Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Highly Efficient and Enantioselective Hydrogenation of Quinoline and Pyridine Derivatives with Ir-Difluorphos Catalyst

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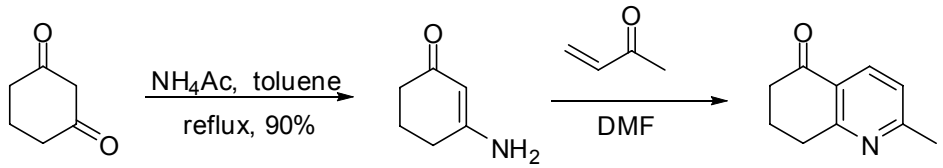
1. General information:

Unless otherwise noted, all experiments were carried out under an atmosphere of nitrogen using standard Schlenk techniques or in a nitrogen-filled glovebox, and all commercially available chemicals were used as received from Aldrich, Acros or Strem without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Model Avance DMX 400 Spectrometer (^{1}H 400 MHz and ^{13}C 106 MHz, respectively). Chemical shifts (δ) are given in ppm and are referenced to residual solvent peaks. All organic solvents were dried using standard, published methods and were distilled before use.

2. The general procedure for the synthesis of pyridine derivatives

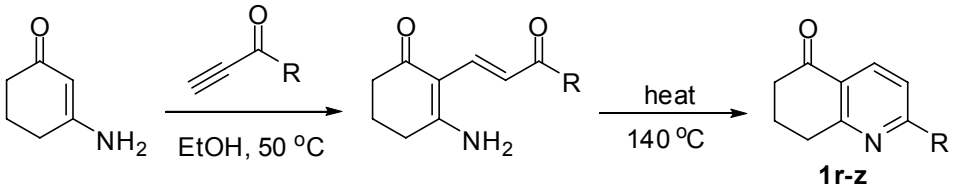
2.1 7, 8-dihydro-2-methylquinolin-5(6H)-one:



1q 50% yield

This compound was synthesized according to the reported literature:[1] To a 100 ml dried flask, 3-Aminocyclohex-2-enone (5.6 g, 50.0 mmol) prepared by reported method[2] and but-3-en-2-one (7.0 g, 100.0 mmol) were refluxed in DMF (50 ml) for 1 h. Then the solvent was removed at reduced pressure. The residue was purified by column chromatography on silica gel using Et_2O/hexane in 6:1 as an eluent gave colourless oil. Yield: 4.0 g (50%). ^{1}H and ^{13}C NMR spectra identical with reference[3]

2.2 Compounds from **1r** to **1z**:



1r-z

A solution of 3-aminocyclohex-2-enone (222 mg, 2 mmol) and propargylic ketone (4.7 mmol) in ethanol (10 ml) was stirred at 50 °C for 12 h, cooled and then evaporated *in vacuo*. Purification by flash chromatography on silica, eluting with

ethyl ether and then methanol gave a yellow solid, which was heated at 140 ^{o}C for 2h in a flask with a dry tube and allowed to cool to give pyridines.

7, 8-dihydro-2-propyl-quinolin-5(6H)-one (1r), brown liquid, 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.18 (d, *J* = 8.00 Hz, 1H), 7.10-7.12 (d, *J* = 8.05 Hz, 1H), 3.09-3.12 (m, 2H), 2.75-2.79 (m, 2H), 2.64-2.67 (m, 2H), 2.16-2.19 (m, 2H), 1.71-1.77 (m, 2H), 0.95-0.99 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.75, 168.04, 164.07, 136.02, 126.78, 122.20, 41.65, 39.31, 33.41, 23.81, 22.75, 14.67 ppm; HRMS (ESI) calcd. for $C_{12}H_{15}NO$ $[M+H]^+$: 190.1232, found: 190.1240

7, 8-dihydro-2-pentyl-quinolin-5(6H)-one (1s), brown liquid, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.17 (d, *J* = 8.03 Hz, 1H), 7.10-7.12 (d, *J* = 8.01 Hz, 1H), 3.08-3.12 (m, 2H), 2.76-2.80 (m, 2H), 2.63-2.67 (m, 2H), 2.15-2.19 (m, 2H), 1.68-1.72 (m, 2H), 1.31-1.35 (m, 4H), 0.86-0.89 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.77, 168.30, 164.07, 136.04, 126.74, 122.13, 39.72, 39.31, 33.42, 32.41, 30.29, 23.28, 22.75, 14.77 ppm; HRMS (ESI) calcd. for $C_{14}H_{19}NO$ $[M+H]^+$: 218.1545, found: 218.1553

7, 8-dihydro-2-hexyl-quinolin-5(6H)-one (1t), brown liquid, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.18 (d, *J* = 8.04 Hz, 1H), 7.11-7.13 (d, *J* = 8.03 Hz, 1H), 3.09-3.12 (m, 2H), 2.77-2.81 (m, 2H), 2.64-2.67 (m, 2H), 2.16-2.19 (m, 2H), 1.69-1.73 (m, 2H), 1.28-1.34 (m, 6H), 0.85-0.89 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.78, 168.32, 164.08, 136.04, 126.75, 122.14, 39.76, 39.31, 33.43, 32.44, 30.57, 29.90, 23.32, 22.76, 14.83 ppm; HRMS (ESI) calcd. for $C_{15}H_{22}NO$ $[M+H]^+$: 232.1701, found: 232.1700

7,8-dihydro-2-heptyl-quinolin-5(6H)-one (1u), brown liquid, 74% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.19 (d, *J* = 8.02 Hz, 1H), 7.11-7.13 (d, *J* = 8.06 Hz, 1H), 3.10-3.13 (m, 2H), 2.78-2.82 (m, 2H), 2.65-2.68 (m, 2H), 2.17-2.20 (m, 2H), 1.69-1.73 (m, 2H), 1.26-1.35 (m, 8H), 0.85-0.89 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.77, 168.33, 164.08, 136.04, 126.75, 122.13, 39.77, 39.32, 33.44, 32.52, 30.62, 30.20, 29.91, 23.41, 22.77, 14.85 ppm; HRMS (ESI) calcd. for $C_{16}H_{23}NO$ $[M+H]^+$: 246.1858, found: 246.1865

7, 8-dihydro-2-octyl-quinolin-5(6H)-one (1v), brwon liquid, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.16 (d, *J* = 8.00 Hz, 1H), 7.09-7.11 (d, *J* = 8.05 Hz, 1H), 3.08-3.11 (m, 2H), 2.76-2.80 (m, 2H), 2.62-2.66 (m, 2H), 2.15-2.18 (m, 2H), 1.67-1.71 (m, 2H), 1.24-1.34 (m, 10H), 0.83-0.86 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.73, 168.30, 164.06, 136.02, 126.73, 122.12, 39.75, 39.30, 33.41, 32.60, 30.60, 30.23, 30.19, 29.96, 23.41, 22.75, 14.87 ppm; HRMS (ESI) calcd. for $C_{17}H_{26}NO$ $[M+H]^+$: 260.2014, found: 260.2022

7,8-dihydro-2-decyl-quinolin-5(6H)-one (1w), brown liquid, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.18 (d, *J* = 8.04 Hz, 1H), 7.11-7.13 (d, *J* = 8.04 Hz, 1H), 3.09-3.12 (m, 2H), 2.77-2.81 (m, 2H), 2.64-2.67 (m, 2H), 2.16-2.21 (m, 2H), 1.68-1.72 (m, 2H), 1.24-1.32 (m, 14H), 0.84-0.88 (m, 3H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.78, 168.33, 164.07, 136.04, 126.74, 122.14, 39.77, 39.31, 33.43, 32.68, 30.61, 30.35, 30.31, 30.23, 30.09, 23.46, 22.76, 14.89 ppm; HRMS (ESI) calcd. for $C_{19}H_{29}NO$ $[M+H]^+$: 288.2327, found: 288.2341

7, 8-dihydro-2-phenylquinolin-5(6H)-one (1x), yellow solid, 82% yield; ^{1}H NMR

(400 MHz, $CDCl_3$) δ 8.31-8.33 (d, *J* = 8.19 Hz, 1H), 8.04-8.06 (m, 2H), 7.69-7.71 (d, *J* = 8.19 Hz, 1H), 7.45-7.51 (m, 3H), 3.20-3.23 (m, 2H), 2.69-2.73 (m, 2H), 2.21-2.24 (m, 2H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.69, 164.60, 161.55, 139.26, 136.62, 130.78, 129.67, 128.27, 127.35, 119.73, 39.41, 33.68, 22.76 ppm; HRMS (ESI) calcd. for $C_{15}H_{13}NO$ $[M+H]^+$: 224.1075, found: 224.1076

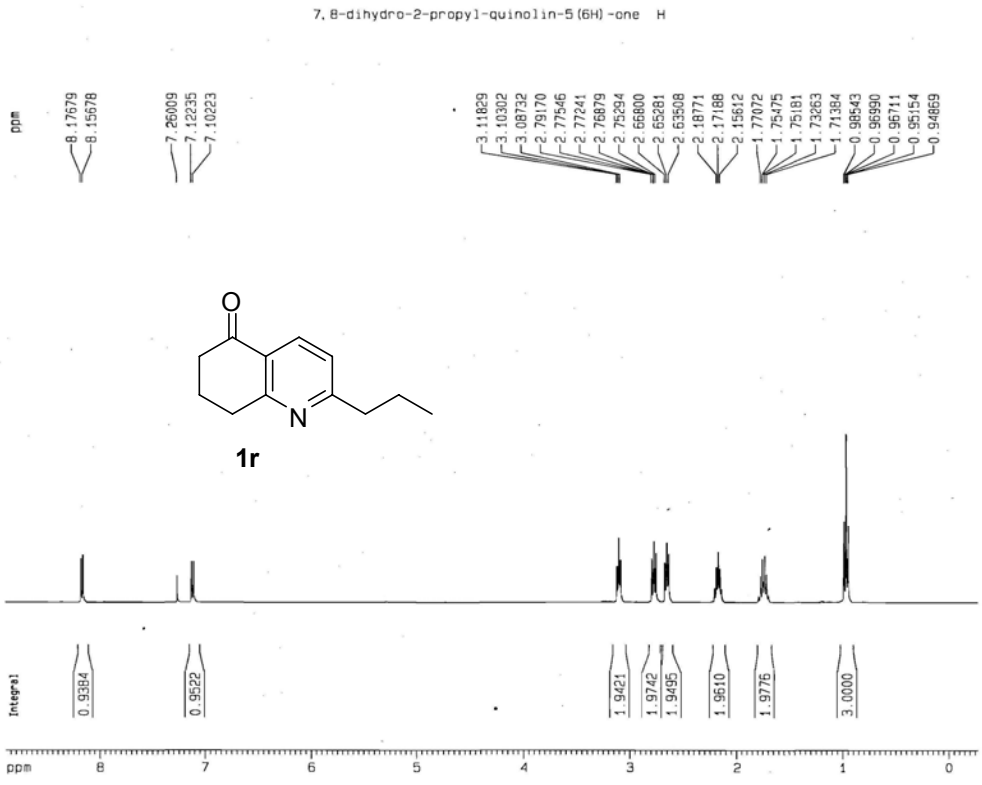
7, 8-dihydro-2-benzyl-quinolin-5(6H)-one (1y), yellow liquid, 81% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15-8.17 (d, *J* = 8.06 Hz, 1H), 7.26-7.32 (m, 5H), 7.05-7.07 (d, *J* = 8.08 Hz, 1H), 4.19 (s, 2H), 3.14-3.17 (m, 2H), 2.66-2.69 (m, 2H), 2.17-2.23 (m, 2H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.65, 166.39, 164.19, 139.25, 136.34, 129.99, 129.50, 127.48, 126.96, 122.51, 45.84, 39.32, 33.42, 22.73 ppm; HRMS (ESI) calcd. for $C_{16}H_{15}NO$ $[M+H]^+$: 238.1232, found: 238.1239

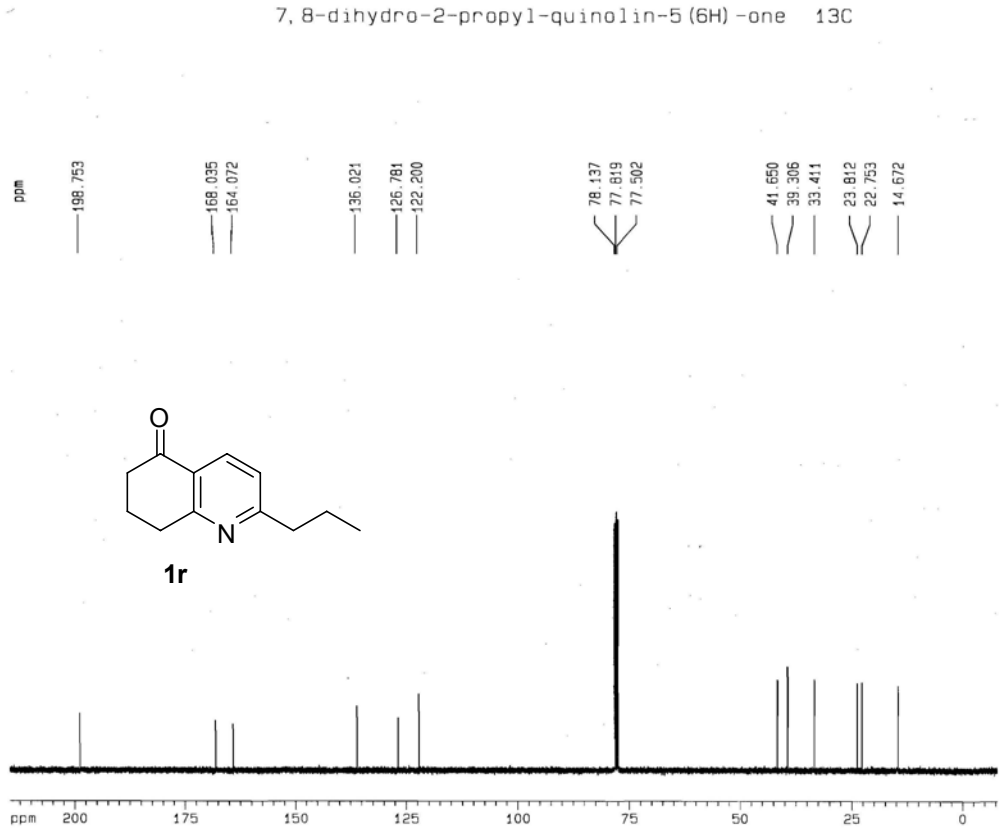
7, 8-dihydro-2-phenethylquinolin-5(6H)-one (1z), yellow liquid, 80% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.14-8.16 (d, *J* = 8.01 Hz, 1H), 7.26-7.29 (m, 2H), 7.18-7.20 (m, 3H), 7.05-7.07 (d, *J* = 8.0 Hz, 1H), 3.11-3.15 (m, 4H), 3.05-3.07 (m, 2H), 2.66-2.69 (m, 2H), 2.18-2.21 (m, 2H) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 198.74, 166.88, 164.21, 141.86, 136.10, 129.22, 126.95, 126.90, 122.45, 41.32, 39.33, 36.45, 33.43, 22.76 ppm; HRMS (ESI) calcd. for $C_{17}H_{17}NO$ $[M+H]^+$: 252.1388, found: 252.1397

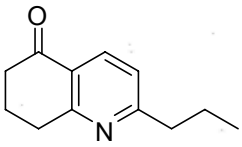
3. References:

1. J. Jampilek, M. Dolezal, J. Kunes, V. Buchta, L. Silva, K. Kralova, *Med. Chem.* **2005,** *1*, 591.

4. ^{1}H and ^{13}C NMR and MS spectra of the trisubstituted pyridine derivatives







1r

Elemental Composition Report **Page 1**

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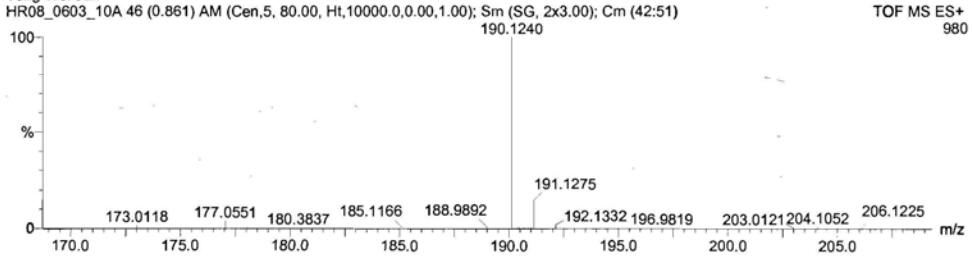
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_10A 46 (0.861) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (42:51) TOF MS ES+
980



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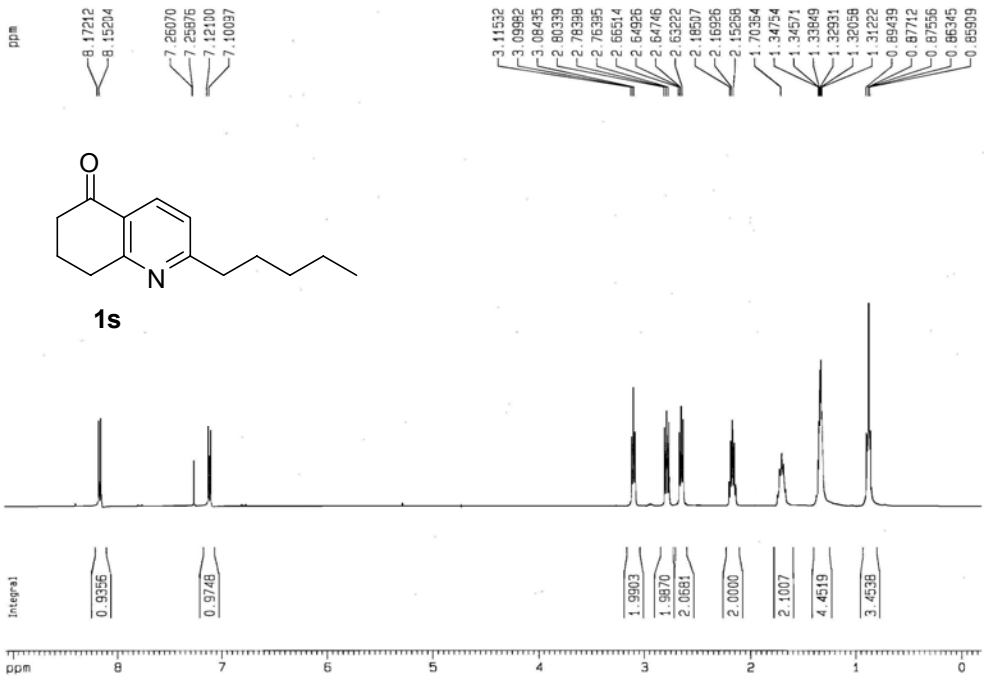
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
190.1240	190.1232	0.8	4.2	5.5	1.3	C12 H16 N O

7,8-dihydro-2-pentyl-quinolin-5(6H)-one H



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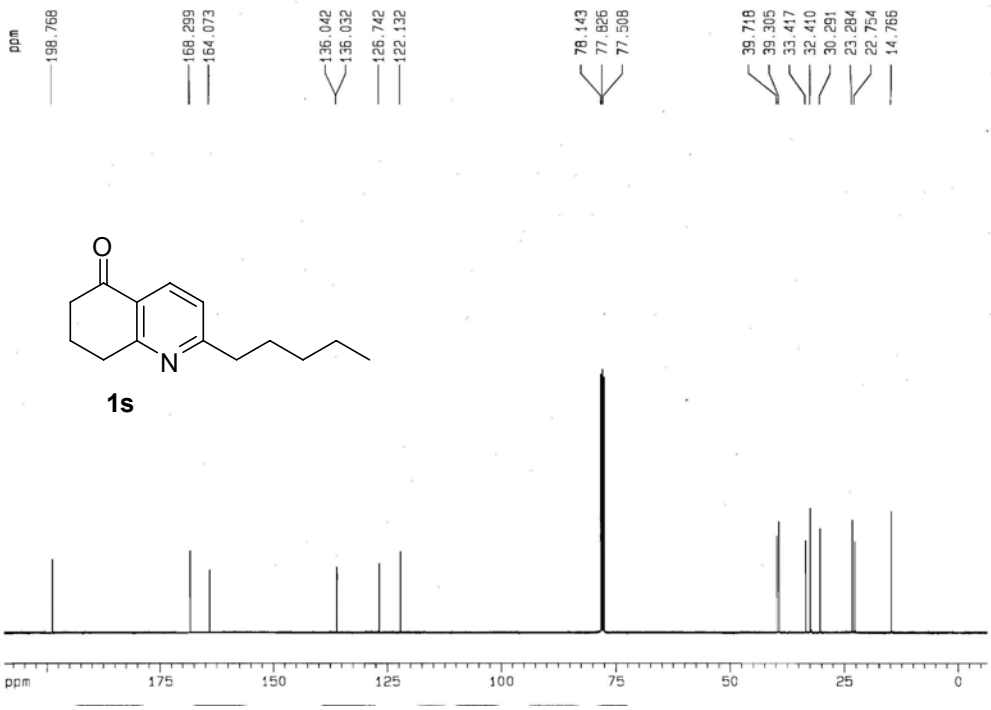
7,8-dihydro-2-pentyl-quinolin-5(6H)-one 13C



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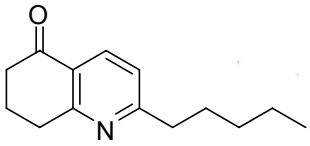

1s

Elemental Composition Report **Page 1**

Single Mass Analysis
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20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
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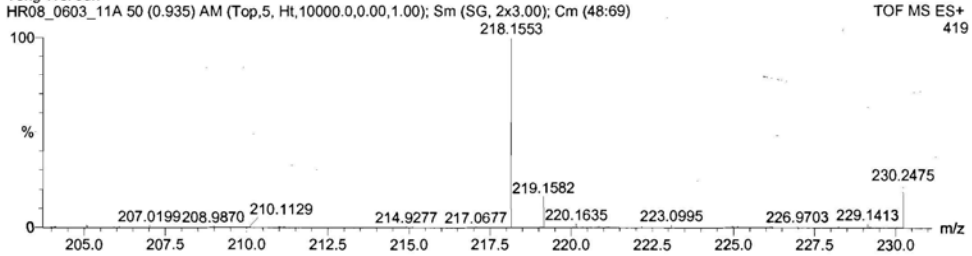
419



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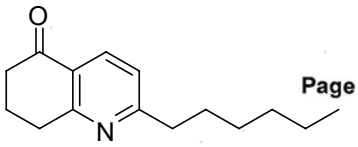

Elemental Composition Report

1t

Single Mass Analysis
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Selected filters: None

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21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
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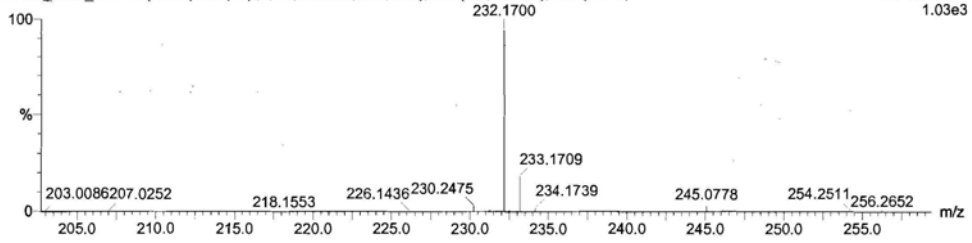

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Maximum:		100.0	20.0	60.0		
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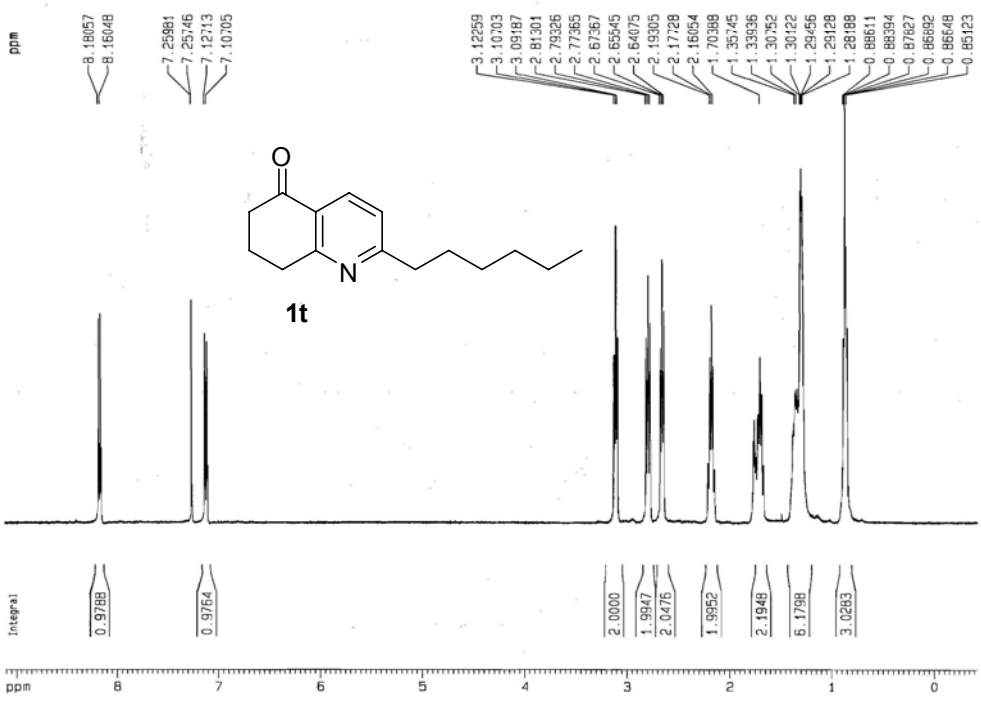
232.1700	232.1701	-0.1	-0.4	5.5	0.2	C15 H22 N O

7, 8-dihydro-2-hexyl-quinolin-5(6H)-one



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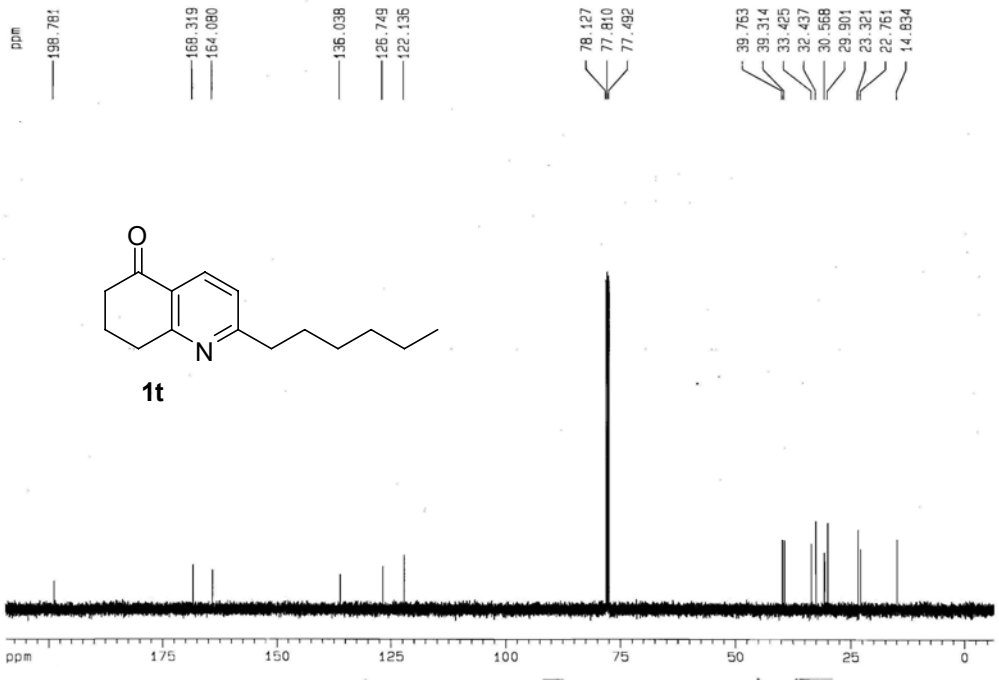
7, 8-dihydro-2-hexyl-quinolin-5(6H)-one 13C



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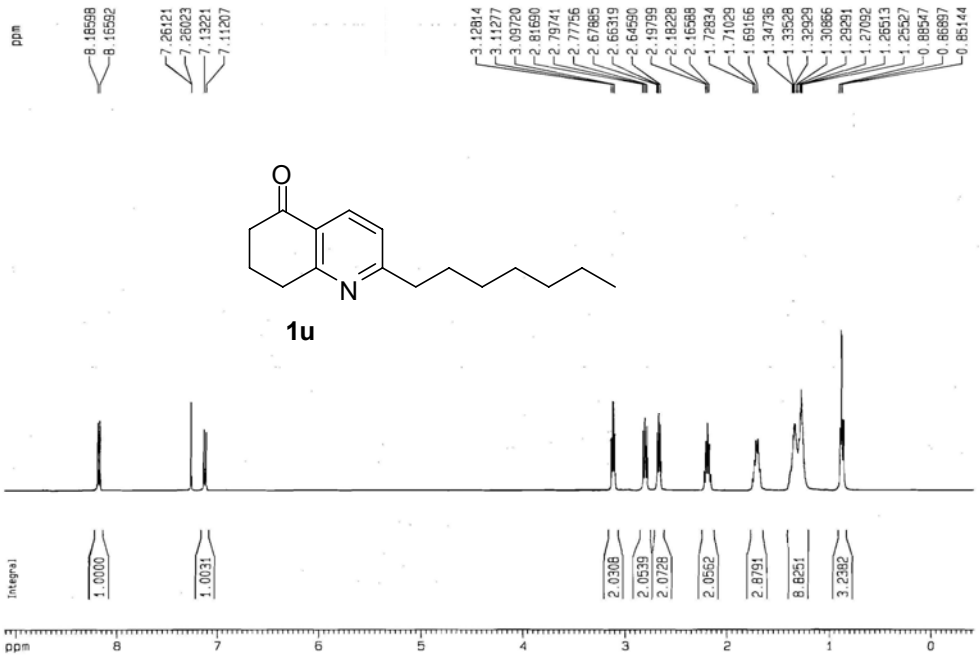

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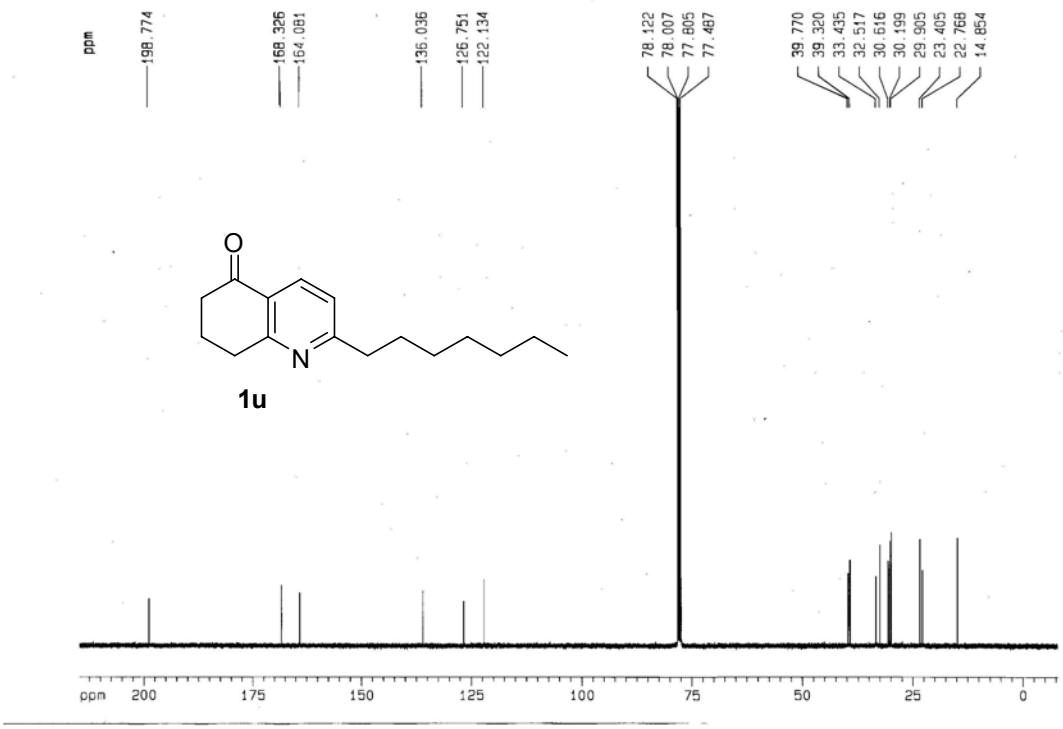
7, 8-dihydro-2-heptylquinolin-5(6H)-one 13C



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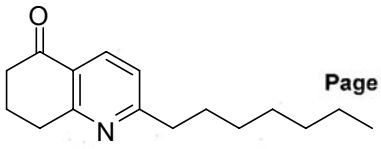

1u

Elemental Composition Report **Page 1**

Single Mass Analysis
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Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
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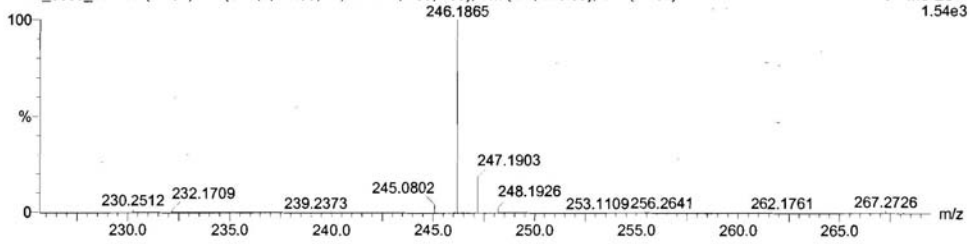
Tong Wei Jun
HR08_0603_13A 50 (0.935) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (50:62) TOF MS ES+ 1.54e3



Minimum:				-1.5		
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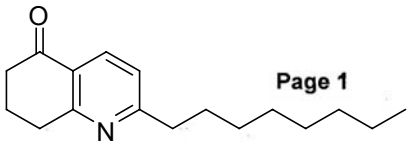

1v

Elemental Composition Report

Single Mass Analysis
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Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
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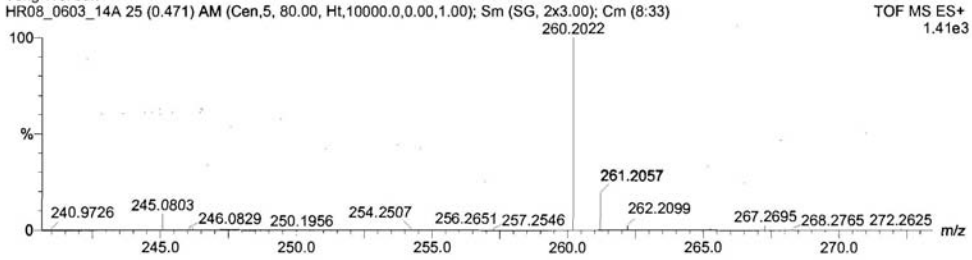

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Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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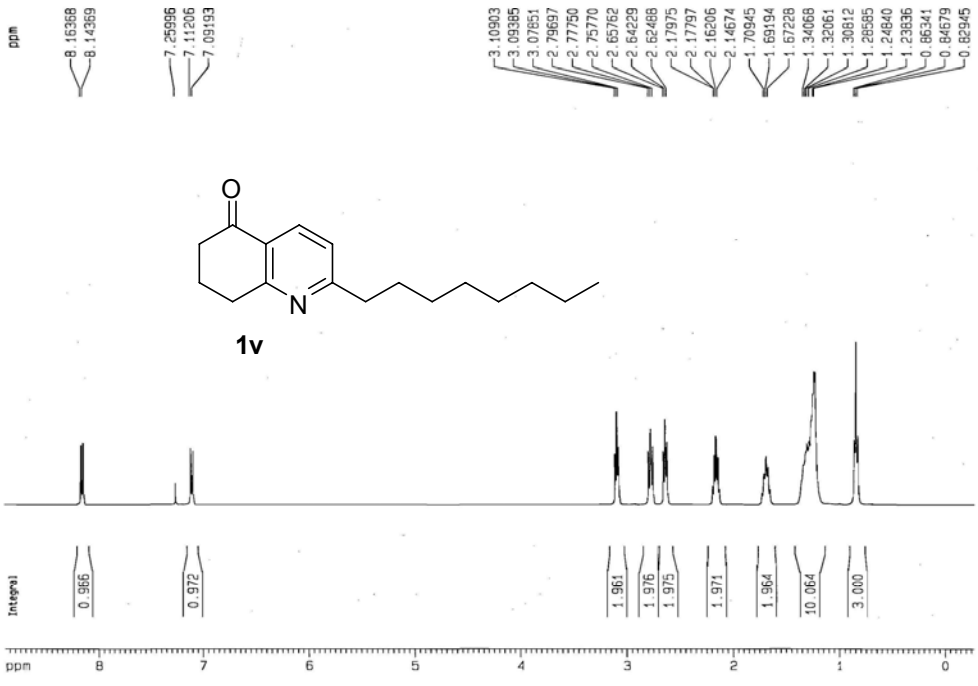
7,8-dihydro-2-octylquinolin-5(6H)-one H



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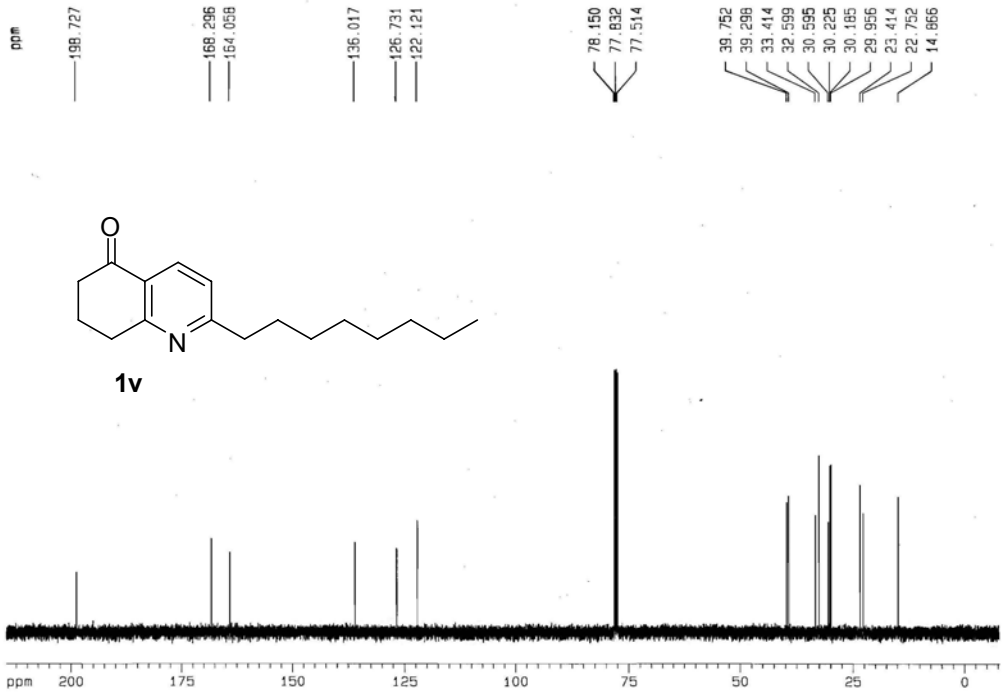
7, 8-dihydro-2-octylquinolin-5 (6H) -one 13C



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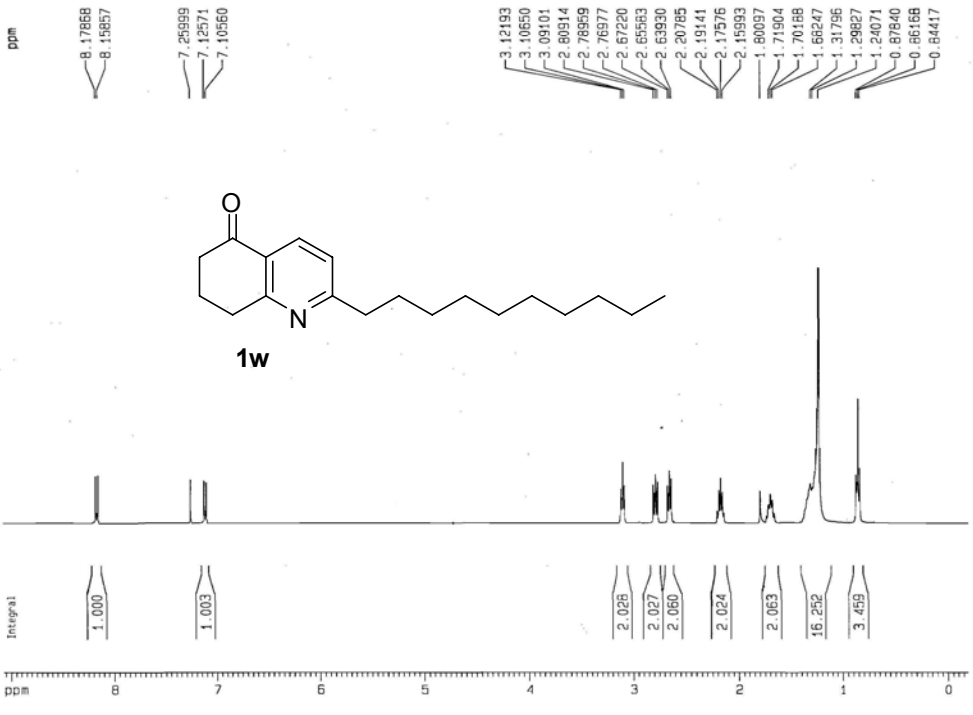
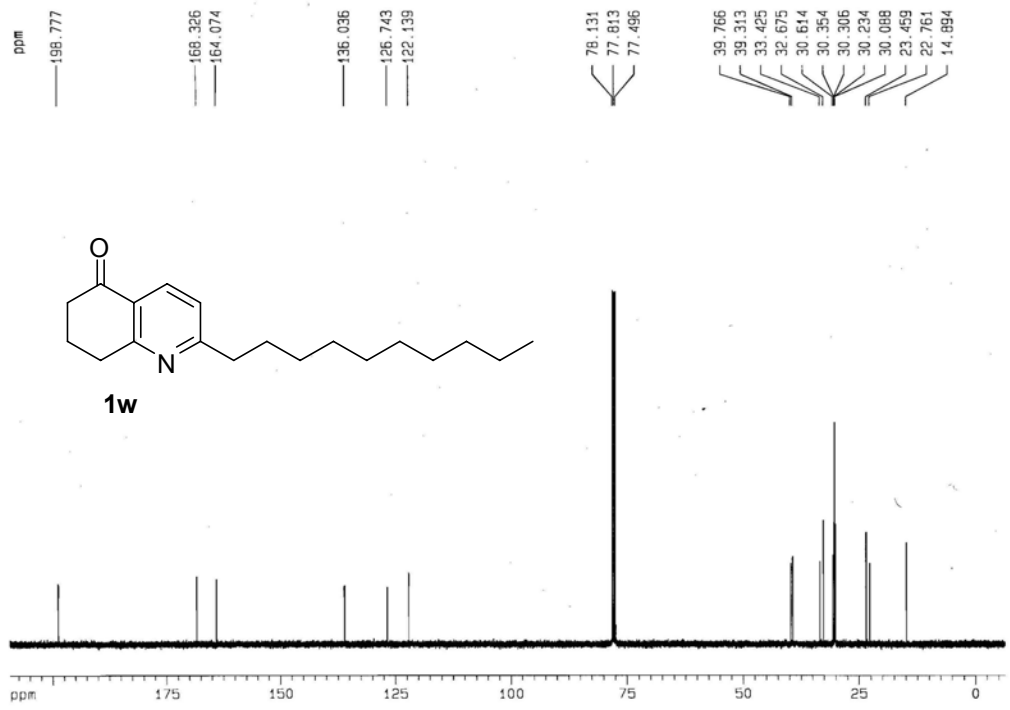
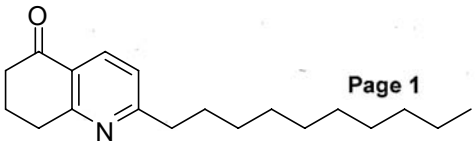
7, 8-dihydro-2-decyl-quinolin-5 (6H) -one H



1w



Elemental Composition Report



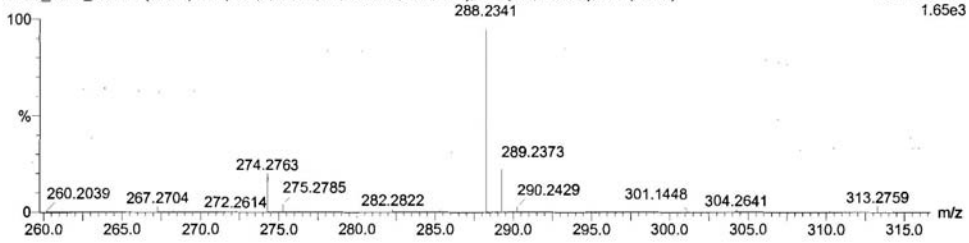
1w

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

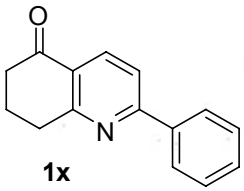
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_15A 71 (1.325) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (56:75)

TOF MS ES+
1.65e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.2341	288.2327	1.4	4.9	5.5	0.2	C19 H30 N O



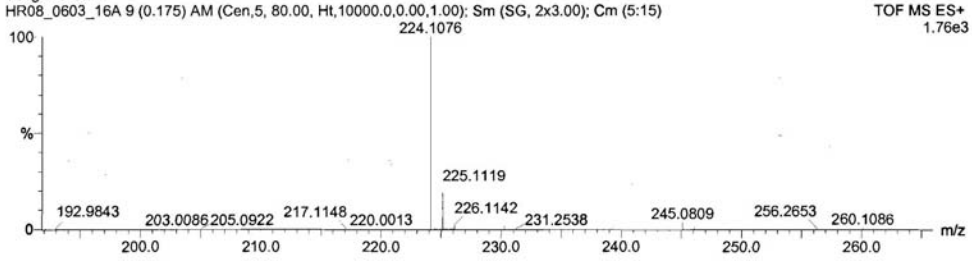
1x

Elemental Composition Report

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

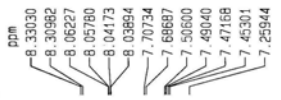
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_16A 9 (0.175) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (5:15)

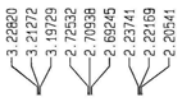
TOF MS ES+
1.76e3

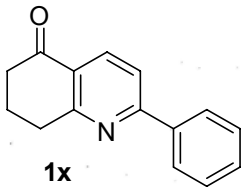


Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.1076	224.1075	0.1	0.4	9.5	2.1	C15 H14 N O

7,8-dihydro-2-phenyl-quinolin-5(6H)-one H







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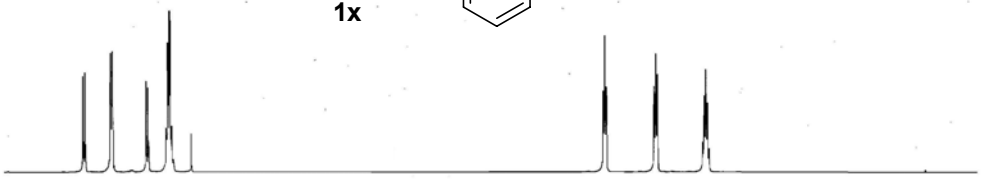
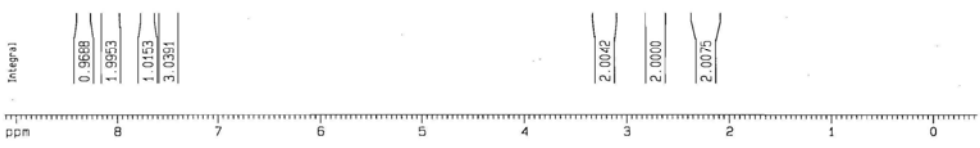
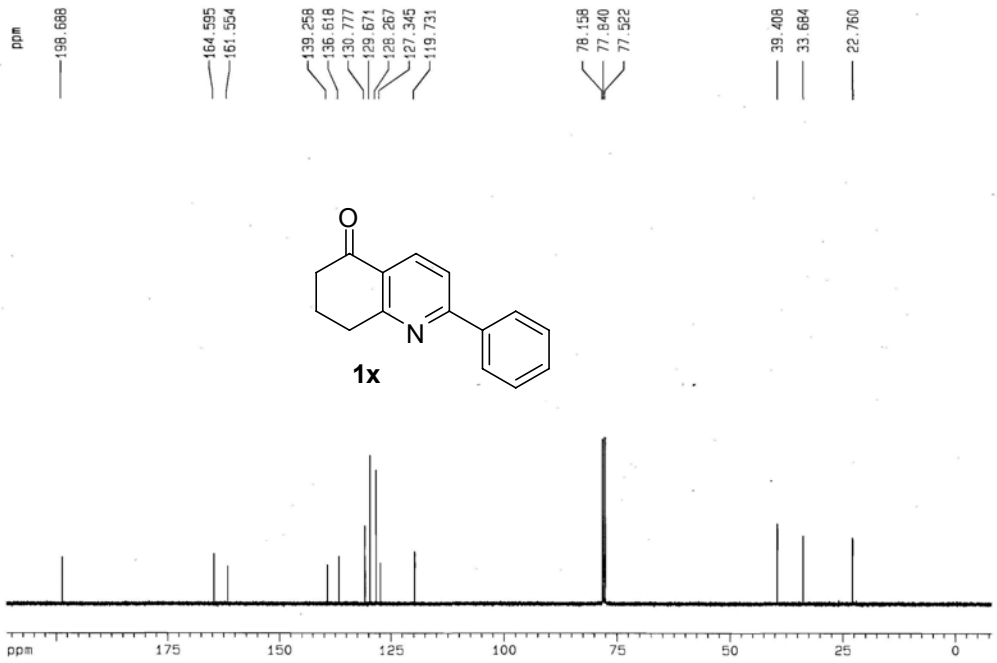


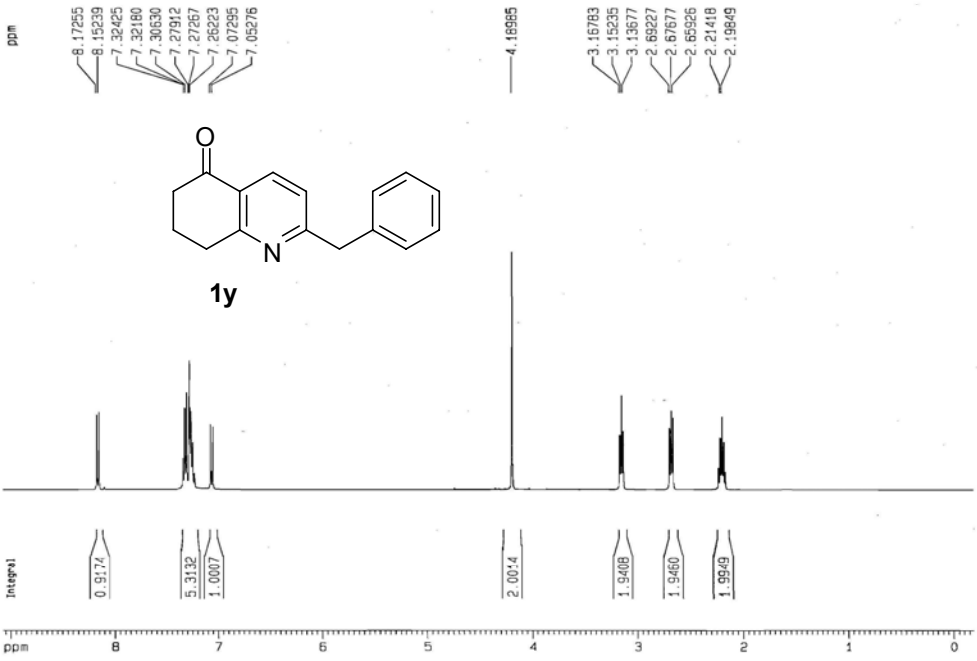


7, 8-dihydro-2-phenyl-quinolin-5(6H)-one 13C

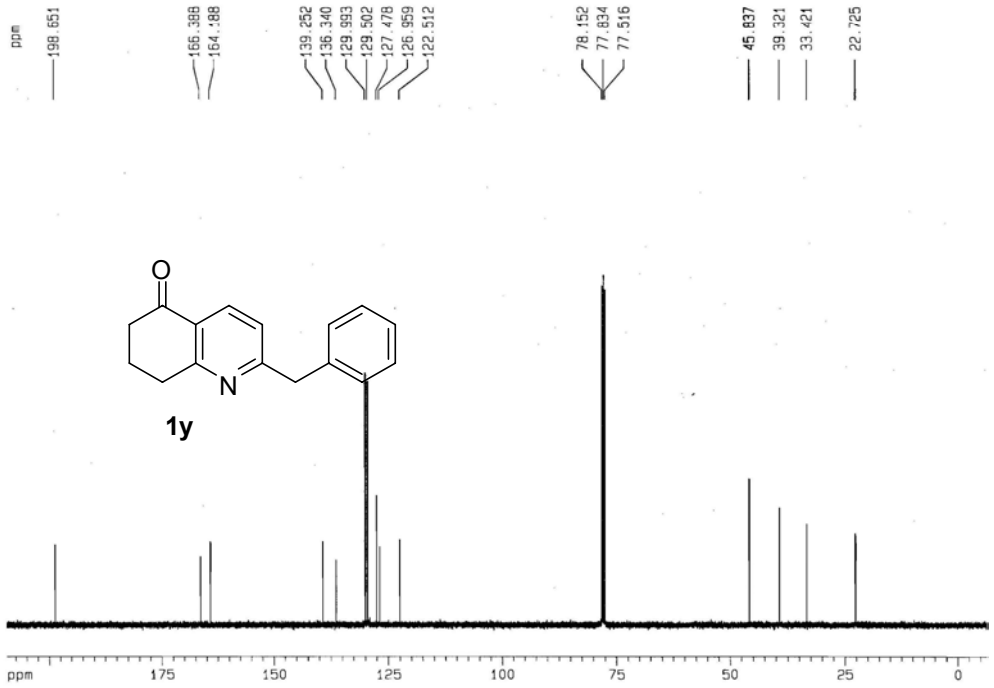


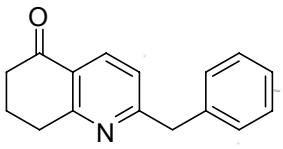
1x

7, 8-dihydro-2-benzyl-quinolin-5(6H)-one H



1y





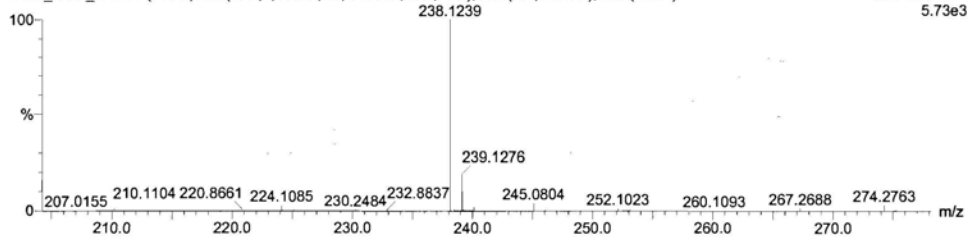
1y

Elemental Composition Report **Page 1**

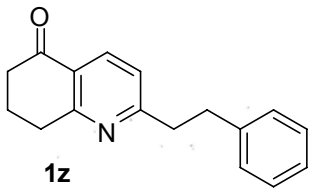
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_17A 77 (1.436) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (62:84) TOF MS ES+
5.73e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
238.1239	238.1232	0.7	2.9	9.5	0.7	C16 H16 N O



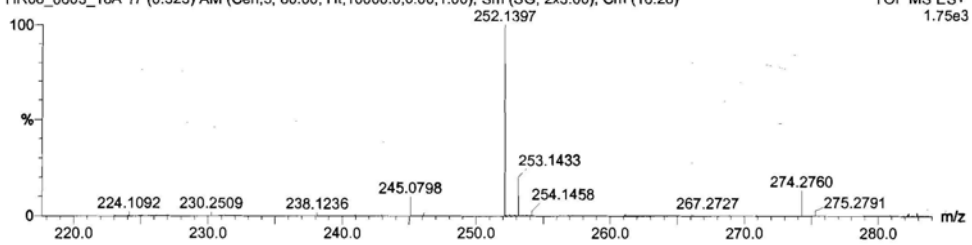
1z

Elemental Composition Report

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

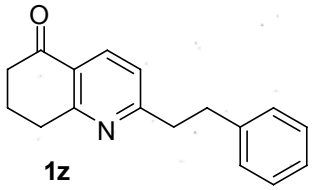
Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_18A 17 (0.323) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (16:28) TOF MS ES+
1.75e3

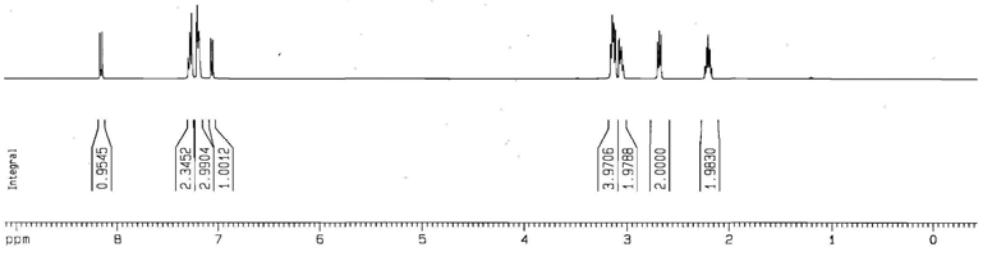


Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.1397	252.1388	0.9	3.6	9.5	0.2	C17 H18 N O

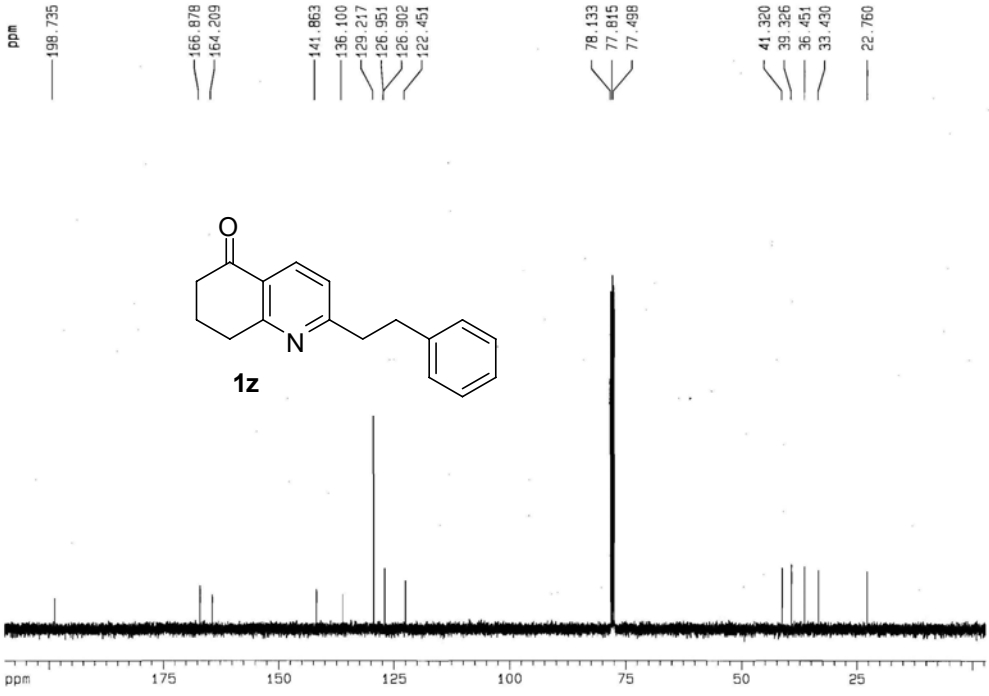
7,8-dihydro-2-ethylphenyl-quinolin-5(6H)-one H



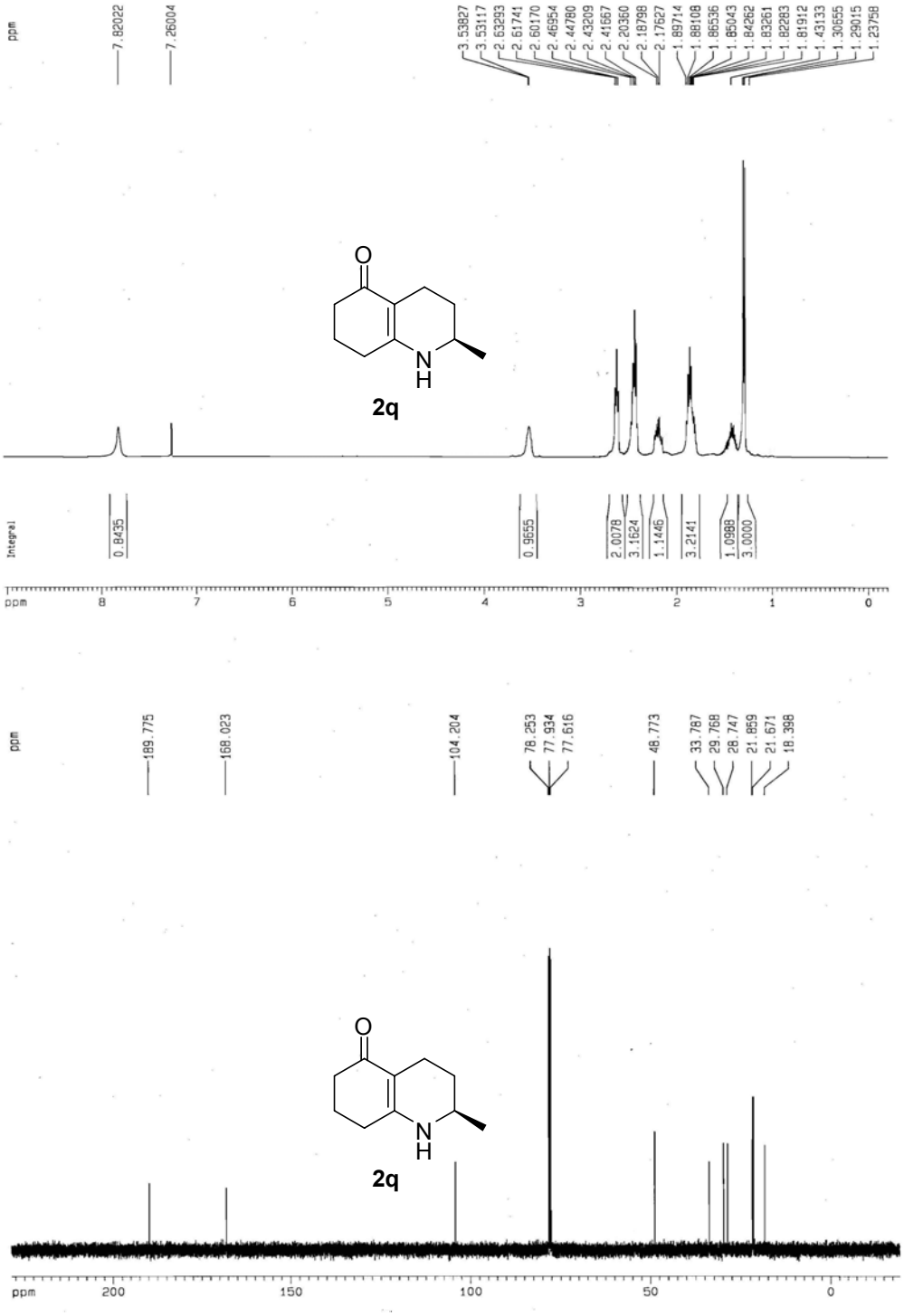
1z

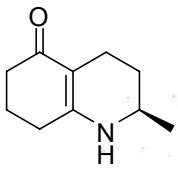


7, 8-dihydro-2-ethylphenyl-quinolin-5(6H)-one 13C



5. ^{1}H and ^{13}C NMR and MS spectra of the reduced pyridines





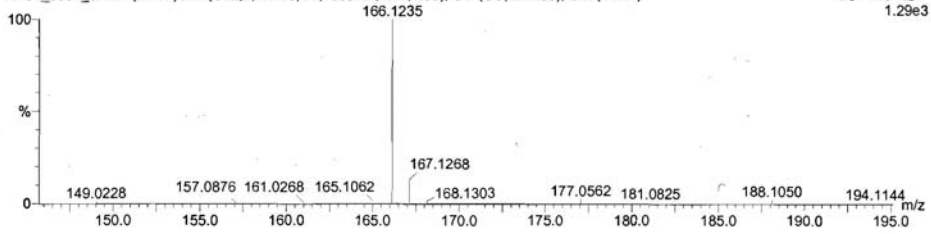
2q

Elemental Composition Report

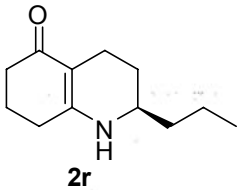
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-3

Tong Wei Jun, py-Methyl
HR08_0604_3A 21 (0.397) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (15:28) TOF MS ES+ 1.29e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
166.1235	166.1232	0.3	1.8	3.5	1.0	C10 H16 N O



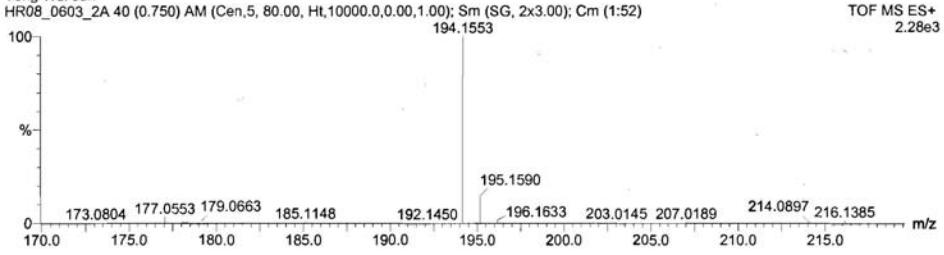
2r

Elemental Composition Report

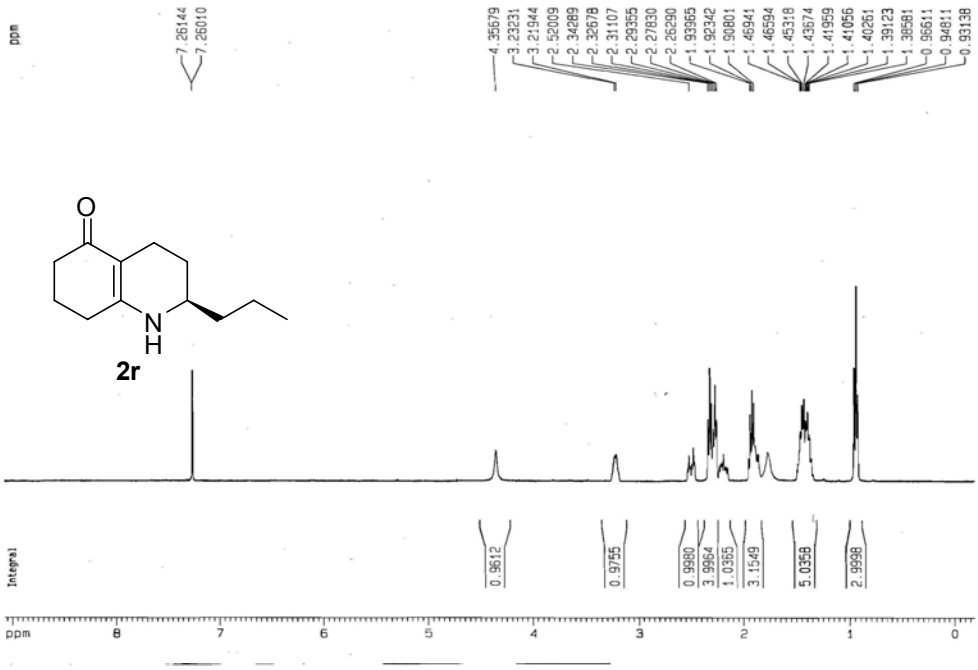
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_2A 40 (0.750) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (1:52) TOF MS ES+ 2.28e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
194.1553	194.1545	0.8	4.1	3.5	1.3	C12 H20 N O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1.92342
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1.45318
1.43674
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H
2r
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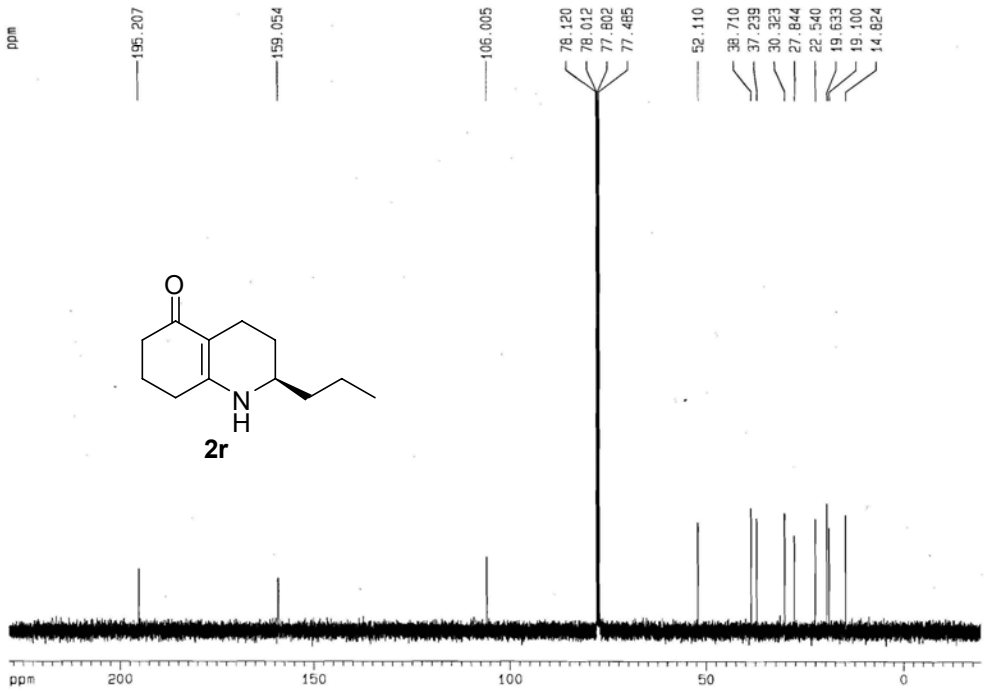
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19.633
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O
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H
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ppm
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150
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50
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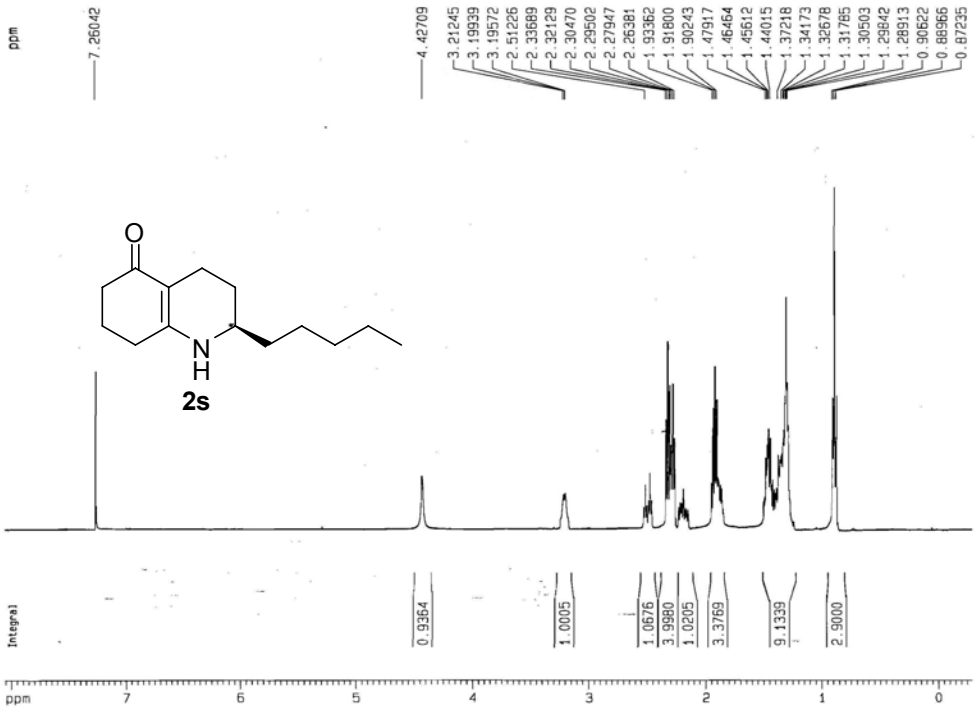
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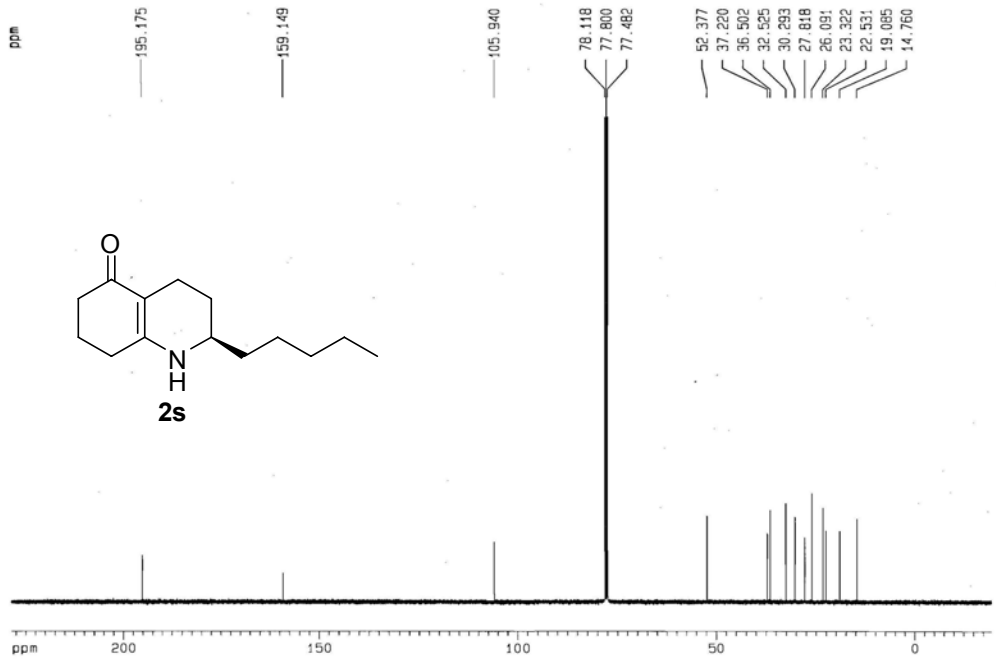
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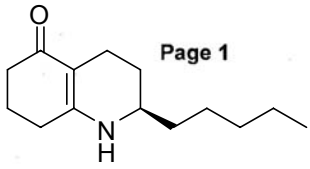
Elemental Composition Report

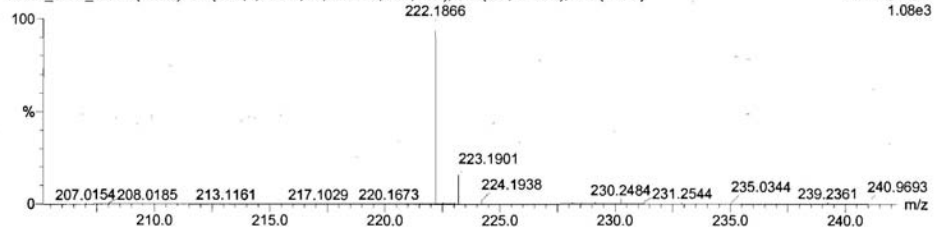


2s

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

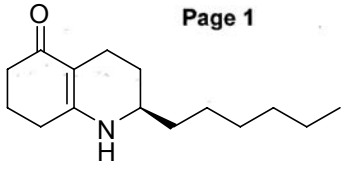
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_3A 30 (0.564) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (15:34) TOF MS ES+ 1.08e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
222.1866	222.1858	0.8	3.6	3.5	0.3	C14 H24 N O

Elemental Composition Report

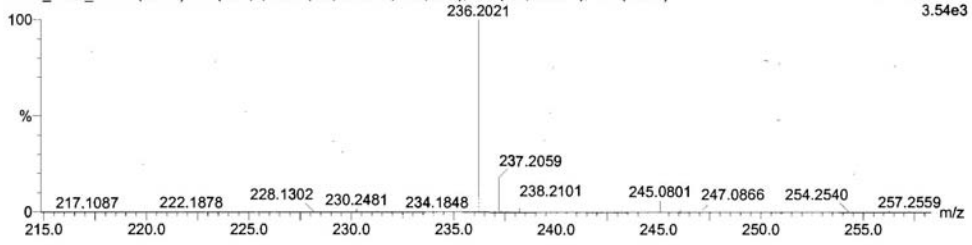


2t

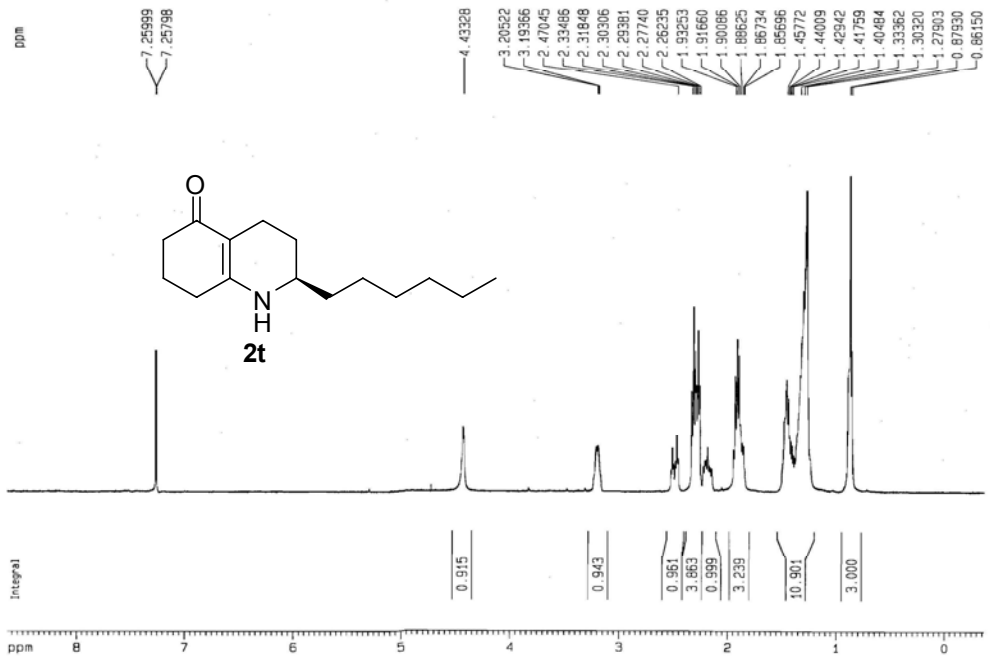
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_4A 70 (1.306) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (46:81) TOF MS ES+ 3.54e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.2021	236.2014	0.7	3.0	3.5	1.2	C15 H26 N O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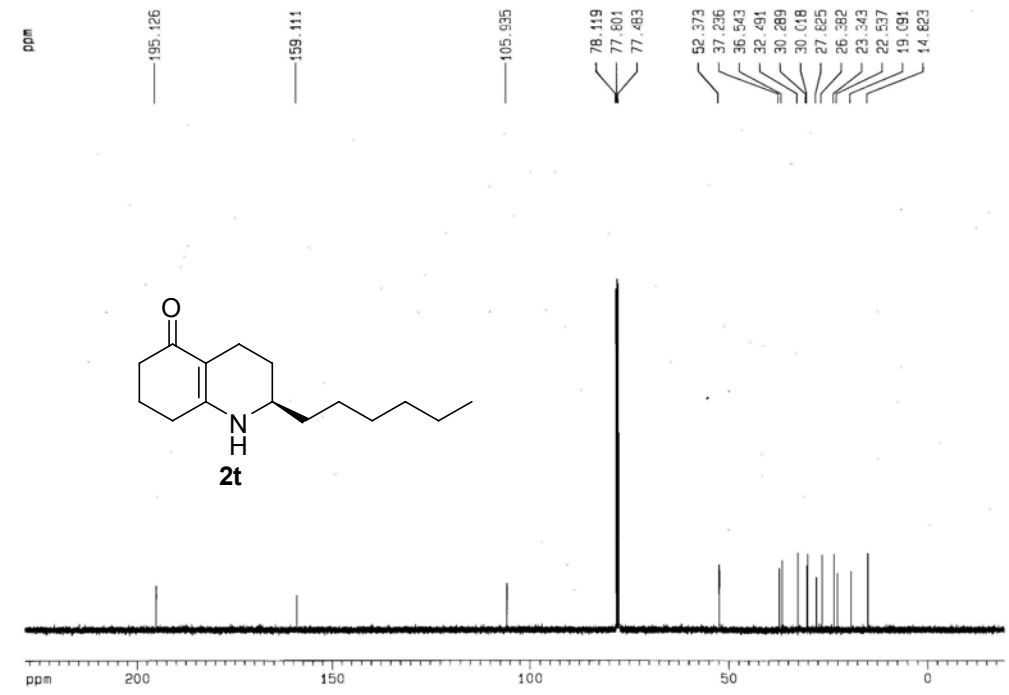
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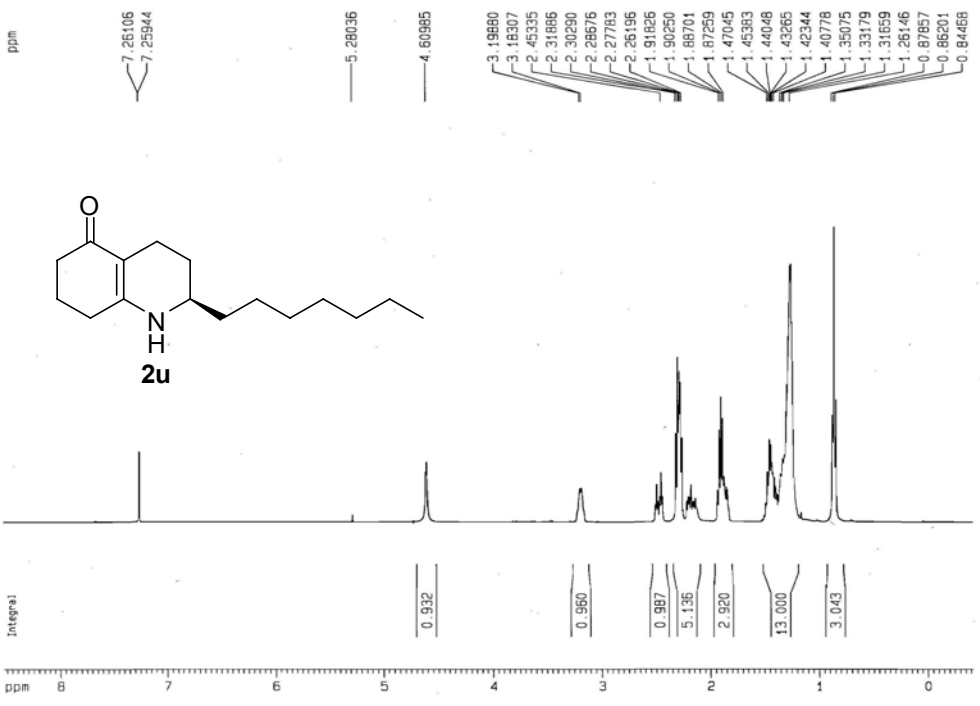
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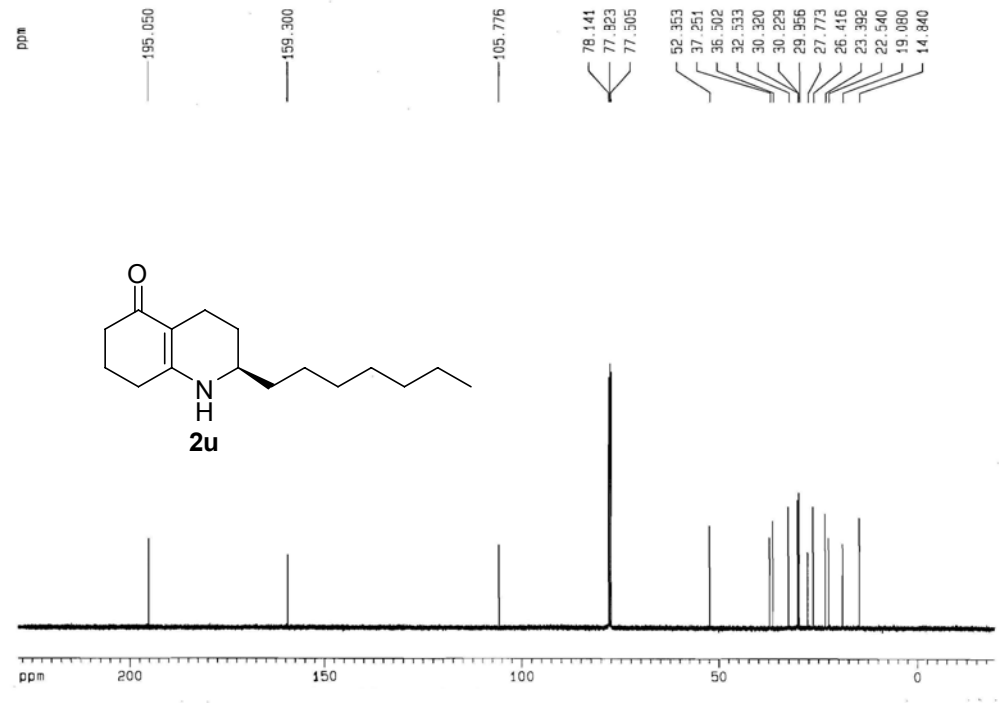
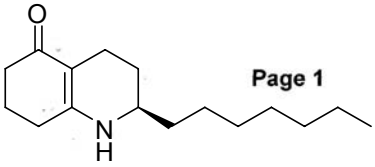
7.26106
7.25944
5.28036
4.60985
3.19880
3.18307
2.45335
2.31886
2.30290
2.28676
2.27783
2.26196
1.91826
1.90250
1.88701
1.87259
1.47045
1.45383
1.44048
1.43265
1.42344
1.40778
1.35075
1.33179
1.31659
1.26146
0.87857
0.86201
0.84468
O
N
H
2u
Integral
0.932
0.960
0.987
5.136
2.920
13.000
3.043
ppm 8 7 6 5 4 3 2 1 0


ppm
195.050
159.300
105.776
78.141
77.823
77.505
52.353
37.251
36.502
32.533
30.320
30.229
29.956
27.773
26.416
23.392
22.540
19.080
14.840
O
N
H
2u
ppm 200 150 100 50 0

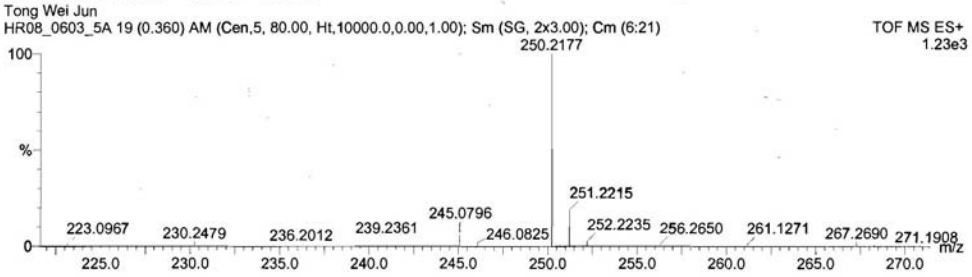


Elemental Composition Report

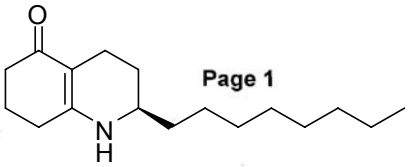
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

2u

Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_5A 19 (0.360) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (6:21) TOF MS ES+ 1.23e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
250.2177	250.2171	0.6	2.4	3.5	0.6	C16 H28 N O

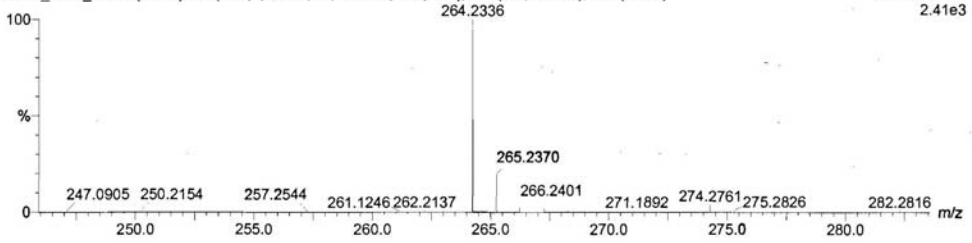


Elemental Composition Report

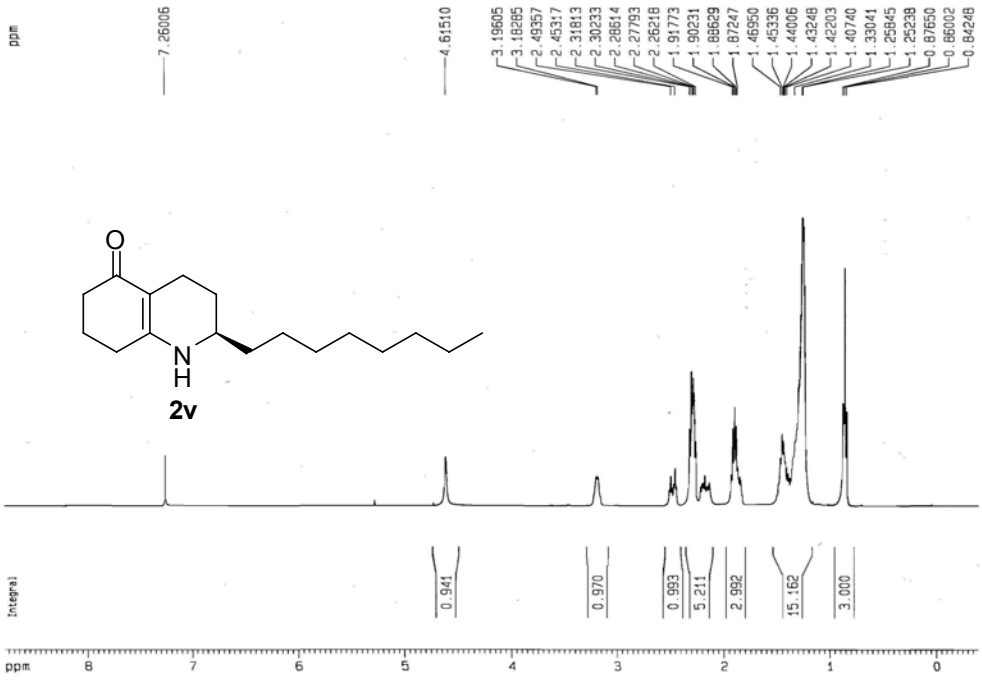
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

2v

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_6A 62 (1.158) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (54:74) TOF MS ES+ 2.41e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
264.2336	264.2327	0.9	3.4	3.5	0.3	C17 H30 N O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3.18285
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2.30233
2.28614
2.27793
2.26218
1.91773
1.90231
1.88629
1.87247
1.46950
1.45336
1.44006
1.43248
1.42203
1.40740
1.33041
1.25845
1.25238
0.87650
0.86002
0.84248
O
N
H
2v
Integral
0.941
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5.211
2.992
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3.000
ppm
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7
6
5
4
3
2
1
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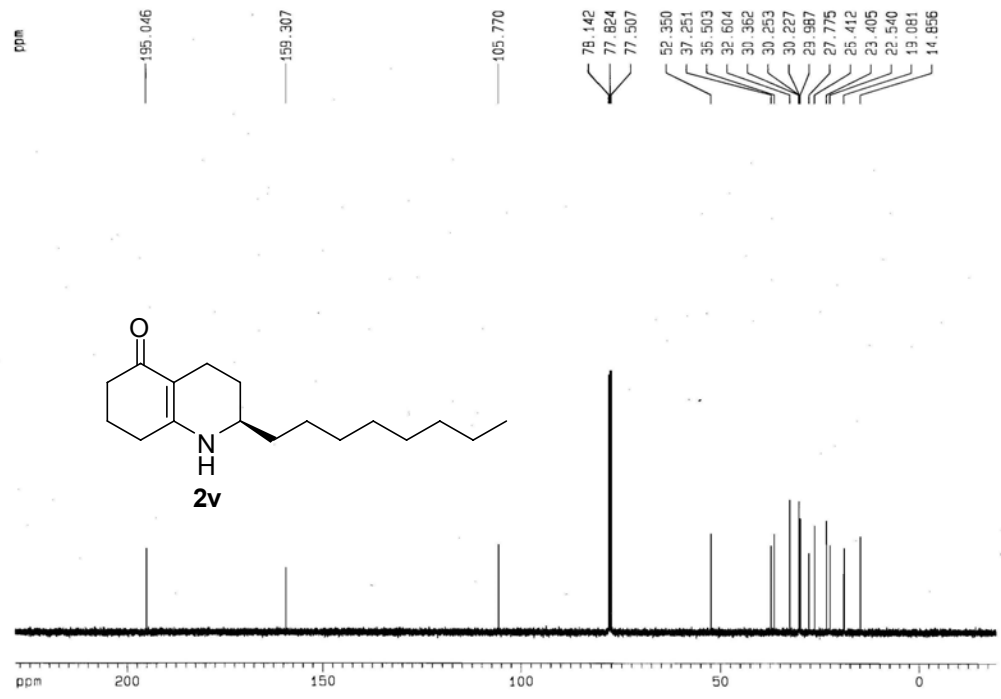
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105.770
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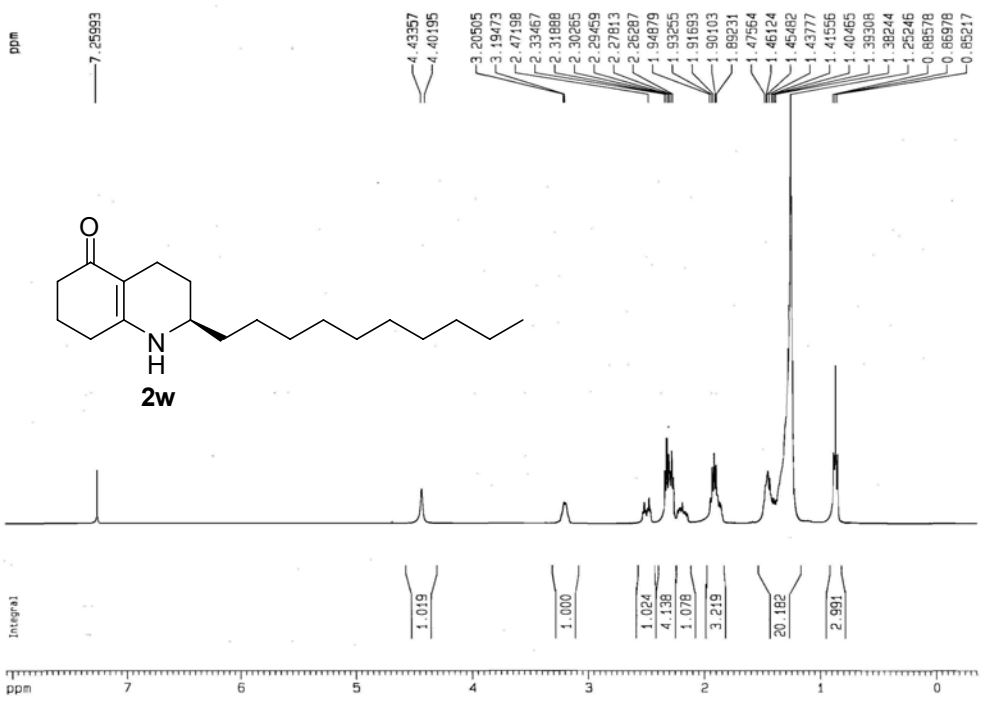
77.824
77.507
52.350
37.251
35.503
32.604
30.362
30.253
30.227
29.987
27.775
25.412
23.405
22.540
19.081
14.856
O
N
H
2v
ppm
200
150
100
50
0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4.40195
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3.19473
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2.31888
2.30265
2.29459
2.27813
2.26287
1.94879
1.93255
1.91693
1.90103
1.89231
1.47564
1.46124
1.45482
1.43777
1.41556
1.40465
1.39308
1.38244
1.25246
0.88578
0.86978
0.85217
O
N
H
2w
Integral
1.019
1.000
1.024
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1.078
3.219
20.182
2.991
ppm
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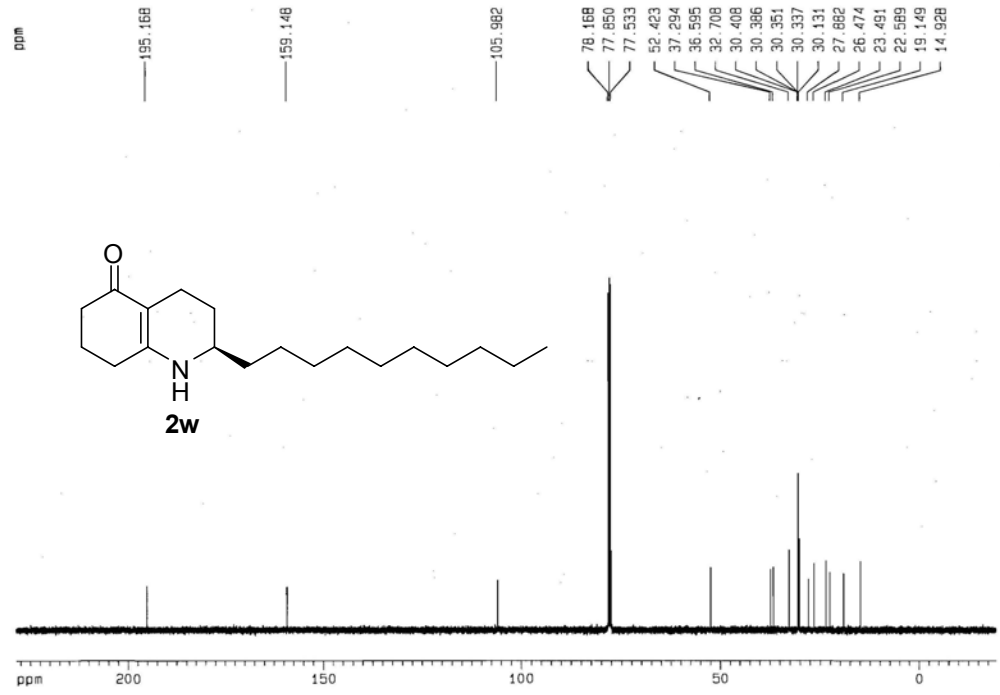
5
4
3
2
1
0


ppm
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105.982
78.168
77.850
77.533
52.423
37.294
36.595
32.708
30.408
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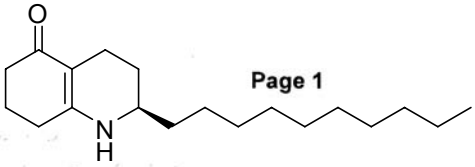
30.337
30.131
27.882
26.474
23.491
22.589
19.149
14.928
O
N
H
2w
ppm
200
150
100
50
0

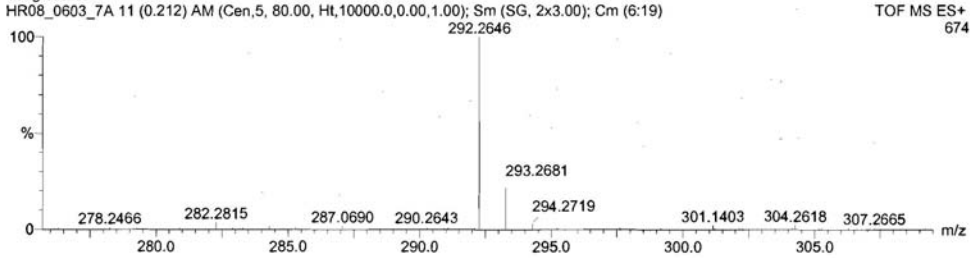
Elemental Composition Report



2w

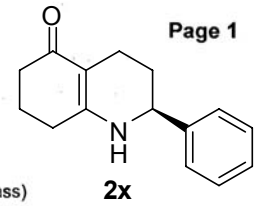
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_7A 11 (0.212) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (6:19) TOF MS ES+ 674



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.2646	292.2640	0.6	2.1	3.5	0.3	C19 H34 N O

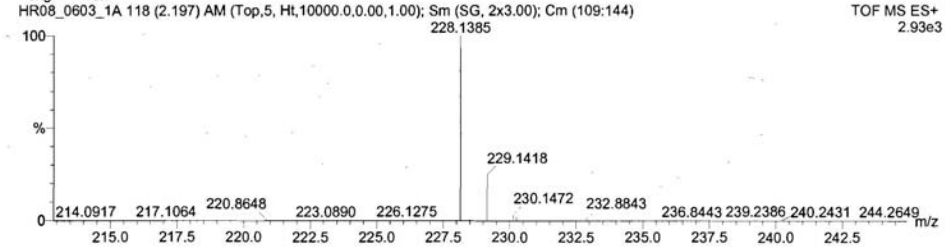
Elemental Composition Report



2x

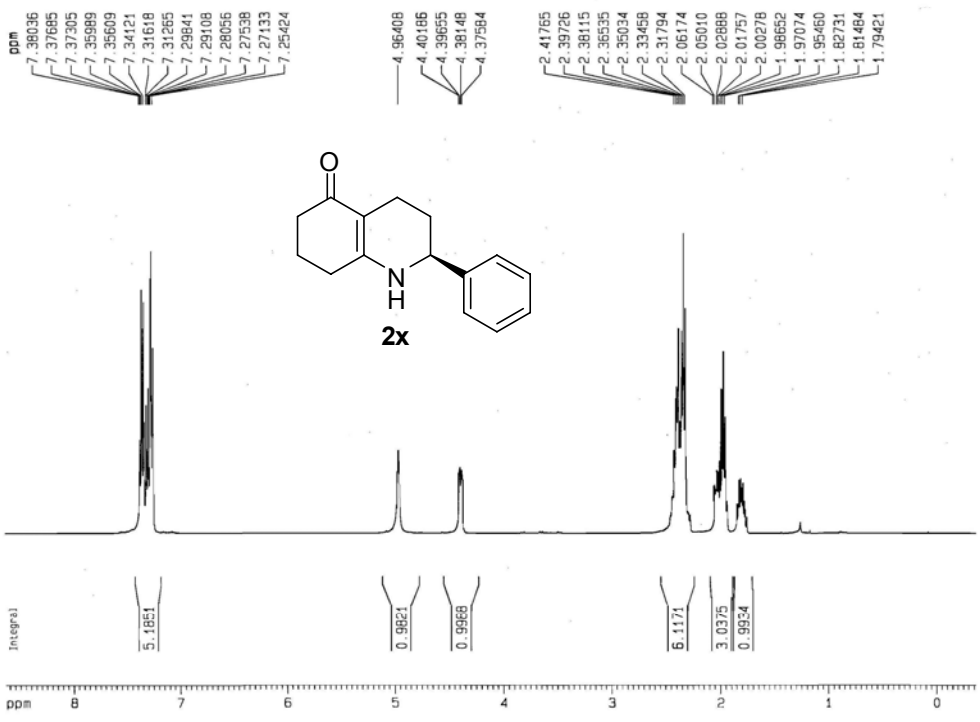
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

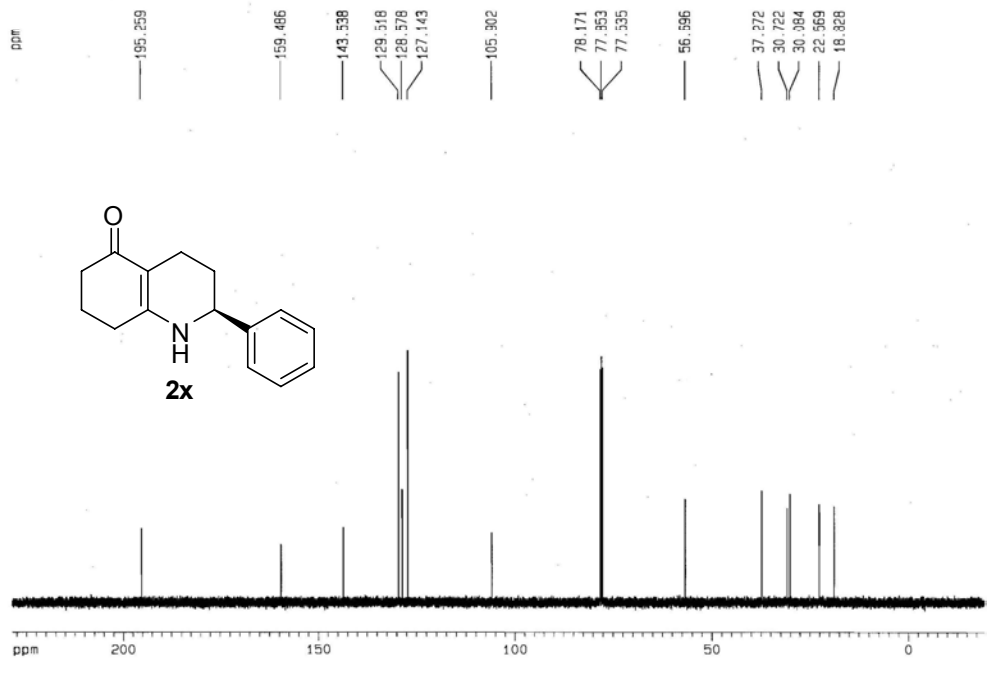
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2
Tong Wei Jun
HR08_0603_1A 118 (2.197) AM (Top,5, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (109:144) TOF MS ES+ 2.93e3



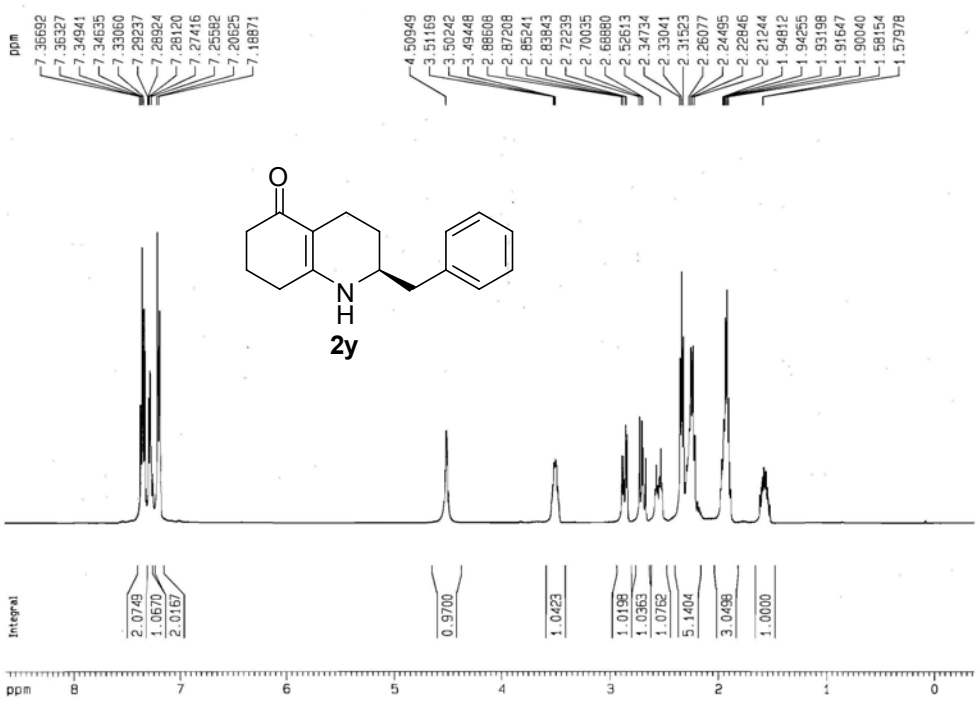
Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
228.1385	228.1388	-0.3	-1.3	7.5	40.5	C15 H18 N O

2-phenyl-2,3,4,6,7,8-hexahydroquinolin-5(1H)-one H

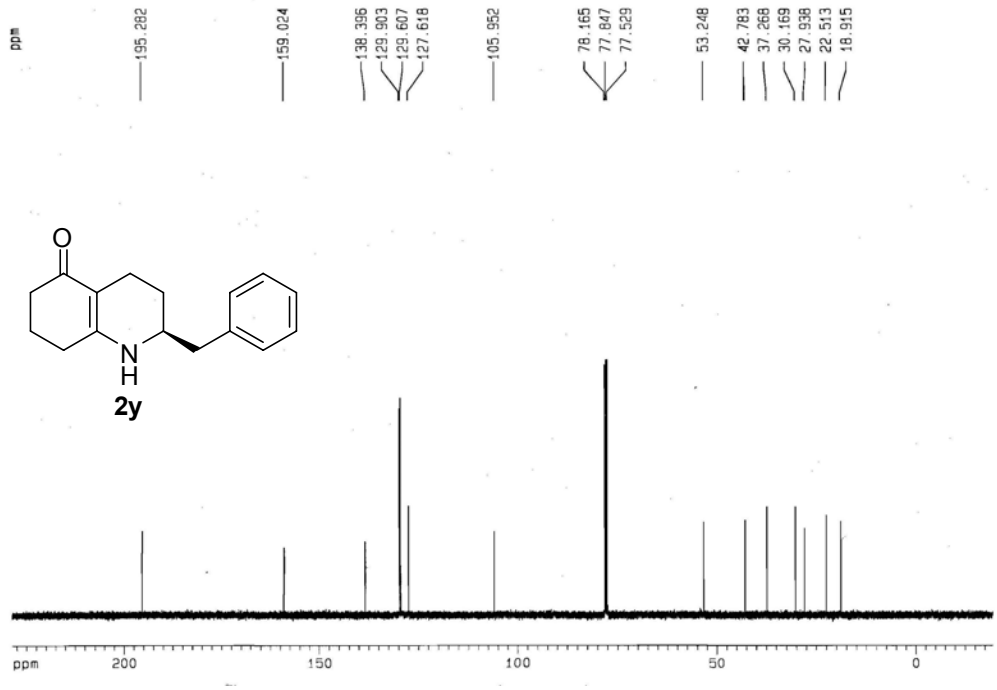




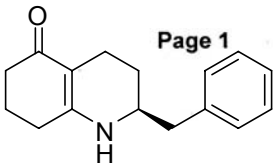
2-benzyl-2, 3, 4, 6, 7, 8-hexahydroquinolin-5(1H)-one H



2-benzyl-2, 3, 4, 6, 7, 8-hexahydroquinolin-5(1H)-one 13C



Elemental Composition Report



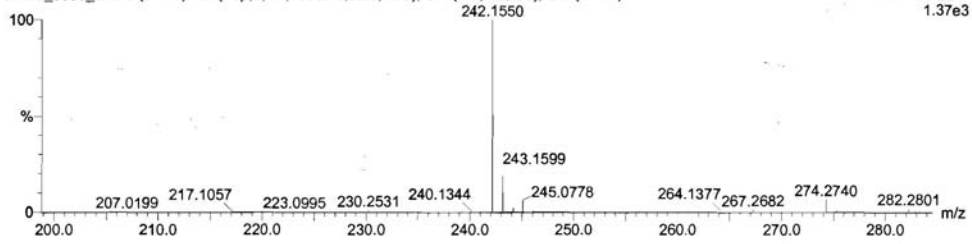
2y

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

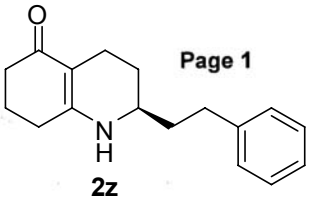
Tong Wei Jun
HR08_0603_9A 40 (0.750) AM (Top,5, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (40:53)

TOF MS ES+
1.37e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
242.1550	242.1545	0.5	2.1	7.5	0.5	C16 H20 N O

Elemental Composition Report



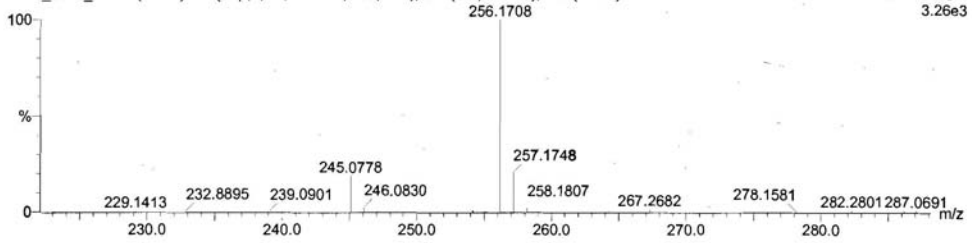
2z

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 60.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-26 H: 0-1000 N: 0-1 O: 0-2

Tong Wei Jun
HR08_0603_8A 34 (0.638) AM (Top,5, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (21:59)

TOF MS ES+
3.26e3



Minimum:				-1.5		
Maximum:		100.0	20.0	60.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.1708	256.1701	0.7	2.7	7.5	1.2	C17 H22 N O

2-ethylphenyl-2, 3, 4, 6, 7, 8-hexahydroquinolin-5(1H)-one H