Electronic Supplementary Material (ESI) for RSC Advances.

Sulfamic acid promoted one-pot multicomponent reaction: A facile synthesis of 4-oxo-tetrahydroindoles under ball milling process†

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Supporting information

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S1. Materials and method:

General Information: The chemicals were procured from S.D. Fine, India and Merck Ltd. without additional purification. The sulfamic acid was purchased from Merck Ltd. (catalogue no. 242780). The reactions were monitored by thin-layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (100–200 mesh) using distilled hexane, ethyl acetate, and dichloromethane. A Retsch 01.462.0220 Agate Grinding Jar (250 mL Capacity) was used for the Planetary Ball Mill 100. All the products were identified compounds and their physical information, FT-IR, mass spectra and 1H NMR was basically the same as those of the genuine samples. Melting points were determined using melting point B-540 apparatus and are uncorrected. HRMS was determined using waters LCT premier XETOF ARE-047 apparatus.

S2. General Procedure for synthesis of 4-oxo-tetrahydroindoles derivatives using ball milling technique: The mixture of dimedone (1 mmol), phenacyl bromide (1 mmol), and aniline (1 mmol) and catalytic amount of sulfamic acid (20 mol %) was taken in one pot under solvent/additives free under ball-milling at 600 rpm with six balls (d = 10 mm) of the equivalent substance using 25 mL stainless steel beaker for 60 min. The ball-milling was carried out at inverted rotation directions, for time durations of 10 min separated by intervals of 30 s. The extraction of the reaction residue was accomplished by elution with ethanol followed by solvent evaporation to furnish the product (4a-n). This methodology was applicable for all the reactions listed in (Table 2). The remaining sulfamic acid was again washed with ethanol followed by acetone, dried under vacuum and reused for next run.

S3. Analytical dada for selected products

1. **6,6-dimethyl-1,2-diphenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4a):** Faint yellow solid; mp: 205-206°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 6H), 2.42 (s, 2H), 2.51 (s, 2H), 6.78 (s, 1H), 7.05-7.07 (m, 2H), 7.12-7.17 (m, 5H), 7.39-7.41 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.6 (2C), 35.5, 37.0, 52.1, 105.6, 120.0, 122.5, 126.8, 127.7 (2C), 128.1 (2C), 128.1 (2C), 128.2, 129.3 (2C), 136.3, 137.7, 144.7, 194.0; HRMS (ESI) [M+1] calcd for $C_{22}H_{22}NO$: 316.1701, found: 316.1689.
2. **1-(4-bromophenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4b):** Brown solid; mp: 170-173°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 6H), 2.41 (s, 2H), 2.50 (s, 2H), 6.77 (s, 1H), 7.00-7.03 (m, 2H), 7.04-7.07 (m, 2H), 7.18-7.20 (m, 3H), 7.52 (dd, J 1,2 = 2.0 Hz, , J 1,3= 6.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.6 (2C), 35.5, 37.0, 52.0, 105.9, 120.2, 122.1, 127.1, 128.2 (2C), 128.3, 129.2 (2C), 131.5 (2C), 132.5 (2C), 136.2, 136.6, 144.4, 193.8; HRMS (ESI) [M+1] calcd for $C_{22}H_{21}NOBr$: 394.0807, found: 394.0810.
3. **6,6-dimethyl-2-phenyl-1-(o-tolyl)-1,5,6,7-tetrahydro-4H-indol-4-one (4c):** Offwhite solid; mp: 168-170°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.05 (d, J = 9.6 Hz, 6H), 1.86 (s, 3H), 2.15 (d, J = 16 Hz, 1H), 2.36-2.50 (m, 3H), 6.83 (s, 1H), 7.08-7.14 (m, 5H), 7.2-7.36 (m, 4H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 17.4, 27.9, 29.2, 35.5, 36.5, 52.1, 104.9, 119.7, 126.9 (2C), 127.4 (2C), 128.1 (2C), 128.6, 129.1, 131.2, 132.0, 136.1, 136.4, 136.9, 144.8, 193.9; HRMS (ESI) [M+1] calcd for $C_{23}H_{24}NO$: 330.1858, found: 330.1846.

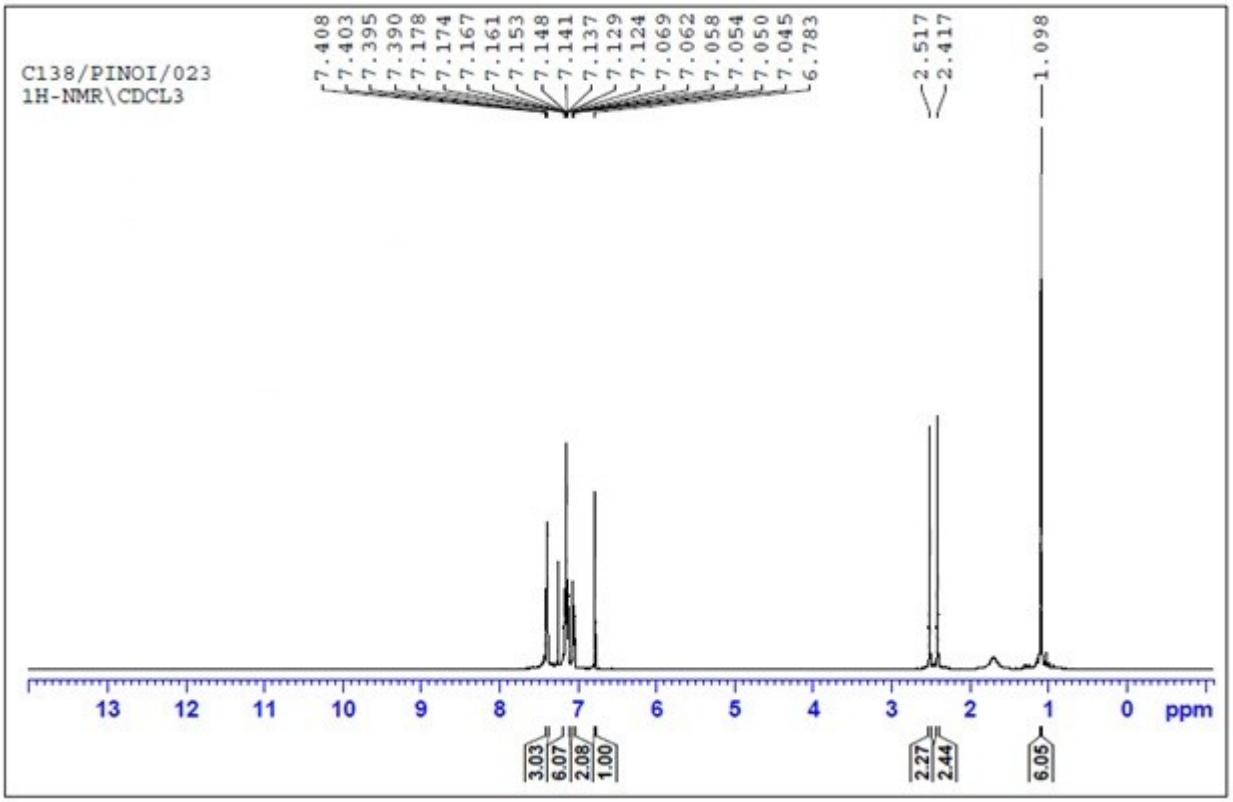
4. **1-(2,3-dimethylphenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4d):** Brown solid; mp: 149-151°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.07 (s, 3H), 1.10 (s, 3H), 1.74 (s, 3H), 2.15 (d, J = 16 Hz, 1H), 2.26 (s, 3H), 2.40- 2.47 (m, 3H), 6.82 (s,1H), 7.06 -7.09 (m, 3H), 7.12-7.14 (m, 3H), 7.18-7.19 (m,1H), 7.22-7.23 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.9, 20.3, 27.9, 29.1, 35.5, 36.5, 52.1, 104.8, 119.5, 126.1, 126.8, 127.4 (2C), 128.1(2C), 130.1, 130.4, 132.0, 133.4, 136.6, 136.8, 138.6, 145.1, 194.0; HRMS (ESI) [M+1] calcd for $C_{24}H_{26}NO$:344.2014, found: 344.2012.
5. **1-(3-chloro-2-methylphenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4e):** Light pink solid; mp: 162-164°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.52 (s, 3H), 1.55 (s, 3H), 2.34 (s, 3H), 2.60 (d, J = 16.4 Hz, 1H), 2.85-2.87 (m, 2H), 2.90 (d, J = 2.8 Hz, 1H), 7.26 (s, 1H), 7.49 (d, J = 2.0Hz, 2H), 7.50-7.60 (m, 3H), 7.61-7.67 (m, 1H), 7.88-7.93 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 15.0, 27.9, 29.1, 35.6, 36.5, 52.0, 105.2, 119.9, 127.3 (2C), 128.3 (2C), 129.3 (2C), 130.1, 131.6, 133.6,135.0, 135.8, 136.7, 138.1, 144.8, 194.0; HRMS (ESI) [M+1] calcd for $C_{23}H_{23}NO$: 364.1468, found: 364.1455.
6. **6,6-dimethyl-1-(naphthalen-1-yl)-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4f):** Brown solid; mp: 162 – 164°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.02 (s, 6H), 2.13 (d, J = 16.4 Hz, 1H), 2.32 -2.42 (m, 3H), 6.91 (s, 1H), 7.01-7.36 (m, 5H), 7.46-7.49 (m, 2H), 7.50-7.56 (m, 3H), 7.92-7.95 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.0, 28.8, 35.5, 36.3, 52.1, 105.1, 119.8, 122.5, 125.2, 126.5, 126.8 (2C), 127.5 (2C), 127.7 (2C), 128.3 (2C), 129.3, 130.9, 131.8, 134.0, 134.2, 137.5, 146.1, 194.0; HRMS (ESI) [M+1] calcd for $C_{26}H_{24}NO$: 366.1858, found: 366.1850.
7. **1-cyclopropyl-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4g):** Off white solid; mp: 162-164°C; ; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.55-0.60 (m, 2H), 0.85-0.95 (m, 2H), 1.17 (s, 6H), 2.37 (s, 2H), 2.80 (s, 2H), 3.20-3.24 (m, 1H), 6.54 (s, 1H), 7.31-7.33 (m, 1H), 7.36-7.40 (m, 2H), 7.45-7.47 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 9.2 (2C), 27.0, 28.7 (2C), 35.5, 37.2, 51.9, 104.6, 119.0, 127.0, 128.1 (2C), 128.3 (2C), 132.8, 137.0, 146.0, 193.6; HRMS (ESI) [M+1] calcd for $C_{19}H_{22}NO$: 280.1701, found: 280.1707.
8. **1-butyl-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4h):** Faint yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.77 (t, J = 7.6 Hz, 3H), 1.10-1.19 (m, 2H), 1.25 (s, 6H), 1.46-1.52 (m, 2H), 2.36 (s, 2H), 2.67 (s, 2H), 3.83 (t, J = 7.6 Hz, 2H), 6.53 (s, 1H), 7.34-7.42 (m, 3H), 7.42-7.49 (m, 1H), 7.58-7.62 (m,1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.5, 19.6, 28.8 (2C), 35.5, 36.5, 40.8, 44.2, 51.9, 105.4, 119.2, 127.7, 128.4 (2C), 129.2 (2C), 130.1, 133.6, 143.3, 193.7 ;HRMS (ESI) [M+1] calcd for $C_{20}H_{26}NO$: 296.2014, found: 296.2000.
9. **1-(4-fluorophenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4i):** Pale yellow solid; mp: 198-200°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 6H), 2.42 (s, 2H), 2.49 (s, 2H), 6.77 (s, 1H), 7.04-7.07 (m, 2H), 7.09-7.12 (m, 4H), 7.17-7.19 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.6 (2C), 35.5, 37.0, 52.0, 105.6, 116.2 & 116.4 (d,^{2}J C,F= 23.0 Hz) (2C), 119.9, 127.0 (2C), 128.2 (3C), 129.3 &129.4 (d,^{3}J C,F= 9.0 Hz) (2C), 131.6, 133.6, 136.3, 144.6, 160.7 & 163 (d,^{1}J C,F=247.0 Hz), 193.9; HRMS (ESI) [M+1] calcd for $C_{22}H_{21}NOF$: 334.1607, found: 334.1600.
10. **2-(4-methoxyphenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4j):** Brown gum; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 6H), 2.42 (s, 2H), 2.49 (s, 2H), 3.69 (s, 3H), 6.77 (s, 1H), 7.04-7.07 (m, 2H), 7.09-7.12 (m, 3H), 7.17-7.19 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.4, 28.7, 35.4, 36.4, 52.1, 55.5, 104.8, 112.1, 119.6, 120.8, 126.4, 126.7, 127.7 (2C), 127.9(2C), 129.6, 130.1, 132.2, 136.7, 145.8, 155.1, 194.0; HRMS (ESI) [M+1] calcd for $C_{23}H_{24}NO_2$: 346.1807,found: 346.1812.
11. **4-(6,6-dimethyl-4-oxo-1-phenyl-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4k):** Pale yellow solid; mp: 204-206°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 6H), 2.43 9s, 2H), 2.51 (s, 2H), 6.91 (s, 1H), 7.11-7.15 (m, 4H), 7.42-7.46 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.5 (2C), 35.5, 36.9, 51.9, 107.7, 118.6, 120.2, 127.5 (2C), 127.9 (2C), 128.8, 129.7 (2C), 131.9 (2C), 132.2, 134.1, 136.2, 137.1, 146.1, 194.0; HRMS (ESI) [M+1] calcd for $C_{23}H_{21}N_2O$:341.1654, found: 341.1644.
12. **4-(6,6-dimethyl-4-oxo-1-(o-tolyl)-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4l):** Brown solid; mp: 170-172°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.07 (s, 3H), 1.11 (s, 3H), 1.85 (s, 3H), 2.16 (d, J = 16.8 Hz, 1H), 2.41-2.50 (m, 3H), 6.96 (s, 1H), 7.13-7.16 (m, 2H), 7.23 (d, J = 1.2 Hz, 1H), 7.28 (d, J = 0.8 Hz, 1H), 7.30-7.37 (m, 1H), 7.39 (d, J = 1.6 Hz, 1H), 7.40-7.43 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 17.2, 27.8, 29.1, 35.5, 36.5, 52.05, 107.1, 110.0, 118.7, 120.1, 127.0 (2C), 127.3, 128.3, 129.7, 131.5, 132.1 (2C), 134.2, 134.2, 135.8, 136.4, 146.1, 193.7; HRMS (ESI) [M+1] calcd for $C_{24}H_{23}N_2O$: 355.1810, found: 355.1805.
13. **4-(1-(2,3-dimethylphenyl)-6,6-dimethyl-4-oxo-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4m):** Brown solid; mp: 173-175°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.36 (s, 3H), 1.40 (s, 3H), 2.02 (s, 3H), 2.46 (d, J = 16.8 Hz, 1H), 2.59 (s, 3H), 2.70-2.77 (m, 3H), 7.36 (s, 1H), 7.38-7.44 (m, 2H), 7.50-7.52 (m, 1H), 7.54-7.55 (m, 1H), 7. 57-7.59 (m, 1H) 7.69-7.72 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 13.8, 20.3, 27.9, 29.0, 35.5, 36.4, 52.0, 107.0, 109.9, 118.7, 120.0, 125.9, 126.5, 127.0 (2C), 131.0 132.0 (2C),

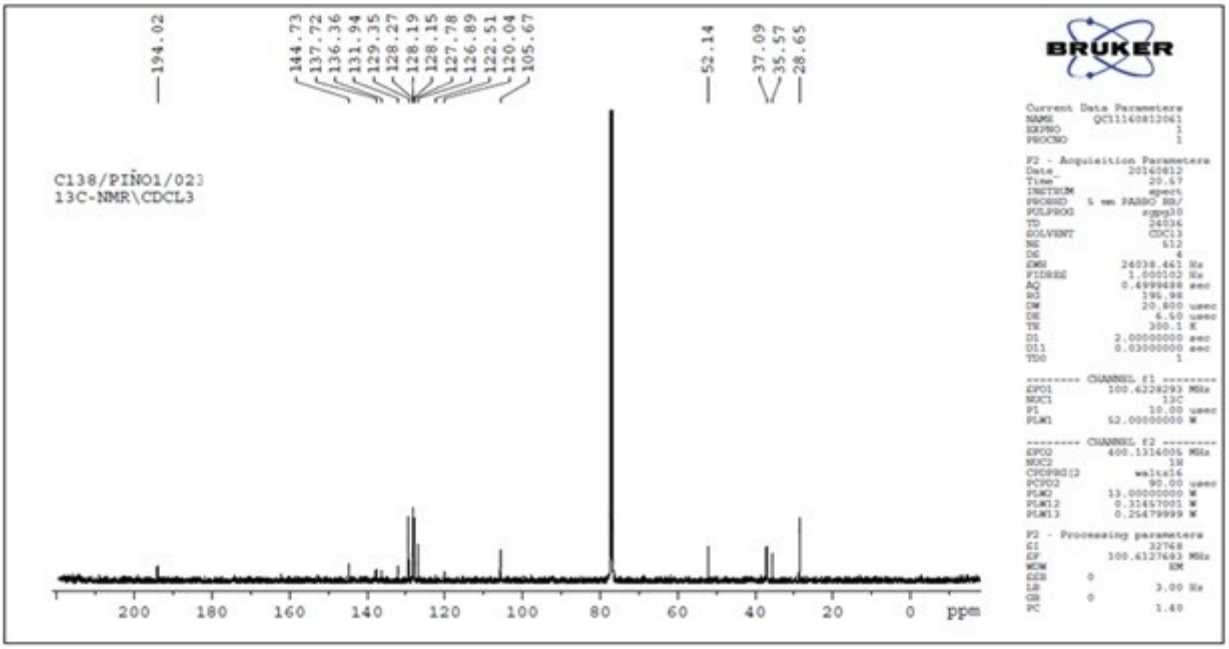
134.3, 134.5, 136.3, 136.4, 139.1, 146.3, 193.8; HRMS (ESI) [M+1] calcd for $C_{25}H_{25}N_2O$:369.1967, found: 369.1951.

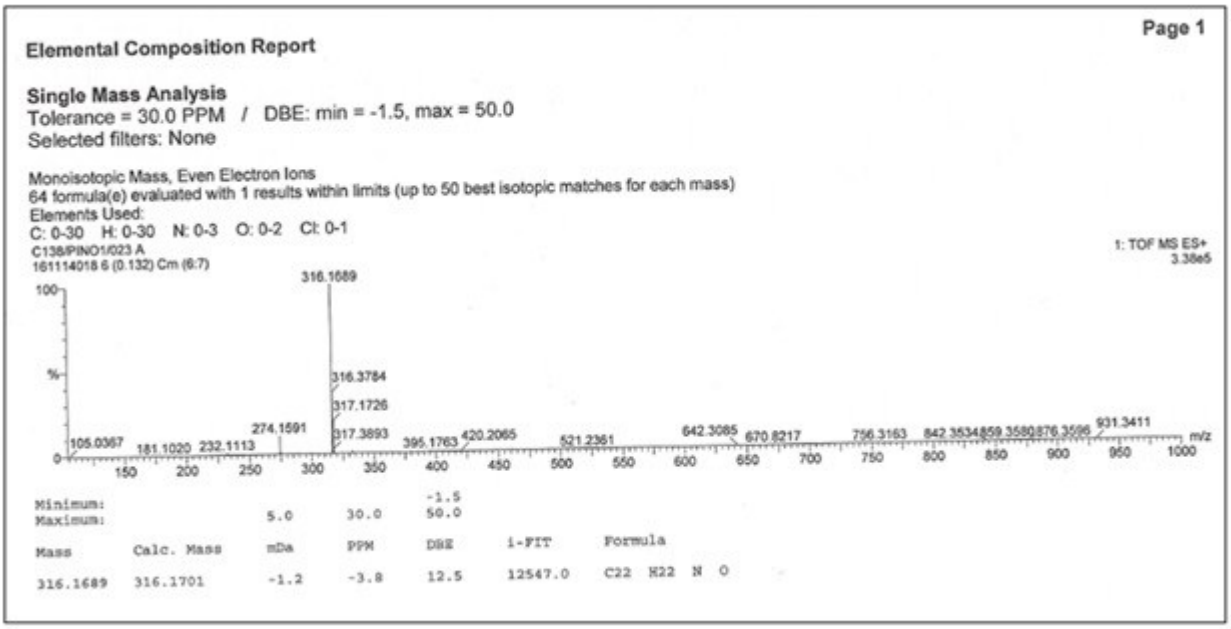
14. **2-(4-chlorophenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4n):** Brown solid; mp:149-151°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.09 (s, 6H), 2.41 (s, 2H), 2.50 (s, 2H), 6.77 (s, 1H), 6.96-6.98 (d, J = 8.4 Hz, 2H), 7.11-7.14 (m, 4H), 7.41-7.42 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 28.6 (2C), 35.5, 37.0, 52.0, 105.9, 120.2, 122.1, 127.1, 128.2 (2C), 128.3, 129.2 (2C), 131.5 (2C), 132.5 (2C), 136.2, 136.6, 144.4, 193.8;HRMS (ESI) ([M] +1) calcd for $C_{22}H_{21}NOCl$: 350.1312, found: 350.1300.

S5. ^{1}H NMR, ^{13}C NMR, MS spectra of compounds (2a-2l):

6,6-dimethyl-1,2-diphenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4a):







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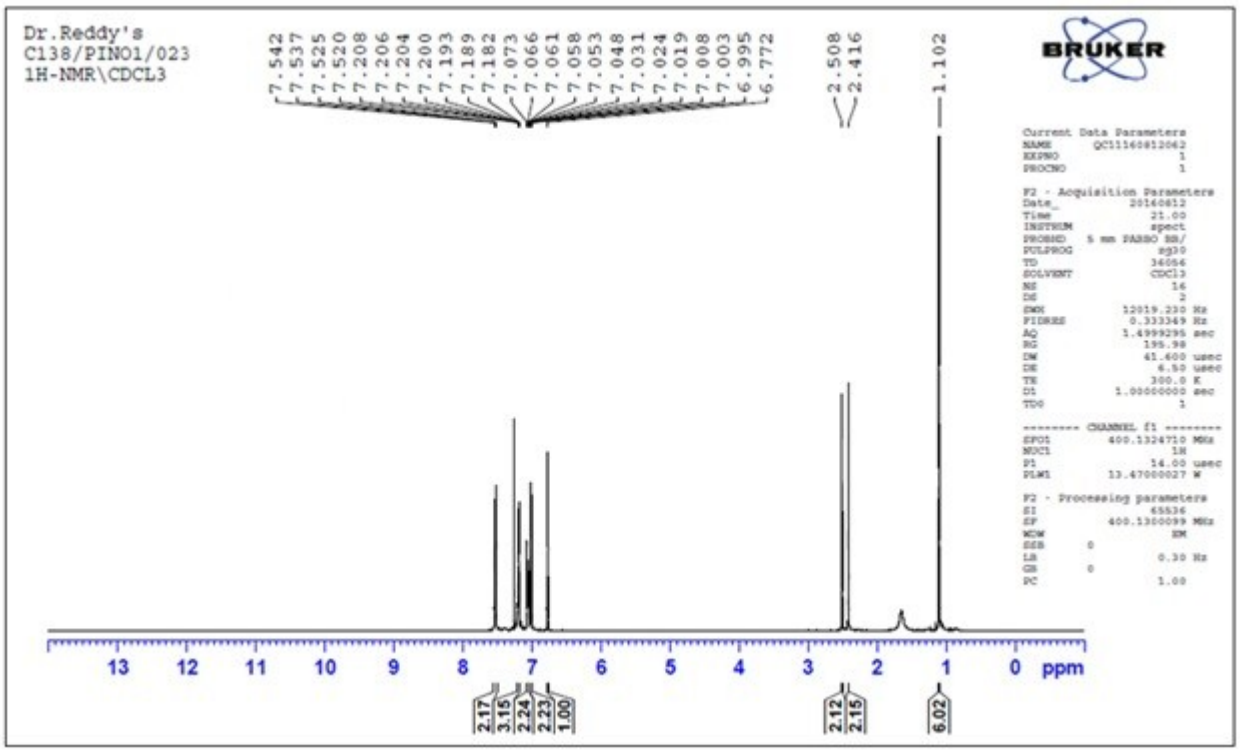

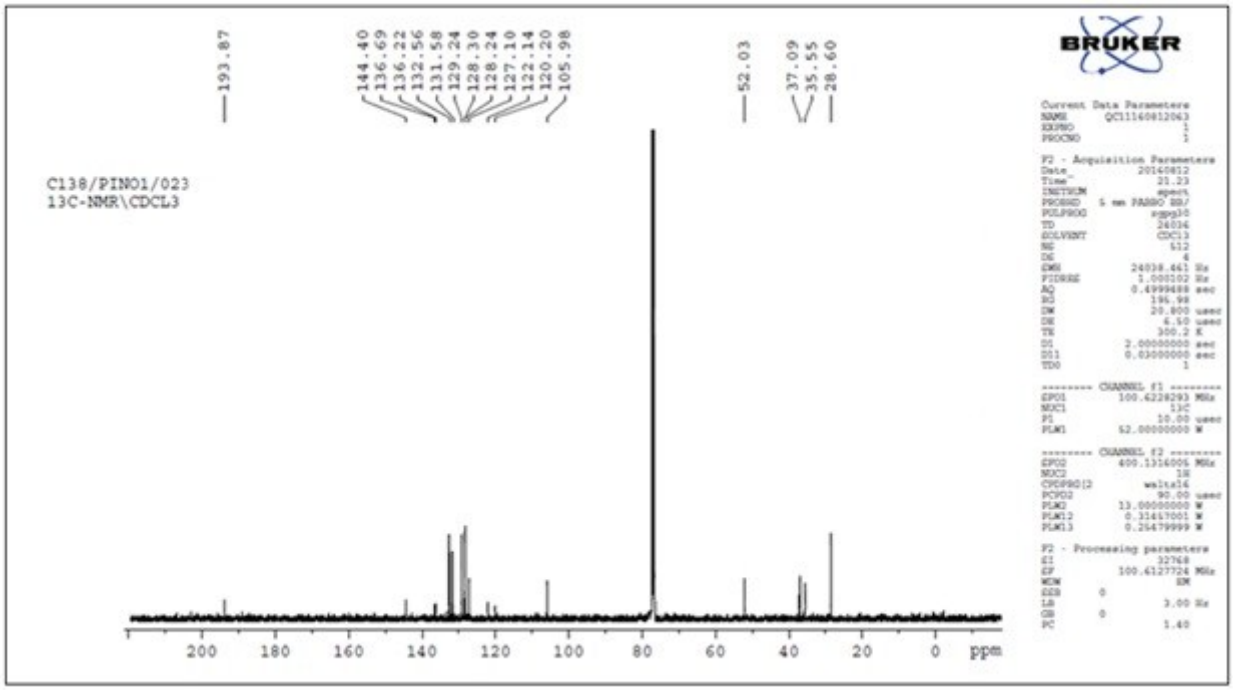

Elemental Composition Report Page 1

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Selected filters: None

Monoisotopic Mass, Even Electron Ions
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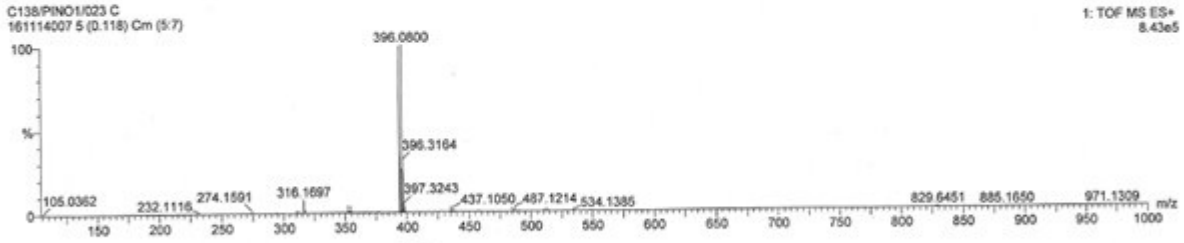

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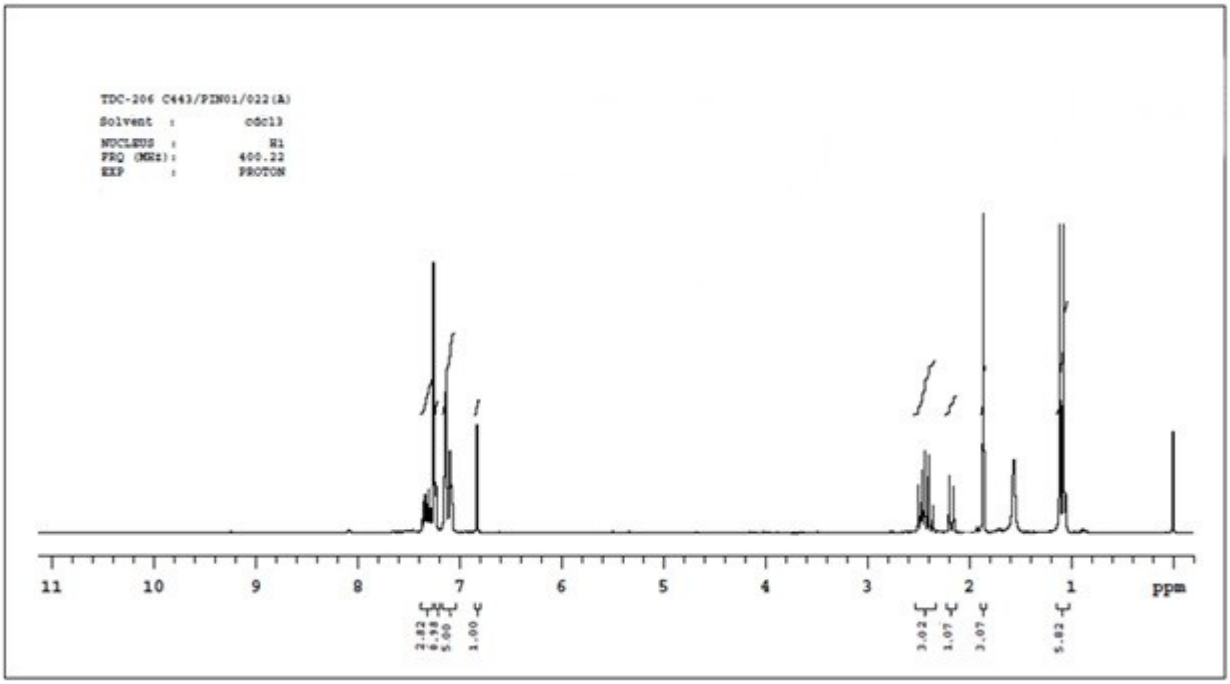

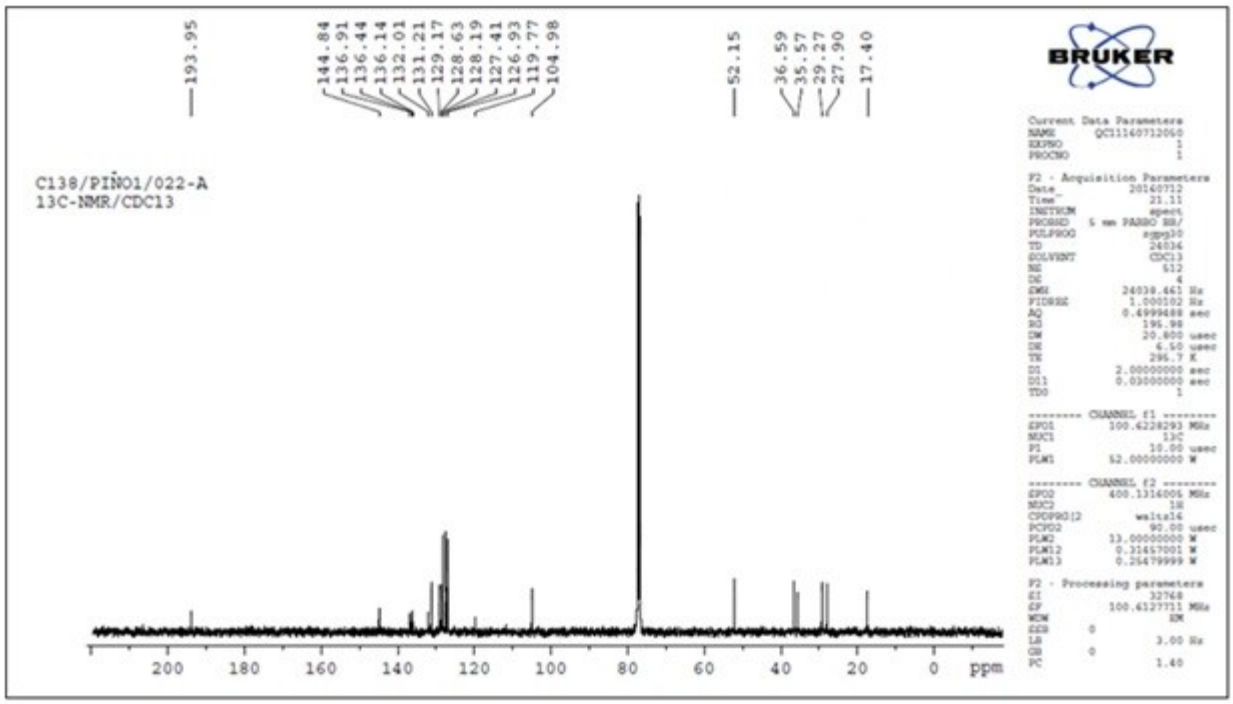

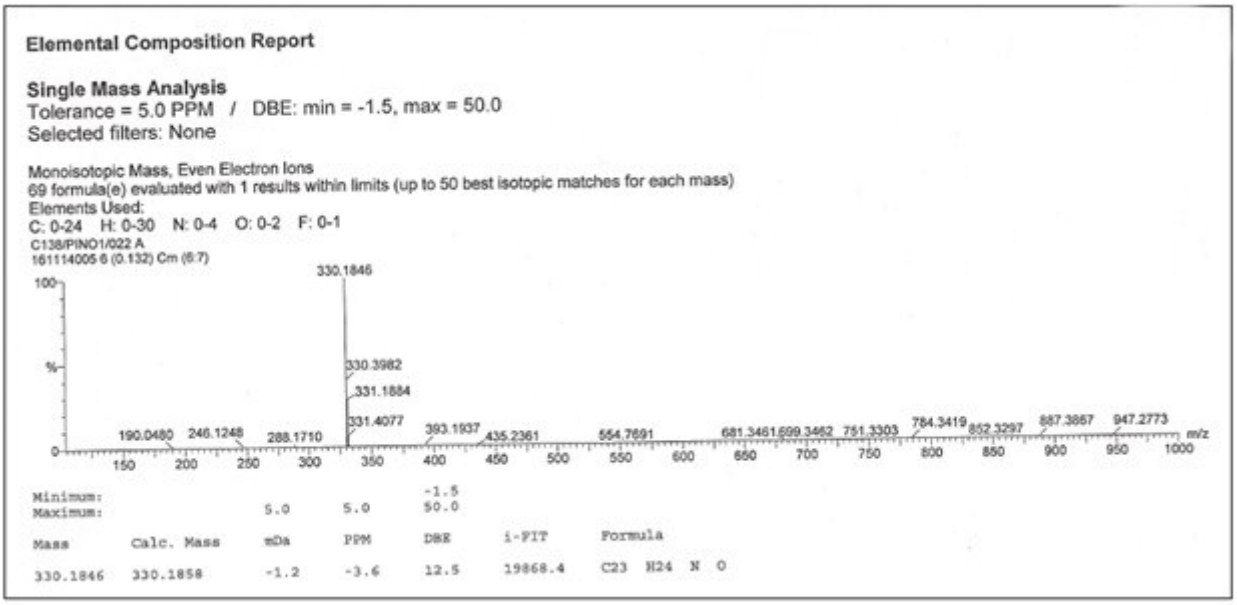

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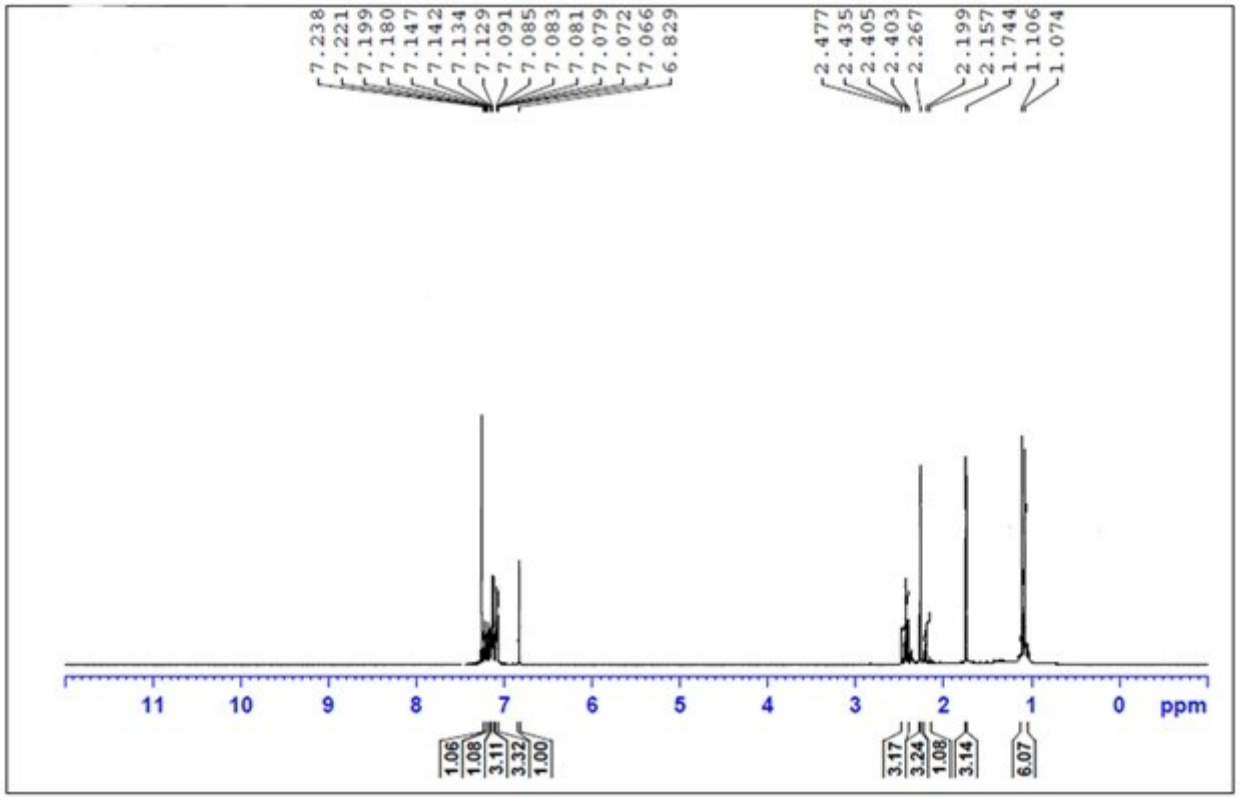

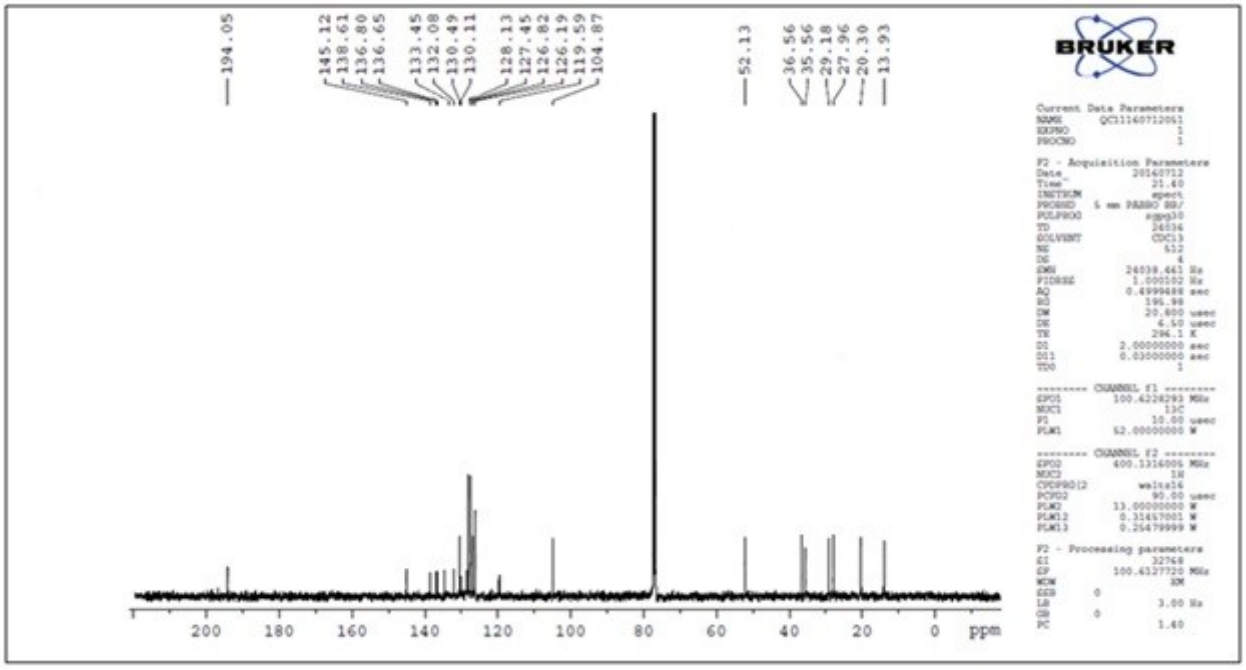

BRUKER

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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
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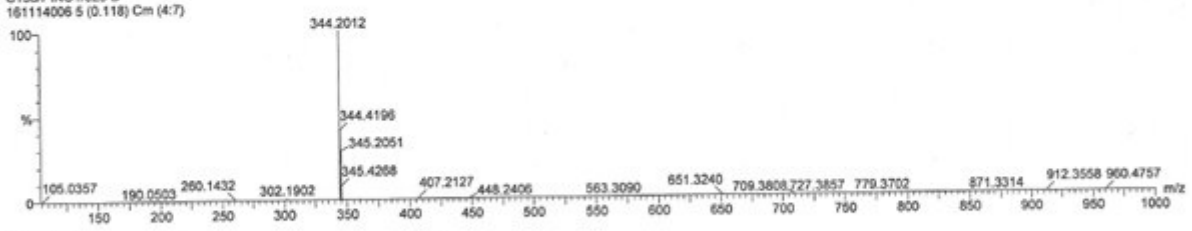

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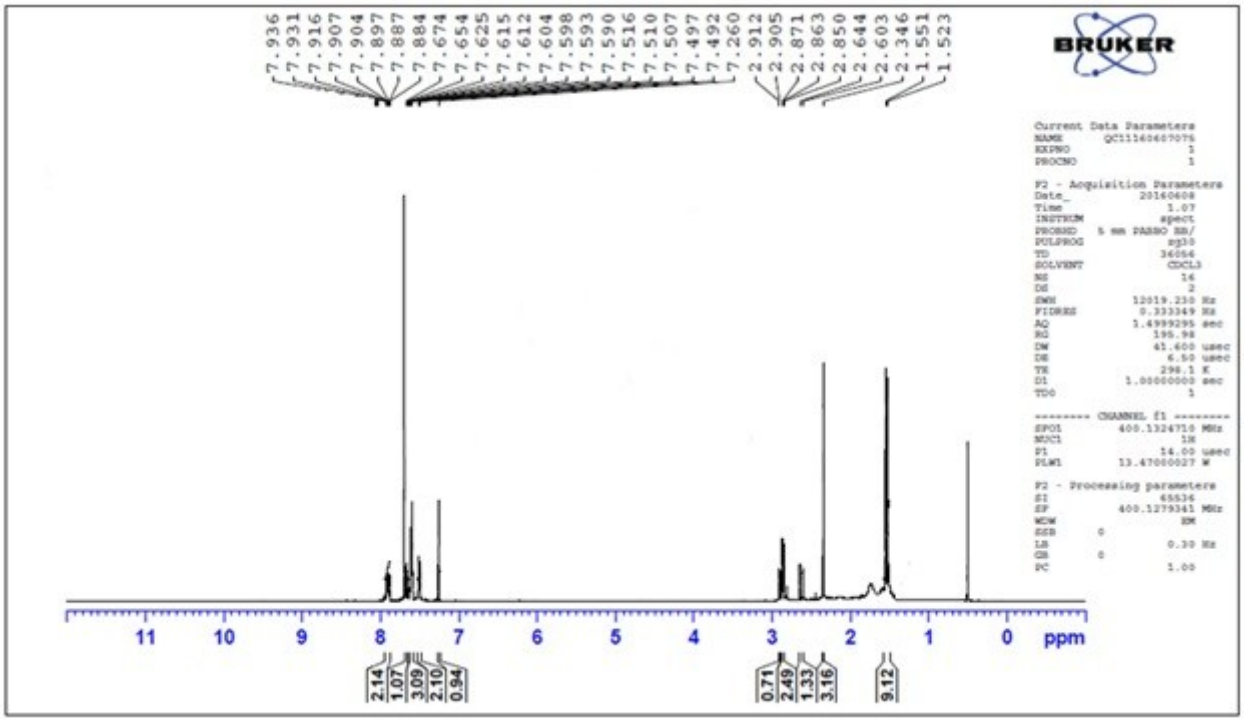
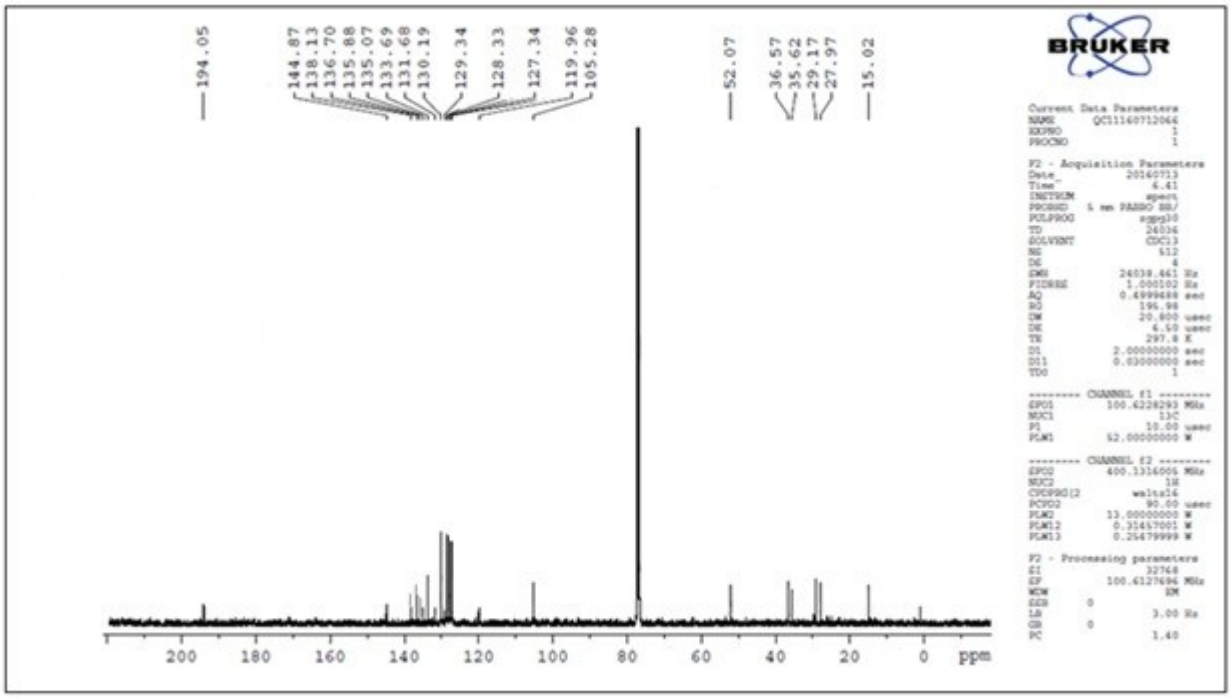
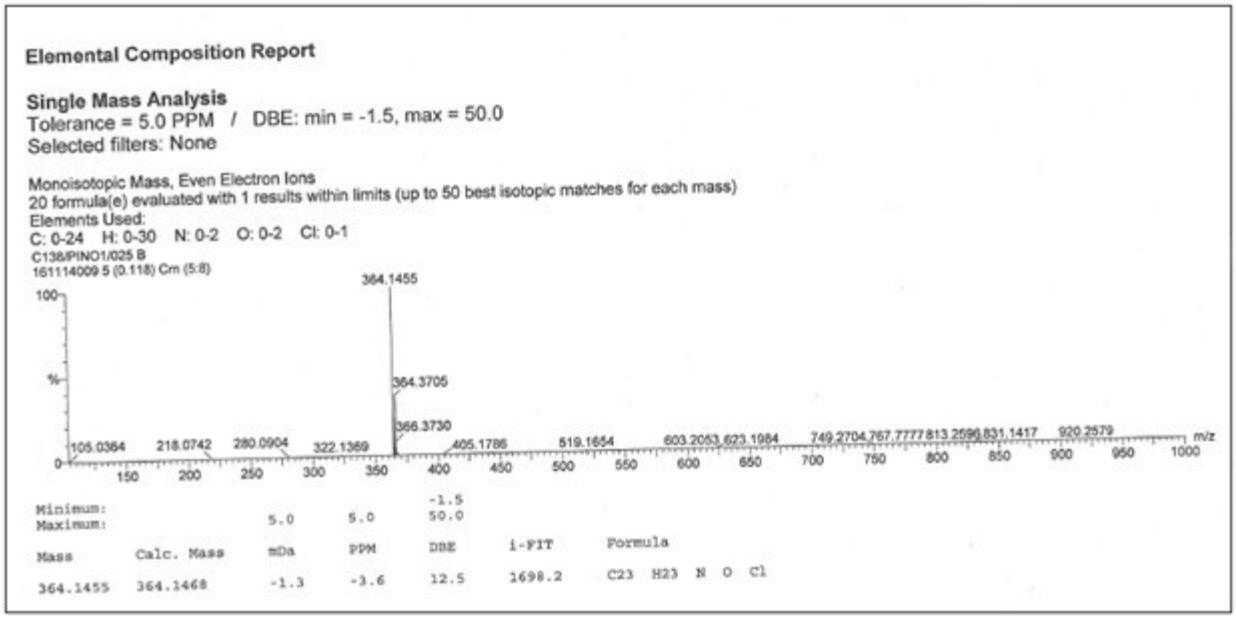
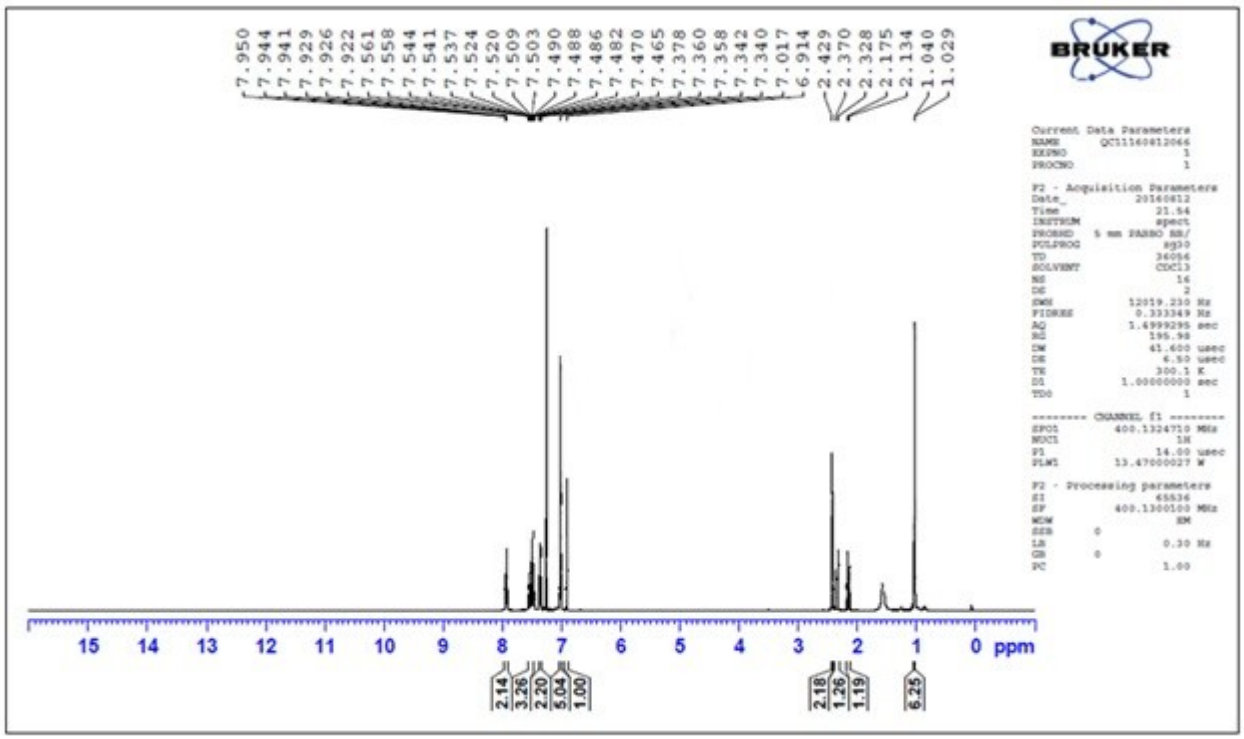
1-(3-chloro-2-methylphenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4e):

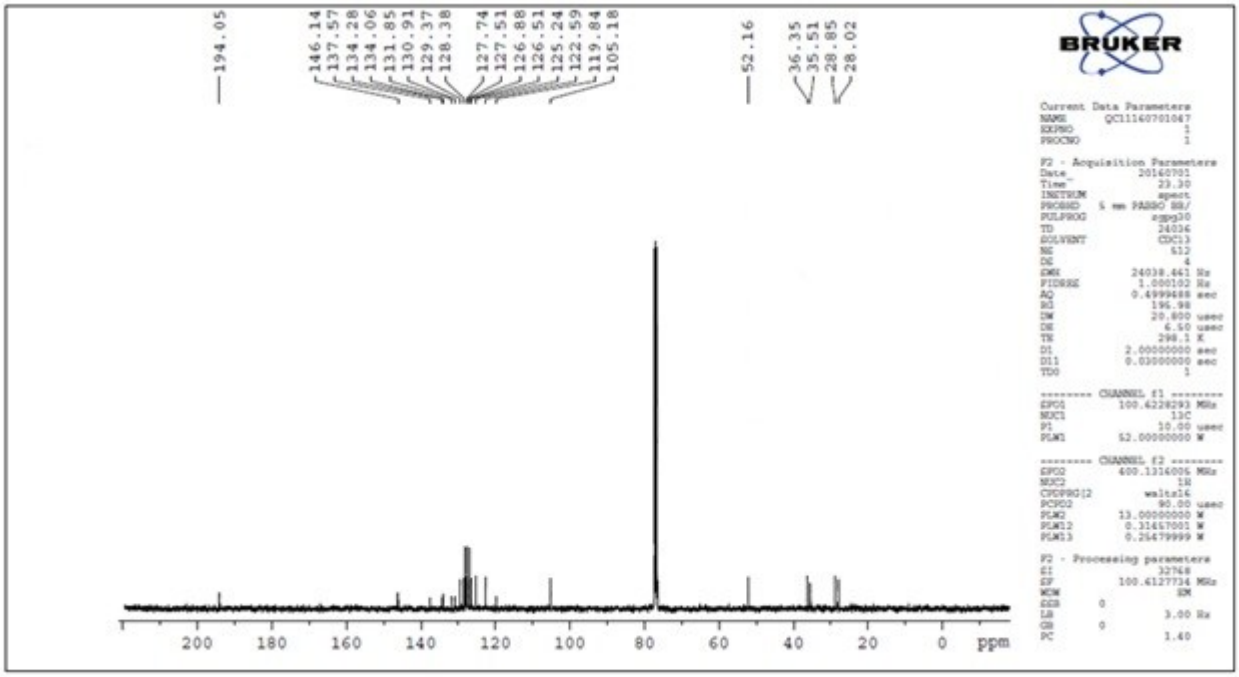






6,6-dimethyl-1-(naphthalen-1-yl)-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4f):



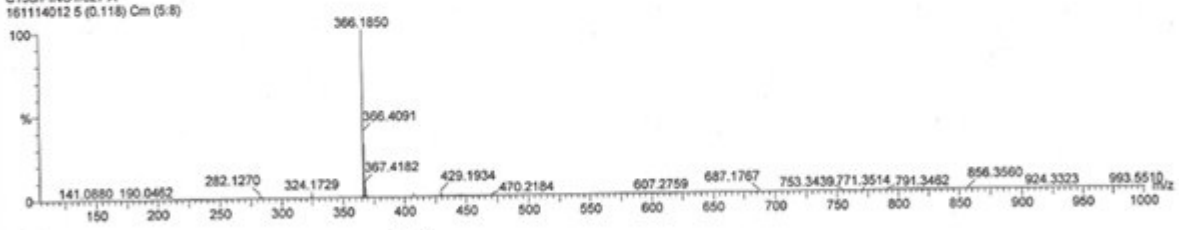


Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

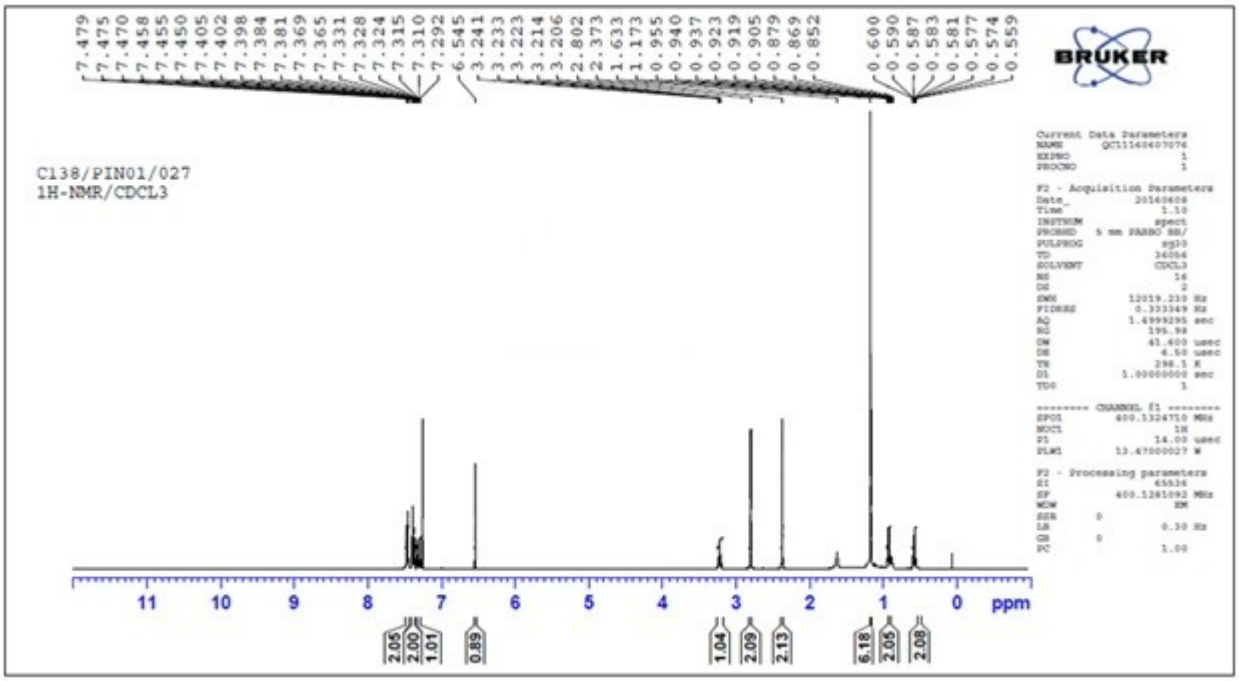
Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-2

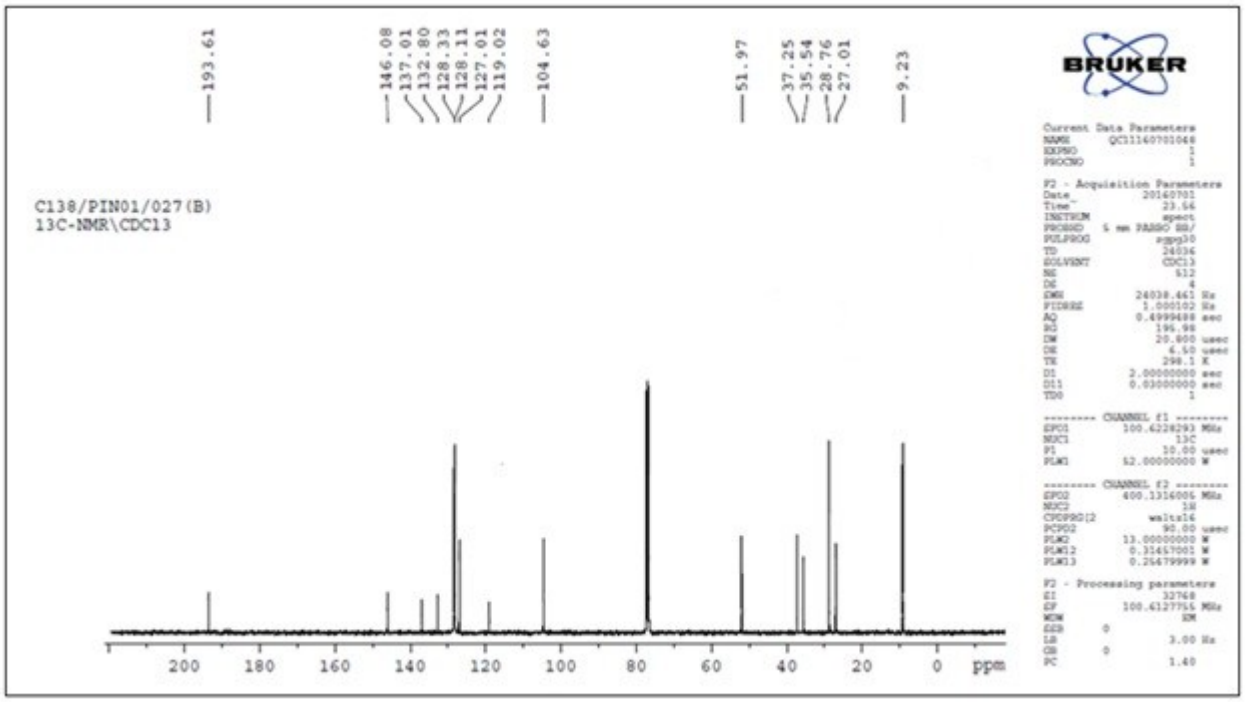
C138/PINO1/027 A
161114012 5 (0.118) Cm (5:8)

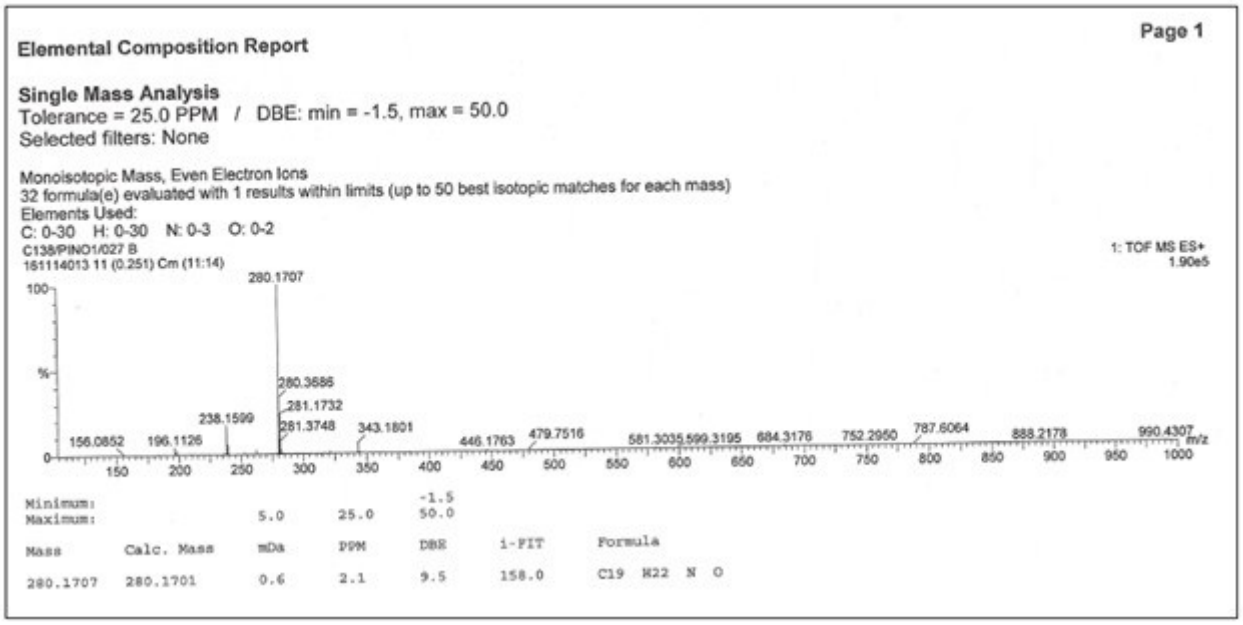


Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
366.1850	366.1858	-0.8	-2.2	15.5	1358.1	C26 H24 N O

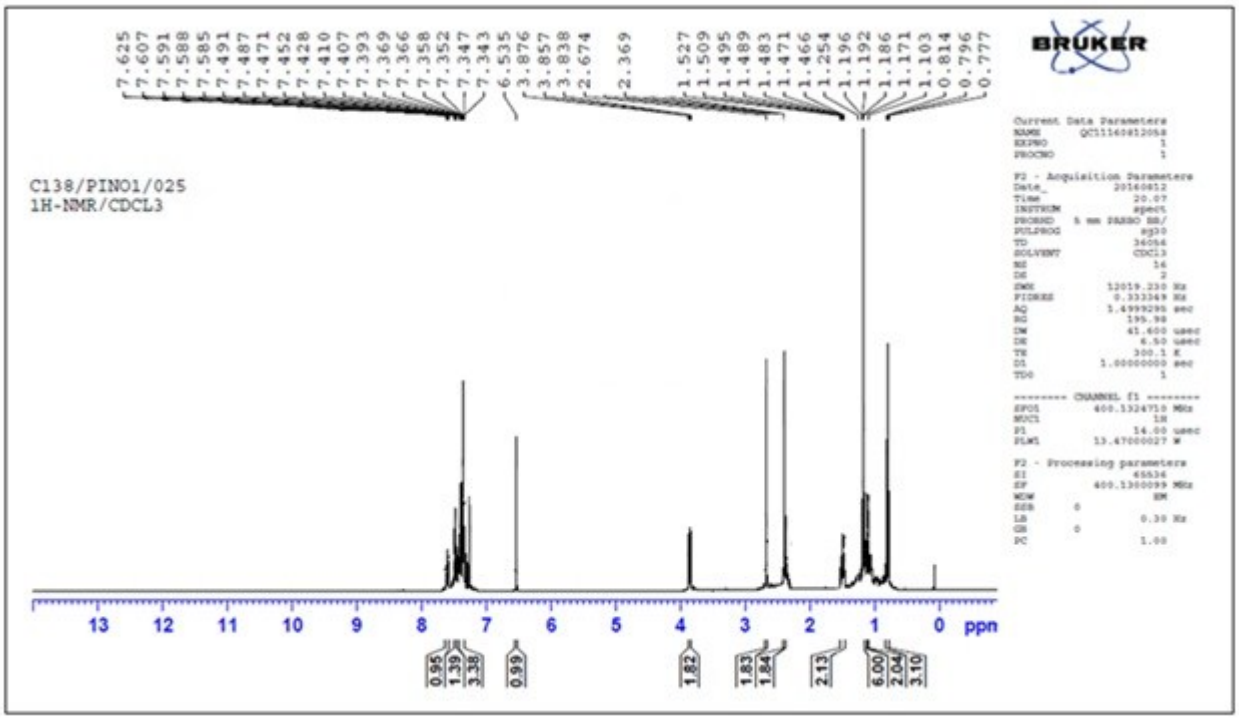
1-cyclopropyl-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4g):

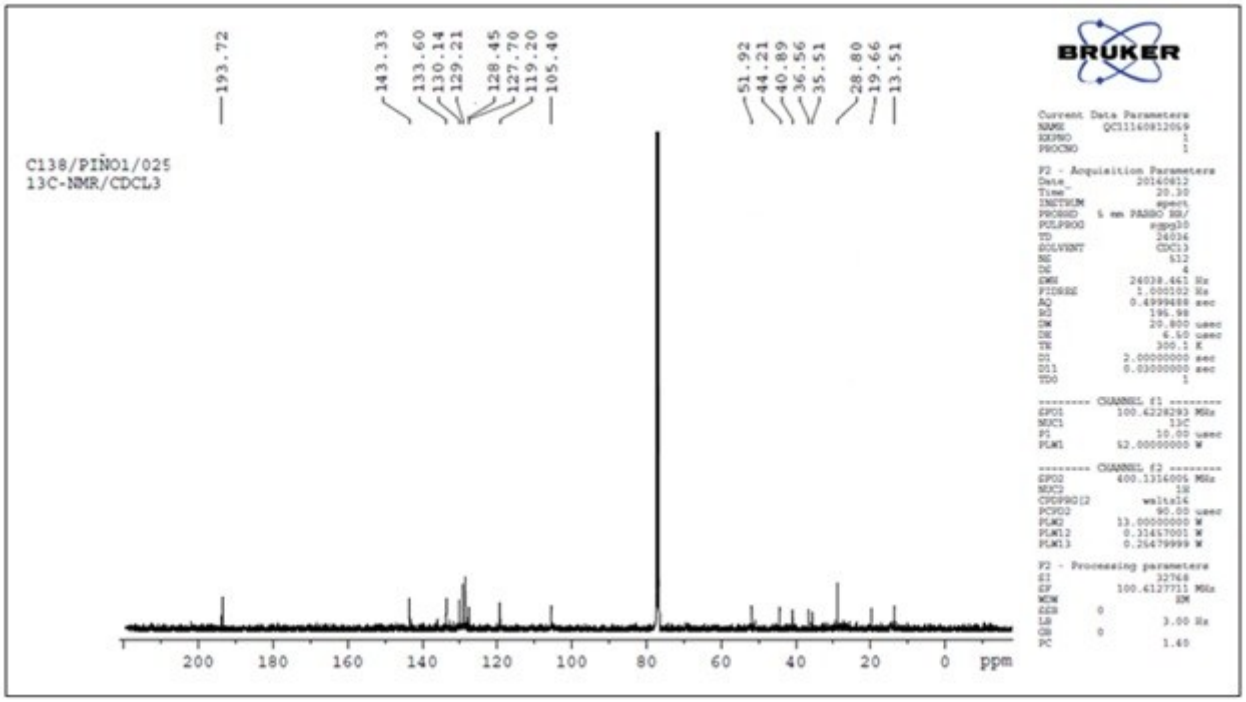


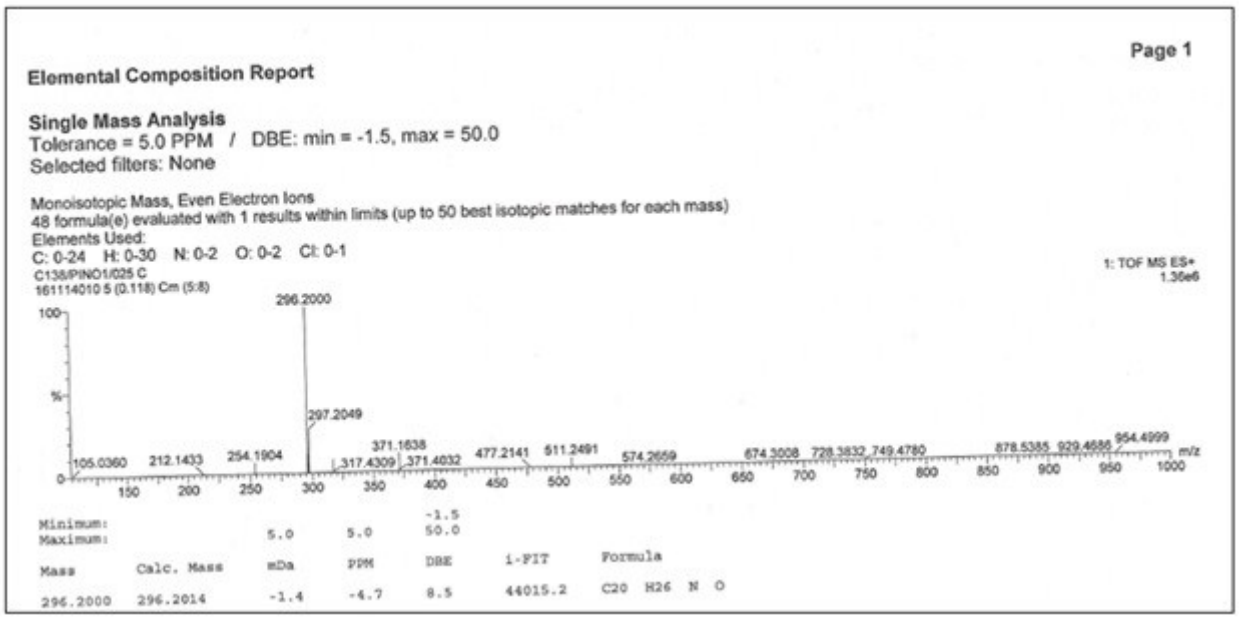




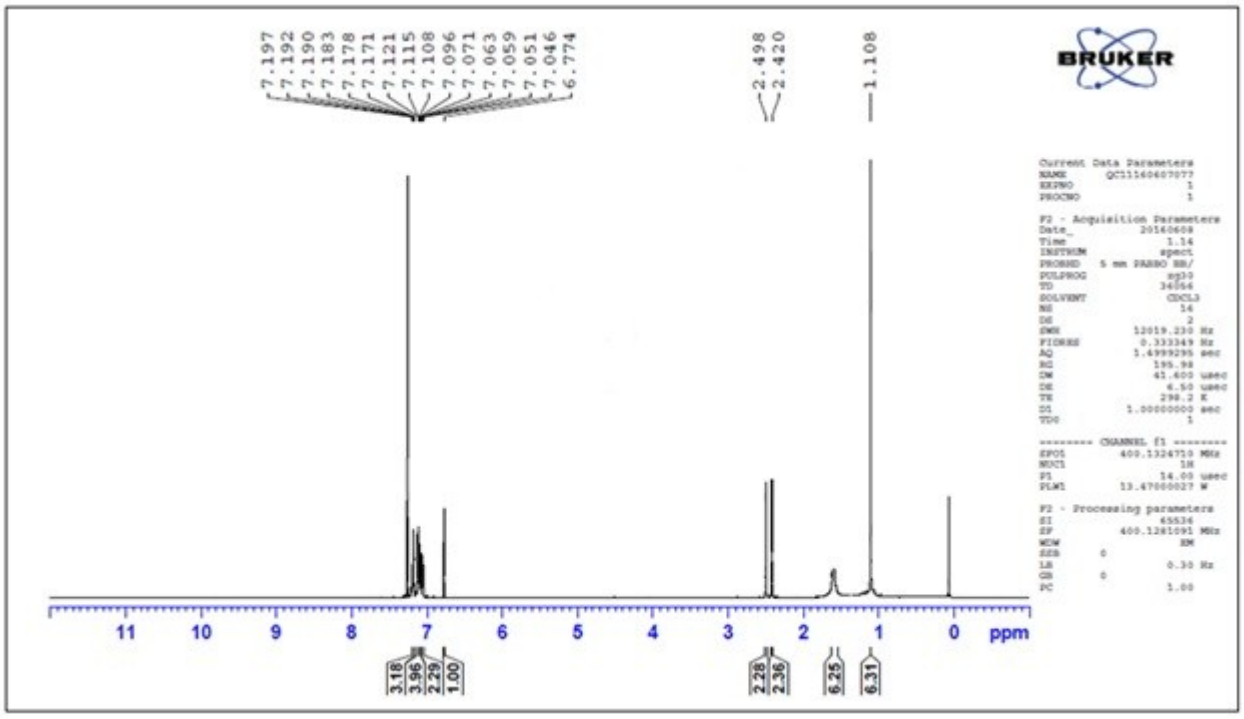
1-butyl-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4h):

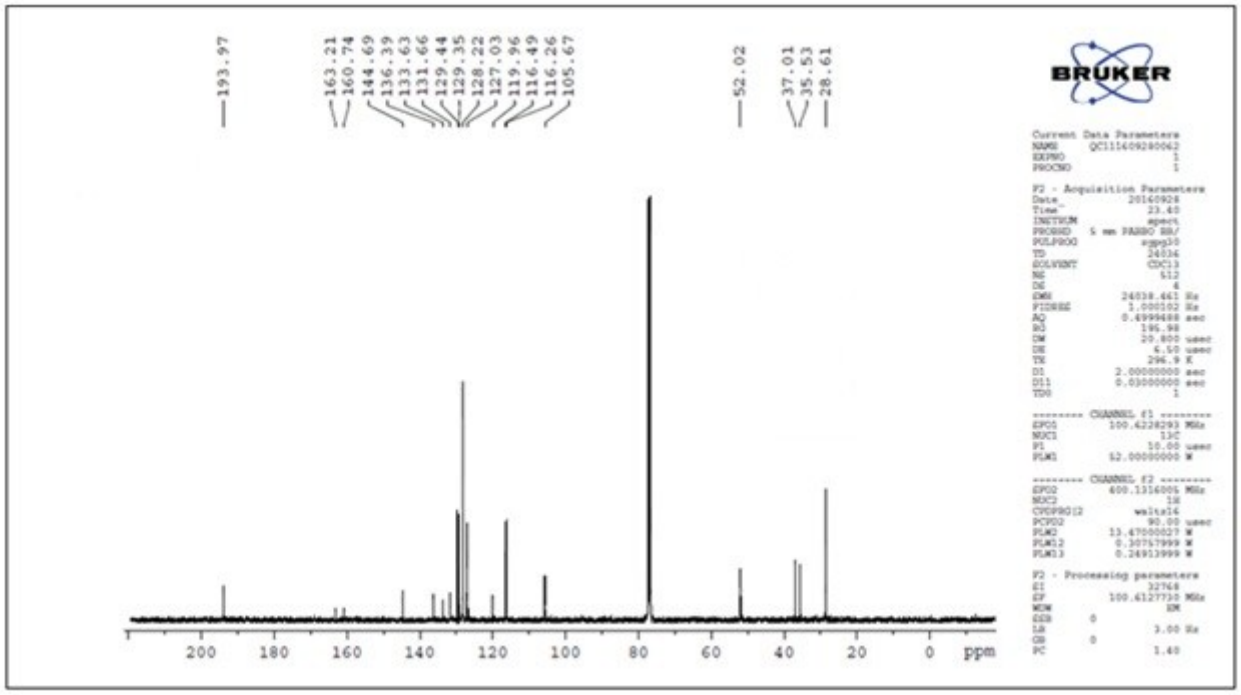


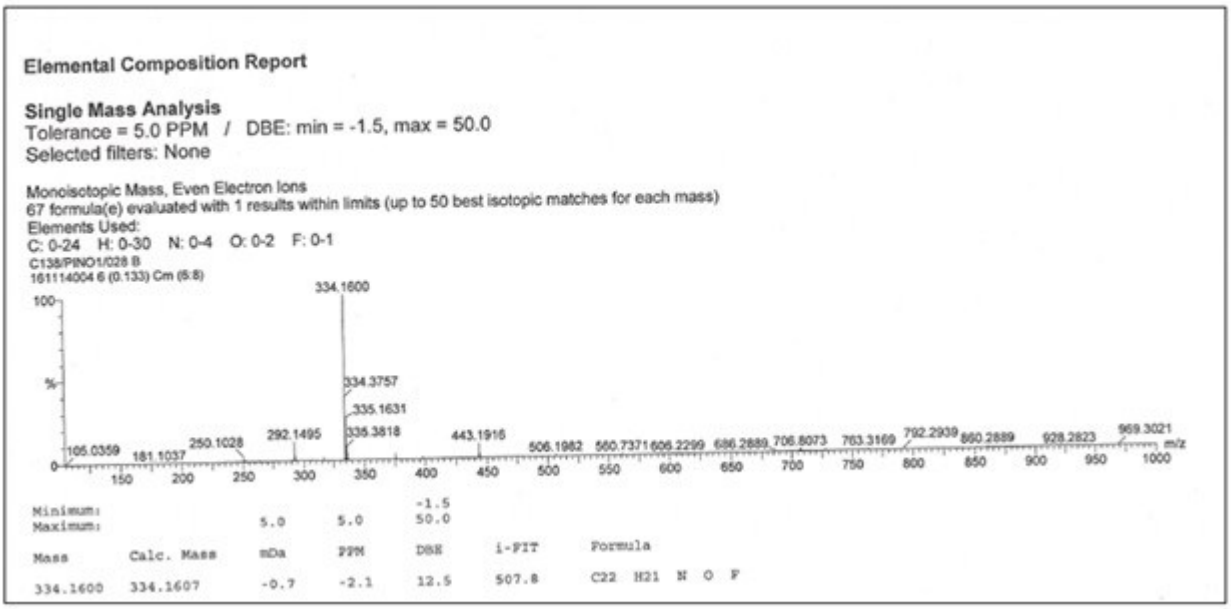

193.72
143.33
133.60
130.14
129.21
128.45
127.70
119.20
105.40
51.92
44.21
40.89
36.56
35.51
28.80
19.66
13.51
C138/PIÑO1/025
13C-NMR/CDCL3
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER


Page 1
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None
Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-30 N: 0-2 O: 0-2 Cl: 0-1
C138/PINO1/025 C
161114010 5 (0.116) Cm (5:8)
1: TOF MS ES+
1.36e6
296.2000
297.2049
105.0360
212.1433
254.1904
317.4309
371.1638
371.4032
477.2141
511.2491
574.2659
674.3008
728.3832
749.4780
878.5385
929.4686
954.4999
m/z
Minimum:
Maximum:
5.0
5.0
-1.5
50.0
Mass
Calc. Mass
mDa
PPM
DBE
i-FIT
Formula
296.2000
296.2014
-1.4
-4.7
8.5
44015.2
C20 H26 N O

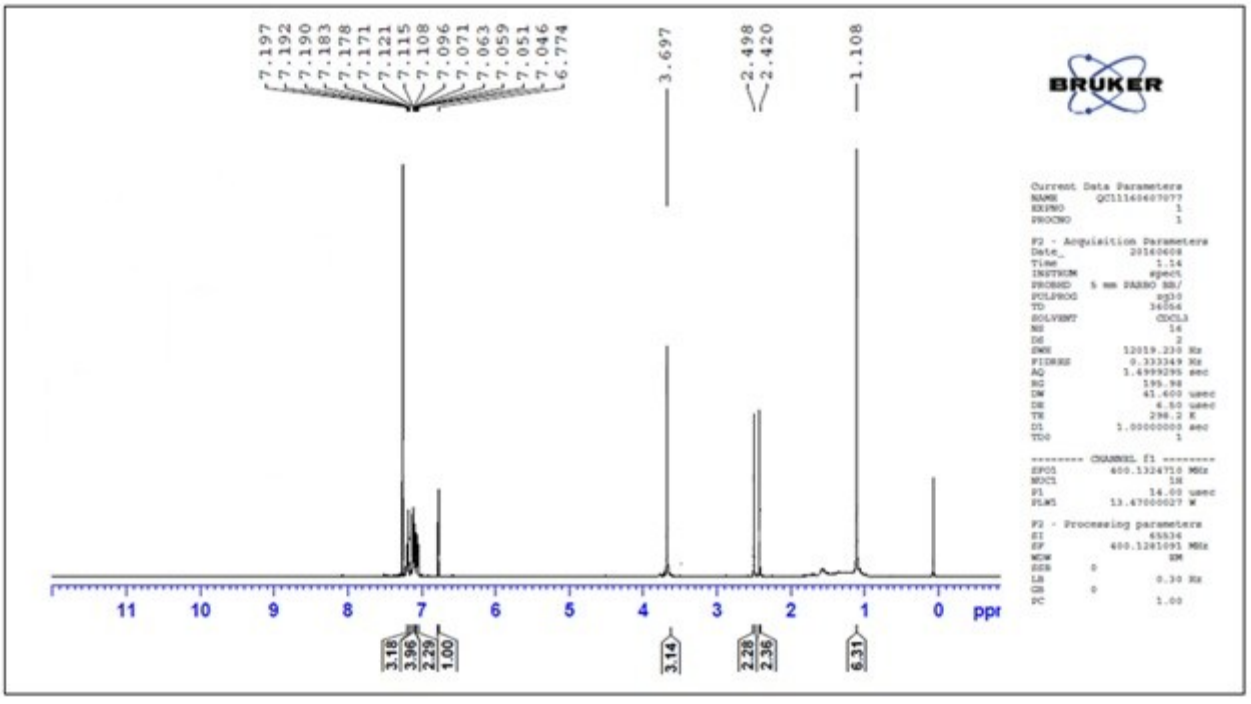
1-(4-fluorophenyl)-6,6-dimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4i):

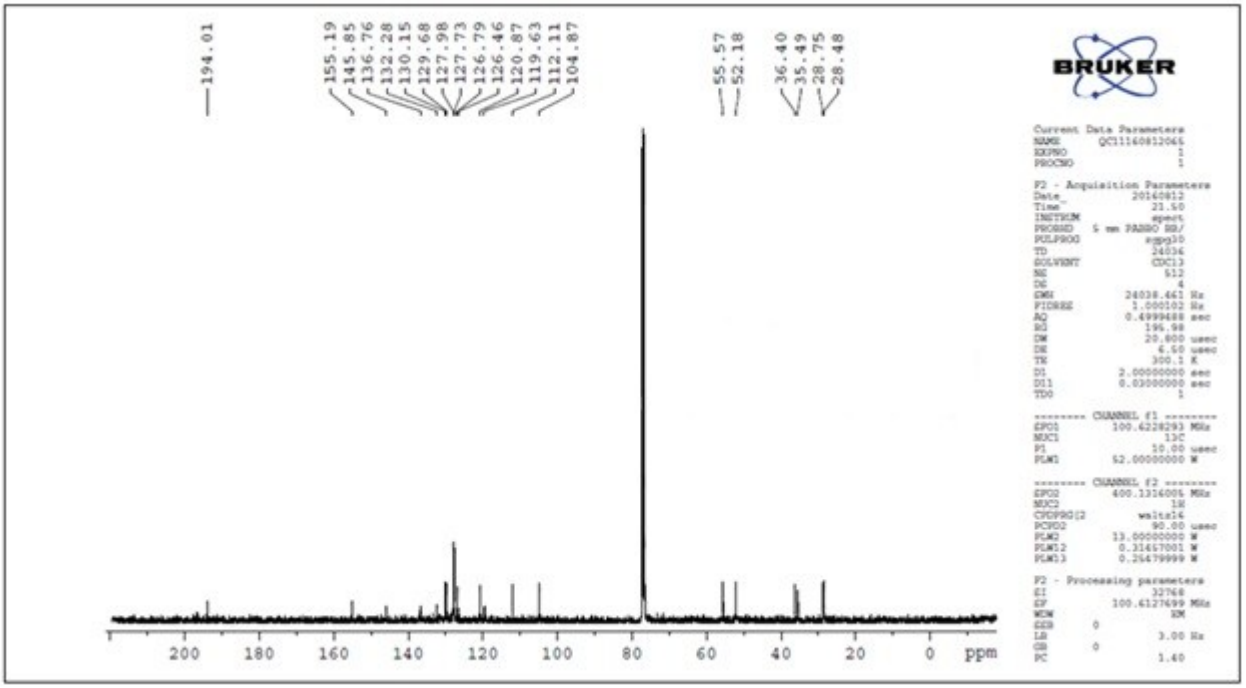






2-(4-methoxyphenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4j):



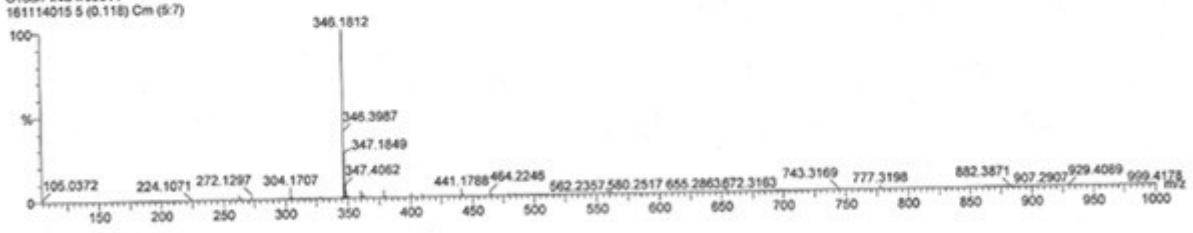


Elemental Composition Report

Single Mass Analysis
Tolerance = 25.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

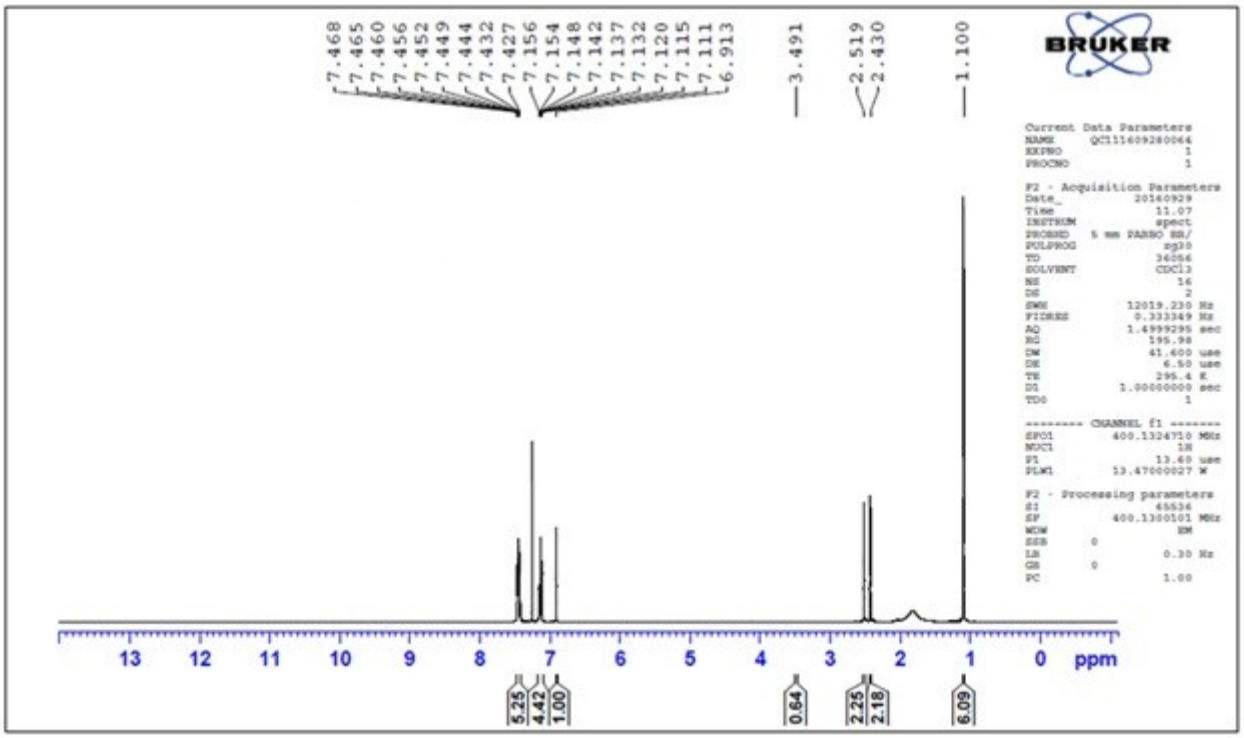
Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-2

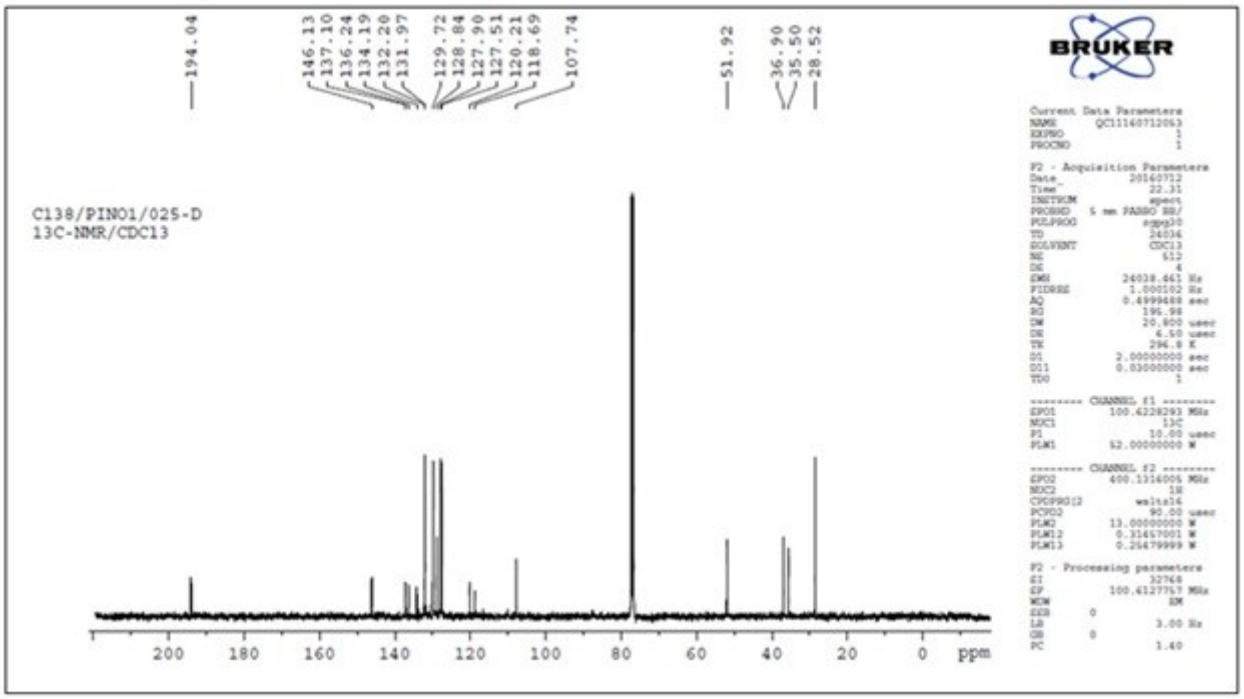
C138/PINO1/030 A
161114015 5 (0.118) Cm (5:7)

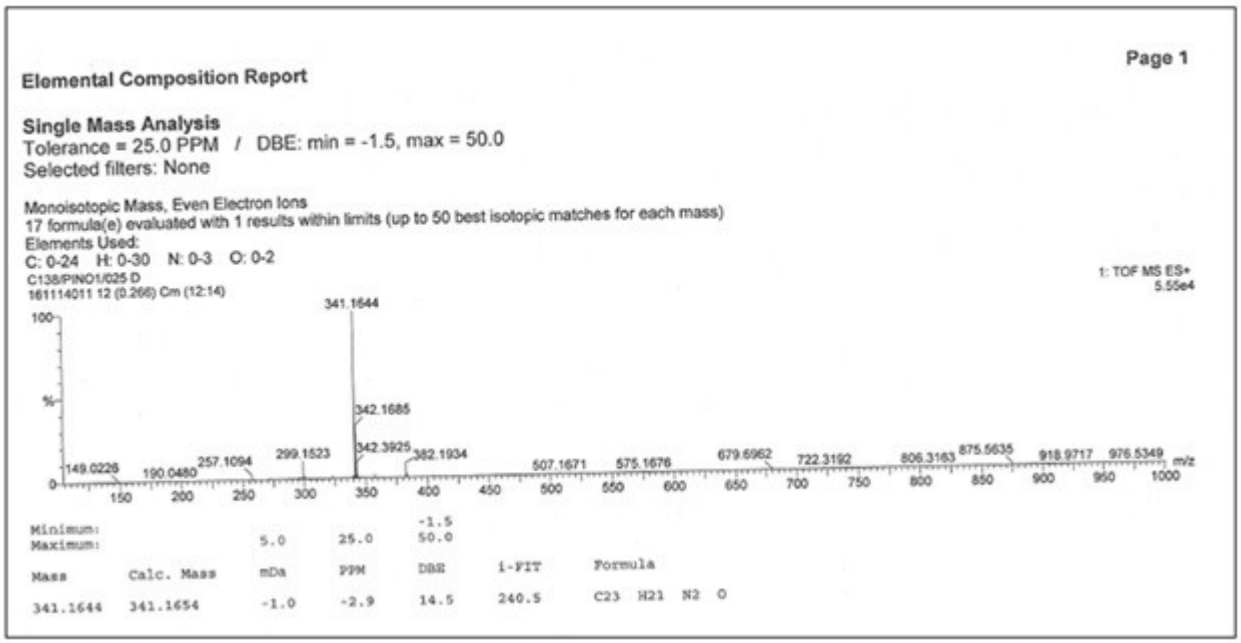


Minimum:				-1.5		
Maximum:		5.0	25.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.1812	346.1807	0.5	1.4	12.5	798.4	C23 H24 N O2

4-(6,6-dimethyl-4-oxo-1-phenyl-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4k):







Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 25.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

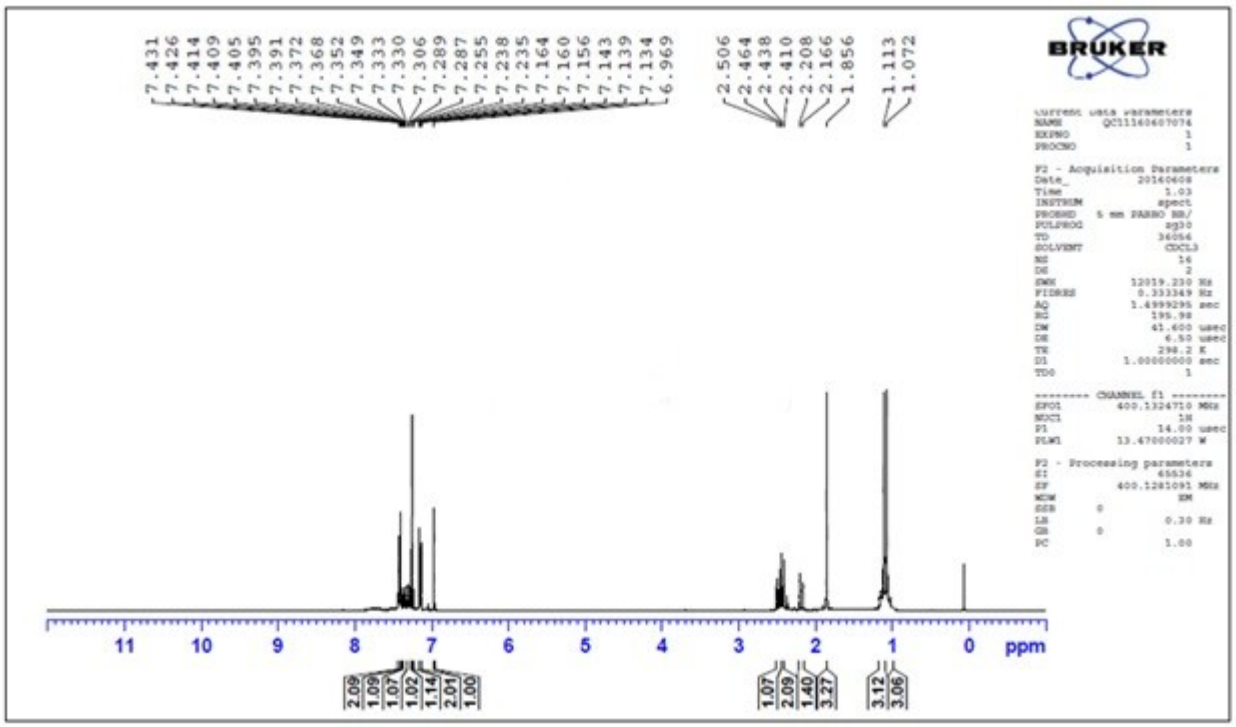
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-30 N: 0-3 O: 0-2

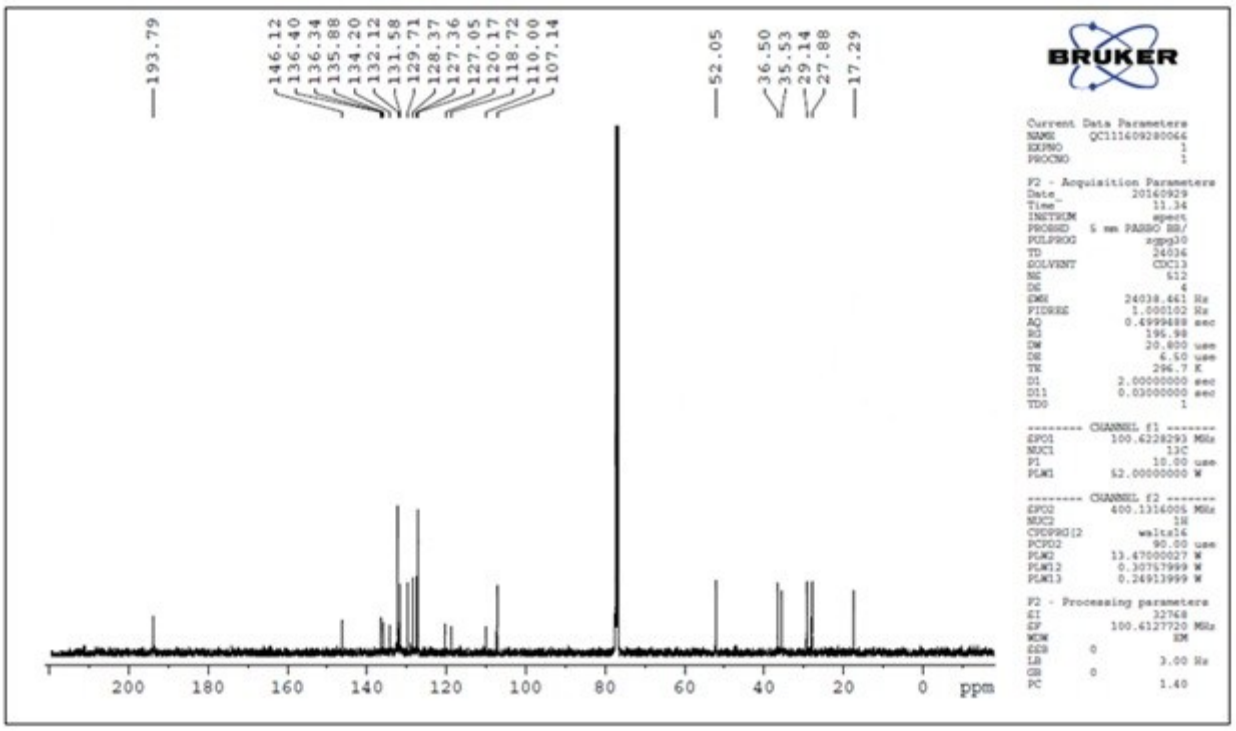
C138/PINO1/025 D
161114011 12 (0.266) Cm (12:14)

1: TOF MS ES+
5.55e4

Minimum:		5.0	25.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
341.1644	341.1654	-1.0	-2.9	14.5	240.5	C23 H21 N2 O

4-(6,6-dimethyl-4-oxo-1-(o-tolyl)-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4l):



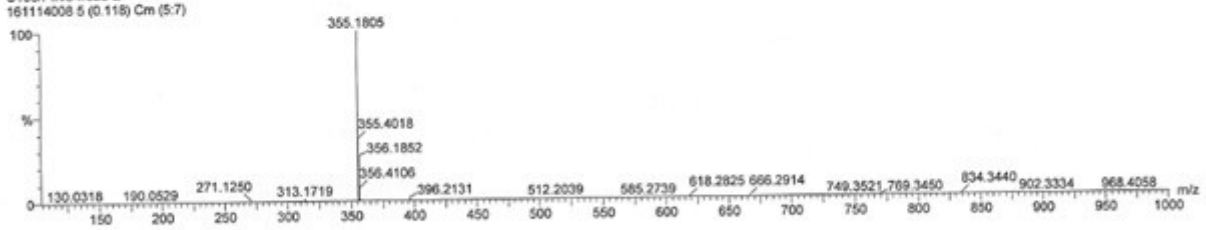


Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

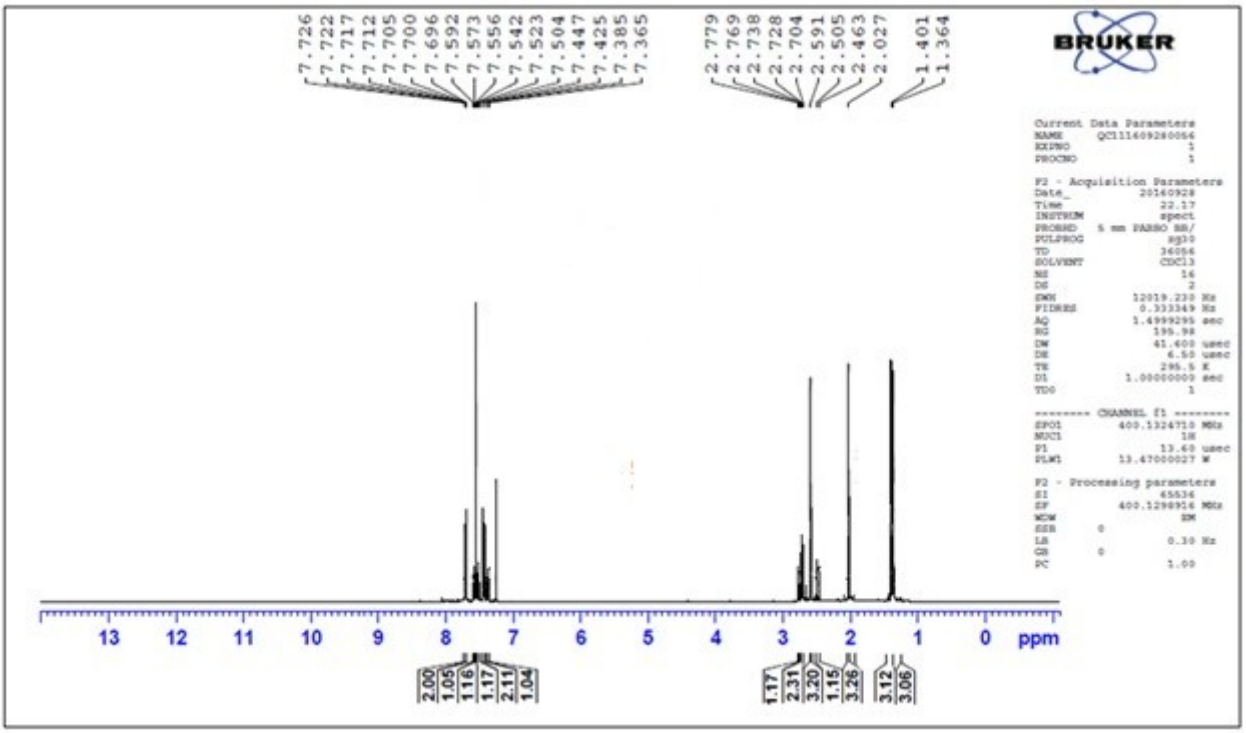
Monoisotopic Mass, Even Electron Ions
58 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-30 N: 0-4 O: 0-2 Br: 0-1

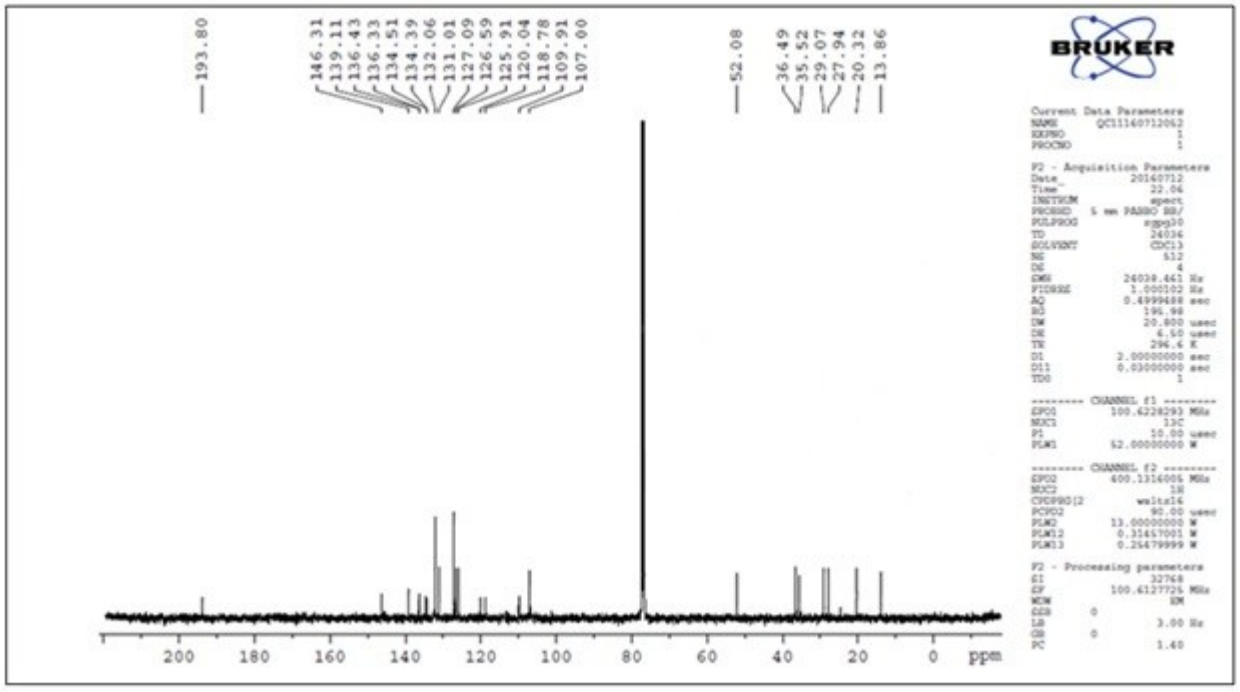
C13&PINO1/023 E
161114008 5 (0.118) Cm (5:7)

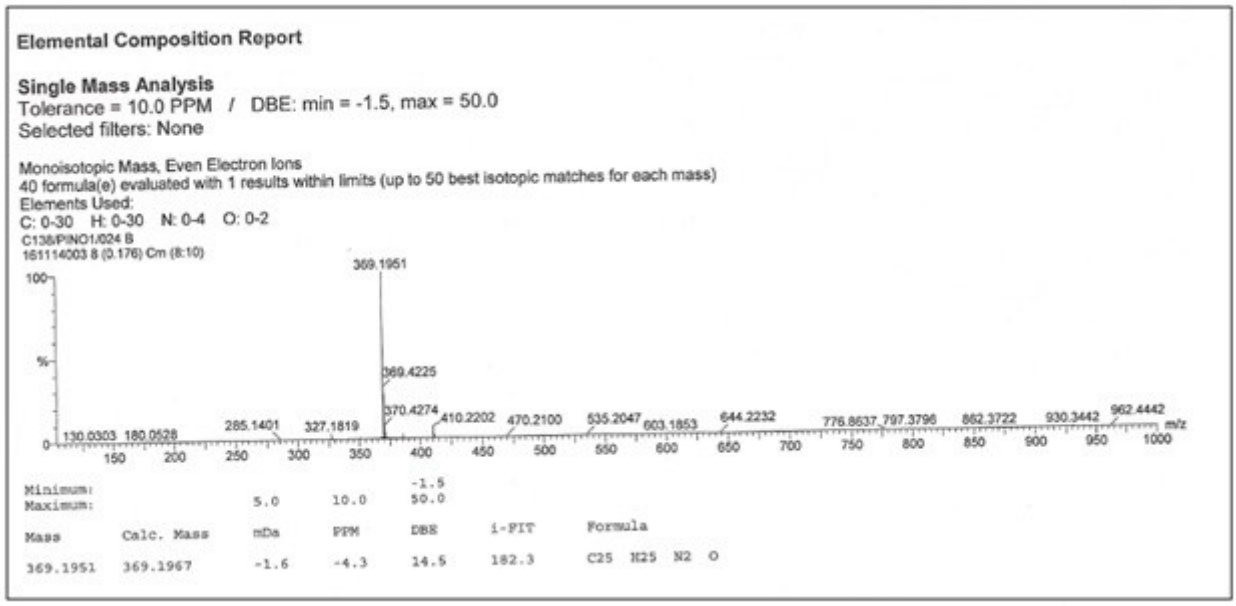


Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
355.1805	355.1810	-0.5	-1.4	14.5	32046.1	C24 H23 N2 O

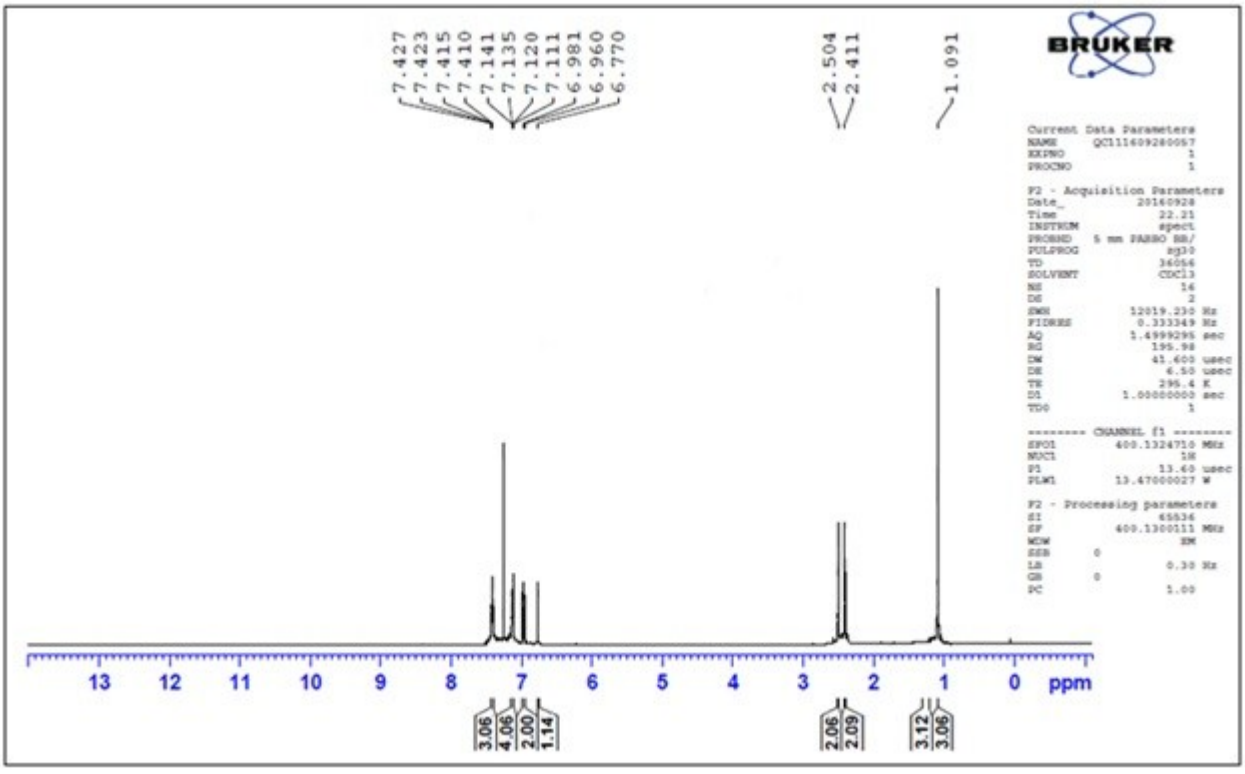
4-(1-(2,3-dimethylphenyl)-6,6-dimethyl-4-oxo-4,5,6,7-tetrahydro-1H-indol-2-yl)benzonitrile (4m):

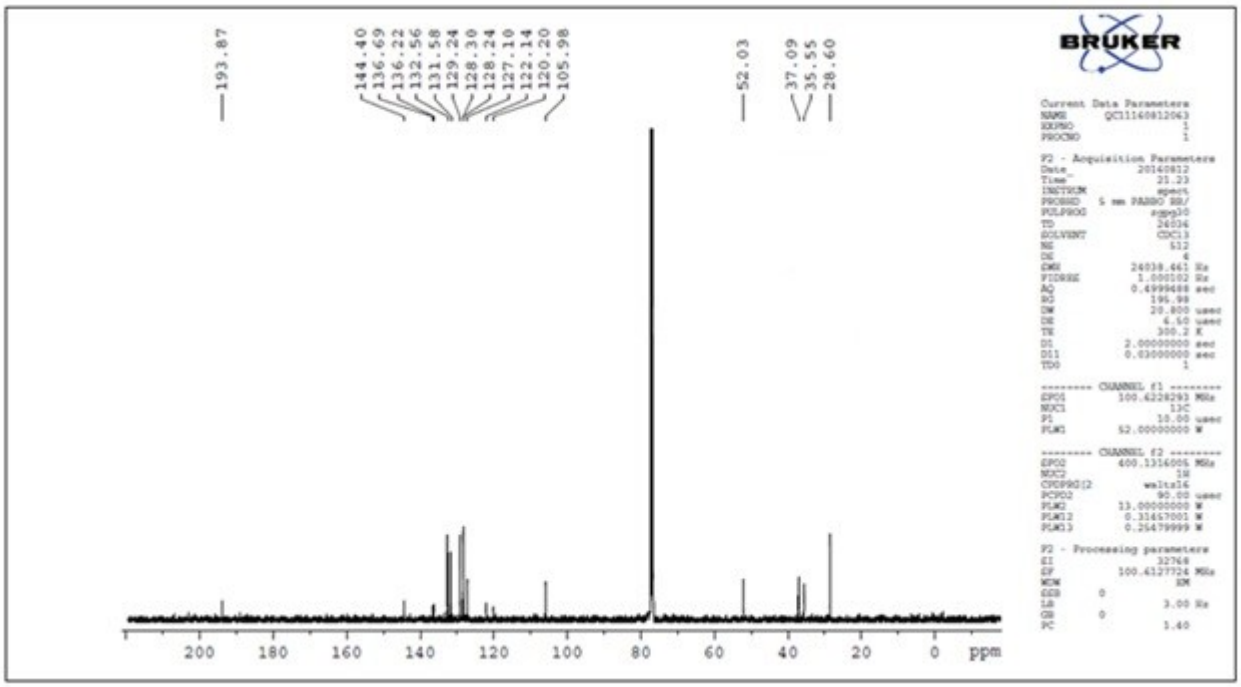






2-(4-chlorophenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indol-4-one (4n):

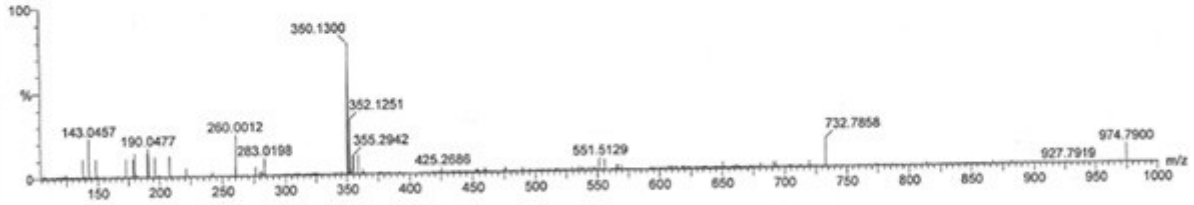




Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-2 O: 0-2 Cl: 0-1
C138/PINO1/030 C
161114017 49 (1.098) Cm (49:50)



Minimum:		5.0	5.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
350.1300	350.1312	-1.2	-3.4	12.5	261.7	C22 H21 N O Cl