

## Supplementary Material

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

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<sup>a</sup>*Sección de Química Orgánica, Facultad de Estudios Superiores Cuautitlán-Universidad Nacional Autónoma de México, Campo 1, Avenida 1 de mayo s/n, Colonia Santa María Guadalupe Las Torres, Cuautitlán Izcalli, Estado de México, C.P. 54740, México.*

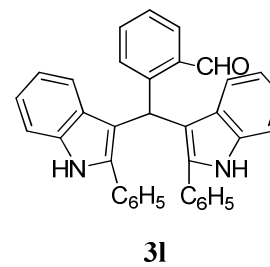
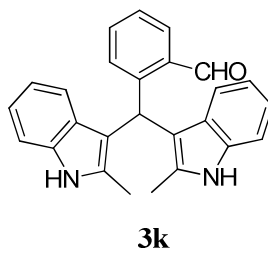
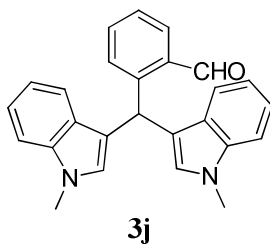
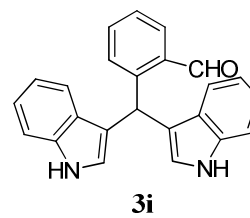
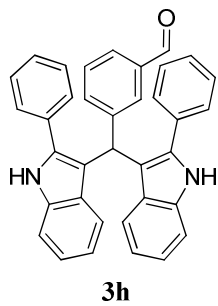
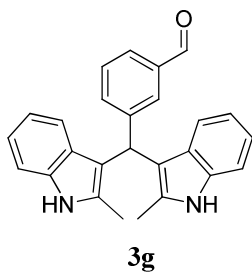
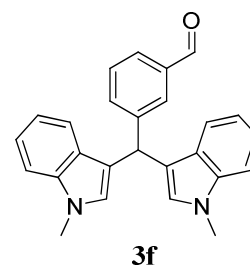
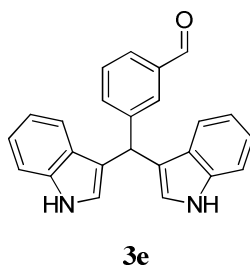
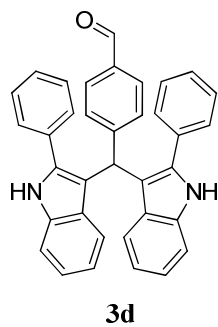
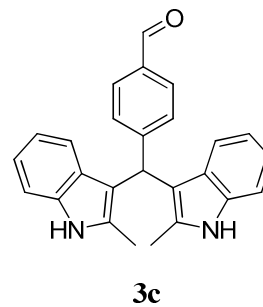
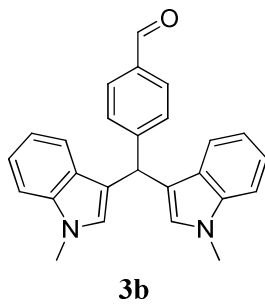
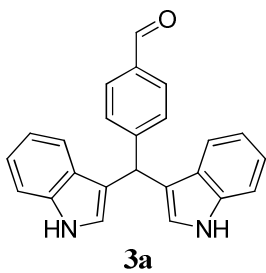
<sup>b</sup>*Instituto de Química-Universidad Nacional Autónoma de México, Ciudad Universitaria, Circuito Exterior, México D.F., C.P. 04510.*

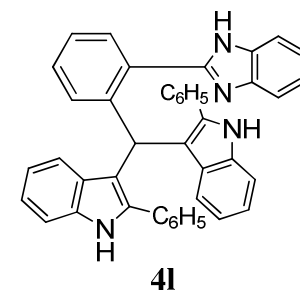
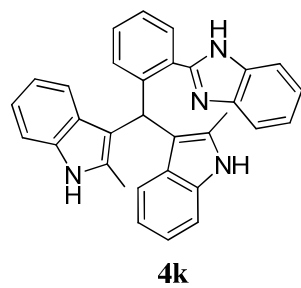
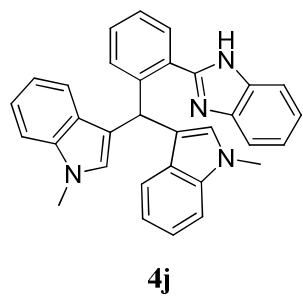
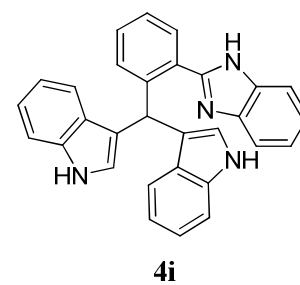
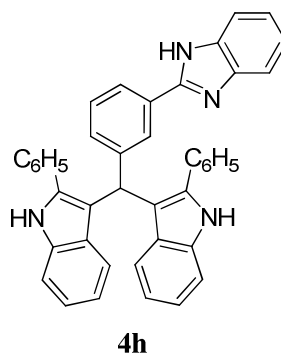
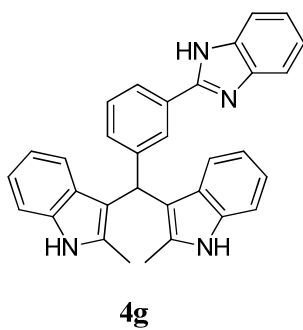
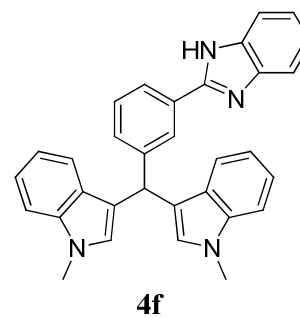
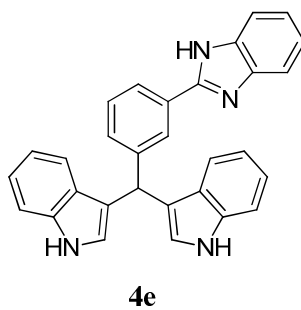
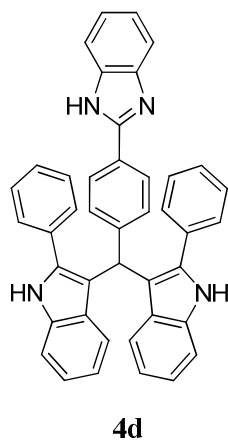
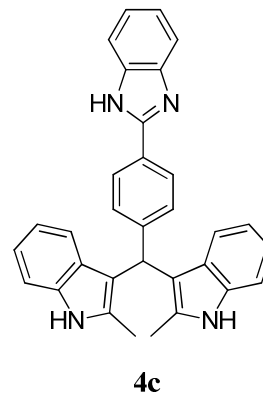
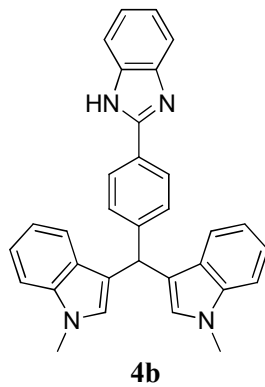
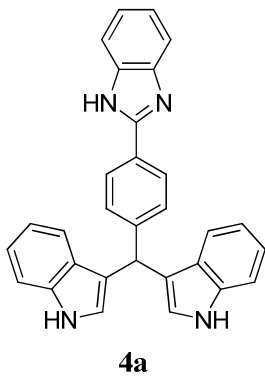
<sup>c</sup>*Departamento de Alimentos y Biotecnología, Facultad de Química, Edificio E, UNAM, Av. Universidad 3000, C.U., Coyoacán, México, D.F., 04510, México.*

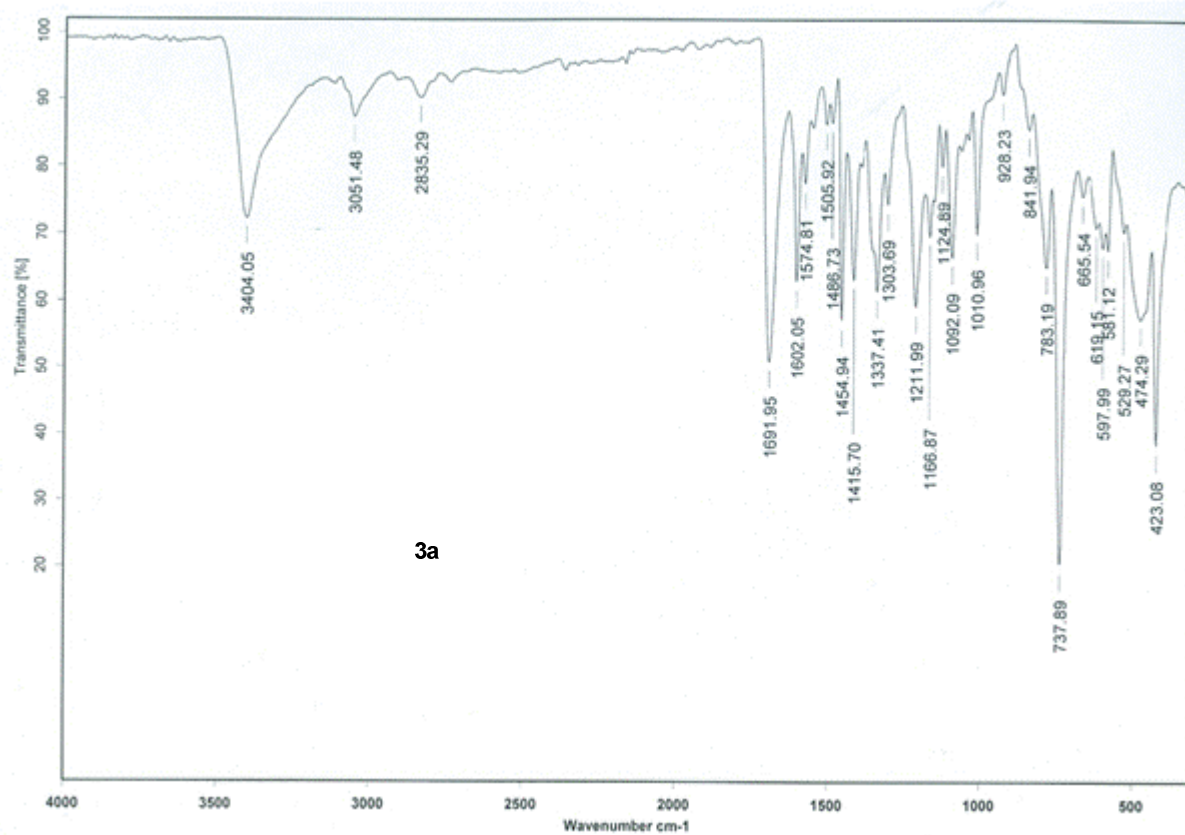
*E-mail: [penieres@unam.mx](mailto:penieres@unam.mx)*

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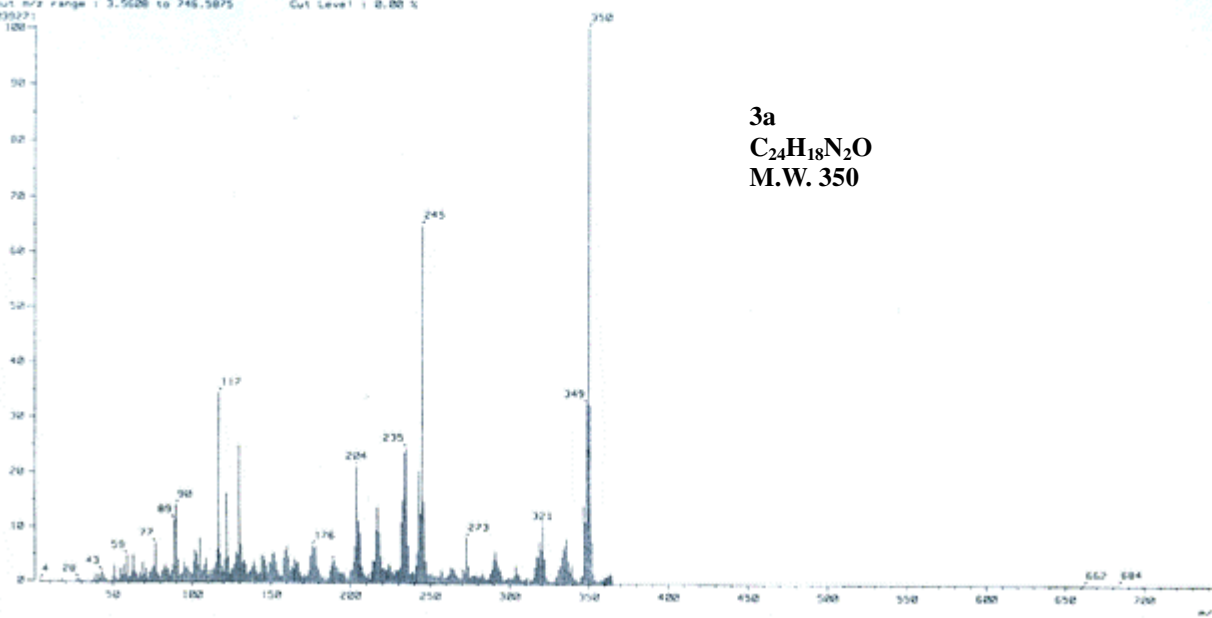
Structure of synthesized compounds	S2
IR, MS, <sup>1</sup> H NMR, <sup>13</sup> C NMR Spectra	S4





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

[ Mass Spectrum ]  
Data : D:\Users\jose-05\ Date : 24-May-2012 17:03  
Sample: 1212 IC11 Ion: FID2500  
Note : Javier Perez  
Inlet : Direct Ion Mode : EI+  
Spectrum Type : Normal Ion [M<sup>+</sup>-Linear]  
RT : 1.99 min Scan : 110,823  
BP : m/z 350.0000 Int. : 98.83  
Output m/z range : 3.5608 to 746.5875 Cut Level : 0.00 %  
103927:



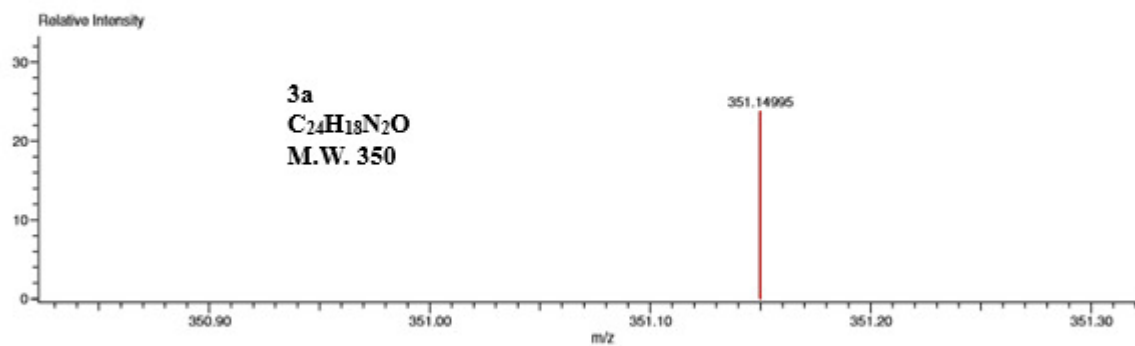
3a  
 $\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}$   
M.W. 350

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...

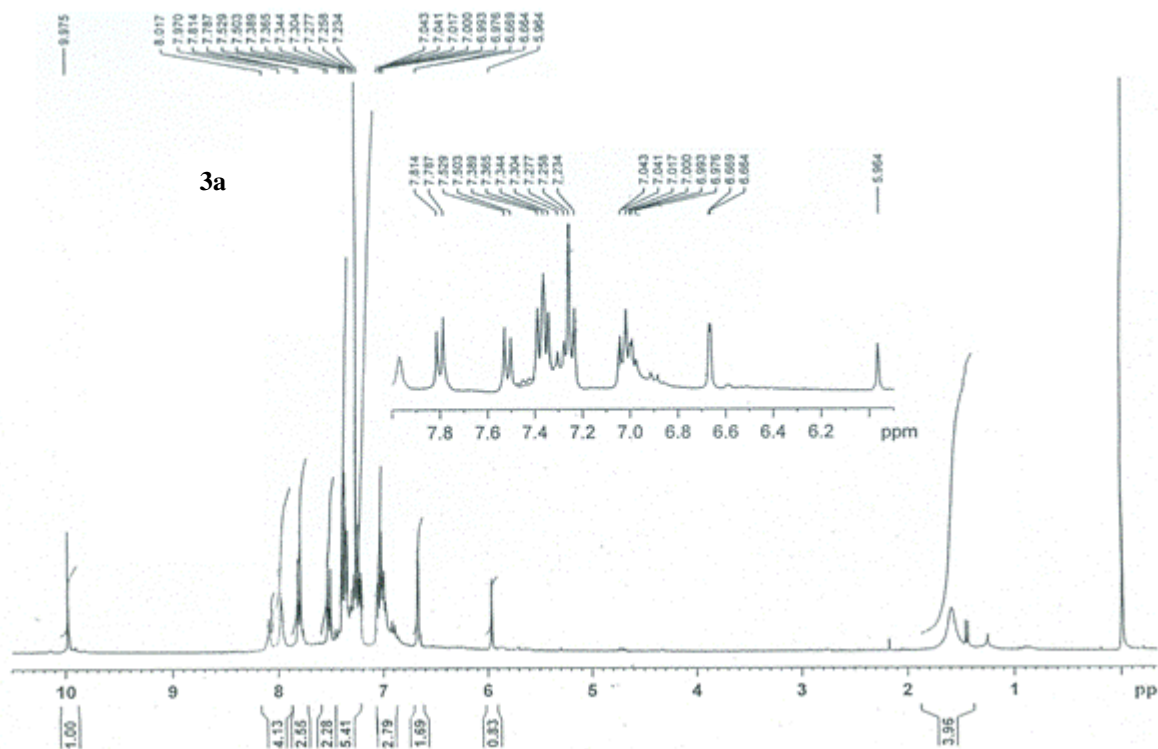
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 Operator:AccuTOF  
 Mass Calibration data:Cal\_Peg\_600  
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 Created by:AccuTOF

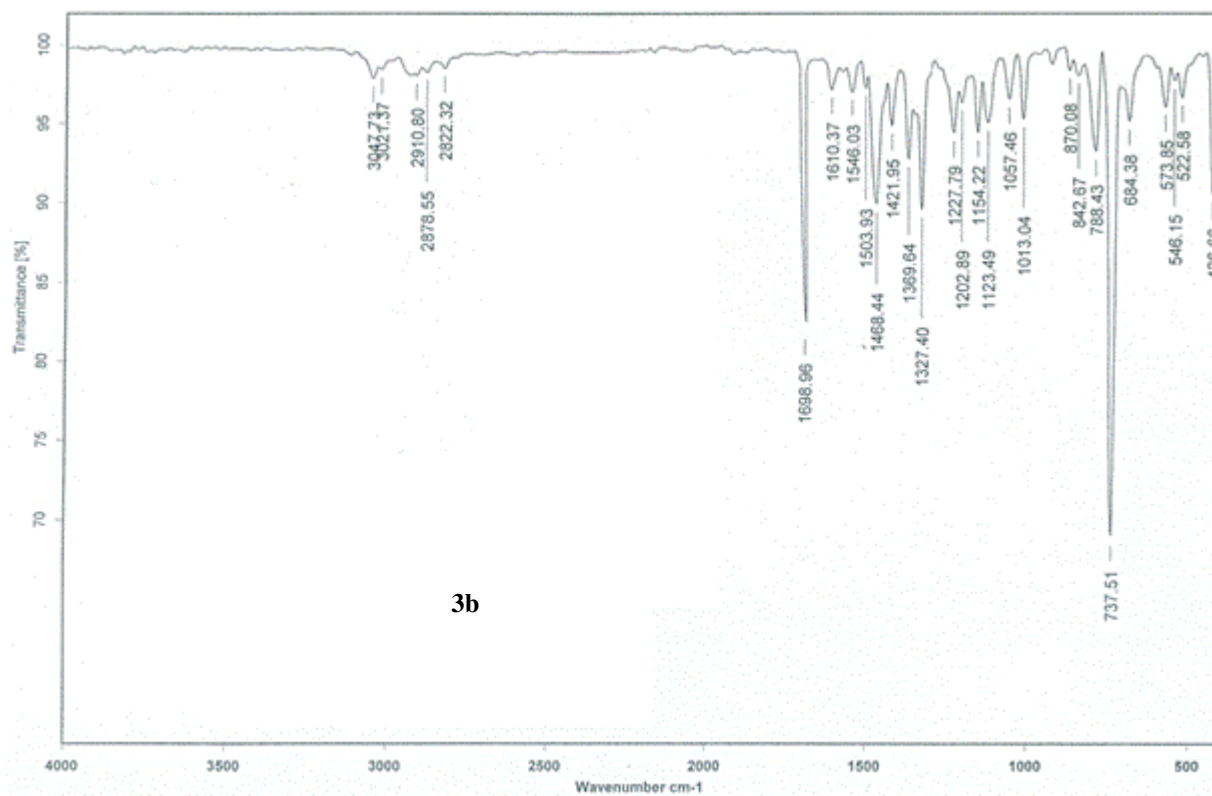
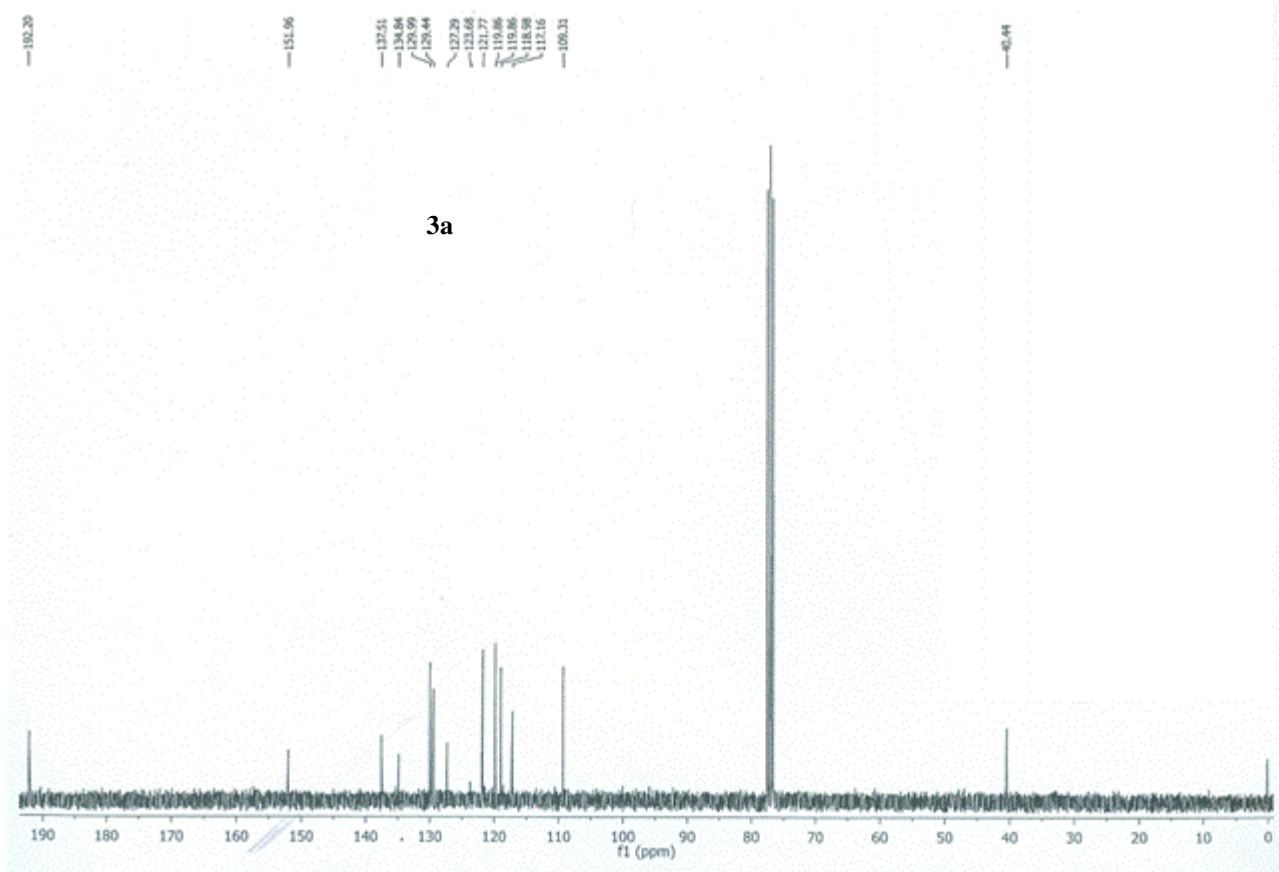
Charge number:1  
 Element:<sup>12</sup>C:0 .. 56, <sup>1</sup>H:0 .. 120, <sup>14</sup>N:0 .. 2, <sup>16</sup>O:0 .. 1  
 Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

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

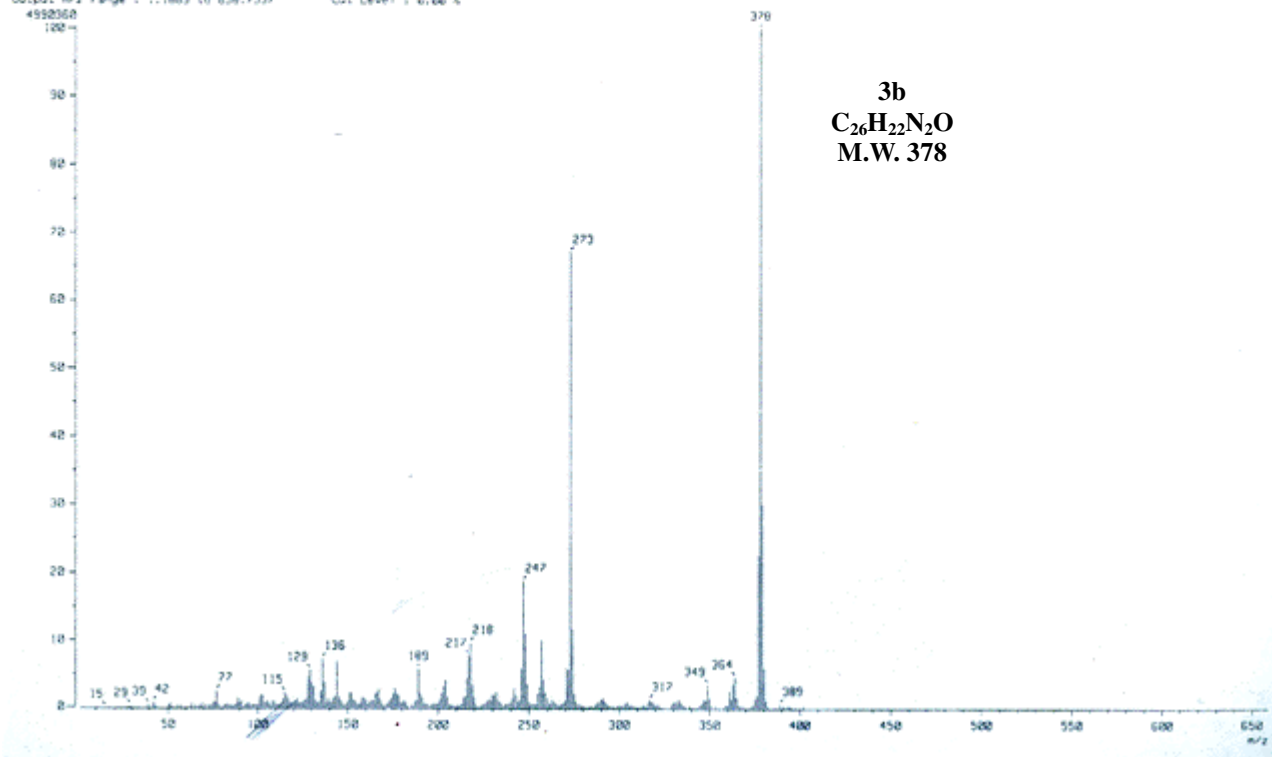


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14995	11159.75	351.14974	0.21	0.61	$^{12}C_{24}^{1}H_{18}^{14}N_2^{16}O_1$	16.5





[ Mass Spectrum ]  
 Date : Dr-Lopez-Jose-055 Date : 24-May-2012 17:32  
 Sample: 1222 IET1 Jeol RXS254R  
 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

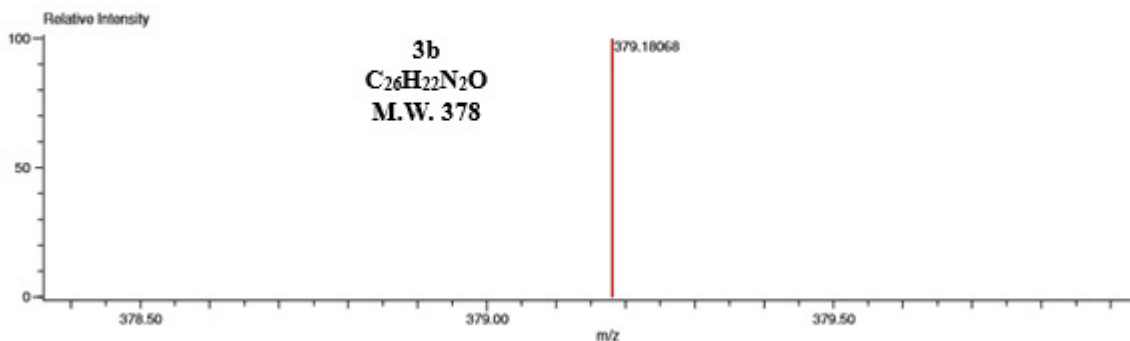
Data:2579 1-Me-p  
 Sample Name:Dr Alvarez Cocilio Operator: Carmen Garcia/ Javier Perez  
 Description:  
 Ionization Mode:ESI-  
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.7...

Acquired:9/3/2015 1:05:14 PM  
 Operator:AccuTOF  
 Mass Calibration data:Cal\_Peg\_600  
 Created:9/3/2015 3:16:29 PM  
 Created by:AccuTOF

Charge number:1  
 Element:<sup>12</sup>C:0 .. 56, <sup>1</sup>H:0 .. 120, <sup>14</sup>N:0 .. 2, <sup>16</sup>O:0 .. 1

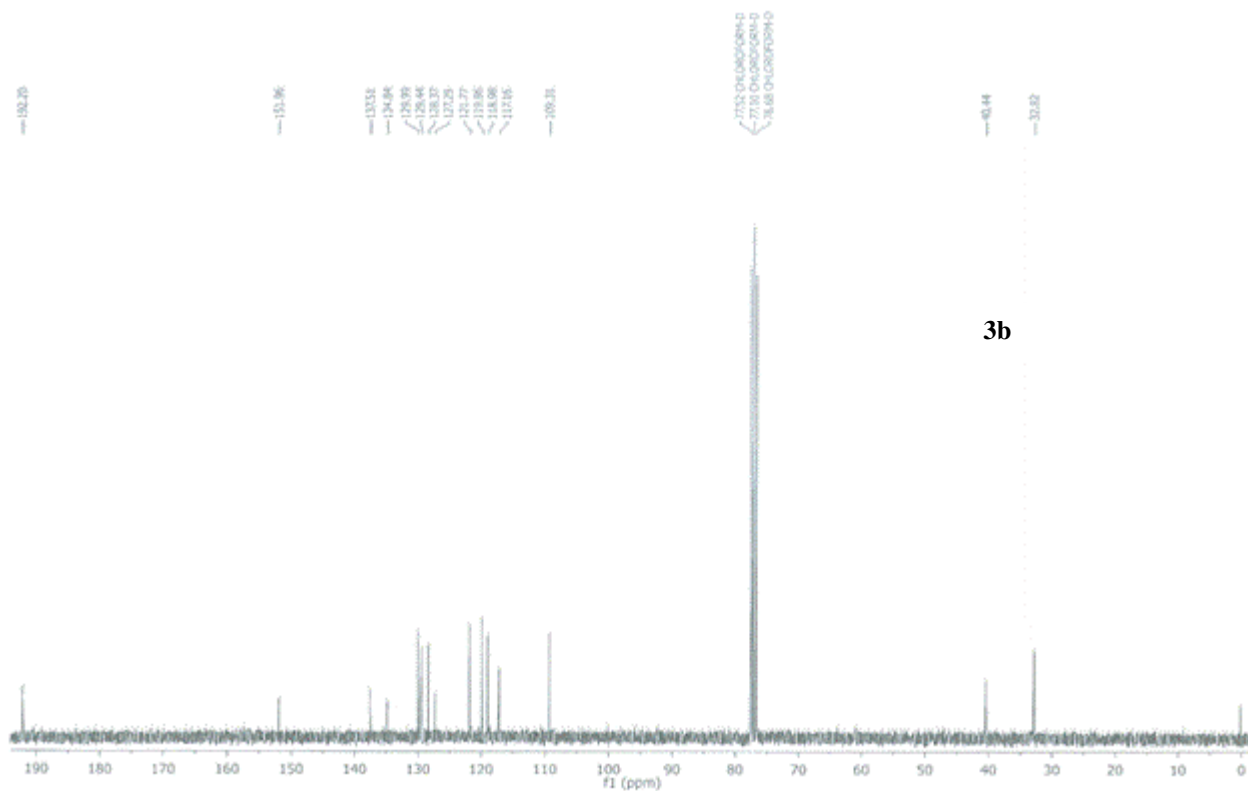
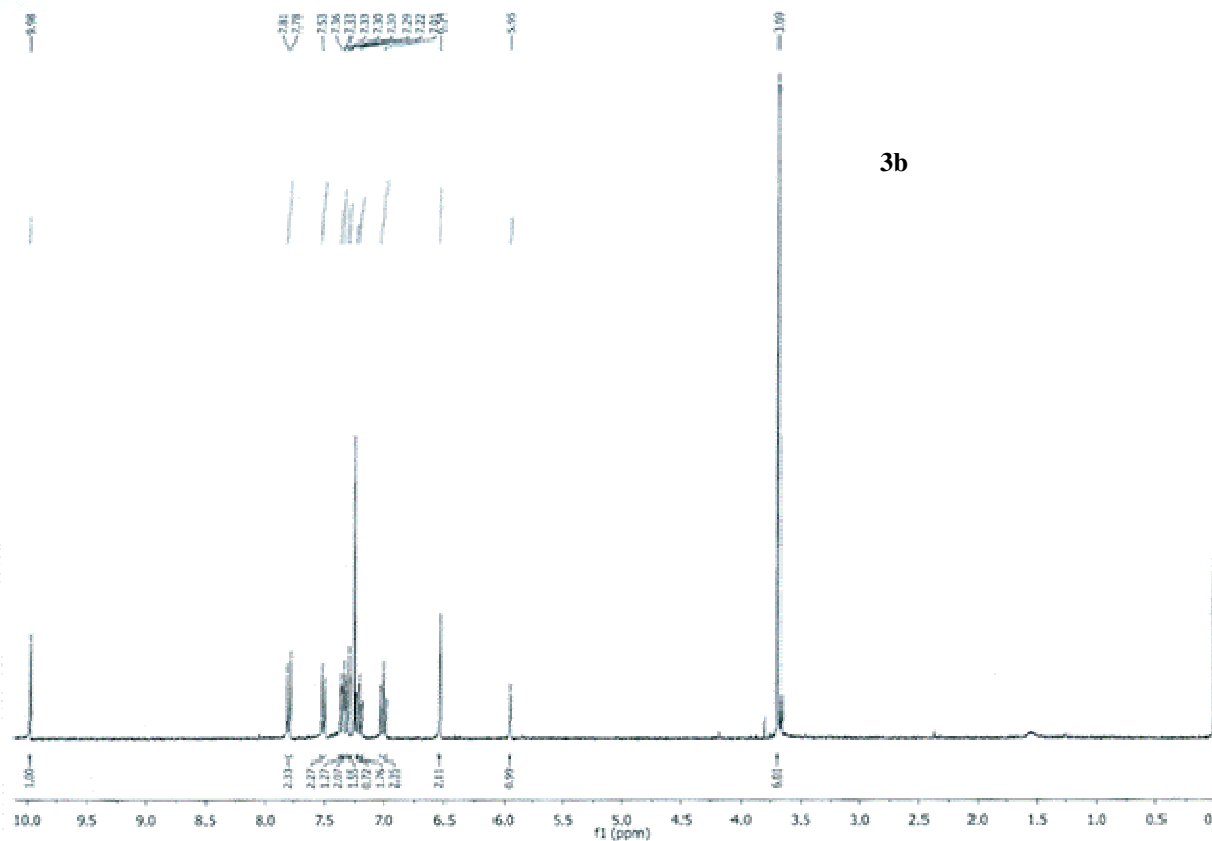
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

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

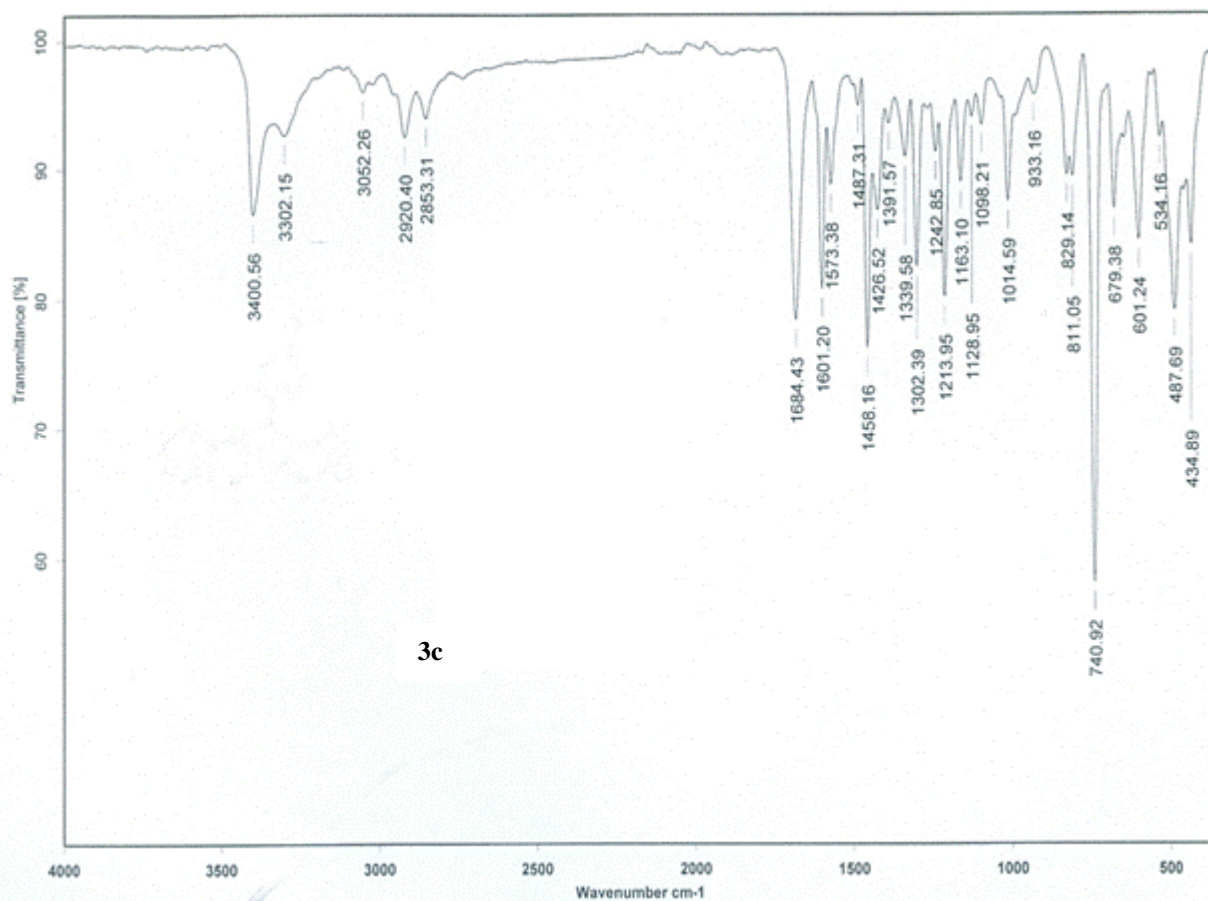


**3b**  
 $C_{26}H_{22}N_2O$   
 M.W. 378

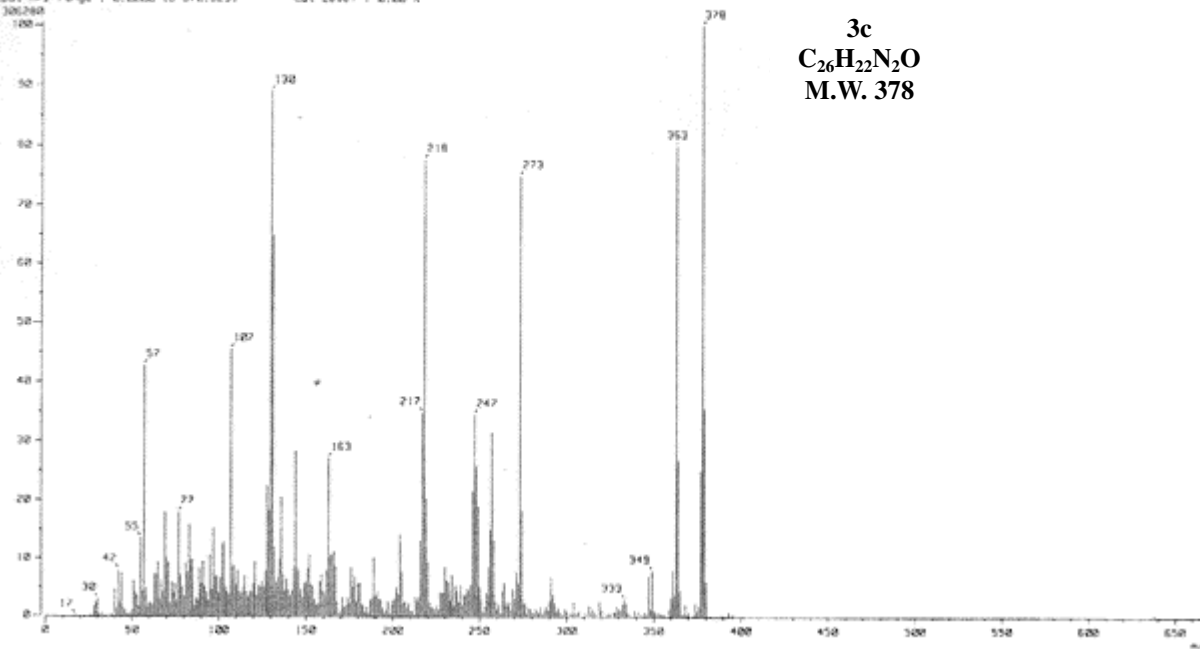
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18068	13748.00	379.18104	-0.36	-0.95	<sup>12</sup> C <sub>26</sub> <sup>1</sup> H <sub>22</sub> <sup>14</sup> N <sub>2</sub> <sup>16</sup> O <sub>1</sub>	16.5







[ Mass Spectrum ]  
 Date : 17-Apr-2012 19:25  
 Sample: 502 IC19 Jeol RMU200M  
 Note : Javier Perez  
 Inlet : Direct Ion Mode : E1+  
 Spectrum Type : Normal Ion (M-Linear)  
 RT : 1.43 min Scan# : 133,55  
 BP : m/z 378.0000 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...

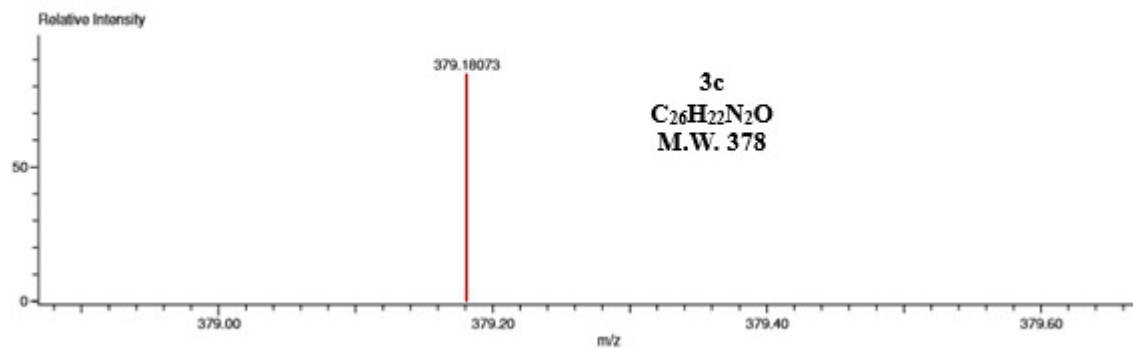
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 Mass Calibration data:Cal\_Pag\_600  
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 Created by:AccuTOF

Charge number:1

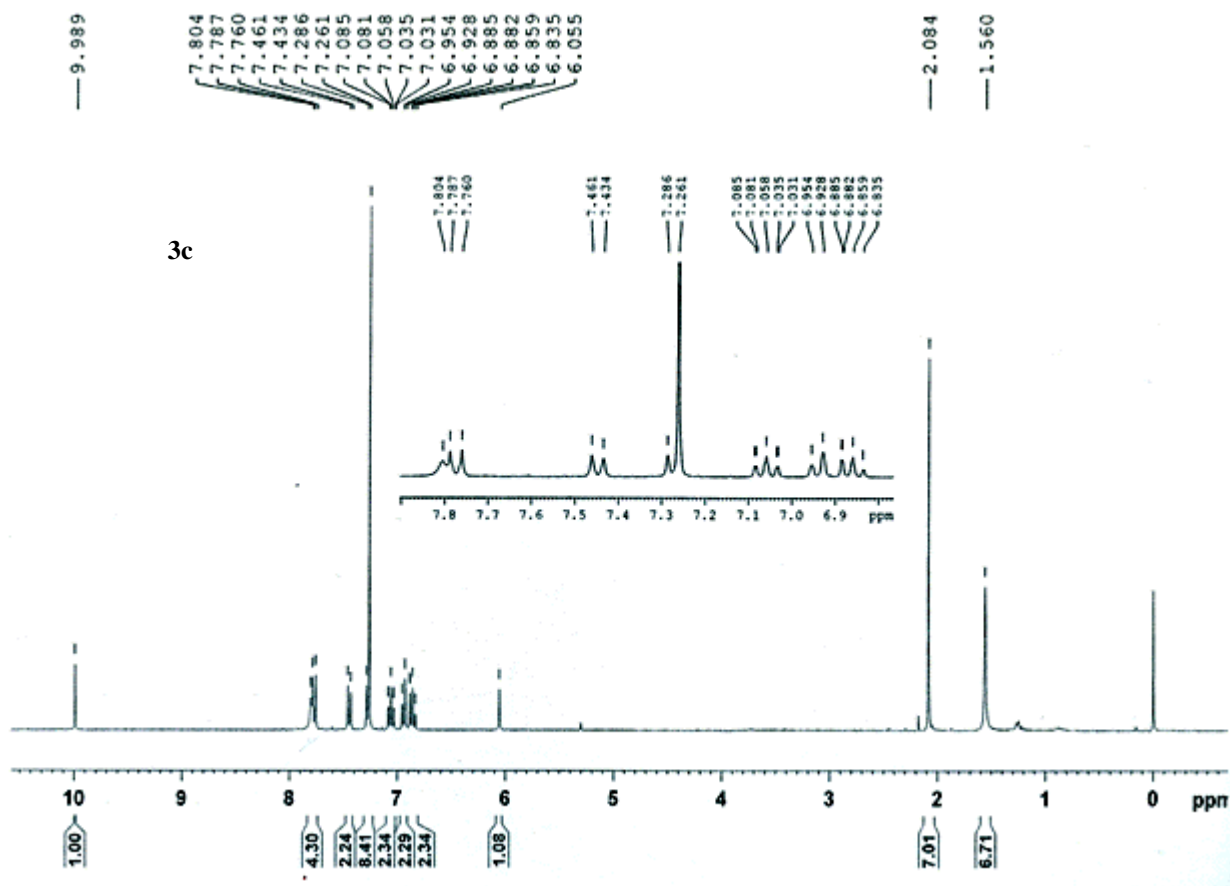
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

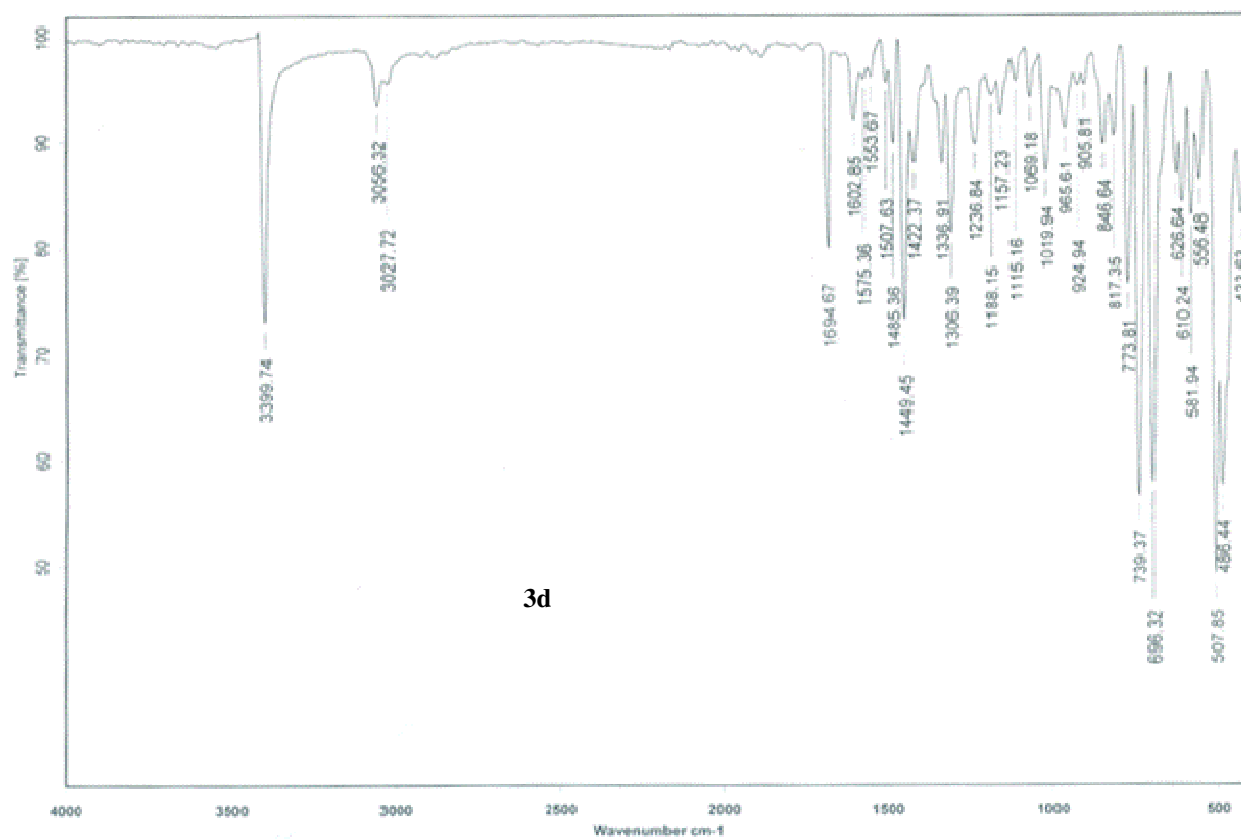
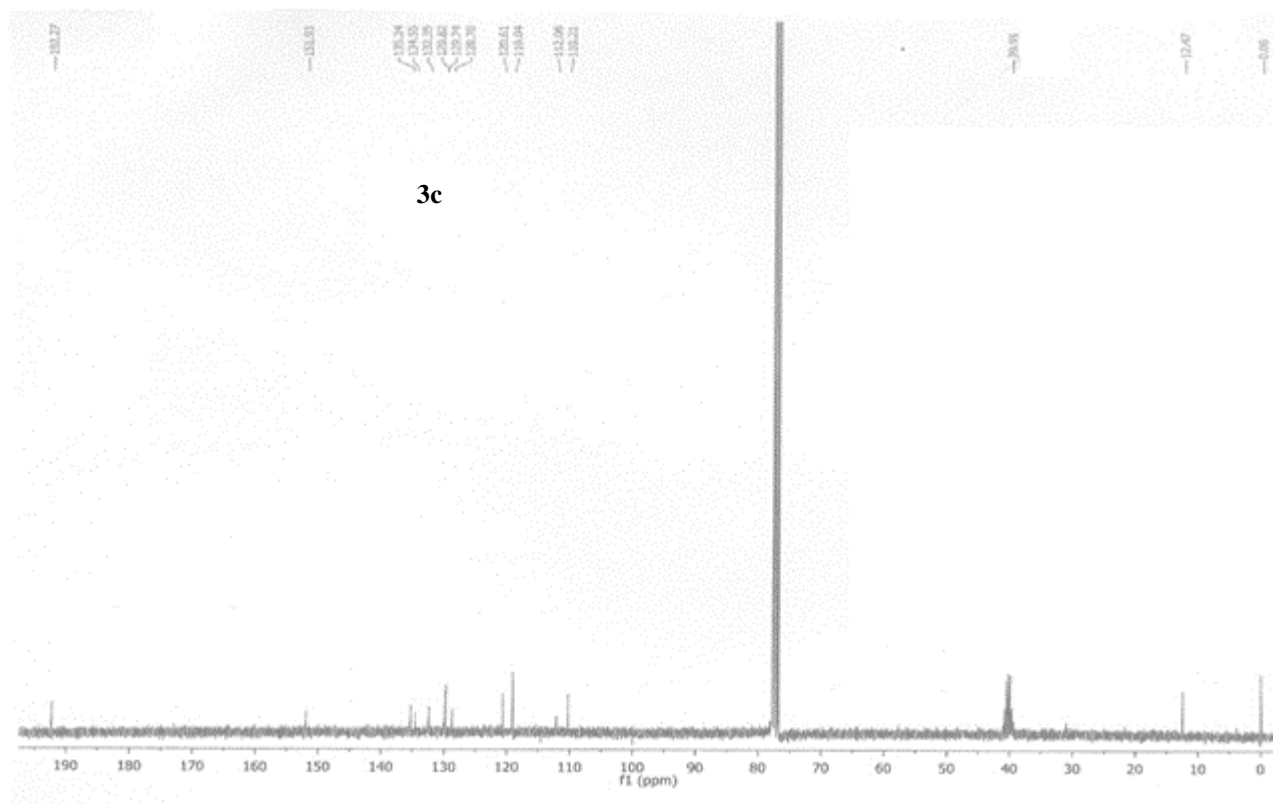
Unsaturation Number:0.0 .. 30.0 (Fraction:Both)

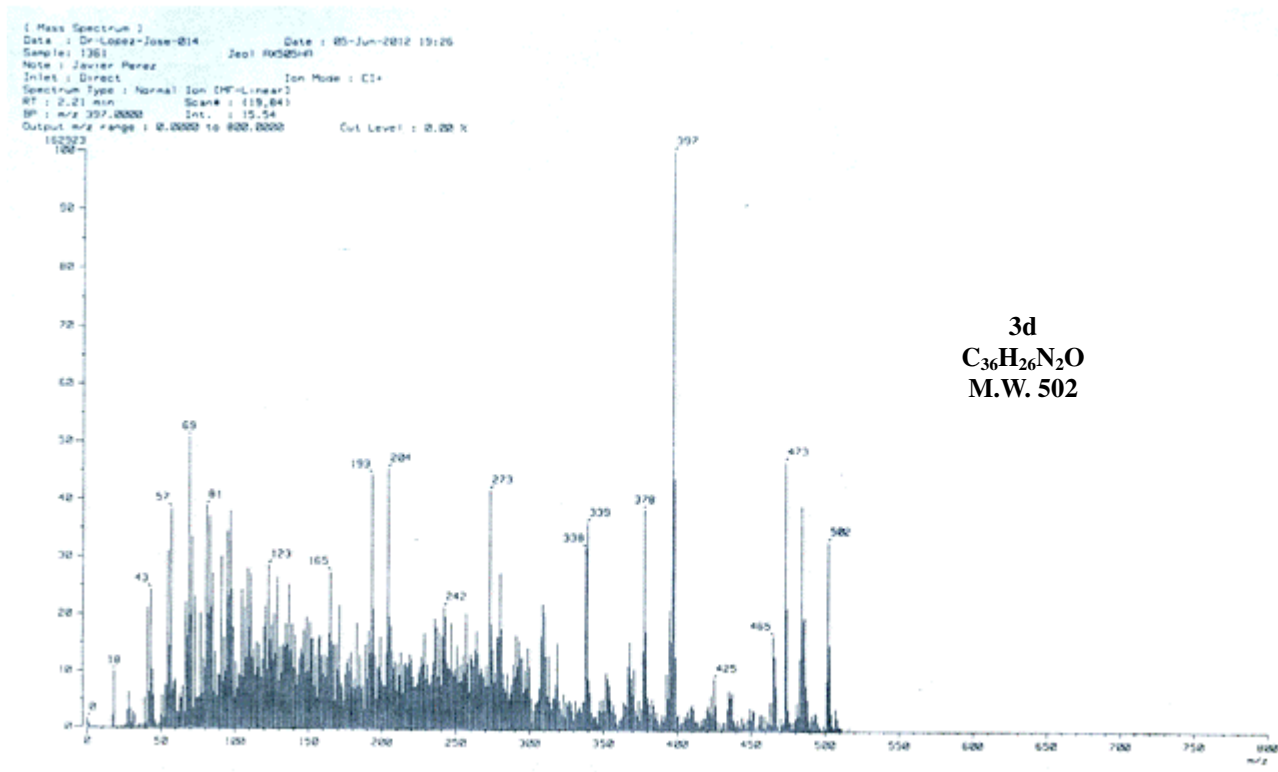
Element:<sup>12</sup>C:0 .. 56, <sup>1</sup>H:0 .. 120, <sup>14</sup>N:0 .. 2, <sup>16</sup>O:0 .. 1



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



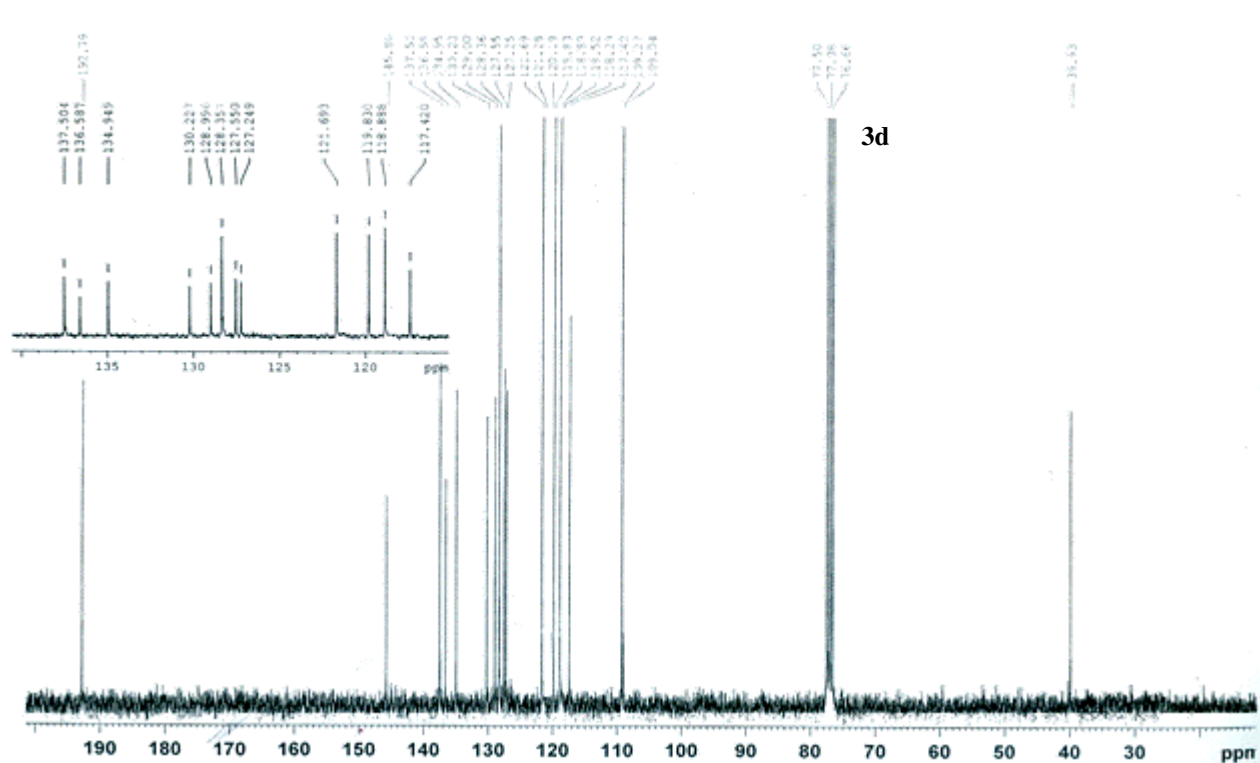
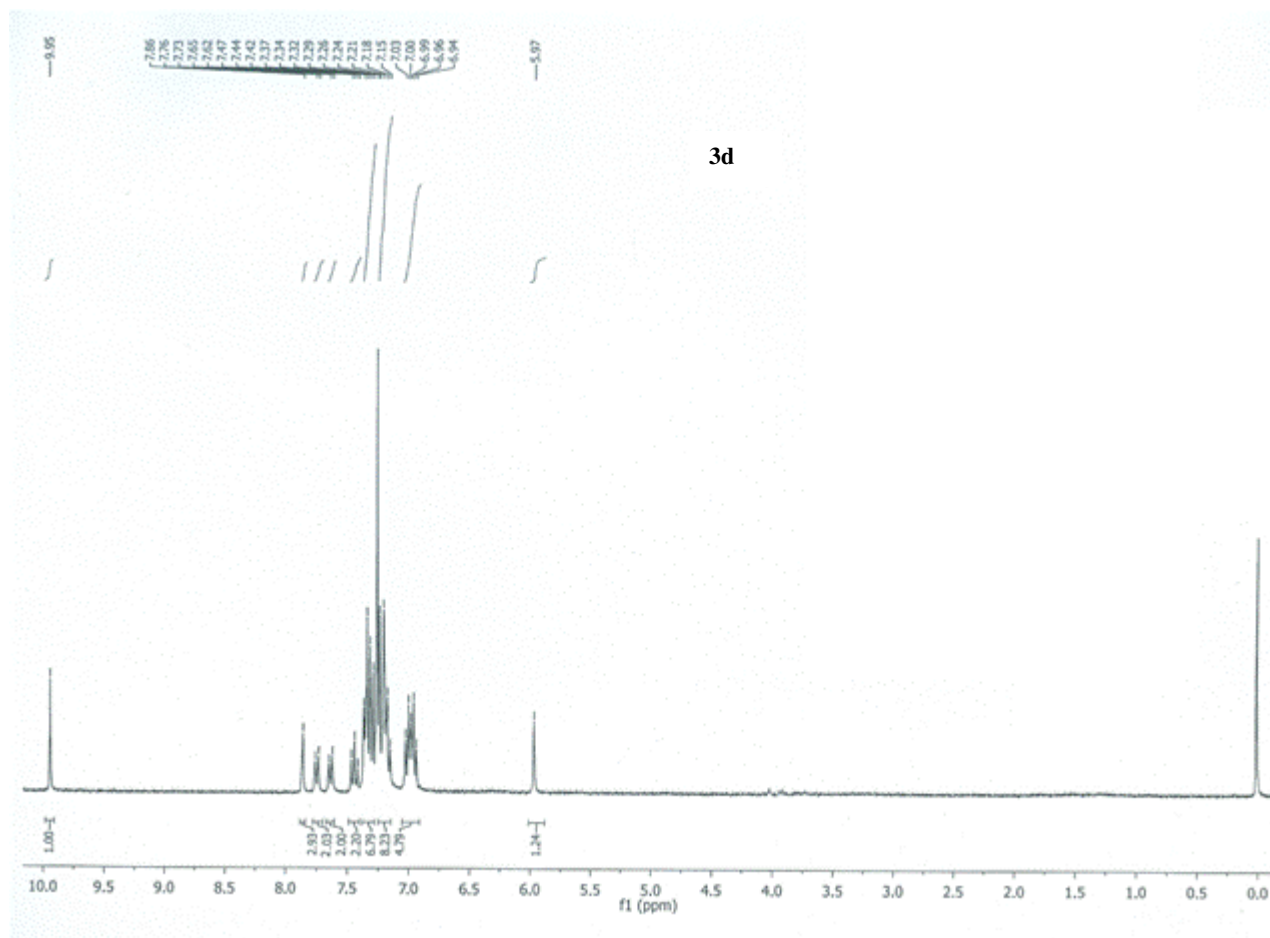


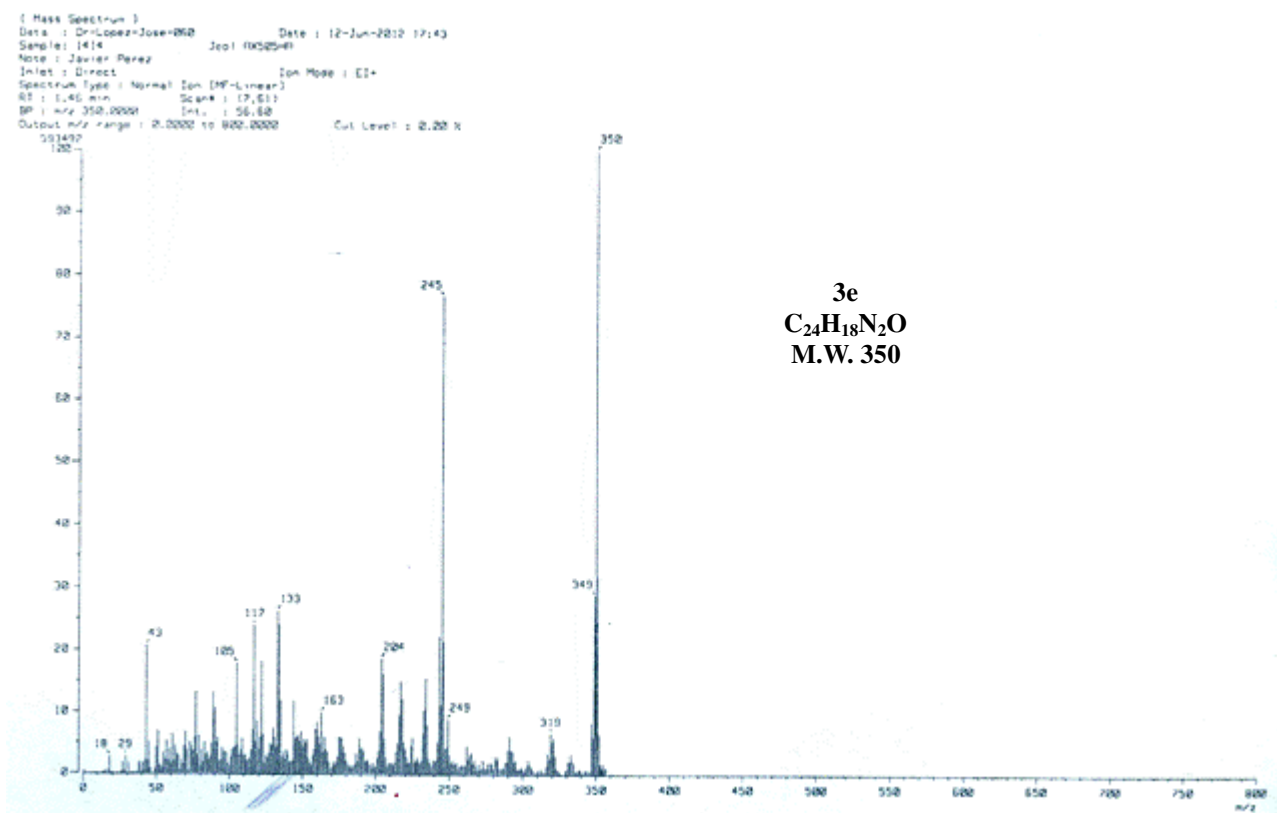
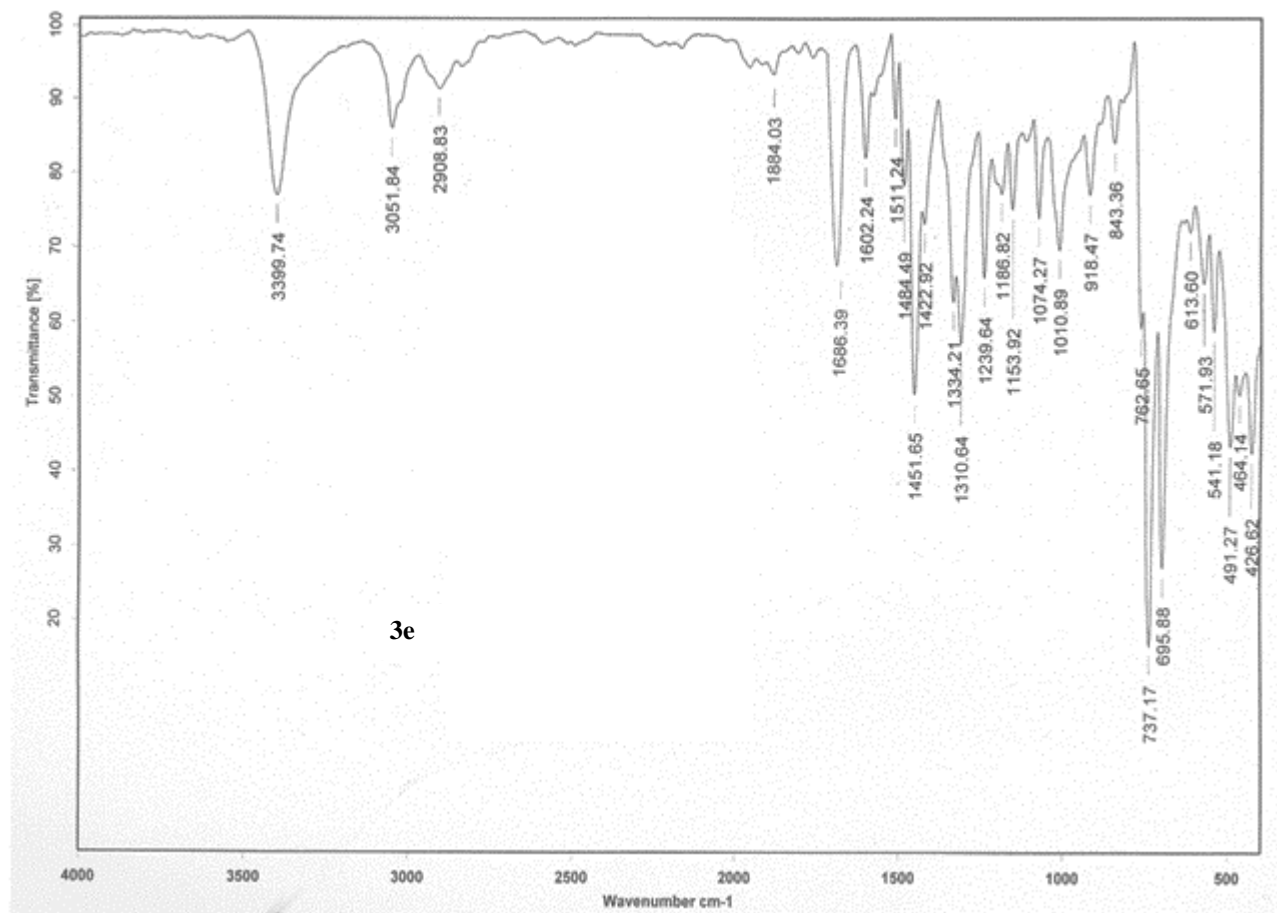


Data : Dr Cecilio-Alvarez059 Date : 02-Sep-2015 11:20  
 Instrument : MStation  
 Sample : 2582 2-ph-p  
 Note : -  
 Inlet : Direct Ion Mode : FAB+  
 RT : 0.75 min Scan# : (6,7)  
 Elements : C 40/0, H 49/0, N 3/0, O 2/0  
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1  
 Unsaturation (U.S.) : -0.5 - 45.0

**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



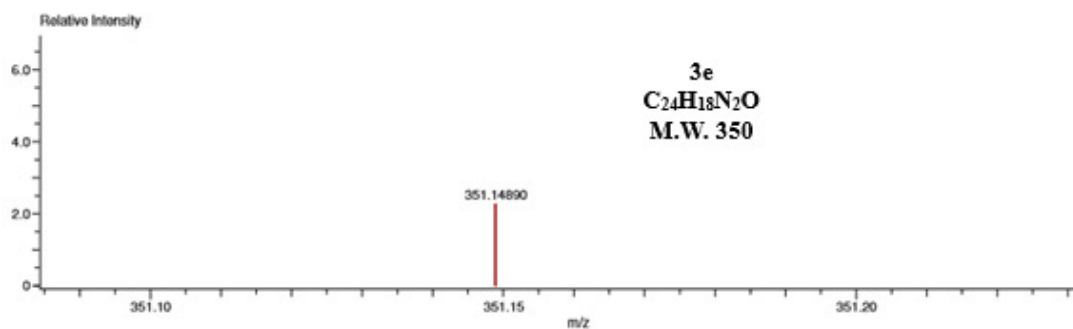


Data:3010 Indol-m  
 Sample Name:Dr Alvarez Cocilio/ Operador: Carmen Garcia-Javier Perez  
 Description:  
 Ionization Mode:ESI+  
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 1.1...

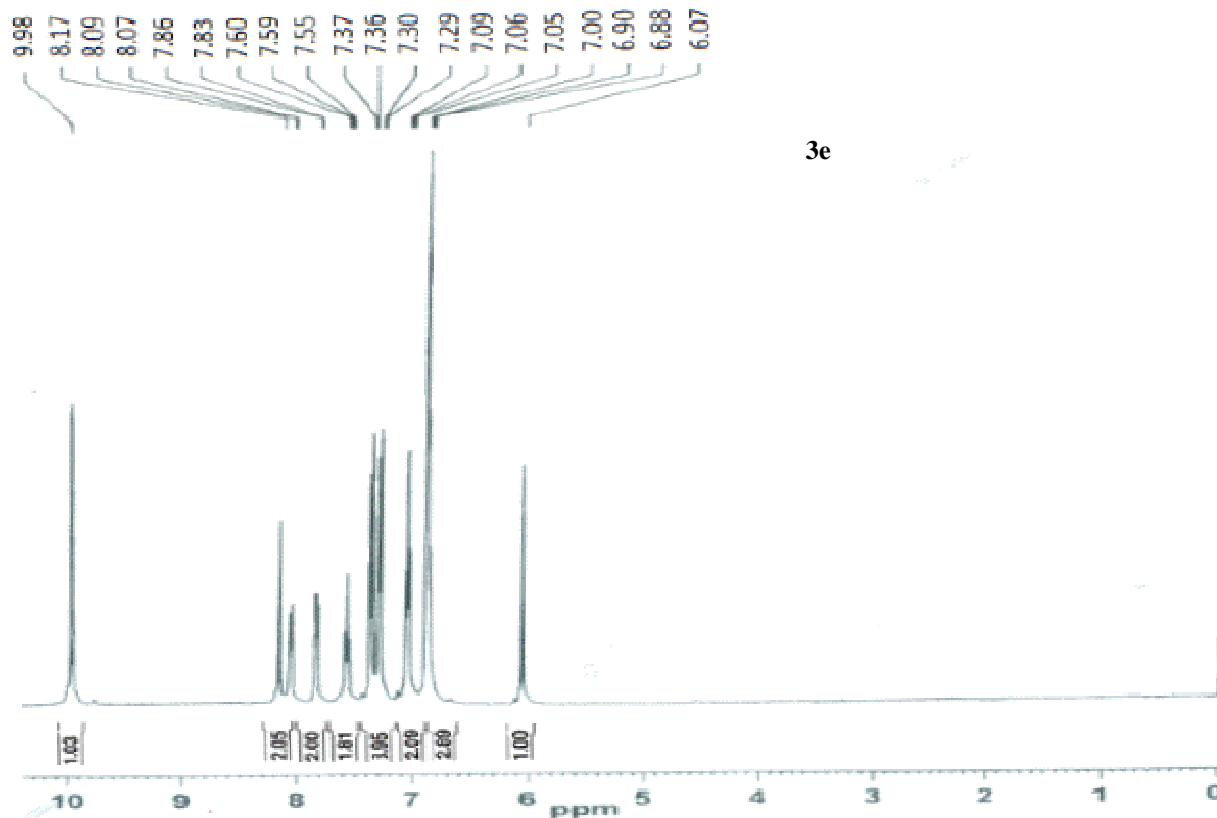
Acquired:9/30/2015 9:44:05 AM  
 Operator:AccuTOF  
 Mass Calibration data:Cal\_Peg\_600  
 Created:9/30/2015 12:15:17 PM  
 Created by:AccuTOF

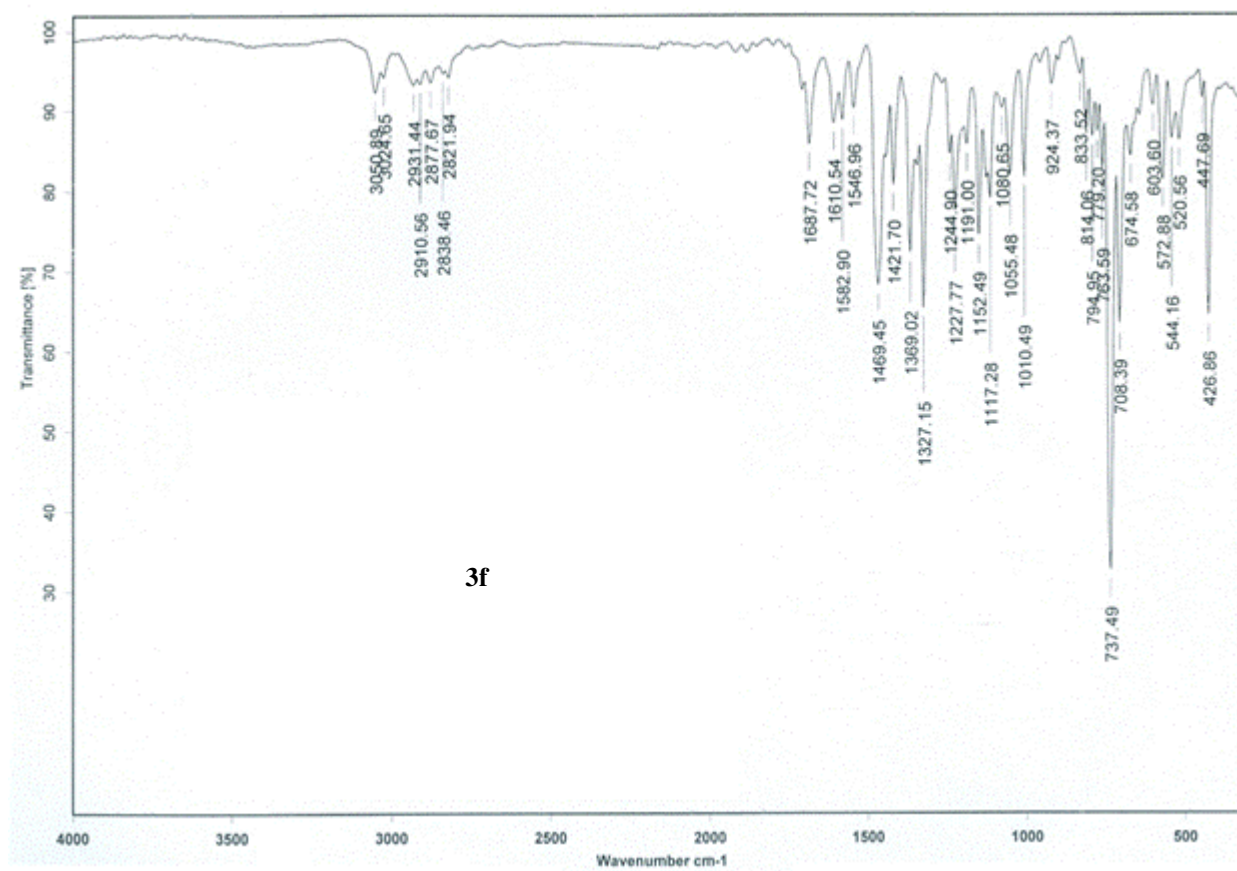
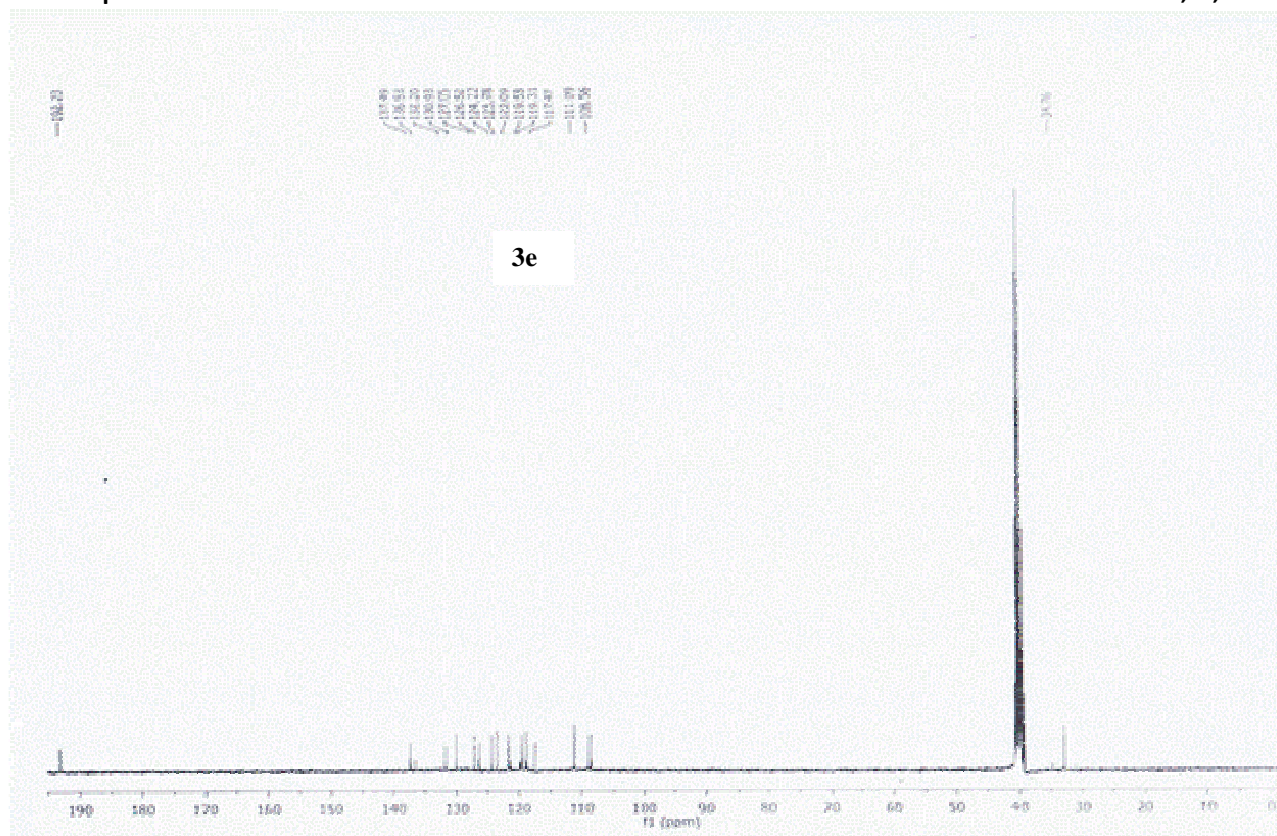
Charge number:1  
 Element:<sup>12</sup>C:0 .. 56, <sup>1</sup>H:0 .. 120, <sup>14</sup>N:0 .. 2, <sup>16</sup>O:0 .. 3  
 Tolerance:3.00(mmu)

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



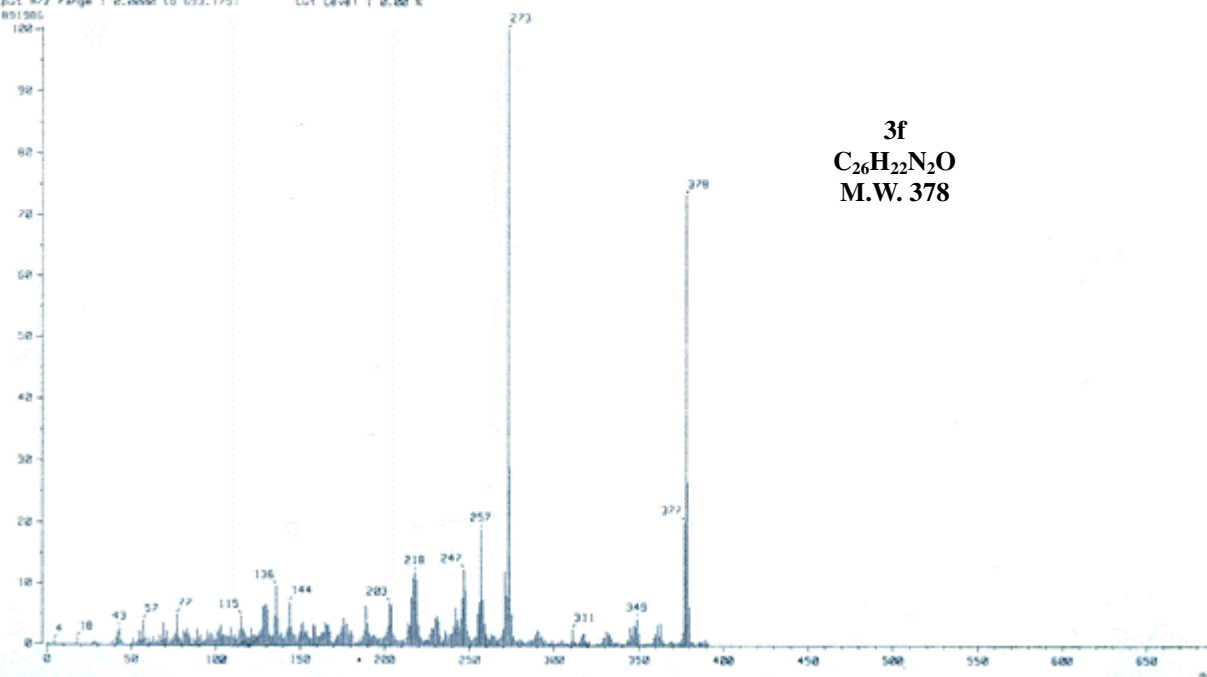
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14890	1386.79	351.14974	-0.84	-2.38	<sup>12</sup> C <sub>24</sub> <sup>1</sup> H <sub>18</sub> <sup>14</sup> N <sub>2</sub> <sup>16</sup> O <sub>1</sub>	16.5







[ Mass Spectrum ]  
 Date : Dr-Lopez-Jose-204 Date : 24-May-2012 17:18  
 Sample : 1213 ICP1 Joel RA50596  
 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

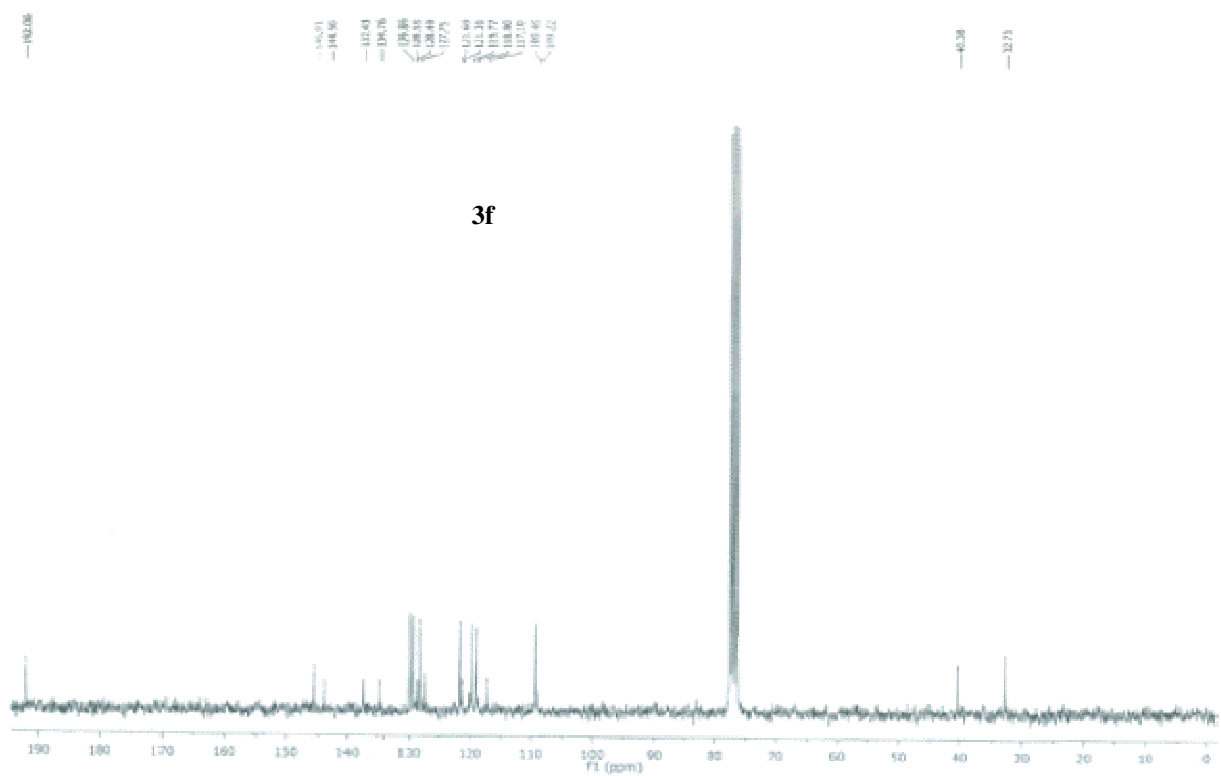
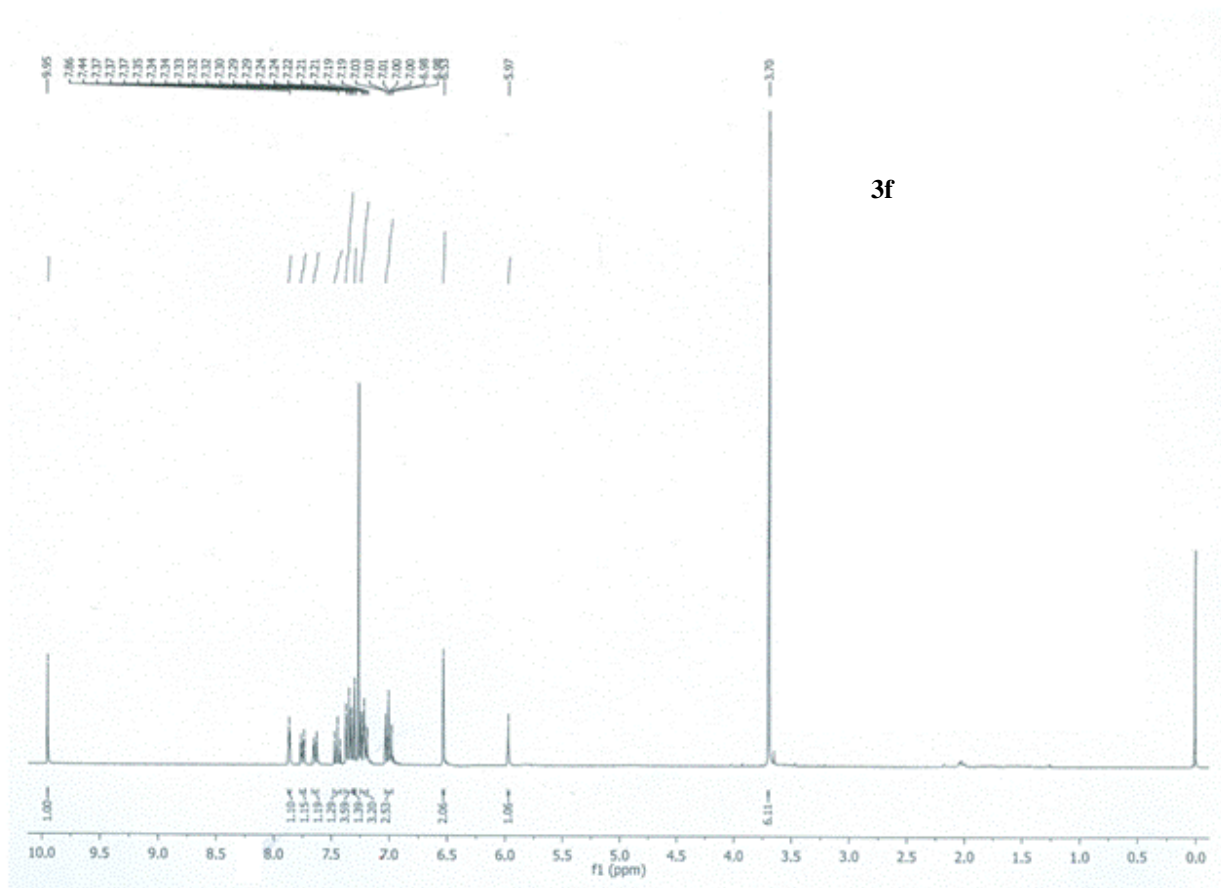


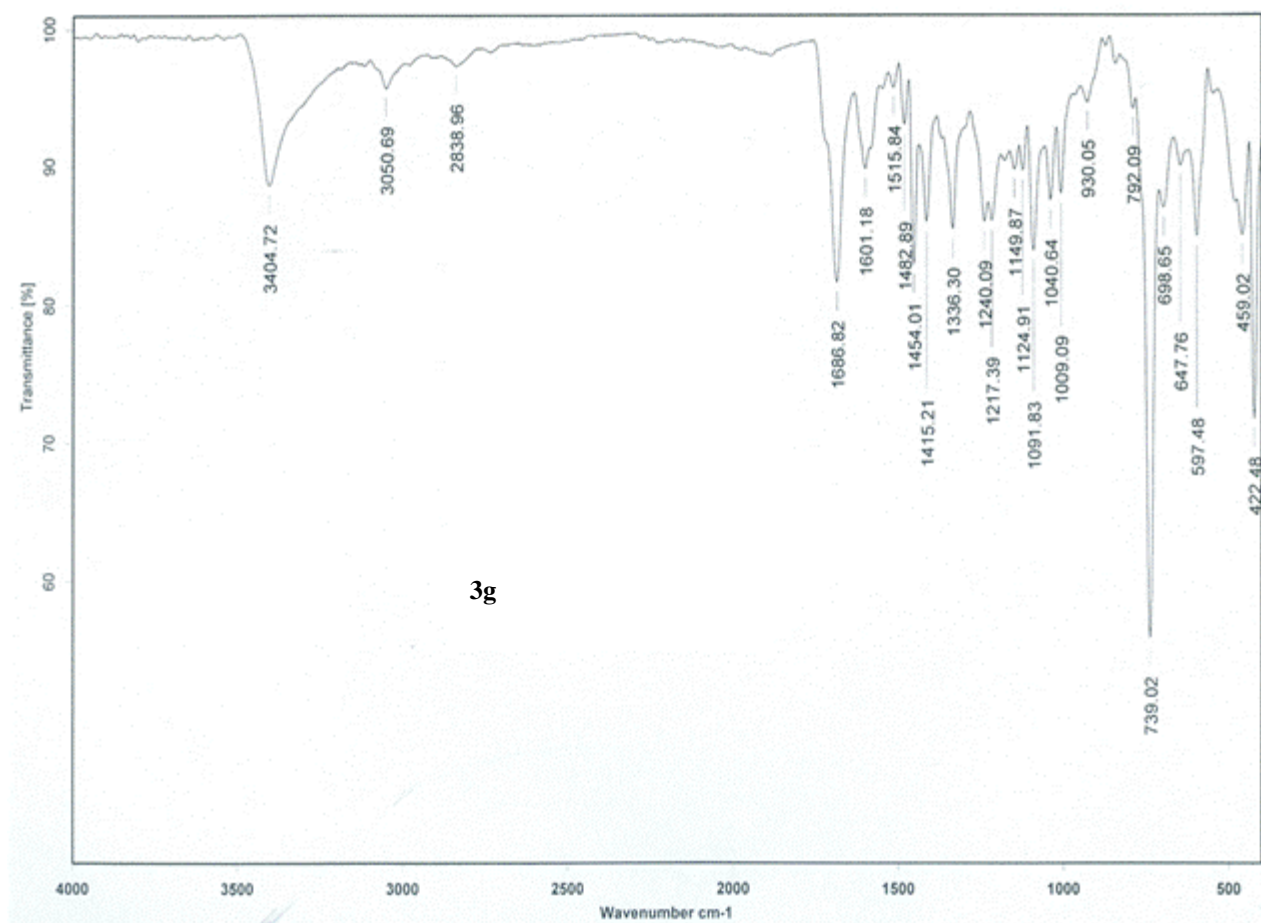
**3f**  
C26H22N2O  
 M.W. 378

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

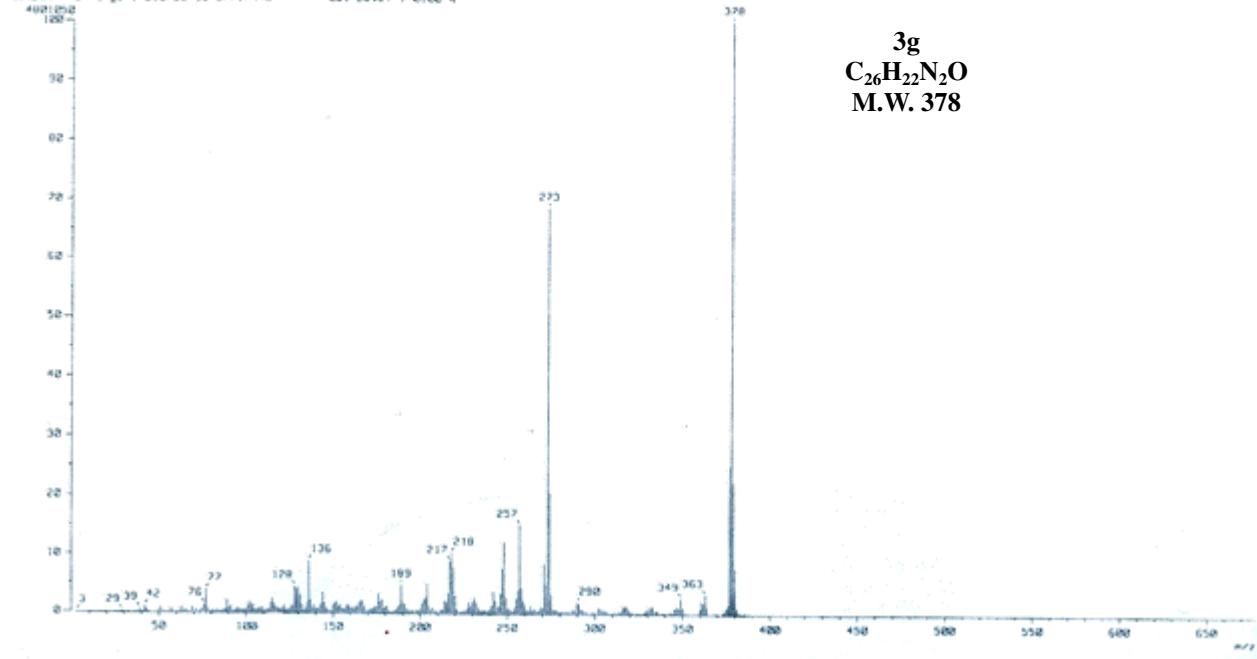
**3f**  
C26H22N2O  
 M.W. 378

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 19:17  
 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 %



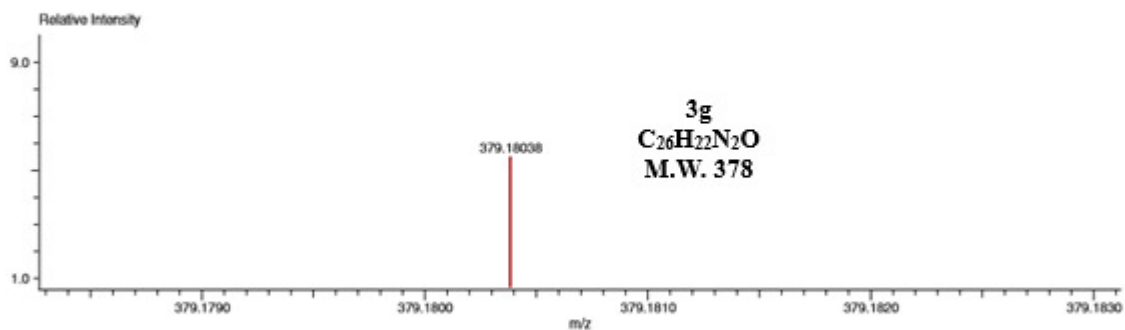
**3g**  
C26H22N2O  
 M.W. 378

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...

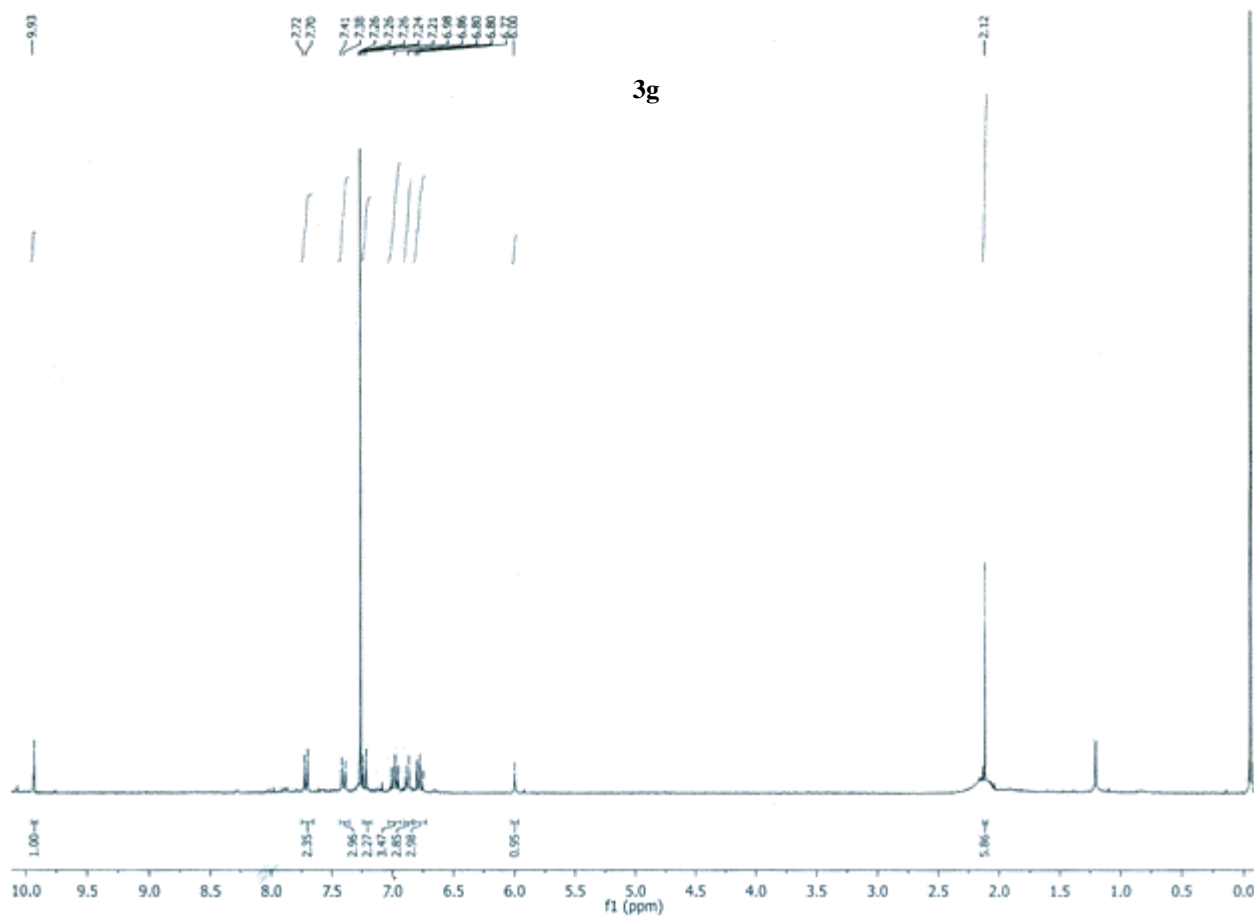
Acquired:9/30/2015 9:49:57 AM  
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 Mass Calibration data:Cal\_Peg\_600  
 Created:9/30/2015 12:56:56 PM  
 Created by:AccuTOF

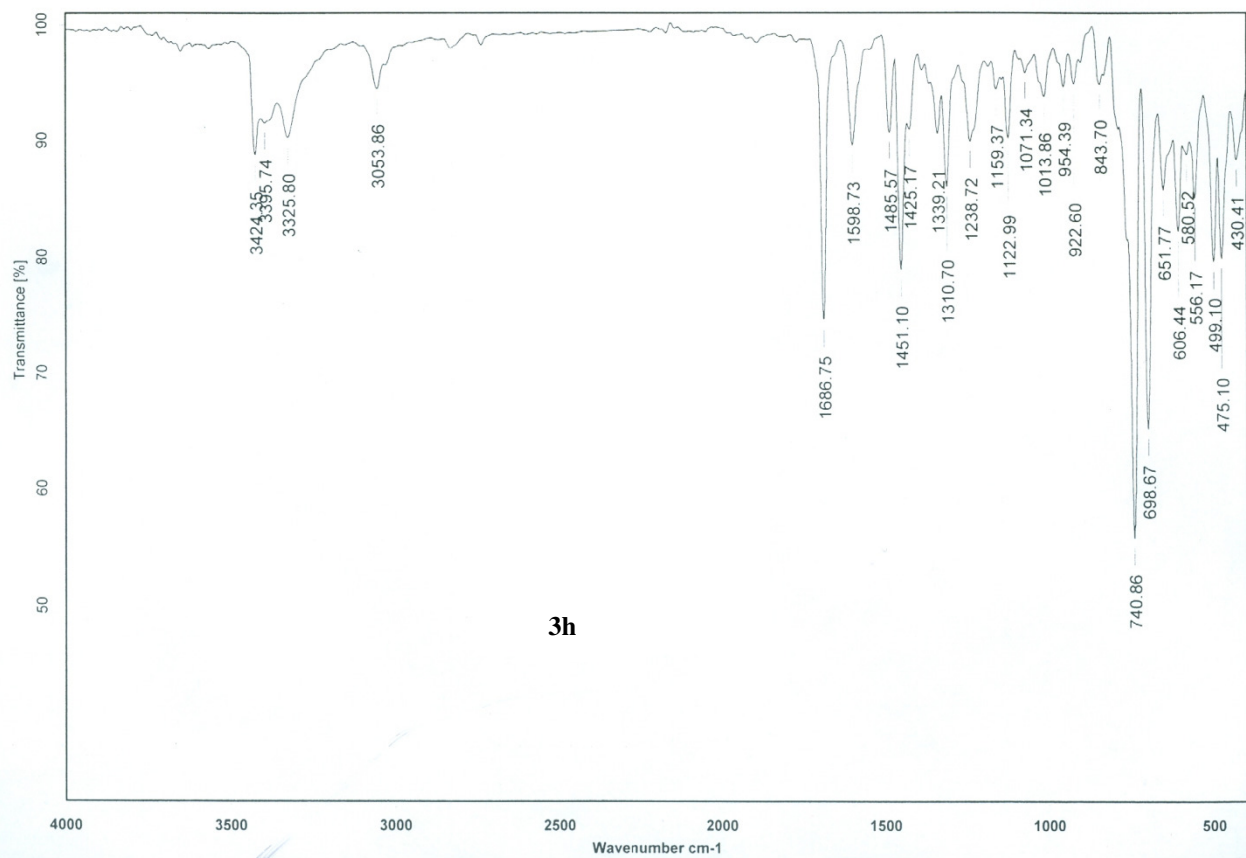
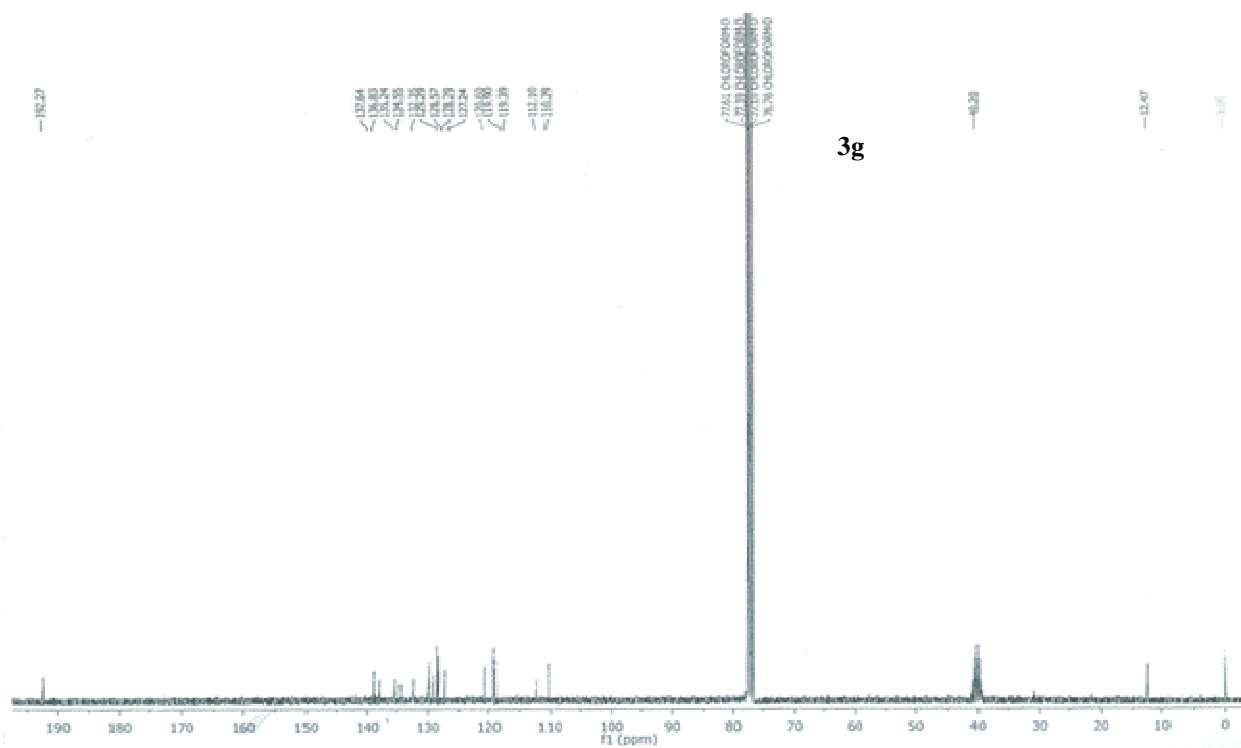
Charge number:1  
 Element:<sup>12</sup>C:0 .. 56, <sup>1</sup>H:0 .. 120, <sup>14</sup>N:0 .. 2, <sup>16</sup>O:0 .. 3  
 Tolerance:3.00(mmu)

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

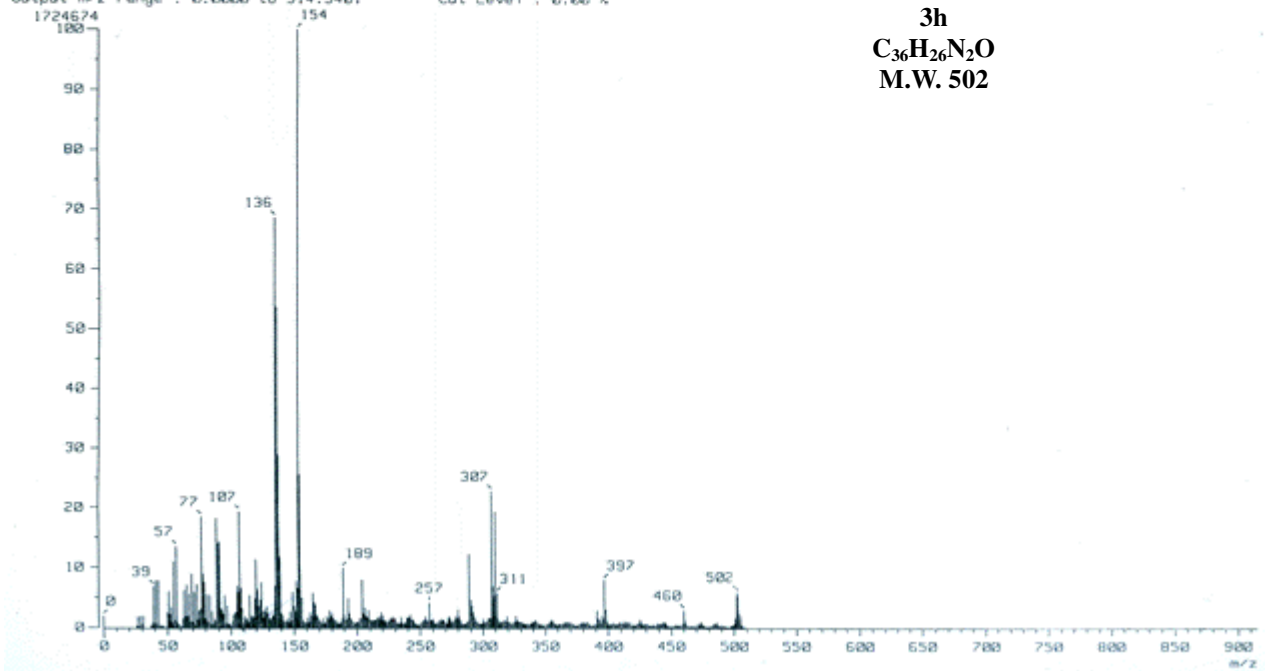


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18038	1642.76	379.18104	-0.65	-1.73	<sup>13</sup> C <sub>26</sub> <sup>1</sup> H <sub>22</sub> <sup>14</sup> N <sub>2</sub> <sup>16</sup> O <sub>1</sub>	16.5





[ 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

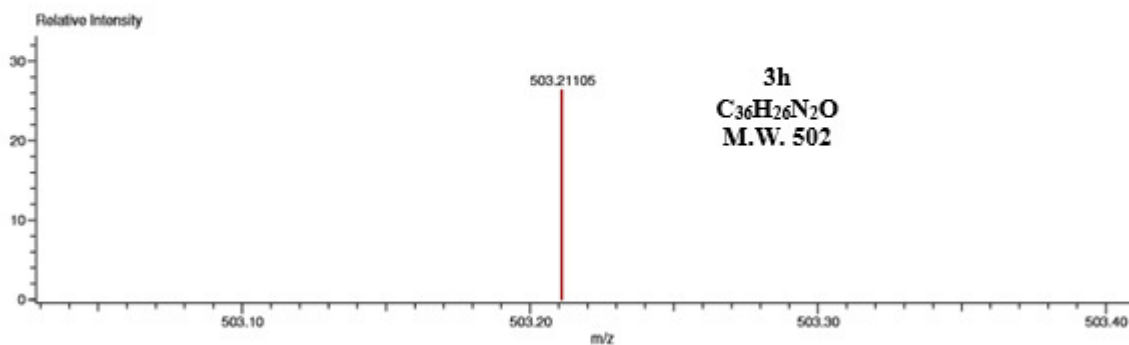
Data:CAT 8  
 Sample Name:  
 Description:  
 Ionization Mode:ESI+  
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.3...

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:<sup>12</sup>C:0 .. 100, <sup>1</sup>H:0 .. 100, <sup>14</sup>N:0 .. 3, <sup>16</sup>O:0 .. 3

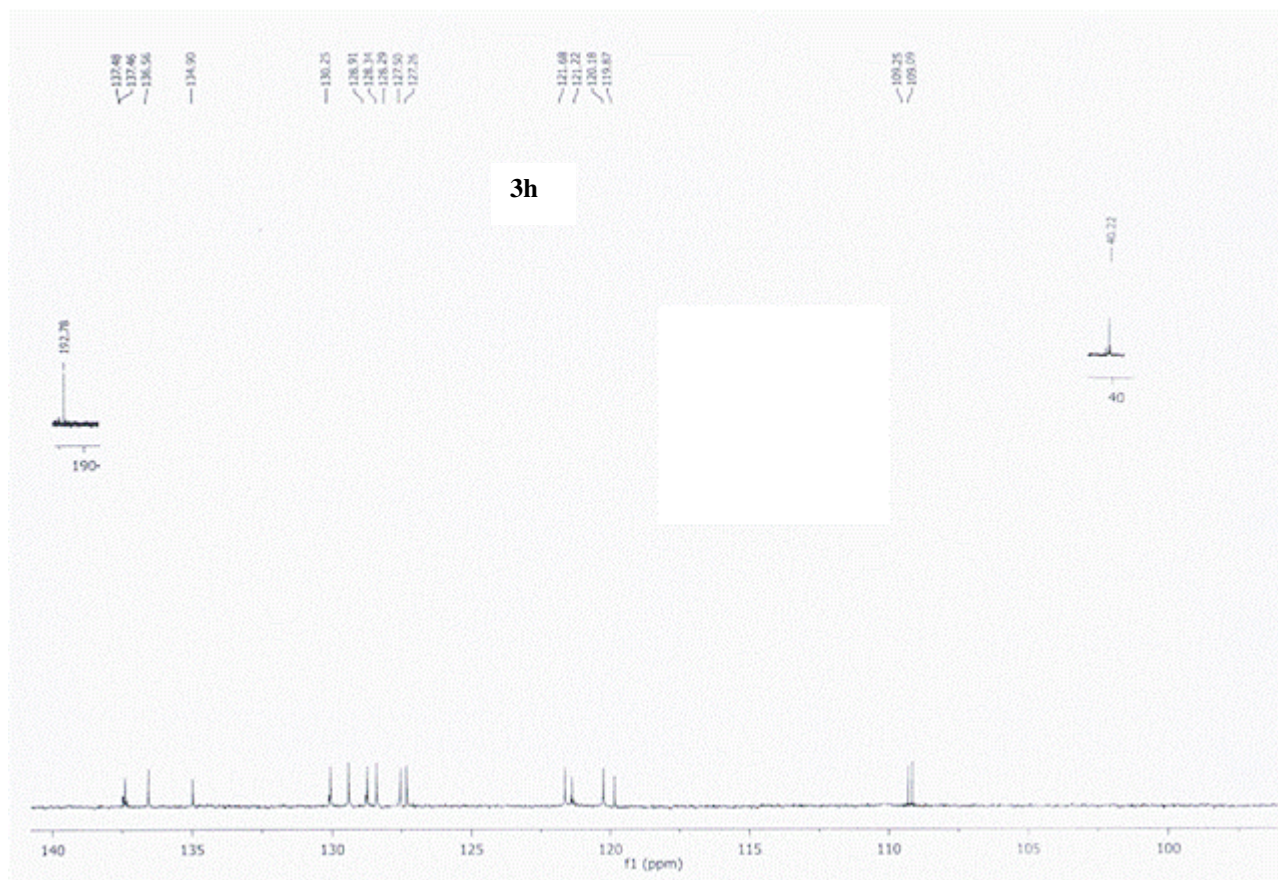
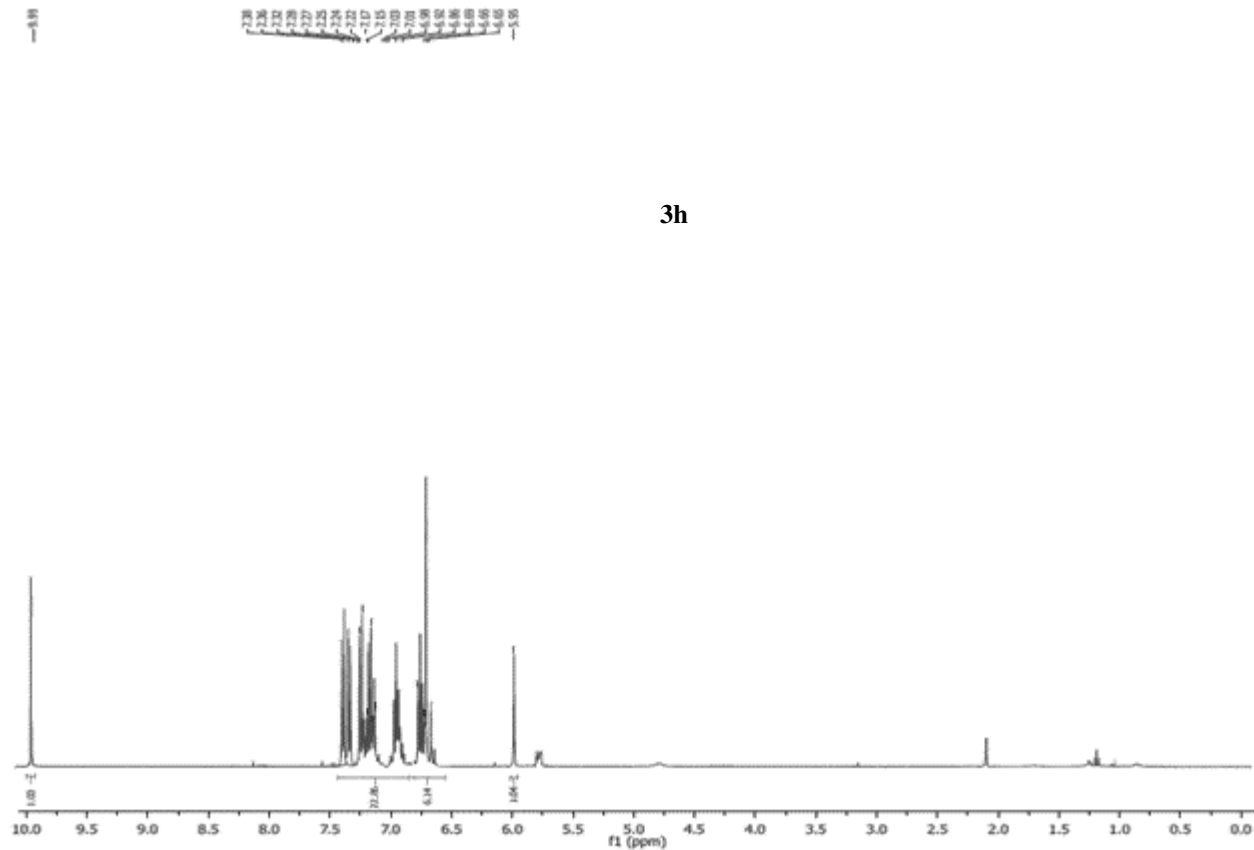
Tolerance:3.00(mmu)

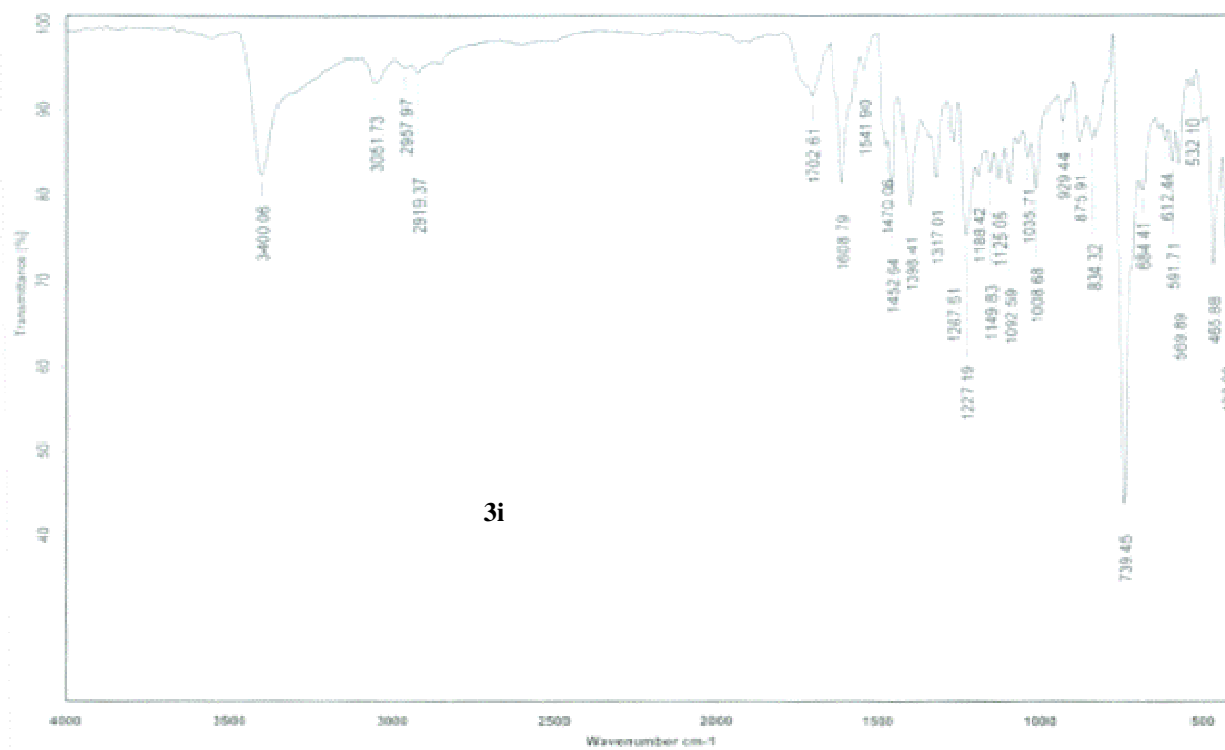
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



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

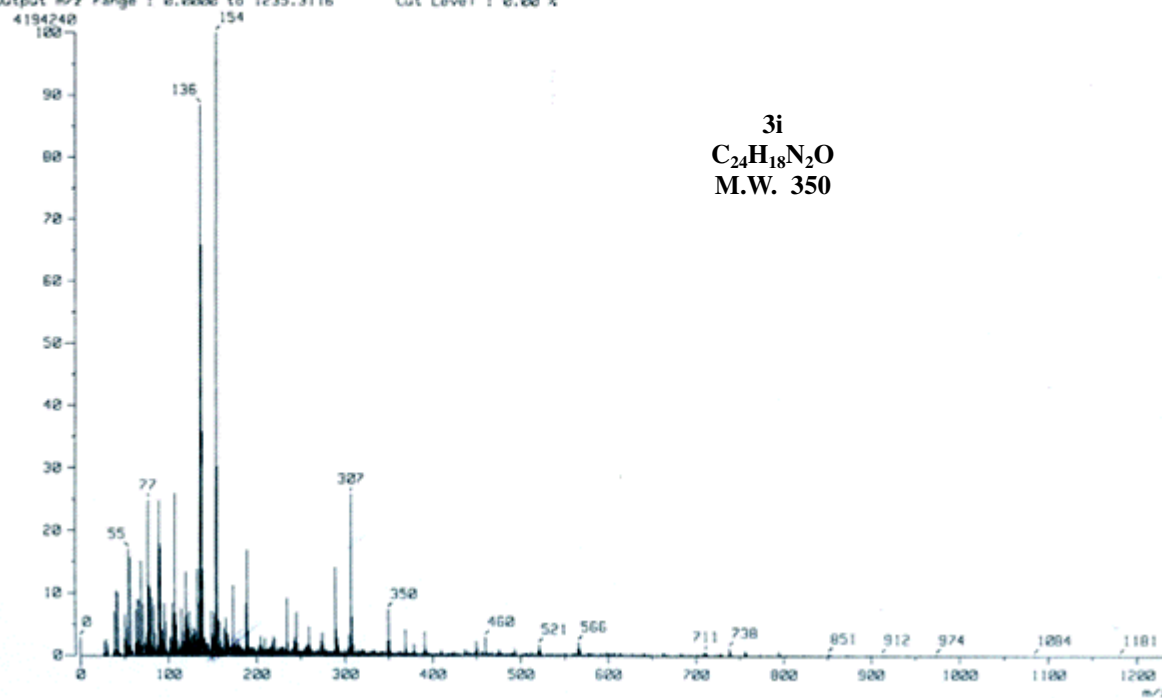
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21105	2115.38	503.21234	-1.28	-2.55	$^{12}C_{36}^{1}H_{26}^{14}N_2^{16}O_1$	24.5





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 %



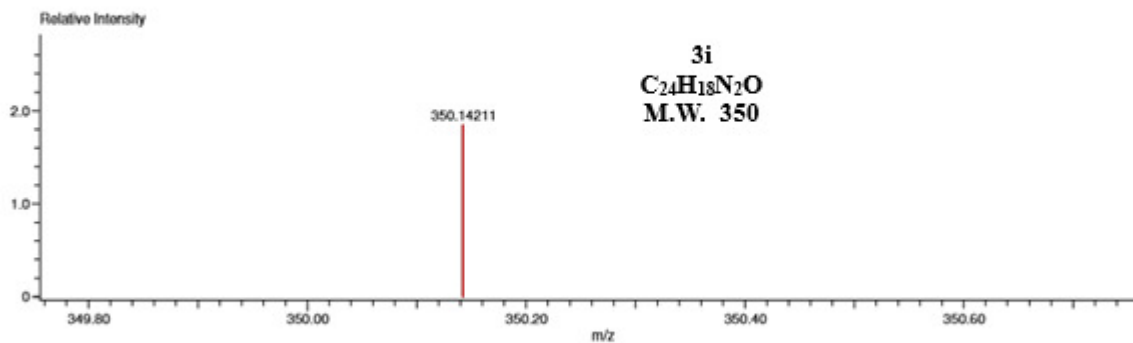
3i  
 $C_{24}H_{18}N_2O$   
 M.W. 350



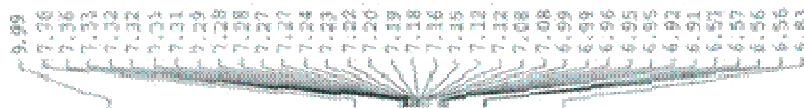
Data: CAT 10  
 Sample Name:  
 Description:  
 Ionization Mode: ESI+  
 History: Determine m/z [Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.7...

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

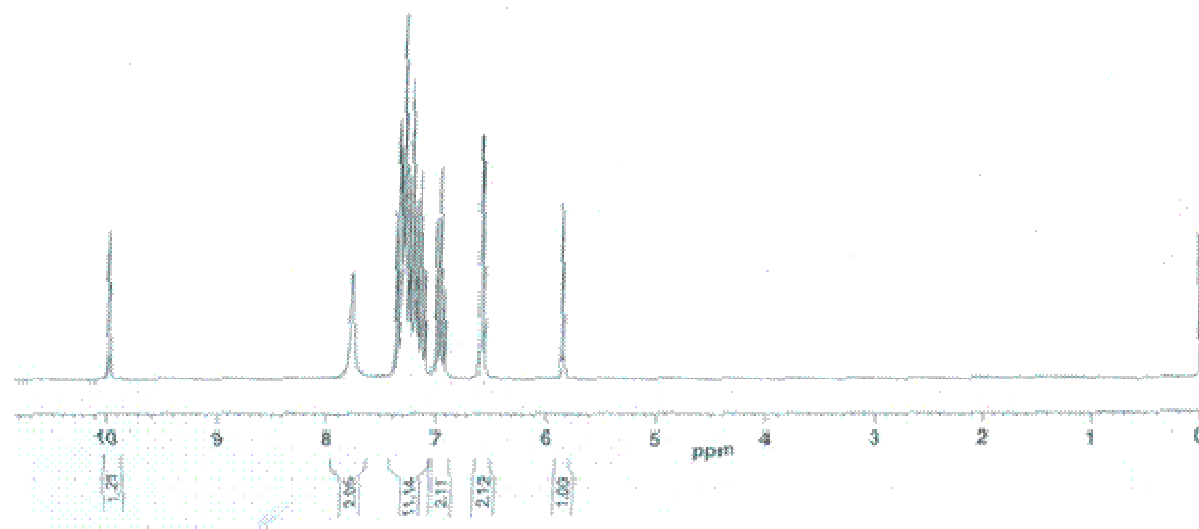
Charge number: 1  
 Element: <sup>12</sup>C: 0 .. 100, <sup>1</sup>H: 0 .. 100, <sup>14</sup>N: 0 .. 3, <sup>16</sup>O: 0 .. 3  
 Tolerance: 3.00 (mmu)  
 Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

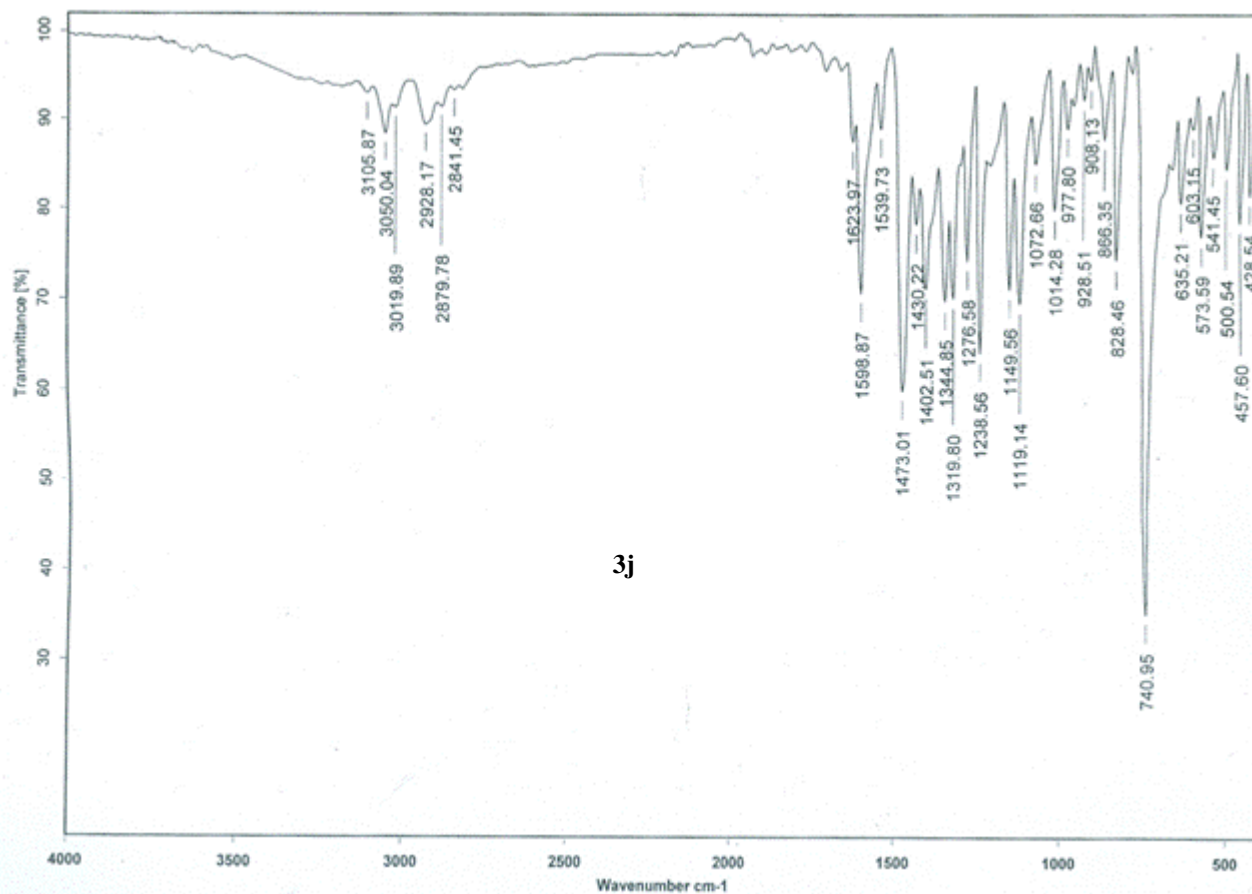
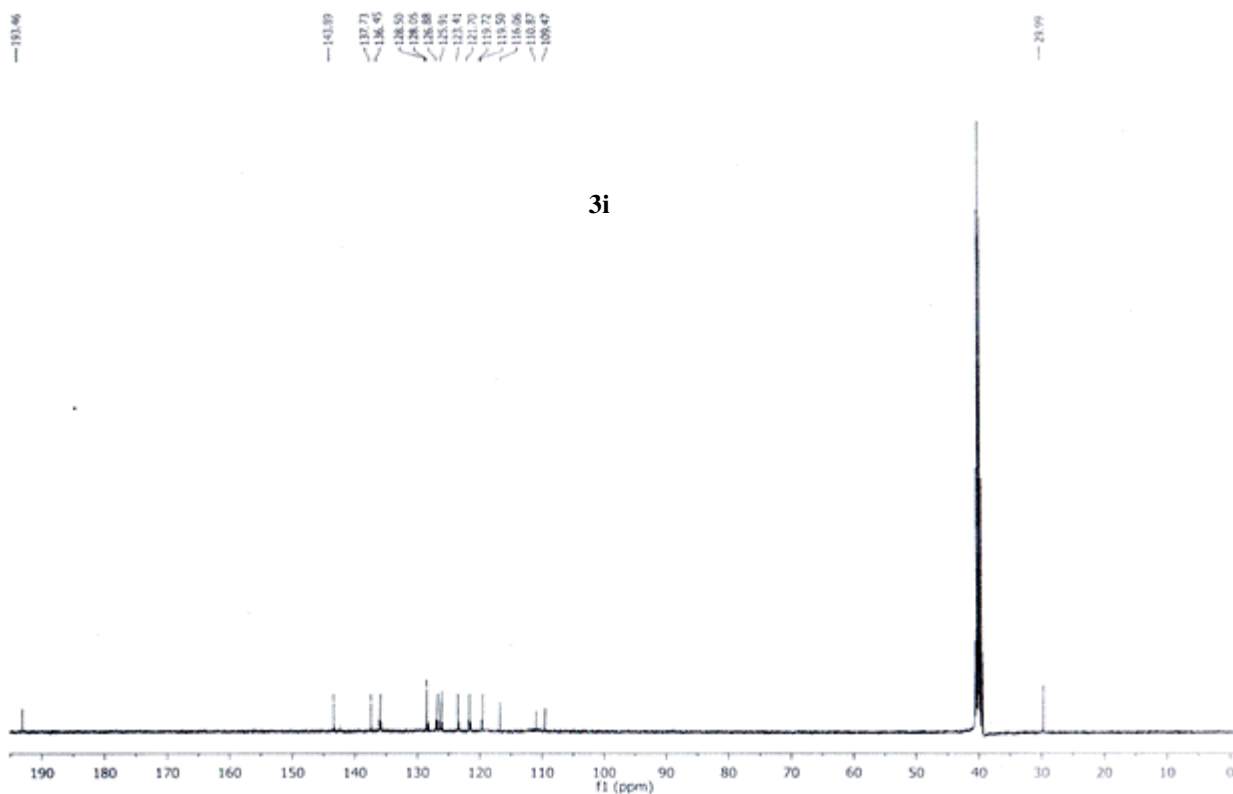


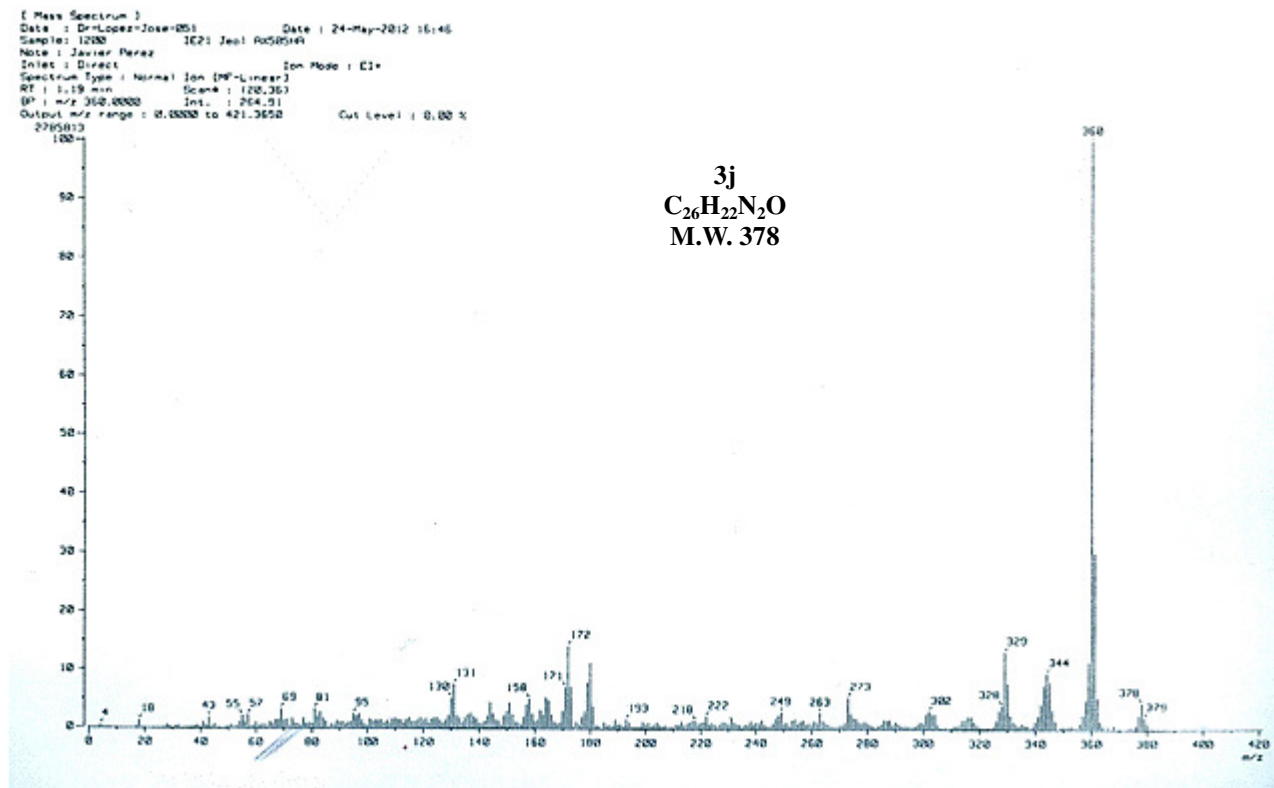
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
350.14211	2134.88	350.14191	0.19	0.55	<sup>12</sup> C <sub>24</sub> <sup>1</sup> H <sub>18</sub> <sup>14</sup> N <sub>2</sub> <sup>16</sup> O <sub>1</sub>	17.0



3i







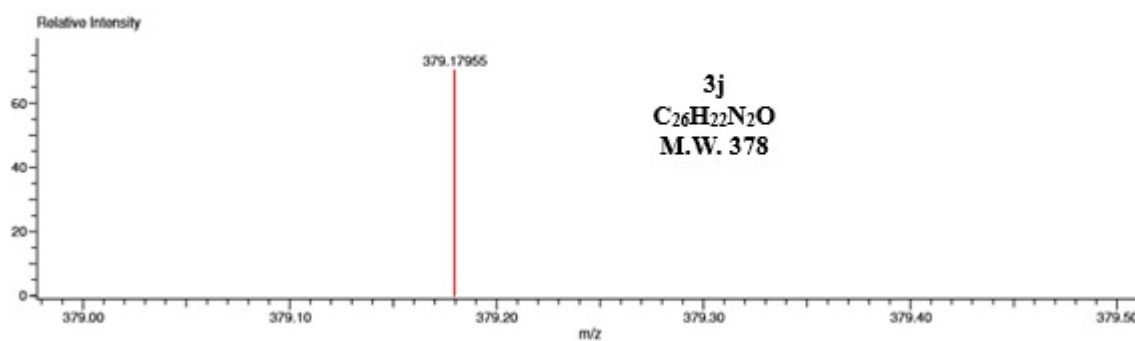
Data:CAT 9  
 Sample Name:  
 Description:  
 Ionization Mode:ESI+  
 History:Determine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%],Average[MS[1] 0.2...]

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

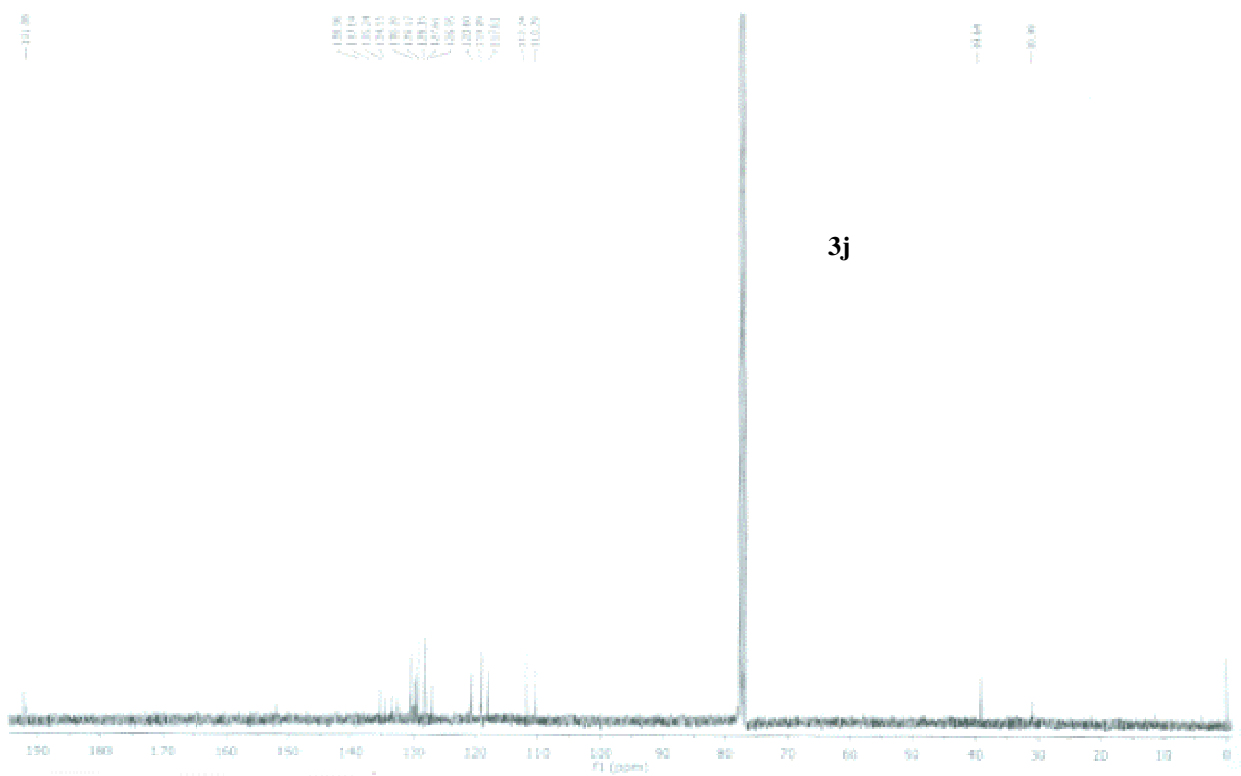
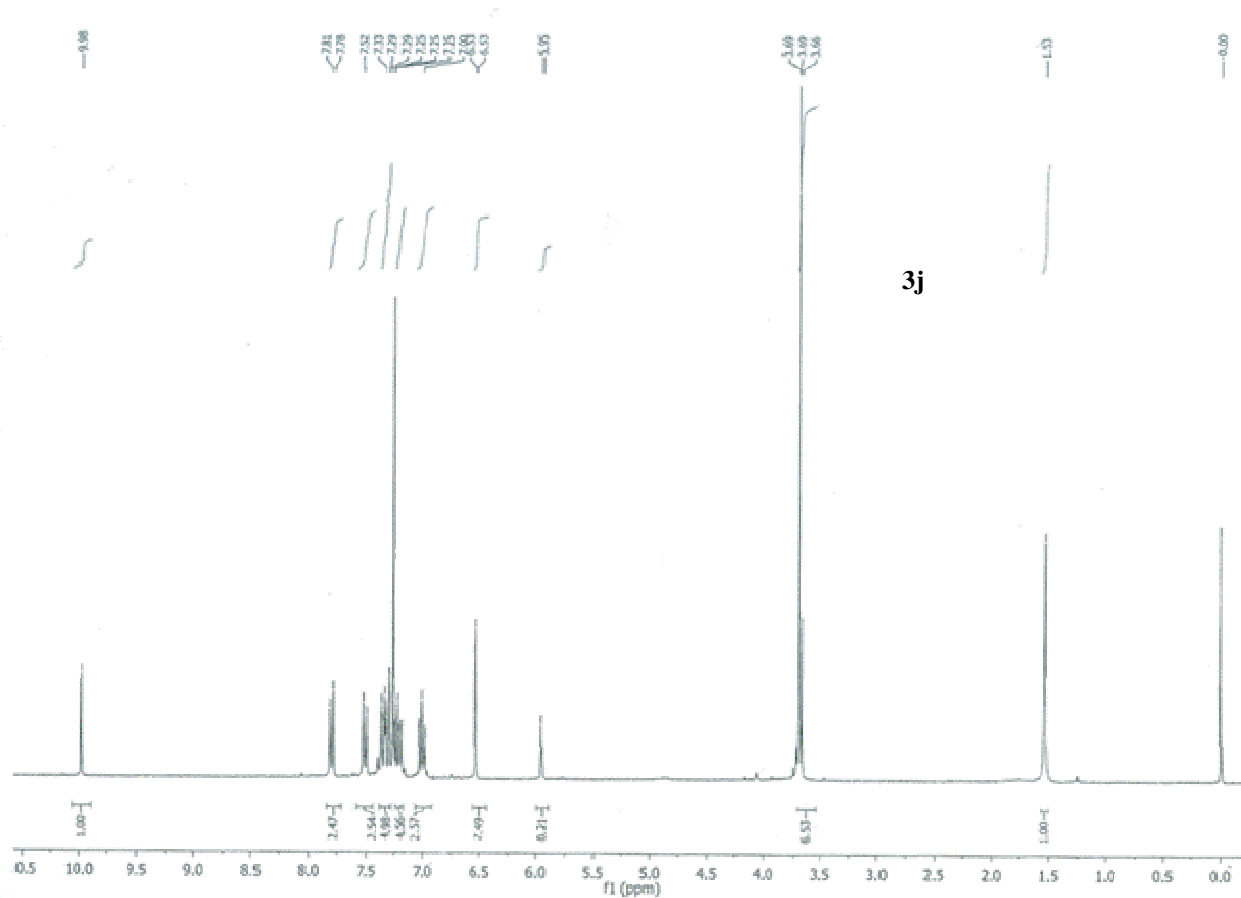
Charge number:1  
 Element: $^{12}C:0 \dots 100$ ,  $^1H:0 \dots 100$ ,  $^{14}N:0 \dots 3$ ,  $^{16}O:0 \dots 3$

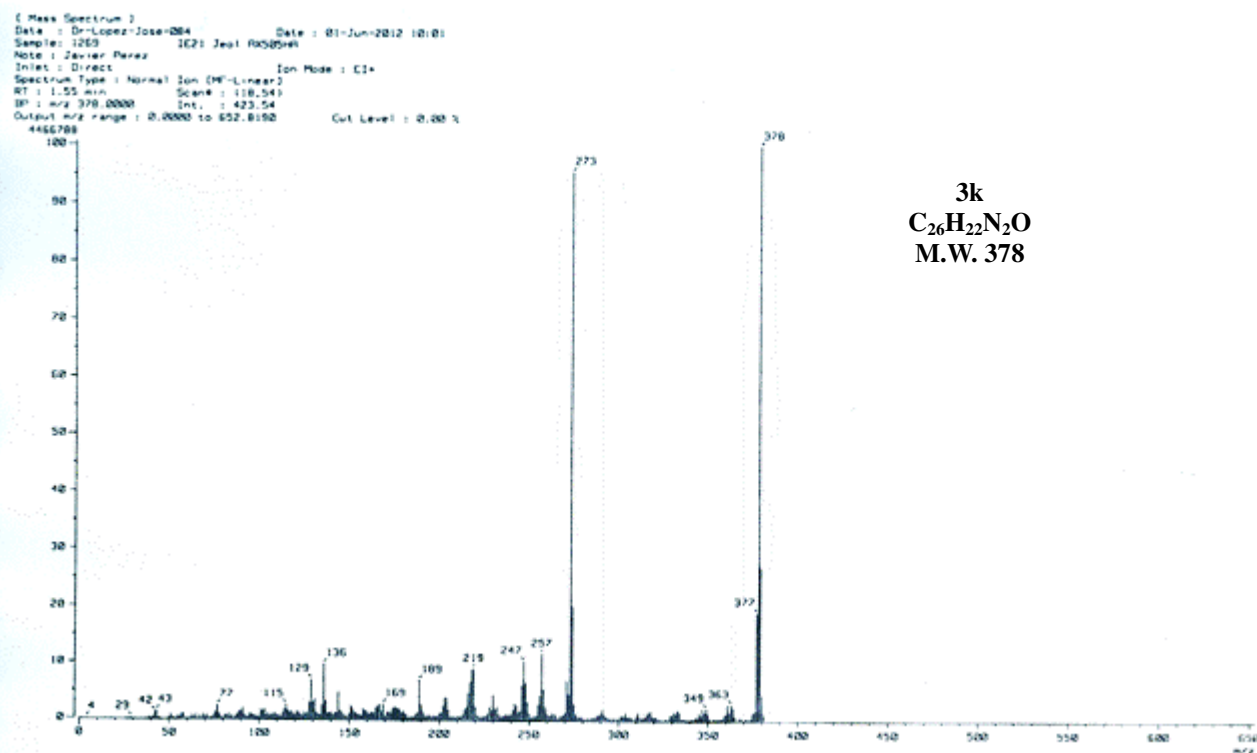
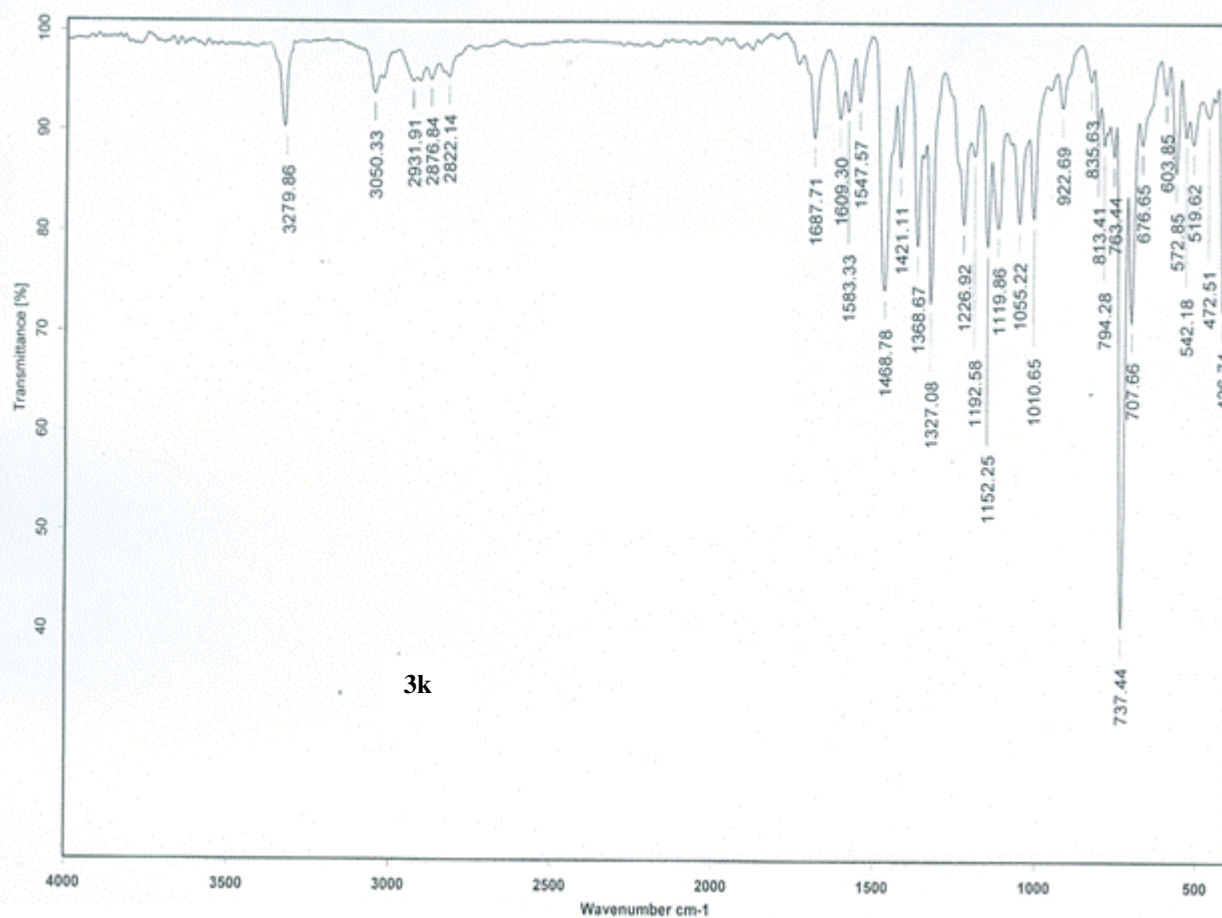
Tolerance:3.00(mmu)

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





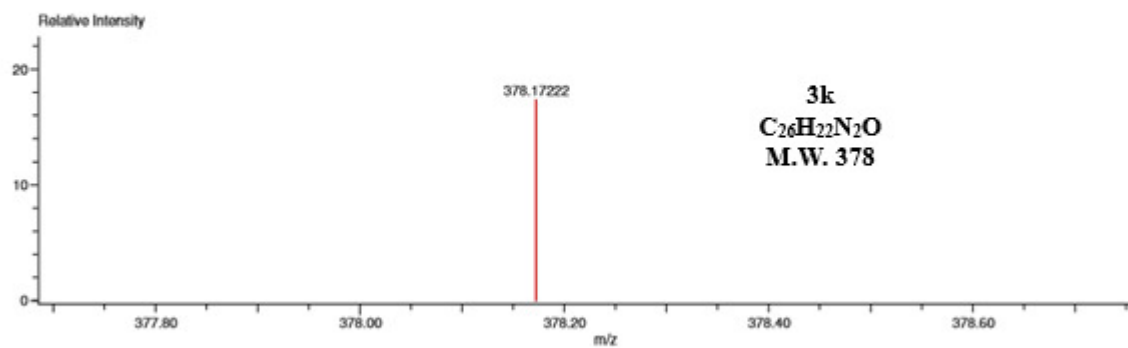
Data: CAT 11  
 Sample Name:  
 Description:  
 Ionization Mode: ESI+  
 History: Determine m/z [Peak Detect [Centroid, 30, Area], Correct Base [5.0%], Correct Base [5.0%], Average [MS [1] 0.8...

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

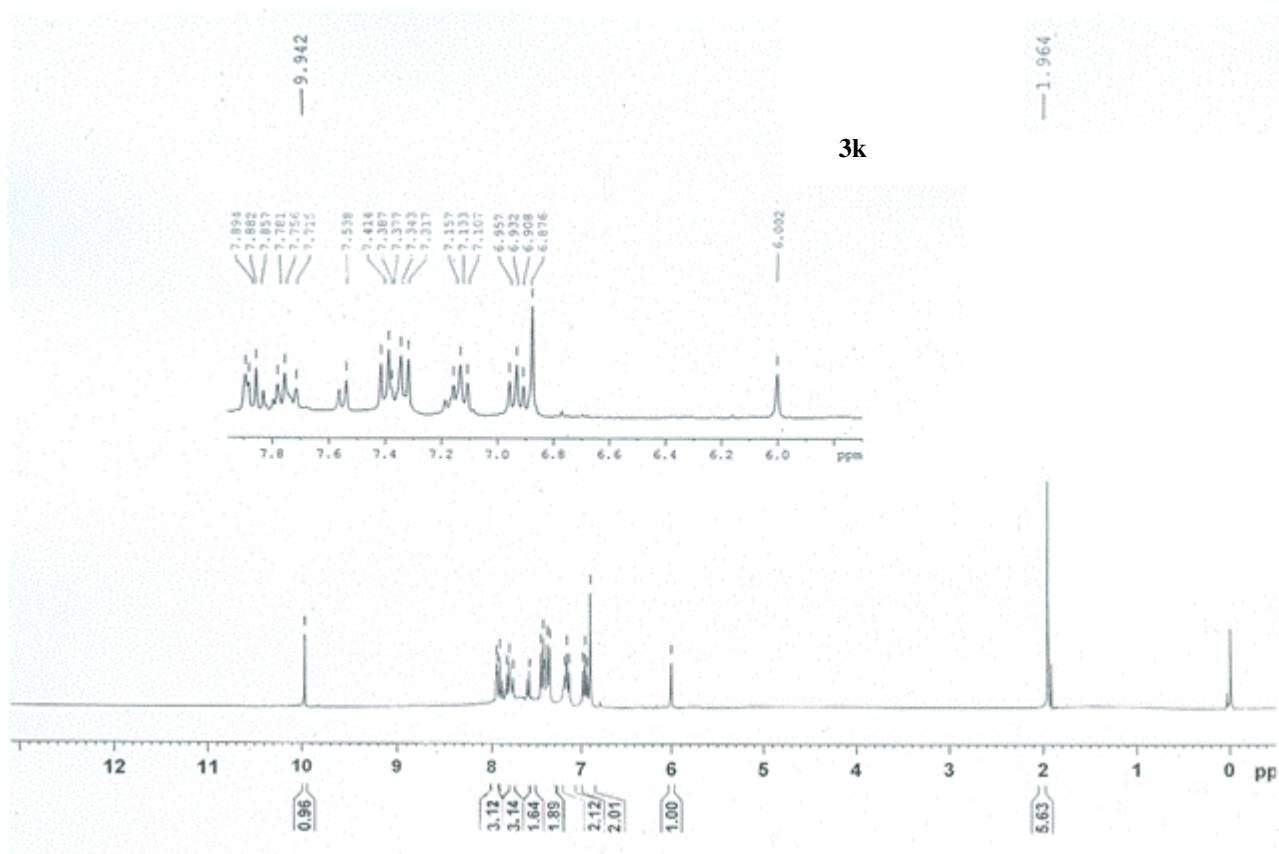
Charge number: 1  
 Element:  $^{12}\text{C}$ : 0 .. 100,  $^1\text{H}$ : 0 .. 100,  $^{14}\text{N}$ : 0 .. 3,  $^{16}\text{O}$ : 0 .. 3

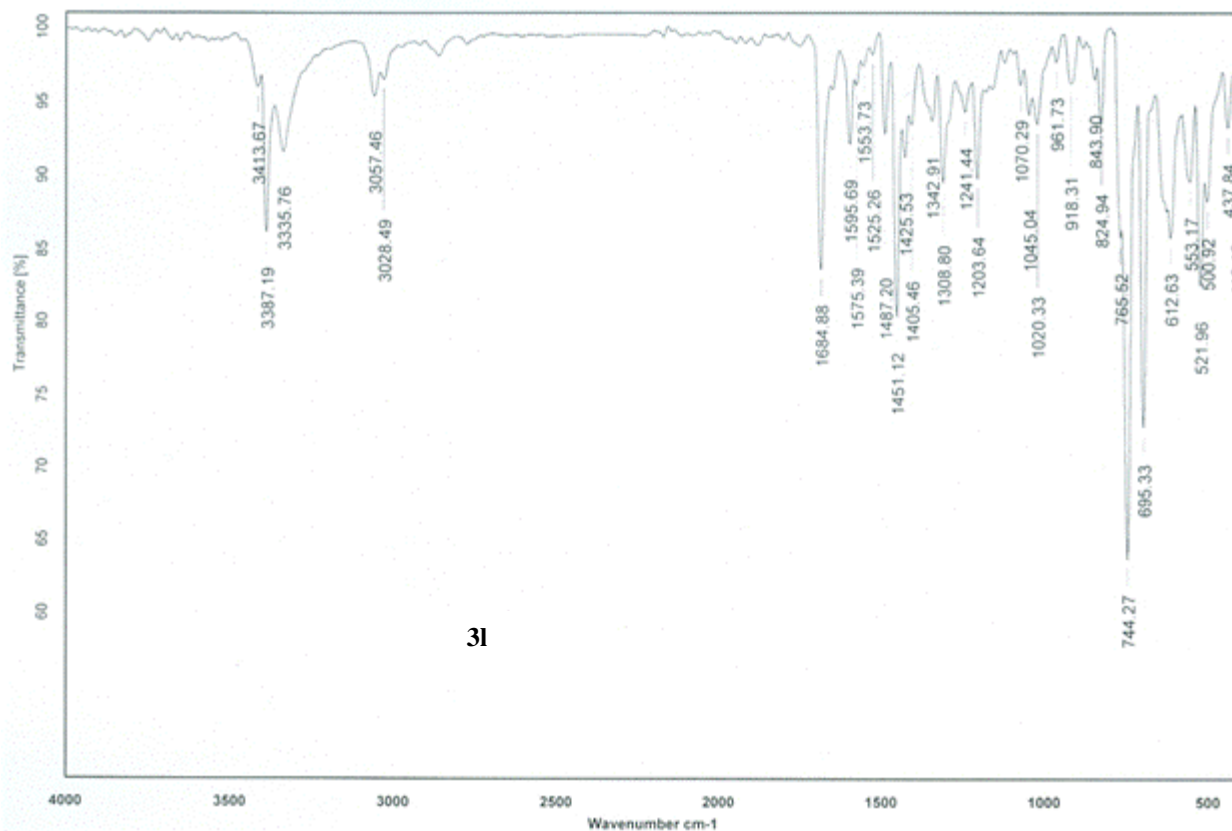
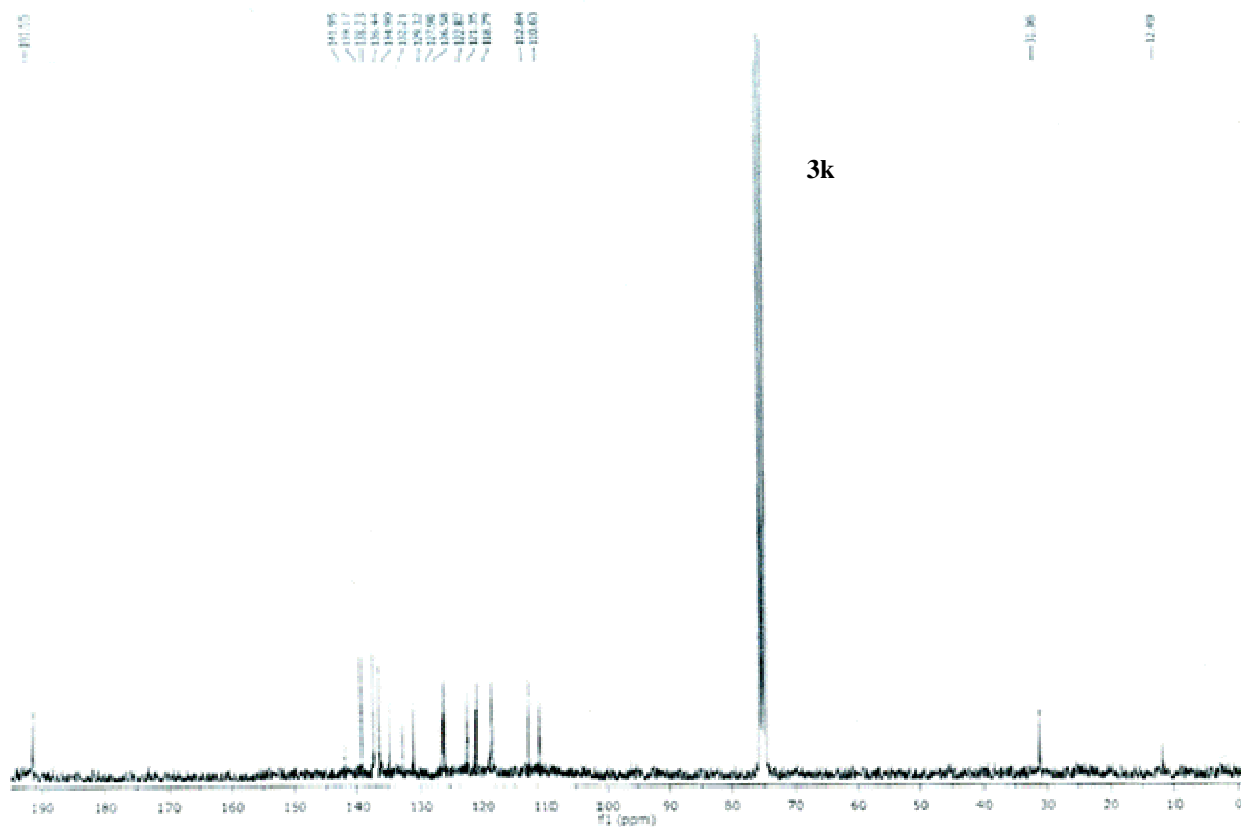
Tolerance: 3.00 (mmu)

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

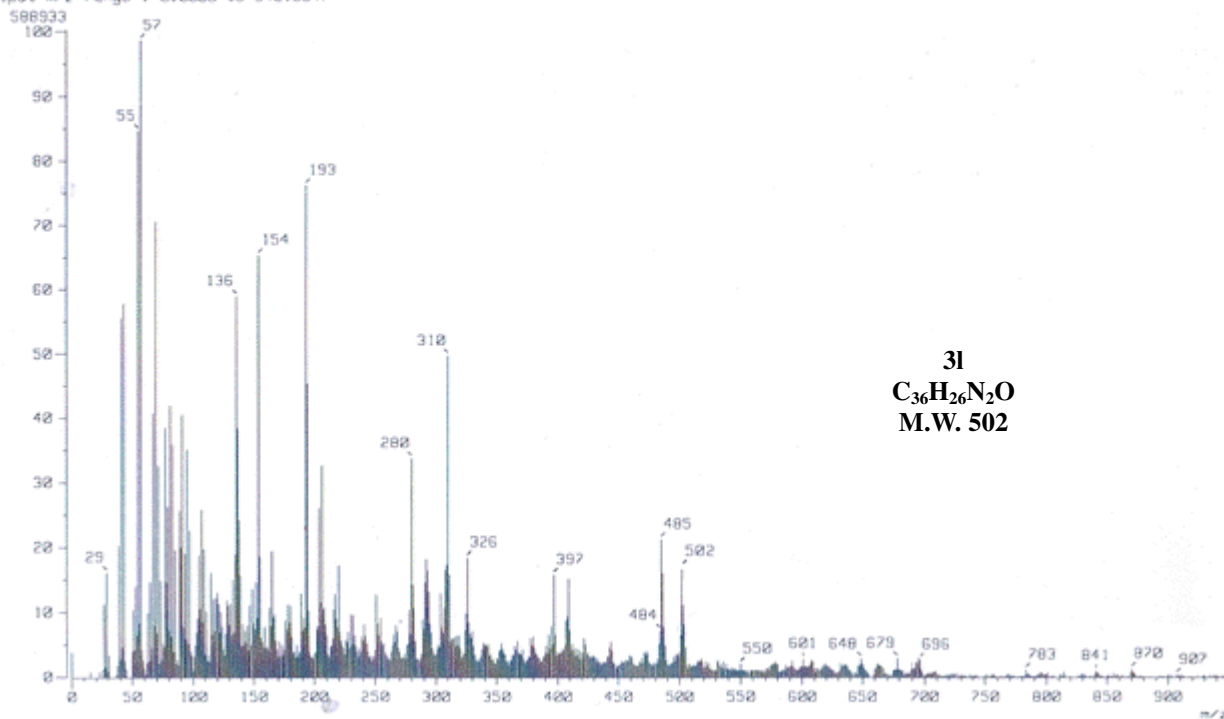


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
378.17222	13695.63	378.17321	-0.99	-2.62	$^{12}\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}$	17.0





[ 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

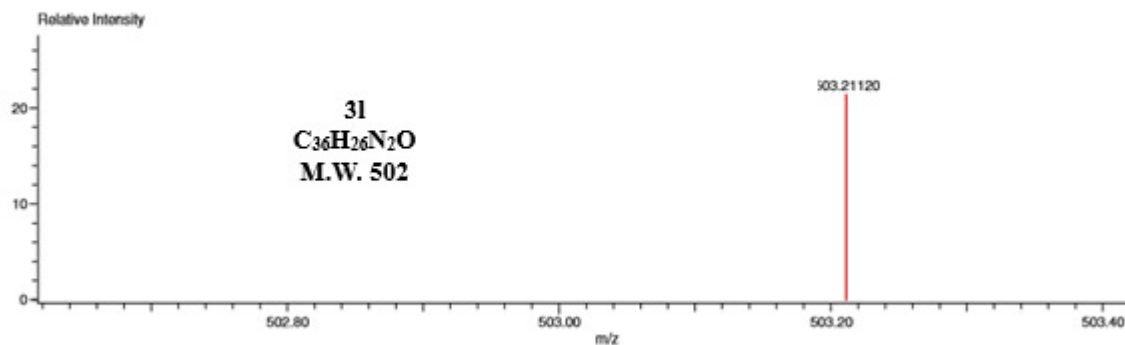
Data:CAT 12  
 Sample Name:  
 Description:  
 Ionization Mode:ESI+  
 History:Determine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%];Average[MS[1] 0.7...

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

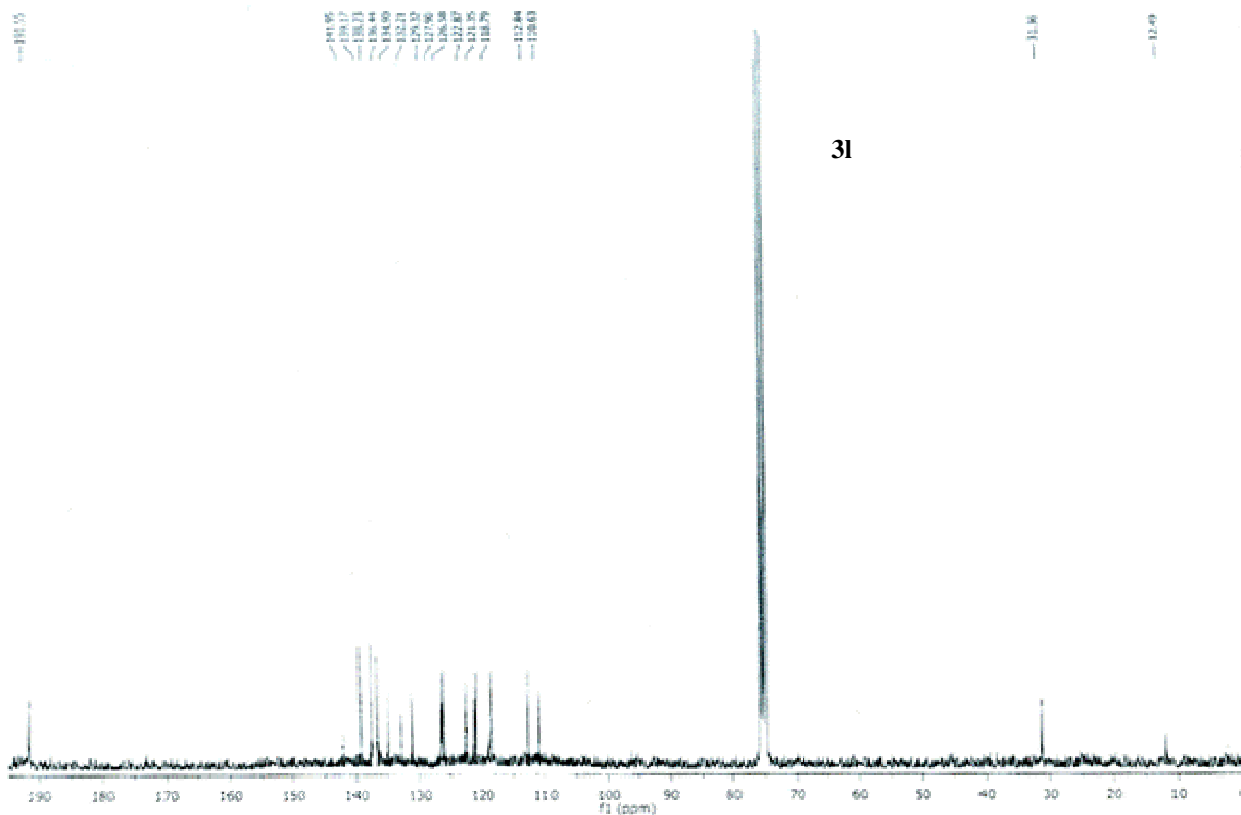
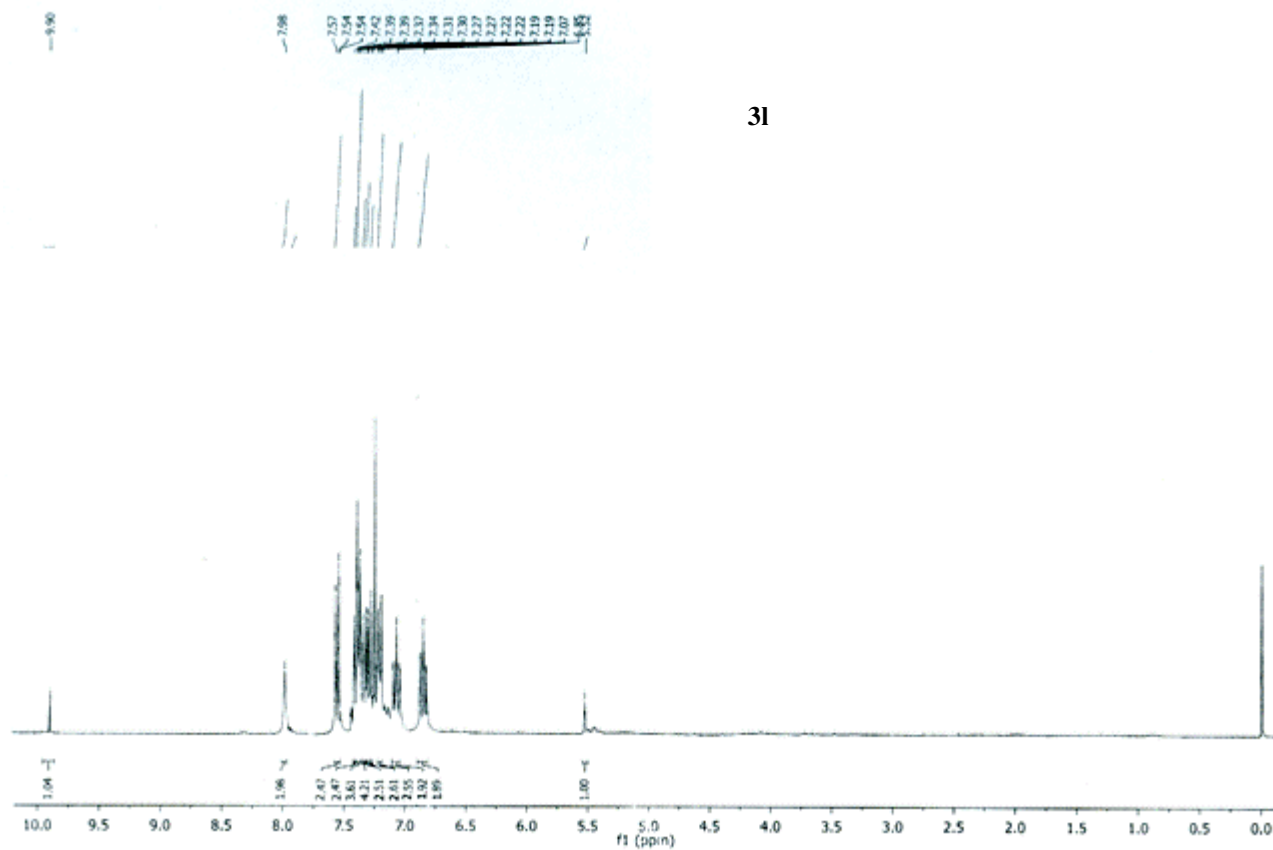
Tolerance:3.00(mmu)

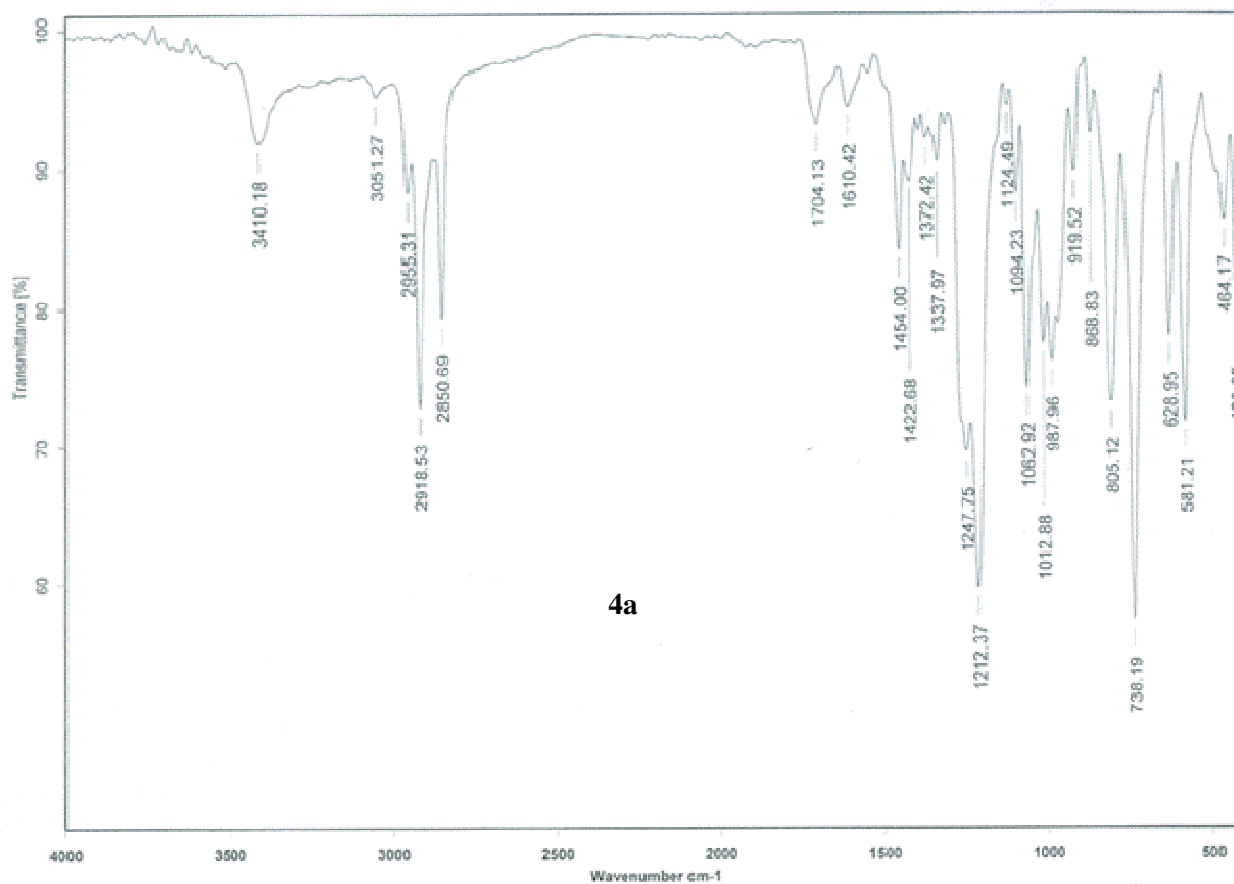
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



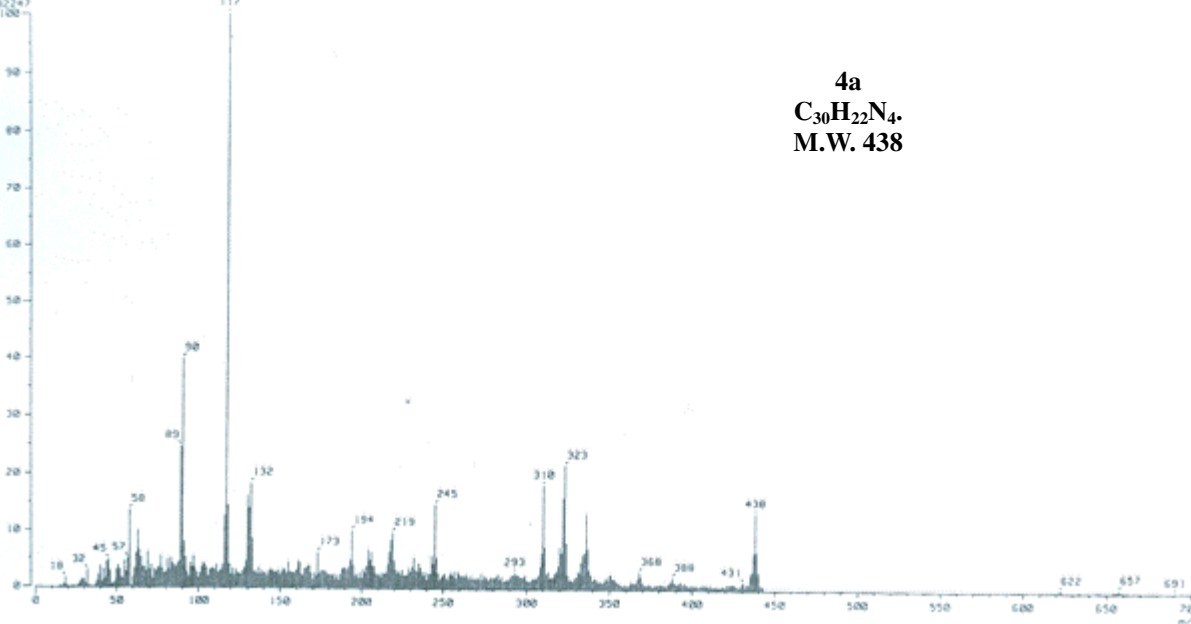
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21120	6693.89	503.21234	-1.13	-2.25	$^{12}C_{36}^{1}H_{27}^{14}N_2^{16}O_1$	24.5







[ Mass Spectrum ]  
 Date : Dr-Lopez-Jose-024 Date : 21-Sep-201  
 Sample: 225 1627 Jeol 4050SAM  
 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...

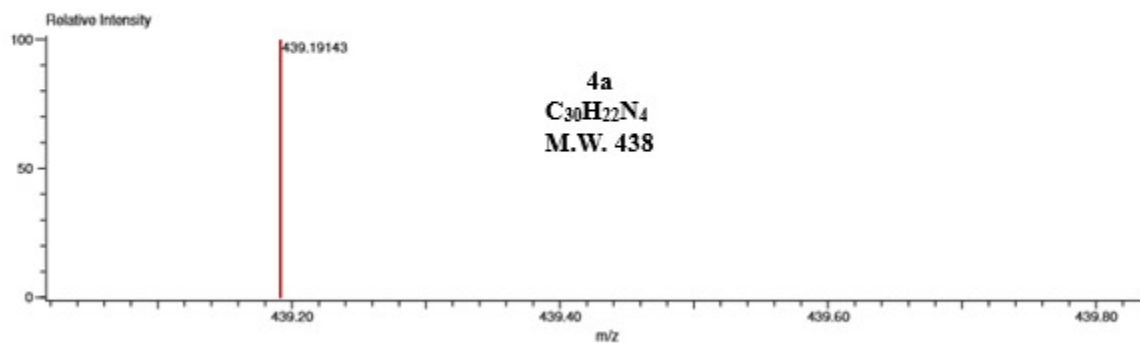
Acquired: 3/31/2016 5:49:59 PM  
 Operator: AccuTOF  
 Mass Calibration data: PEG600  
 Created: 4/11/2016 6:40:29 PM  
 Created by: AccuTOF

Charge number: 1

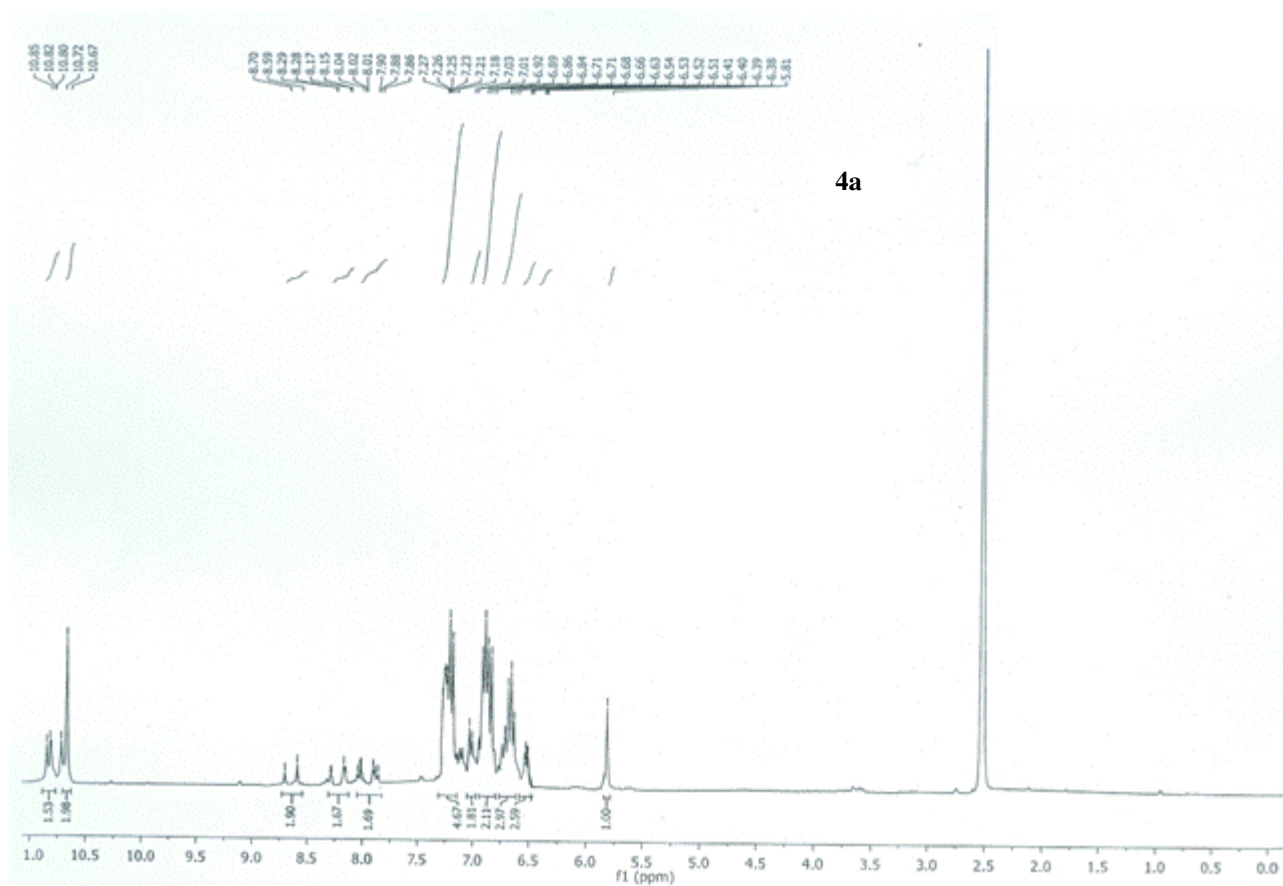
Tolerance: 3.00 (mmu)

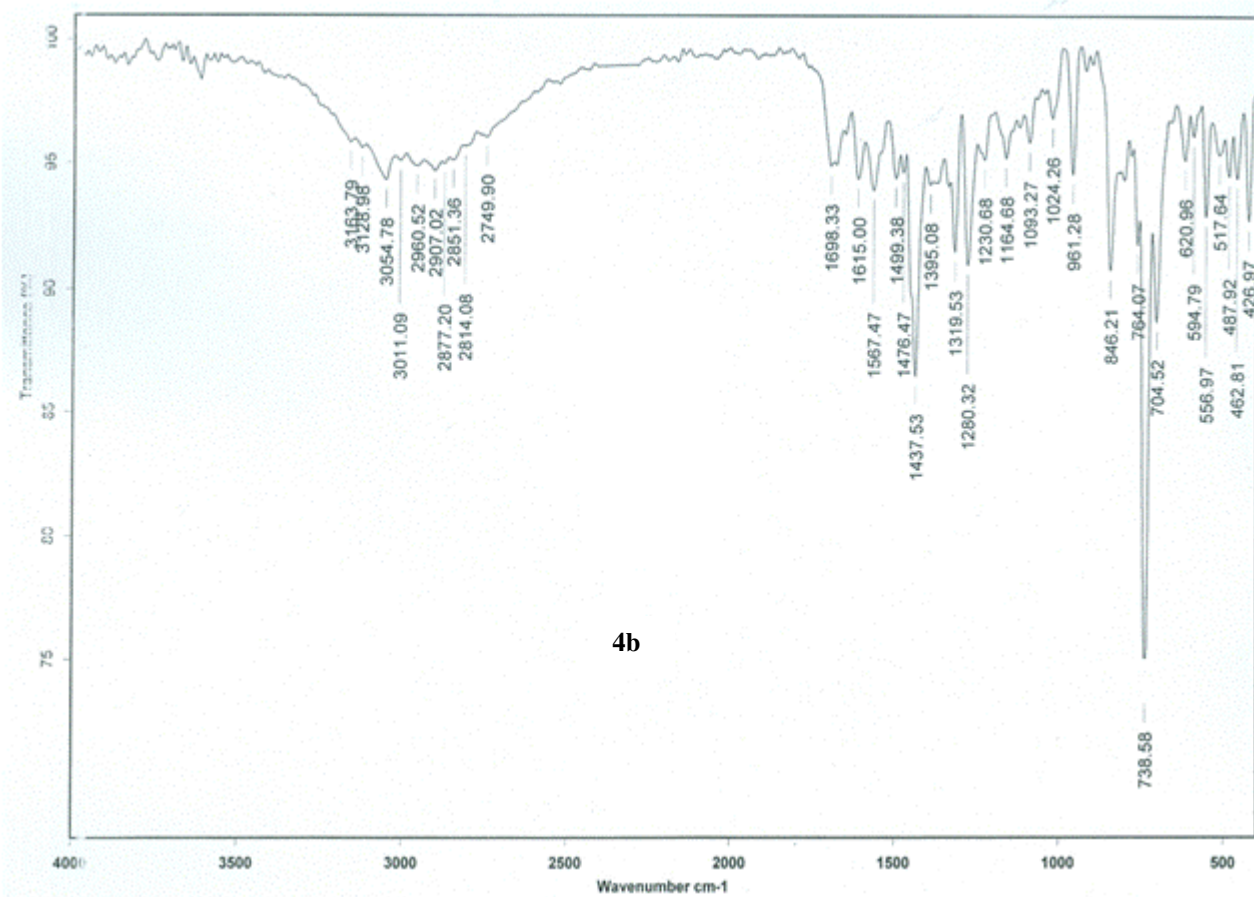
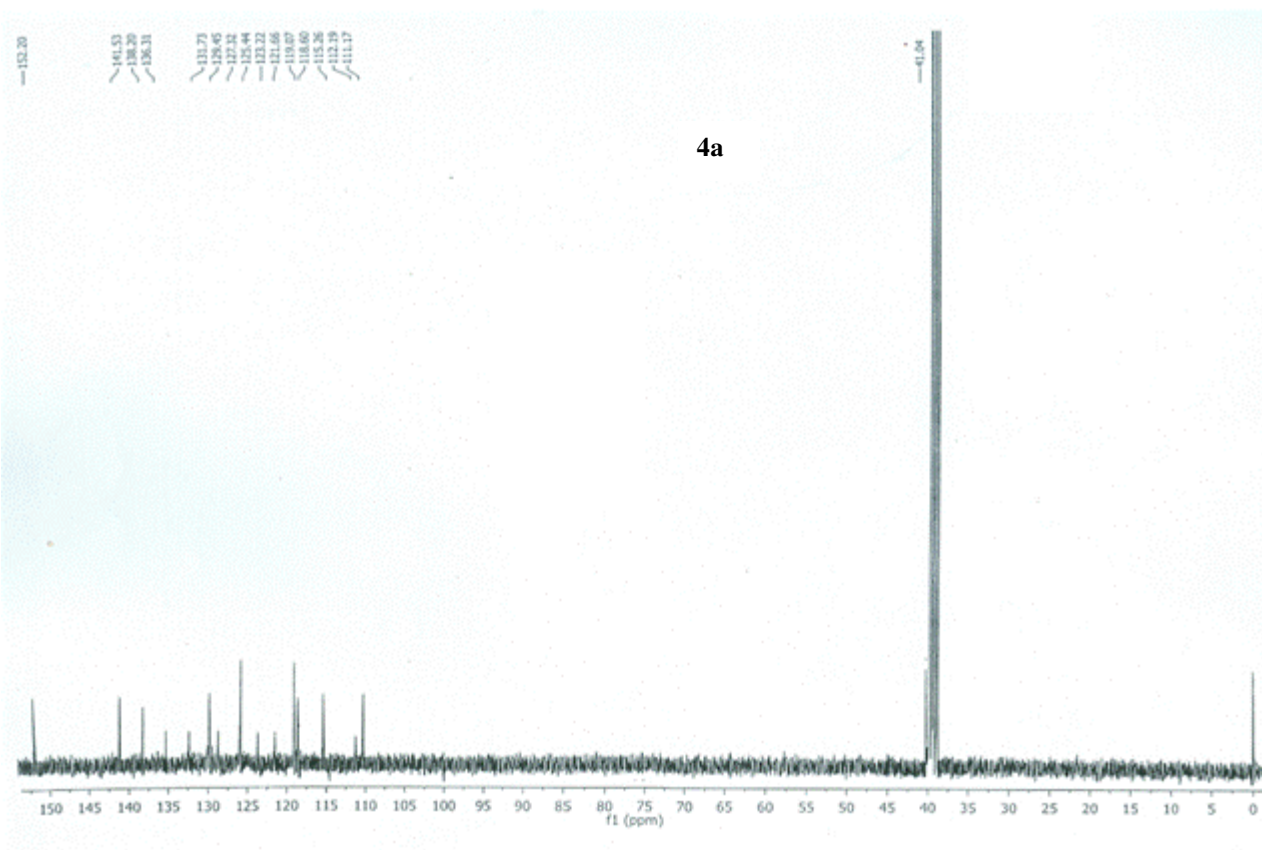
saturation Number: 0.0 .. 32.0 (Fraction: Both)

Element:  $^{13}\text{C}$ : 0 .. 100,  $^1\text{H}$ : 0 .. 100,  $^{14}\text{N}$ : 2 .. 5

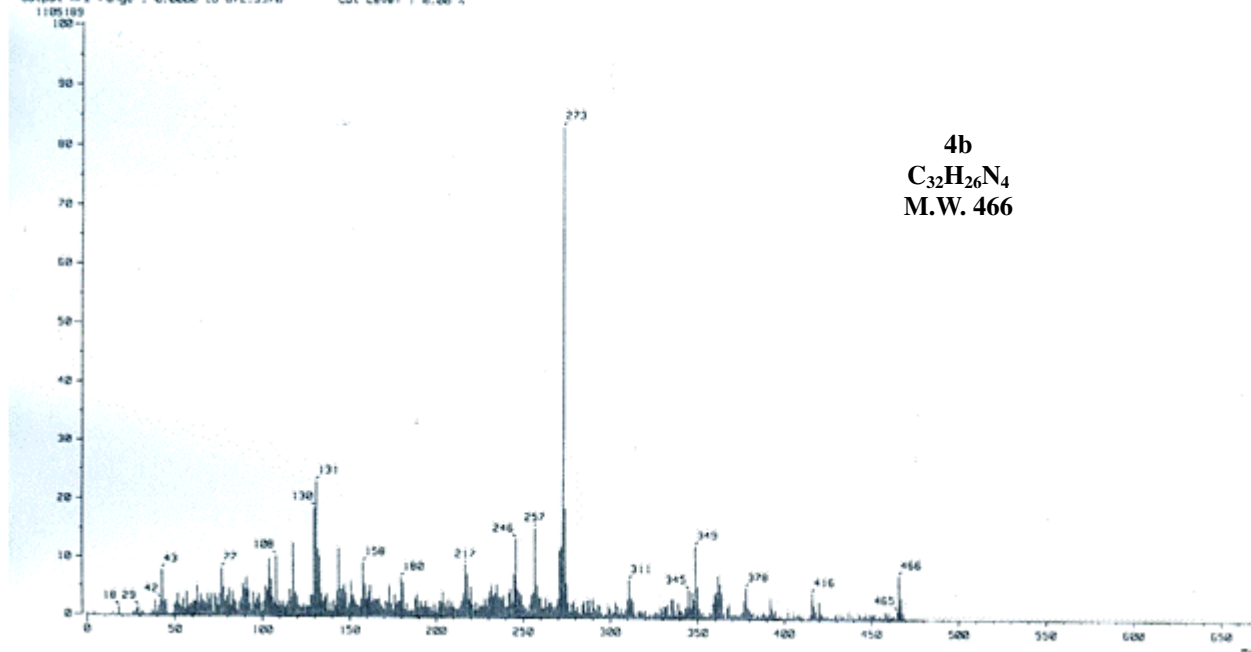


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	$^{12}\text{C}_{30}\text{H}_{22}\text{N}_4$	21.5





Note : Javier Perez  
 Inlet : Direct Ion Mode : ESI+  
 Spectrum Type : Normal Ion (MF-Linear)  
 RT : 1.94 min Scan# : (25,56)  
 BP : m/z 522.0000 Int. : 105.10  
 Output m/z range : 0.0000 to 672.9370 Cut Level : 0.00 %

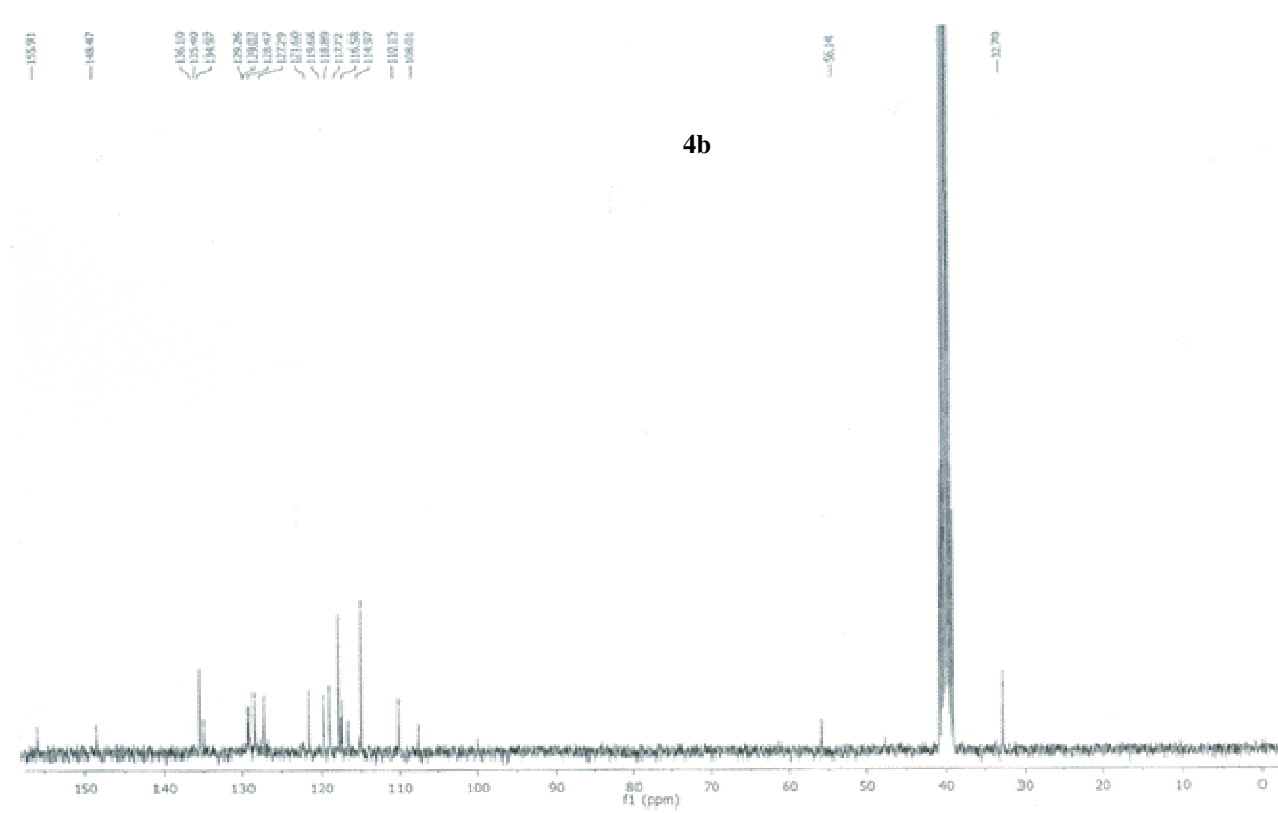
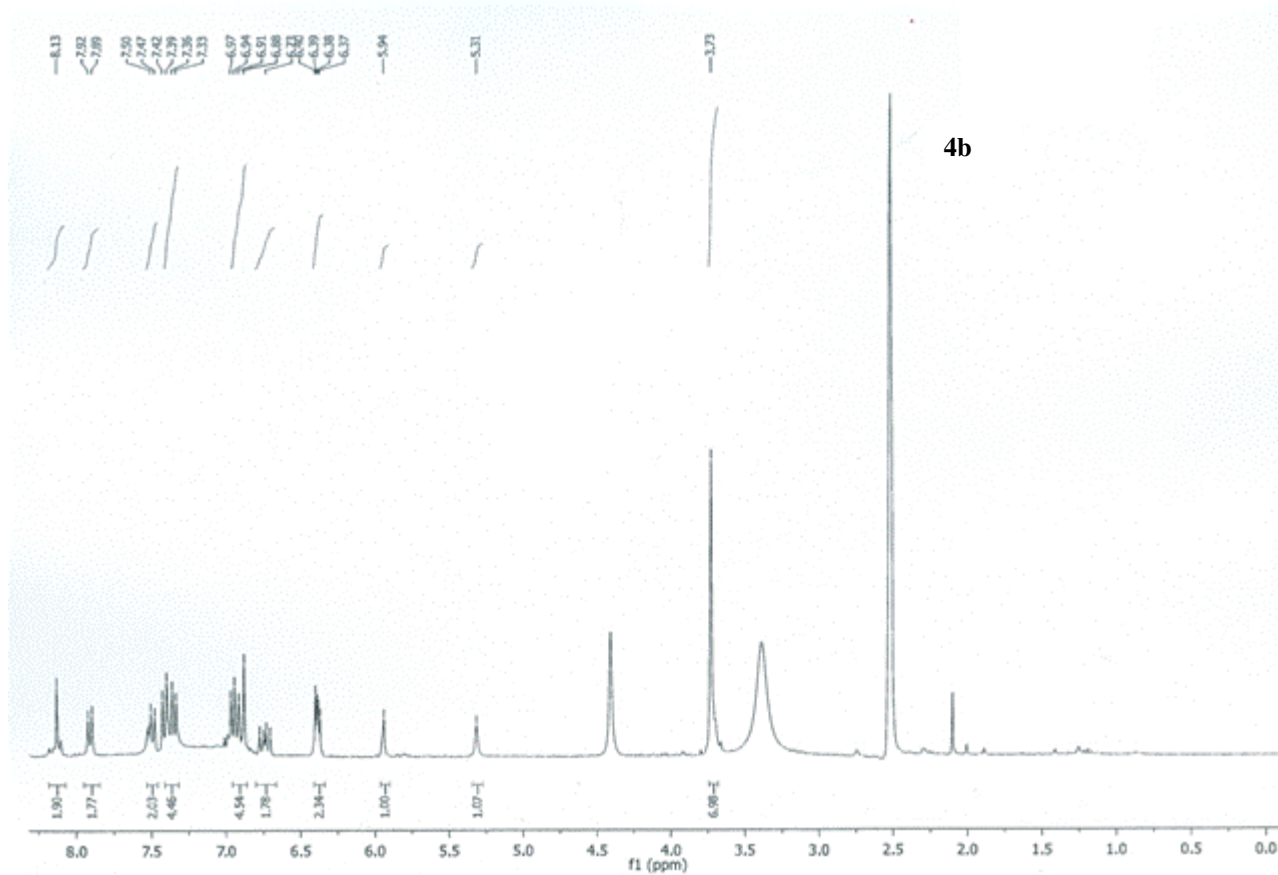


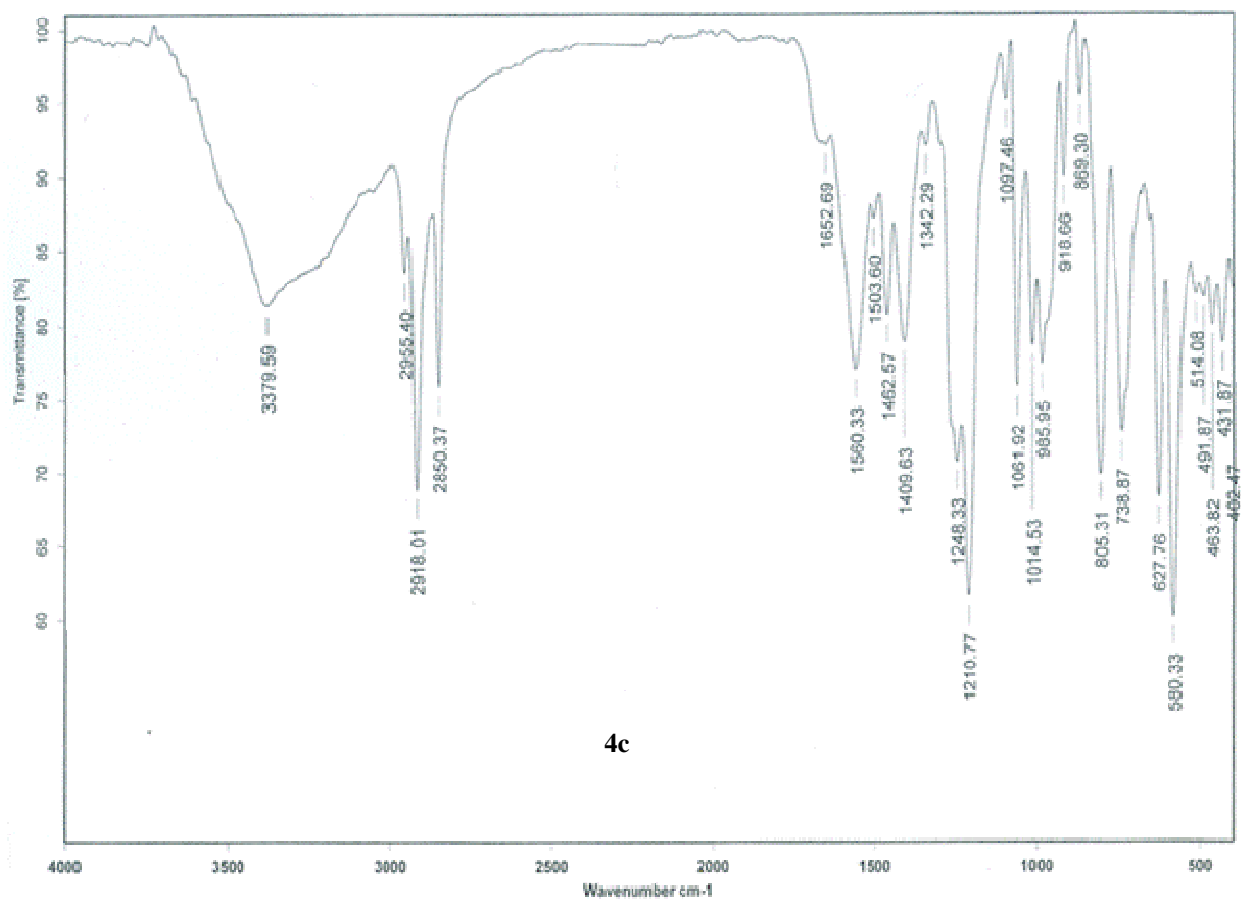
**4b**  
 $C_{32}H_{26}N_4$   
 M.W. 466

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

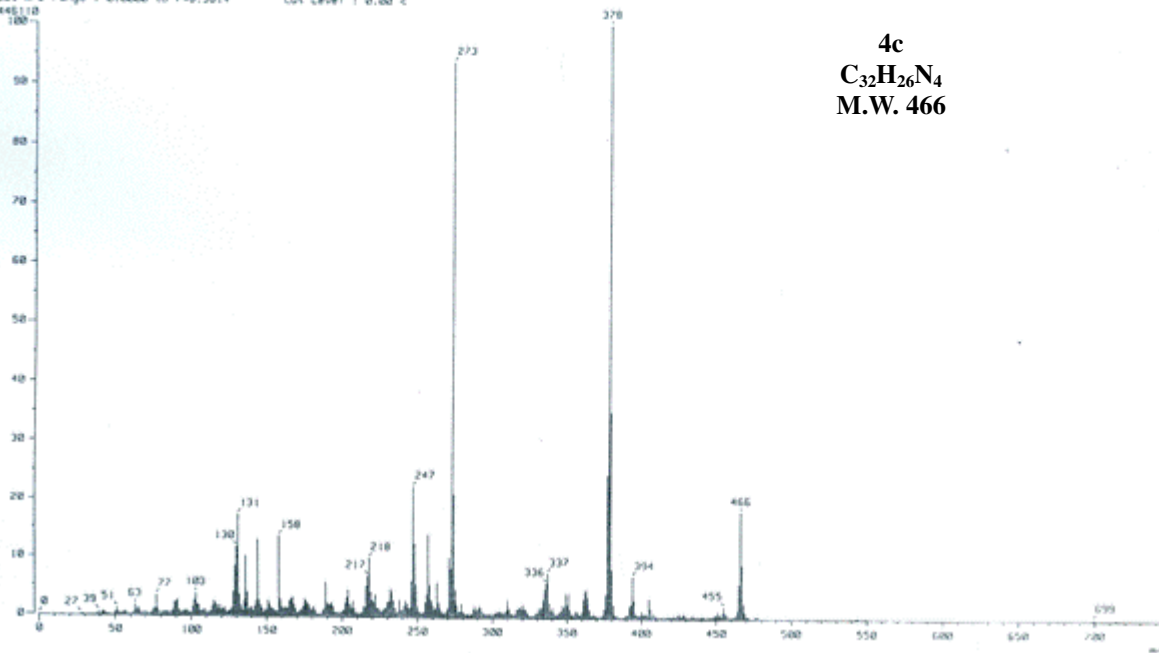
Observed m/z	Int%	Estimated m/z	Err [ppm / mmu]	U.S.	C	H	N
467.2228	68.99	467.2236	-1.7 / -0.8	21.5	32	27	4





4c

[ Mass Spectrum ]  
 Date : Dr-Lopez-Jose-050 Date : 24-May-2012 16:35  
 Sample : 119 IC21 Jeol R030546  
 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

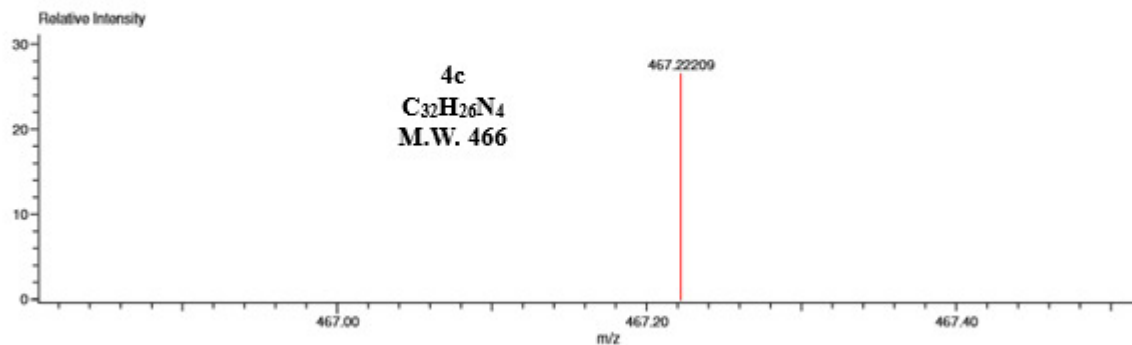
Data: CAT 15  
 Sample Name:  
 Description:  
 Ionization Mode: ESI+  
 History: Determine m/z [Peak Detect [Controid, 30, Area], Correct Base [5.0%], Correct Base [5.0%], Average [MS [1] 2.0...

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

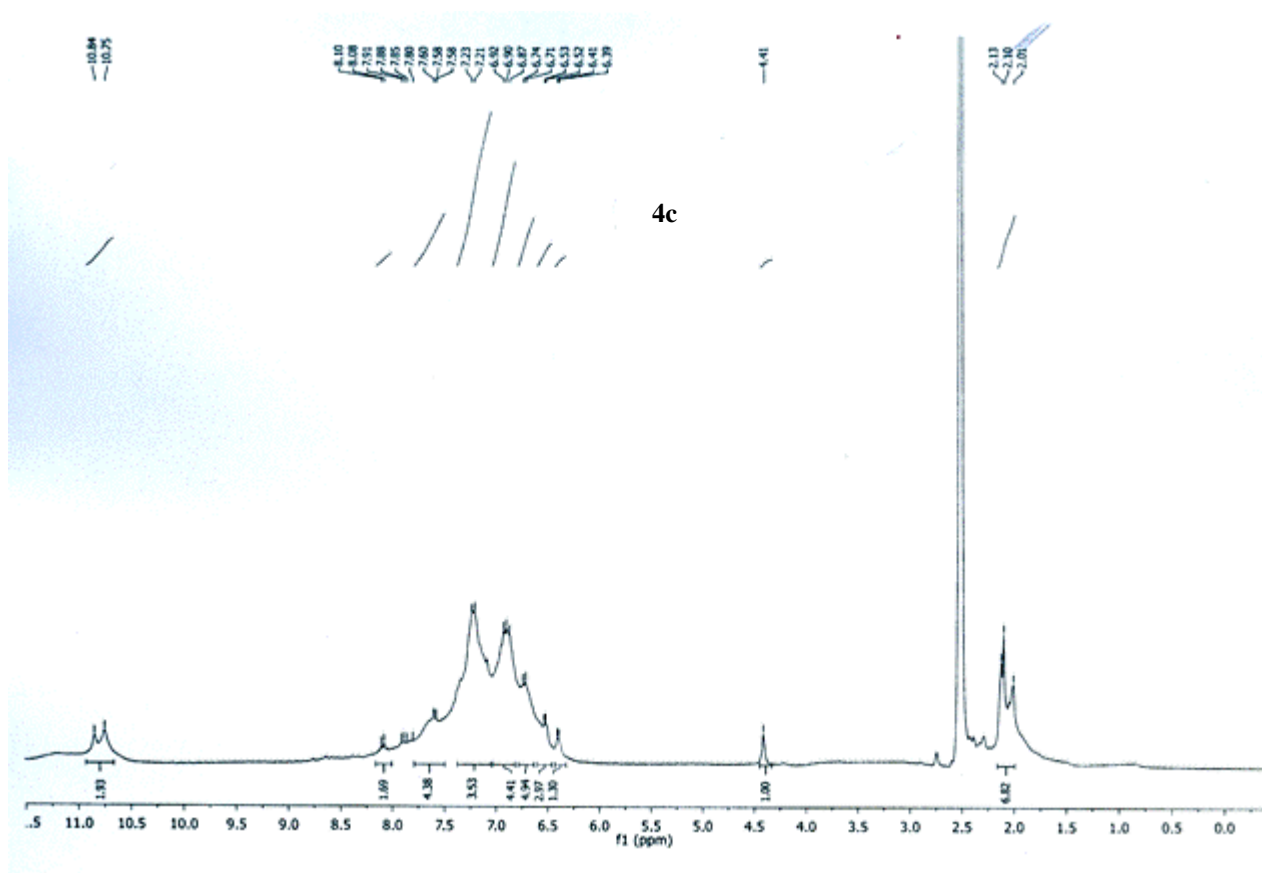
Charge number: 1  
 Element:  $^{12}\text{C}$ : 0 .. 100,  $^1\text{H}$ : 0 .. 100,  $^{14}\text{N}$ : 2 .. 5

Tolerance: 3.00 (mmu)

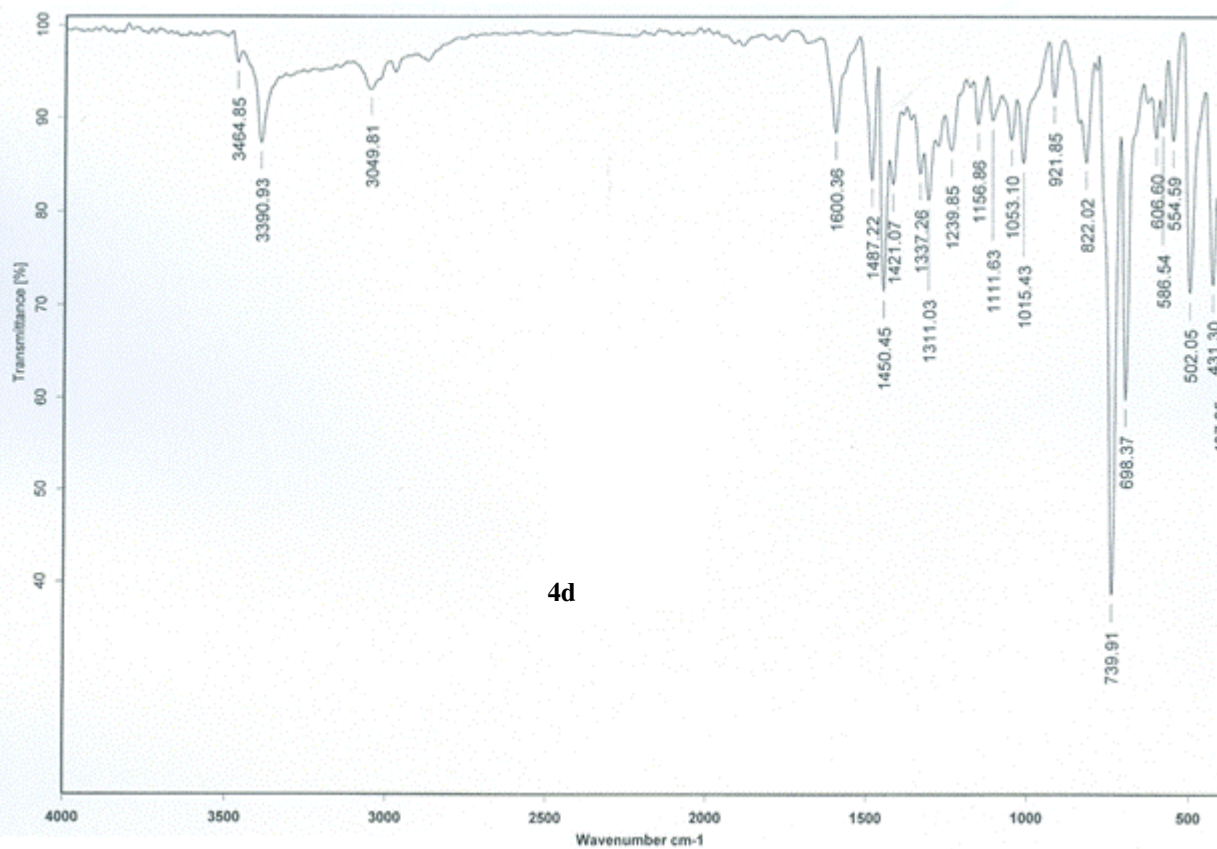
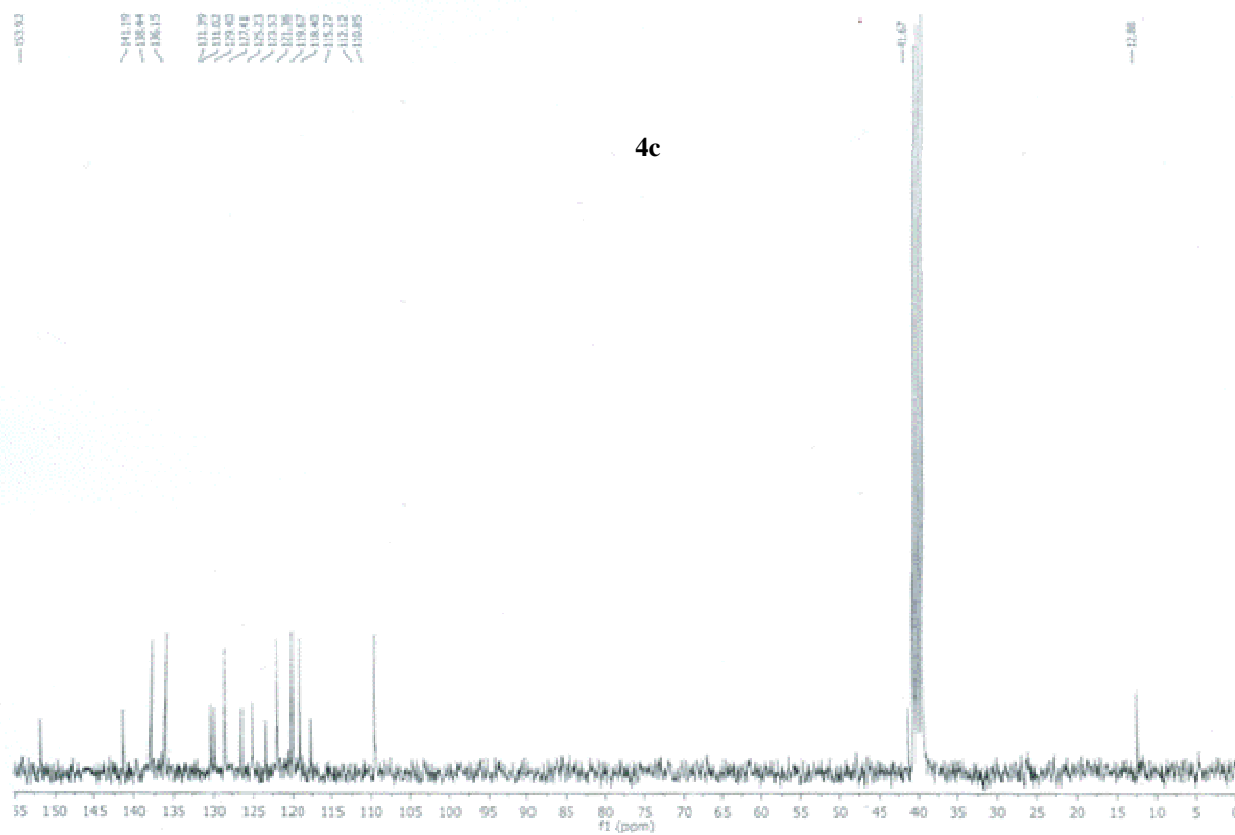
Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)

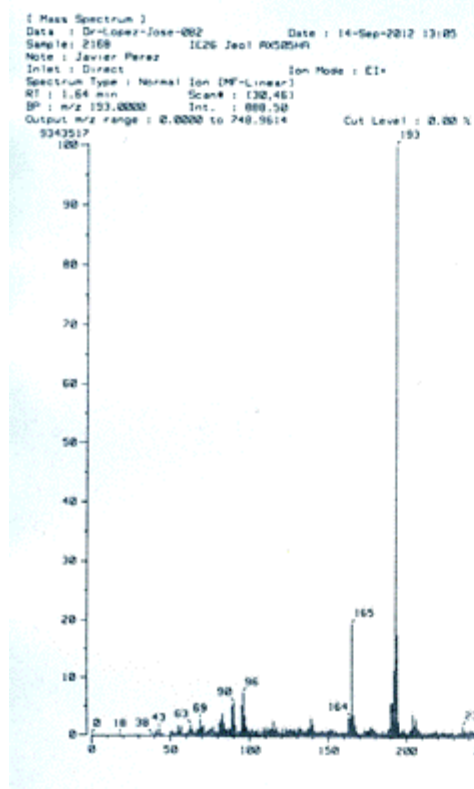


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22209	60294.95	467.22357	-1.46	-3.16	$^{12}\text{C}_{32}\text{H}_{27}\text{N}_4$	21.5









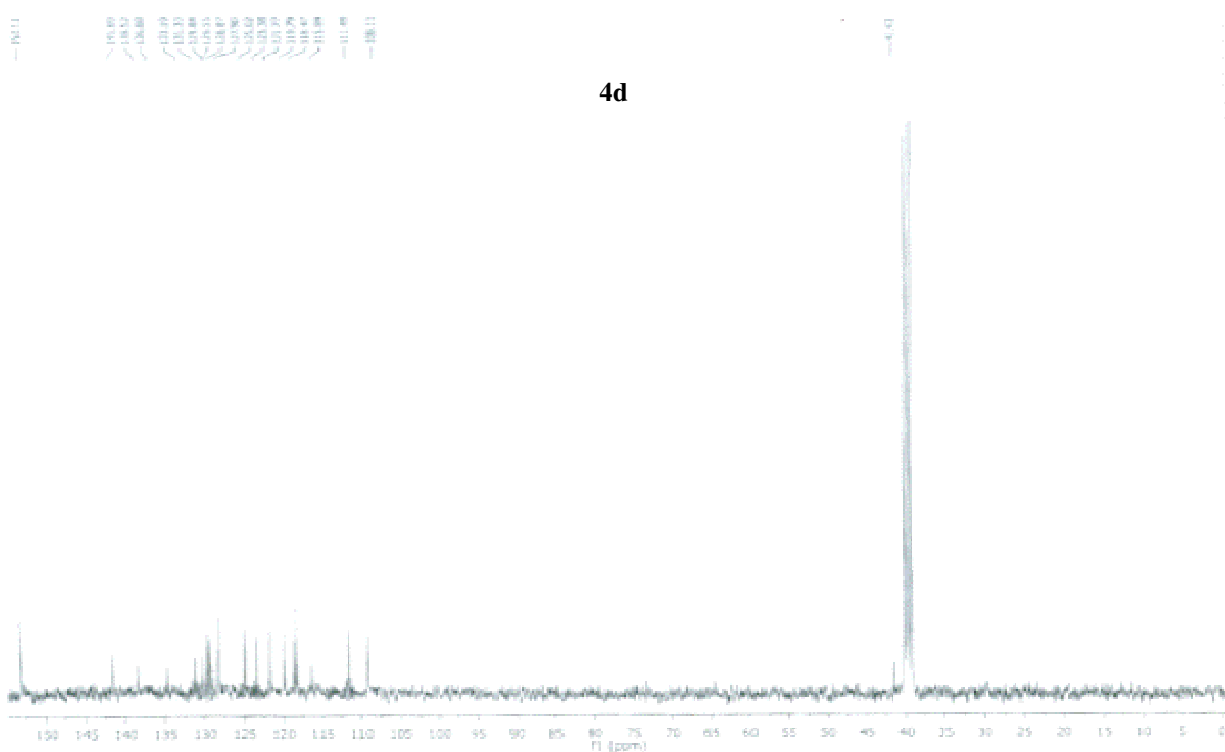
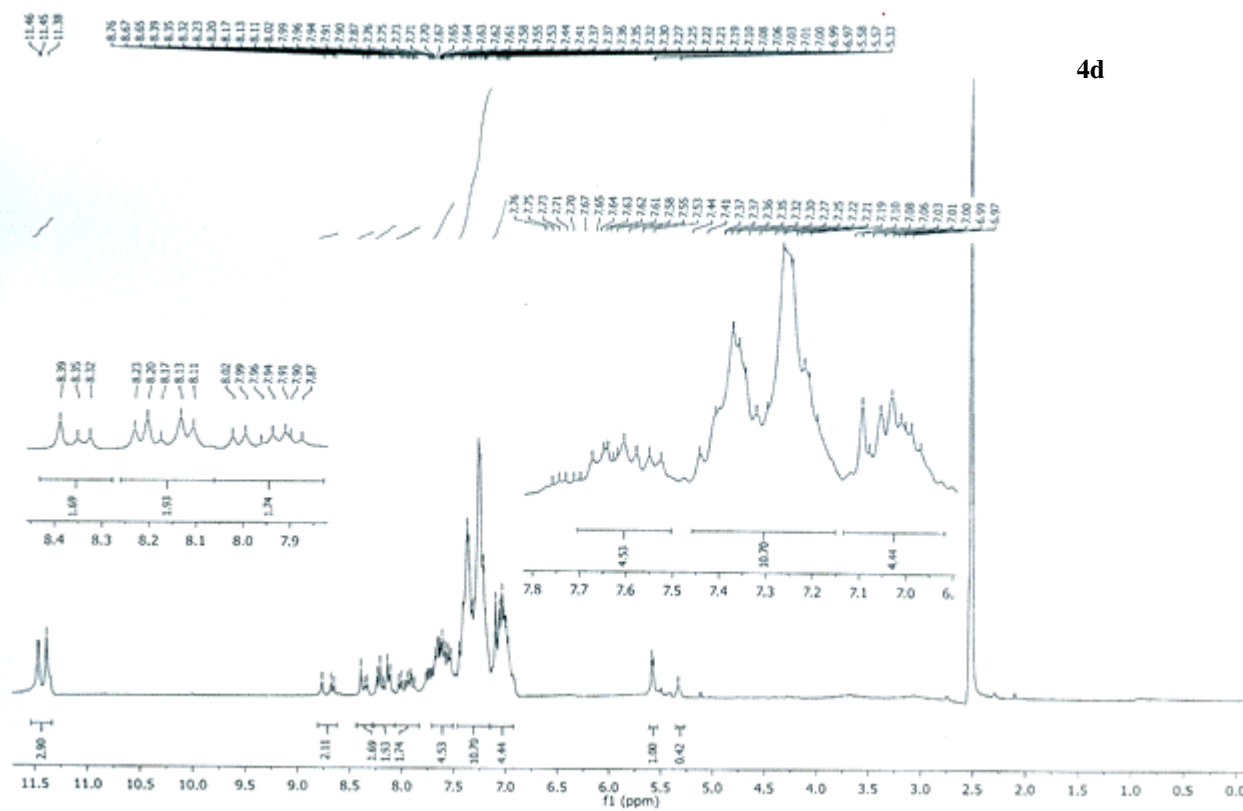
**4d**  
 $C_{42}H_{30}N_4$   
 M.W. 590

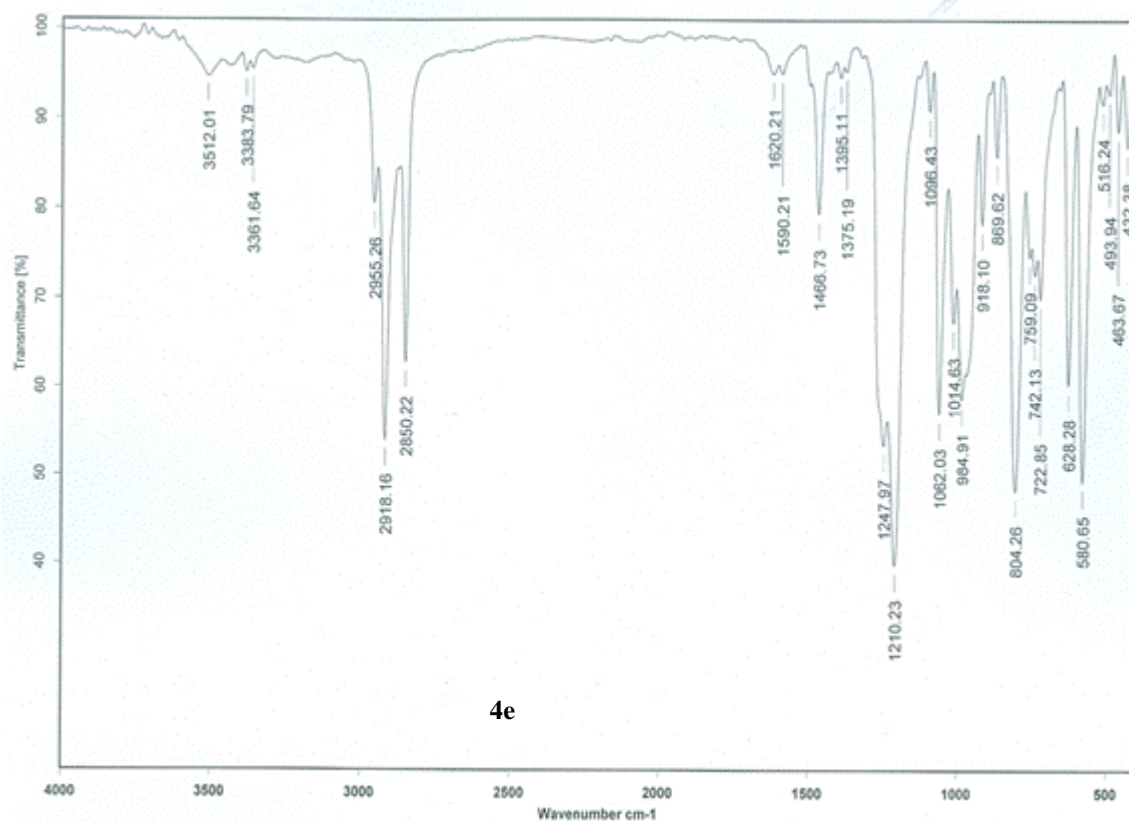
Anal calcd. C 85.40 H 5.12 N 9.48

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

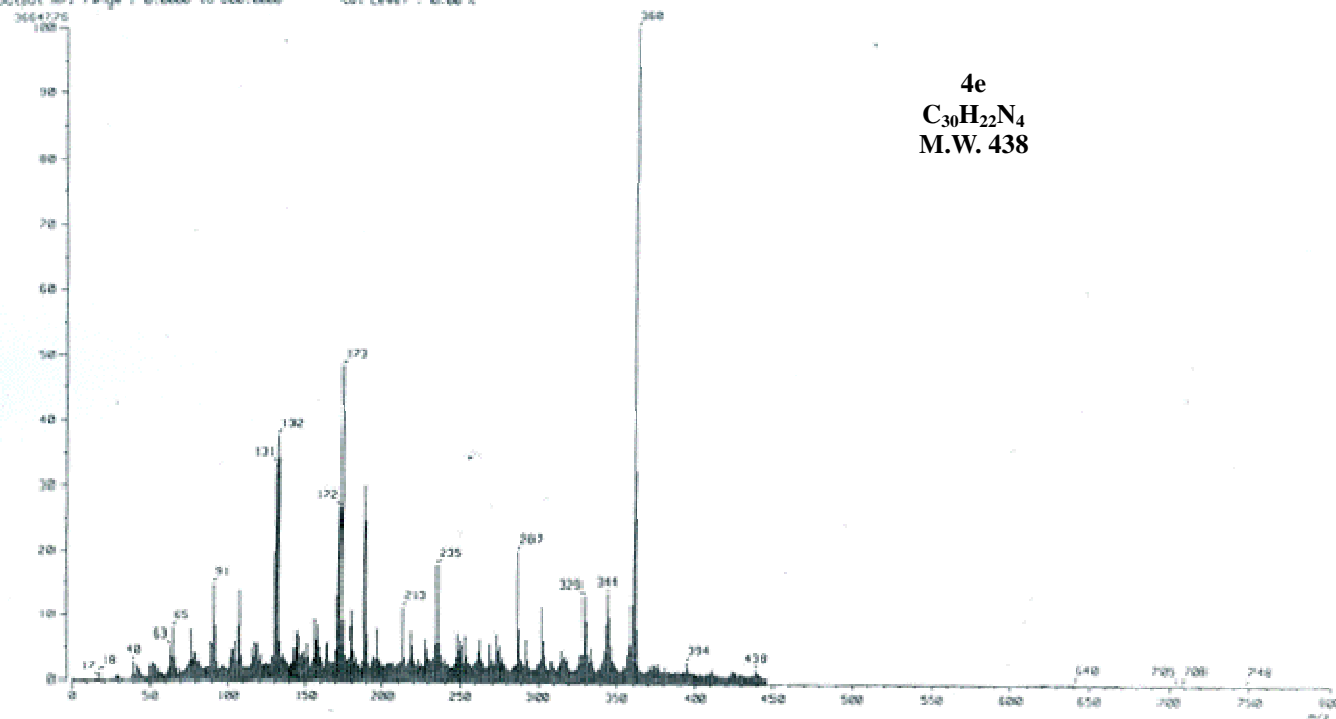
Found

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





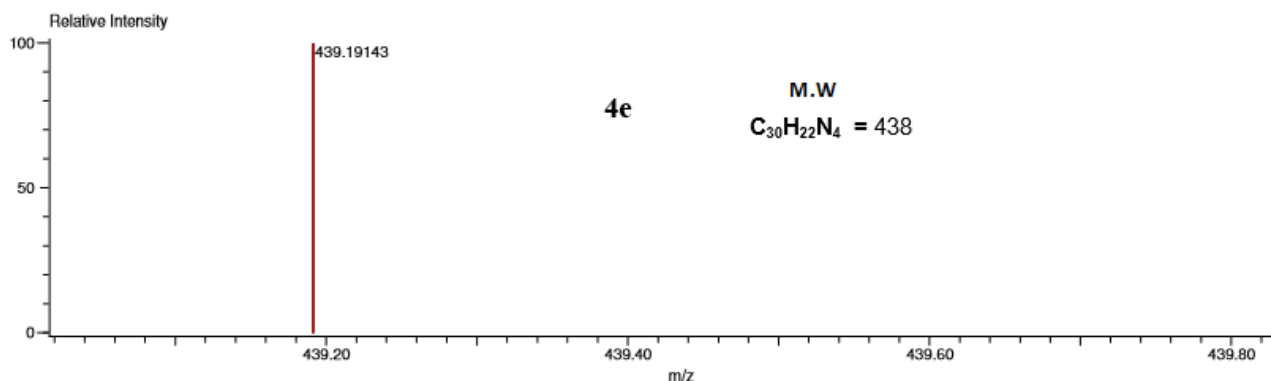
[ Mass Spectrum ]  
 Date : Dr-Rivera-Cecilia-895 Date : 18-Sep-2012 17:59  
 Sample: 2199 IC26 Jsci R55894  
 Note : Javier Perez  
 Inlet : Direct Ion Mode : CI+  
 Spectrum Type : Normal Ion (P1-Linear)  
 RT : 0.69 min Scan : (3,391)  
 BP : m/z 362.0000 Int. : 349.18  
 Output m/z range : 0.0000 to 600.0000  
 Cut Level : 0.00 %



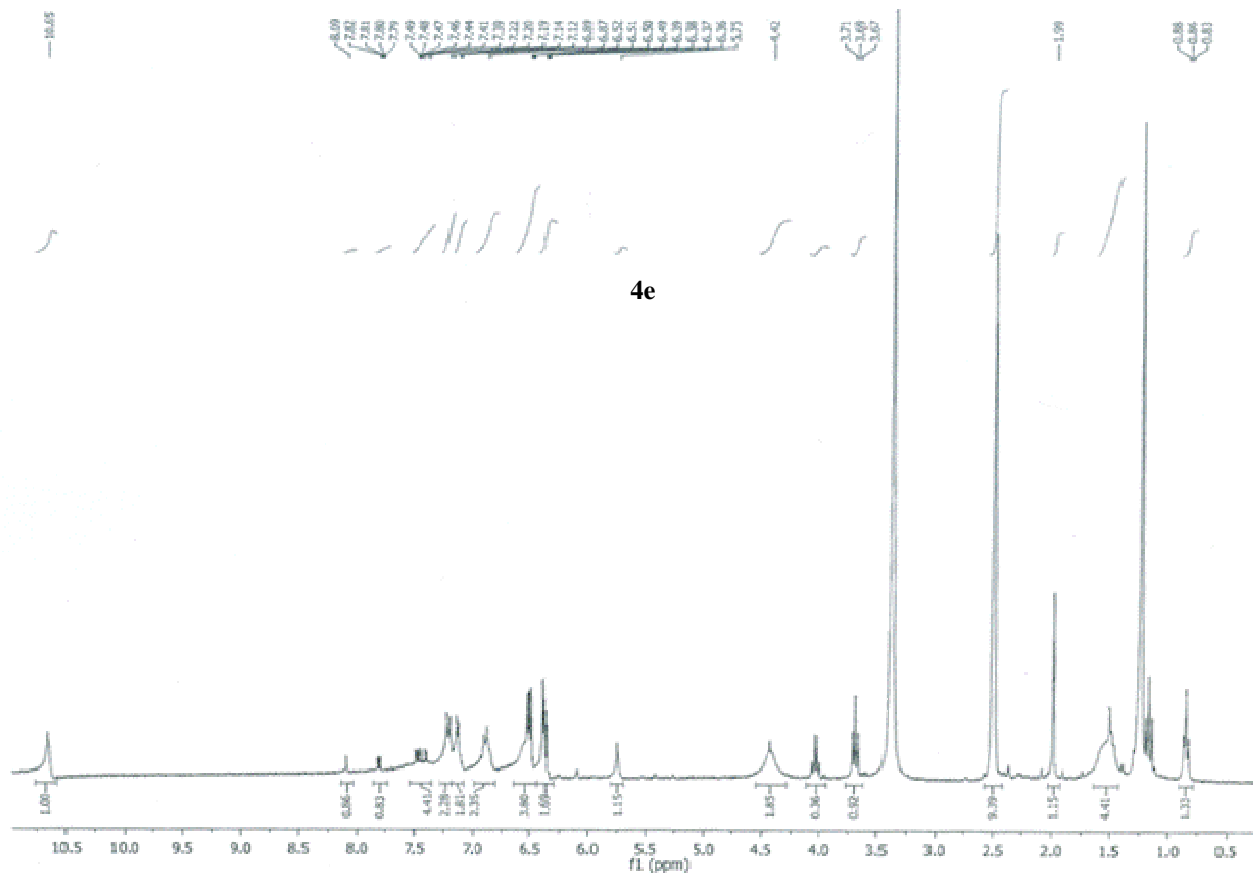
Data: CAT 14  
 Sample Name:  
 Description:  
 Ionization Mode: ESI+  
 History: Determine m/z [Peak Detect [Centroid, 30, Area]; Correct Base [5.0%]; Correct Base [5.0%]; Average [MS[1]] 2.6...

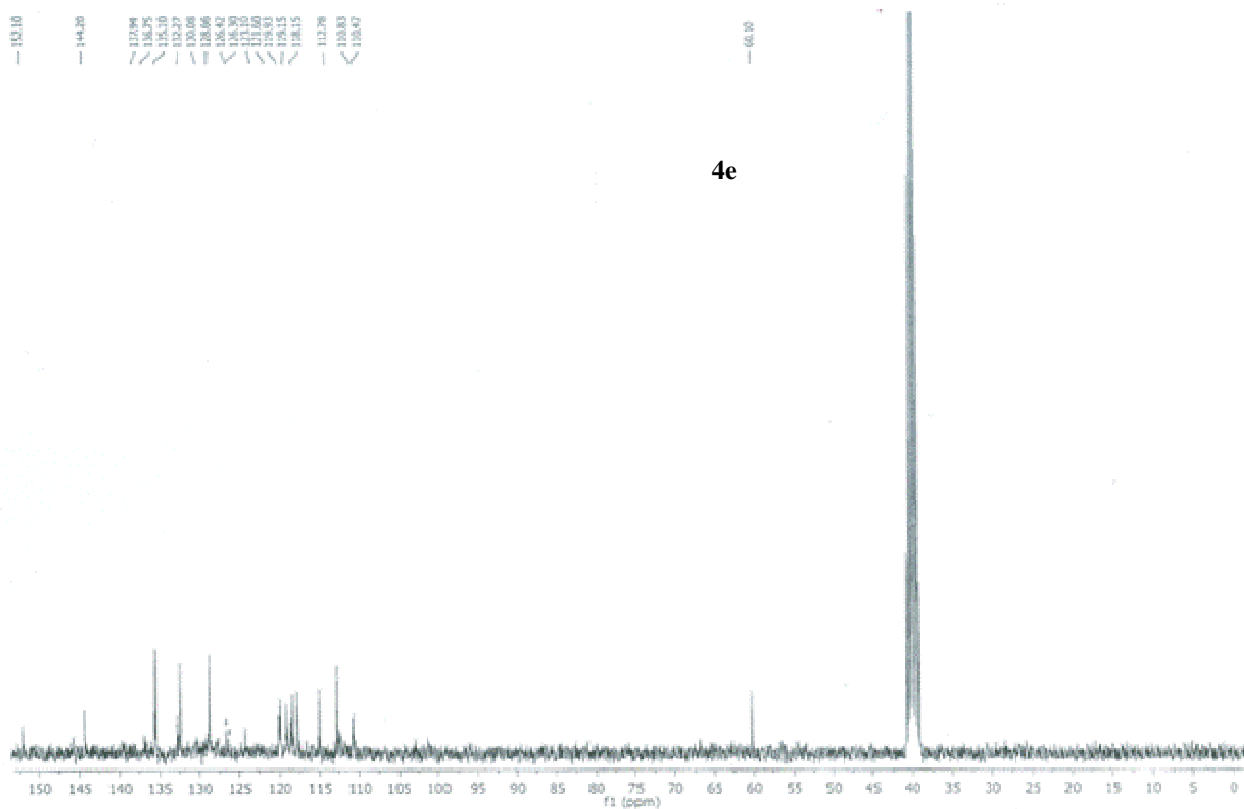
Acquired: 3/31/2016 5:49:59 PM  
 Operator: AccuTOF  
 Mass Calibration data: PEG600  
 Created: 4/11/2016 6:40:29 PM  
 Created by: AccuTOF

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

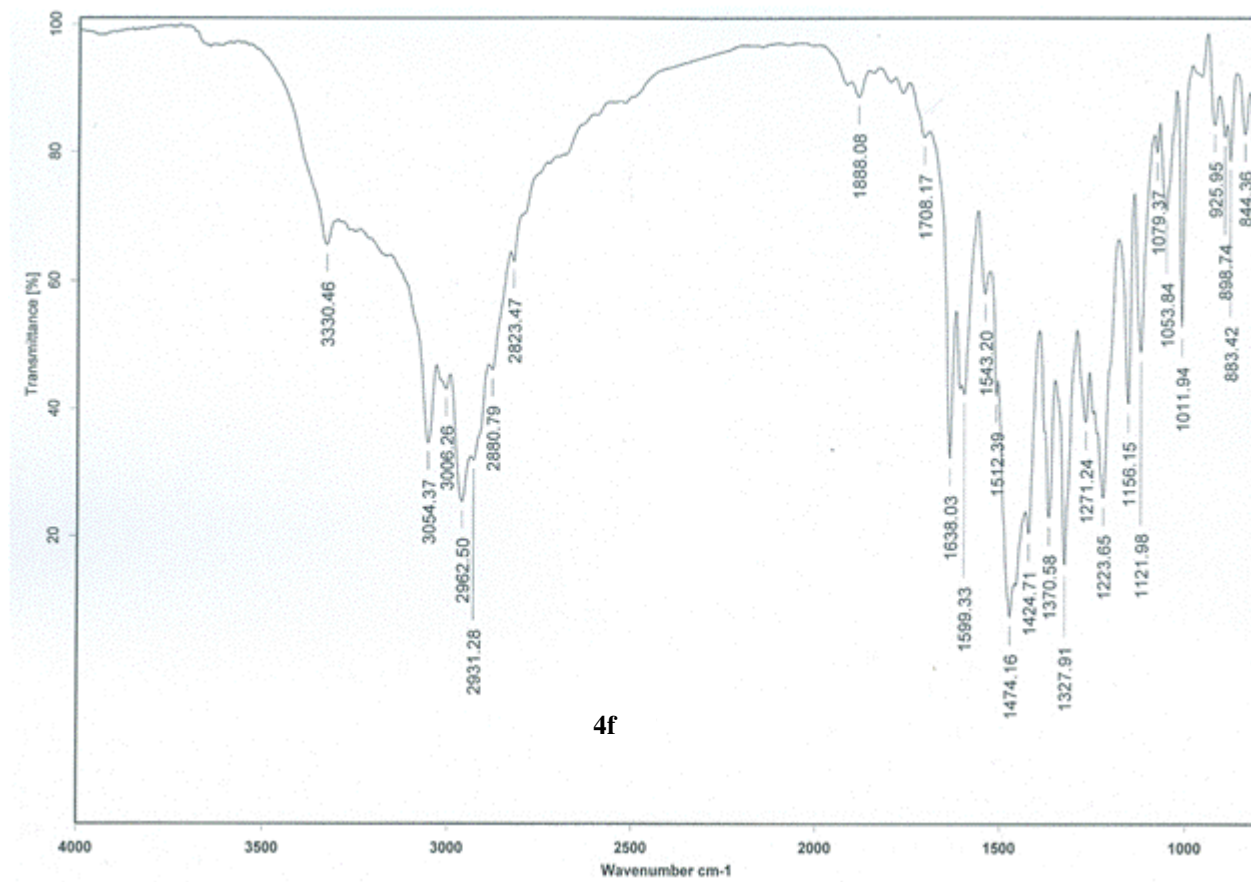


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	<sup>12</sup> C <sub>30</sub> <sup>1</sup> H <sub>22</sub> <sup>14</sup> N <sub>4</sub>	21.5



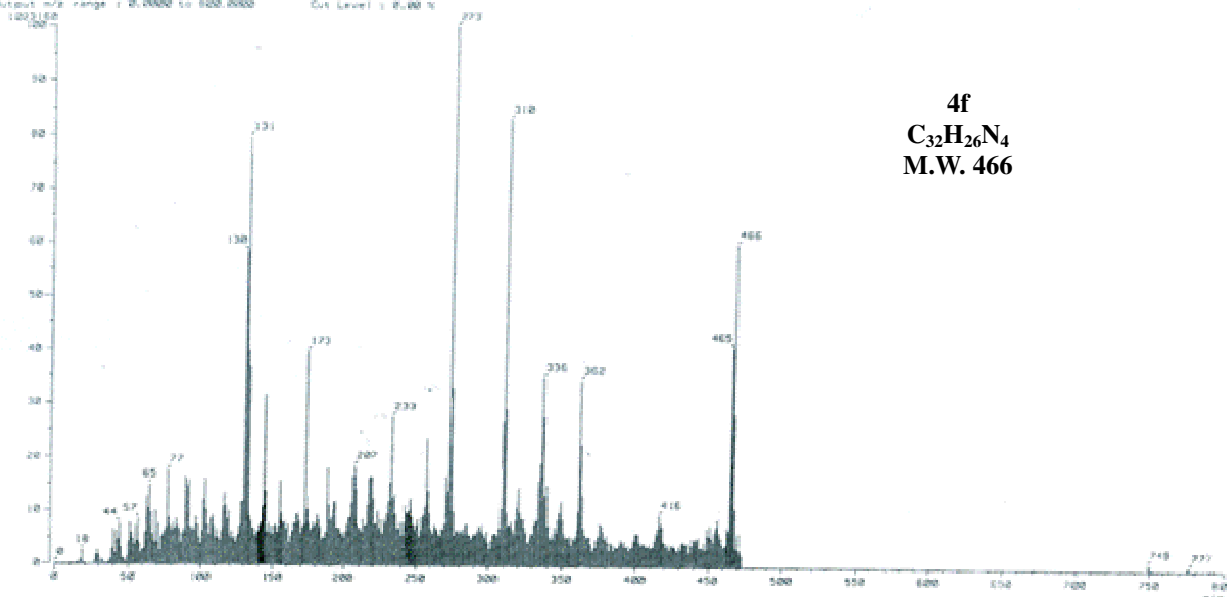


4e



4f

1 Mass Spectrum 3  
 Date : De-Loper-Jose-003 Date : 21-Sep-2016 11:17  
 Sample : 2750 ICP Job: 04503-A  
 MSID : Javier Perez ICP Job: 04503-A  
 Inlet : Direct Ion Mode : ESI+  
 Spectrum Type : Normal Scan (97.500e3)  
 RT : 0.34 min Scan : 110.793  
 BP : 0.02 273.00000 Det. : 97.50  
 Output m/z range : 0.00000 to 800.00000 Cut Level : 0.00 %



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

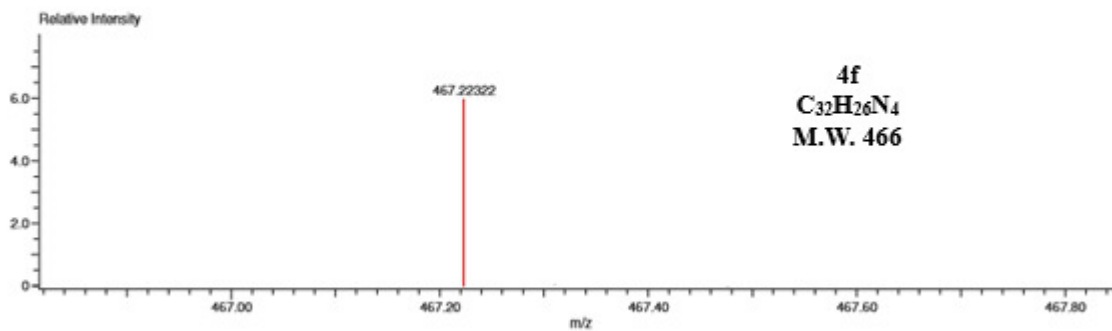
Data:CAT 17  
 Sample Name:  
 Description:  
 Ionization Mode:ESI+  
 History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%];Correct Base[5.0%];Average[MS[1] 0.7...

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

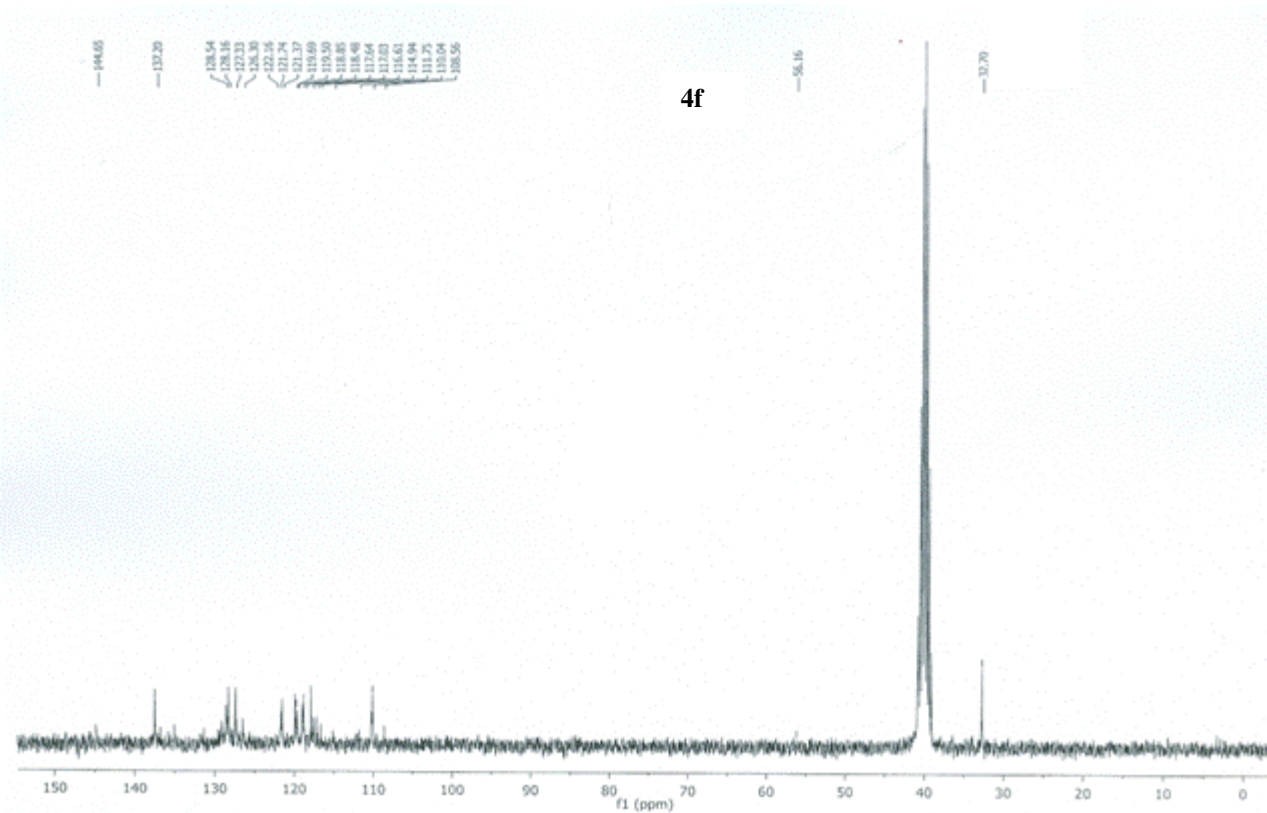
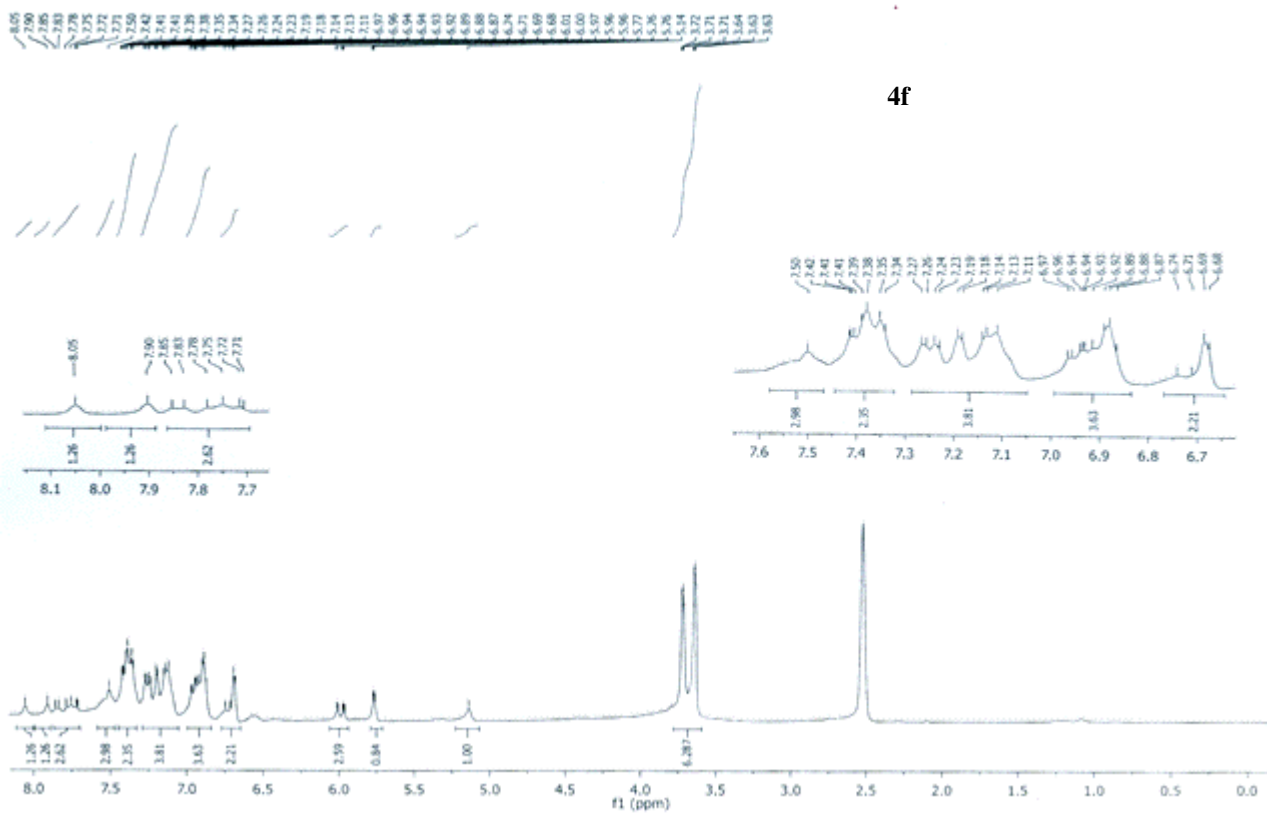
Tolerance:3.00(mmu)

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

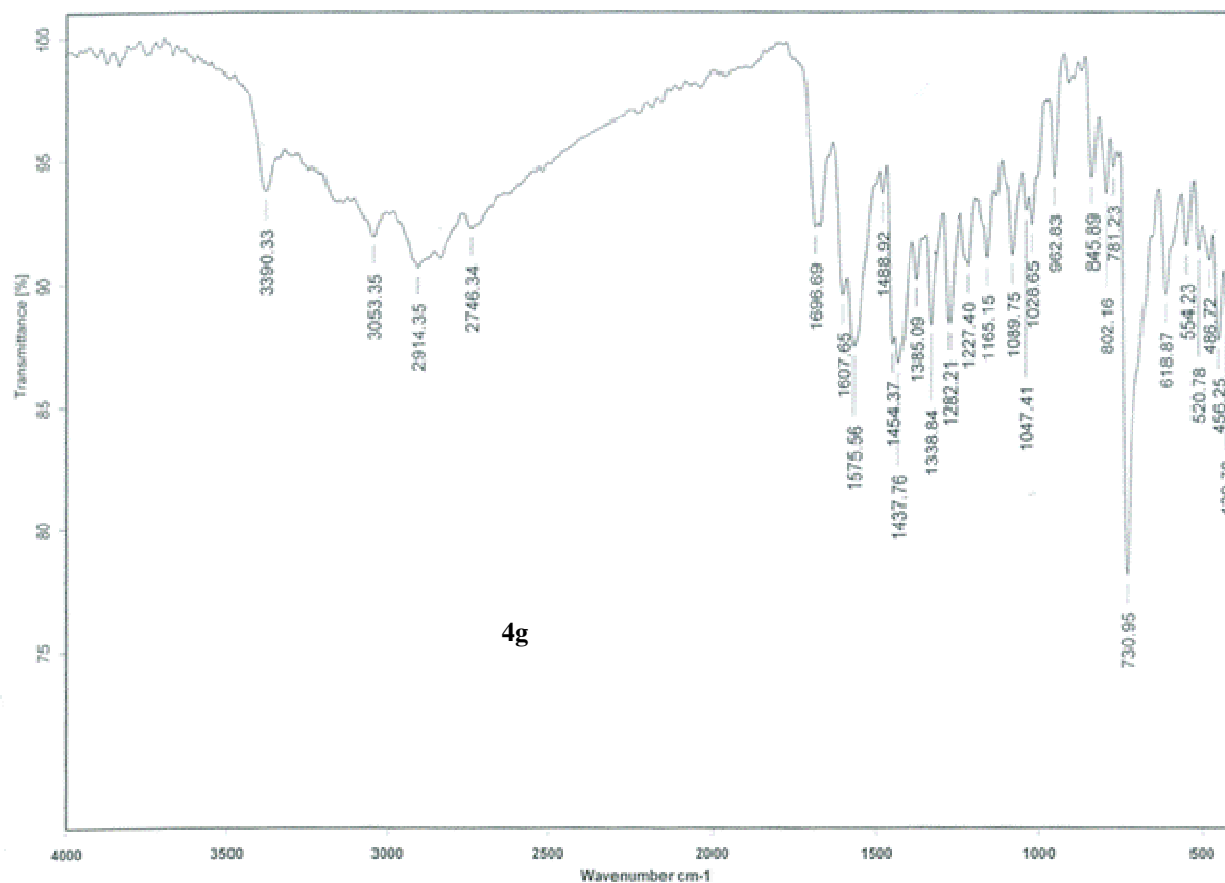


**4f**  
 $C_{32}H_{26}N_4$   
 M.W. 466

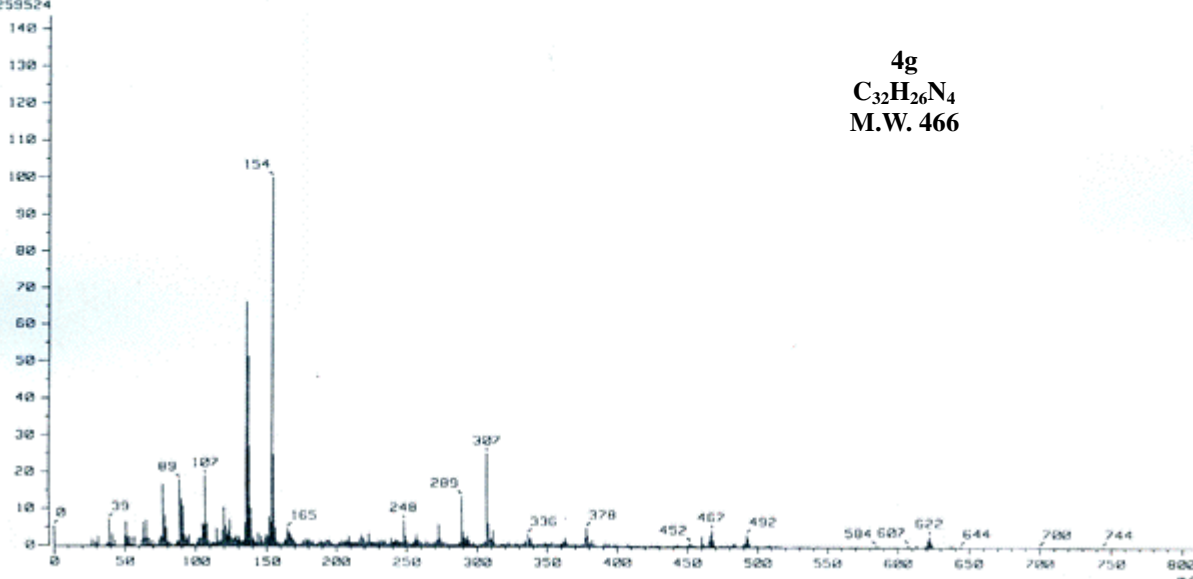
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22322	3587.26	467.22357	-0.35	-0.74	$^{13}C_{32}H_{26}^{14}N_4$	21.5







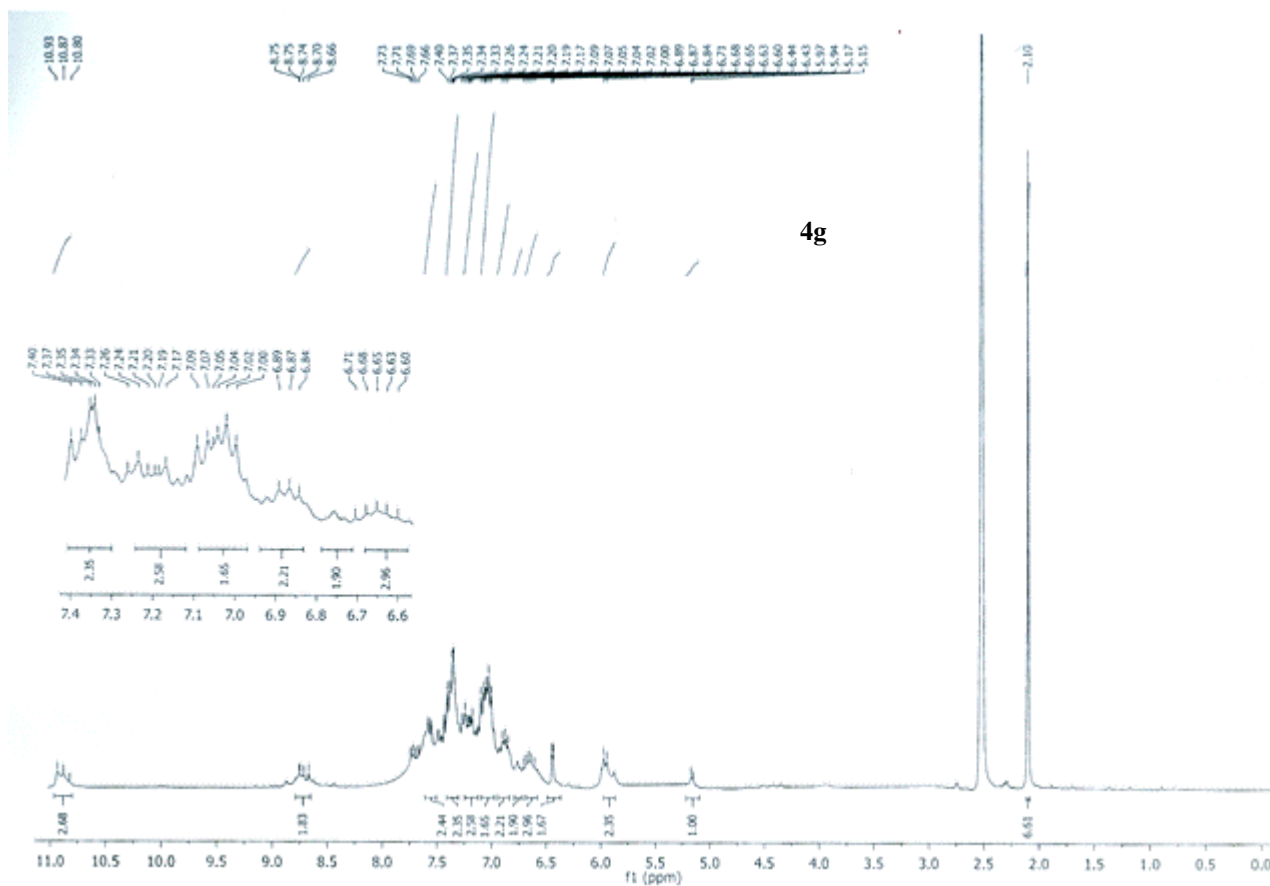
• [ Mass Spectrum ]  
 Date : 17-Oct-2012 11:00  
 Sample: 2398  
 Note : luis-velasco  
 Inlet : Direct Ion Mode : FRB+  
 Spectrum Type : Normal Ion (MF-Linear)  
 RT : 2.47 min Scan# : (3,15)  
 BP : m/z 154.00000 Int. : 216.88  
 Output m/z range : 0.00000 to 815.5786 Cut Level : 0.28 %

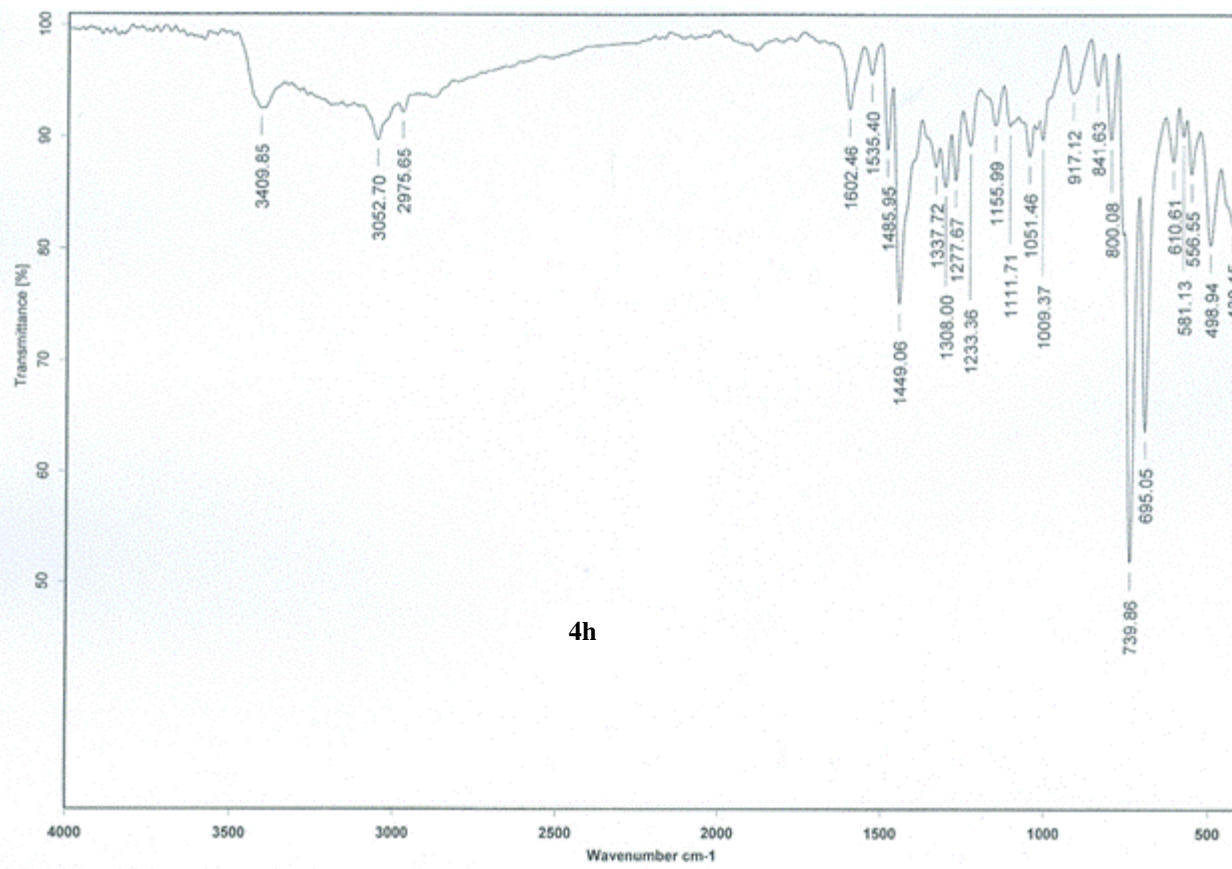
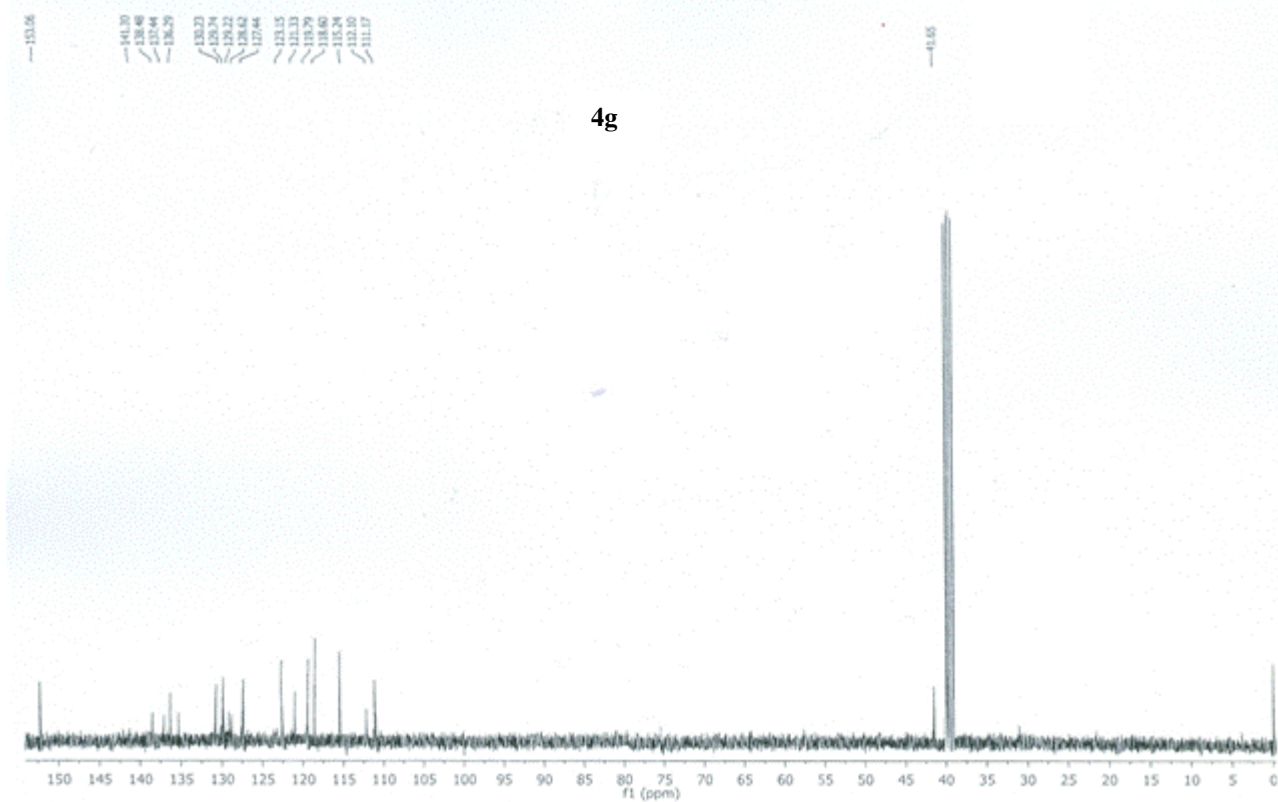


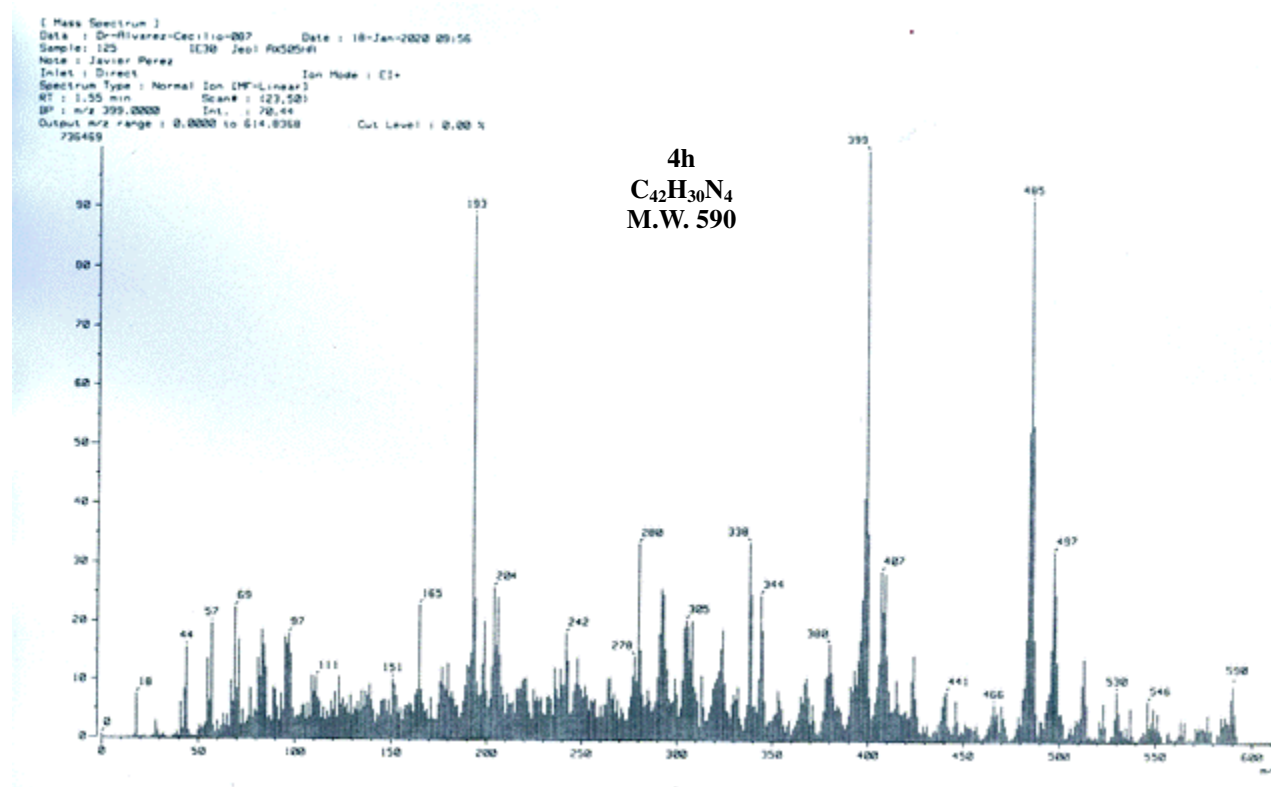
Data : Dr Cecilio Alvarez031 Date : 29-Oct-2015 16:00  
 Instrument : MStation  
 Sample : 3276 2-Me-bz-m  
 Note : -  
 Inlet : Direct Ion Mode : FAB+  
 RT : 3.59 min Scan# : (26,48)  
 Elements : C 34/0, H 49/0, N 5/0  
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1  
 Unsaturation (U.S.) : -0.5 - 34.0

**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







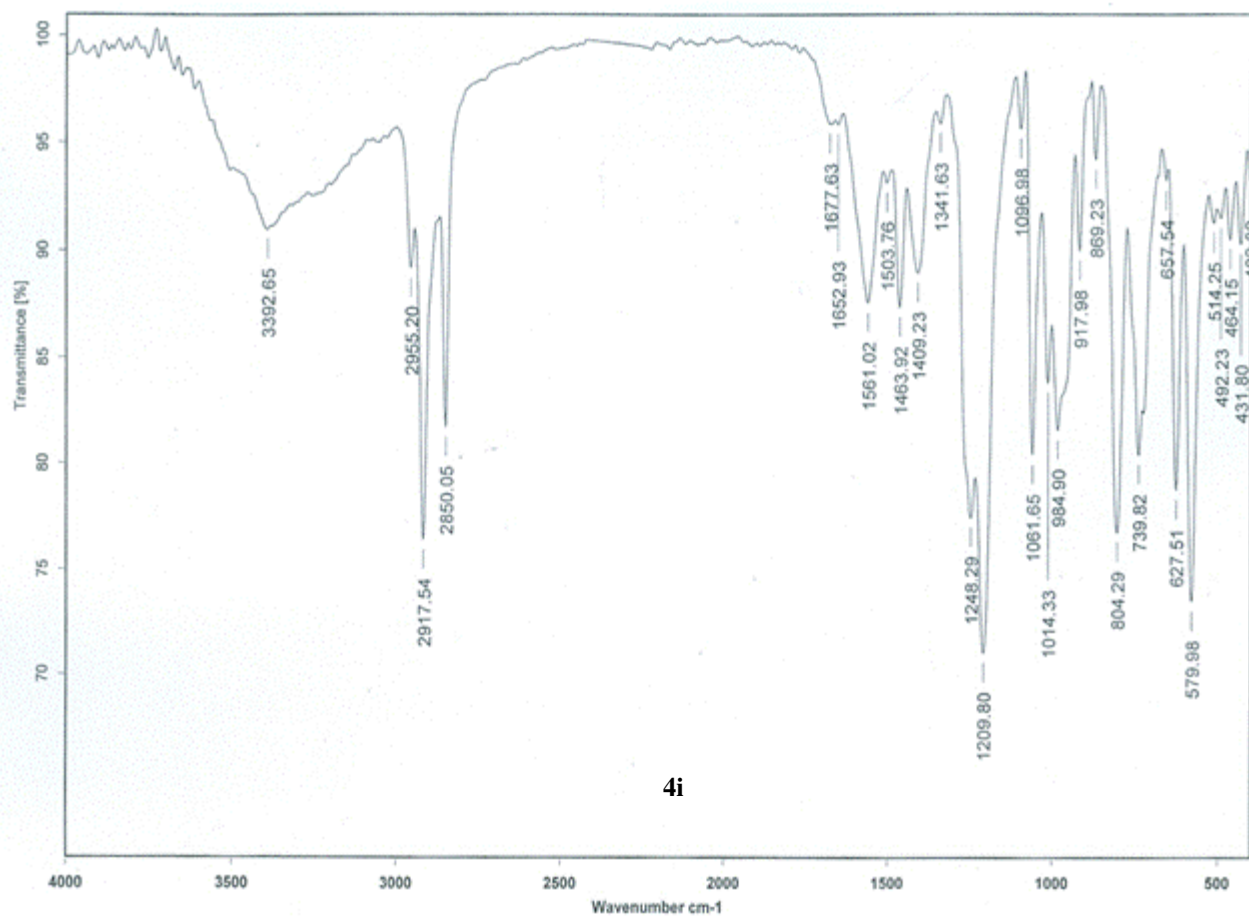
Anal calcd. C 85.40 H 5.12 N 9.48

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

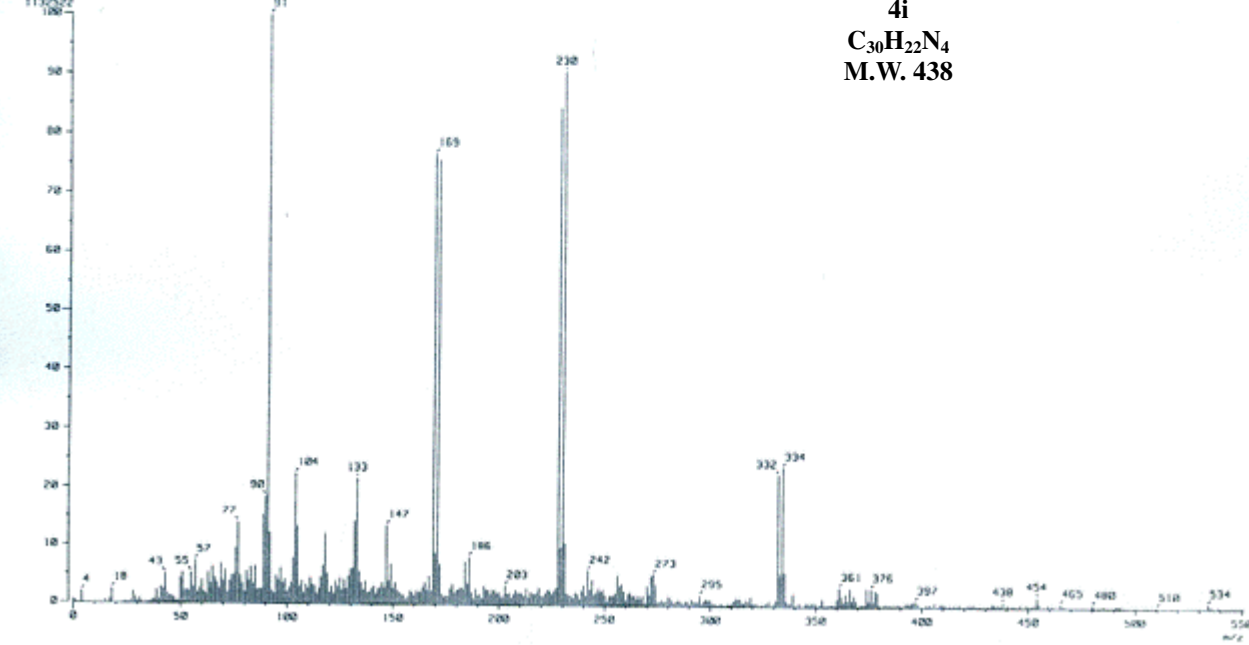
**4h**  
 $C_{42}H_{30}N_4$   
 M.W. 590





4i

[ Mass Spectrum ]  
 Date : Dr-Lopez-Jose-085 Date : 01-Jun-2012 18:16  
 Sample: 1270 ICD1 Jeol HX505sh  
 Note : Javier Perez  
 Inlet : Direct Ion Mode : EI+  
 Spectrum Type : Normal Ion (M<sup>+</sup>-Linear)  
 RT : 0.75 min Scan : (7,29)  
 BP : m/z 91.00000 Int. : 100.01  
 Outset m/z range : 0.00000 to 550.7418 Cut Level : 0.00 %

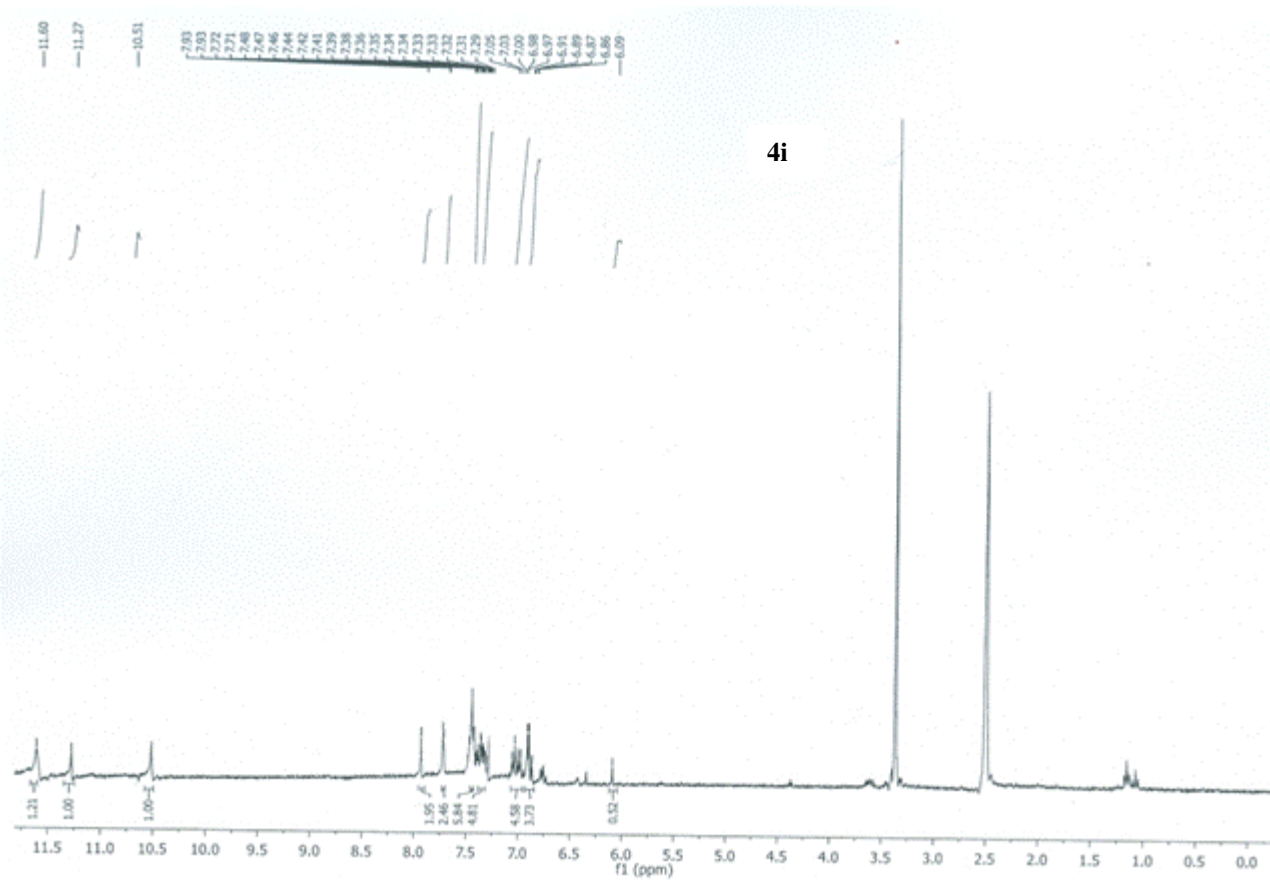


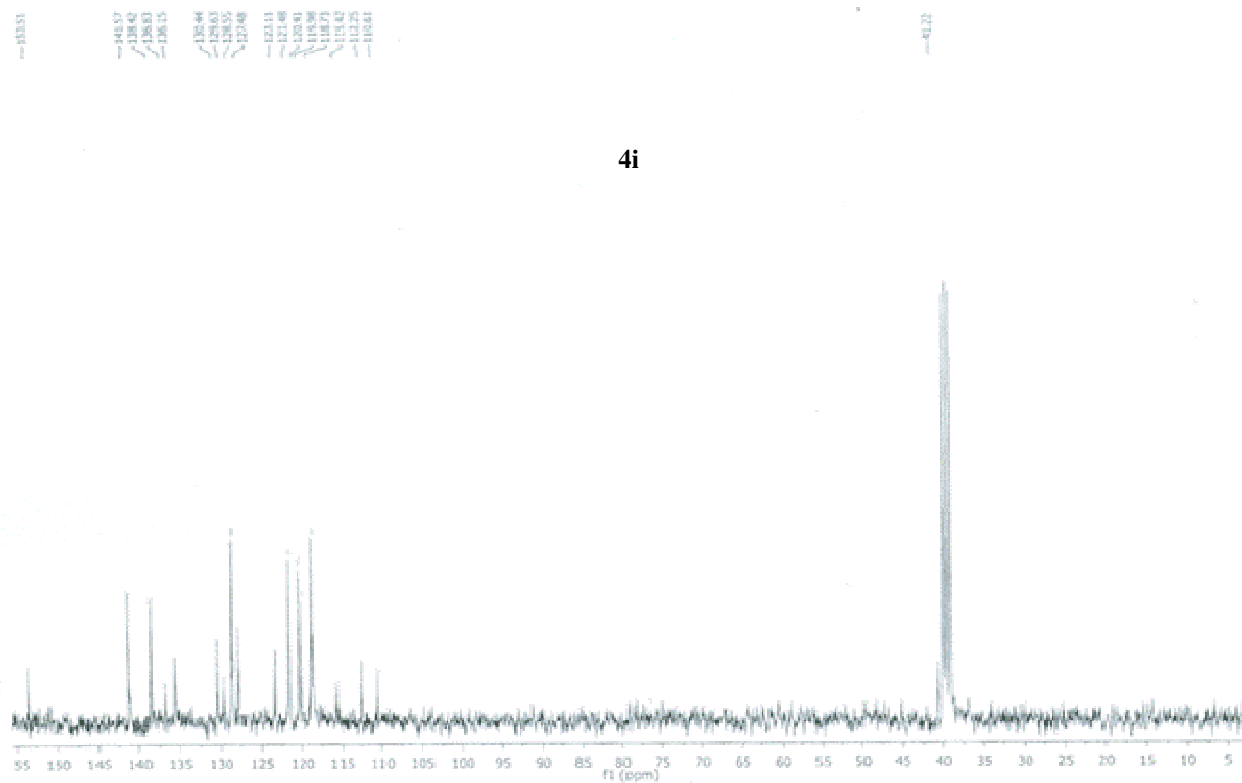
4i  
 $C_{30}H_{22}N_4$   
 M.W. 438

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

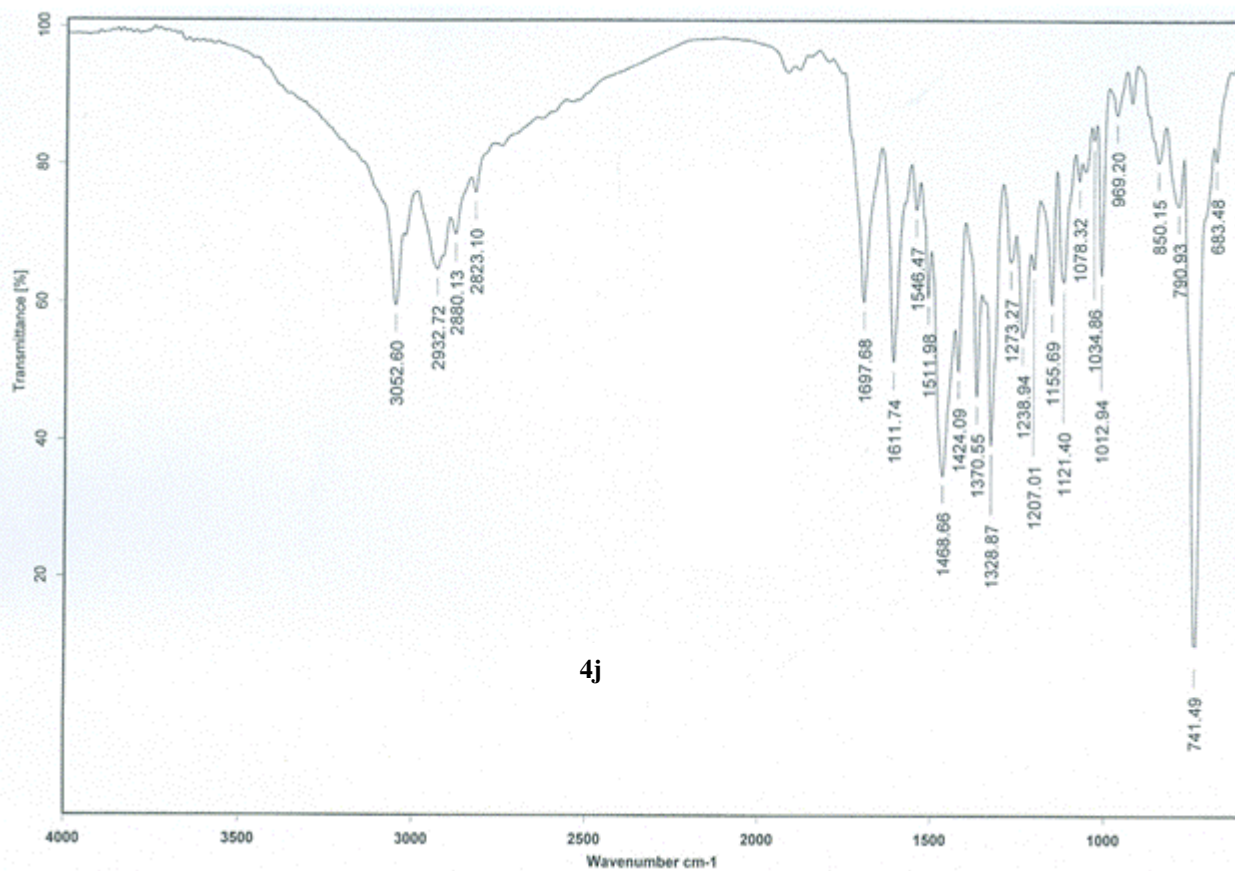
**4i**  
**C<sub>30</sub>H<sub>22</sub>N<sub>4</sub>**  
**M.W. 438**

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





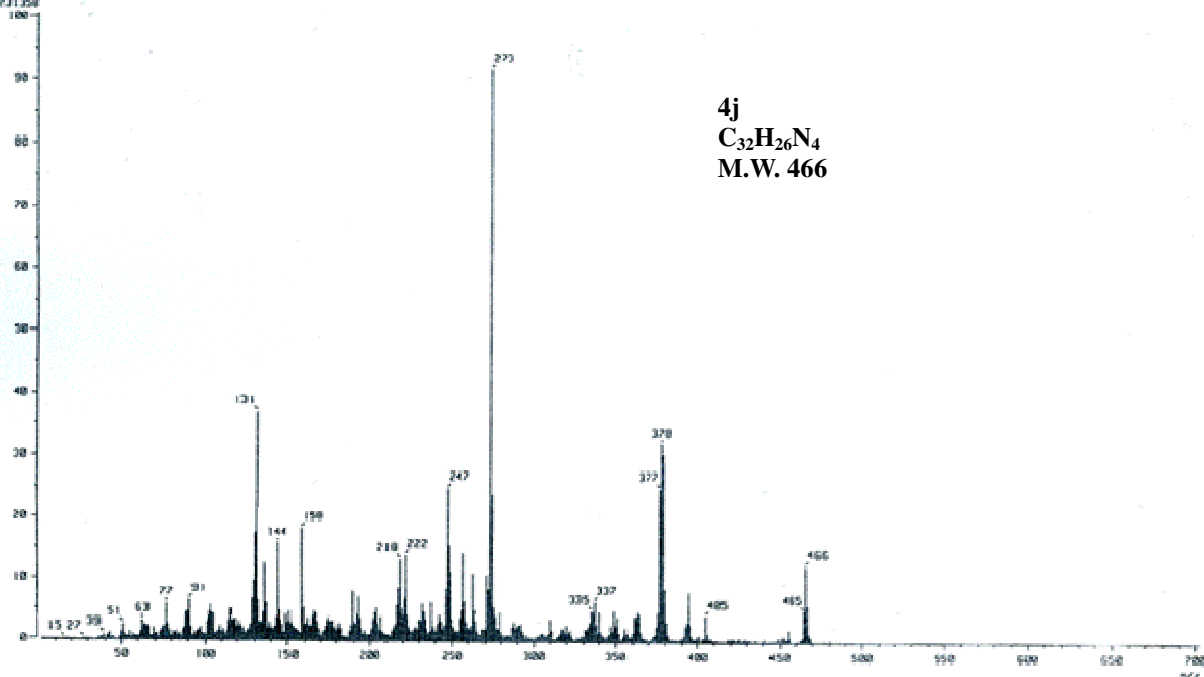
4i



4j

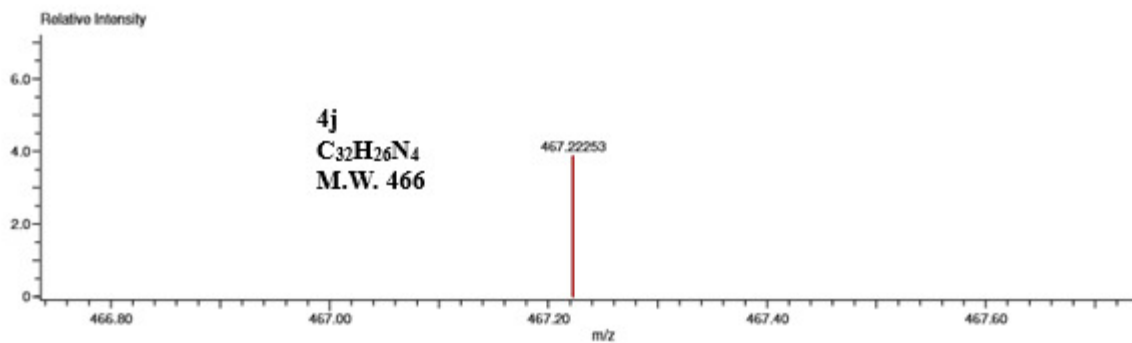


Mass Spectrum 1  
 Date: 24-May-2012 16:23  
 Sample: 1198  
 Inlet: Direct  
 Spectrum Type: Normal Ion (V<sup>+</sup>-Linear)  
 Scan: 410.365  
 SP: 370.0000  
 Output m/z range: 2.2722 to 702.6706  
 Ion Mode: EI+  
 Scale: 110.365  
 Int.: 211.58  
 Cut level: 0.00 A



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

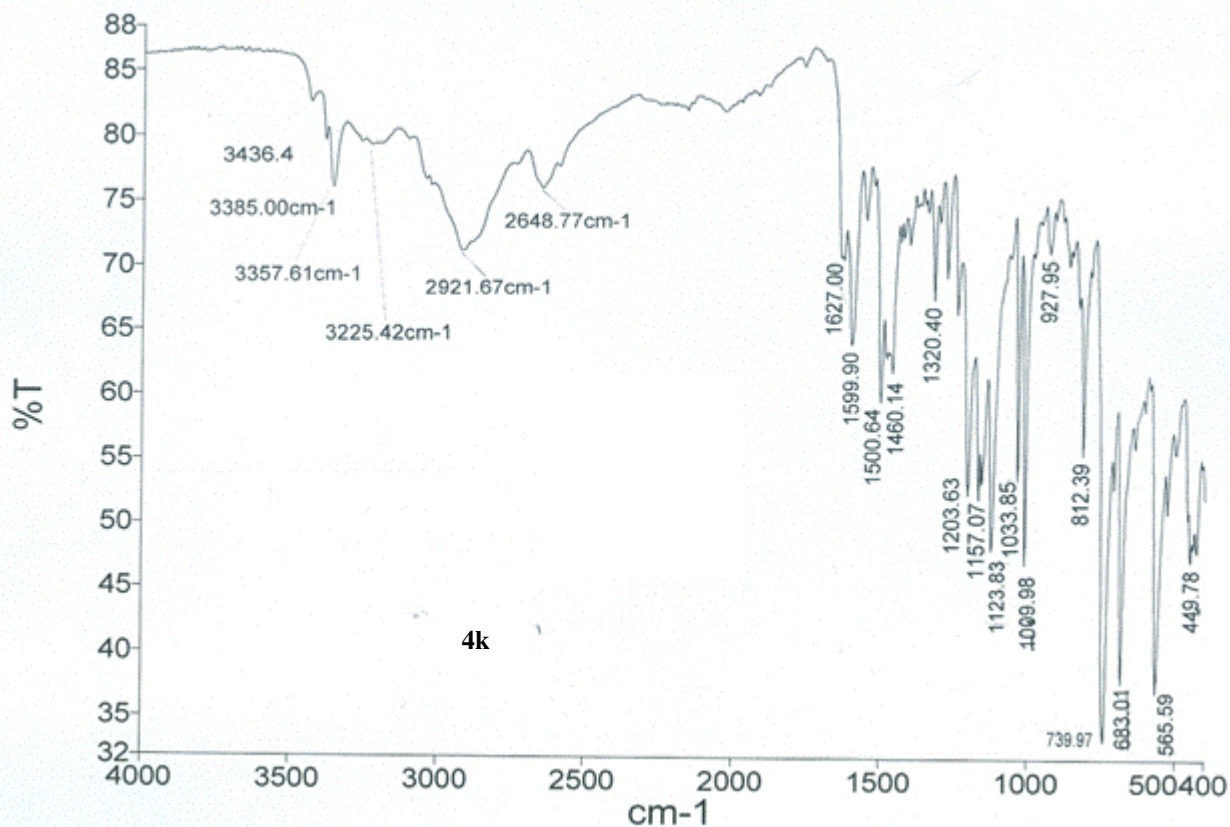
Data: CAT21  
 Sample Name:  
 Description:  
 Ionization Mode: ESI+  
 History: Determine m/z [Peak Detect [Centroid, 30 Area], Correct Base [5.0%], Correct Base [5.0%], Average MS [1] 0.6...  
 Charge number: 1  
 Element: <sup>12</sup>C: 0 .. 100, <sup>1</sup>H: 0 .. 100, <sup>14</sup>N: 2 .. 5  
 Tolerance: 3.00 (mmu)  
 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  
 Unsaturation Number: 0.0 .. 32.0 (Fraction: Both)



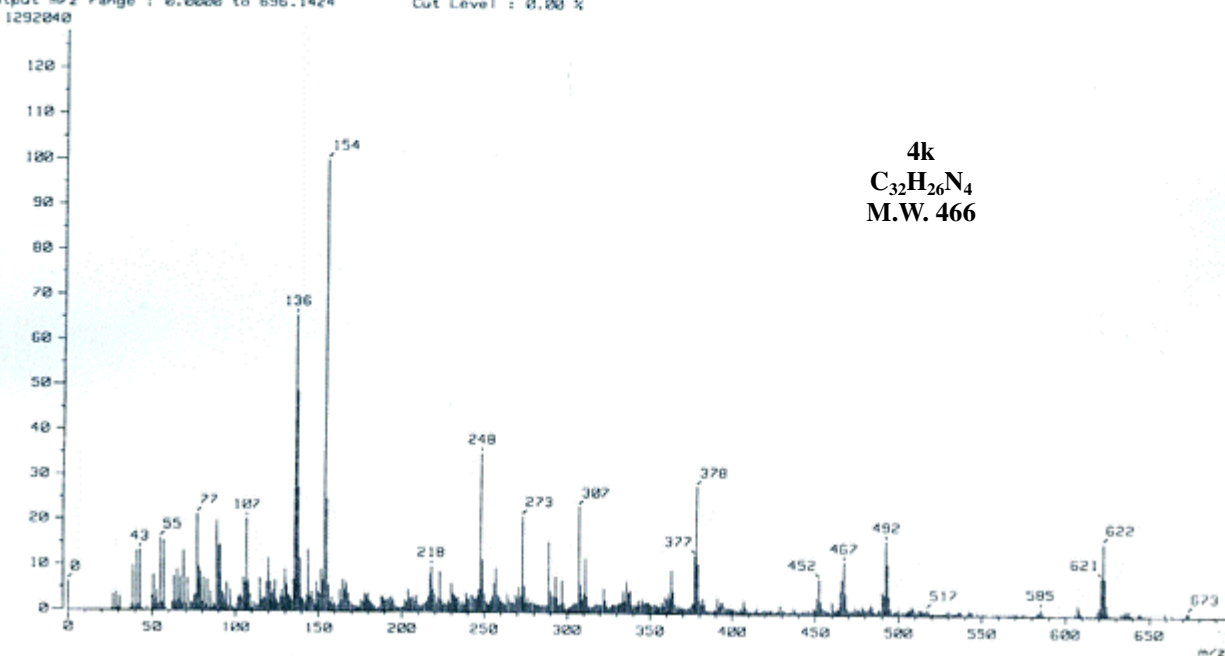
**4j**  
 $C_{32}H_{26}N_4$   
 M.W. 466

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 %

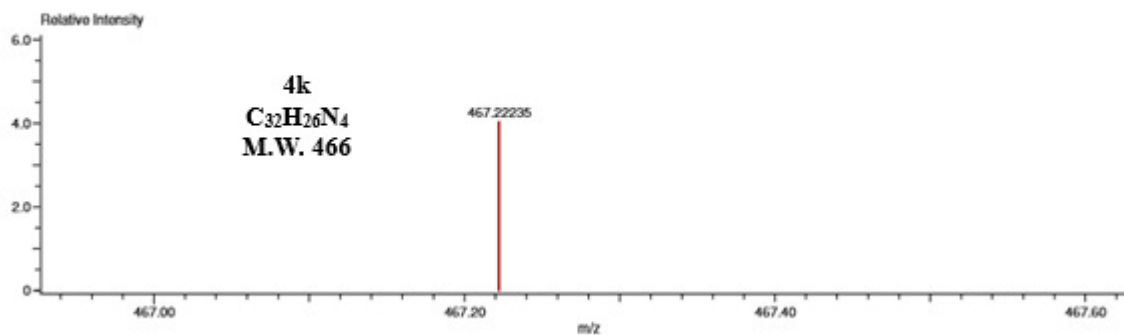


4k  
 $C_{32}H_{26}N_4$   
 M.W. 466

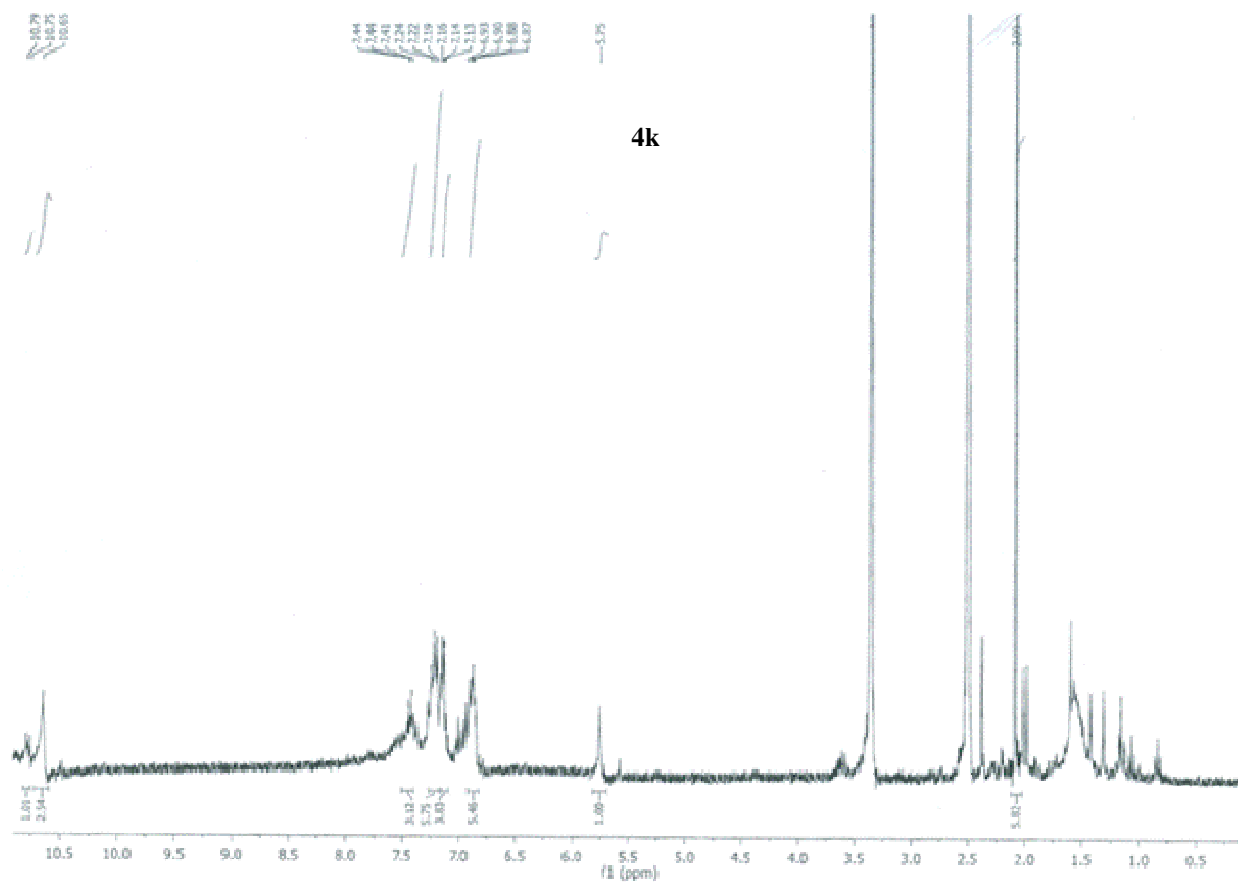
Data:CAT23  
 Sample Name:  
 Description:  
 Ionization Mode:ESI+  
 History:Dotormine m/z[Peak Detect[Centroid,30,Area],Correct Base[5.0%],Correct Base[5.0%];Average[MS[1] 0.2...

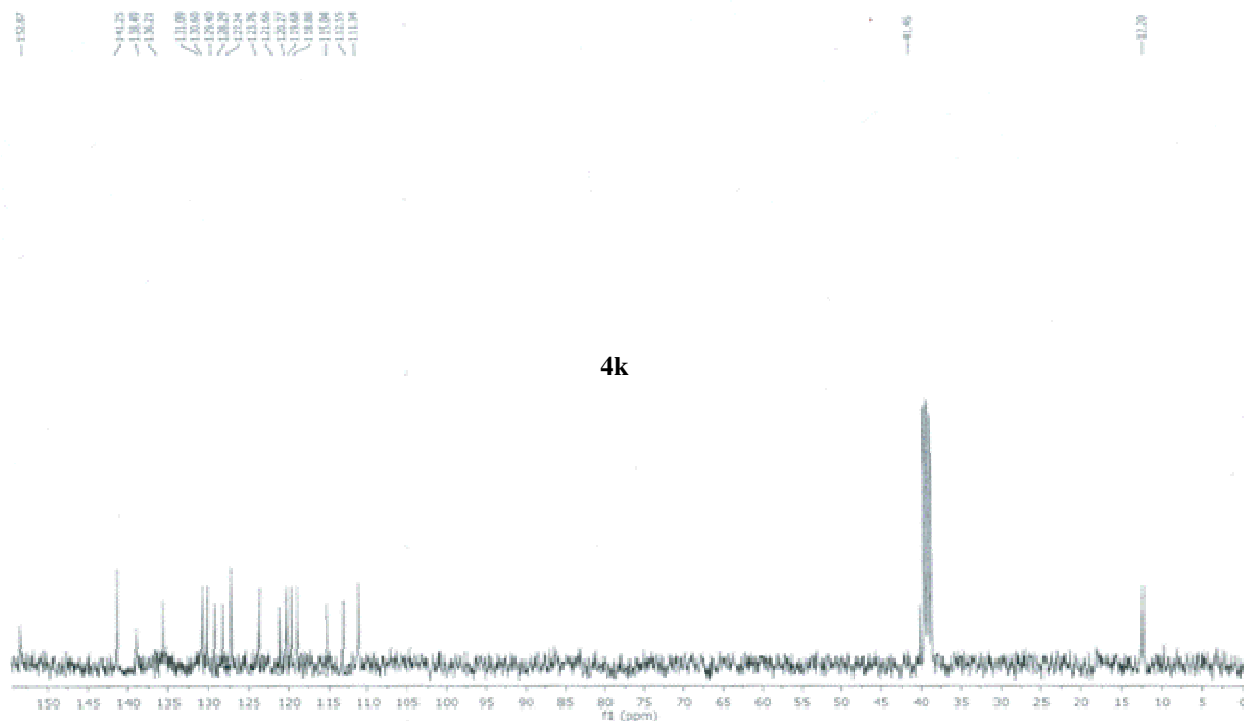
Acquired:4/8/2016 9:06:52 AM  
 Operator:AccuTOF  
 Mass Calibration data:PEG600  
 Created:4/11/2016 7:35:34 PM  
 Created by:AccuTOF

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

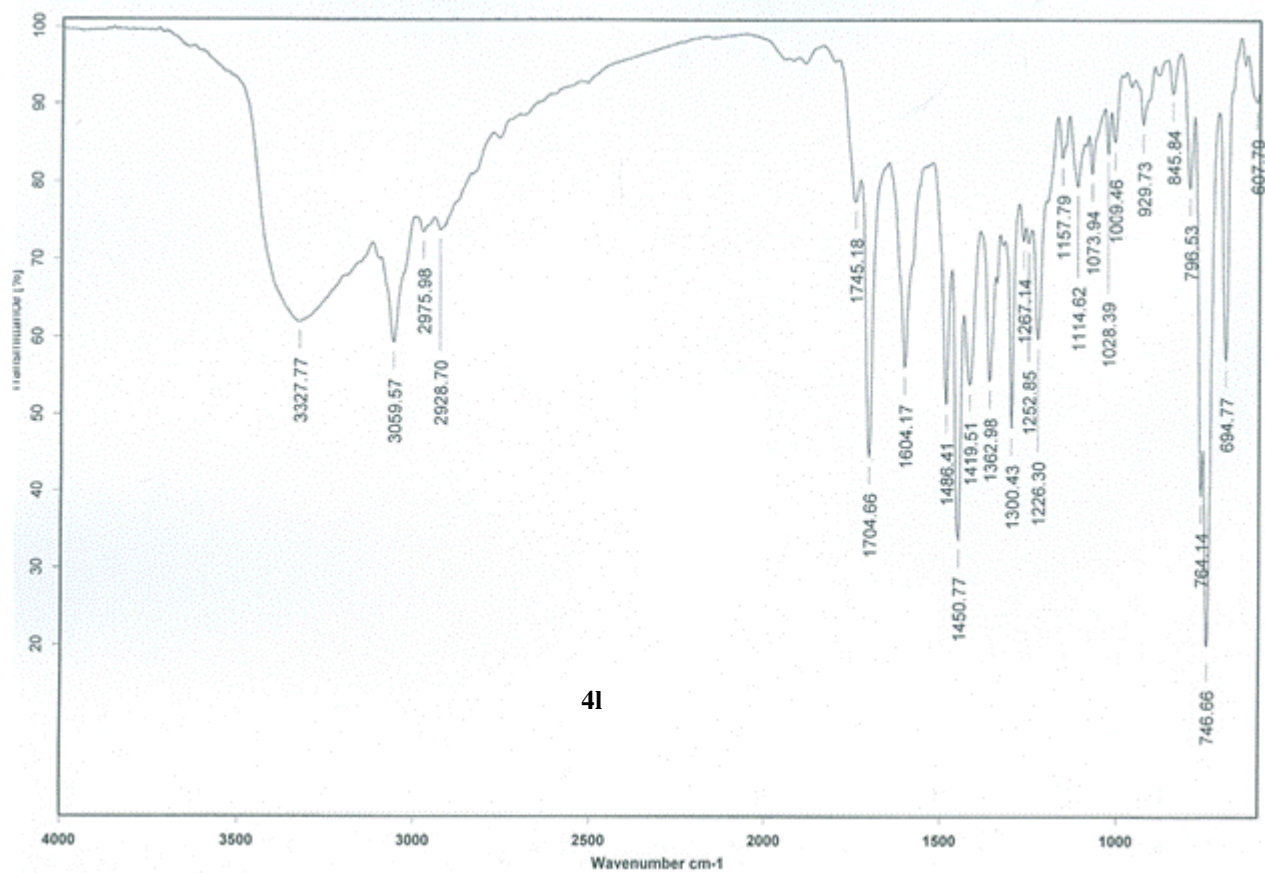


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22235	2357.78	467.22357	-1.22	-2.62	<sup>13</sup> C <sub>32</sub> <sup>1</sup> H <sub>27</sub> <sup>14</sup> N <sub>4</sub>	21.5



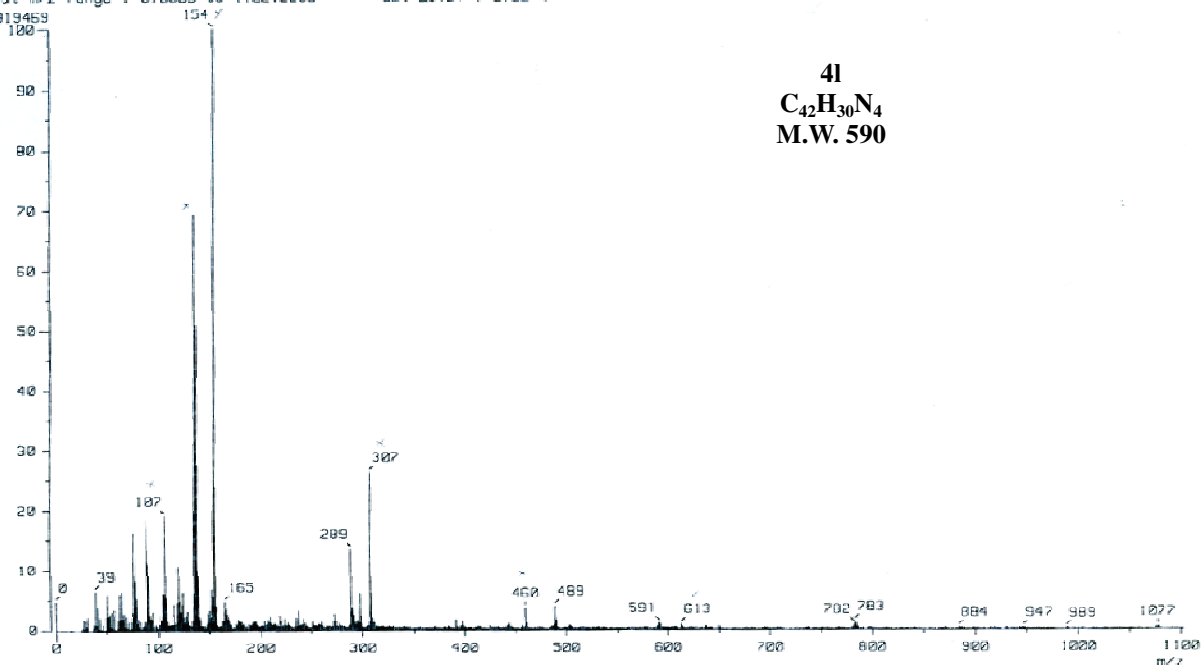


4k



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 %



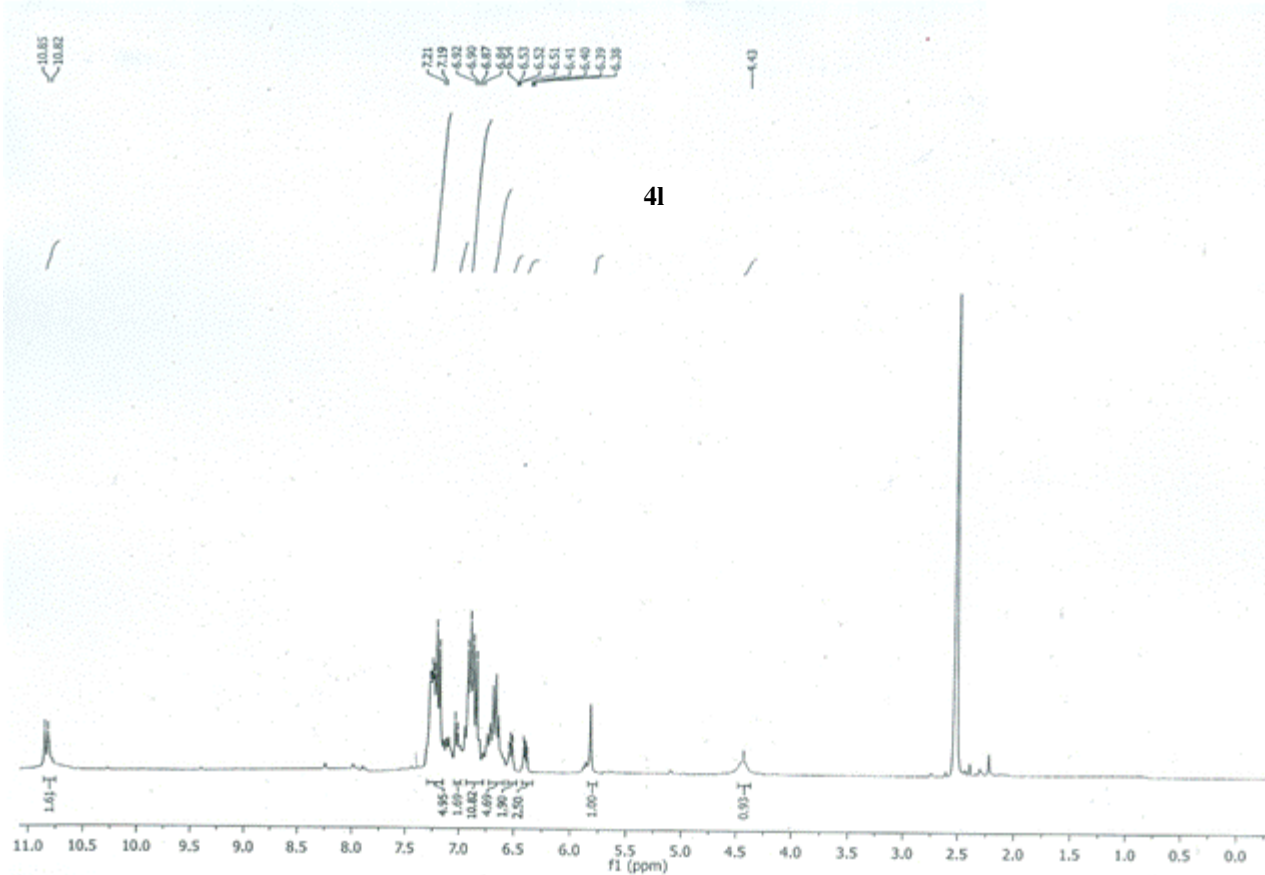
**41**  
 $C_{42}H_{30}N_4$   
 M.W. 590

Anal calcd. C 85.40 H 5.12 N 9.48

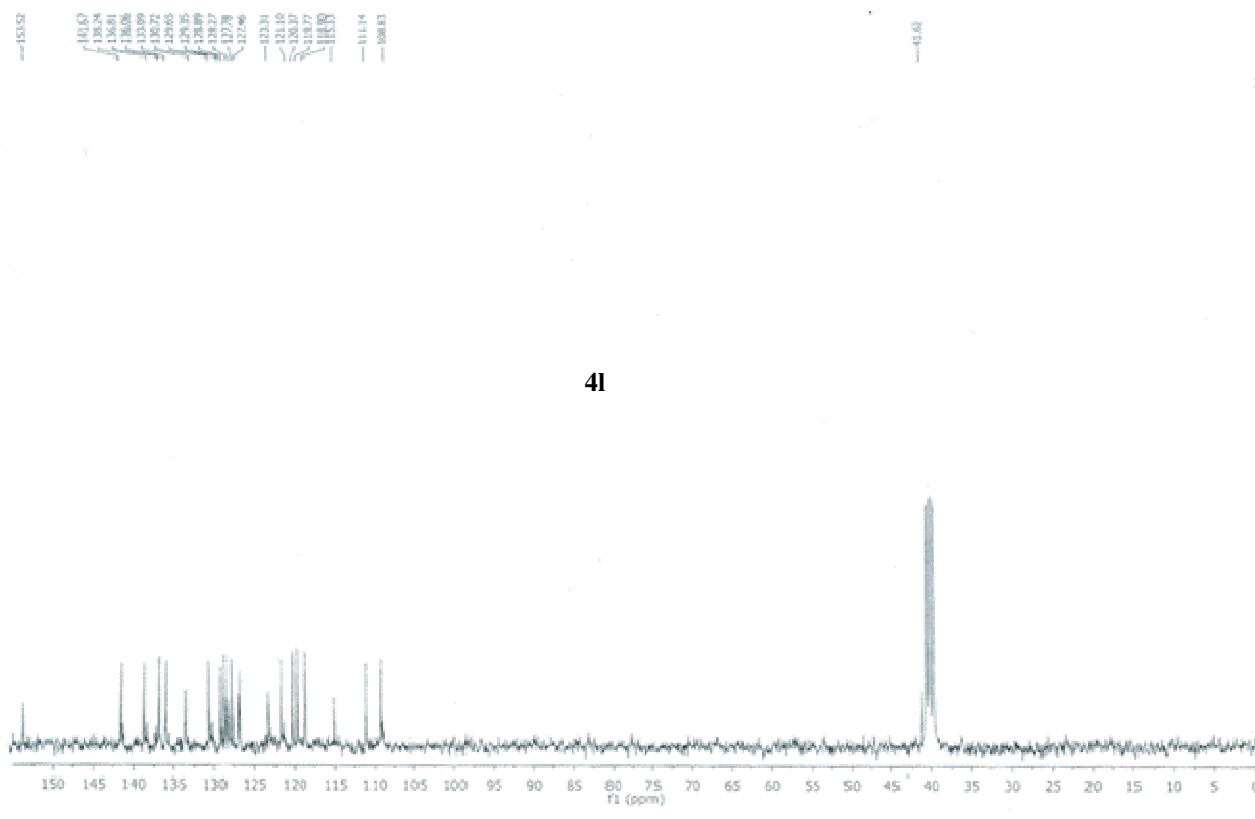
Clave de la muestra	Peso [mg]	N [%]	C [%]	H [%]	S [%]	Fecha de análisis
bz2ph o	2.412	9.37	85.40	4.99	---	27-04-2016

Found

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



41



41