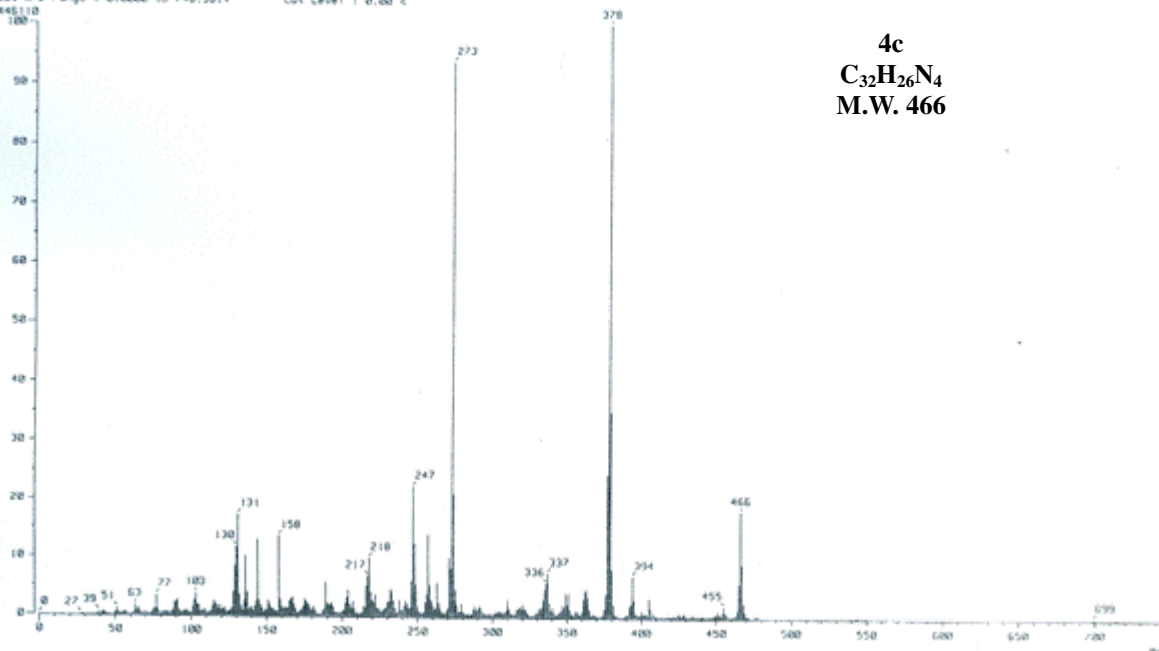
Observed m/z	Int%	Estimated m/z	Err [ppm / mmu] U.S.	C	H	N
467.2228	68.99	467.2236	-1.7 / -0.8 21.5	32	27	4





4c

[Mass Spectrum]
 Date : Dr-Lopez-Jose-050 Date : 24-May-2012 16:35
 Sample: 119 IC21 Jeol R03054
 Note : Javier Perez
 Inlet : Direct Ion Mode : E1+
 Spectrum Type : Normal Ion (MF-Linear)
 RT : 1.64 min Scan : 120,463
 BP : m/z 378,0000 Int. : 805,48
 Output m/z range : 0.0000 to 749.9614 Cut Level : 0.00 %
 8446110



4c
 $C_{32}H_{26}N_4$
 M.W. 466

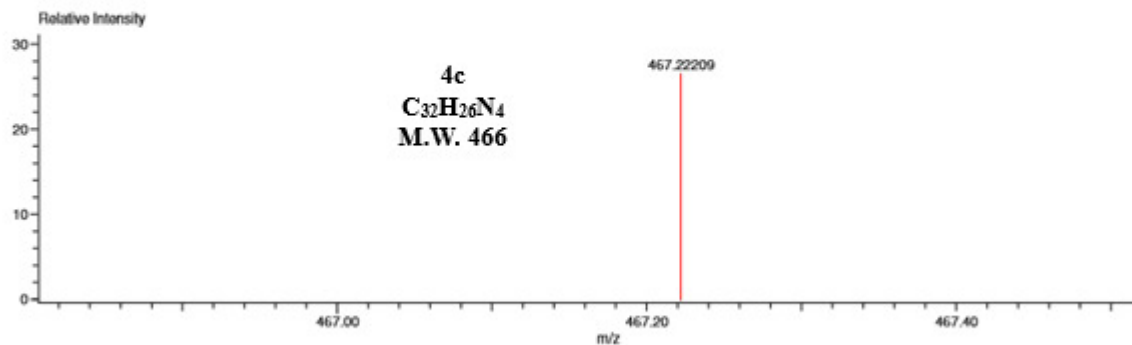
Data: CAT 15
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect [Controid, 30, Area], Correct Base [5.0%], Correct Base [5.0%], Average [MS [1] 2.0...

Acquired: 3/31/2016 5:55:20 PM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 6:57:24 PM
 Created by: AccuTOF

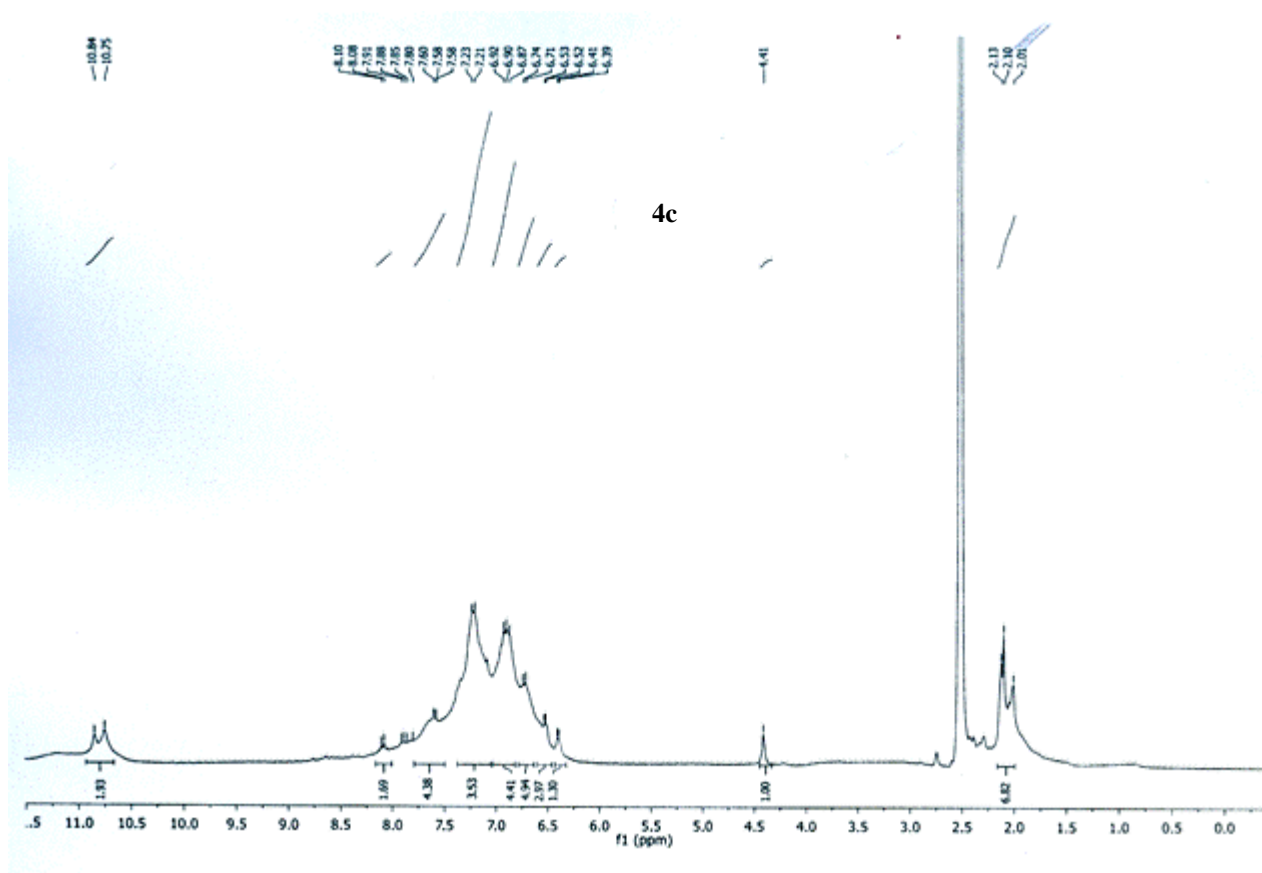
Charge number: 1
 Element: ^{13}C : 0 .. 100, ^1H : 0 .. 100, ^{14}N : 2 .. 5

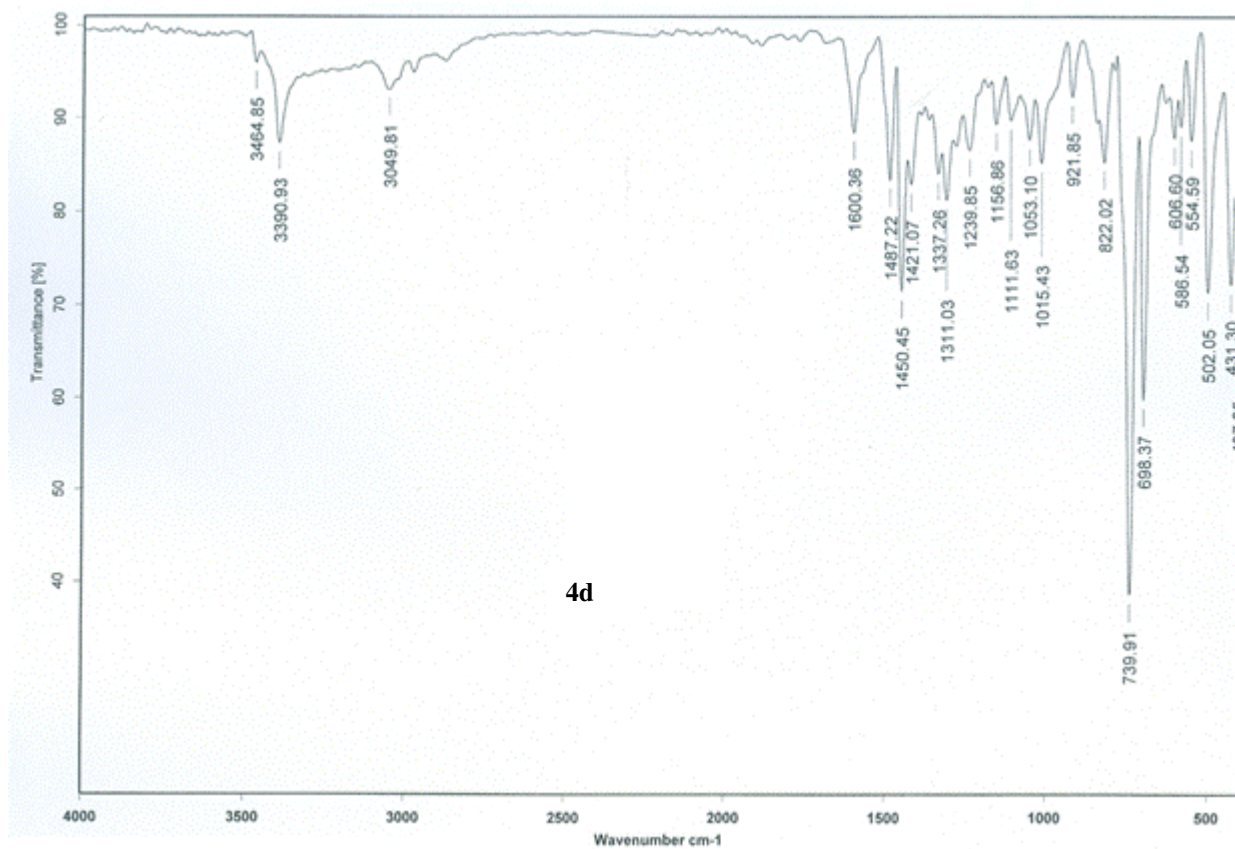
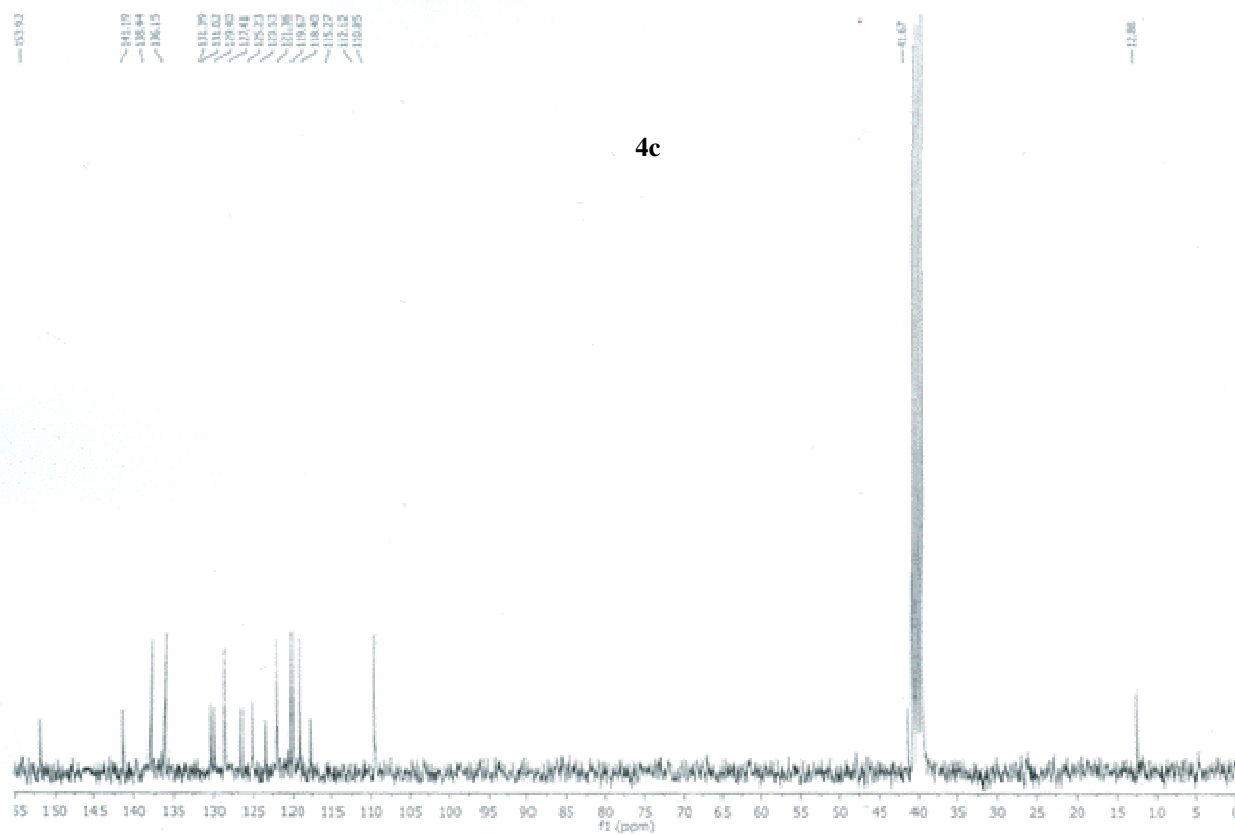
Tolerance: 3.00 (mmu)

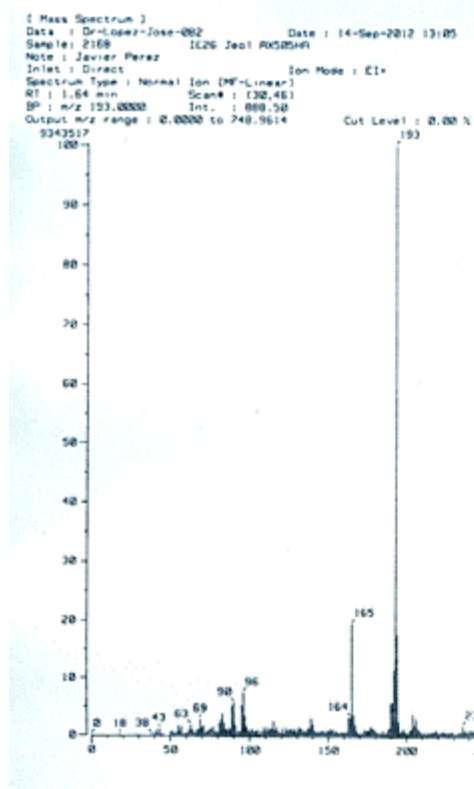
Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22209	60294.95	467.22357	-1.46	-3.16	$^{13}\text{C}_{32}\text{H}_{27}\text{N}_4$	21.5







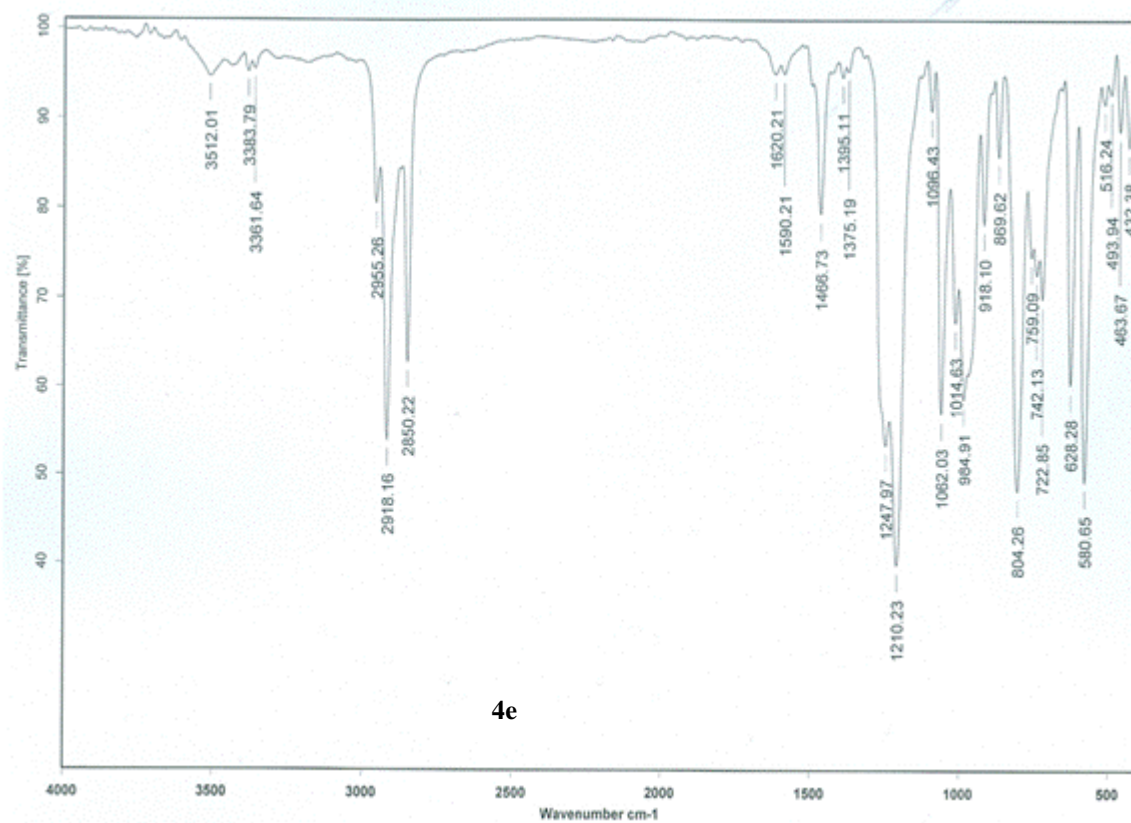
4d
 $C_{42}H_{30}N_4$
 M.W. 590

Anal calcd. C 85.40 H 5.12 N 9.48

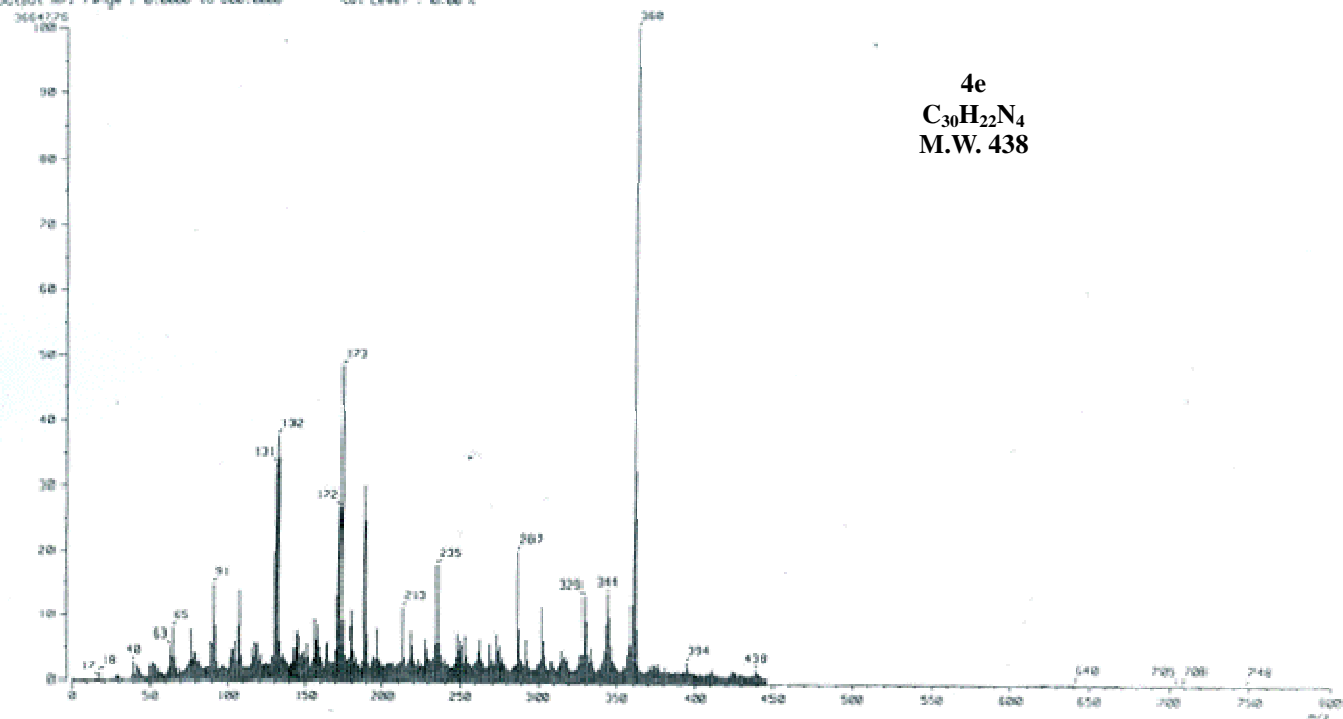
Clave de la muestra	Peso [mg]	N [%]	C [%]	H [%]	S [%]	Fecha de análisis
bz2ph p	2.700	9.43	85.38	5.10	—	27-04-2016

Found

4d
 $C_{42}H_{30}N_4$
 M.W. 590



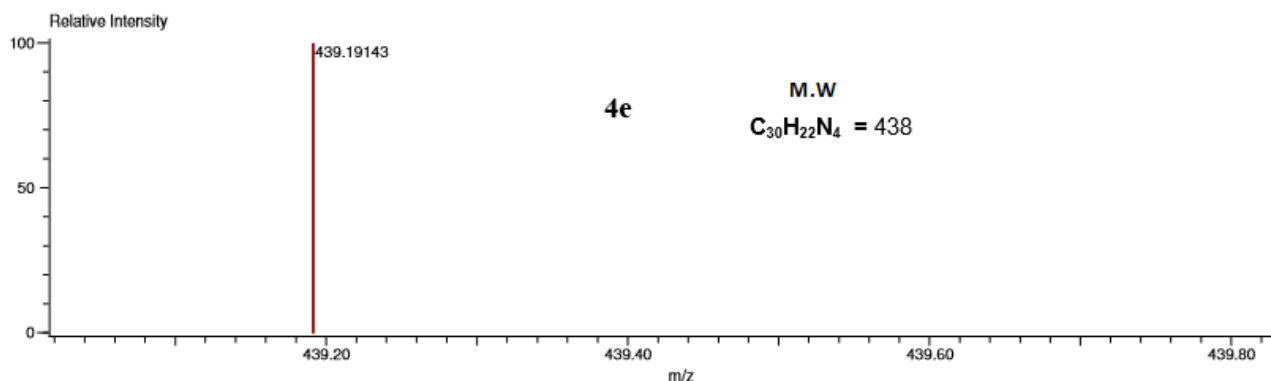
[Mass Spectrum]
Date : Dr-Rivera-Cecilia-895 Date : 18-Sep-2012 17:59
Sample: 2199 IC26 Jsci R55894
Note : Javier Perez
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion (P1-Linear)
RT : 0.69 min Scan# : 13,391
BP : m/z 362.0000 Int. : 349.18
Output m/z range : 0.0000 to 600.0000
Cut Level : 0.00 %



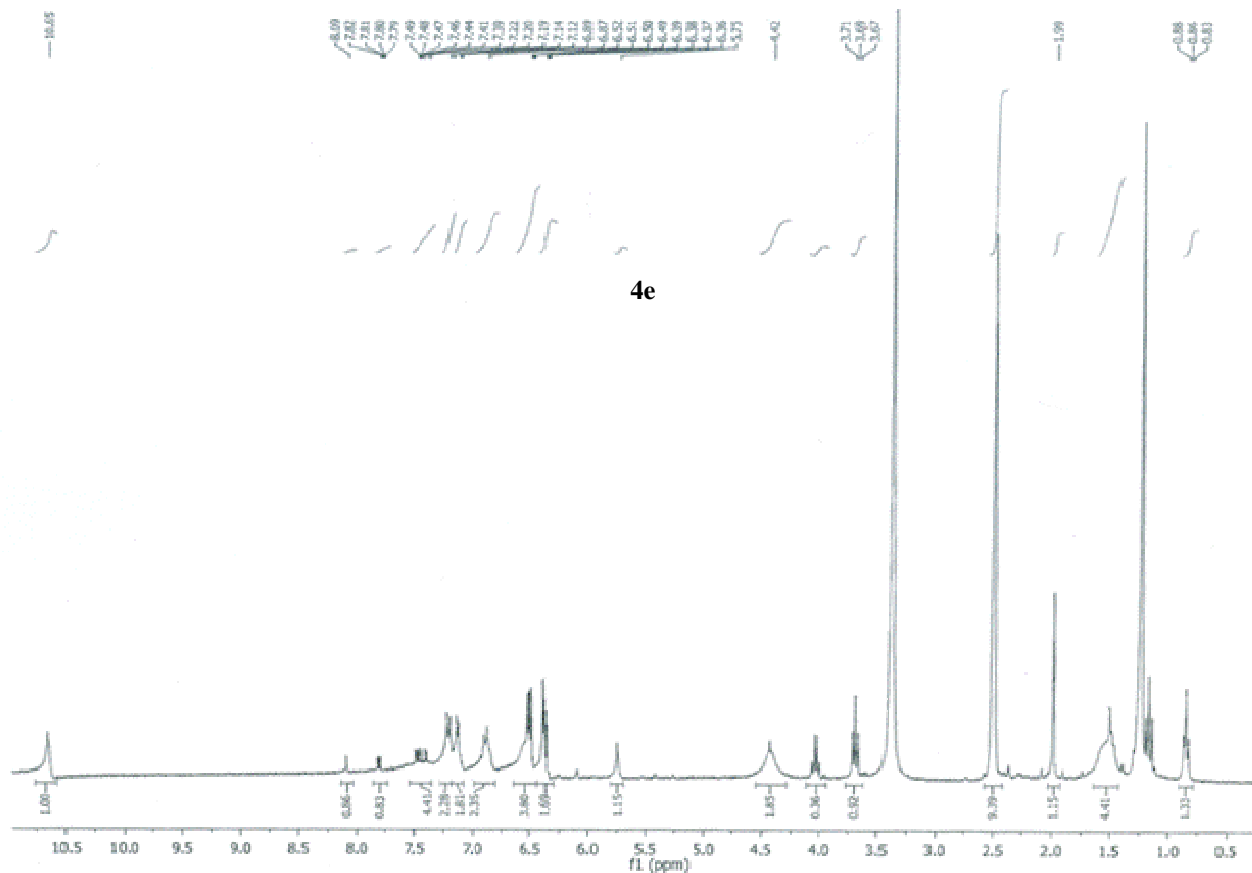
Data: CAT 14
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect [Centroid, 30, Area]; Correct Base [5.0%]; Correct Base [5.0%]; Average [MS[1]] 2.6...

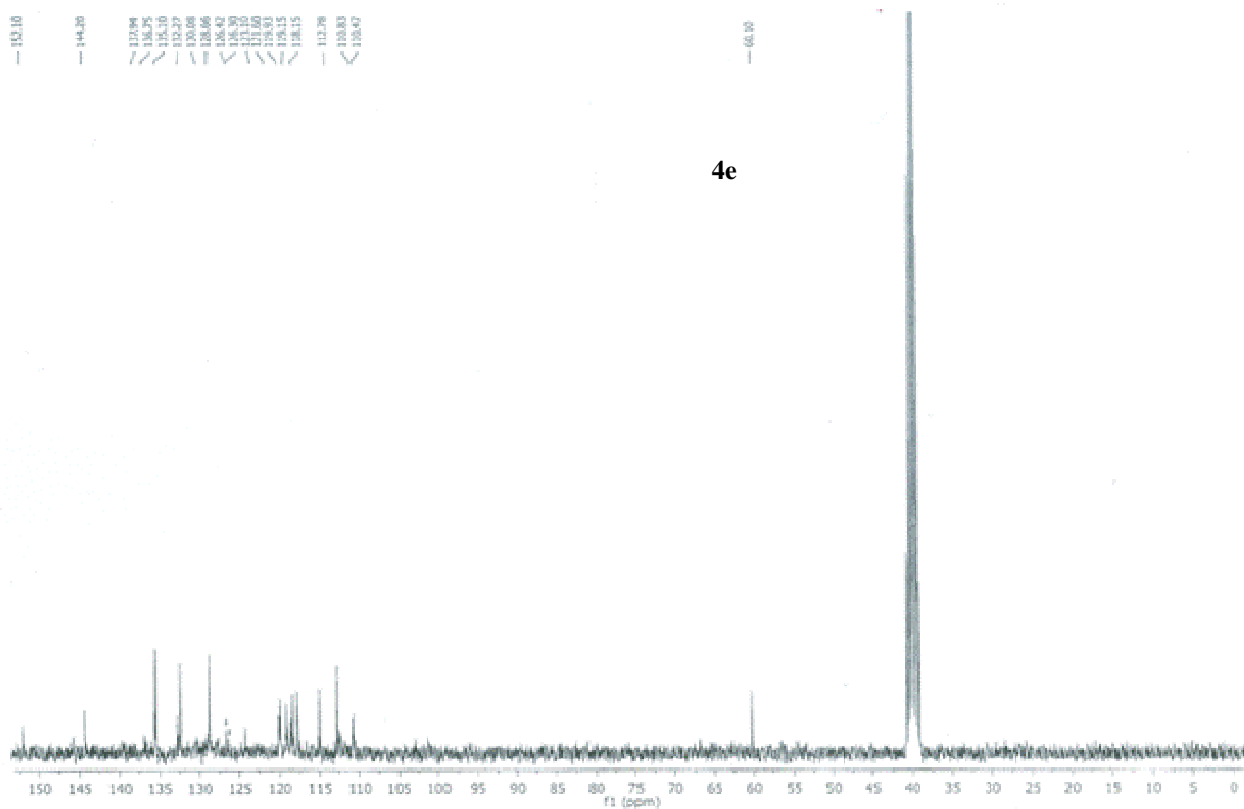
Acquired: 3/31/2016 5:49:59 PM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 6:40:29 PM
 Created by: AccuTOF

Charge number: 1
 Element: ¹²C: 0 .. 100, ¹H: 0 .. 100, ¹⁴N: 2 .. 5
 Tolerance: 3.00 (mmu)
 Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

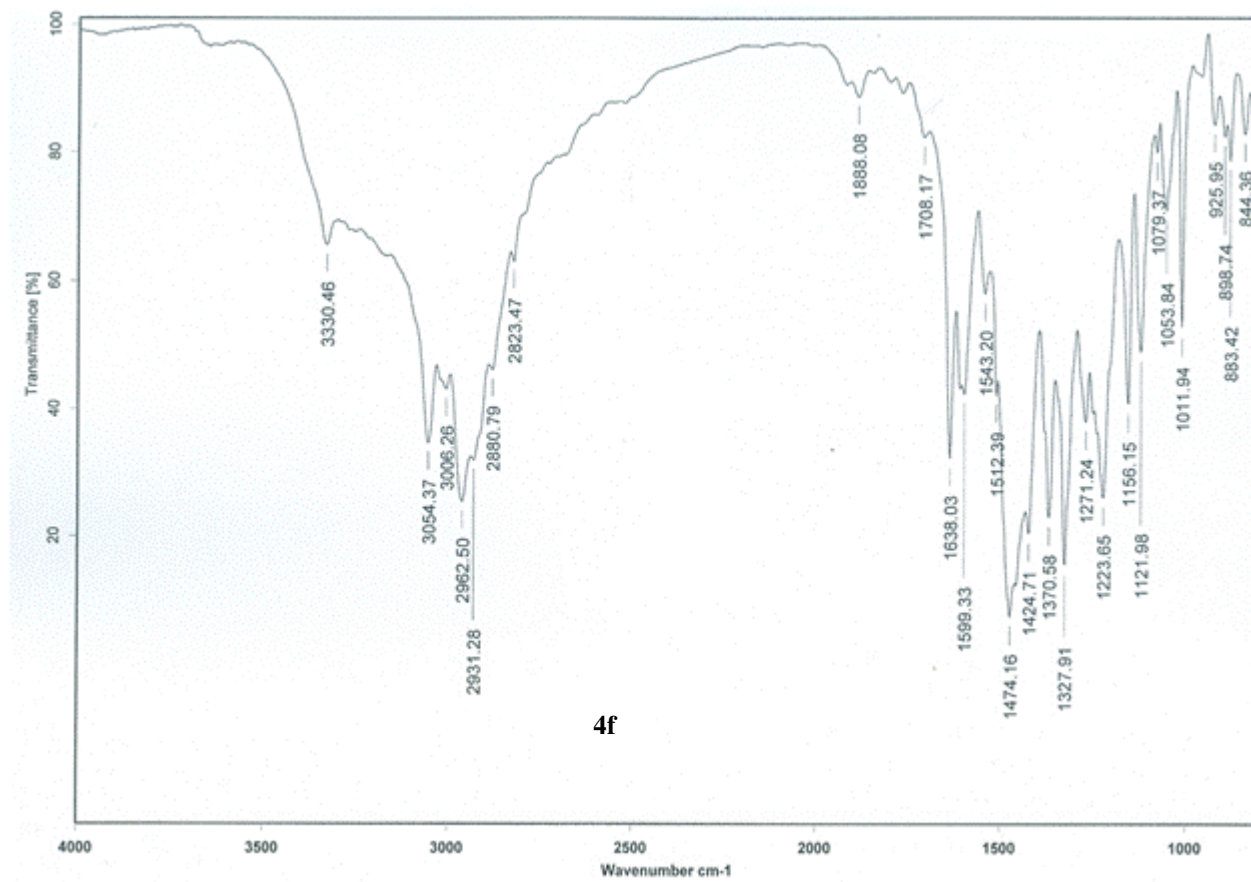


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	¹² C ₃₀ ¹ H ₂₂ ¹⁴ N ₄	21.5



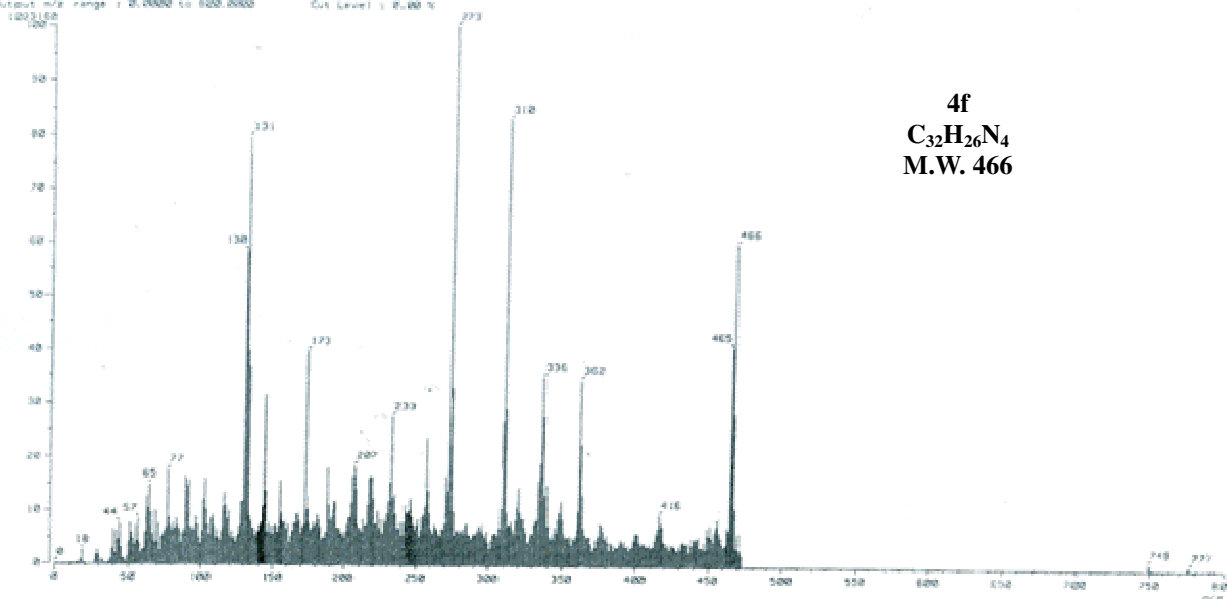


4e



4f

1 Mass Spectrum 3
 Date : De-Logan-Jose-800 Desk : 21-Sep-2016 11:17
 Sample : 2758 ICP Job: R0503-A
 MSID : Javier Perez ICP Mode : ESI+
 Inlet : Direct Ion Mode : ESI+
 Spectrum Type : Normal Scan (90°-10000)
 RT : 0.34 min Scan : 110,793
 BP : m/z 273.80000 Det. : 97.58
 Output m/z range : 0.00000 to 800.00000 Cut Level : 0.00 %



4f
 $C_{32}H_{26}N_4$
 M.W. 466

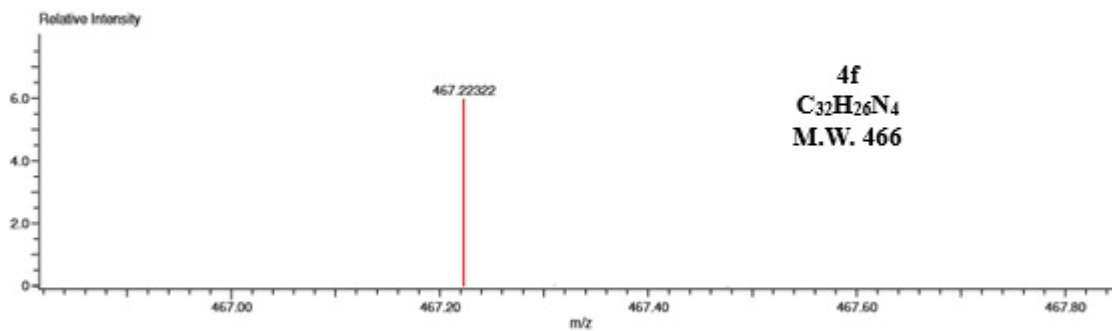
Data:CAT 17
 Sample Name:
 Description:
 Ionization Mode:ESI+
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.7...

Acquired:3/31/2016 6:01:08 PM
 Operator:AccuTOF
 Mass Calibration data:PEG600
 Created:4/11/2016 7:04:54 PM
 Created by:AccuTOF

Charge number:1
 Element: ^{13}C :0 .. 100, 1H :0 .. 100, ^{14}N :2 .. 5

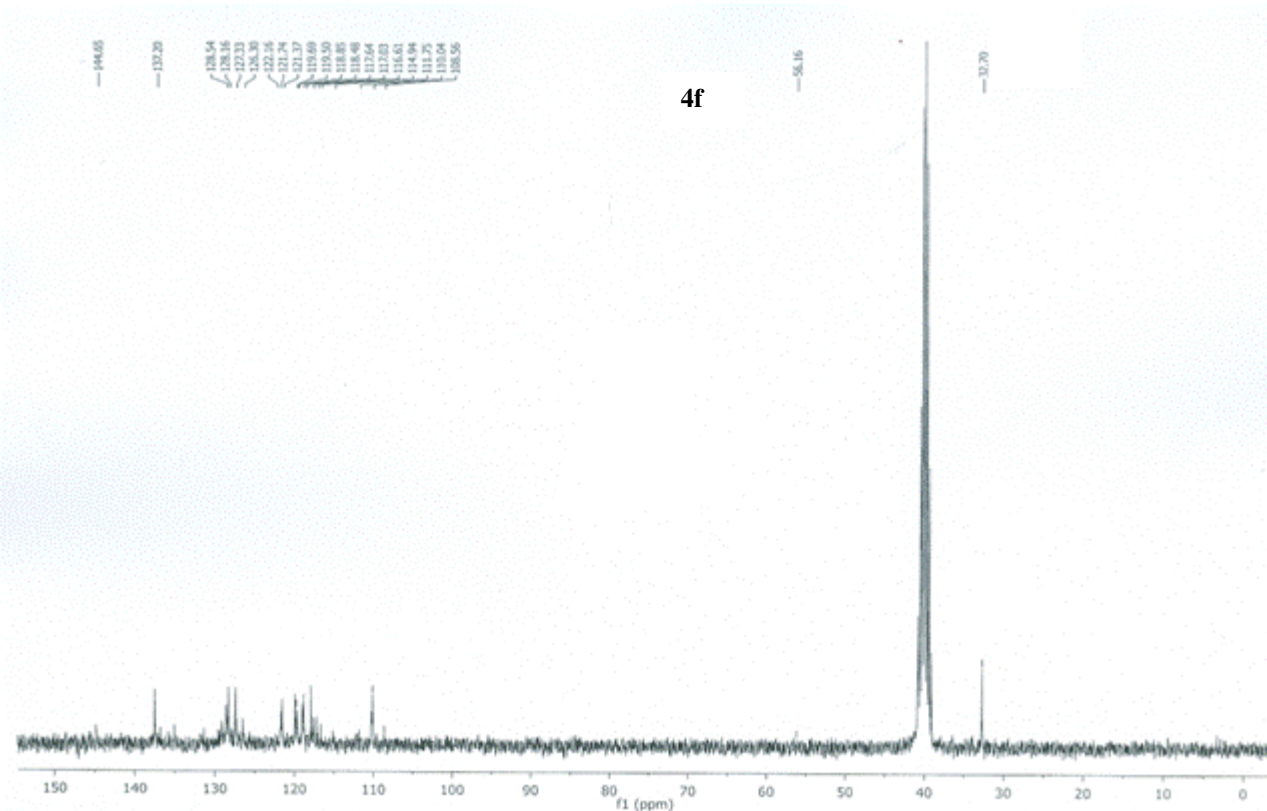
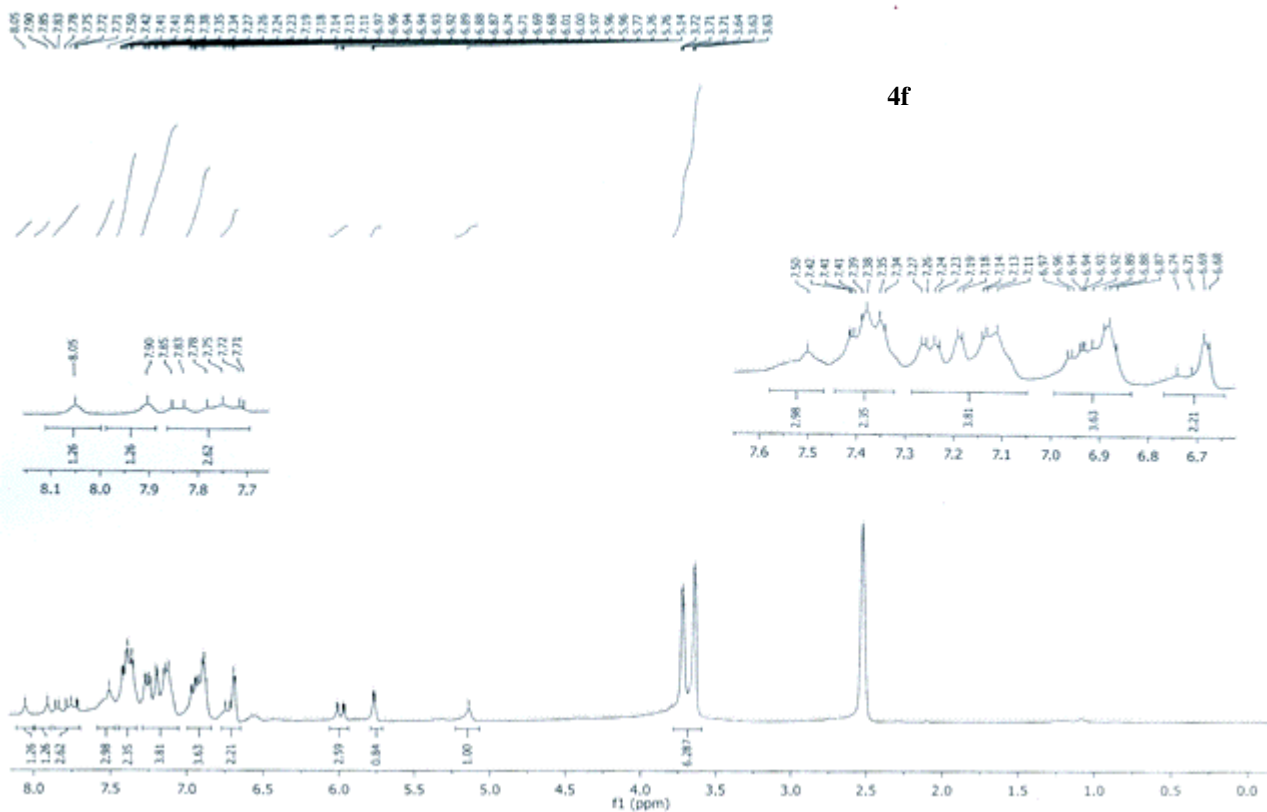
Tolerance:3.00(mmu)

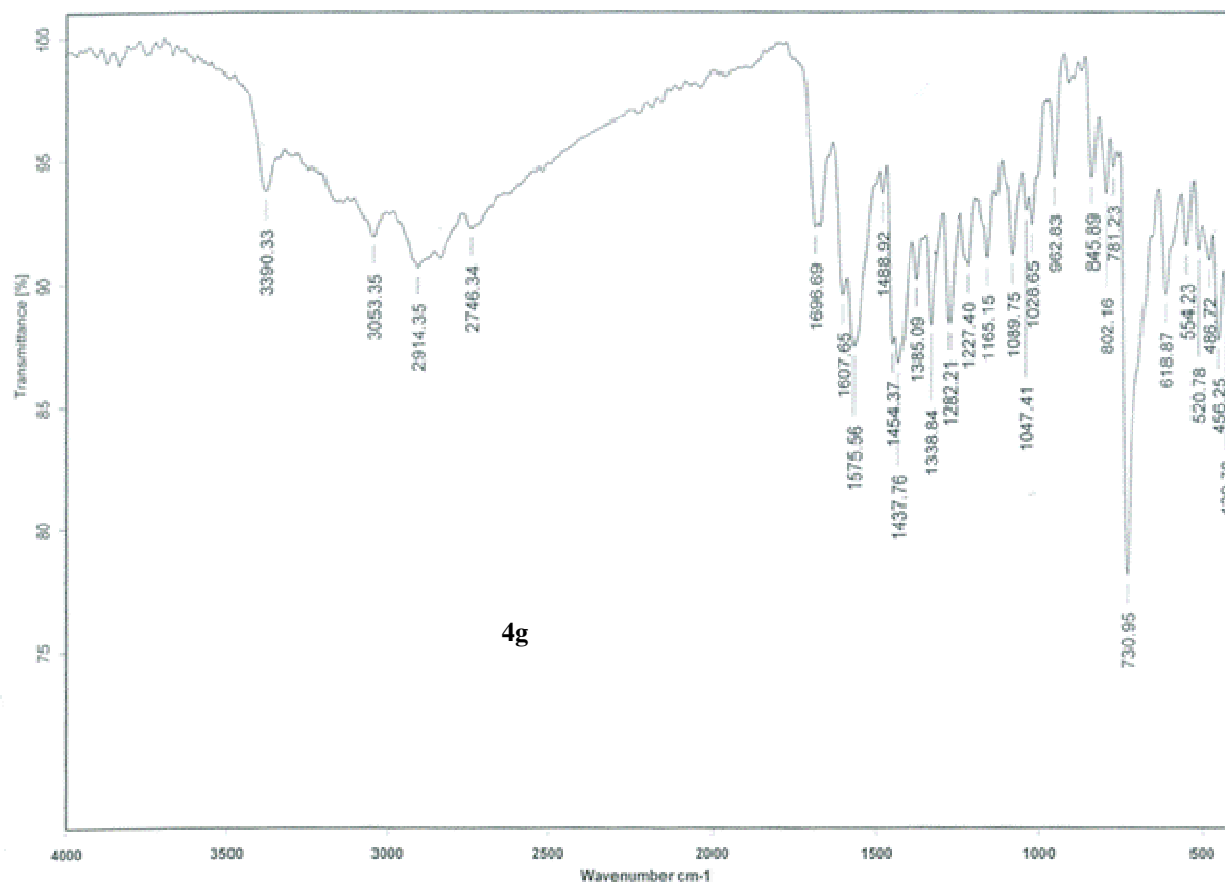
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



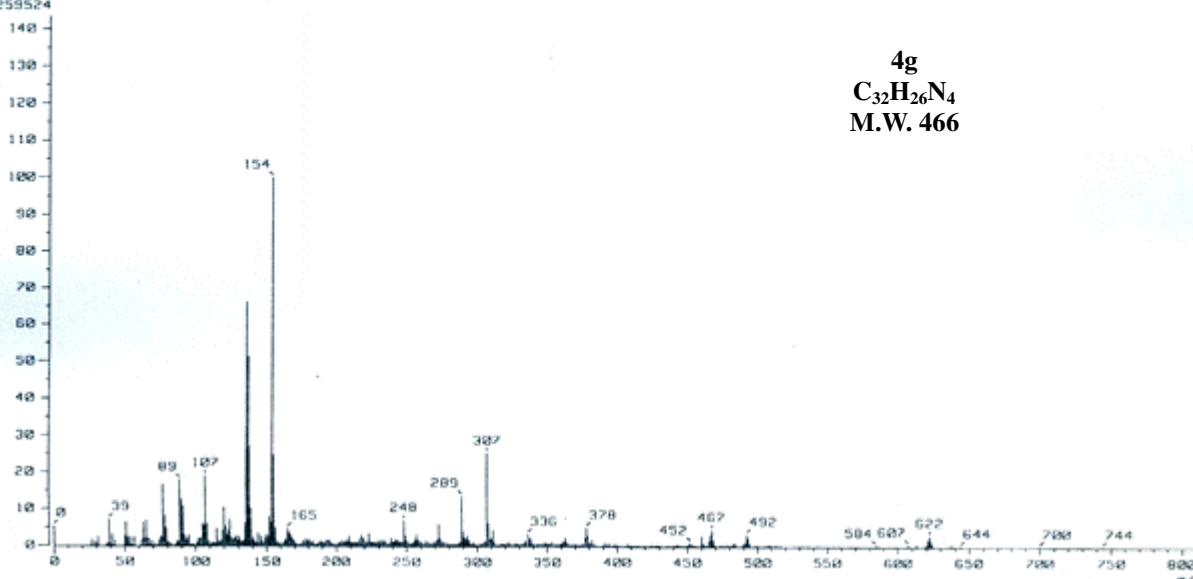
4f
 $C_{32}H_{26}N_4$
 M.W. 466

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22322	3587.26	467.22357	-0.35	-0.74	$^{13}C_{32}H_{26}^{14}N_4$	21.5





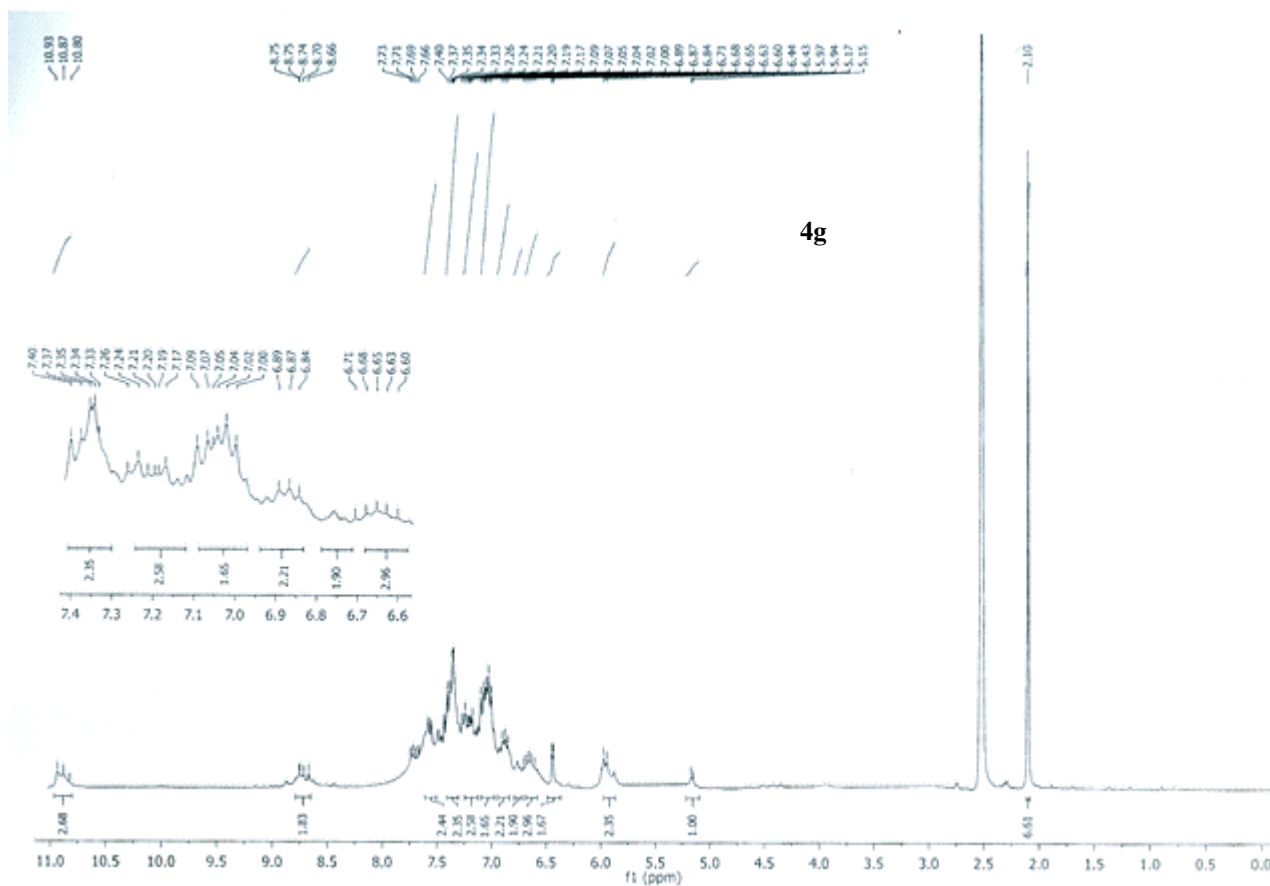
• [Mass Spectrum]
 Data : Dr-Jose-Lopez065 Date : 17-Oct-2012 11:00
 Sample: 2398
 Note : Luis-Velasco
 Inlet : Direct Ion Mode : FRB+
 Spectrum Type : Normal Ion (MF-Linear)
 RT : 2.47 min Scan# : (3,15)
 BP : m/z 154.00000 Int. : 216.88
 Output m/z range : 0.00000 to 815.5786 Cut Level : 0.28 %

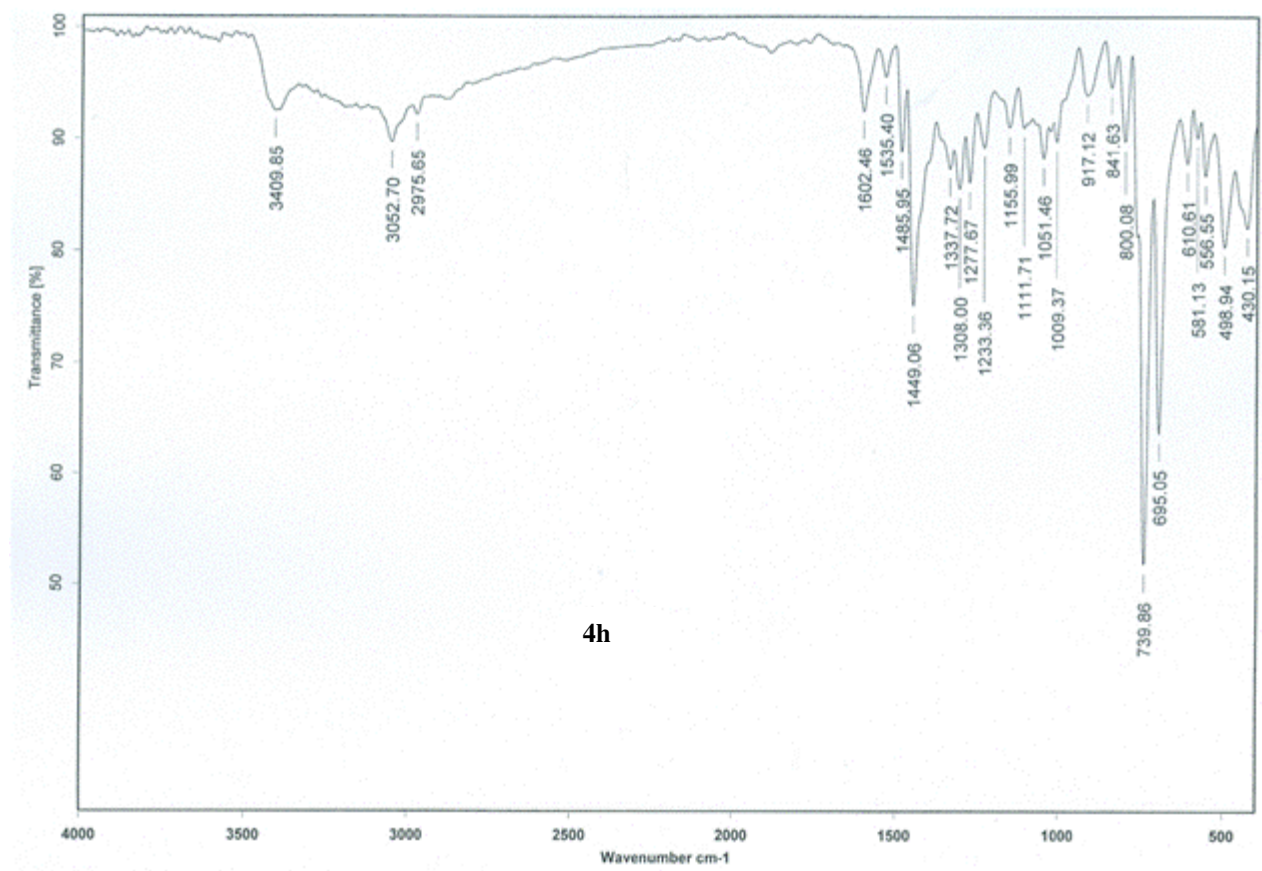
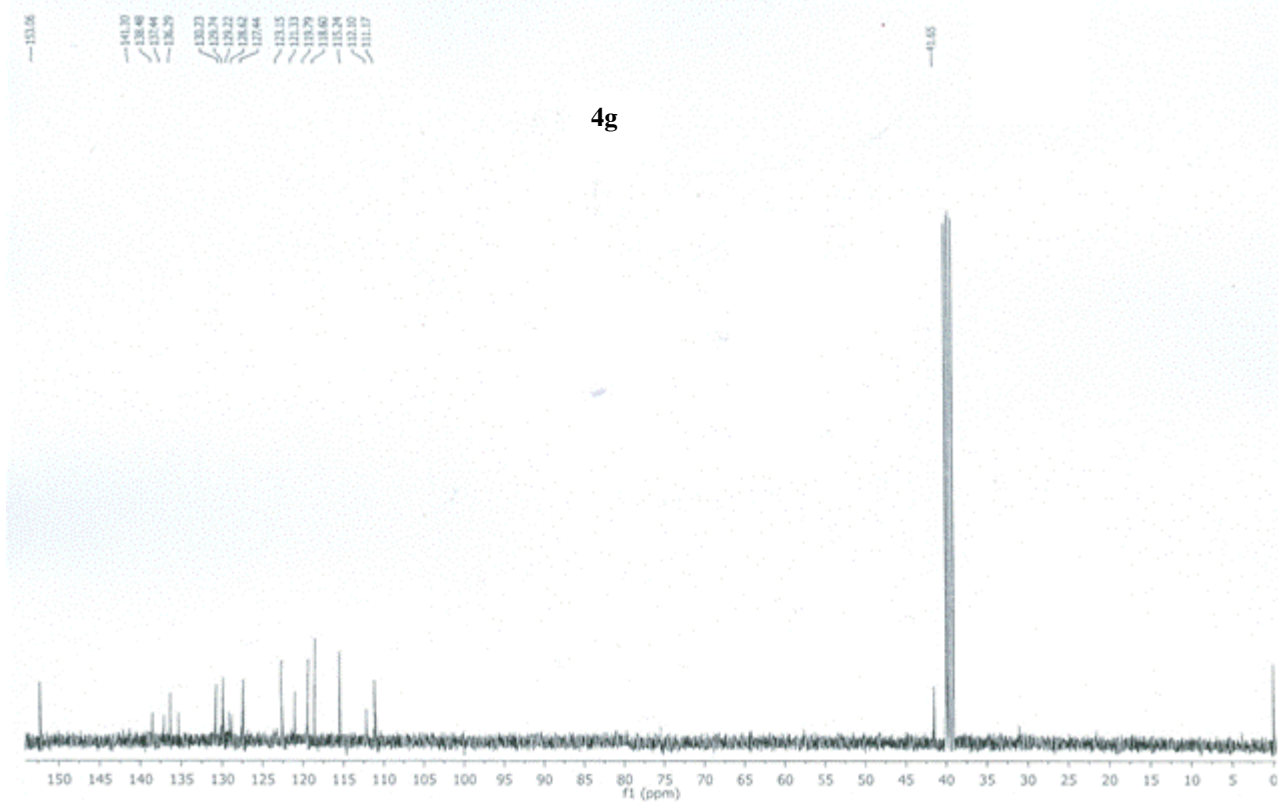


Data : Dr Cecilio Alvarez031 Date : 29-Oct-2015 16:00
 Instrument : MStation
 Sample : 3276 2-Me-bz-m
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 3.59 min Scan# : (26,48)
 Elements : C 34/0, H 49/0, N 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : -0.5 - 34.0

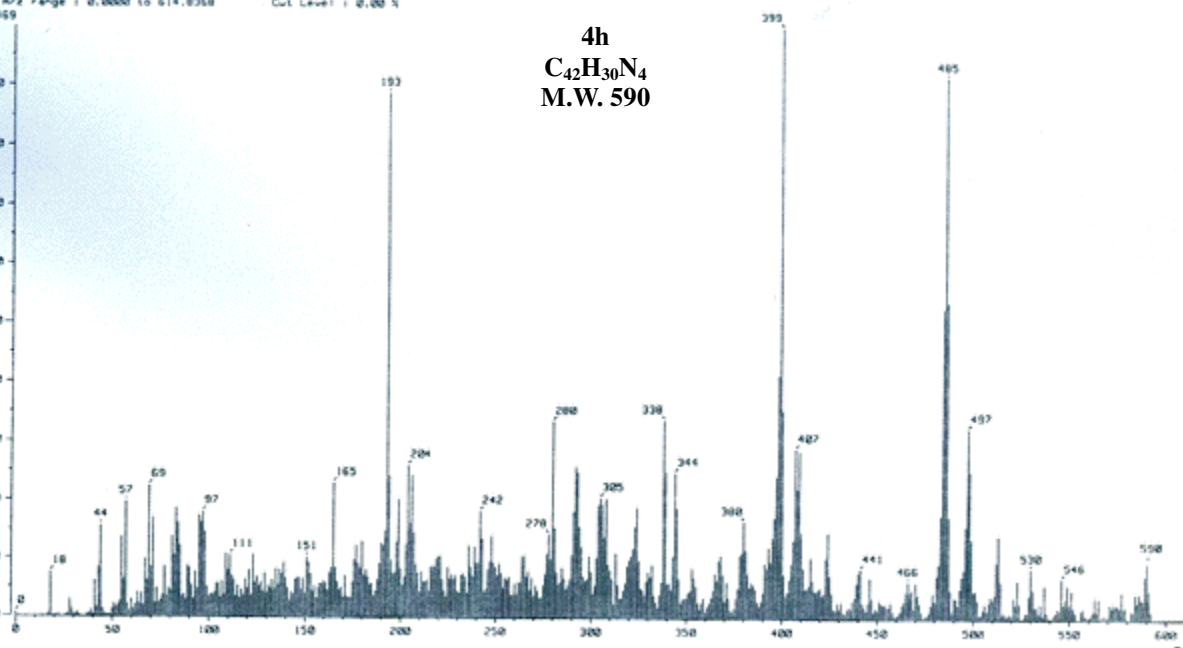
4g
 $C_{32}H_{26}N_4$
 M.W. 466

	Observed m/z	Int%			
	467.2228	68.99			
1	Estimated m/z	Err[ppm / mmu]	U.S.	C	H N
	467.2236	-1.7 / -0.8	21.5	32	27 4





[Mass Spectrum]
 Date : D-Rivera-Cecilio-207 Date : 18-Jan-2020 09:56
 Sample: 125 IC30 Jeol Rx5054f
 Note : Javier Perez
 Inlet : Direct Ion Mode : E1+
 Spectrum Type : Normal Ion (HF-Linear)
 RT : 1.55 min Scan# : (23,52)
 BP : m/z 399.0000 Int. : 70.44
 Output m/z range : 0.0000 to 614.8358 Cut Level : 0.00 %



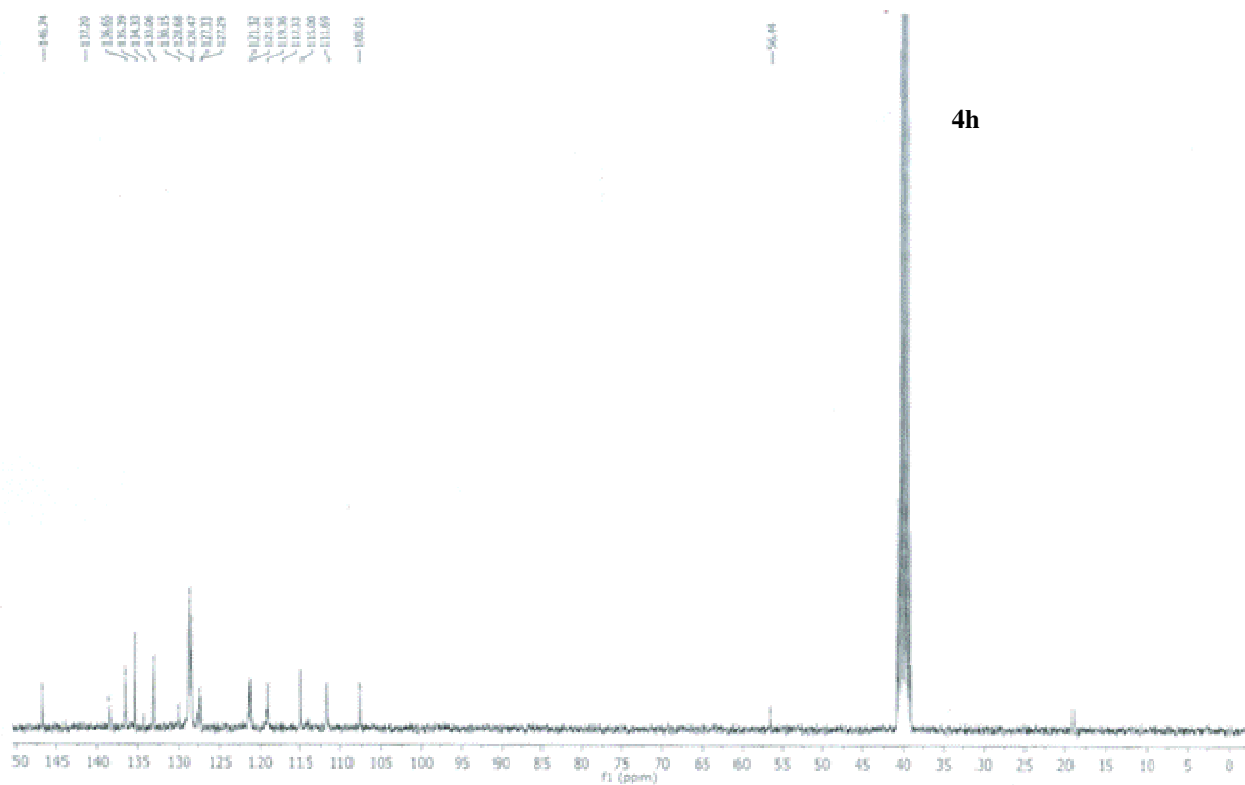
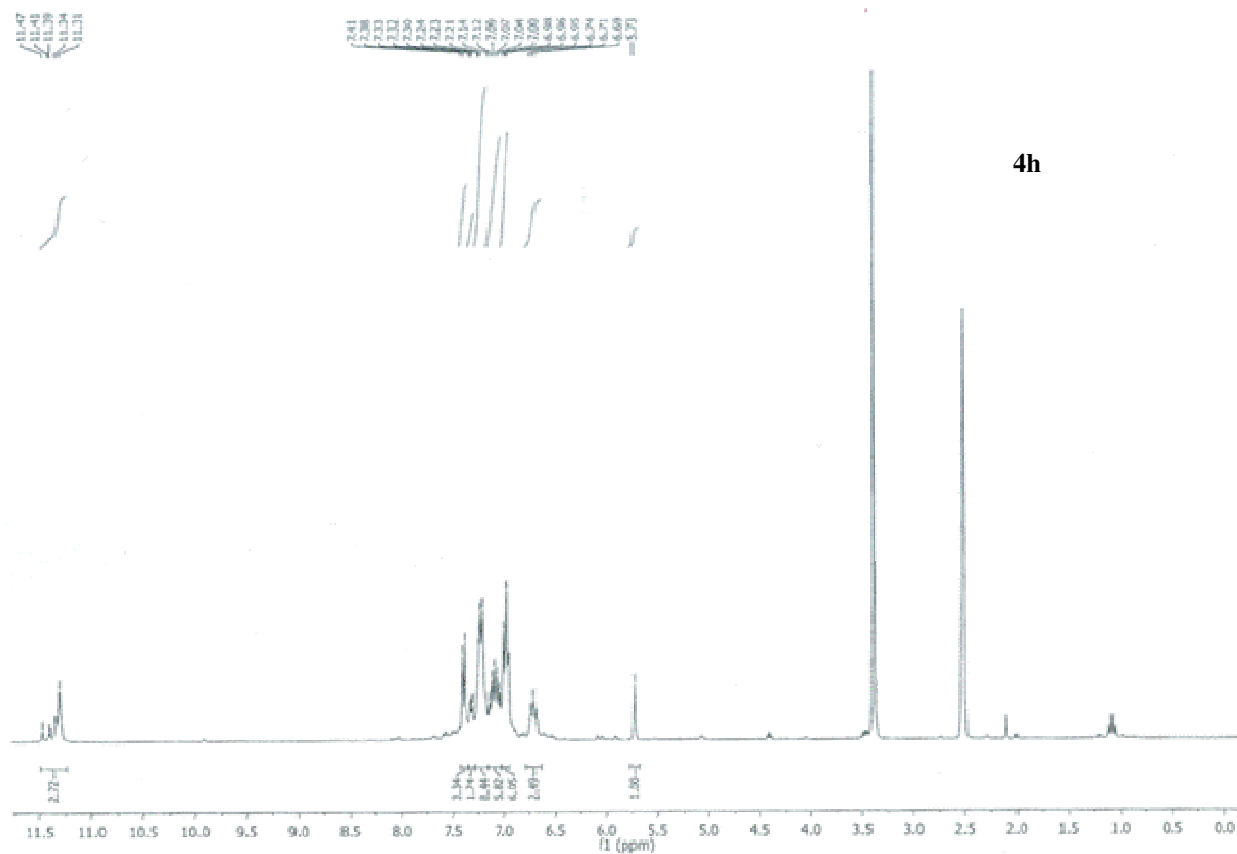
4h
 $C_{42}H_{30}N_4$
 M.W. 590

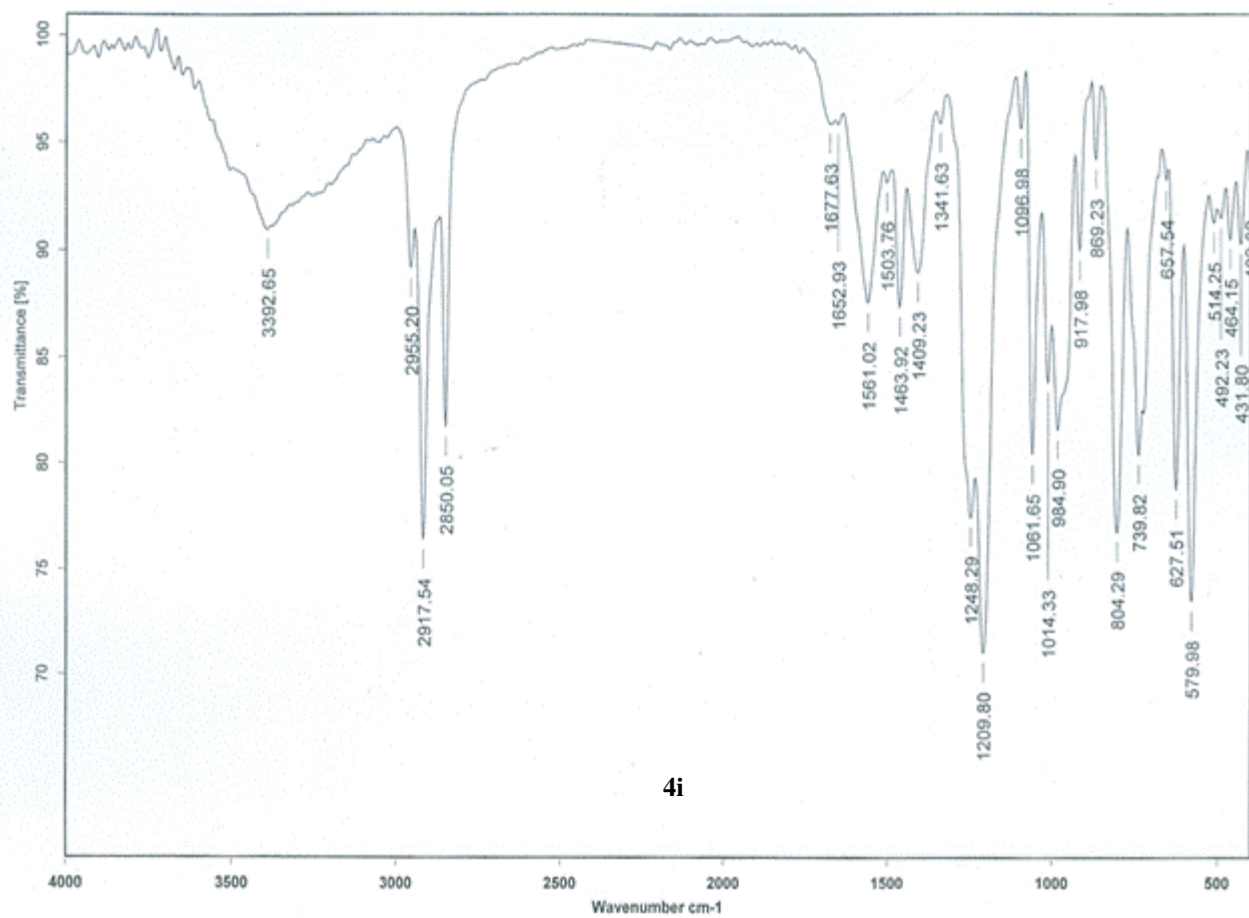
Anal calcd. C 85.40 H 5.12 N 9.48

Clave de la muestra	Peso [mg]	N [%]	C [%]	H [%]	S [%]	Fecha de análisis
bz2ph m	2.647	9.44	85.37	5.01	---	27-04-2016

Found

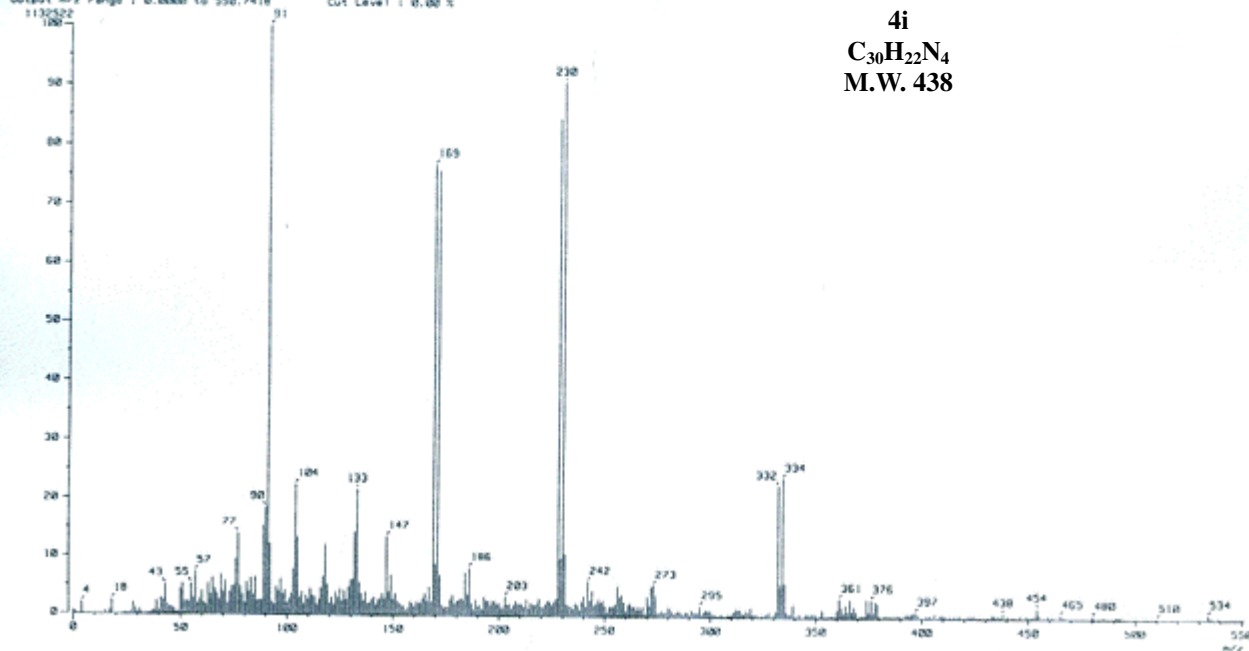
4h
 $C_{42}H_{30}N_4$
 M.W. 590





4i

[Mass Spectrum]
Date : Dr-Lopez-Jose-085 Date : 01-Jun-2012 18:16
Sample: 1270 ICD: Jeol HX505sh
Note : Javier Perez
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion (M⁺-Linear)
RT : 0.75 min Scan : (7,29)
BP : m/z 91.0000 Int. : 100.01
Outlet m/z range : 0.0000 to 550.7418 Cut Level : 0.00 %

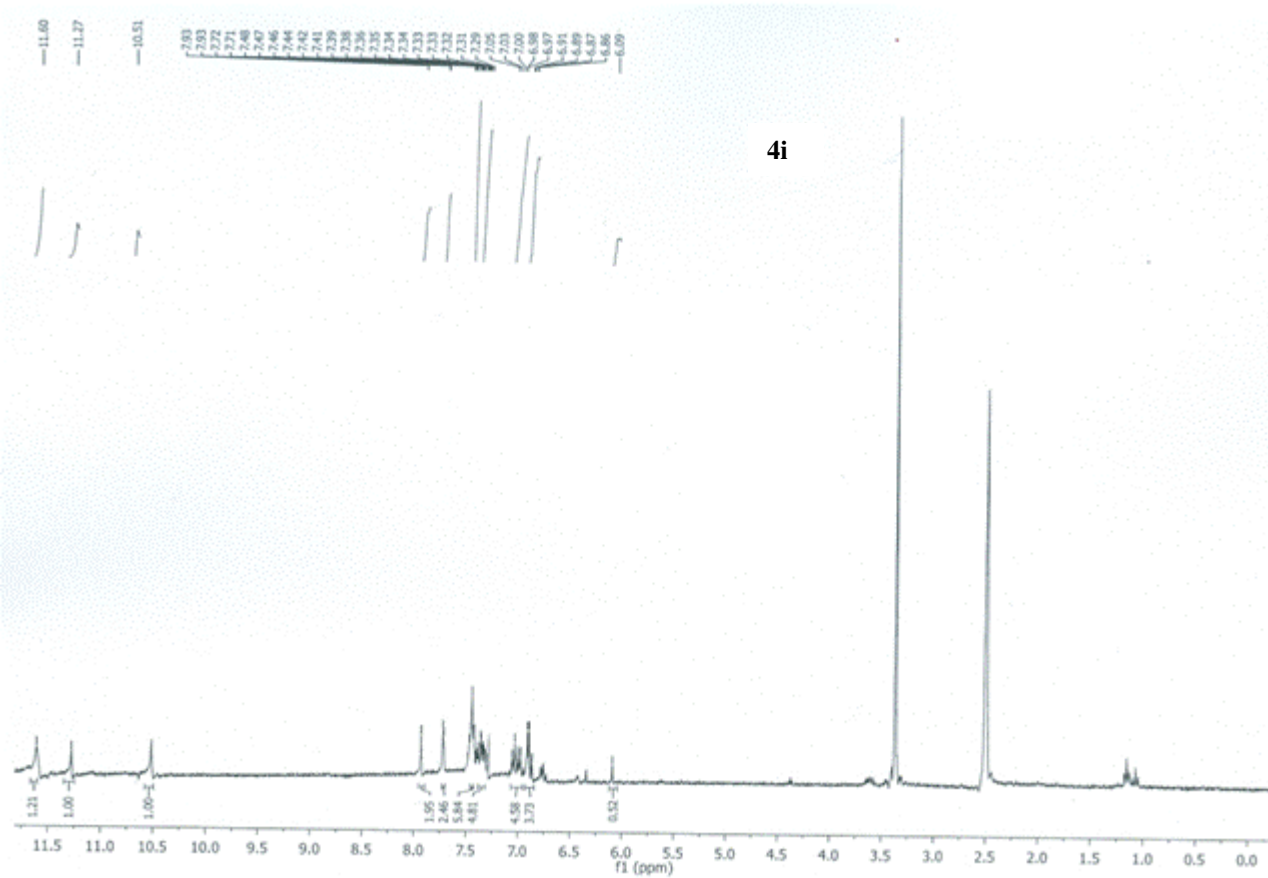


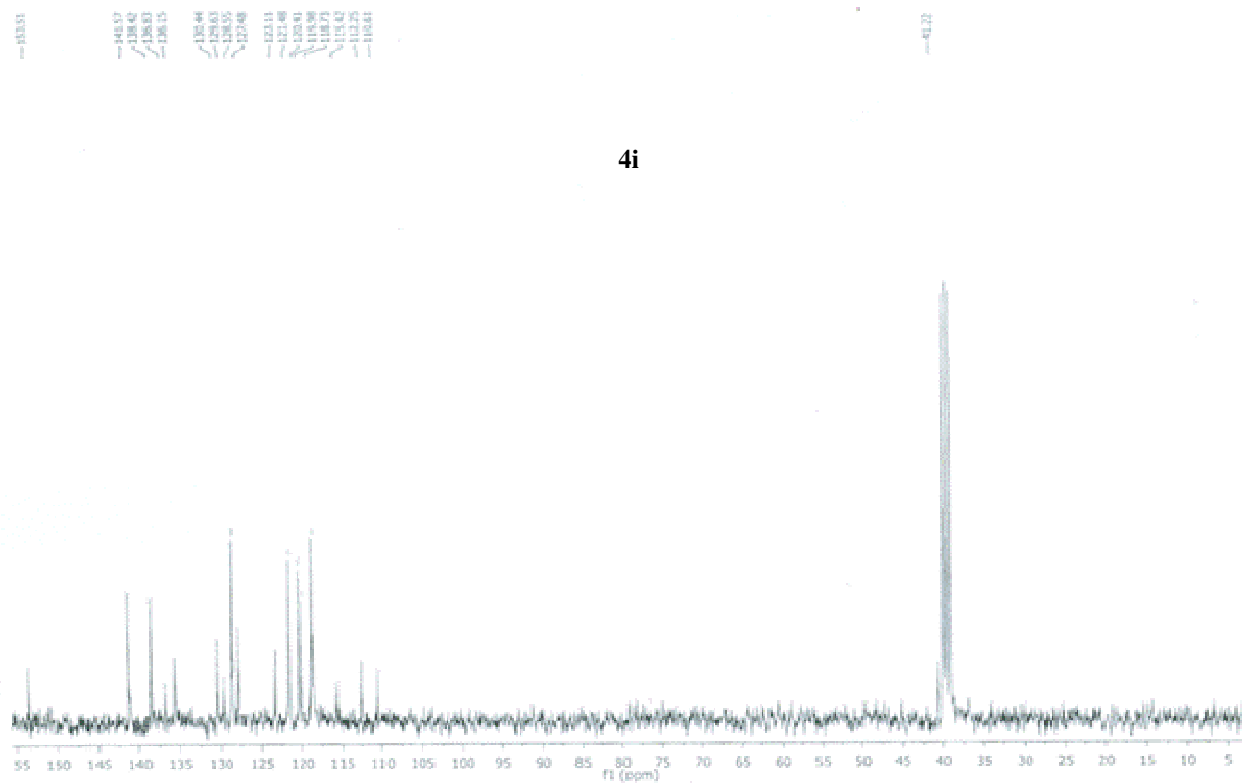
4i
 $C_{30}H_{22}N_4$
M.W. 438

Data: Dr Cecilio Alvarez032 Date: 30-Oct-2015 13:08
Instrument: MStation
Sample: 3565 Indol-bz-o
Note: -
Inlet: Direct Ion Mode: FAB+
RT: 0.47 min Scan#: (4,10)
Elements: C 34/0, H 49/0, N 5/0
Mass Tolerance : 1000ppm, 2mmu if m/z > 2
Unsaturation (U.S.): -0.5 - 34.0

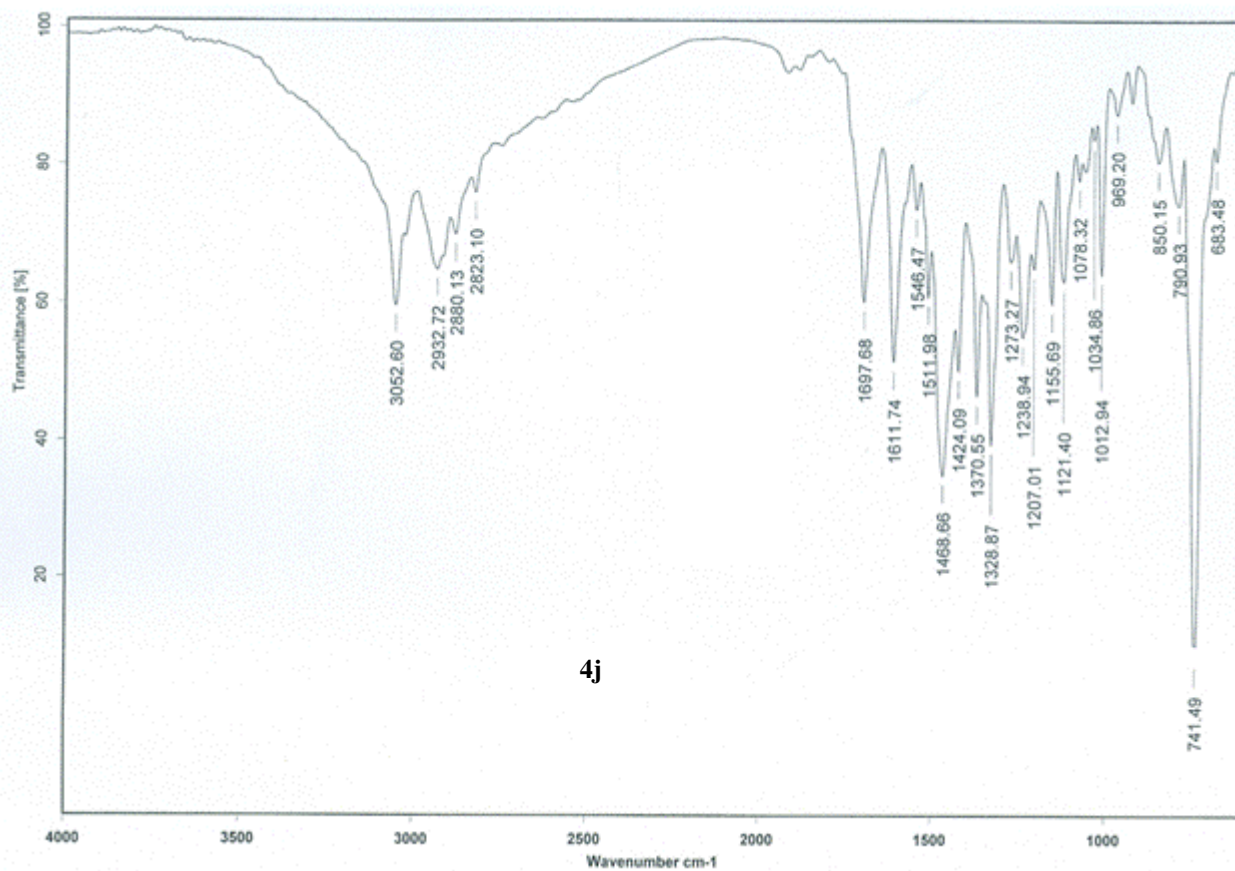
4i
C₃₀H₂₂N₄
M.W. 438

Observed m/z	Int%				
438.1835	2.32				
Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N
1 438.1844	-2.2 / -0.9	22.0	30	22	4



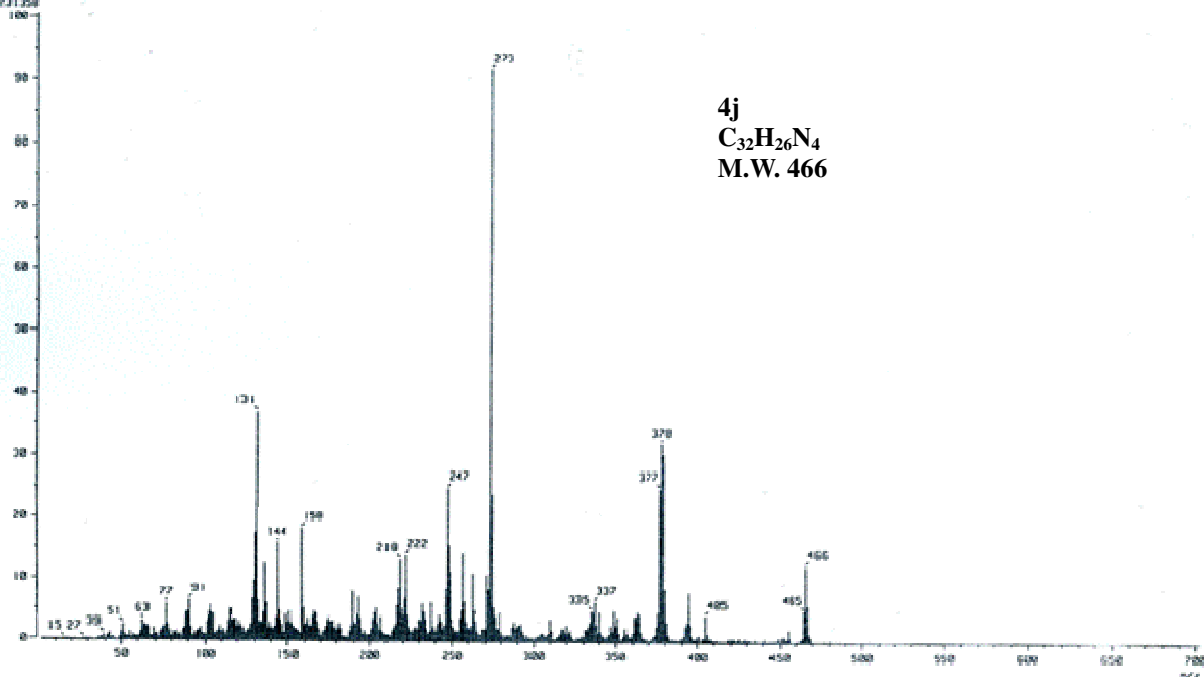


4i



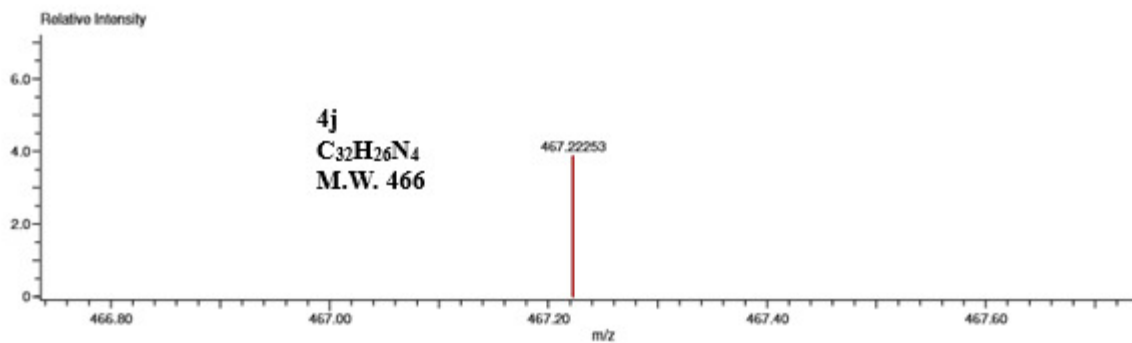
4j

Mass Spectrum 1
 Date: 2/4/May/2012 16:23
 Sample: 1198
 Inlet: Direct
 Spectrum Type: Normal Ion (V⁺-Linear)
 Scan: 410.365
 SP: 370.0000
 Output m/z range: 2.2722 to 702.6706
 Ion Mode: EI+
 Scale: 110.365
 Int.: 211.58
 Cut level: 0.00 A



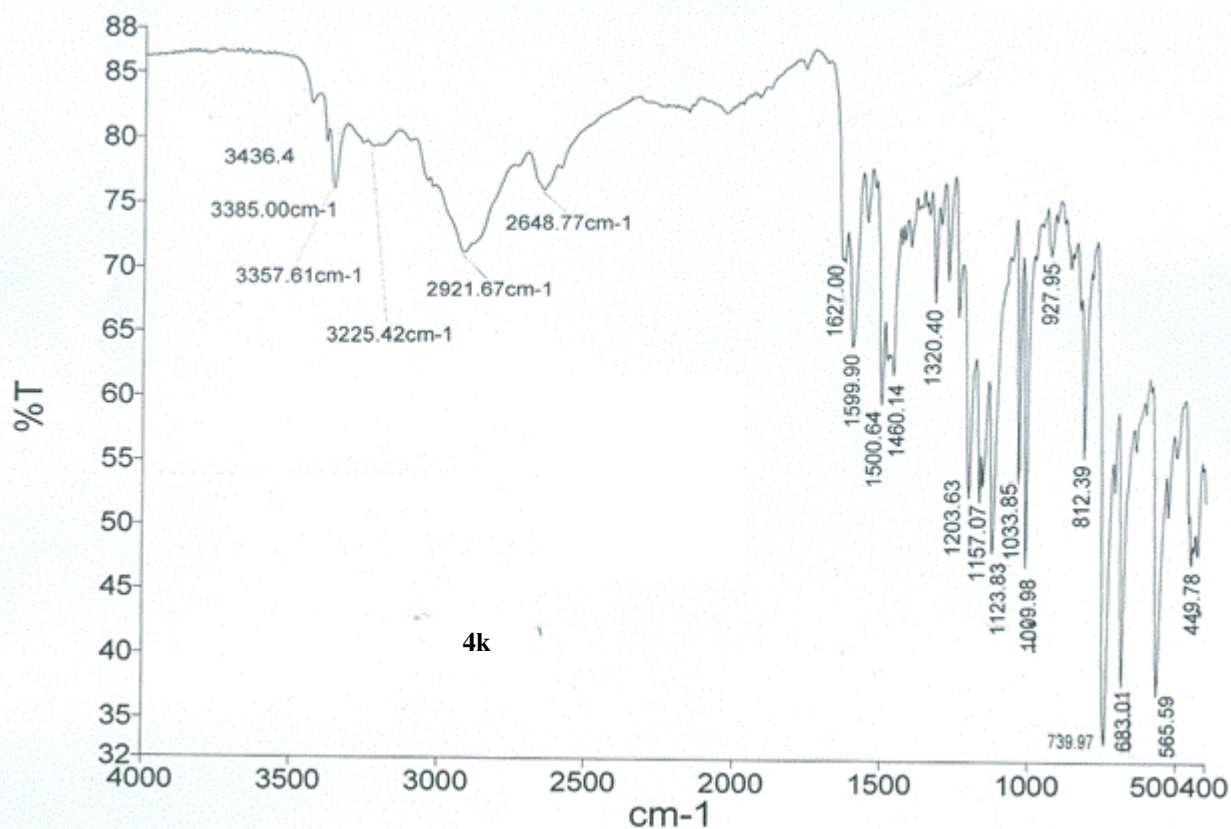
4j
 $C_{32}H_{26}N_4$
 M.W. 466

Data: CAT21
 Sample Name:
 Description:
 Ionization Mode: ESI+
 History: Determine m/z [Peak Detect [Centroid, 30 Area], Correct Base [5.0%]]; Correct Base [5.0%]; Average [MS [1] 0.6...
 Acquired: 4/8/2016 9:01:14 AM
 Operator: AccuTOF
 Mass Calibration data: PEG600
 Created: 4/11/2016 7:18:32 PM
 Created by: AccuTOF
 Charge number: 1
 Tolerance: 3.00 (mmu)
 Element: ¹²C: 0 .. 100, ¹H: 0 .. 100, ¹⁴N: 2 .. 5
 Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

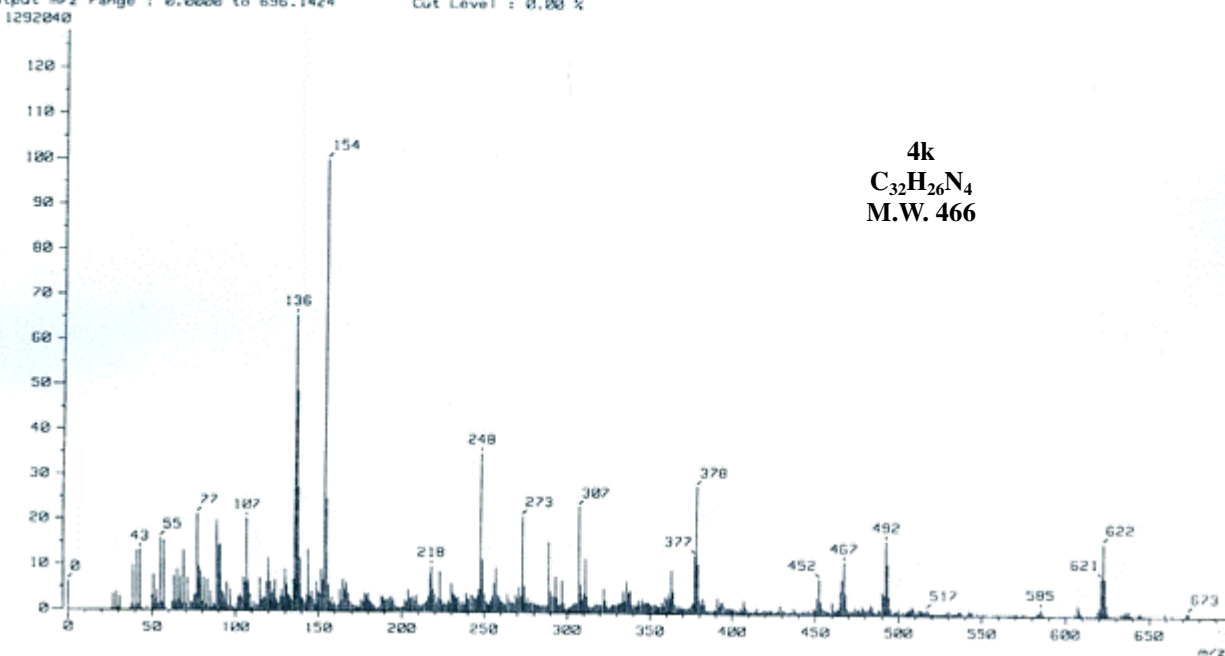


4j
 $C_{32}H_{26}N_4$
 M.W. 466

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22253	3657.25	467.22357	-1.05	-2.24	$^{12}C_{32}H_{26}^{14}N_4$	21.5



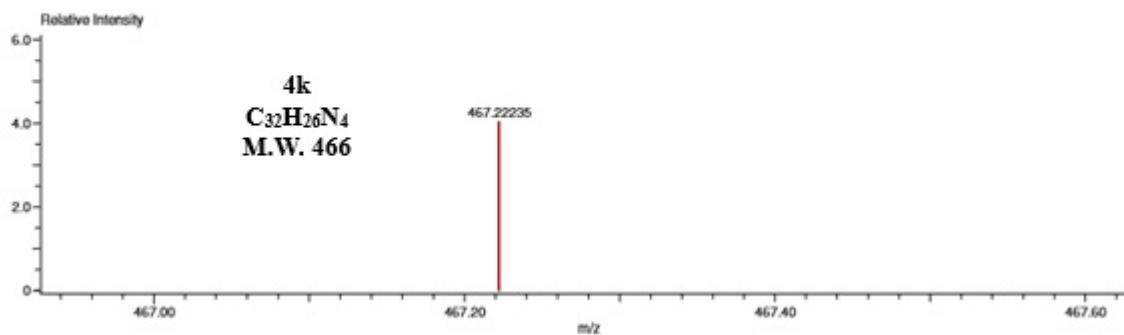
[Mass Spectrum]
 Date : 15-Oct-2012 12:29
 Sample: 2528
 Note : Luis-Velasco
 Inlet : Direct
 Ion Mode : FID+
 Spectrum Type : Normal Ion (MF-Linear)
 RT : 1.55 min Scan# : (2,10)
 BP : m/z 154.0000 Int. : 96.31
 Output m/z range : 0.0000 to 696.1424 Cut Level : 0.00 %



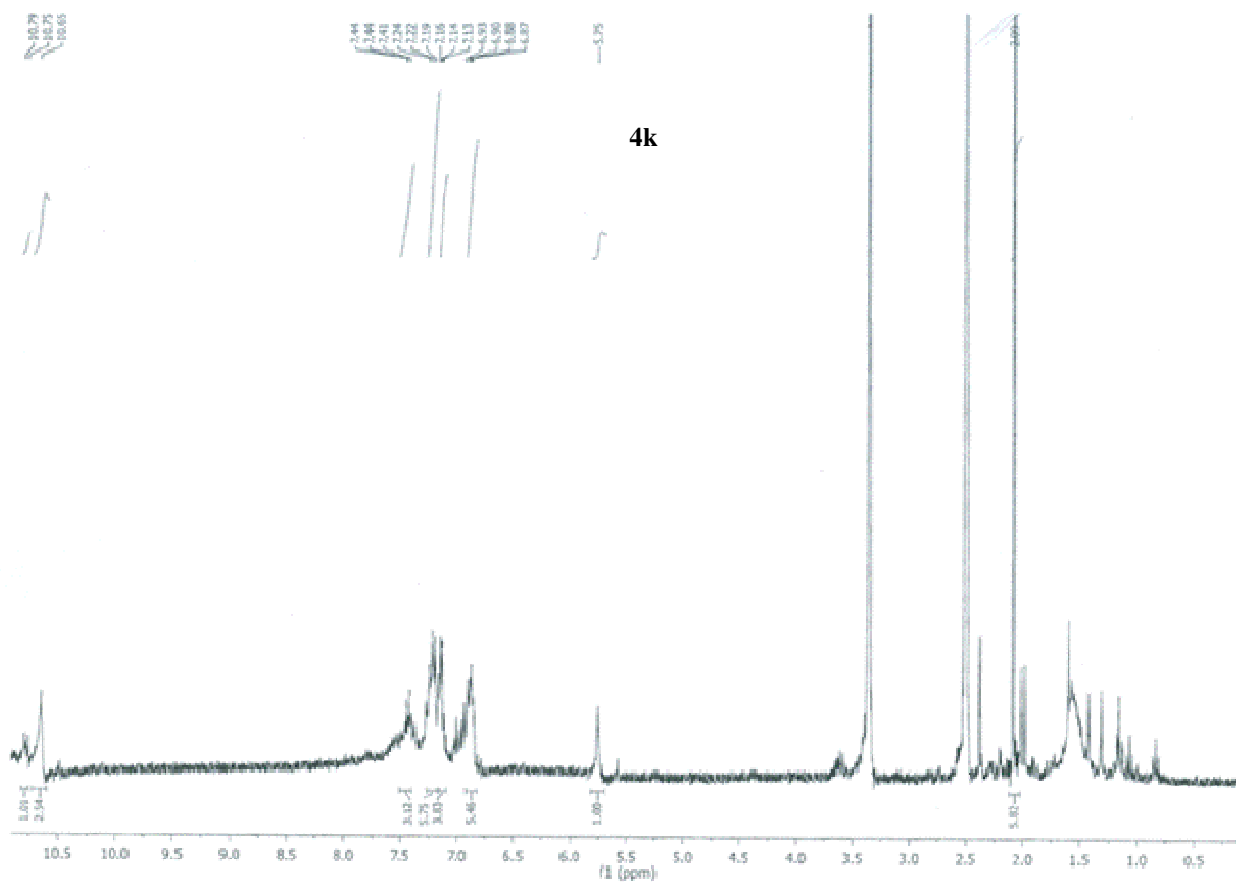
Data:CAT23
 Sample Name:
 Description:
 Ionization Mode:ESI+
 History:Dotormine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%];Average[MS[1] 0.2...

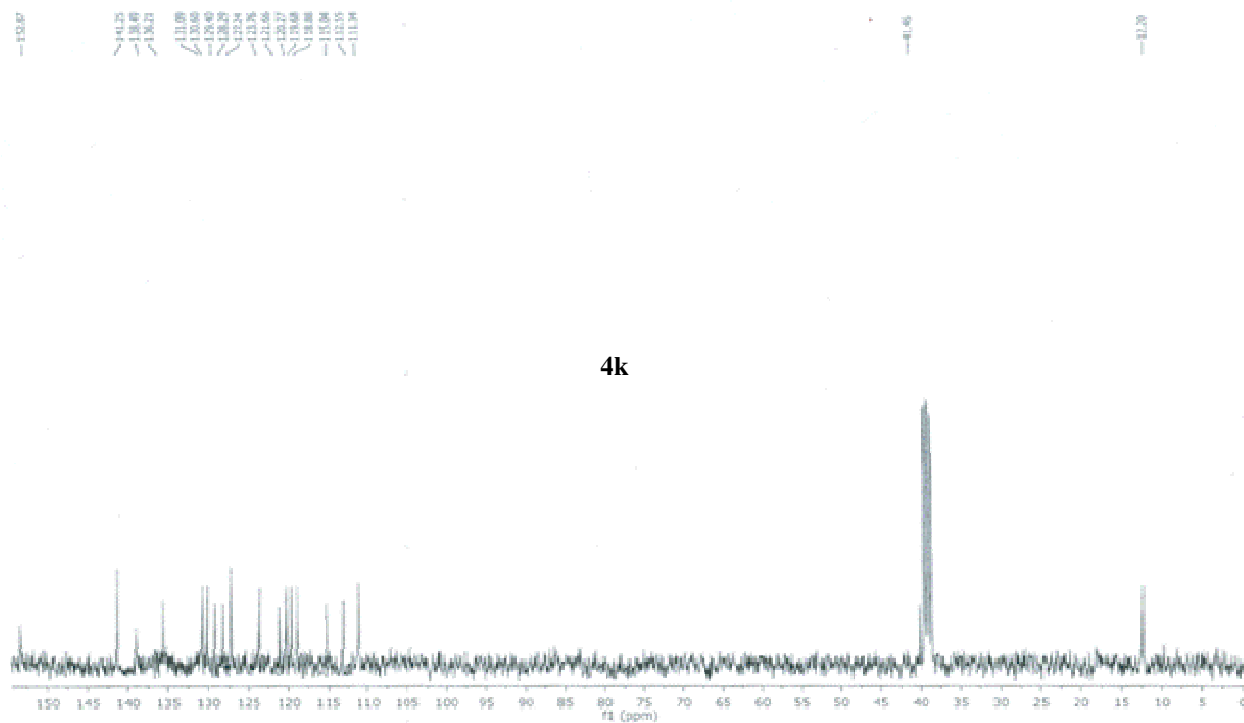
Acquired:4/8/2016 9:06:52 AM
 Operator:AccuTOF
 Mass Calibration data:PEG600
 Created:4/11/2016 7:35:34 PM
 Created by:AccuTOF

Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:0.0 .. 32.0 (Fraction:Both)
 Element:¹³C:0 .. 100, ¹H:0 .. 100, ¹⁴N:2 .. 5

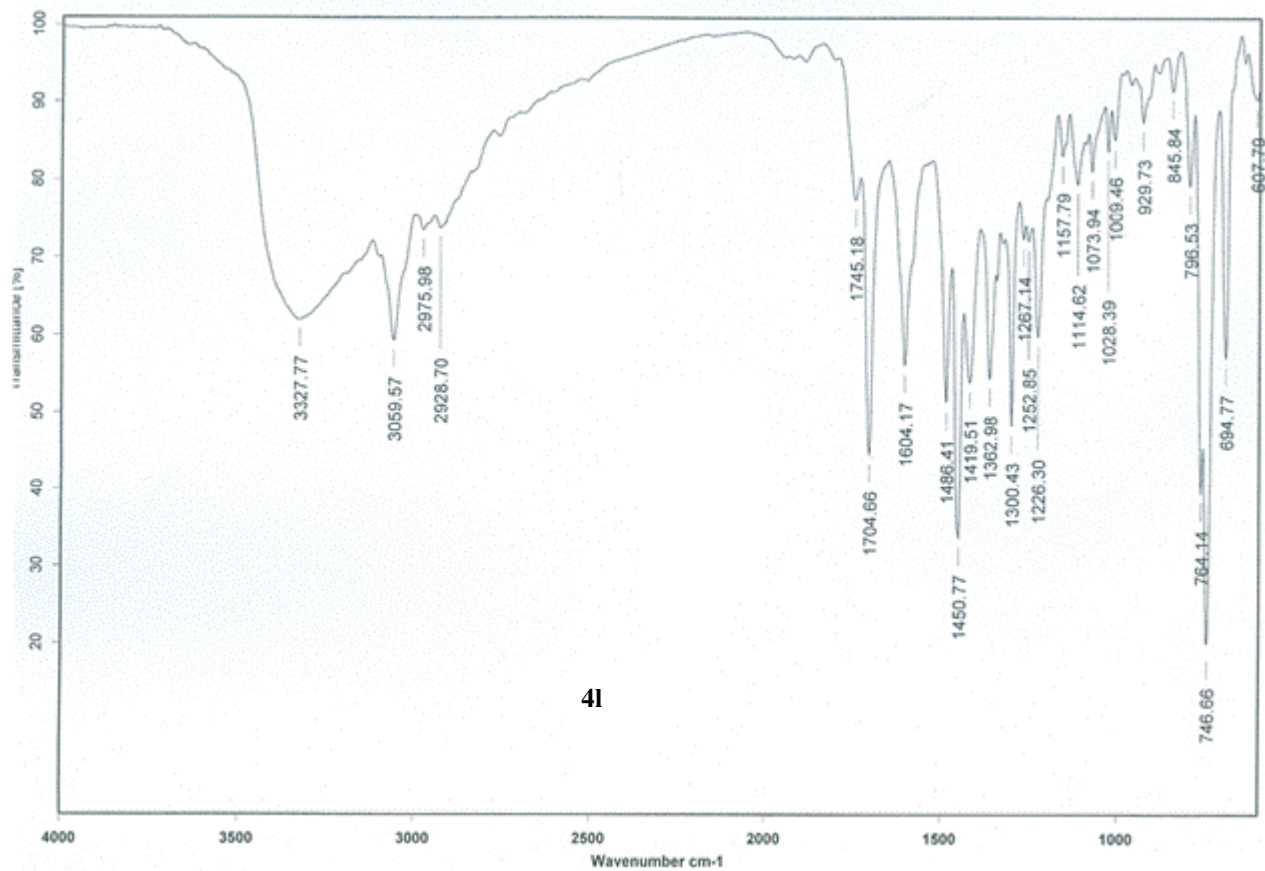


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22235	2357.78	467.22357	-1.22	-2.62	¹³ C ₃₂ ¹ H ₂₇ ¹⁴ N ₄	21.5



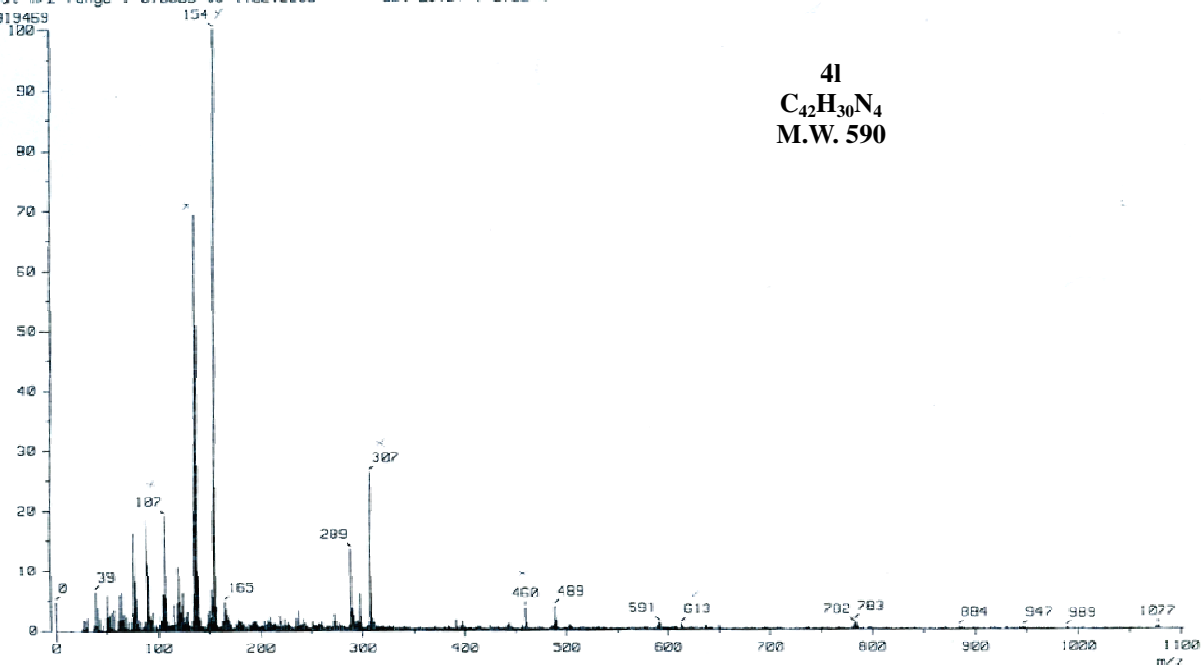


4k



4l

[Mass Spectrum]
 Data : Dr-Cecilio-Rivera2033 Date : 13-Feb-2013 18:22
 Sample: 390 GG
 Note : Luis-Velasco
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 1.55 min Scan# : (3,9)
 BP : m/z 154.0000 Int. : 373.79
 Output m/z range : 0.2000 to 1102.2255 Cut Level : 0.00 %



41
 $C_{42}H_{30}N_4$
 M.W. 590

Anal calcd. C 85.40 H 5.12 N 9.48

Clave de la muestra	Peso [mg]	N [%]	C [%]	H [%]	S [%]	Fecha de análisis
bz2ph o	2.412	9.37	85.40	4.99	---	27-04-2016

Found

41
 $C_{42}H_{30}N_4$
 M.W. 590

