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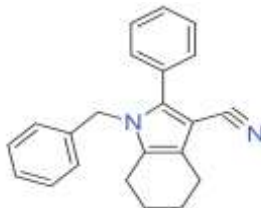
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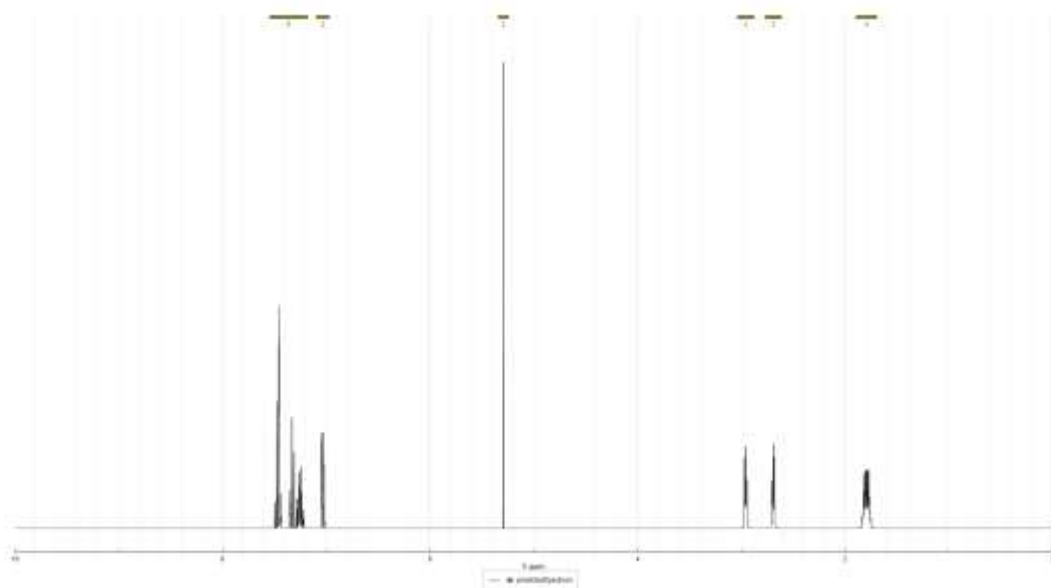
## APPENDICES

### A.1 Predicted $^1\text{H}$ NMR Spectra

#### A.1.1 2-Benzyl-4-cyano-6-phenyl-1,2,3,4-tetrahydroquinoline

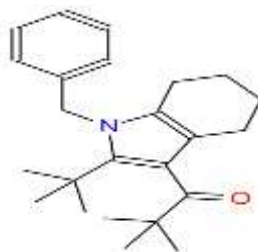


#### 2-Benzyl-4-cyano-6-phenyl-1,2,3,4-tetrahydroquinoline

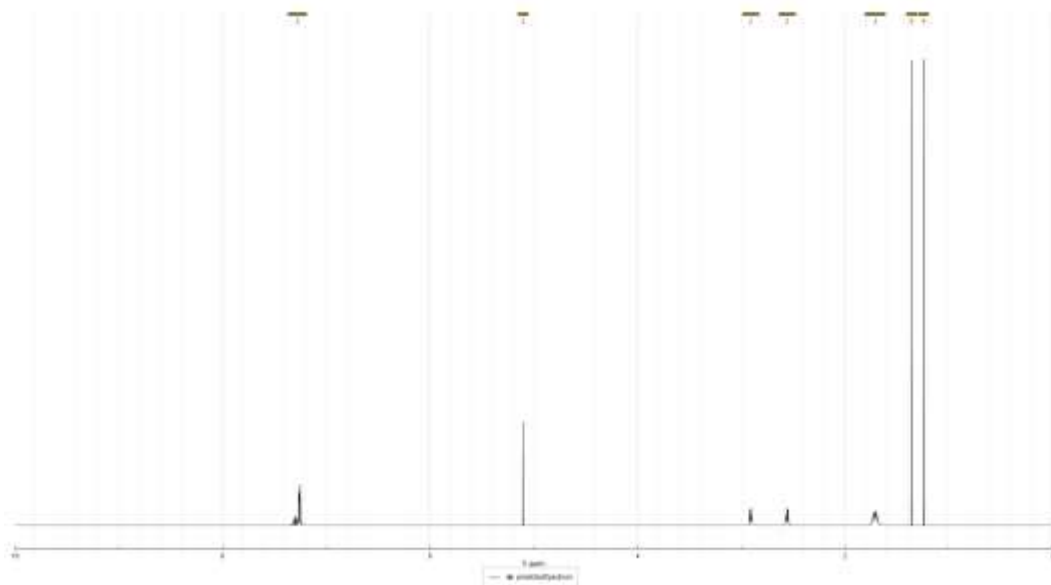


$^1\text{H}$  NMR:  $\delta$  1.69-1.89 (4H, 1.77 (dtdd,  $J = 13.1, 7.0, 2.9, 1.9$  Hz), 1.81 (dtdd,  $J = 13.7, 6.9, 2.9, 1.9$  Hz)), 2.69 (2H, ddd,  $J = 13.3, 7.0, 2.9$  Hz), 2.96 (2H, ddd,  $J = 14.2, 7.0, 2.9$  Hz), 5.29 (2H, s), 7.03 (2H, dddd,  $J = 7.8, 1.5, 1.3, 0.6$  Hz), 7.18-7.54 (8H, 7.24 (tt,  $J = 7.7, 1.5$  Hz), 7.26 (tdd,  $J = 7.5, 1.9, 1.4$  Hz), 7.33 (tdd,  $J = 7.7, 1.8, 0.6$  Hz), 7.45 (dddd,  $J = 7.8, 1.7, 1.4, 0.5$  Hz), 7.47 (dddd,  $J = 7.8, 7.5, 1.4, 0.5$  Hz)).

#### A.1.2 2-(tert-Butyl)-3-(cyclopenta[b]indol-3-yl)-1-(benzyl)pyrrole-3-one

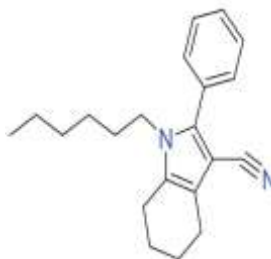


#### 2-(tert-Butyl)-3-(cyclopenta[b]indol-3-yl)-1-(benzyl)pyrrole-3-one



$^1\text{H NMR}$ :  $\delta$  1.24 (9H, s), 1.36 (9H, s), 1.61-1.81 (4H, 1.69 (dtdd,  $J = 13.7, 7.0, 2.9, 1.9$  Hz), 1.73 (dtdd,  $J = 13.9, 6.9, 2.9, 1.9$  Hz)), 2.56 (2H, ddd,  $J = 14.3, 7.0, 2.9$  Hz), 2.91 (2H, ddd,  $J = 14.2, 7.0, 2.9$  Hz), 5.10 (2H, s), 7.19-7.37 (5H, 7.25 (dddd,  $J = 7.8, 1.6, 1.3, 0.6$  Hz), 7.26 (tdd,  $J = 7.7, 1.8, 0.6$  Hz), 7.31 (tt,  $J = 7.7, 1.6$  Hz)).

### A.1.3 6-Hexyl-4-cyano-2,3,4,5-tetrahydrobenzo[h]quinoline



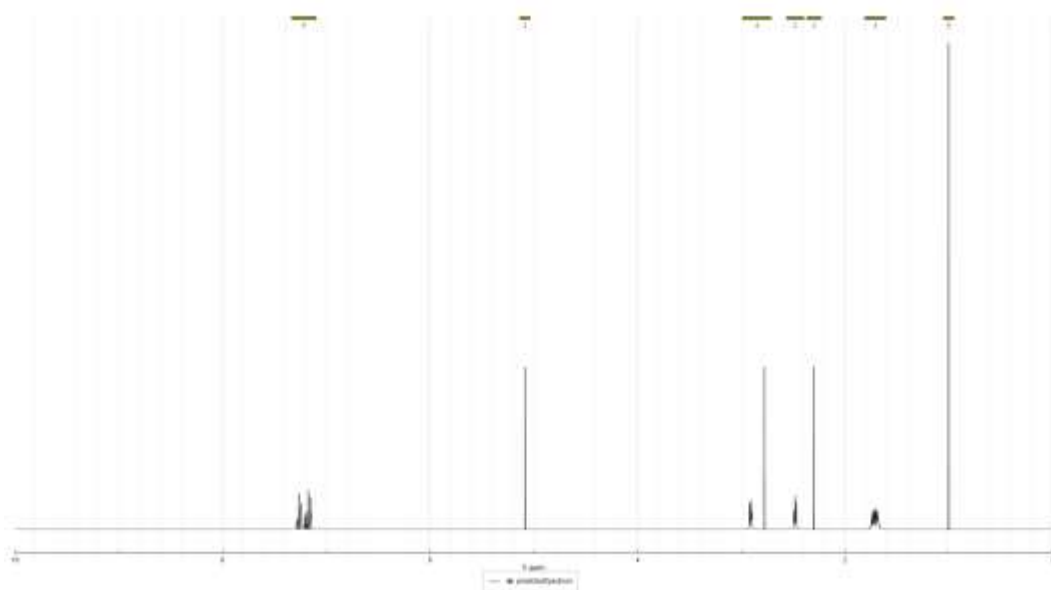
6-Hexyl-4-cyano-2,3,4,5-tetrahydrobenzo[h]quinoline



#### A.1.4 1-(Benzyl)-2,3,4,9-tetrahydro-2-tert-butyl-3-oxo-1H-cyclopenta[b]indole



#### 1-(Benzyl)-2,3,4,9-tetrahydro-2-tert-butyl-3-oxo-1H-cyclopenta[b]indole



$^1\text{H NMR}$ :  $\delta$  1.00 (6H, s), 1.61-1.81 (4H, 1.69 (dtdd,  $J = 13.7, 7.0, 2.9, 1.9$  Hz), 1.72 (dtdd,  $J = 13.8, 6.9, 2.9, 1.9$  Hz)), 2.31 (2H, d,  $J = 16.2$  Hz), 2.48 (2H, ddd,  $J = 16.8, 7.0, 2.9$  Hz), 2.71-2.99 (4H, 2.78 (d,  $J = 11.2$  Hz), 2.91 (ddd,  $J = 14.2, 7.0, 2.9$  Hz)), 5.08 (2H, s), 7.10-7.34 (5H, 7.16 (dddd,  $J = 7.9, 1.6, 1.3, 0.6$  Hz), 7.19 (tt,  $J = 7.7, 1.6$  Hz), 7.26 (dddd,  $J = 7.9, 7.7, 1.9, 0.6$  Hz)).

#### A.2 Reaction Data and Calculation

Theoretical yield

$$= \frac{\text{mass}_{\text{limiting reactant}} \times \text{purity}_{\text{limiting reactant}}}{MW_{\text{limiting reactant}}} \times MW_{\text{product}}$$

Note: 1 mol of 2-hydroxycyclohexanone dimer = 2 mol equivalent of 2-hydroxycyclohexanone

##### 1. Initial Reaction:

2-hydroxycyclohexanone dimer : 0.1176 g (0.51515 mmol)

3-oxo-3-phenylpropanenitrile	:	0.1511 g (1.04092 mmol)
Benzylamine	:	0.1197 g (purity unclear)
Triethylamine	:	0.0554 g (1.11713 mmol)
Theoretical yield	:	0.3260 g
<b>Yield</b>	:	<b>Incalculable</b>
$\frac{0.1176 \text{ g} \times 97\%}{228.28 \text{ g/mol}} \times 2 \text{ mol equiv.} \times \frac{316.44 \text{ g}}{\text{mol}} = 0.3260 \text{ g}$		

**2. Reaction 2,2,6,6-Tetramethyl-3,5-heptanedione and ZnCl<sub>2</sub>:**

2-hydroxycyclohexanone dimer	:	0.2358 g (1.02261 mmol)
2,2,6,6-tetramethyl-3,5-heptanedione	:	0.3735 g (1.94106 mmol)
Benzylamine	:	0.2383 g (purity unclear)
ZnCl <sub>2</sub>	:	0.1450 g (1.04255 mmol)
Theoretical yield	:	0.6823 g
<b>Yield</b>	:	<b>0.07 g (10.25%)</b>

$$\frac{0.3735 \text{ g} \times 99\%}{136.3 \text{ g/mol}} \times \frac{351.52 \text{ g}}{\text{mol}} = 0.6823 \text{ g}$$

**3. Reaction 2,2,6,6-Tetramethyl-3,5-heptanedione and AcOH:**

2-hydroxycyclohexanone dimer	:	0.2354 g (1.020875 mmol)
2,2,6,6-tetramethyl-3,5-heptanedione	:	0.3978 g (2.11550 mmol)
Benzylamine	:	0.2197 g (purity unclear)
AcOH	:	0.1046 g (0.86223 mmol)
Theoretical yield	:	0.7177 g
<b>Yield</b>	:	<b>0.085 g (11.84%)</b>

$$\frac{0.2354 \text{ g} \times 97\%}{228.28 \text{ g/mol}} \times 2 \text{ mol equiv.} \times \frac{351.52 \text{ g}}{\text{mol}} = 0.7177 \text{ g}$$

**4. Reaction 3-oxo-3-phenylpropanenitrile and 1-hexylamine:**

2-hydroxycyclohexanone dimer	:	0.1177 g (0.50012 mmol)
3-oxo-3-phenylpropanenitrile	:	0.1481 g (0.99984 mmol)
1-hexylamine	:	0.1222 g (1.19555 mmol)
Triethylamine	:	0.1084 g (1.0605 mmol)
Theoretical yield	:	0.3064 g
<b>Yield</b>	:	<b>Incalculable</b>

$$\frac{0.1481 \text{ g} \times 99\%}{145.16 \text{ g/mol}} \times \frac{306.438 \text{ g}}{\text{mol}} = 0.3064 \text{ g}$$

**5. Reaction 5,5-dimethyl-1,3-cyclohexanedione and DMAP**

2-hydroxycyclohexanone dimer	:	0.1192 g (0.50650 mmol)
5,5-dimethyl-1,3-cyclohexanedione	:	0.1506 g (1.02061 mmol)
Benzylamine	:	0.2651 g (purity unclear)
4-dimethylaminopyridine (DMAP)	:	0.0623 g (0.50484 mmol)
Theoretical yield	:	0.3210 g

$$\begin{aligned} \text{Yield} & : \quad \mathbf{0.1076 \text{ g (33.50\%)}} \\ & \frac{0.1192 \text{ g} \times 97\%}{228.28 \text{ g/mol}} \times 2 \text{ mol equiv.} \times \frac{307.42 \text{ g}}{\text{mol}} = 0.3210 \text{ g} \end{aligned}$$

**6. Reaction 5,5-dimethyl-1,3-cyclohexanedione and AcOH**

2-hydroxycyclohexanone dimer	:	0.1188 g (0.50480 mmol)
5,5-dimethyl-1,3-cyclohexanedione	:	0.1479 g (1.00231 mmol)
Benzylamine	:	0.2571 g (purity unclear)
AcOH	:	0.0716 g (0.59020 mmol)
Theoretical yield	:	0.3199 g
<b>Yield</b>	:	<b>0.1085 g (33.90%)</b>

$$\frac{0.1479 \text{ g} \times 95\%}{140.18 \text{ g/mol}} \times \frac{307.42 \text{ g}}{\text{mol}} = 0.3199 \text{ g}$$