

## Supporting Information

### Microwave promoted efficient and green synthesis of dihydroquinazolines

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## 1. (a) General Information

Melting points were measured with a Buchi B-540 melting point apparatus and are uncorrected. IR spectra were recorded on a SHIMADZU FTIR-8400. NMR spectra were recorded on Advance DPX 300 MHz FT-NMR spectrometer using tetramethylsilane (TMS) as an internal standard. Mass spectra were recorded on ESQUIRE 3000 Mass spectrometer. All the commercially available reagents were used as received. All experiments were monitored by thin layer chromatography (TLC). TLC was performed on pre-coated silica gel plates (Merck). After elution, plate was visualized under UV illumination at 254 nm for UV active materials. Further visualization was achieved by staining  $\text{KMnO}_4$  and warming in a hot air oven. Column chromatography was performed on silica gel (100-200 mesh, Merck) using ethyl acetate: hexane as eluent.

## 1. (b) Microwave Instrumentation

All MW reactions were carried out in a Synthos 3000 (Anton Paar) microwave reactor. The multitude microwave has a twin magnetron (2.45 GHz) with maximum output power of 1400 W. The output power can be controlled in unpulsed control mode over whole power range which is adjustable in 1 W increments. A Motorola 68xxx series microprocessor system control is used to measure temperature, pressure, time and power during the reaction. The temperature and pressure were monitored throughout the reaction by an infrared detector. The temperature can be measured from 0 to 280 °C with uncertainty  $\pm 1\%$ . The pressure can be measured from 0 to 86 bar with uncertainty  $\pm 0.2$  bar. All parameters like temperature, pressure, time and power are displayed in an illuminated LCD display during the reaction.

## 2. General Procedure for Synthesis of Quinazolines

### 2.(a) Under MW Irradiations Using Urea

2-aminobenzophenone **1** (1 mmol), an aldehyde **2** (1 mmol) and urea (1.5 mmol) were irradiated in a closed vessel in absence of any solvent in a Synthos 3000 microwave reactor at

540 Watt, 140 °C and 10.9 bar for 4 minutes. The crude product mixture was dissolved in ethyl acetate and directly column chromatographed using 2:8 ethyl acetate:hexane as the eluent to get pure 1,2-dihydroquinazoline **3** and quinazoline **4**.

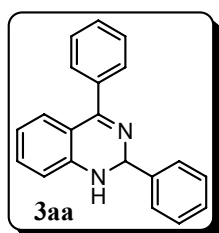
### **2.(b) Under MW Irradiations Using Ammonium Acetate**

2-aminobenzophenone **1** (1 mmol), an aldehyde **2** (1 mmol) and ammonium acetate (1.5 mmol) were irradiated in a closed vessel for 2 min in absence of any solvent in a Synthos 3000 microwave reactor at 540 Watt, 130 °C and 15 bar pressure. The crude product mixture was dissolved in ethyl acetate and directly column chromatographed using 2:8 ethyl acetate:hexane as the eluent to get pure 1,4-dihydroquinazoline **3** and quinazoline **4**.

### **2.(a) Under Classical Conditions Using Ammonium Acetate**

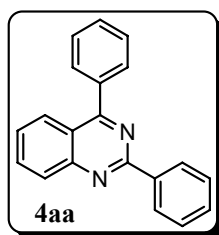
2-aminobenzophenone **1** (1 mmol), an aldehyde **2** (1 mmol) and ammonium acetate (1.5 mmol) were refluxed in acetic acid under air for 10 h. The reaction mixture was poured in water, neutralised with potassium bicarbonate solution and extracted with ethyl acetate and dried over anhydrous sodium sulphate. It was filtered and purified by column chromatography using 2:8 ethyl acetate:hexane as the eluent to get the products 1,4-dihydroquinazoline **3** and quinazoline **4**.

### 3. Characterization data of the Products



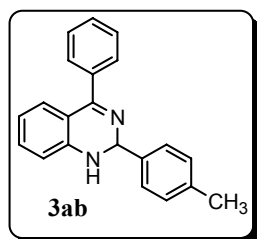
#### 2,4-Diphenyl-1,2-dihydroquinazoline (3aa)

Yellow solid; m.p. 95-97 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.10-8.07 (m, 1H, arom.), 7.62-7.25 (m, 11H, arom.), 6.72-6.66 (m, 2H, arom.), 5.98 (s, 1H, CH), 4.58 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.95, 146.81, 142.42, 137.89, 132.95, 129.29, 129.03, 128.66, 128.58, 128.14, 128.12, 127.32, 118.24, 117.81, 114.31, 72.29; IR (thin film,  $\text{cm}^{-1}$ ) 3328.3, 1615.0, 1538.2, 753.7, 699.1; MS (GCMS,  $m/z$ ) 284.1 [ $\text{M}$ ] $^+$



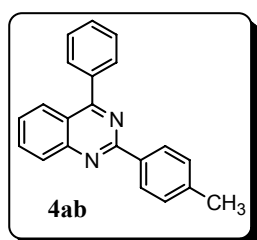
#### 2,4-Diphenylquinazoline (4aa)

Light brown solid; m.p. 115-116 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.71-8.68 (m, 2H, arom.), 8.15-8.12 (m, 2H, arom.), 7.91-7.88 (m, 2H, arom.), 7.61-7.51 (m, 8H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  168.35, 160.26, 152.01, 138.23, 137.69, 133.59, 130.55, 130.23, 129.97, 129.18, 129.10, 128.70, 128.58, 127.15, 127.05, 121.71; IR (thin film,  $\text{cm}^{-1}$ ) 1613.1, 1561.2, 1538.6, 1341.9, 772.0, 699.6; MS (GCMS,  $m/z$ ) 282.1 [ $\text{M}$ ] $^+$



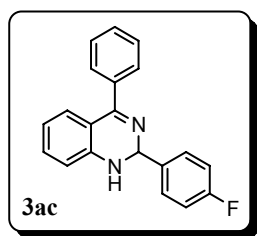
### 2-(4-Methylphenyl)-4-phenyl-1,2-dihydroquinazoline (3ab)

Yellow solid; m.p. 127-129 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.59-7.15 (m, 11H, arom.), 6.71-6.64 (m, 2H, arom.), 5.91 (s, 1H, CH), 4.24 (s, br, 1H, NH), 2.35 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.71, 146.86, 139.62, 138.07, 132.80, 129.39, 129.30, 129.28, 129.15, 128.92, 127.21, 118.15, 117.84, 114.27, 72.26, 21.25; IR (thin film,  $\text{cm}^{-1}$ ) 3392.4, 1614.8, 1561.7, 752.4, 699.7; MS (GCMS,  $m/z$ ) 298.1  $[\text{M}]^+$



### 2-(4-Methylphenyl)-4-phenylquinazoline (4ab)

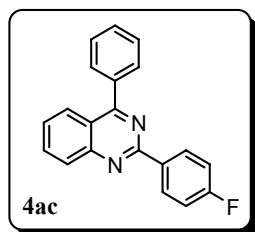
Yellow solid; m.p. 144-146 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.59 (d,  $J = 8.19$  Hz, 2H), 8.15-7.25 (m, 11H, arom.), 2.44 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  167.95, 160.43, 152.37, 138.59, 137.23, 133.17, 130.47, 130.21, 129.90, 129.26, 129.13, 128.38, 128.10, 127.29, 127.12, 121.64, 21.61; IR (thin film,  $\text{cm}^{-1}$ ) 1622.1, 1538.3, 774.6, 700.7; MS (GCMS,  $m/z$ ) 296.1  $[\text{M}]^+$



### 2-(4-Fluorophenyl)-4-phenyl-1,2-dihydroquinazoline (3ac)

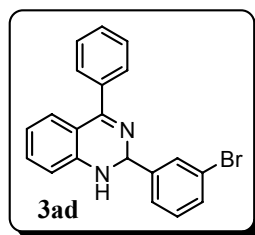
Light brown solid; m.p. 128-130 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.71 (m, 1H, arom.), 8.12-7.04 (m, 10H, arom.), 6.70 (m, 2H, arom.), 5.91 (s, 1H, CH), 4.22 (s, br, 1H, NH);  $^{13}\text{C}$

NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  166.01, 151.95, 146.76, 137.97, 137.58, 133.72, 132.91, 129.22, 129.10, 129.05, 128.18, 127.09, 118.45, 115.32, 114.30, 72.00; IR (thin film, cm<sup>-1</sup>) 3347.5, 1599.6, 1539.7, 1340.3, 775.9, 700.2; MS (GCMS, *m/z*) 302.0 [M]<sup>+</sup>



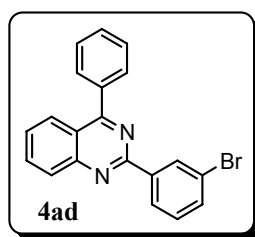
### 2-(4-Fluorophenyl)-4-phenylquinazoline (4ac)

Yellow solid; m.p. 119-120 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  8.72-8.67 (m, 2H, arom.), 8.11-7.16 (m, 11H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  168.21, 160.32, 151.91, 138.27, 137.77, 133.62, 130.70, 130.51, 130.00, 129.74, 129.29, 128.65, 128.23, 127.37, 127.15, 121.34; IR (thin film, cm<sup>-1</sup>) 1622.1, 1539.7, 1340.0, 776.1, 700.6; MS (GCMS, *m/z*) 300.0 [M]<sup>+</sup>



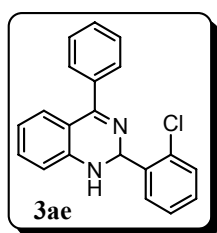
### 2-(3-Bromophenyl)-4-phenyl-1,2-dihydroquinazoline (3ad)

Light yellow solid; m.p. 117-118 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  8.17-7.16 (m, 11H, arom.), 6.75-6.68 (m, 2H, arom.), 5.90 (s, 1H, CH), 4.23 (s, br, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  166.16, 146.59, 144.78, 137.89, 132.98, 131.48, 130.64, 130.25, 129.56, 129.23, 129.01, 128.21, 126.13, 122.75, 118.57, 117.85, 114.37, 72.05; IR (thin film, cm<sup>-1</sup>) 3387.1, 1613.7, 1561.2, 1537.6, 1337.9, 776.3, 699.6; MS (GCMS, *m/z*) 363.9 [M]<sup>+</sup>

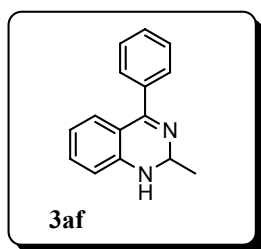


**2-(3-Bromophenyl)-4-phenylquinazoline (4ad)**

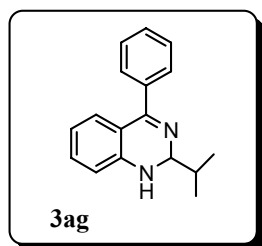
Yellow solid; m.p. 80-82 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.85 (t, 1H,  $J = 1.77$  Hz, arom.), 8.62 (s, 1H, arom.), 8.14-7.39 (m, 11H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  168.72, 160.68, 151.79, 138.12, 137.47, 134.08, 131.00, 130.58, 130.03, 129.76, 129.48, 129.21, 128.75, 128.58, 128.16, 127.35, 127.23, 121.82; IR (thin film,  $\text{cm}^{-1}$ ) 1622.3, 1561.2, 777.1, 701.8; MS (GCMS,  $m/z$ ) 361.5  $[\text{M}]^+$

**2-(2-Chlorophenyl)-4-phenyl-1,2-dihydroquinazoline (3ae)**

Brown gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.76-7.18 (m, 11H, arom.), 6.73-6.65 (m, 2H, arom.), 6.39 (s, 1H, CH), 4.46 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  166.76, 147.08, 139.36, 138.16, 133.04, 132.71, 129.95, 129.72, 129.67, 129.58, 129.39, 128.91, 128.34, 127.36, 118.42, 117.70, 114.59, 69.03; IR (thin film,  $\text{cm}^{-1}$ ) 3388.4, 1614.4, 1468.3, 753.6, 699.6; MS (GCMS,  $m/z$ ) 319.0  $[\text{M}]^+$

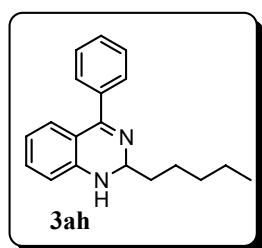
**2-Methyl-4-phenyl-1,2-dihydroquinazoline (3af)**

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.55-7.08 (m, 7H, arom.), 6.70-6.62 (m, 2H, arom.), 4.79 (q,  $J = 6.12$  Hz, 1H, CH), 4.07 (s, br, 1H, NH), 1.62 (d,  $J = 6.12$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  164.71, 146.22, 137.94, 131.63, 130.06, 129.67, 129.18, 128.47, 117.91, 117.55, 114.93, 74.23, 21.94; IR (thin film,  $\text{cm}^{-1}$ ) 3245.6, 1615.1, 1564.4, 1484.7, 1342.7, 754.7, 700.0; MS (GCMS,  $m/z$ ) 222.0  $[\text{M}]^+$



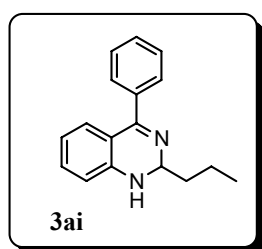
### 2-Isopropyl-4-phenyl-1,2-dihydroquinazoline (3ag)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.55-7.07 (m, 7H, arom.), 6.64 (m, 2H, arom.), 4.70 (d,  $J = 5.82$  Hz, 1H, CH), 4.06 (s, br, 1H, NH), 2.12 (m, 1H,  $\text{CHMe}_2$ ), 1.15 (d,  $J = 6.81$  Hz, 3H,  $\text{CH}_3$ ), 1.08 (d,  $J = 6.72$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.37, 147.33, 138.44, 132.53, 129.23, 129.09, 128.65, 128.16, 117.85, 117.55, 114.07, 74.48, 33.72, 18.14, 17.94; IR (thin film,  $\text{cm}^{-1}$ ) 3299.0, 1615.3, 1564.9, 1486.5, 1348.9, 752.4, 699.7; MS (GCMS,  $m/z$ ) 250.0  $[\text{M}]^+$



### 2-Pentyl-4-phenyl-1,2-dihydroquinazoline (3ah)

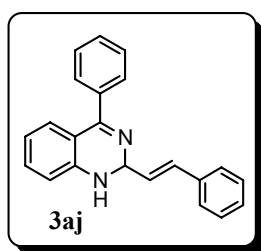
Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.47-7.00 (m, 7H, arom.), 6.63-6.59 (m, 2H, arom.), 4.99 (m, 1H, CH), 4.08 (s, br, 1H, NH), 1.92-1.76 (m, 4H,  $2\text{CH}_2$ ), 1.43-1.17 (m, 4H,  $2\text{CH}_2$ ), 0.08 (m, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  166.46, 147.54, 137.11, 137.05, 129.90, 129.55, 128.55, 127.02, 121.13, 117.64, 114.92, 67.67, 39.78, 31.39, 24.21, 22.66, 14.09; IR (thin film,  $\text{cm}^{-1}$ ) 3343.2, 1615.8, 1564.3, 1485.3, 1343.6, 752.6, 669.7; MS (GCMS,  $m/z$ ) 278.0  $[\text{M}]^+$



### 2-Propyl-4-phenyl-1,2-dihydroquinazoline (3ai)

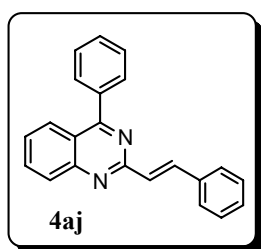


Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.94-6.98 (m, 7H, arom.), 6.55-6.45 (m, 2H, arom.), 4.78 (t,  $J = 6.12$  Hz, 1H, CH), 4.26 (s, br, 1H, NH), 1.94-1.81 (m, 2H,  $\text{CH}_2$ ) 1.52-1.45 (m, 2H,  $\text{CH}_2$ ) 0.8 (t,  $J = 7.32$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  166.33, 147.43, 137.52, 133.04, 129.18, 128.57, 125.17, 127.22, 121.68, 117.07, 115.02, 69.02, 39.14, 31.56, 23.21, 22.65, 14.40; IR (thin film,  $\text{cm}^{-1}$ ) 3341.4, 1615.9, 1564.6, 1485.1, 1344.5, 753.1, 699.9; MS (GCMS,  $m/z$ ) 250.0  $[\text{M}]^+$



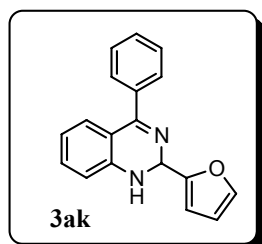
#### 4-Phenyl-2-styryl-1,2-dihydroquinazoline (3aj)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.54-7.01 (m, 14H, arom.), 6.60 (m, 1H, -CH=CH-Ar), 6.50 (d,  $J = 7.98$  Hz, 1H, -CH=CH-Ar), 5.16 (s, br, 1H, NH), 4.91 (t,  $J = 6.06$  Hz, 1H, CH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  164.91, 145.45, 138.32, 135.06, 132.84, 131.42, 129.56, 129.29, 129.13, 128.76, 128.30, 128.11, 127.89, 127.76, 127.55, 127.47, 124.02, 117.67, 114.71, 74.6; IR (thin film,  $\text{cm}^{-1}$ ) 3389.5, 1616.0, 1544.5, 1341.4, 770.0, 699.1; MS (GCMS,  $m/z$ ) 310.0  $[\text{M}]^+$



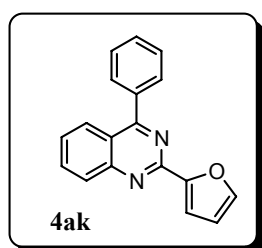
#### 4-Phenyl-2-styrylquinazoline (4aj)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.06-7.14 (m, 16H, arom. & 2CH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  167.21, 159.62, 152.11, 138.43, 137.69, 134.01, 130.97, 130.59, 130.21, 129.89, 129.44, 129.12, 128.91, 128.37, 127.21, 127.07, 126.14, 121.72; IR (thin film,  $\text{cm}^{-1}$ ) 1615.4, 1561.5, 1540.1, 1340.9, 770.1, 699.9; MS (GCMS,  $m/z$ ) 308.0  $[\text{M}]^+$



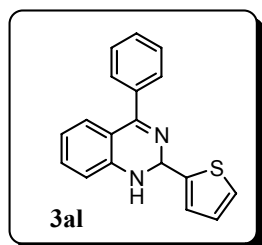
### 2-(2-Furanyl)-4-phenyl-1,2-dihydroquinazoline (3ak)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz) 7.59-7.13 (m, 9H, arom.), 6.67 (m, 2H, arom.), 6.37-6.31 (m, 1H, arom.), 6.11 (s, 1H, CH), 4.71 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) 164.80, 152.75, 145.45, 142.20, 138.31, 131.97, 130.82, 129.76, 129.57, 129.15, 128.87, 128.61, 121.11, 117.03, 115.96, 114.39, 112.45, 74.50; IR (thin film,  $\text{cm}^{-1}$ ) 3340.4, 1615.2., 1537.9, 1483.8, 1340.8, 751.9, 700.7; MS (GCMS,  $m/z$ ) 274.0  $[\text{M}]^+$



### 2-(2-Furanyl)-4-phenylquinazoline (4ak)

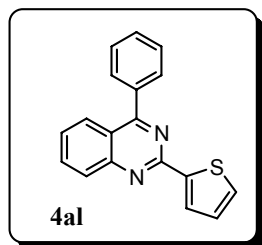
Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.62-7.37 (m, 8H, arom.), 6.85 (d,  $J = 8.43$  Hz, 1H, arom.), 6.57 (t,  $J = 8.40$  Hz, 1H, arom.), 6.33-6.27 (m, 2H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.40, 160.12, 154.92, 149.77, 146.56, 137.28, 132.34, 130.09, 129.89, 129.63, 129.45, 128.82, 128.36, 127.51, 127.37, 127.05, 112.52, 110.83; IR (thin film,  $\text{cm}^{-1}$ ) 3324.3, 1622.7, 1574.7, 1454.8, 1321.5, 751.8, 700.7; MS (GCMS,  $m/z$ ) 272.0  $[\text{M}]^+$



### 2-(2-Thiophenyl)-4-phenyl-1,2-dihydroquinazoline (3al)

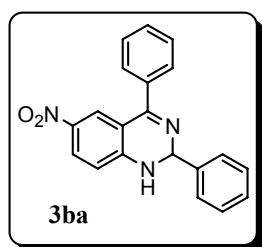
Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz) 7.75-6.49 (m, 12H, arom.), 6.23 (s, 1H, CH), 5.09 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) 161.48, 145.54, 143.21, 133.31, 131.57, 131.23, 130.80, 130.78, 127.65, 126.68, 125.42, 125.35, 124.48, 123.40, 119.03, 116.36, 115.67,

70.24; IR (thin film,  $\text{cm}^{-1}$ ) 3346.2, 1614.8, 1538.9, 1455.4, 1249.5, 752.8, 699.9; MS (GCMS,  $m/z$ ) 290.0  $[\text{M}]^+$



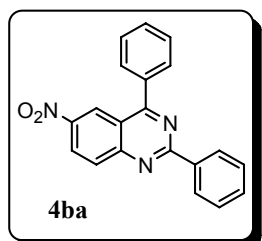
### 2-Thiophenyl-4-phenylquinazoline (4a)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz) 8.09 (d,  $J = 8.63$  Hz, 1H, arom.), 7.86 (d,  $J = 3.14$  Hz, 1H, arom.), 7.62-6.96 (m, 9H, arom.), 6.84 (d,  $J = 8.50$  Hz, 1H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) 160.19, 155.02, 148.15, 135.44, 133.65, 131.68, 130.91, 130.54, 129.25, 128.82, 128.11, 127.31, 127.19, 124.63, 123.45, 118.24, 116.16, 116.112; IR (thin film,  $\text{cm}^{-1}$ ) 3320.8, 1622.6, 1571.7, 1539.1, 1455.5, 1253.3, 752.2, 699.6; MS (GCMS,  $m/z$ ) 288.0  $[\text{M}]^+$



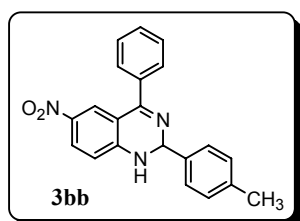
### 6-Nitro-2,4-diphenyl-1,2-dihydroquinazoline (3ba)

Yellow solid; m.p. 160-162  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.13-8.04 (m, 1H, arom.), 7.54-7.38 (m, 11H, arom.), 6.58-6.54 (m, 1H, arom.), 6.27 (s, 1H, CH), 5.17 (s, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  164.04, 151.04, 141.57, 138.12, 136.58, 130.28, 129.12, 129.03, 128.94, 128.77, 128.67, 126.82, 125.45, 114.48, 113.43, 72.48; IR (thin film,  $\text{cm}^{-1}$ ) 3345.5, 1618.4, 1519.7, 1324.0, 771.8, 698.7; MS (GCMS,  $m/z$ ) 329.7  $[\text{M}]^+$

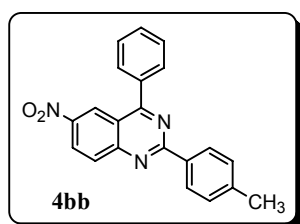


**6-Nitro-2,4-diphenylquinazoline (4ba)**

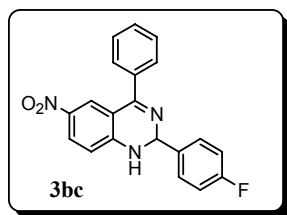
Light yellow solid; sub. 236-238 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 9.07 (d, *J* = 2.43 Hz, 1H, arom.), 8.75-8.63 (m, 3H, arom.), 8.28 (d, *J* = 9.27 Hz, 1H, arom.), 7.93-7.90 (m, 2H, arom.), 7.69-7.67 (m, 3H, arom.), 7.57-7.54 (m, 3H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 170.30, 163.41, 153.94, 145.11, 141.82, 136.44, 133.56, 130.78, 131.18, 130.47, 130.19, 129.85, 129.05, 127.92, 124.39, 120.27; IR (thin film, cm<sup>-1</sup>) 1618.6, 1537.2, 1343.8, 774.3, 701.5; MS (GCMS, *m/z*) 326.8 [M]<sup>+</sup>

**6-Nitro-2-(4-methylphenyl)-4-phenyl-1,2-dihydroquinazoline (3bb)**

Brown solid; m.p. 225-227 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 9.05 (d, *J* = 2.40 Hz, 1H, arom.), 8.62 (m, 3H, arom.), 8.25-7.20 (m, 7H, arom.), 6.60 (d, *J* = 8.61 Hz, 1H, arom.), 6.28 (s, 1H, CH), 5.00 (s, br, 1H, NH), 2.46 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 163.73, 150.98, 142.33, 138.76, 136.42, 130.88, 130.10, 129.55, 129.07, 128.76, 128.63, 126.70, 125.37, 114.59, 113.35, 72.45, 21.24; IR (thin film, cm<sup>-1</sup>) 3370.1, 1618.2, 1537.8, 1329.9, 772.7, 700.1; MS (GCMS, *m/z*) 343.0 [M]<sup>+</sup>

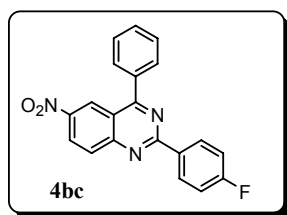
**6-Nitro-2-(4-methylphenyl)-4-phenylquinazoline (4bb)**

Brown solid; m.p. 217-218 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 9.04 (d, *J* = 2.49 Hz, 1H, arom.), 8.64-8.60 (m, 3H, arom.), 8.23 (d, *J* = 9.27 Hz, 1H, arom.), 7.93-7.88 (m, 2H, arom.), 7.69-7.65 (m, 3H, arom.), 7.36 (d, *J* = 8.16 Hz, 2H, arom.), 2.46 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 170.35, 163.47, 154.56, 145.91, 142.31, 136.43, 134.39, 130.92, 130.89, 130.25, 129.54, 129.22, 129.07, 126.92, 124.29, 120.33, 21.69; IR (thin film, cm<sup>-1</sup>) 1685.3, 1603.6, 1536.2, 772.3, 696.4; MS (GCMS, *m/z*) 341.0 [M]<sup>+</sup>



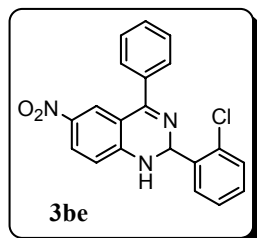
### 6-Nitro-2-(4-fluorophenyl)-4-phenyl-1,2-dihydroquinazoline (3bc)

Brown solid; m.p. 202-204 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.17-8.11 (m, 2H, arom.), 7.55-7.46 (m, 7H, arom.), 7.10 (t, *J* = 8.64 Hz, 2H, arom.), 6.64 (d, *J* = 8.82 Hz, 1H, arom.), 6.26 (s, 1H, CH), 4.97 (s, br, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 165.15, 151.46, 138.87, 137.54, 136.45, 133.00, 132.21, 130.68, 130.31, 129.97, 129.43, 129.29, 129.04, 128.53, 128.20, 127.13, 125.36, 114.11, 113.57, 70.07; IR (thin film, cm<sup>-1</sup>) 3341.1, 1620.4, 1509.2, 1324.3, 772.7, 701.2; MS (GCMS, *m/z*) 347.0 [M]<sup>+</sup>



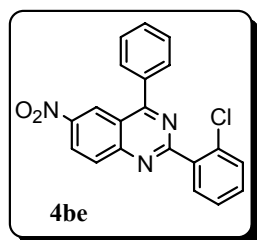
### 6-Nitro-2-(4-fluorophenyl)-4-phenylquinazoline (4bc)

Light yellow solid; m.p. 240-241 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 9.06 (d, *J* = 2.46 Hz, 1H, arom.), 8.78-8.73 (m, 2H, arom.), 8.67-8.63 (dd, *J* = 9.27, 1H, arom.), 8.26 (d, *J* = 9.27, 1H, arom.), 7.92-7.88 (m, 2H, arom.), 7.69-7.67 (m, 2H, arom.), 7.26-7.20 (m, 3H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 170.23, 163.65, 153.80, 146.18, 137.54, 136.00, 133.38, 132.24, 132.02, 131.91, 131.43, 131.27, 130.89, 129.36, 127.55, 127.08, 124.64, 120.71; IR (thin film, cm<sup>-1</sup>) 1619.6, 1598.1, 1537.9, 1339.0, 773.6, 695.8; MS (GCMS, *m/z*) 345.0 [M]<sup>+</sup>



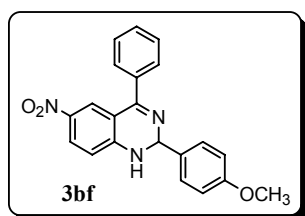
### 6-Nitro-2-(2-chlorophenyl)-4-phenyl-1,2-dihydroquinazoline (3be)

Brown gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.11-8.07 (m, 2H, arom.), 7.61-7.25 (m, 9H, arom.), 6.73 (s, 1H, CH), 6.58 (d,  $J = 8.73$  Hz, 1H, arom.), 5.33 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  165.17, 151.43, 138.29, 137.94, 136.56, 132.17, 130.41, 130.32, 130.00, 129.93, 129.17, 129.14, 129.08, 128.73, 128.64, 127.49, 125.39, 114.03, 113.70, 69.08; IR (thin film,  $\text{cm}^{-1}$ ) 3340.9, 1619.1, 1521.5, 1323.6, 771.0, 700.0; MS (GCMS,  $m/z$ ) 363.0  $[\text{M}]^+$



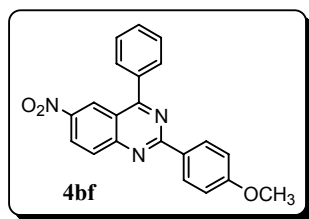
#### 6-Nitro-2-(2-chlorophenyl)-4-phenylquinazoline (4be)

Yellow solid; m.p. 161-163  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  9.15 (d,  $J = 2.40$  Hz, 1H, arom.), 8.72-8.69 (dd,  $J = 9.21$  Hz, 1H, arom.), 8.34 (d,  $J = 9.27$  Hz, 1H, arom.), 7.98-7.90 (m, 3H, arom.), 7.67-7.48 (m, 6H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  170.37, 163.95, 153.97, 146.07, 137.35, 135.95, 133.29, 132.11, 131.18, 131.15, 131.07, 130.90, 130.37, 129.20, 127.19, 127.04, 124.22, 120.21; IR (thin film,  $\text{cm}^{-1}$ ) 1621.1, 1537.6, 1344.2, 770.6, 698.8; MS (GCMS,  $m/z$ ) 361.0  $[\text{M}]^+$



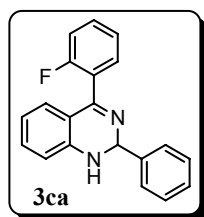
#### 6-Nitro-2-(4-methoxyphenyl)-4-phenyl-1,2-dihydroquinazoline (3bf)

Brown solid; m.p. 158-160  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.10 (s, 1H, arom.) 7.55-7.41 (m, 8H, arom.), 6.93 (d,  $J = 6.69$  Hz, 2H, arom.), 6.58-6.54 (dd,  $J = 8.34$  Hz, 1H, arom.), 6.23 (s, 1H, CH), 5.07 (s, br, 1H, NH), 3.81 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  163.76, 159.99, 151.06, 138.02, 136.71, 134.02, 130.11, 129.14, 128.94, 128.75, 128.64, 125.37, 114.41, 114.12, 113.37, 72.14, 55.38; IR (thin film,  $\text{cm}^{-1}$ ) 3242.4, 1614.0, 1513.3, 1323.8, 1095.3, 772.2, 699.9; MS (GCMS,  $m/z$ ) 359.0  $[\text{M}]^+$



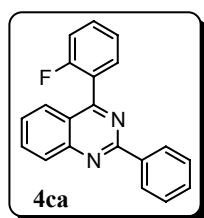
### 6-Nitro-2-(4-methoxyphenyl)-4-phenylquinazoline (4bf)

Brown solid; m.p. 207-209 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.71 (d, *J* = 8.73 Hz, 2H, arom.), 8.20 (d, *J* = 9.24 Hz, 1H, arom.), 7.91-7.82 (m, 3H, arom.), 7.67 (m, 2H, arom.), 7.06-6.99 (m, 4H, arom.), 3.89 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.61, 162.75, 154.62, 144.98, 136.46, 132.02, 131.07, 130.88, 130.67, 130.20, 129.94, 129.71, 129.04, 126.90, 124.31, 120.06, 114.32, 114.08, 55.60; IR (thin film, cm<sup>-1</sup>) 1642.2, 1541.1, 1430.4, 1337.8, 1220.0, 772.8; MS (GCMS, *m/z*) 357.0 [M]<sup>+</sup>



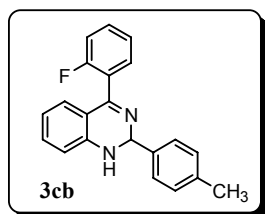
### 2-Phenyl-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3ca)

Yellow gum; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.67-8.64 (dd, *J* = 7.89 Hz, 2H, arom.), 8.15-7.20 (m, 9H, arom.), 6.70-6.60 (m, 2H, arom.), 6.09 (s, 1H, CH), 4.22 (s, br, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.62, 160.53, 145.66, 138.08, 133.94, 133.28, 131.98, 130.63, 129.01, 128.73, 128.63, 128.49, 128.26, 127.29, 127.26, 118.41, 114.03, 72.90; IR (thin film, cm<sup>-1</sup>) 3347.9, 1615.8, 1564.9, 1541.5, 1486.3, 1341.7, 768.1, 709.4; MS (GCMS, *m/z*) 303.2 [M]<sup>+</sup>



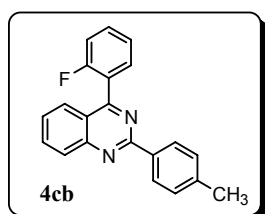
### 2-Phenyl-4-(2-fluorophenyl)quinazoline (4ca)

Yellow solid, 113-115 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.67-8.64 (dd, *J* = 7.98 Hz, 2H, arom.), 8.17 (d, *J* = 8.46 Hz, 1H, arom.), 7.90-7.25 (m, 10H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.60, 160.52, 151.42, 138.11, 133.92, 131.99, 131.77, 131.66, 130.63, 129.03, 128.74, 128.63, 127.25, 126.90, 124.68, 122.47, 116.28, 115.99; IR (thin film, cm<sup>-1</sup>) 1615.8, 1564.7, 1541.2, 1341.3, 1219.0, 769.9, 708.4; MS (GCMS, *m/z*) 301.1 [M]<sup>+</sup>



### 2-(4-Methylphenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3cb)

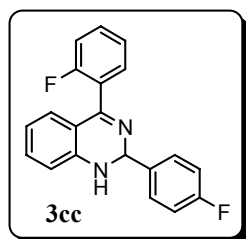
Light yellow solid, m.p. 152-153 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.49-7.11 (m, 9H, arom.), 6.92 (s, 1H, arom.), 6.68-6.58 (m, 2H, arom.), 6.06 (s, 1H, CH), 4.19 (s, br, 1H, NH), 2.35 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 162.19, 145.68, 139.62, 138.16, 133.21, 131.12, 130.78, 129.34, 128.95, 128.24, 127.13, 124.28, 118.28, 117.65, 115.94, 115.65, 114.03, 72.62, 21.26; IR (thin film, cm<sup>-1</sup>) 3391.4, 1616.6, 1565.8, 1486.1, 1450.6, 1341.2, 1219.6, 771.6; MS (LCMS, ESI, *m/z*) 316.4 [M]<sup>+</sup>



### 2-(4-Methylphenyl)-4-(2-fluorophenyl)quinazoline (4cb)

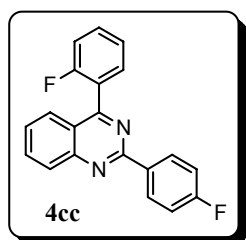
Light yellow solid, m.p. 147-148 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.56 (d, *J* = 8.22 Hz, 2H, arom.), 8.15 (d, *J* = 8.49 Hz, 1H, arom.), 7.90-7.25 (m, 9H, arom.), 2.44 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.48, 160.60, 151.43, 140.83, 135.38, 133.82, 131.99, 131.69, 131.58, 129.37, 128.93, 128.67, 126.86, 126.82, 124.64, 122.37, 116.24, 115.95, 21.58; IR (thin film, cm<sup>-1</sup>) 1614.3, 1564.5, 1541.0, 1485.6, 1341.0, 1218.9, 770.6, 694.9; MS (LCMS, ESI, *m/z*) 314.0 [M]<sup>+</sup>





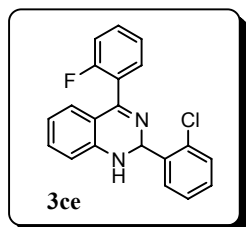
### 2-(4-Fluorophenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3cc)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.69-8.64 (m, 1H, arom.), 8.12-7.05 (m, 9H, arom.), 6.69-6.61 (m, 2H, arom.), 6.06 (s, 1H, CH), 4.19 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  162.47, 145.57, 134.05, 133.32, 131.00, 130.96, 130.88, 129.14, 129.03, 128.90, 128.29, 127.28, 124.33, 118.59, 117.70, 116.00, 115.65, 115.36, 114.06, 72.31; IR (thin film,  $\text{cm}^{-1}$ ) 3399.9, 1616.0, 1541.9, 1509.2, 1451.8, 1341.7, 1221.6, 766.2, 694.0; MS (LCMS, ESI,  $m/z$ ) 320.3  $[\text{M}]^+$



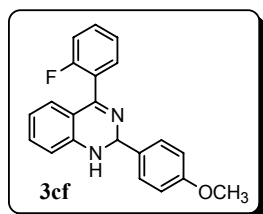
### 2-(4-Fluorophenyl)-4-(2-fluorophenyl)quinazoline (4cc)

White solid; m.p. 146-147  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.69-8.64 (m, 2H, arom.), 8.15 (d,  $J = 8.37$  Hz, 1H, arom.), 7.91-7.16 9 (m, 9H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  164.64, 159.56, 151.36, 134.23, 134.00, 131.89, 131.85, 131.79, 131.68, 130.86, 130.74, 128.91, 127.24, 126.86, 124.60, 122.35, 116.29, 116.00, 115.65, 115.36; IR (thin film,  $\text{cm}^{-1}$ ) 1615.7, 1564.9, 1541.5, 1452.6, 1341.3, 1221.3, 768.0, 618.9; MS (GCMS,  $m/z$ ) 318.0  $[\text{M}]^+$



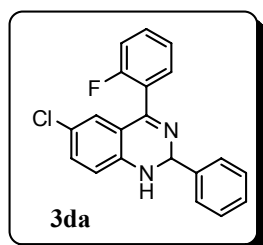
### 2-(2-Chlorophenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3ce)

Brown gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.22-7.14 (m, 12H, arom.), 6.31 (s, 1H, CH), 4.41 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.46, 157.38, 145.71, 139.17, 135.14, 134.56, 133.47, 132.38, 131.99, 131.73, 129.71, 129.62, 127.39, 124.25, 118.49, 117.06, 115.92, 114.24, 69.27; IR (thin film,  $\text{cm}^{-1}$ ) 3349.6, 1615.7, 1582.3, 1546.2, 1481.3, 1450.2, 1303.8, 1219.1, 771.1; MS (GCMS,  $m/z$ ) 336.6  $[\text{M}]^+$



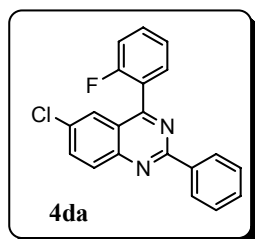
### 2-(4-Methoxyphenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3cf)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.63 (d,  $J = 6.9$  Hz, 1H, arom.), 8.12-6.57 (m, 11H, arom.), 6.03 (s, 1H, CH), 4.15 (s, br, 1H, NH), 3.79 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  164.46, 161.82, 151.45, 145.72, 134.85, 133.85, 133.21, 130.77, 130.37, 128.75, 128.45, 126.83, 118.31, 114.00, 113.92, 72.44, 55.40; IR (thin film,  $\text{cm}^{-1}$ ) 3345.1, 1614.5, 1540.8, 1341.7, 1250.8, 768.8, 700.7; MS (GCMS,  $m/z$ ) 332.1  $[\text{M}]^+$



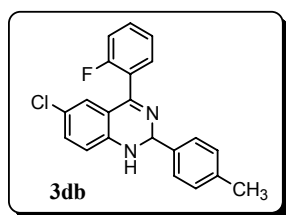
### 6-Chloro-2-phenyl-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3da)

Light brown solid; m.p. 154-156  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.63-8.65 (m, 1H, arom.), 8.12 (d,  $J = 8.97$  Hz, 1H, arom.), 7.59-7.16 (m, 8H, arom.), 6.91 (d,  $J = 2.13$  Hz, 1H, arom.), 6.57 (d,  $J = 8.55$  Hz, 1H, arom.), 6.10 (s, 1H, CH), 4.26 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.30, 144.10, 141.10, 134.92, 133.10, 130.91, 128.77, 128.69, 128.64, 127.69, 127.17, 124.48, 122.89, 118.43, 116.16, 115.88, 115.38, 72.79; IR (thin film,  $\text{cm}^{-1}$ ) 3395.4, 1615.7, 1561.0, 1537.6, 1313.1, 1218.5; MS (GCMS,  $m/z$ ) 337.0  $[\text{M}]^+$



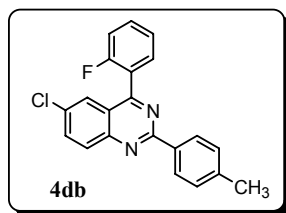
### 6-Chloro-2-phenyl-4-(2-fluorophenyl)quinazoline (4da)

Light yellow solid; m.p. 180-181 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.66-8.62 (m, 2H, arom.), 8.12 (d, *J* = 8.88 Hz, 1H, arom.), 7.85-7.26 (m, 9H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 163.80, 160.72, 149.94, 137.64, 134.89, 132.84, 132.08, 131.98, 131.88, 130.87, 130.74, 128.78, 128.66, 125.67, 124.77, 122.98, 116.45, 116.17; IR (thin film, cm<sup>-1</sup>) 1616.9, 1560.9, 1535.9, 1389.5, 771.9, 703.6; MS (GCMS, *m/z*) 335.0 [M]<sup>+</sup>



### 6-Chloro-2-(4-methylphenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3db)

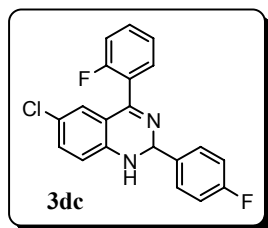
Brown solid; 138-140 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.46-7.40 (m, 4H, arom.), 7.26-7.14 (m, 5H, arom.), 6.89 (t, *J* = 2.28 Hz, 1H, arom.), 6.56 (d, *J* = 8.51 Hz, 1H, arom.), 6.07 (s, 1H, CH), 4.23 (s, br, 1H, NH), 2.35 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 161.11, 144.10, 139.16, 138.36, 133.02, 131.24, 131.14, 130.97, 129.40, 127.64, 127.00, 124.45, 122.77, 118.41, 116.13, 115.85, 115.35, 72.56, 21.25; IR (thin film, cm<sup>-1</sup>) 3332.8, 1615.1, 1561.2, 1538.4, 1219.1, 771.7; MS (GCMS, *m/z*) 351.0 [M]<sup>+</sup>



### 6-Chloro-2-(4-methylphenyl)-4-(2-fluorophenyl)quinazoline (4db)

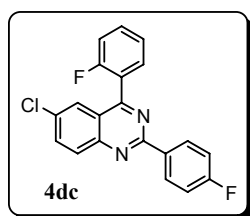
Yellow solid, 189-191 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.83-7.74 (m, 5H, arom.), 7.43-7.23 (m, 6H, arom.), 2.44 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 163.70, 160.81, 149.95,

145.59, 141.17, 134.79, 134.18, 131.91, 130.63, 129.88, 129.73, 129.42, 128.67, 127.01, 125.64, 124.74, 118.49, 116.42, 21.92; IR (thin film,  $\text{cm}^{-1}$ ) 1611.1, 1561.3, 1537.8, 1308.4, 772.2; MS (GCMS,  $m/z$ ) 349.0  $[\text{M}]^+$



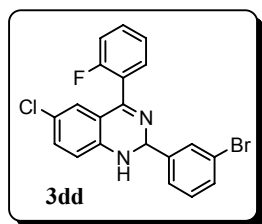
### 6-Chloro-2-(4-fluorophenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3dc)

Yellow solid; m.p. 185-187  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.10-8.07 (m, 1H, arom.), 7.58-7.53 (m, 2H, arom.), 7.44-7.42 (m, 2H, arom.), 7.26-7.05 (m, 4H, arom.), 6.91 (d,  $J = 2.22$  Hz, 1H, arom.), 6.59 (d,  $J = 8.52$  Hz, 1H, arom.), 6.08 (s, 1H, CH), 4.30 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.46, 143.99, 137.91, 133.18, 131.39, 131.28, 130.87, 130.83, 129.04, 128.93, 127.73, 124.50, 123.11, 118.44, 115.91, 115.73, 115.44, 115.23, 72.13; IR (thin film,  $\text{cm}^{-1}$ ) 3235.7, 1614.7, 1561.2, 1509.0, 1451.2, 1344.8, 1219.2, 754.2; MS (GCMS,  $m/z$ ) 354.0  $[\text{M}]^+$



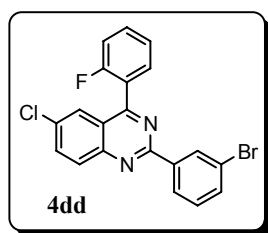
### 6-Chloro-2-(4-fluorophenyl)-4-(2-fluorophenyl)quinazoline (4dc)

Yellow solid; m.p. 210-212  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.68-8.63 (m, 2H, arom.), 8.09 (d,  $J = 8.96$  Hz, 1H, arom.), 7.85-7.16 (m, 8H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  166.48, 163.87, 159.91, 149.90, 134.99, 132.87, 132.13, 132.02, 131.75, 130.90, 130.78, 130.62, 125.68, 124.81, 122.87, 118.88, 116.48, 116.19, 115.74, 115.45; IR (thin film,  $\text{cm}^{-1}$ ) 1630.7, 1539.3, 1508.3, 1218.6, 766.1, 691.8; MS (GCMS,  $m/z$ ) 352.0  $[\text{M}]^+$



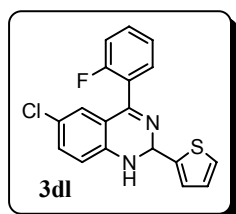
### 6-Chloro-2-(3-bromophenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3dd)

Light yellow solid; m.p. 175-177 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.74 (t,  $J = 1.59$  Hz, 1H, arom.), 7.49-7.18 (m, 8H, arom.), 6.91 (d,  $J = 2.25$  Hz, 1H, arom.), 6.60 (d,  $J = 8.55$  Hz, 1H, arom.), 6.06 (s, 1H, CH), 4.23 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.67, 144.16, 135.12, 133.72, 133.25, 131.62, 130.74, 130.44, 130.35, 130.18, 127.79, 127.26, 125.92, 124.56, 123.32, 122.82, 118.49, 116.22, 115.50, 72.22; IR (thin film,  $\text{cm}^{-1}$ ) 3247.8, 1674.7, 1616.7, 1537.3, 1452.9, 1309.5, 1220.0, 772.1; MS (GCMS,  $m/z$ ) 414.9  $[\text{M}]^+$



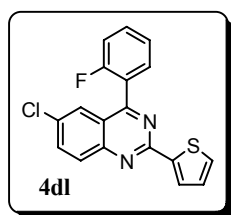
### 6-Chloro-2-(3-bromophenyl)-4-(2-fluorophenyl)quinazoline (4dd)

Light yellow solid; m.p. 156-158 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.01 (s, 1H, arom.), 7.82-7.73 (m, 7H, arom.), 7.45-7.39 (m, 3H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  166.31, 163.85, 160.11, 148.94, 135.26, 133.20, 132.73, 132.59, 131.33, 130.70, 130.37, 129.00, 124.97, 124.62, 122.41, 119.07, 117.36, 116.48, 116.14, 115.78; IR (thin film,  $\text{cm}^{-1}$ ) 1677.2, 1615.2, 1538.4, 1452.0, 1309.2, 759.4; MS (GCMS,  $m/z$ ) 413.9  $[\text{M}+1]^+$



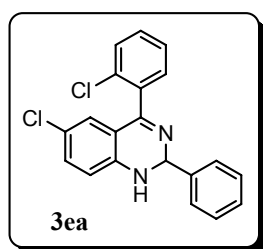
### 6-Chloro-2-(2-thiophenyl)-4-(2-fluorophenyl)-1,2-dihydroquinazoline (3dl)

Yellow solid, m.p. 204-205 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.45-6.92 (m, 9H, arom.), 6.62 (d,  $J = 17.52$  Hz, 1H, arom.), 6.42 (s, 1H, CH), 4.47 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.47, 145.58, 143.23, 133.17, 131.42, 131.31, 130.99, 130.95, 127.74, 126.69, 125.68, 125.15, 124.49, 123.42, 118.70, 116.17, 115.89, 68.30; IR (thin film,  $\text{cm}^{-1}$ ) 3335.8, 1615.3, 1536.7, 1452.3, 1219.4, 759.8, 694.8; MS (GCMS,  $m/z$ ) 344.0  $[\text{M}]^+$



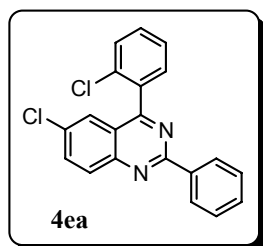
#### 6-Chloro-2-(2-thiophenyl)-4-(2-fluorophenyl)quinazoline (4dl)

Off white solid; m.p. 202-204 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.18-8.16 (dd,  $J = 3.72$  Hz, 1H, arom.), 8.03 (d,  $J = 9.00$  Hz, 1H, arom.), 7.81-7.16 (m, 8H, arom.);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  160.58, 154.27, 148.10, 145.72, 135.45, 133.60, 130.79, 130.31, 129.05, 128.98, 127.92, 127.37, 127.22, 124.63, 123.48, 118.25, 116.18, 116.14; IR (thin film,  $\text{cm}^{-1}$ ) 1634.9, 1616.7, 1536.2, 1454.5, 1385.8, 772.3, 694.6; MS (GCMS,  $m/z$ ) 341.9  $[\text{M}]^+$



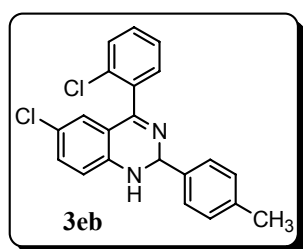
#### 6-Chloro-2-phenyl-4-(2-chlorophenyl)-1,2-dihydroquinazoline (3ea)

Yellow gum;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  8.64-8.61 (m, 1H, arom.), 8.12 (d,  $J = 8.91$  Hz, 1H, arom.), 7.84-7.47 (m, 11H, arom. & CH), 2.63 (s, br, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  161.10, 145.30, 141.65, 134.97, 132.31, 130.88, 129.76, 128.69, 128.43, 127.36, 127.17, 124.21, 124.53, 122.40, 118.18, 116.23, 115.67, 71.98; IR (thin film,  $\text{cm}^{-1}$ ) 3348.8, 1623.0, 1569.3, 1541.2, 1474.1, 1435.2, 1238.5, 755.4, 706.1; MS (GCMS,  $m/z$ ) 352.0  $[\text{M}]^+$



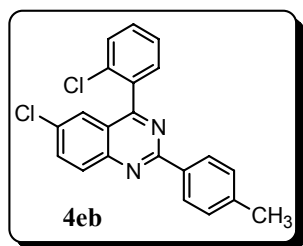
### 6-Chloro-2-phenyl-4-(2-chlorophenyl)quinazoline (4ea)

Yellow solid; m.p. 172-173 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.61-8.64 (m, 3H, arom.), 8.12 (d, *J* = 8.97 Hz, 2H, arom.), 7.84-7.80 (dd, *J* = 8.97 Hz, 2H, arom.), 7.61-7.47 (m, 5H, arom.); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 166.78, 160.51, 148.23, 134.67, 133.42, 132.83, 132.18, 131.28, 130.98, 130.65, 129.84, 129.17, 128.56, 128.34, 127.77, 127.49, 125.56, 122.24; IR (thin film, cm<sup>-1</sup>) 1626.7, 1561.0, 1538.9, 1470.8, 1308.6, 773.9, 705.2; MS (GCMS, *m/z*) 350.0 [M]<sup>+</sup>



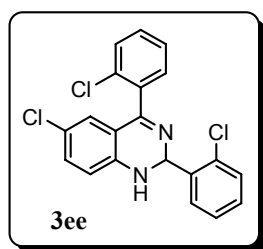
### 6-Chloro-2-(4-methylphenyl)-4-(2-chlorophenyl)-1,2-dihydroquinazoline (3eb)

Light Yellow solid; m.p. 163-164 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.50-7.13 (m, 10H, arom.), 6.73 (s, 1H, CH), 6.54 (d, *J* = 8.52 Hz, 1H, arom.), 4.22 (s, br, 1H, NH), 2.41 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 161.78, 146.10, 141.70, 134.54, 133.98, 130.45, 129.65, 128.32, 128.13, 127.77, 127.44, 127.10, 125.19, 124.52, 124.06, 122.61, 116.73, 115.57, 72.38, 21.26; IR (thin film, cm<sup>-1</sup>) 3247.9, 1622.1, 1567.8, 1474.4, 1434.9, 1343.5, 1244.6, 762.4; MS (GCMS, *m/z*) 366.0 [M]<sup>+</sup>

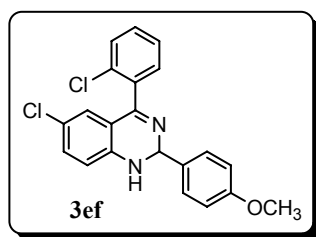


**6-Chloro-2-(4-methylphenyl)-4-(2-chlorophenyl)quinazoline (4eb)**

Light Yellow solid; m.p. 188-189 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.53 (d, *J* = 8.22 Hz, 2H, arom.), 8.09 (d, *J* = 9 Hz, 1H, arom.), 7.82-7.78 (dd, *J* = 9 Hz, 1H, arom.), 7.62-7.49 (m, 5H, arom.), 7.33 (d, *J* = 8.07 Hz, 2H, arom.), 2.43 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 166.30, 160.80, 149.92, 141.18, 136.00, 134.96, 134.82, 132.91, 132.53, 131.12, 130.84, 130.71, 130.18, 129.42, 128.75, 127.08, 125.58, 122.73, 21.59; IR (thin film, cm<sup>-1</sup>) 3384.0, 1594.8, 1561.2, 1538.0, 1470.6, 1419.0, 1385.9, 771.8; MS (GCMS, *m/z*) 364.0 [M]<sup>+</sup>

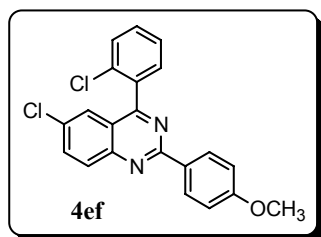
**6-Chloro-2-(2-chlorophenyl)-4-(2-chlorophenyl)-1,2-dihydroquinazoline (3ee)**

Yellow gum; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.52-7.13 (m, 10H, arom.), 6.76 (s, 1H, CH), 6.54 (d, *J* = 8.55 Hz, 1H, arom.), 4.40 (s, br, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.18, 151.34, 144.03, 138.76, 136.44, 132.90, 130.96, 130.64, 130.21, 129.63, 129.25, 129.02, 128.67, 127.82, 127.43, 127.09, 125.39, 115.15, 114.70, 69.37; IR (thin film, cm<sup>-1</sup>) 3346.8, 1623.1, 1569.5, 1541.1, 1435.3, 1341.7, 1238.6, 770.3, 705.8; MS (GCMS, *m/z*) 387.8 [M]<sup>+</sup>

**6-Chloro-2-(4-methoxyphenyl)-4-(2-chlorophenyl)-1,2-dihydroquinazoline (3ef)**

Yellow solid; m.p. 174-176 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.51-6.50 (m, 12H, arom. & CH), 4.24 (s, br, 1H, NH), 3.88 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 162.00, 160.56, 146.44, 141.68, 134.67, 133.77, 131.23, 130.31, 129.29, 129.03, 128.76, 128.49, 127.24, 127.11, 125.90, 124.63, 124.28, 122.82, 116.17, 115.80, 72.37, 55.24; IR (thin film, cm<sup>-1</sup>) 3248.6, 1639.3, 1561.2, 1538.7, 1513.3, 1417.4, 1385.0, 1251.1, 772.1; MS (GCMS, *m/z*) 383.1 [M]<sup>+</sup>





### 6-Chloro-2-(4-methoxyphenyl)-4-(2-chlorophenyl)quinazoline (4ef)

Light Yellow solid; m.p. 199-200 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 8.60-8.57 (dd, *J* = 6.93 Hz, 2H, arom.), 8.07 (d, *J* = 9 Hz, 1H, arom.), 7.81-7.77 (dd, *J* = 9 Hz, 1H, arom.), 7.59-7.49 (m, 5H, arom.), 7.03-7.01 (dd, *J* = 6.96 Hz, 4H, arom.), 3.89 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 166.41, 162.74, 160.88, 149.56, 141.32, 135.98, 134.69, 134.27, 132.46, 131.40, 130.71, 130.29, 130.00, 129.52, 128.68, 127.55, 124.86, 122.50, 55.82; IR (thin film, cm<sup>-1</sup>) 1639.1, 1561.5, 1539.6, 1470.2, 1417.9, 1385.3, 1251.8, 772.1; MS (GCMS, *m/z*) 382.1 [M+1]<sup>+</sup>

