Supplementary Material

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

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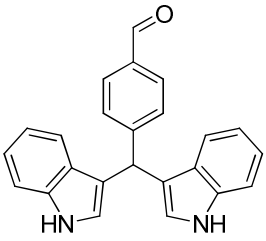
Table of Contents



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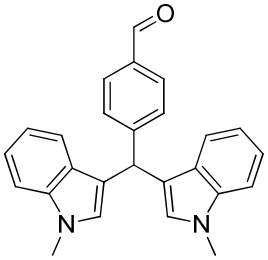

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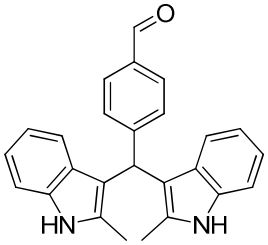

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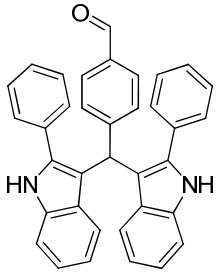

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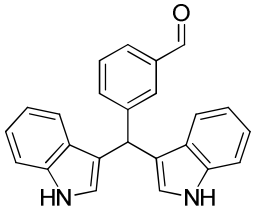

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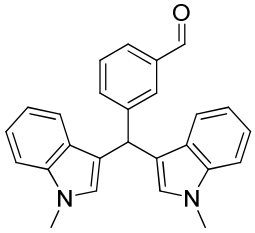

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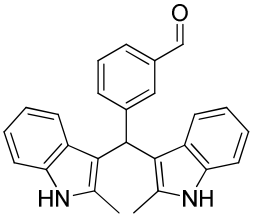

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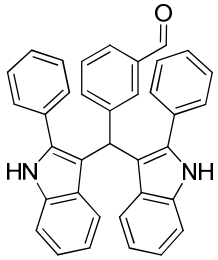

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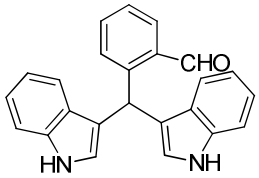

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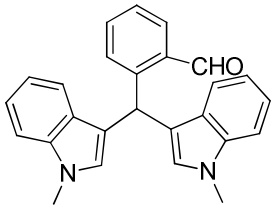

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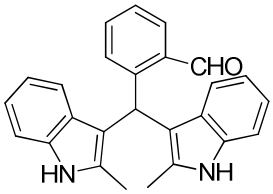

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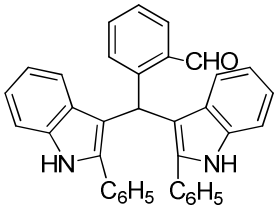

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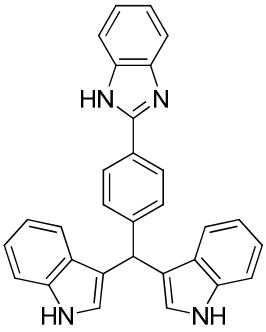

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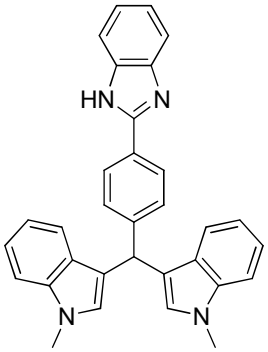

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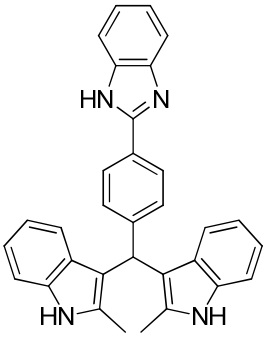

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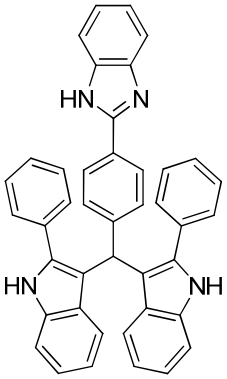

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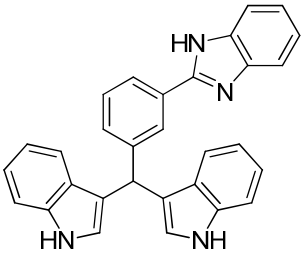

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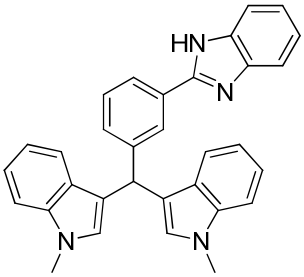

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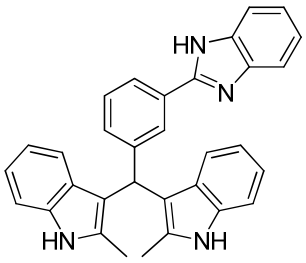

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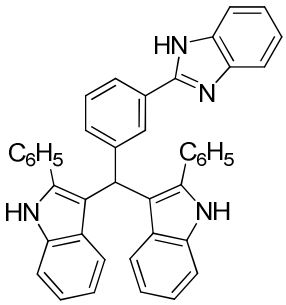

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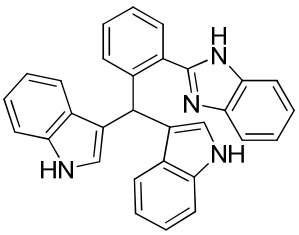

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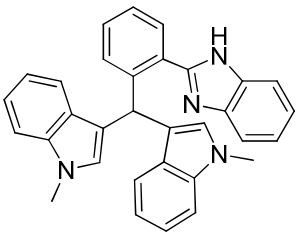

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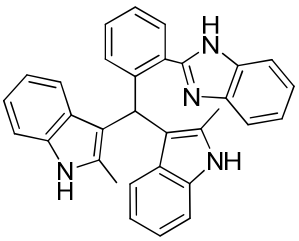

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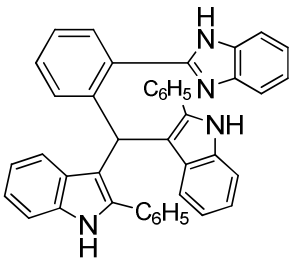

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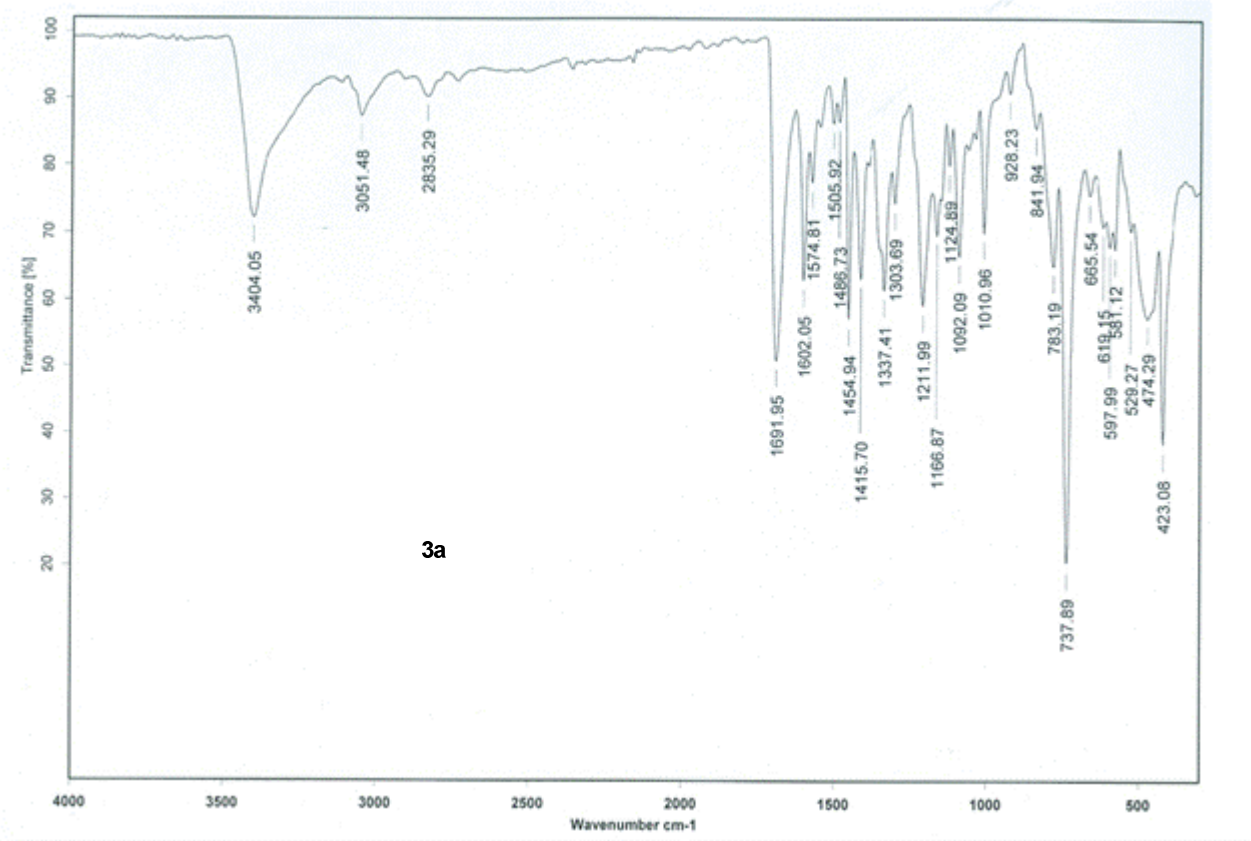
IR, MS, ^{1}H NMR, ^{13}C NMR Spectra



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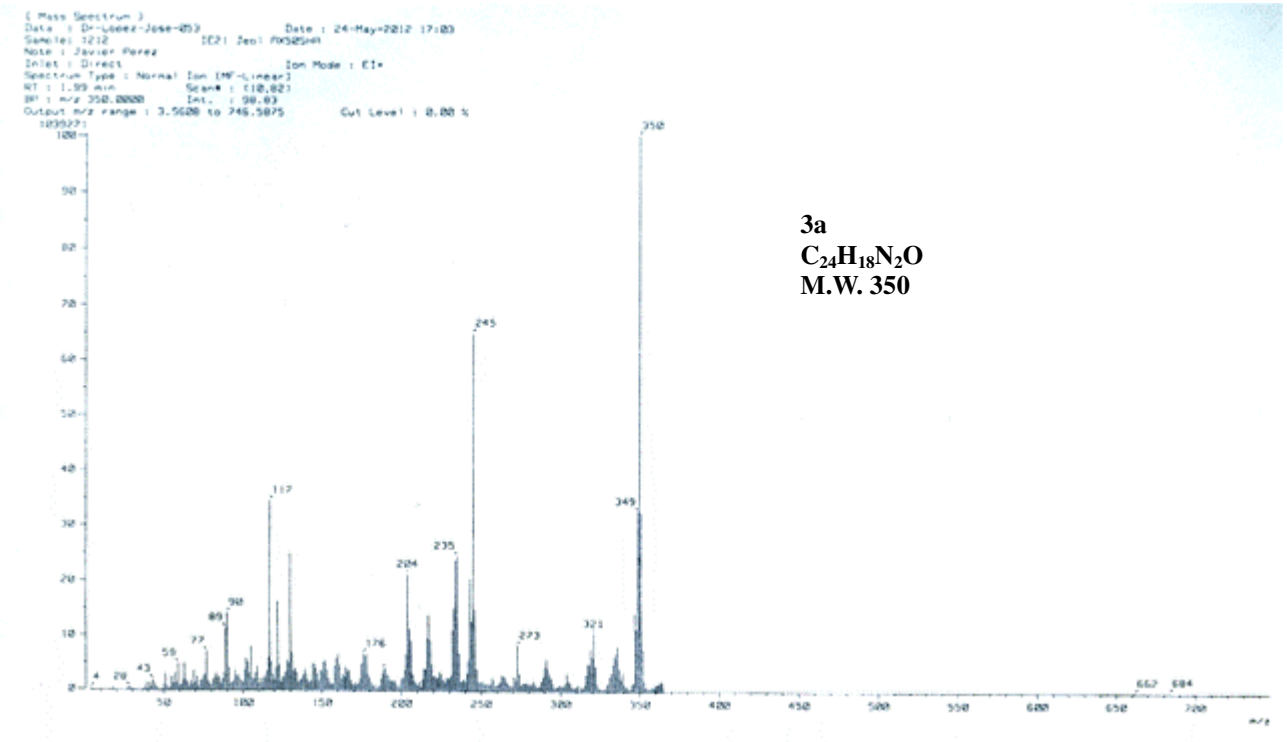


3a
$C_{24}H_{18}N_2O$
M.W. 350

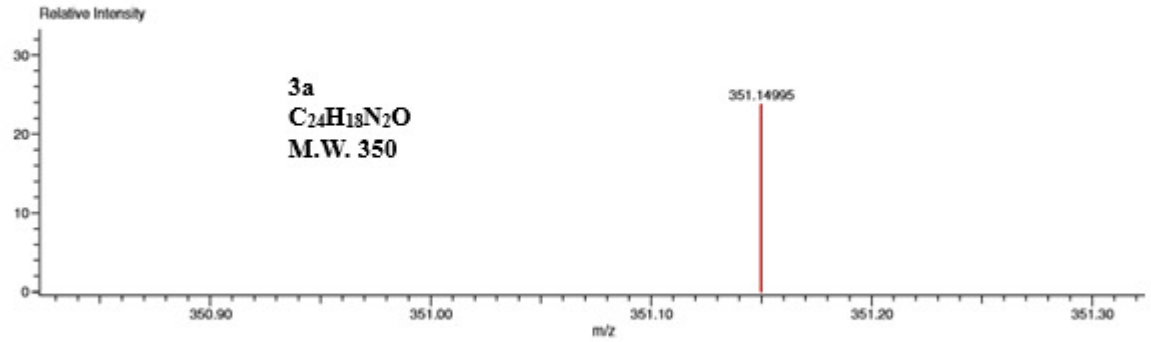
Data:2580 indol-p
Sample Name:Dr Alvarez Cecilio Operador: Carmen Garcia/ Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.6...

Acquired:9/3/2015 1:00:54 PM
Operator:AccuTOF
Mass Calibration data:Cal_Peg_600
Created:9/3/2015 3:23:17 PM
Created by:AccuTOF

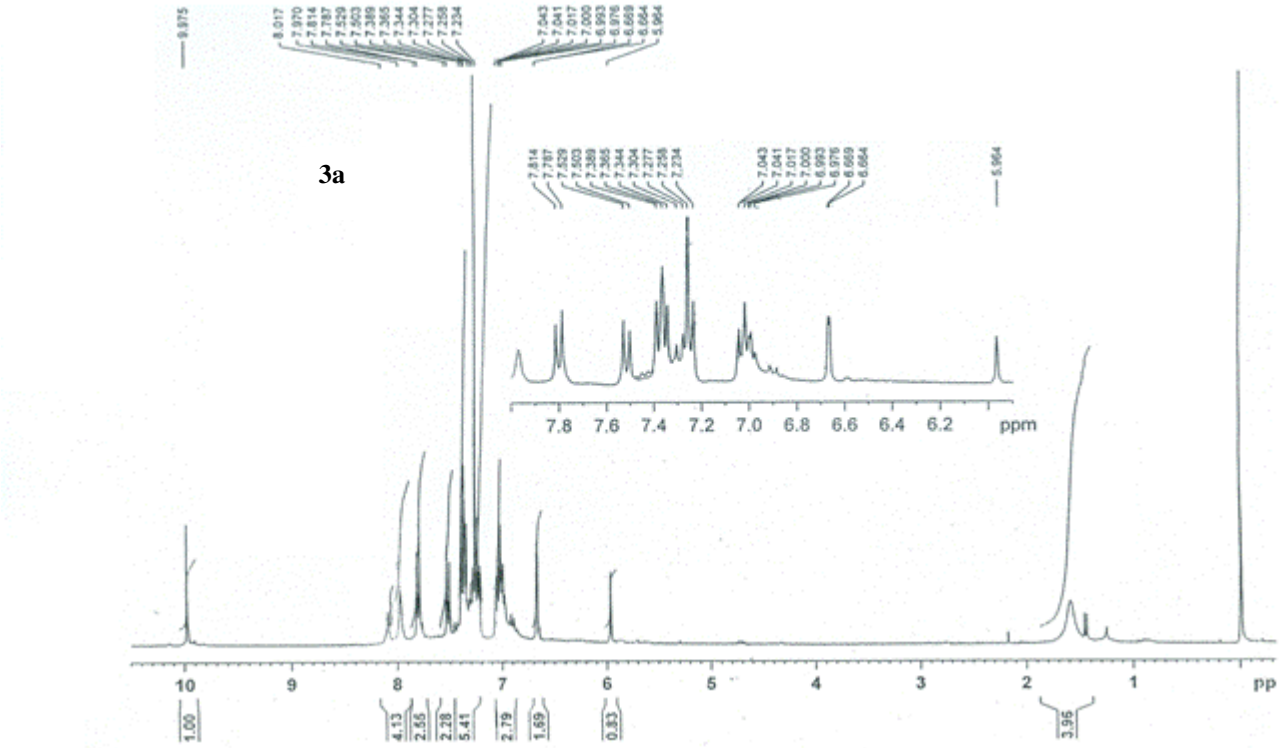
Charge number:1
Element:^{12}C:0 .. 56, ^{1}H:0 .. 120, ^{14}N:0 .. 2, ^{16}O:0 .. 1

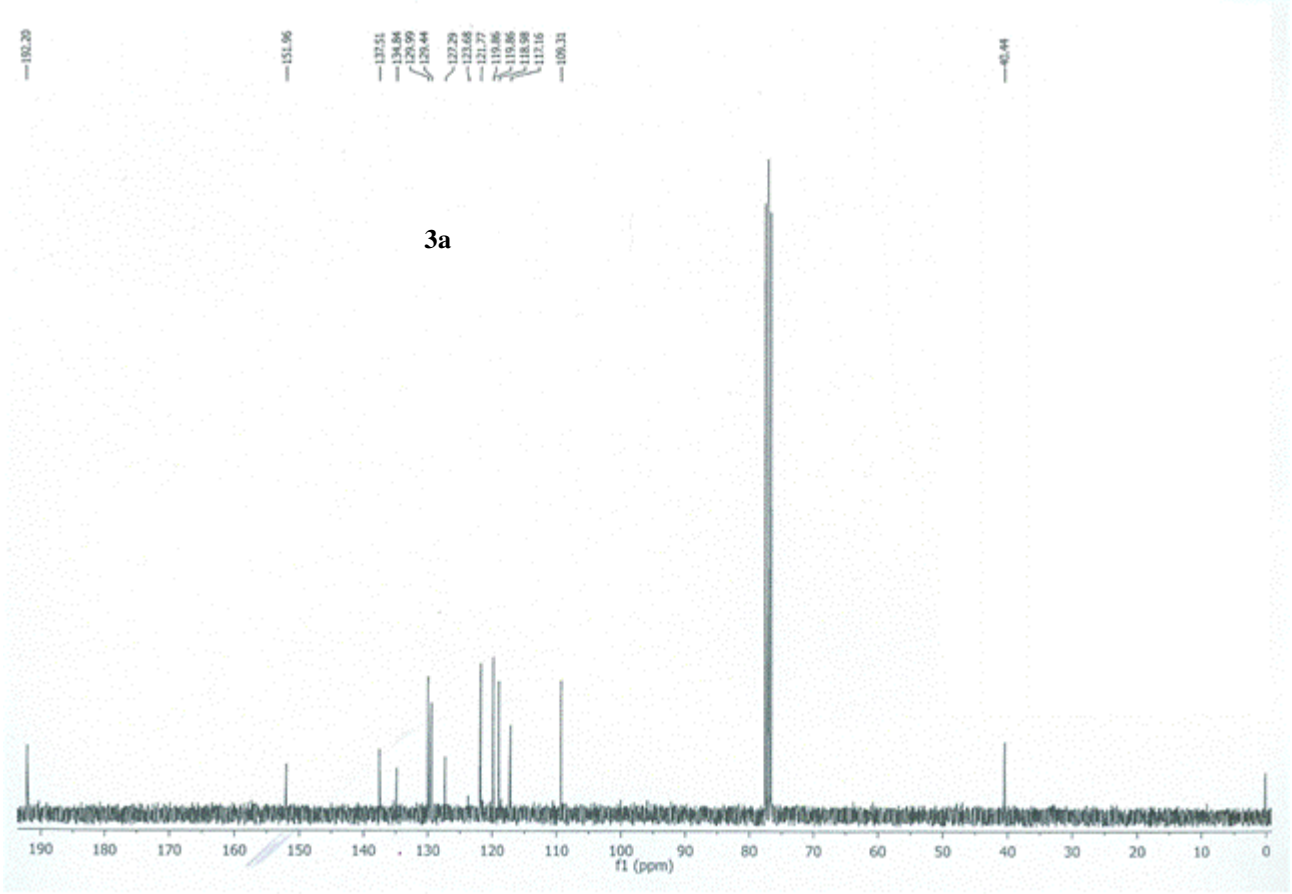
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

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



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14995	11159.75	351.14974	0.21	0.61	$^{12}C_{24}{}^{1}H_{19}{}^{14}N_{2}{}^{16}O_{1}$	16.5





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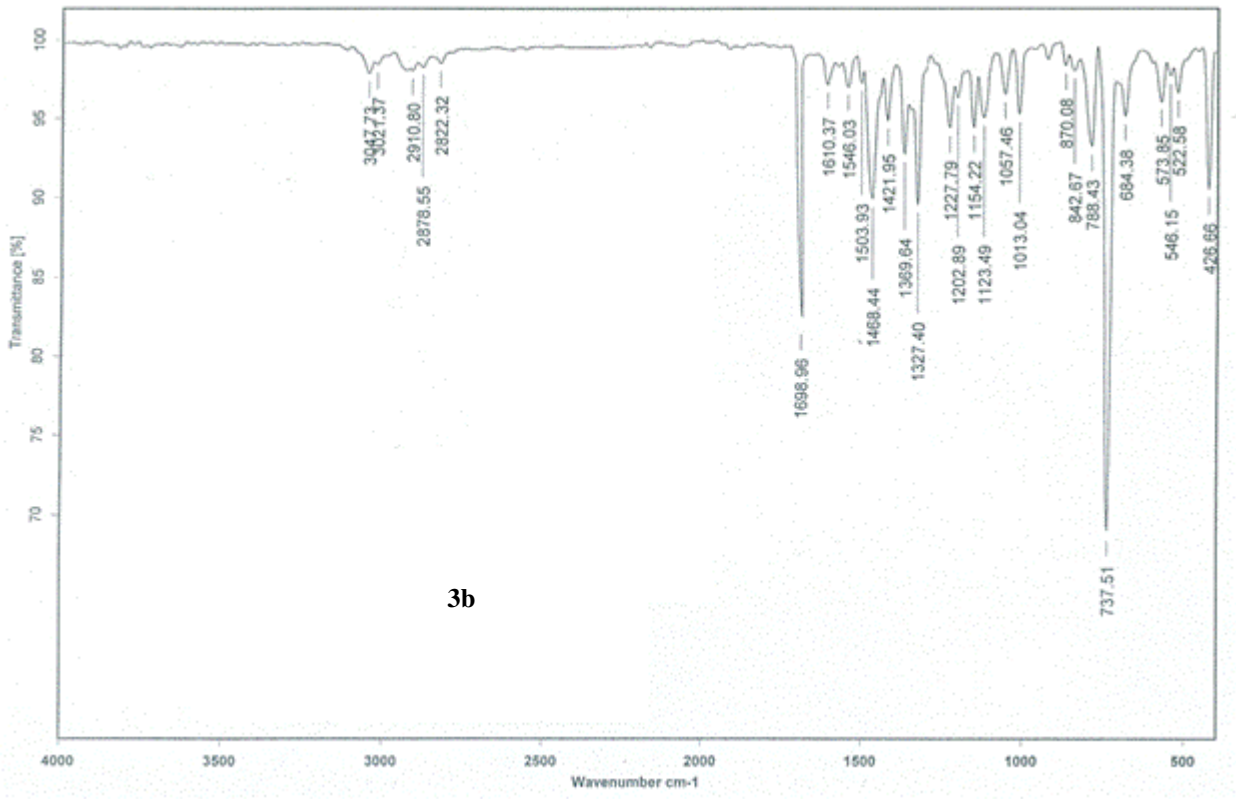

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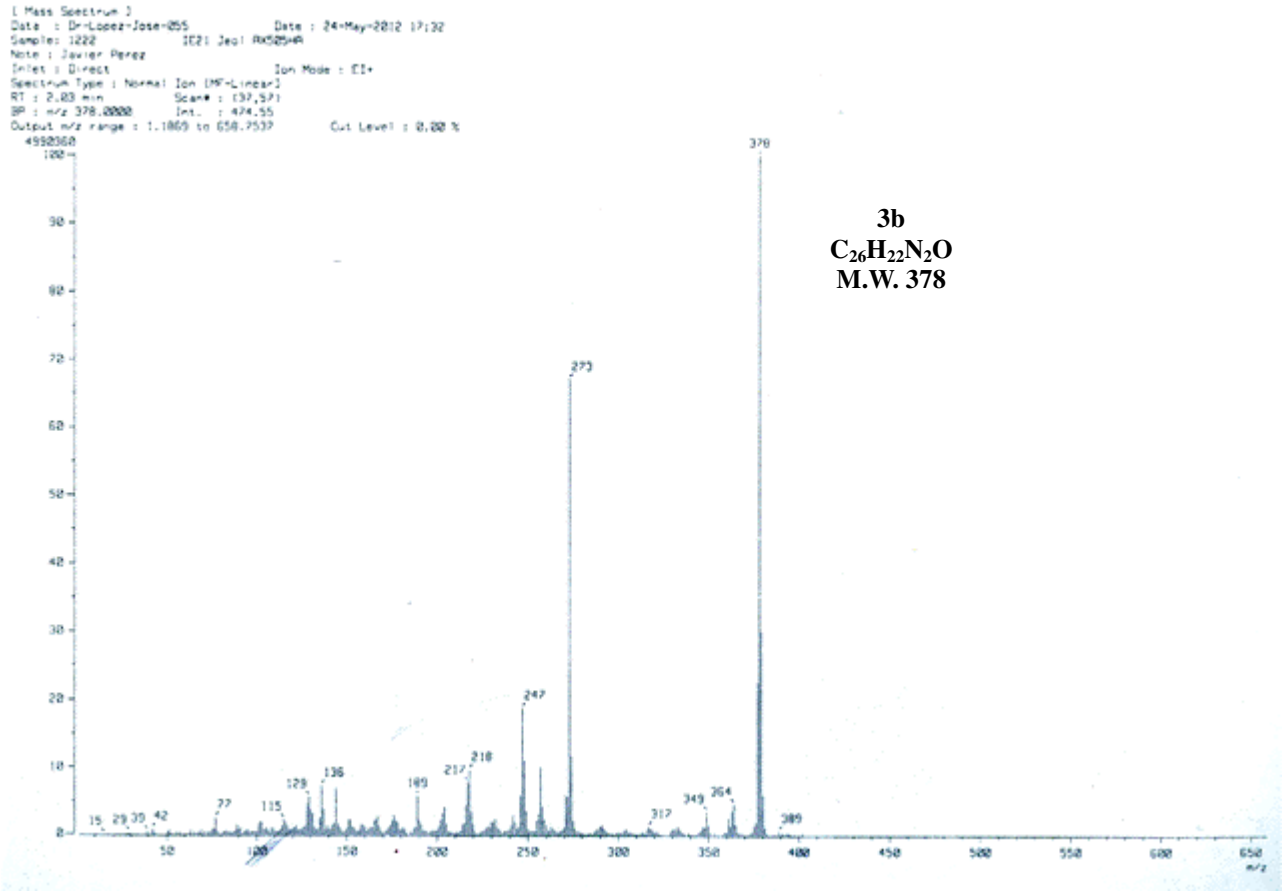
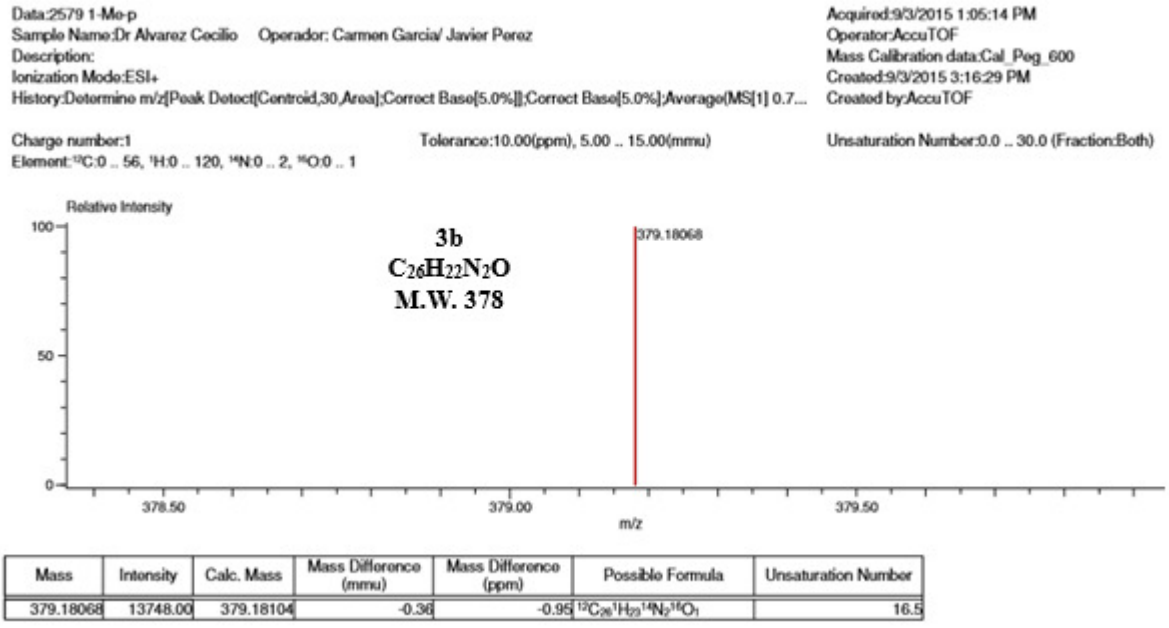
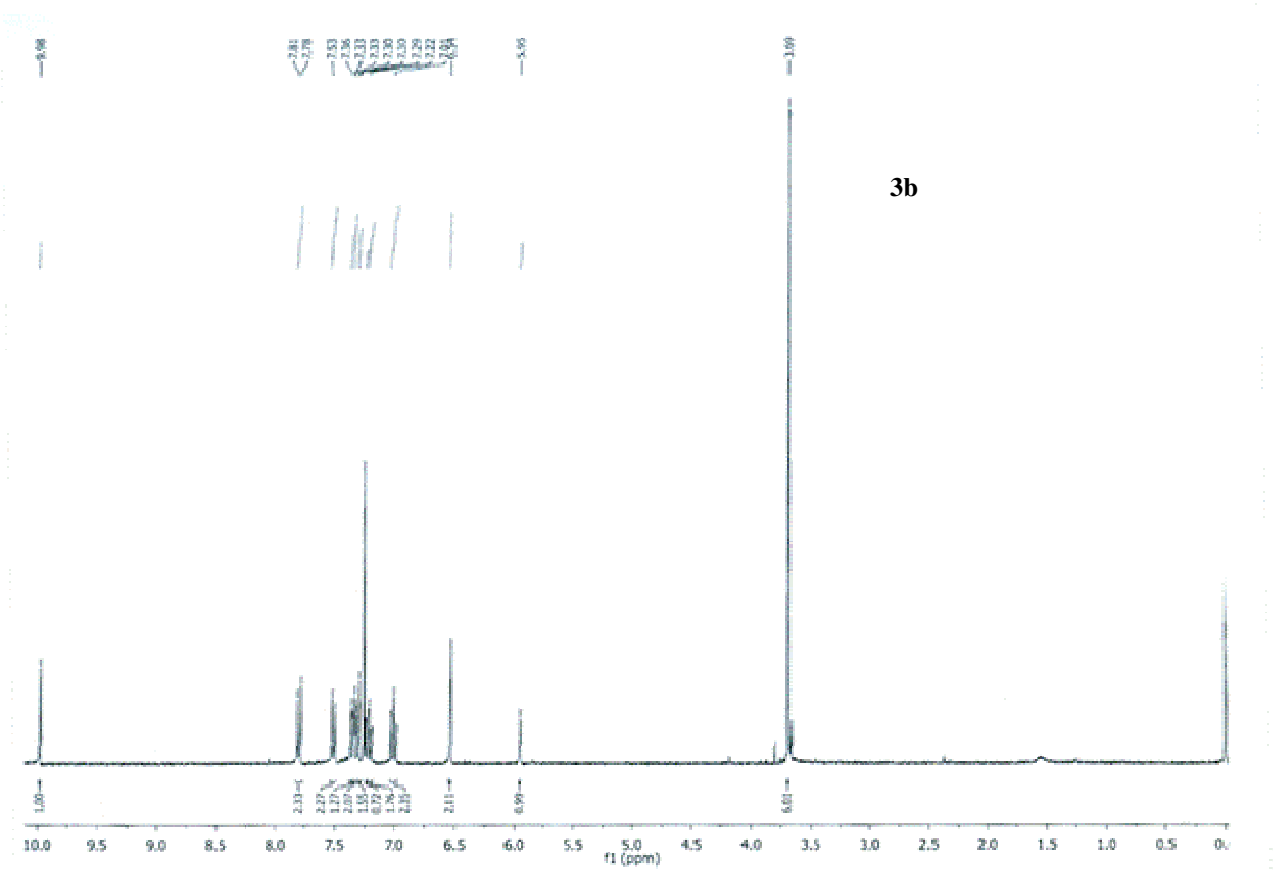
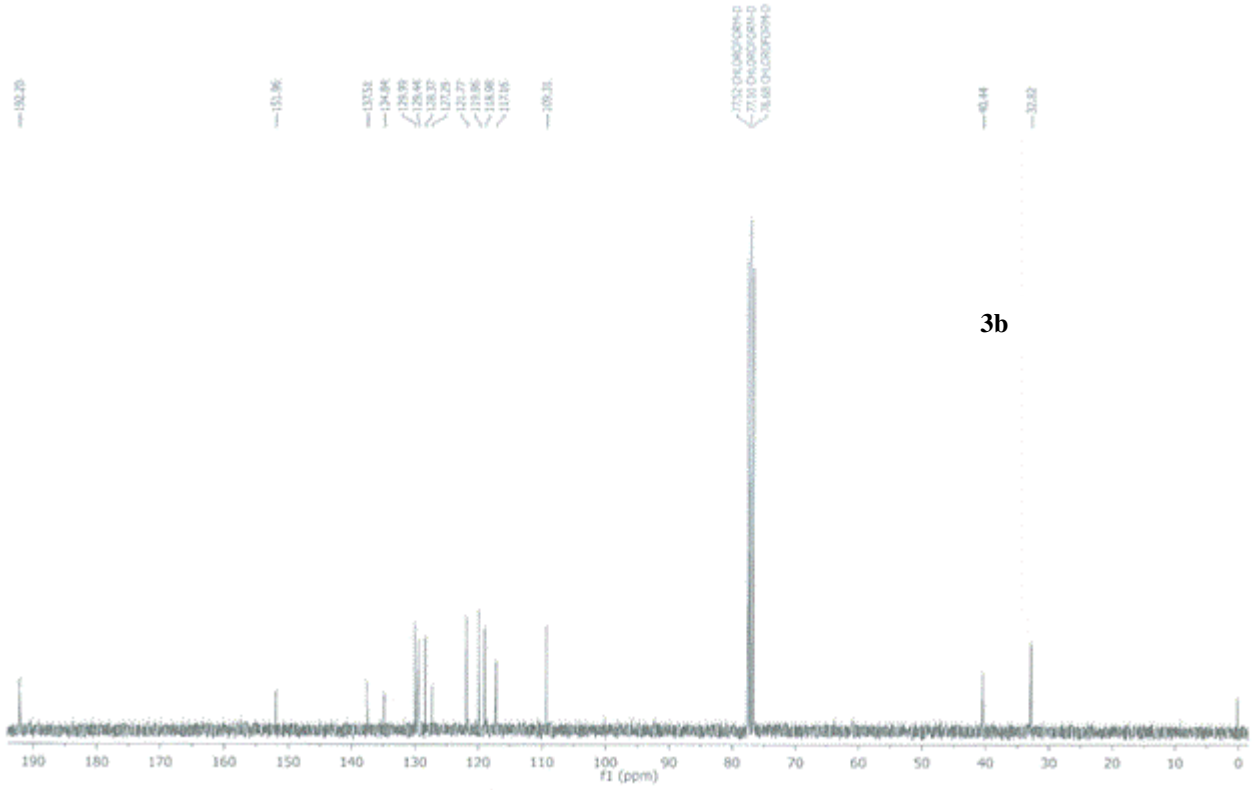
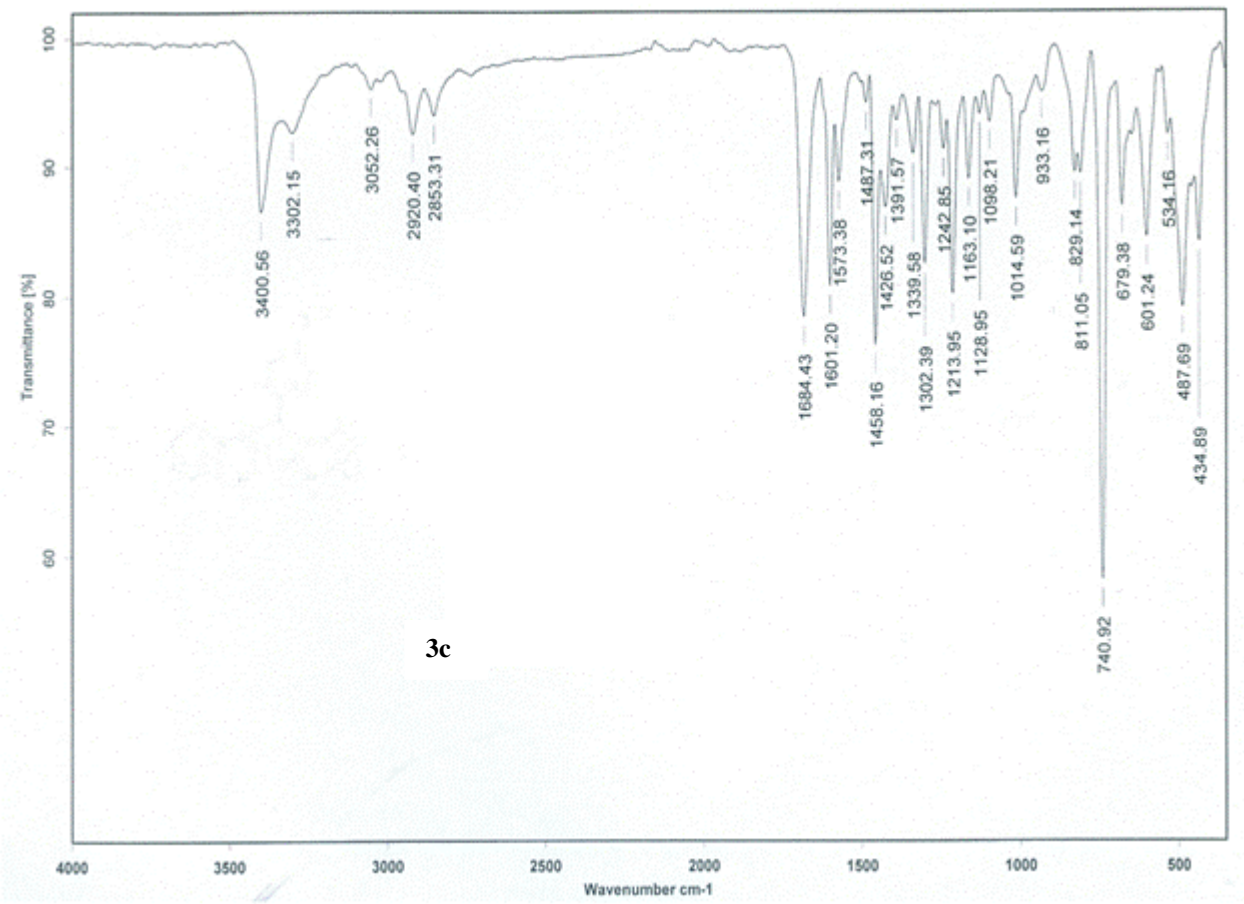




Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18068	13748.00	379.18104	-0.36	-0.95	$^{12}C_{26}{}^{1}H_{23}{}^{14}N_{2}{}^{16}O_{1}$	16.5







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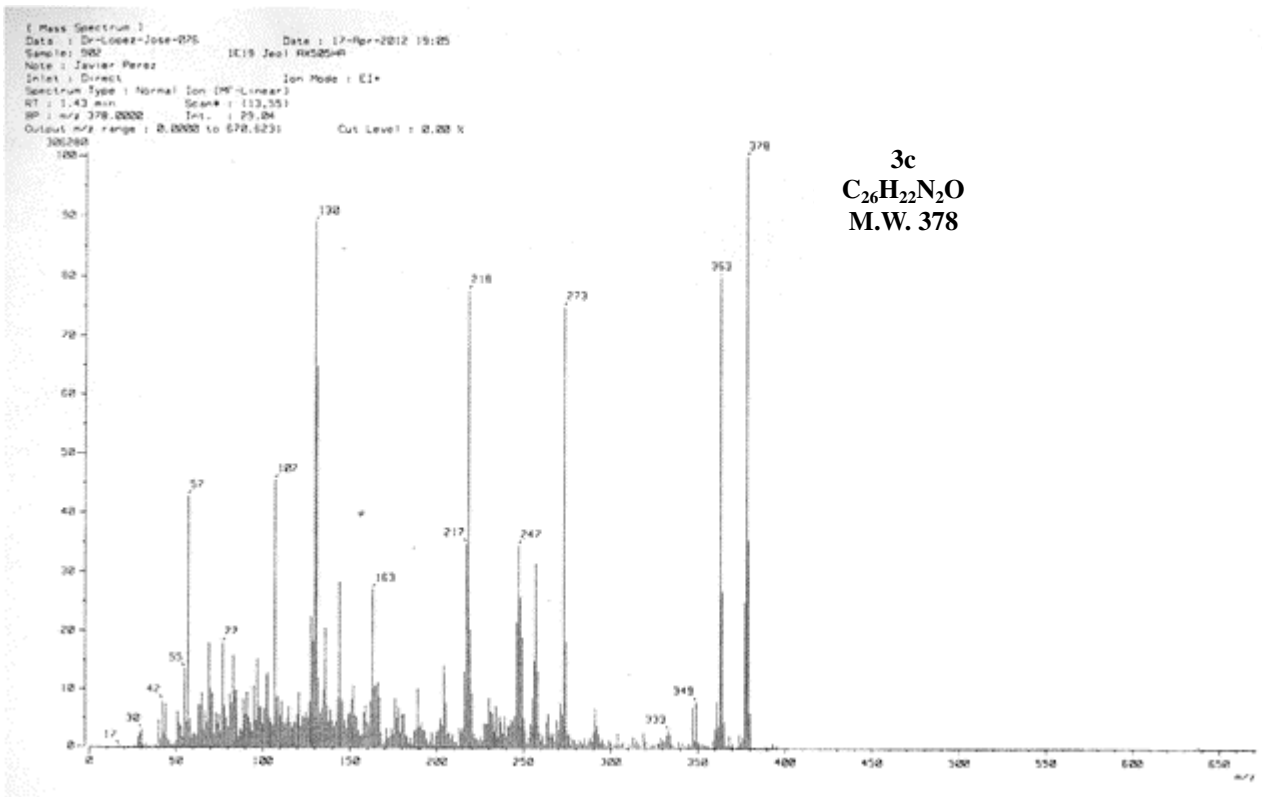


3c
$C_{26}H_{22}N_2O$
M.W. 378

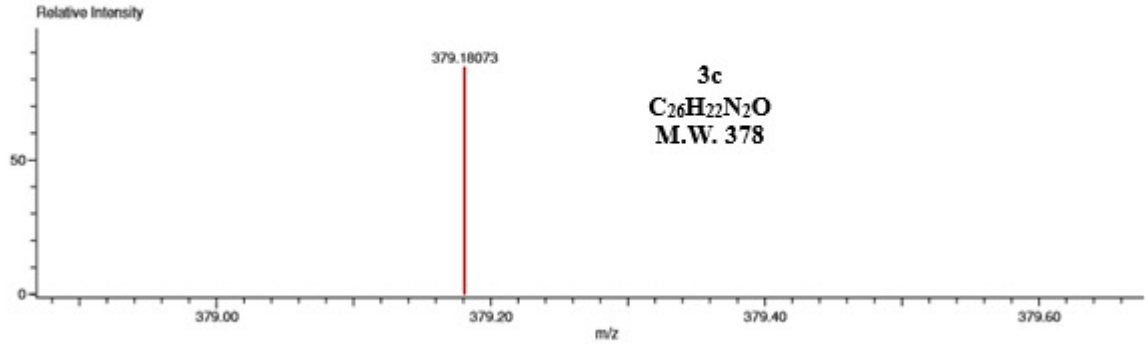
Data:2581 2-Me-p
Sample Name:Dr Alvarez Cecilio Operador: Carmen Garcia/ Javier Perez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.3...

Acquired:9/3/2015 1:03:12 PM
Operator:AccuTOF
Mass Calibration data:Cal_Peg_600
Created:9/3/2015 3:26:52 PM
Created by:AccuTOF

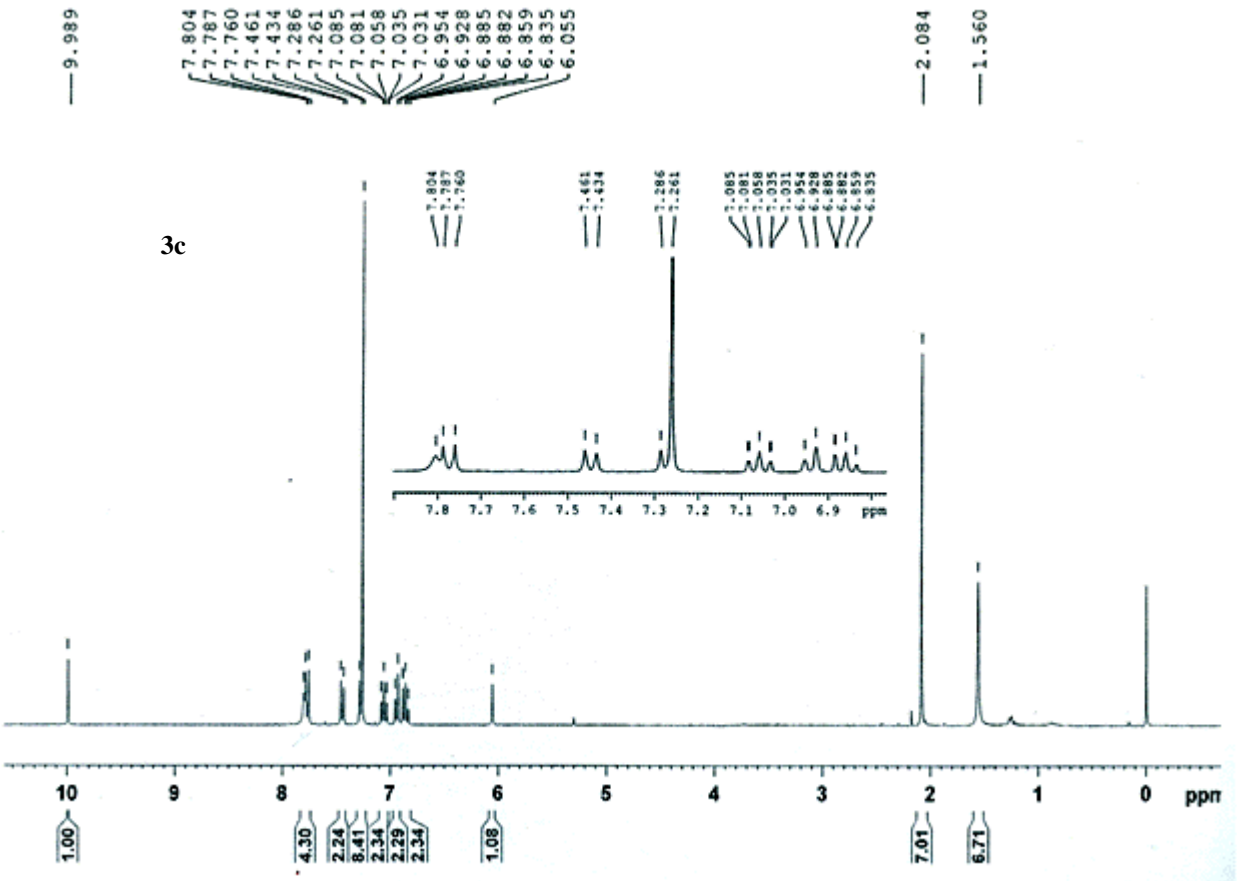
Charge number:1
Element:^{12}C:0 .. 56, ^{1}H:0 .. 120, ^{14}N:0 .. 2, ^{16}O:0 .. 1

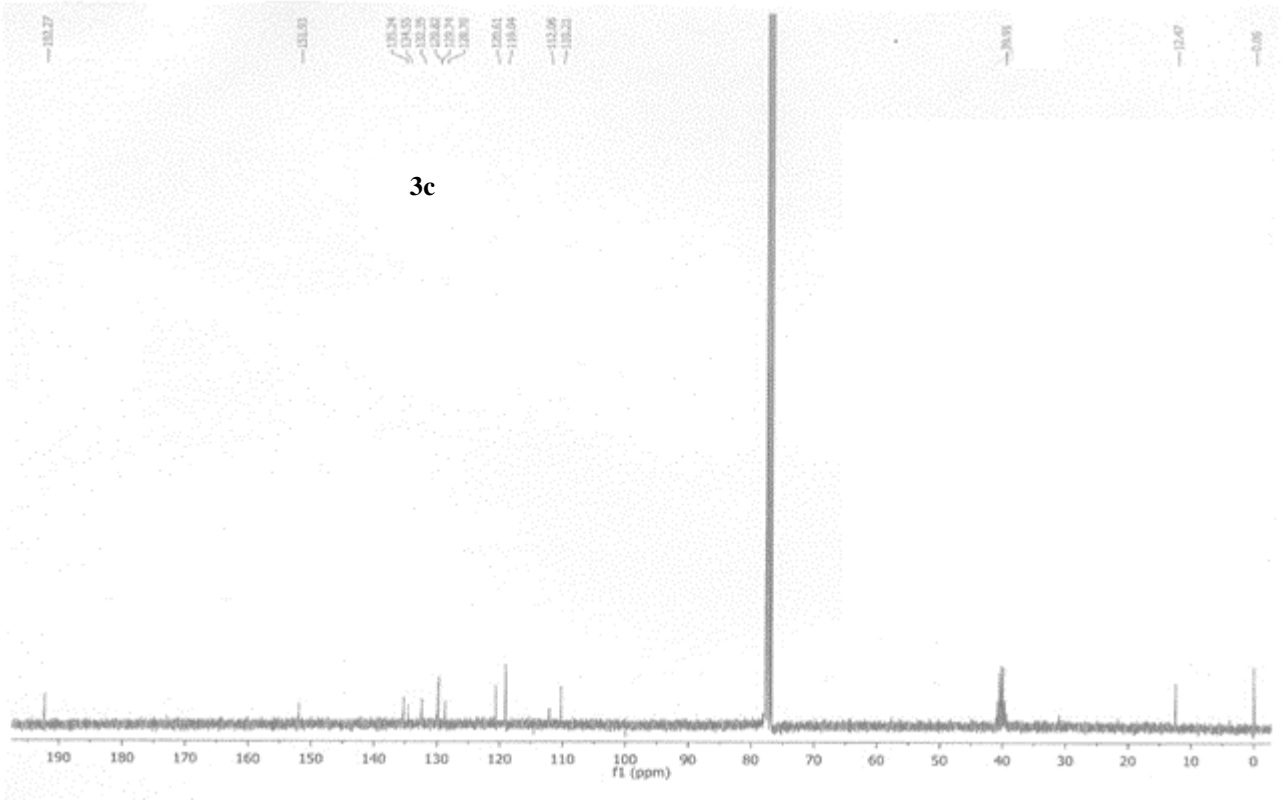
Tolerance:10.00(ppm), 5.00 .. 15.00(mmu)

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



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18073	20083.50	379.18104	-0.31	-0.81	$^{12}C_{26}{}^{1}H_{23}{}^{14}N_2{}^{16}O_1$	16.5





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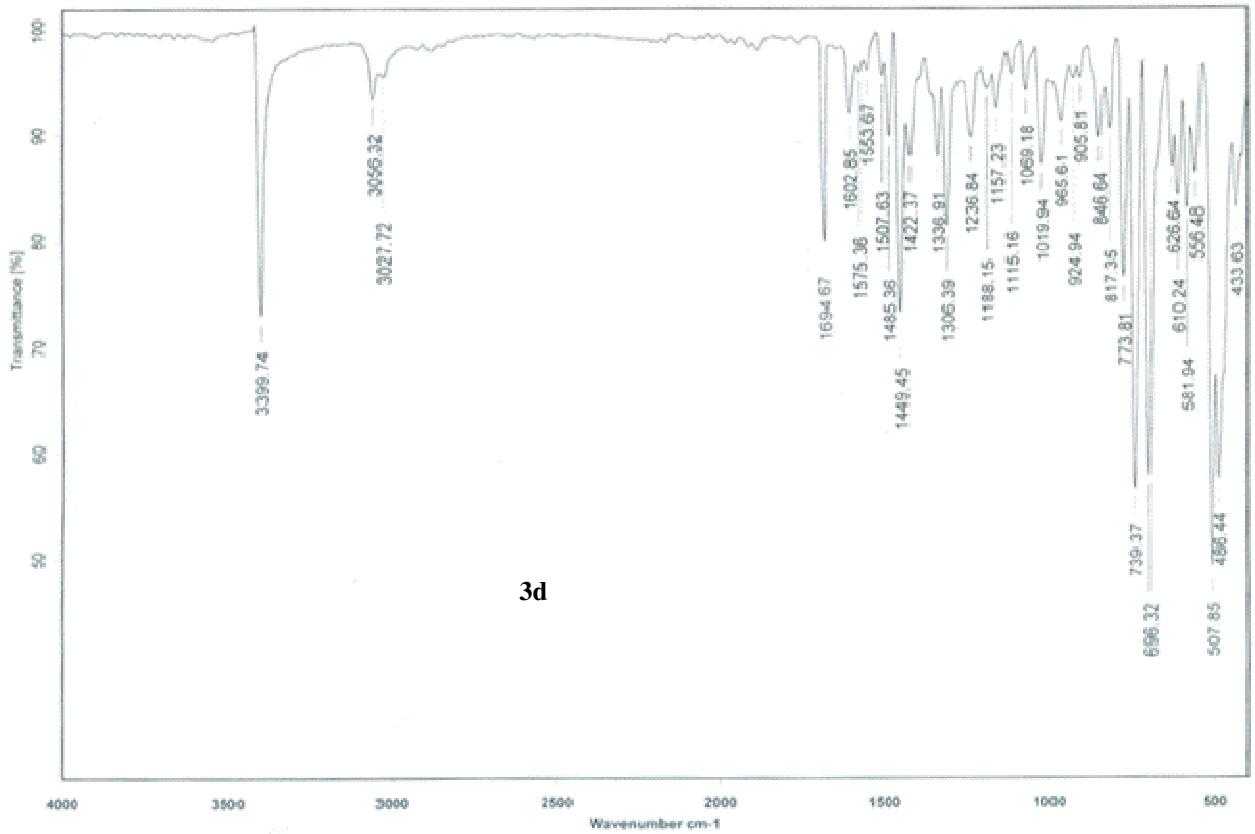

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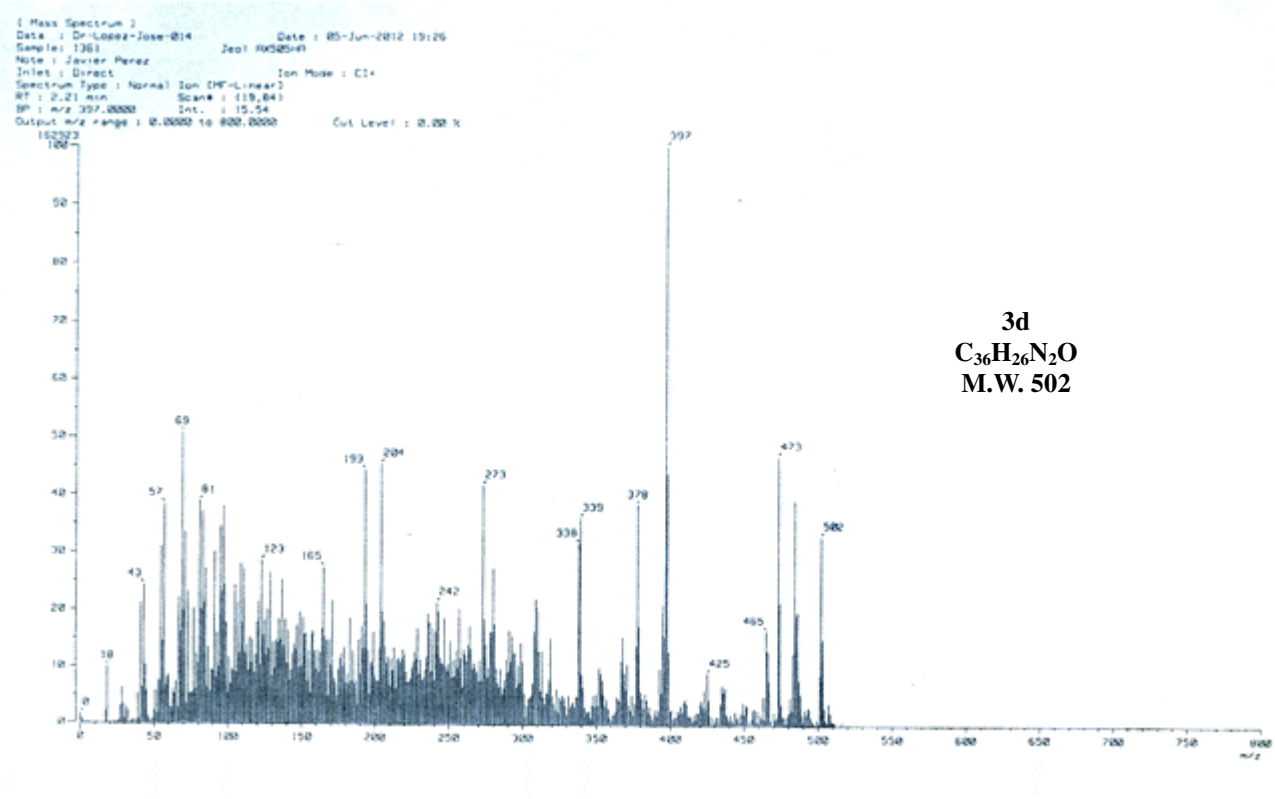
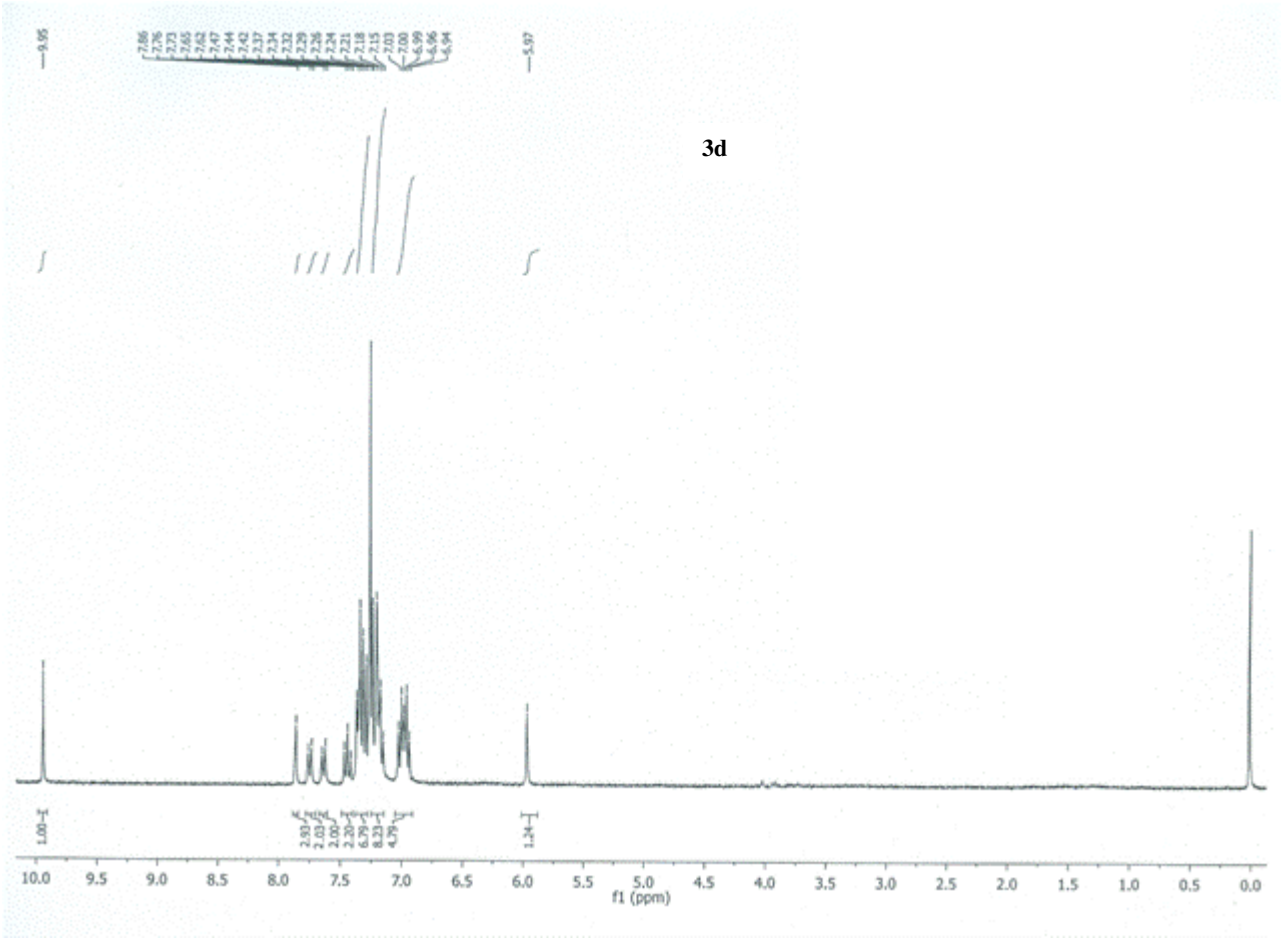


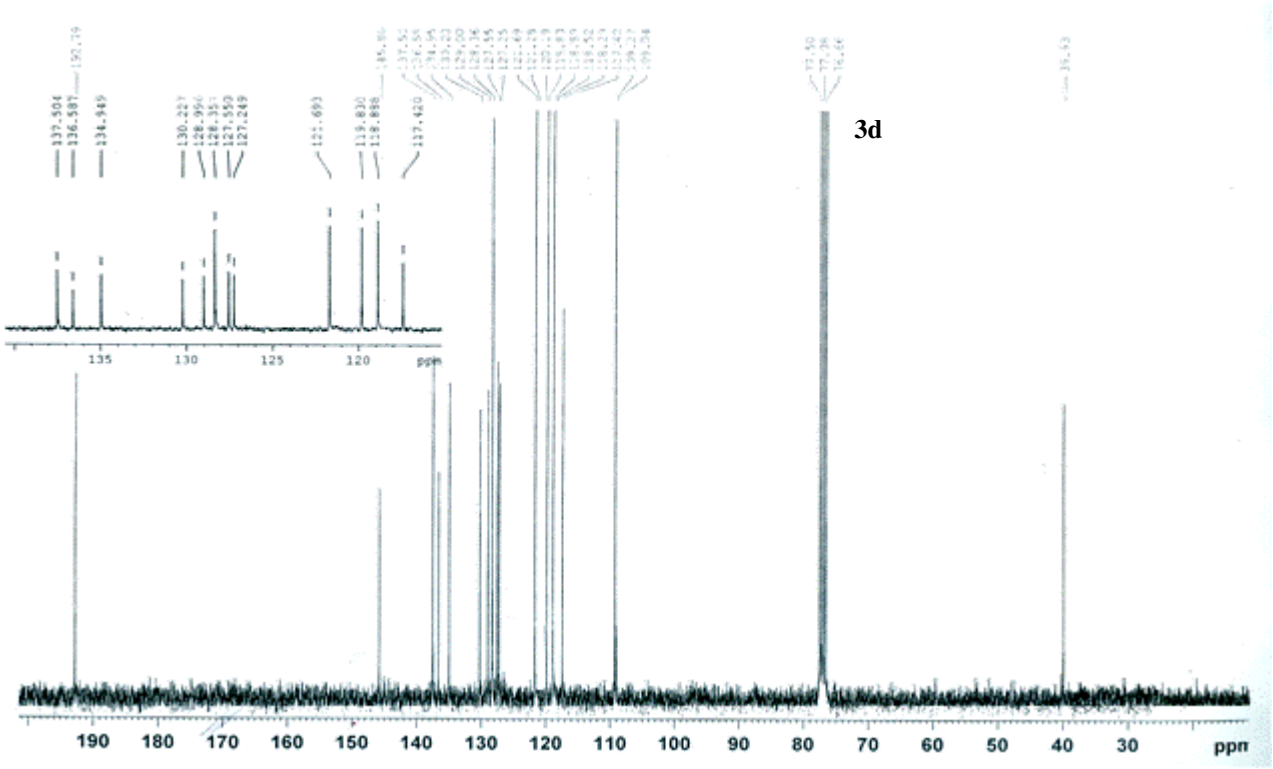
3d
$C_{36}H_{26}N_2O$
M.W. 502

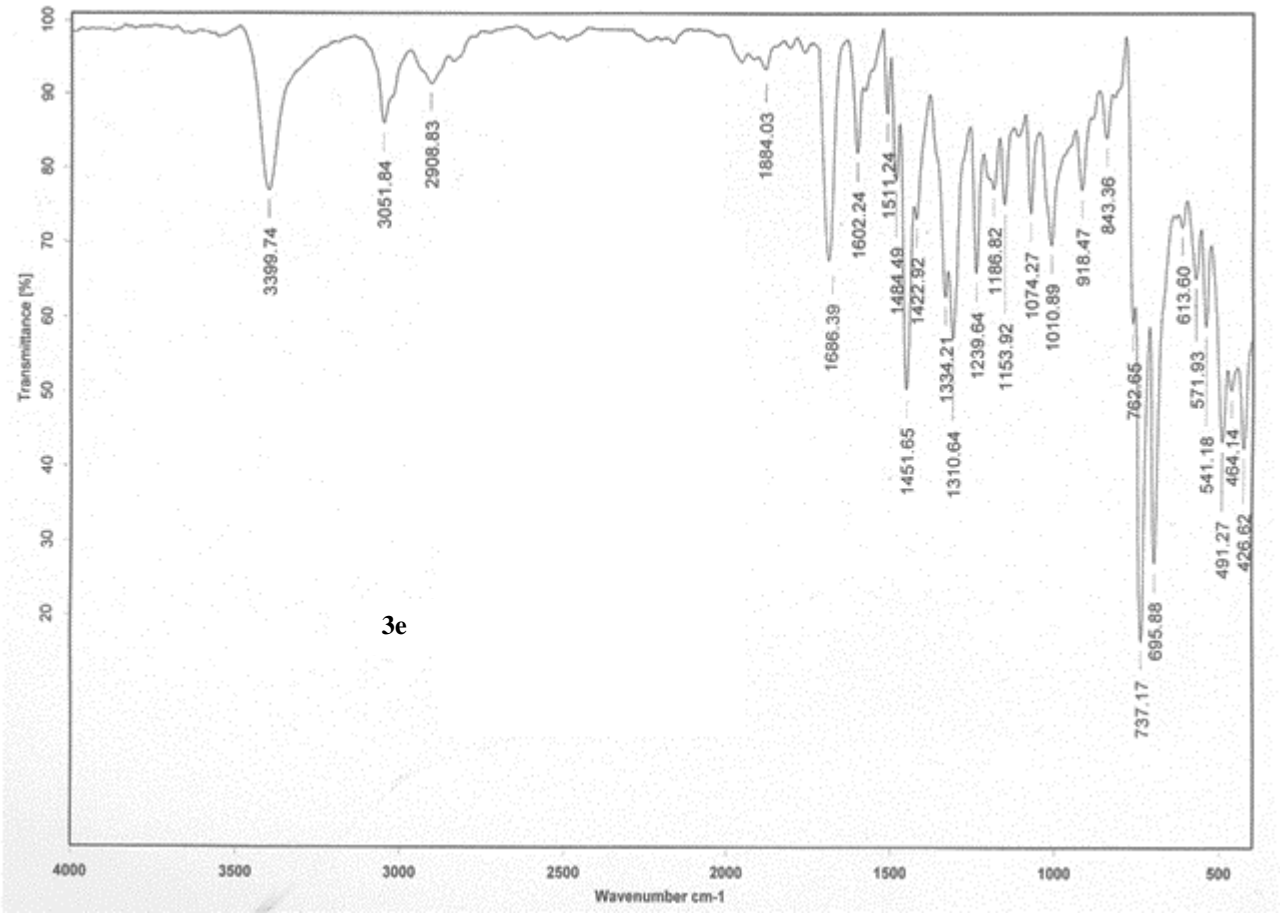
Data : Dr Cecilio-Alvarez059 Date : 02-Sep-2015 11:20
Instrument : MStation
Sample : 2582 2-ph-p
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 0.75 min Scan# : (6,7)
Elements : C 40/0, H 49/0, N 3/0, O 2/0
Mass Tolerance : 1000ppm, 1mmu if m/z > 1
Unsaturation (U.S.) : -0.5 - 45.0

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

	Observed m/z	Int%					
	502.2049	25.03					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	502.2045	+0.8 / +0.4	25.0	36	26	2	1







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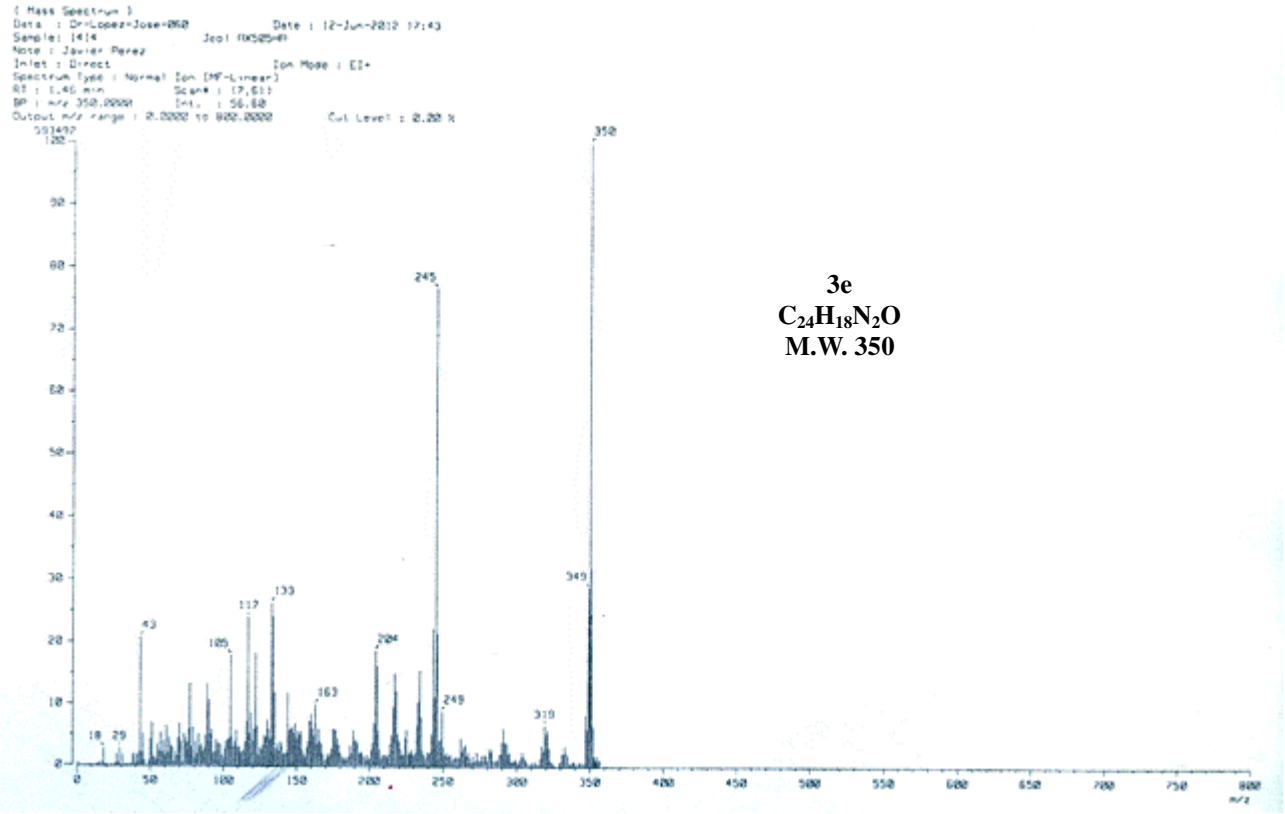
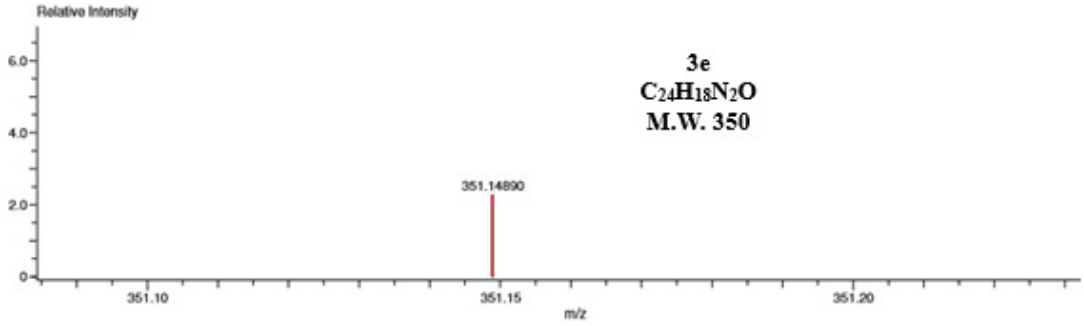


3e
$C_{24}H_{18}N_2O$
M.W. 350

Data:3010 Indol-m
Sample Name:Dr Alvarez Cecilio/ 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...

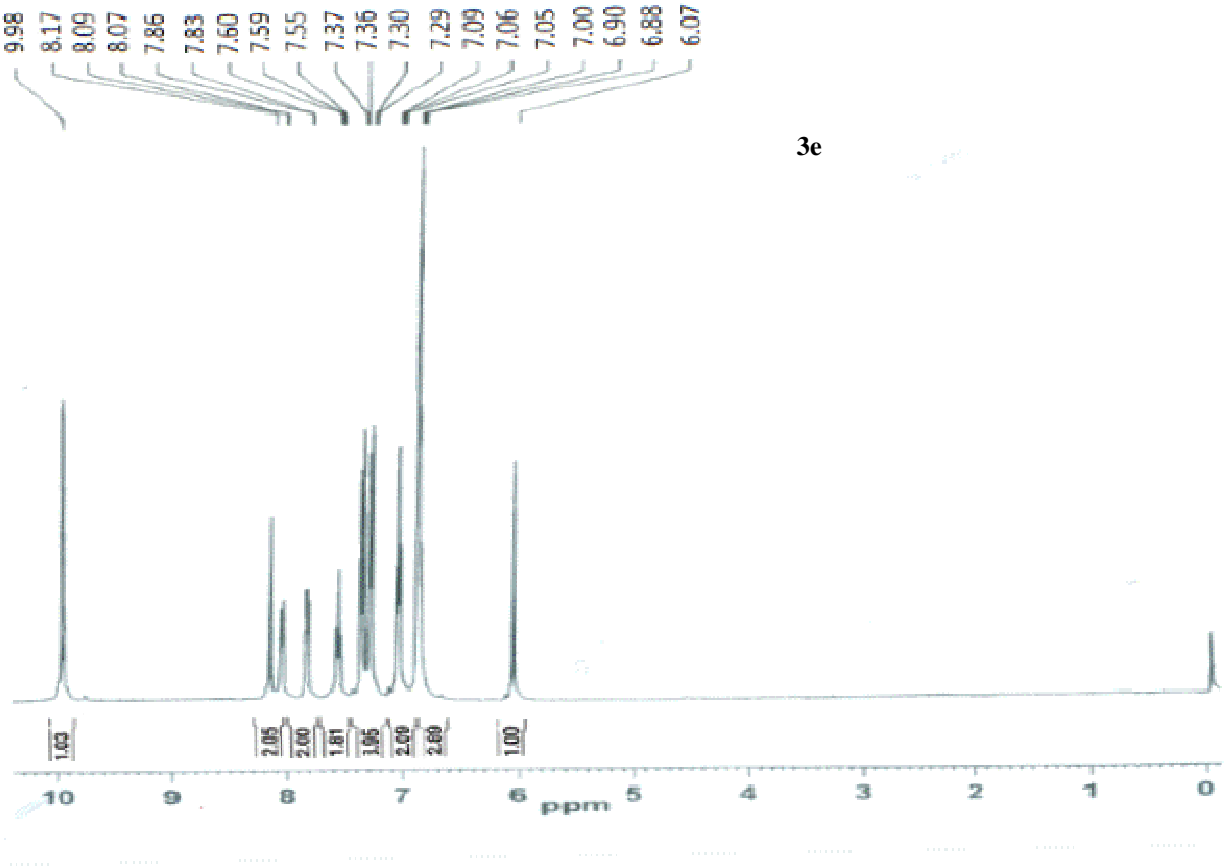
Acquired:9/30/2015 9:44:05 AM
Operator:AccuTOF
Mass Calibration data:Cal_Peg_600
Created:9/30/2015 12:15:17 PM
Created by:AccuTOF

Charge number:1
Tolerance:3.00(mmu)
Unsaturation Number:2.0 .. 20.0 (Fraction:Both)
Element:^{12}C:0 .. 56, ^{1}H:0 .. 120, ^{14}N:0 .. 2, ^{16}O:0 .. 3



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

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
351.14890	1386.79	351.14974	-0.84	-2.38	$^{12}C_{24}{}^{1}H_{19}{}^{14}N_2{}^{16}O_1$	16.5



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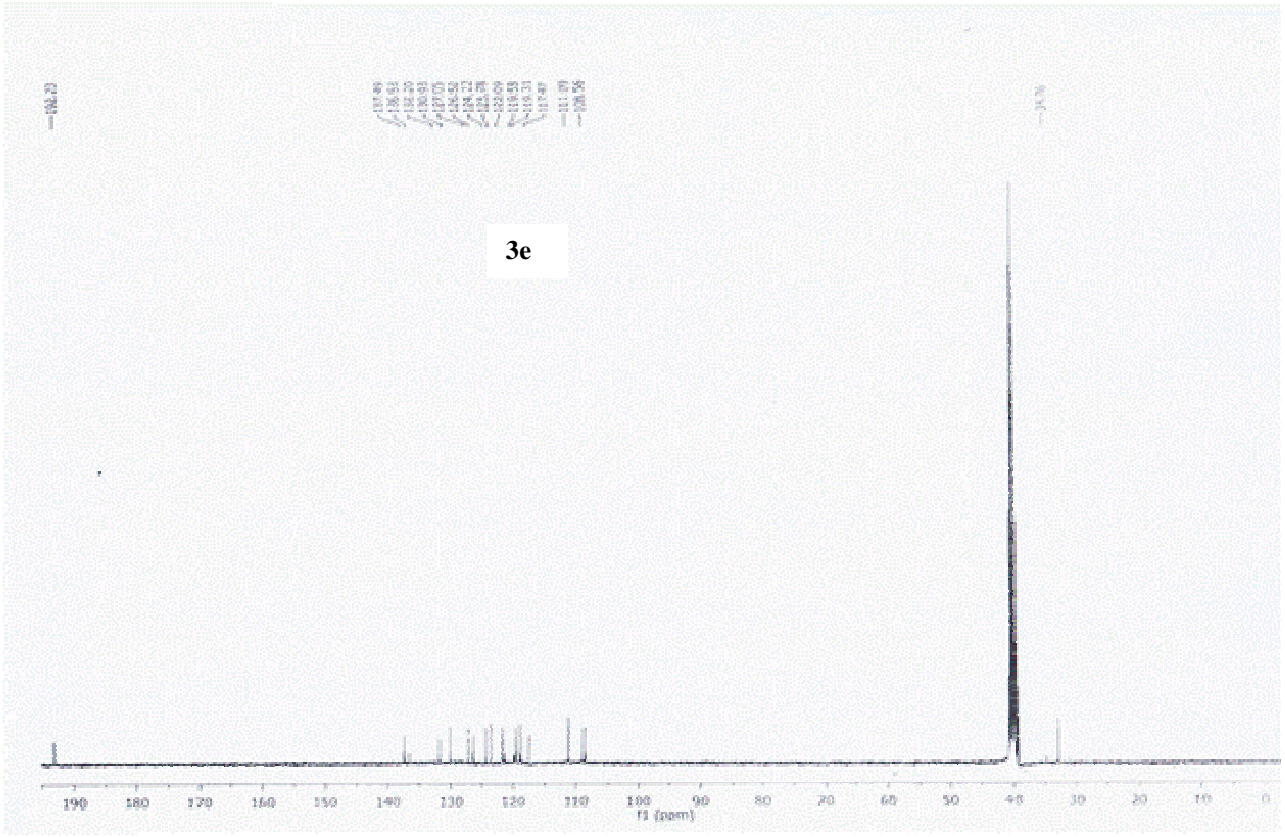
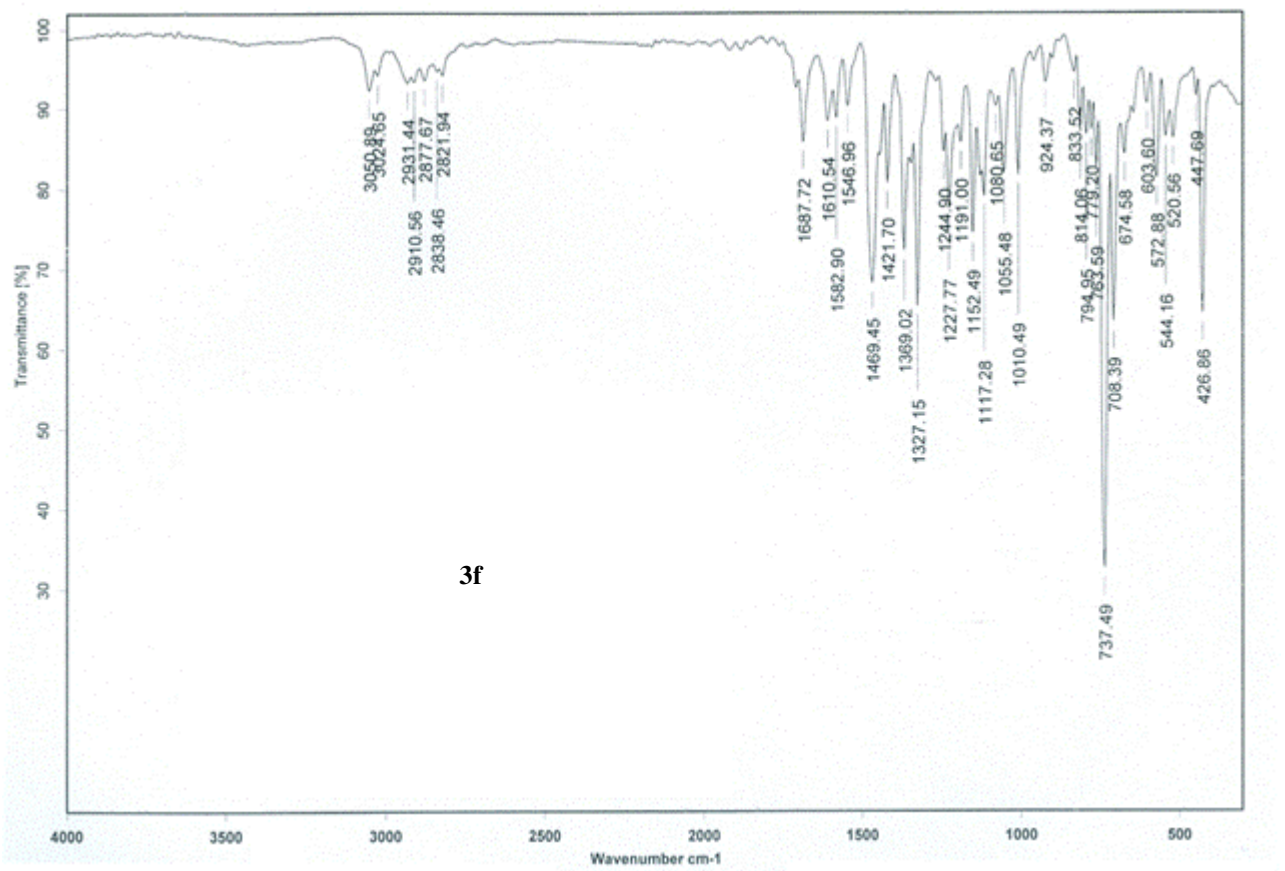
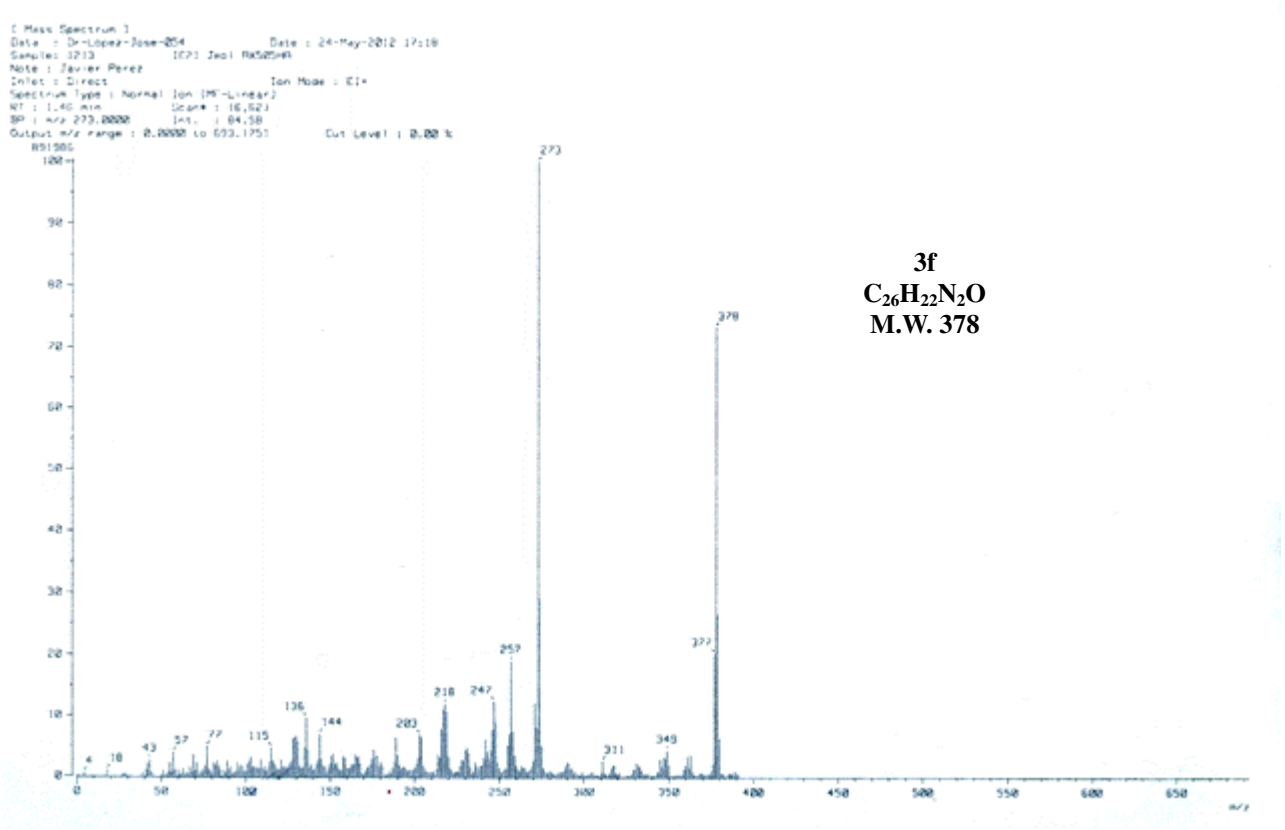


3e



3f

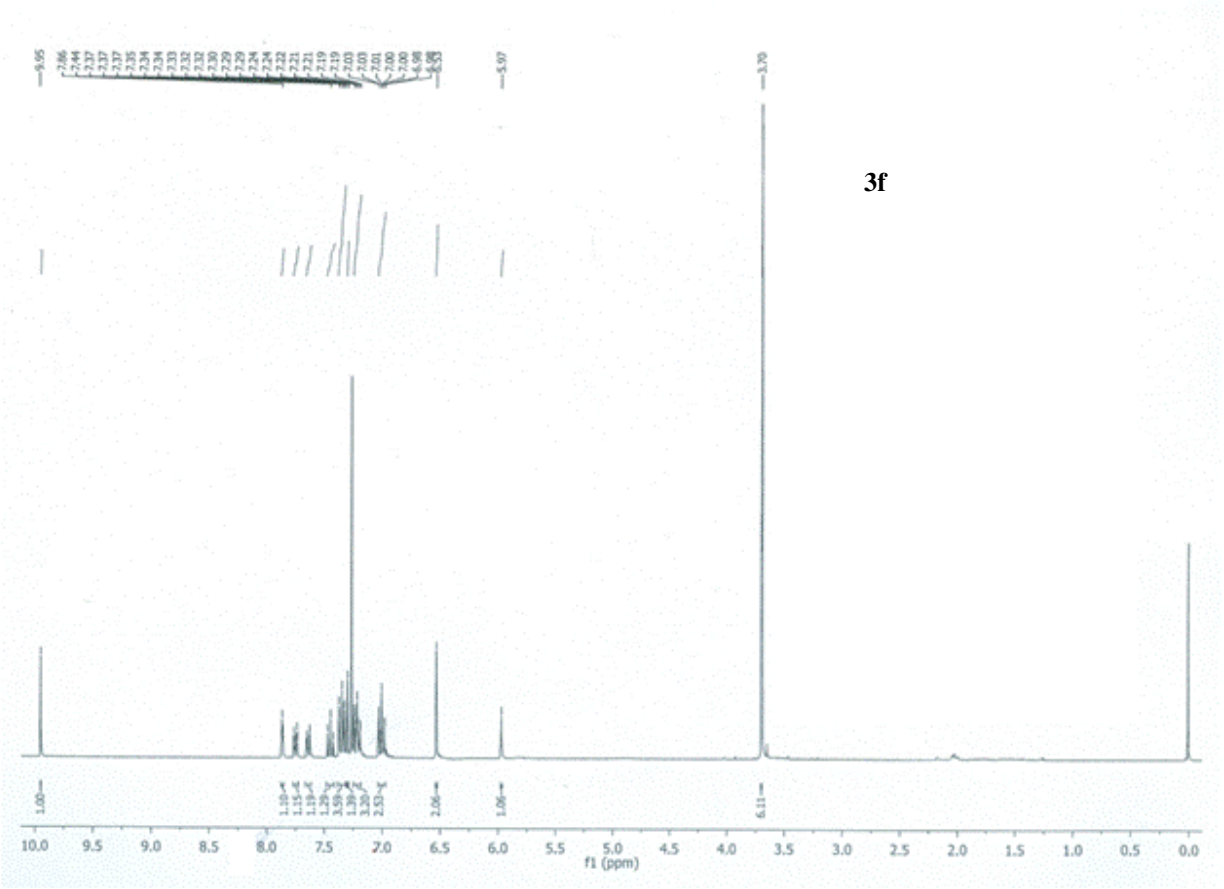


3f
$C_{26}H_{22}N_2O$
M.W. 378

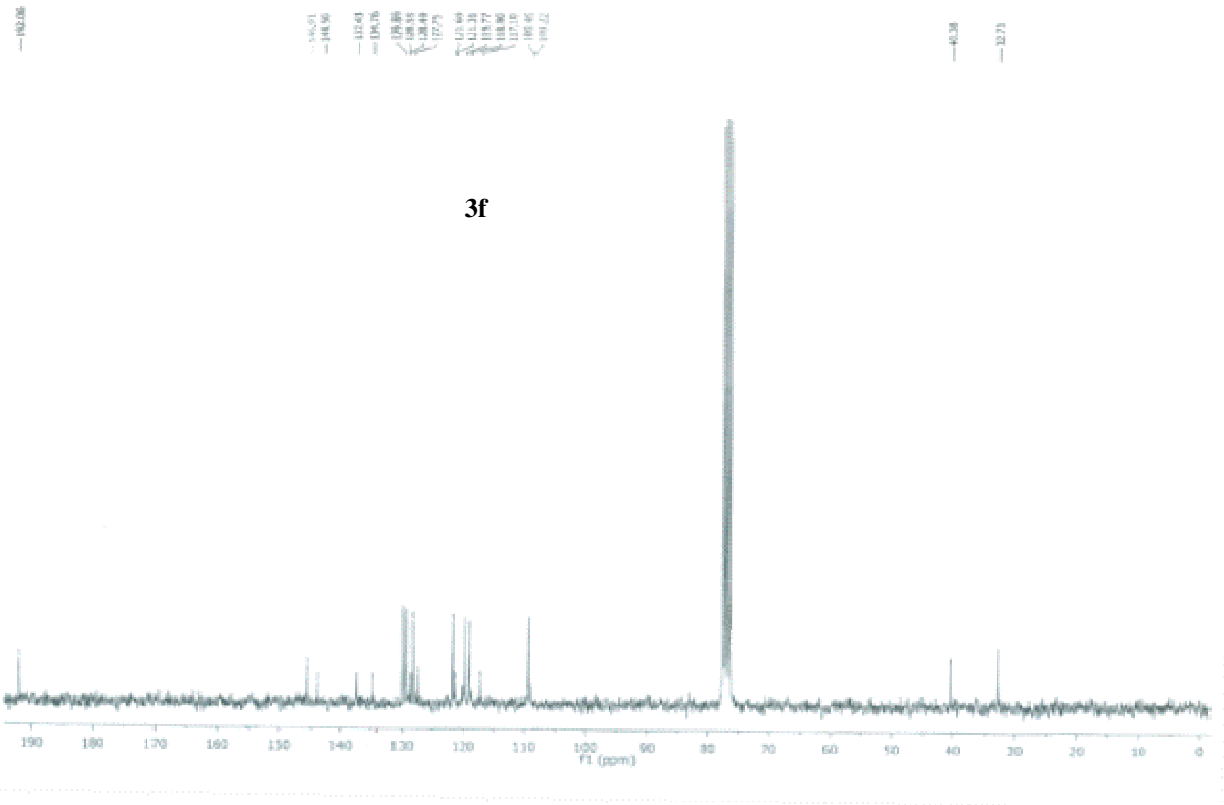
Data : Dr Cecilio Alvarez033 Date : 06-Oct-2015 12:27
Instrument : MStation
Sample : 3011 1-Me-m
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 0.00 min Scan# : (1,4)
Elements : C 30/0, H 49/0, N 3/0, O 2/0
Mass Tolerance : 1000ppm, 1mmu if m/z > 1
Unsaturation (U.S.) : -0.5 - 23.0

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

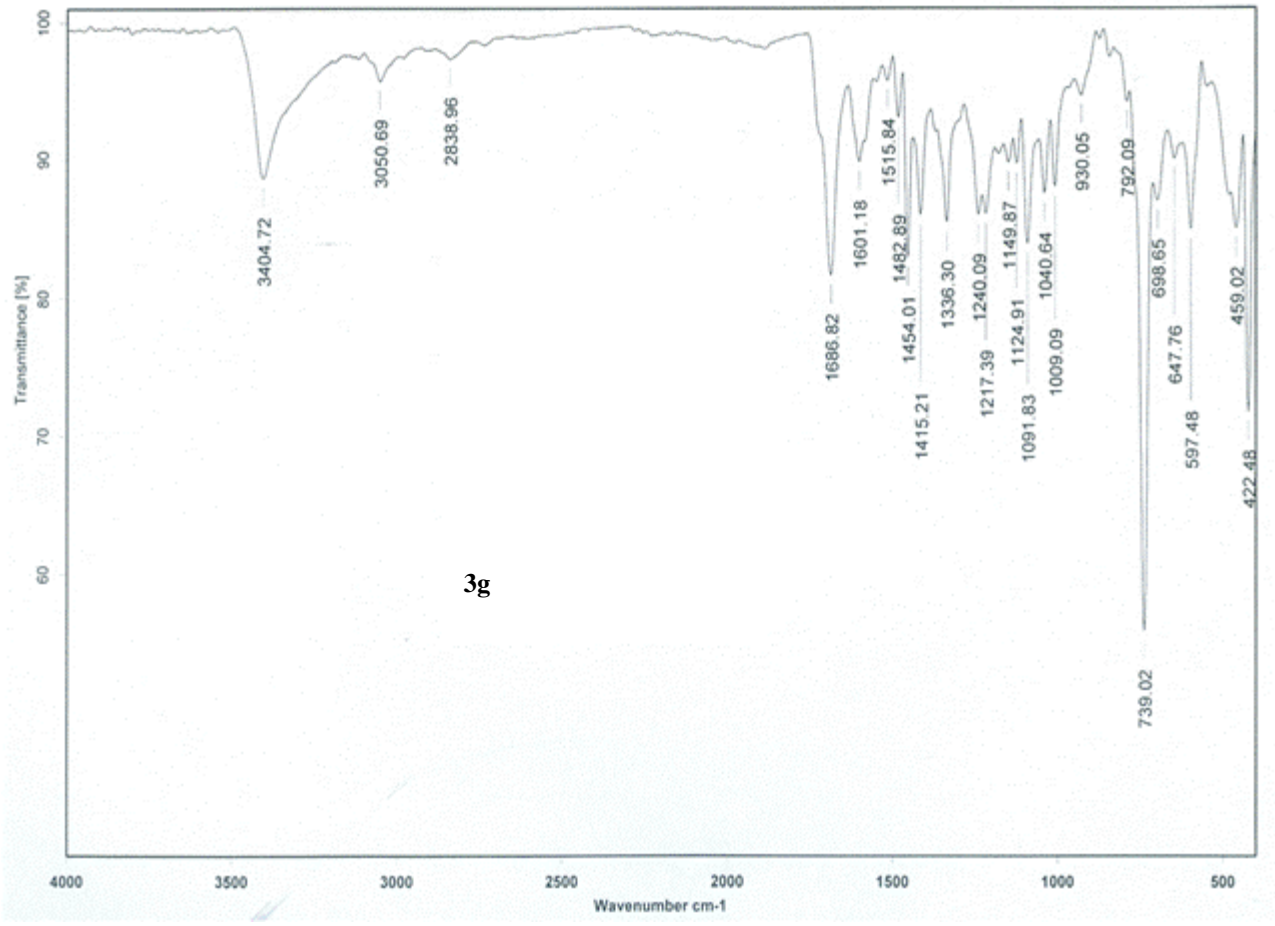
	Observed m/z	Int%	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
	378.1729	43.23							
1			378.1732	-0.8 / -0.3	17.0	26	22	2	1



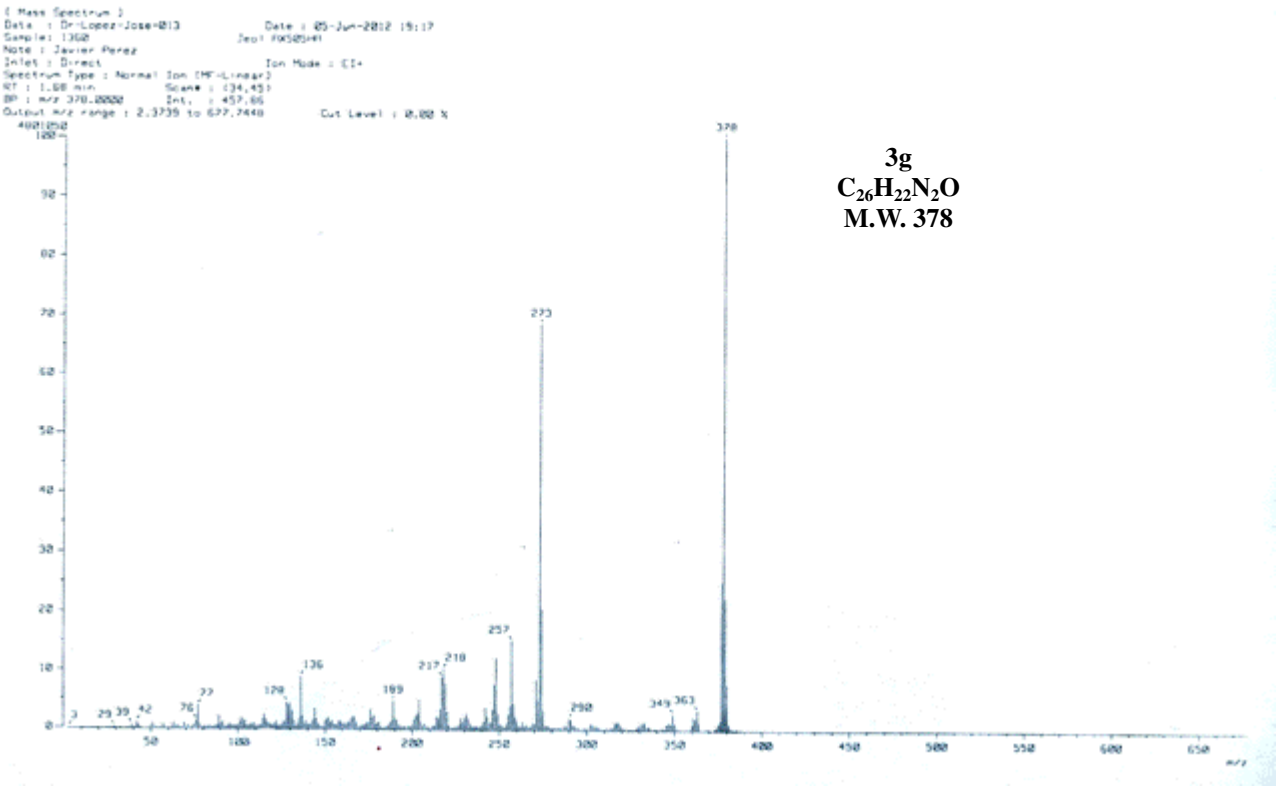
3f



3f



3g

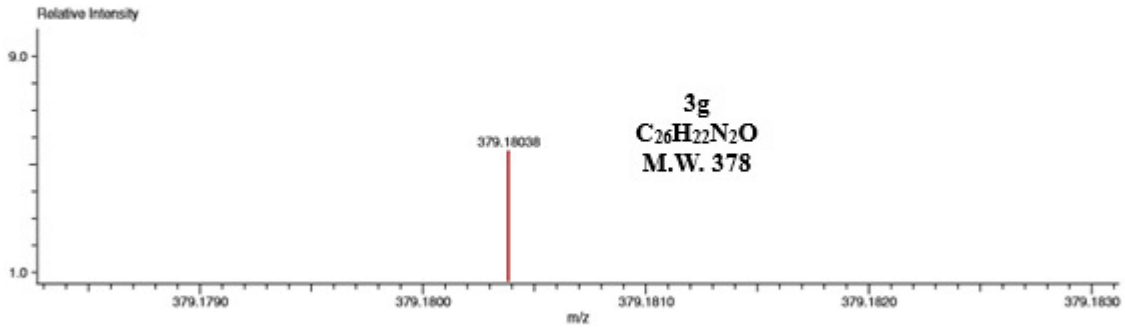


3g
$C_{26}H_{22}N_2O$
M.W. 378

Data:3013 2-Me-m
Sample Name:Dr Alvarez Cecilio/ 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] 0.4...

Acquired:9/30/2015 9:49:57 AM
Operator:AccuTOF
Mass Calibration data:Cal_Peg_600
Created:9/30/2015 12:56:56 PM
Created by:AccuTOF

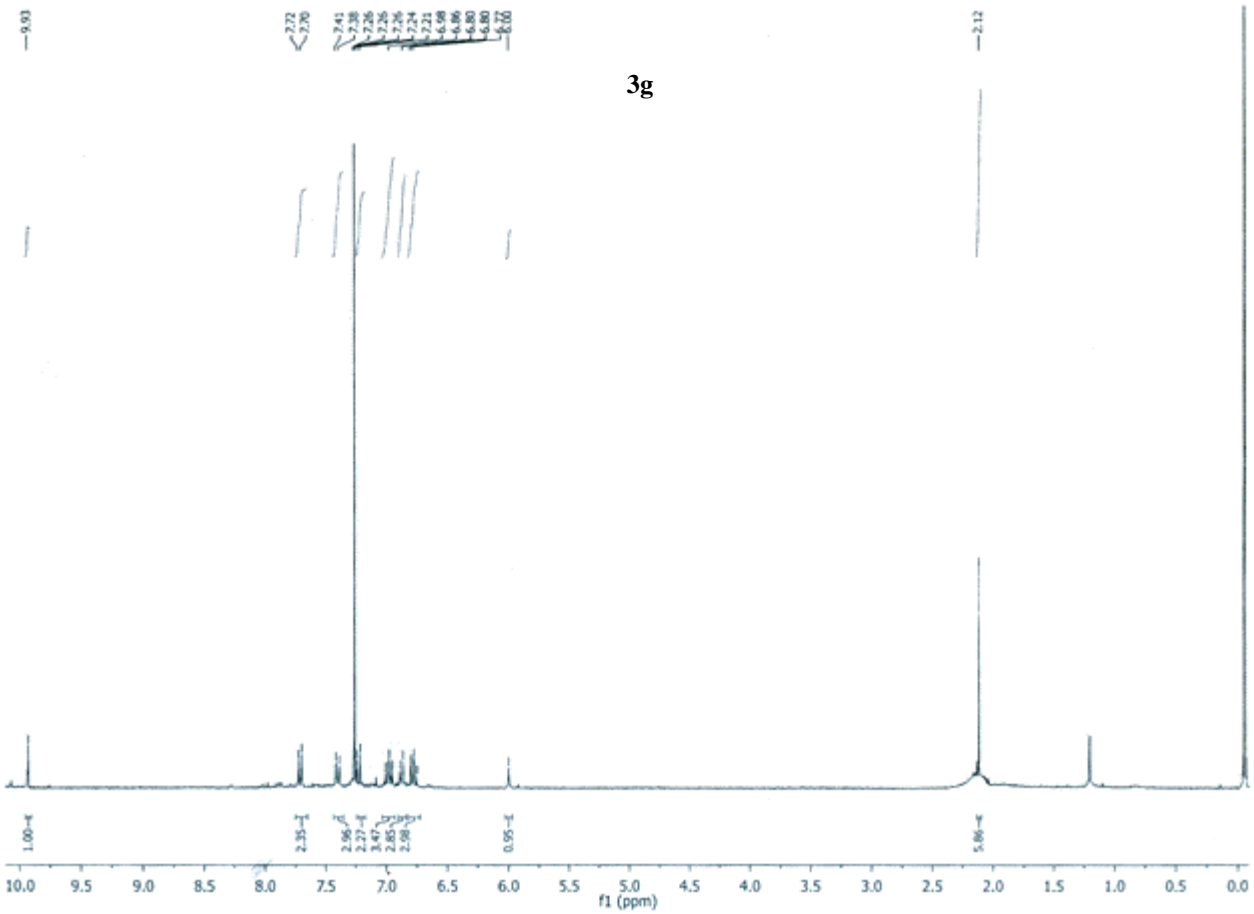
Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:2.0 .. 20.0 (Fraction:Both)
Element:^{12}C:0 .. 56, ^{1}H:0 .. 120, ^{14}N:0 .. 2, ^{16}O:0 .. 3

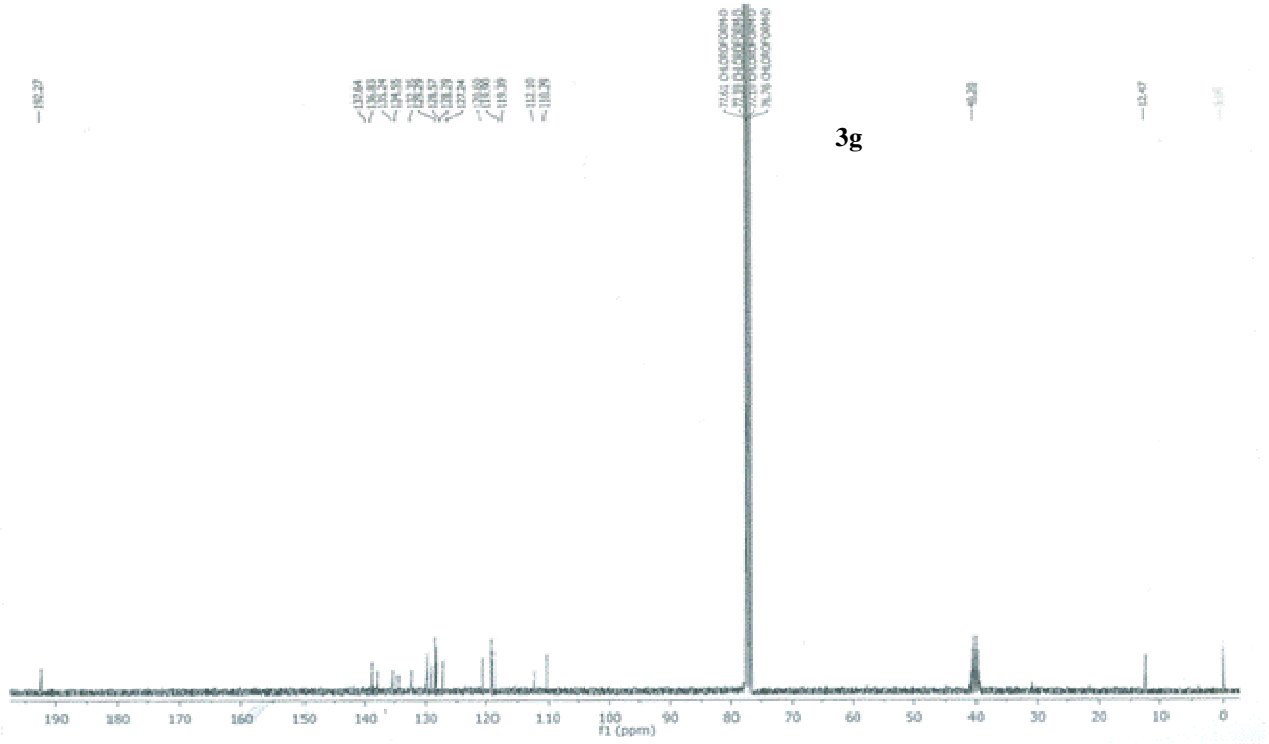


3g
$C_{26}H_{22}N_2O$
M.W. 378

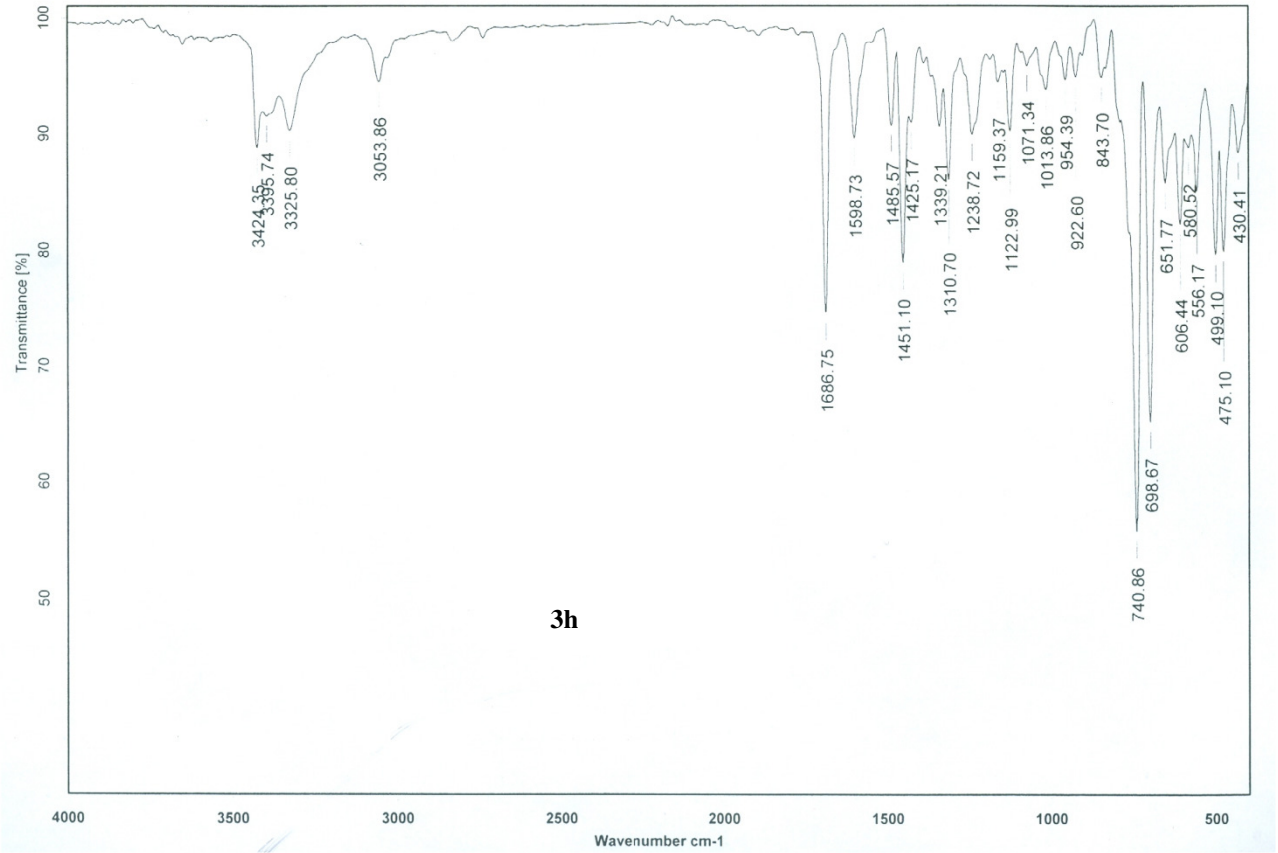
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.18038	1642.76	379.18104	-0.65	-1.73	$^{12}C_{26}{}^{1}H_{23}{}^{14}N_2{}^{16}O_1$	16.5

3g

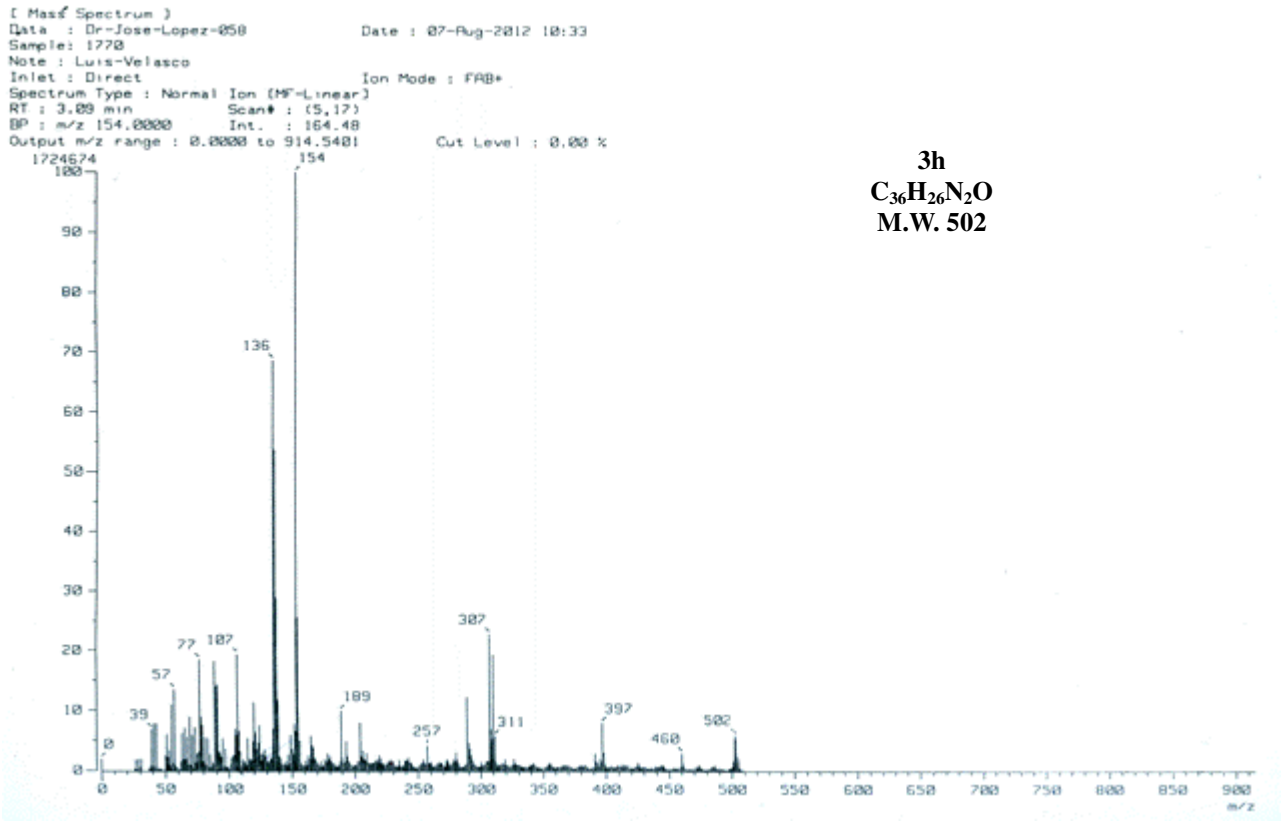




3g



3h



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

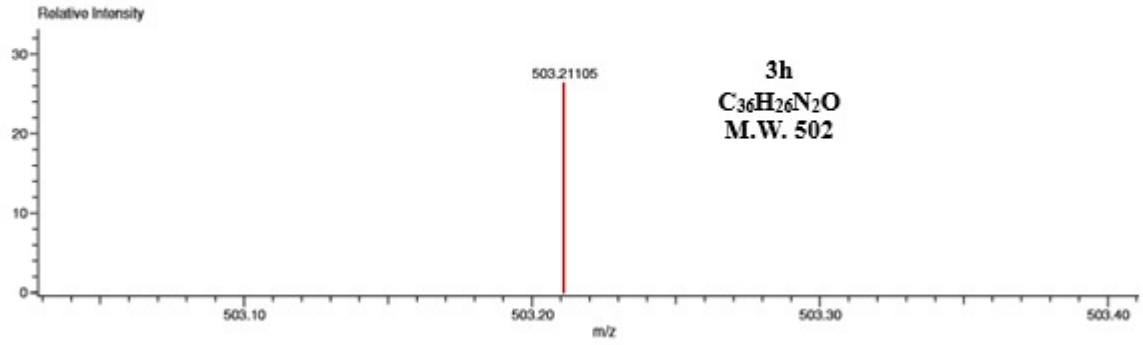
Data:CAT 8
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.3...

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

Tolerance:3.00(mmu)

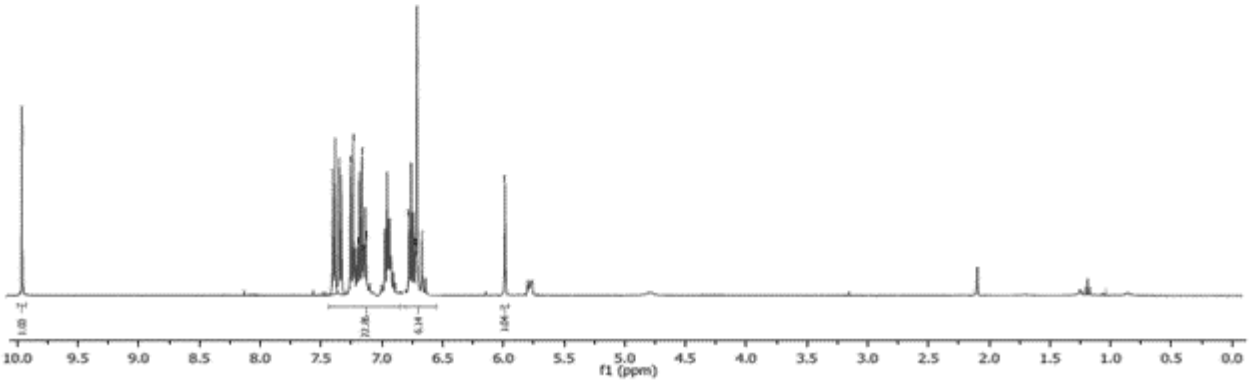
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)

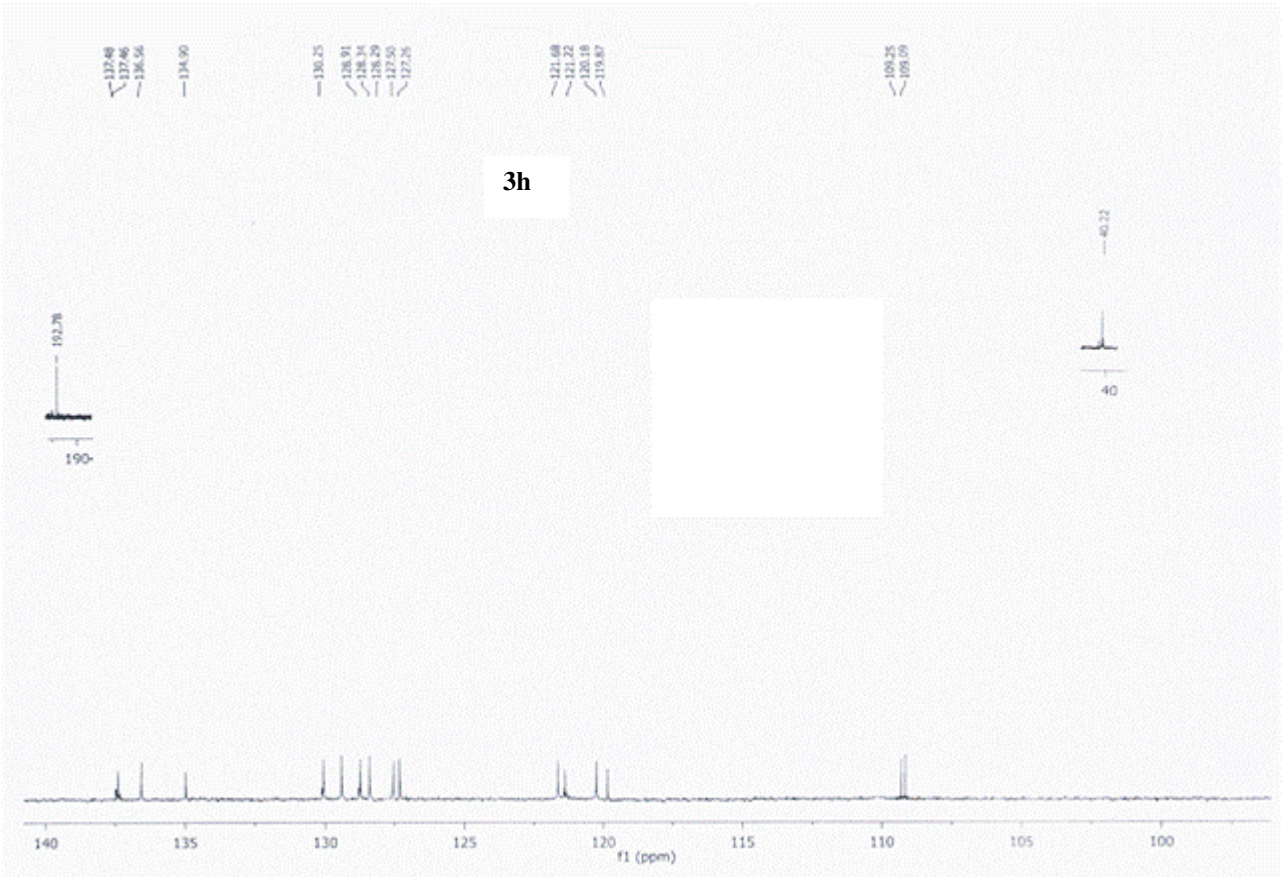


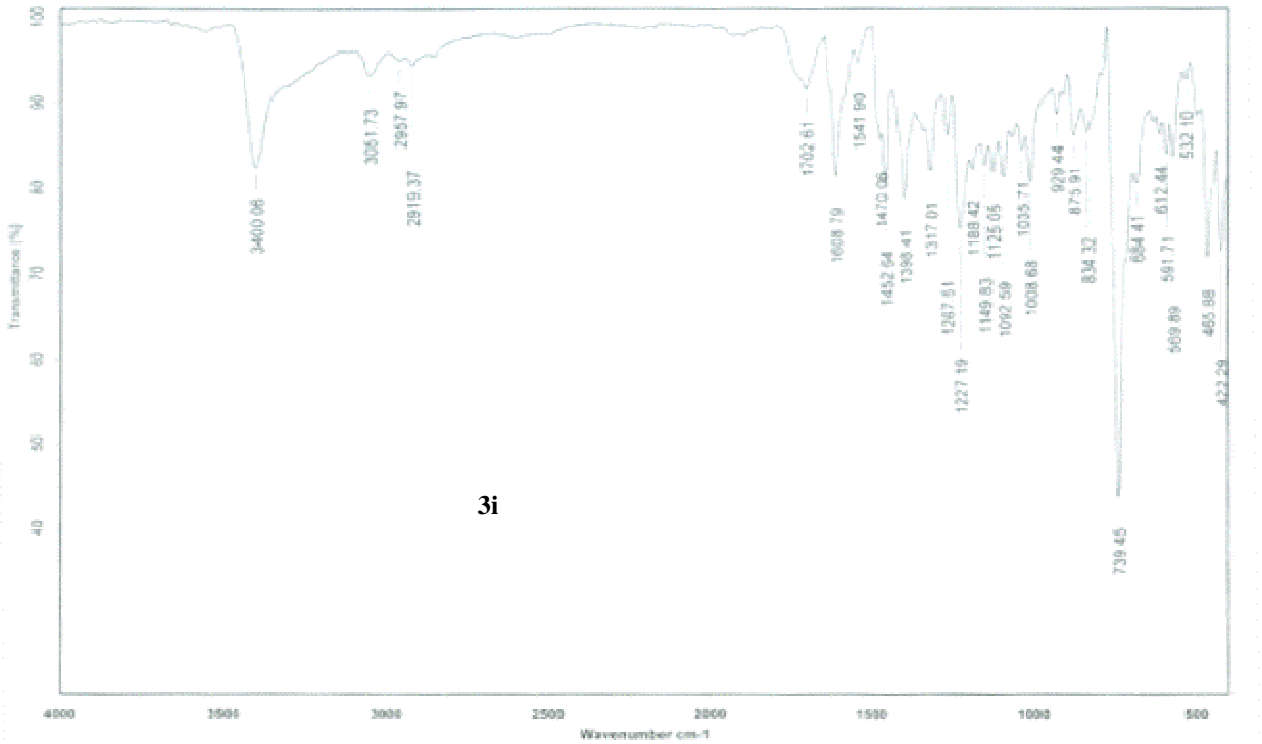
3h
$C_{36}H_{26}N_2O$
M.W. 502

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21105	2115.38	503.21234	-1.28	-2.55	$^{12}C_{36}{}^{1}H_{27}{}^{14}N_2{}^{16}O_1$	24.5

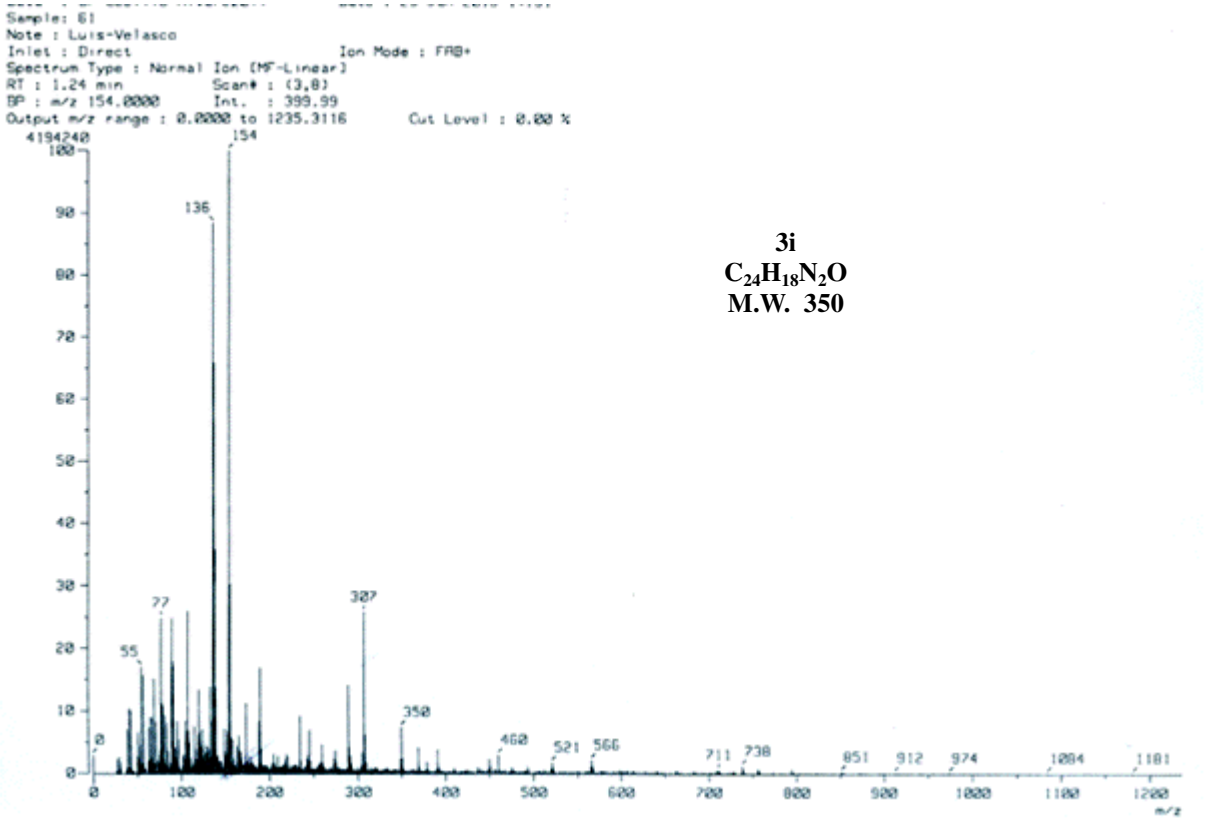
3h







3i



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

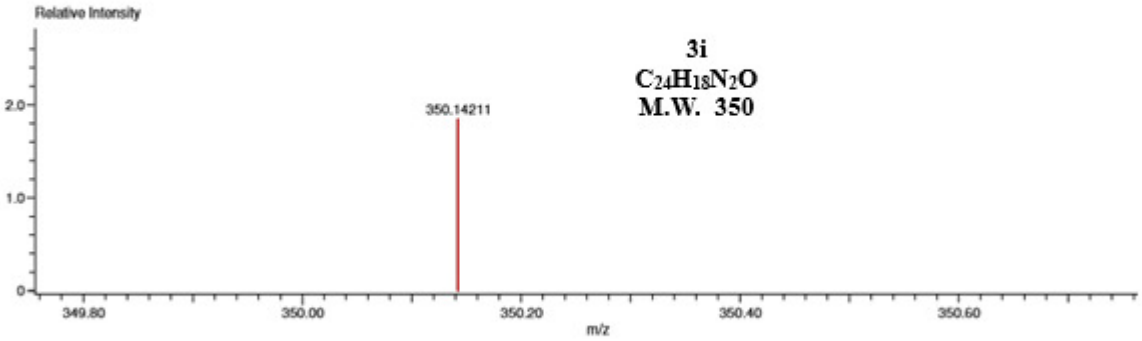
Data:CAT 10
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.7...

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

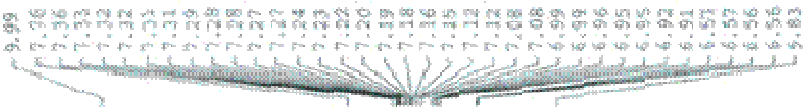
Charge number:1
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:0 .. 3, ^{16}O:0 .. 3

Tolerance:3.00(mmu)

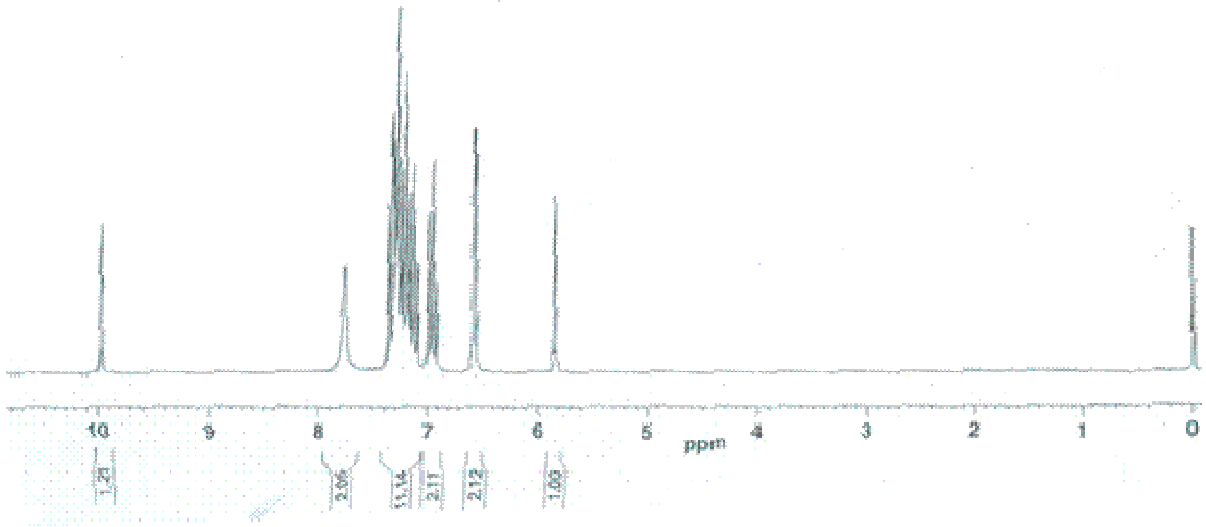
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)

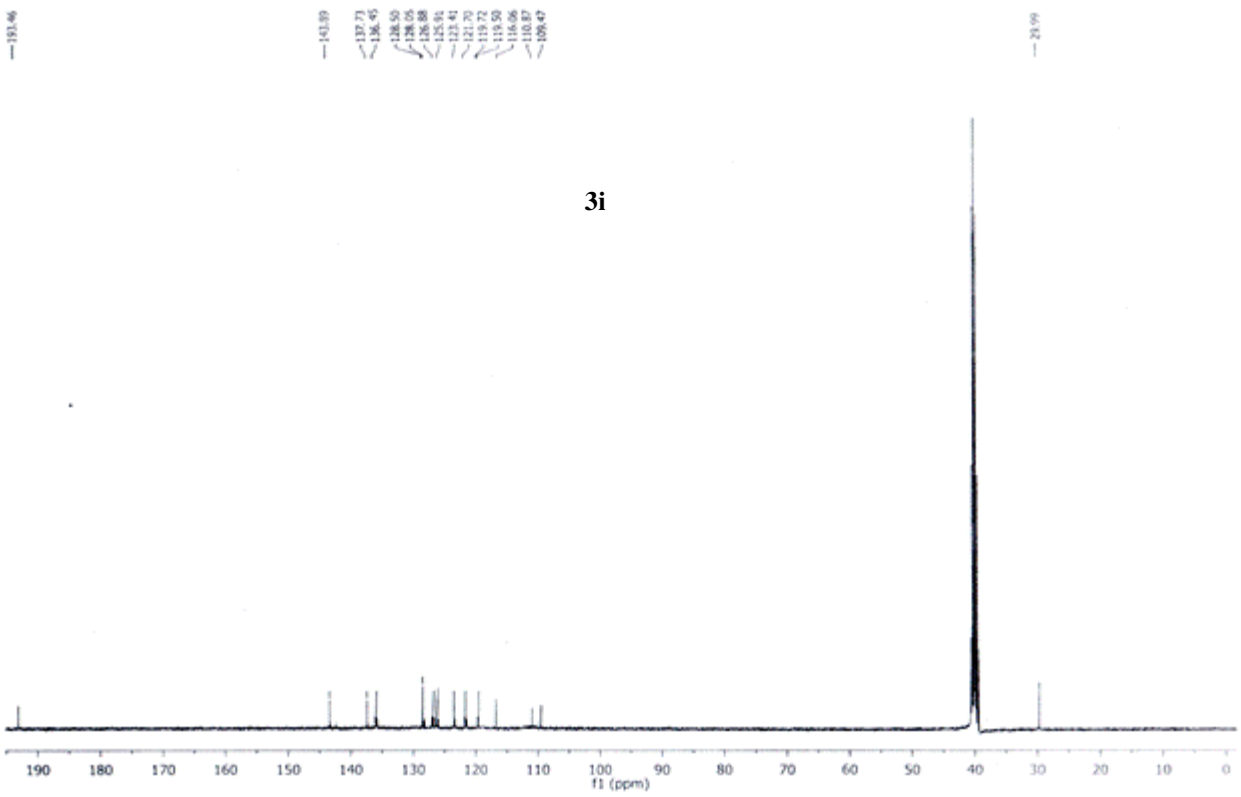


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
350.14211	2134.88	350.14191	0.19	0.55	$^{12}C_{24}{}^{1}H_{18}{}^{14}N_{2}{}^{16}O_{1}$	17.0

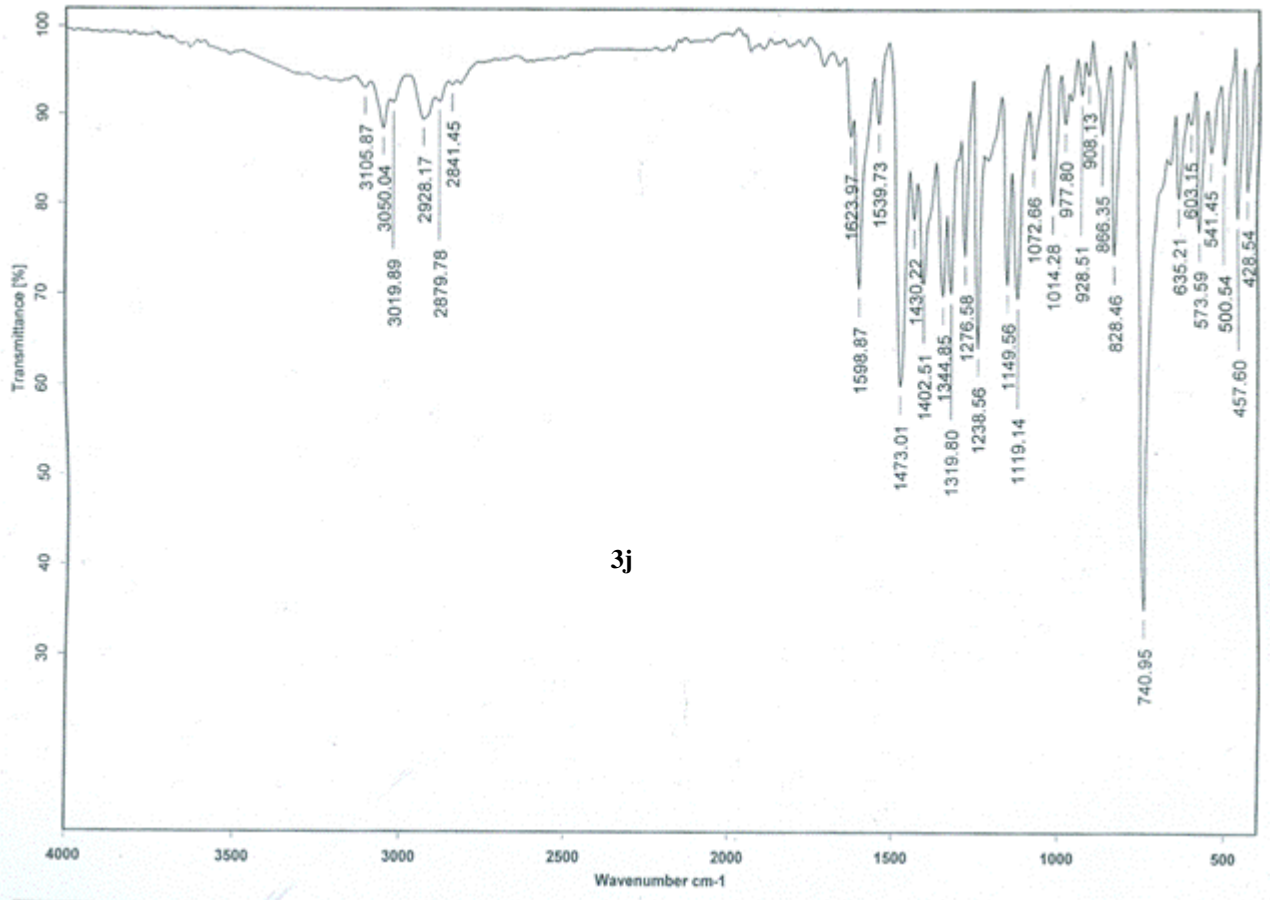


3i

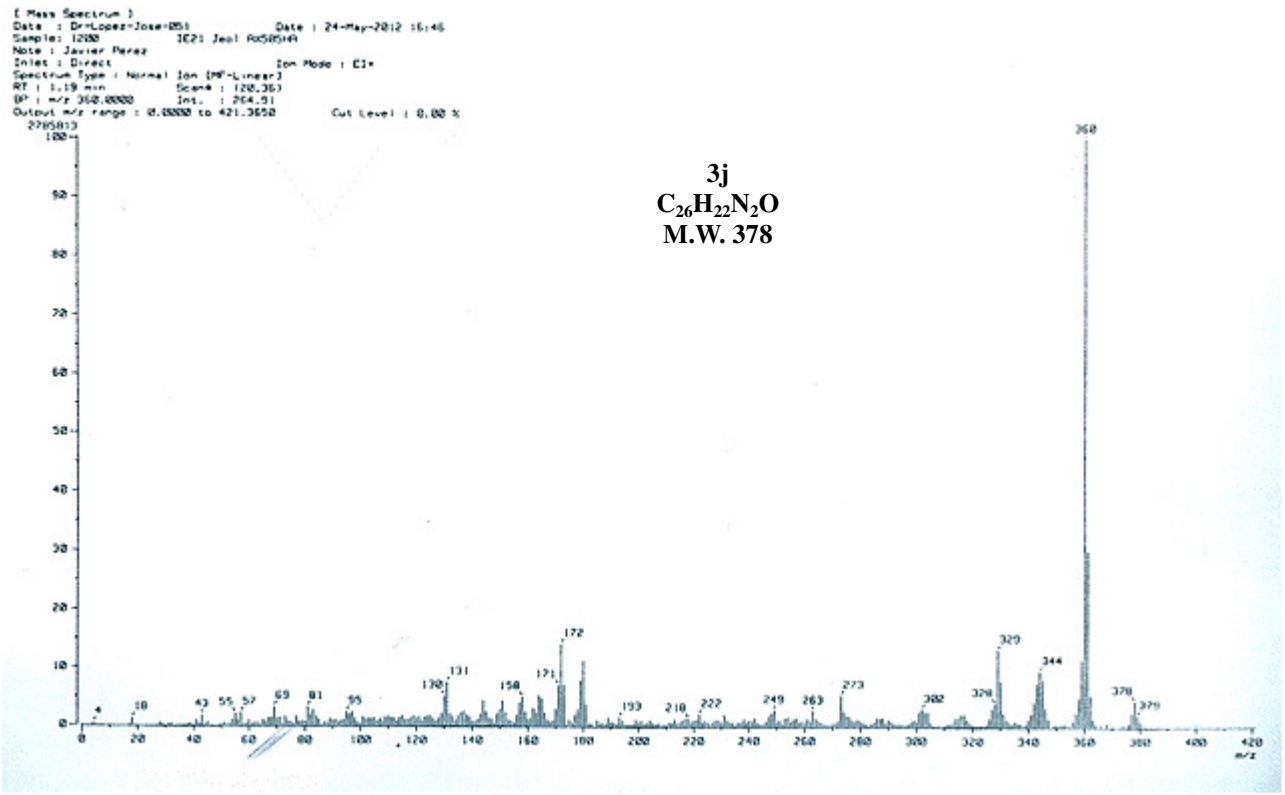




3i



3j



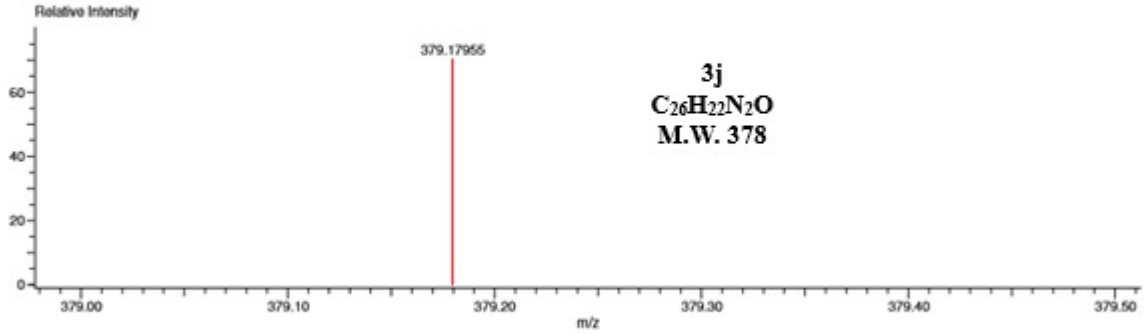
Data:CAT 9
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.2...

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

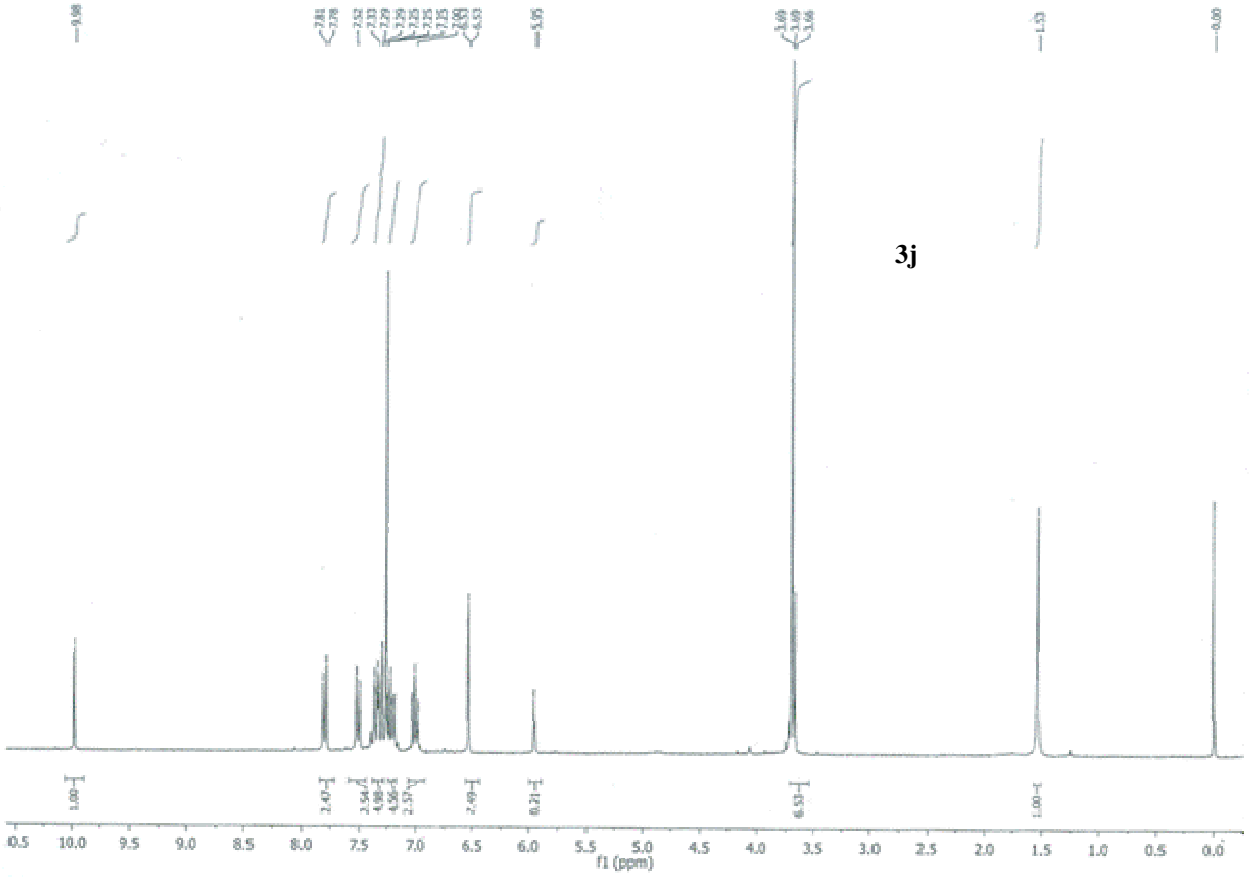
Charge number:1
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:0 .. 3, ^{16}O:0 .. 3

Tolerance:3.00(mmu)

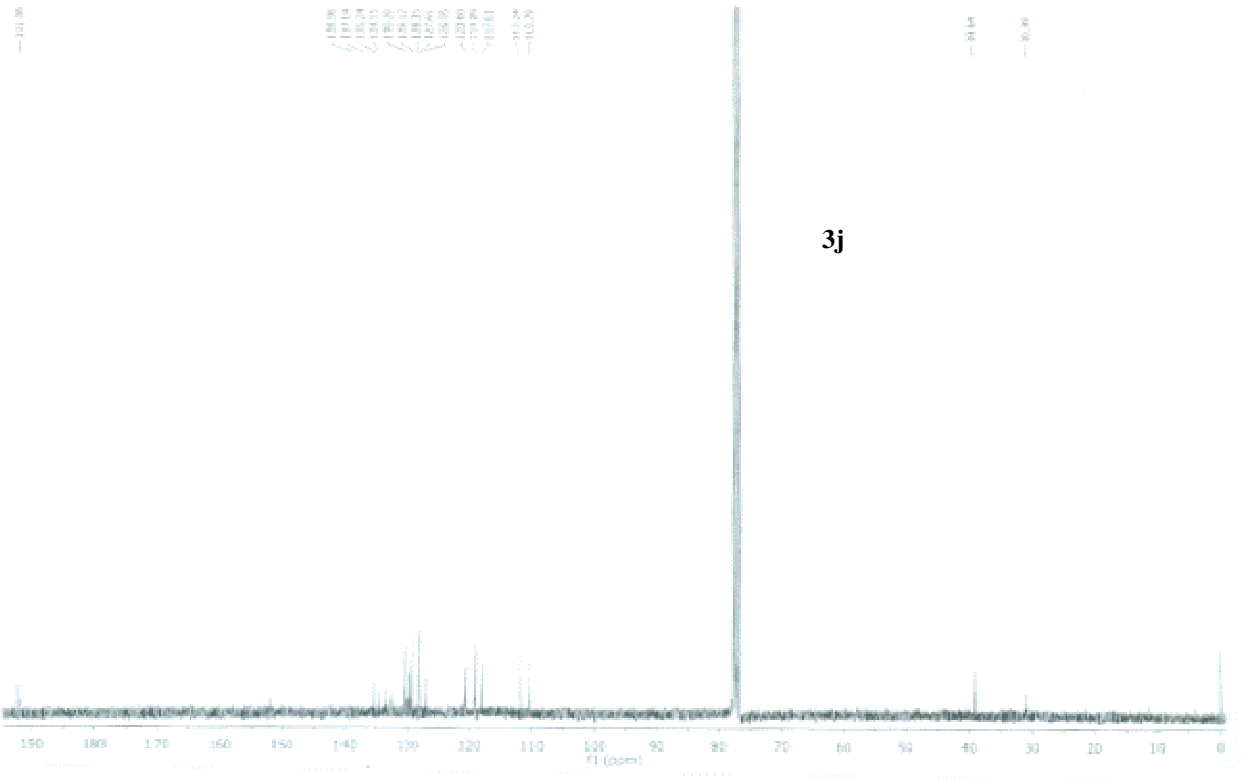
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



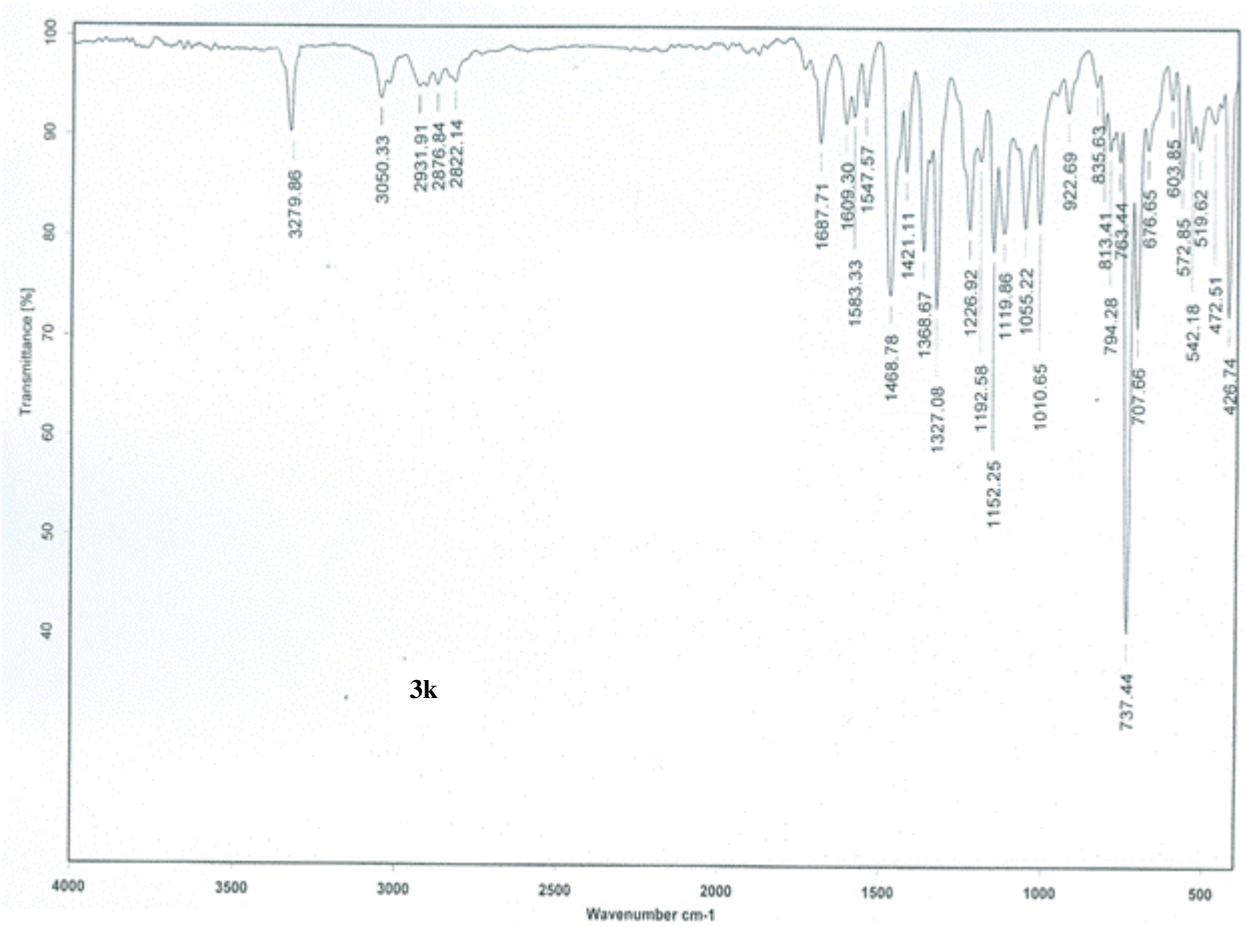
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
379.17955	5429.27	379.18104	-1.49	-3.93	$^{12}C_{26}{}^{1}H_{23}{}^{14}N_2{}^{16}O_1$	16.5



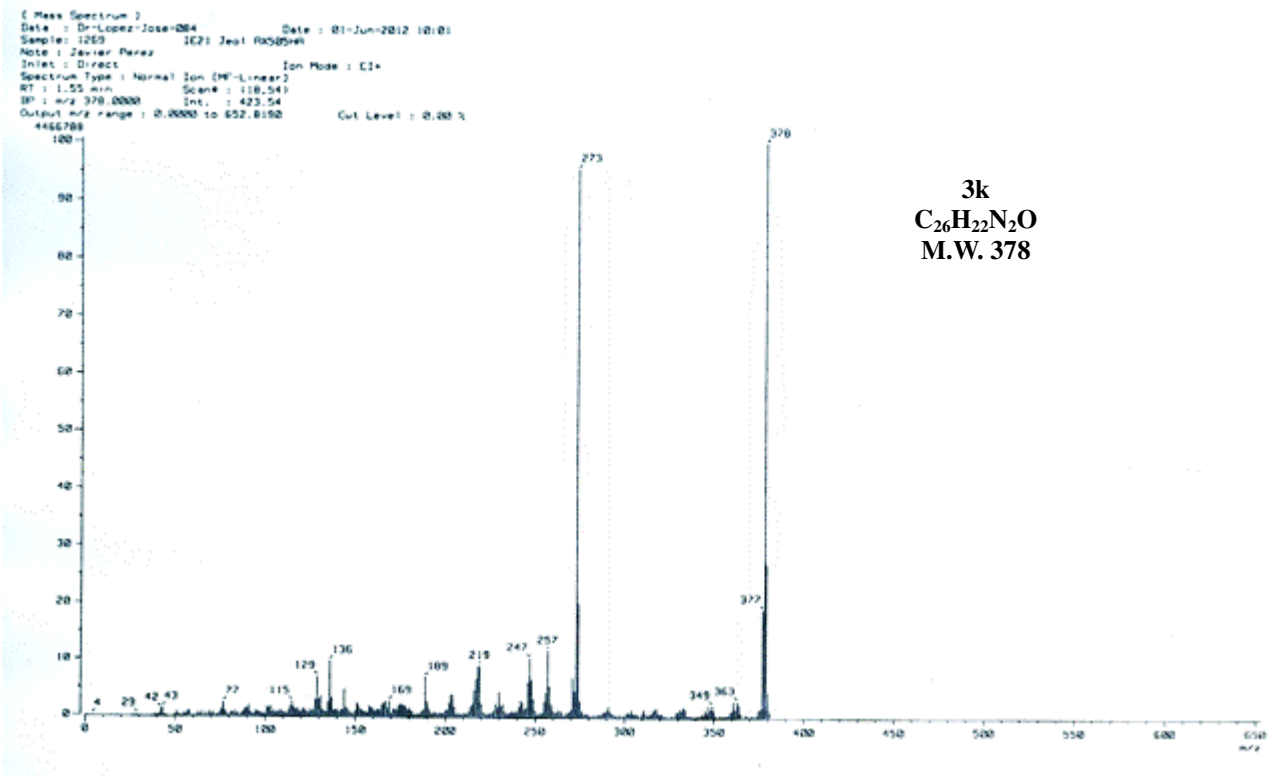
3j



3j



3k



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

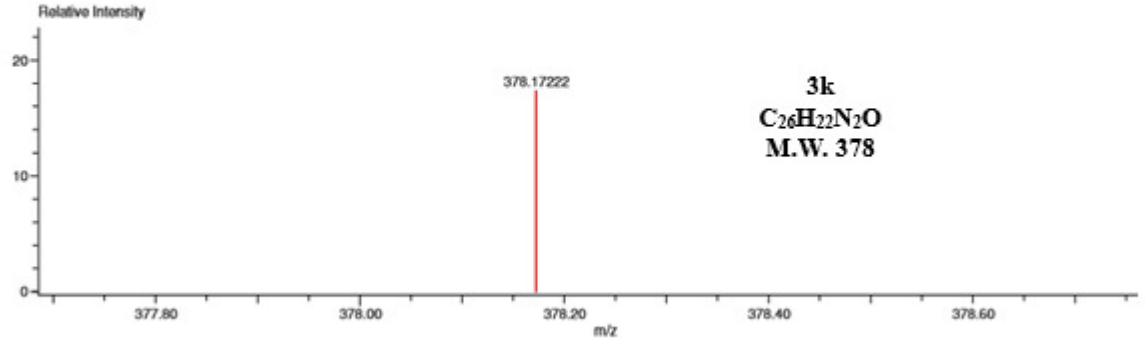
Data:CAT 11
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.8...

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

Tolerance:3.00(mmu)

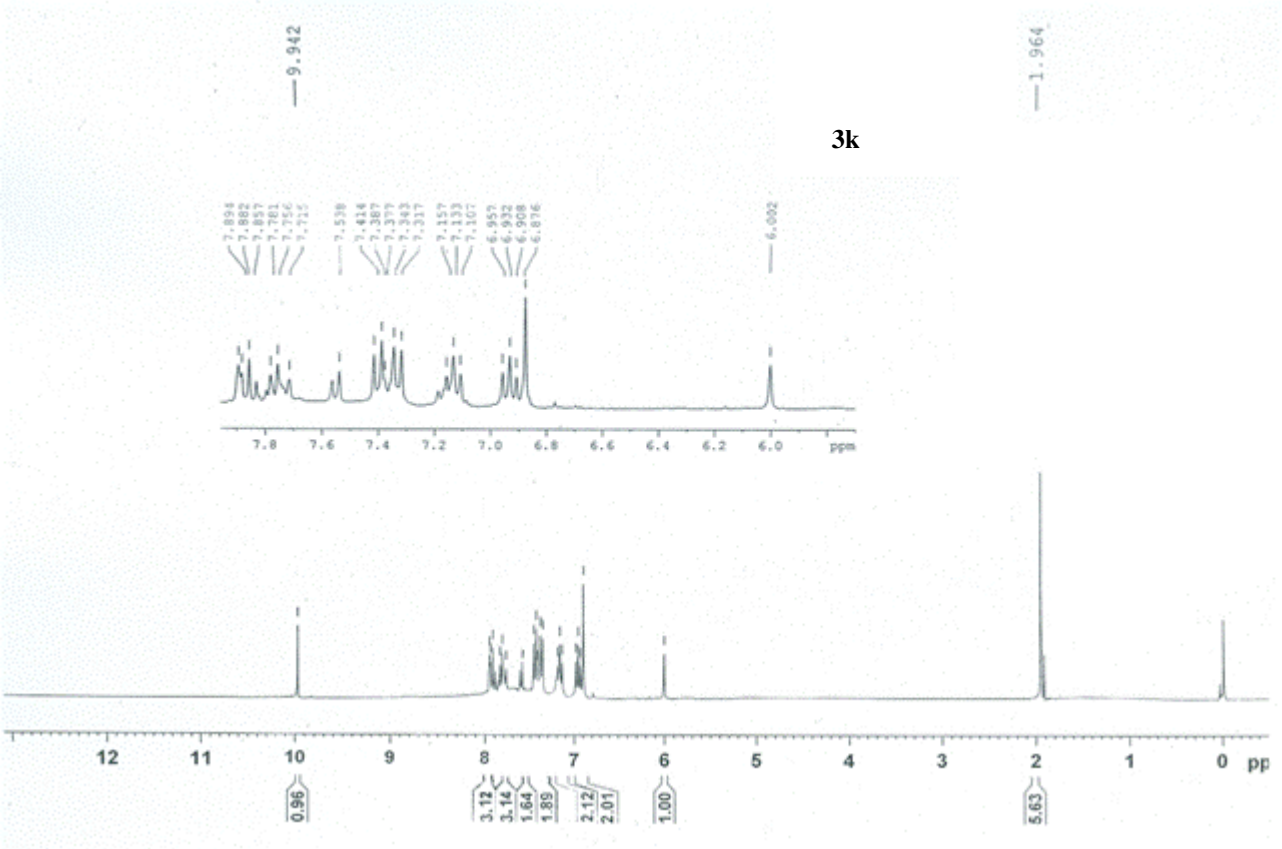
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)

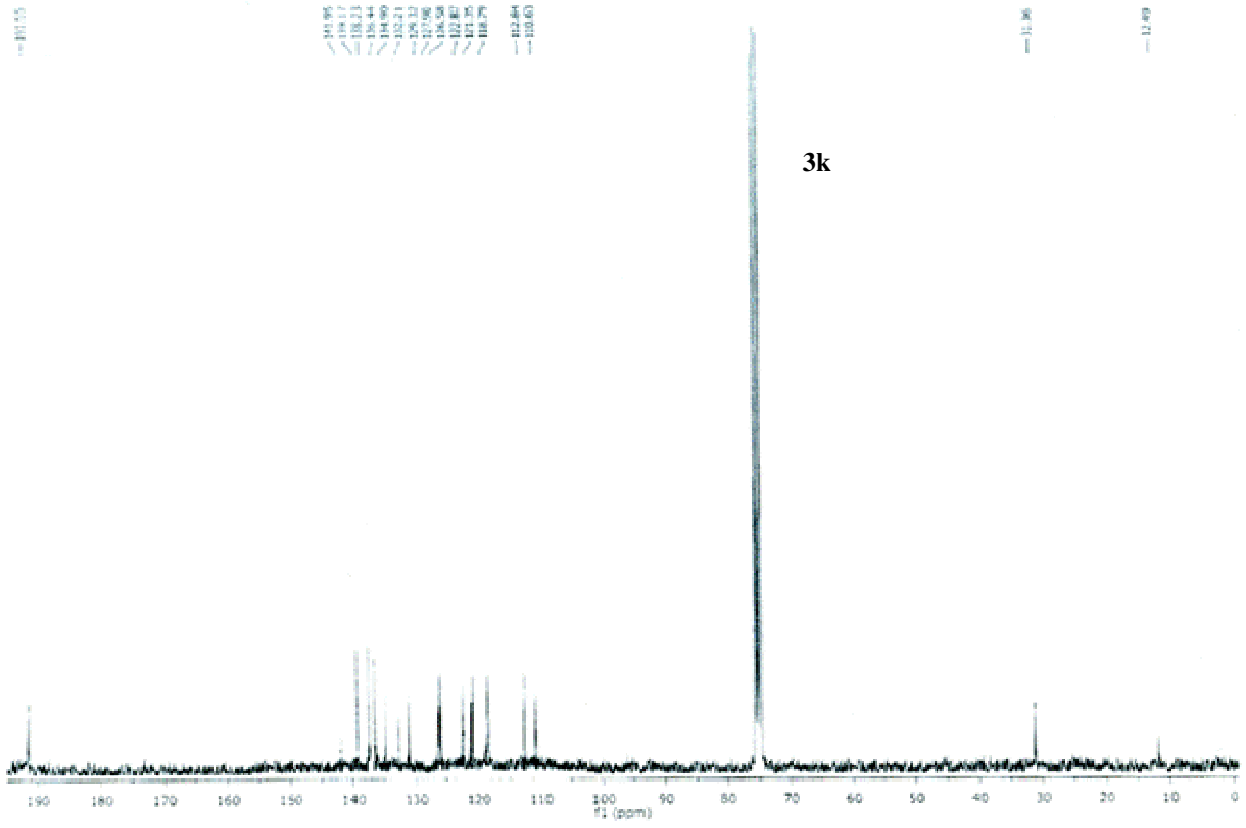


3k
$C_{26}H_{22}N_2O$
M.W. 378

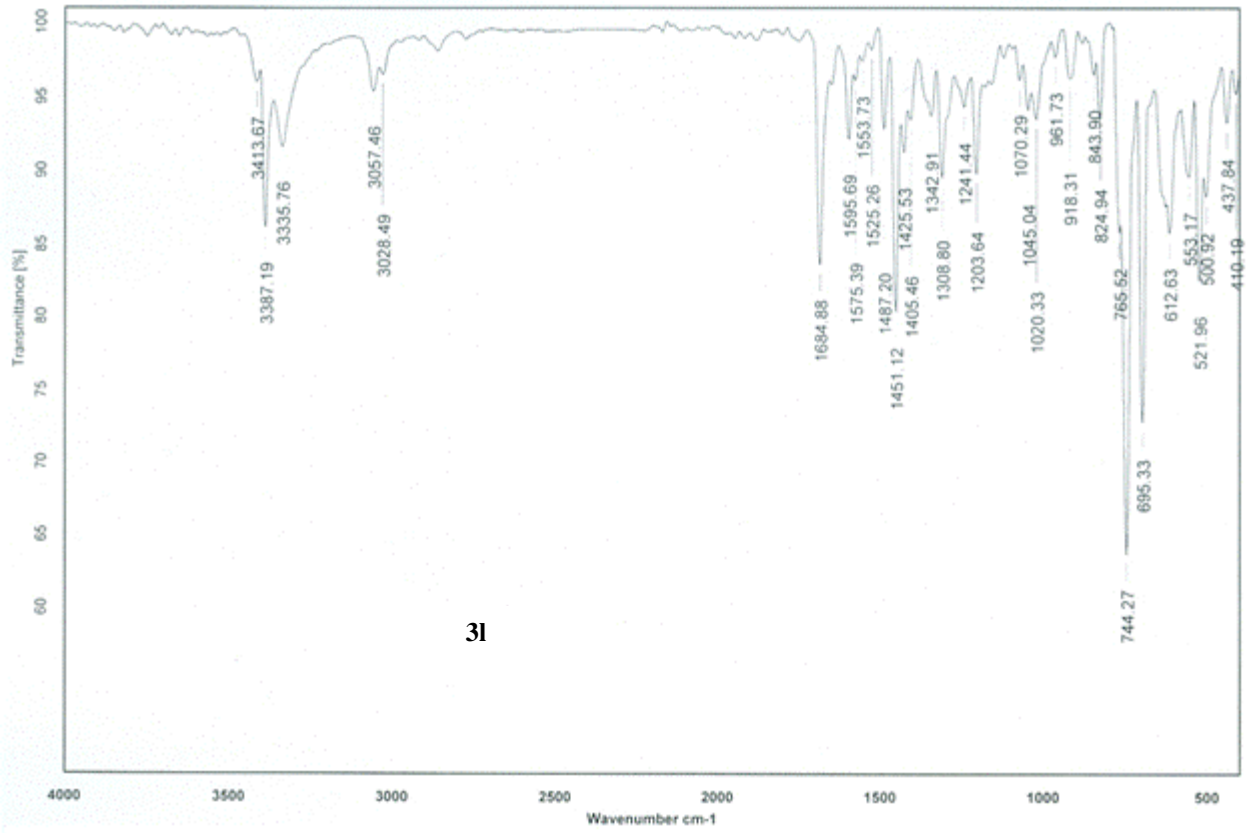
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
378.17222	13695.63	378.17321	-0.99	-2.62	$^{12}C_{26}{}^{1}H_{22}{}^{14}N_2{}^{16}O_1$	17.0

3k

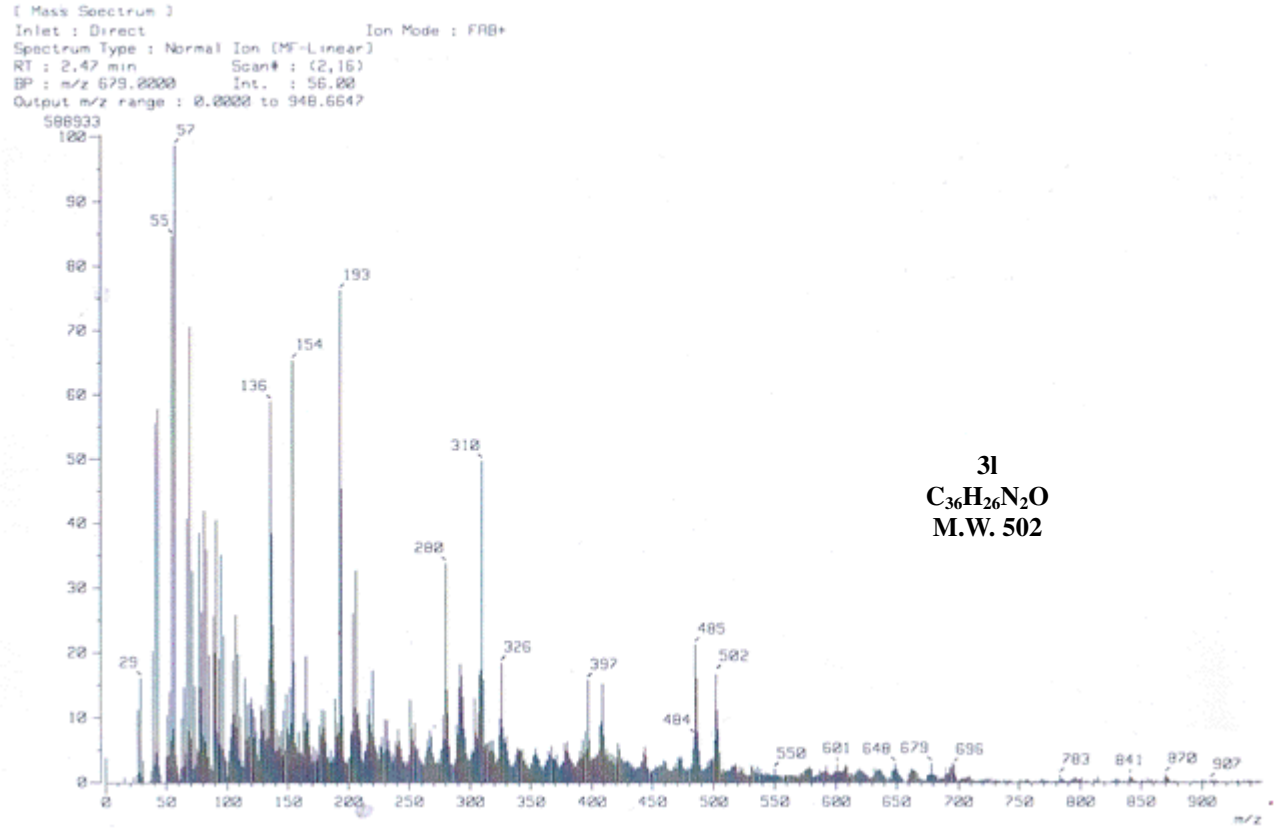




3k



3l



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

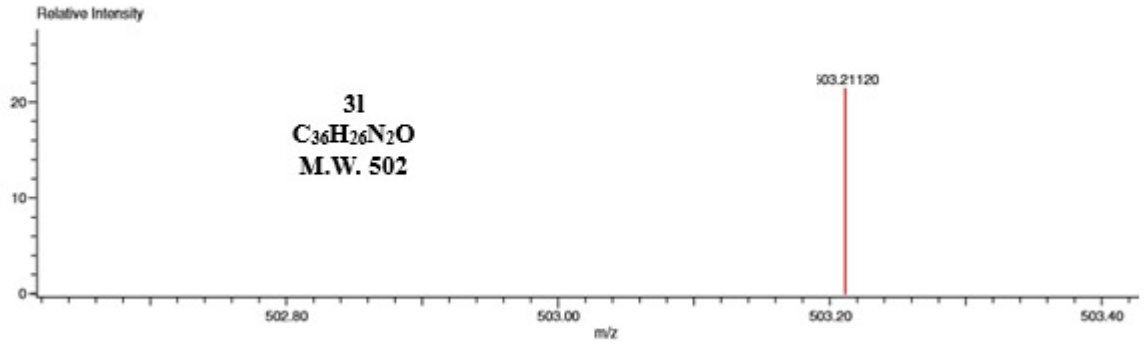
Data:CAT 12
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.7...

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

Tolerance:3.00(mmu)

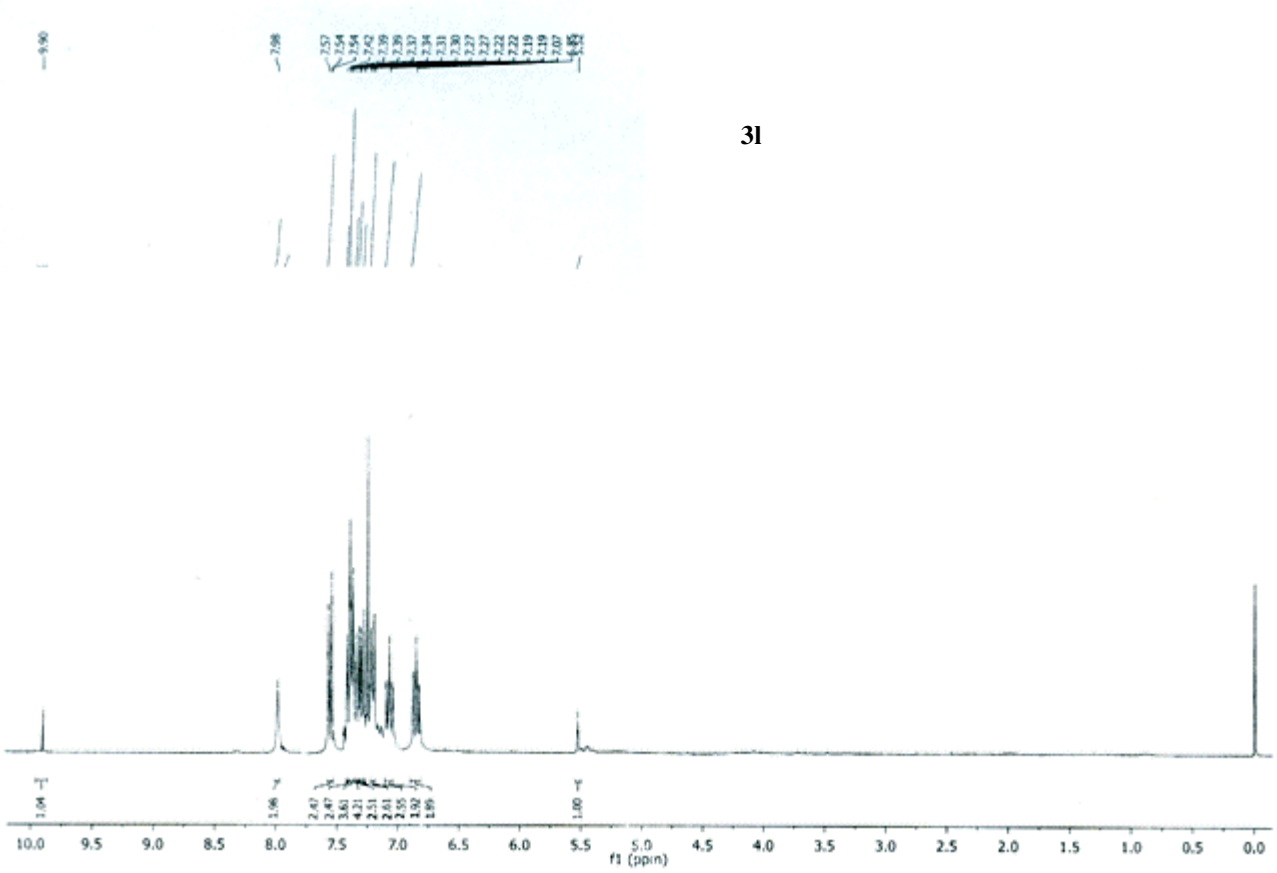
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



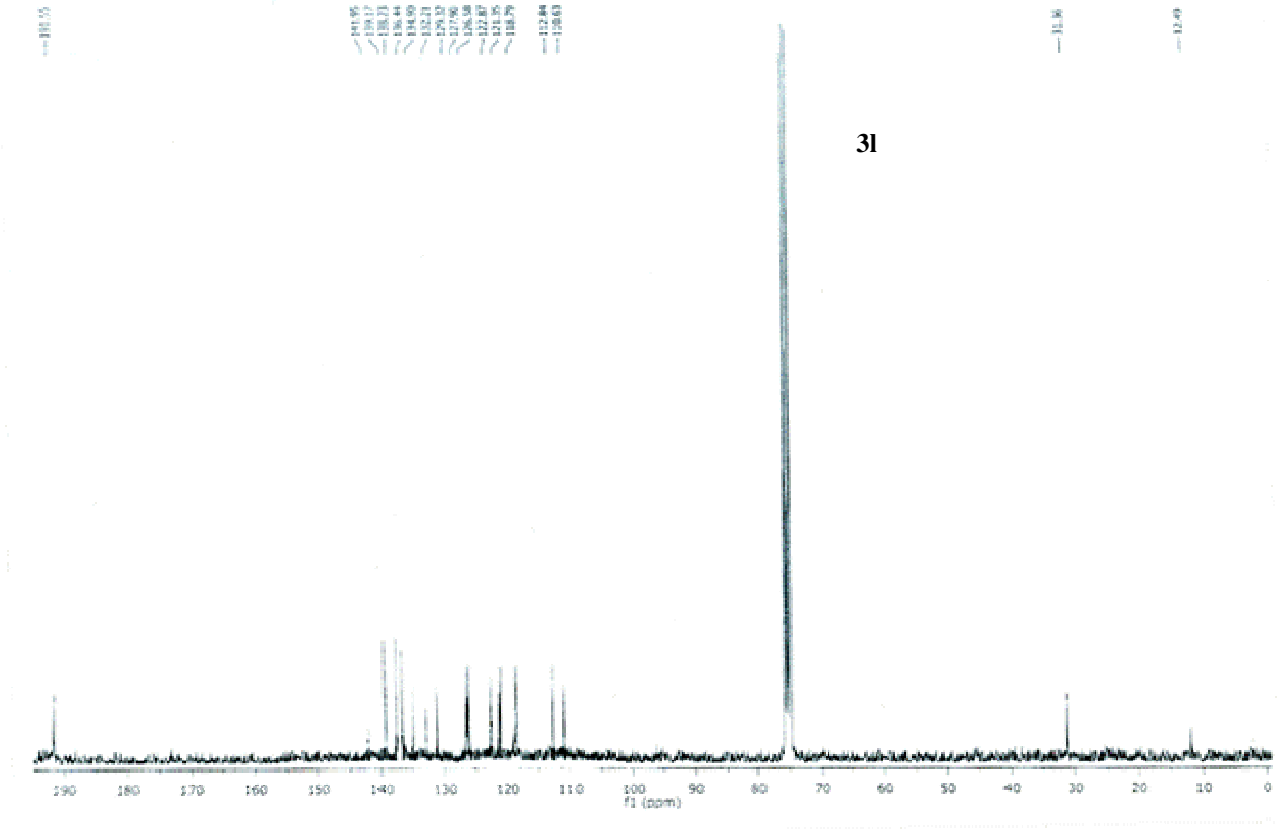
3l
$C_{36}H_{26}N_2O$
M.W. 502

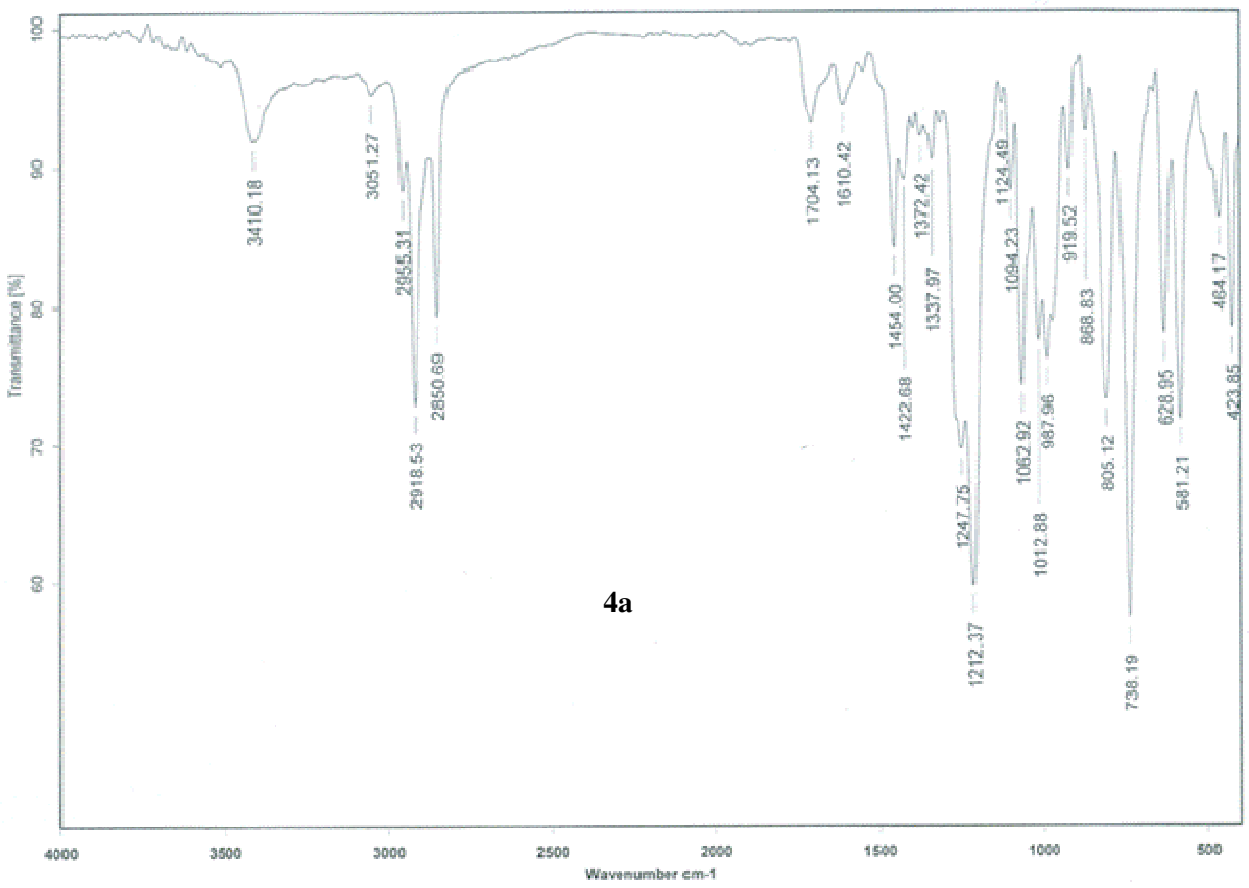
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
503.21120	6693.89	503.21234	-1.13	-2.25	$^{12}C_{36}{}^{1}H_{27}{}^{14}N_2{}^{16}O_1$	24.5

3l

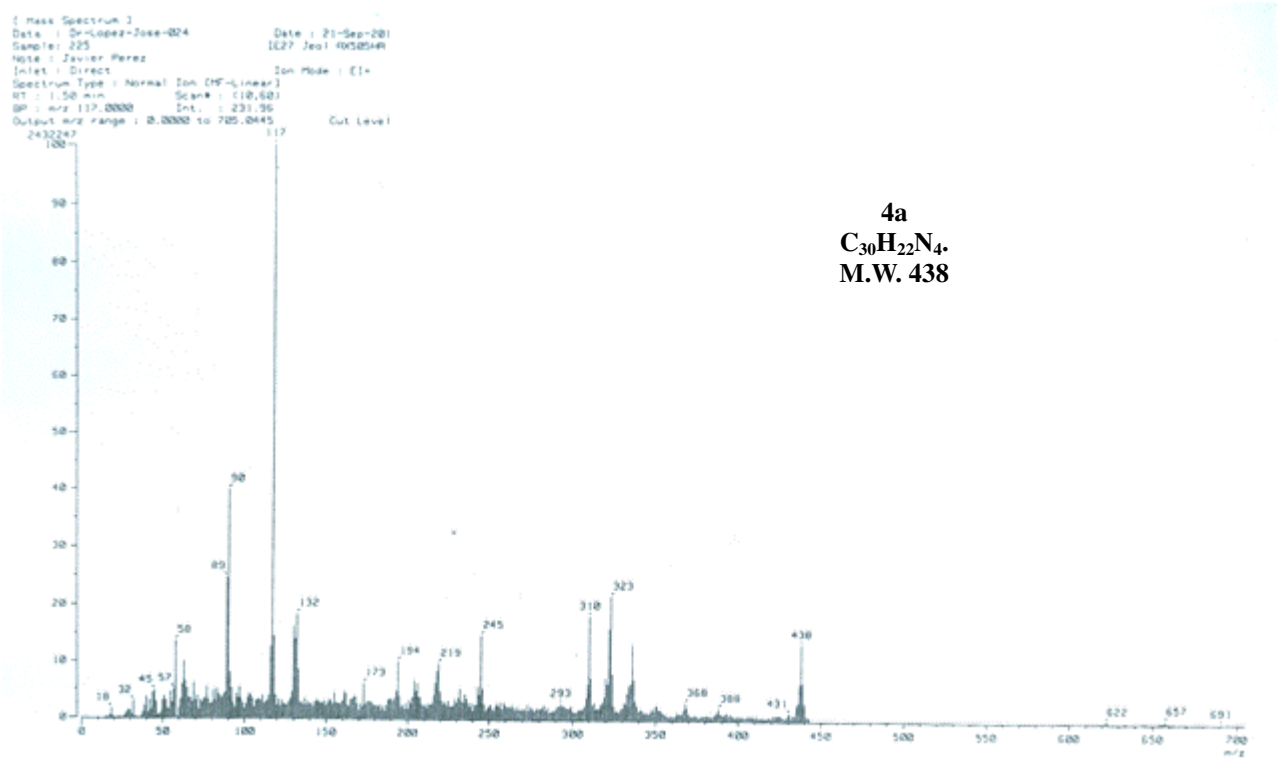


3l





4a



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

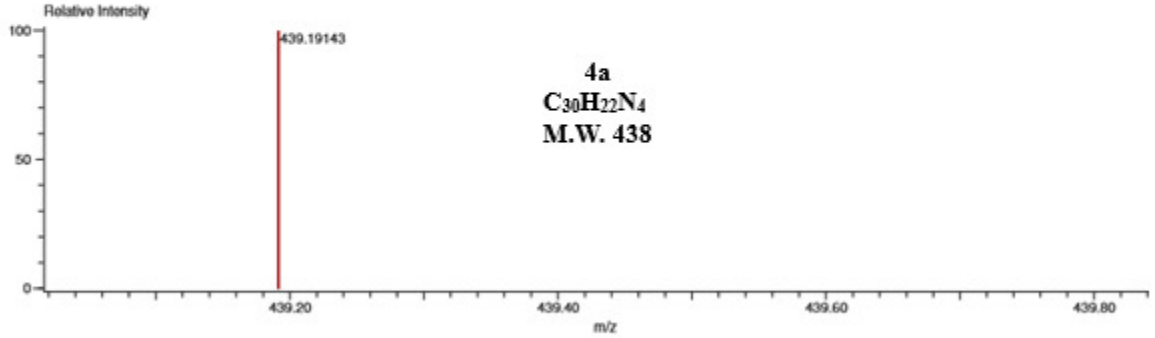
Data:CAT 14
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 2.6...

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:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

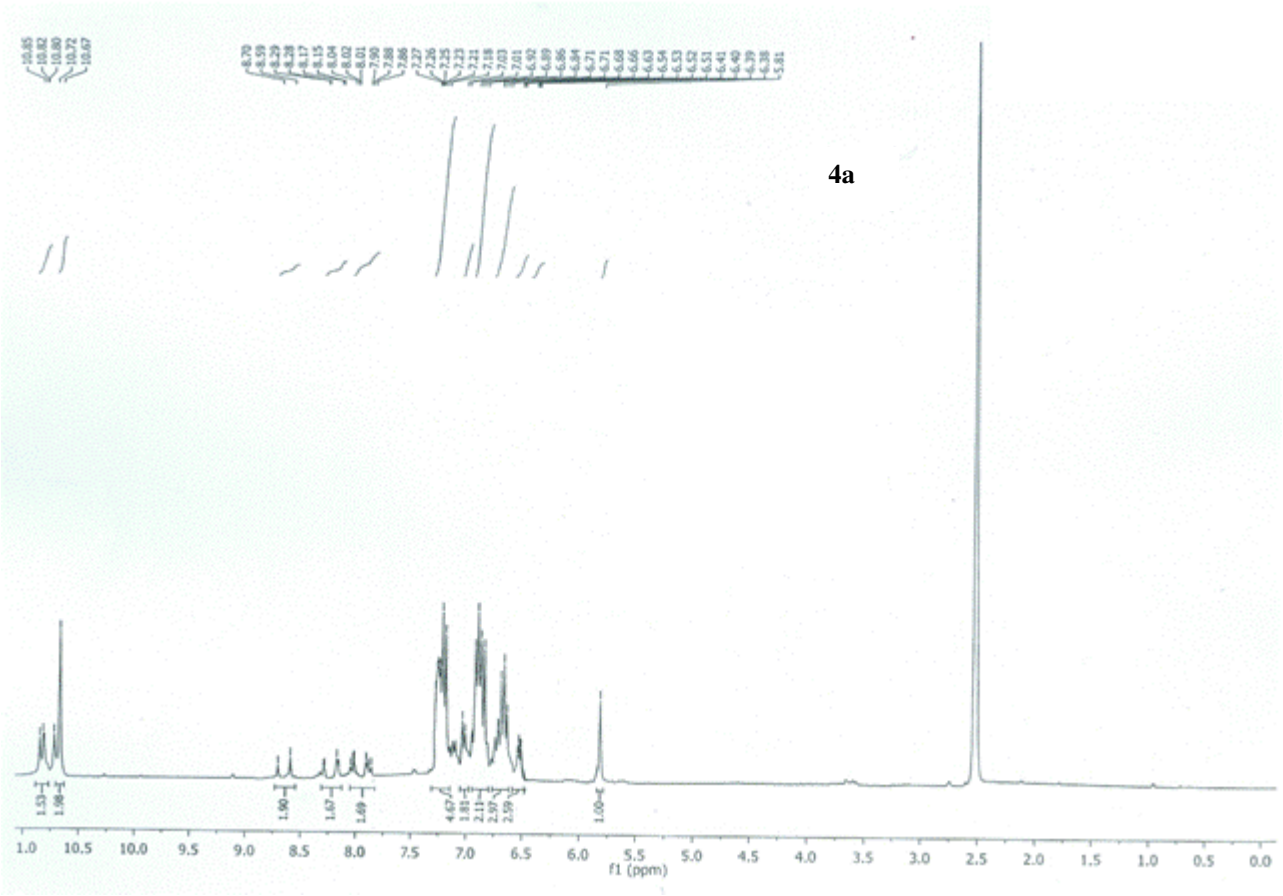
Tolerance:3.00(mmu)

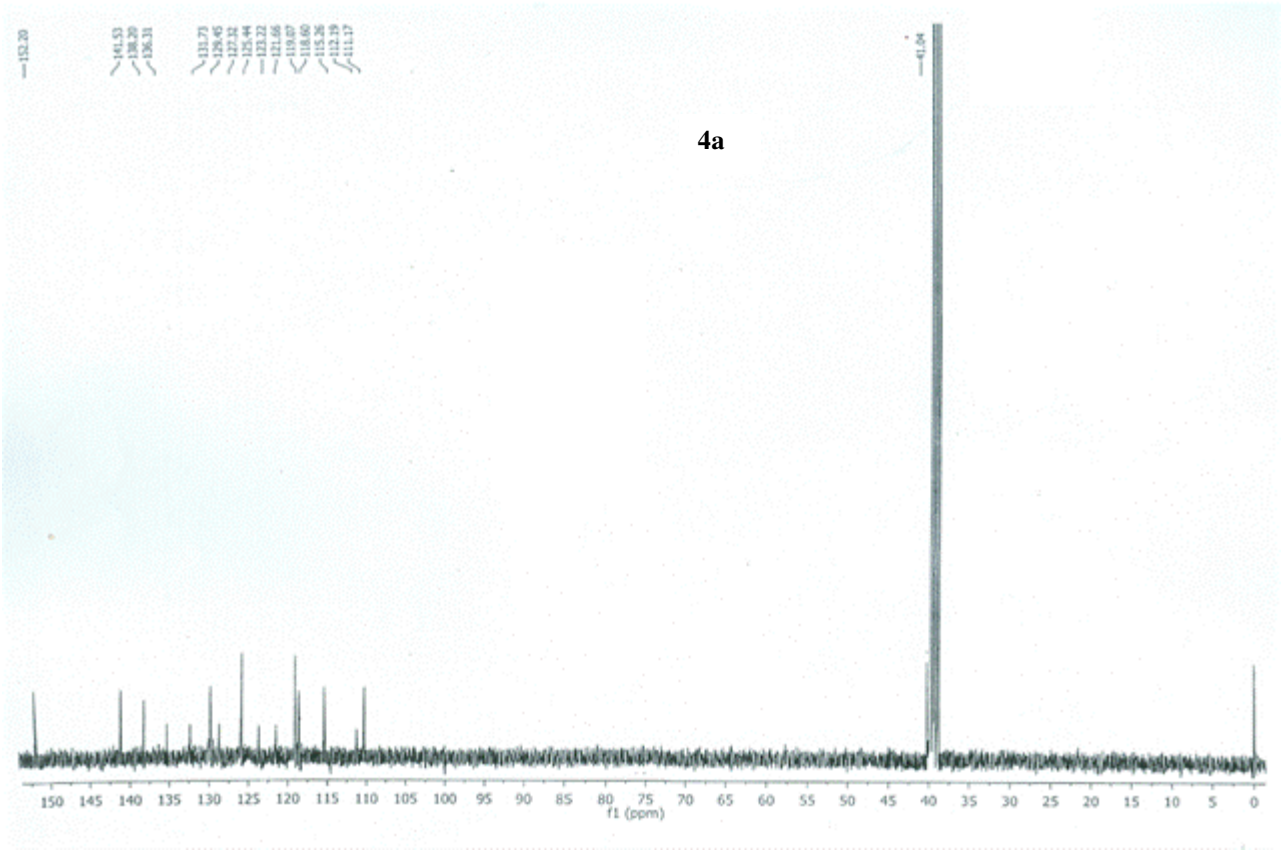
saturation Number:0.0 .. 32.0 (Fraction:Both)



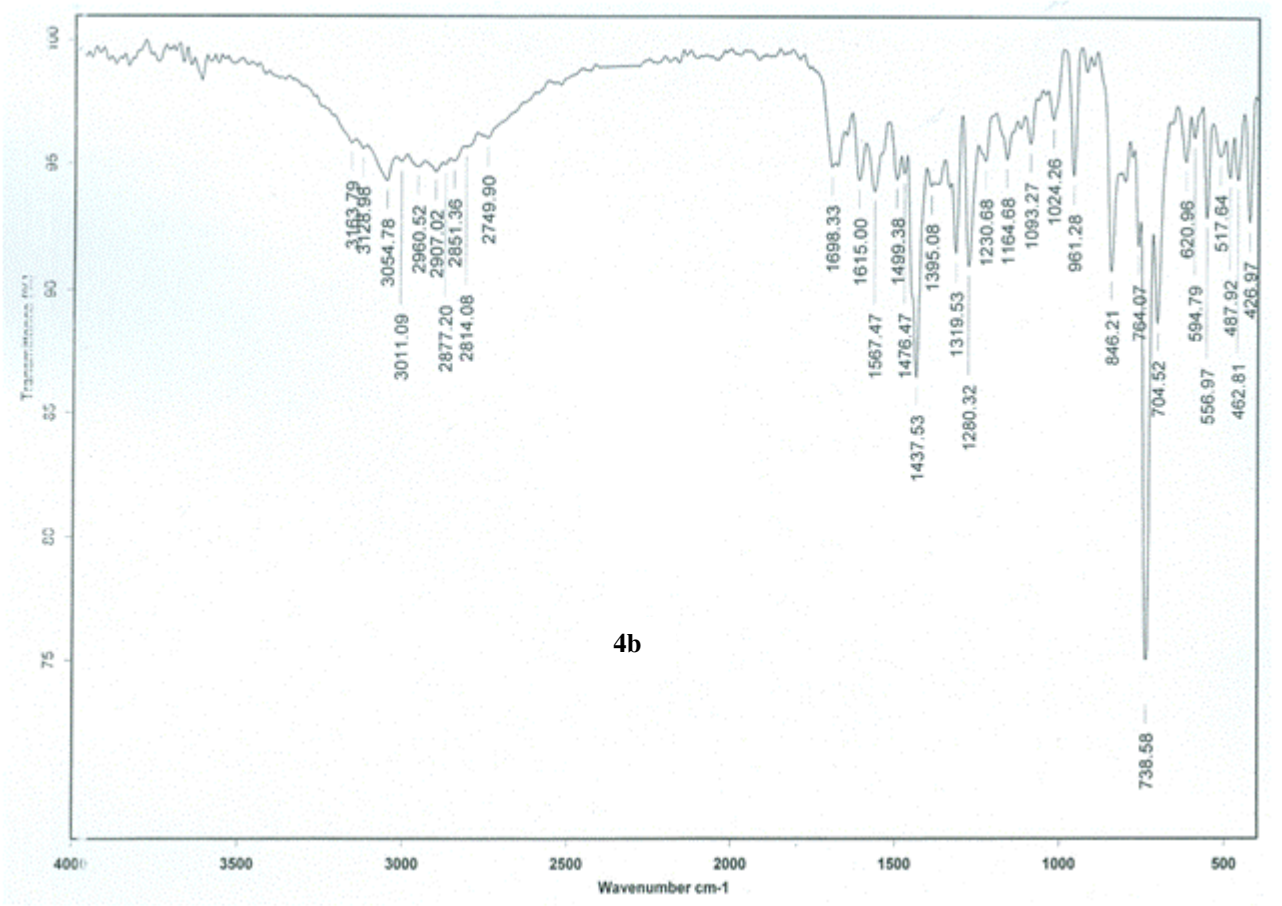
4a
$C_{30}H_{22}N_4$
M.W. 438

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	$^{12}C_{30}{}^{1}H_{23}{}^{14}N_4$	21.5

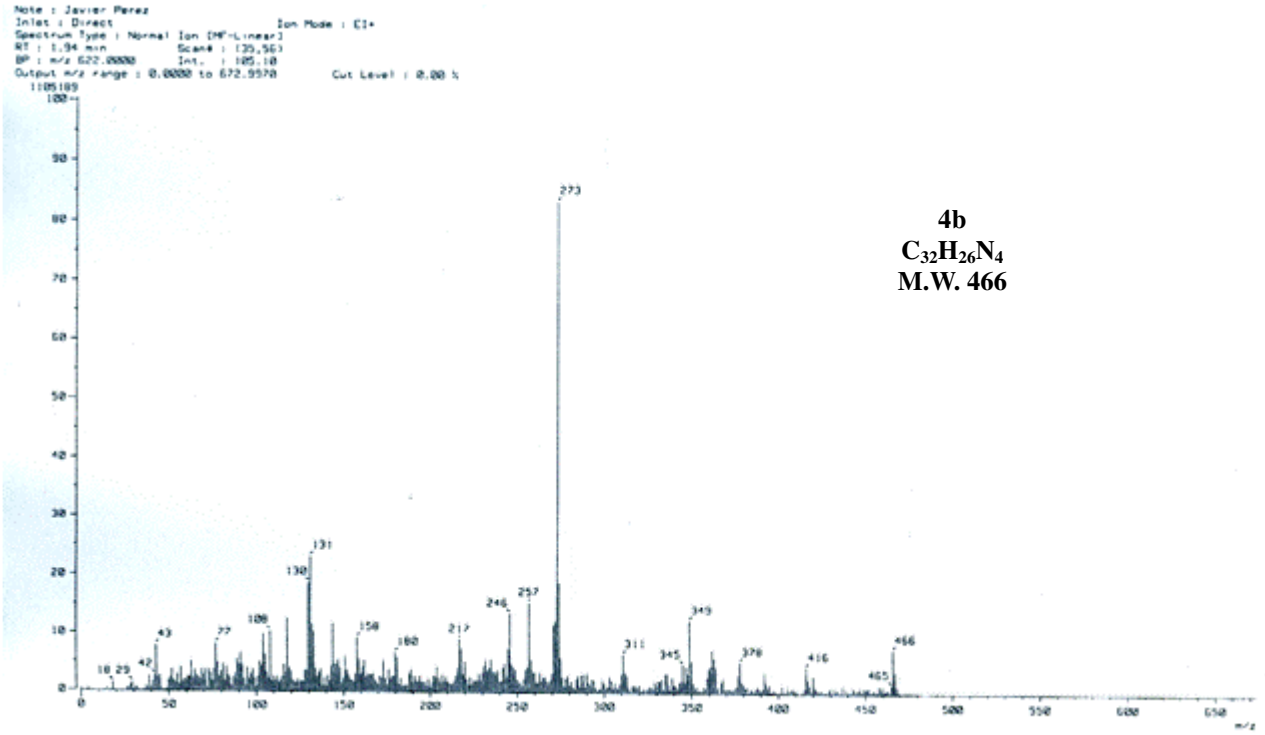




4a



4b

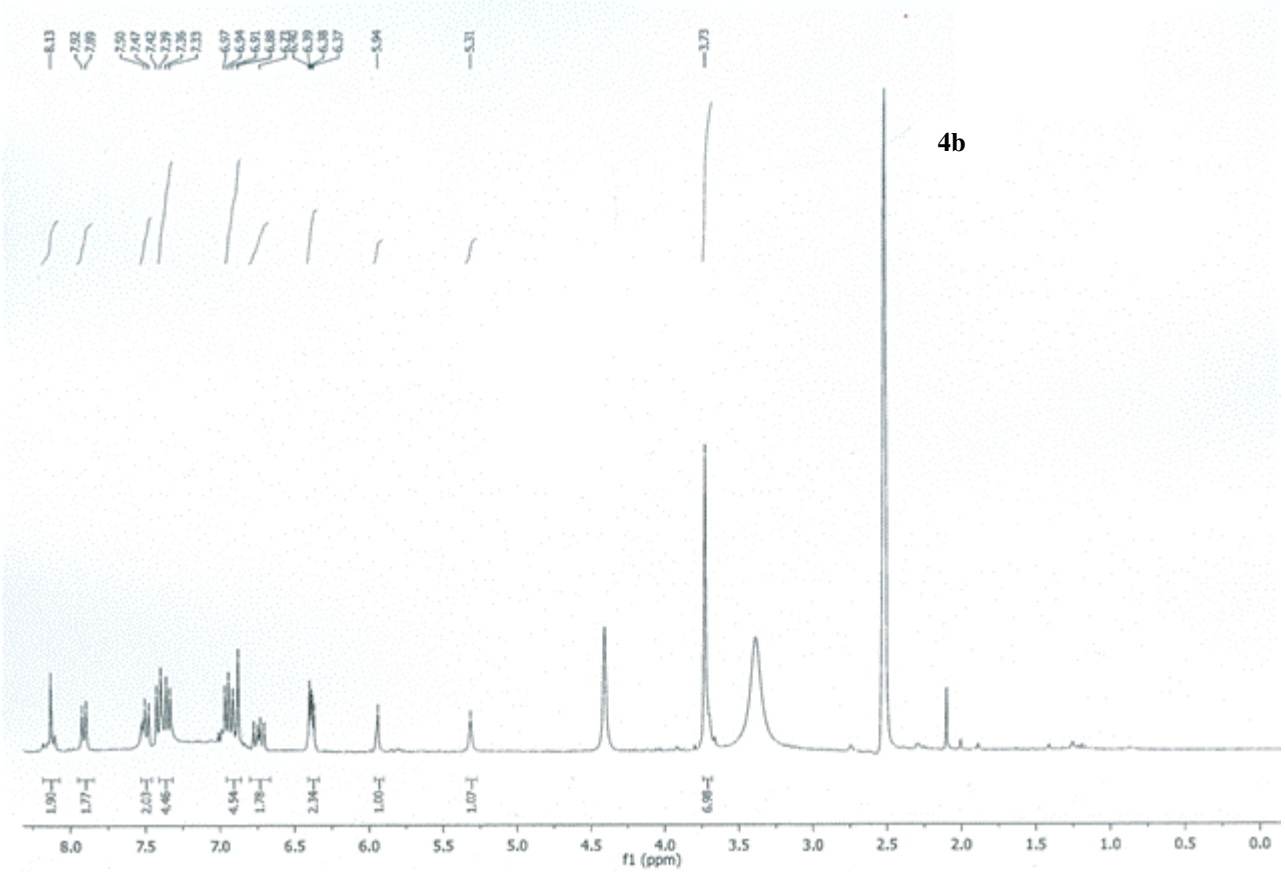


4b
$C_{32}H_{26}N_4$
M.W. 466

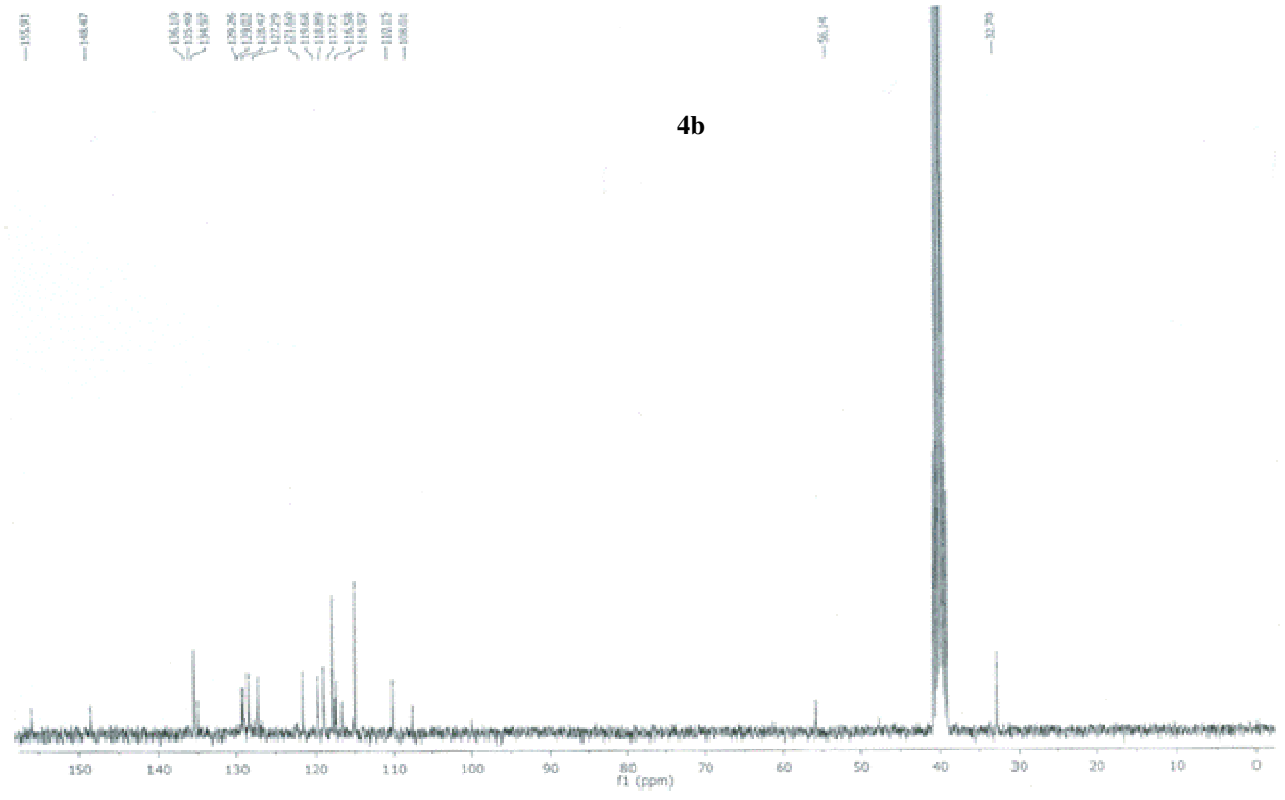
Data : Dr Cecilio Alvarez029 Date : 29-Oct-2015 17:00
Instrument : MStation
Sample : 3275 1-Me-bz-p
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 3.59 min Scan# : (26,48)
Elements : C 34/0, H 49/0, N 5/0
Mass Tolerance : 1000ppm, 1mmu if m/z > 1
Unsaturation (U.S.) : -0.5 - 34.0

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

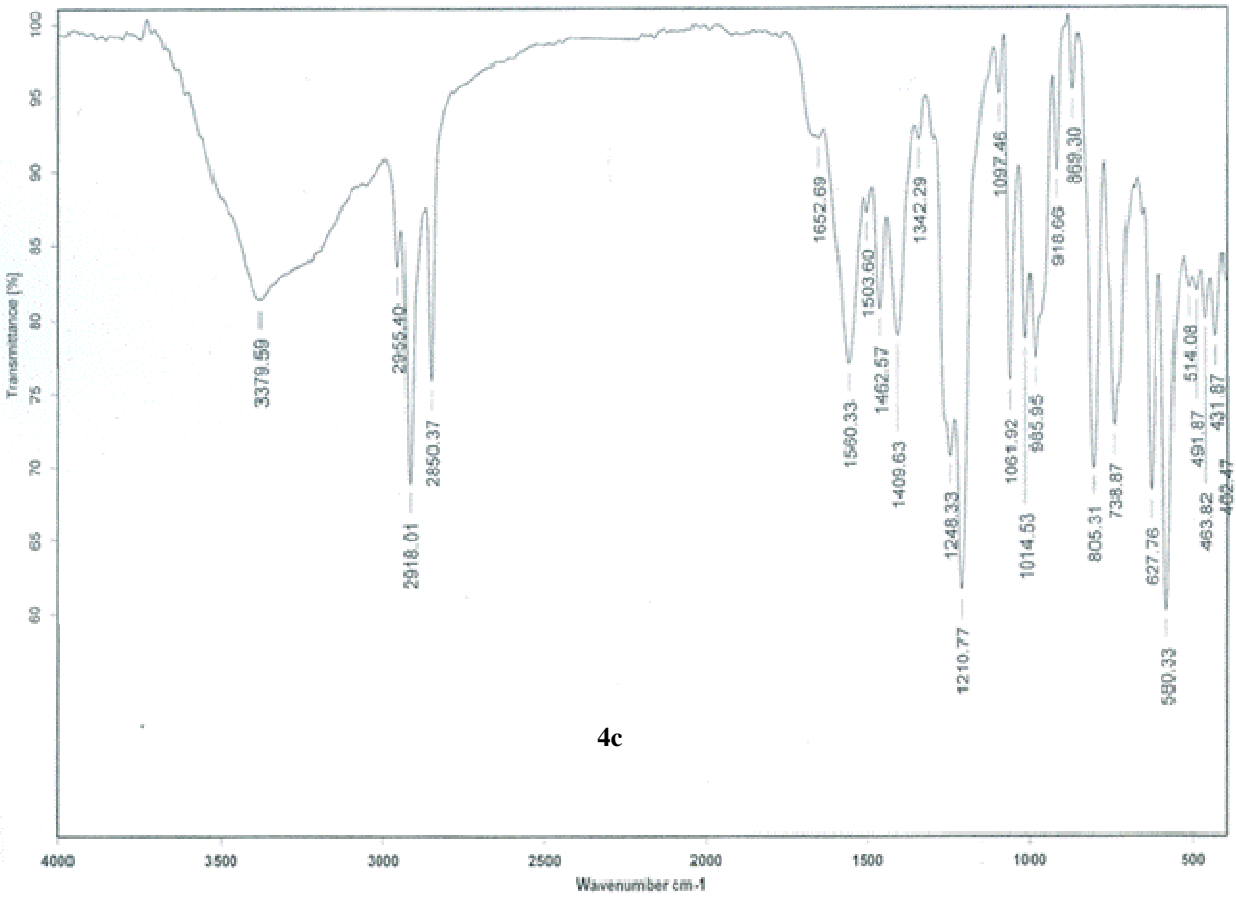
	Observed m/z	Int%				
	467.2228	68.99				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N
1	467.2236	-1.7 / -0.8	21.5	32	27	4



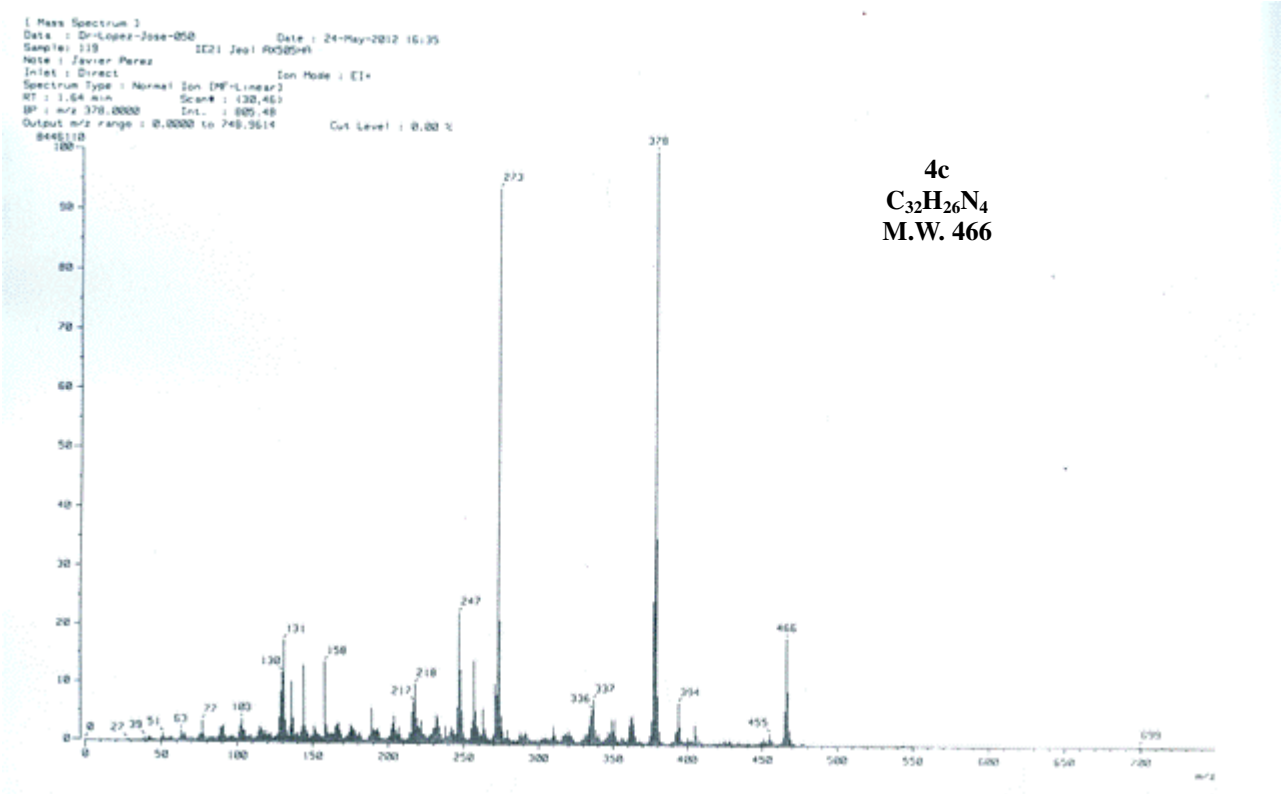
4b



4b



4c



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

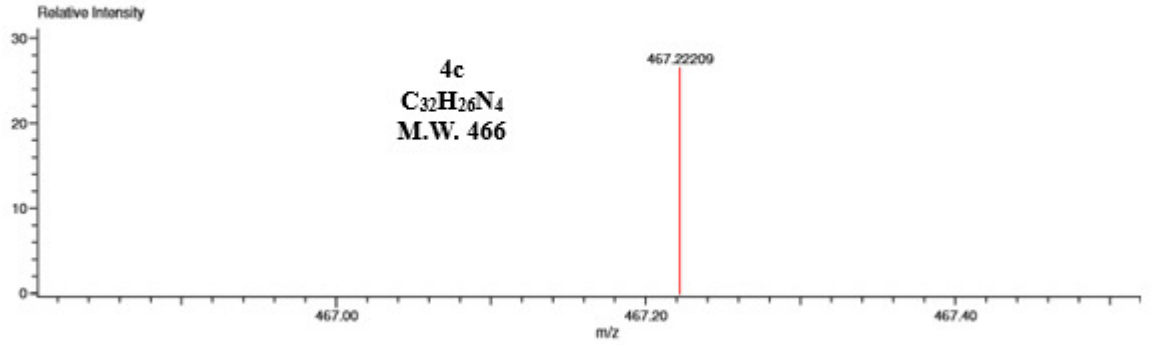
Data:CAT 15
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 2.0...

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

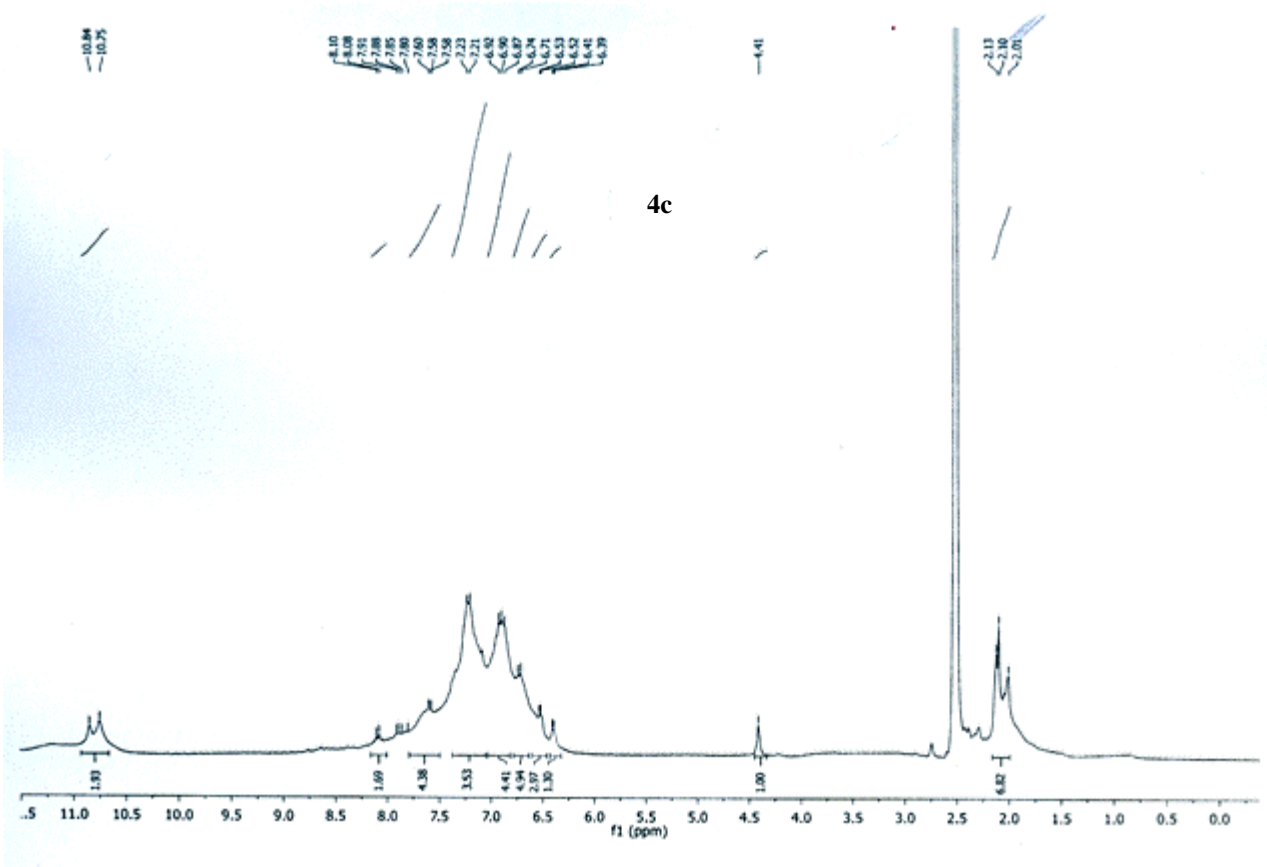
Charge number:1
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

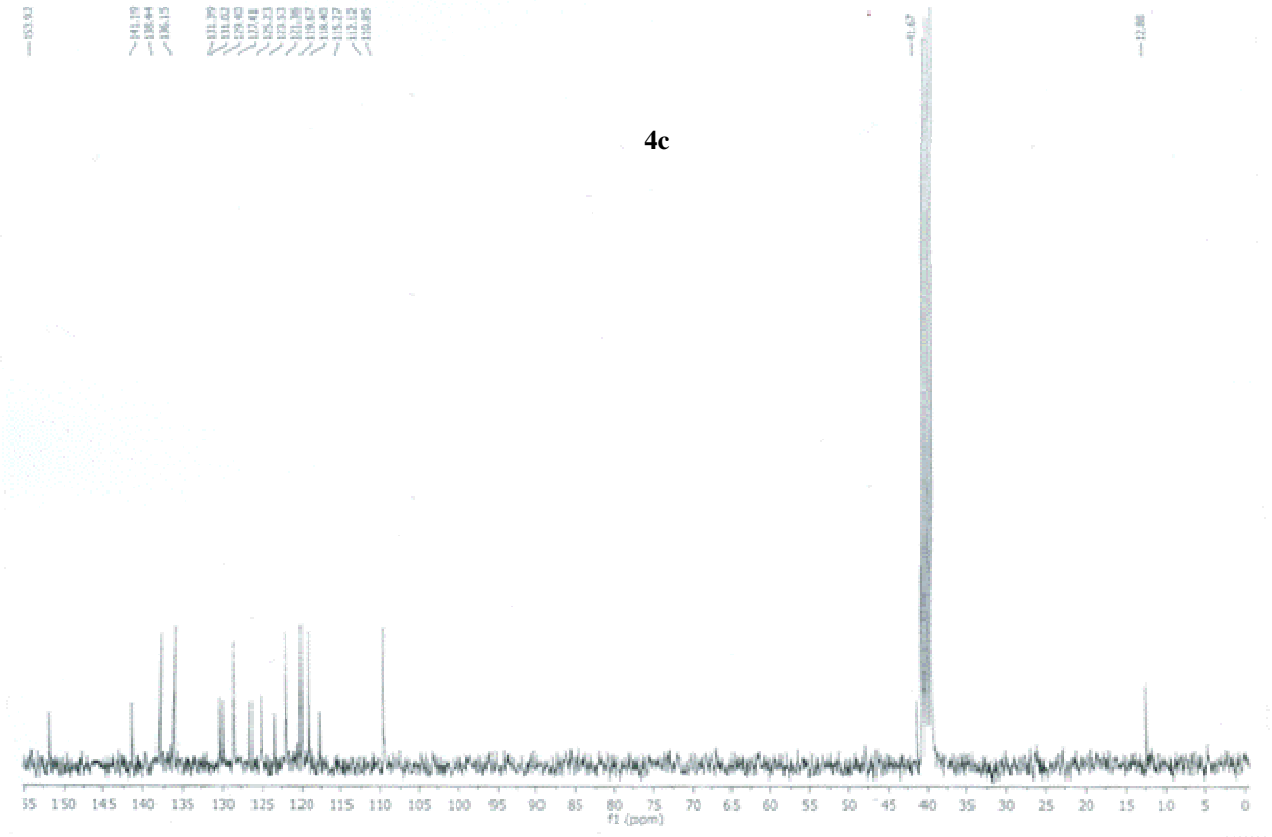
Tolerance:3.00(mmu)

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

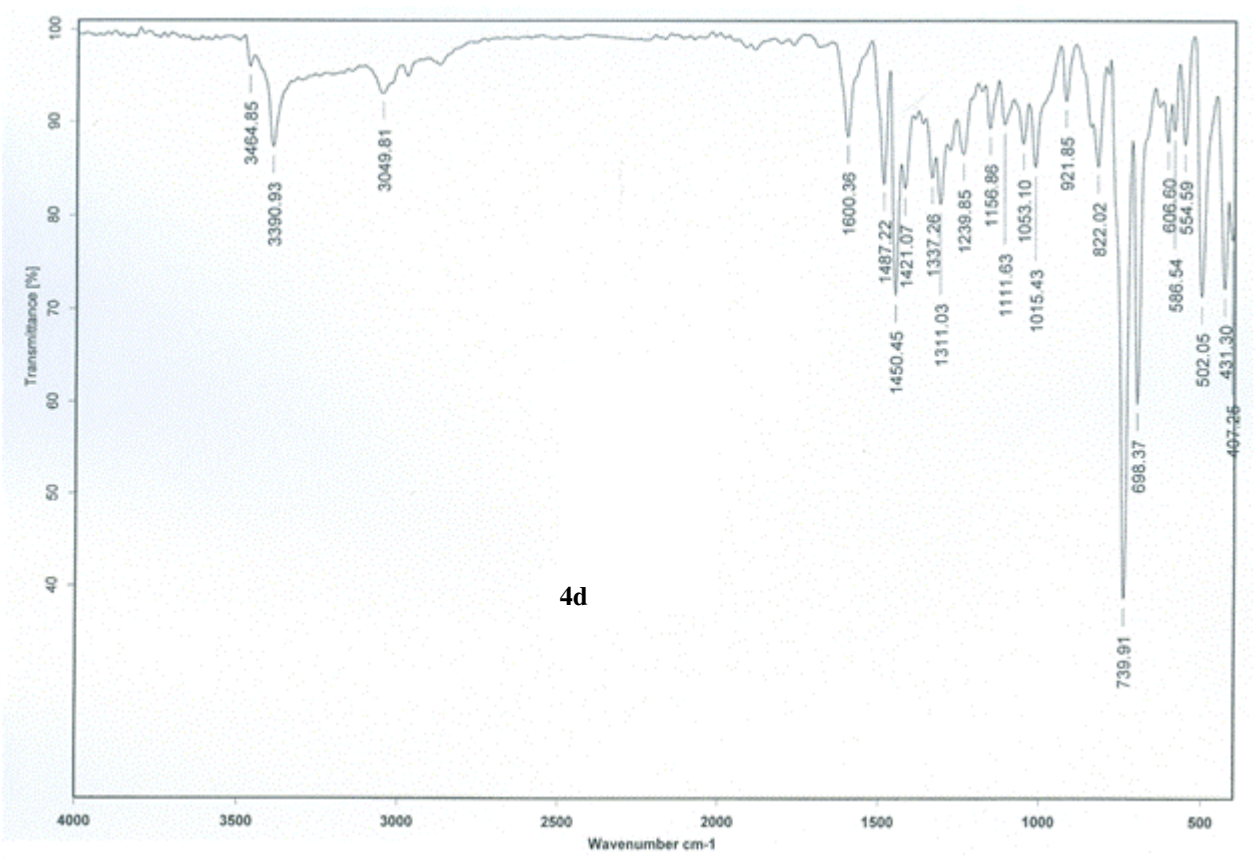


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22209	60294.95	467.22357	-1.48	-3.16	$^{12}C_{32}{}^{1}H_{27}{}^{14}N_4$	21.5

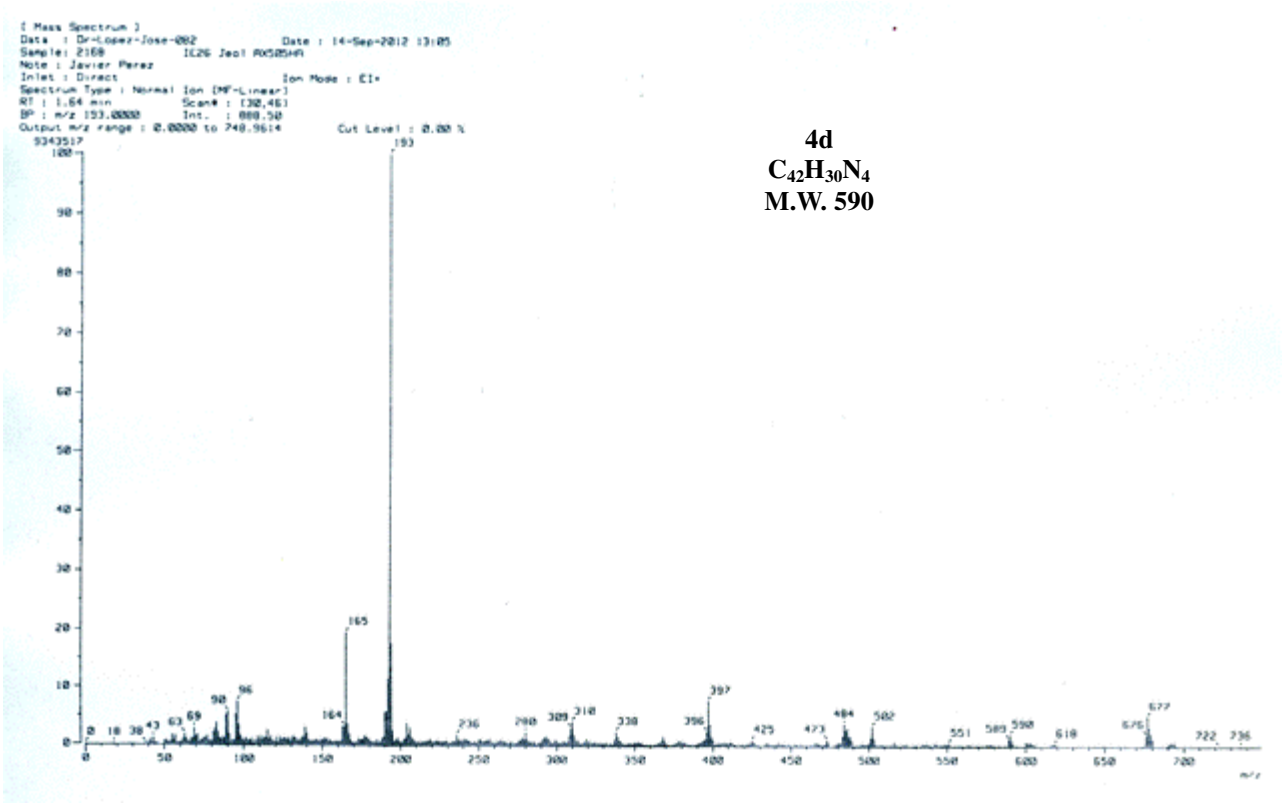




4c



4d



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

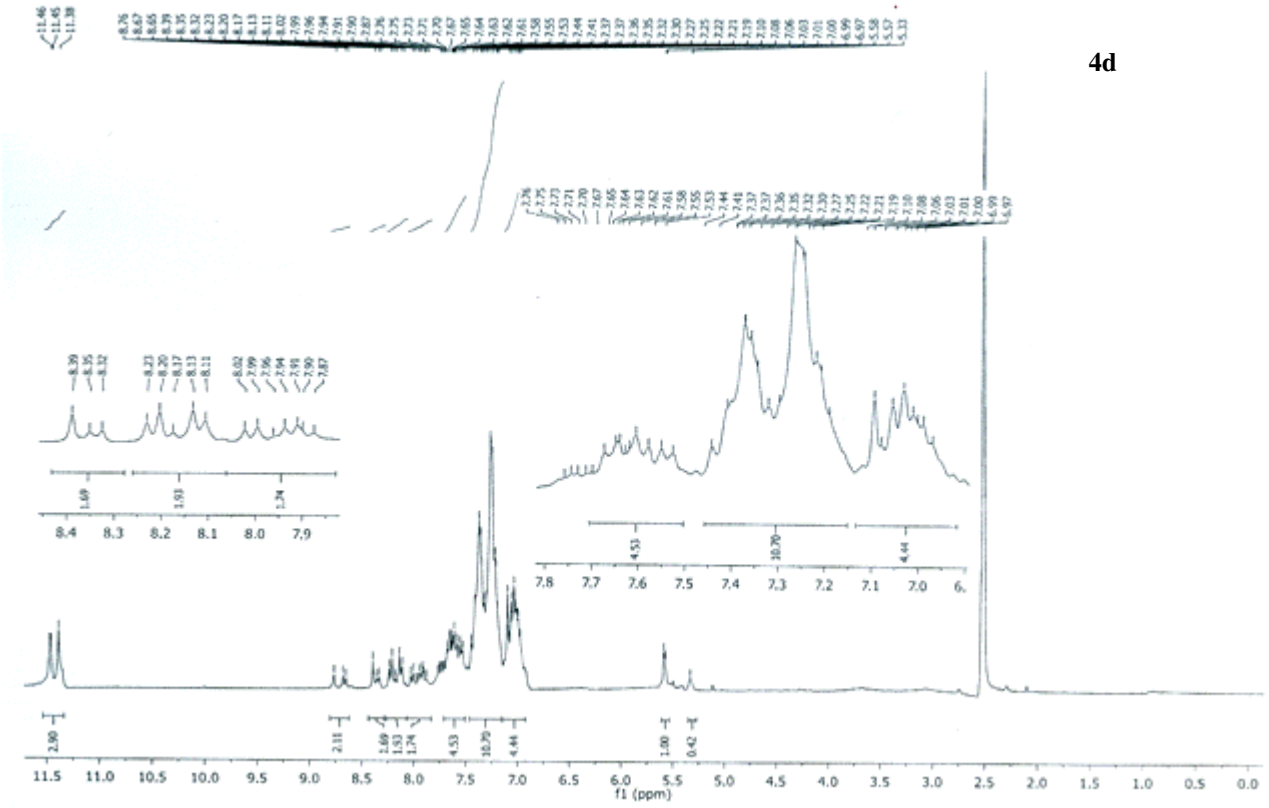
Anal calcd. C 85.40 H 5.12 N 9.48

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

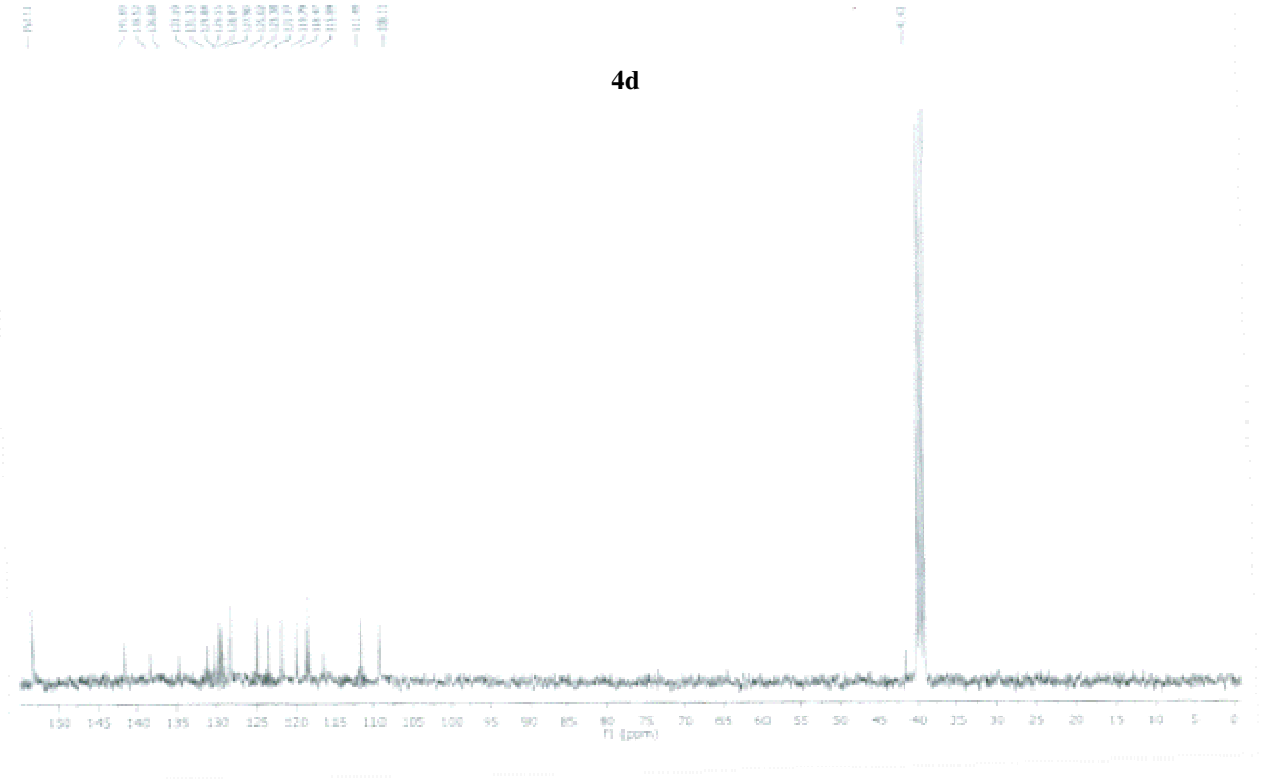
Found

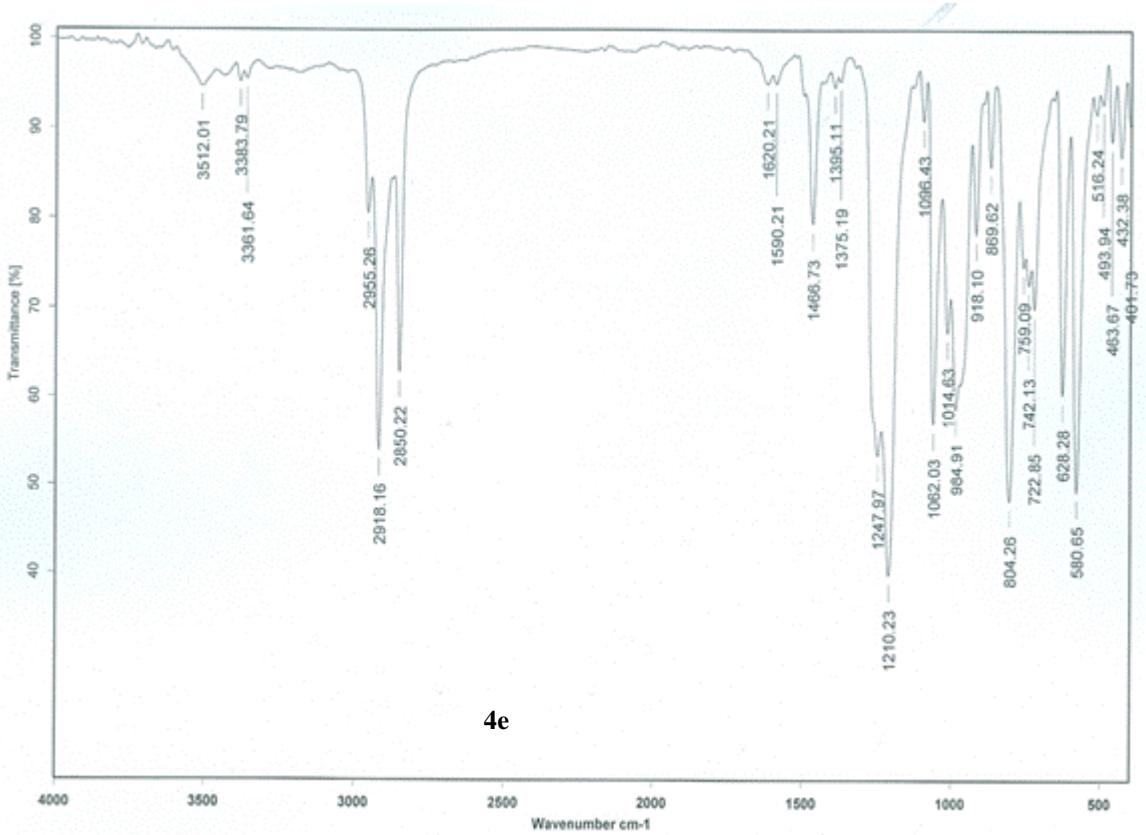
4d
$C_{42}H_{30}N_4$
M.W. 590

4d

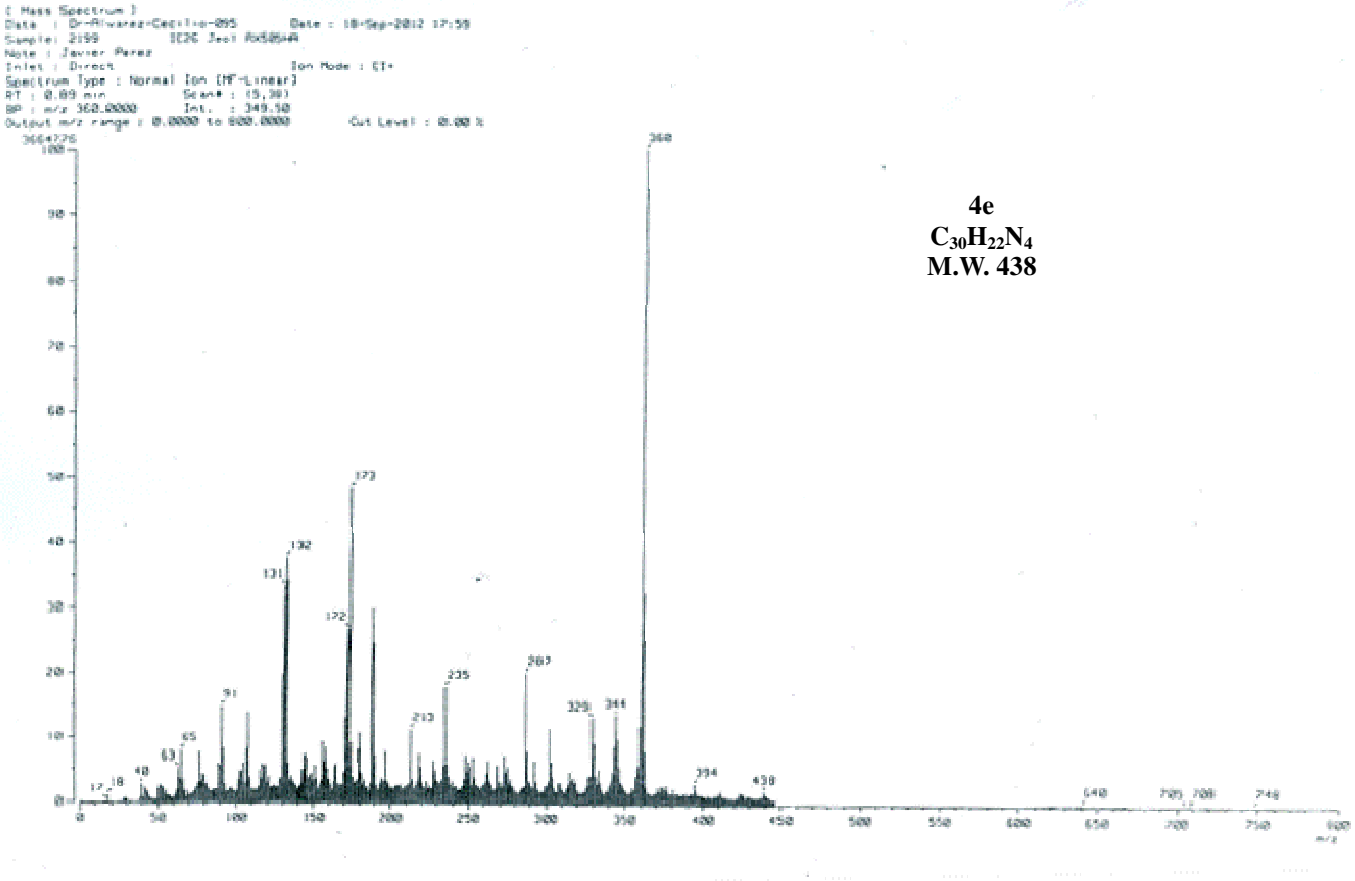


4d





4e

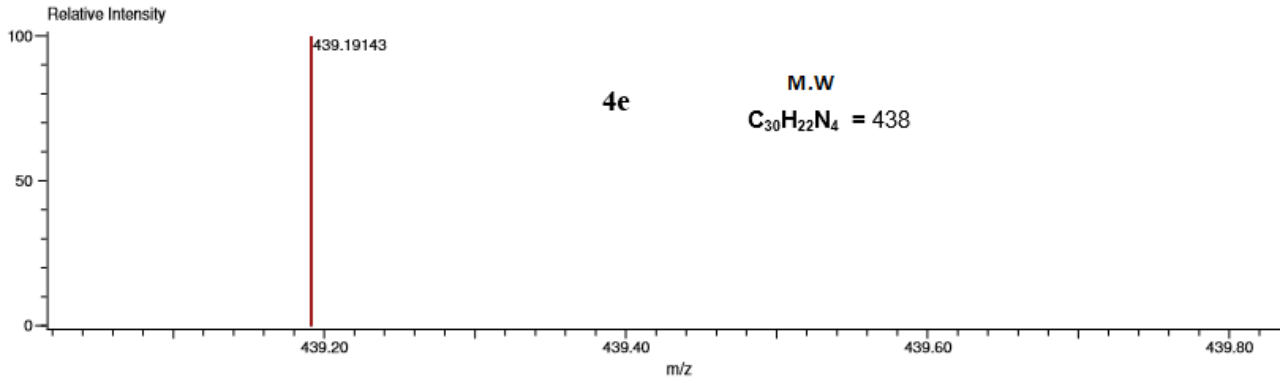


4e
$C_{30}H_{22}N_4$
M.W. 438

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)
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

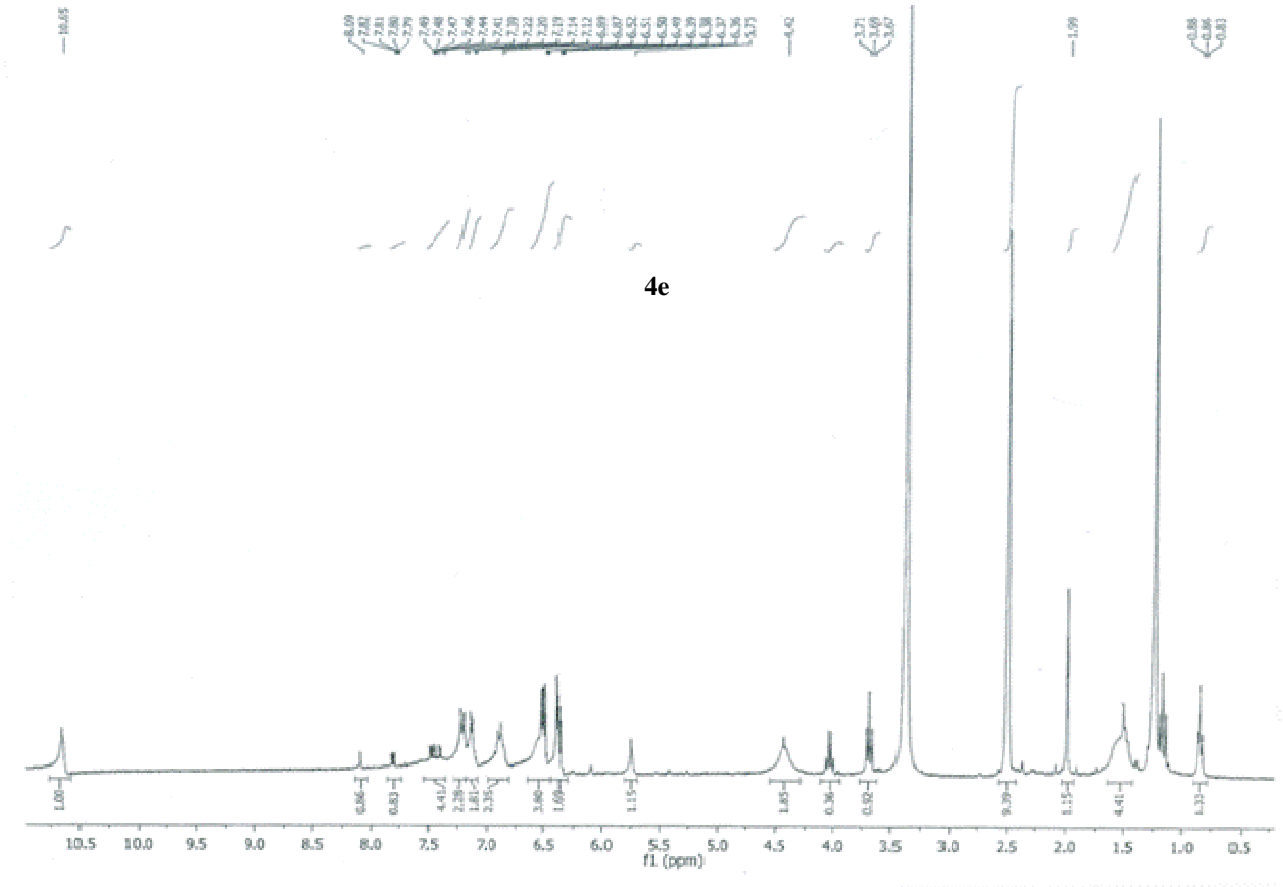


4e

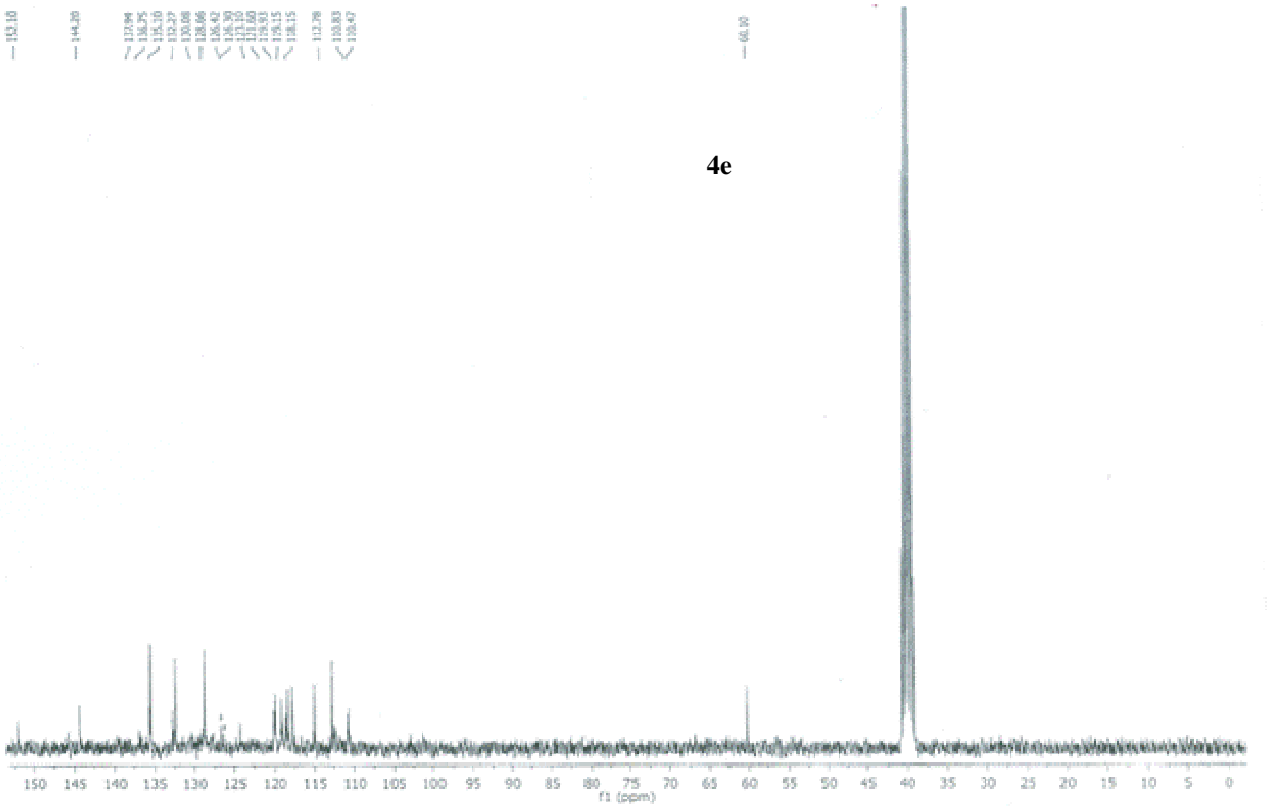
M.W

$C_{30}H_{22}N_4$ = 438

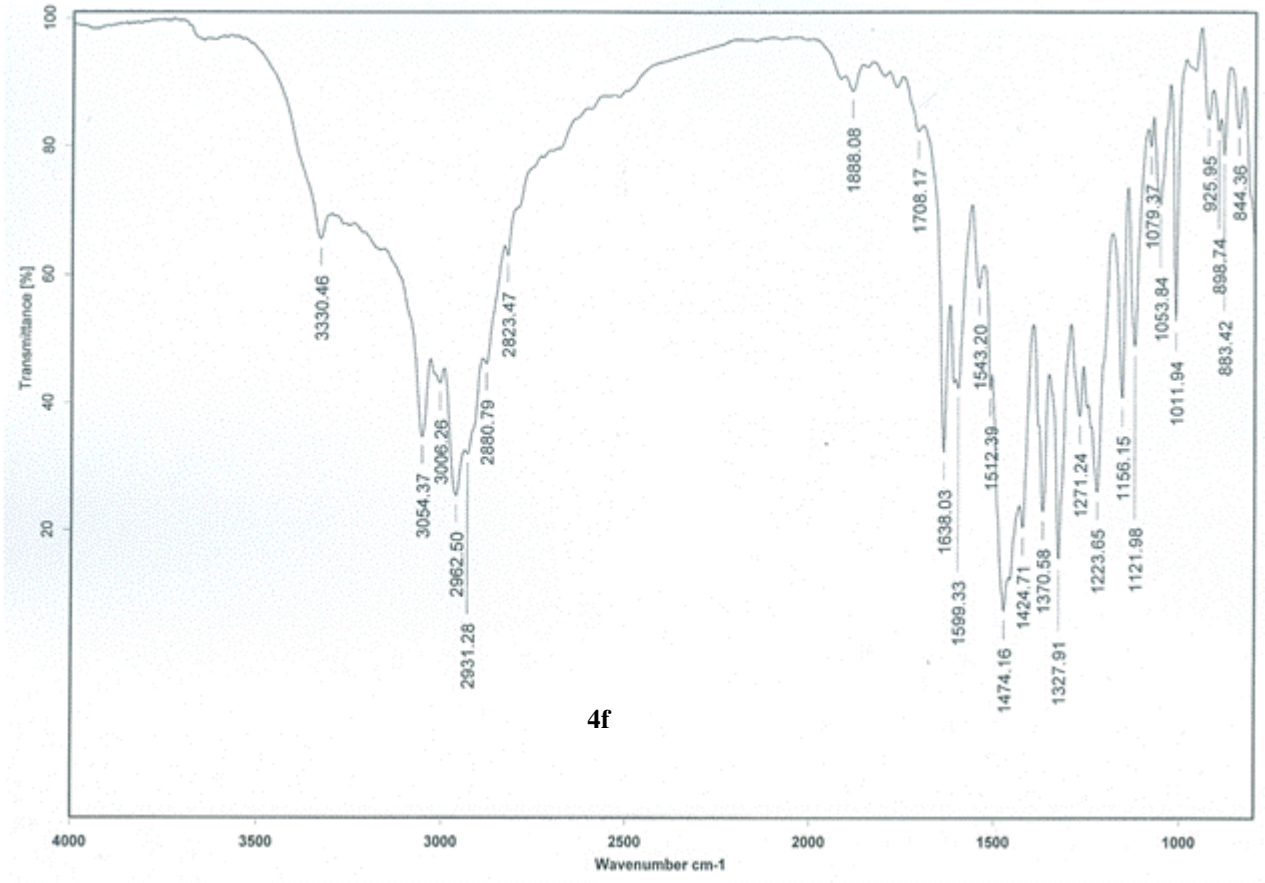
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
439.19143	4035.63	439.19227	-0.84	-1.91	$^{12}C_{30}{}^{1}H_{23}{}^{14}N_4$	21.5



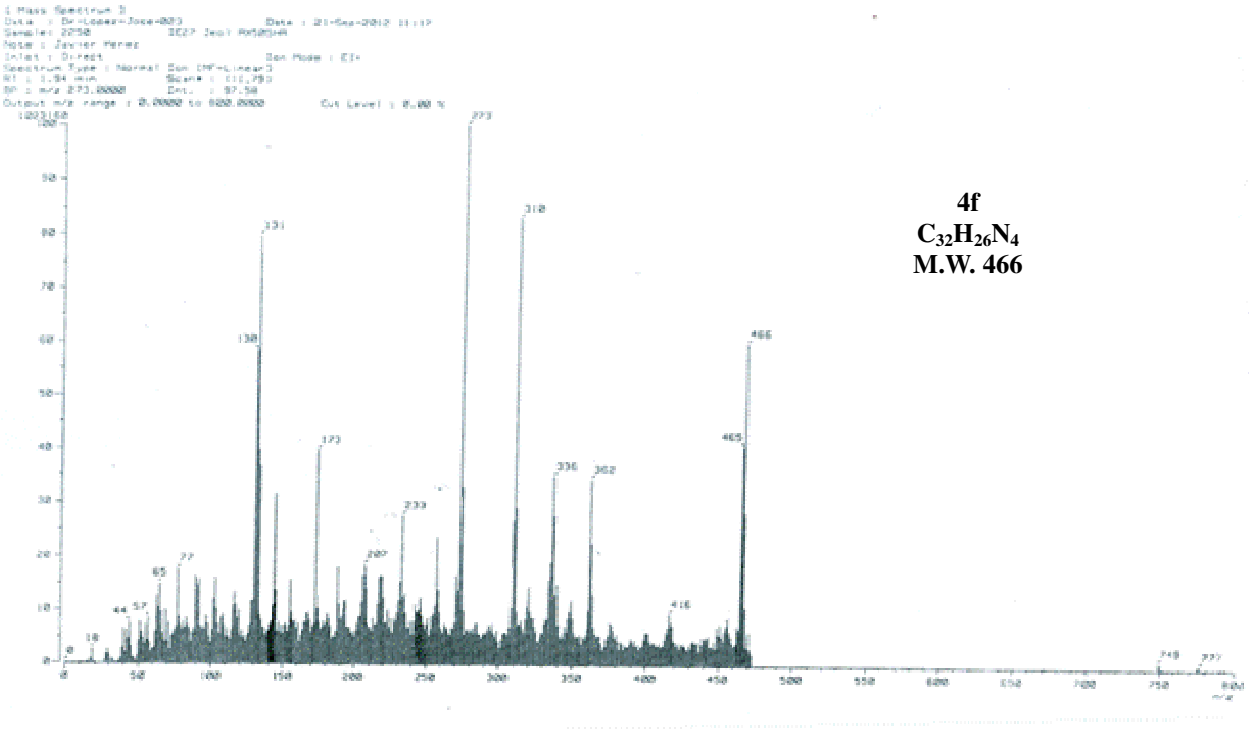
4e



4e



4f



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

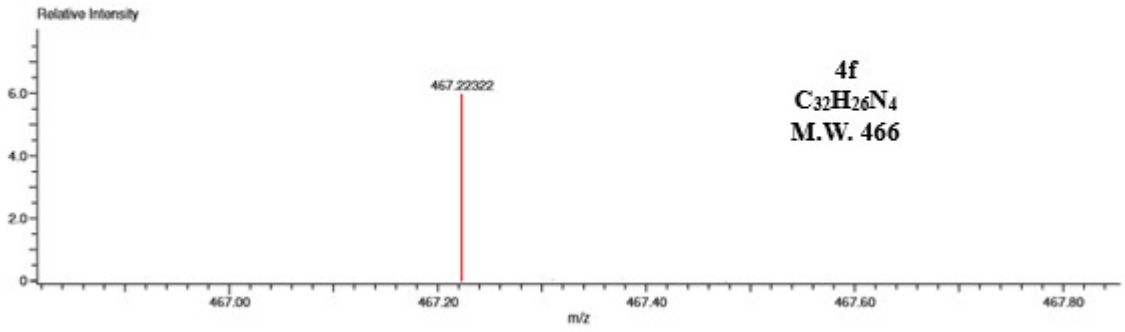
Data:CAT 17
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.7...

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:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

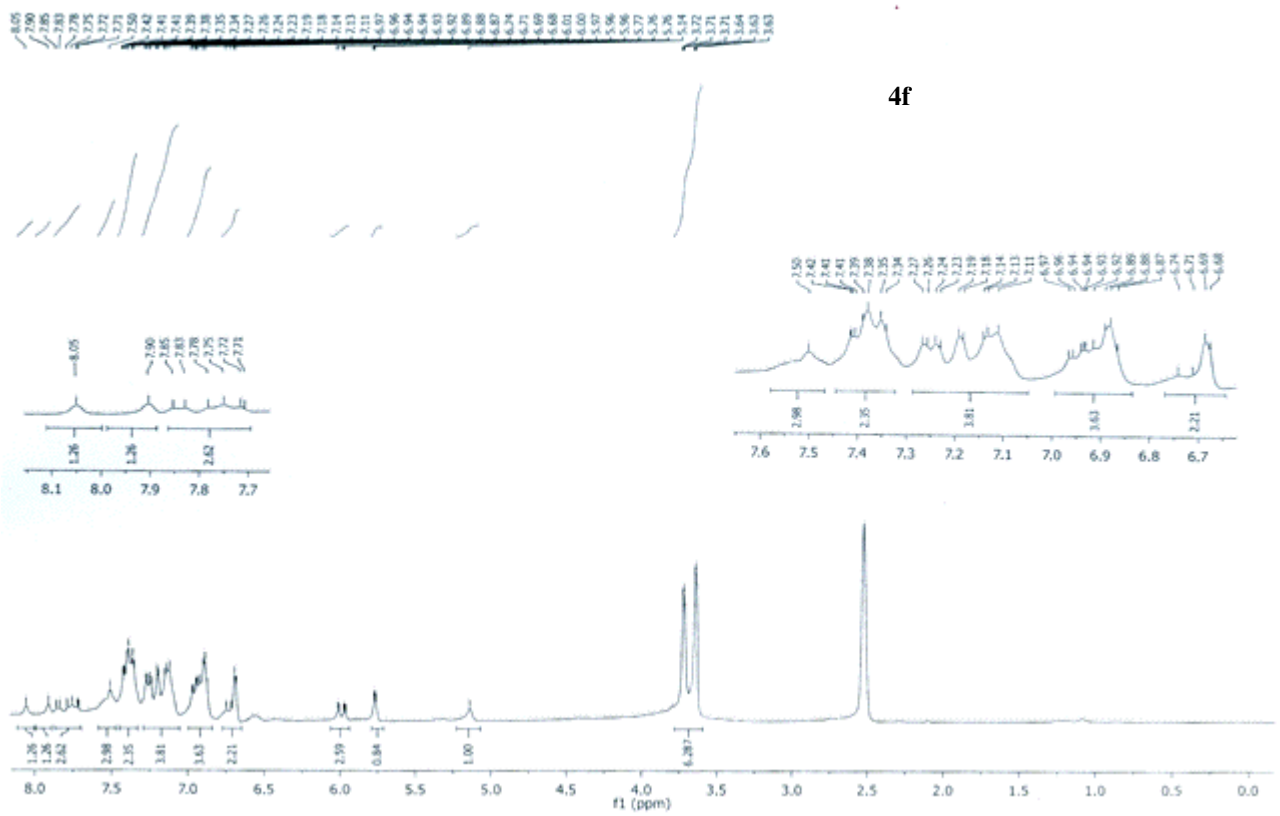
Tolerance:3.00(mmu)

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

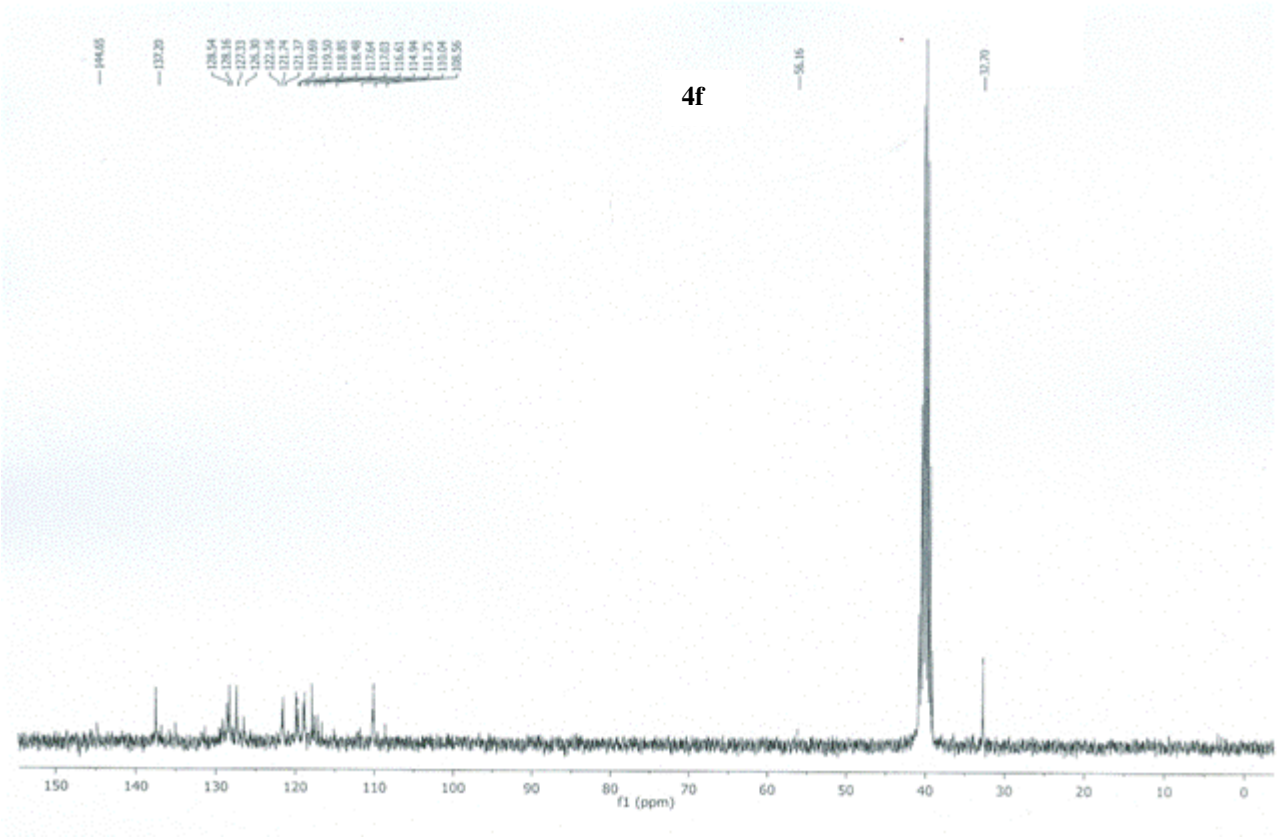


4f
$C_{32}H_{26}N_4$
M.W. 466

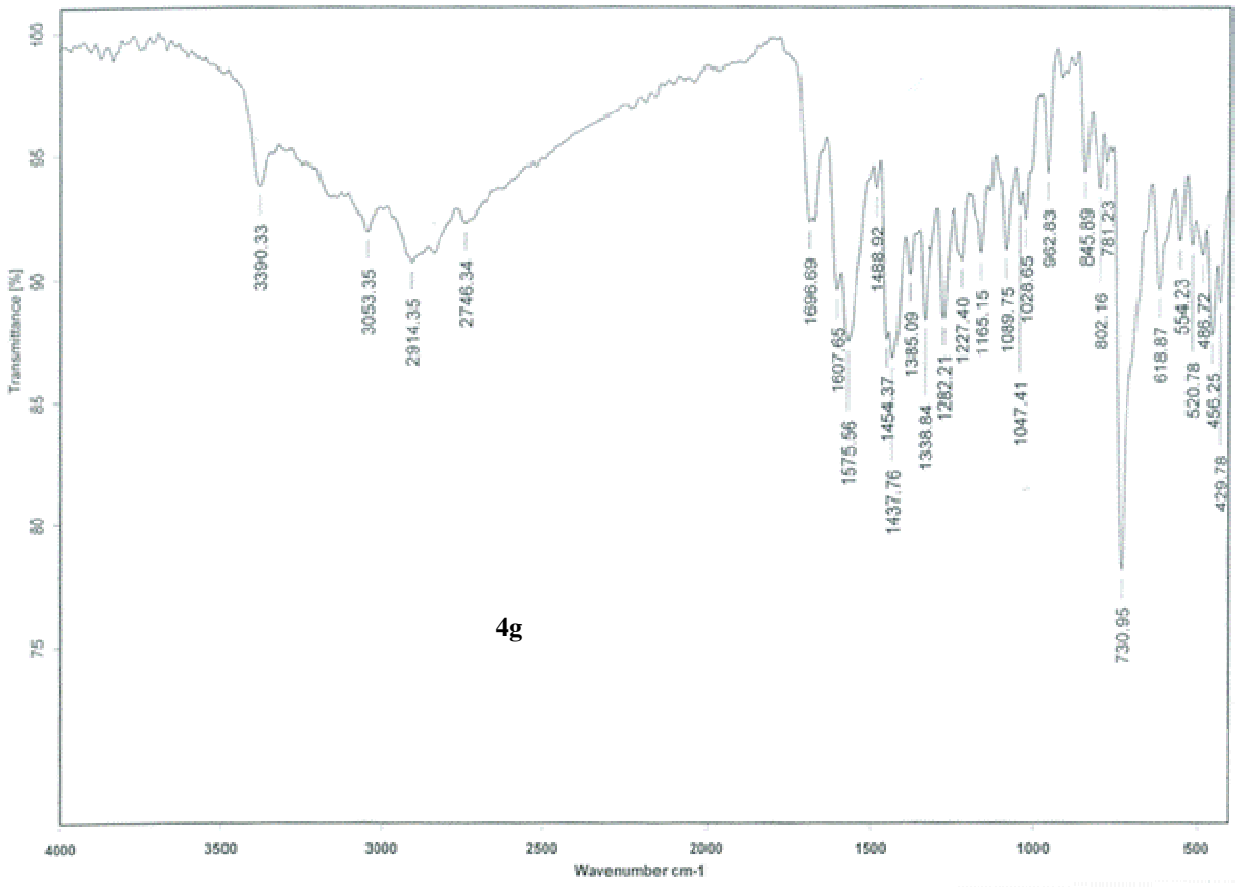
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22322	3587.26	467.22357	-0.35	-0.74	$^{12}C_{32}{}^{1}H_{27}{}^{14}N_4$	21.5



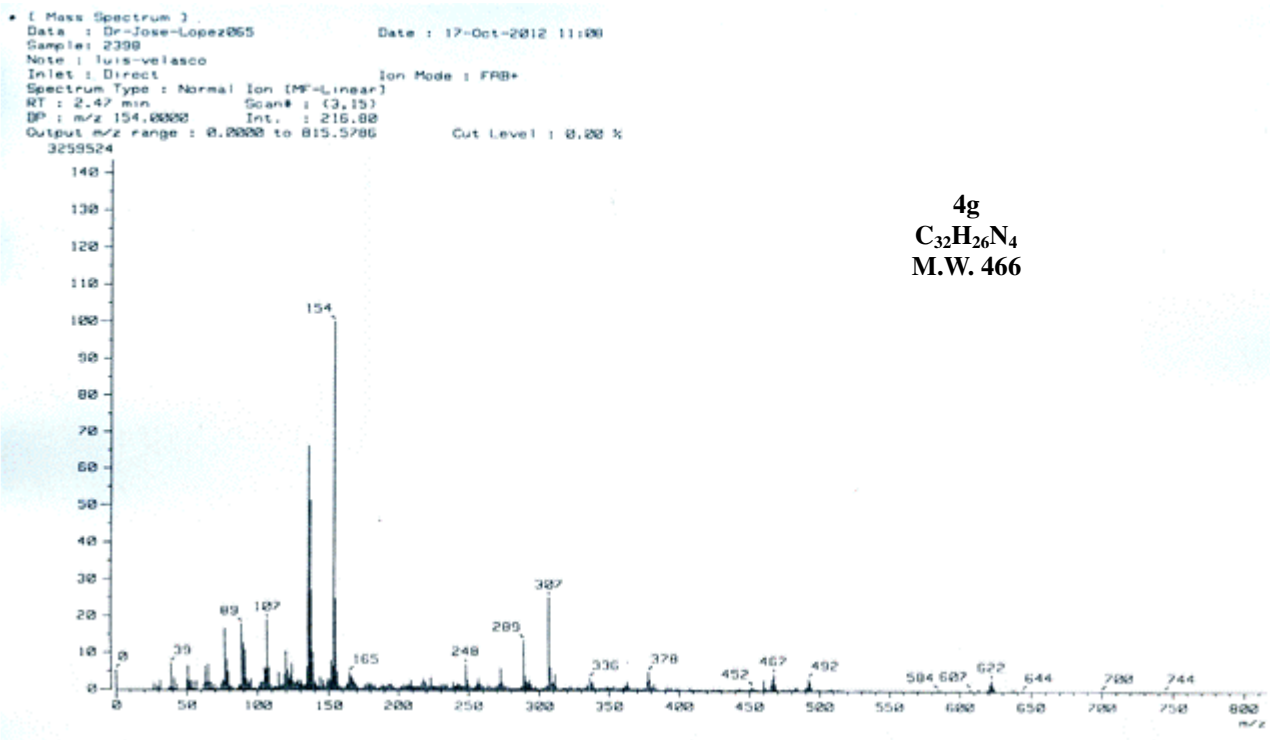
4f



4f



4g

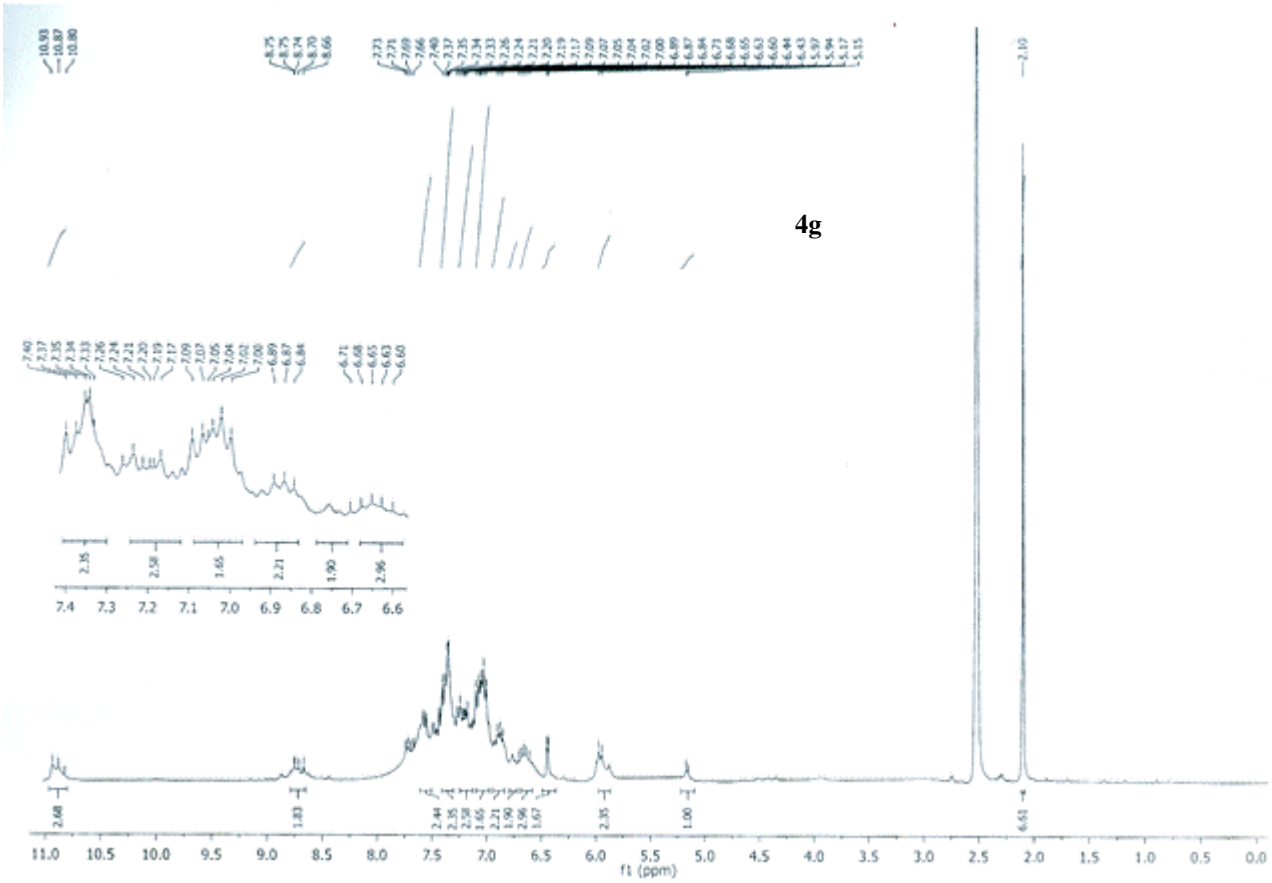


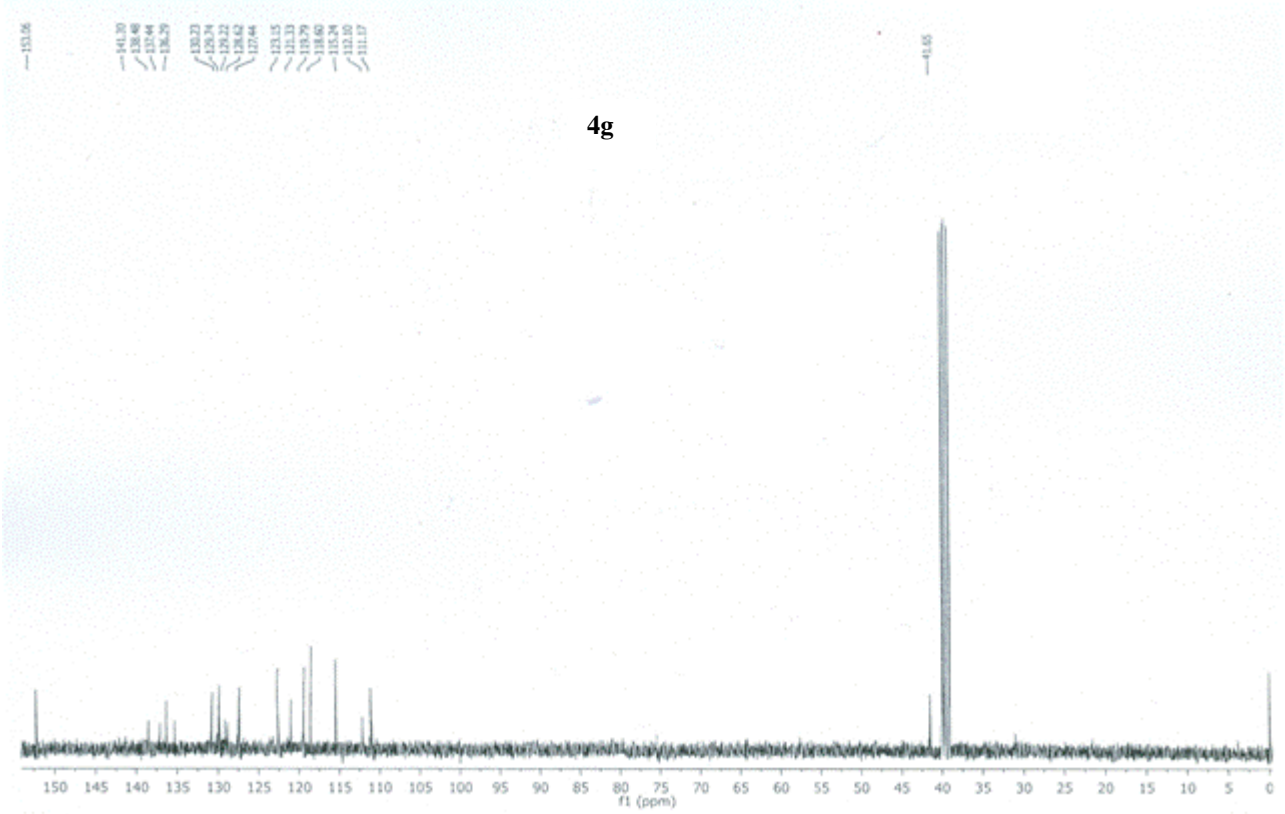
4g
$C_{32}H_{26}N_4$
M.W. 466

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

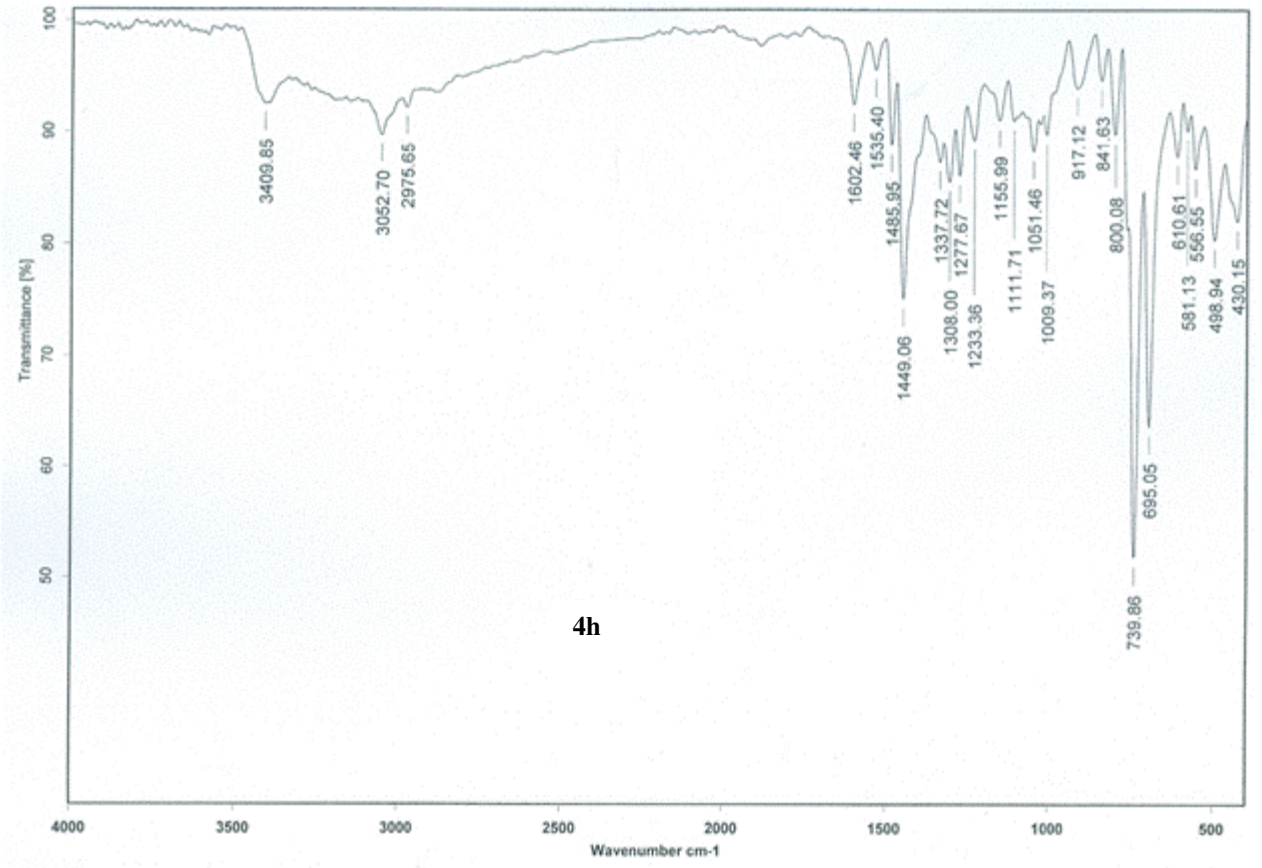
4g
$C_{32}H_{26}N_4$
M.W. 466

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

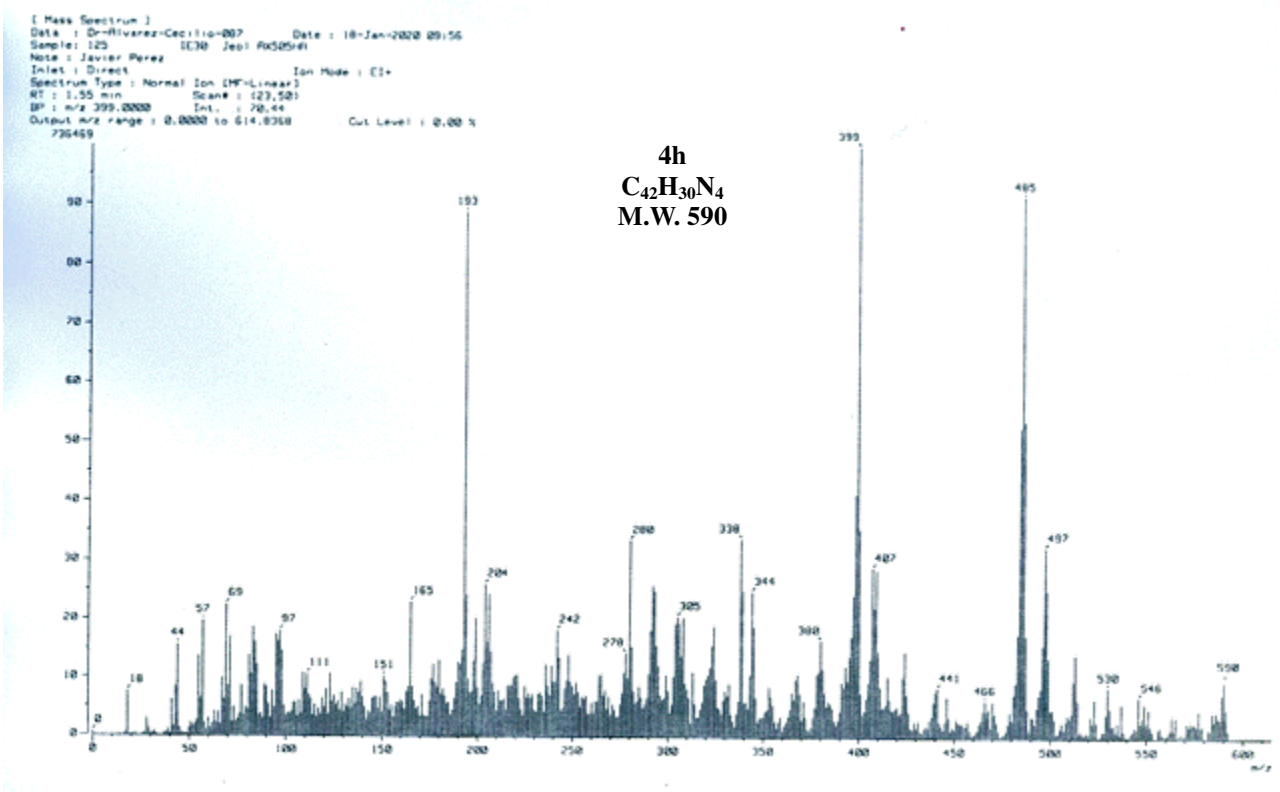




4g



4h



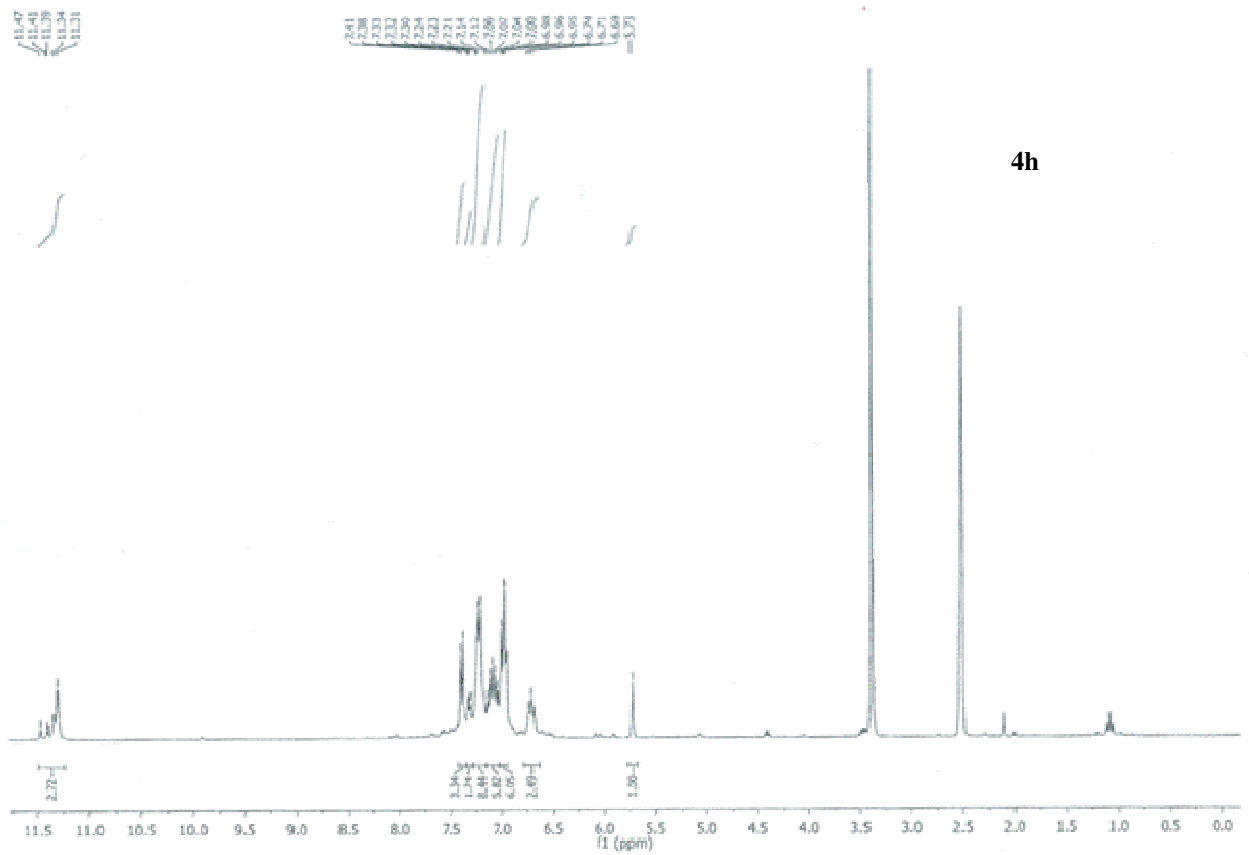
4h
$C_{42}H_{30}N_4$
M.W. 590

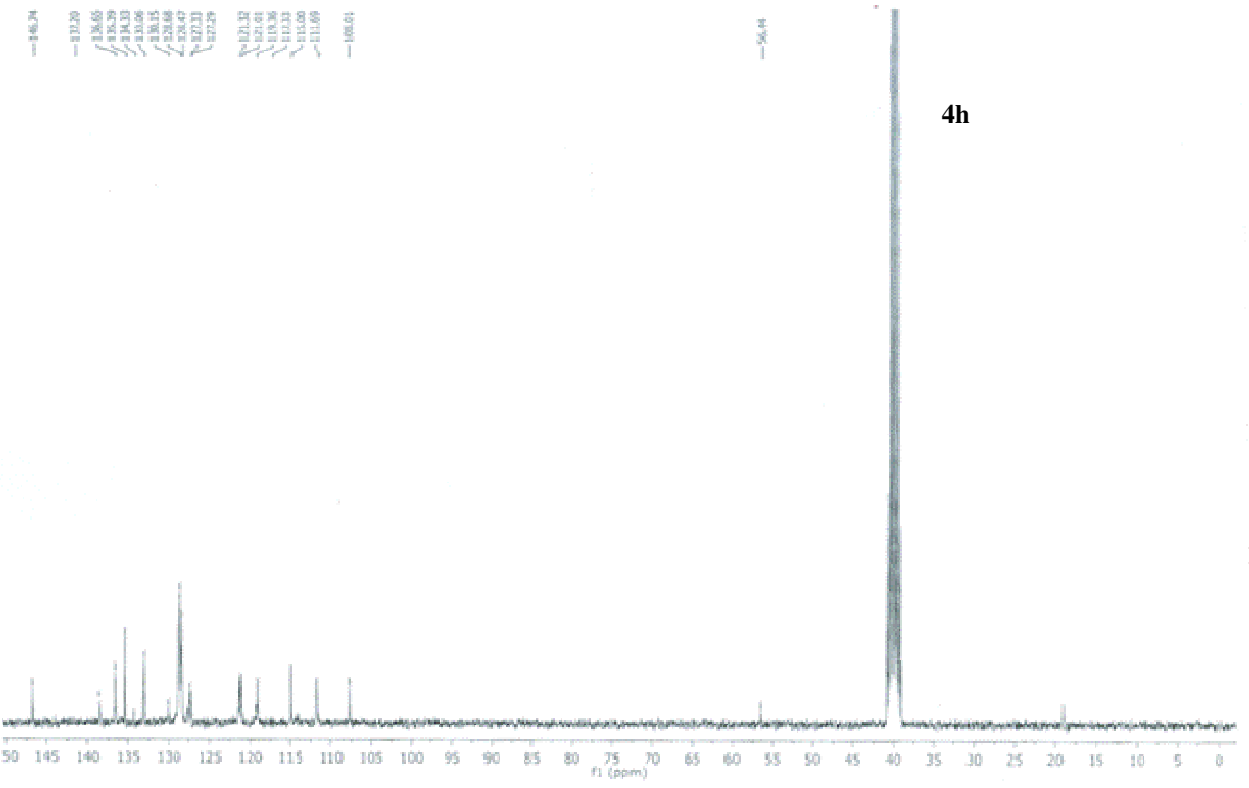
Anal calcd. C 85.40 H 5.12 N 9.48

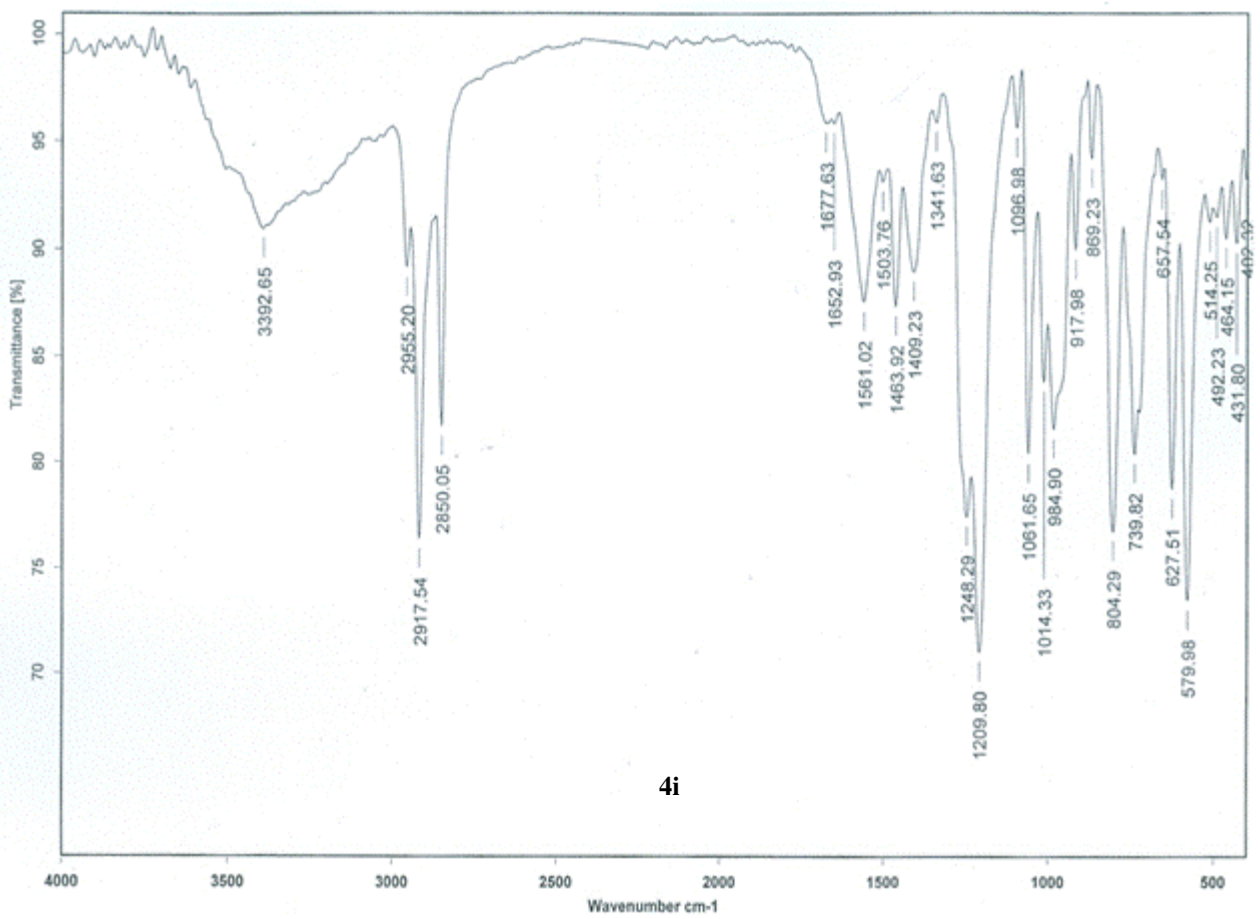
Clave de la muestra	Peso [mg]	N [%]	C [%]	H [%]	S [%]	Fecha de análisis
bz2ph m	2.647	9.44	85.37	5.01	---	27-04-2016

Found

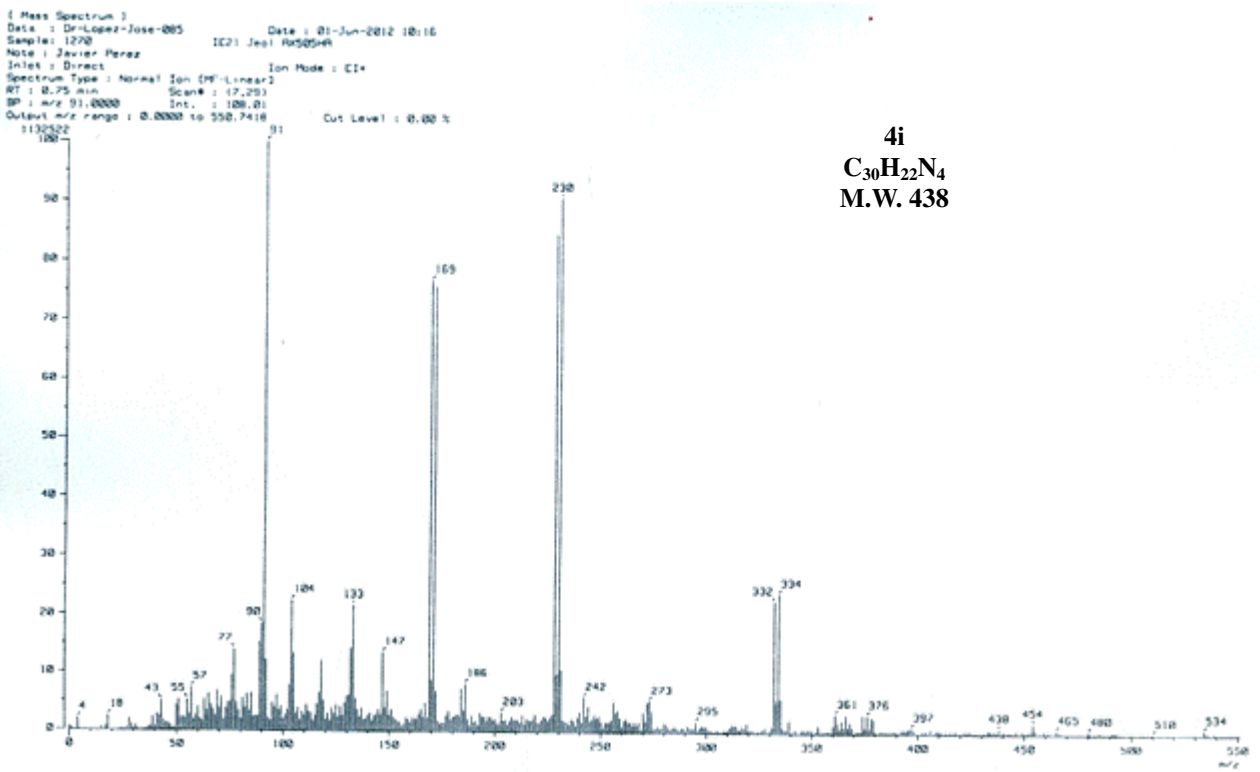
4h
$C_{42}H_{30}N_4$
M.W. 590







4i

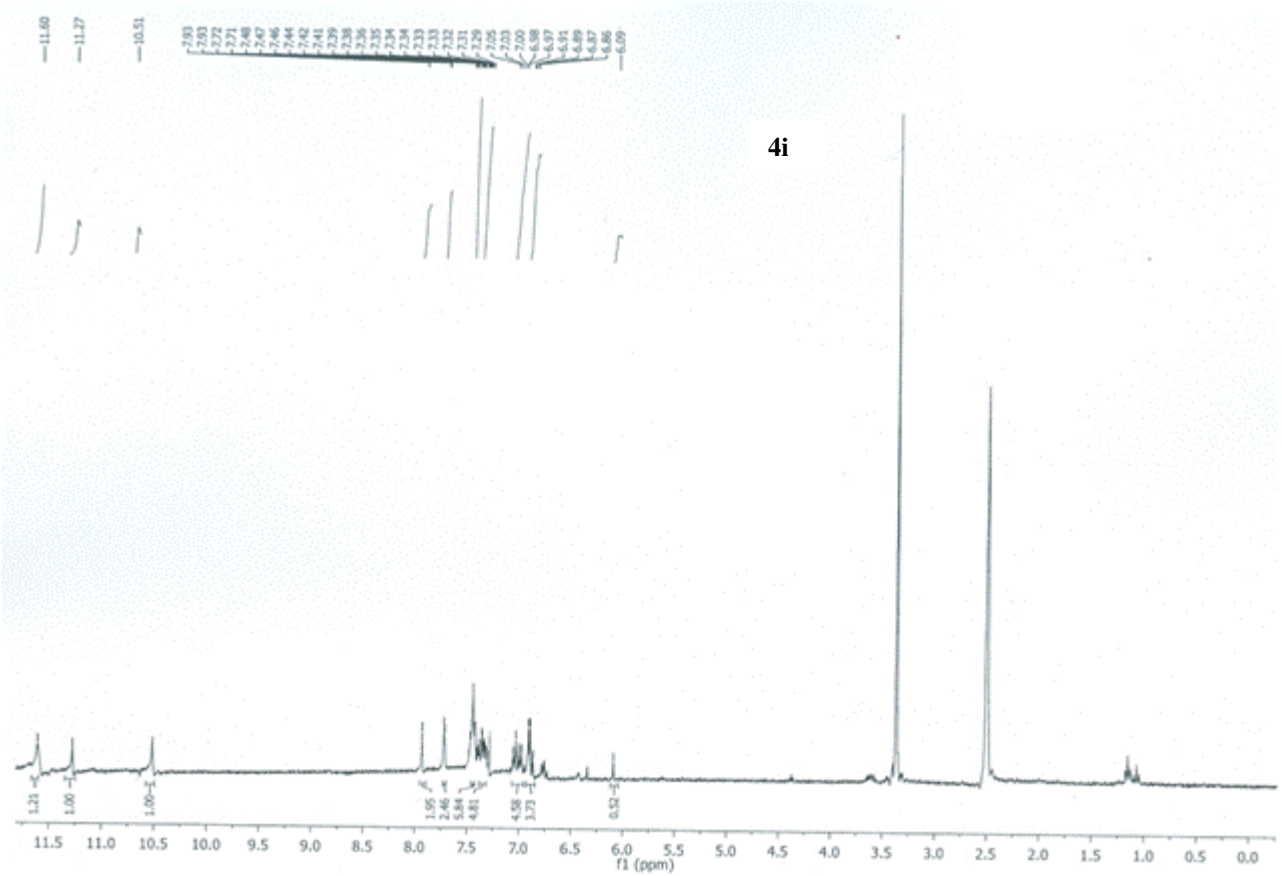


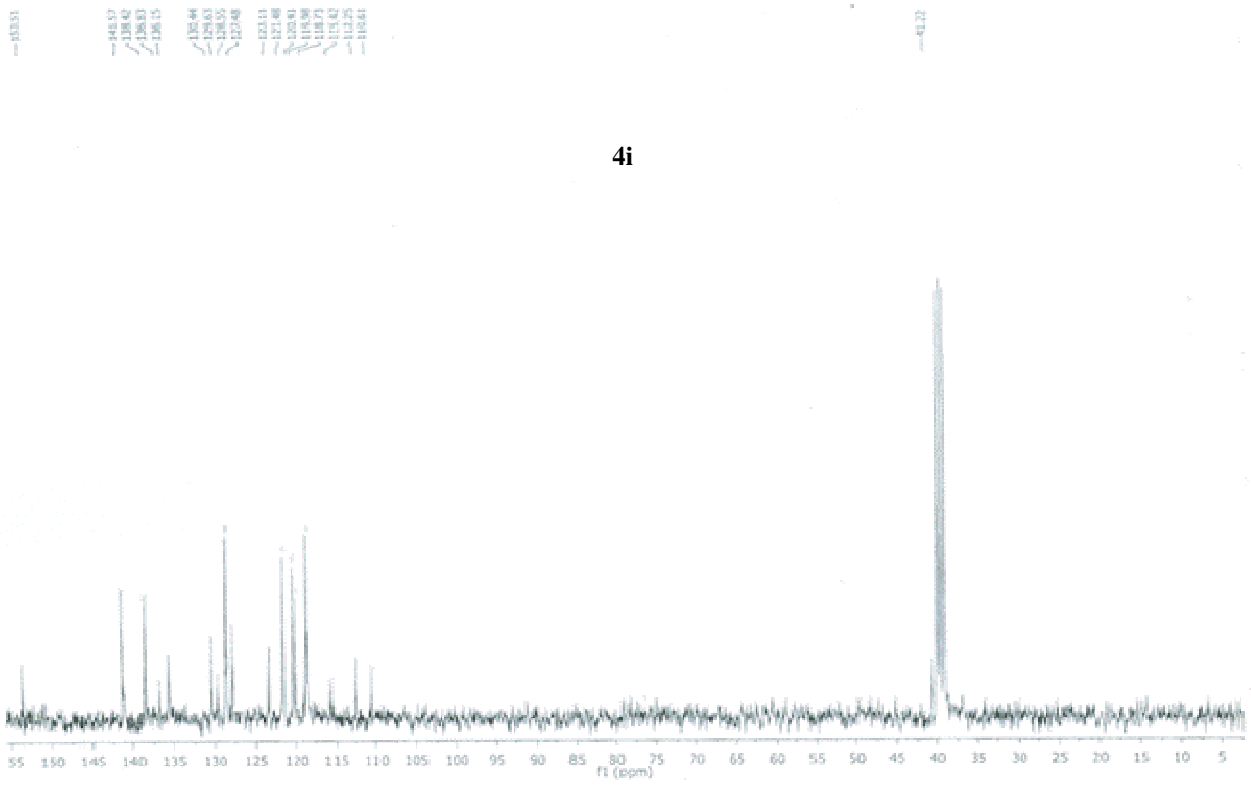
4i
$C_{30}H_{22}N_4$
M.W. 438

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

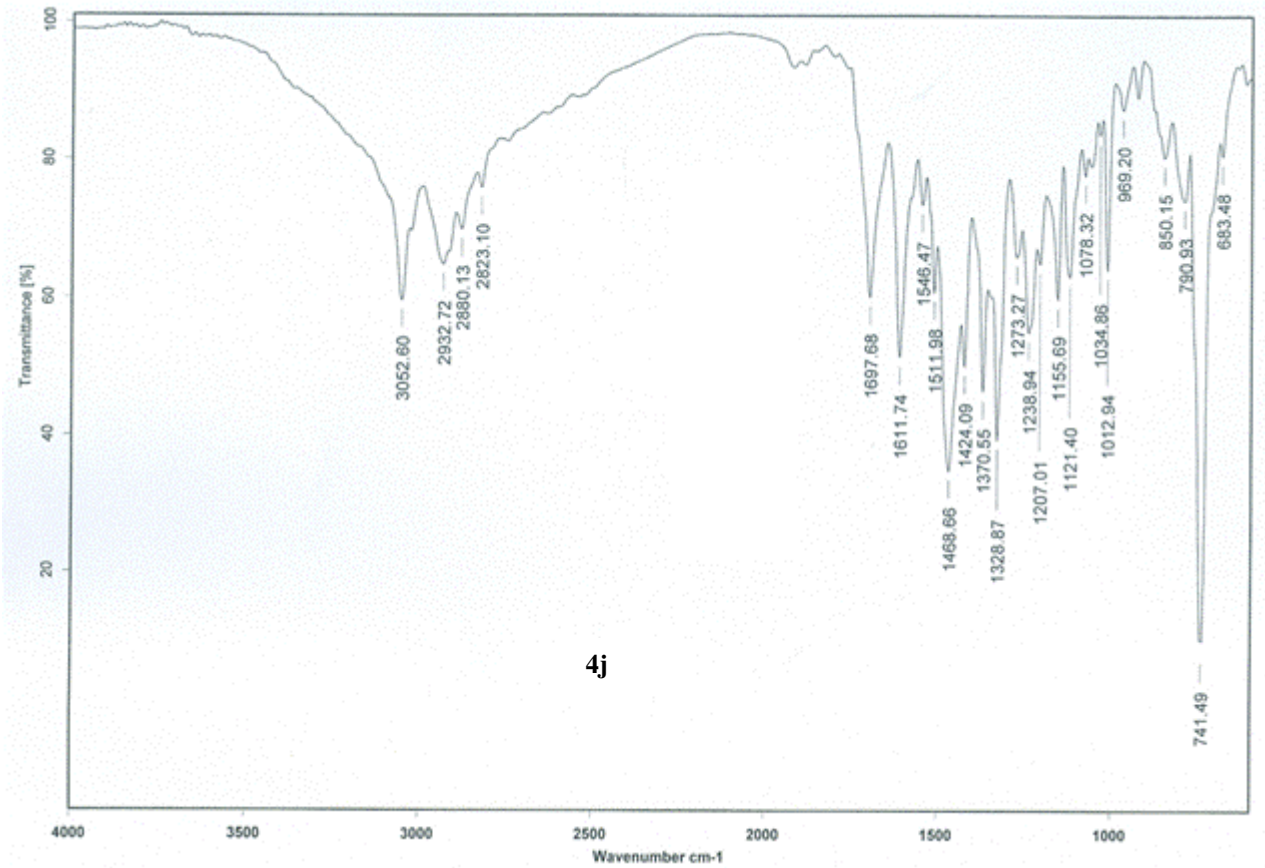
	Observed m/z	Int%				
	438.1835	2.32				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N
1	438.1844	-2.2 / -0.9	22.0	30	22	4

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

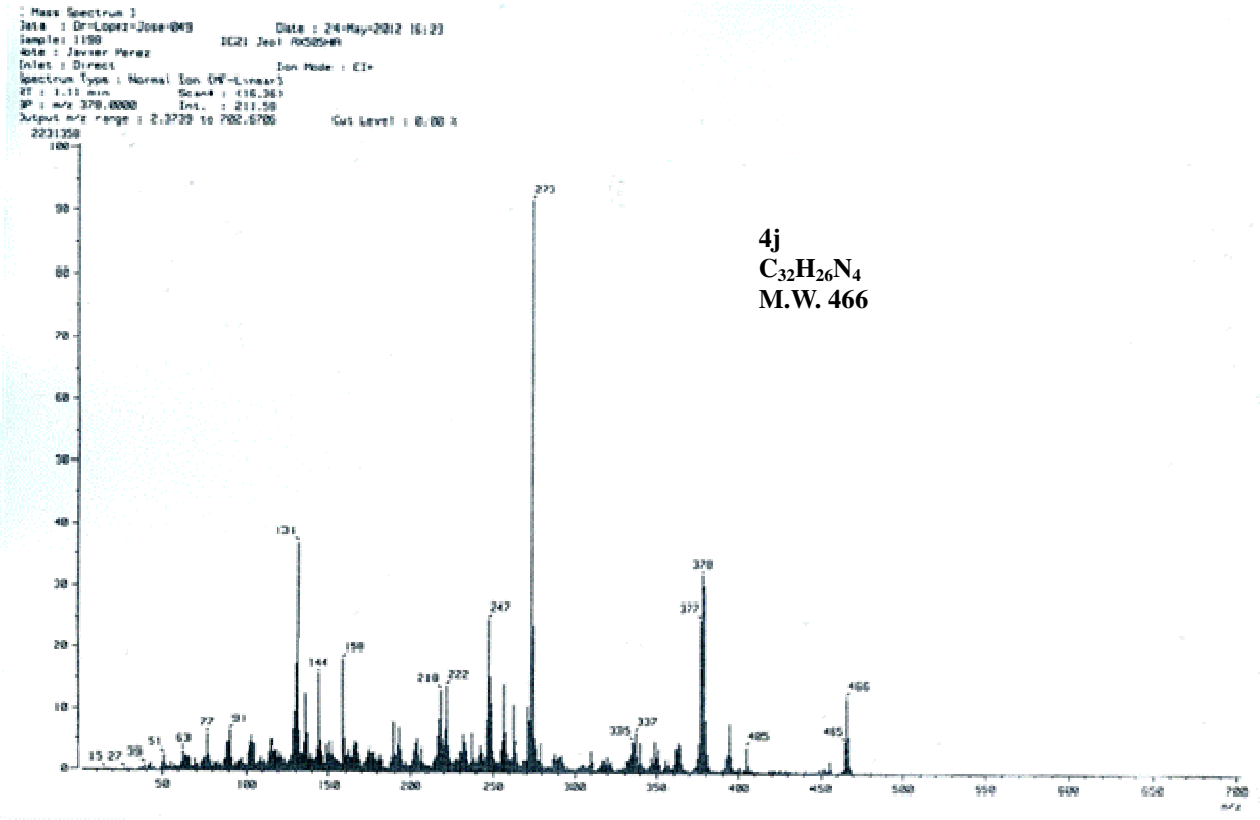




4i



4j



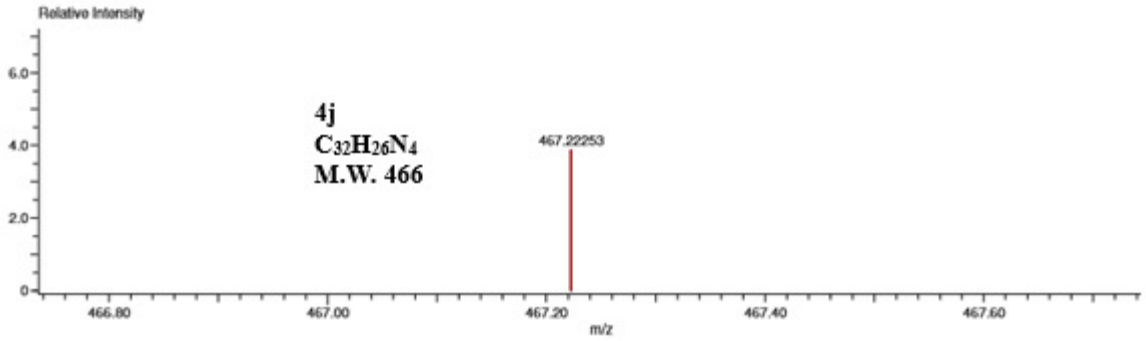
Data:CAT21
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.6...

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

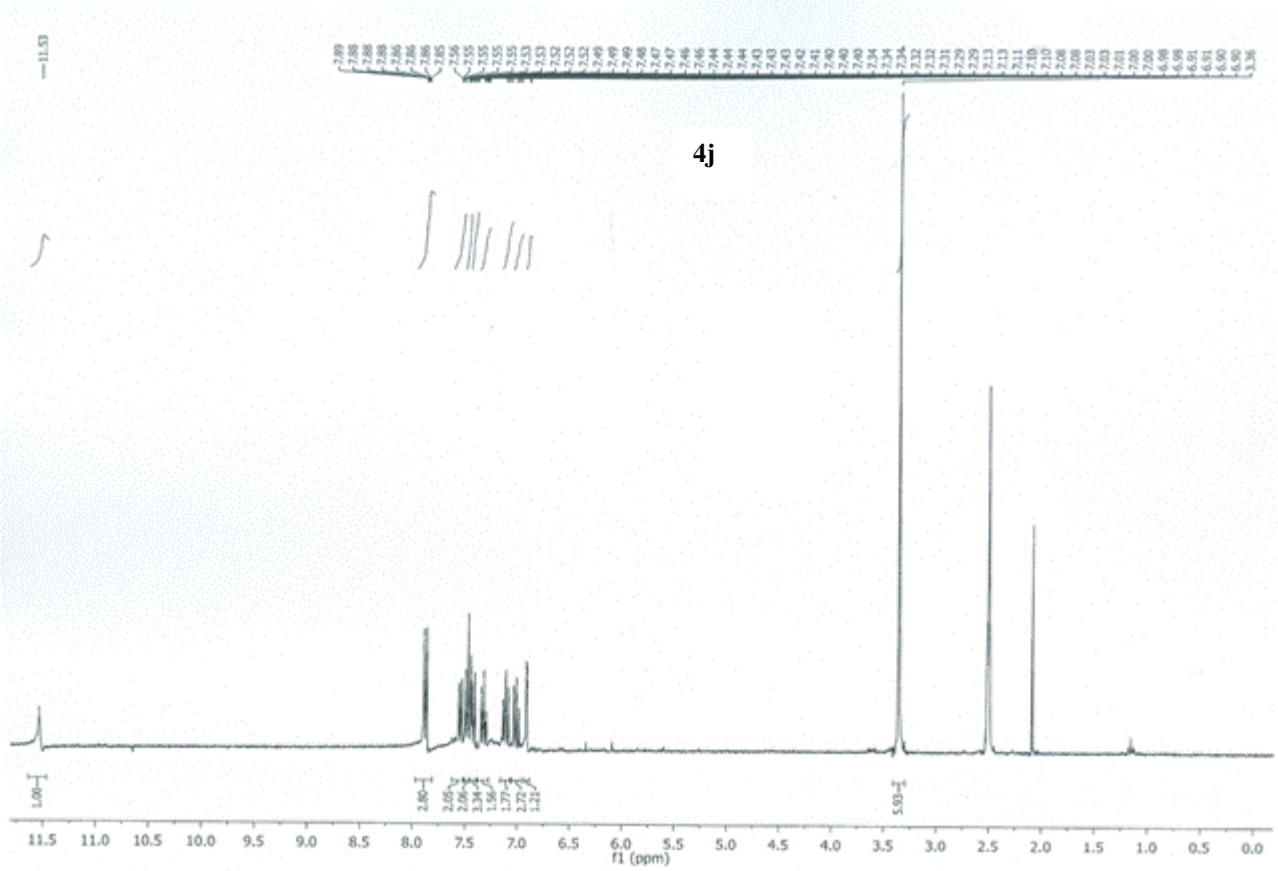
Charge number:1
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

Tolerance:3.00(mmu)

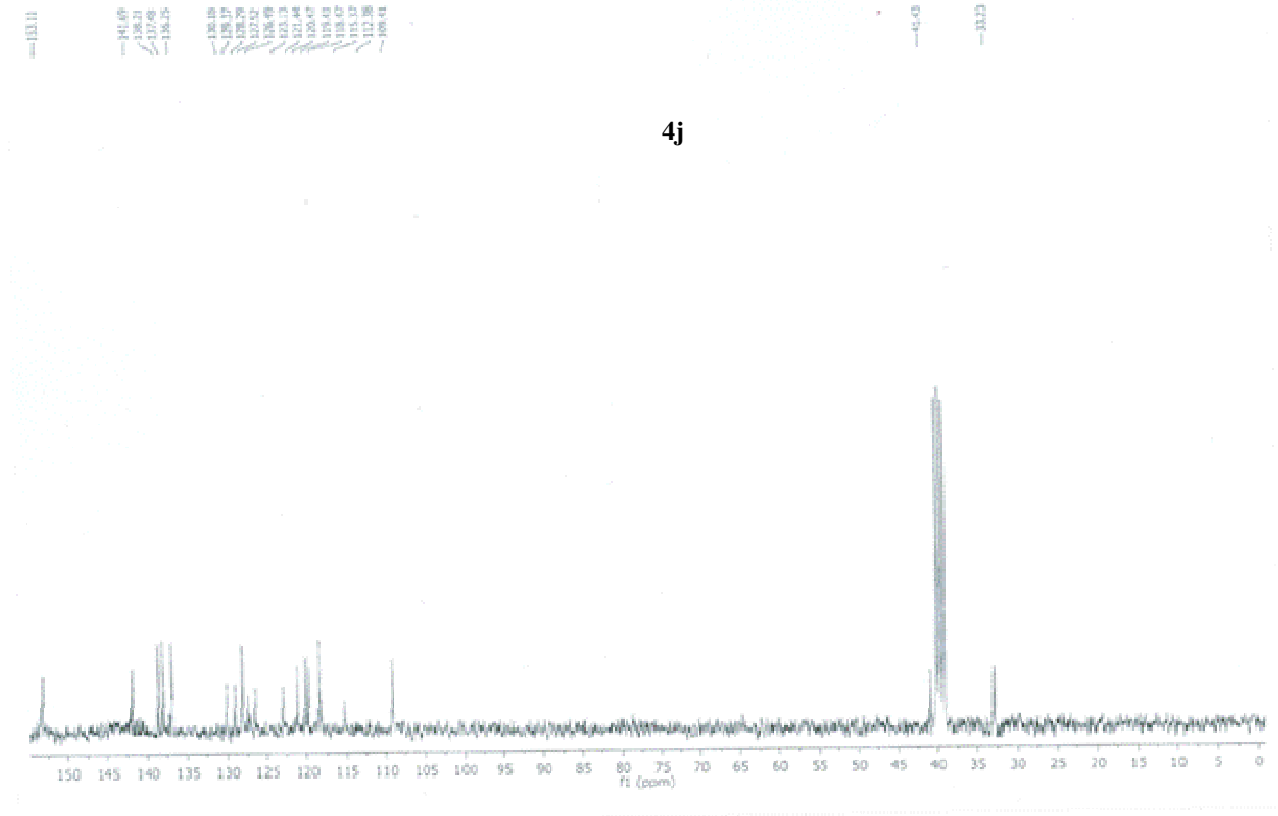
Unsaturation Number:0.0 .. 32.0 (Fraction:Both)



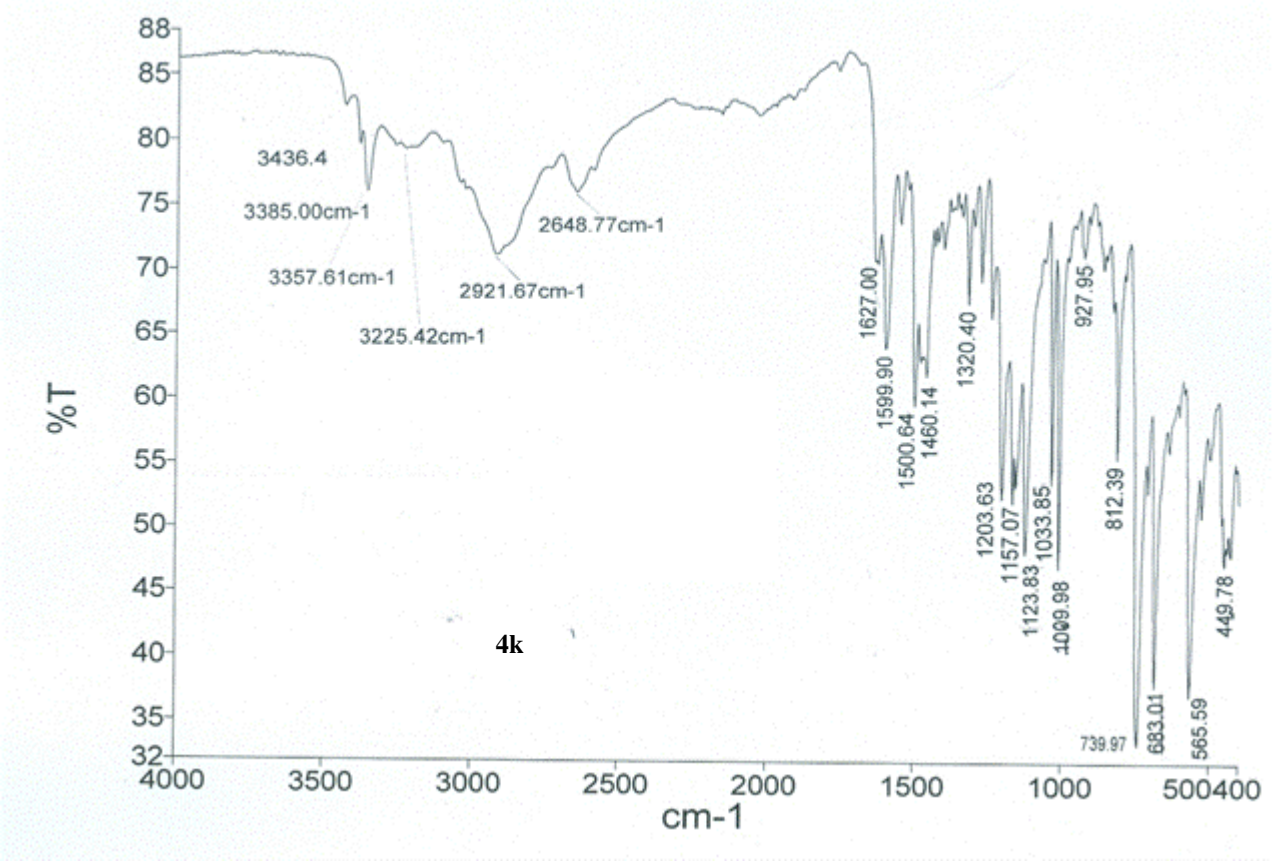
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22253	3657.25	467.22357	-1.05	-2.24	$^{12}C_{32}{}^{1}H_{27}{}^{14}N_4$	21.5



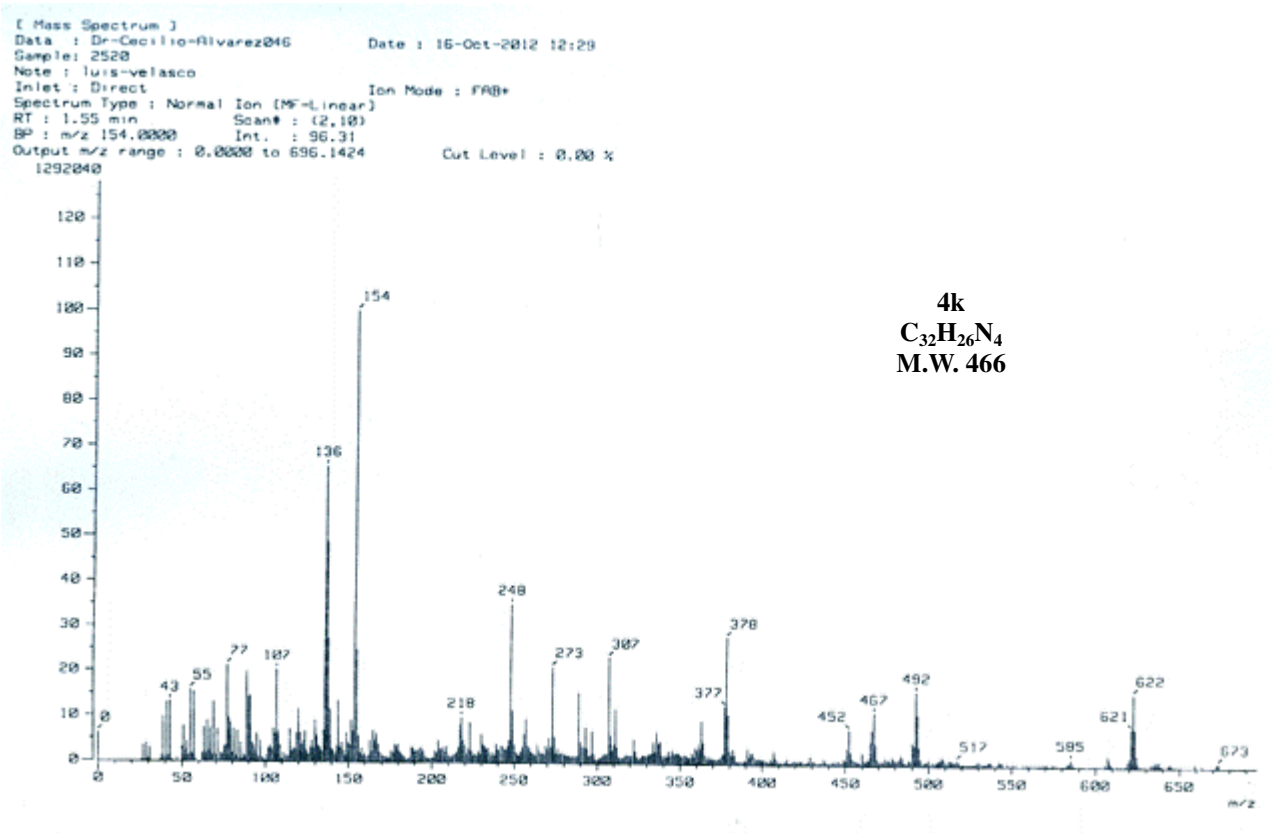
4j



4j



4k



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

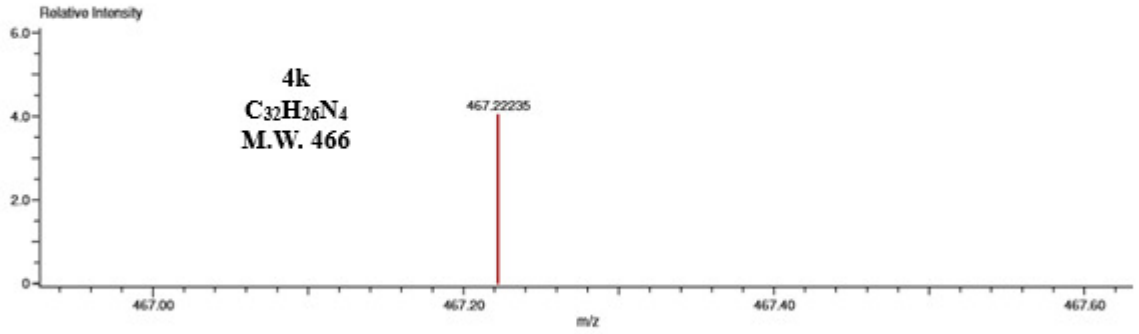
Data:CAT23
Sample Name:
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid;30,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 0.2...

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

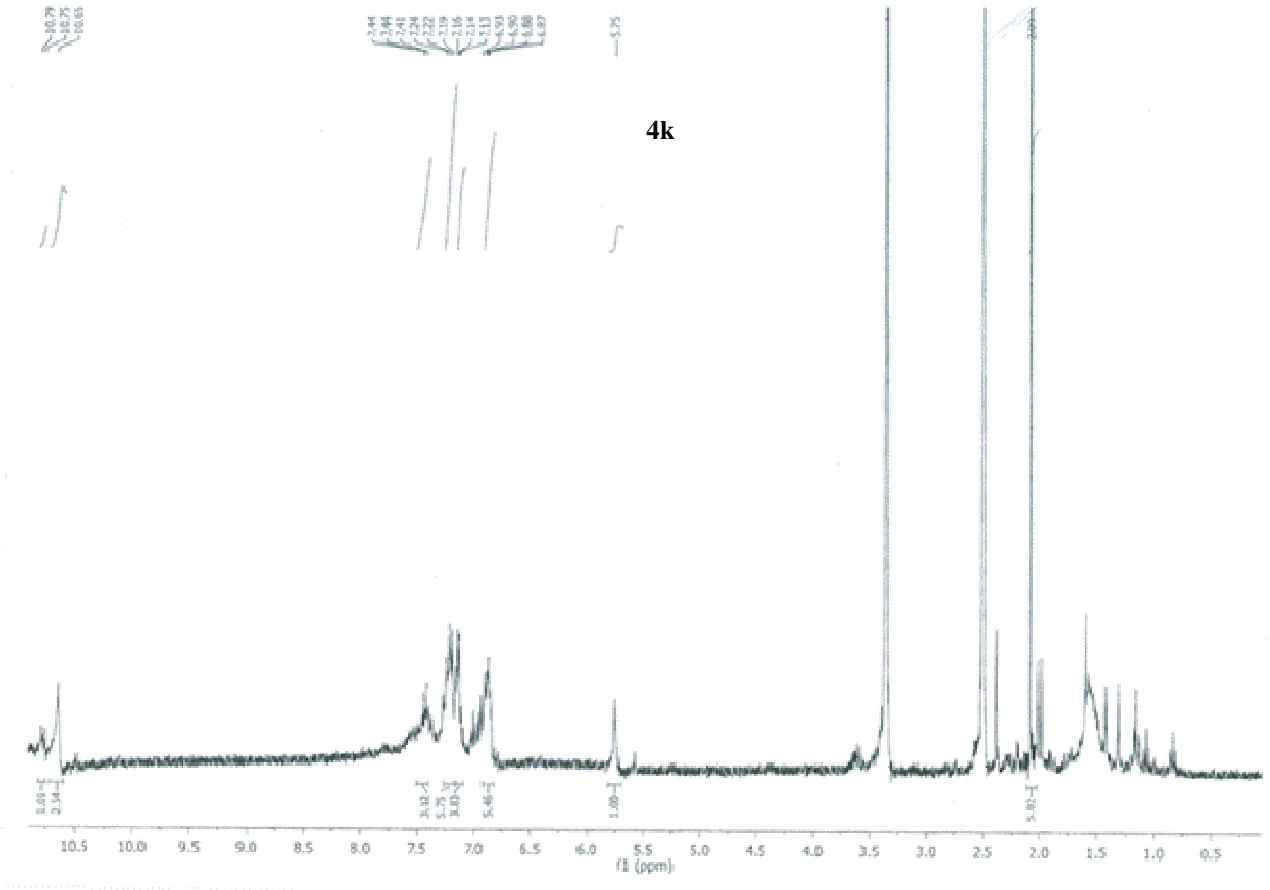
Charge number:1
Element:^{12}C:0 .. 100, ^{1}H:0 .. 100, ^{14}N:2 .. 5

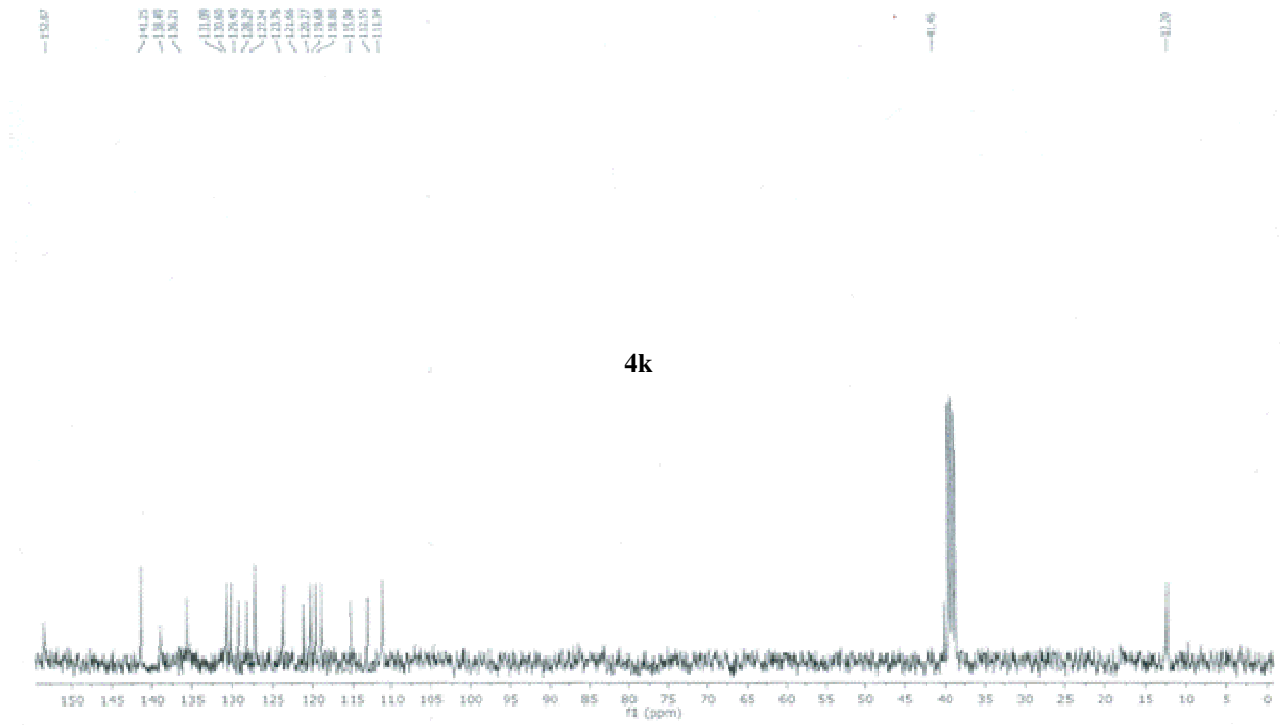
Tolerance:3.00(mmu)

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

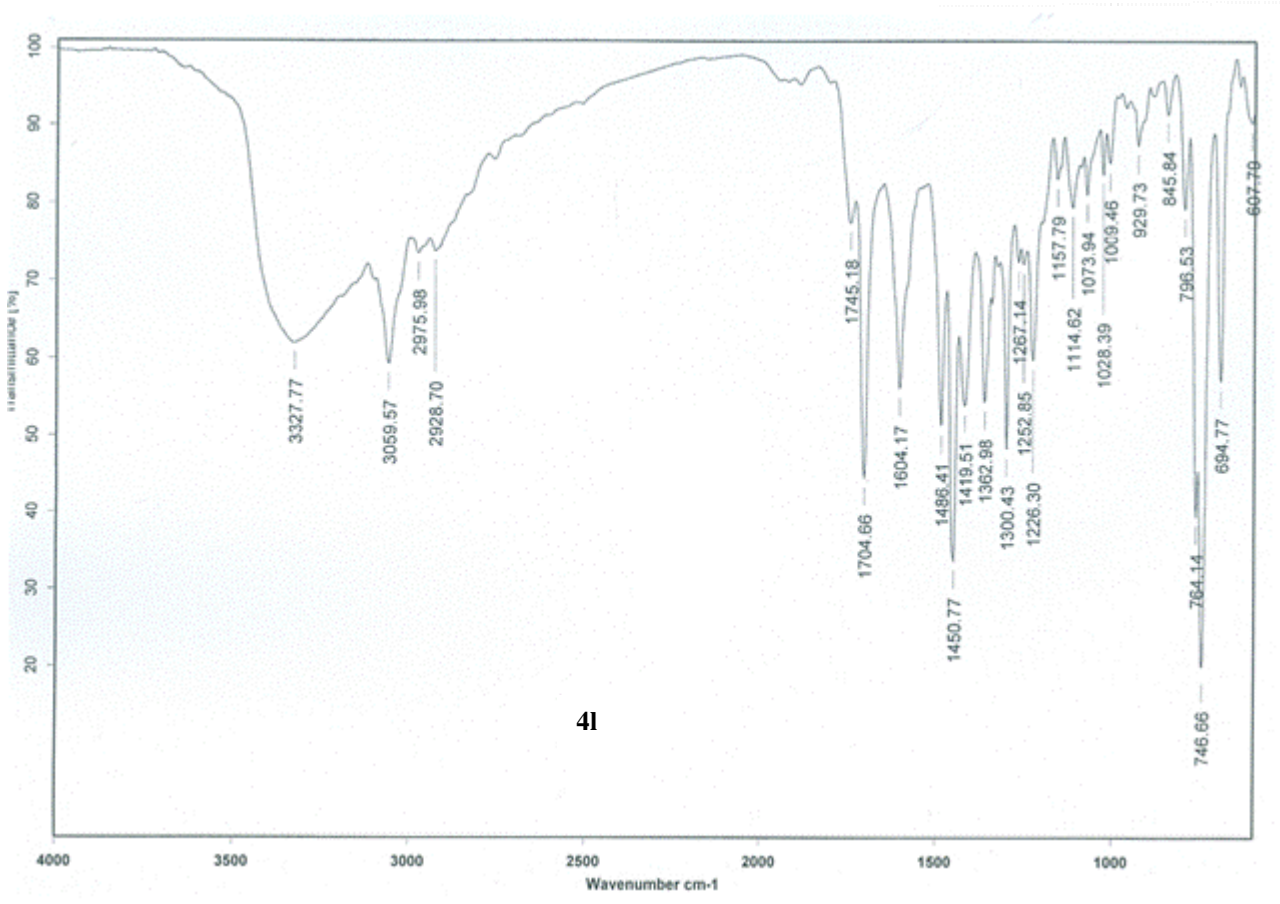


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
467.22235	2357.76	467.22357	-1.22	-2.62	$^{13}C_{32}{}^{1}H_{27}{}^{14}N_4$	21.5

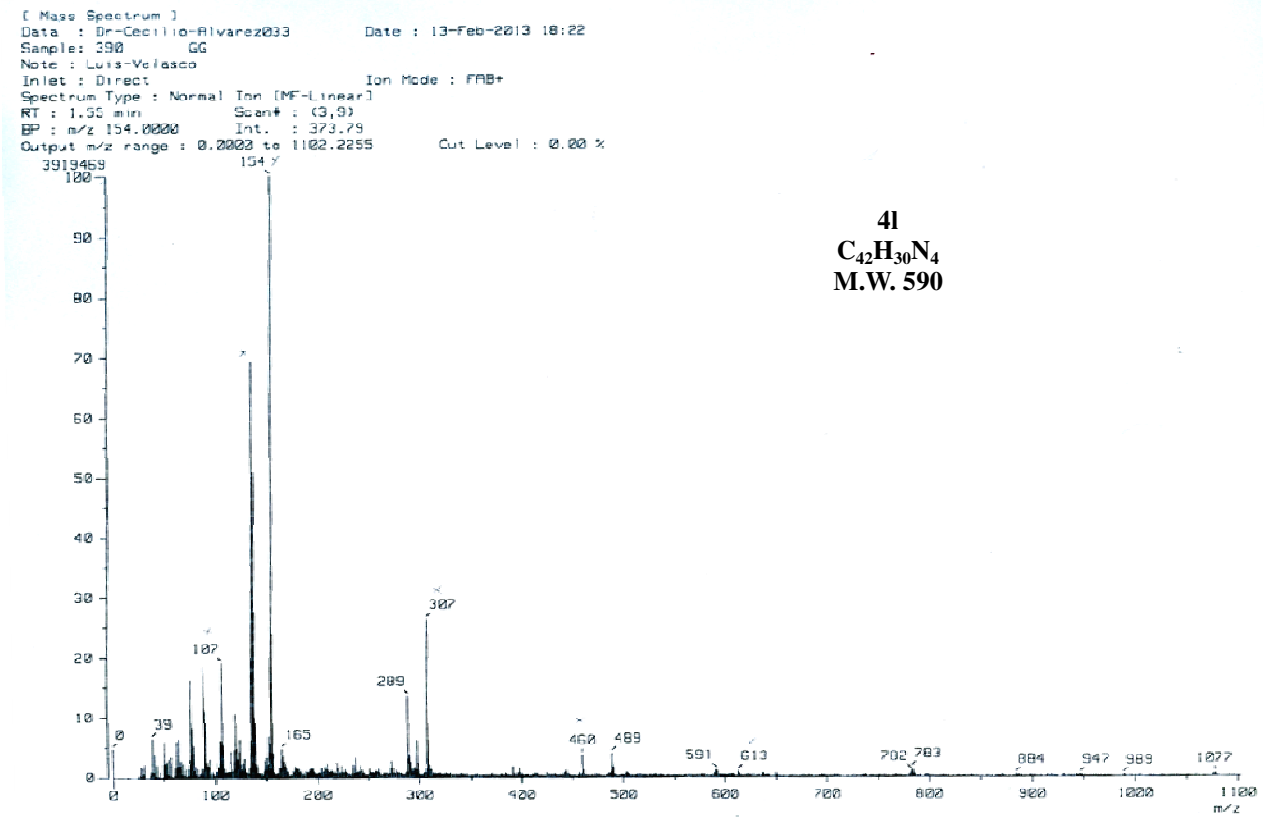




4k



4l



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

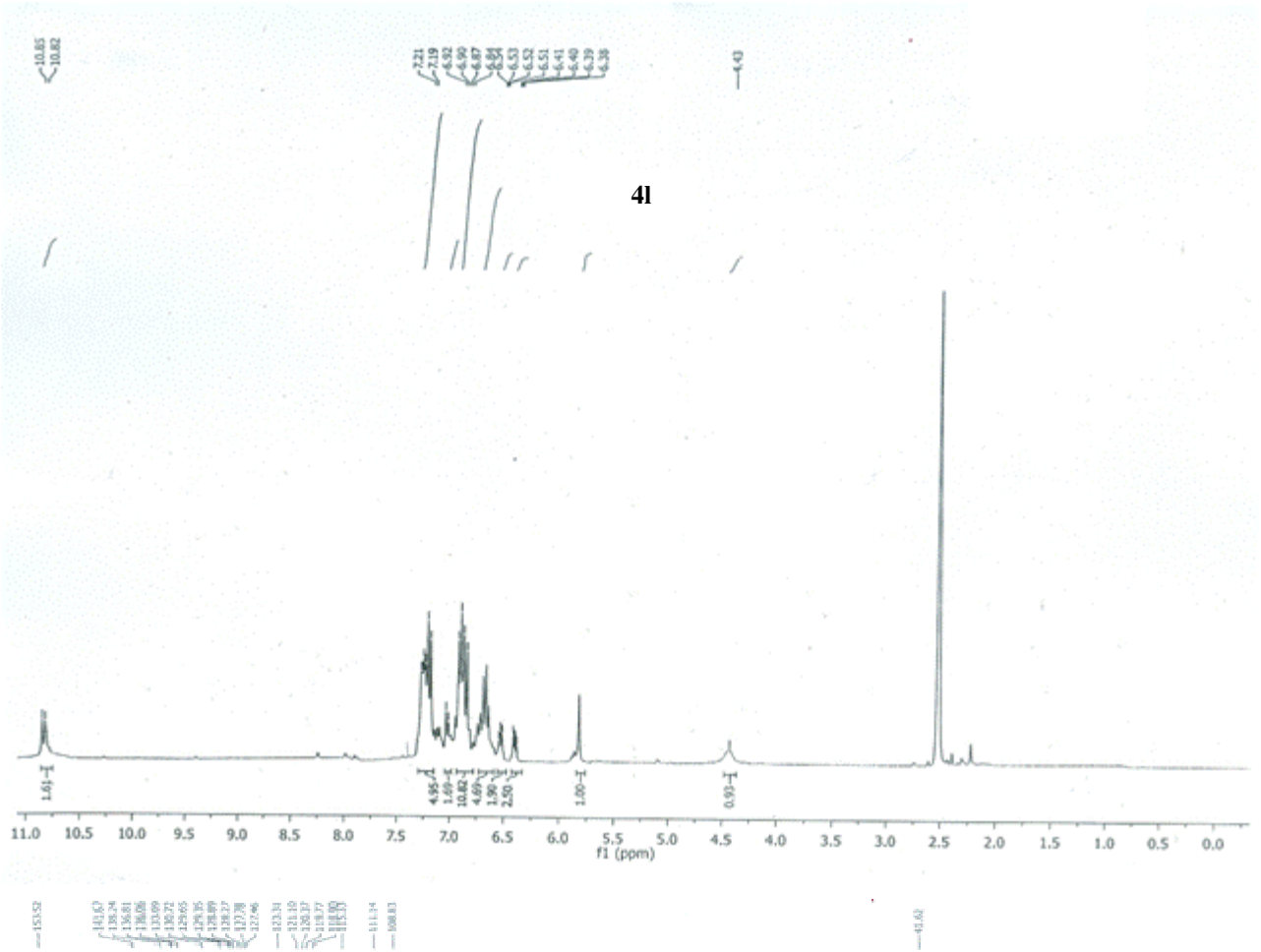
Anal calcd. C 85.40 H 5.12 N 9.48

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

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

4l



4l