

*Supporting Information*

**Tandem Palladium-Catalyzed Addition/Cyclocarbonylation: An Efficient Synthesis of 2-Heteroquinazolin-4(3*H*)-ones**

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**Experimental Section (Supporting Information)**

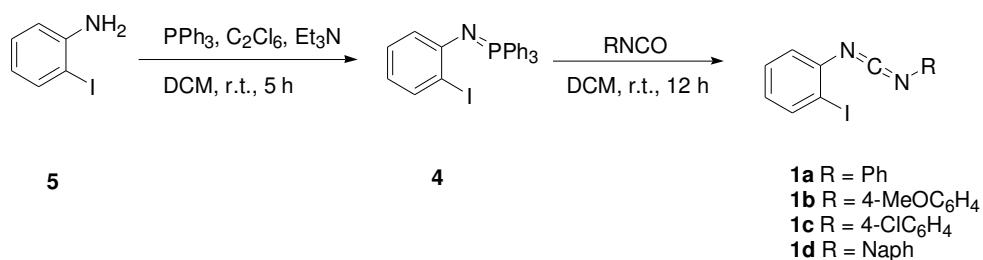
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## I General Considerations

Unless otherwise noted, all the materials were purchased from commercial suppliers and used as received. Solvents were freshly distilled by standard procedure prior to use. Flash chromatography was performed on silica gel 60Å (Aldrich, 200-425 mesh) with the indicated eluant. All  $^1\text{H}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra were recorded on a Bruker 400 MHz spectrometer. The NMR chemical shift values refer to  $\text{CDCl}_3$  ( $\delta(^1\text{H})$ , 7.26 ppm;  $\delta(^{13}\text{C})$ , 77.16 ppm). Mass spectra were obtained on a VG7070E mass spectrometer. IR Spectra were recorded on a Shimadzu FTIR-8400S spectrometer.

## II General Procedure for the Preparation of Starting Materials



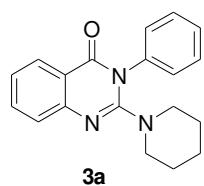
**General Procedure for the Synthesis of Aza-Wittig Reagents 4.<sup>1,2</sup>** To a mixture of 2-iodoaniline (1.00 g, 4.57 mmol), PPh<sub>3</sub> (1.80 g, 6.86 mmol) and C<sub>2</sub>Cl<sub>6</sub> (1.62 g, 6.86 mmol) in dry CH<sub>2</sub>Cl<sub>2</sub> (40 mL), Et<sub>3</sub>N (1.40 g, 13.84 mmol) was added dropwise at 25 °C. After being stirred for 5 h, the reaction mixture was concentrated under reduced pressure. The residue was extracted by EtOAc (100 mL), filtered through Celite (5 cm). All the volatiles were removed under reduced pressure. Isolation by silica gel column chromatography with EtOAc/Hexanes (v/v = 1:6) as the eluant afforded **4** as a white solid (1.30 g, 98%).

**General Procedure for the Synthesis of *O*-iodoarylcarbodiimides 1a-d.**<sup>3, 4, 5</sup> To a

stirred solution of an aza-Wittig reagent **4** (10 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (50 mL), an isocyanate R<sub>2</sub>-NCO (10 mmol) was added dropwise, and then the resulting mixture was stirred at room temperature for 12 h. The solvent was evaporated under reduced pressure. Isolation by silica gel column chromatography with EtOAc/Hexanes (v/v = 1:12) as the eluent afforded the corresponding *o*-idoarylcarbodiimides **1a-d**.

### III General Procedure for the Palladium-Catalyzed Synthesis of 2-Heteroquinazolin-4(3H)-ones

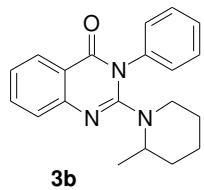
A mixture of **1** (0.50 mmol), K<sub>2</sub>CO<sub>3</sub> (1.00 mmol), Pd(OAc)<sub>2</sub>, (0.020 mmol), PPh<sub>3</sub>, (0.040 mmol), tetrahydrofuran (6 mL) and **2** (0.55 mmol) were sequentially added to a 45 mL glass-lined autoclave. After sealing, the autoclave was purged three times with carbon monoxide and pressurized with 100 psi of CO, and then heated at 80 °C for 15 h. The autoclave was removed from the oil bath and cooled to room temperature prior to the release of excess carbon monoxide. The reaction mixture was filtered and the filtrate was concentrated by rotary evaporator. The residue was purified by flash chromatography on silica gel with a mixture of hexanes and ethyl acetate (7:1 to 3:1) as the eluant to afford the products **3a-u**.



#### 2-(Piperidin-1'-yl)-3-phenylquinazolin-4(3H)-one<sup>6</sup>

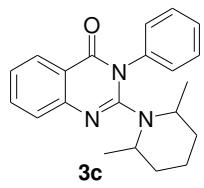
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.20-1.26 (m, 4 H), 1.38-1.44 (m, 2 H), 3.09 (t, J = 4.0 Hz , 4 H), 7.25-7.29 (m, 1 H), 7.35-7.40 (m, 3 H), 7.46-7.52 (m, 3 H), 7.63-7.67

(m, 1 H), 8.16-8.18 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  24.2, 25.0, 50.3, 119.3, 124.5, 125.9, 127.5, 128.0, 128.8, 128.9, 134.6, 137.9, 148.2, 155.0, 163.6; IR (neat)  $\text{cm}^{-1}$ : 1684 [(C=O)]; MS (EI)  $m/z$  305 ( $\text{M}^+$ ).



### 2-(2'-Methylpiperidin-1'-yl)-3-phenylquinazolin-4(3H)-one

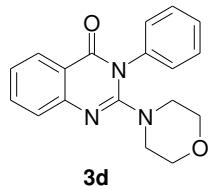
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  1.06 (d,  $J = 6.6$  Hz, 3 H), 1.14-1.25 (m, 2 H), 1.29-1.40 (m, 3 H), 1.45-1.58 (m, 1 H), 2.99-3.10 (m, 1 H), 3.11-3.23 (m, 1 H), 3.63-3.74 (m, 1 H), 7.27-7.40 (m, 4 H), 7.44-7.57 (m, 2 H), 7.50-7.55 (m, 1 H), 7.63-7.74 (m, 1 H), 8.16-8.26 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  16.0, 20.2, 25.0, 30.9, 46.0, 51.8, 119.5, 124.5, 126.1, 127.4, 127.8, 128.7, 128.9, 134.5, 138.0, 148.1, 154.6, 163.7; IR (neat)  $\text{cm}^{-1}$ : 1680 [(C=O)]; MS (EI)  $m/z$  319 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}$  ( $\text{M}^+$ ) 319.1685, found 319.1677.



### 2-(2',6'-Dimethylpiperidin-1'-yl)-3-phenylquinazolin-4(3H)-one

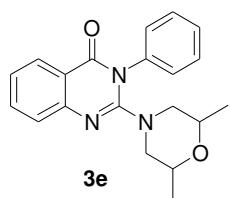
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  0.97 (d,  $J = 6.7$  Hz, 6 H), 1.06-1.18 (m, 2 H), 1.37-1.49 (m, 1 H), 1.55-1.66 (m, 3 H), 3.33-3.46 (m, 2 H), 7.23-7.32 (m, 2 H), 7.35-7.43 (m, 2 H), 7.44-7.50 (m, 2 H), 7.62-7.66 (m, 1 H), 7.66-7.78 (m, 1 H), 8.21-8.33 (m, 1 H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 20.5, 20.7, 32.3, 56.5, 120.3, 125.6, 126.6, 127.4, 127.9, 128.5, 129.6, 134.5, 138.0, 147.8, 156.5, 163.9; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) *m/z* 333 (M<sup>+</sup>); HRMS (EI) *m/z* calcd for C<sub>21</sub>H<sub>23</sub>N<sub>3</sub>O (M<sup>+</sup>) 333.1841, found 333.1850.



### 2-(Morpholin-1'-yl)-3-phenylquinazolin-4(3*H*)-one<sup>6</sup>

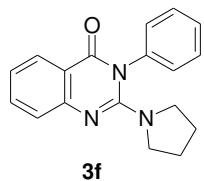
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 3.14 (t, *J* = 8.0 Hz, 4 H), 3.43 (t, *J* = 8.0 Hz, 4 H), 7.29-7.35 (m, 1 H), 7.36-7.45 (m, 3 H), 7.47-7.58 (m, 3 H), 7.65-7.74 (m, 1 H), 8.16-8.24 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 49.4, 66.1, 119.4, 124.9, 126.1, 127.5, 128.4, 128.8, 129.0, 134.7, 137.2, 147.8, 153.8, 163.3; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) *m/z* 307 (M<sup>+</sup>).



### 2-(3',5'-Dimethylmorpholin-1'-yl)-3-phenylquinazolin-4(3*H*)-one

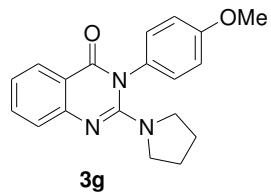
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.01 (d, *J* = 8.0 Hz, 6 H), 2.42-2.52 (m, 2 H), 3.24-3.33 (m, 2 H), 3.34-3.36 (m, 2 H), 7.27-7.33 (m, 1 H), 7.34-7.44 (m, 3 H), 7.45-7.55 (m, 3 H), 7.60-7.73 (m, 1 H), 8.14-8.26 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 18.7, 54.3, 71.0, 119.3, 124.8, 126.0, 127.5, 128.4, 128.8, 128.9, 134.7, 137.4, 147.9, 153.5, 163.3; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) *m/z* 335 (M<sup>+</sup>); HRMS (EI) *m/z* calcd

for C<sub>20</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub> (M<sup>+</sup>) 335.1634, found 335.1610.



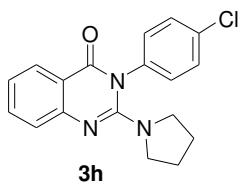
**2-(Pyrrolidin-1'-yl)-3-phenylquinazolin-4(3H)-one<sup>6</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.65-1.77 (m, 4 H), 3.07 (t, J = 16.0 Hz, 4 H), 7.10-7.20 (m, 1 H), 7.33-7.37 (m, 2 H), 7.39-7.49 (m, 4 H), 7.53-7.65 (m, 1 H), 8.08-8.18 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 25.5, 50.0, 117.6, 122.7, 125.1, 127.4, 128.2, 129.1, 129.3, 134.6, 138.0, 149.4, 151.8, 163.8; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) m/z 291 (M<sup>+</sup>).



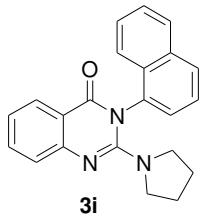
**2-(Pyrrolidin-1'-yl)-3-(4''-methoxyphenyl)quinazolin-4(3H)-one**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.66-1.79 (m, 4 H), 3.04-3.16 (m, 4 H) 3.84 (s, 3 H), 6.93-7.03 (m, 2 H), 7.08-7.20 (m, 1 H), 7.19-7.30 (m, 2 H), 7.37-7.43 (m, 1 H), 7.52-7.63 (m, 1 H), 8.05-8.15 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 25.5, 50.1, 55.5, 114.3, 117.6, 122.6, 125.0, 127.4, 130.2, 130.5, 134.6, 149.4, 152.1, 159.1, 164.1; IR (neat) cm<sup>-1</sup>: 1680 [(C=O)]; MS (EI) m/z 321 (M<sup>+</sup>); HRMS (EI) m/z calcd for C<sub>19</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub> (M<sup>+</sup>) 321.1477, found 321.1476.



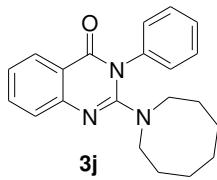
**2-(Pyrrolidin-1'-yl)-3-(4''-chlorophenyl)quinazolin-4(3H)-one<sup>6</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.69-1.82 (m, 4 H), 3.09 (t, *J* = 12.0 Hz, 4 H), 7.12-7.22 (m, 1 H), 7.24-7.35 (m, 2 H), 7.37-7.50 (m, 3 H), 7.56-7.66 (m, 1 H), 8.06-8.15 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 25.5, 50.2, 117.5, 123.0, 125.2, 127.4, 129.3, 130.6, 134.1, 134.8, 136.5, 149.3, 151.6, 163.6; IR (neat) cm<sup>-1</sup>: 1680 [(C=O)]; MS (EI) *m/z* 325 (M<sup>+</sup>).



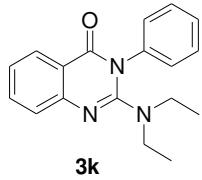
**2-(Pyrrolidin-1'-yl)-3-naphthylquinazolin-4(3H)-one**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.52-1.64 (m, 4 H), 2.89-3.01 (m, 4 H), 7.15-7.24 (m, 1 H), 7.42-7.59 (m, 5 H), 7.58-7.69 (m, 2 H), 7.87-7.96 (m, 2 H), 8.10-8.20 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 25.5, 49.9, 117.4, 122.8, 122.8, 125.1, 125.5, 126.5, 127.2, 127.5, 127.5, 128.6, 129.5, 131.3, 134.1, 134.8, 134.9, 149.7, 152.1, 164.0; IR (neat) cm<sup>-1</sup>: 1680 [(C=O)]; MS (EI) *m/z* 341 (M<sup>+</sup>); HRMS (EI) *m/z* calcd for C<sub>22</sub>H<sub>19</sub>N<sub>3</sub>O (M<sup>+</sup>) 341.1528, found 341.1514.



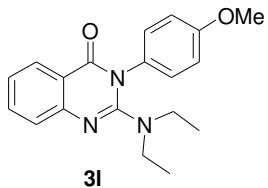
**2-Cyclooctylamino-3-phenylquinazolin-4(3H)-one**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 1.39-1.51 (m, 10 H), 3.27 (t, *J* = 5.5 Hz, 4 H), 7.16-7.25 (m, 1 H), 7.30-7.53 (m, 6 H), 7.58-7.67 (m, 1 H), 8.08-8.16 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 24.5, 26.8, 27.0, 52.2, 118.2, 123.3, 125.5, 127.4, 128.1, 128.8, 129.0, 134.6, 138.4, 148.9, 154.1, 164.2; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) *m/z* 333 (M<sup>+</sup>); HRMS (EI) *m/z* calcd for C<sub>21</sub>H<sub>23</sub>N<sub>3</sub>O (M<sup>+</sup>) 333.1841, found 333.1850.



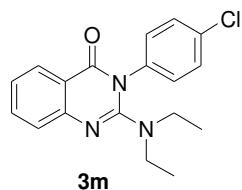
**2-(Diethylamino)-3-phenylquinazolin-4(3H)-one<sup>6</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 0.82 (t, *J* = 7.1 Hz, 6 H), 3.08 (q, *J* = 7.0 Hz, 4 H), 7.21-7.27 (m, 1 H), 7.34-7.41 (m, 1 H), 7.42-7.53 (m, 3 H), 7.60-7.66 (m, 1 H), 8.12-8.20 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 12.6, 45.1, 119.0, 124.2, 125.9, 127.4, 128.0, 129.0, 129.1, 134.5, 138.1, 148.3, 154.0, 163.9; IR (neat) cm<sup>-1</sup>: 1680 [(C=O)]; MS (EI) *m/z* 293 (M<sup>+</sup>).



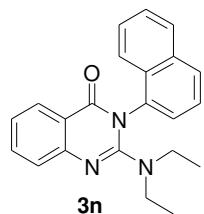
**2-(Diethylamino)-3-(4'-methoylphenyl)quinazolin-4(3*H*)-one**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 0.85 (t, *J* = 7.0 Hz, 6 H), 3.09 (q, *J* = 7.0 Hz, 4 H) 3.82 (s, 3 H), 6.85-7.05 (m, 2 H), 7.17-7.28 (m, 3 H), 7.44-7.52 (m, 1 H), 7.57-7.66 (m, 1 H), 8.09-8.19 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 12.7, 45.0, 55.5, 114.2, 119.0, 124.1, 125.8, 127.3, 129.9, 130.6, 134.5, 148.2, 154.2, 159.0, 164.1; IR (neat) cm<sup>-1</sup>: 1684 [(C=O)]; MS (EI) *m/z* 323 (M<sup>+</sup>); HRMS (EI) *m/z* calcd for C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub> (M<sup>+</sup>) 323.1634, found 323.1631.



**2-(Diethylamino)-3-(4'-chlorophenyl)quinazolin-4(3*H*)-one<sup>6</sup>**

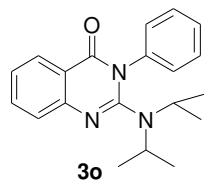
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 0.86 (t, *J* = 7.0 Hz, 6 H), 3.07 (q, *J* = 7.0 Hz, 4 H) 7.20-7.32 (m, 3 H), 7.40-7.53 (m, 3 H), 7.63-7.69 (m, 1 H), 8.11-8.17 (m, 1 H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, 23 °C): δ 12.6, 45.0, 118.9, 124.4, 126.0, 127.4, 129.2, 130.4, 133.9, 134.7, 136.5, 148.1, 153.6, 163.6; IR (neat) cm<sup>-1</sup>: 1680 [(C=O)]; MS (EI) *m/z* 327 (M<sup>+</sup>).



**2-(Diethylamino)-3-naphthylquinazolin-4(3*H*)-one**

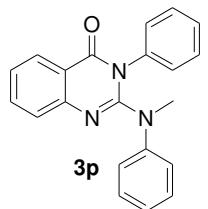
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 23 °C): δ 0.64 (t, *J* = 8.0 Hz, 6 H), 2.97-3.14 (m, 4 H),

7.27-7.35 (m, 1 H), 7.44-7.55 (m, 4 H), 7.56-7.63 (m, 2 H), 7.65-7.72 (m, 1 H), 7.88-8.00 (m, 2 H), 8.16-8.26 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  12.6, 45.4, 119.0, 122.8, 124.3, 125.4, 126.0, 126.4, 127.2, 127.6, 127.7, 128.6, 129.2, 130.4, 134.5, 134.7, 134.9, 148.5, 154.7, 164.2; IR (neat)  $\text{cm}^{-1}$ : 1684 [(C=O)]; MS (EI)  $m/z$  343 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{N}_3\text{O}$  ( $\text{M}^+$ ) 343.1685, found 343.1658.



### **2-(Diisopropylamino)-3-phenylquinazolin-4(3H)-one<sup>6</sup>**

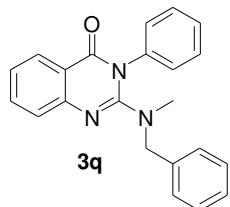
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  1.11 (d,  $J = 6.7$  Hz, 12 H), 3.48-3.61 (m, 2 H), 7.22-7.27 (m, 1 H), 7.27-7.34 (m, 1 H), 7.34-7.41 (m, 1 H), 7.43-7.54 (m, 3 H), 7.61-7.67 (m, 1 H), 8.09-8.21 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  21.7, 49.9, 119.2, 124.0, 126.1, 127.3, 127.9, 128.8, 129.4, 134.4, 138.9, 148.3, 152.8, 164.5; IR (neat)  $\text{cm}^{-1}$ : 1680 [(C=O)]; MS (EI)  $m/z$  321 ( $\text{M}^+$ ).



### **2-(N-methylanilino)-3-phenylquinazolin-4(3H)-one**

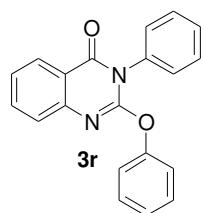
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  3.33 (s, 3 H), 6.56-6.67 (m, 2 H), 6.75-6.85 (m, 2 H), 6.96-7.06 (m, 3 H), 7.07-7.14 (m, 3 H), 7.29-7.38 (m, 1 H), 7.60-7.68 (m, 1 H), 7.69-7.77 (m, 1 H), 8.17-8.27 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  42.7,

119.6, 124.8, 124.9, 125.1, 126.1, 127.4, 127.5, 128.2, 128.8, 129.2, 134.7, 137.1, 147.0, 148.1, 153.0, 163.5; IR (neat)  $\text{cm}^{-1}$ : 1684 [(C=O)]; MS (EI)  $m/z$  327 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{17}\text{N}_3\text{O}$  ( $\text{M}^+$ ) 327.1372, found 327.1371.



### **2-(N-methylbenzylamino)-3-phenylquinazolin-4(3H)-one**

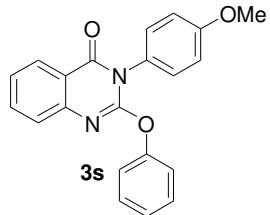
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  2.49 (s, 3 H), 4.35 (s, 2 H), 7.02-7.11 (m, 2 H), 7.18-7.32 (m, 4 H), 7.33-7.42 (m, 3 H), 7.43-7.51 (m, 2 H), 7.52-7.57 (m, 1 H), 7.63-7.72 (m, 1 H), 8.15-8.24 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  38.5, 56.8, 119.0, 124.3, 125.8, 127.3, 127.5, 128.2, 128.3, 128.4, 129.0, 129.1, 134.7, 137.2, 137.8, 148.2, 154.7, 163.7; IR (neat)  $\text{cm}^{-1}$ : 1684 [(C=O)]; MS (EI)  $m/z$  341 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}$  ( $\text{M}^+$ ) 341.1528, found 341.1520.



### **2-Phenoxy-3-phenylquinazolin-4(3H)-one**

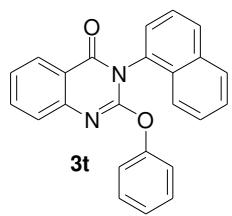
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  7.16-7.22 (m, 2 H), 7.23-7.29 (m, 1 H) 7.33-7.48 (m, 6 H), 7.48-7.52 (m, 1 H), 7.53-7.60 (m, 2 H), 7.63-7.71 (m, 1 H), 8.23-8.30 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  119.6, 121.6, 125.4, 125.9, 126.3, 127.6,

128.3, 129.1, 129.5, 129.6, 134.8, 135.3, 146.9, 151.8, 151.9, 163.0; IR (neat)  $\text{cm}^{-1}$ : 1693 [(C=O)]; MS (EI)  $m/z$  314 ( $M^+$ ); HRMS (EI)  $m/z$  calcd for  $C_{20}\text{H}_{14}\text{N}_2\text{O}_2$  ( $M^+$ ) 314.1055, found 314.1071.



### **2-Phenoxy-3-(4'-methoxyphenyl)quinazolin-4(3H)-one**

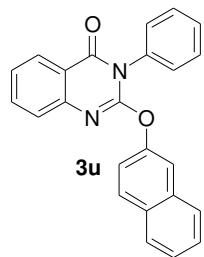
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  3.84 (s, 3 H), 6.99-7.07 (m, 2 H), 7.16-7.19 (m, 2 H), 7.21-7.26 (m, 1 H), 7.27-7.44 (m, 6 H), 7.58-7.69 (m, 1 H), 8.20-8.27 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  55.6, 114.9, 119.6, 121.7, 125.3, 125.9, 126.3, 127.6, 127.8, 129.2, 129.5, 134.8, 146.9, 152.0, 152.2, 159.9, 163.2; IR (neat)  $\text{cm}^{-1}$ : 1697 [(C=O)]; MS (EI)  $m/z$  344 ( $M^+$ ); HRMS (EI)  $m/z$  calcd for  $C_{21}\text{H}_{16}\text{N}_2\text{O}_3$  ( $M^+$ ) 344.1161, found 344.1153.



### **2-Phenoxy-3-naphthylquinazolin-4(3H)-one**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  7.05-7.16 (m, 2 H), 7.19-7.27 (m, 1 H) 7.32-7.39 (m, 2 H), 7.40-7.47 (m, 1 H), 7.52-7.60 (m, 3 H), 7.61-7.79 (m, 4 H), 7.96-8.08 (m, 2 H), 8.31-8.40 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  119.6, 121.7, 121.7,

125.5, 125.7, 126.0, 126.5, 126.7, 127.6, 127.8, 128.8, 129.4, 129.8, 130.1, 130.4, 132.0, 134.6, 135.0, 147.2, 151.8, 152.5, 163.1; IR (neat)  $\text{cm}^{-1}$ : 1693 [(C=O)]; MS (EI)  $m/z$  364 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_2$  ( $\text{M}^+$ ) 364.1212, found 364.1236.



### **2-(2'-Naphthoxyl)-3-phenylquinazolin-4(3*H*)-one**

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  7.33-7.45 (m, 3 H), 7.46-7.56 (m, 5 H), 7.57-7.73 (m, 4 H), 7.79-7.85 (m, 1 H), 7.85-7.93 (m, 2 H), 8.27-8.33 (m, 1 H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ , 23 °C):  $\delta$  118.4, 119.7, 121.4, 125.4, 125.9, 126.3, 126.7, 127.6, 127.7, 127.9, 128.3, 129.1, 129.4, 129.6, 131.5, 133.8, 134.9, 135.3, 146.9, 149.5, 152.0, 163.0; IR (neat)  $\text{cm}^{-1}$ : 1691 [(C=O)]; MS (EI)  $m/z$  364 ( $\text{M}^+$ ); HRMS (EI)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_2$  ( $\text{M}^+$ ) 364.1212, found 364.1224.

### **References**

- (1) Schmittel, M.; Rodríguez, D.; Stenffen, J.-P. *Angew. Chem. Int. Ed.* **2000**, *39*, 2152.
- (2) Huang, N.-Y.; Liu, M.-G.; Ding, M.-W. *J. Org. Chem.* **2009**, *74*, 6874.
- (3) Lv, X.; Bao, W.-L. *J. Org. Chem.* **2009**, *74*, 5618.
- (4) Vicente, J.; Abad, J.-A.; López-Serrano, J. *Organometallics* **2004**, *23*, 4711.
- (5) Vicente, J.; Abad, J.-A.; Clemente, R.; López-Serrano, J. *Organometallics* **2003**, *22*, 4248.
- (6) Ding, M.-W.; Zeng, G.-P.; Wu, T.-J. *Syn. Commun.* **2000**, *30*, 1599.

#### IV NMR Spectra for Products 3a-u

